

# Interfacing the JChem Suite outside of Java

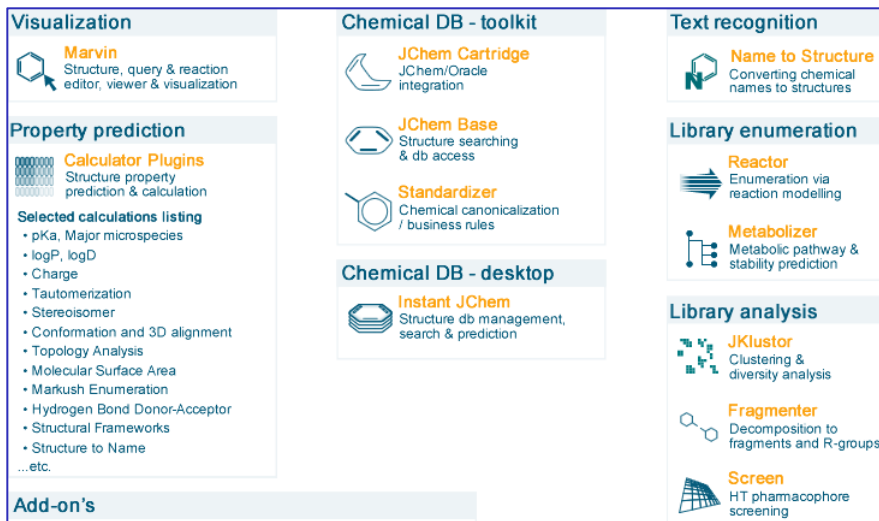
**Jonathan Lee**



**ChemAxon**  
*Solutions for Cheminformatics*

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

# Interfaces to JChem Suite of Tools



## 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

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## Language Strength

- 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

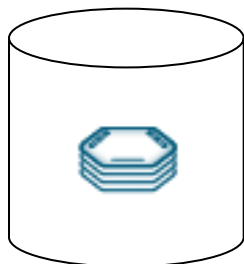
- Do you use a Service Oriented Architecture?

# JChem Cartridge

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

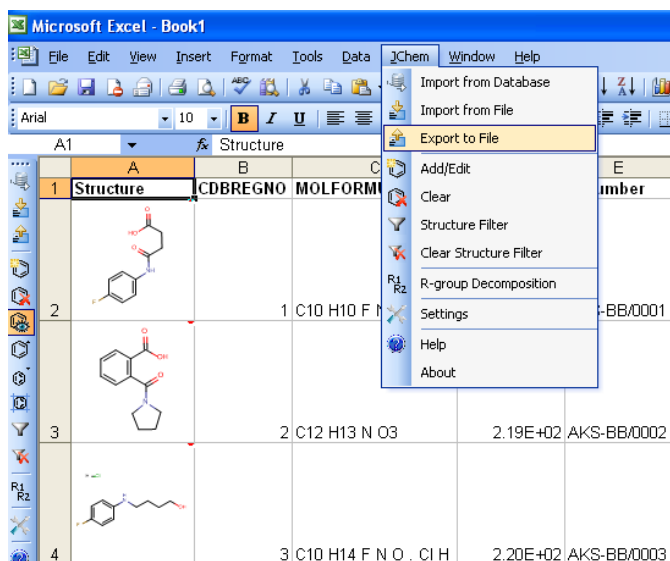
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## **Supports**

- SQL
- Most JChem Modules (Searching, Standardizer, Reactor, Chemical Terms, Calculator Plugins, ...)

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



## Supports

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

# JChem Web Services

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



## Supports

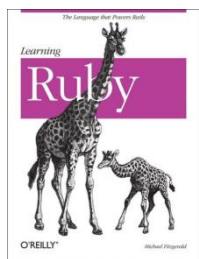
- Web Languages: AJAX/JavaScript, Perl, Python, Ruby, PHP, ...
- App languages: Java, C#, ...
- Growing list of JChem Modules (Searching, Standardization, Chemical Terms, Molecule Conversion...)

