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

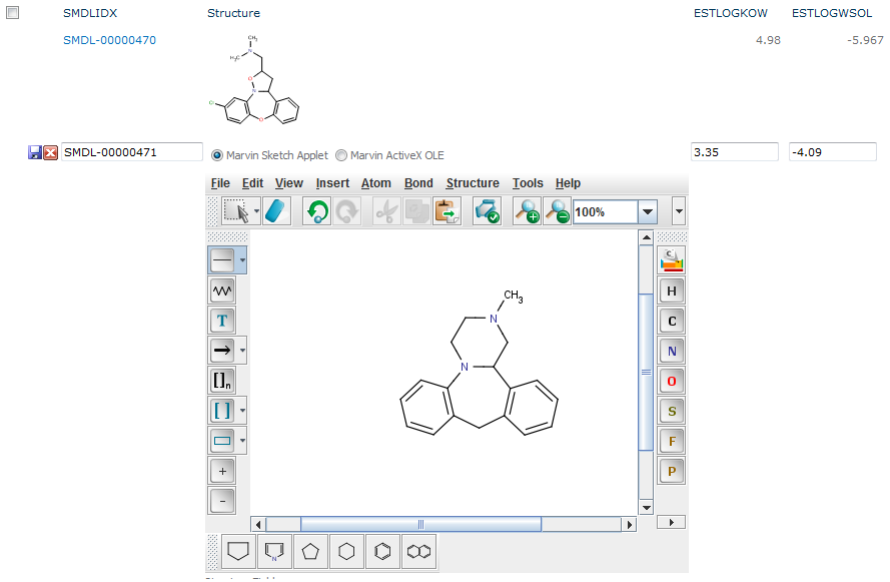
- ChemAxon Structure Field
- ChemAxon Calculated Field (Chemical Terms Field)
- Blog, Discussion Board, Wiki integration
- Structure Filter Web Part

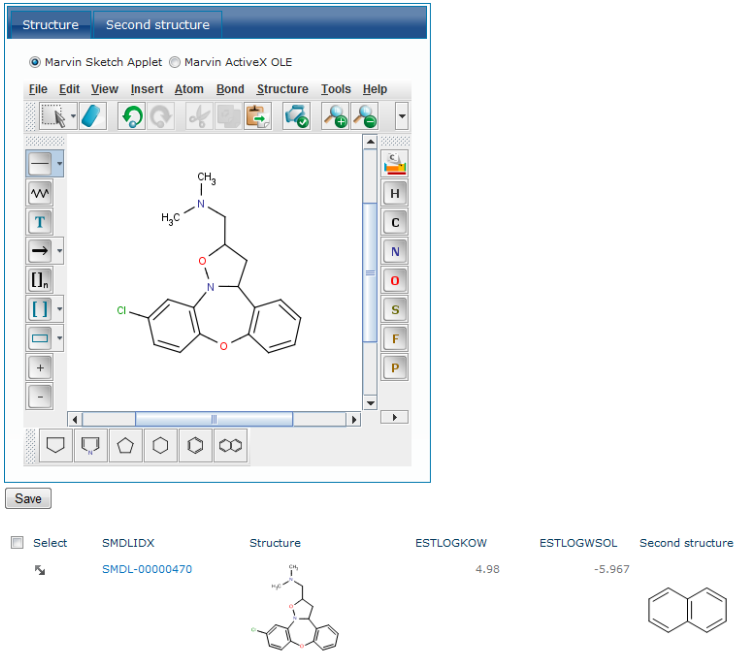
What is new?

