

Interfacing the JChem Suite outside of Java

Jonathan Lee

- **JChem Interfaces**
- **Situational Factors**
- **SQL**
- **.NET**
- **Web Services**
 - Details
 - Demo
- **Workflow Integrations**

Interfaces to JChem Suite of Tools

Visualization

Marvin
Structure, query & reaction editor, viewer & visualization

Property prediction

Calculator Plugins
Structure property prediction & calculation

Selected calculations listing

- pKa, Major microspecies
- logP, logD
- Charge
- Tautomerization
- Stereoisomer
- Conformation and 3D alignment
- Topology Analysis
- Molecular Surface Area
- Markush Enumeration
- Hydrogen Bond Donor-Acceptor
- Structural Frameworks
- Structure to Name
- ...etc.

Add-on's

Chemical DB - toolkit

JChem Cartridge
JChem/Oracle integration

JChem Base
Structure searching & db access

Standardizer
Chemical canonicalization / business rules

Chemical DB - desktop

Instant JChem
Structure db management, search & prediction

JChem for Excel®
Enabling chemistry in Excel

Visualization

Name to Structure
Converting chemical names to structures

Enumeration

Reactor
Enumeration via reaction modelling

Metabolizer
Metabolic pathway & stability prediction

Library analysis

JKluster
Clustering & diversity analysis

Fragmenter
Decomposition to fragments and R-groups

Screen
HT pharmacophore screening



Java

- Direct POJO and Server-side JSP

SQL

- JChem Cartridge for environments with Oracle

.NET

- Interoperability with .NET framework

Web Services

- Platform and Language-Independent

Situational Factors

Applicable Language

- Does Java, .NET, SQL, or other Web language figure prominently?

Data Environment

- Is Oracle the target structure database?

End User Environment

- Will the user have a Desktop Client or a Web Client?

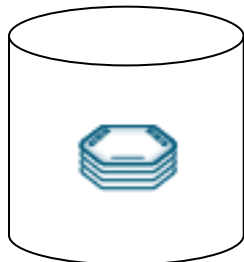
Overall Technical Architecture

- Do you use a Service Oriented Architecture?

JChem Cartridge

- Leverage Oracle Database Advantages
- Stored procedures quickly handle database work
- External communication with JChem Server for process intensive work

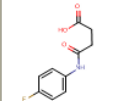
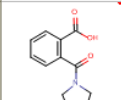
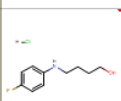
ORACLE®



Supports

- SQL
- Most JChem Modules (Searching, Standardization, Reactor, Chemical Terms, Calculator Plug-in, ...)

- Pure .NET solution for all non-GUI elements
- Marvin .NET GUI components (Marvin 5.3)
- New no cost native .dll is simpler, faster, than earlier JNBridge solution

Structure	CDBREGNO	MOLFORM	Number
	1	C10 H10 F N	-BB/0001
	2	C12 H13 N O3	2.19E+02 AKS-BB/0002
	3	C10 H14 F N O . Cl H	2.20E+02 AKS-BB/0003

Supports

- All .NET languages (C#, VB.NET, ...)
- All of JChem Suite (except Cartridge and Marvin Beans classes)

JChem Web Services

- WS-I, SOAP, and WSDL standards
- Reusable and accessible to other services
- Automated client-side code generation



Supports

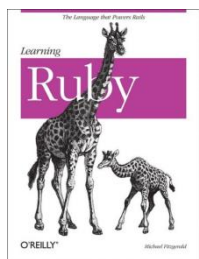
- Web Languages: AJAX/JavaScript, Perl, Python, Ruby, PHP, ...
- App languages: Java, C#, ...
- Growing list of JChem Modules (Searching, Standardization, Chemical Terms, Molecule Conversion)

