

SERVICES

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#



Community

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.



Legio: Combinatorial chemistry GUI tool



Average bond length in pixels (conflicts with -w and -h) -margins <number> <number> Horizontal and vertical margins, in pixels. No margins by defaul -thickness <number> Set relative thickness factor. Default is hydro <none|terminal|hetero|terminalhetero|a Set implicit hydrogen display mode (default is terminalhetero label <normallforceshowlhideterminallforcehide> Set atom label display mode (default is normal [de]arom Force [delaromatizati I Gring be in Ge C and the Content of the Content o omm t to boour abve the molecule or react: iel Viring of Field and Domment n. No default value comments in a comment is a comment is a comment is the comment of talign <left|center right> comercaligner cetter by left to ng fon off> mercetter by default. ighting with thick lines a <graen: olue> ighting with coll r Convon

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ciTou	ch Indigo »API
	System
go	Indian acts like a state machine that consists of
의 	Indigo acts like a state machine that consists of:
System	Objects
Indigo Constructor	Configuration settings
Loading Molecules and Query	Error handling facility
Molecules	It is possible to use more than one Indigo instance at a time. In plain C API, the "active" instance can be switched with
Accessing	indigoSetSession call, while in Python, Java, and C# instance is represented as an object of class Indigo.
Molecules	The objects which belong to Indigo state machine are represented as integer handles in the C API, while in Python, Java, and
Calculating	C# they are wrapped by IndigoD ject class.
Molecule Properties	
Canonical SMILES	Access to configuration settings is done via indigoSetOption*** functions in the C API, while in Python, Java, and C# there is
Saving Molecules	a number of Indigo.setOption methods for that.
Loading Reactions and Query	Error handling in C is done via return codes, indigoGetLastError, and indigoSetErroHandler. In Python, Java, and C#, as
Reactions	soon as some Indigo function terminates with error, an IndigoException is thrown.
Creating Reactions	Several library instances may be created to act simultaneously and independently. However, each instance requires a certain
Accessing	amount of memory, and thus it is recommended to have as few instances as possible.
Reactions	
Saving Reactions	It is absolutely allowable to have multiple Indigo instances within one program and even in different threads. However, using a single Indigo instance across multiple threads will not work as expected: there will be really dedicated Indigo instances per
Layout	each thread.
Rendering	
Aromaticity	From now on, only the Python, Java, and C# interfaces are explained. For those who are interested in plain C interface, please read the <u>C API</u> page.
Reading SDF, RDF, multiline SMILES	read the <u>CALL</u> page.
files	Indigo Constructor
Accessing Molecule	
and Reaction	The constructor of Indigo object accepts a string parameter containing path to the directory where the library binaries (the
Properties	ones that come in the lib directory in the distribution) are located. They should be put somewhere, otherwise the high-level
Exact Match	Indigo library will not work.
Molecule Similarity	Java:
Molecule Substructure Match	
Scaffold Detection	<pre>import com.scitouch.indigo.*;</pre>
R-Group	 Indigo indigo = new Indigo("/path/to/lib");
Deconvolution	
Reaction Products	C#:
Enumeration	using com.scitouch.indigo;
Plain C	daing com.acitoden.indigo;

