What's New with ACD/ChemSketch Version 11.0

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 11.0 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:

- Interface changes to simplify workflow, including the standard Microsoft Windows shortcuts
- Improvements in graphical Structure representation, including the antialiasing option for chemical structure drawing
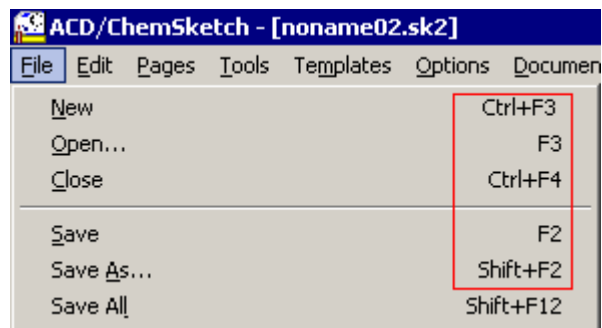- New InChIKey identifier is now supported
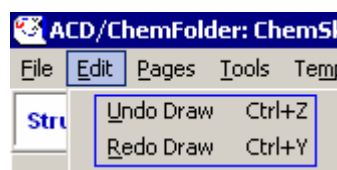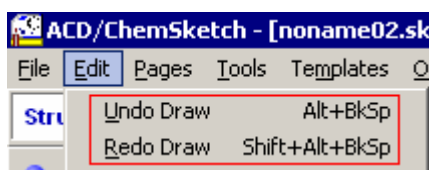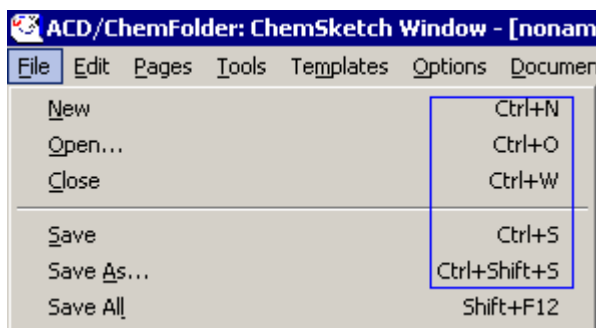
Interface Enhancements

Standard Microsoft Windows shortcuts

Several shortcuts for menu commands have been changed to meet the requirements of Microsoft Windows standards. Some of these shortcuts were already in place in earlier versions, but a number of new ones are replacing the old-style "F+number" shortcuts.
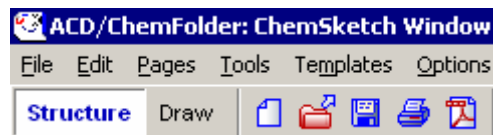
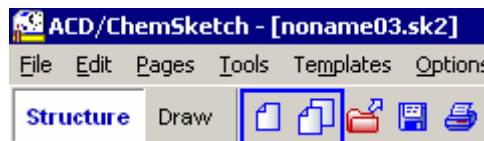**Version 10**:   **Version 11**:

"New Document" button

Our old toolbar button for **New Page** was sometimes confused for the **New Document** button typical of other software applications. Now this button has its common meaning: **New Document**, and the new button, **New Page**, is placed next to it.

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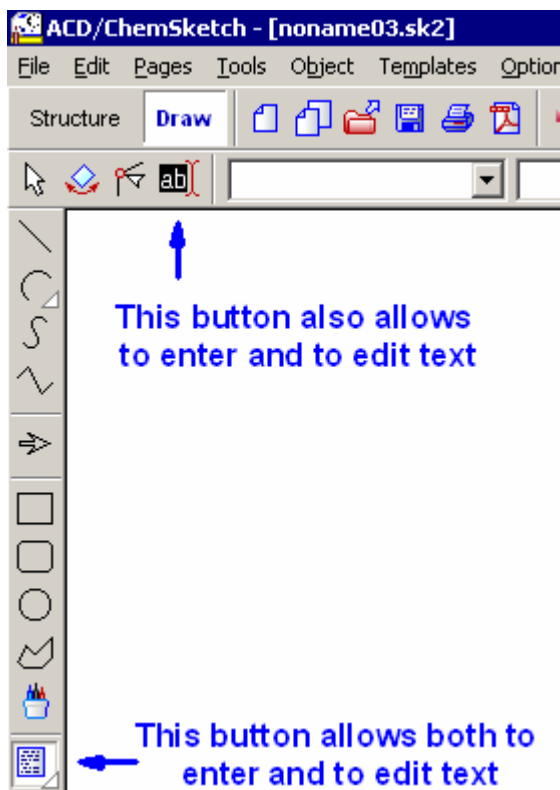Visionary Software   Advancing Research

"Text" button changes improve workflow

Previously we had one button to enter new text—the **Text** button on the left toolbar (*Draw* mode), and another button to edit text—the **Edit Text** button on the Editing top toolbar.

