Bioclipse

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Bioclipse is a free and open source workbench for the life sciences.

Bioclipse is based on the Eclipse Rich Client Platform (RCP) which means that Bioclipse inherits a state-of-the-art plugin architecture, functionality, and visual interfaces from Eclipse, such as help system, software updates, preferences, cross-platform deployment etc.

Bioclipse provides advanced functionality in fields such as cheminformatics, bioinformatics, semantic web, spectrum analysis, drug discovery, safety assessment, and general chemistry education.

Bioclipse (2)

Bioclipse is developed as a collaboration between the Proteochemometric Group , Dept. of Pharmaceutical Biosciences, Uppsala University, Sweden, and the Cheminformatics and Metabolism Team at the European Bioinformatics Institute (EBI).

Bioclipse is released under Eclipse Public License (EPL) + exception, see the License Statement, putting no constraints on choice of backend and/or license for creating plugins for Bioclipse; it is totally open for both open source plugins as well as commercial.

Bioclipse (4)

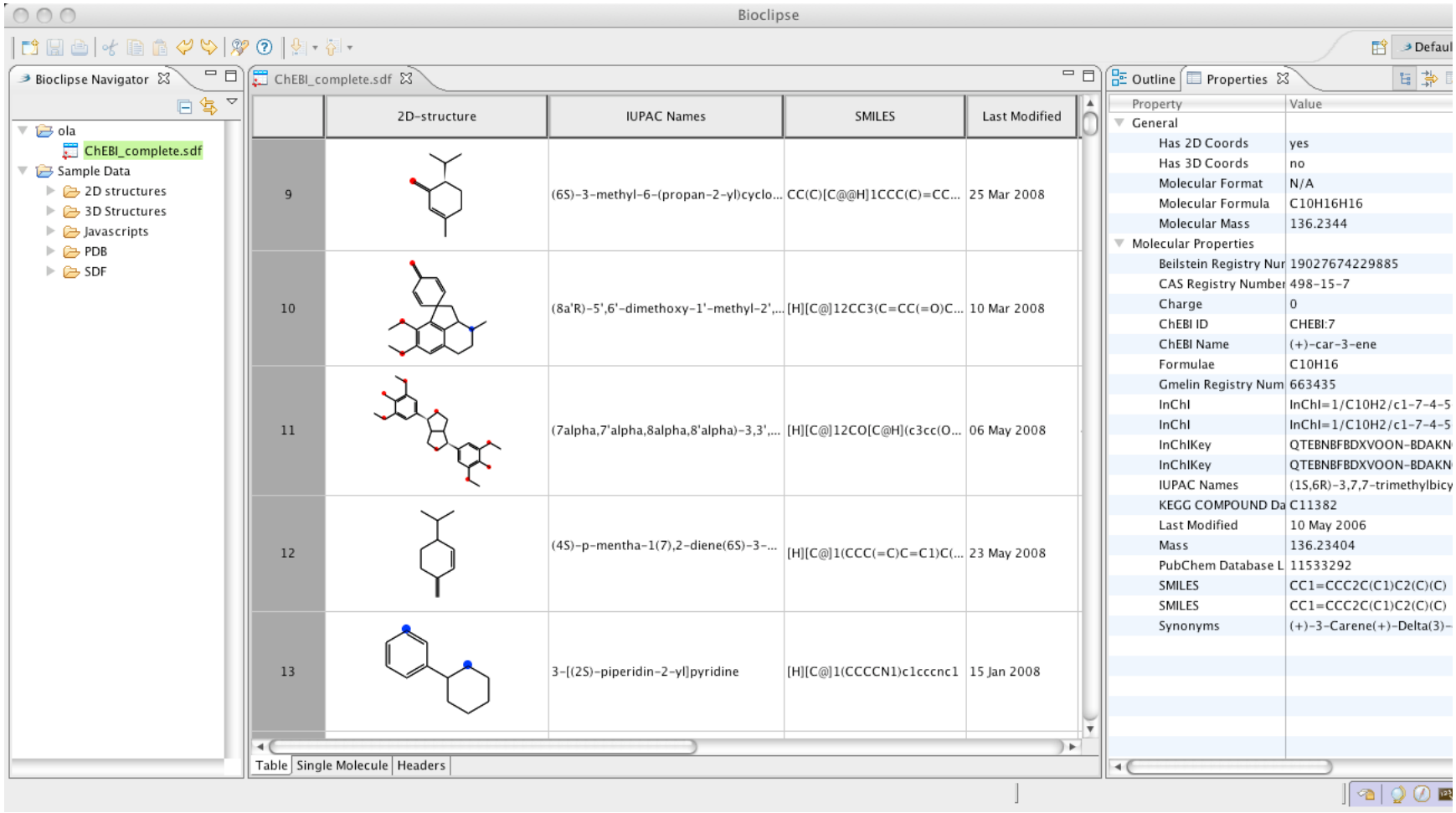
Some examples of functionality is listed below:

