

Quicker, Better, Sketcher

Ákos Papp



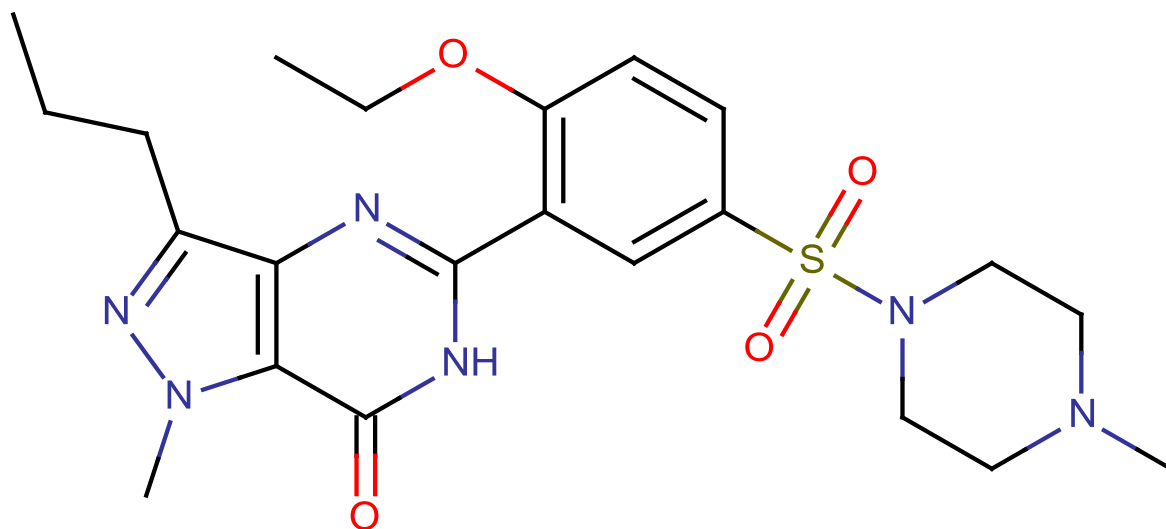
ChemAxon
Solutions for Cheminformatics

- 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



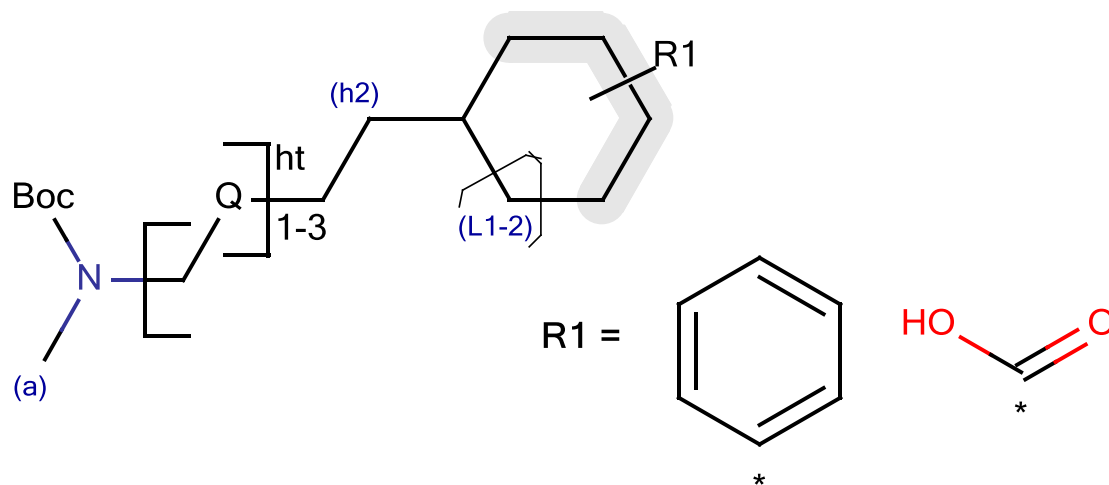