Now both buttons allow users to enter a new text box and edit the existing text with one mouse-click, significantly simplifying the workflow.

Version 11:

Enhanced Zoom commands
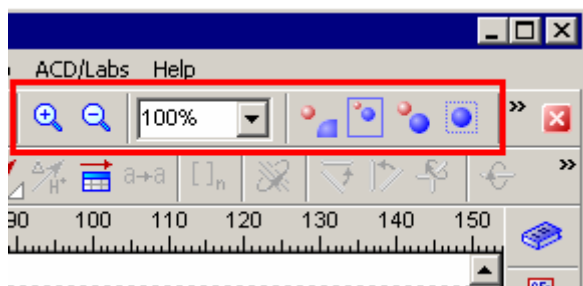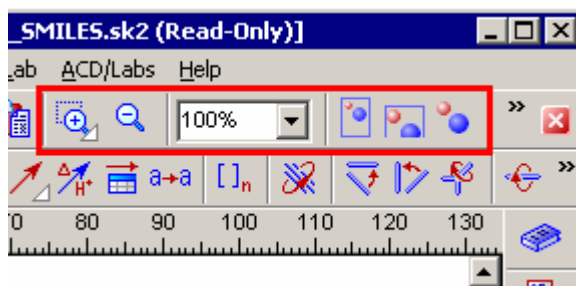
Default zoom is set to the Page Width

Previously, the default zoom option was 100% and, in the to portrait paper layout, a significant gray area was present on the screen. We have listened to our users' requests and reset the default zoom to *Fit Page Width*.
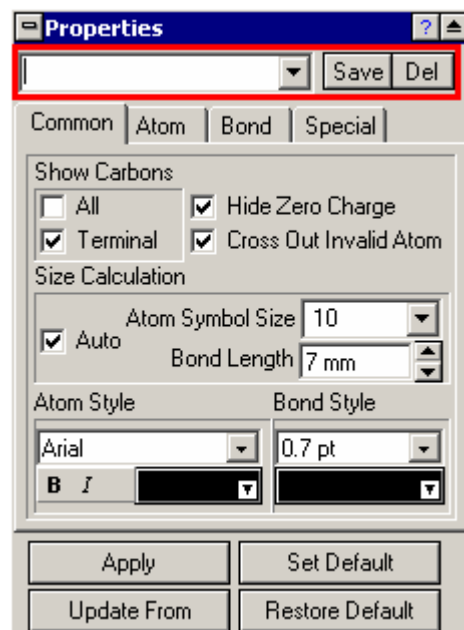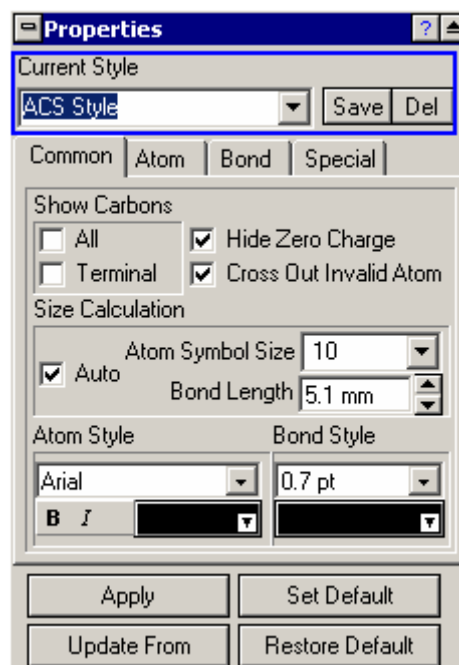
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New "Zoom In" button is added

New zoom button is added that increases the zoom step-by-step on each click of a button.

This is the most commonly accepted way of zooming in. The old button **Zoom Selection** is retained as an additional tool. Also, the rarely used button **Fit Selection** has been removed.

