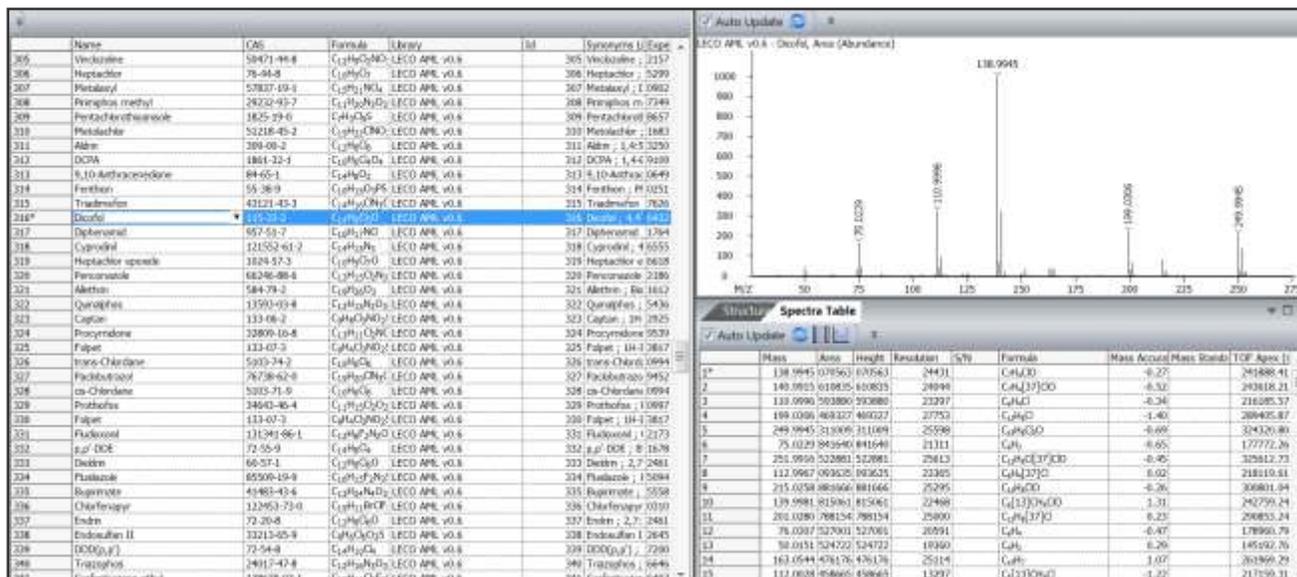# LECO Accurate Mass Library

Mass Spectral Databases

Mass spectral databases are the foundation of identification tools in mass spectrometry. Their use and development has enabled GC-MS to be a dominant and routine technique in many applications of hyphenated MS technologies. Over the past several years, the use of high resolution (accurate mass) mass spectrometry and its data has expanded into all areas of application, which could take advantage of spectral databases specifically developed to exploit these novel instrumentation capabilities. LECO's accurate mass-based spectral database, its curation, and application of novel algorithms result in similarity searches, which are further improved by the information obtained through high performance GC-MS.

Truly take your identification of known unknowns to a new level.

With LECO's new Accurate Mass Library for the Pegasus GC-HRT+ you can now compare your high resolution data to those acquired and curated by leading researchers. Take further advantage of a novel algorithm that calculates a similarity score based on the accuracy of the data (AML Rank).
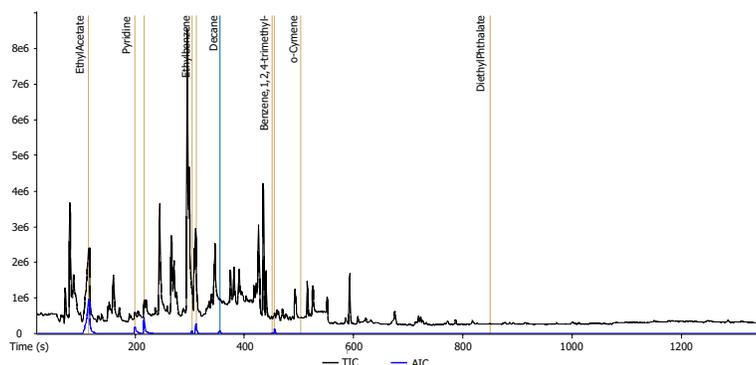
Name	Similarity	AML Rank	Mass Accuracy (ppm)	R.T. (s)	Peak S/N
Ethyl Acetate	820	979	-0.36	114.0	2904
Pyridine	927	926	-0.39	198.7	7770
Toluene	910	919	0.47	215.6	2160
Ethylbenzene	816	881	1.06	303.4	335
o-Xylene	904	861	1.16	310.9	556
Decane	768	664	N/A	354.5	132
Benzene, 1,2,4-trimethyl-	762	814	0.58	450.1	256
D-Limonene	861	851	0.17	455.1	233
o-Cymene	651	776	0.67	502.1	52
Diethyl Phthalate	802	828	N/A	849.5	168
Dodecane	694	761	N/A	1243.6	56

Extra Virgin Olive Oil run on the Pegasus GC-HRT. Shown for only those species that match for AML library.

LECO

EMPOWERING RESULTS

AML Rank and Similarity Score

Accurate Mass Library Rank is a measure of how close the masses align between two spectra and the similarities of the spectra. A number between 0 and 1000, expressing how closely two spectra match, based on mass accuracy. A higher number means a closer match. The spectral masses are paired if they have overlapping mass confidence intervals, which are based on the mass spectrometer's resolution. Each pair is scored by the mass difference relative to a mass tolerance value. The final score for the spectra is the sum of the scores for each pair, weighted by the sum of the abundance of both masses in the pair. The score is not affected by the difference in abundance between the matching masses. In contrast, the NIST similarity score is based on the relative abundances of the matched pairs of masses, and weighs them based on MW and the abundance ratios of adjacent matching peaks. There is no comparison of accurate masses because the masses are grouped into 1 amu wide segments. Therefore, AML rank and NIST similarity are independent metrics, each scoring based on different spectral characteristics.

The similarity metric should be familiar to users who perform conventional NIST library searches. Typically, if a high-resolution spectrum is searched against a nominal mass library, then masses are converted to nominal masses, each spectrum is normalized to a base peak relative abundance of 1000, and the library spectrum is projected onto the reported spectrum. Thus, the similarity metric is penalized for signals present in the reported spectrum, but absent from the library spectrum.

LECO Accurate Mass Spectral Library

- Available on DVD (Part Number 359-011-120) for both Pegasus GC-HRT and GC-HRT$^+$ systems.
- In collaboration with Prof. Albert Lebedev, Moscow State University.
- Approximately 1822 compounds: alkanes, PAH, essential oils, pesticides, and general SVOCs.