



TouchMol for Excel User Manual



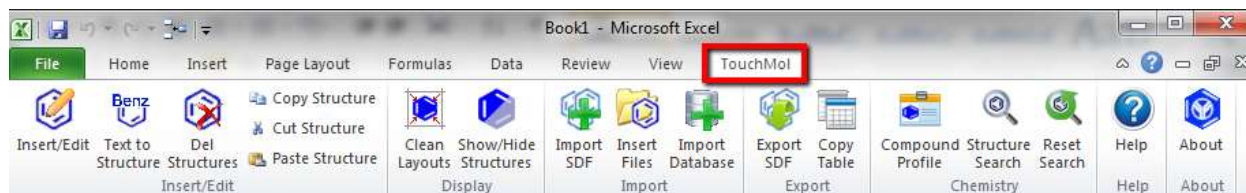
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Getting Started with TouchMol for Excel

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Getting Started with TouchMol for Excel

1. Click **TouchMol** tab

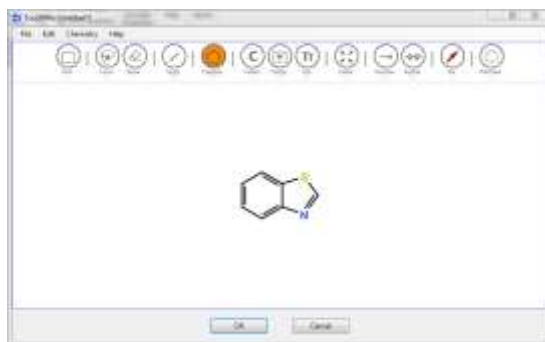


Insert/Edit Structure

1. Select a cell or structure on a Excel sheet, then click **Insert/Edit Structure**



2. Draw or edit chemical or biological structures on TouchMol pop-up window



3. Click OK

Convert Chemical Name/Identifier to Structure

1. Select a cell on a Excel sheet, then click **Text to Structure**



2. Input chemical name, trade name or chemical identifier such as CAS# in the pop-up box

The screenshot shows a dialog box titled 'Name(Voice) to Structure'. It contains a text input field with the word 'Zyrtec' entered. Above the field is the instruction: 'Please type a chemical identifier (IUPAC name, CAS, Trade name, SMILES, InChI etc.)'. To the right of the field is a microphone icon. At the bottom of the dialog box are 'OK' and 'Cancel' buttons.

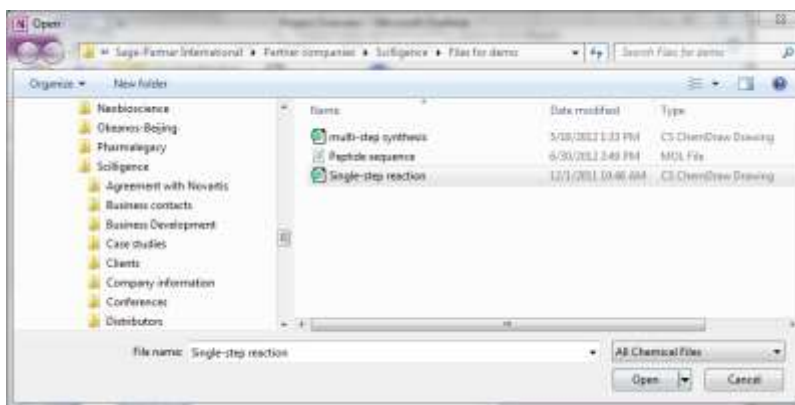
3. Click OK

Insert Structure from Other Chemical File Formats

1. To insert structure or reaction from other chemical file formats, click **Insert File** after selecting a cell on a Excel sheet

