Measurement and Estimation of Electrophilic Reactivity for Predictive Toxicology

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Chemical Reviews

Supporting Information

Table S1. Reactivity Data, Experimental Values, Assay Conditions, Reaction Mechanisms[*]

- CAS number[a]
- Name of Electrophile (El)
- Reference nucleophile (Nu)
- Parameter; Unit
- Value; Standard error; log(Value)
- T/°C; pH; Solvent
- Reaction time
- Ratio Nu:El
- Reference
- Comment
- Chemical reaction mechanism (according to reference)

[a] CAS numbers given for guidance only, individual experiments may have been performed with equivalent compounds, but deviating CAS numbers.
[*] This document was prepared in good faith, however authors or institutions of this document are not responsible for any inaccuracies or errors.

Table S1. Reactivity Data, Experimental Values, Assay Conditions, Reaction Mechanisms

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1	818-61-1	2-Hydroxyethyl acrylate	4-Nitrobenzenethiol	t1/2(NBT)	min	2.45E-01		
2	144-48-9	2-Iodoacetamide	4-Nitrobenzenethiol	t1/2(NBT)	min	1.83E-03		
3	2682-20-4	2-Methyl-2H-isothiazolin-3-one	4-Nitrobenzenethiol	t1/2(NBT)	min	1.60E-03		
4	25567-67-3	3-Chloro-1.2-dinitrobenzene	4-Nitrobenzenethiol	t1/2(NBT)	min	1.25E-02		
5	2497-21-4	4-Hexen-3-one	4-Nitrobenzenethiol	t1/2(NBT)	min	2.77E-02		
6	26172-55-4	5-Chloro-2-methyl-4-isothiazolin-3-one	4-Nitrobenzenethiol	t1/2(NBT)	min	5.83E-05		
7	108-24-7	Acetic anhydride	4-Nitrobenzenethiol	t1/2(NBT)	min	9.83E-04		
8	107-02-8	Acrolein	4-Nitrobenzenethiol	t1/2(NBT)	min	8.25E-02		
9	100-39-0	Benzyl bromide	4-Nitrobenzenethiol	t1/2(NBT)	min	4.67E-05		
10	57-57-8	beta-Propiolactone	4-Nitrobenzenethiol	t1/2(NBT)	min	1.62E-04		
11	88-11-9	Diethylthiocarbamoyl chloride	4-Nitrobenzenethiol	t1/2(NBT)	min	1.52E-03		
12	886-38-4	Diphenylcyclopropenone	4-Nitrobenzenethiol	t1/2(NBT)	min	1.05E-05		
13	140-88-5	Ethyl acrylate	4-Nitrobenzenethiol	t1/2(NBT)	min	7.70E-01		
14	50-00-0	Formaldehyde	4-Nitrobenzenethiol	t1/2(NBT)	min	1.25E-03		
15	55965-84-9	Kathon CG	4-Nitrobenzenethiol	t1/2(NBT)	min	2.17E-04		
16	124-63-0	Methyl sulfonyl chloride	4-Nitrobenzenethiol	t1/2(NBT)	min	7.67E-04		
17	128-53-0	N-Ethylmaleimide	4-Nitrobenzenethiol	t1/2(NBT)	min	3.33E-04		
18		Nitrobenzyl bromide	4-Nitrobenzenethiol	t1/2(NBT)	min	9.83E-06		
19	15646-46-5	Oxazolone	4-Nitrobenzenethiol	t1/2(NBT)	min	9.00E-06		
20	106-51-4	p-Benzoquinone	4-Nitrobenzenethiol	t1/2(NBT)	min	7.33E-06		
21	1939-99-7	Phenylmethanesulfonyl chloride	4-Nitrobenzenethiol	t1/2(NBT)	min	6.00E-03		
22	2892-51-5	Squaric acid	4-Nitrobenzenethiol	t1/2(NBT)	min	6.12E-02		
23	584-84-9	Toluene 2.4-diisocyanate	4-Nitrobenzenethiol	t1/2(NBT)	min	4.50E-04		
24	23726-91-2	(2E)-1-(2.6.6-Trimethyl-1-cyclohexen-1-yl)-2-buten-1-one	Glutathione	t1/2(GSH)	min	52	7	
25	123-73-9	(E)-Crotonaldehyde	Glutathione	t1/2(GSH)	min	> 5200		
26	97-00-7	1-Chloro-2.4-dinitrobenzene	Glutathione	t1/2(GSH)	min	200	70	
27	610-40-2	1-Chloro-3.4-dinitrobenzene	Glutathione	t1/2(GSH)	min	469		
28	610-40-2	1-Chloro-3.4-dinitrobenzene	Glutathione	t1/2(GSH)	min	52		
29	610-40-2	1-Chloro-3.4-dinitrobenzene	Glutathione	t1/2(GSH)	min	8.5		
30	610-40-2	1-Chloro-3.4-dinitrobenzene	Glutathione	t1/2(GSH)	min	4		
31	610-40-2	1-Chloro-3.4-dinitrobenzene	Glutathione	t1/2(GSH)	min	3		
32	1629-60-3	1-Hexen-3-one	Glutathione	t1/2(GSH)	min	3.9		
33	4312-99-6	1-Octen-3-one	Glutathione	t1/2(GSH)	min	9.72		
34	1629-58-9	1-Penten-3-one	Glutathione	t1/2(GSH)	min	3.56		
35	930-68-7	2-Cyclohexen-1-one	Glutathione	t1/2(GSH)	min	492		
36	930-30-3	2-Cyclopenten-1-one	Glutathione	t1/2(GSH)	min	19.4		
37	505-57-7	2-Hexenal	Glutathione	t1/2(GSH)	min	> 5200		
38	95-41-0	2-Hexyl-2-cyclopenten-1-one	Glutathione	t1/2(GSH)	min	17	4	
39	1120-73-6	2-Methyl-2-cyclopenten-1-one	Glutathione	t1/2(GSH)	min	73.1		
40	4643-27-0	2-Octen-4-one	Glutathione	t1/2(GSH)	min	22.3		
41	4643-27-0	2-Octen-4-one	Glutathione	t1/2(GSH)	min	2.3	0.6	

#2	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
2	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
3	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
4	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
5	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
6	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
7	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
8	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
9	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
10	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
11	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
12	25	7.4	PBS 0.1 M, ACN, acetone		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
13	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
14	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
15	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
16	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
17	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
18	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
19	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
20	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
21	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
22	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
23	25	7.4	PBS 0.1 M, ACN, acetone		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
24	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
25	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
26	22	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
27	10	7.5	PSB 50 mM, EDTA buffer 1 mM	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
28	10	8.5	PSB 50 mM, EDTA buffer 1 mM	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
29	10	9.5	PSB 50 mM, EDTA buffer 1 mM	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
30	10	10.5	PSB 50 mM, EDTA buffer 1 mM	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
31	10	11.5	PSB 50 mM, EDTA buffer 1 mM	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
32	25	7.4	PBS, max 20% DMSO	120 min	1:1.38	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
33	25	7.4	PBS, max 20% DMSO	120 min	1:0.79	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
34	25	7.4	PBS, max 20% DMSO	120 min	1:1.40	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
35	20	7.4	PBS 66 mM		1:1	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
36	25	7.4	PBS, max 20% DMSO	120 min	1:10.3	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
37	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
38	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
39	25	7.4	PBS, max 20% DMSO	120 min	1:298	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
40	25	7.4	PBS, max 20% DMSO	120 min	1:8.79	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
41	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773

#3	Comment
1	Assay: Stopped flow; UV(-SH loss 412 nm)
2	Assay: Stopped flow; UV(-SH loss 412 nm)
3	Assay: Stopped flow; UV(-SH loss 412 nm)
4	Assay: Stopped flow; UV(-SH loss 412 nm)
5	Assay: Stopped flow; UV(-SH loss 412 nm)
6	Assay: Stopped flow; UV(-SH loss 412 nm)
7	Assay: Stopped flow; UV(-SH loss 412 nm)
8	Assay: Stopped flow; UV(-SH loss 412 nm)
9	Assay: Stopped flow; UV(-SH loss 412 nm)
10	Assay: Stopped flow; UV(-SH loss 412 nm)
11	Assay: Stopped flow; UV(-SH loss 412 nm)
12	Assay: Stopped flow; UV(-SH loss 412 nm)
13	Assay: Stopped flow; UV(-SH loss 412 nm)
14	Assay: Stopped flow; UV(-SH loss 412 nm)
15	MITZ+ITZ mixture: competing reactions, deviation from ideal kinetics. Assay: Stopped flow; UV(-SH loss 412 nm
16	Assay: Stopped flow; UV(-SH loss 412 nm)
17	Assay: Stopped flow; UV(-SH loss 412 nm)
18	Assay: Stopped flow; UV(-SH loss 412 nm)
19	Assay: Stopped flow; UV(-SH loss 412 nm)
20	Assay: Stopped flow; UV(-SH loss 412 nm)
21	Assay: Stopped flow; UV(-SH loss 412 nm)
22	Assay: Stopped flow; UV(-SH loss 412 nm)
23	Assay: Stopped flow; UV(-SH loss 412 nm)
24	RP-HPLC (El DP, 254 nm).
25	reverse reaction t1/2 ca. 300 min.
26	HPLC-UV(210-300 nm).
27	HPLC-UV(210-300 nm).
28	HPLC-UV(210-300 nm).
29	HPLC-UV(210-300 nm).
30	HPLC-UV(210-300 nm).
31	HPLC-UV(210-300 nm).
32	UV (DTNB; 412 nm), neglects oxidative GSSH formation
33	UV (DTNB; 412 nm), neglects oxidative GSSH formation
34	UV (DTNB; 412 nm), neglects oxidative GSSH formation
35	
36	UV (DTNB; 412 nm), neglects oxidative GSSH formation
37	reverse reaction t1/2 ca. 300 min.
38	RP-HPLC (El DP, 254 nm).
39	UV (DTNB; 412 nm), neglects oxidative GSSH formation
40	UV (DTNB; 412 nm), neglects oxidative GSSH formation
41	RP-HPLC (El DP, 254 nm).

#4	Mechanism
1	Michael-type nucleophilic addition
2	Acylation
3	Michael-type nucleophilic addition: LC-MS analysis inconsistent with MA
4	Nucleophilic aromatic substitution (SNAr)
5	Michael-type nucleophilic addition
6	Michael-type nucleophilic addition: LC-MS analysis inconsistent with MA
7	Acylation: Schiff base former, but reactive to NBT
8	Michael-type nucleophilic addition
9	Nucleophilic substitution
10	Nucleophilic substitution
11	Nucleophilic substitution
12	Michael-type nucleophilic addition
13	Michael-type nucleophilic addition
14	Acylation: Schiff base former, but reactive to NBT
15	Michael-type nucleophilic addition: LC-MS analysis inconsistent with MA
16	Nucleophilic substitution
17	Nucleophilic substitution
18	Nucleophilic substitution
19	Michael-type nucleophilic addition
20	Michael-type nucleophilic addition
21	Nucleophilic substitution
22	Michael-type nucleophilic addition
23	Acylation: Hydrolysis and amine formation
24	Michael-type nucleophilic addition
25	Michael-type nucleophilic addition: adduct unstable
26	
27	
28	
29	
30	
31	
32	Michael-type nucleophilic addition
33	Michael-type nucleophilic addition
34	Michael-type nucleophilic addition
35	Michael-type nucleophilic addition
36	Michael-type nucleophilic addition
37	Michael-type nucleophilic addition: adduct unstable
38	Michael-type nucleophilic addition
39	Michael-type nucleophilic addition
40	Michael-type nucleophilic addition
41	Michael-type nucleophilic addition

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
42	764-39-6	2-Pentenal	Glutathione	t1/2(GSH)	min	> 5200		
43	1119-44-4	3-Heptene-2-one	Glutathione	t1/2(GSH)	min	44.3		
44	1679-36-3	3-Hexyn-2-one	Glutathione	t1/2(GSH)	min	38.5		
45	1193-18-6	3-Methyl-2-cyclohexen-1-one	Glutathione	t1/2(GSH)	min	> 4000		
46	2758-18-1	3-Methyl-2-cyclopenten-1-one	Glutathione	t1/2(GSH)	min	170		
47	2758-18-1	3-Methyl-2-cyclopenten-1-one	Glutathione	t1/2(GSH)	min	> 4000		
48	814-78-8	3-Methyl-3-buten-2-one	Glutathione	t1/2(GSH)	min	276		
49	565-62-8	3-Methyl-3-penten-2-one	Glutathione	t1/2(GSH)	min	54.8		
50	14309-57-0	3-Nonen-2-one	Glutathione	t1/2(GSH)	min	57.8		
51	1669-44-9	3-Octen-2-one	Glutathione	t1/2(GSH)	min	34.9		
52	625-33-2	3-Penten-2-one	Glutathione	t1/2(GSH)	min	23.4		
53		4-Ethoxy-2-pentenal	Glutathione	t1/2(GSH)	min	ca. 100		
54	2497-21-4	4-Hexen-3-one	Glutathione	t1/2(GSH)	min	20.9		
55	29389-17-1	4-Hydroxy-2-decenal	Glutathione	t1/2(GSH)	min	ca. 100		
56	29343-60-0	4-Hydroxy-2-dodecenal	Glutathione	t1/2(GSH)	min	ca. 100		
57	17427-09-7	4-Hydroxy-2-heptenal	Glutathione	t1/2(GSH)	min	ca. 100		
58	17427-08-6	4-Hydroxy-2-hexenal	Glutathione	t1/2(GSH)	min	ca. 100		
59	29343-52-0	4-Hydroxy-2-nonenal	Glutathione	t1/2(GSH)	min	ca. 100		
60	17449-15-9	4-Hydroxy-2-octenal	Glutathione	t1/2(GSH)	min	ca. 100		
61	34424-65-2	4-Hydroxy-2-pentenal	Glutathione	t1/2(GSH)	min	ca. 100		
62	29343-58-6	4-Hydroxy-2-undecenal	Glutathione	t1/2(GSH)	min	ca. 100		
63		4-Hydroxy-4-isopropyl-2-pentenal	Glutathione	t1/2(GSH)	min	ca. 100		
64		4-Isopropyl-3-methylcyclohex-2-en-1-one	Glutathione	t1/2(GSH)	min	> 4000		
65		4-Keto-2-pentenoic acid	Glutathione	t1/2(GSH)	min	48		
66	141-79-7	4-Methyl-3-penten-2-one	Glutathione	t1/2(GSH)	min	72		
67	141-79-7	4-Methyl-3-penten-2-one	Glutathione	t1/2(GSH)	min	340	130	
68	141-79-7	4-Methyl-3-penten-2-one	Glutathione	t1/2(GSH)	min	72000		
69	100-14-1	4-Nitrobenzylchloride	Glutathione	t1/2(GSH)	min	480	120	
70	100-14-1	4-Nitrobenzylchloride	Glutathione	t1/2(GSH)	min	11		
71	100-14-1	4-Nitrobenzylchloride	Glutathione	t1/2(GSH)	min	4		
72	100-14-1	4-Nitrobenzylchloride	Glutathione	t1/2(GSH)	min	144		
73	122-57-6	4-Phenyl-3-buten-2-one	Glutathione	t1/2(GSH)	min	22	5	
74		6.11-Dimethyldodeca-3.5.9-trien-2-one	Glutathione	t1/2(GSH)	min	1600	820	
75	1604-28-0	6-Methyl-3.5-heptadien-2-one	Glutathione	t1/2(GSH)	min	713	44	
76	34256-82-1	Acetochlor	Glutathione	t1/2(GSH)	min	15		
77	107-02-8	Acrolein	Glutathione	t1/2(GSH)	min	1.4		
78	79-10-7	Acrylic acid	Glutathione	t1/2(GSH)	min	166000		
79	15972-60-8	Alachlor	Glutathione	t1/2(GSH)	min	960	110	
80	15972-60-8	Alachlor	Glutathione	t1/2(GSH)	min	8		
81	1912-24-9	Atrazine	Glutathione	t1/2(GSH)	min	459		
82	131860-33-8	Azoxystrobin	Glutathione	t1/2(GSH)	min	6000	2000	
83	23696-85-7	beta-Damascenone	Glutathione	t1/2(GSH)	min	33	9	
84	23184-66-9	Butachlor	Glutathione	t1/2(GSH)	min	43	6	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
42	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
43	25	7.4	PBS, max 20% DMSO	120 min	1:9.21	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
44	25	7.4	PBS, max 20% DMSO	120 min	1:1.90	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
45	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
46	25	7.4	PBS, max 20% DMSO	120 min	1:279	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
47	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
48	20	7.4	PBS 66 mM		1:1	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
49	25	7.4	PBS, max 20% DMSO	120 min	1:106	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
50	25	7.4	PBS, max 20% DMSO	120 min	1:8.21	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
51	25	7.4	PBS, max 20% DMSO	120 min	1:12.7	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
52	25	7.4	PBS, max 20% DMSO	120 min	1:0.82	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
53	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
54	25	7.4	PBS, max 20% DMSO	120 min	1:10.1	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
55	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
56	20	7.4	PBS 66 mM, 10% ethanol		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
57	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
58	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
59	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
60	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
61	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
62	20	7.4	PBS 66 mM, 10% ethanol		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
63	20	7.4	PBS 66 mM		1:1	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
64	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
65	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
66	25	7.4	PBS, max 20% DMSO	120 min	1:291	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
67	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
68	20	7.4	PBS 66 mM		1:400	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
69	22	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
70	22	8.9	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
71	22	10.5	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
72	37	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
73	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
74	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
75	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
76	37	9	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
77	20	7.4	PBS 66 mM		1:1	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
78	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
79	22	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
80	37	9	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
81	37	10.5	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
82	37	9	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
83	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
84	20	9	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385

#	Comment
42	reverse reaction t1/2 ca. 300 min.
43	UV (DTNB; 412 nm), neglects oxidative GSSH formation
44	UV (DTNB; 412 nm), neglects oxidative GSSH formation
45	RP-HPLC (El DP, 254 nm).
46	UV (DTNB; 412 nm), neglects oxidative GSSH formation
47	RP-HPLC (El DP, 254 nm).
48	reverse reaction t1/2 ca. 1.2 min.
49	UV (DTNB; 412 nm), neglects oxidative GSSH formation
50	UV (DTNB; 412 nm), neglects oxidative GSSH formation
51	UV (DTNB; 412 nm), neglects oxidative GSSH formation
52	UV (DTNB; 412 nm), neglects oxidative GSSH formation
53	
54	UV (DTNB; 412 nm), neglects oxidative GSSH formation
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64	RP-HPLC (El DP, 254 nm).
65	
66	UV (DTNB; 412 nm), neglects oxidative GSSH formation
67	RP-HPLC (El DP, 254 nm).
68	reverse reaction t1/2 ca. 1000 min.
69	HPLC-UV(210-300 nm).
70	HPLC-UV(210-300 nm).
71	HPLC-UV(210-300 nm).
72	HPLC-UV(210-300 nm).
73	RP-HPLC (El DP, 254 nm).
74	RP-HPLC (El DP, 254 nm).
75	RP-HPLC (El DP, 254 nm).
76	22C pH 7: NR; HPLC-UV(210-300 nm).
77	
78	
79	HPLC-UV(210-300 nm).
80	HPLC-UV(210-300 nm).
81	23C pH 7: NR; HPLC-UV(210-300 nm).
82	33C pH 7: NR; HPLC-UV(210-300 nm).
83	RP-HPLC (El DP, 254 nm).
84	20C pH 7: NR; HPLC-UV(210-300 nm).

#	Mechanism
42	Michael-type nucleophilic addition: adduct unstable
43	Michael-type nucleophilic addition
44	Michael-type nucleophilic addition
45	Michael-type nucleophilic addition
46	Michael-type nucleophilic addition
47	Michael-type nucleophilic addition
48	Michael-type nucleophilic addition: adduct very unstable
49	Michael-type nucleophilic addition
50	Michael-type nucleophilic addition
51	Michael-type nucleophilic addition
52	Michael-type nucleophilic addition
53	Michael-type nucleophilic addition
54	Michael-type nucleophilic addition
55	Michael-type nucleophilic addition
56	Michael-type nucleophilic addition
57	Michael-type nucleophilic addition
58	Michael-type nucleophilic addition
59	Michael-type nucleophilic addition
60	Michael-type nucleophilic addition
61	Michael-type nucleophilic addition
62	Michael-type nucleophilic addition
63	Michael-type nucleophilic addition
64	Michael-type nucleophilic addition
65	Michael-type nucleophilic addition
66	Michael-type nucleophilic addition
67	Michael-type nucleophilic addition
68	Michael-type nucleophilic addition: adduct stable
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73	Michael-type nucleophilic addition
74	Michael-type nucleophilic addition
75	Michael-type nucleophilic addition
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77	Michael-type nucleophilic addition
78	Michael-type nucleophilic addition
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83	Michael-type nucleophilic addition
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#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
85	99-49-0	Carvone	Glutathione	t1/2(GSH)	min	950	280	
86	1897-45-6	Chlorothalonil	Glutathione	t1/2(GSH)	min	3		
87	5392-40-5	Citral	Glutathione	t1/2(GSH)	min	5200		
88	3724-65-0	Crotonic acid	Glutathione	t1/2(GSH)	min	> 166000		
89	333-41-5	Diazinon	Glutathione	t1/2(GSH)	min	ND		
90	37764-25-3	Dichlormid	Glutathione	t1/2(GSH)	min	634		
91	141-05-9	Diethyl maleate	Glutathione	t1/2(GSH)	min	3.6	1.5	
92	140-88-5	Ethyl acrylate	Glutathione	t1/2(GSH)	min	48.8		
93	623-70-1	Ethyl crotonate	Glutathione	t1/2(GSH)	min	171		
94	623-70-1	Ethyl crotonate	Glutathione	t1/2(GSH)	min	53000		
95	97-63-2	Ethyl methacrylate	Glutathione	t1/2(GSH)	min	379		
96	623-47-2	Ethyl propiolate	Glutathione	t1/2(GSH)	min	30.5		
97	69806-50-4	Fluazifop-butyl	Glutathione	t1/2(GSH)	min	ND		
98	79622-59-6	Fluazinam	Glutathione	t1/2(GSH)	min	22		
99	15457-05-3	Fluorodifen	Glutathione	t1/2(GSH)	min	2300	800	
100	15457-05-3	Fluorodifen	Glutathione	t1/2(GSH)	min	215		
101	61213-25-0	Flurochloridone	Glutathione	t1/2(GSH)	min	798		
102	72178-02-0	Fomesafen	Glutathione	t1/2(GSH)	min	ND		
103	100784-20-1	Halosulfuron-methyl	Glutathione	t1/2(GSH)	min	5300	900	
104	100784-20-1	Halosulfuron-methyl	Glutathione	t1/2(GSH)	min	250	50	
105	96-33-3	Methyl acrylate	Glutathione	t1/2(GSH)	min	30.4		
106	623-43-8	Methyl crotonate	Glutathione	t1/2(GSH)	min	106		
107	80-62-6	Methyl methacrylate	Glutathione	t1/2(GSH)	min	176		
108	922-67-8	Methyl propiolate	Glutathione	t1/2(GSH)	min	20.7		
109	6622-76-0	Methyl tiglate	Glutathione	t1/2(GSH)	min	548		
110	78-94-4	Methyl vinyl ketone	Glutathione	t1/2(GSH)	min	5.2		
111	78-94-4	Methyl vinyl ketone	Glutathione	t1/2(GSH)	min	0.003	0.001	
112	51218-45-2	Metolachlor	Glutathione	t1/2(GSH)	min	70	9	
113	623-15-4	Monofurfurylideneacetone	Glutathione	t1/2(GSH)	min	90	4	
114		N.N-dipropyl-2-chloroacetamide	Glutathione	t1/2(GSH)	min	1777		
115		N.N-dipropyl-2-chloroacetamide	Glutathione	t1/2(GSH)	min	374		
116		N.N-dipropyl-2-chloroacetamide	Glutathione	t1/2(GSH)	min	114		
117		N.N-dipropyl-2-chloroacetamide	Glutathione	t1/2(GSH)	min	29		
118		N.N-dipropyl-2-chloroacetamide	Glutathione	t1/2(GSH)	min	8		
119	141-32-2	n-Butyl acrylate	Glutathione	t1/2(GSH)	min	30.4		
120	128-53-0	N-Ethylmaleimide	Glutathione	t1/2(GSH)	min	0.0001		
121	925-60-0	n-Propyl acrylate	Glutathione	t1/2(GSH)	min	37.3		
122	51218-49-6	Pretilachlor	Glutathione	t1/2(GSH)	min	251		
123	1918-16-7	Propachlor	Glutathione	t1/2(GSH)	min	5		
124	55335-06-3	Triclopyr	Glutathione	t1/2(GSH)	min	2100	600	
125	58138-08-2	Tridiphane	Glutathione	t1/2(GSH)	min	880	290	
126	58138-08-2	Tridiphane	Glutathione	t1/2(GSH)	min	76		
127		Hydroxymethylvinyl ketone	L-Valinamide	t1/2(Amino acid)	min	16		1.2

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
85	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
86	36	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
87	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
88	20	7.4	PBS 66 mM		1:40	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
89	23	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
90	37	9	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
91	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
92	25	7.4	PBS, max 20% DMSO	120 min	1:9.86	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
93	25	7.4	PBS, max 20% DMSO	120 min	1:129	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
94	20	7.4	PBS 66 mM		1:40	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
95	25	7.4	PBS, max 20% DMSO	120 min	1:83.6	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
96	25	7.4	PBS, max 20% DMSO	120 min	1:1.84	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
97	37	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
98	40	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
99	25	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
100	26	10.5	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
101	37	10	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
102	37	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
103	36	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
104	36	9	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
105	25	7.4	PBS, max 20% DMSO	120 min	1:14.6	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
106	25	7.4	PBS, max 20% DMSO	120 min	1:234	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
107	25	7.4	PBS, max 20% DMSO	120 min	1:276	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
108	25	7.4	PBS, max 20% DMSO	120 min	1:2.33	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
109	25	7.4	PBS, max 20% DMSO	120 min	1:116	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
110	20	7.4	PBS 66 mM		1:1	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
111	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
112	37	9	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
113	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
114	10	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
115	25	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
116	37	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
117	50	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
118	65	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
119	25	7.4	PBS, max 20% DMSO	120 min	1:19.4	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
120	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
121	25	7.4	PBS, max 20% DMSO	120 min	1:13.3	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
122	40	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
123	25	9	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
124	37	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
125	25	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
126	26	9	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
127	37	7.4	PBS 10 mM	4-6 h	2:1	Barshteyn N et al., Chem. Res. Toxicol. 22 (2009), 918

#	Comment
85	RP-HPLC (El DP, 254 nm).
86	HPLC-UV(210-300 nm).
87	
88	
89	HPLC-UV(210-300 nm).
90	37C pH 7: NR; HPLC-UV(210-300 nm).
91	RP-HPLC (El DP, 254 nm).
92	UV (DTNB; 412 nm), neglects oxidative GSSH formation
93	UV (DTNB; 412 nm), neglects oxidative GSSH formation
94	reverse reaction t1/2 ca. 200 min.
95	UV (DTNB; 412 nm), neglects oxidative GSSH formation
96	UV (DTNB; 412 nm), neglects oxidative GSSH formation
97	HPLC-UV(210-300 nm).
98	HPLC-UV(210-300 nm).
99	HPLC-UV(210-300 nm).
100	HPLC-UV(210-300 nm).
101	37C pH 7: NR; HPLC-UV(210-300 nm).
102	HPLC-UV(210-300 nm).
103	HPLC-UV(210-300 nm).
104	HPLC-UV(210-300 nm).
105	UV (DTNB; 412 nm), neglects oxidative GSSH formation
106	UV (DTNB; 412 nm), neglects oxidative GSSH formation
107	UV (DTNB; 412 nm), neglects oxidative GSSH formation
108	UV (DTNB; 412 nm), neglects oxidative GSSH formation
109	UV (DTNB; 412 nm), neglects oxidative GSSH formation
110	
111	MVK: RP-HPLC (El DP, 210 nm).
112	20C pH 7: NR; HPLC-UV(210-300 nm).
113	RP-HPLC (El DP, 254 nm).
114	HPLC-UV(210-300 nm).
115	HPLC-UV(210-300 nm).
116	HPLC-UV(210-300 nm).
117	HPLC-UV(210-300 nm).
118	HPLC-UV(210-300 nm).
119	UV (DTNB; 412 nm), neglects oxidative GSSH formation
120	RP-HPLC (El DP, 254 nm).
121	UV (DTNB; 412 nm), neglects oxidative GSSH formation
122	HPLC-UV(210-300 nm).
123	20C pH 7: NR; HPLC-UV(210-300 nm).
124	HPLC-UV(210-300 nm).
125	HPLC-UV(210-300 nm).
126	HPLC-UV(210-300 nm).
127	Assay: HPLC-UV, NMR and ESI-MS

#	Mechanism
85	Michael-type nucleophilic addition
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87	Michael-type nucleophilic addition
88	NOT Michael-type nucleophilic addition
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91	Michael-type nucleophilic addition
92	Michael-type nucleophilic addition
93	Michael-type nucleophilic addition
94	Michael-type nucleophilic addition: adduct very unstable
95	Michael-type nucleophilic addition
96	Michael-type nucleophilic addition
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105	Michael-type nucleophilic addition
106	Michael-type nucleophilic addition
107	Michael-type nucleophilic addition
108	Michael-type nucleophilic addition
109	Michael-type nucleophilic addition
110	Michael-type nucleophilic addition
111	Michael-type nucleophilic addition
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113	Michael-type nucleophilic addition
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119	Michael-type nucleophilic addition
120	Michael-type nucleophilic addition
121	Michael-type nucleophilic addition
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126	
127	diadduct at higher HMVK concentrations

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
128		Hydroxymethylvinyl ketone	L-Valinamide	t1/2(Amino acid)	min	14		1.15
129		Hydroxymethylvinyl ketone	L-Valinamide	t1/2(Amino acid)	min	13.5		1.13
130		Hydroxymethylvinyl ketone	L-Valinamide	t1/2(Amino acid)	min	10		1
131		Hydroxymethylvinyl ketone	N(alpha)-Acetyl lysine	t1/2(Amino acid)	min	105		2.02
132		Hydroxymethylvinyl ketone	N(alpha)-Acetyl lysine	t1/2(Amino acid)	min	55		1.74
133		Hydroxymethylvinyl ketone	N(alpha)-Acetyl lysine	t1/2(Amino acid)	min	45		1.65
134		Hydroxymethylvinyl ketone	N(alpha)-Acetyl lysine	t1/2(Amino acid)	min	8.6		0.93
135		Hydroxymethylvinyl ketone	N-Acetyl cysteine	t1/2(Amino acid)	min	rapid		
136	585-71-7	(1-Bromoethyl)benzene	Glutathione	RC50(GSH)	mM	NR		
137	103-63-9	(2-Bromoethyl)benzene	Glutathione	RC50(GSH)	mM	NR		
138	103-63-9	(2-Bromoethyl)benzene	Glutathione	RC50(GSH)	mM	NR		
139	123-73-9	(E)-Crotonaldehyde	Glutathione	RC50(GSH)	mM	ca. 0.9		
140	123-73-9	(E)-Crotonaldehyde	Glutathione	RC50(GSH)	mM			-0.68
141	123-73-9	(E)-Crotonaldehyde	Glutathione	RC50(GSH)	mM	0.22		-0.66
142	80480-15-5	1-(Bromoacetyl)pyrene	Glutathione	RC50(GSH)	mM	0.058		-1.24
143	80480-15-5	1-(Bromoacetyl)pyrene	Glutathione	RC50(GSH)	mM	0.063		-1.2
144	95-50-1	1.2-Dichlorobenzene	Glutathione	RC50(GSH)	mM	NR		
145	524-42-5	1.2-Naphthoquinone	Glutathione	RC50(GSH)	mM	0.022		-1.66
146	524-42-5	1.2-Naphthoquinone	Glutathione	RC50(GSH)	mM	0.023		-1.64
147	4430-51-7	1.4-Butylenediisothiocyanate	Glutathione	RC50(GSH)	mM	0.038		-1.42
148	106-42-3	1.4-Dimethylbenzene	Glutathione	RC50(GSH)	mM	NR		
149	123-31-9	1.4-Hydroquinone	Glutathione	RC50(GSH)	mM			0.71
150	123-31-9	1.4-Hydroquinone	Glutathione	RC50(GSH)	mM	4.4		0.64
151	106-50-3	1.4-Phenylenediamine	Glutathione	RC50(GSH)	mM			1.33
152	106-50-3	1.4-Phenylenediamine	Glutathione	RC50(GSH)	mM	21		1.32
153	5586-70-9	1.6-Hexanediisothiocyanate	Glutathione	RC50(GSH)	mM	0.035		-1.46
154	4411-26-1	1-Adamantylisothiocyanate	Glutathione	RC50(GSH)	mM	0.22		-0.66
155	57-06-7	1-Allylisothiocyanate	Glutathione	RC50(GSH)	mM	0.053		-1.28
156	584-48-5	1-Bromo-2.4-dinitrobenzene	Glutathione	RC50(GSH)	mM	1		0
157	816-40-0	1-Bromo-2-butanone	Glutathione	RC50(GSH)	mM	0.05		-1.3
158	3355-28-0	1-Bromo-2-butyne	Glutathione	RC50(GSH)	mM	0.36		-0.44
159	110-53-2	1-Bromopentane	Glutathione	RC50(GSH)	mM	NR		
160	5469-26-1	1-Bromopinacolone	Glutathione	RC50(GSH)	mM	0.038		-1.42
161	71-36-3	1-Butanol	Glutathione	RC50(GSH)	mM	NR		
162	592-82-5	1-Butylisothiocyanate	Glutathione	RC50(GSH)	mM	0.13		-0.89
163	97-00-7	1-Chloro-2.4-dinitrobenzene	Glutathione	RC50(GSH)	mM			0.19

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
128	37	7.4	PBS 10 mM	4-6 h	5:1	Barshteyn N et al., Chem. Res. Toxicol. 22 (2009), 918
129	37	9	PBS 10 mM	4-6 h	5:1	Barshteyn N et al., Chem. Res. Toxicol. 22 (2009), 918
130	60	7.4	PBS 10 mM	4-6 h	5:1	Barshteyn N et al., Chem. Res. Toxicol. 22 (2009), 918
131	37	7.4	PBS 10 mM	4-6 h	2:1	Barshteyn N et al., Chem. Res. Toxicol. 22 (2009), 918
132	37	7.4	PBS 10 mM	4-6 h	5:1	Barshteyn N et al., Chem. Res. Toxicol. 22 (2009), 918
133	37	9	PBS 10 mM	4-6 h	5:1	Barshteyn N et al., Chem. Res. Toxicol. 22 (2009), 918
134	60	7.4	PBS 10 mM	4-6 h	5:1	Barshteyn N et al., Chem. Res. Toxicol. 22 (2009), 918
135	37	7.4	PBS 10 mM	4-6 h	2:1	Barshteyn N et al., Chem. Res. Toxicol. 22 (2009), 918
136		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
137		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
138		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
139	20	7.4	PBS 66 mM	30 min	1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
140		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
141		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
142		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
143		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
144		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
145		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
146		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
147		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
148		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
149		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicol. Vitro 20 (2006), 239
150		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
151		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicol. Vitro 20 (2006), 239
152		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
153		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
154		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
155		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
156		7.4	PBS, max. 20% DMSO	120 min	(different)	Gagan EM et al., Arch. Environ. Contam. Toxicol. 52 (2007), 283
157		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
158		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
159		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
160		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
161		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
162		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
163		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicol. Vitro 20 (2006), 239

#	Comment
128	Assay: HPLC-UV, NMR and ESI-MS
129	Assay: HPLC-UV, NMR and ESI-MS
130	Assay: HPLC-UV, NMR and ESI-MS
131	Assay: HPLC-UV, NMR and ESI-MS
132	Assay: HPLC-UV, NMR and ESI-MS
133	Assay: HPLC-UV, NMR and ESI-MS
134	Assay: HPLC-UV, NMR and ESI-MS
135	Assay: HPLC-UV, NMR and ESI-MS
136	not reactive. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
137	not reactive. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
138	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
139	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
140	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
141	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
142	extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
143	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
144	inactive at soluble level. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
145	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
146	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
147	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
148	inactive at soluble level. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
149	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
150	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
151	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
152	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
153	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
154	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
155	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
156	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
157	extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
158	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
159	not reactive. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
160	extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
161	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
162	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
163	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm

#	Mechanism
128	Michael-type nucleophilic addition: monoadduct; diadduct at higher HMVK concentrations
129	Michael-type nucleophilic addition: monoadduct; diadduct at higher HMVK concentrations
130	Michael-type nucleophilic addition: monoadduct; diadduct at higher HMVK concentrations
131	Michael-type nucleophilic addition: monoadduct+autooxidated octameric cyclic diadduct at epsilon-N
132	Michael-type nucleophilic addition: monoadduct+autooxidated octameric cyclic diadduct at epsilon-N
133	Michael-type nucleophilic addition: monoadduct+autooxidated octameric cyclic diadduct at epsilon-N
134	Michael-type nucleophilic addition: monoadduct+autooxidated octameric cyclic diadduct at epsilon-N
135	instantaneous; Michael-type nucleophilic addition: monoadduct
136	NOT Nucleophilic substitution, second order (SN2)
137	NOT Nucleophilic substitution, second order (SN2)
138	NOT Nucleophilic substitution, second order (SN2)
139	Michael-type nucleophilic addition
140	Michael-type nucleophilic addition
141	Michael-type nucleophilic addition
142	Nucleophilic substitution, second order (SN2)
143	Nucleophilic substitution, second order (SN2)
144	No protein binding
145	Michael-type nucleophilic addition
146	Michael-type nucleophilic addition
147	Michael-type nucleophilic addition
148	No protein binding
149	(Metabolically activated) pro-Michael addition
150	Pre-Michael addition of aromatic hydrocarbons
151	(Metabolically activated) pro-Michael addition
152	Pre-Michael addition of aromatic hydrocarbons
153	Michael-type nucleophilic addition
154	Michael-type nucleophilic addition
155	Michael-type nucleophilic addition
156	Nucleophilic aromatic substitution (SNAr)
157	Nucleophilic substitution, second order (SN2)
158	Nucleophilic substitution, second order (SN2)
159	NOT Nucleophilic substitution, second order (SN2)
160	Nucleophilic substitution, second order (SN2)
161	No protein binding
162	Michael-type nucleophilic addition
163	Nucleophilic aromatic substitution (SNAr)

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
164	97-00-7	1-Chloro-2.4-dinitrobenzene	Glutathione	RC50(GSH)	mM	1.5		0.18
165	13547-70-1	1-Chloropinacoline	Glutathione	RC50(GSH)	mM	0.75		-0.12
166	56601-42-4	1-Cyclopropylisothiocyanate	Glutathione	RC50(GSH)	mM	0.067		-1.17
167	245640-94-1	1-Decylisothiocyanate	Glutathione	RC50(GSH)	mM	0.069		-1.16
168	1072-32-8	1-Dodecylisothiocyanate	Glutathione	RC50(GSH)	mM	NR		
169	4426-83-9	1-Heptylisothiocyanate	Glutathione	RC50(GSH)	mM	0.056		-1.25
170	1629-60-3	1-Hexen-3-one	Glutathione	RC50(GSH)	mM	0.08	0.01	-1.1
171	1629-60-3	1-Hexen-3-one	Glutathione	RC50(GSH)	mM	0.052		-1.28
172	1629-60-3	1-Hexen-3-one	Glutathione	RC50(GSH)	mM	0.052		-1.28
173	1629-60-3	1-Hexen-3-one	Glutathione	RC50(GSH)	mM	0.052		-1.28
174	4404-45-9	1-Hexylisothiocyanate	Glutathione	RC50(GSH)	mM	0.088		-1.06
175	551-06-4	1-Naphthylisothiocyanate	Glutathione	RC50(GSH)	mM	0.038		-1.42
176	2562-37-0	1-Nitro-1-cyclohexene	Glutathione	RC50(GSH)	mM	0.028		-1.55
177	4430-43-7	1-Nonylisothiocyanate	Glutathione	RC50(GSH)	mM	0.073		-1.14
178	4312-99-6	1-Octen-3-one	Glutathione	RC50(GSH)	mM	0.11	0.01	-0.96
179	4312-99-6	1-Octen-3-one	Glutathione	RC50(GSH)	mM	0.051		-1.29
180	4430-45-9	1-Octylisothiocyanate	Glutathione	RC50(GSH)	mM	0.065		-1.19
181	1629-58-9	1-Penten-3-one	Glutathione	RC50(GSH)	mM	0.09	0.03	-1.05
182	1629-58-9	1-Penten-3-one	Glutathione	RC50(GSH)	mM	0.051		-1.29
183	1629-58-9	1-Penten-3-one	Glutathione	RC50(GSH)	mM	0.051		-1.29
184	1629-58-9	1-Penten-3-one	Glutathione	RC50(GSH)	mM	0.051		-1.29
185	629-12-9	1-Pentylisothiocyanate	Glutathione	RC50(GSH)	mM	0.15		-0.82
186	24309-48-6	1-Propargylisothiocyanate	Glutathione	RC50(GSH)	mM	0.056		-1.25
187	628-30-8	1-Propylisothiocyanate	Glutathione	RC50(GSH)	mM	0.11		-0.96
188	613-54-7	2-(2-Bromoacetyl)naphthalene	Glutathione	RC50(GSH)	mM	0.066		-1.18
189	613-54-7	2-(2-Bromoacetyl)naphthalene	Glutathione	RC50(GSH)	mM	0.066		-1.18
190	1468-82-2	2-(2-Bromoacetyl)thiophene	Glutathione	RC50(GSH)	mM	0.07		-1.15
191	10531-41-6	2-(2-Bromoacetyl)thiophene	Glutathione	RC50(GSH)	mM	0.077		-1.11
192	10531-41-6	2-(2-Bromoacetyl)thiophene	Glutathione	RC50(GSH)	mM	0.075		-1.12
193	699-18-3	2-(2-Nitrovinyl)furan	Glutathione	RC50(GSH)	mM	0.26		-0.59
194	651-70-7	2-(Trifluoroacetyl)thiophene	Glutathione	RC50(GSH)	mM	1.9		0.28
195	14920-89-9	2.3-Dimethylfuran	Glutathione	RC50(GSH)	mM	NR		
196	611-06-3	2.4-Dichloronitrobenzene	Glutathione	RC50(GSH)	mM			0.57
197	5910-85-0	2.4-Heptadienal	Glutathione	RC50(GSH)	mM	1.1		0.04
198	5910-85-0	2.4-Heptadienal	Glutathione	RC50(GSH)	mM	1.145		0.06
199	142-83-6	2.4-Hexadienal	Glutathione	RC50(GSH)	mM	1.52		0.18
200	527-61-7	2.6-Dimethyl-benzoquinone	Glutathione	RC50(GSH)	mM	0.085		-1.07
201	1193-79-9	2-Acetyl-5-methyl-furan	Glutathione	RC50(GSH)	mM	50		1.7
202		2-Acetyl-5-methylpyrrole	Glutathione	RC50(GSH)	mM	NR		
203	1192-62-7	2-Acetylfuran	Glutathione	RC50(GSH)	mM	13		1.11
204	1072-83-9	2-Acetylpyrrole	Glutathione	RC50(GSH)	mM	1.7		0.23
205	88-15-3	2-Acetylthiophene	Glutathione	RC50(GSH)	mM	47		1.67
206	95-55-6	2-Aminophenol	Glutathione	RC50(GSH)	mM	23		1.36

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
164		7.4	PBS, max. 20% DMSO	120 min	(different)	Gagan EM et al., Arch. Environ. Contam. Toxicol. 52 (2007), 283
165		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
166		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
167		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
168		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
169		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
170	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
171		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
172		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 16 (2005), 313
173		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
174		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
175		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
176		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
177		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
178	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
179		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
180		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
181	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
182		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
183		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 16 (2005), 313
184		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
185		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
186		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
187		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
188		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
189		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
190		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
191		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
192		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
193		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
194		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
195		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
196		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicol. Vitro 20 (2006), 239
197		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
198		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicology 231 (2007), 104
199		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
200		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
201		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
202		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
203		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
204		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
205		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
206		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21

#	Comment
164	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
165	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
166	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
167	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
168	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
169	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
170	low (1 mL) reaction volume. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
171	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
172	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
173	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
174	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
175	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
176	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
177	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
178	low (1 mL) reaction volume. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
179	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
180	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
181	low (1 mL) reaction volume. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
182	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
183	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
184	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
185	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
186	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
187	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
188	extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
189	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
190	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
191	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
192	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
193	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
194	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
195	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
196	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
197	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
198	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
199	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
200	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
201	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
202	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
203	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
204	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
205	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
206	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm

#	Mechanism
164	Nucleophilic aromatic substitution (SNAr)
165	Nucleophilic substitution, second order (SN2)
166	Michael-type nucleophilic addition
167	Michael-type nucleophilic addition
168	NOT Michael-type nucleophilic addition
169	Michael-type nucleophilic addition
170	Michael-type nucleophilic addition
171	Michael-type nucleophilic addition
172	Michael-type nucleophilic addition
173	Michael-type nucleophilic addition
174	Michael-type nucleophilic addition
175	Michael-type nucleophilic addition
176	Michael-type nucleophilic addition
177	Michael-type nucleophilic addition
178	Michael-type nucleophilic addition
179	Michael-type nucleophilic addition
180	Michael-type nucleophilic addition
181	Michael-type nucleophilic addition
182	Michael-type nucleophilic addition
183	Michael-type nucleophilic addition
184	Michael-type nucleophilic addition
185	Michael-type nucleophilic addition
186	Michael-type nucleophilic addition
187	Michael-type nucleophilic addition
188	Nucleophilic substitution, second order (SN2)
189	Nucleophilic substitution, second order (SN2)
190	Michael-type nucleophilic addition
191	Nucleophilic substitution, second order (SN2)
192	Nucleophilic substitution, second order (SN2)
193	Michael-type nucleophilic addition
194	Michael-type nucleophilic addition
195	No protein binding
196	Nucleophilic aromatic substitution (SNAr)
197	Michael-type nucleophilic addition
198	
199	Michael-type nucleophilic addition
200	Michael-type nucleophilic addition
201	Michael-type nucleophilic addition
202	NOT Michael-type nucleophilic addition
203	Michael-type nucleophilic addition
204	Michael-type nucleophilic addition
205	Michael-type nucleophilic addition
206	Pre-Michael addition of aromatic hydrocarbons

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
207	5447-97-2	2-Bromo-2-nitropropane	Glutathione	RC50(GSH)	mM	0.021		-1.68
208	14282-76-9	2-Bromo-3-methylthiophene	Glutathione	RC50(GSH)	mM	NR		
209	2873-18-9	2-Bromo-5-chlorothiophene	Glutathione	RC50(GSH)	mM	NR		
210	765-58-2	2-Bromo-5-methylthiophene	Glutathione	RC50(GSH)	mM	NR		
211	13195-50-1	2-Bromo-5-nitrothiophene	Glutathione	RC50(GSH)	mM	0.7		-0.15
212	683-57-8	2-Bromoacetamide	Glutathione	RC50(GSH)	mM	0.26		-0.59
213	683-57-8	2-Bromoacetamide	Glutathione	RC50(GSH)	mM	0.26		-0.59
214	70-11-1	2-Bromoacetophenone	Glutathione	RC50(GSH)	mM	0.055		-1.26
215	70-11-1	2-Bromoacetophenone	Glutathione	RC50(GSH)	mM	0.053		-1.28
216	80-58-0	2-Bromobutyric acid	Glutathione	RC50(GSH)	mM	16		1.2
217	2052-01-9	2-Bromoisobutyric acid	Glutathione	RC50(GSH)	mM	5.3		0.72
218	19481-82-4	2-Bromopropanenitrile	Glutathione	RC50(GSH)	mM	28		1.45
219	5875-25-2	2-Bromopropionamide	Glutathione	RC50(GSH)	mM	25		1.4
220	1003-09-4	2-Bromothiophene	Glutathione	RC50(GSH)	mM	NR		
221	584-93-0	2-Bromovaleric acid	Glutathione	RC50(GSH)	mM	12		1.08
222	4426-79-3	2-Butylisothiocyanate	Glutathione	RC50(GSH)	mM	0.34		-0.47
223	695-99-8	2-Chloro-1.4-benzoquinone	Glutathione	RC50(GSH)	mM	0.025		-1.6
224	79-07-2	2-Chloroacetamide	Glutathione	RC50(GSH)	mM	16		1.2
225	79-07-2	2-Chloroacetamide	Glutathione	RC50(GSH)	mM	16.9		1.23
226	4170-24-5	2-Chlorobutyric acid	Glutathione	RC50(GSH)	mM	38		1.58
227	96-43-5	2-Chlorothiophene	Glutathione	RC50(GSH)	mM	NR		
228	930-68-7	2-Cyclohexen-1-one	Glutathione	RC50(GSH)	mM	1.1		0.04
229	930-68-7	2-Cyclohexen-1-one	Glutathione	RC50(GSH)	mM	0.37		-0.43
230	930-30-3	2-Cyclopenten-1-one	Glutathione	RC50(GSH)	mM	0.58	0.02	-0.24
231	930-30-3	2-Cyclopenten-1-one	Glutathione	RC50(GSH)	mM	1.2		0.08
232	3208-16-0	2-Ethylfuran	Glutathione	RC50(GSH)	mM	NR		
233	103-11-7	2-Ethylhexyl acrylate	Glutathione	RC50(GSH)	mM	NR		
234	103-11-7	2-Ethylhexyl acrylate	Glutathione	RC50(GSH)	mM	0.44		-0.36
235	872-55-9	2-Ethylthiophene	Glutathione	RC50(GSH)	mM	NR		
236	609-38-1	2-Furamide	Glutathione	RC50(GSH)	mM	0.2		-0.7
237	7187-01-1	2-Furanacrylonitrile	Glutathione	RC50(GSH)	mM	26		1.41
238	3237-22-7	2-Furfurylidenemalononitrile	Glutathione	RC50(GSH)	mM	30		1.48
239	617-90-3	2-Furonitrile	Glutathione	RC50(GSH)	mM	17		1.23
240	31909-58-7	2-Furoylacetonitrile	Glutathione	RC50(GSH)	mM	50		1.7
241	505-57-7	2-Hexenal	Glutathione	RC50(GSH)	mM	ca. 0.9		
242	505-57-7	2-Hexenal	Glutathione	RC50(GSH)	mM	0.76		-0.12
243	818-61-1	2-Hydroxyethyl acrylate	Glutathione	RC50(GSH)	mM	0.28		-0.55
244	818-61-1	2-Hydroxyethyl acrylate	Glutathione	RC50(GSH)	mM	0.27		-0.57
245	818-61-1	2-Hydroxyethyl acrylate	Glutathione	RC50(GSH)	mM			-0.57
246	818-61-1	2-Hydroxyethyl acrylate	Glutathione	RC50(GSH)	mM	0.268		-0.57
247	868-77-9	2-Hydroxyethyl methacrylate	Glutathione	RC50(GSH)	mM	33		1.52
248	923-26-2	2-Hydroxypropyl methacrylate	Glutathione	RC50(GSH)	mM	28		1.85
249	923-26-2	2-Hydroxypropyl methacrylate	Glutathione	RC50(GSH)	mM	28.25		1.45

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
207		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
208		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
209		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
210		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
211		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
212		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
213		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
214		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
215		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
216		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
217		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
218		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
219		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
220		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
221		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
222		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
223		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
224		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
225		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
226		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
227		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
228	20	7.4	PBS 66 mM	30 min	1:1	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
229		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
230	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
231		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
232		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
233		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
234		7.4	Methanol:PBS 1:1	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
235		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
236		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
237		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
238		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
239		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
240		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
241	20	7.4	PBS 66 mM	30 min	1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
242		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 16 (2005), 313
243	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004
244		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
245		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
246		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicology 231 (2007), 104
247		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
248		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
249		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicology 231 (2007), 104

#	Comment
207	extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
208	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
209	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
210	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
211	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
212	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
213	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
214	extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
215	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
216	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
217	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
218	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
219	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
220	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
221	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
222	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
223	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
224	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
225	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
226	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
227	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
228	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
229	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
230	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
231	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
232	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
233	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
234	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
235	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
236	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
237	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
238	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
239	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
240	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
241	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
242	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
243	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
244	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
245	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
246	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
247	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
248	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
249	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm

#	Mechanism
207	Nucleophilic halogen abstraction. GS+Hal-R --> GS-Hal+H-R --> GSSG
208	NOT Nucleophilic substitution, second order (SN2): no halo-sp3-C
209	NOT Nucleophilic substitution, second order (SN2): no halo-sp3-C
210	NOT Nucleophilic substitution, second order (SN2): halo-sp3-C
211	Michael-type nucleophilic addition
212	Nucleophilic substitution, second order (SN2)
213	Nucleophilic substitution, second order (SN2)
214	Nucleophilic substitution, second order (SN2)
215	Nucleophilic substitution, second order (SN2)
216	SN2 or alpha-Elimination and carben addition to nucleophile
217	NOT Nucleophilic substitution, second order (SN2)
218	
219	Nucleophilic substitution, second order (SN2)
220	NOT Nucleophilic substitution, second order (SN2): no halo-sp3-C
221	SN2 or alpha-Elimination and carben addition to nucleophile
222	Michael-type nucleophilic addition
223	Michael-type nucleophilic addition
224	Nucleophilic substitution, second order (SN2)
225	Nucleophilic substitution, second order (SN2)
226	SN2 or alpha-Elimination and carben addition to nucleophile
227	NOT Nucleophilic substitution, second order (SN2): no halo-sp3-C
228	Michael-type nucleophilic addition
229	Michael-type nucleophilic addition
230	Michael-type nucleophilic addition
231	Michael-type nucleophilic addition
232	No protein binding
233	Michael-type nucleophilic addition
234	Michael-type nucleophilic addition
235	No protein binding
236	Michael-type nucleophilic addition
237	Michael-type nucleophilic addition
238	Michael-type nucleophilic addition
239	Michael-type nucleophilic addition
240	Michael-type nucleophilic addition
241	Michael-type nucleophilic addition
242	Michael-type nucleophilic addition
243	Michael-type nucleophilic addition
244	Michael-type nucleophilic addition
245	Michael-type nucleophilic addition
246	
247	Michael-type nucleophilic addition
248	Michael-type nucleophilic addition
249	

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
250	144-48-9	2-Iodoacetamide	Glutathione	RC50(GSH)	mM	0.2		-0.7
251	1120-73-6	2-Methyl-2-cyclopenten-1-one	Glutathione	RC50(GSH)	mM	8.4	0.01	0.92
252	623-36-9	2-Methyl-2-pentenal	Glutathione	RC50(GSH)	mM	21		1.32
253	623-36-9	2-Methyl-2-pentenal	Glutathione	RC50(GSH)	mM	21		1.32
254	553-97-9	2-Methyl-benzoquinone	Glutathione	RC50(GSH)	mM	0.046		-1.34
255	1572-52-7	2-Methyleneglutaronitrile	Glutathione	RC50(GSH)	mM	21		1.32
256	4466-24-4	2-n-Butylfuran	Glutathione	RC50(GSH)	mM	NR		
257	609-39-2	2-Nitrofuran	Glutathione	RC50(GSH)	mM	ND		
258	609-40-5	2-Nitrothiophene	Glutathione	RC50(GSH)	mM	NR		
259	3777-69-3	2-n-Pentylfuran	Glutathione	RC50(GSH)	mM	NR		
260	4861-58-9	2-n-Pentylthiophene	Glutathione	RC50(GSH)	mM	NR		
261	4643-27-0	2-Octen-4-one	Glutathione	RC50(GSH)	mM	0.22	0.01	-0.66
262	69626-80-8	2-Octylisothiocyanate	Glutathione	RC50(GSH)	mM	0.15		-0.82
263	764-39-6	2-Pentenal	Glutathione	RC50(GSH)	mM	ca. 0.9		
264	764-39-6	2-Pentenal	Glutathione	RC50(GSH)	mM	0.78		-0.11
265	201224-94-4	2-Pentylisothiocyanate	Glutathione	RC50(GSH)	mM	0.25		-0.6
266	3194-15-8	2-Propionylfuran	Glutathione	RC50(GSH)	mM	NR		
267	98-03-3	2-Thiophenecarboxaldehyde	Glutathione	RC50(GSH)	mM	NR		
268	5813-89-8	2-Thiophenecarboxamide	Glutathione	RC50(GSH)	mM	23		1.36
269	100-69-6	2-Vinylpyridine	Glutathione	RC50(GSH)	mM	2.8		0.45
270	100-69-6	2-Vinylpyridine	Glutathione	RC50(GSH)	mM	2.8		0.45
271	100-69-6	2-Vinylpyridine	Glutathione	RC50(GSH)	mM			0.56
272	29310-88-1	3-(Bromoacetyl)coumarin	Glutathione	RC50(GSH)	mM	0.07		-1.15
273	29310-88-1	3-(Bromoacetyl)coumarin	Glutathione	RC50(GSH)	mM	0.07		-1.15
274	119-84-6	3.4-Dihydrocoumarin	Glutathione	RC50(GSH)	mM			1.23
275	78-59-1	3.5.5-Trimethyl-2-cyclohexen-1-one	Glutathione	RC50(GSH)	mM			1.45
276	932-62-7	3-Acetyl-1-methylpyrrole	Glutathione	RC50(GSH)	mM	NR		
277	2386-25-6	3-Acetyl-2.4-dimethylpyrrole	Glutathione	RC50(GSH)	mM	NR		
278	1072-82-8	3-Acetylpyrrole	Glutathione	RC50(GSH)	mM	NR		
279	591-27-5	3-Aminophenol	Glutathione	RC50(GSH)	mM	NR		
280	40032-73-3	3-Bromo-2-chlorothiophene	Glutathione	RC50(GSH)	mM	NR		
281	814-75-5	3-Bromobutan-2-one	Glutathione	RC50(GSH)	mM	0.07		-1.15
282	221037-28-1	3-Bromofuran	Glutathione	RC50(GSH)	mM	NR		
283	872-31-1	3-Bromothiophene	Glutathione	RC50(GSH)	mM	NR		
284	1423-60-5	3-Butyn-2-one	Glutathione	RC50(GSH)	mM	0.057		-1.24
285	1694-29-7	3-Chloro-2.4-pentanedione	Glutathione	RC50(GSH)	mM	0.2		-0.7
286	4091-39-8	3-Chloro-2-butanone	Glutathione	RC50(GSH)	mM	1.3		0.11
287	4091-39-8	3-Chloro-2-butanone	Glutathione	RC50(GSH)	mM	1.4		0.15
288	542-76-7	3-Chloropropanonitrile	Glutathione	RC50(GSH)	mM	NR		
289	5875-24-1	3-Chloropropionamide	Glutathione	RC50(GSH)	mM	NR		
290	498-60-2	3-Furaldehyde	Glutathione	RC50(GSH)	mM	63		1.8
291	1119-44-4	3-Heptene-2-one	Glutathione	RC50(GSH)	mM	0.43	0.01	-0.37

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
250		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
251	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
252		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 16 (2005), 313
253		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
254		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
255		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
256		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
257		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
258		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
259		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
260		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
261	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
262		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
263	20	7.4	PBS 66 mM	30 min	1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
264		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 16 (2005), 313
265		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
266		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
267		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
268		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
269		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
270		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
271		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
272		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
273		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
274		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicol. Vitro 20 (2006), 239
275		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
276		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
277		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
278		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
279		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
280		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
281		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
282		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
283		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
284		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
285		7.4	PBS, max. 20% DMSO	120 min	(different)	Gagan EM et al., Arch. Environ. Contam. Toxicol. 52 (2007), 283
286		7.4	PBS, max. 20% DMSO	120 min	(different)	Gagan EM et al., Arch. Environ. Contam. Toxicol. 52 (2007), 283
287		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
288		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
289		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
290		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
291	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742

#	Comment
250	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
251	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
252	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
253	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
254	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
255	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
256	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm not quantifiable, color interference.
257	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm)
258	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
259	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
260	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
261	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
262	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
263	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
264	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
265	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
266	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
267	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
268	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
269	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
270	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
271	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
272	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
273	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
274	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
275	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
276	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
277	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
278	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
279	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
280	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
281	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
282	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
283	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
284	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
285	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
286	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
287	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
288	not reactive. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
289	not reactive. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
290	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
291	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm

#	Mechanism
250	Nucleophilic substitution, second order (SN2)
251	Michael-type nucleophilic addition
252	Michael-type nucleophilic addition
253	Michael-type nucleophilic addition
254	Michael-type nucleophilic addition
255	Michael-type nucleophilic addition
256	No protein binding
257	Michael-type nucleophilic addition
258	NOT Michael-type nucleophilic addition
259	No protein binding
260	No protein binding
261	Michael-type nucleophilic addition
262	Michael-type nucleophilic addition
263	Michael-type nucleophilic addition
264	Michael-type nucleophilic addition
265	Michael-type nucleophilic addition
266	NOT Michael-type nucleophilic addition
267	NOT Michael-type nucleophilic addition
268	Michael-type nucleophilic addition
269	Michael-type nucleophilic addition
270	Michael-type nucleophilic addition
271	Michael-type nucleophilic addition
272	Nucleophilic substitution, second order (SN2)
273	Nucleophilic substitution, second order (SN2)
274	Acylation
275	Michael-type nucleophilic addition
276	NOT Michael-type nucleophilic addition
277	NOT Michael-type nucleophilic addition
278	NOT Michael-type nucleophilic addition
279	(Metabolically activated) pro-Michael addition
280	NOT Nucleophilic substitution, second order (SN2): no halo-sp3-C
281	
282	NOT Nucleophilic substitution, second order (SN2): no halo-sp3-C
283	NOT Nucleophilic substitution, second order (SN2): no halo-sp3-C
284	Michael-type nucleophilic addition
285	Nucleophilic substitution, second order (SN2)
286	Nucleophilic substitution, second order (SN2)
287	
288	NOT Nucleophilic substitution, second order (SN2)
289	NOT Nucleophilic substitution, second order (SN2)
290	Michael-type nucleophilic addition
291	Michael-type nucleophilic addition

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
292	1679-36-3	3-Hexyn-2-one	Glutathione	RC50(GSH)	mM	0.16	0.01	-0.8
293	1679-36-3	3-Hexyn-2-one	Glutathione	RC50(GSH)	mM	0.12		-0.92
294	1679-36-3	3-Hexyn-2-one	Glutathione	RC50(GSH)	mM	0.12		-0.92
295	1679-36-3	3-Hexyn-2-one	Glutathione	RC50(GSH)	mM	0.12		-0.92
296	563-80-4	3-Methyl-2-butanone	Glutathione	RC50(GSH)	mM	NR		
297	201224-92-2	3-Methyl-2-butylisothiocyanate	Glutathione	RC50(GSH)	mM	0.32		-0.49
298	2758-18-1	3-Methyl-2-cyclopenten-1-one	Glutathione	RC50(GSH)	mM	26.9	0.5	1.43
299	814-78-8	3-Methyl-3-buten-2-one	Glutathione	RC50(GSH)	mM	15		1.18
300	565-62-8	3-Methyl-3-penten-2-one	Glutathione	RC50(GSH)	mM	5.17	0.8	0.71
301	565-62-8	3-Methyl-3-penten-2-one	Glutathione	RC50(GSH)	mM	10		1
302	565-62-8	3-Methyl-3-penten-2-one	Glutathione	RC50(GSH)	mM	10		1
303	565-62-8	3-Methyl-3-penten-2-one	Glutathione	RC50(GSH)	mM	9.8		0.99
304	565-62-8	3-Methyl-3-penten-2-one	Glutathione	RC50(GSH)	mM	10		1
305	628-03-5	3-Methylbutylisothiocyanate	Glutathione	RC50(GSH)	mM	0.082		-1.09
306	488-17-5	3-Methylcatechol	Glutathione	RC50(GSH)	mM			-0.24
307	488-17-5	3-Methylcatechol	Glutathione	RC50(GSH)	mM	1.04		0.02
308	616-44-4	3-Methylthiophene	Glutathione	RC50(GSH)	mM	NR		
309	34722-01-5	3-n-Butylthiophene	Glutathione	RC50(GSH)	mM	NR		
310	14309-57-0	3-Nonen-2-one	Glutathione	RC50(GSH)	mM	0.44	0.01	-0.36
311	1669-44-9	3-Octen-2-one	Glutathione	RC50(GSH)	mM	0.63	0.01	-0.2
312	1669-44-9	3-Octen-2-one	Glutathione	RC50(GSH)	mM	0.46		-0.34
313	625-33-2	3-Penten-2-one	Glutathione	RC50(GSH)	mM	0.21	0.01	-0.68
314	625-33-2	3-Penten-2-one	Glutathione	RC50(GSH)	mM	0.11		-0.96
315	201224-89-7	3-Pentylisothiocyanate	Glutathione	RC50(GSH)	mM	0.25		-0.6
316	17369-59-4	3-Propylidenephthalide	Glutathione	RC50(GSH)	mM			0.43
317	140-67-0	4-Allylanisole	Glutathione	RC50(GSH)	mM	NR		
318		4-Ethoxy-2-pentenal	Glutathione	RC50(GSH)	mM	ca. 0.3		
319	352530-29-1	4-Ethynylpyridine	Glutathione	RC50(GSH)	mM	4.5		0.65
320	352530-29-1	4-Ethynylpyridine	Glutathione	RC50(GSH)	mM	4.5		0.65
321	2497-21-4	4-Hexen-3-one	Glutathione	RC50(GSH)	mM	0.28	0.01	-0.55
322	2497-21-4	4-Hexen-3-one	Glutathione	RC50(GSH)	mM	0.34		-0.47
323	2497-21-4	4-Hexen-3-one	Glutathione	RC50(GSH)	mM	0.34		-0.47
324	2497-21-4	4-Hexen-3-one	Glutathione	RC50(GSH)	mM	0.34		-0.47
325	29389-17-1	4-Hydroxy-2-decenal	Glutathione	RC50(GSH)	mM	ca. 0.3		
326	29343-60-0	4-Hydroxy-2-dodecenal	Glutathione	RC50(GSH)	mM	ca. 0.3		
327	17427-09-7	4-Hydroxy-2-heptenal	Glutathione	RC50(GSH)	mM	ca. 0.3		
328	17427-08-6	4-Hydroxy-2-hexenal	Glutathione	RC50(GSH)	mM	ca. 0.3		
329	29343-52-0	4-Hydroxy-2-nonenal	Glutathione	RC50(GSH)	mM	ca. 0.3		
330	17449-15-9	4-Hydroxy-2-octenal	Glutathione	RC50(GSH)	mM	ca. 0.3		
331	34424-65-2	4-Hydroxy-2-pentenal	Glutathione	RC50(GSH)	mM	ca. 0.3		
332	29343-58-6	4-Hydroxy-2-undecenal	Glutathione	RC50(GSH)	mM	ca. 0.3		
333		4-Hydroxy-4-isopropyl-2-pentenal	Glutathione	RC50(GSH)	mM	ca. 0.3		
334		4-Keto-2-pentenoic acid	Glutathione	RC50(GSH)	mM	0.15		-0.82

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
292	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
293		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
294		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
295		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
296		7.4	PBS, max. 20% DMSO	120 min	(different)	Gagan EM et al., Arch. Environ. Contam. Toxicol. 52 (2007), 283
297		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
298	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
299	20	7.4	PBS 66 mM	30 min	1:1	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
300	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
301		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
302		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 16 (2005), 313
303		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
304		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
305		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
306		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicol. Vitro 20 (2006), 239
307		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
308		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
309		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
310	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
311	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
312		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
313	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
314		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
315		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
316		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicol. Vitro 20 (2006), 239
317		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
318	20	7.4	PBS 66 mM	30 min	1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
319		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
320		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
321	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
322		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
323		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 16 (2005), 313
324		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
325	20	7.4	PBS 66 mM	30 min	1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
326	20	7.4	PBS 66 mM, 10% ethanol	30 min	1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
327	20	7.4	PBS 66 mM	30 min	1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
328	20	7.4	PBS 66 mM	30 min	1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
329	20	7.4	PBS 66 mM	30 min	1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
330	20	7.4	PBS 66 mM	30 min	1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
331	20	7.4	PBS 66 mM	30 min	1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
332	20	7.4	PBS 66 mM, 10% ethanol	30 min	1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
333	20	7.4	PBS 66 mM	30 min	1:1	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
334	20	7.4	PBS 66 mM	30 min	1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466

#	Comment
292	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
293	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
294	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
295	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
296	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
297	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
298	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
299	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
300	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
301	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
302	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
303	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
304	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
305	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
306	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
307	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
308	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
309	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
310	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
311	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
312	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
313	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
314	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
315	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
316	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
317	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
318	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
319	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
320	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
321	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
322	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
323	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
324	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
325	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
326	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
327	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
328	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
329	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
330	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
331	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
332	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
333	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
334	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm

#	Mechanism
292	Michael-type nucleophilic addition
293	Michael-type nucleophilic addition
294	Michael-type nucleophilic addition
295	Michael-type nucleophilic addition
296	NOT Nucleophilic (aromatic or aliphatic) substitution
297	Michael-type nucleophilic addition
298	Michael-type nucleophilic addition
299	Michael-type nucleophilic addition
300	Michael-type nucleophilic addition
301	Michael-type nucleophilic addition
302	Michael-type nucleophilic addition
303	Michael-type nucleophilic addition
304	Michael-type nucleophilic addition
305	Michael-type nucleophilic addition
306	(Metabolically activated) pro-Michael addition
307	Pre-Michael addition of aromatic hydrocarbons
308	No protein binding
309	No protein binding
310	Michael-type nucleophilic addition
311	Michael-type nucleophilic addition
312	Michael-type nucleophilic addition
313	Michael-type nucleophilic addition
314	Michael-type nucleophilic addition
315	Michael-type nucleophilic addition
316	Acylation
317	(Metabolically activated) pro-Michael addition
318	Michael-type nucleophilic addition
319	Michael-type nucleophilic addition
320	Michael-type nucleophilic addition
321	Michael-type nucleophilic addition
322	Michael-type nucleophilic addition
323	Michael-type nucleophilic addition
324	Michael-type nucleophilic addition
325	Michael-type nucleophilic addition
326	Michael-type nucleophilic addition
327	Michael-type nucleophilic addition
328	Michael-type nucleophilic addition
329	Michael-type nucleophilic addition
330	Michael-type nucleophilic addition
331	Michael-type nucleophilic addition
332	Michael-type nucleophilic addition
333	Michael-type nucleophilic addition
334	Michael-type nucleophilic addition

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
335	5362-56-1	4-Methyl-2-pentenal	Glutathione	RC50(GSH)	mM	1.1		0.04
336	5362-56-1	4-Methyl-2-pentenal	Glutathione	RC50(GSH)	mM	1.1		0.04
337	141-79-7	4-Methyl-3-penten-2-one	Glutathione	RC50(GSH)	mM	31.4	4.8	1.5
338	141-79-7	4-Methyl-3-penten-2-one	Glutathione	RC50(GSH)	mM	166		2.22
339	141-79-7	4-Methyl-3-penten-2-one	Glutathione	RC50(GSH)	mM	28		1.45
340	141-79-7	4-Methyl-3-penten-2-one	Glutathione	RC50(GSH)	mM			1.45
341	141-79-7	4-Methyl-3-penten-2-one	Glutathione	RC50(GSH)	mM	28		1.45
342	100-11-8	4-Nitrobenzylbromide	Glutathione	RC50(GSH)	mM	0.22		-0.66
343	122-57-6	4-Phenyl-3-buten-2-one	Glutathione	RC50(GSH)	mM	3.7		0.57
344	122-57-6	4-Phenyl-3-buten-2-one	Glutathione	RC50(GSH)	mM	3.526		0.55
345	1817-57-8	4-Phenyl-3-butyn-2-one	Glutathione	RC50(GSH)	mM	0.05		-1.3
346	100-43-6	4-Vinylpyridine	Glutathione	RC50(GSH)	mM	0.31		-0.51
347	100-43-6	4-Vinylpyridine	Glutathione	RC50(GSH)	mM			-0.17
348	1119-51-3	5-Bromo-1-pentene	Glutathione	RC50(GSH)	mM	NR		
349	1899-24-7	5-Bromo-2-furaldehyde	Glutathione	RC50(GSH)	mM	10		1
350	5414-21-1	5-Bromopentanenitrile	Glutathione	RC50(GSH)	mM	NR		
351	2067-33-6	5-Bromovaleric acid	Glutathione	RC50(GSH)	mM	NR		
352	21508-19-0	5-Chloro-2-furaldehyde	Glutathione	RC50(GSH)	mM	50		1.7
353	50478-16-5	5-Chloro-2-thiophene carbonitrile	Glutathione	RC50(GSH)	mM	NR		
354	7283-96-7	5-Chlorothiophene-2-carbaldehyde	Glutathione	RC50(GSH)	mM	61		1.79
355	109-49-9	5-Hexen-2-one	Glutathione	RC50(GSH)	mM	25		1.4
356	5048-19-1	5-Hexenenitrile	Glutathione	RC50(GSH)	mM	NR		
357	2689-65-8	5-Iodo-2-furaldehyde	Glutathione	RC50(GSH)	mM	12		1.08
358	620-02-0	5-Methyl-2-furfural	Glutathione	RC50(GSH)	mM	3.7		0.57
359	698-63-5	5-Nitro-2-furaldehyde	Glutathione	RC50(GSH)	mM	14		1.15
360	4521-33-9	5-Nitrothiophene-2-carboxaldehyde	Glutathione	RC50(GSH)	mM	5.5		0.74
361	92-48-8	6-Methylcoumarin	Glutathione	RC50(GSH)	mM	NR		
362	67-64-1	Acetone	Glutathione	RC50(GSH)	mM	2752		3.44
363	98-86-2	Acetophenone	Glutathione	RC50(GSH)	mM	NR		
364	107-02-8	Acrolein	Glutathione	RC50(GSH)	mM	0.05		-1.3
365	107-02-8	Acrolein	Glutathione	RC50(GSH)	mM	0.086		-1.07
366	107-02-8	Acrolein	Glutathione	RC50(GSH)	mM	0.086		-1.07
367	79-10-7	Acrylic acid	Glutathione	RC50(GSH)	mM	380		2.58
368	999-55-3	Allyl acrylate	Glutathione	RC50(GSH)	mM	3.5		0.54
369	106-95-6	Allyl bromide	Glutathione	RC50(GSH)	mM	0.038		-1.42
370	107-05-1	Allyl chloride	Glutathione	RC50(GSH)	mM	0.85		-0.07
371	556-56-9	Allyl iodide	Glutathione	RC50(GSH)	mM	0.032		-1.49
372	96-05-9	Allyl methacrylate	Glutathione	RC50(GSH)	mM	0.14		-0.85
373	16212-05-8	Allyl phenyl sulfone	Glutathione	RC50(GSH)	mM	NR		
374	122-40-7	alpha-Amyl cinnamaldehyde	Glutathione	RC50(GSH)	mM	NR		
375	122-40-7	alpha-Amyl cinnamaldehyde	Glutathione	RC50(GSH)	mM	NR		
376	122-40-7	alpha-Amyl cinnamaldehyde	Glutathione	RC50(GSH)	mM	NR		
377	7492-44-6	alpha-Butylcinnamic aldehyde	Glutathione	RC50(GSH)	mM	NR		

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
335		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 16 (2005), 313
336		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
337	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
338	20	7.4	PBS 66 mM	30 min	1:400	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
339		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 16 (2005), 313
340		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
341		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
342		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
343		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
344		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicology 231 (2007), 104
345		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
346		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
347		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
348		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
349		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
350		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
351		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
352		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
353		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
354		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
355		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 16 (2005), 313
356		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
357		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
358		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
359		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
360		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
361		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
362		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
363		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
364	20	7.4	PBS 66 mM	30 min	1:1	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
365		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
366		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
367	20	7.4	PBS 66 mM	30 min	1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
368		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
369		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
370		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
371		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
372	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004
373		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
374		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
375		7.4	Methanol:PBS 1:1	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
376		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicology 231 (2007), 104
377		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21

#	Comment
335	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
336	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
337	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
338	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
339	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
340	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
341	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
342	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
343	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
344	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
345	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
346	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
347	reported pEC50 = 0.12. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
348	not reactive. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
349	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
350	not reactive. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
351	not reactive. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
352	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
353	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
354	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
355	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
356	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
357	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
358	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
359	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
360	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
361	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
362	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
363	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
364	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
365	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
366	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
367	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
368	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
369	extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
370	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
371	extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
372	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
373	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
374	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
375	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
376	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
377	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm

#	Mechanism
335	Michael-type nucleophilic addition
336	Michael-type nucleophilic addition
337	Michael-type nucleophilic addition
338	Michael-type nucleophilic addition
339	Michael-type nucleophilic addition
340	Michael-type nucleophilic addition
341	Michael-type nucleophilic addition
342	Nucleophilic substitution, second order (SN2)
343	Michael-type nucleophilic addition
344	
345	Michael-type nucleophilic addition
346	Michael-type nucleophilic addition
347	Michael-type nucleophilic addition
348	NOT Nucleophilic substitution, second order (SN2)
349	Michael-type nucleophilic addition
350	NOT Nucleophilic substitution, second order (SN2)
351	NOT Nucleophilic substitution, second order (SN2)
352	Michael-type nucleophilic addition
353	NOT Michael-type nucleophilic addition
354	Michael-type nucleophilic addition
355	Michael-type nucleophilic addition
356	NOT Michael-type nucleophilic addition
357	Michael-type nucleophilic addition
358	Michael-type nucleophilic addition
359	Michael-type nucleophilic addition
360	Michael-type nucleophilic addition
361	NOT Michael-type nucleophilic addition
362	No protein binding
363	NOT Nucleophilic substitution, second order (SN2)
364	Michael-type nucleophilic addition
365	Michael-type nucleophilic addition
366	Michael-type nucleophilic addition
367	Michael-type nucleophilic addition
368	Michael-type nucleophilic addition
369	Nucleophilic substitution, second order (SN2)
370	Nucleophilic substitution, second order (SN2)
371	Nucleophilic substitution, second order (SN2)
372	Michael-type nucleophilic addition
373	NOT Michael-type nucleophilic addition
374	NOT Michael-type nucleophilic addition
375	NOT Michael-type nucleophilic addition
376	
377	NOT Michael-type nucleophilic addition

