MassWorks Rx™ **GC/ID** **NEW V3.0**

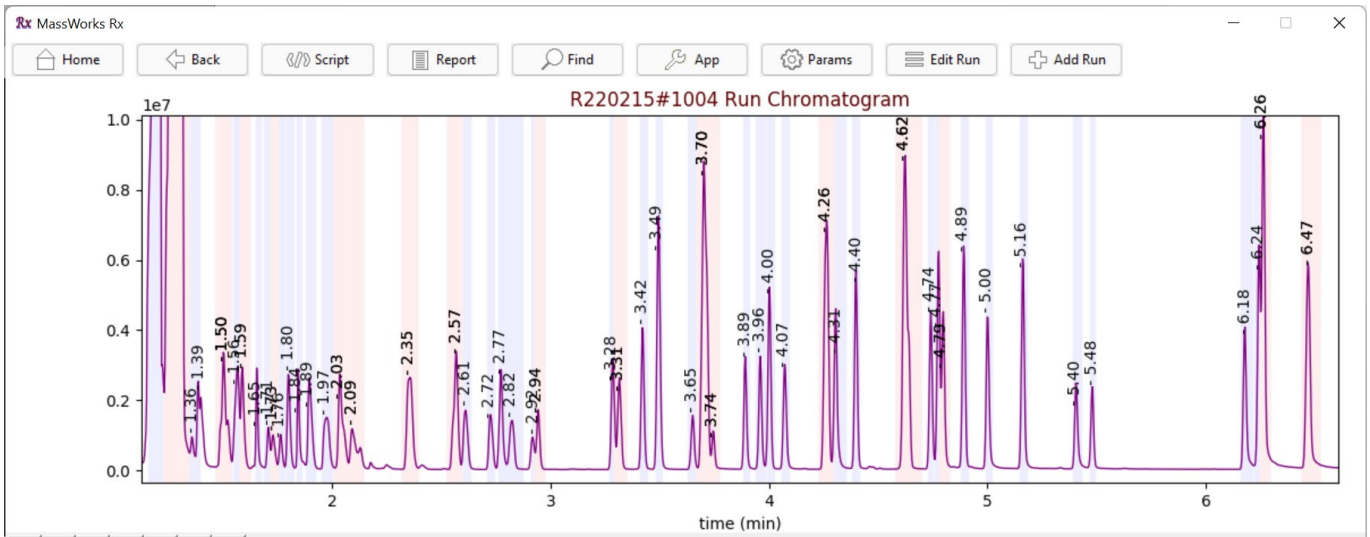
Fully Automated and Highly Confident GC/MS Compound ID

GC/ID is fully automated data processing software that provides dramatic improvements for GC/MS qualitative and now, semi-quantitative analysis. By incorporating Cerno's proven TrueCal™ calibration technology for *accurate mass formula ID* along with conventional library search, a significant improvement in compound ID certainty is achieved on single quad GC/MS systems. For the first time GC/ID also provides an entirely automated method of quantitatively utilizing the NIST, Wiley or user generated retention index (RI) values to provide yet a third orthogonal metric for compound ID.

GC/ID takes full advantage of the new NIST20 libraries which incorporate accurately calculated RI values by Artificial Intelligence (AI) along with accurate experimental RI values to provide 100% coverage of RI for the entire library! V3 further improves the powerful new approach used to identify and deconvolve mixtures and the background of co-eluting peaks to minimize the mis-identification of compounds in complex samples.

These features can save the analyst hundreds of hours per year while increasing compound ID confidence and minimizing the number of "unidentified" peaks due to interferences, unresolved peaks, or just ambiguous library search results. GC/ID can automatically process an entire sequence of GC/MS runs from most vendor instruments including the popular Agilent GC/MSD. It also provides an easy-to-use review mode to audit results and generate reports in either PDF or spreadsheet formats.

Formula ID is a feature normally only available on high resolution MS instruments. Combined with library search and RI match, these three metrics can be "blended" into an overall match quality or used independently providing dramatic improvements and valuable time savings in GC/MS compound ID.



