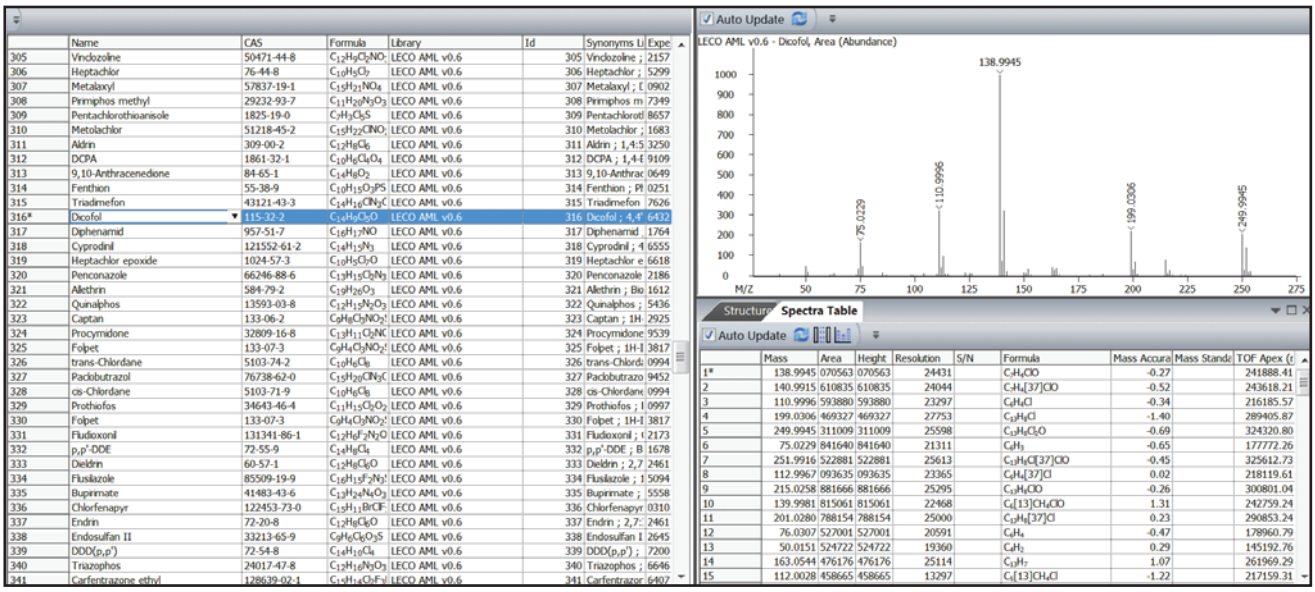
LECO Accurate Mass Library

Mass Spectral Databases



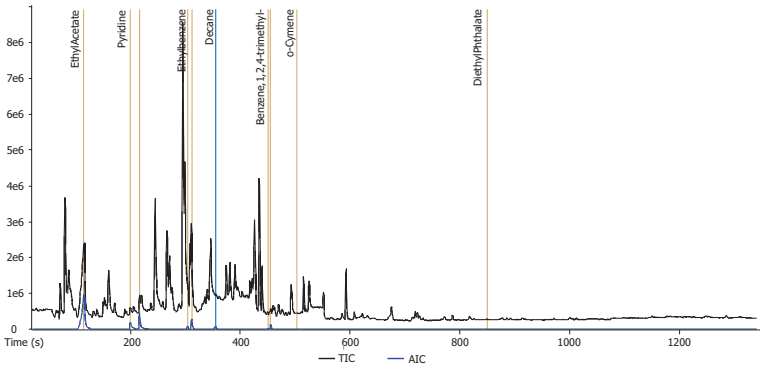
	Name	CAS	Formula	Library	Id	Synonyms Li	Expe
305	Vinclozoline	50471-44-8	$C_{12}H_9Cl_2NO_3$	LECO AML v0.6	305	Vinclozoline ;	2157
306	Heptachlor	76-44-8	$C_{10}H_5Cl_7$	LECO AML v0.6	306	Heptachlor ;	5299
307	Metalaxyl	57837-19-1	$C_{15}H_{21}NO_4$	LECO AML v0.6	307	Metalaxyl ; [	0902
308	Pirimiphos methyl	29232-93-7	$C_{11}H_{20}N_3O_3PS$	LECO AML v0.6	308	Pirimiphos m	7349
309	Pentachlorothioanisole	1825-19-0	$C_7H_3Cl_5S$	LECO AML v0.6	309	Pentachlorotl	8657
310	Metolachlor	51218-45-2	$C_{15}H_{22}ClNO_2$	LECO AML v0.6	310	Metolachlor ;	1683
311	Aldrin	309-00-2	$C_{12}H_8Cl_6$	LECO AML v0.6	311	Aldrin ; 1,4:5	3250
312	DCPA	1861-32-1	$C_{10}H_6Cl_4O_4$	LECO AML v0.6	312	DCPA ; 1,4-E	9109
313	9,10-Anthracenedione	84-65-1	$C_{14}H_8O_2$	LECO AML v0.6	313	9,10-Anthrac	0649
314	Fenthion	55-38-9	$C_{10}H_{15}O_3PS_2$	LECO AML v0.6	314	Fenthion ; Pt	0251
315	Triadimefon	43121-43-3	$C_{14}H_{16}ClN_3O_2$	LECO AML v0.6	315	Triadimefon	7626
316*	Dicofol	115-32-2	$C_{14}H_9Cl_5O$	LECO AML v0.6	316	Dicofol ; 4,4'	6432
317	Diphenamid	957-51-7	$C_{16}H_{17}NO$	LECO AML v0.6	317	Diphenamid	1764
318	Cyprodinil	121552-61-2	$C_{14}H_{15}N_3$	LECO AML v0.6	318	Cyprodinil ; 4	6555
319	Heptachlor epoxide	1024-57-3	$C_{10}H_5Cl_7O$	LECO AML v0.6	319	Heptachlor e	6618
320	Penconazole	66246-88-6	$C_{13}H_{15}Cl_2N_3$	LECO AML v0.6	320	Penconazole	2186
321	Allethrin	584-79-2	$C_{19}H_{26}O_3$	LECO AML v0.6	321	Allethrin ; Bio	1612
322	Quinalphos	13593-03-8	$C_{12}H_{15}N_2O_3PS$	LECO AML v0.6	322	Quinalphos ;	5436
323	Captan	133-06-2	$C_9H_8Cl_3NO_2S$	LECO AML v0.6	323	Captan ; 1H-	2925
324	Procymidone	32809-16-8	$C_{13}H_{11}Cl_2NO_2$	LECO AML v0.6	324	Procymidone	9539
325	Folpet	133-07-3	$C_9H_4Cl_3NO_2S$	LECO AML v0.6	325	Folpet ; 1H-I	3817
326	trans-Chlordane	5103-74-2	$C_{10}H_6Cl_8$	LECO AML v0.6	326	trans-Chlord	0994
327	Paclobutrazol	76738-62-0	$C_{15}H_{20}ClN_3O$	LECO AML v0.6	327	Paclobutrazo	9452
328	cis-Chlordane	5103-71-9	$C_{10}H_6Cl_8$	LECO AML v0.6	328	cis-Chlordane	0994
329	Prothiofos	34643-46-4	$C_{11}H_{15}Cl_2O_2PS_2$	LECO AML v0.6	329	Prothiofos ; [	0997
330	Folpet	133-07-3	$C_9H_4Cl_3NO_2S$	LECO AML v0.6	330	Folpet ; 1H-I	3817
