

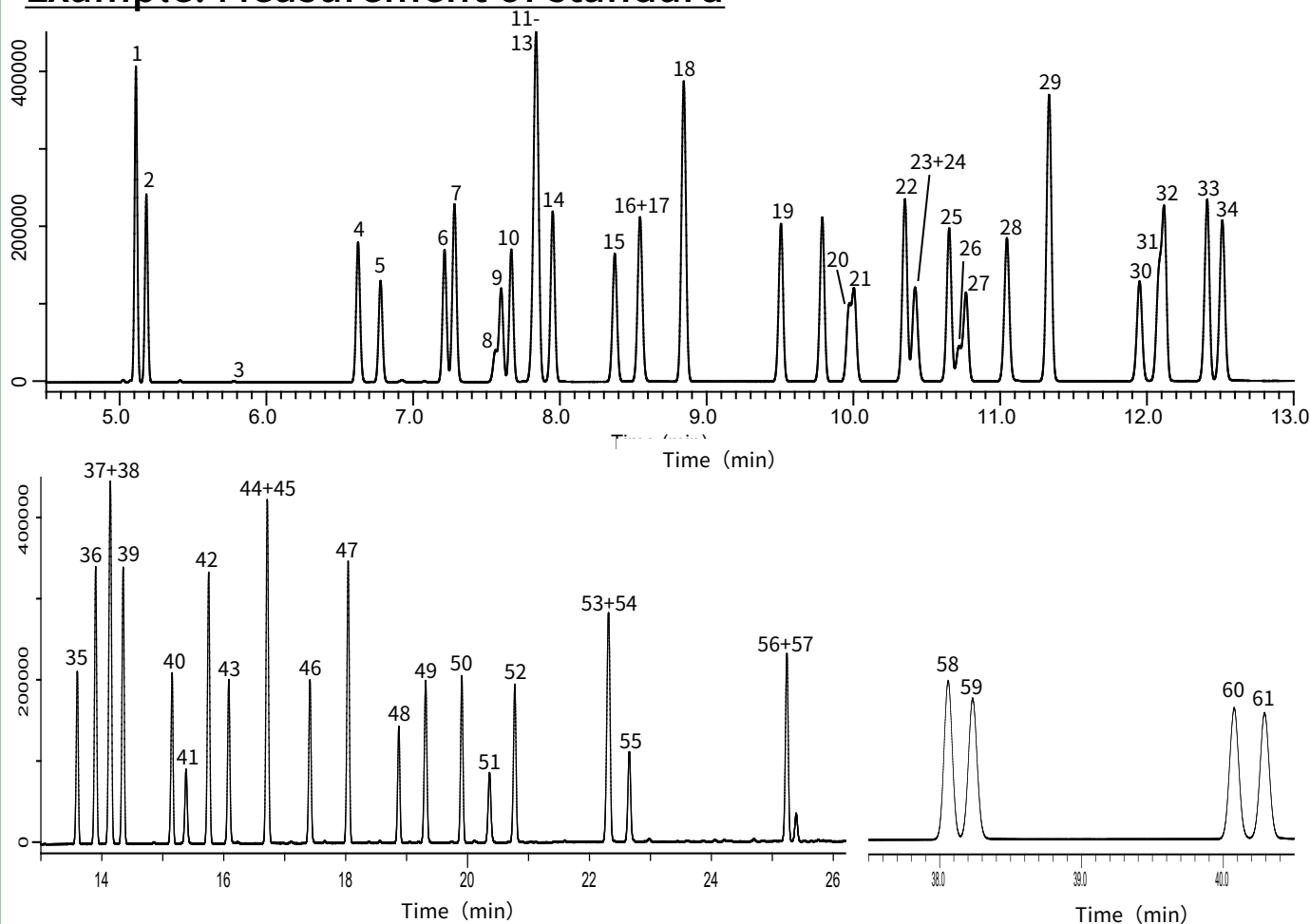
Analytical and Retention Index of 61 Components of Organic Solvents - Using InertCap WAX

