

Supplementary data for the article:

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## SUPPLEMENTARY MATERIAL

### Linear modeling of the soil-water partition coefficient normalized to organic carbon content by reversed-phase thin-layer chromatography

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**TABLE S1** List of standard compounds and unknowns accompanied with the list of  $\log K_{OC}$  values measured by soil sorption experiments (U.S. EPA); Molar mass  $M$ ; Abraham's solvatochromic parameters ( $A$  – hydrogen bond proton donating ability,  $B$  – hydrogen bond proton accepting ability,  $S$  – dipolarity/polarizability,  $E$  – molar refractivity in excess,  $V$  – McGowan's molar molecular volume); Acidity constants  $pK_a$ ; Ionization degree  $\alpha$  at  $pH = 6$

No	Compound	$\log K_{OC}$	Ref	$M$ (g/mol)	Solvatochromic parameters					$pK_a^b$	Ref	$\alpha$ (%) <sup>b</sup> $pH = 6$
					$A$	$B$	$S$	$E$	$V$			
<i>Standard compounds</i>												
1	Phenol	1.90	A1	94.12	0.60	0.30	0.89	0.81	0.775	9.99	B1	0.01
2	<b>4-Nitrophenol</b>	2.37	A1	139.12	0.82	0.26	1.72	1.07	0.949	7.18	B1	<b>6.20</b>
3	Benzyl Alcohol	1.10	A2	109.14	0.39	0.56	0.87	0.80	0.916	-	-	-
4	1-Naphthylamine	3.51	A1	143.20	0.20	0.57	1.26	1.67	1.185	3.92 <sup>a</sup>	B2	99.2 <sup>a</sup>
5	1-Naphthol	3.10	A1	144.18	0.60	0.37	1.05	1.52	1.144	9.34	B3	0.05
6	2,4-Dichlorophenol	2.81	A1	163.00	0.53	0.19	0.84	0.96	1.020	7.65	B1	2.19
7	Anthracene	4.31	A1	178.24	0.00	0.28	1.34	2.29	1.454	-	-	-
8	Acetophenone	1.80	A2	120.16	0.00	0.48	1.01	0.82	1.014	-	-	-
9	<b>2,4,6-Trichlorophenol</b>	3.03	A1	197.45	0.42	0.15	0.94	1.07	1.142	6.42	B1	<b>27.55</b>
10	Ethyl- <i>p</i> -hydroxybenzoate	2.21	A1	166.19	0.69	0.45	1.35	0.86	1.272	8.50	B4	0.32
11	<i>p</i> -Anisidine	1.93	A3	123.17	0.16	0.66	1.26	1.05	1.016	5.36 <sup>a</sup>	B5	81.36
12	1,2,3-Benzotriazole	1.69	A1	119.14	0.62	0.48	1.70	1.47	0.864	8.37	B3	0.42
13	Diphenylamine	2.78	A1	169.24	0.08	0.51	1.08	1.59	1.424	0.78 <sup>a</sup>	B6	>99.9 <sup>a</sup>
14	2,2'-Dipiridyl	1.60	A1	156.20	0.00	0.81	1.33	1.38	1.242	4.33 <sup>a</sup>	B7	>97.91 <sup>a</sup>
15	4-Bromoaniline	1.96	A1	172.03	0.31	0.30	1.19	1.19	0.991	3.86 <sup>a</sup>	B8	>99.2 <sup>a</sup>
16	Benzophenone	2.63	A1	182.23	0.00	0.50	1.50	1.45	1.481	-	-	-
17	<b>4-Aminobenzoic acid</b>	1.70	A4	137.15	0.94	0.69	1.61	1.08	1.032	2.38	B9	<b>99.98</b>
18	Pyrene	4.90	A1	202.26	0.00	0.25	1.52	2.60	1.585	-	-	-
19	Benzo[ <i>a</i> ]pyrene	5.95	A2	252.32	0.00	0.31	1.84	3.32	1.954	-	-	-
20	Fluorene	3.70	A1	166.23	0.00	0.25	1.06	1.59	1.357	-	-	-
21	Acenaphthene	3.59	A1	154.22	0.00	0.26	1.14	1.75	1.259	-	-	-
22	Naphthalene	2.96	A1	128.18	0.00	0.20	0.92	1.34	1.085	-	-	-
23	Phenanthrene	4.35	A1	178.24	0.00	0.29	1.29	2.06	1.454	-	-	-
24	Dibenz[ <i>a,h</i> ]anthracene	6.22	A1	278.36	0.00	0.35	1.99	3.43	2.192	-	-	-
25	Benz[ <i>a</i> ]anthracene	5.30	A1	228.30	0.00	0.29	1.66	2.71	1.823	-	-	-
26	Simazine	2.10	A1	201.69	0.33	0.95	1.20	1.55	1.479	1.62 <sup>a</sup>	B10	>99.9 <sup>a</sup>
27	Propazine	2.40	A1	229.75	0.30	0.97	1.14	1.47	1.761	1.85 <sup>a</sup>	B10	>99.9 <sup>a</sup>
28	Ametryn	2.59	A1	227.38	0.26	1.07	1.27	1.50	1.802	4.10 <sup>a</sup>	B11	>98.8 <sup>a</sup>
29	Prometryn	2.85	A1	241.41	0.26	1.10	1.26	1.51	1.940	4.05 <sup>a</sup>	B11	>98.9 <sup>a</sup>

