GGA SOFTWARE SERVICES

SciTouch Open-source software

Indigo: Universal Cheminformatics API

Capabilities

- ► **Support of popular data formats**: SMILES, SMARTS, Molfile, Rxnfile, SDF, RDF, GZip
- ► **Portability over modern platforms and languages**: Linux/Windows/Mac OS X, 32/64 bit, Java/Python/C#
- ► **Outstanding performance**: Original algorithms, fast C++ implementation

Functionality

Calculation of structure properties:
Canonical (isomeric) SMILES, molecular weight, molecular formula

Rendering of molecules and reactions:
PNG, SVG, PDF formats supported. Query features supported.
Also automatic SMILES layout, colors, highlighted fragments, titles, ...

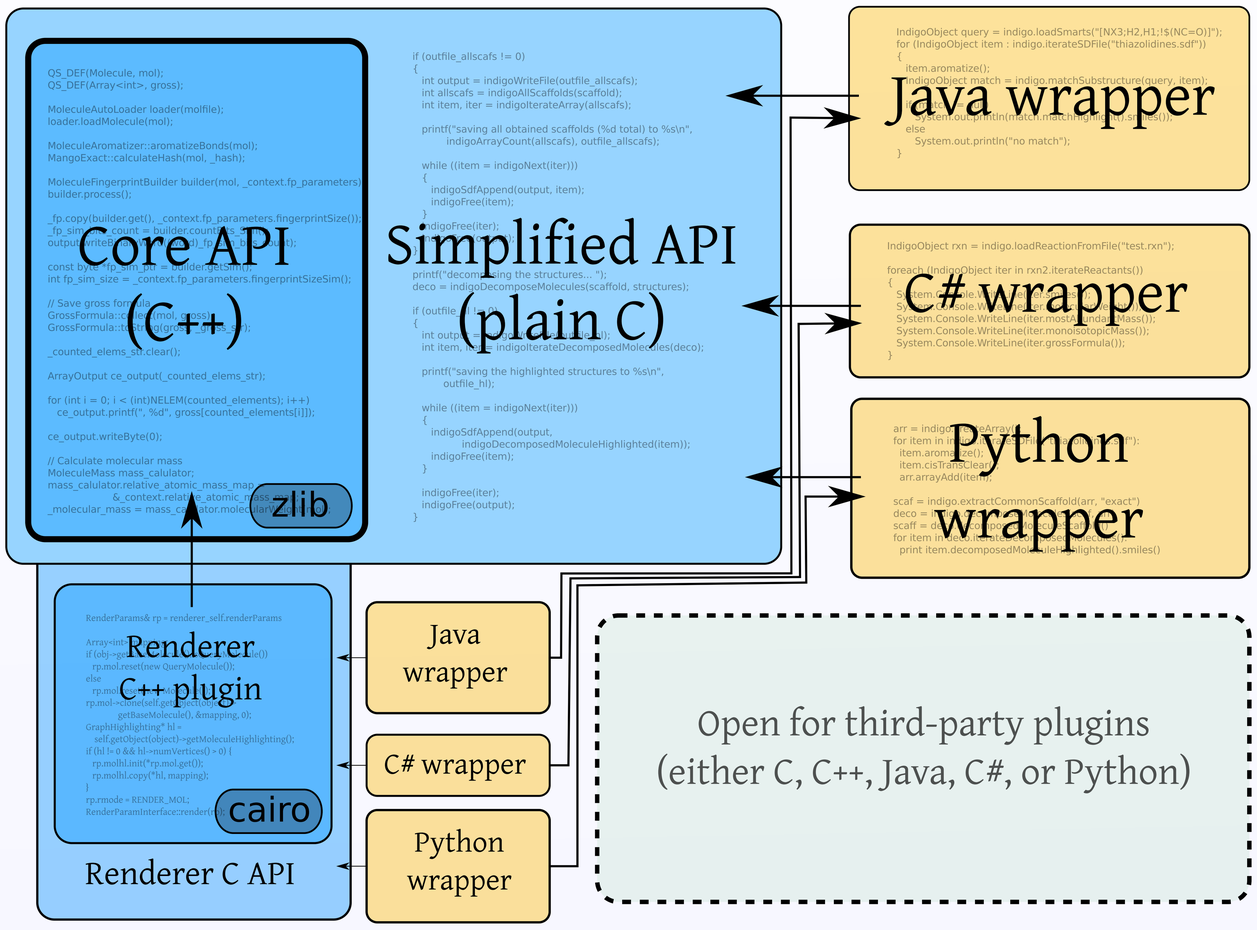
Molecule and reaction search:
Exact/Substructure/SMARTS matching. Options for matching tautomers, resonance structures, Markush structures. Original fingerprints. Various similarity measures.

Scaffold detection and R-Group decomposition:
Maximum common substructure of arbitrary amount of input structures

Reaction atom-to-atom mapping:
Calculate a new AAM or alter an existing AAM

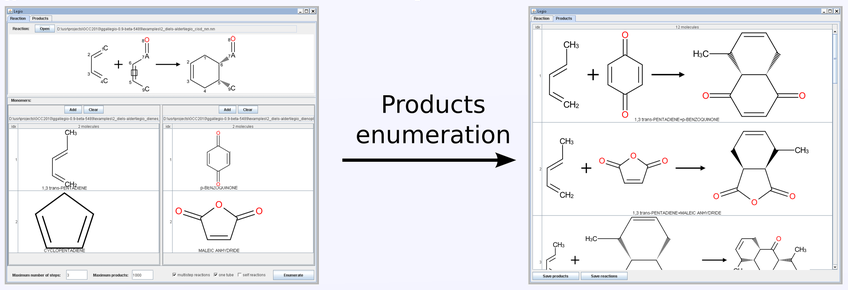
Combinatorial chemistry:
Enumeration of reaction products from available monomers.
Support of query features, perception of stereochemistry transformation.
Intramolecular reactions. Automatic screening of duplicates.

