

# 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<sup>®</sup>

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




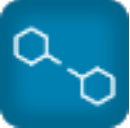




# The Art of Componentry

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- 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

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- 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

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- 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

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- 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](http://www.chemaxon.com/products.html)
- **Forum**  
[www.chemaxon.com/forum](http://www.chemaxon.com/forum)
- **Presentations and posters**  
[www.chemaxon.com/conf](http://www.chemaxon.com/conf)
- **Download**  
[www.chemaxon.com/download.html](http://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 "Marvin and Calculator Plugin Demo" featuring a rich editing interface and a list of supported file types (MOL, MOL2, SDF, etc.).
- Middle-Right Screenshot:** A screenshot of the JChem Base tool interface, showing a chemical structure and associated data.
- Bottom Screenshot:** A screenshot of the "Technical Support Forum" showing a list of support topics with columns for Topic, Posts, and Last Post.

Topic	Posts	Last Post
Structure editing, viewing and file formats	827	4/18
Support for MarvinSketch, MarvinView and MarvinCenter	40	4/18
MarvinSpace	40	3/26
Development discussion area for OpenBabel, 3D rendering, Marvin and small molecule viewer	351	3/14
Structure based prediction and Chemical Terms	251	3/14
Support for Calculator Plugins operation through Oracle, JPL, Marvin, Instant JChem and Chemical Terms	426	3/14
Structure search and chemical database	426	3/14
Support for JChem Base and JChem Cartridge	179	3/14
Instant JChem	179	3/14
Discussion area for Instant JChem (Structure database GUI, both Calculator Plugin processor etc)	74	3/14
Structure conversion algorithm / standardization	164	3/14
Support for ChEMBLviewer	164	3/14
Library management, virtual synthesis and metabolite generation	108	3/14
Support for Reactor and Fragmenter	108	3/14
Virtual screening, clustering and molecular descriptors	4	3/14
Support for Inven and Shifter	4	3/14
License Issues	4	3/14
Support for the technical questions related to license handling	4	3/14