

Supporting Information for:

Hierarchical Bayesian Approach To Reduce Uncertainty in the Aquatic Effect Assessment of Realistic Chemical Mixtures

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A. Toxicity data for the 13 APIs in the mixture

Table S1. EC50 data for mixture of 13 APIs.

Chemical	Species	Endpoint	C (mg/L)	Reference
5-Fluorouracil	Daphnia magna	immobilisation	15	Zoumková et al. (1)
5-Fluorouracil	Daphnia magna	immobilisation	36	Zoumková et al. (1)
5-Fluorouracil	Daphnia magna	reproduction	0.1	Zoumková et al. (1)
5-Fluorouracil	Desmodesmus subspicatus	growth	48	Zoumková et al. (1)
5-Fluorouracil	Pimephales promelas	growth	400	DeYoung et al. (2)
5-Fluorouracil	Pimephales promelas	mortality	2420	DeYoung et al. (2)
5-Fluorouracil	Pseudokirchneriella subcapitata	growth	0.11	Zoumková et al. (1)
5-Fluorouracil	Pseudomonas putida	growth	0.027	Zoumková et al. (1)
5-Fluorouracil	Pseudomonas putida	growth	0.044	Zoumková et al. (1)
5-Fluorouracil	Vibrio fischeri	luminescence	0.122	Backhaus and Grimme (3)
5-Fluorouracil	Xenopus laevis	growth	0.000015	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	growth	0.000039	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	growth	0.000052	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	growth	0.000058	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	growth	0.00006	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	growth	0.000063	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	growth	0.000069	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	growth	0.00008	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	growth	0.000089	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	growth	0.00009	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	growth	0.000092	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	growth	0.0001	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	growth	0.00011	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	growth	0.00012	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	growth	0.000126	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	growth	0.000132	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	growth	0.00014	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	growth	0.000141	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	growth	0.00018	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	growth	80	DeYoung et al. (2)
5-Fluorouracil	Xenopus laevis	mortality	0.00031	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	mortality	0.00041	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	mortality	0.00045	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	mortality	0.0005	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	mortality	0.00054	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	mortality	0.00065	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	mortality	0.00092	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	mortality	0.00095	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	mortality	0.00095	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	mortality	0.00126	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	mortality	0.00126	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	mortality	0.00127	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	mortality	0.00128	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	mortality	0.0014	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	mortality	0.00148	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	mortality	0.00151	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	mortality	0.00158	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	mortality	0.00173	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	mortality	0.00178	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	mortality	0.00179	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	mortality	0.00213	Gaudet-Hull et al. (4)
5-Fluorouracil	Xenopus laevis	mortality	530	DeYoung et al. (2)
Cefuroxime	Oncorhynchus mykiss	unknown	100	FASS (5)
Cefuroxime	Pseudomonas putida	growth	0.389	Kümmerer (6)
Chlortetracycline	Daphnia magna	immobilisation	225	Park and Choi (7)
Chlortetracycline	Daphnia magna	immobilisation	380	Park and Choi (7)
Chlortetracycline	Daphnia magna	immobilisation	193.6	Kim et al. (8)
Chlortetracycline	Daphnia magna	immobilisation	321.6	Kim et al. (8)
Chlortetracycline	Daphnia magna	immobilisation	328.4	Kim et al. (8)
Chlortetracycline	Daphnia magna	immobilisation	391.8	Kim et al. (8)
Chlortetracycline	Daphnia magna	immobilisation	111.2	Kim et al. (8)
Chlortetracycline	Daphnia magna	immobilisation	132.5	Kim et al. (8)
Chlortetracycline	Daphnia magna	immobilisation	198.4	Kim et al. (8)
Chlortetracycline	Daphnia magna	immobilisation	288	Kim et al. (8)
Chlortetracycline	Daphnia magna	morphological changes	128	Muller (9)
Chlortetracycline	Daphnia magna	morphological changes	88	Muller (9)
Chlortetracycline	Lemna gibba	carotenoids conc.	1.62	Brain et al. (10)
Chlortetracycline	Lemna gibba	chlorophyll A conc.	0.63	Brain et al. (10)

Chlortetracycline	Lemna gibba	chlorophyll B conc.	0.65	Brain et al. (10)
Chlortetracycline	Lemna gibba	growth	0.219	Brain et al. (10)
Chlortetracycline	Lemna gibba	reproduction	0.318	Brain et al. (10)
Chlortetracycline	Microcystis aeruginosa	growth	0.05	Halling-Sørensen (11)
Chlortetracycline	Moina macrocopa	mortality	515	Park and Choi (7)
Chlortetracycline	Moina macrocopa	mortality	272	Park and Choi (7)
Chlortetracycline	Oryzias latipes	mortality	88.4	Park and Choi (7)
Chlortetracycline	Oryzias latipes	mortality	78.9	Park and Choi (7)
Chlortetracycline	Plasmodium falciparum	protein content	0.36	Divo et al. (12)
Chlortetracycline	Plasmodium falciparum	protein content	3.69	Divo et al. (12)
Chlortetracycline	Plasmodium falciparum	protein content	12.45	Divo et al. (12)
Chlortetracycline	Plasmodium falciparum	protein content	15.80	Divo et al. (12)
Chlortetracycline	Plasmodium falciparum	protein synthesis	0.000000026	Divo et al. (12)
Chlortetracycline	Plasmodium falciparum	protein synthesis	0.000000033	Divo et al. (12)
Chlortetracycline	Pseudokirchneriella subcapitata	growth	1.8	Yang et al. (13)
Chlortetracycline	Pseudokirchneriella subcapitata	growth	3.1	Halling-Sørensen (11)
Chlortetracycline	Pseudomonas putida	growth	0.241	Kümmerer (6)
Chlortetracycline	Vibrio fischeri	luminescence	13	Park and Choi (7)
Ciprofloxacin	Daphnia magna	immobilisation	1.1	Kim et al. (8)
Ciprofloxacin	Daphnia magna	immobilisation	1.2	Kim et al. (8)
Ciprofloxacin	Daphnia magna	immobilisation	1.3	Kim et al. (8)
Ciprofloxacin	Daphnia magna	mortality	65.3	Martins et al. (2012)
Ciprofloxacin	Daphnia magna	reproduction	12.8	Martins et al. (2012)
Ciprofloxacin	Lemna gibba	carotenoids conc.	1.762	Brain et al. (10)
Ciprofloxacin	Lemna gibba	chlorophyll A conc.	1.279	Brain et al. (10)
Ciprofloxacin	Lemna gibba	chlorophyll B conc.	0.992	Brain et al. (10)
Ciprofloxacin	Lemna gibba	growth	0.697	Brain et al. (10)
Ciprofloxacin	Lemna minor	growth	3.75	Martins et al. (14)
Ciprofloxacin	Lemna minor	reproduction	0.203	Robinson et al. (15)
Ciprofloxacin	Microcystis aeruginosa	growth	0.017	Robinson et al. (15)
Ciprofloxacin	Microcystis aeruginosa	growth	0.005	Halling-Sørensen et al. (16)
Ciprofloxacin	Pseudokirchneriella subcapitata	growth	18.7	Robinson et al. (15)
Ciprofloxacin	Pseudokirchneriella subcapitata	growth	6.7	Yang et al. (13)
Ciprofloxacin	Pseudokirchneriella subcapitata	growth	4.83	Martins et al. (14)
Ciprofloxacin	Pseudokirchneriella subcapitata	growth	3	Golet et al. (17)
Ciprofloxacin	Pseudokirchneriella subcapitata	growth	2.97	Halling-Sørensen et al. (16)
Ciprofloxacin	Pseudomonas putida	growth	0.08	Kümmerer et al. (18)
Ciprofloxacin	Sludge bacteria	growth	0.61	Halling-Sørensen et al. (16)
Ciprofloxacin	Vibrio fischeri	mortality	11.5	Martins et al. (14)
Cyclophosphamide	Danio rerio	development	1227	Weigt et al. (19)
Cyclophosphamide	Danio rerio	mortality	2193	Weigt et al. (19)
Cyclophosphamide	Pseudokirchneriella subcapitata	growth	930	Zouneková et al. (1)
Erythromycin	Anabaena cylindrica	growth	0.035	Ando et al. (20)
Erythromycin	Anabaena flos-aquae	growth	0.27	Ando et al. (20)
Erythromycin	Anabaena variabilis	growth	0.43	Ando et al. (20)
Erythromycin	Anabaena sp.	growth	0.022	González-Pleiter et al. (21)
Erythromycin	Ankistrodesmus falcatus	mortality	10	El-Bassat et al. (22)
Erythromycin	Brachionus calyciflorus	growth	0.94	Isidori et al. (23)
Erythromycin	Brachionus calyciflorus	mortality	27.53	Isidori et al. (23)
Erythromycin	Brachionus calyciflorus	mortality	28	El-Bassat et al. (22)
Erythromycin	Ceriodaphnia dubia	abundance	0.22	Isidori et al. (23)
Erythromycin	Ceriodaphnia dubia	immobilisation	10.23	Isidori et al. (23)
Erythromycin	Chlorella pyrenoidosa	unknown	2	NCCOS (24)
Erythromycin	Chlorella vulgaris	growth	33.8	Eguchi et al. (25)
Erythromycin	Chlorella vulgaris	mortality	12	El-Bassat et al. (22)
Erythromycin	Daphnia longispina	mortality	24	El-Bassat et al. (22)
Erythromycin	Daphnia magna	mortality	22.45	Isidori et al. (23)
Erythromycin	Daphnia magna	mortality	207.83	Ji et al. (26)
Erythromycin	Daphnia magna	mortality	210.57	di Delupis et al. (27)
Erythromycin	Daphnia magna	mortality	387.7	di Delupis et al. (27)
Erythromycin	Lemna minor	growth	5.62	Pomati et al. (28)
Erythromycin	Litopenaeus vannamei	mortality	29.2	Williams et al. (29)
Erythromycin	Litopenaeus vannamei	mortality	22.7	Williams et al. (29)
Erythromycin	Litopenaeus vannamei	mortality	37.7	Williams et al. (29)
Erythromycin	Litopenaeus vannamei	mortality	49.8	Williams et al. (29)
Erythromycin	Litopenaeus vannamei	mortality	30.8	Williams et al. (29)
Erythromycin	Litopenaeus vannamei	mortality	85	Williams et al. (29)
Erythromycin	Litopenaeus vannamei	unknown	0.0377	NCCOS (24)
Erythromycin	Litopenaeus vannamei	unknown	0.0498	NCCOS (24)
Erythromycin	Microcystis aeruginosa	abundance	0.023	Ando et al. (20)
Erythromycin	Microcystis wesenbergii	abundance	0.023	Ando et al. (20)
Erythromycin	Moina macrocopa	immobilisation	135.52	Ji et al. (26)
Erythromycin	Morone saxatilis	mortality	349	Williams et al. (29)
Erythromycin	Nostoc sp.	abundance	0.2	Ando et al. (20)
Erythromycin	Paramecium caudatum	mortality	16	El-Bassat et al. (22)

Erythromycin	Pseudokirchneriella subcapitata	abundance	0.02	Isidori et al. (23)
Erythromycin	Pseudokirchneriella subcapitata	growth	0.13	Christensen et al. (30)
Erythromycin	Pseudokirchneriella subcapitata	growth	0.15	Christensen et al. (30)
Erythromycin	Pseudokirchneriella subcapitata	growth	0.19	Christensen et al. (30)
Erythromycin	Pseudokirchneriella subcapitata	growth	0.24	Christensen et al. (30)
Erythromycin	Pseudokirchneriella subcapitata	growth	0.35	González-Pleiter et al. (21)
Erythromycin	Pseudokirchneriella subcapitata	growth	0.0366	Eguchi et al. (25)
Erythromycin	Pseudomonas putida	growth	0.054	Kümmerer (6)
Erythromycin	Salvelinus namaycush	mortality	410	Marking et al. (31)
Erythromycin	Salvelinus namaycush	mortality	818	Marking et al. (31)
Erythromycin	Synechococcus leopoliensis	growth	0.16	Ando et al. (20)
Erythromycin	Synechococcus sp.	growth	0.23	Ando et al. (20)
Erythromycin	Thamnocephalus platyurus	mortality	17.68	Isidori et al. (23)
Levofloxacin	aerobic bacteria	respiration	10	Kümmerer et al. (32)
Levofloxacin	aerobic bacteria	respiration	1	Kümmerer et al. (32)
Levofloxacin	Anabaena sp.	growth	4.8	González-Pleiter et al. (21)
Levofloxacin	Lemna gibba	reproduction	0.194	Brain et al. (10)
Levofloxacin	Lemna gibba	carotenoids conc.	1.413	Brain et al. (10)
Levofloxacin	Lemna gibba	chlorophyll A conc.	0.942	Brain et al. (10)
Levofloxacin	Lemna gibba	chlorophyll B conc.	0.473	Brain et al. (10)
Levofloxacin	Lemna gibba	growth	0.185	Brain et al. (10)
Levofloxacin	Lemna minor	reproduction	0.051	Robinson et al. (15)
Levofloxacin	Microcystis aeruginosa	chlorophyll A conc.	0.0079	Robinson et al. (15)
Levofloxacin	Pseudokirchneriella subcapitata	chlorophyll A conc.	7.4	Robinson et al. (15)
Methotrexate	Danio rerio	mortality	85	Henschel et al. (33)
Methotrexate	Danio rerio	pulse rate	142	Henschel et al. (33)
Methotrexate	Scenedesmus subspicatus	growth	260	Henschel et al. (33)
Methotrexate	Tetrahymena pyriformis	growth	45	Henschel et al. (33)
Methotrexate	Vibrio fischeri	luminescence	1220	Henschel et al. (33)
Methotrexate	Xenopus laevis	growth	546	Gaudet-Hull et al. (4)
Ofloxacin	Brachionus calyciflorus	growth	0.53	Isidori et al. (23)
Ofloxacin	Brachionus calyciflorus	mortality	29.88	Isidori et al. (23)
Ofloxacin	Ceriodaphnia dubia	growth	3.13	Isidori et al. (23)
Ofloxacin	Ceriodaphnia dubia	immobilisation	17.41	Isidori et al. (23)
Ofloxacin	Ceriodaphnia dubia	mortality	26.7	Ferrari et al. (34)
Ofloxacin	Cyclotella meneghiniana	growth	0.0906	Ferrari et al. (34)
Ofloxacin	Daphnia magna	immobilisation	31.75	Isidori et al. (23)
Ofloxacin	Daphnia magna	mortality	76.58	Ferrari et al. (34)
Ofloxacin	Lemna gibba	carotenoids conc.	1.374	Brain et al. (10)
Ofloxacin	Lemna gibba	chlorophyll A conc.	0.989	Brain et al. (10)
Ofloxacin	Lemna gibba	chlorophyll B conc.	0.84	Brain et al. (10)
Ofloxacin	Lemna gibba	growth	0.532	Brain et al. (10)
Ofloxacin	Lemna minor	reproduction	0.653	Robinson et al. (15)
Ofloxacin	Lemna minor	abundance	0.126	Robinson et al. (15)
Ofloxacin	Microcystis aeruginosa	chlorophyll A conc.	0.021	Robinson et al. (15)
Ofloxacin	Pseudokirchneriella subcapitata	chlorophyll A conc.	12.1	Robinson et al. (15)
Ofloxacin	Pseudokirchneriella subcapitata	growth	4.74	Ferrari et al. (34)
Ofloxacin	Pseudokirchneriella subcapitata	growth	1.44	Isidori et al. (23)
Ofloxacin	Pseudokirchneriella subcapitata	reproduction	4.7	REMPHARMAWATER report
Ofloxacin	Pseudomonas putida	growth	0.01	Ayscough (35)
Ofloxacin	Pseudomonas putida	growth	0.265	Kümmerer (6)
Ofloxacin	Scenedesmus vacuolatus	unknown	82.8	Backhaus et al. (36)
Ofloxacin	Synechococcus leopolensis	growth	0.016	Ferrari et al. (34)
Ofloxacin	Thamnocephalus platyurus	mortality	33.98	Isidori et al. (23)
Ofloxacin	Vibrio fischeri	luminescence	0.0135	Ferrari et al. (34)
Ofloxacin	Vibrio fischeri	luminescence	0.01359	Backhaus and Grimme (3)
Ofloxacin	Vibrio fischeri	luminescence	90	Backhaus et al. (37)
Oxytetracycline	Artemia franchiscana	mortality	540.5	Sahul Hameed and Balasubramanian (38)
Oxytetracycline	Brachionus calyciflorus	growth	1.87	Isidori et al. (23)
Oxytetracycline	Brachionus calyciflorus	mortality	34.21	Isidori et al. (23)
Oxytetracycline	Brachionus koreanus	mortality	300	Rhee et al. (39)
Oxytetracycline	Ceratophyllum demersum	morphological changes	0.2976	Hanson et al. (40)
Oxytetracycline	Ceriodaphnia dubia	growth	0.18	Isidori et al. (23)
Oxytetracycline	Ceriodaphnia dubia	mortality	18.65	Isidori et al. (23)
Oxytetracycline	Chlorella vulgaris	growth	7.05	Eguchi et al. (25)
Oxytetracycline	Chlorella vulgaris	growth	6.4	Pro et al. (41)
Oxytetracycline	Daphnia magna	mortality	831.6	Park and Choi (7)
Oxytetracycline	Daphnia magna	mortality	621.2	Park and Choi (7)
Oxytetracycline	Daphnia magna	mortality	22.64	Isidori et al. (23)
Oxytetracycline	Daphnia magna	reproduction	46.2	Wollenberger et al. (42)
Oxytetracycline	Egeria densa	growth	0.2746	Hanson et al. (40)
Oxytetracycline	Egeria densa	growth	0.2804	Hanson et al. (40)
Oxytetracycline	Egeria densa	growth	0.2396	Hanson et al. (40)
Oxytetracycline	Egeria densa	growth	0.2823	Hanson et al. (40)
Oxytetracycline	Egeria densa	growth	0.3324	Hanson et al. (40)

Oxytetracycline	Egeria densa	growth	0.3104	Hanson et al. (40)
Oxytetracycline	Egeria densa	growth	0.403	Hanson et al. (40)
Oxytetracycline	Hydra attenuata	morphological changes	40.13	Quinn et al. (43)
Oxytetracycline	Lemna gibba	chlorophyll A conc.	1.179	Brain et al. (10)
Oxytetracycline	Lemna gibba	chlorophyll B conc.	1.152	Brain et al. (10)
Oxytetracycline	Lemna gibba	growth	1.01	Brain et al. (10)
Oxytetracycline	Lemna gibba	reproduction	1.401	Brain et al. (10)
Oxytetracycline	Lemna minor	reproduction	4.92	Pro et al. (41)
Oxytetracycline	Litopenaeus vannamei	mortality	214.1	Williams et al. (29)
Oxytetracycline	Litopenaeus vannamei	mortality	61.1	Williams et al. (29)
Oxytetracycline	Litopenaeus vannamei	mortality	135.7	Williams et al. (29)
Oxytetracycline	Litopenaeus vannamei	mortality	238.4	Williams et al. (29)
Oxytetracycline	Litopenaeus vannamei	unknown	0.0616	NCCOS (24)
Oxytetracycline	Microcystis aeruginosa	growth	0.207	Holten Lützhøft et al. (44)
Oxytetracycline	Microcystis aeruginosa	photosynthesis inhibition	5.4	van der Grinten et al. (45)
Oxytetracycline	Moina macrocopa	mortality	137.1	Park and Choi (7)
Oxytetracycline	Moina macrocopa	mortality	126.7	Park and Choi (7)
Oxytetracycline	Morone saxatilis	mortality	150	Hughes (46)
Oxytetracycline	Morone saxatilis	mortality	125	Hughes (46)
Oxytetracycline	Morone saxatilis	mortality	100	Hughes (46)
Oxytetracycline	Morone saxatilis	mortality	75	Hughes (46)
Oxytetracycline	Morone saxatilis	unknown	62.5	NCCOS (24)
Oxytetracycline	Oryzias latipes	mortality	110.1	Park and Choi (7)
Oxytetracycline	Oryzias latipes	mortality	215.4	Park and Choi (7)
Oxytetracycline	Plasmodium falciparum	protein content	0.1580304	Divo et al. (12)
Oxytetracycline	Plasmodium falciparum	protein content	1.340864	Divo et al. (12)
Oxytetracycline	Plasmodium falciparum	protein content	15.32416	Divo et al. (12)
Oxytetracycline	Plasmodium falciparum	protein content	18.67632	Divo et al. (12)
Oxytetracycline	Plasmodium falciparum	protein synthesis	0.000000032	Divo et al. (12)
Oxytetracycline	Plasmodium falciparum	protein synthesis	0.000000039	Divo et al. (12)
Oxytetracycline	Pseudokirchneriella subcapitata	abundance	0.17	Isidori et al. (23)
Oxytetracycline	Pseudokirchneriella subcapitata	growth	4.18	De Liguoro et al. (47)
Oxytetracycline	Pseudokirchneriella subcapitata	growth	4.5	Holten Lützhøft et al. (44)
Oxytetracycline	Pseudokirchneriella subcapitata	growth	0.342	Eguchi et al. (25)
Oxytetracycline	Pseudokirchneriella subcapitata	growth	1.3	Christensen et al. (30)
Oxytetracycline	Pseudokirchneriella subcapitata	growth	1.4	Christensen et al. (30)
Oxytetracycline	Pseudokirchneriella subcapitata	growth	2	Christensen et al. (30)
Oxytetracycline	Pseudokirchneriella subcapitata	growth	0.47	Christensen et al. (30)
Oxytetracycline	Pseudokirchneriella subcapitata	unknown	5	NCCOS (24)
Oxytetracycline	Pseudokirchneriella subcapitata	photosynthesis inhibition	0.6	van der Grinten et al. (45)
Oxytetracycline	Rhodomonas salina	growth	1.6	Holten Lützhøft et al. (44)
Oxytetracycline	Rhodomonas salina	unknown	1.7	NCCOS (24)
Oxytetracycline	Salvelinus namaycush	mortality	341	Marking et al. (31)
Oxytetracycline	Salvelinus namaycush	mortality	251	Marking et al. (31)
Oxytetracycline	Salvelinus namaycush	mortality	840	Marking et al. (31)
Oxytetracycline	Thamnocephalus platyurus	mortality	25	Isidori et al. (23)
Oxytetracycline	Vibrio fischeri	luminescence	64.5	Isidori et al. (23)
Oxytetracycline	Vibrio fischeri	luminescence	87	Park and Choi (7)
Oxytetracycline	Vibrio fischeri	luminescence	235.4	Park and Choi (7)
Oxytetracycline	Vibrio fischeri	luminescence	121.01	Lalumera et al. (48)
Tamoxifen	Acartia tonsa	reproduction	0.049	Andersen et al. (49)
Tamoxifen	Lepomis macrochirus	mortality	0.23	Brixham ELR BL5483
Tamoxifen	Oncorhynchus mykiss	mortality	0.41	Brixham ELR BL5482
Tamoxifen	Oncorhynchus mykiss	mortality	0.32	Brixham ELR BL3656
Tamoxifen	Pseudokirchneriella subcapitata	growth	0.0092	AstraZeneca (50)
Tamoxifen	Strongylocentrotus purpuratus	development	0.00005	Roepke et al. (51)
Tetracycline	Anabaena sp.	growth	6.2	González-Pleiter et al. (21)
Tetracycline	Artemia salina	mortality	10	Metcalf et al. (52)
Tetracycline	Crassostrea gigas	mortality	550	Cardwell et al. (53)
Tetracycline	Crassostrea gigas	reproduction	85	Cardwell et al. (53)
Tetracycline	Daphnia magna	mortality	11	FASS (5)
Tetracycline	Daphnia magna	reproduction	44.8	Wollenberger et al. (42)
Tetracycline	Lemna gibba	chlorophyll A conc.	2.592	Brain et al. (10)
Tetracycline	Lemna gibba	chlorophyll B conc.	4.569	Brain et al. (10)
Tetracycline	Lemna gibba	growth	0.723	Brain et al. (10)
Tetracycline	Lemna gibba	reproduction	1.114	Brain et al. (10)
Tetracycline	Lemna minor	growth	1.06	Pomati et al. (28)
Tetracycline	Microcystis aeruginosa	chlorophyll conc.	0.09	Halling-Sørensen et al. (16)
Tetracycline	Pseudokirchneriella subcapitata	growth	1	Yang et al. (13)
Tetracycline	Pseudokirchneriella subcapitata	unknown	0.31	FASS (5)
Tetracycline	Pseudokirchneriella subcapitata	chlorophyll conc.	2.2	Halling-Sørensen et al. (16)
Tetracycline	Pseudokirchneriella subcapitata	growth	3.31	González-Pleiter et al. (21)
Tetracycline	Pseudomonas putida	growth	0.322	Kümmerer (6)
Tetracycline	Salvelinus namaycush	mortality	279	Marking et al. (31)
Tetracycline	Salvelinus namaycush	mortality	475.7	Marking et al. (31)

Tetracycline	Salvelinus namaycush	mortality	800	Marking et al. (31)
Tetracycline	Salvelinus namaycush	mortality	220	Marking et al. (31)
Tetracycline	Vibrio fischeri	luminescence	0.0251	Backhaus and Grimme (3)
Tetracycline	Vibrio fischeri	luminescence	19.6	Backhaus et al. (54)
Tetracycline	Vibrio fischeri	luminescence	19.9	Backhaus et al. (54)
Tetracycline	Vibrio fischeri	luminescence	0.0241	Backhaus et al. (54)
Trimethoprim	Anabaena variabilis	abundance	11	Ando et al. (20)
Trimethoprim	Brachionus koreanus	mortality	189.5	Rhee et al. (39)
Trimethoprim	Danio rerio	unknown	123	FASS (5)
Trimethoprim	Danio rerio	unknown	100	NCCOS (24)
Trimethoprim	Daphnia magna	unknown	120	FASS (5)
Trimethoprim	Daphnia magna	unknown	123	Halling-Sørensen et al. (16)
Trimethoprim	Daphnia magna	immobilisation	120.7	Kim et al. (55)
Trimethoprim	Daphnia magna	immobilisation	167.4	Kim et al. (55)
Trimethoprim	Daphnia magna	immobilisation	92	Park and Choi (7)
Trimethoprim	Daphnia magna	immobilisation	155.6	Park and Choi (7)
Trimethoprim	Daphnia magna	immobilisation	149	De Liguoro et al. (56)
Trimethoprim	Microcystis aeruginosa	chlorophyll A conc.	112	Holten Lützhøft et al. (44)
Trimethoprim	Microcystis aeruginosa	growth	112	Halling-Sørensen et al. (16)
Trimethoprim	Microcystis aeruginosa	photosynthesis inhibition	6.9	van der Grinten et al. (45)
Trimethoprim	Microcystis aeruginosa	abundance	150	Ando et al. (20)
Trimethoprim	Moina macrocopa	immobilisation	54.8	Park and Choi (7)
Trimethoprim	Moina macrocopa	immobilisation	144.8	Park and Choi (7)
Trimethoprim	Nostoc sp.	growth	53	Ando et al. (20)
Trimethoprim	Pseudokirchneriella subcapitata	growth	40	Yang et al. (13)
Trimethoprim	Pseudokirchneriella subcapitata	growth	130	Holten Lützhøft et al. (44)
Trimethoprim	Pseudokirchneriella subcapitata	growth	80.3	Eguchi et al. (25)
Trimethoprim	Pseudokirchneriella subcapitata	growth	110	Halling-Sørensen et al. (16)
Trimethoprim	Pseudokirchneriella subcapitata	unknown	70	FASS (5)
Trimethoprim	Pseudomonas putida	growth	0.19	Kümmerer (6)
Trimethoprim	Rhodomonas salina	growth	16	Holten Lützhøft et al. (44)
Trimethoprim	Scenedesmus capricornutum	growth	110	FASS (5)
Trimethoprim	Sludge bacteria	growth	17.8	Halling-Sørensen et al. (16)
Trimethoprim	Vibrio fischeri	luminescence	176.7	Kim et al. (55)
Trimethoprim	Vibrio fischeri	luminescence	165.1	Kim et al. (55)

B. Toxicity data for the chemicals included in the chemical inventory

Table S2. Chemicals included in chemical inventory.

CAS RN	Name	$\bar{X}$ logEC50	SlogEC50	n _{species}	class
56840610	((3-Nitrophenyl)hydrazono)propanedioic acid	5.18E-02	7.22E-02	4	1
67564914	(+)-cis-4-[3-(4-tert-butylphenyl)-2-methylpropyl]-2,6-dimethylmorpholine	5.85E-01	5.84E-02	6	1
319868	(1alpha,2alpha,3alpha,4beta,5alpha,6beta)-1,2,3,4,5,6-hexachlorocyclohexane	9.54E-02	9.75E-01	7	1
319857	(1alpha,2beta,3alpha,4beta,5alpha,6beta)-1,2,3,4,5,6-hexachlorocyclohexane	2.25E-01	2.00E-02	3	1
465736	(1alpha,4alpha,4beta,5beta,8beta,8alpha)-1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-1,4:5,8-dimethanonaphthalene	-2.07E+00	4.53E-02	2	1
22431625	(1R-trans)-3-(Cyclopentylidenemethyl)-2,2-dimethyl-cyclopropanecarboxylic acid, (5-Phenylmethyl)-3-furanyl)methyl ester	-3.27E+00	1.60E+00	18	1
3084626	(2,4,5-Trichlorophenoxy)acetic acid, 2-Butoxypropyl ester	-3.94E-02	1.24E+00	3	1
3966118	(2,4-Dichlorophenoxy)acetic acid 2-butoxy-1-methylethyl ester	2.22E-01	1.25E-01	4	1
4834495	(2,4-Dichlorophenoxy)acetic acid compd with N-9-octadecenyl-1,3-propanediamine (2:1)	-2.48E-01	3.69E-02	2	1
8015358	(2,4-Dichlorophenoxy)acetic acid, Mixt. with (2,4,5-Trichlorophenoxy) acetic acid	-8.98E-02	2.12E-01	4	1
7166190	(2-bromo-2-nitrovinyl)benzene	-4.90E-01	6.59E-01	3	1
2698411	(2-chlorobenzylidene)malononitrile	7.85E-01	6.02E-01	4	1
951428	(2-endo,5-exo)-5-Chloro-6-(((methylamino)carbonyl)oxy)imino)bicyclo(2.2.1)heptane-2-carbonitrile	9.59E-01	1.06E-01	2	1
83794	(2R,6aS,12aS)-1,2,6,6a,12,12a-hexahydro-2-isopropenyl-8,9-dimethoxychromeno[3,4-b]furo[2,3-h]chromen-6-one	-6.11E-01	1.10E+00	68	1
18530568	(3alpha,4alpha,5alpha,7alpha,7aalpha)-1,1-dimethyl-3-(octahydro-4,7-methano-1H-inden-5-yl)urea	1.12E+00	3.47E-01	4	1
80330332	(3-Phenoxyphenyl)methyl ester, 3-(2,2-Dichloroethenyl)-2,2-dimethylcyclopropane carboxylic acid mixt. with 5-[[[2-(2-butoxyethoxy)ethoxy]methyl]-6-propyl-1,3-benzodioxole	-2.71E+00	4.33E-01	4	1
63821863	(4-Chloro-2-methylphenoxy)acetic acid sodium salt mxt with 6-Chloro-N,N-diethyl-1,3,5-triazine-2,4-diamine and N-(1,1-di	1.30E+00	7.72E-02	3	1
1.41E+08	(5-Cyclopropyl-4-isoxazolyl)[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl]methanone	-7.03E-01	1.71E+00	3	1
102998	(Acetato)-3-pyridyl mercury	9.26E-01	5.74E-02	6	1
21564170	(benzothiazol-2-ylthio)methyl thiocyanate	-1.94E+00	5.50E-01	5	1
19902046	(E,E)-2-(bis(3,7-Dimethyl-2,6-octadienyl)amino)ethanol	-1.25E-01	4.24E-01	27	1
96093	(epoxyethyl)benzene	1.21E+00	6.51E-02	3	1
12054852	(NH4)6Mo7O24.4H2O	2.00E-02	4.30E-01	2	1
5989275	(R)-p-mentha-1,8-diene	1.16E+00	8.00E-01	4	1
8003427	(T-4)-Bis(dimethylcarbomodithioato-s,s')zinc, Mixt. with 2(3H)-Benzothiazolone zinc salt	-2.55E-01	3.29E-02	3	1
8063523	(Z)-9-Octadecen-1-ol, Hydrogen sulfate, Sodium salt mixt. with hexadecyl sodium salt	8.47E-01	4.40E-02	2	1
20056922	(Z)-dodec-7-enol	5.18E-01	5.12E-03	2	1
29118874	(Z)-N-(((Methylamino)carbonyl)oxy)ethanimidothioic acid, 2-Cyanoethyl ester	5.17E-01	1.33E-02	3	1
7173628	(Z)-N-9-octadecenylpropane-1,3-diamine	-3.89E-02	3.47E-02	4	1
112903	(Z)-octadec-9-enylamine	1.12E-01	1.14E-01	4	1
9004813	.alpha.-(1-Oxododecyl)-.omega.-hydroxypoly(oxy-1,2-ethanediyl)	1.78E+00	3.97E-01	2	1
51811791	.alpha.-(Nonylphenyl)-.omega.-hydroxypoly(oxy-1,2-ethanediyl)phosphate	1.17E+00	2.63E-02	5	1
57213691	[(3,5,6-trichloro-2-pyridyl)oxy]acetic acid, compound with triethylamine (1:1)	2.44E+00	3.27E-01	9	1
1803185	[(Diethylthiocarbamoyl)thio]triphenyl stannane	-3.62E+00	4.90E-01	3	1
8067989	[(Dimethoxyphosphinothioyl)thiol]butanedioic acid, Diethyl ester mixt. with O,O-dimethyl O-(3-methyl-4-nitrophenyl)phosp	-5.64E-02	3.61E-01	3	1
31430861	[(tetrachlorophthaloyl)bis(oxy)]bis(tributylstannane)	-2.63E+00	4.80E-01	3	1
55349547	[[[(Diethylamino)thioxomethyl]thio]tris(phenylmethyl)stannane	-2.70E+00	1.33E-01	3	1
1.1E+08	[[[Methoxyphenyl]thio]methyl]benzoic acid	4.64E-01	3.01E-03	2	1
66523566	[[1,2-Ethanediyl bis[carbomodithioato]](2-)]manganese mixt. with [[1,2-Ethanediylbis[carbomodithiato]] (2-) zinc and alu	1.50E+00	5.79E-02	2	1
1740198	[1R-(1alpha,4beta,10alpha)]-1,2,3,4,4a,9,10,10a-octahydro-7-isopropyl-1,4a-dimethylphenanthren-1-carboxylic acid	2.97E-01	1.17E-01	11	1
475207	[1S-(1alpha,3beta,4alpha,8alpha)]-decahydro-4,8,8-trimethyl-9-methylene-1,4-methanoazulene	-2.08E-01	7.75E-01	4	1
79127803	[2-(Phenoxyphenoxy)ethyl]carbamic acid, Ethyl ester	-5.56E-01	1.89E+00	9	1
992201	[2aR-[2a alpha,3 beta,5 beta(E),5a alpha,6 alpha,6a alpha,8 beta,9a beta,10a alpha,10b alpha,10c beta]]-3-(Acetyloxy)-8-	1.83E+00	4.50E-01	7	1
569642	[4-[alpha-[4-(dimethylamino)phenyl]benzylidene]cyclohexa-2,5-dien-1-ylidene]dimethylammonium chloride	-2.44E-02	1.30E+00	34	1

