Quicker, Better, Sketcher

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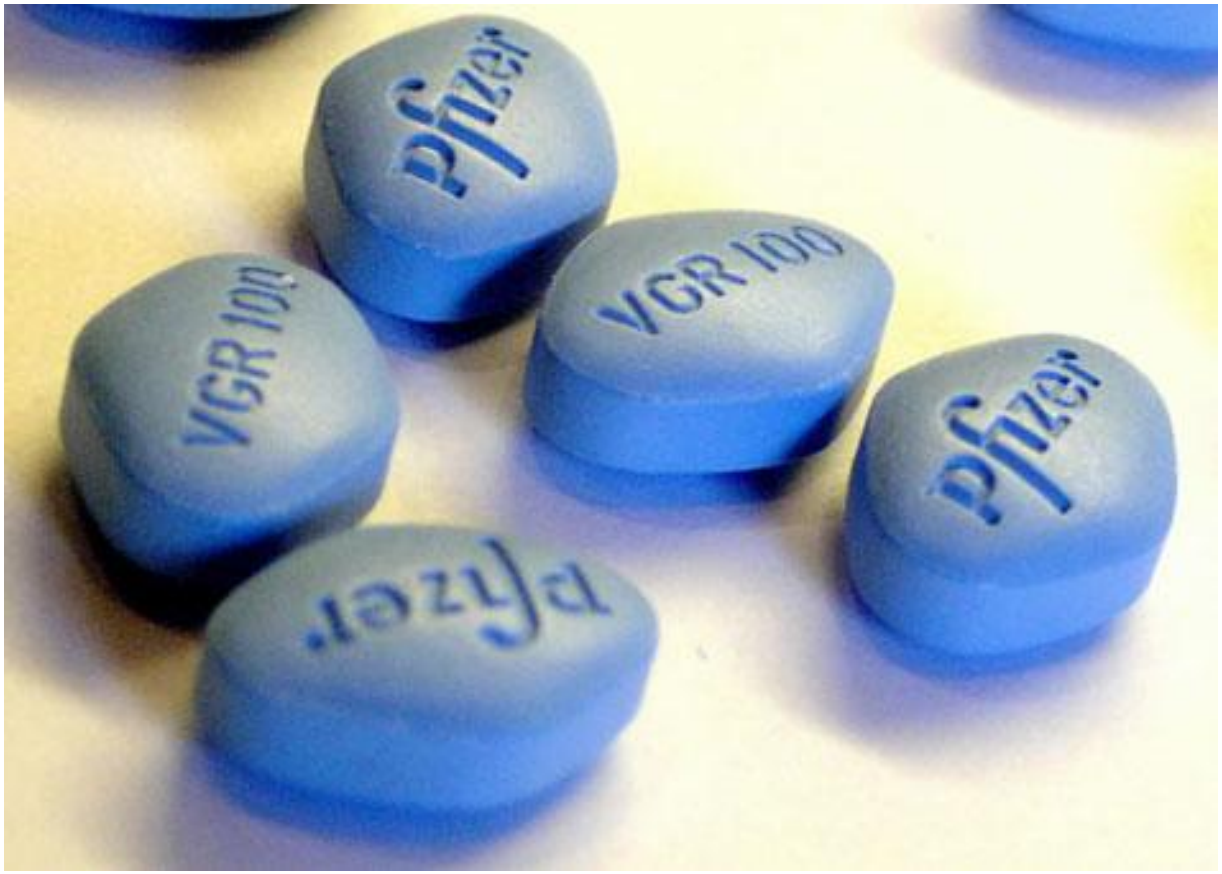
ChemAxon