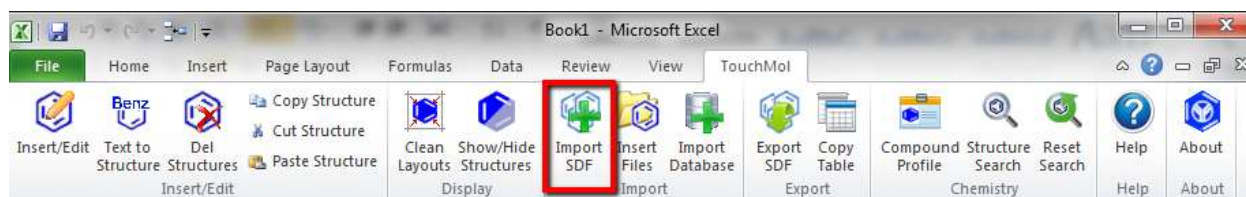


2. Select the chemical file, then click **Open**



Import SDF File

1. To import a SDF file, click **Import SDF**



2. Browse and select a sdf file
3. Click **Open**

Export SDF File

1. Select data in a Excel sheet to be exported into a sdf file
2. Click **Export SDF**



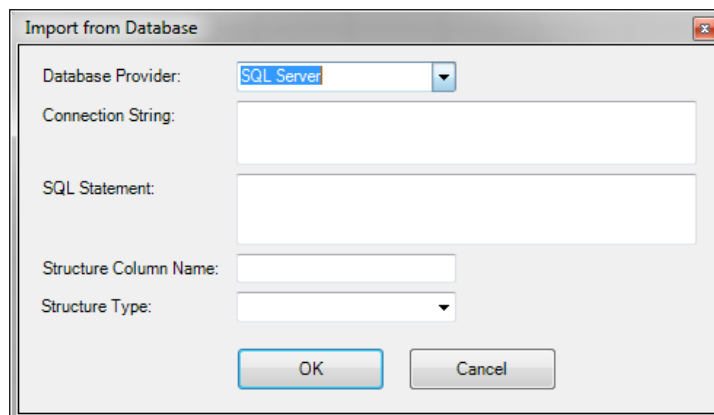
3. Input a file name, then click **Save**

Import Structures and Associated Data from Databases

1. To import structures and their associated data from a corporate database, click **Import Database**



2. Select database type (SQL or Oracle); input Connection String, SQL statement, and Structure Column Name; select Structure Type

A screenshot of the 'Import from Database' dialog box. The 'Database Provider' dropdown menu is set to 'SQL Server'. Below it are text input fields for 'Connection String', 'SQL Statement', and 'Structure Column Name'. At the bottom, there is a 'Structure Type' dropdown menu and two buttons: 'OK' and 'Cancel'.

3. Click **OK**

Note: To load structures and their associated data from corporate databases, configuration of TouchMol for Excel is required.

Show Compound Profile of a Selected Structure

1. Select a chemical structure, then click **Compound Profile**



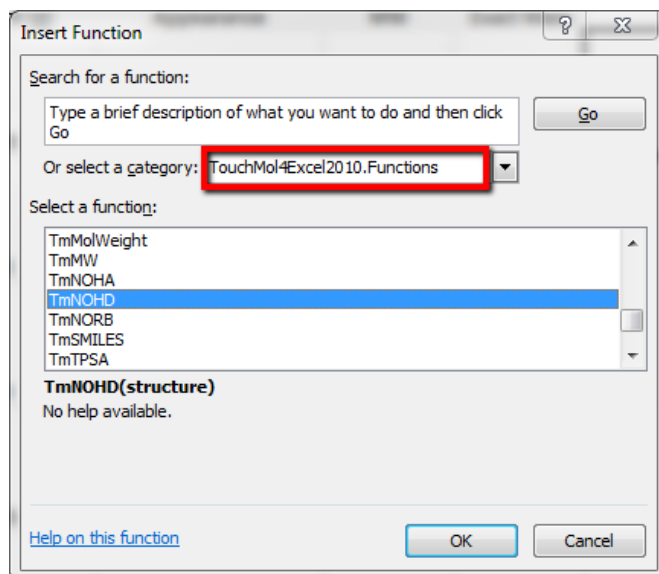
Note: Compound profile can include calculated properties, bioassay data from public and internal corporate databases. To access bioassay data in corporate databases, configuration of TouchMol for Excel is required.

Insert Calculated Property Using Column Formula

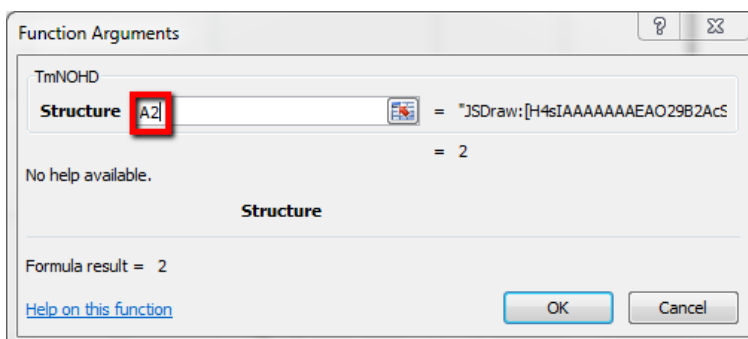
1. Select a cell on the row of a structure that its property will be calculated from
2. Use standard Excel column formula operation (input "=")
3. Select **More Functions** from the function dropdown manual

	B	C	D	E	F	G	H	I
	Purity (%)	Amount (g)	Appearance	MW	Exact Mass			
	97	100	white solid	359.97666	357.81452	=		
	95	78	off white solid	357.17656	355.93537			
	98	89	light yellow solid	373.17596	371.93027			

- In the Insert Function pop-up window, select the category **TouchMol4Excel2010.Functions**; select calculated property function, e.g., **TmNOHD** (total number of hydrogen bond donor); then click **OK**



- In the Function Arguments pop-up window, input the cell coordinate of a structure that its property will be calculated from, then click **OK**



Structure Search in an Excel Spreadsheet

- Click **Structure Search**



- Input a structure in the TouchMol pop-up window, then click **OK**

Note: Structure search results will only display structures that contain the inputted substructure. Associated data with these search hits will also be displayed.