35367385	1-(4-chlorophenyl)-3-(2,6-difluorobenzoyl)urea	-1.35E+00	4.61E+00	45	1
8027007	1,1'-(2-Nitrobutylidene)bis(4-chlorobenzene), Mixt. with 1,1'-(2-Nitropropylidene)bis(4-chlorobenzene)	-9.35E-01	6.44E-01	6	1
26258708	1,1'-(2-Nitropropylidene)bis[4-ethoxybenzene]	-1.47E+00	1.01E+00	3	1
630206	1,1,1,2-tetrachloroethane	1.35E+00	5.49E-03	2	1
71556	1,1,1-trichloroethane	1.90E+00	1.15E-01	8	1
79345	1,1,2,2-tetrachloroethane	1.33E+00	1.32E-01	8	1
79005	1,1,2-trichloroethane	1.94E+00	9.90E-02	25	1
72560	1,1-dichloro-2,2-bis(4-ethylphenyl)ethane	-1.37E+00	4.85E-01	5	1
75354	1,1-dichloroethylene	2.16E+00	1.56E-01	7	1
78999	1,1-dichloropropane	1.71E+00	1.63E-01	2	1
4685147	1,1'-dimethyl-4,4'-bipyridinium	1.34E+00	7.79E-01	34	1
590669	1,1-dimethylcyclohexane	8.11E-01	4.28E-03	2	1
12002538	1,1-dimethylethyl 4(or 5)-chloro-2-methylcyclohexanecarboxylate	1.08E+00	6.16E-03	2	1
24307264	1,1-dimethylpiperidinium chloride	2.73E+00	1.62E+00	2	1
110974	1,1'-iminodipropyl-2-ol	2.83E+00	9.19E-02	2	1
14788977	1,1'-Sulfinylbis(1,2,2-trichloro)ethane	-1.10E+00	1.98E-01	3	1
634662	1,2,3,4-tetrachlorobenzene	-1.01E-01	5.73E-02	4	1
119642	1,2,3,4-tetrahydronaphthalene	1.14E+00	1.14E+00	2	1
634902	1,2,3,5-tetrachlorobenzene	4.51E-01	4.09E-01	7	1
87616	1,2,3-trichlorobenzene	2.16E-01	2.99E-01	7	1
96184	1,2,3-trichloropropane	6.07E-01	3.10E+00	3	1
95943	1,2,4,5-tetrachlorobenzene	4.46E-01	5.59E-01	10	1
95932	1,2,4,5-tetramethylbenzene	9.00E-01	6.67E-01	2	1
288880	1,2,4-triazole	1.41E+00	1.38E+00	3	1
120821	1,2,4-trichlorobenzene	4.24E-01	3.10E-01	37	1
95636	1,2,4-trimethylbenzene	8.46E-01	2.18E-02	3	1
2634335	1,2-benzisothiazol-3(2H)-one	1.20E+00	7.92E-02	2	1
5395755	1,2-bis(ethylthio)ethane	1.62E+00	4.89E-02	2	1
96128	1,2-dibromo-3-chloropropane	1.38E+00	2.48E-01	6	1
106934	1,2-dibromoethane	1.29E+00	1.83E-01	7	1
3209221	1,2-dichloro-3-nitrobenzene	6.37E-01	4.69E-02	4	1
99547	1,2-dichloro-4-nitrobenzene	4.23E-01	1.12E-02	3	1
95501	1,2-dichlorobenzene	1.07E+00	2.40E-01	16	1
107062	1,2-dichloroethane	2.22E+00	4.19E-01	14	1
78875	1,2-dichloropropane	2.14E+00	1.41E-01	9	1
72480	1,2-dihydroxyanthraquinone	3.18E-01	3.72E-02	2	1
49866877	1,2-dimethyl-3,5-diphenyl-1H-pyrazolium	1.39E+00	2.96E+00	4	1
583573	1,2-dimethylcyclohexane	3.38E-01	1.25E-01	2	1
528290	1,2-dinitrobenzene	3.76E-01	7.15E-01	2	1
71706075	1,3,3,5,5-Pentanitropiperidine	7.70E-01	1.48E-01	2	1
4005510	1,3,4-thiadiazol-2-amine	2.49E+00	1.11E+00	2	1
108703	1,3,5-trichlorobenzene	6.24E-01	1.46E+00	2	1
99354	1,3,5-trinitrobenzene	-5.86E-02	1.01E-01	6	1
110883	1,3,5-trioxane	4.08E+00	7.05E-02	3	1
109466	1,3-dibutyl-2-thiourea	8.86E-01	5.71E-01	3	1
8003198	1,3-Dichloro-1-propene mixt. with 1,2-Dichloropropane	4.67E-01	1.10E-01	6	1
611063	1,3-dichloro-4-nitrobenzene	6.23E-01	3.04E-02	5	1
618622	1,3-dichloro-5-nitrobenzene	3.96E-01	2.89E-01	3	1
541731	1,3-dichlorobenzene	1.21E+00	3.47E-01	10	1
96231	1,3-dichloropropan-2-ol	2.24E-01	2.55E+01	4	1
142289	1,3-dichloropropane	1.90E+00	2.00E-01	8	1
542756	1,3-dichloropropene	5.45E-01	1.32E-01	20	1
105555	1,3-diethyl-2-thiourea	2.08E+00	6.36E-02	3	1
1630177	1,3-Dimethyl-5-(4-nitrophenoxy)benzene	1.30E+00	3.80E-03	2	1
591219	1,3-dimethylcyclohexane	8.87E-01	1.80E-02	2	1
575417	1,3-dimethylnaphthalene	1.13E-01	2.75E-02	2	1
99650	1,3-dinitrobenzene	7.31E-01	3.05E-01	7	1
646060	1,3-dioxolane	3.95E+00	1.56E-02	2	1
102089	1,3-diphenyl-2-thiourea	1.55E+00	1.51E-01	2	1
89612	1,4-dichloro-2-nitrobenzene	6.39E-01	4.71E-02	4	1
106467	1,4-dichlorobenzene	9.91E-01	2.95E-01	16	1

589902	1,4-dimethylcyclohexane	5.66E-01	1.29E-01	2	1
100254	1,4-dinitrobenzene	3.14E-01	2.59E-01	4	1
123911	1,4-dioxane	3.82E+00	3.88E-02	5	1
130154	1,4-naphthoquinone	-7.20E-01	2.86E+00	4	1
3698837	1,5-dichloro-2,4-dinitrobenzene	-1.28E+00	1.94E-02	5	1
2245387	1,6,7-trimethylnaphthalene	1.53E-01	8.53E-01	2	1
115311	1,7,7-trimethylbicyclo[2.2.1]hept-2-yl thiocyanatoacetate	6.93E-03	4.12E-01	10	1
57055397	12,14-dichlorodehydroabiatic acid	-1.36E-01	1.49E-01	4	1
941980	1'-acetonaphthone	9.05E-01	1.80E-02	2	1
78966	1-aminopropan-2-ol	2.79E+00	3.06E-01	3	1
109706	1-bromo-3-chloropropane	1.74E+00	3.44E-02	2	1
112298	1-bromodecane	1.68E-01	2.44E+00	2	1
4316421	1-butyylimidazole	1.20E+00	2.97E-01	2	1
106898	1-chloro-2,3-epoxypropane	1.41E+00	3.54E-02	8	1
97007	1-chloro-2,4-dinitrobenzene	-1.12E-01	1.43E-01	5	1
88733	1-chloro-2-nitrobenzene	1.30E+00	1.10E-01	5	1
121733	1-chloro-3-nitrobenzene	7.38E-01	4.46E-01	8	1
100005	1-chloro-4-nitrobenzene	8.72E-01	2.42E-01	9	1
90131	1-chloronaphthalene	1.28E-03	1.25E-01	8	1
502396	1-cyano-3-(methylmercurio)guanidine	-1.09E+00	3.14E-04	2	1
78273	1-ethynylcyclohexanol	2.73E+00	2.13E-01	2	1
350469	1-fluoro-4-nitrobenzene	1.85E+00	3.04E-01	2	1
119380	1-isopropyl-3-methylpyrazol-5-yl dimethylcarbamate	2.89E-01	4.74E+00	3	1
2303255	1-Methyl-3-(4-nitrophenoxy)benzene	9.93E-01	4.87E-02	4	1
59756604	1-methyl-3-phenyl-5-[3-(trifluoromethyl)phenyl]-4-pyridone	8.01E-01	4.68E-01	20	1
36557274	1-Methylethyl ester, 11-methoxy-3,7,11-trimethyl-2,4-dodecadienoic acid	2.28E-01	6.69E-02	10	1
81406373	1-methylheptyl [(4-amino-3,5-dichloro-6-fluoropyridin-2-yl)oxy]acetate	1.11E+00	3.41E-03	6	1
90120	1-methylnaphthalene	7.68E-01	1.43E-01	6	1
120945	1-methylpyrrolidine	1.03E+00	5.72E-01	2	1
16058267	1-Methyltetradecylamine, Acetate	3.26E-01	1.00E-01	3	1
90153	1-naphthol	6.41E-01	2.13E-01	13	1
86873	1-naphthylacetic acid	2.16E+00	8.52E-02	9	1
134327	1-naphthylamine	1.47E+00	4.29E-01	2	1
86577	1-nitronaphthalene	9.74E-01	1.42E-01	2	1
118956	2-(1-Methylethyl)-4,6-dinitrophenol	-1.37E-01	7.94E-01	6	1
96300979	2-(1-Methylethyl)phenyldiphenyl ester phosphoric acid mixture w/triphenyl phosphate	4.00E-01	4.37E-02	6	1
6119922	2-(1-methylheptyl)-4,6-dinitrophenyl crotonate	-2.96E-01	1.09E-01	5	1
15067524	2-(2,4,5-Trichlorophenoxy)propanoic acid, 2-Butoxypropyl ester	6.78E-02	3.33E-01	15	1
2317240	2-(2,4,5-Trichlorophenoxy)propionic acid, 2-Butoxy-1-methylethyl ester	2.76E-01	4.11E-02	5	1
1982429	2-(2,4-dichlorophenoxy)acetamide	9.41E-01	3.36E-01	2	1
57571058	2-(2,4-Dichlorophenoxy)propanoic acid, 2-Butoxyethyl ester mixture with 2-Butoxyethyl(2,4-dichlorophenoxy) acetate	4.93E-01	7.72E-02	6	1
112345	2-(2-butoxyethoxy)ethanol	3.39E+00	4.18E-02	6	1
112561	2-(2-butoxyethoxy)ethyl thiocyanate	7.27E-01	8.59E-04	3	1
111900	2-(2-ethoxyethoxy)ethanol	4.15E+00	7.28E-02	11	1
93652	2-(4-chloro-o-tolyloxy)propionic acid	1.12E+00	3.85E-01	4	1
1.5E+08	2-(4-Methoxy[1,1'-biphenyl]-3-ylhydrazine carboxylic acid, 1-Methylethyl ester	-2.22E-01	7.13E-02	11	1
55792615	2'-(octyloxy)acetanilide	3.08E-01	8.58E-01	2	1
66827381	2-(p-Chlorophenyl)-2-isopropylacetic acid, Cyano(p-phenoxyphenyl)methyl ester	-1.64E+00	2.47E-01	4	1
112276	2,2'-(ethylenedioxy)diethanol	4.69E+00	1.35E-01	5	1
102716	2,2',2''-nitrioltriethanol	3.33E+00	3.34E-01	5	1
302170	2,2,2-trichloroethane-1,1-diol	2.03E+00	2.84E+00	3	1
115208	2,2,2-trichloroethanol	2.41E+00	1.16E-02	14	1
33979032	2,2',4,4',6,6'-hexachlorobiphenyl	-7.93E-01	1.95E-03	2	1
2437798	2,2',4,4'-tetrachlorobiphenyl	-1.17E+00	8.88E-02	4	1
37680732	2,2',4,5,5'-pentachlorobiphenyl	-6.00E-01	1.21E-02	2	1
79947	2,2',6,6'-tetrabromo-4,4'-isopropylidenediphenol	-5.46E-01	1.53E+00	6	1
2896700	2,2,6,6-tetramethyl-4-oxopiperidinoxy	-8.88E-01	9.22E-01	6	1
5567157	2,2'-[(3,3'-dichlorobiphenyl-4,4'-diyl)bis(azo)]bis[N-(4-chloro-2,5-dimethoxyphenyl)-3-oxobutyramide]	1.64E+00	8.12E-04	3	1
27541884	2,2-dichloro-N-(3-chloro-1,4-naphthoquinon-2-yl)acetamide	2.85E-02	1.25E-01	2	1
75990	2,2-dichloropropionic acid	2.47E+00	1.04E+00	19	1

70382	2,2-Dimethyl-3-(2-methyl-1-propenyl)cyclopropanecarboxylic acid, (2,4-Dimethylphenyl)methyl ester	-1.09E+00	3.10E-01	4	1
111400	2,2'-iminodi(ethylamine)	2.62E+00	2.87E-01	5	1
111422	2,2'-iminodiethanol	2.41E+00	6.01E-01	17	1
111466	2,2'-oxydiethanol	4.18E+00	9.66E-01	2	1
62046371	2,3 (or 3,4)-Dichlorobenzenemethanol methylcarbamate	-5.28E-02	1.10E+00	2	1
16022698	2,3,4,5,6-Pentachlorobenzenemethanol	2.23E-01	9.51E-03	3	1
634833	2,3,4,5-tetrachloroaniline	-3.89E-01	1.63E-01	5	1
4901513	2,3,4,5-tetrachlorophenol	-9.23E-02	1.37E-01	6	1
58902	2,3,4,6-tetrachlorophenol	-8.39E-03	2.39E-01	26	1
634673	2,3,4-trichloroaniline	1.47E-01	7.36E-02	5	1
54135807	2,3,4-trichloroanisole	-2.99E-01	1.95E-02	2	1
38444858	2,3,4'-Trichlorobiphenyl	-1.12E+00	3.00E-03	2	1
15950660	2,3,4-trichlorophenol	3.35E-01	3.61E-02	6	1
3481207	2,3,5,6-tetrachloroaniline	-7.79E-01	8.96E-02	2	1
935955	2,3,5,6-tetrachlorophenol	2.73E-01	3.04E-01	9	1
50737	2,3,5-Trichlorobenzoic acid	2.03E+00	1.88E-02	2	1
933788	2,3,5-trichlorophenol	2.79E-01	6.66E-02	4	1
1162658	2,3,6a-alpha,9a-alpha-tetrahydro-4-methoxycyclopenta[c]furo[3',2':4,5]furo[2,3-h]chromene-1,11-dione	-2.10E-02	9.29E-02	2	1
50317	2,3,6-TBA	2.13E+00	3.37E+00	3	1
50375105	2,3,6-trichloroanisole	-1.69E-01	1.37E-02	2	1
933755	2,3,6-trichlorophenol	7.84E-01	8.17E-02	5	1
18292972	2,3,6-Trinitrotoluene	-5.61E-01	3.19E-01	2	1
1.22E+08	2,3-bis(1,2-Dicarboxyethoxy)butanedioic acid hexasodium salt mixt. with 2-(1,2-dicarboxyethoxy)-3-hydroxybutanedioic aci	2.29E+00	9.17E-02	11	1
96139	2,3-dibromopropan-1-ol	2.36E+00	1.91E-01	3	1
1984594	2,3-dichloroanisole	1.62E-01	3.30E-01	2	1
576249	2,3-dichlorophenol	5.00E-01	7.11E-02	5	1
602017	2,3-dinitrotoluene	1.05E-01	1.25E-01	7	1
526750	2,3-xilenol	1.09E+00	1.42E-03	2	1
87592	2,3-xylidine	1.36E+00	2.65E-01	2	1
93765	2,4,5-T	1.21E+00	6.38E-01	28	1
636306	2,4,5-trichloroaniline	1.97E-01	4.13E-01	5	1
95954	2,4,5-trichlorophenol	8.95E-02	6.61E-02	18	1
118796	2,4,6-tribromophenol	-5.91E-02	1.36E+00	2	1
634935	2,4,6-trichloroaniline	5.70E-01	8.67E-02	2	1
87401	2,4,6-trichloroanisole	-8.62E-01	8.74E-01	2	1
88062	2,4,6-trichlorophenol	4.23E-01	1.24E-01	28	1
527606	2,4,6-trimethylphenol	1.35E+00	5.42E-01	4	1
118967	2,4,6-trinitrotoluene	6.96E-01	1.75E-01	12	1
94757	2,4-D	1.66E+00	9.58E-01	65	1
64047887	2,4-Dichloro-6-nitrophenol, Sodium salt	5.19E-01	2.66E-01	5	1
60168889	2,4'-dichloro-alpha-(pyrimidin-5-yl)benzhydryl alcohol	1.85E-01	2.19E-01	6	1
554007	2,4-dichloroaniline	6.99E-01	3.15E-01	18	1
120832	2,4-dichlorophenol	7.91E-01	4.79E-01	22	1
10202923	2,4-dinitro-3-methylaniline	8.59E-01	6.96E-02	2	1
5267276	2,4-dinitro-5-methylaniline	4.36E-01	6.18E-03	2	1
616739	2,4-Dinitro-5-methylphenol	5.25E-01	7.57E-04	2	1
97029	2,4-dinitroaniline	4.28E-01	1.37E+00	3	1
51285	2,4-dinitrophenol	1.06E+00	5.66E-01	25	1
121142	2,4-dinitrotoluene	6.04E-01	3.18E-01	17	1
1320189	2,4-D-propyleneglycol butyl ether	1.02E-01	1.70E-01	14	1
105679	2,4-xilenol	1.09E+00	3.23E-01	20	1
95681	2,4-xylidine	1.75E+00	5.82E-01	2	1
1420048	2',5-dichloro-4'-nitrosalicylanilide--2-aminoethanol (1:1)	-4.93E-01	5.82E-01	80	1
95829	2,5-dichloroaniline	7.27E-01	2.08E-01	4	1
5138932	2,5-Dichlorobenzenesulfonic acid, Sodium salt	3.57E+00	1.34E-02	2	1
583788	2,5-dichlorophenol	5.02E-01	4.55E-02	4	1
619158	2,5-dinitrotoluene	3.23E-01	8.72E-02	2	1
31473537	2,5-Furandione, Polymer with 1-Tetradecene	1.24E+00	5.03E-01	12	1
95874	2,5-xilenol	1.42E+00	8.34E-01	3	1

99309	2,6-dichloro-4-nitroaniline	5.01E-01	2.94E-01	6	1
608311	2,6-dichloroaniline	3.83E-01	1.10E-01	3	1
1984652	2,6-dichloroanisole	3.26E-01	6.44E-02	2	1
2008584	2,6-dichlorobenzamide	2.44E+00	8.13E-02	5	1
50306	2,6-dichlorobenzoic acid	2.12E+00	2.81E-03	2	1
87650	2,6-dichlorophenol	1.05E+00	1.35E-01	11	1
385002	2,6-difluorobenzoic acid	1.70E+00	1.27E-01	5	1
24544045	2,6-diisopropylaniline	1.23E+00	7.38E-03	2	1
581420	2,6-dimethylnaphthalene	-4.90E-01	3.54E-01	2	1
877430	2,6-dimethylquinoline	1.24E+00	2.11E-01	17	1
70343065	2,6-dinitro-3-methylaniline	9.97E-01	1.58E-02	2	1
606202	2,6-dinitrotoluene	1.44E+00	1.41E-01	4	1
128370	2,6-di-tert-butyl-p-cresol	3.84E-01	1.89E-01	4	1
576261	2,6-xylenol	1.10E+00	6.35E-01	7	1
87627	2,6-xylidine	1.99E+00	2.47E-03	3	1
3648360	2-[2-[4-[(2-chloroethyl)methylamino]phenyl]vinyl]-1,3,3-trimethyl-3H-indolium chloride	1.86E+00	7.09E-02	3	1
93083	2'-acetonaphthone	6.44E-01	6.73E-02	3	1
1745819	2-allylphenol	1.09E+00	5.55E-02	5	1
96913	2-amino-4,6-dinitrophenol	1.70E+00	2.10E-02	2	1
141435	2-aminoethanol	2.35E+00	1.82E-01	9	1
95841	2-amino-p-cresol	6.51E-01	3.50E-02	2	1
615361	2-bromoaniline	1.39E+00	7.45E-01	2	1
95567	2-bromophenol	1.25E+00	8.62E-01	2	1
20679587	2-butene-1,4-diyl bis(bromoacetate)	-5.12E-01	1.47E-01	5	1
111762	2-butoxyethanol	3.12E+00	1.65E-02	7	1
19398131	2-butoxyethyl 2-(2,4,5-trichlorophenoxy)propionate	3.96E-01	6.36E-01	13	1
53404312	2-butoxyethyl 2-(2,4-dichlorophenoxy)propionate	-1.38E-02	3.39E-02	6	1
2545597	2-butoxyethyl 2,4,5-trichlorophenoxyacetate	8.29E-02	1.84E-01	7	1
1929733	2-butoxyethyl 2,4-dichlorophenoxyacetate	5.89E-01	5.33E-01	29	1
19480434	2-butoxyethyl 4-chloro-o-tolyloxyacetate	3.47E-01	1.64E-01	2	1
3766812	2-butylphenyl methylcarbamate	5.99E-01	1.01E+00	16	1
961115	2-chloro-1-(2,4,5-trichlorophenyl)vinyl dimethyl phosphate	-3.69E-01	8.94E-03	3	1
3397624	2-chloro-4,6-diamino-1,3,5-triazine	1.23E+00	4.50E-01	3	1
121879	2-chloro-4-nitroaniline	8.59E-01	4.00E-01	2	1
121868	2-chloro-4-nitrotoluene	8.22E-01	3.49E-02	2	1
74070465	2-chloro-6-nitro-3-phenoxyaniline	1.70E-02	5.02E-01	7	1
83421	2-chloro-6-nitrotoluene	8.92E-01	3.79E-02	6	1
2464371	2-chloro-9-hydroxy-9H-fluorene-9-carboxylic acid	-4.11E-03	2.49E+00	3	1
95512	2-chloroaniline	1.24E+00	6.64E-01	6	1
766518	2-chloroanisole	9.00E-01	2.02E-02	2	1
89985	2-chlorobenzaldehyde	7.02E-01	4.93E-02	3	1
2051607	2-chlorobiphenyl	1.24E-01	9.27E-02	5	1
107073	2-chloroethanol	1.88E+00	3.05E-01	15	1
16672870	2-chloroethylphosphonic acid	2.57E+00	5.23E-01	7	1
50563365	2-chloro-N-(2,6-dimethylphenyl)-N-(2-methoxyethyl)acetamide	6.34E-01	6.01E-01	6	1
64902723	2-chloro-N-[[[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino]carbonyl]benzenesulphonamide	1.81E-01	2.16E+00	12	1
95578	2-chlorophenol	1.21E+00	2.03E-01	14	1
3942549	2-chlorophenyl methylcarbamate	7.31E-01	1.68E+00	7	1
95498	2-chlorotoluene	1.44E+00	2.56E-01	3	1
57966957	2-cyano-N-[(ethylamino)carbonyl]-2-(methoxyimino)acetamide	1.56E+00	4.57E-02	4	1
111159	2-ethoxyethyl acetate	2.14E+00	4.30E-01	9	1
578541	2-ethylaniline	1.50E+00	1.77E-01	3	1
104767	2-ethylhexan-1-ol	1.49E+00	1.71E-01	5	1
103117	2-ethylhexyl acrylate	1.84E+00	2.21E-01	3	1
1241947	2-ethylhexyl diphenyl phosphate	-5.30E-01	3.66E-01	2	1
6283869	2-ethylhexyl lactate	1.71E+00	8.57E-02	2	1
104756	2-ethylhexylamine	9.49E-01	4.92E-02	3	1
98011	2-furaldehyde	1.56E+00	2.59E-01	8	1
75865	2-hydroxy-2-methylpropiononitrile	-1.51E-01	4.52E-02	3	1
868779	2-hydroxyethyl methacrylate	1.92E+00	3.86E-01	2	1
5464711	2-Hydroxypropanoic acid, Octyl ester	1.32E+00	1.02E-01	3	1
23060142	2-Mercaptodiethylsuccinate	1.61E+00	8.20E-03	2	1

2539175	2-methoxy-3,4,5,6-tetrachlorophenol, tetrachloroguaiacol	-1.70E-01	4.00E-01	5	1
2668248	2-Methoxy-4,5,6-trichlorophenol	-1.18E-02	7.94E-01	4	1
3811492	2-methoxy-4H-1,3,2-benzodioxaphosphorin 2-sulphide	6.80E-01	9.23E-02	5	1
123886	2-methoxyethylmercury chloride	2.16E-01	3.49E-01	7	1
149315	2-Methyl-1,3-pentanediol	3.96E+00	5.26E-02	10	1
121299	2-methyl-4-oxo-3-(penta-2,4-dienyl)cyclopent-2-enyl [1R-[1alpha[S*(Z)](3beta)-3-(3-methoxy-2-methyl-3-oxoprop-1-enyl)-2,2-dimethylcyclopropanecarboxylate	-2.12E+00	1.60E-01	2	1
121211	2-methyl-4-oxo-3-(penta-2,4-dienyl)cyclopent-2-enyl [1R-[1alpha[S*(Z)],3beta]]-chrysanthemate	-5.11E-01	4.59E+00	5	1
64036437	2-Methylbenzothiazolethiol	6.70E-01	1.17E-01	5	1
75854	2-methylbutan-2-ol	3.61E+00	5.80E-02	3	1
583608	2-methylcyclohexanone	2.65E+00	3.05E-03	2	1
534225	2-methylfuran	2.77E+00	6.77E-02	2	1
91576	2-methylnaphthalene	1.84E-01	4.25E-02	6	1
107415	2-methylpentane-2,4-diol	3.77E+00	5.09E-02	9	1
78831	2-methylpropan-1-ol	3.09E+00	2.60E-01	18	1
75650	2-methylpropan-2-ol	3.67E+00	3.66E-02	4	1
109068	2-methylpyridine	2.98E+00	1.17E-03	2	1
655765	2-Methylquinoline, Sulfate (1:1)	1.53E+00	5.65E-02	13	1
64722	2-Naphthacenecarboxamide, 7-chloro-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-, monohydrochloride, [4S-(4alpha,4aalpha,5aalpha,6beta,12aalpha)]-	3.51E-01	2.52E+00	3	1
135193	2-naphthol	5.54E-01	3.56E-01	12	1
88744	2-nitroaniline	1.77E+00	6.04E-01	4	1
91236	2-nitroanisole	1.98E+00	8.86E-02	6	1
4920778	2-nitro-m-cresol	1.47E+00	7.59E-02	2	1
119335	2-nitro-p-cresol	1.52E+00	1.35E-01	2	1
88755	2-nitrophenol	1.16E+00	5.51E-01	10	1
89623	2-nitro-p-toluidine	1.61E+00	9.36E-02	2	1
88722	2-nitrotoluene	1.54E+00	6.40E-02	8	1
13146855	2-Pentadecanamine	2.63E-01	1.07E-01	4	1
122996	2-phenoxyethanol	2.36E+00	6.58E-02	2	1
504290	2-pyridylamine	1.76E+00	1.37E+00	2	1
1948330	2-tert-butylhydroquinone	-1.63E-01	6.73E-01	4	1
8065369	3-(1-Ethylpropyl)-phenol, Methylcarbamate, Mixt. with 3-(1-Methylbutyl)phenyl methylcarbamate	-1.90E+00	1.52E+00	6	1
98119347	3-(2,2-Dichloroethenyl)-2,2-dimethylcyclopropanecarboxylic acid (3-phenoxyphenyl)methyl ester mixt. with N-(3,4-dichloro	-6.57E-02	4.37E-02	3	1
3692908	3-(2-Propynyloxy)phenol methylcarbamate	-5.98E-01	8.17E-01	2	1
36734197	3-(3,5-dichlorophenyl)-2,4-dioxo-N-isopropylimidazolidine-1-carboxamide	4.77E-01	1.81E-01	10	1
56073075	3-(3-biphenyl-4-yl-1,2,3,4-tetrahydro-1-naphthyl)-4-hydroxycoumarin	-6.42E-01	2.56E-01	2	1
57465288	3,3',4,4',5-pentachlorobiphenyl	-2.95E+00	2.55E+00	3	1
1.11E+08	3,3-Dibutyl-N,N,6-triethyl-5-thioxo-2,4-dithia-6-aza-3-stannaooctanethioamide	-2.43E+00	8.68E-02	3	1
91941	3,3'-dichlorobenzidine	1.64E-01	4.08E-02	2	1
39196184	3,3-dimethyl-1-(methylthio)butanone-O-(N-methylcarbamoyl)oxime	-6.84E-01	8.18E-02	2	1
464073	3,3-dimethylbutan-2-ol	2.59E+00	2.48E-02	3	1
1656480	3,3'-oxydipropiononitrile	3.71E+00	1.73E-02	3	1
18472872	3,4,5,6-tetrachloro-2-(1,4,5,8-tetrabromo-6-hydroxy-3-oxoxanthen-9-yl)benzoic acid	8.31E-01	2.90E+00	2	1
57057837	3,4,5-Trichloroguaiacol	-1.66E-01	3.34E-03	2	1
609198	3,4,5-trichlorophenol	-1.34E-01	1.32E-01	4	1
2686999	3,4,5-trimethylphenyl methylcarbamate	-1.05E+00	2.12E+00	3	1
95761	3,4-dichloroaniline	4.92E-01	5.31E-01	33	1
95772	3,4-dichlorophenol	3.88E-01	3.87E-02	6	1
518752	3,4-dihydro-8-hydroxy-3,4,5-trimethyl-6H-6-oxobenzo(c)pyran-7-carboxylic acid	-1.98E+00	2.56E-01	2	1
610399	3,4-dinitrotoluene	3.34E-01	4.97E-02	2	1
95658	3,4-xylenol	1.03E+00	4.26E-02	4	1
95647	3,4-xylydine	1.00E+00	5.80E-01	2	1
2425107	3,4-xylyl methylcarbamate	6.82E-01	7.53E-01	11	1
78591	3,5,5-trimethylcyclohex-2-enone	2.21E+00	2.08E-01	9	1
3452979	3,5,5-trimethylhexan-1-ol	1.17E+00	2.72E-03	2	1
6515384	3,5,6-trichloro-2-pyridone	5.22E-01	1.22E-01	8	1
3281967	3,5-Dibromo-4-hydroxy-4'-nitroazobenzene	-5.75E-02	8.89E-03	4	1

1689845	3,5-dibromo-4-hydroxybenzonitrile	-1.42E-01	7.93E-01	20	1
626437	3,5-dichloroaniline	4.05E-01	1.17E-01	5	1
33719743	3,5-dichloroanisole	7.46E-01	3.02E-03	2	1
591355	3,5-dichlorophenol	4.07E-01	1.50E-01	14	1
500992	3,5-dimethoxyphenol	1.50E+00	9.61E-01	2	1
35572782	3,5-dinitro-2-methylaniline	7.27E-01	4.10E-01	3	1
19406510	3,5-dinitro-4-methylaniline	4.74E-01	1.49E-01	3	1
618871	3,5-dinitroaniline	9.54E-01	1.05E-01	6	1
618859	3,5-dinitrotoluene	1.50E+00	4.68E-02	2	1
108689	3,5-xyleneol	1.53E+00	3.28E-01	4	1
3055978	3,6,9,12,15,18,21-heptaaxatritriacontanol	2.92E-02	1.96E-01	2	1
86408	3,6-diamino-10-methylacridinium chloride	1.09E+00	1.57E-02	2	1
8048520	3,6-Diamino-10-methylacridinium, Chloride, Mixt. with 3,6-Acridinediamine	1.36E+00	6.28E-01	12	1
1702176	3,6-dichloropyridine-2-carboxylic acid	1.77E+00	5.62E-01	8	1
3401807	3,6-dichlorosalicylic acid	1.96E+00	5.09E-02	2	1
56207397	3,6-dinitro-o-toluidine	1.33E-01	8.79E-02	2	1
122101	3-[(Dimethoxyphosphinyl)oxy]-2-pentenedioic acid, Dimethyl ester	-5.71E-01	1.97E-01	2	1
19666309	3-[2,4-dichloro-5-(1-methylethoxy)phenyl]-5-(1,1-dimethylethyl)-1,3,4-oxadiazol-2(3H)-one	1.93E-01	1.62E-01	5	1
77736	3a,4,7,7a-tetrahydro-4,7-methanoindene	1.05E+00	4.04E-01	13	1
28434006	3-allyl-2-methyl-4-oxocyclopent-2-en-1-yl [1R-[1alpha(S*),3beta]]-2,2-dimethyl-3-(2-methylprop-1-enyl)cyclopropanecarboxylate	-1.65E+00	1.69E-01	4	1
591275	3-aminophenol	3.13E-01	2.94E-02	2	1
563473	3-chloro-2-methylpropene	1.07E+00	1.07E-02	2	1
6491027	3'-Chloro-3-nitrosalicylanilide	-2.33E-01	1.26E-01	22	1
61213250	3-chloro-4-(chloromethyl)-1-[3-(trifluoromethyl)phenyl]pyrrolidin-2-one	6.33E-01	2.29E-02	4	1
7745893	3-Chloro-4-methyl benzeneamine hydrochloride	1.21E+00	4.94E-02	10	1
5367282	3-chloro-6-nitrotoluene	1.37E+00	5.78E-02	2	1
108429	3-chloroaniline	1.15E+00	4.88E-01	7	1
2845898	3-chloroanisole	8.08E-01	1.85E-03	2	1
2051618	3-chlorobiphenyl	2.46E-01	2.80E-01	4	1
17109363	3-Chloro-N-(2-chloro-4-nitrophenyl)-5-(1,1-dimethylethyl)-6-hydroxy-2-methylbenzamide	-1.99E+00	6.88E-01	24	1
108430	3-chlorophenol	1.00E+00	1.76E-01	8	1
627305	3-chloropropan-1-ol	2.59E+00	3.08E-01	3	1
96242	3-chloropropane-1,2-diol	3.38E+00	6.27E-03	2	1
107051	3-chloropropene	1.40E+00	8.15E-01	7	1
95749	3-chloro-p-toluidine	1.13E+00	3.49E-01	8	1
51235042	3-cyclohexyl-6-dimethylamino-1-methyl-1,2,3,4-tetrahydro-1,3,5-triazine-2,4-dione	2.01E-01	3.46E+00	33	1
886862	3-ethoxycarbonylanilinium methanesulfonate	1.78E+00	1.14E-02	4	1
99069	3-hydroxybenzoic acid	1.89E+00	7.37E-03	5	1
64006	3-isopropylphenyl methylcarbamate	-1.23E+00	5.66E-01	3	1
150196	3-methoxyphenol	1.73E+00	2.48E-02	2	1
108996	3-methylpyridine	2.55E+00	3.02E-01	2	1
1.1E+08	3-Nitro-4-[(phenylsulfinyl)methyl]benzoic acid	1.20E-01	1.95E-04	2	1
1.03E+08	3-Nitro-4-[(phenylsulfonyl)methyl]benzoic acid	-2.01E-01	8.57E-04	2	1
1.03E+08	3-Nitro-4-[(phenylthio)methyl]benzoic acid	3.11E-01	2.03E-05	2	1
1.1E+08	3-Nitro-4-[[[(4-nitrophenyl)sulfinyl]methyl]benzoic acid	3.54E-02	8.01E-06	2	1
1.03E+08	3-Nitro-4-[[[(4-nitrophenyl)sulfonyl]methyl]benzoic acid	-2.08E-01	9.82E-05	2	1
1.03E+08	3-Nitro-4-[[[(4-nitrophenyl)thio]methyl]benzoic acid	1.09E-01	5.71E-06	2	1
99092	3-nitroaniline	1.58E+00	6.45E-01	4	1
619249	3-nitrobenzonitrile	1.73E+00	4.75E-03	2	1
603838	3-nitro-o-toluidine	1.41E+00	1.67E-01	2	1
83410	3-nitro-o-xylene	7.31E-01	1.26E-02	3	1
554847	3-nitrophenol	6.94E-01	5.21E-01	5	1
119324	3-nitro-p-toluidine	1.28E+00	3.43E-02	2	1
99081	3-nitrotoluene	1.41E+00	5.06E-02	6	1
39515510	3-phenoxybenzaldehyde	1.05E+00	7.33E-02	5	1
3739386	3-phenoxybenzoic acid	1.61E+00	1.26E-01	6	1
26002802	3-phenoxybenzyl 2-dimethyl-3-(methylpropenyl)cyclopropanecarboxylate	-1.22E+00	2.59E+00	6	1
13826352	3-phenoxybenzyl alcohol	1.04E+00	2.38E-02	5	1
140669	4-(1,1,3,3-tetramethylbutyl)phenol	-7.63E-01	2.35E-01	7	1
96300968	4-(1,1-Dimethylethyl)phenyl diphenyl ester phosphoric acid mixt. with triphenyl phosphate	1.86E-01	1.58E-01	6	1
94826	4-(2,4-dichlorophenoxy)butyric acid	1.45E+00	2.80E-01	6	1

