Advanced Chemistry Development

ACD/Labs

Products and Solutions Catalogue

Advanced Chemistry Development, Inc. (ACD/Labs)

We are a global chemistry software company developing desktop and enterprise solutions to effectively use the wealth of scientific knowledge generated among the many branches of chemical, biochemical, and pharmaceutical R&D. Using our deep understanding of chemical disciplines, advanced mathematical algorithms, and computer science, our solutions help guide on-going research, aid decision-making, and speed the development of new chemical entities for the marketplace.

Our clients and partners in pharmaceutical companies, chemical companies, academic institutions, and government organizations span the globe. We are recognized as the industry standard in NMR spectrum, physicochemical, and ADMET property predictions, and a market leader in analytical vendor-neutral databasing, processing, and analysis for MS and NMR. Our chemical drawing and nomenclature products continue to gain prominence in the industry.

Founded in 1994 and headquartered in Toronto, Canada, ACD/Labs employs a team of over 160 dedicated individuals, including many PhD-level scientists from varying chemical disciplines. Our expertise lies in vendor-neutral spectroscopic data processing and prediction, property prediction, analytical knowledge management, and interactive reporting of scientific data. These software solutions integrate analytical data with chemical structures and physicochemical and ADMET property prediction to help organizations protect and leverage valuable research knowledge.
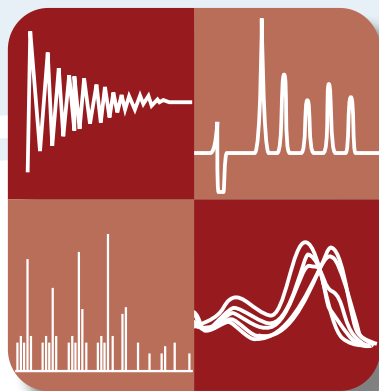
Our Commitment

ACD/Labs is committed to providing the industry standard in comprehensive and innovative predictive, chemical, spectroscopic, chromatographic, and database management software solutions while developing and maintaining customer loyalty. These objectives are accomplished through:
  · Adopting and developing state-of-the-art algorithms
  · Maintaining the highest standards in the development of our products
  · Continuously improving our existing products and customer support
  · Providing the highest standards of customer support

Table of Contents

Analytical Data Handling

ACD/Labs' analytical data handling software offers vendor-neutral spectroscopic and chromatographic data handling, processing and prediction, interactive reporting, and integration of analytical data with chemical structures. Our software packages include a full range of tools for experts and simpler tools for occasional users.

Table of Contents/Analytical Data Handling

ACD/NMR Predictors

Software for fast and accurate prediction of NMR spectra, chemical shifts, and coupling constants.

ACD/NMR Predictors include predictions for ^{1}H, ^{13}C, ^{15}N, ^{19}F, and ^{31}P nuclei for 1D spectra, and ^{1}H and ^{13}C (and ^{15}N) for 2D spectral prediction. With the simple input of a chemical structure, you can predict NMR spectra in seconds. All predictors use both HOSE code and neural net algorithms to provide the most accurate chemical shifts in the prediction of spectra, also taking into account stereochemistry. NMR predictors also include full processing functionality and the ability to train predictions with your own experimental data.

The predictors are available as three distinct packages:
· Individual purchase of ^{1}H and/or ^{13}C predictor
· XNMR Suite, which includes ^{15}N, ^{19}F, and ^{31}P predictors
· NMR Predictor Suite - ^{1}H, ^{13}C, ^{15}N, ^{19}F, ^{31}P, and 2D NMR predictor

Features

· Calculate and display accurate chemical shifts and coupling constants for ^{1}H, ^{13}C, ^{15}N, ^{19}F, and ^{31}P
· Solvent-specific prediction of 1H and ^{13}C spectra
· Recognize tautomeric forms before prediction
· Process experimental spectra from a variety of NMR data formats
· Train the predictors with experimental data to improve prediction accuracy in novel and proprietary chemical spaces
· Automatically verify and assign experimental spectra when a structure is attached with one button-click

Benefits

· Ease interpretation of spectra for non-routine experiments and complex structures
· Quickly verify and auto-assign experimental spectra to a chemical structure
· Reduce instrument time by estimating ^{15}N chemical shifts and narrowing down the experimental acquisition range for these experiments

· Visualize and compare predicted and experimental spectra on the same screen
· Use the software as a teaching tool by generating simulated spectra and hiding the associated chemical structure
· Easily build a central, fully searchable repository of NMR data in the User (training) Database

Application Note

Improving NMR Shift Predictions with Database Training

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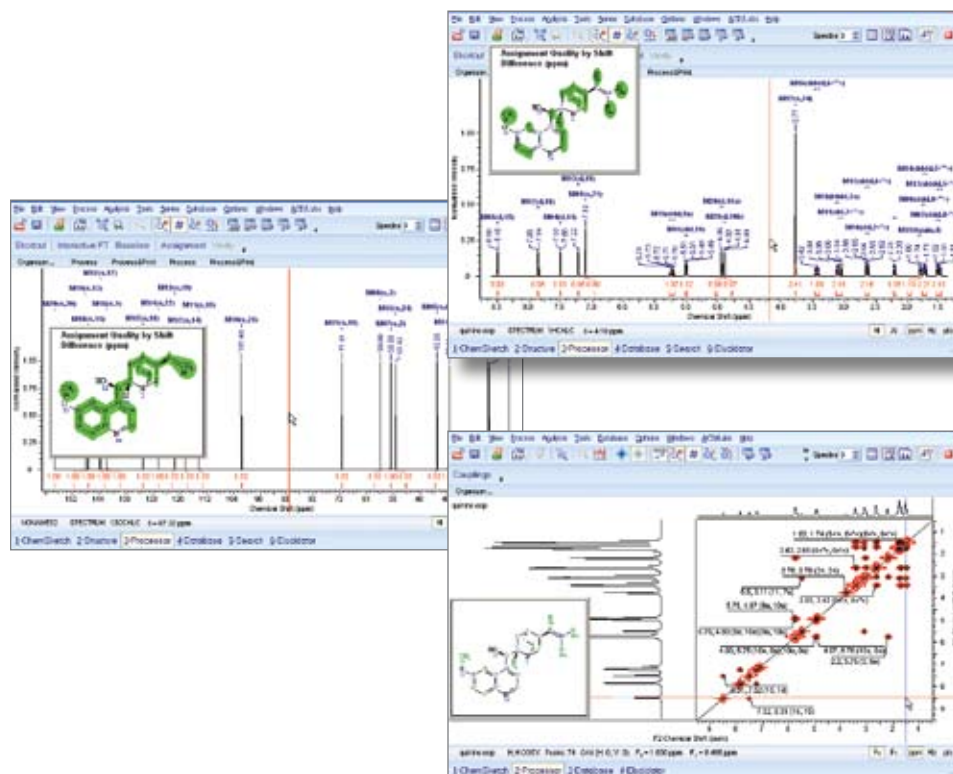
Full List of Features

Prediction Features

· Calculate and display accurate chemical shifts and coupling constants

· HOSE code and neural net prediction algorithms

· Display the Calculation Protocol window, enabling you to see the fragments contributing to each calculated shift

· Interactively highlight the relationship between a tabular value and its associated numbered nuclear center

· Use the included ACD/ChemSketch with its full-featured capabilities of drawing chemical structures and creating reports. It also includes ACD/Dictionary and ACD/Tautomers to quickly and easily draw complex structures and check their tautomeric forms.

Specific to ^1H and ^{13}C Predictors Only:

· Contains a History window that displays all of the structures used for spectral calculations during the current program session. This window allows you to load (or save) all of the structures to (or from) a file on a disk, print them, and then import a new list of up to 99 structures from an SDfile.

· Perform solvent-specific predictions—choose from a list of solvents to include in the prediction dataset

· Set the desired frequency for predicted spectra

· Set the desired line widths for predicted spectra

· Save predicted spectra and chemical structures for later review

· View predicted spectra in Hz or ppm units

· Utilize fully interactive zooming features to focus on various spectral regions of predicted spectra

· Hide chemical structures so that produced spectra can be used as a teaching tool

"The software is an extraordinarily practical and convenient compendium of NMR data that effectively replaces the time-consuming task of looking up individual NMR data from... [disparate] resources."

Brian Pagenkopf,
J.A.C.S., 2005, 127, 3232

Databasing Features

· Build user databases with chemical structures and experimental ^1H chemical shifts to improve predictions

· Automatically search the database for exact matches before generating a prediction

· Search databases by structure, substructure, structural similarity, multiple structure fragments, chemical shift, coupling constant, solvent, chemical formula, molecular weight, NMR technique, and literature reference, as well as assigned chemical shifts and spin systems

· Search databases by shift correlations

· Search the database for similar structures to the one selected with one of five different algorithms: Tanimoto, Dice, Cosine, Hamming distance, and Euclidean distance

· Search the database for more stable tautomers when performing a structure search

· Update or change a structure in the predictor database with the structure exchange tool

· View the user database in One Record, Tile, or Table view mode

· Sort the chemical shift search results by Hit Quality Index (HQI)

· Estimation of chemical shifts when right-clicking

· Search stereoisomeric structures with the stereo search option

· Substructure search query can include Markush structures

· Customize the database window layout with Forms view. Arrange out the database window panes according to your preference and save the customized layout setting.