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
378	101-86-0	alpha-Hexylcinnamaldehyde	Glutathione	RC50(GSH)	mM	NR		
379	101-86-0	alpha-Hexylcinnamaldehyde	Glutathione	RC50(GSH)	mM	NR		
380	101-39-3	alpha-Methyl cinnamic aldehyde	Glutathione	RC50(GSH)	mM	PR		
381	101-39-3	alpha-Methyl cinnamic aldehyde	Glutathione	RC50(GSH)	mM	25		1.4
382	100-39-0	Benzyl bromide	Glutathione	RC50(GSH)	mM	0.19		-0.72
383	57-57-8	beta-Propiolactone	Glutathione	RC50(GSH)	mM			0.27
384	590-17-0	Bromoacetonitrile	Glutathione	RC50(GSH)	mM	0.55		-0.26
385	563-70-2	Bromonitromethane	Glutathione	RC50(GSH)	mM	0.03		-1.52
386	123-72-8	Butyraldehyde	Glutathione	RC50(GSH)	mM	NR		
387	120-80-9	Catechol	Glutathione	RC50(GSH)	mM	12		1.08
388	120-80-9	Catechol	Glutathione	RC50(GSH)	mM	10		1
389	107-14-2	Chloroacetonitrile	Glutathione	RC50(GSH)	mM	14		1.15
390	108-90-7	Chlorobenzene	Glutathione	RC50(GSH)	mM	NR		
391	104-55-2	Cinnamaldehyde	Glutathione	RC50(GSH)	mM			0.02
392	104-55-2	Cinnamaldehyde	Glutathione	RC50(GSH)	mM	1		0
393	104-55-2	Cinnamaldehyde	Glutathione	RC50(GSH)	mM	1.15		0.06
394	621-82-9	Cinnamic acid	Glutathione	RC50(GSH)	mM			1.51
395	104-54-1	Cinnamic alcohol	Glutathione	RC50(GSH)	mM	NR		
396	104-54-1	Cinnamic alcohol	Glutathione	RC50(GSH)	mM	NR		
397	1476-11-5	cis-1.4-Dichloro-2-butene	Glutathione	RC50(GSH)	mM	1		0
398	5392-40-5	Citral	Glutathione	RC50(GSH)	mM	12		1.08
399	5392-40-5	Citral	Glutathione	RC50(GSH)	mM			0.31
400	91-64-5	Coumarin	Glutathione	RC50(GSH)	mM			1.57
401	91-64-5	Coumarin	Glutathione	RC50(GSH)	mM	NR		
402	91-64-5	Coumarin	Glutathione	RC50(GSH)	mM	NR		
403	93-51-6	Creosol	Glutathione	RC50(GSH)	mM	NR		
404	93-51-6	Creosol	Glutathione	RC50(GSH)	mM	NR		
405	3724-65-0	Crotonic acid	Glutathione	RC50(GSH)	mM	> 380		
406	110-83-8	Cyclohexene	Glutathione	RC50(GSH)	mM	NR		
407	1122-82-3	Cyclohexylisothiocyanate	Glutathione	RC50(GSH)	mM	0.098		-1.01
408	33522-03-1	Cyclopentylisothiocyanate	Glutathione	RC50(GSH)	mM	0.1		-1
409	685-87-0	Diethyl bromomalonate	Glutathione	RC50(GSH)	mM	0.025		-1.6
410	631-22-1	Diethyl dibromomalonate	Glutathione	RC50(GSH)	mM	0.012		-1.92
411	623-91-6	Diethyl fumarate	Glutathione	RC50(GSH)	mM	0.2		-0.7
412	141-05-9	Diethyl maleate	Glutathione	RC50(GSH)	mM	2.1		0.32
413	141-05-9	Diethyl maleate	Glutathione	RC50(GSH)	mM	3.28		0.52
414	533-68-6	Ethyl 2-bromobutyrate	Glutathione	RC50(GSH)	mM	1.6		0.2
415	600-00-0	Ethyl 2-bromoisobutyrate	Glutathione	RC50(GSH)	mM	0.66		-0.18
416	535-11-5	Ethyl 2-bromopropionate	Glutathione	RC50(GSH)	mM	1.7		0.23
417	615-83-8	Ethyl 2-bromovalerate	Glutathione	RC50(GSH)	mM	1.7		0.23
418	57382-97-5	Ethyl 2-thiopheneacetate	Glutathione	RC50(GSH)	mM	NR		
419	141-78-6	Ethyl acetate	Glutathione	RC50(GSH)	mM	NR		
420	140-88-5	Ethyl acrylate	Glutathione	RC50(GSH)	mM	0.47	0.009	-0.33

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
378		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
379		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicology 231 (2007), 104
380		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
381		7.4	Methanol:PBS 1:1	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
382		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
383		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicol. Vitro 20 (2006), 239
384		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
385		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
386		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
387		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
388		7.4	Methanol:PBS 1:1	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
389		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
390		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
391		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicol. Vitro 20 (2006), 239
392		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
393		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicology 231 (2007), 104
394		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicol. Vitro 20 (2006), 239
395		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
396		7.4	Methanol:PBS 1:1	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
397		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
398	20	7.4	PBS 66 mM, 10% ethanol	30 min	1:10	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
399		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicol. Vitro 20 (2006), 239
400		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicol. Vitro 20 (2006), 239
401		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
402		7.4	Methanol:PBS 1:1	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
403		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
404		7.4	Methanol:PBS 1:1	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
405	20	7.4	PBS 66 mM	30 min	1:40	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
406		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
407		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
408		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
409		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
410		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
411		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
412		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
413		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicology 231 (2007), 104
414		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
415		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
416		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
417		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
418		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
419		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
420	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742

#	Comment
378	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
379	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
380	partial response at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
381	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
382	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
383	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
384	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
385	extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
386	no effect at 200 mM. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
387	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
388	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
389	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
390	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
391	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
392	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
393	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
394	unreactive. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
395	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
396	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
397	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
398	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
399	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
400	weak MA. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
401	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
402	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
403	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
404	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
405	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
406	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
407	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
408	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
409	extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
410	extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
411	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
412	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
413	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
414	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
415	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
416	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
417	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
418	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
419	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
420	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm

#	Mechanism
378	NOT Michael-type nucleophilic addition
379	
380	Michael-type nucleophilic addition
381	Michael-type nucleophilic addition
382	Nucleophilic substitution, second order (SN2)
383	Nucleophilic substitution, second order (SN2)
384	
385	Nucleophilic halogen abstraction. GS+Hal-R --> GS-Hal+H-R --> GSSG
386	NOT Michael-type nucleophilic addition
387	Pre-Michael addition of aromatic hydrocarbons
388	Pre-Michael addition of aromatic hydrocarbons
389	
390	No protein binding
391	Michael-type nucleophilic addition
392	Michael-type nucleophilic addition
393	
394	
395	(Metabolically activated) pro-Michael addition
396	(Metabolically activated) pro-Michael addition
397	Nucleophilic substitution, second order (SN2)
398	Michael-type nucleophilic addition
399	Schiff base formation
400	Michael-type nucleophilic addition
401	NOT Michael-type nucleophilic addition
402	NOT Michael-type nucleophilic addition
403	(Metabolically activated) pro-Michael addition
404	(Metabolically activated) pro-Michael addition
405	NOT Michael-type nucleophilic addition
406	NOT Michael-type nucleophilic addition
407	Michael-type nucleophilic addition
408	Michael-type nucleophilic addition
409	Nucleophilic halogen abstraction. GS+Hal-R --> GS-Hal+H-R --> GSSG
410	Nucleophilic halogen abstraction. GS+Hal-R --> GS-Hal+H-R --> GSSG
411	Michael-type nucleophilic addition
412	Michael-type nucleophilic addition
413	
414	Nucleophilic substitution, second order (SN2)
415	beta-Elimination and Michael addition
416	Nucleophilic substitution, second order (SN2)
417	Nucleophilic substitution, second order (SN2)
418	No protein binding: ester narcotic
419	NOT Nucleophilic substitution, second order (SN2)
420	Michael-type nucleophilic addition

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
421	140-88-5	Ethyl acrylate	Glutathione	RC50(GSH)	mM	1.85		0.27
422	140-88-5	Ethyl acrylate	Glutathione	RC50(GSH)	mM	0.52		-0.28
423	140-88-5	Ethyl acrylate	Glutathione	RC50(GSH)	mM	0.37		-0.43
424	140-88-5	Ethyl acrylate	Glutathione	RC50(GSH)	mM			-0.29
425	140-88-5	Ethyl acrylate	Glutathione	RC50(GSH)	mM	0.52		-0.28
426	140-88-5	Ethyl acrylate	Glutathione	RC50(GSH)	mM	0.516		-0.29
427	105-36-2	Ethyl bromoacetate	Glutathione	RC50(GSH)	mM	0.085		-1.07
428	105-36-2	Ethyl bromoacetate	Glutathione	RC50(GSH)	mM	0.086		-1.07
429	105-39-5	Ethyl chloroacetate	Glutathione	RC50(GSH)	mM	3		0.48
430	105-39-5	Ethyl chloroacetate	Glutathione	RC50(GSH)	mM	3.06		0.49
431	623-70-1	Ethyl crotonate	Glutathione	RC50(GSH)	mM	34.8	0.2	1.54
432	623-70-1	Ethyl crotonate	Glutathione	RC50(GSH)	mM	122		2.09
433	623-70-1	Ethyl crotonate	Glutathione	RC50(GSH)	mM	23		1.36
434	623-70-1	Ethyl crotonate	Glutathione	RC50(GSH)	mM	23		1.36
435	459-72-3	Ethyl fluoroacetate	Glutathione	RC50(GSH)	mM	NR		
436	16205-90-6	Ethyl hex-2-ynoate	Glutathione	RC50(GSH)	mM	0.96		-0.02
437	623-48-3	Ethyl iodoacetate	Glutathione	RC50(GSH)	mM	0.029		-1.54
438	623-48-3	Ethyl iodoacetate	Glutathione	RC50(GSH)	mM	0.029		-1.54
439	97-63-2	Ethyl methacrylate	Glutathione	RC50(GSH)	mM	NR		
440	97-63-2	Ethyl methacrylate	Glutathione	RC50(GSH)	mM	42		1.62
441	97-63-2	Ethyl methacrylate	Glutathione	RC50(GSH)	mM	NR		1
442	97-63-2	Ethyl methacrylate	Glutathione	RC50(GSH)	mM	NR		
443	623-47-2	Ethyl propiolate	Glutathione	RC50(GSH)	mM	0.13	0.01	-0.89
444	623-47-2	Ethyl propiolate	Glutathione	RC50(GSH)	mM	0.091		-1.04
445	623-47-2	Ethyl propiolate	Glutathione	RC50(GSH)	mM	0.091		-1.04
446	105-37-3	Ethyl propionate	Glutathione	RC50(GSH)	mM	NR		
447	105-37-3	Ethyl propionate	Glutathione	RC50(GSH)	mM	NR		
448	4341-76-8	Ethyl tetrolate	Glutathione	RC50(GSH)	mM	1.3		0.11
449	4341-76-8	Ethyl tetrolate	Glutathione	RC50(GSH)	mM	1.31		0.12
450	97-90-5	Ethylene glycol dimethacrylate	Glutathione	RC50(GSH)	mM	5.6		0.75
451	97-90-5	Ethylene glycol dimethacrylate	Glutathione	RC50(GSH)	mM	NR		1.45
452	7367-82-0	Ethyl-trans-2-octenoate	Glutathione	RC50(GSH)	mM	3.2		0.51
453	7367-82-0	Ethyl-trans-2-octenoate	Glutathione	RC50(GSH)	mM	NR		
454	13894-21-8	Ethynyl-p-tolyl sulfone	Glutathione	RC50(GSH)	mM	0.06		-1.22
455	97-53-0	Eugenol	Glutathione	RC50(GSH)	mM			1.17
456	110-00-9	Furan	Glutathione	RC50(GSH)	mM	NR		
457	98-01-1	Furfural	Glutathione	RC50(GSH)	mM	NR		
458	591-78-6	Hexan-2-one	Glutathione	RC50(GSH)	mM			2.04
459	110-54-3	Hexane	Glutathione	RC50(GSH)	mM	NR		
460	624-75-9	Iodoacetonitrile	Glutathione	RC50(GSH)	mM	0.45		-0.35
461	106-63-8	Isobutyl acrylate	Glutathione	RC50(GSH)	mM	1.7		0.23
462	97-86-9	Isobutyl methacrylate	Glutathione	RC50(GSH)	mM	5		0.7

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
421	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004
422		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
423		7.4	Methanol:PBS 1:1	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
424		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
425		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
426		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicology 231 (2007), 104
427		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
428		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
429		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
430		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
431	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
432	20	7.4	PBS 66 mM	30 min	1:40	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
433		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 16 (2005), 313
434		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
435		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
436		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
437		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
438		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
439	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
440		7.4	Methanol:PBS 1:1	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
441		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
442		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
443	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
444		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 16 (2005), 313
445		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
446		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
447		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
448		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
449		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
450		7.4	Methanol:PBS 1:1	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
451		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
452		7.4	Methanol:PBS 1:1	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
453		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
454		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
455		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicol. Vitro 20 (2006), 239
456		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
457		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
458		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
459		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
460		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
461	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004
462	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004

#	Comment
421	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
422	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
423	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
424	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
425	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
426	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
427	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
428	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
429	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
430	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
431	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
432	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
433	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
434	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
435	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
436	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
437	extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
438	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm 50% GSH degradation not achieved at saturation limit.
439	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm)
440	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
441	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
442	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
443	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
444	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
445	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
446	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
447	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
448	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
449	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
450	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
451	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
452	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
453	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
454	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
455	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
456	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
457	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
458	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
459	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
460	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
461	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
462	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm

#	Mechanism
421	Michael-type nucleophilic addition
422	Michael-type nucleophilic addition
423	Michael-type nucleophilic addition
424	Michael-type nucleophilic addition
425	Michael-type nucleophilic addition
426	
427	Nucleophilic substitution, second order (SN2)
428	Nucleophilic substitution, second order (SN2)
429	Nucleophilic substitution, second order (SN2)
430	Nucleophilic substitution, second order (SN2)
431	Michael-type nucleophilic addition
432	Michael-type nucleophilic addition
433	Michael-type nucleophilic addition
434	Michael-type nucleophilic addition
435	NOT Nucleophilic substitution, second order (SN2)
436	Michael-type nucleophilic addition
437	Nucleophilic substitution, second order (SN2)
438	Nucleophilic substitution, second order (SN2)
439	Michael-type nucleophilic addition
440	Michael-type nucleophilic addition
441	NOT Michael-type nucleophilic addition
442	NOT Michael-type nucleophilic addition
443	Michael-type nucleophilic addition
444	Michael-type nucleophilic addition
445	Michael-type nucleophilic addition
446	NOT Michael-type nucleophilic addition
447	NOT Michael-type nucleophilic addition
448	Michael-type nucleophilic addition
449	Michael-type nucleophilic addition
450	Michael-type nucleophilic addition
451	NOT Michael-type nucleophilic addition
452	Michael-type nucleophilic addition
453	NOT Michael-type nucleophilic addition
454	Michael-type nucleophilic addition
455	(Metabolically activated) pro-Michael addition
456	No protein binding
457	NOT Nucleophilic substitution, second order (SN2): no halo-sp3-C
458	Michael-type nucleophilic addition
459	No protein binding
460	
461	Michael-type nucleophilic addition
462	Michael-type nucleophilic addition

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
463	591-82-2	Isobutylisothiocyanate	Glutathione	RC50(GSH)	mM	0.08		-1.1
464	97-54-1	Isoeugenol	Glutathione	RC50(GSH)	mM			0.32
465	97-54-1	Isoeugenol	Glutathione	RC50(GSH)	mM	NR		
466	4245-35-6	Isopentyl acrylate	Glutathione	RC50(GSH)	mM	0.93		-0.03
467	4655-34-9	Isopropyl methacrylate	Glutathione	RC50(GSH)	mM	NR		
468	3196-15-4	Methyl 2-bromobutyrate	Glutathione	RC50(GSH)	mM	3.5		0.54
469	3196-15-4	Methyl 2-bromobutyrate	Glutathione	RC50(GSH)	mM	3.54		0.55
470	5445-22-7	Methyl 2-bromooctanoate	Glutathione	RC50(GSH)	mM	NR		
471	611-13-2	Methyl 2-furoate	Glutathione	RC50(GSH)	mM	22		1.34
472	111-12-6	Methyl 2-octynoate	Glutathione	RC50(GSH)	mM	0.26		-0.59
473	5454-83-1	Methyl 5-bromovalerate	Glutathione	RC50(GSH)	mM	NR		
474	5454-83-1	Methyl 5-bromovalerate	Glutathione	RC50(GSH)	mM	NR		
475	96-33-3	Methyl acrylate	Glutathione	RC50(GSH)	mM	0.42	0.01	-0.38
476	96-33-3	Methyl acrylate	Glutathione	RC50(GSH)	mM	0.45		-0.35
477	96-33-3	Methyl acrylate	Glutathione	RC50(GSH)	mM	0.5		-0.3
478	96-33-3	Methyl acrylate	Glutathione	RC50(GSH)	mM	0.41		-0.39
479	96-33-3	Methyl acrylate	Glutathione	RC50(GSH)	mM	0.55		-0.26
480	96-32-2	Methyl bromoacetate	Glutathione	RC50(GSH)	mM	0.066		-1.18
481	96-32-2	Methyl bromoacetate	Glutathione	RC50(GSH)	mM	0.067		-1.17
482	96-34-4	Methyl chloroacetate	Glutathione	RC50(GSH)	mM	2.8		0.45
483	96-34-4	Methyl chloroacetate	Glutathione	RC50(GSH)	mM	2.93		0.47
484	623-43-8	Methyl crotonate	Glutathione	RC50(GSH)	mM	32.6	0.5	1.51
485	623-43-8	Methyl crotonate	Glutathione	RC50(GSH)	mM	25		1.4
486	623-43-8	Methyl crotonate	Glutathione	RC50(GSH)	mM	25		1.4
487	80-62-6	Methyl methacrylate	Glutathione	RC50(GSH)	mM	74.1	1.1	1.87
488	80-62-6	Methyl methacrylate	Glutathione	RC50(GSH)	mM	7.42		0.87
489	80-62-6	Methyl methacrylate	Glutathione	RC50(GSH)	mM	70		1.85
490	80-62-6	Methyl methacrylate	Glutathione	RC50(GSH)	mM	43		1.63
491	80-62-6	Methyl methacrylate	Glutathione	RC50(GSH)	mM	75		1.88
492	80-62-6	Methyl methacrylate	Glutathione	RC50(GSH)	mM	76		1.88
493	80-62-6	Methyl methacrylate	Glutathione	RC50(GSH)	mM	76		1.88
494	922-67-8	Methyl propiolate	Glutathione	RC50(GSH)	mM	0.14	0.01	-0.85
495	922-67-8	Methyl propiolate	Glutathione	RC50(GSH)	mM	0.091		-1.04
496	922-67-8	Methyl propiolate	Glutathione	RC50(GSH)	mM	0.095		-1.02
497	23326-27-4	Methyl tetrolate	Glutathione	RC50(GSH)	mM	4.3		0.63
498	23326-27-4	Methyl tetrolate	Glutathione	RC50(GSH)	mM	1.27		0.1
499	6622-76-0	Methyl tiglate	Glutathione	RC50(GSH)	mM	NR		
500	6622-76-0	Methyl tiglate	Glutathione	RC50(GSH)	mM	6.1		0.79
501	7367-81-9	Methyl trans-2-octenoate	Glutathione	RC50(GSH)	mM	5.8		0.76
502	78-94-4	Methyl vinyl ketone	Glutathione	RC50(GSH)	mM	0.05		-1.3
503	78-94-4	Methyl vinyl ketone	Glutathione	RC50(GSH)	mM			-1.1

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
463		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
464		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicol. Vitro 20 (2006), 239
465		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
466		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
467		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
468		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
469		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
470		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
471		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
472		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
473		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
474		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
475	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
476		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
477		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
478		7.4	Methanol:PBS 1:1	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
479		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
480		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
481		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
482		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
483		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
484	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
485		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 16 (2005), 313
486		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
487	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
488	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004
489		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
490		7.4	Methanol:PBS 1:1	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
491		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 16 (2005), 313
492		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
493		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
494	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
495		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
496		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
497		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 16 (2005), 313
498		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
499	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
500		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
501		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
502	20	7.4	PBS 66 mM	30 min	1:1	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
503		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413

#	Comment
463	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
464	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
465	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
466	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
467	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
468	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
469	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
470	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
471	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
472	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
473	not reactive. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
474	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
475	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
476	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
477	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
478	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
479	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
480	extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
481	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
482	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
483	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
484	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
485	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
486	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
487	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
488	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
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493	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
494	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
495	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
496	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
497	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
498	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm 50% GSH degradation not achieved at saturation limit.
499	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm) RC50 too high: very low water solubility.
500	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm)
501	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
502	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
503	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm

#	Mechanism
463	Michael-type nucleophilic addition
464	(Metabolically activated) pro-Michael addition
465	(Metabolically activated) pro-Michael addition
466	Michael-type nucleophilic addition
467	NOT Michael-type nucleophilic addition
468	Nucleophilic substitution, second order (SN2)
469	Nucleophilic substitution, second order (SN2)
470	NOT Nucleophilic substitution, second order (SN2)
471	Michael-type nucleophilic addition
472	Michael-type nucleophilic addition
473	NOT Nucleophilic substitution, second order (SN2)
474	NOT Nucleophilic substitution, second order (SN2)
475	Michael-type nucleophilic addition
476	Michael-type nucleophilic addition
477	Michael-type nucleophilic addition
478	Michael-type nucleophilic addition
479	Michael-type nucleophilic addition
480	Nucleophilic substitution, second order (SN2)
481	Nucleophilic substitution, second order (SN2)
482	Nucleophilic substitution, second order (SN2)
483	Nucleophilic substitution, second order (SN2)
484	Michael-type nucleophilic addition
485	Michael-type nucleophilic addition
486	Michael-type nucleophilic addition
487	Michael-type nucleophilic addition
488	Michael-type nucleophilic addition
489	Michael-type nucleophilic addition
490	Michael-type nucleophilic addition
491	Michael-type nucleophilic addition
492	Michael-type nucleophilic addition
493	Michael-type nucleophilic addition
494	Michael-type nucleophilic addition
495	Michael-type nucleophilic addition
496	Michael-type nucleophilic addition
497	Michael-type nucleophilic addition
498	Michael-type nucleophilic addition
499	Michael-type nucleophilic addition
500	Michael-type nucleophilic addition
501	Michael-type nucleophilic addition
502	Michael-type nucleophilic addition
503	Michael-type nucleophilic addition

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
504	78-94-4	Methyl vinyl ketone	Glutathione	RC50(GSH)	mM	0.09		-1.05
505	5445-17-0	Methyl-2-bromopropionate	Glutathione	RC50(GSH)	mM	1.5		0.18
506	5445-17-0	Methyl-2-bromopropionate	Glutathione	RC50(GSH)	mM	1.04		0.02
507	4755-81-1	Methyl-2-chloroacetoacetate	Glutathione	RC50(GSH)	mM	0.3		-0.52
508	2396-77-2	Methyl-2-hexenoate	Glutathione	RC50(GSH)	mM	1.2		0.08
509	111-80-8	Methyl-2-nonynoate	Glutathione	RC50(GSH)	mM	0.27		-0.57
510	111-80-8	Methyl-2-nonynoate	Glutathione	RC50(GSH)	mM	0.264		-0.58
511	3395-91-3	Methyl-3-bromopropionate	Glutathione	RC50(GSH)	mM	8.62		0.94
512	4897-84-1	Methyl-4-bromobutyrate	Glutathione	RC50(GSH)	mM	48.44		1.69
513	141-32-2	n-Butyl acrylate	Glutathione	RC50(GSH)	mM	0.55	0.007	-0.26
514	141-32-2	n-Butyl acrylate	Glutathione	RC50(GSH)	mM	0.8		-0.1
515	109-73-9	n-Butylamine	Glutathione	RC50(GSH)	mM	NR		
516	1122-60-7	Nitrocyclohexane	Glutathione	RC50(GSH)	mM	NR		
517	111-87-5	n-Octanol	Glutathione	RC50(GSH)	mM	NR		
518	2998-23-4	n-Pentyl acrylate	Glutathione	RC50(GSH)	mM	0.81		-0.09
519	925-60-0	n-Propyl acrylate	Glutathione	RC50(GSH)	mM	0.49	0.006	-0.31
520	925-60-0	n-Propyl acrylate	Glutathione	RC50(GSH)	mM	0.8		-0.1
521	2210-28-8	n-Propyl methacrylate	Glutathione	RC50(GSH)	mM	NR		
522	111-65-9	Octane	Glutathione	RC50(GSH)	mM	NR		
523	124-07-2	Octanoic acid	Glutathione	RC50(GSH)	mM	NR		
524	15646-46-5	Oxazolone	Glutathione	RC50(GSH)	mM			-0.45
525	150-13-0	p-Aminobenzoic acid	Glutathione	RC50(GSH)	mM			1.6
526	106-51-4	p-Benzoquinone	Glutathione	RC50(GSH)	mM	0.046		-1.34
527	106-51-4	p-Benzoquinone	Glutathione	RC50(GSH)	mM	0.047		-1.33
528	106-51-4	p-Benzoquinone	Glutathione	RC50(GSH)	mM			-1.33
529	106-51-4	p-Benzoquinone	Glutathione	RC50(GSH)	mM	0.0465		-1.33
530	96-22-0	Pentan-3-one	Glutathione	RC50(GSH)	mM	NR		
531	2111-75-3	Perillaldehyde	Glutathione	RC50(GSH)	mM	5.5		0.74
532	2111-75-3	Perillaldehyde	Glutathione	RC50(GSH)	mM	NR		
533	536-74-3	Phenyl acetylene	Glutathione	RC50(GSH)	mM	NR		
534	620-72-4	Phenyl bromoacetate	Glutathione	RC50(GSH)	mM	0.072		-1.14
535	1562-34-1	Phenyl vinyl sulfonate	Glutathione	RC50(GSH)	mM	0.081		-1.09
536	20451-53-0	Phenyl vinyl sulfoxide	Glutathione	RC50(GSH)	mM	17		1.23
537	2579-22-8	Phenylpropargyl aldehyde	Glutathione	RC50(GSH)	mM	0.025		-1.6
538	85-44-9	Phthalic anhydride	Glutathione	RC50(GSH)	mM			0.05
539	10477-47-1	Propargyl acrylate	Glutathione	RC50(GSH)	mM	0.21		-0.68
540	6750-04-5	Propargyl benzoate	Glutathione	RC50(GSH)	mM	NR		
541	79-05-0	Propionamide	Glutathione	RC50(GSH)	mM	NR		
542	35223-80-4	Propyl bromoacetate	Glutathione	RC50(GSH)	mM	0.075		-1.12
543	35223-80-4	Propyl bromoacetate	Glutathione	RC50(GSH)	mM	0.089		-1.05
544	5396-24-7	Propyl chloroacetate	Glutathione	RC50(GSH)	mM	2.7		0.43
545	5396-24-7	Propyl chloroacetate	Glutathione	RC50(GSH)	mM	2.75		0.44
546	110-86-1	Pyridine	Glutathione	RC50(GSH)	mM	NR		

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
504		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
505		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
506		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
507		7.4	PBS, max. 20% DMSO	120 min	(different)	Gagan EM et al., Arch. Environ. Contam. Toxicol. 52 (2007), 283
508		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
509		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
510		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicology 231 (2007), 104
511		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
512		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
513	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
514		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
515		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
516		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
517		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
518		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
519	25	7.4	PBS, max. 20% DMSO	120 min	(different)	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
520		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
521		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
522		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
523		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
524		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicol. Vitro 20 (2006), 239
525		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicol. Vitro 20 (2006), 239
526		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
527		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
528		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
529		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicology 231 (2007), 104
530		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
531		7.4	Methanol:PBS 1:1	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
532		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
533		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
534		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
535		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
536		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
537		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
538		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicol. Vitro 20 (2006), 239
539		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
540		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
541		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
542		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
543		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
544		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
545		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
546		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359

#	Comment
504	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
505	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
506	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
507	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
508	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
509	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
510	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
511	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
512	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
513	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
514	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
515	no effect at 1000 mM. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
516	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
517	inactive at soluble level. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
518	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
519	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
520	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
521	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
522	inactive at soluble level. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
523	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
524	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
525	unreactive. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
526	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
527	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
528	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
529	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
530	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
531	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
532	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
533	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
534	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
535	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
536	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
537	RC50 extrapolated. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
538	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
539	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
540	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
541	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
542	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
543	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
544	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
545	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
546	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm

#	Mechanism
504	Michael-type nucleophilic addition
505	Nucleophilic substitution, second order (SN2)
506	Nucleophilic substitution, second order (SN2)
507	Nucleophilic substitution, second order (SN2)
508	Michael-type nucleophilic addition
509	Michael-type nucleophilic addition
510	
511	Nucleophilic substitution, second order (SN2)
512	Nucleophilic substitution, second order (SN2)
513	Michael-type nucleophilic addition
514	Michael-type nucleophilic addition
515	NOT Michael-type nucleophilic addition
516	NOT Michael-type nucleophilic addition
517	No protein binding
518	Michael-type nucleophilic addition
519	Michael-type nucleophilic addition
520	Michael-type nucleophilic addition
521	NOT Michael-type nucleophilic addition
522	No protein binding
523	No protein binding
524	Acylation
525	
526	Michael-type nucleophilic addition
527	Michael-type nucleophilic addition
528	Michael-type nucleophilic addition
529	
530	NOT Michael-type nucleophilic addition
531	Michael-type nucleophilic addition
532	NOT Michael-type nucleophilic addition
533	NOT Michael-type nucleophilic addition
534	Nucleophilic substitution, second order (SN2)
535	Michael-type nucleophilic addition
536	Michael-type nucleophilic addition
537	Michael-type nucleophilic addition
538	Acylation
539	Michael-type nucleophilic addition
540	NOT Michael-type nucleophilic addition
541	NOT Nucleophilic substitution, second order (SN2)
542	Nucleophilic substitution, second order (SN2)
543	Nucleophilic substitution, second order (SN2)
544	Nucleophilic substitution, second order (SN2)
545	Nucleophilic substitution, second order (SN2)
546	NOT Michael-type nucleophilic addition

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
547	109-97-7	Pyrrole	Glutathione	RC50(GSH)	mM	NR		
548	4513-94-4	Pyrrole-2-carbonitrile	Glutathione	RC50(GSH)	mM	NR		
549	1003-29-8	Pyrrole-2-carboxaldehyde	Glutathione	RC50(GSH)	mM	NR		
550	108-46-3	Resorcinol	Glutathione	RC50(GSH)	mM	NR		
551	151-21-3	Sodium lauryl sulfate	Glutathione	RC50(GSH)	mM	NR		
552	100-42-5	Styrene	Glutathione	RC50(GSH)	mM	NR		
553	100-42-5	Styrene	Glutathione	RC50(GSH)	mM	NR		
554	1663-39-4	tert-Butyl acrylate	Glutathione	RC50(GSH)	mM	1.5		0.18
555	5292-43-3	tert-Butyl bromoacetate	Glutathione	RC50(GSH)	mM	0.085		-1.07
556	5292-43-3	tert-Butyl bromoacetate	Glutathione	RC50(GSH)	mM	0.075		-1.12
557	107-59-5	tert-Butyl chloroacetate	Glutathione	RC50(GSH)	mM	3.4		0.53
558	107-59-5	tert-Butyl chloroacetate	Glutathione	RC50(GSH)	mM	3.37		0.53
559	590-42-1	tert-Butylisothiocyanate	Glutathione	RC50(GSH)	mM	6.2		0.79
560	17701-76-7	tert-Octylisothiocyanate	Glutathione	RC50(GSH)	mM	NA		
561	597-97-7	tert-Pentylisothiocyanate	Glutathione	RC50(GSH)	mM	0.75		-0.12
562	110-02-1	Thiophene	Glutathione	RC50(GSH)	mM	NR		
563	1003-31-2	Thiophene-2-carbonitrile	Glutathione	RC50(GSH)	mM	NR		
564	498-62-4	Thiophene-3-carboxaldehyde	Glutathione	RC50(GSH)	mM	NR		
565	110-57-6	trans-1.4-Dichloro-2-butene	Glutathione	RC50(GSH)	mM	1		0
566	7348-71-2	trans-1-Bromo-2-pentene	Glutathione	RC50(GSH)	mM	0.46		-0.34
567	3913-81-3	trans-2-Decenal	Glutathione	RC50(GSH)	mM	0.17		-0.77
568	6728-26-3	trans-2-Hexenal	Glutathione	RC50(GSH)	mM	0.4		-0.4
569	6728-26-3	trans-2-Hexenal	Glutathione	RC50(GSH)	mM			-0.05
570	6728-26-3	trans-2-Hexenal	Glutathione	RC50(GSH)	mM	0.76		-0.12
571	2548-87-0	trans-2-Octenal	Glutathione	RC50(GSH)	mM	0.28		-0.55
572	1576-87-0	trans-2-Pentenal	Glutathione	RC50(GSH)	mM	0.33		-0.48
573	1576-87-0	trans-2-Pentenal	Glutathione	RC50(GSH)	mM	0.78		-0.11
574	1576-87-0	trans-2-Pentenal	Glutathione	RC50(GSH)	mM	0.78		-0.11
575	13991-37-2	trans-2-Pentenoic acid	Glutathione	RC50(GSH)	mM	37		1.57
576	39511-08-5	trans-3-(2-Furyl)acrolein	Glutathione	RC50(GSH)	mM	6.6		0.82
577	552-30-7	Trimellitic anhydride	Glutathione	RC50(GSH)	mM			0.18
578	110-62-3	Valeraldehyde	Glutathione	RC50(GSH)	mM	NR		
579	2177-18-6	Vinyl acrylate	Glutathione	RC50(GSH)	mM	0.11		-0.96
580	2177-18-6	Vinyl acrylate	Glutathione	RC50(GSH)	mM	0.11		-0.96
581	14861-06-4	Vinyl crotonate	Glutathione	RC50(GSH)	mM	4.3		0.63
582	14861-06-4	Vinyl crotonate	Glutathione	RC50(GSH)	mM	4.3		0.63
583	4245-37-8	Vinyl methacrylate	Glutathione	RC50(GSH)	mM	4.5		0.65
584	101-39-3	alpha-Methyl cinnamic aldehyde	Cys-Peptide (AcRFAACAA)	RC50(Cys-P.)	mM	>10		
585	23726-91-2	beta-Damascone	Cys-Peptide (AcRFAACAA)	RC50(Cys-P.)	mM	1.78		0.25
586	79-77-6	beta-Ionone	Cys-Peptide (AcRFAACAA)	RC50(Cys-P.)	mM	8.93		0.95
587	104-55-2	Cinnamaldehyde	Cys-Peptide (AcRFAACAA)	RC50(Cys-P.)	mM	2.74		0.44
588	5392-40-5	Citral	Cys-Peptide (AcRFAACAA)	RC50(Cys-P.)	mM	7.03		0.85
589	141-05-9	Diethyl maleate	Cys-Peptide (AcRFAACAA)	RC50(Cys-P.)	mM	0.31		-0.51

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
547		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
548		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
549		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
550		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
551		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicol. Vitro 20 (2006), 239
552		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
553		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
554		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
555		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
556		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
557		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
558		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 18 (2007), 21
559		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
560		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
561		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Environ. Toxicol. Pharmacol. 23 (2007), 10
562		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
563		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
564		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
565		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
566		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
567		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
568		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
569		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
570		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
571		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
572		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Contact Dermatitis 60 (2009), 21
573		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
574		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
575		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., Chem. Res. Toxicol. 20 (2007), 1359
576		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. (2010), in press
577		7.4	PBS, max. 20% DMSO	120 min	(different)	Aptula N et al., Toxicol. Vitro 20 (2006), 239
578		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 17 (2006), 413
579		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 16 (2005), 313
580		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
581		7.4	PBS, max. 20% DMSO	120 min	(different)	Schultz TW et al., SAR QSAR Environ. Res. 16 (2005), 313
582		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
583		7.4	PBS, max. 20% DMSO	120 min	(different)	Yarbrough et al., Chem. Res. Toxicol. 20 (2007), 558
584	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
585	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
586	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
587	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
588	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
589	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220

#	Comment
547	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
548	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
549	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
550	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
551	unreactive. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
552	no effect at 100 mM. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
553	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
554	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
555	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
556	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
557	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
558	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
559	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
560	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
561	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
562	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
563	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
564	not reactive at saturation. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
565	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
566	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
567	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
568	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
569	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
570	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
571	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
572	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
573	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
574	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
575	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
576	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
577	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
578	no effect at 100 mM. Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
579	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
580	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
581	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
582	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
583	Assay: room temperature; UV (absorption free SH after reaction with DTNB=5,5'-dithiobis(2-nitrobenzoic acid); 412 nm
584	LC-MS. Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.
585	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.
586	LC-MS. Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.
587	LC-MS. Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.
588	LC-MS. Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.
589	LC-MS. Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.

#	Mechanism
547	No protein binding
548	NOT Michael-type nucleophilic addition
549	NOT Michael-type nucleophilic addition
550	(Metabolically activated) pro-Michael addition
551	
552	No protein binding
553	NOT Michael-type nucleophilic addition
554	Michael-type nucleophilic addition
555	Nucleophilic substitution, second order (SN2)
556	Nucleophilic substitution, second order (SN2)
557	Nucleophilic substitution, second order (SN2)
558	Nucleophilic substitution, second order (SN2)
559	Michael-type nucleophilic addition
560	Michael-type nucleophilic addition
561	Michael-type nucleophilic addition
562	No protein binding
563	NOT Michael-type nucleophilic addition
564	NOT Michael-type nucleophilic addition
565	Nucleophilic substitution, second order (SN2)
566	Nucleophilic substitution, second order (SN2)
567	Michael-type nucleophilic addition
568	Michael-type nucleophilic addition
569	Michael-type nucleophilic addition
570	Michael-type nucleophilic addition
571	Michael-type nucleophilic addition
572	Michael-type nucleophilic addition
573	Michael-type nucleophilic addition
574	Michael-type nucleophilic addition
575	Michael-type nucleophilic addition
576	Michael-type nucleophilic addition
577	Acylation
578	NOT Michael-type nucleophilic addition
579	Michael-type nucleophilic addition
580	Michael-type nucleophilic addition
581	Michael-type nucleophilic addition
582	Michael-type nucleophilic addition
583	Michael-type nucleophilic addition
584	Mass spectrometry confirms adduct formation
585	
586	Adduct + mass 32 (oxidation)
587	Mass spectrometry confirms adduct formation
588	Adduct confirmed (traces)
589	Mass spectrometry confirms adduct formation

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
590	97-53-0	Eugenol	Cys-Peptide (AcRFAACAA)	RC50(Cys-P.)	mM	4.27		0.63
591	56973-85-4	Galbanone	Cys-Peptide (AcRFAACAA)	RC50(Cys-P.)	mM	6.5		0.81
592	97-54-1	Isoeugenol	Cys-Peptide (AcRFAACAA)	RC50(Cys-P.)	mM	0.63		-0.2
593	357650-26-1	Pomarose	Cys-Peptide (AcRFAACAA)	RC50(Cys-P.)	mM	0.4		-0.4
594	2634-33-5	1.2-Benzisothiazolin-3-one	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	<0.125		
595	106-50-3	1.4-Phenylenediamine	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.51		
596	97-00-7	1-Chloro-2.4-dinitrobenzene	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.07		
597	431-03-8	2.3-Butanedione	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	1.86		
598	5910-85-0	2.4-Heptadienal	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.52		
599	95-55-6	2-Aminophenol	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	>1		
600	818-61-1	2-Hydroxyethyl acrylate	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.08		
601	149-30-4	2-Mercaptobenzothiazole	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.2		
602	2682-20-4	2-Methyl-2H-isothiazolin-3-one	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	<0.125		
603	140-67-0	4-Allylanisole	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.82		
604	100-11-8	4-Nitrobenzylbromide	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	<0.125		
605	122-57-6	4-Phenyl-3-buten-2-one	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	1.08		
606	100-43-6	4-Vinylpyridine	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.46		
607	26172-55-4	5-Chloro-2-methyl-4-isothiazolin-3-one	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	<0.125		
608	13706-86-0	5-Methyl-2.3-hexanedione	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.39		
609	101-86-0	alpha-Hexylcinnamaldehyde	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	>1		
610	101-39-3	alpha-Methyl cinnamic aldehyde	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	>10		
611	100-39-0	Benzyl bromide	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.14		
612	23726-91-2	beta-Damascone	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	2.14		
613	23726-91-2	beta-Damascone	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.7		-0.15
614	79-77-6	beta-Ionone	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	6.53		0.81
615	2426-08-6	Butyl glycidyl ether	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	3.75		
616	104-55-2	Cinnamaldehyde	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.7		
617	104-55-2	Cinnamaldehyde	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	1.39		0.14
618	5392-40-5	Citral	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	4.86		0.69
619	103-95-7	Cyclamen aldehyde	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	1.26		
620	141-05-9	Diethyl maleate	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.42		
621	141-05-9	Diethyl maleate	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.31		-0.51
622	886-38-4	Diphenylcyclopropenone	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.41		
623	140-88-5	Ethyl acrylate	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.15		
624	97-90-5	Ethylene glycol dimethacrylate	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	>1		
625	97-53-0	Eugenol	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	2.5		
626	97-53-0	Eugenol	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	2.26		0.35
627	19317-11-4	Farnesal	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	>1		
628	3326-32-7	Fluorescein-5-isothiocyanate	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.03		
629	50-00-0	Formaldehyde	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	1.81		
630	56973-85-4	Galbanone	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	2.63		0.42
631	56973-85-4	Galbanone	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	1.28		
632	111-30-8	Glutaraldehyde	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.14		

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
590	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
591	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
592	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
593	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
594	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
595	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
596	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
597	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
598	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
599	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
600	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
601	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
602	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
603	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
604	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
605	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
606	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
607	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
608	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
609	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
610	30	7.5	PBS 20 mM	150 min	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
611	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
612	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
613	30	7.5	PBS 20 mM	150 min	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
614	30	7.5	PBS 20 mM	150 min	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
615	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
616	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
617	30	7.5	PBS 20 mM	150 min	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
618	30	7.5	PBS 20 mM	150 min	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
619	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
620	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
621	30	7.5	PBS 20 mM	150 min	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
622	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
623	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
624	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
625	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
626	30	7.5	PBS 20 mM	150 min	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
627	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
628	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
629	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
630	30	7.5	PBS 20 mM	150 min	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
631	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
632	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464

#	Comment
590	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
591	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
592	LC-MS. Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
593	LC-MS. Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
594	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
595	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
596	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
597	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
598	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
599	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
600	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
601	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
602	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
603	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
604	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
605	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
606	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
607	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
608	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
609	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
610	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
611	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
612	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
613	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
614	LC-MS. Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
615	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
616	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
617	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
618	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
619	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
620	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
621	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
622	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
623	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
624	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
625	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
626	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
627	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
628	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
629	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
630	LC-MS. Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
631	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
632	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)

#	Mechanism
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592	various adducts
593	Mass spectrometry confirms adduct formation
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614	Adduct + mass 32 (oxidation)
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630	Mass spectrometry confirms adduct formation
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632	

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
633	107-22-2	Glyoxal	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.52		
634	93-53-8	Hydratropic aldehyde	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	>1		
635	107-75-5	Hydroxycitronellal	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.4		
636	39236-46-9	Imidazolidinyl urea	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	>1		
637	97-54-1	Isoeugenol	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.57		-0.24
638	97-54-1	Isoeugenol	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.47		
639	80-54-6	Lilial	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	1.01		
640	111-80-8	Methyl-2-nonynoate	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	1.16		
641	35691-65-7	Methyldibromo glutaronitrile	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	<0.125		
642	150-75-4	Metol	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	<0.125		
643	15646-46-5	Oxazolone	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.17		
644	106-51-4	p-Benzoquinone	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	<0.125		
645	2111-75-3	Perillaldehyde	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	1.5		
646	122-78-1	Phenylacetaldehyde	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	1.64		
647	357650-26-1	Pomarose	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.26		-0.59
648	357650-26-1	Pomarose	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.35		
649	121-79-9	Propyl gallate	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	>1		
650	116-26-7	Safranal	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	1.42		
651	224031-70-3	Spirogalbanone	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	2.92		
652	137-26-8	Tetramethylthiuram disulfide	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	<0.125		
653	3913-81-3	trans-2-Decenal	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.59		
654	6728-26-3	trans-2-Hexenal	Cor1C-420 (AcNKKCDLF)	RC50(Cor1)	mM	0.24		
655	101-39-3	alpha-Methyl cinnamic aldehyde	N-Acetyl cysteine	RC50(AcCys)	mM	>10		
656	23726-91-2	beta-Damascone	N-Acetyl cysteine	RC50(AcCys)	mM	>10		
657	79-77-6	beta-Ionone	N-Acetyl cysteine	RC50(AcCys)	mM	>10		
658	104-55-2	Cinnamaldehyde	N-Acetyl cysteine	RC50(AcCys)	mM	3.06		0.49
659	5392-40-5	Citral	N-Acetyl cysteine	RC50(AcCys)	mM	>10		
660	141-05-9	Diethyl maleate	N-Acetyl cysteine	RC50(AcCys)	mM	0.48		-0.32
661	97-53-0	Eugenol	N-Acetyl cysteine	RC50(AcCys)	mM	>10		
662	56973-85-4	Galbanone	N-Acetyl cysteine	RC50(AcCys)	mM	>10		
663	97-54-1	Isoeugenol	N-Acetyl cysteine	RC50(AcCys)	mM	1.42		0.15
664	357650-26-1	Pomarose	N-Acetyl cysteine	RC50(AcCys)	mM	1.55		0.19
665	2045-23-0	4-((2-Chloroethyl)amino)benzoic acid	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	0		
666	2045-21-8	4-((2-Chloroethyl)ethylamino)benzoic acid	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	17		
667	2045-17-2	4-(Bis(2-bromoethyl)amino)acetanilide	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	252		
668	2045-17-2	4-(Bis(2-bromoethyl)amino)acetanilide	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	40		
669	2045-42-3	4-(Bis(2-chloroethyl)amino)benzamide	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	0.5		
670	2045-11-6	4-(Bis(2-iodoethyl)amino)acetanilide	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	263		
671	2045-11-6	4-(Bis(2-iodoethyl)amino)acetanilide	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	40		
672	2045-13-8	4-(Bis(2-iodoethyl)amino)benzoic acid	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	68.8		
673	1208-03-3	4-Bis(2-chloroethyl)aminobenzaldehyde	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	0.33		
674	2045-16-1	Acetic acid. thio-S-(bis(2-bromoethylamino)phenyl ester	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	38.9		

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
633	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
634	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
635	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
636	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
637	30	7.5	PBS 20 mM	150 min	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
638	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
639	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
640	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
641	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
642	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
643	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
644	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
645	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
646	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
647	30	7.5	PBS 20 mM	150 min	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
648	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
649	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
650	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
651	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
652	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
653	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
654	37	7.5	PBS 0.1 M, ACN	150 min	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
655	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
656	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
657	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
658	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
659	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
660	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
661	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
662	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
663	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
664	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
665	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
666	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
667	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
668	50	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
669	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
670	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
671	50	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
672	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
673	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
674	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167

#	Comment
633	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
634	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
635	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
636	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
637	LC-MS. Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
638	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
639	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
640	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
641	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
642	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
643	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
644	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
645	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
646	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
647	LC-MS. Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
648	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
649	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
650	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
651	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
652	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
653	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
654	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
655	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
656	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
657	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
658	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
659	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
660	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
661	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
662	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
663	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
664	Assay: UV (unreacted Cys after reaction with monobromobimane; 385 nm excit., 480 emiss.)
665	Assay: Rate constants relative to hydrolysis
666	Assay: Rate constants relative to hydrolysis
667	Assay: Rate constants relative to hydrolysis
668	Assay: Rate constants relative to hydrolysis
669	Assay: Rate constants relative to hydrolysis
670	Assay: Rate constants relative to hydrolysis
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672	Assay: Rate constants relative to hydrolysis
673	Assay: Rate constants relative to hydrolysis
674	Assay: Rate constants relative to hydrolysis

#	Mechanism
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637	Adduct + mass 16 (oxidation)
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647	Mass spectrometry confirms adduct formation
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665	Nucleophilic substitution, second order (SN2)
666	Nucleophilic substitution, second order (SN2)
667	Nucleophilic substitution, second order (SN2)
668	Nucleophilic substitution, second order (SN2)
669	Nucleophilic substitution, second order (SN2)
670	Nucleophilic substitution, second order (SN2)
671	Nucleophilic substitution, second order (SN2)
672	Nucleophilic substitution, second order (SN2)
673	Nucleophilic substitution, second order (SN2)
674	Nucleophilic substitution, second order (SN2)

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
675	2045-16-1	Acetic acid. thio-S-(bis(2-bromoethylamino)phenyl ester	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	2.5		
676	1507-07-9	Acetic acid. thio-S-(bis(2-chloroethylamino)phenyl ester	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	2.7		
677	553-27-5	Aniline mustard	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	13		
678	553-27-5	Aniline mustard	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	1		
679	1141-37-3	Benzoic acid nitrogen mustard	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	4.6		
680	1492-93-9	Fluoroacetyl-N-(p-aminophenyl)-nitrogen mustard	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	16.4		
681	1492-93-9	Fluoroacetyl-N-(p-aminophenyl)-nitrogen mustard	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	0.75		
682	1204-69-9	Hydroxyaniline mustard	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	48.6		
683	1204-69-9	Hydroxyaniline mustard	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	21.6		
684	148-78-7	IC40	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	14		
685	148-78-7	IC40	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	0.4		
686	2045-44-5	Isopropyl p-(bis(2-chloroethyl)amino)-carbanilate	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	32		
687	2045-44-5	Isopropyl p-(bis(2-chloroethyl)amino)-carbanilate	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	3.05		
688	1215-16-3	Lonin 3	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	29.6		
689	1215-16-3	Lonin 3	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	2		
690	51-75-2	Mechlorethamine	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	492		
691	51-75-2	Mechlorethamine	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	80		
692	92-49-9	N-(2-Chloroethyl)-N-ethylaniline	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	32		
693	92-49-9	N-(2-Chloroethyl)-N-ethylaniline	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	5		
694	1669-85-8	N-(2-Chloroethyl)-N-methylaniline	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	4.9		
695	1669-85-8	N-(2-Chloroethyl)-N-methylaniline	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	0.4		
696	2045-18-3	N-(Bis(2-bromoethyl)amino)benzoic acid	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	46.7		
697	935-06-8	N-(Chloroethyl)aniline	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	1.3		
698	2045-19-4	N.N-Bis(2-bromoethyl)aniline	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	123		
699	2045-19-4	N.N-Bis(2-bromoethyl)aniline	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	18.6		
700	29523-51-1	N.N-Bis(2-iodoethyl)aniline	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	158		
701	29523-51-1	N.N-Bis(2-iodoethyl)aniline	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	20.2		
702		N4-(2-Bromoethyl)-N4-(2-bromopropyl)sulfanilamide	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	6.1		
703		N4-(2-Bromoethyl)-N4-(2-bromopropyl)sulfanilamide	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	0.67		
704	2045-20-7	N4-(2-Chloroethyl)-N4-(2-chloropropyl)sulfanilamide	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	0.8		
705		N4-(2-Iodoethyl)-N4-(2-iodopropyl)sulfanilamide	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	3.1		
706	955-79-3	N4.N4-Bis(2-bromoethyl)sulfanilamide	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	7.5		
707	955-79-3	N4.N4-Bis(2-bromoethyl)sulfanilamide	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	0.4		

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
675	50	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
676	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
677	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
678	50	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
679	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
680	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
681	50	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
682	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
683	50	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
684	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
685	50	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
686	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
687	50	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
688	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
689	50	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
690	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
691	50	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
692	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
693	50	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
694	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
695	50	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
696	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
697	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
698	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
699	50	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
700	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
701	50	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
702	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
703	50	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
704	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
705	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
706	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
707	50	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167

#	Comment
675	Assay: Rate constants relative to hydrolysis
676	Assay: Rate constants relative to hydrolysis
677	Assay: Rate constants relative to hydrolysis
678	Assay: Rate constants relative to hydrolysis
679	Assay: Rate constants relative to hydrolysis
680	Assay: Rate constants relative to hydrolysis
681	Assay: Rate constants relative to hydrolysis
682	Assay: Rate constants relative to hydrolysis
683	Assay: Rate constants relative to hydrolysis
684	Assay: Rate constants relative to hydrolysis
685	Assay: Rate constants relative to hydrolysis
686	Assay: Rate constants relative to hydrolysis
687	Assay: Rate constants relative to hydrolysis
688	Assay: Rate constants relative to hydrolysis
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690	Assay: Rate constants relative to hydrolysis
691	Assay: Rate constants relative to hydrolysis
692	Assay: Rate constants relative to hydrolysis
693	Assay: Rate constants relative to hydrolysis
694	Assay: Rate constants relative to hydrolysis
695	Assay: Rate constants relative to hydrolysis
696	Assay: Rate constants relative to hydrolysis
697	Assay: Rate constants relative to hydrolysis
698	Assay: Rate constants relative to hydrolysis
699	Assay: Rate constants relative to hydrolysis
700	Assay: Rate constants relative to hydrolysis
701	Assay: Rate constants relative to hydrolysis
702	Assay: Rate constants relative to hydrolysis
703	Assay: Rate constants relative to hydrolysis
704	Assay: Rate constants relative to hydrolysis
705	Assay: Rate constants relative to hydrolysis
706	Assay: Rate constants relative to hydrolysis
707	Assay: Rate constants relative to hydrolysis

#	Mechanism
675	Nucleophilic substitution, second order (SN2)
676	Nucleophilic substitution, second order (SN2)
677	Nucleophilic substitution, second order (SN2)
678	Nucleophilic substitution, second order (SN2)
679	Nucleophilic substitution, second order (SN2)
680	Nucleophilic substitution, second order (SN2)
681	Nucleophilic substitution, second order (SN2)
682	Nucleophilic substitution, second order (SN2)
683	Nucleophilic substitution, second order (SN2)
684	Nucleophilic substitution, second order (SN2)
685	Nucleophilic substitution, second order (SN2)
686	Nucleophilic substitution, second order (SN2)
687	Nucleophilic substitution, second order (SN2)
688	Nucleophilic substitution, second order (SN2)
689	Nucleophilic substitution, second order (SN2)
690	Nucleophilic substitution, second order (SN2)
691	Nucleophilic substitution, second order (SN2)
692	Nucleophilic substitution, second order (SN2)
693	Nucleophilic substitution, second order (SN2)
694	Nucleophilic substitution, second order (SN2)
695	Nucleophilic substitution, second order (SN2)
696	Nucleophilic substitution, second order (SN2)
697	Nucleophilic substitution, second order (SN2)
698	Nucleophilic substitution, second order (SN2)
699	Nucleophilic substitution, second order (SN2)
700	Nucleophilic substitution, second order (SN2)
701	Nucleophilic substitution, second order (SN2)
702	Nucleophilic substitution, second order (SN2)
703	Nucleophilic substitution, second order (SN2)
704	Nucleophilic substitution, second order (SN2)
705	Nucleophilic substitution, second order (SN2)
706	Nucleophilic substitution, second order (SN2)
707	Nucleophilic substitution, second order (SN2)

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
708	1669-83-6	N4.N4-Bis(2-chloroethyl)sulfanilamide	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	3.1		
709	2045-41-2	N4.N4-Bis(2-chloroethyl)sulfanilamide	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	0.1		
710	334-22-5	Nornitrogen mustard	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	10		
711	10477-72-2	Phenylacetic mustard	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	41.6		
712	10477-72-2	Phenylacetic mustard	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	2.6		
713	2067-58-5	Phenylenediamine mustard	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	42		
714	2067-58-5	Phenylenediamine mustard	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	17.2		
715	51-18-3	TEM	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	6.2		
716	545-55-1	TEPA	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	3.5		
717	302-49-8	Uredepa	4-Nitrobenzylpyridine	krel(NBP)	1 = OH[-]	2.95		
718	23726-91-2	(2E)-1-(2.6.6-Trimethyl-1-cyclohexen-1-yl)-2-buten-1-one	Glutathione	krel(GSH): DEM	1 = DEM	0.069		
719	95-41-0	2-Hexyl-2-cyclopenten-1-one	Glutathione	krel(GSH): DEM	1 = DEM	0.21		
720	4643-27-0	2-Octen-4-one	Glutathione	krel(GSH): DEM	1 = DEM	1.57		
721	1193-18-6	3-Methyl-2-cyclohexen-1-one	Glutathione	krel(GSH): DEM	1 = DEM	<0.001		
722	2758-18-1	3-Methyl-2-cyclopenten-1-one	Glutathione	krel(GSH): DEM	1 = DEM	<0.001		
723		4-Isopropyl-3-methylcyclohex-2-en-1-one	Glutathione	krel(GSH): DEM	1 = DEM	<0.001		
724	141-79-7	4-Methyl-3-penten-2-one	Glutathione	krel(GSH): DEM	1 = DEM	0.01		
725	122-57-6	4-Phenyl-3-buten-2-one	Glutathione	krel(GSH): DEM	1 = DEM	0.16		
726		6.11-Dimethyldodeca-3.5.9-trien-2-one	Glutathione	krel(GSH): DEM	1 = DEM	0.002		
727	1604-28-0	6-Methyl-3.5-heptadien-2-one	Glutathione	krel(GSH): DEM	1 = DEM	0.005		
728	23696-85-7	beta-Damascenone	Glutathione	krel(GSH): DEM	1 = DEM	0.11		
729	99-49-0	Carvone	Glutathione	krel(GSH): DEM	1 = DEM	0.004		
730	141-05-9	Diethyl maleate (DEM)	Glutathione	krel(GSH): DEM	1 = DEM	1		
731	78-94-4	Methyl vinyl ketone	Glutathione	krel(GSH): DEM	1 = DEM	1200		
732	623-15-4	Monofurfurylideneacetone	Glutathione	krel(GSH): DEM	1 = DEM	0.036		
733	128-53-0	N-Ethylmaleimide	Glutathione	krel(GSH): DEM	1 = DEM	36000		
734	99-54-7	1.2-Dichloro-4-nitrobenzene	Glutathione	krel(GSH): CDNB	1 = CDNB	3.20E-03		
735	97-00-7	1-Chloro-2.4-dinitrobenzene	Glutathione	krel(GSH): CDNB	1 = CDNB	1.00E+00		
736	121-17-5	2-Chloro-5-(trifluoromethyl)-nitrobenzene	Glutathione	krel(GSH): CDNB	1 = CDNB	5.50E-02		
737	1930-72-9	4-Chloro-3.5-dinitro-benzonitrile	Glutathione	krel(GSH): CDNB	1 = CDNB	7.26E+02		
738		Ethyl 4-chloro-3.5-dinitrobenzoate	Glutathione	krel(GSH): CDNB	1 = CDNB	1.59E+01		
739		3-(2-Bromoethyl)-5.5-dimethyldihydro-2(3H)-furanone (2B)	n-Butylamine	krel(BuNH2): 3-MeCl-Lac	1 = 3-MeCl-Lac	0.05		
740		3-(2-Chloroethyl)-5.5-dimethyldihydro-2(3H)-furanone (2A)	n-Butylamine	krel(BuNH2): 3-MeCl-Lac	1 = 3-MeCl-Lac	0.01		
741		3-(3'-Bromopropyl)-5.5'-dimethyldihydro-2(3H)-furanone (3B)	n-Butylamine	krel(BuNH2): 3-MeCl-Lac	1 = 3-MeCl-Lac	0.1		
742		3-(Bromomethyl)-5.5-dimethyldihydro-2(3H)-furanone (1B)	n-Butylamine	krel(BuNH2): 3-MeCl-Lac	1 = 3-MeCl-Lac	8.94		
743		3-(Chloromethyl)-5.5-dimethyldihydro-2(3H)-furanone	n-Butylamine	krel(BuNH2): 3-MeCl-Lac	1 = 3-MeCl-Lac	1		

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
708	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
709	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
710	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
711	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
712	50	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
713	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
714	50	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
715	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
716	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
717	80	4.2	Ethanol, hydrogen phthalate buffer			Bardos TJ et al., J. Med. Chem. 8 (1965), 167
718	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
719	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
720	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
721	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
722	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
723	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
724	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
725	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
726	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
727	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
728	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
729	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
730	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
731	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
732	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
733	50	7.4	Ethanol		38:1	Portoghese PS et al., Fd. Chem. Toxicol. 27 (1989), 773
734	25	7.5	PBS 0.1 M	15 min	5:1	Hulbert P et al., J. Pharmaceut. Biomed. Anal. 8 (1990), 1009
735	25	7.5	PBS 0.1 M	15 min	1:1	Hulbert P et al., J. Pharmaceut. Biomed. Anal. 8 (1990), 1009
736	25	7.5	PBS 0.1 M, add. DMSO	15 min	5:1	Hulbert P et al., J. Pharmaceut. Biomed. Anal. 8 (1990), 1009
737	25	6.5	PBS 0.1 M	15 min	1:1	Hulbert P et al., J. Pharmaceut. Biomed. Anal. 8 (1990), 1009
738	25	6.5	PBS 0.1 M, add. DMSO	15 min	1:1	Hulbert P et al., J. Pharmaceut. Biomed. Anal. 8 (1990), 1009
739				48 h (Me) 27 d (Et)	1:1	Franot C et al., Chem. Res. Toxicol. 7 (1994), 297
740				48 h (Me) 27 d (Et)	1:1	Franot C et al., Chem. Res. Toxicol. 7 (1994), 297
741				48 h (Me) 27 d (Et)	1:1	Franot C et al., Chem. Res. Toxicol. 7 (1994), 297
742				48 h (Me) 27 d (Et)	1:1	Franot C et al., Chem. Res. Toxicol. 7 (1994), 297
743				48 h (Me) 27 d (Et)	1:1	Franot C et al., Chem. Res. Toxicol. 7 (1994), 297

#	Comment
708	Assay: Rate constants relative to hydrolysis
709	Assay: Rate constants relative to hydrolysis
710	Assay: Rate constants relative to hydrolysis
711	Assay: Rate constants relative to hydrolysis
712	Assay: Rate constants relative to hydrolysis
713	Assay: Rate constants relative to hydrolysis
714	Assay: Rate constants relative to hydrolysis
715	Assay: Rate constants relative to hydrolysis
716	Assay: Rate constants relative to hydrolysis
717	Assay: Rate constants relative to hydrolysis
718	Assay: k relative to Diethylmaleate; RP-HPLC (El DP, 254 nm); reactive pH 3-5, low reactive pH up to 9, extrapolated to pH 7.4
719	Assay: k relative to Diethylmaleate; RP-HPLC (El DP, 254 nm); reactive pH 3-5, low reactive pH up to 9, extrapolated to pH 7.4
720	Assay: k relative to Diethylmaleate; RP-HPLC (El DP, 254 nm); reactive pH 3-5, low reactive pH up to 9, extrapolated to pH 7.4
721	Assay: k relative to Diethylmaleate; RP-HPLC (El DP, 254 nm); reactive pH 3-5, low reactive pH up to 9, extrapolated to pH 7.4
722	Assay: k relative to Diethylmaleate; RP-HPLC (El DP, 254 nm); reactive pH 3-5, low reactive pH up to 9, extrapolated to pH 7.4
723	Assay: k relative to Diethylmaleate; RP-HPLC (El DP, 254 nm); reactive pH 3-5, low reactive pH up to 9, extrapolated to pH 7.4
724	Assay: k relative to Diethylmaleate; RP-HPLC (El DP, 254 nm); reactive pH 3-5, low reactive pH up to 9, extrapolated to pH 7.4
725	Assay: k relative to Diethylmaleate; RP-HPLC (El DP, 254 nm); reactive pH 3-5, low reactive pH up to 9, extrapolated to pH 7.4
726	Assay: k relative to Diethylmaleate; RP-HPLC (El DP, 254 nm); reactive pH 3-5, low reactive pH up to 9, extrapolated to pH 7.4
727	Assay: k relative to Diethylmaleate; RP-HPLC (El DP, 254 nm); reactive pH 3-5, low reactive pH up to 9, extrapolated to pH 7.4
728	Assay: k relative to Diethylmaleate; RP-HPLC (El DP, 254 nm); reactive pH 3-5, low reactive pH up to 9, extrapolated to pH 7.4
729	Assay: k relative to Diethylmaleate; RP-HPLC (El DP, 254 nm); reactive pH 3-5, low reactive pH up to 9, extrapolated to pH 7.4
730	Assay: k relative to Diethylmaleate; RP-HPLC (El DP, 254 nm); reactive pH 3-5, low reactive pH up to 9, extrapolated to pH 7.4 MVK: RP-HPLC (El DP, 210 nm).
731	Assay: k relative to Diethylmaleate; reactive pH 3-5, low reactive pH up to 9, extrapolated to pH 7.4
732	Assay: k relative to Diethylmaleate; RP-HPLC (El DP, 254 nm); reactive pH 3-5, low reactive pH up to 9, extrapolated to pH 7.4
733	Assay: k relative to Diethylmaleate; RP-HPLC (El DP, 254 nm); reactive pH 3-5, low reactive pH up to 9, extrapolated to pH 7.4
734	UV (GSH-conjugate). Assay: k relative to 1-Chloro-2,4-dinitrobenzene
735	UV (GSH-conjugate). Assay: k relative to 1-Chloro-2,4-dinitrobenzene
736	UV (GSH-conjugate). Assay: k relative to 1-Chloro-2,4-dinitrobenzene
737	UV (GSH-conjugate). Assay: k relative to 1-Chloro-2,4-dinitrobenzene
738	UV (GSH-conjugate). Assay: k relative to 1-Chloro-2,4-dinitrobenzene
739	Assay: NMR (Integration of reference 3-RCl-Lac vs. Test); 0.025 mmol Test+BuNH2; BuNH2: SN2 or Elimination
740	Assay: NMR (Integration of reference 3-RCl-Lac vs. Test); 0.025 mmol Test+BuNH2; BuNH2: SN2 or Elimination
741	Assay: NMR (Integration of reference 3-RCl-Lac vs. Test); 0.025 mmol Test+BuNH2; BuNH2: SN2 or Elimination
742	Assay: NMR (Integration of reference 3-RCl-Lac vs. Test); 0.025 mmol Test+BuNH2; BuNH2: SN2 or Elimination
743	Assay: NMR (Integration of reference 3-RCl-Lac vs. Test); 0.025 mmol Test+BuNH2; BuNH2: SN2 or Elimination

#	Mechanism
708	Nucleophilic substitution, second order (SN2)
709	Nucleophilic substitution, second order (SN2)
710	Nucleophilic substitution, second order (SN2)
711	Nucleophilic substitution, second order (SN2)
712	Nucleophilic substitution, second order (SN2)
713	Nucleophilic substitution, second order (SN2)
714	Nucleophilic substitution, second order (SN2)
715	Nucleophilic substitution, second order (SN2)
716	Nucleophilic substitution, second order (SN2)
717	Nucleophilic substitution, second order (SN2)
718	Michael-type nucleophilic addition
719	Michael-type nucleophilic addition
720	Michael-type nucleophilic addition
721	Michael-type nucleophilic addition
722	Michael-type nucleophilic addition
723	Michael-type nucleophilic addition
724	Michael-type nucleophilic addition
725	Michael-type nucleophilic addition
726	Michael-type nucleophilic addition
727	Michael-type nucleophilic addition
728	Michael-type nucleophilic addition
729	Michael-type nucleophilic addition
730	Michael-type nucleophilic addition
731	Michael-type nucleophilic addition
732	Michael-type nucleophilic addition
733	Michael-type nucleophilic addition
734	
735	
736	
737	
738	
739	Nucleophilic substitution, second order (SN2)
740	
741	Nucleophilic substitution, second order (SN2)
742	Nucleophilic substitution, second order (SN2)
743	Nucleophilic substitution, second order (SN2)

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
744		3-[(Mesyloxy)ethyl]-5.5-dimethyldihydro-2(3H)-furanone (2C)	n-Butylamine	krel(BuNH2): 3-MeCl-Lac	1 = 3-MeCl-Lac	0.04		
745		3-[(Mesyloxy)methyl]-5.5-dimethyldihydro-2(3H)-furanone (1C)	n-Butylamine	krel(BuNH2): 3-MeCl-Lac	1 = 3-MeCl-Lac	1.5		
746		3-[[(Phenylsulfonyl)oxy]ethyl]-5.5-dimethyldihydro-2(3H)-furanone (2F)	n-Butylamine	krel(BuNH2): 3-MeCl-Lac	1 = 3-MeCl-Lac	0.04		
747		3-[[(Phenylsulfonyl)oxy]methyl]-5.5-dimethyldihydro-2(3H)-furanone (1F)	n-Butylamine	krel(BuNH2): 3-MeCl-Lac	1 = 3-MeCl-Lac	1.31		
748		3-[[[(4-Chlorophenyl)sulfonyl]oxy]ethyl]-5.5-dimethyldihydro-2(3H)-furanone (2G)	n-Butylamine	krel(BuNH2): 3-MeCl-Lac	1 = 3-MeCl-Lac	0.09		
749		3-[[[(4-Chlorophenyl)sulfonyl]oxy]methyl]-5.5-dimethyldihydro-2(3H)-furanone (1G)	n-Butylamine	krel(BuNH2): 3-MeCl-Lac	1 = 3-MeCl-Lac	2.13		
750		3-[[[(4-Methoxyphenyl)sulfonyl]oxy]ethyl]-5.5-dimethyldihydro-2(3H)-furanone (2E)	n-Butylamine	krel(BuNH2): 3-MeCl-Lac	1 = 3-MeCl-Lac	0.03		
751		3-[[[(4-Methoxyphenyl)sulfonyl]oxy]methyl]-5.5-dimethyldihydro-2(3H)-furanone (1E)	n-Butylamine	krel(BuNH2): 3-MeCl-Lac	1 = 3-MeCl-Lac	1.01		
752		5.5-Dimethyl-3-[(tosyloxy)ethyl]-dihydro-2(3H)-furanone (2D)	n-Butylamine	krel(BuNH2): 3-MeCl-Lac	1 = 3-MeCl-Lac	0.03		
753		5.5-Dimethyl-3-[(tosyloxy)methyl]-dihydro-2(3H)-furanone (1D)	n-Butylamine	krel(BuNH2): 3-MeCl-Lac	1 = 3-MeCl-Lac	1.25		
754		5.5-Dimethyl-3-[[[(4-nitrophenyl)sulfonyl]oxy]-ethylldihydro-2(3H)-furanone (2H)	n-Butylamine	krel(BuNH2): 3-MeCl-Lac	1 = 3-MeCl-Lac	0.24		
755		5.5-Dimethyl-3-[[[(4-nitrophenyl)sulfonyl]oxy]-methylldihydro-2(3H)-furanone (1H)	n-Butylamine	krel(BuNH2): 3-MeCl-Lac	1 = 3-MeCl-Lac	49.99		
756		5.5-Dimethyl-3-methylenedihydro-2(3H)-furanone (1L)	n-Butylamine	krel(BuNH2): 3-MeCl-Lac	1 = 3-MeCl-Lac	0.98		
757		5.5-Dimethyl-3-(thiocyanatoethyl)-dihydro-2(3H)-furanone (2I)	n-Butylamine	krel(BuNH2): 3-MeCl-Lac	1 = 3-MeCl-Lac	<0.01		
758		5.5-Dimethyl-3-(thiocyanatomethyl)-dihydro-2(3H)-furanone (1I)	n-Butylamine	krel(BuNH2): 3-MeCl-Lac	1 = 3-MeCl-Lac	1.51		
759	98-09-9	Benzenesulfonyl chloride	Aniline	krel(Aniline)	1 = (Nu=Water)			5.15
760	98-88-4	Benzoyl chloride	Aniline	krel(Aniline)	1 = (Nu=Water)			6.38
761	74-83-9	Methyl bromide	Aniline	krel(Aniline)	1 = (Nu=Water)			4.49
762	505-60-2	Mustard cation	Aniline	krel(Aniline)	1 = (Nu=Water)			4.6
763	98-88-4	Benzoyl chloride	Acetate	krel(Acetate)	1 = (Nu=Water)			2.86
764	100-44-7	Benzyl chloride	Acetate	krel(Acetate)	1 = (Nu=Water)			2.51
765	57-57-8	beta-Propiolactone	Acetate	krel(Acetate)	1 = (Nu=Water)			2.49
766	106-89-8	Epichlorohydrin	Acetate	krel(Acetate)	1 = (Nu=Water)			2.54
767	505-60-2	Mustard cation	Acetate	krel(Acetate)	1 = (Nu=Water)			2.72
768	3460-18-2	1.4-Dibromo-2-nitrobenzene	Piperidine	k1(Piperidine)	min-1	2.27E-02		-1.64
769	3460-18-2	1.4-Dibromo-2-nitrobenzene	Piperidine	k1(Piperidine)	min-1	4.23E-02		-1.37

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
744				48 h (Me) 27 d (Et)	1:1	Franot C et al., Chem. Res. Toxicol. 7 (1994), 297
745				48 h (Me) 27 d (Et)	1:1	Franot C et al., Chem. Res. Toxicol. 7 (1994), 297
746				48 h (Me) 27 d (Et)	1:1	Franot C et al., Chem. Res. Toxicol. 7 (1994), 297
747				48 h (Me) 27 d (Et)	1:1	Franot C et al., Chem. Res. Toxicol. 7 (1994), 297
748				48 h (Me) 27 d (Et)	1:1	Franot C et al., Chem. Res. Toxicol. 7 (1994), 297
749				48 h (Me) 27 d (Et)	1:1	Franot C et al., Chem. Res. Toxicol. 7 (1994), 297
750				48 h (Me) 27 d (Et)	1:1	Franot C et al., Chem. Res. Toxicol. 7 (1994), 297
751				48 h (Me) 27 d (Et)	1:1	Franot C et al., Chem. Res. Toxicol. 7 (1994), 297
752				48 h (Me) 27 d (Et)	1:1	Franot C et al., Chem. Res. Toxicol. 7 (1994), 297
753				48 h (Me) 27 d (Et)	1:1	Franot C et al., Chem. Res. Toxicol. 7 (1994), 297
754				48 h (Me) 27 d (Et)	1:1	Franot C et al., Chem. Res. Toxicol. 7 (1994), 297
755				48 h (Me) 27 d (Et)	1:1	Franot C et al., Chem. Res. Toxicol. 7 (1994), 297
756				48 h (Me) 27 d (Et)	1:1	Franot C et al., Chem. Res. Toxicol. 7 (1994), 297
757				48 h (Me) 27 d (Et)	1:1	Franot C et al., Chem. Res. Toxicol. 7 (1994), 297
758				48 h (Me) 27 d (Et)	1:1	Franot C et al., Chem. Res. Toxicol. 7 (1994), 297
759	0.5		Acetone:water 1:1			Swain CG et al., J. Am. Chem. Soc. 75 (1953), 141
760	0.5		Acetone:water 1:1			Swain CG et al., J. Am. Chem. Soc. 75 (1953), 141
761	49.8		Acetone:water 1:1			Swain CG et al., J. Am. Chem. Soc. 75 (1953), 141
762	49.8		Water:ethanol 95:5			Swain CG et al., J. Am. Chem. Soc. 75 (1953), 141
763	0.5		Acetone:water 1:1			Swain CG et al., J. Am. Chem. Soc. 75 (1953), 141
764	50		Water:dioxane 39:61			Swain CG et al., J. Am. Chem. Soc. 75 (1953), 141
765	25		Water			Swain CG et al., J. Am. Chem. Soc. 75 (1953), 141
766	20		Water			Swain CG et al., J. Am. Chem. Soc. 75 (1953), 141
767	25		Water:ethanol 95:5			Swain CG et al., J. Am. Chem. Soc. 75 (1953), 141
768	25				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
769	35				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273

#	Comment
744	Assay: NMR (Integration of reference 3-RCl-Lac vs. Test); 0.025 mmol Test+BuNH2; BuNH2: SN2 or Elimination
745	Assay: NMR (Integration of reference 3-RCl-Lac vs. Test); 0.025 mmol Test+BuNH2; BuNH2: SN2 or Elimination
746	Assay: NMR (Integration of reference 3-RCl-Lac vs. Test); 0.025 mmol Test+BuNH2; BuNH2: SN2 or Elimination
747	Assay: NMR (Integration of reference 3-RCl-Lac vs. Test); 0.025 mmol Test+BuNH2; BuNH2: SN2 or Elimination
748	Assay: NMR (Integration of reference 3-RCl-Lac vs. Test); 0.025 mmol Test+BuNH2; BuNH2: SN2 or Elimination
749	Assay: NMR (Integration of reference 3-RCl-Lac vs. Test); 0.025 mmol Test+BuNH2; BuNH2: SN2 or Elimination
750	Assay: NMR (Integration of reference 3-RCl-Lac vs. Test); 0.025 mmol Test+BuNH2; BuNH2: SN2 or Elimination
751	Assay: NMR (Integration of reference 3-RCl-Lac vs. Test); 0.025 mmol Test+BuNH2; BuNH2: SN2 or Elimination
752	Assay: NMR (Integration of reference 3-RCl-Lac vs. Test); 0.025 mmol Test+BuNH2; BuNH2: SN2 or Elimination
753	Assay: NMR (Integration of reference 3-RCl-Lac vs. Test); 0.025 mmol Test+BuNH2; BuNH2: SN2 or Elimination
754	Assay: NMR (Integration of reference 3-RCl-Lac vs. Test); 0.025 mmol Test+BuNH2; BuNH2: SN2 or Elimination
755	Assay: NMR (Integration of reference 3-RCl-Lac vs. Test); 0.025 mmol Test+BuNH2; BuNH2: SN2 or Elimination
756	Assay: NMR (Integration of reference 3-RCl-Lac vs. Test); 0.025 mmol Test+BuNH2; BuNH2: SN2 or Elimination
757	Assay: NMR (Integration of reference 3-RCl-Lac vs. Test); 0.025 mmol Test+BuNH2; BuNH2: SN2 or Elimination
758	Assay: NMR (Integration of reference 3-RCl-Lac vs. Test); 0.025 mmol Test+BuNH2; BuNH2: SN2 or Elimination
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#	Mechanism
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745	Nucleophilic substitution, second order (SN2)
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747	Nucleophilic substitution, second order (SN2)
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749	Nucleophilic substitution, second order (SN2)
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751	Nucleophilic substitution, second order (SN2)
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753	Nucleophilic substitution, second order (SN2)
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755	Nucleophilic substitution, second order (SN2)
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757	Nucleophilic substitution, second order (SN2)
758	Nucleophilic substitution, second order (SN2)
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768	Nucleophilic aromatic substitution (SNAr)
769	Nucleophilic aromatic substitution (SNAr)

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
770		1-Bromo-2-nitronaphthalene	Piperidine	k1(Piperidine)	min-1	9.20E-02		-1.04
771		1-Bromo-2-nitronaphthalene	Piperidine	k1(Piperidine)	min-1	1.83E-02		-1.74
772		1-Bromo-4-(tert-butyl)-2-nitrobenzene	Piperidine	k1(Piperidine)	min-1	4.94E-04		-3.31
773		1-Bromo-4-(tert-butyl)-2-nitrobenzene	Piperidine	k1(Piperidine)	min-1	9.99E-04		-3
774		1-Bromo-4-ethoxy-2-nitrobenzene	Piperidine	k1(Piperidine)	min-1	4.37E-05		-4.36
775		1-Bromo-4-ethoxy-2-nitrobenzene	Piperidine	k1(Piperidine)	min-1	9.43E-05		-4.03
776	446-09-3	1-Bromo-4-fluoro-2-nitrobenzene	Piperidine	k1(Piperidine)	min-1	7.55E-04		-3.12
777	446-09-3	1-Bromo-4-fluoro-2-nitrobenzene	Piperidine	k1(Piperidine)	min-1	1.56E-03		-2.81
778	90-11-9	1-Bromonaphthalene	Piperidine	k1(Piperidine)	min-1	1.43E-05		-4.84
779		1-Chloro-2-nitronaphthalene	Piperidine	k1(Piperidine)	min-1	7.70E-02		-1.11
780		1-Chloro-2-nitronaphthalene	Piperidine	k1(Piperidine)	min-1	1.41E-02		-1.85
781	90-13-1	1-Chloronaphthalene	Piperidine	k1(Piperidine)	min-1	2.50E-06		-5.6
782		1-Iodo-2-nitronaphthalene	Piperidine	k1(Piperidine)	min-1	1.40E-02		-1.85
783		1-Iodo-2-nitronaphthalene	Piperidine	k1(Piperidine)	min-1	1.78E-03		-2.75
784	90-14-2	1-Iodonaphthalene	Piperidine	k1(Piperidine)	min-1	2.83E-05		-4.55
785		2-Bromo-1-nitronaphthalene	Piperidine	k1(Piperidine)	min-1	1.00E-02		-2
786		2-Bromo-1-nitronaphthalene	Piperidine	k1(Piperidine)	min-1	1.52E-03		-2.82
787	41513-04-6	2-Bromo-5-chloronitrobenzene	Piperidine	k1(Piperidine)	min-1	1.62E-02		-1.79
788	41513-04-6	2-Bromo-5-chloronitrobenzene	Piperidine	k1(Piperidine)	min-1	3.07E-02		-1.51
789		2-Bromo-5-iodonitrobenzene	Piperidine	k1(Piperidine)	min-1	1.57E-02		-1.8
790		2-Bromo-5-iodonitrobenzene	Piperidine	k1(Piperidine)	min-1	3.11E-02		-1.51
791	580-13-2	2-Bromonaphthalene	Piperidine	k1(Piperidine)	min-1	2.48E-05		-4.61
792	577-19-5	2-Bromonitrobenzene	Piperidine	k1(Piperidine)	min-1	2.90E-03		-2.54
793	577-19-5	2-Bromonitrobenzene	Piperidine	k1(Piperidine)	min-1	5.63E-03		-2.25
794		2-Chloro-1-nitronaphthalene	Piperidine	k1(Piperidine)	min-1	7.80E-03		-2.11
795		2-Chloro-1-nitronaphthalene	Piperidine	k1(Piperidine)	min-1	1.31E-03		-2.88
796	91-58-7	2-Chloronaphthalene	Piperidine	k1(Piperidine)	min-1	3.10E-06		-5.51
797		2-Iodo-1-nitronaphthalene	Piperidine	k1(Piperidine)	min-1	1.30E-03		-2.89
798		2-Iodo-1-nitronaphthalene	Piperidine	k1(Piperidine)	min-1	1.30E-04		-3.89
799		2-Iodonaphthalene	Piperidine	k1(Piperidine)	min-1	3.52E-06		-5.45
800		4-Bromo-3-nitroaniline	Piperidine	k1(Piperidine)	min-1	3.90E-07		-6.41
801		4-Bromo-3-nitroaniline	Piperidine	k1(Piperidine)	min-1	8.00E-07		-6.1
802	5344-78-5	4-Bromo-3-nitroanisole	Piperidine	k1(Piperidine)	min-1	5.22E-05		-4.28
803	5344-78-5	4-Bromo-3-nitroanisole	Piperidine	k1(Piperidine)	min-1	1.17E-04		-3.93
804		4-Bromo-3-nitrobenzoic acid	Piperidine	k1(Piperidine)	min-1	7.31E-03		-2.14
805		4-Bromo-3-nitrobenzoic acid	Piperidine	k1(Piperidine)	min-1	1.44E-02		-1.84
806		4-Bromo-3-nitrophenol	Piperidine	k1(Piperidine)	min-1	1.70E-06		-5.77
807		4-Bromo-3-nitrophenol	Piperidine	k1(Piperidine)	min-1	4.40E-06		-5.36
808	5326-34-1	4-Bromo-3-nitrotoluene	Piperidine	k1(Piperidine)	min-1	4.23E-04		-3.37
809	5326-34-1	4-Bromo-3-nitrotoluene	Piperidine	k1(Piperidine)	min-1	8.70E-04		-3.06
810		4-Bromo-N.N.N-trimethyl-3-nitroanilinium salt	Piperidine	k1(Piperidine)	min-1	3.50E-06		-5.46

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
770	25				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
771	0				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
772	25				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
773	35				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
774	25				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
775	35				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
776	25				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
777	35				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
778	165				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
779	25				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
780	0				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
781	165				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
782	25				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
783	0				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
784	165				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
785	25				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
786	0				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
787	25				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
788	35				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
789	25				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
790	35				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
791	165				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
792	25				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
793	35				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
794	25				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
795	0				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
796	165				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
797	25				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
798	0				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
799	165				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
800	25				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
801	35				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
802	25				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
803	35				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
804	25				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
805	35				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
806	25				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
807	35				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
808	25				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
809	35				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
810	25				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273

#	Comment
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800	extremely slowly, does not justify Arrhenius parameters.
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806	extremely slowly, does not justify Arrhenius parameters.
807	extremely slowly, does not justify Arrhenius parameters.
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810	extremely slowly, does not justify Arrhenius parameters.

