Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

SUPPORTING INFORMATION

Quantifying the Equilibrium Partitioning of Substituted Polycyclic Aromatic Hydrocarbons in Aerosols and Clouds using COSMOtherm

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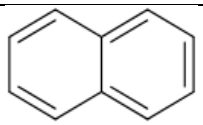
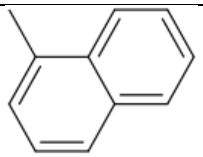
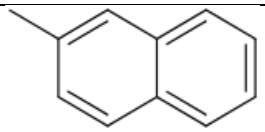
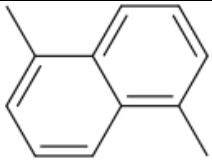
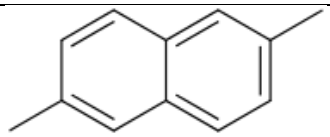
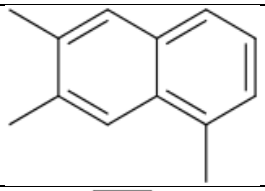
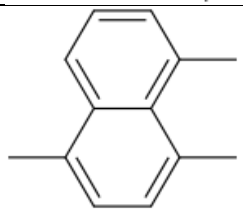
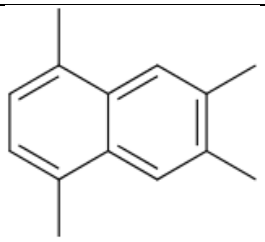
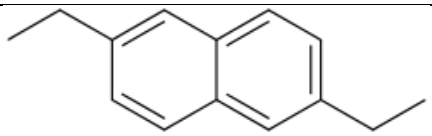
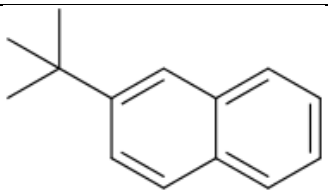
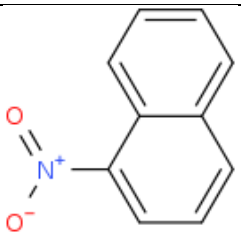
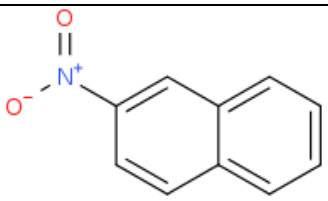
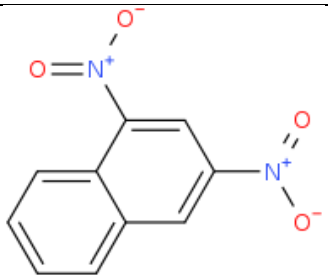
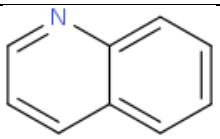
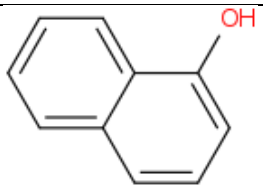
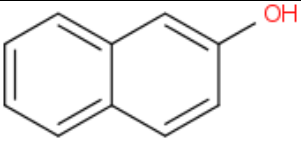
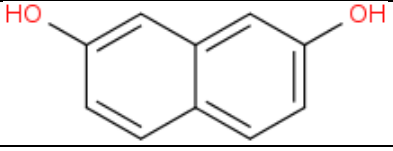
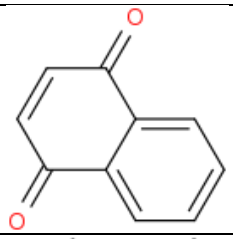
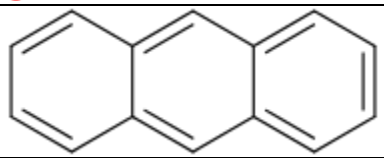
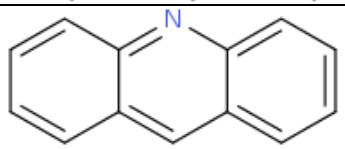
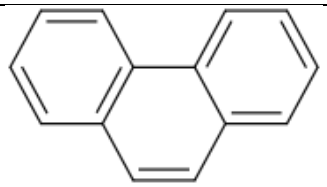
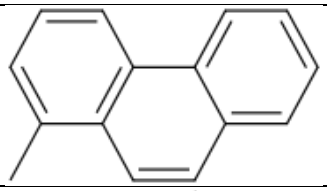
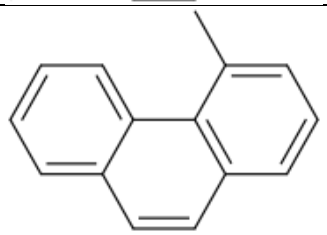
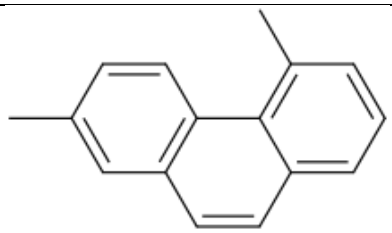
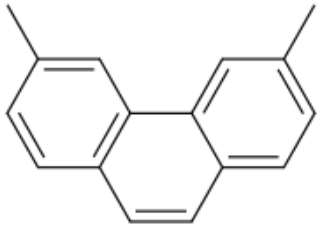
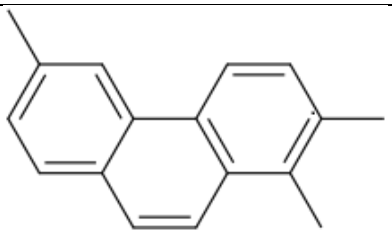
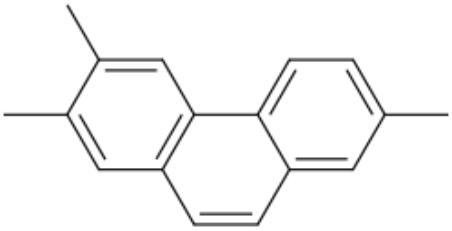
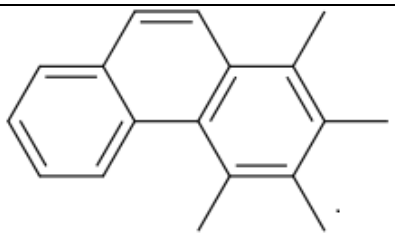
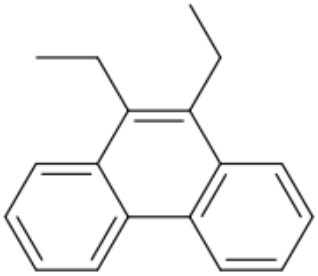
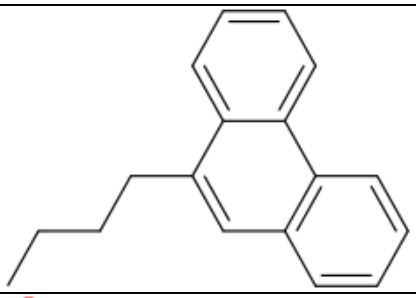
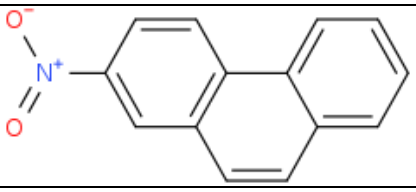
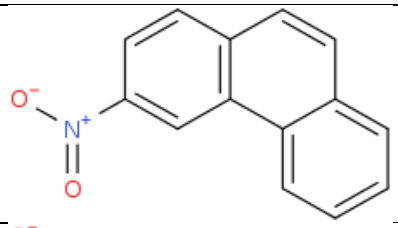
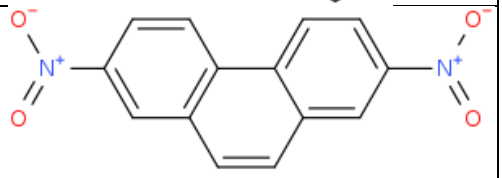
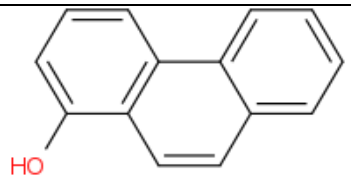
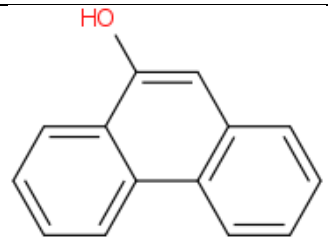
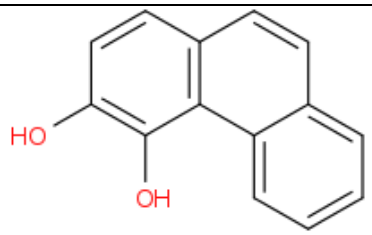
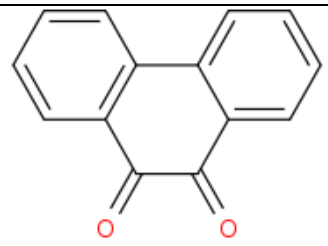
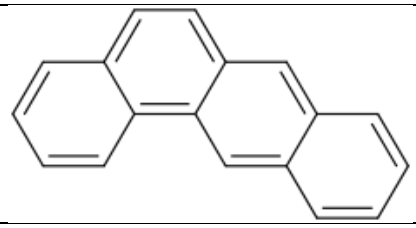
Table S1. Names and structures of PAHs and SPAHs

