ChemAxon SharePoint Technologies

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ChemAxon

Solutions for Cheminformatics

Introduction

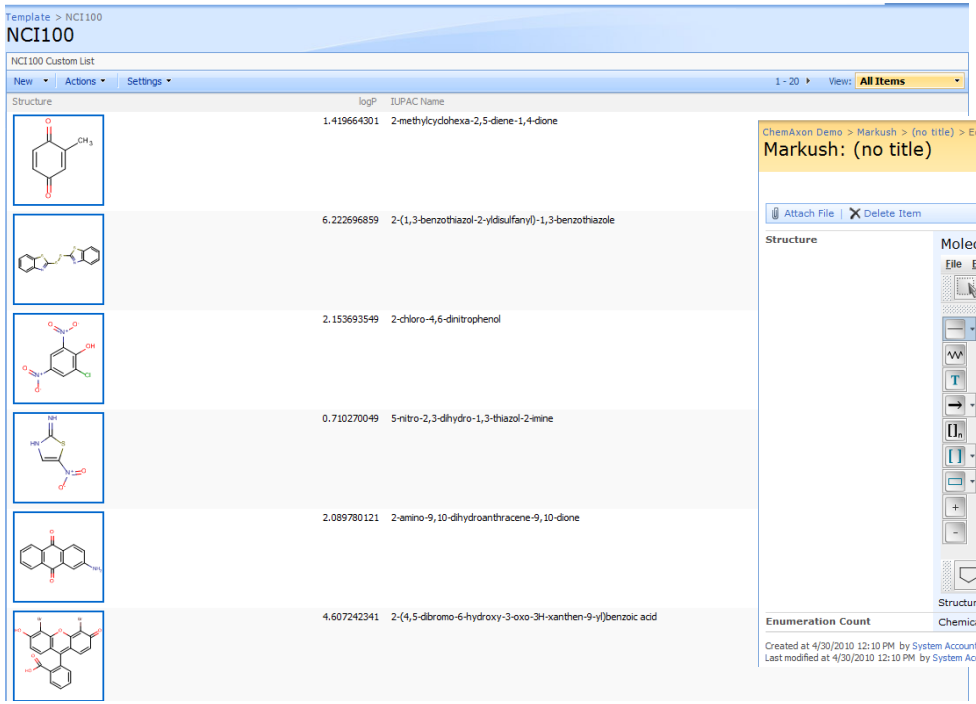
- Integrate Marvin and JChem functionality in SharePoint
  - .NET based API, Marvin Applet
- Use SharePoint's powerful features:
  - Lists, Collaboration Features, Custom ASP.NET based Web Parts, Search, Web Services, Workflow
- Access and manage all research related data from a single place
- JChem for SharePoint : General SharePoint integration
- JChem Search for SharePoint : Indexing and searching structures enterprise wide

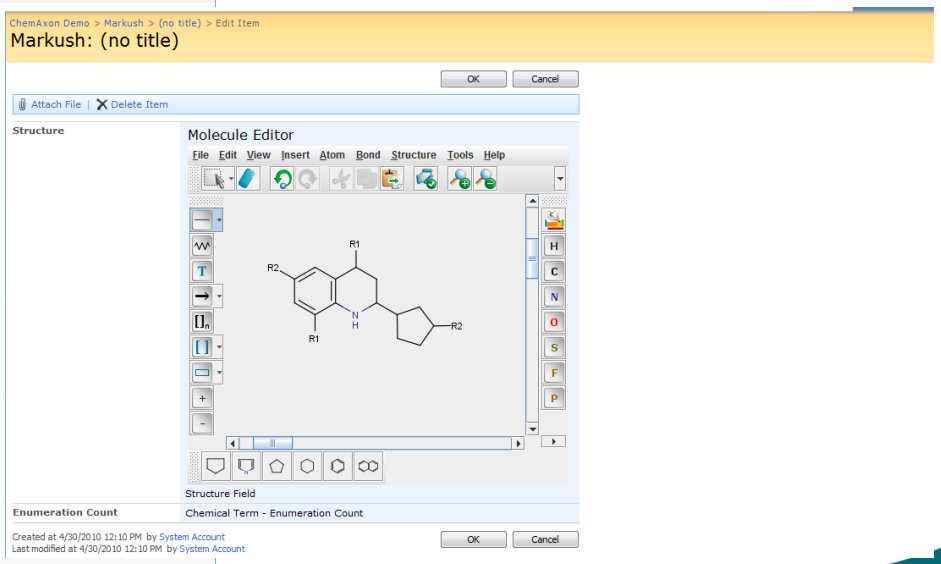
Features

- Handle and filter structures in SharePoint Lists
- Calculate structure based predictions in lists
- Handle structures in Blogs, Wiki, and Discussion Board
- Import, Export and modify lists using a desktop tool

ChemAxon Structure Field

- Render structures
  - Render multiple formats stored (MOL, SMILES, MRV,…)
  - Specify display settings, and image size
- Edit structures
  - Add, edit structure by drawing them in Marvin Sketch Applet





