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Further Bioclipse QSAR functionality development

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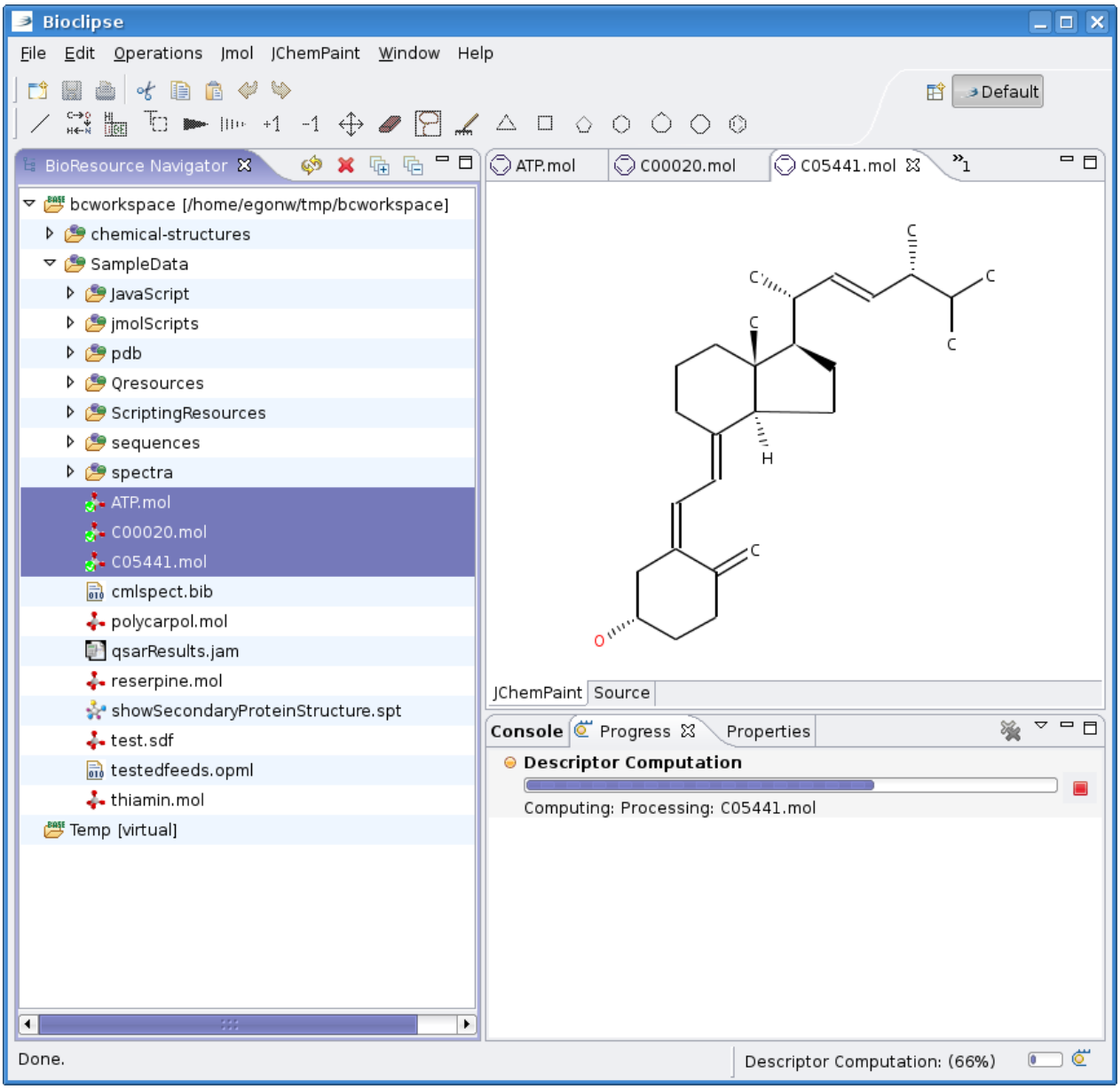
I had some time to work some more on the QSAR functionality in Bioclipse. There is still much to do, but it is getting there. The calculation of a QSAR descriptor data matrix



