Supporting Information

Maximizing chromatographic information from environmental extracts by GCxGC-ToFMS

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Contents:

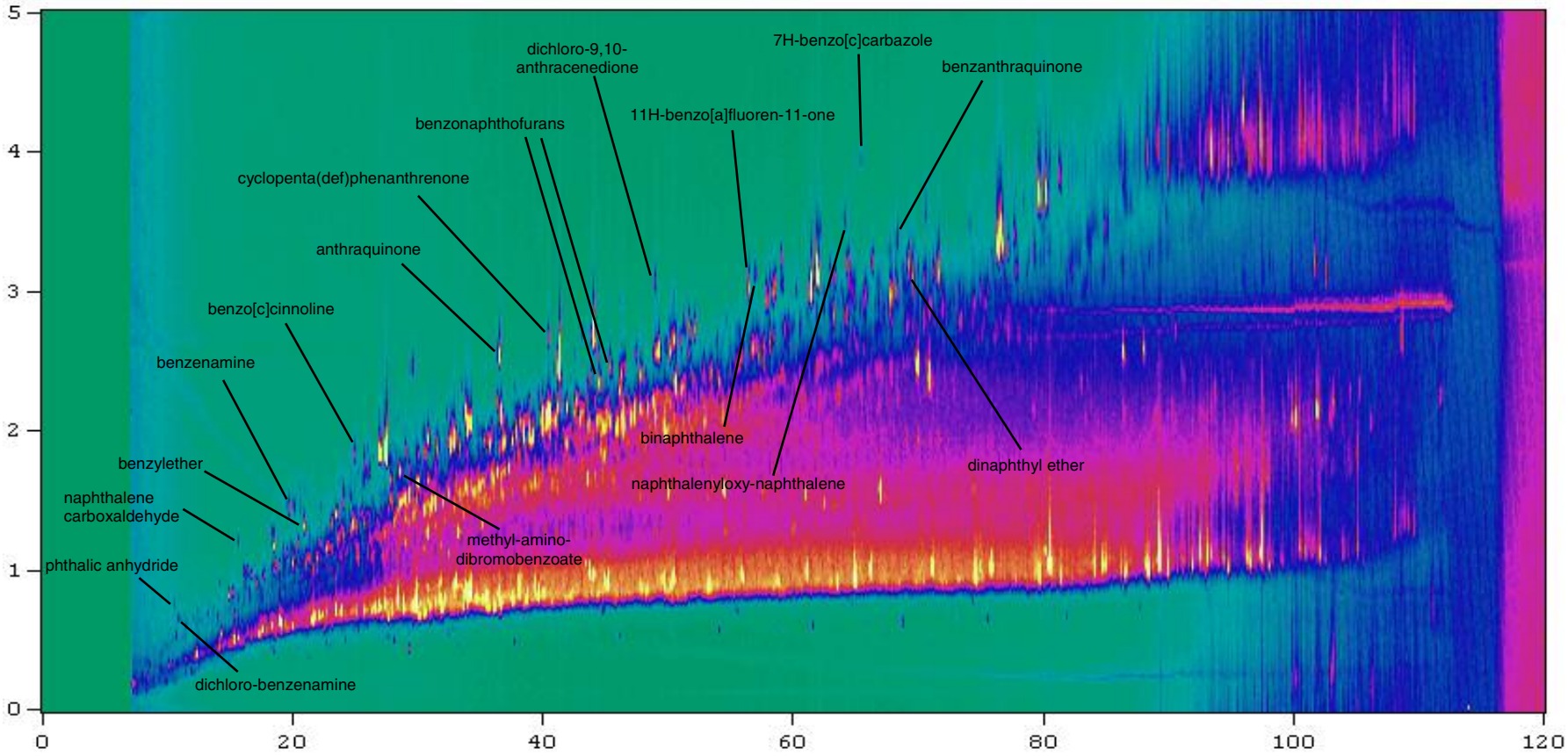
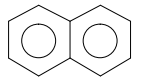
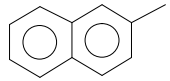
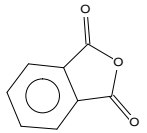
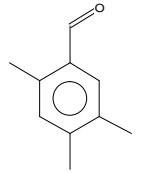
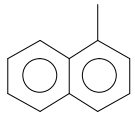
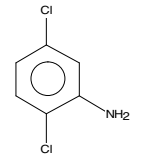
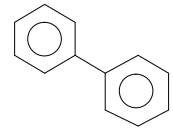
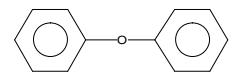
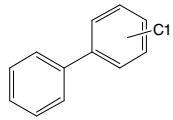
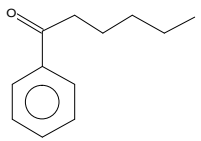
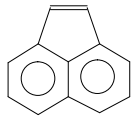
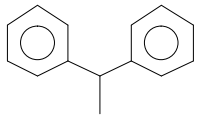
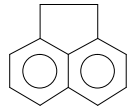
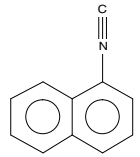
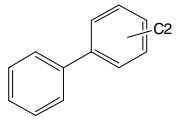
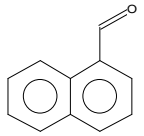
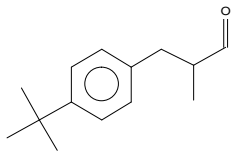
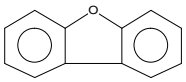
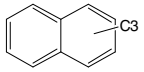
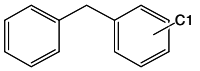


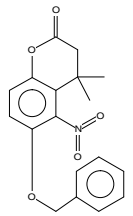
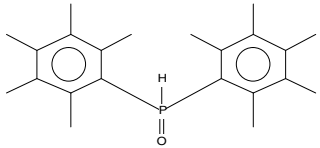
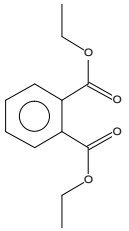
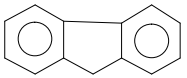
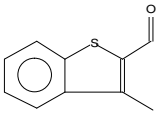
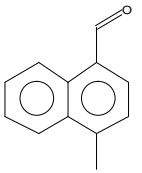
FIGURE A. GCxGC chromatogram of Elbe extract fraction 2 in the Total Ion Current mode. Examples of peaks of compounds separated from the matrix and identified with AMDIS.

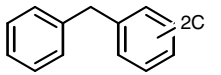
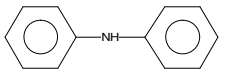
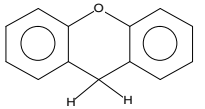
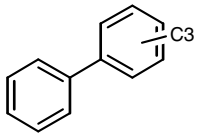
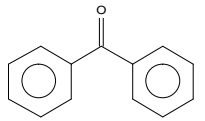
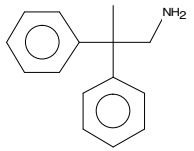
Tabel A. List of compounds identified in fraction 2 of Elbe sediment. The table lists only peaks separated from the matrix. Identification is based on a manual deconvolution and NIST-MS search. Some identities were confirmed by injections of the standards. The structures pesented in the table (with the CAS numbers) are only probable NIST library hits; e.g. a place of alkylation or halogenation on an aryl ring can be different.

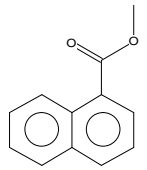
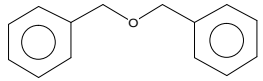
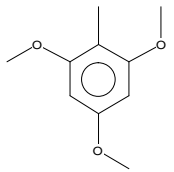
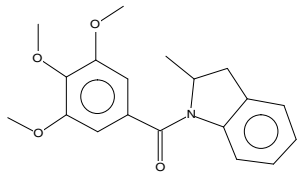
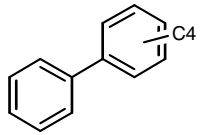
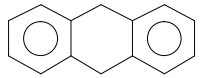
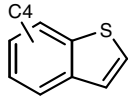
Compound	Substructure Identification[E]	R.T. (min) [A]	% NIST[B]	CAS	MW[C]	Kow[D]	Structure
Naphthalene	STANDARD	8.432		91-20-3	128	3.37	
2-Methylnaphthalene	CH2/3, AR, ArC, CH3	10.268	13	91-57-6		3.87	
Phthalic anhydride	ArCO, >C=O, ArCOO, C-O	10.523	44	85-44-9	148		
Benzaldehyde-3C	Ph-2sub	10.602	49	5779-72-6	138	3.35	
1-Methylnaphthalene	STANDARD	10.685		90-12-0		3.87	
Dichloro-benzenamine	Ph-Nsat, Ph-2sub, Cl , N-C	10.854	27	95-82-9	161	2.75	
Benzaldehyde-3C	ArC, Ph-all, CH3, PhCO	11.437	41		148		e.a.

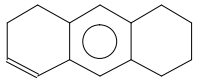
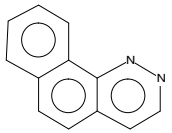
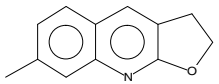
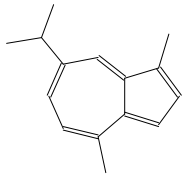
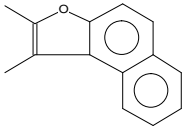
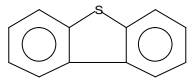
Biphenyl	AR, HCUNS, Ph-all	12.021	72	92-52-4	154		
Diphenyl ether	AR, CH&O, Ph-O	12.522	88	101-84-8	170		
Biphenyl-1C	AR, ph, -CH2/3-, AR-CHx	13.356	25		168		
1-Phenyl-hexanone	Ph-all, -CH2/3-, CH3, PhCO	13.938	48	942-92-7	176	3.64	
Acenaphthylene	STANDARD	14.025	49	208-96-8	152	4.07	
Biphenyl-1C	AR, ph, -CH2/3-, AR-CHx	14.857	27		168	4.63	e.a.
1,1'-Ethylidenebis- benzene	AR, -CH2/3-	15.106	21	612-00-0	182	4.15	
Acenaphthene	STANDARD	15.109	66	83-32-9	154	3.98	
Biphenyl-1C	AR, Ar-CHx	15.191	30		168		e.a.

