

ISIS/Application Development Kit Professional: Rapid Application Development for Cheminformatics

Evolution of the ISIS/ADK Pro

Cheminformatics application development is becoming significantly faster and provides more user value than was possible even a few years ago. The progression towards open systems and smaller, best-of-breed functional software components has helped speed application development. Integrating ActiveX and OLE/COM controls on the desktop has enabled new software applications in cheminformatics. These new applications can be designed and constructed rapidly, in some cases days instead of years.

In 1995 MDL released the ISIS/Object Library to support the increasing demands of developing software applications from industry-standard application development tools. Combined with the flexibility in the ISIS server technology for chemical, relational, and textual database integration, these tools have provided unparalleled support for third-party development environments such as Microsoft Visual Basic, Microsoft Office VBA, PowerBuilder, and Delphi. MDL's standard ISIS/ADK provides two OCXs, the ISIS Form Box Control and the ISIS Database Control, as well as access to the rich intrinsic library of ISIS/Base. The ISIS Database Control provides a link to an ISIS/Base local database or an ISIS/Host remote database. The ISIS Form Box Control provides a multipurpose form box that can display text or structural data from the connected database. The standard ISIS/ADK tools are provided without additional charge as part of the standard ISIS/Development license, and are described in the ISIS/ADK Help.

As MDL has released additional applications layered on the rich ISIS client-server framework, it has developed a common set of application building

blocks and custom controls that further speed application development. These building blocks are discrete functional software units with defined and documented software interfaces. They can be dropped into custom cheminformatics applications to satisfy common requirements so developers can focus on the important, value-added capabilities unique to their own discovery operations. These tools are now available as a complete package under the name ISIS/ADK Pro.

ISIS/ADK Pro

MDL has a unique perspective on application development since we develop both our own applications and open-architecture tools that support hundreds of companies with cheminformatics application development. From this viewpoint several common requirements stand out as important for many cheminformatics applications. Applications should

- Connect the user to the database(s) for read/write operations
- Allow the user to submit queries of chemical structures and/or textual/numerical data

- Hyperlink to ISIS/Draw for structure drawing as input or refinements of queries
- Display boxes, marquees, grids, or spreadsheets of chemical structures and data
- Allow the user to perform list handling and list logic operations on the lists returned by the searches
- Allow the user to select fields in the database to perform operations for sorting, viewing, and data export and import

Login Dialog

The Login Dialog Object (Figure 1) provides a convenient, flexible way of prompting the user for database connection information and forming the connection. By predefining all the connection information, the developer can simplify the connection process so that the user need only to enter a password. If more information is required, the Login Dialog can collect it before making the connection.

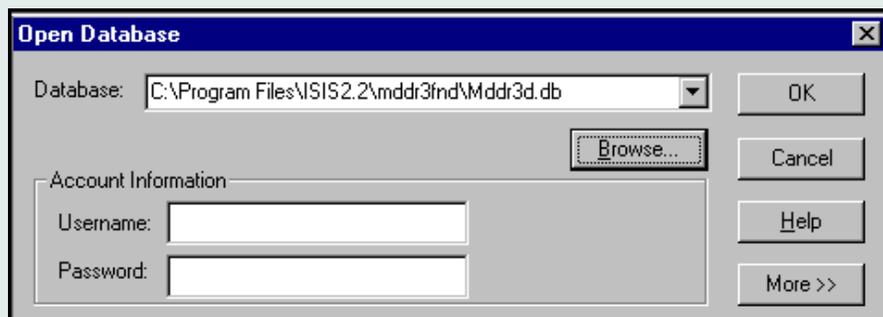


Figure 1: Login Dialog provides simplified end-user access to complex, integrated data sources.

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Query Builder Control

The MDL Query Builder Control provides a grid-style interface through which users can build complex structure and data queries. This control can be used to create custom query dialogs similar to the query dialog in MDL's ISIS for Microsoft Excel. Developers can design their own query dialogs, either blank or preloaded with canned queries, and create queries that involve both chemical structures and text/numeric clauses simultaneously. The Query Builder provides an automatic hotlink to ISIS/Draw for creating the depth of chemical structure queries that chemists rely upon from MDL.

Query Builder Dialog

The Query Builder Dialog Object (Figure 2) provides a simpler, prebuilt dialog that contains much of the same grid-style interface as the Query Builder Control and the identical basic functionality. It can be used easily with little or no customization, even in development environments that provide no form or dialog builder.

Field Selector Dialog

The Field Selector Dialog (Figure 3) allows the user to select a group of fields from a list of available fields in the database definition. The Field Selector also allows the user to order the field if required for display or export of data to a file or another program.

