GT053

GL Sciences Inc.

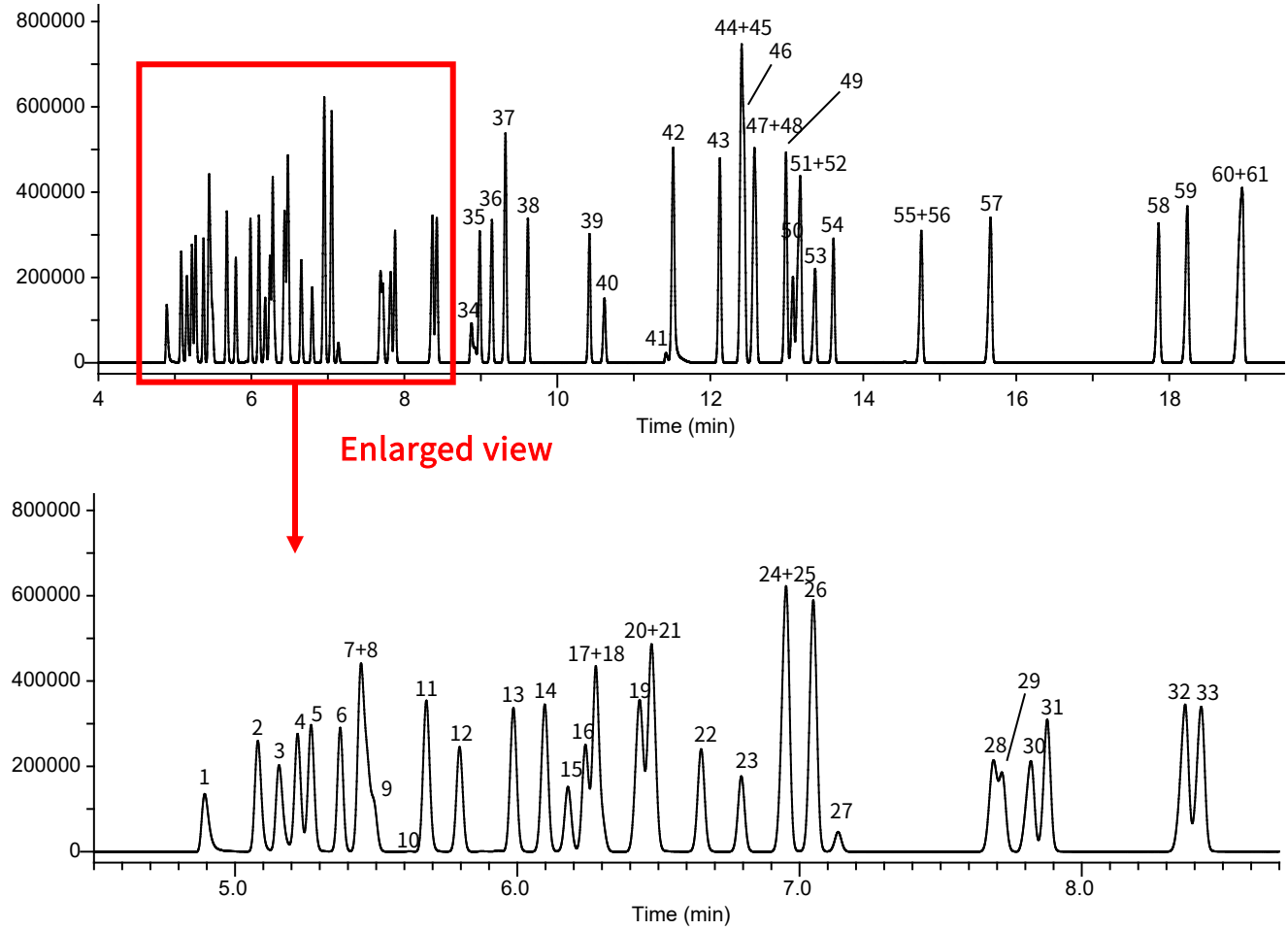
Analytical and Retention Index of 61 Components of Organic Solvents - Using InertCap 1

The retention index is a relatively representative index of the retention ratio of straight-chain alkanes and is used to study constituents based on the number of carbons in the molecule. It is one of the most useful pieces of information for qualitative analysis.

