Electronic Supplementary Material (ESI) for Analytical Methods.

Supplementary information

Manuscript Title: Application of multi-location peak parking approach for calculation of second dimensional retention indices for improved volatile compound identification with cryogen-free comprehensive heart cut two-dimensional gas chromatography

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Table S-1. The cyclic multiple H/C events with the 0.2 min H/C window consisting of 25 runs.

Run 1		Run 2		Run 3		Run 4		Run 5		Run 6		Run 7		Run 8		Run 9		Run 10	
8.5	On	8.7	On	8.9	On	9.1	On	9.3	On	9.5	On	9.7	On	9.9	On	10.1	On	10.3	On
8.7	Off	8.9	Off	9.1	Off	9.3	Off	9.5	Off	9.7	Off	9.9	Off	10.1	Off	10.3	Off	10.5	Off
13.5	On	13.7	On	13.9	On	14.1	On	14.3	On	14.5	On	14.7	On	14.9	On	15.1	On	15.3	On
13.7	Off	13.9	Off	14.1	Off	14.3	Off	14.5	Off	14.7	Off	14.9	Off	15.1	Off	15.3	Off	15.5	Off
18.5	On	18.7	On	18.9	On	19.1	On	19.3	On	19.5	On	19.7	On	19.9	On	20.1	On	20.3	On
18.7	Off	18.9	Off	19.1	Off	19.3	Off	19.5	Off	19.7	Off	19.9	Off	20.1	Off	20.3	Off	20.5	Off
23.5	On	23.7	On	23.9	On	24.1	On	24.3	On	24.5	On	24.7	On	24.9	On	25.1	On	25.3	On
23.7	Off	23.9	Off	24.1	Off	24.3	Off	24.5	Off	24.7	Off	24.9	Off	25.1	Off	25.3	Off	25.5	Off
28.5	On	28.7	On	28.9	On	29.1	On	29.3	On	29.5	On	29.7	On	29.9	On	30.1	On	30.3	On
28.7	Off	28.9	Off	29.1	Off	29.3	Off	29.5	Off	29.7	Off	29.9	Off	30.1	Off	30.3	Off	30.5	Off
33.5	On	33.7	On	33.9	On	34.1	On	34.3	On	34.5	On	34.7	On	34.9	On	35.1	On	35.3	On
33.7	Off	33.9	Off	34.1	Off	34.3	Off	34.5	Off	34.7	Off	34.9	Off	35.1	Off	35.3	Off	35.5	Off
38.5	On	38.7	On	38.9	On	39.1	On	39.3	On	39.5	On	39.7	On	39.9	On	40.1	On	40.3	On
38.7	Off	38.9	Off	39.1	Off	39.3	Off	39.5	Off	39.7	Off	39.9	Off	40.1	Off	40.3	Off	40.5	Off
43.5	On	43.7	On	43.9	On	44.1	On	44.3	On	44.5	On	44.7	On	44.9	On	45.1	On	45.3	On
43.7	Off	43.9	Off	44.1	Off	44.3	Off	44.5	Off	44.7	Off	44.9	Off	45.1	Off	45.3	Off	45.5	Off
48.5	On	48.7	On	48.9	On	49.1	On	49.3	On	49.5	On	49.7	On	49.9	On	50.1	On	50.3	On
48.7	Off	48.9	Off	49.1	Off	49.3	Off	49.5	Off	49.7	Off	49.9	Off	50.1	Off	50.3	Off	50.5	Off

