ChemAxon

20th anniversary

Serving drug discovery with cutting-edge software

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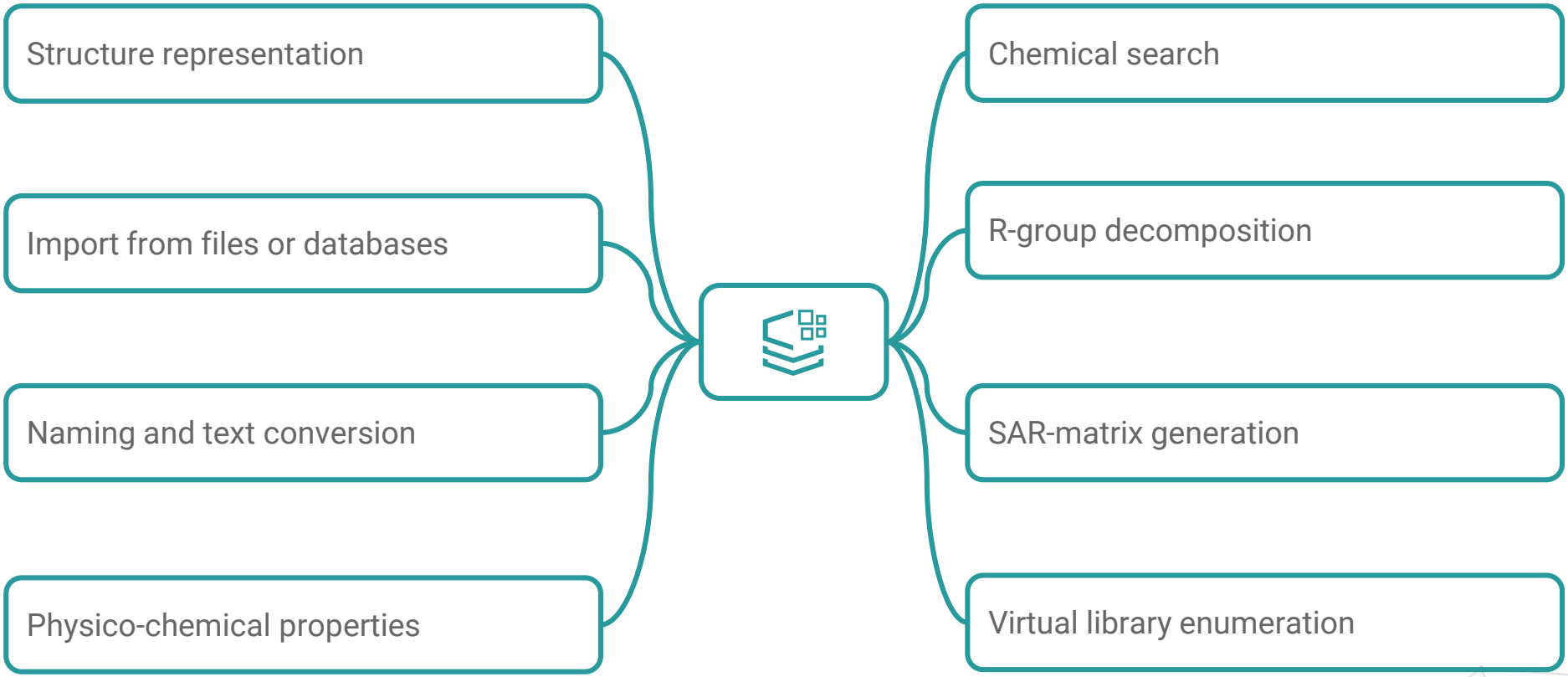
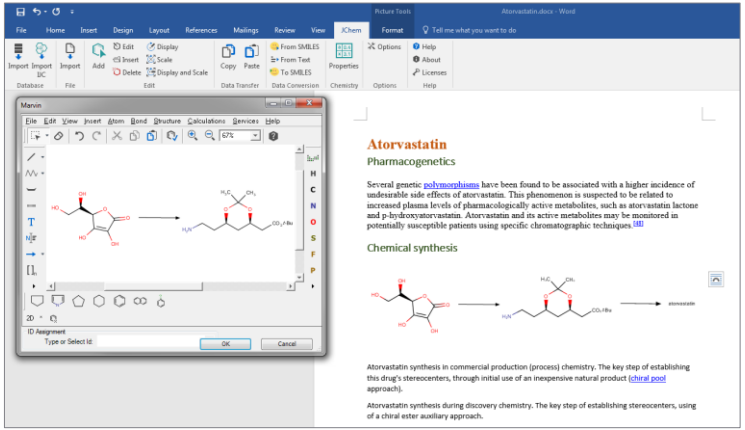
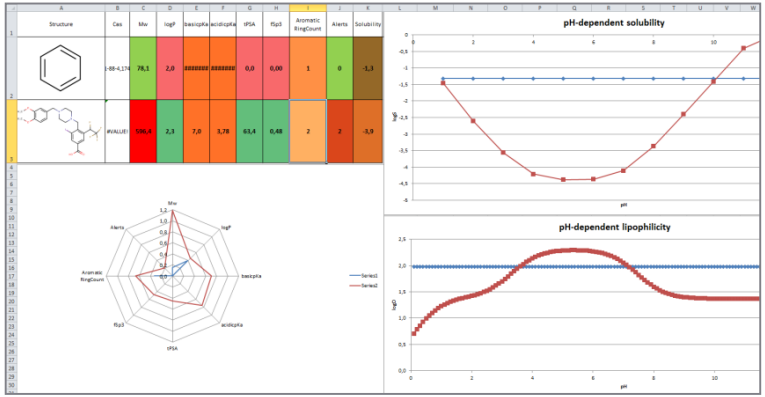
Application Scientist

