

2<sup>th</sup>  
20

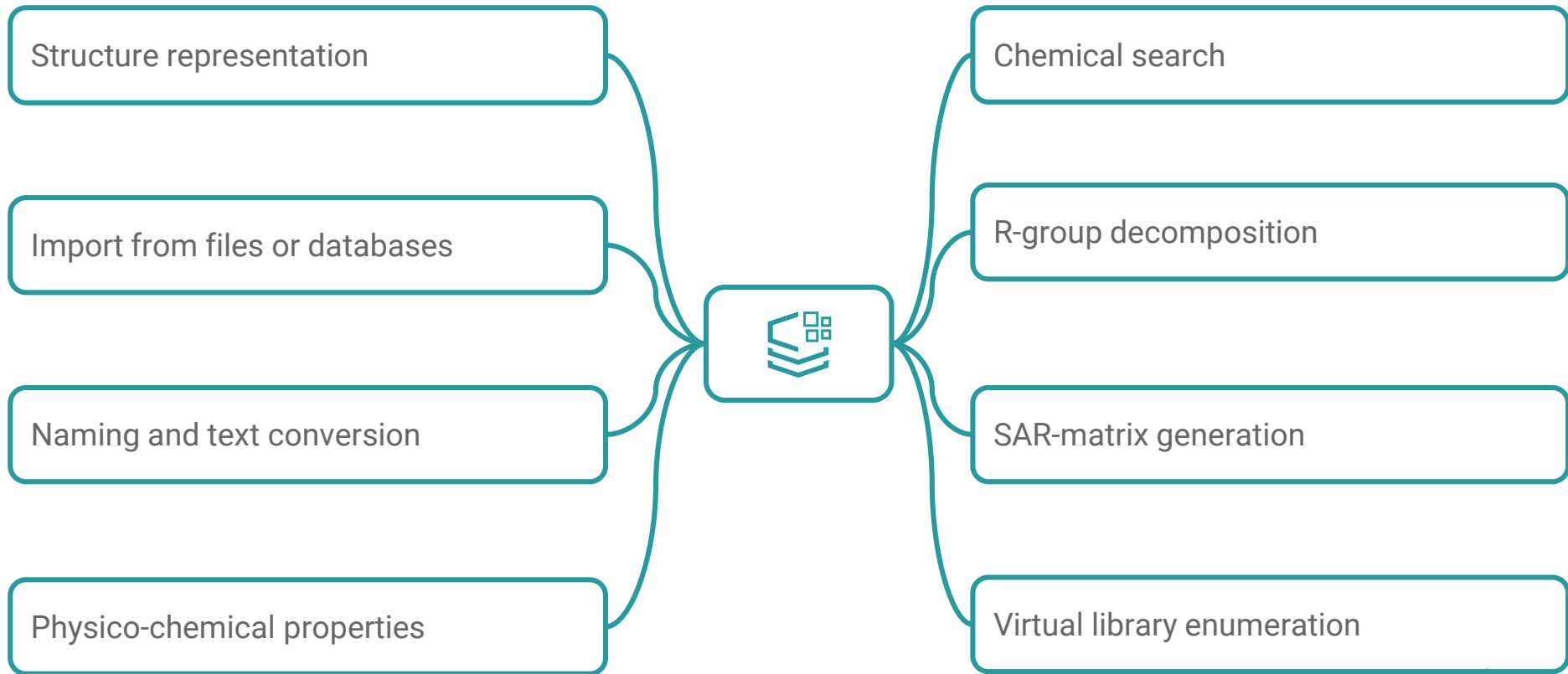
**anniversary**

**Serving drug discovery with  
cutting-edge software**



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Application Scientist

# Live Chemistry in Microsoft Office



# JChem for Office

**Atorvastatin Pharmacogenetics**

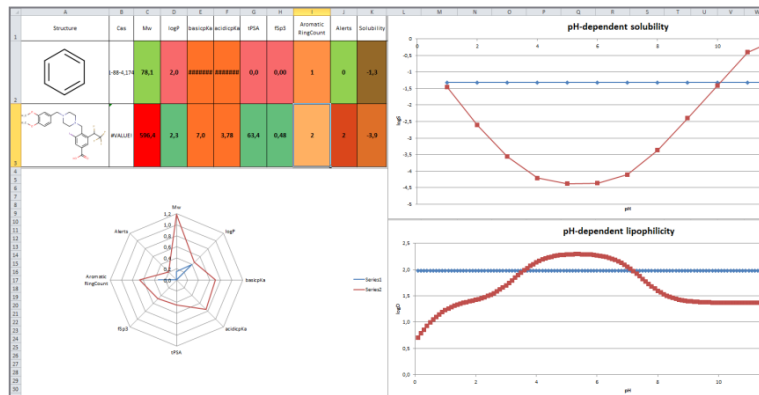
Several genetic [polymorphisms](#) have been found to be associated with a higher incidence of undesirable side effects of atorvastatin. This phenomenon is suspected to be related to increased plasma levels of pharmacologically active metabolites, such as atorvastatin lactone and  $\beta$ -hydroxyatorvastatin. Atorvastatin and its active metabolites may be monitored in potentially susceptible patients using specific chromatographic techniques.<sup>[1]</sup>

