

CeuticalSoft

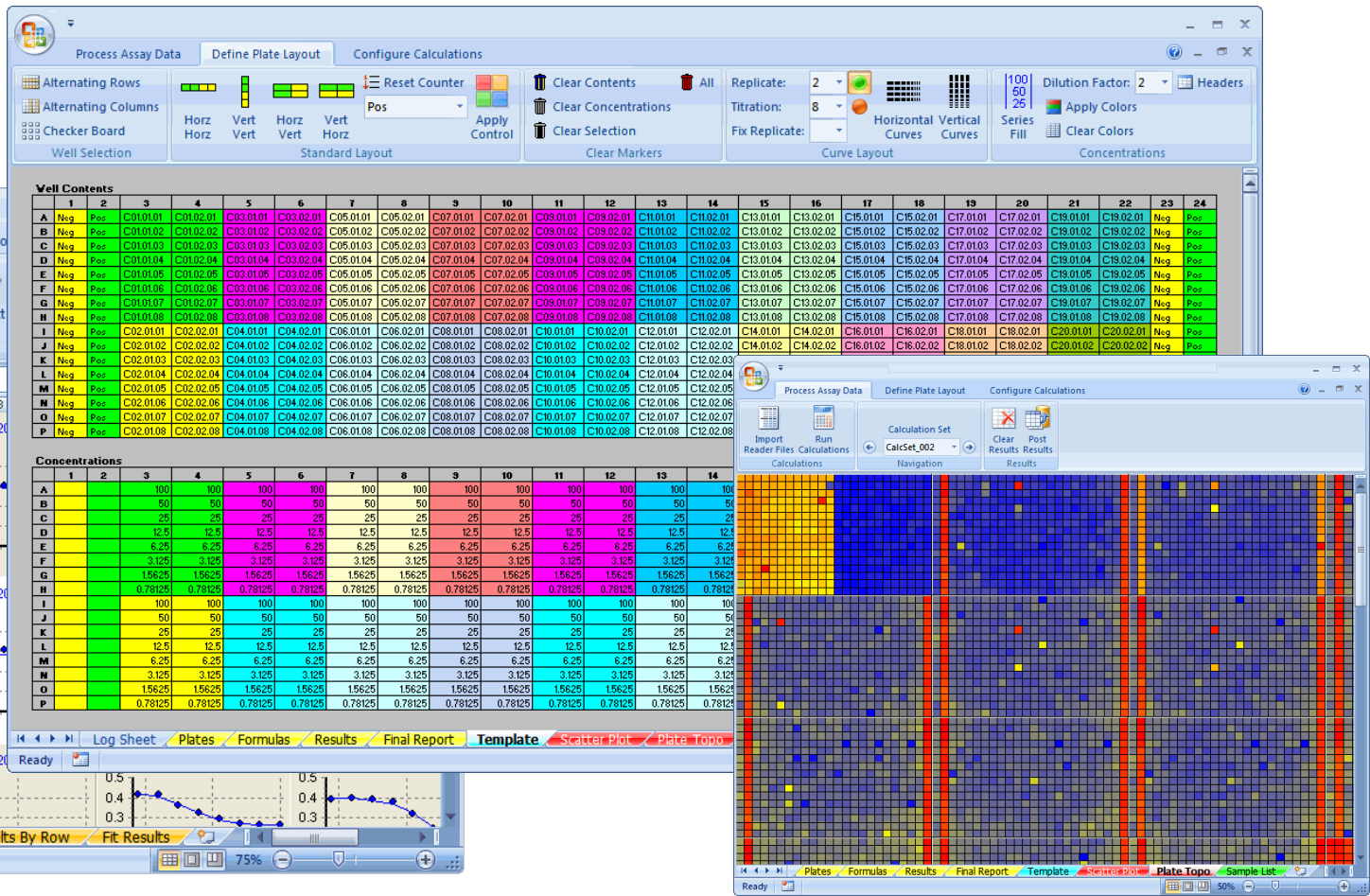
Discovery IT Solutions

CeuticalSoft is a Life Science IT company offering products, services and customized solutions for Pharmaceutical and Biotechnology companies worldwide.

