GT071

GL Sciences Inc.

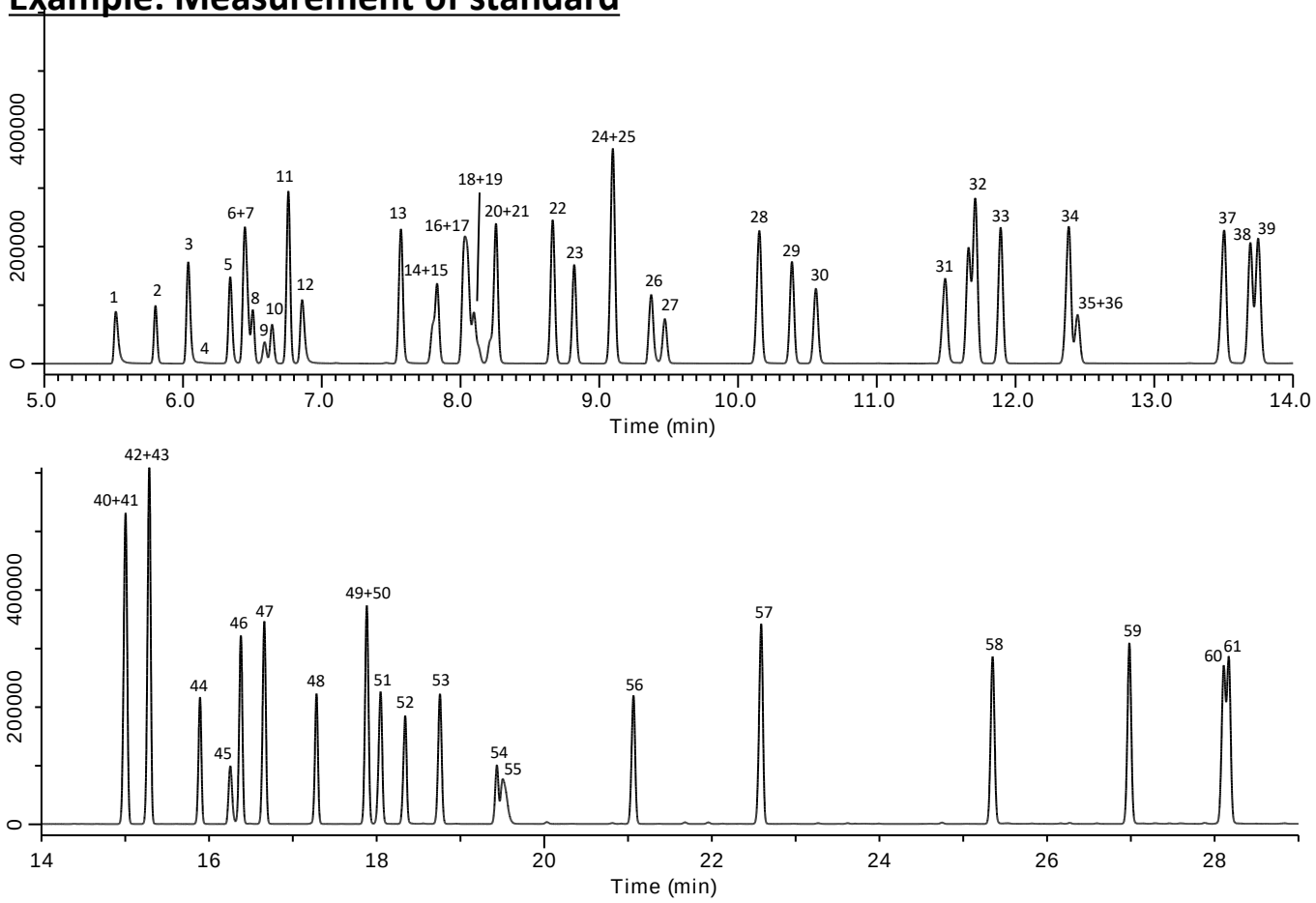
Analysis and Retention Index for 61 Components of Organic Solvents - Using InertCap 1701

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 1701 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 1701 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	: Split flow 150 mL/min 240 ˚C
Detection	: FID Range 10^0 240 ˚C
Sample Size	: Mixed evenly 0.2 µL

Chromatographic conditions described above.

For isothermal analysis, adjust the pressure so that the linear velocity is constant.

