

Quicker, Better, Sketcher

Ákos Papp

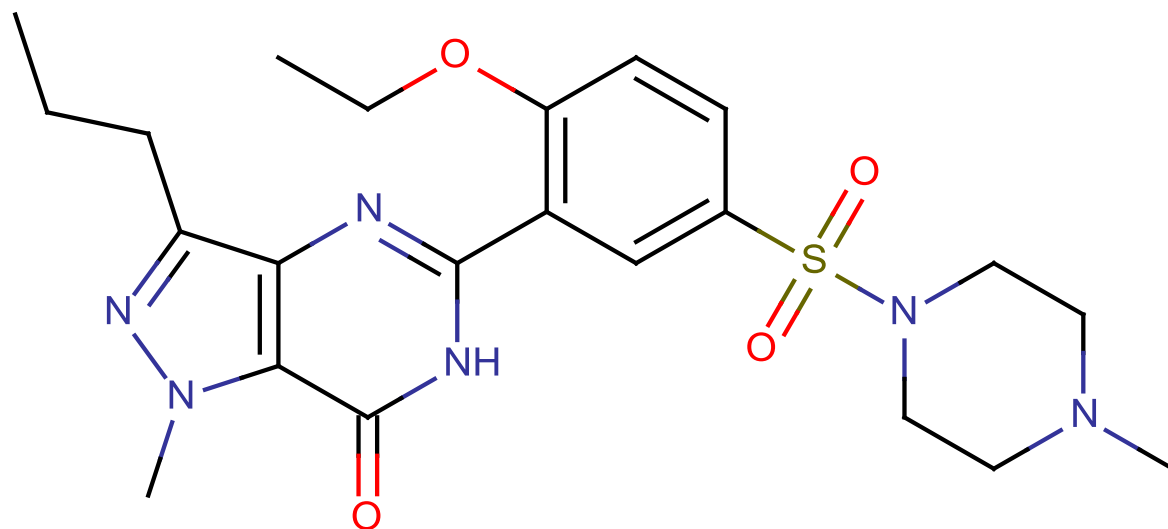


- Tips and tricks for quick drawing
 - Sketching a molecule
 - Autorecognition during paste
 - Sketching a query
- Latest features you might not be aware
- Top features coming in version 5.4

