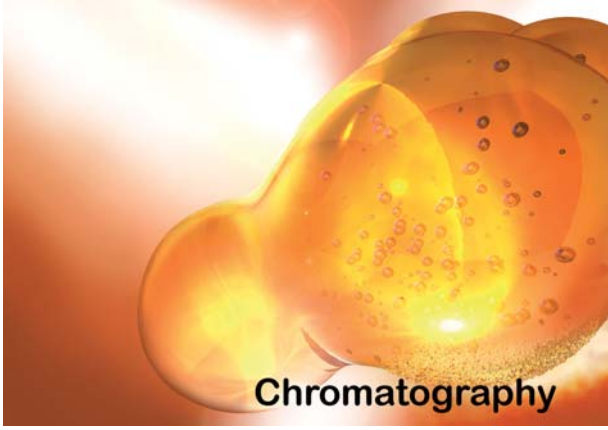

Application Note

Linear Retention Index Function (LRI) in GCMSsolution 2.4
An excellent help for identification confirmation of target compounds in complex chromatograms

Whenever a complex analysis has to be done with a large number of peaks and interfering matrix signals GCMS identification may be time consuming and/or difficult. Examples are the analysis of flavours and fragrances or the screening of pollutants in environmental/food matrices. As a help for identification the concept of linear retention index (LRI, Temperature ramp condition) may be applied. The concept is well known for a long time but now the standard Shimadzu GCMSsolution 2.4 software offer an easy and practical handling of this concept. The procedure is visualized in figure 1.

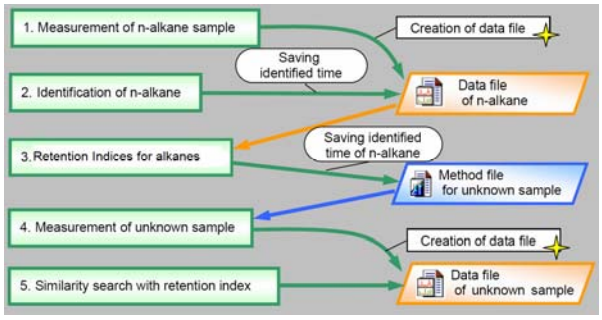

Fig. 1: Flow diagram for the LRI concept

The procedure is described in more detail in the following. In figure 2 the TIC relative to a n-alkane mix is shown together with the compound table after identification.

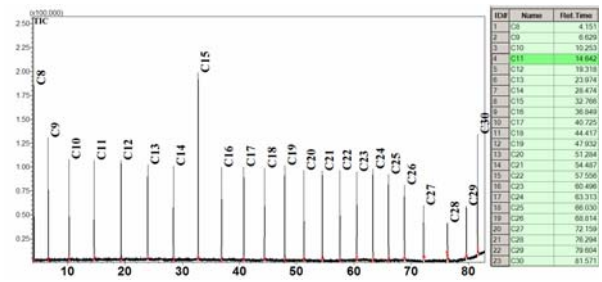

Fig. 2: TIC of an n-alkane mix recorded under temperature ramp condition.

The compound table is stored in the data file (all in one data file structure of GCMSsolution software).

The method for the unknown samples with the LRI calibration can either be derived from the alkane file or freely created using the GCMS real time or GCMS analysis editor (off line method development) offering maximum flexibility. In any way the retention index calculation based on the n-alkanes are stored in the method. Here as an example the GCMS analysis editor is used.

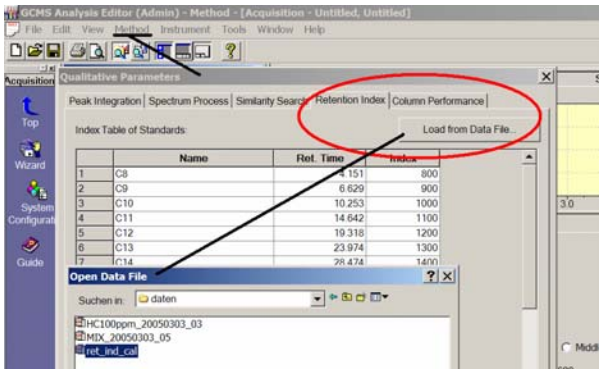

Fig.3: Method qualitative parameters. The LRI is automatically calculated from the carbon number in the name field multiplied by 100.

With the “Load from Data File” button the alkane data file is selected and the list of alkanes together with the retention times is read from the alkane file. The LRI is automatically calculated. Finally the method is saved. The next step is to record the unknown sample and to make an identification by library search. The figure 4 shows a part of a TIC where two peaks (fenchol and terpineole) elute close together resulting in spectra for each compound which are interfered by the other. However due to the alkane calibration each scan point on the TIC trace is correlated with an LRI indicated in the lower part of figure 4. The LRI for the 2 peaks are 1090 and 1091.

