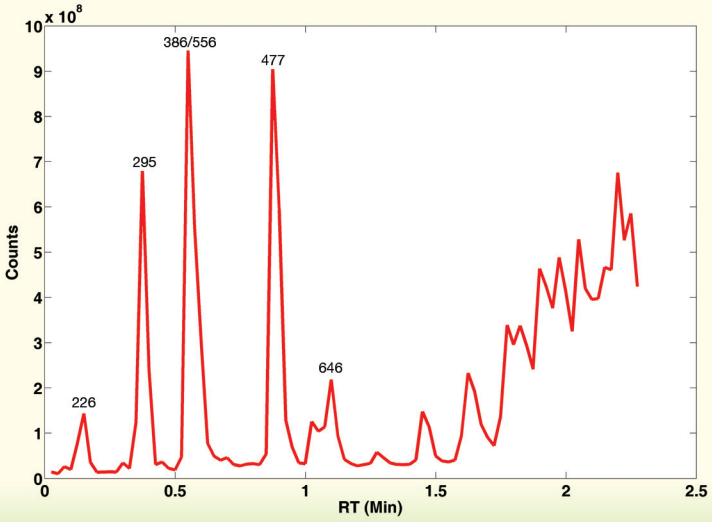
AutoID™

Formula ID software for automated analysis, e.g., with open access quadrupole MS

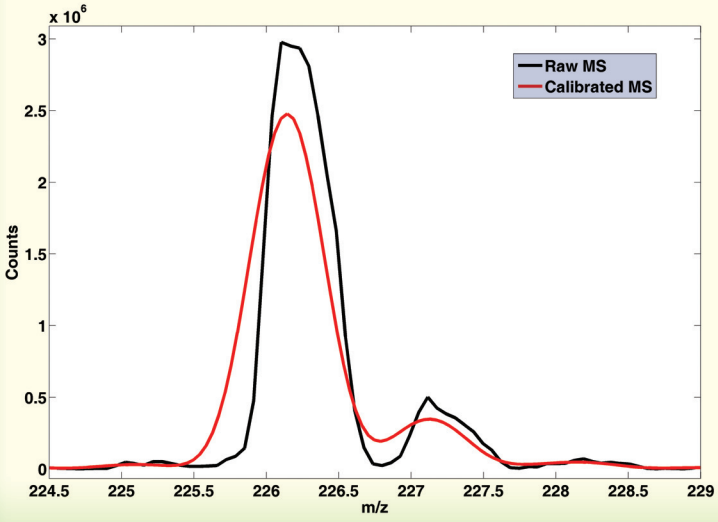
Automated MS calibration and formula ID with high mass accuracy and SPECTRAL ACCURACY

Cerno Bioscience proudly introduces **AutoID**™, a new MS software product built from its flagship MassWorks™ premium software, which won the Most Innovative Product award at PittCon 2006 for enabling formula ID on even a single quadrupole MS, a capability typically reserved for higher resolution MS systems. Details of this innovative MS processing technology have recently been published in a cover feature article in Anal. Chem. **2010**, 82, 7055-7062. By automating this patented calibration and formula ID process on the widely available workhorse quadrupole MS systems, AutoID brings the 100x improvement in mass accuracy and the unparalleled spectral accuracy (up to 99.9%) seamlessly to a routine laboratory at all times. With both accurate mass and high spectral accuracy, AutoID allows any user to either confirm a given formula or propose possible formulas in a fully automated fashion without any human intervention or manual operations.

AutoID™ completely removes the manual steps required of a conventional formula determination process, including the introduction of calibration standard(s), the user selection of ions and elemental parameters, the report generation and delivery. For highly automated applications such as those in open access or walk-up environment, AutoID not only brings the formula ID capability to non-expert MS users including synthetic or medicinal chemists but also reduces the burden placed on analytical chemists or mass spectrometrists who support these functions. With the formula ID capability now seamlessly available to non-expert users on a routine yet reliable quadrupole MS system, significant savings in time, effort, and hardware costs can be achieved.



