

JChem for SharePoint

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ChemAxon
Solutions for Cheminformatics

Introduction

- JChem for SharePoint:
 - What it is
 - Features
- Architecture Changes introduced in 1.0
- Roadmap

JChem for SharePoint

- Product name covering all ChemAxon components related to Microsoft SharePoint
 - Including JChem for SharePoint Search
- Composed of smaller building blocks
 - SharePoint allows certain extension points for these
 - Web Parts
 - Custom List Fields
 - ...
- Infrastructure to include chemistry in SharePoint
 - Open to 3rd party components, and integrations

Past Features – US UGM 2010

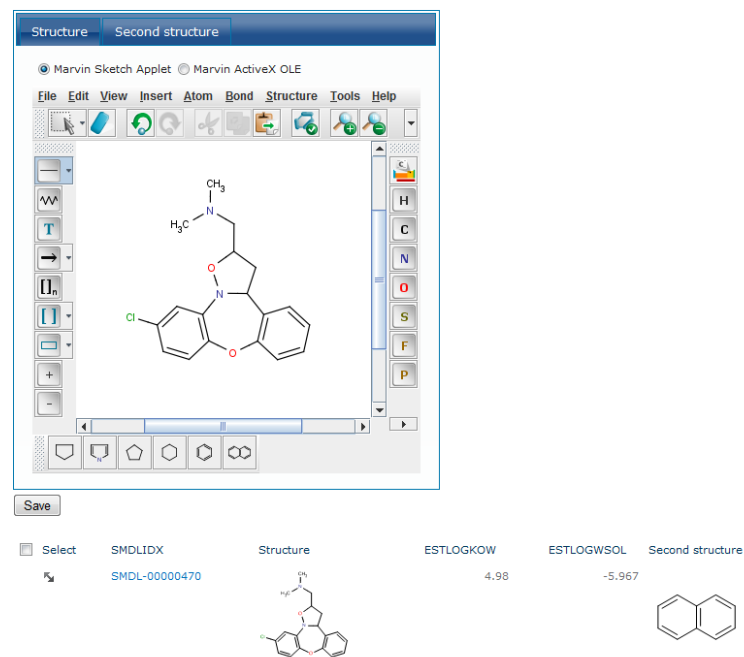
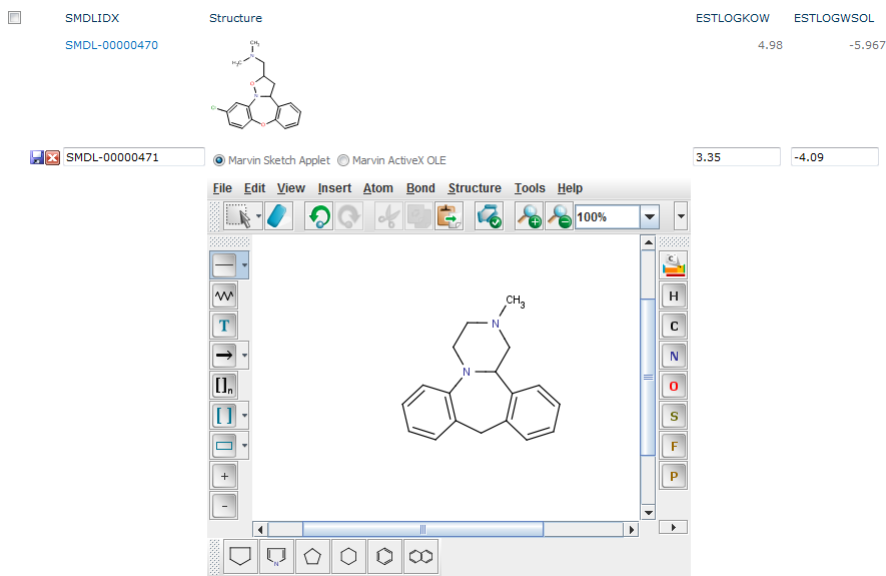
- ChemAxon Structure Field
- ChemAxon Calculated Field (Chemical Terms Field)
- Blog, Discussion Board, Wiki integration
- Structure Filter Web Part

What is new?

