cerno BIOSCIENCE

GC/ID New Version 5.0

Fully Automated and Highly Confident GC/MS Compound ID

GC/ID™ is an advanced, vendor agnostic software solution that enhances the performance of your GC/MS library search and compound identification process. It is designed to validate the search results automatically, resulting in dramatically improved ID accuracy and efficiency. With Cerno's GC/ID, you can expect a more streamlined and accurate workflow, leading to rapid and confident outcomes in your research and analysis.

Challenges with Library Search

Despite its huge popularity, library search results are often ambiguous and in some instances can fail to produce any useful results. There are several reasons, including unresolved chromatographic peaks (mixtures), column bleed and background interferences, the spectral similarity of closely related compounds, or the absence of the compound in the library. As a result, it's essential to explore alternative search strategies to ensure you get the results you're looking for rapidly and with confidence.

Built in Analytical Expertise

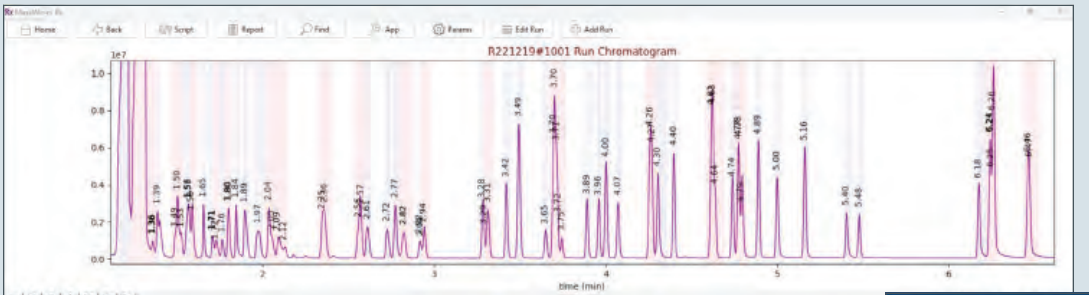
Confident Unknown ID typically requires a high degree of user expertise and can be tedious and time-consuming.

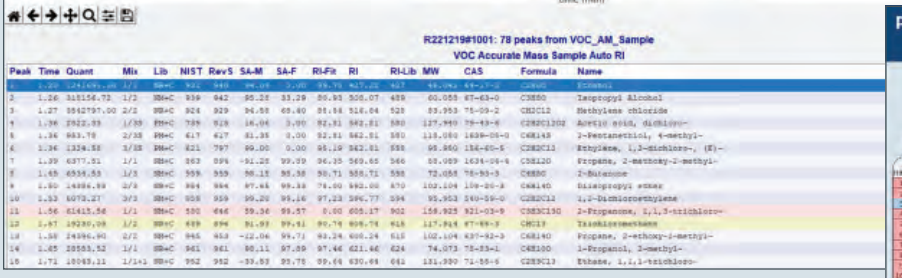
GC/ID is the only processing software that incorporates "Composite Scoring" in a fully automated system that is fast and easy to use, turning every analyst into an expert. The results are processed and presented in a way that enables any analyst to review and interpret runs in minutes instead of hours.

Feature	Benefit
Vendor Agnostic	Compatible with all GC/MS systems
Forward Search	Uses industry-standard NIST library search
Reverse Search	Used for automatic match quality check and mixture detection
Retention Index (RI) Match	Confirms correct compound, eliminates incorrect matches
Auto | External RI Calibration	Easy and flexible RI calibration with or without standards
Accurate Mass Formula Confirmation	Additional compound confirmation, aids to ID compounds not in library
Composite Scoring	Mixture Detection & Deconvolution | Library Search | Retention Index | Accurate Mass
Full Spectrum Deconvolution	Reduces false spectral matches, resolves co-eluting compounds
Colored Highlighter	Combines all the above metrics to identify the "True" answer
PDF/Excel Reports	Easily create hyperlinked PDF reports or directly paste to Excel
Custom LIMS Report	Powerful Python scripting allows for easy and flexible LIMS integration
Python Scripting	Python scripting can customize the product to your needs
NetCDF File Format	New support for NetCDF file format in addition to most native vendor formats
64-bit Application	Up to 70% faster with greater stability

Improve efficiency and save time for science with GC/ID, latest version 5.0 software. A powerful and fully automated application that provides quick and accurate identification, confirmation, and quantitation of both target and unknown compounds.