No	Compound	log <i>K</i> <sub>OC</sub>	Ref	<i>M</i> (g/mol)	Solvatochromic parameters					p <i>K</i> <sub>a</sub> <sup>b</sup>	Ref	α (%) <sup>b</sup> pH = 6
					<i>A</i>	<i>B</i>	<i>S</i>	<i>E</i>	<i>V</i>			
<i>Unknowns</i>												
30	3-Nitrophenol	-		139.12	0.79	0.23	1.57	1.05	0.949	8.36	B1	0.43
31	2-Naphthol	-		144.18	0.61	0.40	1.08	1.52	1.144	9.67	B12	0.02
32	4-Hydroxybenzaldehyde	-		122.13	0.85	0.37	1.54	1.01	0.932	7.61	B3	2.40
33	2-Aminophenol	-		109.14	0.60	0.66	1.10	1.11	0.875	9.44 (-OH)	B1	0.00
34	4- <i>t</i> -Butylphenol	-		150.24	0.56	0.41	0.89	0.81	1.339	10.31	B1	0.00
35	2,6-Dimethylphenol	-		122.18	0.39	0.39	0.79	0.86	1.057	10.59	B1	0.00
36	4-Methoxyphenol	-		124.15	0.57	0.48	1.17	0.90	0.975	10.27	B1	0.01
37	Methyl- <i>p</i> -hydroxybenzoate	-		152.16	0.69	0.45	1.37	0.90	1.131	8.47	B4	0.34
38	2-Nitrobenzaldehyde	-		151.13	0.00	0.38	1.59	1.12	1.047	-	-	-
39	3-Nitrobenzaldehyde	-		151.13	0.00	0.48	1.49	1.10	1.047	-	-	-
40	Phthalimide	-		147.14	0.39	0.44	1.97	1.18	1.021	8.3	B13	0.50
41	Oxazepam	-		286.73	0.45	1.60	1.10	2.35	1.992	10.9 (-OH)	B14	0.00
42	Lorazepam	-		321.18	0.45	1.63	1.28	2.51	2.114	11.5 (-OH)	B15	0.00
43	Clonazepam	-		315.73	0.33	1.50	1.75	2.46	2.107	10.5 (-OH)	B16	0.00
44	Bromazepam	-		316.17	0.33	1.62	1.38	2.31	1.940	11.0 (-OH)	B17	0.00
45	Diazepam	-		284.76	0.00	1.25	1.57	2.08	2.074	3.40 <sup>a</sup>	B18	99.75 <sup>a</sup>
46	Nitrazepam	-		281.29	0.47	1.10	2.17	2.21	1.985	10.8	B15	0.00
47	Chlordiazepoxide	-		299.78	0.13	0.94	1.65	1.95	2.174	4.80 <sup>a</sup>	B18	94.06 <sup>a</sup>
48	Clobazam	-		300.76	0.00	1.47	2.49	2.29	2.133	6.65 <sup>a</sup>	B19	18.30 <sup>a</sup>
49	Medazepam	-		270.78	0.00	0.67	1.40	1.92	2.058	6.20 <sup>a</sup>	B20	38.69 <sup>a</sup>
50	Chrysene	-		228.30	0.00	0.29	1.66	2.71	1.823	-	-	-

<sup>a</sup>Dissociation degree is referred to the positively charged (protonated) form

<sup>b</sup>Compounds marked in bold are present in negatively charged form under studied chromatographic conditions

**TABLE S2** Retention factors of calibration set of compounds and unknowns - given as  $R_M$ , and  $\log k$  values in the case of TLC and HPLC experiments respectively

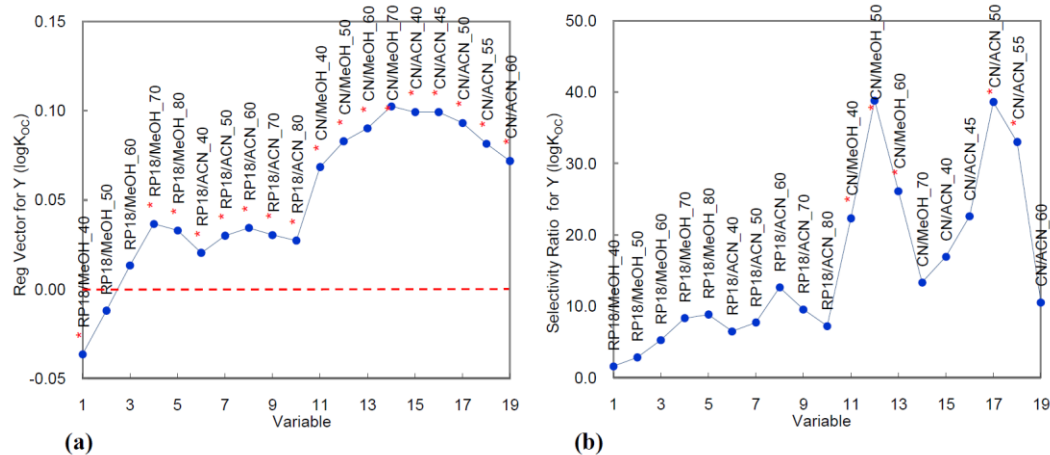
Comp. no.	HPLC $\log k$	TLC																			
		RP18 MeOH					RP18 ACN					CN MeOH					CNACN				
		40%	50%	60%	70%	80%	40%	50%	60%	70%	80%	40%	50%	60%	70%	40%	45%	50%	55%	60%	
1	-0.040	0.580	0.267	0.057	-0.175	-0.367	0.475	0.261	-0.276	-0.690	-0.738	0.010	-0.285	-0.409	-0.479	-0.076	-0.192	-0.318	-0.460	-0.558	
2	-0.064	0.706	0.395	0.184	-0.059	-0.267	0.513	0.232	-0.187	-0.632	-0.738	0.337	0.005	-0.181	-0.302	0.044	-0.042	-0.220	-0.344	-0.460	
3	-0.265	0.629	0.329	0.064	-0.161	-0.324	0.347	0.109	-0.295	-0.632	-0.660	-0.151	-0.402	-0.494	-0.592	-0.180	-0.233	-0.369	-0.486	-0.586	
