

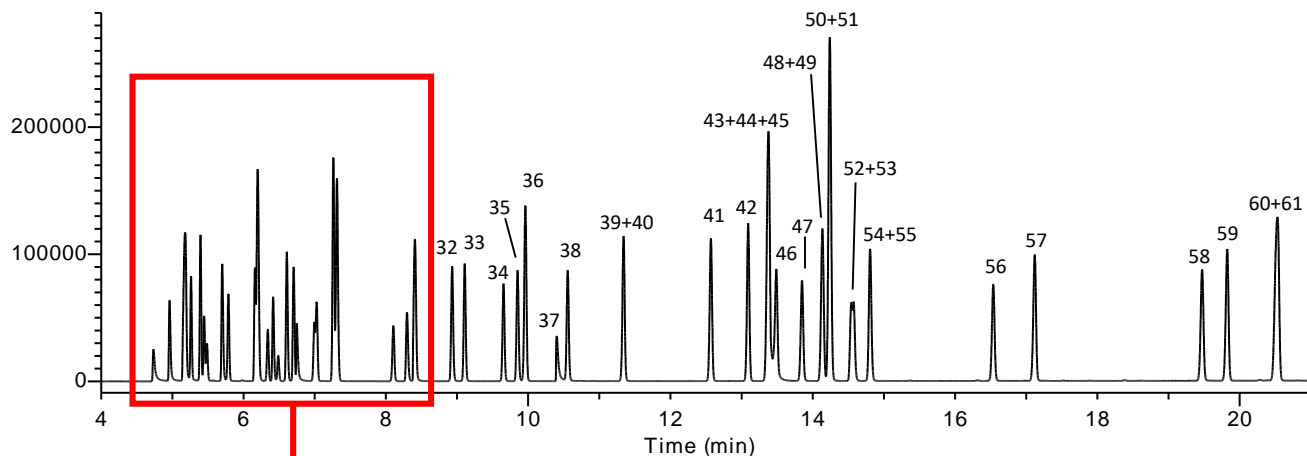
Analytical ad Retention Index of 61 Components of Organic Solvents - Using InertCap 5

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.

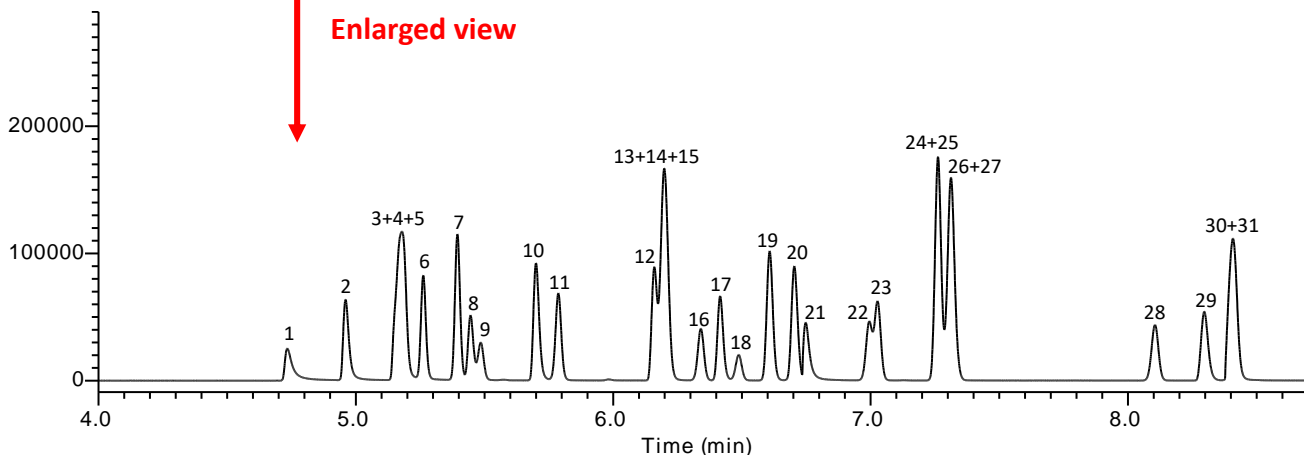
The retention index can be determined because in isothermal analysis the logarithm of the retention ratio for straight-chain alkanes is linearly related to the number of carbons, and the retention ratio is also linear to the number of carbons in thermal rise analysis.

In this report, InertCap 5 was used to determine the retention index of 61 components in organic solvents by isothermal analysis and temperature rise analysis .