Fast ways for entering a drug



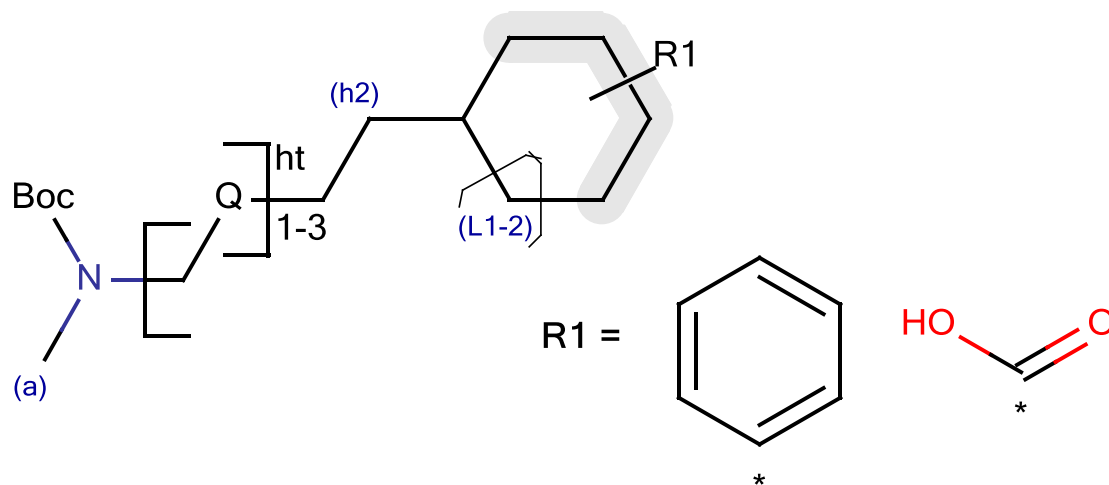
Sketching a Molecule



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

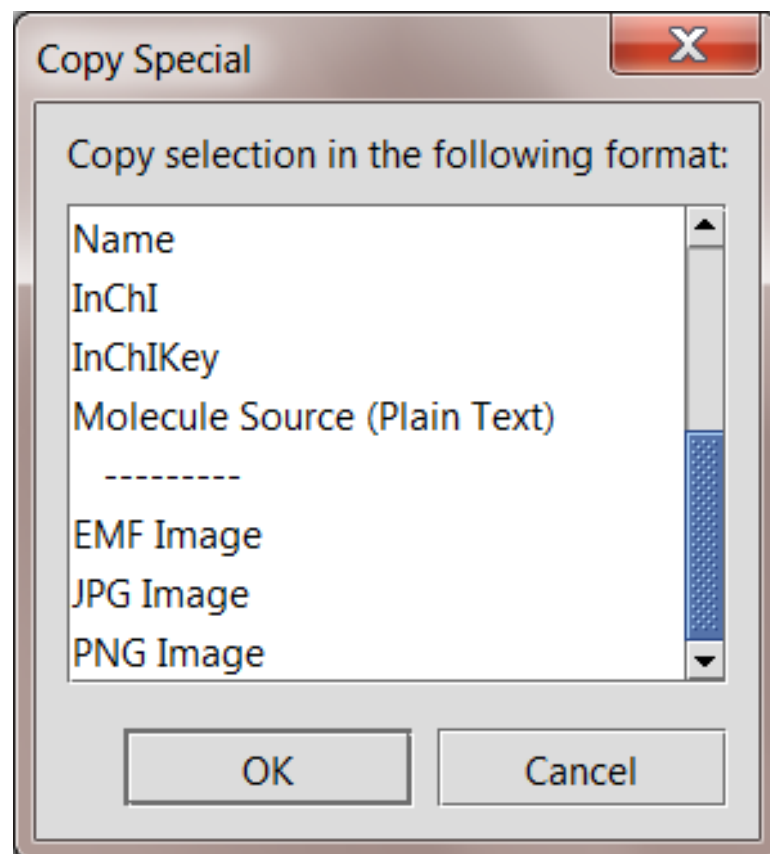
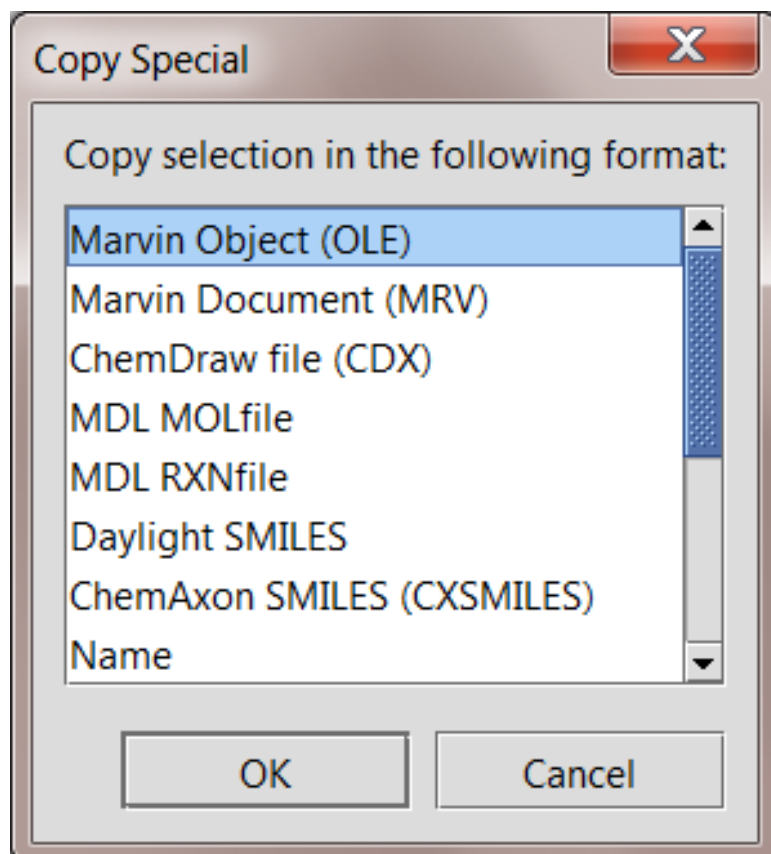
Sketching of a Query