# 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>
```



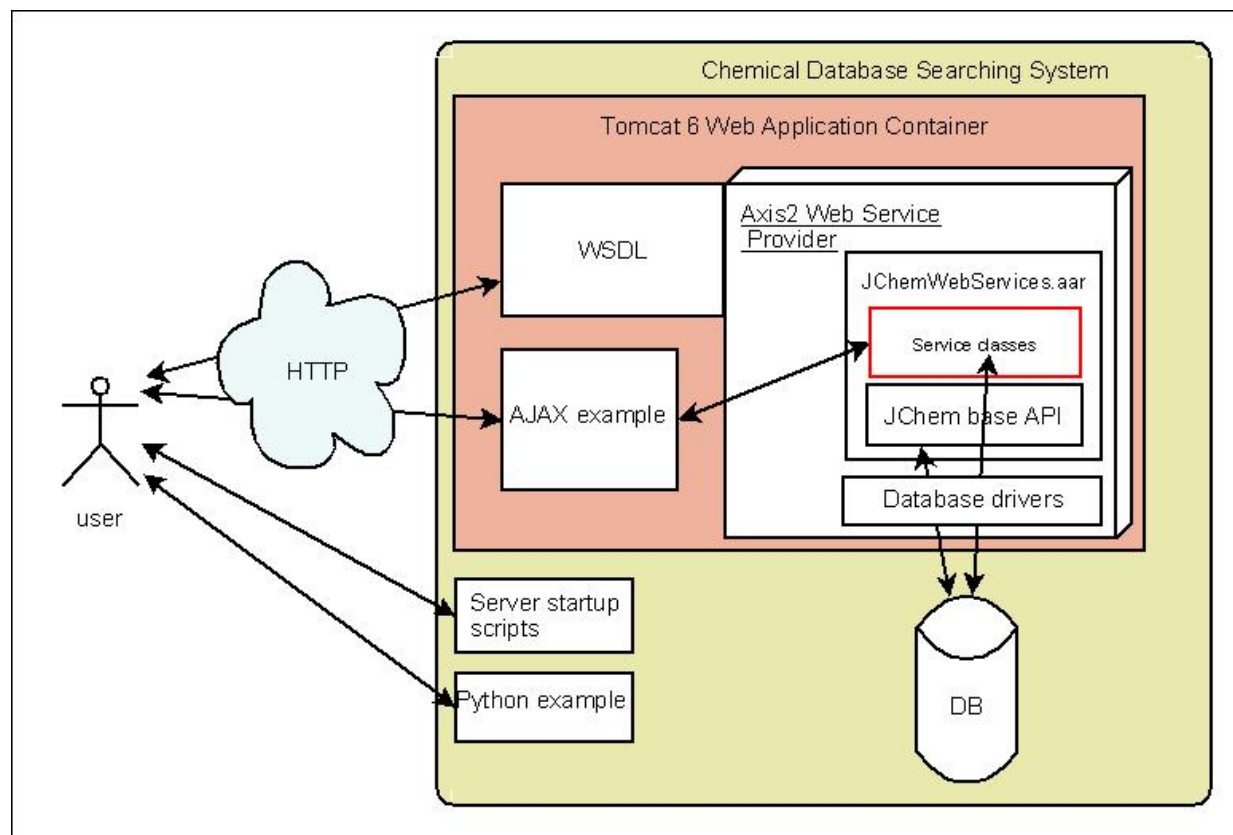
JChem Web Services



# 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


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- Database Related Services
  - JChem Search Service
  - Relational Table Service
  - Data Manipulation Service
  - Connection Service
- Molecular Conversion Service
- Standardization Service
- Chemical Terms Evaluation Service
- Reactor Service
- Future Services (SQL Execution, Molecule Search, Markush/R Group Decomposition, DB Table Management, Expanded Batch Processing)



# AJAX Demo of JChem Web Services

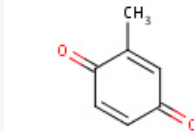
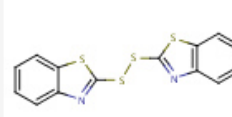
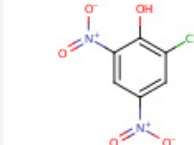
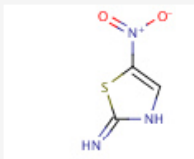
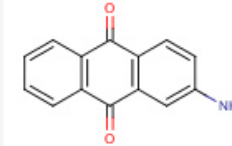
JChemSearch Web Service - [www.chemaxon.com/ajax](http://www.chemaxon.com/ajax)

  
ChemAxon

Navigation

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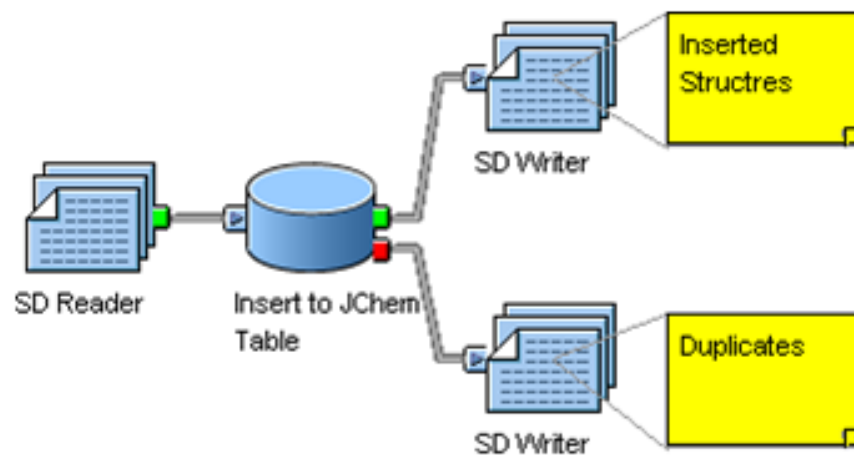
Hit alignment Results: 250251 Select table nci

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

# Workflow Integrations

**ChemAxon components exist for several workflow software vendors**

- Pipeline Pilot
- KNIME (by Infocom)
- Inforsense (IDBS)



# Find out more about JChem Cartridge

- **Product descriptions & links**

[www.chemaxon.com/products/jchem-cartridge/](http://www.chemaxon.com/products/jchem-cartridge/)

- **Forum**

[www.chemaxon.com/forum/forum7.html](http://www.chemaxon.com/forum/forum7.html)

- **Presentations and posters**

[www.chemaxon.com/conf/JChemCartridge.ppt](http://www.chemaxon.com/conf/JChemCartridge.ppt)

- **Download**

[www.chemaxon.com/download/jchem/](http://www.chemaxon.com/download/jchem/)

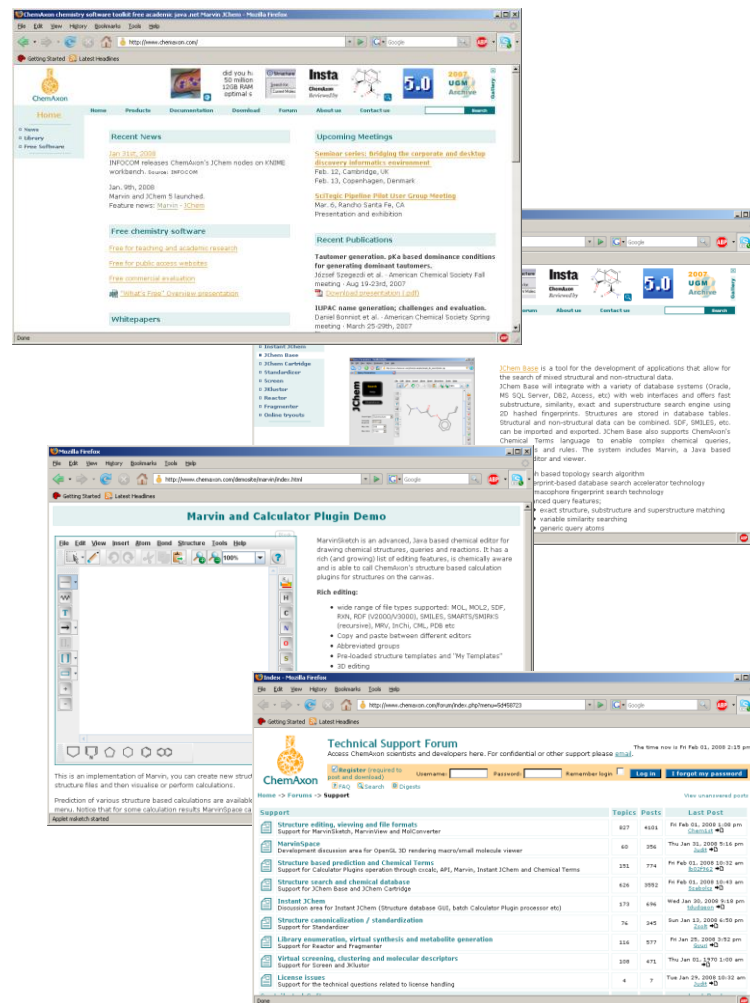