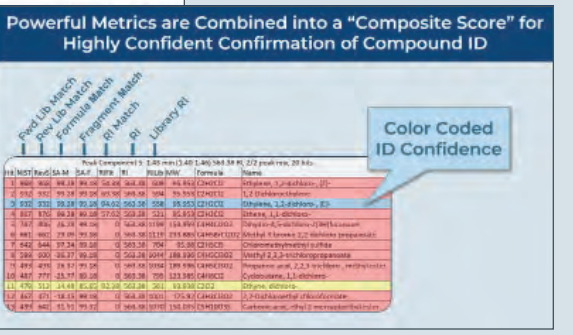
Unknown ID with the Highest Confidence and Fastest Review





GC/ID tells you at a glance each peak's ID confidence by color coding the results using Magic Highlighter™:

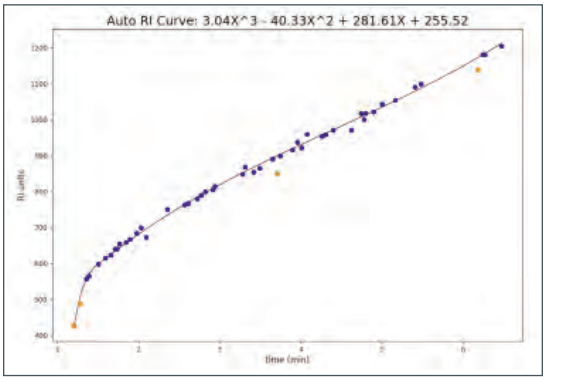
Blue=High **Yellow**=Medium **Red**=Low. This is done automatically by evaluating, for each peak, the purity (Mix), forward and reverse match value (NIST, RevS), the Retention Index match (RI Fit), the compound formula of the molecular ion by accurate mass/spectral accuracy (SA-M) as well as fragment ions (SA-F).



Powerful but Easy Retention Index Verification

Retention Index is perhaps the most powerful metric for confirming a library search ID. Many compounds have very similar spectra, but significantly different RIs, in particular, isomers. However, utilizing RI has traditionally been tedious and, without RI values for all library spectra, frustrating. That has all changed with modern libraries (e.g., NIST20, NIST23) with nearly 100% RI coverage using experimental and accurately calculated RI by AI (Artificial Intelligence) modeling. Even if the library does not have RI values, GC/ID can calculate them from the structures as needed. This is a game changer.

Just as importantly, for calibrating the GC for RI, GC/ID makes it effortless using its patented Auto RI™ technology, which automatically calibrates the GC from the sample itself. You can even process previously acquired data and enhance the results with RI, all without separate RI calibration standards. For those samples which may require a separate calibration, GC/ID makes it easy to fully calibrate the GC with a simple n-alkane sample, or even your standard system suitability mixture.



Auto RI is a revolutionary approach for calculating RI from unknown samples without the need for tedious and time-consuming calibration runs.