Specific to 2D NMR Predictor

Prediction Features

· Simulate 2D NMR spectra for H,H COSY (2J-3J Long-Range); C,H COSY (HSQC, HSQC-DEPT, HMQC, HMBC); C,H COSY(HSQC-TOCSY); N,H COSY* (Direct and Long-Range); C,C COSY/HSQC-TOCSY (2J-3J and Long-Range); C,C COSY (INADEQUATE, Direct, and Long-Range); H,H J-resolved (2J-3J and Long-Range); and C,H J-resolved (2J-3J and Long-Range)

· Predict multiplicity-edited 2D spectra

· Predict un-decoupled direct correlations

· Display data as intensity or contour plots

· View tables of shifts and coupling constants

· Correct chemical shifts or coupling constant values and recalculate the spectrum

· Simulate experimental conditions by specifying the spectrometer frequency and line width

· Transpose spectra to simulate experiments with direct or indirect detection

· Simulate experiments with long-range detection by turning on the long-range coupling constants option

· Use heteronuclear couplings for all the experiments

· Simulate a H,H COSY spectrum using a set of chemical shifts and coupling constants

· Print high-quality spectra and create reports directly in ACD/ChemSketch or through a variety of word processing software packages

· Improve the 2D NMR predictions by entering your own measurements and assignments in the ACD/CNMR and ACD/HNMR Predictor databases

Databasing Features

· Update the database with the predicted spectra along with their chemical structures, as well as miscellaneous information copied to User Data and Notes

· Search by full spectrum or one or more spectral regions, chemical shifts, spectral parameters, chemical structure and substructure, formula, molecular weight, and user data text

· Perform spectrum searches according to Euclidean distance, or squared or absolute difference methods; the search hits will be ranked by HQI (Hit Quality Index)

· Control data that is entered into your corporate databases with Data Forms Manager

· Manage remote databases through a local or global network with an Oracle-based SQL client-server system

ACD/NMR Processor

Software for processing, analysis, and assignment of 1D and 2D NMR data.

ACD/NMR Processor provides a desktop solution for otherwise tedious processing and analysis tasks. It eases the interpretation of both 1D and 2D NMR data with advanced processing, analysis, and assignment tools. In addition to 1D NMR data, ACD/NMR Processor provides exceptional capabilities for all 2D NMR data from experiments such as COSY, HETCOR, TOCSY, and HMQC/HMBC/HSQC.

Features

· Provides tools for basic spectral manipulations such as the Fourier transform, weighting functions, manual and automated phase correction, baseline correction, and calibration
· Supports the import of FID and FT data from all major spectrometer vendor formats, including Bruker, Varian, and JEOL
· Attach structures to spectra and easily assign correlations by clicking and dragging from atom to spectral peak
· Handle spectral series, synchronize spectra, and add or subtract two spectra
· Macro capabilities include templates and a macro organizer for completely automated data processing
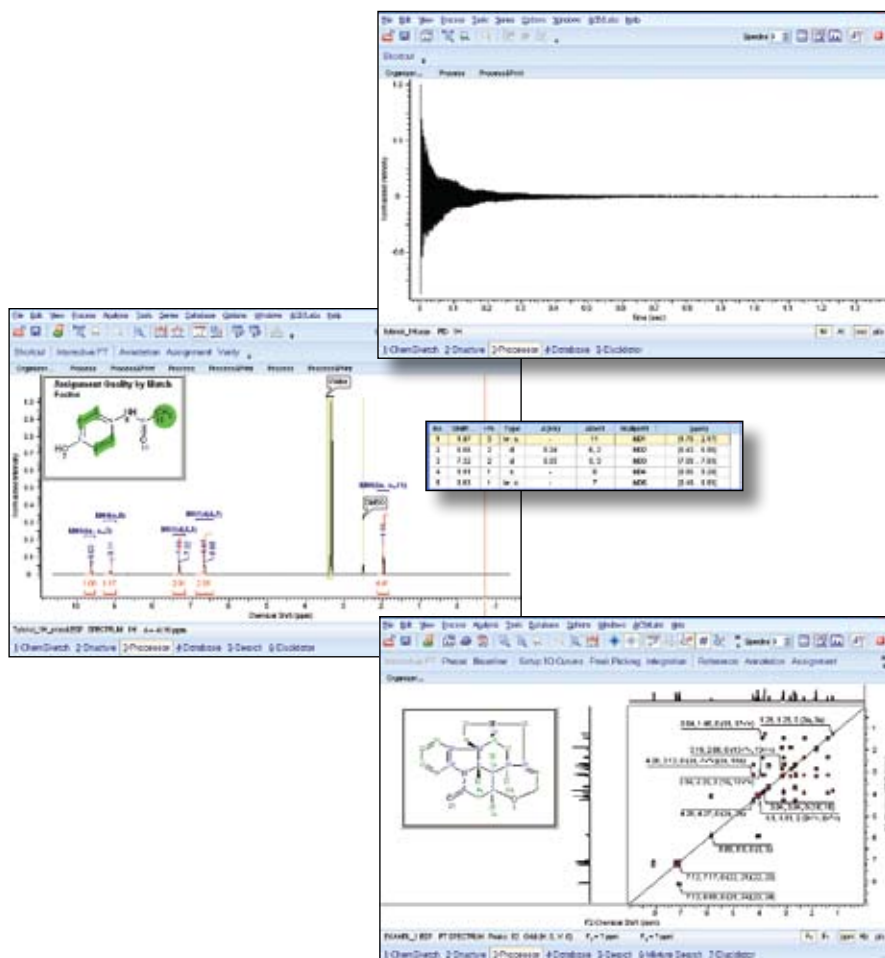
Benefits

· Process NMR data and manipulate spectra remote from the instrument
· Obtain clear, concise, and consistent reports of NMR data for publication/reporting
· Reduce the burden of 2D NMR verification and evaluation

Application Note

A Quick and Easy Way to Process ¹H NMR Spectra Manually

Full List of Features

General Features

- ACD/NMR Processor includes 1D and 2D NMR processing capabilities and ACD/ChemSketch
- Automatically obtain summary information when importing complex vendor formats using multiple directories
- Preview spectra for import/export
- Full audit trail feature (History) tracks all applied processing commands
- Macro capabilities include templates and a macro organizer for completely automated data processing
- Carry out basic spectral manipulations such as Fourier transform, weighting functions, manual and automated phase correction, baseline correction, and calibration
- Apply manual and automated peak picking and integration
- Data can be displayed as intensity or contour plots

- Apply Magnitude spectrum, Power spectrum, and Symmetrization commands
- Suppress the diagonal in homonuclear experiments
- Merge multiplets
- Apply Transpose spectrum and Reverse spectrum commands
- Apply color-coded gridlines
- Peak picking gridlines can be transferred from one spectrum to another
- Remove t1 noise with differential scaling, or edit the spectrum automatically or manually
- View individual slices and 3D projections; simultaneously view and manipulate the spectrum in 3D
- Save any cross-section (sum of cross-sections) as a 1D spectrum
- Attach 1D spectra to the 2D spectrum

- Attach a chemical structure and additional data to the spectrum
- Annotate signals and spectral regions
- Assign diagonal and cross-peaks to any atom or portion of a chemical structure manually or automatically
- Create a 2D spectrum from a set of chemical shifts and couplings
- Set the display mode for each dimension independently (view F1 or F2 in Phase-Sensitive, Magnitude, or Power mode)
- View multiple spectra in Tile or Replace modes
- Synchronize axes in a multiple-window display
- Cut and paste into other applications with high resolution
- Add and subtract two spectra
- Print spectra and create reports with ACD/ChemSketch

"ACD/Labs' NMR Processors have helped increase the effiiency in our lab... all of our chemists are now able to manipulate their NMR data at their convenience, eliminating lengthy line-ups in our walk-up lab."

Dr. R. C. Gadwood,
President and CEO, Kalexsyn

Supported Formats for Import/Export

Vendor	File Format	Required Parameter Files	Optional Parameter Files
Acorn NMR, Inc.	*.fid, *.nmr, *.2d		
ASCII†	*.txt; *.prn, *.csv, *.asc		
Bruker Corporation	*.ser, *.rr, *.fid, *.1r, *.ser, *.2rr, *.* (DISNMR)	acqus, procs, acqu2, proc2s, *.fqs, *.fa1, *.fa2, *.fp1, *.fp2	title, intrng, *.tit, *.ti2
GE	*.raw, *.* (Nicolet)		
JCAMP†	*.dx; *.jdx		
JEOL Ltd.	*.als, *.nmfid, *.nmf, *.nmdata, *.nmd, *.gxd, *.bin, *.* (Delta)	*.gxp, *.hdr	exp.param, exp.par
Lybrics	*.*		
MSI Felix	*.*		
Tecmag	*.tnt, *.* (MacNMR)		
Thermo Scientific†	*.spc		
Varian, Inc.	data, *.fdf, fid0001.fdf, *.txt, fid, phasefile	acq, proc, procpar	acq_2, text

† File export is also supported (only 1D NMR is supported for JCAMP)

ACD/NMR Workbook

Software for synchronous work-up and assignment of entire NMR datasets (1D and 2D).