- 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



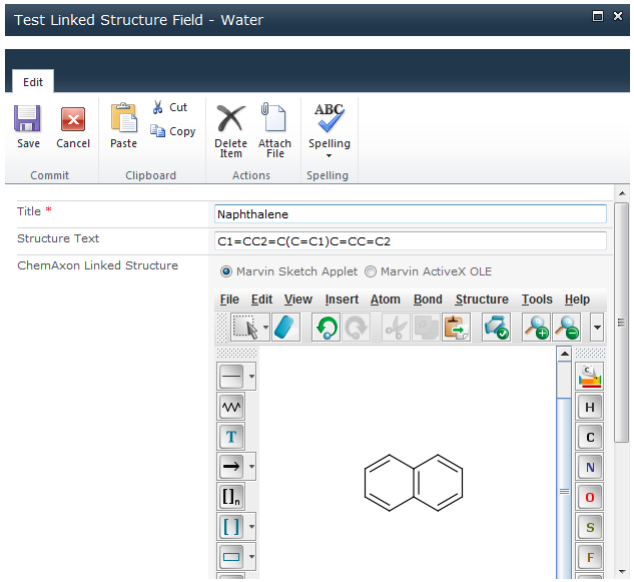


External List Support

- 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

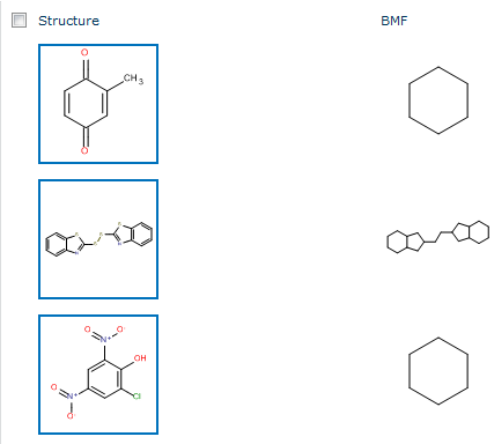
ChemAxon Linked Structure Field

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



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 exisitng structure
  - Chemical Terms expressions resulting in structure

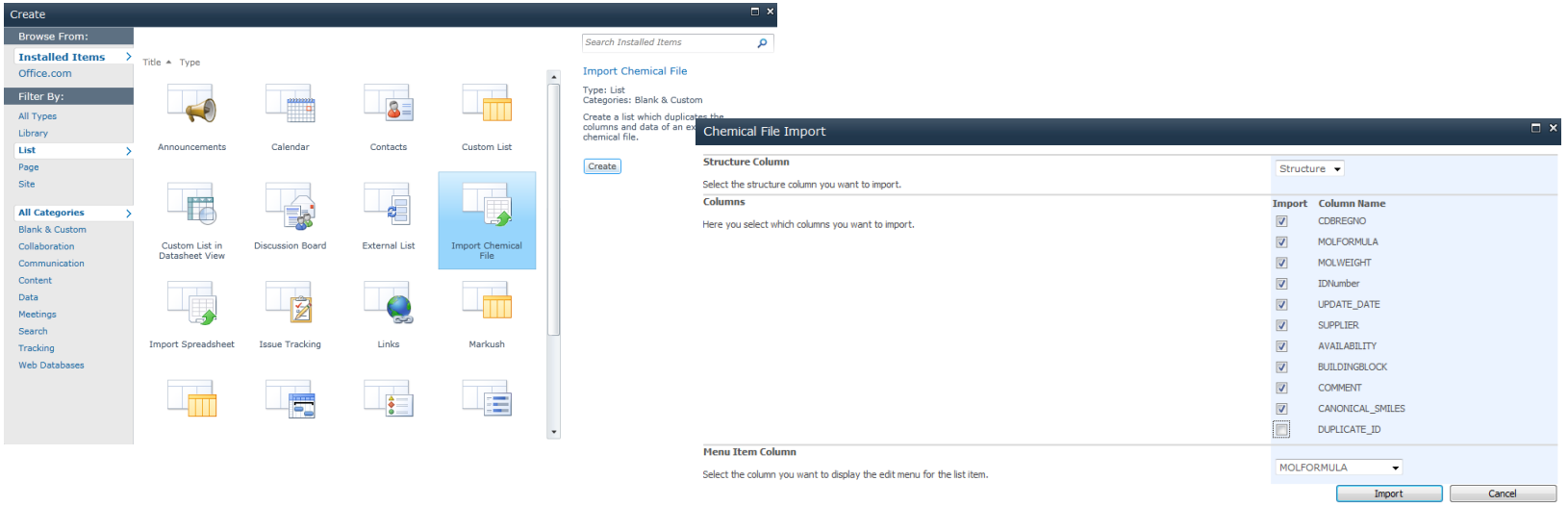


Demonstration

- 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

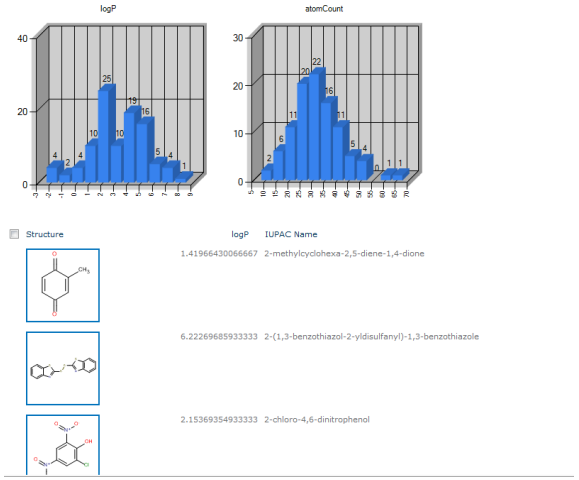


Demonstration

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

Visualization

- Samples for
  - Visifire – Silverlight
  - Microsoft Charts



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