Responses to Comments on Manuscript amt-2020-267 (Orbitool: A software tool for analyzing online Orbitrap mass spectrometry data)

We thank Dr. Myriam Guillevic for her concerns on the public availability of Orbitool. As clarified below, Orbitool is an open-source code. In the following paragraphs, the comments are shown as sans-serif dark red texts and our responses are shown as serif black texts.

Reviewer #1, Dr. Myriam Guillevic

We would like to make a brief technical comment regarding naming of the released code/version.

In Cai et al., the authors write that the newly developed software is Open Source. Technically, this means that the source code (.py files in Python, as written by the authors), should be made available, so that other people can check each step of the process and read the algorithms. However, as also mentioned by the reviewers, so far what is available is an executable version to install, after registration. Also on the project webpage <https://orbitrap.catalyse.cnrs.fr/>, it is clearly stated that " an executable Orbitool is available". We downloaded the zip file and we found indeed only the executable, with Python bytecode (.pyd and .dll files).

It would be good if the authors clarify the description of what is exactly made available to registered users.

If the authors wish to make only an executable available, to avoid other scientists to check or re-use the source code, this is called a 'Freeware' version, i.e. users have no access to the source code but the executable is available for free. If you do not make the source code available, you cannot call it 'Open Source', please use 'Freeware' instead, so that users don't get confused.

Or, if the authors plan to release the source code along with the executable in the future, please mention this clearly (e.g., where the source code will be hosted).

Response: Both the source codes (.py files) and the executable software (.exe file) are now publically available on the website.

We have added the following text on the website:

"<u>Researchers who are not familiar with Python can directly run the Orbitool.exe file without a Python programming</u> language on their computer. An executable can be downloaded using the following link...

Source codes (.py files) are publically available in the following files..."

In addition to providing open-source codes, we aim to facilitate researchers to use Orbitool in a more flexible way. Researchers who are experienced with Python programming can modify Orbitool and add new features by themselves. They can also use the Orbitool functions without following the standing data processing procedure or relying on the graphical user interface. We are currently refactoring the codes and adding brief comments so that it will take less effort to understand the codes. Classes and functions will be defined in a more general way to facilitate customized applications.