

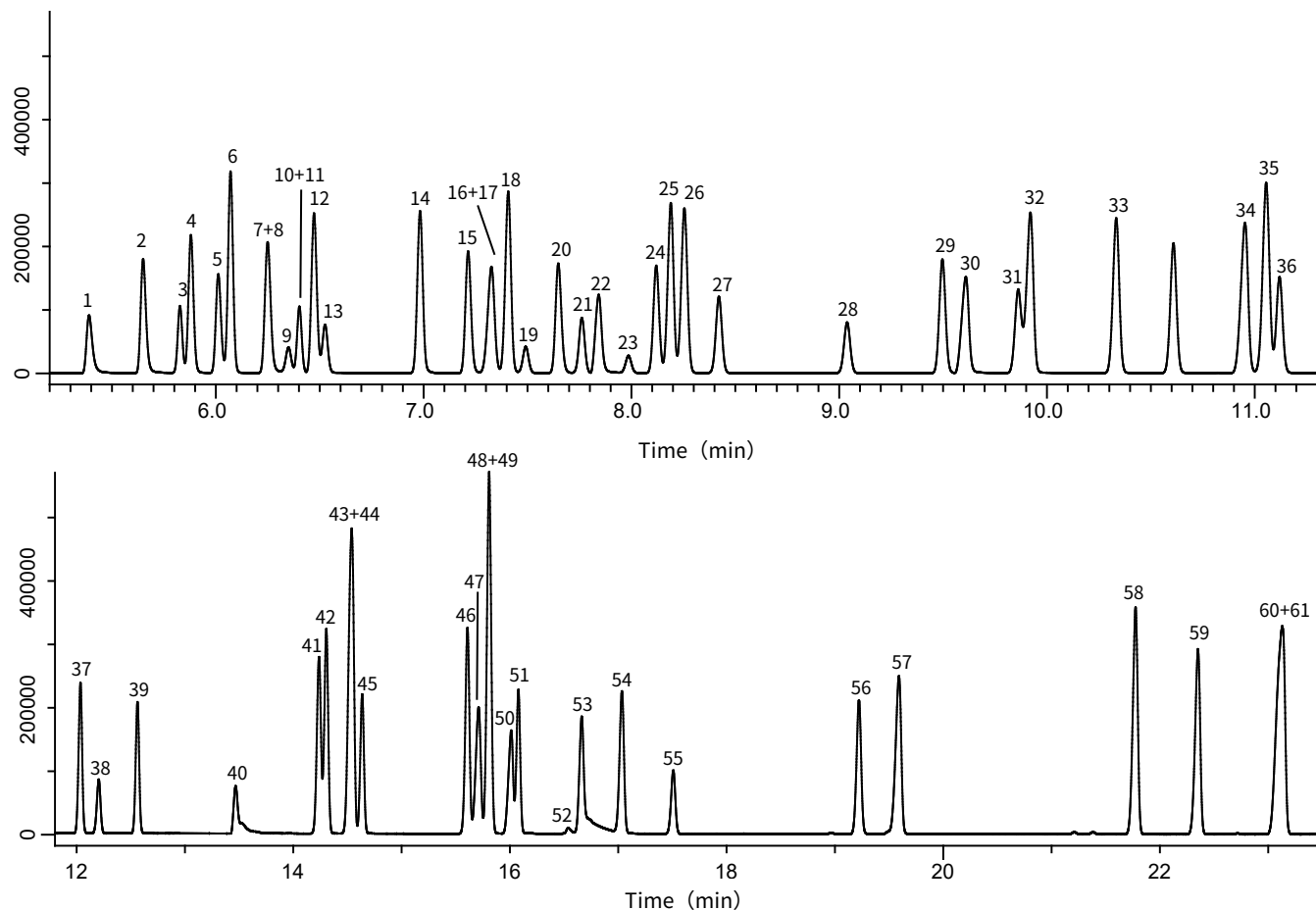
Analysis and Retention Indicators for 61 Organic Solvents - Using InertCap 25

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 25 was used to determine the retention index of 61 components of organic solvents by isothermal and temperature rise analysis..

