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Bioclipse: A Rich Client for the Life Sciences

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Introduction

Bioclipse is a workbench for the life sciences built on the Eclipse Rich Client Platform (RCP). Leveraging on the powerful architecture of Eclipse, Bioclipse delivers an extensible platform and workbench for scientists, teachers, and students in fields like biotechnology, biochemistry, pharmacology, molecular biology, and general chemistry. Bioclipse has an extensive set of graphical editors, and also provides many new extension points tailored towards the life science domain. All functionality is available from the Bioclipse Scripting Language (BSL) as well as from the user interface (see fig. 1).

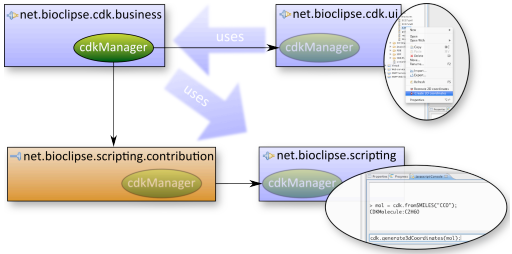

Fig 1: *Overview of the Bioclipse architecture describing the use of Managers to collect business code, where the same manager can be called both from the GUI and the scripting language.*

Cheminformatics

Cheminformatics concerns the management, analysis, and visualization of chemical structures and related information. Bioclipse is equipped with editors, views, and wizards for single molecules in 2D, large collection of molecules, and interactive 3D visualizations. The underlying cheminformatics framework is mainly based on the Chemistry Development Kit (CDK).

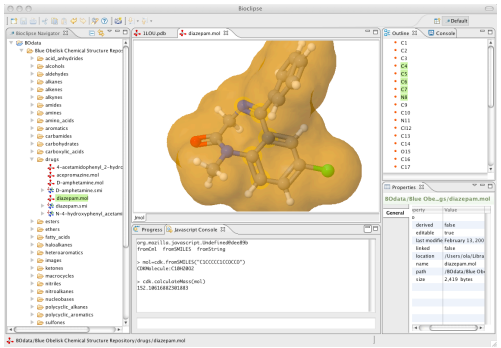

Fig 2: *Screenshot of a 3D visualization of a drug using the JmolEditor in Bioclipse. The Javascript Console (bottom, center) can be used as an alternative to the GUI for controlling the rendering.*

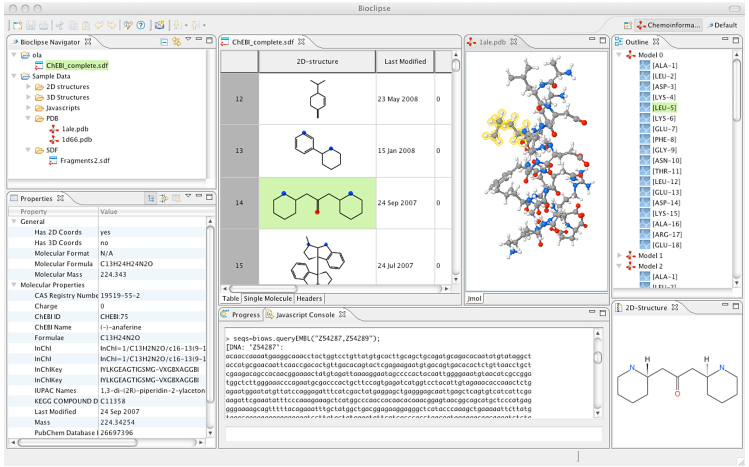

Fig 3: *Screenshot from Bioclipse 2.0 showing the Molecules Table (top middle panel) with chemical structures and properties in a spreadsheet-like editor and the selected structure rendered in a separate 2D view (bottom right panel), and computed properties (bottom left panel). Also shown is a 3D structure where monomers are selected in the outline (top rightmost panel) and highlighted in the interactive Jmol 3D-Editor (top right panel). The Javascript console (bottom middle panel) can be used to execute scripting commands, and shows the result of a Web service query to download two proteins from the European Molecular Biology Laboratory (EMBL) database.*

Bioinformatics

Bioinformatics concerns primarily the management and analysis of biological sequences (DNA, RNA, and proteins). Bioclipse is equipped with graphical editors for editing sequences, and makes use of several Web services for retrieving data from public repositories, and for performing various analyses.

Drug discovery

Bioclipse is equipped with many features that simplify pharmacological research and drug discovery. A feature for prediction of chemical interactions based on computational models is available. A second feature provides decision support for drug safety assessment. A third feature includes functionality to mine chemical databases for interesting compounds (virtual screening).

eScience

eScience denotes the increasing part of science which makes use of high performance computing and distributed resources. Bioclipse aims at being the most advanced platform in life science providing access to eScience resources, and important features in Bioclipse includes the access to service-oriented resources such as Web services and networked databases. Connections to grids and workflows are in the pipeline.

www.bioclipse.net

Data analysis

The majority of scientific analyses in Bioclipse ends with some sort of data analysis. We are currently implementing a data analysis engine based on the statistical language R, integrated with the other Bioclipse features.

Links

Bioclipse:	http://www.bioclipse.net
Bioclipse blog:	http://bioclipse.blogspot.com/
CDK:	http://cdk.sourceforge.net/

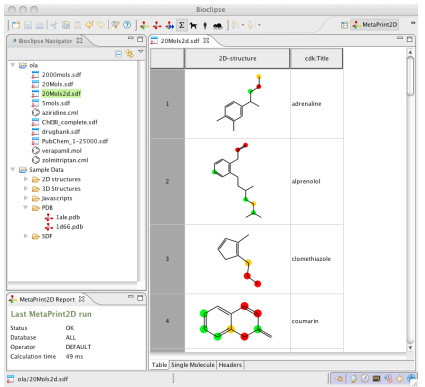

Fig 4: *Screenshot of the MetaPrint2D feature for Bioclipse to highlight atoms in drugs which are likely of undergo metabolization in the liver. The feature was developed in collaboration with AstraZeneca, and is used in active drug discovery projects.*