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

oogle groups	Google groups	Google groups			
💪 indigo-general	🔧 indigo-dev	ע indigo-bugs			
Discussions	Discussions	Discussions			
iew: <u>Topic list</u> , Topic summary	View: Topic list, Topic summary	View: <u>Topic list</u> , Topic summary			
escription: Indigo project general topics	Description: Indigo project development topics	Description: Indigo project bug reports			
Introducing Legio and Chemdiff We are pleased to present our new Java GUI applications based on Indigo API: Legio and Chem Simply speaking, this utility can predict molecules that we can obtain from a specified set of re By Mikhail Rybalkin - Oct 21 - <u>1 new of 1 message - Report as span</u> Bingo 1.5 Release Billo all, Bingo 1.5 is finally released: [link] Major changes from the 1.4 branch are: * Aromatic database * SMARTS matching has been implemented * General Tversky similarity metric is as improved performancemore.» By Dmitry Pavlov - Oct 18 - <u>1 new of 1 message - Report as span</u> <i>Hold</i> all, Indigo API has grown up to version 0.9, which means that we are close to 1.0 now. [lin Python bindings have been very much extended. C# bindings are now available for download: documentation has appearedmore.» By Dmitry Pavlov - Oct 13 - <u>1 new of 1 message - Report as span</u> <i>Hold</i> all, Bingo 1.5 goes from 'beta' to 'release candidate'. We are indebted to all of you who he ads aggestions. Without your feedback, we never would be able to achieve the quality we have everybody who is using Bingo 1.4 or some beta version of Bingo 1.5 tomore.» By Dmitry Pavlov - Sep 30 - <u>1 new of 1 message - Report as span</u> Hold all: while testing bingo in complex queries its performance is very low. I have two entities that are related with the many-to-many relationship. (Many companies may own many molect represented by 3 tables (molecule_structure, company and supply). The table supply establishmore.» By Pavlo Musienko - Sep 3 - <u>1 new of 7 messages - Report as span</u> Eff: doth think so. To	 Iterating through the property values of mol/rxn files contained in sd/rd files. Hello, I'm using Indigo for .NET and attempting to iterate through the names and values of profile. I'm using to following code: (using Indigo indigo = new Indigo(1)) { foreach (IndigoObject ioM By Josh van Eikeren - Nov 3 - 2 new of 2 messages - Report as spam Java Wrapper: Input CML for loadMolecule method Hello, I'm using indigo indigo = new Indigo(1) { foreach (IndigoObject ioM By Josh van Eikeren - Nov 3 - 2 new of 2 messages - Report as spam Java Wrapper: Input CML for loadMolecule method Hello Corey,Unfortunately, no. At this moment CML is supported only as "save-only" moleculing of the users, so we did not implement the loader. It may be good if you share your opinit be useful, given that the Molfile and SMILES loaders are more 2 By Dmitry Pavlov - Oct 18 - 4 new of 4 messages - Report as spam GLIBC_2.7 Hi. Indigo-depict requires GLIBC_2.7 not available for Red hat OS. Would it be possible to comp Claudio By claudio R - Oct 15 - 9 new of 9 messages - Report as spam Dingo java wrapper: Output a MDL file Hi, I would like to use the Dingo java wrapper to add coordinates to a an MDL file. This is easily render nocoordinate.mol However, I have not been able to use the java wrappe Dingo('Ib/Dingo') more 2 By Corey Dow-Hygelund - Sep 2 - 4 new of 4 messages - Report as spam Bingo - Tversky similarity searches As a very new user, I see that Bingo is able to do searches using the Tversky similarity metric t (equivalent to the Dice index'). In its more general form the Tversky metric has adjustable part the 'query' and 'hit fingerprints , i.e more 2 By Chris Earnshaw - Aug 4 - 2 new of 2 messages - Report as spam Quasi-static Variables Browsing the code, I have encountered the widespread use of "Quasi-	 Memory and Rendering Issues with Indigo for .NET Hi Dmity, I've spent the last few days integrating the latest build of Indigo for .NET (5489) in the most part, indigo is working well - the API is excellent. A core issue that I've been experie stability. In my implementation, I don't persist any Indigo objects; <u>more ></u> By Josh van Eikeren - Nov 3 - <u>1 new of 1 message - Report as span</u> Dingo: core dump in powerPC compile Hello, I am running openSUSE 11.1 on a PowerMac Quad G5. Therefore I had to compile ding - I downloaded and unpacked dingo-src 4740.2;p - cd dingo-src 4740/dingo - , /all-release.inu. doesn't seem to build, but the ppc (32bit) version does. So I copied the files from dingo-rg-lif By Ruediger Goetz - Oct 7 - <u>5 new of 5 messages - Report as span</u> Bingo - Tversky similarity searches Hello Chris, Thank you for the inquiry. Indeed, there was a mistake in the documentation. The correct, and we have just fixed the documentation. Also, we have found a minor bug in the s can possibly cut out some right results. This week we will publish the <u>more ></u> By Mikhail Rybalkin - Oct 7 - <u>1 new of 1 message - Report as spam</u> Cano: Problematic Smiles Hi, I found a problem for some smiles where the canonization is not working properly. Cano i smiles (*JC=1C(=0)NZC=CSC2(=RC=1C).(*)[CN3CCC(=C(c1ccc(F)cc1)=C1CCN(<*)CC1] ey M W - Sep 20 - <u>8 new of 8 messages - Report as spam</u> Bingo occasionally matching the substitution of (OH) group with aromatic si Hello all: Looks like bingo 'occasionally' matches the substitution of (OH) group under Search Hydrogens in aromatic smiles i.e. the SearchSub with [H]OC1ccccc1' occasionally matches f structure 'C=C(10)(CN2CCC1C2C2(0)C1=C2E = C(0C)C=CC2=(C=C1(1).)), which obvious! By Pavlo Musienko - Sep 5 - <u>3 new of 3 messages - Report as spam</u> Dingo.SearchExact error for component smiles under pyodbc			