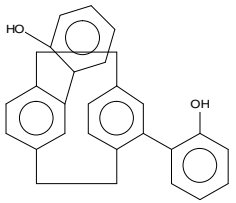
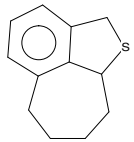
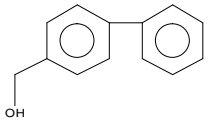
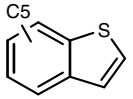
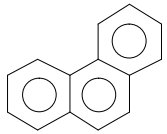
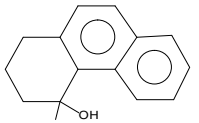
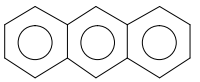
Isocyano-naphthalene	AR, N, Naph, CN, CH&N, PAH	15.279	70	1984-04-9	153		
Biphenyl-2C	HCUNS, AR, Ph-all, ArC	15.523	15		182		
Naphthalene-carboxaldehyde	naph, >C=O	15.613	77	66-77-3	156	2.89	
Lilial	CH3, >C=O	16.106	40	80-54-6	204		
Dibenzofuran	AR, HCUNS	16.11	30	132-64-9	153		
Isocyano-naphthalene	N, naph	16.115	72		153		e.a.
Naphthalene-3C	naph, CH3	16.274	24		170		
Diphenylmethane-1C	Ph-all, Ph-2sub, CH3	16.36	36		182	4.56	
Naphthalene-3C	CH3, naph	16.44	35		170		e.a.
Phenylmethyl-benzene-1C	Ph-all, Ar-CHx, CH3	16.610	21		180		e.a.
Naphthalene-3C	Naph, CH3	17.025			170		e.a.

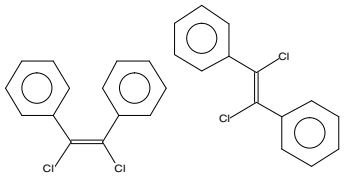
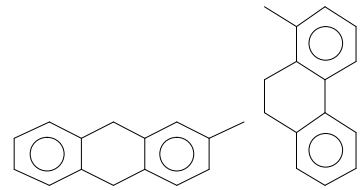
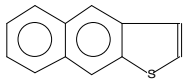
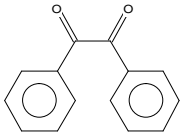
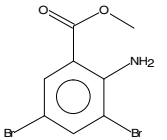
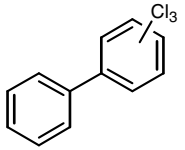
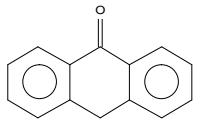
6-benzyloxy-3,4-dihydro-4,4-dimethyl-5-nitro-coumarin	Ph-all, O, hetcyc, Ar-CHx, ether, N	17.126	22	N/A	327		
Bis(pentamethylphenyl)-phosphine oxide	O, CH3, ether, hetcyc, CH2	17.459	43	122085-61-4	342		
Naphthalene-3C	naph, CH3	17.692			170		e.a.
Diethyl phthalate	ArCOO, Ph-2sub	18.198	63	84-66-2	222		
Biphenyl-2C	Ph-2sub, CH3, PhCH3, Ar-Ar	18.444	22		182		e.a.
Fluorene	STANDARD	18.446		86-73-7	180	4.18	
Naphthalene-3C	Naph, CH3	18.611	32		170		e.a.
Biphenyl-2C	PhCH3, PH-2sub, Ph-all	18.944	30		182		e.a.
Methyl-benzo[b]thiophene-carboxaldehyde	O, AR, hetcyc, >C=O,	18.951	48	22053-74-3	176		
Methyl-naphthalenecarboxaldehyde	AR, ArC, naph, O	19.284	57	33738-48-6	170		

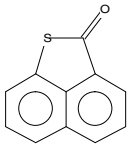
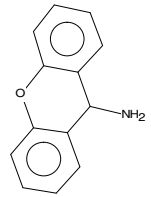
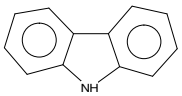
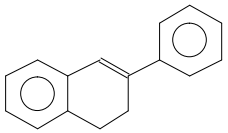
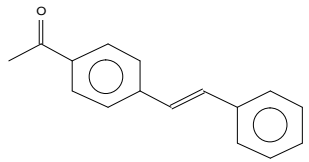
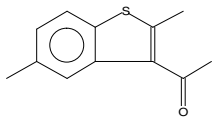
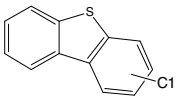
Methyl-benzo[b]thiophene-carboxaldehyde	AR, hetcyc, O, S, >C=O, CH3, ArS	19.451	56		176		e.a.
Diphenylmethane-2C	AR, Ph-all, CH3, CH2/3	19.529	33		196		
Benzenamine, N-phenyl-	Ph-all, N, ArN, Ph-Nsat	19.618	52	122-39-4	169		
9H-Xanthene	AR, O, C-O	19.863	30	92-83-1	182	4.23	
Biphenyl-3C	ArC, Ph-all, CH3, -CH2/3-	19.944	21		196		
Benzophenone	Ph-all, PhCO	20.035	70	119-61-9	182		
2,2-Diphenylpropylamine	PhCsat, AR, Ph-all, CH3	20.195	42	34611-07-9	211		
9H-Xanthene	O, AR, >C=O	20.447	46		182		e.a.
Methyl-naphthalenecarboxaldehyde	AR, O, C-O, Ph-all, -OH	20.535	29		170		e.a.

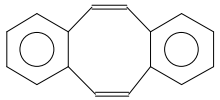
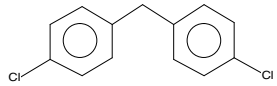
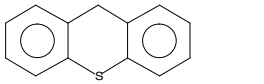
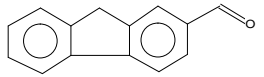
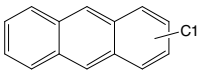
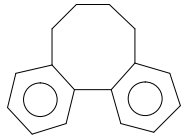
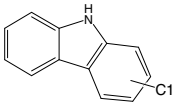
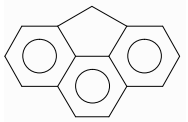
Naphthalenecarboxylic acid-methyl ester	naph, ArCO, >C=O, ArCOO	20.617	31	2459-24-7	186	
Methyl-naphthalenecarboxaldehyde	hetcyc, AR, S, S-C, ArS, O, >C=O, CH3	20.620	51		176	e.a.
Benzylether	PhCH2, O, C-O	20.865	41	103-50-4	198	
Methyl-naphthalenecarboxaldehyde	AR, O, Ph-O, >C=O	21.203	35		170	e.a.
Biphenyl-3C	-CH2/3- AR, Ph-all	21.278	31		196	e.a.
2,4,6-trimethoxytoluene	AR, Ph-all, O, OCH3, CH3, ether	21.455	17	14107-97-2	182	
2,3-dihydro-1-(3,4,5-trimethoxybenzoyl)-2-methyl-indole	O, AR, >C=O, Ph-all, CH3, hetcyc, ARCO	21.619	47	333352-31-1	327	
Biphenyl-4C	AR, Ph-all, Ar-C, CH3	22.197	22		210	
9,10-dihydro-anthracene	AR, CH2	22.201	36	613-31-0	180	
Benzo[b]thiophene-4C	Ar.R, CH3, hetcyc, S, AR-CHx	24.288	25	16587-45-4	190	

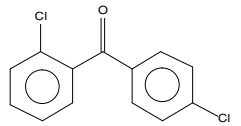
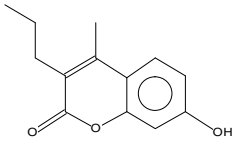
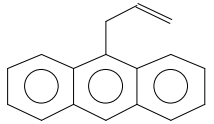
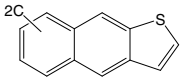
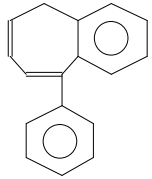
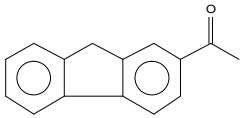
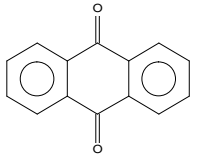
Anthracene, 1,2,3,4,5,6-hexahydro-	AR	24.536	11	6109-22-4	184		
UNKNOWN	AR, Ph-all, O, CH2/3	24.540					
Diphenylmethane-2C	AR , Ph-all, CH2/3, Ph-2sub	24.614	26		196		e.a.
Naphthalene-4C	AR, naph, Ar-CHx	24.619	51		184		e.a.
Benzo[b]thiophene-4C	AR, hetcyc, CH2/3, S	24.704	29		190		e.a.
Naphthalene-4C	AR, naph, Ar-CHx	24.869	38		184		e.a.
Benzo[c]cinnoline	AR, .N.	24.874	33	230-31-9	180		
2,3-Dihydro-7-methylfuro(2,3-b)quinoline	AR, N, O, hetcyc, .N.	25.038	23	73863-57-7	185		
UNKNOWN	AR, O, CH3, S, N, hetcyc, N-C, halogen	25.125					
1,2,3,4,5,6-hexahydro-anthracene	AR, -CH2/3-, CH3, cond, naph	25.205	22		184		e.a.
Biphenyl-4C	AR, CH3	25.367	25		210		e.a.
1,4-dimethyl-7-(1-methylethyl)-azulene	CH3, CH2/3, cond, AR	25.445	36	489-84-9	198		
Naphtho[2,1-b]furan-2C	AR, ArC, O, Ph-All	25.615	5	129812-23-3	196		
Dibenzothiophene	STANDARD	25.623	53	132-65-0	184	4.38	

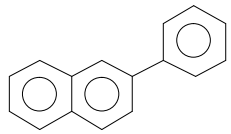
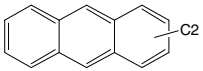
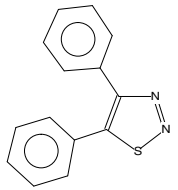
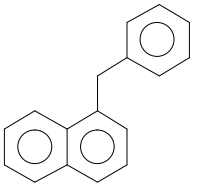
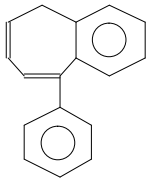
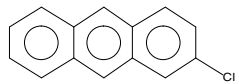
5,12-Di-(2-hydroxyphenyl)paracyclophane	AR, ArC, Ph-all, CH2/3 O	25.867	21	N/A	392		
Naphthalene-4C	AR, -CH2/3-	25.955	46		184		e.a.
2,6,7,8,9,9a-hexahydro-cyclohepta[cd][2]-benzothiophene	AR, S	25.958	48	199807-57-3	190		
Hydroxymethylbiphenyl	AR, ph, O, C-O	26.122	14	3597-91-9	184		
1,2,3,4,5,6-hexahydro-anthracene	naph, ArC, cond, Ar-CH2,3, CH3	26.457	15		184		e.a.
Benzo[b]thiophene-5C	AR, CH3, hetcyc, ArC, O, S	26.705	21		204		
Phenanthrene	STANDARD	26.958	30		178	4.46	
1,2,3,4-tetrahydro-4-methyl-4-phenanthrenol	AR, AR.C, CH2, CH3	27.369	42	77536-58-4	212		
Anthracene	STANDARD	27.375	22	120-20-7	178	4.5	

