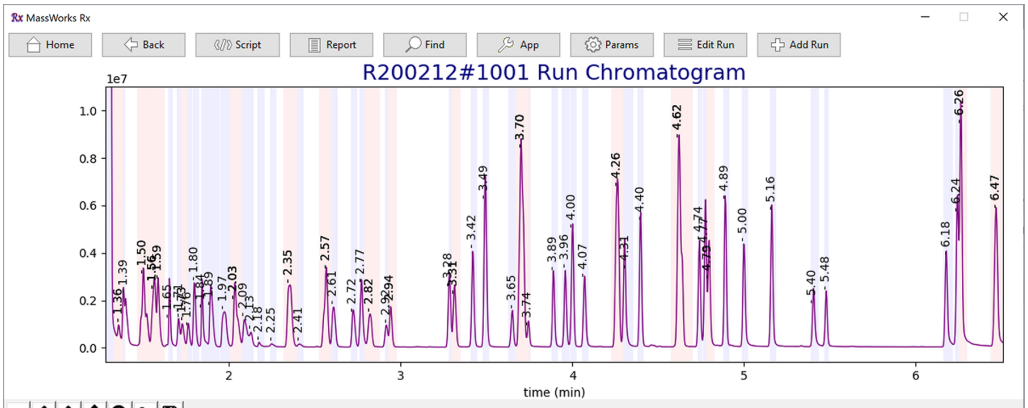
MassWorks Rx™ **GC/ID** **NEW V1.1**

Fully Automated and Highly Confident GC/MS Compound ID

GC/ID is a fully automated data processing software that provides dramatic improvements for GC/MS qualitative analysis. By incorporating Cerno's proven TrueCal™ calibration technology for accurate mass formula ID along with conventional NIST library search, a significant improvement in compound ID certainty is achieved on single quad GC/MS systems. GC/ID also provides, for the first time, an entirely automated method of quantitatively utilizing the NIST retention index values to provide yet a third orthogonal metric for compound ID. V1.1 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 instruments. Combined with library search and retention index values, 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.



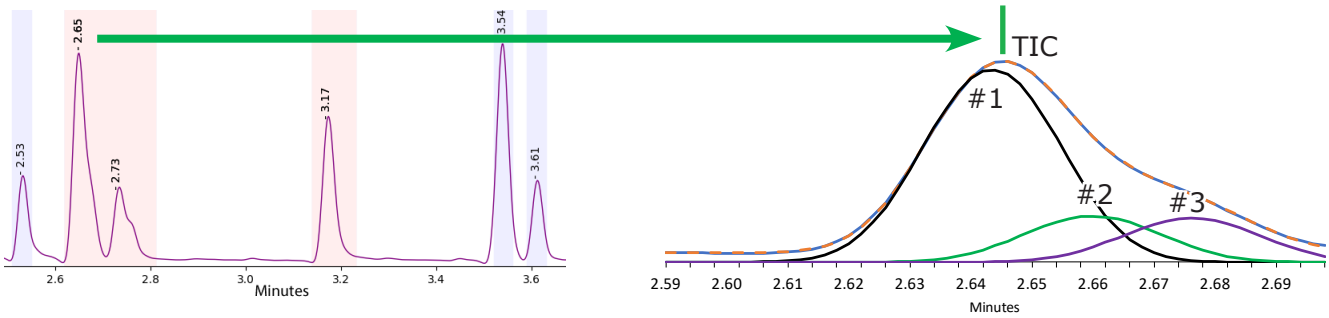
R200212#1001: 78 peaks from JPCerno_Split_Pro_LowR_2