- Product line sold through [OpenHTS](#) subscription.
- [Consulting](#) for process automation, custom development, integration, migration, cloud solutions.
 - Chip Allee – CEO
 - 20 years experience in Drug Discovery and Discovery IT
 - Jeff Moore – CTO
 - 20 years experience in Cheminformatics and Discovery IT



OpenHTS Excel Modules



Core OpenHTS Excel Modules

Core Modules

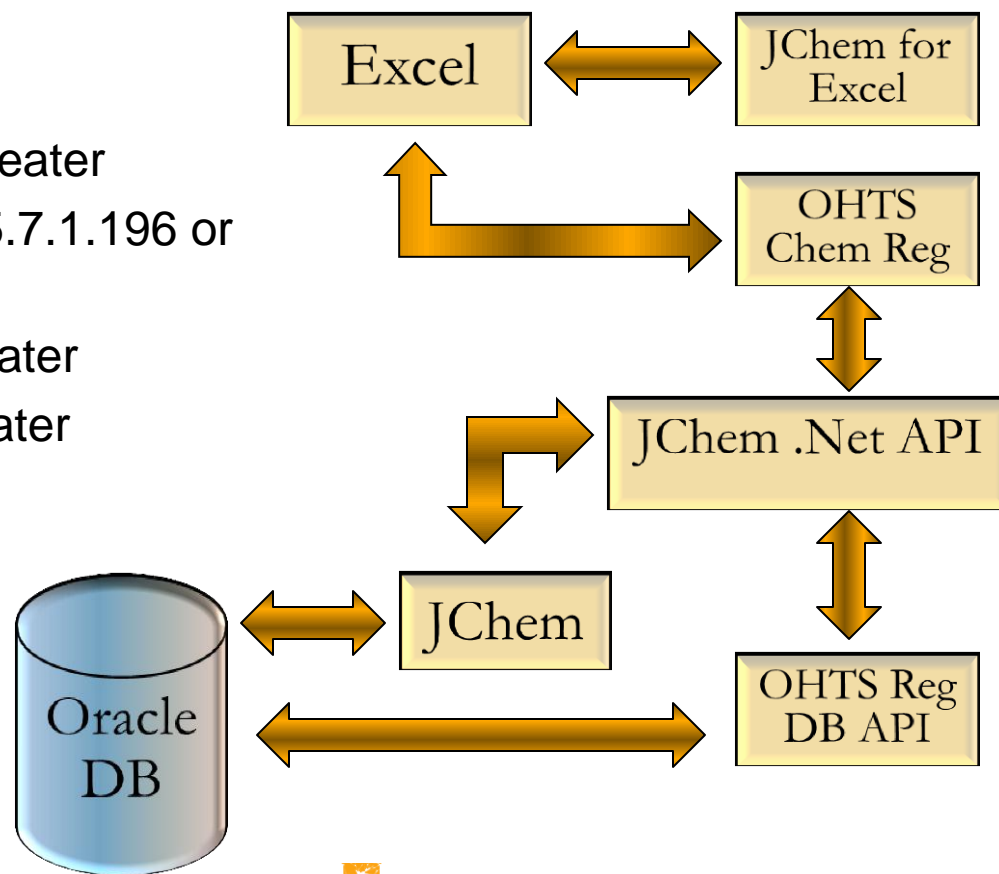
- **Kinetiture** - Kinetic data analysis (FDSS, FLIPR, Etc.)
- **Curvature** - Automated dose response curve fitting
- **Calcature** - Automated plate calculations
- **RegMaster** – JChem4XL Compound Registration
- **10XY** - Orthogonal plate mixing
- **Templature** - Plate layout templates
- **Filature** - Plate reader file conversion