4	0.487	1.252	0.868	0.533	0.199	-0.064	0.916	0.617	0.204	-0.131	-0.285	0.564	0.179	0.034	-0.130	0.268	0.233	0.057	-0.114	-0.202	
5	0.443	1.444	1.007	0.589	0.240	-0.040	0.916	0.591	0.152	-0.235	-0.389	0.623	0.192	-0.034	-0.183	0.220	0.199	-0.038	-0.172	-0.291	
6	0.248	1.358	1.183	0.710	0.323	0.017	0.876	0.644	0.169	-0.196	-0.345	0.536	0.146	-0.097	-0.285	0.325	0.172	-0.064	-0.192	-0.313	
7	0.664	1.688	1.721	1.612	1.092	0.641	1.555	1.466	0.973	0.602	0.322	1.284	0.822	0.490	0.143	0.654	0.548	0.396	0.239	-0.019	
8	0.187	0.979	0.725	0.363	0.088	-0.150	0.668	0.457	0.107	-0.238	-0.361	0.125	-0.105	-0.299	-0.418	0.108	0.003	-0.180	-0.337	-0.436	
9	0.382	1.521	1.130	0.777	0.458	0.209	0.985	0.703	0.384	0.062	-0.137	0.649	0.252	0.009	-0.233	0.440	0.333	0.092	-0.076	-0.306	
10	0.219	1.127	0.809	0.388	0.088	-0.174	0.596	0.314	-0.043	-0.457	-0.606	0.187	-0.099	-0.327	-0.467	0.025	-0.003	-0.213	-0.359	-0.521	
11	-0.431	0.575	0.348	0.113	-0.161	-0.324	0.418	0.239	0.020	-0.398	-0.490	0.406	0.265	0.145	0.016	0.318	0.219	0.097	-0.088	-0.205	
12	-0.390	0.502	0.239	-0.009	-0.244	-0.446	0.194	-0.017	-0.368	-0.845	-1.038	-0.138	-0.339	-0.481	-0.518	-0.207	-0.261	-0.362	-0.529	-0.558	
13	0.317	1.521	1.227	0.929	0.538	0.199	1.474	1.098	0.640	0.183	-0.053	0.987	0.543	0.161	0.000	0.673	0.645	0.303	0.120	-0.142	
14	0.366	1.179	0.823	0.444	0.182	-0.034	0.679	0.526	0.287	0.016	-0.027	0.051	-0.153	-0.338	-0.402	0.083	0.035	-0.095	-0.185	-0.306	
15	0.228	1.127	0.789	0.528	0.138	-0.115	0.805	0.555	0.215	-0.183	-0.341	0.382	0.077	-0.148	-0.216	0.193	0.126	-0.019	-0.133	-0.320	
16	0.624	1.730	1.310	0.692	0.501	0.177	1.344	1.007	0.597	0.163	-0.060	0.665	0.208	-0.081	-0.213	0.053	0.032	-0.100	-0.275	-0.438	
17	-0.341	-0.309	-0.419	-0.579	-0.586	-0.763	-0.251	-0.329	-0.634	-1.028	-1.071	-0.245	-0.462	-0.570	-0.597	0.199	0.086	-0.198	-0.331	-0.502	
18	0.787	2.035	1.721	1.693	1.225	0.790	1.736	1.371	1.129	0.741	0.455	1.549	0.872	0.490	0.243	0.910	0.815	0.499	0.294	0.058	
19	0.909	2.035	2.026	1.693	2.024	1.241	2.041	1.522	1.398	1.028	0.764	1.648	1.245	0.807	0.446	1.048	0.956	0.625	0.452	0.135	
20	0.815	1.730	1.541	1.168	0.958	0.562	1.555	1.273	0.861	0.461	0.185	1.206	0.580	0.250	0.035	0.651	0.604	0.241	0.146	-0.077	
21	0.716	2.035	2.026	1.113	0.787	0.387	1.736	1.178	0.823	0.368	0.140	1.126	0.516	0.224	0.006	0.625	0.479	0.213	0.127	-0.116	
22	0.514	2.035	2.026	1.040	0.611	0.309	1.242	1.074	0.668	0.249	0.020	1.086	0.468	0.207	-0.009	0.558	0.462	0.197	0.106	-0.126	
23	1.026	2.035	2.026	1.512	1.036	0.635	1.736	1.350	0.983	0.546	0.464	1.319	0.733	0.356	0.082	0.767	0.614	0.265	0.205	-0.064	
24	1.198	2.035	2.026	1.524	1.383	0.940	2.041	1.522	1.297	1.091	0.826	1.601	1.253	0.768	0.417	1.053	0.922	0.567	0.436	0.168	
25	0.967	2.035	2.026	1.693	1.457	1.041	2.041	1.702	1.297	0.897	0.527	1.493	1.201	0.670	0.327	0.998	0.829	0.448	0.359	0.142	