Sketching a Molecule



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

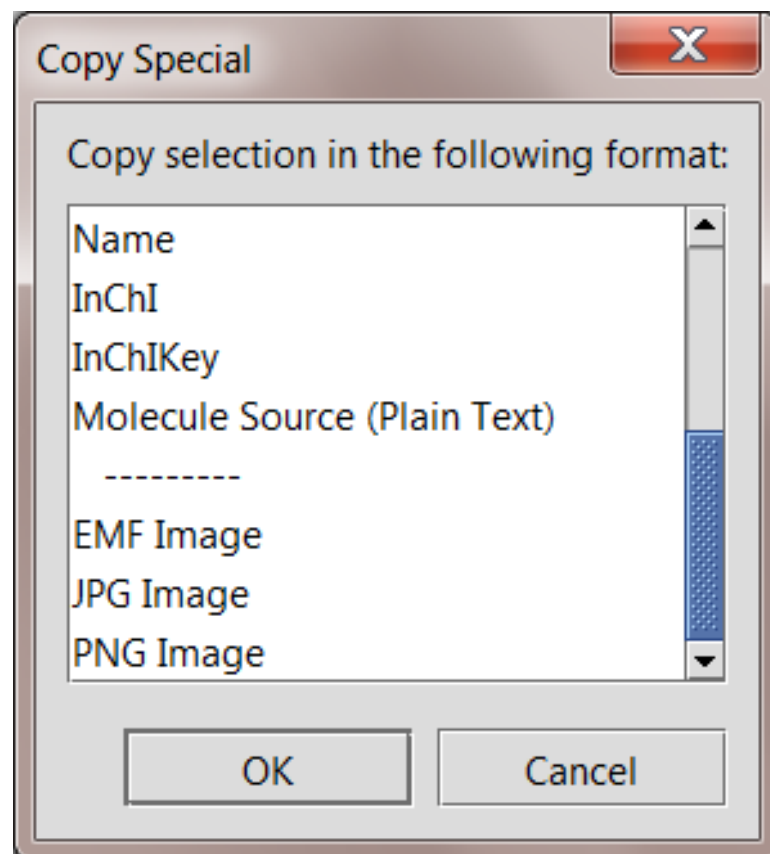
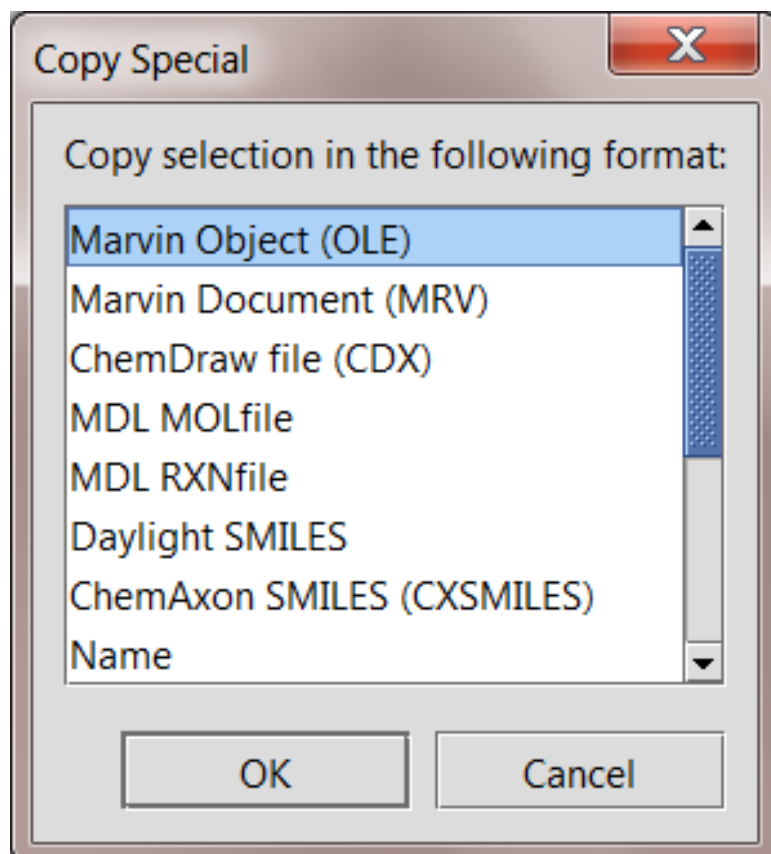
Sketching of a Query