The retention index can be determined because in isothermal analysis the logarithm of the retention ratio for straight-chain alkanes is linearly related to the number of carbons, and the retention ratio is also linear to the number of carbons in thermal rise analysis.

In this report, InertCap 1 was used to determine the retention index of 61 components of organic solvents by isothermal and temperature-rise analysis.

Example: Measurement of standard



Conditions

System	: GC - FID
Column	: InertCap 1 0.25 mm I.D. x 60 m df = 0.25 µm
Col. Temp.	: 40 ˚C - 5 ˚C/min - 220 ˚C
Carrier Gas	: He 160 kPa
Injection 240 ℃	: Split flow 150 mL/min
Detection	: FID Range 10^0 240 ˚C
Sample Size	: Mixed evenly 0.2 µL

Chromatographic terms described above.

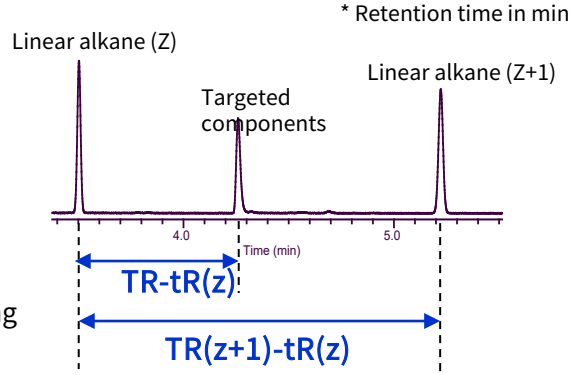
Only temperature was changed for isothermal analysis conditions.

Retention index in the temperature-raising analysis

Peak No.	Component	RI	RT	Peak No.	Component	RI	RT
1	Methanol	357	4.893	32	3-Methyl-1-butanol (Isoamyl alcohol)	715	8.343
2	Ethanol	426	5.077				
3	Acetonitrile	445	5.154	33	4-Methyl-2-pentanone (MIBK)	717	8.408
4	Acetone	460	5.218				
5	2-Propanol (Isopropyl alcohol)	471	5.264	34	N,N-Dimethylformamide	735	8.861
				35	Isobutyl acetate	739	8.975
6	Diethyl ether	497	5.369	36	1-Pentanol(Amyl alcohol)	745	9.118
7	tert-Butanol	506	5.438	37	Toluene	752	9.313
8	Methyl acetate	509	5.463	38	2-Hexanone(MBK)	763	9.601
9	Dichloromethane	512	5.488	39	n-Butyl acetate	795	10.407
10	Carbon disulfide	527	5.623	40	Tetrachloroethylene	802	10.608
11	1-Propanol	532	5.670	41	N,N-Dimethylacetamide	826	11.407
12	trans-1,2-Dichloroethylene	546	5.790	42	Chlorobenzene	829	11.503
13	2-Butanone(MEK)	567	5.978	43	Ethylbenzene	848	12.113
14	2-Butanol	579	6.085	44	Isopentyl acetate (Isoamyl acetate)	857	12.386
15	cis-1,2-Dichloroethylene	589	6.172				
16	Ethyl acetate	595	6.229	45	m-Xylene	857	12.387
17	n-Hexane	600	6.271	46	p-Xylene	858	12.423
18	Chloroform	601	6.289	47	Cyclohexanone	861	12.542
19	2-Methyl-1-propanol (Isobutyl alcohol)	608	6.412	48	Cyclohexanol	862	12.561
				49	Styrene	875	12.970
20	2-Methoxyethanol (Methyl cellosolve)	610	6.446	50	2-Ethoxyethyl acetate (Cellosolve acetate)	877	13.056
21	Tetrahydrofuran	611	6.465	51	1,1,2,2-Tetrachloroethane	879	13.103
22	1,2-Dichloroethane	622	6.638	52	o-Xylene	880	13.146
23	1,1,1-Trichloroethane	630	6.783	53	2-Butoxyethanol (Butyl cellosolve)	886	13.330
24	1-Butanol	639	6.923				
25	Isopropyl acetate	639	6.936	54	n-Pentyl acetate	894	13.592
26	Benzene	645	7.034	55	4-Methylcyclohexanol	926	14.695
27	Carbon tetrachloride	651	7.133	56	4-Methylcyclohexanone	927	14.745
28	1,4-Dioxane	683	7.676	57	Phenol	952	15.638
29	Trichloroethylene	685	7.711	58	1,2-Dichlorobenzene	1016	17.847
30	2-Ethoxyethanol (Cellosolve)	691	7.801	59	o-Cresol	1026	18.193
				60	p-Cresol	1046	18.895
31	n-Propyl acetate	695	7.868	61	m-Cresol	1047	18.932

