

JChem for Excel in Drug Discovery

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ChemAxon
Solutions for Cheminformatics

What is new since last year?

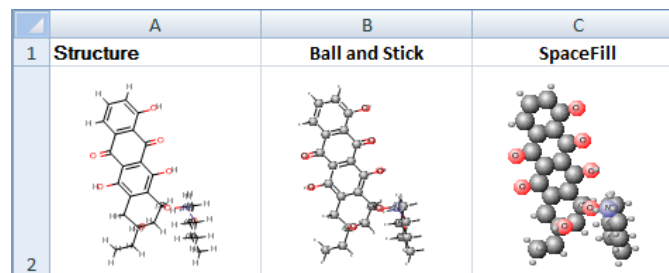
- Marvin .NET Included
- Structure drawing settings
- Image and Structure resulting functions
 - Display Options, Plug-Ins, Structural Framework,..
 - Standardizer, Reactor
- Copy-Paste (from-to)
 - Marvin, other popular editors
 - Other Office applications with OLE
 - Workbook-workbook
- Convert to Structure
 - From SMILES
- API
- Fast startup

What is (will be) new in 5.3.x?

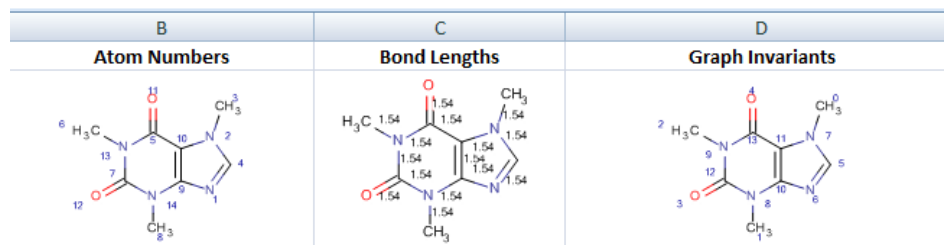
- Third party editors:
 - ChemDraw®,
 - ISIS Draw®, Symyx Draw®
- Third party cartridges:
 - Symyx Cartridge®,
 - IDBS Cartridge®
- Marvin OLE Support in Marvin .NET
 - No need for Java for any of the features
- Customizable UI

Image Resulting Functions

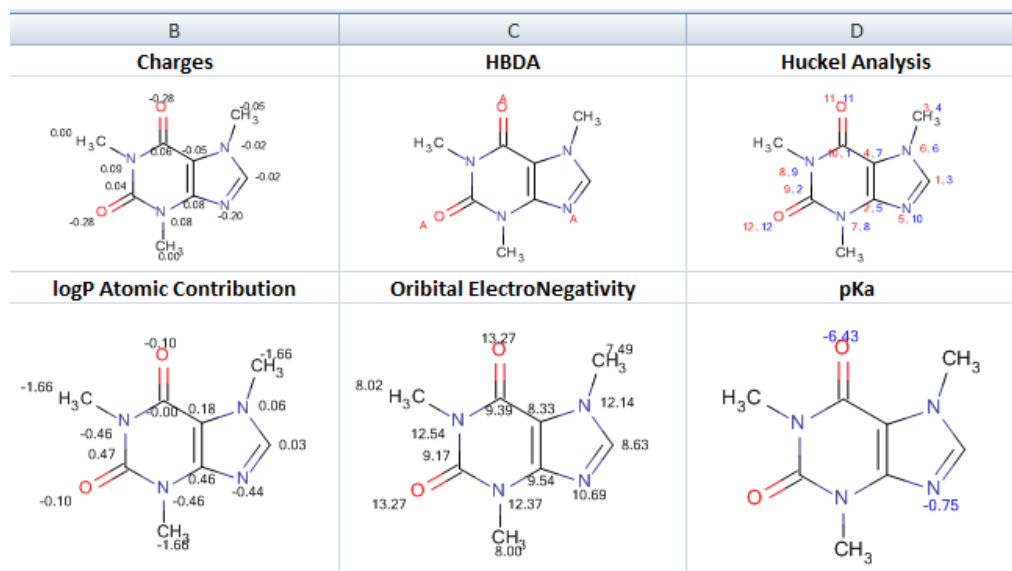
- **Rendering**



- **Display Options**

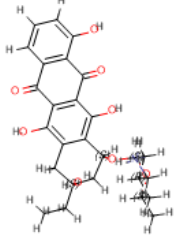
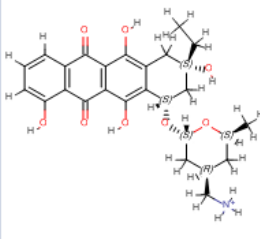
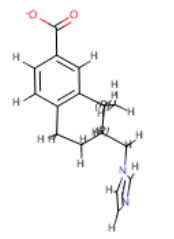
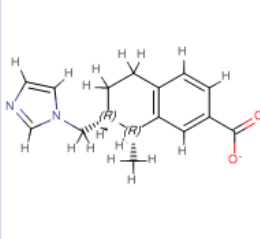
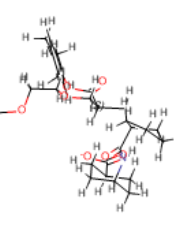
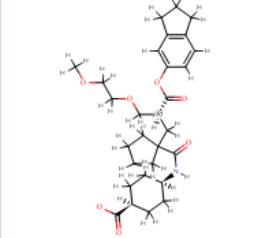