Solutions for Cheminformatics

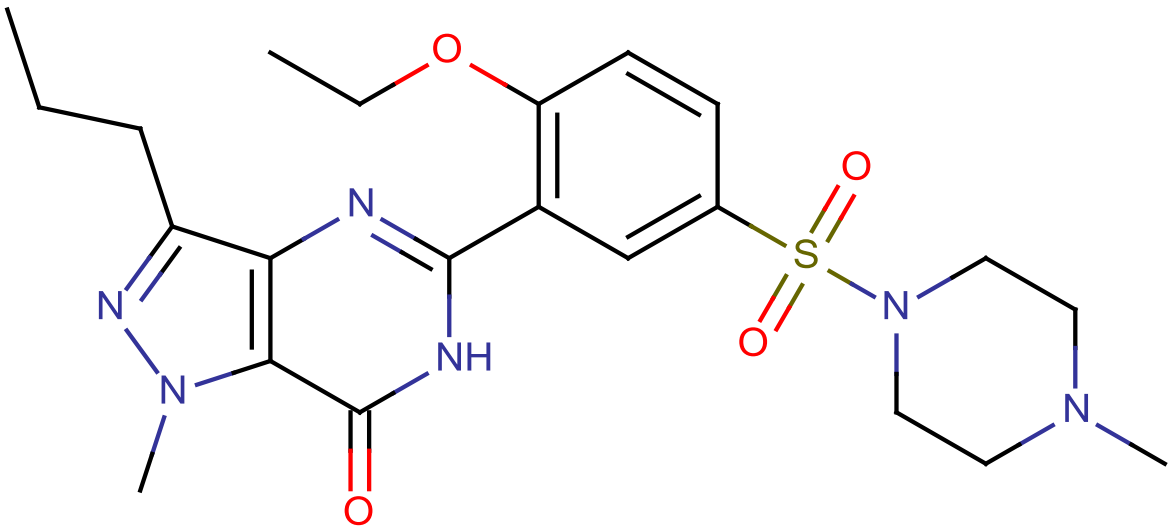
Content

- Tips and tricks for quick drawing
  - Sketching a molecule
  - Autorecognition during paste
  - Sketching a query
- Latest features you might not be aware
- Top features coming in version 5.4

Fast ways for entering a drug



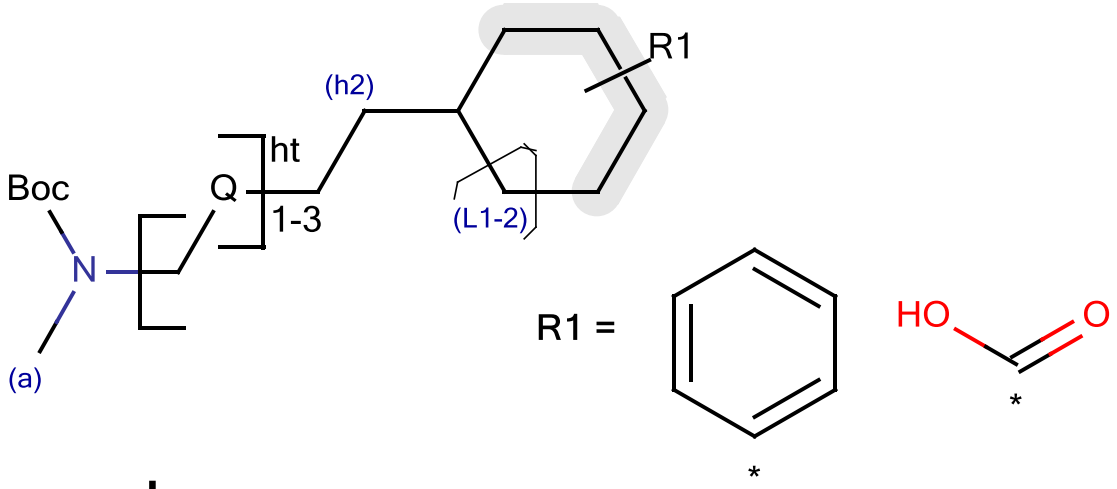
Sketching a Molecule



Tricks used:

- Shortcuts
  - 1: single bond
  - 2: double bond
  - O,N,S: atoms
  - Esc: select mode
- Quick multiple clicking at a terminal atom: chain
- Sprout drawing
- 2D clean

