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GIGA-D-17-00039
"From chromatogram to analyte to metabolite. How to pick horses for courses from the massive web-resources for mass spectral plant metabolomics"
Original Submission

Hiroshi Tsugawa (Reviewer 1)

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Comments to Editor:

Comments to Author:

This review has been well-written already, but I have some comments as listed below which should be considered by authors.

1. The paper is too long. Should all of the local- or web applications that you introduced be highlighted in this paper? As you mentioned in the future perspective, many of the tools are already 'out of dates', never updated for a long time, and never used for metabolomics research anymore. But I really feel a 'value' in this paper especially for an 'education' purpose too. Therefore, I highly would like authors to add 'the date of last update' for each tool (or as much as possible) cited in this manuscript. As you know, the evaluation of GO analysis tools is now performed like that: http://www.nature.com/nmeth/journal/v13/n9/full/nmeth.3963.html?WT.ec_id=NMETH-201609&spMailingID=52180959&spUserID=MzcwMzk3NDY5OTES1&spJobID=985584826&spReportId=OTg1NTg0ODI2S0

I know your review is not for the evaluation. But you have to add the information of 'recommended'-, 'activity-', 'special interest' or 'outstanding interest' as a lot of reviews do. See like COCB reviews: http://www.sciencedirect.com/science/journal/13675931/36/supp/C.

2. Please transfer ms2lda and ms2analyzer to 'annotation' section.
3. I think MS-DIAL is not only for DIA-MS, but also all other techniques such as GC/MS and DDA.
4. Please transfer mathdamp and spectconnect to data processing section.
5. In metabolite annotation section, cite CASMI, and see MS-FINDER and CSI-IOKR are also interesting tools which have been recently developed.
6. UNPD database should be cited as natural product database.
7. You said 'Metline currently contains 961,829 molecules'. Ok my question is: how many records do contain MS/MS information?

I am looking forward to seeing your improved manuscript.
Thanks,

More Reviewer Details

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