GT065

GL Sciences Inc.

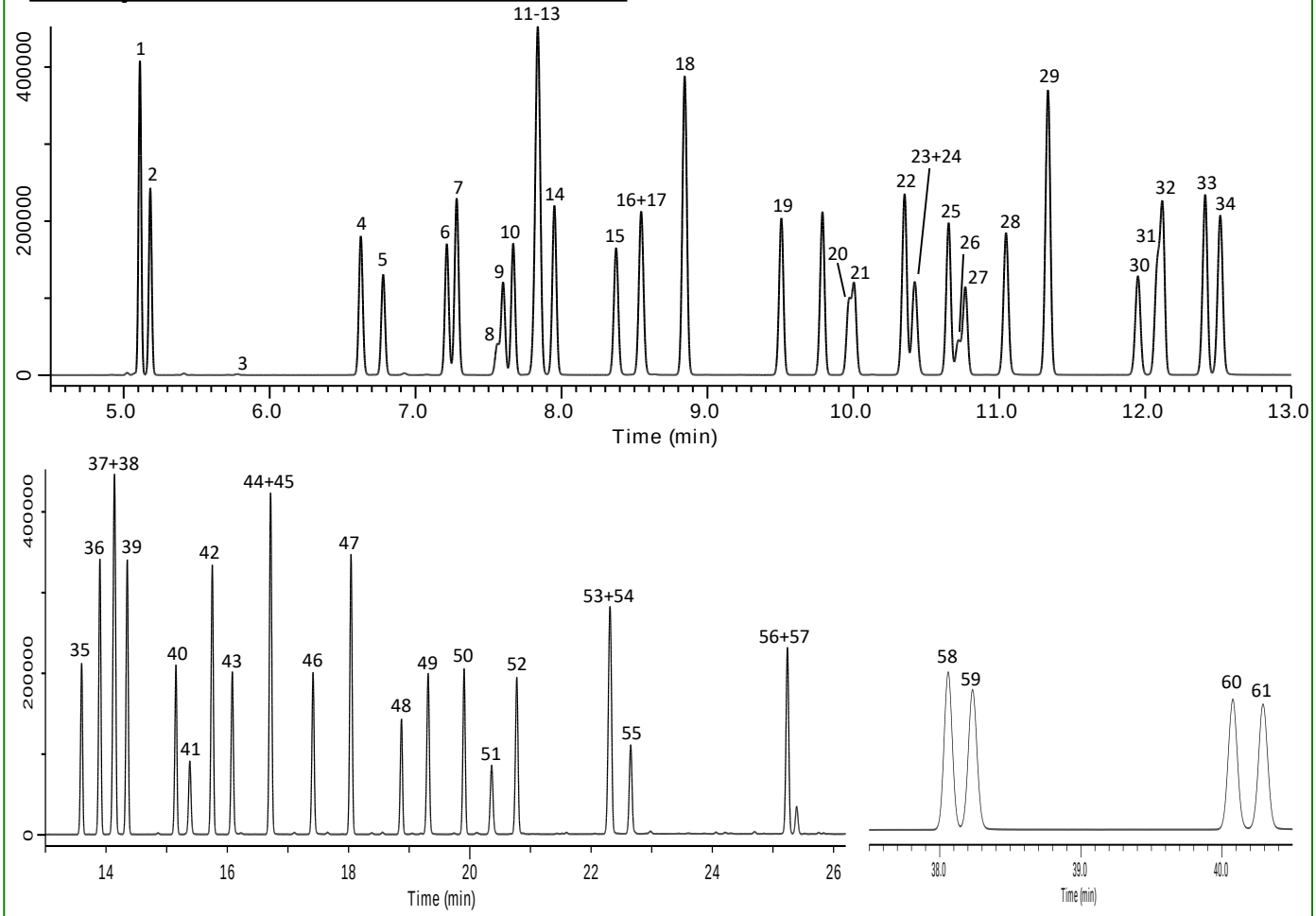
# Analytical and Retention Index of 61 Components of Organic Solvents - Using InertCap WAX