R220215#1004: 72 peaks from VOC_AM_Sample

VOC Accurate Mass Sample Auto RI

Peak	Time	Quant	Mix	NIST	RevS	SA-M	SA-F	RIFit	RI-SS	MW	CAS	Formula	Name
1	1.20	1278699.62	1/1	931	940	94.09	0.00	96.87	39	46.042	64-17-5	C2H6O	Ethanol
2	1.28	318905.53	1/2	939	942	95.31	33.29	86.00	34	60.058	67-63-0	C3H8O	Isopropyl Alcohol
3	1.28	3542048.25	2/2	924	930	94.57	68.34	75.00	26	83.953	75-09-2	CH2Cl2	Methylene chloride
4	1.36	6092.44	1/1+1	980	980	99.00	99.46	98.81	4	95.953	156-60-5	C2H2Cl2	Ethylene, 1,2-dichloro-, (E)-
5	1.39	6377.51	1/1	863	894	-91.21	99.89	96.60	7	88.089	1634-04-4	C5H12O	Propane, 2-methoxy-2-methyl-
6	1.50	6934.85	1/3	959	959	98.15	98.37	99.34	119	72.058	78-93-3	C4H8O	2-Butanone
7	1.50	14387.20	2/3	954	954	97.64	99.33	71.34	9	102.104	108-20-3	C6H14O	Diisopropyl ether
8	1.50	6072.64	3/3	959	959	99.20	99.16	95.34	-1	95.953	540-59-0	C2H2Cl2	1,2-Dichloroethylene
9	1.56	36138.38	1/1	581	647	59.28	99.57	0.00	-1	159.925	921-03-9	C3H3Cl3O	2-Propanone, 1,1,3-trichloro-
10	1.59	9537.87	1/2	639	896	91.98	99.42	98.75	39	117.914	67-66-3	CHCl3	Trichloromethane
11	1.59	12101.38	2/2	945	953	-12.06	99.72	98.75	5	102.104	637-92-3	C6H14O	Propane, 2-ethoxy-2-methyl-

GC/ID processes an entire run in a few minutes, calculates the NIST match value (NIST) for each peak, verifies the compound formula by accurate mass/spectral accuracy via M+ (SA-M) as well as fragment ions (SA-F), and then performs retention index match (RI Fit). ***The new "Magic Highlighter" color codes questionable compound IDs based on all these metrics to save you time and provide you with the highest confidence in compound ID.***

Key Features of GC/ID and New Features in V3.0

- Forward and reverse search using the industry standard NIST search engine
- Accurate mass with high Spectral Accuracy for confident formula ID confirmations
- Formula ID for molecular ions and/or fragments
- Powerful Retention Index Match against NIST comprehensive RI database
- Powerful Deconvolution of Co-eluted Peaks
- **New!** A patented method for generating RI without standards!
- **New!** "Magic Highlighter" color codes problem IDs visually to speed analyst review
- **New!** Conveniently processes legacy centroid data with deconvolution and RI validation
- **New!** Semi-Quant, a simple but smart Semi-Quantitative analysis tool
- **New!** Build custom User Libraries directly from GC/ID
- Supports NIST, Wiley, and other third-party or User Libraries
- Full Automation including Report Generation

3.0 adds some additional powerful and ground breaking capabilities to a product already rich in innovation, including:

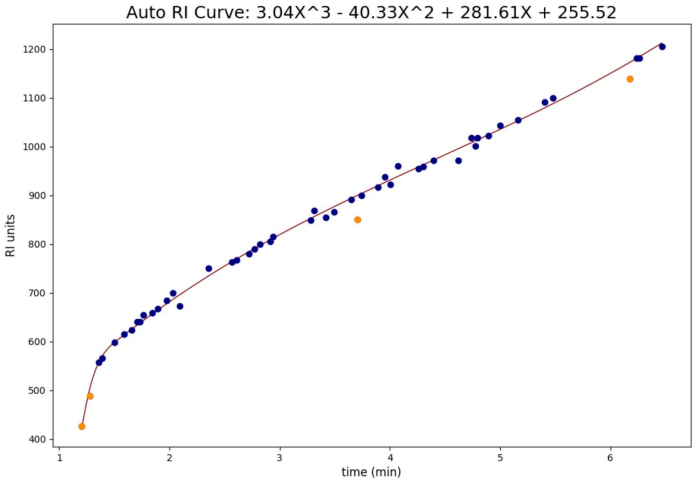
Magic Highlighter is a new way to visualize the quality of each peak ID. Blending four important metrics (Fwd Search, Rev Search, Retention Index and Formula ID (via Spectral Accuracy) to signify High, Medium, and Low compound ID confidence in a color-coded system that dramatically accelerates the review process. This is a powerful aid to speed the analyst review and minimize compound mis-identification.