ACD/NMR Workbook* allows you to import, process, and analyze your 1D and 2D NMR data, and then, using the new NMRSync technology, you can synchronize peak picking and assignment throughout your entire dataset. When you pick a correlation in an HMBC spectrum, it results in automatic creation of a multiplet in the ^{1}H and ^{13}C spectra. Assign a multiplet in your 1D ^{1}H, and all other relevant peaks and correlations are assigned to atoms in the chemical structure. You can also store assigned spectra along with chemical structures, data tables, and other associated data easily in a fully searchable database.

Features

· Full processing of data (from FT and FID) for all major instrument vendor formats
· Synchronous work-up of 1D and 2D NMR data
· Automatic alignment and attachment of 1D curves upon import for spectra pertaining to one sample
· Project management console captures all data associated with one sample for at-a-glance review
· Database all the knowledge gained from your NMR datasets and create professional reports with assigned spectra and all associated data

Benefits

· Faster, better, and more uniform handling of NMR data
· Immediate access to all data in one place

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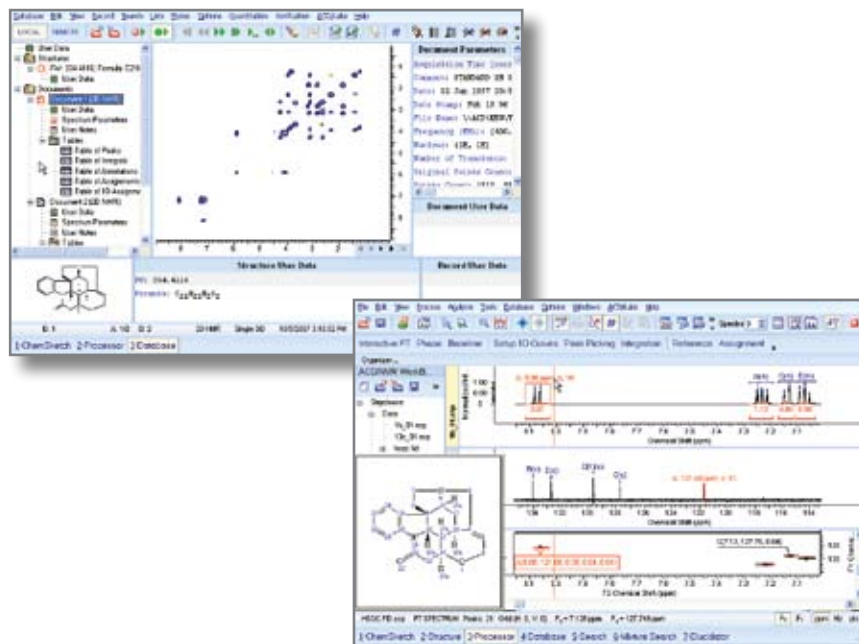
* Previously sold as ACD/2D NMR Manager

Full List of Features

General Features

· Import different vendor data formats including Bruker, JEOL, Varian, TECMAG, and CHEMAGNETICS

· Capture all NMR data associated with one sample in the NMR Workbook console

· Automatically process any variety of 1D and 2D experiments with the help of scripting and macro functionality

· Full audit trail feature (History) tracks every processing command. One-click import and processing of entire dataset macro programs that are easily created from a template building tool or the processing history.

· Automatic alignment and attachment of 1D curves upon import for spectra pertaining to one sample

· Attach a chemical structure and additional data to the spectrum, and use them in your analysis

· Organize and compare multiple spectra in Tile or Full window modes, or make two spectra transparent to create an overlay mode

· Create professional, high-quality reports in Adobe PDF, ACD/ChemSketch, or other formats

Processing Features

· Automatically process all data associated with one sample upon directory import

· Carry out basic spectral manipulations such as the Fourier transform, weighting functions, manual and automated phase correction, baseline correction, and calibration

· Automatic synchronizing and alignment of data relative to ^{1}H and ^{13}C spectra

· Apply Linear Prediction

· Multiply the first point of an FID by a set factor

· Apply Magnitude spectrum, Power spectrum, and Symmetrization commands

Analysis Features

· Attach chemical structures to all spectra

· NMRSync synchronizes multiplet creation and peak picking throughout an NMR dataset

· NMRSync synchronizes assignments made to atoms in a chemical structure across all data in an NMR dataset

· Automatically (or manually) pick peaks; perform peak and/or bucket integration

· Annotate signals and spectrum regions

· Automatically (or manually) set dark regions to ignore impurities signals and artifacts during all analyses

· Display the data as intensity, contour plots, or as a 3D surface

· View slices and 3D projections; simultaneously view and manipulate the spectrum in 3D

Databasing Features

· Build a spectral database of all experimental spectra associated with different samples in one simple step. Individual database records can include chemical structures, analysis results (table of peaks, table of assignments, annotations), as well as miscellaneous information copied to User Data and Notes

· Create external links from database records to entire NMR datasets associated with samples, raw data files, etc.

· Search by full spectrum or spectral region(s), peaks, spectral parameters, chemical structure and substructure, formula, molecular weight, and user data text

· Perform spectrum searches according to Euclidean distance, or squared or absolute difference methods; the search hits will be ranked by HQI (Hit Quality Index)

· Control data that is entered into your corporate databases with Data Forms Manager

· Manage remote databases through a local or global network with an Oracle-based SQL client-server system

· Simultaneously update an NMR Predictor chemical shift database to train NMR predictions (Note: This capability requires additional licenses of ACD/HNMR and/or CNMR Predictor)

Supported Formats for Import/Export

Vendor	File Format	Required Parameter Files	Optional Parameter Files
Acorn NMR, Inc.	*.fid, *.nmr, *.2d		
ASCII†	*.txt; *.prn, *.csv, *.asc		
Bruker Corporation	*.ser, *.rr, *.fid, *.1r, *.ser, *.2rr, *.* (DISNMR)	acqus, procs, acqu2, proc2s, *.fqs, *.fa1, *.fa2, *.fp1, *.fp2	title, intrng, *.tit, *.ti2
GE	*.raw, *.* (Nicolet)		
JCAMP†	*.dx; *.jdx		
JEOL Ltd.	*.als, *.nmfid, *.nmf, *.nmdata, *.nmd, *.gxd, *.bin, *.* (Delta)	*.gxp, *.hdr	exp.param, exp.par
Lybrics	*.*		
MSI Felix	*.*		
Tecmag	*.tnt, *.* (MacNMR)		
Thermo Scientific†	*.spc		
Varian, Inc.	data, *.fdf, fid0001.fdf, *.txt, fid,phasefile	acq, proc, proc-par	acq_2, text

† File export is also supported (only 1D NMR is supported for JCAMP)

ACD/1D NMR Assistant

NMR software for synthetic chemists.

ACD/1D NMR Assistant was designed specifically with the chemist in mind. While it includes all of ACD/Labs' powerful processing features and prediction algorithms for 1D NMR, the interface is simple and offers the functionality and capabilities most suited to a routine non-expert user. You can choose to manually or automatically process and analyze NMR data, and have the software verify your assigned structure. With ^{1}H and ^{13}C NMR predictors running in the background, you will receive a match factor between your experimental spectrum and the predicted spectrum for the proposed structure.

Features

· Fully process NMR data from all
  major vendor formats for 1D ^{1}H,
  ^{13}C, ^{15}N, ^{19}F, and ^{31}P
· Assignment assistance—with Multiplet
  Assignment Preview (MAP) for ^{1}H
  spectra, hover over a multiplet and get
  real-time feedback on which atoms
  should be assigned to it
· Automatic creation of multiplet reports
· Assistance in structure verification (for
  1H)—automatically confirm whether
  your proposed structure is consistent
  with the data, with the option to auto
  assign for quicker reporting
· Macro capabilities include templates
  and a macro organizer for completely
  automated data processing and
  analysis
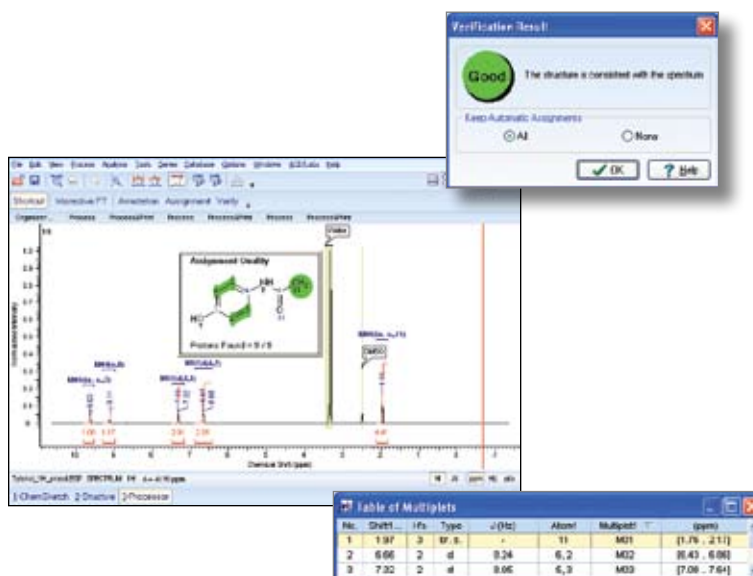
Benefits