Live Chemistry in Microsoft Office


Structure representation
Import from files or databases
Naming and text conversion
Physico-chemical properties
Chemical search
R-group decomposition
SAR-matrix generation
Virtual library enumeration





JChem for Office

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

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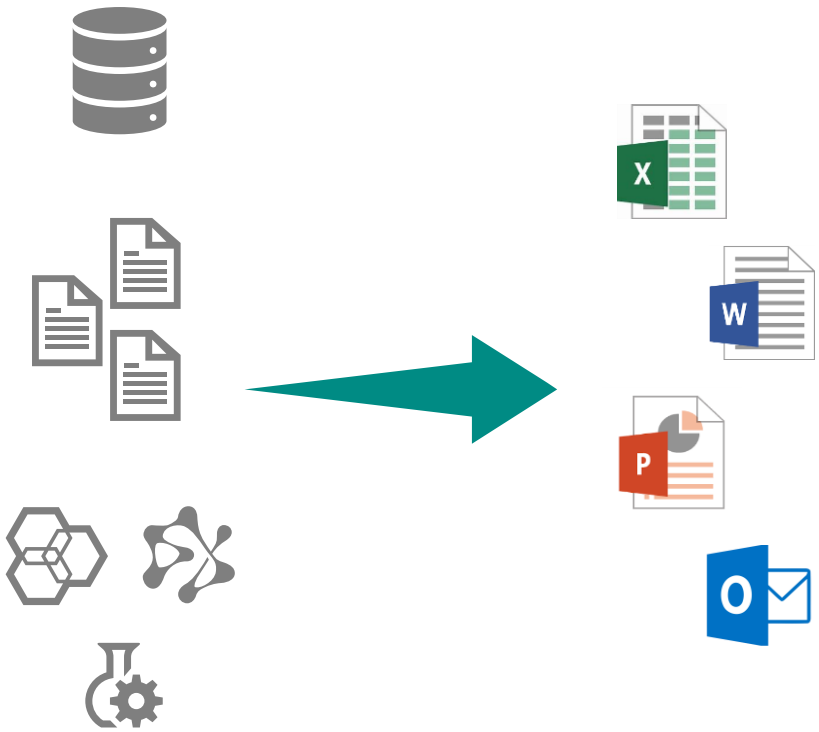
Import



