

**A d v a n c e d
C h e m i s t r y
D e v e l o p m e n t**

ACD/Labs

What's New with ACD/ChemSketch Version 12.0

For more than a decade, ACD/Labs has been fully dedicated to building integrated solutions that enable data transfer and connection within chemical organizations. We remain committed to the adoption and creation of the latest technological and industrial advances, empowering our customers' research and development efforts with the foremost chemical capabilities. Each year, we release newer versions of our software to provide enhanced capabilities and superior integration between existing and new technologies.

New capabilities for ACD/ChemSketch 12.0 have resulted from collaboration with our users, as well as feedback from industry experts. We appreciate your input and encourage you to contact us with ideas or suggestions for new features by visiting support.acdlabs.com. In addition, we invite you to join us at one of the seminars we will be holding throughout the year to discuss our products and learn more about the current version. Visit www.acdlabs.com/events/ for a list of upcoming events.

Among the key features of ACD/ChemSketch presented below, are:

- Expanded ACD/Dictionary
- New customizable interface appearance & style
- Copy all generated tautomers in one click
- Improved atom numbering positioning
- Resize and Rotate tools simplification
- Set standard InChI options (updated IUPAC recommendation)



Expanded ACD/Dictionary

More names and structures added in ACD/Dictionary

The Dictionary has been expanded to over 30,000 well-known structures. Associated with these structures, there is over 165,000 corresponding chemical names and registry numbers, so that you can look up your queries easily. Dictionary entries span systematic names, trivial chemical names, brand names, and various registry numbers.

The Dictionary allows you to find and copy a chemical structure from the Dictionary in seconds, avoiding unnecessary drawing efforts and mistakes.

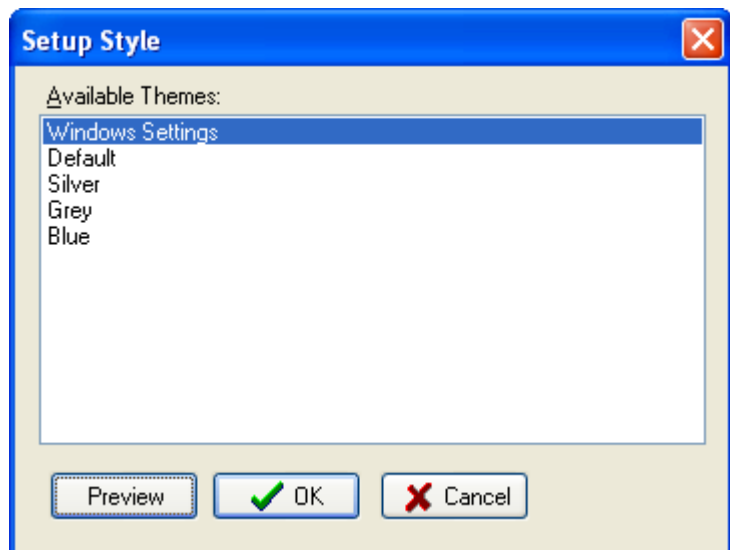
The screenshot shows the ACD/Dictionary window. On the left, a 'Quick Search' list contains entries from TTFD to TU, with 'TTP' highlighted. Below the list is a checkbox for 'Show All Names of Structure' and an 'Advanced Search' section with a search button. On the right, the 'Show/Search' panel has checkboxes for 'Systematic Names', 'Other Names', and 'Registry Numbers'. Below these are buttons for 'Category', 'Enzymes', and 'Undefine', and a dropdown menu currently set to '<Not defined>'. The main display area shows the chemical structure of triphenyl phosphite, c1ccccc1OP(=O)(Oc2ccccc2)Oc3ccccc3. At the bottom of the window are 'OK', 'Cancel', and 'Help' buttons.



Interface Enhancements

*New customizable **interface appearance & style***

The interface style and appearance has been refreshed. The background color, buttons, and other graphic controls can be made to conform to the Windows setting, the classic ACD/Labs view, or you can create your own theme and preference.



*Resize and Rotate **tools simplification***

The interface was simplified and behavior made more consistent. Previously, there was a slight discrepancy in Drawing versus Structure modes when it came to selecting, moving, rotating, and resizing structures and drawings.

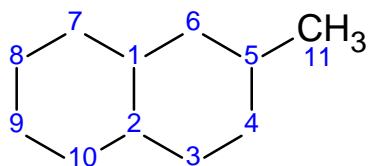
The new interface controls for manipulating images and structure objects are made similar to those used by Microsoft Word, ChemDraw, and many other applications. This effectively merges several tools into one, creating a simpler, more user-friendly interface.

Chemical Structure Representation

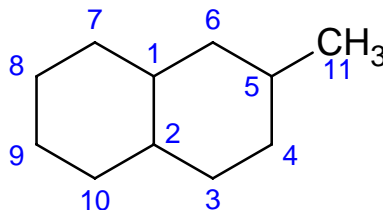
Improved atom numbering position

In previous versions, the default position of atom numbers overlapped at the center of the atom node. In the current version, the numbering is positioned near the atom node instead in accordance with current common preferences.

