MDL's Reagent Selector

MDL's Reagent Selector offers scientists engaged in medium- and high-throughput synthesis integrated tools for selecting reagents, locating and obtaining compounds from in-house inventories, and "shopping" for reagents from databases of commercial suppliers. Developed for synthetic, medicinal, and combinatorial chemists, Reagent Selector's detailed architecture is also designed to help IT professionals easily administer and customize the system in a variety of ways that unify and accelerate the scientist's workflow. For example, administrators can create an Oracle-based Concordance database that functions as a virtual "reagent datamart." The Concordance database presents a consolidated view of in-house and commercial repositories where inventory sources can be standardized and searches extend over multiple databases at once.

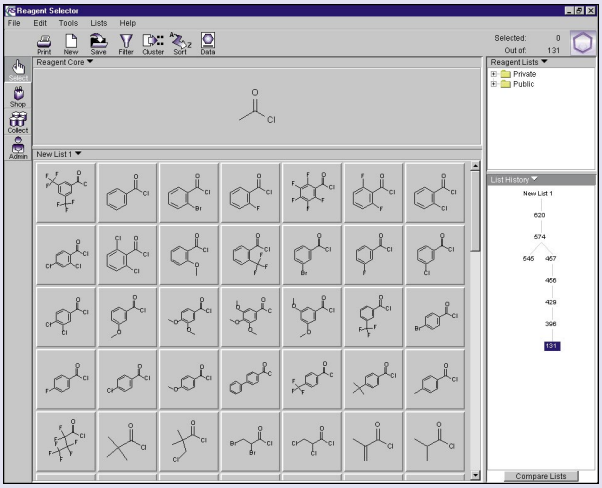

Figure 1: *Reagent Selector's intuitive interface includes an interactive grid for selecting reagents with a mouse click, a public and private folder pane that facilitates the storage and sharing of lists, and a list history pane for tracking steps in filtering, sorting, and clustering and for interactively refining lists.*

Wide-Ranging Capabilities within an Intuitive Interface

Reagent Selector's features include

- **An interactive selection grid:** The selection mode is designed for easy inspection of chemical structures and navigation throughout the selection process.
- **Multiple filters and the ability to add more:** Researchers can refine lists based on functional groups, cost, purity, calculated properties, and source databases. The software comes standard with a general class of functional-group filters, and administrators can add others as well as new properties that extend Reagent Selector's filtering capabilities.
- **Flexible clustering:** Reagent Selector comes out-of-the-box with K-MEANS, a nonhierarchical, distance-based clustering algorithm that provides fast, accurate results with small and very large populations of molecules. Administrators can easily customize Reagent Selector to add commercial or proprietary clustering algorithms. The system's intuitive display allows users to easily drill down into specific clusters or select structures from several clusters.
- **List history:** A list history pane enables scientists to move back and forth between the reagent lists generated by searching, filtering, and clustering operations.
- **Private and public storage:** Scientists can store reagent lists in private or publicly accessible folders that allow researchers to share information easily.
- **Collection and shopping modes:** In the collection mode, researchers can determine the real-time availability of compounds in corporate inventories. The shopping area includes a virtual "shopping cart" that allows researchers to gather multiple items based on supplier, ordering, and product information contained in MDL's Available Chemicals Directory (ACD).
- **Easy integration with logistics:** Selection and shopping lists are stored in Oracle tables and can be easily integrated with purchasing systems and inventory management systems. For indirect purchasing, users can export shopping lists to ASCII tables, which can then be imported into Microsoft Excel and/or emailed to purchasing departments. Reagent Selector can also easily integrate with other in-house or MDL applications, including SMART and Central Library. For example, Central Library can directly import and clip reagent lists from Reagent Selector.