The collage includes several screenshots from the ChemAxon website and forums:

- Recent News:** A screenshot of the 'Recent News' section on the ChemAxon website, dated Feb 13, 2007. It lists several news items, including 'INFOCAMP releases ChemAxon's JChem nodes on KXNDE workbench', 'Maven and JChem 5 launched', and 'Free chemistry software'.
- Harvin and Calculator Plugin Demo:** A screenshot of a demo page for 'Harvin and Calculator Plugin'. It describes Harvin as an advanced, Java-based chemical editor for drawing chemical structures, queries, and reactions. It lists features such as 'Rich editing' (wide range of file types supported, copy and paste between editors, etc.) and '3D editing'.
- Technical Support Forum:** A screenshot of the 'Technical Support Forum' on the ChemAxon website. It includes a table of support topics with columns for 'Support', 'Topics', 'Posts', and 'Last Post'.

Support	Topics	Posts	Last Post
Structure editing, viewing and file formats Support for MarvinSketch, MarvinView and MarvinCenter	827	4081	Feb 03, 2007 9:00 am Global
MarvinSpace Development discussion area for Open3D, 3D rendering, macros/email molecule viewer	60	306	Thu Jan 31, 2007 9:16 pm Global
Structure based prediction and Chemical Terms Support for Calculator Plugin operation through Oracle, API, Marvin, Instant JChem and Chemical Terms	351	174	Fri Feb 02, 2007 10:02 am Global
Structure search and chemical database Support for JChem Base and JChem Cartridge	426	1082	Fri Feb 02, 2007 10:43 am Global
Instant JChem Discussion area for Instant JChem (Structure database GUI), both Calculator Plugin processor etc)	173	416	Wed Jan 30, 2007 9:18 pm Global
Structure canonicalization / standardization Support for Standardizer	76	245	Sun Jan 28, 2007 9:30 pm Global
