

Matrix support in Bioclipse

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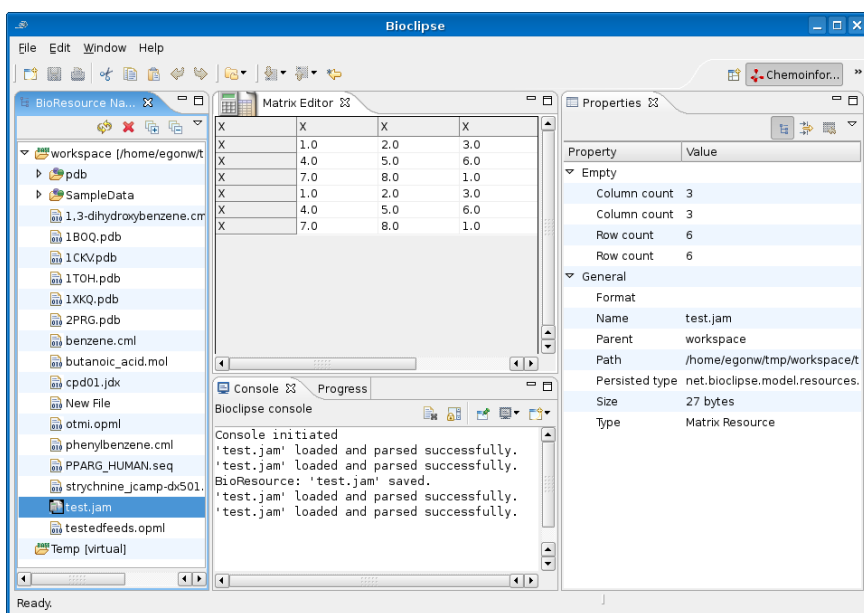
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chem-bla-ics

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:

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.

References