#	Mechanism
770	Nucleophilic aromatic substitution (SNAr)
771	Nucleophilic aromatic substitution (SNAr)
772	Nucleophilic aromatic substitution (SNAr)
773	Nucleophilic aromatic substitution (SNAr)
774	Nucleophilic aromatic substitution (SNAr)
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783	Nucleophilic aromatic substitution (SNAr)
784	Nucleophilic aromatic substitution (SNAr)
785	Nucleophilic aromatic substitution (SNAr)
786	Nucleophilic aromatic substitution (SNAr)
787	Nucleophilic aromatic substitution (SNAr)
788	Nucleophilic aromatic substitution (SNAr)
789	Nucleophilic aromatic substitution (SNAr)
790	Nucleophilic aromatic substitution (SNAr)
791	Nucleophilic aromatic substitution (SNAr)
792	Nucleophilic aromatic substitution (SNAr)
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798	Nucleophilic aromatic substitution (SNAr)
799	Nucleophilic aromatic substitution (SNAr)
800	Nucleophilic aromatic substitution (SNAr)
801	Nucleophilic aromatic substitution (SNAr)
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804	Nucleophilic aromatic substitution (SNAr)
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806	Nucleophilic aromatic substitution (SNAr)
807	Nucleophilic aromatic substitution (SNAr)
808	Nucleophilic aromatic substitution (SNAr)
809	Nucleophilic aromatic substitution (SNAr)
810	Nucleophilic aromatic substitution (SNAr)

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
811		4-Bromo-N.N.N-trimethyl-3-nitroanilinium salt	Piperidine	k1(Piperidine)	min-1	**7.50E-06**		**-5.12**
812	108-86-1	Bromobenzene	Piperidine	k1(Piperidine)	min-1	**8.70E-06**		**-5.06**
813	108-90-7	Chlorobenzene	Piperidine	k1(Piperidine)	min-1	**1.10E-06**		**-5.96**
814	591-50-4	Iodobenzene	Piperidine	k1(Piperidine)	min-1	**1.57E-05**		**-4.8**
815	818-61-1	2-Hydroxyethyl acrylate	4-Nitrobenzenethiol	k1(NBT) | k1s | k1i | k1r	min-1	**3.18**	0.6	**0.5**
816	144-48-9	2-Iodoacetamide	4-Nitrobenzenethiol	k1(NBT) | k1s | k1i | k1r	min-1	**211.8**	42.6	**2.33**
817	2682-20-4	2-Methyl-2H-isothiazolin-3-one	4-Nitrobenzenethiol	k1(NBT) | k1s | k1i | k1r	min-1	**432**	78	**2.64**
818	25567-67-3	3-Chloro-1.2-dinitrobenzene	4-Nitrobenzenethiol	k1(NBT) | k1s | k1i | k1r	min-1	**52.2**	12	**1.72**
819	2497-21-4	4-Hexen-3-one	4-Nitrobenzenethiol	k1(NBT) | k1s | k1i | k1r	min-1	**25.08**	7.8	**1.4**
820	26172-55-4	5-Chloro-2-methyl-4-isothiazolin-3-one	4-Nitrobenzenethiol	k1(NBT) | k1s | k1i | k1r	min-1	**11580**	360	**4.06**
821	108-24-7	Acetic anhydride	4-Nitrobenzenethiol	k1(NBT) | k1s | k1i | k1r	min-1	**705.6**	98.4	**2.85**
822	107-02-8	Acrolein	4-Nitrobenzenethiol	k1(NBT) | k1s | k1i | k1r	min-1	**9.6**	1.2	**0.98**
823	100-39-0	Benzyl bromide	4-Nitrobenzenethiol	k1(NBT) | k1s | k1i | k1r	min-1	**14880**	1470	**4.17**
824	57-57-8	beta-Propiolactone	4-Nitrobenzenethiol	k1(NBT) | k1s | k1i | k1r	min-1	**4284**	438	**3.63**
825	88-11-9	Diethylthiocarbamoyl chloride	4-Nitrobenzenethiol	k1(NBT) | k1s | k1i | k1r	min-1	**372.6**	44.4	**2.57**
826	886-38-4	Diphenylcyclopropenone	4-Nitrobenzenethiol	k1(NBT) | k1s | k1i | k1r	min-1	**66300**	5760	**4.82**
827	140-88-5	Ethyl acrylate	4-Nitrobenzenethiol	k1(NBT) | k1s | k1i | k1r	min-1	**1.08**	0.12	**0.03**
828	50-00-0	Formaldehyde	4-Nitrobenzenethiol	k1(NBT) | k1s | k1i | k1r	min-1	**55.8**	46.8	**1.75**
829	55965-84-9	Kathon CG	4-Nitrobenzenethiol	k1(NBT) | k1s | k1i | k1r	min-1	**3516**	318	**3.55**
830	124-63-0	Methyl sulfonyl chloride	4-Nitrobenzenethiol	k1(NBT) | k1s | k1i | k1r	min-1	**1284**	360	**3.11**
831	128-53-0	N-Ethylmaleimide	4-Nitrobenzenethiol	k1(NBT) | k1s | k1i | k1r	min-1	**2226**	756	**3.35**
832		Nitrobenzyl bromide	4-Nitrobenzenethiol	k1(NBT) | k1s | k1i | k1r	min-1	**76800**	7380	**4.89**
833	15646-46-5	Oxazolone	4-Nitrobenzenethiol	k1(NBT) | k1s | k1i | k1r	min-1	**77400**	7020	**4.89**

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
811	35				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
812	165				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
813	165				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
814	165				Nu excess	Bunnet JF et al., Chem. Rev. 49 (1951), 273
815	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
816	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
817	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
818	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
819	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
820	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
821	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
822	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
823	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
824	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
825	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
826	25	7.4	PBS 0.1 M, ACN, acetone		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
827	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
828	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
829	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
830	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
831	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
832	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
833	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918

#	Comment
811	extremely slowly, does not justify Arrhenius parameters.
812	
813	
814	
	k1s 2.82E+00 | k1i 4.80E-03 | k1r 3.66E-04.
815	Assay: Stopped flow; UV(-SH loss 412 nm); k1 = Overall kinetics | k1s = from slope | k1i = from intercept | k1r = initial rate; k1(pH=5.5) = 10* k1(7.4)
	fits second-order plots; k1s 3.78E+02 | k1i 1.80E-03 | k1r 1.80E-05.
816	Assay: Stopped flow; UV(-SH loss 412 nm); k1 = Overall kinetics | k1s = from slope | k1i = from intercept | k1r = initial rate; k1(pH=5.5) = 10* k1(7.4)
	k1s 4.02E+02 | k1i 1.20E-03 | k1r 1.38E-01.
817	Assay: Stopped flow; UV(-SH loss 412 nm); k1 = Overall kinetics | k1s = from slope | k1i = from intercept | k1r = initial rate; k1(pH=5.5) = 10* k1(7.4)
	k1s 5.58E+01 | k1i 1.20E-04 | k1r 1.26E-03.
818	Assay: Stopped flow; UV(-SH loss 412 nm); k1 = Overall kinetics | k1s = from slope | k1i = from intercept | k1r = initial rate; k1(pH=5.5) = 10* k1(7.4)
	k1s 2.22E+01 | k1i 5.34E-01 | k1r 1.20E-02.
819	Assay: Stopped flow; UV(-SH loss 412 nm); k1 = Overall kinetics | k1s = from slope | k1i = from intercept | k1r = initial rate; k1(pH=5.5) = 10* k1(7.4)
	fits second-order plots; k1s 1.18E+04 | k1i 3.60E-03 | k1r 2.34E+00.
820	Assay: Stopped flow; UV(-SH loss 412 nm); k1 = Overall kinetics | k1s = from slope | k1i = from intercept | k1r = initial rate; k1(pH=5.5) = 10* k1(7.4)
	k1s 7.24E+02 | k1i 3.18E-01 | k1r 1.50E-01.
821	Assay: Stopped flow; UV(-SH loss 412 nm); k1 = Overall kinetics | k1s = from slope | k1i = from intercept | k1r = initial rate; k1(pH=5.5) = 10* k1(7.4)
	k1s 6.00E+00 | k1i 3.00E-03 | k1r 1.20E-03.
822	Assay: Stopped flow; UV(-SH loss 412 nm); k1 = Overall kinetics | k1s = from slope | k1i = from intercept | k1r = initial rate; k1(pH=5.5) = 10* k1(7.4)
	k1s 1.48E+04 | k1i 3.60E-02 | k1r 3.60E+00.
823	Assay: Stopped flow; UV(-SH loss 412 nm); k1 = Overall kinetics | k1s = from slope | k1i = from intercept | k1r = initial rate; k1(pH=5.5) = 10* k1(7.4)
	k1s 5.08E+03 | k1i 1.80E-03 | k1r 6.00E-04.
824	Assay: Stopped flow; UV(-SH loss 412 nm); k1 = Overall kinetics | k1s = from slope | k1i = from intercept | k1r = initial rate; k1(pH=5.5) = 10* k1(7.4)
	k1s 4.58E+02 | k1i 1.20E-02 | k1r 5.22E-04.
825	Assay: Stopped flow; UV(-SH loss 412 nm); k1 = Overall kinetics | k1s = from slope | k1i = from intercept | k1r = initial rate; k1(pH=5.5) = 10* k1(7.4)
	k1s 6.50E+04 | k1i 1.20E-03 | k1r 1.80E-04.
826	Assay: Stopped flow; UV(-SH loss 412 nm); k1 = Overall kinetics | k1s = from slope | k1i = from intercept | k1r = initial rate; k1(pH=5.5) = 10* k1(7.4)
	k1s 9.00E-01 | k1i 6.00E-04 | k1r 1.02E-04.
827	Assay: Stopped flow; UV(-SH loss 412 nm); k1 = Overall kinetics | k1s = from slope | k1i = from intercept | k1r = initial rate; k1(pH=5.5) = 10* k1(7.4)
	k1s 4.98E+02 | k1i 7.80E-01 | k1r 1.80E-01.
828	Assay: Stopped flow; UV(-SH loss 412 nm); k1 = Overall kinetics | k1s = from slope | k1i = from intercept | k1r = initial rate; k1(pH=5.5) = 10* k1(7.4)
	fit 2nd order; MITZ+ITZ mixture; k1s 3.09E+03 | k1i 3.00E-02 | k1r 1.32E+00.
829	Assay: Stopped flow; UV(-SH loss 412 nm); k1 = Overall kinetics | k1s = from slope | k1i = from intercept | k1r = initial rate; k1(pH=5.5) = 10* k1(7.4)
	fits second-order plots; k1s 9.00E+02 | k1i 2.46E-01 | k1r 7.20E-02.
830	Assay: Stopped flow; UV(-SH loss 412 nm); k1 = Overall kinetics | k1s = from slope | k1i = from intercept | k1r = initial rate; k1(pH=5.5) = 10* k1(7.4)
	k1s 2.09E+03 | k1i 3.60E-04 | k1r 6.00E-01.
831	Assay: Stopped flow; UV(-SH loss 412 nm); k1 = Overall kinetics | k1s = from slope | k1i = from intercept | k1r = initial rate; k1(pH=5.5) = 10* k1(7.4)
	k1s 7.02E+04 | k1i 4.44E-01 | k1r 6.84E+00.
832	Assay: Stopped flow; UV(-SH loss 412 nm); k1 = Overall kinetics | k1s = from slope | k1i = from intercept | k1r = initial rate; k1(pH=5.5) = 10* k1(7.4)
	fits second-order plots; k1s 8.06E+04 | k1i 4.80E-02 | k1r 3.60E-04.
833	Assay: Stopped flow; UV(-SH loss 412 nm); k1 = Overall kinetics | k1s = from slope | k1i = from intercept | k1r = initial rate; k1(pH=5.5) = 10* k1(7.4)

#	Mechanism
811	Nucleophilic aromatic substitution (SNAr)
812	Nucleophilic aromatic substitution (SNAr)
813	Nucleophilic aromatic substitution (SNAr)
814	Nucleophilic aromatic substitution (SNAr)
815	Michael-type nucleophilic addition
816	Acylation
817	Michael-type nucleophilic addition: LC-MS analysis inconsistent with MA
818	Nucleophilic aromatic substitution (SNAr)
819	Michael-type nucleophilic addition
820	Michael-type nucleophilic addition: LC-MS analysis inconsistent with MA
821	Acylation: Schiff base former, but reactive to NBT
822	Michael-type nucleophilic addition
823	Nucleophilic substitution
824	Nucleophilic substitution
825	Nucleophilic substitution
826	Michael-type nucleophilic addition
827	Michael-type nucleophilic addition
828	Acylation: Schiff base former, but reactive to NBT
829	Michael-type nucleophilic addition: LC-MS analysis inconsistent with MA
830	Nucleophilic substitution
831	Nucleophilic substitution
832	Nucleophilic substitution
833	Michael-type nucleophilic addition

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
834	106-51-4	p-Benzoquinone	4-Nitrobenzenethiol	k1(NBT) | k1s | k1i | k1r	min-1	99600	5160	5
835	1939-99-7	Phenylmethanesulfonyl chloride	4-Nitrobenzenethiol	k1(NBT) | k1s | k1i | k1r	min-1	115.2	20.4	2.06
836	2892-51-5	Squaric acid	4-Nitrobenzenethiol	k1(NBT) | k1s | k1i | k1r	min-1	11.34	1.2	1.05
837	584-84-9	Toluene 2.4-diisocyanate	4-Nitrobenzenethiol	k1(NBT) | k1s | k1i | k1r	min-1	1206	204	3.08
838	2426-07-5	1.2.7.8-Diepoxyoctane	4-Nitrobenzylpyridine	k1(NBP)	min-1			-3.15
839	78-87-5	1.2-Dichloropropane	4-Nitrobenzylpyridine	k1(NBP)	min-1	NR		
840	106-88-7	1.2-Epoxybutane	4-Nitrobenzylpyridine	k1(NBP)	min-1			-3.35
841	2404-44-6	1.2-Epoxydecane	4-Nitrobenzylpyridine	k1(NBP)	min-1			-3.35
842	2855-19-8	1.2-Epoxydodecane	4-Nitrobenzylpyridine	k1(NBP)	min-1			-3.32
843	7320-37-8	1.2-Epoxyhexadecane	4-Nitrobenzylpyridine	k1(NBP)	min-1			-3.62
844	1436-34-6	1.2-Epoxyhexane	4-Nitrobenzylpyridine	k1(NBP)	min-1			-3.42
845	2984-50-1	1.2-Epoxyoctane	4-Nitrobenzylpyridine	k1(NBP)	min-1			-3.41
846	1464-53-5	1.3-Butadiene diepoxide	4-Nitrobenzylpyridine	k1(NBP)	min-1			-2.68
847	618-62-2	1.3-Dichloro-5-nitrobenzene	4-Nitrobenzylpyridine	k1(NBP)	min-1	NR		
848	541-73-1	1.3-Dichlorobenzene	4-Nitrobenzylpyridine	k1(NBP)	min-1	NR		
849	142-28-9	1.3-Dichloropropane	4-Nitrobenzylpyridine	k1(NBP)	min-1			-5.1
850	542-75-6	1.3-Dichloropropene	4-Nitrobenzylpyridine	k1(NBP)	min-1	4.22E+03		3.63
851	542-75-6	1.3-Dichloropropene	4-Nitrobenzylpyridine	k1(NBP)	min-1			-3.69
852	542-75-6	1.3-Dichloropropene	4-Nitrobenzylpyridine	k1(NBP)	min-1			-3.5
853	542-75-6	1.3-Dichloropropene	4-Nitrobenzylpyridine	k1(NBP)	min-1			-3.9
854	628-76-2	1.5-Dichloropentane	4-Nitrobenzylpyridine	k1(NBP)	min-1			-5.23
855	97-00-7	1-Chloro-2.4-dinitrobenzene	4-Nitrobenzylpyridine	k1(NBP)	min-1			-2.71
856	111-44-4	2.2'-Dichlorodiethyl ether	4-Nitrobenzylpyridine	k1(NBP)	min-1			-4.9
857	78-88-6	2.3-Dichloro-1-propene	4-Nitrobenzylpyridine	k1(NBP)	min-1	2.02E+02		2.31
858	78-88-6	2.3-Dichloro-1-propene	4-Nitrobenzylpyridine	k1(NBP)	min-1			-4.3
859	554-00-7	2.4-Dichloroaniline	4-Nitrobenzylpyridine	k1(NBP)	min-1	NR		
860	107-20-0	2-Chloroacetaldehyde	4-Nitrobenzylpyridine	k1(NBP)	min-1	NR		
861	760-23-6	3.4-Dichloro-1-butene	4-Nitrobenzylpyridine	k1(NBP)	min-1			-5.3
862	563-52-0	3-Chloro-1-butene	4-Nitrobenzylpyridine	k1(NBP)	min-1			-5.2
863	563-47-3	3-Chloro-2-methylpropene	4-Nitrobenzylpyridine	k1(NBP)	min-1	1.28E+03		3.11
864	100-11-8	4-Nitrobenzylbromide	4-Nitrobenzylpyridine	k1(NBP)	min-1			-1.32
865	100-11-8	4-Nitrobenzylbromide	4-Nitrobenzylpyridine	k1(NBP)	min-1			-3
866	106-95-6	Allyl bromide	4-Nitrobenzylpyridine	k1(NBP)	min-1	1.24E+05		5.09
867	107-05-1	Allyl chloride	4-Nitrobenzylpyridine	k1(NBP)	min-1	5.32E+02		2.73
868	107-05-1	Allyl chloride	4-Nitrobenzylpyridine	k1(NBP)	min-1			-4.02
869	107-05-1	Allyl chloride	4-Nitrobenzylpyridine	k1(NBP)	min-1			-3.55
870	94-99-5	alpha.2.4-Trichlorotoluene	4-Nitrobenzylpyridine	k1(NBP)	min-1			-3.14
871	626-16-4	alpha.alpha'-Dichloro-m-xylene	4-Nitrobenzylpyridine	k1(NBP)	min-1			-3.26
872	3132-64-7	alpha-Epibromohydrin	4-Nitrobenzylpyridine	k1(NBP)	min-1			-2.88

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
834	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
835	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
836	25	7.4	PBS 0.1 M, ACN		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
837	25	7.4	PBS 0.1 M, ACN, acetone		10:1 - 1:100	Chipinda I et al., Chem. Res. Toxicol. 23 (2010), 918
838	37	7.4	Ethylene glycol, acetone, TRIS-buff	90 min	90:1	Deneer JW et al., Aquat. Toxicol. 13 (1988), 195
839	80		2-Butanone	60 min	30:1	Hermens J et al., Toxicol. Environ. Chem. 9 (1985), 219
840	37	7.4	Ethylene glycol, acetone, TRIS-buff	90 min	90:1	Deneer JW et al., Aquat. Toxicol. 13 (1988), 195
841	37	7.4	Ethylene glycol, acetone, TRIS-buff	90 min	90:1	Deneer JW et al., Aquat. Toxicol. 13 (1988), 195
842	37	7.4	Ethylene glycol, acetone, TRIS-buff	90 min	90:1	Deneer JW et al., Aquat. Toxicol. 13 (1988), 195
843	37	7.4	Ethylene glycol, acetone, TRIS-buff	90 min	90:1	Deneer JW et al., Aquat. Toxicol. 13 (1988), 195
844	37	7.4	Ethylene glycol, acetone, TRIS-buff	90 min	90:1	Deneer JW et al., Aquat. Toxicol. 13 (1988), 195
845	37	7.4	Ethylene glycol, acetone, TRIS-buff	90 min	90:1	Deneer JW et al., Aquat. Toxicol. 13 (1988), 195
846	37	7.4	Ethylene glycol, acetone, TRIS-buff	90 min	90:1	Deneer JW et al., Aquat. Toxicol. 13 (1988), 195
847	80		2-Butanone	60 min	30:1	Hermens J et al., Toxicol. Environ. Chem. 9 (1985), 219
848	80		2-Butanone	60 min	30:1	Hermens J et al., Toxicol. Environ. Chem. 9 (1985), 219
849	80		2-Butanone	60 min	30:1	Hermens J et al., Toxicol. Environ. Chem. 9 (1985), 219
850	60		Ethyl methyl ketone, triethylamine	60 min	7:1	Eder E et al., Chem. Biol. Interactions 38 (1982), 303
851	80		2-Butanone	60 min	30:1	Hermens J et al., Toxicol. Environ. Chem. 9 (1985), 219
852	80		2-Butanone	60 min	30:1	Verhaar HJM et al., Environ. Toxicol. Chem 15 (1996), 1011
853	80		2-Butanone	60 min	30:1	Verhaar HJM et al., Environ. Toxicol. Chem 15 (1996), 1011
854	80		2-Butanone	60 min	30:1	Hermens J et al., Toxicol. Environ. Chem. 9 (1985), 219
855	80		2-Butanone	60 min	30:1	Hermens J et al., Toxicol. Environ. Chem. 9 (1985), 219
856	80		2-Butanone	60 min	30:1	Hermens J et al., Toxicol. Environ. Chem. 9 (1985), 219
857	60		Ethyl methyl ketone, triethylamine	60 min	7:1	Eder E et al., Chem. Biol. Interactions 38 (1982), 303
858	80		2-Butanone	60 min	30:1	Hermens J et al., Toxicol. Environ. Chem. 9 (1985), 219
859	80		2-Butanone	60 min	30:1	Hermens J et al., Toxicol. Environ. Chem. 9 (1985), 219
860	37	7.4	Acetone, TRIS-HCl buffer	60 min	1:775	Barbin A et al., Biochem. Biophys. Res. Commun. 67 (1975), 596
861	80		2-Butanone	60 min	30:1	Verhaar HJM et al., Environ. Toxicol. Chem 15 (1996), 1011
862	80		2-Butanone	60 min	30:1	Hermens J et al., Toxicol. Environ. Chem. 9 (1985), 219
863	60		Ethyl methyl ketone, triethylamine	60 min	7:1	Eder E et al., Chem. Biol. Interactions 38 (1982), 303
864	80		2-Butanone	60 min	30:1	Hermens J et al., Toxicol. Environ. Chem. 9 (1985), 219
865	37	7.4	Ethylene glycol, acetone, TRIS-buff	90 min	90:1	Deneer JW et al., Aquat. Toxicol. 13 (1988), 195
866	60		Ethyl methyl ketone, triethylamine	60 min	7:1	Eder E et al., Chem. Biol. Interactions 38 (1982), 303
867	60		Ethyl methyl ketone, triethylamine	60 min	7:1	Eder E et al., Chem. Biol. Interactions 38 (1982), 303
868	80		2-Butanone	60 min	30:1	Hermens J et al., Toxicol. Environ. Chem. 9 (1985), 219
869	37	7.4	Ethylene glycol, acetone, TRIS-buff	90 min	90:1	Deneer JW et al., Aquat. Toxicol. 13 (1988), 195
870	80		2-Butanone	60 min	30:1	Hermens J et al., Toxicol. Environ. Chem. 9 (1985), 219
871	80		2-Butanone	60 min	30:1	Hermens J et al., Toxicol. Environ. Chem. 9 (1985), 219
872	37	7.4	Ethylene glycol, acetone, TRIS-buff	90 min	90:1	Deneer JW et al., Aquat. Toxicol. 13 (1988), 195

#	Comment
	k1s 9.46E+04 | k1i 6.36E-01 | k1r 4.18E+01.
834	Assay: Stopped flow; UV(-SH loss 412 nm); k1 = Overall kinetics | k1s = from slope | k1i = from intercept | k1r = initial rate; k1(pH=5.5) = 10* k1(7.4)
	k1s 1.32E+02 | k1i 2.40E-03 | k1r 5.40E-04.
835	Assay: Stopped flow; UV(-SH loss 412 nm); k1 = Overall kinetics | k1s = from slope | k1i = from intercept | k1r = initial rate; k1(pH=5.5) = 10* k1(7.4)
	k1s 1.05E+01 | k1i 1.80E-04 | k1r 1.20E-03.
836	Assay: Stopped flow; UV(-SH loss 412 nm); k1 = Overall kinetics | k1s = from slope | k1i = from intercept | k1r = initial rate; k1(pH=5.5) = 10* k1(7.4)
	fits second-order plots; k1s 1.53E+03 | k1i 6.60E+00 | k1r 1.20E-01.
837	Assay: Stopped flow; UV(-SH loss 412 nm); k1 = Overall kinetics | k1s = from slope | k1i = from intercept | k1r = initial rate; k1(pH=5.5) = 10* k1(7.4)
838	no significant hydrolysis observed. Assay: UV (ca. 560 nm)
839	non-reactive in NBP test. Assay: UV (ca. 560 nm)
840	no significant hydrolysis observed. Assay: UV (ca. 560 nm)
841	no significant hydrolysis observed. Assay: UV (ca. 560 nm)
842	no significant hydrolysis observed. Assay: UV (ca. 560 nm)
843	no significant hydrolysis observed. Assay: UV (ca. 560 nm)
844	no significant hydrolysis observed. Assay: UV (ca. 560 nm)
845	no significant hydrolysis observed. Assay: UV (ca. 560 nm)
846	no significant hydrolysis observed. Assay: UV (ca. 560 nm)
847	non-reactive in NBP test. Assay: UV (ca. 560 nm)
848	non-reactive in NBP test. Assay: UV (ca. 560 nm)
849	Assay: UV (ca. 560 nm)
850	trans-Isomer. Assay: UV (ca. 560 nm)
851	Assay: UV (ca. 560 nm)
852	cis-isomer. Assay: UV (ca. 560 nm)
853	trans-isomer. Assay: UV (ca. 560 nm)
854	Assay: UV (ca. 560 nm)
855	Assay: UV (ca. 560 nm)
856	Assay: UV (ca. 560 nm)
857	Assay: UV (ca. 560 nm)
858	Assay: UV (ca. 560 nm)
859	non-reactive in NBP test. Assay: UV (ca. 560 nm)
860	Assay: UV (ca. 560 nm)
861	Assay: UV (ca. 560 nm)
862	Assay: UV (ca. 560 nm)
863	Assay: UV (ca. 560 nm)
864	estimated by curve fitting for first order kinetics. Assay: UV (ca. 560 nm)
865	no significant hydrolysis observed. Assay: UV (ca. 560 nm)
866	Assay: UV (ca. 560 nm)
867	Assay: UV (ca. 560 nm)
868	Assay: UV (ca. 560 nm)
869	no significant hydrolysis observed. Assay: UV (ca. 560 nm)
870	Assay: UV (ca. 560 nm)
871	Assay: UV (ca. 560 nm)
872	no significant hydrolysis observed. Assay: UV (ca. 560 nm)

#	Mechanism
834	Michael-type nucleophilic addition
835	Nucleophilic substitution
836	Michael-type nucleophilic addition
837	Acylation: Hydrolysis and amine formation
838	
839	NOT Nucleophilic substitution, second order (SN2)
840	
841	
842	
843	
844	
845	
846	
847	NOT Nucleophilic aromatic substitution (SNAr)
848	NOT Nucleophilic aromatic substitution (SNAr)
849	Nucleophilic substitution, second order (SN2)
850	Nucleophilic substitution and direct DNA-alkylatior
851	Nucleophilic substitution, second order (SN2)
852	Nucleophilic substitution, second order (SN2)
853	Nucleophilic substitution, second order (SN2)
854	Nucleophilic substitution, second order (SN2)
855	Nucleophilic aromatic substitution (SNAr)
856	Nucleophilic substitution, second order (SN2)
857	Nucleophilic substitution and direct DNA-alkylatior
858	Nucleophilic substitution, second order (SN2)
859	NOT Nucleophilic aromatic substitution (SNAr)
860	
861	Nucleophilic substitution, second order (SN2)
862	Nucleophilic substitution, second order (SN2)
863	Nucleophilic substitution and direct DNA-alkylatior
864	Nucleophilic substitution, second order (SN2)
865	
866	Nucleophilic substitution and direct DNA-alkylatior
867	Nucleophilic substitution and direct DNA-alkylatior
868	Nucleophilic substitution, second order (SN2)
869	
870	Nucleophilic substitution, second order (SN2)
871	Nucleophilic substitution, second order (SN2)
872	

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
873	100-44-7	Benzyl chloride	4-Nitrobenzylpyridine	k1(NBP)	min-1			-3.55
874	100-44-7	Benzyl chloride	4-Nitrobenzylpyridine	k1(NBP)	min-1			-3
875	2104-96-3	Bromophos	4-Nitrobenzylpyridine	k1(NBP)	min-1			-4.11
876	78-95-5	Chloroacetone	4-Nitrobenzylpyridine	k1(NBP)	min-1			-2.73
877	7763-77-1	Chloroethylene oxide	4-Nitrobenzylpyridine	k1(NBP)	min-1	0.43		-0.37
878	591-97-9	Crotyl chloride	4-Nitrobenzylpyridine	k1(NBP)	min-1	2.57E+03		3.41
879	591-97-9	Crotyl chloride	4-Nitrobenzylpyridine	k1(NBP)	min-1			-3.7
880	2636-26-2	Cyanophos	4-Nitrobenzylpyridine	k1(NBP)	min-1			-4.58
881	3070-16-4	Demethyl-fenthion	4-Nitrobenzylpyridine	k1(NBP)	min-1			-5.31
882	2463-84-5	Dicapthon	4-Nitrobenzylpyridine	k1(NBP)	min-1			-4
883	106-89-8	Epichlorohydrin	4-Nitrobenzylpyridine	k1(NBP)	min-1			-2.85
884	75-56-9	Epoxypropane	4-Nitrobenzylpyridine	k1(NBP)	min-1			-3.27
885	107-06-2	Ethylene dichloride	4-Nitrobenzylpyridine	k1(NBP)	min-1			-5.86
886	122-14-5	Fenitrothion	4-Nitrobenzylpyridine	k1(NBP)	min-1			-4.59
887	55-38-9	Fenthion	4-Nitrobenzylpyridine	k1(NBP)	min-1			-5.05
888	50-00-0	Formaldehyde	4-Nitrobenzylpyridine	k1(NBP)	min-1	NR		
889	556-52-5	Glycidol	4-Nitrobenzylpyridine	k1(NBP)	min-1			-3.29
890	87-68-3	Hexachloro-1.3-butadiene	4-Nitrobenzylpyridine	k1(NBP)	min-1			-2.03
891	18181-70-9	Iodofenphos	4-Nitrobenzylpyridine	k1(NBP)	min-1			-4.28
892	298-00-0	Methyl parathion	4-Nitrobenzylpyridine	k1(NBP)	min-1			-4.36
893	18936-52-2	Methylisocyanothion	4-Nitrobenzylpyridine	k1(NBP)	min-1			-4.04
894	624-65-7	Propargyl chloride	4-Nitrobenzylpyridine	k1(NBP)	min-1			-3.98
895	299-84-3	Ronnel	4-Nitrobenzylpyridine	k1(NBP)	min-1			-4.23
896	96-09-3	Styrene oxide	4-Nitrobenzylpyridine	k1(NBP)	min-1			-3.19
897	33576-92-0	SV5	4-Nitrobenzylpyridine	k1(NBP)	min-1			-5.52
898	110-57-6	trans-1.4-Dichloro-2-butene	4-Nitrobenzylpyridine	k1(NBP)	min-1			-3.34
899	79-01-6	Trichloroethene	4-Nitrobenzylpyridine	k1(NBP)	min-1	NR		
900	2607-52-5	2.6-Di-tert-butyl-4-methylene-2.5-cyclohexadienone	Lysine	k1(Lys)	min-1	7.20E-02		-1.14
901		2-tert-Butyl-6-methyl-4-methylene-2.5-cyclohexadienone	Lysine	k1(Lys)	min-1	7.20E+00		0.86
902		6-tert-Butyl-2-(2-hydroxy-1.1-dimethylethyl)-4-methylene-2.5-cyclohexadienone	Lysine	k1(Lys)	min-1	5.94E-01		-0.23
903	2607-52-5	2.6-Di-tert-butyl-4-methylene-2.5-cyclohexadienone	Histidine	k1(His)	min-1	7.20E-02		-1.14
904	2607-52-5	2.6-Di-tert-butyl-4-methylene-2.5-cyclohexadienone	Histidine	k1(His)	min-1	NR		
905		2-tert-Butyl-6-methyl-4-methylene-2.5-cyclohexadienone	Histidine	k1(His)	min-1	7.20E+00		0.86
906		2-tert-Butyl-6-methyl-4-methylene-2.5-cyclohexadienone	Histidine	k1(His)	min-1	2.46E-01		-0.61
907		6-tert-Butyl-2-(2-hydroxy-1.1-dimethylethyl)-4-methylene-2.5-cyclohexadienone	Histidine	k1(His)	min-1	7.20E-01		-0.14

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
873	80		2-Butanone	60 min	30:1	Hermens J et al., Toxicol. Environ. Chem. 9 (1985), 219
874	37	7.4	Ethylene glycol, acetone, TRIS-buff	90 min	90:1	Deneer JW et al., Aquat. Toxicol. 13 (1988), 195
875	22		2-Butanone	60 min	30:1	Schüürmann G, Environ. Toxicol. Chem 9 (1990), 417
876	80		2-Butanone	60 min	30:1	Hermens J et al., Toxicol. Environ. Chem. 9 (1985), 219
877	37	7.4	Acetone, TRIS-HCl buffer	60 min	1:775	Barbin A et al., Biochem. Biophys. Res. Commun. 67 (1975), 596
878	60		Ethyl methyl ketone, triethylamine	60 min	7:1	Eder E et al., Chem. Biol. Interactions 38 (1982), 303
879	80		2-Butanone	60 min	30:1	Hermens J et al., Toxicol. Environ. Chem. 9 (1985), 219
880	22		2-Butanone	60 min	30:1	Schüürmann G, Environ. Toxicol. Chem 9 (1990), 417
881	22		2-Butanone	60 min	30:1	Schüürmann G, Environ. Toxicol. Chem 9 (1990), 417
882	22		2-Butanone	60 min	30:1	Schüürmann G, Environ. Toxicol. Chem 9 (1990), 417
883	37	7.4	Ethylene glycol, acetone, TRIS-buff	90 min	90:1	Deneer JW et al., Aquat. Toxicol. 13 (1988), 195
884	37	7.4	Ethylene glycol, acetone, TRIS-buff	90 min	90:1	Deneer JW et al., Aquat. Toxicol. 13 (1988), 195
885	80		2-Butanone	60 min	30:1	Hermens J et al., Toxicol. Environ. Chem. 9 (1985), 219
886	22		2-Butanone	60 min	30:1	Schüürmann G, Environ. Toxicol. Chem 9 (1990), 417
887	22		2-Butanone	60 min	30:1	Schüürmann G, Environ. Toxicol. Chem 9 (1990), 417
888	80		2-Butanone	60 min	30:1	Hermens J et al., Toxicol. Environ. Chem. 9 (1985), 219
889	37	7.4	Ethylene glycol, acetone, TRIS-buff	90 min	90:1	Deneer JW et al., Aquat. Toxicol. 13 (1988), 195
890	80		2-Butanone	60 min	30:1	Hermens J et al., Toxicol. Environ. Chem. 9 (1985), 219
891	22		2-Butanone	60 min	30:1	Schüürmann G, Environ. Toxicol. Chem 9 (1990), 417
892	22		2-Butanone	60 min	30:1	Schüürmann G, Environ. Toxicol. Chem 9 (1990), 417
893	22		2-Butanone	60 min	30:1	Schüürmann G, Environ. Toxicol. Chem 9 (1990), 417
894	80		2-Butanone	60 min	30:1	Verhaar HJM et al., Environ. Toxicol. Chem 15 (1996), 1011
895	22		2-Butanone	60 min	30:1	Schüürmann G, Environ. Toxicol. Chem 9 (1990), 417
896	37	7.4	Ethylene glycol, acetone, TRIS-buff	90 min	90:1	Deneer JW et al., Aquat. Toxicol. 13 (1988), 195
897	22		2-Butanone	60 min	30:1	Schüürmann G, Environ. Toxicol. Chem 9 (1990), 417
898	80		2-Butanone	60 min	30:1	Hermens J et al., Toxicol. Environ. Chem. 9 (1985), 219
899	80		2-Butanone	60 min	30:1	Hermens J et al., Toxicol. Environ. Chem. 9 (1985), 219
900	25	7.4	PBS 50 mM		1:10	Bolton JL et al., Chem. Biol. Interact. 107 (1997), 185
901	25	7.4	PBS 50 mM		1:10	Bolton JL et al., Chem. Biol. Interact. 107 (1997), 185
902	25	7.4	PBS 50 mM		1:10	Bolton JL et al., Chem. Biol. Interact. 107 (1997), 185
903	25	7.4	PBS 50 mM		1:10	Bolton JL et al., Chem. Biol. Interact. 107 (1997), 185
904	25	7.4	PBS 50 mM		1:10	Bolton JL et al., Chem. Biol. Interact. 107 (1997), 185
905	25	7.4	PBS 50 mM		1:10	Bolton JL et al., Chem. Biol. Interact. 107 (1997), 185
906	25	7.4	PBS 50 mM		1:10	Bolton JL et al., Chem. Biol. Interact. 107 (1997), 185
907	25	7.4	PBS 50 mM		1:10	Bolton JL et al., Chem. Biol. Interact. 107 (1997), 185

#	Comment
873	Assay: UV (ca. 560 nm)
874	no significant hydrolysis observed. Assay: UV (ca. 560 nm)
875	Assay: UV (ca. 560 nm)
876	Assay: UV (ca. 560 nm)
877	very fast, alkylation finished after 90s, t1/2=1.6 min. Assay: UV (ca. 560 nm)
878	Assay: UV (ca. 560 nm)
879	Assay: UV (ca. 560 nm)
880	Assay: UV (ca. 560 nm)
881	Assay: UV (ca. 560 nm)
882	Assay: UV (ca. 560 nm)
883	no significant hydrolysis observed. Assay: UV (ca. 560 nm)
884	no significant hydrolysis observed. Assay: UV (ca. 560 nm)
885	Assay: UV (ca. 560 nm)
886	Assay: UV (ca. 560 nm)
887	Assay: UV (ca. 560 nm)
888	non-reactive in NBP test. Assay: UV (ca. 560 nm)
889	no significant hydrolysis observed. Assay: UV (ca. 560 nm)
890	estimated by curve fitting for first order kinetics. Assay: UV (ca. 560 nm)
891	Assay: UV (ca. 560 nm)
892	Assay: UV (ca. 560 nm)
893	Assay: UV (ca. 560 nm)
894	Assay: UV (ca. 560 nm)
895	Assay: UV (ca. 560 nm)
896	no significant hydrolysis observed. Assay: UV (ca. 560 nm)
897	Assay: UV (ca. 560 nm)
898	Assay: UV (ca. 560 nm)
899	non-reactive in NBP test. Assay: UV (ca. 560 nm)
900	Assay: HPLC/UV: N-alpha (230 nm+280 nm)
901	Assay: HPLC/UV: N-alpha (230 nm+280 nm)
902	Assay: HPLC/UV: N-alpha (230 nm+280 nm)
903	N in alpha position. Assay: HPLC/UV (230 nm+280 nm)
904	N in pi/tau position. Assay: HPLC/UV (230 nm+280 nm)
905	N in alpha position. Assay: HPLC/UV (230 nm+280 nm)
906	N in pi/tau position. Assay: HPLC/UV (230 nm+280 nm)
907	N in alpha position. Assay: HPLC/UV (230 nm+280 nm)

#	Mechanism
873	Nucleophilic substitution, second order (SN2)
874	
875	Acetylcholinesterase inhibition
876	Nucleophilic substitution, second order (SN2)
877	
878	Nucleophilic substitution and direct DNA-alkylatior
879	Nucleophilic substitution, second order (SN2)
880	Acetylcholinesterase inhibition
881	Acetylcholinesterase inhibition
882	Acetylcholinesterase inhibition
883	
884	
885	Nucleophilic substitution, second order (SN2)
886	Acetylcholinesterase inhibition
887	Acetylcholinesterase inhibition
888	NOT Nucleophilic substitution, second order (SN2)
889	
890	Nucleophilic substitution, second order (SN2)
891	Acetylcholinesterase inhibition
892	Acetylcholinesterase inhibition
893	Acetylcholinesterase inhibition
894	Nucleophilic substitution, second order (SN2)
895	Acetylcholinesterase inhibition
896	
897	Acetylcholinesterase inhibition
898	Nucleophilic substitution, second order (SN2)
899	NOT Nucleophilic substitution, second order (SN2)
900	
901	
902	
903	
904	
905	
906	
907	

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
908		6-tert-Butyl-2-(2-hydroxy-1.1-dimethylethyl)-4-methylene-2.5-cyclohexadienone	Histidine	k1(His)	min-1	NR		
909	2607-52-5	2.6-Di-tert-butyl-4-methylene-2.5-cyclohexadienone	Cysteine	k1(Cys)	min-1	4.62E-01		-0.34
910		2-tert-Butyl-6-methyl-4-methylene-2.5-cyclohexadienone	Cysteine	k1(Cys)	min-1	1.50E+01		1.18
911		6-tert-Butyl-2-(2-hydroxy-1.1-dimethylethyl)-4-methylene-2.5-cyclohexadienone	Cysteine	k1(Cys)	min-1	2.58E+00		0.41
912		3.4'-Dimethoxybenzhydrylacetate	- not k determining -	k1(ACN-SN1)	min-1	2.30E-08		-7.63
913		3-Methoxy-4'-methylbenzhydrylacetate	- not k determining -	k1(ACN-SN1)	min-1	2.30E-08		-7.63
914		3-Methoxybenzhydrylacetate	- not k determining -	k1(ACN-SN1)	min-1	2.40E-08		-7.62
915	776-74-9	Benzhydryl bromide	- not k determining -	k1(ACN-SN1)	min-1	ND		
916	90-99-3	Benzhydryl chloride	- not k determining -	k1(ACN-SN1)	min-1	7.80E-09		-8.11
917	2607-52-5	2.6-Di-tert-butyl-4-methylene-2.5-cyclohexadienone	N(alpha)-Acetyl lysine	k1(AcLys)	min-1	NR		
918		2-tert-Butyl-6-methyl-4-methylene-2.5-cyclohexadienone	N(alpha)-Acetyl lysine	k1(AcLys)	min-1	2.16E-01		-0.67
919		6-tert-Butyl-2-(2-hydroxy-1.1-dimethylethyl)-4-methylene-2.5-cyclohexadienone	N(alpha)-Acetyl lysine	k1(AcLys)	min-1	NR		
920		3-Nitro-alpha-nitrostilbene	2-Mercaptoethanol	k(Thiolate) | K | k-1	M-1 min-1	1.61E+07	3.00E+06	7.21
921		4-Bromo-alpha-nitrostilbene	2-Mercaptoethanol	k(Thiolate) | K | k-1	M-1 min-1	7.26E+06	1.80E+05	6.86
922		4-Methyl-alpha-nitrostilbene	2-Mercaptoethanol	k(Thiolate) | K | k-1	M-1 min-1	2.23E+06	1.20E+05	6.35
923		4-Nitro-alpha-nitrostilbene	2-Mercaptoethanol	k(Thiolate) | K | k-1	M-1 min-1	1.93E+07	4.20E+06	7.28
924	1215-07-2	alpha-Nitrostilbene	2-Mercaptoethanol	k(Thiolate) | K | k-1	M-1 min-1	3.49E+06	3.60E+04	6.54
925	1215-07-2	alpha-Nitrostilbene	2-Mercaptoethanol	k(Thiolate) | K | k-1	M-1 min-1	3.49E+06		6.54
926		beta-Methoxy-alpha-nitrostilbene	2-Mercaptoethanol	k(Thiolate) | K | k-1	M-1 min-1	2.34E+04		4.37
927		Methoxybenzylidene Meldrum's acid	2-Mercaptoethanol	k(Thiolate) | K | k-1	M-1 min-1	2.64E+06	1.20E+04	6.42
928	1215-07-2	alpha-Nitrostilbene	Ethanethiolate	k(Thiolate) | K | k-1	M-1 min-1	4.01E+06		6.6
929	1215-07-2	alpha-Nitrostilbene	Methyl 3-mercaptopropionate	k(Thiolate) | K | k-1	M-1 min-1	3.49E+06		6.54
930	1215-07-2	alpha-Nitrostilbene	Methyl thioglycolate	k(Thiolate) | K | k-1	M-1 min-1	1.71E+06		6.23
931	370-86-5	Carbonyl cyanide p-trifluoromethoxyphenylhydrazone	2-Mercaptoethanol	k(Thiolate)	M-1 min-1	1.68E+04		4.23
932	586-96-9	Nitrosobenzene	2-Mercaptoethanol	k(Thiolate)	M-1 min-1	7.80E+04		4.89

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
908	25	7.4	PBS 50 mM		1:10	Bolton JL et al., Chem. Biol. Interact. 107 (1997), 185
909	25	7.4	PBS 50 mM		1:10	Bolton JL et al., Chem. Biol. Interact. 107 (1997), 185
910	25	7.4	PBS 50 mM		1:10	Bolton JL et al., Chem. Biol. Interact. 107 (1997), 185
911	25	7.4	PBS 50 mM		1:10	Bolton JL et al., Chem. Biol. Interact. 107 (1997), 185
912	23		ACN			Peters KS, Chem. Rev. 107 (2007), 859
913	23		ACN			Peters KS, Chem. Rev. 107 (2007), 859
914	23		ACN			Peters KS, Chem. Rev. 107 (2007), 859
915	23		ACN			Peters KS, Chem. Rev. 107 (2007), 859
916	23		ACN			Peters KS, Chem. Rev. 107 (2007), 859
917	25	7.4	PBS 50 mM		1:10	Bolton JL et al., Chem. Biol. Interact. 107 (1997), 185
918	25	7.4	PBS 50 mM		1:10	Bolton JL et al., Chem. Biol. Interact. 107 (1997), 185
919	25	7.4	PBS 50 mM		1:10	Bolton JL et al., Chem. Biol. Interact. 107 (1997), 185
920	20	7.5	DMSO:H20 1:1, N-Me-morpholine buf			Bernasconi CF et al., J. Am. Chem. Soc. 110 (1988), 7506
921	20	7.5	DMSO:H20 1:1, N-Me-morpholine buf			Bernasconi CF et al., J. Am. Chem. Soc. 110 (1988), 7506
922	20	7.5	DMSO:H20 1:1, N-Me-morpholine buf			Bernasconi CF et al., J. Am. Chem. Soc. 110 (1988), 7506
923	20	7.5	DMSO:H20 1:1, N-Me-morpholine buf			Bernasconi CF et al., J. Am. Chem. Soc. 110 (1988), 7506
924	20	7.5	DMSO:H20 1:1, N-Me-morpholine buf			Bernasconi CF et al., J. Am. Chem. Soc. 110 (1988), 7506
925	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
926	20		DMSO:water 1:1			Bernasconi CF et al., J. Org. Chem. 64 (1999), 2897
927	20		DMSO:water 1:1			Bernasconi CF et al., J. Am. Chem. Soc. 120 (1998), 7461
928	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
929	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
930	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
931	25	7.5	Citrate/phosphate 0.1 M, 1% MeOH		25:1	Drobnica L et al., Biochim. Biophys. Acta 585 (1979), 462
932	37	7.4				Eyer P, Biological Oxidation of Nitrogen in Orga... (1985), 386

#	Comment
908	N in pi/tau position. Assay: HPLC/UV (230 nm+280 nm)
909	Assay: HPLC/UV (230 nm+280 nm)
910	Assay: HPLC/UV (230 nm+280 nm)
911	Assay: HPLC/UV (230 nm+280 nm)
	k(GS) 3.6E-08 | k(SSIP) 7.8E-08 | k(FR) 4.8E-08.
912	Assay: SN1 R: [101]; 1. Contact ion pair > reactant | 2. CIP > Solvent-separated ion pair | 3. SSIP > CIP rate-determining step (=k1) | 4. Free ion formation
	k(GS) 1.3E-07 | k(SSIP) 1.8E-07 | k(FR) 4.8E-08.
913	Assay: SN1 R: [101]; 1. Contact ion pair > reactant | 2. CIP > Solvent-separated ion pair | 3. SSIP > CIP rate-determining step (=k1) | 4. Free ion formation
	k(GS) 1.8E-07 | k(SSIP) 2.1E-07 | k(FR) 4.8E-08.
914	Assay: SN1 R: [101]; 1. Contact ion pair > reactant | 2. CIP > Solvent-separated ion pair | 3. SSIP > CIP rate-determining step (=k1) | 4. Free ion formation
	k(GS) 1.9E-07 | k(SSIP) 3.4E-07 | k(FR) ND.
915	Assay: SN1 R: [101]; 1. Contact ion pair > reactant | 2. CIP > Solvent-separated ion pair | 3. SSIP > CIP rate-determining step (=k1) | 4. Free ion formation
	k(GS) 2.3E-07 | k(SSIP) 1.7E-07 | k(FR) 4.7E-08.
916	Assay: SN1 R: [101]; 1. Contact ion pair > reactant | 2. CIP > Solvent-separated ion pair | 3. SSIP > CIP rate-determining step (=k1) | 4. Free ion formation
917	Assay: HPLC/UV: N-epsilon (230 nm+280 nm)
918	Assay: HPLC/UV: N-epsilon (230 nm+280 nm)
919	Assay: HPLC/UV: N-epsilon (230 nm+280 nm)
	{OCC[S-]}; K 4.18(78)E+07 | k-1 3.86(8)E-01 | k2 (proton.) 4.75(30)E+01.
920	Assay: Stopped-flow UV(max. abs.); Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
	{OCC[S-]}; K 2.08(9)E+07 | k-1 3.50(12)E-01 | k2 (proton.) 3.53(8)E+01.
921	Assay: Stopped-flow UV(max. abs.); Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
	{OCC[S-]}; K 5.01(31)E+06 | k-1 4.46(14)E-01 | k2 (proton.) 2.44(10)E+01.
922	Assay: Stopped-flow UV(max. abs.); Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
	{OCC[S-]}; K 6.84(1.52)E+07 | k-1 2.80(12)E-01 | k2 (proton.) 3.34(24)E+01.
923	Assay: Stopped-flow UV(max. abs.); Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
	{OCC[S-]}; K 8.28(27)E+06 | k-1 4.21(13)E-01 | k2 (proton.) 2.75(8)E+01.
924	Assay: Stopped-flow UV(max. abs.); Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
925	Ion: {OCC[S-]}. Assay: Stopped-flow UV(max. abs.); Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
926	Ion: {OCC[S-]}. Assay: Stopped-flow UV(max. abs.); Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
927	Ion: {OCC[S-]}. Assay: Stopped-flow UV(max. abs.); Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
928	Assay: Stopped-flow UV(max. abs.); Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
929	Ion: {COC(=O)CC[S-]}. Assay: Stopped-flow UV(max. abs.); Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
930	Ion: {COC(=O)C[S-]}. Assay: Stopped-flow UV(max. abs.); Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
931	UV(200-800 nm); reactive: non-diss. CCP + RS[-] (pH < pKa).
932	

#	Mechanism
908	
909	
910	
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912	Nucleophilic substitution, first order (SN1)
913	Nucleophilic substitution, first order (SN1)
914	Nucleophilic substitution, first order (SN1)
915	Nucleophilic substitution, first order (SN1)
916	Nucleophilic substitution, first order (SN1)
917	
918	
919	
920	Nucleophilic olefinic addition
921	Nucleophilic olefinic addition
922	Nucleophilic olefinic addition
923	Nucleophilic olefinic addition
924	Nucleophilic olefinic addition
925	Nucleophilic olefinic addition
926	Vinylic nucleophilic substitution
927	Vinylic nucleophilic substitution
928	Nucleophilic olefinic addition
929	Nucleophilic olefinic addition
930	Nucleophilic olefinic addition
931	Nucleophilic olefinic addition
932	

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
933	79-06-1	Acrylamide	beta-Mercaptoacetic acid	k(Thiolate)	M-1 min-1	2.80E+03		3.440909
934	107-13-1	Acrylonitrile	beta-Mercaptoacetic acid	k(Thiolate)	M-1 min-1	1.62E+04		4.209515
935	107-13-1	Acrylonitrile	beta-Mercaptoacetic acid	k(Thiolate)	M-1 min-1	1.62E+00		0.21
936	96-33-3	Methyl acrylate	beta-Mercaptoacetic acid	k(Thiolate)	M-1 min-1	6.60E+04		4.819544
937	586-96-9	Nitrosobenzene	Cysteamine	k(Thiolate)	M-1 min-1	7.20E+05		5.86
938	370-86-5	Carbonyl cyanide p-trifluoromethoxyphenylhydrazone	Dithiothreitol	k(Thiolate)	M-1 min-1	2.46E+03		3.39
939	107-13-1	Acrylonitrile	Mercaptoacetic acid	k(Thiolate)	M-1 min-1	2.34E+00		0.37
940	555-60-2	Carbonyl cyanide m-chlorophenyl hydrazone	Mercaptoacetic acid	k(Thiolate)	M-1 min-1	3.28E+06		6.52
941	306-18-3	Carbonyl cyanide phenylhydrazone	Mercaptoacetic acid	k(Thiolate)	M-1 min-1	1.48E+06		6.17
942	370-86-5	Carbonyl cyanide p-trifluoromethoxyphenylhydrazone	Mercaptoacetic acid	k(Thiolate)	M-1 min-1	9.54E+04		4.98
943	370-86-5	Carbonyl cyanide p-trifluoromethoxyphenylhydrazone	Mercaptoacetic acid	k(Thiolate)	M-1 min-1	5.33E+06		6.73
944	586-96-9	Nitrosobenzene	Monothioglycerol	k(Thiolate)	M-1 min-1	1.00E+05		5.01
945	586-96-9	Nitrosobenzene	tert-Butylthiol	k(Thiolate)	M-1 min-1	2.40E+02		2.38
946	586-96-9	Nitrosobenzene	Thiophenol	k(Thiolate)	M-1 min-1	1.90E+03		3.28
947		1.1-Dinitro-2.2-diphenylethylene	Piperidine	k(Piperidine) | K | k-1	M-1 min-1	4.10E+02		2.61
948		2-(2.4-dinitrophenyl)-3-phenylprop-2-enenitrile	Piperidine	k(Piperidine) | K | k-1	M-1 min-1	3.68E+03		3.57
949		2-(Phenylmethylidene)propanedinitrile	Piperidine	k(Piperidine) | K | k-1	M-1 min-1			
950	3695-95-2	2-(p-Nitrophenyl)-3-phenylacrylonitrile	Piperidine	k(Piperidine) | K | k-1	M-1 min-1	1.60E+03		3.19
951	4335-90-4	3-Benzylidene acetylacetone	Piperidine	k(Piperidine) | K | k-1	M-1 min-1	4.90E+02		2.69
952	1215-07-2	alpha-Nitrostilbene	Piperidine	k(Piperidine) | K | k-1	M-1 min-1	7.02E+03		3.85
953	2700-22-3	Benzylidene malononitrile	Piperidine	k(Piperidine) | K | k-1	M-1 min-1	1.26E+07		7.1
954	2700-22-3	Benzylidene malononitrile	Piperidine	k(Piperidine) | K | k-1	M-1 min-1	4.21E+06		6.62
955		Benzylidene Meldrum's acid	Piperidine	k(Piperidine) | K | k-1	M-1 min-1	4.01E+07		7.6
956		Benzylidene Meldrum's acid	Piperidine	k(Piperidine) | K | k-1	M-1 min-1	1.62E+07		7.21
957	102-96-5	beta-Nitrostyrene	Piperidine	k(Piperidine) | K | k-1	M-1 min-1	6.84E+04		4.84
958	102-96-5	beta-Nitrostyrene	Piperidine	k(Piperidine) | K | k-1	M-1 min-1	3.97E+04		4.6
959	584-48-5	1-Bromo-2.4-dinitrobenzene	Piperidine	k(Piperidine)	M-1 min-1	1.16E+00		0.07
960	3466-32-8	1-Bromo-4-(methylsulphonyl)benzene	Piperidine	k(Piperidine)	M-1 min-1	2.10E-05		-4.68
961	97-00-7	1-Chloro-2.4-dinitrobenzene	Piperidine	k(Piperidine)	M-1 min-1	1.15E+00		0.06
962	97-00-7	1-Chloro-2.4-dinitrobenzene	Piperidine	k(Piperidine)	M-1 min-1	9.20E-01		-0.04
963	3623-15-2	1-Phenyl-2-propyn-1-one	Piperidine	k(Piperidine)	M-1 min-1	2514		3.4
964	99-90-1	4-Bromoacetophenone	Piperidine	k(Piperidine)	M-1 min-1	5.20E-06		-5.28
965	623-00-7	4-Bromobenzonitrile	Piperidine	k(Piperidine)	M-1 min-1	1.19E-05		-4.92
966	586-78-7	4-Bromonitrobenzene	Piperidine	k(Piperidine)	M-1 min-1	3.87E-04		-3.41
967	100-00-5	4-Chloronitrobenzene	Piperidine	k(Piperidine)	M-1 min-1	6.80E-05		-4.17
968	97-00-7	1-Chloro-2.4-dinitrobenzene	Phenolate. Sodium	k(Phenolate)	M-1 min-1	9.00E-01		-0.05
969	97-00-7	1-Chloro-2.4-dinitrobenzene	Phenolate. Sodium	k(Phenolate)	M-1 min-1	4.29E-01		-0.37
970	97-00-7	1-Chloro-2.4-dinitrobenzene	Phenolate. Sodium	k(Phenolate)	M-1 min-1	1.06E+00		0.03
971	97-00-7	1-Chloro-2.4-dinitrobenzene	Phenolate. Sodium	k(Phenolate)	M-1 min-1	9.70E-01		-0.01
972	97-00-7	1-Chloro-2.4-dinitrobenzene	Phenolate. Sodium	k(Phenolate)	M-1 min-1	1.98E+00		0.3

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
933	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
934	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
935	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
936	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
937	37	7.4				Eyer P, Biological Oxidation of Nitrogen in Orga... (1985), 386
938	25	7.5	Citrate/phosphate 0.1 M, 1% MeOH		25:1	Drobnica L et al., Biochim. Biophys. Acta 585 (1979), 462
939	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
940	25	6	Phthalate buffer 0.1 M, 1% MeOH		40:1	Drobnica L et al., Biochim. Biophys. Acta 585 (1979), 462
941	25	6.55	Phthalate buffer 0.1 M, 1% MeOH		40:1	Drobnica L et al., Biochim. Biophys. Acta 585 (1979), 462
942	25	7.5	Citrate/phosphate 0.1 M, 1% MeOH		25:1	Drobnica L et al., Biochim. Biophys. Acta 585 (1979), 462
943	25	5.8	Phthalate buffer 0.1 M, 1% MeOH		40:1	Drobnica L et al., Biochim. Biophys. Acta 585 (1979), 462
944	37	7.4				Eyer P, Biological Oxidation of Nitrogen in Orga... (1985), 386
945	37	7.4				Eyer P, Biological Oxidation of Nitrogen in Orga... (1985), 386
946	37	7.4				Eyer P, Biological Oxidation of Nitrogen in Orga... (1985), 386
947	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
948	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
949	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
950	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
951	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
952	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
953	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
954	20		Water			Bernasconi CF, Tetrahedron 45 (1989), 4017
955	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
956	20		Water			Bernasconi CF, Tetrahedron 45 (1989), 4017
957	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
958	20		Water			Bernasconi CF, Tetrahedron 45 (1989), 4017
959	25					Bunnet JF et al., Chem. Rev. 49 (1951), 273
960	99		Benzene			Bunnet JF et al., Chem. Rev. 49 (1951), 273
961	25					Bunnet JF et al., Chem. Rev. 49 (1951), 273
962	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
963	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., Bull. Korean Chem. Soc. 29 (2008), 767
964	99		Benzene			Bunnet JF et al., Chem. Rev. 49 (1951), 273
965	99		Benzene			Bunnet JF et al., Chem. Rev. 49 (1951), 273
966	99		Benzene			Bunnet JF et al., Chem. Rev. 49 (1951), 273
967	99		Benzene			Bunnet JF et al., Chem. Rev. 49 (1951), 273
968	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
969	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
970	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
971	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
972	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273

#	Comment
933	Titration.
934	Titration.
935	Titration.
936	Titration.
937	
938	UV(200-800 nm); reactive: non-diss. CCP + RS[-] (pH < pKa).
939	Titration.
940	UV(200-800 nm); reactive: non-diss. CCP + RS[-] (pH < pKa).
941	UV(200-800 nm); reactive: non-diss. CCP + RS[-] (pH < pKa).
942	UV(200-800 nm); reactive: non-diss. CCP + RS[-] (pH < pKa).
943	UV(200-800 nm); reactive: non-diss. CCP + RS[-] (pH < pKa).
944	
945	
946	
947	K 6.80E-02 | k-1 6.00E+03 | pKa 6.22. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
948	K 1.29E-02 | k-1 2.84E+05 | pKa 8.13. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
949	K 1.55E+01. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
950	K 3.57E-04 | k-1 4.72E+06 | pKa 8.67. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
951	K 5.47E+01 | k-1 9.0E+00 | pKa 13.5. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
952	K 4.50E+01 | k-1 1.6E+02 | pKa 9.73. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
953	K 1.54E+01 | k-1 8.16E+05 | pKa 10.28. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
954	K 4.50E+00 | k-1 9.36E+05 | pKa 10.92. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
955	K 1.35E+07 | k-1 2.96E+00. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
956	K 2.08E+07 | k-1 7.80E-01 | pKa 11.64. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
957	K 3.18E+01 | k-1 2.2E+03 | pKa 8.3. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
958	K 7.90E+02 | k-1 5.0E+01 | pKa 8.44. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
959	
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963	UV(max. abs. enaminone) and 1H-NMR.
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969	
970	Nu: 2-Cresolate, sodium.
971	Nu: 3-Cresolate, sodium.
972	Nu: 4-Cresolate, sodium.

#	Mechanism
933	Michael-type nucleophilic addition
934	Michael-type nucleophilic addition
935	Michael-type nucleophilic addition
936	Michael-type nucleophilic addition
937	
938	Nucleophilic olefinic addition
939	Michael-type nucleophilic addition
940	Nucleophilic olefinic addition
941	Nucleophilic olefinic addition
942	Nucleophilic olefinic addition
943	Nucleophilic olefinic addition
944	
945	
946	
947	Nucleophilic olefinic addition
948	Nucleophilic olefinic addition
949	Nucleophilic olefinic addition
950	Nucleophilic olefinic addition
951	Nucleophilic olefinic addition
952	Nucleophilic olefinic addition
953	NOT Nucleophilic olefinic addition: formation of aldehyde
954	Nucleophilic olefinic addition
955	Nucleophilic olefinic addition
956	Nucleophilic olefinic addition
957	Nucleophilic olefinic addition
958	Nucleophilic olefinic addition
959	Nucleophilic aromatic substitution (SNAr)
960	Nucleophilic aromatic substitution (SNAr)
961	Nucleophilic aromatic substitution (SNAr)
962	Nucleophilic aromatic substitution (SNAr)
963	Michael-type nucleophilic addition
964	Nucleophilic aromatic substitution (SNAr)
965	Nucleophilic aromatic substitution (SNAr)
966	Nucleophilic aromatic substitution (SNAr)
967	Nucleophilic aromatic substitution (SNAr)
968	
969	
970	
971	
972	

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
973	591-12-8	alpha-Angelicalactone	4-Nitrobenzylpyridine	k(NBP)	M-1 min-1	360000	6000	5.56
974	3068-88-0	beta-Butyrolactone	4-Nitrobenzylpyridine	k(NBP)	M-1 min-1	0.04	0.002	-1.4
975	57-57-8	beta-Propiolactone	4-Nitrobenzylpyridine	k(NBP)	M-1 min-1	0.47	0.04	-0.33
976	542-28-9	delta-Valerolactone	4-Nitrobenzylpyridine	k(NBP)	M-1 min-1	NR		
977	674-82-8	Diketene	4-Nitrobenzylpyridine	k(NBP)	M-1 min-1	3.66		0.56
978	150-13-0	p-Aminobenzoic acid	4-Nitrobenzylpyridine	k(NBP)	M-1 min-1	NR		
979		1.1-Dinitro-2.2-diphenylethylene	Morpholine	k(Morpholine) | K | k-1	M-1 min-1	5.70E+01		1.76
980		2-(2.4-dinitrophenyl)-3-phenylprop-2-enenitrile	Morpholine	k(Morpholine) | K | k-1	M-1 min-1	3.82E+02		2.58
981	3695-95-2	2-(p-Nitrophenyl)-3-phenylacrylonitrile	Morpholine	k(Morpholine) | K | k-1	M-1 min-1	6.60E+01		1.82
982	4335-90-4	3-Benzylidene acetylacetone	Morpholine	k(Morpholine) | K | k-1	M-1 min-1	1.07E+02		2.03
983	1215-07-2	alpha-Nitrostilbene	Morpholine	k(Morpholine) | K | k-1	M-1 min-1	1.06E+03		3.02
984	2700-22-3	Benzylidene malononitrile	Morpholine	k(Morpholine) | K | k-1	M-1 min-1	7.32E+05		5.86
985	2700-22-3	Benzylidene malononitrile	Morpholine	k(Morpholine) | K | k-1	M-1 min-1	3.54E+06		6.55
986		Benzylidene Meldrum's acid	Morpholine	k(Morpholine) | K | k-1	M-1 min-1	1.91E+07		7.28
987		Benzylidene Meldrum's acid	Morpholine	k(Morpholine) | K | k-1	M-1 min-1	1.05E+07		7.02
988	102-96-5	beta-Nitrostyrene	Morpholine	k(Morpholine) | K | k-1	M-1 min-1	1.30E+04		4.11
989	102-96-5	beta-Nitrostyrene	Morpholine	k(Morpholine) | K | k-1	M-1 min-1	8.22E+03		3.91
990		1-(3-Nitrophenyl)-2-propyn-1-one	Morpholine	k(Morpholine)	M-1 min-1	2070		3.32
991		1-(4-Chlorophenyl)-2-propyn-1-one	Morpholine	k(Morpholine)	M-1 min-1	864		2.94
992		1-(4-Cyanophenyl)-2-propyn-1-one	Morpholine	k(Morpholine)	M-1 min-1	1884		3.28
993	16469-68-4	1-(4-Methoxyphenyl)-2-propyn-1-one	Morpholine	k(Morpholine)	M-1 min-1	278.4		2.44
994		1-(4-Methylphenyl)-2-propyn-1-one	Morpholine	k(Morpholine)	M-1 min-1	515.4		2.71
995	3623-15-2	1-Phenyl-2-propyn-1-one	Morpholine	k(Morpholine)	M-1 min-1	690		2.84
996		1.2.3-Trichloro-4.5-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	2.35E+00		0.37
997	6379-46-0	1.2.3-Trichloro-4.6-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	3.30E+00		0.52
998	17700-09-3	1.2.3-Trichloro-4-nitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	1.91E-03		-2.72
999	17700-09-3	1.2.3-Trichloro-4-nitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	8.30E-03		-2.08
1000	20098-48-0	1.2.3-Trichloro-5-nitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	8.14E-03		-2.09
1001	20098-48-0	1.2.3-Trichloro-5-nitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	2.46E-02		-1.61
1002	95-94-3	1.2.4.5-Tetrachlorobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	NR		
1003	2678-21-9	1.2.4-Trichloro-3.5-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	3.20E-01		-0.49
1004		1.2.4-Trichloro-3.6-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	8.00E-01		-0.1
1005		1.2.4-Trichloro-3-nitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	4.70E-05		-4.33
1006		1.2.4-Trichloro-3-nitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	1.57E-04		-3.8
1007	89-69-0	1.2.4-Trichloro-5-nitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	7.29E-03		-2.14
1008	89-69-0	1.2.4-Trichloro-5-nitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	2.31E-02		-1.64
1009	120-82-1	1.2.4-Trichlorobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	NR		
1010	610-31-1	1.2.4-Trinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	very great		

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
973	25		Dioxane:water 3:7	20 min - 3d	10:1	Fernández-Rodríguez, E et al., Int. J. Chem. Kinet. 39 (2007), 591
974	25		Dioxane:water 3:7	20 min - 3d	1:180	Manso JA et al., Chem. Res. Toxicol. 18 (2005), 1161
975	25		Dioxane:water 3:7	20 min - 3d	1:180	Manso JA et al., Chem. Res. Toxicol. 18 (2005), 1161
976	35		Dioxane:water 3:7	20 min - 3d	10:1	Manso JA et al., Chem. Res. Toxicol. 18 (2005), 1161
977	25		Dioxane:water 3:7	20 min - 3d	10:1	Gómez-Bombarelli R et al., Chem. Res. Toxicol. 21 (2008), 1964
978	35		Dioxane:water 3:7	20 min - 3d	10:1	Manso JA et al., Chem. Res. Toxicol. 18 (2005), 1161
979	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
980	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
981	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
982	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
983	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
984	20		Water			Bernasconi CF, Tetrahedron 45 (1989), 4017
985	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
986	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
987	20		Water			Bernasconi CF, Tetrahedron 45 (1989), 4017
988	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
989	20		Water			Bernasconi CF, Tetrahedron 45 (1989), 4017
990	25		Self-buffered (NH3*HCl+NaOH)		20:1 (>)	Um I-H et al., Bull. Korean Chem. Soc. 29 (2008), 767
991	25		Self-buffered (NH3*HCl+NaOH)		20:1 (>)	Um I-H et al., Bull. Korean Chem. Soc. 29 (2008), 767
992	25		Self-buffered (NH3*HCl+NaOH)		20:1 (>)	Um I-H et al., Bull. Korean Chem. Soc. 29 (2008), 767
993	25		Self-buffered (NH3*HCl+NaOH)		20:1 (>)	Um I-H et al., Bull. Korean Chem. Soc. 29 (2008), 767
994	25		Self-buffered (NH3*HCl+NaOH)		20:1 (>)	Um I-H et al., Bull. Korean Chem. Soc. 29 (2008), 767
995	25		Self-buffered (NH3*HCl+NaOH)		20:1 (>)	Um I-H et al., Bull. Korean Chem. Soc. 29 (2008), 767
996	0		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
997	0		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
998	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
999	35		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1000	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1001	35		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1002	0		Methanol			Landsteiner et al., J. Exp. Med. 64 (1936), 625
1003	0		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1004	0		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1005	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1006	35		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1007	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1008	35		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1009	0		Methanol			Landsteiner et al., J. Exp. Med. 64 (1936), 625
1010	0		Methanol			Landsteiner et al., J. Exp. Med. 64 (1936), 625

#	Comment
973	Assay: UV(max abs. 450-590 nm); solvent ratios from 3:7 to 7:1 and T from 15C to 35C in paper
974	Assay: UV(max abs. 450-590 nm); solvent ratios from 3:7 to 7:1 and T from 15C to 35C in paper
975	Assay: UV(max abs. 450-590 nm); solvent ratios from 3:7 to 7:1 and T from 15C to 35C in paper
976	no reaction. Assay: UV(max abs. 450-590 nm); solvent ratios from 3:7 to 7:1 and T from 15C to 35C in paper
977	Assay: UV(max abs. 450-590 nm); solvent ratios from 3:7 to 7:1 and T from 15C to 35C in paper
978	no reaction. Assay: UV(max abs. 450-590 nm); solvent ratios from 3:7 to 7:1 and T from 15C to 35C in paper
979	K 4.E-04 | k-1 1.4E+05 | pKa 3.94. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa; pKa0: reprotonatior
980	K 9.5E-05 | k-1 4.00E+06 | pKa 5.83. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa; pKa0: reprotonation
981	K 1.36E-06 | k-1 4.87E+07 | pKa 6.37. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa; pKa0: reprotonatior
982	K 0.64 | k-1 1.67E+02 | pKa 11.26. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa; pKa0: reprotonatior
983	K 0.34 | k-1 3.1E+03 | pKa 7.26. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa; pKa0: reprotonatior K 2.86E-02 | k-1 2.56E+07 | pKa 8.29 | reproton. pKa0 8.86.
984	Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa; pKa0: reprotonation K 0.23 | k-1 1.56E+07 | pKa 8 | reproton. pKa0 8.43.
985	Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa; pKa0: reprotonation
986	K 7.76E+04 | k-1 2.47E+02. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa; pKa0: reprotonatior
987	K 8.80E+04 | k-1 1.19E+02 | pKa 8.90. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa; pKa0: reprotonatior
988	K 0.22 | k-1 6.0E+04 | pKa 6.15. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa; pKa0: reprotonatior
989	K 1.44 | k-1 5.70E+03 | pKa 5.87. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa; pKa0: reprotonatior
990	Assay: UV(max. abs. enaminone) and 1H-NMR
991	Assay: UV(max. abs. enaminone) and 1H-NMR
992	Assay: UV(max. abs. enaminone) and 1H-NMR
993	Assay: UV(max. abs. enaminone) and 1H-NMR
994	Assay: UV(max. abs. enaminone) and 1H-NMR
995	Assay: UV(max. abs. enaminone) and 1H-NMR
996	
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1003	
1004	
1005	
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1007	
1008	
1009	
1010	

#	Mechanism
	Nucleophilic heterocycle ring opening:
973	entropy strain-catalysed, early lactone ring cleavage
974	Nucleophilic heterocycle ring opening
975	Nucleophilic heterocycle ring opening
976	NOT Nucleophilic heterocycle ring opening
	Acyl transfer and carboxylate aminolysis:
977	acyl fission in contrast to other lactones: low energy barrier fast hydrolysis
978	NOT Nucleophilic heterocycle ring opening
979	Nucleophilic olefinic addition: deprotonation partially rate limiting
980	Nucleophilic olefinic addition
981	Nucleophilic olefinic addition: deprotonation partially rate limiting: low I
982	Nucleophilic olefinic addition
983	Nucleophilic olefinic addition
984	Nucleophilic olefinic addition
985	Nucleophilic olefinic addition: pKa partially rate limiting: low intrinsic barrier
986	Nucleophilic olefinic addition
987	Nucleophilic olefinic addition
988	Nucleophilic olefinic addition
989	Nucleophilic olefinic addition
990	Michael-type nucleophilic addition
991	Michael-type nucleophilic addition
992	Michael-type nucleophilic addition
993	Michael-type nucleophilic addition
994	Michael-type nucleophilic addition
995	Michael-type nucleophilic addition
996	Nucleophilic aromatic substitution (SNAr)
997	Nucleophilic aromatic substitution (SNAr)
998	Nucleophilic aromatic substitution (SNAr)
999	Nucleophilic aromatic substitution (SNAr)
1000	Nucleophilic aromatic substitution (SNAr)
1001	Nucleophilic aromatic substitution (SNAr)
1002	
1003	Nucleophilic aromatic substitution (SNAr)
1004	Nucleophilic aromatic substitution (SNAr)
1005	Nucleophilic aromatic substitution (SNAr)
1006	Nucleophilic aromatic substitution (SNAr)
1007	Nucleophilic aromatic substitution (SNAr)
1008	Nucleophilic aromatic substitution (SNAr)
1009	
1010	

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1011		1.2.5-Trichloro-3.4-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	6.75E-01		-0.17
1012		1.2.5-Trichloro-3-nitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	8.30E-04		-3.08
1013		1.2.5-Trichloro-3-nitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	2.63E-03		-2.58
1014		1.2-Dichloro-3.5-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	4.10E-01		-0.39
1015	6306-39-4	1.2-Dichloro-4.5-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	3.60E-01		-0.44
1016	6306-39-4	1.2-Dichloro-4.5-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	3.26E-01		-0.49
1017	99-54-7	1.2-Dichloro-4-nitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	5.50E-04		-3.26
1018	99-54-7	1.2-Dichloro-4-nitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	2.90E-01		-0.54
1019	99-54-7	1.2-Dichloro-4-nitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	1.83E-05		-4.74
1020	95-50-1	1.2-Dichlorobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	6.40E-04		-3.19
1021	528-29-0	1.2-Dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	8.50E-03		-2.07
1022	528-29-0	1.2-Dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	6.95E-02		-1.16
1023	6284-83-9	1.3.5-Trichloro-2.4-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	6.10E-02		-1.21
1024	18708-70-8	1.3.5-Trichloro-2-nitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	1.89E-04		-3.72
1025	99-35-4	1.3.5-Trinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	1.57E+00		0.2
1026	13633-34-6	1.3-Dichloro-2.5-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	1.45E-01		-0.84
1027	601-88-7	1.3-Dichloro-2-nitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	2.30E-03		-2.64
1028	618-62-2	1.3-Dichloro-5-nitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	ND		
1029	541-73-1	1.3-Dichlorobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	8.40E-04		-3.08
1030		1.4-Dichloro-2.3-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	2.61E-02		-1.58
1031		1.4-Dichloro-2.5-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	6.91E-01		-0.16
1032	2213-82-3	1.4-Dichloro-2.6-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	2.48E-02		-1.61
1033	89-61-2	1.4-Dichloro-2-nitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	1.05E-04		-3.98
1034	89-61-2	1.4-Dichloro-2-nitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	6.50E-02		-1.19
1035	89-61-2	1.4-Dichloro-2-nitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	5.50E-01		-0.26
1036	89-61-2	1.4-Dichloro-2-nitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	2.97E-06		-5.53
1037	106-46-7	1.4-Dichlorobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	1.90E-04		-3.72
1038	100-25-4	1.4-Dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	2.22E-02		-1.65
1039	100-25-4	1.4-Dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	2.38E-01		-0.62
1040	584-48-5	1-Bromo-2.4-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	1.12E+00		0.05
1041	584-48-5	1-Bromo-2.4-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	4.05E-01		-0.39
1042	88-88-0	1-Chloro-2.4.6-trinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	very great		
1043	97-00-7	1-Chloro-2.4-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	1.51E+00		0.18
1044	97-00-7	1-Chloro-2.4-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	1.11E-01		-0.95
1045	2401-85-6	1-Chloro-2.4-dinitronaphthalene	Methylate. Sodium	k(Methylate)	M-1 min-1	2.00E+01		1.3
1046	2401-85-6	1-Chloro-2.4-dinitronaphthalene	Methylate. Sodium	k(Methylate)	M-1 min-1	8.4		0.92
1047	610-40-2	1-Chloro-3.4-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	4.37E-01		-0.36
1048	610-40-2	1-Chloro-3.4-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	3.31E-02		-1.48
1049	70-34-8	1-Fluoro-2.4-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	6.86E+02		2.84
1050		2.3-Dichloro-1.5-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	4.09E-01		-0.39
1051	3209-22-1	2.3-Dichloronitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	3.00E-02		-1.52
1052	3209-22-1	2.3-Dichloronitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	2.40E-01		-0.62
1053		2.4-Dichloro-1.3-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	2.13E-02		-1.67