Version 11



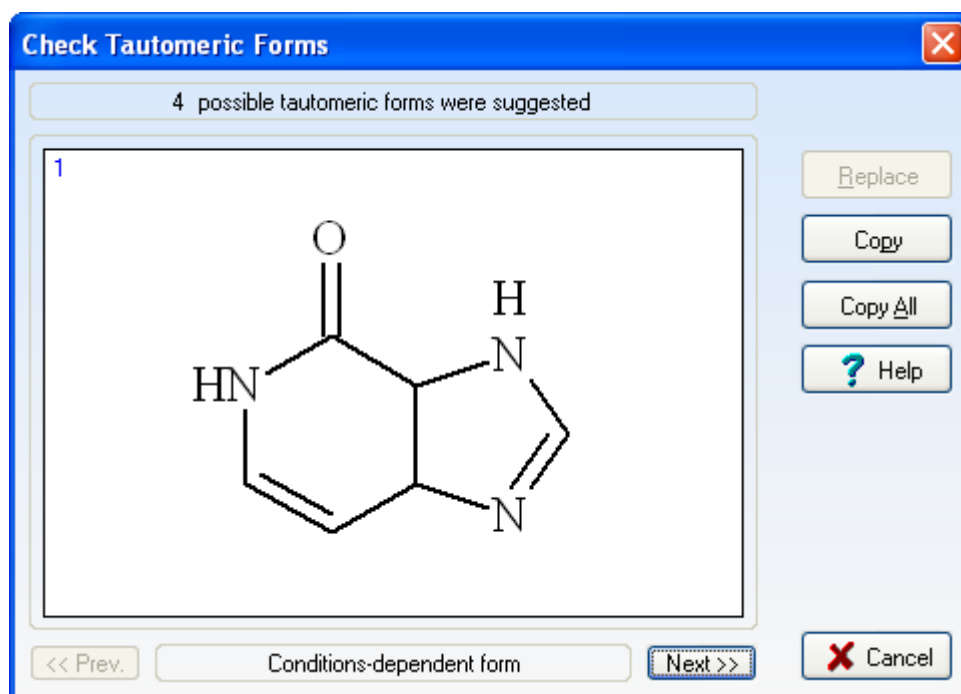
Version 12



Copy all generated tautomers in one click

The "tautomer verification tool" generates various reasonable tautomeric forms for a given structure. It is now possible to copy all tautomeric forms generated by this tool to ChemSketch.

This makes it easy to report the various tautomeric forms of a given structure.

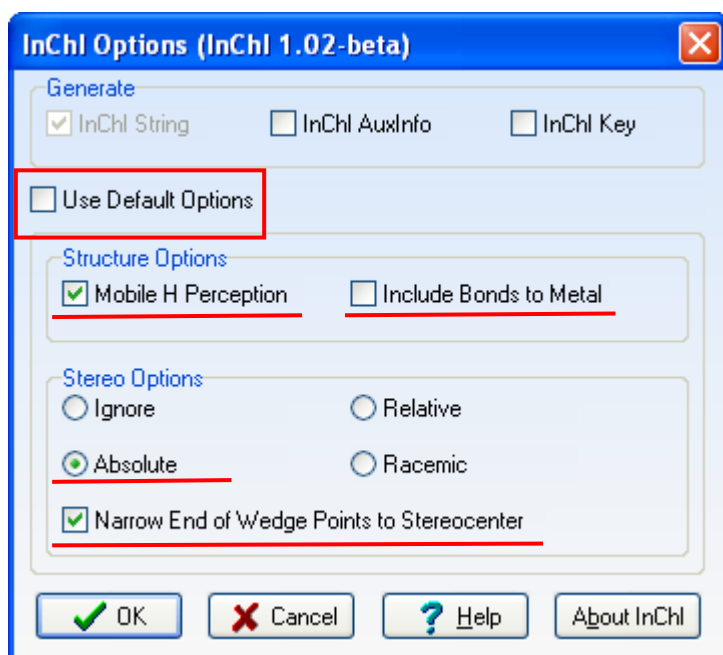


Set Standard InChI Options (Updated IUPAC Recommendations)

New InChI Options proposed by IUPAC were implemented. The options include:

- Mobile Hydrogen Perception (taking tautomerism into account)
- Excluded bonds to metal
- Absolute stereoconfiguration
- Taking into account narrow ends of stereobonds only

The IUPAC International Chemical Identifier (InChI™) is a non-proprietary identifier enabling unambiguous identification of chemical substances for electronic handling of chemical structural information. These new IUPAC options for InChI reflect the decisions made by the IUPAC InChI project group, and are intended to increase the role of InChI and InChI key as a universal structure identifier.



Additional Improvements

Correct SMILE and InChI for Zero Valent Metals

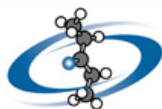
The SMILE or InChI for zero valent metals has been corrected so that improper non-explicit hydrogens are not automatically added. For example, drawing Be in ChemSketch leads to the [Be] and InChI=1/Be SMILES and InChI, respectively, and not [BeH2] and InChI=1/Be.2H as was previously the case.

Template Window Resolution

A previous issue with the resolution of the Template Window while resizing has been resolved for version 12.



To learn more about this product, please download our catalog from <http://www.acdlabs.com/download/catalogs/drawcat.pdf> or visit our Web site (<http://www.acdlabs.com/chemsketch/>).



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