

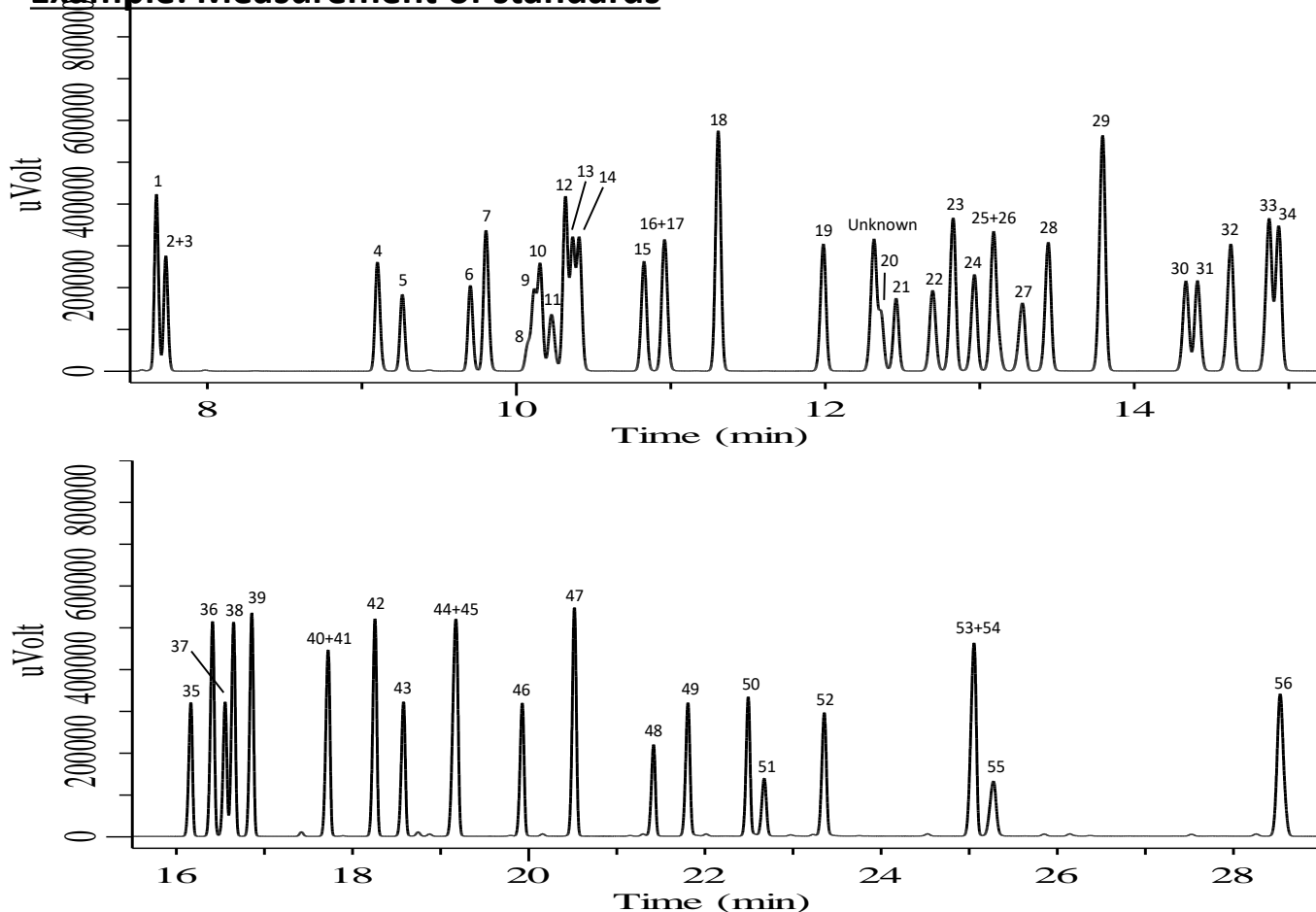
# Analysis and Retention Index of 61 Components of Organic Solvents using Nitrogen Carrier Gas - Using InertCap Pure-WAX

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 report, InertCap Pure WAX was used to determine the isothermal and temperature-rise retention indices of 61 organic solvents using nitrogen as the carrier gas.

