chem-bla-ics

Further Bioclipse QSAR functionality development

Egon Willighagen

Published July 26, 2007

Citation

Willighagen, E. (2007, July 26). Further Bioclipse QSAR functionality development. *Chem-bla-ics*. https://doi.org/10.59350/d98p9-06w80

Keywords

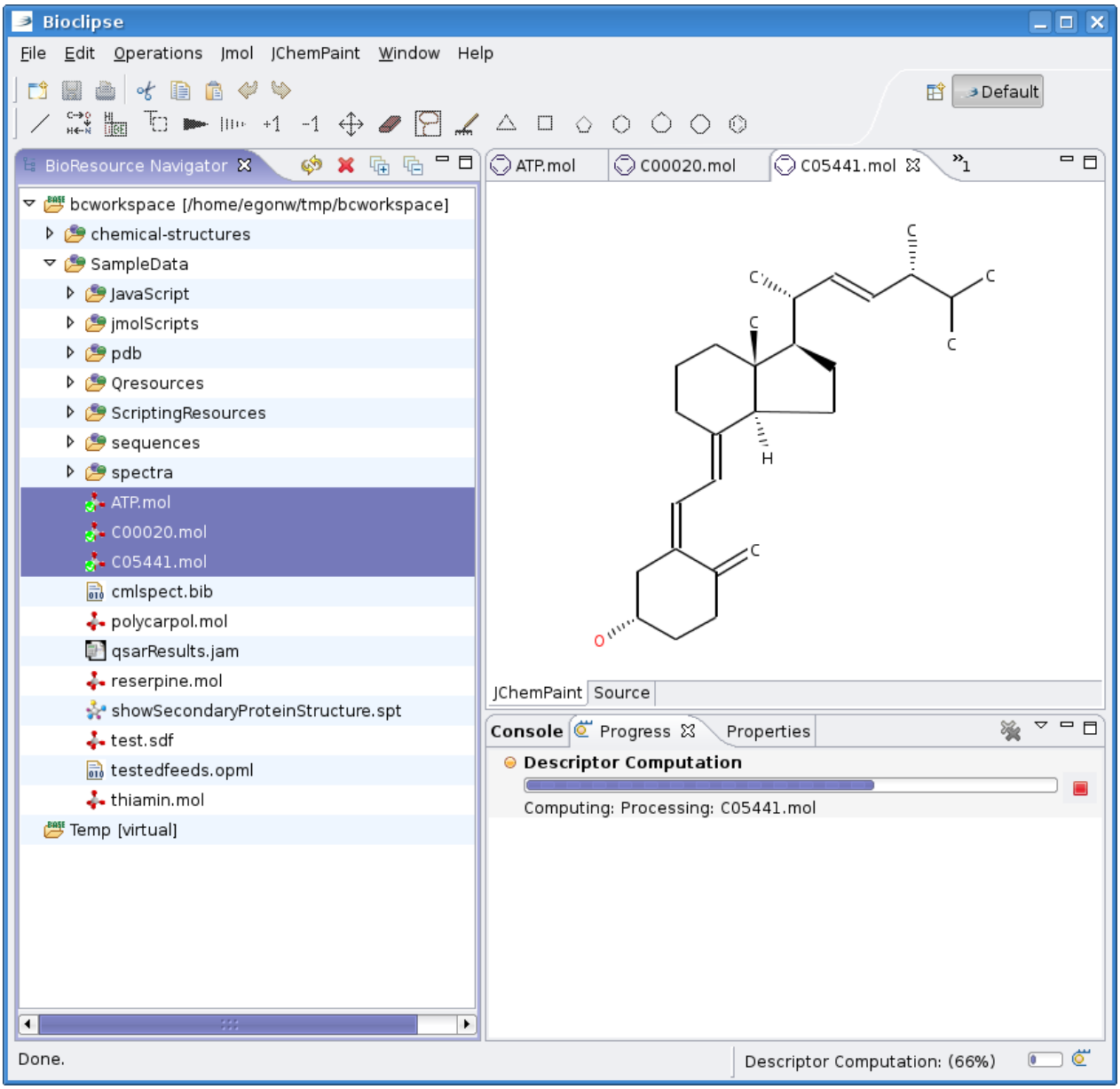
Cdk, Qsar, Bioclipse, Joelib

Copyright

Copyright © Egon Willighagen 2007. Distributed under the terms of the Creative Commons Attribution 4.0 International License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

