MassWorks Rx™ **GC/ID** **NEW V4.0**

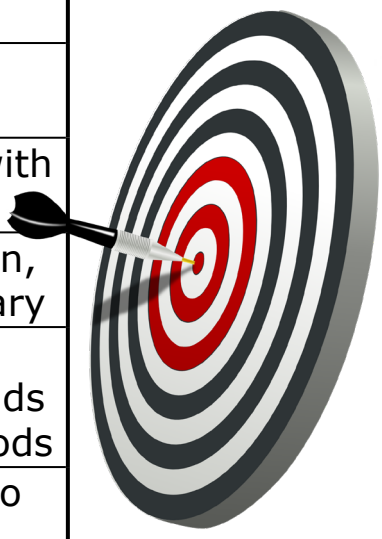
Fully Automated and Highly Confident GC/MS Compound ID

If the confident identification of unknown compounds by GC/MS is important to you, you need GC/ID. GC/ID is the only software that combines library search, automatic Retention Index calibration and matching, Accurate Mass, and the most powerful deconvolution tools into a total solution. This allows GC/ID to automatically and reliably identify unknown compounds with an unparalleled degree of confidence while saving the analyst many hours of tedious review for each and every peak in a run.

We are all very familiar with the challenges of compound ID by GC/MS. Typically, for each peak a spectrum is searched against a library of compounds to produce a "Hit" list. The Hit list is a ranked list of the best library matches. The problem is that the list is not definitive, and the top match is often not the correct match. In addition, the peak may be a mixture of co-eluting compounds or contain a high background which can severely degrade the search results. Or, even more challenging, the compound might not even be in the library.

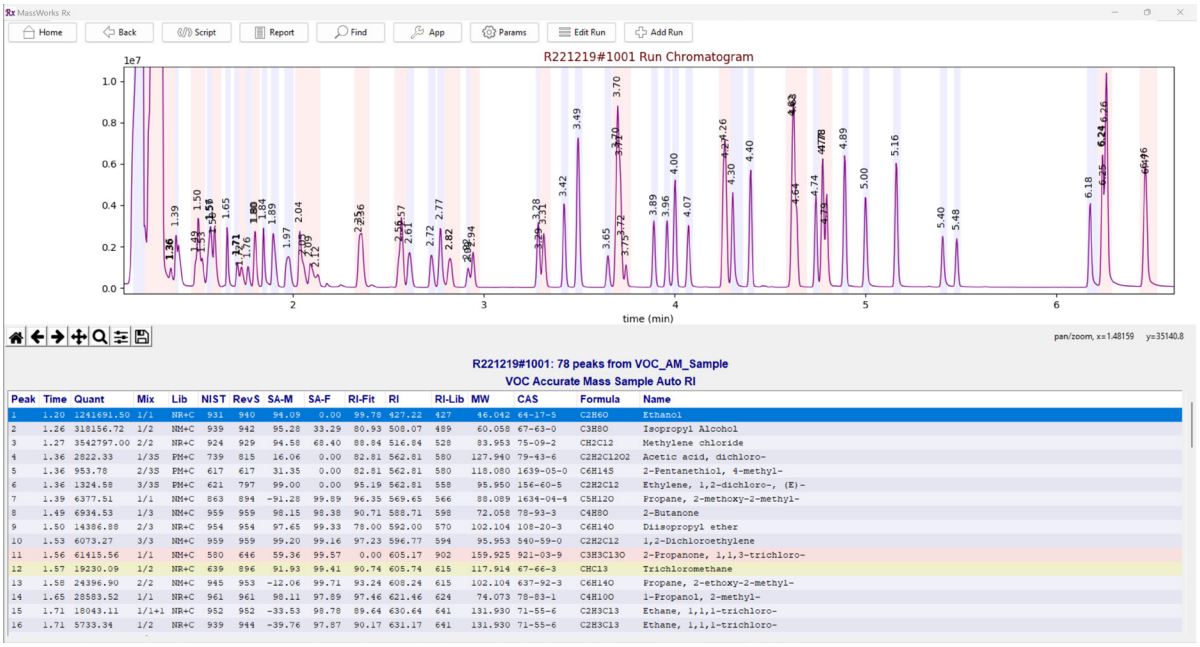
Just like in a court of law, we need a sound body of evidence to make a confident unknown ID. GC/ID provides a broad collection of metrics which compliment library search to dramatically improve the quality, reliability, and confidence in identifying unknowns. And the best part is GC/ID is fully automated with the most likely answer conveniently highlighted for each peak, making the analyst's job in reviewing data fast and efficient while minimizing miss-identified compounds.