OpenHTS Compound Registration

Powered by JChem

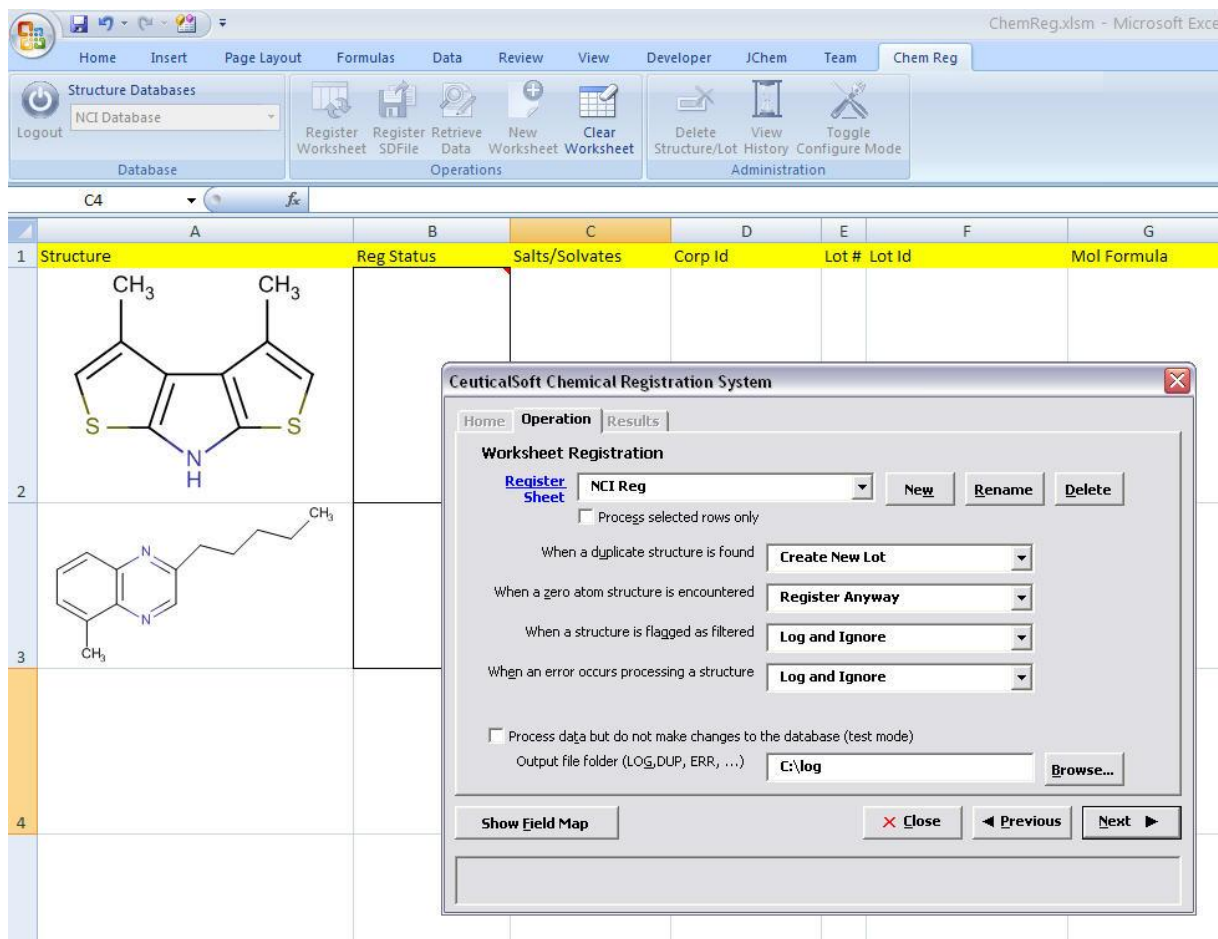
- Architecture

- JChem 5.7.0 or greater
- JChem for Excel 5.7.1.196 or greater
- Oracle 10G or greater
- Excel 2007 or greater



OpenHTS Compound Registration

Powered by JChem



The screenshot shows a Microsoft Excel spreadsheet titled "ChemReg.xlsm" with a ribbon menu including "Home", "Insert", "Page Layout", "Formulas", "Data", "Review", "View", "Developer", "JChem", "Team", and "Chem Reg". The "Chem Reg" ribbon contains sections for "Structure Databases", "Operations", and "Administration".