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<br>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<br>240 ˚C |
| **Detection** | : FID Range 10^0<br>240 ˚C |
| **Sample Size** | : Mixed evenly<br>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 | *n-Hexane* | 599 | 5.122 | 34 | 2-Methyl-1-propanol (Isobutyl alcohol) | 1093 | 12.526 |
| 2 | Ethyl ether | 616 | 5.189 | | | | |
| 3 | Carbon disulfide | 735 | 5.813 | 35 | Isopentyl acetate (Isoamyl acetate) | 1126 | 13.612 |
| 4 | Acetone | 820 | 6.632 | | | | |
| 5 | Methyl acetate | 831 | 6.784 | 36 | Ethylbenzene | 1135 | 13.922 |
| 6 | *Trans-1,2-Dichloroethylene* | 861 | 7.218 | 37 | 1-Butanol | 1142 | 14.145 |
| 7 | Tetrahydrofuran | 866 | 7.293 | 38 | *p-Xylene* | 1143 | 14.168 |
| 8 | Carbon tetrachloride | 885 | 7.576 | 39 | *m-Xylene* | 1149 | 14.375 |
| 9 | 1,1,1-Trichloroethane | 888 | 7.613 | 40 | *N-Pentyl acetate* | 1173 | 15.172 |
| 10 | Ethyl acetate | 893 | 7.676 | 41 | 2-Methoxyethanol (Methyl cellosolve) | 1179 | 15.394 |
| 11 | Methanol | 902 | 7.821 | | | | |
| 12 | Tert-Butanol | 903 | 7.838 | 42 | *o-Xylene* | 1190 | 15.730 |
| 13 | Isopropyl acetate | 903 | 7.862 | 43 | 3-Methyl-1-butanol (Isoamyl alcohol) | 1201 | 16.108 |
| 14 | Methyl ethyl ketone | 908 | 7.954 | | | | |
| 15 | 2-Propanol (Isopropyl alcohol) | 927 | 8.381 | 44 | 2-Ethoxyethanol (Cellosolve) | 1219 | 16.670 |
| 16 | Ethanol | 935 | 8.549 | 45 | Chlorobenzene | 1219 | 16.686 |
| 17 | Dichloromethane | 935 | 8.549 | 46 | 1-Pentanol(Amyl alcohol) | 1243 | 17.441 |
| 18 | Benzene | 949 | 8.862 | 47 | Styrene | 1263 | 18.070 |
| 19 | *n-Propyl acetate* | 979 | 9.525 | 48 | 2-Ethoxyethyl acetate (Cellosolve acetate) | 1289 | 18.898 |
| 20 | *Cis-1,2-Dichloroethylene* | 1000 | 9.967 | | | | |
| 21 | Trichloroethylene | 1001 | 10.020 | 49 | Cyclohexanone | 1301 | 19.292 |
| 22 | 4-Methyl-2-pentanone (MIBK) | 1014 | 10.366 | 50 | 1-Methylcyclohexanol | 1321 | 19.938 |
| | | | | 51 | *N,N-Dimethylformamide* | 1333 | 20.310 |
| 23 | Acetonitrile | 1016 | 10.425 | 52 | 4-Methylcyclohexanone | 1349 | 20.810 |
| 24 | Isobutyl acetate | 1018 | 10.468 | 53 | 2-Butoxyethanol (Butyl cellosolve) | 1394 | 22.259 |
| 25 | 2-Butanol | 1025 | 10.659 | | | | |
| 26 | Chloroform | 1027 | 10.719 | 54 | Cyclohexanol | 1395 | 22.293 |
| 27 | Tetrachloroethylene | 1029 | 10.779 | 55 | *N,N-Dimethylacetamide* | 1406 | 22.614 |
| 28 | 1-Propanol | 1039 | 11.054 | 56 | 1,1,2,2-Tetrachloroethane | 1502 | 25.248 |
| 29 | Toluene | 1050 | 11.348 | 57 | 1,2-Dichlorobenzene | 1503 | 25.268 |
| 30 | 1,4-Dioxane | 1072 | 11.967 | 58 | *o-Cresol* | 2029 | 38.084 |
| 31 | 1,2-Dichloroethane | 1077 | 12.087 | 59 | Phenol | 2036 | 38.256 |
| 32 | *n-Butyl acetate* | 1078 | 12.138 | 60 | *p-Cresol* | 2112 | 40.101 |
| 33 | 2-Hexanone(MBK) | 1089 | 12.434 | 61 | *m-Cresol* | 2121 | 40.316 |

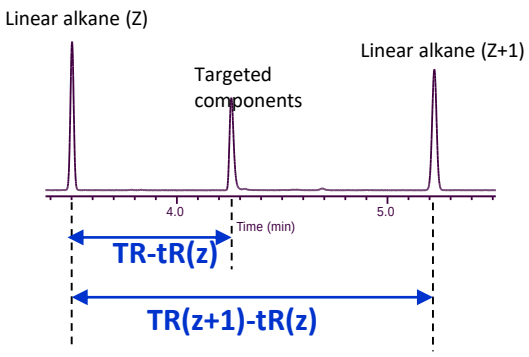
In the case of temperature programming...

* 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.

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

T R = retention time of the target ingredient
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)



## Retention index in isothermal analysis-1

| Peak No. (gradient temp.) | Component | 40℃ | | 80℃ | | 120℃ | | 160℃ | |
|---|---|---|---|---|---|---|---|---|---|
| | | Retention index | Retention time | Retention index | Retention time | Retention index | Retention time | Retention index | Retention time |
| 1 | *N-Hexane* | 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 | *Trans-1,2-Dichloroethylene* | 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 | *N-Propyl acetate* | 980 | 13.977 | 983 | 6.460 | 984 | 4.954 | 987 | 4.393 |
| 20 | *Cis-1,2-Dichloroethylene* | 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 | *n-Butyl acetate* | 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.

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

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)

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