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

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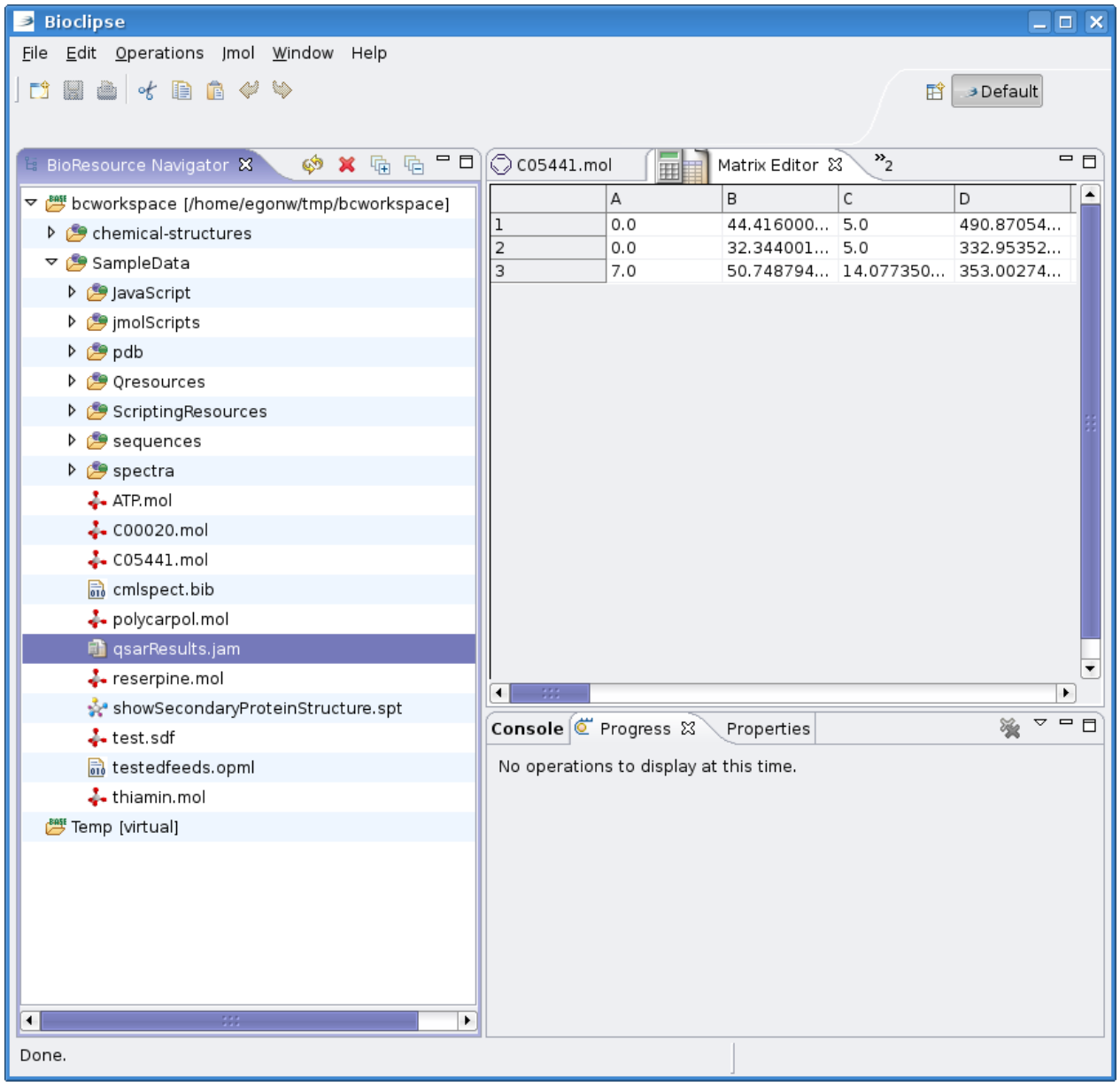

Things that remain to be done:

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