ChemAxon Chemical Terms Field

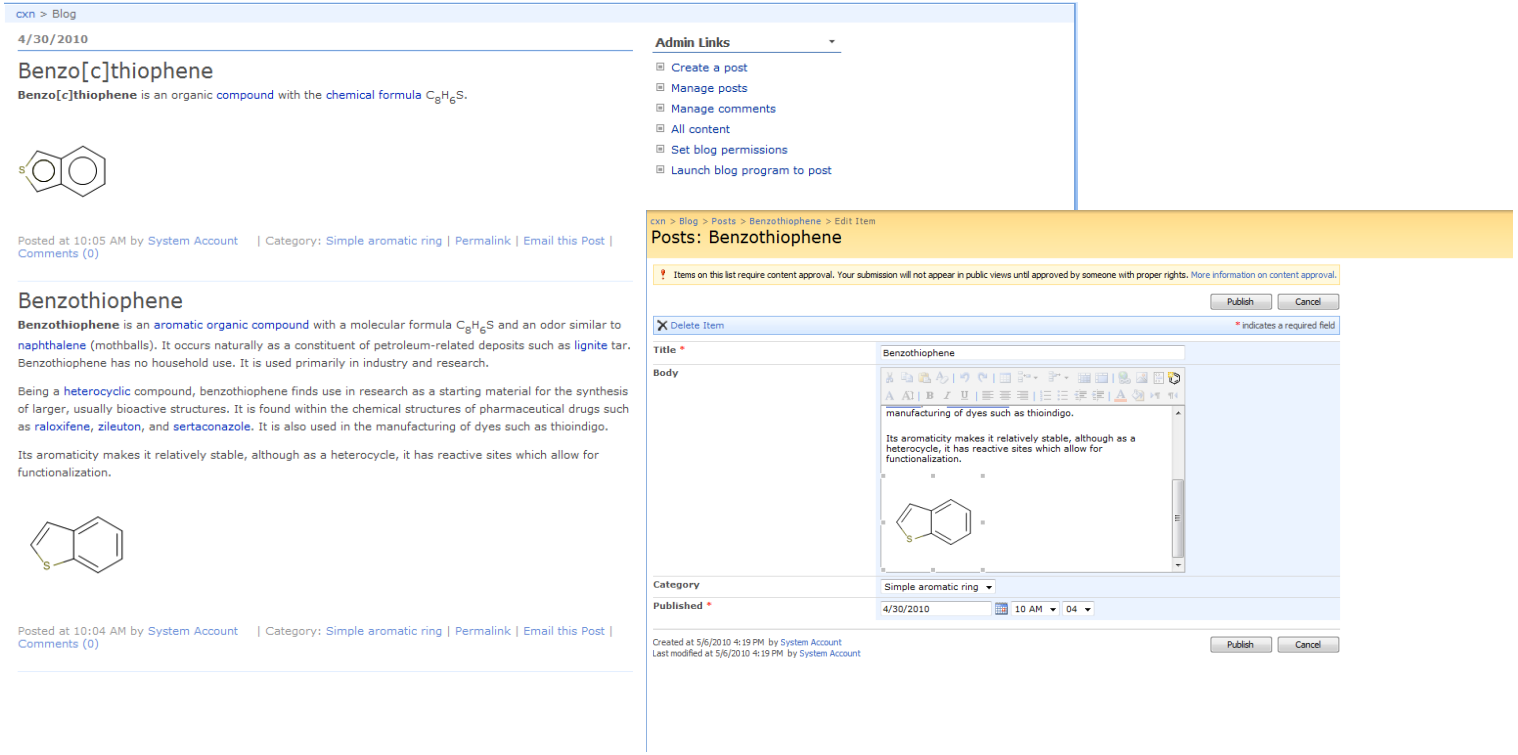
- Calculate structural property predictions using Chemical Terms
- Most Chemical Terms functions
  - Composition,Mass, MolFormula…
  - AtomCount,BondCount,ChiralCenterCount,RingCount…
  - log*P*,log*D*, pK_a, PSA, H-bond donor/acceptors
  - Bioavailability, GhoseFilter,LeadLikeness,Lipinski rule of 5…
  - SubstructureMatch, Dissimilarity
  - IUPAC Name
- Sortable, filterable
  - Dynamically changing its type
- Calculated result change on:
  - Structure edit
  - Expression change

Demonstration

- Create List with Structure Field
  - Create Chemical Terms Fields
  - Edit Structures
  - See changes in versioning
  - Delete, recycle deleted item

Collaboration Features

- Blogs, Wiki, Discussion Board
- Add, edit structures with Marvin Sketch Applet
- Resize structure images

