Journal of Cheminformatics

POSTER PRESENTATION Open Access

Indigo: universal cheminformatics API

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From 6th German Conference on Chemoinformatics, GCC 2010
Goslar, Germany. 7-9 November 2010

Indigo is a universal portable open-source library which allows developers and chemists to solve various cheminformatics tasks. The library has grown out from a collection of more specific tools we have developed during the past years. Proper wrappers for popular programming languages are provided, as well as some command-line and GUI tools useful for scientists. All software is available under the terms of the GPL license.

The core of Indigo is a C++ cheminformatics library, which has been developed with two things in mind: performance and important chemical features. Plain C wrapper is provided for the core library, and other wrappers are built around it for Python, Java, and C# languages (support of Ruby is coming soon). The main chemical features of Indigo are:

- Support of popular chemistry formats: Molfiles/Rxnfiles v2000 and v3000, SDF, RDF, SMILES, SMARTS, SMIRKS
- Tehrahedral and cis-trans stereochemistry support
- Molecule and reaction rendering to PNG, SVG, PDF files
- Molecule and reaction layout (depiction)
- Aromatization and kekulization
- Canonical (isomeric) SMILES computation
- Exact and substructure matching for molecule and reactions, SMARTS and SMIRKS
- matching, highlighting support
- Matching or tautomers and resonance structures
- Molecule and reaction fingerprinting, similarity computation
- Molecular weight, molecular formula computation
- Maximum Common Substructure (MCS) computation
- R-Group deconvolution and scaffold detection
- Combinatorial chemistry

The pre-compiled static and dynamic binaries of the Indigo library are available, as well as binaries of command-line utilities and GUI tools. The library allows multi-threaded use. All binaries are provided for Windows, Linux and Mac OS X, both 32-bit and 64-bit Intel architectures.

The site of Indigo is http://scitouch.net/indigo (to be opened in August 2010).

Published: 19 April 2011

doi:10.1186/1758-2946-3-S1-P4
Cite this article as: Pavlov *et al.*: Indigo: universal cheminformatics API. *Journal of Cheminformatics* 2011 **3**(Suppl 1):P4.

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