

Supplementary material for the article:

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## SUPPLEMENTARY MATERIAL

### How to compare the separation selectivity of HPLC columns properly?

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**Table S1** Retention parameters for 67 solutes and ten chromatographic columns given as  $\log k$  values; Data have been retrieved from ref. [1]  
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Compound No.	Inertsil	Symmetry	SB-100	SB-90	SB-300	Eclipse	YMC 15	YMC 16	YMC 17	Discovery	VARC*
1	0.675	0.581	0.484	0.480	-0.025	0.51	0.528	0.514	0.530	0.255	0.4532
2	0.888	0.803	0.702	0.692	0.176	0.734	0.748	0.736	0.752	0.471	0.6702
3	1.090	1.010	0.91	0.895	0.369	0.947	0.955	0.949	0.957	0.672	0.8754
4	1.107	1.036	0.924	0.908	0.379	0.964	0.976	0.966	0.979	0.693	0.8932
5	1.322	1.247	1.143	1.123	0.585	1.188	1.194	1.184	1.196	0.901	1.1083
6	1.552	1.478	1.373	1.347	0.802	1.424	1.426	1.419	1.429	1.127	1.3377
7	1.049	0.958	0.860	0.853	0.333	0.890	0.912	0.899	0.913	0.629	0.8296
8	1.110	1.027	0.920	0.907	0.382	0.957	0.973	0.956	0.955	0.691	0.8878
9	1.120	1.037	0.928	0.916	0.392	0.965	0.981	0.972	0.986	0.701	0.8998
10	1.251	1.145	1.057	1.046	0.519	1.093	1.112	1.111	1.111	0.817	1.0262
11	0.952	0.857	0.757	0.748	0.232	0.787	0.806	0.793	0.809	0.528	0.7269
12	0.248	0.130	0.066	0.080	-0.396	0.078	0.110	0.086	0.105	-0.160	0.0347
13	0.521	0.388	0.333	0.346	-0.144	0.343	0.377	0.353	0.370	0.092	0.2979
14	0.717	0.595	0.538	0.55	0.046	0.551	0.582	0.561	0.576	0.290	0.5006
15	0.721	0.587	0.538	0.552	0.052	0.554	0.588	0.565	0.580	0.292	0.5029
16	-0.249	-0.376	-0.38	-0.345	-0.785	-0.413	-0.374	-0.399	-0.380	-0.622	-0.4323
17	0.623	0.516	0.437	0.440	-0.061	0.457	0.483	0.464	0.481	0.202	0.4042
18	-0.07	-0.186	-0.236	-0.215	-0.666	-0.237	-0.195	-0.220	-0.200	-0.456	-0.2681
19	0.204	0.096	0.051	0.074	-0.39	0.045	0.084	0.062	0.08	-0.178	0.0128
20	0.567	0.470	0.434	0.449	-0.025	0.424	0.458	0.437	0.453	0.190	0.3857
21	0.055	-0.066	-0.129	-0.111	-0.564	-0.119	-0.076	-0.100	-0.080	-0.332	-0.1522
22	0.33	0.208	0.138	0.154	-0.308	0.154	0.196	0.174	0.194	-0.063	0.1177
23	0.158	0.028	-0.043	-0.031	-0.436	-0.039	0.039	0.024	0.032	-0.234	-0.0502
24	0.055	-0.088	-0.142	-0.119	-0.552	-0.131	-0.083	-0.109	-0.092	-0.331	-0.1592
25	0.525	0.417	0.353	0.361	-0.11	0.369	0.405	0.384	0.402	0.129	0.3235
26	1.069	0.964	0.887	0.893	0.377	0.906	0.948	0.931	0.938	0.645	0.8558