TABLE S2 Continues

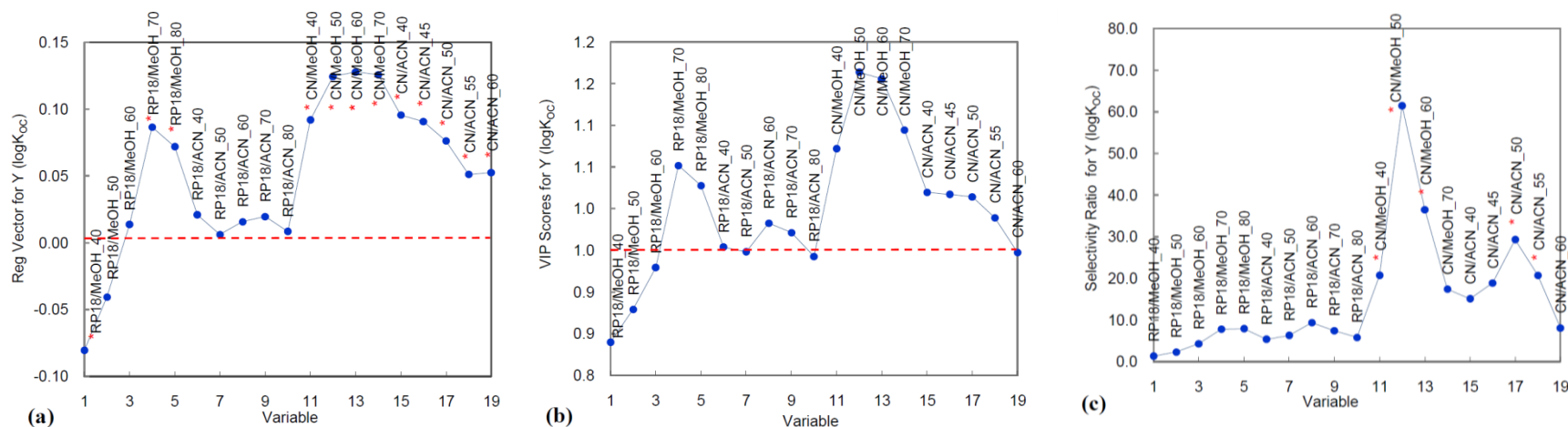
Comp. no.	HPLC log <i>k</i>	TLC																			
		RP18 MeOH					RP18 ACN					CN MeOH					CN ACN				
		40%	50%	60%	70%	80%	40%	50%	60%	70%	80%	40%	50%	60%	70%	40%	45%	50%	55%	60%	
26	0.084	1.421	1.007	0.518	0.171	-0.067	0.742	0.427	0.124	-0.147	-0.296	0.214	-0.086	-0.254	-0.418	0.089	-0.093	-0.173	-0.280	-0.357	
27	0.277	2.035	1.412	0.868	0.429	0.129	1.145	0.788	0.380	0.062	-0.100	0.454	0.027	-0.135	-0.387	0.543	0.393	-0.013	-0.063	-0.236	
28	0.380	1.733	1.419	1.033	0.473	0.208	1.029	0.585	0.375	0.094	-0.085	0.406	0.101	-0.166	-0.383	0.169	0.140	0.051	-0.053	-0.110	
29	0.461	1.733	1.548	1.175	0.638	0.307	1.341	0.746	0.543	0.190	0.034	0.538	0.177	-0.127	-0.337	0.224	0.172	0.076	0.003	-0.078	
30	0.038	0.830	0.540	0.290	-0.113	-0.237	0.612	0.049	-0.190	-0.490	-0.768	0.240	-0.027	-0.278	-0.427	-0.122	-0.172	-0.340	-0.403	-0.492	
31	0.426	1.424	0.950	0.593	0.120	-0.081	0.880	0.243	0.043	-0.285	-0.529	0.430	0.101	-0.176	-0.341	-0.036	-0.033	-0.200	-0.294	-0.373	
32	-0.134	0.476	0.146	-0.027	-0.415	-0.455	0.288	-0.179	-0.439	-0.834	-1.037	-0.073	-0.330	-0.501	-0.568	-0.278	-0.339	-0.494	-0.572	-0.625	
33	-0.147	0.255	0.024	-0.119	-0.456	-0.546	0.243	-0.141	-0.391	-0.654	-0.965	0.063	-0.085	-0.223	-0.296	-0.020	-0.096	-0.141	-0.253	-0.377	
34	0.383	1.733	1.356	0.850	0.349	0.087	1.061	0.489	0.269	-0.104	-0.306	0.402	0.024	-0.292	-0.490	0.527	0.230	-0.004	-0.208	-0.104	
35	0.117	1.083	0.811	0.566	0.113	-0.078	0.851	0.352	0.154	-0.197	-0.430	0.215	-0.043	-0.317	-0.439	0.341	0.162	-0.029	-0.157	-0.291	
36	-0.123	0.555	0.203	0.068	-0.364	-0.425	0.364	-0.061	-0.287	-0.593	-0.957	-0.066	-0.294	-0.406	-0.503	-0.089	-0.252	-0.319	-0.412	-0.605	
37	0.214	0.913	0.526	0.258	-0.190	-0.297	0.467	-0.012	-0.200	-0.533	-0.811	0.040	-0.224	-0.467	-0.512	-0.102	-0.238	-0.336	-0.439	-0.595	
38	0.098	1.051	0.453	0.201	-0.196	-0.320	0.726	0.250	0.082	-0.244	-0.521	0.095	-0.111	-0.357	-0.387	0.115	-0.070	-0.147	-0.256	-0.312	
39	0.064	0.874	0.540	0.290	-0.113	-0.250	0.709	0.220	0.069	-0.244	-0.546	0.185	-0.037	-0.285	-0.348	0.102	-0.089	-0.157	-0.277	-0.326	
40	-0.006	0.633	0.332	0.104	-0.301	-0.373	0.320	-0.104	-0.245	-0.579	-0.831	-0.047	-0.238	-0.475	-0.578	-0.135	-0.350	-0.366	-0.483	-0.576	
41	0.470	1.553	1.164	0.690	0.196	-0.054	0.680	0.157	-0.040	-0.345	-0.564	0.243	-0.046	-0.331	-0.477	0.062	-0.238	-0.272	-0.384	-0.549	
42	0.590	1.553	1.235	0.665	0.173	-0.124	0.709	0.185	-0.027	-0.320	-0.573	0.303	-0.027	-0.313	-0.473	0.115	-0.185	-0.224	-0.347	-0.513	
43	0.445	1.553	1.056	0.593	0.097	-0.109	0.802	0.263	0.037	-0.264	-0.582	0.480	0.231	-0.130	-0.311	0.246	-0.083	-0.112	-0.243	-0.392	
44	0.362	1.424	0.959	0.562	0.081	-0.109	0.592	0.160	0.037	-0.214	-0.333	0.112	-0.147	-0.387	-0.469	0.030	-0.238	-0.258	-0.333	-0.496	
45	0.721	1.733	1.318	1.013	0.553	0.260	1.258	0.729	0.502	0.190	0.037	0.534	0.245	-0.118	-0.296	0.388	0.036	0.022	-0.138	-0.229	
46	0.405	1.424	1.046	0.640	0.120	-0.109	0.795	0.243	0.005	-0.299	-0.546	0.476	0.217	-0.095	-0.264	0.217	-0.127	-0.131	-0.305	-0.377	
47	0.522	1.553	1.101	0.690	0.113	-0.094	0.775	0.220	-0.018	-0.299	-0.555	0.476	0.197	-0.095	-0.275	0.204	-0.039	-0.141	-0.298	-0.355	
48	0.627	1.733	1.266	0.717	0.183	-0.048	1.019	0.430	0.183	-0.107	-0.322	0.480	0.221	-0.102	-0.293	0.303	-0.020	-0.051	-0.236	-0.291	
49	1.076	2.068	2.038	2.033	1.314	0.847	2.037	1.488	1.417	0.951	0.727	1.719	1.136	0.795	0.440	1.135	0.760	0.490	0.316	0.144	
50	0.742	2.068	2.038	2.033	1.724	1.204	2.037	1.570	1.316	0.842	0.610	2.024	1.547	0.697	0.232	1.305	0.931	0.595	0.443	0.236	

**TABLE S3** Simple – the least square – univariate calibration models based on individual TLC experiments; Models are given in a form of  $\log K_{OC} = a + bR_M$ ; statistically satisfactory models are marked in bold.