Cheminformatics

- Cheminformatics in Bioclipse is mainly based on the Chemistry Development Kit (CDK), and contains a framework for managing and analyzing chemical compounds.
- Bioclipse supports editing in 2D, processing large collections of molecules in tables, calculation of various types of properties, and much more cheminformatics functionality.
- The Jmol application is integrated in Bioclipse as an editor, and provides advanced interactive 3D visualizations.

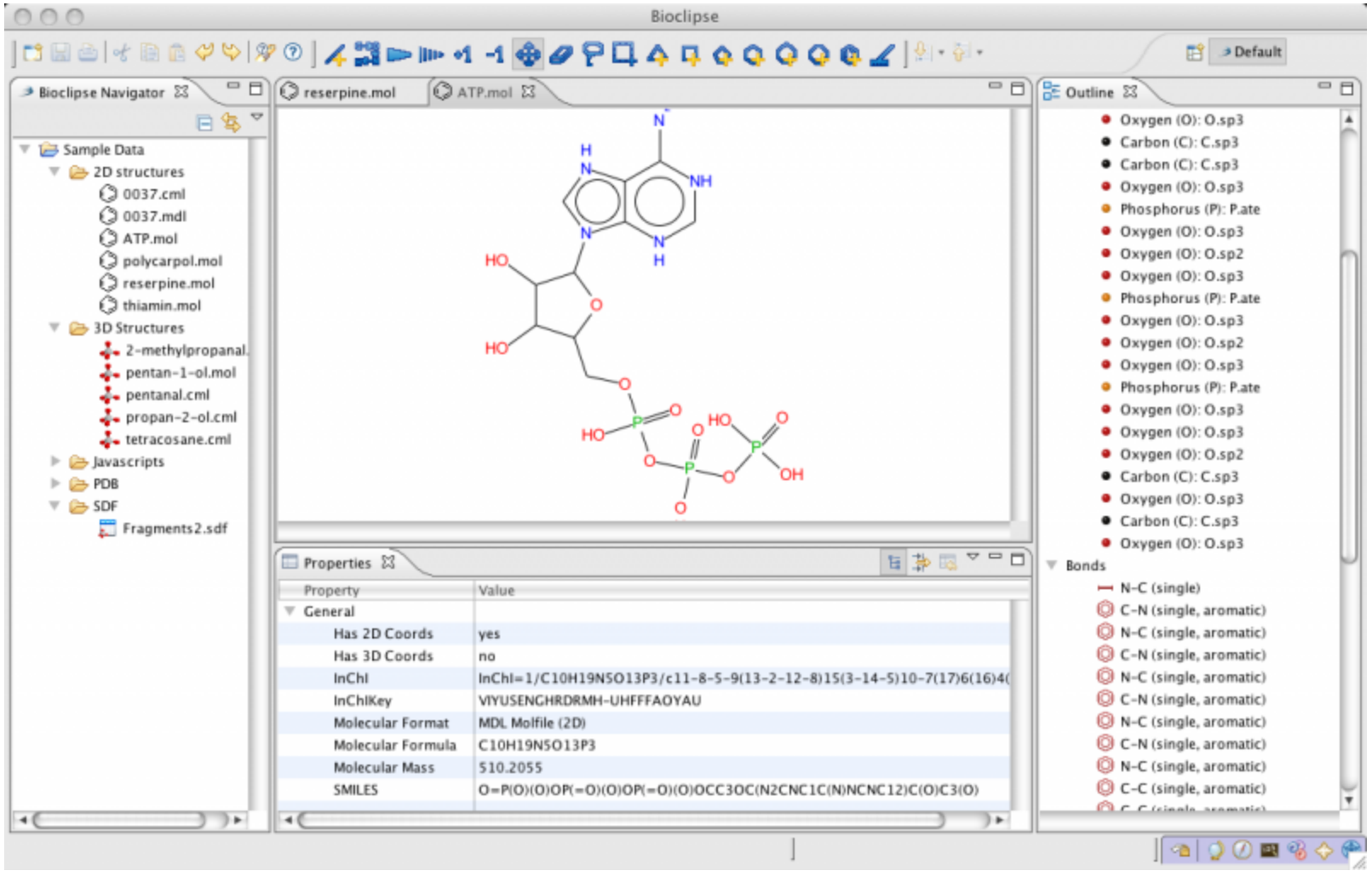
Bioclipse (5)

