

Symyx Draw

Symyx 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

Symyx 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, Symyx Draw offers flexible integration with custom Java® and .NET applications as well as integration with Symyx 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

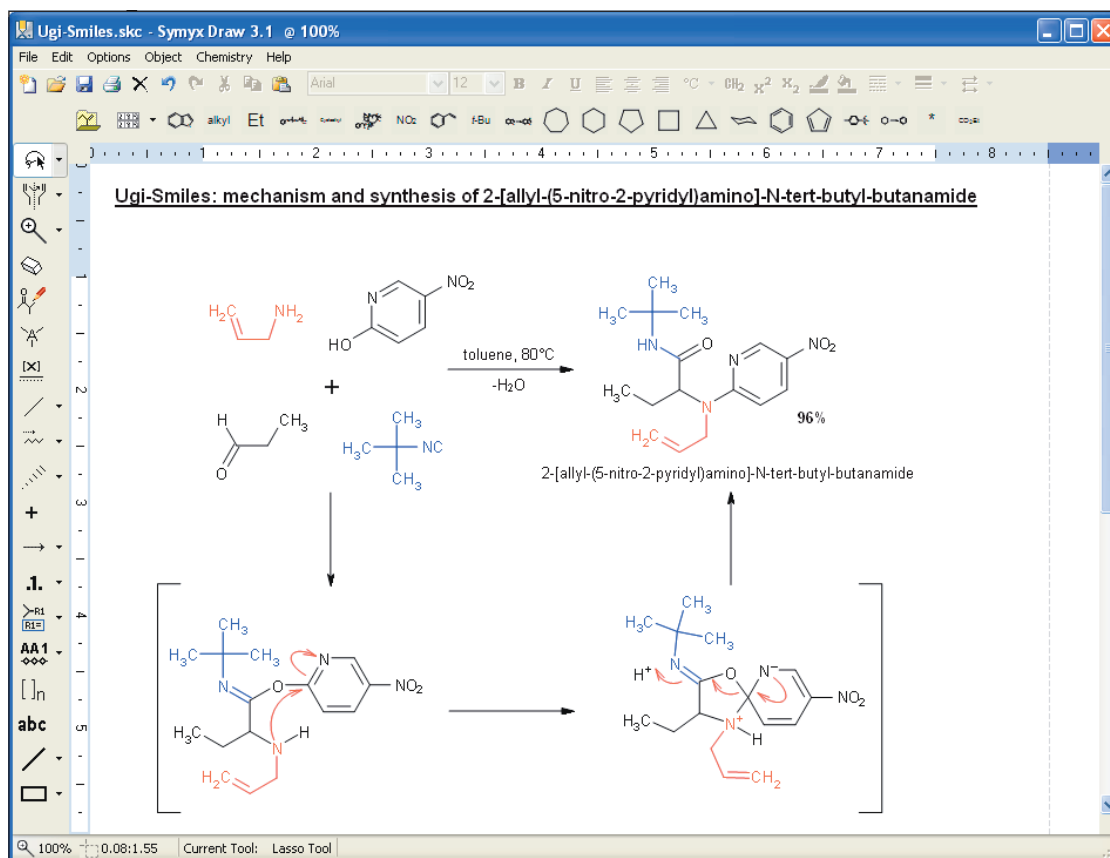


Figure 1: Drawing a synthesis suitable for high-quality printing is simple with Symyx Draw. The product name displayed below the structure was generated automatically using the included structure-to-name generator.

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 Symyx NEMA algorithm

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

For developers—Add structure drawing and display to your applications, and customize according to your organizational workflows

Use Symyx Draw in Microsoft Internet Explorer® browser

- Symyx Draw supports Microsoft XP, Vista, and Office 2003/2007 software
 - Easily extend the Symyx 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

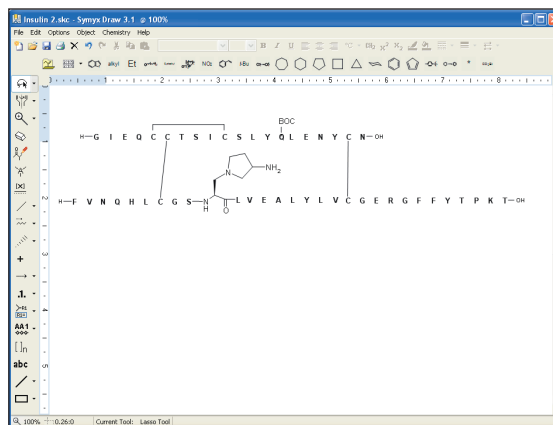


Figure 2: Easily create, register, search, and present 1- and 3-letter peptides, DNA, and RNA. Modify sequences to include unnatural residues. Use templates to add protecting groups.

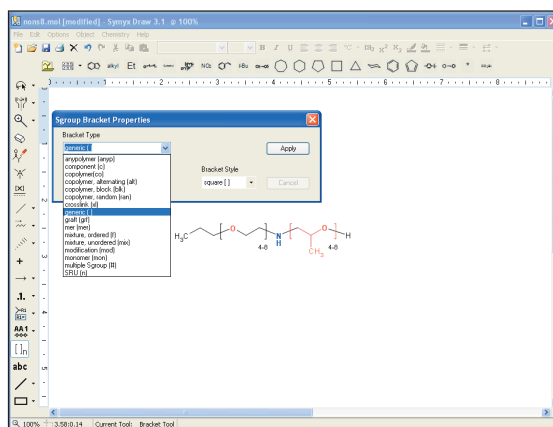


Figure 3: All polymer, mixture, and formulation Sgroup features are supported. In this example, a combination of Generic and data Sgroups is used to represent a Markush structure.

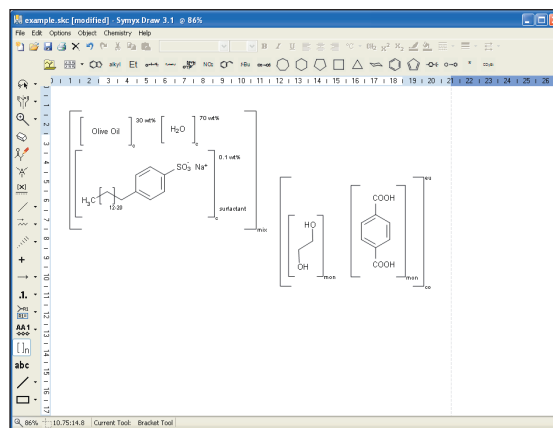


Figure 4: Polymers, mixtures, and formulations. An example of a complex mixture containing a Markush structure and a source-based representation of polyethylene terephthalate (PET) are depicted.



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