Design



Applications

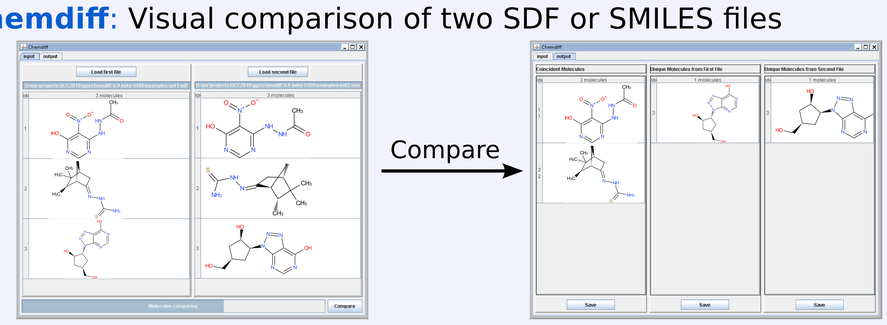
Legio: Combinatorial chemistry GUI tool



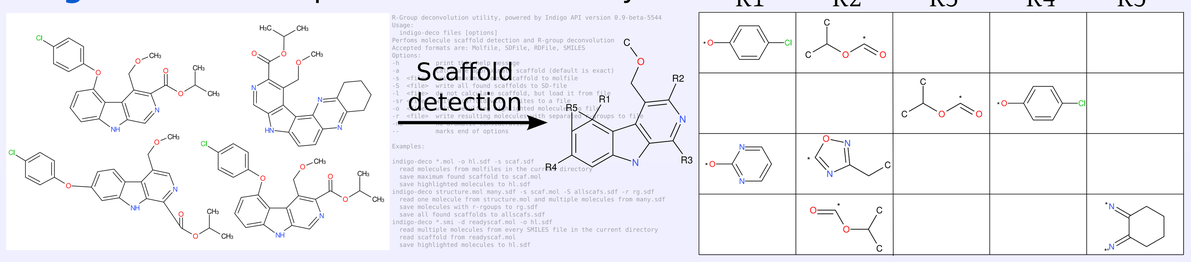
indigo-depict: Molecule and reaction rendering utility

indigo-cano: Canonical SMILES generator

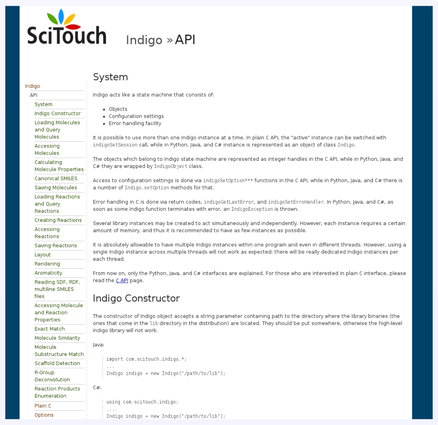
chemdiff: Visual comparison of two SDF or SMILES files



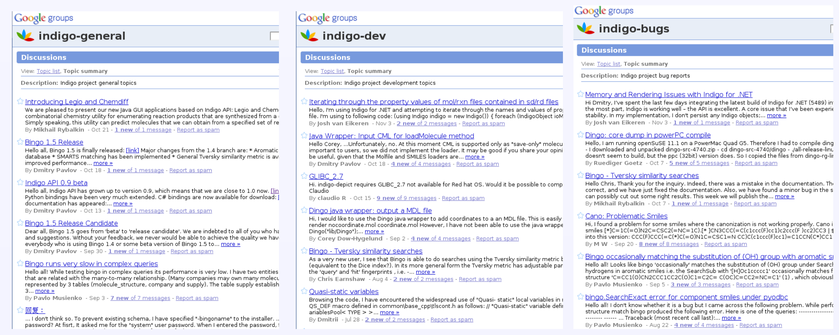
indigo-deco: R-Group deconvolution utility



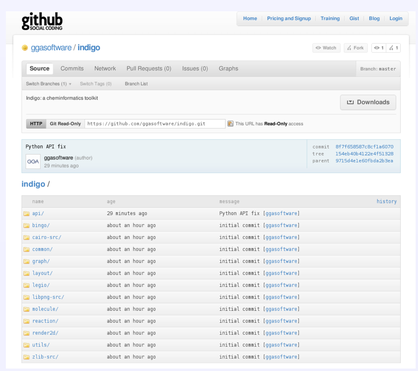
Community



http://scitouch.net
Product information, documentation, downloads



http://groups.google.com/group/indigo-general
http://groups.google.com/group/indigo-dev
http://groups.google.com/group/indigo-bugs
Public discussion lists



http://github.com/ggasoftware
Complete source code (GPL v3)

http://blueobelisk.shapado.com
BlueObelisk question board

http://ctr.wikia.com
Code examples for different toolkits