MASH Explorer App

MASH Explorer, developed by the Ying Ge research group, is a comprehensive, universal, and user-friendly, free software environment for top-down proteomics. MASH Explorer allows data import from various vendor data formats. This software accommodates several deconvolution and database search pipelines for spectral deconvolution and protein identifications. The program also allows quantification of various proteoforms in different biological/experimental conditions. MASH Explorer allows visualization of the complex top-down and tandem mass spectra for the validation of deconvolution and protein identification results. It is developed by an interdisciplinary team consisting of experts in top-down mass spectrometry-based proteomics, computational data science, and bioinformatics/biostatistics.

More information can be found on the MASH Explorer Website.

MASH Explorer Citation

Please cite the following publications if the software is used:

- Wu, Z.; Roberts, D.S.; Melby, J.A.; Wenger, K.; Wetzel, M.; Gu, Y.; Ramanathan, S.G.; Bayne, E.F.; Liu, X.; Sun, R.; Ong, I.M.; McIlwain, S.J.; **Ge, Y.** MASH Explorer: A Universal Software Environment for Top-Down Proteomics., *J. Proteome Res.*, 2020, Online ahead of print.
- Cai, W.; Guner, H.; Gregorich, Z.R.; Chen, A.J.; Ayaz - Guner, S.; Peng, Y.; Valeja, S.G.; Liu, X.; Ge, Y. MASH Suite Pro: A Comprehensive Software Tool for Top - down Proteomics, *Mol. Cell. Proteomics*. Epub ahead of print.mcp.O115.054387.

Also, please cite the supporting software you use within MASH Explorer (see “Supporting Software References” below).

Development Information

This application is written in C# using Microsoft Visual Studio Professional 2015.

Funding

MASH Explorer software development is supported by NIH grant R01GM125085-01A1.

License

Installation Requirements

Please see our Installation Guide for a detailed description of how to install the required supporting software. The same information can be found in the **User Installation Guide** (C:\Program Files\Human Proteomics Program\MASH Explorer\doc\User Installation Guide.pdf) included with your MASH Explorer download.

Getting Started

The Getting Started Webpage and the **Getting Started file** (C:\Program Files\Human Proteomics Program\MASH Explorer\doc\GettingStarted.pdf) document included with the MASH Explorer download contains sample data files and a tutorial of how to use Discovery Mode and Targeted Mode.

User Manual

Please see the **User Manual** (C:\Program Files\Human Proteomics Program\MASH Explorer\doc\MASH_Explorer_User_Manual.pdf) included with the MASH Explorer download, for a detailed description of how to use MASH Explorer's functions. (You can also access the user manual from the MASH Explorer User Resources page.)

Supported Mass Spectra Data Files

- Thermo *.raw files
- Bruker *.d and *.ascii files

- *.mzXML files
- *.mzML files
- *.mgf files
- Waters *.raw files

Supported Algorithms

Informed Proteomics:

- ProMex and MSPathFinderT Website
- Manual and Other Information

MS-Align+:

- Ms-Deconv Information
- MS-Align+ Information

pTop:

- pParseTD Manual and Other Information
- pTop Manual and Other Information

THRASH:

- THRASH Paper

TopPIC:

- Manual and Other Information

OpenMS:

- FLASHDeconv information

UniDec:

- UniDec information
- UniDec software license

Versions

The current MASH Explorer software is version 2.2. A description of software updates and release notes can be found in the **Release Notes** (C:\Program Files\Human Proteomics Program\MASH Explorer\doc\ReleaseNotes.pdf). (You can also access the release notes from the MASH Explorer User Resources page.)

User Support

Please email mash-support@g-groups.wisc.edu for technical assistance. The MASH Explorer development team responds to these emails.

Email Lists

MASH Explorer Announcements: mash-announce@g-groups.wisc.edu (Note that you cannot send email to this list – it is only for the MASH team to send announcements to MASH users.)

- Provides emails with news about MASH Explorer software updates
- To join, go to https://groups.google.com/a/g-groups.wisc.edu/g/mash-announce and click the "Ask to join group" button.
- To leave the group once you've joined, go to https://groups.google.com/a/g-groups.wisc.edu/g/mash-announce/membership and click the "Leave group" button.

MASH Explorer Forum: mashforum@googlegroups.com.

- Provides a forum for MASH users to post questions, etc. Questions can be answered by other MASH users or by the MASH team.
- To join, go to https://groups.google.com/g/mashforum and click the "Ask to join group" button.
- To leave the group once you've joined, go to https://groups.google.com/g/mashforum and click the "Leave group" button.

MASH Explorer Team

Active Team Members

- Dr. Ying Ge, Principal Investigator
- Dr. Irene Ong, Co-Investigator
- Dr. Sean McIlwain, Co-Investigator
- Dr. Xiaowen Liu, Collaborator
- Dr. Ruixiang Sun, Collaborator
- Kent Wenger, Software Developer
- Jake Melby, Graduate Student
- David Roberts, Graduate Student
- Eli Larson, Graduate Student
- Anna Janicek, Undergraduate Assistant

Previous Team Members

- Dr. Wenxuan Cai
- Yiwen Gu Sudharshanan
- Govindaraj Ramanathan
- Molly Wetzel, Software Developer
- Yiran Yan, Undergraduate Assistant
- Zhijie (Abe) Wu, Graduate Student
- Kyndalanne Pike, Graduate Student

Supporting Software References

Please cite the appropriate publications from the following list according to the supporting software that you use within MASH Explorer.