Auto RI is a revolutionary, patented system for automatic Retention Index calibration without the need to run any standards, saving you time and enabling enhanced analysis of previously collected data. You can now add powerful RI scoring to any run by simply reprocessing it with GC/ID, even with legacy centroid data!

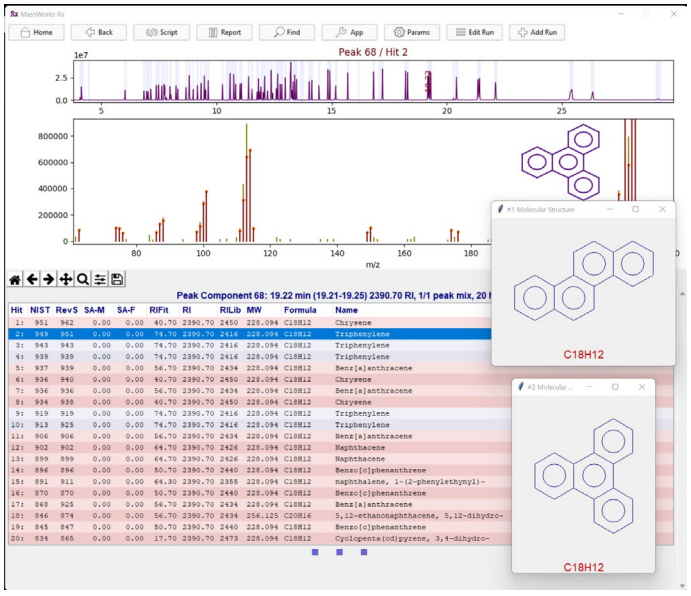
Semi-Quant is a simple but powerful tool for semi-quantitative analysis. Easily setup Target and Reference peaks by retention time, retention index, or even by compound ID (as determined by search). Even mixture peaks can be used in quant thanks to the powerful deconvolution feature in GC/ID.

Centroid Data processing is now supported. This means that you will not get formula ID information, but you will get all the other features of GC/ID including rapid processing, peak deconvolution and Retention Index match. And, with the new Auto RI you can reprocess old runs to automatically add accurate RI information for a more confident analysis.

There are many other improvements to GC/ID including the ability to directly add new compounds to a NIST User Library with a simple click of the mouse. An improved user interface makes reviewing runs easier and more convenient than ever. Improved NIST search results from an advanced algorithm that filters out spectral noise which can degrade search quality, and much more.