Chromatography system	<i>a</i>	<i>b</i>	$RMSE_{Cal}$	$RMSE_{Pred}$	$R^2_{Cal}$	$R^2_{Pred}$	<i>n</i>	<i>F</i>	<i>p</i>
RP-18 MeOH_40	0.74±0.52	1.61±0.34	0.916	0.974	0.5163	0.4538	29	28.81	<1·10 <sup>-5</sup>
RP-18 MeOH_50	1.12±0.36	1.62±0.27	0.795	0.864	0.6354	0.5699	29	47.06	<1·10 <sup>-5</sup>
RP-18 MeOH_60	1.47±0.24	1.97±0.25	0.659	0.718	0.7494	0.7033	29	80.74	<1·10 <sup>-5</sup>
<b>RP-18 MeOH_70</b>	<b>2.00±0.14</b>	<b>2.11±0.19</b>	<b>0.500</b>	<b>0.527</b>	<b>0.8557</b>	<b>0.8397</b>	<b>29</b>	<b>160.17</b>	<b>&lt;1·10<sup>-5</sup></b>
<b>RP-18 MeOH_80</b>	<b>2.57±0.12</b>	<b>2.60±0.25</b>	<b>0.516</b>	<b>0.557</b>	<b>0.8465</b>	<b>0.8210</b>	<b>29</b>	<b>148.90</b>	<b>&lt;1·10<sup>-5</sup></b>
RP-18 ACN_40	0.87±0.29	2.00±0.24	0.629	0.710	0.7721	0.7094	29	91.45	<1·10 <sup>-5</sup>
RP-18 ACN_50	1.28±0.25	2.26±0.28	0.642	0.687	0.7625	0.7282	29	86.66	<1·10 <sup>-5</sup>
RP-18 ACN_60	2.08±0.16	2.24±0.25	0.589	0.637	0.8001	0.7664	29	108.07	<1·10 <sup>-5</sup>
RP-18 ACN_70	2.92±0.13	2.19±0.25	0.597	0.641	0.7948	0.7635	29	104.61	<1·10 <sup>-5</sup>
RP-18 ACN_80	3.33±0.15	2.40±0.30	0.642	0.680	0.7624	0.7333	29	86.64	<1·10 <sup>-5</sup>
<b>CN-MeOH_40</b>	<b>1.55±0.16</b>	<b>2.21±0.19</b>	<b>0.471</b>	<b>0.506</b>	<b>0.8722</b>	<b>0.8522</b>	<b>29</b>	<b>184.31</b>	<b>&lt;1·10<sup>-5</sup></b>
<b>CN-MeOH_50</b>	<b>2.27±0.10</b>	<b>2.67±0.19</b>	<b>0.403</b>	<b>0.441</b>	<b>0.9062</b>	<b>0.8878</b>	<b>29</b>	<b>260.93</b>	<b>&lt;1·10<sup>-5</sup></b>
<b>CN-MeOH_60</b>	<b>2.94±0.10</b>	<b>3.36±0.26</b>	<b>0.439</b>	<b>0.474</b>	<b>0.8892</b>	<b>0.8706</b>	<b>29</b>	<b>216.65</b>	<b>&lt;1·10<sup>-5</sup></b>
<b>CN-MeOH_70</b>	<b>3.69±0.13</b>	<b>4.13±0.40</b>	<b>0.531</b>	<b>0.556</b>	<b>0.8373</b>	<b>0.8220</b>	<b>29</b>	<b>138.92</b>	<b>&lt;1·10<sup>-5</sup></b>
CN-ACN_40	1.75±0.18	3.33±0.35	0.568	0.614	0.8142	0.7831	29	118.34	<1·10 <sup>-5</sup>
CN-ACN_45	2.00±0.16	3.50±0.36	0.557	0.598	0.8214	0.7938	29	124.17	<1·10 <sup>-5</sup>
<b>CN-ACN_50</b>	<b>2.72±0.12</b>	<b>4.43±0.44</b>	<b>0.537</b>	<b>0.568</b>	<b>0.8340</b>	<b>0.8140</b>	<b>29</b>	<b>135.68</b>	<b>&lt;1·10<sup>-5</sup></b>
CN-ACN_55	3.29±0.13	4.39±0.46	0.562	0.600	0.8182	0.7926	29	121.53	<1·10 <sup>-5</sup>
CN-ACN_60	4.26±0.20	5.37±0.63	0.615	0.643	0.7819	0.7618	29	96.81	<1·10 <sup>-5</sup>



**Figure S1.** PCR model – variable statistics demonstrating different impact of chromatographic systems in overall logK<sub>OC</sub> modelling; Regression vector plot (a) and sensitivity ratio diagram (b); Regression coefficients statistically significantly different from zero and points with high sensitivity ratio are marked by asterisk.



**Figure S2.** PLS model – variable statistics demonstrating different impact of chromatographic systems in overall logK<sub>OC</sub> modelling; Regression vector plot (a), VIP score graph (b) and sensitivity ratio diagram (c); Regression coefficients statistically significantly different from zero ( $p = 0.05$ ) and points with high sensitivity ratio are marked by asterisk.



PLS and PCR variable diagnostic plots demonstrate differences of individual chromatographic systems in contribution to the overall model. In the case of PCR 17 regression coefficients are statistically different from zero (tested by a t-test of cross-validated values, at the significance level  $p = 0.05$ ). The exceptions are only two coefficients associated with chromatographic systems: RP18/MeOH\_50 and RP18/MeOH\_60 (Figure S1a). According to the values of sensitivity ratio (cut-off value = 20) five out of seventeen coefficients, corresponding to the chromatographic systems based on CN-silica in combination with methanol content of 40 – 60% v/v, and acetonitrile content of 50 – 55% v/v, may be considered as the mostly influential ones (**Figure S1b**).

In the case of the PLS model there are 13 statistically significant regression coefficients. The exceptions are 6 coefficients associated with chromatographic systems mostly obtained on RP18-silica in combination with acetonitrile-water mixtures (**Figure S2a**). Since the VIP scores describe the average contribution of variables to the overall model, it is easy to perceive those ones that contribute better than the average ( $VIP > 1$ ). In that sense, thirteen chromatographic systems contributes to the overall PLS model better than the average, most of them are obtained on CN-silica layers in combination with methanol or acetonitrile as organic modifier (Figure S2b). Selectivity ratio plot (**Figure S2c**) indicates that the most influential chromatographic systems (cut-off value = 20) are those based on CN-silica in combination with methanol content of 40 – 60% v/v, and acetonitrile of 50 – 55% v/v (**Figure S2c**).

Clearly, the use of CN-silica layers has a stronger impact to the overall modeling of  $\log K_{OC}$  than RP18-modified beds. This could lead to a presumption that CN-modified layers should be more suitable for chromatographic determination of  $\log K_{OC}$  than hydrophobic, long alkyl-chain modified silica. This is in accordance with OECD guideline recommendations regarding the achieved accuracy.