Retention index in the temperature rise analysis

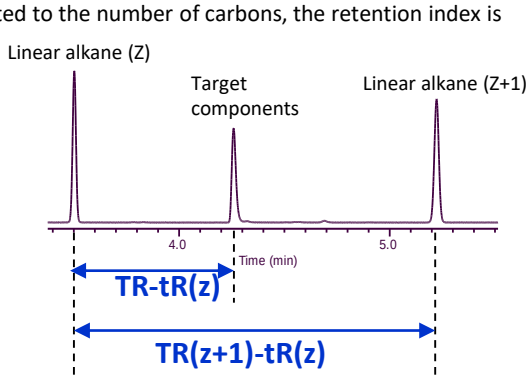
Peak No.	Peak name	Retention index	Retention time	Peak No.	Peak name	Retention index	Retention time
1	Methanol	481	5.437	32	Toluene	820	11.635
2	Ethyl ether	523	5.737	33	4-Methyl-2-pentanone (MIBK)	826	11.831
3	Ethanol	548	5.968				
4	Carbon disulfide	562	6.098	34	Isobutyl acetate	836	12.174
5	Acetone	581	6.269	35	3-Methyl-1-butanol (Isoamyl alcohol)	841	12.333
6	2-Propanol (Isopropyl alcohol)	593	6.382				
				36	Tetrachloroethylene	842	12.371
7	Methyl acetate	595	6.399	37	1-Pentanol(Amyl alcohol)	874	13.448
8	*N-Hexane*	599	6.440	38	*n-Butyl acetate*	879	13.623
9	Dichloromethane	604	6.520	39	2-Hexanone(MBK)	881	13.684
10	*Trans-1,2-Dichloroethylene*	607	6.574	40	Chlorobenzene	917	14.918
11	Tert-Butanol	614	6.697	41	Ethylbenzene	917	14.935
12	Acetonitrile	620	6.867	42	*p-Xylene*	924	15.202
13	1-Propanol	660	7.517	43	*m-Xylene*	925	15.208
14	*cis-1,2-Dichloroethylene*	672	7.728	44	Isopentyl acetate (Isoamyl acetate)	941	15.809
15	Ethyl acetate	674	7.768				
16	Methyl ethyl ketone	685	7.958	45	*N,N-Dimethylformamide*	952	16.205
17	Tetrahydrofuran	687	7.985	46	*o-Xylene*	955	16.301
18	1,1,1-Trichloroethane	689	8.023	47	Styrene	963	16.584
19	Carbon tetrachloride	691	8.059	48	*n-Pentyl acetate*	980	17.207
20	Chloroform	695	8.138	49	2-Ethoxyethyl acetate (Cellosolve acetate)	997	17.802
21	2-Butanol	699	8.202				
22	Benzene	714	8.595	50	1-Methylcyclohexanol	997	17.823
23	Isopropyl acetate	720	8.753	51	Cyclohexanol	1002	17.983
24	1,2-Dichloroethane	729	9.023	52	2-Butoxyethanol (Butyl cellosolve)	1009	18.263
25	2-Methyl-1-propanol (Isobutyl alcohol)	730	9.043				
				53	Cyclohexanone	1021	18.768
26	2-Methoxyethanol (Methyl cellosolve)	740	9.325	54	1,1,2,2-Tetrachloroethane	1038	19.428
				55	*N,N-Dimethylacetamide*	1039	19.450
27	Trichloroethylene	743	9.397	56	4-Methylcyclohexanone	1079	21.003
28	1-Butanol	769	10.103	57	1,2-Dichlorobenzene	1128	22.623
29	*n-Propyl acetate*	777	10.317	58	Phenol	1214	25.276
30	1,4-Dioxane	783	10.491	59	*o-Cresol*	1265	26.903
31	2-Ethoxyethanol (Cellosolve)	815	11.445	60	*p-Cresol*	1301	28.028
				61	*m-Cresol*	1303	28.086

* Retention time in minutes

In the case of temperature programming...

