



ChemAxon

# Comparing chemistry in Microsoft Excel

## Ease of Managing Chemistry in Microsoft Excel

	JChem for Excel 5.10	Accord for Excel 7.1 Standard and Enterprise edition	Iseentris for Excel (PE 3.3)	ChemBio Office 12.0/ ChemDraw for Excel
Support of standard chemistry sketching applications <small>AccordDraw, CASDraw, ChemDraw, DS Viewer Pro, MarvinSketch, SymyxDraw, IsisDraw</small>	<small>SymyxDraw, ChemDraw, IsisDraw, MarvinSketch</small>	<small>AccordDraw, CASDraw, ChemDraw, DS Viewer Pro, MarvinSketch, SymyxDraw</small>	SymyxDraw	ChemDraw
Copy and paste between sheets or workbooks	Yes	Yes	Yes	Yes
Undoing the last chemical structure modification	Yes	No	No	No
Image, OLE object copy-paste and conversion	Yes	Yes	Yes	Yes
Customizable chemical structure display (stereo configurations, hydrogens, atom/bond properties, etc), customizable UI	Yes	No	No	No
Working environment	Excel sheet	Accord-enabled sheet	Excel sheet	ChemOffice-enabled sheet
SMILES, Chime, InChi, IUPAC conversion	All	SMILES	Chime, SMILES	SMILES
ID visualization upon hiding the molecular structure	Yes	Yes	No	Yes
Support for workflow tools	Yes	Yes	No	No

## Chemical data management through Microsoft Excel

Easy-to-use wizard interface to query and retrieve data from databases	MySQL, Oracle	AEI DB, MS Access, Oracle Enterprise Edition	MySQL, Iseentris DB, Oracle	No <small>ChemFinder List</small>
Fast and robust chemical structure file import	Yes	No	Yes	Yes
Name to structure conversion upon import	Yes	No	No	No
Batch reaction file import and management	Yes	Yes	Yes	No
Markush structure import	Yes	No	No	No
Customizable chemical structure export to databases	No	Yes <small>Enterprise Edition</small>	Yes	No

## Interaction with Microsoft Excel

### 1. Built-in chemistry functions

Physico-chemical parameter prediction: pKa, logP-logD	Add-on	Add-on	No	Yes
Partial charge calculations	Add-on	No	No	No
Topology analysis	Add-on	No	Yes	Yes
Molecular descriptors (indices, surface areas)	Add-on	No	No	Yes
Stereoisomer and tautomer count prediction	Add-on	No	No	No
2D structure cleaning	Yes	Yes	No	No
IUPAC name generation	Add-on	No	No	No
ADME property prediction	No	Add-on	No	No
Thermodynamic property prediction	No	No	No	Yes

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<b>Interaction with Microsoft Excel</b> <small>continued</small>				
<b>2. Chemical structures in 3 Dimensions</b>				
Conformations	Yes	No	No	No
3D structure cleaning	Yes	No	No	No
3D Molecular Descriptors: projection area, surface area, energy	Yes	No	No	Yes
<b>Direct Medicinal Chemistry Support in Microsoft Excel 2003/2007/2010</b>				
<b>Structure Searches and Filtering</b>				
Searches and filtering when importing from databases	Yes	Yes	Yes	No
Scaffold alignment and coloring	Yes	Yes	Yes	No
Structure filter	Yes	Yes	Yes	Yes
Similarity searches	Yes	Yes	No	Yes
<b>R-group decomposition</b>				
Pivoting/Direct SAR support	No	No	Yes	No
Decomposition in Excel	Yes	Yes	Yes	Yes
<b>Virtual library enumeration</b>				
Reaction enumeration	Add-on	Add-on	Yes	Yes
Enumeration engine as Excel function	Add-on	No	No	No
Reaction library	Add-on	No	No	No
Flexible reactants/products/reaction placement, usability	Flexible	Fixed	No	Fixed
Markush enumeration	No	Add-on	Yes	No
<b>Publishing and Reporting</b>				
Multiple structure cleaning	Yes	Yes	No	No
Multiple image generation	Yes	Yes	No	No
Multiple standardization	Yes	No	No	No

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