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Other interface changes:

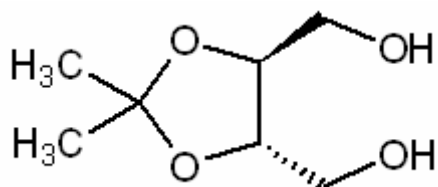A title for the **Current Style** list has been added in the **Properties** dialog box.

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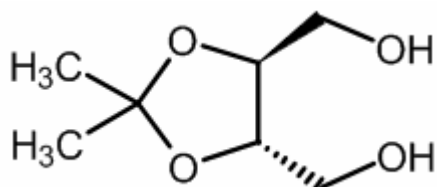
Improvements in Structure Representation

Antialiasing option for chemical structures

The new version of ACD/ChemSketch supports antialiasing that displays chemical structures drawn with smooth lines. Antialiasing is a computer rendering technique that blurs the hard edges and adds shaded pixels to create the appearance of smoothness. This addresses the common issue with printers and computer monitors, when, due to the relatively low resolution, the tilted lines appear "stairlike" instead of smooth straight lines or curves. For example, compare the two pictures below:

Without antialiasing:

With antialiasing:

For different graphical applications, both images with and without antialiasing are used. The antialiasing option can be set in the **General** tab (from the **Options** menu, choose **Preferences**).

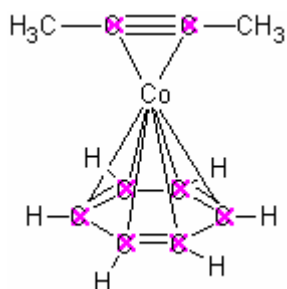*Support of different presentation of coordination structures*

Treat some bonds to metal atoms as coordination bonds

ACD/Labs supports the usage of a special *coordination bond* to represent a specific bonding between a ligand and a metal center in coordination structures. Such a bond indicates a connection but does not affect the valence of the corresponding atoms.
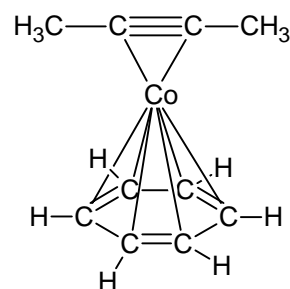
However, chemists often use the regular *single bond* to represent a coordination that leads to formal violation of valence rules. Such a violation is marked in ACD/ChemSketch by "crossed atoms". The new version of ACD/ChemSketch now supports the single bond indicating the coordination, without interpreting it as valence violation.

(This option has also allowed better nomenclature generation of coordination structures by ACD/Name and other ACD/Labs nomenclature packages.)
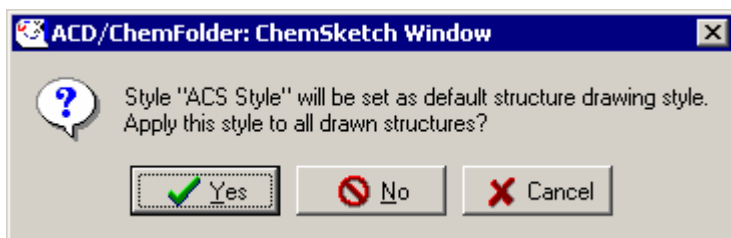
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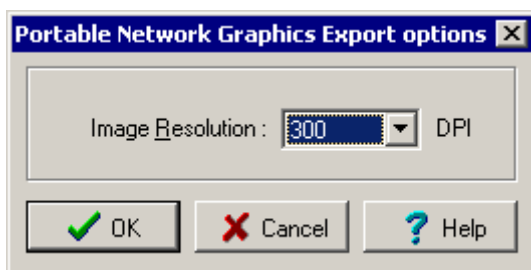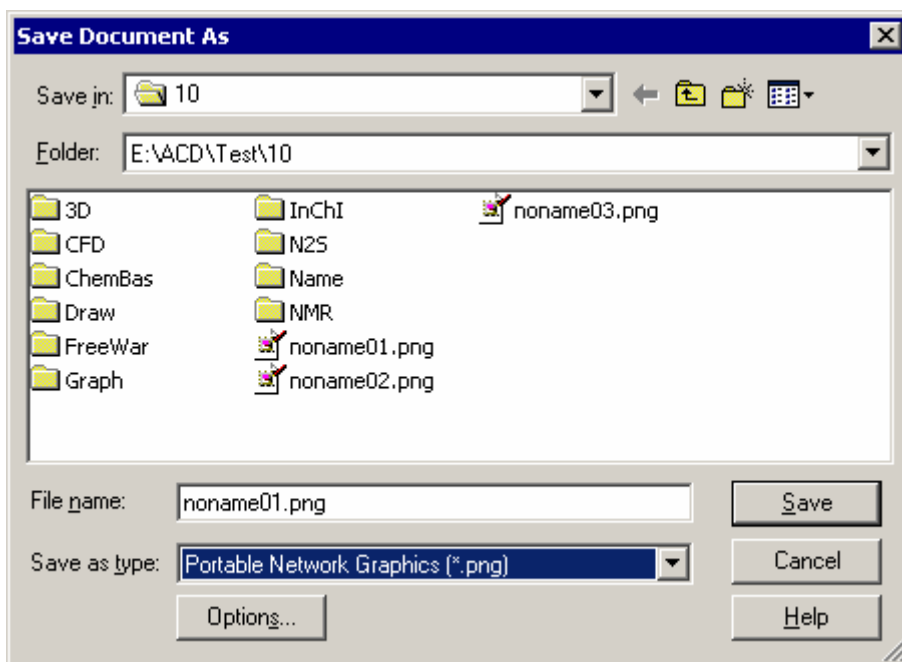## More flexibility in applying the Structure Drawing Style