3572063	4-(3-oxobutyl)phenyl acetate	1.24E+00	2.69E-03	2	1
133324	4-(indol-3-yl)butyric acid	2.01E+00	1.95E-01	3	1
2050682	4,4'-dichlorobiphenyl	-9.49E-01	5.21E-03	2	1
80057	4,4'-isopropylidenediphenol	3.29E-01	7.44E-01	9	1
3734483	4,5,6,7,8,8-hexachloro-3a,4,7,7a-tetrahydro-4,7-methano-1H-indene	-4.42E-01	9.67E-02	2	1
2460493	4,5-Dichloro-2-methoxyphenol	9.31E-01	5.17E-01	4	1
3428248	4,5-dichloropyrocatechol	-3.17E-03	7.08E-01	4	1
1570656	4,6-dichloro-o-cresol	1.86E-01	2.38E-01	3	1
616728	4,6-dinitro-m-xylene	1.14E+00	1.19E-01	2	1
1.1E+08	4-[(4-Nitrophenylsulfonyl)methyl]benzoic acid	7.71E-02	5.35E-04	2	1
71964926	4-[(Phenylsulfonyl)methyl]benzoic acid	-2.04E-01	2.41E-05	2	1
88382494	4-[(Phenylthio)methyl]benzoic acid	1.05E+00	2.62E-03	2	1
1.1E+08	4-[[[(4-Aminophenyl)sulfinyl]methyl]-3-nitrobenzoic acid	2.61E-01	1.39E-04	2	1
1.03E+08	4-[[[(4-Aminophenyl)sulfonyl]methyl]-3-nitrobenzoic acid	-1.74E-01	8.40E-05	2	1
1.1E+08	4-[[[(4-Aminophenyl)sulfonyl]methyl]benzoic acid	8.81E-01	8.01E-06	2	1
1.03E+08	4-[[[(4-Aminophenyl)thio]methyl]-3-nitrobenzoic acid	1.97E-01	3.42E-05	2	1
1.1E+08	4-[[[(4-Aminophenyl)thio]methyl]benzoic acid	9.41E-01	8.13E-03	2	1
1.1E+08	4-[[[(4-Bromophenyl)sulfinyl]methyl]-3-nitrobenzoic acid	2.72E-02	2.08E-04	2	1
1.03E+08	4-[[[(4-Bromophenyl)sulfonyl]methyl]-3-nitrobenzoic acid	-3.43E-01	1.14E-03	2	1
1.1E+08	4-[[[(4-Bromophenyl)sulfonyl]methyl]benzoic acid	4.39E-01	1.80E-04	2	1
1.1E+08	4-[[[(4-Bromophenyl)thio]methyl]benzoic acid	9.38E-01	1.02E-05	2	1
1.1E+08	4-[[[(4-Chlorophenyl)sulfonyl]methyl]benzoic acid	-4.69E-01	3.27E-04	2	1
88382518	4-[[[(4-Chlorophenyl)thio]methyl]benzoic acid	9.29E-01	8.25E-03	2	1
1.1E+08	4-[[[(4-Methoxyphenyl)sulfonyl]methyl]benzoic acid	6.55E-01	3.12E-04	2	1
1.03E+08	4-[[[(4-Methylphenyl)sulfonyl]methyl]-3-nitrobenzoic acid	-1.58E-01	1.95E-05	2	1
1.03E+08	4-[[[(4-Methylphenyl)sulfonyl]methyl]-3-nitrobenzoic acid	-2.25E-01	2.66E-05	2	1
1.1E+08	4-[[[(4-Methylphenyl)sulfonyl]methyl]benzoic acid	-1.23E+00	1.07E-02	2	1
1.03E+08	4-[[[(4-Methylphenyl)thio]methyl]-3-nitrobenzoic acid	-2.68E-01	5.18E-04	2	1
88382507	4-[[[(4-Methylphenyl)thio]methyl]benzoic acid	1.04E+00	1.53E-03	2	1
1.1E+08	4-[[[(4-Nitrophenyl)thio]methyl]benzoic acid	7.62E-01	4.78E-05	2	1
1.03E+08	4-[[[(Chlorophenyl)thio]methyl]-3-nitrobenzoic acid	-2.33E-01	2.48E-04	2	1
93152	4-allylveratrole	8.62E-01	5.72E-03	2	1
109273	4-amidino-N'-nitroso-1-tetrazene-1-carboximidohydrazide	3.59E+00	2.76E+00	3	1
6753475	4-amino-3,5,6-trichloropyridine-2-carboxylic acid, compound with 1,1',1''-nitrilotripropan-2-ol (1:1)	2.00E+00	4.24E-02	4	1
3096706	4-amino-3,5-xyleneol	-3.21E-01	4.37E-01	5	1
123308	4-aminophenol	-3.05E-01	1.36E-01	3	1
106401	4-bromoaniline	1.74E+00	8.88E-03	2	1
5015758	4-Bromobenzenesulfonic acid, Sodium salt	3.21E+00	8.60E-02	2	1
106412	4-bromophenol	1.17E+00	3.07E-01	2	1
101553	4-bromophenyl phenyl ether	4.24E-01	1.33E+00	2	1
20115348	4-Chloro-2-nitrophenyl-p-nitrophenyl ether	1.19E+00	6.05E-02	4	1
89598	4-chloro-2-nitrotoluene	9.99E-01	3.01E-02	6	1
89601	4-chloro-3-nitrotoluene	1.09E+00	2.31E-02	2	1
106478	4-chloroaniline	1.16E+00	2.55E-01	19	1
623121	4-chloroanisole	7.11E-01	5.42E-03	2	1
104881	4-chlorobenzaldehyde	1.04E+00	4.21E-01	3	1
2051629	4-chlorobiphenyl	-9.38E-02	5.03E-02	4	1
1570645	4-chloro-o-cresol	5.60E-01	6.70E-01	5	1
106489	4-chlorophenol	1.28E+00	7.44E-01	26	1
95885	4-chlororesorcinol	1.57E+00	4.94E+00	2	1
106434	4-chlorotoluene	1.03E+00	1.33E-01	3	1
37529309	4-decylaniline	-1.60E+00	3.18E-01	2	1
589162	4-ethylaniline	1.19E+00	4.79E-01	5	1
123079	4-ethylphenol	1.26E+00	2.95E-01	3	1
39905572	4-hexyloxyaniline	3.83E-02	4.53E-01	2	1
56073100	4-hydroxy-3-(3-(4'-bromo-4-biphenyl)-1,2,3,4-tetrahydro-1-naphthyl)coumarin	-4.96E-01	1.68E-01	10	1
123422	4-hydroxy-4-methylpentan-2-one	3.30E+00	6.18E-01	4	1
99967	4-hydroxybenzoic acid	1.90E+00	2.43E-01	2	1
767000	4-hydroxybenzonitrile	1.71E+00	5.70E-01	3	1
613376	4-methoxy-1,1'-biphenyl	-5.57E-01	7.80E-03	2	1
95807	4-methyl-m-phenylenediamine	2.25E+00	1.95E+00	3	1

108112	4-methylpentan-2-ol	2.69E+00	3.40E-02	2	1
108101	4-methylpentan-2-one	2.99E+00	9.67E-02	6	1
108894	4-methylpyridine	2.73E+00	3.34E-02	2	1
100016	4-nitroaniline	1.30E+00	1.07E+00	8	1
100174	4-nitroanisole	1.56E+00	6.41E-02	4	1
619727	4-nitrobenzonitrile	1.54E+00	4.69E-02	2	1
2581342	4-nitro-m-cresol	7.88E-01	2.88E-01	4	1
99514	4-nitro-o-xylene	9.96E-01	3.31E-03	4	1
100298	4-nitrophenetole	1.27E+00	7.21E-02	3	1
100027	4-nitrophenol	1.10E+00	1.41E-01	32	1
99990	4-nitrotoluene	1.50E+00	1.24E-01	5	1
16245797	4-octylaniline	-1.22E+00	2.71E-01	2	1
14938353	4-pentylphenol	3.73E-01	3.83E-02	4	1
939231	4-phenylpyridine	1.37E+00	5.14E-02	2	1
99718	4-sec-butylphenol	6.23E-02	7.45E-02	2	1
98544	4-tert-butylphenol	7.24E-01	1.68E-01	4	1
98511	4-tert-butyltoluene	5.88E-01	2.46E-02	2	1
63284719	5-(2-chloro-4'-fluorobenzhydryl)-4-hydroxypyrimidine	7.00E-01	7.60E-02	5	1
71662118	5-(morpholinomethyl)-3-[(5-nitrofurfurylidene)amino]oxazolidin-2-one [R-(R*,R*)]-tartrate	1.41E+00	1.02E+00	2	1
33813206	5,6-dihydro-3H-imidazo[2,1-c]-1,2,4-dithiazole-3-thione	-2.25E-01	5.63E-01	14	1
41483436	5-butyl-2-ethylamino-6-methylpyrimidin-4-yl dimethylsulfamate	3.61E-01	1.16E-01	4	1
481390	5-hydroxy-1,4-naphthoquinone	-6.92E-01	7.01E-01	11	1
41814782	5-methyl[1,2,4]triazolo[3,4-b]benzo[1,3]thiazole	1.10E+00	4.50E-01	5	1
110123	5-methylhexan-2-one	2.60E+00	1.88E-01	4	1
578461	5-methyl-o-nitroaniline	1.08E+00	2.00E-01	2	1
99558	5-nitro-o-toluidine	1.35E+00	1.21E-01	4	1
2917193	5-sec-Butyl-2-chlorophenyl methylcarbamate	-1.49E+00	4.34E-01	2	1
15662336	6-(1-alpha,5a-beta,8a-beta,9-pentahydroxy-7-beta-isopropyl-2-beta,5-beta,8-beta-trimethylperhydro-8b-alpha,9-epoxy-5,8-ethanocyclopenta[1,2-b]indenyl) pyrrole-2-carboxylate	1.06E+00	2.11E-01	3	1
5964625	6,6'-[Sulfonylbis(p-phenyleneazo)]dithymol	-6.31E-02	1.19E-01	3	1
329895	6-aminonicotinamide	1.62E+00	1.82E+00	2	1
8066113	6-Chloro-N-(1,1-dimethylethyl)-N'-ethyl-1,3,5-triazine-2,4-diamine mixt. with N-(1,1-dimethylethyl)-N'-ethyl-6-(methylth	5.36E-01	1.09E-01	4	1
22936863	6-chloro-N-cyclopropyl-N'-isopropyl-1,3,5-triazine-2,4-diamine	7.32E-01	1.18E-02	2	1
4684940	6-chloropicolinic acid	9.65E-01	6.27E-01	7	1
1653403	6-Methyl-1-heptanol	1.61E+00	1.15E-01	2	1
700389	6-nitro-m-cresol	1.25E+00	2.91E-01	3	1
408275	8-Fluoro-1-octanol	3.78E-01	5.15E-02	3	1
81889	9-(2-carboxyphenyl)-3,6-bis(diethylamino)xanthylum chloride	2.00E+00	3.14E-01	10	1
84117	9,10-phenanthrenequinone	-2.80E-01	1.74E-02	3	1
779022	9-methylanthracene	-1.40E+00	6.61E-01	3	1
65195553	Abamectin	-1.66E+00	1.10E+00	2	1
28288053	ABG-6070	-1.58E+00	7.89E-01	3	1
514103	abietic acid	2.61E-01	3.58E-01	3	1
2312734	Accel	7.62E-01	5.23E-02	2	1
83329	acenaphthene-	-5.96E-02	1.64E-01	21	1
30560191	acephate-	2.13E+00	2.76E+00	18	1
75070	acetaldehyde-	1.89E+00	1.43E-01	8	1
75398	acetaldehyde--ammonia	2.31E+00	1.04E-01	2	1
103902	Acetaminophen	2.30E+00	5.97E-01	22	2
103844	acetanilide-	2.03E+00	1.84E-03	2	1
64197	acetic acid, of a concentration of more than 10 per cent, by weight, of acetic acid	2.38E+00	2.66E-01	13	1
108247	acetic-anhydride-	2.75E+00	4.36E-01	3	1
67641	Acetone	3.86E+00	4.46E-01	46	1
75058	Acetonitrile	3.23E+00	1.33E-01	7	1
50782	Acetylsalicylic acid	2.39E+00	2.97E-01	13	2
260946	acridine-	8.91E-02	3.91E-01	21	1
107028	acrylaldehyde-	-8.45E-01	4.36E-01	27	1
79061	acrylamide-	2.16E+00	1.16E-01	12	1
79107	acrylic-acid-	2.49E+00	6.45E-01	5	1
107131	acrylonitrile-	1.34E+00	8.03E-02	23	1

9003569	Acrylonitrile, Polymer with 1,3-Butadiene and Styrene	1.28E+00	5.96E-02	13	1
111693	adiponitrile-	2.86E+00	3.58E-02	5	1
87501119	Adogen 570	-2.53E-02	5.19E-02	4	1
8065756	Aerazine-50	5.29E-01	1.21E-03	2	1
1757182	Akton	-8.78E-01	9.49E-01	7	1
15972608	Alachlor	2.06E-01	1.08E+00	35	1
8034999	Alamine 21	3.16E-01	1.13E-01	4	1
37191381	Albegal B	-8.90E-02	2.42E+00	3	1
68131408	Alcohols, C11-15-secondary, Ethoxylated	9.25E-01	1.26E-01	2	1
68439463	Alcohols, C9-11, Ethoxylated	8.39E-01	9.11E-03	3	1
116063	Aldicarb	-2.39E-01	1.19E+00	43	1
1646873	Aldicarb sulfoxide	1.05E-01	1.24E+00	3	1
1646884	Aldoxycarb	6.20E-01	1.51E+00	5	1
309002	Aldrin	-1.22E+00	1.15E+00	77	1
63513779	Alfloc	3.67E+00	2.94E-01	6	1
8046637	Aliquat 221	-3.17E-02	1.64E-01	4	1
63449412	Alkyl dimethylbenzyl ammonium chloride	-2.18E-01	7.67E-01	11	1
23526025	Allaric acid, 2-O-alpha-D-glucopyranosyl-4-(dihydrogen phosphate), 4',5'-anhydride with adenosine	1.71E+00	1.38E-01	2	1
584792	allethrin	-1.51E+00	3.41E-01	24	1
107186	allyl-alcohol-	4.54E-02	3.03E-01	9	1
107119	allylamine-	1.43E+00	2.73E-01	26	1
57067	allyl-isothiocyanate-	-1.09E+00	1.06E-03	2	1
109579	allylthiourea	3.02E+00	5.43E-01	2	1
6392467	allyxycarb	3.55E-01	2.56E-03	4	1
9002931	alpha-(4-(1,1,3,3-Tetramethylbutyl)phenyl)-omega-hydroxypoly(oxy-1,2-ethanediyl)	1.35E+00	1.57E-01	5	1
9016459	alpha-(Nonylphenyl)-omega-hydroxypoly(oxy-1,2-ethanediyl)	9.07E-01	1.59E-01	26	1
88302	alpha,alpha,alpha-trifluoro-4-nitro-m-cresol	9.36E-01	3.25E-01	84	1
654660	alpha,alpha,alpha-Trifluoro-4-nitro-m-cresol, Sodium salt	6.28E-01	1.91E-01	30	1
80159	alpha,alpha-dimethylbenzyl hydroperoxide	1.09E+00	7.38E-03	2	1
9036195	alpha-[(1,1,3,3-Tetramethylbutyl)phenyl]-omega-hydroxypoly(oxy-1,2-ethanediyl)	8.15E-01	5.72E-01	12	1
319846	alpha-BHC	9.25E-02	4.54E-01	18	1
100447	alpha-chlorotoluene	7.51E-01	6.93E-02	6	1
65732072	alpha-cyano-3-phenoxybenzyl [1R-[1alpha(S*),3beta]]-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate	-3.85E+00	5.28E-01	5	1
39515418	alpha-cyano-3-phenoxybenzyl 2,2,3,3-tetramethylcyclopropanecarboxylate	-2.36E+00	3.56E-01	7	1
66841256	alpha-cyano-3-phenoxybenzyl 2,2-dimethyl-3-(1,2,2,2-tetrabromoethyl)cyclopropanecarboxylate	-3.16E+00	6.62E-01	4	1
68085858	alpha-cyano-3-phenoxybenzyl 3-(2-chloro-3,3,3-trifluoroprop-1-enyl)-2,2-dimethylcyclopropanecarboxylate	-2.66E+00	2.02E+00	9	1
68359375	alpha-cyano-4-fluoro-3-phenoxybenzyl 3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate	-2.58E+00	7.20E-01	16	1
67375308	alpha-Cypermethrin	-3.18E+00	9.25E-01	10	1
34398011	alpha-Undecyl-omega-hydroxypoly(oxy-1,2-ethanediyl)	6.48E-01	1.08E-02	2	1
7784250	aluminium ammonium bis(sulfate)	1.81E+00	4.11E-03	2	1
13473900	aluminium-nitrate-	6.56E-01	1.50E-03	2	1
1302427	aluminium-sodium-dioxide-	3.16E+00	7.72E-01	3	1
10043013	aluminium-sulphate-	7.05E-01	1.70E+00	21	1
768945	amantadine	1.49E+00	1.63E-02	2	1
12642136	Amberlite LA-1	-7.33E-02	1.58E-01	3	1
67485294	Amdro	-1.98E+00	1.48E+00	12	1
3309680	American Cyanamid 12009	-1.53E+00	8.10E-01	3	1
834128	ametryn	-4.85E-01	1.67E+00	38	1
60139	amfetamine-sulfate	2.03E+00	6.59E-01	2	2
1.21E+08	Amidosulfuron	1.61E+00	6.70E-03	2	1
63231505	Amines, C15-18-alkyl, Unsatd.	-3.58E-01	1.42E-01	5	1
61791637	Amines, N-coco alkyltrimethylenedi-	9.74E-02	5.81E-02	4	1
61791580	Amines, N-tall-oil alkyltrimethylenedi-	-7.17E-02	1.84E-02	4	1
68814959	Amines, tri-C8-10-alkyl	-6.76E-01	2.31E-02	2	1
2032599	aminocarb	1.15E-01	1.02E+00	36	1
1066519	Aminomethylphosphonic acid	2.49E+00	2.60E-01	3	1
33089611	amitraz	-7.47E-01	2.15E+00	10	1

50486	Amitriptyline	7.23E-01	8.49E-01	12	2
61825	amitrole	1.85E+00	1.61E+00	13	1
7664417	ammonia, anhydrous	6.20E-01	1.70E+00	58	1
1336216	ammonia, in aqueous solution	9.95E-01	1.40E-01	6	1
14798039	Ammonium	1.86E+00	4.75E-01	7	1
1076466	ammonium 3-amino-2,5-dichlorobenzoate	3.36E+00	1.80E-02	4	1
7783202	Ammonium sulfate	1.62E+00	1.65E+00	20	1
12125029	ammonium-chloride-	9.39E-01	8.96E-01	179	1
7788989	ammonium-chromate-	1.64E-02	3.96E-01	3	1
3226366	ammonium-dimethyldithiocarbamate-	2.24E-01	9.65E-02	4	1
6484522	ammonium-nitrate-	1.90E+00	4.65E-01	9	1
7773060	ammonium-sulfamidate-	2.93E+00	1.41E-01	6	1
7803556	ammonium-trioxovanadate-	9.40E-01	3.50E-01	4	1
10350819	Amopyroquin dihydrochloride	1.44E+00	4.69E-02	6	1
26787780	Amoxicillin	6.99E-01	9.23E+00	5	3
300629	Amphetamine	2.60E+00	3.15E+00	2	2
69534	Ampicillin	2.17E+00	3.38E-01	4	3
121255	amprolium	2.60E+00	1.78E-01	4	1
1.21E+08	Anastrozole	1.76E+00	5.50E-02	3	4
12771685	ancymidol	1.95E+00	8.99E-02	2	1
101053	anilazine	-4.70E-01	4.38E-01	22	1
62533	aniline-	1.69E+00	9.56E-01	52	1
100663	anisole-	1.82E+00	4.57E-01	3	1
120127	Anthracene	-1.29E+00	5.26E-01	15	1
84651	anthraquinone-	6.74E-01	1.59E+00	5	1
11118722	Antimycin	-1.92E+00	1.43E+00	47	1
1397940	Antimycin A	-3.52E+00	9.98E-01	39	1
72674056	AOS	9.58E-01	2.22E-01	8	1
75022229	Arafosfotion	5.79E-01	2.21E+00	3	1
140578	Aramite	-7.26E-01	6.49E-02	7	1
60649265	Armeen DML 15D	3.84E-01	5.75E-02	3	1
52038489	Armohib 25	-2.94E+00	7.14E-04	2	1
12674112	Aroclor 1016	-1.13E+00	5.38E-01	19	1
11104282	Aroclor 1221	1.18E-02	3.74E-01	4	1
11141165	Aroclor 1232	-7.00E-02	1.49E+00	5	1
53469219	Aroclor 1242	-1.18E+00	7.55E-01	21	1
12672296	Aroclor 1248	-1.25E+00	8.94E-01	9	1
11097691	Aroclor 1254	-1.28E+00	1.61E+00	29	1
11096825	Aroclor 1260	-7.45E-01	1.96E+00	6	1
37324235	Aroclor 1262	1.61E-01	4.73E+00	2	1
11100144	Aroclor 1268	5.29E-01	2.74E+00	2	1
7440382	Arsenic	4.20E-01	5.89E-01	14	1
37337136	Arsenic acid (H3AsO4), Chromated copper salt (2:3)	-3.04E-01	1.62E+00	4	1
7631892	arsenic acid, sodium salt	1.99E+00	5.67E-01	8	1
15502746	Arsenite (AsO3)	-3.14E-01	1.66E-01	2	1
76578148	Assure	3.25E-01	1.74E-01	6	1
3337711	asulam	1.59E+00	1.39E-02	2	1
29122687	Atenolol	2.51E+00	3.70E-01	7	2
1081341	a-terthienyl	-2.06E+00	1.02E-01	7	1
53763001	Atlas 1901	1.90E+00	3.98E-02	3	1
1.35E+08	Atorvastatin	8.34E-01	1.69E+00	6	2
1912249	Atrazine	-6.95E-02	1.04E+00	128	1
51558	Atropine	3.06E+00	5.67E-01	7	2
71751412	Avermectin B1	-1.66E+00	2.58E+00	7	1
1.2E+08	Avolan UL 75	5.76E-01	5.74E-02	3	1
60207310	azaconazole	1.51E+00	7.17E-02	10	1
11141176	Azadirachtin	9.58E-01	2.88E-01	5	1
35575963	Azamethiphos	-1.53E-01	1.92E+00	13	1
2642719	azinthos-ethyl	-1.94E+00	1.31E+00	7	1
86500	azinthos-methyl	-1.47E+00	1.95E+00	69	1
151564	aziridine-	9.39E-01	6.26E-01	2	1
83905015	Azithromycin	1.79E-01	7.22E+00	2	3

103333	azobenzene-	-5.85E-03	4.65E-01	4	1
41083118	azocyclotin	-1.48E+00	1.01E+00	7	1
1.32E+08	azoxystrobin-propyl	-3.85E-02	6.67E-02	4	1
275514	azulene-	7.90E-01	1.55E-01	4	1
1405874	Bacitracin	1.63E+00	5.27E-02	2	3
1405896	bacitracin-zinc	1.61E+00	6.38E-02	2	1
81732469	Bambuterol	2.26E+00	3.41E-01	2	2
101279	barban	2.27E-01	5.65E-01	9	1
7440393	barium-	1.98E+00	3.63E-01	3	1
27949526	BEBP (O-butyl-S-ethyl-S-benzylphosphorodithioate)	1.10E+00	3.27E-03	4	1
3813056	Benazolin	2.10E+00	2.05E-01	4	1
22781233	Bendiocarb	-6.16E-01	6.53E-01	14	1
1861401	Benfluralin	7.40E-01	5.73E-01	9	1
82560541	Benfuracarb	-6.14E-01	9.11E-01	3	1
15310017	Benodanil	8.94E-01	1.55E-02	2	1
17804352	Benomyl	4.11E-01	1.24E+00	17	1
741582	Bensulide	-1.61E-02	1.66E-01	6	1
17606314	Bensultap	1.33E+00	1.32E-01	3	1
25057890	Bentazone	2.24E+00	7.39E-01	11	1
225116	Benz[a]acridine	-1.08E+00	1.08E+00	2	1
100527	Benzaldehyde	1.43E+00	4.83E-01	10	1
71432	Benzene	1.98E+00	3.79E-01	46	1
68411303	Benzenesulfonic acid, C10-13-alkyl derivs., sodium salts	7.80E-01	2.39E-01	3	1
8046535	Benzenesulfonic acid, Sodium salt, Alkyl derivs.	9.32E-01	5.03E-01	8	1
121540	benzethonium-chloride	7.89E-01	1.79E-01	9	1
92875	benzidine-	5.48E-01	6.52E-01	2	1
50328	Benzo[a]pyrene	-1.42E+00	1.72E+00	6	1
95158	benzo[b]thiophene	1.24E+00	2.25E-02	2	1
85029	benzo[f]quinoline	1.85E-01	6.68E-02	3	1
230273	benzo[h]quinoline	1.48E-01	1.55E-01	3	1
94097	benzocaine	1.45E+00	1.30E-02	15	1
65850	benzoic-acid-	2.13E+00	3.33E-01	10	1
100470	benzonitrile-	1.99E+00	1.68E-01	10	1
119619	benzophenone-	4.86E-01	8.25E-01	3	1
149304	benzothiazole-2-thiol	4.20E-01	2.17E-01	4	1
29104301	benzoximate	1.06E+00	5.78E-01	5	1
98884	benzoyl-chloride-	1.91E+00	2.38E-01	2	1
22212562	benzoylprop-ethyl	5.21E-01	6.36E-02	2	1
100516	benzyl-alcohol	2.33E+00	8.53E-01	7	1
85687	benzyl-butyl-phthalate-	5.19E-01	7.91E-01	20	1
51158180	Berol TL-188	2.31E+00	2.89E-01	5	1
51158191	Berol TL-198	2.64E+00	1.26E-01	4	1
39433084	Beycostat IP4A	1.53E+00	3.64E-02	2	1
41859670	Bezafibrate	1.19E+00	1.72E+00	8	2
608731	BHC-or-HCH	-4.92E-01	1.13E+00	37	1
82657043	Bifenthrin	-2.63E+00	1.96E+00	14	1
485314	binapacryl	-1.20E-01	2.01E+00	13	1
28434017	bioresmethrin-	-2.09E+00	3.27E-01	2	1
92524	biphenyl-	2.82E-01	1.65E-01	7	1
90437	biphenyl-2-ol	6.63E-01	6.96E-02	5	1
92693	biphenyl-4-ol	7.06E-01	4.05E-02	2	1
31895224	bis(1,2,3-trithiacyclohexyldimethylammonium) oxalate	-3.18E-01	6.76E-01	6	1
1445756	bis(1-methylethyl) methylphosphonate	2.94E+00	1.49E-01	8	1
111911	bis(2-chloroethoxy)methane	2.28E+00	7.36E-04	2	1
111444	bis(2-chloroethyl) ether	2.40E+00	1.70E-01	3	1
298077	bis(2-ethylhexyl) hydrogen phosphate	1.52E+00	3.45E-03	2	1
117817	bis(2-ethylhexyl) phthalate	1.19E+00	2.40E+00	11	1
541093	bis(acetato-O)dioxouranium	9.20E-01	2.38E-01	3	1
10102064	bis(nitrato-O)dioxouranium	1.04E+00	1.10E+00	7	1
56359	Bis(tri-n-butyltin)oxide	-1.82E+00	1.39E+00	68	1
1262211	bis(triphenyltin) oxide	-2.37E+00	8.67E-01	3	1
13356086	bis(tris(2-methyl-2-phenylpropyl)tin) oxide	-1.72E+00	1.58E+00	11	1

2437298	bis[[4-[4-(dimethylamino)benzhydrylidene]cyclohexa-2,5-dien-1-ylidene]dimethylammonium] oxalate, dioxalate	-5.82E-02	1.49E+00	5	1
55179312	bitertanol	3.65E-01	4.25E-01	9	1
56902080	Bithiophene	5.02E-02	8.41E-02	2	1
2079007	Blasticidin-S	5.82E-01	3.46E-02	4	1
1303964	Borax	2.36E+00	2.14E-01	5	1
8011630	Bordeaux mixture	4.98E-01	1.38E-02	2	1
10043353	boric acid	2.91E+00	2.52E+00	19	1
1333739	Boric acid, sodium salt	2.08E+00	6.70E-02	2	1
11126435	BP 1002	1.30E+00	2.47E-01	8	1
39278825	BP 1100	2.19E+00	8.27E-02	2	1
39403844	BP 1100 x	3.53E+00	1.66E-03	2	1
314409	bromacil	1.51E+00	1.58E+00	6	1
15541454	Bromate	2.14E+00	3.87E-01	3	1
7726956	bromine-	-8.68E-01	1.83E+00	2	1
13863417	bromine-chloride-	-4.71E-01	9.73E-02	8	1
79083	bromoacetic-acid-	7.75E-01	2.16E+00	2	1
108861	bromobenzene-	5.72E-01	1.02E-01	3	1
96638721	Bromocide	1.88E-02	1.61E-02	2	1
108850	bromocyclohexane-	6.76E-01	1.82E-02	4	1
13181174	bromofenoxim	-2.39E-01	2.31E-01	9	1
75252	bromoform-	1.45E+00	6.88E-02	10	1
74839	bromomethane-	3.91E-01	7.19E-01	8	1
1204213	bromomethyl 2,5-dimethoxyphenyl ketone	-1.06E+00	5.58E-02	5	1
2104963	bromophos- (ISO); bromofos	-1.79E+00	6.38E-01	11	1
4824786	bromophos-ethyl	-4.13E-01	6.28E-01	9	1
18181801	bromopropylate-	6.18E-02	2.82E-01	13	1
1.16E+08	Bromuconazole	-1.06E-01	3.06E-01	4	1
52517	bronopol	-4.97E-01	8.26E-01	7	1
357573	brucine-	1.43E+00	3.26E-02	2	1
2282340	Bufencarb	-1.87E+00	7.41E-01	5	1
69327760	Buprofezin	1.52E+00	1.07E+00	3	1
1423605	but-3-yn-2-one	1.39E+00	6.10E+00	2	1
36335678	Butamifos	-5.95E-03	1.61E+00	3	1
71363	butan-1-ol	3.13E+00	1.76E-01	11	1
78922	butan-2-ol	3.50E+00	2.55E-02	6	1
109795	butane-1-thiol	3.16E+00	3.65E-02	2	1
78933	butanone-	3.60E+00	4.31E-02	7	1
34681102	butocarboxim	1.32E+00	2.76E-01	5	1
126227	butonate	6.25E-01	3.03E-01	4	1
34681237	butoxycarboxim	1.72E+00	3.33E+00	3	1
94804	butyl 2,4-dichlorophenoxyacetate	5.60E-01	2.59E-01	17	1
2314092	butyl 9-hydroxy-9H-fluorene-9-carboxylate	1.03E+00	8.62E-01	4	1
109739	butylamine-	2.06E+00	3.88E-01	6	1
2008415	butylate	7.11E-01	5.03E-01	5	1
138227	butyl-lactate-	2.39E+00	2.10E-01	3	1
97881	butyl-methacrylate-	2.10E+00	5.30E-05	2	1
123728	butyraldehyde-	2.04E+00	3.58E-01	4	1
107926	butyric-acid-	2.45E+00	1.55E-01	6	1
24151937	C 19490	8.29E-01	3.29E-03	5	1
3844459	C.I. Acid Blue 9; C.I. Food Blue 2	2.69E+00	7.01E-02	6	1
633965	C.I. Acid Orange 7	2.61E+00	3.06E-01	2	1
8004873	C.I. Basic Violet 1	1.90E+00	1.88E+00	7	1
66455149	C12-13 Alcohols, Ethoxylated	2.94E-01	4.04E-01	3	1
68131395	C12-15 Alcohols, Ethoxylated	7.94E-02	7.42E-02	7	1
68951677	C14-15 Alcohols, Ethoxylated	2.92E-01	1.45E-01	16	1
58082	Caffeine	1.70E+00	5.87E+00	7	2
10043524	Calcium chloride	3.45E+00	2.00E-01	13	1
26264062	Calcium dodecylbenzenesulphonate	8.55E-01	7.36E-02	7	1
1305620	calcium hydroxide, not obtained from the product of calcining natural materials	1.90E+00	1.52E-01	3	1
7778543	Calcium hypochlorite	-6.11E-01	3.28E-01	27	1
1344816	Calcium polysulfide	1.20E+00	8.61E-02	7	1

7778189	Calcium sulfate	3.49E+00	3.19E-04	3	1
58561663	Calgon M-500	4.98E-01	1.10E-01	4	1
8001352	camphechlor	-1.60E+00	1.09E+00	79	1
79925	camphene-	1.06E+00	1.09E+00	4	1
66419383	Capacitor 21	-2.09E+00	2.83E-01	8	1
2425061	captafol	-2.73E-01	1.30E+00	20	1
133062	captan	-3.48E-01	7.34E-01	39	1
62571862	Captopril	1.87E+00	1.83E-01	3	2
298464	Carbamazepine	1.41E+00	7.54E-01	23	2
63252	carbaryl- (ISO); carbaril	1.32E-02	1.36E+00	199	1
86748	carbazole-	2.47E-01	1.55E-01	2	1
10605217	carbendazim	4.17E-01	1.16E+00	15	1
16118493	carbetamide-	1.26E+00	2.65E+00	8	1
1563662	Carbofuran	-3.79E-01	1.53E+00	67	1
1563388	Carbofuran phenol	8.60E-01	8.81E-04	2	1
75150	carbon-disulfide-	1.35E+00	5.53E-01	6	1
786196	carbophenothion- (ISO); carbofenotion	-1.29E+00	1.70E+00	25	1
55285148	carbosulfan	-5.94E-01	4.48E-01	3	1
5234684	carboxin	6.63E-01	1.32E+00	3	1
1.29E+08	Carfentrazone-ethyl	-1.32E+00	1.77E+00	3	1
15263533	Cartap	-3.62E-01	5.16E-01	17	1
4.01E+08	Ceftaroline	-2.51E-02	1.24E+01	2	3
12788964	Celanol PS 19	9.68E-01	9.58E-07	2	1
26183528	Cemulsol 870	1.06E+00	4.24E-03	2	1
57090	cetrimonium-bromide	-7.09E-01	4.64E-01	8	1
112027	cetrimonium-chloride	-4.77E-01	1.28E+00	9	1
123035	cetylpyridinium-chloride	-7.02E-02	2.35E-01	6	1
23504076	CGA 13608	1.98E-01	6.84E-01	4	1
95266403	CGA 163935	1.15E+00	5.79E-01	10	1
99607702	CGA 185072	4.01E-01	4.90E-01	5	1
8003461	Chemagro 2635	-1.16E+00	7.16E-01	3	1
2439012	chinomethionate	1.01E+00	1.69E+00	6	1
9012764	Chitosan	-1.30E+00	8.02E-03	2	1
133904	chloramben	2.06E+00	6.89E-03	4	1
10599903	chloramide-	-5.28E-01	5.53E-01	24	1
56757	Chloramphenicol	1.88E+00	2.09E+00	16	3
14866683	Chlorate	-1.03E+00	1.48E-02	3	1
52623844	Chlorax	3.36E+00	1.35E-02	2	1
13360457	chlorbromuron	5.22E-01	8.85E-01	15	1
1967164	chlorbufam	1.23E+00	3.38E-02	4	1
57749	chlordane	-1.16E+00	3.67E-01	33	1
12789036	Chlordane	-1.37E+00	8.57E-01	41	1
143500	chlordecone	-1.13E+00	4.83E-01	29	1
6164983	chlordimeform	1.65E+00	7.15E-02	7	1
85347	chlorfenac	1.20E+00	2.77E-01	5	1
80068	chlorfenethol	4.52E-02	1.93E-01	4	1
14437173	chlorfenprop-methyl	-1.94E+00	9.98E-01	7	1
80331	chlorfenson	6.18E-03	6.57E-02	3	1
470906	Chlorfenvinphos	-6.18E-01	1.85E+00	36	1
1698608	Chloridazon	1.43E+00	7.64E-01	10	1
7782505	chlorine-	-4.75E-01	6.12E-01	39	1
10049044	chlorine-dioxide-	2.64E+00	3.45E+00	4	1
24934916	chlormephos	-3.22E-01	9.74E-01	3	1
999815	Chlormequat chloride	2.08E+00	2.13E+00	3	1
999815	chlormequat-chloride	2.60E+00	9.62E-01	2	1
1836777	chlornitrofen-	8.71E-02	1.20E+00	15	1
107200	chloroacetaldehyde-	4.65E-01	3.84E-01	3	1
79118	chloroacetic-acid-	8.54E-01	3.67E+00	3	1
108907	chlorobenzene-	1.06E+00	7.19E-01	16	1
510156	chlorobenzilate	5.21E-01	4.02E-01	9	1
59507	chlorocresol	9.04E-01	2.92E-01	9	1
67663	chloroform-	1.76E+00	6.74E-01	31	1