Example: Measurement of standards



Conditions

System	: GC - FID
Column	: InertCap 25 0.25 mm I.D. x 60 m df = 0.25 μ m
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 ¹⁰ 240 °C
Sample Size	: Mixed evenly 0.2 μ L

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.	Component	Retention index	Retention time	Peak No.	Component	Retention index	Retention time
1	Methanol	418	5.362	32	3-Methyl-1-butanol (Isoamyl alcohol)	781	9.894
2	Ethanol	498	5.623	33	4-Methyl-2-pentanone (MIBK)	798	10.302
3	Ethyl ether	523	5.802	34	1-Pentanol (Amyl alcohol)	818	10.926
4	2-Propanol (Isopropyl alcohol)	530	5.853	35	Toluene	820	11.017
5	Acetone	548	5.985	36	Isobutyl acetate	822	11.083
6	Tert-Butanol	556	6.045	37	2-Hexanone (MBK)	851	12.005
7	Acetonitrile	580	6.219	38	Tetrachloroethylene	855	12.160
8	Methyl acetate	581	6.227	39	<i>n</i> -Butyl acetate	867	12.525
9	Carbon disulfide	590	6.298	40	<i>N,N</i> -Dimethylformamide	895	13.448
10	Dichloromethane	594	6.323	41	Chlorobenzene	916	14.194
11	<i>n</i> -Hexane	600	6.377	42	Ethylbenzene	918	14.265
12	1-Propanol	605	6.448	43	<i>p</i> -Xylene	924	14.476
13	<i>Trans</i> -1,2-Dichloroethylene	609	6.502	44	<i>m</i> -Xylene	925	14.500
14	2-Butanol	639	6.955	45	Isopentyl acetate (Isoamyl acetate)	927	14.588
15	Methyl ethyl ketone	654	7.186	46	<i>o</i> -Xylene	955	15.567
16	<i>cis</i> -1,2-Dichloroethylene	661	7.281	47	Cyclohexanol	958	15.663
17	Ethyl acetate	662	7.300	48	1-Methylcyclohexanol	960	15.747
18	2-Methyl-1-propanol (Isobutyl alcohol)	667	7.376	49	Styrene	960	15.767
19	Chloroform	672	7.452	50	2-Butoxyethanol (Butyl cellosolve)	966	15.963
20	Tetrahydrofuran	683	7.617	51	<i>n</i> -Pentyl acetate	968	16.021
21	1,1,1-Trichloroethane	691	7.732	52	<i>N,N</i> -Dimethylacetamide	981	16.487
22	2-Methoxyethanol (Methyl cellosolve)	697	7.824	53	2-Ethoxyethyl acetate (Cellosolve acetate)	984	16.617
23	Carbon tetrachloride	703	7.950	54	Cyclohexanone	995	16.991
24	Isopropyl acetate	709	8.088	55	1,1,2,2-Tetrachloroethane	1007	17.441
25	1-Butanol	712	8.163	56	4-Methylcyclohexanone	1051	19.187
26	Benzene	714	8.222	57	Phenol	1059	19.527
27	1,2-Dichloroethane	721	8.387	58	1,2-Dichlorobenzene	1118	21.683
28	Trichloroethylene	746	9.003	59	<i>o</i> -Cresol	1141	22.385
29	<i>n</i> -Propyl acetate	764	9.464	60	<i>p</i> -Cresol	1164	23.078
30	2-Ethoxyethanol (Cellosolve)	769	9.588	61	<i>m</i> -Cresol	1165	23.113
31	1,4-Dioxane	779	9.823				

※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.

