

Further Bioclipse QSAR functionality development



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Keywords

Cdk, Qsar, Bioclipse, Joelib

Abstract

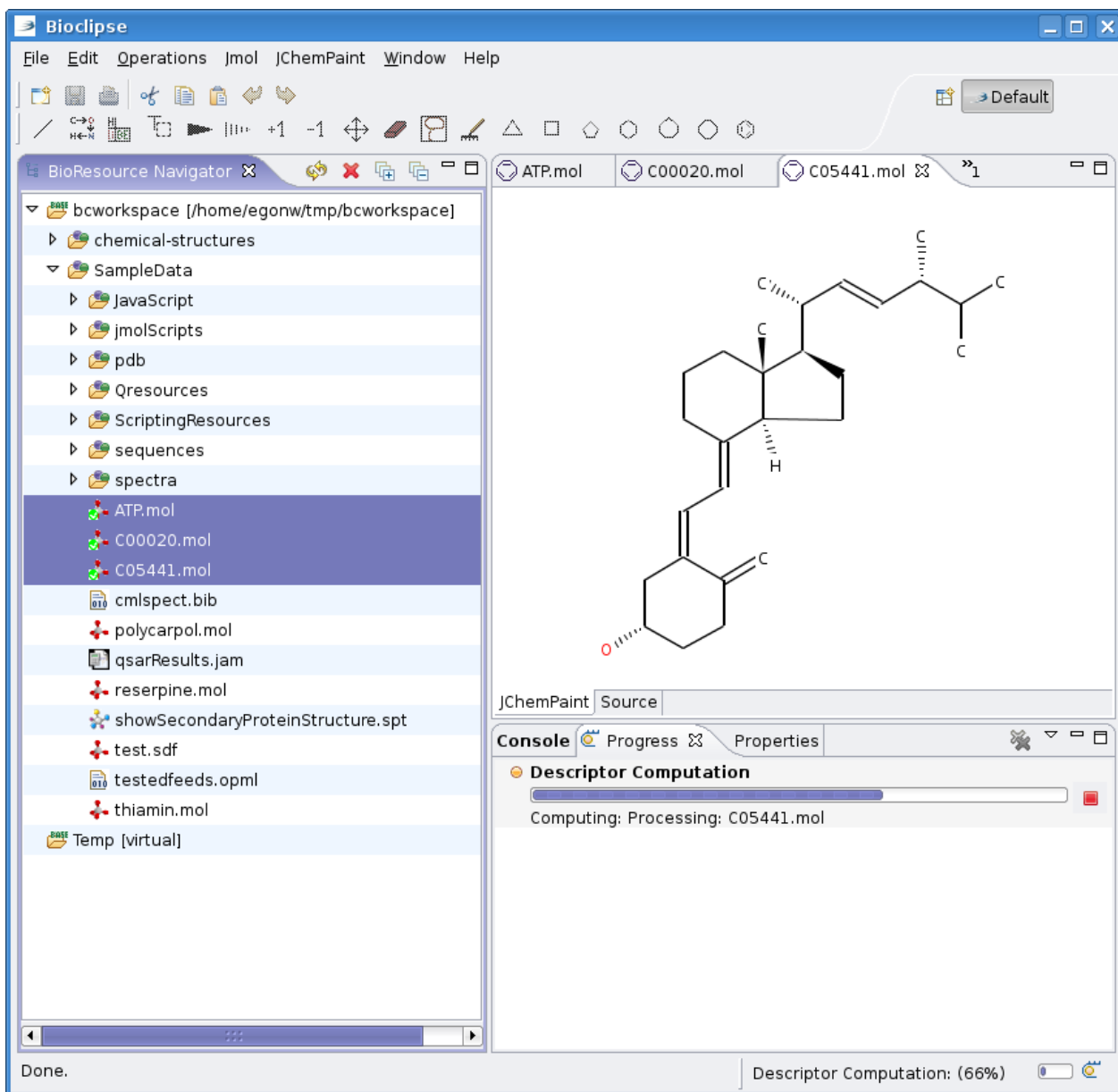
I had some time to work some more on the QSAR functionality in Bioclipse. There is still much to do, but it is getting there.

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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:

Bioclipse

File Edit Operations Jmol Window Help

BioResource Navigator

bcworkspace [/home/egonw/tmp/bcworkspace]

- chemical-structures
- SampleData
 - JavaScript
 - jmolScripts
 - pdb
 - Qresources
 - ScriptingResources
 - sequences
 - spectra
- ATP.mol
- C00020.mol
- C05441.mol
- cmlspect.bib
- polycarpol.mol
- qsarResults.jam
- reserpine.mol
- showSecondaryProteinStructure.spt
- test.sdf
- testedfeeds.opml
- thiamin.mol
- Temp [virtual]

Matrix Editor

	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

No operations to display at this time.

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