Hit	Lib	NIST	RevS	SA-M	SA-F	RI-Fit	RI	RI-Lib	MW	CAS	Formula	Name
1:	PM+C	916	919	-95.96	99.14	0.00	996.54	1184	136.090	264628-23-1	C9H12O	7-Methylene-9-oxabicyclo[6.1.0]non-2-ene
2:	PM+C	914	915	-96.60	99.14	0.00	996.54	1126	136.130	19485-20-2	C10H16	Tricyclo[5.3.0.0(4,8)]decane
3:	PM+C	914	916	-96.60	99.14	0.00	996.54	1338	136.130	514-95-4	C10H16	1,5,5-Trimethyl-6-methylene-cyclohexene
4:	PM+C	914	915	-95.96	99.14	0.00	996.54	1149	136.090	0	C9H12O	7-Methylene-9-oxa-bicyclo[3.3.1]non-2-ene
5:	PR+C	911	913	-96.60	99.14	53.46	996.54	950	136.130	471-84-1	C10H16	Bicyclo[2.2.1]heptane, 7,7-dimethyl-2-methylene-
6:	PM+C	908	913	-96.60	99.14	53.46	996.54	950	136.130	471-84-1	C10H16	Bicyclo[2.2.1]heptane, 7,7-dimethyl-2-methylene-
7:	PR+C	906	907	-96.60	99.14	86.46	996.54	983	136.130	5113-87-1	C10H16	Cyclohexene, 3-methyl-6-(1-methylethenyl)-, (3R-t
8:	PM+C	905	906	-95.96	99.14	0.00	996.54	1238	136.090	0	C9H12O	3-Methylene-bicyclo[3.2.1]oct-6-en-8-ol
9:	PM+C	904	905	-95.96	99.14	0.00	996.54	1173	136.090	0	C9H12O	5-Methylene-1,3a,4,5,6,6a-hexahydropentalen-1-ol
10:	PM+C	904	915	-96.60	99.14	43.46	996.54	940	136.130	497-32-5	C10H16	Bicyclo[2.2.1]heptane, 2,2-dimethyl-5-methylene-

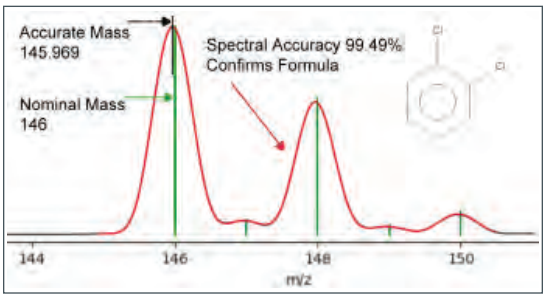
Retention Index matching is particularly powerful for complex samples like natural products. In this example all the top matches have excellent NIST match results, but the correct compound can be easily identified as the 7th best match based on RI. GC/ID automatically reviews all the match metrics and color codes each Hit (Magic Highlighter) to indicate low confidence matches (red) and highlights the high confidence match (light blue) automatically.

Accurate Mass for Benchtop GC/MS

High resolution accurate mass instruments such as TOF or Orbitrap can help confirm unknowns by formula ID. They can also help to determine the structures of compounds not in the library by identifying the formula of the molecular ion and the fragment ions. GC/ID brings those capabilities to the benchtop single quad through its published and patented, award winning TrueCal™ technology.

To achieve better mass accuracy and confirm the identification of molecular ion and fragment ion formula, run your instrument in Profile mode instead of Centroid mode. At the end of the run, briefly turn on the tune gas (PFTBA), and GC/ID will automatically calibrate your single quad. This results in up to 100 times better mass accuracy and, more importantly, up to 99.9% spectral accuracy.

For compounds not in the library, formula ID is a valuable tool towards proposing possible structures. The technology applies to all MS instrumentation, from routine benchtops to state-of-the-art high-resolution instruments.