## Example: Measurement of standards



### Conditions

<b>System</b>	: GC - FID
<b>Column</b>	: InertCap Pure-WAX 0.25 mm I.D. x 60 m df = 0.25 $\mu$ m
<b>Col. Temp.</b>	: 40 $^{\circ}$ C - 5 $^{\circ}$ C/min - 220 $^{\circ}$ C
<b>Carrier Gas</b>	: N <sub>2</sub> 90 kPa
<b>Injection</b>	: Split 1:50 240 $^{\circ}$ C
<b>Detection</b>	: FID Range 10 <sup>10</sup> 240 $^{\circ}$ C
<b>Sample Size</b>	: Mixed evenly 0.2 $\mu$ 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	<i>n</i> -Hexane	598	7.690	34	2-Methyl-1-propanol (Isobutyl alcohol)	1065	14.953
2	Ethyl ether	611	7.745	35	Isopentyl acetate (Isoamyl acetate)	1098	16.211
3	Carbon disulfide	613	7.750	36	Ethylbenzene	1109	16.384
4	Acetone	808	9.113	37	1-Butanol	1114	16.572
5	Methyl acetate	819	9.276	38	<i>P</i> -Xylene	1117	16.617
6	<i>Trans</i> -1,2-Dichloroethylene	848	9.718	39	<i>M</i> -Xylene	1123	16.821
7	Tetrahydrofuran	855	9.819	40	<i>N</i> -Pentyl acetate	1149	17.793
8	Carbon tetrachloride	873	10.091	41	2-Methoxyethanol (Methyl cellosolve)	1152	17.728
9	1,1,1-Trichloroethane	876	10.131	42	<i>O</i> -Xylene	1168	18.218
10	Ethyl acetate	878	10.170	43	3-Methyl-1-butanol (Isoamyl alcohol)	1180	18.600
11	Methanol	882	10.223	44	Chlorobenzene	1195	19.226
12	<i>Tert</i> -Butanol	888	10.324	45	2-Ethoxyethanol (Cellosolve)	1198	19.162
13	Isopropyl acetate	892	10.376	46	1-Pentanol (Amyl alcohol)	1222	19.953
14	Methyl ethyl ketone	895	10.421	47	Styrene	1239	20.489
15	2-Propanol (Isopropyl alcohol)	915	10.833	48	2-Ethoxyethyl acetate (Cellosolve acetate)	1264	21.472
16	Dichloromethane	920	10.964	49	Cyclohexanone	1276	21.871
17	Ethanol	921	10.966	50	1-Methylcyclohexanol	1297	22.554
18	Benzene	936	11.324	51	<i>N,N</i> -Dimethylformamide	1305	22.690
19	<i>n</i> -Propyl acetate	966	12.007	52	4-Methylcyclohexanone	1322	23.434
20	<i>cis</i> -1,2-Dichloroethylene	982	12.372	53	Cyclohexanol	1369	25.094
21	Trichloroethylene	987	12.473	54	2-Butoxyethanol (Butyl cellosolve)	1369	25.117
22	Acetonitrile	997	12.703	55	<i>N,N</i> -Dimethylacetamide	1375	25.303
23	4-Methyl-2-pentanone (MIBK)	1002	12.848	56	1,2-Dichlorobenzene	1434	28.613
24	Isobutyl acetate	1006	12.983	57	1,1,2,2-Tetrachloroethane	—	—
25	2-Butanol	1010	13.101	58	Phenol	—	—
26	Chloroform	1011	13.130	59	<i>O</i> -Cresol	—	—
27	Tetrachloroethylene	1014	13.304	60	<i>P</i> -Cresol	—	—
28	1-Propanol	1020	13.455	61	<i>M</i> -Cresol	—	—
29	Toluene	1031	13.819				
30	1,4-Dioxane	1047	14.349				
31	1,2-Dichloroethane	1049	14.423				
32	<i>n</i> -Butyl acetate	1054	14.695				
33	2-Hexanone (MBK)	1062	14.946				

\* 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.

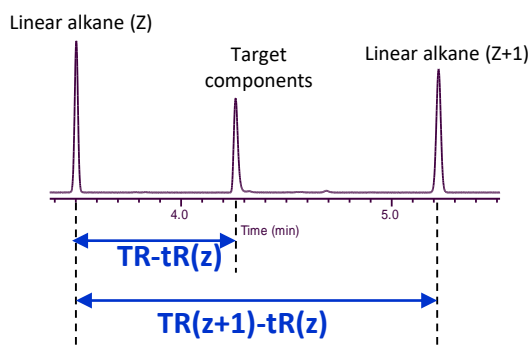
$$\text{Retention index } I = 100 \times \frac{\text{TR} - \text{tR}}{\text{TR}(Z+1) - \text{tR}(Z)} + 100 \times Z$$

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)



