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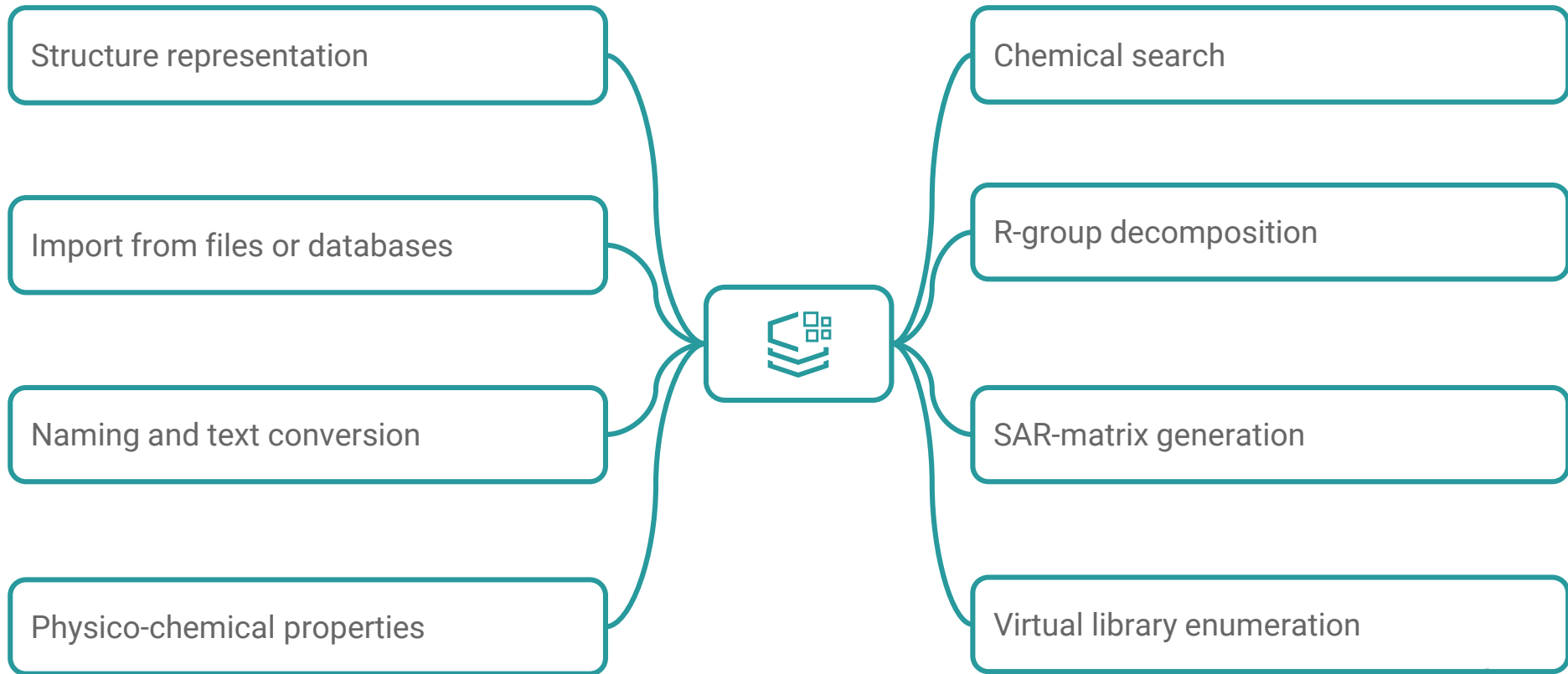
anniversary

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



Dóra Barna, PhD
Application Scientist

Live Chemistry in Microsoft Office



JChem for Office

The screenshot shows the JChem for Office application window. The main area displays text about Atorvastatin Pharmacogenetics, including a paragraph about genetic polymorphisms and a chemical synthesis reaction. A smaller window in the foreground shows a chemical structure editor with a benzene ring and a hydroxyl group.

