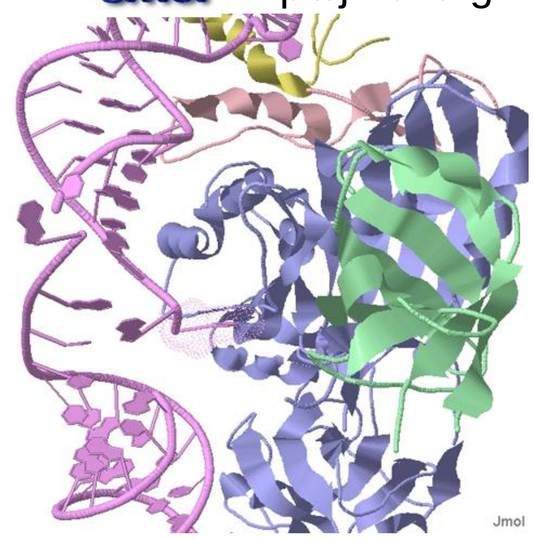
View metadata, citation and similar papers at core.ac.uk
brought to you by CORE
provided by Apollo

The **Blue Obelisk** community

Introduction

The Internet has brought together a group of chemists who are driven by wanting to do things better, but are frustrated with the Closed systems that chemists currently have to work with. They share a belief in the concepts of **Open Data, Open Standards and Open Source**. And they express this in software, data, algorithms, specifications, tutorials, demonstrations, articles and anything that helps get the message across.

Jmol http://jmol.org



OpenSMILES Specification

<< Previous: n/a Up: Table of Contents Next: Formal Grammar >>

Contributors:
Richard Apodaca, Noel O'Boyle, Andrew Dalke, John van Drie, Peter Ertl, Geoff Hutchison, Craig A. James, Greg Landrum, Chris Morley, Egon Willighagen, Hans De Winter

This document formally defines an open specification version of the SMILES language, a typographical line notation for specifying chemical structure. It is hosted under the banner of the Blue Obelisk project, with the intent to solicit contributions and comments from the entire computational chemistry community.

http://opensmiles.org

Cheminformatics Toolkits

RDKit
Open-Source Cheminformatics and Machine Learning

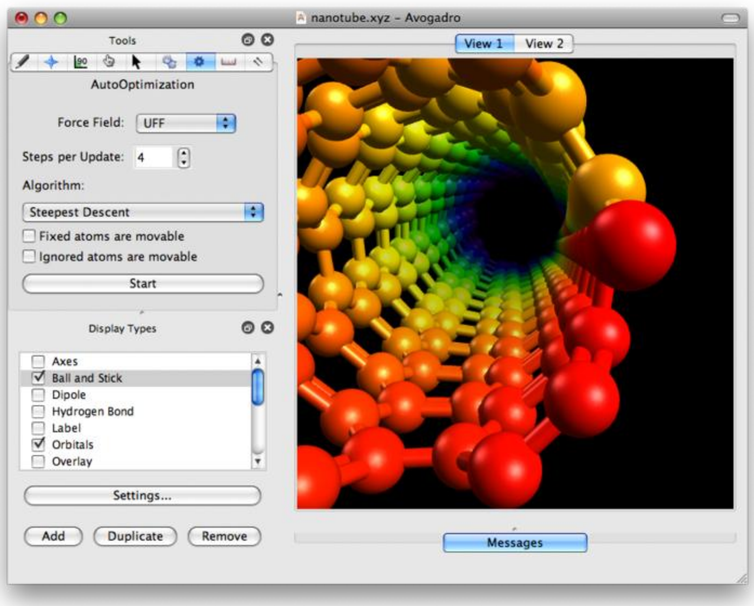
Open Babel

CDK

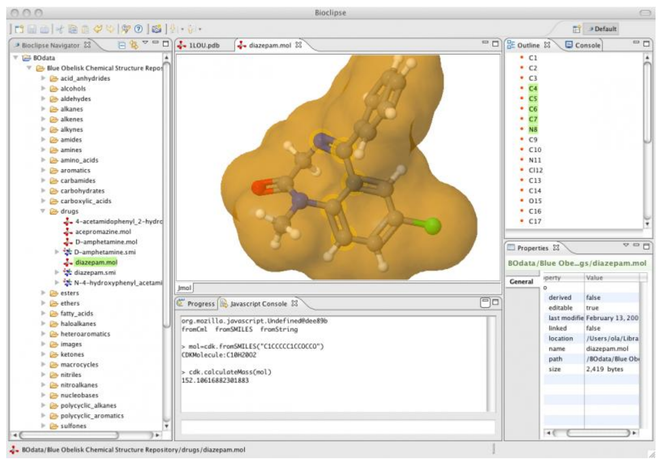
Cinfony

Indigo

Avogadro http://avogadro.sf.net



Bioclipse http://bioclipse.net



Welcome to cclib

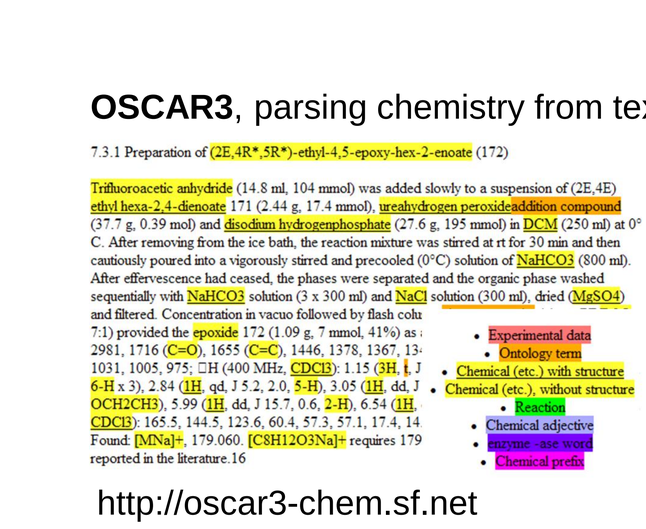
cclib is an open source library, written in Python, for parsing and interpreting the results of computational chemistry packages. The current version, **cclib 1.0**, parses output files from ADF, GAMESS (US), GAMESS-UK, Gaussian, Jaguar, Molpro, ORCA and Firefly. See what's new in **cclib 1.0**.