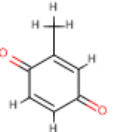

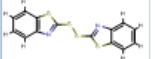
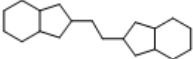
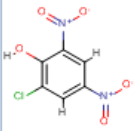

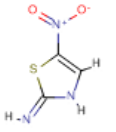

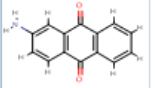
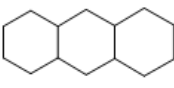
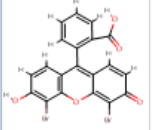
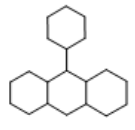
- **Plug-Ins**



Structure Resulting Functions

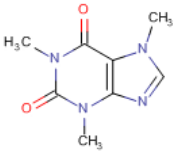
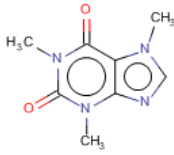
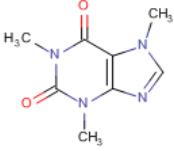
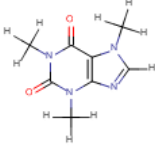
- 2D Clean - Structural Framework

	A	B
1	Structure	2D Cleaned
2		
3		
4		

	A	B
1	Structure	Framework
2		
3		
4		
5		
6		
7		

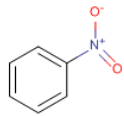
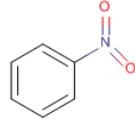
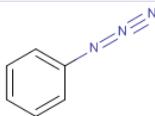
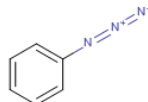
Functions - Standardizer

- Simple

	A	B	C
1		aromatize	
2		addexplicitH	

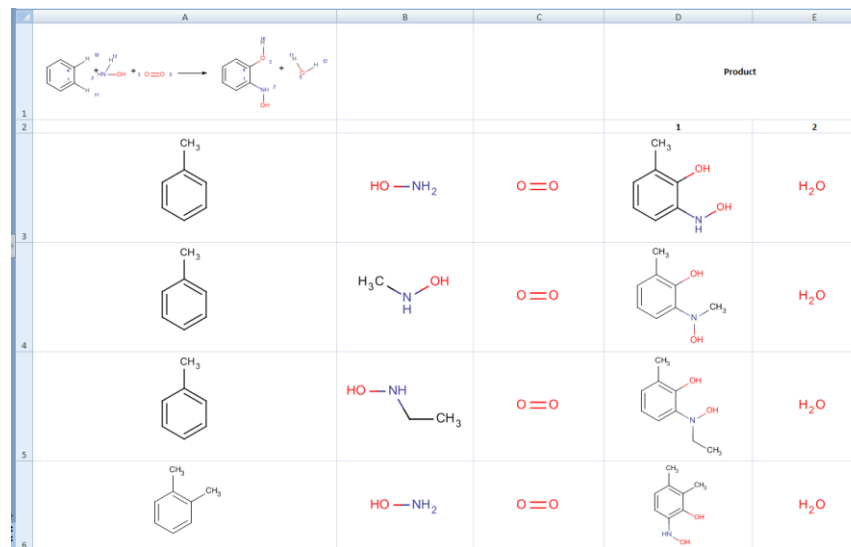
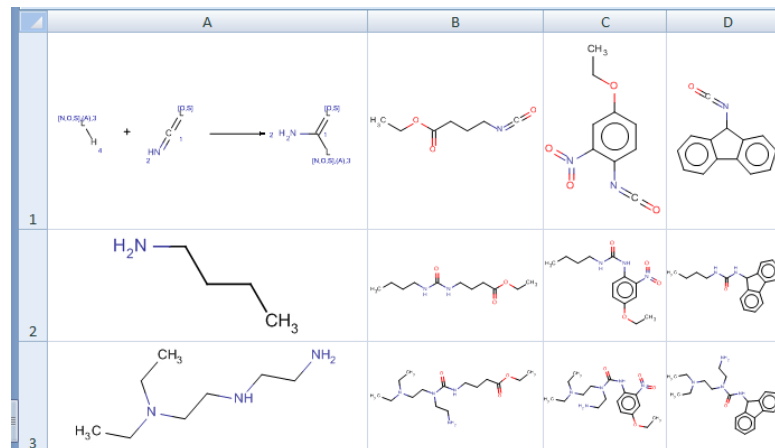
- Custom

- Complex, multi step

	A	B	C
1		Converting nitro mesomers	
2		$[O:-2][N+:1]=O>>[O:2]=[N:1]=O$	
3		Converting azide mesomers	
4		$N=[N:1]\#[N:2]>>N=[N+:1]=[N:-2]$	

Functions - Reactor

- **Matrix Arrangement**
- **Multiple products, product lists**
- **Products, reactions**
- **Reactivity, selectivity rules**



Demonstration

- Virtual library generation
- Compound profiling
- Sorting by scaffold structure
- Descriptor visualization using radar chart
- R-group decomposition
- Structural similarity visualization
- Structure canonicalization

Future Developments

- Import from Database
 - Import related tables: 1-1, 1-N
 - Relational data mapping, merged rows, outlines.
 - Preview data in grid, before placing in Excel
 - Load and save queries
 - Hierarchical AND / OR criteria
 - IJC
- Import from Web Services
 - JChem, PubChem, ChemSpider,...
- SharePoint integration
- R-Group Decomposition
 - Multiple query structures
- Markush Structure enumeration
- ...