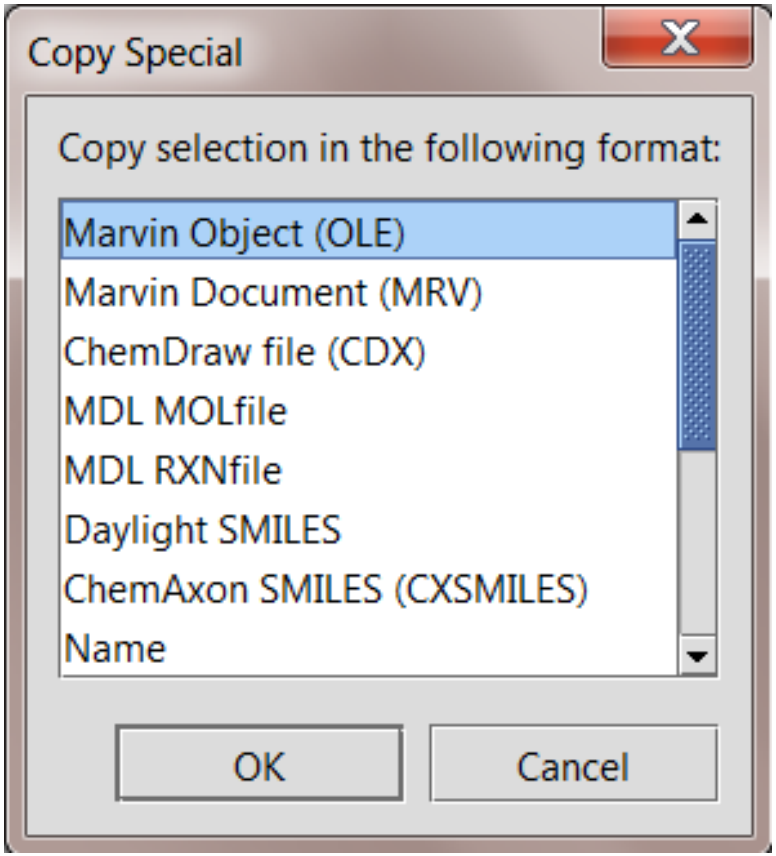
Sketching of a Query

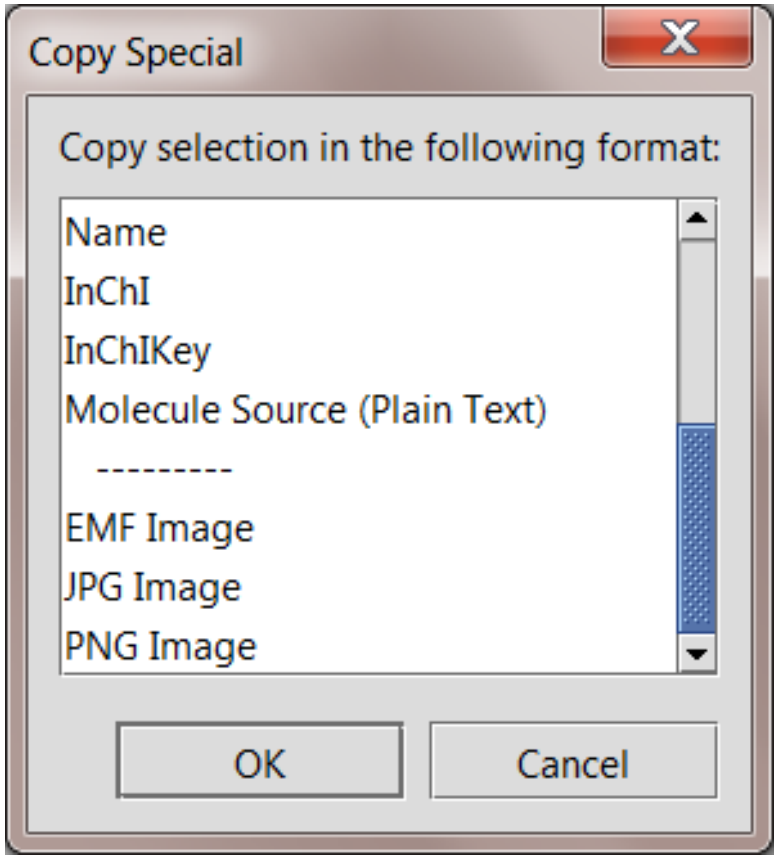


Tricks used:

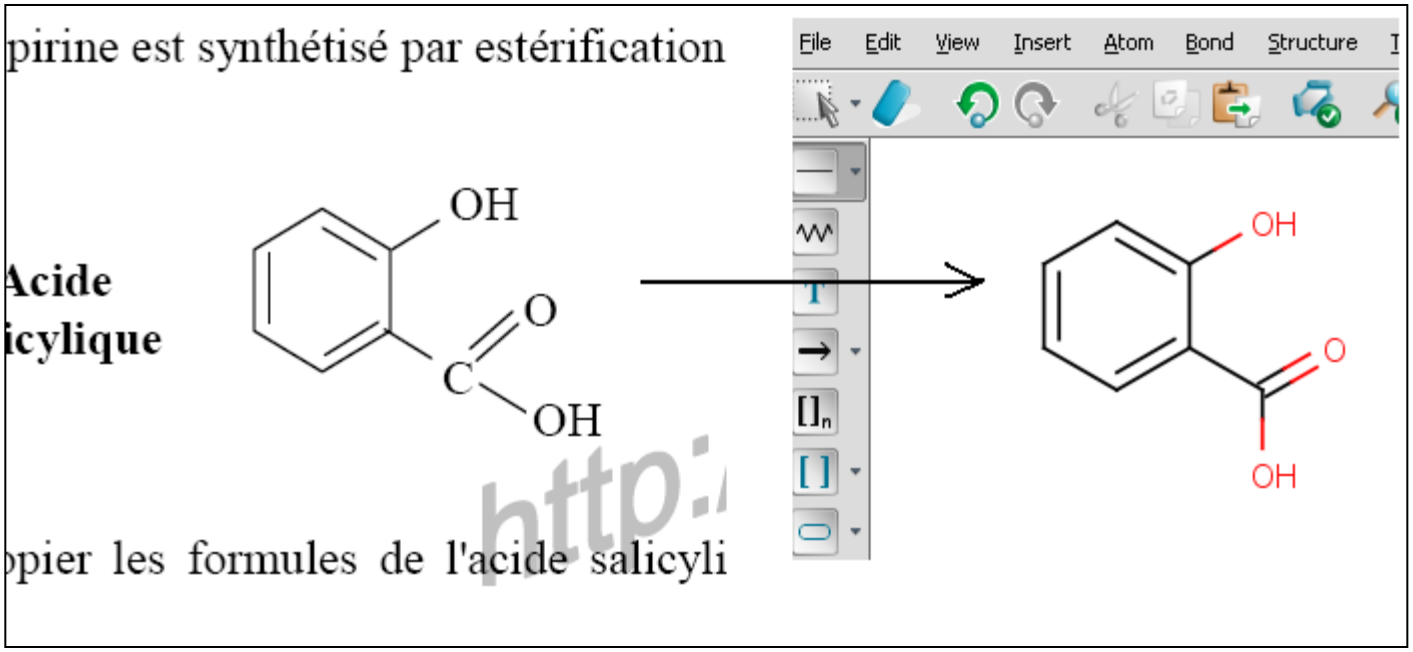
- Shortcuts
  - .a: aromatic atom
  - .h#: implicit Hs
  - R#: R atoms
- Abbreviated groups
- Link node
- Position variation
- Multiple group
- R-groups

