

Quicker, Better, Sketcher

Ákos Papp



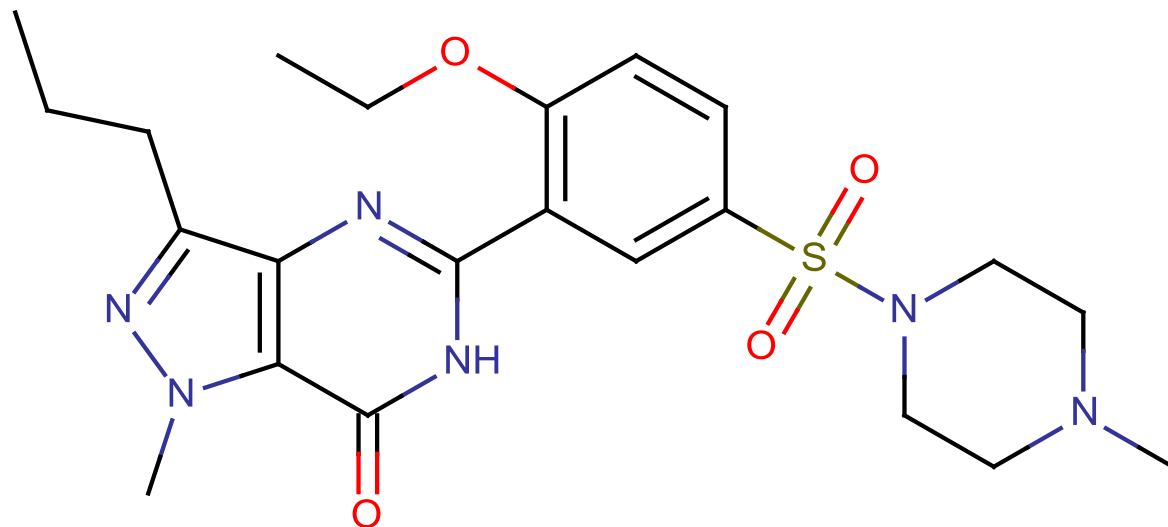
ChemAxon
Solutions for Cheminformatics

- 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



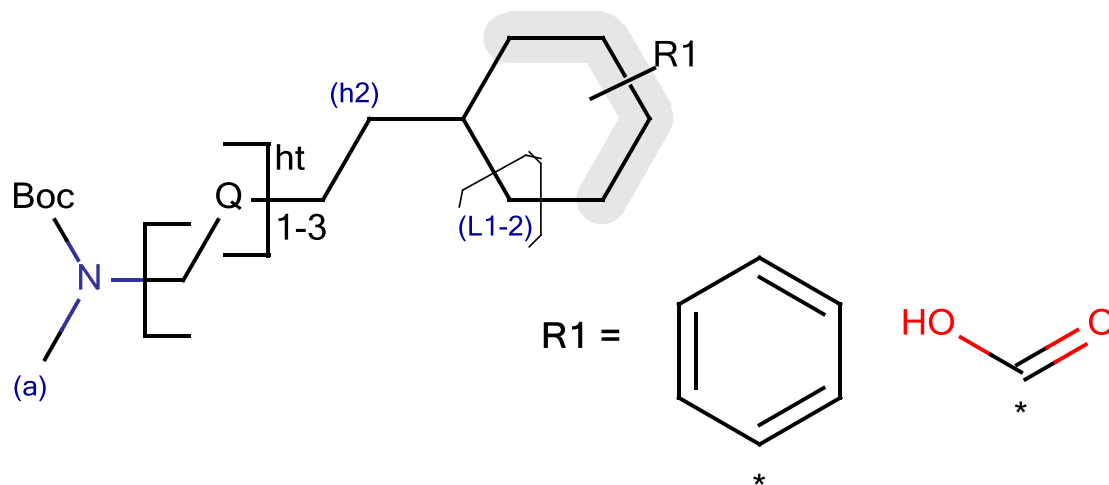
