

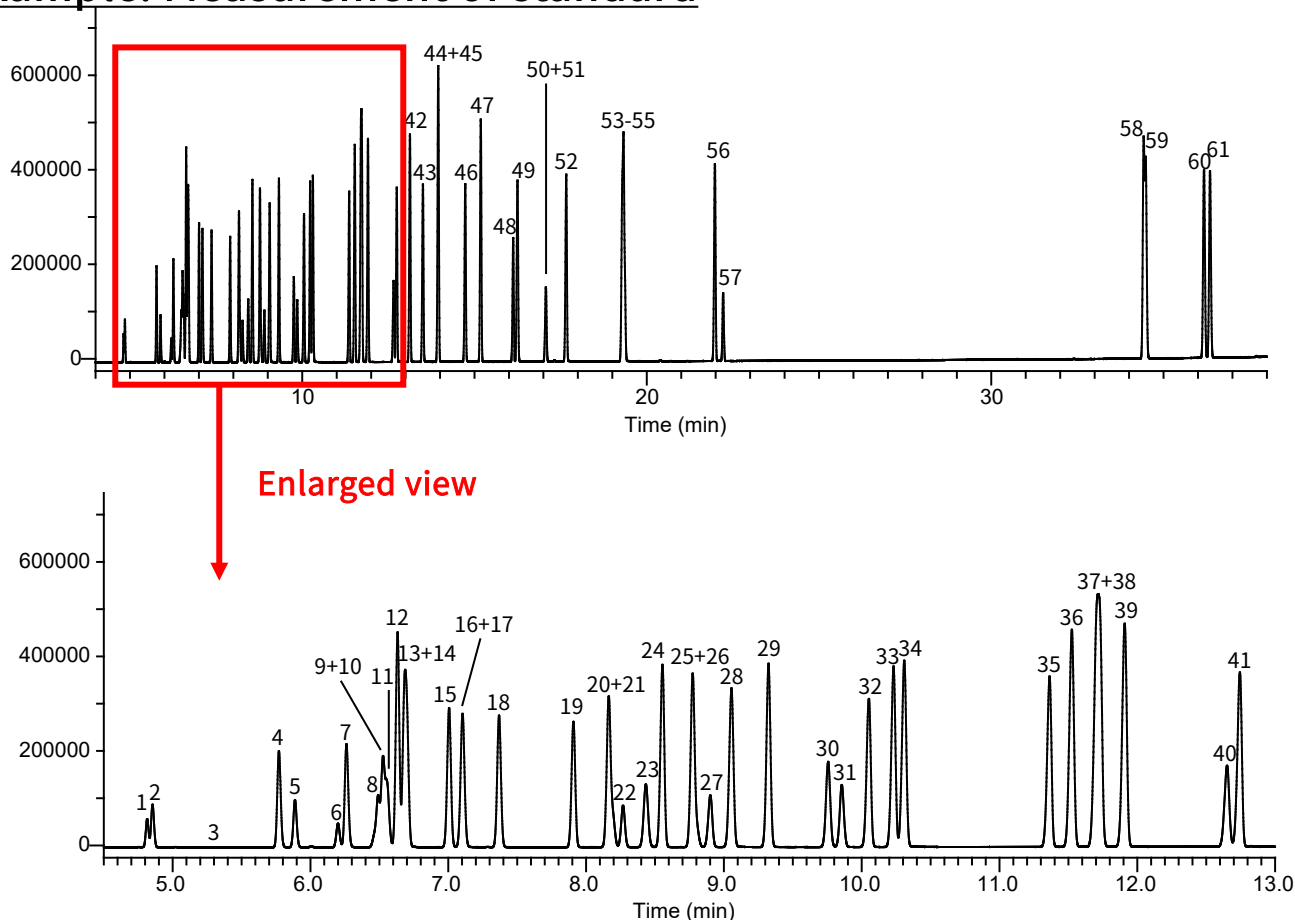
Analytical and Retention Index of 61 Components of Organic Solvents - Using InertCap Pure-WAX

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 application, InertCap Pure WAX was used to determine the retention index of 61 components in organic solvents using isothermal and temperature-rise analysis.

Example: Measurement of standard



Conditions

System	: GC - FID
Column	: InertCap Pure-WAX 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.

Only the temperature was changed for isothermal analysis.

