The Journal of Open Source Software

mzEasy

Chase M Clark[1]

1 University of Illinois at Chicago

DOI: 10.21105/joss.00804

Software

- Review
- Repository
- Archive

Submitted: 02 July 2018
Published: 03 July 2018

Summary

An increase in access to liquid chromatography-mass spectrometry (LC-MS/MS) and advanced algorithms (often cloud-based) has led to a surge in users whose time is often better spent with advanced analyses than converting and evaluating, holistically, their raw data. However, conversion of raw spectra to open access formats and ensuring data is of good quality are necessary steps for proper use in later analyses. Unfortunately, users unfamiliar with conversion software often miss needed settings or are unsure how to proceeed, adding a barrier of entry to the use of more advanced analysis pipelines.

mzEasy provides a simple interface with MSConvert (Chambers et al. 2012) to convert raw MS files to the "mzXML" open access format (Pedrioli et al. 2004) and auto-generate quality control graphs (with an option to save graphs as a pre-assembled manuscript image). Importantly, mzEasy doesn't require (or have options for) adjusting/selecting any settings other than what image format to save plots as.

mzEasy is auto-configured to convert vendor files to mzXML with settings required for analyses such as GNPS (Wang et al. 2016) and is meant for anyone uneasy with using MSConvertGUI. It is also designed for users that want access to parallelized MSConvert and/or a simple way to generate quality control plots that are pre-arranged for easy publication/sharing.

Features:

- Available for download as a Windows executable for easy installation.
- Interfaces with MSConvert for conversion of raw mass spectrometry data.
- Provides the option to run conversion in parallel (# of cores minus one).
- Creates graphs to assess, broadly, the quality of an LC-MS/MS file.
- Allows export of graphs as pre-assembled figure, in multiple image formats.
- Automatic updates for future improvements.

Availability:

- Download from: chasemc.github.io/mzEasy
- Source code available at: github.com/chasemc/mzEasy

Software Requirements:

- Windows operating system
- ProteoWizard (proteowizard.sourceforge.net)

mzEasy was written in R (R Core Team 2018) and utilizes Shiny (Chang et al. 2018), RInno (Hill and Pang 2018), mzR (Chambers et al. 2012), and ggplot2 (Wickham 2009).

References

Chambers, Matthew C, Brendan Maclean, Robert Burke, Dario Amodei, Daniel L Ruderman, Steffen Neumann, Laurent Gatto, et al. 2012. "A Cross-Platform Toolkit for Mass Spectrometry and Proteomics." *Nature Biotechnology* 30 (10). Nature Research:918–20. https://doi.org/10.1038/nbt.2377.

Chang, Winston, Joe Cheng, JJ Allaire, Yihui Xie, and Jonathan McPherson. 2018. *Shiny: Web Application Framework for R*. https://CRAN.R-project.org/package=shiny.

Hill, Jon, and W. Lee Pang. 2018. *RInno: An Installation Framework for Shiny Apps*. www.ficonsulting.com.

Pedrioli, Patrick G A, Jimmy K Eng, Robert Hubley, Mathijs Vogelzang, Eric W Deutsch, Brian Raught, Brian Pratt, et al. 2004. "A Common Open Representation of Mass Spectrometry Data and its Application to Proteomics Research." *Nature Biotechnology* 22 (11). Nature Publishing Group:1459–66. https://doi.org/10.1038/nbt1031.

R Core Team. 2018. *R: A Language and Environment for Statistical Computing*. Vienna, Austria: R Foundation for Statistical Computing. https://www.R-project.org/.

Wang, Mingxun, Jeremy J Carver, Vanessa V Phelan, Laura M Sanchez, Neha Garg, Yao Peng, Don Duy Nguyen, et al. 2016. "Sharing and Community Curation of Mass Spectrometry Data with Global Natural Products Social Molecular Networking." *Nature Biotechnology* 34 (8):828–37. https://doi.org/10.1038/nbt.3597.

Wickham, Hadley. 2009. *Ggplot2: Elegant Graphics for Data Analysis*. Springer-Verlag New York. http://ggplot2.org.