Run 11		Run 12		Run 13		Run 14		Run 15		Run 16		Run 17		Run 18		Run 19		Run 20	
10.5	On	10.7	On	10.9	On	11.1	On	11.3	On	11.5	On	11.7	On	11.9	On	12.1	On	12.3	On
10.7	Off	10.9	Off	11.1	Off	11.3	Off	11.5	Off	11.7	Off	11.9	Off	12.1	Off	12.3	Off	12.5	Off
15.5	On	15.7	On	15.9	On	16.1	On	16.3	On	16.5	On	16.7	On	16.9	On	17.1	On	17.3	On
15.7	Off	15.9	Off	16.1	Off	16.3	Off	16.5	Off	16.7	Off	16.9	Off	17.1	Off	17.3	Off	17.5	Off
20.5	On	20.7	On	20.9	On	21.1	On	21.3	On	21.5	On	21.7	On	21.9	On	22.1	On	22.3	On
20.7	Off	20.9	Off	21.1	Off	21.3	Off	21.5	Off	21.7	Off	21.9	Off	22.1	Off	22.3	Off	22.5	Off
25.5	On	25.7	On	25.9	On	26.1	On	26.3	On	26.5	On	26.7	On	26.9	On	27.1	On	27.3	On
25.7	Off	25.9	Off	26.1	Off	26.3	Off	26.5	Off	26.7	Off	26.9	Off	27.1	Off	27.3	Off	27.5	Off
30.5	On	30.7	On	30.9	On	31.1	On	31.3	On	31.5	On	31.7	On	31.9	On	32.1	On	32.3	On
30.7	Off	30.9	Off	31.1	Off	31.3	Off	31.5	Off	31.7	Off	31.9	Off	32.1	Off	32.3	Off	32.5	Off
35.5	On	35.7	On	35.9	On	36.1	On	36.3	On	36.5	On	36.7	On	36.9	On	37.1	On	37.3	On
35.7	Off	35.9	Off	36.1	Off	36.3	Off	36.5	Off	36.7	Off	36.9	Off	37.1	Off	37.3	Off	37.5	Off
40.5	On	40.7	On	40.9	On	41.1	On	41.3	On	41.5	On	41.7	On	41.9	On	42.1	On	42.3	On
40.7	Off	40.9	Off	41.1	Off	41.3	Off	41.5	Off	41.7	Off	41.9	Off	42.1	Off	42.3	Off	42.5	Off
45.5	On	45.7	On	45.9	On	46.1	On	46.3	On	46.5	On	46.7	On	46.9	On	47.1	On	47.3	On
45.7	Off	45.9	Off	46.1	Off	46.3	Off	46.5	Off	46.7	Off	46.9	Off	47.1	Off	47.3	Off	47.5	Off
50.5	On	50.7	On	50.9	On	51.1	On	51.3	On	51.5	On	51.7	On	51.9	On	52.1	On	52.3	On
50.7	Off	50.9	Off	51.1	Off	51.3	Off	51.5	Off	51.7	Off	51.9	Off	52.1	Off	52.3	Off	52.5	Off

Run 21		Run 22		Run 23		Run 24		Run 25	
12.5	On	12.7	On	12.9	On	13.1	On	13.3	On
12.7	Off	12.9	Off	13.1	Off	13.3	Off	13.5	Off
17.5	On	17.7	On	17.9	On	18.1	On	18.3	On
17.7	Off	17.9	Off	18.1	Off	18.3	Off	18.5	Off
22.5	On	22.7	On	22.9	On	23.1	On	23.3	On
22.7	Off	22.9	Off	23.1	Off	23.3	Off	23.5	Off
27.5	On	27.7	On	27.9	On	28.1	On	28.3	On
27.7	Off	27.9	Off	28.1	Off	28.3	Off	28.5	Off
32.5	On	32.7	On	32.9	On	33.1	On	33.3	On
32.7	Off	32.9	Off	33.1	Off	33.3	Off	33.5	Off
37.5	On	37.7	On	37.9	On	38.1	On	38.3	On
37.7	Off	37.9	Off	38.1	Off	38.3	Off	38.5	Off
42.5	On	42.7	On	42.9	On	43.1	On	43.3	On
42.7	Off	42.9	Off	43.1	Off	43.3	Off	43.5	Off
47.5	On	47.7	On	47.9	On	48.1	On	48.3	On
47.7	Off	47.9	Off	48.1	Off	48.3	Off	48.5	Off
52.5	On	52.7	On	52.9	On	53.1	On	53.3	On
52.7	Off	52.9	Off	53.1	Off	53.3	Off	53.5	Off

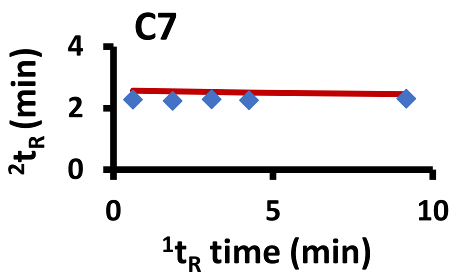
Table S-2. The multi-location peak parking for the construction of *n*-alkane isovolatility curves.