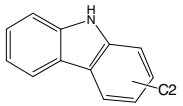
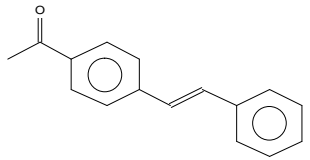
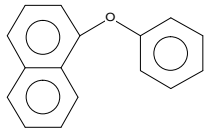
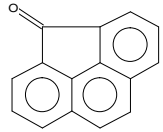
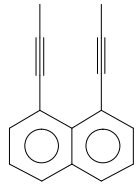
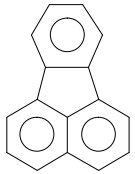
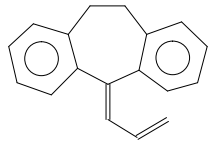
Dichlorostilbene (trans or cis)	Cl, AR, Ph-all, Ar-C=C, ArCl, C=CX	27.788	33	5216-32-0 951-86-0	248		
Methyl-9,10-dihydro-anthracene or methyl- 9,10-dihydro-phenanthrene	AR, CH2/3, ArC, CH2, CH3	28.205	29	948-67-4 95676-48-5	194		
Naphtho[2,3-b]thiophene	S, hetcyc, S-C, Ar.S, AR ArS	28.211	44	268-77-9	184		
Benzil	Ph, Ar-CO, -C=O	28.378	6	134-81-6	210	3.38	
Methyl 2-amino-3,5-dibromobenzoate	AR, Br, N, Ar-Br, Ph-all, O, C-O, Br=2, Ph-4sub, >C=O, ArN, ether, -O-, Ph-Nsat, C=OO, ArCOO	28.538	98	606-00-8	307		
9,10-dihydro-anthracene-1C or 9,10-dihydro-phenanthrene-1C	CH2/3, AR, ArC, -CH2/3-, Ar.C, CH3	28.618	29		194		e.a.
Trichloro-biphenyl	Cl, ArCl, Ar-Ar	28.872	40				
Anthrone	AR, O	29.041	34	90-44-8	194	3.66	

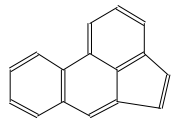
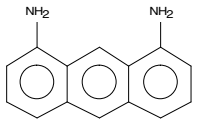
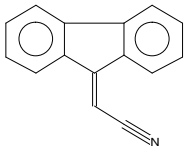
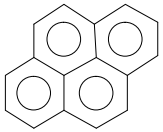
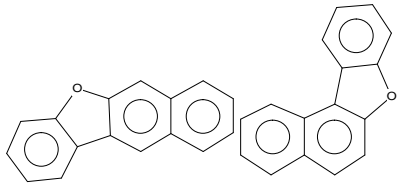
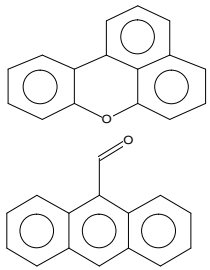
2H-Naphtho[1,8-bc]thiophen-2-one	>C=O, hetcyc, AR, O, .C=O, S, ArCO, S-C	29.132	81	20760-29-6	186	
9H-Xanthen-9-ylamine	AR, O, C-O, Ph-all, Ph-2sub, ether	29.210	8	N/A	197	
Dichlorostilbene (trans or cis)	AR, Ph-all, Cl, 1C=#C, Ar-C=C	29.371	38		248	e.a.
Carbazole	N, AR, .N., N-C, hetcyc	29.551	31	86-74-8	167	
9,10-dihydro-anthracene-1C or 9,10-dihydro-phenanthrene-1C	AR, ArC, HCUNS, CH3, Ar.C	30.038	28		194	e.a.
1,2-Dihydro-3-phenylnaphthalene	AR, Ph-all, CH2, ArC	30.040	13	20669-52-7	206	
Ethanone, 1-[4-(2-phenylethenyl)phenyl]-	AR, >C=O	30.207	42	3112-03-6	222	
3-Acetyl-2,5-dimethylbenzo(b)thiophene	-CH2/3-1, Ar-C, O	30.376	34	6179-04-0	204	
Dibenzothiophene-1C	S, ArC, hetcyc	30.540	52	16587-52-3	198	

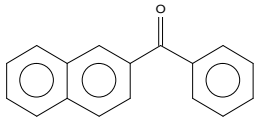
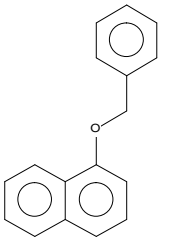
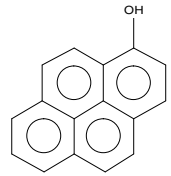
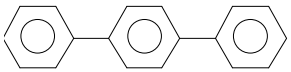
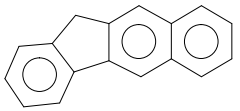
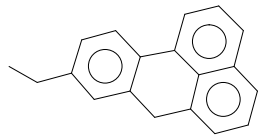
Dibenzo[a,e]cyclooctene	HCUNS	30.792	14	262-89-5	204		
Dichlorodiphenyl-methane	Cl, Ph-Cl	30.958	42	101-76-8	236	5.3	
Dibenzothiophene-1C	ArC, hetcyc, S	31.541	48		198		e.a.
Thioxanthene	ArC, hetcyc, S	32.043	36	261-31-4	198	4.55	
Fluorenecarboxaldehyde	AR, O, >C=O	32.296	46	30084-90-3	194		
Anthracene- or Phenanthrene-1C	An/Phen, ArC	32.625	22		192		
Thioxanthene	ArC, S, hetcyc, ArS	32.712	42		198		e.a.
Anthracene- or Phenanthrene-1C	An/Phen, ArC	32.875	18		192		e.a.
Dibenzo[a,c]cyclooctene, 5,6,7,8-tetrahydro-	ArC	33.291	13	1082-12-8	208		
Anthracene- or Phenanthrene-1C	An/Phen, Ar-C	33.375	25		192		e.a.
9H-Carbazole-1C	.N., ArN, ?NH?, CH3	33.549	16		181	3.84	
4H-Cyclopenta[def]phenanthrene	4+brid, CH2	33.796	91	203-64-5	190	4.6	
Anthracene- or Phenanthrene-1C	An/Phen, ArCH3	33.961	27		192		e.a
Anthracene- or Phenanthrene-1C	An/Phen, ArCH3	34.128	25		192		e.a.

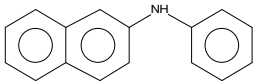
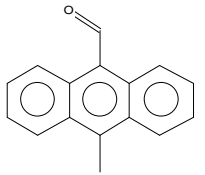
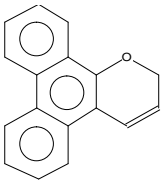
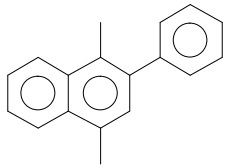
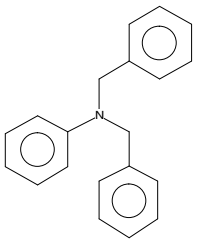
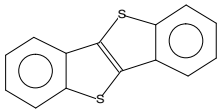
Dichlorobenzophenone	PhCO, Ph-2sub, Cl, ArCl, ArCOAr	34.628	33	85-29-0	250	4.44	
7-hydroxy-4-methyl-3-propyl-coumarin	AR, -CH2/3-, O, hetcyc, >C=O, CCH3, C-O	34.877	40	19491-93-1	218		
Propenl-anthracene	AR, cond, Ph-all, PAH	35.127	45	23707-65-5	218		
Naphtho[2,3-b]thiophene-2C	AR, Ar-C, -CH2/3-,	35.292	61		212		
Naphtho[2,3-b]thiophene-2C	S, Ar-C, hetcyc	35.792	58		212		e.a.
9H-Carbazole-1C	N, Ar-N, .N., CH3, ?NH?	36.055	26		181		e.a.
9-Phenyl-5H-benzocycloheptene	cond, Ph-all	36.293	20	138089-71-1	218		
Acetylfluorene	O, CH3, cond	36.380	48	781-73-7	208		
Anthraquinone	.C=O, O2, ArCOAr	36.469	71	84-65-1		3.39	

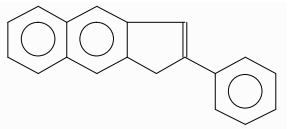
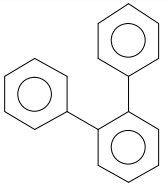
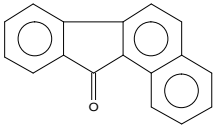
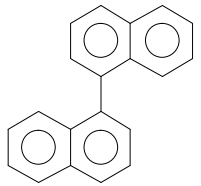
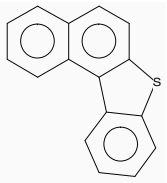
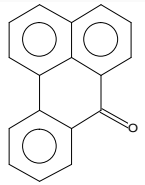
Phenyl-naphthelene	cond, PAH, Ph-all, naph	36.628	31	612-94-2	204		
Naphtho[2,3-b]thiophene-2C	S, Ar-C, hetcyc	36.875	57		212		e.a
Phenanthrene- or Anthracene-2C	An/Phen, ArC	37.542	26		206		
1,2,3-Thiadiazole, 4,5-diphenyl-	hetcyc, S, Ph-all, 1C=#C	37.629	64	5393-99-7	238		
Phenylmethyl-naphthalene	ArC, ph, CH2	37.715	25	611-45-0	218		
Dichlorobenzophenone	Cl2, Ph-2sub, PhCO, PhCl	37.793	20		250	4.44	e.a.
9-Phenyl-5H-benzocycloheptene	cond, Ph-all, Ar-CHx	37.796	25	138089-71-1	218		
Naphtho[2,3-b]thiophene-2C	S, ArC, hetcyc, O, Ph-all, S-C, CH3	37.877	75		212		e.a.
UNKNOWN	Ar, CH3, N, Ar-CHx, Ar.N	38.041					
2-Chloroanthracene	STANDARD	38.046	32	17135-78-3	212	4.99	
Naphtho[2,3-b]thiophene-C2	S, ArC, hetcyc, O, Ph-all, S-C, CH3	38.127	51		212		e.a.