Compound No.	Inertsil	Symmetry	SB-100	SB-90	SB-300	Eclipse	YMC 15	YMC 16	YMC 17	Discovery	VARC*
27	0.220	0.116	0.055	0.067	-0.419	0.059	0.082	0.060	0.079	-0.182	0.0137
28	0.560	0.446	0.388	0.397	-0.100	0.395	0.423	0.402	0.418	0.124	0.3453
29	0.378	0.250	0.202	0.219	-0.266	0.204	0.238	0.213	0.23	-0.043	0.1625
30	0.149	0.069	-0.038	-0.02	-0.446	-0.037	0.029	0.015	0.032	-0.239	-0.0486
31	0.336	0.217	0.175	0.191	-0.294	0.171	0.201	0.178	0.195	-0.076	0.1294
32	0.910	0.785	0.739	0.745	0.236	0.752	0.780	0.759	0.773	0.479	0.6958
33	1.034	0.910	0.866	0.872	0.355	0.884	0.911	0.889	0.902	0.601	0.8224
34	1.125	0.992	0.950	0.956	0.438	0.968	0.999	0.962	0.99	0.684	0.9064
35	0.988	0.844	0.817	0.829	0.318	0.830	0.866	0.840	0.853	0.545	0.773
36	1.109	0.957	0.937	0.950	0.433	0.954	0.996	0.978	0.978	0.656	0.8948
37	0.992	0.858	0.824	0.834	0.321	0.839	0.870	0.847	0.860	0.555	0.780
38	1.097	0.953	0.921	0.932	0.418	0.938	0.976	0.953	0.961	0.650	0.8799
39	-0.124	-0.274	-0.212	-0.159	-0.621	-0.280	-0.223	-0.253	-0.239	-0.509	-0.2894
40	-0.106	-0.258	-0.205	-0.159	-0.602	-0.260	-0.202	-0.231	-0.218	-0.491	-0.2732
41	0.123	-0.003	-0.045	-0.029	-0.474	-0.041	0.002	-0.023	-0.006	-0.267	-0.0763
42	0.201	0.085	0.042	0.053	-0.353	0.042	0.095	0.074	0.091	-0.162	0.0168
43	0.448	0.301	0.289	0.311	-0.155	0.284	0.324	0.298	0.312	0.031	0.2443
44	0.209	0.007	0.053	0.079	-0.400	0.039	0.075	0.047	0.064	-0.21	-0.0037
45	-0.973	-0.994	-0.736	-0.698	-1.240	-1.063	-1.103	-1.139	-1.118	-1.354	-1.0418
46	-0.306	-0.328	-0.113	-0.126	-0.407	-0.165	-0.224	-0.158	-0.141	-0.239	-0.2207
47	-0.689	-0.685	-0.412	-0.419	-0.656	-0.471	-0.563	-0.484	-0.458	-0.524	-0.5361
48	-0.995	-0.959	-0.642	-0.645	-0.871	-0.700	-0.818	-0.721	-0.694	-0.728	-0.7773
49	-0.379	-0.407	-0.19	-0.196	-0.467	-0.240	-0.298	-0.237	-0.214	-0.309	-0.2937
50	-0.757	-0.757	-0.459	-0.467	-0.736	-0.508	-0.637	-0.551	-0.525	-0.596	-0.5993
51	0.543	0.478	0.449	0.433	-0.039	0.425	0.441	0.434	0.447	0.202	0.3813
52	0.777	0.722	0.685	0.664	0.185	0.664	0.680	0.673	0.688	0.437	0.6175
53	1.013	0.967	0.923	0.897	0.409	0.904	0.920	0.914	0.930	0.674	0.8551
54	0.061	-0.040	-0.068	-0.100	-0.579	-0.084	-0.068	-0.083	-0.068	-0.309	-0.1338

