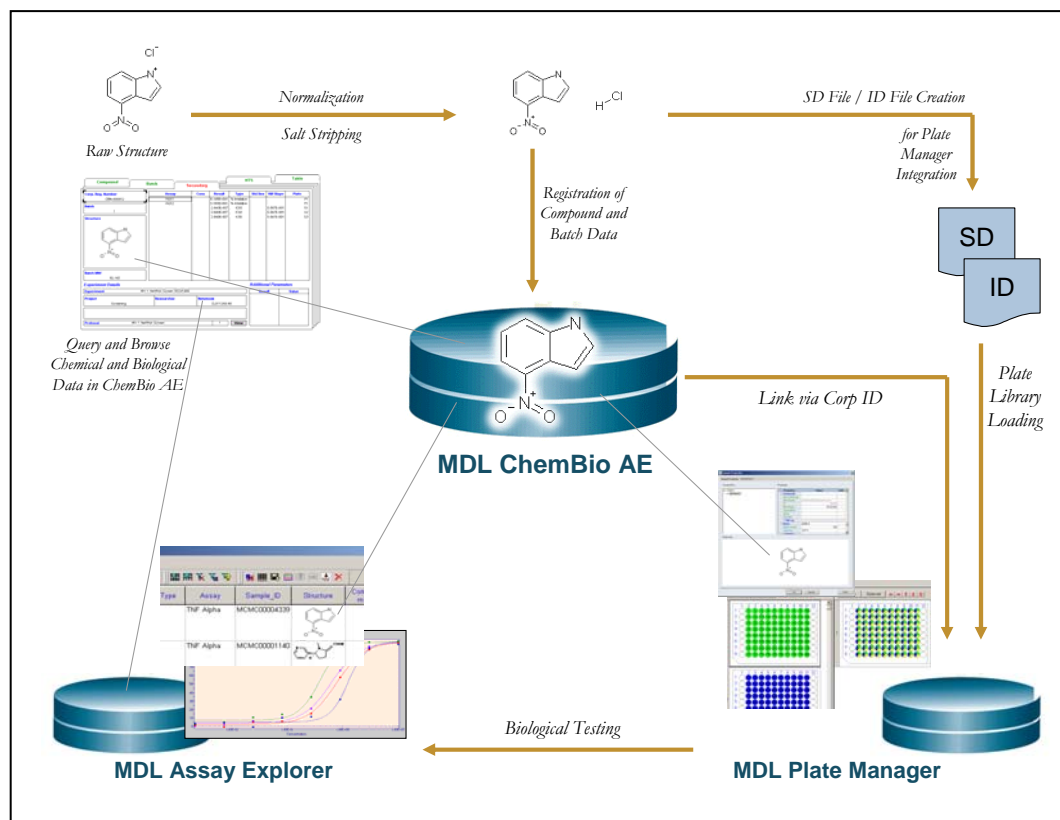


# MDL® ChemBio AE

MDL® ChemBio AE is an out-of-the-box chemical registration and retrieval system for scientists to store compound and batch data and search chemical and biological data. Structures are normalized and deduplicated during registration of single compounds or collections of compounds from SDfiles.



MDL ChemBio AE integrates with MDL® Assay Explorer and MDL® Plate Manager, serving as the central structure repository. Compounds are registered in ChemBio AE and plate information is loaded into Plate Manager. Biological testing information is stored in Assay Explorer. Compound summary data is searched and displayed in ChemBio AE.

## Register Compound and Batch

MDL ChemBio AE enables registration of compound and batch data

- Normalize structures to conform to corporate structure representation rules via MDL® Cheshire
- Check for duplicates
- Generate batch molecular weight and formula automatically
- Generate corporate ID's
- Register multiple batches for a given parent structure
- Register compounds via SDfile with flexible field mapping utility

## Search and View Data

MDL ChemBio AE allows searching and viewing of chemical and biological data via MDL® ISIS/Base interface

- Structure-based searches, including similarity, exact match, and substructure searches
- Text or numeric searches on any field in the database
- Combined searches on multiple fields
- Integrated chemical and biological information searches on shared Assay Explorer data



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### About MDL and Elsevier Life Sciences

A wholly owned subsidiary of Elsevier, Inc., MDL is part of the Elsevier Life Sciences division. Over 1,000 life science companies supercharge their discovery engines with MDL software solutions to generate fresh ideas and make breakthrough discoveries. By synchronizing and streamlining the sharing and management of vital information and knowledge, MDL enables scientists to work more efficiently and invent drugs faster. MDL is headquartered in San Leandro, CA with offices worldwide. For more information, visit [www.mdl.com](http://www.mdl.com).

Elsevier Life Sciences combines Elsevier's wide array of life science content products with MDL's extensive informatics, database, workflow, and decision support solutions. This unique combination enables Elsevier Life Sciences to bring unparalleled solutions to researchers, significantly advancing the efficient, cost-effective development of new medicines.

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## Administration

MDL ChemBio AE provides sophisticated administration capabilities

- Modify and delete chemical data
- Manage lookup tables, including users, projects, and analytical procedures
- Manage the flexible SDfile field mapping utility
- Manage user access through flexible security roles

## Flexibility

The built-in flexibility of ChemBio AE enables user-friendly data registration

- Flexible lookup data
- Custom fields at Compound level
- Custom fields at Batch level
- Flexible integration to analytical data

## Integration with MDL Assay Explorer

By integrating with Assay Explorer, biologists and chemists can easily share information on lead candidates and assay results. Structures and compound data stored in ChemBio AE are accessible via Assay Explorer, and the biological assay results for a compound are in turn searchable and viewable in ChemBio AE.

## Integration with MDL Plate Manager

The integration between ChemBio AE and Plate Manager dramatically simplifies the process of creating and formatting plates from purchased libraries. During registration of library SD files the crucial information needed by Plate Manager is registered into the ChemBio AE database, and readily imported into Plate Manager. And, since ChemBio AE serves as the central structure repository, maintenance of the corporate structure database needs only occur in one place.

## Benefits

- Consistent corporate structure registration and representation
- Normalized, deduplicated, and centralized structure database
- Keystone of a complete, out-of-the-box discovery workflow solution integrating chemistry and biology, data analysis, and plate management.

*A user-friendly guide to chemical registration. Data consistency is achieved through flexible lookup tables.*

*View data in the familiar and proven ISIS/Base environment.*