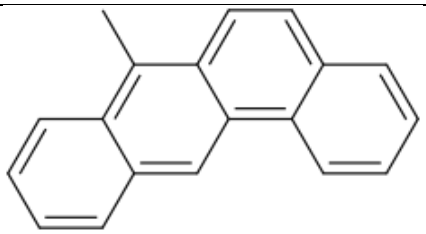
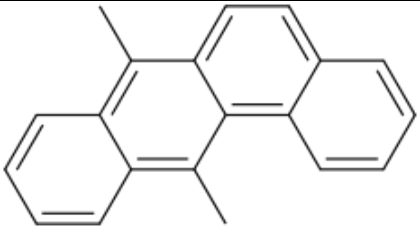
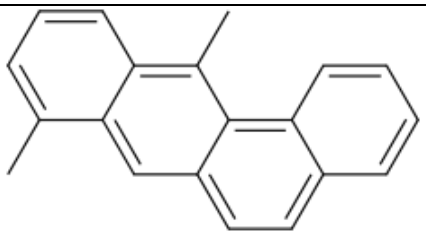
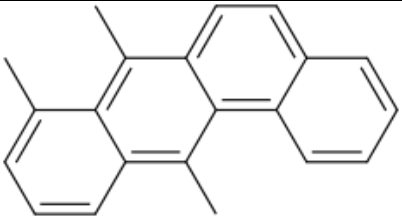
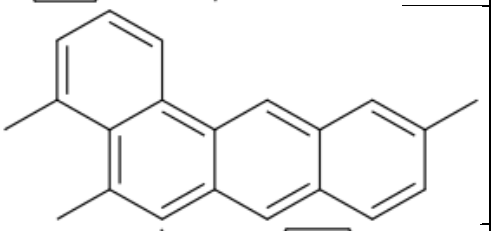
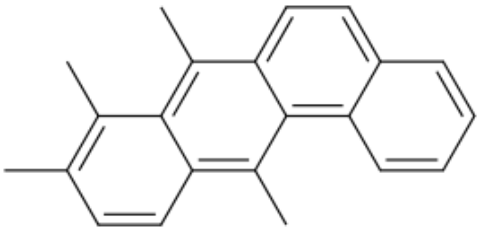
Compound	Type	Substituent	Structure
Naphthalene	PAH		
1-Methylnaphthalene	Alkyl-PAH	Me	
2-Methylnaphthalene	Alkyl-PAH	Me	
1,5-Dimethylnaphthalene	Alkyl-PAH	Di-Me	
2,6-Dimethylnaphthalene	Alkyl-PAH	Di-Me	
2,3,5-Trimethylnaphthalene	Alkyl-PAH	Tri-Me	
1,4,5-Trimethylnaphthalene	Alkyl-PAH	Tri-Me	
1,4,6,7-Tetramethylnaphthalene	Alkyl-PAH	Tetra-Me	

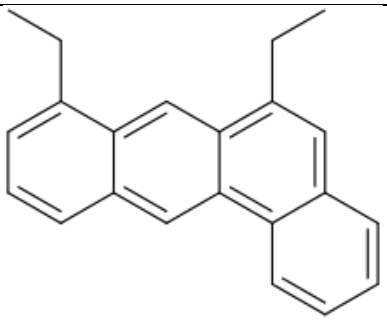
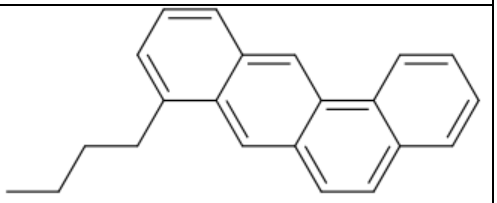
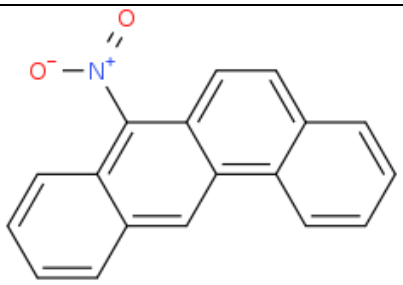
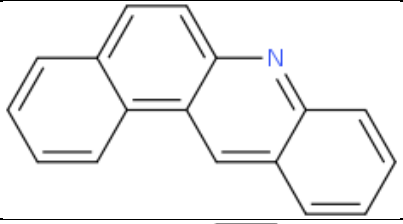
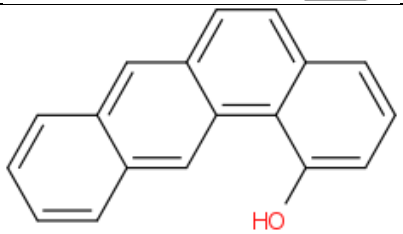
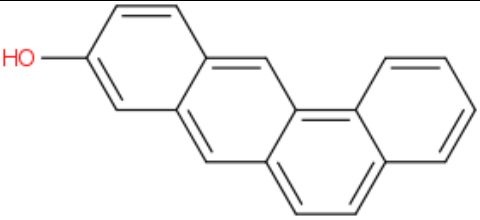
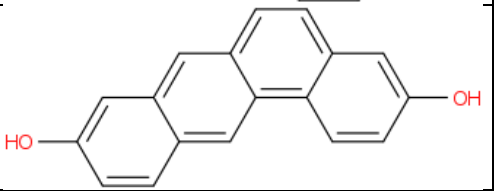
2,6-Diethylnaphthalene	Alkyl-PAH	Di-Et	
2-tert-Butylnaphthalene	Alkyl-PAH	But	
1-Nitronaphthalene	Nitro-PAH	NO_2	
2-Nitronaphthalene	Nitro-PAH	NO_2	
1,3-Dinitronaphthalene	Nitro-PAH	Di-NO_2	
Quinoline	Azaarene	N	
1-Naphthol	Hydroxy-PAH	OH	
2-Naphthol	Hydroxy-PAH	OH	
2,7-Dihydroxynaphthalene	Hydroxy-PAH	Di-OH	

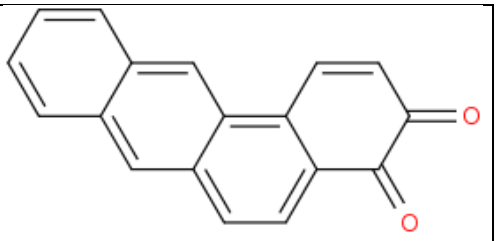
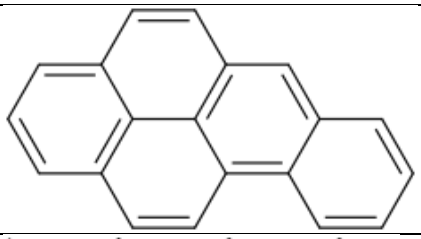
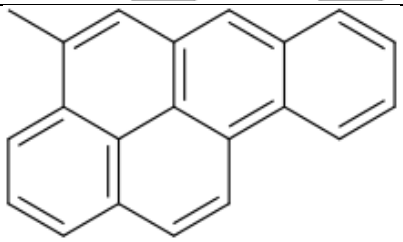
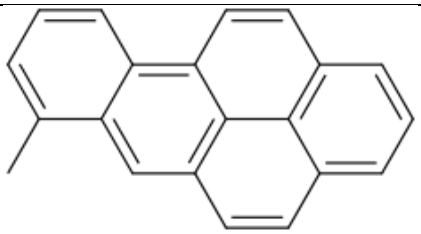
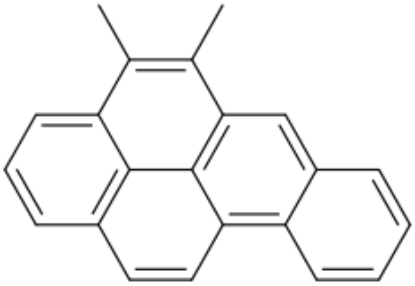
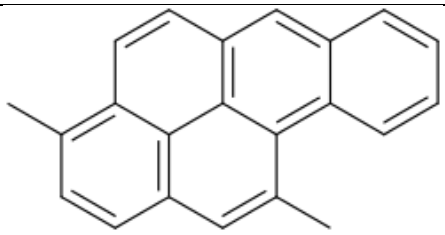
1,4-Naphthoquinone	Dione	Di-O	
Anthracene	PAH		
Acridine	Azaarene	N	
Phenanthrene	PAH		
1-Methylphenanthrene	Alkyl-PAH	Me	
4-Methylphenanthrene	Alkyl-PAH	Me	
2,5-Dimethylphenanthrene	Alkyl-PAH	Di-Me	
3,6-Dimethylphenanthrene	Alkyl-PAH	Di-Me	