Copy Special dialog

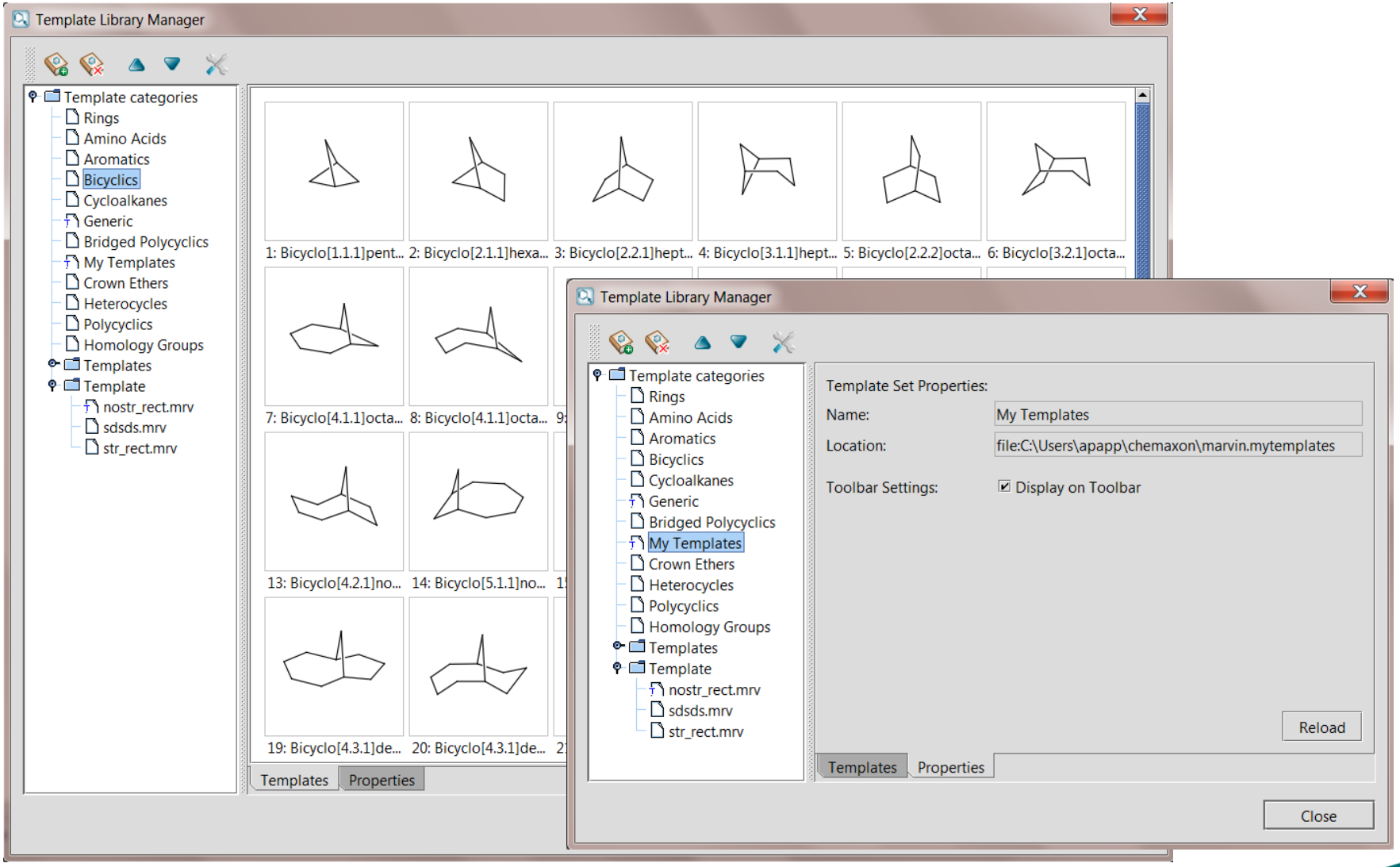




