

Protein support in Bioclipse using Jmol and the CDK

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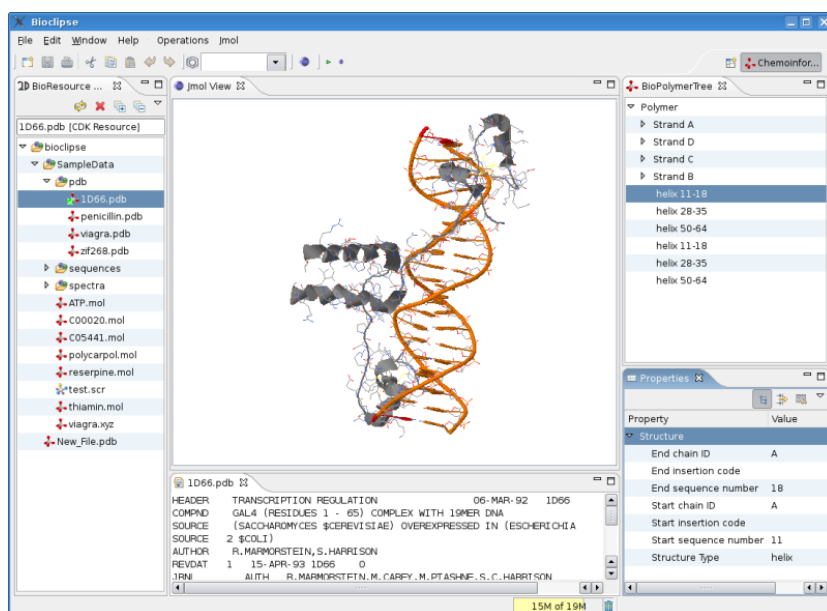
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Keywords

Bioclipse, Jmol, Cdk



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chem-bla-ics

I have not blogged for about a week now, and been too busy with other things, like finishing my PhD articles/manuscript, [my new job at the CUBIC](#) where I [continued the work](#) on proper protein support in [Bioclipse](#) using the [CDK](#) and [Jmol](#):

Screenshot of Bioclipse with a protein visualized with Jmol in the middle.

The latter involves getting the [CdkJmolAdapter](#), the interface between the CDK and Jmol, [updated for changes](#) since the [Jmol as 3D viewer for CDK](#) article in [CDK News](#), the open access journal for CDK related projects.

The screenshot is not showing the actual status: the `CdkJmolAdapter` does not propagate all information to Jmol correctly; as you can see in the screenshot in the `BioPolymerTree` and `Property` views, the CDK now reads the structure information from the PDB file, and I verified that Jmol really extracts this using the `StructureIterator`, but the secondary structure does not show up yet. I believe the problem is in the `AtomIterator`: issuing the `select protein` script, selects zero atoms.

The above screenshot is using a workaround, and was made by using Jmol's own IO instead of the `CdkJmolAdapter`. But I'm very close and think I will be able to fix this soon.

References