chem-bla-ics

Matrix support in Bioclipse

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Keywords

Bioclipse, Chemometrics, Qsar, Cdk

Abstract

With chemometrics in mind (QSAR, data mining, ...), I have started working on matrix support in Bioclipse, because the matrix is the important step between (bio-)molecular content and statistical analysis. I implemented this such that the actual matrix implementation can be freely chosen, that is, bc_statistical provides a IMatrixImplementation extension point.

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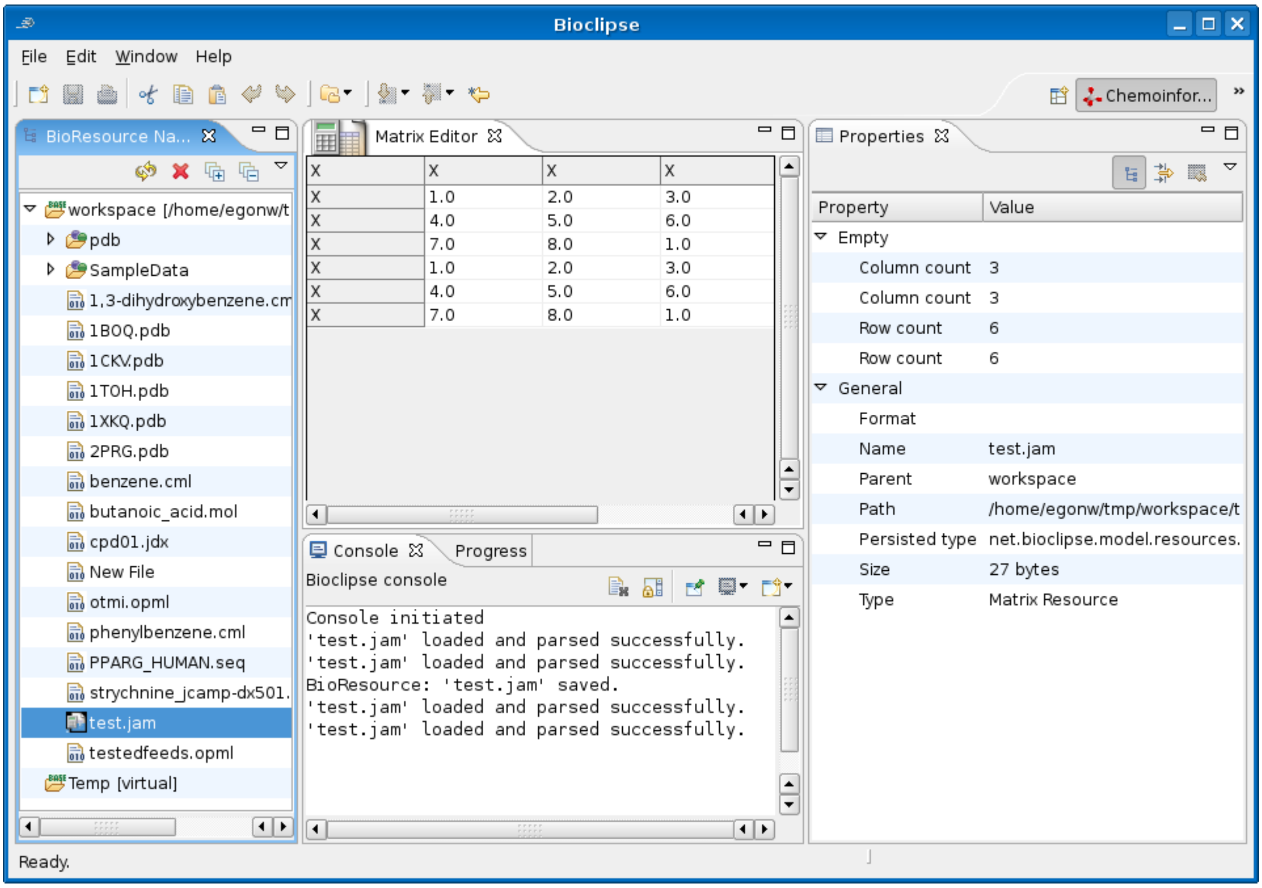
With chemometrics in mind (QSAR, data mining, …), I have started working on matrix support in Bioclipse, because the matrix is the important step between (bio-)molecular content and statistical analysis. I implemented this such that the actual matrix implementation can be freely chosen, that is, bc_statistical provides a `IMatrixImplementation` extension point. The plugin bc_jama provides a JAMA based extension for this, but other implementations are possible, and possibly useful.

The second component provided by the new statistics plugin, is the MatrixResource, a BioResource for documents (e.g. files on the harddisk) that represent a matrix. However, Bioclipse can create such matrices on the fly too, and these do not necessarily have to be stored on disk, as is general for BioResource's. This makes it possible for other plugins to create matrices from other resources: for example, the CDK plugin can now have an action that converts a SDF file into a QSAR data matrix.

The MatrixResource can be edited using a plain text editor, and a more visually attractive graphical editor based on the KTable SWT widget:



X	X	X	X
X	1.0	2.0	3.0
X	4.0	5.0	6.0
X	7.0	8.0	1.0
X	1.0	2.0	3.0
X	4.0	5.0	6.0
X	7.0	8.0	1.0

Property	Value
Empty	
Column count	3
Column count	3
Row count	6
Row count	6
General	
Format	
Name	test.jam
Parent	workspace
Path	/home/egonw/tmp/workspace/t
Persisted type	net.bioclipse.model.resources.
Size	27 bytes
Type	Matrix Resource

Bioclipse console

```
Console initiated
'test.jam' loaded and parsed successfully.
'test.jam' loaded and parsed successfully.
BioResource: 'test.jam' saved.
'test.jam' loaded and parsed successfully.
'test.jam' loaded and parsed successfully.
```

The next step is to work on column and row names, and replace those uninformative X's. As you can see in the Properties View, I also need to tweak adding and removing advanced properties a bit. And then it is time to have the CDK plugin create a QSAR data matrix.