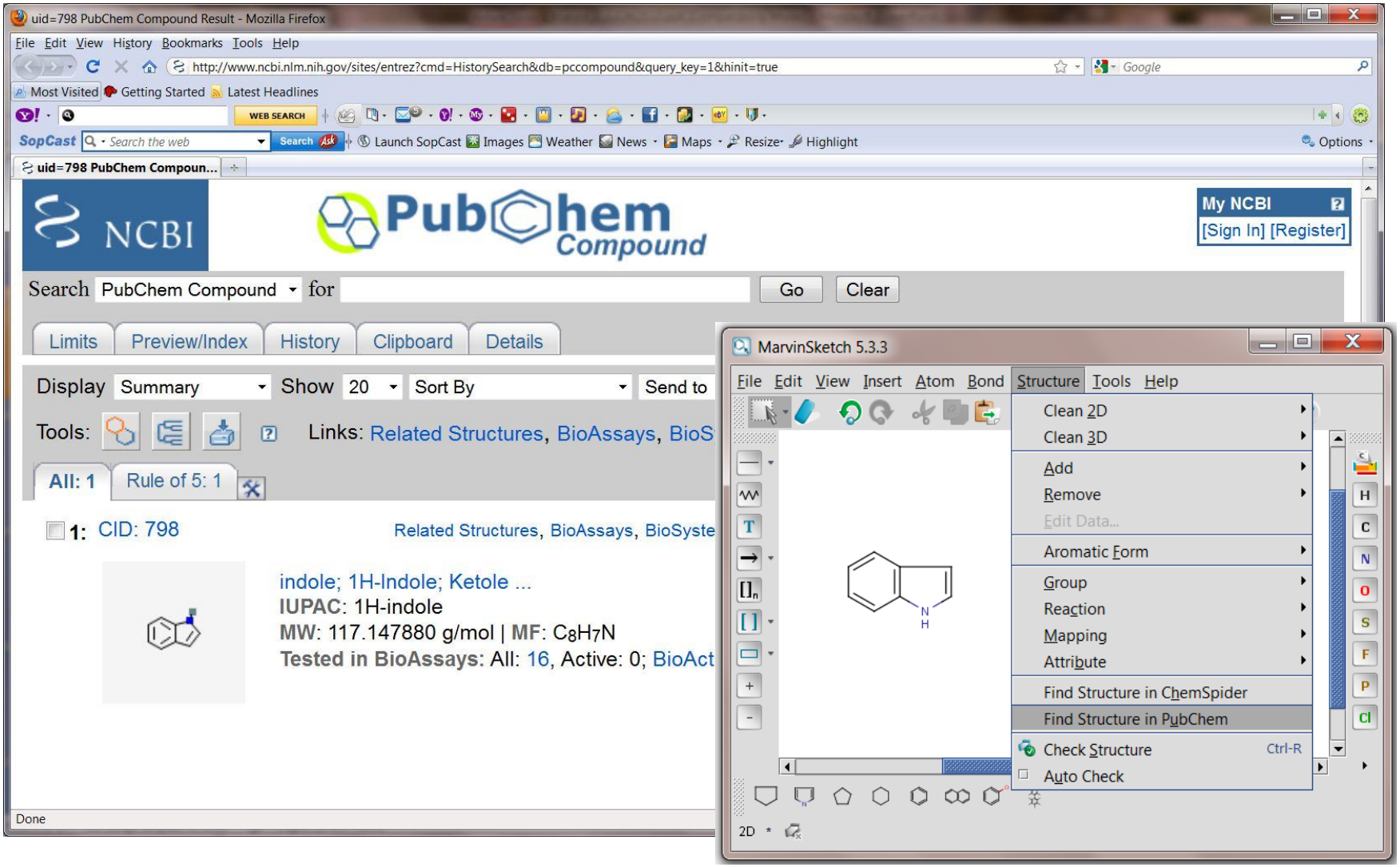
Converting Images to Structure using OSRA