Feature	Benefit
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 or 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
Advanced Deconvolution	Minimizes false spectral matches and resolves co-eluting compounds not solvable via traditional methods
Colored Highlighter	Combines all the above metrics to identify the "True" answer
Vendor Agnostic	Works with all brands of GC/MS systems



GC/ID provides a powerful set of Search and Confirmation metrics unsurpassed in the industry. These features are automatically applied to your data with the correct ID conveniently indicated in the search "Hit" list.

Unknown ID with the Highest Confidence and Fastest Review



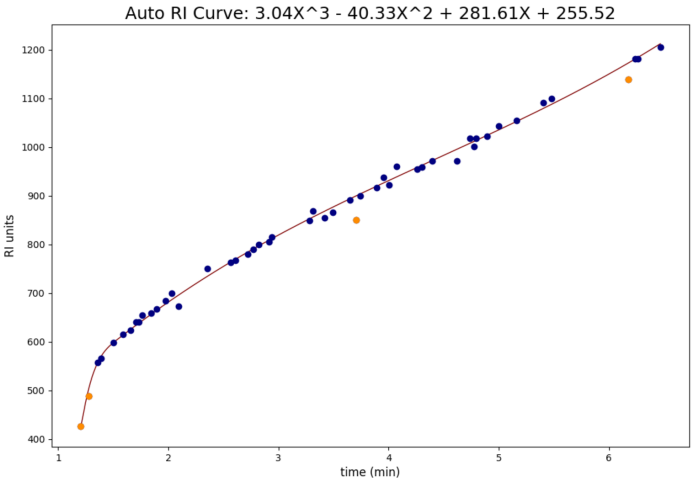
Peak	Time	Quant	Mix	Lib	NIST	RevS	SA-M	SA-F	RI-Fit	RI	RI-Lib	MW	CAS	Formula	Name
1	1.20	1241691.50	1/1	NR+C	931	940	94.09	0.00	99.78	427.22	427	46.042	64-17-5	C2H6O	Ethanol
2	1.26	318156.72	1/2	NM+C	939	942	95.28	33.29	80.93	508.07	489	60.058	67-63-0	C3H8O	Isopropyl Alcohol
3	1.27	3542797.00	2/2	NR+C	924	929	94.58	68.40	88.84	516.84	528	83.953	75-09-2	CH2Cl2	Methylene chloride
4	1.36	2822.33	1/3S	PM+C	739	815	16.06	0.00	82.81	562.81	580	127.940	79-43-6	C2H2Cl2O2	Acetic acid, dichloro-
5	1.36	953.78	2/3S	PM+C	617	617	31.35	0.00	82.81	562.81	580	118.080	1639-05-0	C6H14S	2-Pentanethiol, 4-methyl-
6	1.36	1324.58	3/3S	PM+C	621	797	99.00	0.00	95.19	562.81	558	95.950	156-60-5	C2H2Cl2	Ethylene, 1,2-dichloro-, (E)-
7	1.39	6377.51	1/1	NM+C	863	894	-91.28	99.89	96.35	569.65	566	88.089	1634-04-4	C5H12O	Propane, 2-methoxy-2-methyl-
8	1.49	6934.53	1/3	NM+C	959	959	98.15	98.38	90.71	588.71	598	72.058	78-93-3	C4H8O	2-Butanone
9	1.50	14386.88	2/3	NR+C	954	954	97.65	99.33	78.00	592.00	570	102.104	108-20-3	C6H14O	Diisopropyl ether
10	1.53	6073.27	3/3	NM+C	959	959	99.20	99.16	97.23	596.77	594	95.953	540-59-0	C2H2Cl2	1,2-Dichloroethylene
11	1.56	61415.56	1/1	NM+C	580	646	59.36	99.57	0.00	605.17	902	159.925	921-03-9	C3H3Cl3O	2-Propanone, 1,1,3-trichloro-
12	1.57	19230.09	1/2	NR+C	639	896	91.93	99.41	90.74	605.74	615	117.914	67-66-3	CHCl3	Trichloromethane
13	1.58	24396.90	2/2	NM+C	945	953	-12.06	99.71	93.24	608.24	615	102.104	637-92-3	C6H14O	Propane, 2-ethoxy-2-methyl-
14	1.65	28583.52	1/1	NR+C	961	961	98.11	97.89	97.46	621.46	624	74.073	78-83-1	C4H10O	1-Propanol, 2-methyl-
15	1.71	18043.11	1/1+1	NR+C	952	952	-33.53	98.78	89.64	630.64	641	131.930	71-55-6	C2H3Cl3	Ethane, 1,1,1-trichloro-
16	1.71	5733.34	1/2	NR+C	939	944	-39.76	97.87	90.17	631.17	641	131.930	71-55-6	C2H3Cl3	Ethane, 1,1,1-trichloro-