## 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</i> -Hexane	600	7.495	600	7.233	600	7.676	600	7.452
2	Ethyl ether	616	7.573	605	7.243	598	7.675	631	7.465
3	Carbon disulfide	615	7.572	606	7.244	600	7.676	643	7.470
4	Acetone	808	9.816	812	7.874	817	7.940	825	7.585
5	Methyl acetate	824	10.192	822	7.933	821	7.948	832	7.591
6	<i>Trans</i> -1,2-Dichloroethylene	855	11.141	855	8.145	855	8.023	869	7.659
7	Tetrahydrofuran	854	11.103	873	8.286	888	8.114	920	7.687
8	Carbon tetrachloride	875	11.880	884	8.380	893	8.127	906	7.701
9	1,1,1-Trichloroethane	876	11.916	887	8.409	898	8.143	924	7.693
10	Ethyl acetate	882	12.193	882	8.368	881	8.093	896	7.657
11	Methanol	890	12.569	884	8.383	874	8.041	867	7.657
12	<i>Tert</i> -Butanol	898	12.916	882	8.361	864	8.047	854	7.612
13	Isopropyl acetate	895	12.758	894	8.472	890	8.119	885	7.677
14	Methyl ethyl ketone	893	12.650	900	8.537	908	8.175	926	7.695
15	2-Propanol (Isopropyl alcohol)	924	14.334	910	8.631	894	8.130	879	7.638
16	Dichloromethane	926	14.437	923	8.772	922	8.222	930	7.701
17	Ethanol	928	14.560	918	8.719	906	8.168	892	7.653
18	Benzene	933	14.865	950	9.115	967	8.399	983	7.811
19	<i>N</i> -Propyl acetate	969	17.634	972	9.442	973	8.426	972	7.793
20	<i>cis</i> -1,2-Dichloroethylene	984	19.028	987	9.682	991	8.513	1002	7.817
21	Trichloroethylene	985	19.095	994	9.807	1002	8.570	1010	7.858
22	Acetonitrile	992	19.836	1002	9.963	1014	8.633	1021	7.854
23	4-Methyl-2-pentanone (MIBK)	997	20.397	1009	10.092	1019	8.660	1027	7.891
24	Isobutyl acetate	1007	21.555	1011	10.136	1013	8.626	1014	7.865
25	2-Butanol	1018	23.109	1010	10.108	998	8.548	992	7.799
26	Chloroform	1013	22.330	1016	10.233	1017	8.652	1023	7.858
27	Tetrachloroethylene	1008	21.803	1028	10.503	1044	8.806	1076	7.978
28	1-Propanol	1029	24.744	1023	10.401	1013	8.629	1004	7.821
29	Toluene	1024	24.037	1046	10.953	1067	8.975	1087	8.027
30	1,4-Dioxane	1042	26.861	1063	11.419	1083	9.098	1099	8.059
31	1,2-Dichloroethane	1053	28.842	1062	11.389	1071	9.009	1084	7.999
32	<i>n</i> -Butyl acetate	1061	30.444	1070	11.605	1074	9.028	1078	8.004
33	2-Hexanone(MBK)	1063	30.962	1080	11.917	1092	9.172	1101	8.066
34	2-Methyl-1-propanol (Isobutyl alcohol)	1079	34.420	1076	11.809	1068	8.982	1059	7.937

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  $t'R = t_R - t_0$   
 $T_0$  = hold-up time (elution time of non-retentive components)

## Retention index in isothermal analysis-2

Peak No.	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
35	Isopentyl acetate (Isoamyl acetate)	1107	42.040	1120	13.378	1125	9.483	1130	8.148
36	Ethylbenzene	1101	40.399	1129	13.808	1152	9.777	1173	8.294
37	1-Butanol	1129	48.925	1130	13.847	1124	9.472	1115	8.103
38	<i>p</i> -Xylene	1107	42.171	1137	14.133	1160	9.866	1181	8.324
39	<i>m</i> -Xylene	1113	43.922	1143	14.433	1166	9.943	1188	8.348
40	<i>n</i> -Pentyl acetate	1157	59.524	1168	15.772	1175	10.051	1181	8.324
41	2-Methoxyethanol (Methyl cellosolve)	1149	56.356	1167	15.712	1179	10.102	1196	8.372
42	<i>o</i> -Xylene	1152	57.659	1183	16.695	1211	10.566	1236	8.559
43	3-Methyl-1-butanol (Isoamyl alcohol)	1191	77.198	1190	17.245	1191	10.266	1183	8.330
44	Chlorobenzene	1180	70.726	1209	18.483	1237	11.009	1265	8.705
45	2-Ethoxyethanol (Cellosolve)	1194	78.787	1210	18.565	1220	10.721	1227	8.513
46	1-Pentanol(Amyl alcohol)	1213	90.267	1237	20.737	1234	10.951	1228	8.520
47	Styrene	1216	92.514	1249	21.839	1273	11.730	1297	8.887
48	2-Ethoxyethyl acetate (Cellosolve acetate)	1223	97.195	1283	25.450	1284	11.965	1284	8.813
49	Cyclohexanone	1219	94.608	1281	25.215	1320	12.895	1362	9.349
50	1-Methylcyclohexanol	1225	98.379	1311	29.169	1324	12.991	1340	9.178
51	<i>N,N</i> -Dimethylformamide	1223	97.548	1269	23.883	1337	13.381	1366	9.383
52	4-Methylcyclohexanone	1224	97.888	1322	30.901	1363	14.251	1406	9.748
53	Cyclohexanol	1229	101.734	1383	42.798	1397	15.557	1413	9.818
54	2-Butoxyethanol (Butyl cellosolve)	1229	101.695	1383	42.985	1398	15.594	1411	9.796
55	<i>N,N</i> -Dimethylacetamide	1228	101.248	1378	41.668	1408	16.024	1437	10.079
56	1,2-Dichlorobenzene	—	—	1459	64.015	1496	20.663	1530	11.369
57	1,1,2,2-Tetrachloroethane	—	—	—	—	—	—	1498	10.898
58	Phenol	—	—	—	—	—	—	1985	32.757
59	<i>o</i> -Cresol	—	—	—	—	—	—	1982	32.503
60	<i>p</i> -Cresol	—	—	—	—	—	—	2058	41.521
61	<i>m</i> -Cresol	—	—	—	—	—	—	2065	42.580

\* Retention time in minutes

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