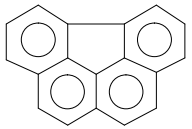
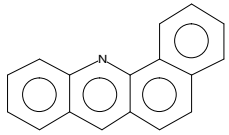
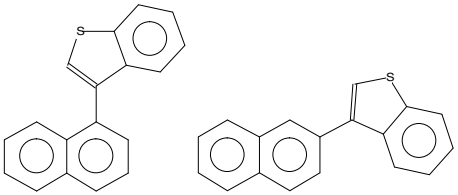
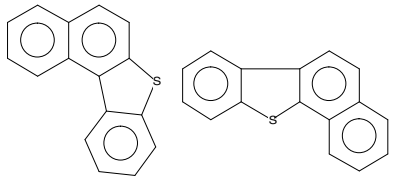
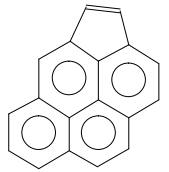
Naphtho[2,3-b]thiophene-C2	S, ArC, hetcyc, O, Ph-all, S-C, CH3	38.794	85				e.a.
Carbazole-2C	ArN	39.132	17	18992-68-2	195		
Ethanone, 1-[4-(2-phenylethenyl)phenyl]-	O, Ph-all,	39.378	23	3112-03-6	222		
Naphthyl phenyl ether	Ar, Ph-all	39.384	26	3402-76-4	220		
Cyclopenta(def)phenanthrenone	AR, .C=O, cond	40.387	99	5737-13-3	204		
Dipropynylnaphthalene	AR, HC, PAH	40.884	20	22360-77-6	204		
Fluoranthene	STANDARD	41.301		26-44-0	202	4.90	
5-(2-Propenylidene)-10,11-dihydro-5H-dibenzo[a,d]cycloheptene	AR, Ph-all, Ar-C	42.216	63	24755-73-5	232		

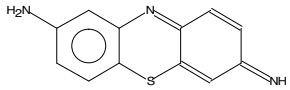
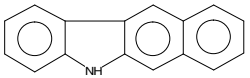
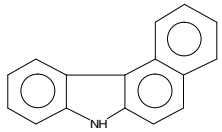
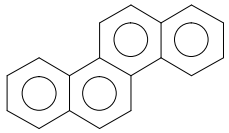
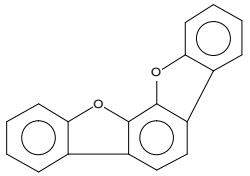
PAH MW=202	PAH	42.552	60	201-06-9	202		
UNKNOWN	AR, CH3, -CH2/3-, 4-brid, cond, An/Phen,	42.798			232		
Anthracenediamine	AR, N, CH2/3	43.138	22	139312-39-3	208		
Cyanomethylenefluorene	N1, cond, PAH, 4+brid, CN	43.472	27	4425-74-5	203		
Pyrene	STANDARD	43.978			202	4.88	
Benzonaphthofuran or Benzo[k]xanthene	Ar, hetcyc, PAH, O	44.465		243-42-5	218		
Anthracenecarboxaldehyde	-C=O, An/Phen,	44.557	64	642-31-9	206		
UNKNOWN	CH, cond, PAH, Ph-all, naph	44.886					e.a.
Benzonaphthofuran or	Hetcyc, PAH, O,	45.384			218		e.a.

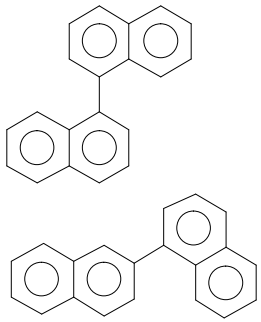
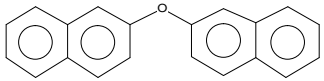
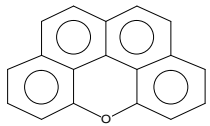
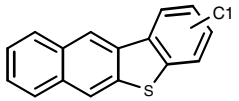
Benzo[k]xanthene							
UNKNOWN	Cl, Ar, -CH2/3-, CH3, N, O, Ph-all	46.048			305		
Methanone, 2-naphthalenylphenyl	naph, ArCOAr	46.142	86	644-13-3	232		
Benzonaphthofuran or Benzo[k]xanthene	AR, cond, hetcyc, O, PAH	46.217	57		218		e.a.
Naphthalene, 1-(phenylmethoxy)-	PhCH2, OCH2, ether	46.55	68	607-58-9	234		
Hydroxypyrene	AR, cond, PAH, O, hetcyc,	46.970	62	5315-79-7	218		
Benzonaphthofuran or Benzo[k]xanthene	AR, cond, O, hetcyc	47.469	34		218		e.a.
p-Terphenyl	Ph-all, Ph-2sub, Ar-Ar	48.216	46	92-94-4	230	6.03	
11H-Benzo[b]fluorene	PAH, cond, ArC, CH2/3,	49.219	52	243-17-4	216	5.77	
9-Ethyl-7H-benzo[de]anthracene	cond, PAH	49.804	38	N/A	244		
11H-Benzo[b]fluorene	PAH, cond, ArCH2/3	50.219	53		216		e.a.
11H-Benzo[b]fluorene	PAH, cond, ArCH2/3	50.304	30		216		e.a.

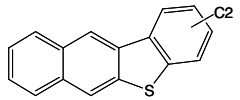
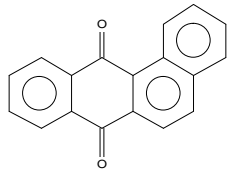
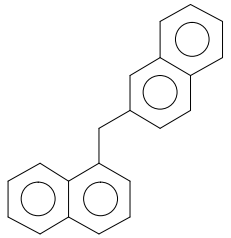
Naphthalenamine, N-phenyl-	N, Ph-all, PAH, ArN	50.476	39	135-88-6	219	4.38	
UNKNOWN	AR, O, Ph-all	51.048			272		
UNKNOWN	AR, cond, Ph-all	51.054			219		
10-Methylanthracene-9-carboxaldehyde	An/Phen, ArCH3, ArCHO	51.306	41	7072-00-6	220		
2H-Phenanthro[9,10-b]pyran	PAH, hetcyc, C-O	51.967	94	217-67-4	232		
phenyl-naphthalene-2C	HC, Ph-all, Naph, CH3	52.800	43	51036-91-0	232		
UNKNOWN	Ph-all, -CH2/3-, CH3, >C<, Cl	53.384			272		
UNKNOWN	hetcyc, cond, .N., O, PAH, Ph-all	53.887			245		
UNKNOWN	AR, Ph-all, cond, CH2,	54.049			234		
Benzenemethanamine, N-phenyl-N-(phenylmethyl)-	Ph-all, Ar-C, CH2, N	54.386	15	91-73-6	273	5.29	
[1]Benzothieno[3,2-b][1]benzothiophene	hetcyc, S,	54.724	56	248-70-4	240		

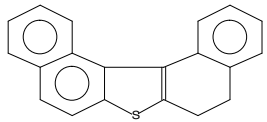
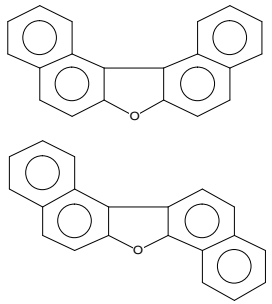
Phenyl-benz[f]indene	AR, AR-CHx, PAH, Ar-CH3,	54.969	17	N/A	242		
o-Terphenyl	AR, Ph-all,	55.970	21	84-15-1	230		
UNKNOWN	AR, O, -CH2/3-	56.304			230		
11H-Benzo[a]fluoren-11-one	AR, PAH, >C=O, .C=O	56.477	58	479-79-8	230		
o-Terphenyl	AR.Ph-all,	56.803	36		230		e.a.
Binaphthalene	PAH, naph, Ar-Ar	56.979	31	604-53-5	254	6.11	
UNKNOWN	AR, Ph-all, O, >C=O, Ar-C=C	57.218					
Benzo[b]naphtho[1,2-d]thiophene	Ar.S, hetcyc, S-C, PAH, cond	57.892	68	205-43-6	234	5.19	
7H-Benz[de]anthracen-7-one	PAH, >C=O	58.145	58	82-05-3	230	4.81	

Benzo[ghi]fluoranthene	cond, PAH	58.393	59	203-12-3	226		
PAH MW=228	AR, PAH	58.561	63		228		
Benzacridine	PAH, .N.	58.978	76	225-51-4	229	4.49	
Naphthenyl-benzothiophene	hetcyc,S, Ph-all	59.064	46	55712-59-9 55712-60-2	260		
Benzonaphthothiophene	Ar.S, S, CH&S, hetcyc, PAH	59.227	60	205-43-6 239-35-0	234	5.19	
Benzonaphthothiophene	Ar.S, CH&S, hetcyc, PAH	60.063	53		234		e.a.
Benzonaphthothiophene	Ar.S, CH&S, hetcyc, PAH	60.310	60		234		e.a.
Benzonaphthothiophene	Ar.S, CH&S, hetcyc, PAH	60.480	49		234		e.a.
Cyclopenta[cd]pyrene	cond, PAH,	60.981	76	27208-37-3	226		

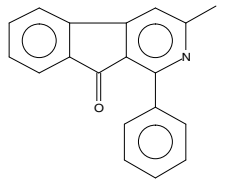
Amino-imino-phenothiazine	AR, hetcyc, .N., Ar.S	60.984	53	6470-71-9	227		
UNKNOWN	AR, hetcyc, cond, O	61.223			244		
Benzoacridine	PAH, .N.	61.393	62		229	4.48	e.a.
Benzoacridine	PAH	61.895	38		228		e.a.
Benzocarbazole	N, PAH, .N., cond	62.151	39	243-28-7 205-25-4	217	4.47	 
UNKNOWN	cond, PAH, O, hetcyc, N	62.475			245		
UNKNOWN	Ar-C, Ph-all, N-C, cond	62.891			244		
Chrysene	STANDARD	62.895		218-01-9	228	5.81	
Benzobisbenzofuran	AR, O, O2, hetcyc, .O.	63.055	15	222-23-1	258		
UNKNOWN	AR, hetcyc, Cl, S, Ar-Cl, CH3	63.224			249		