Julia giereon, group, margo http://groups.google.com/group/indigo-dev http://groups.google.com/group/indigo-bugs Public discussion lists

l1 months ago

832 time:

Latest activity 7 months ago

Related question

"Ligand libraries" generation

(and optimization) free tools

What is the proper format of a SMILES (.smi) file?

Has anyone got Dingo to work

count_matches(subsearch, mol):

indigo.countSubstructureMatches(subsearch, mol)



N(CC(=0)N1C(CSC1cCC(C)SCNC(=0)C1CSC(=C(CCC(=0)c1ccc(F)ccCN1CCOC[COH]1CNC(=0)C1CSC(c2cccc2)N1C(=0)CN(C)c1ccCCCCCCC1SCC(C(=0)NC2CC2)N1C(=0)CSc1[n]c2ccccc2[s]1 =C(CC1CCCC10Cc1ccccc1)N1C(SCC1C(=0)NC1CC1)c1cccc

=C(CC1CCCC10Cc1ccccc1)N1C(SCC1C(=0)NC1CC1)C1CC2C

chemdiff: Visual comparison of two SDF or SMILES files





indigo-deco: R-Group deconvolution utility







	ndigo		 Watch 	4 Fork	1			
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Complete source code (GPL v3)

	dmitry pavlov 🔌	Has anyone got Dingo to work?			
	227 •7	Draw a colored sphere from cartesian coordinates in pymol			
	Federation	Is Balloon a "free" equivalent for CORINA?			
10 months ago david garcía aristegui said:	nu bay and tast #111 bast regards	Get coordinates of beads covering the surface of a protein			
Thank you for the info, tomorrow i will install Dingo in my linux bo	ux and test it::: best regards.	How to get an experimental ligand structure from the PDB?			
10 months ago dmitry pavlov said: OK, please note that you should have cairo graphics library inst	alled on your Linux box.	Is there a webservice that can convert a MOL file to a SMILES string?			
10 months ago david garcía aristegui said: The cairo graphics library is available via apt-get?		Which formats fall into "Open Data, Open Source, and Open			

Answered 10 months

Dmitry

Link

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

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de, and Selzer (J. Med. Chem., 43:3714-3717 face area (PSA). Part of it involves summing tions. Each fragment corresponds to a SMAR of this task is get an idea of how to do a set nal table. In this case it's a data table from T SQL, listed at http://www.gnova.com/book/tps a in the file contains three tab-separated field fragment contribution. The first field is the p match defined in the second column. The las definition contains a typo, it should be "[N+1	of SMARTS matches when t of SMARTS matches when t J O'Donnell's CHORD chemis a.tab 다 and available for use ds. The first line is the heade artial surface area contributi st column is a comment. Not	ased on fragr the data com <mark>stry extension</mark> e here with p er. The other ion, for each te that the fin	ment nes in from n ^ው for ermission. lines SMARTS rst	Recent Wiki Dpavlov edit s seconds ago A Wikia con Working wit Egonw edite string to ca Dpavlov edit stereochem in SMILES fi	ed Calculat tributor edi h SD tag d d Convert a nonical SMI ed Change istry of cer	ted lata a SMILES ILES
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= indigo.Indigo()						
<pre>place to store the pattern definition = collections.namedtuple("Pattern" ms = []</pre>		"])				
the patterns from the tpsa.tab file, ne in open("tpsa.tab").readlines()[1 xtract the fields .ue, smarts, comment = line.split("\	:]:	ine				
<pre>search = indigo.loadSmarts(smarts)</pre>						
tore for later use terns.append(Pattern(float(value),	subsearch))					
er function to count how many times	a substructure matches					

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