- Click **Reset Search** to display all structures on a spreadsheet



Sort Data Column

- Highlighted data columns/area including the structure column and the column to be sorted
- Use Excel standard sorting functions to sort a column; structures in the structure column will move accordingly as well

Clean Layouts

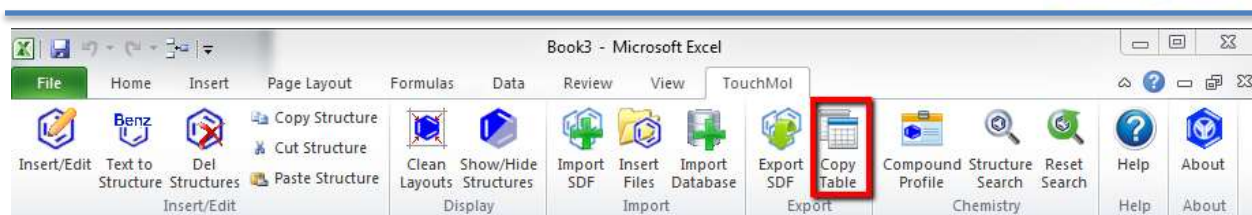
- If any structure is not aligned with a cell after sorting or copy/paste, select the structure or the whole spreadsheet
- Click **Clean Layouts**



Copy Table

Copy Table from Excel to Word

- Select data including structures on a spreadsheet
- Click **Copy Table**



3. Open Word, then click **Paste** or **Ctrl-V**

Copy Table into PowerPoint

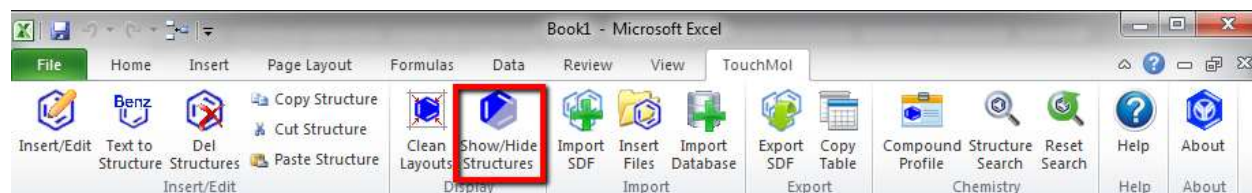
1. To copy table into PowerPoint, select the table pasted into Word
2. Click **Copy** or **Ctrl-C**
3. Open PowerPoint and right-click to see the paste options
4. Click **Embed [E]** or **Picture**

Copy Table into OneNote

1. To copy table into OneNote, select the table pasted into Word
2. Click **Copy** or **Ctrl-C**
3. Open OneNote and right-click to see the paste options
4. Click **Keep Sourcing Formatting, Merge Formatting** or **Picture**

Show/Hide Structures

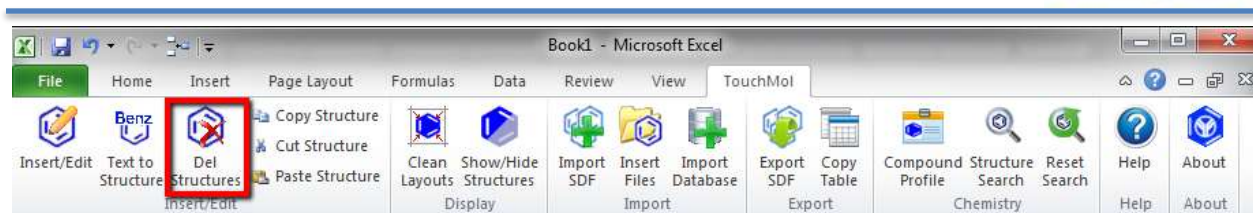
1. To hide all structures in a spreadsheet, click **Show/Hide Structures**



2. To re-display structures, click **Show/Hide Structures** again

Delete Structures in a Selected Area

1. Select an area on a spreadsheet with the structures to be deleted
2. Click **Del Structures**



Other Editing Functions

1. Copy a structure or reaction: click **Copy Structure**
2. Cut a structure or reaction: click **Cut Structure**
3. Paste a structure or reaction: click **Paste Structure**