Ilustration: Work with collections of molecular structures



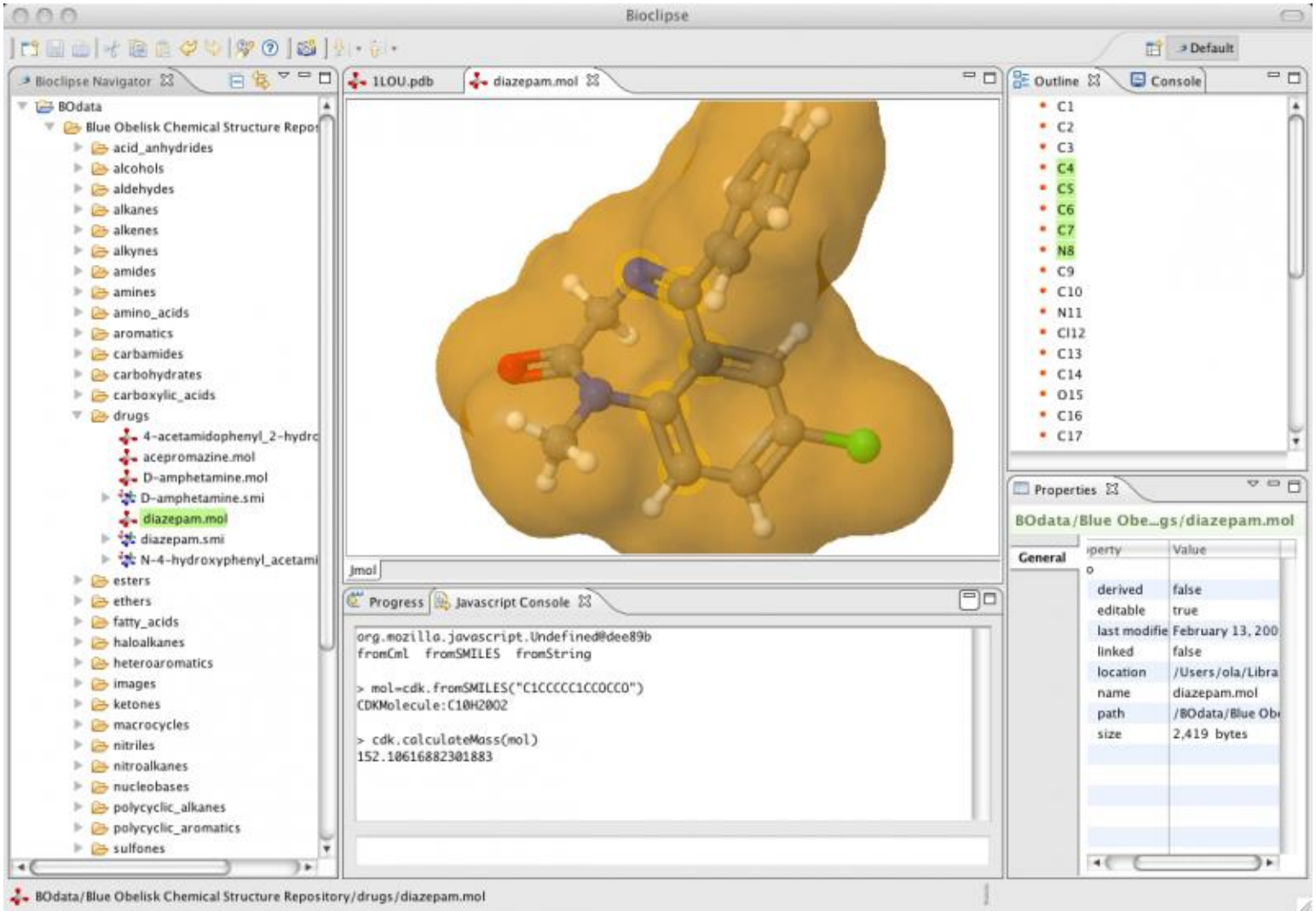
Bioclipse (6)

