

# ISIS/Base

## Flexible, Efficient, Integrated Scientific Data Management

ISIS/Base is a database management system for storing, searching, and retrieving chemical structures and associated scientific data with customizable forms. It can be used as a stand-alone desktop package or as a client to ISIS/Host.

### ISIS/Base

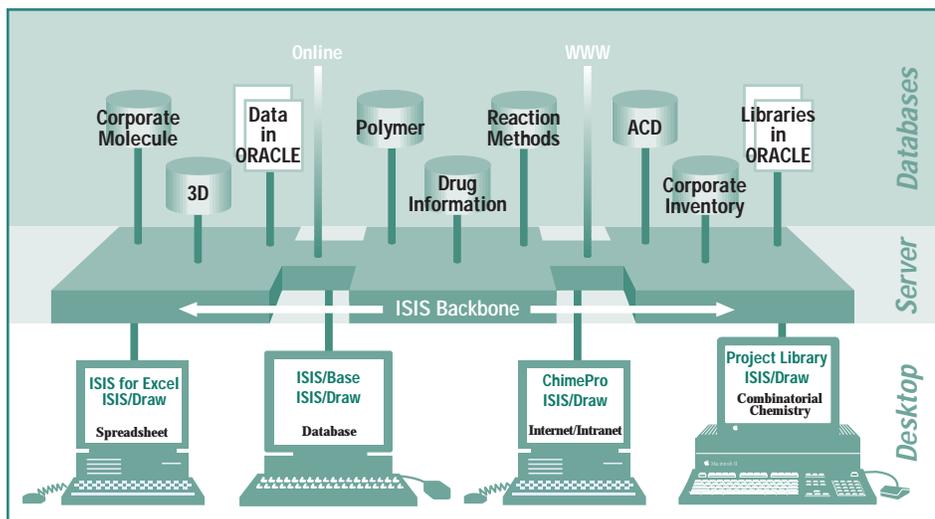
- ▶ **Create desktop databases:** Store your project data in a way that suits you.
- ▶ **Query with customizable forms:** Form-based searching is as easy as filling in the blanks. You can even combine chemical structure searches with text and numeric queries. Many form properties are customizable, with logically organized menus and a Table Tool that helps you plan and outline a form before creating it.
- ▶ **Control data display with sorting:** Sorting operations can be defined at the application level or performed interactively by the user. Sort on any field, including lower level database fields, and sort by up to three fields at any parent level in remote databases. The sort order is preserved when the list is saved.
- ▶ **Create calculated fields in forms:** Produce fields that contain derived data, such as the average or medium of several activity measurements for a compound. ISIS/Base allows you to view and sort on aggregate values—maximum, minimum, mean, median, sum, and count.
- ▶ **Analyze research results:** Export data to Microsoft Excel, where you can use ISIS for Excel—MDL's Excel add-in—to create SAR or SPR tables.
- ▶ **Manipulate lists of results:** Generate temporary lists automatically; add, subtract, and intersect lists; save lists that include results from any data source; discard, move, and copy items within a list.
- ▶ **Design your reports:** You can preview forms before printing; save page orientations with forms; and create, save, and print headers and footers.
- ▶ **Customize Applications:** Use development tools to create your own dialog boxes, tool bars, buttons, and special forms; control vocabulary and user access to specific functions; and automate procedures such as data registration.

The top screenshot displays a 'Chem/Ste Project Database' window. It features a chemical structure on the left and a form on the right with fields for 'Company ID', 'Name', 'Formula', and 'MW'. Below these fields is a table titled 'WAS Resorption' with columns for 'Resor 1', 'Resor 2', 'Resor 3', and 'Resor 4'. The bottom screenshot shows a 'STRUCTURE' window with a chemical structure and a table with columns for 'WAS Resorption' and 'Molecules'.

*Figure 1: Here ISIS/Base is used to build a desktop chemical/biological project that displays the chemical structure along with fields of data and tables of research results. Each field in the database—whether text, numeric, or structural—is searchable. Another application is built to access a remote ISIS/Host polymer database which tracks the properties of a series of polymers under different conditions.*

The top screenshot shows an 'Inventory Management System' window with fields for 'Company ID', 'Chemical Name', 'Formula', and 'Molecular Weight'. Below these fields is a table with columns for 'Batch ID', 'Location', 'Amount (gms)', 'Supplier', and 'Checked Out'. The bottom left screenshot shows a similar form with a chemical structure. The bottom right screenshot shows a dialog box with a 'List' field and buttons for 'Add', 'Subtract', and 'Intersect'.

*Figure 2: Form based searching makes information retrieval as easy as fill-in-the-box. Once your results are displayed, you can move specific items to a list for later reference. List handling capabilities enable you to add, subtract, or intersect saved lists.*



### Expand Your Capabilities with ISIS/Base as the Client to ISIS/Host

- ▶ **Register, search, and view data in server-based databases:** You can work with servers located anywhere in the world by simply linking ISIS/Base to ISIS/Host, MDL's server-based information management system, which transparently integrates 2D and 3D structure, reaction, polymer, relational, and other specialized databases.
- ▶ **Perform a full range of structure-based searches:** Search molecule, reaction, and relational databases with a variety of search types, including substructure, flexible exact match, similarity, Rgroup, 3D, polymer, reaction substructure, formula, numeric, and text.

### The ISIS Family

For the past five years, 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/Base can be used alone to manage local databases or as the client of ISIS/Host to provide access to information from virtually anywhere on your corporate information system.

Because of the integrated nature of ISIS tools, organizations can choose the way they want to present scientific information. Some researchers may prefer ISIS for Microsoft Excel, which provides access to databases from within a spreadsheet program. Others may like the ease of use offered by a Web browser, now available with MDL's Chemscape series. ISIS/Base is perfect for scientists who want a form-based front-end where they can create advanced search and display forms for chemical information.

### About MDL

MDL Information Systems, Inc. is a leading provider of integrated solutions that accelerate high-throughput discovery and development in the life science and chemical industries. Our software systems, databases, and services help customers manage, communicate, and analyze the volumes of data associated with modern R & D workflows. With applications supporting chemical and biological information management, bioinformatics, automated synthesis and screening, and materials science, MDL is committed to keeping pace with new technologies in the pharmaceutical, chemical, and biotechnology industries. MDL has offices worldwide with headquarters in San Leandro, California.

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