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1011	0		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1012	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1013	35		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1014	0		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1015	0		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1016	0		Methanol			Landsteiner et al., J. Exp. Med. 64 (1936), 625
1017	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1018	85		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1019	0		Methanol			Landsteiner et al., J. Exp. Med. 64 (1936), 625
1020	175		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1021	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1022	45		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1023	0		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1024	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1025	0		Methanol			Landsteiner et al., J. Exp. Med. 64 (1936), 625
1026	0		Methanol			Landsteiner et al., J. Exp. Med. 64 (1936), 625
1027	85		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1028	0		Methanol			Landsteiner et al., J. Exp. Med. 64 (1936), 625
1029	175		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1030	0		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1031	0		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1032	0		Methanol			Landsteiner et al., J. Exp. Med. 64 (1936), 625
1033	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1034	85		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1035	110		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1036	0		Methanol			Landsteiner et al., J. Exp. Med. 64 (1936), 625
1037	175		Methanol			Landsteiner et al., J. Exp. Med. 64 (1936), 625
1038	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1039	45		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1040	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1041	15		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1042	0		Methanol			Landsteiner et al., J. Exp. Med. 64 (1936), 625
1043	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1044	0		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1045	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1046	15		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1047	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1048	0		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1049	15		Methanol			Landsteiner et al., J. Exp. Med. 64 (1936), 625
1050	0		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1051	85		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1052	110		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1053	0		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273

#	Comment
1011	
1012	
1013	
1014	
1015	per nitro group: 1.8E-01.
1016	
1017	
1018	
1019	
1020	
1021	per nitro group: 4.2E-3.
1022	
1023	per chlorine atom: 3.0E-02.
1024	per chlorine atom: 9.5E-05.
1025	
1026	
1027	per chlorine atom: 1.2E-3.
1028	reaction irregular.
1029	
1030	per nitro group: 1.31E-02.
1031	per nitro group: 3.46E-01.
1032	
1033	
1034	
1035	
1036	
1037	
1038	per nitro group: 1.11E-02.
1039	
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#	Mechanism
1011	Nucleophilic aromatic substitution (SNAr)
1012	Nucleophilic aromatic substitution (SNAr)
1013	Nucleophilic aromatic substitution (SNAr)
1014	Nucleophilic aromatic substitution (SNAr)
1015	Nucleophilic aromatic substitution (SNAr)
1016	
1017	Nucleophilic aromatic substitution (SNAr)
1018	Nucleophilic aromatic substitution (SNAr)
1019	
1020	Nucleophilic aromatic substitution (SNAr)
1021	Nucleophilic aromatic substitution (SNAr)
1022	Nucleophilic aromatic substitution (SNAr)
1023	Nucleophilic aromatic substitution (SNAr)
1024	Nucleophilic aromatic substitution (SNAr)
1025	
1026	
1027	Nucleophilic aromatic substitution (SNAr)
1028	
1029	Nucleophilic aromatic substitution (SNAr)
1030	Nucleophilic aromatic substitution (SNAr)
1031	Nucleophilic aromatic substitution (SNAr)
1032	
1033	Nucleophilic aromatic substitution (SNAr)
1034	Nucleophilic aromatic substitution (SNAr)
1035	Nucleophilic aromatic substitution (SNAr)
1036	
1037	
1038	Nucleophilic aromatic substitution (SNAr)
1039	Nucleophilic aromatic substitution (SNAr)
1040	Nucleophilic aromatic substitution (SNAr)
1041	Nucleophilic aromatic substitution (SNAr)
1042	
1043	Nucleophilic aromatic substitution (SNAr)
1044	Nucleophilic aromatic substitution (SNAr)
1045	Nucleophilic aromatic substitution (SNAr)
1046	Nucleophilic aromatic substitution (SNAr)
1047	Nucleophilic aromatic substitution (SNAr)
1048	Nucleophilic aromatic substitution (SNAr)
1049	
1050	Nucleophilic aromatic substitution (SNAr)
1051	Nucleophilic aromatic substitution (SNAr)
1052	Nucleophilic aromatic substitution (SNAr)
1053	Nucleophilic aromatic substitution (SNAr)

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1054	3698-83-7	2.4-Dichloro-1.5-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	1.20E+00		0.08
1055	611-06-3	2.4-Dichloronitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	5.00E-04		-3.3
1056	611-06-3	2.4-Dichloronitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	1.05E-02		-1.98
1057		2.4-Dinitro-5-methoxychlorobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	4.70E-01		-0.33
1058		2.4-Dinitro-5-methoxychlorobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	3.70E-02		-1.43
1059		2.4-Dinitro-5-methoxychlorobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	2.00E-01		-0.7
1060		2.4-Dinitro-5-methoxychlorobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	3.00E-01		-0.52
1061		2-Bromo-1.6.8-trinitronaphthalene	Methylate. Sodium	k(Methylate)	M-1 min-1	1.00E+01		1
1062		2-Bromo-1.6.8-trinitronaphthalene	Methylate. Sodium	k(Methylate)	M-1 min-1	1.2		0.08
1063		2-Bromo-5-nitrobenzonitrile	Methylate. Sodium	k(Methylate)	M-1 min-1	2.05E-01		-0.69
1064		2-Bromo-5-nitrobenzonitrile	Methylate. Sodium	k(Methylate)	M-1 min-1	6.35E-01		-0.2
1065	606-21-3	2-Chloro-1.3-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	4.60E-02		-1.34
1066	606-21-3	2-Chloro-1.3-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	2.89E-03		-2.54
1067	619-16-9	2-Chloro-1.4-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	5.59E-01		-0.25
1068	619-16-9	2-Chloro-1.4-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	3.18E-02		-1.5
1069		2-Chloro-1.6.8-trinitronaphthalene	Methylate. Sodium	k(Methylate)	M-1 min-1	3.70E+01		1.57
1070		2-Chloro-1.6.8-trinitronaphthalene	Methylate. Sodium	k(Methylate)	M-1 min-1	2.2		0.34
1071	16588-02-6	2-Chloro-5-nitrobenzonitrile	Methylate. Sodium	k(Methylate)	M-1 min-1	2.60E-01		-0.59
1072	16588-02-6	2-Chloro-5-nitrobenzonitrile	Methylate. Sodium	k(Methylate)	M-1 min-1	8.24E-01		-0.08
1073	88-73-3	2-Chloronitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	9.00E-06		-5.05
1074	88-73-3	2-Chloronitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	6.20E-03		-2.21
1075		2-Fluoronitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	7.00E-03		-2.15
1076	27811-88-7	3.4.5-Trichloro-1.2-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	2.35E+00		0.37
1077		3.4-Dichloro-1.2-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	3.33E-01		-0.48
1078	28689-08-9	3.5-Dichloro-1.2-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	1.28E-01		-0.89
1079	25567-67-3	3-Chloro-1.2-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	1.00E-01		-1
1080	25567-67-3	3-Chloro-1.2-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	7.45E-03		-2.13
1081	99-65-0	3-Dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	ND		
1082	97-07-4	3-Nitro-4-chlorophenyl methyl sulfone	Methylate. Sodium	k(Methylate)	M-1 min-1	1.59E-01		-0.8
1083		4.5-Dimethoxy-1.2-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	2.90E-03		-2.54
1084		4.5-Dimethoxy-1.2-dinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	8.80E-03		-2.06
1085		4-Bromo-3-nitrobenzonitrile	Methylate. Sodium	k(Methylate)	M-1 min-1	1.02E-02		-1.99
1086	28260-61-9	4-Chloro-1.2.3-trinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	1.07E+01		1.03
1087	5465-65-6	4'-Chloro-3'-nitroacetophenone	Methylate. Sodium	k(Methylate)	M-1 min-1	1.87E-02		-1.73
1088	939-80-0	4-Chloro-3-nitrobenzonitrile	Methylate. Sodium	k(Methylate)	M-1 min-1	1.42E-02		-1.85
1089		4-Chloro-N.N.N-trimethyl-3-nitroanilinium salt	Methylate. Sodium	k(Methylate)	M-1 min-1	5.00E-02		-1.3
1090	100-00-5	4-Chloronitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	2.31E-02		-1.64
1091	100-00-5	4-Chloronitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	9.87E-07		-6.01
1092	28260-61-9	5-Chloro-1.2.3-trinitrobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	7.50E+00		0.88
1093		5-Chloro-2.4-dinitroanisole	Methylate. Sodium	k(Methylate)	M-1 min-1	3.70E-02		-1.43
1094	118-74-1	Hexachlorobenzene	Methylate. Sodium	k(Methylate)	M-1 min-1	NR		
1095	107-13-1	Acrylonitrile	DL-alpha-Methylmethionine	k(Met): Met-Derivatives	M-1 min-1	7.68E+04		4.89

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1054	0		Methanol			Landsteiner et al., J. Exp. Med. 64 (1936), 625
1055	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1056	50		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1057	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1058	0		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1059	15		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1060	20		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1061	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1062	0		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1063	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1064	35		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1065	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1066	0		Methanol			Landsteiner et al., J. Exp. Med. 64 (1936), 625
1067	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1068	0		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1069	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1070	0		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1071	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1072	35		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1073	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1074	85		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1075	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1076	0		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1077	0		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1078	0		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1079	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1080	0		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1081	0		Methanol			Landsteiner et al., J. Exp. Med. 64 (1936), 625
1082	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1083	35		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1084	45		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1085	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1086	0		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1087	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1088	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1089	25		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1090	85		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1091	0		Methanol			Landsteiner et al., J. Exp. Med. 64 (1936), 625
1092	0		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1093	0		Methanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1094	175		Methanol			Landsteiner et al., J. Exp. Med. 64 (1936), 625
1095	30	8.4				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672

#	Comment
1054	per chlorine atom: 0.6E-01.
1055	
1056	
1057	
1058	
1059	
1060	
1061	
1062	
1063	in eqilibrium with imino esters.
1064	
1065	
1066	
1067	
1068	
1069	
1070	
1071	in eqilibrium with imino esters.
1072	
1073	calc. based on 85C.
1074	
1075	
1076	
1077	
1078	
1079	
1080	
1081	reaction irregular.
1082	
1083	per nitro group: 1.5E-03.
1084	
1085	in eqilibrium with imino esters.
1086	
1087	
1088	in eqilibrium with imino esters.
1089	
1090	
1091	
1092	
1093	
1094	
1095	

#	Mechanism
1054	
1055	Nucleophilic aromatic substitution (SNAr)
1056	Nucleophilic aromatic substitution (SNAr)
1057	Nucleophilic aromatic substitution (SNAr)
1058	Nucleophilic aromatic substitution (SNAr)
1059	Nucleophilic aromatic substitution (SNAr)
1060	Nucleophilic aromatic substitution (SNAr)
1061	Nucleophilic aromatic substitution (SNAr)
1062	Nucleophilic aromatic substitution (SNAr)
1063	Nucleophilic aromatic substitution (SNAr)
1064	Nucleophilic aromatic substitution (SNAr)
1065	Nucleophilic aromatic substitution (SNAr)
1066	
1067	Nucleophilic aromatic substitution (SNAr)
1068	Nucleophilic aromatic substitution (SNAr)
1069	Nucleophilic aromatic substitution (SNAr)
1070	Nucleophilic aromatic substitution (SNAr)
1071	Nucleophilic aromatic substitution (SNAr)
1072	Nucleophilic aromatic substitution (SNAr)
1073	Nucleophilic aromatic substitution (SNAr)
1074	Nucleophilic aromatic substitution (SNAr)
1075	Nucleophilic aromatic substitution (SNAr)
1076	Nucleophilic aromatic substitution (SNAr)
1077	Nucleophilic aromatic substitution (SNAr)
1078	Nucleophilic aromatic substitution (SNAr)
1079	Nucleophilic aromatic substitution (SNAr)
1080	Nucleophilic aromatic substitution (SNAr)
1081	
1082	Nucleophilic aromatic substitution (SNAr)
1083	Nucleophilic aromatic substitution (SNAr)
1084	Nucleophilic aromatic substitution (SNAr)
1085	Nucleophilic aromatic substitution (SNAr)
1086	Nucleophilic aromatic substitution (SNAr)
1087	Nucleophilic aromatic substitution (SNAr)
1088	Nucleophilic aromatic substitution (SNAr)
1089	Nucleophilic aromatic substitution (SNAr)
1090	Nucleophilic aromatic substitution (SNAr)
1091	
1092	Nucleophilic aromatic substitution (SNAr)
1093	Nucleophilic aromatic substitution (SNAr)
1094	
1095	Michael-type nucleophilic addition

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1096	107-13-1	Acrylonitrile	DL-Methionine	k(Met): Met-Derivatives	M-1 min-1	1.82E+06		6.26
1097	107-13-1	Acrylonitrile	L-Methionyl-L-methionine	k(Met): Met-Derivatives	M-1 min-1	2.00E+06		6.3
1098	123-73-9	(E)-Crotonaldehyde	4-Dimethylaminopyridine	k'(Me2NPyr) | k''(H-Add)	M-1 min-1 (M-1)	0.5	0.1	-0.32
1099	21351-43-9	1-Methyl-4-vinylpyridinium cation (iodide)	4-Dimethylaminopyridine	k'(Me2NPyr) | k''(H-Add)	M-1 min-1 (M-1)	3.1	0.1	0.49
1100	100-13-0	4-Nitrostyrene	4-Dimethylaminopyridine	k'(Me2NPyr) | k''(H-Add)	M-1 min-1 (M-1)	NR		
1101	107-02-8	Acrolein	4-Dimethylaminopyridine	k'(Me2NPyr) | k''(H-Add)	M-1 min-1 (M-1)	143	5	2.16
1102	79-06-1	Acrylamide	4-Dimethylaminopyridine	k'(Me2NPyr) | k''(H-Add)	M-1 min-1 (M-1)	0.037	0.001	-1.44
1103	107-13-1	Acrylonitrile	4-Dimethylaminopyridine	k'(Me2NPyr) | k''(H-Add)	M-1 min-1 (M-1)	0.242	0.002	-0.62
1104	78-85-3	Methacrolein	4-Dimethylaminopyridine	k'(Me2NPyr) | k''(H-Add)	M-1 min-1 (M-1)	1.1	0.2	0.03
1105	96-33-3	Methyl acrylate	4-Dimethylaminopyridine	k'(Me2NPyr) | k''(H-Add)	M-1 min-1 (M-1)	0.876	0.024	-0.06
1106	78-94-4	Methyl vinyl ketone	4-Dimethylaminopyridine	k'(Me2NPyr) | k''(H-Add)	M-1 min-1 (M-1)	33	1	1.52
1107	3680-02-2	Methyl vinyl sulfone	4-Dimethylaminopyridine	k'(Me2NPyr) | k''(H-Add)	M-1 min-1 (M-1)	4.95	0.05	0.69
1108	2680-03-7	N.N-Dimethylacrylamide	4-Dimethylaminopyridine	k'(Me2NPyr) | k''(H-Add)	M-1 min-1 (M-1)	0.0109	0.0002	-1.96
1109	4436-24-2	(2.3-Epoxypropyl)benzene	2'-Deoxyguanosine	k(GUA)	M-1 min-1			-2.09
1110	6388-74-5	(4-Nitrophenyl)oxirane	2'-Deoxyguanosine	k(GUA)	M-1 min-1			-1.89
1111	106-88-7	1.2-Epoxybutane	2'-Deoxyguanosine	k(GUA)	M-1 min-1			-3.02
1112	78-88-6	2.3-Dichloro-1-propene	2'-Deoxyguanosine	k(GUA)	M-1 min-1			-1.38
1113	1838-94-4	2-Methyl-2-vinyloxirane	2'-Deoxyguanosine	k(GUA)	M-1 min-1	NR		
1114	100-14-1	4-Nitrobenzylchloride	2'-Deoxyguanosine	k(GUA)	M-1 min-1	NR		
1115	100-44-7	Benzyl chloride	2'-Deoxyguanosine	k(GUA)	M-1 min-1	SN1		
1116	106-89-8	Epichlorohydrin	2'-Deoxyguanosine	k(GUA)	M-1 min-1			-2.3
1117	96-09-3	Styrene oxide	2'-Deoxyguanosine	k(GUA)	M-1 min-1			-2.15
1118	123-73-9	(E)-Crotonaldehyde	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	4.71E+01	5-10%	1.67
1119	123-73-9	(E)-Crotonaldehyde	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	1.60E+01		1.21
1120	123-73-9	(E)-Crotonaldehyde	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	7.50E+01		1.88
1121	123-73-9	(E)-Crotonaldehyde	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	5.00E+01		1.7
1122	123-73-9	(E)-Crotonaldehyde	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	3.20E+01		1.5
1123	123-73-9	(E)-Crotonaldehyde	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	4.00E+01		1.6
1124	123-73-9	(E)-Crotonaldehyde	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	1.50E+01		1.18
1125	123-73-9	(E)-Crotonaldehyde	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	1.60E+01		1.21
1126	123-73-9	(E)-Crotonaldehyde	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	2.90E+01		1.46

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1096	30	8.4				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1097	30	8.4				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1098	25		Aqueous solution		(different)	Heo CKM et al., J. Org. Chem. 57 (1992), 3570
1099	25		Aqueous solution		(different)	Heo CKM et al., J. Org. Chem. 57 (1992), 3570
1100	25		Aqueous solution		(different)	Heo CKM et al., J. Org. Chem. 57 (1992), 3570
1101	25		Aqueous solution		(different)	Heo CKM et al., J. Org. Chem. 57 (1992), 3570
1102	25		Aqueous solution		(different)	Heo CKM et al., J. Org. Chem. 57 (1992), 3570
1103	25		Aqueous solution		(different)	Heo CKM et al., J. Org. Chem. 57 (1992), 3570
1104	25		Aqueous solution		(different)	Heo CKM et al., J. Org. Chem. 57 (1992), 3570
1105	25		Aqueous solution		(different)	Heo CKM et al., J. Org. Chem. 57 (1992), 3570
1106	25		Aqueous solution		(different)	Heo CKM et al., J. Org. Chem. 57 (1992), 3570
1107	25		Aqueous solution		(different)	Heo CKM et al., J. Org. Chem. 57 (1992), 3570
1108	25		Aqueous solution		(different)	Heo CKM et al., J. Org. Chem. 57 (1992), 3570
1109	30	7.65	PBS 15 mM		1:50 - 1:200	Harder A et al., Environ. Sci. Technol. 37 (2003), 4955
1110	30	7.65	PBS 15 mM		1:50 - 1:200	Harder A et al., Environ. Sci. Technol. 37 (2003), 4955
1111	30	7.65	PBS 15 mM		1:50 - 1:200	Harder A et al., Environ. Sci. Technol. 37 (2003), 4955
1112	30	7.65	PBS 15 mM		1:50 - 1:200	Harder A et al., Environ. Sci. Technol. 37 (2003), 4955
1113	30	7.65	PBS 15 mM		1:50 - 1:200	Harder A et al., Environ. Sci. Technol. 37 (2003), 4955
1114	30	7.65	PBS 15 mM		1:50 - 1:200	Harder A et al., Environ. Sci. Technol. 37 (2003), 4955
1115	30	7.65	PBS 15 mM		1:50 - 1:200	Harder A et al., Environ. Sci. Technol. 37 (2003), 4955
1116	30	7.65	PBS 15 mM		1:50 - 1:200	Harder A et al., Environ. Sci. Technol. 37 (2003), 4955
1117	30	7.65	PBS 15 mM		1:50 - 1:200	Harder A et al., Environ. Sci. Technol. 37 (2003), 4955
1118	20	7.4	PBS 66 mM		1:20 (k-1 1:2)	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1119	20	7.4	no buffer		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1120	20	7.4	PBS 0.1 M		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1121	20	7.4	TRIS (77-86-1) 0.1 M		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1122	20	7.4	Triethanolamine buffer 0.1 M		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1123	20	7.4	Borate buffer 0.1 M		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1124	20	7.4	Acetate buffer 0.1 M		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1125	20	7.4	Formiate buffer 0.1 M		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1126	20	7.4	Ammoniumchloride buffer 0.1 M		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466

#	Comment
1096	
1097	
	k'' (se) 1518 (30) | Keq 3.2E-04 | Kadd 6.0E+01.
1098	Assay: UV(max. abs.); Adducts 1H-NMR; k'=Nu addition; k''=H addition; Keq=k'/k''; Kadd=Keq*(Ka/Kw); other Nu in paper
	k'' (se) 34 (1) | Keq 0.093 | Kadd 1.9E+03.
1099	Assay: UV(max. abs.); Adducts 1H-NMR; k'=Nu addition; k''=H addition; Keq=k'/k''; Kadd=Keq*(Ka/Kw); other Nu in paper
	NR = extremely slow; kOH 0.0006.
1100	Assay: UV(max. abs.); Adducts 1H-NMR; k'=Nu addition; k''=H addition; Keq=k'/k''; Kadd=Keq*(Ka/Kw); other Nu in paper
	k'' (se) 336 (18) | Keq 0.43 | Kadd 7.9E+03.
1101	Assay: UV(max. abs.); Adducts 1H-NMR; k'=Nu addition; k''=H addition; Keq=k'/k''; Kadd=Keq*(Ka/Kw); other Nu in paper
	k'' (se) 0.011 (0.002) | Keq 3.2 | Kadd 6.0E+04.
1102	Assay: UV(max. abs.); Adducts 1H-NMR; k'=Nu addition; k''=H addition; Keq=k'/k''; Kadd=Keq*(Ka/Kw); other Nu in paper
	k'' (se) 0.25 (0.02) | Keq 0.96 | Kadd 2.0E+04.
1103	Assay: UV(max. abs.); Adducts 1H-NMR; k'=Nu addition; k''=H addition; Keq=k'/k''; Kadd=Keq*(Ka/Kw); other Nu in paper
	k'' (se) 540 (60) | Keq 2.0E-03 | Kadd 4.0E+01.
1104	Assay: UV(max. abs.); Adducts 1H-NMR; k'=Nu addition; k''=H addition; Keq=k'/k''; Kadd=Keq*(Ka/Kw); other Nu in paper
1105	Assay: UV(max. abs.); Adducts 1H-NMR; k'=Nu addition; k''=H addition; Keq=k'/k''; Kadd=Keq*(Ka/Kw); other Nu in paper
	k'' (se) 24 (1) | Keq 1.38 | Kadd 2.6E+04.
1106	Assay: UV(max. abs.); Adducts 1H-NMR; k'=Nu addition; k''=H addition; Keq=k'/k''; Kadd=Keq*(Ka/Kw); other Nu in paper
	k'' (se) 1.4 (0.2) | Keq 3.4 | Kadd 6.4E+04.
1107	Assay: UV(max. abs.); Adducts 1H-NMR; k'=Nu addition; k''=H addition; Keq=k'/k''; Kadd=Keq*(Ka/Kw); other Nu in paper
	k'' (se) 0.0044 (0.0005) | Keq 2.5 | Kadd 4.8E+04.
1108	Assay: UV(max. abs.); Adducts 1H-NMR; k'=Nu addition; k''=H addition; Keq=k'/k''; Kadd=Keq*(Ka/Kw); other Nu in paper
1109	Assay: RP-HPLC-UV (252 nm)
1110	Assay: RP-HPLC-UV (252 nm)
1111	Assay: RP-HPLC-UV (252 nm)
1112	Assay: RP-HPLC-UV (252 nm)
1113	Assay: RP-HPLC-UV (252 nm)
1114	Assay: RP-HPLC-UV (252 nm)
1115	Assay: RP-HPLC-UV (252 nm)
1116	Assay: RP-HPLC-UV (252 nm)
1117	Assay: RP-HPLC-UV (252 nm)
	K 4.16E-05 | k-1 1.81E-03.
1118	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate)
1119	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate
1120	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate
1121	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate
1122	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate
1123	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate
1124	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate
1125	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate
1126	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate

#	Mechanism
1096	Michael-type nucleophilic addition
1097	Michael-type nucleophilic addition
1098	Michael-type nucleophilic addition
1099	Michael-type nucleophilic addition
1100	Michael-type nucleophilic addition
1101	Michael-type nucleophilic addition
1102	Michael-type nucleophilic addition
1103	Michael-type nucleophilic addition
1104	Michael-type nucleophilic addition
1105	Michael-type nucleophilic addition: no H-addition: ester hydrolysis
1106	Michael-type nucleophilic addition
1107	Michael-type nucleophilic addition
1108	Michael-type nucleophilic addition
1109	
1110	
1111	
1112	
1113	
1114	
1115	Nucleophilic substitution, first order (SN1)
1116	
1117	
1118	Michael-type nucleophilic addition
1119	Michael-type nucleophilic addition
1120	Michael-type nucleophilic addition
1121	Michael-type nucleophilic addition
1122	Michael-type nucleophilic addition
1123	Michael-type nucleophilic addition
1124	Michael-type nucleophilic addition
1125	Michael-type nucleophilic addition
1126	Michael-type nucleophilic addition

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1127	123-73-9	(E)-Crotonaldehyde	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	1.70E+01		1.23
1128	930-68-7	2-Cyclohexen-1-one	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	2.02E+01	5-10%	1.3
1129	505-57-7	2-Hexenal	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	1.98E+01	5-10%	1.3
1130	764-39-6	2-Pentenal	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	2.83E+01	5-10%	1.45
1131	814-78-8	3-Methyl-3-buten-2-one	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	3.60E+01	5-10%	1.56
1132		4-Ethoxy-2-pentenal	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	1.10E+02	5-10%	2.04
1133	29389-17-1	4-Hydroxy-2-decenal	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	1.18E+02	5-10%	2.07
1134	29343-60-0	4-Hydroxy-2-dodecenal	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	1.46E+02	5-10%	2.17
1135	17427-09-7	4-Hydroxy-2-heptenal	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	1.10E+02	5-10%	2.04
1136	17427-08-6	4-Hydroxy-2-hexenal	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	9.36E+01	5-10%	1.97
1137	29343-52-0	4-Hydroxy-2-nonenal	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	6.54E+01	5-10%	1.82
1138	17449-15-9	4-Hydroxy-2-octenal	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	1.04E+02	5-10%	2.02
1139	34424-65-2	4-Hydroxy-2-pentenal	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	1.31E+02	5-10%	2.12
1140	29343-58-6	4-Hydroxy-2-undecenal	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	8.82E+01	5-10%	1.95
1141		4-Hydroxy-4-isopropyl-2-pentenal	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	2.14E+00	5-10%	0.33
1142		4-Keto-2-pentenoic acid	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	2.05E+02	5-10%	2.31
1143	141-79-7	4-Methyl-3-penten-2-one	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	1.38E-01	5-10%	-0.86
1144	107-02-8	Acrolein	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	7.26E+03	5-10%	3.86
1145	79-06-1	Acrylamide	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	7.80E-01		-0.11
1146	79-10-7	Acrylic acid	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	6.00E-02		-1.22
1147	5392-40-5	Citral	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	1.94E+00	5-10%	0.29
1148	3724-65-0	Crotonic acid	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	NR		
1149	71-63-6	Digitoxin	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	NR		
1150	140-88-5	Ethyl acrylate	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	1.46E+01		1.16

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1127	20	7.4	Natriumchloride 0.5 M		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1128	20	7.4	PBS 66 mM		1:1 (k-1 1:2)	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1129	20	7.4	PBS 66 mM		1:20 (k-1 1:2)	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1130	20	7.4	PBS 66 mM		1:20 (k-1 1:2)	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1131	20	7.4	PBS 66 mM		1:1 (k-1 1:10)	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1132	20	7.4	PBS 66 mM		1:20 (k-1 1:2)	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1133	20	7.4	PBS 66 mM		1:20 (k-1 1:2)	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1134	20	7.4	PBS 66 mM, 10% ethanol		1:20 (k-1 1:2)	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1135	20	7.4	PBS 66 mM		1:20 (k-1 1:2)	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1136	20	7.4	PBS 66 mM		1:20 (k-1 1:2)	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1137	20	7.4	PBS 66 mM		1:20 (k-1 1:2)	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1138	20	7.4	PBS 66 mM		1:20 (k-1 1:2)	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1139	20	7.4	PBS 66 mM		1:20 (k-1 1:2)	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1140	20	7.4	PBS 66 mM, 10% ethanol		1:20 (k-1 1:2)	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1141	20	7.4	PBS 66 mM		1:1 (k-1 1:2)	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1142	20	7.4	PBS 66 mM		1:20 (k-1 1:2)	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1143	20	7.4	PBS 66 mM		1:400 (k-1 1:2)	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1144	20	7.4	PBS 66 mM		1:1 (k-1 1:2)	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1145	20	7.4	PBS 66 mM		1:10	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1146	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1147	20	7.4	PBS 66 mM, 10% ethanol		1:10 (k-1 1:20)	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1148	20	7.4	PBS 66 mM		1:40 (k-1 1:2)	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1149	20	7.4	PBS 66 mM		1:40	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1150	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466

#	Comment
1127	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate
	K 1.53E-05 (calc.) | k-1 3.10E-04.
1128	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate)
	K 1.42E-04 (calc.) | k-1 2.82E-03.
1129	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate)
	K 7.38E-05 | k-1 2.06E-03.
1130	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate)
	K 1.50E-02 | k-1 5.40E-01 (calc.).
1131	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate)
	K 9.60E-06 | k-1 1.05E-03.
1132	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate)
	K 4.85E-07 (calc.) | k-1 5.70E-05.
1133	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate)
	K 5.42E-07 (calc.) | k-1 7.56E-05.
1134	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate)
	K 2.50E-07 (calc.) | k-1 2.74E-05.
1135	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate)
	K 2.63E-07 (calc.) | k-1 2.46E-05.
1136	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate)
	K 8.85E-07 (calc.) | k-1 5.76E-05.
1137	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate)
	K 4.89E-07 | k-1 4.49E-05.
1138	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate)
	K 2.96E-07 | k-1 3.36E-05.
1139	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate)
	K 6.38E-07 | k-1 5.62E-05.
1140	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate)
	K 2.31E-05 | k-1 4.66E-05.
1141	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate)
	K 6.07E-07 | k-1 1.39E-04.
1142	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate)
	K 4.80E-03 | k-1 6.72E-04.
1143	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate)
	K 1.40E-08 | k-1 1.06E-04.
1144	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate)
1145	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate
1146	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate
	K 1.63E-04 | k-1 3.00E-04.
1147	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate)
1148	Crotonate. Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate
1149	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate
1150	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate)

#	Mechanism
1127	Michael-type nucleophilic addition
1128	Michael-type nucleophilic addition
1129	Michael-type nucleophilic addition
1130	Michael-type nucleophilic addition
1131	Michael-type nucleophilic addition
1132	Michael-type nucleophilic addition
1133	Michael-type nucleophilic addition
1134	Michael-type nucleophilic addition
1135	Michael-type nucleophilic addition
1136	Michael-type nucleophilic addition
1137	Michael-type nucleophilic addition
1138	Michael-type nucleophilic addition
1139	Michael-type nucleophilic addition
1140	Michael-type nucleophilic addition
1141	Michael-type nucleophilic addition
1142	Michael-type nucleophilic addition
1143	Michael-type nucleophilic addition
1144	Michael-type nucleophilic addition
1145	Michael-type nucleophilic addition
1146	Michael-type nucleophilic addition
1147	Michael-type nucleophilic addition
1148	NOT Michael-type nucleophilic addition
1149	NOT Michael-type nucleophilic addition
1150	Michael-type nucleophilic addition

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1151	623-70-1	Ethyl crotonate	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	1.86E-01	5-10%	-0.73
1152	78-94-4	Methyl vinyl ketone	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	1.91E+03	5-10%	3.28
1153	626-98-2	Pent-2-enoic acid	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	NR		
1154	508-52-1	Strophanthidin G	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	NR		
1155	630-60-4	Strophanthin G	Glutathione	k'(GSH) | K | k-1	mol-1 min-1	NR		
1156	4436-24-2	(2.3-Epoxypropyl)benzene	Glutathione	k(GSH)	M-1 min-1			-0.42
1157		(3.4-dioxocyclohexa-1.5-dien-1-yl)-acetic acid	Glutathione	k(GSH)	M-1 min-1	3.70E+07	10%	7.57
1158	6388-74-5	(4-Nitrophenyl)oxirane	Glutathione	k(GSH)	M-1 min-1			-0.12
1159		(E)-(Phenylimino)thiourea	Glutathione	k(GSH)	M-1 min-1	1.23E+02		2.09
1160		(E)-{[4-(pentyloxy)phenyl]imino}thiourea	Glutathione	k(GSH)	M-1 min-1	1.51E+01		1.18
1161		(E)-1-[(4-hexylphenyl)imino]-3.3-dimethylthiourea	Glutathione	k(GSH)	M-1 min-1	4.30E-01		-0.36
1162		(E)-1-[(4-hexylphenyl)imino]-3.3-dimethylurea	Glutathione	k(GSH)	M-1 min-1	1.40E-02		-1.84
1163		(E)-3.3-dimethyl-1-(phenylimino)thiourea	Glutathione	k(GSH)	M-1 min-1	2.30E+00		0.36
1164		(E)-3.3-dimethyl-1-(phenylimino)urea	Glutathione	k(GSH)	M-1 min-1	7.80E-02		-1.11
1165		(E)-3.3-dimethyl-1-{[4-(pentyloxy)phenyl]imino}thiourea	Glutathione	k(GSH)	M-1 min-1	7.80E-02		-1.11
1166		(E)-3.3-dimethyl-1-{[4-(pentyloxy)phenyl]imino}urea	Glutathione	k(GSH)	M-1 min-1	2.40E-03		-2.62
1167	123-73-9	(E)-Crotonaldehyde	Glutathione	k(GSH)	M-1 min-1	160	5	2.2
1168	99-54-7	1.2-Dichloro-4-nitrobenzene	Glutathione	k(GSH)	M-1 min-1	0.012		-1.92
1169	106-88-7	1.2-Epoxybutane	Glutathione	k(GSH)	M-1 min-1			-0.82
1170	97-00-7	1-Chloro-2.4-dinitrobenzene	Glutathione	k(GSH)	M-1 min-1	4.20E+04	2.00E+03	4.62
1171	97-00-7	1-Chloro-2.4-dinitrobenzene	Glutathione	k(GSH)	M-1 min-1	0.72		-0.14
1172	97-00-7	1-Chloro-2.4-dinitrobenzene	Glutathione	k(GSH)	M-1 min-1	0.42		-0.38
1173	97-00-7	1-Chloro-2.4-dinitrobenzene	Glutathione	k(GSH)	M-1 min-1	3.8		0.58
1174	97-00-7	1-Chloro-2.4-dinitrobenzene	Glutathione	k(GSH)	M-1 min-1			0.58
1175	610-40-2	1-Chloro-3.4-dinitrobenzene	Glutathione	k(GSH)	M-1 min-1	0.32		-0.5
1176	610-40-2	1-Chloro-3.4-dinitrobenzene	Glutathione	k(GSH)	M-1 min-1	2.9		0.46
1177	610-40-2	1-Chloro-3.4-dinitrobenzene	Glutathione	k(GSH)	M-1 min-1	17		1.24
1178	610-40-2	1-Chloro-3.4-dinitrobenzene	Glutathione	k(GSH)	M-1 min-1	36		1.56
1179	610-40-2	1-Chloro-3.4-dinitrobenzene	Glutathione	k(GSH)	M-1 min-1	50		1.7
1180	1629-60-3	1-Hexen-3-one	Glutathione	k(GSH)	M-1 min-1	1173	30	3.07
1181	4312-99-6	1-Octen-3-one	Glutathione	k(GSH)	M-1 min-1	1074	13	3.03
1182	1629-58-9	1-Penten-3-one	Glutathione	k(GSH)	M-1 min-1	1261	63	3.1
1183		2.3-(1.3-Cyclopentylene)-N-ethylmaleimide	Glutathione	k(GSH)	M-1 min-1	1.74E+04		4.24
1184	527-17-3	2.3.5.6-Tetramethyl-benzoquinone	Glutathione	k(GSH)	M-1 min-1	113	11	2.05

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1151	20	7.4	PBS 66 mM		1:40 (k-1 1:2)	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1152	20	7.4	PBS 66 mM		1:1 (k-1 1:2)	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1153	20	7.4	PBS 66 mM		1:40 (k-1 1:2)	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1154	20	7.4	PBS 66 mM		1:40	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1155	20	7.4	PBS 66 mM		1:40	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1156	30	7.65	PBS		1:4 - 1:20	Harder A et al., Environ. Sci. Technol. 37 (2003), 4955
1157		6.96	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1158	30	7.65	PBS		1:4 - 1:20	Harder A et al., Environ. Sci. Technol. 37 (2003), 4955
1159			30% Ethanol			Kosover EM, Chem. Biochem. React. 6 (2009), 549
1160			30% Ethanol			Kosover EM, Chem. Biochem. React. 6 (2009), 549
1161			30% Ethanol			Kosover EM, Chem. Biochem. React. 6 (2009), 549
1162			30% Ethanol			Kosover EM, Chem. Biochem. React. 6 (2009), 549
1163			30% Ethanol			Kosover EM, Chem. Biochem. React. 6 (2009), 549
1164			30% Ethanol			Kosover EM, Chem. Biochem. React. 6 (2009), 549
1165			30% Ethanol			Kosover EM, Chem. Biochem. React. 6 (2009), 549
1166			30% Ethanol			Kosover EM, Chem. Biochem. React. 6 (2009), 549
1167	25	8	PBS 0.1 M, DMSO		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1027
1168	25	7.5	PBS 0.1 M	15 min	5:1	Hulbert P et al., J. Pharmaceut. Biomed. Anal. 8 (1990), 1009
1169	30	7.65	PBS		1:4 - 1:20	Harder A et al., Environ. Sci. Technol. 37 (2003), 4955
1170	50	9.2	PBS 0.1 M		2.5:1 to 200:1	van der Aar EM et al., Biochem. J. 320 (1996), 531
1171	22	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1172	25	6.5	PBS 0.1 M	15 min	1:1	Hulbert P et al., J. Pharmaceut. Biomed. Anal. 8 (1990), 1009
1173	25	7.5	PBS 0.1 M	15 min	1:1	Hulbert P et al., J. Pharmaceut. Biomed. Anal. 8 (1990), 1009
1174	25	7.5	PBS 0.1 M	15 min	1:1	Hulbert P et al., J. Pharmaceut. Biomed. Anal. 8 (1990), 1009
1175	10	7.5	PSB 50 mM, EDTA buffer 1 mM	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1176	10	8.5	PSB 50 mM, EDTA buffer 1 mM	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1177	10	9.5	PSB 50 mM, EDTA buffer 1 mM	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1178	10	10.5	PSB 50 mM, EDTA buffer 1 mM	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1179	10	11.5	PSB 50 mM, EDTA buffer 1 mM	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1180	25	7.4	PBS, max 20% DMSO	120 min	1:1.38	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1181	25	7.4	PBS, max 20% DMSO	120 min	1:0.79	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1182	25	7.4	PBS, max 20% DMSO	120 min	1:1.40	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1183	25	7.2	Aqueous buffer			Kosover EM, Chem. Biochem. React. 6 (2009), 549
1184	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 608

#	Comment
	K 1.65E-02 | k-1 3.45E-03.
1151	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate)
	K 3.60E-09 | k-1 7.14E-06.
1152	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate)
1153	2-Pentenoate. Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate
1154	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate
1155	Assay: UV (DTNB 412 nm; Carbonyl 222 nm); rate limiting: low pH = addition anion, high pH = proton transfer (stabilizes intermediate
1156	RP-HPLC-UV (GAS derivat. o-Phthaldialdehyde excit. 350 nm, emis. 420 nm).
1157	
1158	RP-HPLC-UV (GAS derivat. o-Phthaldialdehyde excit. 350 nm, emis. 420 nm).
1159	
1160	
1161	
1162	estimated from k ratio for related compounds.
1163	
1164	
1165	
1166	estimated from k ratio for related compounds.
1167	UV (DTNB, 412 nm).
1168	UV (GSH-conjugate).
1169	RP-HPLC-UV (GAS derivat. o-Phthaldialdehyde excit. 350 nm, emis. 420 nm).
1170	UV (GSH-conjugate).
1171	HPLC-UV(210-300 nm).
1172	UV (GSH-conjugate).
1173	UV (GSH-conjugate).
1174	est. from pH 6.5: k2(est. pH 7.5) = 10*k2(exp. pH 6.5); UV.
1175	HPLC-UV(210-300 nm).
1176	HPLC-UV(210-300 nm).
1177	HPLC-UV(210-300 nm).
1178	HPLC-UV(210-300 nm).
1179	HPLC-UV(210-300 nm).
1180	UV (DTNB; 412 nm).
1181	UV (DTNB; 412 nm).
1182	UV (DTNB; 412 nm).
1183	UV(325 nm); carried out at concentrations with GSH reaction only.
1184	UV(DTNB, 412 nm).

#	Mechanism
1151	Michael-type nucleophilic addition
1152	Michael-type nucleophilic addition
1153	NOT Michael-type nucleophilic addition
1154	NOT Michael-type nucleophilic addition
1155	NOT Michael-type nucleophilic addition
1156	
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1167	Michael-type nucleophilic addition
1168	
1169	
1170	Nucleophilic aromatic substitution (SNAr)
1171	
1172	
1173	
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1176	
1177	
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1179	
1180	Michael-type nucleophilic addition
1181	Michael-type nucleophilic addition
1182	Michael-type nucleophilic addition
1183	Michael-type nucleophilic addition
1184	

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1185	935-92-2	2.3.5-Trimethyl-benzoquinone	Glutathione	k(GSH)	M-1 min-1	376	45	2.58
1186	78-88-6	2.3-Dichloro-1-propene	Glutathione	k(GSH)	M-1 min-1			0.36
1187		2.3-Dimethyl-N-ethylmaleimide	Glutathione	k(GSH)	M-1 min-1	4.40E-01		-0.36
1188		2.3-Tetramethylene-N-ethylmaleimide	Glutathione	k(GSH)	M-1 min-1	1.77E+00		0.25
1189	615-93-0	2.5-Dichloro-benzoquinone	Glutathione	k(GSH)	M-1 min-1	6052	600	3.78
1190	530-55-2	2.6-Dimethoxy-benzoquinone	Glutathione	k(GSH)	M-1 min-1	696	70	2.84
1191	527-61-7	2.6-Dimethyl-benzoquinone	Glutathione	k(GSH)	M-1 min-1	1601	177	3.2
1192	583-63-1	2-Benzoquinone	Glutathione	k(GSH)	M-1 min-1	1.60E+08	10%	8.19
1193		2-Bromo-1-chloro-4-nitrobenzene	Glutathione	k(GSH)	M-1 min-1	1.00E+02	2.00E+01	2
1194	5447-97-2	2-Bromo-2-nitropropane	Glutathione	k(GSH)	M-1 min-1			2.9
1195	41513-04-6	2-Bromo-5-chloronitrobenzene	Glutathione	k(GSH)	M-1 min-1	4.80E+03	1.00E+02	3.68
1196	3958-82-5	2-Bromo-benzoquinone	Glutathione	k(GSH)	M-1 min-1	1435	180	3.16
1197	584-93-0	2-Bromovaleric acid	Glutathione	k(GSH)	M-1 min-1			0.28
1198	121-17-5	2-Chloro-5-(trifluoromethyl)-nitrobenzene	Glutathione	k(GSH)	M-1 min-1	0.21		-0.68
1199	6361-21-3	2-Chloro-5-nitrobenzaldehyde	Glutathione	k(GSH)	M-1 min-1	5.10E+02	1.00E+01	2.71
1200		2-Chloro-5-nitrobenzoic acid butyl ester	Glutathione	k(GSH)	M-1 min-1	3.90E+02	5.00E+01	2.59
1201	6307-82-0	2-Chloro-5-nitrobenzoic acid methyl ester	Glutathione	k(GSH)	M-1 min-1	4.30E+02	1.00E+01	2.63
1202		2-Chloro-5-nitrobenzoic acid tert-butyl ester	Glutathione	k(GSH)	M-1 min-1	2.90E+02	2.00E+01	2.46
1203	34052-37-4	2-Chloro-5-nitrobenzophenone	Glutathione	k(GSH)	M-1 min-1	2.80E+02	1.00E+01	2.45
1204	930-30-3	2-Cyclopenten-1-one	Glutathione	k(GSH)	M-1 min-1	25.6	0.1	1.41
1205	2370-63-0	2-Ethoxy ethyl methacrylate	Glutathione	k(GSH)	M-1 min-1	0.25	0.04	-0.6
1206	818-61-1	2-Hydroxyethyl acrylate	Glutathione	k(GSH)	M-1 min-1	102	10	2.01
1207	818-61-1	2-Hydroxyethyl acrylate	Glutathione	k(GSH)	M-1 min-1	50.9	2.24	1.71
1208	818-61-1	2-Hydroxyethyl acrylate	Glutathione	k(GSH)	M-1 min-1			1.71
1209	923-26-2	2-Hydroxypropyl methacrylate	Glutathione	k(GSH)	M-1 min-1	4	0.5	0.55
1210	1120-73-6	2-Methyl-2-cyclopenten-1-one	Glutathione	k(GSH)	M-1 min-1	0.2	0.001	-0.7
1211	1838-94-4	2-Methyl-2-vinyloxirane	Glutathione	k(GSH)	M-1 min-1			-0.55
1212	553-97-9	2-Methyl-benzoquinone	Glutathione	k(GSH)	M-1 min-1	2423	225	3.38
1213	4643-27-0	2-Octen-4-one	Glutathione	k(GSH)	M-1 min-1	26.1	0.5	1.42
1214	3602-55-9	2-tert-Butyl-benzoquinone	Glutathione	k(GSH)	M-1 min-1	846	80	2.93
1215	4091-39-8	3-Chloro-2-butanone	Glutathione	k(GSH)	M-1 min-1			1.08
1216	1119-44-4	3-Heptene-2-one	Glutathione	k(GSH)	M-1 min-1	12.5	0.3	1.1
1217	1679-36-3	3-Hexyn-2-one	Glutathione	k(GSH)	M-1 min-1	80	1.3	1.9
1218	2758-18-1	3-Methyl-2-cyclopenten-1-one	Glutathione	k(GSH)	M-1 min-1	0.074	0.002	-1.13
1219	565-62-8	3-Methyl-3-penten-2-one	Glutathione	k(GSH)	M-1 min-1	0.779	0.018	-0.11
1220	14309-57-0	3-Nonen-2-one	Glutathione	k(GSH)	M-1 min-1	10.8	0.2	1.03
1221	1669-44-9	3-Octen-2-one	Glutathione	k(GSH)	M-1 min-1	11.4	0.2	1.06
1222	625-33-2	3-Penten-2-one	Glutathione	k(GSH)	M-1 min-1	26.7	0.9	1.43
1223		4-[(1Z)-3-oxo-3-phenylprop-1-en-1-yl]-1.2-benzoquinone	Glutathione	k(GSH)	M-1 min-1	3.50E+08	10%	8.54
1224		4-Bromo-1.2-benzoquinone	Glutathione	k(GSH)	M-1 min-1	2.00E+08	10%	8.31
1225	31222-02-3	4-Chloro-1.2-benzoquinone	Glutathione	k(GSH)	M-1 min-1	2.30E+08	10%	8.36

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1185	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 608
1186	30	7.65	PBS		1:4 - 1:20	Harder A et al., Environ. Sci. Technol. 37 (2003), 4955
1187	25	7.2	Aqueous buffer			Kosover EM, Chem. Biochem. React. 6 (2009), 549
1188	25	7.1	Aqueous buffer			Kosover EM, Chem. Biochem. React. 6 (2009), 549
1189	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 608
1190	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 608
1191	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 608
1192		7.12	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1193	50	9.2	PBS 0.1 M		2.5:1 to 200:1	van der Aar EM et al., Biochem. J. 320 (1996), 531
1194		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
1195	50	9.2	PBS 0.1 M		2.5:1 to 200:1	van der Aar EM et al., Biochem. J. 320 (1996), 531
1196	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 608
1197		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
1198	25	7.5	PBS 0.1 M, add. DMSO	15 min	5:1	Hulbert P et al., J. Pharmaceut. Biomed. Anal. 8 (1990), 1009
1199	50	9.2	PBS 0.1 M		2.5:1 to 200:1	van der Aar EM et al., Biochem. J. 320 (1996), 531
1200	50	9.2	PBS 0.1 M		2.5:1 to 200:1	van der Aar EM et al., Biochem. J. 320 (1996), 531
1201	50	9.2	PBS 0.1 M		2.5:1 to 200:1	van der Aar EM et al., Biochem. J. 320 (1996), 531
1202	50	9.2	PBS 0.1 M		2.5:1 to 200:1	van der Aar EM et al., Biochem. J. 320 (1996), 531
1203	50	9.2	PBS 0.1 M		2.5:1 to 200:1	van der Aar EM et al., Biochem. J. 320 (1996), 531
1204	25	7.4	PBS, max 20% DMSO	120 min	1:10.3	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1205	20	8.8	Tetraborate buffer	24 h	1:4 - 1:16	Freidig AP et al., Environ. Toxicol. Chem. 18 (1999), 1133
1206	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004
1207	20	8.8	Tetraborate buffer	1 h	1:4 - 1:16	Freidig AP et al., Environ. Toxicol. Chem. 18 (1999), 1133
1208	30	7.65	PBS		1:4 - 1:20	Harder A et al., Environ. Sci. Technol. 37 (2003), 4955
1209	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004
1210	25	7.4	PBS, max 20% DMSO	120 min	1:298	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1211	30	7.65	PBS		1:4 - 1:20	Harder A et al., Environ. Sci. Technol. 37 (2003), 4955
1212	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 608
1213	25	7.4	PBS, max 20% DMSO	120 min	1:8.79	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1214	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 608
1215		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
1216	25	7.4	PBS, max 20% DMSO	120 min	1:9.21	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1217	25	7.4	PBS, max 20% DMSO	120 min	1:1.90	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1218	25	7.4	PBS, max 20% DMSO	120 min	1:279	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1219	25	7.4	PBS, max 20% DMSO	120 min	1:106	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1220	25	7.4	PBS, max 20% DMSO	120 min	1:8.21	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1221	25	7.4	PBS, max 20% DMSO	120 min	1:12.7	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1222	25	7.4	PBS, max 20% DMSO	120 min	1:0.82	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1223		7.2	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1224		6.97	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1225		7.11	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498

#	Comment
1185	UV(DTNB, 412 nm).
1186	RP-HPLC-UV (GAS derivat. o-Phthaldialdehyde excit. 350 nm, emis. 420 nm).
1187	UV(305 nm).
1188	UV(307.5 nm).
1189	UV(DTNB, 412 nm).
1190	UV(DTNB, 412 nm).
1191	UV(DTNB, 412 nm).
1192	
1193	UV (GSH-conjugate).
1194	RC50 assay.
1195	UV (GSH-conjugate).
1196	UV(DTNB, 412 nm).
1197	RC50 assay.
1198	UV (GSH-conjugate).
1199	UV (GSH-conjugate).
1200	UV (GSH-conjugate).
1201	UV (GSH-conjugate).
1202	UV (GSH-conjugate).
1203	UV (GSH-conjugate).
1204	UV (DTNB; 412 nm).
1205	UV (GSH derivat. o-phthalaldehyde, excit 350 nm, emiss. 420 nm).
1206	UV(DTNB, 412 nm).
1207	UV (GSH derivat. o-phthalaldehyde, excit 350 nm, emiss. 420 nm).
1208	RP-HPLC-UV (GAS derivat. o-Phthaldialdehyde excit. 350 nm, emis. 420 nm).
1209	UV(DTNB, 412 nm).
1210	UV (DTNB; 412 nm), assum. pseudo 1st order, accounts for oxidative GSSH formation
1211	RP-HPLC-UV (GAS derivat. o-Phthaldialdehyde excit. 350 nm, emis. 420 nm).
1212	UV(DTNB, 412 nm).
1213	UV (DTNB; 412 nm).
1214	UV(DTNB, 412 nm).
1215	RC50 assay.
1216	UV (DTNB; 412 nm).
1217	UV (DTNB; 412 nm).
1218	UV (DTNB; 412 nm), assum. pseudo 1st order, accounts for oxidative GSSH formation
1219	UV (DTNB; 412 nm), assum. pseudo 1st order, accounts for oxidative GSSH formation
1220	UV (DTNB; 412 nm).
1221	UV (DTNB; 412 nm).
1222	UV (DTNB; 412 nm).
1223	
1224	
1225	

#	Mechanism
1185	
1186	
1187	NOT Michael-type nucleophilic addition
1188	NOT Michael-type nucleophilic addition
1189	
1190	
1191	
1192	
1193	Nucleophilic aromatic substitution (SNAr)
1194	Nucleophilic halogen abstraction. GS+Hal-R --> GS-Hal+H-R --> GSSG
1195	Nucleophilic aromatic substitution (SNAr)
1196	
1197	Nucleophilic substitution, second order (SN2)
1198	
1199	Nucleophilic aromatic substitution (SNAr)
1200	Nucleophilic aromatic substitution (SNAr)
1201	Nucleophilic aromatic substitution (SNAr)
1202	Nucleophilic aromatic substitution (SNAr)
1203	Nucleophilic aromatic substitution (SNAr)
1204	Michael-type nucleophilic addition
1205	Michael-type nucleophilic addition
1206	Michael-type nucleophilic addition
1207	Michael-type nucleophilic addition
1208	
1209	Michael-type nucleophilic addition
1210	Michael-type nucleophilic addition
1211	
1212	
1213	Michael-type nucleophilic addition
1214	
1215	
1216	Michael-type nucleophilic addition
1217	Michael-type nucleophilic addition
1218	Michael-type nucleophilic addition
1219	Michael-type nucleophilic addition
1220	Michael-type nucleophilic addition
1221	Michael-type nucleophilic addition
1222	Michael-type nucleophilic addition
1223	
1224	
1225	

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1226	777-37-7	4-Chloro-3-(trifluoromethyl)-nitrobenzene	Glutathione	k(GSH)	M-1 min-1	1.10E+02	1.00E+01	2.04
1227	1930-72-9	4-Chloro-3.5-dinitro-benzonitrile	Glutathione	k(GSH)	M-1 min-1	305		2.48
1228	1930-72-9	4-Chloro-3.5-dinitro-benzonitrile	Glutathione	k(GSH)	M-1 min-1			3.48
1229	100-00-5	4-Chloronitrobenzene	Glutathione	k(GSH)	M-1 min-1	<0.001		
1230		4-Ethylaminium-1.2-benzoquinone	Glutathione	k(GSH)	M-1 min-1	4.90E+08	10%	8.69
1231	2497-21-4	4-Hexen-3-one	Glutathione	k(GSH)	M-1 min-1	24.2	0.2	1.38
1232	29343-52-0	4-Hydroxy-2-nonenal	Glutathione	k(GSH)	M-1 min-1	8706	606	3.94
1233		4-Isopropyl-1.2-benzoquinone	Glutathione	k(GSH)	M-1 min-1	1.10E+08	10%	8.03
1234	69818-23-1	4-Methoxy-1.2-benzoquinone	Glutathione	k(GSH)	M-1 min-1	1.80E+07	10%	7.26
1235	3131-54-2	4-Methyl-1.2-benzoquinone	Glutathione	k(GSH)	M-1 min-1	7.20E+07	10%	7.86
1236	141-79-7	4-Methyl-3-penten-2-one	Glutathione	k(GSH)	M-1 min-1	0.208	0.007	-0.68
1237		4-Methylaminium-1.2-benzoquinone	Glutathione	k(GSH)	M-1 min-1	7.20E+08	10%	8.86
1238		4-Methylthio-1.2-benzoquinone	Glutathione	k(GSH)	M-1 min-1	1.10E+08	10%	8.03
1239		4-n-Butoxy-1.2-benzoquinone	Glutathione	k(GSH)	M-1 min-1	1.00E+07	10%	7.01
1240		4-n-Butylthio-1.2-benzoquinone	Glutathione	k(GSH)	M-1 min-1	8.40E+07	10%	7.92
1241	100-11-8	4-Nitrobenzylbromide	Glutathione	k(GSH)	M-1 min-1			1.95
1242	100-14-1	4-Nitrobenzylchloride	Glutathione	k(GSH)	M-1 min-1	0.3		-0.52
1243	100-14-1	4-Nitrobenzylchloride	Glutathione	k(GSH)	M-1 min-1	12.6		1.1
1244	100-14-1	4-Nitrobenzylchloride	Glutathione	k(GSH)	M-1 min-1	32		1.51
1245	100-14-1	4-Nitrobenzylchloride	Glutathione	k(GSH)	M-1 min-1	1		-0.02
1246	100-14-1	4-Nitrobenzylchloride	Glutathione	k(GSH)	M-1 min-1			0.43
1247		4-n-Propoxy-1.2-benzoquinone	Glutathione	k(GSH)	M-1 min-1	9.00E+06	10%	6.95
1248		4-n-Propylthio-1.2-benzoquinone	Glutathione	k(GSH)	M-1 min-1	9.00E+07	10%	7.95
1249	103560-62-9	4-Oxo-2-nonenal	Glutathione	k(GSH)	M-1 min-1	79.8	3	1.9
1250	1129-21-1	4-tert-Butyl-1.2-benzoquinone	Glutathione	k(GSH)	M-1 min-1	7.20E+07	10%	7.86
1251		4-Trifluoromethoxy-1.2-benzoquinone	Glutathione	k(GSH)	M-1 min-1	3.00E+08	10%	8.48
1252	34256-82-1	Acetochlor	Glutathione	k(GSH)	M-1 min-1	10.2		1.01
1253	107-02-8	Acrolein	Glutathione	k(GSH)	M-1 min-1	437	11	2.64
1254	107-02-8	Acrolein	Glutathione	k(GSH)	M-1 min-1			3.92
1255	79-06-1	Acrylamide	Glutathione	k(GSH)	M-1 min-1			-0.33
1256	79-06-1	Acrylamide	Glutathione	k(GSH)	M-1 min-1			-1.02
1257	79-06-1	Acrylamide	Glutathione	k(GSH)	M-1 min-1			-0.15
1258	79-06-1	Acrylamide	Glutathione	k(GSH)	M-1 min-1			-0.23
1259	107-13-1	Acrylonitrile	Glutathione	k(GSH)	M-1 min-1			0.87
1260	107-13-1	Acrylonitrile	Glutathione	k(GSH)	M-1 min-1	10.86		1.04
1261	107-13-1	Acrylonitrile	Glutathione	k(GSH)	M-1 min-1	1.04E+01		1.02
1262	107-13-1	Acrylonitrile	Glutathione	k(GSH)	M-1 min-1	2.21E+02		2.34
1263	107-13-1	Acrylonitrile	Glutathione	k(GSH)	M-1 min-1			0.87
1264	15972-60-8	Alachlor	Glutathione	k(GSH)	M-1 min-1	0.144		-0.84
1265	15972-60-8	Alachlor	Glutathione	k(GSH)	M-1 min-1	0.31		-0.51
1266	999-55-3	Allyl acrylate	Glutathione	k(GSH)	M-1 min-1			1.292
1267	96-05-9	Allyl methacrylate	Glutathione	k(GSH)	M-1 min-1	3	0.1	0.54
1268	96-05-9	Allyl methacrylate	Glutathione	k(GSH)	M-1 min-1	0.51	0.22	-0.29

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1226	50	9.2	PBS 0.1 M		2.5:1 to 200:1	van der Aar EM et al., Biochem. J. 320 (1996), 531
1227	25	6.5	PBS 0.1 M	15 min	1:1	Hulbert P et al., J. Pharmaceut. Biomed. Anal. 8 (1990), 1009
1228	25	7.5	PBS 0.1 M	15 min	1:1	Hulbert P et al., J. Pharmaceut. Biomed. Anal. 8 (1990), 1009
1229	25	7.5	PBS 0.1 M	15 min	100:1	Hulbert P et al., J. Pharmaceut. Biomed. Anal. 8 (1990), 1009
1230		7.11	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1231	25	7.4	PBS, max 20% DMSO	120 min	1:10.1	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1232	23	7.4	PBS 50 mM		> 1:10	Doorn JA et al., Chem. Biol. Interact. 143 (2003), 93
1233		7.12	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1234		7.08	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1235		7.08	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1236	25	7.4	PBS, max 20% DMSO	120 min	1:291	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1237		7.2	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1238		7.19	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1239		7.17	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1240		7.19	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1241		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
1242	22	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1243	22	8.9	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1244	22	10.5	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1245	37	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1246	30	7.65	PBS		1:4 - 1:20	Harder A et al., Environ. Sci. Technol. 37 (2003), 4955
1247		7.2	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1248		7.16	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1249	23	7.4	PBS 50 mM		> 1:10	Doorn JA et al., Chem. Biol. Interact. 143 (2003), 93
1250		7.2	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1251		6.89	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1252	37	9	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1253	25	8	PBS 0.1 M, DMSO		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1027
1254	20	8.8	Tetraborate buffer 0.4 mM	3 min	El excess	Freidig AP et al., Environ. Sci. Technol. 33 (1999), 3038
1255	20	8.8	Tetraborate buffer 0.4 mM	50 min	El excess	Freidig AP et al., Environ. Sci. Technol. 33 (1999), 3038
1256		7.4			El excess	LoPachin RM et al., Toxicol. Sci. 98 (2007), 561
1257		8.8			El excess	LoPachin RM et al., Toxicol. Sci. 98 (2007), 561
1258	30	7.65	PBS		1:4 - 1:20	Harder A et al., Environ. Sci. Technol. 37 (2003), 4955
1259	20	8.8	Tetraborate buffer 0.4 mM	50 min	El excess	Freidig AP et al., Environ. Sci. Technol. 33 (1999), 3038
1260	30	8.12				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1261	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1262	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1263	30	7.65	PBS		1:4 - 1:20	Harder A et al., Environ. Sci. Technol. 37 (2003), 4955
1264	22	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1265	37	9	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1266	25	7.4	PBS, max 20% DMSO	120 min		Wondrousch D et al., J. Phys. Chem. Lett. 1 (2010), 1605
1267	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004
1268	20	8.8	Tetraborate buffer	24 h	1:4 - 1:16	Freidig AP et al., Environ. Toxicol. Chem. 18 (1999), 1133

#	Comment
1226	UV (GSH-conjugate).
1227	UV (GSH-conjugate).
1228	est. from pH 6.5: k2(est. pH 7.5) = 10*k2(exp. pH 6.5); UV.
1229	37C: NR; UV (GSH-conjugate).
1230	
1231	UV (DTNB; 412 nm).
1232	Room temperature, UV (DTNB 412 nm).
1233	
1234	
1235	
1236	UV (DTNB; 412 nm), assum. pseudo 1st order, accounts for oxidative GSSH formation
1237	
1238	
1239	
1240	
1241	RC50 assay.
1242	HPLC-UV(210-300 nm).
1243	HPLC-UV(210-300 nm).
1244	HPLC-UV(210-300 nm).
1245	HPLC-UV(210-300 nm).
1246	RP-HPLC-UV (GAS derivat. o-Phthaldialdehyde excit. 350 nm, emis. 420 nm).
1247	
1248	
1249	Room temperature, UV (DTNB 412 nm).
1250	
1251	
1252	22C pH 7: NR; HPLC-UV(210-300 nm).
1253	UV (DTNB, 412 nm).
1254	HPLC-UV (205 nm).
1255	HPLC-UV (205 nm).
1256	UV (DTNB 412 nm).
1257	UV (DTNB 412 nm).
1258	RP-HPLC-UV (GAS derivat. o-Phthaldialdehyde excit. 350 nm, emis. 420 nm).
1259	HPLC-UV (205 nm).
1260	other pH in paper.
1261	
1262	k(NH2) of GSH.
1263	RP-HPLC-UV (GAS derivat. o-Phthaldialdehyde excit. 350 nm, emis. 420 nm).
1264	HPLC-UV(210-300 nm).
1265	HPLC-UV(210-300 nm).
1266	UV (DTNB; 412 nm).
1267	UV(DTNB, 412 nm).
1268	UV (GSH derivat. o-phthalaldehyde, excit 350 nm, emiss. 420 nm).

#	Mechanism
1226	Nucleophilic aromatic substitution (SNAr)
1227	
1228	
1229	
1230	
1231	Michael-type nucleophilic addition
1232	Michael-type nucleophilic addition
1233	
1234	
1235	
1236	Michael-type nucleophilic addition
1237	
1238	
1239	
1240	
1241	Nucleophilic substitution, second order (SN2)
1242	
1243	
1244	
1245	
1246	
1247	
1248	
1249	Michael-type nucleophilic addition
1250	
1251	
1252	
1253	Michael-type nucleophilic addition
1254	Michael-type nucleophilic addition
1255	Michael-type nucleophilic addition
1256	Michael-type nucleophilic addition
1257	Michael-type nucleophilic addition
1258	
1259	Michael-type nucleophilic addition
1260	Michael-type nucleophilic addition
1261	Michael-type nucleophilic addition
1262	Michael-type nucleophilic addition
1263	
1264	
1265	
1266	Michael-type nucleophilic addition
1267	Michael-type nucleophilic addition
1268	Michael-type nucleophilic addition

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1269	1912-24-9	Atrazine	Glutathione	k(GSH)	M-1 min-1	0.3		-0.52
1270	131860-33-8	Azoxystrobin	Glutathione	k(GSH)	M-1 min-1	0		
1271	100-44-7	Benzyl chloride	Glutathione	k(GSH)	M-1 min-1	NR		
1272	2495-37-6	Benzyl methacrylate	Glutathione	k(GSH)	M-1 min-1	0.33	0.05	-0.49
1273	79-08-3	Bromoacetic acid	Glutathione	k(GSH)	M-1 min-1	8.5	0.7	0.93
1274	590-17-0	Bromoacetonitrile	Glutathione	k(GSH)	M-1 min-1			1.79
1275	23184-66-9	Butachlor	Glutathione	k(GSH)	M-1 min-1	3.42		0.53
1276	306-18-3	Carbonyl cyanide phenylhydrazone	Glutathione	k(GSH)	M-1 min-1	2.07E+05	8.40E+03	5.32
1277	370-86-5	Carbonyl cyanide p-trifluoromethoxyphenylhydrazone	Glutathione	k(GSH)	M-1 min-1	1.07E+04		4.03
1278	79-11-8	Chloroacetic acid	Glutathione	k(GSH)	M-1 min-1	0.15	0.01	-0.83
1279	107-14-2	Chloroacetonitrile	Glutathione	k(GSH)	M-1 min-1			0.23
1280	118-75-2	Chloroanil	Glutathione	k(GSH)	M-1 min-1	4116	440	3.61
1281	1897-45-6	Chlorothalonil	Glutathione	k(GSH)	M-1 min-1	46.8		1.67
1282	1072-87-3	Citraconimide	Glutathione	k(GSH)	M-1 min-1	3.10E+02		2.49
1283	5392-40-5	Citral	Glutathione	k(GSH)	M-1 min-1	2	2	0.29
1284	333-41-5	Diazinon	Glutathione	k(GSH)	M-1 min-1	NR		
1285	37764-25-3	Dichlormid	Glutathione	k(GSH)	M-1 min-1	0.234		-0.63
1286	623-91-6	Diethyl fumarate	Glutathione	k(GSH)	M-1 min-1			2.05
1287	623-91-6	Diethyl fumarate	Glutathione	k(GSH)	M-1 min-1			2.05
1288	106-89-8	Epichlorohydrin	Glutathione	k(GSH)	M-1 min-1			0.15
1289		Ethyl 4-chloro-3.5-dinitrobenzoate	Glutathione	k(GSH)	M-1 min-1	6.67		0.82
1290		Ethyl 4-chloro-3.5-dinitrobenzoate	Glutathione	k(GSH)	M-1 min-1			1.82
1291	140-88-5	Ethyl acrylate	Glutathione	k(GSH)	M-1 min-1	10.6	0.1	1.03
1292	140-88-5	Ethyl acrylate	Glutathione	k(GSH)	M-1 min-1	57	4	1.76
1293	140-88-5	Ethyl acrylate	Glutathione	k(GSH)	M-1 min-1	39.7	1.87	1.6
1294	140-88-5	Ethyl acrylate	Glutathione	k(GSH)	M-1 min-1			1.6
1295	140-88-5	Ethyl acrylate	Glutathione	k(GSH)	M-1 min-1	26.6	6	1.42
1296	140-88-5	Ethyl acrylate	Glutathione	k(GSH)	M-1 min-1	32.8		1.52
1297	105-36-2	Ethyl bromoacetate	Glutathione	k(GSH)	M-1 min-1			2.49
1298	105-39-5	Ethyl chloroacetate	Glutathione	k(GSH)	M-1 min-1			0.7
1299	623-70-1	Ethyl crotonate	Glutathione	k(GSH)	M-1 min-1	0.161	0.002	-0.79
1300	623-48-3	Ethyl iodoacetate	Glutathione	k(GSH)	M-1 min-1			2.76
1301	97-63-2	Ethyl methacrylate	Glutathione	k(GSH)	M-1 min-1	0.058	0.005	-1.24
1302	97-63-2	Ethyl methacrylate	Glutathione	k(GSH)	M-1 min-1	4	0.7	0.59
1303	97-63-2	Ethyl methacrylate	Glutathione	k(GSH)	M-1 min-1	0.139	0.022	-0.86
1304	623-47-2	Ethyl propiolate	Glutathione	k(GSH)	M-1 min-1	105	5	2.02
1305	97-90-5	Ethylene glycol dimethacrylate	Glutathione	k(GSH)	M-1 min-1	0.83	0.12	-0.08
1306	69806-50-4	Fluazifop-butyl	Glutathione	k(GSH)	M-1 min-1	NR		
1307	79622-59-6	Fluazinam	Glutathione	k(GSH)	M-1 min-1	6.6		0.82
1308	15457-05-3	Fluorodifen	Glutathione	k(GSH)	M-1 min-1	0.06		-1.22
1309	15457-05-3	Fluorodifen	Glutathione	k(GSH)	M-1 min-1	0.011		-0.96
1310	61213-25-0	Flurochloridone	Glutathione	k(GSH)	M-1 min-1	0.174		-0.76

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1269	37	10.5	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1270	37	9	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1271	30	7.65	PBS		1:4 - 1:20	Harder A et al., Environ. Sci. Technol. 37 (2003), 4955
1272	20	8.8	Tetraborate buffer	24 h	1:4 - 1:16	Freidig AP et al., Environ. Toxicol. Chem. 18 (1999), 1133
1273	37.5	7.4	Hydrogen carbonate buffer	40 min	(different)	Dickens F, Biochem. J. 17 (1933), 1141
1274		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
1275	20	9	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1276	25	4	Citrate/phosphate 0.2 M			Drobnica L et al., Biochim. Biophys. Acta 585 (1979), 462
1277	25	7.5	Citrate/phosphate 0.1 M, 1% MeOH		25:1	Drobnica L et al., Biochim. Biophys. Acta 585 (1979), 462
1278	37.5	7.4	Hydrogen carbonate buffer	40 min	(different)	Dickens F, Biochem. J. 17 (1933), 1141
1279		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
1280	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 608
1281	36	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1282	25	7.2	Aqueous buffer			Kosover EM, Chem. Biochem. React. 6 (2009), 549
1283	25	8	PBS 0.1 M, DMSO		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1027
1284	23	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1285	37	9	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1286	20	8.8	Tetraborate buffer 0.4 mM	50 min	El excess	Freidig AP et al., Environ. Sci. Technol. 33 (1999), 3038
1287	20	8.8	Tetraborate buffer	1 h	1:4 - 1:16	Freidig AP et al., Environ. Toxicol. Chem. 18 (1999), 1133
1288	30	7.65	PBS		1:4 - 1:20	Harder A et al., Environ. Sci. Technol. 37 (2003), 4955
1289	25	6.5	PBS 0.1 M, add. DMSO	15 min	1:1	Hulbert P et al., J. Pharmaceut. Biomed. Anal. 8 (1990), 1009
1290	25	7.5	PBS 0.1 M, add. DMSO	15 min	1:1	Hulbert P et al., J. Pharmaceut. Biomed. Anal. 8 (1990), 1009
1291	25	7.4	PBS, max 20% DMSO	120 min	1:9.86	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1292	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004
1293	20	8.8	Tetraborate buffer	1 h	1:4 - 1:16	Freidig AP et al., Environ. Toxicol. Chem. 18 (1999), 1133
1294	30	7.65	PBS		1:4 - 1:20	Harder A et al., Environ. Sci. Technol. 37 (2003), 4955
1295	37	7.4	PBS	45 min	1:4	McCarthy TJ et al., Fund. Appl. Toxicol. 22 (1994), 543
1296	37	7.4	PBS	40 min	2.5:1	Potter DW et al., Toxicol. Lett. 62 (1992), 275
1297		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
1298		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
1299	25	7.4	PBS, max 20% DMSO	120 min	1:129	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1300		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
1301	25	7.4	PBS, max 20% DMSO	120 min	1:83.6	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1302	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004
1303	37	7.4	PBS	45 min	1:400	McCarthy TJ et al., Fund. Appl. Toxicol. 22 (1994), 543
1304	25	7.4	PBS, max 20% DMSO	120 min	1:1.84	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1305	37	7.4	PBS	45 min	1:40	McCarthy TJ et al., Fund. Appl. Toxicol. 22 (1994), 543
1306	37	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1307	40	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1308	25	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1309	26	10.5	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1310	37	10	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385

#	Comment
1269	23C pH 7: NR; HPLC-UV(210-300 nm).
1270	33C pH 7: NR; HPLC-UV(210-300 nm).
1271	RP-HPLC-UV (GAS derivat. o-Phthaldialdehyde excit. 350 nm, emis. 420 nm).
1272	UV (GSH derivat. o-phthalaldehyde, excit 350 nm, emiss. 420 nm).
1273	manometric measurement (CO2 evolution); no units in paper.
1274	RC50 assay.
1275	20C pH 7: NR; HPLC-UV(210-300 nm).
1276	
1277	UV(200-800 nm); reactive: non-diss. CCP + RS[-] (pH < pKa).
1278	manometric measurement (CO2 evolution); no units in paper.
1279	RC50 assay.
1280	UV(DTNB, 412 nm).
1281	HPLC-UV(210-300 nm).
1282	UV(270 nm).
1283	UV (DTNB, 412 nm).
1284	HPLC-UV(210-300 nm).
1285	37C pH 7: NR; HPLC-UV(210-300 nm).
1286	HPLC-UV (205 nm).
1287	UV (GSH derivat. o-phthalaldehyde, excit 350 nm, emiss. 420 nm).
1288	RP-HPLC-UV (GAS derivat. o-Phthaldialdehyde excit. 350 nm, emis. 420 nm).
1289	UV (GSH-conjugate).
1290	est. from pH 6.5: k2(est. pH 7.5) = 10*k2(exp. pH 6.5); UV.
1291	UV (DTNB; 412 nm).
1292	UV(DTNB, 412 nm).
1293	UV (GSH derivat. o-phthalaldehyde, excit 350 nm, emiss. 420 nm).
1294	RP-HPLC-UV (GAS derivat. o-Phthaldialdehyde excit. 350 nm, emis. 420 nm).
1295	UV (DTNB, 412 nm).
1296	HPLC-Scintillator; Use of [14C]-ethyl acrylate.
1297	RC50 assay.
1298	RC50 assay.
1299	UV (DTNB; 412 nm), assum. pseudo 1st order, accounts for oxidative GSSH formation
1300	RC50 assay.
1301	UV (DTNB; 412 nm), assum. pseudo 1st order, accounts for oxidative GSSH formation
1302	UV(DTNB, 412 nm).
1303	UV (DTNB, 412 nm).
1304	UV (DTNB; 412 nm).
1305	0.406 ± 0.059* | * = Bifunct. ester calc. as two indep. esters; UV (DTNB).
1306	HPLC-UV(210-300 nm).
1307	HPLC-UV(210-300 nm).
1308	HPLC-UV(210-300 nm).
1309	HPLC-UV(210-300 nm).
1310	37C pH 7: NR; HPLC-UV(210-300 nm).