Retention index using temperature rise analysis

Peak No.	Component	RI	RT	Peak No.	Component	RI	RT
1	<i>n</i> -Hexane	603	4.838	34	2-Methyl-1-propanol (Isobutyl alcohol)	1073	10.330
2	Diethyl ether	616	4.874	35	Isopentyl acetate (Isoamyl acetate)	1115	11.400
3	Carbon disulfide	727	5.276	36	Ethylbenzene	1121	11.568
4	Acetone	808	5.785	37	1-Butanol	1126	11.723
5	Methyl acetate	820	5.910	38	<i>p</i> -Xylene	1128	11.773
6	<i>trans</i> -1,2-Dichloroethylene	849	6.225	39	<i>m</i> -Xylene	1135	11.952
7	Tetrahydrofuran	855	6.290	40	2-Methoxyethanol (Methyl cellosolve)	1160	12.670
8	Carbon tetrachloride	874	6.493	41	<i>n</i> -Pentyl acetate	1164	12.775
9	1,1,1-Trichloroethane	876	6.520	42	<i>o</i> -Xylene	1178	13.168
10	Ethyl acetate	879	6.550	43	3-Methyl-1-butanol (Isoamyl alcohol)	1191	13.532
11	Methanol	882	6.583	44	2-Ethoxyethanol (Cellosolve)	1207	13.977
12	<i>tert</i> -Butanol	888	6.648	45	Chlorobenzene	1207	13.993
13	Isopropyl acetate	893	6.705	46	1-Pentanol(Amyl alcohol)	1233	14.762
14	2-Butanone(MEK)	895	6.721	47	Styrene	1249	15.229
15	2-Propanol (Isopropyl alcohol)	914	7.021	48	2-Ethoxyethyl acetate (Cellosolve acetate)	1281	16.157
16	Ethanol	920	7.121	49	Cyclohexanone	1286	16.290
17	Dichloromethane	921	7.143	50	Methylcyclohexanol	1311	17.045
18	Benzene	936	7.401	51	<i>N,N</i> -Dimethylformamide	1313	17.088
19	<i>n</i> -Propyl acetate	967	7.943	52	Methylcyclohexanone	1333	17.698
20	Isobutyl acetate	982	8.201	53	Cyclohexanol	1387	19.323
21	<i>cis</i> -1,2-Dichloroethylene	983	8.224	54	2-Butoxyethanol (Butylcellosolve)	1388	19.346
22	Trichloroethylene	987	8.303	55	<i>N,N</i> -Dimethylacetamide	1389	19.380
23	Acetonitrile	996	8.455	56	1,2-Dichlorobenzene	1483	22.010
24	4-Methyl-2-pentanone (MIBK)	1003	8.588	57	1,1,2,2-Tetrachloroethane	1492	22.247
25	2-Butanol	1011	8.791	58	<i>o</i> -Cresol	1977	34.454
26	Chloroform	1013	8.833	59	Phenol	1980	34.518
27	Tetrachloroethylene	1016	8.928	60	<i>p</i> -Cresol	2057	36.214
28	1-Propanol	1022	9.069	61	<i>m</i> -Cresol	2065	36.388
29	Toluene	1034	9.366				
30	1,4-Dioxane	1051	9.790				
31	1,2-Dichloroethane	1055	9.889				
32	<i>n</i> -Butyl acetate	1064	10.091				
33	2-Hexanone(MBK)	1071	10.268				

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 calculated using the following equation.

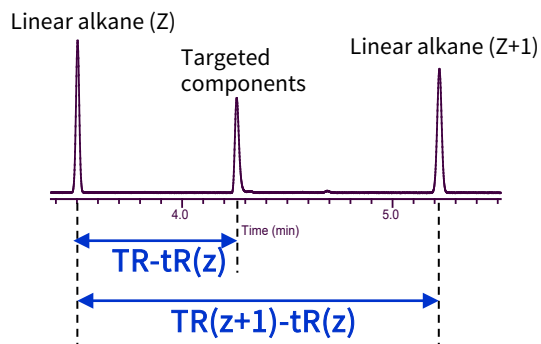
$$\text{Retention index } I = 100 \times \frac{\text{TR} - \text{tR}(Z)}{\text{TR}(Z+1) - \text{tR}(Z)} + 100 \times Z$$

TR = retention time of the target compound

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 tR(Z)