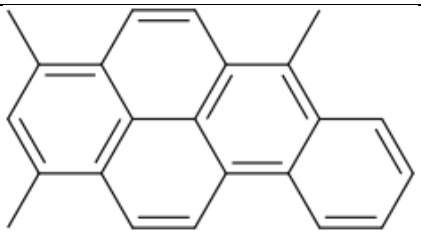
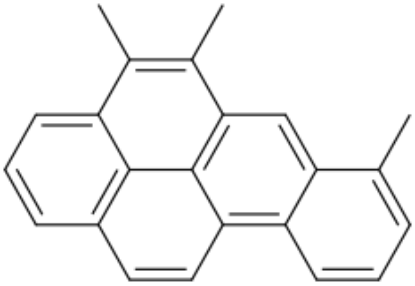
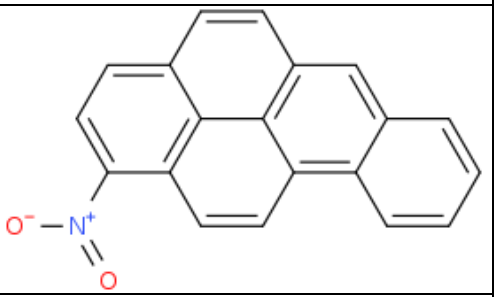
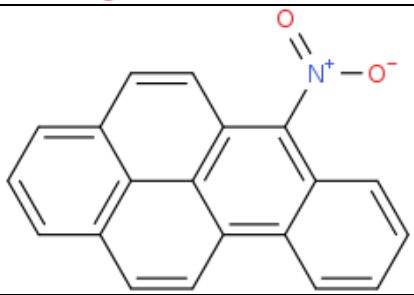
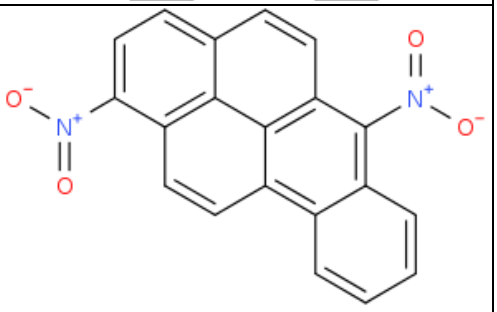
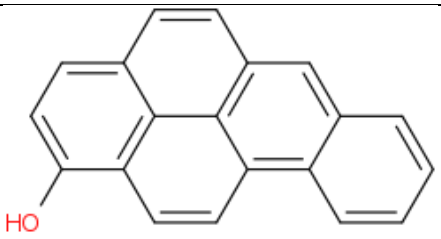
1,2,6-Trimethylphenanthrene	Alkyl-PAH	Tri-Me	
2,3,7-Trimethylphenanthrene	Alkyl-PAH	Tri-Me	
1,2,3,4-Tetramethylphenanthrene	Alkyl-PAH	Tetra-Me	
9,10-Diethylphenanthrene	Alkyl-PAH	Di-Et	
9-Butylphenanthrene	Alkyl-PAH	But	
2-Nitrophenanthrene	Nitro-PAH	NO_2	

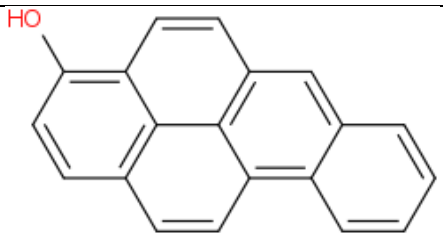
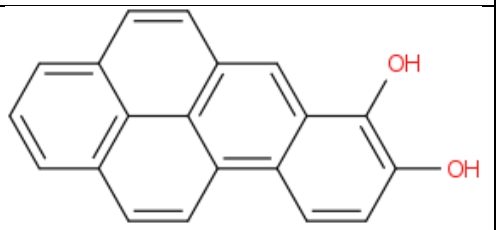
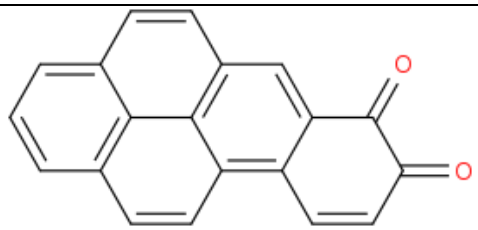
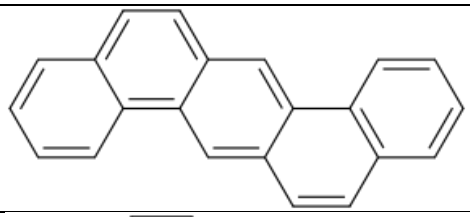
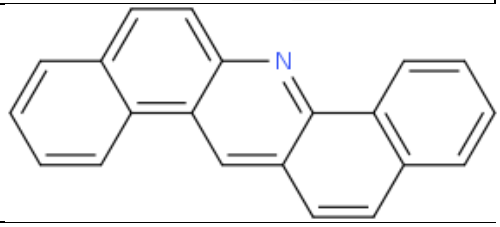
3-Nitrophenanthrene	Nitro-PAH	NO_2	
2,7-Dinitrophenanthrene	Nitro-PAH	Di-NO_2	
1-Hydroxyphenanthrene	Hydroxy-PAH	OH	
9-Hydroxyphenanthrene	Hydroxy-PAH	OH	
3,4-Dihydroxyphenanthrene	Hydroxy-PAH	Di-OH	
9,10-Phenanthrenedione	Dione	Di-O	
Benz(a)anthracene	PAH		

7-Methylbenz[a]anthracene	Alkyl-PAH	Me	
7,12-Dimethylbenz[a]anthracene	Alkyl-PAH	Di-Me	
8,12-Dimethylbenz[a]anthracene	Alkyl-PAH	Di-Me	
7,8,12-Trimethylbenz(a)anthracene	Alkyl-PAH	Tri-Me	
4,5,10-Trimethylbenz(a)anthracene	Alkyl-PAH	Tri-Me	
7,8,9,12-Tetramethylbenz(a)anthracene	Alkyl-PAH	Tetra-Me	

6,8-Diethylbenz[a]anthracene	Alkyl-PAH	Di-Et	
8-n-Butylbenz[a]anthracene	Alkyl-PAH	But	
7-Nitrobenz(a)anthracene	Nitro-PAH	NO_2	
Benz[a]acridine	Azaarene	N	
1-Hydroxybenz[a]anthracene	Hydroxy-PAH	OH	
9-Hydroxy-benz[a]anthracene	Hydroxy-PAH	OH	
3,9-Benz[a]anthracene-diol	Hydroxy-PAH	Di-OH	

Benz[a]anthracene-3,4-dione	Dione	Di-O	
Benzo[a]pyrene	PAH		
4-Methylbenzo[a]pyrene	Alkyl-PAH	Me	
7-Methylbenzo[a]pyrene	Alkyl-PAH	Me	
4,5-Dimethylbenzo[a]pyrene	Alkyl-PAH	Di-Me	
3,11-Dimethylbenzo[a]pyrene	Alkyl-PAH	Di-Me	

1,3,6-Trimethylbenzo[a]pyrene	Alkyl-PAH	Tri-Me	
4,5,7-Trimethylbenzo(a)pyrene	Alkyl-PAH	Tri-Me	
1-Nitrobenzo[a]pyrene	Nitro-PAH	NO_2	
6-Nitrobenzo[a]pyrene	Nitro-PAH	NO_2	
1,6-Dinitrobenzo[a]pyrene	Nitro-PAH	Di-NO_2	
1-Hydroxybenzo[a]pyrene	Hydroxy-PAH	OH	

3-Hydroxybenzo[a]pyrene	Hydroxy-PAH	OH	
Benzo[a]pyrene-7,8-diol	Hydroxy-PAH	Di-OH	
Benzo(a)pyrene-7,8-dione	Dione	Di-O	
Dibenz(a,h)anthracene	PAH		
Dibenz(a,h)acridine	Azaarene	N	