74873	chloromethane-	2.59E+00	4.77E-02	2	1
54057	Chloroquine	1.46E+00	3.31E+00	8	2
1897456	chlorothalonil-	-6.89E-01	1.09E+00	36	1
15545489	chlorotoluron	8.07E-01	2.22E+00	14	1
1067147	chlorotriethylplumbane-	-1.91E-01	5.44E-01	4	1
1520781	chlorotrimethylplumbane-	3.42E-01	6.61E-01	4	1
3151415	Chlorotris(phenylmethyl)stannane	-3.09E+00	1.67E-01	3	1
1982474	chloroxuron	-8.75E-02	1.23E+00	10	1
14816207	chlorphoxim	-2.16E+00	4.36E-02	3	1
50533	Chlorpromazine	9.52E-02	3.51E-01	3	2
101213	chlorpropham	6.59E-01	1.69E-01	16	1
2921882	chlorpyrifos	-2.09E+00	1.52E+00	162	1
5598130	chlorpyrifos-methyl	-1.18E+00	1.45E+00	22	1
1861321	chlorthal-dimethyl	1.33E+00	1.61E+00	6	1
21923239	chlorthiophos-	-2.54E+00	4.05E+00	2	1
7440473	Chromium	7.56E-01	8.53E-01	52	1
2207014	cis-1,2-dimethylcyclohexane	6.77E-01	5.62E-02	2	1
10061015	cis-1,3-dichloropropene	8.15E-01	1.67E-02	3	1
15663271	Cisplatin	4.17E-01	5.00E-01	4	4
59729338	Citalopram	6.99E-01	3.09E-01	3	2
59355532	Citrex S5	4.02E+00	4.70E-01	2	1
77929	citric-acid-	2.72E+00	2.43E-01	3	1
1.27E+08	Clam-Trol CT 1	4.49E-01	3.67E-01	4	1
81103119	Clarithromycin	4.47E-01	3.15E+00	5	3
1.14E+08	clodinafop	1.85E+00	1.68E-02	4	1
1.26E+08	clodinafop	5.92E-02	1.30E+00	5	1
1.06E+08	Clodinafop-propargyl	-4.61E-01	3.56E-02	3	1
637070	Clofibrate	6.84E-01	1.02E+00	6	2
55600345	Clophen A 30	-1.22E-01	7.18E-01	2	1
7440484	cobalt-	2.08E-02	1.91E+00	3	1
66845292	Cocnq (Copper-2-oxy-3-chloro-1,4-naphthoquinone)	6.93E-01	6.99E-03	4	1
137291	copper bis(dimethyldithiocarbamate)	-5.06E-01	1.99E-01	2	1
61912876	Copper count-N	-7.05E-01	1.78E+00	3	1
3251238	Copper dinitrate	-6.28E-01	5.17E-01	37	1
20427592	Copper hydroxide	3.35E-01	2.08E+00	8	1
7758896	Copper monochloride	-8.15E-01	3.00E-01	10	1
1332407	Copper oxychloride	2.09E-01	1.16E+00	11	1
29204931	Copper-2-hydroxy-1,4-naphthoquinone	8.83E-01	3.19E-02	4	1
28275801	Copper-bis(ethylenediamine)dodecylbenzenesulfonate)	2.58E-01	1.17E-01	4	1
39362293	Corexit	1.79E+00	7.41E-01	2	1
12774300	Corexit 7664	2.54E+00	1.65E+00	9	1
60617063	Corexit 9527	1.56E+00	1.53E+00	9	1
1.72E+08	Corexit 9554	1.78E+00	5.01E-01	3	1
56724	coumaphos- (ISO); coumafos	-5.45E-01	2.95E+00	24	1
91645	coumarin-	1.32E+00	1.40E-01	3	1
5836293	coumatetralyl	1.92E+00	5.92E-01	4	1
1319773	cresol	1.42E+00	1.69E-01	6	1
4170303	crotonaldehyde-	1.48E+00	2.14E+00	5	1
7700176	crotoxyphos	-7.15E-01	9.83E-01	12	1
299865	crufomate	1.26E+00	1.83E-01	7	1
15096523	cryolite, natural	1.21E+00	3.95E-01	3	1
98828	cumene-	1.19E+00	5.20E-01	9	1
3251294	Cuprous nitrate	-1.52E+00	9.97E-02	2	1
12772064	Cutrine	7.40E-01	2.24E+00	12	1
66555337	Cutrine Plus	-4.81E-01	1.25E+00	2	1
21689849	Cyanatryn	1.58E+00	1.28E-01	2	1
21725462	cyanazine-	6.18E-01	1.09E+00	15	1
57125	Cyanide	-1.09E-01	8.44E-01	8	1
51630581	cyano (3-phenoxybenzyl)-2-(4-chlorophenyl)-3-methylbutyrate	-2.62E+00	1.54E+00	59	1
13067931	Cyanofenphos	4.29E-02	3.80E-02	3	1
506683	cyanogen-bromide-	-4.74E-01	4.26E-02	2	1
2636262	cyanophos	1.56E+00	4.19E-02	5	1

1.2E+08	cyazofamid	-8.04E-01	3.41E-01	3	1
1134232	cycloate	5.21E-01	2.48E-02	4	1
4904614	cyclododeca-1,5,9-triene	4.03E-01	7.92E-02	2	1
544252	cycloheptatriene-	1.39E+00	9.54E-02	2	1
628922	cycloheptene-	2.03E+00	1.07E-03	2	1
110827	cyclohexane-	2.16E+00	9.47E-01	13	1
108930	cyclohexanol-	2.92E+00	1.76E-02	4	1
108941	cyclohexanone-	2.84E+00	4.01E-03	3	1
110838	Cyclohexene	1.66E+00	9.18E-01	5	1
622457	cyclohexyl-acetate-	2.13E+00	1.09E-01	2	1
108918	cyclohexylamine-	1.88E+00	2.07E-01	6	1
91656	cyclohexyldiethylamine-	1.21E+00	2.77E-02	2	1
111784	cycloocta-1,5-diene	1.26E+00	2.74E-02	2	1
96413	cyclopentanol-	3.15E+00	1.03E-02	2	1
120923	cyclopentanone-	3.35E+00	4.02E-02	2	1
1.01E+08	Cycloxydim	2.09E+00	1.53E-01	4	1
13121705	cyhexatin	-2.05E+00	2.44E+00	16	1
52315078	cypermethrin	-3.06E+00	1.49E+00	79	1
39515407	cyphenothrin	-1.71E+00	1.41E+00	3	1
1.13E+08	Cyproconazole	7.39E-01	1.10E+00	5	1
94361076	cyproconazole	5.02E-01	1.20E+00	4	1
147944	Cytarabine	1.32E+00	1.37E-01	3	4
1596845	daminozide	2.22E+00	2.37E-01	4	1
533744	dazomet-	1.72E-01	3.67E-01	9	1
50293	DDT	-1.42E+00	1.42E+00	227	1
112301	decan-1-ol	6.05E-01	2.37E-01	6	1
706149	decan-4-olide	2.31E+00	2.24E+00	2	1
124185	decane-	-2.24E-02	5.84E+00	4	1
2026246	dehydroabietylamine-acetate-	-1.10E+00	1.91E-01	3	1
52918635	deltamethrin	-2.25E+00	3.85E+00	45	1
8065483	Demeton	-4.21E-01	8.80E-01	17	1
8022002	Demeton-methyl	4.13E-02	1.28E+00	15	1
919868	demeton-S-methyl	1.51E+00	3.19E-03	4	1
53763216	Dermol	2.29E+00	5.32E-02	4	2
1007289	Desethyl simazine	6.93E-01	6.05E-01	2	1
30125634	Desethyl-terbutylazine	1.45E+00	5.78E-02	2	1
13684565	desmedipham	-3.40E-01	3.70E-01	6	1
1014693	desmetryn	4.35E-01	2.48E+00	8	1
11113603	Destruxin	1.82E+00	2.14E-01	2	1
50022	Dexamethasone	6.50E-01	2.19E+00	5	2
10311849	dialifos	4.05E-01	4.11E-01	2	1
2303164	di-allate	8.88E-01	1.28E-02	3	1
124027	diallylamine-	1.38E+00	1.72E-03	2	1
7398698	diallyldimethylammonium-chloride-	4.25E-02	1.12E-01	2	1
131179	diallyl-phthalate-	5.73E-01	8.03E-01	3	1
37228356	Diam-26	1.13E-02	7.54E-02	4	1
3566107	diammonium ethylenebis[dithiocarbamate]	1.13E+00	1.75E-01	5	1
7783280	diammonium hydrogenorthophosphate, with an iron content not exceeding 0,03% by weight on the dry anhydrous product	8.15E-01	2.27E+00	3	1
7727540	diammonium-peroxodisulfate-	2.08E+00	4.44E-01	8	1
439145	Diazepam	1.90E+00	8.66E-01	12	2
333415	Diazinon	-5.80E-01	1.66E+00	113	1
132649	dibenzofuran-	3.79E-01	6.04E-02	6	1
132650	dibenzothiophene-	-5.18E-01	2.19E-01	3	1
124481	dibromochloromethane-	1.72E+00	1.79E-02	2	1
51249059	dibutyl [1-(butylamino)cyclohexyl]phosphonate	8.10E-01	2.24E-01	5	1
1770805	dibutyl 1,4,5,6,7,7-hexachlorobicyclo[2.2.1]hept-5-ene-2,3-dicarboxylate	7.41E-01	1.53E-01	2	1
111922	dibutylamine-	1.55E+00	3.29E-01	3	1
563257	dibutyldifluorostannane-	-9.00E-01	2.48E-01	2	1
142961	dibutyl-ether-	1.87E+00	1.16E-01	4	1
105759	dibutyl-fumarate-	-1.64E-01	1.27E-02	5	1
84742	dibutyl-phthalate-	1.45E-01	3.27E-01	21	1

1067330	dibutyltin di(acetate)	-9.41E-01	4.08E-03	2	1
683181	dibutyltin-dichloride-	-1.22E+00	3.69E+00	7	1
77587	dibutyltin-dilaurate-	-9.39E-03	7.25E-02	3	1
818086	dibutyltin-oxide-	-1.01E-01	1.10E-02	2	1
1918009	dicamba-	1.71E+00	1.39E+00	14	1
2463845	Dicapthon	-6.25E-01	1.84E+00	4	1
1194656	dichlobenil	1.18E+00	4.15E-01	38	1
97176	dichlofenthion	-6.77E-02	9.75E-01	18	1
1085989	dichlofluanid	-4.05E-01	1.14E+00	11	1
117806	dichlone	-7.61E-01	4.17E-01	20	1
3400097	Dichloramine	-9.08E-01	3.31E-01	4	1
79436	Dichloroacetic acid	2.55E+00	1.25E+00	3	2
1135995	dichlorodiphenylstannane-	-1.49E+00	3.66E+00	6	1
1300216	dichloroethane-	2.71E+00	1.75E-03	2	1
75092	dichloromethane-	2.47E+00	2.54E-01	13	1
97234	dichlorophen	-7.69E-02	6.83E-01	6	1
25167811	dichlorophenol-	5.85E-01	9.20E-02	2	1
120365	Dichlorprop	2.28E+00	6.28E-01	13	1
15165670	Dichlorprop-P	2.36E+00	1.68E-01	3	1
62737	Dichlorvos	-2.97E-01	2.04E+00	114	1
15307865	Diclofenac	1.18E+00	8.76E-01	17	2
115322	dicofol	-1.58E-01	4.53E-01	28	1
141662	dicrotophos	4.00E-01	4.14E-01	13	1
2954941	Dicyclohexyltin	-5.65E-01	1.50E+00	2	1
7173515	Didecyldimethylammoniumchloride	-4.78E-01	8.61E-01	20	1
3401749	didodecyldimethylammonium-chloride-	-1.80E-01	1.23E-01	4	1
3972132	DIDT	-7.30E-01	1.71E-01	3	1
60571	dieldrin	-1.57E+00	1.00E+00	126	1
2227170	dienochlor-	-4.04E-01	6.81E-01	7	1
87130209	Diethofencarb	7.44E-01	6.16E-02	2	1
311455	diethyl 4-nitrophenyl phosphate	-1.52E+00	1.25E+00	12	1
109897	diethylamine-	2.14E+00	3.88E-01	7	1
60297	diethyl-ether-	3.11E+00	3.54E-01	4	1
623916	diethyl-fumarate-	7.15E-01	7.58E-03	2	1
598027	diethyl-hydrogen-phosphate-	1.81E+00	1.58E+00	2	1
55185	diethylnitrosoamine-	2.17E+00	8.08E-01	6	1
95921	diethyl-oxalate-	2.60E+00	6.90E-02	3	1
84662	diethyl-phthalate-	1.63E+00	2.66E-01	18	1
56531	diethylstilbestrol	-7.21E-01	1.21E+00	2	1
866557	diethyltin-dichloride-	-1.28E+00	6.43E+00	4	1
134623	diethyltoluamide	2.21E+00	5.43E-02	2	1
1.19E+08	Difenoconazole	-3.12E-02	7.76E-03	6	1
14214325	difenoxuron	5.70E-01	2.15E+00	4	1
83164334	Diflufenican	1.65E+00	1.13E-01	3	1
20830755	Digoxin	2.81E+00	1.66E+00	7	2
7783064	dihydrogen-sulfide-	-5.30E-01	1.71E+00	33	1
84695	diisobutyl-phthalate-	2.16E-01	1.37E-01	2	1
28553120	di-isononyl phthalate	3.31E-01	2.29E-01	4	1
10552746	diisopropyl 5-nitroisophthalate	1.48E-01	8.97E-02	5	1
108189	diisopropylamine-	2.09E+00	4.06E-01	15	1
108203	diisopropyl-ether-	3.21E+00	5.13E-01	4	1
55914	diisopropyl-phosphorofluoridate-	1.08E+00	2.08E-02	2	1
57157809	diisotridecylamine-	-3.14E-01	4.61E-02	2	1
42399417	Diltiazem	1.47E+00	4.00E-01	4	2
22936750	dimethametryn	7.97E-01	1.11E-02	5	1
81777891	Dimethazone	1.02E+00	1.49E-01	5	1
1.64E+08	Dimethenamid-P	-7.63E-01	1.19E+00	10	1
60515	dimethoate	2.21E-01	2.18E+00	70	1
1.1E+08	Dimethomorph	1.15E+00	1.10E-01	3	1
1773893	dimethyl 1,4,5,6,7,7-hexachlorobicyclo[2.2.1]hept-5-ene-2,3-dicarboxylate	3.17E-01	1.26E-02	4	1
63148629	Dimethyl siloxanes and silicones	1.20E+00	2.24E-01	5	1
124403	dimethylamine	1.82E+00	5.77E-01	6	1

6369977	dimethylammonium 2,4,5-trichlorophenoxyacetate	2.28E+00	2.45E-01	8	1
2008391	dimethylammonium 2,4-dichlorophenoxyacetate	2.16E+00	8.66E-01	25	1
107642	dimethyldioctadecylammonium-chloride-	1.72E+00	1.06E+00	3	1
28804888	dimethylnaphthalene-	-1.99E-01	4.73E-01	5	1
62759	dimethylnitrosoamine-	2.27E+00	1.69E+00	6	1
131113	dimethyl-phthalate-	2.02E+00	1.27E-01	15	1
77781	dimethyl-sulfate-	1.03E+00	4.53E-02	2	1
67685	dimethyl-sulfoxide	4.51E+00	6.19E-02	9	1
753731	dimethyltin-dichloride-	-2.27E-01	4.68E+00	5	1
131895	dinex	-5.43E-01	9.57E-02	2	1
148016	dinitolmide	2.14E+00	7.78E-03	2	1
29091052	dinitramine	5.04E-02	1.96E-02	10	1
534521	Dinitro-o-cresol	2.20E-01	4.22E-01	18	1
973217	dinobuton	-1.51E+00	4.07E-01	3	1
39300453	dinocap	-1.32E+00	2.79E-01	6	1
88857	dinoseb	-3.59E-01	3.79E-01	29	1
2813958	dinoseb-acetate-	-1.36E+00	6.87E-01	5	1
1420071	dinoterb	-8.87E-01	1.01E+00	8	1
6988212	dioxacarb	1.36E+00	4.75E-02	6	1
78342	dioxathion- (ISO); dioxation	-7.25E-01	1.67E+00	25	1
1314643	dioxo[sulphato(2-)-O]uranium	8.48E-01	2.79E-01	5	1
957517	diphenamid	1.79E+00	2.56E-02	8	1
122394	diphenylamine-	3.28E-01	8.21E-02	4	1
101848	diphenyl-ether-	2.00E-01	1.05E-01	6	1
57410	Diphenylhydantoin	1.45E+00	2.30E-01	7	2
38638050	diphenyl-nonylphenyl-phosphate-	1.64E+00	2.32E-01	2	1
26444495	diphenyl-tolyl-phosphate-	-1.52E-01	2.27E-02	3	1
7727211	dipotassium-peroxodisulfate-	2.66E+00	1.85E-01	7	1
7790581	dipotassium-trioxotellurate-	1.89E+00	6.08E-01	2	1
2764729	Diquat	3.03E-01	2.00E+00	34	1
85007	diquat-dibromide	7.83E-01	1.98E+00	36	1
6385600	disodium (endo,endo)-7-oxabicyclo[2.2.1]hept-5-ene-2,3-dicarboxylate	1.51E+00	5.21E+00	2	1
518478	disodium 2-(3-oxo-6-oxidoxanthen-9-yl)benzoate	3.26E+00	1.74E-01	6	1
27344418	disodium 2,2'-([1,1'-biphenyl]-4,4'-diyldivinylene)bis(benzenesulphonate)	1.97E+00	9.99E-02	3	1
16090021	disodium 4,4'-bis[(4-anilino-6-morpholino-1,3,5-triazin-2-yl)amino]stilbene-2,2'-disulphonate	2.36E+00	1.75E+00	3	1
13863315	disodium 4,4'-bis[(4-anilino-4-[(2-hydroxyethyl)methylamino]-1,3,5-triazin-2-yl)amino]stilbene-2,2'-disulphonate	1.89E+00	5.19E-02	3	1
10048950	disodium arsenate(V) heptahydrate	2.27E+00	2.88E-01	2	1
1330434	disodium tetraborate, anhydrous	2.17E+00	6.42E-01	4	1
497198	disodium-carbonate-	2.68E+00	1.39E-01	12	1
16893859	disodium-hexafluorosilicate-	1.95E+00	1.32E-01	2	1
7778430	disodium-hydrogenarsenate-	1.12E+00	1.21E+00	19	1
144218	disodium-methylarsonate-	2.36E+00	7.88E-01	4	1
7631950	disodium-molybdate-	2.50E+00	1.97E+00	8	1
62760	disodium-oxalate-	3.18E+00	1.63E-01	3	1
7775271	disodium-peroxodisulfate-	2.66E+00	2.18E-01	6	1
7757826	disodium-sulfate-	3.10E+00	7.61E-01	15	1
1313822	disodium-sulfide-	3.67E-01	1.14E+00	26	1
12058661	disodium-tin-trioxide-	1.20E+00	3.46E-01	2	1
13472452	disodium-wolframate-	1.78E+00	1.03E+00	5	1
1.15E+08	Dispolene 32S	2.61E+00	2.89E-01	5	1
64742478	Distillates (petroleum), hydrotreated light	7.62E-01	4.62E-02	4	1
97778	disulfiram	-8.12E-01	9.08E-01	5	1
298044	disulfoton	-3.55E-01	1.01E+00	32	1
12656698	Dithane	-5.35E-01	4.28E-02	2	1
3347226	dithianon	-1.40E-01	2.35E+00	15	1
148185	ditiocarb-sodium	1.70E-01	4.83E-01	4	1
330541	diuron	-2.71E-01	1.52E+00	75	1
299854	DMPA	-1.38E+00	2.40E+00	3	1
2312767	DNOC-sodium	6.45E-02	5.00E-01	5	1
2385855	dodecachloropentacyclo[5.2.1.0-{2,6}-0-{3,9}-0-{5,8}-]decane	7.48E-02	1.14E+00	8	1
112538	dodecan-1-ol	2.66E-02	1.42E-02	4	1

124221	dodecylamine-	-1.15E+00	5.31E-02	2	1
1886813	dodecyl-benzenesulphonate-	9.43E-01	7.87E-02	3	1
27176870	dodecylbenzenesulphonic-acid-	1.01E+00	1.77E-01	5	1
112005	dodecyltrimethylammonium-chloride-	-1.88E-01	6.16E-01	7	1
1593777	dodemorph	2.85E-01	1.36E+00	7	1
66231172	Dodigen 95	-3.50E+00	5.91E-01	2	1
2439103	dodine	5.79E-02	2.97E-01	14	1
23214928	Doxorubicin	4.83E-01	1.92E-01	4	4
53384397	DTAS	1.35E+00	9.97E-03	4	1
74871402	Dubaral SP	9.89E-01	6.19E-02	6	1
56257911	Duomeen L 15	7.46E-02	6.34E-02	4	1
60004	edetic-acid	2.11E+00	5.09E-02	4	1
17109498	edifenphos-	4.32E-01	3.09E-01	9	1
15271417	endo-3-Chloro-exo-6-cyano-2-norbornanone, o-(Methylcarbamoyl) oxime	2.38E-01	1.47E+00	3	1
115297	endosulfan	-1.73E+00	1.89E+00	151	1
1031078	Endosulfan sulfate	-3.98E-01	1.52E-01	2	1
959988	Endosulfan, alpha	-1.98E+00	2.14E+00	7	1
33213659	Endosulfan, beta	-1.66E+00	4.51E-01	5	1
145733	endothal-	1.17E+00	1.41E+00	22	1
17439940	endothal-ammonium	2.05E+00	5.28E-02	9	1
2164070	endothal-potassium	2.22E+00	1.74E-01	8	1
129679	endothal-sodium	1.88E+00	6.79E-01	12	1
72208	endrin	-2.10E+00	2.03E+00	144	1
93106606	Enrofloxacin	8.15E-01	2.31E+00	7	3
1.06E+08	epoxyconazool	6.40E-01	6.48E-02	6	1
1.06E+08	epoxyconazool	4.16E-01	3.65E-01	5	1
105602	epsilon-caprolactam	3.48E+00	7.70E-02	3	1
759944	EPTC	1.02E+00	2.95E-01	17	1
136254	Erbon	9.87E-01	4.10E-01	3	1
66829058	Erional NWS	1.65E+00	2.56E-01	4	1
66230044	Esfenvalerate	-2.80E+00	1.35E+00	11	1
37226281	Essolvane	1.42E+00	1.71E-01	10	1
50282	Estradiol	-2.18E+00	3.35E+00	24	2
53167	Estrone	-1.80E+00	3.00E+00	6	2
107211	Ethane-1,2-diol	4.42E+00	7.07E-01	8	1
64175	Ethanol	3.65E+00	6.06E-01	17	1
57636	Ethinylestradiol	-1.53E+00	4.45E+00	30	1
29973135	ethiofencarb	9.09E-01	1.03E+00	5	1
563122	ethion	-7.10E-01	1.97E+00	28	1
23947606	Ethirimol	1.67E+00	5.80E-03	4	1
80844071	Ethofenprox	7.33E-01	4.37E-01	2	1
26225796	ethofumesate-	1.21E+00	4.22E-01	11	1
61791240	Ethomeen S/25	3.49E-01	1.42E-01	5	1
13194484	Ethoprophos	-2.74E-01	1.72E+00	18	1
4329037	Ethoxychlor	-3.91E-01	2.34E+00	4	1
72490018	ethyl [2-(4-phenoxyphenoxy)ethyl]carbamate	7.45E-02	3.89E-02	9	1
533233	ethyl 2,4-dichlorophenoxyacetate	2.89E-01	6.58E-02	4	1
22212551	ethyl N-benzoyl-N-(3,4-dichlorophenyl)-DL-alaninate	8.02E-02	4.92E-03	2	1
14324551	Ethyl ziram	-5.02E-01	4.36E-01	3	1
141786	ethyl-acetate-	2.82E+00	2.16E-01	29	1
141979	ethyl-acetoacetate-	2.74E+00	5.27E-02	2	1
140885	ethyl-acrylate-	7.25E-01	1.17E-01	3	1
75047	ethylamine-	2.50E+00	4.93E-01	2	1
100414	ethylbenzene-	1.46E+00	3.53E-01	16	1
93890	ethyl-benzoate-	1.21E+00	8.01E-02	3	1
105544	ethyl-butyrate-	2.56E+00	4.29E-01	3	1
1678917	ethylcyclohexane-	7.60E-01	1.06E-01	2	1
111557	ethylene di(acetate)	1.92E+00	1.93E-03	2	1
107153	Ethylenediamine	2.18E+00	3.94E-01	9	1
333186	ethylenediammonium-dichloride-	9.52E-01	6.13E-01	2	1
75218	ethylene-oxide-	2.27E+00	1.29E-01	4	1
96457	Ethylenethiourea	2.95E+00	1.16E+00	8	1

120934	Ethyleneurea	3.24E+00	1.88E+00	4	1
97643	ethyl-lactate-	2.92E+00	2.36E-01	3	1
107277	ethylmercury-chloride-	-7.54E-01	1.04E+00	3	1
2235258	ethylmercury-dihydrogen-phosphate-	1.55E-01	7.66E-01	3	1
333437	Ethylphosphonodithioic acid, O-Ethyl S-(4-methylphenyl) ester	-2.00E+00	7.78E-01	3	1
105373	ethyl-propionate-	2.20E+00	2.58E-01	24	1
118616	ethyl-salicylate-	1.27E+00	1.43E-03	2	1
2809214	Etidronic acid	-3.18E-01	2.78E-01	9	2
33125972	etomidate	3.53E-02	1.23E-01	4	1
33419420	Etoposide	2.22E+00	4.60E-01	3	4
2593159	Etridiazole	4.55E-01	1.15E-01	7	1
38260547	Etrimfos	-3.48E-01	2.11E+00	11	1
1.32E+08	Famoxadone	-1.53E+00	5.32E-01	4	1
504245	fampridine	1.18E+00	3.71E-01	11	1
72509763	Felodipine	-5.25E-01	2.78E-01	4	2
140567	fenamino-sulf	1.24E+00	2.50E-01	8	1
22224926	Fenamiphos	-1.35E+00	1.63E+00	9	1
14255880	fenazaflor	-4.85E-01	3.97E-03	3	1
1.03E+08	Fenchlorazole-ethyl	-4.11E-01	6.27E-02	5	1
299843	fenchlorphos- (ISO); fenclofos	-5.39E-01	9.82E-01	16	1
122145	fenitrothion	-7.04E-01	2.07E+00	164	1
2255176	Fenitrothion oxygen analog	-6.38E-01	4.73E+00	2	1
49562289	Fenofibrate	7.50E-01	4.81E-01	6	2
93721	fenoprop	9.47E-01	5.10E-01	16	1
71283802	Fenoxaprop-P-ethyl	-1.13E-01	1.50E-01	4	1
74738173	Fenpiclonil	-9.44E-02	8.69E-02	6	1
64257847	Fenpropathrin	-2.40E+00	1.52E+00	7	1
67306030	Fenpropimorph	2.57E-01	3.88E-01	6	1
80386	fenson	8.36E-01	5.83E-03	2	1
115902	fensulfothion	-4.52E-01	2.23E+00	6	1
55389	fenthion	-1.03E+00	1.70E+00	126	1
900958	fentin-acetate	-1.65E+00	1.96E+00	34	1
639587	fentin-chloride	-2.10E+00	1.69E+00	28	1
379522	fentin-fluoride	-1.26E+00	7.13E-01	5	1
76879	fentin-hydroxide	-1.75E+00	1.86E+00	31	1
101428	fenuron	8.28E-01	1.41E+00	7	1
14484641	ferbam	-1.68E-01	1.45E+00	22	1
51222390	Finasol OSR 2	2.07E+00	2.28E+00	4	1
67298322	Finasol OSR 5	1.90E+00	1.54E-01	2	1
39412516	Finasol SC	1.59E+00	4.71E-02	5	1
74665842	Fire-trol 100	2.34E+00	8.13E-02	3	1
74665864	Fire-trol 931	2.62E+00	3.57E-01	4	1
1.46E+08	florasulam	-1.73E+00	4.14E-01	5	1
69806504	Fluazifop-butyl	2.63E-01	1.49E-01	5	1
79241466	Fluazifop-p-butyl	2.02E-01	1.86E-01	6	1
79622596	Fluazinam	-1.02E+00	3.33E-02	5	1
33245395	fluchloralin	-1.28E+00	8.94E-01	8	1
70124775	flucythrinate	-3.19E+00	9.61E-01	16	1
1.31E+08	Fludioxonil	-2.70E-01	8.18E-02	3	1
42835256	Flumequine	7.53E-01	1.12E+00	9	3
2164172	fluometuron-	1.05E+00	1.04E+00	11	1
206440	Fluoranthene	-1.29E+00	8.04E-01	43	1
86737	fluorene-	2.69E-01	3.98E-01	12	1
144490	fluoroacetic-acid-	2.09E+00	3.73E-01	3	1
15457053	fluorodifen	7.91E-01	8.11E-01	6	1
13738631	Fluoronitrofen	7.81E-01	1.51E-01	5	1
54910893	Fluoxetine	1.66E-01	2.46E+00	16	2
69377817	Fluroxypyr	1.31E+00	1.11E-01	3	1
66332965	Flutolanil	1.16E+00	2.09E-01	13	1
69409945	Fluvalinate	-2.04E+00	1.06E+00	5	1
1.03E+08	Fluvalinate-tau	-2.42E+00	7.97E-02	4	1
54739183	Fluvoxamine	2.58E-01	5.67E-01	8	2

52341330	FMC-35171	-2.76E+00	7.29E-01	14	1
133073	Folpet	-2.04E-01	8.73E-01	26	1
944229	fonofos	-9.28E-01	1.34E+00	12	1
66767393	fonofos	-1.50E+00	1.56E+00	4	1
1.73E+08	Foramsulfuron	-2.23E-01	7.14E+00	3	1
50000	Formaldehyde	1.82E+00	5.84E-01	48	1
64186	Formic acid	2.68E+00	3.95E-01	4	1
2540821	Formothion	1.40E+00	5.83E-02	6	1
39148248	Fosetyl-aluminium	2.04E+00	2.49E-01	7	1
5598527	Fospirate	-2.59E+00	1.02E-02	2	1
98886443	Fosthiazate	8.20E-01	1.35E+00	3	1
27355222	Fthalide	2.36E+00	3.93E-01	3	1
3878191	fuberidazole	5.11E-01	4.10E-01	4	1
57646307	Furalaxyl	1.63E+00	1.15E-01	8	1
67458	furazolidone	-3.42E-01	1.30E+00	5	1
98000	furfuryl-alcohol-	2.64E+00	2.45E-01	2	1
54319	Furosemide	2.10E+00	1.46E+00	5	2
55818865	Fyrquel GT	2.81E-01	4.91E-02	7	1
53763318	Gamlen D	1.19E+00	9.86E-02	3	1
11100042	Gamlen Oil Spill Remover	1.06E+00	4.47E-02	5	1
1.84E+08	Gefitinib	2.50E-01	1.17E-01	2	4
95058814	Gemcitabine	1.90E+00	4.54E-02	3	4
25812300	Gemfibrozil	1.43E+00	8.32E-01	17	2
2.45E+08	Genapol OXD 080	-6.32E-01	2.00E+00	7	1
106241	geraniol-	5.67E-01	1.82E-02	3	1
1.63E+08	Geranol	5.28E-01	9.94E-03	3	1
1310538	germanium-dioxide-	-6.18E-01	1.40E+00	3	1
77182822	Glufosinate-ammonium	1.18E+00	8.71E-01	6	1
556229	glyodin	-7.21E-02	4.06E-01	2	1
107222	glyoxal-	2.24E+00	1.15E-01	2	1
1071836	glyphosate	1.43E+00	8.84E-01	38	1
81591813	Glyphosate-trimethylsulfonium	9.47E-01	1.66E+00	6	1
9000300	Guar-gum-	1.98E+00	2.56E-01	2	1
1.08E+08	Guazatine	9.88E-01	1.63E+00	4	1
12616352	Halowax 1013	-5.76E-01	3.74E-01	2	1
12616363	Halowax 1014	-8.70E-01	1.31E+00	3	1
87237487	Haloxypop ethoxyethyl ester	8.24E-01	9.38E-01	5	1
72619320	Haloxypop-P-methyl	8.66E-02	5.53E-02	2	1
592767	hept-1-ene	2.46E+00	4.86E-02	2	1
76448	heptachlor	-1.25E+00	7.52E-01	80	1
1024573	heptachlor-epoxide-	-2.00E+00	2.15E+00	5	1
111706	heptan-1-ol	1.88E+00	7.33E-02	29	1
142825	heptane-	2.54E+00	1.20E+00	8	1
23560590	Heptenophos	-2.73E-01	3.50E+00	7	1
25637994	hexabromocyclododecane-	-1.47E+00	5.15E-01	2	1
118741	hexachlorobenzene-	-3.13E-01	2.79E+00	9	1
87683	hexachlorobuta-1,3-diene	-7.48E-02	7.90E-01	16	1
77474	hexachlorocyclopentadiene-	-3.07E-02	1.80E+00	5	1
67721	hexachloroethane-	5.04E-01	2.28E-01	19	1
70304	hexachlorophene	-1.45E+00	6.09E-01	3	1
112696	hexadecyldimethylamine-	4.65E-01	3.76E-02	3	1
680319	hexamethylphosphoric-triamide-	3.78E+00	3.33E-03	2	1
111273	hexan-1-ol	2.47E+00	2.65E-01	9	1
626937	hexan-2-ol	2.67E+00	5.07E-02	4	1
623370	hexan-3-ol	2.68E+00	3.28E-02	2	1
110543	hexane-	1.72E+00	2.37E+00	12	1
142621	hexanoic-acid-	2.28E+00	9.06E-02	2	1
111262	hexylamine-	1.44E+00	2.02E-01	2	1
12797874	Houghtosafe 1120	6.25E-01	3.55E-01	8	1
1399800	Hyamine 2389	4.75E-01	2.06E-03	2	1
14235860	hydrargaphen	1.35E-01	1.35E-02	4	1
302012	hydrazine-	-1.66E-01	1.01E+00	16	1

14729829	Hydrazine compd. with copper sulfate	-5.42E-01	1.60E-01	3	1
122667	hydrazobenzene-	3.50E-01	1.46E-01	2	1
7722841	Hydrogen peroxide	1.26E+00	5.36E-01	14	1
7647010	hydrogen-chloride-	2.42E+00	1.23E-03	3	1
74908	hydrogen-cyanide-	-7.55E-01	4.40E-01	5	1
123319	hydroquinone-	-3.97E-01	7.42E-01	12	1
66330889	Hydrothol 191	1.05E-01	9.02E-02	9	1
10004441	Hymexazol	2.43E+00	4.95E-01	6	1
14380611	Hypochlorite	-4.14E-01	5.47E-02	2	1
7790923	hypochlorous-acid-	-5.87E-01	2.18E-02	3	1
15687271	Ibuprofen	1.43E+00	8.05E-01	17	2
70903514	Idet 51	1.47E+00	1.67E-02	2	1
35554440	imazalil	4.73E-01	2.75E-02	3	1
73790280	Imazalil	3.02E-01	5.23E-02	5	1
81405858	Imazamethabenz-methyl	2.24E+00	3.83E-02	5	1
81334341	Imazapyr-acid	5.46E-01	2.58E-02	2	1
1.38E+08	Imidacloprid	1.23E+00	3.24E+00	8	1
50497	Imipramine	-1.15E-01	2.32E-01	2	2
87514	indol-3-ylacetic acid	1.31E+00	9.53E-01	3	1
120729	indole-	4.87E-01	4.74E-01	2	1
1.74E+08	Indoxacarb	-2.04E-01	6.04E-04	2	1
7553562	iodine-	1.99E-01	1.05E-01	3	1
18181709	iodofenphos-	-7.88E-01	6.14E-01	12	1
823041	Iodophenylmercury	-1.25E+00	1.05E-01	5	1
1.45E+08	Iodosulfuron-methyl-sodium	-2.12E+00	1.85E+00	2	1
1689834	ioxynil	2.95E-01	6.21E-01	14	1
5827054	IPSP	-1.80E+00	7.92E-02	2	1
7439896	iron-	9.38E-01	1.52E-01	5	1
12040572	Iron chloride	1.40E+00	1.83E-01	6	1
6047138	iron(2+) dipotassium [R-(R*,R*)]-ditartrate	3.28E+00	1.12E-04	2	1
297789	isobenzan	-5.41E-01	4.75E+00	9	1
110190	isobutyl-acetate-	2.59E+00	1.95E-01	4	1
106638	isobutyl-acrylate-	3.60E-01	2.87E-03	2	1
79312	isobutyric-acid-	2.97E+00	4.84E-01	3	1
25339177	iso-decyl alcohol	8.23E-01	1.70E-01	2	1
96300957	Isodecylidiphenyl ester phosphoric acid mixt. with triphenyl phosphate	9.72E-01	4.19E-01	5	1
29761215	isodecyl-diphenyl-phosphate-	1.91E+00	7.57E+00	3	1
25311711	isofenphos-	-4.01E-01	2.97E+00	5	1
54853	Isoniazid	2.46E+00	9.08E-01	10	2
26952216	isooctan-1-ol	1.64E+00	3.16E-01	2	1
25168154	isooctyl (2,4,5-trichlorophenoxy)acetate	1.28E+00	1.90E-03	2	1
25168267	isooctyl (2,4-dichlorophenoxy)acetate	9.67E-01	4.18E-01	3	1
32534955	isooctyl 2-(2,4,5-trichlorophenoxy)propionate	9.93E-01	2.66E-01	2	1
123922	isopentyl-acetate-	2.07E+00	1.13E-01	2	1
19329896	isopentyl-lactate-	2.17E+00	2.57E-02	2	1
5835267	Isopimaric acid	-3.59E-01	1.78E-01	2	1
78795	isoprene-	2.04E+00	1.18E-01	4	1
2631405	isoprocarb	5.02E-01	1.13E+00	12	1
33820530	isopropalin	-9.45E-01	6.69E-01	2	1
108214	isopropyl-acetate-	2.71E+00	1.86E-01	4	1
75310	isopropylamine-	2.56E+00	3.79E-01	2	1
617516	isopropyl-lactate-	3.03E+00	2.98E-02	2	1
28108998	isopropylphenyl-diphenyl-phosphate-	-4.08E-01	7.50E-02	2	1
50512351	Isoprothiolane	9.31E-01	2.98E-02	3	1
34123596	Isoproturon	1.76E-01	2.58E+00	20	1
119653	isoquinoline-	1.27E+00	8.29E-02	4	1
8401749	Isothan dL-1	-2.78E-01	1.54E-01	4	1
53763385	Jansolve 60	1.65E+00	1.96E-02	2	1
19408469	Kasugamycin	7.41E-01	2.70E-02	7	1
37353632	Kc300 (trichlorinated form)	-2.53E-01	3.00E-01	2	1
22071154	Ketoprofen	8.03E-01	2.98E-01	4	2
52769672	Komeen (copper-ethylenediamine complex(elemental copper 8%))	9.05E-01	2.19E+00	3	1