**TABLE S4** Chromatographically determined and computationally estimated log $K_{OC}$  values

No.	Compound	TLC									HPLC	LSER		EPI Suite	
		PCR	PLS	RP18/ MeOH 70% v/v	RP18/ MeOH 80% v/v	CN/ MeOH 40% v/v	CN/ MeOH 50% v/v	CN/ MeOH 6 % v/v	CN/ MeOH 70% v/v	CN/ ACN 50% v/v		Poole	Nguyen	MCI	KOW
<i>Standard compounds</i>															
1	Phenol	1.41	1.47	1.63	1.62	1.57	1.50	1.57	1.71	1.31	1.49	1.65	1.58	2.27	1.90
2	4-Nitrophenol	1.94	2.07	1.88	1.88	2.30	2.28	2.33	2.44	1.75	1.40	1.85	2.18	2.46	2.37
3	Benzyl Alcohol	1.17	1.20	1.66	1.73	1.22	1.19	1.28	1.24	1.08	0.66	1.44	1.32	1.33	1.12
4	Naphthylamine	2.83	2.83	2.42	2.41	2.80	2.74	3.06	3.15	2.98	3.41	2.67	2.53	3.40	1.95
5	1-Naphthol	2.63	2.64	2.51	2.47	2.93	2.78	2.83	2.94	2.55	3.25	3.02	2.71	3.31	2.67
6	2,4-Dichlorophenol	2.56	2.56	2.68	2.62	2.74	2.66	2.61	2.51	2.44	2.54	2.62	2.48	2.69	2.78
7	Anthracene	4.38	4.42	4.31	4.24	4.39	4.46	4.59	4.28	4.48	4.06	4.46	4.27	4.21	3.86
8	Acetophenone	1.97	1.96	2.19	2.18	1.83	1.99	1.94	1.96	1.92	2.31	1.67	1.81	1.71	1.99
9	2,4,6-Trichlorophenol	2.97	2.96	2.97	3.12	2.99	2.94	2.97	2.73	3.13	3.02	3.01	2.94	3.25	3.28
10	Ethyl- <i>p</i> -hydroxybenzoate	1.77	1.79	2.19	2.12	1.97	2.00	1.84	1.76	1.78	2.43	2.23	2.30	2.20	2.39
11	<i>p</i> -Anisidine	2.87	2.96	1.66	1.73	2.45	2.97	3.43	3.76	3.15	0.06	1.42	1.52	1.65	1.48
12	1,2,3-Benzotriazole	1.13	1.21	1.49	1.41	1.25	1.36	1.32	1.55	1.12	0.21	1.65	1.82	1.72	1.79
13	Diphenylamine	3.80	3.76	3.14	3.09	3.73	3.72	3.48	3.69	4.07	2.79	3.35	3.14	2.92	2.82
14	2,2'-Dipiridylum	2.16	2.06	2.39	2.49	1.67	1.86	1.80	2.03	2.30	2.97	1.93	1.93	3.09	2.11
15	4-Bromoaniline	2.50	2.49	2.29	2.27	2.40	2.47	2.44	2.80	2.64	2.46	2.30	2.38	2.05	2.15
16	Benzophenone	2.51	2.50	3.06	3.04	3.02	2.82	2.67	2.81	2.28	3.91	3.04	3.21	3.06	2.88
17	4-Aminobenzoic acid	1.40	1.46	0.77	0.59	1.01	1.03	1.02	1.22	1.84	0.39	1.29	1.33	0.90	0.59
18	Pyrene	4.81	4.83	4.59	4.63	4.97	4.59	4.59	4.70	4.93	4.51	5.02	4.84	4.74	4.24
19	Benzo[ <i>a</i> ]pyrene	5.57	5.73	6.28	5.81	5.19	5.59	5.66	5.54	5.50	4.95	6.31	6.00	5.77	5.32
20	Fluorene	4.00	4.00	4.02	4.04	4.22	3.81	3.78	3.83	3.79	4.61	3.72	3.63	3.96	3.63
21	Acenaphthene	3.77	3.69	3.66	3.58	4.04	3.64	3.69	3.72	3.67	4.25	3.60	3.51	3.70	3.40
22	Naphthalene	3.60	3.51	3.29	3.38	3.95	3.52	3.64	3.65	3.60	3.51	3.03	2.99	3.19	2.86
23	Phenanthrene	4.23	4.20	4.19	4.23	4.47	4.22	4.14	4.03	3.90	5.38	4.21	4.08	4.22	3.87
24	Dibenz[ <i>a,h</i> ]anthracene	5.42	5.47	4.92	5.02	5.09	5.61	5.53	5.41	5.24	6.01	6.79	6.49	6.28	5.68
25	Benz[ <i>a</i> ]anthracene	5.16	5.23	5.08	5.29	4.85	5.47	5.19	5.04	4.71	5.16	5.51	5.33	5.25	5.00
26	Simazine	2.01	1.95	2.36	2.40	2.03	2.04	2.09	1.96	1.95	1.94	2.52	2.15	2.17	2.18
27	Propazine	2.78	2.61	2.91	2.91	2.56	2.34	2.49	2.09	2.67	2.64	3.07	2.65	2.54	2.34
28	Ametryn	2.65	2.53	3.00	3.12	2.45	2.54	2.38	2.11	2.95	3.02	2.90	2.54	2.63	2.36
29	Prometryn	2.89	2.77	3.35	3.37	2.74	2.74	2.51	2.30	3.06	3.31	3.18	2.77	2.82	3.51

