

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

Template > NCI100
NCI100

NCI100 Custom List

New Actions Settings 1 - 20 View: All Items

Structure	logP	IUPAC Name
	1.419664301	2-methylcyclohexa-2,5-diene-1,4-dione
	6.222696859	2-(1,3-benzothiazol-2-ylsulfanyl)-1,3-benzothiazole
	2.153693549	2-chloro-4,6-dinitrophenol
	0.710270049	5-nitro-2,3-dihydro-1,3-thiazol-2-imine
	2.089780121	2-amino-9,10-dihydroanthracene-9,10-dione
	4.607242341	2-(4,5-dibromo-6-hydroxy-3-oxo-3H-xanthen-9-yl)benzoic acid

ChemAxon Demo > Markush > (no title) > Edit Item

Markush: (no title)

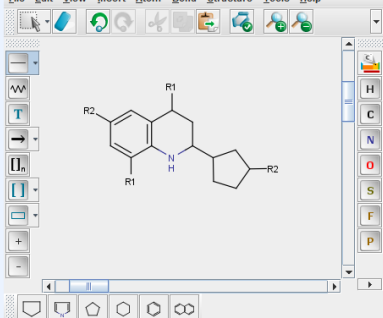
Attach File Delete Item

OK Cancel

Structure

Molecule Editor

File Edit View Insert Atom Bond Structure Tools Help



Structure Field

Enumeration Count

Chemical Term - Enumeration Count

Created at 4/30/2010 12:10 PM by System Account
Last modified at 4/30/2010 12:10 PM by System Account

OK Cancel

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

The screenshot displays a web application interface with two main sections: a blog post view and an edit form.

Blog Post View (Left):

- Header: cxn > Blog
- Date: 4/30/2010
- Title: Benzo[c]thiophene
- Text: Benzo[c]thiophene is an organic compound with the chemical formula C_8H_6S .
- Chemical Structure:
- Metadata: Posted at 10:05 AM by System Account | Category: Simple aromatic ring | Permalink | Email this Post | Comments (0)
- Title: Benzothiophene
- Text: Benzothiophene is an aromatic organic compound with a molecular formula C_8H_6S and an odor similar to naphthalene (mothballs). It occurs naturally as a constituent of petroleum-related deposits such as lignite tar. Benzothiophene has no household use. It is used primarily in industry and research.
- Text: Being a heterocyclic compound, benzothiophene finds use in research as a starting material for the synthesis of larger, usually bioactive structures. It is found within the chemical structures of pharmaceutical drugs such as raloxifene, zileuton, and sertaconazole. It is also used in the manufacturing of dyes such as thioindigo.
- Text: Its aromaticity makes it relatively stable, although as a heterocycle, it has reactive sites which allow for functionalization.
- Chemical Structure:
- Metadata: Posted at 10:04 AM by System Account | Category: Simple aromatic ring | Permalink | Email this Post | Comments (0)

Edit Form (Right):

- Header: cxn > Blog > Posts > Benzothiophene > Edit Item
- Title: Posts: Benzothiophene
- Warning: Items on this list require content approval. Your submission will not appear in public views until approved by someone with proper rights. More information on content approval.
- Buttons: Publish, Cancel
- Section: Delete Item (with a red X icon)
- Text: * indicates a required field
- Form Fields:
 - Title: Benzothiophene
 - Body:

manufacturing of dyes such as thioindigo.

Its aromaticity makes it relatively stable, although as a heterocycle, it has reactive sites which allow for functionalization.
 - Category: Simple aromatic ring
 - Published: 4/30/2010 10 AM 04
- Footer: Created at 5/6/2010 4:19 PM by System Account; Last modified at 5/6/2010 4:19 PM by System Account
- Buttons: Publish, Cancel

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

cxn > NCI100
NCI100

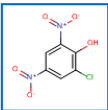
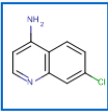
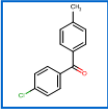
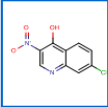
NCI100 Custom List

Select a list: NCI100

Select a molecule field: Structure

Search Type: Substructure 

New Actions Settings View: All Items

Structure	logP	IUPAC Name
	2.153693549	2-chloro-4,6-dinitrophenol
	1.906019194	7-chloroquinolin-4-amine
	4.550064919	(4-chlorophenyl)(4-methylphenyl)methanone
	2.371364015	7-chloro-3-nitroquinolin-4-ol

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:
 - ncalin@chemaxon.com
 - tpelcz@chemaxon.com