The goals of **cclib**

- to facilitate the implementation of algorithms that are not specific to a particular computational chemistry package
- to provide a simple and standard interface to the results of computational chemistry calculations, particularly those results that are useful for algorithms or visualisation
- to maximise interoperability with other open source computational chemistry and cheminformatic software libraries

http://cclib.sf.net

OSCAR3, parsing chemistry from text



7.3.1 Preparation of (2E,4R*,5R*)-ethyl-4,5-epoxy-hex-2-enoate (172)

Trifluoroacetic anhydride (14.8 ml, 104 mmol) was added slowly to a suspension of (2E,4E) ethyl hexa-2,4-dienoate 171 (2.44 g, 17.4 mmol), ureahydrogen peroxideaddition compound (37.7 g, 0.39 mol) and disodium hydrogenphosphate (27.6 g, 195 mmol) in DCM (250 ml) at 0° C. After removing from the ice bath, the reaction mixture was stirred at rt for 30 min and then cautiously poured into a vigorously stirred and precooled (0°C) solution of NaHCO3 (800 ml). After effervescence had ceased, the phases were separated and the organic phase washed sequentially with NaHCO3 solution (3 x 300 ml) and NaCl solution (300 ml), dried (MgSO4) and filtered. Concentration in vacuo followed by flash colu
7:1) provided the epoxide 172 (1.09 g, 7 mmol, 41%) as
2981, 1716 (C=O), 1655 (C=C), 1446, 1378, 1367, 13
1031, 1005, 975; □H (400 MHz, CDCl3): 1.15 (3H, t, J
6-H x 3), 2.84 (1H, qd, J 5.2, 2.0, 5-H), 3.05 (1H, dd, J
OCH2CH3), 5.99 (1H, dd, J 15.7, 0.6, 2-H), 6.54 (1H,
CDCl3): 165.5, 144.5, 123.6, 60.4, 57.3, 57.1, 17.4, 14
Found: [MNa]+, 179.060. [C8H12O3Na]+ requires 179
reported in the literature.16

- Experimental data
- Ontology term
- Chemical (etc.) with structure
- Chemical (etc.), without structure
- Reaction
- Chemical adjective
- enzyme -ase word
- Chemical prefix

http://oscar3-chem.sf.net

Cheminformatics Databases

Pgchem::tigress

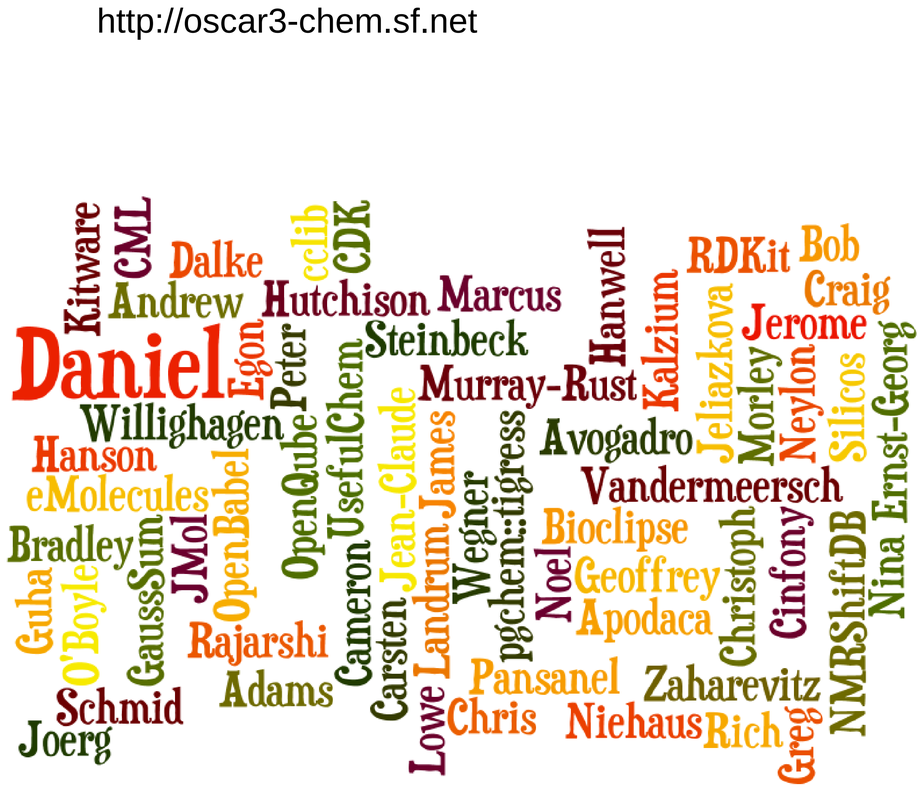
Mychem

ORCHEM

ambit

ChemiSQL

Bingo



And much more...!

Want to get involved?

Membership is informal and open to anyone with an interest in open data, open standards or open source in chemistry. Just send an email to our public mailing list and introduce yourself. There are also regular meetups at chemistry conferences so keep an eye out for announcements.

http://www.blueobelisk.org
blueobelisk-discuss@lists.sourceforge.net