Example: Measurement of standard



Enlarged view



Conditions

System	: GC - FID
Column	: InertCap 5 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 192 mL/min 240 °C
Detection	: FID Range 10 ⁰ 240 °C
Sample Size	: Mixed evenly 0.1 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	Methanol	380	4.752	32	3-Methyl-1-butanol (Isoamyl alcohol)	730	8.938
2	Ethanol	440	4.968	33	4-Methyl-2-pentanone (MIBK)	736	9.117
3	Acetonitrile	484	5.164	34	<i>N</i> -Butyl acetate	756	9.679
4	Acetone	487	5.176	35	1-Pentanol (Amyl alcohol)	763	9.856
5	2-Propanol (Isopropyl alcohol)	491	5.192	36	Toluene	767	9.974
6	Diethyl ether	504	5.270	37	<i>N,N</i> -Dimethylformamide	782	10.401
7	Tert-Butanol	517	5.399	38	2-Hexanone (MBK)	787	10.564
8	Methyl acetate	522	5.453	39	Tetrachloroethylene	813	11.350
9	Dichloromethane	526	5.485	40	Isobutyl acetate	813	11.356
10	1-Propanol	549	5.712	41	Chlorobenzene	848	12.583
11	Trans-1,2-Dichloroethylene	557	5.787	42	Ethylbenzene	864	13.110
12	2-Butanone (MEK)	596	6.169	43	<i>M</i> -Xylene	871	13.378
13	Carbon disulfide	598	6.198	44	<i>N,N</i> -Dimethylacetamide	872	13.398
14	<i>N</i> -Hexane	599	6.207	45	<i>P</i> -Xylene	872	13.400
15	2-Butanol	600	6.217	46	Isopentyl acetate (Isoamyl acetate)	875	13.501
16	<i>Cis</i> -1,2-Dichloroethylene	607	6.353	47	Cyclohexanol	885	13.853
17	Ethyl acetate	612	6.428	48	1-Methylcyclohexanol	897	14.149
18	Chloroform	615	6.499	49	Styrene	894	14.154
19	2-Methyl-1-propanol (Isobutyl alcohol)	622	6.616	50	Cyclohexanone	897	14.253
20	Tetrahydrofuran	627	6.713	51	<i>O</i> -Xylene	897	14.254
21	2-Methoxyethanol (Methyl cellosolve)	629	6.759	52	2-Ethoxyethyl acetate (Cellosolve acetate)	905	14.545
22	1,1,1-Trichloroethane	643	7.008	53	2-Butoxyethanol (Butyl cellosolve)	906	14.577
23	1,2-Dichloroethane	644	7.039	54	<i>N</i> -Pentyl acetate	912	14.813
24	1-Butanol	656	7.268	55	1,1,2,2-Tetrachloroethane	913	14.826
25	Isopropyl acetate	657	7.269	56	4-Methylcyclohexanone	960	16.550
26	Benzene	659	7.323	57	Phenol	976	17.128
27	Carbon tetrachloride	660	7.343	58	1,2-Dichlorobenzene	1042	19.492
28	Trichloroethylene	701	8.121	59	<i>O</i> -Cresol	1052	19.843
29	1,4-Dioxane	708	8.308	60	<i>P</i> -Cresol	1071	20.515
30	2-Ethoxyethanol (Cellosolve)	711	8.401	61	<i>M</i> -Cresol	1072	20.548
31	<i>N</i> -Propyl acetate	712	8.425				

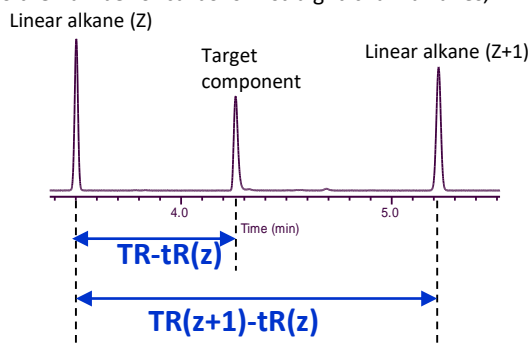
In the case of temperature programming...

*Retention time in minutes

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

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

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)



