Identification Grading System™ (IGS™)

Available with ChromaTOF® brand software

Bring the Power of Accurate Mass and Confidence to your Identification Problems

LECO's new *Identification Grading System (IGS)* eases data review by allowing users to quickly see, justify, have confidence in, and report on which chemicals are in a particular sample. This in turn allows a user to make confident decisions on what to do next.

Stop Guessing What is in Your Sample: KNOW

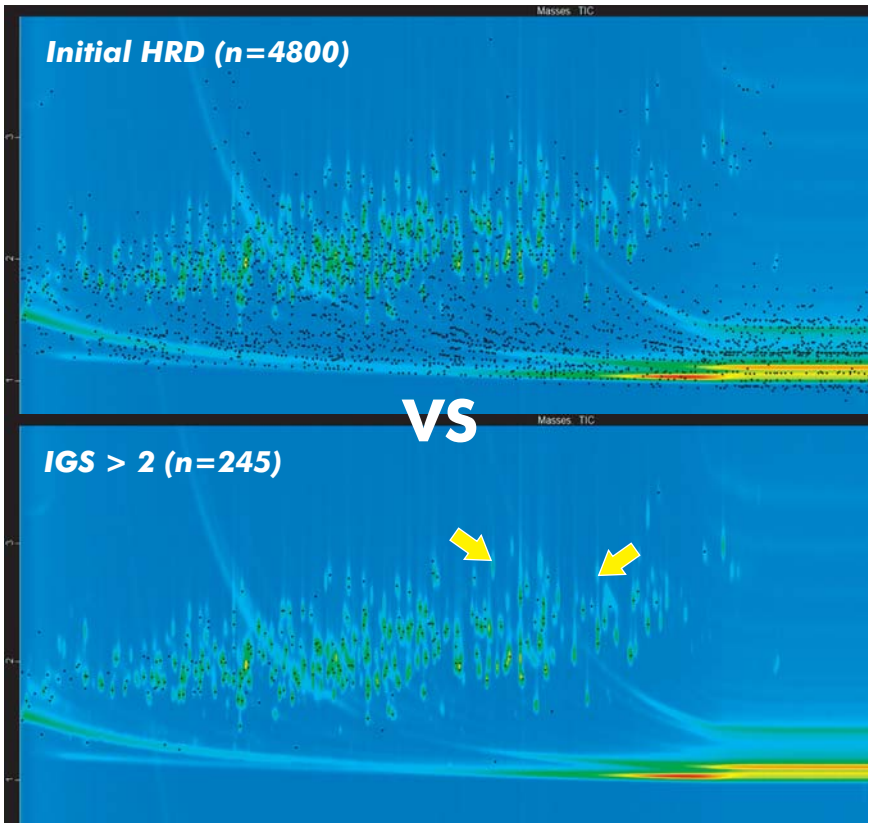
The *IGS* uses all the available chemical information generated from the Pegasus® GC-HRT+ 4D to add confidence to your unknown unknown identification process.

- The *IGS* gives a grade to a particular identification based on 4 criteria:
  1. *Presence and accurate mass of a molecular ion*
  2. *Presence and good correlation of a spectral similarity score from a curated library*
  3. *Accurate masses of sensible potential formulae of fragmented ions corresponding to a spectral library hit*
  4. *Matching retention index from the library hit*

The higher the value of the grade the more confident you can be in your identification.

- The true power of identification can only be realized with the combined power of GCxGC and high resolution time-of-flight mass spectrometry (TOFMS).
  - GCxGC separates coeluting species and gives cleaner mass spectra than other techniques.
  - TOFMS enables unskewed mass spectra across a chromatographic peak even across very narrow second dimensional peak; which, when combined with deconvolution, yields the highest quality spectra that you can generate.

Born out of the EPA's Non-Targeted Analysis Collaborative Trial (ENTACT), the *IGS* is LECO's solution to the time-intensive process of data review.



Here is an example of the unfiltered deconvolution results from a GCxGC-TOFMS analysis of a sample from the EPA's ENTACT project: *https://doi.org/10.1007/s00216-018-1435-6* By applying the *IGS* filter, we can quickly view only the most confident identifications. This simplification is dramatic and enables you to immediately begin investigating the "unknown unknowns", indicated by arrows in the diagram.

