

JChem for SharePoint

Tamas Pelcz



ChemAxon
Solutions for Cheminformatics

Introduction

- What is JChem for SharePoint: Covers all ChemAxon components not related to Microsoft SharePoint Search
- Past – New Features
- Architecture Changes for 1.0

JChem for SharePoint

- Covers all ChemAxon components not related to Microsoft SharePoint Search
- SharePoint allows certain extension points:
 - Web Parts
 - Custom List Fields
 - ...
- Some of these components building block could be used separately

Past Features

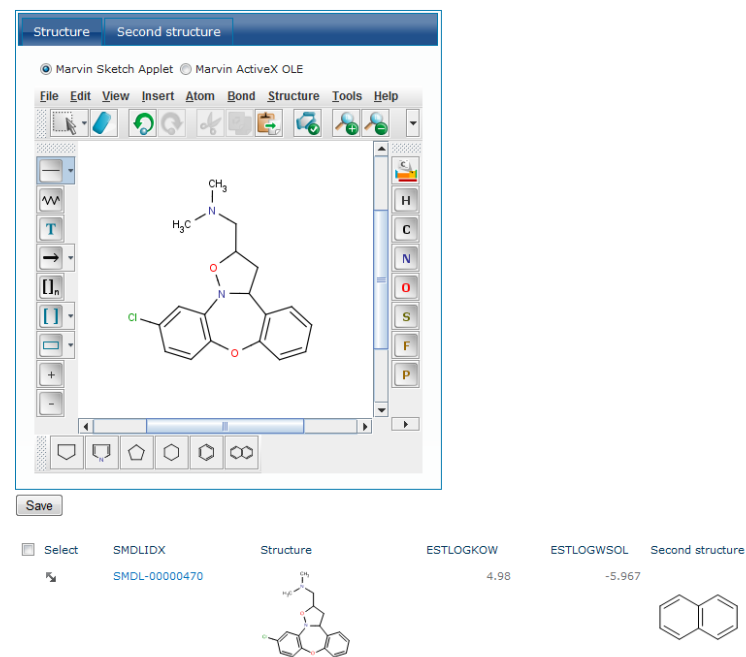
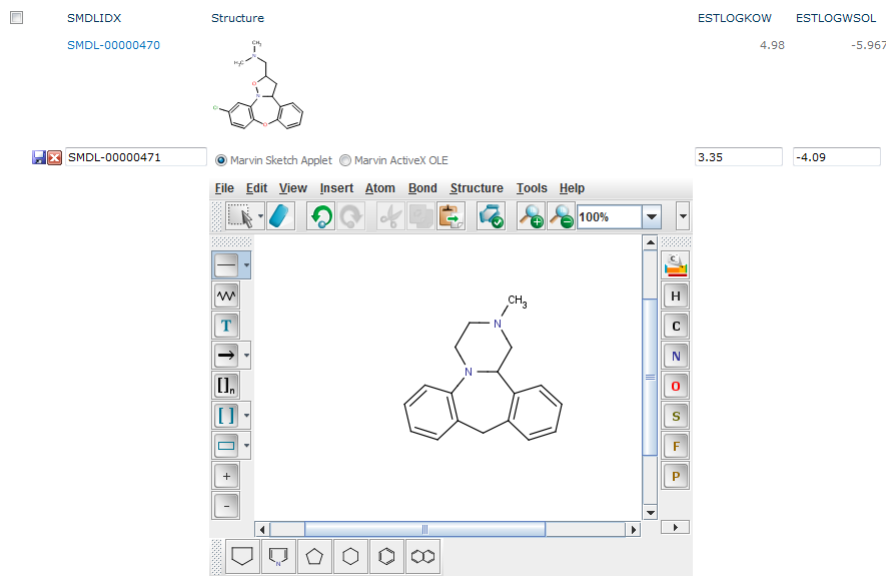
- ChemAxon Structure Field
- ChemAxon Calculated Field (Chemical Terms Field)
- Blog, Discussion Board, Wiki integration
- Structure Filter Web Part

What is new?

- SharePoint 2010 integration
 - Will stop further develop SharePoint 2007 integration
 - Full Firefox and Google Chrome support
- ChemAxon Structure Field
 - Inline editing
- ChemAxon Linked Structure Field
- ChemAxon Calculated Structure Field
- Import – Export Web Parts
- Visualization (Charting) Samples with Microsoft Chart and Visifire
- WCF Web Services

Structure Editing – Inline – connected web part, OLE

- Inline (SharePoint 2010): edit in-place without dialog
- Connected web part – structures are displayed in a connected Marvin Sketch
- OLE: Edit structures with a desktop editor



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

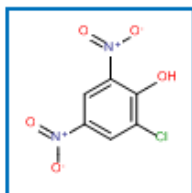
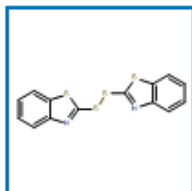
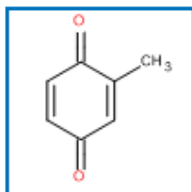
The screenshot shows a window titled "Test Linked Structure Field - Water". The interface includes an "Edit" menu with options like Save, Cancel, Paste, Copy, Delete Item, Attach File, and Spelling. Below the menu, there are three fields: "Title" containing "Naphthalene", "Structure Text" containing 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 icons 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 "Propane" (marked as 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".

