

Interactive comment on “FATES: A Flexible Analysis Toolkit for the Exploration of Single Particle Mass Spectrometer Data” by Camille M. Sultana et al.

Anonymous Referee #1

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This is a great piece of coding and work. Owing to the great variety of data formats of particle mass spectra and the copious numbers and types of clustering and relational information that is sought, having the flexibility provided by FATES is critical. The authors have included every iteration of data analysis and presentation that I could think of. Nonetheless, I am confident that the user base for this wonderful analytical tool will grow quickly and with the added insight of many users will become even more useful.

I have two primary concerns however: (1) Operation has been demonstrated only with the authors' data format. I believe that, before publication, the authors should experiment with different data formats from the intended users of the program. I could find little discussion of how data entry for specific formats is or will be accomplished. Having

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had a copy of the program to test would have been very beneficial. Unfortunately, the link in the manuscript is not working. (2) How will the authors overcome the potential limitation of becoming obsolete, or at least not readily upgradeable or adaptable, with future versions of Matlab, as is the case suffered by YAADA.

Again, overall I feel that the authors are providing a very important to harmonize particle mass spectrometer data across a user base of data formats that has developed quite haphazardly over the past decade or so. In my opinion though, I believe that publication at this point is precocious until the program has been tested to some extent by others.

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