Секция «Биоинформатика»

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

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Natural products (NPs) have an unparalleled track record in pharmacology that includes many antibiotics and other bioactive compounds [1]. One of the leading experimental techniques for high-throughput NP discovery is tandem mass spectrometry (MS/MS) which allows rapid and low-cost scanning of thousands of compounds. Further analysis of vast amounts of experimental MS/MS data requires appropriate computational methods [5]. Due to the small size of present reference spectral libraries for NPs, often the only way to interpret the data is to use in silico fragmentation software and large chemical databases of NPs. These tools identify unknown compounds by comparing and ranking theoretical MS/MS fragmentations from target structures to experimental MS/MS peaks. Despite the recent progress in the development of in silico database search tools for NPs [2,3], these instruments are still in their infancy and require validation of their outputs.

As shown in many proteomics studies, visualization of MS/MS peptide fragmentation is a powerful method for validation of in silico identification results [4]. At the moment, there are multiple widely used tools for this problem. Though, visualization of NP MS/MS fragmentation is a much more difficult task preventing the use of conventional proteomics software. NPs represent a widely diverse chemical class of compounds. In contrast to linear peptides, many NPs have cyclic, branched, or more complex structures. Furthermore, MS/MS peptide fragmentation paradigm relies on the breakage of peptide bonds while some NPs such as polyketides do not include peptide bonds at all.

Here we present NPvis, a versatile interactive visualizer for MS/MS fragmentation of NPs. NPvis can work with compounds of an arbitrary chemical structure including all classes of NPs. The tool accepts as input molecules in popular chemical formats such as SMILES and MDL MOL as well as MS/MS data in common formats like mzML and MGF. NPvis allows users to match any annotated experimental peak to the corresponding chemical structure fragmentation. Our tool is embedded into the output of widely used in silico identification tools at the GNPS web platform [5] and also available as a command-line utility.

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### References

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