No.	Run No.	Injection	Temperature program
Set 1	Parking	*n*-alkane standards	35°C → 100°C with ramp rate 20°C/min
	Run-off	blank vial	The same with perfume sample in off mode
	Parking	*n*-alkane standards	35°C → 100°C with ramp rate 20°C/min
	Run-on	blank vial	The same with perfume sample in on mode
Set 2	Parking	*n*-alkane standards	35°C → 120°C with ramp rate 20°C/min
	Run-off	blank vial	The same with perfume sample in off mode
	Parking	*n*-alkane standards	35°C → 120°C with ramp rate 20°C/min
	Run-on	blank vial	The same with perfume sample in on mode
Set 3	Parking	*n*-alkane standards	35°C → 140°C with ramp rate 20°C/min
	Run-off	blank vial	The same with perfume sample in off mode
	Parking	*n*-alkane standards	35°C → 140°C with ramp rate 20°C/min
	Run-on	blank vial	The same with perfume sample in on mode
Set 4	Parking	*n*-alkane standards	35°C → 160°C with ramp rate 20°C/min
	Run-off	blank vial	The same with perfume sample in off mode
	Parking	*n*-alkane standards	35°C → 160°C with ramp rate 20°C/min
	Run-on	blank vial	The same with perfume sample in on mode
Set 5	Parking	*n*-alkane standards	35°C → 180°C with ramp rate 20°C/min
	Run-off	blank vial	The same with perfume sample in off mode
	Parking	*n*-alkane standards	35°C → 180°C with ramp rate 20°C/min
	Run-on	blank vial	The same with perfume sample in on mode
Set 6	Parking	*n*-alkane standards	35°C → 200°C with ramp rate 20°C/min
	Run-off	blank vial	The same with perfume sample in off mode
	Parking	*n*-alkane standards	35°C → 200°C with ramp rate 20°C/min
	Run-on	blank vial	The same with perfume sample in on mode
Set 7	Parking	*n*-alkane standards	35°C → 220°C with ramp rate 20°C/min
	Run-off	blank vial	The same with perfume sample in off mode
	Parking	*n*-alkane standards	35°C → 220°C with ramp rate 20°C/min
	Run-on	blank vial	The same with perfume sample in on mode
Set 8	Parking	*n*-alkane standards	35°C → 240°C with ramp rate 20°C/min
	Run-off	blank vial	The same with perfume sample in off mode
	Parking	*n*-alkane standards	35°C → 240°C with ramp rate 20°C/min
	Run-on	blank vial	The same with perfume sample in on mode
Set 9	Parking	*n*-alkane standards	35°C → 240°C with ramp rate 20°C/min and hold 2 min
	Run-off	blank vial	The same with perfume sample in off mode
	Parking	*n*-alkane standards	35°C → 240°C with ramp rate 20°C/min and hold 2 min
	Run-on	blank vial	The same with perfume sample in on mode
Set 10	Parking	*n*-alkane standards	35°C → 240°C with ramp rate 20°C/min and hold 4 min
	Run-off	blank vial	The same with perfume sample in off mode