- SharePoint 2010 integration
 - Will stop further develop SharePoint 2007 integration
 - Full Firefox and Google Chrome support
- ChemAxon Structure Field
 - Inline editing, 3rd party editor support
- ChemAxon Linked Structure Field
- ChemAxon Calculated Field – External Web Services
- ChemAxon Calculated Structure Field
- Import – Export Web Parts
- Visualization (Charting) Samples with Microsoft Chart and Visifire
- Service Application based architecture
- ...

Structure Editing – Inline – 3rd party

- Inline (SharePoint 2010): edit in-place without dialog
- Connected web part – structures are displayed in a connected editor
- 3rd party editor: ChemDraw



External List Support

- Usual requirement: I want to import 1 million structures there, fast...
 - Standard Lists are not the best place to put those
 - They are designed to be flexible, therefore less performant
- Solution: External Lists
- Could be attached to existing databases
- Present: Sample for editing structures in a SQL Server table.
 - Requires some programming for the schema mapping
- Roadmap:
 - External Data Column – get structures for corporate IDs from a database
 - Flexible, user configurable schema mapping with custom fields
 - Database schema modification
 - Import – export
 - Oracle support
 - Structure indexed search

ChemAxon Linked Structure Field

- Structures are stored in a different field
- SMILES, IUPAC Name, any other format
- No need for content migration, simply add a new field

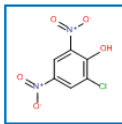
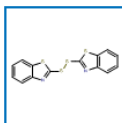
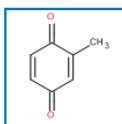
The screenshot shows a window titled "Test Linked Structure Field - Water". The interface includes an "Edit" menu with options like Save, Cancel, Paste, Copy, Delete Item, Attach File, and Spelling. Below the menu, there are three fields: "Title" containing "Naphthalene", "Structure Text" containing the SMILES string "C1=CC2=C(C=C1)C=CC=C2", and "ChemAxon Linked Structure" which is set to "Marvin Sketch Applet". A toolbar with various drawing tools is visible, and a skeletal structure of naphthalene is displayed in the center.

The diagram illustrates the linked structure field concept. It shows three columns: "Title" with the entry "Propane NEW", "Structure Text" with the SMILES string "CCC", and "ChemAxon Linked Structure" with a skeletal structure of propane (H₃C-CH₂-CH₃). Below these columns is a button labeled "Add new item".

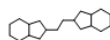
ChemAxon Calculated Fields

- External Web Service Support
- Calculated Image Field - Web Part
- Calculated Structure Field: Creates and stores a new (calculated) structure based on an existing structure
 - Chemical Terms expressions resulting in structure

Structure



BMF



Demonstration

- Editing a structure in external lists
- Inline edit a linked structure field
 - Linked structure changes
 - Calculated value changes
 - Calculated structure changes
- Calculated Image Web Part

Import - Export

- Import – Export SDF and other chemical file formats to/from lists, JChem for Excel workbooks
- Custom Parsers (skips structure parsing) - ~1000% performance gain
- Append, template support and column matching
- Asynchronous upload of files with a progress bar

The screenshot displays the 'Create' application interface. On the left, a sidebar shows navigation options like 'Browse From: Installed Items', 'Filter By: All Types', and 'All Categories'. The main area shows a grid of icons for various list types, with 'Import Chemical File' highlighted. A 'Chemical File Import' dialog box is open, showing options for 'Structure Column' and 'Columns'. The 'Columns' section has a table with checked boxes for various chemical data fields.