TABLE S4 Continues

No.	Compound	TLC									HPLC	LSER		EPI Suite		
		PCR	PLS	RP18/ MeOH 70% v/v	RP18/ MeOH 80% v/v	CN/ MeOH 40% v/v	CN/ MeOH 50% v/v	CN/ MeOH 60% v/v	CN/ MeOH 70% v/v	CN/ ACN 50% v/v		Poole	Nguyen	MCI	KOW	
	<i>Unknowns</i>															
30	3-Nitrophenol	2.33	2.43	1.76	1.96	2.08	2.19	2.01	1.93	1.22	1.77	1.99	2.24	2.46	2.42	
31	2-Naphthol	2.81	2.82	2.26	2.36	2.50	2.54	2.35	2.28	1.84	3.19	2.94	2.64	3.30	2.59	
32	4-Hydroxybenzaldehyde	1.58	1.69	1.13	1.39	1.39	1.38	1.26	1.34	0.53	1.14	1.66	1.83	1.15	1.61	
33	2-Aminophenol	2.56	2.66	1.04	1.15	1.69	2.04	2.19	2.47	2.10	1.10	1.35	1.17	1.96	1.41	
34	4- <i>t</i> -Buthylphenol	3.30	3.13	2.74	2.80	2.44	2.33	1.96	1.66	2.71	3.03	2.71	2.53	3.11	2.92	
35	2,6-Dimethylphenol	3.09	3.00	2.24	2.37	2.03	2.15	1.88	1.88	2.60	2.06	2.21	2.05	2.70	2.40	
36	4-Methoxyphenol	1.99	2.04	1.23	1.47	1.41	1.48	1.57	1.61	1.31	1.18	1.65	1.65	2.08	2.02	
37	Methyl- <i>p</i> -hydroxybenzoate	2.01	2.03	1.60	1.80	1.64	1.67	1.37	1.57	1.23	2.41	1.94	2.03	1.94	2.11	
38	2-Nitrobenzaldehyde	2.69	2.61	1.59	1.74	1.76	1.97	1.74	2.09	2.07	1.99	1.86	2.33	1.24	1.88	
39	3-Nitrobenzaldehyde	2.77	2.75	1.76	1.92	1.96	2.17	1.98	2.25	2.03	1.86	1.71	2.08	1.24	1.73	
40	Phthalimide	1.85	1.90	1.37	1.60	1.45	1.63	1.34	1.30	1.10	1.61	1.54	2.09	0.15	1.10	
41	Oxazepam	2.36	2.35	2.42	2.43	2.09	2.14	1.83	1.72	1.52	3.35	3.37	2.27	2.76	1.73	
42	Lorazepam	2.48	2.43	2.37	2.25	2.22	2.19	1.89	1.74	1.73	3.79	3.64	2.58	2.98	1.81	
43	Clonazepam	2.99	2.98	2.21	2.29	2.61	2.88	2.50	2.41	2.23	3.26	3.47	2.86	4.06	2.45	
44	Bromazepam	2.37	2.30	2.17	2.29	1.80	1.87	1.64	1.75	1.58	2.95	2.95	2.12	3.56	2.21	
45	Diazepam	3.57	3.48	3.17	3.25	2.73	2.92	2.55	2.47	2.82	4.26	3.55	3.17	3.88	2.44	
46	Nitrazepam	2.98	3.01	2.26	2.29	2.61	2.85	2.62	2.60	2.14	3.11	3.43	3.32	3.85	2.36	
47	Chlordiazepoxide	2.99	3.00	2.24	2.33	2.61	2.79	2.62	2.56	2.10	3.54	4.21	3.98	5.48	2.23	
48	Clobazam	3.20	3.13	2.39	2.45	2.61	2.85	2.60	2.48	2.50	3.92	2.82	2.93	2.54	2.03	
49	Medazepam	6.33	6.37	4.78	4.78	5.35	5.30	5.62	5.51	4.89	5.56	4.61	4.37	4.48	3.30	
50	Chrysene	6.66	6.79	5.64	5.71	6.02	6.39	5.29	4.65	5.36	4.34	5.51	5.33	5.26	5.04	

**TABLE S5a** Comparison of chromatographic and *in silico* methods;

Collection of normalized SRD values

<b>Method</b>	<b>SRD</b>
TLC (CN/MeOH_40)	9.60
TLC (CN/MeOH_50)	10.72
LSER (Poole)	12.80
TLC (RP18/MeOH_80)	13.60
TLC (RP18/MeOH_70)	13.76
TLC (CN/MeOH_60)	14.08
LSER (Nguyen)	15.36
TLC (PCR)	16.48
TLC (PLS)	17.60
HPLC	18.08
TLC (CN/MeOH_70)	19.04
EPI (MCI)	19.84
TLC (CN/ACN_50)	20.00
EPI (KOW)	21.60

**TABLE S5b** Normalized SRD values obtained by the sevenfold jack-knife resampling procedure

<b>Method</b>	<b>SRD1</b>	<b>SRD2</b>	<b>SRD3</b>	<b>SRD4</b>	<b>SRD5</b>	<b>SRD6</b>	<b>SRD7</b>	<b>Median</b>
TLC (CN/MeOH_40)	8.8	9.7	11.7	10.0	10.0	10.6	7.6	<b>9.96</b>
TLC (CN/MeOH_50)	11.3	8.7	13.2	11.5	10.6	10.4	10.4	<b>10.61</b>
LSER (Poole)	13.6	11.3	14.7	14.3	11.7	11.9	13.2	<b>13.20</b>
TLC (RP18/MeOH_80)	13.4	12.6	18.2	13.4	13.4	13.2	12.6	<b>13.38</b>
TLC (RP18/MeOH_70)	13.6	13.4	18.0	13.2	13.4	13.2	12.1	<b>13.42</b>
TLC (CN/MeOH_60)	13.8	13.2	18.4	15.2	12.6	12.8	14.1	<b>13.83</b>
LSER (Nguyen)	16.6	14.1	17.3	16.2	15.4	12.3	15.8	<b>15.80</b>
TLC (PCR)	17.0	16.0	19.3	18.2	14.3	13.4	17.5	<b>17.01</b>
TLC (PLS)	18.6	16.5	20.3	17.7	14.5	15.2	19.3	<b>17.75</b>
HPLC	18.4	16.5	20.6	19.3	19.0	16.0	18.6	<b>18.61</b>
TLC (CN/MeOH_70)	19.5	17.3	24.2	19.7	17.3	17.3	19.3	<b>19.26</b>
EPI (MCI)	20.4	16.7	21.6	20.8	19.9	19.3	19.5	<b>19.91</b>
TLC (CN/ACN_50)	21.5	18.4	22.3	22.3	18.6	18.0	18.8	<b>18.83</b>
EPI (KOW)	21.1	20.6	26.8	23.8	19.9	20.8	20.1	<b>20.78</b>

**TABLE S6** LSER regression coefficients of TLC systems given as the value  $\pm$  standard deviation;  $I$  – intercept,  $a$  – hydrogen bond basicity,  $b$  – hydrogen bond acidity,  $s$  – dipolarity/polarizability,  $e$  – molar refraction in excess, and  $\nu$  – ability for formation of a vacant space; Stationary phase octadecyl (RP18)-modified silica and cyano (CN)-modified silica; Mobile phases: mixtures of methanol (MeOH) and acetonitrile (ACN) with water in different proportions (v/v); Statistical parameters:  $R^2$  – squared determination coefficient,  $S.D.$  – standard error of the model,  $F$  – Fisher’s statistic,  $P$  – significance of  $F$ ,  $n$  – number of calibration points (compounds)