#	Mechanism
1269	
1270	
1271	Nucleophilic substitution, first order (SN1)
1272	Michael-type nucleophilic addition
1273	
1274	
1275	
1276	Nucleophilic olefinic addition
1277	Nucleophilic olefinic addition
1278	
1279	
1280	
1281	
1282	Michael-type nucleophilic addition
1283	Michael-type nucleophilic addition
1284	
1285	
1286	Michael-type nucleophilic addition
1287	Michael-type nucleophilic addition
1288	
1289	
1290	
1291	Michael-type nucleophilic addition
1292	Michael-type nucleophilic addition
1293	Michael-type nucleophilic addition
1294	
1295	
1296	
1297	Nucleophilic substitution, second order (SN2)
1298	Nucleophilic substitution, second order (SN2)
1299	Michael-type nucleophilic addition
1300	Nucleophilic substitution, second order (SN2)
1301	Michael-type nucleophilic addition
1302	Michael-type nucleophilic addition
1303	
1304	Michael-type nucleophilic addition
1305	
1306	
1307	
1308	
1309	
1310	

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1311	72178-02-0	Fomesafen	Glutathione	k(GSH)	M-1 min-1	NR		
1312	100784-20-1	Halosulfuron-methyl	Glutathione	k(GSH)	M-1 min-1	0		
1313	100784-20-1	Halosulfuron-methyl	Glutathione	k(GSH)	M-1 min-1	0		
1314	2499-95-8	Hexyl acrylate	Glutathione	k(GSH)	M-1 min-1	31	2	1.48
1315	2499-95-8	Hexyl acrylate	Glutathione	k(GSH)	M-1 min-1	20.3	1.73	1.31
1316	25584-83-2	Hydroxyl propyl acrylate	Glutathione	k(GSH)	M-1 min-1			1.47
1317	25584-83-2	Hydroxyl propyl acrylate	Glutathione	k(GSH)	M-1 min-1	42.1	5.73	1.47
1318	25584-83-2	Hydroxyl propyl acrylate	Glutathione	k(GSH)	M-1 min-1			1.47
1319	64-69-7	Iodoacetic acid	Glutathione	k(GSH)	M-1 min-1	14.9	1.2	1.17
1320	624-75-9	Iodoacetonitrile	Glutathione	k(GSH)	M-1 min-1			1.4
1321	106-63-8	Isobutyl acrylate	Glutathione	k(GSH)	M-1 min-1	65	0.5	1.81
1322	106-63-8	Isobutyl acrylate	Glutathione	k(GSH)	M-1 min-1			1.62
1323	106-63-8	Isobutyl acrylate	Glutathione	k(GSH)	M-1 min-1	29.3	3.34	1.62
1324	106-63-8	Isobutyl acrylate	Glutathione	k(GSH)	M-1 min-1			1.62
1325	106-63-8	Isobutyl acrylate	Glutathione	k(GSH)	M-1 min-1			1.47
1326	97-86-9	Isobutyl methacrylate	Glutathione	k(GSH)	M-1 min-1	1.4	0.4	0.14
1327	97-86-9	Isobutyl methacrylate	Glutathione	k(GSH)	M-1 min-1	0.19	0.04	-0.73
1328	4655-34-9	Isopropyl methacrylate	Glutathione	k(GSH)	M-1 min-1	NR		-1
1329	3196-15-4	Methyl 2-bromobutyrate	Glutathione	k(GSH)	M-1 min-1			0.71
1330	96-33-3	Methyl acrylate	Glutathione	k(GSH)	M-1 min-1	11.4	0.3	1.06
1331	96-33-3	Methyl acrylate	Glutathione	k(GSH)	M-1 min-1	61	1	1.78
1332	96-33-3	Methyl acrylate	Glutathione	k(GSH)	M-1 min-1	52	5	1.72
1333	623-43-8	Methyl crotonate	Glutathione	k(GSH)	M-1 min-1	0.164	0.005	-0.79
1334	80-62-6	Methyl methacrylate	Glutathione	k(GSH)	M-1 min-1	0.072	0.004	-1.14
1335	80-62-6	Methyl methacrylate	Glutathione	k(GSH)	M-1 min-1	6	2	0.78
1336	80-62-6	Methyl methacrylate	Glutathione	k(GSH)	M-1 min-1	0.2	0.04	-0.7
1337	80-62-6	Methyl methacrylate	Glutathione	k(GSH)	M-1 min-1	3.25E-01	5.90E-02	-0.49
1338	922-67-8	Methyl propiolate	Glutathione	k(GSH)	M-1 min-1	117	8	2.07
1339	6622-76-0	Methyl tiglate	Glutathione	k(GSH)	M-1 min-1	0.007	0.001	-2.15
1340	7367-81-9	Methyl trans-2-octenoate	Glutathione	k(GSH)	M-1 min-1			-0.105
1341	78-94-4	Methyl vinyl ketone	Glutathione	k(GSH)	M-1 min-1	7620	360	3.88
1342	51218-45-2	Metolachlor	Glutathione	k(GSH)	M-1 min-1	2.1		0.32
1343		N.N-dipropyl-2-chloroacetamide	Glutathione	k(GSH)	M-1 min-1	0.084		-1.08
1344		N.N-dipropyl-2-chloroacetamide	Glutathione	k(GSH)	M-1 min-1	0.39		-0.41
1345		N.N-dipropyl-2-chloroacetamide	Glutathione	k(GSH)	M-1 min-1	1.3		0.1
1346		N.N-dipropyl-2-chloroacetamide	Glutathione	k(GSH)	M-1 min-1	5.1		0.71
1347		N.N-dipropyl-2-chloroacetamide	Glutathione	k(GSH)	M-1 min-1	18		1.26
1348	141-32-2	n-Butyl acrylate	Glutathione	k(GSH)	M-1 min-1	8.54	0.2	0.93
1349	141-32-2	n-Butyl acrylate	Glutathione	k(GSH)	M-1 min-1	38.7	3.3	1.59
1350	97-88-1	n-Butyl methacrylate	Glutathione	k(GSH)	M-1 min-1	NR		
1351	31217-72-8	N-Ethyl-2-methylmaleimide	Glutathione	k(GSH)	M-1 min-1	2.81E+02		2.45
1352	128-53-0	N-Ethylmaleimide	Glutathione	k(GSH)	M-1 min-1	1.38E+05		5.14
1353	128-53-0	N-Ethylmaleimide	Glutathione	k(GSH)	M-1 min-1	2.26E+06	9.60E+04	6.35

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1311	37	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1312	36	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1313	36	9	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1314	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004
1315	20	8.8	Tetraborate buffer	1 h	1:4 - 1:16	Freidig AP et al., Environ. Toxicol. Chem. 18 (1999), 1133
1316	20	8.8	Tetraborate buffer	1 h	El excess	Freidig AP et al., Environ. Sci. Technol. 33 (1999), 3038
1317	20	8.8	Tetraborate buffer	1 h	1:4 - 1:16	Freidig AP et al., Environ. Toxicol. Chem. 18 (1999), 1133
1318	20	8.8	Tetraborate buffer	1 h	1:4 - 1:16	Freidig AP et al., Environ. Toxicol. Chem. 18 (1999), 1133
1319	37.5	7.4	Hydrogen carbonate buffer	40 min	(different)	Dickens F, Biochem. J. 17 (1933), 1141
1320		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
1321	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004
1322	20	8.8	Tetraborate buffer	1 h	El excess	Freidig AP et al., Environ. Sci. Technol. 33 (1999), 3038
1323	20	8.8	Tetraborate buffer	1 h	1:4 - 1:16	Freidig AP et al., Environ. Toxicol. Chem. 18 (1999), 1133
1324	20	8.8	Tetraborate buffer	1 h	1:4 - 1:16	Freidig AP et al., Environ. Toxicol. Chem. 18 (1999), 1133
1325	30	7.65	PBS		1:4 - 1:20	Harder A et al., Environ. Sci. Technol. 37 (2003), 4955
1326	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004
1327	20	8.8	Tetraborate buffer	24 h	1:4 - 1:16	Freidig AP et al., Environ. Toxicol. Chem. 18 (1999), 1133
1328	20	8.8	Tetraborate buffer	24 h	1:4 - 1:16	Freidig AP et al., Environ. Toxicol. Chem. 18 (1999), 1133
1329		7.4	PBS, max. 20% DMSO	120 min	(different)	Roberts DW et al., Chem. Res. Toxicol. 23 (2010), 228
1330	25	7.4	PBS, max 20% DMSO	120 min	1:14.6	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1331	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004
1332	37	7.4	PBS	45 min	1:4	McCarthy TJ et al., Fund. Appl. Toxicol. 22 (1994), 543
1333	25	7.4	PBS, max 20% DMSO	120 min	1:234	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1334	25	7.4	PBS, max 20% DMSO	120 min	1:276	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1335	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004
1336	20	8.8	Tetraborate buffer	24 h	1:4 - 1:16	Freidig AP et al., Environ. Toxicol. Chem. 18 (1999), 1133
1337	37	7.4	PBS	45 min	1:400	McCarthy TJ et al., Fund. Appl. Toxicol. 22 (1994), 543
1338	25	7.4	PBS, max 20% DMSO	120 min	1:2.33	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1339	25	7.4	PBS, max 20% DMSO	120 min	1:116	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1340	25	7.4	PBS, max 20% DMSO	120 min		Wondrousch D et al., J. Phys. Chem. Lett. 1 (2010), 1605
1341	20	8.8	Tetraborate buffer, water, methanol	max. 24h	El excess	Freidig AP, Models for Risk Assessment of Reactive Chemicals i (2000)
1342	37	9	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1343	10	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1344	25	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1345	37	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1346	50	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1347	65	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1348	25	7.4	PBS, max 20% DMSO	120 min	1:19.4	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1349	37	7.4	PBS	45 min	1:4	McCarthy TJ et al., Fund. Appl. Toxicol. 22 (1994), 543
1350	37	7.4	PBS	45 min	1:400	McCarthy TJ et al., Fund. Appl. Toxicol. 22 (1994), 543
1351	25	7.2	Aqueous buffer			Kosover EM, Chem. Biochem. React. 6 (2009), 549
1352	25	7.3	Aqueous buffer			Kosover EM, Chem. Biochem. React. 6 (2009), 549
1353	25	4	Citrate/phosphate 0.2 M			Drobnica L et al., Biochim. Biophys. Acta 585 (1979), 462

#	Comment
1311	HPLC-UV(210-300 nm).
1312	HPLC-UV(210-300 nm).
1313	HPLC-UV(210-300 nm).
1314	UV(DTNB, 412 nm).
1315	UV (GSH derivat. o-phthalaldehyde, excit 350 nm, emiss. 420 nm).
1316	HPLC-UV [53].
1317	paper: log k=1.62; UV (GSH deriv. o-phthalaldehyde: ex. 350 nm, em. 420 nm).
1318	UV (GSH derivat. o-phthalaldehyde, excit 350 nm, emiss. 420 nm).
1319	manometric measurement (CO2 evolution); no units in paper.
1320	RC50 assay.
1321	UV(DTNB, 412 nm).
1322	HPLC-UV [53].
1323	paper: log k=1.47; UV (GSH deriv. o-phthalaldehyde: ex. 350 nm, em. 420 nm).
1324	UV (GSH derivat. o-phthalaldehyde, excit 350 nm, emiss. 420 nm).
1325	RP-HPLC-UV (GAS derivat. o-Phthaldialdehyde excit. 350 nm, emis. 420 nm).
1326	UV(DTNB, 412 nm).
1327	UV (GSH derivat. o-phthalaldehyde, excit 350 nm, emiss. 420 nm).
1328	UV (GSH derivat. o-phthalaldehyde, excit 350 nm, emiss. 420 nm).
1329	RC50 assay.
1330	UV (DTNB; 412 nm).
1331	UV(DTNB, 412 nm).
1332	UV (DTNB, 412 nm).
1333	UV (DTNB; 412 nm), assum. pseudo 1st order, accounts for oxidative GSSH formation
1334	UV (DTNB; 412 nm), assum. pseudo 1st order, accounts for oxidative GSSH formation
1335	UV(DTNB, 412 nm).
1336	UV (GSH derivat. o-phthalaldehyde, excit 350 nm, emiss. 420 nm).
1337	UV (DTNB, 412 nm).
1338	UV (DTNB; 412 nm).
1339	UV (DTNB; 412 nm), assum. pseudo 1st order, accounts for oxidative GSSH formation
1340	UV (DTNB; 412 nm).
1341	HPLC-UV (isoindole; ex. 350 nm, em. 420 nm).
1342	20C pH 7: NR; HPLC-UV(210-300 nm).
1343	HPLC-UV(210-300 nm).
1344	HPLC-UV(210-300 nm).
1345	HPLC-UV(210-300 nm).
1346	HPLC-UV(210-300 nm).
1347	HPLC-UV(210-300 nm).
1348	UV (DTNB; 412 nm).
1349	UV (DTNB, 412 nm).
1350	UV (DTNB, 412 nm).
1351	UV(300 nm); stable in buffer.
1352	estimated from lower pH.
1353	

#	Mechanism
1311	
1312	
1313	
1314	Michael-type nucleophilic addition
1315	Michael-type nucleophilic addition
1316	Michael-type nucleophilic addition
1317	Michael-type nucleophilic addition
1318	Michael-type nucleophilic addition
1319	
1320	
1321	Michael-type nucleophilic addition
1322	Michael-type nucleophilic addition
1323	Michael-type nucleophilic addition
1324	Michael-type nucleophilic addition
1325	
1326	Michael-type nucleophilic addition
1327	Michael-type nucleophilic addition
1328	NOT Michael-type nucleophilic addition
1329	Nucleophilic substitution, second order (SN2)
1330	Michael-type nucleophilic addition
1331	Michael-type nucleophilic addition
1332	
1333	Michael-type nucleophilic addition
1334	Michael-type nucleophilic addition
1335	Michael-type nucleophilic addition
1336	Michael-type nucleophilic addition
1337	
1338	Michael-type nucleophilic addition
1339	Michael-type nucleophilic addition
1340	Michael-type nucleophilic addition
1341	Michael-type nucleophilic addition
1342	
1343	
1344	
1345	
1346	
1347	
1348	Michael-type nucleophilic addition
1349	
1350	
1351	Michael-type nucleophilic addition
1352	Michael-type nucleophilic addition
1353	Nucleophilic olefinic addition

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1354	586-96-9	Nitrosobenzene	Glutathione	k(GSH)	M-1 min-1	3.00E+05		5.48
1355	925-60-0	n-Propyl acrylate	Glutathione	k(GSH)	M-1 min-1	10.2	0.3	1.01
1356	106-51-4	p-Benzoquinone	Glutathione	k(GSH)	M-1 min-1	1712	148	3.23
1357	103-72-0	Phenyl isothiocyanate	Glutathione	k(GSH)	M-1 min-1	3.53E+04	1.44E+03	4.55
1358	51218-49-6	Pretilachlor	Glutathione	k(GSH)	M-1 min-1	0.588		-0.23
1359	1918-16-7	Propachlor	Glutathione	k(GSH)	M-1 min-1	32.4		1.51
1360	10477-47-1	Propargyl acrylate	Glutathione	k(GSH)	M-1 min-1			1.711
1361	13861-22-8	Propargyl methacrylate	Glutathione	k(GSH)	M-1 min-1			-0.658
1362	16755-07-0	Showdomycin	Glutathione	k(GSH)	M-1 min-1	1.77E+04		4.25
1363	96-09-3	Styrene oxide	Glutathione	k(GSH)	M-1 min-1			0.11
1364	1663-39-4	tert-Butyl acrylate	Glutathione	k(GSH)	M-1 min-1			0.398
1365	5292-43-3	tert-Butyl bromoacetate	Glutathione	k(GSH)	M-1 min-1	1.00E+02	3.00E+00	2
1366	17831-71-9	Tetraethyleneglycol diacrylate	Glutathione	k(GSH)	M-1 min-1	143	4	2.16
1367	109-17-1	Tetraethyleneglycol dimethacrylate	Glutathione	k(GSH)	M-1 min-1	1.45	0.17	0.16
1368	2455-24-5	Tetrahydrofurfuryl methacrylate	Glutathione	k(GSH)	M-1 min-1	0.3	0.03	-0.52
1369	25152-84-5	trans.trans.2.4-Decadienal	Glutathione	k(GSH)	M-1 min-1	25	1	1.39
1370	5910-87-2	trans.trans-2.4-Nonadienal	Glutathione	k(GSH)	M-1 min-1	17	2	1.23
1371	557-48-2	trans-2-cis-6-Nonadienal	Glutathione	k(GSH)	M-1 min-1	65	1	1.82
1372	18829-55-5	trans-2-Heptenal	Glutathione	k(GSH)	M-1 min-1	56	4	1.75
1373	6728-26-3	trans-2-Hexenal	Glutathione	k(GSH)	M-1 min-1	54	5	1.73
1374	18829-56-6	trans-2-Nonenal	Glutathione	k(GSH)	M-1 min-1	39	4	1.59
1375	2548-87-0	trans-2-Octenal	Glutathione	k(GSH)	M-1 min-1	43	4	1.64
1376	1576-87-0	trans-2-Pentenal	Glutathione	k(GSH)	M-1 min-1	89	2	1.95
1377	55335-06-3	Triclopyr	Glutathione	k(GSH)	M-1 min-1	0		
1378	58138-08-2	Tridiphane	Glutathione	k(GSH)	M-1 min-1	0.156		-0.81
1379	58138-08-2	Tridiphane	Glutathione	k(GSH)	M-1 min-1	0.032		-1.49
1380	107-13-1	Acrylonitrile	Diglycine	k(Gly)	M-1 min-1	5.72E+06		6.76
1381	3623-15-2	1-Phenyl-2-propyn-1-one	Glycine	k(Gly)	M-1 min-1	67.8		1.83
1382	79-06-1	Acrylamide	Glycine	k(Gly)	M-1 min-1	1.56E+07		7.19
1383	107-13-1	Acrylonitrile	Glycine	k(Gly)	M-1 min-1	1.22E+08		8.09
1384	107-13-1	Acrylonitrile	Glycine	k(Gly)	M-1 min-1	2.35E+06		6.37
1385	96-33-3	Methyl acrylate	Glycine	k(Gly)	M-1 min-1	4.56E+08		8.66
1386	3623-15-2	1-Phenyl-2-propyn-1-one	Glycine ethyl ester	k(Gly)	M-1 min-1	27.96		1.45
1387		1-(3-Nitrophenyl)-2-propyn-1-one	N-Glycylglycine	k(Gly)	M-1 min-1	126.6		2.1
1388		1-(4-Chlorophenyl)-2-propyn-1-one	N-Glycylglycine	k(Gly)	M-1 min-1	51.3		1.71
1389		1-(4-Cyanophenyl)-2-propyn-1-one	N-Glycylglycine	k(Gly)	M-1 min-1	130.2		2.11
1390	16469-68-4	1-(4-Methoxyphenyl)-2-propyn-1-one	N-Glycylglycine	k(Gly)	M-1 min-1	16.02		1.2
1391		1-(4-Methylphenyl)-2-propyn-1-one	N-Glycylglycine	k(Gly)	M-1 min-1	27.96		1.45
1392	3623-15-2	1-Phenyl-2-propyn-1-one	N-Glycylglycine	k(Gly)	M-1 min-1	35.7		1.55
1393	107-13-1	Acrylonitrile	Tetraglycine	k(Gly)	M-1 min-1	4.99E+06		6.7
1394	107-13-1	Acrylonitrile	Triglycine	k(Gly)	M-1 min-1	5.34E+06		6.73
1395	95-50-1	1.2-Dichlorobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	2.20E-05		-4.66
1396	528-29-0	1.2-Dinitrobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	1.30E-02		-1.89

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1354	37	7.4				Eyer P, Biological Oxidation of Nitrogen in Orga... (1985), 386
1355	25	7.4	PBS, max 20% DMSO	120 min	1:13.3	Böhme A et al., Chem. Res. Toxicol. 22 (2009), 742
1356	25	8	PBS 0.1 M	10-180 min	El excess	Chan K et al., J. Appl. Toxicol. 28 (2008), 608
1357	25	4	Citrate/phosphate 0.2 M			Drobnica L et al., Biochim. Biophys. Acta 585 (1979), 462
1358	40	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1359	25	9	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1360	25	7.4	PBS, max 20% DMSO	120 min		Wondrousch D et al., J. Phys. Chem. Lett. 1 (2010), 1605
1361	25	7.4	PBS, max 20% DMSO	120 min		Wondrousch D et al., J. Phys. Chem. Lett. 1 (2010), 1605
1362	25	7.2	Aqueous buffer			Kosover EM, Chem. Biochem. React. 6 (2009), 549
1363	30	7.65	PBS		1:4 - 1:20	Harder A et al., Environ. Sci. Technol. 37 (2003), 4955
1364	25	7.4	PBS, max 20% DMSO	120 min		Wondrousch D et al., J. Phys. Chem. Lett. 1 (2010), 1605
1365	50	9.2	PBS 0.1 M		2.5:1 to 200:1	van der Aar EM et al., Biochem. J. 320 (1996), 531
1366	37	7.4	PBS	45 min	1:4	McCarthy TJ et al., Fund. Appl. Toxicol. 22 (1994), 543
1367	37	7.4	PBS	45 min	1:40	McCarthy TJ et al., Fund. Appl. Toxicol. 22 (1994), 543
1368	20	8.8	Tetraborate buffer	24 h	1:4 - 1:16	Freidig AP et al., Environ. Toxicol. Chem. 18 (1999), 1133
1369	25	8	PBS 0.1 M, DMSO		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1027
1370	25	8	PBS 0.1 M, DMSO		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1027
1371	25	8	PBS 0.1 M, DMSO		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1027
1372	25	8	PBS 0.1 M, DMSO		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1027
1373	25	8	PBS 0.1 M, DMSO		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1027
1374	25	8	PBS 0.1 M, DMSO		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1027
1375	25	8	PBS 0.1 M, DMSO		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1027
1376	25	8	PBS 0.1 M, DMSO		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1027
1377	37	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1378	25	7	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1379	26	9	EDTA buffer	max. 16h	50:1	Clarke ED et al., Pestic. Sci. 54 (1998), 385
1380	30	8.4				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1381	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1382	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1383	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1384	30	8.4				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1385	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1386	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1387	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1388	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1389	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1390	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1391	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1392	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1393	30	8.4				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1394	30	8.4				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1395	150		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1396	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273

#	Comment
1354	
1355	UV (DTNB; 412 nm).
1356	UV(DTNB, 412 nm).
1357	
1358	HPLC-UV(210-300 nm).
1359	20C pH 7: NR; HPLC-UV(210-300 nm).
1360	UV (DTNB; 412 nm).
1361	UV (DTNB; 412 nm).
1362	UV(280 nm).
1363	RP-HPLC-UV (GAS derivat. o-Phthaldialdehyde excit. 350 nm, emis. 420 nm).
1364	UV (DTNB; 412 nm).
1365	UV (GSH-conjugate).
1366	UV (DTNB, 412 nm).
1367	0.725 ± 0.087* | * = Bifunct. ester calc. as two indep. esters; UV (DTNB).
1368	UV (GSH derivat. o-phthalaldehyde, excit 350 nm, emiss. 420 nm).
1369	UV (DTNB, 412 nm).
1370	UV (DTNB, 412 nm).
1371	UV (DTNB, 412 nm).
1372	UV (DTNB, 412 nm).
1373	UV (DTNB, 412 nm).
1374	UV (DTNB, 412 nm).
1375	UV (DTNB, 412 nm).
1376	UV (DTNB, 412 nm).
1377	HPLC-UV(210-300 nm).
1378	HPLC-UV(210-300 nm).
1379	HPLC-UV(210-300 nm).
1380	
1381	UV(max. abs. enaminone) and 1H-NMR.
1382	
1383	
1384	other pH values in paper.
1385	
1386	UV(max. abs. enaminone) and 1H-NMR.
1387	UV(max. abs. enaminone) and 1H-NMR.
1388	UV(max. abs. enaminone) and 1H-NMR.
1389	UV(max. abs. enaminone) and 1H-NMR.
1390	UV(max. abs. enaminone) and 1H-NMR.
1391	UV(max. abs. enaminone) and 1H-NMR.
1392	UV(max. abs. enaminone) and 1H-NMR.
1393	
1394	
1395	per chlorine atom: 1.1E-05.
1396	

#	Mechanism
1354	
1355	Michael-type nucleophilic addition
1356	
1357	Nucleophilic olefinic addition
1358	
1359	
1360	Michael-type nucleophilic addition
1361	Michael-type nucleophilic addition
1362	Michael-type nucleophilic addition
1363	
1364	Michael-type nucleophilic addition
1365	Nucleophilic aromatic substitution (SNAr)
1366	
1367	
1368	Michael-type nucleophilic addition
1369	Michael-type nucleophilic addition
1370	Michael-type nucleophilic addition
1371	Michael-type nucleophilic addition
1372	Michael-type nucleophilic addition
1373	Michael-type nucleophilic addition
1374	Michael-type nucleophilic addition
1375	Michael-type nucleophilic addition
1376	Michael-type nucleophilic addition
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1380	Michael-type nucleophilic addition
1381	Michael-type nucleophilic addition
1382	Michael-type nucleophilic addition
1383	Michael-type nucleophilic addition
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1386	Michael-type nucleophilic addition
1387	Michael-type nucleophilic addition
1388	Michael-type nucleophilic addition
1389	Michael-type nucleophilic addition
1390	Michael-type nucleophilic addition
1391	Michael-type nucleophilic addition
1392	Michael-type nucleophilic addition
1393	Michael-type nucleophilic addition
1394	Michael-type nucleophilic addition
1395	Nucleophilic aromatic substitution (SNAr)
1396	Nucleophilic aromatic substitution (SNAr)

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1397	528-29-0	1.2-Dinitrobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	3.92E-02		-1.41
1398	528-29-0	1.2-Dinitrobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	1.17E-01		-0.93
1399	541-73-1	1.3-Dichlorobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	5.60E-05		-4.25
1400	106-46-7	1.4-Dichlorobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	2.00E-05		-4.8
1401	100-25-4	1.4-Dinitrobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	1.06E-01		-0.97
1402	100-25-4	1.4-Dinitrobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	3.54E-02		-1.45
1403	100-25-4	1.4-Dinitrobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	1.11E-01		-0.95
1404	584-48-5	1-Bromo-2.4-dinitrobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	2.46E+00		0.39
1405	584-48-5	1-Bromo-2.4-dinitrobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	2.20E-01		-0.66
1406	584-48-5	1-Bromo-2.4-dinitrobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	1.02		0.01
1407	584-48-5	1-Bromo-2.4-dinitrobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	1.89		0.28
1408	97-00-7	1-Chloro-2.4-dinitrobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	4.95E+00		0.69
1409	97-00-7	1-Chloro-2.4-dinitrobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	3.90E-01		-0.41
1410	97-00-7	1-Chloro-2.4-dinitrobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	1.05		0.02
1411	97-00-7	1-Chloro-2.4-dinitrobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	1.63		0.21
1412	97-00-7	1-Chloro-2.4-dinitrobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	2.9		0.46
1413	97-00-7	1-Chloro-2.4-dinitrobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	2.98		0.47
1414	97-00-7	1-Chloro-2.4-dinitrobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	3.26		0.51
1415	2401-85-6	1-Chloro-2.4-dinitronaphthalene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	4.42E+01		1.65
1416	348-51-6	1-Chloro-2-fluorobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	4.80E-03		-2.32
1417		1-Chloro-3-fluorobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	3.30E-03		-2.48
1418	98-56-6	1-Chloro-4-(trifluoromethyl)benzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	3.50E-04		-3.46
1419	352-33-0	1-Chloro-4-fluorobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	7.00E-04		-3.15
1420	402-44-8	1-Fluoro-4-(trifluoromethyl)benzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	2.70E-01		-0.57
1421	709-49-9	1-Iodo-2.4-dinitrobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	2.28E-01		-0.64
1422	709-49-9	1-Iodo-2.4-dinitrobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	4.55E-01		-0.34
1423		2.4-Dinitro-5-ethoxychlorobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	1.10E+00		0.04
1424		2.4-Dinitro-5-ethoxychlorobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	1.12E-01		-0.95
1425		2.4-Dinitro-5-ethoxychlorobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	2.20E-01		-0.66
1426		2.4-Dinitro-5-ethoxychlorobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	4.70E-01		-0.33
1427		2.4-Dinitro-5-ethoxychlorobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	6.10E-01		-0.21
1428		2-Bromo-1.6.8-trinitronaphthalene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	5.70E+00		0.76
1429		2-Bromo-5-nitrobenzonitrile	Ethylate. Sodium	k(Ethylate)	M-1 min-1	1.67		0.22
1430		2-Bromo-5-nitrobenzonitrile	Ethylate. Sodium	k(Ethylate)	M-1 min-1	5.50E-01		-0.26
1431	606-21-3	2-Chloro-1.3-dinitrobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	8.82E-01		-0.05
1432		2-Chloro-1.6.8-trinitronaphthalene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	rapid		
1433	16588-02-6	2-Chloro-5-nitrobenzonitrile	Ethylate. Sodium	k(Ethylate)	M-1 min-1	2.54		0.4
1434	16588-02-6	2-Chloro-5-nitrobenzonitrile	Ethylate. Sodium	k(Ethylate)	M-1 min-1	8.17E-01		-0.09
1435	98-15-7	3-Chlorobenzotrifluoride	Ethylate. Sodium	k(Ethylate)	M-1 min-1	3.50E-05		-4.46
1436	401-80-9	3-Fluorobenzotrifluoride	Ethylate. Sodium	k(Ethylate)	M-1 min-1	6.50E-03		-2.19
1437		4-Bromo-3-nitrobenzonitrile	Ethylate. Sodium	k(Ethylate)	M-1 min-1	3.08E-02		-1.51
1438	5264-65-3	4-Chloro-3.5-dinitrotoluene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	1.55E-01		-0.81
1439	939-80-0	4-Chloro-3-nitrobenzonitrile	Ethylate. Sodium	k(Ethylate)	M-1 min-1	4.24E-02		-1.37

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1397	35		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1398	45		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1399	150		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1400	150		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1401	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1402	35		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1403	45		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1404	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1405	0		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1406	15		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1407	15		Ethanol			Landsteiner et al., J. Exp. Med. 64 (1936), 625
1408	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1409	0		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1410	10		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1411	15		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1412	20		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1413	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1414	15		Ethanol			Landsteiner et al., J. Exp. Med. 64 (1936), 625
1415	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1416	150		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1417	150		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1418	150		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1419	150		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1420	150		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1421	15		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1422	15		Ethanol			Landsteiner et al., J. Exp. Med. 64 (1936), 625
1423	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1424	0		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1425	10		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1426	15		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1427	20		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1428	15		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1429	35		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1430	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1431	50		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1432	0		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1433	35		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1434	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1435	150		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1436	150		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1437	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1438	50		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1439	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273

#	Comment
1397	
1398	
1399	per chlorine atom: 2.8E-05.
1400	per chlorine atom: 8.E-06.
1401	
1402	
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#	Mechanism
1397	Nucleophilic aromatic substitution (SNAr)
1398	Nucleophilic aromatic substitution (SNAr)
1399	Nucleophilic aromatic substitution (SNAr)
1400	Nucleophilic aromatic substitution (SNAr)
1401	Nucleophilic aromatic substitution (SNAr)
1402	Nucleophilic aromatic substitution (SNAr)
1403	Nucleophilic aromatic substitution (SNAr)
1404	Nucleophilic aromatic substitution (SNAr)
1405	Nucleophilic aromatic substitution (SNAr)
1406	Nucleophilic aromatic substitution (SNAr)
1407	
1408	Nucleophilic aromatic substitution (SNAr)
1409	Nucleophilic aromatic substitution (SNAr)
1410	Nucleophilic aromatic substitution (SNAr)
1411	Nucleophilic aromatic substitution (SNAr)
1412	Nucleophilic aromatic substitution (SNAr)
1413	Nucleophilic aromatic substitution (SNAr)
1414	
1415	Nucleophilic aromatic substitution (SNAr)
1416	Nucleophilic aromatic substitution (SNAr)
1417	Nucleophilic aromatic substitution (SNAr)
1418	Nucleophilic aromatic substitution (SNAr)
1419	Nucleophilic aromatic substitution (SNAr)
1420	Nucleophilic aromatic substitution (SNAr)
1421	Nucleophilic aromatic substitution (SNAr)
1422	
1423	Nucleophilic aromatic substitution (SNAr)
1424	Nucleophilic aromatic substitution (SNAr)
1425	Nucleophilic aromatic substitution (SNAr)
1426	Nucleophilic aromatic substitution (SNAr)
1427	Nucleophilic aromatic substitution (SNAr)
1428	Nucleophilic aromatic substitution (SNAr)
1429	Nucleophilic aromatic substitution (SNAr)
1430	Nucleophilic aromatic substitution (SNAr) in eqilibrium with imino esters
1431	Nucleophilic aromatic substitution (SNAr)
1432	Nucleophilic aromatic substitution (SNAr)
1433	Nucleophilic aromatic substitution (SNAr)
1434	Nucleophilic aromatic substitution (SNAr) in eqilibrium with imino esters
1435	Nucleophilic aromatic substitution (SNAr)
1436	Nucleophilic aromatic substitution (SNAr)
1437	Nucleophilic aromatic substitution (SNAr) in eqilibrium with imino esters
1438	Nucleophilic aromatic substitution (SNAr)
1439	Nucleophilic aromatic substitution (SNAr) in eqilibrium with imino esters

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1440	100-00-5	4-Chloronitrobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	4.30E-04		-3.37
1441	350-46-9	4-Fluoronitrobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	1.45E-01		-0.84
1442	2213-81-2	4-tert-Butyl-2.6-dinitrochlorobenzene	Ethylate. Sodium	k(Ethylate)	M-1 min-1	2.73E-01		-0.56
1443	108-73-6	1.3.5-Trihydroxybenzene	4.6-Dinitrobenzofuroxan	k(DNBF)	M-1 min-1	47400		4.68
1444	621-23-8	1.3.5-Trimethoxybenzene	4.6-Dinitrobenzofuroxan	k(DNBF)	M-1 min-1	1230		3.09
1445	151-10-0	1.3-Dimethoxybenzene	4.6-Dinitrobenzofuroxan	k(DNBF)	M-1 min-1	31.2		1.49
1446	500-99-2	3.5-Dimethoxyphenol	4.6-Dinitrobenzofuroxan	k(DNBF)	M-1 min-1	7380		3.87
1447	108-46-3	Resorcinol	4.6-Dinitrobenzofuroxan	k(DNBF)	M-1 min-1	96		1.98
1448	2634-33-5	1.2-Benzisothiazolin-3-one	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	462		
1449	5910-85-0	2.4-Heptadienal	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	1.83		0.2581513
1450	818-61-1	2-Hydroxyethyl acrylate	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	22.2		3.178151
1451	2682-20-4	2-Methyl-2H-isothiazolin-3-one	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	307.8		
1452	122-57-6	4-Phenyl-3-buten-2-one	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	0.768		-0.1118487
1453	100-43-6	4-Vinylpyridine	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	4.602		0.6581513
1454	23726-94-5	alpha-Damascone	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	1.65		0.2181513
1455	101-86-0	alpha-Hexylcinnamaldehyde	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	NR		
1456	101-39-3	alpha-Methyl cinnamic aldehyde	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	0.042		-1.371849
1457	103-41-3	Benzyl cinnamate	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	0.018		-1.791849
1458	104-55-2	Cinnamaldehyde	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	1.302		0.1181512
1459	5392-40-5	Citral	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	NR		
1460	141-05-9	Diethyl maleate	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	5.598		3.878151
1461	886-38-4	Diphenylcyclopropenone	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	6.12		
1462	140-88-5	Ethyl acrylate	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	6.42		0.8081512
1463	97-90-5	Ethylene glycol dimethacrylate	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	0.468		-0.3318487
1464	19317-11-4	Farnesal	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	NR		
1465	56973-85-4	Galbanone	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	>2.22		0.35
1466	111-80-8	Methyl-2-nonynoate	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	ND		
1467	15646-46-5	Oxazolone	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	22.26		
1468	106-51-4	p-Benzoquinone	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	>924		2.97
1469	2111-75-3	Perillaldehyde	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	ND		

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1440	40		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1441	40		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1442	50		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1443	25		DMSO:water 1:1		Rct excess	Terrier F et al., J. Phys. Org. Chem. 11 (1998), 707
1444	25		DMSO:water 1:1		Rct excess	Terrier F et al., J. Phys. Org. Chem. 11 (1998), 707
1445	25		DMSO:water 1:1		Rct excess	Terrier F et al., J. Phys. Org. Chem. 11 (1998), 707
1446	25		DMSO:water 1:1		Rct excess	Terrier F et al., J. Phys. Org. Chem. 11 (1998), 707
1447	25		DMSO:water 1:1		Rct excess	Terrier F et al., J. Phys. Org. Chem. 11 (1998), 707
1448	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1449	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1450	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1451	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1452	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1453	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1454	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1455	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1456	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1457	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1458	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1459	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1460	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1461	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1462	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1463	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1464	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1465	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1466	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1467	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1468	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1469	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592

#	Comment
1440	
1441	
1442	
1443	Assay: Low pH; stopped flow apparatus
1444	Assay: Low pH; stopped flow apparatus
1445	Assay: Low pH; stopped flow apparatus
1446	Assay: Low pH; stopped flow apparatus
1447	Assay: Low pH; stopped flow apparatus
1448	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h)
1449	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h)
1450	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h
1451	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h)
1452	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h
1453	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h
1454	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h no significant reaction.
1455	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h) calculated as mean of 3 time points.
1456	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h) calculated by t=1440 min point only.
1457	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h)
1458	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h) no significant reaction.
1459	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h)
1460	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h
1461	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h)
1462	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h
1463	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h no significant reaction, but peptide dimerization (Cor1: only oxidization).
1464	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h)
1465	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h
1466	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h)
1467	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h)
1468	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h kinetics cannot be derived; LC-MS.
1469	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h)

#	Mechanism
1440	Nucleophilic aromatic substitution (SNAr)
1441	Nucleophilic aromatic substitution (SNAr)
1442	Nucleophilic aromatic substitution (SNAr)
1443	Electrophilic aromatic substitution (SEAr)
1444	Electrophilic aromatic substitution (SEAr)
1445	Electrophilic aromatic substitution (SEAr)
1446	Electrophilic aromatic substitution (SEAr)
1447	Electrophilic aromatic substitution (SEAr)
1448	NOT Michael-type nucleophilic addition: 1:1 adduct, peptide dimerization (Cor1: adduct + oxidization)
1449	Michael-type nucleophilic addition: 1:1 adducts + oxidization (Cor1: oxidization only)
1450	Michael-type nucleophilic addition: 1:1 adducts
1451	NOT Michael-type nucleophilic addition: 1:1 adduct, peptide dimerization (Cor1: adduct + oxidization)
1452	Michael-type nucleophilic addition: 1:1 adducts
1453	Michael-type nucleophilic addition: 1:1 adducts
1454	Michael-type nucleophilic addition: 1:1 adducts
1455	Michael-type nucleophilic addition: no significant reaction, but peptide dimerization (Cor1: only oxidization)
1456	Michael-type nucleophilic addition: 1:1 adducts (<20%)
1457	Michael-type nucleophilic addition: 1:1 adducts
1458	Michael-type nucleophilic addition: 1:1 adducts only (Cor1: adduct + oxidization)
1459	Schiff base formation
1460	Michael-type nucleophilic addition: 1:1 adducts
1461	Michael-type nucleophilic ring opening: 1:1 adducts (40%) + ring opening products
1462	Michael-type nucleophilic addition: 1:1 adducts
1463	Michael-type nucleophilic addition: 1:1 adducts
1464	Schiff base formation: no significant reaction, but peptide dimerization (Cor1: only oxidization)
1465	Michael-type nucleophilic addition: 1:1 adducts
1466	Michael-type nucleophilic addition: 1:1 adducts (70%) + oxidization + peptide dimerization (Cor1: adducts only)
1467	NOT Michael-type nucleophilic addition: complex products, no direct MA adducts or oxidization
1468	Michael-type nucleophilic addition: adducts, but reoxid. to quinone
1469	Schiff base formation: 1:1 adducts + oxidization

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1470	357650-26-1	Pomarose	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	4.752		0.6781512
1471	116-26-7	Safranal	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	ND		
1472	224031-70-3	Spirogalbanone	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	>0.468		-0.33
1473	3913-81-3	trans-2-Decenal	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	5.646		0.7581512
1474	6728-26-3	trans-2-Hexenal	Cys-Peptide (AcRFAACAA)	k(Cys-P.)	M-1 min-1	14.28		1.158151
1475	107-13-1	Acrylonitrile	beta-Mercaptoisoleucine	k(Cys-Derivatives)	M-1 min-1	2.65E-01		-0.58
1476	107-13-1	Acrylonitrile	beta-Mercaptoisoleucine	k(Cys-Derivatives)	M-1 min-1	2.65E-01		-0.58
1477	107-13-1	Acrylonitrile	beta-Mercaptoisoleucine	k(Cys-Derivatives)	M-1 min-1	3.36E+02		2.53
1478	107-13-1	Acrylonitrile	Cysteine ethyl ester	k(Cys-Derivatives)	M-1 min-1	1.10E+01		1.04
1479	107-13-1	Acrylonitrile	Cysteine ethyl ester	k(Cys-Derivatives)	M-1 min-1	8.52E+01		1.93
1480	107-13-1	Acrylonitrile	Homocysteine	k(Cys-Derivatives)	M-1 min-1	7.2	0.36	0.86
1481	107-13-1	Acrylonitrile	Homocysteine	k(Cys-Derivatives)	M-1 min-1	7.20E+00		0.86
1482	107-13-1	Acrylonitrile	Homocysteine	k(Cys-Derivatives)	M-1 min-1	2.52E+02		2.4
1483	107-13-1	Acrylonitrile	N-Acetyl cysteine	k(Cys-Derivatives)	M-1 min-1	3.44E+00		0.54
1484	107-13-1	Acrylonitrile	N-Acetyl penicillamine	k(Cys-Derivatives)	M-1 min-1	6.24E-02		-1.2
1485	107-13-1	Acrylonitrile	N-Acetyl-beta-mercaptoisoleucine	k(Cys-Derivatives)	M-1 min-1	3.50E-02		-1.45
1486	107-13-1	Acrylonitrile	Penicillamine	k(Cys-Derivatives)	M-1 min-1	3.92E-01		-0.41
1487	107-13-1	Acrylonitrile	Penicillamine	k(Cys-Derivatives)	M-1 min-1	3.90E-01		-0.41
1488	107-13-1	Acrylonitrile	Penicillamine	k(Cys-Derivatives)	M-1 min-1	5.66E+02		2.75
1489	123-73-9	(E)-Crotonaldehyde	Cysteine	k'(Cys)	mol-1 min-1	1.00E+03		3
1490	123-73-9	(E)-Crotonaldehyde	Cysteine	k'(Cys)	mol-1 min-1	9.90E+02		3
1491	123-73-9	(E)-Crotonaldehyde	Thioglycolic acid ethylester	k'(Cys)	mol-1 min-1	6.00E+00		0.78
1492	123-73-9	(E)-Crotonaldehyde	Thioglycolic acid ethylester	k'(Cys)	mol-1 min-1	1.20E+02		2.08
1493		(3.4-dioxocyclohexa-1.5-dien-1-yl)-acetic acid	Cysteine	k(Cys)	M-1 min-1	8.40E+07	10%	7.92
1494	123-73-9	(E)-Crotonaldehyde	Cysteine	k(Cys)	M-1 min-1	5.30E+02		2.73
1495	123-73-9	(E)-Crotonaldehyde	Cysteine	k(Cys)	M-1 min-1		0.11 (log)	3.31
1496	583-63-1	2-Benzoquinone	Cysteine	k(Cys)	M-1 min-1	3.20E+08	10%	8.5
1497	100-50-5	3-Cyclohexene-1-carboxaldehyde	Cysteine	k(Cys)	M-1 min-1		0.03 (log)	2.42
1498		4-[(1Z)-3-oxo-3-phenylprop-1-en-1-yl]-1.2-benzoquinone	Cysteine	k(Cys)	M-1 min-1	1.30E+09	10%	9.12
1499		4-Bromo-1.2-benzoquinone	Cysteine	k(Cys)	M-1 min-1	4.80E+08	10%	8.68
1500	31222-02-3	4-Chloro-1.2-benzoquinone	Cysteine	k(Cys)	M-1 min-1	6.00E+08	10%	8.78
1501		4-Ethylaminium-1.2-benzoquinone	Cysteine	k(Cys)	M-1 min-1	1.60E+09	10%	9.19
1502	29343-52-0	4-Hydroxy-2-nonenal	Cysteine	k(Cys)	M-1 min-1			2.716
1503	16931-17-2	4-Hydroxypentenal	Cysteine	k(Cys)	M-1 min-1	1.50E+03		3.18
1504		4-Isopropyl-1.2-benzoquinone	Cysteine	k(Cys)	M-1 min-1	1.40E+08	10%	8.14
1505	69818-23-1	4-Methoxy-1.2-benzoquinone	Cysteine	k(Cys)	M-1 min-1	2.40E+07	10%	7.38
1506	3131-54-2	4-Methyl-1.2-benzoquinone	Cysteine	k(Cys)	M-1 min-1	2.00E+08	10%	8.31
1507		4-Methylaminium-1.2-benzoquinone	Cysteine	k(Cys)	M-1 min-1	1.90E+09	10%	9.27

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1470	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1471	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1472	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1473	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1474	25	7.5	PBS 0.1 M (75%), ACN (25%)	3 - 1440 min	1:2 - 1:30	Roberts DW et al., Chem. Res. Toxicol. 22 (2009), 592
1475	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1476	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1477	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1478	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1479	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1480	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1481	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1482	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1483	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1484	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1485	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1486	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1487	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1488	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1489	20	7.4	PBS 0.1 M		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1490	20	7.4	no buffer		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1491	20	7.4	no buffer		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1492	20	7.4	PBS 0.1 M		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1493		6.97	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1494	20	7.5				Esterbauer H et al., Tetrahedron 32 (1976), 285
1495		7	PBS, Acetone		1:10	Deneer JW et al., Aquat. Toxicol. 12 (1988), 185
1496		7.13	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1497		7	PBS, Acetone		1:10	Deneer JW et al., Aquat. Toxicol. 12 (1988), 185
1498		7.2	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1499		6.95	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1500		7.11	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1501		7.12	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1502		7.4			El excess	LoPachin RM et al., Toxicol. Sci. 107 (2009), 171
1503	20	7.5				Esterbauer H et al., Tetrahedron 32 (1976), 285
1504		7.13	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1505		7.12	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1506		7.1	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1507		7.2	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498

#	Comment
1470	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h kinetics cannot be derived; LC-MS.
1471	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h)
1472	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h
1473	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h
1474	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm); Light protected; corrected for drowning out effects; LC-MS analysis (after 24h
1475	other pH in paper. Assay: Mikroamp. Titration
1476	Assay: Mikroamp. Titration
1477	k(NH2) of beta-Mercaptoisoleucine. Assay: Mikroamp. Titratior
1478	Assay: Mikroamp. Titration
1479	k(NH2) of Cysteine ethyl ester. Assay: Mikroamp. Titratior
1480	Assay: Mikroamp. Titration
1481	Assay: Mikroamp. Titration
1482	k(NH2) of DL-Homocysteine. Assay: Mikroamp. Titration
1483	Assay: Mikroamp. Titration
1484	Assay: Mikroamp. Titration
1485	Assay: Mikroamp. Titration
1486	other pH: paper. Assay: Mikroamp. Titration
1487	Assay: Mikroamp. Titration
1488	k(NH2) of Penicillamine. Assay: Mikroamp. Titration
1489	
1490	k'(Cys) not increased by buffers.
1491	
1492	
1493	
1494	
1495	HPLC-UV(230 nm).
1496	
1497	HPLC-UV(230 nm).
1498	
1499	
1500	
1501	
1502	UV (DTNB 412 nm).
1503	Cys-diadduct formation k = 66 M-1 min-1.
1504	
1505	
1506	
1507	

#	Mechanism
1470	Michael-type nucleophilic addition: 1:1 adducts
1471	Schiff base formation: 1:1 adducts (Cor1: adduct + oxidization)
1472	Michael-type nucleophilic addition: 1:1 adducts
1473	Michael-type nucleophilic addition: 1:1 adducts + oxidization (10%
1474	Michael-type nucleophilic addition: 1:1 adducts
1475	Michael-type nucleophilic addition
1476	Michael-type nucleophilic addition
1477	Michael-type nucleophilic addition
1478	Michael-type nucleophilic addition
1479	Michael-type nucleophilic addition
1480	Michael-type nucleophilic addition
1481	Michael-type nucleophilic addition
1482	Michael-type nucleophilic addition
1483	Michael-type nucleophilic addition
1484	Michael-type nucleophilic addition
1485	Michael-type nucleophilic addition
1486	Michael-type nucleophilic addition
1487	Michael-type nucleophilic addition
1488	Michael-type nucleophilic addition
1489	Michael-type nucleophilic addition
1490	Michael-type nucleophilic addition: fast intramol. proton transfe
1491	Michael-type nucleophilic addition
1492	Michael-type nucleophilic addition
1493	
1494	Michael-type nucleophilic addition: formation of monoadduct: rate determining step
1495	
1496	
1497	
1498	
1499	
1500	
1501	
1502	Michael-type nucleophilic addition
1503	Michael-type nucleophilic addition: formation of monoadduct: rate determining: Cys-diadduct
1504	
1505	
1506	
1507	

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1508		4-Methylthio-1.2-benzoquinone	Cysteine	k(Cys)	M-1 min-1	1.70E+08	10%	8.24
1509		4-n-Butoxy-1.2-benzoquinone	Cysteine	k(Cys)	M-1 min-1	3.00E+07	10%	7.48
1510		4-n-Butylthio-1.2-benzoquinone	Cysteine	k(Cys)	M-1 min-1	1.90E+08	10%	8.27
1511		4-n-Propoxy-1.2-benzoquinone	Cysteine	k(Cys)	M-1 min-1	2.40E+07	10%	7.38
1512		4-n-Propylthio-1.2-benzoquinone	Cysteine	k(Cys)	M-1 min-1	1.30E+08	10%	8.12
1513	1129-21-1	4-tert-Butyl-1.2-benzoquinone	Cysteine	k(Cys)	M-1 min-1	1.30E+08	10%	8.12
1514		4-Trifluoromethoxy-1.2-benzoquinone	Cysteine	k(Cys)	M-1 min-1	7.20E+08	10%	8.86
1515	75-07-0	Acetaldehyde	Cysteine	k(Cys)	M-1 min-1		0.03 (log)	2.96
1516	107-02-8	Acrolein	Cysteine	k(Cys)	M-1 min-1			4.374
1517	107-02-8	Acrolein	Cysteine	k(Cys)	M-1 min-1	1.32E+04		4.12
1518	79-06-1	Acrylamide	Cysteine	k(Cys)	M-1 min-1			-0.026
1519	79-06-1	Acrylamide	Cysteine	k(Cys)	M-1 min-1			-0.72
1520	79-06-1	Acrylamide	Cysteine	k(Cys)	M-1 min-1			0.63
1521	107-13-1	Acrylonitrile	Cysteine	k(Cys)	M-1 min-1	1.29E+01		1.11
1522	107-13-1	Acrylonitrile	Cysteine	k(Cys)	M-1 min-1	8.04E+00		0.91
1523	107-13-1	Acrylonitrile	Cysteine	k(Cys)	M-1 min-1	2.64E+02		2.42
1524	107-18-6	Allyl alcohol	Cysteine	k(Cys)	M-1 min-1	NR		
1525	100-52-7	Benzaldehyde	Cysteine	k(Cys)	M-1 min-1		0.02 (log)	1.39
1526	123-72-8	Butyraldehyde	Cysteine	k(Cys)	M-1 min-1		0.03 (log)	2.44
1527	370-86-5	Carbonyl cyanide p-trifluoromethoxyphenylhydrazone	Cysteine	k(Cys)	M-1 min-1	5.75E+03		3.76
1528	2043-61-0	Cyclohexanaecarboxaldehyde	Cysteine	k(Cys)	M-1 min-1		0.04 (log)	3.58
1529	112-81-2	Decaldehyde	Cysteine	k(Cys)	M-1 min-1		0.02 (log)	2.46
1530	97-96-1	Diethylacetaldehyde	Cysteine	k(Cys)	M-1 min-1		0.07 (log)	3.73
1531	50-00-0	Formaldehyde	Cysteine	k(Cys)	M-1 min-1		0.03 (log)	2.61
1532	98-01-1	Furfural	Cysteine	k(Cys)	M-1 min-1		0.02 (log)	0.74
1533	66-25-1	Hexaldehyde	Cysteine	k(Cys)	M-1 min-1		0.04 (log)	2.42
1534	78-84-2	Isobutyraldehyde	Cysteine	k(Cys)	M-1 min-1		0.03 (log)	2.29
1535	590-86-3	Isovaleraldehyde	Cysteine	k(Cys)	M-1 min-1		0.06 (log)	3.47
1536	78-94-4	Methyl vinyl ketone	Cysteine	k(Cys)	M-1 min-1			3.826
1537	111-71-7	n-Heptanal	Cysteine	k(Cys)	M-1 min-1		0.11 (log)	4.6
1538	586-96-9	Nitrosobenzene	Cysteine	k(Cys)	M-1 min-1	7.20E+05		5.86
1539	124-13-0	Octylaldehyde	Cysteine	k(Cys)	M-1 min-1		0.03 (log)	2.37
1540	123-38-6	Propionaldehyde	Cysteine	k(Cys)	M-1 min-1	NR		
1541	123-38-6	Propionaldehyde	Cysteine	k(Cys)	M-1 min-1		0.02 (log)	2.79
1542		Thiocarbamate-S-oxide	Cysteine	k(Cys)	M-1 min-1	49.2	1.8	1.691965
1543		Thiocarbamate-S-oxide	Cysteine	k(Cys)	M-1 min-1	3743.04	12.48	3.573225
1544	110-62-3	Valeraldehyde	Cysteine	k(Cys)	M-1 min-1		0.03 (log)	2.67
1545	79-06-1	Acrylamide	Cysteine ethyl ester	k(Cys)	M-1 min-1			-0.43
1546	79-06-1	Acrylamide	Cysteine ethyl ester	k(Cys)	M-1 min-1			0.01
1547		1.1-Dinitro-2.2-diphenylethylene	n-Butylamine	k(BuNH2) | K | k-1	M-1 min-1	2.40E+03		3.38

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1508		7.2	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1509		7.2	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1510		7.18	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1511		7.2	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1512		7.19	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1513		7.2	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1514		6.86	Water		El excess	Cooksey CJ et al., Quant. Struct. Act. Relat. 15 (1996), 498
1515		7	PBS, Acetone		1:10	Deneer JW et al., Aquat. Toxicol. 12 (1988), 185
1516		7.4			El excess	LoPachin RM et al., Toxicol. Sci. 107 (2009), 171
1517	20	7.5				Esterbauer H et al., Tetrahedron 32 (1976), 285
1518		7.4			El excess	LoPachin RM et al., Toxicol. Sci. 107 (2009), 171
1519		7.4			El excess	LoPachin RM et al., Toxicol. Sci. 98 (2007), 561
1520		8.8			El excess	LoPachin RM et al., Toxicol. Sci. 98 (2007), 561
1521	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1522	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1523						Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1524		7.4			El excess	LoPachin RM et al., Toxicol. Sci. 107 (2009), 171
1525		7	PBS, Acetone		1:10	Deneer JW et al., Aquat. Toxicol. 12 (1988), 185
1526		7	PBS, Acetone		1:10	Deneer JW et al., Aquat. Toxicol. 12 (1988), 185
1527	25	7.5	Citrate/phosphate 0.1 M, 1% MeOH		25:1	Drobnica L et al., Biochim. Biophys. Acta 585 (1979), 462
1528		7	PBS, Acetone		1:10	Deneer JW et al., Aquat. Toxicol. 12 (1988), 185
1529		7	PBS, Acetone		1:10	Deneer JW et al., Aquat. Toxicol. 12 (1988), 185
1530		7	PBS, Acetone		1:10	Deneer JW et al., Aquat. Toxicol. 12 (1988), 185
1531		7	PBS, Acetone		1:10	Deneer JW et al., Aquat. Toxicol. 12 (1988), 185
1532		7	PBS, Acetone		1:10	Deneer JW et al., Aquat. Toxicol. 12 (1988), 185
1533		7	PBS, Acetone		1:10	Deneer JW et al., Aquat. Toxicol. 12 (1988), 185
1534		7	PBS, Acetone		1:10	Deneer JW et al., Aquat. Toxicol. 12 (1988), 185
1535		7	PBS, Acetone		1:10	Deneer JW et al., Aquat. Toxicol. 12 (1988), 185
1536		7.4			El excess	LoPachin RM et al., Toxicol. Sci. 107 (2009), 171
1537		7	PBS, Acetone		1:10	Deneer JW et al., Aquat. Toxicol. 12 (1988), 185
1538	37	7.4				Eyer P, Biological Oxidation of Nitrogen in Orga... (1985), 386
1539		7	PBS, Acetone		1:10	Deneer JW et al., Aquat. Toxicol. 12 (1988), 185
1540		7.4			El excess	LoPachin RM et al., Toxicol. Sci. 107 (2009), 171
1541		7	PBS, Acetone		1:10	Deneer JW et al., Aquat. Toxicol. 12 (1988), 185
1542	18	11.22	Inorganic phosphate buffer 0.1M	1-10 min	1.6:1 - 16:1	Wang X et al., Chem. Res. Toxicol. 21 (2008), 2120
1543	18	8.07	TRIS buffer 0.1M	1-10 min	1.6:1 - 16:1	Wang X et al., Chem. Res. Toxicol. 21 (2008), 2120
1544		7	PBS, Acetone		1:10	Deneer JW et al., Aquat. Toxicol. 12 (1988), 185
1545		7.4			El excess	LoPachin RM et al., Toxicol. Sci. 98 (2007), 561
1546		8.8			El excess	LoPachin RM et al., Toxicol. Sci. 98 (2007), 561
1547	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017

#	Comment
1508	
1509	
1510	
1511	
1512	
1513	
1514	
1515	HPLC-UV(230 nm).
1516	UV (DTNB 412 nm).
1517	
1518	UV (DTNB 412 nm).
1519	UV (DTNB 412 nm).
1520	UV (DTNB 412 nm).
1521	other pH in paper.
1522	
1523	k(NH2) of Cysteine.
1524	UV (DTNB 412 nm).
1525	HPLC-UV(230 nm).
1526	HPLC-UV(230 nm).
1527	UV(200-800 nm); reactive: non-diss. CCP + RS[-] (pH < pKa).
1528	HPLC-UV(230 nm).
1529	HPLC-UV(230 nm).
1530	HPLC-UV(230 nm).
1531	HPLC-UV(230 nm).
1532	HPLC-UV(230 nm).
1533	HPLC-UV(230 nm).
1534	HPLC-UV(230 nm).
1535	HPLC-UV(230 nm).
1536	UV (DTNB 412 nm).
1537	HPLC-UV(230 nm).
1538	
1539	HPLC-UV(230 nm).
1540	UV (DTNB 412 nm).
1541	HPLC-UV(230 nm).
1542	stopped-flow/DAD+PMT; other pH: bell shape, k(max) at pH 7.6, see paper.
1543	stopped-flow/DAD+PMT; log k=1.10 at pH=8.8.
1544	HPLC-UV(230 nm).
1545	UV (DTNB 412 nm).
1546	UV (DTNB 412 nm).
1547	K 1.1E+02 | k-1 2.2E+01 | pKa 5.91. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa

#	Mechanism
1508	
1509	
1510	
1511	
1512	
1513	
1514	
1515	
1516	Michael-type nucleophilic addition
1517	Michael-type nucleophilic addition: formation of monoadduct: rate determining step
1518	Michael-type nucleophilic addition
1519	Michael-type nucleophilic addition
1520	Michael-type nucleophilic addition
1521	Michael-type nucleophilic addition
1522	Michael-type nucleophilic addition
1523	Michael-type nucleophilic addition
1524	NOT Michael-type nucleophilic addition
1525	
1526	
1527	Nucleophilic olefinic addition
1528	
1529	
1530	
1531	
1532	
1533	
1534	
1535	
1536	Michael-type nucleophilic addition
1537	
1538	
1539	
1540	NOT Michael-type nucleophilic addition
1541	
1542	Disulfide formation
1543	Disulfide formation: +Cys-H --> CSSC + {NC(=O}S}
1544	
1545	Michael-type nucleophilic addition
1546	Michael-type nucleophilic addition
1547	Nucleophilic olefinic addition

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1548		2-(2.4-dinitrophenyl)-3-phenylprop-2-enenitrile	n-Butylamine	k(BuNH2) | K | k-1	M-1 min-1	2.30E+02		2.36
1549	3695-95-2	2-(p-Nitrophenyl)-3-phenylacrylonitrile	n-Butylamine	k(BuNH2) | K | k-1	M-1 min-1	1.06E+02		2.03
1550		Benzylidene Meldrum's acid	n-Butylamine	k(BuNH2) | K | k-1	M-1 min-1	3.36E+06		6.53
1551		beta-Methoxy-alpha-nitrostilbene	n-Butylamine	k(BuNH2) | K | k-1	M-1 min-1	87		1.94
1552	102-96-5	beta-Nitrostyrene	n-Butylamine	k(BuNH2) | K | k-1	M-1 min-1	1.90E+03		3.27
1553	123-73-9	(E)-Crotonaldehyde	n-Butylamine	k(BuNH2)	M-1 min-1	0.44	0.01	-0.36
1554	584-48-5	1-Bromo-2.4-dinitrobenzene	n-Butylamine	k(BuNH2)	M-1 min-1	5.53E-03		-2.26
1555	97-00-7	1-Chloro-2.4-dinitrobenzene	n-Butylamine	k(BuNH2)	M-1 min-1	5.71E-03		-2.24
1556	818-61-1	2-Hydroxyethyl acrylate	n-Butylamine	k(BuNH2)	M-1 min-1	NR		
1557	923-26-2	2-Hydroxypropyl methacrylate	n-Butylamine	k(BuNH2)	M-1 min-1	NR		
1558		3-(2-Bromoethyl)-5.5-dimethyldihydro-2(3H)-furanone (2B)	n-Butylamine	k(BuNH2)	M-1 min-1	8.80E-06		-5.06
1559		3-(3'-Bromopropyl)-5.5'-dimethyldihydro-2(3H)-furanone (3B)	n-Butylamine	k(BuNH2)	M-1 min-1	1.81E-05		-4.74
1560		3-(Bromomethyl)-5.5-dimethyldihydro-2(3H)-furanone (1B)	n-Butylamine	k(BuNH2)	M-1 min-1	1.66E-03		-2.78
1561	619-73-8	4-Nitrobenzyl alcohol	n-Butylamine	k(BuNH2)	M-1 min-1	NR		
1562	4450-68-4	4-Nitrobenzyl tosylate	n-Butylamine	k(BuNH2)	M-1 min-1	2.50E-03		-2.6
1563	100-11-8	4-Nitrobenzylbromide	n-Butylamine	k(BuNH2)	M-1 min-1	8.80E-02		-1.06
1564	100-14-1	4-Nitrobenzylchloride	n-Butylamine	k(BuNH2)	M-1 min-1	4.90E-04		-3.31
1565		4-Nitrobenzylfluoride	n-Butylamine	k(BuNH2)	M-1 min-1	5.00E-09		-8.3
1566	3145-86-6	4-Nitrobenzyliodide	n-Butylamine	k(BuNH2)	M-1 min-1	4.30E-01		-0.37
1567	99-99-0	4-Nitrotoluene	n-Butylamine	k(BuNH2)	M-1 min-1	NR		
1568	107-02-8	Acrolein	n-Butylamine	k(BuNH2)	M-1 min-1	25.58	6.3	1.41
1569	96-05-9	Allyl methacrylate	n-Butylamine	k(BuNH2)	M-1 min-1	NR		
1570		C16-1.3-Sultone	n-Butylamine	k(BuNH2)	M-1 min-1	2.90E-02		-1.54
1571		C16-1.4-Sultone	n-Butylamine	k(BuNH2)	M-1 min-1	2.60E-03		-2.59
1572	5392-40-5	Citral	n-Butylamine	k(BuNH2)	M-1 min-1	0.81	0.2	-0.09
1573	140-88-5	Ethyl acrylate	n-Butylamine	k(BuNH2)	M-1 min-1	NR		
1574	97-63-2	Ethyl methacrylate	n-Butylamine	k(BuNH2)	M-1 min-1	NR		
1575	2499-95-8	Hexyl acrylate	n-Butylamine	k(BuNH2)	M-1 min-1	NR		
1576	106-63-8	Isobutyl acrylate	n-Butylamine	k(BuNH2)	M-1 min-1	NR		
1577	97-86-9	Isobutyl methacrylate	n-Butylamine	k(BuNH2)	M-1 min-1	0.71	3	-0.15
1578	96-33-3	Methyl acrylate	n-Butylamine	k(BuNH2)	M-1 min-1	NR		
1579	80-62-6	Methyl methacrylate	n-Butylamine	k(BuNH2)	M-1 min-1	NR		
1580	25152-84-5	trans.trans.2.4-Decadienal	n-Butylamine	k(BuNH2)	M-1 min-1	4.72	1.3	0.67
1581	5910-87-2	trans.trans-2.4-Nonadienal	n-Butylamine	k(BuNH2)	M-1 min-1	1.46	0.1	0.16
1582	557-48-2	trans-2-cis-6-Nonadienal	n-Butylamine	k(BuNH2)	M-1 min-1	0.94	0.6	-0.03
1583	18829-55-5	trans-2-Heptenal	n-Butylamine	k(BuNH2)	M-1 min-1	2.81	0.3	-0.45
1584	6728-26-3	trans-2-Hexenal	n-Butylamine	k(BuNH2)	M-1 min-1	0.4	0.1	-0.4
1585	18829-56-6	trans-2-Nonenal	n-Butylamine	k(BuNH2)	M-1 min-1	0.69	0.05	-0.16
1586	2548-87-0	trans-2-Octenal	n-Butylamine	k(BuNH2)	M-1 min-1	0.23	0.1	-0.64

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1548	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
1549	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
1550	20		Water			Bernasconi CF, Tetrahedron 45 (1989), 4017
1551	20		DMSO:water 1:1			Bernasconi CF et al., J. Org. Chem. 64 (1999), 2897
1552	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
1553	25	8.5	Borate buffer 0.1 M, DMSO		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1027
1554	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1555	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1556		8.5	Borate buffer 0.1 M		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004
1557		8.5	Borate buffer 0.1 M		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004
1558			CDCl3		5:1	Franot C et al., Chem. Res. Toxicol. 7 (1994), 297
1559			CDCl3		5:1	Franot C et al., Chem. Res. Toxicol. 7 (1994), 297
1560			CDCl3		5:1	Franot C et al., Chem. Res. Toxicol. 7 (1994), 297
1561	23		1,4-Dioxan			Roberts DW et al., Fd. Chem. Toxicol. 21 (1983), 811
1562	23		1,4-Dioxan			Roberts DW et al., Fd. Chem. Toxicol. 21 (1983), 811
1563	23		1,4-Dioxan			Roberts DW et al., Fd. Chem. Toxicol. 21 (1983), 811
1564	23		1,4-Dioxan			Roberts DW et al., Fd. Chem. Toxicol. 21 (1983), 811
1565	23		1,4-Dioxan			Roberts DW et al., Fd. Chem. Toxicol. 21 (1983), 811
1566	23		1,4-Dioxan			Roberts DW et al., Fd. Chem. Toxicol. 21 (1983), 811
1567	23		1,4-Dioxan			Roberts DW et al., Fd. Chem. Toxicol. 21 (1983), 811
1568	25	8.5	Borate buffer 0.1 M, DMSO		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1027
1569		8.5	Borate buffer 0.1 M		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004
1570	100		Ethanol			Roberts DW et al., J. Theor. Biol. 99 (1982), 807
1571	100		Ethanol			Roberts DW et al., J. Theor. Biol. 99 (1982), 807
1572	25	8.5	Borate buffer 0.1 M, DMSO		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1027
1573		8.5	Borate buffer 0.1 M		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004
1574		8.5	Borate buffer 0.1 M		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004
1575		8.5	Borate buffer 0.1 M		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004
1576		8.5	Borate buffer 0.1 M		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004
1577		8.5	Borate buffer 0.1 M		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004
1578		8.5	Borate buffer 0.1 M		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004
1579		8.5	Borate buffer 0.1 M		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1004
1580	25	8.5	Borate buffer 0.1 M, DMSO		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1027
1581	25	8.5	Borate buffer 0.1 M, DMSO		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1027
1582	25	8.5	Borate buffer 0.1 M, DMSO		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1027
1583	25	8.5	Borate buffer 0.1 M, DMSO		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1027
1584	25	8.5	Borate buffer 0.1 M, DMSO		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1027
1585	25	8.5	Borate buffer 0.1 M, DMSO		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1027
1586	25	8.5	Borate buffer 0.1 M, DMSO		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1027

#	Comment
1548	K 5.70E-03 | k-1 4.06E+04 | pKa 7.76. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
1549	K 9.88E-05 | k-1 1.07E+06 | pKa 8.30. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
1550	K 3.41E+06 | k-1 9.84E-01 | pKa 10.60. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
1551	Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
1552	K 24.8 | k-1 7.50E+01 | pKa 8.62. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
1553	UV (Fluorescamine: 390 nm excit., 475 nm emiss.).
1554	other amines in paper.
1555	other amines in paper.
1556	UV (Fluorescamine; 390 nm excit., 475 emiss.).
1557	UV (Fluorescamine; 390 nm excit., 475 emiss.).
1558	H-NMR.
1559	H-NMR.
1560	H-NMR.
1561	
1562	
1563	
1564	
1565	estimated from k determined at 84C.
1566	
1567	
1568	UV (Fluorescamine: 390 nm excit., 475 nm emiss.).
1569	UV (Fluorescamine; 390 nm excit., 475 emiss.).
1570	
1571	
1572	UV (Fluorescamine: 390 nm excit., 475 nm emiss.).
1573	UV (Fluorescamine; 390 nm excit., 475 emiss.).
1574	UV (Fluorescamine; 390 nm excit., 475 emiss.).
1575	UV (Fluorescamine; 390 nm excit., 475 emiss.).
1576	UV (Fluorescamine; 390 nm excit., 475 emiss.).
1577	UV (Fluorescamine; 390 nm excit., 475 emiss.).
1578	UV (Fluorescamine; 390 nm excit., 475 emiss.).
1579	UV (Fluorescamine; 390 nm excit., 475 emiss.).
1580	UV (Fluorescamine: 390 nm excit., 475 nm emiss.).
1581	UV (Fluorescamine: 390 nm excit., 475 nm emiss.).
1582	UV (Fluorescamine: 390 nm excit., 475 nm emiss.).
1583	UV (Fluorescamine: 390 nm excit., 475 nm emiss.).
1584	UV (Fluorescamine: 390 nm excit., 475 nm emiss.).
1585	UV (Fluorescamine: 390 nm excit., 475 nm emiss.).
1586	UV (Fluorescamine: 390 nm excit., 475 nm emiss.).

#	Mechanism
1548	Nucleophilic olefinic addition
1549	Nucleophilic olefinic addition
1550	Nucleophilic olefinic addition
1551	Vinylic nucleophilic substitution
1552	Nucleophilic olefinic addition
1553	Michael addition or Schiff base formation
1554	Nucleophilic aromatic substitution (SNAr)
1555	Nucleophilic aromatic substitution (SNAr)
1556	
1557	
1558	Nucleophilic substitution, second order (SN2): reacts via SN2 or Elimination
1559	Nucleophilic substitution, second order (SN2): reacts via SN2 or Elimination
1560	Nucleophilic substitution, second order (SN2): reacts via SN2 or Elimination
1561	
1562	
1563	
1564	
1565	
1566	
1567	
1568	Michael addition or Schiff base formation
1569	
1570	
1571	
1572	Michael addition or Schiff base formation
1573	
1574	
1575	
1576	
1577	
1578	
1579	
1580	Michael addition or Schiff base formation
1581	Michael addition or Schiff base formation
1582	Michael addition or Schiff base formation
1583	Michael addition or Schiff base formation
1584	Michael addition or Schiff base formation
1585	Michael addition or Schiff base formation
1586	Michael addition or Schiff base formation

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1587	1576-87-0	trans-2-Pentenal	n-Butylamine	k(BuNH2)	M-1 min-1	0.62	0.05	-0.21
1588		1.1-Dinitro-2.2-diphenylethylene	Aniline	k(Aniline) | K | k-1	M-1 min-1	6.00E+01		1.78
1589	102-96-5	beta-Nitrostyrene	Aniline	k(Aniline) | K | k-1	M-1 min-1	3.00E+03		3.48
1590	584-48-5	1-Bromo-2.4-dinitrobenzene	Aniline	k(Aniline)	M-1 min-1	2.71E-02		-1.57
1591	584-48-5	1-Bromo-2.4-dinitrobenzene	Aniline	k(Aniline)	M-1 min-1	1.04E-02		-1.98
1592	584-48-5	1-Bromo-2.4-dinitrobenzene	Aniline	k(Aniline)	M-1 min-1	1.85E-02		-1.73
1593	584-48-5	1-Bromo-2.4-dinitrobenzene	Aniline	k(Aniline)	M-1 min-1	1.39E-02		-1.86
1594	584-48-5	1-Bromo-2.4-dinitrobenzene	Aniline	k(Aniline)	M-1 min-1	3.19E-02		-1.5
1595	584-48-5	1-Bromo-2.4-dinitrobenzene	Aniline	k(Aniline)	M-1 min-1	5.73E-03		-2.24
1596	97-00-7	1-Chloro-2.4-dinitrobenzene	Aniline	k(Aniline)	M-1 min-1	8.50E-03		-2.07
1597	97-00-7	1-Chloro-2.4-dinitrobenzene	Aniline	k(Aniline)	M-1 min-1	1.79E-02		-1.75
1598	97-00-7	1-Chloro-2.4-dinitrobenzene	Aniline	k(Aniline)	M-1 min-1	9.75E-03		-2.01
1599	97-00-7	1-Chloro-2.4-dinitrobenzene	Aniline	k(Aniline)	M-1 min-1	2.13E-02		-1.67
1600	97-00-7	1-Chloro-2.4-dinitrobenzene	Aniline	k(Aniline)	M-1 min-1	1.93E-03		-2.71
1601	2401-85-6	1-Chloro-2.4-dinitronaphthalene	Aniline	k(Aniline)	M-1 min-1	1.31E+00		0.12
1602	709-49-9	1-Iodo-2.4-dinitrobenzene	Aniline	k(Aniline)	M-1 min-1	7.90E-03		-2.1
1603	709-49-9	1-Iodo-2.4-dinitrobenzene	Aniline	k(Aniline)	M-1 min-1	1.39E-03		-2.86
1604	584-48-5	1-Bromo-2.4-dinitrobenzene	Benzylamine	k(Amine)	M-1 min-1	2.78E-02		-1.56
1605	97-00-7	1-Chloro-2.4-dinitrobenzene	Benzylamine	k(Amine)	M-1 min-1	2.71E-02		-1.57
1606	3623-15-2	1-Phenyl-2-propyn-1-one	Benzylamine	k(Amine)	M-1 min-1	73.2		1.86
1607	3623-15-2	1-Phenyl-2-propyn-1-one	Ethanolamine	k(Amine)	M-1 min-1	42.18		1.63
1608		1-(3-Nitrophenyl)-2-propyn-1-one	Ethylamine	k(Amine)	M-1 min-1	256.8		2.41
1609		1-(4-Chlorophenyl)-2-propyn-1-one	Ethylamine	k(Amine)	M-1 min-1	109.8		2.04
1610		1-(4-Cyanophenyl)-2-propyn-1-one	Ethylamine	k(Amine)	M-1 min-1	261.6		2.42
1611	16469-68-4	1-(4-Methoxyphenyl)-2-propyn-1-one	Ethylamine	k(Amine)	M-1 min-1	36.9		1.57
1612		1-(4-Methylphenyl)-2-propyn-1-one	Ethylamine	k(Amine)	M-1 min-1	59.04		1.77
1613	3623-15-2	1-Phenyl-2-propyn-1-one	Ethylamine	k(Amine)	M-1 min-1	79.8		1.9
1614		1-(3-Nitrophenyl)-2-propyn-1-one	Hydrazine	k(Amine)	M-1 min-1	579.6		2.76
1615		1-(4-Chlorophenyl)-2-propyn-1-one	Hydrazine	k(Amine)	M-1 min-1	332.4		2.52
1616		1-(4-Cyanophenyl)-2-propyn-1-one	Hydrazine	k(Amine)	M-1 min-1	594		2.77
1617	16469-68-4	1-(4-Methoxyphenyl)-2-propyn-1-one	Hydrazine	k(Amine)	M-1 min-1	205.8		2.31
1618		1-(4-Methylphenyl)-2-propyn-1-one	Hydrazine	k(Amine)	M-1 min-1	247.8		2.39
1619	584-48-5	1-Bromo-2.4-dinitrobenzene	Hydrazine	k(Amine)	M-1 min-1	3.71E-01		-0.43
1620	97-00-7	1-Chloro-2.4-dinitrobenzene	Hydrazine	k(Amine)	M-1 min-1	3.58E-01		-0.45
1621	3623-15-2	1-Phenyl-2-propyn-1-one	Hydrazine	k(Amine)	M-1 min-1	264.6		2.42
1622	584-48-5	1-Bromo-2.4-dinitrobenzene	Methylamine	k(Amine)	M-1 min-1	1.52E-01		-0.82
1623	584-48-5	1-Bromo-2.4-dinitrobenzene	Methylamine	k(Amine)	M-1 min-1	6.08E-02		-1.22
1624	584-48-5	1-Bromo-2.4-dinitrobenzene	Methylamine	k(Amine)	M-1 min-1	2.10E+00		0.32
1625	584-48-5	1-Bromo-2.4-dinitrobenzene	Methylamine	k(Amine)	M-1 min-1	1.17E-02		-1.93
1626	97-00-7	1-Chloro-2.4-dinitrobenzene	Methylamine	k(Amine)	M-1 min-1	1.88E-01		-0.73
1627	97-00-7	1-Chloro-2.4-dinitrobenzene	Methylamine	k(Amine)	M-1 min-1	6.15E-02		-1.21
1628	97-00-7	1-Chloro-2.4-dinitrobenzene	Methylamine	k(Amine)	M-1 min-1	2.09E+00		0.32
1629	97-00-7	1-Chloro-2.4-dinitrobenzene	Methylamine	k(Amine)	M-1 min-1	1.08E-02		-1.97

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1587	25	8.5	Borate buffer 0.1 M, DMSO		1:10	Chan K et al., J. Appl. Toxicol. 28 (2008), 1027
1588	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
1589	20		DMSO:water 1:1			Bernasconi CF, Tetrahedron 45 (1989), 4017
1590	50		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1591	35		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1592	45		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1593	35		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1594	35		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1595	50		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1596	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1597	50		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1598	35		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1599	35		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1600	50		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1601	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1602	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1603	50		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1604	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1605	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1606	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1607	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1608	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1609	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1610	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1611	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1612	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1613	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1614	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1615	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1616	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1617	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1618	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1619	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1620	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1621	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1622	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1623	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1624	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1625	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1626	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1627	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1628	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273
1629	25		Ethanol			Bunnet JF et al., Chem. Rev. 49 (1951), 273

#	Comment
1587	UV (Fluorescamine: 390 nm excit., 475 nm emiss.).
1588	K 2.00E-07 | k-1 3.00E+08 | pKa -0.5. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
1589	K 1.30E-06 | k-1 2.28E+08 | pKa 2.2. Assay: Rate limiting step: K = k1("R2NH + C=C --> Adduct")/k-1; fast deprotonation pKa
1590	
1591	
1592	
1593	Nu: 3-Aminotoluene.
1594	Nu: 4-Aminotoluene.
1595	Nu: Methylaniline.
1596	other anilines in paper.
1597	
1598	Nu: 3-Aminotoluene.
1599	Nu: 4-Aminotoluene.
1600	Nu: Methylaniline.
1601	
1602	
1603	Nu: Methylaniline.
1604	
1605	
1606	UV(max. abs. enaminone) and 1H-NMR.
1607	UV(max. abs. enaminone) and 1H-NMR.
1608	UV(max. abs. enaminone) and 1H-NMR.
1609	UV(max. abs. enaminone) and 1H-NMR.
1610	UV(max. abs. enaminone) and 1H-NMR.
1611	UV(max. abs. enaminone) and 1H-NMR.
1612	UV(max. abs. enaminone) and 1H-NMR.
1613	UV(max. abs. enaminone) and 1H-NMR.
1614	UV(max. abs. enaminone) and 1H-NMR.
1615	UV(max. abs. enaminone) and 1H-NMR.
1616	UV(max. abs. enaminone) and 1H-NMR.
1617	UV(max. abs. enaminone) and 1H-NMR.
1618	UV(max. abs. enaminone) and 1H-NMR.
1619	
1620	
1621	UV(max. abs. enaminone) and 1H-NMR.
1622	
1623	Nu: Heptylamine.
1624	Nu: Dimethylamine.
1625	Nu: Diethylamine.
1626	
1627	Nu: Heptylamine.
1628	Nu: Dimethylamine.
1629	Nu: Diethylamine.