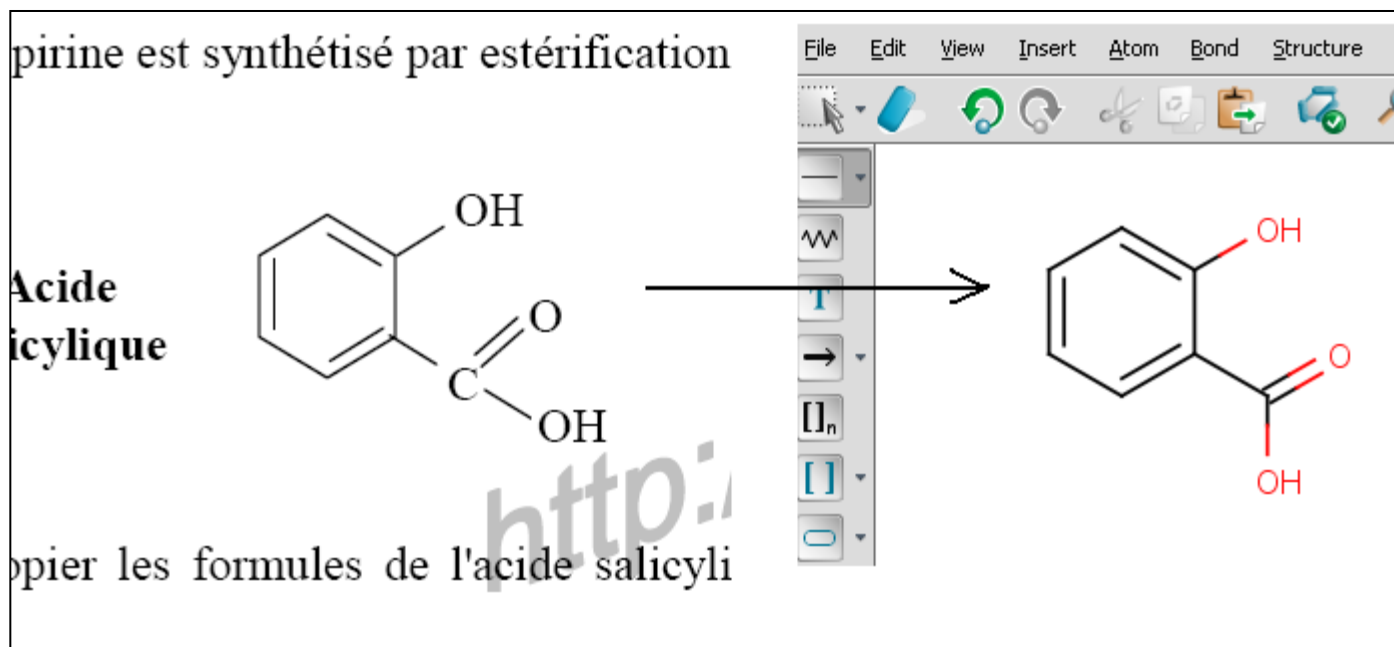
Tricks used:

- 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 'Name' field with 'My Templates', a 'Location' field with 'file:C:\Users\apapp\chemaxon\marvin.mytemplates', and a 'Toolbar Settings' section with a checked 'Display on Toolbar' option. There are 'Reload', 'Templates', 'Properties', and 'Close' buttons.

Template Library Manager

Template categories

- Rings
- Amino Acids
- Aromatics
- Bicyclics
- Cycloalkanes
- Generic
- Bridged Polycyclics
- My Templates
- Crown Ethers
- Heterocycles
- Polycyclics
- Homology Groups
- Templates
- Template
 - nostr_rect.mrv
 - sdsds.mrv
 - str_rect.mrv

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... 21: Bicyclo[4.3.1]de...

