

Out-of-the-box Enterprise Cheminformatics

Extensible and customizable to meet your organization's needs

Easy web-based access to flexible tools and discovery data

## Accord Enterprise Informatics

Accord Enterprise Informatics (AEI) is an out-of-the-box, Oracle®-based enterprise-wide solution for the management of chemical structures, related biological, chemical & inventory data, experimental results and registration information. AEI provides you with a comprehensive set of tools to enable you to collaborate, work effectively and make quicker decisions by providing easy access to key discovery data.

AEI leverages Oracle® to provide a data management solution that helps you to share your data seamlessly within and across workgroups, to identify potential leads and to facilitate crucial decisions faced during the competitive drug discovery process.

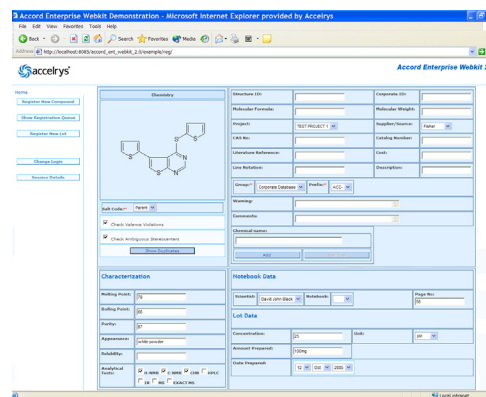
AEI provides seamless integration of data, querying, and reporting across chemistry and biology databases. This robust, flexible, and scalable solution is well suited to meet the ever-changing needs of research operations.

Since all Accelrys 2D chemistry products share a common chemistry engine, you can quickly learn to rely on a consistent set of features to minimize possible confusion and reduce training costs as tools are deployed from the desktop to the integrated enterprise.

By searching on structures, reactions and other data types, you can quickly identify hits, create customizable reports using Accord for Excel Enterprise or the Accord Enterprise Webkit, and share these hit lists automatically with colleagues. Hit lists are available in all AEI applications via the built-in list manager common to all AEI applications to enable you to seamlessly share information across research groups and between different teams.

### Advanced Chemistry

Accord Enterprise Informatics uses the Accord Chemistry Engine, which forms the backbone of the system. The Accord engine endows the system with powerful chemistry capabilities and is capable of handling a wide range of organic, organometallic and inorganic molecules and reactions, isotopes, charges, radicals, delocalised pi-systems and more. Accord understands aromaticity the way chemists do using the Hückel rule, and can interpret a comprehensive range of stereochemical designations, both chiral and geometric. In addition, a wide range of chemical formats are supported, including molfile, SDfile, rxn files and SMILES strings.



Registering a compound into AEI from a simple web page built using the Accord Enterprise Webkit.

### **Corporate Registration**

AEI enables you to register structures, structure lots, samples and reactions, along with associated information such as project name, chemical name, etc. Major features of registration include:

- Structures can be registered one at a time, or in bulk, using SDfiles
- Reactions, reactants and products can all be registered into the system
- Complete duplicate checking ensures only one copy of a compound is registered; duplicates can be registered as a new lot, rejected or registered again
- Flexible security rules can be configured to control access to structures, lots and registration functionality
- A variety of flexible corporate identifier configurations are available out-of-the-box
- Optional registrar role is available to enable all registrations to pass through a central master user or users
- Automated salt stripping for compounds can be initiated as part of the registration workflow
- Compounds can be associated with multiple batches
- Compounds can be registered into multiple databases simultaneously, depending on the configuration of your security and business rules

### **Comprehensive Biological Data Management**

AEI enables you to manage all of the biological data associated with your drug discovery efforts. Through AEI, you can define and manage entities such as assays, assay protocols, result types, units, concentration and volume. Any number of different result types, units and associated entities can be defined, giving you the ability to manage data from a variety of assay types and experiments including biochemical, cell-based and animal-based studies.

The system's flexible biological capabilities are further enhanced by the ability to define result data hierarchies, enabling you to create relationships between different datasets so that you can store final and intermediate results, as well as raw data and curve-fit parameters. Once defined, relationships are retained for subsequent viewing and reanalysis of datasets, giving you the ability to drill-up and down between primary and derived data when assessing the quality and outcome of experimental studies.

