

Displays chemical structures, reactions, metal complexes, stereochemistry, and more...

ADME, Tox, pKa/logD and QSAR prediction, library enumeration, property calculation and full stereochemistry display in MS Excel®

Reporting, publishing, plotting, and graphing

Compatible with common sketching applications

R-group analysis and substituent handling

Sub-structure, exact structure and similarity filtering

Clean and align structures

Accord for Excel

Accord for Excel enables the popular Excel spreadsheet to understand chemistry the way you do—using the language of structure diagrams, reactions, and stereochemistry.

Accord for Excel allows scientists to display chemical structures and reactions, perform chemical calculations, analyze R-groups, and query by substructure or similarity directly within Excel. The chemistry capabilities are ideal in Excel because most scientists are familiar with the productivity tools graphing, plotting, organizing, reporting, publishing, and analysis capabilities already; we improved Excel by adding chemistry to the spreadsheets repertoire.

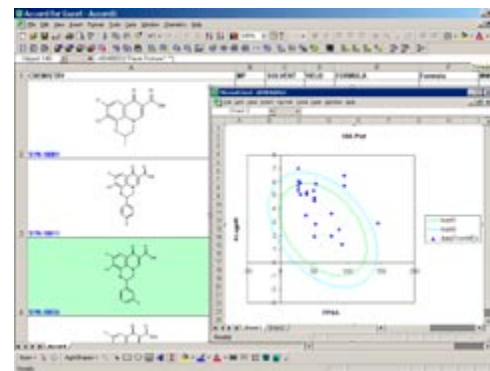
Live Chemistry in your spreadsheets

Accord chemical objects are 'live', not static pictures as in other imitations. Live chemistry means related data such as molecular weight, AlogP and Lipinski's 'rule-of-five' changes automatically when the structure changes, just like other calculated data in Excel. Chemistry diagrams in a selected region can be easily expanded or collapsed to save space, all at the click of a button.

Extending Accord for Excel

A wide range of validated predictive ADME models and intuitive library enumeration and physical property prediction methods can be provided to scientists through add-on modules that extend Accord for Excel's capabilities. Add-ons reduce the need to relearn a new application for each function. The add-ons, described in more detail below, include:

- ADME/Tox add-on
- CombiChem add-on
- pKa/logD add-on.



Structures can be analyzed using the ADME models and fast QSAR properties to design 'drug-likeness' into compounds and libraries early-on in the drug-discovery process.

Plus a new **Pipeline Pilot wizard** enables you to send your chemical data to external protocols, giving you the ability to calculate any in-house properties & descriptors you require, cluster datasets, search databases – anything you can already do using Pipeline Pilot.

Fast QSAR Descriptors

Standard properties that can be calculated in Accord for Excel include: Lipinski's rule-of-5, AlogP98, Rotatable bonds count, H-bond donor count, H-bond acceptor count, Molecular Weight, MW, MlogP, E-state keys, Balaban Indices, Chi Index, Information content, Kappa index, Molar refractivity, Molecular flexibility, Sub-graph count, Wiener Index, Zagreb index, Elemental formula, Composition formula, and more...

Powerful Filtering Capabilities

Filter tables of molecules or reactions using exact, substructure or similarity search options. Full stereochemical matching and substructure highlighting are available. With Accord you can organize and explore your data right within Excel.

R-Group Analysis

Produce publication quality R-group tables. Draw in a core structure using your favorite chemical editor and then simply select the R-Group Table command. The result is a structure of each R-group, clipped at the attachment point. Use Accord for Excel's customizable substituent libraries to name R-group attachments.

Publishing and Reporting

Accord's inbuilt chemical intelligence makes it easy to create publication quality tables containing chemical moieties and associated data. You can publish your results to HTML in seconds or create reports with ease by pasting your data into Microsoft Office® applications.

Fast and Flexible Chemistry Import and Export

Pull in data from a variety of systems in standard chemical formats such as SD, RD files, or SMILES strings. Accord also supports a variety of formats for transferring chemical structures via the clipboard. File formats supported include:

- MDL SD and RD Files
- MDL Molfiles, Rxnfiles & Sketch files
- CS ChemDraw
- CAS CXF/CXG
- SMD 4.3
- SMILES
- Questel DARC-F1
- v3000 mol
- 3D mol.

Compatible Sketching Applications

Accord for Excel is compatible with standard 2D sketching and 3D viewing applications, such as:

- ISIS/Draw
- ChemDraw
- CASDraw 2000
- DS ViewerPro.

pKa/logD Add-on

The new pKa/logD add-on gives scientists the ability to quickly and easily predict lipophilicity & ionisability of compounds within Excel – calculate & visualise multiple ionisable groups, and generate lipophilicity profiles

ADME Add-on

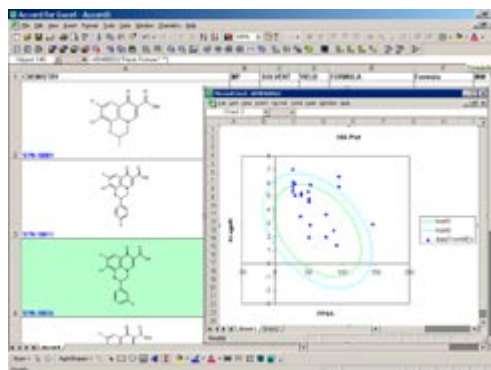
Accord for Excel's ADME add-on enables scientists to compute and predict absorption, distribution, metabolism, and excretion (ADME) properties for chemical libraries, screening collections, and synthesis candidates. The ADME add-on includes:

- Blood Brain Barrier permeation model
- Human Intestinal Absorption model
- Aqueous Solubility model
- Serum Protein Binding model
- 2D PSA - Fast Polar Surface Area
- CYP 2D6 inhibition
- Hepatotoxicity

CombiChem Add-on

Accord for Excel CombiChem Add-on provides an intuitive, step-by-step interface to generate combinatorial library structures directly within Accord for Excel. Just specify a generic reaction scheme, create or import reagent lists and at the push of a button, the enumerated library is generated directly within the Excel spreadsheet. Chemical libraries may be profiled and refined

by using the predictive ADME models and QSAR property descriptors (Lipinski's 'rule-of-five', AlogP98, etc.). After profiling, swapping reagents



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with other possible alternatives that provide better physiochemical properties can be extremely useful in designing drug-like libraries.

Chemexplorer

None of us are as organised as we'd like to be. Now you don't need to worry about losing your reports and data of interest. Search your local machine or network by substructure, exact structure or similarity. Chemexplorer™ is now included as standard in Accord for Excel and lets you search SDF, RD, SMILES, MS Word & Excel files for embedded chemistry.

System Requirements

- Windows 2000 or XP
- Microsoft Excel 2000, 2002, 2003.

Publications

Scientific validation and publication information for these ADME models can be found at:

<http://www.accelrys.com/products/cerius2/refs.html#adme>

Find out more about using Accord for Excel with SciFinder by registering for the white paper at:

http://www.accelrys.com/reference/publications/pub_lipinski.php