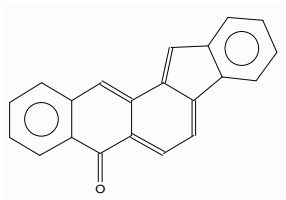
Binaphthalene	cond, PAH, naph, Ar-AR	63.395	18	604-53-5 4325-74-0	254	6.11	
Binaphthalene	cond, PAH, naph, Ar-AR	63.893	10		254		e.a.
Binaphthalene	cond, PAH, naph, Ar-AR	63.976	22		254		e.a.
Dinaphthyl ether	AR, O cond, PAH, naph, Ar-O-Ar	64.152	70	613-80-9	270		
UNKNOWN	AR, hetcyc, Cl, S, Ar-Cl, CH3	64.307			249		
Naphthenyl-benzothiophene	Ar, S, hetcyc, 1C=#C, Ph-all	64.396	48		260		e.a.
Naphtho[2,1,8,7-klmn]xanthene	PAH, cond,	64.561	63	191-37-7	242		
Benzocarbazole	N, Ar, cond, PAH, hetcyc	64.74	35		217		e.a.
UNKNOWN	hetcyc, S, Ar-CHx, CH3, N, halogen, PAH	65.308			263		
Benzocarbazole	N, cond, PAH, .N.	65.492	26		217		e.a.
Benzonaphthothiophene-1C		65.725	34		248		
Naphthenyl-benzothiophene	S, hetcyc, cond, PAH, Ph-all, naph	66.397	51		260		e.a.
UNKNOWN	AR, N, Cl,	67.648			266		

Benzonaphthothiophene-2C	Ar, CH3, hetcyc, S,O	67.890	75	24964-12-3	262		
Benz[a]anthracene-7,12-dione	ArCO, .CO, cond, O2, PAH	68.315	81	2498-66-0	258	4.4	
Dinaphthyl ether	PAH, O	69.312	55		270	6.4	e.a.
PAH228-C1	ArCH3, PAH	69.645	10		242		
Naphthalenylmethyl-naphthalene	PAH, Ar-CH2, naph	69.732	49	611-48-3	268		
Benzonaphthothiophene-2C	hetcyc, S, CH3, PAH, .S.	70.473	75		262		e.a.
Binaphthalene	PAH, naph, Ar-Ar	70.478	25		254		\ e.a.
UNKNOWN	AR, N, hetcyc, .N., O, halogen	70.646			266		
Dinaphthyl ether	AR, O, Ph-all,	70.652	21				e.a.
Benzonaphthothiophene-2C	hetcyc, S, cond, CH3	70.892	75		262		e.a.
Benzonaphthothiophene-2C	hetcyc, S, cond, CH3	71.058	75		262		e.a.
Binaphthalene	PAH, naph, Ar-Ar	71.311					e.a.
Benzonaphthothiophene-2C	hetcyc, S, cond, CH3	71.390	54		262		e.a.
Naphthenyl-benzothiophene	S, AR, ArS, hetcyc, Ar.S, CH&S	71.646	41		260		e.a.
Benzonaphthothiophene-2C	Hetcyc, S, cond, CH3	71.974	61		262		e.a.
UNKNOWN	N, Ar, hetcyc, halogen, CH3	72.489					

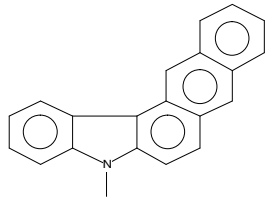
Benzonaphthothiophene-2C	hetcyc, S, cond, CH3	72.558	45		262	e.a.
UNKNOWN	hetcyc, N, cond, PAH, O	74.152			255	
Dihydro-dinaphthothiophene	AR, hetcyc, S, CH&S	75.489	30	16587-62-5	286	
UNKNOW	Cl, PAH	75.898			278	
PAH MW=252 (2-3 peaks)	PAH, HCUNS	76.316	33		252	
Dinaphthofuran	O, hetcyc, ether	77.232		194-63-8 207-93-2	268	
PAH MW=252	PAH, HCUNS	77.733	27		252	
UNKNOWN	AR, O, hetcyc, ether	77.823			258	
Dinaphthofuran	O, hetcyc, ether	77.979	5		268	e.a.
UNKNOWN	hetcyc, Ph-all, N	78.404			258	
Dinaphthofuran	Ar, O, hetcyc	78.729	35		268	e.a.
Dinaphthofuran	Ar, O, hetcyc	78.897	8		268	e.a.
UNKNOWN	hetcyc, Ph-all, O, ether	79.155			258	
Dinaphthofuran	Ar, O, hetcyc	79.315	4		268	e.a.
PAH MW=252	PAH, 4+brid, HCUNS	79.738	26		252	
UNKNOWN	AR, N, O ether, hetcyc,	79.814			268	
PAH MW=252	PAH, 4+brid, HCUNS	80.239	24		252	
Dinaphthofuran	AR, hetcyc, O, ether	80.481	12		268	e.a.
PAH MW=252	PAH, 4+brid, HCUNS	81.324	24		252	

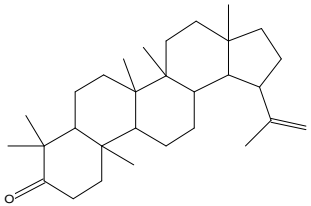
PAH 252-C1	AR, 4+brid, C2/3	81.480	35		266
PAH 252-C1	AR, 4+brid, C2/3	82.312	57		266
PAH 252-C1	AR, 4+brid, C2/3	82.647	51		266
PAH 252-C1	AR, 4+brid, C2/3	82.897	44		266
UNKNOWN	AR, Ph-all, O, hetcyc	83.310			271
PAH 252-C1	AR, PAH, 4+brid, C2/3	83.650	53		266
PAH 252-C1	AR, PAH, 4+brid, C2/3	84.068	38		266
PAH MW=266	AR, PAH, 4+brid, C2/3	84.317	39		266
Methyl-phenyl-azafluorenone	AR, O, hetcyc, .N., Ph-all, Ndbl	84.896	53	62578-45-4	271
PAH 252-C1	AR, 4+brid, PAH	84.900	69		266
PAH 252-C1	AR, 4+brid, PAH	85.151	38		266
PAH 252-C1	AR, 4+brid, PAH	86.068	21		266
UNKNOWN	AR, Ph-all, CH3	86.313			362
UNKNOWN	CH2/3, O, N, AR, ether, -Ch2/3-, .N., halogen	86.386			345
UNKNOWN	AR, N,O, hetcyc	86.489			263
UNKNOWN	O, ether, hetcyc, CH2	88.053			345
UNKNOWN	AR, Ph-all, CH3	88.48			362
7H-Indeno[2,1-a]anthracen-7-one	AR, O >=O	89.49	14	27582-45-2	280
UNKNOWN	hetcyc, AR, halogen, N, S, O	89.902			380
UNKNOWN	O, C-O, CH3, ether, hetcyc	90.555			330

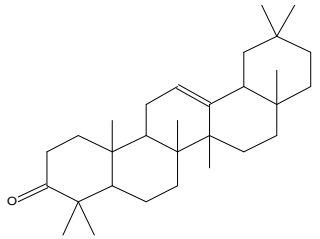




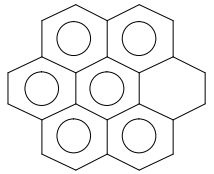
PAH MW=278	4+brid, AR, PAH	91.158	29		278
Methylnaphthocarbazole	AR, CH3, hetcyc, N	91.9	37	100025-44-3	281
PAH MW=276	AR, PAH, 4+brid	92.493	33		276
PAH MW=278	4+brid, AR, PAH	92.738	30		278
PAH MW=276	4+brid, AR, PAH	93.493	43		276
PAH MW=278	AR, 4+brid, PAH	94.074	20		278
PAH MW=278	4+brid, AR, PAH	95.077	20		278
PAH MW=278	4+brid, AR, PAH	95.412	18		278
UNKNOWN	hetcyc, -CH2/3-, AR, .N., CH3, O, ether,	95.978			327
PAH MW=276	4+brid, AR, PAH	95.997	31		276
PAH MW=276	AR, PAH, 4+brid	96.081	61		276
UNKNOWN	AR, cond, O	98.146			342
Lup-20(29)-en-3-one	CCH3, NoAr-Cy, O	99.878	17	1617-70-5	424
4,4,6a,6b,8a,11,11,14b-Octamethyl-1,4,4a,5,6,6a,6b,7,8,8a,9,10,11,12,12a,14,14a,14b-octadecahydro-2H-picen-3-one	noAr_cy, CCH3, cond, O	100.211	25	N/A	424
UNKNOWN	AR, .N., hetcyc, O	101.73			325
UNKNOWN	AR, N	102.563			325







PAH with MW=302	cond, PAH	107.335	24		302
PAH with MW=302	PAH, cond	108.086	10		302
Dihydrocoronene	AR, PAH, 4+brid	111.105	49	107716-56-3	302