#	Mechanism
1587	Michael addition or Schiff base formation
1588	Nucleophilic olefinic addition: deprotonation partially rate limiting
1589	Nucleophilic olefinic addition
1590	Nucleophilic aromatic substitution (SNAr)
1591	Nucleophilic aromatic substitution (SNAr)
1592	Nucleophilic aromatic substitution (SNAr)
1593	Nucleophilic aromatic substitution (SNAr)
1594	Nucleophilic aromatic substitution (SNAr)
1595	Nucleophilic aromatic substitution (SNAr)
1596	Nucleophilic aromatic substitution (SNAr)
1597	Nucleophilic aromatic substitution (SNAr)
1598	Nucleophilic aromatic substitution (SNAr)
1599	Nucleophilic aromatic substitution (SNAr)
1600	Nucleophilic aromatic substitution (SNAr)
1601	Nucleophilic aromatic substitution (SNAr)
1602	Nucleophilic aromatic substitution (SNAr)
1603	Nucleophilic aromatic substitution (SNAr)
1604	Nucleophilic aromatic substitution (SNAr)
1605	Nucleophilic aromatic substitution (SNAr)
1606	Michael-type nucleophilic addition
1607	Michael-type nucleophilic addition
1608	Michael-type nucleophilic addition
1609	Michael-type nucleophilic addition
1610	Michael-type nucleophilic addition
1611	Michael-type nucleophilic addition
1612	Michael-type nucleophilic addition
1613	Michael-type nucleophilic addition
1614	Michael-type nucleophilic addition
1615	Michael-type nucleophilic addition
1616	Michael-type nucleophilic addition
1617	Michael-type nucleophilic addition
1618	Michael-type nucleophilic addition
1619	Nucleophilic aromatic substitution (SNAr)
1620	Nucleophilic aromatic substitution (SNAr)
1621	Michael-type nucleophilic addition
1622	Nucleophilic aromatic substitution (SNAr)
1623	Nucleophilic aromatic substitution (SNAr)
1624	Nucleophilic aromatic substitution (SNAr)
1625	Nucleophilic aromatic substitution (SNAr)
1626	Nucleophilic aromatic substitution (SNAr)
1627	Nucleophilic aromatic substitution (SNAr)
1628	Nucleophilic aromatic substitution (SNAr)
1629	Nucleophilic aromatic substitution (SNAr)

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1630		1-(3-Nitrophenyl)-2-propyn-1-one	Trifluoroethylamine	k(Amine)	M-1 min-1	8.28		0.92
1631		1-(4-Chlorophenyl)-2-propyn-1-one	Trifluoroethylamine	k(Amine)	M-1 min-1	3.192		0.5
1632		1-(4-Cyanophenyl)-2-propyn-1-one	Trifluoroethylamine	k(Amine)	M-1 min-1	9.12		0.96
1633	16469-68-4	1-(4-Methoxyphenyl)-2-propyn-1-one	Trifluoroethylamine	k(Amine)	M-1 min-1	0.1044		-0.98
1634		1-(4-Methylphenyl)-2-propyn-1-one	Trifluoroethylamine	k(Amine)	M-1 min-1	1.68		0.23
1635	3623-15-2	1-Phenyl-2-propyn-1-one	Trifluoroethylamine	k(Amine)	M-1 min-1	2.442		0.39
1636	107-13-1	Acrylonitrile	alpha-Aminoisobutyric acid	k(Ala)	M-1 min-1	4.45E+05		5.65
1637	107-13-1	Acrylonitrile	beta-Alanine	k(Ala)	M-1 min-1	1.15E+06		6.06
1638	107-13-1	Acrylonitrile	beta-Alanine	k(Ala)	M-1 min-1	5.81E+01		1.76
1639	107-13-1	Acrylonitrile	beta-Methoxy-alpha-alanine	k(Ala)	M-1 min-1	2.36E+06		6.37
1640	107-13-1	Acrylonitrile	Cycloleucine	k(Ala)	M-1 min-1	5.80E+05		5.76
1641	107-13-1	Acrylonitrile	DL-alpha-Alanine	k(Ala)	M-1 min-1	1.34E+06		6.13
1642	107-13-1	Acrylonitrile	DL-alpha-Phenyl-alpha-alanine	k(Ala)	M-1 min-1	1.00E+05		5
1643	107-13-1	Acrylonitrile	DL-Norleucine	k(Ala)	M-1 min-1	1.23E+06		6.09
1644	107-13-1	Acrylonitrile	DL-Phenylalanine	k(Ala)	M-1 min-1	2.11E+06		6.32
1645	107-13-1	Acrylonitrile	epsilon-Aminocaproic acid	k(Ala)	M-1 min-1	7.26E+05		5.86
1646	107-13-1	Acrylonitrile	iso-Valine	k(Ala)	M-1 min-1	4.29E+05		5.63
1647	107-13-1	Acrylonitrile	L-alpha-Alanyl-L-alpha-alanine	k(Ala)	M-1 min-1	3.35E+06		6.52
1648	29343-52-0	4-Hydroxy-2-nonenal	N(alpha)-Acetyl lysineamide	k(AcPeptideamide)	M-1 min-1	0.4476	0.0366	-0.35
1649	103560-62-9	4-Oxo-2-nonenal	N(alpha)-Acetyl lysineamide	k(AcPeptideamide)	M-1 min-1	0.0798	0.005	-1.1
1650	29343-52-0	4-Hydroxy-2-nonenal	N-Acetyl argininamide	k(AcPeptideamide)	M-1 min-1	0.03666	0.0051	-1.44
1651	103560-62-9	4-Oxo-2-nonenal	N-Acetyl argininamide	k(AcPeptideamide)	M-1 min-1	ND		
1652	29343-52-0	4-Hydroxy-2-nonenal	N-Acetyl cysteamine	k(AcPeptideamide)	M-1 min-1	11130	1755	4.05
1653	103560-62-9	4-Oxo-2-nonenal	N-Acetyl cysteamine	k(AcPeptideamide)	M-1 min-1	72.78	1.61	1.86
1654	29343-52-0	4-Hydroxy-2-nonenal	N-Acetyl histamine	k(AcPeptideamide)	M-1 min-1	1.326	0.102	0.12
1655	103560-62-9	4-Oxo-2-nonenal	N-Acetyl histamine	k(AcPeptideamide)	M-1 min-1	0.1284	0.0187	-0.89
1656	29343-52-0	4-Hydroxy-2-nonenal	Peptide (Cys+Arg)	k(AcPeptideamide)	M-1 min-1	53220	5298	4.73
1657	103560-62-9	4-Oxo-2-nonenal	Peptide (Cys+Arg)	k(AcPeptideamide)	M-1 min-1	407.4	38.76	2.61
1658	303-38-8	2.3-Dihydroxybenzoic acid	2-Acetylcyclopentanone	k(ACP)	M-1 min-1	6.48E+04	2.16E+03	4.81
1659	99-50-3	3.4-Dihydroxybenzoic acid	2-Acetylcyclopentanone	k(ACP)	M-1 min-1	4.58E+04	1.62E+03	4.66
1660	934-00-9	3-Methoxycatechol	2-Acetylcyclopentanone	k(ACP)	M-1 min-1	2.77E+04	1.56E+03	4.44
1661	488-17-5	3-Methylcatechol	2-Acetylcyclopentanone	k(ACP)	M-1 min-1	4.02E+04	1.68E+03	4.6
1662	120-80-9	Catechol	2-Acetylcyclopentanone	k(ACP)	M-1 min-1	5.22E+04	2.52E+03	4.72
1663	303-38-8	2.3-Dihydroxybenzoic acid	2-Acetylcyclohexanone	k(ACH)	M-1 min-1	3.42E+04	1.62E+03	4.53
1664	99-50-3	3.4-Dihydroxybenzoic acid	2-Acetylcyclohexanone	k(ACH)	M-1 min-1	1.86E+04	1.50E+03	4.27
1665	934-00-9	3-Methoxycatechol	2-Acetylcyclohexanone	k(ACH)	M-1 min-1	1.20E+04	1.32E+03	4.08
1666	488-17-5	3-Methylcatechol	2-Acetylcyclohexanone	k(ACH)	M-1 min-1	1.68E+04	1.38E+03	4.23
1667	120-80-9	Catechol	2-Acetylcyclohexanone	k(ACH)	M-1 min-1	2.10E+04	1.50E+03	4.32
1668	107-02-8	Acrolein	N-Acetyl cysteine	k(AcCys)	M-1 min-1			2.11
1669	79-06-1	Acrylamide	N-Acetyl cysteine	k(AcCys)	M-1 min-1			-1.873
1670	79-06-1	Acrylamide	N-Acetyl cysteine	k(AcCys)	M-1 min-1			0.16
1671	107-18-6	Allyl alcohol	N-Acetyl cysteine	k(AcCys)	M-1 min-1	NR		
1672	96-33-3	Methyl acrylate	N-Acetyl cysteine	k(AcCys)	M-1 min-1			-0.115

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1630	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1631	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1632	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1633	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1634	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1635	25		Self-buffered (NH3*HCl+NaOH)		>20:1	Um I-H et al., J. Org. Chem. 70 (2005), 7530
1636	30	8.4				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1637	30	8.4				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1638	30	8.1				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1639	30	8.4				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1640	30	8.4				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1641	30	8.4				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1642	30	8.4				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1643	30	8.4				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1644	30	8.4				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1645	30	8.4				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1646	30	8.4				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1647	30	8.4				Friedman M et al., J. Am. Chem. Soc. 87 (1965), 3672
1648	23	7.4	PBS 50 mM		1:10 (>)	Doorn JA et al., Chem. Biol. Interact. 143 (2003), 93
1649	23	7.4	PBS 50 mM		1:10 (>)	Doorn JA et al., Chem. Biol. Interact. 143 (2003), 93
1650	23	7.4	PBS 50 mM		1:10 (>)	Doorn JA et al., Chem. Biol. Interact. 143 (2003), 93
1651	23	7.4	PBS 50 mM		1:10 (>)	Doorn JA et al., Chem. Biol. Interact. 143 (2003), 93
1652	23	7.4	PBS 50 mM		1:10 (>)	Doorn JA et al., Chem. Biol. Interact. 143 (2003), 93
1653	23	7.4	PBS 50 mM		1:10 (>)	Doorn JA et al., Chem. Biol. Interact. 143 (2003), 93
1654	23	7.4	PBS 50 mM		1:10 (>)	Doorn JA et al., Chem. Biol. Interact. 143 (2003), 93
1655	23	7.4	PBS 50 mM		1:10 (>)	Doorn JA et al., Chem. Biol. Interact. 143 (2003), 93
1656	23	7.4	PBS 50 mM		1:10 (>)	Doorn JA et al., Chem. Biol. Interact. 143 (2003), 93
1657	23	7.4	PBS 50 mM		1:10 (>)	Doorn JA et al., Chem. Biol. Interact. 143 (2003), 93
1658	25	6.8	PBS 0.2 M		1:1	Nematollahi D et al., J. Phys. Org. Chem. 20 (2007), 49
1659	25	6.8	PBS 0.2 M		1:1	Nematollahi D et al., J. Phys. Org. Chem. 20 (2007), 49
1660	25	6.8	PBS 0.2 M		1:1	Nematollahi D et al., J. Phys. Org. Chem. 20 (2007), 49
1661	25	6.8	PBS 0.2 M		1:1	Nematollahi D et al., J. Phys. Org. Chem. 20 (2007), 49
1662	25	6.8	PBS 0.2 M		1:1	Nematollahi D et al., J. Phys. Org. Chem. 20 (2007), 49
1663	25	6.8	PBS 0.2 M		1:1	Nematollahi D et al., J. Phys. Org. Chem. 20 (2007), 49
1664	25	6.8	PBS 0.2 M		1:1	Nematollahi D et al., J. Phys. Org. Chem. 20 (2007), 49
1665	25	6.8	PBS 0.2 M		1:1	Nematollahi D et al., J. Phys. Org. Chem. 20 (2007), 49
1666	25	6.8	PBS 0.2 M		1:1	Nematollahi D et al., J. Phys. Org. Chem. 20 (2007), 49
1667	25	6.8	PBS 0.2 M		1:1	Nematollahi D et al., J. Phys. Org. Chem. 20 (2007), 49
1668		7.4			El excess	LoPachin RM et al., Toxicol. Sci. 98 (2007), 561
1669		7.4			El excess	LoPachin RM et al., Toxicol. Sci. 98 (2007), 561
1670		8.8			El excess	LoPachin RM et al., Toxicol. Sci. 98 (2007), 561
1671		7.4			El excess	LoPachin RM et al., Toxicol. Sci. 98 (2007), 561
1672		7.4			El excess	LoPachin RM et al., Toxicol. Sci. 98 (2007), 561

#	Comment
1630	UV(max. abs. enaminone) and 1H-NMR.
1631	UV(max. abs. enaminone) and 1H-NMR.
1632	UV(max. abs. enaminone) and 1H-NMR.
1633	UV(max. abs. enaminone) and 1H-NMR.
1634	UV(max. abs. enaminone) and 1H-NMR.
1635	UV(max. abs. enaminone) and 1H-NMR.
1636	
1637	
1638	k(NH2) of beta-Alanine.
1639	
1640	
1641	
1642	
1643	
1644	
1645	
1646	
1647	
1648	Assay: Room temperature, UV (Abs. at 224 nm [HNE], 228 nm [ONE], 412 nm [Cys with DTNB])
1649	Assay: Room temperature, UV (Abs. at 224 nm [HNE], 228 nm [ONE], 412 nm [Cys with DTNB])
1650	Assay: Room temperature, UV (Abs. at 224 nm [HNE], 228 nm [ONE], 412 nm [Cys with DTNB])
1651	Assay: Room temperature, UV (Abs. at 224 nm [HNE], 228 nm [ONE], 412 nm [Cys with DTNB])
1652	Assay: Room temperature, UV (Abs. at 224 nm [HNE], 228 nm [ONE], 412 nm [Cys with DTNB])
1653	Assay: Room temperature, UV (Abs. at 224 nm [HNE], 228 nm [ONE], 412 nm [Cys with DTNB])
1654	Assay: Room temperature, UV (Abs. at 224 nm [HNE], 228 nm [ONE], 412 nm [Cys with DTNB])
1655	Assay: Room temperature, UV (Abs. at 224 nm [HNE], 228 nm [ONE], 412 nm [Cys with DTNB])
1656	Assay: Room temperature, UV (Abs. at 224 nm [HNE], 228 nm [ONE], 412 nm [Cys with DTNB])
1657	Assay: Room temperature, UV (Abs. at 224 nm [HNE], 228 nm [ONE], 412 nm [Cys with DTNB])
1658	Assay: Cyclic voltammetry; pH dependence in paper
1659	Assay: Cyclic voltammetry; pH dependence in paper
1660	Assay: Cyclic voltammetry; pH dependence in paper
1661	Assay: Cyclic voltammetry; pH dependence in paper
1662	Assay: Cyclic voltammetry; pH dependence in paper
1663	Assay: Cyclic voltammetry; pH dependence in paper
1664	Assay: Cyclic voltammetry; pH dependence in paper
1665	Assay: Cyclic voltammetry; pH dependence in paper
1666	Assay: Cyclic voltammetry; pH dependence in paper
1667	Assay: Cyclic voltammetry; pH dependence in paper
1668	Assay: UV (DTNB 412 nm)
1669	Assay: UV (DTNB 412 nm)
1670	UV (DTNB 412 nm). Assay: UV (DTNB 412 nm)
1671	Assay: UV (DTNB 412 nm)
1672	Assay: UV (DTNB 412 nm)

#	Mechanism
1630	Michael-type nucleophilic addition
1631	Michael-type nucleophilic addition
1632	Michael-type nucleophilic addition
1633	Michael-type nucleophilic addition
1634	Michael-type nucleophilic addition
1635	Michael-type nucleophilic addition
1636	Michael-type nucleophilic addition
1637	Michael-type nucleophilic addition
1638	Michael-type nucleophilic addition
1639	Michael-type nucleophilic addition
1640	Michael-type nucleophilic addition
1641	Michael-type nucleophilic addition
1642	Michael-type nucleophilic addition
1643	Michael-type nucleophilic addition
1644	Michael-type nucleophilic addition
1645	Michael-type nucleophilic addition
1646	Michael-type nucleophilic addition
1647	Michael-type nucleophilic addition
1648	Michael-type nucleophilic addition
1649	Michael-type nucleophilic addition
1650	Michael-type nucleophilic addition
1651	
1652	Michael-type nucleophilic addition
1653	Michael-type nucleophilic addition
1654	Michael-type nucleophilic addition
1655	Michael-type nucleophilic addition
1656	Michael-type nucleophilic addition
1657	Michael-type nucleophilic addition
1658	Michael-type nucleophilic addition
1659	Michael-type nucleophilic addition
1660	Pre-Michael addition of aromatic hydrocarbons
1661	Michael-type nucleophilic addition
1662	Michael-type nucleophilic addition
1663	Michael-type nucleophilic addition
1664	Michael-type nucleophilic addition
1665	Pre-Michael addition of aromatic hydrocarbons
1666	Michael-type nucleophilic addition
1667	Michael-type nucleophilic addition
1668	Michael-type nucleophilic addition
1669	Michael-type nucleophilic addition
1670	Michael-type nucleophilic addition
1671	NOT Michael-type nucleophilic addition
1672	Michael-type nucleophilic addition

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1673	78-94-4	Methyl vinyl ketone	N-Acetyl cysteine	k(AcCys)	M-1 min-1			1.815
1674	128-53-0	N-Ethylmaleimide	N-Acetyl cysteine	k(AcCys)	M-1 min-1			3.948
1675	123-38-6	Propionaldehyde	N-Acetyl cysteine	k(AcCys)	M-1 min-1	NR		
1676	123-73-9	(E)-Crotonaldehyde	Glutathione	Free GSH	%	46.8		
1677	930-68-7	2-Cyclohexen-1-one	Glutathione	Free GSH	%	32		
1678	505-57-7	2-Hexenal	Glutathione	Free GSH	%	67		
1679	764-39-6	2-Pentenal	Glutathione	Free GSH	%	56		
1680	814-78-8	3-Methyl-3-buten-2-one	Glutathione	Free GSH	%	99		
1681		4-Ethoxy-2-pentenal	Glutathione	Free GSH	%	26.4		
1682	29389-17-1	4-Hydroxy-2-decenal	Glutathione	Free GSH	%	4.7		
1683	29343-60-0	4-Hydroxy-2-dodecenal	Glutathione	Free GSH	%	7.1		
1684	17427-09-7	4-Hydroxy-2-heptenal	Glutathione	Free GSH	%	4.9		
1685	17427-08-6	4-Hydroxy-2-hexenal	Glutathione	Free GSH	%	5		
1686	29343-52-0	4-Hydroxy-2-nonenal	Glutathione	Free GSH	%	8.5		
1687	17449-15-9	4-Hydroxy-2-octenal	Glutathione	Free GSH	%	6.7		
1688	34424-65-2	4-Hydroxy-2-pentenal	Glutathione	Free GSH	%	5.2		
1689	29343-58-6	4-Hydroxy-2-undecenal	Glutathione	Free GSH	%	7.7		
1690		4-Hydroxy-4-isopropyl-2-pentenal	Glutathione	Free GSH	%	38		
1691		4-Keto-2-pentenoic acid	Glutathione	Free GSH	%	7.5		
1692	141-79-7	4-Methyl-3-penten-2-one	Glutathione	Free GSH	%	98		
1693	107-02-8	Acrolein	Glutathione	Free GSH	%	1.2		
1694	5392-40-5	Citral	Glutathione	Free GSH	%	70.5		
1695	3724-65-0	Crotonic acid	Glutathione	Free GSH	%	NR		
1696	623-70-1	Ethyl crotonate	Glutathione	Free GSH	%	99		
1697	78-94-4	Methyl vinyl ketone	Glutathione	Free GSH	%	0.6		
1698	626-98-2	Pent-2-enoic acid	Glutathione	Free GSH	%	NR		
1699	70-34-8	1-Fluoro-2.4-dinitrobenzene	Lys-Tyr-Peptide (H-Lys-Tyr-OH)	EC50(LysTyr)	mM/mM	0.077	0.041	-1.11
1700	75-07-0	Acetaldehyde	Lys-Tyr-Peptide (H-Lys-Tyr-OH)	EC50(LysTyr)	mM/mM	0.164	0.037	-0.79
1701	75-05-8	Acetonitrile	Lys-Tyr-Peptide (H-Lys-Tyr-OH)	EC50(LysTyr)	mM/mM	4.22E-05	9.10E-06	-4.37
1702	100-52-7	Benzaldehyde	Lys-Tyr-Peptide (H-Lys-Tyr-OH)	EC50(LysTyr)	mM/mM	0.406	0.084	-0.39
1703	605-65-2	Dansyl chloride	Lys-Tyr-Peptide (H-Lys-Tyr-OH)	EC50(LysTyr)	mM/mM	0.713	0.348	-0.15
1704	50-00-0	Formaldehyde	Lys-Tyr-Peptide (H-Lys-Tyr-OH)	EC50(LysTyr)	mM/mM	0.509	0.032	-0.29
1705	111-30-8	Glutaraldehyde	Lys-Tyr-Peptide (H-Lys-Tyr-OH)	EC50(LysTyr)	mM/mM	0.575	0.046	-0.24
1706	85-44-9	Phthalic anhydride	Lys-Tyr-Peptide (H-Lys-Tyr-OH)	EC50(LysTyr)	mM/mM	1.061	0.057	0.03
1707	584-84-9	Toluene 2.4-diisocyanate	Lys-Tyr-Peptide (H-Lys-Tyr-OH)	EC50(LysTyr)	mM/mM	2.62	0.663	0.42
1708	407-25-0	Trifluoroacetic anhydride	Lys-Tyr-Peptide (H-Lys-Tyr-OH)	EC50(LysTyr)	mM/mM	0.019	0.001	-1.72
1709	2508-19-2	Trinitrobenzenesulfonic acid	Lys-Tyr-Peptide (H-Lys-Tyr-OH)	EC50(LysTyr)	mM/mM	0.03	0.06	-1.52
1710	95-94-3	1.2.4.5-Tetrachlorobenzene	Aniline	DPE(Aniline)	% Depletion	<5		
1711	120-82-1	1.2.4-Trichlorobenzene	Aniline	DPE(Aniline)	% Depletion	<5		
1712	610-31-1	1.2.4-Trinitrobenzene	Aniline	DPE(Aniline)	% Depletion	>90		
1713	6306-39-4	1.2-Dichloro-4.5-dinitrobenzene	Aniline	DPE(Aniline)	% Depletion	>90		
1714	99-54-7	1.2-Dichloro-4-nitrobenzene	Aniline	DPE(Aniline)	% Depletion	<5		
1715	99-35-4	1.3.5-Trinitrobenzene	Aniline	DPE(Aniline)	% Depletion	<5		

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1673		7.4			El excess	LoPachin RM et al., Toxicol. Sci. 98 (2007), 561
1674		7.4			El excess	LoPachin RM et al., Toxicol. Sci. 98 (2007), 561
1675		7.4			El excess	LoPachin RM et al., Toxicol. Sci. 98 (2007), 561
1676	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1677	20	7.4	PBS 66 mM		1:1	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1678	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1679	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1680	20	7.4	PBS 66 mM		1:1	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1681	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1682	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1683	20	7.4	PBS 66 mM, 10% ethanol		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1684	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1685	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1686	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1687	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1688	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1689	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1690	20	7.4	PBS 66 mM		1:1	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1691	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1692	20	7.4	PBS 66 mM		1:400	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1693	20	7.4	PBS 66 mM		1:1	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1694	20	7.4	PBS 66 mM		1:20	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1695	20	7.4	PBS 66 mM		1:40	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1696	20	7.4	PBS 66 mM		1:40	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1697	20	7.4	PBS 66 mM		1:1	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1698	20	7.4	PBS 66 mM		1:40	Esterbauer H et al., Z. Naturforsch. 30 (1975), 466
1699		7.4	ACN			Reichardt P et al., Environ. Toxicol. 18 (2003), 29
1700		7.4	ACN			Reichardt P et al., Environ. Toxicol. 18 (2003), 29
1701		7.4	ACN			Reichardt P et al., Environ. Toxicol. 18 (2003), 29
1702		7.4	ACN			Reichardt P et al., Environ. Toxicol. 18 (2003), 29
1703		7.4	ACN			Reichardt P et al., Environ. Toxicol. 18 (2003), 29
1704		7.4	ACN			Reichardt P et al., Environ. Toxicol. 18 (2003), 29
1705		7.4	ACN			Reichardt P et al., Environ. Toxicol. 18 (2003), 29
1706		7.4	ACN			Reichardt P et al., Environ. Toxicol. 18 (2003), 29
1707		7.4	ACN			Reichardt P et al., Environ. Toxicol. 18 (2003), 29
1708		7.4	ACN			Reichardt P et al., Environ. Toxicol. 18 (2003), 29
1709		7.4	ACN			Reichardt P et al., Environ. Toxicol. 18 (2003), 29
1710	100		Ethanol (abs.)	2 h		Landsteiner et al., J. Exp. Med. 64 (1936), 625
1711	100		Ethanol (abs.)	2 h		Landsteiner et al., J. Exp. Med. 64 (1936), 625
1712	100		Ethanol (abs.)	2 h		Landsteiner et al., J. Exp. Med. 64 (1936), 625
1713	100		Ethanol (abs.)	2 h		Landsteiner et al., J. Exp. Med. 64 (1936), 625
1714	100		Ethanol (abs.)	2 h		Landsteiner et al., J. Exp. Med. 64 (1936), 625
1715	100		Ethanol (abs.)	2 h		Landsteiner et al., J. Exp. Med. 64 (1936), 625

#	Comment
1673	Assay: UV (DTNB 412 nm)
1674	Assay: UV (DTNB 412 nm)
1675	Assay: UV (DTNB 412 nm)
1676	Assay: % of GSH in equilibrium if 0.1 mM GSH is allowed to react with 0.1 mM carbonyl, calc. by k
1677	Assay: % of GSH in equilibrium if 0.1 mM GSH is allowed to react with 0.1 mM carbonyl, calc. by k
1678	Assay: % of GSH in equilibrium if 0.1 mM GSH is allowed to react with 0.1 mM carbonyl, calc. by k
1679	Assay: % of GSH in equilibrium if 0.1 mM GSH is allowed to react with 0.1 mM carbonyl, calc. by k
1680	Assay: % of GSH in equilibrium if 0.1 mM GSH is allowed to react with 0.1 mM carbonyl, calc. by k
1681	Assay: % of GSH in equilibrium if 0.1 mM GSH is allowed to react with 0.1 mM carbonyl, calc. by k
1682	Assay: % of GSH in equilibrium if 0.1 mM GSH is allowed to react with 0.1 mM carbonyl, calc. by k
1683	Assay: % of GSH in equilibrium if 0.1 mM GSH is allowed to react with 0.1 mM carbonyl, calc. by k
1684	Assay: % of GSH in equilibrium if 0.1 mM GSH is allowed to react with 0.1 mM carbonyl, calc. by k
1685	Assay: % of GSH in equilibrium if 0.1 mM GSH is allowed to react with 0.1 mM carbonyl, calc. by k
1686	Assay: % of GSH in equilibrium if 0.1 mM GSH is allowed to react with 0.1 mM carbonyl, calc. by k
1687	Assay: % of GSH in equilibrium if 0.1 mM GSH is allowed to react with 0.1 mM carbonyl, calc. by k
1688	Assay: % of GSH in equilibrium if 0.1 mM GSH is allowed to react with 0.1 mM carbonyl, calc. by k
1689	Assay: % of GSH in equilibrium if 0.1 mM GSH is allowed to react with 0.1 mM carbonyl, calc. by k
1690	Assay: % of GSH in equilibrium if 0.1 mM GSH is allowed to react with 0.1 mM carbonyl, calc. by k
1691	Assay: % of GSH in equilibrium if 0.1 mM GSH is allowed to react with 0.1 mM carbonyl, calc. by k
1692	Assay: % of GSH in equilibrium if 0.1 mM GSH is allowed to react with 0.1 mM carbonyl, calc. by k
1693	Assay: % of GSH in equilibrium if 0.1 mM GSH is allowed to react with 0.1 mM carbonyl, calc. by k
1694	Assay: % of GSH in equilibrium if 0.1 mM GSH is allowed to react with 0.1 mM carbonyl, calc. by k
1695	Assay: % of GSH in equilibrium if 0.1 mM GSH is allowed to react with 0.1 mM carbonyl, calc. by k
1696	Assay: % of GSH in equilibrium if 0.1 mM GSH is allowed to react with 0.1 mM carbonyl, calc. by k
1697	Assay: % of GSH in equilibrium if 0.1 mM GSH is allowed to react with 0.1 mM carbonyl, calc. by k
1698	2-Pentenoate. Assay: % of GSH in equilibrium if 0.1 mM GSH is allowed to react with 0.1 mM carbonyl, calc. by k
1699	Assay: HPLC/MS; Factor of Reactivity
1700	Assay: HPLC/MS; Factor of Reactivity
1701	Assay: HPLC/MS; Factor of Reactivity
1702	Assay: HPLC/MS; Factor of Reactivity
1703	Assay: HPLC/MS; Factor of Reactivity
1704	Assay: HPLC/MS; Factor of Reactivity
1705	Assay: HPLC/MS; Factor of Reactivity
1706	Assay: HPLC/MS; Factor of Reactivity
1707	Assay: HPLC/MS; Factor of Reactivity
1708	Assay: HPLC/MS; Factor of Reactivity
1709	Assay: HPLC/MS; Factor of Reactivity
1710	Assay: Steam bath; >90 = more than 90% liberation of halogen
1711	Assay: Steam bath; >90 = more than 90% liberation of halogen
1712	Assay: Steam bath; >90 = more than 90% liberation of halogen
1713	Assay: Steam bath; >90 = more than 90% liberation of halogen
1714	Assay: Steam bath; >90 = more than 90% liberation of halogen
1715	Assay: Steam bath; >90 = more than 90% liberation of halogen

#	Mechanism
1673	Michael-type nucleophilic addition
1674	Michael-type nucleophilic addition
1675	NOT Michael-type nucleophilic addition
1676	Michael-type nucleophilic addition
1677	Michael-type nucleophilic addition
1678	Michael-type nucleophilic addition
1679	Michael-type nucleophilic addition
1680	Michael-type nucleophilic addition
1681	Michael-type nucleophilic addition
1682	Michael-type nucleophilic addition
1683	Michael-type nucleophilic addition
1684	Michael-type nucleophilic addition
1685	Michael-type nucleophilic addition
1686	Michael-type nucleophilic addition
1687	Michael-type nucleophilic addition
1688	Michael-type nucleophilic addition
1689	Michael-type nucleophilic addition
1690	Michael-type nucleophilic addition
1691	Michael-type nucleophilic addition
1692	Michael-type nucleophilic addition
1693	Michael-type nucleophilic addition
1694	Michael-type nucleophilic addition
1695	NOT Michael-type nucleophilic addition
1696	Michael-type nucleophilic addition
1697	Michael-type nucleophilic addition
1698	NOT Michael-type nucleophilic addition
1699	
1700	
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#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1716	13633-34-6	1.3-Dichloro-2.5-dinitrobenzene	Aniline	DPE(Aniline)	% Depletion	>90		
1717	618-62-2	1.3-Dichloro-5-nitrobenzene	Aniline	DPE(Aniline)	% Depletion	<5		
1718	2213-82-3	1.4-Dichloro-2.6-dinitrobenzene	Aniline	DPE(Aniline)	% Depletion	>90		
1719	89-61-2	1.4-Dichloro-2-nitrobenzene	Aniline	DPE(Aniline)	% Depletion	<5		
1720	106-46-7	1.4-Dichlorobenzene	Aniline	DPE(Aniline)	% Depletion	<5		
1721	584-48-5	1-Bromo-2.4-dinitrobenzene	Aniline	DPE(Aniline)	% Depletion	>90		
1722	88-88-0	1-Chloro-2.4.6-trinitrobenzene	Aniline	DPE(Aniline)	% Depletion	>90		
1723	97-00-7	1-Chloro-2.4-dinitrobenzene	Aniline	DPE(Aniline)	% Depletion	>90		
1724	70-34-8	1-Fluoro-2.4-dinitrobenzene	Aniline	DPE(Aniline)	% Depletion	>90		
1725	709-49-9	1-Iodo-2.4-dinitrobenzene	Aniline	DPE(Aniline)	% Depletion	>90		
1726	3698-83-7	2.4-Dichloro-1.5-dinitrobenzene	Aniline	DPE(Aniline)	% Depletion	>90		
1727	99-65-0	3-Dinitrobenzene	Aniline	DPE(Aniline)	% Depletion	<5		
1728	100-00-5	4-Chloronitrobenzene	Aniline	DPE(Aniline)	% Depletion	<5		
1729	118-74-1	Hexachlorobenzene	Aniline	DPE(Aniline)	% Depletion	<5		
1730	123-31-9	1.4-Hydroquinone	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	0.42	1.26	
1731	106-50-3	1.4-Phenylenediamine	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	-12.6	2.75	
1732	3344-77-2	12-Bromo-1-dodecanol	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	1.68	1.82	
1733	109-65-9	1-Bromobutane	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	-3.74	4.81	
1734	71-36-3	1-Butanol	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	-8.36	6.03	
1735	97-00-7	1-Chloro-2.4-dinitrobenzene	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	93.3	11.1	
1736	5910-85-0	2.4-Heptadienal	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	3.01	0.9	
1737	874-23-7	2-Acetylcyclohexanone	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	20	1.02	
1738	818-61-1	2-Hydroxyethyl acrylate	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	3.73	2.78	
1739	923-26-2	2-Hydroxypropyl methacrylate	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	0.1	6.24	
1740	119-84-6	3.4-Dihydrocoumarin	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	6.6	4.5	
1741	3775-21-1	3-Methyl-4-phenyl-1.2.5-thiazole-1.1-dioxide	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	29	1.44	
1742	100-11-8	4-Nitrobenzylbromide	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	99.9	0.14	
1743	92-48-8	6-Methylcoumarin	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	3.66	2.94	
1744	101-86-0	alpha-Hexylcinnamaldehyde	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	-7.3	2.45	
1745	100-52-7	Benzaldehyde	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	-10.5	9.97	
1746	100-39-0	Benzyl bromide	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	60.5	0.91	
1747	104-55-2	Cinnamaldehyde	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	-4.19	4.18	
1748	104-54-1	Cinnamic alcohol	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	16.6	2.63	
1749	103-95-7	Cyclamen aldehyde	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	5.16	1.77	
1750	140-88-5	Ethyl acrylate	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	-0.64	1.03	
1751	50-00-0	Formaldehyde	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	1.27	2.4	
1752	111-30-8	Glutaraldehyde	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	0.86	2.7	
1753	56-81-5	Glycerol	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	-0.64	3.89	
1754	107-22-2	Glyoxal	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	-0.13	1.57	
1755	107-75-5	Hydroxycitronellal	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	4.45	1.38	
1756	97-54-1	Isoeugenol	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	11.7	0.44	
1757	50-21-5	Lactic acid	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	-4.77	3.41	
1758	143-15-7	Lauryl bromide	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	-4.27	4.43	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1716	100		Ethanol (abs.)	2 h		Landsteiner et al., J. Exp. Med. 64 (1936), 625
1717	100		Ethanol (abs.)	2 h		Landsteiner et al., J. Exp. Med. 64 (1936), 625
1718	100		Ethanol (abs.)	2 h		Landsteiner et al., J. Exp. Med. 64 (1936), 625
1719	100		Ethanol (abs.)	2 h		Landsteiner et al., J. Exp. Med. 64 (1936), 625
1720	100		Ethanol (abs.)	2 h		Landsteiner et al., J. Exp. Med. 64 (1936), 625
1721	100		Ethanol (abs.)	2 h		Landsteiner et al., J. Exp. Med. 64 (1936), 625
1722	100		Ethanol (abs.)	2 h		Landsteiner et al., J. Exp. Med. 64 (1936), 625
1723	100		Ethanol (abs.)	2 h		Landsteiner et al., J. Exp. Med. 64 (1936), 625
1724	100		Ethanol (abs.)	2 h		Landsteiner et al., J. Exp. Med. 64 (1936), 625
1725	100		Ethanol (abs.)	2 h		Landsteiner et al., J. Exp. Med. 64 (1936), 625
1726	100		Ethanol (abs.)	2 h		Landsteiner et al., J. Exp. Med. 64 (1936), 625
1727	100		Ethanol (abs.)	2 h		Landsteiner et al., J. Exp. Med. 64 (1936), 625
1728	100		Ethanol (abs.)	2 h		Landsteiner et al., J. Exp. Med. 64 (1936), 625
1729	100		Ethanol (abs.)	2 h		Landsteiner et al., J. Exp. Med. 64 (1936), 625
1730	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1731	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1732	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1733	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1734	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1735	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1736	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1737	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1738	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1739	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1740	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1741	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1742	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1743	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1744	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1745	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1746	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1747	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1748	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1749	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1750	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1751	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1752	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1753	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1754	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1755	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1756	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1757	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1758	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401

#	Comment
1716	Assay: Steam bath; >90 = more than 90% liberation of halogen
1717	Assay: Steam bath; >90 = more than 90% liberation of halogen
1718	Assay: Steam bath; >90 = more than 90% liberation of halogen
1719	Assay: Steam bath; >90 = more than 90% liberation of halogen
1720	Assay: Steam bath; >90 = more than 90% liberation of halogen
1721	Assay: Steam bath; >90 = more than 90% liberation of halogen
1722	Assay: Steam bath; >90 = more than 90% liberation of halogen
1723	Assay: Steam bath; >90 = more than 90% liberation of halogen
1724	Assay: Steam bath; >90 = more than 90% liberation of halogen
1725	Assay: Steam bath; >90 = more than 90% liberation of halogen
1726	Assay: Steam bath; >90 = more than 90% liberation of halogen
1727	Assay: Steam bath; >90 = more than 90% liberation of halogen
1728	Assay: Steam bath; >90 = more than 90% liberation of halogen
1729	Assay: Steam bath; >90 = more than 90% liberation of halogen
1730	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1731	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1732	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1733	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1734	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1735	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1736	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1737	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1738	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1739	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1740	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1741	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1742	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1743	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1744	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1745	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1746	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1747	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1748	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1749	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1750	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1751	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1752	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1753	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1754	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1755	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1756	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1757	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1758	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard

#	Mechanism
1716	
1717	
1718	
1719	
1720	
1721	
1722	
1723	
1724	
1725	
1726	
1727	
1728	
1729	
1730	No protein binding
1731	No protein binding
1732	Nucleophilic substitution, second order (SN2)
1733	Nucleophilic substitution, second order (SN2)
1734	No protein binding
1735	Nucleophilic aromatic substitution (SNAr)
1736	Michael-type nucleophilic addition
1737	unknown adduct
1738	No protein binding
1739	No protein binding
1740	No protein binding
1741	Acylation: Ac and MPT hydrolysis
1742	Nucleophilic substitution, second order (SN2)
1743	No protein binding
1744	No protein binding
1745	No protein binding
1746	Nucleophilic substitution, second order (SN2)
1747	No protein binding
1748	No protein binding
1749	No protein binding
1750	No protein binding
1751	No protein binding
1752	No protein binding
1753	No protein binding
1754	No protein binding
1755	No protein binding
1756	No protein binding
1757	No protein binding
1758	No protein binding

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1759	1166-52-5	Lauryl gallate	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	-2.04	5.12	
1760	15646-46-5	Oxazolone	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	22.7	3.41	
1761	106-51-4	p-Benzoquinone	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	0.25	1.32	
1762	93-99-2	Phenyl benzoate	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	-0.54	3.39	
1763	122-78-1	Phenylacetaldehyde	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	-0.61	7.81	
1764	69-72-7	Salicylic acid	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	-5.85	1.33	
1765	3913-81-3	trans-2-Decenal	Tyr-Peptide (AcFAAYAA)	DP(Tyr-P.): Aleksic	% Depletion	6.95	1.62	
1766	123-31-9	1.4-Hydroquinone	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	83.8	0.16	
1767	106-50-3	1.4-Phenylenediamine	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	-3	1.86	
1768	3344-77-2	12-Bromo-1-dodecanol	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	5.22	8.92	
1769	109-65-9	1-Bromobutane	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	3.61	3.11	
1770	71-36-3	1-Butanol	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	5.96	9.99	
1771	97-00-7	1-Chloro-2.4-dinitrobenzene	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	39.8	6.63	
1772	5910-85-0	2.4-Heptadienal	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	90.2	0.76	
1773	874-23-7	2-Acetylcyclohexanone	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	35.7	5.14	
1774	818-61-1	2-Hydroxyethyl acrylate	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	55.3	3.92	
1775	923-26-2	2-Hydroxypropyl methacrylate	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	6.96	9.67	
1776	119-84-6	3.4-Dihydrocoumarin	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	61.3	0.62	
1777	3775-21-1	3-Methyl-4-phenyl-1.2.5-thiazole-1.1-dioxide	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	90.2	2.16	
1778	100-11-8	4-Nitrobenzylbromide	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	100	0	
1779	92-48-8	6-Methylcoumarin	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	9.79	4.99	
1780	101-86-0	alpha-Hexylcinnamaldehyde	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	1.55	2.28	
1781	100-52-7	Benzaldehyde	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	82.1	0.49	
1782	100-39-0	Benzyl bromide	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	94.8	0.8	
1783	104-55-2	Cinnamaldehyde	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	81.3	0.62	
1784	104-54-1	Cinnamic alcohol	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	32.8	3.23	
1785	103-95-7	Cyclamen aldehyde	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	81.4	0.8	
1786	140-88-5	Ethyl acrylate	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	30	2.11	
1787	50-00-0	Formaldehyde	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	100	0	
1788	111-30-8	Glutaraldehyde	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	96.2	0	
1789	56-81-5	Glycerol	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	-3.66	1.84	
1790	107-22-2	Glyoxal	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	100	0	
1791	107-75-5	Hydroxycitronellal	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	91.2	0.57	
1792	97-54-1	Isoeugenol	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	95.6	0.23	
1793	50-21-5	Lactic acid	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	-11.7	0.55	
1794	143-15-7	Lauryl bromide	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	-14.6	2.57	
1795	1166-52-5	Lauryl gallate	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	6.17	1.91	
1796	15646-46-5	Oxazolone	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	96	0	
1797	106-51-4	p-Benzoquinone	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	100	0	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1759	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1760	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1761	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1762	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1763	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1764	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1765	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1766	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1767	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1768	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1769	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1770	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1771	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1772	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1773	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1774	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1775	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1776	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1777	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1778	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1779	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1780	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1781	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1782	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1783	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1784	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1785	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1786	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1787	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1788	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1789	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1790	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1791	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1792	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1793	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1794	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1795	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1796	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1797	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401

#	Comment
1759	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1760	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1761	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1762	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1763	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1764	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1765	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1766	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1767	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1768	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1769	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1770	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1771	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1772	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1773	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1774	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1775	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1776	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1777	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1778	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1779	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1780	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1781	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1782	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1783	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1784	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1785	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1786	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1787	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1788	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1789	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1790	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1791	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1792	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1793	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1794	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1795	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1796	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1797	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard

#	Mechanism
1759	No protein binding
1760	Acylation: Three possible adducts; hydrolysis products
1761	No protein binding
1762	Acylation: Loss of phenyl group
1763	No protein binding
1764	No protein binding
1765	No protein binding
1766	Michael-type nucleophilic addition: Double MA adduct and cyclised diquinone cross-linking
1767	No protein binding
1768	Nucleophilic substitution, second order (SN2)
1769	No protein binding
1770	No protein binding
1771	Nucleophilic aromatic substitution (SNAr)
1772	Schiff base formation
1773	Schiff base formation
1774	Michael-type nucleophilic addition: MA followed by hydrolysis
1775	No protein binding
1776	Acylation or Michael addition
1777	Pre-Schiff base formation: SB of MPT hydrolysis product
1778	Nucleophilic substitution, second order (SN2): Single+double adducts (N-terminal and -COOH terminal)
1779	Acylation or Michael addition
1780	Schiff base formation
1781	Schiff base formation
1782	Nucleophilic substitution, second order (SN2)
1783	Schiff base formation
1784	Michael-type nucleophilic addition: MA, evidence of SB adduct (oxidation to aldehyde, contamination?)
1785	Schiff base formation
1786	Michael-type nucleophilic addition
1787	Schiff base formation
1788	Gluturaldehyde polymerisation, multiple adducts
1789	No protein binding
1790	Schiff base formation
1791	Schiff base formation
1792	Pre-Michael addition of aromatic hydrocarbons
1793	No protein binding
1794	No protein binding
1795	No protein binding
1796	Imine formation with ethanol loss
1797	Michael-type nucleophilic addition: Triple MA adduct and cyclised diquinone cross-linked species

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1798	93-99-2	Phenyl benzoate	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	-2.02	0.81	
1799	122-78-1	Phenylacetaldehyde	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	92.1	0.26	
1800	69-72-7	Salicylic acid	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	2.47	1.79	
1801	3913-81-3	trans-2-Decenal	N-term-Peptide (FAAAAA)	DP(N-term.): Aleksic	% Depletion	49.3	0.88	
1802	104-27-8	1-(4-Methoxyphenyl)-1-penten-3-one	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	8.3	2.3	
1803	2634-33-5	1.2-Benzisothiazolin-3-one	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	ND		
1804	109-65-9	1-Bromobutane	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	0.2	1.2	
1805	71-36-3	1-Butanol	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	1.2	2.5	
1806	97-00-7	1-Chloro-2.4-dinitrobenzene	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	13.4	9	
1807	1118-71-4	2.2.6.6-Tetramethyl-3.5-heptanedione	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	0.6	1.9	
1808	431-03-8	2.3-Butanedione	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	23.7	1.3	
1809	5910-85-0	2.4-Heptadienal	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	19.8	3.5	
1810	874-23-7	2-Acetylcyclohexanone	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	-4.6	2.2	
1811	818-61-1	2-Hydroxyethyl acrylate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	38.2	2.4	
1812	923-26-2	2-Hydroxypropyl methacrylate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	ND		
1813	149-30-4	2-Mercaptobenzothiazole	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	-1.9	1.2	
1814	2682-20-4	2-Methyl-2H-isothiazolin-3-one	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	2.6	9.4	
1815	100-69-6	2-Vinylpyridine	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	0.1	11.3	
1816	140-67-0	4-Allylanisole	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	-0.9	1.3	
1817	99-96-7	4-Hydroxybenzoic acid	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	2.2	1.2	
1818	100-06-1	4-Methoxyacetophenone	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	-0.8	0.7	
1819	122-57-6	4-Phenyl-3-buten-2-one	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	-2.2	0.5	
1820	26172-55-4	5-Chloro-2-methyl-4-isothiazolin-3-one	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	3.9	3.2	
1821	13706-86-0	5-Methyl-2.3-hexanedione	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	5	1.1	
1822	92-48-8	6-Methylcoumarin	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	0.2	2.5	
1823	122-40-7	alpha-Amyl cinnamaldehyde	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	2.2	1.2	
1824	101-86-0	alpha-Hexylcinnamaldehyde	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	1	1.5	
1825	20048-27-5	Bandrowski's base	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	11.6	2.5	
1826	100-52-7	Benzaldehyde	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	-1.5	1.2	
1827	94-36-0	Benzoyl peroxide	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	28.6	8.1	
1828	120-51-4	Benzyl benzoate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	2.9	0.9	
1829	25646-71-3	CD3	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	18.9	2.5	
1830	108-90-7	Chlorobenzene	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	1.4	0.8	
1831	104-55-2	Cinnamaldehyde	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	27.5	1.7	
1832	91-64-5	Coumarin	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	-9.9	2.9	
1833	103-95-7	Cyclamen aldehyde	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	0.3	0.4	
1834	141-05-9	Diethyl maleate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	33.4	0.6	
1835	84-66-2	Diethyl phthalate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	0.7	1	
1836	886-38-4	Diphenylcyclopropenone	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	0.3	4.1	
1837	140-88-5	Ethyl acrylate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	24	20.7	
1838	94-02-0	Ethyl benzoylacetate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	-0.6	0.6	
1839	121-32-4	Ethyl vanillin	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	ND		
1840	97-90-5	Ethylene glycol dimethacrylate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	4.5	1.6	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1798	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1799	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1800	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1801	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1802		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1803		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1804		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1805		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1806		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1807		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1808		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1809		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1810		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1811		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1812		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1813		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1814		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1815		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1816		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1817		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1818		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1819		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1820		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1821		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1822		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1823		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1824		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1825		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1826		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1827		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1828		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1829		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1830		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1831		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1832		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1833		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1834		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1835		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1836		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1837		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1838		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1839		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1840		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417

#	Comment
1798	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1799	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1800	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1801	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1802	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1803	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1804	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1805	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1806	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1807	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1808	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1809	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1810	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1811	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1812	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1813	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1814	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1815	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1816	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1817	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1818	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1819	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1820	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1821	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1822	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1823	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1824	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1825	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1826	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1827	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1828	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1829	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1830	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1831	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1832	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1833	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1834	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1835	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1836	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1837	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1838	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1839	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1840	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD

#	Mechanism
1798	No protein binding
1799	Schiff base formation
1800	No protein binding
1801	Michael addition or Schiff base formation and multiple cross-linked species
1802	
1803	
1804	
1805	
1806	
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#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1841	19317-11-4	Farnesal	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	5.9	0.6	
1842	27072-45-3	Fluorescein isothiocynate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	15.5	0.3	
1843	50-00-0	Formaldehyde	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	0.7	0.6	
1844	111-30-8	Glutaraldehyde	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	66	2.2	
1845	56-81-5	Glycerol	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	-0.6	1.2	
1846	107-22-2	Glyoxal	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	29.7	6.2	
1847	110-54-3	Hexane	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	-0.7	0.3	
1848	93-53-8	Hydratropic aldehyde	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	8.8	2.1	
1849	107-75-5	Hydroxycitronellal	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	10.6	1.2	
1850	39236-46-9	Imidazolidinyl urea	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	0.2	1	
1851	67-63-0	Isopropanol	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	-1.3	0.1	
1852	110-27-0	Isopropyl myristate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	3.5	2.5	
1853	55965-84-9	Kathon CG	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	4.5	1	
1854	50-21-5	Lactic acid	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	3.2	0.4	
1855	1166-52-5	Lauryl gallate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	6.8	0.6	
1856	80-54-6	Lilial	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	0.8	0.8	
1857	119-36-8	Methyl salicylate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	2.4	0.8	
1858	111-80-8	Methyl-2-nonynoate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	2.5	2.9	
1859	99-76-3	Methylparaben	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	-0.6	2.3	
1860	150-75-4	Metol	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	34.2	3.8	
1861	112-05-0	Nonanoic acid	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	-4.1	3.9	
1862	764-85-2	Nonanoyl chloride	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	-1.1	9.3	
1863	124-07-2	Octanoic acid	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	-0.3	0.7	
1864	144-62-7	Oxalic acid	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	0	1.4	
1865	15646-46-5	Oxazolone	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	42.9	3.2	
1866	112-67-4	Palmitoyl chloride	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	0.2	0.4	
1867	106-51-4	p-Benzoquinone	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	55.6	3	
1868	2111-75-3	Perillaldehyde	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	13.3	0.5	
1869	122-78-1	Phenylacetaldehyde	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	12.9	0.5	
1870	85-44-9	Phthalic anhydride	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	9.9	0.8	
1871	121-79-9	Propyl gallate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	13.5	11.7	
1872	94-13-3	Propyl paraben	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	-0.7	0.2	
1873	57-55-6	Propylene glycol	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	0.2	2	
1874	108-46-3	Resorcinol	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	-0.9	1.7	
1875	69-72-7	Salicylic acid	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	-6.9	2.7	
1876	2892-51-5	Squaric acid	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	3.2	1.3	
1877	63-74-1	Sulfanilamide	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	0.3	1.6	
1878	121-57-3	Sulphanilic acid	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	-0.3	1.6	
1879	7426-07-5	Tetrachlorosalicylanilide	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	-0.2	0.7	
1880	6728-26-3	trans-2-Hexenal	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	2.8	1.8	
1881	552-30-7	Trimellitic anhydride	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	6.5	0.7	
1882	121-33-5	Vanillin	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	0.2	2	
1883	75-35-4	Vinylidene dichloride	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick (1:10)	% Depletion	-0.8	7.8	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1841		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1842		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1843		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1844		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1845		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1846		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1847		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1848		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1849		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1850		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1851		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1852		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1853		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1854		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1855		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1856		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1857		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1858		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1859		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1860		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1861		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1862		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1863		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1864		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1865		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1866		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1867		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1868		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1869		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1870		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1871		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1872		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1873		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1874		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1875		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1876		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1877		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1878		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1879		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1880		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1881		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1882		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1883		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417

#	Comment
1841	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1842	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1843	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1844	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1845	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1846	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1847	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1848	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1849	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1850	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1851	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1852	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1853	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1854	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1855	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1856	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1857	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1858	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1859	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1860	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1861	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1862	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1863	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1864	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1865	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1866	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1867	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1868	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1869	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1870	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1871	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1872	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1873	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1874	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1875	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1876	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1877	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1878	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1879	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1880	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1881	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1882	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
1883	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD

#	Mechanism
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#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1884	104-27-8	1-(4-Methoxyphenyl)-1-penten-3-one	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**14.3**	3.2	
1885	2634-33-5	1.2-Benzisothiazolin-3-one	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**9.7**	2.5	
1886	123-31-9	1.4-Hydroquinone	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**51.1**	6.5	
1887	109-65-9	1-Bromobutane	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**1.2**	0.4	
1888	71-36-3	1-Butanol	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**1.2**	0.8	
1889	97-00-7	1-Chloro-2.4-dinitrobenzene	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**14.7**	4.2	
1890	1118-71-4	2.2.6.6-Tetramethyl-3.5-heptanedione	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**0**	0.2	
1891	431-03-8	2.3-Butanedione	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**27**	3.9	
1892	5910-85-0	2.4-Heptadienal	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**23.9**	5	
1893	874-23-7	2-Acetylcyclohexanone	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**12.5**	0.5	
1894	818-61-1	2-Hydroxyethyl acrylate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**88.9**	0.3	
1895	923-26-2	2-Hydroxypropyl methacrylate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**-13.6**	7.8	
1896	149-30-4	2-Mercaptobenzothiazole	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**-3**	0.6	
1897	2682-20-4	2-Methyl-2H-isothiazolin-3-one	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**-5.6**	5.2	
1898	100-69-6	2-Vinylpyridine	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**-16.9**	16.2	
1899	119-84-6	3.4-Dihydrocoumarin	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**7.5**	1	
1900	591-27-5	3-Aminophenol	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**1.2**	1.7	
1901	109-55-7	3-Dimethylaminopropylamine	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**1.8**	1.9	
1902	140-67-0	4-Allylanisole	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**-0.8**	1.8	
1903	99-96-7	4-Hydroxybenzoic acid	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**2.2**	2.1	
1904	100-06-1	4-Methoxyacetophenone	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**0.1**	0.3	
1905	122-57-6	4-Phenyl-3-buten-2-one	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**1.5**	0.9	
1906	26172-55-4	5-Chloro-2-methyl-4-isothiazolin-3-one	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**35.1**	14	
1907	13706-86-0	5-Methyl-2.3-hexanedione	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**7.5**	1.1	
1908	92-48-8	6-Methylcoumarin	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**4**	5.6	
1909	122-40-7	alpha-Amyl cinnamaldehyde	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**3.9**	1.5	
1910	101-86-0	alpha-Hexylcinnamaldehyde	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**-1.6**	2.9	
1911	20048-27-5	Bandrowski's base	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**4.2**	17	
1912	100-52-7	Benzaldehyde	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**-1.7**	1.4	
1913	94-36-0	Benzoyl peroxide	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**81.3**	2.9	
1914	120-51-4	Benzyl benzoate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**3**	5.3	
1915	25646-71-3	CD3	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**13.6**	0.5	
1916	108-90-7	Chlorobenzene	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**1.3**	0.2	
1917	104-55-2	Cinnamaldehyde	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**43.2**	4.1	
1918	5392-40-5	Citral	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**16.9**	0.3	
1919	91-64-5	Coumarin	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**-14.9**	22	
1920	103-95-7	Cyclamen aldehyde	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**1**	0.4	
1921	141-05-9	Diethyl maleate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**85.5**	1.6	
1922	84-66-2	Diethyl phthalate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**-0.7**	0.9	
1923	886-38-4	Diphenylcyclopropenone	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**-0.7**	3.8	
1924	140-88-5	Ethyl acrylate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**93.7**	1.3	
1925	94-02-0	Ethyl benzoylacetate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**1.9**	0.4	
1926	121-32-4	Ethyl vanillin	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	**9.7**	5.5	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1884		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1885		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1886		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
1887		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1888		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1889		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1890		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1891		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1892		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1893		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1894		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1895		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1896		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1897		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1898		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1899		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
1900		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
1901		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
1902		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1903		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1904		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1905		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1906		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1907		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1908		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1909		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1910		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1911		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1912		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1913		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1914		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1915		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1916		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1917		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1918		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
1919		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1920		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1921		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1922		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1923		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1924		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1925		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1926		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417

#	Comment
1884	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1885	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1886	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1887	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1888	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1889	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1890	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1891	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1892	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1893	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1894	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1895	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1896	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1897	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1898	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1899	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1900	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1901	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1902	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1903	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1904	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1905	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1906	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1907	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1908	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1909	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1910	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1911	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1912	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1913	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1914	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1915	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1916	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1917	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1918	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1919	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1920	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1921	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1922	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1923	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1924	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1925	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1926	Assay: room temperature 0.5 : 25 mM; HPLC-DAD

#	Mechanism
1884	
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#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1927	97-90-5	Ethylene glycol dimethacrylate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	12.4	3	
1928	19317-11-4	Farnesal	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	8.5	13.6	
1929	27072-45-3	Fluorescein isothiocynate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	61.1	1.5	
1930	50-00-0	Formaldehyde	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	11.2	3.5	
1931	111-30-8	Glutaraldehyde	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	85.4	3.5	
1932	56-81-5	Glycerol	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	2.1	0.9	
1933	107-22-2	Glyoxal	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	67.8	1.9	
1934	110-54-3	Hexane	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	-5.1	0.6	
1935	93-53-8	Hydratropic aldehyde	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	21.2	1.6	
1936	107-75-5	Hydroxycitronellal	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	6.5	2	
1937	39236-46-9	Imidazolidinyl urea	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	1.3	1.9	
1938	67-63-0	Isopropanol	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	0.5	0.5	
1939	110-27-0	Isopropyl myristate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	-4	17.3	
1940	55965-84-9	Kathon CG	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	3.9	1	
1941	50-21-5	Lactic acid	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	0.8	0.5	
1942	1166-52-5	Lauryl gallate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	8.7	4.2	
1943	80-54-6	Lilial	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	0.7	0.2	
1944	119-36-8	Methyl salicylate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	1.6	0.3	
1945	111-80-8	Methyl-2-nonynoate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	3.2	4	
1946	99-76-3	Methylparaben	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	-0.4	0.8	
1947	150-75-4	Metol	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	44.7	3.8	
1948	112-05-0	Nonanoic acid	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	-9.6	2.9	
1949	764-85-2	Nonanoyl chloride	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	-6.3	1.8	
1950	124-07-2	Octanoic acid	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	0.9	0.1	
1951	144-62-7	Oxalic acid	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	-0.9	0.7	
1952	15646-46-5	Oxazolone	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	49.6	1.8	
1953	112-67-4	Palmitoyl chloride	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	26.6	1.3	
1954	106-51-4	p-Benzoquinone	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	91	0.2	
1955	2111-75-3	Perillaldehyde	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	13.8	0.5	
1956	122-78-1	Phenylacetaldehyde	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	22.6	1.9	
1957	85-44-9	Phthalic anhydride	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	75	3.9	
1958	121-79-9	Propyl gallate	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	26.6	10.7	
1959	94-13-3	Propyl paraben	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	-0.2	1.3	
1960	57-55-6	Propylene glycol	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	0.6	0.7	
1961	108-46-3	Resorcinol	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	-0.8	1.9	
1962	69-72-7	Salicylic acid	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	ND	ND	
1963	2892-51-5	Squaric acid	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	4.8	4.9	
1964	63-74-1	Sulfanilamide	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	0.8	0.5	
1965	121-57-3	Sulphanilic acid	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	0.5	1	
1966	7426-07-5	Tetrachlorosalicylanilide	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	9	24	
1967	6728-26-3	trans-2-Hexenal	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	3.6	2.6	
1968	552-30-7	Trimellitic anhydride	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	43.7	4.9	
1969	121-33-5	Vanillin	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	-6.6	3.6	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1927		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1928		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1929		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1930		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1931		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1932		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1933		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1934		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1935		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1936		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1937		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
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1939		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
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1941		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1942		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1943		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1944		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1945		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
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1963		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1964		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1965		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1966		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1967		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1968		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1969		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417

#	Comment
1927	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
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1930	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1931	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1932	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1933	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1934	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1935	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1936	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1937	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1938	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1939	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1940	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1941	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1942	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1943	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1944	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1945	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1946	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1947	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1948	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1949	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1950	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1951	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1952	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1953	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1954	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1955	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1956	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1957	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1958	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1959	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1960	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1961	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1962	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1963	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1964	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1965	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1966	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1967	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1968	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1969	Assay: room temperature 0.5 : 25 mM; HPLC-DAD

#	Mechanism
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#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
1970	75-35-4	Vinylidene dichloride	Lys-Peptide (AcRFAAKAA)	DP(Lys-P.): Gerberick	% Depletion	-4.3	18.2	
1971	123-31-9	1.4-Hydroquinone	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	98.2	0.26	
1972	106-50-3	1.4-Phenylenediamine	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	25	5.61	
1973	3344-77-2	12-Bromo-1-dodecanol	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	13	8.63	
1974	109-65-9	1-Bromobutane	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	0.04	1.46	
1975	71-36-3	1-Butanol	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	6.27	4.17	
1976	97-00-7	1-Chloro-2.4-dinitrobenzene	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	97.7	0.9	
1977	5910-85-0	2.4-Heptadienal	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	90.7	2.02	
1978	874-23-7	2-Acetylcyclohexanone	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	49.6	1.03	
1979	818-61-1	2-Hydroxyethyl acrylate	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	100	0	
1980	923-26-2	2-Hydroxypropyl methacrylate	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	33.1	1.65	
1981	119-84-6	3.4-Dihydrocoumarin	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	38.1	3.2	
1982	3775-21-1	3-Methyl-4-phenyl-1.2.5-thiazole-1.1-dioxide	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	61.5	10.5	
1983	100-11-8	4-Nitrobenzylbromide	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	100	0	
1984	92-48-8	6-Methylcoumarin	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	12.7	3.48	
1985	101-86-0	alpha-Hexylcinnamaldehyde	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	6.27	3.21	
1986	100-52-7	Benzaldehyde	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	26.7	0.14	
1987	100-39-0	Benzyl bromide	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	77.3	1.61	
1988	104-55-2	Cinnamaldehyde	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	58.8	1.64	
1989	104-54-1	Cinnamic alcohol	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	8.38	3.17	
1990	103-95-7	Cyclamen aldehyde	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	7.19	5.48	
1991	140-88-5	Ethyl acrylate	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	94	2.75	
1992	50-00-0	Formaldehyde	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	26.2	6.26	
1993	111-30-8	Glutaraldehyde	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	100	0	
1994	56-81-5	Glycerol	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	1.04	2.23	
1995	107-22-2	Glyoxal	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	42.7	1.41	
1996	107-75-5	Hydroxycitronellal	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	10.9	6.48	
1997	97-54-1	Isoeugenol	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	96.1	0.71	
1998	50-21-5	Lactic acid	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	1.16	0.26	
1999	143-15-7	Lauryl bromide	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	10.2	1.9	
2000	1166-52-5	Lauryl gallate	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	85.3	2.53	
2001	15646-46-5	Oxazolone	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	99.2	0.17	
2002	106-51-4	p-Benzoquinone	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	100	0	
2003	93-99-2	Phenyl benzoate	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	20.3	5.6	
2004	122-78-1	Phenylacetaldehyde	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	100	0	
2005	69-72-7	Salicylic acid	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	-9.06	5.93	
2006	3913-81-3	trans-2-Decenal	Lys-Peptide (AcFAAKAA)	DP(Lys-P.): Aleksic	% Depletion	57.9	3.77	
2007	123-31-9	1.4-Hydroquinone	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	31.9	0.41	
2008	106-50-3	1.4-Phenylenediamine	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	27.3	3.79	
2009	3344-77-2	12-Bromo-1-dodecanol	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	9.94	2.96	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
1970		10.2	Acetate buffer 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
1971	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1972	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1973	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1974	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1975	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1976	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1977	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1978	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1979	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1980	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1981	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1982	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1983	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1984	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1985	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1986	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1987	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1988	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1989	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1990	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1991	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1992	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1993	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1994	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1995	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1996	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1997	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1998	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
1999	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2000	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2001	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2002	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2003	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2004	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2005	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2006	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2007	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2008	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2009	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401

#	Comment
1970	Assay: room temperature 0.5 : 25 mM; HPLC-DAD
1971	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1972	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1973	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1974	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1975	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1976	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1977	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1978	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1979	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1980	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1981	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1982	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1983	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1984	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1985	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1986	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1987	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1988	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1989	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1990	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1991	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1992	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1993	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1994	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1995	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1996	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1997	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1998	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
1999	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2000	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2001	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2002	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2003	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2004	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2005	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2006	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2007	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2008	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2009	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard

#	Mechanism
1970	
1971	Cross-linking via Schiff base formation: Cyclised diquinone cross-link species
	Pre-Michael addition of aromatic hydrocarbons:
1972	MA of quinine diimine after PPD oxidisation
1973	Nucleophilic substitution, second order (SN2)
1974	Nucleophilic substitution, second order (SN2)
1975	No protein binding
1976	Nucleophilic aromatic substitution (SNAr)
1977	Schiff base formation
1978	Schiff base formation
	Michael-type nucleophilic addition:
1979	Single+double adduct and hydrolysis products
1980	Michael-type nucleophilic addition: MA followed by hydrolysis
1981	Acylation or Michael addition
1982	Schiff base formation: SB from MPT hydrolysis product
1983	Nucleophilic substitution, second order (SN2): Single and double adducts
1984	Acylation or Michael addition
1985	Michael addition or Schiff base formation
1986	Schiff base formation
1987	Nucleophilic substitution, second order (SN2): Single+double+triple adduct
1988	Michael addition or Schiff base formation
1989	No protein binding
1990	Schiff base formation
	Michael-type nucleophilic addition:
1991	Single+double adduct and hydrolysis products
1992	Schiff base formation
1993	Cross-linking via Schiff base formation
1994	No protein binding
1995	Schiff base formation
1996	Schiff base formation
1997	Pre-Michael addition of aromatic hydrocarbons: Single+double adduct
1998	No protein binding
1999	No protein binding
2000	Schiff base formation
2001	Acylation: Loss of ethanol, imine formation
2002	Cross-linking via Schiff base formation: Cyclised diquinone cross-link species
2003	Acylation
2004	Schiff base formation
2005	No protein binding
2006	Michael addition or Schiff base formation: MA and SB double adduct
2007	Pre-Michael addition of aromatic hydrocarbons
2008	Cross-linking via Schiff base formation: probably, multiple adducts
2009	No protein binding

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2010	109-65-9	1-Bromobutane	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	3.31	2.01	
2011	71-36-3	1-Butanol	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	-4.95	1.66	
2012	97-00-7	1-Chloro-2.4-dinitrobenzene	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	5.87	9.2	
2013	5910-85-0	2.4-Heptadienal	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	14.5	1.64	
2014	874-23-7	2-Acetylcyclohexanone	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	3.93	1.66	
2015	818-61-1	2-Hydroxyethyl acrylate	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	14.1	6.83	
2016	923-26-2	2-Hydroxypropyl methacrylate	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	17.1	2.6	
2017	119-84-6	3.4-Dihydrocoumarin	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	2.6	1.85	
2018	3775-21-1	3-Methyl-4-phenyl-1.2.5-thiazole-1.1-dioxide	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	3.5	6.82	
2019	100-11-8	4-Nitrobenzylbromide	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	84.8	7.54	
2020	92-48-8	6-Methylcoumarin	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	7.26	3.38	
2021	101-86-0	alpha-Hexylcinnamaldehyde	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	-2.64	8.63	
2022	100-52-7	Benzaldehyde	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	36.2	0.97	
2023	100-39-0	Benzyl bromide	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	40.1	10.1	
2024	104-55-2	Cinnamaldehyde	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	18.9	4.16	
2025	104-54-1	Cinnamic alcohol	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	4.94	1.72	
2026	103-95-7	Cyclamen aldehyde	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	3.41	0.82	
2027	140-88-5	Ethyl acrylate	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	3.94	4.63	
2028	50-00-0	Formaldehyde	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	-11.1	5.63	
2029	111-30-8	Glutaraldehyde	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	1.45	3.38	
2030	56-81-5	Glycerol	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	-8.93	1.04	
2031	107-22-2	Glyoxal	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	4.04	6.8	
2032	107-75-5	Hydroxycitronellal	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	6.36	1.23	
2033	97-54-1	Isoeugenol	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	21.6	5.14	
2034	50-21-5	Lactic acid	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	9.44	2.85	
2035	143-15-7	Lauryl bromide	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	4.87	9.31	
2036	1166-52-5	Lauryl gallate	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	-5.29	5.19	
2037	15646-46-5	Oxazolone	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	-7.63	3.61	
2038	106-51-4	p-Benzoquinone	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	100	0	
2039	93-99-2	Phenyl benzoate	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	9.75	3.88	
2040	122-78-1	Phenylacetaldehyde	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	-0.13	4.37	
2041	69-72-7	Salicylic acid	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	2.56	1.24	
2042	3913-81-3	trans-2-Decenal	His-Peptide (AcFAAHAA)	DP(His-P.): Aleksic	% Depletion	17.9	5.32	
2043	104-27-8	1-(4-Methoxyphenyl)-1-penten-3-one	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	1.7	2.1	
2044	2634-33-5	1.2-Benzisothiazolin-3-one	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	ND		
2045	123-31-9	1.4-Hydroquinone	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	30	0.9	
2046	71-36-3	1-Butanol	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	0.5	0.4	
2047	97-00-7	1-Chloro-2.4-dinitrobenzene	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	0.3	4.9	
2048	818-61-1	2-Hydroxyethyl acrylate	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	8.2	4.3	
2049	923-26-2	2-Hydroxypropyl methacrylate	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	ND		
2050	119-84-6	3.4-Dihydrocoumarin	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	1.8	2.8	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2010	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2011	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2012	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2013	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2014	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2015	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2016	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2017	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2018	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2019	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2020	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2021	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2022	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2023	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2024	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2025	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2026	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2027	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2028	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2029	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2030	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2031	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2032	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2033	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2034	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2035	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2036	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2037	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2038	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2039	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2040	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2041	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2042	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2043		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2044		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2045		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2046		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2047		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2048		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2049		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2050		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332

#	Comment
2010	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2011	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2012	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2013	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2014	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2015	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2016	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2017	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2018	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2019	Simultaneous analysis: 82.34(1.51)%. Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2020	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2021	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2022	Simultaneous analysis: 14.53(3.05)%. Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2023	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2024	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2025	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2026	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2027	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2028	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2029	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2030	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2031	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2032	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2033	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2034	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2035	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2036	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2037	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2038	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2039	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2040	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2041	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2042	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2043	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2044	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2045	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2046	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2047	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2048	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2049	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2050	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD

#	Mechanism
2010	No protein binding
2011	No protein binding
2012	Nucleophilic aromatic substitution (SNAr)
2013	Michael-type nucleophilic addition
2014	No protein binding
	Michael-type nucleophilic addition:
2015	Single+double adduct and hydrolysis products
2016	No protein binding
2017	No protein binding
2018	No protein binding
	Nucleophilic substitution, second order (SN2):
2019	SN2 on His and terminal -COOH group
2020	No protein binding
2021	No protein binding
2022	Schiff base formation: Single+double adducts
2023	Nucleophilic substitution, second order (SN2)
2024	Michael-type nucleophilic addition
2025	No protein binding
2026	No protein binding
2027	Michael-type nucleophilic addition
2028	No protein binding
2029	No protein binding
2030	No protein binding
2031	No protein binding
2032	unknown adduct
2033	Pre-Michael addition of aromatic hydrocarbons
2034	No protein binding
2035	No protein binding
2036	No protein binding
2037	No protein binding
2038	Michael-type nucleophilic addition
2039	No protein binding
2040	No protein binding
2041	No protein binding
2042	Michael-type nucleophilic addition
2043	
2044	
2045	
2046	
2047	
2048	
2049	
2050	

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2051	591-27-5	3-Aminophenol	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	2	2.4	
2052	109-55-7	3-Dimethylaminopropylamine	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	1.9	2.5	
2053	99-96-7	4-Hydroxybenzoic acid	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	-0.4	0.2	
2054	13706-86-0	5-Methyl-2.3-hexanedione	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	23.1	3.9	
2055	92-48-8	6-Methylcoumarin	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	1.6	2.5	
2056	122-40-7	alpha-Amyl cinnamaldehyde	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	-1.1	1.7	
2057	101-86-0	alpha-Hexylcinnamaldehyde	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	-0.4	1.5	
2058	120-51-4	Benzyl benzoate	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	-2.5	0.8	
2059	25646-71-3	CD3	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	-8.9	4	
2060	108-90-7	Chlorobenzene	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	-1.8	2	
2061	104-55-2	Cinnamaldehyde	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	3.8	7.8	
2062	5392-40-5	Citral	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	7.9	1	
2063	141-05-9	Diethyl maleate	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	0.5	0.8	
2064	84-66-2	Diethyl phthalate	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	0.7	2.8	
2065	886-38-4	Diphenylcyclopropenone	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	1	3.1	
2066	97-90-5	Ethylene glycol dimethacrylate	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	1.2	1.8	
2067	111-30-8	Glutaraldehyde	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	2.7	1	
2068	56-81-5	Glycerol	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	0.2	0.6	
2069	110-54-3	Hexane	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	-1.8	3.5	
2070	107-75-5	Hydroxycitronellal	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	5.6	6.2	
2071	50-21-5	Lactic acid	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	-0.8	1.3	
2072	1166-52-5	Lauryl gallate	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	0.1	1	
2073	80-54-6	Lilial	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	0.4	0.3	
2074	119-36-8	Methyl salicylate	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	0.5	1.1	
2075	124-07-2	Octanoic acid	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	0.7	0.3	
2076	15646-46-5	Oxazolone	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	4.9	11.6	
2077	106-51-4	p-Benzoquinone	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	94	3.8	
2078	122-78-1	Phenylacetaldehyde	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	3.1	0.8	
2079	85-44-9	Phthalic anhydride	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	4.6	5.8	
2080	2892-51-5	Squaric acid	His-Peptide (AcRFAAHAA)	DP(His-P.)	% Depletion	3.1	0.4	
2081		(Z)-Ethyl 2-acetyldec-2-enoate	Glutathione	DP(GSH): Natsch	% Depletion	30.9	3	
2082	16510-27-3	1-(Cyclopropylmethyl)-4-methoxybenzene	Glutathione	DP(GSH): Natsch	% Depletion	1	6.9	
2083	3910-35-8	1.1.3-Trimethyl-3-phenylindane	Glutathione	DP(GSH): Natsch	% Depletion	4.4	5.6	
2084	97-00-7	1-Chloro-2.4-dinitrobenzene	Glutathione	DP(GSH): Natsch	% Depletion	93.5	7.2	
2085	54440-17-4	2.3-Dihydro-2.3.3-trimethyl-1H-inden-1-one	Glutathione	DP(GSH): Natsch	% Depletion	-0.5	3.6	
2086	6658-48-6	2-Methyl-3-(4-(2-methylpropyl)phenyl)-propanal	Glutathione	DP(GSH): Natsch	% Depletion	6.1	5.1	
2087	10032-15-2	2-Methyl-butanoic acid hexyl ester	Glutathione	DP(GSH): Natsch	% Depletion	ND	ND	
2088	928-95-0	2-trans-Hexenol	Glutathione	DP(GSH): Natsch	% Depletion	-1	4	
2089	119-84-6	3.4-Dihydrocoumarin	Glutathione	DP(GSH): Natsch	% Depletion	-7.1	1.3	
2090	259854-71-2	3-Methyl-(5Z)-5-cyclotetradecen-1-one	Glutathione	DP(GSH): Natsch	% Depletion	1	1.6	
2091	65442-31-1	6-(1-methylpropyl)quinoline	Glutathione	DP(GSH): Natsch	% Depletion	3.2	4.9	
2092	26330-65-4	6-Ethyl-3-methyl-6-octen-1-ol	Glutathione	DP(GSH): Natsch	% Depletion	7.7	1.4	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2051		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2052		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2053		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2054		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2055		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2056		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2057		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2058		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2059		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2060		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2061		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2062		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2063		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2064		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2065		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2066		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2067		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2068		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2069		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2070		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2071		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2072		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2073		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2074		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2075		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2076		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2077		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2078		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2079		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2080		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2081	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2082	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2083	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2084	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2085	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2086	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2087	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2088	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2089	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2090	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2091	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2092	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220

#	Comment
2051	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2052	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2053	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2054	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2055	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2056	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2057	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2058	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2059	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2060	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2061	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2062	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2063	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2064	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2065	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2066	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2067	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2068	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2069	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2070	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2071	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2072	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2073	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2074	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2075	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2076	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2077	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2078	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2079	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2080	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2081	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2082	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2083	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2084	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2085	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2086	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2087	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2088	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2089	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2090	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2091	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2092	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]

#	Mechanism
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#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2093		6-Methoxy-2.6-dimethyl octanal	Glutathione	DP(GSH): Natsch	% Depletion	**8.2**	1.4	
2094	362467-67-2	7-(3-Methylbutyl)-2H-1.5-benzodioxepin-3(4H)-one	Glutathione	DP(GSH): Natsch	% Depletion	**45.4**	5.7	
2095	101-86-0	alpha-Hexylcinnamaldehyde	Glutathione	DP(GSH): Natsch	% Depletion	**32.3**	3.1	
2096	101-39-3	alpha-Methyl cinnamic aldehyde	Glutathione	DP(GSH): Natsch	% Depletion	**12.6**	2.3	
2097	123-69-3	Ambrettolide	Glutathione	DP(GSH): Natsch	% Depletion	**-0.8**	3.1	
2098	100-51-6	Benzyl alcohol	Glutathione	DP(GSH): Natsch	% Depletion	**-0.7**	10.8	
2099	120-51-4	Benzyl benzoate	Glutathione	DP(GSH): Natsch	% Depletion	**-2.1**	0.1	
2100	103-41-3	Benzyl cinnamate	Glutathione	DP(GSH): Natsch	% Depletion	**6.9**	2.3	
2101	118-58-1	Benzyl salicylate	Glutathione	DP(GSH): Natsch	% Depletion	**-6.7**	3.6	
2102	23726-91-2	beta-Damascone	Glutathione	DP(GSH): Natsch	% Depletion	**81.5**	0.4	
2103	79-77-6	beta-Ionone	Glutathione	DP(GSH): Natsch	% Depletion	**5.7**	4.2	
2104	495-62-5	Bisabolene	Glutathione	DP(GSH): Natsch	% Depletion	**-5.4**	3.2	
2105	28940-11-6	Calone	Glutathione	DP(GSH): Natsch	% Depletion	**ND**	ND	
2106	104-55-2	Cinnamaldehyde	Glutathione	DP(GSH): Natsch	% Depletion	**21.3**	3.3	
2107	104-54-1	Cinnamic alcohol	Glutathione	DP(GSH): Natsch	% Depletion	**-1.8**	4.4	
2108	2277-19-2	cis-6-Nonenal	Glutathione	DP(GSH): Natsch	% Depletion	**ND**	ND	
2109	5392-40-5	Citral	Glutathione	DP(GSH): Natsch	% Depletion	**21.2**	3	
2110		Citrathal R	Glutathione	DP(GSH): Natsch	% Depletion	**18.1**	9.1	
2111	68039-49-6	Cyclal C	Glutathione	DP(GSH): Natsch	% Depletion	**-2.1**	2.1	
2112	103-95-7	Cyclamen aldehyde	Glutathione	DP(GSH): Natsch	% Depletion	**4.1**	4.1	
2113	477218-42-1	Cyclopropanecarboxylic acid-2-[1-(3.3-dimethylcyclohexyl)ethoxy]-2-methylpropyl ester	Glutathione	DP(GSH): Natsch	% Depletion	**1.5**	2.5	
2114	141-05-9	Diethyl maleate	Glutathione	DP(GSH): Natsch	% Depletion	**99**	0.2	
2115	84-66-2	Diethyl phthalate	Glutathione	DP(GSH): Natsch	% Depletion	**-4.6**	1.1	
2116	2785-87-7	Dihydroeugenol	Glutathione	DP(GSH): Natsch	% Depletion	**0**	0.8	
2117	105-95-3	Ethylene brassylate	Glutathione	DP(GSH): Natsch	% Depletion	**8.6**	1.1	
2118	97-53-0	Eugenol	Glutathione	DP(GSH): Natsch	% Depletion	**ND**	ND	
2119	50-00-0	Formaldehyde	Glutathione	DP(GSH): Natsch	% Depletion	**90.5**	2.3	
2120	56973-85-4	Galbanone	Glutathione	DP(GSH): Natsch	% Depletion	**61.4**	1.9	
2121	106-24-1	Geraniol	Glutathione	DP(GSH): Natsch	% Depletion	**-9.2**	0.8	
2122	56-81-5	Glycerol	Glutathione	DP(GSH): Natsch	% Depletion	**-8.9**	3	
2123	24851-98-7	Hedione	Glutathione	DP(GSH): Natsch	% Depletion	**3**	2.3	
2124	107-75-5	Hydroxycitronellal	Glutathione	DP(GSH): Natsch	% Depletion	**38.3**	0.8	
2125	97-54-1	Isoeugenol	Glutathione	DP(GSH): Natsch	% Depletion	**55.1**	3.3	
2126	110-27-0	Isopropyl myristate	Glutathione	DP(GSH): Natsch	% Depletion	**-2.2**	7.3	
2127	1166-52-5	Lauryl gallate	Glutathione	DP(GSH): Natsch	% Depletion	**24.4**	9.9	
2128	80-54-6	Lilial	Glutathione	DP(GSH): Natsch	% Depletion	**13.6**	1.3	
2129	78-70-6	Linalool	Glutathione	DP(GSH): Natsch	% Depletion	**-9.2**	5.1	
2130	475-20-7	Longifolene	Glutathione	DP(GSH): Natsch	% Depletion	**ND**	ND	
2131	31906-04-4	Lyral	Glutathione	DP(GSH): Natsch	% Depletion	**8.2**	6.4	
2132	111-12-6	Methyl 2-octynoate	Glutathione	DP(GSH): Natsch	% Depletion	**ND**	ND	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2093	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2094	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2095	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2096	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2097	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2098	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2099	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2100	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2101	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2102	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2103	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2104	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2105	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2106	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2107	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2108	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2109	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2110	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2111	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2112	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2113	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2114	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2115	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2116	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2117	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2118	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2119	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2120	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2121	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2122	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2123	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2124	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2125	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2126	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2127	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2128	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2129	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2130	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2131	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2132	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220