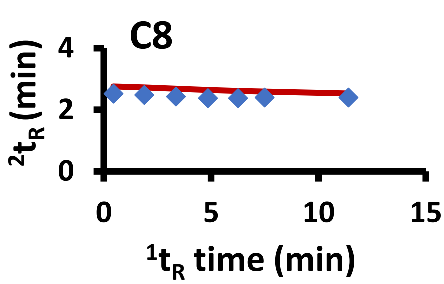
	Parking	*n*-alkane standards	35°C → 240°C with ramp rate 20°C/min and hold 4 min
	Run-on	blank vial	The same with perfume sample in on mode
Set 11	Parking	*n*-alkane standards	35°C → 240°C with ramp rate 20°C/min and hold 6 min
	Run-off	blank vial	The same with perfume sample in off mode
	Parking	*n*-alkane standards	35°C → 240°C with ramp rate 20°C/min and hold 6 min
	Run-on	blank vial	The same with perfume sample in on mode
Set 12	Parking	*n*-alkane standards	35°C → 240°C with ramp rate 20°C/min and hold 8 min
	Run-off	blank vial	The same with perfume sample in off mode
	Parking	*n*-alkane standards	35°C → 240°C with ramp rate 20°C/min and hold 8 min
	Run-on	blank vial	The same with perfume sample in on mode
Set 13	Parking	*n*-alkane standards	35°C → 240°C with ramp rate 20°C/min and hold 10 min
	Run-off	blank vial	The same with perfume sample in off mode
	Parking	*n*-alkane standards	35°C → 240°C with ramp rate 20°C/min and hold 10 min
	Run-on	blank vial	The same with perfume sample in on mode
Set 14	Parking	*n*-alkane standards	35°C → 240°C with ramp rate 20°C/min and hold 12 min
	Run-off	blank vial	The same with perfume sample in off mode
	Parking	*n*-alkane standards	35°C → 240°C with ramp rate 20°C/min and hold 12 min
	Run-on	blank vial	The same with perfume sample in on mode
Set 15	Parking	*n*-alkane standards	35°C → 240°C with ramp rate 20°C/min and hold 14 min
	Run-off	blank vial	The same with perfume sample in off mode
	Parking	*n*-alkane standards	35°C → 240°C with ramp rate 20°C/min and hold 14 min
	Run-on	blank vial	The same with perfume sample in on mode
Set 16	Parking	*n*-alkane standards	35°C → 240°C with ramp rate 20°C/min and hold 16 min
	Run-off	blank vial	The same with perfume sample in off mode
	Parking	*n*-alkane standards	35°C → 240°C with ramp rate 20°C/min and hold 16 min
	Run-on	blank vial	The same with perfume sample in on mode

Table S-3. The fitting curve parameters of the isovolatility curves of *n*-alkanes.

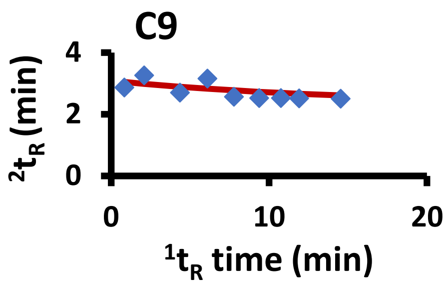
p1	p2	p3	p4	p5
-0.00385456	-0.61813	-26.47746735	5.555882	-3.952407
C7 (Experimental $^{1}t_R$ (min))	Experimental $^{1}t_R$ (min)	Calculated $^{2}t_R$ (min)	Difference^2 (min^2)	
9.177	2.307	2.449	0.020084	
4.251	2.264	2.508	0.059293	
3.08	2.286	2.524	0.0567	
1.855	2.234	2.543	0.095348	
0.618	2.28	2.563	0.080138	



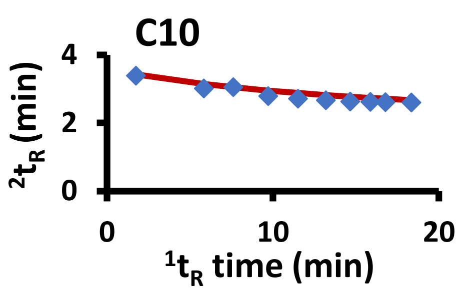
p1	p2	p3	p4	p5
-0.00385	-0.61813	-26.4775	5.555882	-3.95241
C8 (Experimental $^{1}t_R$ (min))	Experimental $^{1}t_R$ (min)	Calculated $^{2}t_R$ (min)	Difference^2 (min^2)	
11.396	2.404	2.529	0.015683	
7.497	2.398	2.595	0.038875	
6.252	2.384	2.620	0.0556	
4.857	2.383	2.650	0.071183	
3.358	2.435	2.685	0.062597	
1.882	2.485	2.724	0.056935	
0.454	2.529	2.765	0.055486	