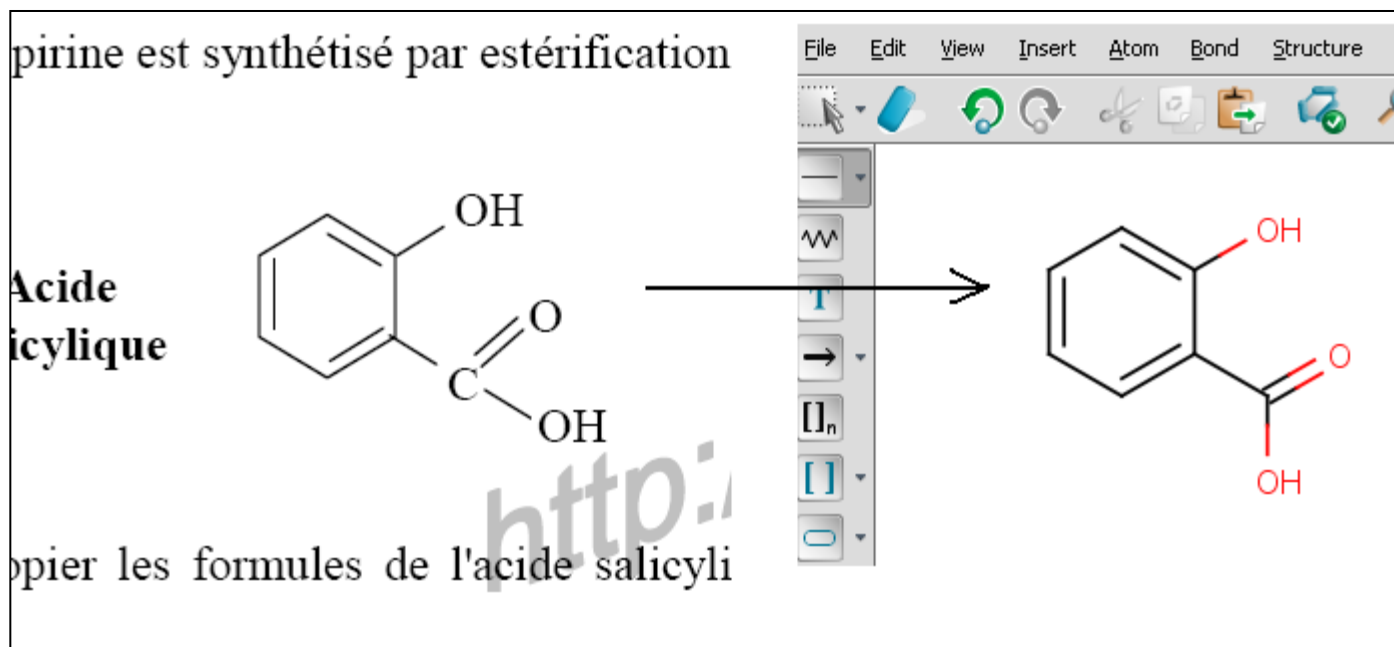
Tricks used:

- 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 '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

