

# JChem for Excel in Drug Discovery

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**ChemAxon**  
*Solutions for Cheminformatics*

# What is new since last year?

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- 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

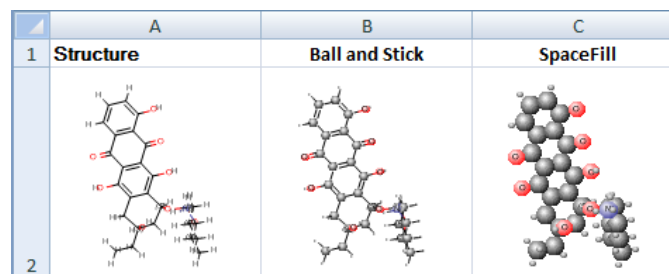
# What is (will be) new in 5.3.x?

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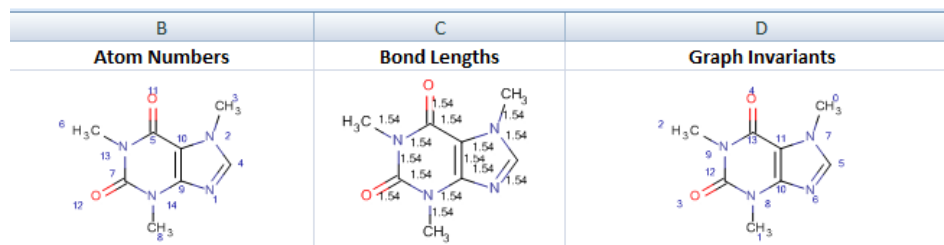
- Third party editors:
  - ChemDraw®,
  - ISIS Draw®, Symyx Draw®
- Third party cartridges:
  - Symyx Cartridge®,
  - IDBS Cartridge®
- Marvin OLE Support in Marvin .NET
  - No need for Java for any of the features
- Customizable UI

# Image Resulting Functions

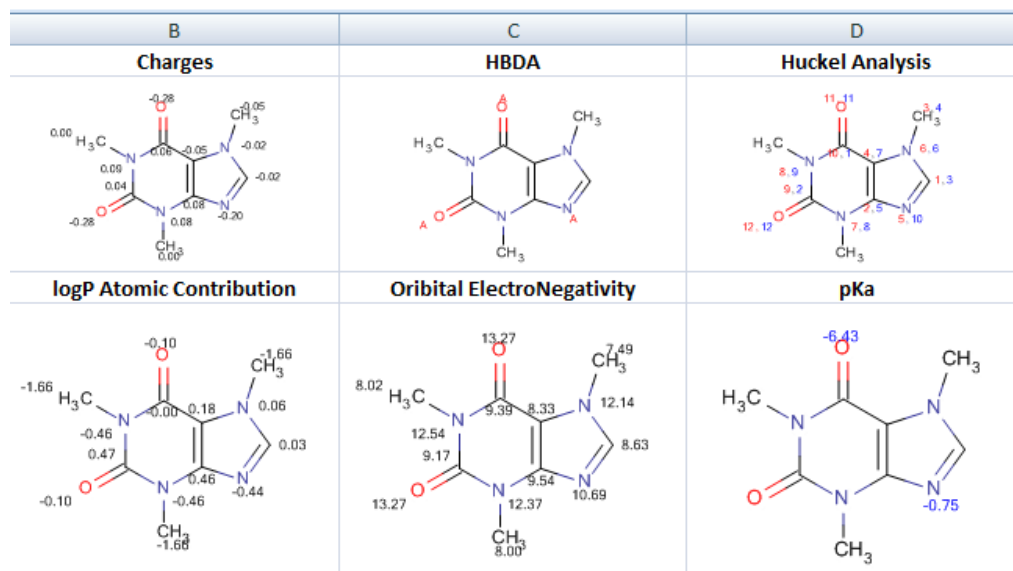
- **Rendering**



- **Display Options**

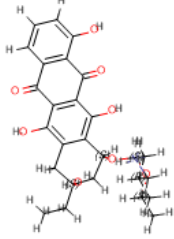
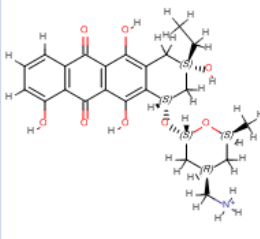
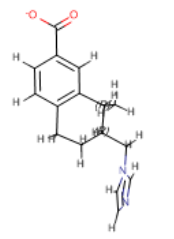
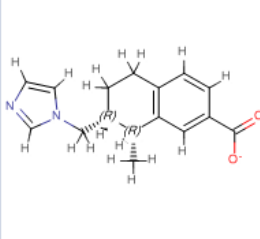
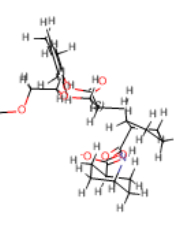
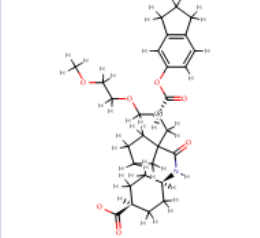