#	Comment
2093	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2094	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2095	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2096	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2097	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2098	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2099	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2100	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2101	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2102	LC-MS. Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2103	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2104	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2105	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2106	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2107	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2108	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2109	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2110	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2111	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2112	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2113	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2114	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2115	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2116	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2117	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2118	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2119	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2120	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2121	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2122	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2123	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2124	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2125	LC-MS. Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2126	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2127	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2128	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2129	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2130	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2131	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2132	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]

#	Mechanism
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2102	Mass spectrometry confirms adduct formation
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2125	GSH-adduct is dimer and trimer of iso-eugenol
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#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2133	4707-47-5	Methyl atrarate	Glutathione	DP(GSH): Natsch	% Depletion	-3	2.6	
2134	119-36-8	Methyl salicylate	Glutathione	DP(GSH): Natsch	% Depletion	5.6	8.8	
2135	99-76-3	Methylparaben	Glutathione	DP(GSH): Natsch	% Depletion	-14	1.1	
2136	15646-46-5	Oxazolone	Glutathione	DP(GSH): Natsch	% Depletion	98.4	0.1	
2137	(495-62-5)	Oxidised Bisabolene	Glutathione	DP(GSH): Natsch	% Depletion	25.8	0.2	
2138	(475-20-7)	Oxidised Longifolene	Glutathione	DP(GSH): Natsch	% Depletion	ND	ND	
2139	60-12-8	Phenyl ethyl alcohol	Glutathione	DP(GSH): Natsch	% Depletion	-0.3	0.9	
2140	122-78-1	Phenylacetaldehyde	Glutathione	DP(GSH): Natsch	% Depletion	20.4	2.3	
2141	357650-26-1	Pomarose	Glutathione	DP(GSH): Natsch	% Depletion	82.2	0.3	
2142	57-55-6	Propylene glycol	Glutathione	DP(GSH): Natsch	% Depletion	-4	8.5	
2143	110-86-1	Pyridine	Glutathione	DP(GSH): Natsch	% Depletion	-3.9	3.9	
2144	69-72-7	Salicylic acid	Glutathione	DP(GSH): Natsch	% Depletion	-6.8	2.3	
2145	224031-70-3	Spirogalbanone	Glutathione	DP(GSH): Natsch	% Depletion	32.5	4.1	
2146	3913-81-3	trans-2-Decenal	Glutathione	DP(GSH): Natsch	% Depletion	36	1.4	
2147	6728-26-3	trans-2-Hexenal	Glutathione	DP(GSH): Natsch	% Depletion	61.9	2.2	
2148	104-46-1	trans-Anethole	Glutathione	DP(GSH): Natsch	% Depletion	2.1	3	
2149	121-33-5	Vanillin	Glutathione	DP(GSH): Natsch	% Depletion	-2.8	3.2	
2150	104-27-8	1-(4-Methoxyphenyl)-1-penten-3-one	Glutathione	DP(GSH): Gerberick	% Depletion	-0.2	1.5	
2151	2634-33-5	1.2-Benzisothiazolin-3-one	Glutathione	DP(GSH): Gerberick	% Depletion	14.5	1.3	
2152	123-31-9	1.4-Hydroquinone	Glutathione	DP(GSH): Gerberick	% Depletion	76.5	6.1	
2153	109-65-9	1-Bromobutane	Glutathione	DP(GSH): Gerberick	% Depletion	4	3.3	
2154	71-36-3	1-Butanol	Glutathione	DP(GSH): Gerberick	% Depletion	6.1	7.5	
2155	97-00-7	1-Chloro-2.4-dinitrobenzene	Glutathione	DP(GSH): Gerberick	% Depletion	43.6	2.6	
2156	1118-71-4	2.2.6.6-Tetramethyl-3.5-heptanedione	Glutathione	DP(GSH): Gerberick	% Depletion	5.4	8.2	
2157	431-03-8	2.3-Butanedione	Glutathione	DP(GSH): Gerberick	% Depletion	0.5	4.1	
2158	5910-85-0	2.4-Heptadienal	Glutathione	DP(GSH): Gerberick	% Depletion	93	2.5	
2159	874-23-7	2-Acetylcyclohexanone	Glutathione	DP(GSH): Gerberick	% Depletion	4.3	4.1	
2160	818-61-1	2-Hydroxyethyl acrylate	Glutathione	DP(GSH): Gerberick	% Depletion	98.1	1.8	
2161	923-26-2	2-Hydroxypropyl methacrylate	Glutathione	DP(GSH): Gerberick	% Depletion	5.5	4.8	
2162	149-30-4	2-Mercaptobenzothiazole	Glutathione	DP(GSH): Gerberick	% Depletion	24	5.9	
2163	2682-20-4	2-Methyl-2H-isothiazolin-3-one	Glutathione	DP(GSH): Gerberick	% Depletion	73	5.8	
2164	100-69-6	2-Vinylpyridine	Glutathione	DP(GSH): Gerberick	% Depletion	38	0.7	
2165	119-84-6	3.4-Dihydrocoumarin	Glutathione	DP(GSH): Gerberick	% Depletion	2.3	2.6	
2166	591-27-5	3-Aminophenol	Glutathione	DP(GSH): Gerberick	% Depletion	2	2.4	
2167	109-55-7	3-Dimethylaminopropylamine	Glutathione	DP(GSH): Gerberick	% Depletion	2.8	5.2	
2168	140-67-0	4-Allylanisole	Glutathione	DP(GSH): Gerberick	% Depletion	17.8	3.1	
2169	99-96-7	4-Hydroxybenzoic acid	Glutathione	DP(GSH): Gerberick	% Depletion	1	5.8	
2170	100-06-1	4-Methoxyacetophenone	Glutathione	DP(GSH): Gerberick	% Depletion	2.5	3.2	
2171	122-57-6	4-Phenyl-3-buten-2-one	Glutathione	DP(GSH): Gerberick	% Depletion	58.5	3.9	
2172	26172-55-4	5-Chloro-2-methyl-4-isothiazolin-3-one	Glutathione	DP(GSH): Gerberick	% Depletion	74.7	8.5	
2173	13706-86-0	5-Methyl-2.3-hexanedione	Glutathione	DP(GSH): Gerberick	% Depletion	-2.6	9.9	
2174	92-48-8	6-Methylcoumarin	Glutathione	DP(GSH): Gerberick	% Depletion	-1.6	8.6	
2175	122-40-7	alpha-Amyl cinnamaldehyde	Glutathione	DP(GSH): Gerberick	% Depletion	0.2	10.1	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2133	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2134	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2135	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2136	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2137	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2138	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2139	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2140	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2141	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2142	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2143	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2144	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2145	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2146	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2147	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2148	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2149	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2150	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2151	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2152	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2153	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2154	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2155	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2156	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2157	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2158	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2159	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2160	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2161	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2162	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2163	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2164	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2165	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2166	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2167	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2168	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2169	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2170	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2171	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2172	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2173	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2174	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2175	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417

#	Comment
2133	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2134	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2135	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2136	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2137	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2138	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2139	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2140	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2141	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2142	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2143	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2144	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2145	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2146	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2147	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2148	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2149	Assay: Unreacted GSH detected with enzymatic test; R: [Tietze, 1969]
2150	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2151	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2152	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2153	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2154	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2155	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2156	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2157	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2158	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2159	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2160	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2161	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2162	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2163	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2164	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2165	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2166	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2167	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2168	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2169	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2170	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2171	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2172	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2173	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2174	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2175	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])

#	Mechanism
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#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2176	101-86-0	alpha-Hexylcinnamaldehyde	Glutathione	DP(GSH): Gerberick	% Depletion	-2.6	3.2	
2177	20048-27-5	Bandrowski's base	Glutathione	DP(GSH): Gerberick	% Depletion	30	9.3	
2178	100-52-7	Benzaldehyde	Glutathione	DP(GSH): Gerberick	% Depletion	6.8	2.6	
2179	94-36-0	Benzoyl peroxide	Glutathione	DP(GSH): Gerberick	% Depletion	100	0	
2180	120-51-4	Benzyl benzoate	Glutathione	DP(GSH): Gerberick	% Depletion	0.7	5.5	
2181	25646-71-3	CD3	Glutathione	DP(GSH): Gerberick	% Depletion	63.6	13.6	
2182	108-90-7	Chlorobenzene	Glutathione	DP(GSH): Gerberick	% Depletion	3.2	2.3	
2183	104-55-2	Cinnamaldehyde	Glutathione	DP(GSH): Gerberick	% Depletion	46.7	5.2	
2184	5392-40-5	Citral	Glutathione	DP(GSH): Gerberick	% Depletion	37.5	14.4	
2185	91-64-5	Coumarin	Glutathione	DP(GSH): Gerberick	% Depletion	1	3.8	
2186	103-95-7	Cyclamen aldehyde	Glutathione	DP(GSH): Gerberick	% Depletion	10.4	5.5	
2187	141-05-9	Diethyl maleate	Glutathione	DP(GSH): Gerberick	% Depletion	83.3	4.5	
2188	84-66-2	Diethyl phthalate	Glutathione	DP(GSH): Gerberick	% Depletion	10.9	13.3	
2189	886-38-4	Diphenylcyclopropenone	Glutathione	DP(GSH): Gerberick	% Depletion	22	7.5	
2190	140-88-5	Ethyl acrylate	Glutathione	DP(GSH): Gerberick	% Depletion	89.8	-4.5	
2191	94-02-0	Ethyl benzoylacetate	Glutathione	DP(GSH): Gerberick	% Depletion	3.9	3	
2192	121-32-4	Ethyl vanillin	Glutathione	DP(GSH): Gerberick	% Depletion	-0.7	3.1	
2193	97-90-5	Ethylene glycol dimethacrylate	Glutathione	DP(GSH): Gerberick	% Depletion	3.6	5.6	
2194	19317-11-4	Farnesal	Glutathione	DP(GSH): Gerberick	% Depletion	10	2.6	
2195	27072-45-3	Fluorescein isothiocynate	Glutathione	DP(GSH): Gerberick	% Depletion	92.6	1.5	
2196	50-00-0	Formaldehyde	Glutathione	DP(GSH): Gerberick	% Depletion	37.5	3.5	
2197	111-30-8	Glutaraldehyde	Glutathione	DP(GSH): Gerberick	% Depletion	20.8	4	
2198	56-81-5	Glycerol	Glutathione	DP(GSH): Gerberick	% Depletion	1.2	4.2	
2199	107-22-2	Glyoxal	Glutathione	DP(GSH): Gerberick	% Depletion	33	6.3	
2200	110-54-3	Hexane	Glutathione	DP(GSH): Gerberick	% Depletion	-0.8	4.1	
2201	93-53-8	Hydratropic aldehyde	Glutathione	DP(GSH): Gerberick	% Depletion	3.7	3.9	
2202	107-75-5	Hydroxycitronellal	Glutathione	DP(GSH): Gerberick	% Depletion	-1.8	3.9	
2203	39236-46-9	Imidazolidinyl urea	Glutathione	DP(GSH): Gerberick	% Depletion	30.7	3	
2204	67-63-0	Isopropanol	Glutathione	DP(GSH): Gerberick	% Depletion	1.4	6.8	
2205	110-27-0	Isopropyl myristate	Glutathione	DP(GSH): Gerberick	% Depletion	4.9	-8.7	
2206	55965-84-9	Kathon CG	Glutathione	DP(GSH): Gerberick	% Depletion	46.7	9.3	
2207	50-21-5	Lactic acid	Glutathione	DP(GSH): Gerberick	% Depletion	-1.1	11.1	
2208	1166-52-5	Lauryl gallate	Glutathione	DP(GSH): Gerberick	% Depletion	42.2	13.6	
2209	80-54-6	Lilial	Glutathione	DP(GSH): Gerberick	% Depletion	7.7	0.8	
2210	119-36-8	Methyl salicylate	Glutathione	DP(GSH): Gerberick	% Depletion	4.2	3.5	
2211	111-80-8	Methyl-2-nonynoate	Glutathione	DP(GSH): Gerberick	% Depletion	92.7	4.1	
2212	99-76-3	Methylparaben	Glutathione	DP(GSH): Gerberick	% Depletion	3.4	4.2	
2213	150-75-4	Metol	Glutathione	DP(GSH): Gerberick	% Depletion	86.1	3.4	
2214	112-05-0	Nonanoic acid	Glutathione	DP(GSH): Gerberick	% Depletion	4	6.5	
2215	764-85-2	Nonanoyl chloride	Glutathione	DP(GSH): Gerberick	% Depletion	79	13	
2216	124-07-2	Octanoic acid	Glutathione	DP(GSH): Gerberick	% Depletion	-1.6	3.1	
2217	144-62-7	Oxalic acid	Glutathione	DP(GSH): Gerberick	% Depletion	-2.9	3.1	
2218	15646-46-5	Oxazolone	Glutathione	DP(GSH): Gerberick	% Depletion	22.6	9.5	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2176	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2177	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2178	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2179	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2180	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2181	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2182	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2183	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2184	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2185	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2186	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2187	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2188	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2189	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2190	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2191	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2192	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2193	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2194	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2195	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2196	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2197	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2198	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2199	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2200	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2201	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2202	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2203	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2204	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2205	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2206	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2207	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2208	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2209	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2210	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2211	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2212	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2213	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2214	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2215	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2216	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2217	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2218	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417

#	Comment
2176	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2177	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2178	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2179	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2180	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2181	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2182	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2183	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2184	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2185	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2186	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2187	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2188	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2189	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2190	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2191	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2192	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2193	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2194	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2195	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2196	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2197	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2198	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2199	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2200	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2201	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2202	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2203	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2204	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2205	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2206	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2207	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2208	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2209	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2210	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2211	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
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2214	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2215	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2216	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2217	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2218	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])

#	Mechanism
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#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2219	112-67-4	Palmitoyl chloride	Glutathione	DP(GSH): Gerberick	% Depletion	77	14.1	
2220	106-51-4	p-Benzoquinone	Glutathione	DP(GSH): Gerberick	% Depletion	100	0	
2221	2111-75-3	Perillaldehyde	Glutathione	DP(GSH): Gerberick	% Depletion	10.2	4.7	
2222	122-78-1	Phenylacetaldehyde	Glutathione	DP(GSH): Gerberick	% Depletion	-4.7	0.7	
2223	85-44-9	Phthalic anhydride	Glutathione	DP(GSH): Gerberick	% Depletion	100	0	
2224	121-79-9	Propyl gallate	Glutathione	DP(GSH): Gerberick	% Depletion	19.7	4.3	
2225	94-13-3	Propyl paraben	Glutathione	DP(GSH): Gerberick	% Depletion	-1	6	
2226	57-55-6	Propylene glycol	Glutathione	DP(GSH): Gerberick	% Depletion	4.2	2.5	
2227	108-46-3	Resorcinol	Glutathione	DP(GSH): Gerberick	% Depletion	3.6	6.2	
2228	69-72-7	Salicylic acid	Glutathione	DP(GSH): Gerberick	% Depletion	-8.2	-5.2	
2229	2892-51-5	Squaric acid	Glutathione	DP(GSH): Gerberick	% Depletion	16.5	4	
2230	63-74-1	Sulfanilamide	Glutathione	DP(GSH): Gerberick	% Depletion	12.8	4.5	
2231	121-57-3	Sulphanilic acid	Glutathione	DP(GSH): Gerberick	% Depletion	-6	2.3	
2232	7426-07-5	Tetrachlorosalicylanilide	Glutathione	DP(GSH): Gerberick	% Depletion	0.7	2.3	
2233	6728-26-3	trans-2-Hexenal	Glutathione	DP(GSH): Gerberick	% Depletion	68	3.9	
2234	552-30-7	Trimellitic anhydride	Glutathione	DP(GSH): Gerberick	% Depletion	97.6	4	
2235	121-33-5	Vanillin	Glutathione	DP(GSH): Gerberick	% Depletion	1.5	4.7	
2236	75-35-4	Vinylidene dichloride	Glutathione	DP(GSH): Gerberick	% Depletion	0	5.3	
2237		(Z)-Ethyl 2-acetyldec-2-enoate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	77.5	13.2	
2238	16510-27-3	1-(Cyclopropylmethyl)-4-methoxybenzene	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	-1.56	1.25	
2239	3910-35-8	1.1.3-Trimethyl-3-phenylindane	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	12.8	6.7	
2240	97-00-7	1-Chloro-2.4-dinitrobenzene	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	100	0	
2241	54440-17-4	2.3-Dihydro-2.3.3-trimethyl-1H-inden-1-one	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	7.6	1.65	
2242	818-61-1	2-Hydroxyethyl acrylate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	89.4		
2243	6658-48-6	2-Methyl-3-(4-(2-methylpropyl)phenyl)-propanal	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	100	0	
2244	10032-15-2	2-Methyl-butanoic acid hexyl ester	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	8.6	5.5	
2245	928-95-0	2-trans-Hexenol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	17.6	1.4	
2246	119-84-6	3.4-Dihydrocoumarin	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	4	9.4	
2247	259854-71-2	3-Methyl-(5Z)-5-cyclotetradecen-1-one	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	6	3.1	
2248	65442-31-1	6-(1-methylpropyl)quinoline	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	6.3	2.4	
2249	26330-65-4	6-Ethyl-3-methyl-6-octen-1-ol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	-3.1	7.2	
2250		6-Methoxy-2.6-dimethyl octanal	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	52	5.9	
2251	362467-67-2	7-(3-Methylbutyl)-2H-1.5-benzodioxepin-3(4H)-one	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	100	0	
2252	101-86-0	alpha-Hexylcinnamaldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	63.7	9	
2253	101-39-3	alpha-Methyl cinnamic aldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	7.5	4.7	
2254	123-69-3	Ambrettolide	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	8.3	4.47	
2255	8001-54-5	Benzalkonium chloride	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	-6.8		
2256	100-51-6	Benzyl alcohol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	5.5	0.8	
2257	120-51-4	Benzyl benzoate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	0.2	0.8	
2258	100-39-0	Benzyl bromide	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	97.8		
2259	103-41-3	Benzyl cinnamate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	-1.5	2.7	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2219	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2220	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2221	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2222	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2223	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2224	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2225	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2226	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2227	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2228	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2229	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2230	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2231	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2232	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2233	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2234	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2235	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2236	25	7.4	PBS	15 min	1:100	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2237	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2238	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2239	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2240	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2241	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2242	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2243	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2244	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2245	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2246	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2247	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2248	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2249	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2250	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2251	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2252	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2253	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2254	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2255	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2256	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2257	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2258	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2259	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220

#	Comment
2219	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2220	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2221	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2222	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2223	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2224	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2225	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2226	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2227	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2228	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2229	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2230	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2231	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2232	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2233	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2234	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2235	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2236	Assay: 0.2 GSH : 20 mM El; RP-HPLC (Derivat. of GSH/GSSH with DNFB; R: [Farris, Reed 1987])
2237	Assay: HPLC-DAD 214 nm
2238	Assay: HPLC-DAD 214 nm
2239	Assay: HPLC-DAD 214 nm
2240	Assay: HPLC-DAD 214 nm
2241	Assay: HPLC-DAD 214 nm
2242	Assay: HPLC-DAD 214 nm
2243	Assay: HPLC-DAD 214 nm
2244	Assay: HPLC-DAD 214 nm
2245	Assay: HPLC-DAD 214 nm
2246	Assay: HPLC-DAD 214 nm
2247	Assay: HPLC-DAD 214 nm
2248	Assay: HPLC-DAD 214 nm
2249	Assay: HPLC-DAD 214 nm
2250	Assay: HPLC-DAD 214 nm
2251	Assay: HPLC-DAD 214 nm
2252	Assay: HPLC-DAD 214 nm
2253	LC-MS. Assay: HPLC-DAD 214 nm
2254	Assay: HPLC-DAD 214 nm
2255	Assay: HPLC-DAD 214 nm
2256	Assay: HPLC-DAD 214 nm
2257	Assay: HPLC-DAD 214 nm
2258	Assay: HPLC-DAD 214 nm
2259	Assay: HPLC-DAD 214 nm

#	Mechanism
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2253	Mass spectrometry confirms adduct formation
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#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2260	118-58-1	Benzyl salicylate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	-9.5	6.7	
2261	23726-91-2	beta-Damascone	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	100	0	
2262	79-77-6	beta-Ionone	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	52.5	1.42	
2263	495-62-5	Bisabolene	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	-3.7	9.5	
2264	28940-11-6	Calone	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	3.8	0.7	
2265	104-55-2	Cinnamaldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	85.9	12.5	
2266	104-54-1	Cinnamic alcohol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	10.8	2	
2267	2277-19-2	cis-6-Nonenal	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	53.4	6.6	
2268	5392-40-5	Citral	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	94.8	5.3	
2269		Citrathal R	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	100	0	
2270	68039-49-6	Cyclal C	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	100	0	
2271	103-95-7	Cyclamen aldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	100	0	
2272	477218-42-1	Cyclopropanecarboxylic acid-2-[1-(3.3-dimethylcyclohexyl)ethoxy]-2-methylpropyl ester	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	10.8	3.5	
2273		Cydrane	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	9		
2274	141-05-9	Diethyl maleate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	98.2	1.6	
2275	84-66-2	Diethyl phthalate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	0.5	1.02	
2276	2785-87-7	Dihydroeugenol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	0.8	2.89	
2277	105-95-3	Ethylene brassylate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	-2.2	18.3	
2278	107-15-3	Ethylenediamine	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	15.9		
2279	97-53-0	Eugenol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	54.3	0	
2280	50-00-0	Formaldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	66.9	1.5	
2281	56973-85-4	Galbanone	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	75.5	4.73	
2282	106-24-1	Geraniol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	-1.39	1.14	
2283	56-81-5	Glycerol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	4.2	6	
2284	24851-98-7	Hedione	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	4.1	2.3	
2285	107-75-5	Hydroxycitronellal	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	77.1	4.18	
2286	97-54-1	Isoeugenol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	100	0	
2287	110-27-0	Isopropyl myristate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	4.2	0.9	
2288	1166-52-5	Lauryl gallate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	94.4	0.9	
2289	80-54-6	Lilial	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	47	3.7	
2290	78-70-6	Linalool	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	1.7	2.5	
2291	475-20-7	Longifolene	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	2.1	5.6	
2292	31906-04-4	Lyral	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	95.2	2	
2293	111-12-6	Methyl 2-octynoate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	100	0	
2294	4707-47-5	Methyl atrarate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	100	0	
2295	119-36-8	Methyl salicylate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	2.4	0.35	
2296	99-76-3	Methylparaben	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	1.2	1.08	
2297	7786-81-4	Nickel(II) sulfate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	35.5		
2298	15646-46-5	Oxazolone	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	95.4	1.7	
2299	(495-62-5)	Oxidised Bisabolene	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	100	0	
2300	(475-20-7)	Oxidised Longifolene	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	0.5	10.1	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2260	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2261	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2262	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2263	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2264	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2265	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2266	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2267	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2268	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2269	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2270	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2271	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2272	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2273	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2274	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2275	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2276	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2277	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2278	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2279	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2280	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2281	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2282	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2283	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2284	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2285	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2286	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2287	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2288	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2289	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2290	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2291	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2292	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2293	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2294	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2295	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2296	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2297	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2298	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2299	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2300	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220

#	Comment
2260	Assay: HPLC-DAD 214 nm
2261	Assay: HPLC-DAD 214 nm
2262	LC-MS. Assay: HPLC-DAD 214 nm
2263	Assay: HPLC-DAD 214 nm
2264	Assay: HPLC-DAD 214 nm
2265	LC-MS. Assay: HPLC-DAD 214 nm
2266	Assay: HPLC-DAD 214 nm
2267	Assay: HPLC-DAD 214 nm
2268	LC-MS. Assay: HPLC-DAD 214 nm
2269	Assay: HPLC-DAD 214 nm
2270	Assay: HPLC-DAD 214 nm
2271	Assay: HPLC-DAD 214 nm
2272	Assay: HPLC-DAD 214 nm
2273	Assay: HPLC-DAD 214 nm
2274	LC-MS. Assay: HPLC-DAD 214 nm
2275	Assay: HPLC-DAD 214 nm
2276	Assay: HPLC-DAD 214 nm
2277	Assay: HPLC-DAD 214 nm
2278	rated non-significant. Assay: HPLC-DAD 214 nm
2279	Assay: HPLC-DAD 214 nm
2280	Assay: HPLC-DAD 214 nm
2281	Assay: HPLC-DAD 214 nm
2282	Assay: HPLC-DAD 214 nm
2283	Assay: HPLC-DAD 214 nm
2284	Assay: HPLC-DAD 214 nm
2285	Assay: HPLC-DAD 214 nm
2286	LC-MS. Assay: HPLC-DAD 214 nm
2287	Assay: HPLC-DAD 214 nm
2288	Assay: HPLC-DAD 214 nm
2289	Assay: HPLC-DAD 214 nm
2290	Assay: HPLC-DAD 214 nm
2291	Assay: HPLC-DAD 214 nm
2292	Assay: HPLC-DAD 214 nm
2293	Assay: HPLC-DAD 214 nm
2294	Assay: HPLC-DAD 214 nm
2295	Assay: HPLC-DAD 214 nm
2296	Assay: HPLC-DAD 214 nm
2297	Assay: HPLC-DAD 214 nm
2298	Assay: HPLC-DAD 214 nm
2299	Assay: HPLC-DAD 214 nm
2300	Assay: HPLC-DAD 214 nm

#	Mechanism
2260	
2261	
2262	Adduct + mass 32 (oxidation)
2263	
2264	
2265	Mass spectrometry confirms adduct formation
2266	
2267	
2268	Adduct confirmed (traces)
2269	
2270	
2271	
2272	
2273	
2274	Mass spectrometry confirms adduct formation
2275	
2276	
2277	
2278	
2279	
2280	
2281	
2282	
2283	
2284	
2285	
2286	various adducts
2287	
2288	
2289	
2290	
2291	
2292	
2293	
2294	
2295	
2296	
2297	
2298	
2299	
2300	

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2301	60-12-8	Phenyl ethyl alcohol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	4	1.9	
2302	122-78-1	Phenylacetaldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	65.8	2.73	
2303	357650-26-1	Pomarose	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	100	0	
2304	57-55-6	Propylene glycol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	12.8	6.8	
2305	110-86-1	Pyridine	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	9.9	7.2	
2306	69-72-7	Salicylic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	-20.8	12	
2307	151-21-3	Sodium lauryl sulfate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	7.2		
2308	224031-70-3	Spirogalbanone	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	98.8	2.13	
2309	3913-81-3	trans-2-Decenal	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	100	0	
2310	6728-26-3	trans-2-Hexenal	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	100	0	
2311	104-46-1	trans-Anethole	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	21.7	9	
2312	121-33-5	Vanillin	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Natsch	% Depletion	36.8	20.1	
2313	104-27-8	1-(4-Methoxyphenyl)-1-penten-3-one	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	75.8	12.6	
2314	2634-33-5	1.2-Benzisothiazolin-3-one	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	83.5	1.6	
2315	109-65-9	1-Bromobutane	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	47.6	24.1	
2316	71-36-3	1-Butanol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	-4.1	4.3	
2317	97-00-7	1-Chloro-2.4-dinitrobenzene	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	100	0	
2318	1118-71-4	2.2.6.6-Tetramethyl-3.5-heptanedione	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	-3.7	0.6	
2319	431-03-8	2.3-Butanedione	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	75.5	16.8	
2320	5910-85-0	2.4-Heptadienal	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	93.4	2.7	
2321	874-23-7	2-Acetylcyclohexanone	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	40.8	8.5	
2322	818-61-1	2-Hydroxyethyl acrylate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	92.2	0.1	
2323	923-26-2	2-Hydroxypropyl methacrylate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	96.5	1.5	
2324	149-30-4	2-Mercaptobenzothiazole	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	99.2	0.7	
2325	2682-20-4	2-Methyl-2H-isothiazolin-3-one	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	100	0	
2326	100-69-6	2-Vinylpyridine	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	90.3	0.1	
2327	140-67-0	4-Allylanisole	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	61.5	5.4	
2328	99-96-7	4-Hydroxybenzoic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	14	14	
2329	100-06-1	4-Methoxyacetophenone	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	-3.3	1.4	
2330	122-57-6	4-Phenyl-3-buten-2-one	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	96.5	3	
2331	26172-55-4	5-Chloro-2-methyl-4-isothiazolin-3-one	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	87.8	6	
2332	13706-86-0	5-Methyl-2.3-hexanedione	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	69.6	7.3	
2333	92-48-8	6-Methylcoumarin	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	-0.3	3.9	
2334	122-40-7	alpha-Amyl cinnamaldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	0.7	10.6	
2335	101-86-0	alpha-Hexylcinnamaldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	1	2.4	
2336	20048-27-5	Bandrowski's base	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	96.3	0.1	
2337	100-52-7	Benzaldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	-2.2	2.6	
2338	94-36-0	Benzoyl peroxide	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	80.6	3.7	
2339	120-51-4	Benzyl benzoate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	-2.2	5.5	
2340	25646-71-3	CD3	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	83	1.1	
2341	108-90-7	Chlorobenzene	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	-2.7	2.2	
2342	104-55-2	Cinnamaldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	88.6	1.4	
2343	91-64-5	Coumarin	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	-14.5	10.1	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2301	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2302	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2303	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2304	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2305	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2306	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2307	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2308	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2309	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2310	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2311	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2312	30		PBS 20 mM	24 h	1:100	Natsch A et al., Toxicol. Vitro 21 (2007), 1220
2313		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2314		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2315		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2316		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2317		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2318		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2319		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2320		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2321		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2322		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2323		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2324		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2325		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2326		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2327		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2328		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2329		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2330		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2331		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2332		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2333		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2334		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2335		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2336		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2337		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2338		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2339		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2340		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2341		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2342		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2343		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417

#	Comment
2301	Assay: HPLC-DAD 214 nm
2302	Assay: HPLC-DAD 214 nm
2303	LC-MS. Assay: HPLC-DAD 214 nm
2304	Assay: HPLC-DAD 214 nm
2305	Assay: HPLC-DAD 214 nm
2306	Assay: HPLC-DAD 214 nm
2307	Assay: HPLC-DAD 214 nm
2308	Assay: HPLC-DAD 214 nm
2309	LC-MS. Assay: HPLC-DAD 214 nm
2310	LC-MS. Assay: HPLC-DAD 214 nm
2311	Assay: HPLC-DAD 214 nm
2312	Assay: HPLC-DAD 214 nm
2313	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2314	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2315	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2316	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2317	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2318	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2319	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2320	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2321	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2322	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2323	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2324	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2325	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2326	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2327	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2328	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2329	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2330	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2331	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2332	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2333	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2334	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2335	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2336	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2337	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2338	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2339	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2340	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2341	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2342	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2343	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD

#	Mechanism
2301	
2302	
2303	Mass spectrometry confirms adduct formation
2304	
2305	
2306	
2307	
2308	
2309	Adduct + mass 32 (oxidation)
2310	Mass spectrometry confirms adduct formation
2311	
2312	
2313	
2314	
2315	
2316	
2317	
2318	
2319	
2320	
2321	
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#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2344	103-95-7	Cyclamen aldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	46.1	9.7	
2345	141-05-9	Diethyl maleate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	100	0	
2346	84-66-2	Diethyl phthalate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	3.3	4.6	
2347	886-38-4	Diphenylcyclopropenone	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	100	0	
2348	140-88-5	Ethyl acrylate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	97.6	2.1	
2349	94-02-0	Ethyl benzoylacetate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	0.5	0.5	
2350	121-32-4	Ethyl vanillin	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	ND		
2351	97-90-5	Ethylene glycol dimethacrylate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	100	0	
2352	19317-11-4	Farnesal	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	71.1	6.7	
2353	27072-45-3	Fluorescein isothiocynate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	100	0	
2354	50-00-0	Formaldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	75	3	
2355	111-30-8	Glutaraldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	70	4.7	
2356	56-81-5	Glycerol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	0.9	1.9	
2357	107-22-2	Glyoxal	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	94	8.5	
2358	110-54-3	Hexane	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	0.3	2.3	
2359	93-53-8	Hydratropic aldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	100	0	
2360	107-75-5	Hydroxycitronellal	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	55.8	3.6	
2361	39236-46-9	Imidazolidinyl urea	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	74.7	2.3	
2362	67-63-0	Isopropanol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	-3.1	0.3	
2363	110-27-0	Isopropyl myristate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	-2.2	2.9	
2364	55965-84-9	Kathon CG	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	99.5	0.9	
2365	50-21-5	Lactic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	11.5	21	
2366	1166-52-5	Lauryl gallate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	100	0	
2367	80-54-6	Lilial	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	71.6	15.5	
2368	119-36-8	Methyl salicylate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	0.8	7.7	
2369	111-80-8	Methyl-2-nonynoate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	100	0	
2370	99-76-3	Methylparaben	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	-5.4	6.3	
2371	150-75-4	Metol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	38.3	3.1	
2372	112-05-0	Nonanoic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	5.2	4.6	
2373	764-85-2	Nonanoyl chloride	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	23	11	
2374	124-07-2	Octanoic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	2.7	3.7	
2375	144-62-7	Oxalic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	-5.8	7.7	
2376	15646-46-5	Oxazolone	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	89.3	2.6	
2377	112-67-4	Palmitoyl chloride	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	60.1	5.2	
2378	106-51-4	p-Benzoquinone	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	97.1	2.8	
2379	2111-75-3	Perillaldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	85	0.7	
2380	122-78-1	Phenylacetaldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	81.1	3.7	
2381	85-44-9	Phthalic anhydride	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	-5.5	2	
2382	121-79-9	Propyl gallate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	97.7	2.4	
2383	94-13-3	Propyl paraben	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	21.8	6.3	
2384	57-55-6	Propylene glycol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	-3	0.6	
2385	108-46-3	Resorcinol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	2.3	2	
2386	69-72-7	Salicylic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	9.3	5.6	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2344		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2345		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2346		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2347		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2348		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2349		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2350		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2351		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2352		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2353		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2354		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2355		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2356		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2357		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2358		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2359		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2360		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2361		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2362		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2363		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2364		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2365		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2366		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2367		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2368		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2369		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2370		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2371		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2372		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2373		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2374		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2375		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2376		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2377		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2378		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2379		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2380		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2381		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2382		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2383		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2384		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2385		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2386		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417

#	Comment
2344	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2345	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2346	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2347	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2348	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2349	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2350	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2351	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2352	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2353	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2354	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2355	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2356	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2357	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2358	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2359	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2360	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2361	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2362	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2363	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2364	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2365	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2366	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2367	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2368	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2369	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2370	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2371	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2372	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2373	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2374	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2375	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2376	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2377	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2378	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2379	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2380	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2381	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2382	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2383	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2384	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2385	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2386	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD

#	Mechanism
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#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2387	2892-51-5	Squaric acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	94.3	4.2	
2388	63-74-1	Sulfanilamide	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	-2.1	0.2	
2389	121-57-3	Sulphanilic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	1.4	4.1	
2390	7426-07-5	Tetrachlorosalicylanilide	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	96.5	0.7	
2391	6728-26-3	trans-2-Hexenal	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	93	1	
2392	552-30-7	Trimellitic anhydride	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	-14.8	5.7	
2393	121-33-5	Vanillin	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	34.2	5.1	
2394	75-35-4	Vinylidene dichloride	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick (1:50)	% Depletion	4	1.7	
2395	104-27-8	1-(4-Methoxyphenyl)-1-penten-3-one	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	29.9	5.6	
2396	2634-33-5	1.2-Benzisothiazolin-3-one	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	97.7	0.1	
2397	123-31-9	1.4-Hydroquinone	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	83.3	0.9	
2398	106-50-3	1.4-Phenylenediamine	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	95.2		
2399	106-50-3	1.4-Phenylenediamine	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	95.2		
2400	109-65-9	1-Bromobutane	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	13.8	3.6	
2401	71-36-3	1-Butanol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	-0.4	1.4	
2402	71-36-3	1-Butanol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	2.2		
2403	71-36-3	1-Butanol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	2.2		
2404	97-00-7	1-Chloro-2.4-dinitrobenzene	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	100	0	
2405	3386-33-2	1-Chlorooctadecane	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	3.4		
2406	579-07-7	1-Phenyl-1.2-propanedione	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	92.1		
2407	1118-71-4	2.2.6.6-Tetramethyl-3.5-heptanedione	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	1.4	13.6	
2408	431-03-8	2.3-Butanedione	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	79	20.8	
2409	431-03-8	2.3-Butanedione	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	79.9		
2410	431-03-8	2.3-Butanedione	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	79.9		
2411	5910-85-0	2.4-Heptadienal	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	97.3	0.1	
2412	5910-85-0	2.4-Heptadienal	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	84.6		
2413	874-23-7	2-Acetylcyclohexanone	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	18.2	4.4	
2414	95-55-6	2-Aminophenol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	100		
2415	95-55-6	2-Aminophenol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	100		
2416	10520-81-7	2-Bromotetradecanoic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	29.3		
2417	10520-81-7	2-Bromotetradecanoic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	29.3		
2418	818-61-1	2-Hydroxyethyl acrylate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	92.6	0.5	
2419	818-61-1	2-Hydroxyethyl acrylate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	83.5		
2420	923-26-2	2-Hydroxypropyl methacrylate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	58.4	5.9	
2421	149-30-4	2-Mercaptobenzothiazole	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	97.5	4.2	
2422	149-30-4	2-Mercaptobenzothiazole	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	100		
2423	149-30-4	2-Mercaptobenzothiazole	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	100		
2424	2682-20-4	2-Methyl-2H-isothiazolin-3-one	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	97.9	0.3	
2425	100-69-6	2-Vinylpyridine	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	92.1	0.4	
2426	119-84-6	3.4-Dihydrocoumarin	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	ND		
2427	591-27-5	3-Aminophenol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	6.6	1.5	
2428	109-55-7	3-Dimethylaminopropylamine	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	10.2	3.4	
2429	140-67-0	4-Allylanisole	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	20.6	5.6	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2387		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2388		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2389		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2390		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2391		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2392		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2393		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2394		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:50	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2395		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2396		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2397		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2398		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2399		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2400		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2401		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2402		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2403		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2404		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2405		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2406		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2407		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2408		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2409		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2410		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2411		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2412		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2413		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2414		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2415		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2416		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2417		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2418		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2419		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2420		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2421		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2422		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2423		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2424		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2425		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2426		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2427		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2428		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2429		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417

#	Comment
2387	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2388	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2389	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2390	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2391	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2392	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2393	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2394	Assay: room temperature; 0.5 : 25 mM; HPLC-DAD
2395	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2396	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2397	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2398	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2399	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2400	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2401	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2402	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2403	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2404	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2405	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2406	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2407	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2408	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2409	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2410	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2411	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2412	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2413	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2414	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2415	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2416	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2417	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2418	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2419	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2420	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2421	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2422	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2423	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2424	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2425	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2426	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2427	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2428	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2429	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD

#	Mechanism
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#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2430	140-67-0	4-Allylanisole	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	38.5		
2431	140-67-0	4-Allylanisole	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	38.5		
2432	99-96-7	4-Hydroxybenzoic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	-0.3	0.8	
2433	99-96-7	4-Hydroxybenzoic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	0		
2434	99-96-7	4-Hydroxybenzoic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	0		
2435	100-06-1	4-Methoxyacetophenone	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	4.7	5	
2436	100-06-1	4-Methoxyacetophenone	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	6.4		
2437	100-11-8	4-Nitrobenzylbromide	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	96		
2438	100-11-8	4-Nitrobenzylbromide	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	96		
2439	122-57-6	4-Phenyl-3-buten-2-one	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	94.7	2.3	
2440	122-57-6	4-Phenyl-3-buten-2-one	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	91.3		
2441	122-57-6	4-Phenyl-3-buten-2-one	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	91.3		
2442	26172-55-4	5-Chloro-2-methyl-4-isothiazolin-3-one	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	96.3	2.8	
2443	26172-55-4	5-Chloro-2-methyl-4-isothiazolin-3-one	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	94.8		
2444	26172-55-4	5-Chloro-2-methyl-4-isothiazolin-3-one	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	94.8		
2445	13706-86-0	5-Methyl-2.3-hexanedione	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	25.8	4	
2446	92-48-8	6-Methylcoumarin	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	1.4	0.3	
2447	92-48-8	6-Methylcoumarin	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	3.6		
2448	122-40-7	alpha-Amyl cinnamaldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	0.6	0.2	
2449	101-86-0	alpha-Hexylcinnamaldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	-0.3	1.2	
2450	20048-27-5	Bandrowski's base	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	87.5	0.3	
2451	100-52-7	Benzaldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	7.2	8.8	
2452	100-52-7	Benzaldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	7		
2453	100-52-7	Benzaldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	7		
2454	8001-54-5	Benzalkonium chloride	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	-6.8		
2455	98-11-3	Benzenesulfonic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	0		
2456	94-09-7	Benzocaine	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	11.6		
2457	65-85-0	Benzoic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	0		
2458	94-36-0	Benzoyl peroxide	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	100	0	
2459	120-51-4	Benzyl benzoate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	0.2	1.1	
2460	100-39-0	Benzyl bromide	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	97.8		
2461	2426-08-6	Butyl glycidyl ether	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	84.8		
2462	2426-08-6	Butyl glycidyl ether	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	84.8		
2463	25646-71-3	CD3	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	90.1	1.1	
2464	108-90-7	Chlorobenzene	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	0.4	0.2	
2465	104-55-2	Cinnamaldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	70.6	1	
2466	104-55-2	Cinnamaldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	90.5		
2467	104-55-2	Cinnamaldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	90.5		
2468	5392-40-5	Citral	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	85.7	3.2	
2469	5392-40-5	Citral	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	34.7		
2470	5392-40-5	Citral	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	34.7		
2471	91-64-5	Coumarin	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	1	4.6	
2472	93-51-6	Creosol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	15.4		

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2430		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2431		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2432		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2433		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2434		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2435		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2436		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2437		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2438		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2439		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2440		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2441		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2442		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2443		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2444		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2445		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2446		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2447		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2448		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2449		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2450		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2451		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2452		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2453		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2454		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2455		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2456		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2457		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2458		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2459		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2460		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2461		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2462		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2463		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2464		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2465		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2466		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2467		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2468		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2469		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2470		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2471		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2472		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106

#	Comment
2430	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2431	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2432	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2433	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2434	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2435	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2436	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2437	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2438	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2439	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2440	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2441	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2442	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2443	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2444	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2445	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2446	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2447	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2448	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2449	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2450	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2451	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2452	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2453	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2454	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2455	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2456	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2457	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2458	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2459	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2460	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2461	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2462	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2463	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2464	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2465	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2466	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2467	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2468	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2469	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2470	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2471	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2472	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD

#	Mechanism
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#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2473	103-95-7	Cyclamen aldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	18.9	8.1	
2474	103-95-7	Cyclamen aldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	59.9		
2475	103-95-7	Cyclamen aldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	59.9		
2476	141-05-9	Diethyl maleate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	100	0	
2477	141-05-9	Diethyl maleate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	100		
2478	84-66-2	Diethyl phthalate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	0.8	1.7	
2479	64-67-5	Diethyl sulfate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	24		
2480	886-38-4	Diphenylcyclopropenone	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	98.8	2	
2481	140-88-5	Ethyl acrylate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	96.4	0.3	
2482	140-88-5	Ethyl acrylate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	101.1		
2483	94-02-0	Ethyl benzoylacetate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	2.3	5.5	
2484	121-32-4	Ethyl vanillin	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	1.1	17	
2485	97-90-5	Ethylene glycol dimethacrylate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	87.3	5	
2486	97-90-5	Ethylene glycol dimethacrylate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	58.4		
2487	19317-11-4	Farnesal	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	16.4	3.5	
2488	19317-11-4	Farnesal	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	36.7		
2489	19317-11-4	Farnesal	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	36.7		
2490	27072-45-3	Fluorescein isothiocynate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	100	0	
2491	50-00-0	Formaldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	60.4	4.1	
2492	50-00-0	Formaldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	56.5		
2493	50-00-0	Formaldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	56.5		
2494	111-30-8	Glutaraldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	30.2	0.5	
2495	56-81-5	Glycerol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	-3.8	5.2	
2496	107-22-2	Glyoxal	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	56.5	1.7	
2497	107-22-2	Glyoxal	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	90.8		
2498	107-22-2	Glyoxal	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	90.8		
2499	110-54-3	Hexane	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	-0.4	0.8	
2500	93-53-8	Hydratropic aldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	48.2	7.1	
2501	107-75-5	Hydroxycitronellal	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	17.5	1.7	
2502	107-75-5	Hydroxycitronellal	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	46.7		
2503	107-75-5	Hydroxycitronellal	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	46.7		
2504	39236-46-9	Imidazolidinyl urea	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	52.3	6	
2505	39236-46-9	Imidazolidinyl urea	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	46.1		
2506	39236-46-9	Imidazolidinyl urea	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	46.1		
2507	97-54-1	Isoeugenol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	98.4		
2508	97-54-1	Isoeugenol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	98.4		
2509	67-63-0	Isopropanol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	-10	17	
2510	67-63-0	Isopropanol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	0.3		
2511	110-27-0	Isopropyl myristate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	0.8	1.7	
2512	55965-84-9	Kathon CG	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	99.1	1.6	
2513	50-21-5	Lactic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	-0.9	0.3	
2514	50-21-5	Lactic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	2.5		
2515	50-21-5	Lactic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	2.5		

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2473		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2474		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2475		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2476		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 81 (2004), 332
2477		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2478		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2479		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2480		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2481		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2482		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2483		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2484		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2485		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2486		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2487		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2488		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2489		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2490		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2491		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2492		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2493		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2494		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2495		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2496		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2497		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2498		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2499		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2500		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2501		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2502		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2503		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2504		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2505		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2506		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2507		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2508		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2509		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2510		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2511		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2512		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2513		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2514		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2515		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106

#	Comment
2473	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2474	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2475	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2476	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2477	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2478	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2479	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2480	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2481	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2482	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2483	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2484	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2485	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2486	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2487	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2488	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2489	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2490	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2491	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2492	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2493	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2494	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2495	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2496	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2497	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2498	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2499	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2500	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2501	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2502	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2503	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2504	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2505	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2506	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2507	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2508	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2509	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2510	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2511	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2512	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2513	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2514	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2515	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD

#	Mechanism
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#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2516	1166-52-5	Lauryl gallate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	90.9	13.1	
2517	80-54-6	Lilial	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	14	6.4	
2518	119-36-8	Methyl salicylate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	0.3	0.8	
2519	111-80-8	Methyl-2-nonynoate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	100	0	
2520	35691-65-7	Methyldibromo glutaronitrile	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	75.8		
2521	35691-65-7	Methyldibromo glutaronitrile	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	75.8		
2522	99-76-3	Methylparaben	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	3.6	6.8	
2523	99-76-3	Methylparaben	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	3.6		
2524	150-75-4	Metol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	100	0	
2525	112-05-0	Nonanoic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	-3.7	6.1	
2526	764-85-2	Nonanoyl chloride	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	18.2	3	
2527	124-07-2	Octanoic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	-1	0.7	
2528	124-07-2	Octanoic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	0		
2529	124-07-2	Octanoic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	0.04		
2530	144-62-7	Oxalic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	0.9	5.8	
2531	15646-46-5	Oxazolone	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	75.5	1.4	
2532	15646-46-5	Oxazolone	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	75.8		
2533	15646-46-5	Oxazolone	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	75.8		
2534	112-67-4	Palmitoyl chloride	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	25.5	6.6	
2535	106-51-4	p-Benzoquinone	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	99	1.8	
2536	106-51-4	p-Benzoquinone	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	91.6		
2537	106-51-4	p-Benzoquinone	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	91.6		
2538	61-33-6	Penicillin G	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	18.5		
2539	61-33-6	Penicillin G	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	18.5		
2540	2111-75-3	Perillaldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	31.9	3.3	
2541	93-99-2	Phenyl benzoate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	38.5		
2542	122-78-1	Phenylacetaldehyde	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	60.7	13.3	
2543	85-44-9	Phthalic anhydride	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	-1.9	1	
2544	121-79-9	Propyl gallate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	59.9	35.2	
2545	121-79-9	Propyl gallate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	62.2		
2546	121-79-9	Propyl gallate	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	62.2		
2547	94-13-3	Propyl paraben	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	8.2	2.3	
2548	57-55-6	Propylene glycol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	-0.9	17.5	
2549	108-46-3	Resorcinol	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	1.6	5.6	
2550	116-26-7	Safranal	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	100		
2551	116-26-7	Safranal	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	100		
2552	69-72-7	Salicylic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	3.5	4.2	
2553	2892-51-5	Squaric acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	46.9	8.7	
2554	63-74-1	Sulfanilamide	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	-1.3	17.3	
2555	121-57-3	Sulphanilic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	5.3	5.5	
2556	121-57-3	Sulphanilic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	3.3		
2557	121-57-3	Sulphanilic acid	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	3.3		
2558	7426-07-5	Tetrachlorosalicylanilide	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	36.8	20	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2516		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2517		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2518		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2519		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2520		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2521		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2522		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2523		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2524		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2525		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2526		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2527		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2528		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2529		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2530		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2531		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2532		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2533		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2534		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2535		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2536		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2537		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2538		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2539		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2540		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2541		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2542		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2543		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2544		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2545		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2546		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2547		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2548		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2549		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2550		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2551		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2552		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2553		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2554		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2555		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2556		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2557		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2558		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417

#	Comment
2516	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2517	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2518	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2519	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2520	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2521	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2522	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2523	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2524	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2525	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2526	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2527	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2528	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2529	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2530	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2531	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2532	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2533	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2534	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2535	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2536	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2537	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2538	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2539	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2540	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2541	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2542	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2543	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2544	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2545	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2546	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2547	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2548	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2549	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2550	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2551	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2552	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2553	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2554	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2555	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2556	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2557	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2558	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD

#	Mechanism
2516	
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#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2559	137-26-8	Tetramethylthiuram disulfide	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	99.4		
2560	137-26-8	Tetramethylthiuram disulfide	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	99.4		
2561	6728-26-3	trans-2-Hexenal	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	97.9	0.3	
2562	552-30-7	Trimellitic anhydride	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	-1.1	5.7	
2563	121-33-5	Vanillin	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	3.2	5.5	
2564	75-35-4	Vinylidene dichloride	Cys-Peptide (AcRFAACAA)	DP(Cys-P.): Gerberick	% Depletion	2.4	1.7	
2565	123-31-9	1.4-Hydroquinone	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	100	0	
2566	106-50-3	1.4-Phenylenediamine	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	99	0.82	
2567	3344-77-2	12-Bromo-1-dodecanol	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	51.1	11.6	
2568	109-65-9	1-Bromobutane	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	11	4.68	
2569	71-36-3	1-Butanol	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	10.1	9.61	
2570	97-00-7	1-Chloro-2.4-dinitrobenzene	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	97.4	0.31	
2571	5910-85-0	2.4-Heptadienal	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	90.8	0.39	
2572	874-23-7	2-Acetylcyclohexanone	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	74.8	1.8	
2573	818-61-1	2-Hydroxyethyl acrylate	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	100	0	
2574	923-26-2	2-Hydroxypropyl methacrylate	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	100	0	
2575	119-84-6	3.4-Dihydrocoumarin	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	-5.13	2.84	
2576	3775-21-1	3-Methyl-4-phenyl-1.2.5-thiazole-1.1-dioxide	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	100	0	
2577	100-11-8	4-Nitrobenzylbromide	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	95	0.48	
2578	92-48-8	6-Methylcoumarin	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	-7.59	0.78	
2579	101-86-0	alpha-Hexylcinnamaldehyde	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	7.59	1.9	
2580	100-52-7	Benzaldehyde	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	100	0	
2581	100-39-0	Benzyl bromide	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	100	0	
2582	104-55-2	Cinnamaldehyde	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	97.3	0	
2583	104-54-1	Cinnamic alcohol	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	22.7	1.13	
2584	103-95-7	Cyclamen aldehyde	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	33.5	2.79	
2585	140-88-5	Ethyl acrylate	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	92.4	0.14	
2586	50-00-0	Formaldehyde	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	31.5	2.16	
2587	111-30-8	Glutaraldehyde	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	74.4	1.15	
2588	56-81-5	Glycerol	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	-1.47	2.07	
2589	107-22-2	Glyoxal	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	-7.23	1.5	
2590	107-75-5	Hydroxycitronellal	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	72.7	4.18	
2591	97-54-1	Isoeugenol	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	90.4	0.14	
2592	50-21-5	Lactic acid	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	-12.7	0.38	
2593	143-15-7	Lauryl bromide	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	74.4	11.3	
2594	1166-52-5	Lauryl gallate	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	72.8	3.77	
2595	15646-46-5	Oxazolone	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	82.3	0.38	
2596	106-51-4	p-Benzoquinone	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	100	0	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2559		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2560		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Natsch A et al., Toxicol. Sci. 107 (2009), 106
2561		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2562		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2563		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2564		7.5	PBS 0.1 M, DMSO, ACN	24 h	1:10	Gerberick GF et al., Toxicol. Sci. 97 (2007), 417
2565	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2566	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2567	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2568	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2569	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2570	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2571	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2572	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2573	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2574	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2575	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2576	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2577	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2578	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2579	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2580	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2581	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2582	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2583	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2584	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2585	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2586	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2587	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2588	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2589	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2590	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2591	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2592	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2593	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2594	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2595	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2596	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401

#	Comment
2559	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2560	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2561	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2562	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2563	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2564	Assay: room temperature; 0.5 : 5 mM; HPLC-DAD
2565	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2566	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2567	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2568	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2569	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2570	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2571	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2572	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2573	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2574	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2575	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2576	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2577	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2578	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2579	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2580	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2581	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2582	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2583	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2584	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2585	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2586	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2587	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2588	Simultaneous analysis: -4.03(1.51)%. Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2589	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2590	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2591	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2592	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2593	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2594	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2595	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2596	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard

#	Mechanism
2559	
2560	
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2565	Pre-Michael addition of aromatic hydrocarbons, followed by sulphoxide or sulphone formation
2566	Michael-type nucleophilic addition: MA followed by sulphoxide and sulphone formation, Cys-peptide dimerisation
2567	Nucleophilic substitution, second order (SN2)
2568	Nucleophilic substitution, second order (SN2)
2569	No protein binding
2570	Nucleophilic aromatic substitution (SNAr) Cys-peptide dimerisation
2571	Michael addition or Schiff base formation, both followed by sulphoxide and sulphone formation
2572	Schiff base formation: SB and sulphone formation
2573	Michael-type nucleophilic addition
2574	Michael-type nucleophilic addition: MA followed by hydrolysis
2575	No protein binding: Cys-peptide dimerisation
2576	Michael-type nucleophilic addition
2577	Nucleophilic substitution, second order (SN2): Adduct on -SH and terminal -COOH
2578	Acylation or Michael addition: Cys-peptide dimerisation
2579	No protein binding
2580	No protein binding: Cys-peptide dimerisation
2581	Nucleophilic substitution, second order (SN2): Single+double+triple adducts, Cys-peptide dimerisation
2582	Michael addition or Schiff base formation: Cys-peptide dimerisation
2583	Michael-type nucleophilic addition
2584	No protein binding: Cys-peptide dimerisation
2585	Michael-type nucleophilic addition
2586	Schiff base formation
2587	Schiff base formation: double adduct, polymerisation of glutaraldehyde
2588	No protein binding
2589	No protein binding: no adducts
2590	No protein binding: Cys-peptide dimerisation
2591	Pre-Michael addition of aromatic hydrocarbons
2592	No protein binding
2593	Nucleophilic substitution, second order (SN2): Cys-peptide dimerisation
2594	Schiff base formation: Cys-peptide dimerisation
2595	Michael-type nucleophilic addition: MA followed by hydrolysis
2596	Michael-type nucleophilic addition

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2597	93-99-2	Phenyl benzoate	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	**76.2**	3.16	
2598	122-78-1	Phenylacetaldehyde	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	**100**	0	
2599	69-72-7	Salicylic acid	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	**-8.59**	2.87	
2600	3913-81-3	trans-2-Decenal	Cys-Peptide (AcFAACAA)	DP(Cys-P.): Aleksic	% Depletion	**91.7**	0.38	
2601	2634-33-5	1.2-Benzisothiazolin-3-one	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**69.8**	0.5	
2602	106-50-3	1.4-Phenylenediamine	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**102.4**	0.1	
2603	71-36-3	1-Butanol	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**12.8**	13.4	
2604	97-00-7	1-Chloro-2.4-dinitrobenzene	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**100.6**	0.1	
2605	431-03-8	2.3-Butanedione	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**99.8**	0.1	
2606	5910-85-0	2.4-Heptadienal	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**100**	0	
2607	95-55-6	2-Aminophenol	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**99.6**	0.5	
2608	10520-81-7	2-Bromotetradecanoic acid	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**40.9**	9.4	
2609	818-61-1	2-Hydroxyethyl acrylate	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**100.7**	0.2	
2610	149-30-4	2-Mercaptobenzothiazole	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**84.8**	0.5	
2611	2682-20-4	2-Methyl-2H-isothiazolin-3-one	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**97.7**	1.3	
2612		4-(6-methylheptan-2-yloxy)butanal	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**40.8**	2.8	
2613	140-67-0	4-Allylanisole	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**63.9**	1	
2614	99-96-7	4-Hydroxybenzoic acid	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**17.7**	14.5	
2615	100-06-1	4-Methoxyacetophenone	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**11.6**	1.4	
2616	100-11-8	4-Nitrobenzylbromide	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**99.9**	0.3	
2617	122-57-6	4-Phenyl-3-buten-2-one	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**64**	1.4	
2618	100-43-6	4-Vinylpyridine	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**104.4**	0.1	
2619	26172-55-4	5-Chloro-2-methyl-4-isothiazolin-3-one	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**100.5**	0.1	
2620	13706-86-0	5-Methyl-2.3-hexanedione	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**70.7**	4.1	
2621	101-86-0	alpha-Hexylcinnamaldehyde	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**103.5**	0.6	
2622	101-39-3	alpha-Methyl cinnamic aldehyde	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**20**	6.4	
2623	100-52-7	Benzaldehyde	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**27**	1.9	
2624	8001-54-5	Benzalkonium chloride	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**20.4**	2.5	
2625	100-51-6	Benzyl alcohol	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**17.2**	1.2	
2626	120-51-4	Benzyl benzoate	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**5.8**	3.1	
2627	100-39-0	Benzyl bromide	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**98.5**	0.5	
2628	103-41-3	Benzyl cinnamate	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**12.1**	0.75	
2629	23726-91-2	beta-Damascone	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**95**	3	
2630	2426-08-6	Butyl glycidyl ether	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**46.3**	1.9	
2631	1952-67-6	Calypsone	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**37.9**	22.3	
2632	104-55-2	Cinnamaldehyde	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**61.5**	3.1	
2633	5392-40-5	Citral	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**14.6**	0.65	
2634	103-95-7	Cyclamen aldehyde	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**62.9**	2	
2635	141-05-9	Diethyl maleate	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**100.4**	0.2	
2636	84-66-2	Diethyl phthalate	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**12.9**	1.3	
2637	2785-87-7	Dihydroeugenol	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**11.1**	0.76	
2638	886-38-4	Diphenylcyclopropenone	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	**103.1**	1.3	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2597	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2598	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2599	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2600	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2601	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2602	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2603	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2604	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2605	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2606	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2607	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2608	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2609	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2610	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2611	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2612	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2613	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2614	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2615	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2616	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2617	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2618	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2619	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2620	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2621	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2622	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2623	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2624	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2625	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2626	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2627	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2628	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2629	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2630	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2631	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2632	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2633	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2634	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2635	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2636	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2637	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2638	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464

#	Comment
2597	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2598	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2599	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2600	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2601	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2602	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2603	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2604	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2605	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2606	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2607	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2608	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2609	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2610	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2611	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2612	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2613	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2614	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2615	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2616	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2617	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2618	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2619	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2620	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2621	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2622	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2623	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2624	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2625	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2626	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2627	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2628	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2629	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2630	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2631	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2632	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2633	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2634	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2635	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2636	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2637	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2638	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)

#	Mechanism
2597	Acylation: Ac with loss of phenyl, Cys-peptide dimerisation
2598	No protein binding: Cys-peptide dimerisation
2599	No protein binding
2600	Michael-type nucleophilic addition: MA followed by sulphone formation, Cys-peptide dimerisation
2601	Oxidization + Adduct formation
2602	Oxidization + Adduct formation
2603	not reactive
2604	Adduct formation, HCl elimination
2605	Oxidization
2606	Oxidization
2607	Oxidization + Adduct formation
2608	Adduct formation, HBr elimination
2609	Adduct formation
2610	Oxidization + Adduct formation
2611	Oxidization + Adduct formation
2612	Oxidization
2613	Oxidization
2614	not reactive
2615	not reactive
2616	Adduct formation, HBr elimination
2617	Adduct formation
2618	Adduct formation
2619	Oxidization + Adduct formation
2620	Oxidization
2621	Oxidization
2622	Adduct formation
2623	not reactive
2624	not reactive, peak originates from test chemica
2625	not reactive
2626	not reactive
2627	Adduct formation, HBr elimination
2628	Adduct formation
2629	Adduct formation
2630	Adduct formation
2631	Oxidization
2632	Oxidization + Adduct formation
2633	Adduct formation
2634	Oxidization
2635	Adduct formation
2636	not reactive
2637	not reactive
2638	(Di-) Adduct formation

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2639	140-88-5	Ethyl acrylate	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	100.8	0.1	
2640	97-90-5	Ethylene glycol dimethacrylate	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	62.9	1.2	
2641	97-53-0	Eugenol	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	58.4	0.4	
2642	19317-11-4	Farnesal	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	80.2	2	
2643	3326-32-7	Fluorescein-5-isothiocyanate	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	106.6	0.1	
2644	50-00-0	Formaldehyde	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	86.2	1.4	
2645	56973-85-4	Galbanone	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	67.2	0.8	
2646	111-30-8	Glutaraldehyde	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	97.4	0.14	
2647	107-22-2	Glyoxal	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	92.9	0.9	
2648	93-53-8	Hydratropic aldehyde	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	50.6	3.1	
2649	107-75-5	Hydroxycitronellal	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	43.6	3.9	
2650	39236-46-9	Imidazolidinyl urea	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	97.8	0.5	
2651	97-54-1	Isoeugenol	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	95.1	0.3	
2652	50-21-5	Lactic acid	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	10.7	1.4	
2653	80-54-6	Lilial	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	64.6	3.8	
2654	78-70-6	Linalool	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	11.9	0.8	
2655	119-36-8	Methyl salicylate	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	10.7	4.6	
2656	111-80-8	Methyl-2-nonynoate	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	104.3	0.8	
2657	35691-65-7	Methyldibromo glutaronitrile	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	100.7	0.1	
2658	99-76-3	Methylparaben	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	10.2	5.6	
2659	150-75-4	Metol	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	101.1	0.1	
2660	764-85-2	Nonanoyl chloride	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	30.8	1	
2661	124-07-2	Octanoic acid	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	23.5	8	
2662	15646-46-5	Oxazolone	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	96.9	0.6	
2663	106-51-4	p-Benzoquinone	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	102	0	
2664	61-33-6	Penicillin G	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	16	8.6	
2665	2111-75-3	Perillaldehyde	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	58.2	0.9	
2666	60-12-8	Phenyl ethyl alcohol	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	13.1	2.2	
2667	122-78-1	Phenylacetaldehyde	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	95.4	1.4	
2668	85-44-9	Phthalic anhydride	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	18.2	1.25	
2669	357650-26-1	Pomarose	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	100	0.2	
2670	121-79-9	Propyl gallate	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	100.6	0.1	
2671	116-26-7	Safranal	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	90.5	1.1	
2672	69-72-7	Salicylic acid	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	8.4	1.62	
2673	151-21-3	Sodium lauryl sulfate	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	12.8	3.3	
2674	224031-70-3	Spirogalbanone	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	61.4	0.3	
2675	121-57-3	Sulphanilic acid	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	8.1	7.4	
2676	137-26-8	Tetramethylthiuram disulfide	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	20	6.4	
2677	3913-81-3	trans-2-Decenal	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	95.3	0.3	
2678	6728-26-3	trans-2-Hexenal	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	93.8	2.2	
2679	552-30-7	Trimellitic anhydride	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	5.9	1.51	
2680	121-33-5	Vanillin	Cor1C-420 (AcNKKCDLF)	DP(Cor1): SH	% Depletion	57	0.9	
2681	2634-33-5	1.2-Benzisothiazolin-3-one	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	95.8	3.6	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2639	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2640	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2641	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2642	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2643	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2644	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2645	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2646	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2647	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2648	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2649	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2650	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2651	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2652	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2653	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2654	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2655	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2656	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2657	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2658	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2659	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2660	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2661	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2662	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2663	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2664	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2665	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2666	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2667	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2668	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2669	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2670	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2671	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2672	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2673	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2674	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2675	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2676	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2677	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2678	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2679	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2680	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2681	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464

#	Comment
2639	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2640	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2641	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2642	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2643	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2644	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2645	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2646	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2647	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2648	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2649	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2650	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2651	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2652	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2653	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2654	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2655	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2656	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2657	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2658	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2659	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2660	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2661	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2662	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2663	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2664	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2665	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2666	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2667	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2668	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2669	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2670	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2671	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2672	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2673	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2674	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2675	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2676	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2677	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2678	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2679	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2680	Assay: Free SH groups by fluorescence with monobromobimane (385/480 nm)
2681	Assay: LC-MS

#	Mechanism
2639	Adduct formation
2640	Adduct formation
2641	Oxidization
2642	Oxidization
2643	Oxidization + Adduct formation
2644	Oxidization + Adduct formation
2645	Adduct formation
2646	Cross-linking
2647	Adduct formation
2648	Oxidization
2649	Oxidization
2650	Oxidization + Adduct formation
2651	Oxidization + Adduct formation
2652	not reactive
2653	Oxidization
2654	not reactive
2655	not reactive
2656	Adduct formation
2657	Oxidization + Adduct formation
2658	not reactive
2659	Adduct formation
2660	Adduct formation, HCl elimination
2661	not reactive
2662	Adduct formation
2663	Adduct formation
2664	not reactive
2665	Oxidization + Adduct formation
2666	not reactive
2667	Oxidization
2668	(Di-) Adduct formation
2669	Adduct formation
2670	Oxidization + Adduct formation
2671	Oxidization + Adduct formation
2672	not reactive
2673	not reactive, peptide micelle formation
2674	Adduct formation
2675	not reactive
2676	Adduct formation, elimination at disulfide bridge
2677	Adduct formation
2678	Oxidization + Adduct formation
2679	not reactive
2680	not reactive
2681	Oxidization + Adduct formation

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2682	106-50-3	1.4-Phenylenediamine	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	>98		
2683	71-36-3	1-Butanol	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	4.6	2.6	
2684	97-00-7	1-Chloro-2.4-dinitrobenzene	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	>98		
2685	431-03-8	2.3-Butanedione	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	>98		
2686	5910-85-0	2.4-Heptadienal	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	>98		
2687	95-55-6	2-Aminophenol	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	>98		
2688	10520-81-7	2-Bromotetradecanoic acid	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	23.4	1.9	
2689	818-61-1	2-Hydroxyethyl acrylate	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	98.4	2.9	
2690	149-30-4	2-Mercaptobenzothiazole	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	97.8	3.7	
2691	2682-20-4	2-Methyl-2H-isothiazolin-3-one	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	89	0.7	
2692		4-(6-methylheptan-2-yloxy)butanal	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	34.6	7.2	
2693	140-67-0	4-Allylanisole	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	56.1	0.4	
2694	99-96-7	4-Hydroxybenzoic acid	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	4.1	6.1	
2695	100-06-1	4-Methoxyacetophenone	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	-3.8	7.4	
2696	100-11-8	4-Nitrobenzylbromide	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	>98		
2697	122-57-6	4-Phenyl-3-buten-2-one	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	64.9	3	
2698	100-43-6	4-Vinylpyridine	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	>98		
2699	26172-55-4	5-Chloro-2-methyl-4-isothiazolin-3-one	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	>98	0	
2700	13706-86-0	5-Methyl-2.3-hexanedione	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	75.9	1.3	
2701	101-86-0	alpha-Hexylcinnamaldehyde	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	93.3	0.2	
2702	101-39-3	alpha-Methyl cinnamic aldehyde	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	8.9	6.4	
2703	100-52-7	Benzaldehyde	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	5.3	9	
2704	8001-54-5	Benzalkonium chloride	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	8.1	11.2	
2705	100-51-6	Benzyl alcohol	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	1.9	7.3	
2706	120-51-4	Benzyl benzoate	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	-4.4	8.3	
2707	100-39-0	Benzyl bromide	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	>98		
2708	103-41-3	Benzyl cinnamate	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	1.5	4.7	
2709	23726-91-2	beta-Damascone	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	99.7	0	
2710	2426-08-6	Butyl glycidyl ether	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	32.5	2.2	
2711	1952-67-6	Calypsone	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	43.8	21.7	
2712	104-55-2	Cinnamaldehyde	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	47.9	0.9	
2713	5392-40-5	Citral	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	3	8.5	
2714	103-95-7	Cyclamen aldehyde	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	61.1	2.2	
2715	141-05-9	Diethyl maleate	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	>98		
2716	84-66-2	Diethyl phthalate	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	-2	2.2	
2717	2785-87-7	Dihydroeugenol	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	-4.8	9.5	
2718	886-38-4	Diphenylcyclopropenone	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	97.9	3.6	
2719	140-88-5	Ethyl acrylate	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	>98		
2720	97-90-5	Ethylene glycol dimethacrylate	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	63.2	4.2	
2721	97-53-0	Eugenol	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	52.8	2.7	
2722	19317-11-4	Farnesal	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	61.6	3.5	
2723	3326-32-7	Fluorescein-5-isothiocyanate	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	>98		
2724	50-00-0	Formaldehyde	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	91.5	0.7	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2682	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2683	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2684	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2685	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2686	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2687	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2688	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2689	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2690	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2691	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2692	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2693	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2694	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2695	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2696	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2697	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2698	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2699	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2700	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2701	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2702	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2703	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2704	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2705	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2706	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2707	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2708	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2709	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2710	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2711	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2712	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2713	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2714	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2715	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2716	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2717	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2718	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2719	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2720	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2721	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2722	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2723	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2724	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464

#	Comment
2682	Assay: LC-MS
2683	Assay: LC-MS
2684	Assay: LC-MS
2685	Assay: LC-MS
2686	Assay: LC-MS
2687	Assay: LC-MS
2688	Assay: LC-MS
2689	Assay: LC-MS
2690	Assay: LC-MS
2691	Assay: LC-MS
2692	Assay: LC-MS
2693	Assay: LC-MS
2694	Assay: LC-MS
2695	Assay: LC-MS
2696	Assay: LC-MS
2697	Assay: LC-MS
2698	Assay: LC-MS
2699	Assay: LC-MS
2700	Assay: LC-MS
2701	Assay: LC-MS
2702	Assay: LC-MS
2703	Assay: LC-MS
2704	Assay: LC-MS
2705	Assay: LC-MS
2706	Assay: LC-MS
2707	Assay: LC-MS
2708	Assay: LC-MS
2709	Assay: LC-MS
2710	Assay: LC-MS
2711	Assay: LC-MS
2712	Assay: LC-MS
2713	Assay: LC-MS
2714	Assay: LC-MS
2715	Assay: LC-MS
2716	Assay: LC-MS
2717	Assay: LC-MS
2718	Assay: LC-MS
2719	Assay: LC-MS
2720	Assay: LC-MS
2721	Assay: LC-MS
2722	Assay: LC-MS
2723	Assay: LC-MS
2724	Assay: LC-MS

#	Mechanism
2682	Oxidization + Adduct formation
2683	not reactive
2684	Adduct formation, HCl elimination
2685	Oxidization
2686	Oxidization
2687	Oxidization + Adduct formation
2688	Adduct formation, HBr elimination
2689	Adduct formation
2690	Oxidization + Adduct formation
2691	Oxidization + Adduct formation
2692	Oxidization
2693	Oxidization
2694	not reactive
2695	not reactive
2696	Adduct formation, HBr elimination
2697	Adduct formation
2698	Adduct formation
2699	Oxidization + Adduct formation
2700	Oxidization
2701	Oxidization
2702	Adduct formation
2703	not reactive
2704	not reactive, peak originates from test chemica
2705	not reactive
2706	not reactive
2707	Adduct formation, HBr elimination
2708	Adduct formation
2709	Adduct formation
2710	Adduct formation
2711	Oxidization
2712	Oxidization + Adduct formation
2713	Adduct formation
2714	Oxidization
2715	Adduct formation
2716	not reactive
2717	not reactive
2718	(Di-) Adduct formation
2719	Adduct formation
2720	Adduct formation
2721	Oxidization
2722	Oxidization
2723	Oxidization + Adduct formation
2724	Oxidization + Adduct formation

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2725	56973-85-4	Galbanone	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	59.9	8.6	
2726	111-30-8	Glutaraldehyde	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	>98		
2727	107-22-2	Glyoxal	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	>98		
2728	93-53-8	Hydratropic aldehyde	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	42.9	6.1	
2729	107-75-5	Hydroxycitronellal	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	34.2	3.6	
2730	39236-46-9	Imidazolidinyl urea	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	97.9	3.7	
2731	97-54-1	Isoeugenol	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	91.1	1	
2732	50-21-5	Lactic acid	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	-5.3	2.2	
2733	80-54-6	Lilial	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	65.1	3.3	
2734	78-70-6	Linalool	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	-2.3	7	
2735	119-36-8	Methyl salicylate	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	-1.2	3.6	
2736	111-80-8	Methyl-2-nonynoate	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	>98		
2737	35691-65-7	Methyldibromo glutaronitrile	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	>98		
2738	99-76-3	Methylparaben	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	1	3.6	
2739	150-75-4	Metol	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	97.7	3.7	
2740	764-85-2	Nonanoyl chloride	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	16.9	5	
2741	124-07-2	Octanoic acid	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	5.3	7	
2742	15646-46-5	Oxazolone	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	>98		
2743	106-51-4	p-Benzoquinone	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	98.4	2.8	
2744	61-33-6	Penicillin G	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	-2.7	25.9	
2745	2111-75-3	Perillaldehyde	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	55.5	2.5	
2746	60-12-8	Phenyl ethyl alcohol	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	-4.7	5.6	
2747	122-78-1	Phenylacetaldehyde	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	95.7	3.7	
2748	85-44-9	Phthalic anhydride	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	>98		
2749	357650-26-1	Pomarose	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	98		
2750	121-79-9	Propyl gallate	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	97.9	3.7	
2751	116-26-7	Safranal	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	88.3	1.1	
2752	69-72-7	Salicylic acid	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	-9.2	16.4	
2753	151-21-3	Sodium lauryl sulfate	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	65.8	2.1	
2754	224031-70-3	Spirogalbanone	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	60	2.1	
2755	121-57-3	Sulphanilic acid	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	1.4	4.3	
2756	137-26-8	Tetramethylthiuram disulfide	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	>98		
2757	3913-81-3	trans-2-Decenal	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	93.7	0.2	
2758	6728-26-3	trans-2-Hexenal	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	93.1	0.3	
2759	552-30-7	Trimellitic anhydride	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	-10.5	18	
2760	121-33-5	Vanillin	Cor1C-420 (AcNKKCDLF)	DP(Cor1)	% Depletion	3.6	5	
2761	123-31-9	1.4-Hydroquinone	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	-1.08	1.66	
2762	106-50-3	1.4-Phenylenediamine	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	22.6	8.75	
2763	3344-77-2	12-Bromo-1-dodecanol	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	11.7	1.16	
2764	109-65-9	1-Bromobutane	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	-4.4	1.14	
2765	71-36-3	1-Butanol	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	4.43	16.5	
2766	97-00-7	1-Chloro-2.4-dinitrobenzene	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	-1.73	4.9	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2725	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2726	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2727	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2728	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2729	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2730	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2731	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2732	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2733	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2734	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2735	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2736	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2737	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2738	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2739	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2740	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2741	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2742	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2743	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2744	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2745	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2746	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2747	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2748	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2749	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2750	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2751	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2752	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2753	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2754	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2755	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2756	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2757	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2758	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2759	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2760	37	7.5	PBS 0.1 M, ACN	24 h - 31 h	1:10	Natsch A et al., Toxicol. Sci. 106 (2008), 464
2761	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2762	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2763	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2764	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2765	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2766	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401

#	Comment
2725	Assay: LC-MS
2726	Assay: LC-MS
2727	Assay: LC-MS
2728	Assay: LC-MS
2729	Assay: LC-MS
2730	Assay: LC-MS
2731	Assay: LC-MS
2732	Assay: LC-MS
2733	Assay: LC-MS
2734	Assay: LC-MS
2735	Assay: LC-MS
2736	Assay: LC-MS
2737	Assay: LC-MS
2738	Assay: LC-MS
2739	Assay: LC-MS
2740	Assay: LC-MS
2741	Assay: LC-MS
2742	Assay: LC-MS
2743	Assay: LC-MS
2744	Assay: LC-MS
2745	Assay: LC-MS
2746	Assay: LC-MS
2747	Assay: LC-MS
2748	Assay: LC-MS
2749	Assay: LC-MS
2750	Assay: LC-MS
2751	Assay: LC-MS
2752	Assay: LC-MS
2753	Assay: LC-MS
2754	Assay: LC-MS
2755	Assay: LC-MS
2756	Assay: LC-MS
2757	Assay: LC-MS
2758	Assay: LC-MS
2759	Assay: LC-MS
2760	Assay: LC-MS
2761	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2762	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2763	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2764	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2765	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2766	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard

#	Mechanism
2725	Adduct formation
2726	Cross-linking
2727	Adduct formation
2728	Oxidization
2729	Oxidization
2730	Oxidization + Adduct formation
2731	Oxidization + Adduct formation
2732	not reactive
2733	Oxidization
2734	not reactive
2735	not reactive
2736	Adduct formation
2737	Oxidization + Adduct formation
2738	not reactive
2739	Adduct formation
2740	Adduct formation, HCl elimination
2741	not reactive
2742	Adduct formation
2743	Adduct formation
2744	not reactive
2745	Oxidization + Adduct formation
2746	not reactive
2747	Oxidization
2748	(Di-) Adduct formation
2749	Adduct formation
2750	Oxidization + Adduct formation
2751	Oxidization + Adduct formation
2752	not reactive
2753	not reactive, peptide micelle formation
2754	Adduct formation
2755	not reactive
2756	Adduct formation, elimination at disulfide bridge
2757	Adduct formation
2758	Oxidization + Adduct formation
2759	not reactive
2760	not reactive
2761	No protein binding
	Pre-Michael addition of aromatic hydrocarbons:
2762	MA of quinine diimine after PPD oxidisation
2763	No protein binding
2764	No protein binding
2765	No protein binding
2766	No protein binding