[A] Retention time
[B] Probability of the NIST library match
[C] Molecular weight
[D] Octanol-water partition coefficient – values from ChemIDPlus Advanced, United States national Library of Medicine (http://chem.sis.nlm.nih.gov/chemidplus/)
[E] Possible substructures identified by NIST-MS search with probability above 50%; abbreviations are explained below

e.a.- example above
4+brid four bridging atoms in ring cluster, **AR** aromatic rings, **An/Phen** anthracene or phenanthrene, **Ar-Ar** aryl-aryl non ring bond, **ArC** aromatic carbon attached to carbon, **Ar-C** aromatic ring-saturated carbon atom bond, **ArCH3** aryl methane group, **Ar-CH2/3** aromatic bond to methyl or methylene group, **Ar-CHx** aromatic-saturated carbon bond, **ArCO** aryl carbonyl, **ArCOO** aryl ester, **ArN** aromatic carbon-nitrogen bond, **Ar.NH** aryl carbon attached to NH in ring, **ArNO2** aryl nitro, **Ar-O** aromatic ring-oxygen atom bond, **ArS** aryl sulphide, **Ar.S** aromatic-sulphur bond in ring, **ARSO2** aromatic SO2 bond, **>C<** quaternary carbon, **carbcy** contains carbon-only rings, **CCH3** methyl bonded to carbon, **CH2/3** primary or secondary saturated carbon, **CH2** methylene group, **CH3** methyl, -**CH2/3-** methylene or methyl group (chain), **-CH2/3-1** exactly one methylene or methyl group (chain), **CH3+alkyl** methylene attached to saturated C-atoms (chain), **CH&N** contains only carbon, hydrogen and nitrogen, **CH&O** contains only carbon, hydrogen and oxygen, **C=C** carbon-carbon double bond, **CN** cyano, **C-O** carbon-oxygen bond, **>C=O** carbonyl group, **.C=O** ring carbonyl, **cond** condensed ring structure (1,2-overlap), **COO** ester group, **-(C=O)-O.** methyl ester, **CO-O/OH** carboxyl or ester, **HC** hydrocarbon, **hetcyc** ring containing at least one hetero atom, **HCUNS** unsaturated carbon, **imino** double bonded, trivalent nitrogen, **N** contains nitrogen**, .N.** any nitrogen atom in ring, **naph** naphthalene ring, **N-C** nitrogen-carbon single bond, **N=C** nitrogen-carbon double bond, **Ndbl** doubly bonded nitrogen atom**,** **?NH?** secondary amine (not alkyl, aryl), **noAr** no aromatic rings, **noAr_cy** rings present, but not aromatic, **noN&O** no nitrogen or oxygen,

O contains oxygen, **-O-** oxygen in chain, **O2** contains two oxygen atoms, **OCH3** methoxy,
OCH2/O. ether oxygen attached to methyl or methylene, **O=COC=O** anhydride, **PAH** condensed polynuclear aromatic compound,
ONS-self OO, NN or SS bond, **ph** phenyl group, **Ph-2sub** phenyl with 2 substituents, **Ph-2+sub** phenyl with 2 or more substituents,
Ph-all isolated benzenoid ring**, PhCH2** phenyl with methylene substituent, **PhCO** phenyl carbonyl,
PhCsat phenyl attached to saturated carbon atom, **Ph-Nsat** phenyl amine, **Ph-sub** substituted phenyl, **S** contains sulphur

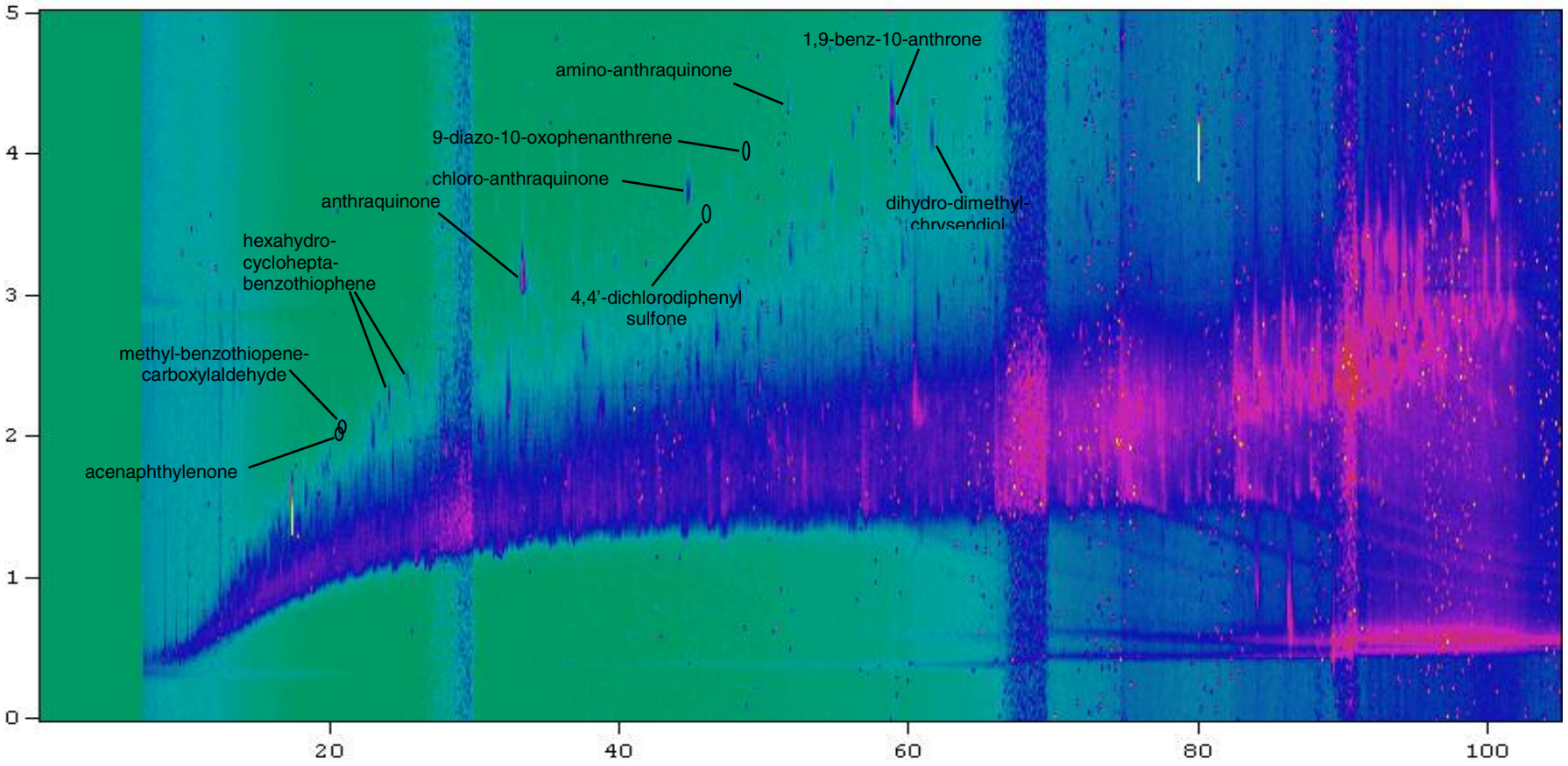
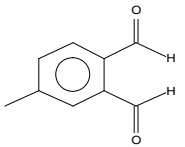
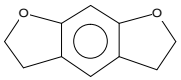
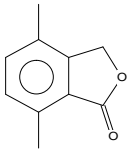
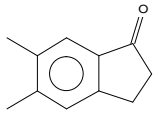
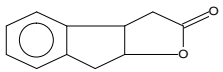
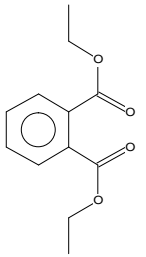
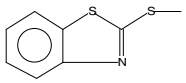
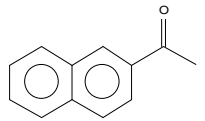
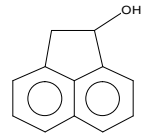
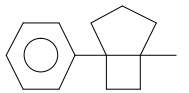
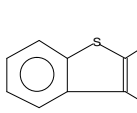
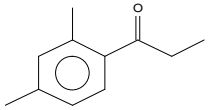
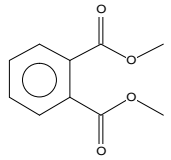
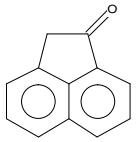
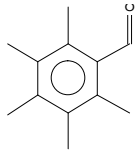
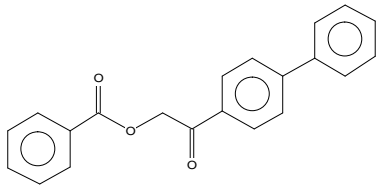
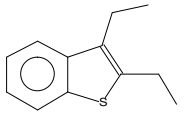
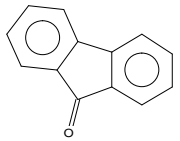
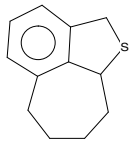
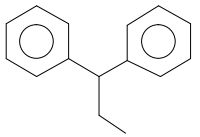
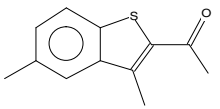


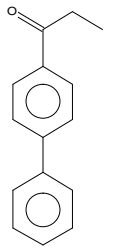
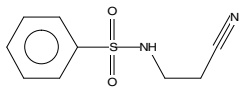
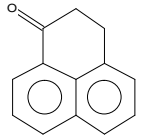
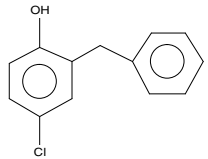
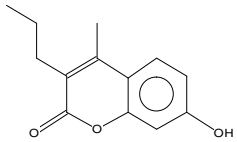
FIGURE B. GCxGC chromatograms of the Elbe extract fraction 3 in the Total Ion Current mode. Example of peaks of compounds separated from the matrix and identified with AMDIS.

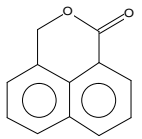
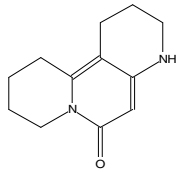
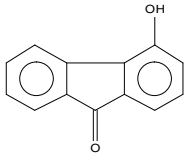
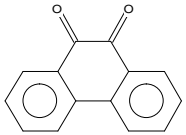
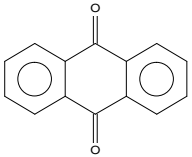
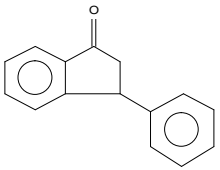
Tabel B. List of compounds identified in fraction 2 of Elbe sediment. The table lists only peaks separated from the matrix. Identification is based on a manual deconvolution and NIST-MS search. Some identities were confirmed by injections of the standards. The structures pesented in the table (with the CAS numbers) are only probable NIST library hits; e.g. a place of alkylation or halogenation on an aryl ring can be different.