The spreadsheet has columns labeled "Structure", "Reg Status", "Salts/Solvates", "Corp Id", "Lot #", "Lot Id", and "Mol Formula". Rows 1 and 2 contain chemical structures: a thienopyrrole derivative and a quinoline derivative.

A dialog box titled "CeuticalSoft Chemical Registration System" is open, showing the "Operation" tab. It includes a "Register Sheet" button, a dropdown menu set to "NCI Reg", and buttons for "New", "Rename", and "Delete". There are also checkboxes for "Process selected rows only" and "Process data but do not make changes to the database (test mode)". Several dropdown menus allow for handling duplicates, zero atoms, and errors. The "Output file folder" is set to "C:\log".

OpenHTS Compound Registration

Powered by JChem

- Application Scope
 - Any JChem structure table can be enabled for registration
 - Registration typically involves creation and management of a compound lot table but this is not required
 - Access to functionality (create, update, delete, etc.) controlled and enforced with Oracle roles on a structure table basis

OpenHTS Compound Registration

Powered by JChem

The screenshot shows a Microsoft Excel spreadsheet titled 'ChemReg.xlsm' with a 'Table Tools' ribbon. The spreadsheet contains a table with the following data:

Field Manager	SDFile Field Name	Data Type	Database Field
	<i>CidId</i>	<i>Integer</i>	
	<i>MolWeight</i>	<i>Real Number</i>	NCI_OPEN_09_03.E_MULTIFRAG NCI_OPEN_09_03.E_NAME
	<i>Formula</i>	<i>Text</i>	NCI_OPEN_09_03.E_NSC
	<i>NSC</i>	<i>Integer</i>	NCI_OPEN_09_03.E_SMILES NCI_OPEN_09_03.E_SOURCE
	<i>CAS RN</i>	<i>Text</i>	NCI_OPEN_09_03.E_TAUTO_HASH NCI_OPEN_09_03.E_THREED_SOURCE NCI_OPEN_09_03.E_UNIQUE_ID
	<i>E_STEREO_SPECIFIED</i>	<i>Text</i>	
	<i>E_STEREO_TAUTO_HASH</i>	<i>Text</i>	NCI_OPEN_09_03.E_STEREO_TAUTO_HASH
	<i>E_ORIGIN</i>	<i>Text</i>	NCI_OPEN_09_03.E_ORIGIN
	<i>E_DB_YEAR</i>	<i>Integer</i>	NCI_OPEN_09_03.E_DB_YEAR
	<i>E_DB_TYPE</i>	<i>Text</i>	NCI_OPEN_09_03.E_DB_TYPE
	<i>E_SAMPLES_AVAIL</i>	<i>Text</i>	NCI_OPEN_09_03.E_SAMPLES_AVAIL
	<i>E_SUPPLIER_TYPE</i>	<i>Text</i>	NCI_OPEN_09_03.E_SUPPLIER_TYPE

Overlaid on the spreadsheet is a dialog box titled 'Microsoft Chemical Registration'. The 'Field Mapping Sheet' dropdown is set to 'NCI Structure Template'. The 'Fill in database fields if possible' checkbox is checked. The 'Apply Mapping' button is visible.

OpenHTS Compound Registration

Powered by JChem

- Field Mapping
 - Mapping of SDFFile fields and worksheet columns to structure/lot fields in the database is supported
 - Mapping can be simple 1:1 or complex Excel formulae may be used to manipulate data from SDFFile to conform to standards
 - Multiple mapping templates supported

OpenHTS Compound Registration

Powered by JChem

- Corporate Id Management
 - By default corporate ids are generated from CD_ID with optional prefix and formatting template
 - e.g., STR-000445
 - Or, a different sequence can be used for id generation (i.e., CD_ID not same or corp id #)
 - Or, ids can be generated using a custom PL/SQL extension
 - Lot Ids are handled in a similar way