VOC Analysis with RI calibration

Peak	Time	Area	Mix	NIST	SA-M	SA-F	RIFit	RI	MW	CAS	Formula	Name
33	2.57	32943.93	1/2	920	99.2	99.4	96.3	767	92.063	108-88-3	C7H8	Toluene
34	2.57	15527.12	2/2	967	99.0	99.5	96.3	767	109.969	1061-02-6	C3H4Cl2	1-Propene, 1,3-dichloro-, (E)-
35	2.61	24905.75	1/1	944	99.0	99.0	96.0	772	131.930	79-00-5	C2H3Cl3	Ethane, 1,1,2-trichloro-
36	2.72	25257.63	1/1	948	98.1	99.5	94.0	786	111.985	142-28-9	C3H6Cl2	Propane, 1,3-dichloro-
37	2.77	36018.47	1/1	939	99.3	99.6	98.1	792	100.089	591-78-6	C6H12O	2-Hexanone
38	2.82	18987.3	1/2	957	96.1	99.1	98.2	798	205.813	124-48-1	CHBr2Cl	Methane, dibromochloro-
39	2.82	6118.36	2/2	750	95.5	99.2	98.2	798	114.141	111-65-9	C8H18	Octane
40	2.92	6584.37	1/1	953	98.1	98.9	97.5	809	185.868	106-93-4	C2H4Br2	Ethane, 1,2-dibromo-
41	2.94	7787.7	1/2	959	98.1	99.2	97.5	811	163.875	127-18-4	C2Cl4	Tetrachloroethylene
42	2.94	2620.49	2/2	950	96.8	99.2	94.5	811	185.868	106-93-4	C2H4Br2	Ethane, 1,2-dibromo-
43	3.28	25139.87	1/1	972	99.2	99.8	99.9	849	112.008	108-90-7	C6H5Cl	Benzene, chloro-
44	3.31	19713.67	1/2	965	-31.2	98.5	83.1	852	165.891	630-20-6	C2H2Cl4	Ethane, 1,1,1,2-tetrachloro-

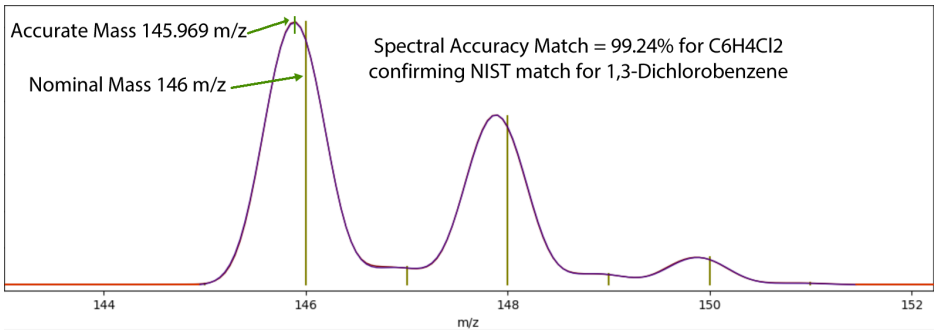
GC/ID processes an entire run in a few minutes and calculates the NIST match value (NIST) for each peak, verifies the compound formula ID by accurate mass/spectral accuracy (SA-M) as well as fragement ions (SA-F) and then calculates the peak's retention index (RI Fit). ***These additional metrics can dramatically improve compound identification confidence.***

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.

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



The profile spectral overlay of the calculated "True" MS (Blue) and the calibrated (Red) MS are identical to within 99.24% spectral accuracy confirming the NIST compound formula for more confident compound ID. This is a feature previously only available in high resolution MS.

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

The "NIST" match results (Red) cannot ID the correct compound (Ethylene, 1,2-dichloro-,Z) and neither can the formula ID from spectral accuracy (SA). "RI Fit" (Blue) easily distinguishes the correct hit and the (NIST+SA+RI Fit) blended "Match" value (Green) clearly identifies the correct compound.

HIT	Match	NIST	SA	RI Fit	Formula	Name
1	95.44%	911	99.35%	96.29%	C2H2Cl2	Ethylene, 1,2-dichloro-, (Z)-
2	86.88%	915	99.35%	52.71%	C2H2Cl2	Ethylene, 1,2-dichloro-, (E)-
3	73.78%	851	99.35%	15.71%	C2H2Cl2	Ethene, 1,1-dichloro-
4	71.80%	718	49.47%	-1.00%	C4H4Cl2O2	Dihydro-4,5-dichloro-2(3H)furanon
5	70.10%	759	99.35%	15.71%	C2H2Cl2	Ethene, 1,1-dichloro-

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 creation of additional 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. Contact us today for a demo or to learn how GC/ID can make your lab more productive.

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FOR MORE INFORMATION
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