No.	Chrom.system	$I$	$a$	$b$	$s$	$e$	$\nu$	$R^2$	$S.D.$	$F$	$P$	$n$
1	MeOH 40%	0.72 $\pm$ 0.19	-0.50 $\pm$ 0.15	-0.660 $\pm$ 0.13	-0.52 $\pm$ 0.12	0.030 $\pm$ 0.12	1.30 $\pm$ 0.20	0.8314	0.248	43.39	6.36 $\cdot$ 10 <sup>-16</sup>	50
2	MeOH 50%	0.47 $\pm$ 0.18	-0.52 $\pm$ 0.15	-0.876 $\pm$ 0.13	-0.59 $\pm$ 0.14	0.161 $\pm$ 0.11	1.29 $\pm$ 0.19	0.8671	0.241	57.40	3.60 $\cdot$ 10 <sup>-18</sup>	50
3	MeOH 60%	0.04 $\pm$ 0.15	-0.40 $\pm$ 0.12	-0.942 $\pm$ 0.10	-0.461 $\pm$ 0.094	0.181 $\pm$ 0.085	1.21 $\pm$ 0.16	0.8934	0.200	73.75	2.92 $\cdot$ 10 <sup>-20</sup>	50
4	MeOH 70%	-0.26 $\pm$ 0.14	-0.37 $\pm$ 0.11	-1.00 $\pm$ 0.09	-0.417 $\pm$ 0.084	0.352 $\pm$ 0.076	0.94 $\pm$ 0.14	0.9159	0.178	95.84	1.64 $\cdot$ 10 <sup>-22</sup>	50
5	MeOH 80%	-0.41 $\pm$ 0.10	-0.32 $\pm$ 0.08	-0.81 $\pm$ 0.07	-0.307 $\pm$ 0.064	0.245 $\pm$ 0.057	0.77 $\pm$ 0.11	0.9220	0.135	104.09	3.12 $\cdot$ 10 <sup>-23</sup>	50
6	ACN 40%	0.49 $\pm$ 0.13	-0.57 $\pm$ 0.10	-1.00 $\pm$ 0.09	-0.352 $\pm$ 0.079	0.156 $\pm$ 0.072	1.05 $\pm$ 0.13	0.9185	0.168	99.20	8.24 $\cdot$ 10 <sup>-23</sup>	50
7	ACN 50%	0.49 $\pm$ 0.14	-0.67 $\pm$ 0.11	-0.93 $\pm$ 0.09	-0.409 $\pm$ 0.084	0.226 $\pm$ 0.075	0.75 $\pm$ 0.14	0.9032	0.177	82.13	3.54 $\cdot$ 10 <sup>-21</sup>	50
8	ACN 60%	0.01 $\pm$ 0.12	-0.67 $\pm$ 0.09	-0.875 $\pm$ 0.08	-0.318 $\pm$ 0.073	0.193 $\pm$ 0.066	0.81 $\pm$ 0.12	0.9230	0.154	105.41	2.42 $\cdot$ 10 <sup>-23</sup>	50
9	ACN 70%	-0.40 $\pm$ 0.11	-0.665 $\pm$ 0.09	-0.789 $\pm$ 0.07	-0.313 $\pm$ 0.066	0.198 $\pm$ 0.060	0.80 $\pm$ 0.11	0.9331	0.140	122.83	1.08 $\cdot$ 10 <sup>-24</sup>	50
10	ACN 80%	-0.50 $\pm$ 0.13	-0.68 $\pm$ 0.10	-0.725 $\pm$ 0.09	-0.347 $\pm$ 0.079	0.177 $\pm$ 0.071	0.75 $\pm$ 0.13	0.8986	0.167	77.95	9.90 $\cdot$ 10 <sup>-21</sup>	50
11	MeOH 40%	-0.01 $\pm$ 0.15	-0.35 $\pm$ 0.12	-1.02 $\pm$ 0.10	-0.298 $\pm$ 0.090	0.349 $\pm$ 0.081	0.80 $\pm$ 0.15	0.8957	0.191	75.56	1.82 $\cdot$ 10 <sup>-20</sup>	50
12	MeOH 50%	-0.39 $\pm$ 0.12	-0.30 $\pm$ 0.10	-0.820 $\pm$ 0.08	-0.138 $\pm$ 0.075	0.313 $\pm$ 0.067	0.62 $\pm$ 0.13	0.8983	0.158	77.74	1.04 $\cdot$ 10 <sup>-20</sup>	50
13	MeOH 60%	-0.40 $\pm$ 0.11	-0.273 $\pm$ 0.09	-0.632 $\pm$ 0.07	-0.142 $\pm$ 0.068	0.262 $\pm$ 0.061	0.41 $\pm$ 0.11	0.8648	0.143	56.28	5.23 $\cdot$ 10 <sup>-18</sup>	50
14	MeOH 70%	-0.406 $\pm$ 0.094	-0.271 $\pm$ 0.08	-0.452 $\pm$ 0.06	-0.081 $\pm$ 0.058	0.227 $\pm$ 0.052	0.19 $\pm$ 0.10	0.8351	0.123	44.56	3.92 $\cdot$ 10 <sup>-16</sup>	50
15	ACN 40%	-0.038 $\pm$ 0.14	-0.28 $\pm$ 0.11	-0.661 $\pm$ 0.09	-0.222 $\pm$ 0.084	0.160 $\pm$ 0.076	0.62 $\pm$ 0.14	0.8037	0.178	36.03	1.71 $\cdot$ 10 <sup>-14</sup>	50
16	ACN 45%	0.040 $\pm$ 0.13	-0.26 $\pm$ 0.10	-0.710 $\pm$ 0.09	-0.269 $\pm$ 0.077	0.192 $\pm$ 0.070	0.49 $\pm$ 0.13	0.8218	0.164	40.58	2.13 $\cdot$ 10 <sup>-15</sup>	50
17	ACN 50%	-0.143 $\pm$ 0.093	-0.296 $\pm$ 0.07	-0.448 $\pm$ 0.06	-0.166 $\pm$ 0.057	0.160 $\pm$ 0.052	0.327 $\pm$ 0.10	0.8338	0.121	44.15	4.64 $\cdot$ 10 <sup>-16</sup>	50
18	ACN 55%	-0.242 $\pm$ 0.089	-0.279 $\pm$ 0.07	-0.431 $\pm$ 0.06	-0.188 $\pm$ 0.055	0.168 $\pm$ 0.049	0.306 $\pm$ 0.10	0.8375	0.116	45.35	2.85 $\cdot$ 10 <sup>-16</sup>	50
19	ACN 60%	-0.409 $\pm$ 0.088	-0.260 $\pm$ 0.07	-0.371 $\pm$ 0.06	-0.116 $\pm$ 0.054	0.066 $\pm$ 0.049	0.340 $\pm$ 0.089	0.7761	0.115	30.50	2.95 $\cdot$ 10 <sup>-13</sup>	50

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