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

Example: Measurement of standard



Conditions

System	: GC - FID
Column	: InertCap WAX 0.25 mm I.D. × 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 ¹⁰ 240 °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.	Component	Retention index	Retention time	Peak No.	Component	Retention index	Retention time
1	<i>n</i> -Hexane	599	5.122	34	2-Methyl-1-propanol (Isobutyl alcohol)	1093	12.526
2	Ethyl ether	616	5.189	35	Isopentyl acetate (Isoamyl acetate)	1126	13.612
3	Carbon disulfide	735	5.813	36	Ethylbenzene	1135	13.922
4	Acetone	820	6.632	37	1-Butanol	1142	14.145
5	Methyl acetate	831	6.784	38	<i>p</i> -Xylene	1143	14.168
6	<i>Trans</i> -1,2-Dichloroethylene	861	7.218	39	<i>m</i> -Xylene	1149	14.375
7	Tetrahydrofuran	866	7.293	40	<i>N</i> -Pentyl acetate	1173	15.172
8	Carbon tetrachloride	885	7.576	41	2-Methoxyethanol (Methyl cellosolve)	1179	15.394
9	1,1,1-Trichloroethane	888	7.613	42	<i>o</i> -Xylene	1190	15.730
10	Ethyl acetate	893	7.676	43	3-Methyl-1-butanol (Isoamyl alcohol)	1201	16.108
11	Methanol	902	7.821	44	2-Ethoxyethanol (Cellosolve)	1219	16.670
12	Tert-Butanol	903	7.838	45	Chlorobenzene	1219	16.686
13	Isopropyl acetate	903	7.862	46	1-Pentanol (Amyl alcohol)	1243	17.441
14	Methyl ethyl ketone	908	7.954	47	Styrene	1263	18.070
15	2-Propanol (Isopropyl alcohol)	927	8.381	48	2-Ethoxyethyl acetate (Cellosolve acetate)	1289	18.898
16	Ethanol	935	8.549	49	Cyclohexanone	1301	19.292
17	Dichloromethane	935	8.549	50	1-Methylcyclohexanol	1321	19.938
18	Benzene	949	8.862	51	<i>N,N</i> -Dimethylformamide	1333	20.310
19	<i>n</i> -Propyl acetate	979	9.525	52	4-Methylcyclohexanone	1349	20.810
20	<i>Cis</i> -1,2-Dichloroethylene	1000	9.967	53	2-Butoxyethanol (Butyl cellosolve)	1394	22.259
21	Trichloroethylene	1001	10.020	54	Cyclohexanol	1395	22.293
22	4-Methyl-2-pentanone (MIBK)	1014	10.366	55	<i>N,N</i> -Dimethylacetamide	1406	22.614
23	Acetonitrile	1016	10.425	56	1,1,2,2-Tetrachloroethane	1502	25.248
24	Isobutyl acetate	1018	10.468	57	1,2-Dichlorobenzene	1503	25.268
25	2-Butanol	1025	10.659	58	<i>o</i> -Cresol	2029	38.084
26	Chloroform	1027	10.719	59	Phenol	2036	38.256
27	Tetrachloroethylene	1029	10.779	60	<i>p</i> -Cresol	2112	40.101
28	1-Propanol	1039	11.054	61	<i>m</i> -Cresol	2121	40.316
29	Toluene	1050	11.348				
30	1,4-Dioxane	1072	11.967				
31	1,2-Dichloroethane	1077	12.087				
32	<i>n</i> -Butyl acetate	1078	12.138				
33	2-Hexanone (MBK)	1089	12.434				

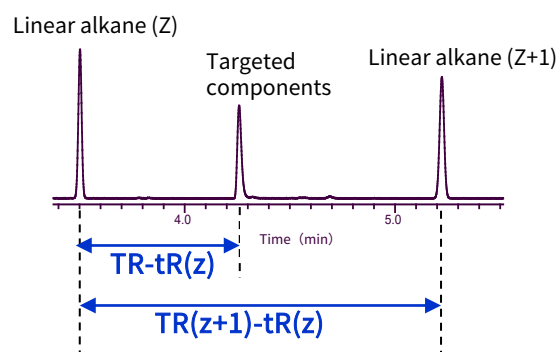
In the case of temperature programming...

* Retention time in minutes

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 ingredient
 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)



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	<i>N-Hexane</i>	600	5.102	597	4.613	600	4.388	608	4.192
2	Ethyl ether	623	5.149	619	4.638	620	4.398	625	4.175
3	Carbon disulfide	734	5.937	758	4.916	788	4.537	814	4.250
4	Acetone	823	7.274	829	5.192	837	4.605	848	4.290
5	Methyl acetate	837	7.522	838	5.232	839	4.608	844	4.268
6	<i>Trans-1,2-Dichloroethylene</i>	867	8.395	868	5.402	870	4.662	865	4.282
7	Tetrahydrofuran	866	8.348	885	5.512	903	4.729	920	4.325
8	Carbon tetrachloride	885	8.953	895	5.583	905	4.735	925	4.329
9	1,1,1-Trichloroethane	886	8.984	899	5.613	911	4.748	923	4.328
10	Ethyl acetate	893	9.244	894	5.582	894	4.711	891	4.301
11	Methanol	903	9.590	899	5.616	890	4.702	879	4.292
12	Tert-Butanol	907	9.752	893	5.573	878	4.678	875	4.308
13	Isopropyl acetate	904	9.663	904	5.651	900	4.724	897	4.306
14	Methyl ethyl ketone	905	9.708	915	5.746	925	4.781	929	4.333
15	2-Propanol (Isopropyl alcohol)	934	11.023	923	5.809	909	4.744	897	4.306
16	Ethanol	941	11.387	933	5.905	923	4.777	912	4.318
17	Dichloromethane	940	11.449	939	5.956	940	4.819	933	4.337
18	Benzene	945	11.690	964	6.224	982	4.945	1000	4.408
19	<i>N-Propyl acetate</i>	980	13.977	983	6.460	984	4.954	987	4.393
20	<i>Cis-1,2-Dichloroethylene</i>	998	15.572	1003	6.726	1008	5.040	1014	4.426
21	Trichloroethylene	997	15.381	1007	6.788	1016	5.071	1028	4.445
22	4-Methyl-2-pentanone (MIBK)	1009	16.445	1021	7.014	1032	5.135	1044	4.467
23	Acetonitrile	1011	16.613	1024	7.056	1037	5.158	1053	4.480
24	Isobutyl acetate	1017	17.283	1021	7.011	1023	5.099	1032	4.468
25	2-Butanol	1030	18.557	1023	7.037	1013	5.057	1000	4.408
26	Chloroform	1027	18.444	1031	7.178	1033	5.142	1036	4.455
27	Tetrachloroethylene	1021	17.662	1040	7.342	1059	5.263	1070	4.487
28	1-Propanol	1044	20.178	1038	7.311	1030	5.126	1026	4.442
29	Toluene	1040	19.755	1061	7.757	1082	5.382	1094	4.528
30	1,4-Dioxane	1062	22.597	1081	8.212	1100	5.486	1122	4.601
31	1,2-Dichloroethane	1075	24.559	1081	8.218	1090	5.428	1106	4.570
32	<i>n-Butyl acetate</i>	1078	25.039	1082	8.227	1085	5.398	1079	4.502
33	2-Hexanone(MBK)	1083	25.777	1094	8.543	1106	5.522	1109	4.555

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

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