Transforming Analytical Data into Knowledge with Software for Metabolite Studies

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Introduction

Advanced Chemistry Development, Inc., (ACD/Labs) has been developing specialized software for chemical and pharmaceutical research for over 16 years. Our expertise includes multi-technique, multi-instrument data handling, knowledge management of analytical and separations data, chemical drawing, and prediction software for a range of chemical properties as well as spectra and chromatograms.

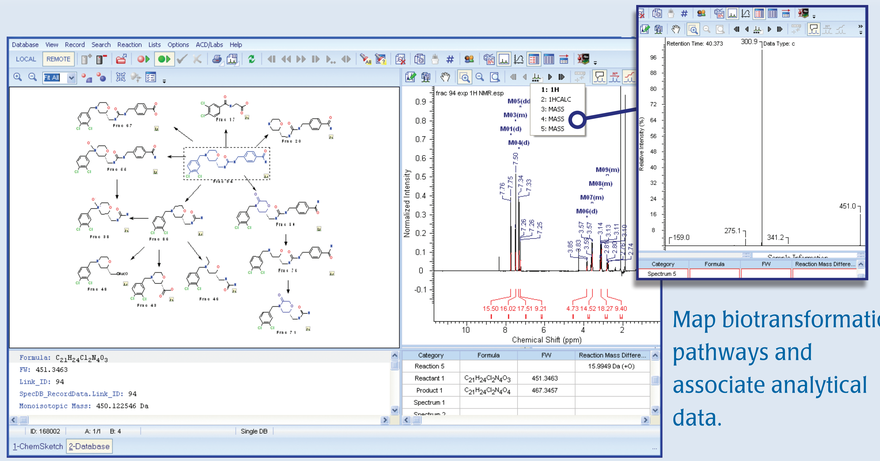
Combining these capabilities, ACD/Labs provides software solutions to speed and enhance research efforts in a variety of industries, including pharmaceuticals, toxicology, forensics, environmental regulation and monitoring, and food safety.

All-In-One Data Handling and Interpretation

ACD/Labs analytical software provides capabilities to process and interpret MS, NMR, UV, Raman, chromatographic data, and other spectroscopic techniques, in almost any vendor format. This all-in-one approach to analytical data handling provides enormous flexibility to analyze and interpret a wide variety of experimental data types within a single interface.

Advanced Analytical Interpretation

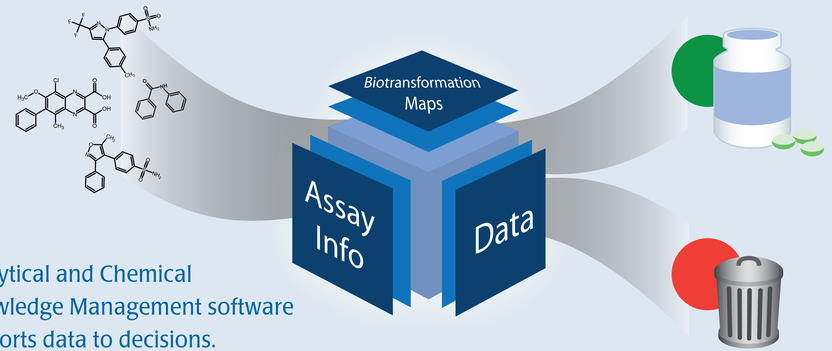
Specialized interpretation capabilities include powerful deconvolution tools, target analysis, structure verification, and more. Quickly extract relevant components from LC/MS data. Automatically assign $[M+H]^+$ or $[M-H]^-$, adduct ions, multimers, neutral losses, and possible fragment ions for each component. Resolve overlapping peaks for complicated LC/MS data, and identify co-eluting components.



Map biotransformation pathways and associate analytical data.

ACD/Labs Metabolism Solution

Uniting all these capabilities, ACD/Labs offers a software solution for Metabolite studies helping researchers relate disparate sources of analytical and chemical data to structural information. Quickly identify recurring metabolites by comparing data to a knowledgebase of information comprised of prior research efforts, including analytical data and interpretations. Easily elucidate structures of unknown metabolites using advanced computer algorithms to verify structure-spectrum correlations. Gain greater insight into the safety profiles of metabolites with structure-based predictions for toxicity and health-related properties.



Analytical and Chemical Knowledge Management software supports data to decisions.

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Knowledge Management

Research knowledge is valuable and should be captured and protected so that it can be leveraged for future use. ACD/Labs software builds libraries of analytical and chemical information, relating metabolite structures to analytical information, including spectral and chromatographic data. Further, associate compound properties of structures with metadata. The ability to collect data from almost any instrument provides a means of centralizing data across multiple research groups and organizations.

Chemical Drawing

Research rarely involves simple linear reactions; however depicting these complex interactions can be challenging. ACD/Labs drawing software allows you to draw complex biotransformation pathways and reaction schema, to incorporate partially elucidated structures with Markush representations, and to relate a variety of chemical and spectral information to each structure in the reaction.

Property Prediction

Fragment-based predictions for a wide array of physicochemical and ADME properties, along with toxicological endpoints, provide greater insight into compounds and metabolites, helping researchers make better decisions to advance research efforts.

Summary

ACD/Labs software enables the transformation of chemical and analytical information into knowledge within a single, integrated platform, complementing your organization's knowledge management infrastructure. Capturing, preserving, and leveraging accumulated knowledge serves to benefit organizations in active research efforts and supports future projects.