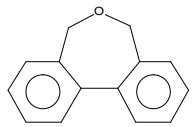
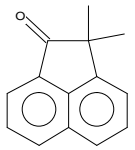
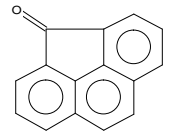
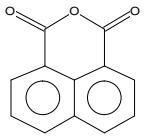
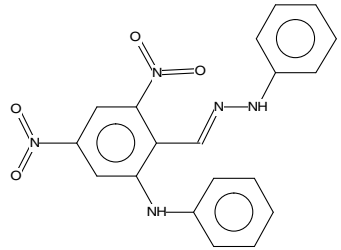
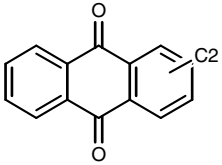
Compound	Substructure Identification[E]	R.T. (min)[A]	% NIST[B]	CAS	MW[C]	Kow[D]	Structure
Phthalaldehyde-1C	O, Ar, >C=O, CH3	15.529	27	15158-36-8	148		
Dihydrofuranno(3,2-f)coumaran	AR, O2, ether, CH2, hetcyc	17.031	17	57052-75-2	162		
1,3-2H-isobenzofuranone-2C	AR, CH2, CH3, O, ArCO, O2, ether	17.617	25	54598-91-3	162		
Indanone-2C	CH3, O, AR	17.866	14	16440-97-4	160		
2H-Indeno[2,1-b]furan-2-one, 3,3a,8,8a-tetrahydro-	AR, Ph-all, CH3, O	18.114	11	80343-98-2	174		
Diethyl phthalate	O, >C=O, AR, C-O, CH2, Ph-all, ether	18.281	51	84-66-2			
Methylthio-benzothiazole	ArS, N-C	18.867	43	615-22-5	181	3.15	

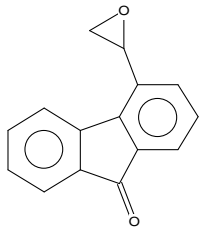
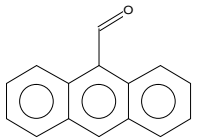
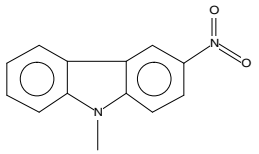
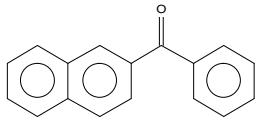
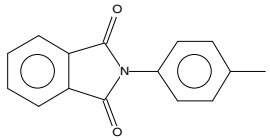
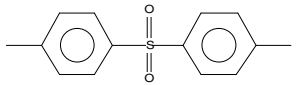
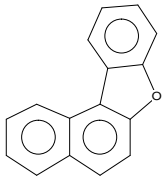
Naphthyl-methyl-ketone	naph, O, -C=O, CH3	19.117	36	93-08-3	170	2.85	
Acenaphthenol	O, AR, Ph-all, OH	19.534	6	6306-07-6	170		
5-Methyl-1-phenylbicyclo[3,2,0]heptane	AR, Ph-all, CH2	19.785	32	N/A	186		
Benzothiophene-carboxaldehyde-1C	S, ArS, hetcyc, CH3, O, -C=O	19.953	54	22053-74-3	176		
Phenyl-propanone-2C	ArCO, -CH2/3-, CH3	19.957	48	35031-55-1	162		
UNKNOWN	AR, O, Cl, ArCl, Ph-all, PhCl, -C=O, N-C	20.036			213		
UNKNOWN	AR, O, >C=O, Cl/Br, N-C, hetcyc	20.120			229		
Dimethyl phthalate	O, AR, ether, -CH2/3-, CH3, ArCOO, -(C=O)-O.	20.294	11	131-11-3	194		
UNKNOWN	AR, N, PAH, ArN, O	20.706			168		
Acenaphthylenone	AR, PAH, CO	20.708	77	2235-15-6	168		
Benzothiophene-carboxaldehyde-1C	S, AR, hetcyc, O, CH3, >C=O	20.873	77		176		e.a.

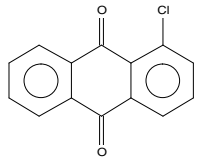
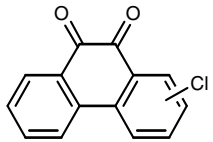
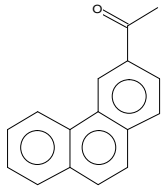
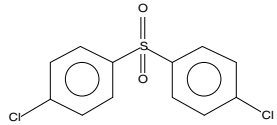
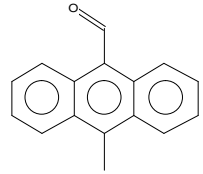
Pentamethylbenzaldehyde	-CH2/3-, CH3, O, AR, >C=O	21.124	3	17432-38-1	176	
Ethanone, 2-(benzoyloxy)-1-[1,1'-biphenyl]-4-yl	PhCO, O, ArCOR, CH2	22.290	10	4347-61-9	316	
Benzothiophene-4C	CH3, AR, CCH3, hetcyc, S	22.706	24	54789-20-7	190	
Fluorenone	STANDARD	23.375	20	486-25-9	180	
UNKNOWN	naph, Ar-CHx, Cl, no N&O	23.706			183	
Cyclohepta[cd][2]benzothiophene, 2,6,7,8,9,9a-hexahydro	AR, O, CH3, hetcyc, C	24.044	13	199807-57-3	190	
1,1'-propylidenebis-benzene	Ph, ph-all, ph-CH, O	24.460	19	1530-03-6	196	
Acetyllbenzothiophene-2C	-CH2/3-, CH3, AR, >C=O, Ar-CHx, CCH3, hetcyc	24.707	28	6179-05-1	204	
UNKNOWN	Cl, AR, S, hetcyc	24.961			189	

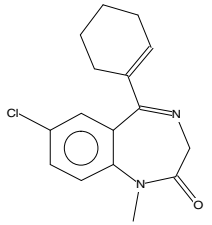
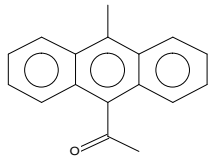
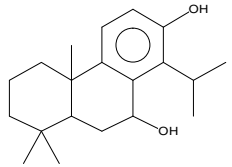
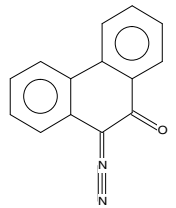
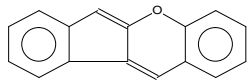
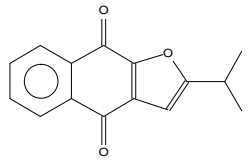
Biphenylethyl-ketone	O, AR, >C=O, PhCO, Ph-2sub	25.131	62	37940-57-1	210		
UNKNOWN	AR, PAH	25.208			176		
N-(2-Cyano-ethyl)-benzenesulfonamide	Ar-S, Ph-all, N, ArSO2, ?NH?	25.219	39	2619-21-8			
Cyclohepta[cd][2]benzothiophene, 2,6,7,8,9,9a-hexahydro-	O, AR, hetcyc, >C=O, CH3	25.378	35		190		e.a.
2,3-Dihydro-1-oxo-1H-phenalene	AR, >C=O, PAH	26.215	51	518-85-4	182		
UNKNOWN	AR, O, CH3	26.377			204		
Acetyllbenzothiophene-2C	AR, O, CH3, Ar-CH3, hetcyc	26.543	11				e.a.
Clorophene	Cl, Ph-all, C-O, Ph-Cl, OH	30.551	84	120-32-1	218	4.18	
UNKNOWN	AR, hetcyc, S, CH3	30.967			206		
Hydroxycoumarin-4C	AR, CH3, hetcyc, O, ether, COO	31.465	55	19491-93-1	218		
UNKNOWN	hetcyc, AR, .N., O, CH2, CH3	31.468			204		

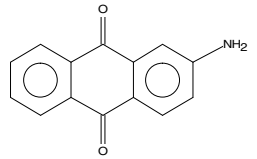
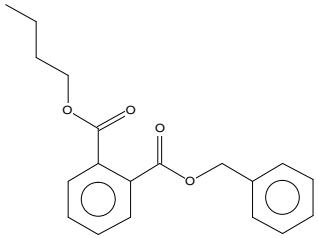
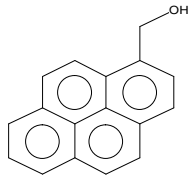
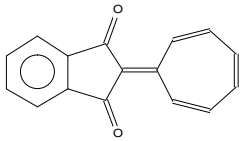
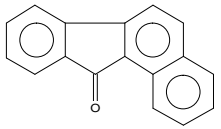
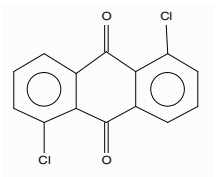
Naphthalide	ArCO, naph, C-O	31.482	72	518-86-5	184	
UNKNOWN	O, AR, >C=O, Ph-all, ARCO, N, Cl	31.732			184	
2,3,4,6,8,9,10,11-Octahydro-6-oxo-1H-pyrido(3,2-a)quinolizine	hetcyc, AR, CH2, .N., O, ether, NH2	31.968	14	26226-34-6	204	
UNKNOWN	N, AR, O, >C=O, ArN	32.307			209	
Hydroxy-fluorenone	AR, O, ArCO, hetcyc, OH	32.641	64	1986-00-1	196	
2,3,4,6,8,9,10,11-Octahydro-6-oxo-1H-pyrido(3,2-a)quinolizine	hetcyc, AR, CH2, O, N, .N., CH3, ArN	32.804	39		204	e.a.
9,10-Phenanthrenedione	AR, ArCO, O2, ArCOAr	32.975	65	84-11-7	208	
Anthraquinone	STANDARD	33.307	61	84-65-1	208	
Phenyl-1-indanone	AR, CH2, .C=O	34.134	10	16618-72-7	208	

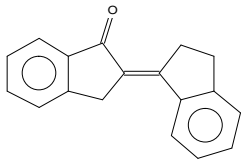
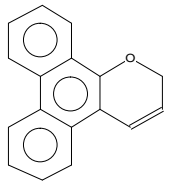
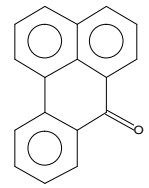
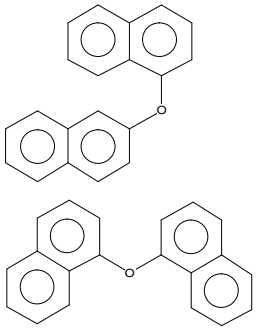
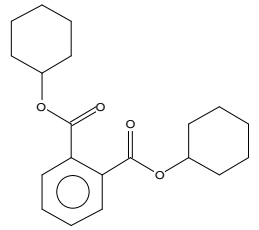
5,7-dihydro-dibenz[c,e]oxepin	AR, Ph-all	34.226	43	1136-22-7	196		
Acenaphthenone-2C	AR, CH2, O	35.561	39	18086-43-6	196		
Cyclopenta(def)phenanthrenone	AR, N, C=O	36.727	88	5737-13-3	204		
1,8-Naphthalic anhydride	O-COC-O, Ar.CO. PAH	36.905	82	81-84-5	198	3.24	
2,4-dinitro-6-phenylamino-phenylhydrazone-benzaldehyde	AR, N-C, Ph-all, O, ArN, N-odd, -CH2/3-, N=C, imino, ONS-self	37.550	24	N/A	377		
Anthraquinone-2C	ArCO, O2, CH3	39.560	41		222		

