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Welcome to San Diego!!

Alex Drijver, CEO

ChemAxon

Solutions for Cheminformatics

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.

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

Add-on's

Markush Search
Store & search Markush structures

JChem WebServices
Web services integration interface

Visualization

Name to Structure
Converting chemical names to structures

Enumeration

Reactor
Enumeration via reaction modelling

Metabolizer
Metabolic pathway & stability prediction

Library analysis

JKlustor
Clustering & diversity analysis

Fragmenter
Decomposition to fragments and R-groups

Screen
HT pharmacophore screening

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The Art of Componentry

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

JChem development history

2000

Oracle, MySQL, SQLServer, Access, hashed **fingerprints**, **substructure** and **similarity**

2001

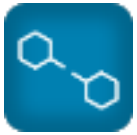
Clustering, diversity

2002

DB2, PostgreSQL, **Rgroup** searching

2003

Reaction searching, fragmentation, **reaction processing**, standardization, **pharmacophores**, **screening**



2004

Cartridge, enhanced stereo searching, **recursive SMARTS**, **Chemical Terms**, **virtual synthesis**

2005

R-decomposition, **R-enumeration**, **reaction library**, custom fingerprints, random synthesis, link nodes…

2006

Tautomer search, **Instant JChem** reaction similarity, **Library MCS**, GUI for Standardizer/ Reactor …

2007

Calculated columns, Installer, Tautomer Duplicate filtering, Query tables, **Markush tables**, Speed enhancements for JChem **Cartridge**, form design, relational data for **Instant JChem** ...

2008

Position variation queries, **Instant JChem**:
- Federated search,
- **Cartridge support**...

2009

JChem for Excel
JChem Web Services, AJAX
Polymer search
Data Sgroup search
Faster SSS
Metabolizer

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Key Development Issues

- Following development needs of the clients
  - Medium term paln 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

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Surf's Up!!

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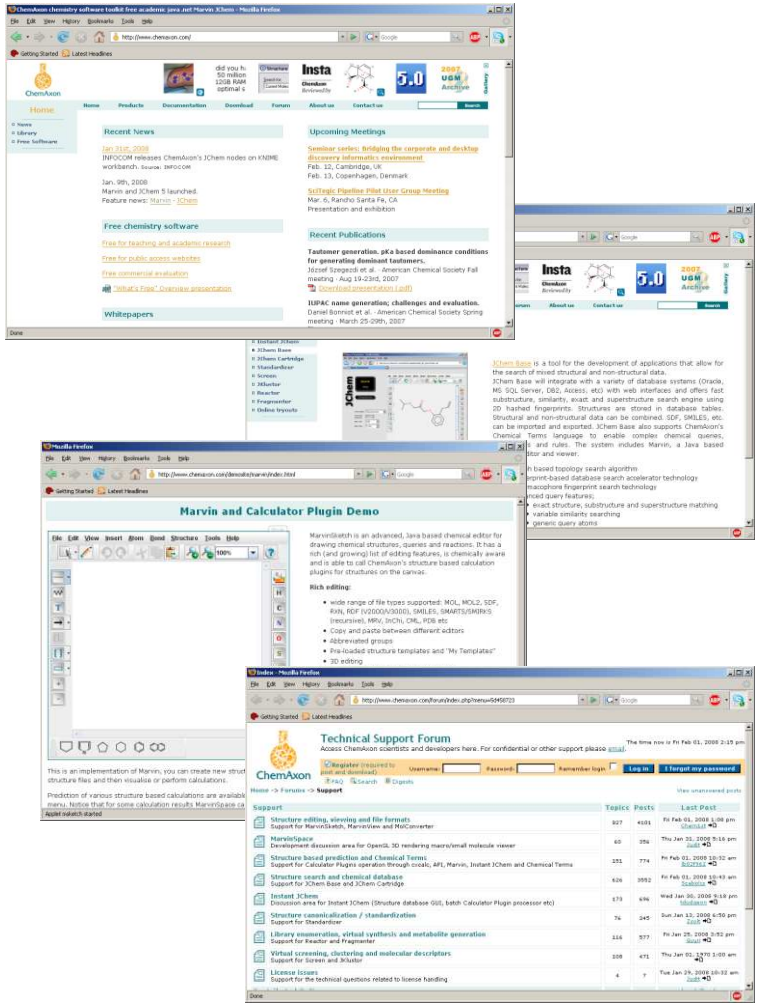

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