Sketching a Molecule



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

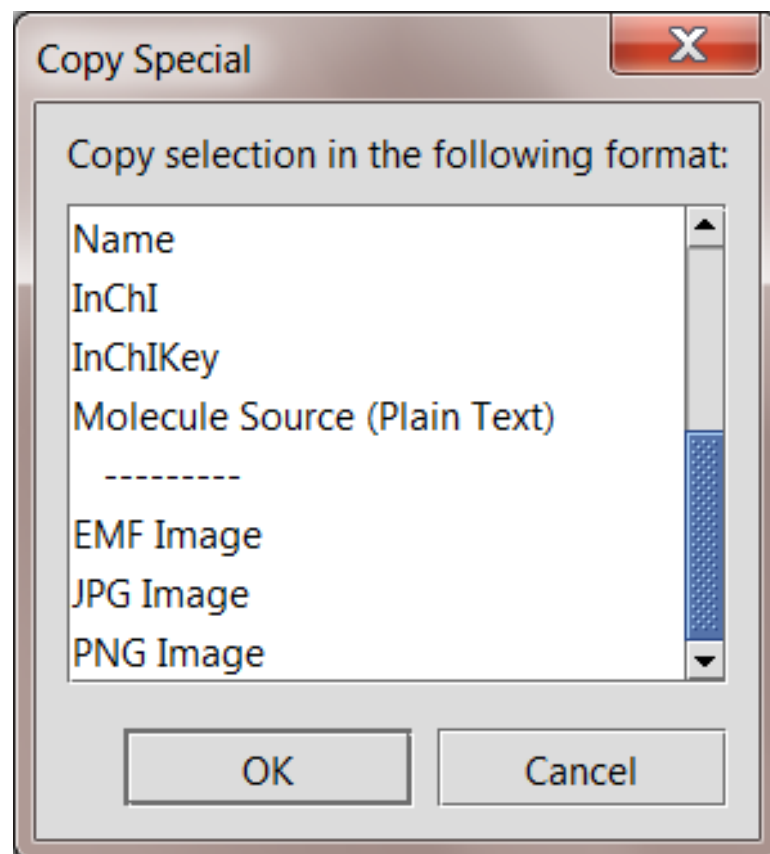
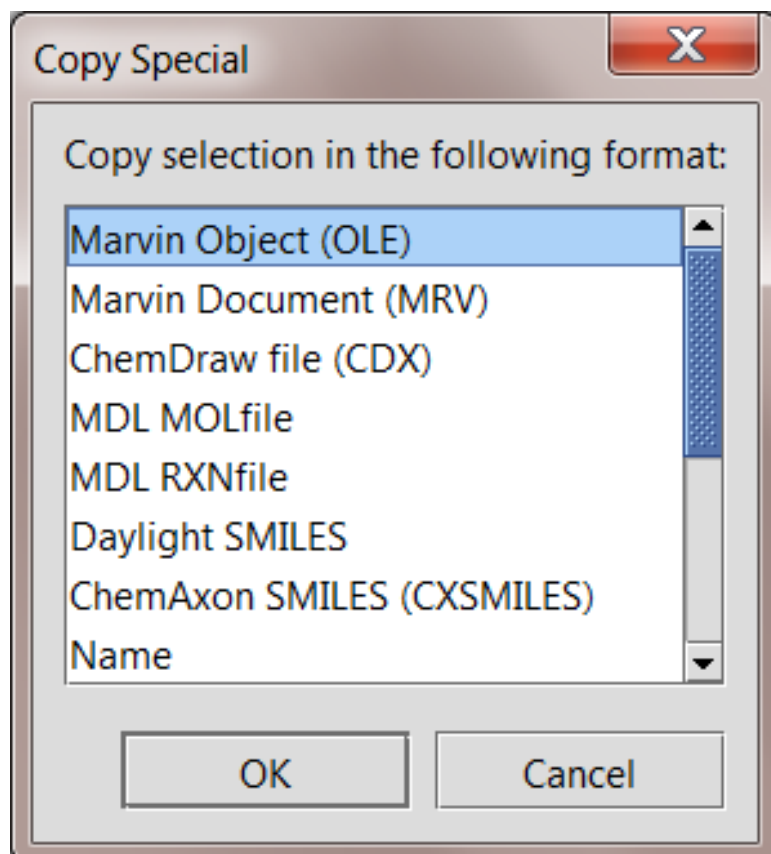
Sketching of a Query