Unlocking the Scripting Menagerie

python

```
loc = ChemicalTermsWS_client.ChemicalTermsWSLocator()
evaluator = loc.getChemicalTermsWSHTTP(Soap11Endpoint())
req = ChemicalTermsWS_client.evaluator.evaluateReturnNumRequest()
req.Target = 'CC=CC'
req.Expression = 'logp'
resp = evaluator.evaluateReturnNum(req)
```

perl 



```
var xhr = new XMLHttpRequest();
xhr.open(method, url, async);
xhr.setRequestHeader('Content-Type', 'text/xml; charset=utf-8');
xhr.send(createEvaluateReturnNumRequest("CC=CC", "logp"))
```



```
<soap:Body>
  <evaluateReturnNum xmlns="http://webservice.jchem.chemaxon">
    <target>CC=CC</target>
    <expression>logp</expression>
  </evaluateReturnNum>
</soap:Body>
```

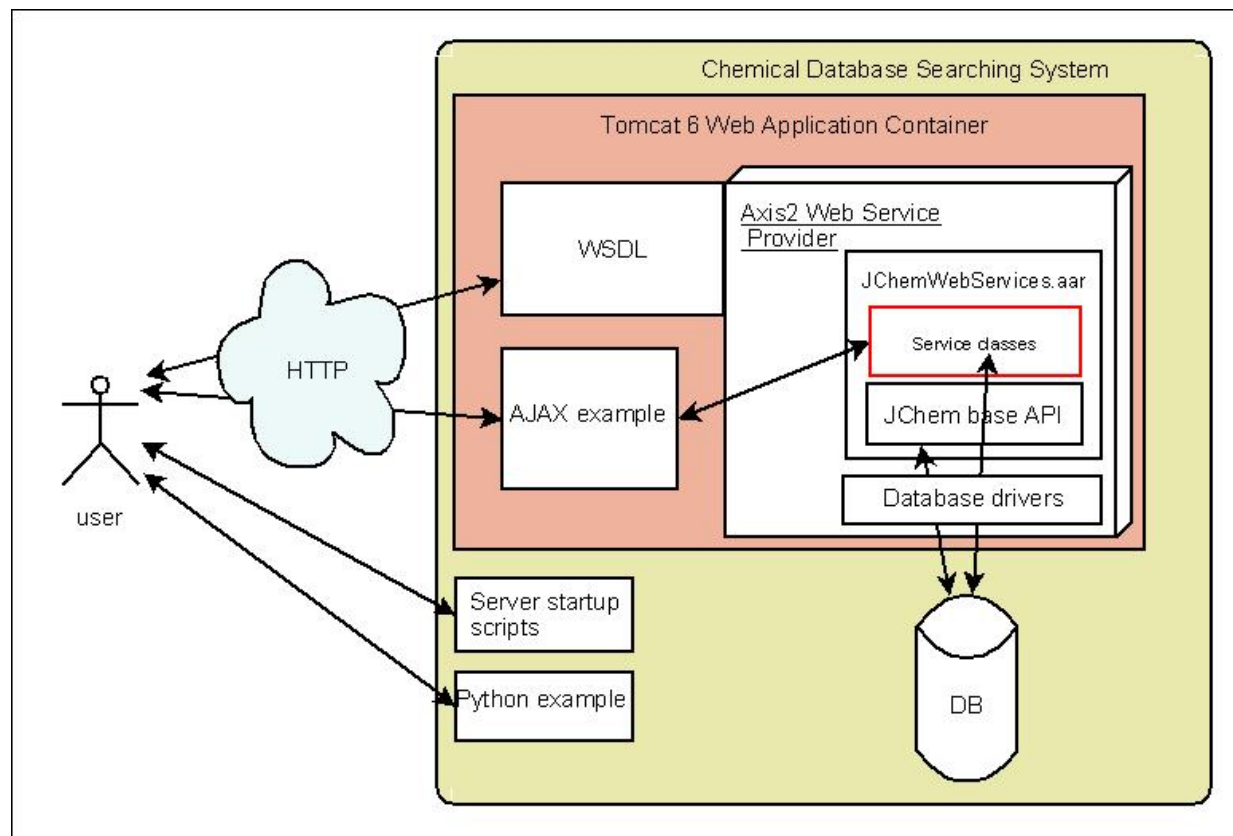


JChem Web Services

JChem WS Server Architecture

Apache Open Source Components

- Axis2 Web Service Engine and Tomcat Web Container



OS List

- Windows
- Unix
- Linux (SUSE, Red Hat, Ubuntu, Gentoo)
- Mac OS X

Current and Future Services

- JChem Search Service
- Standardization Service
- Molecular Conversion Service
- Chemical Terms Evaluation Service