Ilustration: Editing of chemical structure



Bioclipse (7)

Ilustration: Compound visualized in 3D with Jmol



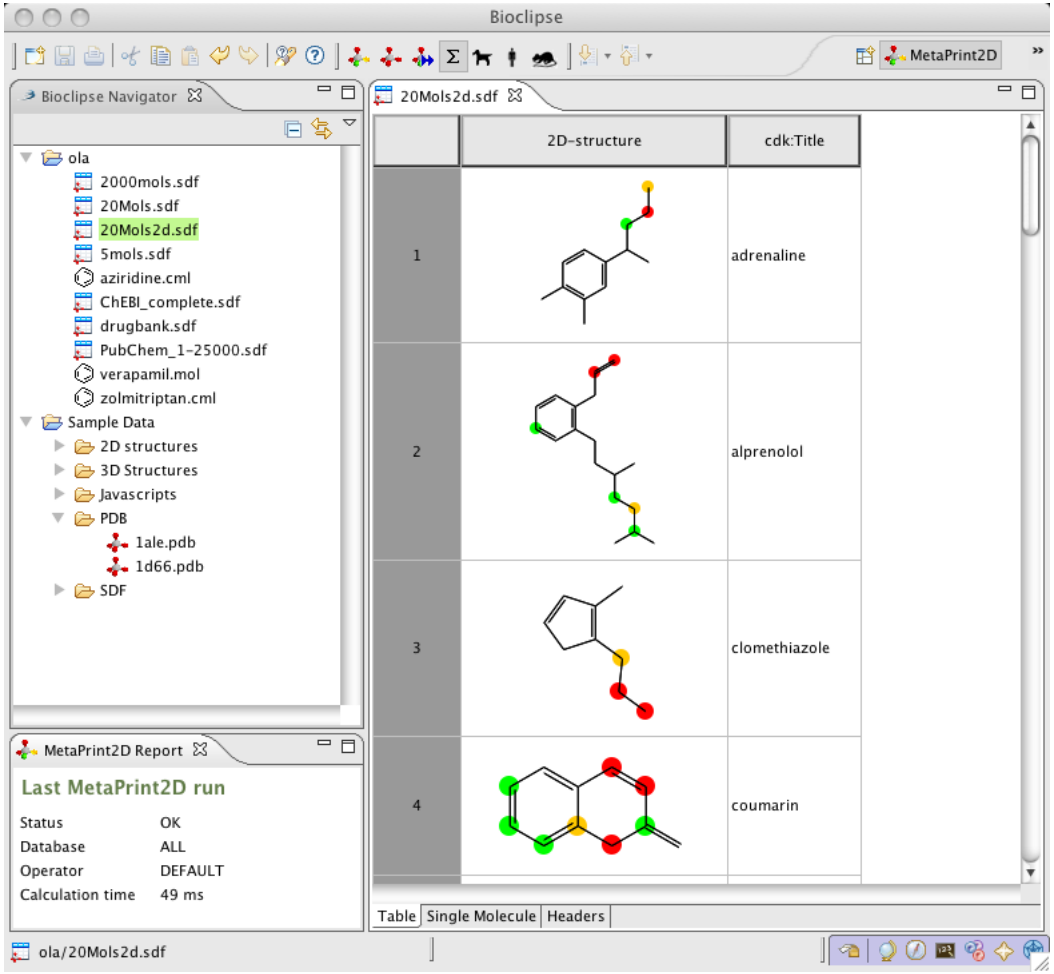
Bioclipse (8)

Pharmacology and Drug Discovery

- Bioclipse is equipped with many features that simplify pharmacological research and drug discovery. Quantitative Structure-Activity Relationships (QSAR) is a methodology to relates the responses between several chemical structures and a target, for example to measure the toxicity of drugs in the human body, described by mathematical descriptors and modelled using statistical methods.
- QSAR models can for example predict if a compound is toxic, and scientists can get decision support for changing the chemical structure before even testing it in the wet lab.
- Bioclipse has many features to work with QSAR and similar fields. A QSAR Project is available with a Builder on a QSAR project file, completely describing the project model. A editor is available, with tabs to select chemical structures, choose mathematical descriptions (descriptors), and all other metadata for performing the analysis.

