

For targeted proteomics, a plugin for browsing public mass spectrometry data

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Biologists often envision their hypotheses within a set of protein interactions, networks, and pathways. In turn, their experiments may focus on measuring an explicit subset of these proteins, corresponding to a targeted proteomics experiment. To date, however, designing a targeted proteomics experiment is very time-consuming, and is typically done only by mass spectrometry specialists.

Numerous publications have taken up the challenge of improving protein assay design. Their proposals largely rely on methods that use previously identified peptide/spectrum matches and that tap several large repositories of tandem <u>mass spectrometry data</u> for proteomics. But the methods they propose typically grow out of a mass spectrometry perspective, without higher-order biological context.

To address this challenge, a new paper describes a software plugin that explores public mass spectrometry data. Developed for the popular Skyline tool, the "Biodiversity Plugin" is the work of a team led by PNNL's Michael G. Degan and Samuel H. Payne, along with colleagues at the University of Texas. The primary goal of the new plugin is to help users identify data that addresses their hypotheses. This is accomplished by presenting the data in an intuitive pathway-centric visualization.

The Biodiversity Plugin comes prepackaged with data from the draft human proteome, as well as from the PNNL Biodiversity Library, a corpus of 3 million peptides (230,000 proteins) in 112 bacteria and archaea. After users have identified relevant data, the plugin seamlessly



imports that data into Skyline, the community standard tool for assay design and data analysis. The plugin can be customized with personal data, which can then be browsed and also imported into Skyline.

More information: Michael G. Degan et al. A Skyline Plugin for Pathway-Centric Data Browsing, *Journal of The American Society for Mass Spectrometry* (2016). DOI: 10.1007/s13361-016-1448-3

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