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2767	5910-85-0	2.4-Heptadienal	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	74.5	0.31	
2768	874-23-7	2-Acetylcyclohexanone	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	53.6	8.33	
2769	818-61-1	2-Hydroxyethyl acrylate	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	10.8	9.02	
2770	923-26-2	2-Hydroxypropyl methacrylate	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	8.46	4.47	
2771	119-84-6	3.4-Dihydrocoumarin	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	-1.62	6.89	
2772	3775-21-1	3-Methyl-4-phenyl-1.2.5-thiazole-1.1-dioxide	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	0.92	8.24	
2773	100-11-8	4-Nitrobenzylbromide	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	14.6	5.86	
2774	92-48-8	6-Methylcoumarin	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	-4.76	1.83	
2775	101-86-0	alpha-Hexylcinnamaldehyde	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	-17.8	7.62	
2776	100-52-7	Benzaldehyde	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	36.5	5.27	
2777	100-39-0	Benzyl bromide	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	3.24	6.14	
2778	104-55-2	Cinnamaldehyde	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	14.4	8.54	
2779	104-54-1	Cinnamic alcohol	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	16.2	1.38	
2780	103-95-7	Cyclamen aldehyde	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	11.8	3.73	
2781	140-88-5	Ethyl acrylate	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	-4.92	4.66	
2782	50-00-0	Formaldehyde	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	34	3.32	
2783	111-30-8	Glutaraldehyde	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	6.24	8.7	
2784	56-81-5	Glycerol	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	-3.17	5.23	
2785	107-22-2	Glyoxal	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	100	0	
2786	107-75-5	Hydroxycitronellal	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	0.97	4.64	
2787	97-54-1	Isoeugenol	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	6.16	2.91	
2788	50-21-5	Lactic acid	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	12.5	3.55	
2789	143-15-7	Lauryl bromide	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	-9.6	4.43	
2790	1166-52-5	Lauryl gallate	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	3.02	4.79	
2791	15646-46-5	Oxazolone	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	-15.3	4.03	
2792	106-51-4	p-Benzoquinone	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	20	8.69	
2793	93-99-2	Phenyl benzoate	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	-9.32	4.05	
2794	122-78-1	Phenylacetaldehyde	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	35	1.61	
2795	69-72-7	Salicylic acid	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	-7.02	3.04	
2796	3913-81-3	trans-2-Decenal	Arg-Peptide (AcFAARAA)	DP(Arg-P.): Aleksic	% Depletion	10.4	1.95	
2797	123-31-9	1.4-Hydroquinone	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	3.54	0.84	
2798	106-50-3	1.4-Phenylenediamine	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	1.65	1.65	
2799	3344-77-2	12-Bromo-1-dodecanol	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	-2.39	1.67	
2800	109-65-9	1-Bromobutane	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	-3.3	3.23	
2801	71-36-3	1-Butanol	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	-2.64	5.8	
2802	97-00-7	1-Chloro-2.4-dinitrobenzene	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	6.79	3.01	
2803	5910-85-0	2.4-Heptadienal	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	6.68	7.65	
2804	874-23-7	2-Acetylcyclohexanone	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	11	1.24	
2805	818-61-1	2-Hydroxyethyl acrylate	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	-3.94	6.14	
2806	923-26-2	2-Hydroxypropyl methacrylate	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	10.2	4.77	
2807	119-84-6	3.4-Dihydrocoumarin	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	12.9	2.68	
2808	3775-21-1	3-Methyl-4-phenyl-1.2.5-thiazole-1.1-dioxide	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	-13.2	6.93	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2767	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2768	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2769	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2770	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2771	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2772	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2773	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2774	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2775	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2776	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2777	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2778	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2779	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2780	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2781	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2782	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2783	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2784	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2785	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2786	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2787	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2788	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2789	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2790	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2791	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2792	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2793	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2794	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2795	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2796	37	10	Carbonate buffer 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2797	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2798	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2799	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2800	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2801	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2802	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2803	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2804	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2805	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2806	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2807	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2808	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401

#	Comment
2767	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2768	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2769	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2770	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2771	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2772	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2773	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2774	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2775	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2776	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2777	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2778	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2779	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2780	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2781	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2782	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2783	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2784	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2785	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2786	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2787	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2788	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2789	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2790	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2791	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2792	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2793	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2794	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2795	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2796	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2797	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2798	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2799	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2800	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2801	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2802	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2803	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2804	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2805	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2806	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2807	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2808	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard

#	Mechanism
2767	unknown adducts
2768	Formation of a ring like structure
2769	No protein binding
2770	No protein binding
2771	No protein binding
2772	Pre-Schiff base formation: SB of MPT hydrolysis product
2773	Nucleophilic substitution, second order (SN2)
2774	No protein binding
2775	No protein binding
2776	Schiff base formation
2777	Nucleophilic substitution, second order (SN2)
2778	Michael addition or Schiff base formation: MA adduct and double MA+SB adduct
2779	No protein binding
2780	No protein binding
2781	No protein binding
2782	Schiff base formation: Single+double+triple adduct
2783	Schiff base formation
2784	No protein binding
2785	Schiff base formation: Single+double adduct and ring like structure formation
2786	No protein binding
2787	No protein binding
2788	No protein binding
2789	No protein binding
2790	No protein binding
2791	No protein binding
2792	No protein binding
2793	No protein binding
2794	unknown adducts
2795	No protein binding
2796	No protein binding
2797	No protein binding
2798	No protein binding
2799	No protein binding
2800	No protein binding
2801	No protein binding
2802	No protein binding
2803	No protein binding
2804	No protein binding
2805	No protein binding
2806	No protein binding
2807	No protein binding
2808	No protein binding

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2809	100-11-8	4-Nitrobenzylbromide	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	24.1	0.74	
2810	92-48-8	6-Methylcoumarin	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	8.68	1.04	
2811	101-86-0	alpha-Hexylcinnamaldehyde	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	5.85	0.76	
2812	100-52-7	Benzaldehyde	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	4.62	1.7	
2813	100-39-0	Benzyl bromide	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	-0.08	0.27	
2814	104-55-2	Cinnamaldehyde	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	12.6	2.74	
2815	104-54-1	Cinnamic alcohol	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	1.17	3.74	
2816	103-95-7	Cyclamen aldehyde	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	5.87	1.41	
2817	140-88-5	Ethyl acrylate	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	3.4	0.98	
2818	50-00-0	Formaldehyde	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	4.92	1.2	
2819	111-30-8	Glutaraldehyde	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	9.57	1.42	
2820	56-81-5	Glycerol	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	3.48	1.42	
2821	107-22-2	Glyoxal	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	1.42	1.26	
2822	107-75-5	Hydroxycitronellal	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	3.69	1.63	
2823	97-54-1	Isoeugenol	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	12.1	6.61	
2824	50-21-5	Lactic acid	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	1.41	1.69	
2825	143-15-7	Lauryl bromide	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	7.86	1.04	
2826	1166-52-5	Lauryl gallate	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	-8.45	4.42	
2827	15646-46-5	Oxazolone	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	-3.56	8.29	
2828	106-51-4	p-Benzoquinone	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	3.38	0.91	
2829	93-99-2	Phenyl benzoate	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	10.3	0.39	
2830	122-78-1	Phenylacetaldehyde	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	-3.98	1.45	
2831	69-72-7	Salicylic acid	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	-21	9.17	
2832	3913-81-3	trans-2-Decenal	Ala-Peptide (AcFAAAAA)	DP(Ala-P.): Aleksic	% Depletion	2.51	1.31	
2833	542-75-6	1.3-Dichloropropene	4-Nitrobenzylpyridine	DE(NBP)	Extinktion	2.24		
2834	542-75-6	1.3-Dichloropropene	4-Nitrobenzylpyridine	DE(NBP)	Extinktion	1.933		
2835	57-06-7	1-Allylisothiocyanate	4-Nitrobenzylpyridine	DE(NBP)	Extinktion	0.182		
2836	57-06-7	1-Allylisothiocyanate	4-Nitrobenzylpyridine	DE(NBP)	Extinktion	0.04		
2837	590-21-6	1-Chloro-1-propene	4-Nitrobenzylpyridine	DE(NBP)	Extinktion	0		
2838	13417-43-1	1-Chloro-2-methyl-2-butene	4-Nitrobenzylpyridine	DE(NBP)	Extinktion	2.057		
2839	930-66-5	1-Chlorocyclohexene	4-Nitrobenzylpyridine	DE(NBP)	Extinktion	0		
2840	78-88-6	2.3-Dichloro-1-propene	4-Nitrobenzylpyridine	DE(NBP)	Extinktion	0.248		
2841	557-98-2	2-Chloro-1-propene	4-Nitrobenzylpyridine	DE(NBP)	Extinktion	0		
2842	563-52-0	3-Chloro-1-butene	4-Nitrobenzylpyridine	DE(NBP)	Extinktion	NA		
2843	2441-97-6	3-Chloro-1-cyclohexene	4-Nitrobenzylpyridine	DE(NBP)	Extinktion	0.312		
2844	5166-35-8	3-Chloro-2-methyl-1-butene	4-Nitrobenzylpyridine	DE(NBP)	Extinktion	NA		
2845	563-47-3	3-Chloro-2-methylpropene	4-Nitrobenzylpyridine	DE(NBP)	Extinktion	0.57		
2846	927-73-1	4-Chloro-1-butene	4-Nitrobenzylpyridine	DE(NBP)	Extinktion	0		
2847	106-95-6	Allyl bromide	4-Nitrobenzylpyridine	DE(NBP)	Extinktion	54		
2848	107-05-1	Allyl chloride	4-Nitrobenzylpyridine	DE(NBP)	Extinktion	0.285		
2849	556-56-9	Allyl iodide	4-Nitrobenzylpyridine	DE(NBP)	Extinktion	164		

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2809	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2810	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2811	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2812	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2813	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2814	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2815	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2816	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2817	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2818	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2819	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2820	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2821	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2822	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2823	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2824	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2825	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2826	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2827	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2828	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2829	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2830	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2831	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2832	37	7.5	PBS 50 mM, ACN	24 h	1:100	Aleksic M et al., Toxicol. Sci. 108 (2009), 401
2833	80		Ethyl methyl ketone (reflux)	10 min	6.6:1	Eder E et al., Chem. Biol. Interactions 38 (1982), 303
2834	80		Ethyl methyl ketone (reflux)	10 min	6.6:1	Eder E et al., Chem. Biol. Interactions 38 (1982), 303
2835	100		Ethylene glycol (reflux)	10 min	6.6:1	Eder E et al., Biochem. Pharmacol. 29 (1980), 993
2836	80		Ethyl methyl ketone (reflux)	10 min	6.6:1	Eder E et al., Chem. Biol. Interactions 38 (1982), 303
2837	80		Ethyl methyl ketone (reflux)	10 min	6.6:1	Neudecker T et al., Biochem. Pharmacol. 29 (1980), 2611
2838	80		Ethyl methyl ketone (reflux)	10 min	6.6:1	Eder E et al., Chem. Biol. Interactions 38 (1982), 303
2839	80		Ethyl methyl ketone (reflux)	10 min	6.6:1	Neudecker T et al., Biochem. Pharmacol. 29 (1980), 2611
2840	80		Ethyl methyl ketone (reflux)	10 min	6.6:1	Eder E et al., Chem. Biol. Interactions 38 (1982), 303
2841	80		Ethyl methyl ketone (reflux)	10 min	6.6:1	Neudecker T et al., Biochem. Pharmacol. 29 (1980), 2611
2842	80		Ethyl methyl ketone (reflux)	10 min	6.6:1	Eder E et al., Chem. Biol. Interactions 38 (1982), 303
2843	80		Ethyl methyl ketone (reflux)	10 min	6.6:1	Eder E et al., Chem. Biol. Interactions 38 (1982), 303
2844	80		Ethyl methyl ketone (reflux)	10 min	6.6:1	Eder E et al., Chem. Biol. Interactions 38 (1982), 303
2845	80		Ethyl methyl ketone (reflux)	10 min	6.6:1	Eder E et al., Chem. Biol. Interactions 38 (1982), 303
2846	80		Ethyl methyl ketone (reflux)	10 min	6.6:1	Neudecker T et al., Biochem. Pharmacol. 29 (1980), 2611
2847	80		Ethyl methyl ketone (reflux)	10 min	6.6:1	Eder E et al., Chem. Biol. Interactions 38 (1982), 303
2848	80		Ethyl methyl ketone (reflux)	10 min	6.6:1	Eder E et al., Chem. Biol. Interactions 38 (1982), 303
2849	80		Ethyl methyl ketone (reflux)	10 min	6.6:1	Eder E et al., Chem. Biol. Interactions 38 (1982), 303

#	Comment
2809	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2810	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2811	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2812	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2813	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2814	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2815	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2816	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2817	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2818	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2819	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2820	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2821	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2822	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2823	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2824	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2825	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2826	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2827	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2828	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2829	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2830	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2831	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2832	Assay: LC-Tandem-MS(Electrospray); includes AcFAGAGA as internal standard
2833	Assay: Alkylating activity; UV(560 nm); DE560 > 0.04: reactive
2834	Assay: Alkylating activity; UV(560 nm); DE560 > 0.04: reactive
2835	Assay: Alkylating activity; UV(560 nm); DE560 > 0.04: reactive
2836	not reactive. Assay: Alkylating activity; UV(560 nm); DE560 > 0.04: reactive
2837	Assay: Alkylating activity; UV(560 nm); DE560 > 0.04: reactive
2838	Assay: Alkylating activity; UV(560 nm); DE560 > 0.04: reactive
2839	Assay: Alkylating activity; UV(560 nm); DE560 > 0.04: reactive
2840	Assay: Alkylating activity; UV(560 nm); DE560 > 0.04: reactive
2841	Assay: Alkylating activity; UV(560 nm); DE560 > 0.04: reactive
2842	not applicable. Assay: Alkylating activity; UV(560 nm); DE560 > 0.04: reactive
2843	Assay: Alkylating activity; UV(560 nm); DE560 > 0.04: reactive
2844	not applicable. Assay: Alkylating activity; UV(560 nm); DE560 > 0.04: reactive
2845	Assay: Alkylating activity; UV(560 nm); DE560 > 0.04: reactive
2846	Assay: Alkylating activity; UV(560 nm); DE560 > 0.04: reactive
2847	Assay: Alkylating activity; UV(560 nm); DE560 > 0.04: reactive
2848	Assay: Alkylating activity; UV(560 nm); DE560 > 0.04: reactive
2849	Assay: Alkylating activity; UV(560 nm); DE560 > 0.04: reactive

#	Mechanism
2809	Nucleophilic substitution, second order (SN2): Single adduct at -COOH terminus
2810	No protein binding
2811	No protein binding
2812	No protein binding
2813	No protein binding
2814	No protein binding
2815	No protein binding
2816	No protein binding
2817	No protein binding
2818	No protein binding
2819	No protein binding
2820	No protein binding
2821	No protein binding
2822	No protein binding
2823	No protein binding
2824	No protein binding
2825	No protein binding
2826	No protein binding
2827	No protein binding
2828	No protein binding
2829	No protein binding
2830	No protein binding
2831	No protein binding
2832	No protein binding
2833	Nucleophilic substitution and direct DNA-alkylation
2834	Nucleophilic substitution and direct DNA-alkylation
2835	NOT Nucleophilic substitution and direct DNA-alkylation
2836	NOT Nucleophilic substitution and direct DNA-alkylation
2837	NOT Nucleophilic substitution and direct DNA-alkylation
2838	Nucleophilic substitution and direct DNA-alkylation
2839	NOT Nucleophilic substitution and direct DNA-alkylation
2840	Nucleophilic substitution and direct DNA-alkylation
2841	NOT Nucleophilic substitution and direct DNA-alkylation
	NOT Nucleophilic substitution and direct DNA-alkylation:
2842	Elimination and HCl formation instead
2843	Nucleophilic substitution and direct DNA-alkylation
	NOT Nucleophilic substitution and direct DNA-alkylation:
2844	Elimination and HCl formation instead
2845	Nucleophilic substitution and direct DNA-alkylation
2846	NOT Nucleophilic substitution and direct DNA-alkylation
2847	Nucleophilic substitution and direct DNA-alkylation
2848	Nucleophilic substitution and direct DNA-alkylation
2849	Nucleophilic substitution and direct DNA-alkylation

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2850	6728-21-8	Allyl methanesulfonate	4-Nitrobenzylpyridine	DE(NBP)	Extinktion	105		
2851	100-44-7	Benzyl chloride	4-Nitrobenzylpyridine	DE(NBP)	Extinktion	2.923		
2852	2211-69-0	cis-2-Chloro-2-butene	4-Nitrobenzylpyridine	DE(NBP)	Extinktion	0		
2853	591-97-9	Crotyl chloride	4-Nitrobenzylpyridine	DE(NBP)	Extinktion	1.035		
2854	106-89-8	Epichlorohydrin	4-Nitrobenzylpyridine	DE(NBP)	Extinktion	1.237		
2855		2.3-Dimethyl-2.3-epoxy-1.4-naphthoquinone	Glutathione	dc/dt(GSH)	M/min	1.80E-05		
2856	15254-69-0	2.3-Epoxy-1.4-benzoquinone	Glutathione	dc/dt(GSH)	M/min	1.17E-04		
2857		2.3-Epoxy-1.4-naphthoquinone	Glutathione	dc/dt(GSH)	M/min	2.40E-04		
2858		2-Methyl-2.3-epoxy-1.4-naphthoquinone	Glutathione	dc/dt(GSH)	M/min	1.23E-04		
2859		6-Methyl-2.3-epoxy-1.4-benzoquinone	Glutathione	dc/dt(GSH)	M/min	1.10E-05		
2860		0-Cyano-N-[4-(trifluoromethyl)phenyl]-methanecarbohydrazonoyl cyanide	Glutathione	beta(GSH)	lg k(RS[-])/pKa	0.7		
2861	39834-44-1	1a.9a-Dihydro-phenanthro(1.2-b)oxirene	Glutathione	beta(GSH)	lg k(RS[-])/pKa	0.2		
2862	39834-45-2	1a.9c-Dihydro-phenanthro(3.4-b)oxirene	Glutathione	beta(GSH)	lg k(RS[-])/pKa	0.2		
2863		2-(Pyridin-2-yldisulfanyl)pyridine	Glutathione	beta(GSH)	lg k(RS[-])/pKa	0.23		
2864	5429-56-1	2-Acetamidoacrylic acid	Glutathione	beta(GSH)	lg k(RS[-])/pKa	0.21		
2865	144-48-9	2-Iodoacetamide	Glutathione	beta(GSH)	lg k(RS[-])/pKa	0.32		
2866		4-(Pyridin-4-yldisulfanyl)pyridine	Glutathione	beta(GSH)	lg k(RS[-])/pKa	0.34		
2867	830-03-5	4-Nitrophenyl acetate	Glutathione	beta(GSH)	lg k(RS[-])/pKa	0.38		
2868		7-Oxabicyclo[4.1.0]hepta-1.3.5-triene	Glutathione	beta(GSH)	lg k(RS[-])/pKa	0.2		
2869	585-08-0	9.10-Epoxy-9.10-dihydrophenanthrene	Glutathione	beta(GSH)	lg k(RS[-])/pKa	0.2		
2870	107-13-1	Acrylonitrile	Glutathione	beta(GSH)	lg k(RS[-])/pKa	0.45		
2871	622-78-6	Benzyl isothiocyanate	Glutathione	beta(GSH)	lg k(RS[-])/pKa	0.56		
2872	622-78-6	Benzyl isothiocyanate	Glutathione	beta(GSH)	lg k(RS[-])/pKa	0.38		
2873	69-78-3	Dithionitrobenzoic acid	Glutathione	beta(GSH)	lg k(RS[-])/pKa	0.4-0.5		
2874	75-21-8	Ethylene oxide	Glutathione	beta(GSH)	lg k(RS[-])/pKa	0.3		
2875	27025-41-8	Glutathione disulfide	Glutathione	beta(GSH)	lg k(RS[-])/pKa	0.5		
2876	129-73-7	Leucomalachite green	Glutathione	beta(GSH)	lg k(RS[-])/pKa	0.3		
2877	27030-97-3	N-(4-(2-Benzimidazolyl)phenyl)maleimide	Glutathione	beta(GSH)	lg k(RS[-])/pKa	0.42		
2878	128-53-0	N-Ethylmaleimide	Glutathione	beta(GSH)	lg k(RS[-])/pKa	0.9		
2879		Organic mercury(II) halogenides	Glutathione	beta(GSH)	lg k(RS[-])/pKa	0		
2880	103-72-0	Phenyl isothiocyanate	Glutathione	beta(GSH)	lg k(RS[-])/pKa	0.54		
2881	103-72-0	Phenyl isothiocyanate	Glutathione	beta(GSH)	lg k(RS[-])/pKa	0.43		
2882	555-60-2	Carbonyl cyanide m-chlorophenyl hydrazone	Benzylmercaptan	Adduct(R-SH)	(yes/no)	yes		
2883	306-18-3	Carbonyl cyanide phenylhydrazone	Benzylmercaptan	Adduct(R-SH)	(yes/no)	yes		
2884	586-96-9	Nitrosobenzene	Monothioglycerol	Adduct(R-SH)	(yes/no)	yes		
2885	2682-20-4	2-Methyl-2H-isothiazolin-3-one	Propanethiolate. Sodium	Adduct(R-SH)	(yes/no)	yes		
2886	26172-55-4	5-Chloro-2-methyl-4-isothiazolin-3-one	Propanethiolate. Sodium	Adduct(R-SH)	(yes/no)	yes		
2887	93-11-8	2-Naphthalenesulfonyl chloride	Thiolacetic acid	Adduct(R-SH)	(yes/no)	no		
2888	98-09-9	Benzenesulfonyl chloride	Thiophenol	Adduct(R-SH)	(yes/no)	no		

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2850	80		Ethyl methyl ketone (reflux)	10 min	6.6:1	Eder E et al., Chem. Biol. Interactions 38 (1982), 303
2851	80		Ethyl methyl ketone (reflux)	10 min	6.6:1	Eder E et al., Chem. Biol. Interactions 38 (1982), 303
2852	80		Ethyl methyl ketone (reflux)	10 min	6.6:1	Neudecker T et al., Biochem. Pharmacol. 29 (1980), 2611
2853	80		Ethyl methyl ketone (reflux)	10 min	6.6:1	Eder E et al., Chem. Biol. Interactions 38 (1982), 303
2854	80		Ethyl methyl ketone (reflux)	10 min	6.6:1	Eder E et al., Biochem. Pharmacol. 29 (1980), 993
2855	37	7.65	PBS 0.1 M		1:1	Brunmark A et al., Free Radic. Biol. Med. 6 (1989), 149
2856	37	7.65	PBS 0.1 M		1:1	Brunmark A et al., Free Radic. Biol. Med. 6 (1989), 149
2857	37	7.65	PBS 0.1 M		1:1	Brunmark A et al., Free Radic. Biol. Med. 6 (1989), 149
2858	37	7.65	PBS 0.1 M		1:1	Brunmark A et al., Free Radic. Biol. Med. 6 (1989), 149
2859	37	7.65	PBS 0.1 M		1:1	Brunmark A et al., Free Radic. Biol. Med. 6 (1989), 149
2860			Aqueous medium			Douglas KT, Glutathione Conjugation (1988), 1
2861			Aqueous medium			Douglas KT, Glutathione Conjugation (1988), 1
2862			Aqueous medium			Douglas KT, Glutathione Conjugation (1988), 1
2863			Aqueous medium			Douglas KT, Glutathione Conjugation (1988), 1
2864			Aqueous medium			Douglas KT, Glutathione Conjugation (1988), 1
2865			Aqueous medium			Douglas KT, Glutathione Conjugation (1988), 1
2866			Aqueous medium			Douglas KT, Glutathione Conjugation (1988), 1
2867			Aqueous medium			Douglas KT, Glutathione Conjugation (1988), 1
2868			Aqueous medium			Douglas KT, Glutathione Conjugation (1988), 1
2869			Aqueous medium			Douglas KT, Glutathione Conjugation (1988), 1
2870			Aqueous medium			Douglas KT, Glutathione Conjugation (1988), 1
2871			Aqueous medium			Douglas KT, Glutathione Conjugation (1988), 1
2872			Aqueous medium			Douglas KT, Glutathione Conjugation (1988), 1
2873			Aqueous medium			Douglas KT, Glutathione Conjugation (1988), 1
2874			Aqueous medium			Douglas KT, Glutathione Conjugation (1988), 1
2875			Aqueous medium			Douglas KT, Glutathione Conjugation (1988), 1
2876			Aqueous medium			Douglas KT, Glutathione Conjugation (1988), 1
2877			Aqueous medium			Douglas KT, Glutathione Conjugation (1988), 1
2878			95% Ethanol			Douglas KT, Glutathione Conjugation (1988), 1
2879			Aqueous medium			Douglas KT, Glutathione Conjugation (1988), 1
2880			Aqueous medium			Douglas KT, Glutathione Conjugation (1988), 1
2881			Aqueous medium			Douglas KT, Glutathione Conjugation (1988), 1
2882	25		Water+NaOH	2h	5:1	Drobnica L et al., Biochim. Biophys. Acta 585 (1979), 462
2883	25		Water, methanol	2h	5:1	Drobnica L et al., Biochim. Biophys. Acta 585 (1979), 462
2884	20	7.4	PBS			Klehr H et al., Biol. Chem. Hoppe-Seyler 366 (1985), 755
2885			Water+NaOH		10:1	Alvarez-Sánchez R et al., Chem. Res. Toxicol. 16 (2003), 627
2886			Water+NaOH		10:1	Alvarez-Sánchez R et al., Chem. Res. Toxicol. 16 (2003), 627
2887			Aqueous, NaOH	4 h	1:0.3	Saunders BC, Biochem. J. 27 (1933), 397
2888			Water+NaOH		10:1	Saunders BC, Biochem. J. 27 (1933), 397

#	Comment
2850	Assay: Alkylating activity; UV(560 nm); DE560 > 0.04: reactive
2851	Assay: Alkylating activity; UV(560 nm); DE560 > 0.04: reactive
2852	Assay: Alkylating activity; UV(560 nm); DE560 > 0.04: reactive
2853	Assay: Alkylating activity; UV(560 nm); DE560 > 0.04: reactive
2854	Assay: Alkylating activity; UV(560 nm); DE560 > 0.04: reactive
2855	Assay: HPLC (Electrochemical Det., GSSG after NADPH oxidation)
2856	Assay: HPLC (Electrochemical Det., GSSG after NADPH oxidation)
2857	Assay: HPLC (Electrochemical Det., GSSG after NADPH oxidation)
2858	Assay: HPLC (Electrochemical Det., GSSG after NADPH oxidation)
2859	Assay: HPLC (Electrochemical Det., GSSG after NADPH oxidation)
2860	R: [Drobnica and Sturdik 1979]. Assay: Bronsted data for attacks on various electrophiles of GS[-]
2861	R: [Bruice et al. 1976]. Assay: Bronsted data for attacks on various electrophiles of GS[-
2862	R: [Bruice et al. 1976]. Assay: Bronsted data for attacks on various electrophiles of GS[-
2863	R: [Shipton and Brocklehurst 1978; Brocklehurst and Little 1972]. Assay: Bronsted data for attacks on various electrophiles of GS[-
2864	R: [Snow et al 1975]. Assay: Bronsted data for attacks on various electrophiles of GS[-
2865	R: [Byers 1977]. Assay: Bronsted data for attacks on various electrophiles of GS[-
2866	R: [Grimshaw et al. 1979]. Assay: Bronsted data for attacks on various electrophiles of GS[-
2867	R: [Ogilvie et al. 1964]. Assay: Bronsted data for attacks on various electrophiles of GS[-
2868	R: [Reuben and Bruice 1976]. Assay: Bronsted data for attacks on various electrophiles of GS[-
2869	R: [Bruice et al. 1976]. Assay: Bronsted data for attacks on various electrophiles of GS[-
2870	R: [Friedman et al 1965]. Assay: Bronsted data for attacks on various electrophiles of GS[-
2871	Other thiol, R: [Drobnica et al 1975]. Assay: Bronsted data for attacks on various electrophiles of GS[-
2872	R: [Podhradsky et al. 1979]. Assay: Bronsted data for attacks on various electrophiles of GS[-
2873	R: [Szajewski and Whitesides 1980; Wilson et al. 1978]. Assay: Bronsted data for attacks on various electrophiles of GS[-
2874	R: [Danely and Noel 1960]. Assay: Bronsted data for attacks on various electrophiles of GS[-
2875	R: [Szajewski and Whitesides 1980]. Assay: Bronsted data for attacks on various electrophiles of GS[-
2876	R: [Reuben and Bruice 1976]. Assay: Bronsted data for attacks on various electrophiles of GS[-
2877	R: [Sekine et al 1974]. Assay: Bronsted data for attacks on various electrophiles of GS[-
2878	R: [Semenow-Garwood 1972]. Assay: Bronsted data for attacks on various electrophiles of GS[-
2879	R: [Sanyal and Khalifah 1979]. Assay: Bronsted data for attacks on various electrophiles of GS[-
2880	Other thiol, R: [Drobnica et al 1975]. Assay: Bronsted data for attacks on various electrophiles of GS[-
2881	R: [Podhradsky et al 1979]. Assay: Bronsted data for attacks on various electrophiles of GS[-
2882	radiochromatogramm of [35S], stable in aqueous media. Assay: 13C NMR
2883	radiochromat. of [35S], NMR, elem. anal.. Assay: 13C NMR
2884	Assay: 13C NMR
2885	very fast. Assay: 13C NMR
2886	very fast; Thiole: not soluble. Assay: 13C NMR
2887	Assay: 13C NMR
2888	Assay: 13C NMR

#	Mechanism
2850	Nucleophilic substitution and direct DNA-alkylatior
2851	Nucleophilic substitution and direct DNA-alkylatior
2852	NOT Nucleophilic substitution and direct DNA-alkylatior
2853	Nucleophilic substitution and direct DNA-alkylatior
2854	Nucleophilic substitution and direct DNA-alkylatior
2855	Michael-type nucleophilic addition
2856	Michael-type nucleophilic addition
2857	Michael-type nucleophilic addition
2858	Michael-type nucleophilic addition
2859	Michael-type nucleophilic addition
2860	
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2881	
2882	Nucleophilic olefinic addition
2883	Nucleophilic olefinic addition: AN of RSH at (CN), stable in aqueous solutior
2884	--> ArNH-SR (-->ArNH2) + ArNH-SOR
2885	--> open hemithioacetal --> thioenolate
2886	addition-elimination --> open mercaptoacrylamide only
2887	Oxidation, disulfide formation, no protein-adduct formation: quantitative dithioglycolic acid (-SS-)
2888	Oxidation, disulfide formation, no protein-adduct formation --> quantitative sulphinic acid; R: [Otto 1891]

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2889	106-51-4	p-Benzoquinone	Proline	Adduct(Pro)	(yes/no)	yes		
2890	2682-20-4	2-Methyl-2H-isothiazolin-3-one	Phenolate. Sodium	Adduct(Phenolate)	(yes/no)	no		
2891	26172-55-4	5-Chloro-2-methyl-4-isothiazolin-3-one	Phenolate. Sodium	Adduct(Phenolate)	(yes/no)	yes		
2892	2607-52-5	2.6-Di-tert-butyl-4-methylene-2.5-cyclohexadienone	Gly-His-Lys	Adduct(Peptide): Tripeptide	(yes/no)	no		
2893		2-tert-Butyl-6-methyl-4-methylene-2.5-cyclohexadienone	Gly-His-Lys	Adduct(Peptide): Tripeptide	(yes/no)	yes		
2894		6-tert-Butyl-2-(2-hydroxy-1.1-dimethylethyl)-4-methylene-2.5-cyclohexadienone	Gly-His-Lys	Adduct(Peptide): Tripeptide	(yes/no)	yes		
2895	50-00-0	Formaldehyde	Peptide intramolecular cross-linking (AcLXENXLLXFNH2)	Adduct(Peptide): Series	(yes/no)	yes		
2896	50-00-0	Formaldehyde	Peptide intramolecular cross-linking (AcLXENXLLXFNH2)	Adduct(Peptide): Series	(yes/no)	yes		
2897	50-00-0	Formaldehyde	Peptide intramolecular cross-linking (AcLXENXLLXFNH2)	Adduct(Peptide): Series	(yes/no)	no		
2898	50-00-0	Formaldehyde	Peptide intramolecular cross-linking (AcLXENXLLXFNH2)	Adduct(Peptide): Series	(yes/no)	no		
2899	50-00-0	Formaldehyde	Peptide intramolecular cross-linking (AcLXENXLLXFNH2)	Adduct(Peptide): Series	(yes/no)	yes		
2900	50-00-0	Formaldehyde	Peptide series (AcVELXVLL)	Adduct(Peptide): Series	(yes/no)	yes		
2901	50-00-0	Formaldehyde	Peptide series (AcVELXVLL)	Adduct(Peptide): Series	(yes/no)	yes		
2902	50-00-0	Formaldehyde	Peptide series (AcVELXVLL)	Adduct(Peptide): Series	(yes/no)	yes		
2903	50-00-0	Formaldehyde	Peptide series (AcVELXVLL)	Adduct(Peptide): Series	(yes/no)	no		
2904	50-00-0	Formaldehyde	Peptide series (AcVELXVLL)	Adduct(Peptide): Series	(yes/no)	no		
2905	50-00-0	Formaldehyde	Peptide series (AcVELXVLL)	Adduct(Peptide): Series	(yes/no)	no		
2906	50-00-0	Formaldehyde	Peptide series (AcVELXVLL)	Adduct(Peptide): Series	(yes/no)	yes		
2907	1129-21-1	4-tert-Butyl-1.2-benzoquinone	Peptide. Nucleophilic (H-PHCKRM-OH)	Adduct(Peptide): Nucleophilic	(yes/no)	yes		
2908	106-51-4	p-Benzoquinone	Peptide. Nucleophilic (H-PHCKRM-OH)	Adduct(Peptide): Nucleophilic	(yes/no)	yes		
2909	29343-52-0	4-Hydroxy-2-nonenal	Peptide (Arg)	Adduct(Peptide): Model	(yes/no)	no		
2910	103560-62-9	4-Oxo-2-nonenal	Peptide (Arg)	Adduct(Peptide): Model	(yes/no)	yes		
2911	29343-52-0	4-Hydroxy-2-nonenal	Peptide (Cys+Arg)	Adduct(Peptide): Model	(yes/no)	yes		
2912	103560-62-9	4-Oxo-2-nonenal	Peptide (Cys+Arg)	Adduct(Peptide): Model	(yes/no)	yes		

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2889				30 min	1:1 - 1:256	Woker G et al., Helv. Chim. Acta 20 (1937), 1260
2890			Water	50 d	10:1	Alvarez-Sánchez R et al., Chem. Res. Toxicol. 16 (2003), 627
2891			Water	15 d	10:1	Alvarez-Sánchez R et al., Chem. Res. Toxicol. 16 (2003), 627
2892	25	7.4	Water	1 h	El excess	Bolton JL et al., Chem. Biol. Interact. 107 (1997), 185
2893	25	7.4	Water	1 h	El excess	Bolton JL et al., Chem. Biol. Interact. 107 (1997), 185
2894	25	7.4	Water	1 h	El excess	Bolton JL et al., Chem. Biol. Interact. 107 (1997), 185
2895	35	7.2	PBS	48 h	1:50	Metz B et al., J. Biol. Chem. 279 (2004), 6235
2896	35	7.2	PBS	48 h	1:50	Metz B et al., J. Biol. Chem. 279 (2004), 6235
2897	35	7.2	PBS	48 h	1:50	Metz B et al., J. Biol. Chem. 279 (2004), 6235
2898	35	7.2	PBS	48 h	1:50	Metz B et al., J. Biol. Chem. 279 (2004), 6235
2899	35	7.2	PBS	48 h	1:50	Metz B et al., J. Biol. Chem. 279 (2004), 6235
2900	35	7.2	PBS	48 h	1:50	Metz B et al., J. Biol. Chem. 279 (2004), 6235
2901	35	7.2	PBS	48 h	1:50	Metz B et al., J. Biol. Chem. 279 (2004), 6235
2902	35	7.2	PBS	48 h	1:50	Metz B et al., J. Biol. Chem. 279 (2004), 6235
2903	35	7.2	PBS	48 h	1:50	Metz B et al., J. Biol. Chem. 279 (2004), 6235
2904	35	7.2	PBS	48 h	1:50	Metz B et al., J. Biol. Chem. 279 (2004), 6235
2905	35	7.2	PBS	48 h	1:50	Metz B et al., J. Biol. Chem. 279 (2004), 6235
2906	35	7.2	PBS	48 h	1:50	Metz B et al., J. Biol. Chem. 279 (2004), 6235
2907	26	3.3	Acetate buffer/PBS (pH 7.4) Borate buffer (pH 8.4)	<5 min	1:1 - 1:8	Ahlfors SR et al., Skin Pharmacol. Appl. Skin Physiol. 16 (2003), 59
2908	26	3.3	Acetate buffer/PBS (pH 7.4) Borate buffer (pH 8.4)	<5 min	1:1 - 1:8	Ahlfors SR et al., Skin Pharmacol. Appl. Skin Physiol. 16 (2003), 59
2909	37	7.4	Tricine buffer 10 mM	16-18 h	1:20	Doorn JA et al., Chem. Biol. Interact. 143 (2003), 93
2910	37	7.4	Tricine buffer 10 mM	16-18 h	1:20	Doorn JA et al., Chem. Biol. Interact. 143 (2003), 93
2911	37	7.4	Tricine buffer 10 mM	16-18 h	1:20	Doorn JA et al., Chem. Biol. Interact. 143 (2003), 93
2912	37	7.4	Tricine buffer 10 mM	16-18 h	1:20	Doorn JA et al., Chem. Biol. Interact. 143 (2003), 93

#	Comment
2889	raspberry red, control yellow. Assay: Visual intensity of colour, compared to contro
2890	Assay: 13C NMR
2891	weak; Phenol: NR. Assay: 13C NMR
2892	Assay: HPLC-Thermospray MS (m/z 120-600)
2893	Assay: HPLC-Thermospray MS (m/z 120-600)
2894	Assay: HPLC-Thermospray MS (m/z 120-600)
2895	Assay: HPLC-MS
2896	Assay: HPLC-MS
2897	Assay: HPLC-MS
2898	Assay: HPLC-MS
2899	Assay: HPLC-MS
2900	Assay: HPLC-MS
2901	Assay: HPLC-MS
2902	Assay: HPLC-MS
2903	Assay: HPLC-MS
2904	Assay: HPLC-MS
2905	Assay: HPLC-MS
2906	Assay: HPLC-MS
2907	red:hydroquinone, unstable ox:quinone at pH 3.3,5.4,7.4,8.5. Assay: HPLC, 1H- and 13C-NMR, FAB-MS
2908	red: hydroquinone and ox: quinone at pH 3.3,5.4,7.4,8.5. Assay: HPLC, 1H- and 13C-NMR, FAB-MS
2909	Assay: MALDI-TOF-MS, post-source decay analysis
2910	Assay: MALDI-TOF-MS, post-source decay analysis
2911	Assay: MALDI-TOF-MS, post-source decay analysis
2912	Assay: MALDI-TOF-MS, post-source decay analysis

#	Mechanism
2889	Michael-type nucleophilic addition
2890	
	Nucleophilic substitution:
2891	addition-elimination --> O-alkylation (cyclic adducts) + minor o-/p-C-alkylation
2892	small amount at Gly-NH-alpha
2893	adducts at Gly and Lys
2894	adducts at Gly and Lys
	Cross-linking via Schiff base formation:
2895	H2CO-Gly-Adduct cross-linking with His,Lys,Arg; with primary Leu only
	Methylol adducts on amino groups yielding Schiff bases:
2896	adducts at His,Lys,Arg; at primary Leu only
	NOT Cross-linking via Schiff base formation:
2897	H2CO-Gly-Adduct: no cross-linking with Ala,Glu,Asn,Leu,Phe
2898	NOT Schiff base formation: no adduct at Ala,Glu,Asn,Leu,Phe
2899	Schiff base formation: adduct at Lys
	Cross-linking via Schiff base formation:
2900	H2CO-AcArgOMe-Adduct: cross-linking with Cys,Lys
	Cross-linking via Schiff base formation:
2901	H2CO-Gly-Adduct cross-linking with peptides containing C,H,N,Q,R,W,Y
	Methylol adducts on amino groups yielding Schiff bases:
2902	adducts at Cys,Arg,Trp; Lys with NaCNBH3: eps-NH2 --> eps-NMe2
	NOT Cross-linking via Schiff base formation:
2903	H2CO-AcArgOMe-Adduct: no cross-linking with His,Asn,Gln,Arg,Trp
	NOT Cross-linking via Schiff base formation:
2904	H2CO-Gly-Adduct cross-linking with peptides containing A,D,F,K,M,P,S,T
	NOT Schiff base formation:
2905	no adducts with peptides cont. His,Lys (yes: +NaCNBH3),A,D,F,M,N,P,Q,S,T,Y
2906	Schiff base formation: adducts at Trp
2907	Michael-type nucleophilic addition: Cys adduct only
2908	Michael-type nucleophilic addition: Cys adduct only
2909	NOT Michael-type nucleophilic addition
	Michael-type nucleophilic addition:
2910	adduct at Arg: reactive toward dicarbonyl compounds
2911	Michael-type nucleophilic addition: adduct at Cys
	Michael-type nucleophilic addition:
2912	adduct at Cys and Arg: reactive toward dicarbonyl compounds

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2913	29343-52-0	4-Hydroxy-2-nonenal	Peptide (His)	Adduct(Peptide): Model	(yes/no)	yes		
2914	103560-62-9	4-Oxo-2-nonenal	Peptide (His)	Adduct(Peptide): Model	(yes/no)	yes		
2915	29343-52-0	4-Hydroxy-2-nonenal	Peptide (Lys)	Adduct(Peptide): Model	(yes/no)	yes		
2916	103560-62-9	4-Oxo-2-nonenal	Peptide (Lys)	Adduct(Peptide): Model	(yes/no)	yes		
2917	29343-52-0	4-Hydroxy-2-nonenal	Peptide (Lys+Arg)	Adduct(Peptide): Model	(yes/no)	yes		
2918	103560-62-9	4-Oxo-2-nonenal	Peptide (Lys+Arg)	Adduct(Peptide): Model	(yes/no)	yes		
2919	29343-52-0	4-Hydroxy-2-nonenal	Peptide (Met)	Adduct(Peptide): Model	(yes/no)	no		
2920	103560-62-9	4-Oxo-2-nonenal	Peptide (Met)	Adduct(Peptide): Model	(yes/no)	no		
2921	2682-20-4	2-Methyl-2H-isothiazolin-3-one	General Peptide (H2N-VLSPADKTNW-GHEYRMFQIG-CO2H)	Adduct(Peptide): General	(yes/no)	no		
2922	26172-55-4	5-Chloro-2-methyl-4-isothiazolin-3-one	General Peptide (H2N-VLSPADKTNW-GHEYRMFQIG-CO2H)	Adduct(Peptide): General	(yes/no)	yes		
2923	106-51-4	p-Benzoquinone	Lysine	Adduct(Lys)	(yes/no)	yes		
2924	106-51-4	p-Benzoquinone	Ornithine	Adduct(Lys)	(yes/no)	yes		
2925	2682-20-4	2-Methyl-2H-isothiazolin-3-one	Imidazole	Adduct(Imidazole)	(yes/no)	no		
2926	26172-55-4	5-Chloro-2-methyl-4-isothiazolin-3-one	Imidazole	Adduct(Imidazole)	(yes/no)	yes		
2927	2607-52-5	2.6-Di-tert-butyl-4-methylene-2.5-cyclohexadienone	Histidine	Adduct(His)	(yes/no)	no		
2928		6-tert-Butyl-2-(2-hydroxy-1.1-dimethylethyl)-4-methylene-2.5-cyclohexadienone	Histidine	Adduct(His)	(yes/no)	yes		
2929	106-51-4	p-Benzoquinone	Histidine	Adduct(His)	(yes/no)	yes		
2930	2682-20-4	2-Methyl-2H-isothiazolin-3-one	Glutathione	Adduct(GSH): NMR	(yes/no)	yes		
2931	26172-55-4	5-Chloro-2-methyl-4-isothiazolin-3-one	Glutathione	Adduct(GSH): NMR	(yes/no)	very fast		
2932	97-00-7	1-Chloro-2.4-dinitrobenzene	Glutathione	Adduct(GSH)	(yes/no)	yes		
2933	624-76-0	2-Iodoethanol	Glutathione	Adduct(GSH)	(yes/no)	yes		
2934	93-11-8	2-Naphthalenesulfonyl chloride	Glutathione	Adduct(GSH)	(yes/no)	no		
2935	64-69-7	Iodoacetic acid	Glutathione	Adduct(GSH)	(yes/no)	yes		
2936	106-51-4	p-Benzoquinone	Glutathione	Adduct(GSH)	(yes/no)	no		
2937	100-44-7	Benzyl chloride	Thiolacetic acid	Adduct(GSH)	(yes/no)	no		
2938	107-02-8	Acrolein	Glu-C. no Cys	Adduct(Glu-C)	(yes/no)	no		
2939	107-02-8	Acrolein	Glu-C. with Cys	Adduct(Glu-C)	(yes/no)	yes		
2940	107-02-8	Acrolein	Glu-C. with Cys	Adduct(Glu-C)	(yes/no)	no		
2941	140-88-5	Ethyl acrylate	2'-Deoxyguanosine	Adduct(DNA)	(yes/no)	no		

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2913	37	7.4	Tricine buffer 10 mM	16-18 h	1:20	Doorn JA et al., Chem. Biol. Interact. 143 (2003), 93
2914	37	7.4	Tricine buffer 10 mM	16-18 h	1:20	Doorn JA et al., Chem. Biol. Interact. 143 (2003), 93
2915	37	7.4	Tricine buffer 10 mM	16-18 h	1:20	Doorn JA et al., Chem. Biol. Interact. 143 (2003), 93
2916	37	7.4	Tricine buffer 10 mM	16-18 h	1:20	Doorn JA et al., Chem. Biol. Interact. 143 (2003), 93
2917	37	7.4	Tricine buffer 10 mM	16-18 h	1:20	Doorn JA et al., Chem. Biol. Interact. 143 (2003), 93
2918	37	7.4	Tricine buffer 10 mM	16-18 h	1:20	Doorn JA et al., Chem. Biol. Interact. 143 (2003), 93
2919	37	7.4	Tricine buffer 10 mM	16-18 h	1:20	Doorn JA et al., Chem. Biol. Interact. 143 (2003), 93
2920	37	7.4	Tricine buffer 10 mM	16-18 h	1:20	Doorn JA et al., Chem. Biol. Interact. 143 (2003), 93
2921		7.7	PBS 0.1 M, ACN	15 d	1:40	Alvarez-Sánchez R et al., Bioorg. Med. Chem. Lett. 14 (2004), 365
2922		7.7	PBS 0.1 M, ACN	15 d	1:40	Alvarez-Sánchez R et al., Bioorg. Med. Chem. Lett. 14 (2004), 365
2923				30 min	1:1 - 1:256	Woker G et al., Helv. Chim. Acta 20 (1937), 1260
2924				30 min	1:1 - 1:256	Woker G et al., Helv. Chim. Acta 20 (1937), 1260
2925			Water	50d	10:1	Alvarez-Sánchez R et al., Chem. Res. Toxicol. 16 (2003), 627
2926			Water	45 d	10:1	Alvarez-Sánchez R et al., Chem. Res. Toxicol. 16 (2003), 627
2927						Bolton JL et al., Chem. Biol. Interact. 107 (1997), 185
2928						Bolton JL et al., Chem. Biol. Interact. 107 (1997), 185
2929				30 min	1:1 - 1:256	Woker G et al., Helv. Chim. Acta 20 (1937), 1260
2930		7.7	PBS 0.1 M, ACN		10:1 detox. 1:40 tox.	Alvarez-Sánchez R et al., Bioorg. Med. Chem. Lett. 14 (2004), 365
2931		7.7	PBS 0.1 M, ACN		10:1 detox. 1:40 tox.	Alvarez-Sánchez R et al., Bioorg. Med. Chem. Lett. 14 (2004), 365
2932			Aqueous, NaOH	10 min	1:1	Saunders BC, Biochem. J. 28 (1934), 1977
2933		7.65		280 min		Goddard DR et al., Biochem. J. 29 (1935), 1009
2934			Aqueous, NaOH	4 h	1:2	Saunders BC, Biochem. J. 27 (1933), 397
2935		7.57		11 min		Goddard DR et al., Biochem. J. 29 (1935), 1009
2936				30 min	1:1 - 1:256	Woker G et al., Helv. Chim. Acta 20 (1937), 1260
2937			Aqueous, NaOH	10 h	1:1.2	Saunders BC, Biochem. J. 28 (1934), 1977
2938	37	7.4	NH4HCO3 buffer 0.1 M	30 min	1:15	Cai J et al., Chem. Res. Toxicol. 22 (2009), 708
2939	37	7.4	NH4HCO3 buffer 0.1 M	30 min	1:15	Cai J et al., Chem. Res. Toxicol. 22 (2009), 708
2940	37	7.4	NH4HCO3 buffer 0.1 M	30 min	1:15	Cai J et al., Chem. Res. Toxicol. 22 (2009), 708
2941	37	7.4	PBS 25 mM	24 h	1:1	McCarthy TJ et al., Fund. Appl. Toxicol. 22 (1994), 543

#	Comment
2913	Assay: MALDI-TOF-MS, post-source decay analysis
2914	Assay: MALDI-TOF-MS, post-source decay analysis
2915	Assay: MALDI-TOF-MS, post-source decay analysis
2916	Assay: MALDI-TOF-MS, post-source decay analysis
2917	Assay: MALDI-TOF-MS, post-source decay analysis
2918	Assay: MALDI-TOF-MS, post-source decay analysis
2919	Assay: MALDI-TOF-MS, post-source decay analysis
2920	Assay: MALDI-TOF-MS, post-source decay analysis
2921	Assay: 13C NMR and 1H(13C) HMBC+HSQC
2922	Assay: 13C NMR and 1H(13C) HMBC+HSQC
2923	salmon pink (1:1,1:2 too acidic, yellow), control yellow. Assay: Visual intensity of colour, compared to contro
2924	purple (1:1 too acidic, yellow), control yellow. Assay: Visual intensity of colour, compared to contro
2925	Assay: 13C NMR and 1H(13C) HMBC; room temperature
2926	very slow. Assay: 13C NMR and 1H(13C) HMBC; room temperature
2927	Assay: 1H-NMR (5.0 ppm imidazole-alkyl singlet)
2928	Assay: 1H-NMR (5.0 ppm imidazole-alkyl singlet)
2929	Visual intensity of colour, compared to control; cherry-red; alpha-NH2-Add.. Assay: 1H-NMR (5.0 ppm imidazole-alkyl singlet
2930	fast. Assay: 13C NMR and 1H(13C) HMBC+HSQC
2931	Assay: 13C NMR and 1H(13C) HMBC+HSQC
2932	
2933	slow,about 50% GSH depletion; room temperature; titration with iodine (alcoholic).
2934	elemental analysis of sulphinic acid.
2935	100% GSH depletion; room temperature; titration with iodine (alcoholic).
2936	Visual intensity of colour, compared to control: intensive orange.
2937	
2938	Assay: ESI-MS(-MS), reactivity at terminal -NH2 checked by blocking with SFB
2939	Assay: ESI-MS(-MS), reactivity at terminal -NH2 checked by blocking with SFB
2940	Assay: ESI-MS(-MS), reactivity at terminal -NH2 checked by blocking with SFB
2941	no adducts with dG, dC, dA, T at 37C or 50C; HPLC.

#	Mechanism
2913	Michael-type nucleophilic addition: adduct at His
2914	Michael-type nucleophilic addition: adduct at His
2915	Michael-type nucleophilic addition: adduct at Lys
2916	Michael-type nucleophilic addition: adduct at Lys
2917	Michael-type nucleophilic addition: adduct at Lys
2918	Michael-type nucleophilic addition: adduct at Lys and Arg: reactive toward dicarbonyl compounds
2919	NOT Michael-type nucleophilic addition
2920	NOT Michael-type nucleophilic addition
2921	
2922	adducts at His, Lys (epsilon-N), Val (alpha-N)
2923	Michael-type nucleophilic addition
2924	Michael-type nucleophilic addition
2925	
2926	Nucleophilic substitution: addition-elimination at MCI pos. 5 --> cyclic adduct, no hydrolysis
2927	
2928	
2929	Michael-type nucleophilic addition
2930	initial G-SH attack --> S-N cleaves --> -SS-MI. GSH excess ->> hemithioacetal
2931	--> mercaptothioester. MCI excess ->> thioamide, intram. attack of a-NH2
2932	Nucleophilic aromatic substitution (SNAr) --> S-2,4-Dinitrophenylglutathione; S now blocked, NH2-adduct with iodoacetic acid
2933	
2934	Oxidation, disulfide formation, no protein-adduct formation: GSH ox. --> GSSG + sulphinic acid
2935	
2936	NOT Michael-type nucleophilic addition
2937	Nucleophilic substitution: some S-adducts, free NH2 group
2938	NOT Michael addition or Schiff base formation: no adducts without Cys in peptide
2939	Michael addition or Schiff base formation: adducts: 1. Cys, 2. terminal -NH2, 3. Lys-NH2 via close Cys-MA intermediate
2940	NOT Schiff base formation: no direct adducts at Lys (epsilon-NH2)
2941	

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2942	3249-28-3	Muconaldehyde	2'-Deoxyguanosine	Adduct(DNA)	(yes/no)	yes		
2943	3249-28-3	Muconaldehyde	2'-Deoxyguanosine	Adduct(DNA)	(yes/no)	yes		
2944		N-Acetoxy-3-aminobenzanthrone	2'-Deoxyguanosine	Adduct(DNA)	(yes/no)	yes		
2945	107-20-0	2-Chloroacetaldehyde	Adenosine	Adduct(DNA)	(yes/no)	yes		
2946	7763-77-1	Chloroethylene oxide	Adenosine	Adduct(DNA)	(yes/no)	yes		
2947	75-01-4	Vinyl chloride	Adenosine	Adduct(DNA)	(yes/no)	no		
2948	97-00-7	1-Chloro-2.4-dinitrobenzene	Cysteine	Adduct(Cys)	(yes/no)	yes		
2949	624-76-0	2-Iodoethanol	Cysteine	Adduct(Cys)	(yes/no)	yes		
2950	93-11-8	2-Naphthalenesulfonyl chloride	Cysteine	Adduct(Cys)	(yes/no)	no		
2951	100-44-7	Benzyl chloride	Cysteine	Adduct(Cys)	(yes/no)	yes		
2952	306-18-3	Carbonyl cyanide phenylhydrazone	Cysteine	Adduct(Cys)	(yes/no)	yes		
2953	64-69-7	Iodoacetic acid	Cysteine	Adduct(Cys)	(yes/no)	yes		
2954	64-69-7	Iodoacetic acid	Cysteine	Adduct(Cys)	(yes/no)	yes		
2955	93-11-8	2-Naphthalenesulfonyl chloride	S-Benzylcysteine	Adduct(Cys)	(yes/no)	yes		
2956	2682-20-4	2-Methyl-2H-isothiazolin-3-one	n-Butylamine	Adduct(BuNH2)	(yes/no)	no		
2957	26172-55-4	5-Chloro-2-methyl-4-isothiazolin-3-one	n-Butylamine	Adduct(BuNH2)	(yes/no)	yes		
2958	106-51-4	p-Benzoquinone	Arginine	Adduct(Arg)	(yes/no)	yes		
2959	26172-55-4	5-Chloro-2-methyl-4-isothiazolin-3-one	N(alpha)-Acetyl lysine	Adduct(AcCys)	(yes/no)	yes		
2960	2682-20-4	2-Methyl-2H-isothiazolin-3-one	N-Acetyl cysteine	Adduct(AcCys)	(yes/no)	yes		
2961	103560-62-9	4-Oxo-2-nonenal	N-Acetyl cysteine	Adduct(AcCys)	(yes/no)	yes		
2962	103560-62-9	4-Oxo-2-nonenal	N-Acetyl cysteine	Adduct(AcCys)	(yes/no)	yes		
2963	26172-55-4	5-Chloro-2-methyl-4-isothiazolin-3-one	N-Acetyl cysteine	Adduct(AcCys)	(yes/no)	yes		
2964	2634-33-5	1.2-Benzisothiazolin-3-one	Lysine	%Dissociation(Lys)	%R/Rmax	0.01	0.4	
2965	109-65-9	1-Bromobutane	Lysine	%Dissociation(Lys)	%R/Rmax	-0.22	0.07	
2966	89-02-1	2.4-Dinitrobenzenesulfonic acid	Lysine	%Dissociation(Lys)	%R/Rmax	0.53	0.42	
2967	119-84-6	3.4-Dihydrocoumarin	Lysine	%Dissociation(Lys)	%R/Rmax	-0.91	0.39	
2968	591-27-5	3-Aminophenol	Lysine	%Dissociation(Lys)	%R/Rmax	-1.18	1.13	
2969	109-55-7	3-Dimethylaminopropylamine	Lysine	%Dissociation(Lys)	%R/Rmax	-1.77	0.36	
2970	122-40-7	alpha-Amyl cinnamaldehyde	Lysine	%Dissociation(Lys)	%R/Rmax	0.02	0.09	
2971	101-86-0	alpha-Hexylcinnamaldehyde	Lysine	%Dissociation(Lys)	%R/Rmax	1.67	0.23	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2942	37	7.4	PBS	16 h	2:1	McCarthy TJ et al., Fund. Appl. Toxicol. 22 (1994), 543
2943	37	7.4	PBS 10 mM	6 h	1:1	Schatz-Kornbrust E et al., Toxicologist 11 (1991), 253
2944	37		THF, DMF, water	6 h	1:1	da Costa GG et al., Chem. Res. Toxicol. 22 (2009), 1860
2945	37	7	Ethanol, citrate buffer	2 h	1:5	Barbin A et al., Biochem. Biophys. Res. Commun. 67 (1975), 596
2946	37	7	Ethanol, citrate buffer	15 min	1:5	Barbin A et al., Biochem. Biophys. Res. Commun. 67 (1975), 596
2947						Barbin A et al., Biochem. Biophys. Res. Commun. 67 (1975), 596
2948			Aqueous, NaOH	10 min	1:1	Saunders BC, Biochem. J. 28 (1934), 1977
2949		7.64	PBS	280 min		Goddard DR et al., Biochem. J. 29 (1935), 1009
2950			Aqueous, NaOH	4 h	1:2	Saunders BC, Biochem. J. 27 (1933), 397
2951			Aqueous, NaOH			Saunders BC, Biochem. J. 27 (1933), 397
2952	25		Water, methanol, carbonate buffer		10:1	Drobnica L et al., Biochim. Biophys. Acta 585 (1979), 462
2953	45	7.15	PBS			Rapkine L, Sociéte de Biologie 112 (1933), 790
2954		7.55	PBS	11 min		Goddard DR et al., Biochem. J. 29 (1935), 1009
2955			Aqueous, NaOH	4 h	1:2	Saunders BC, Biochem. J. 27 (1933), 397
2956			Water	50d	10:1	Alvarez-Sánchez R et al., Chem. Res. Toxicol. 16 (2003), 627
2957			Water	24h	10:1	Alvarez-Sánchez R et al., Chem. Res. Toxicol. 16 (2003), 627
2958				30 min	1:1 - 1:256	Woker G et al., Helv. Chim. Acta 20 (1937), 1260
2959		7.7	PBS 0.1 M, ACN	1d	1:3: cat. 0.1 AcCys	Alvarez-Sánchez R et al., Chem. Res. Toxicol. 16 (2003), 627
2960		7.7	PBS 0.1 M, ACN		10:1+1:1+1:40	Alvarez-Sánchez R et al., Chem. Res. Toxicol. 16 (2003), 627
2961	37	7.4	PBS 0.1 M BSA bovine serum albumin	72 h	1:1	Shimozu Y et al., Chem. Res. Toxicol. 22 (2009), 957
2962	37	7.4	PBS 0.1 M	1h (MA) - 72 h	1:1	Shimozu Y et al., Chem. Res. Toxicol. 22 (2009), 957
2963		7.7	PBS 0.1 M, ACN		10:1+1:1+1:40	Alvarez-Sánchez R et al., Chem. Res. Toxicol. 16 (2003), 627
2964	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2965	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2966	25		PBS	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2967	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2968	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2969	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2970	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2971	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308

#	Comment
2942	radiochromatogram; [R: Latriano 1989].
2943	RP-HPLC-UV(265 nm,340 nm), complex pattern.
2944	ESI-MS/MS.
2945	GC analysis.
2946	GC analysis.
2947	yes after air oxidation/microsomal activation.
2948	room temperature; titration with alcoholic iodine.
2949	slow, about 25% Cys depletion..
2950	elemental analysis.
2951	room temperature; titration with alcoholic iodine.
2952	1H-NMR, elem. analysis.
2953	
2954	100% depletion of Cys..
2955	room temperature; titration with alcoholic iodine.
2956	products in trace amounts. Assay: 13C NMR and 1H(13C) HMBC+HSQC
2957	fast, 100% depletion. Assay: 13C NMR and 1H(13C) HMBC+HSQC
2958	deep purple, control yellow. Assay: Visual intensity of colour, compared to contro
2959	without AcCys: NR. Assay: 13C NMR
2960	slow. Assay: 13C NMR
2961	SDS-PAGE. Assay: 13C NMR
2962	NMR+HMBC. Assay: 13C NMR
2963	very fast; MCl excess: NR; catal. activ. for AcLys. Assay: 13C NMR
2964	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2965	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2966	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2967	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2968	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2969	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2970	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2971	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution

#	Mechanism
2942	multiple adducts
2943	
2944	
2945	3-B-D-ribofuranosyl-imidazo-[2,l-i]purine adduct
2946	
2947	
2948	Nucleophilic aromatic substitution (SNAr) --> S-2,4-Dinitrophenylcysteine
2949	
	Oxidation, disulfide formation, no protein-adduct formation
2950	--> quantitative sulphinic acid + dinaphthalene-2-sulphonyl-1-cystine
2951	
2952	Nucleophilic olefinic addition of RSH at (CN), stable in aqueous solution
2953	Nucleophilic substitution: S-adduct
2954	
2955	Nucleophilic substitution: quantitative adducts
2956	
2957	Addition-elimination (at MCI pos.5) --> open mercaptothioester
2958	Michael-type nucleophilic addition
2959	--> -SH attack --> open -SS- / +AcLys --> thioacyl chloride ->>
2960	--> disulfide only
	Cross-linking via Schiff base formation:
2961	secondary reactions of MA products with BSA-NH2 (SB)
	Michael addition and 2-cyclopentenone type dicarbonyl cyclisation
2962	CHO-MA (pos-3) major, CO-MA (pos-2) minor; still C=O functionality
2963	--> open mercaptothioester
2964	
2965	
2966	
2967	
2968	
2969	
2970	
2971	

#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2972	120-51-4	Benzyl benzoate	Lysine	%Dissociation(Lys)	%R/Rmax	-0.15	0.05	
2973	5392-40-5	Citral	Lysine	%Dissociation(Lys)	%R/Rmax	-0.17	0.89	
2974	103-95-7	Cyclamen aldehyde	Lysine	%Dissociation(Lys)	%R/Rmax	-0.07	0.07	
2975	84-66-2	Diethyl phthalate	Lysine	%Dissociation(Lys)	%R/Rmax	-0.1	0.03	
2976	97-53-0	Eugenol	Lysine	%Dissociation(Lys)	%R/Rmax	-0.63	0.65	
2977	111-30-8	Glutaraldehyde	Lysine	%Dissociation(Lys)	%R/Rmax	15.04	9.44	
2978	107-75-5	Hydroxycitronellal	Lysine	%Dissociation(Lys)	%R/Rmax	-0.41	0.18	
2979	97-54-1	Isoeugenol	Lysine	%Dissociation(Lys)	%R/Rmax	0.19	0.17	
2980	80-54-6	Lilial	Lysine	%Dissociation(Lys)	%R/Rmax	-0.03	0.04	
2981	31906-04-4	Lyral	Lysine	%Dissociation(Lys)	%R/Rmax	-0.09	0.26	
2982	106-51-4	p-Benzoquinone	Lysine	%Dissociation(Lys)	%R/Rmax	9.71	6.07	
2983	122-78-1	Phenylacetaldehyde	Lysine	%Dissociation(Lys)	%R/Rmax	0.94	0.82	
2984	2508-19-2	Trinitrobenzenesulfonic acid	Lysine	%Dissociation(Lys)	%R/Rmax	1.6	1.88	
2985	2634-33-5	1.2-Benzisothiazolin-3-one	Histidine	%Dissociation(His)	%R/Rmax	-0.05	ND	
2986	109-65-9	1-Bromobutane	Histidine	%Dissociation(His)	%R/Rmax	-0.43	ND	
2987	89-02-1	2.4-Dinitrobenzenesulfonic acid	Histidine	%Dissociation(His)	%R/Rmax	-0.03	ND	
2988	119-84-6	3.4-Dihydrocoumarin	Histidine	%Dissociation(His)	%R/Rmax	0.05	0.16	
2989	591-27-5	3-Aminophenol	Histidine	%Dissociation(His)	%R/Rmax	-0.42	ND	
2990	109-55-7	3-Dimethylaminopropylamine	Histidine	%Dissociation(His)	%R/Rmax	-3.3	3.35	
2991	122-40-7	alpha-Amyl cinnamaldehyde	Histidine	%Dissociation(His)	%R/Rmax	0.02	ND	
2992	101-86-0	alpha-Hexylcinnamaldehyde	Histidine	%Dissociation(His)	%R/Rmax	-0.01	ND	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2972	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2973	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2974	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2975	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2976	25		10% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2977	25		PBS	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2978	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2979	25		10 % DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2980	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2981	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2982	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2983	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2984	25		PBS	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2985	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2986	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2987	25		PBS	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2988	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2989	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2990	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2991	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2992	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308

#	Comment
2972	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2973	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2974	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2975	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2976	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2977	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2978	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2979	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2980	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2981	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2982	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2983	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2984	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2985	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2986	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2987	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2988	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2989	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2990	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2991	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2992	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution

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#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
2993	120-51-4	Benzyl benzoate	Histidine	%Dissociation(His)	%R/Rmax	**-0.04**	0.08	
2994	5392-40-5	Citral	Histidine	%Dissociation(His)	%R/Rmax	**0.24**	0.54	
2995	103-95-7	Cyclamen aldehyde	Histidine	%Dissociation(His)	%R/Rmax	**-0.15**	0.12	
2996	84-66-2	Diethyl phthalate	Histidine	%Dissociation(His)	%R/Rmax	**-0.07**	0.07	
2997	97-53-0	Eugenol	Histidine	%Dissociation(His)	%R/Rmax	**0.48**	ND	
2998	111-30-8	Glutaraldehyde	Histidine	%Dissociation(His)	%R/Rmax	**-0.31**	ND	
2999	107-75-5	Hydroxycitronellal	Histidine	%Dissociation(His)	%R/Rmax	**-0.32**	ND	
3000	97-54-1	Isoeugenol	Histidine	%Dissociation(His)	%R/Rmax	**-0.45**	ND	
3001	80-54-6	Lilial	Histidine	%Dissociation(His)	%R/Rmax	**-0.34**	1.03	
3002	31906-04-4	Lyral	Histidine	%Dissociation(His)	%R/Rmax	**-0.03**	0.04	
3003	106-51-4	p-Benzoquinone	Histidine	%Dissociation(His)	%R/Rmax	**3.48**	2.29	
3004	122-78-1	Phenylacetaldehyde	Histidine	%Dissociation(His)	%R/Rmax	**-0.65**	0.09	
3005	2508-19-2	Trinitrobenzenesulfonic acid	Histidine	%Dissociation(His)	%R/Rmax	**5.96**	ND	
3006	2634-33-5	1.2-Benzisothiazolin-3-one	Cysteine	%Dissociation(Cys)	%R/Rmax	**1.43**	0.86	
3007	109-65-9	1-Bromobutane	Cysteine	%Dissociation(Cys)	%R/Rmax	**-0.29**	0.6	
3008	89-02-1	2.4-Dinitrobenzenesulfonic acid	Cysteine	%Dissociation(Cys)	%R/Rmax	**0.08**	0.05	
3009	119-84-6	3.4-Dihydrocoumarin	Cysteine	%Dissociation(Cys)	%R/Rmax	**-0.13**	0.03	
3010	591-27-5	3-Aminophenol	Cysteine	%Dissociation(Cys)	%R/Rmax	**3.28**	5.54	
3011	109-55-7	3-Dimethylaminopropylamine	Cysteine	%Dissociation(Cys)	%R/Rmax	**3.99**	9.63	
3012	122-40-7	alpha-Amyl cinnamaldehyde	Cysteine	%Dissociation(Cys)	%R/Rmax	**-0.14**	0.2	
3013	101-86-0	alpha-Hexylcinnamaldehyde	Cysteine	%Dissociation(Cys)	%R/Rmax	**1.06**	1.28	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
2993	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2994	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2995	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2996	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2997	25		10% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2998	25		PBS	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
2999	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3000	25		10 % DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3001	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3002	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3003	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3004	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3005	25		PBS	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3006	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3007	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3008	25		PBS	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3009	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3010	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3011	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3012	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3013	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308

#	Comment
2993	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2994	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2995	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2996	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2997	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2998	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
2999	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3000	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3001	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3002	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3003	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3004	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3005	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3006	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3007	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3008	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3009	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3010	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3011	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3012	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3013	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution

#	Mechanism
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#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
3014	120-51-4	Benzyl benzoate	Cysteine	%Dissociation(Cys)	%R/Rmax	**-0.12**	0.13	
3015	5392-40-5	Citral	Cysteine	%Dissociation(Cys)	%R/Rmax	**0.22**	0.13	
3016	103-95-7	Cyclamen aldehyde	Cysteine	%Dissociation(Cys)	%R/Rmax	**0.04**	0.17	
3017	84-66-2	Diethyl phthalate	Cysteine	%Dissociation(Cys)	%R/Rmax	**-0.05**	0.35	
3018	97-53-0	Eugenol	Cysteine	%Dissociation(Cys)	%R/Rmax	**0.19**	0.71	
3019	111-30-8	Glutaraldehyde	Cysteine	%Dissociation(Cys)	%R/Rmax	**3.06**	2.27	
3020	107-75-5	Hydroxycitronellal	Cysteine	%Dissociation(Cys)	%R/Rmax	**-0.05**	0.16	
3021	97-54-1	Isoeugenol	Cysteine	%Dissociation(Cys)	%R/Rmax	**0.36**	0.52	
3022	80-54-6	Lilial	Cysteine	%Dissociation(Cys)	%R/Rmax	**0.08**	0.26	
3023	31906-04-4	Lyral	Cysteine	%Dissociation(Cys)	%R/Rmax	**-0.09**	0.01	
3024	106-51-4	p-Benzoquinone	Cysteine	%Dissociation(Cys)	%R/Rmax	**1.88**	1.95	
3025	122-78-1	Phenylacetaldehyde	Cysteine	%Dissociation(Cys)	%R/Rmax	**1.92**	2.77	
3026	2508-19-2	Trinitrobenzenesulfonic acid	Cysteine	%Dissociation(Cys)	%R/Rmax	**35.4**	54.77	
3027	2634-33-5	1.2-Benzisothiazolin-3-one	Lysine	%Association(Lys)	%R/Rmax	**1.05**	0.58	
3028	109-65-9	1-Bromobutane	Lysine	%Association(Lys)	%R/Rmax	**-0.9**	0.08	
3029	89-02-1	2.4-Dinitrobenzenesulfonic acid	Lysine	%Association(Lys)	%R/Rmax	**0.87**	0.31	
3030	119-84-6	3.4-Dihydrocoumarin	Lysine	%Association(Lys)	%R/Rmax	**1.3**	0.64	
3031	591-27-5	3-Aminophenol	Lysine	%Association(Lys)	%R/Rmax	**-2.45**	1.38	
3032	109-55-7	3-Dimethylaminopropylamine	Lysine	%Association(Lys)	%R/Rmax	**-8.37**	2.4	
3033	122-40-7	alpha-Amyl cinnamaldehyde	Lysine	%Association(Lys)	%R/Rmax	**25.51**	33.79	
3034	101-86-0	alpha-Hexylcinnamaldehyde	Lysine	%Association(Lys)	%R/Rmax	**22.03**	25.01	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
3014	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3015	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3016	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3017	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3018	25		10% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3019	25		PBS	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3020	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3021	25		10 % DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3022	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3023	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3024	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3025	25		5% DMSO	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3026	25		PBS	115 s (after End Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3027	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3028	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3029	25		PBS	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3030	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3031	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3032	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3033	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3034	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308

#	Comment
3014	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3015	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3016	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3017	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3018	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3019	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3020	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3021	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3022	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3023	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3024	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3025	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3026	Assay: Dissociation Phase, Late Stability; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3027	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3028	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3029	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3030	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3031	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3032	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3033	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3034	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution

#	Mechanism
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#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
3035	120-51-4	Benzyl benzoate	Lysine	%Association(Lys)	%R/Rmax	0.01	0.01	
3036	5392-40-5	Citral	Lysine	%Association(Lys)	%R/Rmax	4.44	3.05	
3037	103-95-7	Cyclamen aldehyde	Lysine	%Association(Lys)	%R/Rmax	0.22	0.03	
3038	84-66-2	Diethyl phthalate	Lysine	%Association(Lys)	%R/Rmax	-0.19	0.13	
3039	97-53-0	Eugenol	Lysine	%Association(Lys)	%R/Rmax	5.83	3.15	
3040	111-30-8	Glutaraldehyde	Lysine	%Association(Lys)	%R/Rmax	13.37	8.48	
3041	107-75-5	Hydroxycitronellal	Lysine	%Association(Lys)	%R/Rmax	0.02	0.04	
3042	97-54-1	Isoeugenol	Lysine	%Association(Lys)	%R/Rmax	9.6	2.98	
3043	80-54-6	Lilial	Lysine	%Association(Lys)	%R/Rmax	0.51	0.13	
3044	31906-04-4	Lyral	Lysine	%Association(Lys)	%R/Rmax	0.45	0.3	
3045	106-51-4	p-Benzoquinone	Lysine	%Association(Lys)	%R/Rmax	13.83	10.08	
3046	122-78-1	Phenylacetaldehyde	Lysine	%Association(Lys)	%R/Rmax	7.33	1.79	
3047	2508-19-2	Trinitrobenzenesulfonic acid	Lysine	%Association(Lys)	%R/Rmax	13.1	2.44	
3048	2634-33-5	1.2-Benzisothiazolin-3-one	Histidine	%Association(His)	%R/Rmax	1.21	ND	
3049	109-65-9	1-Bromobutane	Histidine	%Association(His)	%R/Rmax	-0.82	ND	
3050	89-02-1	2.4-Dinitrobenzenesulfonic acid	Histidine	%Association(His)	%R/Rmax	0.21	ND	
3051	119-84-6	3.4-Dihydrocoumarin	Histidine	%Association(His)	%R/Rmax	1.33	1.24	
3052	591-27-5	3-Aminophenol	Histidine	%Association(His)	%R/Rmax	0.24	ND	
3053	109-55-7	3-Dimethylaminopropylamine	Histidine	%Association(His)	%R/Rmax	-6.54	4.86	
3054	122-40-7	alpha-Amyl cinnamaldehyde	Histidine	%Association(His)	%R/Rmax	0.74	ND	
3055	101-86-0	alpha-Hexylcinnamaldehyde	Histidine	%Association(His)	%R/Rmax	1.03	ND	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
3035	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3036	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3037	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3038	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3039	25		10% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3040	25		PBS	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3041	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3042	25		10 % DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3043	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3044	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3045	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3046	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3047	25		PBS	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3048	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3049	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3050	25		PBS	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3051	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3052	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3053	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3054	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3055	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308

#	Comment
3035	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3036	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3037	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3038	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3039	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3040	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3041	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3042	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3043	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3044	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3045	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3046	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3047	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3048	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3049	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3050	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3051	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3052	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3053	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3054	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3055	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution

#	Mechanism
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#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
3056	120-51-4	Benzyl benzoate	Histidine	%Association(His)	%R/Rmax	0.03	0.08	
3057	5392-40-5	Citral	Histidine	%Association(His)	%R/Rmax	1.07	0.9	
3058	103-95-7	Cyclamen aldehyde	Histidine	%Association(His)	%R/Rmax	-0.18	0.61	
3059	84-66-2	Diethyl phthalate	Histidine	%Association(His)	%R/Rmax	-0.07	0.02	
3060	97-53-0	Eugenol	Histidine	%Association(His)	%R/Rmax	3.98	ND	
3061	111-30-8	Glutaraldehyde	Histidine	%Association(His)	%R/Rmax	-1	ND	
3062	107-75-5	Hydroxycitronellal	Histidine	%Association(His)	%R/Rmax	0.21	ND	
3063	97-54-1	Isoeugenol	Histidine	%Association(His)	%R/Rmax	5.24	ND	
3064	80-54-6	Lilial	Histidine	%Association(His)	%R/Rmax	-0.66	0.37	
3065	31906-04-4	Lyral	Histidine	%Association(His)	%R/Rmax	0.4	0.19	
3066	106-51-4	p-Benzoquinone	Histidine	%Association(His)	%R/Rmax	5.51	3.41	
3067	122-78-1	Phenylacetaldehyde	Histidine	%Association(His)	%R/Rmax	2.02	0.05	
3068	2508-19-2	Trinitrobenzenesulfonic acid	Histidine	%Association(His)	%R/Rmax	24.24	ND	
3069	2634-33-5	1.2-Benzisothiazolin-3-one	Cysteine	%Association(Cys)	%R/Rmax	7.67	3.34	
3070	109-65-9	1-Bromobutane	Cysteine	%Association(Cys)	%R/Rmax	-0.58	0.76	
3071	89-02-1	2.4-Dinitrobenzenesulfonic acid	Cysteine	%Association(Cys)	%R/Rmax	2.09	1.53	
3072	119-84-6	3.4-Dihydrocoumarin	Cysteine	%Association(Cys)	%R/Rmax	2.3	0.41	
3073	591-27-5	3-Aminophenol	Cysteine	%Association(Cys)	%R/Rmax	6.02	4.92	
3074	109-55-7	3-Dimethylaminopropylamine	Cysteine	%Association(Cys)	%R/Rmax	8.85	2.48	
3075	122-40-7	alpha-Amyl cinnamaldehyde	Cysteine	%Association(Cys)	%R/Rmax	1.39	0.93	
3076	101-86-0	alpha-Hexylcinnamaldehyde	Cysteine	%Association(Cys)	%R/Rmax	6.21	2.07	

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
3056	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3057	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3058	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3059	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3060	25		10% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3061	25		PBS	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3062	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3063	25		10 % DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3064	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3065	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3066	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3067	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3068	25		PBS	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3069	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3070	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3071	25		PBS	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3072	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3073	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3074	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3075	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3076	25		5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308

#	Comment
3056	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3057	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3058	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3059	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3060	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3061	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3062	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3063	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3064	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3065	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3066	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3067	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3068	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3069	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3070	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3071	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3072	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3073	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3074	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3075	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3076	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution

#	Mechanism
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#	CAS	Electrophile (El)	Nucleophile (Nu)	Parameter	Unit	Value	Error	log(Val)
3077	120-51-4	Benzyl benzoate	Cysteine	%Association(Cys)	%R/Rmax	**0.43**	0.57	
3078	5392-40-5	Citral	Cysteine	%Association(Cys)	%R/Rmax	**1.58**	0.09	
3079	103-95-7	Cyclamen aldehyde	Cysteine	%Association(Cys)	%R/Rmax	**1.79**	0.19	
3080	84-66-2	Diethyl phthalate	Cysteine	%Association(Cys)	%R/Rmax	**-0.2**	0.47	
3081	97-53-0	Eugenol	Cysteine	%Association(Cys)	%R/Rmax	**3.25**	0.84	
3082	111-30-8	Glutaraldehyde	Cysteine	%Association(Cys)	%R/Rmax	**2.19**	0.79	
3083	107-75-5	Hydroxycitronellal	Cysteine	%Association(Cys)	%R/Rmax	**0.46**	0.3	
3084	97-54-1	Isoeugenol	Cysteine	%Association(Cys)	%R/Rmax	**5.48**	0.79	
3085	80-54-6	Lilial	Cysteine	%Association(Cys)	%R/Rmax	**1.92**	0.87	
3086	31906-04-4	Lyral	Cysteine	%Association(Cys)	%R/Rmax	**1.16**	0.17	
3087	106-51-4	p-Benzoquinone	Cysteine	%Association(Cys)	%R/Rmax	**4.72**	2.65	
3088	122-78-1	Phenylacetaldehyde	Cysteine	%Association(Cys)	%R/Rmax	**9.94**	4.22	
3089	2508-19-2	Trinitrobenzenesulfonic acid	Cysteine	%Association(Cys)	%R/Rmax	**30**	60.82	

PBS = Aqueous phosphate buffer solution (other abbreviations are explained in the main document).
CAS numbers are given for guidance only, individual experiments may have been performed with equivalent compounds, but deviating CAS numbers.

#	T/°C	pH	Solvent	Time	Ratio Nu:El	Reference
3077	25	5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3078	25	5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3079	25	5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3080	25	5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3081	25	10% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3082	25	PBS	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3083	25	5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3084	25	10 % DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3085	25	5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3086	25	5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3087	25	5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3088	25	5% DMSO	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308
3089	25	PBS	50 s (after Init. Inj.)	Nu immob.	Achilleos C et al., Toxicol. Vitro 23 (2009), 308

#	Comment
3077	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3078	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3079	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3080	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3081	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3082	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3083	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3084	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3085	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3086	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3087	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3088	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution
3089	Assay: Association Phase, Late Binding; SPR (Surface plasmon resonance), immobilized peptide, analyte in solution

#	Mechanism
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