The redundant **Apply Style** command has been removed. A new message box (below) has been added in its place. By clicking **Yes**, the user can easily apply the new style to already drawn objects.

As well, all styles for the American Chemical Society (ACS) and Royal Society of Chemistry (RSC) journals are combined into two corresponding styles—**ACS Style** and **RSC Style**—making the choice of style quicker and simpler.
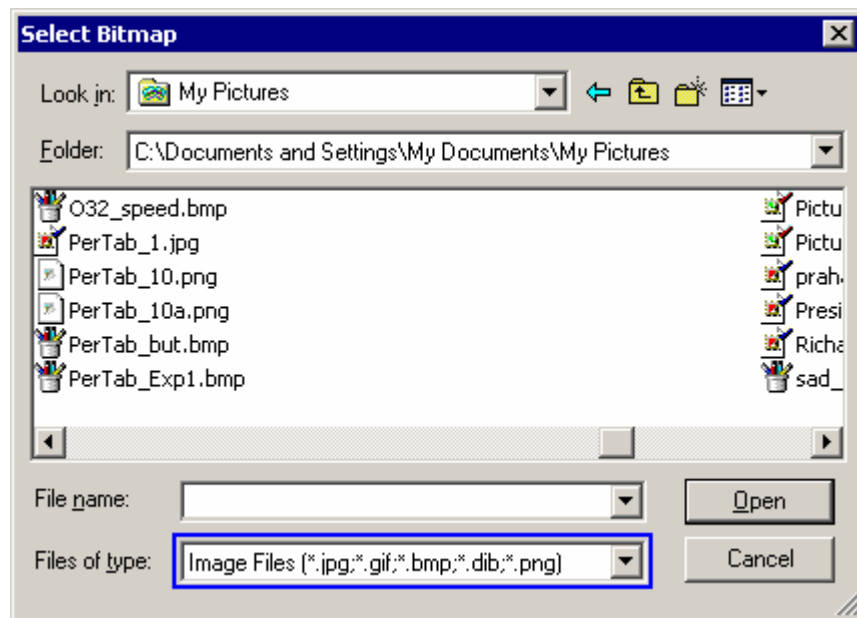
Improved handling of images

Support PNG format export for images

New export option is supported: .PNG (Portable Network Graphics) image file format with variable resolution.