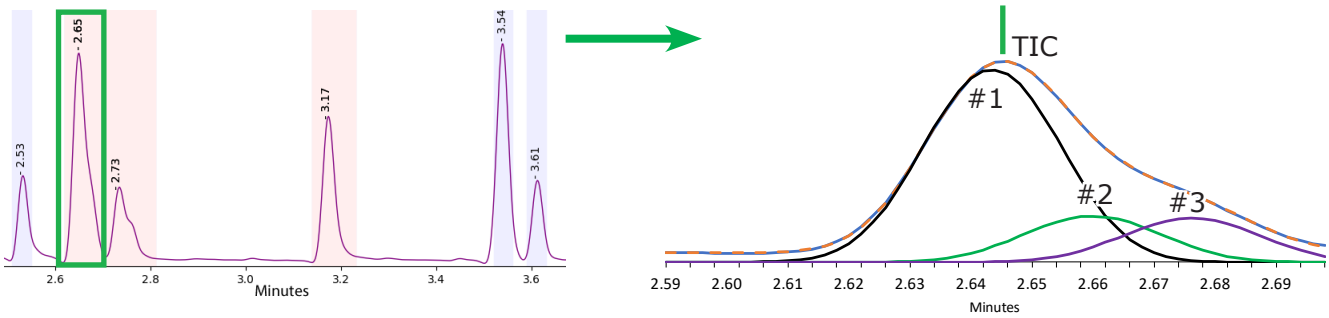


Auto RI is a revolutionary approach for calculating RI from samples without the need for tedious and time consuming separate calibration runs.



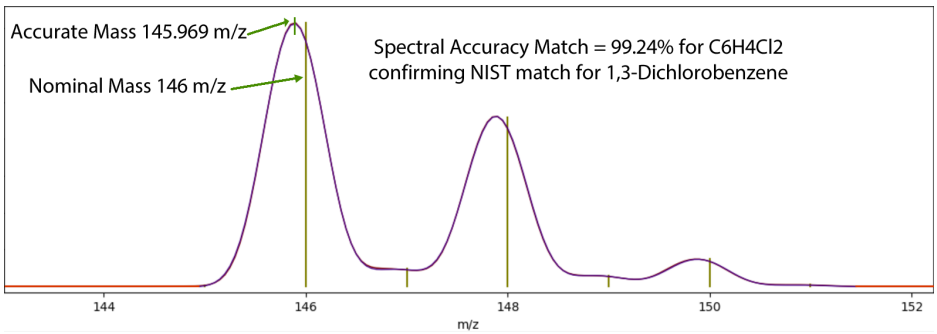
Even without accurate mass or an external RI calibration, GC/ID provides powerful deconvoluton and confident ID using Auto RI with centroid data to correctly ID the isomer Triphenylene. GC/ID processed this entire run in less than 5 seconds!

GC/ID automatically identifies "mixture" peaks and not only indicates the number of unresolved compounds, but also generates the "pure" MS



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

GC/ID confirms each NIST library match by validating the formula using accurate mass/spectral accuracy



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

Retention Index match (RI Fit) provides a powerful quantitative metric to readily ID the right compound, even when the library search values are close or ambiguous

The new "Magic Highlighter" makes quick work of identifying the correct compound even when the top NIST matches are similar. By combining RI data with Fwd and Rev Search and confirmation of ions by accurate mass, the correct compound (Hit 3) is easily identified.

Hit	NIST	RevS	SA-M	SA-F	RIFit	RI	RILib	MW	Formula	Name
1:	968	968	99.28	99.18	54.38	563.38	609	95.953	C2H2Cl2	Ethylene, 1,2-dichloro-, (Z)-
2:	932	932	99.28	99.18	69.38	563.38	594	95.953	C2H2Cl2	1,2-Dichloroethylene
3:	932	932	99.28	99.18	94.62	563.38	558	95.953	C2H2Cl2	Ethylene, 1,2-dichloro-, (E)-
4:	867	876	99.28	99.18	57.62	563.38	521	95.953	C2H2Cl2	Ethene, 1,1-dichloro-
5:	787	806	26.28	99.18	0.00	563.38	1199	153.959	C4H4Cl2O2	Dihydro-4,5-dichloro-2(3H)furanone
6:	661	662	-29.09	99.18	0.00	563.38	1119	233.885	C4H5BrCl2O2	Methyl 3-bromo-2,2-dichloro-propanoate
7:	642	644	97.24	99.18	0.00	563.38	704	95.980	C2H5ClS	Chloromethylmethyl sulfide

GC/ID is the first major breakthrough in GC/MS 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 or to learn how GC/ID V3 can make your lab more productive.

GC/ID 3.0

The Ultimate GC/MS ID/Semi-Quant Solution

- **Modern Python Scripting (Custom Automation)**
- **GC/MS Vendor Agnostic**
- **Library Search**
- **Deconvolution**
- **Automation**
- **Semi-Quant**
- **Report & Review**

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