

Accurate Mass Results Acceptable for Publication in the Journal of Organic Chemistry (JOC)

Since the introduction of its innovative MS calibration and analysis software, Cerno Bioscience has received many similar questions from potential users, especially academic users, on the acceptability of MassWorks accurate mass results for publication in JOC-type journals, even with data from unit mass resolution GC/MS or LC/MS systems. Cerno has closely followed the evolution of the JOC requirement for compound identification over the years, from the initial 5ppm mass accuracy with HRMS, the +/-3mDa mass accuracy without explicitly requiring HRMS, to the current “MS accurate mass (historically called HRMS or exact mass) data” as stated in

http://pubs.acs.org/paragonplus/submission/joceph/joceph_authguide.pdf

with the relevant paragraphs copied below,

“Identity. Evidence for documenting the identity of new compounds should include both proton and carbon NMR data and either MS accurate mass (HRMS) or elemental analysis data. Where other types of physical and spectroscopic methods are useful or necessary for confirming structure assignments, it is appropriate to include a summary of the data in the experimental section, but except as noted below, these additional data types are not required for routine compound characterization in JOC. Such data types include IR, UV-visible, low resolution MS, GCMS, LCMS, 2D NMR, X-ray crystallography, and chiroptical methods.

“Elemental Analysis and Accurate Mass Measurement. For most new compounds except large biomacromolecules (see below) and polymers, either combustion elemental analysis or **mass-spectrometric accurate mass (historically called high resolution mass spectrometry [HRMS] or "exact mass") data** should be reported to support the molecular formula assignment. The data should be reported in ACS Style Guide format and should include the molecular formulas on which the theoretical (Calc) values are based.”

Cerno MassWorks does provide accurate mass measurement, which is conventionally obtained via HRMS, and our understanding of the language is that **either** accurate mass **or** (historically called) HRMS would be sufficient. It is interesting to note that this guideline no longer requires 5ppm or +/-3mDa mass error, since another metric termed Spectral Accuracy, as published by Cerno in a cover feature article in *Anal. Chem.* **2010**, *82*, 7055-7062, has proven to be more important for compound characterization or unknown identification.

We have recently sought clarification from JOC on the exact interpretation of this requirement with the following official response,

JOC does not endorse specific procedure, instrument, or software for obtaining the required data **as long as it is capable of providing the required measurements.**

Based on this response, Cerno Bioscience concludes that MassWorks accurate mass obtained from unit mass resolution GC/MS or LC/MS for organic compound characterization is acceptable for JOC-type of publications.

More Information

Please contact Cerno Bioscience directly for more information.