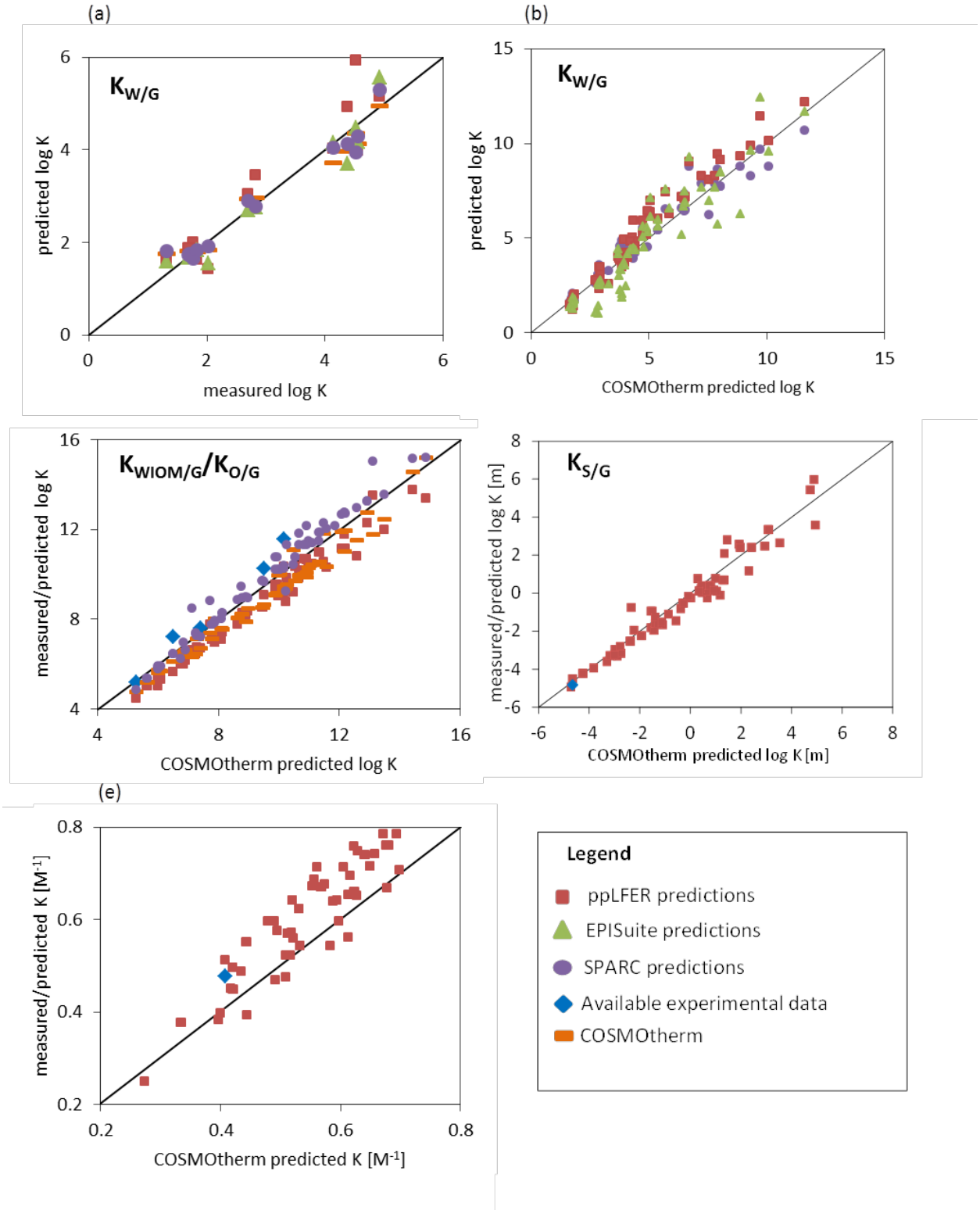


Figure S1 Comparison of COSMOtherm predicted partition coefficients with available experimental data, and with other prediction methods. The lines indicate 1:1 agreement.

Table S2 Mean difference (MD) and mean absolute difference (MAD) between measured data and predicted data.

Measured vs. predicted log $K_{W/G}$	**MD**	**MAD**	**n**
COSMOtherm	0.06	0.22	13
ppLFER	-0.20	0.43	13
SPARC	0.02	0.20	13
EPISuite	0.06	0.21	13
Measured log $K_{O/G}$ vs. predicted log $K_{WIOM/G}$			
COSMOtherm	-0.49	0.52	6
ppLFER	-1.02	1.02	6
Measured vs. predicted log $K_{O/G}$			
COSMOtherm	-1.07	1.07	6
Measured vs. predicted log $K_{S/G}$ for naphthalene			
COSMOtherm	-0.18	0.18	1
ppLFER	-0.37	0.37	1
Measured vs. predicted K_S for naphthalene			
COSMOtherm	0.07	0.07	1
ppLFER	-0.03	0.03	1

Table S3 Mean difference (MD) and mean absolute difference (MAD) between COSMOtherm predicted data and other prediction methods.

COSMOtherm vs ppLFER	**MD**	**MAD**	**n**
log $K_{W/G}$	-0.37	0.52	68
log $K_{WIOM/G}$	0.69	0.71	68
log $K_{S/G}$	0.18	0.46	68
K_S	-0.06	0.07	68
COSMOtherm vs SPARC			
log $K_{W/G}$	-0.15	0.39	68
log $K_{WIOM/G}$	-0.28	0.40	68
COSMOtherm vs EPISuite			
log $K_{W/G}$	0.14	0.64	68

Table S4. Environmental conditions for measured gas-partitioning data

Reference	Environmental Conditions
Wei et al.[1]	Urban/Industrial area in Xi'an, central China Samples collected in September. Average temperature: 19.5 °C Organic Carbon in TSP ~32.34μg/m^3
Li et al.[2]	Urban and Rural areas in Northern China Reported median concentrations of samples collected over 12 months. Average temperature: 11.23 °C Organic Carbon in TSP ~35 μg/m^3
Tomaz et al.[3]	Urban site in Grenoble, France Reported mean concentrations of samples collected over 12 months Average temperature: 13.64 °C Organic Carbon in TSP ~20 μg/m^3

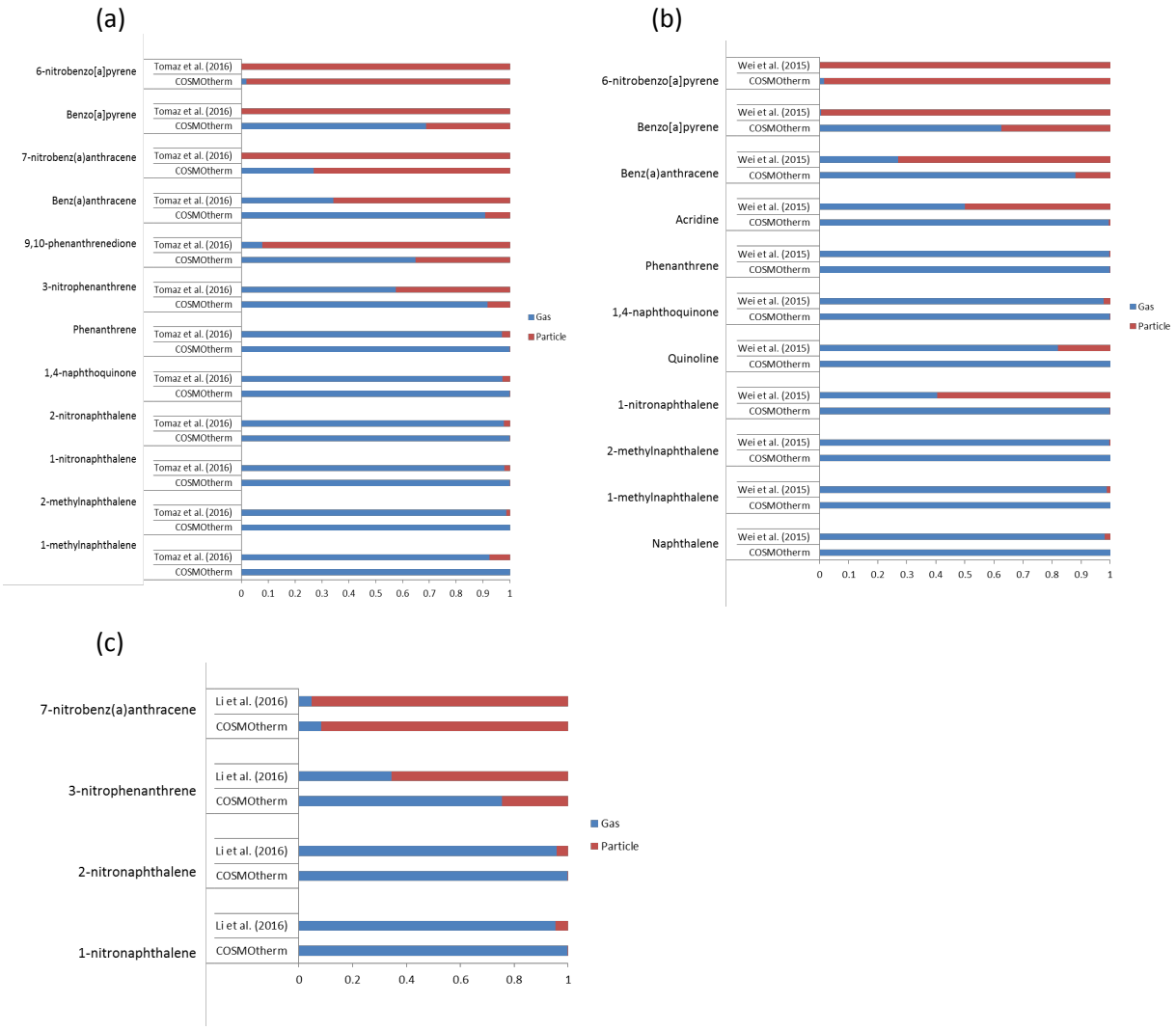


Figure S2 Comparison of measured gas-particle partitioning data with COSMOtherm predicted data at the following temperatures: (a) 13.64°C, (b) 19.5°C and (c) 11.23°C; which correspond to the average temperatures at which $K_{P/G}$ (partitioning coefficient between particle and gas phase) was measured for these compounds.