Using a universal calibration mixture, raw profile mode MS data are automatically acquired at given time intervals (e.g., once daily) or according to a preset schedule.



Once a calibration data acquisition is complete, AutoID automatically creates a new MS calibration to correct for both m/z and peak shape. This calibration will be then used to analyze all subsequent samples until a new calibration becomes available.

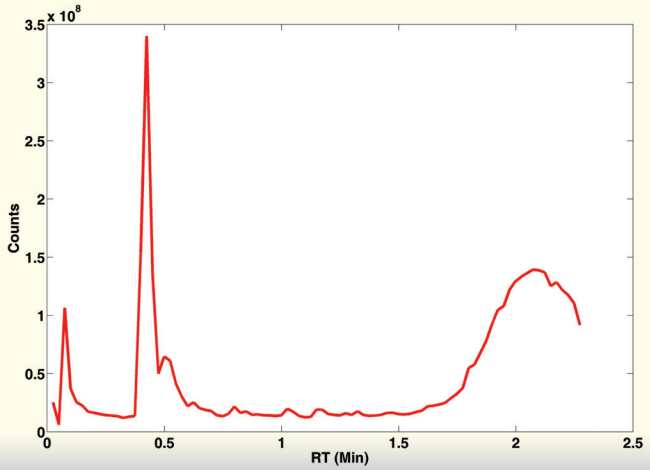
AutoID™

After a calibration is completed, AutoID sends a calibration report to the administrator summarizing the results

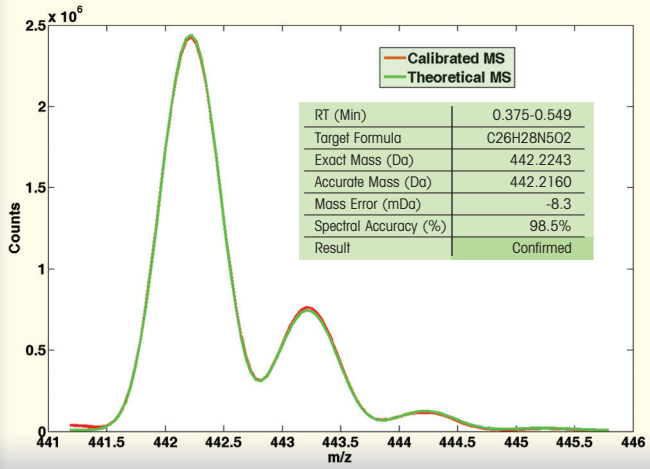
RT (Min)	Standard Formula	Exact Mass	Accurate Mass	Mass Error (mDa)	Spectral Accuracy(%)	Pass
0.075-0.200	C12H20NO3	226.1443	226.1443	0.0	98.88	Y
0.325-0.425	C14H19N2O5	295.1294	295.1295	0.1	98.23	Y
0.574-0.749	C21H32N5O2	386.2556	386.2555	-0.1	99.56	Y
0.824-0.949	C29H34N2O2Cl	477.2309	477.2266	-4.3	99.10	Y
0.525-0.674	C28H38N5O7	556.2771	556.2774	0.2	99.30	Y
1.074-1.199	C25H30I2NO3	646.0315	646.0316	0.1	99.43	Y

TARGET FORMULA CONFIRMATION

When a user submits a sample for analysis with a target formula for confirmation, AutoID automatically processes the acquired MS data as soon as the data acquisition is complete and applies the currently effective calibration to the sample data to provide accurate mass (to a few mDa) and spectral accuracy (up to 99.9%) confirmation of the target formula, with the results summarized in a report to be automatically sent to the end user.