Compound No.	Inertsil	Symmetry	SB-100	SB-90	SB-300	Eclipse	YMC 15	YMC 16	YMC 17	Discovery	VARC*
55	0.396	0.275	0.248	0.247	-0.238	0.231	0.257	0.241	0.254	-0.018	0.1893
56	0.884	0.765	0.728	0.716	0.268	0.714	0.764	0.746	0.759	0.484	0.6828
57	1.104	1.009	0.955	0.936	0.476	0.951	0.995	0.981	0.993	0.720	0.912
58	0.480	0.357	0.326	0.326	-0.109	0.315	0.369	0.348	0.362	0.096	0.287
59	0.695	0.497	0.471	0.494	0.120	0.349	0.441	0.406	0.414	0.171	0.4058
60	0.770	0.706	0.645	0.641	0.200	0.632	0.672	0.659	0.677	0.433	0.6035
61	0.987	0.936	0.867	0.858	0.410	0.856	0.893	0.884	0.901	0.656	0.8248
62	1.206	1.169	1.093	1.078	0.626	1.083	1.119	1.124	1.130	0.883	1.0511
63	-0.144	-0.278	-0.293	-0.268	-0.656	-0.342	-0.273	-0.299	-0.286	-0.524	-0.3363
64	-0.268	-0.436	-0.475	-0.448	-0.806	-0.539	-0.441	-0.48	-0.465	-0.709	-0.5067
65	-0.004	-0.136	-0.149	-0.126	-0.510	-0.207	-0.138	-0.165	-0.152	-0.393	-0.198
66	0.145	0.033	-0.02	-0.016	-0.436	-0.027	0.023	0.001	0.019	-0.230	-0.0508
67	-0.081	-0.208	-0.245	-0.227	-0.626	-0.240	-0.211	-0.237	-0.214	-0.453	-0.2742

\*Virtual average reference column

**Table S2** Selectivity parameters of chromatographic columns; *H* – hydrophobicity, *B* – hydrogen-bond basicity, *A* – hydrogen-bond acidity, *S* – steric resistance, *C* – ion exchange capacity; Selectivity parameters depends on the temperature; current values apply on 35 °C. Except of VARC the rest of data have been taken from the ref. [1] Copyright Elsevier: license number 3995960369478, License date Nov 25, 2016.

No.	Column short name	<i>H</i>	<i>S</i>	<i>A</i>	<i>B</i>	<i>C</i>
1	Inertsil	1.0048	-0.0126	-0.1285	-0.0255	-0.3501
2	Symmetry	1.0498	-0.0588	0.0104	-0.0289	-0.2071
3	SB-100	0.9981	0.0211	0.2715	0.0064	0.0854
4	SB-90	0.9666	0.0418	0.2642	0.0093	0.0505
5	SB-300	0.8945	0.0426	0.1092	0.0761	0.2204
6	Eclipse	1.0355	-0.0084	-0.0202	-0.0325	0.0443
7	YMC 15	1.0022	0.0022	-0.1362	-0.0128	-0.0960
8	YMC 16	1.0106	-0.0077	-0.1317	-0.0105	0.0088
9	YMC 17	1.0106	-0.0067	-0.1357	-0.0099	0.0135
10	Discovery	0.9861	-0.0226	-0.1279	0.0163	0.1899
11	VARC*	0.9967	-0.0011	-0.0024	-0.0011	-0.0039

\*Virtual average reference column

**Table S3** Column comparison by Sum of Ranking Differences (SRD) and Generalized Pairwise Correlation Method (GPCM) using VARC as a reference; List of SRD and GPCM conditional Fisher's exact test with probability weighted (CE-PW) ordering scores, *i*) obtained from primary retention data and *ii*) using hydrophobic-subtraction method (HSM) parameters

No.	SRD				GPCM			
	<i>Based on primary retention data</i>		<i>Based on HSM parameters</i>		<i>Based on primary retention data</i>		<i>Based on HSM parameters</i>	
	Column	Score	Column	Score	Column	Score	Column	Score
1	YMC 16	0.980	Inertsil	0.00	YMC 16	0.980	Inertsil	0.00
2	YMC 15	1.248	YMC 15	16.67	YMC 17	0.987	YMC 15	1.06
3	YMC 17	1.248	Symmetry	33.33	YMC 15	0.994	Symmetry	45.73
4	SB-100	2.139	Eclipse	50.00	SB-100	3.056	YMC 16	46.00
5	SB-90	2.228	YMC 16	50.00	Eclipse	3.065	YMC 17	46.00
6	Eclipse	2.228	YMC 17	50.00	SB-90	3.069	SB-100	51.30
7	Inertsil	2.585	Discovery	50.00	Inertsil	3.332	SB-90	51.30
8	Symmetry	3.209	SB-100	66.67	Symmetry	3.334	Eclipse	51.34
9	Discovery	3.565	SB-90	66.67	Discovery	4.110	Discovery	51.31
10	SB-300	5.169	SB-300	66.67	SB-300	5.169	SB-300	66.67