Atorvastatin Pharmacogenetics

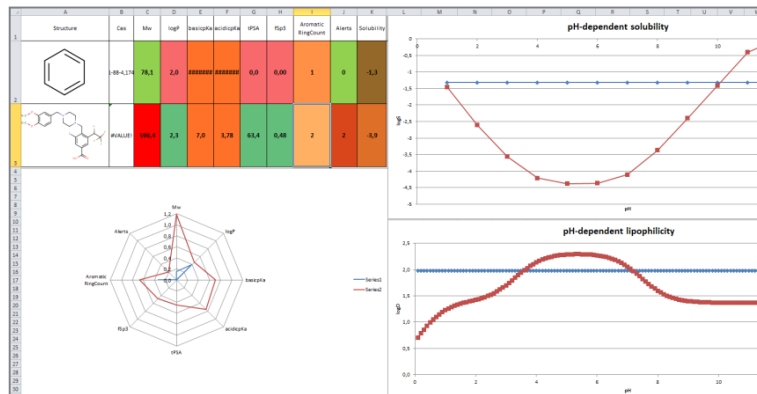
Several genetic [polymorphisms](#) have been found to be associated with a higher incidence of undesirable side effects of atorvastatin. This phenomenon is suspected to be related to increased plasma levels of pharmacologically active metabolites, such as atorvastatin lactone and β -hydroxyatorvastatin.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

Chemical synthesis

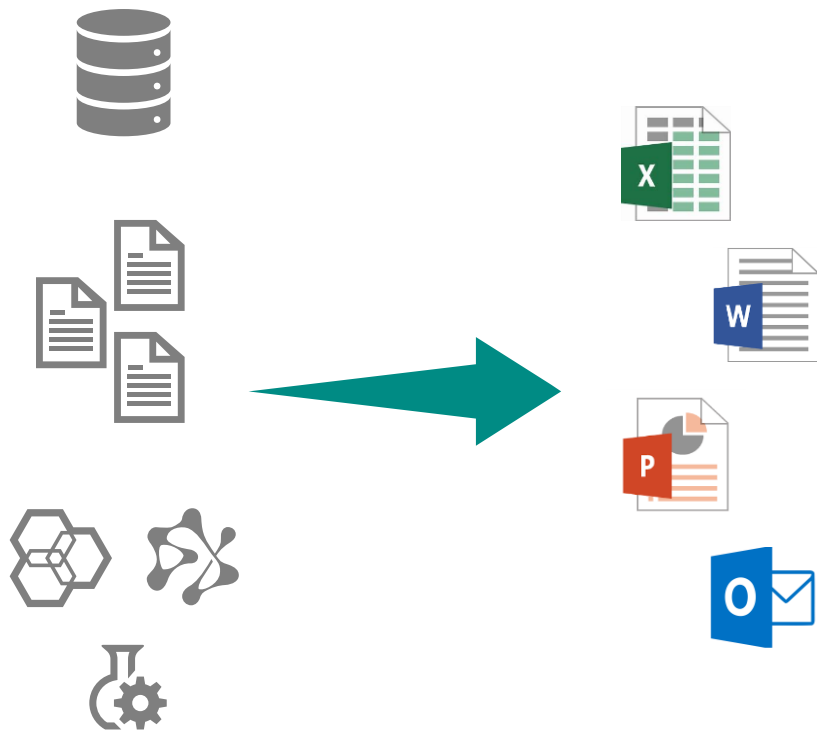
Atorvastatin synthesis in commercial production (process chemistry). The key step of establishing this drug's stereocenters, through initial use of an inexpensive natural product ([chiral pool](#) approach).

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)CC1CC2N(O)1c3cccc3Occcc24</chem>	4.79	-5.644