OpenHTS Compound Registration

Powered by JChem

- Advanced Functionality
 - Custom Integration
 - An extensible API is provided that allows creations of data other than lot (e.g., mother plates, general samples)
 - Structure Filtering
 - Structures may be excluded from registration based on structural features and/or other criteria such as MW.
 - For example, in an SDF file any structure having a heavy metal can be automatically excluded
 - Salt/Solvate stripping
 - Salt “molecules” can be removed based on a salt database
 - Lot MW and MF calculated based on salt codes
 - Lots can have different salt codes (this is common in pharma)

OpenHTS Compound Registration

Powered by JChem

- Advanced Functionality (continued)
 - Audit Trail
 - All data changes (including insert/update/delete) are audited with who/what/why.
 - Previous field values (including structure) are retained when updates/deletes occur
 - Can be configured to force entry of change reasons
 - Configurable Application
 - Full featured application probably not suitable for all users
 - Most options can be locked down and/or hidden from casual users to simplify their experience

OpenHTS Compound Registration

Powered by JChem

- Conclusions
 - A full-featured registration system based on
 - Excellent chemistry software implemented in JChem
 - Familiar and popular Excel application
 - Extensive industry experience





Structure Databases

NCI Database

Logout

Database

Register
WorksheetRegister
SDFFileRetrieve
DataNew
WorksheetClear
Worksheet

Operations

Delete
Structure/LotView
HistoryToggle
Configure Mode

Administration

C4

fx

A

B

C

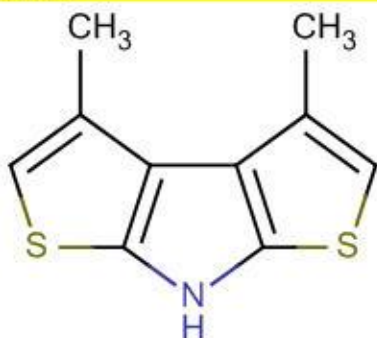
D

E

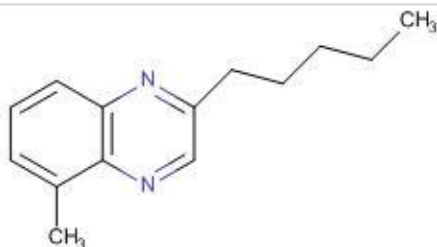
F

G

1	Structure	Reg Status	Salts/Solvates	Corp Id	Lot #	Lot Id	Mol Formula
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2



3

4

CeuticalSoft Chemical Registration System

Home Operation Results

Worksheet Registration

Register
Sheet

NCI Reg

New

Rename

Delete

 Process selected rows only

When a duplicate structure is found

Create New Lot

When a zero atom structure is encountered

Register Anyway

When a structure is flagged as filtered

Log and Ignore

When an error occurs processing a structure

Log and Ignore

 Process data but do not make changes to the database (test mode)

Output file folder (LOG,DUP, ERR, ...)

C:\log

Browse...