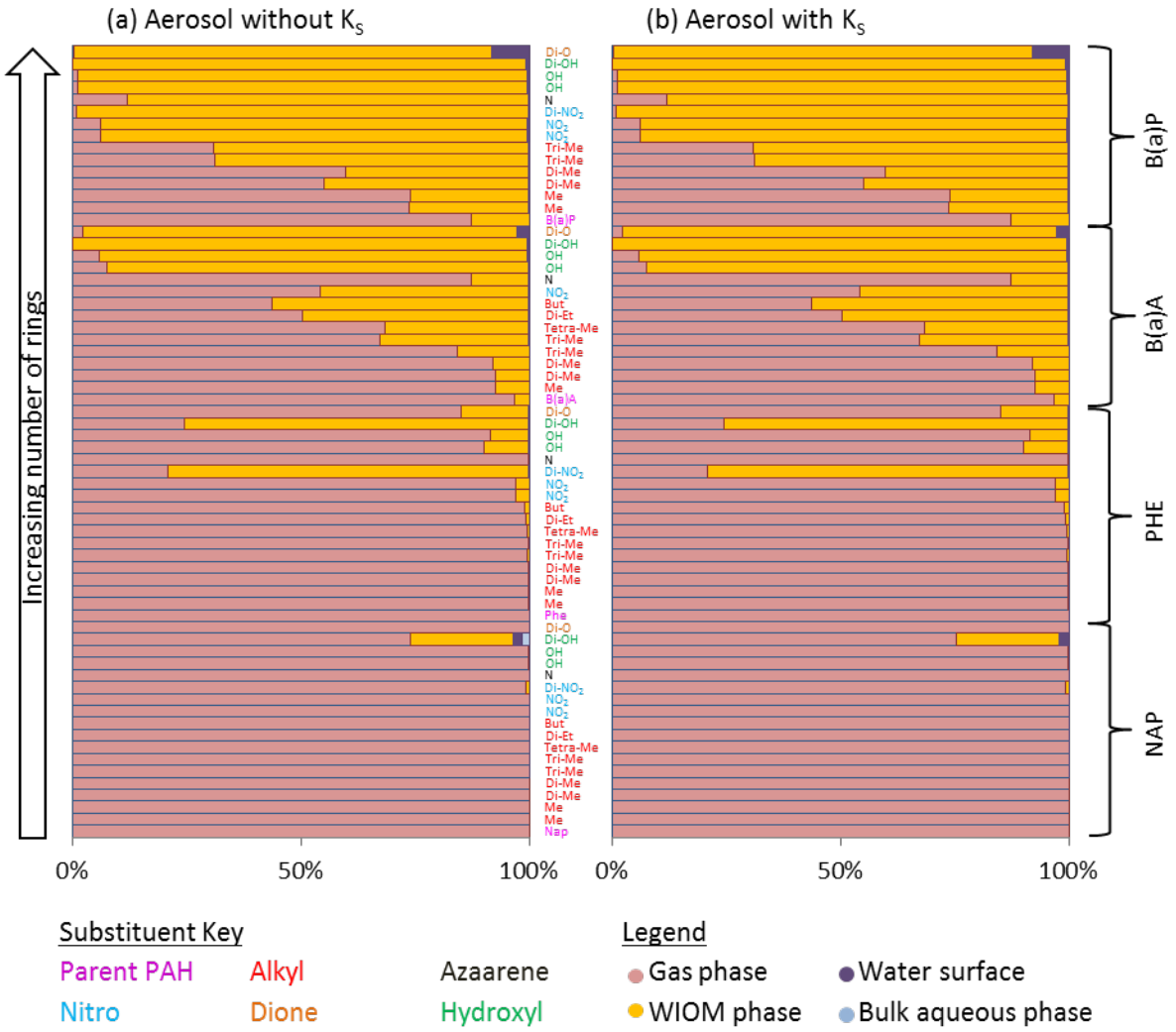


Figure S3 Aerosol phase partitioning (a) without and (b) with the consideration of the salting out effect. The slight partitioning of 2,7-dihydroxynaphthalene to the bulk aqueous phase is seen in (a) but not in (b), due to the salting out effect.

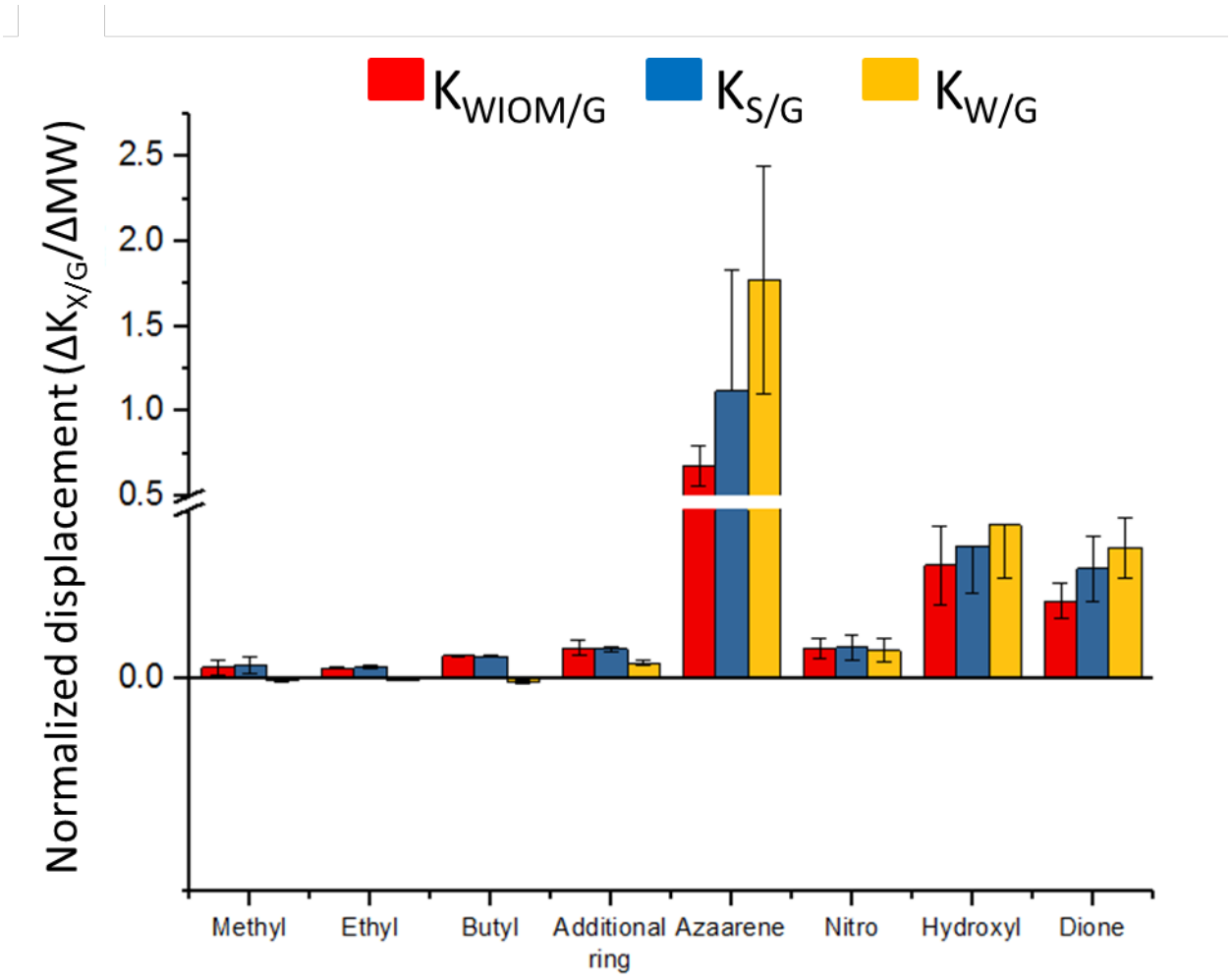


Figure S4 Average change in the COSMOtherm-predicted values of $K_{WIOM/G}$, $K_{S/G}$ and $K_{W/G}$ upon addition of different functional groups to polycyclic aromatic hydrocarbons after normalization by change in molecular weight.

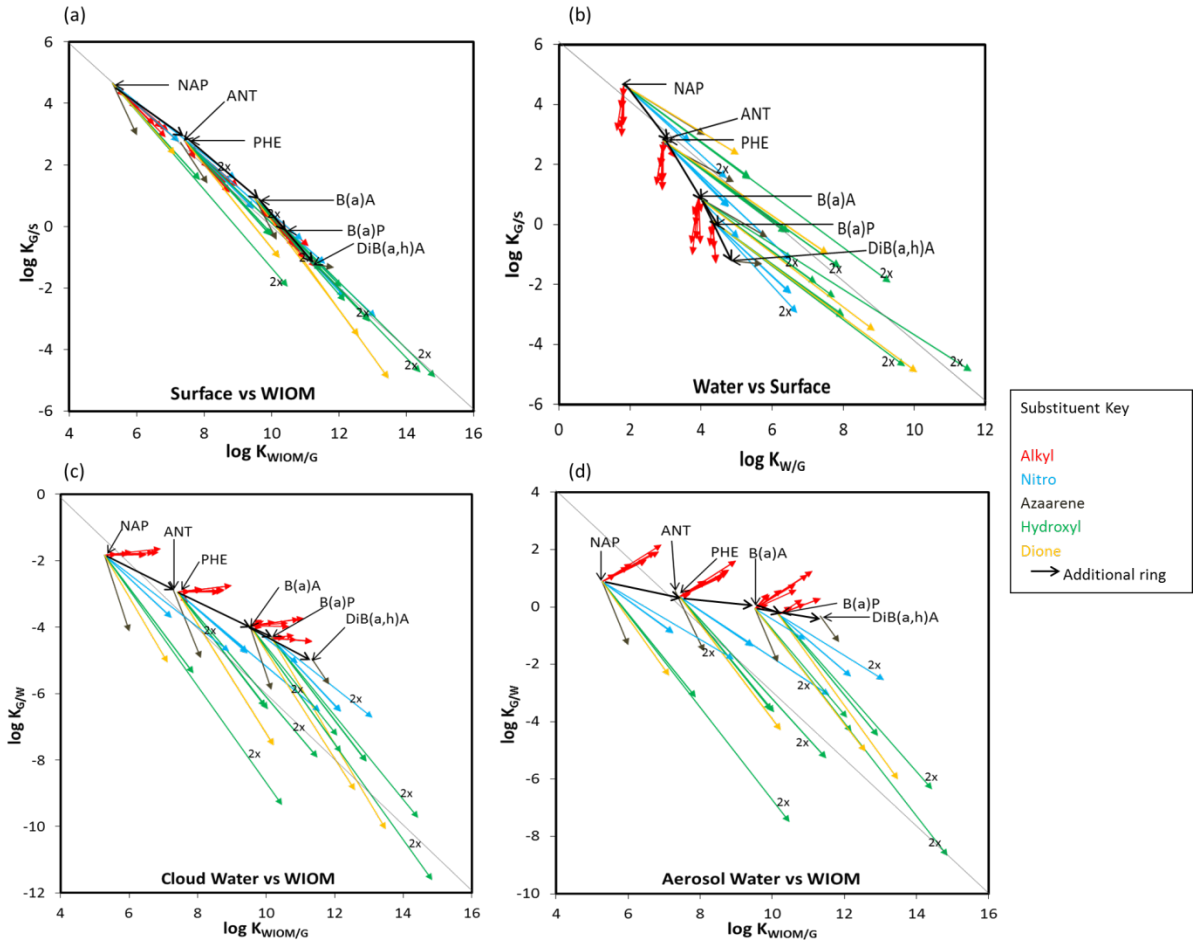
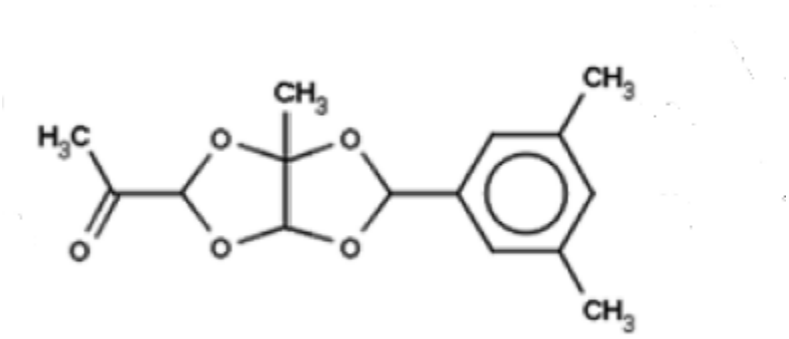


