

Further Bioclipse QSAR functionality development

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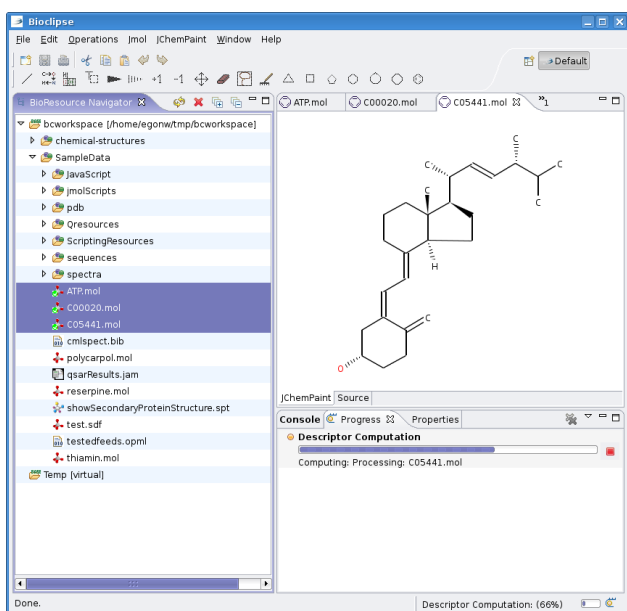
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Keywords

Cdk, Qsar, Bioclipse, Joelib



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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:

Things that remain to be done:

- work on a SDF resource
- a graph view for the matrix
- [R](#) functionality for the matrices
- [JOELib](#) support