DATASHEET

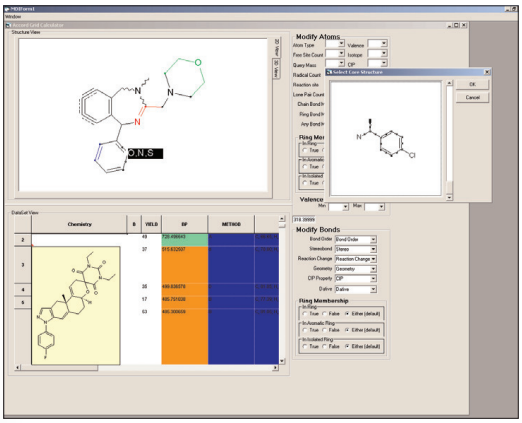
ACCORD SDK

Imagine being able to deliver the software solutions your organization needs, without sacrificing the open standards and quality you demand. What if you could tune your favorite desktop applications into chemistry? Now you can with the Accord SDK.

THE ACCORD SDK: CHEMICAL APPLICATION DEVELOPMENT MADE SIMPLE

'Plug and play' cheminformatics toolkit

With over 1000 API functions, Accord SDK lets you develop customised software to meet your exacting needs. Functions for property calculation, library enumeration, file I/O and high quality chemical depiction are all available and can be used in most development environments – C, C++, VB, .Net, Perl & Java among many others. With support for over 20 common chemical file formats, the SDK can be used to either integrate & enhance your existing software or to develop new chemically-aware applications from scratch.



An application built with the Accord Chemistry SDK allowing CombiChem enumeration, chemical database searching, and prediction of ADME properties

Highest quality chemistry

Based on the Accord Chemistry Engine, the Accord SDK gives you programmatic access to import,manipulate, search and predict properties of molecular & reaction data, with support for advanced queries, organometallics, Markush schema and polymers. Multiple search types are supported including substructure, Exact, Flexible matching and various similarity coefficients.Over 100 molecular descriptors & properties can be calculated from 2D structure, giving you the power to discover new chemical entities & drugs more quickly and efficiently than ever before.

Reusable Components

The Accord SDK provides you with a set of reusable chemical functions that provide the ideal building blocks from which to assemble your own custom solutions. If you want to process chemical data in an SD file, modify atoms in a SMARTS query or perform a substructure search, you can using the Accord SDK. This lets you focus on delivering the application solutions your organization needs in record time.

The Accord SDK provides software functions for performing the following types of operations on chemical entities such as molecules, reactions, molecular fragments:

- Import and Export
- Exact, Substructure and Similarity Searching
- Depiction, Layout and Printing
- Over 100 chemical descriptor & property calculations
- Local database creation, indexing & searching
- Similarity calculations
- Enumeration of combinatorial libraries

Because Accord has an open architecture, application developers can choose to store chemical objects in their preferred database or file system.

Quick & Easy Integration

The Accord SDK supports industry-standard integration protocols, which means it works smoothly within most popular desktop environments.This allows you to focus on your application requirements, using the Accord SDK as appropriate to perform chemical tasks, using the development environment you already know.

Open and Extensible

Because Accord understands standard chemical exchange formats such as SD, RD, SMILES (including stereochemical SMILES) and SMD, it is easy to swap data with other chemical information and modeling systems.

There are a number of extra modules available to expand the functionality of the SDK. A good example is the CombiChem add-on, which allows you to enumerate compound libraries based on a generic reaction and lists of reagents. Other modules are available for molecular property calculations, such as ADME/Tox properties & pKa/logD prediction.

Display & Editing Chemistry

Chemical diagrams produced by Accord can be cut and pasted between supported third-party chemical drawing packages, such as ISIS™/Draw, ChemDraw™ and CAS Draw, for modification.

Extend other Accord™ software

Using the SDK, you can write scripts in PL/SQL or VBA to extend the capabilities of Accord Chemistry Cartridge and Accord for Excel - adding all the functionality available in Accord into MS Excel and Oracle databases.

SAMPLE APPLICATIONS

Accelrys provides numerous sample applications, including source code, which developers are free to use as a basis for their own applications.Examples include a chemical import/export utility, a fingerprint calculator and an SVG image generator.

Applications that have been built utilizing Accord capabilities include:

- LIMS submission systems
- Combichem Enumeration systems
- Reagent inventory systems
- Electronic Laboratory notebooks
- Property prediction applications
- Lead optimization software.

To learn more about Informatics, go to
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