· Process NMR data and manipulate
  spectra on the chemist's desktop,
  remote from the instrument
· Save time on reports, patents, and
  publications with automatic creation
  of multiplet reports in standard journal
  and custom formats
· An affordable way to provide a
  complete NMR software package to
  chemists

Full List of Features

Processing Features

· Automatically obtain summary information when importing complex vendor formats using multiple directories

· Preview spectra for import/export

· Full audit trail feature (History) tracks all applied processing commands

· Macro capabilities include templates and a macro organizer for completely automated data processing

· Carry out basic spectral manipulations such as the Fourier transform, weighting functions, manual and automated phase correction, baseline correction, and calibration

· Apply manual and automated peak picking and integration

· Attach a chemical structure to the spectrum

· Annotate signals and spectral regions

· Assign diagonal and cross-peaks to any atom or portion of a chemical structure manually or automatically

· Set the display mode for each dimension independently (view F1 or F2 in Phase-Sensitive, Magnitude, or Power mode)

· View multiple spectra in Tile or Replace modes

· Cut and paste into other applications with high resolution

· Print spectra and create reports

Prediction Features

· HOSE code and neural net prediction algorithms

· Recognize tautomeric forms

· Choose from a list of solvents when verifying structure

Supported Formats for Import/Export

Vendor	File Format	Required Parameter Files	Optional Parameter Files
Acorn NMR, Inc.	*.fid, *.nmr, *.2d		
ASCII†	*.txt; *.prn, *.csv, *.asc		
Bruker Corporation	*.ser, *.rr, *.fid, *.1r, *.ser, *.2rr, *.* (DIS-NMR)	acqus, procs, acqu2, proc2s, *.fqs, *.fa1, *.fa2, *.fp1, *.fp2	title, intrng, *.tit, *.ti2
GE	*.raw, *.* (Nicolet)		
JCAMP†	*.dx; *.jdx		
JEOL Ltd.	*.als, *.nmfid, *.nmf, *.nmdata, *.nmd, *.gxd, *.bin, *.* (Delta)	*.gxp, *.hdr	exp.param, exp.par
Lybrics	*.*		
MSI Felix	*.*		
Tecmag	*.tnt, *.* (MacNMR)		
Thermo Scientific†	*.spc		
Varian, Inc.	data, *.fdf, fid0001.fdf, *.txt, fid,phasefile	acq, proc, procpar	acq_2, text

† File export is also supported (only 1D NMR is supported for JCAMP)

ACD/1D NMR Expert

Software for high-throughput processing, verification, and quantitation of 1D NMR data.

With ACD/1D NMR Expert, standard processing, analysis, verification, and databasing of results can be automated to reduce data bottlenecks for high-throughput chemistry. It will also automatically evaluate the correspondence between chemical structures and their respective 1D NMR datasets for large batches of compounds, with user-defined thresholds for "incorrect," "ambiguous," and "correct" matches between experimental and predicted spectra. Reaction progress can be monitored using Quanalyst, which compares and measures nearly all spectral attributes, including integral area, multiplet coupling patterns, peak locations, and peaks/multiplet areas from overlapping components. Database records for individual wells can be browsed by clicking on the interactive well-plate diagram.

Features

· Automated high-throughput processing, analysis, and databasing
· Database spectra, chemical structures, and user data for up to 384 well-plates at a time
· Automated structure verification— evaluate the match factor between experimental and predicted data for your structure
· Monitor reaction progress by calculating reagent conversion
· Create reports including spectra, structures, data tables, and plate graphics
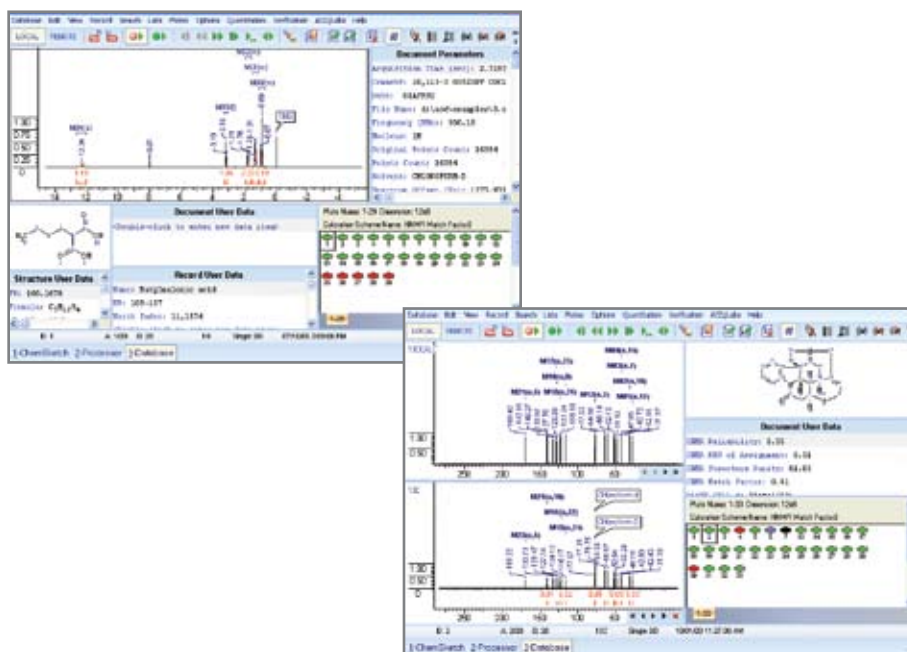
Benefits

· Reduce the time spent on manual evaluation of large NMR datasets
· Automatically process and store 1D datasets with associated chemical structures, customizable user data, and spectrum parameters
· Automatically evaluate the correspondence of the proposed chemical structure with 1D NMR data

Poster

Validating the Quality of Large Collections of NMR Spectra Automatically

Full List of Features

ACD/2D NMR Expert also includes ACD/1D NMR Manager and the ^{1}H and ^{13}C ACD/NMR Predictors.

Structure Verification

· Verify the ^{1}H NMR or ^{13}C, or 2D NMR spectrum-to-structure match in batch mode

· The match factor measures the correspondence between the experimental spectrum and the attached structure and gives the RMS of assignment and structure purity

· Combine the match factors for ^{1}H, ^{13}C, and 2D spectra to get a more reliable result

· Fully customizable layout for verification

· 96 and 384 well-plates available

· Show and store the verification protocol

· Include or exclude exchangeable protons in the verification

· Control the spectrum peak shape for the calculated spectra

· Apply weighting factors to chemical shifts, integral, and multiplicity parameters for verification analysis

· Recognize verification results at a glance by color-coding the results according to parameters of your choice: match factor, RMS of assignment and structure purity, etc.

· Account for solvents and mixtures with a customizable list

· Use dark regions to define impurities and other superfluous signals in spectra

· Calculate and insert the ^{1}H, ^{13}C, or 2D NMR spectra automatically into the database for a given structure

· Load the experimental and calculated spectra simultaneously and display them side-by-side for comparison

· Generate reports for the verification in tabular or plate form

· Report particular spectrum regions in experimental and calculated spectra for visual comparison

· Calculate a wide variety of spectrum responses with the built-in Quanalyst tool

· Analyze the integral in user-defined regions of the spectra

· Fully customizable layout for quantitation

· Plate can be colored according to quantitation results

· Advanced graph object available to visualize and report quantitation results

· Perform operations on the data of interest for more in-depth analyses

· Generate reports in plate, tabular, diagram, and multi-spectral formats

· Perform a quantitative analysis for several spectrum responses at a time

· Analyze a wide range of 2D NMR experiments to verify spectrum-to-structure matches in batch mode

Advanced Verification Options for 1D NMR Spectra

· Use reagent structures to enhance verification reliability

· Check the proposed structures for tautomeric forms and/or E/Z isomers

· Selectively increase or decrease verification weights of the region of interest

· Set reagent or product ratio as a spectrum acceptance test for verification

Databasing

· Create a database using import, drag-and-drop, or macro procedures

· One-click access to spectra in a processed database

· View records in a database as a combinatorial plate

· Multi-spectral report for selected spectral region or entire spectral range

· Display and report plate verification or quantitation results

Supported Formats for Import/Export

Vendor	File Format	Required Parameter Files	Optional Parameter Files
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GE	*.raw, *.* (Nicolet)		
JCAMP†	*.dx; *.jdx		
JEOL Ltd.	*.als, *.nmfid, *.nmf, *.nmdata, *.nmd, *.gxd, *.bin, *.* (Delta)	*.gxp, *.hdr	exp.param, exp.par
Lybrics	*.*		
MSI Felix	*.*		
Tecmag	*.tnt, *.* (MacNMR)		
Thermo Scientific†	*.spc		
Varian, Inc.	data, *.fdf, fid0001.fdf, *.txt, fid, phasefile	acq, proc, procpar	acq_2, text

† File export is also supported (only 1D NMR is supported for JCAMP)

ACD/2D NMR Expert

Software for high-throughput processing, interpretation, and databasing of 1D and 2D NMR data.

