

Further Bioclipse QSAR functionality development

Egon Willighagen 

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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

The screenshot displays the Bioclipse software interface. The main window shows a workspace with a file explorer on the left and a central canvas displaying a complex chemical structure. The file explorer lists several files, including ATP.mol, C00020.mol, and C05441.mol, which are highlighted in blue. The central canvas shows a chemical structure with a complex ring system and a side chain. The bottom of the interface features a console window with a progress bar and the text "Descriptor Computation" and "Computing: Processing: C05441.mol". The status bar at the bottom indicates "Done." and "Descriptor Computation: (66%)".

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
 - cmspect.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