

# 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

## Open Source Discovery IT

- OpenHTS is an open source software depository and user community built on a comprehensive collection of Microsoft Excel modules, ChemAxon cheminformatics, database schemas and stored procedures.
  - Subscribers can integrate, configure, customize and support their own deployments or they can opt for turn-key solutions delivered and supported by CeuticalSoft.
  - Engineered and refined over many years for use in Life Science laboratories.
  - Subscribers have access to the entire software library and are free to deploy unlimited copies within their organization.



# OpenHTS Excel Modules

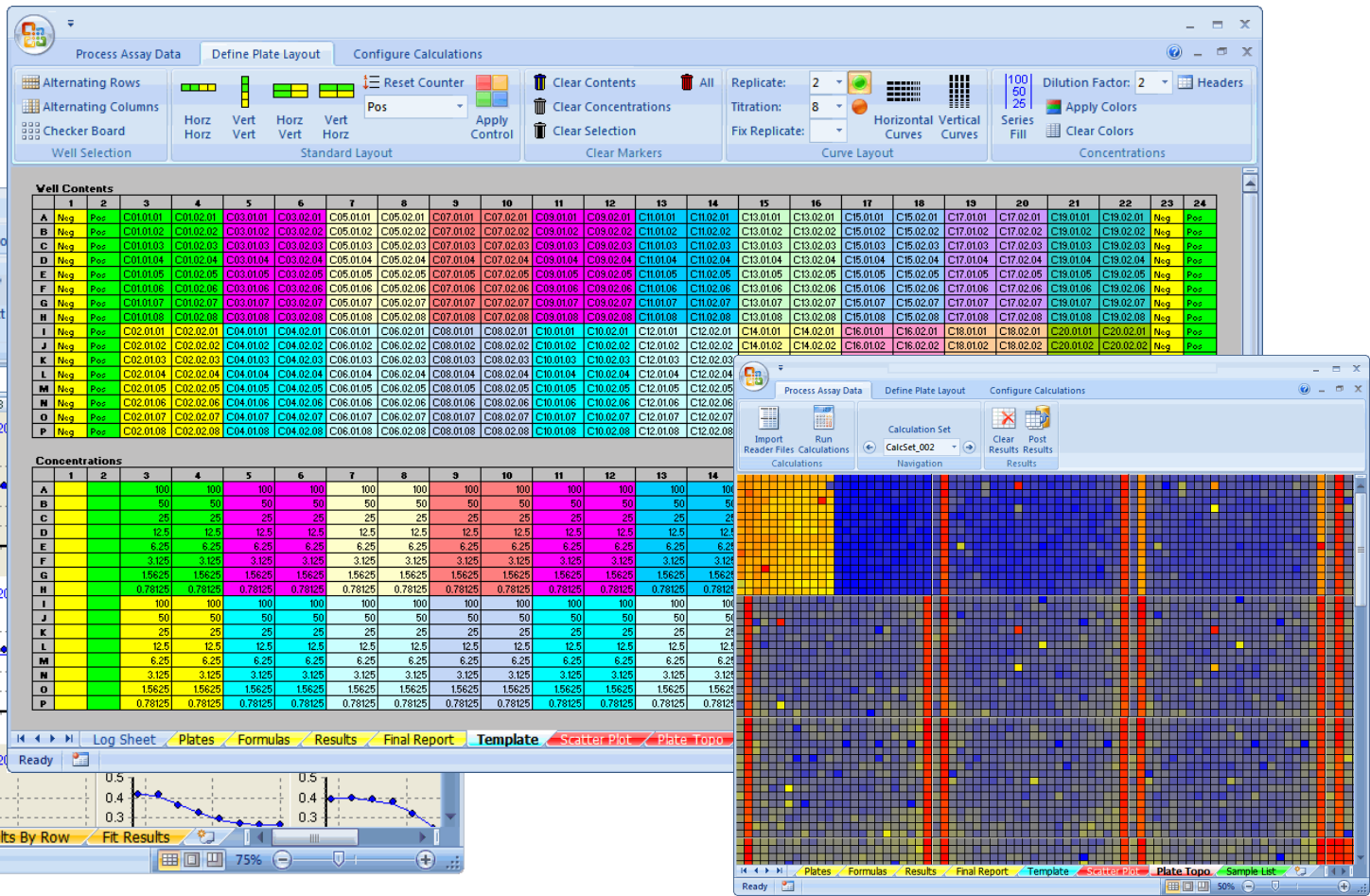
## Core Modules

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

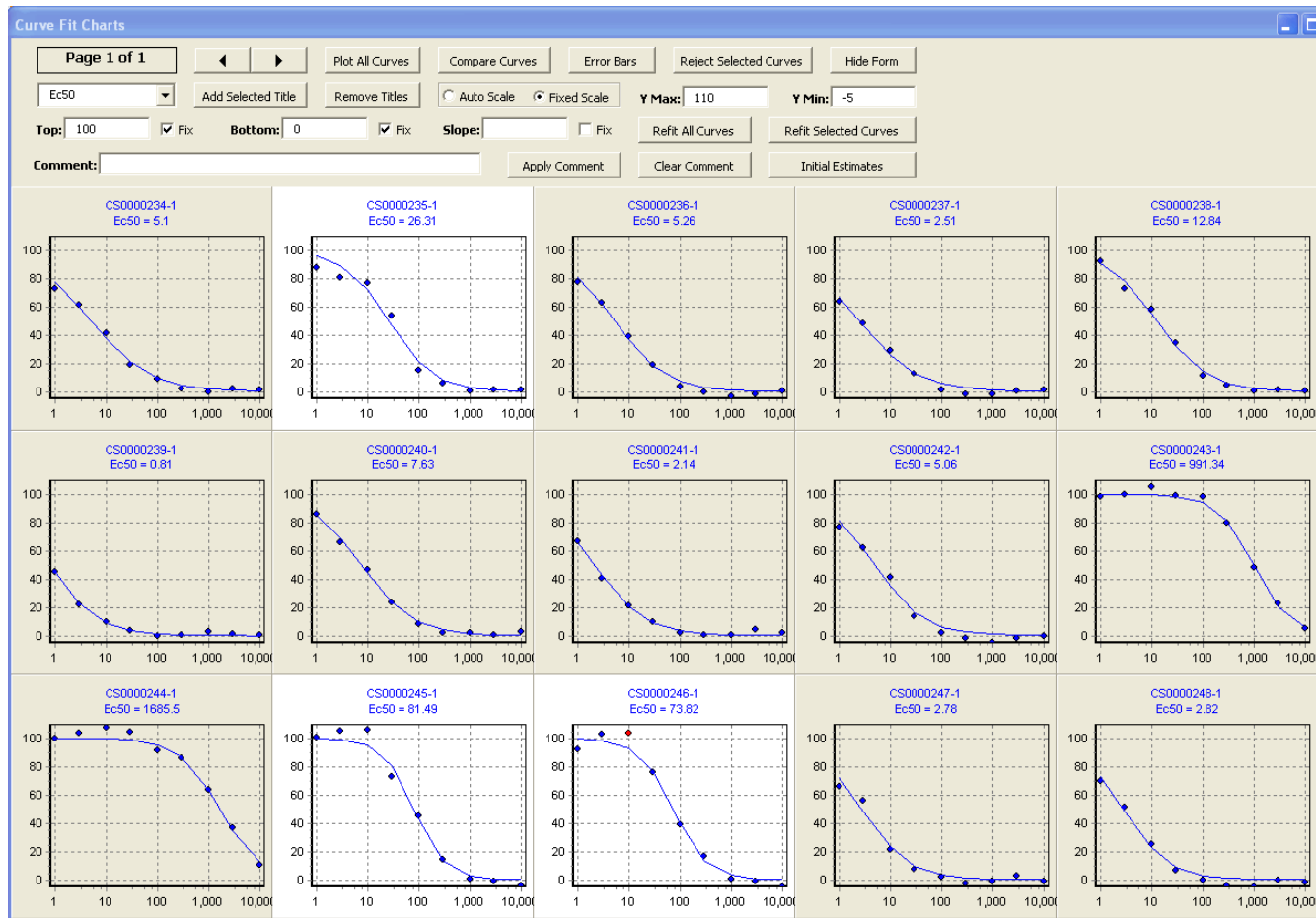
## Components

- **Regmaster** - Sample and plate registration
- **PCRTist** - Expression profiling
- **CurveStore** - Curve storage and retrieval
- **TraceStore** - Kinetic trace storage and retrieval
- **HCSa** - High content screening data analysis