Bioclipse (9)

Ilustration: Predicting site-of-metabolism on multiple molecules



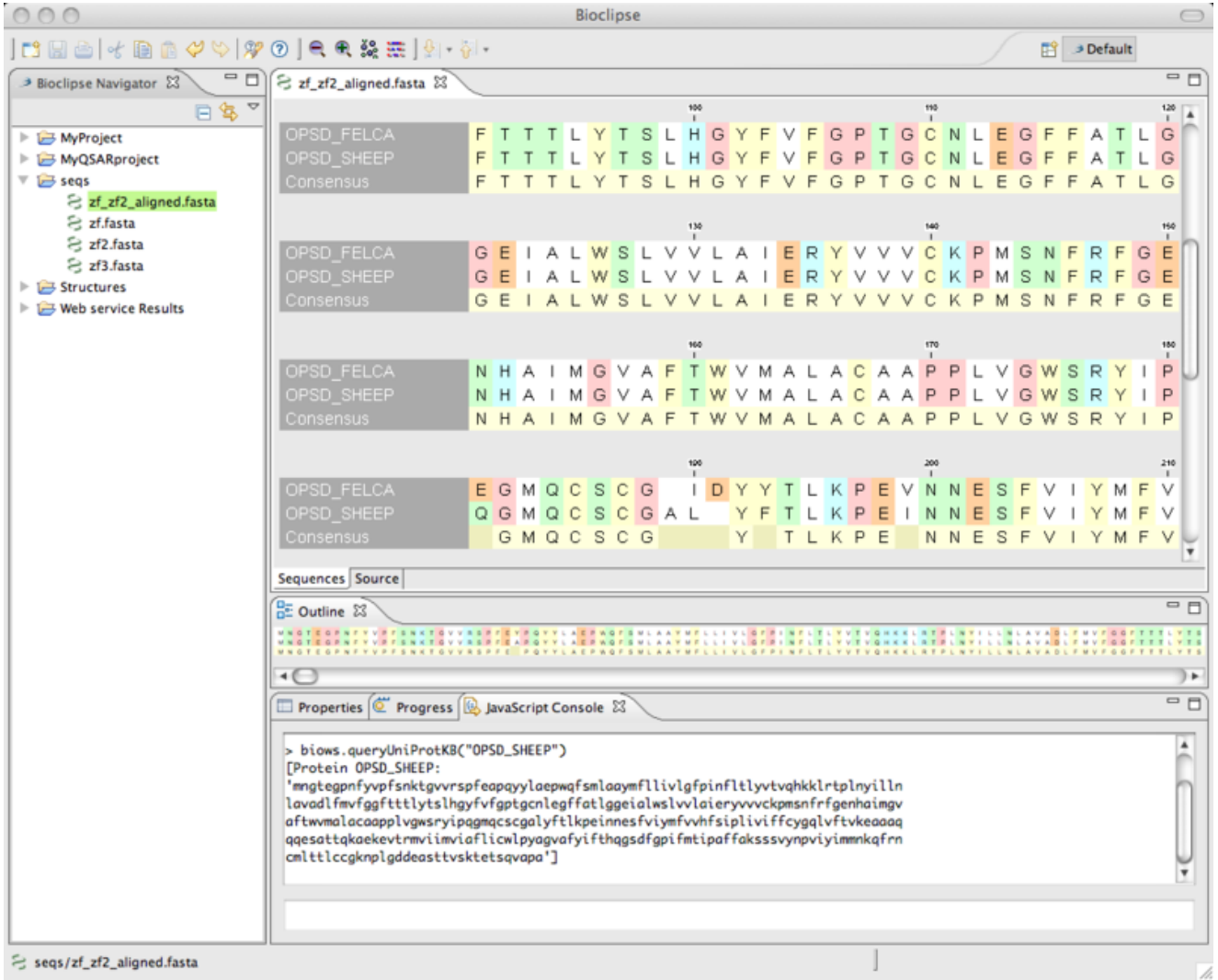
Bioclipse (10)

Bioinformatics

- Bioinformatics in Bioclipse concerns primarily the management and analysis of biological sequences (DNA, RNA, and protein).
- Bioinformatics in Bioclipse relies heavily on BioJava, which provides core bioinformatics functionality, and a graphical editor for sequence alignments.
- Various clients for Web services are also available to facilitate downloading of e.g. biological sequences and annotations, as well as for bioinformatcs analysis.

