





# Compound Registration

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# Outline

-  Warm-up Demo
-  News in 6.1
-  Demo of the major new features
-  Future developments

# Demo, part1: Warm-up

Compound Registration    Registration    Bulkloader    Staging    **Amendment**    Audit    Search    Salt search    Administration    LOCAL    logged in as demouser. version: 6.0.0    Help    Logout

Structure browser    Structure Editing    Perform Quality Checks

CXN43A    Amend    Delete    Undelete    Rename LnbRef    History    Change Restriction Level    Change Molweight

CXN43  
CXN43A  
N7334

Matching structures in the database

Multi-Component Structure

Unique    1. Component Match - CXN45    1 / 1

Cc1ccc2ccccc2c1C(=O)[O-] X%    C1=CC=CC=C1C1=CC=CC=C1 45-55%    Cc1ccc2ccccc2c1C(=O)O CXN44 21-44%    C1=CC=CC=C2C=CC=CC12 CXN42 56-79%

PCN: CXN45  
Match Type: Component Match

Accept

Salts and Solvates


+ Add salt    + Add solvate

Parent Multiplicity 1

Salt components

potassium 1

# News in 6.1: Salt/solvate bulk import

 **Compound Registration**    Registration    Bulkloader    Staging    Amendr

Import salts or solvates    Add salt or solvate    Delete submission    Bulk restrict

## Import salt or solvates

### 1. File selection

Please select a file to upload

[Choose SDF file](#)    No file selected yet

This file contains:

- Salts
- Solvates
- Salts and solvates

[Continue](#)

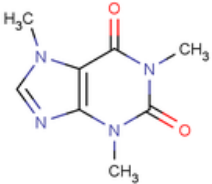
# News in 6.1: Customizable Search page

## SEARCH QUERY

Structure	PCN <span>⌵</span>	LN <span>⌵</span>	Project	MolWeight (Structure) <span>⌵</span>	MolWeight (Structure + Salt) <span>⌵</span>
Click here to draw the structure query	Ignore <span>⌵</span> <input type="text"/>	Ignore <span>⌵</span> <input type="text"/>	Ignore <span>⌵</span> <input type="text"/>	Ignore <span>⌵</span> <input type="text"/>	Ignore <span>⌵</span> <input type="text"/>

## SEARCH RESULTS

Displaying 1 result

	CXN1	CXN1-001		194.1906	194.1906
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# News in 6.1: Hide Version; configurable lot ID

Structure browser

N9373

CXN1  
N9373

Structure Editing

Amend Delete Undelete Rename LnbRef History Change Restriction Level

Molweight: 194.1906	Molecular Formula:	CST: --	Created on: ...	Modified on:
Restriction: 0	Submitter:	Registered by: ADMIN	Modified by:	
Lot Number: CXN1-001	LnbRef: N9373			
CAS Number:	IUPAC Name:	Specified Formula:		

Type: Single

The image shows the chemical structure of caffeine (1,3,7-trimethylxanthine). It consists of a fused pyrimidine-imidazole ring system. The pyrimidine ring has two carbonyl groups (C=O) and a methyl group (CH<sub>3</sub>) attached to the nitrogen at position 1. The imidazole ring has two methyl groups (CH<sub>3</sub>) attached to the nitrogens at positions 3 and 7. The structure is drawn with blue lines for the rings and red lines for the carbonyl groups and oxygen atoms.

# News in 6.1: Project based access control

## Access control

Users Groups **Projects**

Add new project...

Filter projects:

Search Show all

Project name	Project members	
<a href="#">PROJECT_A</a>	user1, user2	
<a href="#">PROJECT_B</a>	user1, user3	

## Update project

Project name:

PROJECT\_B

Users:

Add user to project

User name	User permissions	
<a href="#">user1</a>	READ, WRITE_OWN	
<a href="#">user3</a>	READ	

Update project

# News in 6.1: Marvin JS integration

The screenshot displays the Marvin JS software interface. At the top, there are two red buttons labeled "Register" and "Register with CN", followed by a text input field for "Chem. Sig. Text" and a blue button with a question mark. Below this is a toolbar with various icons for file operations and editing. The main workspace is a large white area containing the Marvin for JavaScript logo (a stylized hexagon with a hand cursor), the text "Marvin for JavaScript Version 6.0", and the ChemAxon logo. On the right side, there is a vertical toolbar with chemical symbols: H, C, N, O, S, F, P, Cl, Br, I, \*, A, R. At the bottom, there are several small icons representing different chemical structures or functions.



# Demo, part2: Major new features

**Search**

**SEARCH OPTIONS**

Search type  
Exact

2D  
 Tautomer

Search

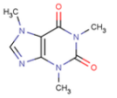
Export results

**SEARCH QUERY**

Structure	Salt info	PCN	LN	LNBREF	Proj
Click here to draw the structure query		Ignore	Ignore	Ignore	Ignore

**SEARCH RESULTS**

Displaying 1 result

	CXN1	CXN1-001	N9373	
---	------	----------	-------	--

number of results to show

**Structure browser**

N9373

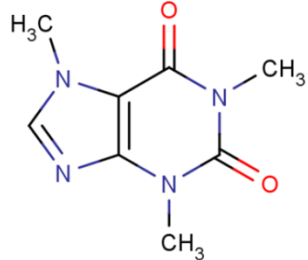
- CXN1
  - N9373

**Structure Editing**

Amend Delete Undelete Rename LnbRef History Change Restriction Level

Molweight: 194.1906 Molecular Formula: CST: ... Created on: ... Modified on: ...  
Restriction: 0 Submitter: Registered by: ADMIN Modified by: ...  
Lot Number: CXN1-001 LnbRef: N9373  
CAS Number: IUPAC Name: Specified Formula: ...

Type: Single



# Future Features



## E-WorkBook

Submission 74

Registration of restricted matches is not allowed. The structure to be registered has an Exact match a restricted compound with PCN GSK34.

Details

LnbRef:  CST:  Restriction:

Molweight:  Molecular formula:

Truncated values can be displayed in a tooltip on mouse hover

Recheck Save Restore

GSK Unmarked Chiral Without Chiral Flag Checker: UnmarkedChiral/Without ChiralFlag

Rare Element Checker: 1 rare element found

Additional data Stereo panel

Comments

General comments	Stereocenters	Double bonds
Stereo comment: Racemic mixture	7 Total stereocenters	2 Total Double Bonds
Geoisomer comment: Unknown	6 Resolved known	1 Major
	0 Resolved, unknown, known relative	1 Mixture of Cis and Trans
	0 Racemic Known relative	
	1 Racemic	

Double bond

- Unknown
- Mixture (45-55)
- As drawn (80-100)
- Major (56-79)

Stereo bond

- Absolute
- Major
- Major as range
- Relative, Racemic
- Racemic (45-55)
- Unknown, resolved
- Unknown, relative
- No information

Cancel Assign

Actions

Register Register with CN

Assign Unlock Show hits

Salts and Solvates

Add salt Add solvate

Parent multiplicity: 1

Salt components: HCl 2

Solvate components: H2O 1

Switches

- Analyze Salt Solvate fragments
- Register New Lots Under Matching Version
- Register New Versions Under Matching Parent
- Register 2D Parent Matches
- Register Tautomer Parent Matches
- Register 2D-Tautomer Parent
- Register if matches are restricted
- Perform quality checks

This might be a combinations of options and structures/selections when not all the options are available (in case it doesn't makes sense to assign them)



Libraries

Projects

Scafolds

EXCLUSIVE

R2 Carboxyl

R3

R4

# Summary



Easy  
integration



Easy  
configuration

# The Team

UGM