**Table S4a** Collection of SRD-COVAT\* scores based on primary retention data

	YMC 16	YMC 17	YMC 15	Eclipse	SB-100	SB-90	Inertsil	Discovery	Symmetry	SB-300
YMC 16	0.00	0.85	1.20	1.96	2.50	2.41	3.30	3.34	3.52	5.39
YMC 17	0.85	0.00	1.52	1.43	2.50	2.54	3.52	3.25	3.83	5.30
YMC 15	1.20	1.52	0.00	2.54	2.94	2.23	2.54	4.41	3.25	5.53
Eclipse	1.96	1.43	2.54	0.00	2.76	3.07	3.03	3.25	3.34	6.37
SB-100	2.50	2.50	2.94	2.76	0.00	1.69	3.97	3.43	4.32	4.10
SB-90	2.41	2.54	2.23	3.07	1.69	0.00	3.65	4.59	4.59	4.55
Inertsil	3.30	3.52	2.54	3.03	3.97	3.65	0.00	5.88	3.34	7.26
Discovery	3.34	3.25	4.41	3.25	3.43	4.59	5.88	0.00	4.55	4.68
Symmetry	3.52	3.83	3.25	3.34	4.32	4.59	3.34	4.55	0.00	7.75
SB-300	5.39	5.30	5.53	6.37	4.10	4.55	7.26	4.68	7.75	0.00

\* Comparison with One VArIable at a Time: all columns were selected as a reference column once and only once.

**Table S4b** Collection of GPCM(CE-PW)-COVAT\* scores based on primary retention data

	YMC 17	YMC 16	YMC 15	Eclipse	SB-100	SB-90	Discovery	Inertsil	Symmetry	SB-300
YMC 17	0.00	0.89	1.20	1.07	2.19	2.27	1.74	3.56	3.42	2.73
YMC 16	1.17	0.00	0.90	2.82	2.19	2.27	1.74	3.56	3.41	2.73
YMC 15	1.18	0.90	0.00	3.51	2.20	1.71	3.81	1.59	2.99	3.34
Eclipse	1.48	2.68	2.97	0.00	2.19	2.28	2.12	2.78	2.57	3.96
SB-100	3.21	3.27	3.27	3.51	0.00	0.87	2.43	3.96	4.67	1.22
SB-90	3.49	3.27	2.96	3.52	0.57	0.00	4.49	3.56	5.93	1.23
Discovery	3.51	3.27	4.15	3.86	2.75	4.27	0.00	6.34	4.25	1.83
Inertsil	3.51	3.56	2.68	3.51	4.11	3.14	5.88	0.00	3.41	5.16
Symmetry	3.51	3.57	3.27	3.51	4.11	4.55	4.14	3.17	0.00	5.17
SB-300	5.26	5.35	5.35	6.33	4.37	4.27	4.83	7.13	7.66	0.00

\* Comparison with One VArIable at a Time: all columns were selected as a reference column once and only once.



**Table S4c** Collection of SRD-COVAT\* scores based on HSM data

	YMC 16	YMC 17	Eclipse	Discovery	SB-300	SB-100	SB-90	YMC 15	Inertsil	Symmetry
YMC 16	0.00	0.00	16.67	16.67	33.33	50.00	50.00	33.33	50.00	66.67
YMC 17	0.00	0.00	16.67	16.67	33.33	50.00	50.00	33.33	50.00	66.67
Eclipse	16.67	16.67	0.00	33.33	33.33	33.33	33.33	50.00	50.00	66.67
Discovery	16.67	16.67	33.33	0.00	33.33	50.00	50.00	33.33	50.00	50.00
SB-300	33.33	33.33	33.33	33.33	0.00	33.33	33.33	66.67	66.67	50.00
SB-100	50.00	50.00	33.33	50.00	33.33	0.00	0.00	66.67	66.67	33.33
SB-90	50.00	50.00	33.33	50.00	33.33	0.00	0.00	66.67	66.67	33.33
YMC 15	33.33	33.33	50.00	33.33	66.67	66.67	66.67	0.00	16.67	50.00
Inertsil	50.00	50.00	50.00	50.00	66.67	66.67	66.67	16.67	0.00	33.33
Symmetry	66.67	66.67	66.67	50.00	50.00	33.33	33.33	50.00	33.33	0.00

\* Comparison with One VArIable at a Time: all columns were selected as a reference column once and only once.