Show Field Map

Close

Previous

Next

Home Insert Page Layout Formulas Data Review View Developer JChem Team Chem Reg

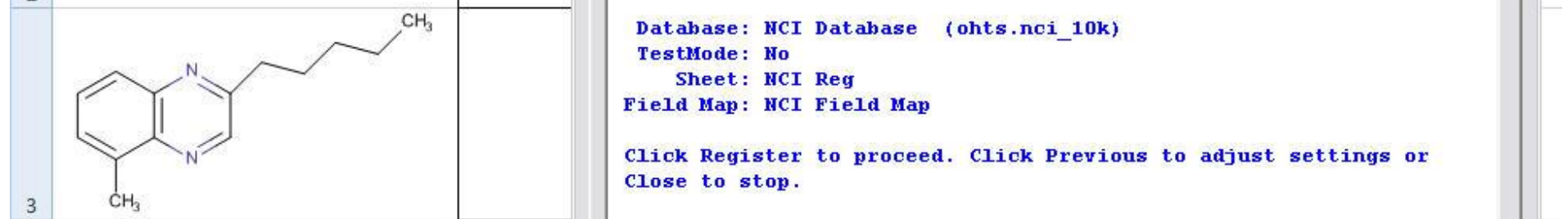
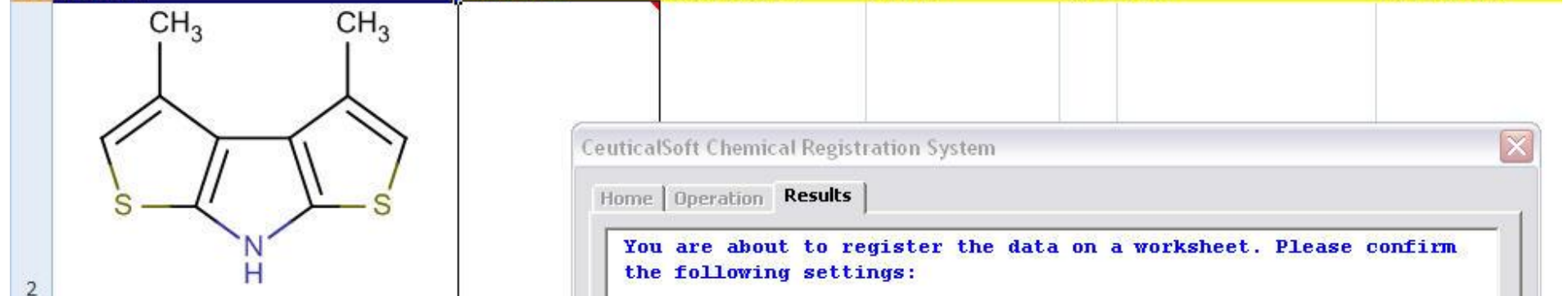
Structure Databases
Logout NCI Database Database

Register Worksheet Register SDFFile Retrieve Data New Worksheet Clear Worksheet Operations

Delete Structure/Lot View History Toggle Administration

A1 Structure

	A	B	C	D	E	F	G
1	Structure	Reg Status	Salts/Solvates	Corp Id	Lot #	Lot Id	Mol Formula



4							
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CeuticalSoft Chemical Registration System

Home Operation Results

You are about to register the data on a worksheet. Please confirm the following settings:

Database: NCI Database (ohts.nci_10k)
 TestMode: No
 Sheet: NCI Reg
 Field Map: NCI Field Map

Click Register to proceed. Click Previous to adjust settings or Close to stop.

Register View Log

Show Field Map Close Previous Next

Structures Examined: 2, Fields: 16 Sheet: NCI Reg

	A	B	C	D	E	F	G	H	I	J
1	Structure	Reg Status	Salts/Solvates	Corp Id	Lot #	Lot Id	Mol Formula	Mol Weigh	Lot Formula	Lot Weight/NS
2		Added Structure/Lot								
3		New Lot		STR-00010253	1	STR-00010253/001	C ₁₀ H ₉ NS ₂	207.315	C ₁₀ H ₉ NS ₂	207.315
4										
5										
6										
7										
8										
9										

CeuticalSoft Chemical Registration System

Home | Operation | **Results**

Registration Complete:

- Total: 2
- Errors: 0
- New Structures: 1
- New Lots: 1
- UpToDate: 0
- Updated: 0
- Reverted: 0
- ToEmptyFile: 0
- ToDupFile: 0
- ToFilterFile: 0
- ToErrorFile: 0
- Ignored: 0

Register X View Log

Show Field Map X Close < Previous Next >

Done, Total: 2 Errors: 0 New Structures: 1 New Lots: 1 UpToDate: 0 Updated: 0 Reverted: 0 ToEmptyFile: 0 ToDupFile: 0 ToFilterFile: 0 ToErrorFile: 0 Ignored: 0



