chem-bla-ics

MetWare screenshot: spectrum support

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Published August 20, 2008

Citation

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

Keywords

Metware, Xml, Java

Abstract

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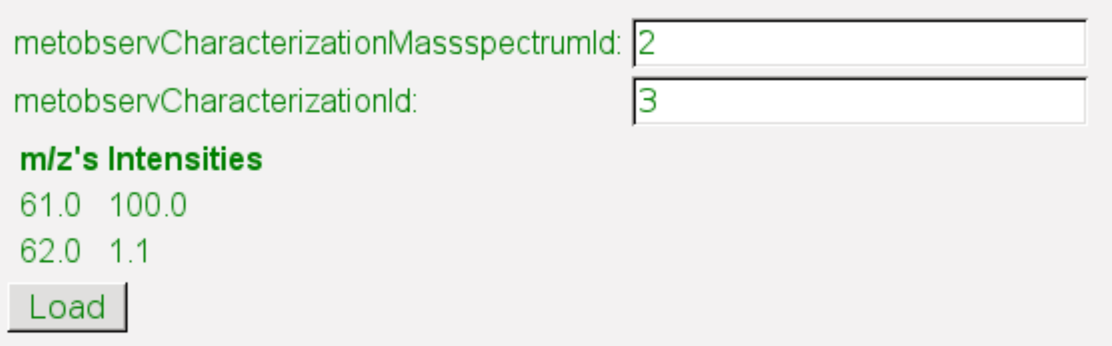
Not visually attractive, but that will be solved when Steffen gets his hands on it. For now, I'm happy with a table formatting. Reason: it uses XML Schema to define a dataType, which is recognized by our code generators in MetWare (see also this presentation), and used to create a easy to use Java API,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

```
<h:dataTable value="#{metobservCharacterizationMassspectrum.spectralPoints.points}" var="
  <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:



metobservCharacterizationMassspectrumId: 2

metobservCharacterizationId: 3

m/z's	Intensities
61.0	100.0
62.0	1.1

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.