



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 from the ChemAxon website:

- Top-left:** Home page with sections for 'Recent News', 'Free chemistry software', and 'Upcoming Meetings'.
- Top-right:** Insta software page with a '5.0' version indicator and a '2007 UGM' award badge.
- Bottom-left:** Marvin and Calculator Plugin Demo page, featuring a chemical structure editor interface and a list of supported file formats.
- Bottom-right:** 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 01, 2008 9:00 am Closed
Support for MarvinSketch, MarvinView and ProConnecter			
MarvinSpace	60	306	Thu Jan 31, 2008 9:16 pm Closed
Development discussion area for Open3D, 3D rendering, macros/email molecule viewer			
Structure based prediction and Chemical Terms	351	174	Fri Feb 01, 2008 10:02 am Closed
Support for Calculator Plugins operation through cracks, API, Marvin, Instant XChem and Chemical Terms			
Structure search and chemical database	426	1982	Fri Feb 01, 2008 10:43 am Closed
Support for XChem Base and XChem Cartridge			
Instant XChem			
Discussion area for Instant XChem (Structure database GUI, both Calculator Plugin processor etc)	179	496	Wed Jan 30, 2008 9:10 pm Closed
Structure conversion/translation / standardization	76	245	Fri Jan 31, 2008 9:52 am Closed
Library enumeration, virtual synthesis and metabolite generation	116	517	Fri Jan 31, 2008 9:52 am Closed
Support for Reactor and Fragmenter			
Virtual screening, clustering and molecular descriptors	308	471	Thu Jan 31, 2008 1:00 am Closed
Support for Solver and Shutter			
License Issues	4	1	Thu Jan 24, 2008 10:12 am Closed
Support for the technical questions related to license handling			