Retention index in isothermal analysis-1

Peak No. (gradient)	Component	40°C		80°C		120°C		160°C	
		RI	RT	RI	RT	RI	RT	RI	RT
1	<i>n</i> -Hexane	601	4.759	602	4.934	600	5.208	600	5.466
2	Diethyl ether	620	4.820	622	4.958	616	5.215	620	5.471
3	Carbon disulfide	726	5.363	748	5.178	765	5.330	798	5.540
4	Acetone	809	6.279	816	5.401	814	5.393	827	5.560
5	Methyl acetate	824	6.528	826	5.441	822	5.405	826	5.559
6	<i>trans</i> -1,2-Dichloroethylene	855	7.143	858	5.592	854	5.456	858	5.585
7	Tetrahydrofuran	854	7.108	874	5.681	887	5.517	900	5.625
8	Carbon tetrachloride	875	7.628	885	5.750	893	5.528	902	5.627
9	1,1,1-Trichloroethane	876	7.648	889	5.773	898	5.538	904	5.628
10	Ethyl acetate	882	7.828	884	5.744	880	5.502	875	5.600
11	Methanol	887	7.963	881	5.727	866	5.477	855	5.583
12	<i>tert</i> -Butanol	896	8.235	883	5.736	862	5.468	850	5.578
13	Isopropyl acetate	895	8.193	895	5.811	888	5.519	884	5.608
14	2-Butanone(MEK)	892	8.118	902	5.863	907	5.559	909	5.633
15	2-Propanol (Isopropyl alcohol)	922	9.144	911	5.924	892	5.527	875	5.600
16	Ethanol	926	9.318	919	5.987	903	5.551	887	5.612
17	Dichloromethane	926	9.297	925	6.034	921	5.593	920	5.643
18	Benzene	933	9.573	951	6.263	965	5.713	983	5.713
19	<i>n</i> -Propyl acetate	969	11.372	972	6.489	971	5.731	969	5.697
20	Isobutyl acetate	982	12.149	985	6.641	985	5.777	981	5.712
21	<i>cis</i> -1,2-Dichloroethylene	984	12.313	988	6.673	991	5.798	996	5.730
22	Trichloroethylene	985	12.358	995	6.757	1002	5.837	1010	5.749
23	Acetonitrile	991	12.802	1004	6.873	1011	5.873	1020	5.765
24	4-Methyl-2-pentanone (MIBK)	996	13.139	1009	6.951	1017	5.893	1025	5.773
25	2-Butanol	1017	14.773	1010	6.962	997	5.818	980	5.710
26	Chloroform	1013	14.477	1017	7.068	1015	5.888	1015	5.757
27	Tetrachloroethylene	1009	14.099	1029	7.245	1046	6.020	1065	5.837
28	1-Propanol	1029	15.838	1023	7.159	1011	5.871	996	5.730
29	Toluene	1025	15.536	1048	7.568	1066	6.117	1083	5.870
30	1,4-Dioxane	1044	17.378	1064	7.885	1081	6.198	1099	5.902
31	1,2-Dichloroethane	1056	18.792	1064	7.879	1070	6.139	1078	5.862
32	<i>n</i> -Butyl acetate	1064	19.730	1071	8.018	1072	6.148	1074	5.853
33	2-Hexanone(MBK)	1066	20.005	1080	8.220	1088	6.240	1098	5.901
34	2-Methyl-1-propanol (Isobutyl alcohol)	1081	22.104	1077	8.148	1065	6.114	1052	5.815

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

* Retention time in minutes

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

t_R = retention time of the target compound
 $t_R(Z)$ = 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 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)

Maintenance retention index in isothermal analysis-2

Peak No. (gradient)	Component	40°C		80°C		120°C		160°C	
		RI	RT	RI	RT	RI	RT	RI	RT
35	Isopentyl acetate (Isoamyl acetate)	1112	27.306	1120	9.254	1124	6.465	1125	5.958
36	Ethylbenzene	1106	26.265	1131	9.574	1151	6.668	1172	6.077
37	1-Butanol	1132	31.393	1127	9.559	1122	6.452	1112	5.929
38	<i>p</i> -Xylene	1112	27.432	1138	9.807	1159	6.733	1180	6.101
39	<i>m</i> -Xylene	1118	28.563	1144	10.014	1165	6.788	1185	6.113
40	2-Methoxyethanol (Methyl cellosolve)	1151	36.154	1167	10.851	1176	6.883	1183	6.109
41	<i>n</i> -Pentyl acetate	1160	38.651	1169	10.942	1173	6.855	1174	6.083
42	<i>o</i> -Xylene	1156	37.532	1185	11.598	1209	7.213	1233	6.269
43	3-Methyl-1-butanol (Isoamyl alcohol)	1194	49.562	1195	12.038	1188	6.993	1180	6.101
44	2-Ethoxyethanol (Cellosolve)	1197	50.563	1211	12.830	1218	7.311	1223	6.235
45	Chlorobenzene	1184	46.110	1211	12.872	1236	7.526	1263	6.387
46	1-Pentanol(Amyl alcohol)	1235	67.991	1237	14.339	1231	7.463	1224	6.238
47	Styrene	1225	63.008	1251	15.223	1273	8.023	1295	6.523
48	2-Ethoxyethyl acetate (Cellosolve acetate)	1281	96.976	1284	17.698	1282	8.163	1279	6.453
49	Cyclohexanone	1240	70.549	1282	17.499	1319	8.812	1358	6.858
50	Methylcyclohexanol	1297	109.952	1311	20.213	1322	8.870	1334	6.722
51	<i>N,N</i> -Dimethylformamide	1278	94.764	1308	19.900	1334	9.111	1361	6.878
52	Methylcyclohexanone	1281	96.647	1323	21.454	1362	9.738	1402	7.148
53	Cyclohexanol	—	—	1384	29.637	1396	10.629	1409	7.203
54	2-Butoxyethanol (Butylcellosolve)	—	—	1385	29.795	1397	10.655	1406	7.178
55	<i>N,N</i> -Dimethylacetamide	—	—	1378	28.655	1406	10.903	1433	7.391
56	1,2-Dichlorobenzene	—	—	1458	44.486	1495	14.203	1533	8.385
57	1,1,2,2-Tetrachloroethane	—	—	1493	54.496	1495	14.234	1501	8.014
58	<i>o</i> -Cresol	—	—	—	—	1967	105.964	1979	24.126
59	Phenol	—	—	—	—	1963	103.939	1981	24.288
60	<i>p</i> -Cresol	—	—	—	—	2035	147.323	2055	30.847
61	<i>m</i> -Cresol	—	—	—	—	2042	152.010	2062	31.603

*Retention time in minutes

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