

Solubility Data in Bioclipse #1

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Published November 18, 2008

Citation

Willighagen, E. (2008, November 18). Solubility Data in Bioclipse #1. *Chem-bla-ics*. <https://doi.org/10.59350/ydgv3-52978>

Keywords

Bioclipse, Rdf

Abstract

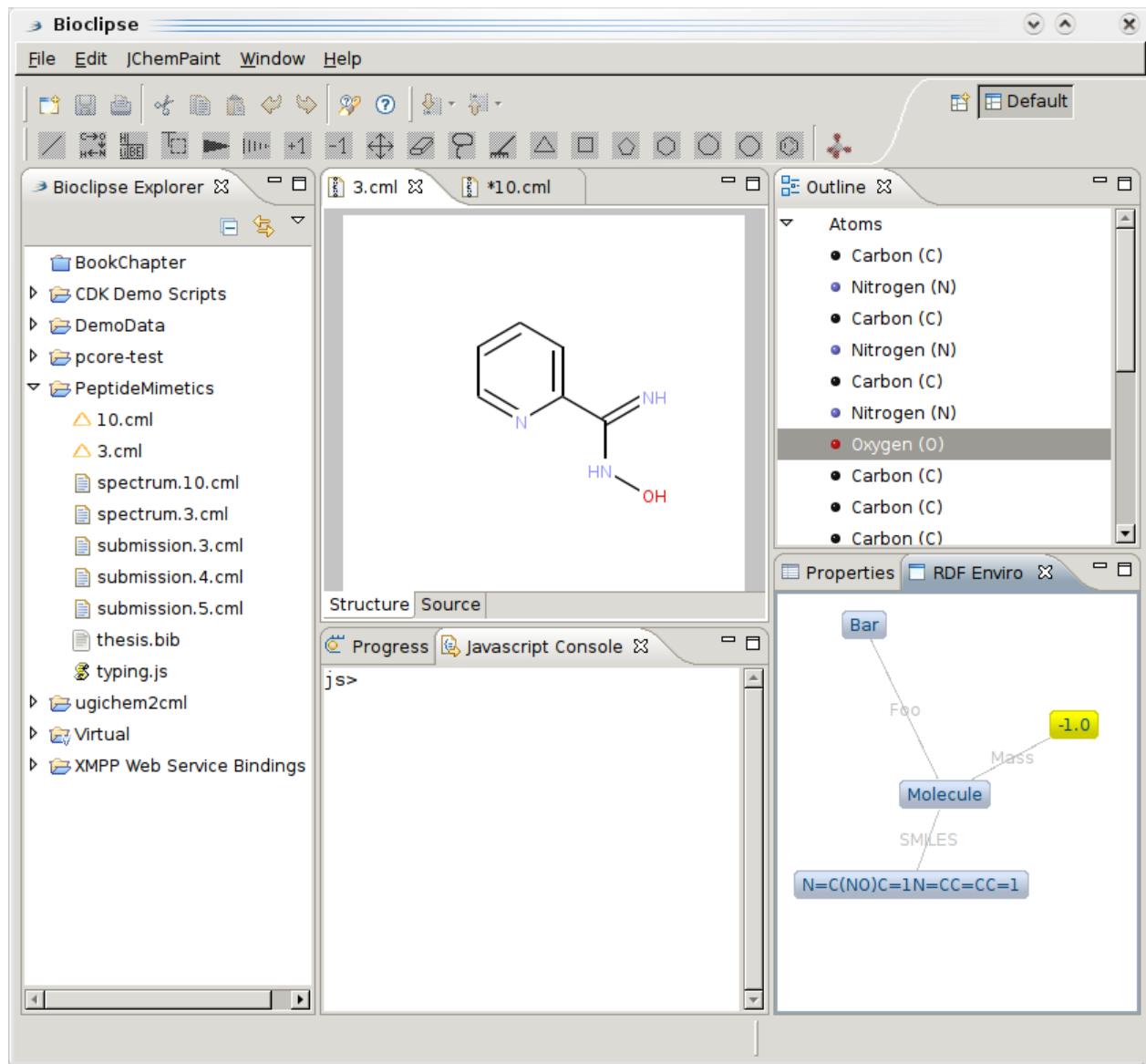
I am working on converting Jean-Claude's Solubility data to RDF (after Pierre's model, see here, here, and here, here for first data exploration), so that I can integrate it with data from DBpedia, Freebase, rdf.openmolecules.net, etc. Bioclipse will be the workbench in which this will be visualized, and just got graph depiction online using Zest.

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chem-bla-ics

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Next stops:

- create a Eclipse package for Jena
- read the Solubility data (does anyone know a Java library to read from Google Docs?)
- create a virtual database of Solubility compounds (possibly StructureDB-based)
- Use the CDK to autoextract chemical triples