**Chemical synthesis**

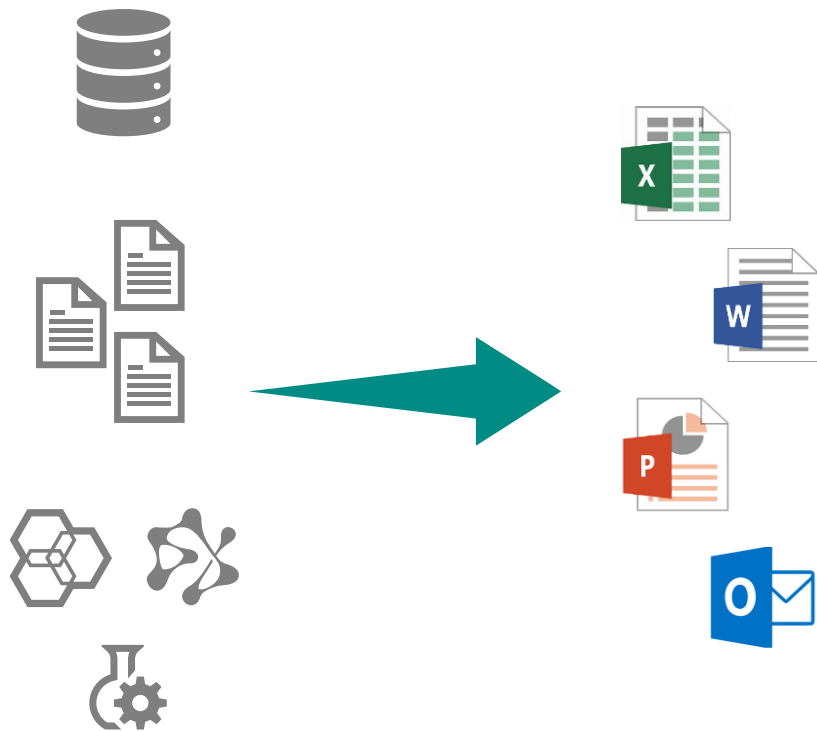
Atorvastatin synthesis in commercial production (process chemistry). The key step of establishing this drug's stereocenters, through initial use of an inexpensive natural product [chiral pool](#) approach.

Atorvastatin synthesis during discovery chemistry. The key step of establishing stereocenters, using of a chiral ester auxiliary approach.

- Live molecules
- Import from several sources
- Chemical intelligence
- Pre-defined display settings for easy reporting
- Well-known environment



# Import



- Chemical file
- Relational database
- JChem Web Services
- Instant JChem, Plexus Suite
- N2S and S2N conversion
- Extracts structures from documents

# Property calculations

The screenshot displays the ChemAxon JChem software interface. The main window shows a table with columns for Structure, Reference, SMILES, LogP, and LogS. A 'Compound Characteristics' radar chart is overlaid on the table, showing various calculated properties for the selected compound. The table contains five rows of data, each representing a different chemical structure and its associated properties.

Structure	Reference	SMILES	LogP	LogS
	Chem. Lett. 12(2)-2002 243-248	<chem>CN(C)CC1CC2N(O)1c3cc(C)ccc3Occcc24</chem>	4.98	-5.967
	471 Bloorg. Med. Chem. Lett. 12(2);		3.35	-4.09
	472 Bloorg. Med. Chem. Lett. 12(2);		4.3	-5.122
	473 Bloorg. Med. Chem. Lett. 12(2)-2002 243-248	<chem>CN(C)CCC1CC2N(O)1c3cccc3Occcc24</chem>	4.79	-5.644

- Elemental analysis
- Protonation, partitioning
- H-bond donor/acceptor
- Isomers, tautomers
- Topology, geometry
- Drug-likeness filters
- Charge

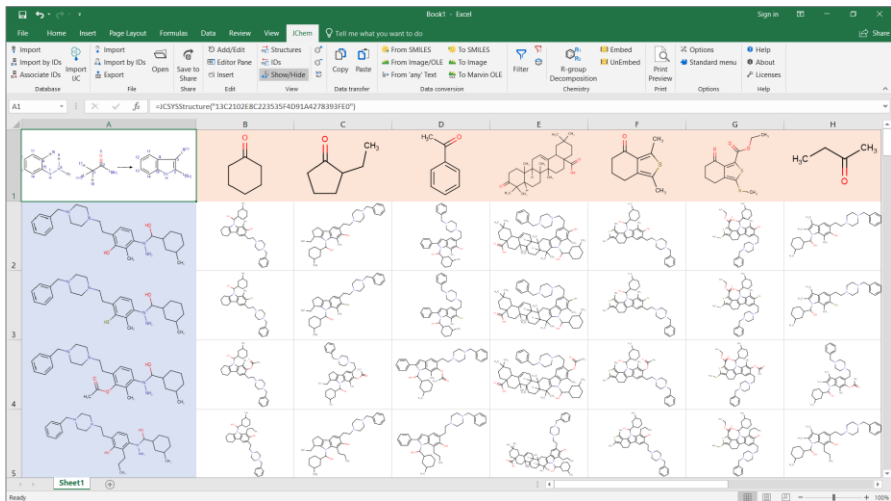
# Chemical search

- Substructure
- Full structure
- Duplicate
- Superstructure
- Similarity
- Search options
- Hit alignment