Of the known compounds entered into the sample from this particular example (which was provided to LECO as a blind sample), *IGS* identified approximately 80% of the known peaks. The combination of GCxGC and high resolution TOF was proven to be necessary for this confidence. See: *https://pubs.acs.org/doi/10.1021/es5002105*

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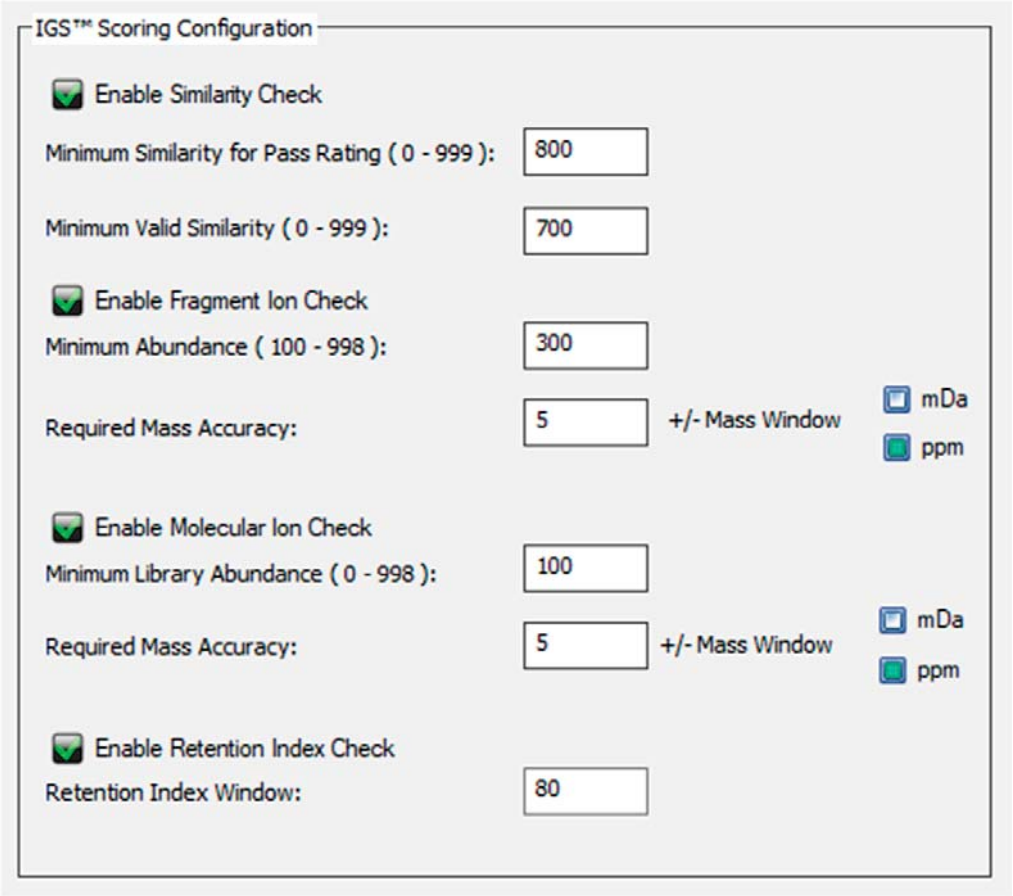
EMPOWERING RESULTS

How IGS is set up and used in the software



Hit Table - 2D Serum Two 1uL s10

Hit	Name	Library	IGS Score	IGS Concerns	Similarity	CAS
>1*	Secbumeton	replib	4.0		804	26259-45-(
2	Secbumeton	mainlib	4.0		795	26259-45-(
3	Secbumeton	Wiley Pesticides v2	3.0	RI:0	829	26259-45-(
4	Sebuthylazine-A (-Cl,+	Wiley DesignerDrugs 2	3.0	RI:0	802	26259-45-(
5	1,3,5-Triazine-2,4-dian	mainlib	2.0	SS:0 ; RI:0	669	13532-26-8
6	Terbumeton	Wiley Pesticides v2	2.0	SS:0 ; RI:0	579	33693-04-8
7	DOF 2PROP	Wiley DesignerDrugs 2	1.0	SS:0 ; RI:0 ; M+:0	566	
8	Terbumeton	replib	0.5	SS:0 ; RI:-	590	33693-04-8
9	Terbumeton	replib	0.5	SS:0 ; RI:-	552	33693-04-8
10	1,3,5-Triazine-2,4-dian	mainlib	-0.5	SS:0 ; RI:0 ; M+:-	629	55702-51-7
11	Atraton	Wiley Pesticides v2	-0.5	SS:0 ; RI:0 ; M+:-	622	1610-17-9
12	1,3,5-Triazin-2(1H)-on	mainlib	-0.5	SS:0 ; RI:0 ; M+:-	616	7374-53-0

Inside of LECO's *ChromaTOF* software, the hit table which links directly to an individual deconvolution result. The highest *IGS* score is used to prioritize this table. The top hit goes into a full summary of all identification results.

This table can use multiple libraries (as shown, even user created libraries) and each individual result can be analyzed and compared by the operator.

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