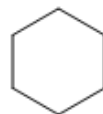
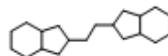
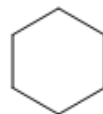
ChemAxon Calculated Structure Field

- Creates and stores a new (calculated) structure based on an existing structure
 - Chemical Terms expressions resulting in structure

Structure



BMF



Demonstration

- Inline edit a linked structure field
 - Linked structure changes
 - Calculated value changes
 - Calculated structure changes

Import - Export

- Import – Export SDF and other chemical file formats to/from lists
- Import – Export Simple JChem for Excel workbooks
- Asynchronous upload of files with a progress bar

The screenshot displays the 'Create' dialog box in a software application. The 'Import Chemical File' option is highlighted. A secondary dialog box, 'Chemical File Import', is open, showing the 'Structure Column' and 'Columns' sections. The 'Columns' section lists various chemical data fields with checkboxes for selection.

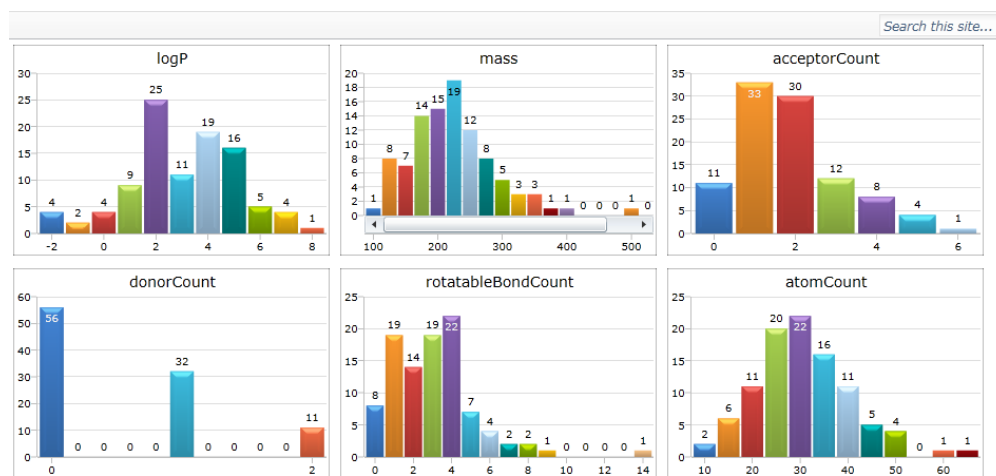
Import	Column Name
<input checked="" type="checkbox"/>	CDBREGNO
<input checked="" type="checkbox"/>	MOLFORMULA
<input checked="" type="checkbox"/>	MOLWEIGHT
<input checked="" type="checkbox"/>	IDNumber
<input checked="" type="checkbox"/>	UPDATE_DATE
<input checked="" type="checkbox"/>	SUPPLIER
<input 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

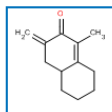
- Import an SDFFile
 - Add atom count column
 - Change a structure
- Export to an SDFFile
- Import Jchem for Excel Workbook
- Export to Jchem for Excel Workbook

Visualization

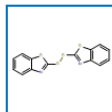
- Samples for
 - Visifire – Silverlight
 - Microsoft Charts



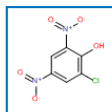
Structure



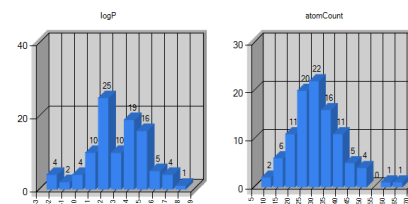
3.28866768833333 1-methyl-3-methylidene-2,3,4,4a,5,6,7,8-octahydronaphthalen-2-one



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

Problems

- Scalability – how many users, structures?
- Overload of SharePoint infrastructure with chemistry
- Load Balancing, SharePoint Farms
- Response Time
- Can this crash a SharePoint server?
- ...
- The solution is...

JChem for SharePoint 1.0

- New WCF and Service Application based architecture
 - Image generation, calculations, filtering, import and export
- Asynchronous, batch based processing
 - Real and fake progress display
- Processor intensive calculations could be externalized and distributed between servers
- Shared state in SQL server, ASP.NET state service

JChem for SharePoint 1.0

- Structure Image generation
- Calculated Field and Calculated Structure Field
 - Calculations will run in background
- Structure Filter
 - Filtering will run in background, Item IDs returned
- Import-Export
 - File passed to background service
 - File generated by background service

Plans – Feature Enhancements

- 3rd party editor support
 - Desktop (ActiveX), web (Applet, JS)
- Ribbon Integration
- Structure Filter:
 - Filter standard fields, AND/OR, load-save queries

Plans – Chemistry

- Database Search
 - JChem Base, JChem Cartridge
 - Markush
- Structure Checker – List, Collaboration
- Standardizer

Team

- Calin Naghi



- Catalin Boldan



- Ionut Lupsan



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