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	397	4.749	368	4.334	354	4.146	347	3.915
2	Ethanol	459	5.032	442	4.422	427	4.184	432	3.937
3	Acetonitrile	493	5.258	492	4.517	478	4.220	480	3.955
4	Acetone	496	5.283	494	4.523	481	4.223	483	3.956
5	2-Propanol (Isopropyl alcohol)	501	5.323	493	4.521	475	4.218	478	3.954
6	Diethyl ether	510	5.405	506	4.552	490	4.231	496	3.962
7	Tert-Butanol	529	5.602	523	4.598	510	4.250	507	3.967
8	Methyl acetate	534	5.656	530	4.618	516	4.256	519	3.972
9	Dichloromethane	537	5.690	540	4.648	537	4.210	542	3.983
10	1-Propanol	564	6.059	555	4.699	543	4.285	547	3.986
11	Trans-1,2-Dichloroethylene	567	6.155	570	4.752	568	4.318	577	4.043
12	2-Butanone(MEK)	600	6.731	597	4.883	591	4.353	594	4.055
13	Carbon disulfide	544	5.821	557	4.702	595	4.359	600	4.062
14	N-Hexane	600	6.743	602	4.904	594	4.358	602	4.063
15	2-Butanol	605	6.856	599	4.890	591	4.352	594	4.055
16	cis-1,2-Dichloroethylene	610	6.968	615	4.974	613	4.390	622	4.074
17	Ethyl acetate	619	7.182	612	4.960	600	4.358	598	4.058
18	Chloroform	620	7.215	624	5.031	624	4.410	613	4.073
19	2-Methyl-1-propanol (Isobutyl alcohol)	633	7.566	624	5.030	615	4.394	623	4.075
20	Tetrahydrofuran	635	7.632	638	5.114	638	4.439	630	4.086
21	2-Methoxyethanol (Methyl cellosolve)	641	7.817	636	5.105	632	4.427	640	4.088
22	1,1,1-Trichloroethane	648	8.069	656	5.248	660	4.488	655	4.107
23	1,2-Dichloroethane	651	8.156	657	5.252	659	4.485	653	4.105
24	1-Butanol	670	8.874	660	5.277	652	4.469	636	4.091
25	Isopropyl acetate	668	8.792	660	5.274	650	4.464	648	4.095
26	Benzene	664	8.645	673	5.388	679	4.536	677	4.128
27	Carbon tetrachloride	665	8.677	674	5.399	681	4.542	679	4.130
28	Trichloroethylene	700	10.329	707	5.727	713	4.636	711	4.164
29	1,4-Dioxane	711	10.989	713	5.787	715	4.645	711	4.164
30	2-Ethoxyethanol (Cellosolve)	720	11.551	713	5.794	711	4.630	701	4.153
31	n-Propyl acetate	718	11.463	712	5.776	706	4.614	703	4.148

Case of isothermal analysis...

*Retention time in minutes

Because the retention ratio of straight-chain alkanes is linearly related to the number of carbons in straight-chain alkanes, 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.)	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
32	3-Methyl-1-butanol (Isoamyl alcohol)	741	13.103	732	6.028	728	4.689	719	4.173
33	4-Methyl-2-pentanone (MIBK)	743	13.262	741	6.160	742	4.738	734	4.192
34	<i>n</i> -Butyl acetate	764	15.219	758	6.411	753	4.783	750	4.205
35	1-Pentanol(Amyl alcohol)	773	16.217	764	6.516	760	4.814	750	4.213
36	Toluene	766	15.407	776	6.722	785	4.928	787	4.269
37	<i>N,N</i> -Dimethylformamide	798	19.228	784	6.887	786	4.934	784	4.264
38	2-Hexanone(MBK)	792	18.424	790	7.001	790	4.954	784	4.265
39	Tetrachloroethylene	807	20.508	819	7.672	831	5.193	838	4.365
40	Isobutyl acetate	819	22.421	812	7.502	807	5.048	796	4.285
41	Chlorobenzene	841	26.552	855	8.704	868	5.463	878	4.459
42	Ethylbenzene	857	30.202	868	9.173	879	5.551	885	4.477
43	<i>m</i> -Xylene	865	32.134	876	9.458	886	5.612	891	4.494
44	<i>N,N</i> -Dimethylacetamide	898	42.159	875	9.421	876	5.525	875	4.450
45	<i>P</i> -Xylene	866	32.305	876	9.481	886	5.616	892	4.496
46	Isopentyl acetate (Isoamyl acetate)	881	36.514	875	9.453	872	5.497	865	4.426
47	Cyclohexanol	886	38.149	888	9.964	897	5.715	905	4.531
48	1-Methylcyclohexanol	891	39.810	899	10.436	958	6.422	924	4.588
49	Styrene	885	37.885	897	10.336	908	5.828	920	4.577
50	Cyclohexanone	890	39.466	900	10.480	913	5.881	925	4.592
51	<i>o</i> -Xylene	887	38.477	899	10.470	912	5.868	925	4.592
52	2-Ethoxyethyl acetate (Cellosolve acetate)	917	49.315	905	10.708	896	5.712	888	4.485
53	2-Butoxyethanol (Butyl cellosolve)	911	46.973	907	10.837	909	5.838	911	4.551
54	<i>N</i> -Pentyl acetate	919	50.144	913	11.107	908	5.832	905	4.531
55	1,1,2,2-Tetrachloroethane	907	45.505	914	11.183	924	5.997	936	4.627
56	4-Methylcyclohexanone	950	65.552	960	13.994	975	6.671	991	4.841
57	Phenol	992	94.428	978	15.330	973	6.634	975	4.771
58	1,2-Dichlorobenzene	—	118.783	1035	21.129	1055	8.216	1076	5.294
59	<i>o</i> -Cresol	—	176.945	1056	23.918	1052	8.152	1058	5.183
60	<i>p</i> -Cresol	—	216.979	1075	26.747	1074	8.720	1072	5.243
61	<i>m</i> -Cresol	—	219.423	1076	26.923	1075	8.737	1073	5.249

*Retention time in minutes

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