**Table S4d** Collection of GPCM(CE-PW)-COVAT\* scores based on HSM data

	Eclipse	YMC 16	YMC 17	Discovery	SB-100	SB-90	SB-300	YMC 15	Inertsil	Symmetry
Eclipse	0.00	4.52	4.52	20.60	31.19	31.19	31.43	33.30	51.28	66.58
YMC 16	17.78	0.00	0.00	10.26	40.04	40.04	31.40	23.86	46.15	66.67
YMC 17	17.78	0.00	0.00	10.26	40.04	40.04	31.40	23.86	46.15	66.67
Discovery	26.72	4.62	4.62	0.00	53.37	53.37	31.43	33.40	51.28	66.48
SB-100	26.72	39.97	39.97	61.58	0.00	0.00	31.43	66.61	51.28	28.64
SB-90	26.72	39.97	39.97	61.58	0.00	0.00	31.43	66.61	51.28	28.64
SB-300	26.72	40.02	40.02	20.60	31.19	31.19	0.00	66.67	66.67	28.59
YMC 15	40.07	31.18	31.18	46.24	66.67	66.67	66.67	0.00	0.09	47.62
Inertsil	62.05	39.92	39.92	61.47	53.27	53.27	66.53	9.63	0.00	28.69
Symmetry	66.67	66.67	66.67	66.67	40.09	40.09	31.44	57.03	46.09	0.00

\* Comparison with One VArIable at a Time: all columns were selected as a reference column once and only once.

**Table S5a** Distances of chromatographic columns compared to the VARC.

<b>Column</b>	<b>Fs</b>	<b>EUC</b>	<b>MNH</b>	<b>CHD</b>	<b>COR</b>	<b>SPR</b>	<b>KNT</b>	<b>GPCM</b>	<b>SRD</b>	<b>COS</b>
<i>Based on primary retention data</i>										
Inertsil	-	9.9	80	1.85	0.0101	0.0032	0.0301	3.33	2.58	0.021
Symmetry	-	5.2	39	1.51	0.0042	0.0042	0.0353	3.33	3.21	0.005
SB-100	-	3.7	22	1.58	0.0025	0.0021	0.0256	3.06	2.14	0.005
SB-90	-	3.9	24	1.78	0.0024	0.0020	0.0258	3.07	2.23	0.007
SB-300	-	19.7	159	2.61	0.0082	0.0092	0.0668	5.17	5.17	0.273
Eclipse	-	2.5	18	0.82	0.0009	0.0021	0.0247	3.06	2.23	0.002
YMC 15	-	3.6	29	0.56	0.0010	0.0010	0.0131	0.99	1.25	0.003
YMC 16	-	2.9	23	0.67	0.0006	0.0007	0.0111	0.98	0.98	0.002
YMC 17	-	3.7	30	0.87	0.0006	0.0010	0.0131	0.99	1.25	0.004
Discovery	-	9.3	74	1.61	0.0058	0.0050	0.0419	4.11	3.57	0.049
<b>Column</b>	<b>Fs</b>	<b>EUC</b>	<b>MNH</b>	<b>CHD</b>	<b>COR</b>	<b>SPR</b>	<b>KNT</b>	<b>GPCM</b>	<b>SRD</b>	<b>COS</b>
<i>Based on HSM selectivity column parameters</i>										
Inertsil	3.24	2.43	4.61	2.10	0.0331	0.0000	0.0000	0.00	0.00	0.0612
Symmetry	1.98	2.84	5.54	2.00	0.0129	0.4000	0.6000	45.7	33.3	0.0200
SB-100	1.72	2.01	3.57	1.76	0.0328	0.8000	0.8000	51.3	66.7	0.0395
SB-90	1.61	2.43	4.32	1.71	0.0318	0.8000	0.8000	51.3	66.7	0.0384
SB-300	2.39	4.19	8.66	2.56	0.0182	1.0000	0.8000	66.7	66.7	0.0414
Eclipse	0.61	1.47	2.65	1.04	0.0021	0.7000	0.8000	51.3	50.0	0.0017
YMC 15	1.12	1.11	2.05	0.86	0.0070	0.1000	0.2000	1.10	16.7	0.0129
YMC 16	0.73	1.08	2.01	0.83	0.0070	0.6000	0.6000	46.0	50.0	0.0081
YMC 17	0.76	0.99	1.79	0.86	0.0079	0.6000	0.6000	46.0	50.0	0.0088
Discovery	1.92	1.73	3.35	1.18	0.0334	0.7000	0.8000	51.3	50.0	0.0267