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

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



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 temp.)	Compound	40℃		80℃		120℃		160℃	
		Retention index	Retention time	Retention index	Retention time	Retention index	Retention time	Retention index	Retention time
1	Methanol	497	5.553	486	4.768	466	4.489	473	4.234
2	Ethyl ether	536	5.923	533	4.888	523	4.543	520	4.257
3	Ethanol	565	6.301	552	4.951	536	4.557	533	4.263
4	Carbon disulfide	570	6.378	588	5.093	597	4.641	610	4.310
5	Acetone	589	6.698	590	5.102	587	4.625	591	4.297
6	2-Propanol (Isopropyl alcohol)	602	6.953	589	5.099	574	4.606	569	4.283
7	Methyl acetate	599	6.905	601	5.157	591	4.632	593	4.298
8	*N-Hexane*	600	6.952	600	5.162	600	4.643	600	4.301
9	Dichloromethane	607	7.057	612	5.213	613	4.668	621	4.318
10	*Trans-1,2-Dichloroethylene*	611	7.152	616	5.234	617	4.676	623	4.320
11	Tert-Butanol	625	7.491	612	5.211	599	4.645	594	4.299
12	Acetonitrile	625	7.493	630	5.316	632	4.705	644	4.337
13	1-Propanol	674	9.075	660	5.521	649	4.740	644	4.337
14	*Cis-1,2-Dichloroethylene*	677	9.195	684	5.716	689	4.840	697	4.389
15	Ethyl acetate	682	9.441	679	5.673	673	4.798	670	4.361
16	Methyl ethyl ketone	689	9.761	691	5.788	692	4.848	696	4.388
17	Tetrahydrofuran	687	9.760	697	5.843	704	4.884	713	4.407
18	1,1,1-Trichloroethane	688	9.787	699	5.868	709	4.898	718	4.413
19	Carbon tetrachloride	689	9.841	701	5.888	711	4.907	722	4.417
20	Chloroform	697	10.107	701	5.880	704	4.883	710	4.403
21	2-Butanol	706	10.586	694	5.816	685	4.829	681	4.372
22	Benzene	712	11.025	724	6.141	734	4.983	751	4.455
23	Isopropyl acetate	725	11.814	721	6.109	716	4.921	710	4.403
24	1,2-Dichloroethane	729	12.108	740	6.347	750	5.043	760	4.468
25	2-Methyl-1-propanol (Isobutyl alcohol)	741	12.847	728	6.193	720	4.933	714	4.408
26	2-Methoxyethanol (Methyl cellosolve)	746	13.233	747	6.440	750	5.042	753	4.458
27	Trichloroethylene	743	13.109	754	6.537	763	5.098	773	4.487
28	1-Butanol	779	16.403	768	6.762	760	5.083	755	4.460
29	*n-Propyl acetate*	781	16.617	779	6.959	777	5.158	773	4.487
30	1,4-Dioxane	782	16.718	790	7.167	798	5.266	808	4.546
31	2-Ethoxyethanol (Cellosolve)	817	21.161	817	7.749	820	5.383	822	4.573

In the case of isothermal analysis...

* Retention time in minutes

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)

Retention index in isothermal analysis-2

Peak No. (gradient temp.)	Compound	40℃		80℃		120℃		160℃	
		Retention index	Retention time	Retention index	Retention time	Retention index	Retention time	Retention index	Retention time
32	Toluene	815	20.858	827	7.984	839	5.508	855	4.642
33	4-Methyl-2-pentanone (MIBK)	826	22.571	830	8.056	834	5.473	837	4.603
34	Isobutyl acetate	840	25.025	838	8.283	837	5.489	835	4.598
35	3-Methyl-1-butanol (Isoamyl alcohol)	851	27.188	840	8.336	834	5.472	830	4.588
36	Tetrachloroethylene	834	24.068	849	8.603	864	5.686	880	4.702
37	1-Pentanol(Amyl alcohol)	884	35.199	873	9.387	867	5.705	863	4.659
38	*n-Butyl acetate*	882	34.650	881	9.649	879	5.802	878	4.696
39	2-Hexanone(MBK)	880	33.943	883	9.762	888	5.880	892	4.734
40	Chlorobenzene	902	40.569	919	11.311	937	6.383	957	4.937
41	Ethylbenzene	906	42.059	919	11.313	932	6.324	947	4.902
42	*p-Xylene*	914	44.449	926	11.676	939	6.400	953	4.922
43	*m-Xylene*	914	44.848	926	11.682	939	6.402	953	4.922
44	Isopentyl acetate (Isoamyl acetate)	943	56.978	943	12.576	942	6.436	943	4.886
45	*N,N-Dimethylformamide*	948	59.275	956	13.376	965	6.735	977	5.013
46	*o-Xylene*	941	55.464	956	13.369	971	6.812	989	5.062
47	Styrene	949	59.477	963	13.858	977	6.906	994	5.082
48	*n-Pentyl acetate*	983	79.227	982	15.198	980	6.948	980	5.023
49	2-Ethoxyethyl acetate (Cellosolve acetate)	—	96.785	999	16.636	993	7.146	989	5.062
50	1-Methylcyclohexanol	993	86.396	997	16.451	1005	7.351	1018	5.193
51	Cyclohexanol	—	91.594	1001	16.847	1008	7.400	1020	5.200
52	2-Butoxyethanol (Butyl cellosolve)	—	97.440	1010	17.638	1015	7.516	1021	5.207
53	Cyclohexanone	999	90.342	1017	18.360	1038	7.977	1062	5.423
54	1,1,2,2-Tetrachloroethane	—	119.147	1037	20.462	1046	8.153	1060	5.412
55	*N,N-Dimethylacetamide*	—	132.512	1045	21.483	1053	8.295	1063	5.432
56	4-Methylcyclohexanone	—	151.449	1077	25.887	1100	9.509	1125	5.852
57	1,2-Dichlorobenzene	—	—	1114	32.368	1140	10.839	1168	6.222
58	Phenol	—	—	1223	64.848	1213	14.209	1209	6.658
59	*o-Cresol*	—	—	1272	89.957	1265	17.527	1264	7.365
60	*p-Cresol*	—	—	1311	116.593	1302	20.613	1299	7.922
61	*m-Cresol*	—	—	1313	118.129	1304	20.802	1301	7.957

* Retention time in minutes

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