GC/ID tells you at a glance each peak's ID confidence by color coding the results (Magic Highlighter): Blue=High, Yellow=Medium and 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. But 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) 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 few 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-

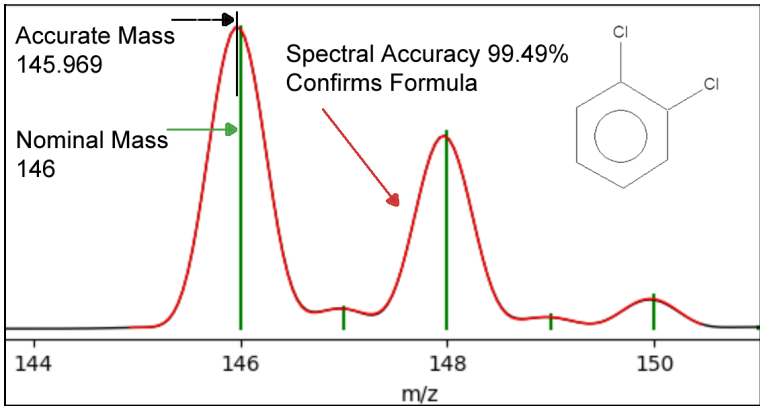
Retention Index matching is particularly powerful for complex samples like natural products. In this example all the top matches have excellent NIST match results, but the correct compound can be easily identified as the 7th best match based on RI. GC/ID automatically reviews all the match metrics and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

Unknown Formula Confirmation without the Expense of High Resolution 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.

By simply running your instrument in Profile mode (vs the usual Centroid mode), and briefly turning on the tune gas (PFTBA) at the end of your run, GC/ID will automatically calibrate your single quad to obtain 100 times better mass accuracy, and perhaps more importantly, up to 99.9% spectral accuracy, to confirm and identify molecular ion and fragment ion formula.

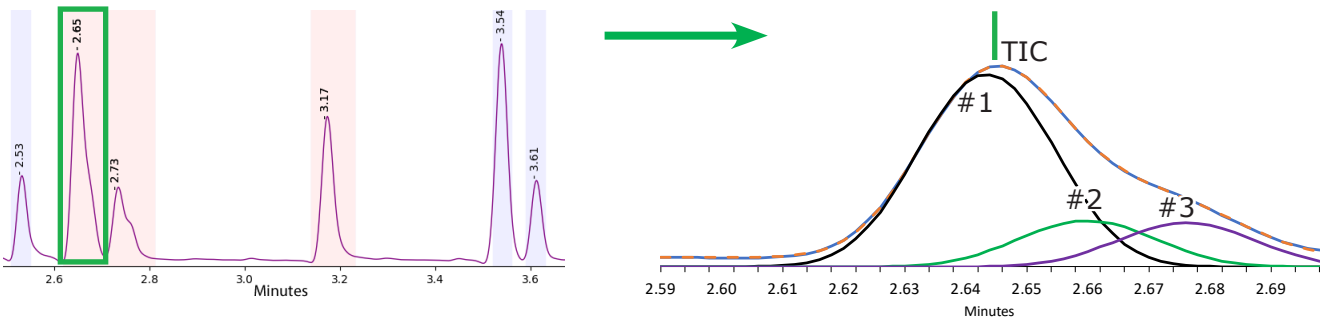
For compounds not in the library, formula ID is a valuable tool towards proposing possible structures.



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 Most Advanced and Reliable Peak Deconvolution

Co-eluting chromatographic peaks remain a frequent challenge for nearly every GC/MS analysis. Conventional deconvolution typically examines the XICs (extracted ion chromatograms) and often fails to determine the correct number of co-eluting compounds (this method will typically over-fit, i.e., return more spectra of "pure" compounds than what is actually in the peak) which tends to produce false library matches. GC/ID improves upon this approach by first using Principal Component Analysis (PCA) to estimate the number of components more confidently in a peak, before deconvoluting them into pure component spectra.