**Table S5b** Similarity measures of chromatographic columns calculated from distances (VARC was the reference).

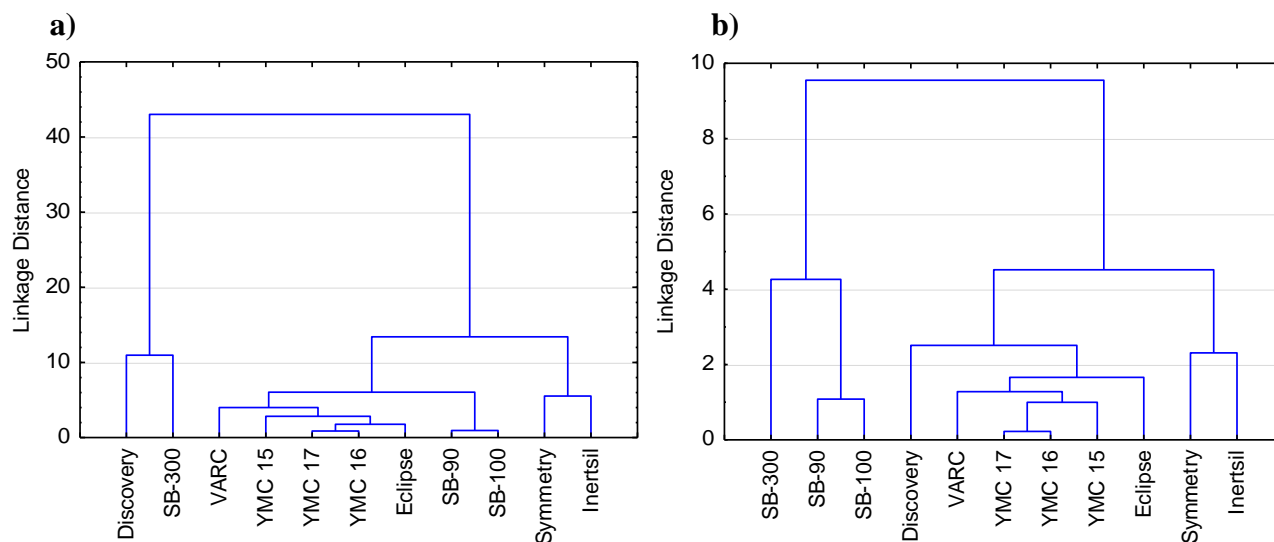
Column	Fs <sup>a</sup>	EUC <sup>a</sup>	MNH <sup>a</sup>	CHD <sup>a</sup>	COR <sup>b</sup>	SPR <sup>b</sup>	KNT <sup>b</sup>	GPCM <sup>a</sup>	SRD <sup>a</sup>	COS <sup>b</sup>
<i>Based on primary retention data</i>										
Inertsil	-	0.092	0.012	0.351	0.858	0.921	0.757	0.231	0.279	0.958
Symmetry	-	0.161	0.025	0.399	0.909	0.909	0.737	0.231	0.238	0.990
SB-100	-	0.215	0.044	0.388	0.930	0.935	0.775	0.247	0.319	0.989
SB-90	-	0.203	0.040	0.360	0.930	0.937	0.774	0.246	0.310	0.986
SB-300	-	0.048	0.006	0.277	0.872	0.864	0.641	0.162	0.162	0.528
Eclipse	-	0.284	0.051	0.549	0.957	0.935	0.779	0.246	0.310	0.996
YMC 15	-	0.219	0.034	0.641	0.955	0.955	0.839	0.502	0.445	0.993
YMC 16	-	0.253	0.041	0.599	0.966	0.961	0.852	0.505	0.505	0.995
YMC 17	-	0.211	0.033	0.534	0.965	0.956	0.839	0.503	0.445	0.992
Discovery	-	0.097	0.013	0.383	0.893	0.900	0.714	0.196	0.219	0.904
Column	Fs <sup>a</sup>	EUC <sup>a</sup>	MNH <sup>a</sup>	CHD <sup>a</sup>	COR <sup>b</sup>	SPR <sup>b</sup>	KNT <sup>b</sup>	GPCM <sup>a</sup>	SRD <sup>a</sup>	COS <sup>b</sup>
<i>Based on HSM selectivity column parameters</i>										
Inertsil	0.236	0.291	0.178	0.322	0.745	1.000	1.000	1.000	1.000	0.881
Symmetry	0.336	0.260	0.153	0.333	0.840	0.200	0.083	0.021	0.029	0.960
SB-100	0.367	0.332	0.219	0.363	0.746	0.020	0.020	0.019	0.015	0.922
SB-90	0.383	0.291	0.188	0.369	0.750	0.020	0.020	0.019	0.015	0.925
SB-300	0.295	0.193	0.103	0.281	0.810	0.000	0.020	0.015	0.015	0.919
Eclipse	0.623	0.405	0.274	0.490	0.935	0.046	0.020	0.019	0.020	0.997
YMC 15	0.471	0.474	0.328	0.538	0.882	0.564	0.400	0.486	0.057	0.974
YMC 16	0.577	0.482	0.333	0.547	0.882	0.083	0.083	0.021	0.020	0.984
YMC 17	0.569	0.502	0.359	0.539	0.875	0.083	0.083	0.021	0.020	0.983
Discovery	0.343	0.366	0.230	0.459	0.744	0.046	0.020	0.019	0.020	0.947