Figure S5 Effects of molecular attributes on the affinity of a compound for different atmospheric phases. The starting point of the arrows indicates the position of the parent PAH while the arrows show the displacement resulting from the addition of a particular substituent. Arrows labelled with 2x indicate diols (green) and di-nitro (blue) substituents.

Table S5: Calculation of total surface area and ratios for clouds and aerosols.

	Cloud 1	Cloud 2	Aerosol 1	Aerosol 2
LWC / m^3 of air (m^3)	3.00E-07		1.00E-11	
Radius of droplet (m)	1.00E-03	1.00E-04	1.00E-06	1.00E-07
Volume of one spherical droplet(m^3)	4.19E-09	4.19E-12	4.19E-18	4.19E-21
Number of droplets	72	71620	2387324	2387324146
Surface area of one droplet (m^2)	1.26E-05	1.26E-07	1.26E-11	1.26E-13
Total surface area (m^2/m^3)	9.00E-04	9.00E-03	3.00E-05	3.00E-04
V_{WIOM} (m^3)	1.00E-11	1.00E-11	1.00E-11	1.00E-11
V_G (m^3)	1	1	1	1
Water surface area-to-water volume ratio	3.00E+03	3.00E+04	3.00E+06	3.00E+07
Water surface area-to-WIOM volume ratio	9.00E+07	9.00E+08	3.00E+06	3.00E+07



WIOM B

Figure S6 Structure of WIOMB which is used as a surrogate for the organic phase. Proposed by Kalberer et al.[4]

Table S6: Partitioning and salting-out coefficients at 25 °C predicted by different techniques.

	COSMOtherm				ppLFER				SPARC		EPISuite
Compound	K_S	log $K_{W/G}$	log $K_{WIOM/G}$	log $K_{S/G}$	K_S	log $K_{W/G}$	log $K_{WIOM/G}$	log $K_{S/G}$	log $K_{W/G}$	log $K_{WIOM/G}$	log $K_{W/G}$
Naphthalene	0.408	1.829	5.281	-4.648	0.511	1.998	4.472	-4.461	1.653	4.830	1.745
1-Methylnaphthalene	0.443	1.801	5.639	-4.242	0.551	1.882	5.008	-4.235	1.749	5.370	1.677
2-Methylnaphthalene	0.444	1.797	5.651	-4.231	0.551	1.882	5.008	-4.235	1.741	5.366	1.674
1,5-Dimethylnaphthalene	0.479	1.772	6.010	-3.832	0.597	1.631	5.325	-3.950	1.837	5.914	1.844
2,6-Dimethylnaphthalene	0.490	1.725	6.106	-3.832	0.597	1.631	5.325	-3.950	1.821	5.906	1.582
2,3,5-Trimethyl naphthalene	0.520	1.809	6.509	-3.304	0.641	1.430	5.647	-3.614	1.964	6.465	1.539
1,4,5-Trimethyl naphthalene	0.521	1.808	6.519	-3.305	0.641	1.430	5.647	-3.614	1.909	6.459	1.539
1,4,6,7-Tetramethylnaphthalene	0.556	1.753	6.861	-2.891	0.686	1.200	5.978	-3.330	2.062	6.975	1.496
2,6-Diethylnaphthalene	0.574	1.627	6.930	-3.104	0.676	1.456	6.153	-3.315	1.594	6.619	1.335
2-tert-Butylnaphthalene	0.553	1.752	6.754	-3.198	0.672	1.473	5.980	-3.300	1.346	6.248	1.255
1-Nitronaphthalene	0.420	3.701	7.254	-2.746	0.496	4.033	6.436	-3.174	4.056	7.366	4.143
2-Nitronaphthalene	0.420	3.691	7.257	-2.748	0.496	4.033	6.436	-3.174	4.081	7.361	4.438
1,3-Dinitronaphthalene	0.436	4.723	8.934	-1.539	0.487	5.934	8.183	-1.829	5.540	8.990	5.595
Quinoline	0.418	4.108	6.003	-2.958	0.451	3.986	4.997	-2.979	4.287	5.762	4.166
1-Naphthol	0.335	5.383	7.875	-1.531	0.377	6.025	6.946	-0.956	5.438	7.868	5.610
2-Naphthol	0.335	5.382	7.876	-1.502	0.377	6.025	6.946	-0.956	5.429	7.924	5.951
2,7-Dihydroxynaphthalene	0.275	9.334	10.480	1.944	0.249	9.869	9.199	2.558	8.250	10.431	9.633
1,4-Naphthoquinone	0.401	5.063	7.139	-2.325	0.398	6.981	6.631	-0.772	6.408	8.487	7.094
Anthracene	0.518	2.887	7.305	-2.727	0.572	3.467	6.735	-2.648	2.870	7.270	2.678
Acridine	0.510	4.923	8.102	-1.394	0.523	5.145	7.096	-1.279	5.295	8.032	5.561
Phenanthrene	0.496	2.937	7.421	-2.793	0.575	3.453	6.704	-2.553	2.768	7.206	2.762
1-Methylphenanthrene	0.531	2.920	7.787	-2.366	0.624	3.040	7.106	-2.534	2.893	7.752	2.696
4-Methylphenanthrene	0.531	2.918	7.783	-2.366	0.624	3.040	7.106	-2.534	2.893	7.752	2.696
2,5-Dimethylphenanthrene	0.568	2.848	8.137	-1.909	0.669	2.790	7.424	-2.249	3.063	8.293	2.593
3,6-Dimethylphenanthrene	0.568	2.859	8.150	-1.904	0.669	2.790	7.424	-2.249	3.055	8.289	1.398
1,2,6-Trimethylphenanthrene	0.605	2.933	8.631	-1.429	0.714	2.560	7.754	-1.965	3.298	8.870	2.550
2,3,7-Trimethylphenanthrene	0.562	3.276	7.722	-2.203	0.714	2.560	7.754	-1.965	3.260	8.825	2.550
1,2,3,4-Tetramethylphenanthrene	0.622	2.913	8.749	-1.106	0.759	2.309	8.072	-1.681	3.547	9.450	2.507
9,10-Diethylphenanthrene	0.629	2.867	8.782	-1.408	0.748	2.615	8.252	-1.614	2.921	8.963	0.999
9-Butylphenanthrene	0.657	2.738	8.990	-1.297	0.742	2.763	8.352	-1.607	2.604	8.949	1.070
2-Nitrophenanthrene	0.513	4.762	9.465	-0.579	0.568	5.192	8.535	-1.474	5.113	9.713	5.081
3-Nitrophenanthrene	0.513	4.784	9.467	-0.586	0.568	5.192	8.535	-1.474	5.137	9.707	4.536
2,7-Dinitrophenanthrene	0.522	6.531	11.580	1.208	0.559	7.093	10.282	-0.128	7.326	12.016	7.486
1-Hydroxyphenanthrene	0.422	6.478	10.042	0.274	0.449	7.184	9.045	0.745	6.546	10.223	6.661
9-Hydroxyphenanthrene	0.421	6.390	9.969	0.275	0.449	7.184	9.045	0.745	6.548	10.224	5.174
3,4-Dihydroxyphenanthrene	0.397	7.916	11.489	1.437	0.383	9.444	10.538	2.789	8.644	12.292	5.710
9,10-Phenanthrenedione	0.493	7.570	10.231	1.020	0.470	8.063	8.761	0.764	6.203	9.258	6.957