Future Enhancements

- Reactor
- SQL Execution
- Relational Table Searching
- Data Manipulation
- Batch Processing

AJAX Demo of JChem Web Services

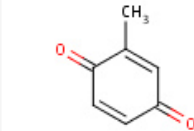
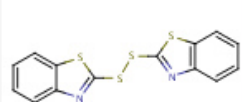
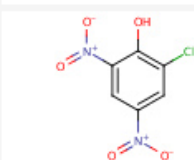
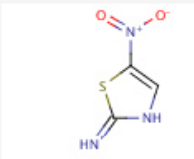
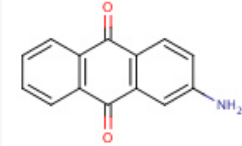
JChemSearch Web Service - www.chemaxon.com/ajax


ChemAxon

Navigation

- Query
- Insert
- Export
- Print
- About

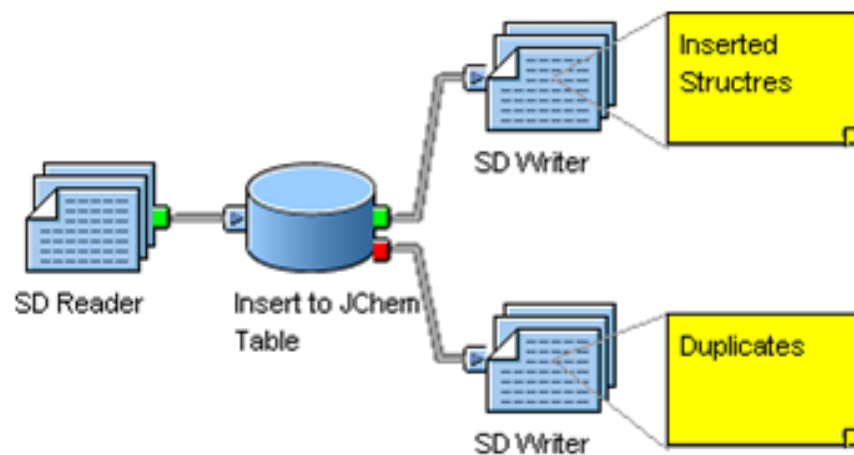
Hit alignment Results: 250251 Select table

No.	Structure	ID	Formula	Molweight	Timestamp
1		1	C ₇ H ₆ O ₂	122.1213	2008-12-02 11:45:03.0
2		2	C ₁₄ H ₈ N ₂ S ₄	332.487	2008-12-02 11:45:03.0
3		3	C ₆ H ₃ ClN ₂ O ₅	218.551	2008-12-02 11:45:03.0
4		4	C ₃ H ₃ N ₃ O ₂ S	145.14	2008-12-02 11:45:03.0
5		5	C ₁₄ H ₉ NO ₂	223.2268	2008-12-02 11:45:03.0

Workflow Integrations

ChemAxon components exist for several workflow software vendors

- Accelrys Pipeline Pilot
- KNIME Workbench (by Infocom)
- Inforsense Analytics



Find out more about JChem Cartridge

- **Product descriptions & links**

www.chemaxon.com/product/jchem_cartridge.html

- **Forum**

www.chemaxon.com/forum/forum7.html

- **Presentations and posters**

www.chemaxon.com/conf/JChemCartridge.ppt

- **Download**

www.chemaxon.com/jchem/download.html

The collage includes several screenshots:

