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Supplement of

Molecular corridors and parameterizations of volatility in the evolution of organic aerosols

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Table S1. Statistics for comparison of the volatility of nitrogen- and sulfur-containing compounds predicted by the EPI Suite (E) and the Eq. (1) (P).

	Number	Median_E[a]	Median_P[b]	Mean_E[c]	Mean_P[d]	MB[e]	MAGE[f]	R[g]
CHN compounds								
Primary amine	222	4.92	4.82	4.38	4.17	0.21	0.92	0.93
Secondary amine	322	3.94	3.75	3.80	3.27	0.53	0.96	0.94
Tetiary amine	473	3.22	2.23	3.01	1.80	1.21	1.35	0.93
Quaternary amine	158	-2.55	2.05	-3.38	2.04	-5.42	5.42	0.86
Heterocyclic ring	1209	1.35	1.53	1.27	1.32	-0.05	1.03	0.88
Imine	249	1.00	0.35	0.52	0.07	0.45	1.23	0.93
Nitriles	282	3.53	3.60	3.41	3.35	0.06	0.74	0.93
CHON compounds								
Amide	5117	-0.10	0.47	-0.49	-0.11	-0.41	1.67	0.84
Imine	741	0.35	-0.09	-0.37	-0.66	0.29	1.78	0.89
Primary amine	576	2.74	2.78	2.57	2.36	0.21	1.53	0.70
Secondary amine	748	1.10	0.87	0.78	0.55	0.23	1.40	0.85
Tetiary amine	2130	0.63	-0.42	0.26	-0.54	0.80	1.67	0.85
Quaternary amine	225	-4.05	-0.23	-4.65	-0.65	-4.00	4.00	0.86
Nitroso	15	3.95	2.78	3.80	2.57	1.23	1.29	0.82
Nitro	750	2.18	0.71	1.92	0.35	1.56	1.76	0.88
Organonitrate	9	3.50	0.30	3.06	0.70	2.36	2.86	0.94
Alkyl nitrite	3	8.39	4.58	8.00	4.46	3.54	3.54	0.99
Azole	425	-0.24	-0.52	-1.27	-1.24	-0.04	1.79	0.84
Pyrimidine	1600	0.68	0.30	0.26	-0.08	0.34	1.40	0.84
Purine	369	-1.38	-1.65	-2.82	-2.56	-0.56	1.69	0.86
Amino acid	400	-1.52	2.05	-1.54	1.63	3.17	3.30	0.62
nitrile	356	2.38	1.40	2.23	1.01	1.21	1.64	0.81
CHOS compounds								
Organosulfate	17	1.45	1.90	-0.87	0.14	-1.01	1.42	0.98
Sulfonate	295	-1.25	-0.79	-2.05	-1.33	-0.73	2.25	0.82
Sulfone	173	1.33	0.86	1.16	0.76	0.40	0.92	0.89
Sulfoxides	12	1.52	2.30	2.38	2.82	-0.45	0.88	0.94
Sulfite	7	5.64	3.14	5.45	2.89	2.56	2.56	0.95
CHONS compounds								
Organosulfate	8	-4.01	-2.42	-4.03	-2.80	-1.23	1.52	0.96
Sulfonate	601	-8.65	-7.44	-10.94	-10.41	-1.79	2.22	0.97
Sulfone	85	-2.12	-4.42	-3.70	-5.95	1.66	2.09	0.94
Sulfonamide	648	-1.03	-2.72	-1.67	-3.35	1.67	1.91	0.91
Organic amide	178	-3.27	-3.43	-4.08	-4.21	0.12	1.66	0.93
Thioamide	244	-0.21	-0.85	-0.74	-1.54	0.80	1.49	0.87
Heterocyclic ring	1315	-1.15	-0.89	-1.98	-1.68	-0.33	1.55	0.90
Amino acid	45	-1.98	1.35	-1.54	0.92	-2.47	2.57	0.91
Thioate	58	0.30	-0.28	-0.28	-1.56	1.28	1.94	0.86
thiocarbamate	36	-2.67	-1.55	-3.64	-2.44	-1.20	1.62	0.92

[a]Median $\log_{10}(C_o)$ predicted by the EPI Suite (μg m^{-3}).

[b]Median $\log_{10}(C_o)$ predicted by the Eq. (1) (μg m^{-3}).

[c]Mean $\log_{10}(C_o)$ predicted by the EPI Suite (μg m^{-3}).

[d]Mean $\log_{10}(C_o)$ predicted by the Eq. (1) (μg m^{-3}).

[e]Mean bias (μg m^{-3}).

[f]Mean absolute gross error (μg m^{-3}).

[g]Correlation coefficient.