With ACD/2D NMR Expert, you can automate standard processing, analysis, verification, and databasing of 1D and 2D NMR data for many spectra at once. It will also automatically evaluate the correspondence between chemical structures and their respective 1D and 2D NMR data-sets for large batches of compounds, with user-defined thresholds for "incorrect," "ambiguous," and "correct" matches between experimental and predicted spectra. Reaction progress can be monitored using Quanalyst, which compares and measures nearly all spectral attributes, including integral area, multiplet coupling patterns, peak locations, and peaks/multiplet areas from overlapping components. Database records for individual wells can be browsed by clicking on the interactive well-plate diagram.
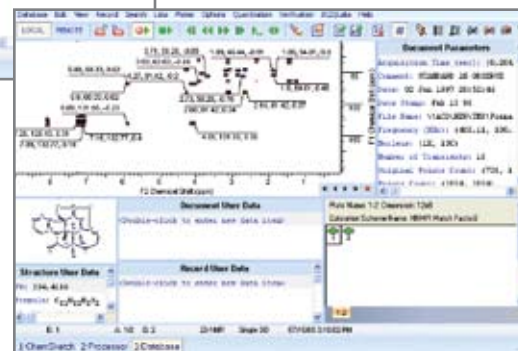
Features

· Automated high-throughput processing, analysis, and databasing
· Database spectra, chemical structures, and user data for up to 382 well-plates at a time
· Combined verification−collective analysis of 1D and 2D NMR data for structure verification
· Monitor reaction progress by calculating reagent conversion
· Create reports including spectra, structures, data tables, and plate graphics
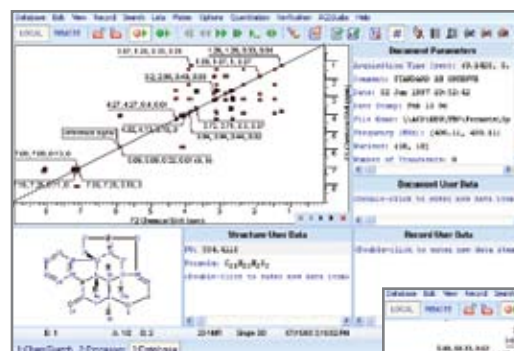
Benefits

· Reduce the time spent on manual evaluation of large NMR datasets
· Automatically process and store 1D and 2D NMR data with associated chemical structures, customizable user data, and spectrum parameters
· Automatically evaluate the correspondence of the proposed chemical structure with the 1D and 2D NMR data

Poster

Automated Evaluation of a Chemical Structure with Only 1D ^{1}H and 2D ^{1}H-^{13}C HSQC

Full List of Features

ACD/2D NMR Expert also includes ACD/1D NMR Manager and the ^{1}H and ^{13}C ACD/NMR Predictors.

Structure Verification

· Verify the ^{1}H NMR or ^{13}C NMR spectrum-to-structure match in batch mode

· The match factor measures the correspondence between the experimental spectrum and the attached structure and gives the RMS of assignment and structure purity

· Fully customizable layout for verification

· 96 and 384 well-plates available as well as many advanced operations with plate

· Show and store the protocol of verification

· Include or exclude exchangeable protons in the verification

· Control the spectrum peak shape for calculated spectra

· Apply weighting factors to chemical shifts, integral, and multiplicity parameters for verification analysis

· Recognize verification results at a glance by color-coding the results according to parameters of your choice: Match Factor, RMS of assignment, structure purity, etc.

· Account for solvents and mixtures with a customizable list

· Use dark regions to define impurities and other superfluous signals in spectra

· Calculate and insert the ^{1}H or ^{13}C NMR spectrum automatically into the database for a given structure

· Load the experimental and calculated spectra simultaneously and display them side-by-side for comparison

· Generate reports for the verification in tabular or plate form

· Report particular spectral regions in experimental and calculated spectra for visual comparison

· Calculate a wide variety of spectrum responses with the built-in Quanalyst tool

· Analyze the integral in user-defined regions of the spectra

· Fully customizable layout for quantitation

· Plate can be colored according to quantitation results

· Advanced graph object available to visualize and report quantitation results

· Perform operations on the data of interest for more in-depth analyses

· Generate reports in plate, tabular, diagram, and multi-spectral formats

· Perform a quantitative analysis for several spectrum responses at a time

Advanced Verification Options for 1D NMR Spectra

· Use reagent structures to enhance verification reliability

· Check the proposed structures for tautomeric forms and/or E/Z isomers

· Selectively increase or decrease verification weights of the region of interest

· Set reagent or product ratio as a spectrum acceptance test for verification

Databasing

· Create a database using import, drag-and-drop, or macro procedures

· One-click access to spectra in a processed database

· View records in a database as a combinatorial plate

· Multi-spectral report for selected spectral region or entire spectral range

· Display and report plate verification or quantitation results

Supported Formats for Import/Export

Vendor	File Format	Required Parameter Files	Optional Parameter Files
Acorn NMR, Inc.	*.fid, *.nmr, *.2d		
ASCII†	*.txt; *.prn, *.csv, *.asc		
Bruker Corporation	*.ser, *.rr, *.fid, *.1r, *.ser, *.2rr, *.* (DISNMR)	acqus, procs, acqu2, proc2s, *.fqs, *.fa1, *.fa2, *.fp1, *.fp2	title, intrng, *.tit, *.ti2
GE	*.raw, *.* (Nicolet)		
JCAMP†	*.dx; *.jdx		
JEOL Ltd.	*.als, *.nmfid, *.nmf, *.nmdata, *.nmd, *.gxd, *.bin, *.* (Delta)	*.gxp, *.hdr	exp.param, exp.par
Lybrics	*.*		
MSI Felix	*.*		
Tecmag	*.tnt, *.* (MacNMR)		
Thermo Scientific†	*.spc		
Varian, Inc.	data, *.fdf, fid0001.fdf, *.txt, fid, phasefile	acq, proc, procpar	acq_2, text

† File export is also supported (only 1D NMR is supported for JCAMP)

ACD/1D NMR Manager

Software to process and assign 1D NMR spectra, and store the knowledge gained from your experiments in an easy-to-search database.

Part of the SpecManager Family

ACD/1D NMR Manager is the complete toolset for processing, interpreting, and databasing your 1D NMR data. This package includes a wide array of processing and databasing capabilities. You can import data from all major NMR instrument vendor formats, and carry out basic, advanced, or automated processing. Attach or paste a chemical structure to your spectrum and easily assign multiplets to atoms. When interpretation is complete, database your experimental spectra, chemical structure, as well as the knowledge obtained from your experiment and all associated information. The resulting database record can be searched by structure, chemical shift, multiplet, and other search methods.

Features

· Real-time vendor-neutral processing− apply all processing features automatically or on the fly, with the ability to preview your results before applying them
· Important information in half the time−peak picking, multiplet patterns, and coupling constants are generated automatically while integrating peaks
· True spectrum-to-structure integration −assign multiplets to atoms, and retain the assignments to share knowledge and improve NMR predictions.
· Efficient knowledge management− store not only spectra but also knowledge obtained from the spectra in a repository with comprehensive searching options.

Benefits

· Desktop viewing and processing capabilities away from the instrument and in the comfort of your own lab or office.
· A standardized format and methods to treat NMR data across your organization.
· Instantly generate formatted multiplet reports for patents, reports, and publications

· Easily store and retrieve all the knowledge and information associated with 1D NMR data in your organization or lab with a fully searchable database (including chemical structure, spectrum assignments, parameters, user data, etc.)
· Quickly and easily create professional reports containing spectra, chemical structures, multiplet reports, assignment tables, and more
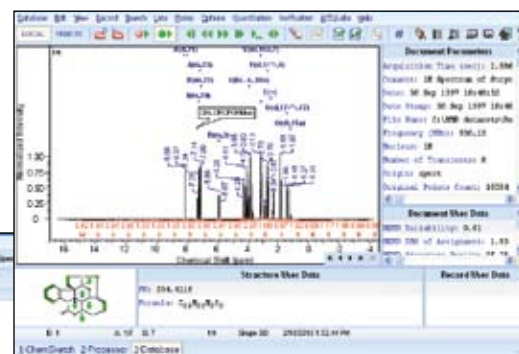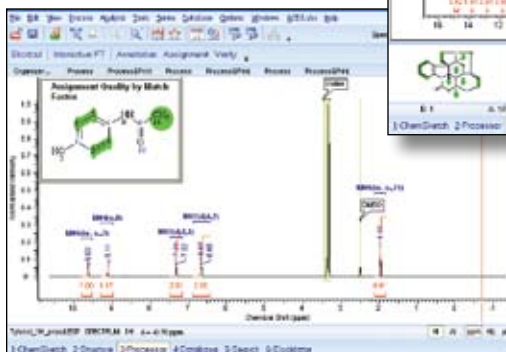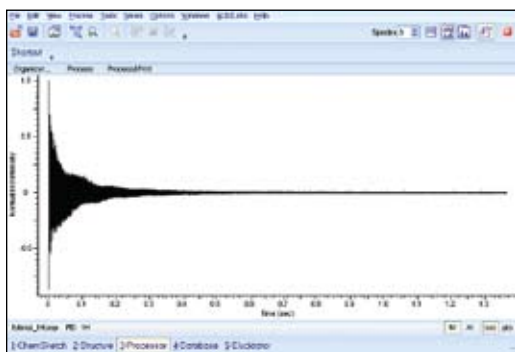
Full List of Features

