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

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Response to comment 1: We are sorry that the link in the manuscript was not working for you to explore the toolkit. We believe that we have fixed the permissions on github so that it is now open to the public to download. Please let us know if you continue to have trouble. Along with the code we have provided a very comprehensive, 33 page, FATES manual. Over ten pages are dedicated to describing the raw data formats, data importation process, current FATES structure, and instructions for altering for adapting the structures and code for compatibility with different data formats. Due to the very detailed nature of this description we do not believe it is appropriate for discussion in the paper, though of course the information is important to provide to users. In
addition we will work on acquiring raw data from an outside SPMS group to validate the adaptability of FATES to different data formats.

Response to comment 2: As mentioned briefly in the paper YAADA was particularly susceptible to updates to MATLAB and difficult to maintain because the YAADA framework created and then utilized data types which were not native to MATLAB. Because YAADA constructed 6 new data classes YAADA couldn’t automatically leverage many of the built-in MATLAB data handling functions. Numerous scripts had to be included in YAADA to perform very simple operations mirroring the capabilities of functions already in MATLAB. Because FATES utilizes native MATLAB data types the code base required to operate the FATES toolkit is decreased by over an order of magnitude from YAADA. In addition, in FATES we have attempted to leverage matrix operations and low-level operations whenever applicable which are unlikely to be affected by foreseeable MATLAB updates. While any toolkit is going to require maintenance eventually as MATLAB updates, we believe that due to the relatively small and simple code base maintenance should not only be minimal but it would likely be straightforward to take advantage of future MATLAB enhancements. We also believe that by offering FATES on a platform built to promote open-source software development (github) it will be much easier for the community to collaborate and improve FATES.