# OpenHTS Excel Modules



# OpenHTS Excel Modules



# OpenHTS Excel Modules

Curve Fitting   Define Plate Layout   Configure Calculations

Import   Fit Curves   Fit Selected Curves  
 Fit Calculations

Unhide Charts   Plot Selected Curves   Plot All Curves   Compare Selected Curves   Go To Fit Results  
 Curve Plot Options

Clear Sample List   Clear Exp Data   Clear Fit Results   Post Fit Results  
 Fit Results

Curve Fitting   Define Plate Layout   Configure Calculations

Alternating Rows   Alternating Columns   Checker Board  
 Well Selection

Horz   Vert   Horz   Vert   Replicate:   Reset Counter   Apply Control  
 Standard Layout

Clear Selection   Clear Markers

Replicate:   Titration:   Fix Replicate:   Horizontal Curves   Vertical Curves  
 Curve Layout

100   50   25   Apply Colors   Clear Colors   Series Fill   Dilution Factor:  
 Concentrations

Process Assay Data   Define Plate Layout   Configure Calculations

Import   Run Calculations   Calculate Saved Data  
 Calculations

Show All Plates on Raw Data Plot  
 Show All Plates on Results Plot  
 Navigate Calculation Sets

Delete Calc Set   Clear Results   Post Results   Result Name:   Result Type:  
 Results

Plot Results   Set Threshold   Get Structure

Show Numbers    Show Sample Names    Show Outlier Tags   Select All Plates   Conditional Formatting   Zoom

Results Topo

Process Assay Data   Define Plate Layout   Configure Calculations

Plate:   Map Plate   Map Control   Clear Selection   Clear All  
 Formula Mapping

Import Sample File   Toggle Config Mode   Reset Calc Set   Reinitialize App   Export Protocol   Import Protocol  
 Module Configuration

# OpenHTS Oracle Modules

- OpenHTS Core - tables and stored procedures responsible for managing the OpenHTS Excel modules.
  - OpenHTS Inventory - tables and stored procedures used for plate and compound registration and management.
  - The OpenHTS Data Publishing - tables and procedures for storing and managing assay results.
  - The OpenHTS Chemistry - based on ChemAxon technology and provides compound registration and heterogeneous (biology/chemistry) query and reporting.
- \* Modules are interchangeable with existing corporate databases except for OpenHTS Core

# OpenHTS Benefits

- Perpetual access to a growing body of drug discovery modules for no additional fee.
- Mutual benefit derived from subscriber contributions.
- OpenHTS modules are highly refined and tested in diverse laboratory environments.
- Native Excel modules take full advantage of Excel capabilities.
- Extremely lean and simplified VBA code easily modified by Scientists.
- Instant user acceptance with users already comfortable with Excel.

# OpenHTS Benefits

- Role based deployment options.
- Multiple deployment configurations. Workbooks, Templates, Sharepoint.
- Easy integration with existing Excel solutions, macros, reports, etc.
- Easy integration with existing databases and applications.
- OpenHTS modules are highly configurable so they can adapt to existing laboratory processes.
- OpenHTS is commercial open source software so it is governed and maintained by CeuticalSoft. This ensures only professional grade development makes it into OpenHTS modules.