Bioclipse (11)

Ilustration: Sequence Editor displaying a wrapped alignment



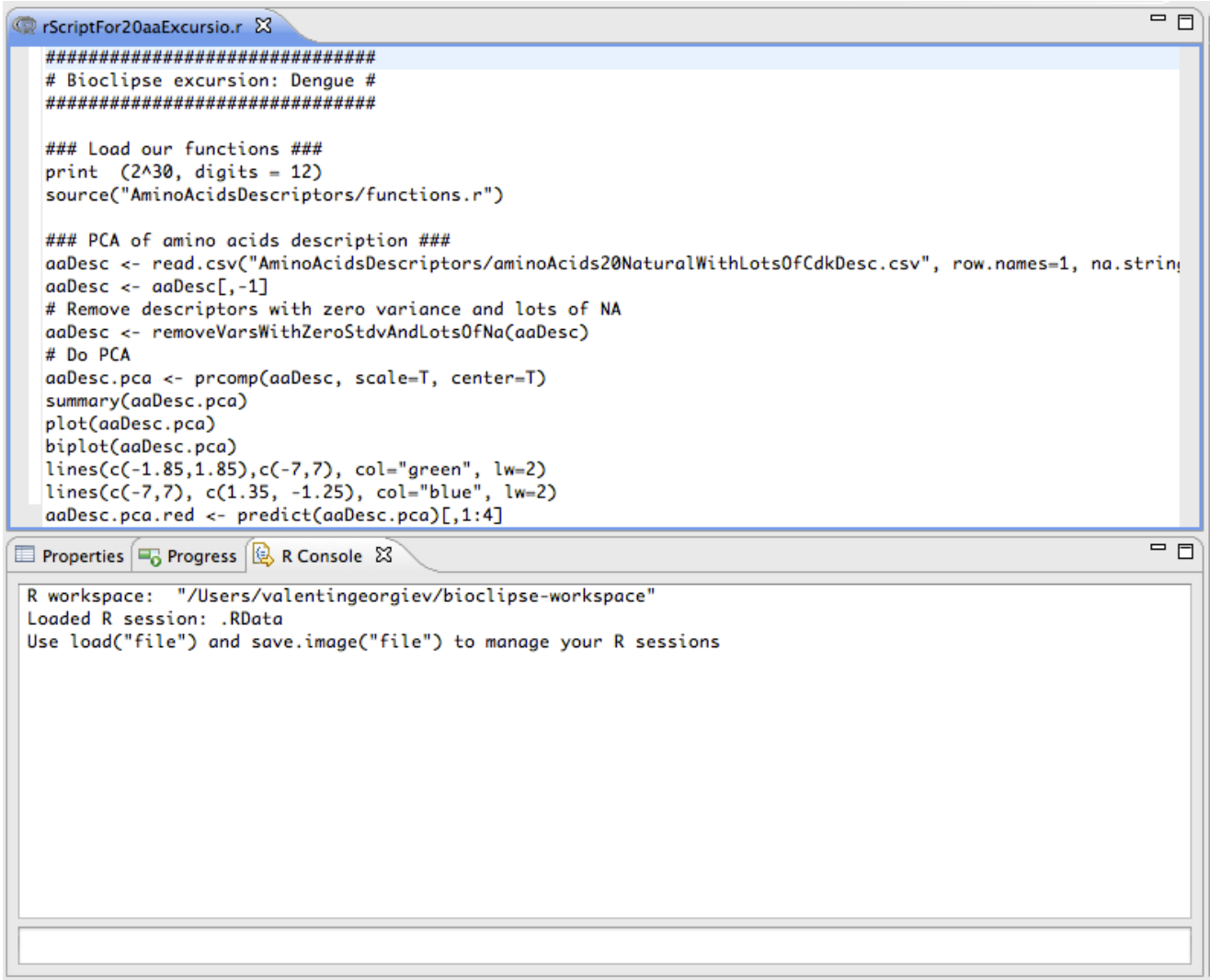
Bioclipse (12)

Bioclipse-R Itegration

- The statistical computing language R is now integrated in Bioclipse.
- R is a free and open source software that runs on Windows, Mac OS, and a wide variety of UNIX platforms and similar systems (including FreeBSD and GNU/Linux).
- The Bioclipse-R feature provides a graphical R editor and a interactive R console for easy running of R scripts, snippets and commands, and the plotting capabilities of R.