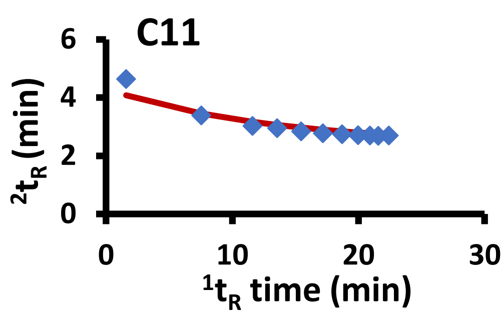
p1	p2	p3	p4	p5
-0.00385	-0.61813	-26.4775	5.555882	-3.95241
C9 (Experimental ^1t_R (min))	Experimental ^1t_R (min)	Calculated ^2t_R (min)	Difference^2 (min^2)	
14.545	2.497	2.607	0.012017	
11.912	2.508	2.663	0.024083	
10.769	2.527	2.691	0.026861	
9.377	2.518	2.728	0.043919	
7.788	2.565	2.774	0.043609	
6.108	3.15	2.828	0.103364	
4.363	2.696	2.892	0.038596	
2.111	3.262	2.988	0.075274	
0.85	2.867	3.048	0.032811	



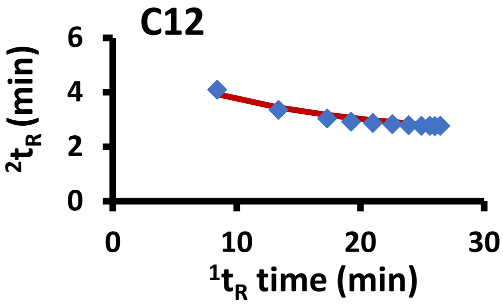
p1	p2	p3	p4	p5
-0.00385	-0.61813	-26.4775	5.555881842	-3.95241
C10 (Experimental ^1t_R (min))	Experimental ^1t_R (min)	Calculated ^2t_R (min)	Difference^2 (min^2)	
18.337	2.602	2.673	0.005020066	
16.779	2.606	2.712	0.011274317	
15.874	2.619	2.737	0.013913933	
14.664	2.623	2.773	0.022357936	
13.181	2.664	2.820	0.024433453	
11.513	2.712	2.880	0.028313731	
9.708	2.786	2.954	0.028098746	
7.62	3.051	3.051	1.12627E-07	
5.826	3.007	3.148	0.019944698	
1.751	3.388	3.425	0.001337495	



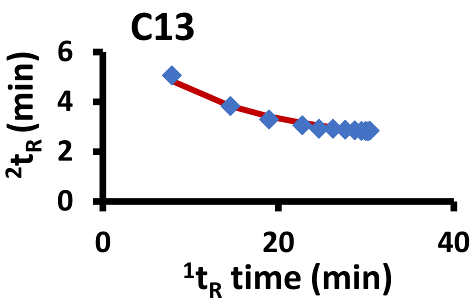
p1	p2	p3	p4	p5
-0.00385	-0.61813	-26.477467	5.555881842	-3.95241
C11 (Experimental ^1t_R (min))	Experimental ^1t_R (min)	Calculated ^2t_R (min)	Difference^2 (min^2)	
22.397	2.69	2.727	0.001401442	
21.549	2.683	2.751	0.004691942	
20.912	2.698	2.770	0.005256092	
19.961	2.703	2.800	0.009495367	
18.692	2.732	2.844	0.012450379	
17.167	2.773	2.901	0.016318598	
15.447	2.836	2.973	0.018800886	
13.543	2.95	3.065	0.013114085	
11.587	3.022	3.173	0.022771187	
7.532	3.382	3.457	0.00559798	
1.587	4.631	4.084	0.299661613	



p1	p2	p3	p4	p5
-0.00385	-0.61813	-26.4775	5.555882	-3.95241
C12 (Experimental ^1t_R (min))	Experimental ^1t_R (min)	Calculated ^2t_R (min)	Difference^2 (min^2)	
26.465	2.767	2.773	3.92E-05	
26.03	2.75	2.787	0.001354	
25.612	2.767	2.800	0.001102	
24.923	2.767	2.823	0.003151	
23.907	2.792	2.859	0.004492	
22.593	2.829	2.909	0.006465	
21.011	2.875	2.977	0.010339	
19.258	2.916	3.061	0.020979	
17.302	3.03	3.169	0.019223	
13.384	3.349	3.440	0.008263	
8.413	4.09	3.933	0.024682	