2425663	Korax	-5.69E-01	3.00E-01	3	1
1.43E+08	Kresoxim-methyl	-7.77E-01	4.36E-03	2	1
79334	L-(+)-lactic acid	2.70E+00	2.08E-01	2	1
78977	lactonitrile-	-2.69E-03	1.53E-02	3	1
91465086	Lambda-cyhalothrin	-3.16E+00	1.34E+00	10	1
42615292	LAS	4.94E-01	5.41E-01	73	1
143077	Lauric acid	1.44E+00	1.08E-03	2	1
8001545	lauryldimethylbenzylammonium chloride	-1.18E-01	4.37E-01	15	1
13826658	Lead nitrite	1.33E+00	4.39E-03	2	1
2164081	Lenacil	-1.86E-01	3.74E+00	6	1
21609905	leptophos-	-1.09E-01	3.19E+00	20	1
137586	Lidocaine	2.20E+00	3.87E-01	6	2
8061516	Lignosulfonic acid, Sodium salt	2.30E+00	4.90E+00	2	1
154212	Lincomycin	8.80E-01	1.96E+00	6	3
859187	lincomycin-hydrochloride	2.52E+00	8.08E-03	2	1
58899	lindane	-7.98E-01	1.30E+00	180	1
9002920	linear dodecanol (ethoxylate)10	6.55E-01	1.26E-01	11	1
330552	linuron	-6.65E-01	1.96E+00	21	1
7439932	Lithium	2.41E+00	2.23E+00	6	2
7447418	lithium-chloride-	1.41E+00	6.40E-01	9	1
98079517	Lomefloxacin	-6.03E-01	1.31E+00	5	3
71212107	Lotos 71	1.79E+00	3.89E-01	4	1
75330755	Lovastatin	-6.36E-02	3.78E+00	2	2
58561787	Magnifloc 521c	4.31E-01	4.29E-04	2	1
1634782	Malaoxon	-1.36E+00	1.65E+00	2	1
121755	Malathion	-3.89E-01	1.79E+00	244	1
10071133	Maleic hydrazide	2.62E+00	6.78E-01	2	1
110167	maleic-acid-	1.86E+00	6.60E-01	4	1
108316	maleic-anhydride-	2.34E+00	9.12E-02	5	1
141822	malonic-acid-	2.31E+00	3.46E-02	2	1
109773	malononitrile-	1.58E-01	1.58E-01	5	1
8018017	Mancozeb	1.89E-01	6.11E-01	23	1
12427382	Maneb	1.78E-01	1.07E+00	39	1
94746	MCPA	1.59E+00	9.33E-01	22	1
94815	MCPB	1.30E+00	3.74E-01	6	1
108394	m-cresol	1.41E+00	1.40E-01	7	1
2595542	mecarbam	3.67E-01	2.19E+00	7	1
32887017	Mecillinam	2.86E-01	4.54E+00	2	3
7085190	Mecoprop	2.11E+00	4.98E-01	10	1
16484778	Mecoprop-p	1.97E+00	4.37E-01	3	1
61687	Mefenamic acid	8.11E-01	3.34E-02	4	2
58275	menadione	-5.05E-01	4.12E-01	2	1
83896	mepacrine	1.85E+00	4.95E-01	6	1
150765	mequinol	1.51E+00	1.41E-01	4	1
2032657	mercaptodimethur	-3.51E-01	1.02E+00	23	1
10045940	mercury-dinitrate-	-2.01E+00	4.65E-01	5	1
108678	mesitylene-	1.33E+00	1.39E-01	4	1
1.04E+08	Mesotrione	1.65E-01	2.20E+00	4	1
57837191	Metalaxyl	1.78E+00	3.28E-01	5	1
41394052	Metamitron	1.52E+00	1.65E+00	6	1
137428	metam-sodium	-4.72E-01	2.04E-01	6	1
108383	meta-xylene	1.23E+00	3.56E-01	9	1
67129082	Metazachlor	8.56E-01	6.42E-01	6	1
657249	Metformin	2.12E+00	1.26E-01	3	2
18691979	methabenzthiazuron-	8.68E-01	1.24E+00	6	1
10265926	methamidophos	-1.66E-01	8.32E+00	10	1
67293747	Methanesulfonic acid, 2,3-Dihydro-3,3-dimethyl-2-ethoxy-5-benzofuranyl ester	2.03E-01	3.24E-01	2	1
124630	methanesulfonyl-chloride-	1.11E+00	9.07E-03	2	1
67561	methanol-	3.75E+00	6.33E-01	15	1
100970	methenamine	4.74E+00	2.50E-02	4	1
950378	methidathion	1.01E-01	1.87E+00	20	1
7379513	Methiocarb phenol	7.54E-01	4.85E-02	3	1

16752775	Methomyl	-8.75E-02	1.07E+00	59	1
40596698	Methoprene	-3.31E-03	1.93E+00	14	1
841065	methoprotryne	1.33E+00	9.32E-02	6	1
72435	methoxychlor	-1.44E+00	1.07E+00	109	1
51338273	methyl 2-(4-(2,4-dichlorophenoxy)phenoxy)propionate	-4.06E-01	4.58E-02	2	1
74222972	methyl 2-[[[(4,6-dimethyl-2-pyrimidinyl)amino]carbonyl]amino]sulphonyl]benzoate	3.32E+00	2.10E-01	5	1
59063	methyl 4-acetamido-2-ethoxybenzoate	1.88E+00	2.19E-01	3	1
1122549	methyl 4-pyridyl ketone	2.57E+00	2.40E-01	2	1
42576023	methyl 5-(2,4-dichlorophenoxy)-2-nitrobenzoate	2.06E-01	4.47E+00	8	1
55634918	methyl 5-[1-[(allyloxy)amino]butylidene]-2,2-dimethyl-4,6-dioxocyclohexanecarboxylate	2.77E+00	1.06E+00	3	1
55635137	methyl 5-[1-[(allyloxy)imino]butyl]-2,2-dimethyl-4,6-dioxocyclohexanecarboxylate, sodium salt	2.46E+00	2.49E-01	8	1
52756259	methyl N-benzoyl-N-(3-chloro-4-fluorophenyl)-DL-alaninate	7.13E-01	5.59E-02	3	1
25474413	Methyl(phenylthio)carbamic acid, 3-(1-Methylpropyl)phenyl ester	-1.65E+00	9.08E-02	4	1
96333	methyl-acrylate-	1.14E+00	2.11E-01	4	1
74895	methylamine	2.34E+00	3.03E-01	4	1
134203	methyl-anthranilate-	1.29E+00	4.02E-02	4	1
35745110	Methylarsonic acid, Ammonium iron (3+) salt	1.89E+00	2.10E-04	2	1
2752810	Methylcarbamic acid, 6-Chloro-m-cumenyl ester	-1.47E+00	6.72E-01	2	1
12407862	Methylcarbamic acid, Mixt. with 2,3,5- and 3,4,5-Trimethylphenyl esters	5.87E-01	5.58E-01	2	1
7286842	Methylchloramben	2.85E-01	1.22E-02	4	1
108872	methylcyclohexane-	1.84E+00	1.70E+00	7	1
144547	methylthiocarbamic-acid-	-7.22E-03	8.97E-01	5	1
6317186	methylene-dithiocyanate-	-5.38E-01	5.90E-01	7	1
60344	methylhydrazine-	2.04E-01	1.18E-01	6	1
556616	Methyl-isothiocyanate	-7.14E-01	1.22E-01	7	1
80626	methyl-methacrylate-	2.65E+00	3.75E-02	7	1
1321944	methylnaphthalene-	4.62E-01	4.27E-01	2	1
77758	methylpentynol	3.08E+00	5.57E-03	10	1
554121	methyl-propionate-	2.96E+00	4.81E-02	2	1
61734	methylthionium-chloride	1.68E+00	4.49E-01	13	1
2533826	Methylthioarsine	3.88E-01	1.23E-01	6	1
5137553	methyltriocylammonium-chloride-	-2.86E-01	6.71E-01	8	1
953173	Methyl-trithion	-6.75E-01	1.35E+00	13	1
9006422	Metiram	3.68E-01	7.00E-01	19	1
3060897	metobromuron	1.46E+00	3.49E-01	14	1
51218452	Metolachlor	1.24E-02	8.90E-01	22	1
51384511	Metoprolol	1.71E+00	2.98E-01	9	2
19937598	metoxuron-	1.29E+00	2.07E+00	11	1
21087649	metribuzin-	-9.21E-02	2.78E+00	21	1
443481	Metronidazole	2.08E+00	6.35E-01	6	3
74223646	Metsulfuron methyl	-1.52E+00	3.51E+00	6	1
7786347	Mevinphos	-1.12E+00	1.27E+00	32	1
315184	mexacarbate	3.36E-02	1.98E+00	47	1
2212671	molinate	6.58E-01	6.68E-01	34	1
7439987	molybdenum-	1.66E+00	1.70E-01	3	1
57055386	Monochlorodehydroabietic acid	2.10E-02	1.37E-01	4	1
6923224	monocrotophos	4.32E-01	2.13E+00	26	1
1746812	monolinuron	8.52E-01	2.50E+00	14	1
150685	monuron	2.07E-01	1.67E+00	16	1
110918	morpholine-	2.17E+00	1.85E-01	8	1
61949766	m-phenoxybenzyl cis-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate	-2.15E+00	1.26E+00	3	1
61949777	m-phenoxybenzyl trans-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate	-1.86E+00	4.49E-01	3	1
780110	m-tert-butylphenyl methylcarbamate	1.35E+00	4.15E-03	2	1
108441	m-toluidine	9.08E-01	5.51E+00	2	1
1129415	m-tolyl methylcarbamate	1.15E+00	2.28E-01	5	1
88671890	Myclobutanil	7.33E-01	1.90E-01	2	1
1.27E+08	N-(2,3-Dichloro-4-hydroxyphenyl)-1-methylcyclohexane carboxamide	8.84E-01	4.30E-01	6	1
3416179	N-(2-Methylpropyl)-a,a-diphenylbenzenemethanamine	-9.89E-01	4.96E-01	2	1
7149793	N-(3-chloro-4-methylphenyl)acetamide	1.70E+00	8.34E-02	6	1
69581335	N-(3-chlorophenyl)-N-(tetrahydro-2-oxo-3-furyl)cyclopropanecarboxamide	1.76E+00	1.29E-01	4	1
1.42E+08	N-(4-Fluorophenyl)-N-(1-methylethyl)-2-[[5-(trifluoromethyl)-1,3,4-thiadiazol-2-	-3.20E-01	2.09E+00	8	1

	yl]oxy]acetamide				
23184669	N-(butoxymethyl)-2-chloro-2',6'-diethylacetanilide	-1.79E-01	6.21E-01	22	1
34911461	N,4-dihydroxy-alpha-oxobenzeneacetimidoyl chloride	5.95E-01	6.41E-01	2	1
1.16E+08	N,N'-1,2-Ethanediylbis(N-(carboxymethyl)glycine trisodium salt mixt. with dodecanamide (1:1)	1.19E+00	1.56E-01	6	1
91667	N,N-diethylaniline	1.01E+00	3.73E-01	3	1
8067490	N,N-Dimethyl-alpha-phenylbenzeneacetamide, Mixt. with 2,6-Dinitro-N,N-dipropyl-4-(trifluoromethyl)benzenamine	-6.38E-01	4.39E-02	2	1
121697	N,N-dimethylaniline	1.65E+00	1.18E-01	11	1
68122	N,N-dimethylformamide	4.08E+00	1.82E-01	9	1
57147	N,N-dimethylhydrazine	9.89E-01	3.40E-01	9	1
2163793	N,N-Dimethyl-N'-(octahydro-4,7-methano-1H-inden-5-yl)urea	1.18E+00	3.70E-01	4	1
99978	N,N-dimethyl-p-toluidine	1.59E+00	2.60E-02	2	1
142596	nabam	3.27E-01	4.35E-01	7	1
35440530	Na-c10-hydroxamate	4.40E-01	3.15E-01	2	1
300765	naled	-7.47E-01	1.47E+00	37	1
389082	Nalidixic acid	4.02E-01	2.46E+00	2	3
8030306	Naphtha-	7.14E-01	7.17E-02	7	1
91203	Naphthalene	6.47E-01	4.64E-01	39	1
120183	naphthalene-2-sulfonic acid	2.36E+00	2.63E-02	3	1
1338245	naphthenic-acid-	1.24E+00	1.50E-01	5	1
22204531	Naproxen	1.49E+00	6.12E-01	20	2
33878501	N-Benzoyl-N-(3,4-dichlorophenyl)-L-alanine, Ethyl ester	7.87E-02	1.08E-02	5	1
123864	n-butyl acetate	2.07E+00	2.62E-01	8	1
1126790	n-butyl phenyl ether	5.02E-01	3.19E-02	3	1
1118463	n-butylin trichloride	-1.43E+00	1.18E+01	4	1
66215278	N-cyclopropyl-1,3,5-triazine-2,4,6-triamine	1.24E+00	3.96E+00	6	1
5538954	N-dodecylpropane-1,3-diamine	1.08E-01	7.77E-02	4	1
555373	neburon-	-1.34E+00	2.86E-01	20	1
1404042	Neomycin	2.84E-01	2.48E+00	3	2
103695	N-ethylaniline	1.42E+00	4.13E-01	5	1
50657	niclosamide	-1.12E+00	1.93E-01	16	1
1.12E+08	Nicosulfuron	1.92E+00	7.02E-03	3	1
500221	nicotinaldehyde-	1.67E+00	4.17E-01	2	1
54115	Nicotine	1.34E+00	2.17E+00	11	2
65305	nicotine-sulfate-	1.01E+00	2.00E-01	6	1
13411160	nifurpirinol	5.73E-01	1.45E-01	17	1
4726141	nitralin	2.97E-01	3.66E+00	4	1
1929824	nitrapyrin-	4.82E-01	4.95E-01	4	1
139139	nitrilotriacetic-acid-	2.35E+00	1.37E-01	8	1
98953	nitrobenzene-	1.47E+00	3.46E-01	17	1
1836755	nitrofen	2.85E-01	3.82E-01	25	1
59870	nitrofural	1.40E+00	4.62E-01	6	1
67209	Nitrofurantoin	0.00E+00	2.00E+00	2	3
10102440	nitrogen-dioxide-	1.58E+00	2.30E-01	5	1
55630	Nitroglycerin	1.01E+00	4.13E-01	13	2
86306	nitrosodiphenylamine-	1.05E+00	4.85E-02	2	1
100618	N-methylaniline	1.45E+00	8.50E-01	8	1
5903139	N-Methyl-N-(1-naphthyl)fluoroacetatamide	1.24E+00	1.10E-01	4	1
70896081	Nokomis 3	1.79E+00	9.98E-02	4	1
143088	nonan-1-ol	1.20E+00	8.78E-02	4	1
112050	Nonanoic acid	1.59E+00	3.64E-01	2	1
112209	nonylamine-	3.45E-01	2.04E-04	2	1
25154523	nonylphenol-	-4.42E-01	3.96E-01	14	1
70458967	Norfloxacin	-3.20E-01	9.63E-01	12	3
72695	Nortriptyline	-3.54E-01	1.22E-02	2	2
59708542	N-Phenyl-N-[1-(3-phenylpropyl)-4-piperidinyl]propamide	-2.11E+00	3.40E-01	2	1
28159980	N'-tert-butyl-N-cyclopropyl-6-(methylthio)-1,3,5-triazine-2,4-diamine	-2.83E+00	3.44E-02	2	1
34643464	O-(2,4-dichlorophenyl) O-ethyl S-propyl dithiophosphate	1.27E-01	7.80E-01	8	1
7533791	O-(2,5-Dichloro-4-iodophenyl)O,O-diethylester phosphorothioic acid	-1.92E-01	2.71E+00	2	1
500287	O-(3-chloro-4-nitrophenyl) O,O-dimethyl thiophosphate	-9.47E-02	1.26E+00	6	1
41198087	O-(4-bromo-2-chlorophenyl) O-ethyl S-propyl phosphorothioate	-1.78E+00	1.40E+00	8	1

3244904	O,O,O',O'-tetrapropyl pyrophosphorothioate	-1.73E+00	4.44E-01	2	1
119120	O,O-diethyl O-(1,6-dihydro-6-oxo-1-phenylpyridazin-3-yl) thiophosphate	2.84E-01	1.98E+00	6	1
18854018	O,O-diethyl O-5-phenylisoxazol-3-ylphosphorothioate	2.65E-01	2.33E-01	3	1
1112385	O,O-Dimethyl ester, Phosphorodithioic acid	1.52E+00	2.26E-02	2	1
756809	O,O-dimethyl hydrogen dithiophosphate	1.41E+00	5.44E-02	3	1
52608	O-[3,5-Dimethyl-4-(methylthio)phenyl]O,O-diethyl ester phosphorothioic acid	-6.16E-01	1.46E-01	2	1
141333	O-butyl hydrogen dithiocarbonate , sodium salt	1.79E+00	1.65E-02	2	1
22555164	O-Butyl-O-methyl-O(1,2,5-thiadiazolyl-3)phosphorothioate	-1.70E+00	2.18E+00	2	1
95487	o-cresol	1.55E+00	1.76E-01	35	1
27304138	Octachlor epoxide	-1.16E+00	3.26E+00	2	1
25267156	Octachloro-2-pinene	-1.97E+00	7.40E-02	3	1
111875	octan-1-ol	1.46E+00	2.20E-01	12	1
106683	octan-3-one	2.30E+00	3.49E-01	2	1
111659	octane-	-1.96E+00	2.16E+00	2	1
111864	octylamine-	2.92E-02	7.04E-01	3	1
35400432	O-ethyl O-(4-methylthiophenyl) S-propyl dithiophosphate	1.06E-01	2.11E+00	13	1
2104645	O-ethyl O-4-nitrophenyl phenylphosphonothioate	-9.74E-01	1.82E+00	36	1
16058256	Oleic acid compd. with 1-Methyltetradecylamine(1:1)	6.09E-01	1.10E-01	3	1
16058314	Oleic acid compd. with N-(1-methyltetradecyl)-1,3-propanediamine (1:1)	2.14E-01	8.50E-02	4	1
16058325	Oleic acid compd. with N-(1-Methyltetradecyl)-1,3-propanediamine(2:1)	1.07E-01	9.34E-02	4	1
73590586	Omeprazole/Esomeprazole	1.56E+00	1.63E-01	3	2
1113026	Omethoate	1.07E+00	2.13E+00	12	1
34622587	Orbencarb	4.77E-01	5.90E-03	2	1
83987	Orphenadrine	1.42E+00	7.58E-01	11	2
95476	ortho-xylene	1.21E+00	3.89E-01	16	1
19044883	Oryzalin	-4.56E-01	6.63E-03	2	1
95534	o-toluidine	1.77E+00	3.99E-01	9	1
77732093	Oxadixyl	2.39E+00	2.43E-01	4	1
144627	Oxalic acid	2.90E+00	1.17E+00	2	1
10380286	oxine-copper	3.24E-01	1.10E+00	7	1
14698294	Oxolinic acid	1.07E-01	1.54E+00	5	3
5259881	oxycarboxin	1.33E+00	2.33E-01	3	1
301122	oxydemeton-methyl	4.95E-01	7.63E-01	14	1
693210	oxydiethylene-dinitrate-	2.35E+00	7.40E-02	9	1
42874033	oxyfluorfen	-5.21E-01	4.09E+00	7	1
10028156	ozone-	-4.01E-01	2.37E-01	10	1
80466	p-(1,1-dimethylpropyl)phenol	5.16E-02	2.36E-01	3	1
72548	p,p'-DDD	-1.50E+00	1.35E+00	32	1
72559	p,p'-DDE	-1.11E+00	2.14E+00	12	1
76738620	Paclobutrazol	1.36E+00	5.64E-02	8	1
104949	p-anisidine	9.32E-01	1.09E+00	2	1
950356	Paraoxon-methyl	-6.80E-01	2.04E+00	3	1
1910425	Paraquat-dichloride	6.65E-01	1.76E+00	34	1
56382	Parathion	-1.13E+00	2.05E+00	140	1
298000	parathion-methyl	-3.15E-02	2.12E+00	123	1
106423	para-xylene	1.21E+00	5.96E-01	7	1
1263894	paromomycin-sulfate	3.00E+00	3.77E-02	2	1
61869087	Paroxetine	6.86E-01	1.13E+00	6	2
106514	p-benzoquinone	-1.11E+00	3.93E-04	2	1
80002	p-chlorophenyl phenyl sulphone	5.82E-01	2.00E-01	4	1
140385	p-Chlorophenylurea	1.63E+00	1.11E-01	9	1
106445	p-cresol	1.17E+00	1.68E-01	12	1
99876	p-cymene	1.13E+00	2.37E-01	4	1
104438	p-dodecylphenol	-8.39E-01	4.49E-04	2	1
1114712	pebulate	1.31E+00	2.05E-01	8	1
66246886	Penconazole	4.72E-01	9.78E-02	8	1
66063056	Pencycuron	1.00E+00	7.27E-01	8	1
40487421	Pendimethaline	-1.69E-01	8.87E-01	13	1
527208	pentachloroaniline-	-8.87E-01	2.66E-01	2	1
1825214	Pentachloroanisole	-8.76E-01	9.50E-01	2	1
608935	pentachlorobenzene-	-9.63E-02	1.04E+00	13	1
76017	pentachloroethane-	1.34E+00	3.19E-01	7	1

82688	Pentachloronitrobenzene	4.09E-01	5.46E-01	2	1
87865	Pentachlorophenol	-2.17E-01	7.35E-01	160	1
15773350	Pentachlorophenol copper salt	-6.38E-01	6.16E-01	3	1
3772949	pentachlorophenyl-laurate-	1.39E+00	4.61E-01	2	1
2176627	pentachloropyridine-	-3.72E-02	1.71E-01	2	1
78115	pentaerithrityl-tetranitrate	4.19E+00	1.12E-01	2	1
71410	pentan-1-ol	2.73E+00	4.41E-02	12	1
123546	pentane-2,4-dione	1.93E+00	2.00E-01	15	1
2307688	pentanochlor-	1.28E+00	3.99E-02	5	1
7758294	pentasodium-triphosphate-	2.35E+00	2.86E-01	3	1
628637	pentyl-acetate-	2.24E+00	4.06E-01	4	1
110587	pentylamine-	2.13E+00	2.75E-02	2	1
6382065	pentyl-lactate-	2.20E+00	5.99E-02	2	1
37262616	Pep:eugenol (7:3)	1.22E+00	4.65E-04	2	1
79210	Peracetic acid	2.96E-01	9.01E-01	3	1
121824	perhydro-1,3,5-trinitro-1,3,5-triazine	8.79E-01	1.48E-02	4	1
52645531	Permethrin	-1.80E+00	2.11E+00	107	1
8002059	Petroleum-	1.01E+00	7.73E-02	2	1
85018	Phenanthrene	-4.51E-01	1.40E-01	15	1
229878	phenanthridine-	-2.03E-01	7.19E-01	3	1
2275141	phenkapton-	4.06E-01	2.40E+00	8	1
13684634	Phenmedipham	6.44E-01	6.64E-01	11	1
50066	Phenobarbital	3.12E+00	5.73E-01	10	2
108952	Phenol	1.79E+00	7.33E-01	224	1
84852153	Phenol, 4-nonyl-, branched	-1.12E+00	1.00E-01	11	1
2597037	phenthoate	-1.15E+00	1.72E+00	36	1
14548460	phenyl 4-pyridyl ketone	2.18E+00	5.89E-02	2	1
103822	phenylacetic-acid-	1.74E+00	1.20E+00	3	1
62384	phenylmercury-acetate-	-9.90E-01	6.77E-01	21	1
1192898	phenylmercury-bromide-	6.33E-01	3.67E-01	6	1
100561	phenylmercury-chloride-	-9.84E-01	2.01E-01	5	1
118558	phenyl-salicylate-	7.51E-02	1.36E-03	2	1
2446697	p-hexylphenol	-3.84E-01	2.28E-01	2	1
298022	phorate	-8.96E-01	2.14E+00	26	1
2310170	phosalone	-5.75E-01	1.57E+00	20	1
56646050	Phoschek 202	2.24E+00	4.68E-01	6	1
39341156	Phos-chek 259	2.32E+00	1.76E-01	6	1
1.77E+08	Phoschek WD 881	1.20E+00	4.10E-02	4	1
947024	phosfolan	9.35E-01	8.90E-02	4	1
732116	phosmet	-5.76E-01	1.26E+00	27	1
13171216	Phosphamidon	6.38E-01	2.20E+00	48	1
2665283	Phosphoric acid, 2-Chloro-1-(2,4,5-trichlorophenyl)ethenyl diethyl ester	-4.74E-01	2.66E-01	3	1
2782709	Phosphorodithioic acid, S,S'-(Phenylmethylene) O,O,O',O'-tetramethyl ester	-3.20E-01	3.00E+00	5	1
1174830	Phosphorothioic acid, O,O'-(Sulfonyldi-p-phenylene) O,O,O',O'-tetramethyl ester	-3.00E-01	1.30E-01	3	1
2274999	Phosphorothioic acid, S,S'-Benzylidene O,O,O',O'-tetramethyl ester	-1.04E+00	2.56E-01	5	1
7723140	phosphorus-	-1.43E+00	2.40E-01	8	1
13350715	Photoaldrin	-1.22E+00	6.20E-02	2	1
13366739	Photodieldrin	-1.60E+00	1.47E-01	5	1
33442830	Photoheptachlor	-1.81E+00	2.55E-01	3	1
3212280	Photoisodrin	-1.90E+00	1.98E-02	2	1
14816183	Phoxim	-6.59E-01	1.08E+00	16	1
253521	phthalazine-	1.97E+00	4.86E-01	3	1
85449	phthalic-anhydride-	1.76E+00	8.71E-01	3	1
1918021	picloram	1.49E+00	3.63E-01	17	1
1.17E+08	Picoxystrobin	1.77E+00	6.42E-02	5	1
88891	picric-acid-	2.09E+00	1.55E-01	12	1
124878	picrotoxin-	1.36E+00	3.86E-01	2	1
94622	piperine-	1.35E+00	4.08E-01	2	1
51036	Piperonyl butoxide	1.89E-01	1.72E-01	18	1
23103982	pirimicarb-	1.51E+00	1.02E+00	22	1
29232937	Pirimiphos methyl	-8.91E-01	2.05E+00	31	1
75989	pivalic-acid-	3.31E+00	2.69E-01	2	1

104405	p-nonylphenol	-4.74E-01	5.53E-02	16	1
31512740	Poly[oxy-1,2-ethanediyl(dimethyliminio)-1,2-ethane diyl(dimethyliminio-1,2-ethanediyl dichloride	-4.80E-01	4.53E-01	5	1
53763556	Polyclens	1.34E+00	1.39E-01	4	1
11113807	Polyoxin	9.07E-01	3.53E-01	5	1
68333799	Polyphosphoric acids, ammonium salts	2.81E+00	2.81E-01	4	1
25322694	Polypropylene glycol	3.02E+00	8.72E-02	2	1
53466721	Polystream (mixed polychlorinated benzenes)	-2.52E-01	1.20E-04	2	1
9009523	Polysub 164	8.52E-01	6.48E-02	3	1
25655418	Polyvinyl pyrrolidoneiodine	2.17E+00	1.23E+00	2	1
7440097	potassium-	2.17E+00	4.02E-01	2	1
2818168	potassium 2-(2,4,5-trichlorophenoxy)propionate	2.00E+00	1.91E-05	2	1
5746178	potassium 2-(2,4-dichlorophenoxy)propionate	2.27E+00	1.81E-01	4	1
1929868	potassium 2-(4-chloro-2-methylphenoxy)propionate	2.00E+00	7.34E-03	2	1
2545600	potassium 4-amino-3,5,6-trichloropyridine-2-carboxylate	1.60E+00	5.35E-01	7	1
28300745	potassium antimony tartrate hemihydrate	1.22E+00	2.19E-01	3	1
5871170	Potassium diethyl thiophosphate	1.91E+00	1.73E-02	2	1
1310583	potassium hydroxide, in aqueous solution	2.06E+00	4.67E-02	2	1
140896	potassium O-ethyl dithiocarbonate	1.53E+00	6.57E-02	2	1
2720732	potassium O-pentyl dithiocarbonate	8.66E-01	3.03E-01	2	1
7778805	potassium sulfate, containing in the dry state more than 52 per cent by weight of K2O	2.96E+00	2.29E-01	7	1
20762601	potassium-azide-	7.71E-01	1.15E-01	7	1
584087	potassium-carbonate-	2.85E+00	6.09E-03	3	1
3811049	potassium-chlorate-	2.55E+00	1.04E-01	2	1
7447407	potassium-chloride-	2.93E+00	2.73E-01	29	1
7789006	potassium-chromate-	1.05E+00	1.24E+00	45	1
151508	potassium-cyanide-	-2.84E-01	9.72E-01	27	1
7778509	potassium-dichromate-	9.26E-01	1.37E+00	179	1
7778770	potassium-dihydrogenorthophosphate-	6.11E-01	7.28E-01	5	1
7681110	potassium-iodide-	2.75E+00	3.14E-01	2	1
7757791	potassium-nitrate-	1.42E+00	1.22E+00	9	1
7778747	potassium-perchlorate-	1.38E+00	1.71E+00	3	1
7722647	potassium-permanganate-	3.99E-01	4.56E-01	34	1
333200	potassium-thiocyanate-	1.72E+00	4.50E-01	3	1
106503	p-phenylenediamine	1.61E+00	1.35E-01	2	1
50248	Prednisolone	3.55E-01	1.97E+00	2	2
51218496	Pretilachlor	-1.21E+00	3.82E+00	4	1
721506	Prilocaine	2.08E+00	6.80E-02	3	2
67747095	Prochloraz	-1.06E-02	3.70E-01	7	1
14088712	proclonol	1.88E-01	1.39E-01	2	1
32809168	Procymidone	1.50E+00	1.03E+00	3	1
1610180	prometon	1.07E+00	4.87E-01	12	1
7287196	Prometryn	-2.00E-01	1.55E+00	19	1
72574959	Pro-noxfish	-1.44E+00	2.22E+00	2	1
107197	prop-2-yn-1-ol	5.79E-01	3.64E-01	3	1
1918167	Propachlor	-2.97E-01	9.18E-01	16	1
24579735	Propamocarb	2.54E+00	2.33E-02	6	1
25606411	Propamocarb hydrochloride	2.54E+00	8.17E-06	3	1
71238	propan-1-ol	3.55E+00	5.00E-02	28	1
67630	propan-2-ol	3.82E+00	1.15E-01	7	1
57556	propane-1,2-diol	3.57E+00	9.46E-03	2	1
709988	propanil	8.39E-01	3.52E-01	36	1
7292162	Propaphos	1.12E+00	1.23E-03	2	1
1.11E+08	Propaquizafop	-4.26E-01	1.24E-01	4	1
2312358	propargite-	1.03E-01	1.25E+00	2	1
139402	propazine	9.14E-01	8.19E-01	6	1
31218834	Propetamphos	-1.42E-01	1.77E+00	10	1
122429	propham	1.25E+00	3.08E-01	12	1
60207901	Propiconazole	3.01E-01	9.27E-01	24	1
123386	propionaldehyde-	2.06E+00	6.49E-03	2	1
79094	propionic-acid-	2.42E+00	4.58E-01	4	1
2078548	Propofol	8.12E-02	4.27E-01	5	2

114261	Propoxur	-7.50E-02	1.14E+00	56	1
1.81E+08	propoxycarbazone-sodium	-2.49E-02	2.81E+00	3	1
525666	Propranolol	7.08E-01	1.01E+00	22	2
109604	propyl-acetate-	2.37E+00	2.36E-01	4	1
107108	propylamine-	2.74E+00	1.31E-01	2	1
103651	propylbenzene-	5.36E-01	6.89E-01	5	1
77996	propylidynetrimethanol-	4.04E+00	7.74E-02	3	1
23950585	Propyzamide	3.96E-01	3.01E+00	5	1
52888809	Prosulfocarb	3.96E-02	1.46E-01	11	1
140932	proxan-sodium	1.45E+00	1.56E+00	2	1
106490	p-toluidine	9.68E-01	2.14E+00	5	1
39429715	Purifloc C-31	-1.77E-01	5.34E-02	5	1
66594329	Pydraul 115E	1.01E+00	3.97E-01	6	1
66594318	Pydraul 50E	2.76E-01	2.02E-01	20	1
77458016	Pyraclofos	-1.07E+00	2.76E-03	2	1
13457186	Pyrazophos	-1.66E-01	1.93E+00	21	1
71561110	Pyrazoxyfen	-3.48E-01	1.81E+00	8	1
129000	pyrene-	-1.84E+00	5.68E-01	9	1
8003347	Pyrethrins-and-Pyrethroids-	-1.51E+00	2.46E-01	26	1
96489713	Pyridaben	-2.66E+00	2.22E-01	4	1
40020017	Pyridafol	1.05E+00	2.62E-01	2	1
55512339	Pyridate	1.36E+00	9.29E-01	4	1
123331	pyridazine-3,6(1H,2H)-dione	2.21E+00	4.17E-01	5	1
110861	pyridine-	2.25E+00	8.56E-01	34	1
100709	pyridine-2-carbonitrile	2.84E+00	1.26E-03	2	1
1086028	pyridinitril	1.07E+00	2.30E+00	5	1
88283414	Pyrifenox	4.28E-02	1.02E+00	7	1
58140	Pyrimethamine	8.66E-01	6.47E-02	5	2
53112280	Pyrimethanil	1.05E+00	1.66E-01	5	1
55949387	Pyrimidinol (6-isopropyl-4-methyl-2-pyrimidinol)	3.05E+00	1.68E-03	2	1
95737681	Pyriproxyfen	-1.58E+00	2.77E+00	4	1
120809	pyrocatechol-	8.60E-01	2.24E-02	2	1
57369321	Pyroquilon	1.53E+00	2.02E-02	7	1
68424851	Quaternary ammonium compounds, benzyl-C12-16-alkyldimethyl, chlorides	3.11E-01	2.66E-01	3	1
68391037	Quaternary ammonium compounds, C12-18-alkyltrimethyl, chlorides	-4.13E-01	3.92E-02	2	1
68514954	Quaternary ammonium compounds, di-C12-20-alkyldimethyl, chlorides	7.34E-01	5.84E-01	6	1
61789773	Quaternary ammonium compounds, dicoco alkyldimethyl, chlorides	-9.05E-02	1.14E-01	4	1
68783788	Quaternary ammonium compounds, dimethylditallow alkyl, chlorides	-1.42E-01	9.57E-01	8	1
1.12E+08	Quetiapine	1.12E+00	1.15E-01	3	2
13593038	quinalphos	-4.49E-01	1.61E+00	16	1
56542	Quinidine	1.56E+00	9.70E-01	6	2
90717036	Quinmerac	1.89E+00	8.06E-02	4	1
2797515	Quinoclamine	-2.49E-02	3.82E-01	8	1
148243	quinolin-8-ol	1.16E+00	1.89E-02	2	1
91225	quinoline-	1.68E+00	2.21E-01	16	1
66357355	Ranitidine	-4.83E-01	4.64E-01	3	2
8002139	Rape-oil-	9.56E-01	5.63E-02	8	1
5349280	REE (Ethyl thiocyanatoacetate)	1.55E+00	1.07E-02	4	1
10453868	resmethrin	-2.34E+00	2.15E-01	11	1
10453868	resmethrin	-2.53E+00	3.58E-01	17	1
108463	resorcinol-	1.35E+00	1.38E+00	7	1
1.23E+08	Rimsulfuron	7.54E-01	1.24E+00	3	1
25875518	robenidine	-8.16E-01	1.89E-01	4	1
12738464	Rodine 213	-2.78E+00	3.47E-04	2	1
76560695	Rodine 31A	-2.13E+00	6.89E-05	2	1
26027383	Rokafenol N-8	1.19E+00	1.38E-02	5	1
84057954	Ropivacaine	1.63E+00	1.63E-02	3	2
11121485	Rose Bengal	1.92E+00	8.53E-04	2	1
66829047	Rotanina W	1.18E+00	1.48E+00	4	1
38641940	Roundup	1.42E+00	9.66E-01	32	1
80214831	Roxithromycin	1.06E+00	2.74E+00	4	3
2937533	S-(2-aminoethyl) hydrogen thiosulphate	1.38E+00	1.42E-01	3	1