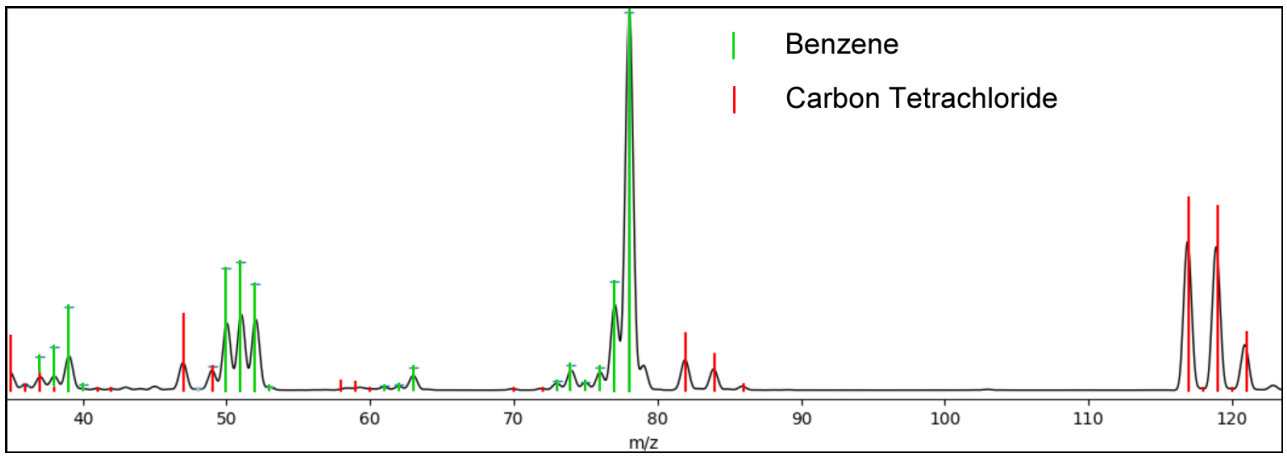


The peak at 2.65 min actually contains 3 co-eluting peaks which GC/ID deconvolves as shown. GC/ID provides improvements over classic deconvolution and, unlike conventional approaches, minimizes over fitting and eliminates false spectra.

Search Mixture Deconvolution (SMD)

When there is not enough retention time separation between co-eluting compounds, all conventional deconvolution approaches will fail. It is a mathematical certainty!

For these cases of co-elution, Cerno applies a different approach, one that deconvolves spectra from co-eluting peaks even if the retention times are identical. SMD is a new approach to deconvolution which directly fits the mixture spectra with all possible library spectra using multiple linear regression to find which "pure" spectra provide the "best" fit to the mixture spectrum. Of course, there are two problems to solve, 1) how to identify potential "mixture" peaks and 2) how to select a reasonable subset of compounds from the library to perform the fit (otherwise finding the best fit using all compounds from the library becomes an intractable problem). To identify likely mixture peaks, we can compare forward and reverse search. Once we do this, we can select a subset of the library to perform the fitting by finding compounds that have a high reverse search score, and that have an RI value close to the peak. Once the best spectra are found that provide the best fit, we return these spectra as the most likely match candidates.



An SMD plot showing the search results from the co-elution of Benzene and Carbon Tetrachloride. The black profile mode spectrum is a mixture of the 2 compounds, the green centroids are the library spectrum of Benzene, while the red represents Carbon Tetrachloride, and together they explain the mixture. Applying conventional deconvolution approaches, from any vendor, will fail in this case where the separation of the peaks is minimal (if any).

Unfortunately, to obtain all possible spectral matches for SMD, we need to search every compound in the library using reverse search and then filter them by RI. Traditional library search, like NIST and PBM, typically employs a pre-filtering algorithm based on using a small number of the largest peaks in the spectrum. This dramatically speeds up the search by reducing the number of library spectra needed for search. Unfortunately, many times these algorithms don't work well with mixtures or low signal-to-noise spectra and can filter out exactly the spectrum we are looking for. CPS is a special library search developed by Cerno to dramatically speed up unfiltered library searching of every spectrum in a library, a requirement for SMD. CPS full library search is typically much faster than a traditional filtered search despite the increased computational load. A traditional NIST search can still be used, and only when a peak deconvolution calls for SMD, it will automatically switch to CPS.

GC/ID is the First Major GC/MS Breakthrough in Decades

GC/MS library search has been a powerful tool for the ID of organic compounds for decades. However, besides continued expansion of spectral libraries, hardware improvements in terms of sensitivity and ease of use, no significant progress has been made to assist the analyst in determining the correct match from a long list of possible hits without the tedious and time-consuming manual review or even re-analysis, **until now!** Contact us today for a demo with your data to learn how GC/ID V4 can make your lab more productive.

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