1D NMR Spectrum Processing Features and Key Capabilities

· Import a wide variety of NMR data formats, including vendor-specific files

· JCAMP export of structure, spectra, and tables of assignment and peaks

· Preview a spectrum before opening a file

· Full audit trail feature (History) tracks every applied processing command

· Macro capabilities include templates and a macro organizer for completely automated data processing

· Multiple window display: Tile, Replace, or Overlay mode

· Synchronize the axes in a multiple window display

· Flexible zooming options

· Zero filling, weighting functions, FID shift, and Fourier transform

· Interactive apodization so that you get immediate feedback for changing the windowing parameters

· Calculation of Power and Magnitude spectra

· Automated and manual phase correction

· Macro for phasing a spectrum by a reference spectrum (PhasebyFile)

· Automated and manual baseline correction over the whole spectrum or region of interest

· Automated and manual peak picking

· Automated and manual spectrum integration

· Automated and manual referencing:

  · Automated referencing includes TMS and solvent peak(s) detection in ^{1}H and ^{13}C spectra

  · Manual referencing includes a list of references and solvents for ^{1}H, ^{13}C, ^{15}N, ^{19}F, and ^{31}P spectra referencing; the list can be extended with custom references for all nuclei

· Construction of a table of multiplets and coupling constants

· Solvent suppression (filtering in the time or frequency domain)

· Various tools for editing spectral data

· Addition or subtraction of two spectra

· Ability to attach a chemical structure to a spectrum

· Mouse-click assignment of single peaks, multiplets, and spectral regions to atoms in structures

· Text annotation of one or more peaks or regions of interest in a spectrum

· Quantitative analysis for series of spectra (Quanalyst) with results graphed

· Put impurities signals and artifacts into dark regions to be ignored during all analyses

· Standard and Intelligent bucketing procedures for metabonomics applications

· Fit peaks by a number of analytical functions

· Calculate the signal-to-noise ratio for any peak

· Store processed spectra along with complete analysis information (structures, table of peaks, table of assignments, table of annotations, table of multiplets, coupling constants, and audit trail) in the .ESP file

· Preparation of high-quality reports, including spectra, structures, annotations, and tables using full integration with ACD/ChemSketch

Databasing Features

· Update the database with the experimental spectra along with their chemical structures, analysis results (table of peaks, annotation), as well as miscellaneous information copied to User Data and Notes

· Populate user databases with thousands of spectra in one step with the Group Macro batch processing tool

· Search by full spectrum or one or more spectral regions, peaks, spectral parameters, chemical structure and substructure, formula, molecular weight, and user data text

· Perform spectrum searches according to Euclidean distance, or squared or absolute difference methods; the search hits will be ranked by HQI (Hit Quality Index)

· Control data that is entered into your corporate databases with Data Forms Manager

· Manage remote databases through a local or global network with an Oracle-based SQL client-server system

Supported Formats for Import/Export

Vendor	File Format	Required Parameter Files	Optional Parameter Files
Acorn NMR, Inc.	*.fid, *.nmr, *.2d		
ASCII†	*.txt; *.prn, *.csv, *.asc		
Bruker Corporation	*.ser, *.rr, *.fid, *.1r, *.ser, *.2rr, *.* (DIS-NMR)	acqus, procs, acqu2, proc2s, *.fqs, *.fa1, *.fa2, *.fp1, *.fp2	title, intrng, *.tit, *.ti2
GE	*.raw, *.* (Nicolet)		
JCAMP†	*.dx; *.jdx		
JEOL Ltd.	*.als, *.nmfid, *.nmf, *.nmdata, *.nmd, *.gxd, *.bin, *.* (Delta)	*.gxp, *.hdr	exp.param, exp.par
Lybrics	*.*		
MSI Felix	*.*		
Tecmag	*.tnt, *.* (MacNMR)		
Thermo Scientific†	*.spc		
Varian, Inc.	data, *.fdf, fid0001.fdf, *.txt, fid, phasefile	acq, proc, procpar	acq_2, text

† File export is also supported (only 1D NMR is supported for JCAMP)

Third-Party Databases

Access and search highly-curated NMR databases.

ACD/Labs' NMR data libraries give chemists access to meticulously examined experimental NMR data, complete with assigned structures and references. Databases are available for ^{1}H, ^{13}C, ^{15}N, ^{19}F, and ^{31}P (each of these databases is used for the appropriate ACD/Labs Predictor). Each standalone database contains chemical shifts, original literature references, molecular formula, molecular weight, and the IUPAC name for each structure record, and does not require any additional software.

Three sets of spectral NMR databases are available (^{1}H and ^{13}C): ACD/Polymer Database (439 records), the Aldrich NMR Library for ACD/Labs (over 35,000 records), and the Chenomx Metabolite Library for ACD/Labs (300 common metabolites found in biofluids). ACD/1D NMR Manager is required to access and browse these databases. ACD/1D NMR Manager also allows you to recreate the FID, re-process, and analyze individual spectra.

Features

· Search by chemical shift, coupling constants, molecular formula, molecular weight, or spin system
· Search for exact structure or substructure matches; identify fragments from successive substructure searches through color-coded highlights.
· Perform structure similarity searches by the Tanimoto, Cosine, Dice, Hamming Distance, and Euclidean Distance algorithms to find exact matches and related structures
· Search the database for more stable tautomers when performing a structure search
· Various result viewing options—review a single record, browse multiple databases in table view or tile view, and select records interactively

Benefits

· Quickly identify unknowns and impurities
· Check starting materials before beginning large/involved syntheses
· Ease dereplication and elucidation problems
· Reduce instrument time and narrow down the experimental acquisition range for ^{15}N NMR experiments
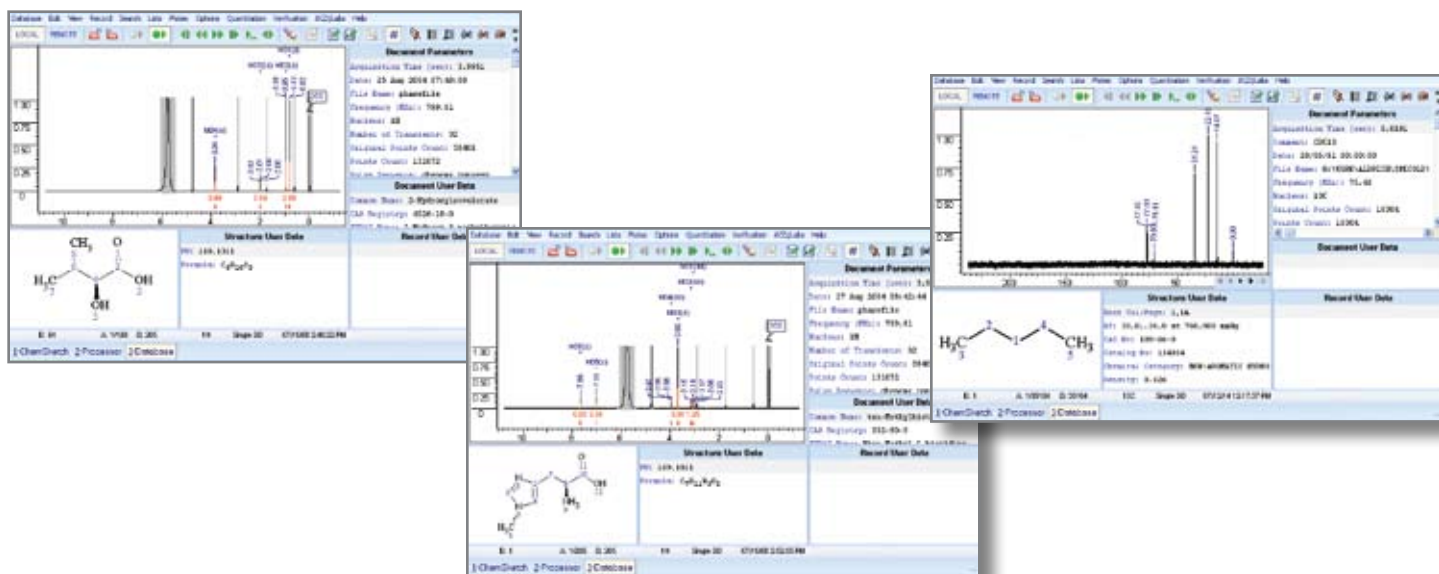
ACD/MS Processor

Software for processing and interpreting all types of MS data.

Process your mass spectral data with software designed for convenient analysis, interpretation, and reporting of results. Whether you have a single mass spectrum (MS), tandem mass spectra (MS/MS, MS/MS/MS, ... MSn), or a hyphenated dataset (LC/MS, LC/DAD, CE/MS, and GC/MS), ACD/MS Processor allows you to process all of your mass spectral data in a consistent manner, no matter which instrument make or model was used to acquire the data.