2674911	S-(2-ethylsulfinyl-1-methylethyl) O,O-dimethyl phosphorothioate	1.37E+00	2.32E-02	4	1
3309873	S-(4-Chlorophenyl)O,O-dimethyl ester phosphorothioic acid	1.19E+00	2.18E-02	4	1
150505	S,S',S"-tributyl phosphorotrithioite	8.50E-01	1.64E-01	3	1
78488	S,S,S-tributylphosphorotrithioate	-4.38E-01	1.66E+00	18	1
28249776	S-4-chlorobenzyl diethylthiocarbamate	1.42E-01	3.17E-01	46	1
90028	salicylaldehyde-	8.18E-01	1.69E-01	27	1
87172	salicylanilide-	-3.80E-01	4.24E+00	2	1
69727	Salicylic acid	2.24E+00	3.48E-01	7	2
57425613	SAN-75	1.08E+00	6.72E-01	6	1
8047152	saponin-	2.08E+00	5.37E-02	6	1
78587050	Savey	5.42E-01	2.01E-01	4	1
26087478	S-benzyl diisopropyl phosphorothioate	9.62E-01	1.07E-01	16	1
152169	schradan	2.63E+00	7.40E-01	5	1
1.11E+08	Scourge II	-2.86E+00	1.00E-01	2	1
3687136	SD-7727	5.95E-01	5.73E-03	2	1
26259450	secbumeton-	1.47E+00	1.34E-02	4	1
7783008	selenious-acid-	-5.43E-02	4.57E-02	3	1
7782492	selenium-	6.73E-01	7.46E-01	18	1
2578281	Seleno-dL-methionine	6.80E-01	5.17E+00	2	1
53572615	Selest	1.18E+00	2.32E-01	4	1
79617962	Sertraline	-4.46E-01	5.53E-01	13	2
74051802	Sethoxydim	1.19E+00	2.89E-01	17	1
66829036	Siarczanol N 2	1.31E+00	4.67E-01	4	1
1.77E+08	Silv-ex(fire suppressant)	7.04E-01	1.07E+00	4	1
122349	Simazine	4.25E-01	1.44E+00	50	1
1014706	simetryn	-1.05E+00	1.09E+00	50	1
79902639	Simvastatin	1.30E+00	3.71E-01	4	2
95312940	Slick-A-way	1.47E+00	3.52E-02	3	1
53763647	Slickgone 1	1.15E+00	1.95E-01	4	1
53763658	Slickgone 2	1.01E+00	2.29E-01	4	1
53763670	Slix	1.36E+00	2.15E-01	7	1
87392129	S-metolachlor	-1.22E+00	1.33E+00	3	1
127208	sodium 2,2-dichloropropionate	2.65E+00	2.31E-02	4	1
2439001	sodium 2,3,6-trichlorophenylacetate	1.14E+00	2.31E-01	6	1
2702729	sodium 2,4-dichlorophenoxyacetate	1.37E+00	4.22E+00	16	1
50540619	Sodium 2,5-dichloro-4-bromophenol	-1.07E-01	3.40E-02	5	1
13150000	sodium 2-[2-[2-(dodecyloxy)ethoxy]ethoxy]ethyl sulphate	1.24E+00	8.93E-01	2	1
587984	sodium 3-(p-anilinophenylazo)benzenesulphonate	1.54E+00	2.47E-01	2	1
6416688	sodium 4-(2H-naphtho[1,2-d]triazol-2-yl)stilbene-2-sulphonate	3.21E+00	9.52E-03	2	1
6062266	sodium 4-(4-chloro-o-tolyloxy)butyrate	1.58E+00	2.54E-01	6	1
5138909	sodium 4-chlorobenzenesulfonate	3.71E+00	3.03E-02	2	1
3653483	sodium 4-chloro-o-tolyloxyacetate	2.54E+00	3.59E-02	6	1
825901	sodium 4-hydroxybenzenesulfonate	3.87E+00	2.18E-02	2	1
3567257	sodium 5-chloro-2-[4-chloro-2-[[[(3,4-dichlorophenyl)amino]carbonyl]amino]phenoxy]benzenesulphonate	8.98E-01	1.36E-03	2	1
128563	sodium 9,10-dihydro-9,10-dioxoanthracene-1-sulfonate	2.02E+00	1.21E-01	2	1
12680487	Sodium chromate (unknown formula)	2.40E-01	3.68E+00	2	1
2386530	sodium dodecane-1-sulphonate	1.54E+00	4.44E-01	6	1
25155300	sodium dodecylbenzenesulphonate, pure	9.33E-01	3.42E-01	17	1
7631905	sodium hydrogensulfite, in aqueous solution	2.19E+00	4.44E-02	5	1
1310732	sodium hydroxide, solid	2.02E+00	7.70E-02	4	1
127526	sodium N-chlorobenzenesulfonamide	2.25E+00	3.51E-02	2	1
7631994	sodium nitrate, other than natural	3.21E+00	2.84E-01	23	1
10042849	Sodium nitrilotriacetate	2.14E+00	6.54E-02	3	1
1191500	sodium n-tetradecyl sulfate	3.26E-01	3.72E-01	3	1
140909	sodium O-ethyl dithiocarbonate	5.30E-01	1.94E+00	2	1
25306756	sodium O-isobutyl dithiocarbonate	1.23E+00	8.98E-01	2	1
36551210	sodium O-sec-butyl dithiocarbonate	1.58E+00	8.54E-01	2	1
5896548	sodium pentadecane-1-sulphonate	1.07E+00	2.70E-01	3	1
26970821	Sodium selenite pentahydrate	3.06E-01	3.32E-01	11	1
127093	sodium-acetate-	3.81E+00	3.22E-02	5	1
26628228	sodium-azide-	8.19E-01	5.09E-01	13	1

7647156	sodium-bromide-	1.85E+00	4.61E+00	12	1
156547	sodium-butyrate-	3.49E+00	8.36E-02	2	1
7775099	sodium-chlorate-	3.26E+00	6.47E-01	13	1
7647145	sodium-chloride-	3.83E+00	1.54E-01	43	1
7775113	sodium-chromate-	1.23E+00	7.76E-01	24	1
143339	sodium-cyanide-	-2.23E-01	6.62E-01	45	1
142870	sodium-decyl-sulphate-	2.32E+00	2.42E-01	2	1
10588019	sodium-dichromate-	3.57E-01	2.65E+00	14	1
124652	sodium-dimethylarsinate-	1.60E+00	1.43E-01	4	1
128041	sodium-dimethyldithiocarbamate-	-8.23E-01	1.75E+00	4	1
7784465	sodium-dioxoarsenate-	1.11E+00	7.79E-01	40	1
151213	sodium-dodecyl-sulfate-	8.03E-01	3.99E-01	81	1
15708415	sodium-feredetate	1.90E+00	6.81E-02	7	1
7681494	sodium-fluoride-	2.58E+00	1.73E+00	24	1
1120010	sodium-hexadecyl-sulfate-	-1.82E-01	1.17E-03	2	1
144558	sodium-hydrogencarbonate-	3.08E+00	6.85E-01	6	1
7681529	sodium-hypochlorite-	-2.43E-01	5.97E-01	92	1
7681552	sodium-iodate-	2.11E+00	3.36E-01	2	1
7681825	sodium-iodide-	1.67E+00	7.19E+00	2	1
15120179	sodium-metaarsenate-	4.66E-01	5.77E-01	2	1
13718268	sodium-metavanadate-	9.14E-01	3.00E-01	17	1
2163806	sodium-methylarsonate-	2.16E+00	4.54E-01	15	1
61790134	sodium-naphthenate-	1.21E+00	9.89E-02	5	1
7632000	sodium-nitrite-	1.60E+00	8.69E-01	60	1
131522	sodium-pentachlorophenolate-	-3.33E-01	4.87E-01	110	1
137406	sodium-propionate-	3.60E+00	1.03E-02	2	1
13410010	sodium-selenate-	1.01E+00	1.08E+00	39	1
10102188	sodium-selenite-	9.03E-01	6.53E-01	44	1
7757837	sodium-sulfite-	3.00E+00	3.27E-01	7	1
11067826	sodium-tetrapropylenebenzenesulphonate-	1.42E+00	7.12E-02	6	1
7772987	sodium-thiosulfate-	3.59E+00	5.04E-01	3	1
6106418	sodium-valerate-	3.48E+00	9.84E-02	2	1
1.68E+08	Spinosad	3.29E-01	4.82E-01	5	1
8025818	Spiramycin	-9.70E-01	3.55E+00	2	3
1929777	S-propyl dipropylthiocarbamate	4.57E-01	4.30E-01	9	1
85409172	Stannane, tributyl-, mono(naphthenoxy) derivs.	-2.39E+00	1.43E+00	6	1
81406373	Starane	-3.75E-01	2.41E-01	4	1
13071799	S-tert-butylthiomethyl O,O-diethylphosphorodithioate	-2.03E+00	1.26E+00	14	1
57921	Streptomycin	2.78E-01	3.02E+00	6	3
8001501	Strobane	-1.19E+00	6.51E-01	14	1
57249	strychnine-	-4.14E-02	7.30E-04	2	1
60413	strychnine-sulfate-	4.01E-01	2.52E-01	2	1
82713	styphnic-acid-	3.01E+00	1.29E+00	3	1
100425	styrene-	1.33E+00	3.23E-01	14	1
99105778	Sulcotrione	1.16E+00	2.92E+00	2	1
68359	Sulfadiazine	9.59E-01	1.21E+00	7	3
723466	Sulfamethoxazole	6.83E-01	2.06E+00	18	3
68608151	Sulfonic acids, alkane, sodium salts	9.89E-01	2.48E-04	2	1
3689245	sulfotep	-1.95E+00	1.52E+00	7	1
7704349	Sulfur, precipitated, sublimed or colloidal	1.55E+00	6.89E+00	2	1
76930580	Sulfuric acid diammonium salt mixt. with diammonium hydrogen phosphate	2.31E+00	1.71E-01	4	1
8066771	Sulfuric acid monododecyl ester sodium salt, Mixt. with Tetradecyl sodium sulfate	8.46E-01	2.25E-02	2	1
13772162	Sulfuric acid, Ammonium iron salt (2:1:1), Decahydrate	1.39E+00	1.90E-02	2	1
7664939	sulfuric-acid-	1.63E+00	1.32E-05	2	1
3761602	Sulfurous acid, 2-Chloroethyl 2-(2-(4-(1,1-dimethylethyl)phenoxy)-1-methylethoxy)-1-methylethyl ester	1.05E+00	4.44E-01	5	1
3.41E+08	Sunitinib	-1.59E-01	5.08E-02	2	4
58561889	Superfloc 330	-2.11E-01	5.28E-02	5	1
8011765	Superphosphates-	2.92E+00	1.37E+00	9	1
1E+08	Suquin	-3.61E+00	4.84E-02	2	1
67167026	Swanic 6L	2.25E-01	5.64E-01	5	1
75139616	Swaryl 10C	1.21E+00	2.11E-02	2	1

75139627	Swascofix CD 38	1.38E+00	1.24E-02	2	1
1918189	Swep	7.46E-01	7.22E-02	7	1
61791262	Tallow alkyl amines, Ethoxylated	6.62E-01	2.16E-01	13	1
1401554	tannic-acid-	7.68E-01	1.57E+00	7	1
650511	TCA	2.43E+00	1.78E+00	16	1
1.08E+08	Tebuconazole	5.68E-01	3.89E-01	10	1
1.12E+08	Tebufenozide	2.74E-01	6.14E-01	5	1
1.19E+08	Tebufenpyrad	-1.02E+00	5.64E-01	3	1
117180	tecnazene	-2.23E-01	6.93E-02	7	1
83121180	Teflubenzuron	-1.05E+00	9.51E+00	3	1
3383968	temephos- (ISO); temefos	-1.19E+00	2.49E+00	113	1
107493	TEPP	-1.31E-02	6.01E-01	9	1
1.5E+08	Tepraloxymid	4.85E-01	7.62E-01	5	1
33693048	terbumeton	1.25E+00	1.77E-01	6	1
5915413	Terbuthylazine	3.64E-01	1.59E+00	15	1
886500	Terbutryn	-4.35E-01	1.64E+00	19	1
540885	tert-butyl acetate	2.96E+00	2.72E-01	4	1
1663394	tert-butyl acrylate	1.49E+00	3.42E-02	2	1
1634044	tert-butyl methyl ether	3.11E+00	1.63E-01	2	1
25013165	tert-butyl-4-methoxyphenol	5.29E-01	2.12E-01	5	1
75649	tert-butylamine	1.76E+00	2.40E-01	3	1
98066	tert-butylbenzene	1.76E+00	5.71E-03	2	1
56803373	tert-butylphenyl diphenyl phosphate	-6.73E-01	4.53E-02	2	1
58220	Testosterone	3.71E-01	6.05E-02	3	2
1461252	tetrabutyltin-	-7.93E-01	6.87E-01	6	1
16903358	tetrachloroauric-acid-	6.65E-01	7.91E-01	3	1
1198556	tetrachlorocatechol	2.53E-01	4.89E-02	4	1
127184	tetrachloroethylene-	9.14E-01	4.28E-01	27	1
56235	Tetrachloromethane	1.27E+00	9.35E-01	16	1
25167833	Tetrachlorophenol	-6.47E-01	1.24E-01	8	1
22248799	Tetrachlorvinphos	2.45E-01	2.44E-01	4	1
116290	tetradifon	-1.00E-01	3.42E-01	10	1
78002	tetraethyllead-	-8.99E-01	3.01E-01	8	1
597648	tetraethyltin-	-1.23E+00	3.94E-01	3	1
109999	tetrahydrofuran-	3.52E+00	5.11E-02	3	1
4136918	Tetra-isopropylthiuram disulfide	-1.95E+00	1.65E-02	2	1
7696120	Tetramethrin	-1.10E-01	1.04E+00	8	1
2782914	tetramethyl-2-thiourea	2.61E+00	3.77E-01	5	1
80126	Tetramethylenedisulfotetramine	-1.28E+00	6.35E-02	3	1
75741	tetramethyllead-	-1.65E-01	1.22E+00	9	1
97745	tetramethylthiuram-monosulfide-	-5.10E-01	1.02E+00	5	1
632224	tetramethylurea-	3.06E+00	2.12E-01	4	1
13943583	tetrapotassium-hexacyanoferrate-	8.55E-01	2.05E+00	4	1
11067815	tetrapropylenebenzenesulphonic-acid-	1.49E+00	1.47E-01	18	1
2556425	tetrapropylthioperoxycarbamic-acid-	-5.39E-01	9.31E-01	3	1
64028	tetrasodium-ethylenediaminetetraacetate-	3.01E+00	2.57E-02	2	1
7722885	tetrasodium-pyrophosphate-	2.65E+00	2.36E-01	4	1
57036290	TFM-2B (3-trifluoromethyl-4-nitrophenyl + bayer 73)	8.38E-01	2.62E-01	21	1
7440280	thallium-	3.25E-01	1.32E+00	8	1
58559	Theophylline	2.83E+00	3.99E-01	9	2
148798	Thiabendazole	6.27E-01	4.27E-01	6	1
1.12E+08	Thiacloprid	1.01E+00	1.99E+00	5	1
62555	thioacetamide-	1.84E+00	7.09E-01	2	1
302045	Thiocyanate	8.52E-01	1.64E+00	2	1
8004055	Thiocyanic acid, Ammonium salt, Mixt. with 1H-1,2,4-Triazol-3-amine	1.99E+00	1.90E+00	6	1
76188642	Thiocyanic acid, Methylene ester mixt. with sulfonylbis[trichloromethane]	-8.14E-01	2.33E-01	2	1
463569	thiocyanic-acid-	1.42E+00	5.62E-01	3	1
59669260	Thiodicarb	-1.43E-01	5.17E-01	13	1
54648	thiomersal	1.41E+00	2.84E-01	7	1
640153	Thiometon	6.43E-01	4.61E-01	18	1
23564058	Thiophanate methyl	1.01E+00	3.58E-01	9	1
50522	Thioridazine	1.35E-01	5.08E-01	6	2

79196	thiosemicarbazide-	1.20E+00	7.98E-02	2	1
62566	thiourea-	8.82E-01	1.04E-02	2	1
492228	thioxanthen-9-one	-6.70E-01	1.87E+00	3	1
137268	Thiram	-6.58E-01	1.23E+00	30	1
89838	thymol-	7.93E-01	1.96E-01	7	1
55297955	Tiamulin	-8.58E-01	2.65E+00	3	3
7646788	tin-tetrachloride-	1.54E+00	5.40E-01	5	1
57018049	Tolclofos-methyl	3.34E-01	2.87E-01	8	1
108883	Toluene	1.77E+00	4.44E-01	46	1
731271	Tolylfluanid	-8.80E-01	4.63E-01	8	1
8067558	Tordon 101	1.65E+00	2.44E-01	2	1
127651	tosylchloramide-sodium	9.41E-01	4.10E-01	7	1
66860808	Toxicant AC	-1.07E+00	8.51E-01	2	1
64924670	trans-(+)-7-Bromo-6-chloro-3-[3-(3-hydroxy-2-piperidinyl)-2-oxopropyl]-4-(3H)-quinazoline monohydrobromide	1.46E-01	1.99E+00	4	1
55219653	triadimenol	8.04E-01	1.67E-01	6	1
2303175	Triallate	-2.43E-01	7.79E-01	13	1
1.12E+08	Triazamate	-3.34E-01	1.41E+00	4	1
24017478	Triazophos	-5.26E-01	2.17E+00	7	1
598163	tribromoethylene-	7.83E-01	4.02E-02	3	1
5847530	tributyl[(diethylthiocarbamoyl)thio]stannane	-3.33E+00	2.85E-01	3	1
6517255	Tributylhydroxy stannane sulfamate	-3.04E+00	1.97E+00	3	1
56360	Tributyltin acetate	-2.01E+00	1.23E+00	13	1
4342363	tributyltin-benzoate-	-1.87E+00	1.78E-01	3	1
1461229	tributyltin-chloride-	-2.39E+00	1.28E+00	41	1
1983104	tributyltin-fluoride-	-2.42E+00	3.48E-01	11	1
3090366	tributyltin-laurate-	-1.71E+00	2.86E-01	3	1
3090355	tributyltin-oleate-	-1.59E+00	2.36E-02	2	1
52686	Trichlorfon	-6.68E-02	1.90E+00	92	1
76039	trichloroacetic-acid-	3.07E+00	1.27E+00	13	1
12002481	trichlorobenzene-	6.79E-01	6.73E-02	2	1
25323891	Trichloroethane	1.20E+00	2.07E-01	2	1
79016	trichloroethylene	1.74E+00	2.67E-01	37	1
993168	trichloromethylstannane-	-9.56E-01	5.92E+00	6	1
327980	trichloronat	-1.39E+00	1.30E+00	8	1
1124192	trichlorophenylstannane-	-1.40E+00	1.43E+01	2	1
306525	Triclofos	1.22E+00	6.06E-01	5	1
55335063	Triclopyr	7.34E-01	3.31E-01	14	1
64700567	Triclopyr, butoxyethyl ester	4.43E-01	7.96E-01	11	1
3380345	triclosan	-4.49E-01	4.76E-05	2	1
1330785	Tricresyl phosphate	4.31E-01	1.34E+00	16	1
2869343	tridecylamine-	-1.39E+00	8.65E-02	2	1
81412433	Tridemorph	1.51E-01	2.81E-01	4	1
112243	trientine	1.05E+00	4.63E-01	2	1
1912261	trietazine-	4.61E-01	1.21E-01	10	1
121448	triethylamine-	2.35E+00	2.58E-01	3	1
2008460	triethylammonium (2,4,5-trichlorophenoxy)acetate	6.74E-01	8.54E-01	3	1
78400	Triethyl-phosphate	3.04E+00	3.71E-02	4	1
2767546	triethyltin-bromide-	-1.27E+00	4.21E-01	6	1
1420060	trifenmorph	-8.16E-01	2.68E-01	7	1
1.42E+08	Trifloxystrobin	-1.17E+00	4.88E-01	19	1
68694111	Triflumizole	4.15E-01	4.01E-01	6	1
1582098	trifluralin	-2.82E-01	8.05E-01	50	1
1.27E+08	Triflusulfuron methyl ester	1.29E+00	5.03E+00	2	1
26644462	Triforine	1.27E+00	1.29E+00	2	1
593817	trimethylammonium-chloride-	-5.00E-01	3.25E-01	4	1
1066451	trimethyltin-chloride-	-8.40E-01	2.06E+00	9	1
688733	tri-n-butyltin hydride	-2.53E+00	2.79E+00	7	1
1.04E+08	Trinexapac	1.95E+00	1.77E-02	2	1
78308	tri-o-tolyl phosphate	4.17E-01	3.89E-02	3	1
115866	Triphenyl-phosphate	2.46E-01	7.80E-01	19	1
101020	triphenyl-phosphite-	-2.46E-01	7.47E-02	5	1

17523089	triphenyltin N,N-diethyldithiocarbamate	-3.17E+00	6.11E-02	2	1
13746662	tripotassium-hexacyanoferrate-	1.34E+00	1.25E+00	12	1
2279767	tripropyltin-chloride-	-3.43E+00	4.69E+00	5	1
126727	tris(2,3-dibromopropyl) phosphate	1.29E-01	1.30E-01	3	1
78513	Tris(2-butoxyethyl) phosphate	1.43E+00	1.14E-01	4	1
13674845	tris(2-chloro-1-methylethyl)phosphate	1.90E+00	1.73E-01	10	1
115968	tris(2-chloroethyl) phosphate	2.27E+00	3.82E-01	11	1
2569019	tris(2-hydroxyethyl)ammonium (o,p-dichlorophenoxy)acetate	2.13E+00	1.02E-01	2	1
126716	Tris(iso-butyl)phosphate	1.59E+00	3.26E-01	7	1
126738	Tris(n-butyl)phosphate	1.23E+00	4.65E-01	25	1
13674878	tris[2-chloro-1-(chloromethyl)ethyl] phosphate	6.51E-01	2.02E-01	5	1
34128013	trisodium (carboxylatomethoxy)succinate	3.33E+00	3.63E-02	7	1
15281911	trisodium tetra(cyano-C)cuprate(3-)	-2.11E-01	2.17E-01	2	1
13464374	trisodium-arsenite-	1.11E+00	3.74E-01	10	1
68042	trisodium-citrate-	3.19E+00	2.15E-01	2	1
5064313	trisodium-nitritotriacetate-	3.09E+00	4.48E-01	18	1
7601549	trisodium-orthophosphate-	2.43E+00	2.16E-01	4	1
1330785	tritolytl-phosphate-	4.71E-01	1.18E+00	15	1
2893789	troclosene-sodium	-5.28E-01	9.07E-02	3	1
7440337	tungsten-	8.28E-01	2.67E-01	2	1
1401690	Tylosin	3.52E-01	4.95E+00	3	3
1.04E+08	UC-84572	-3.18E+00	1.44E-01	10	1
112425	undecan-1-ol	2.63E-01	9.76E-02	4	1
7307553	undecylamine-	-3.78E-01	1.80E-01	2	1
83657221	Uniconazole	1.79E+00	1.00E-01	10	1
57136	Urea	3.30E+00	1.54E+00	8	1
8027858	Ureabor	2.67E+00	4.82E-02	2	1
51796	urethane	3.36E+00	2.59E-01	2	1
73561167	Utinal 302	3.02E+00	2.79E-01	4	1
109524	valeric-acid-	2.01E+00	1.62E-01	4	1
99661	Valproic acid	1.67E+00	5.40E-01	3	2
2275232	Vamidothion	2.23E+00	2.76E+00	5	1
4.44E+08	Vandetanib	9.96E-02	5.25E-01	3	4
52539	Verapamil	1.48E+00	6.68E-01	10	2
50471448	Vinclozolin	1.25E+00	2.06E-01	7	1
108054	vinyl-acetate-	1.56E+00	7.91E-02	7	1
23135220	Vydate	3.02E-01	4.56E-01	12	1
81812	Warfarin	2.00E+00	2.38E+00	8	2
8050848	Wescodyne	1.89E+00	3.72E-01	2	1
1.07E+08	X-77	7.79E-01	1.22E-01	4	1
98726739	XA 2020	-7.93E-01	5.17E-01	2	1
90471	xanthen-9-one	-7.32E-01	1.28E-01	3	1
1330207	xylene, mixed isomers, pure	1.74E+00	4.02E-01	19	1
16039535	Zinc dilactate	8.43E-01	5.42E-01	2	1
13597449	Zinc sulfite	1.16E+00	3.46E-01	2	1
12122677	Zineb	7.36E-01	1.16E+00	14	1
137304	Ziram	-5.62E-01	4.79E-01	19	1
1.39E+08	Zolmitriptan	2.54E+00	2.94E-01	3	2

Class: 1=non-pharmaceutical compound; 2=pharmaceutical compound (no antibiotic or anticancer drug); 3=antibiotic; 4=anticancer drug.

C. Description and syntax of the OpenBUGS model

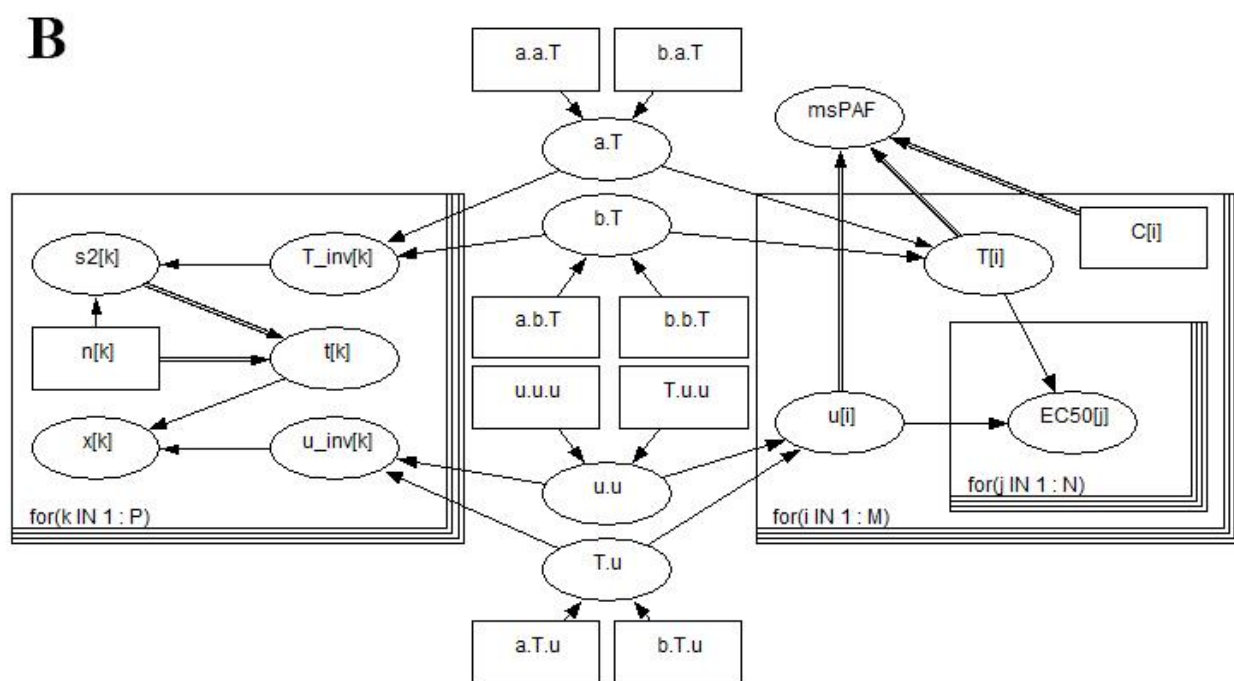
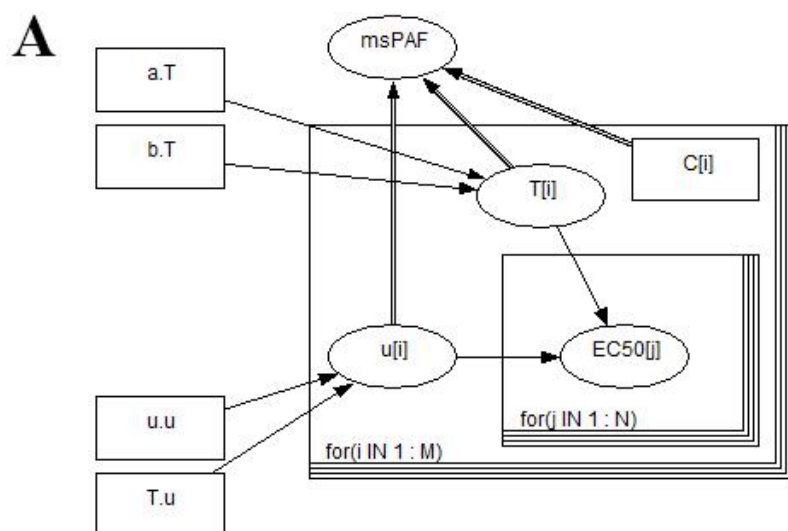
The OpenBUGS program enables the user to define deterministic nodes, stochastic nodes, and constants, as well as their relationships, either logical (functional dependence, indicated in the syntax with an arrow) or stochastic (stochastic dependence, indicated in the syntax with a tilde). The nodes (and constants) represent parameters and probability distributions. Additionally, repetitive structures ('for-loops') can be implemented. Figure S1 contains a graphical representation of the models in the form of a Directed Acyclic Graph (DAG). In a DAG, an ellipse represents either a deterministic or a stochastic node, while rectangles represent constants. Furthermore, hollow arrows point at a deterministic node, whose value then is a logical function of the values of the source nodes, and solid arrows point at a stochastic node, whose distribution then is determined by parameters given by source nodes. Repetitive structures are represented by plates.

In Figure S1, the SSD parameters $\mu_{\log EC50}$ and $\tau_{\log EC50}$ of each individual chemical i in the mixture of M chemicals are represented by $u[i]$ and $T[i]$, respectively. In Figure S1A, the constants $u.u$, $T.u$, $a.T$ and $b.T$ represent the prior parameters μ , τ , α and β , respectively. In Figures S1B and S1C, $u.u$ and $T.u$ represent the parameters of the inter-chemical distribution on $\mu_{\log EC50}$, i.e., $N(\mu, \tau)$, and $a.T$ and $b.T$ represent the parameters of the inter-chemical distribution on $\tau_{\log EC50}$, i.e., $\Gamma(\alpha, \beta)$. As a consequence, their rectangular nodes are replaced by elliptical nodes. Additionally, the third hypothesis (Figure S1C) includes Q different sets of inter-chemical distributions on $\mu_{\log EC50}$ and $\tau_{\log EC50}$, one for each API group l . Furthermore, the non-informative hyperprior distributions on the parameters of the inter-chemical distributions are characterized with two hyperparameters each.

In the hierarchical models (Figures S1B and S1C), each individual chemical k in the (sub)set of P chemicals is used to update the inter-chemical distributions on $\mu_{\log EC50}$ and $\tau_{\log EC50}$. For this, their individual $\mu_{\log EC50}$ and $\tau_{\log EC50}$ values are used, which are represented by $u_inv[k]$ and $T_inv[k]$, respectively. Their inference depends on their sample mean $\bar{x}_{\log EC50}$ and sample variance (the reciprocal of the sample precision $t_{\log EC50}$), which are represented by $x[k]$ and $s2[k]$, respectively. Additionally, their n_{species} , represented by $n[k]$, and the sample precision of the sample mean, represented by $t[k]$, are used.

Finally, the constant $C[i]$ represents the log-transformed surface water concentration, and $EC50[j]$ represents the log-transformed $EC50$ value j in a total set of N $EC50$ values. In the syntax, each $EC50$ value is assigned an identification number ($ID[j]$) corresponding with the relevant chemical i . This number is used to correctly update the SSD parameters of each individual chemical in the mixture with its own specific toxicity data. Something similar is done in the syntax for the hierarchical model with the third hypothesis (Figure S1C), in

order to correctly update the prior distributions with the relevant data: each chemical in the inventory, as well as each chemical in the mixture, is assigned a class number ($\text{class_inv}[k]$ or $\text{class}[i]$, respectively).