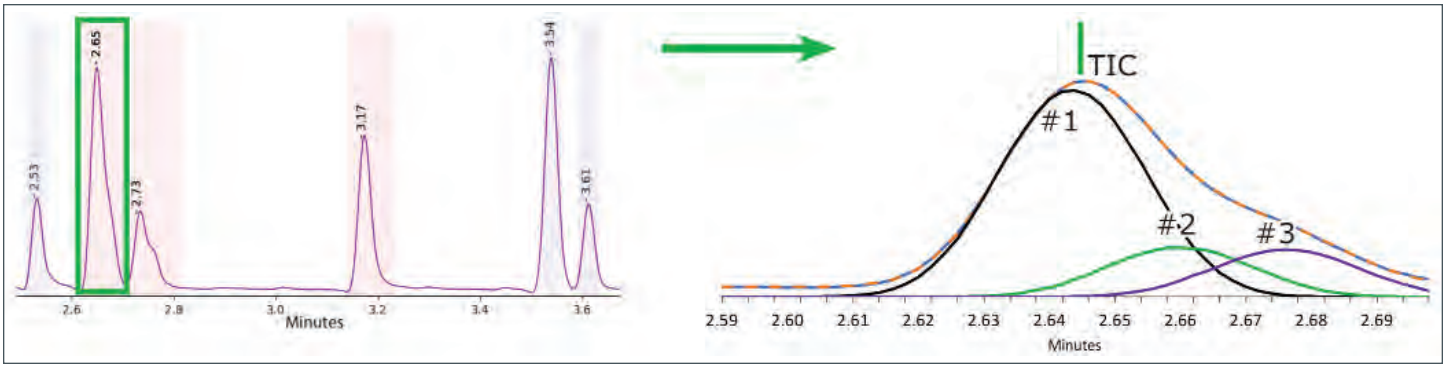


The profile mode spectral overlay of the calculated "True" MS (**Red**) and the calibrated (**Black**) MS shows nearly a perfect match with 99.24% spectral accuracy confirming the NIST compound formula for more confident ID. This is a capability previously only available in high resolution MS instruments.