	COSMOtherm				ppLFER				SPARC		EPISuite
Compound	K_S	log $K_{W/G}$	log $K_{WIOM/G}$	log $K_{S/G}$	K_S	log $K_{W/G}$	log $K_{WIOM/G}$	log $K_{S/G}$	log $K_{W/G}$	log $K_{WIOM/G}$	log $K_{W/G}$
benz(a)anthracene	0.588	3.944	9.528	-0.883	0.640	4.934	9.086	-0.686	4.133	9.661	3.688
7-Methylbenz(a)anthracene	0.617	4.018	9.901	-0.392	0.695	4.219	9.217	-0.835	4.342	10.212	2.451
7,12-Dimethylbenz(a)anthracene	0.641	3.775	9.896	-0.317	0.740	3.969	9.535	-0.549	4.541	10.764	2.255
8,12-Dimethylbenz(a)anthracene	0.641	3.813	9.939	-0.261	0.740	3.969	9.535	-0.549	4.532	10.759	3.320
7,8,12-Trimethylbenz(a)anthracene	0.671	3.842	10.267	0.044	0.786	3.718	9.853	-0.265	4.702	11.311	2.060
4,5,10-Trimethylbenz(a)anthracene	0.693	3.985	10.684	0.653	0.786	3.718	9.853	-0.265	4.676	11.298	3.560
7,8,9,12-Tetramethylbenz(a)anthracene	0.706	3.867	10.662	0.494	0.831	3.468	10.171	0.020	4.889	11.834	1.866
6,8-Diethylbenz(a)anthracene	0.737	3.758	10.994	1.045	0.819	3.794	10.363	0.086	4.313	11.466	3.355
8-n-Butylbenz(a)anthracene	0.752	3.725	11.109	0.647	0.814	3.922	10.451	0.093	4.056	11.413	2.994
7-Nitrobenz(a)anthracene	0.594	5.073	10.926	0.449	0.640	6.351	10.634	0.227	6.370	12.150	6.092
Benz(a)acridine	0.597	5.875	10.158	0.438	0.596	6.254	9.191	0.371	6.370	10.393	6.572
1-Hydroxybenz(a)anthracene	0.515	7.255	12.081	1.977	0.522	8.293	11.140	2.395	7.882	12.664	7.671
9-Hydroxybenz(a)anthracene	0.516	7.778	12.190	2.432	0.522	8.293	11.140	2.395	7.881	12.724	7.671
3,9-Benz(a)anthracene diol	0.445	11.623	14.870	4.912	0.393	12.186	13.396	5.959	10.658	15.226	11.654
Benz(a)anthracene-3,4-dione	0.583	8.899	12.595	3.566	0.542	9.299	10.829	2.630	8.757	12.964	6.245
Benzo[a]pyrene	0.612	4.324	10.165	-0.094	0.653	5.937	10.360	0.265	3.934	10.244	4.480
4-Methylbenzo[a]pyrene	0.649	4.300	10.551	0.369	0.715	5.028	10.351	0.102	4.056	10.787	4.437
7-Methylbenzo[a]pyrene	0.649	4.281	10.543	0.381	0.715	5.028	10.351	0.102	4.056	10.787	4.437
4,5-Dimethylbenzo[a]pyrene	0.676	4.365	10.910	0.832	0.760	4.797	10.682	0.386	4.219	11.329	4.394
3,11-Dimethylbenzo[a]pyrene	0.680	4.237	10.827	0.736	0.760	4.797	10.682	0.386	4.160	11.334	4.394
1,3,6-Trimethylbenzo[a]pyrene	0.713	4.418	11.341	1.335	0.806	4.546	10.999	0.670	4.216	11.853	4.351
4,5,7-Trimethylbenzo[a]pyrene	0.713	4.416	11.348	1.310	0.806	4.546	10.999	0.670	4.290	11.876	4.351
1-Nitrobenzo[a]pyrene	0.623	6.517	12.183	2.304	0.660	7.179	11.780	1.162	6.419	12.739	6.883
6-Nitrobenzo[a]pyrene	0.624	6.542	12.175	2.304	0.660	7.179	11.780	1.162	6.491	12.741	6.883
1,6-Dinitrobenzo[a]pyrene	0.627	6.708	13.099	2.955	0.652	9.031	13.523	2.457	8.789	15.039	9.288
1-Hydroxybenzo[a]pyrene	0.532	8.027	12.927	3.046	0.542	9.122	12.286	3.330	7.731	13.244	8.463
3-Hydroxybenzo[a]pyrene	0.532	8.026	12.928	3.104	0.542	9.122	12.286	3.330	7.729	13.244	8.463
Benzo[a]pyrene-7,8-diol	0.510	9.741	14.431	4.753	0.474	11.432	13.783	5.425	9.662	15.178	12.445
Benzo[a]pyrene-7,8-dione	0.614	10.082	13.485	4.954	0.562	10.127	11.974	3.565	8.796	13.556	9.579
Dibenz(a,h)anthracene	0.699	4.942	11.340	1.246	0.707	6.434	11.368	1.347	4.510	11.470	5.298
Dibenz(a,h)acridine	0.678	5.713	11.861	1.334	0.667	7.433	11.302	2.071	6.507	12.178	7.582

Table S7: SMILES code and solute descriptors predicted by ABSOLV (*Solute descriptors obtained from UFZ-LSER database[5]).

Compound	Smiles	Σa_2^H	Σb_2^H	logL[16]	π_2^H	R_2	Vi
Naphthalene*	C1=CC=CC2=CC=CC=C12	0.000	0.200	5.161	0.920	1.340	1.085
1-Methylnaphthalene	CC1=CC=CC2=CC=CC=C12	0.000	0.170	5.804	0.960	1.300	1.226
2-Methylnaphthalene	CC1=CC2=CC=CC=C2C=C1	0.000	0.170	5.804	0.960	1.300	1.226
1,5-Dimethylnaphthalene	CC1=CC=CC2=C(C=CC=C12)C	0.000	0.170	6.275	0.900	1.320	1.367
2,6-Dimethylnaphthalene	CC1=CC2=CC=C(C=C2C=C1)C	0.000	0.170	6.275	0.900	1.320	1.367
2,3,5-Trimethyl naphthalene	CC1=CC2=CC=CC(=C2C=C1C)C	0.000	0.180	6.747	0.840	1.350	1.508
1,4,5-Trimethyl naphthalene	CC1=CC=C(C2=C(C=CC=C12)C)C	0.000	0.180	6.747	0.840	1.350	1.508
1,4,6,7-Tetramethylnaphthalene	CC1=CC=C(C2=CC(=C(C=C12)C)C)C	0.000	0.180	7.219	0.790	1.370	1.649
2,6-Diethylnaphthalene	C(C)C1=CC2=CC=C(C=C2C=C1)CC	0.000	0.180	7.264	0.910	1.320	1.649
2-tert-Butylnaphthalene	C(C)(C)(C)C1=CC2=CC=CC=C2C=C1	0.000	0.220	6.953	0.900	1.280	1.649
1-Nitronaphthalene	[N+](=O)([O-])C1=CC=CC2=CC=CC=C12	0.000	0.270	6.813	1.590	1.540	1.260
2-Nitronaphthalene	[N+](=O)([O-])C1=CC2=CC=CC=C2C=C1	0.000	0.270	6.813	1.590	1.540	1.260
1,3-Dinitronaphthalene	[N+](=O)([O-])C1=CC(=CC2=CC=CC=C12)[N+](=O)[O-]	0.000	0.370	8.294	2.160	1.810	1.434
Quinoline	N1=CC=CC2=CC=CC=C12	0.000	0.460	5.445	1.150	1.320	1.044
1-Naphthol	C1(=CC=CC2=CC=CC=C12)O	0.500	0.450	6.150	1.230	1.500	1.144
2-Naphthol	C1=C(C=CC2=CC=CC=C12)O	0.500	0.450	6.150	1.230	1.500	1.144
2,7-Dihydroxynaphthalene	OC1=CC2=CC(=CC=C2C=C1)O	1.000	0.720	6.969	1.440	1.730	1.203
1,4-Naphthoquinone	C1(C=CC(C2=CC=CC=C12)=O)=O	0.000	0.770	6.582	1.760	1.390	1.160
Anthracene*	C1=CC=C2C=C3C=CC=CC3=CC2=C1	0.000	0.280	7.568	1.340	2.290	1.454
Acridine	C1=CC=CC2=NC3=CC=CC=C3C=C12	0.000	0.520	7.819	1.470	2.040	1.413
Phenanthrene*	C1=CC=CC=2C3=CC=CC=C3C=CC12	0.000	0.290	7.632	1.290	2.060	1.454
1-Methylphenanthrene	CC1=CC=CC=2C3=CC=CC=C3C=CC12	0.000	0.230	8.177	1.280	2.020	1.595
4-Methylphenanthrene	CC1=CC=CC=2C=CC3=CC=CC=C3C12	0.000	0.230	8.177	1.280	2.020	1.595
2,5-Dimethylphenanthrene	CC1=CC=2C=CC3=CC=CC(=C3C2C=C1)C	0.000	0.230	8.649	1.220	2.040	1.736
3,6-Dimethyl phenanthrene	CC=1C=CC=2C=CC3=CC=C(C=C3C2C1)C	0.000	0.230	8.649	1.220	2.040	1.736
1,2,6-Trimethylphenanthrene	CC1=C(C=CC=2C3=CC(=CC=C3C=CC12)C)C	0.000	0.230	9.121	1.170	2.070	1.877
2,3,7-Trimethylphenanthrene	CC1=CC=2C=CC3=CC(=CC=C3C2C=C1C)C	0.000	0.230	9.121	1.170	2.070	1.877
1,2,3,4-Tetramethylphenanthrene	CC1=C(C(=C(C=2C3=CC=CC=C3C=CC12)C)C)C	0.000	0.230	9.592	1.110	2.090	2.018
9,10-Diethylphenanthrene	C(C)C=1C2=CC=CC=C2C=2C=CC=CC2C1CC	0.000	0.240	9.638	1.230	2.040	2.018
9-Butylphenanthrene	C(CCC)C=1C2=CC=CC=C2C=2C=CC=CC2C1	0.000	0.240	9.661	1.300	2.010	2.018
2-Nitrophenanthrene	[N+](=O)([O-])C1=CC=2C=CC3=CC=CC=C3C2C=C1	0.000	0.330	9.187	1.910	2.260	1.629
3-Nitrophenanthrene	[N+](=O)([O-])C=1C=CC=2C=CC3=CC=CC=C3C2C1	0.000	0.330	9.187	1.910	2.260	1.629
2,7-Dinitrophenanthrene	[N+](=O)([O-])C1=CC=2C=CC3=CC(=CC=C3C2C=C1)[N+](=O)[O-]	0.000	0.430	10.668	2.480	2.530	1.803
1-Hydroxyphenanthrene	OC1=CC=CC=2C3=CC=CC=C3C=CC12	0.500	0.510	8.524	1.550	2.220	1.513
9-Hydroxyphenanthrene	OC=1C2=CC=CC=C2C=2C=CC=CC2C1	0.500	0.510	8.524	1.550	2.220	1.513

