

# Press Release

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## **New: FFNSC-MS library Higher accuracy in the identification of unknown fragrances**

### **Spectral library for fragrance and flavour compounds using LRI/ Helpful in the differentiation of isomers and homologues**

Shimadzu, one of the world leaders in analytical instrumentation, has introduced its new FFNSC-MS library (Flavours and Fragrances Natural and Synthetic Compounds) that contains approximately 1,200 mass spectra of various flavour and fragrance compounds. The spectra were acquired using a Shimadzu GCMS-QP2010 system in the laboratory of Professor Luigi Mondello at the University of Messina, Italy. For this purpose, only pure substances were used. In order to offer users the highest possible accuracy and reliability for the identification of unknown samples, the linear retention index (LRI) of each compound was determined in addition to the mass spectra and included in the spectral library.

### **Automatic LRI calculation**

Each compound possesses its own specific LRI. The retention times of the components of a hydrocarbon standard are used as a reference. The GCMSsolution software (from version 2.4) automatically carries

out the LRI calculation for each peak of an unknown sample, after separation and determination of the hydrocarbon standard using the same column. The LRI is solely dependent on the type of stationary phase in the column. The column dimensions, on the other hand, are irrelevant.

A temperature program is used for the separation. Even after exchanging the column, the LRI values remain constant if the same stationary phase is being used. For the current library a non-polar standard dimethyl siloxane column with a 5% phenyl-substitution was used.

### **MS library searches using the LRI**

For each compound in the FFNSC library, the LRI was calculated and stored. During the library search the library spectra are compared with those of the unknown compounds, and the stored LRI data are also compared with the values that the software has calculated for each individual peak. This is extremely helpful for the correct determination of compounds showing very similar fragmentation patterns, such as homologues or isomers of terpenes. The acquired mass spectra are of excellent quality, as the FFNSC library is entirely based on standards of pure compounds. When mass spectra and LRI data are combined, identification of unknown compounds reaches a hitherto unrivalled level of accuracy.

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