

Interactive comment on “Orbitool: A software tool for analyzing online Orbitrap mass spectrometry data” by Runlong Cai et al.

Anonymous Referee #2

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Summary and recommendation:

In this study, Cai et al. describe the development of a new software tool for the analysis of Orbitrap data, focusing in particular on data treatment procedures that are common in atmospheric sciences. The authors demonstrate the usefulness of the developed procedures and explain how the algorithms process the data. Moreover, they show examples of laboratory and field data that were processed using the new software. The software is planned as an open source tool and freely available on the internet after user registration.

In my opinion, the authors did a very good job and created an impressive tool for Orbitrap data analysis, which follows routines that are familiar to the CIMS community. I agree with the authors that Orbitrap mass spectrometers will play a more and more

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important role in atmospheric sciences in the future. Therefore, a software tool tailored to the needs of online Orbitrap MS data is highly desirable and will certainly help CI-TOFMS users to transition to CI-Orbitrap MS.

The manuscript is well-written and explains in a reader-friendly manner all modules of the software. Therefore, I have only some minor comments, which should be addressed before final publication in AMT.

Minor comments:

- 1) P6L17f: I cannot follow the authors explanation on the averaging weight for the spectra. Could you explain in more detail why the scan number is more important than the duration of a single scan?
- 2) P7L5: How do the authors define background here? Is it only electronic background? As far as I know there is already a built-in background subtraction of signals by the acquisition software from the manufacturer.
- 3) P7L9f: For readers less familiar with the common procedures in the CIMS community, it might be helpful to explain shortly why the noise estimation is conducted in the mass defect range of 0.5-0.8 Da.
- 4) P8L13f: The description of the peak width normalization should be revised. Currently, it remains unclear why the peaks are normalized to 200 Da after dividing them by the square root of m.
- 5) P9L13: As far as I know, the default setting of XCalibur is to remove lock masses and reference signals from the mass spectra. Could the authors check again?
- 6) P10L4ff: It remains unclear whether isotopic patterns of candidate formulae are considered in the formula assignment procedure. If they are not considered so far, I would suggest to include this in future versions of the software. Even if the isotopic signals might deviate at low concentrations from the expected intensity, it would still be reasonable to check for the presence of such signals. Could the authors comment on

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this?

- 7) P12L19: Over which time span were the spectra averaged that are shown in Fig. 4?
- 8) P13L10f: Could the authors provide a list of observed signals and assigned molecular formulas in the supporting material? Moreover, do the authors suggest the presence of gas-phase organosulfates and nitrooxy organosulfates which are among the CHOS and CHONS compounds?

- 9) P14L15ff: Several authors are missing in the list of "Author Contributions" (i.e., C.G., M.E., C.H., and P.Y.)

Technical comments:

- 1) Abstract / L2: replace "wildly-used" with "widely-used"
- 2) P3L1: replace "produce" with "emit" (or a similar verb)
- 3) P6L15: replace "within each time bin" with "for each time bin"
- 4) P6L23: better use "ion polarity" instead of "charge polarity"
- 5) P7L1: replace "positively charged spectra" with "spectra from positive mode" (and accordingly for "negatively charged spectra")
- 6) P8L22: word missing after "this"
- 7) P10L6: better use "ion polarity" instead of "charge polarity"
- 8) P10L20 and P11L11: replace "exported into file" by "exported into other file formats"
- 9) P11L8: replace "These" by "The"
- 10) P12L14: remove "50th"
- 11) P13L1: replace "then" by "the"
- 12) Figure 3: It is difficult to distinguish the colors of the different percentiles

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- 13) Figure 4: typos in the legend ("denoized" should read as "denoised")

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