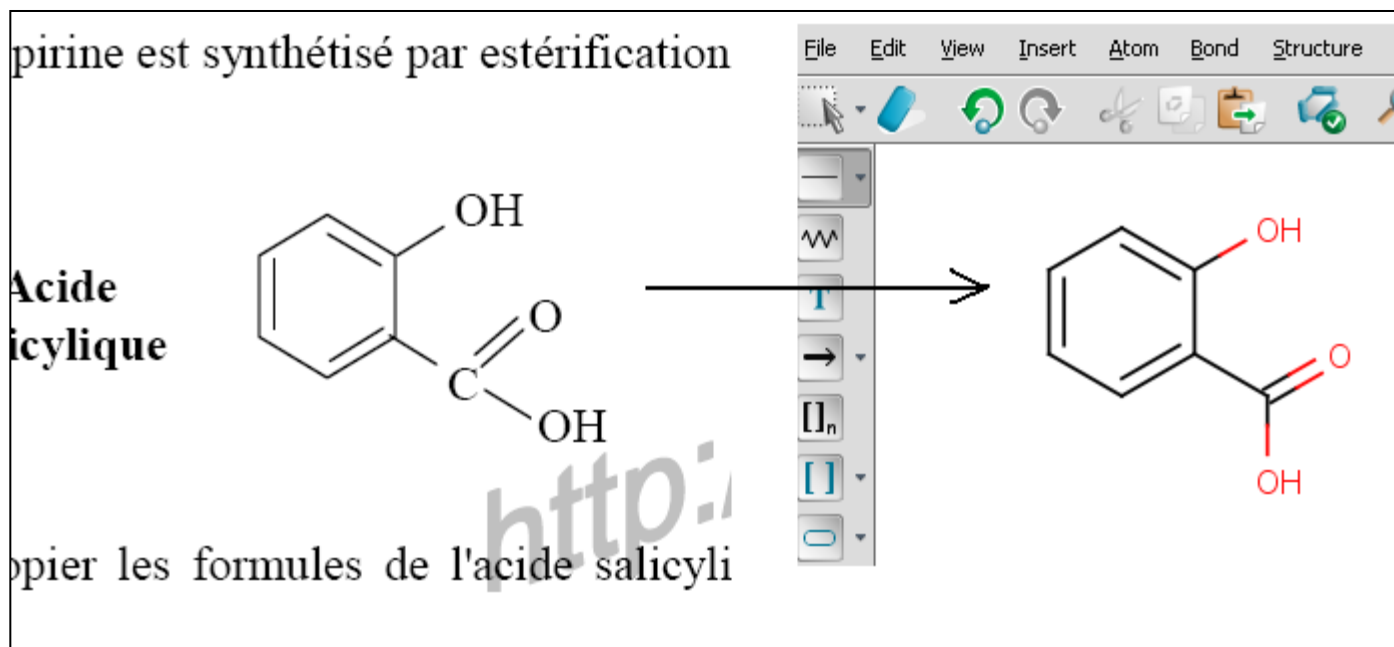
Tricks used:

- 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

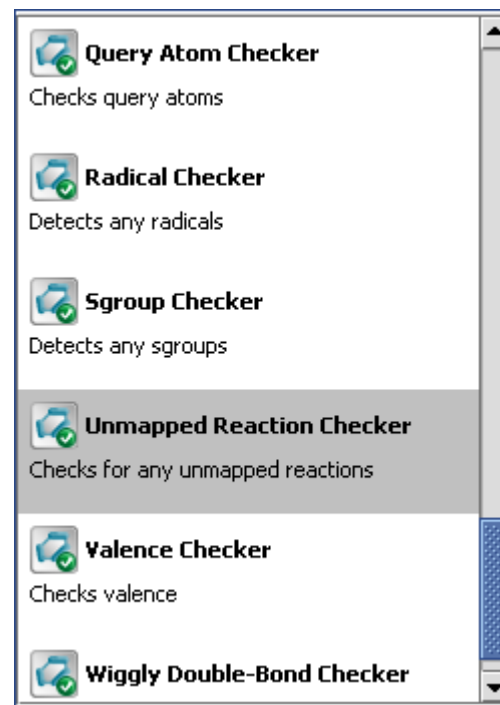
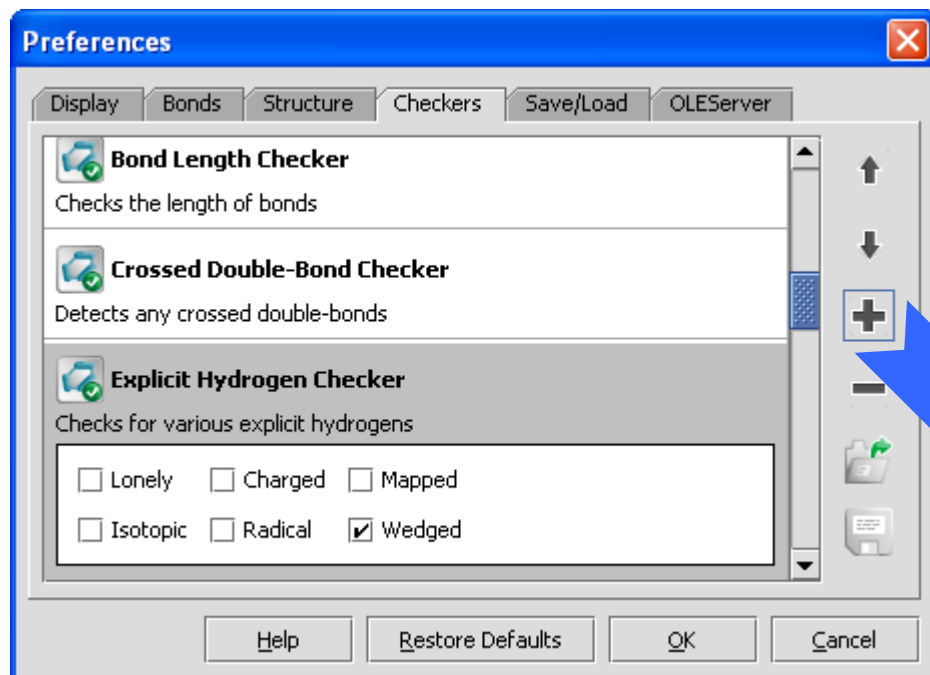
The image displays the 'Template Library Manager' software interface. The main window shows a grid of 20 bicyclic templates, each with a skeletal structure and a label. The labels are: 1: Bicyclo[1.1.1]pent..., 2: Bicyclo[2.1.1]hexa..., 3: Bicyclo[2.2.1]hept..., 4: Bicyclo[3.1.1]hept..., 5: Bicyclo[2.2.2]octa..., 6: Bicyclo[3.2.1]octa..., 7: Bicyclo[4.1.1]octa..., 8: Bicyclo[4.1.1]octa..., 9: Bicyclo[4.1.1]octa..., 10: Bicyclo[4.1.1]octa..., 11: Bicyclo[4.1.1]octa..., 12: Bicyclo[4.1.1]octa..., 13: Bicyclo[4.2.1]no..., 14: Bicyclo[5.1.1]no..., 15: Bicyclo[5.1.1]no..., 16: Bicyclo[5.1.1]no..., 17: Bicyclo[5.1.1]no..., 18: Bicyclo[5.1.1]no..., 19: Bicyclo[4.3.1]de..., 20: Bicyclo[4.3.1]de... The left sidebar shows a tree view of 'Template categories' including Rings, Amino Acids, Aromatics, Bicyclics, Cycloalkanes, Generic, Bridged Polycyclics, My Templates, Crown Ethers, Heterocycles, Polycyclics, Homology Groups, Templates, and Template. The 'Template' folder is expanded, showing sub-items: nostr_rect.mrv, sdsds.mrv, and str_rect.mrv. A 'Template Library Manager' dialog box is open in the foreground, showing the 'Template Set Properties' for 'My Templates'. The dialog box has a toolbar with icons for adding, deleting, and refreshing. The 'Template Set Properties' section includes: Name: My Templates, Location: file:C:\Users\apapp\chemaxon\marvin.mytemplates, and Toolbar Settings: Display on Toolbar. There is a 'Reload' button and a 'Close' button at the bottom right. The dialog box also has a 'Templates' tab and a 'Properties' tab.

Direct search in ChemSpider and PubChem

The image displays a web browser window showing a search result for PubChem Compound CID: 798. The browser address bar shows the URL: http://www.ncbi.nlm.nih.gov/sites/entrez?cmd=HistorySearch&db=pccompound&query_key=1&hinit=true. The search results show the compound name "indole; 1H-Indole; Ketole ..." and its IUPAC name "1H-indole". The molecular weight (MW) is 117.147880 g/mol and the molecular formula (MF) is C₈H₇N. The results also indicate that the compound has been tested in 16 BioAssays, with 0 being active.

Overlaid on the browser window is the MarvinSketch 5.3.3 software interface. The "Structure" menu is open, showing options such as "Clean 2D", "Clean 3D", "Add", "Remove", "Edit Data...", "Aromatic Form", "Group", "Reaction", "Mapping", "Attribute", "Find Structure in ChemSpider", "Find Structure in PubChem", "Check Structure", and "Auto Check". The main canvas of MarvinSketch displays the chemical structure of indole.