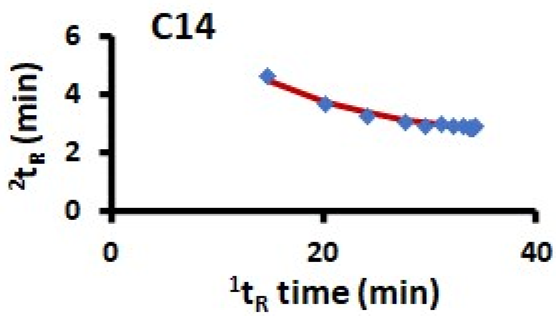


p1	p2	p3	p4	p5
-0.00385	-0.61813	-26.4775	5.555882	-3.95241
C13 (Experimental ^1t_R (min))	Experimental ^1t_R (min)	Calculated ^2t_R (min)	Difference^2 (min^2)	
30.416	2.832	2.813	0.000362	
30.197	2.813	2.820	5.37E-05	
29.947	2.82	2.829	7.88E-05	
29.469	2.826	2.846	0.000386	
28.703	2.849	2.874	0.00061	
27.611	2.874	2.916	0.001799	
26.22	2.92	2.976	0.003124	
24.617	2.919	3.052	0.017774	
22.724	3.05	3.155	0.011045	
18.937	3.29	3.411	0.014698	
14.514	3.821	3.827	3.45E-05	
7.83	5.062	4.842	0.048537	

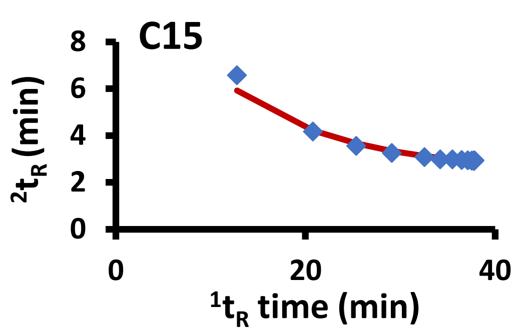


p1	p2	p3	p4	p5
-0.00385	-0.61813	-26.4774674	5.555882	-3.95241
14 (Experimental ^1t_R (min))	Experimental ^1t_R (min)	Calculated ^2t_R (min)	Difference^2 (min^2)	
34.207	2.889	2.848	0.001674	
34.095	2.874	2.852	0.000479	
33.946	2.881	2.858	0.000551	
33.639	2.88	2.869	0.000124	
33.086	2.901	2.890	0.000124	

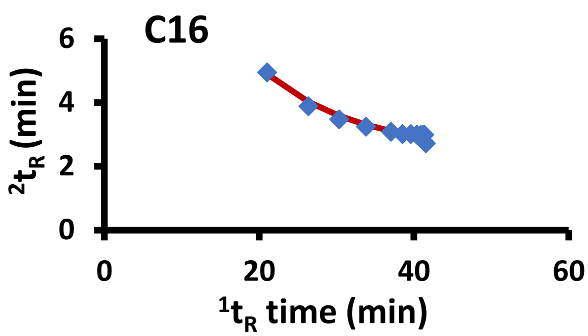
32.222	2.913	2.924	0.00013	
31.035	2.953	2.976	0.000507	
29.593	2.941	3.044	0.010569	
27.798	3.067	3.140	0.005281	
24.164	3.265	3.379	0.012977	
20.097	3.656	3.743	0.007493	
14.652	4.61	4.471	0.019421	



p1	p2	p3	p4	p5
-0.00385	-0.61813	-26.47746735	5.555882	-3.95241
C15 (Experimental ^1t_R (min))	Experimental ^1t_R (min)	Calculated ^2t_R (min)	Difference^2 (min^2)	
37.831	2.944	2.879	0.004161	
37.785	2.917	2.881	0.001278	
37.689	2.928	2.885	0.001856	
37.503	2.926	2.892	0.001148	
37.112	2.946	2.908	0.001478	
36.459	2.957	2.934	0.000515	
35.485	2.977	2.977	1.44E-07	
34.213	2.981	3.037	0.003091	
32.563	3.081	3.123	0.001788	
29.096	3.259	3.345	0.007391	
25.33	3.553	3.665	0.012615	
20.789	4.171	4.211	0.001604	
12.765	6.574	5.921	0.426483	