SHIMADZU
Solutions for Science
since 1875

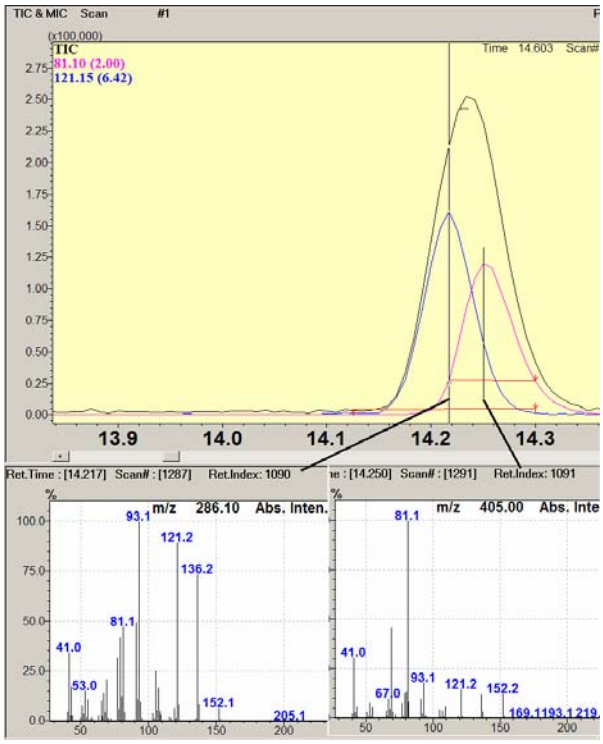

Fig. 4: Peaks of fenchol and terpineol at selected mass traces and spectra at the top.

So even without background subtraction it is possible to differentiate the two peaks by the difference in LRI.
In addition it is possible to perform a library search with or without an LRI filter. The parameters how to do it are also set in the qualitative parameter window. This is shown in figure 5.

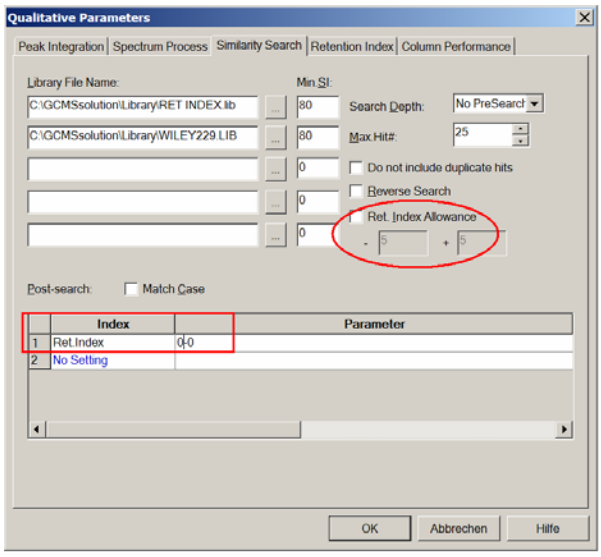

Fig. 5: Method qualitative parameters – similarity search tab.

Retention index allowance filter can been set as well as retention index range filter. The library search can be performed simultaneously in up to 5 libraries (commercial or private). Here as an example one with and one without LRI entries is used. Figure 6 indicates the library search result of the raw spectra indicated in figure 4. Two lists of matches with decreasing similarity indices SI are shown.

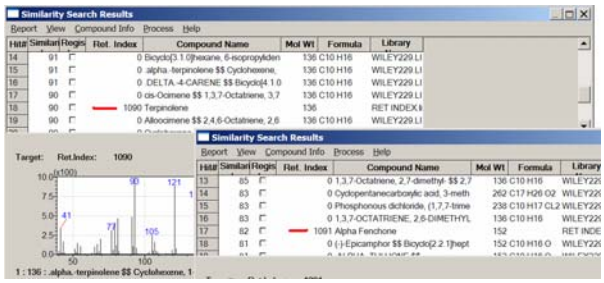

Fig. 6: Library search results using two libraries. One with the other without LRI entries. Among the list the hits from the private library containg LRIs are marked by the red dash.

When using the LRI filter with allowance of ±1 only one hit in each case remains. This is shown in figure 7.

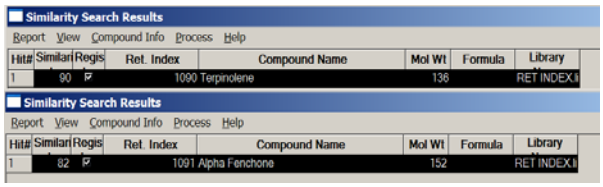

Fig. 7: Library search results using an LRI filter

With background subtraction the similarities are of course much higher as demonstrated in figure 8 for the compound terpinolene.

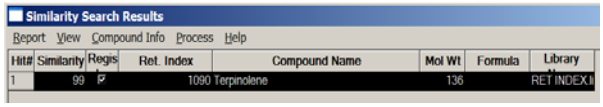

Fig. 8: Library search result for terpinolene with LRI filter and spectrum background subtraction.

The LRI function of GCMSsolution 2.4 offers a convenient help in routine identification work of complex chromatograms. At the same time library searches can be done with libraries which contain or do not contain LRIs.

The given specifications serve purely as technical information for the user.
No guarantee is given on technical specification of the described product and/or procedures.