



ChemAxon

Solutions for Cheminformatics

Partnering ChemAxon



”Discovery consists of seeing what everybody else has seen and thinking what nobody else has thought.”

Albert Szent-Györgyi (1893-1986)

What do I expect from in Silico Drug Discovery Solutions?

- decrease research costs
- enable better experiment design
- provide better access to data
- increase collaboration across groups
- reduce duplication and redundancy in experiments
- Leverage work already done
- Increase operating efficiency

What can I expect from a single vendor system?

- *Theory:*

Reduces cost, simplifies interface, only one piece of code

- *Reality:*

- *Price changes, long customization*
- *Revolver selling/ packaging*
- *Functionality /Best of breed*
- *Migration trap*





35 Integrator Partners

- Analysis and reporting
- Biological Data Management
- ELN
- Scientific Publishing
- Data Mining
- Workflow/pipeline tools
- Online Education
- SAR
- Laboratory Information Management
- Analytical chemistry
- Chemical inventory
- Chemical registration
- Sample management
- Patent search
- Toxicity and metabolites prediction

Can ChemAxon satisfy all my cheminformatics needs?

- *NO - not ChemAxon alone*
- *YES – having many options and the freedom of choice*

Applications integrating ChemAxon

	Target Identification	Hit Generation	Lead Generation	Lead Optimization
Knowledge database and management				
ELN				
Scientific Publishing				
Data Mining/ Analysis/ Visulisation				
Workflow/pipeline tools				
LIMS				
Chemical inventory				
Chemical registration				
Sample management				
SAR analysis				
Toxicity and metabolites prediction, ADMET				

Use cases

- Celgene/ using SEURAT and DeltaSoft Registration
- Abbott / using SEURAT and Pipeline Pilot
- Evotec/ using Contur ELN and KNIME

Consultants



**INFORMATICS
MATTERS**

Informatics solutions for drug discovery



**JOHN McNEIL
& Company, Inc.**



PHASTEC

What's hot

- .NET implementations
- JChem Web services programming interface
- JChem for Sharepoint

Find out more

- **ChemAxon's Partners**
www.chemaxon.com/partner.html
- **Product descriptions & links**
www.chemaxon.com/products.html
- **Forum**
www.chemaxon.com/forum
- **Presentations and posters**
www.chemaxon.com/conf
- **Download**
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The collage consists of four screenshots:

- Top-left:** ChemAxon homepage. Sections include: Recent News (e.g., INFOCOM releases ChemAxon's JChem nodes on KXNDE workbench), Upcoming Meetings (e.g., Seminar series: Bridging the corporate and desktop), and Recent Publications (e.g., Topomer generation, pKa based dominance conditions).
- Top-right:** Insta software interface. Features a '5.0' version badge and a '2007 UGM' award badge. Text: 'Insta is 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. Text: 'MarvinBatch 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 structures on the canvas.' Lists rich editing features like file types, copy/paste, and 3D editing.
- Bottom-right:** Technical Support Forum. Includes a search bar and a table of support topics and posts.

Support Topic	Topics	Posts	Last Post
Structure editing, viewing and file formats	827	4081	Fri Feb 01, 2008 9:00 am
Support for MarvinBatch, MarvinView and ProConverter	40	306	Fri Feb 01, 2008 9:16 pm
MarvinSpace	60	374	Fri Feb 01, 2008 10:02 am
Development discussion area for Open3D, 3D rendering, macros/email molecule viewer	351	374	Fri Feb 01, 2008 10:02 am
Structure based prediction and Chemical Terms	125	174	Fri Feb 01, 2008 10:02 am
Support for Calculator Plugins operation through cracks, API, Marvin, Instant JChem and Chemical Terms	426	1082	Fri Feb 01, 2008 10:02 am
Structure search and chemical database	426	1082	Fri Feb 01, 2008 10:02 am
Support for JChem Base and JChem Cartridge	173	416	Fri Feb 01, 2008 9:10 am
Instant JChem	76	245	Fri Feb 01, 2008 9:10 am
Discussion area for Instant JChem (Structure database GUI, batch Calculator Plugin processor etc)	116	517	Fri Feb 01, 2008 9:10 am
Structure conversion/translation / standardization	116	517	Fri Feb 01, 2008 9:10 am
Library enumeration, virtual synthesis and metabolite generation	116	517	Fri Feb 01, 2008 9:10 am
Support for Reactor and Fragmenter	116	517	Fri Feb 01, 2008 9:10 am
Virtual screening, clustering and molecular descriptors	116	517	Fri Feb 01, 2008 9:10 am
Support for Solver and Shutter	116	517	Fri Feb 01, 2008 9:10 am
License Issues	4	7	Fri Feb 01, 2008 10:02 am
Support for the technical questions related to license handling	4	7	Fri Feb 01, 2008 10:02 am