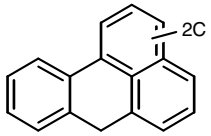
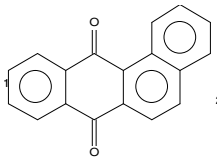
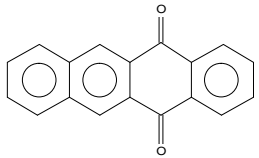
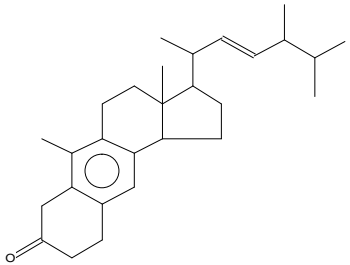
9-Keto-fluorenylethylene oxide	AR, O, .C=O, ArCOAr,	39.643	24	53221-10-6	222		
Anthracenecarboxaldehyde	AR, >C=O, PAH, Anth/Phen	40.313	12	642-31-9	206		
Anthracenecarboxaldehyde	AR, >C=O, PAH, Anth/Phen	40.980			206		e.a.
Methyl-nitro-carbazole	AR, O, ArNO2	41.148	29	61166-05-0	226		
2-Naphthalenylphenyl-methanone	naph, ArCO, ph	42.232	89	644-13-3	232		
2-p-Tolylisoindole-1,3-dione	>C=O, hetcyc, ArCO, N, Ph-all	42.983	12	2142-03-2	237		
p-Talylsulfone	O, Ph-all, S, Ph-2sub, Ar-S, Ar-CHx	44.069	74	599-66-6	246	3.7	
Benzonaphthofuran	C-O, hetcyc, ether, PAH	44.562	17	239-30-5	218		

1-chloroanthraquinone	STANDARD	44.734		82-44-0	242		
Chloro-phenanthrenequinone	ArCl, >C=O, O2	44.985	75		242		
Acetylphenanthrene	Anth/Phen, Ar-COCH3,	45.147	36	2039-76-1	220		
4,4'-Dichlorodiphenyl sulfone	Cl, PhCl, O, hetcyc, S, O2	46.065	33	80-07-9	286	3.9	
Anthraquinone-2C	A, O, >C=O, O2, CH3	46.227	34		236		e.a.
Methylanthracene carboxaldehyde	Anth/Phen, O, >C=O, CH3	46.563	63	7072-00-6	220		
Methylanthracene carboxaldehyde	Anth/Phen, O, >C=O, CH3	47.063	37		220		e.a.
Methylanthracene carboxaldehyde	AR, O, >C=O, CH3	47.48	26		220		e.a.

Tetrazepam	AR, O, CH3, hetcyc, Ar.S, Cl	47.651	72	10379-14-3	288	3.2	
Methylanthracene carboxaldehyde	Anth/Phen, O, >C=O, CH3	48.065	20		220		e.a.
1-(10-Methylanthracen-9-yl)ethanone	AR, CH3, PAH, O	48.396	42	36778-18-4	234		
14-isopropyl-podocarpa-8,11,13-triene-7á,13-diol	CH3+alkyl, cond, CH&O, >C=O, AR, C-O	48.549	22	24338-19-0	302		
9-Diazo-10-phenanthrone	AR, O, N, hetcyc, >C=O, .N., Ndbl	48.822	58	7509-44-6	220		
Indeno[2,1-b]chromene,	AR, cond, O, C-O, PAH, hetcyc, ether	49.237	31	243-24-3	218		
2-isopropyl-naphtho[2,3-b]furan-4,9-dione	AR, CH3, cond, O, hetcyc, PAH, ether,	50.647	11	13019-43-7	240		
Anthraquinone-2C	AR, O2, .C=O, CH3, ArCOAr	51.142	22		236		e.a.

Amino-anthraquinone	N, ArN, .C=O	51.662	73	117-79-3	223	3.31	
Benzyl butyl phthalate	AR, ArCOO, OCH2/O.	51.728	78	85-68-7	312	4.73	
Pyrenemethanol	PAH, cond, C-O, OH	52.152	41	24463-15-8	232		
1-(10-Methylanthracen-9-yl)ethanone	ARC, CH3, O, Ph-all	52.428	41		234		e.a.
2-(2,4,6-Cycloheptatrienylidene)-1,3-indandione	AR, >C=O,	52.903	58	3178-28-7	234		
11H-Benzo[a]fluoren-11-one	PAH, cond, O, ArCOAr	53.402	20	479-79-8	230		
11H-Benzo[a]fluoren-11-one	PAH, cond, .C=O	54.562	41		230		e.a.
11H-Benzo[a]fluoren-11-one	PAH, cond, .C=O	54.818	61		230		e.a.
1,5-Dichloroanthracenequinone	STANDARD		48	82-46-2	276		
Dichloroanthracenequinone	ArCOAr, ArCl	56.158	48		276		e.a.

1H-Inden-1-one, 2-(2,3-dihydro-1H-inden-1-ylidene)-2,3-dihydro	Ph-all, O,	56.900	25	5706-06-9	246		
2H-Phenanthro[9,10-b]pyran	cond, PAH, O	57.243	37	217-67-4	232		
1,9-benz-10-anthrone	STANDARD	58.744		82-05-3	230	4.81	
Naphthylether	PAH, naph, ArOAr	59.325	63	611-49-4 607-52-3	270		
1,2-Benzenedicarboxylic acid, dicyclohexyl ester	ArCOO, Ph-2sub	59.559	64	84-61-7	330	6.2	

7H-benzo[de]anthracene-2C	AR, cond, C-O, ph	60.900	49		244		
UNKNOWN	AR, PAH	61.497			232		
UNKNOWN	AR, ph-all, PAH	61.657			290		
7H-benzo[de]anthracene-2C	AR, cond, O, PAH,	62.574	29		246		e.a.
Benz(a)anthracene-7,12-dione	STANDARD	63.157		2498-66-0	258	4.4.	
Naphthylether	PAH, O, ether, ArOAr	65.409	80		270		e.a.
Naphthylether	O, PAH, naph, Ar-O-Ar	66.579	24		270		e.a.
5, 12-naphthacenequinone	STANDARD	66.91	76	1090-13-7	258		
Anthiaergostan-5,7,9,22-tetraen-3-one	>C<, O, CCH3, >C=O, noAr_cy	91.311	52	64110-74-3	392		
UNKNOWN	O, C-O, CH2, CH3, >C=O, >C<, ether, CO-O/OH	95.820			374		
UNKNOWN	CH2, cond, O, CH3+alkyl, >C<, AR, O	98.149			390		
UNKNOWN	CH2, O, CH3+alkyl, cond, noAR_cy	98.645			404		

[A] Retention time
[B] Probability of the NIST library match
[C] Molecular weight
[D] Octanol-water partition coefficient – values from ChemIDPlus Advanced, United States national Library of Medicine (http://chem.sis.nlm.nih.gov/chemidplus/)
[E] Possible substructures identified by NIST-MS search with probability above 50%; abbreviations are explained below

e.a.- example above
4+brid four bridging atoms in ring cluster, **AR** aromatic rings, **An/Phen** anthracene or phenanthrene, **Ar-Ar** aryl-aryl non ring bond,
ArC aromatic carbon attached to carbon, **Ar-C** aromatic ring-saturated carbon atom bond, **ArCH3** aryl methane group,
Ar-CH2/3 aromatic bond to methyl or methylene group, **Ar-CHx** aromatic-saturated carbon bond, **ArCO** aryl carbonyl, **ArCOO** aryl ester,
ArN aromatic carbon-nitrogen bond, **Ar.NH** aryl carbon attached to NH in ring, **ArNO2** aryl nitro, **Ar-O** aromatic ring-oxygen atom bond,
ArS aryl sulphide, **Ar.S** aromatic-sulphur bond in ring, **ARSO2** aromatic SO2 bond, **>C<** quaternary carbon,
carbcy contains carbon-only rings, **CCH3** methyl bonded to carbon, **CH2/3** primary or secondary saturated carbon, **CH2** methylene group,
CH3 methyl, -**CH2/3-** methylene or methyl group (chain), **-CH2/3-1** exactly one methylene or methyl group (chain),
CH3+alkyl methylene attached to saturated C-atoms (chain), **CH&N** contains only carbon, hydrogen and nitrogen,
CH&O contains only carbon, hydrogen and oxygen, **C=C** carbon-carbon double bond, **CN** cyano, **C-O** carbon-oxygen bond,
>C=O carbonyl group, **.C=O** ring carbonyl, **cond** condensed ring structure (1,2-overlap), **COO** ester group, **-(C=O)-O.** methyl ester,
CO-O/OH carboxyl or ester, **HC** hydrocarbon, **hetcyc** ring containing at least one hetero atom, **HCUNS** unsaturated carbon,
imino double bonded, trivalent nitrogen, **N** contains nitrogen**, .N.** any nitrogen atom in ring, **naph** naphthalene ring,
N-C nitrogen-carbon single bond, **N=C** nitrogen-carbon double bond, **Ndbl** doubly bonded nitrogen atom**,**
?NH? secondary amine (not alkyl, aryl), **noAr** no aromatic rings, **noAr_cy** rings present, but not aromatic, **noN&O** no nitrogen or oxygen,
O contains oxygen, **-O-** oxygen in chain, **O2** contains two oxygen atoms, **OCH3** methoxy,
OCH2/O. ether oxygen attached to methyl or methylene, **O=COC=O** anhydride, **PAH** condensed polynuclear aromatic compound,
ONS-self OO, NN or SS bond, **ph** phenyl group, **Ph-2sub** phenyl with 2 substituents, **Ph-2+sub** phenyl with 2 or more substituents,
Ph-all isolated benzenoid ring**, PhCH2** phenyl with methylene substituent, **PhCO** phenyl carbonyl,
PhCsat phenyl attached to saturated carbon atom, **Ph-Nsat** phenyl amine, **Ph-sub** substituted phenyl, **S** contains sulphur