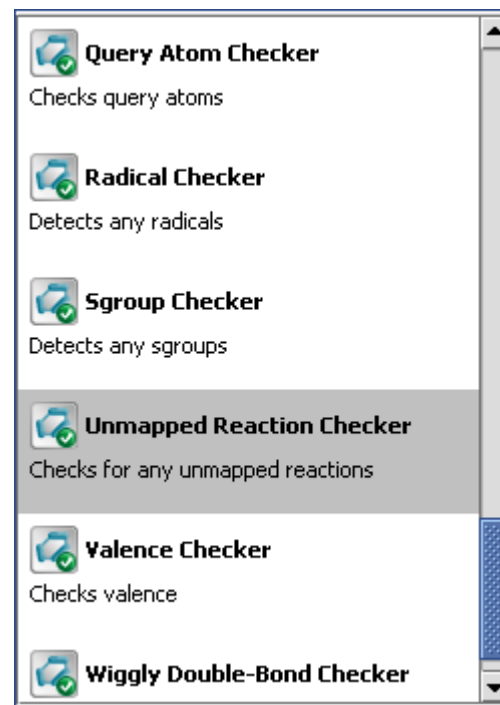
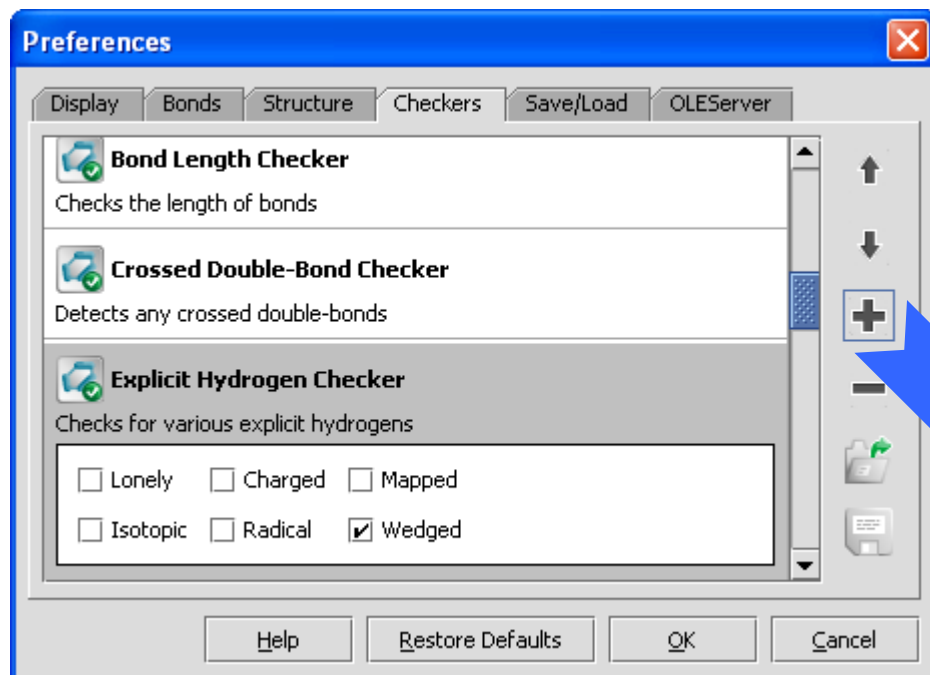
Close

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 Compound search interface is visible, with the search term "PubChem Compound" entered. The search results show the entry for CID 798, which is indole. The chemical structure of indole is displayed, along with its IUPAC name (1H-indole), molecular weight (117.147880 g/mol), and molecular formula (C₈H₇N). The search results also indicate that indole has been tested in 16 BioAssays, with 0 active and 16 inactive.

Overlaid on the browser window is the MarvinSketch 5.3.3 software interface. The "Structure" menu is open, showing options for cleaning the structure (Clean 2D, Clean 3D), adding or removing atoms, and editing data. The "Find Structure" options are highlighted, showing "Find Structure in ChemSpider" and "Find Structure in PubChem". The "Check Structure" option is also visible, with a "Ctrl-R" shortcut. The chemical structure of indole is shown in the MarvinSketch workspace.