Features

· Process data from different instrument models and makes
· Automatically assign mass fragments to spectral peaks
· CODA algorithm and COMPARELCMS for LC/MS data
· COmponent Detection Algorithm (CODA) and COMPARELCMS for LC/MS data
· Attach chemical structures to spectra, including Markush representations
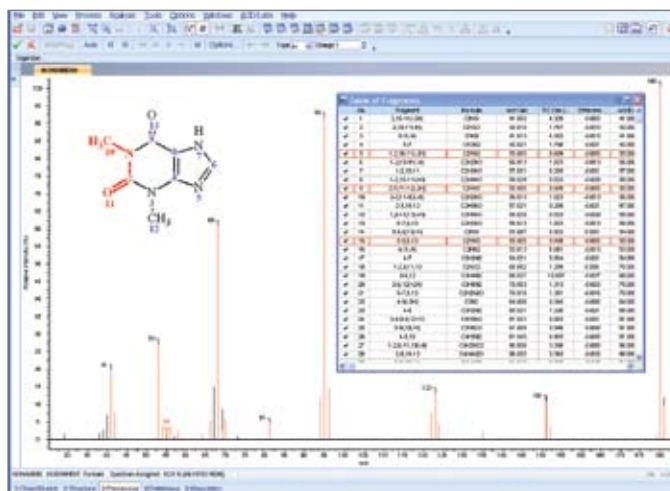
Benefits

· Consistent, uniform data processing
· Reduce noise and extract relevant information from data sets
· Create reports quickly and easily
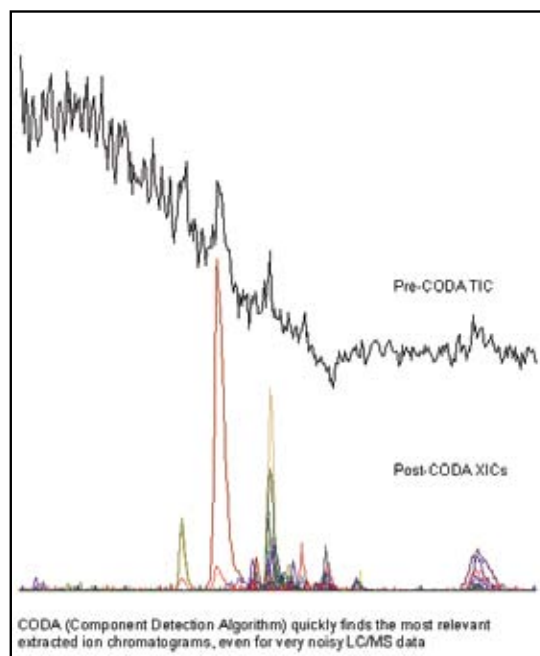
CODA (Component Detection Algorithm) quickly finds the most relevant extracted ion chromatograms, even for very noisy LC/MS data

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Add additional capabilities to ACD/MS Processor:

ACD/IntelliTarget screens samples for the presence or absence of known compounds specified by formula or monoisotopic mass. In the process $[M+H]^+$ or $[M-H]^-$, adduct, multimer, and fragment ions are automatically assigned.

ACD/IntelliXtract extracts all components in a given dataset, assigns $[M+H]^+$ or $[M-H]^-$, adduct, multimer, and fragment ions, and can reconstruct a pure component spectrum for each.

ACD/MS Fragmenter provides a convenient way to review the fragmentation pathways and possible structure configurations for a particular fragment automatically assigned to a spectral peak by ACD/MS Manager. You can also easily create a report illustrating the possible fragmentation schemes.

Full List of Features

Mass Spectrum Analysis

· Import and process MS data from many different instrument makes and models

· Automatically assign mass fragments to an experimental spectrum

· Choose positive or negative ionization modes

· For positive ions, select from three sets of fragmentation rules (EI, APCI and ESI, and CI)

· For negative ions, select from three sets of fragmentation rules (Electron Capture, Deprotonation, and Hydride Attachment)

· Assignment Quality Index (AQI) indicates the quality of fragment assignment.

· Use Formulae Generator to generate the possible molecular or fragment ion formulae

· Calculate the isotope pattern for single, multiple charged, protonated, or deprotonated ions

· Display a spectrum of neutral losses derived from the current mass spectrum

· Apply flexible spectral subtraction options

· Search for mass differences (specified by either formula or mass) between selected peaks in Compare Mass Spectra using a correlation analysis algorithm for finding similarity between mass spectra

· Annotate the spectra aided by the mass loss or formula loss autocalculator

· Automate data processing with macro programs

LC/MS Processing

· Use CODA to reduce noise and background

· Find small differences between similar LC/MS or GC/MS datasets with COMPARELCMS

· Combine the spectra under a chromatographic peak into a single spectrum

· Subtract major component mass spectra from the entire LC/MS dataset to better distinguish the low concentration components

· Smooth chromatograms according to the fast Fourier transform (FFT) or Savitzky-Golay smoothing algorithms

· Automatically find and label peaks with a selected parent mass or mass difference from parent

· Remove baseline effects with the baseline correction algorithm

· Perform peak picking on LC/UV (PDA, DAD) datasets

· Subtract the solvent background from LC/UV datasets

· Convert profile LC/MS data-sets to centroid manually or automatically using macros

Full List of Supported Formats

Vendor	Spectrum File
Agilent Technologies	*.ms, *.yep, *.wiff, *.bin
Applied Biosystems/MDS SCIEX	*.wiff
Bruker Daltonics	*.yep
Hitachi	*.msd; *.dad
JEOL (Japan)	*.jsp, *.jpf, *.jmc, *.spe
MasCom MASPEC II^{32} Data System	*.ms2
Matlab/Eigenvector Research	*.mat
National Institute of Standards and Technology	*.msp, *.sdf
Shimadzu Corporation	*.lcd, *.qgd, *.qld
Thermo	*.raw, *.dat, *.spc
Unidata	*.cdf, *.nc
Varian, Inc.	*.dat, *.xms, *.sms
Waters Corporation	_functns.inf, *.rpt
ASCII	*.txt
JCAMP	*.dx, *.jdx
netCDF	*.cdf, *.nc

ACD/Labs software is compatible with most major vendor file types and formats.

For more detailed information on the compatibility of specific vendor file formats for MS, please visit our website.

www.acdlabs.com/msformats

ACD/MS Fragmenter

Software for the prediction of mass spectral fragmentation.

Predict mass fragmentation in just seconds with ACD/MS Fragmenter. Simply draw a structure, select an ionization technique and polarity, and get instant predictions for almost any MS experiment. ACD/MS Fragmenter predicts fragment ions based on established MS fragmentation rules from the literature and allows you to review the rules to gain a clear understanding of your molecule's fragmentation.

Features

- Predict fragmentation for small molecules of up to 255 atoms plus hydrogens
- Predict fragments from both positive and negative ionization
- Review key fragmentation pathways and ion structures in a convenient fragmentation tree
- Create several types of fragmentation reports including Branch, Scheme, Compact, and Detailed

Benefits

- Gain a better understanding of the fragmentation of your molecule
- Review possible fragment ion structures without bias
- Report fragmentation pathways for reports or publications with ease

Application Notes

Prediction of Negative Ion Mass Fragmentation of Chloramphenicol

Prediction of Mass Fragmentation of Dextromethorphan Under Positive Electrospray Ionization Conditions

Make structure elucidation and confirmation faster and easier by automatically assigning predicted mass fragments to experimental spectra processed in either ACD/MS Processor or ACD/MS Manager.

ACD/MS Databases

Available mass spectral reference databases.

Wiley Registry of Mass Spectral Data, 9th Edition with NIST 2008

The Wiley Registry® 9th Edition/NIST 2008 is the largest mass spectral library commercially available, with over 796,000 mass spectra and over 746,000 spectra with searchable chemical structures. Containing over 667,000 compounds, the Wiley Registry/NIST Library is a must-have for any analytical laboratory.

Applications include pathology, forensics, quality assurance, border control, research and development, commercial deformulation, food safety, food quality, environmental science, and anywhere an unknown compound must be identified or a known compound must be confirmed.