- ChemAxon Homepage:** Features sections for 'Recent News' (e.g., 'INFOCAMP releases ChemAxon's JChem nodes on KXNDE workbench'), 'Upcoming Meetings' (e.g., 'Seminars series: Bridging the corporate and desktop business informatics environment'), and 'Recent Publications' (e.g., 'Customer generation, pKa based dominance conditions for generating dominant tautomers').
- JChem Base:** A screenshot of the software interface with a text box explaining: 'JChem Base is a tool for the development of applications that allow for the search of mixed structural and non-structural data. JChem Base will integrate with a variety of database systems (Oracle, MS SQL Server, DB2, Access, etc) with web interfaces and offers fast substructure, similarity, exact and superstructure search engine using 2D hashed fingerprints. Structures are stored in database tables. Structural and non-structural data can be combined. DSF, SMILES, etc. can be imported and exported. JChem Base also supports ChemAxon's Chemical Terms language to enable complex chemical queries and rules. The system includes Marvin, a Java based editor and viewer.'
- Marvin and Calculator Plugin Demo:** A screenshot of the Marvin editor interface with a text box describing it as 'an advanced, Java based chemical editor for drawing chemical structures, queries and reactions'. It lists features like 'Rich editing' (wide range of file types supported, copy and paste between editors, etc.) and '3D editing'.
- Technical Support Forum:** A screenshot of the forum interface with a table of support topics.

Support	Topics	Posts	Last Post
Structure editing, viewing and file formats	827	4081	16 Feb 01, 2008 1:08 pm
Support for MarvinSketch, MarvinView and MarvinCenter			Deleted
MarvinSpace	60	306	16 Feb 01, 2008 11:16 pm
Environment discussion area for OpenGL 3D rendering main/mml viewer			Deleted
Structure based prediction and Chemical Terms	351	174	16 Feb 01, 2008 10:02 am
Support for Calculator Plugin operation through Oracle, API, Marvin, Instant JChem and Chemical Terms			Deleted
Structure search and chemical database	426	1982	16 Feb 01, 2008 10:43 am
Support for JChem Base and JChem Cartridge			Deleted
Instant JChem			Deleted
Discussion area for Instant JChem (Structure database GUI, both Calculator Plugin processor etc)	173	416	16 Feb 01, 2008 9:18 pm
Structure conversion/translation / standardization	76	245	16 Feb 01, 2008 9:10 pm
Library enumeration, virtual synthesis and metabolite generation	116	517	16 Feb 01, 2008 9:12 am
Support for Reactor and Fragmenter			Deleted
Virtual screening, clustering and molecular descriptors	308	471	16 Feb 01, 2008 1:00 am
Support for Solver and Shaper			Deleted
License Issues	4	1	16 Feb 01, 2008 10:12 am
Support for the technical questions related to license handling			Deleted

Find out more about .NET integration

- **Product descriptions & links**

www.chemaxon.com/NET_support_land.html

- **Forum**

www.chemaxon.com/forum/forum7.html

- **Presentations and posters**

www.chemaxon.com/conf

- **Download**

www.chemaxon.com/jchem/download.html

The collage includes several screenshots:

- ChemAxon Homepage:** Features sections for 'Recent News' (e.g., 'INFOCOM releases ChemAxon's JChem nodes on KXNDE'), 'Upcoming Meetings' (e.g., 'Seminars series: Bridging the corporate and desktop'), and 'Recent Publications' (e.g., 'Customer generation, pKa based dominance conditions').
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- Marvin and Calculator Plugin Demo:** A screenshot of the Marvin editor interface with a text box stating: 'Marvin is an advanced, Java based chemical editor for drawing chemical structures, queries and reactions. It has a rich (and growing) list of editing features, is chemically aware and is able to call ChemAxon's structure based calculation plugins for structure on the canvas.' It lists features like 'Rich editing' and 'Wide range of file types supported'.
- Technical Support Forum:** A screenshot of the forum interface with a search bar and a table of support topics.