Compound	Smiles	Σa_2^H	Σb_2^H	$logL^{16}$	π_2^H	R_2	Vi
3,4-Dihydroxyphenanthrene	OC=1C=CC=2C=CC3=CC=CC=C3C2C1O	0.770	0.650	9.268	1.730	2.370	1.572
9,10-Phenanthrenedione	C1=CC=CC=2C3=CC=CC=C3C(C(C12)=O)=O	0.000	0.800	8.944	2.120	2.070	1.529
benz(a)anthracene*	C1=CC=CC=2C1=C1C=C3C=CC=CC3=CC1=CC2	0.000	0.350	10.291	1.700	2.990	1.823
7-Methylbenz(a)anthracene	CC=1C2=CC=C3C(=C2C=C2C=CC=CC12)C=CC=C3	0.000	0.290	10.551	1.610	2.740	1.964
7,12-Dimethylbenz(a)anthracene	CC=1C2=CC=C3C(=C2C(=C2C=CC=CC12)C)C=CC=C3	0.000	0.290	11.023	1.550	2.760	2.105
8,12-Dimethylbenz(a)anthracene	CC=1C2=CC3=CC=C4C(=C3C(=C2C=CC1)C)C=CC=C4	0.000	0.290	11.023	1.550	2.760	2.105
7,8,12-Trimethylbenz(a)anthracene	CC=1C2=CC=C3C(=C2C(=C2C=CC=C(C12)C)C)C=CC=C3	0.000	0.290	11.494	1.490	2.780	2.246
4,5,10-Trimethylbenz(a)anthracene	c12c3c(c(C)ccc3)c(cc1cc1c(c2)cc(cc1)C)C	0.000	0.290	11.494	1.490	2.780	2.246
7,8,9,12-Tetramethylbenz(a)anthracene	CC=1C2=CC=C3C(=C2C(=C2C=CC(=C(C12)C)C)C)C=CC=C3	0.000	0.290	11.966	1.430	2.810	2.387
6,8-Diethylbenz(a)anthracene	c12c(cc(c3cc4c(cccc4cc13)CC)CC)cccc2	0.000	0.300	12.012	1.560	2.760	2.387
8-n-Butylbenz(a)anthracene	C(CCC)C=1C2=CC3=CC=C4C(=C3C=C2C=CC1)C=CC=C4	0.000	0.300	12.035	1.620	2.730	2.387
7-Nitrobenz(a)anthracene	[N+](=O)([O-])C=1C2=CC=C3C(=C2C=C2C=CC=CC12)C=CC=C3	0.000	0.390	11.561	2.230	2.980	1.998
Benz(a)acridine	n1c2c(cc3c1cccc3)c1c(cc2)cccc1	0.000	0.570	10.193	1.790	2.760	1.782
1-Hydroxybenz(a)anthracene	C1=C2C(=CC3=C1C=CC=C3)C4=C(C=C2)C=CC=C4O	0.500	0.560	10.898	1.870	2.940	1.882
9-Hydroxybenz(a)anthracene	OC1=CC2=CC3=CC=C4C(=C3C=C2C=C1)C=CC=C4	0.500	0.560	10.898	1.870	2.940	1.882
3,9-Benz(a)anthracene diol	c12c3c(ccc1cc1cc(O)ccc1c2)cc(O)cc3	1.000	0.840	11.716	2.080	3.170	1.941
Benz(a)anthracene-3,4-dione	C1=CC(C(C=2C1=C1C=C3C=CC=CC3=CC1=CC2)=O)=O	0.000	0.890	11.330	2.400	2.830	1.898
Benzo[a]pyrene*	C1=CC=C2C=CC=3C=C4C(=C5C=CC1=C2C53)C=CC=C4	0.000	0.370	11.736	1.960	3.630	1.954
4-Methylbenzo[a]pyrene	c12c3c4c(C)cc2cc2c(c1ccc3ccc4)cccc2	0.000	0.310	11.956	1.780	3.340	2.095
7-Methylbenzo[a]pyrene	c12c3c4ccc1c1c(c(ccc1)C)cc2ccc3ccc4	0.000	0.310	11.956	1.780	3.340	2.095
4,5-Dimethylbenzo[a]pyrene	c12c3c4c(C)c(c2cc2c(c1ccc3ccc4)cccc2)C	0.000	0.310	12.428	1.730	3.370	2.235
3,11-Dimethylbenzo[a]pyrene	CC1=C2C=CC=3C=C4C(=C5C(=CC(C=C1)=C2C53)C)C=CC=C4	0.000	0.310	12.428	1.730	3.370	2.235
1,3,6-Trimethylbenzo[a]pyrene	c12c3c4ccc1c1c(cccc1)c(c2ccc3c(C)cc4C)C	0.000	0.310	12.899	1.670	3.390	2.376
4,5,7-Trimethylbenzo[a]pyrene	c12c(cc3c(c(c4cccc5ccc1c3c45)C)C)c(ccc2)C	0.000	0.310	12.899	1.670	3.390	2.376
1-Nitrobenzo[a]pyrene	c12c3c4c(ccc3ccc2cc2c(c1cc4)cccc2)[N+](=O)[O-]	0.000	0.410	12.965	2.410	3.590	2.128
6-Nitrobenzo[a]pyrene	c12c3c4ccc1c1c(cccc1)c(c2ccc3ccc4)[N+](=O)[O-]	0.000	0.410	12.965	2.410	3.590	2.128
1,6-Dinitrobenzo[a]pyrene	C3=CC2=C1C=CC=CC1=C([N+]([O-])=O)C5=C2C4=C3C(=CC=C4C=C5)[N+]([O-])=O	0.000	0.500	14.447	2.980	3.860	2.302
1-Hydroxybenzo[a]pyrene	c12c3c4ccc1c1c(cccc1)cc2ccc3ccc4O	0.500	0.580	12.303	2.050	3.550	2.012
3-Hydroxybenzo[a]pyrene	C1=CC=C2C3=C4C(=CC2=C1)C=CC5=C(C=CC(=C54)C=C3)O	0.500	0.580	12.303	2.050	3.550	2.012
Benzo[a]pyrene-7,8-diol	c12c3c4ccc1c1c(c(c(O)cc1)O)cc2ccc3ccc4	0.770	0.730	13.047	2.230	3.690	2.071
Benzo[a]pyrene-7,8-dione	c1c(c(c2c(c3ccc4c5c(ccc4)ccc(c2)c35)c1)=O)=O	0.000	0.910	12.734	2.580	3.440	2.028
Dibenz(a,h)anthracene*	C1=CC=C2C(=C1)C=CC3=CC4=C(C=CC5=CC=CC=C54)C=C32	0.000	0.440	12.960	2.040	4.000	2.192
Dibenz(a,h)acridine	c12c3c(ccc1nc1c4c(cccc4)ccc1c2)cccc3	0.000	0.630	12.567	2.120	3.470	2.151

References

1. C. Wei, Y. Han, B.A.M. Bandowe, J. Cao, R.-J. Huang, H. Ni, J. Tian, and W. Wilcke, *Sci. Total Environ.*, 2015, **505**, 814-822.
2. W. Li, G. Shen, C. Yuan, C. Wang, H. Shen, H. Jiang, Y. Zhang, Y. Chen, S. Su, N. Lin, and S. Tao, *Atmos. Res*., 2016, **172-173**, 66-73.
3. S. Tomaz, P. Shahpoury, J.-L. Jaffrezo, G. Lammel, E. Perraudin, E. Villenave, and A. Albinet, *Sci. Total Environ*., 2016, **565**, 1071-1083.
4. M. Kalberer, D. Paulsen, M. Sax, M. Steinbacher, J. Dommen, A.S. Prevot, R. Fisseha, E. Weingartner, V. Frankevich, R. Zenobi, and U. Baltensperger, *Science*, 2004, **303**, 1659-1662.
5. S. Endo, T. N. Brown, N. Watanabe, N. Ulrich, G. Bronner, M. H. Abraham, and K. –U. Goss, UFZ-LSER database v 3.1, Leipzig, Germany, Helmholtz Centre for Environmental Research-UFZ. 2015. Available from http://www.ufz.de/lserd