# OpenHTS Compound Registration

## Powered by JChem

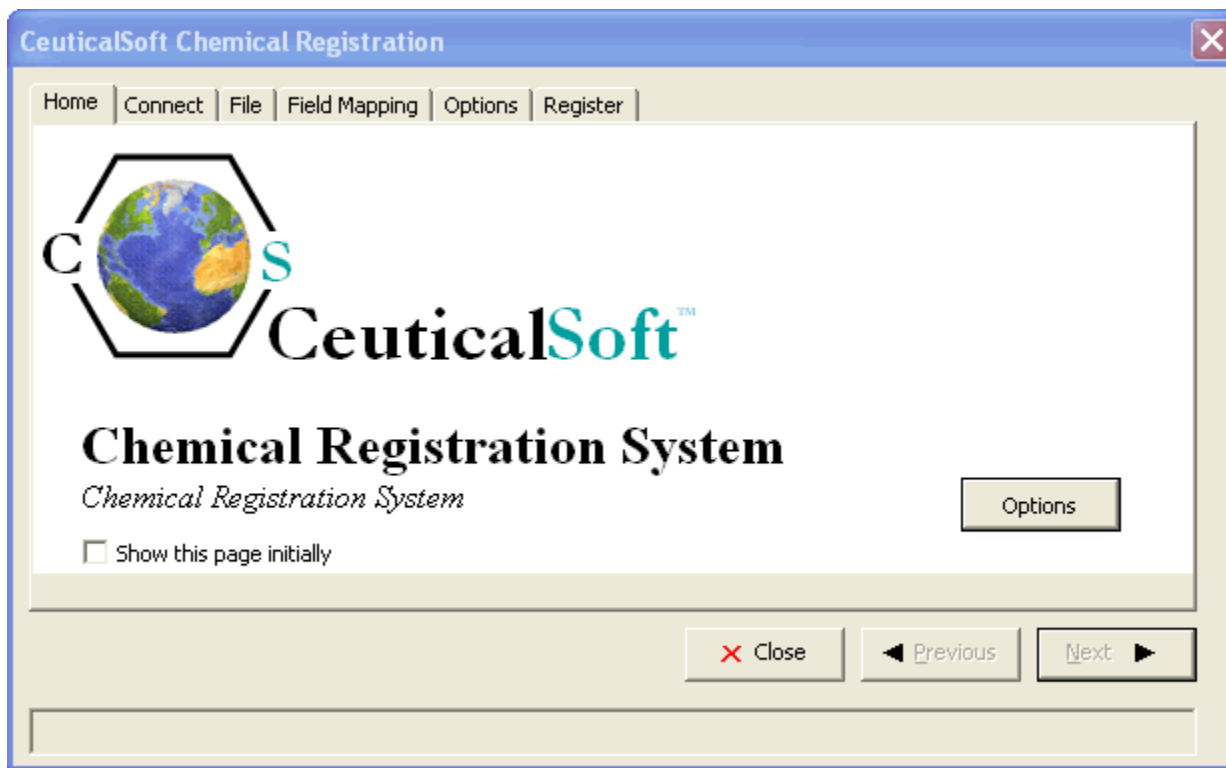
- OpenHTS Compound Registration Module
  - Register structures to any JChem Structure Entity in any Schema
  - Batch registration from SD files (other file types available)
  - Duplicate structure search with automatic lot creation or duplicate allowed mode.
  - Fully integrated with plate registration
  - Structure filtering based on field values
  - Null structure reject/allow
- Extensive user-defined field mapping templates
  - Map to structure, lot, plate, wells and sample tables
  - Field derivatives include merge, split, calculate