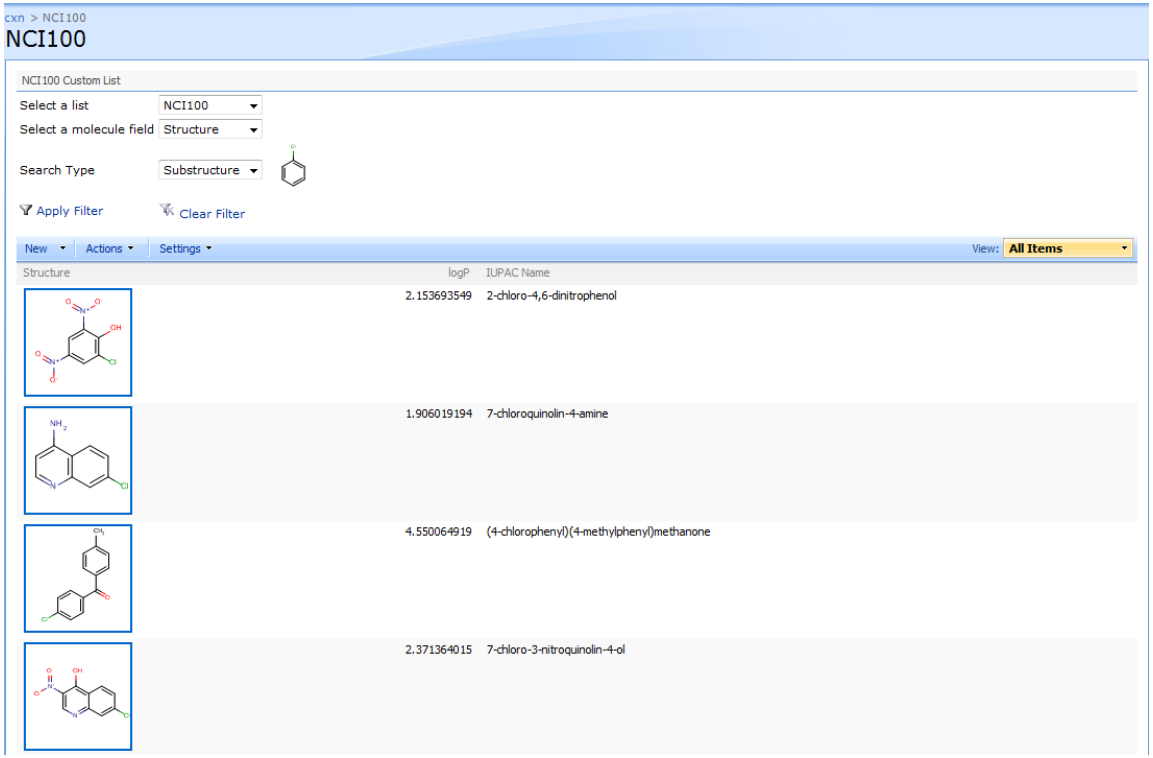


Demonstration

- Show examples for Blog, Discussion Board and Wiki
- Create new Discussion Board

ChemAxon Structure Filter Web Part

- Filter by structure search
  - Supports all JChem query features
- Works for: Lists
- Dynamically select lists and columns to filter



Demonstration

- Filter NCI100 List Structures
- Markush Search using Filter

Import – Export (coming soon)

- Popular file formats:
  - Flat: SDF, MRV, SMILES, IUPAC Names
- Import
  - Create new lists
  - Append to existing lists
- Export

Desktop Editor for SharePoint Content

- Using SharePoint Web Services
- Based on the not yet released ChemAxon .NET components
- Batch Import-Export
- Faster editing and data input

JChem Search for SharePoint - Index

- Crawl and index structures
- Where: SharePoint sites, file system, internal and external websites, databases, e-mail system
- What
  - Structure files: MOL, SDF, CDX, SKC….
  - Extracted from: IUPAC Name, SMILES, InChi
  - Configurable words and synonyms:
    - Brand names: Aspirin, Viagra
    - Corporate ID: PHARMA-00000211
  - Custom
    - OLE Objects
    - JChem for excel workbooks
    - Images
- Security aware

JChem Search for SharePoint - Search

- Custom Search Interface
  - Search for structures, keywords and metadata at the same time
  - Full JChem query feature support:
    - Substructure, similarity, calculated structural properties
    - Markush, polymer
- Web Service Interface
- Hit ranking and relevance
  - The mass amount of information indexed can result in high number of hits. Possible solutions:
    - Structure similarity
    - Structural property similarity
    - Source of extraction
      - IUPAC Name in document title – High score
      - IUPAC Name in text body – Low score
    - Other built in options in SharePoint

Planned Features and Enhancements

- Features
  - Database Search Web Part
  - Database Import-Export
  - Chemical tools web parts
    - Standardizer, structure checker, Reactor, Fragmenter
  - Excel integration
  - Custom InfoPath based forms
  - Workflow based solutions (registration system)
- Enhancements
  - Desktop Editor for structure editing
  - Enhanced client side JavaScript, jQuery
  - Custom SharePoint Web Services
  - Image generation, calculation
  - Silverlight
- SharePoint 2010

Get involved

- Demo server: http://sharepoint.chemaxon.com/
- Deployable web parts: ~ Q3 2010
- Contact:
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