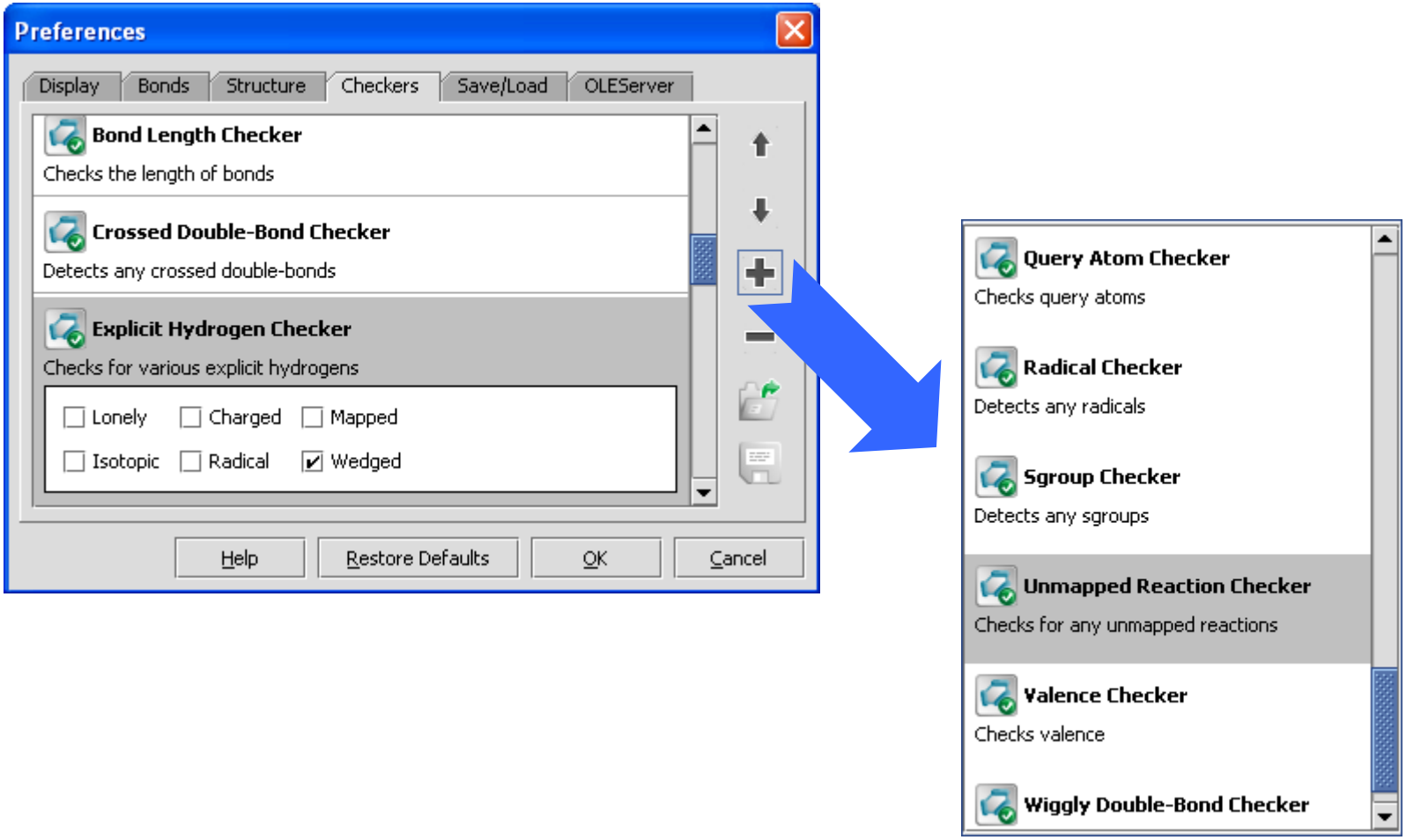
The New Template Library



Direct search in ChemSpider and PubChem



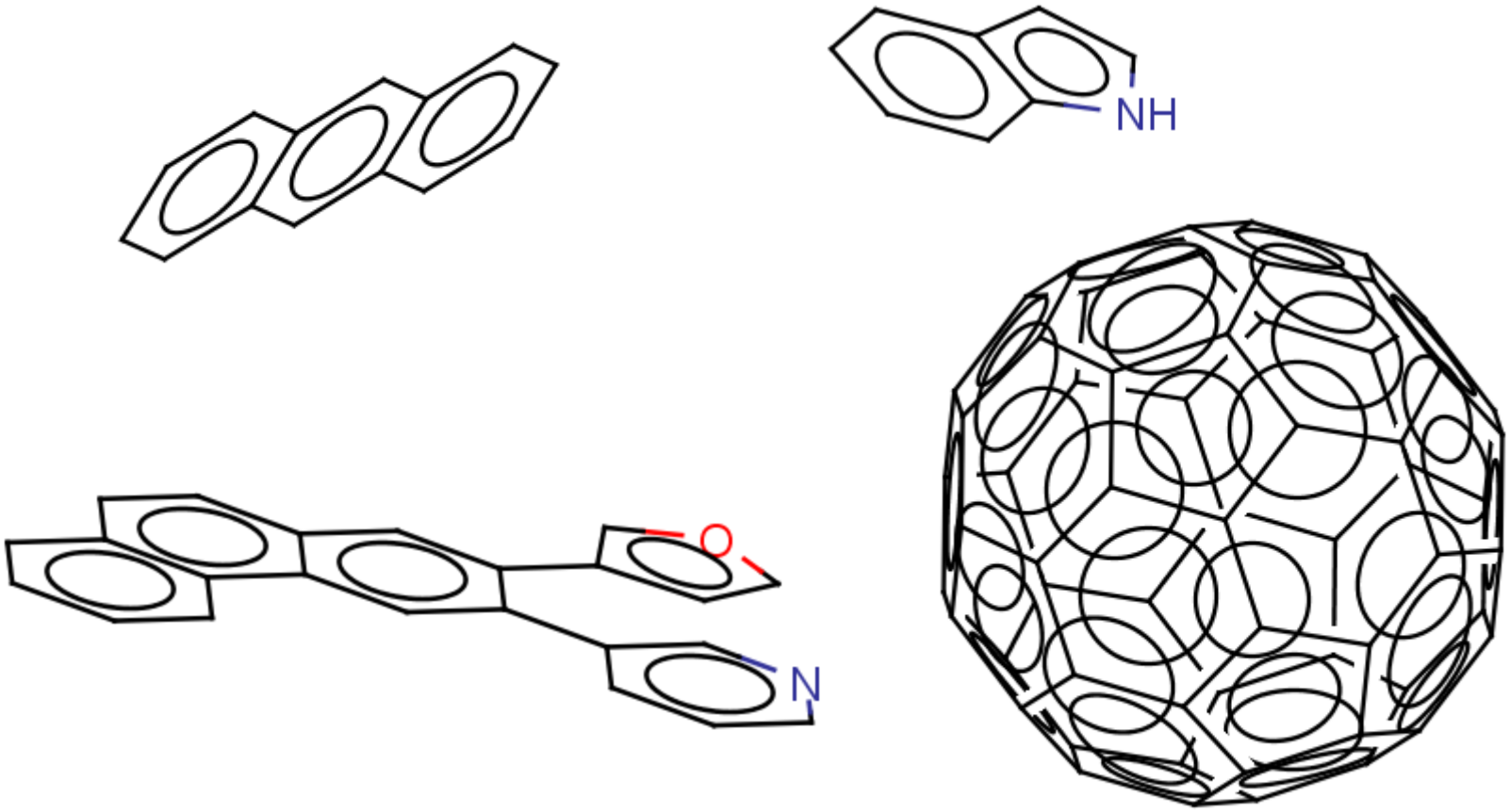
Structure checker in MarvinSketch GUI



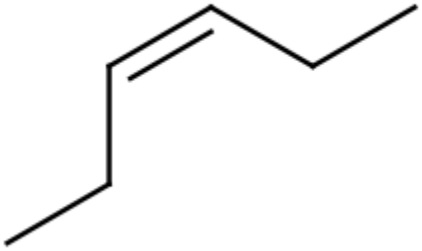
Coming in 5.4

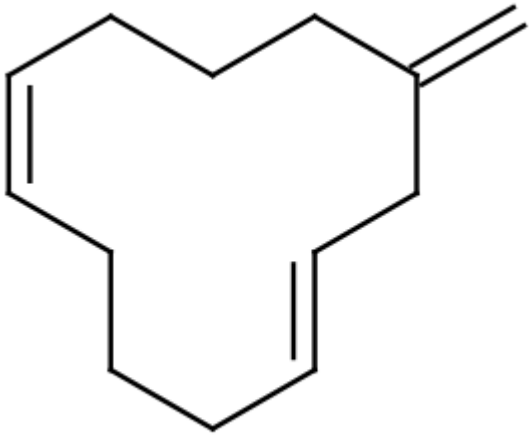
- Improvements towards presentation quality drawings
  - Projected structures (ellipses in aromatic rings)
  - Enhanced double bond drawing
- Improved 3D sketching
  - Enhanced 3D rotation and mirroring features
  - Directed merge of fragments in 3D
- Functionality improvements
  - Multiple, ordered attachment points in Markush structures
  - Atomic property editor
  - Storing molecule source in images (important for MAC docs)
- Technical Improvements
  - Full 64-bit support (MSpace, InChI on MAC, native libraries)
  - Customizable Attach Data dialog
  - Customizable clipboard handling in applets

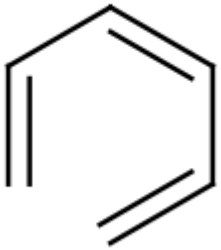
Ellipses in aromatic rings

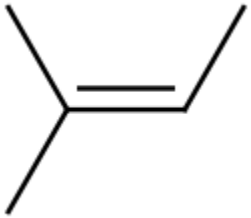


Enhanced double bond drawing









Acknowledgements