CompassXtract: This software uses CompassXtract software. Copyright © 2011 by Bruker Daltonik GmbH. All rights reserved.

DeconEngine: N. Jaitly, A. Mayampurath, K. Littlefield, J. N. Adkins, G. A. Anderson, and R. D. Smith. Decon2LS: An open-source software package for automated processing and visualization of high resolution mass spectrometry data. *BMC Bioinformatics*, 2009, 10: 87. Link

Informed Proteomics: J. Park, P. D. Piehowski, C. Wilkins, M. Zhou, J. Mendoza, G. M. Fujimoto, B. C. Gibbons, J. B. Shaw, Y. Shen, A. K. Shukla, R. J. Moore, T. Liu, V. A. Petyuk, N. Tolic, L. Pasa-Tolic, R. D. Smith, S. H. Payne, and S. Kim. Informed-Proteomics: Open Source Software Package for Top-down Proteomics. *Nature Methods*, 2017, 14: 9. 909-914. Link

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Ms-Deconv: X. Liu, Y. Inbar, P. C. Dorrestein, C. Wynne, N. Edwards, P.Souda, J. P. Whitelegge, V. Bafna, and P. A. Pevzner. Deconvolution and Database Search of Complex Tandem Mass Spectra of Intact Proteins. *Molecular & Cellular Proteomics*, 2010, 9, 12: 2772-2782. Link

MSFileReaderT: MSFileReader file reading tool. Copyright © 2009 - 2014 by Thermo Fisher Scientific, Inc. All rights reserved.

pParseTD: Z.-F. Yuan, C. Liu, H.-P. Wang, R.-X. Sun, Y. Fu, J.-F. Zhang, L.-H. Wang, H. Chi, Y. Li, L.-Y. Xiu, W.-P. Wang, S.-M. He. pParse: a method for accurate determination of monoisotopic peaks in high-resolution mass spectra. *Proteomics*, 2012, 12: 2, 226–235. Link

ProteoWizard: M.C. Chambers, B. MacLean, R. Burke, D. Amode, D.L. Ruderman, S. Neumann, L. Gatto, B. Fischer, B.Pratt, J. Egertson, K. Hoff, D. Kessner, N. Tasman, N. Shulman, B. Frewen, T.A. Baker, M.-Y. Brusniak, C. Paulse, D. Creasy, L. Flashner,K. Kani, C. Moulding, S. L.Seymour, L. M. Nuwaysir, B. Lefebvre, F. Kuhlmann, J. Roark, P. Rainer, S. Detlev, T. Hemenway, A. Huhmer, J. Langridge, B. Connolly, T. Chadick, K. Holly, J. Eckels, E. W. Deutsch, R. L. Moritz, J. E. Katz, D. B. Agus, M. MacCoss, D. L. Tabb, & P. Mallick. A cross-platform toolkit for mass spectrometry and proteomics. *Nature Biotechnology*, 2012, 30, 918-920. Link

pTop: R.-X. Sun, L. Luo, L. Wu, R.-M. Wang, W.-F. Zeng, H. Chi, C. Liu, and S.-M. He. pTop 1.0: a High-accuracy and High-efficiency Search Engine for Intact Protein Identification. *Analytical Chemistry*, 2016, 88, 3082-3090. Link

THRASH: D. M. Horn, R. A. Zubarev, and F. W. McLafferty. Automated reduction and interpretation of high resolution electrospray mass spectra of large molecules, *Journal of the American Society for Mass Spectrometry,* 2000, 11: 4, 320-332. Link

TopPIC Suite: Q. Kou, L. Xun, and X. Liu. TopPIC: a software tool for top-down mass spectrometry-based proteoform identification and characterization. *Bioinformatics*, 2016, 32, 3495-3497. Link

FLASHDeconv: K. Jeong, J. Kim, M. Gaikwad, S. N. Hidayah, L. Heikaus, H. Schlüter, and O. Kohlbacher, "FLASHDeconv: Ultrafast, high-quality feature deconvolution for top-down proteomics," Cell Systems, vol. 10, iss. 2, p. 213–218, 2020. Link

UniDec: M. T. Marty , A. J. Baldwin , E. G. Marklund , G. K. A. Hochberg , J. L. P. Benesch , and C. V. Robinson."Bayesian Deconvolution of Mass and Ion Mobility Spectra: From Binary Interactions to Polydisperse Ensembles"Analytical Chemistry, 2015, DOI: 10.1021/acs.analchem.5b00140. Link

Additional Resources

- UniProt Database Website
- UW Human Proteomics Program
- Ying Ge Research Group

- Consortium for Top-down Proteomics