Library enumeration, virtual synthesis and metabolite generation Support for Reactor and Fragmenter	116	517	Fri Jan 26, 2007 9:52 am Global
Virtual screening, clustering and molecular descriptors Support for Screen and Shaper	308	471	Thu Jan 25, 2007 1:00 am Global
License Issues Support for the technical questions related to license handling	4	7	Thu Jan 25, 2007 10:32 am Global

# Find out more about .NET integration

- **Product descriptions & links**  
[www.chemaxon.com/dotNET/index.html](http://www.chemaxon.com/dotNET/index.html)
- **Forum**  
[www.chemaxon.com/forum/forum85.html](http://www.chemaxon.com/forum/forum85.html)
- **Presentations and posters**  
[www.chemaxon.com/conf](http://www.chemaxon.com/conf)
- **Download**  
[www.chemaxon.com/download/jchem/](http://www.chemaxon.com/download/jchem/)



# Find out more about JChem Web Services

- **Product descriptions & links**

[www.chemaxon.com/products/jchem-web-services/](http://www.chemaxon.com/products/jchem-web-services/)

- **Forum**

[www.chemaxon.com/forum/forum93.html](http://www.chemaxon.com/forum/forum93.html)

- **Presentations and posters**

[www.chemaxon.com/conf](http://www.chemaxon.com/conf)

- **Download**

[www.chemaxon.com/download/jchem-web-services/](http://www.chemaxon.com/download/jchem-web-services/)

The collage consists of four screenshots from the ChemAxon website:

- Top-left:** Home page with sections for 'Recent News', 'Upcoming Meetings', and 'Recent Publications'.
- Top-right:** JChem Base product page, describing it as a tool for the development of applications that allow for the search of mixed structural and non-structural data.
- Bottom-left:** Marvin and Calculator Plugin Demo page, highlighting features like 'Rich editing' and 'Wide range of file types supported'.
- Bottom-right:** Technical Support Forum page, showing a list of support topics and a table of recent posts.