



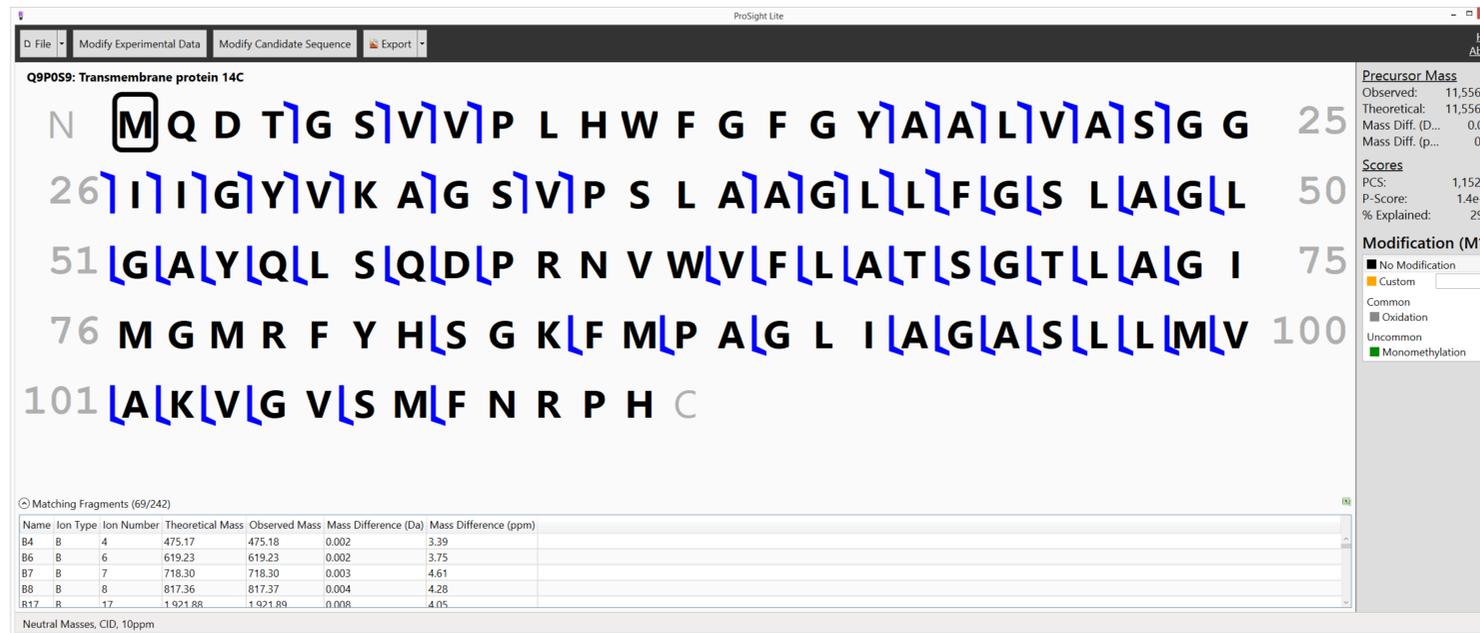
Overview

- ProSight Lite is a free tool that facilitates the matching of tandem mass spectrometry data to a protein candidate sequence
- Post Translational Modifications can be applied in an iterative fashion to test hypotheses
- Fragment maps can be exported in various formats to aid the creation of figures and presentations
- The program installs and updates from the web

Introduction

Many top-down proteomics experiments focus on identifying and localizing post-translational modifications and other sources of mass shift on a known protein sequence. There is a need for a simple application that is freely available, is easy to install and use, can match ion masses, and allows iterative hypothesis testing of PTM locations. ProSight Lite is a free tool for matching a single candidate sequence against a set of mass spectrometric observations. Fixed or variable modifications, including both post-translational and a select number of glycosylations, can be applied to the amino acid sequence. The application reports multiple scores and a matching fragment list. Fragmentation maps can be exported for publication in PNG and SVG formats.