Bioclipse (13)

Ilustration: Integration of the R into Bioclipse workbench



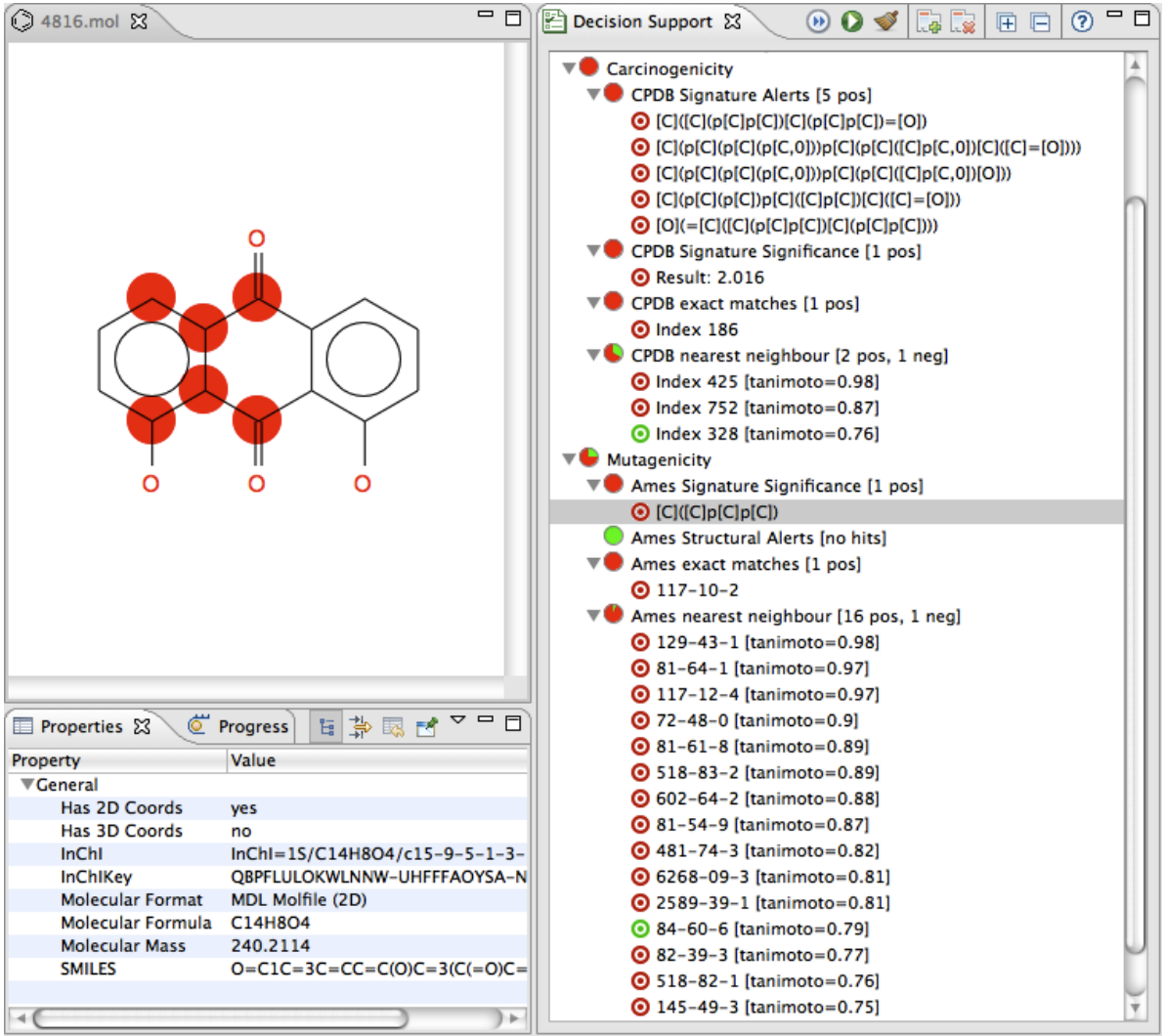
Bioclipse (14)

Decision support

- Bioclipse facilitates working with decision support systems, for example when predicting the susceptibility of a drug for certain patients. By sequencing the DNA of the patient (or e.g. a virus in the patient), it is possible to predict what drugs that would best attack the disease. An example of this is HIVPred, which is implemented as an XMPP cloud service and a plugin in Bioclipse to facilitate invocation.
- Bioclipse also has a feature for decision support in safety assessment with graphical views and editors for executing and integrating various computational models to predict the safety of chemical compounds.