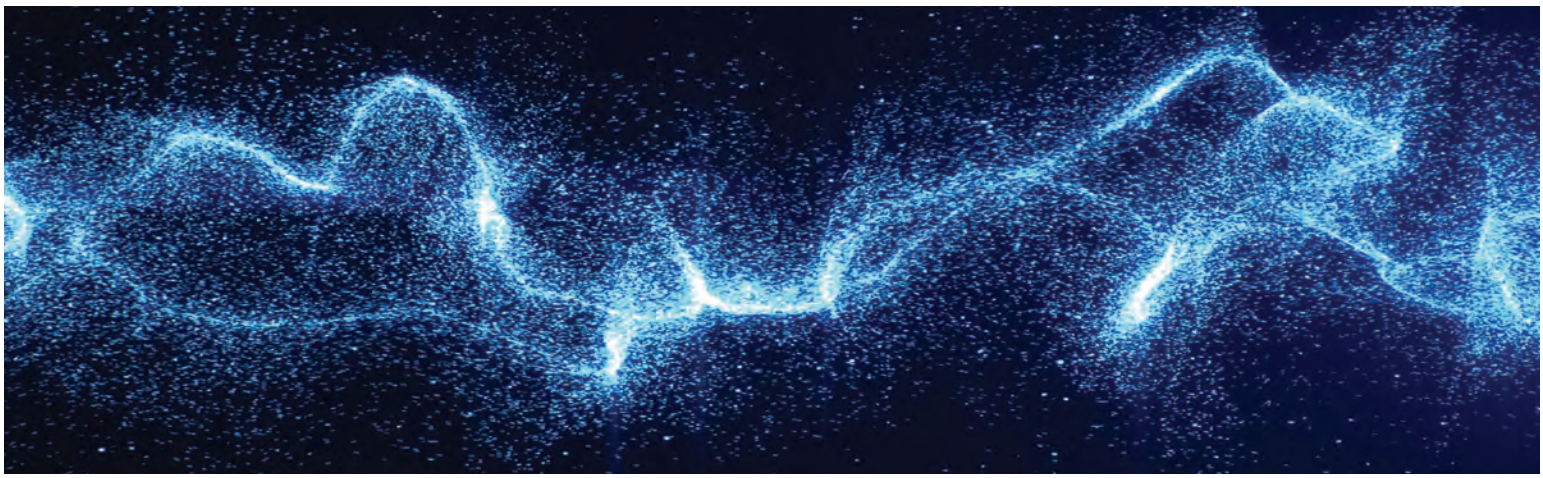
The "Full Spectrum" Peak Deconvolution

Co-eluting chromatographic peaks remain a frequent challenge for nearly every GC/MS analysis. Unlike most "conventional" deconvolution algorithms, which use only a few resolved m/z ions to locate potential coeluting peaks (eXtracted Ion Chromatograms (XIC)), GC/ID uses a patented, "Full Spectrum" Deconvolution (FSD) approach for improved performance and accuracy. This is a multi-step process based on sound statistical methods. An initial "mixture" screening using Principal Component Analysis (PCA) is used to reliably estimate the number of "components" (compounds) included in a chromatographic peak or group of peaks. This step reduces the typical overfitting that can produce erroneous spectra and false IDs when using XIC based approaches. Traditional deconvolution methods often generate "false" spectra, which can severely impact the accuracy of compound identification and mislead analysts. FSD has a number of advantages over traditional deconvolution:

1. Superior quantitation of the underlying peaks using full spectrum fit since the full spectrum is integrated under the peak curve, not just a single ion, the best approach for the quantitative analysis of unknown compounds.
2. Automatic background correction is "free" due to the matrix algebra used as it becomes a static "residual", no need to manually or automatically try to identify and subtract "baseline" spectra.
3. Finally, any deconvolution math will fail if the compounds elute too closely. For these cases, Cerno's Search Mixture Deconvolution (SMD) steps in to identify and resolve them.



The peak at 2.65 min actually contains 3 co-eluting peaks which GC/ID deconvolves as shown. GC/ID provides improvements over classic deconvolution and, unlike conventional approaches, minimizes over fitting and eliminates false spectra. FSD also improves the ability to accurately quantitate co-eluting peaks. Improvements over classic deconvolution and, unlike conventional approaches, minimizes over fitting and eliminates false spectra.

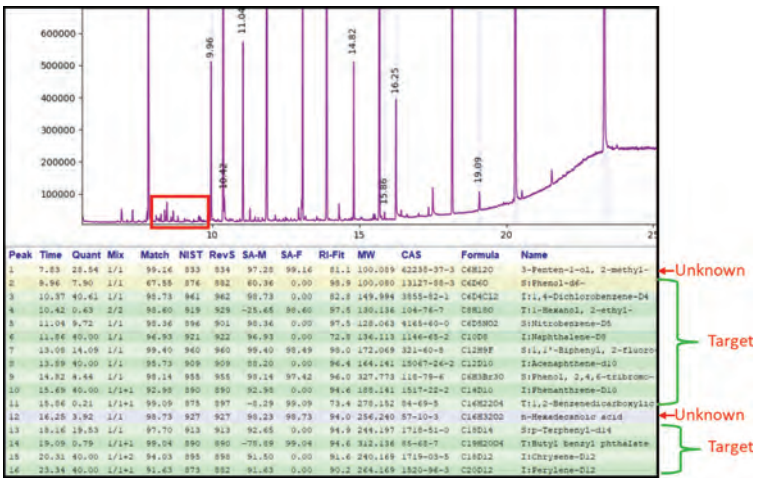


Target and non-Target semi-Quant

Powerful new semi-Quant features have been added to Version 5 including target and non-target analysis. Even co-eluting peaks can be accurately quantified thanks to GC/ID's "Full Spectrum" deconvolution feature. Target compounds are confidently identified with "Composite Scoring", minimizing errors and accelerating review. Peaks can be quantitated by multiple internal standards. Those below an established reporting limit can be filtered from the results table to simplify review.

Targets, surrogates, and internal standards are color coded and tagged to allow the analyst to focus on what's important.