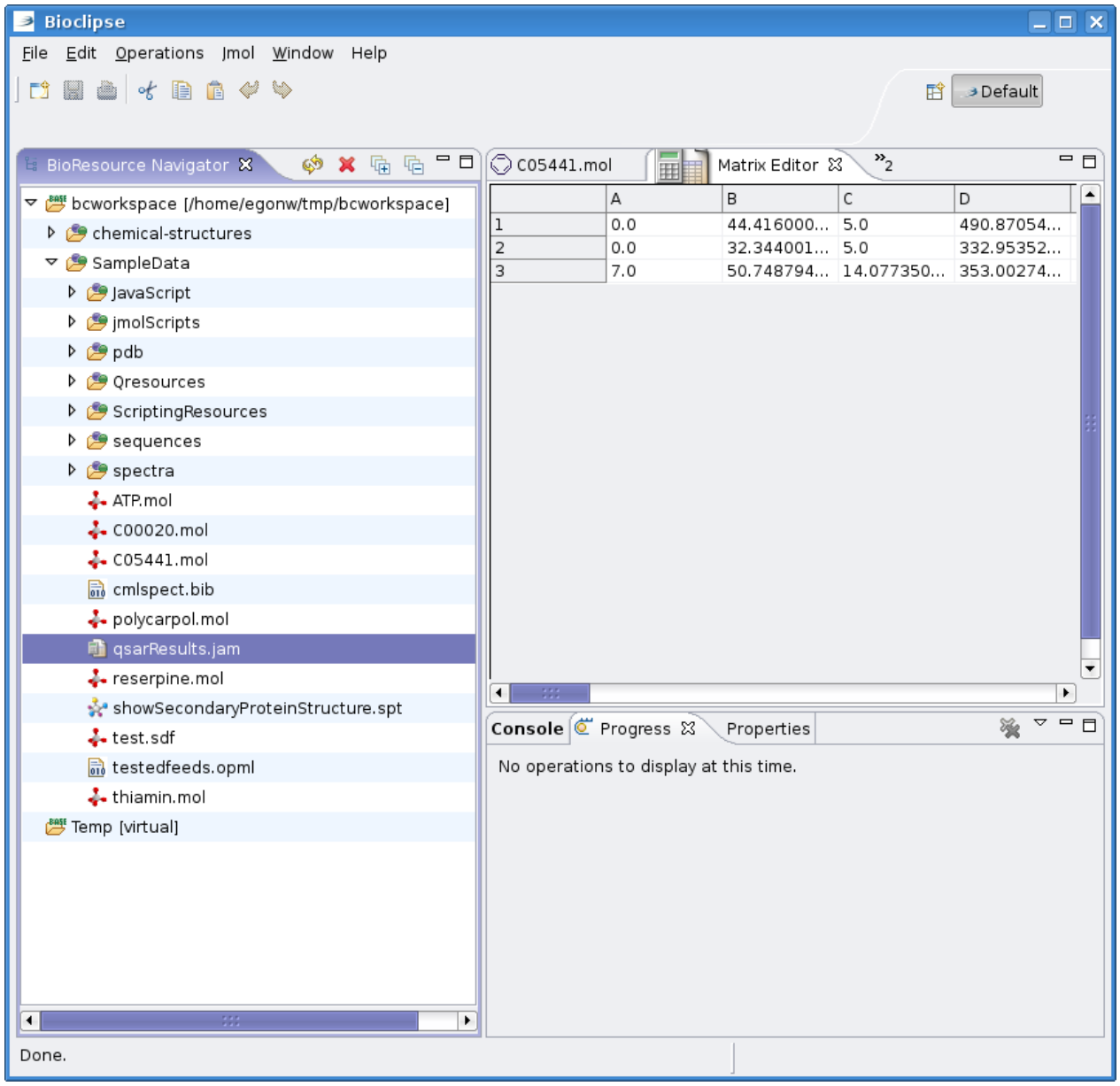
chem-bla-ics

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:

chem-bla-ics



Things that remain to be done:

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