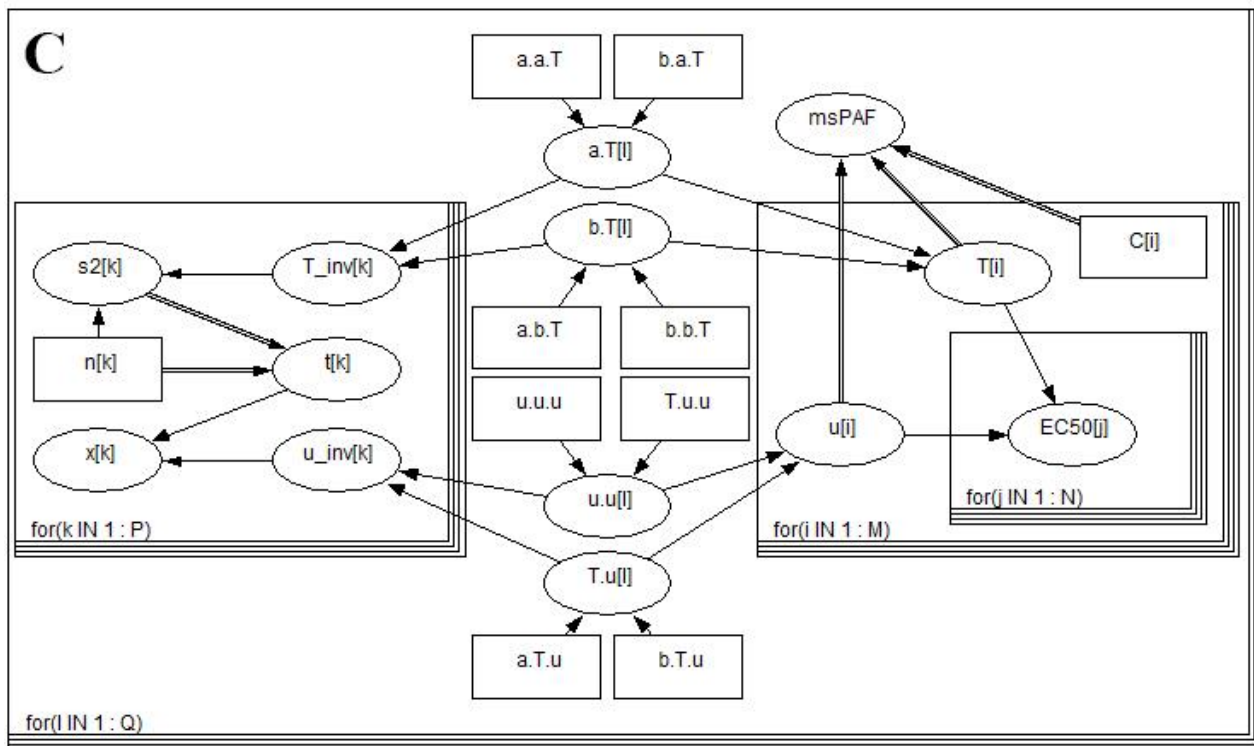
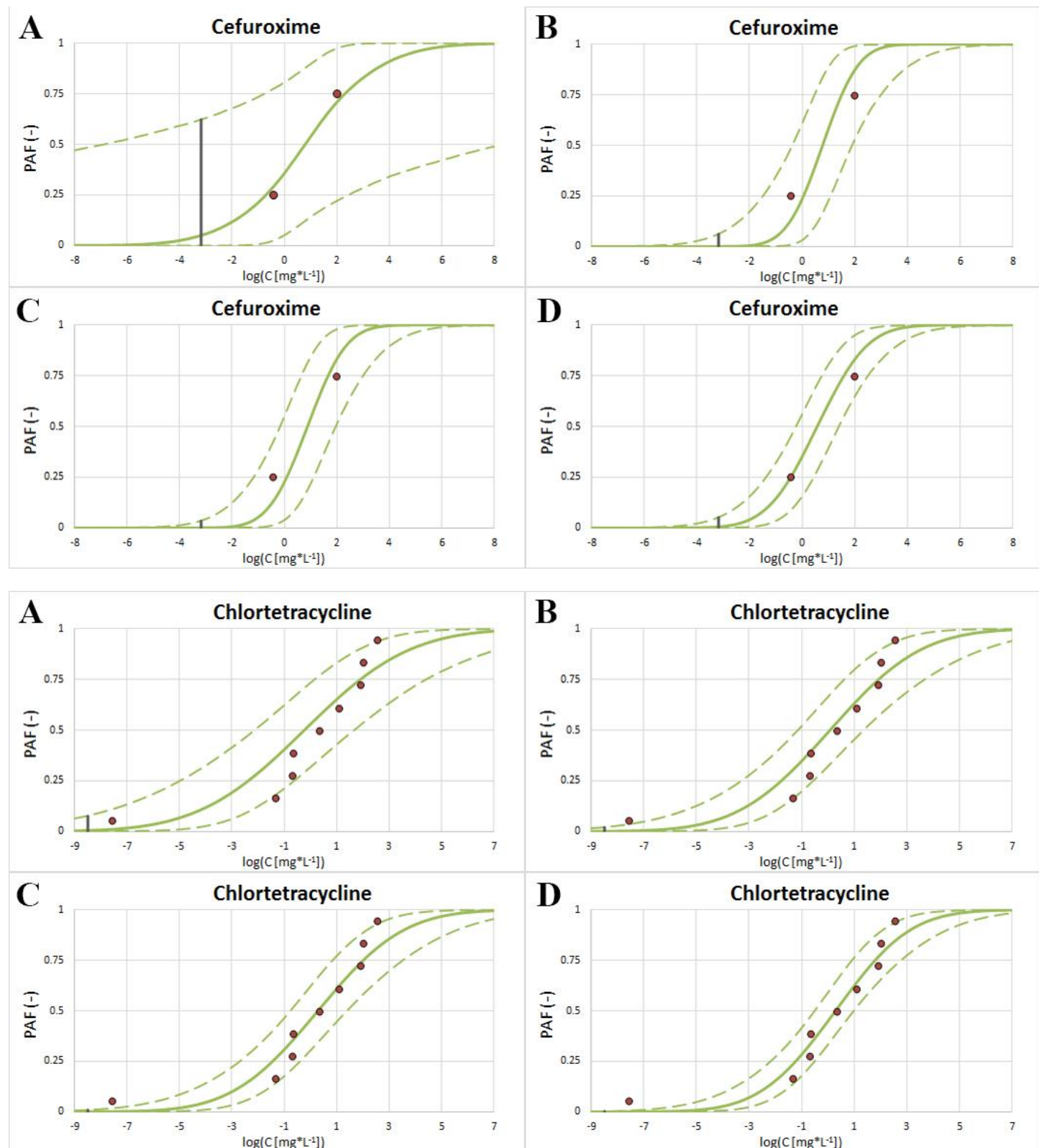
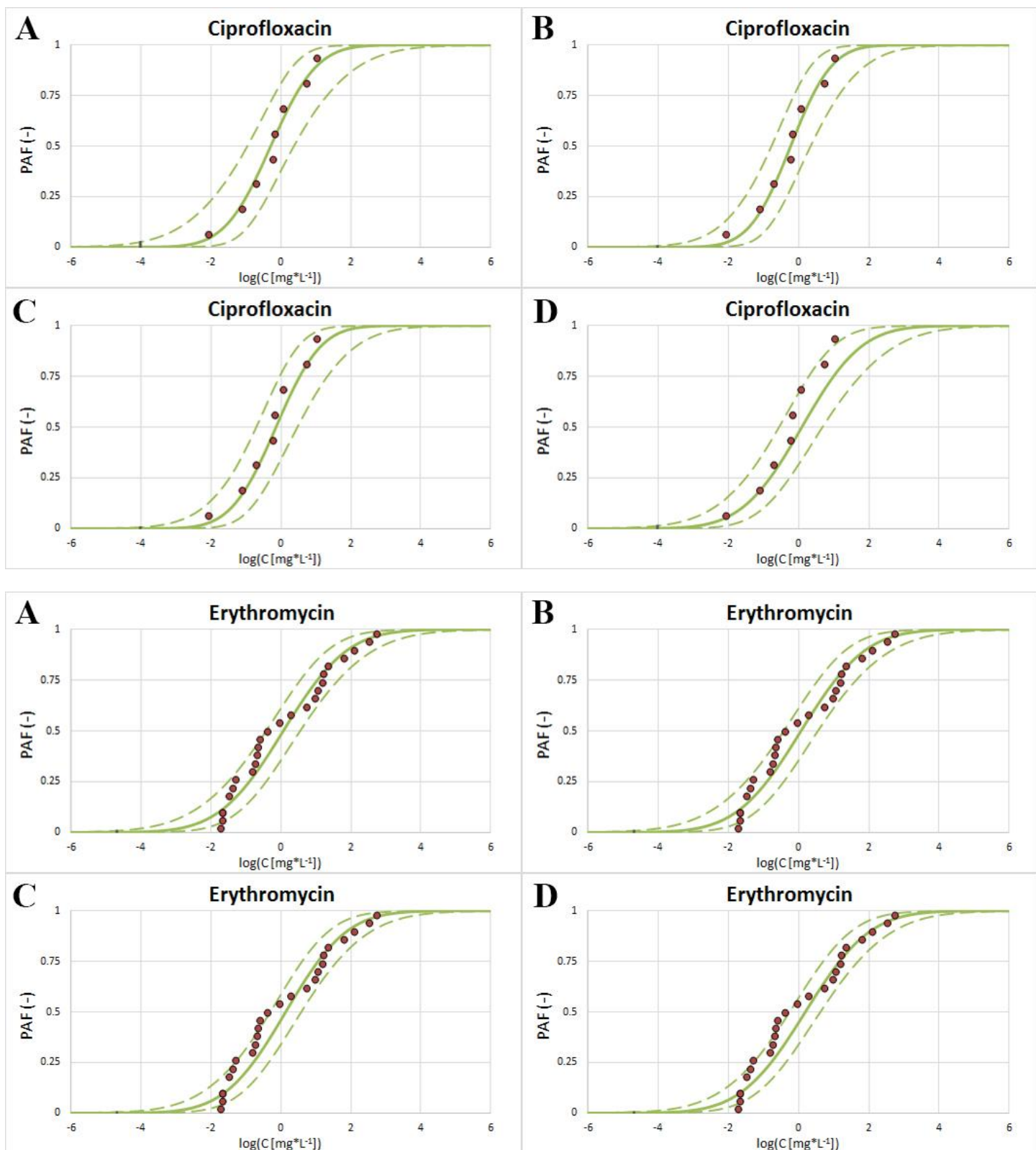


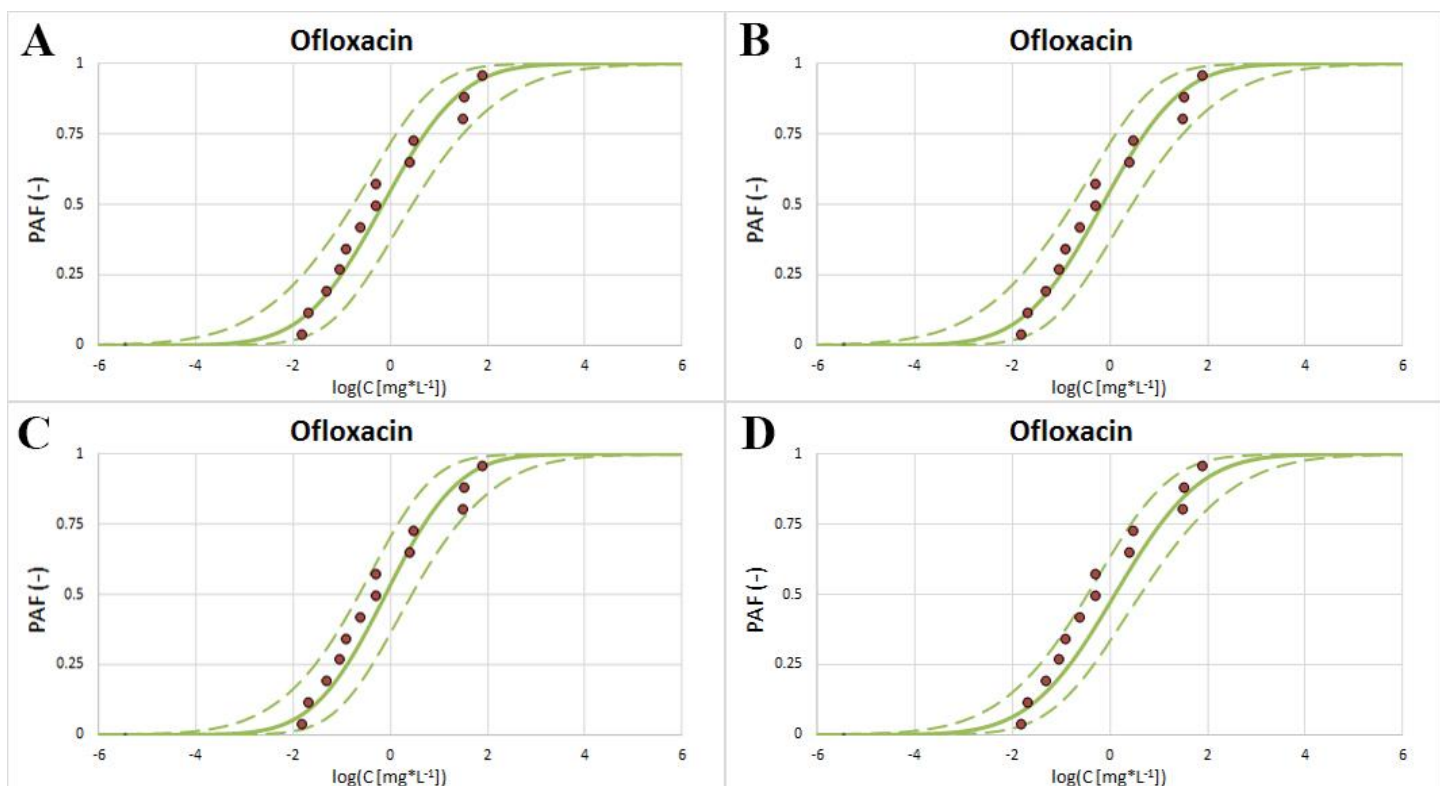
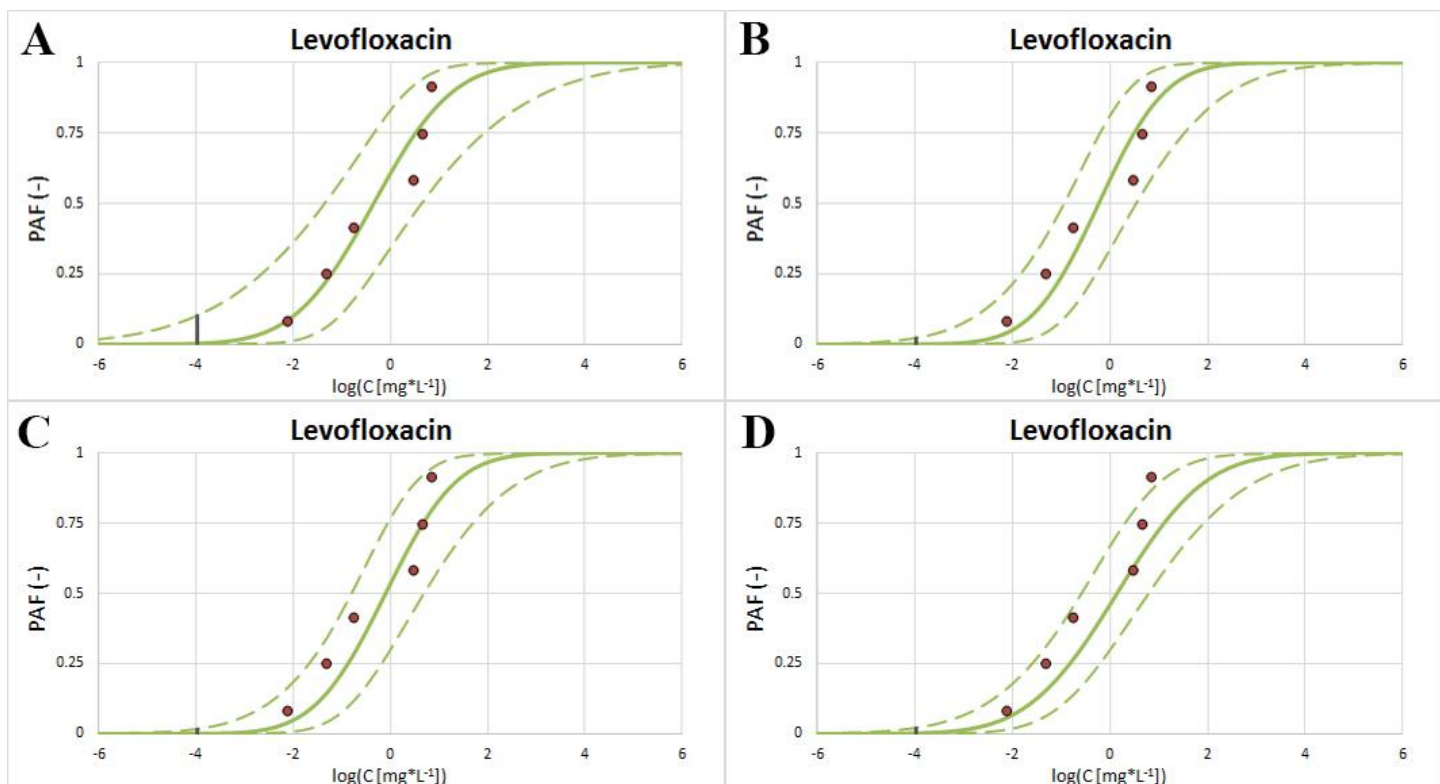
Figure S1. Directed Acyclic Graphs (DAGs) of the OpenBUGS models used for the msPAF calculations via (A) the classical approach, (B) the proposed hierarchical approach with hypotheses 1 and 2, and (C) the proposed hierarchical approach with hypothesis 3. Ellipses: deterministic and stochastic nodes; rectangles: constants; hollow arrows: functional dependence between parameters; solid arrows: stochastic dependence between parameters; plates: repetitive structures.

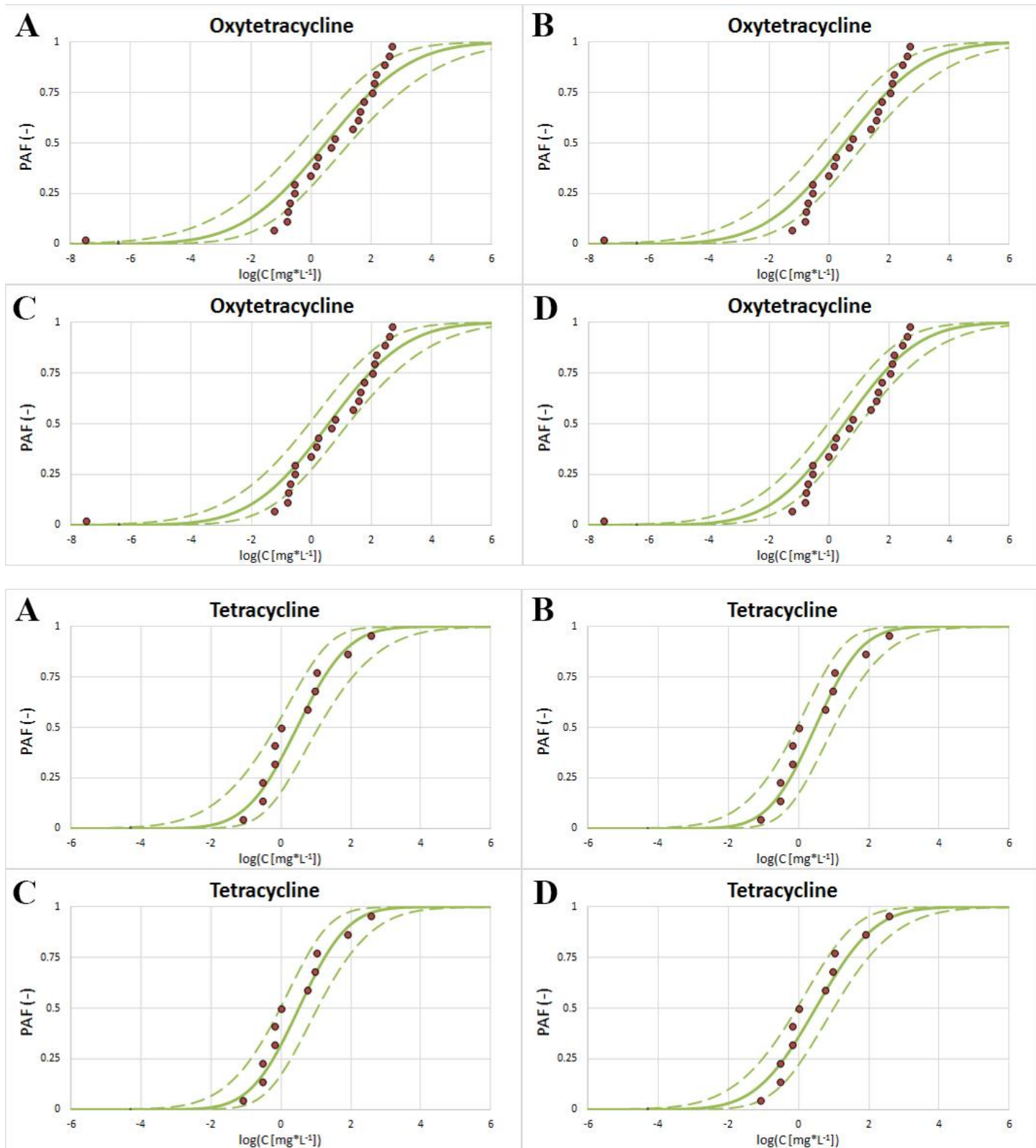
The OpenBUGS syntax and data for msPAF estimations with the classical and hierarchical models can be found at the end of the Supporting Information (pages S60-S146).

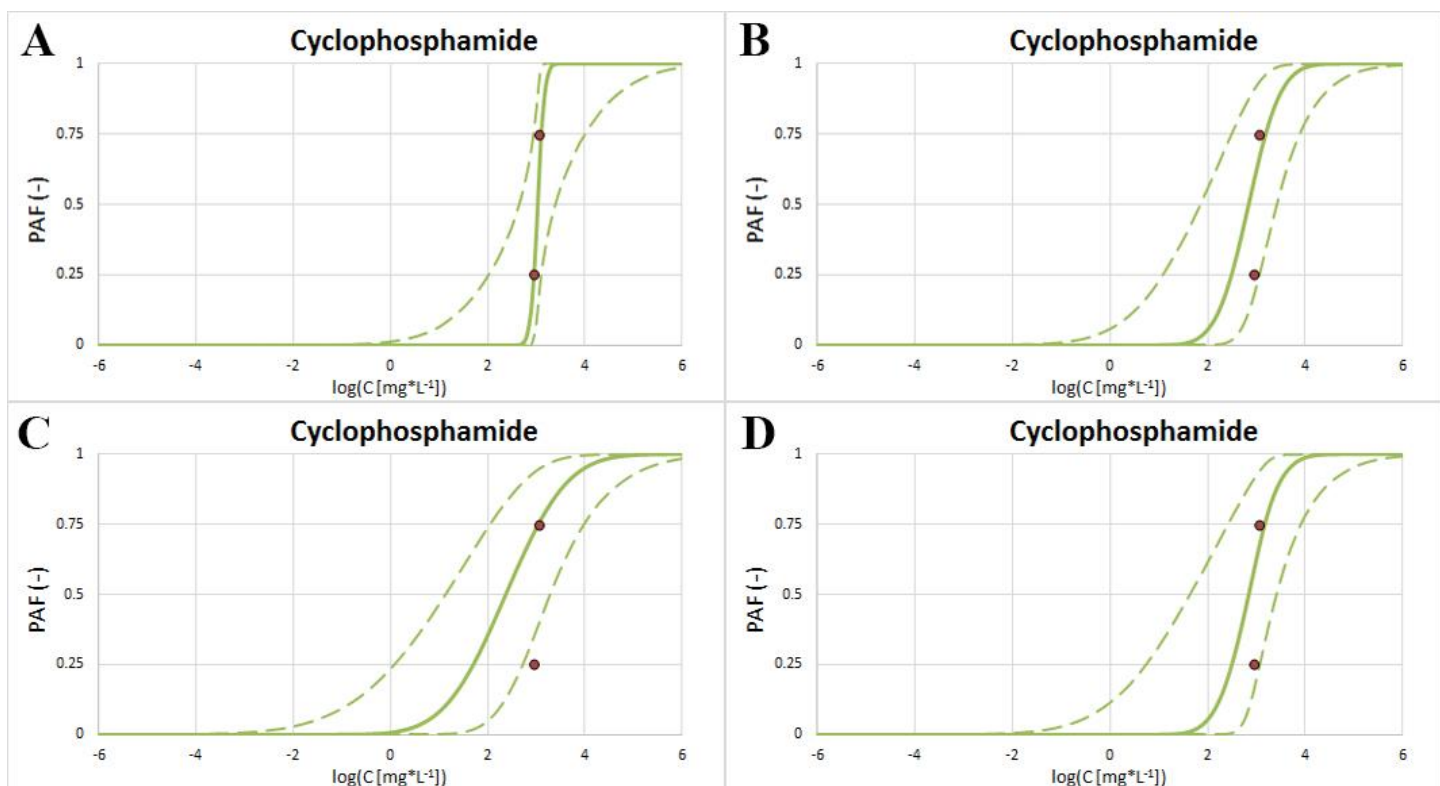
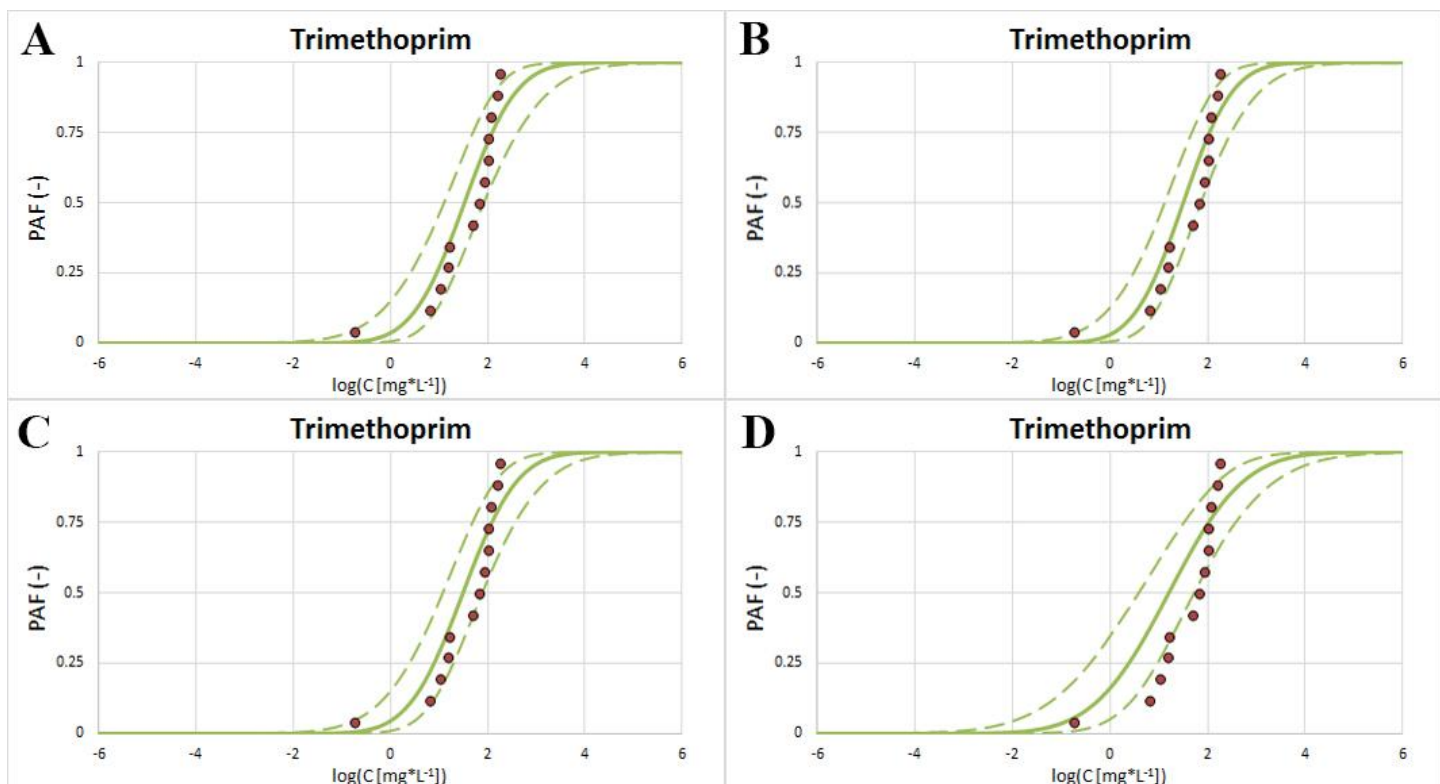
D. Posterior distributions of the SSDs of the chemicals in the mixture

