Atmos. Meas. Tech. Discuss.,
doi:10.5194/amt-2020-267-RC3, 2020

Atmospheric Measurement Techniques Discussions

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

Anonymous Referee #4

Received and published: 30 September 2020

General comment:

The paper presents Orbitool, a novel online software tool for analyzing Orbitrap mass spectrometry data. The paper is within the scope of AMT but is often too superficial in the description of the working principles of the software and there is no real validation of the output. Some specific comments follow.

Specific comments:

p.4, l.1: the mass resolving power of the best TOF analyzers is now more than 50,000. https://www.sciencedirect.com/science/article/pii/S0165993619302018

p.4, l.7-13: this paragraph on source comparison does not belong to this software development article

p.5, l.20: I do not understand what is meant by "long-term atmospheric measurements". Is it related to the averaging feature?

p.6, l.10: even if the orbitrap was recording all the data points, this would not generate an equally spaced grid since the size of the bins (i.e. resolution) is variable with the mass

p.6, l.12: the term "proper averaging" needs to be clarified: what are the different methods to make the average?

p.6, l.15: "time bin" - this concept seems important afterwards but it is not defined

p.6, l.17-18: why making weighted averages?

p.6, l.19-20: why would the mathematical operation of average involve the resolution of the Orbitrap?

p.6, l.19-23: this should be at the beginning of the paragraph; first describe the procedure before going into the details of how it's done and not the other way around

p.7, l.8: the mathematical effect of the average itself causes the noise level to go down (division of a constant level by a higher number of spectra), not the instrumental fact of acquiring more time

p.7, l.8-9: I am guessing that the mass defect range of [0.5, 0.8] Da was chosen because no signal peaks are expected with such a mass defect in the mass range studied?

p.7, l.13: what is "a certain percentile"? I had to wait until p.12, l.16-17 to find the explanation. It should be in the description section, not in the the discussion. See also p.12, l.5-6

p.7, l.17: here, I think it is necessary to develop why the averaged spectrum would have different noise thresholds because according to me, even if the individual spectra have different noise thresholds, the resulting spectrum will in any case have a single

noise level from a statistical point of view. Actually, I don't understand the difference in the final result between option b and option a

p.8, l.1-3: I understand that the orbitrap doesn't generate signals at 0 for the masses it doesn't detect. However, I don't see the link between removing noise, i.e. removing data, and the fact that the orbitrap doesn't populate empty masses. It seems obvious that removing data (noise) reduces the size of the file and thus the number of points to be processed afterwards

p.8, l.9-10: my personal experience is that peaks are not really Gaussian, and I don't seem to see any discussion on why the Gaussian model works in your case. It seems necessary to develop what you say in the caption in the body of the text

p.10, l.9-10: this statement needs a reference or at least more explanations

p.12, l.22: Th here and Da in figures. The same unit should be used throughout the paper

p.13, l.14-15: I'm having a hard time with this sentence (and this paragraph, actually). It's a software article. A software needs to be validated with a systematic validation protocol with other software/publications and the quantification of the performance. It cannot just be like "oh, that's cool, we are seeing things we've already seen and things we don't know anything about"

p.13, l.21: is it Orbitool or rather the fundamental difference between ToF and Orbitrap data? Because nowhere is there any mention of a data storage strategy that is not based on the fact that Orbitrap data is generated in the right way

p.14, l.1: I am not convinced. See my previous comment above

p.14, l5-7: This sentence does not belong to this article

Figure 5: The mass defect as presented in this figure does not match with the definition of the mass defect in p.7, l.9-10: depending on your definition of the nominal mass, it

should be either in the range of [0, 1] or of [-0.5, 0.5]

Interactive comment on Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2020-267, 2020.