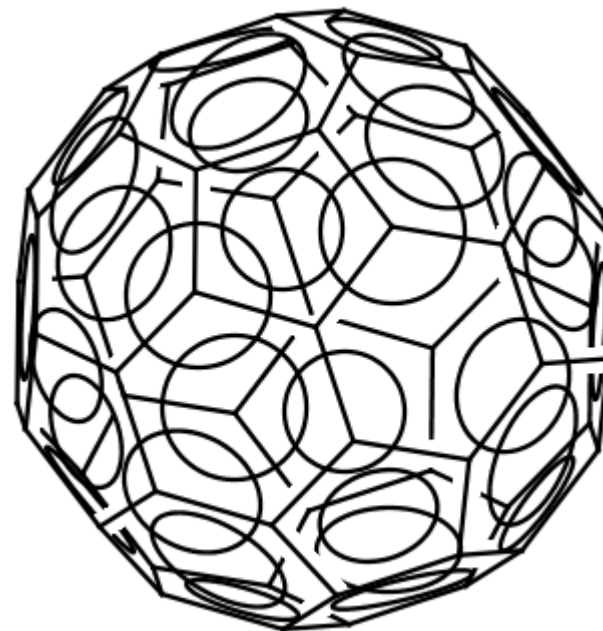
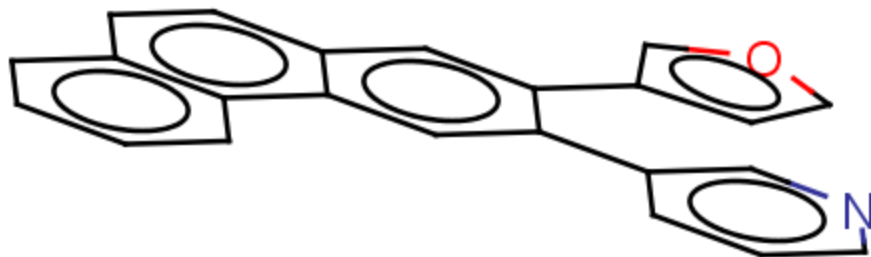
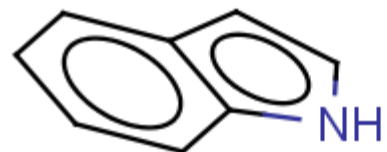
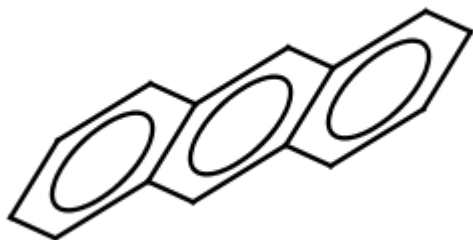
Structure checker in MarvinSketch GUI



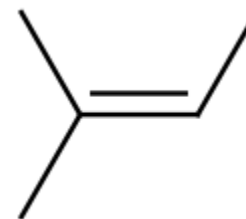
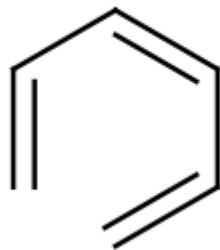
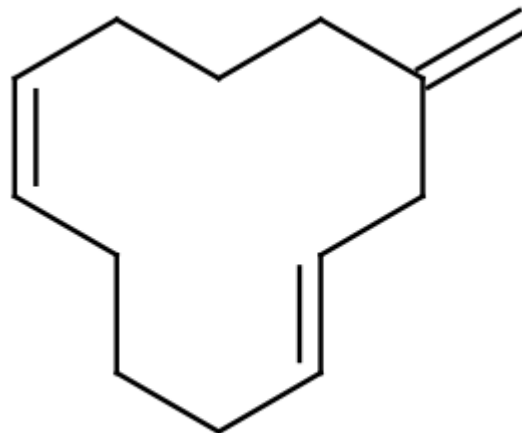
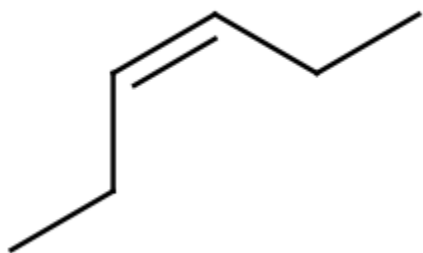
Plans for 5.4

- Improvements towards presentation quality drawings
 - Projected structures (ellipses in aromatic rings)
 - Enhanced double bond drawing
- Easier sketching
 - Markush toolbar
 - Enhanced 3D rotation features
 - Object/structure grouping, align and distribute tools
- Functionality improvements
 - Atomic property editor
 - Chemical terms in MarvinSketch GUI
 - Defining property calculations using chemical terms editor
 - Displaying dynamically calculated properties on the canvas

Ellipses in aromatic rings



Enhanced double bond drawing



Acknowledgements