But, every lab is different, that's where the power of GC/ID's powerful Python scripting can provide the perfect fit to accelerate your laboratory workflow. The scripting tools also allow easy LIMS integration and custom reporting. Finally, since GC/ID is vendor agnostic, it can work with all your GC/MS systems, regardless of the instrument manufacturer or generation.



Peak	Time	Quant	Mix	Match	NIST	RevS	SA-M	SA-F	RI-Fit	MW	CAS	Formula	Name
1	7.83	28.54	1/1	99.14	833	834	97.25	99.16	81.1	100.089	42235-97-3	C6H12O	3-Penten-1-ol, 2-methyl-
2	8.96	7.90	1/1	97.55	874	882	90.96	0.00	98.9	100.080	13127-88-3	C6D6O	SiPhenol-d6-
3	10.37	40.41	1/1	98.73	861	862	98.73	0.00	82.8	149.994	3855-82-1	C6D4Cl2	Ti1,4-Dichlorobenzene-D4
4	10.42	0.63	2/2	98.60	819	929	-25.65	98.60	97.5	130.136	104-76-7	C8H18O	Ti1-Hexanol, 2-ethyl-
5	11.04	9.72	1/1	98.36	896	901	98.36	0.00	97.5	128.063	4165-60-0	C6D4NO2	SiNitrobenzene-D5
6	11.86	40.00	1/1	96.93	921	922	96.93	0.00	72.8	136.113	1146-65-2	C10D8	IiNaphthalene-D8
7	13.08	14.09	1/1	99.40	960	960	99.40	98.49	98.0	172.069	321-60-8	C12H9F	Si1,1'-Biphenyl, 2-fluoro
8	13.89	40.00	1/1	95.73	909	909	88.20	0.00	96.4	164.141	15067-26-2	C12D10	IiAcenaphthene-d10
9	14.82	4.44	1/1	98.14	955	955	98.14	97.42	96.0	327.773	118-79-6	C6H3Br3O	SiPhenol, 2,4,6-tribromo-
10	15.69	40.00	1/1+1	92.98	890	890	92.98	0.00	94.6	188.141	1517-22-2	C14D10	IiPhenanthrene-D10
11	15.86	0.21	1/1+1	99.09	875	897	-8.29	99.09	73.4	270.152	84-69-5	C16H2204	Ti1,2-Benzenedicarboxylic
12	16.25	3.92	1/1	98.73	927	927	98.23	98.73	94.0	256.240	57-10-3	C16H32O2	n-Hexadecanoic acid
13	18.16	19.53	1/1	97.70	913	913	92.65	0.00	94.9	244.197	1718-51-0	C18D14	Sip-Terphenyl-d14
14	19.09	0.79	1/1+1	99.04	890	890	-78.89	99.04	94.6	312.136	85-68-7	C19H2004	TiButyl benzyl phthalate
15	20.31	40.00	1/1+2	94.03	895	898	91.50	0.00	91.6	240.169	1719-03-5	C18D12	IiChrysene-D12
16	23.34	40.00	1/1+1	91.63	873	882	91.63	0.00	90.2	264.169	1520-96-3	C20D12	IiPerylene-D12

Huge reductions in the analysis time of GC/MS runs can be accomplished with powerful Python scripting tailored to your workflow needs. Automatic deconvolution and filtering of compounds below the desired threshold are automatically performed, target compounds clearly highlighted and tagged allows the analyst to focus on only the key compounds, the unknowns in this case.

GC/ID: UnLock the True Power of GC/MS

Experience the speed and efficiency of GC/ID for all your compound analysis needs. Improve efficiency and save time for science with GC/ID, a powerful and fully automated application that provides quick and accurate identification, confirmation, and quantitation of both target and unknown compounds.

Contact us to schedule a demo of GC/ID V5 with your data and see how it can boost your lab's productivity.

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For More Information
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