

09 15-16^S
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Meetingium
32°47.367' -117°15.159'

Welcome to San Diego!!



Alex Drijver, CEO

Product Map

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



Markush Search

Store & search Markush structures



JChem WebServices

Web services integration interface

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




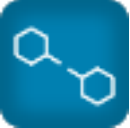




HT pharmacophore screening

The Art of Componentry



- Cheminformatics specialized
- Toolkit / components provider
- Customer decides based on needs, strategies, politics
- Ease or replacement / upgrade

JChem development history

2000	2001	2002	2003	2004
<p>Oracle, MySQL, SQLServer, Access, hashed fingerprints, substructure and similarity</p> 	<p>Clustering, diversity</p> 	<p>DB2, PostgreSQL, Rgroup searching</p>	<p>Reaction searching, fragmentation, reaction processing, standardization, pharmacophores, screening</p>  	<p>Cartridge, enhanced stereo searching, recursive SMARTS, Chemical Terms, virtual synthesis</p>  
2005	2006	2007	2008	2009
<p>R-decomposition, R-enumeration, reaction library, custom fingerprints, random synthesis, link nodes...</p>	<p>Tautomer search, Instant JChem reaction similarity, Library MCS, GUI for Standardizer/Reactor ...</p>  	<p>Calculated columns, Installer, Tautomer Duplicate filtering, Query tables, Markush tables, Speed enhancements for JChem Cartridge, form design, relational data for Instant JChem ...</p>	<p>Position variation queries, Instant JChem: - Federated search, - Cartridge support...</p>	<p>JChem for Excel JChem Web Services, AJAX Polymer search Data Sgroup search Faster SSS Metabolizer</p>

Key Development Issues

- Following development needs of the clients
 - Medium term pains not flavour of the month
- Platform independence
 - Ease of integration
- Common core
- Adapting the core
 - .Net, web services, sharepoint
- History

Languages

- Java – chosen in '98. Portability, web technology, multi-tier.
- IJC and JC4XL demand more direct support of MS technologies -- .Net API, OLE, Sharepoint.
- Web Services API enables use of our technology in from all relevant languages.
- Maintaining and improving the core remain our priority and direction.

Product Strategies

- Focusing on toolkit
- End user apps that are complementing platform/toolkit
- Niche areas of expertise - Markush
- Partnering for applications (ELN, LIMS, Screening)
- New technologies and deliveries – SaaS, hosted services, Sharepoint

Surf's Up!!



Find out more

- **Product descriptions & links**
www.chemaxon.com/products.html
- **Forum**
www.chemaxon.com/forum
- **Presentations and posters**
www.chemaxon.com/conf
- **Download**
www.chemaxon.com/download.html

The collage consists of four screenshots from the ChemAxon website:

- Top Screenshot:** The main website homepage with navigation tabs (Home, Products, Documentation, Download, Forum, About us, Contact us) and sections for 'Recent News', 'Upcoming Meetings', and 'Recent Publications'.
- Middle-Left Screenshot:** A page titled 'Harvin and Calculator Plugin Demo' featuring a chemical structure editor interface and a list of features such as 'Rich editing', 'Wide range of file types supported', and 'Pre-loaded structure templates'.
- Middle-Right Screenshot:** A page for 'JChem Base' describing it as a tool for the development of applications that allow for the search of mixed structural and non-structural data.
- Bottom Screenshot:** The 'Technical Support Forum' page, which includes a search bar, a list of support topics, and a table of recent posts.

Support	Topics	Posts	Last Post
Structure editing, viewing and file formats	827	4081	Fri Feb 05, 2009 1:00 pm Closed
Support for MarvinSketch, MarvinView and MarvinCenter	60	306	Thu Jan 31, 2009 9:16 pm Closed
MarvinSpace	60	306	Thu Jan 31, 2009 9:16 pm Closed
Development discussion area for OpenEye, 3D rendering, Marvin and/or molecule viewer	351	174	Fri Feb 03, 2009 10:02 am Closed
Structure based prediction and Chemical Terms	151	74	Fri Feb 03, 2009 10:02 am Closed
Support for Calculator Plugins operation through cracks, API, Marvin, Instant JChem and Chemical Terms	426	1952	Fri Feb 03, 2009 10:02 am Closed
Structure search and chemical database	426	1952	Fri Feb 03, 2009 10:02 am Closed
Support for JChem Base and JChem Cartridge	426	1952	Fri Feb 03, 2009 10:02 am Closed
Instant JChem	179	416	Wed Jan 29, 2009 9:10 pm Closed
Discussion area for Instant JChem (Structure database GUI, both Calculator Plugin processor etc)	179	416	Wed Jan 29, 2009 9:10 pm Closed
Structure conversion algorithm / standardization	74	345	Wed Jan 29, 2009 9:10 pm Closed
Support for Standardizer	74	345	Wed Jan 29, 2009 9:10 pm Closed
Library enumeration, virtual synthesis and metabolite generation	116	517	Thu Jan 29, 2009 9:10 am Closed
Support for Reactor and Fragmenter	116	517	Thu Jan 29, 2009 9:10 am Closed
Virtual screening, clustering and molecular descriptors	108	471	Thu Jan 29, 2009 1:00 am Closed
Support for Solver and Shaper	108	471	Thu Jan 29, 2009 1:00 am Closed
License Issues	4	7	Tue Jan 29, 2009 10:02 am Closed
Support for the technical questions related to license handling	4	7	Tue Jan 29, 2009 10:02 am Closed