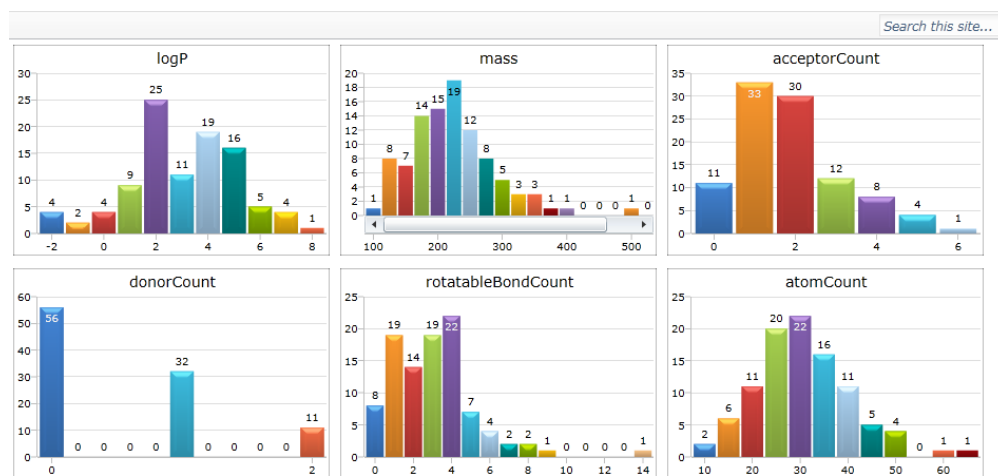
Import	Column Name
<input checked="" type="checkbox"/>	CDBREGNO
<input checked="" type="checkbox"/>	MOLFORMULA
<input checked="" type="checkbox"/>	MOLWEIGHT
<input checked="" type="checkbox"/>	IDNumber
<input checked="" type="checkbox"/>	UPDATE_DATE
<input checked="" type="checkbox"/>	SUPPLIER
<input checked="" type="checkbox"/>	AVAILABILITY
<input checked="" type="checkbox"/>	BUILDINGBLOCK
<input checked="" type="checkbox"/>	COMMENT
<input checked="" type="checkbox"/>	CANONICAL_SMILES
<input type="checkbox"/>	DUPLICATE_ID

Demonstration

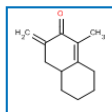
- Import an SDFFile
 - Add atom count column
 - Change a structure
- Export to an SDFFile
- Import Jchem for Excel Workbook
- Export to Jchem for Excel Workbook

Visualization

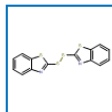
- Samples for
 - Visifire – Silverlight
 - Microsoft Charts



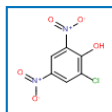
Structure



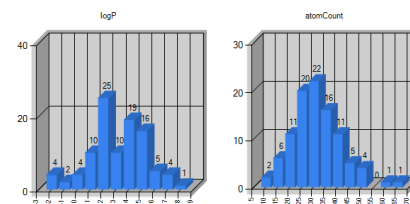
3.28866768833333 1-methyl-3-methylidene-2,3,4,4a,5,6,7,8-octahydronaphthalen-2-one



6.22269685933333 2-(1,3-benzothiazol-2-yl)disulfanyl)-1,3-benzothiazole



2.15369354933333 2-chloro-4,6-dinitrophenol



Structure



1.41966430066667 2-methylcyclohexa-2,5-diene-1,4-dione



6.22269685933333 2-(1,3-benzothiazol-2-yl)disulfanyl)-1,3-benzothiazole



2.15369354933333 2-chloro-4,6-dinitrophenol

How does it fit in corporate SharePoint?

- Scalability – how many users, structures?
- Overload of SharePoint infrastructure with chemistry
- Load Balancing, SharePoint Farms
- Response Time
- Foreign solutions, dlls on SharePoint servers?
- ...

Service Application based architecture 1.0

- Scalable
 - New servers could be added easily
- Offload chemistry to dedicated servers
 - Foreign code could only affect those
- SharePoint Farm Integration, Load Balancing
 - Shared State stored in database
- Asynchronous, batch based processing – 1.3

Planned Roadmap - 2011

- 1.2 October – Major Features
 - External Data Columns
 - External Lists Oracle
 - Web Service Samples
- 1.3 November
 - BPOS-D Feasibility
 - Background, queue based, distributed processing service for calculations
 - Markush Search and enumeration
 - Other enumerations: Conformers, tautomers.

Planned Roadmap - 2012

- Structure Filter
 - Additional fields, AND/OR hierarchies,
 - External Lists
- Structure Checker
 - Lists, collaboration features
- R-Group Decomposition, Reactor, Standardizer, NMR Prediction
- Custom Forms: SharePoint Designer, InfoPath, Silverlight, JavaScript
- Excel Web Access Integration

Team

- Calin Naghi



- Catalin Boldan



Get involved

- Demo server: <http://sharepoint.chemaxon.com/>
 - Anonymous: changes are lost, limited functionality
 - Forum user: Single site, full functionality
 - Active Directory: Separate company site or web application, can try collaborative features
- Deployable web parts