

# ACCELRYS DRAW

Accelrys Draw enables scientists to draw and edit complex molecules and chemical reactions with ease, facilitating the collaborative searching, viewing, communicating and archiving of scientific information.

## FASTER AND MORE EFFICIENT

Accelrys Draw has the same look-and-feel as ISIS/Draw, but brings additional speed and efficiency to chemical structure drawing:

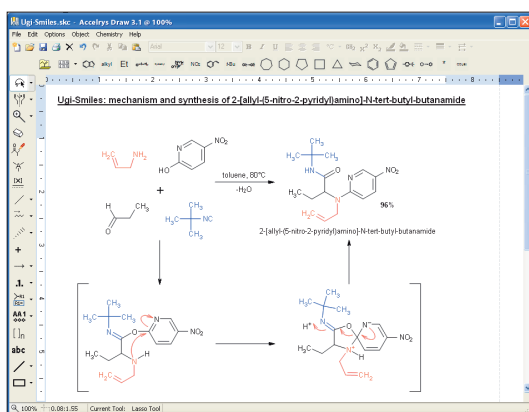
- Continuously draw bonds, pull out rings and add atoms using all-purpose drawing tool
- Drag-and-drop commonly-used structures and chemical abbreviations onto the toolbar for reuse
- Right-click for atom, bond, fragment properties and query options
- Quickly retrace steps using Multiple Undo/Redo

- Easily create structures with Rgroups for queries or enumerations
- Annotate reaction schemes with text, color and a variety of arrow styles
- Easily create publication-quality structures for inclusion in Microsoft Office documents and presentations

## EASY TO INTEGRATE AND CONFIGURE

As an enterprise software application, Accelrys Draw offers flexible integration with custom Java® and .NET applications as well as integration with Accelrys Isentris® and ISIS applications. Use XML to configure the chemical drawing look-and-feel according to the organization's needs.

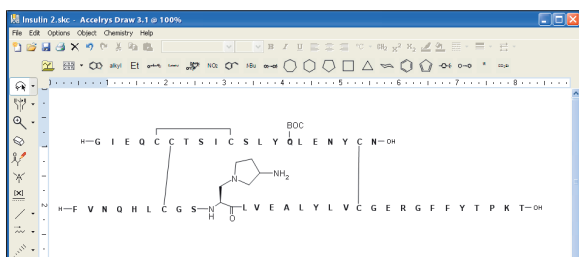
- Create custom add-ins to enhance the scientist's drawing experience
- Integrate with existing desktop applications
- Leverage Web applications for query and browsing



**Figure 1:** Drawing a synthesis suitable for high-quality printing is simple with Accelrys Draw. The product name displayed below the structure was generated automatically using the included structure-to-name generator.

## FOR SCIENTISTS—QUICK AND EFFICIENT STRUCTURE AND QUERY DRAWING

- Structure converter converts structure-to-IUPAC name and IUPAC name-to-structure; structure-to-canonical SMILES and SMILES-to-structure; structure-to-InChI name and InChI name-to-structure; and structure-to-InChI key
- Create and edit ISIS-compatible sketches, edit legacy sketches with improved cleaning of sketches
- Ease the transition with familiar ISIS/Draw-like chemical drawing tools and behaviors
- Create and edit polymers, formulations and mixtures (Sgroups)
- Create and edit Rgroup (Markush) queries including built-in Rgroup query logic
- Create and edit 3D queries, all 3D query features supported including 3D rotate
- Customize symbols including composite symbols
- Choose from large library of protecting group templates
- Take advantage of improved chemical recognition of tetrahedral and geometric stereogenic centers made possible by Accelrys NEMA algorithm

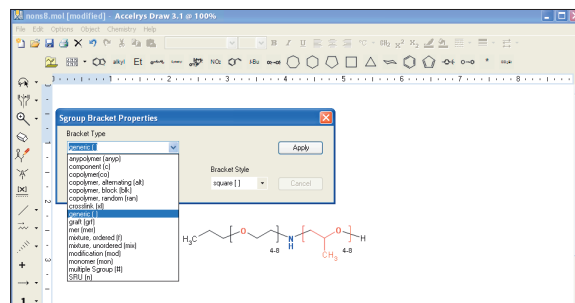


**Figure 2:** Easily create, register, search and present 1- and 3-letter peptides, DNA, and RNA. Modify sequences to include unnatural residues. Use templates to add protecting groups.

## FOR BIOCHEMISTS—DRAW, REGISTER, SEARCH AND REPORT ON CHEMICALLY MODIFIED PEPTIDE OR NUCLEOTIDE SEQUENCES

- Create 1- and 3-letter peptide, DNA or RNA sequences with a Sequence tool
- Use the same tool to draw crossing bonds, disulfide bridges and attach side-chain protecting groups

- Convert text from the clipboard, FASTA, Swiss-Prot, PDB and EMBL files into chemically significant sequences
- Expand residues in a sequence to full structure to illustrate chemical modifications

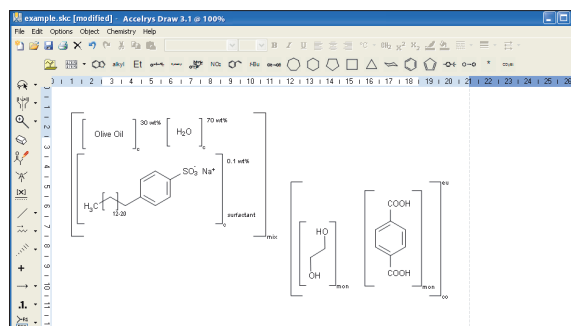


**Figure 3:** All polymer, mixture and formulation Sgroup features are supported. In this example, a combination of Generic and data Sgroups is used to represent a Markush structure.

## FOR DEVELOPERS—ADD STRUCTURE DRAWING AND DISPLAY TO YOUR APPLICATIONS, AND CUSTOMIZE ACCORDING TO YOUR ORGANIZATIONAL WORKFLOWS

- Use Accelrys Draw in Microsoft Internet Explorer® browser
- Accelrys Draw supports Microsoft XP, Vista and Office 2003/2007 software
- Easily extend the Accelrys Draw look-and-feel with custom add-ins, including:
  - 2D-to-3D Structure Converter\*
  - ACD/Labs calculators\*
  - ACD/Name\*
  - Enumerator
  - Bio-availability (Rule of 5)
  - Calculate-As-You-Draw
  - Isotopomer Distribution

\*separate license required



**Figure 4:** Polymers, mixtures and formulations. An example of a complex mixture containing a Markush structure and a source-based representation of polyethylene terephthalate (PET) are depicted.