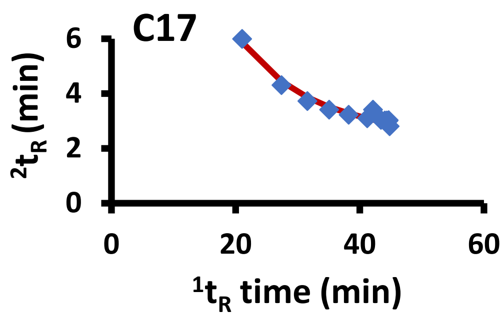


p1	p2	p3	p4	p5
-0.00385456	-0.61813	-26.47746735	5.555882	-3.952407
C16 (Experimental $^{1}t_{R}$ (min))	Experimental $^{1}t_{R}$ (min)	Calculated $^{2}t_{R}$ (min)	Difference^{2} (min^{2})	
41.312	2.985	2.907	0.006086	
41.523	2.723	2.899	0.030839	
41.234	2.971	2.910	0.003707	
41.114	2.976	2.915	0.003726	
40.859	2.979	2.925	0.002874	
40.38	2.988	2.946	0.001805	
39.604	3.007	2.980	0.000749	
38.518	3.008	3.031	0.000517	
37.032	3.083	3.108	0.000607	
33.778	3.244	3.309	0.004288	
30.311	3.473	3.589	0.013533	
26.353	3.883	4.023	0.019497	
21.007	4.944	4.901	0.001857	

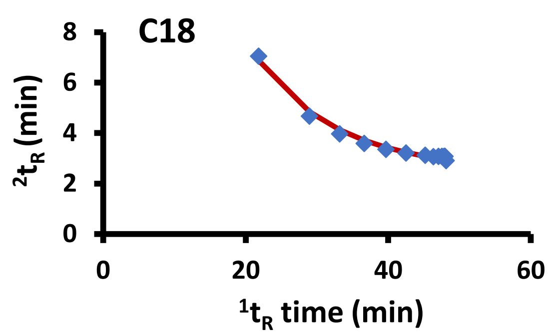


p1	p2	p3	p4	p5
-0.00385	-0.61813	-26.4775	5.555882	-3.95241
C17 (Experimental $^{1}t_{R}$ (min))	Experimental $^{1}t_{R}$ (min)	Calculated $^{2}t_{R}$ (min)	Difference^{2} (min^{2})	
44.67	3.026	2.930	0.009137	
44.851	2.812	2.923	0.012303	
44.627	3.007	2.932	0.005594	
44.557	3.002	2.935	0.00447	
44.379	3.01	2.943	0.004534	
44.043	3.021	2.957	0.004079	
43.437	3.042	2.984	0.003349	
42.163	3.408	3.045	0.131816	
41.226	3.102	3.093	7.3E-05	
38.24	3.229	3.273	0.001942	
35.08	3.409	3.514	0.011129	
31.603	3.725	3.862	0.0188	
27.433	4.309	4.439	0.01697	

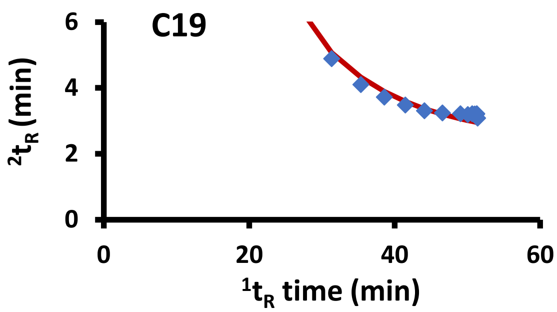
21.042	5.989	5.873	0.013437	



p1	p2	p3	p4	p5
-0.00385	-0.61813	-26.4775	5.555882	-3.95241
C18(Experimental ^1t_R (min))	Experimental ^1t_R (min)	Calculated ^2t_R (min)	Difference^2 (min^2)	
47.957	3.079	2.948	0.017113	
48.106	2.909	2.942	0.001077	
47.932	3.074	2.949	0.015561	
47.888	3.069	2.951	0.013888	
47.768	3.06	2.956	0.010742	
47.526	3.072	2.967	0.011029	
47.06	3.073	2.988	0.007229	
46.339	3.064	3.022	0.001773	
45.198	3.113	3.079	0.001129	
42.505	3.209	3.236	0.000747	
39.679	3.35	3.440	0.008122	
36.625	3.584	3.719	0.018171	
33.19	3.964	4.130	0.027412	
28.949	4.666	4.839	0.029976	
21.815	7.041	6.887	0.023651	