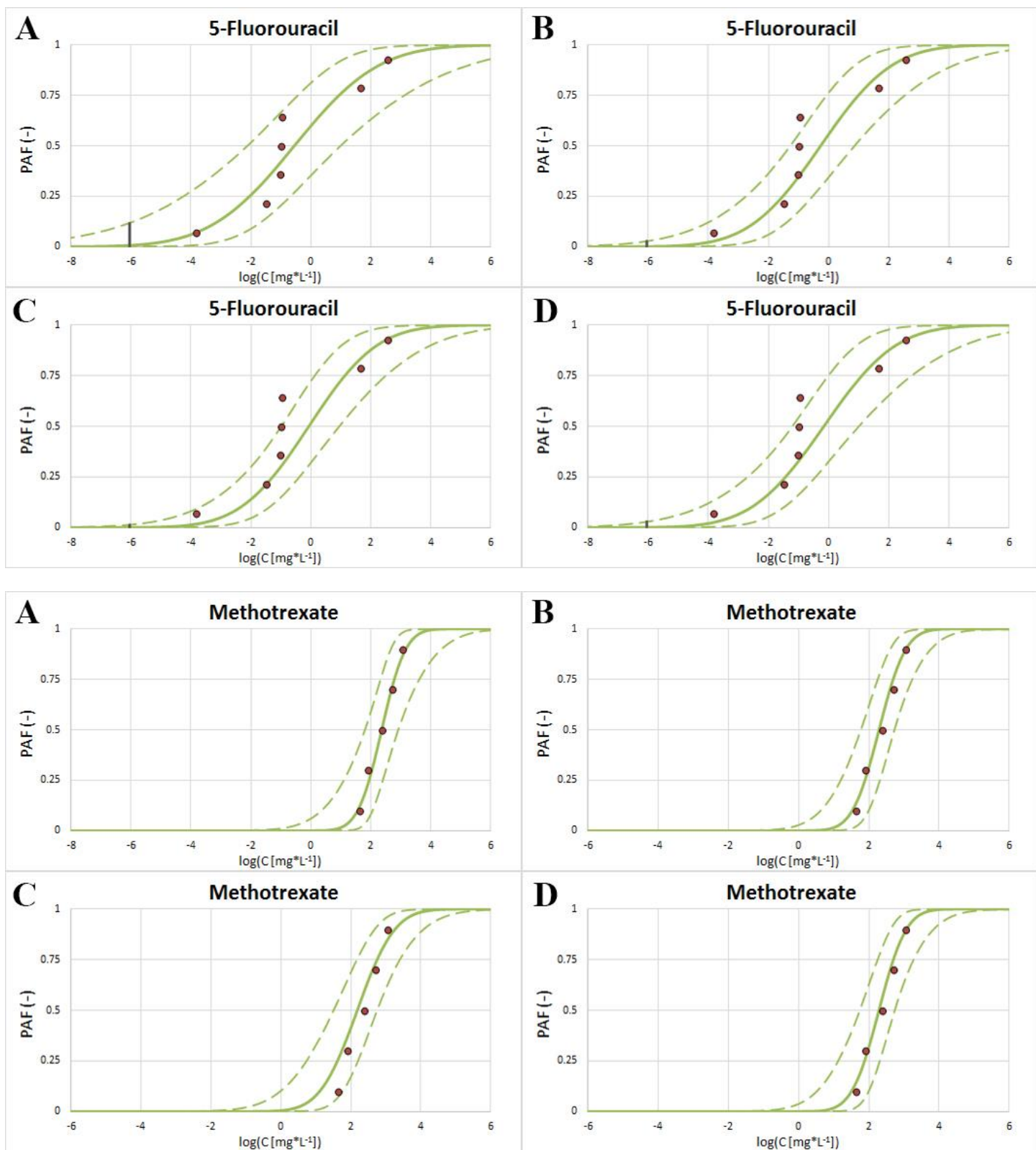












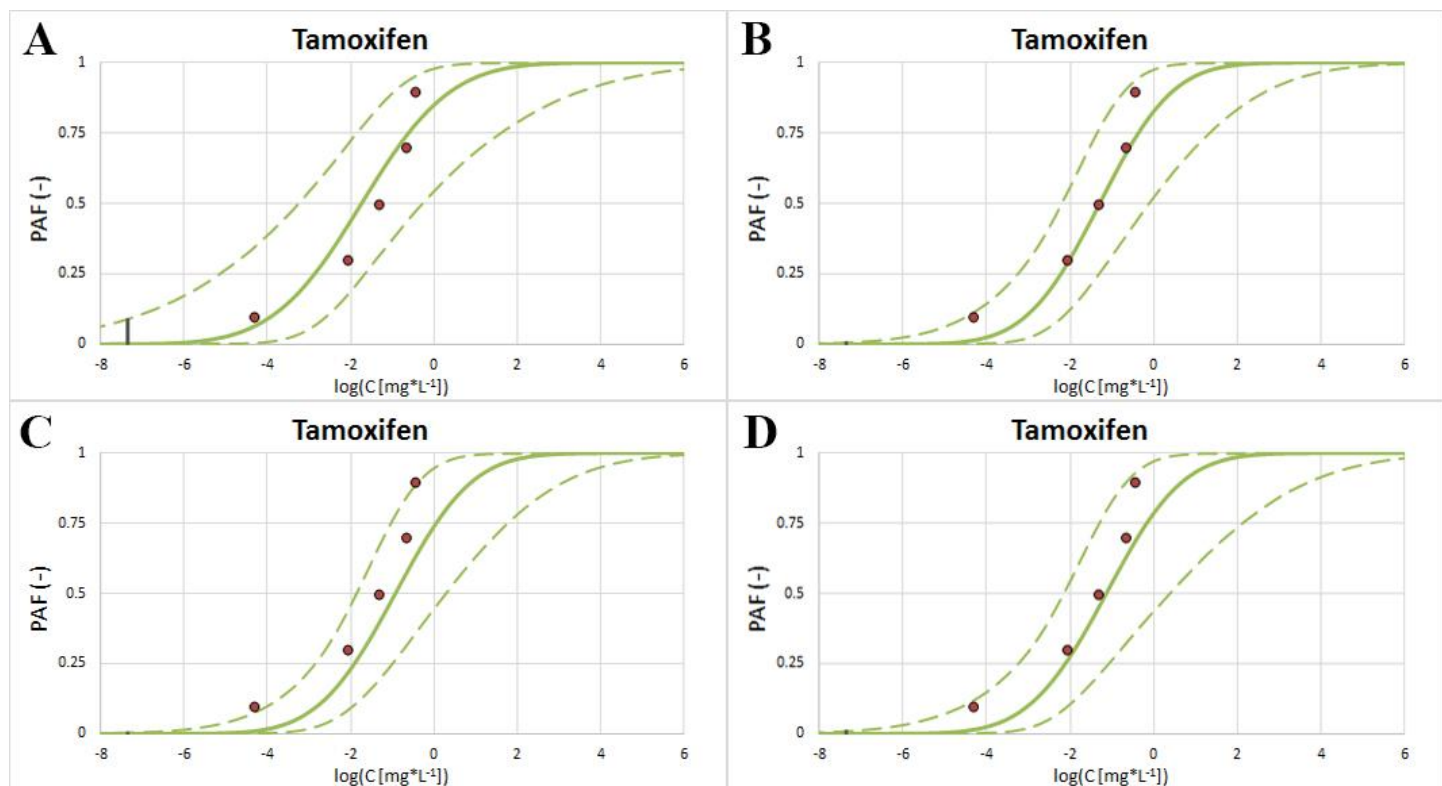
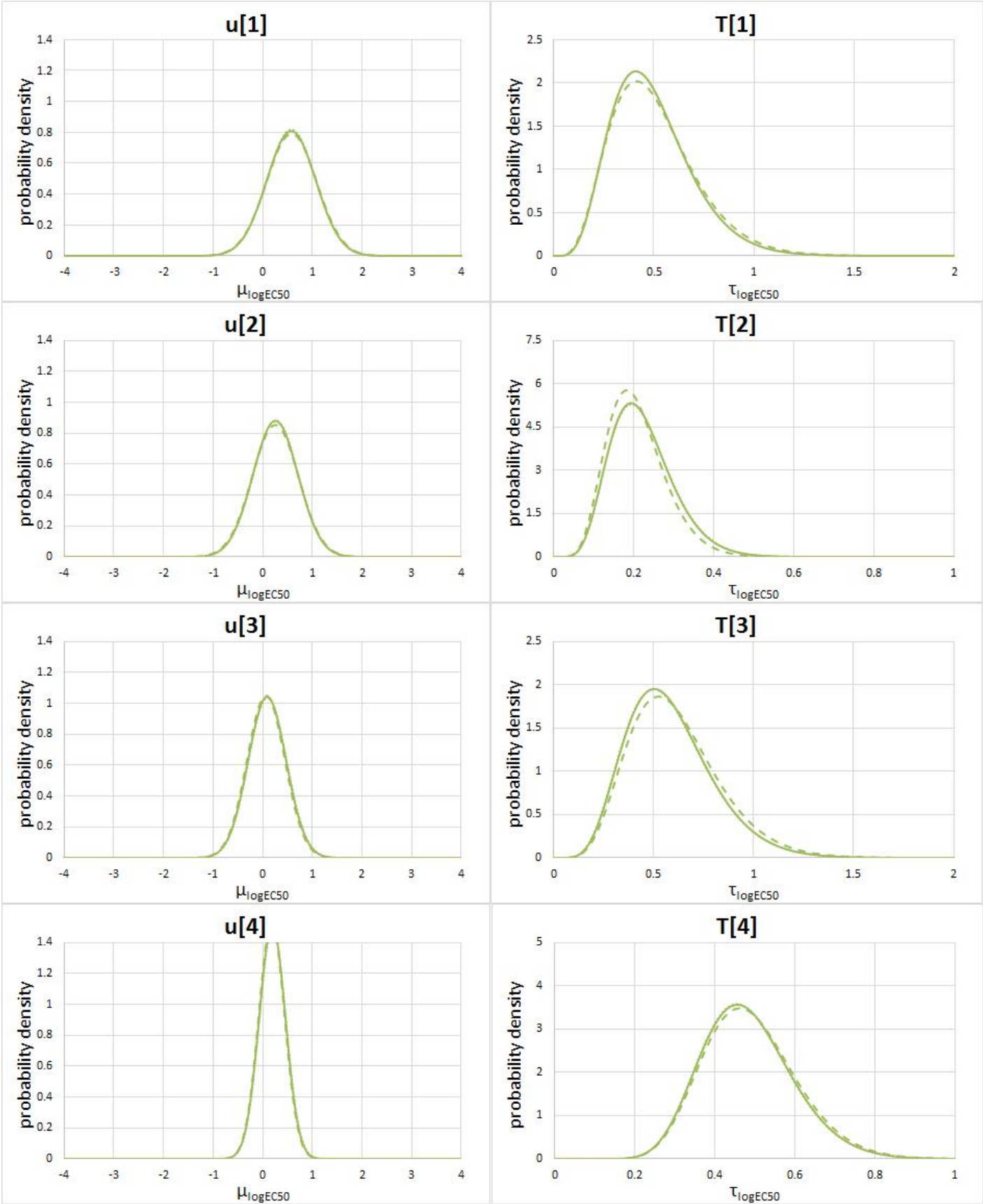
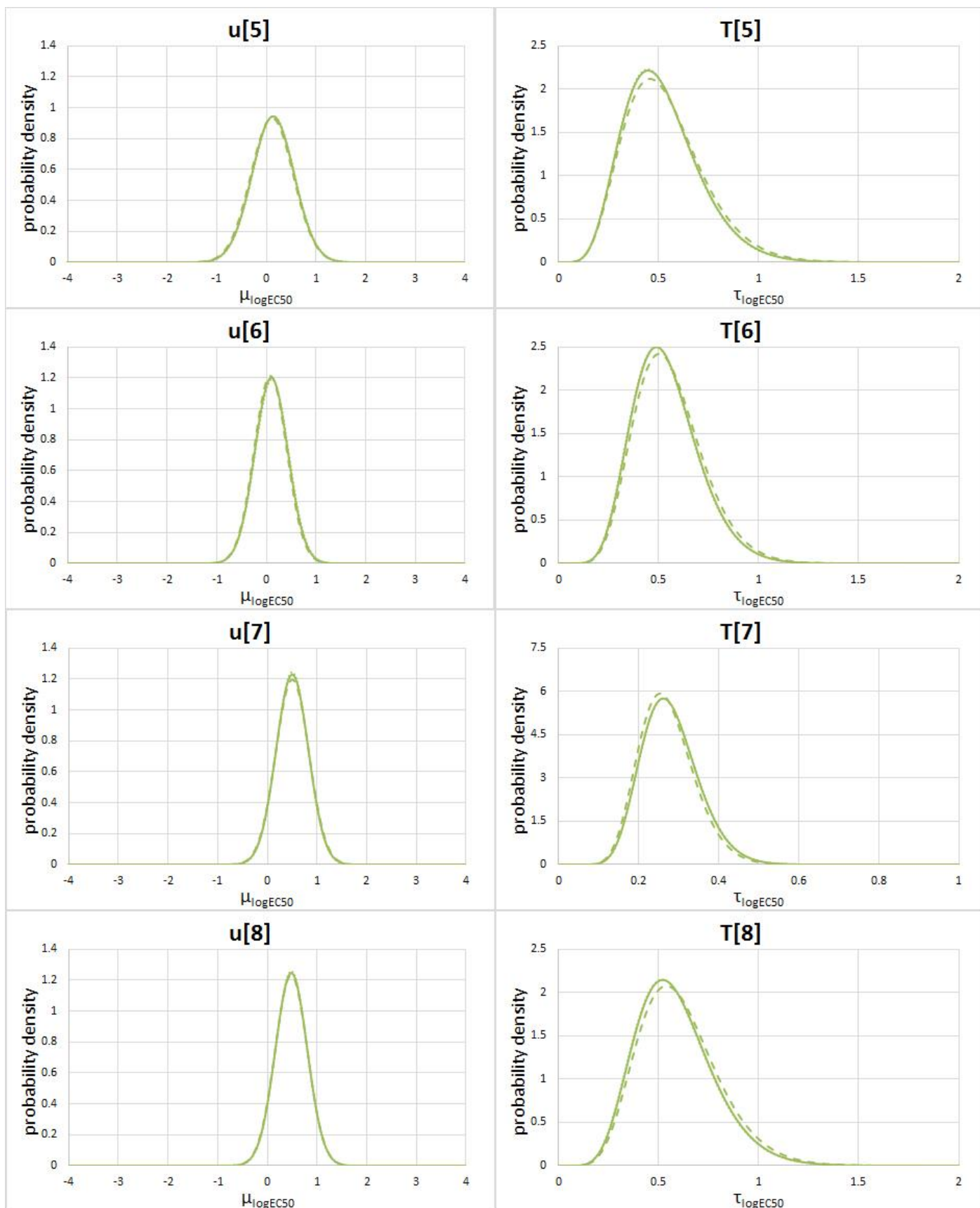
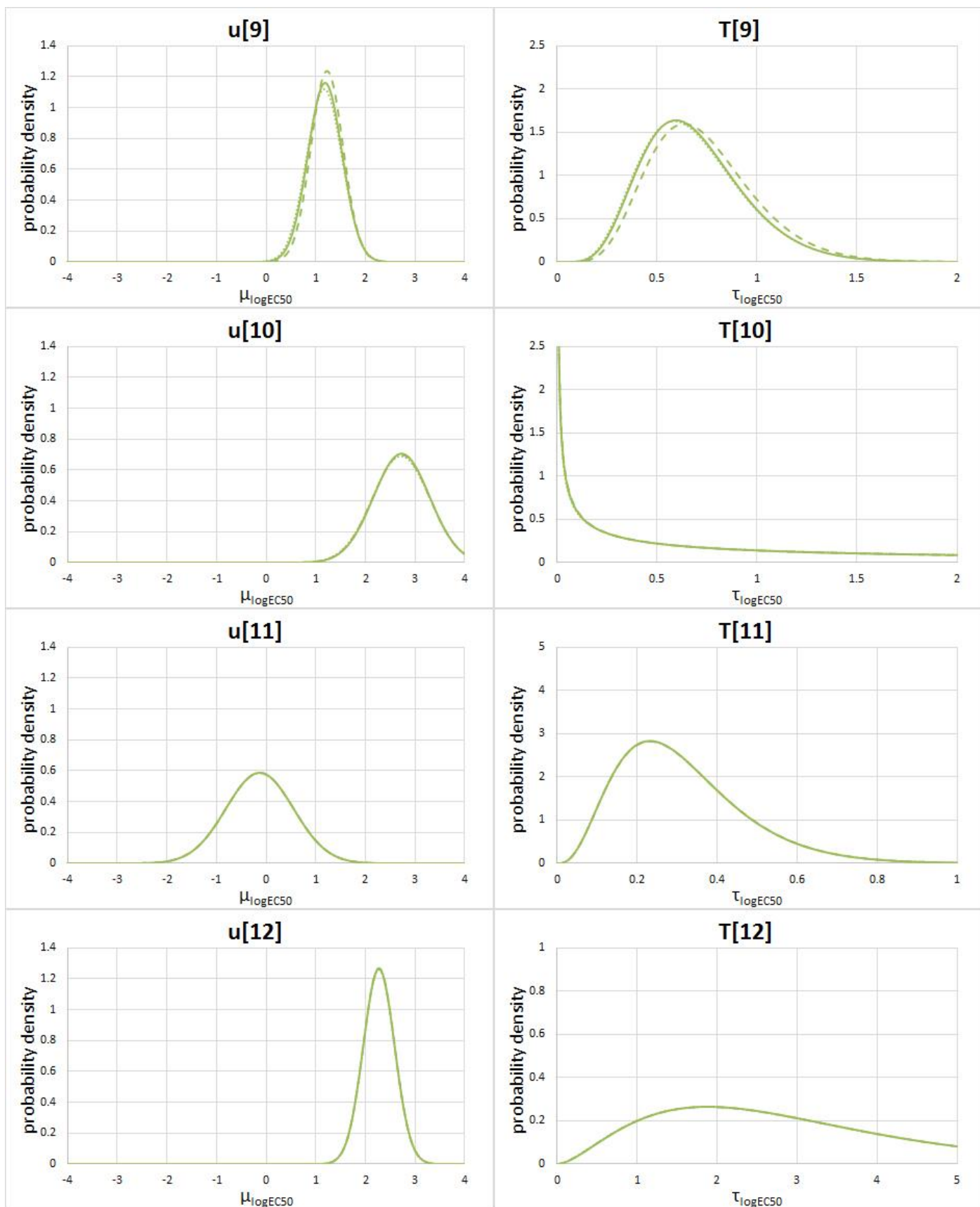


Figure S2. Cumulative density functions of the posterior distributions of species sensitivity distributions (SSDs) for all chemicals in the mixture, after 100.000 MCMC iterations after convergence. A: classical model; B: hierarchical model with hypothesis 1 (i.e., based on the total chemical inventory); C: hierarchical model with hypothesis 2 (i.e., based on all APIs in the chemical inventory); D: hierarchical model with hypothesis 3 (i.e., based on all ABs and all ACs in the chemical inventory). Solid line represents the 50th percentile of the posterior distribution of SSDs, dashed lines the 5th and 95th percentiles of the posterior distribution of SSDs.

E. Posterior distributions of the SSD parameters at different sets of hyperparameters







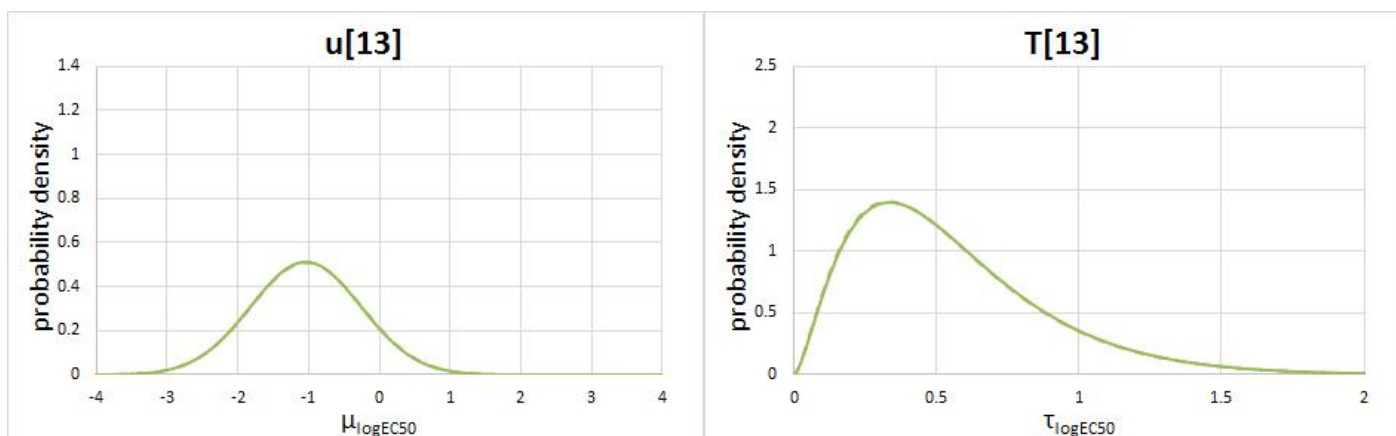


Figure S3. Posterior probability density distributions of $\mu_{\log EC50}$ ($u[]$) and $\tau_{\log EC50}$ ($T[]$) based on all ABs and all ACs in the chemical inventory, with prior distributions parameterised with different hyperparameters. Solid line: $N(0, 1 \cdot 10^{-5})$ and $\Gamma(1 \cdot 10^{-5}, 1 \cdot 10^{-5})$; dashed line: $N(0, 1 \cdot 10^{-2})$ and $\Gamma(1 \cdot 10^{-2}, 1 \cdot 10^{-2})$; dotted line: $N(0, 1 \cdot 10^{-8})$ and $\Gamma(1 \cdot 10^{-8}, 1 \cdot 10^{-8})$. Numbers 1 to 13 correspond with chemicals in the mixture: 1=cefuroxime; 2=chlortetracycline; 3=ciprofloxacin; 4=erythromycin; 5=levofloxacin; 6=ofloxacin; 7=oxytetracycline; 8=tetracycline; 9=trimethoprim; 10=cyclophosphamide; 11=5-fluorouracil; 12=methotrexate; 13=tamoxifen.

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classical model - syntax

```
model
{
# calculating PAFs for each individual chemical in the mixture
# based on separate non-informative priors for each individual chemical

for (i in 1:M) {
  u[i] ~ dnorm(u.u, T.u)
  T[i] ~ dgamma(a.T, b.T)

  sigma[i] <- sqrt(1 / T[i])
  PAF[i] <- phi((C[i] - u[i]) / sigma[i])
  HU[i] <- pow(10, C[i] - u[i])
  UF[i] <- 1 - PAF[i]
}

# updating the SSD-parameters of the individual chemicals in the mixture
for (j in 1:N) {
  EC50[j] ~ dnorm(u[ID[j]], T[ID[j]])
}

# calculating the msPAF - response addition
msUF <- prod(UF[ ])
msPAFra <- 1 - msUF

# calculating the msPAF - concentration addition
TUt看 <- sum(HU[ ])
x.sigma <- mean(sigma[ ])
msPAFca <- phi((log(TUtot) / log(10)) / x.sigma)

# calculating the msPAF - hybrid of response and concentration addition
TU_AB <- HU[1] + HU[2] + HU[3] + HU[4] + HU[5] + HU[6] + HU[7] + HU[8] + HU[9]
x.sigma_AB <- (sigma[1] + sigma[2] + sigma[3] + sigma[4] + sigma[5] + sigma[6] + sigma[7]
+ sigma[8] + sigma[9]) / 9
msPAFca_AB <- phi((log(TU_AB) / log(10)) / x.sigma_AB)
```

```

TU_AC <- HU[10] + HU[11] + HU[12] + HU[13]
x.sigma_AC <- (sigma[10] + sigma[11] + sigma[12] + sigma[13]) / 4
msPAFca_AC <- phi((log(TU_AC) / log(10)) / x.sigma_AC)

msPAFhyb <- 1 - (1 - msPAFca_AB) * (1 - msPAFca_AC)
}

```


classical model - data

list(N=128)

EC50[] ID[]

2 1

-0.410050399 1

2.025846321 2

-0.659555885 2

-1.301029996 2

2.573188067 2

1.921764634 2

-7.533256356 2

0.373317099 2

-0.617982957 2

1.113943352 2

0.078172428 3

-0.156767222 3

-0.692503962 3

-2.035290537 3

0.746348249 3

-1.096910013 3

-0.214670165 3

1.06069784 3

-1.455931956 4

-0.568636236 4

-1.657577319 4

-0.366531544 4

1 4

-0.026872146 4

-0.657577319 4

0.301029996 4

1.079181246 4

1.380211242 4

1.834462291 4

0.749736316 4

-1.363214654	4
-1.638272164	4
-1.638272164	4
2.132003393	4
2.542825427	4
-0.698970004	4
1.204119983	4
-1.698970004	4
-1.26760624	4
2.76276858	4
-0.795880017	4
-0.638272164	4
1.247482261	4
0.5	5
0.681241237	5
-0.732828272	5
-1.292429824	5
-2.102372909	5
0.86923172	5
-0.27572413	6
0.495544338	6
-1.042871802	6
1.50174373	6
-0.274088368	6
-0.899629455	6
-1.677780705	6
0.417070417	6
-1.288377063	6
1.918030337	6
-1.795880017	6
1.531223375	6
-0.594068088	6
2.732795698	7
0.271841607	7
2.477121255	7
-0.526367073	7

-0.744727495	7
0.827184545	7
1.664641976	7
-0.523490856	7
1.60346916	7
0.004321374	7
0.691965103	7
-1.210419288	7
-0.684029655	7
2.119907035	7
1.795880017	7
2.187516509	7
-7.451892707	7
-0.769551079	7
0.204119983	7
2.618902462	7
1.397940009	7
2.050926672	7
0.792391689	8
1	8
1.929418926	8
1.041392685	8
-0.140861703	8
0.025305865	8
-1.045757491	8
-0.508638306	8
-0.492144128	8
2.592112506	8
-0.156800022	8
1.041392685	9
2.277609214	9
2.044952556	9
2.084543179	9
0.838849091	9
1.94977456	9
1.72427587	9

```

1.84509804  9
-0.721246399      9
1.204119983  9
2.041392685  9
1.250420002  9
2.232491811  9
3.088881443 10
2.968482949 10
-1      11
1.681241237 11
2.602059991 11
-0.958607315      11
-1.46259178 11
-0.913640169      11
-3.788566676      11
1.929418926 12
2.414973348 12
1.653212514 12
3.086359831 12
2.737192643 12
-1.30980392 13
-0.638272164      13
-0.441033082      13
-2.036212173      13
-4.301029996      13
END

```

```
list(M=13)
```

```

C[ ]
-3.1765291
-8.4865111
-4.0134149
-4.6827732
-3.9679245
-5.4497547

```

```
-6.3990035  
-4.2934727  
-5.7161427  
-6.5789304  
-6.0402039  
-6.0193919  
-7.3461271  
END
```

```
list(u.u=0, T.u=0.00001, a.T=0.00001, b.T=0.00001)
```

```
#inits
```

```
list(T = c(1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1))
```

hierarchical models 1 & 2 - syntax

model

```
{
# non-informative priors for chemicals' population parameters
u.u ~ dnorm(u.u.u, T.u.u)
T.u ~ dgamma(a.T.u, b.T.u)
a.T ~ dgamma(a.a.T, b.a.T)
b.T ~ dgamma(a.b.T, b.b.T)

for (k in 1:P) {
  # uncertain T of individual chemicals in inventory
  degf[k] <- n[k] -1
  a.s2[k] <- degf[k] / 2
  b.s2[k] <- a.s2[k] * T_inv[k]
  s2[k] ~ dgamma(a.s2[k], b.s2[k])

  # uncertain u of individual chemicals in inventory
  t[k] <- T_inv[k] * n[k]
  x[k] ~ dnorm(u_inv[k], t[k])

  # updating the non-informative priors with u and T values of the individual
chemicals
  u_inv[k] ~ dnorm(u.u, T.u)
  T_inv[k] ~ dgamma(a.T, b.T)
}

# calculating the PAFs of the individual chemicals in the mixture
for (i in 1:M) {
  u[i] ~ dnorm(u.u, T.u)
  T[i] ~ dgamma(a.T, b.T)
  sigma[i] <- sqrt(1 / T[i])
  PAF[i] <- phi((C[i] - u[i]) / sigma[i])
  HU[i] <- pow(10, C[i] - u[i])
  UF[i] <- 1 - PAF[i]
}
```

```

# updating the SSD-parameters of the individual chemicals in the mixture
for (j in 1:N) {
  EC50[j] ~ dnorm(u[ID[j]], T[ID[j]])
}

# calculating the msPAF - response addition
msUF <- prod(UF[ ])
msPAFra <- 1 - msUF

# calculating the msPAF - concentration addition
TUt看 <- sum(HU[ ])
x.sigma <- mean(sigma[ ])
msPAFca <- phi((log(TUt看) / log(10)) / x.sigma)

# calculating the msPAF - hybrid of response and concentration addition
TU_AB <- HU[1] + HU[2] + HU[3] + HU[4] + HU[5] + HU[6] + HU[7] + HU[8] + HU[9]
x.sigma_AB <- (sigma[1] + sigma[2] + sigma[3] + sigma[4] + sigma[5] + sigma[6] + sigma[7]
+ sigma[8] + sigma[9]) / 9
msPAFca_AB <- phi((log(TU_AB) / log(10)) / x.sigma_AB)

TU_AC <- HU[10] + HU[11] + HU[12] + HU[13]
x.sigma_AC <- (sigma[10] + sigma[11] + sigma[12] + sigma[13]) / 4
msPAFca_AC <- phi((log(TU_AC) / log(10)) / x.sigma_AC)

msPAFhyb <- 1 - (1 - msPAFca_AB) * (1 - msPAFca_AC)
}

```


hierarchical model 1 - data

list(P=2043)

x[] s2[] n[]

-0.388723105	1.788335463	244
-1.417434106	1.415452651	227
1.794252092	0.73311679	224
0.013202676	1.359230015	199
-0.797817441	1.30109927	180
0.93877081	0.896346584	179
0.926372439	1.365745323	179
-0.704088762	2.069887623	164
-2.091588486	1.522247174	162
-0.21686118	0.735230838	160
-1.733317768	1.889032746	151
-2.102521981	2.033590806	144
-1.130245609	2.053172754	140
-0.069485888	1.044695187	128
-1.573470758	1.002414755	126
-1.030455029	1.695831584	126
-0.031514116	2.124889606	123
-0.296680429	2.036232178	114
-0.579642625	1.663892278	113
-1.185665343	2.491970225	113
-0.33298861	0.487143456	110
-1.439171168	1.068351823	109
-1.796785061	2.110569511	107
-0.242801733	0.597419862	92
-0.066805111	1.898074654	92
0.936022319	0.324777827	84
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-1.251098754	0.752384726	80
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-1.816475971	1.38636529	68
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END

```

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list(N=128)
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1.921764634	2
-7.533256356	2
0.373317099	2
-0.617982957	2
1.113943352	2
0.078172428	3
-0.156767222	3
-0.692503962	3
-2.035290537	3
0.746348249	3
-1.096910013	3
-0.214670165	3
1.06069784	3
-1.455931956	4
-0.568636236	4
-1.657577319	4
-0.366531544	4
1	4
-0.026872146	4
-0.657577319	4
0.301029996	4
1.079181246	4
1.380211242	4
1.834462291	4
0.749736316	4
-1.363214654	4
-1.638272164	4
-1.638272164	4

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-1.698970004	4
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0.681241237	5
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-1.292429824	5
-2.102372909	5
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-1.795880017	6
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2.477121255	7
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-0.769551079	7
0.204119983	7
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1	8
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-0.508638306	8
-0.492144128	8
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2.277609214	9
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2.041392685 9
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2.232491811 9
3.088881443 10
2.968482949 10
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END

```

```
list(M=13)
```

```

C[ ]
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-3.9679245
-5.4497547
-6.3990035
-4.2934727
-5.7161427

```

-6.5789304

-6.0402039

-6.0193919

-7.3461271

END

```
list(a.a.T=0.00001, b.a.T=0.00001, a.b.T=0.00001, b.b.T=0.00001, u.u.u=0, T.u.u=0.00001,  
a.T.u=0.00001, b.T.u=0.00001)
```

#inits

```
list(T = c(1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1), a.T = 1, b.T = 1, T.u = 1)
```

hierarchical model 2 - data

list(P=106)

x[] s2[] n[]

```
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2.295858198 0.596830878 22
0.707546989 1.005501935 22
1.49359794  0.61215214  20
0.682741116 2.057885536 18
1.176204681 0.876169553 17
1.425474081 0.832262053 17
1.427788582 0.804797032 17
1.881163397 2.085955526 16
0.165664215 2.459455412 16
2.394881016 0.297370573 13
1.005110979 0.413081048 13
-0.445830317      0.552639825 13
-0.320120314      0.963441184 12
0.722985959 0.849195554 12
1.903558982 0.865759262 12
1.338151967 2.166559745 11
1.422086831 0.758262919 11
2.460481812 0.908089223 10
3.118960191 0.57267421  10
1.48248316  0.667972161 10
0.752981191 1.121871878 9
-0.317760826      0.278118427 9
1.705597714 0.297681466 9
2.831403149 0.398540662 9
1.191609808 1.717834586 8
1.462432913 3.314445377 8
0.257941369 0.566652221 8
1.997965341 2.379087476 8
```


0.814504521 2.310425827 7
 0.959313718 1.211308877 7
 2.507973972 0.370046941 7
 3.063837619 0.567254348 7
 1.69543937 5.869524228 7
 2.807038068 1.660869432 7
 1.449993337 0.23021723 7
 2.236585346 0.348340506 7
 0.880414033 1.963507921 6
 2.077161738 0.634620718 6
 0.278227606 3.022989993 6
 0.833602937 1.689452112 6
 0.683773239 1.019683426 6
 -1.796055176 3.003352819 6
 0.750499868 0.481167552 6
 2.202172016 0.386752982 6
 2.412846491 2.231308052 6
 0.685941352 1.127600303 6
 1.56129256 0.969710313 6
 0.135072433 0.507532865 6
 0.699160258 9.229256085 5
 0.447312554 3.154069939 5
 -0.602621214 1.31455017 5
 0.1072445 1.537586016 5
 0.649984957 2.19202074 5
 2.100860948 1.46248324 5
 0.081247108 0.426752046 5
 0.866467005 0.064679077 5
 0.417092992 0.499620586 4
 0.483304422 0.191788578 4
 2.170952905 0.337617499 4
 1.057380814 2.73662798 4
 2.293034322 0.053155764 4
 1.47139416 0.40042951 4
 -0.524507441 0.278380195 4
 0.802932238 0.297920848 4

0.810711769 0.033359082 4
 1.302940838 0.371136328 4
 1.764961629 0.055044861 3
 1.318241597 0.136924549 3
 2.224800604 0.459548906 3
 1.898201733 0.045443127 3
 0.099609146 0.524639796 3
 -0.857667014 2.65343552 3
 0.351989299 4.951423895 3
 2.553951819 1.250883342 3
 1.87441643 0.182963403 3
 0.095244031 0.350740665 3
 0.698738195 0.309498095 3
 2.117574212 0.126492486 3
 0.283763138 2.484306189 3
 1.562990878 0.162902372 3
 2.082336135 0.068036055 3
 1.119294996 0.114526846 3
 -0.482628515 0.464467995 3
 1.625454065 0.016308098 3
 0.371223988 0.060511201 3
 1.669396279 0.539697526 3
 2.537535001 0.293558815 3
 0.249980933 0.116529344 2
 -0.159379381 0.050803574 2
 0.178967424 7.221625143 2
 1.629949228 0.052738403 2
 -0.025090282 12.44917475 2
 0.285621425 4.544932656 2
 0.401637523 2.457257952 2
 0 2 2
 -0.96965108 3.545139635 2
 2.03359624 0.659419899 2
 2.600768292 3.149652278 2
 2.263975979 0.340671685 2
 -0.115311337 0.232044812 2

```

-0.063572378      3.783044526 2
-0.353761203      0.012179569 2
0.354918952 1.972857187 2
END

```

```
list(N=128)
```

```
EC50[ ]      ID[ ]
```

```
2      1
```

```
-0.410050399      1
```

```
2.025846321 2
```

```
-0.659555885      2
```

```
-1.301029996      2
```

```
2.573188067 2
```

```
1.921764634 2
```

```
-7.533256356      2
```

```
0.373317099 2
```

```
-0.617982957      2
```

```
1.113943352 2
```

```
0.078172428 3
```

```
-0.156767222      3
```

```
-0.692503962      3
```

```
-2.035290537      3
```

```
0.746348249 3
```

```
-1.096910013      3
```

```
-0.214670165      3
```

```
1.06069784 3
```

```
-1.455931956      4
```

```
-0.568636236      4
```

```
-1.657577319      4
```

```
-0.366531544      4
```

```
1      4
```

```
-0.026872146      4
```

```
-0.657577319      4
```

```
0.301029996 4
```

```
1.079181246 4
```

1.380211242	4
1.834462291	4
0.749736316	4
-1.363214654	4
-1.638272164	4
-1.638272164	4
2.132003393	4
2.542825427	4
-0.698970004	4
1.204119983	4
-1.698970004	4
-1.26760624	4
2.76276858	4
-0.795880017	4
-0.638272164	4
1.247482261	4
0.5	5
0.681241237	5
-0.732828272	5
-1.292429824	5
-2.102372909	5
0.86923172	5
-0.27572413	6
0.495544338	6
-1.042871802	6
1.50174373	6
-0.274088368	6
-0.899629455	6
-1.677780705	6
0.417070417	6
-1.288377063	6
1.918030337	6
-1.795880017	6
1.531223375	6
-0.594068088	6
2.732795698	7

0.271841607	7
2.477121255	7
-0.526367073	7
-0.744727495	7
0.827184545	7
1.664641976	7
-0.523490856	7
1.60346916	7
0.004321374	7
0.691965103	7
-1.210419288	7
-0.684029655	7
2.119907035	7
1.795880017	7
2.187516509	7
-7.451892707	7
-0.769551079	7
0.204119983	7
2.618902462	7
1.397940009	7
2.050926672	7
0.792391689	8
1	8
1.929418926	8
1.041392685	8
-0.140861703	8
0.025305865	8
-1.045757491	8
-0.508638306	8
-0.492144128	8
2.592112506	8
-0.156800022	8
1.041392685	9
2.277609214	9
2.044952556	9
2.084543179	9

```

0.838849091 9
1.94977456 9
1.72427587 9
1.84509804 9
-0.721246399 9
1.204119983 9
2.041392685 9
1.250420002 9
2.232491811 9
3.088881443 10
2.968482949 10
-1 11
1.681241237 11
2.602059991 11
-0.958607315 11
-1.46259178 11
-0.913640169 11
-3.788566676 11
1.929418926 12
2.414973348 12
1.653212514 12
3.086359831 12
2.737192643 12
-1.30980392 13
-0.638272164 13
-0.441033082 13
-2.036212173 13
-4.301029996 13
END

```

```
list(M=13)
```

```
C[ ]
```

```

-3.1765291
-8.4865111
-4.0134149

```

```
-4.6827732  
-3.9679245  
-5.4497547  
-6.3990035  
-4.2934727  
-5.7161427  
-6.5789304  
-6.0402039  
-6.0193919  
-7.3461271
```

```
END
```

```
list(a.a.T=0.00001, b.a.T=0.00001, a.b.T=0.00001, b.b.T=0.00001, u.u.u=0, T.u.u=0.00001,  
a.T.u=0.00001, b.T.u=0.00001)
```

```
#inits
```

```
list(T = c(1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1), a.T = 1, b.T = 1, T.u = 1)
```

hierarchical model 3 - syntax

```
{
# non-informative priors for chemicals' population parameters
for (l in 1:Q) {
  u.u[l] ~ dnorm(u.u.u, T.u.u)
  T.u[l] ~ dgamma(a.T.u, b.T.u)
  a.T[l] ~ dgamma(a.a.T, b.a.T)
  b.T[l] ~ dgamma(a.b.T, b.b.T)
}

for (k in 1:P) {
  # uncertain T of individual chemicals in inventory
  degf[k] <- n[k] -1
  a.s2[k] <- degf[k] / 2
  b.s2[k] <- a.s2[k] * T_inv[k]
  s2[k] ~ dgamma(a.s2[k], b.s2[k])

  # uncertain u of individual chemicals in inventory
  t[k] <- T_inv[k] * n[k]
  x[k] ~ dnorm(u_inv[k], t[k])

  # updating the non-informative priors with u and T values of the individual
chemicals
  u_inv[k] ~ dnorm(u.u[class_inv[k]], T.u[class_inv[k]])
  T_inv[k] ~ dgamma(a.T[class_inv[k]], b.T[class_inv[k]])
}

# calculating the PAFs of the individual chemicals in the mixture
for (i in 1:M) {
  u[i] ~ dnorm(u.u[class[i]], T.u[class[i]])
  T[i] ~ dgamma(a.T[class[i]], b.T[class[i]])
  sigma[i] <- sqrt(1 / T[i])
  PAF[i] <- phi((C[i] - u[i]) / sigma[i])
  HU[i] <- pow(10, C[i] - u[i])
}
```



```

    UF[i] <- 1 - PAF[i]
  }

# updating the SSD-parameters of the individual chemicals in the mixture
for (j in 1:N) {
  EC50[j] ~ dnorm(u[ID[j]], T[ID[j]])
}

# calculating the msPAF - response addition
msUF <- prod(UF[ ])
msPAFra <- 1 - msUF

# calculating the msPAF - concentration addition
TUt看 <- sum(HU[ ])
x.sigma <- mean(sigma[ ])
msPAFca <- phi((log(TUt看) / log(10)) / x.sigma)

# calculating the msPAF - hybrid of response and concentration addition
TU_AB <- HU[1] + HU[2] + HU[3] + HU[4] + HU[5] + HU[6] + HU[7] + HU[8] + HU[9]
x.sigma_AB <- (sigma[1] + sigma[2] + sigma[3] + sigma[4] + sigma[5] + sigma[6] + sigma[7]
+sigma[8] + sigma[9]) / 9
msPAFca_AB <- phi((log(TU_AB) / log(10)) / x.sigma_AB)

TU_AC <- HU[10] + HU[11] + HU[12] + HU[13]
x.sigma_AC <- (sigma[10] + sigma[11] + sigma[12] + sigma[13]) / 4
msPAFca_AC <- phi((log(TU_AC) / log(10)) / x.sigma_AC)

msPAFhyb <- 1 - (1 - msPAFca_AB) * (1 - msPAFca_AC)
}

```

hierarchical model 3 - data

list(P=33)

x[]	s2[]	n[]	class_inv[]		
0.682741116	2.057885536	18	1		
1.881163397	2.085955526	16	1		
-0.320120314	0.963441184	12	1		
0.752981191	1.121871878	9	1		
0.814504521	2.310425827	7	1		
0.959313718	1.211308877	7	1		
0.880414033	1.963507921	6	1		
2.077161738	0.634620718	6	1		
0.278227606	3.022989993	6	1		
0.699160258	9.229256085	5	1		
0.447312554	3.154069939	5	1		
-0.602621214	1.31455017	5	1		
0.1072445	1.537586016	5	1		
2.170952905	0.337617499	4	1		
1.057380814	2.73662798	4	1		
-0.857667014	2.65343552	3	1		
0.351989299	4.951423895	3	1		
0.178967424	7.221625143	2	1		
1.629949228	0.052738403	2	1		
-0.025090282	12.44917475	2	1		
0.285621425	4.544932656	2	1		
0.401637523	2.457257952	2	1		
0	2	2	1		
-0.96965108	3.545139635	2	1		
0.417092992	0.499620586	4	2		
0.483304422	0.191788578	4	2		
1.318241597	0.136924549	3	2		
2.224800604	0.459548906	3	2		
1.898201733	0.045443127	3	2		
0.099609146	0.524639796	3	2		
0.249980933	0.116529344	2	2		

```

-0.159379381      0.050803574 2      2
1.764961629 0.055044861 3      2
END

```

```
list(N=128)
```

```
EC50[ ]      ID[ ]
```

```
2      1
```

```
-0.410050399      1
```

```
2.025846321 2
```

```
-0.659555885      2
```

```
-1.301029996      2
```

```
2.573188067 2
```

```
1.921764634 2
```

```
-7.533256356      2
```

```
0.373317099 2
```

```
-0.617982957      2
```

```
1.113943352 2
```

```
0.078172428 3
```

```
-0.156767222      3
```

```
-0.692503962      3
```

```
-2.035290537      3
```

```
0.746348249 3
```

```
-1.096910013      3
```

```
-0.214670165      3
```

```
1.06069784 3
```

```
-1.455931956      4
```

```
-0.568636236      4
```

```
-1.657577319      4
```

```
-0.366531544      4
```

```
1      4
```

```
-0.026872146      4
```

```
-0.657577319      4
```

```
0.301029996 4
```

```
1.079181246 4
```

```
1.380211242 4
```

1.834462291	4
0.749736316	4
-1.363214654	4
-1.638272164	4
-1.638272164	4
2.132003393	4
2.542825427	4
-0.698970004	4
1.204119983	4
-1.698970004	4
-1.26760624	4
2.76276858	4
-0.795880017	4
-0.638272164	4
1.247482261	4
0.5	5
0.681241237	5
-0.732828272	5
-1.292429824	5
-2.102372909	5
0.86923172	5
-0.27572413	6
0.495544338	6
-1.042871802	6
1.50174373	6
-0.274088368	6
-0.899629455	6
-1.677780705	6
0.417070417	6
-1.288377063	6
1.918030337	6
-1.795880017	6
1.531223375	6
-0.594068088	6
2.732795698	7
0.271841607	7

2.477121255	7
-0.526367073	7
-0.744727495	7
0.827184545	7
1.664641976	7
-0.523490856	7
1.60346916	7
0.004321374	7
0.691965103	7
-1.210419288	7
-0.684029655	7
2.119907035	7
1.795880017	7
2.187516509	7
-7.451892707	7
-0.769551079	7
0.204119983	7
2.618902462	7
1.397940009	7
2.050926672	7
0.792391689	8
1	8
1.929418926	8
1.041392685	8
-0.140861703	8
0.025305865	8
-1.045757491	8
-0.508638306	8
-0.492144128	8
2.592112506	8
-0.156800022	8
1.041392685	9
2.277609214	9
2.044952556	9
2.084543179	9
0.838849091	9

```

1.94977456  9
1.72427587  9
1.84509804  9
-0.721246399      9
1.204119983  9
2.041392685  9
1.250420002  9
2.232491811  9
3.088881443 10
2.968482949 10
-1      11
1.681241237 11
2.602059991 11
-0.958607315      11
-1.46259178 11
-0.913640169      11
-3.788566676      11
1.929418926 12
2.414973348 12
1.653212514 12
3.086359831 12
2.737192643 12
-1.30980392 13
-0.638272164      13
-0.441033082      13
-2.036212173      13
-4.301029996      13
END

```

```
list(M=13)
```

```

C[ ] class[ ]
-3.1765291  1
-8.4865111  1
-4.0134149  1
-4.6827732  1

```

```

-3.9679245  1
-5.4497547  1
-6.3990035  1
-4.2934727  1
-5.7161427  1
-6.5789304  2
-6.0402039  2
-6.0193919  2
-7.3461271  2
END

```

```

list(Q=2, a.a.T=0.00001, b.a.T=0.00001, a.b.T=0.00001, b.b.T=0.00001, u.u.u=0,
T.u.u=0.00001, a.T.u=0.00001, b.T.u=0.00001)

```

```

#inits
list(T = c(1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1))

```

```

a.T[ ]      b.T[ ]      T.u [ ]
1      1      1
1      1      1
END

```