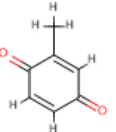

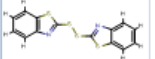
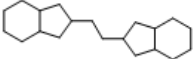
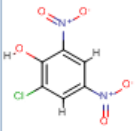

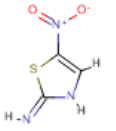

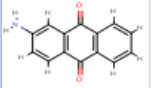
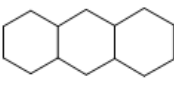
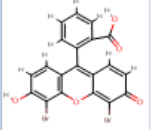
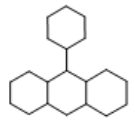
- **Plug-Ins**



# Structure Resulting Functions

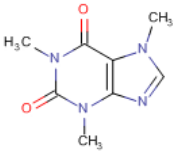
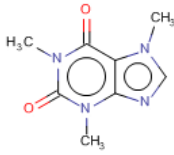
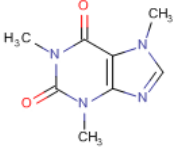
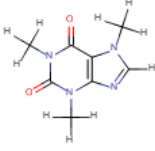
- 2D Clean - Structural Framework

	A	B
1	<b>Structure</b>	<b>2D Cleaned</b>
2		
3		
4		

	A	B
1	<b>Structure</b>	<b>Framework</b>
2		
3		
4		
5		
6		
7		

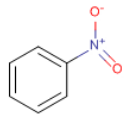
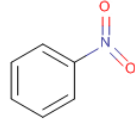
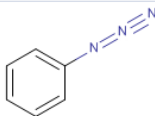
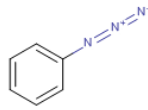
# Functions - Standardizer

- Simple

	A	B	C
1		aromatize	
2		addexplicitH	

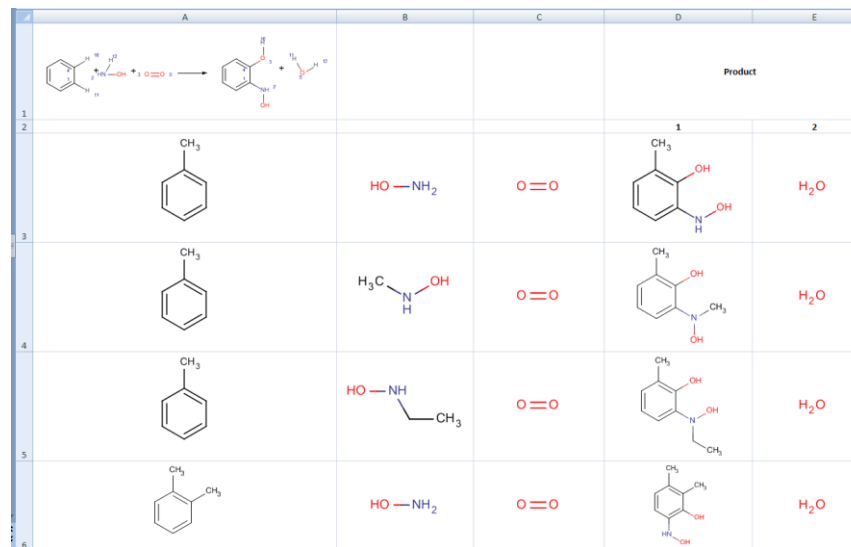
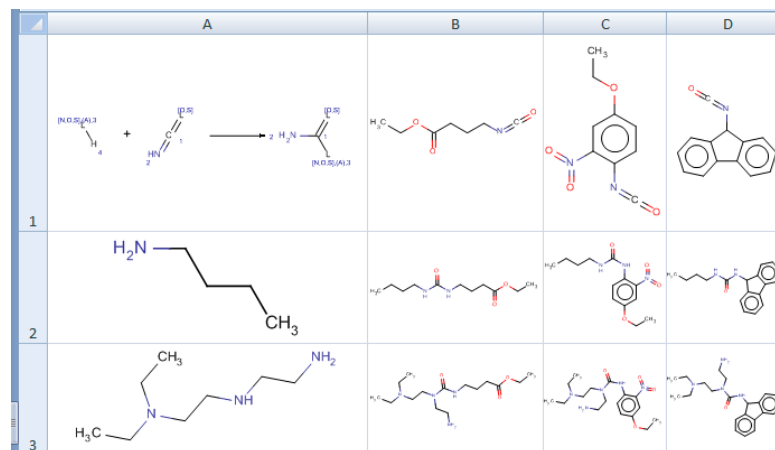
- Custom

- Complex, multi step

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

# Functions - Reactor

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



# Demonstration

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

# Future Developments

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- 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
- ...