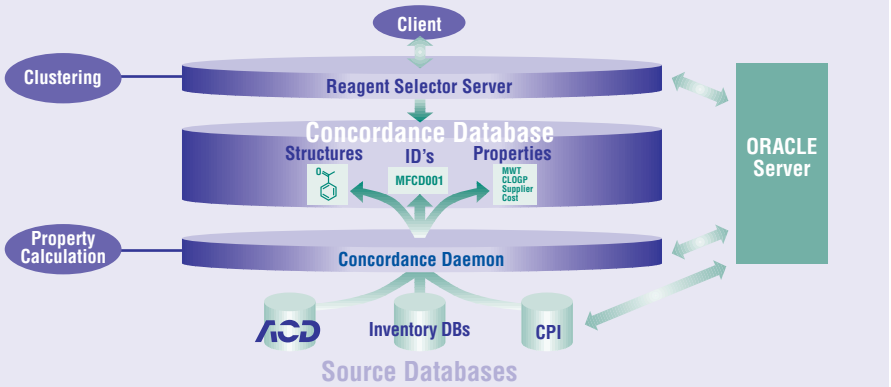

Figure 2: *Reagent Selector's three-tiered architecture includes a database tier illustrated above. The Concordance database provides tight integration of multiple data repositories. A daemon synchronizes the Concordance database with in-house databases and allows administrators to add property calculations or define registration filters.*

The Concordance Database

An extension of MDL's Relational-Chemical Gateway, Reagent Selector's Oracle-based Concordance database allows end-users to search, select, collect, or shop from a unified view of multiple in-house inventories and ACD.

- **No duplicate structures; access to source databases:** The Concordance database contains chemical structures, property calculations, and compound identification numbers from the original databases. The Concordance database consolidates structurally identical hits—it displays no duplicate structures—and yet points to source databases, where users can find a compound's physical location(s) and other non-structural data.
- **Daemon controlled database synchronization:** A server-side Concordance Daemon maintains synchronization between inventory databases and the Concordance database. Administrators can set the daemon to run automatically at intervals specific to each in-house database.

MDL® Information Systems, Inc.

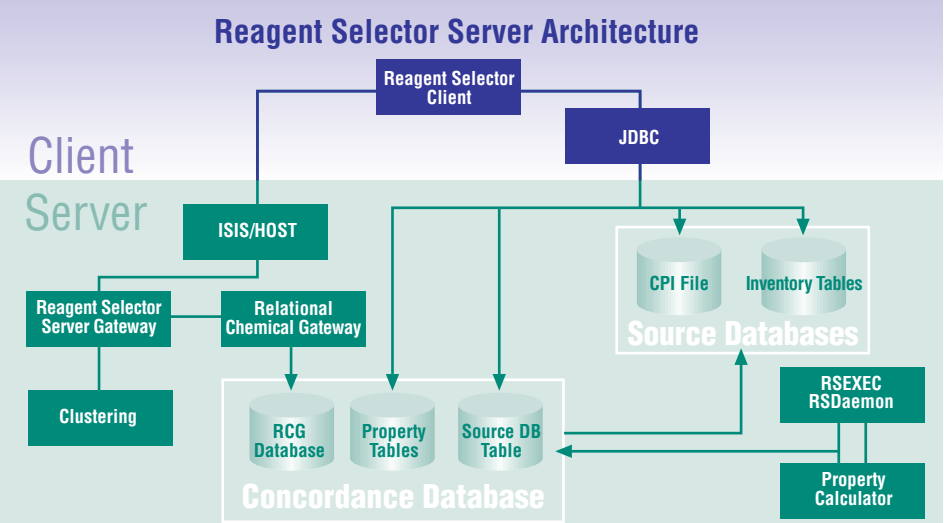

Figure 3: *The Reagent Selector client accesses structures in the Concordance database via ISIS/Host through the Relational-Chemical Gateway and a dedicated gateway. The client accesses non-structural data in inventory and CPI-file databases via JDBC.*

