chem-bla-ics

# MetWare screenshot: spectrum support

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Published August 20, 2008

**Citation**
Willighagen, E. (2008, August 20). MetWare screenshot: spectrum support. *Chem-bla-ics*. https://doi.org/10.59350/9m75g-4rh11

**Keywords**
Metware, Xml, Java

**Abstract**
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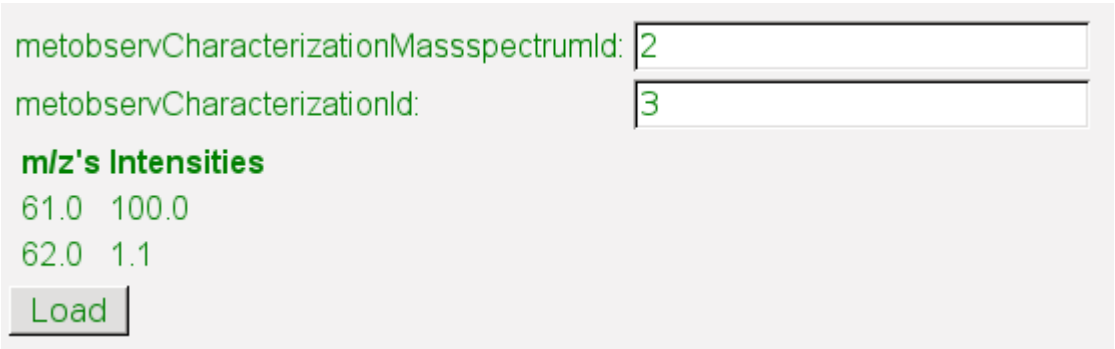
Not visually attractive, but that will be solved when Steffen gets his hands on it. For now, I'm happy with a table formatting. Reason: it uses XML Schema to define a dataType, which is recognized by our code generators in MetWare (see also this presentation ), and used to create a easy to use Java API, which, in turn, can be used in this JSF snippet:

```
<h:dataTable
value="#{metobservCharacterizationMassspectrum.spectralPoints.points}"
var="specpoint">
  <h:column>
    <f:facet name="header"><h:outputText value="m/z's"/></f:facet>
    <h:outputText value="#{specpoint.mz}"/>
  </h:column>
  <h:column>
    <f:facet name="header"><h:outputText value="Intensities"/></f:facet>
    <h:outputText value="#{specpoint.intensity}"/>
  </h:column>
</h:dataTable>
```

The `<dataTable> @value` points (via the `faces-config.xml`) to the `MetobservCharacterizationMassspectrumBean`, which has a `getSpectralPoints()` method (autocreated from the `<skos:Concept> SpectralPoints`, which has a convenience method `List<SpectralPoint> getPoints()`.

`SpectralPoint` in turn has the methods `getIntensity()` and `getMz()` also used in the above JSF snippet. For convenience, `SpectralPointArray` also has two other methods: `double[] getIntensities()` and `double[] getMzs()` (which I'll have to rename to reuse the code for NMR support :).

So, here's the outcome:




Final note, given the dataType, the MetWare bean also has the logic to convert the data back and forth into a SQL serialization, which may eventually use base64 encoding, but currently looks like *61.0,100.0;62.0,1.1*, as defined by the regular expression of the XSD dataType for spectralPointArray.