The Field Selector object can be used for many common tasks such as

- Selecting fields for display after a query operation
- Selecting fields for sorting
- Selecting fields for import or export of data to and from the database
- Selecting fields for mathematical or statistical calculations

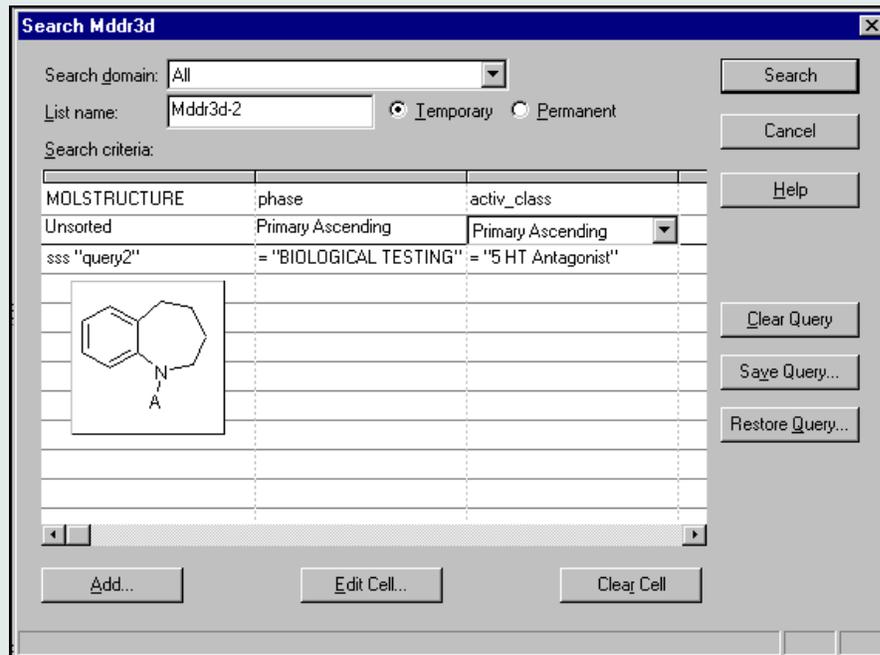


Figure 2: Query Builder Dialog, based on the Query Builder Control, enables applications with a powerful, easy-to-use querying capability for chemical structures and text/numeric data.

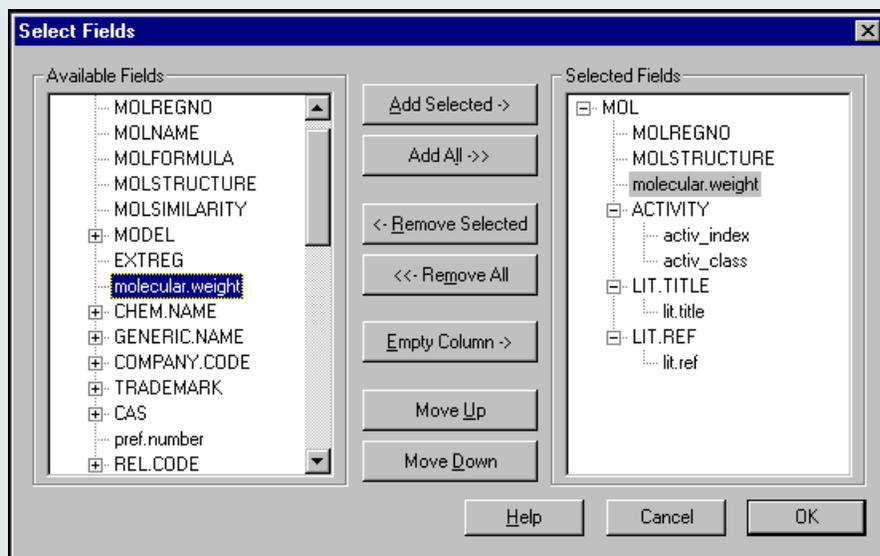


Figure 3: Field Selector Dialog presents easy-to-understand views and control over the logical database definition.

Grid Partner Control

The MDL Grid Partner Control channels data from an ISIS database into Spread 2.5, a third-party spreadsheet control from FarPoint Technologies. This provides a grid or spreadsheet display of graphical, text, and numeric information in an application (Figure 4). Grid Partner Controls can be linked with each other or with ISIS Form Box controls to produce an integrated, multi-level structure and data display.

When combined with the FarPoint Spread control, Grid Partner Control provides a “virtual mode” that retrieves only enough data to fill the displayed cells, but automatically retrieves more as the user scrolls through a list. This provides unrivaled responsiveness for chemical structure display even on a large list of search results.

The developer can access the OCX's properties through a dialog in the container application development environment (Figure 5). This dialog provides consistency and integration with similar property sheets in the ISIS Database and Form Box controls.

List Logic Dialog

The List Logic Dialog (Figure 6) can be used to perform Boolean operations on collections of records in ISIS hit lists. For example, the user can find the intersection between two lists (AND), the union of two lists (OR) or the records from one list that are not in the other list (NOT). The resulting list or lists can be stored as a separate new list.

The List Logic Object can be incorporated directly into the application's user interface so that the user can quickly manipulate lists.