User Interface



The user interface consists of four sections: the menu bar, the fragment map, the modification pane, and the matching fragments grid.

Glycosylation Support



The Proteomics Center of Excellence is working with UniCarbKB to standardize glycosylation searching and reporting.

UniCarbKB is an initiative that aims to promote the creation of an online information storage and search platform for glycomics and glycobiology research. ProSight Lite will be updated in the near future to include access to all of the structures cataloged in UniCarbKB using a web service that is currently under construction. We also plan to make use of UniCarbKB's cross references in UniProt to automatically search for glycosylations based on an accession number. In our initial release, we have manually added a set of 6 common glycosylations.

File Formats



Proteoform Characterization XML
An XML-based format to store experiment metadata, MS/MS observations, and a proteoform hypothesis.



Portable Network Graphics
A raster graphics file format that supports lossless data compression. Very good for a quick email or the web.



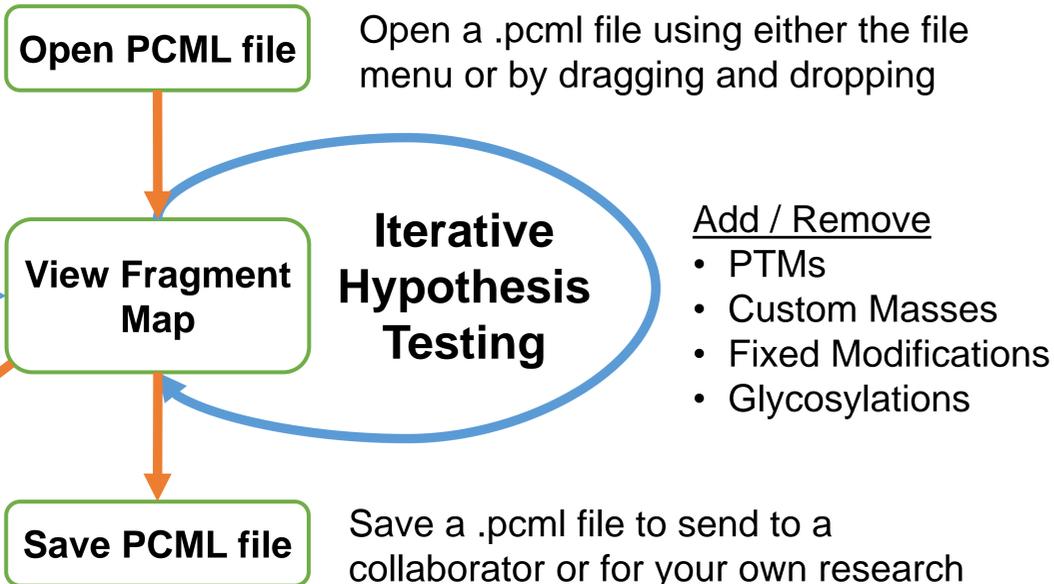
Scalable Vector Graphics
An XML-based vector image format for two-dimensional graphics. Very good when high resolution is needed.

<http://prosightlite.northwestern.edu>

Application Workflow

Requirements

- Tandem Mass Spectrometry Data
- Proteoform Hypothesis



Complex Fragmentation Maps

ProSight Lite supports many complex fragmentation types including ultraviolet photodissociation (UVPD) and combined collisional and electron based dissociations (creating BY and CZ⁺ ions). These complex fragmentations result in up to 6 different ion types.



Acknowledgements

The authors would like to thank the other members of the Top-Down Proteomics Development Team at Northwestern University. This research is supported by the National Science Foundation under grant No. ABI-1062432 to Indiana University (RDL), by Award No. DA018310 from the National Institute on Drug Abuse (NLK), and Award No. GM067193 from the National Institute of General Medical Sciences (NLK).

Future Work

- Expand the number of glycosylations supported (currently we only have 6) and improve the glycosylation selection user interface.
- Listen to the features requested by the community and provide updates and improvements in a timely manner.