

# Further Bioclipse QSAR functionality development

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## Keywords

Cdk, Qsar, Bioclipse, Joelib

## Abstract

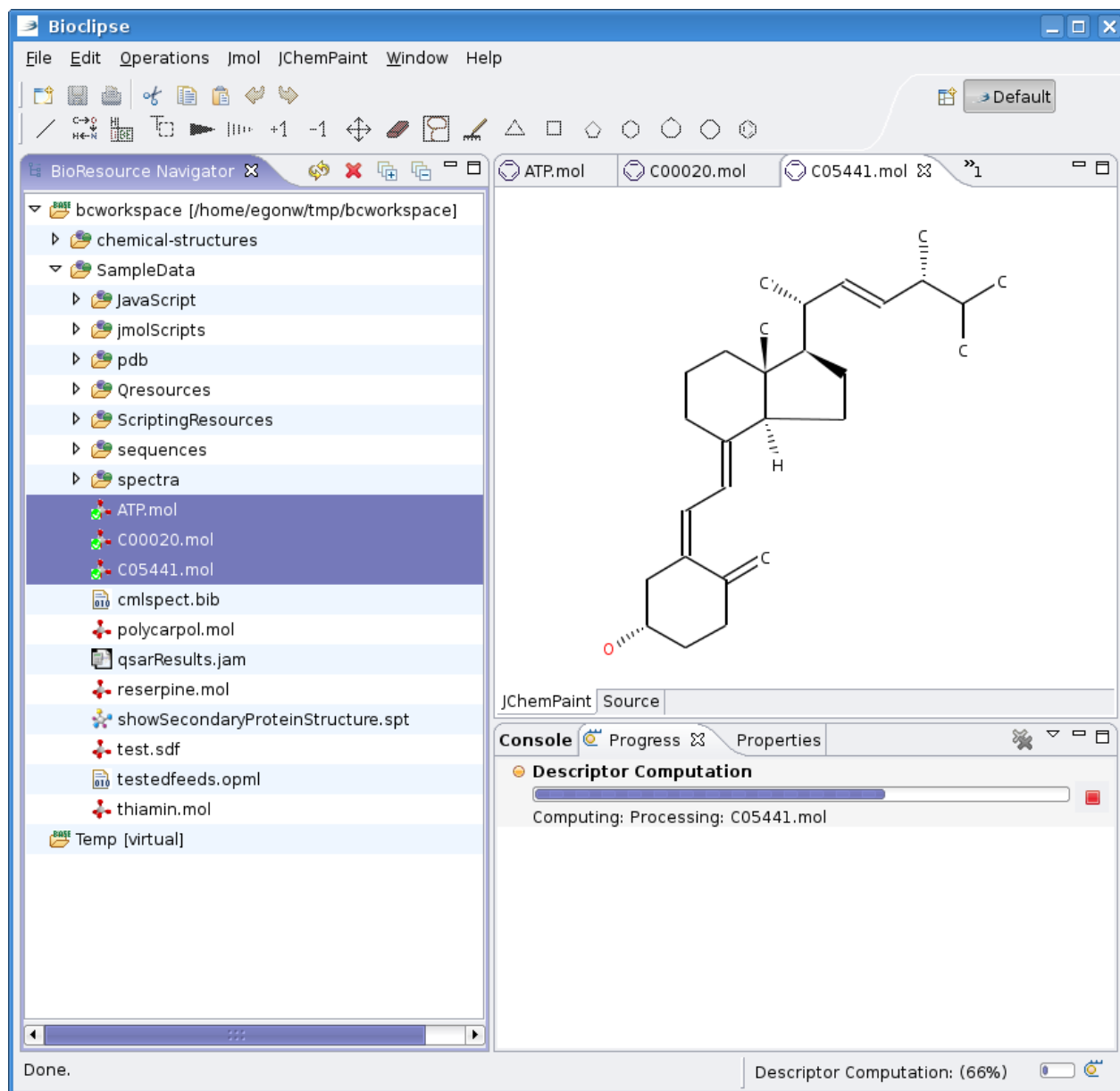
I had some time to work some more on the QSAR functionality in Bioclipse. There is still much to do, but it is getting there.

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## chem-bla-ics

I had some time to [work some more on the QSAR functionality](#) in Bioclipse. There is still much to do, but it is getting there. The calculation of a QSAR descriptor data matrix



This screenshot shows that multi-resource selection is now working, and that the calculation is now a Job. The resulting matrix looks like:

The screenshot shows the Bioclipse application window. The top menu bar includes File, Edit, Operations, Jmol, Window, and Help. Below the menu is a toolbar with icons for file operations and a 'Default' button. The main interface is divided into several panes:

- BioResource Navigator:** A tree view on the left showing the workspace structure. The root is 'bcworkspace [home/egonw/tmp/bcworkspace]'. It contains folders like 'chemical-structures', 'SampleData', and 'sequences'. Under 'SampleData', there are subfolders like 'JavaScript', 'jmolScripts', 'pdb', 'Qresources', 'ScriptingResources', and 'spectra'. A list of files is shown, including 'ATP.mol', 'C00020.mol', 'C05441.mol', 'cmlspect.bib', 'polycarpol.mol', 'qsarResults.jam' (highlighted), 'reserpine.mol', 'showSecondaryProteinStructure.spt', 'test.sdf', 'testedfeeds.opml', and 'thiamin.mol'. A 'Temp [virtual]' folder is also present.
- Matrix Editor:** A pane on the right showing a matrix for 'C05441.mol'. The matrix has 3 rows and 4 columns (A, B, C, D). The data is as follows:

	A	B	C	D
1	0.0	44.416000...	5.0	490.87054...
2	0.0	32.344001...	5.0	332.95352...
3	7.0	50.748794...	14.077350...	353.00274...
- Console:** A pane at the bottom right showing 'No operations to display at this time.'

The status bar at the bottom left says 'Done.'

Things that remain to be done:

- work on a SDF resource
- a graph view for the matrix
- R functionality for the matrices
- JOELib support