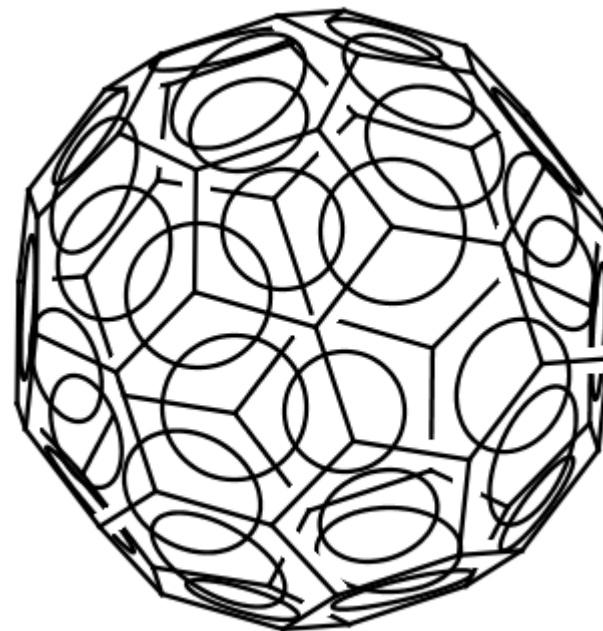
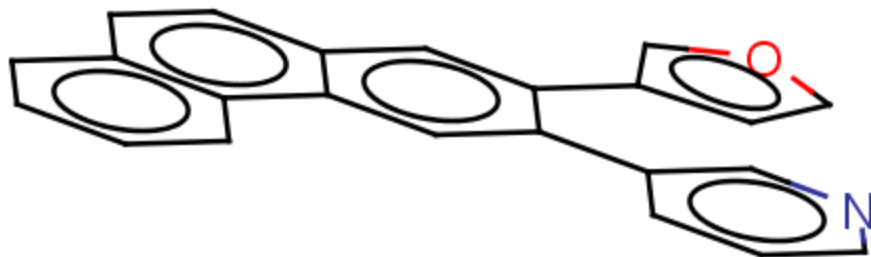
Structure checker in MarvinSketch GUI



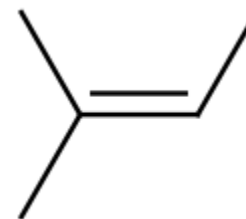
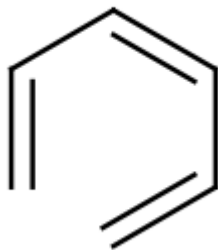
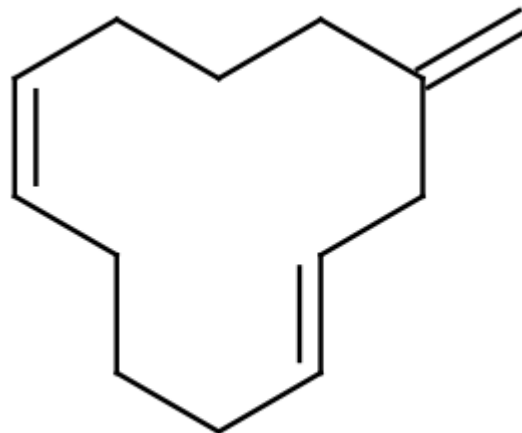
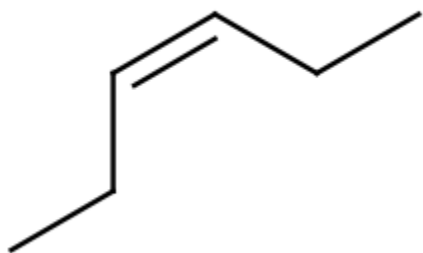
Coming in 5.4

- 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

