

MetWare screenshot: spectrum support #2

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Keywords

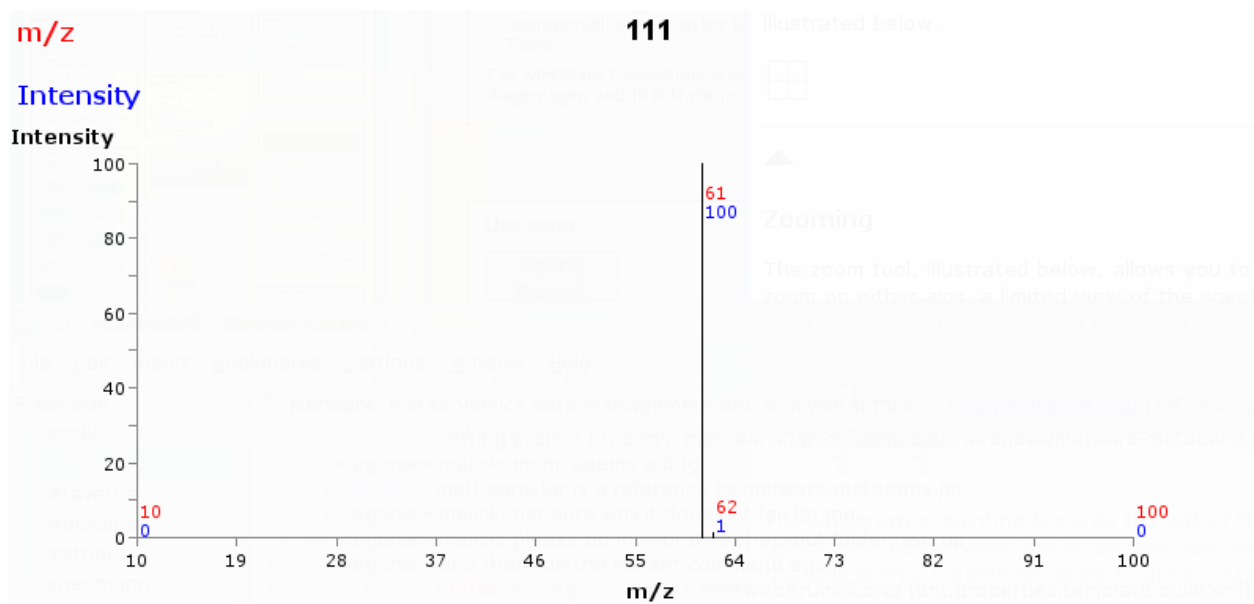
Metware, Metabolomics, Xml, Skos

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chem-bla-ics

As [promised yesterday](#), here's the pretty visualization of the mass spectrum, using JavaScript from the [PRIDE project](#):



Note the manual adding of peaks at 10 and 100 m/z to get the real peaks somewhere in the middle instead of on the left and right border of the graph.

Meanwhile, the search page is now autogenerated too, and the types of searches allowed (min, max in the picture) again depends on the XML Scheme data type defined in the [MetWare SKOS](#):

Metabolite

Molecules which are said to exist play a role of the effect of some metabolism and of which the exact chemical structure is known, including stereochemistry.

Monoisotopic Mass:

min:

max:

2 InChI=1/CH4/h1H4 VNWK TOKETHGBQD-UHFFFAOYAM 16.0313

3

0.0