

**Table S1.** Experimental retention data,  $t_R$  (exp) in min, of test solutes obtained on the Kinetex 5 $\mu$ m EVO C18 column and under isocratic and linear gradient conditions in different eluent pHs modified with ACN or MeOH.

Eluent pH 2 modified with ACN								
solutes	isocratic runs with different $\phi_{ACN}$				linear $\phi_{ACN}$ -gradients from $\phi_0 = 0.3$ to $\phi_f = 0.5$ with different gradient durations, $t_G$ (min)			
	0.3	0.4	0.5	0.37 (opt.)	2.5	5	10	6.5 (opt.)
p-CA	2.175	2.054	1.943	2.094	2.164	2.174	2.175	2.245
p-BA	2.596	2.356	2.124	2.427	2.557	2.587	2.588	2.698
3-BP	7.038	3.861	2.613	4.450	4.238	4.963	5.638	5.326
2B-4NP	7.912	3.997	2.613	4.692	4.319	5.145	5.971	5.578
B	8.951	5.246	3.443	5.991	4.963	5.920	6.887	6.413
4B-2NP	12.75	6.051	3.549	7.259	5.336	6.463	7.984	7.168
2,4-DBP	15.27	6.298	3.534	7.773	5.336	6.604	8.357	7.380
T	16.73	8.065	4.571	9.675	6.263	7.440	9.444	8.296
Eluent pH 3 modified with ACN								
solutes	isocratic runs with different $\phi_{ACN}$				linear $\phi_{ACN}$ -gradients from $\phi_0 = 0.3$ to $\phi_f = 0.5$ with different gradient durations, $t_G$ (min)			
	0.3	0.4	0.5	0.365 (opt.)	5	10	20	6.5 (opt.)
p-CA	4.118	3.060	2.376	3.373	3.806	3.957	4.027	3.846
p-BA	5.074	3.463	2.557	3.926	4.370	4.671	4.863	4.470
3-BP	7.148	3.906	2.638	4.711	5.045	5.759	6.333	5.296
2B-4NP	8.004	4.032	2.617	4.983	5.216	6.081	6.826	5.528
B	9.091	5.296	3.458	6.333	6.001	7.018	7.853	6.373
4B-2NP	12.95	6.131	3.584	7.803	6.545	8.115	9.665	7.108
2,4-DBP	15.52	6.393	3.564	8.437	6.686	8.487	10.43	7.320
T	17.02	8.155	4.596	10.40	7.531	9.575	11.76	8.226
Eluent pH 5 modified with ACN								
solutes	isocratic runs with different $\phi_{ACN}$				linear $\phi_{ACN}$ -gradients from $\phi_0 = 0.3$ to $\phi_f = 0.5$ with different gradient durations, $t_G$ (min)			
	0.3	0.4	0.5	0.365 (opt.)	2.5	5 (opt.)	10	
2B-4NP	5.105	3.057	2.336	3.363	3.705	4.118	4.480	
p-CA	5.382	3.403	2.550	3.846	3.926	4.379	4.772	
p-BA	6.388	3.790	2.648	4.356	4.198	4.812	5.356	
3-BP	7.199	3.901	2.608	4.621	4.289	5.014	5.709	
B	9.132	5.306	3.458	6.212	5.014	5.970	6.957	
4B-2NP	11.93	5.762	3.443	7.048	5.185	6.313	7.722	
2,4-DBP	15.69	6.384	3.880	8.206	5.407	6.655	8.447	
T	17.14	8.175	4.581	10.16	6.333	7.511	9.544	

Eluent pH 7 modified with ACN								
solutes	isocratic runs with different $\varphi_{ACN}$				linear $\varphi_{ACN}$ -gradients from $\varphi_0 = 0.3$ to $\varphi_f = 0.5$ with different gradient durations, $t_G$ (min)			
	0.3	0.4	0.5	0.37 (opt.)	2.5	5	10	6 (opt.)
2B-4NP	1.980	1.656	1.596	1.702	1.953	1.963	1.963	1.963
4B-2NP	3.366	2.306	1.827	2.426	2.960	3.111	3.191	3.141
p-CA	5.356	3.392	2.467	3.765	3.906	4.380	4.762	4.470
p-BA	6.343	3.770	2.648	4.259	4.168	4.803	5.357	4.933
3-BP	7.050	3.916	2.628	4.480	4.248	4.984	5.689	5.155
B	9.041	5.346	3.443	6.051	4.973	5.951	6.957	6.202
2,4-DBP	13.81	6.056	3.443	7.309	5.185	6.444	8.055	6.816
T	16.92	8.225	4.591	9.806	6.262	7.491	9.525	7.934

Eluent pH 9 modified with ACN								
solutes	isocratic runs with different $\varphi_{ACN}$				linear $\varphi_{ACN}$ -gradients from $\varphi_0 = 0.3$ to $\varphi_f = 0.5$ with different gradient durations, $t_G$ (min)			
	0.3	0.4			10	20		
2B-4NP	1.682	1.294			1.682	1.701		
4B-2NP	1.833	1.621			1.822	1.862		
3-BP	4.701	2.315			4.138	4.782		
p-CA	5.291	3.332			4.732	4.963		
2,4-DBP	6.004	3.544			5.104	5.608		
p-BA	6.258	3.705			5.316	5.700		
B	8.941	5.195			6.916	7.702		
T	16.71	7.984			9.494	11.56		

Eluent pH 3 modified with MeOH								
solutes	isocratic runs with different $\varphi_{MeOH}$				linear $\varphi_{MeOH}$ -gradients from $\varphi_0 = 0.4$ to $\varphi_f = 0.6$ with different gradient durations, $t_G$ (min)			
	0.4	0.5	0.6	0.575 (opt.)	5	10	15	20 (opt.)
p-CA	3.856	2.839	2.185	2.330	3.584	3.705	3.765	3.806
p-BA	4.798	3.252	2.366	2.557	4.158	4.450	4.561	4.631
3-BP	8.715	4.576	2.839	3.164	5.578	6.564	7.088	7.410
B	8.947	5.372	3.458	3.867	5.951	7.050	7.551	7.863
2B-4NP	9.991	5.120	3.070	3.461	6.031	7.138	7.793	8.205
4B-2NP	14.80	7.260	4.047	4.639	7.088	8.980	10.08	10.83
2,4-DBP	23.96	9.716	4.711	5.569	8.035	10.60	12.45	13.79
T	18.95	9.444	5.115	5.932	8.095	10.40	11.91	12.95