ISIS/Draw

ISIS/Draw is a chemically intelligent drawing program that understands the fundamentals of chemistry such as valence limits, bond angles, and aromatic ring systems. This understanding enables users to create chemical graphics intuitively, which can be inserted into documents or used to build and search databases of 2D and 3D molecules, polymers, and reactions.

Create Publication Quality Graphics

With ISIS/Draw, scientists can graphically represent almost any kind of chemical or polymer structure for use in reports, publications, and presentations.

- **Sketch large biomolecules with ease and speed:** Draw complicated structures including DNA, RNA, and amino acid sequences using special shortcut tools.
- **Create many types of polymer structures**: including homopolymers; source-based polymers; structure-based polymers; copolymers; crosslinked polymers; branched polymers; graft polymers; and statistical, random, and unspecified copolymers.
- **Control the display of your structures:** Scale atom labels, bonds, and other chemical attributes proportionally to make sketches easier to read.
- **Speed drawing using templates:** Create structures by piecing together predrawn templates of commonly used structures. Design your own template structures to reuse later.
- **Use flexible drawing tools:** Create multiple groups, drag out chains of atoms, automatically scale brackets, easily identify and manipulate specific atoms and bonds, clean structures, and apply various drawing defaults.
- **Publish your drawings:** Use professional format configuration files predefined for specific journals or internal presentations.
- **Post structures on the Web**: Combine ISIS/Draw with MDL's Chemscape to post your structures on any HTML page.

Build Structure Databases

Any chemical structure supported by ISIS/Draw may be registered into an ISIS/Host or ISIS/Base database.

- **Draw all types of structures**: Use your drawings to build databases of 2D and 3D molecules, reactions, and polymers.
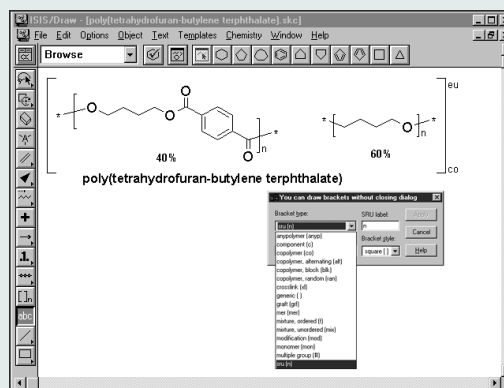

Figure 1: *When drawing polymers in ISIS/Draw, the bracket tool presents the user with a full range of polymer types from which to choose. Data such as weight percentages can be attached to polymer components and searched on later as part of the database.*
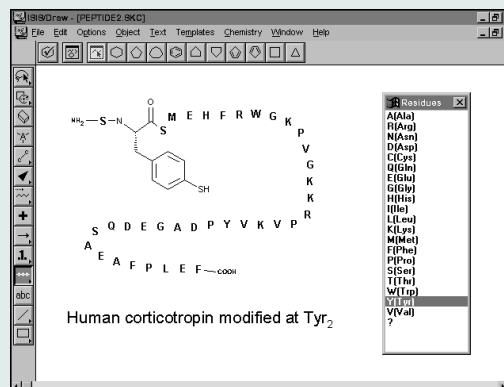