331	Fludioxonil	131341-86-1	$C_{12}H_6F_2N_2O_2$	LECO AML v0.6	331	Fludioxonil ; [	2173
332	p,p'-DDE	72-55-9	$C_{14}H_8Cl_4$	LECO AML v0.6	332	p,p'-DDE ; B	1678
333	Dieldrin	60-57-1	$C_{12}H_8Cl_6O$	LECO AML v0.6	333	Dieldrin ; 2,7	2461
334	Flusilazole	85509-19-9	$C_{16}H_{15}F_2N_3Si$	LECO AML v0.6	334	Flusilazole ; 1	5094
335	Bupirimate	41483-43-6	$C_{13}H_{24}N_4O_3S$	LECO AML v0.6	335	Bupirimate ;	5558
336	Chlorfenapyr	122453-73-0	$C_{15}H_{11}BrClF_3N_2O$	LECO AML v0.6	336	Chlorfenapyr	0310
337	Endrin	72-20-8	$C_{12}H_8Cl_6O$	LECO AML v0.6	337	Endrin ; 2,7-	2461
338	Endosulfan II	33213-65-9	$C_9H_6Cl_6O_3S$	LECO AML v0.6	338	Endosulfan I	2645
339	DDD(p,p')	72-54-8	$C_{14}H_{10}Cl_4$	LECO AML v0.6	339	DDD(p,p') ;	7200
340	Triazophos	24017-47-8	$C_{12}H_{16}N_3O_3PS$	LECO AML v0.6	340	Triazophos ;	6646
341	Carfentrazone ethyl	128639-02-1	$C_{15}H_{14}Cl_2F_3N_3O_3$	LECO AML v0.6	341	Carfentrazor	6407

	Mass	Area	Height	Resolution	S/N	Formula	Mass Accura	Mass Standa	TOF Apex (t
1*	138.9945	070563	070563	24431		C_7H_4ClO	-0.27		241888.41
2	140.9915	610835	610835	24044		$C_7H_4[37]ClO$	-0.52		243618.21
3	110.9996	593880	593880	23297		C_6H_4Cl	-0.34		216185.57
4	199.0306	469327	469327	27753		$C_{13}H_8Cl$	-1.40		289405.87
5	249.9945	311009	311009	25598		$C_{13}H_6Cl_2O$	-0.69		324320.80
6	75.0229	841640	841640	21311		C_6H_3	-0.65		177772.26
7	251.9916	522881	522881	25613		$C_{13}H_6Cl[37]ClO$	-0.45		325612.73
8	112.9967	093635	093635	23365		$C_6H_4[37]Cl$	0.02		218119.61
9	215.0258	881666	881666	25295		$C_{13}H_6ClO$	-0.26		300801.04
10	139.9981	815061	815061	22468		$C_6[13]CH_4ClO$	1.31		242759.24
11	201.0280	788154	788154	25000		$C_{13}H_8[37]Cl$	0.23		290853.24
12	76.0307	527001	527001	20591		C_6H_4	-0.47		178960.79
13	50.0151	524722	524722	19360		C_4H_2	0.29		145192.76
14	163.0544	476176	476176	25114		$C_{13}H_7$	1.07		261969.29
15	112.0028	458665	458665	13297		$C_5[13]CH_4Cl$	-1.22		217159.31

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.

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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 359-011-111) for both Pegasus GC-HRT and GC-HRT^{+} systems.
- In collaboration with Prof. Albert Lebedev, Moscow State University.
- Approximately 760 compounds: alkanes, PAH, essential oils, pesticides, and general SVOCs.

LECO Corporation
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