* Retention time in minutes

$$\text{Retention index I} = 100 \times \frac{TR - tR(Z)}{TR(Z+1) - tR(Z)} + 100 \times Z$$



T R = retention time of the target component
T R(Z) = retention time of straight-chain alkanes that precede the components of interest
T R(Z+1) = retention time of straight-chain alkanes emerging after the components of interest
Z = number of carbons in straight-chain alkanes with a retention time t R(Z)

Retention index in isothermal analysis-1

Peak No. (gradient	Peak No.	40°C		80°C		120°C		160°C	
		RI	RT	RI	RT	RI	RT	RI	RT
1	Methanol	379	4.802	369	5.017	353	5.300	345	5.571
2	Ethanol	438	5.038	423	5.109	351	5.346	346	5.598
3	Acetonitrile	454	5.135	449	5.156	431	5.370	424	5.613
4	Acetone	468	5.227	463	5.187	452	5.388	439	5.621
5	2-Propanol	478	5.307	470	5.201	447	5.384	439	5.621
6	Diethyl ether	495	5.458	490	5.255	475	5.411	458	5.631
7	tert-Butanol	510	5.565	508	5.295	507	5.431	504	5.643
8	Methyl acetate	514	5.606	510	5.303	509	5.433	506	5.643
9	Dichloromethane	516	5.628	518	5.328	523	5.451	526	5.657
10	Carbon disulfide	532	5.802	541	5.408	556	5.499	567	5.688
11	1-Propanol	544	5.956	537	5.394	536	5.468	531	5.660
12	trans-1,2-Dichloroethylene	554	6.105	557	5.478	564	5.513	566	5.687
13	2-Butanone(MEK)	575	6.442	575	5.560	577	5.539	577	5.697
14	2-Butanol	586	6.662	582	5.598	583	5.551	581	5.701
15	cis-1,2-Dichloroethylene	587	6.748	595	5.683	598	5.603	606	5.743
16	Ethyl acetate	599	6.938	593	5.663	590	5.568	586	5.705
17	n-Hexane	600	6.962	600	5.703	600	5.591	600	5.719
18	Chloroform	597	6.958	605	5.743	605	5.619	611	5.748
19	2-Methyl-1-propanol	610	7.286	608	5.764	601	5.609	600	5.737
20	2-Methoxyethanol	611	7.302	615	5.808	612	5.636	614	5.752
21	Tetrahydrofuran	610	7.279	619	5.839	622	5.658	627	5.766
22	1,2-Dichloroethane	622	7.607	632	5.931	635	5.693	642	5.783
23	1,1,1-Trichloroethane	631	7.877	642	6.014	647	5.727	655	5.799
24	1-Butanol	646	8.370	643	6.018	636	5.696	635	5.774
25	Isopropyl acetate	646	8.385	644	6.029	635	5.693	630	5.768
26	Benzene	646	8.386	659	6.155	664	5.778	674	5.824
27	Carbon tetrachloride	651	8.565	664	6.205	670	5.798	679	5.832
28	1,4-Dioxane	682	9.910	690	6.482	693	5.879	699	5.862
29	Trichloroethylene	682	9.933	693	6.519	697	5.898	705	5.873
30	2-Ethoxyethanol	691	10.378	693	6.521	690	5.871	692	5.852
31	n-Propyl acetate	695	10.629	694	6.537	687	5.858	683	5.838
32	3-Methyl-1-butanol	717	12.018	715	6.812	711	5.951	710	5.881
33	4-Methyl-2-pentanone	717	11.978	722	6.903	721	5.998	724	5.904
34	N,N-Dimethylformamide	734	13.278	740	7.198	745	6.113	752	5.958
35	Isobutyl acetate	743	14.022	742	7.227	736	6.065	733	5.920