Figure 2: *Flexible tools in ISIS/Draw make it easy to draw peptides and other large molecules. The Sequence Tool gives you two options: Type in the amino acid abbreviations to build the structure, or simply click on the appropriate amino acid residues in the Residue List. To complete the drawing, orient the structure using the Sequence Shape Tool.*
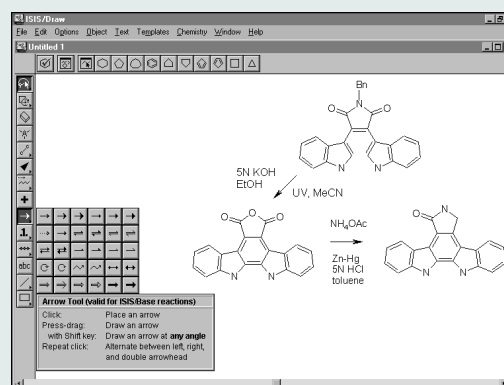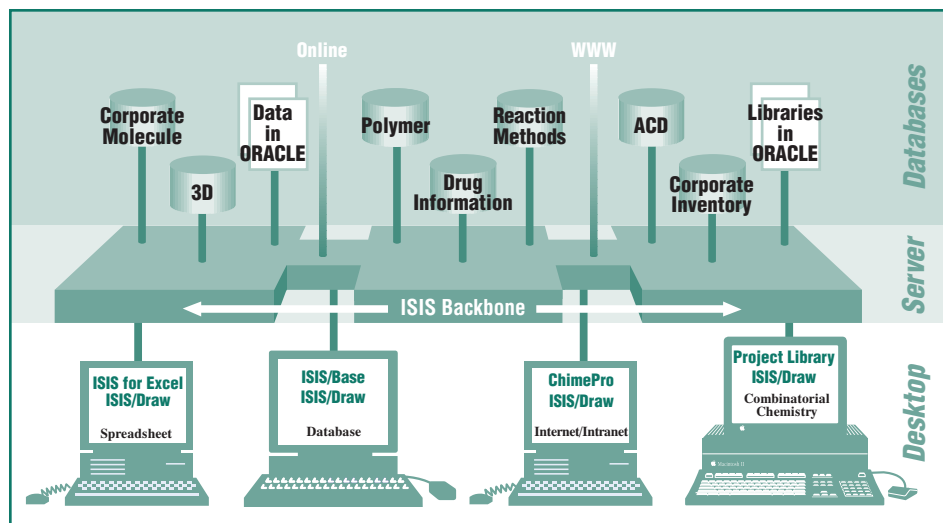

Figure 3: *Use ISIS/Draw to draw reactions for publishing or for inclusion in an ISIS reaction database. The arrow tool provides a variety of options for tailoring your sketch.*

- **Intuitively create reaction databases:** Simply draw the reaction as you would on paper, complete with + signs and arrows; ISIS/Draw will interpret the drawing and produce chemically intelligent reactions.
- **Attach substructure information:** Assign properties or values for any collection of components, atoms and bonds, including IR, NMR, and other spectroscopic data, weight and mole percentages, and tacticity information.

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Compose Database Queries

Use ISIS/Draw to create structure queries for local or server databases of ISIS molecules, polymers, or reactions.

- **Utilize special search options:** Easily define polymer, biomolecule, and 3D searches.
- **Define your structure query:** Use a full range of structure attributes such as substructure; location of single, double, aromatic bonds; lists of atoms; and stereochemistry.
- **Verify suitable structures or reactions:** Chem Inspector automatically checks the validity of structures and reactions for ISIS database registration and searching.

ISIS/Draw Communicates

Because ISIS/Draw adheres to platform standards, you can easily integrate your work with other applications such as Microsoft Word, Microsoft Excel, Lotus 1-2-3, Aldus Persuasion, and Microsoft Powerpoint.

You can move your drawings between applications by simply cutting and pasting. Or, by taking advantage of Publish and Subscribe on the Macintosh or OLE on Windows, you can ensure that the most up-to-date version of your drawing automatically appears everywhere you want it, eliminating repetitive cutting and pasting.

The ISIS Family

Since 1991, ISIS solutions have provided an information management architecture that supports the registration, retrieval, display, and analysis of all types of scientific information. ISIS applications, which support compound discovery research and development, are used by the pharmaceutical, biotech, agrochemical, and chemical industries worldwide. ISIS /Draw works together with MDL's ISIS/Base, ISIS for Microsoft Excel, Chemscape Chime Pro, and Project Library.

About MDL

MDL Information Systems ("MDL") is the recognized leader in discovery informatics for the life sciences and chemistry in industry and academia. MDL software, content, and services provide the enterprise-wide discovery informatics framework for comprehensive and successful discovery research. We are an international business headquartered in San Leandro, CA with offices worldwide. MDL Information Systems, Inc. is a wholly owned subsidiary of Elsevier Science, Inc.