# OpenHTS Compound Registration

Powered by JChem

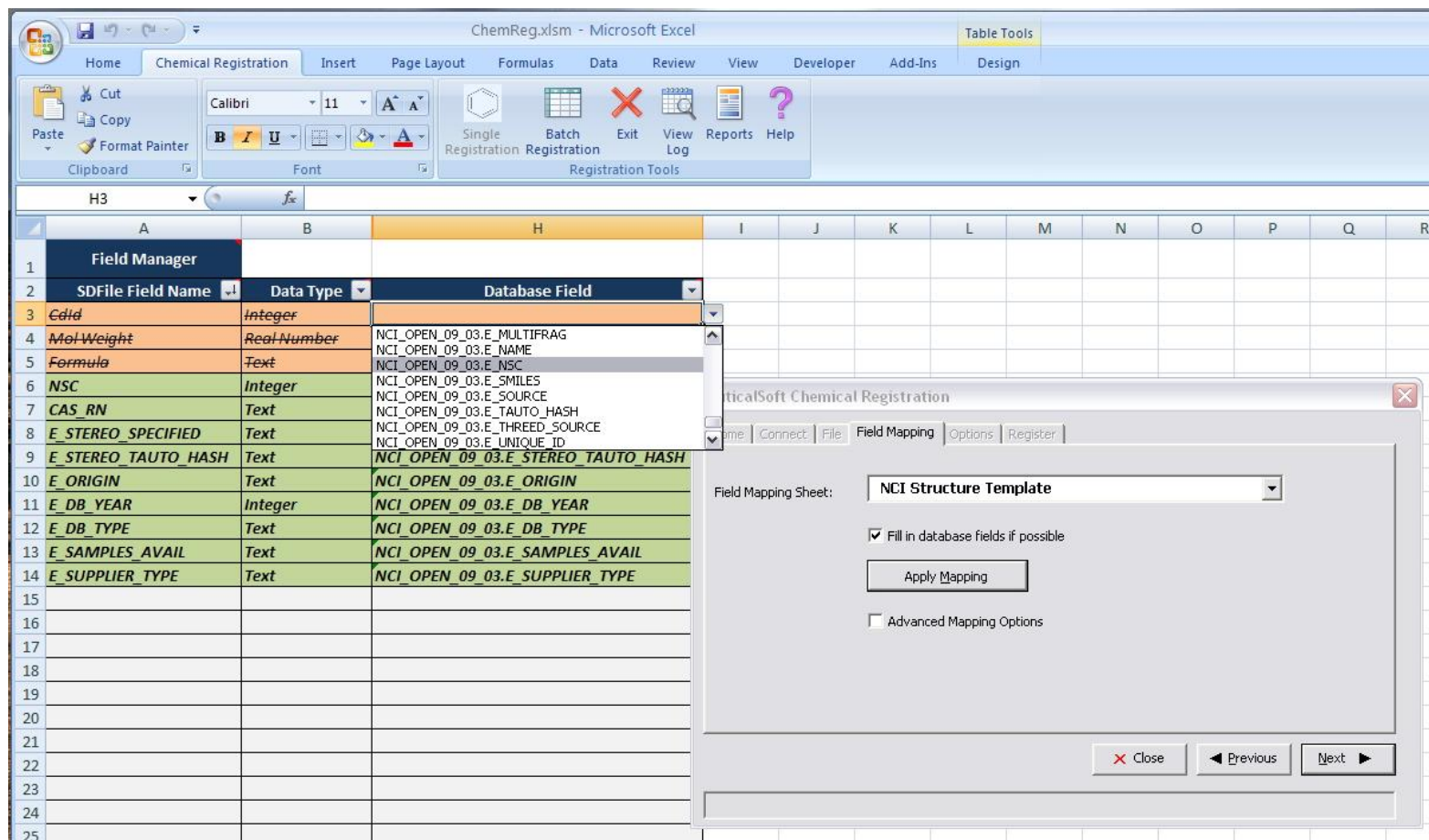


Registration Wizard



# OpenHTS Compound Registration

## Powered by JChem

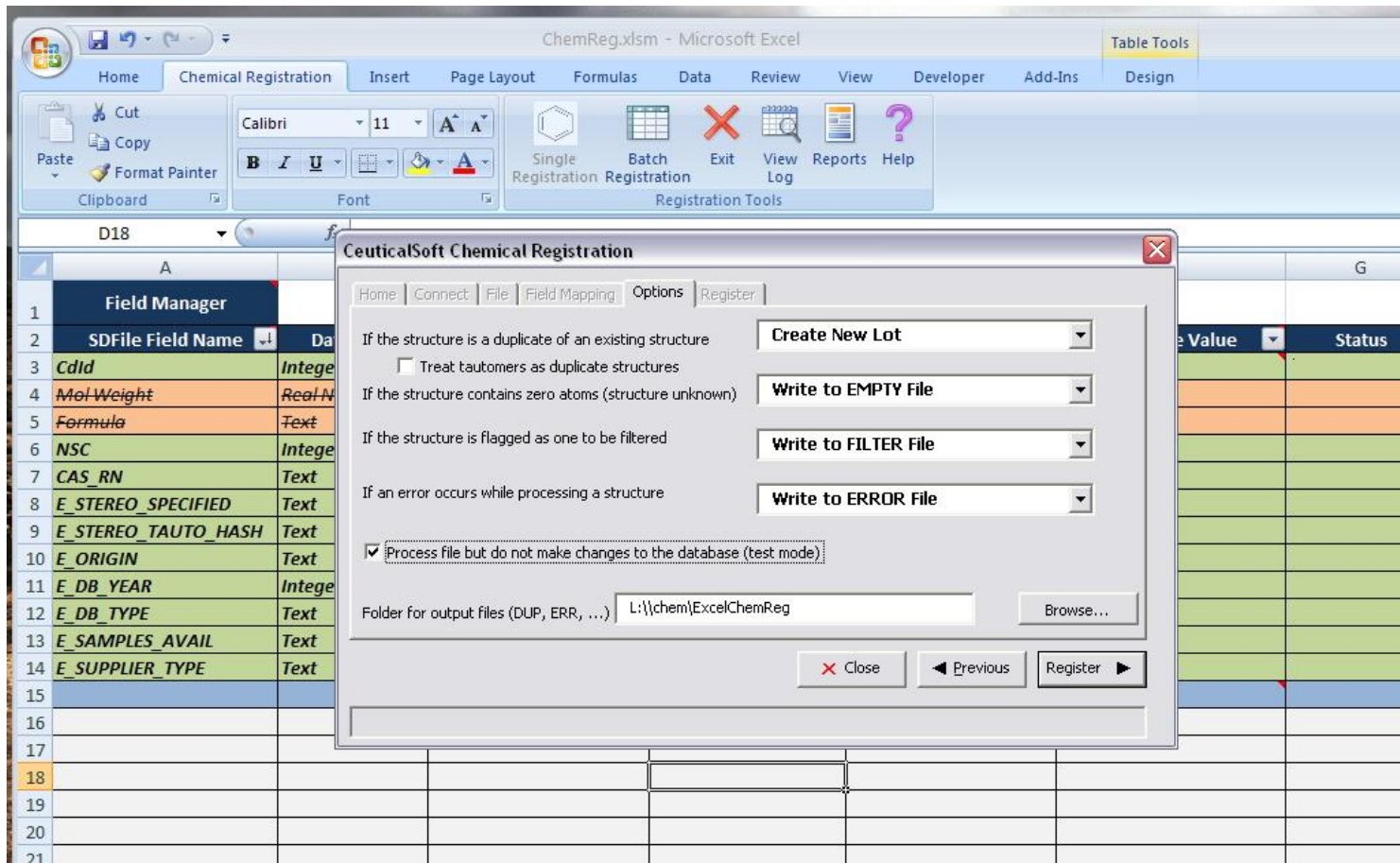


The screenshot shows the Microsoft Excel interface with a spreadsheet titled 'ChemReg.xlsm'. The spreadsheet contains a table with columns for 'SDFFile Field Name', 'Data Type', and 'Database Field'. A dropdown menu is open for the 'Database Field' column, showing a list of database field names. A dialog box titled 'Microsoft Chemical Registration' is overlaid on the spreadsheet, showing the 'Field Mapping Sheet' set to 'NCI Structure Template'. The dialog box has a checked option for 'Fill in database fields if possible' and an 'Apply Mapping' button.

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

# OpenHTS Compound Registration

## Powered by JChem



ChemReg.xlsm - Microsoft Excel

Table Tools

Home Chemical Registration Insert Page Layout Formulas Data Review View Developer Add-Ins Design

Clipboard Font Registration Tools

Single Registration Batch Registration Exit View Log Reports Help

Field Manager

SDFFile Field Name	Data Type
Cdid	Integer
Mol Weight	Real Number
Formula	Text
NSC	Integer
CAS_RN	Text
E_STEREO_SPECIFIED	Text
E_STEREO_TAUTO_HASH	Text
E_ORIGIN	Text
E_DB_YEAR	Integer
E_DB_TYPE	Text