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

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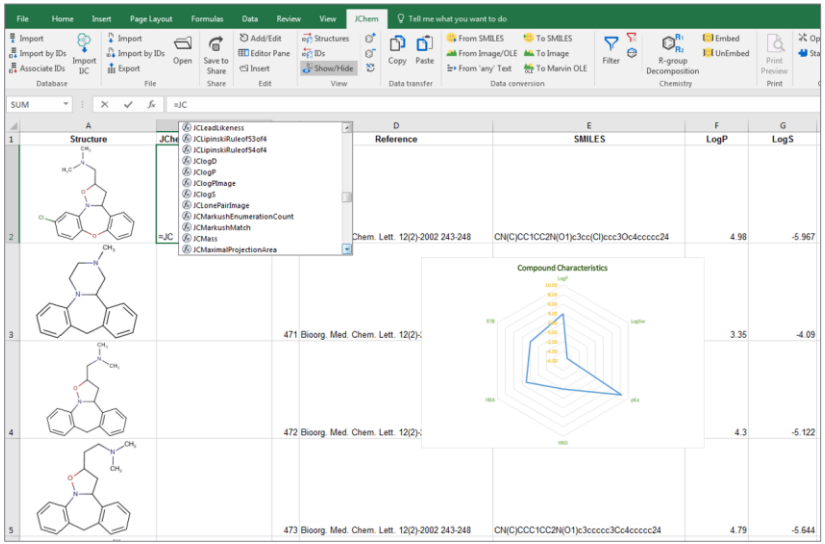
Property calculations



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

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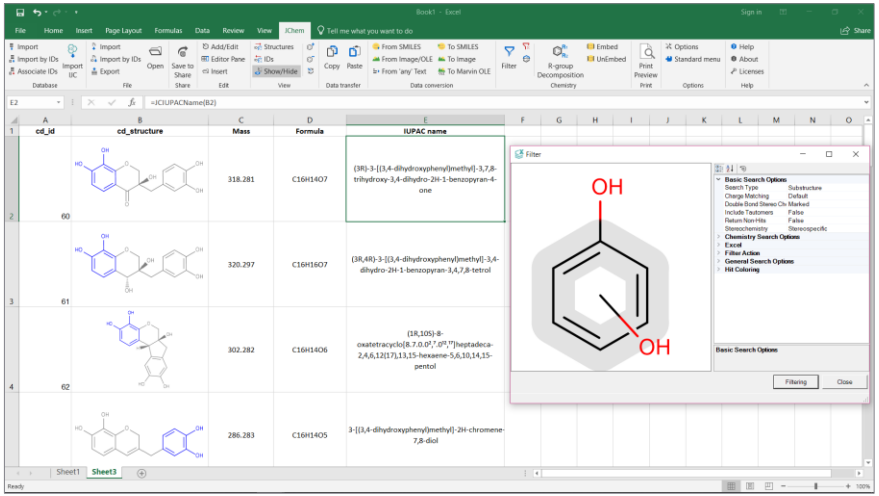
Chemical search



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

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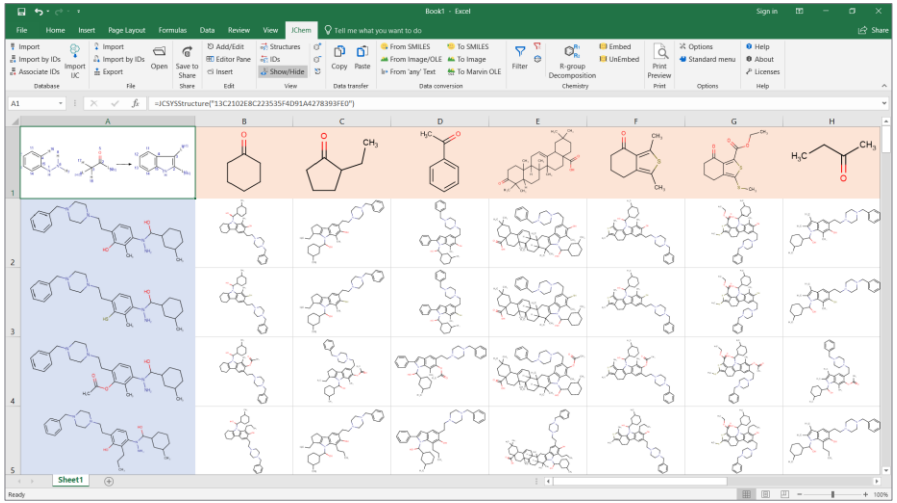
Virtual library generation