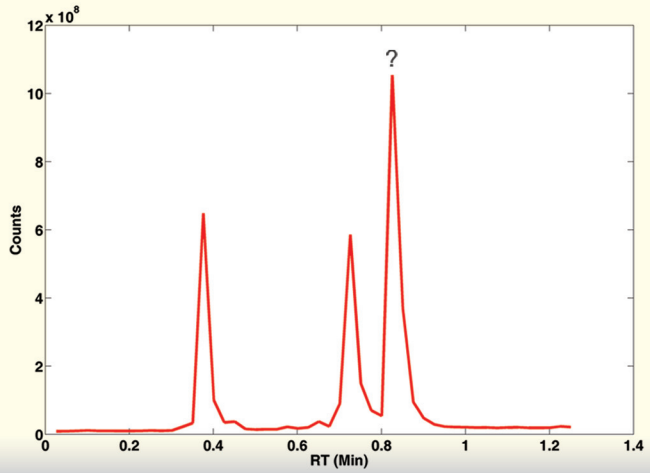
The target compound eluted at RT ~0.5min in a short LC/MS run



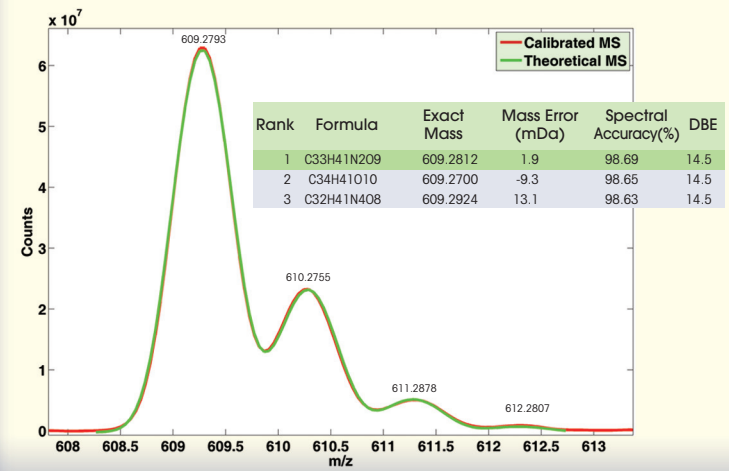
After the MS calibration, the target compound is correctly confirmed with both accurate mass and spectral accuracy.

UNKNOWN FORMULA IDENTIFICATION

If a sample is submitted for analysis without a target formula or if a given target formula could not be confidently confirmed, the sample will be treated as an unknown. In this case, AutoID will proceed to identify possible formulas for a given number of significant chromatographic peaks. An unknown identification report is then generated and automatically sent to the end user.



The unknown compound eluted at RT ~0.83min in a short LC/MS run



The mass spectrum of the unknown compound is calibrated with accurate mass reported. A CLIPS formula search lists a few possible formula candidates for consideration.

Date	Time	User	BatchID	Plate/ Well	Result	Mass Error (mDa)	Spectral Accuracy (%)	PDF Report
1/11/2011	4:00	Rachel Jones	rjones149	3/6	Pass	≤5	≥98.50	C311QC_24
1/11/2011	10:40	Dave Smith	dsmith156	3/16	Confirmed	9.3	99.29	C311_00442
1/11/2011	10:48	Sharon Lee	slee157	3/19	Confirmed	-3.1	99.11	C311_00444
1/11/2011	10:51	Nancy Deng	ndeng158	3/34	Identified	6.5	98.82	C311_00446
1/11/2011	12:13	Megan Johnson	mjohn-son159		Identified	-4.2	99.95	C311_00448
1/12/2011	4:00	Rachel Jones	rjones150	3/6	Pass	≤5	≥98.50	C311QC_25
1/12/2011	7:30	Doug Wong	dwong157	4/16	Identified	5.4	99.29	C311_00512
1/12/2011	8:13	Lilly Brown	lbrown162	4/19	Identified	8.1	99.11	C311_00514
1/12/2011	8:59	Matt Davidson	mdavidso168	4/22	Confirmed	-4.8	98.62	C311_00516
1/12/2011	9:35	Julia Cheung	jcheung173	4/34	Confirmed	-0.5	98.94	C311_00518

MS calibration, formula confirmation and unknown formula ID in one fully automated package with real time display of processed samples

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