MSFragger: Ultrafast and Comprehensive Identification of Peptides from Tandem Mass Spectra

TECHNOLOGY NUMBER: 7143







Technology ID

7143

Category

Software & Content

Inventor

Aleksey Nesvizhskiy Andy Kong

Further information

Drew Bennett

andbenne@umich.edu

NOTICE: April 25, 2025

Effective <u>May 1, 2025</u> the forward licensing and commercial management MSFragger + suite of tools will be handled by Fragmatics, LLC. All inquiries regarding commercial use including trial licenses, full commercial license, embedded licenses, renewals and associated use will be managed by Fragmatics, LLC. All requests should be submitted to info@fragmatics.com or at www.fragmatics.com.

No additional commercial licenses will be managed or initiated by the University of Michigan.

OVERVIEW

Peptide identification from tandem mass spectrometry (MS/MS) data

- Protein-drug interaction, protein-protein interaction analyses
- Biomarker analysis

BACKGROUND

The advent of tandem mass spectrometry (MS/MS) also known as shotgun proteomics has enabled the identification of large numbers of proteins in a biological sample and had become an indispensable tool for academic researchers as well as pharmaceutical and molecular diagnostic companies around the world. Currently, the field of tandem mass spectroscopy represents the biggest share (36%) of the mass spectroscopy market. However, the analysis of large amount data produced by proteomics experiments in addition to the advances in speed of modern instrument and growing interest in protein-drug, protein-protein interaction as well a post-translation modification has produced a significant challenge. While computer clusters are an option to provide additional processing power, but due to their expense, difficulty to maintain, and limited lifespan, there is a need for alternative methods to combat this problem.

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"In our quest to develop a broadly applicable and fast computational strategy for open database search, we designed a novel fragment-ion indexing method that provides orders-of-magnitude improvement in speed over existing tools."

MSFragger is implemented in the cross-platform Java programming language, and is compatible with standard open file formats for mass spectrometry data (mzXML/mzML). The standalone JAR file and the ProteomeDiscoverer node now support reading Thermo RAW files directly. MSFragger writes output in either tabular or pepXML formats, making it fully compatible with downstream data analysis pipelines such as Trans-Proteomic Pipeline and Philosopher.

ADDITIONAL DETAILS

Nesvizhskiy Lab Site

Commercial Users:

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References

 Kong A, et al., MSFragger: ultrafast and comprehensive peptide identification in mass spectrometry-based proteomics.Nat Methods . 2017 May;14(5):513-520. doi: 10.1038/nmeth.4256.