Home Insert Page Layout Formulas Data Review View Developer JChem Team Chem Reg



Structure Databases

NCI Database

Logout

Database

Register
WorksheetRegister
SDFFileRetrieve
DataNew
WorksheetClear
Worksheet

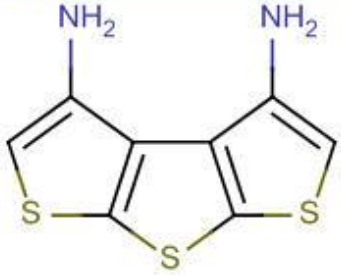
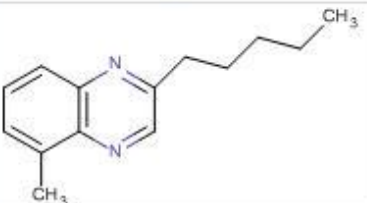
Operations

Delete
Structure/LotView
HistoryToggle
Configure Mode

Administration

A1

fx Structure

	A	B	C	D	E	F	G	H	I
1	Structure	Reg Status	Salts/Solvates	Corp Id	Lot #	Lot Id	Mol Formula	Mol Weigh	Lot Formula
2		Added Structure/Lot							
3		New Lot							
4									
5									

CeuticalSoft Chemical Registration System

Home Operation Results

Worksheet Registration

Register
Sheet

NCI Reg

New

Rename

Delete

 Process selected rows only

When a duplicate structure is found

Create New Lot

When a zero atom structure is encountered

Register Anyway

When a structure is flagged as filtered

Log and Ignore

When an error occurs processing a structure

Log and Ignore

 Process data but do not make changes to the database (test mode)

Output file folder (LOG, DUP, ERR, ...)

C:\log

Browse...

Show Field Map

X Close

◀ Previous

Next ▶



Structure Databases

NCI Database

Logout

Database

Register
WorksheetRegister
SDFFileRetrieve
DataNew
WorksheetClear
Worksheet

Operations

Delete
Structure/LotView
HistoryToggle
Configure Mode

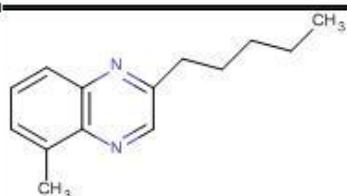
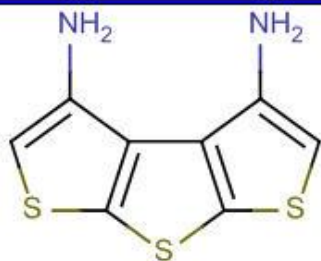
Administration

A2



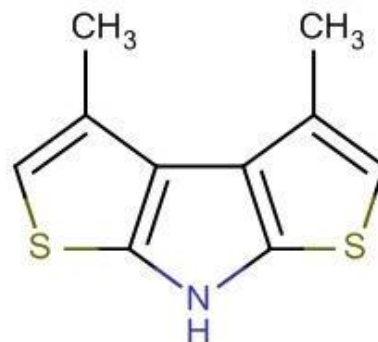
fx Structure

1 Structure Reg Status Salts/Solvates Corp Id Lot # Lot Id Mol Formula Mol Weigh Lot Formula Lot W

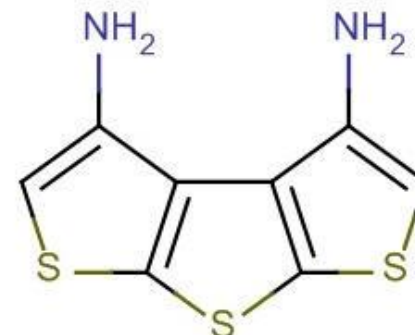


Confirm Changes to Structure/Data for: STR-00010253/001

Database Structure



Modified Structure



Modified Fields

Field Name	Current Value	Modified Value
supplier (nci_10k_lot.supplier)	Internal	Aldrich
supplier lot (nci_10k_lot.supplier_purity (nci_10k_lot.purity))		324-33 98

Reason for Change Recorded wrong structure and supplier.

Accept Changes

Discard Changes