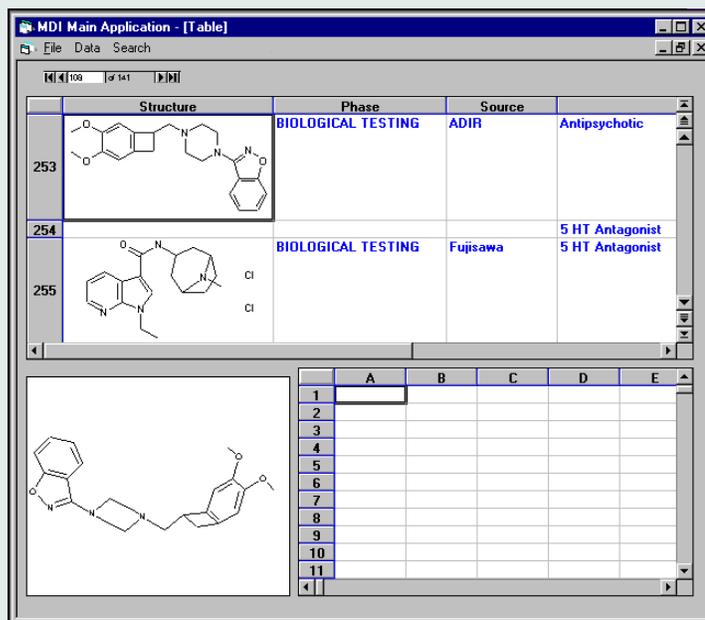


Figure 4: Grid Partner Control provides an efficient and sophisticated interface to chemical structures and related data.

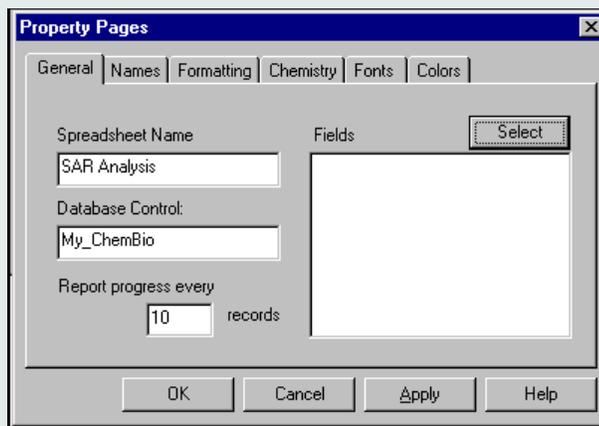


Figure 5: Grid Partner Control properties dialog.

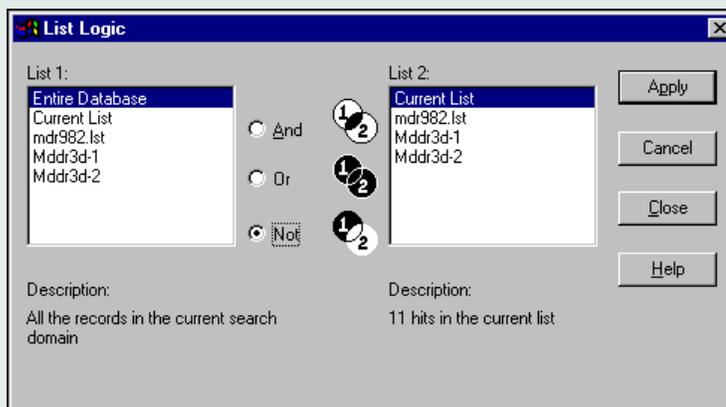


Figure 6: List Logic Dialog allows users to perform powerful Boolean operations on database hit lists.

Hardware and Software Requirements

Hardware

- IBM PC or 100% PC-compatible with a Pentium or higher microprocessor
- VGA or better monitor
- Microsoft Windows compatible mouse

Software

- Windows 95 and Windows NT 4.0 or higher.
- Compatibility with ISIS 2.0 or higher databases
- Compatibility with ISIS/Base and ISIS/Draw 2.2 or higher
- Spread 2.5 control, licensed separately from FarPoint Technologies (<http://www.fpoint.com>).

Memory

- Minimum of 32 MB RAM (recommended)

Hard Disk Space

- Minimum of 10 MB hard disk space

Summary

ISIS/ADK Pro extends the utility of ISIS/ADK by providing common application building blocks that allow developers to build cheminformatics applications more quickly within the ISIS server environment. These high-level application building blocks and OCXs allow developers to focus on technological contributions that are unique to their own discovery operations. ISIS/ADK Pro's prebuilt tools simplify common and mundane application requirements. Users also benefit from a well-tested interface that is reused in multiple cheminformatics applications. If you are interested in learning more about ISIS/ADK Pro, contact an MDL office or your MDL sales representative.

About MDL

MDL Information Systems, Inc., a wholly-owned subsidiary of Elsevier Science, is a leading provider of integrated logistics and decision support systems that enable a high-throughput environment for research and development in the life sciences and chemical industries. Our customers include industrial, government, and academic producers and users of chemical and biological products. MDL's pioneering software systems, databases, and services help customers manage, communicate, and analyze the volumes of data associated with modern research. MDL has specialized applications in the areas of chemical and biological information management, high-throughput synthesis and screening, chemical sourcing, and environmental health and safety. MDL has offices worldwide with headquarters in San Leandro, California.

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