*Retention time in minutes

In the case of isothermal analysis...

Because the logarithm of the retention ratio of straight-chain alkanes is linearly related to the number of carbons, the retention index is given by the following equation.

$$\text{Retention index I} = 100 \times \frac{\text{Log t'R} - \text{log t'R(Z)}}{\text{Log t'R(Z+1)} - \text{log t'R(Z)}} + 100 \times Z$$

T R = retention time of the target component
T R(Z) = retention time of straight-chain alkanes that precede the components of interest
T R(Z+1) = retention time of straight-chain alkanes emerging after the components of interest

Z = number of carbons in straight-chain alkanes with a retention time t R(Z)
T'R = corrected retention time t'R = t R-t 0
T 0 = hold-up time (elution time of non-retentive components)

Retnetion index in isothermal analysis-2

Peak No. (gradient temp.)	Peak No.	40°C		80°C		120°C		160°C	
		RI	RT	RI	RT	Ri	RT	RI	RT
36	(Amyl alcohol)	749	14.625	747	7.311	742	6.094	741	5.935
37	Toluene	748	14.526	761	7.572	768	6.238	778	6.013
38	2-Hexanone(MBK)	764	16.055	768	7.718	768	6.235	770	5.996
39	*n*-Butyl acetate	795	19.963	794	8.313	788	6.364	785	6.031
40	Tetrachloroethylene	795	19.456	806	8.630	816	6.566	828	6.143
41	N,N-Dimethylacetamide	823	24.297	829	9.312	834	6.708	841	6.180
42	Chlorobenzene	820	23.793	835	9.495	847	6.822	861	6.246
43	Ethylbenzene	841	27.727	853	10.132	861	6.965	873	6.285
44	(Isoamyl acetate)	860	32.093	858	10.344	854	6.893	853	6.217
45	*m*-Xylene	850	29.646	861	10.450	869	7.042	879	6.307
46	*p*-Xylene	851	29.898	862	10.495	870	7.054	880	6.313
47	Cyclohexanone	852	30.084	866	10.667	879	7.152	895	6.369
48	Cyclohexanol	858	31.546	865	10.618	872	7.080	884	6.326
49	Styrene	866	33.712	878	11.191	887	7.248	899	6.385
50	(Cellosolve acetate)	886	39.208	878	11.170	869	7.044	863	6.252
51	1,1,2,2-Tetrachloroethane	872	35.111	881	11.343	891	7.290	904	6.405
52	*o*-Xylene	871	34.864	883	11.439	894	7.322	906	6.414
53	(Butyl cellosolve)	886	39.361	887	11.623	888	7.252	891	6.352
54	*n*-Pentyl acetate	898	43.360	894	11.983	889	7.269	887	6.336
55	4-Methylcyclohexanol	920	51.823	926	13.828	935	7.883	947	6.600
56	4-Methylcyclohexanone	913	49.182	928	13.933	942	7.999	960	6.664
57	Phenol	969	79.566	953	15.784	944	8.031	943	6.581
58	1,2-Dichlorobenzene	1000	97.202	1010	21.349	1029	9.797	1050	7.258
59	*o*-Cresol	—	—	1029	23.716	1024	9.684	1028	7.086
60	*p*-Cresol	—	—	1049	26.618	1043	10.188	1043	7.209
61	*m*-Cresol	—	—	1050	26.792	1043	10.208	1044	7.214

*Retention time in minutes

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