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

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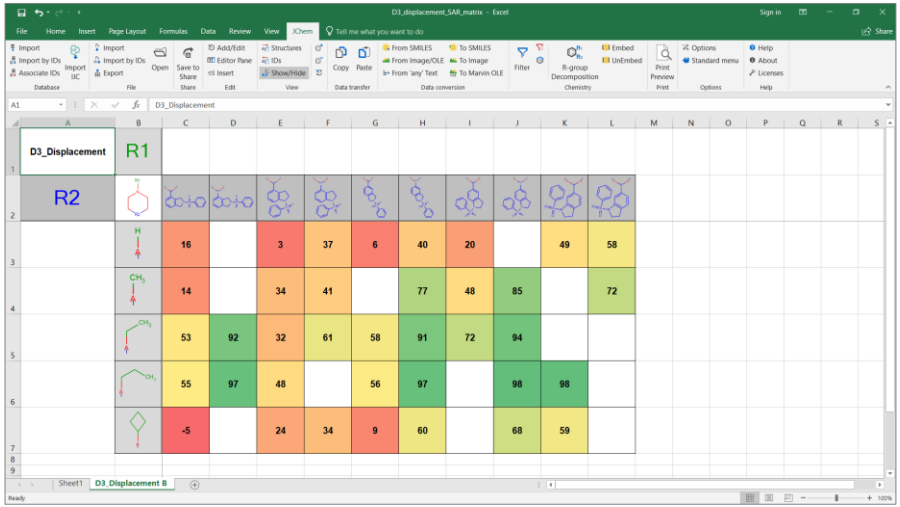
SAR-analysis



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

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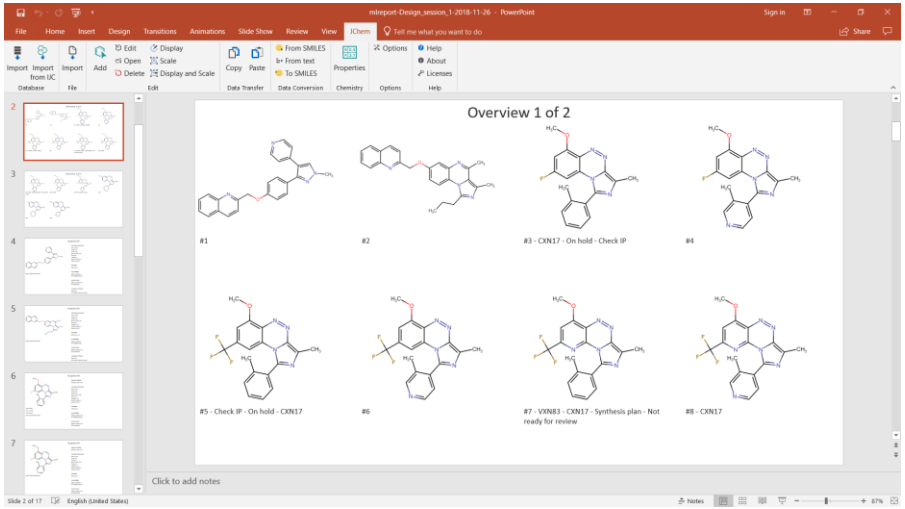
Reporting



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

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Live demo

THANK YOU

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