Support Topic	Topics	Posts	Last Post
Structure editing, viewing and file formats	827	4081	Fri Feb 05, 2009 1:00 pm
Support for MarvinSketch, MarvinView and PdfConverter	40	306	Thu Jan 31, 2009 5:16 pm
MarvinSpace	60	306	Thu Jan 31, 2009 5:16 pm
Development discussion area for Open3D, 3D rendering macros/email molecule viewer	351	374	Fri Feb 03, 2009 10:02 am
Structure based prediction and Chemical Terms	251	374	Fri Feb 03, 2009 10:02 am
Support for Calculator Plugins operation through Oracle, API, Marvin, Instant JChem and Chemical Terms	426	3982	Fri Feb 03, 2009 10:43 am
Structure search and chemical database	426	3982	Fri Feb 03, 2009 10:43 am
Support for JChem Base and JChem Cartridge	426	3982	Fri Feb 03, 2009 10:43 am
Instant JChem	426	3982	Fri Feb 03, 2009 10:43 am
Discussion area for Instant JChem (Structure database GUI, both Calculator Plugin processor etc)	179	496	Fri Feb 03, 2009 9:10 pm
Structure conversion algorithm / standardization	76	245	Fri Feb 03, 2009 9:10 pm
Library enumeration, virtual synthesis and metabolite generation	116	577	Fri Feb 03, 2009 9:10 pm
Support for Reactor and Fragmenter	116	577	Fri Feb 03, 2009 9:10 pm
Virtual screening, clustering and molecular descriptors	108	471	Fri Feb 03, 2009 10:02 am
Support for Solver and Shaper	108	471	Fri Feb 03, 2009 10:02 am
License Issues	4	7	Fri Feb 03, 2009 10:02 am
Support for the technical questions related to license handling	4	7	Fri Feb 03, 2009 10:02 am

Find out more about JChem Web Services

- **Product descriptions & links**

www.chemaxon.com/product/jc_webservices.html

- **Forum**

www.chemaxon.com/forum/forum93.html

- **Presentations and posters**

www.chemaxon.com/conf

- **Download**

www.chemaxon.com/webservices/download.html

The collage consists of four screenshots from the ChemAxon website:

- Top-left:** 'Recent News' section. Articles include: 'INFOCOM releases ChemAxon's JChem nodes on KNIME workflow, source: zeroc.com', 'New commercial evaluation', and 'Whitepaper: Customer generation'.
- Top-right:** 'Upcoming Meetings' section. Meetings include: 'Seminar series: Bridging the corporate and desktop discovery information environment', 'Scientific Pipeline Pilot User Group Meeting', and 'Customer generation, pKa based dominance conditions for generating dominant toolmakers'.
- Bottom-left:** 'Harvin and Calculator Plugin Demo' section. Features include: 'Rich editing: wide range of file types supported, copy and paste between different editors, pre-loaded structure templates and "My Templates", 3D editing'.
- Bottom-right:** 'Technical Support Forum' section. A table of recent posts is shown:

Topic	Posts	Last Post
Structure editing, viewing and file formats	827	4018
Support for MarvinSketch, MarvinView and MarvinCenter	40	306
MarvinSpace	60	306
Development discussion area for Open3D, 3D rendering, main3d/molecule viewer	351	374
Structure based prediction and Chemical Terms	151	174
Support for Calculator Plugin operation through cracks, API, Marvin, Instant JChem and Chemical Terms	426	392
Structure search and chemical database	426	392
Support for JChem Base and JChem Cartridge	173	416
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Discussion area for Instant JChem (Structure database GUI, batch Calculator Plugin processor etc)	173	416
Structure conversion/alignment / standardization	76	245
Support for Standardizer	116	177
Library enumeration, virtual synthesis and metabolite generation	116	177
Support for Reactor and Fragmenter	116	177
Virtual screening, clustering and molecular descriptors	116	177
Support for Solver and Shaper	116	177
License Issues	4	1
Support for the technical questions related to license handling	4	1