The screenshot displays the ChemAxon software interface. The main window shows a table with columns for 'cd\_id', 'cd\_structure', 'Mass', 'Formula', and 'IUPAC name'. The table contains four rows of chemical data. A 'Filter' dialog box is open, showing a chemical structure of a benzene ring with two hydroxyl groups (OH) attached. The dialog includes search options such as 'Substructure', 'Similarity', and 'Full structure'.

cd_id	cd_structure	Mass	Formula	IUPAC name
60		318.281	C16H14O7	[3R]-3-[(1,4-dihydroxyphenyl)methyl]-3,7,8-trihydroxy-3,4-dihydro-2H-1-benzopyran-4-one
61		320.297	C16H16O7	[3R,4R]-3-[(1,4-dihydroxyphenyl)methyl]-3,4-dihydro-2H-1-benzopyran-3,4,7,8-tetraol
62		302.282	C16H14O6	[1R,10S]-6-oxatetracyclo[8.7.0.0 <sup>1,9</sup> .0 <sup>1,7</sup> ]heptadeca-2,4,6,11,12,13,15-hexaene-5,6,10,14,15-pentol
		286.283	C16H14O5	3-[(1,4-dihydroxyphenyl)methyl]-2H-chromene-7,8-diol

# Virtual library generation

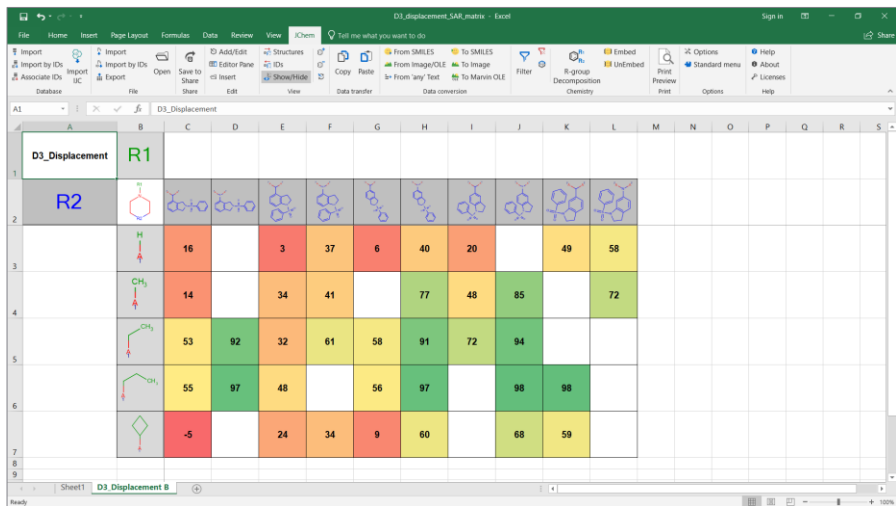


- Reaction-based library enumeration
- Reactivity and selectivity prediction via empirical smart rules



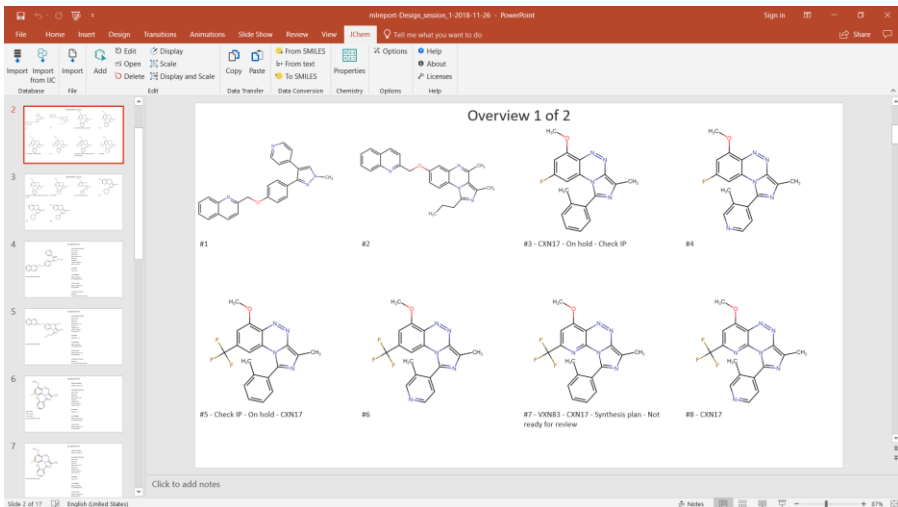
# SAR-analysis

- Decompose your molecules
- SAR-matrix
- Heat map
- Report in PowerPoint



# Reporting

- Pre-defined display options
- Unified structure layout
- Reports with „live” molecules
- Shareable files



# Live demo





# THANK YOU

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