NPvis: interactive visualizer for MS/MS fragmentation of natural products

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Overview

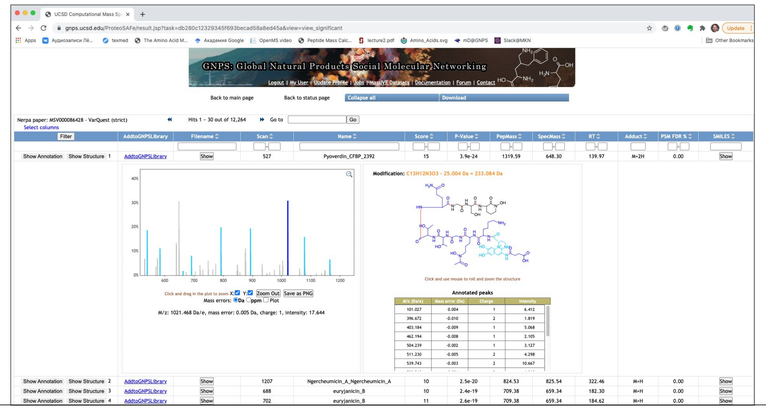
- Natural products (NPs) include many antibiotics and other bioactive compounds [1]
- High-throughput NP discovery is driven by tandem mass spectrometry (MS/MS). Analysis of experimental MS/MS data involves computational methods
- MS/MS can be searched against reference spectral libraries of previously analysed compounds, however they are currently small for NPs. Another approach is to use *in silico* fragmentation software. These tools compare theoretical MS/MS fragmentations of target structures from large chemical NP databases (e.g. the Dictionary of Natural Products [2]) to experimental MS/MS peaks. Despite the recent progress in the NP database search tools development, these instruments are still in their infancy and require validation of their outputs
- Visualization of MS/MS compound fragmentation is a powerful method for validation of *in silico* identification results [3]. Standard proteomics visualization tools are not applicable to NPs due to
  - complex chemical structure (e.g. cyclic, branched)
  - non-standard amino acid residues or absence of amino acids at all (e.g. polyketides, lipids)
  - unclear MS/MS fragmentation patterns (e.g. in the absence of peptide bonds)
- We present NPvis, a versatile interactive visualizer for MS/MS fragmentation of wide range of NPs

Implementation

- NPvis is implemented in JavaScript/JQuery (visualization part) and Python/RDKit (preprocessing)
- Build on top of Lorikeet, an MS/MS visualizer for proteomics http://uwpr.github.io/Lorikeet/
- Fragmentation and compound-MS/MS matching is done with NPDtools (VarQuest [4] / Dereplicator+ [5] /etc) https://cab.spbu.ru/software/npdtools/

Integration with GNPS

- Global Natural Products Social Molecular Networking (GNPS, https://gnps.ucsd.edu/ [6]) is a community-driven platform for storing, sharing and analysing NP MS/MS data
- NPvis is integrated in the output of the GNPS In silico Tools



Input data

Mass spectra: MGF, mzML, mzXML
Compounds: MDL MOL, SMILES, InChIKey, peptide sequence

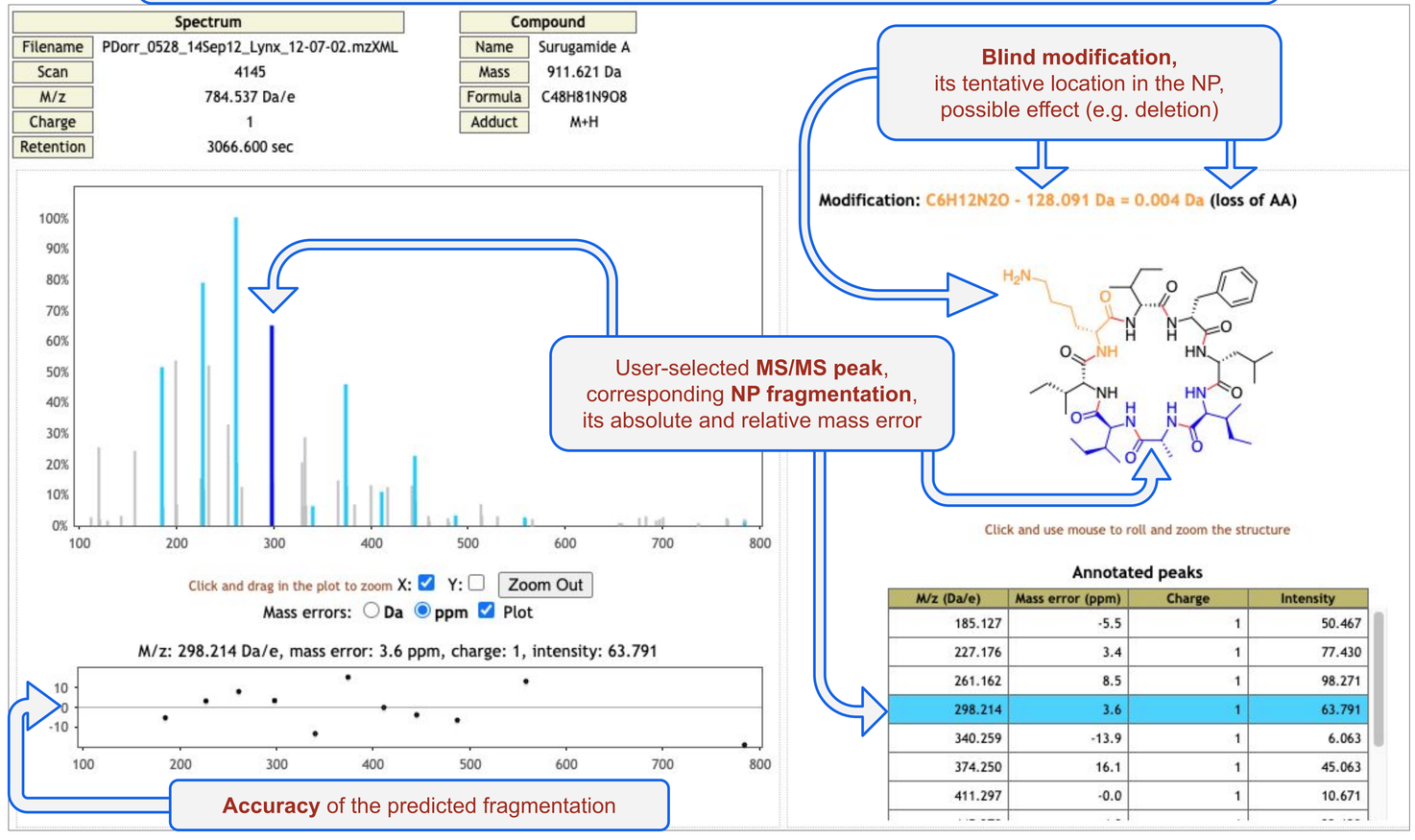
Key features

- Compounds of virtually arbitrary chemical structure
- Non-peptidic MS/MS fragmentation
- Single blind modifications

Coming soon

Improved support for non-peptidic NPs
Release of the command-line version
Web-service at http://cab.cc.spbu.ru/

More examples and info at https://cab.spbu.ru/software/npvis. Stay tuned!



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