- **Administration/configurability:** Reagent Selector includes RSExec, an application that helps program administrators create, customize, manage, or eliminate Concordance databases, as well as modify and remove source databases. Administrators can set registration filters, add clustering algorithms, and manage property calculators that will calculate properties through the Concordance Daemon during the uploading of inventories. Companies can use RSExec to drop in their own property calculators (examples of property calculations are shipped with the product) and store calculated properties in the Concordance database or in external Oracle tables. Administrators can also use RSExec to start, stop, or check the Concordance Daemon.
- **Security:** RSExec manages database security, using system passwords for end-users.
- **Inventory database normalization with Cheshire:** RSExec allows administrators to use Cheshire, MDL's new molecular scripting editor, to standardize inventory databases through the Concordance Daemon before compound representations are registered into the Concordance database. For example, representations of tautomers or salts can be normalized according to a company's business rules throughout multiple inventory databases.

The Concordance database consists of a relational-chemical database and an additional set of tables for administration, property data, lists, and other functions not directly supported by a relational-chemical database. The tables comprising the main Concordance database contain all of the chemical structures and all of the standard relational-chemical data, such as internal registry numbers. The separate administration tables contain additional nonstructural data specific to Reagent Selector, such as information about source databases, the Concordance Daemon log, and property tables. Together, these molecule and data tables support a many-to-one structure relationship in the Concordance database.

The Concordance database can draw from several types of source databases:

- 2D molecule gateway
- Relational molecule 2D databases
- Host library databases (specific structures only) and building-block databases

System Requirements

Client

- Intel or Intel-compatible PC running at greater than 133 MHz (>166 MHz recommended) with the Microsoft Windows 95, Windows NT 4.x, Japanese Microsoft Windows 95, or Japanese Windows NT 4.x operating system
- Apple Power Macintosh
- ISIS/Desktop 2.1.4 or greater

Server

- Digital Alpha computer with OpenVMS 7.1
- SGI computer with IRIX 6.2, 6.3, 6.4
- IBM RISC System/6000 computer with AIX 4.2 or 4.3
- ISIS/Host 3.1
- MDL Available Chemicals Directory database
- MDL Chemical Products Information File database
- Oracle Database Management System

Please contact your local MDL sales representative for specific requirements.

About MDL

MDL Information Systems, Inc. is the recognized leader in discovery informatics for the life science and chemical industries. Our software, content, and services provide the enterprise framework for identifying successful new products. A wholly owned subsidiary of Elsevier Science, MDL has offices worldwide with headquarters in San Leandro, California.

MDL®
Information Systems, Inc.

U.S.A.
World Headquarters & Western Sales
14600 Catalina Street
San Leandro, CA 94577
TEL: (510) 895-1313
FAX: (510) 483-4738
http://www.mdli.com

Eastern Sales
14 Walsh Drive
Parsippany, NJ 07054
TEL: (973) 299-3991
(800) 401-4321
FAX: (973) 299-3994

Midwest Sales
3 Westbrook Corporate Center
Suite 520
Westchester, IL 60154
TEL: (708) 409-8300
FAX: (708) 409-8305

Europe
Headquarters
MDL Information Systems AG
Gewerbestrasse 12
CH-4123 Allschwil 2
Switzerland
TEL: +41 61-486-88-88
FAX: +41 61-486-88-89

Cologne Office
TEL: +49 221-16025-255
FAX: +49 221-16025-68

Authorized Agent Scandinavia
Oslo Office
TEL: +47-22-44575-6
FAX: +47-22-43416-6

Paris Office
TEL: +33 1-45 36 80 00
FAX: +33 1-45 36 80 01

United Kingdom
Headquarters
MDL Information Systems (UK) Limited
Ground Floor, Building 4
Archipelago
Lyon Way
Camberley
Surrey GU16 5ER
England
TEL: 44 (0)1276 701500
FAX: 44 (0)1276 701501

Japan
MDL Information Systems Japan K.K.
Kojimachi M Bldg., 3F
3-12-12 Kojimachi
Chiyoda-ku
Tokyo 102
Japan
TEL: +81-3-3230-2641
FAX: +81-3-3230-2761