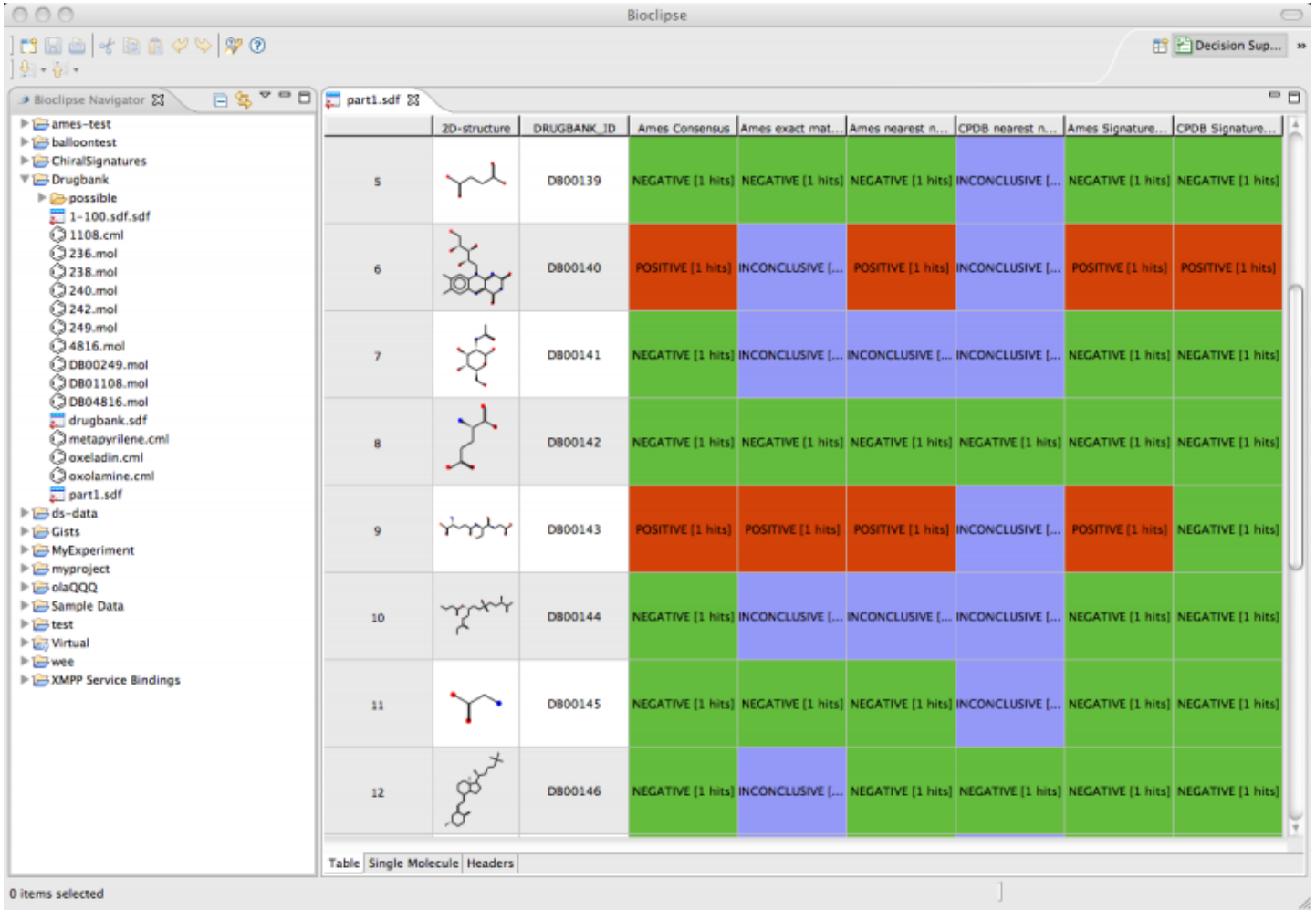
Bioclipse (15)

Ilustration: Chemical liability assessment in the Bioclipse workbench



Bioclipse (16)

Ilustration: Chemical liability assessment for multiple structures with results in spreadsheet



Acknowlegments

Some material of the presentation is taken from

http://research.microsoft.com/en-us/projects/chem4word/

Some material of the presentation is taken from http://www.xml-cml.org/

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