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

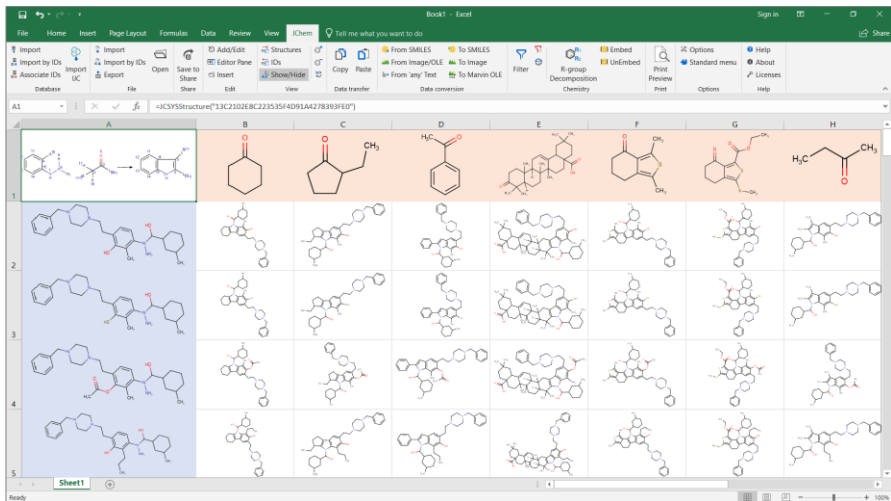
Chemical search

- 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-[(3,4-dihydroxyphenyl)methyl]-3,7,8-trihydroxy-3,4-dihydro-2H-1-benzopyran-4-one
61		320.297	C16H16O7	[3R,4R]-3-[(3,4-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 ^{1,9} .0 ^{1,7}]heptadeca-2,4,6,11,12,13,15-hexaene-5,6,10,14,15-pentol
		286.283	C16H14O5	3-[(3,4-dihydroxyphenyl)methyl]-2H-chromene-7,8-diol

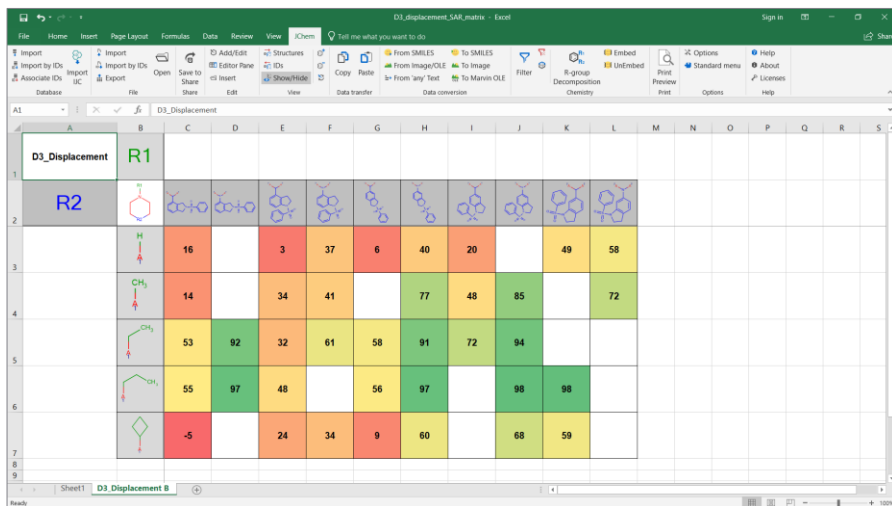
Virtual library generation



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

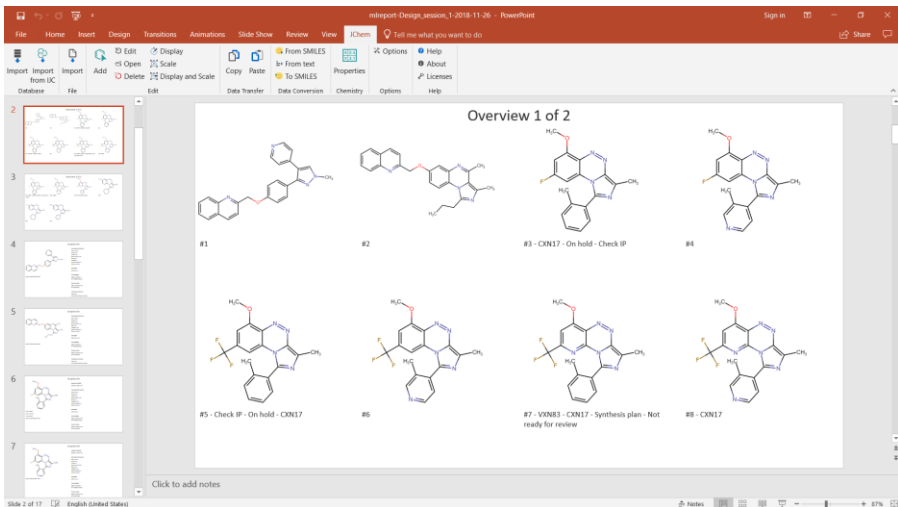
SAR-analysis

- 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

dbarna@chemaxon.com