a Converted from the distances,  $d$ , according to the transformation function:  $S = 1/(1 + d)$

b Converted from the distances,  $d$ , according to the transformation function:  $S = 1 - |d|$

**Table S6** Comparison of similarity measures; List of SRD score values for standardized (STD), range scaled (RNG) and ranked (RNK) data; Measures associated with primary retention data and HSM selectivity parameters are denoted with *ret* and *HSM* respectively.

<b>STD</b>		<b>SCL</b>		<b>RNK</b>	
Similarity measure	Score	Similarity measure	Score	Similarity measure	Score
KNT_ret	14.0	KNT_ret	10.0	KNT_ret	10.0
GPCM_ret	20.0	GPCM_ret	15.0	GPCM_ret	16.0
SRD_ret	20.0	COS_ret	15.0	SRD_ret	16.0
EUC_HSM	24.0	SRD_ret	17.5	COS_ret	16.0
MNH_HSM	24.0	EUC_HSM	20.0	CHD_ret	20.0
CHD_ret	24.0	MNH_HSM	20.0	SPR_ret	20.0
SPR_ret	24.0	EUC_ret	20.0	EUC_HSM	24.0
COS_ret	24.0	CHD_ret	20.0	MNH_HSM	24.0
CHD_HSM	28.0	SPR_ret	20.0	CHD_HSM	24.0
Fs	32.0	CHD_HSM	25.0	EUC_ret	24.0
EUC_ret	32.0	COR_ret	25.0	COR_ret	24.0
COR_ret	32.0	Fs	35.0	Fs	32.0
COR_HSM	40.0	COR_HSM	35.0	COR_HSM	32.0
COS_HSM	40.0	COS_HSM	35.0	COS_HSM	32.0
GPCM_HSM	42.0	MNH_ret	35.0	MNH_ret	40.0
KNT_HSM	44.0	GPCM_HSM	47.5	GPCM_HSM	46.0
SPR_HSM	46.0	SPR_HSM	52.5	KNT_HSM	48.0
MNH_ret	48.0	KNT_HSM	52.5	SPR_HSM	50.0
SRD_HSM	54.0	SRD_HSM	60.0	SRD_HSM	58.0



**Figure S1** HCA of chromatographic columns based on standardized retention factors of compounds (a) and standardized HSM parameters (b)

## Reference

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