Template Set Properties:

Name: My Templates

Location: file:C:\Users\apapp\chemaxon\marvin.mytemplates

Toolbar Settings: Display on Toolbar

Reload

Templates Properties

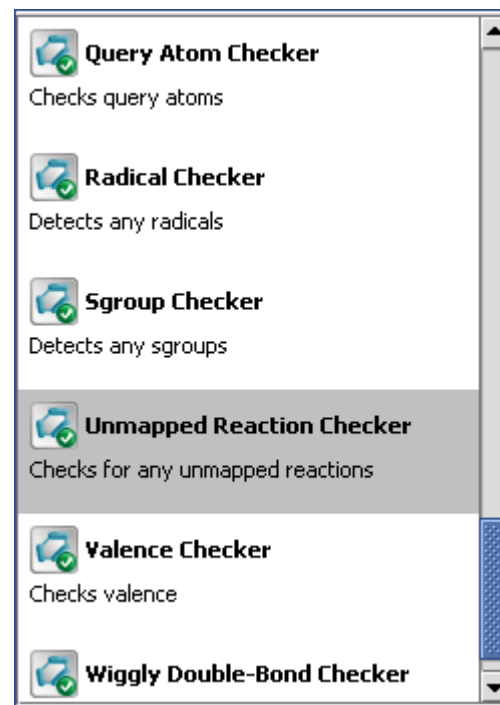
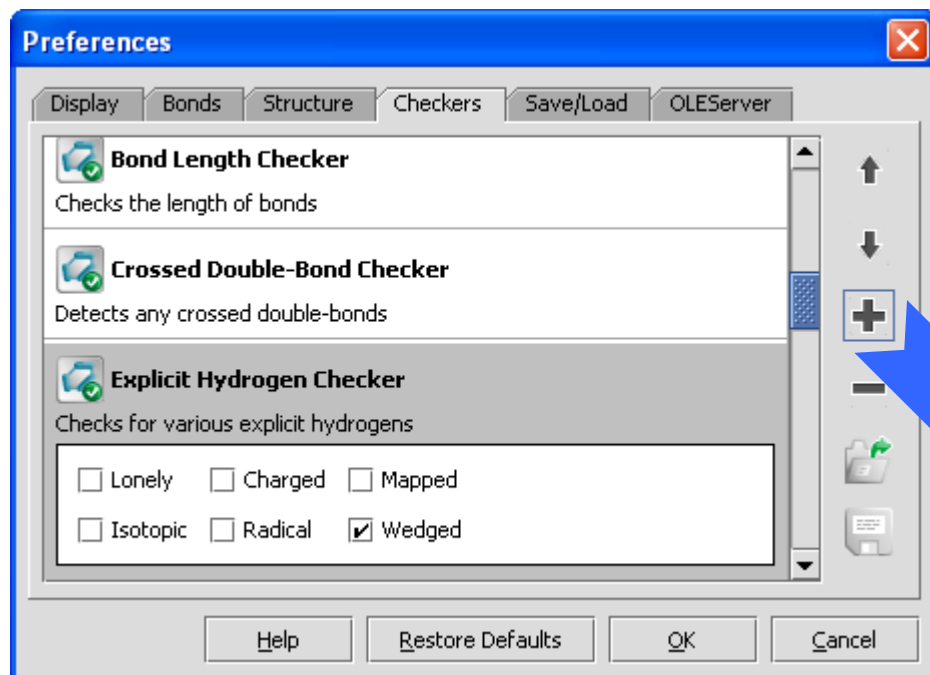
Close

Direct search in ChemSpider and PubChem

The image displays a web browser window showing a PubChem search result for 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 PubChem logo and search bar are visible at the top. The search results show the compound name "indole; 1H-Indole; Ketole ...", its IUPAC name "1H-indole", molecular weight "MW: 117.147880 g/mol", and molecular formula "MF: C₈H₇N". The search was tested in BioAssays, with results: "All: 16, Active: 0; BioAct".

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 shows the chemical structure of indole.