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

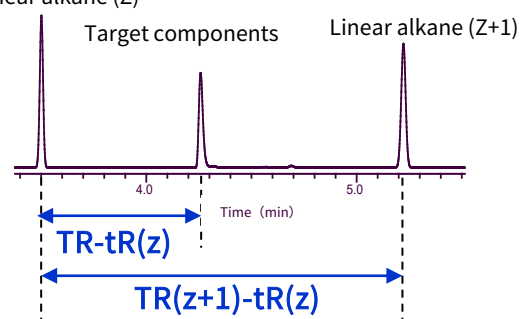
TR = retention time of the target component

TR(Z) = retention time of straight-chain alkanes that precede the components of interest

TR(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 tR(Z)

Linear alkane (Z)



Retention index in isothermal analysis-1

Peak No. (gradient temp.)	Component	40 °C		80 °C		120 °C		160 °C	
		Retention index	Retention time	Retention index	Retention time	Retention index	Retention time	Retention index	Retention time
1	Methanol	436	5.358	428	5.421	428	4.667	405	4.441
2	Ethanol	502	5.682	496	5.529	495	4.707	475	4.460
3	Ethyl ether	533	5.916	528	5.601	529	4.733	506	4.471
4	2-Propanol (Isopropyl alcohol)	542	5.991	535	5.620	536	4.739	515	4.474
5	Acetone	560	6.173	556	5.679	558	4.760	541	4.484
6	Tert-Butanol	567	6.265	561	5.696	557	4.759	551	4.488
7	Acetonitrile	586	6.512	584	5.780	587	4.793	579	4.501
8	Methyl acetate	587	6.527	582	5.770	582	4.787	567	4.495
9	Carbon disulfide	589	6.560	589	5.800	604	4.814	591	4.507
10	Dichloromethane	595	6.646	598	5.835	606	4.817	600	4.512
11	<i>n</i> -Hexane	601	6.741	599	5.840	605	4.815	602	4.508
12	1-Propanol	609	6.873	602	5.855	605	4.815	593	4.508
13	<i>Trans</i> -1,2- <i>Dichloroethylene</i>	611	6.912	614	5.909	624	4.843	619	4.523
14	2-Butanol	648	7.725	643	6.066	646	4.878	638	4.535
15	Methyl ethyl ketone	663	8.122	660	6.171	663	4.909	654	4.546
16	<i>cis</i> -1,2- <i>Dichloroethylene</i>	666	8.231	671	6.249	681	4.947	682	4.567
17	Ethyl acetate	671	8.374	664	6.198	662	4.908	650	4.543
18	2-Methyl-1-propanol (Isobutyl alcohol)	675	8.511	670	6.241	672	4.927	666	4.555
19	Chloroform	677	8.566	681	6.326	691	4.968	692	4.576
20	Tetrahydrofuran	685	8.857	690	6.404	701	4.992	703	4.586
21	1,1,1-Trichloroethane	690	9.056	698	6.471	710	5.015	717	4.598
22	2-Methoxyethanol (Methyl cellosolve)	697	9.309	698	6.474	706	5.004	706	4.588
23	Carbon tetrachloride	700	9.456	711	6.596	726	5.058	737	4.618
24	Isopropyl acetate	713	10.031	705	6.538	701	4.993	690	4.574
25	1-Butanol	716	10.163	711	6.593	712	5.019	706	4.588
26	Benzene	713	10.030	723	6.724	739	5.095	746	4.628
27	1,2-Dichloroethane	722	10.481	728	6.777	738	5.093	743	4.625
28	Trichloroethylene	747	11.886	756	7.123	768	5.192	776	4.663
29	<i>n</i> -Propyl acetate	771	13.633	764	7.249	762	5.171	755	4.638
30	2-Ethoxyethanol (Cellosolve)	772	13.742	773	7.375	778	5.228	779	4.668

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.