p1	p2	p3	p4	p5
-0.00385	-0.61813	-26.4775	5.555881842	-3.95241
C19 (Experimental $^{1}t_R$ (min))	Experimental $^{1}t_R$ (min)	Calculated $^{2}t_R$ (min)	Difference^2 (min^2)	
51.297	3.216	2.955	0.067920515	
51.412	3.085	2.950	0.018115089	
51.285	3.205	2.956	0.0620478	
51.255	3.199	2.957	0.058461319	
51.174	3.191	2.961	0.0530136044	
51.003	3.206	2.968	0.056502738	
50.662	3.212	2.984	0.052156212	
50.071	3.185	3.011	0.030240185	
49.061	3.211	3.061	0.022524899	
46.595	3.237	3.200	0.001401585	
44.094	3.308	3.370	0.003797763	
41.466	3.48	3.588	0.011769917	
38.605	3.72	3.887	0.027796827	
35.355	4.102	4.326	0.050142062	
31.35	4.882	5.073	0.036586598	
24.852	6.971	7.079	0.011609378	



p1	p2	p3	p4	p5
-0.00385	-0.61813	-26.477467	5.555881842	-3.95241
C20 (Experimental $^{1}t_R$ (min))	Experimental $^{1}t_R$ (min)	Calculated $^{2}t_R$ (min)	Difference^2 (min^2)	
54.668	3.4	2.953	0.199392299	
54.657	3.386	2.954	0.18667323	
54.643	3.381	2.955	0.181859391	
54.59	3.392	2.957	0.18935153	
54.471	3.385	2.962	0.178877604	
54.223	3.365	2.973	0.153620255	
53.741	3.348	2.995	0.124608823	
52.908	3.398	3.035	0.131916646	
50.746	3.387	3.150	0.056015542	
48.442	3.385	3.296	0.00789093	
46.131	3.401	3.471	0.004940149	
43.726	3.556	3.692	0.018364573	

41.121	3.791	3.985	0.037668597	
38.224	4.172	4.398	0.051251698	
34.767	4.759	5.053	0.086593158	
29.883	6.18	6.425	0.059844886	

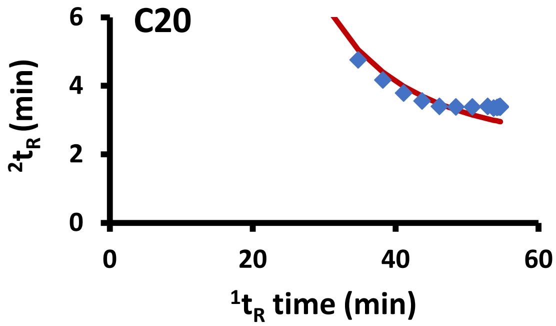


Table S-4. ^{2}I profile of standard compounds compared with the literature data.

Standard compound	Class	$^{1}t_{R}$ (min)	$^{2}t_{R}$ (min)	$^{2}I_{Cal}$	$^{2}I_{Lit}$	$^{2}I_{Lit}$ - $^{2}I_{Cal}$
Propanal	Aldehyde	8.6	3.5	831	799	-32
Methyl propanoate	Ester	10.8	3.8	922	905	-17
Methanol	Alcohol	12	3.5	882	894	11
2-Pentanone	Ketone	13.4	4.2	1016	981	-35
Hydroxyacetone	Alcohol & ketone	13.6	11.8	1285	1276	-9
3-Pentanone	Ketone	13.8	4. 2	1015	980	-35
Propyl acetate	Ester	15.2	3.8	992	973	-19
Hexanal	Aldehyde	15.4	4. 2	1042	1083	41
2-Hexanone	Ketone	20.4	3.9	1098	1106	7
Methyl pentanoate	Ester	22.2	3.6	1079	1085	6