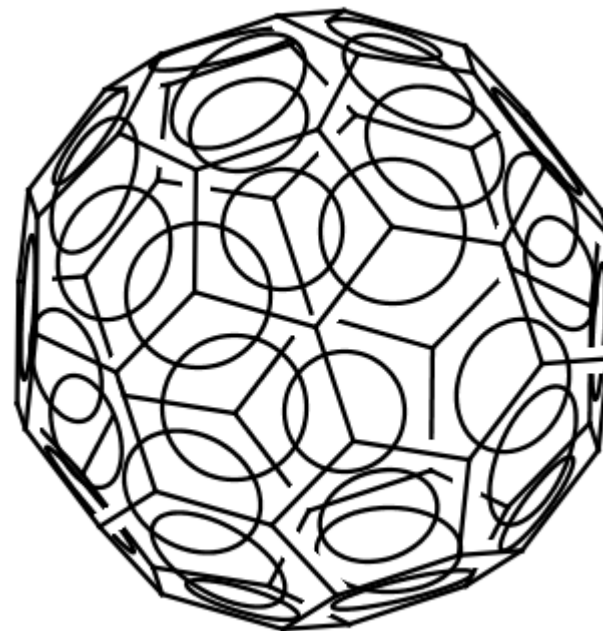
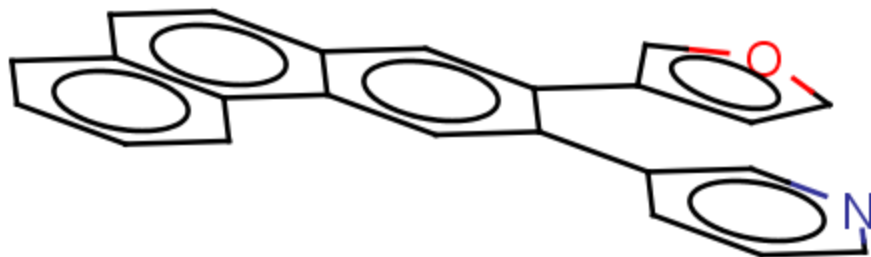
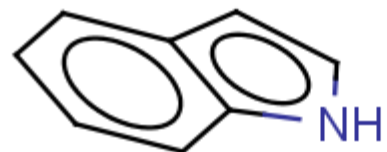
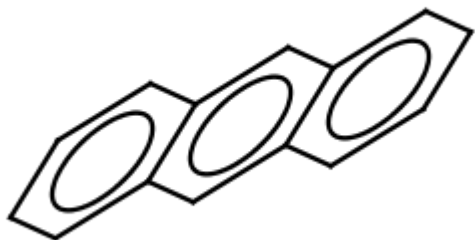
Structure checker in MarvinSketch GUI



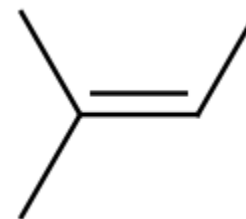
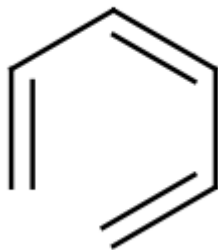
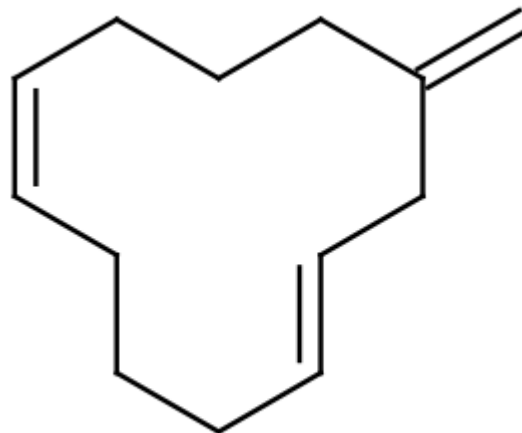
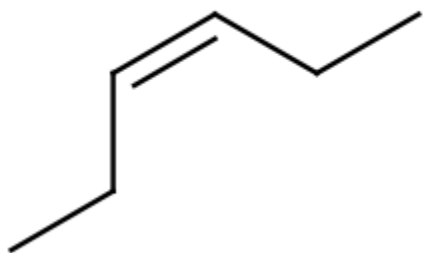
Plans for 5.4

- 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