### **Configurable Row-Level Security**

AEI provides an optional, off-the-shelf security module that you can use to control access to a variety of data and system features including individual structures & reactions, database lists, registration, assays and query resources. The security system is flexible enough to cover almost any conceivable set of security requirements so that you can easily configure the system to meet your own business rules. Whether your requirements are for simple project-level security or for more comprehensive system-wide security to ensure the confidentiality of client data, AEI's security system provides you with the tools that you need to ensure that your data remains secure at all times.

### **Powerful Querying and List Management**

The built-in list manager in AEI stores database lists, queries, hit lists and user-defined structure lists. Lists can be combined, annotated and modified in a variety of ways to enable you to generate lists of interesting actives, compounds or reactions for further investigation or analysis. Any list stored in the list manager can be kept private for your individual use, or can be shared with all users or just selected users that are working on the same project, providing you with an easy way to share information across your workgroup or with fellow team members.

Compound ID	Name	Structure Identifier	Other Data
ACC000001	...	...	...
ACC000002	...	...	...
ACC000003	...	...	...

Viewing hit lists and generating reports from AEI's built-in list manager

**Analysis Report for ACC000023**

Registration Date: 2009-09-24  
Formula: C16H17NO2S  
Weight: 275.395  
Process Date: 2009-09-24

COMPONENT_ID	LOT_ID	RESULT_TYPE	RESULT_VALUE	CONCENTRATION	UNIT_VALUE	PROTOCOL
ACC000023	1	N/N/N	32.7020216427714	35	uM	AL
ACC000023	1	N/N/N	0.0000109044899	100	uM	AL
ACC000023	1	N/N/N	13.1220270751094	100	uM	AL
ACC000023	1	N/N/N	0.57420204790581	0.01	uM	AL
ACC000023	1	N/N/N	0.5718126113119670	0.01	uM	AL
ACC000023	1	N/N/N	0.444010100207479	0.1	uM	AL
ACC000023	1	N/N/N	25.8309000002096	1	uM	AL
ACC000023	1	N/N/N	20.0002010995413	1	uM	AL

Viewing compound property and assay information via an analysis report interface built with the AE Webkit.

Powerful query capabilities are available to enable you to search any data stored in AEI: almost any database field available in AEI can be queried. AEI's built-in data catalogue module makes it easy to extend queries across other internal data sources and tables or external to AEI itself. Queries can be structure-based (exact match, substructure or similarity) and can be combined with other non-structural search terms such as biological assay data, and physical or chemical properties to enable you to return only the specific information that you need. AEI's query capabilities are fully schedulable, allowing you to run project or target-level queries automatically on a regular basis so that you can keep track of project progress.

### Work within a Familiar Environment

Accord for Excel Enterprise seamlessly integrates AEI databases with Microsoft® Excel to provide you with a variety of powerful tools for managing and analyzing data within the familiar Excel environment. Typically used for querying and reporting on data stored in AEI, Accord for Excel Enterprise features sophisticated chemical analysis tools, compound & reaction registration, connectivity to Pipeline Pilot, library enumeration and specialized templates for sending and retrieving data. The rich toolset provided enables you to interactively report on, interrogate and drill-down into datasets right on your desktop.

### Easy Access to Data

The Accord Enterprise Webkit provides you with one of the primary interfaces for managing data within AEI. Built on a customizable, Java-based toolkit, the AE Webkit enables you to access all of your data in a single, web-browser based location, providing you with a 'one-stop shop' for interacting with discovery information. Customizable and easy both to deploy and use, the AE Webkit enables you to readily access the key data that you need to for quick, informed decision-making.

CHEMISTRY	Sample Compound ID	Assay/Protocol	Sample Name	Sample Size	Result Type	Result Value
<chem>C1=CC=C(C=C1)N2C=NC(=C2)C3=CC=CC=C3</chem>	ACC000002	ASSAY 151V2	PLATE A1	AS1	N/N/N	65
<chem>C1=CC=C(C=C1)N2C=NC(=C2)C3=CC=CC=C3</chem>	ACC000003	ASSAY 151V3	PLATE A2	AS1	N/N/N	4
<chem>C1=CC=C(C=C1)N2C=NC(=C2)C3=CC=CC=C3</chem>	ACC000004	ASSAY 151V4	PLATE A3	AS1	BC/N	34

Generating a simple assay report in Accord for Excel Enterprise directly from data stored in AEI