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

$t'R$ = 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 $t'R = t - t_0$
 t_0 = hold-up time (elution time of non-retentive components)

Retention index in isothermal analysis-2

Peak No. (gradient temp.)	Peak name	40 °C		80 °C		120 °C		160 °C	
		Retention index	Retention time	Retention index	Retention time	Retention index	Retention time	Retention index	Retention time
31	1,4-Dioxane	779	14.348	784	7.559	793	5.288	800	4.696
32	3-Methyl-1-butanol (Isoamyl alcohol)	785	14.919	782	7.520	783	5.248	785	4.675
33	4-Methyl-2-pentanone (MIBK)	798	16.212	797	7.800	800	5.318	804	4.702
34	1-Pentanol(Amyl alcohol)	821	18.811	817	8.196	817	5.397	817	4.722
35	Toluene	816	18.158	827	8.423	842	5.522	856	4.788
36	Isobutyl acetate	827	19.633	821	8.294	819	5.403	814	4.717
37	2-Hexanone(MBK)	853	23.747	852	9.077	854	5.595	856	4.788
38	Tetrachloroethylene	848	22.832	863	9.388	880	5.761	896	4.870
39	<i>n</i> -Butyl acetate	872	27.313	866	9.504	863	5.652	859	4.794
40	<i>N,N</i> -Dimethylformamide	893	32.064	896	10.542	903	5.936	911	4.905
41	Chlorobenzene	904	35.043	919	11.554	938	6.250	958	5.035
42	Ethylbenzene	909	36.454	921	11.615	936	6.222	952	5.015
43	<i>p</i> -Xylene	915	38.242	926	11.889	941	6.275	956	5.028
44	<i>m</i> -Xylene	915	38.403	927	11.927	942	6.282	956	5.028
45	Isopentyl acetate (Isoamyl acetate)	932	43.960	927	11.919	925	6.122	923	4.937
46	<i>o</i> -Xylene	942	47.703	956	13.524	973	6.628	992	5.148
47	Cyclohexanol	949	50.887	958	13.629	971	6.604	987	5.128
48	1-Methylcyclohexanol	951	51.507	961	13.805	974	6.643	991	5.142
49	Styrene	948	50.395	961	13.837	977	6.675	994	5.155
50	2-Butoxyethanol (Butyl cellosolve)	963	57.064	966	14.148	972	6.610	979	5.100
51	<i>n</i> -Pentyl acetate	973	62.368	967	14.227	964	6.527	962	5.047
52	<i>N,N</i> -Dimethylacetamide	977	64.292	980	15.137	988	6.813	997	5.164
53	2-Ethoxyethyl acetate (Cellosolve acetate)	996	75.925	984	15.435	976	6.662	977	5.096
54	Cyclohexanone	980	65.905	993	16.134	1011	7.142	1031	5.302
55	1,1,2,2-Tetrachloroethane	998	77.265	1006	17.193	1018	7.248	1033	5.310
56	4-Methylcyclohexanone	1051	108.532	1051	21.915	1068	8.184	1089	5.591
57	Phenol	1084	134.571	1063	23.415	1070	8.220	1083	5.555
58	1,2-Dichlorobenzene	1170	179.045	1115	31.840	1139	10.060	1167	6.128
59	<i>o</i> -Cresol	—	—	1140	37.316	1156	10.607	1163	6.088
60	<i>p</i> -Cresol	—	—	1161	42.598	1171	11.187	1187	6.302
61	<i>m</i> -Cresol	—	—	1162	42.872	1172	11.223	1188	6.308

* Retention time in minutes

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GL Sciences Inc. Japan

22-1 Nishishinjuku 6-chome
Shinjuku-ku, Tokyo
163-1130, Japan

Phone: +81-3-5323-6620
Fax: +81-3-5323-6621
Email: world@glsc.co.jp
Web: www.glsciences.com

GL Sciences Inc. USA

4733 Torrance Blvd. Suite 255
Torrance, CA 90503
USA

Phone: +1-310-265-4424
Fax: +1-310-265-4425
Email: info@glsciencesinc.com
Web: www.glsciencesinc.com

GL Sciences B.V.

Dillenburgstraat 7C
5652AM, Eindhoven
The Netherlands

Phone: +31-40-254-9531
Email: info@glsciences.eu
Web: www.glsciences.eu

GL Sciences (Shanghai) Limited

Tower B, Room 2003
Far East International Plaza
No.317 Xianxia Road, Changning District
Shanghai, China 200051

Phone: +86-21-62782272
Email: contact@glsciences.com.cn
Web: www.glsciences.com.cn

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