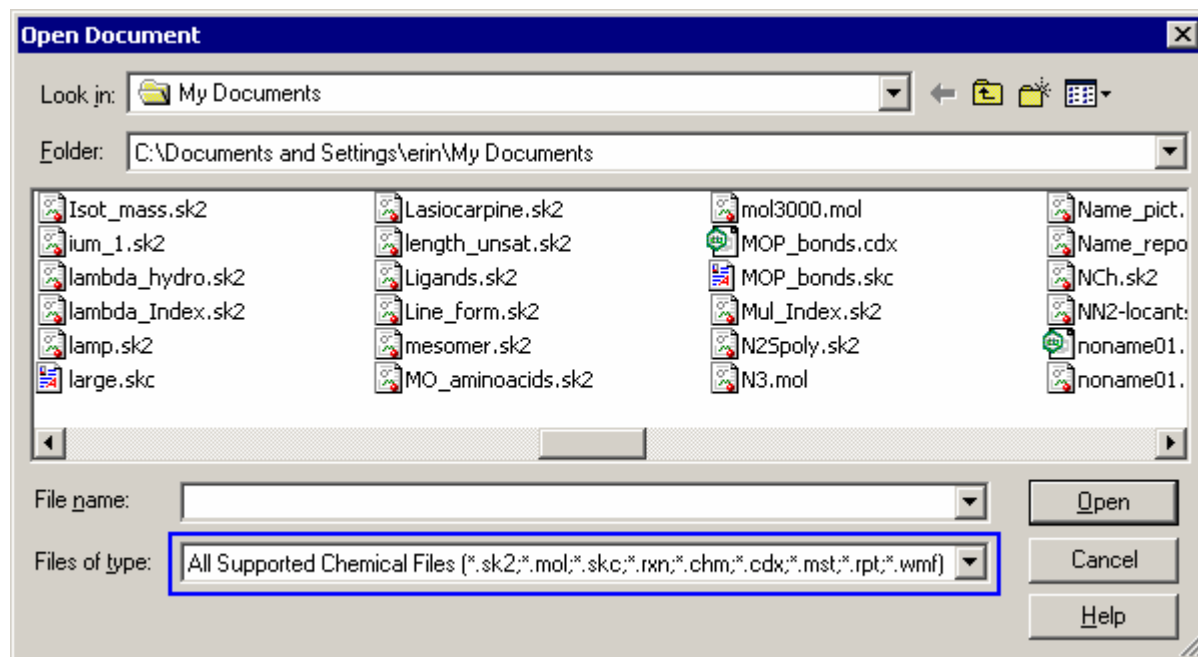Visionary Software   Advancing Research

Improved "Insert Image" tool

The "Insert Image" dialog box now, by default, includes all supported image file formats: .jpg, .gif, .bmp, .dib, and .png.

New "Open File" dialog box offers "All supported chemical files" at-a-glance

An ACD/ChemSketch user opening a new file can either specify the file format to be opened, or see all supported file formats at once:

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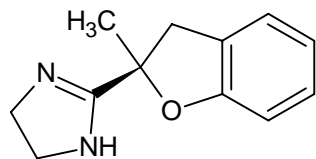## IUPAC International Chemical Identifier (InChI) Improvements

New 1.02 beta version of InChI generation procedures has been integrated and allows users to generate new InChIKeys

New "Generate InChI" button on top toolbar

ACD/Labs further extends the integration of InChI generation procedures into our products.

The IUPAC International Chemical Identifier (InChI™) is a non-proprietary identifier enabling unambiguous identification of chemical substances for electronic handling of chemical structural information. The new 1.02 beta version of InChI generation procedures officially released by IUPAC in September 2007 includes an ability to generate InChIKey—a short, condensed 25-character long representation of the InChI string. This compact representation of InChI codes significantly expands the use of InChI encoding for structure specification and searching over the Internet.
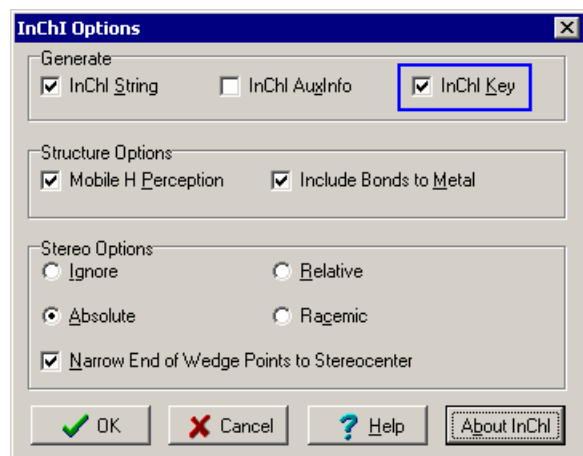
For example:

InChI: 1/C12H14N2O/c1-12(11-13-6-7-14-11)8-9-4-2-3-5-10(9)15-12/h2-5H,6-8H2,1H3,(H,13,14)/t12-/m1/s1

InChIKey: FEGRMCYCYUYYDA-GFCCVEGCBV

InChI generation options (on the **Tools** menu, point to **Generate**, and choose **InChI Options**) now include an option for InChIKey generation:

For quick access of InChI generation, a special button "Generate InChI" has been added to the top toolbar:

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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