E_SAMPLES_AVAIL	Text
E_SUPPLIER_TYPE	Text

CeuticalSoft Chemical Registration

Home Connect File Field Mapping Options Register

If the structure is a duplicate of an existing structure: Create New Lot

Treat tautomers as duplicate structures

If the structure contains zero atoms (structure unknown): Write to EMPTY File

If the structure is flagged as one to be filtered: Write to FILTER File

If an error occurs while processing a structure: Write to ERROR File

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

Folder for output files (DUP, ERR, ...) L:\chem\ExcelChemReg

Close Previous Register



# ChemAxon & OpenHTS

- OpenHTS Enterprise & ChemAxon Integration
  - OpenHTS
    - Assay data management/analysis
    - Plate/Compound inventory management/registration
    - Automation/Instrumentation integration
    - Compound registration
  - ChemAxon
    - Structure storage, retrieval, querying
    - Instant JChem Query/Reporting
    - JChem for XL Query/Reporting
  - Pure Excel Discovery IT Solution





# ChemAxon & OpenHTS

## Future Plans

- Ongoing development of Compound Registration Module
- Complete data management system with comprehensive chemistry/biology capabilities for cost effective annual subscription.
- Ongoing OpenHTS integration with JChem XL.
- Pure SQL Server version with enhanced Sharepoint deployment.

