Indigo: Universal Cheminformatics API

Capabilities

- Support of popular data formats: SMILES, SMARTS, Molfile, Rxtxfile, SDF, RDF, GZ/p
- 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, ...
- 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

Design

- Core API (C++)
- Simplified API (plain C)
- Java wrapper
- C# wrapper
- Python wrapper
- Open for third-party plugins (either C, C++, Java, C#, or Python)

Applications

- Lego: 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 list
- http://github.com/ggasoftware
  - Complete source code (GPL v3)
- http://blueobelisk.shapado.com
  - Code examples for different toolkits
- http://ctr.wikia.com
  - BlueObelisk question board