Each DVD contains the Complete Wiley Registry 9th Edition/NIST 2008 library in a format compatible with ACD/MS Manager and the complete NIST/EPA/NIH 2008 with MS Search.
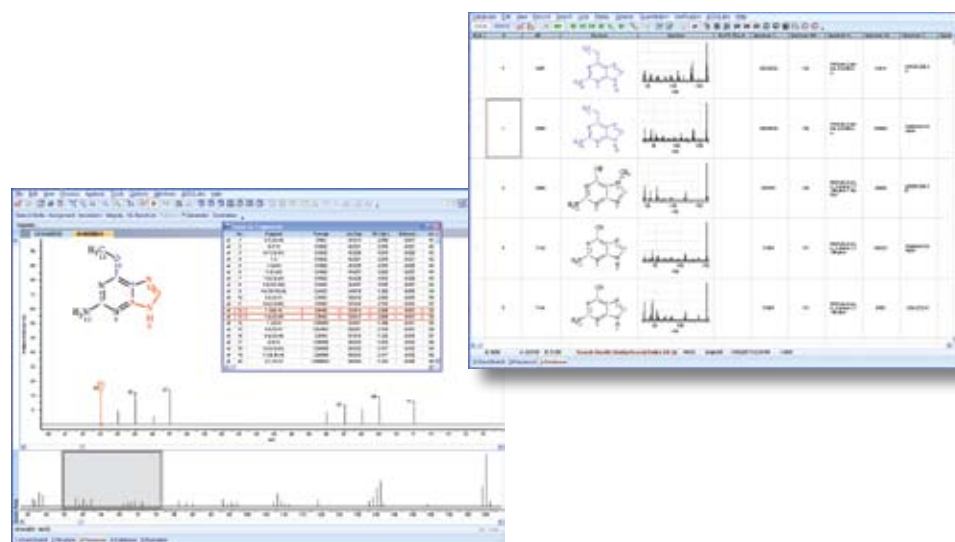
ACD/MS Manager

Software for processing, interpreting, and storing MS data.

ACD/MS Manager allows you to process all types of mass spectrometric data, including data from Thermo, ABSciex, Waters, Agilent, Bruker, Varian, Shimadzu, and other instruments. Unify data processing, build fully searchable databases of mass spectra, and simplify the sharing of information and report generation. Automated options are available to automate routine processing and databasing tasks.

Features

· Process data from different instrument models and makes
· Automatically assign mass fragments to spectral peaks
· COmponent Detection Algorithm (CODA) and COMPARE LCMS for LC/MS data
· Attach chemical structures to spectra, including Markush representations
· Build databases of mass spectra that are searchable by a variety of structure and spectral parameters

Benefits

· Consistent, uniform data processing
· Reduce noise and extract relevant information from datasets
· Create reports quickly and easily
· Store information in a database and easily search it

Add additional capabilities to ACD/MS Manager:

ACD/IntelliTarget screens samples for the presence or absence of known compounds specified by formula or monoisotopic mass. In the process $[M+H]^+$ or $[M-H]^-$, adduct, multimer, and fragment ions are automatically assigned.

ACD/IntelliXtract extracts all components in a given dataset, assigns $[M+H]^+$ or $[M-H]^-$, adduct, multimer, and fragment ions, and can reconstruct a pure component spectrum for each.

ACD/MS Fragmenter provides a convenient way to review the fragmentation pathways and possible structure configurations for a particular fragment automatically assigned to a spectral peak by ACD/MS Manager. You can also easily create a report illustrating the possible fragmentation schemes.

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Full List of Processing Features

Mass Spectrum Analysis

· Import and process MS data from many different instrument makes and models

· Automatically assign mass fragments to an experimental spectrum

· Choose positive or negative ionization modes

· For positive ions, select from three sets of fragmentation rules (EI, APCI and ESI, and CI)

· For negative ions, select from three sets of fragmentation rules (Electron Capture, Deprotonation, and Hydride Attachment)

· Assignment Quality Index (AQI) indicates the quality of fragment assignment.

· Use Formulae Generator to generate the possible molecular or fragment ion formulae

· Calculate the isotope pattern for single, multiple charged, protonated, or deprotonated ions

· Display a spectrum of neutral losses derived from the current mass spectrum.

· Apply flexible spectral subtraction options

· Search for mass differences (specified by either formula or mass) between selected peaks in Compare Mass Spectra using a correlation analysis algorithm for finding similarity between mass spectra

· Annotate the spectra aided by the mass loss or formula loss autocalculator

· Automate data processing with macro programs

LC/MS Processing

· Use CODA to reduce noise and background

· Find small differences between similar LC/MS or GC/MS datasets with COMPARELCMS

· Combine the spectra under a chromatographic peak into a single spectrum

· Subtract major component mass spectra from the entire LC/MS dataset to better distinguish the low concentration components

· Smooth chromatograms according to the fast Fourier transform (FFT) or Savitzky-Golay smoothing algorithms.

· Automatically find and label peaks with a selected parent mass or mass difference from parent

· Remove baseline effects with the baseline correction algorithm.

· Perform peak picking on LC/UV (PDA, DAD) datasets

· Subtract the solvent background from LC/UV datasets

· Convert profile LC/MS datasets to centroid manually or automatically using macros

Full List of Database Features

· Store thousands of spectra simultaneously with the Group Macro command

· Search by peaks, spectra, formulae, molecular weights, full and partial chemical structure, and user data text

· Search using Markush structures to find database entries for all possible structures

· Search for different tautomeric forms of a structure

· Hyperlink directly to electronic files, such as images and documents, in a database field

· Create and search a database of neutral loss spectra

· Show detailed analysis of information, such as peak labels and annotations, in the database curve windowpane

· Browse and visualize the database's content in One Record view, Table view, and Tile view

· Store and display images (BMP, JPEG, GIF, PNG) directly in the database screen form
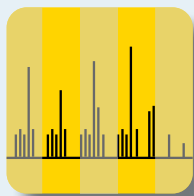

ACD/Labs software is compatible with most major vendor file types and formats.

For more detailed information on the compatibility of specific vendor file formats for MS, please visit our website.

www.acdlabs.com/msformats

Full List of Supported Formats

Vendor	Spectrum File
Agilent Technologies	*.ms, *.yep, *.wiff, *.bin
Applied Biosystems/MDS SCIEX	*.wiff
Bruker Daltonics	*.yep
Hitachi	*.msd; *.dad
JEOL (Japan)	*.jsp, *.jpf, *.jmc, *.spe
MasCom MASPEC II[32] Data System	*.ms2
Matlab/Eigenvector Research	*.mat
National Institute of Standards and Technology	*.msp, *.sdf
Shimadzu Corporation	*.lcd, *.qgd, *.qld
Thermo	*.raw, *.dat, *.spc
Unidata	*.cdf, *.nc
Varian, Inc.	*.dat, *.xms, *.sms
Waters Corporation	_functns.inf, *.rpt
ASCII	*.txt
JCAMP	*.dx, *.jdx
netCDF	*.cdf, *.nc

ACD/IntelliXtract

Deconvolution software for ACD/MS Manager and ACD/MS Processor.

A tool to quickly extract relevant components from LC/MS Data.

ACD/IntelliXtract extracts all chromatographic components in LC/MS datasets and assigns $[M+H]^+$ or $[M-H]^-$ for each component. Whether used to complement manual data examination or for fully automated analysis, ACD/IntelliXtract can reduce interpretation time and confirm the presence of co-eluting or trace components that otherwise may have been overlooked. ACD/IntelliXtract will help analysts quickly understand their results and extract the information of interest.

Features

· Automatically assign [M+H]+ or [M-H]-
  for each component
· Resolve overlapping peaks and
  identify co-eluting components
· View reconstructed pure component
  spectra for each chromatographic
  component
· Automatically analyze batches
  of samples

Benefits

· Find all relevant components, even at
  low concentrations or when co-eluting
  with other components
· Reduce interpretation time with
  advanced filters
· Work with data from most major
  instrument vendors

Post-processing

Pre-processing
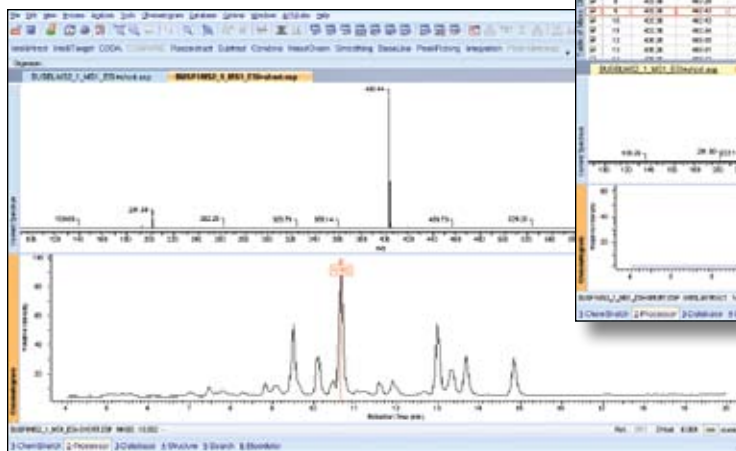
Application Notes

**Extraction and Elucidation
of Metabolites Using Related
Fragment Screening**

**Software-guided Identification of
Dextromethorphan Metabolites
with ACD/IntelliXtract**

ACD/IntelliXtract uses a unique algorithm based on CODA technology used by ACD/MS Manager. The process, called componentization begins with peak extraction, which is followed by interpretation of the mass spectrum associated with each extracted component. This step considers the expected $^{12}C/^{13}C$ ratios, adducts, multimers, isotopes, neutral losses, and fragment ions, providing reliable spectrum interpretation and protonated or deprotonated molecule assignment. Componentization ensures that all relevant components are detected, even when they exist only at trace concentrations or co-elute with other components.

Full List of Processing Features

General Features

· Compatible with positive or negative ionization mode data

· Compatible with different ionization modes (ESI, APCI, APPI, EI, CI, LC-FAB, etc.)

· Work with mass accuracies from 0.00001 to 1 Da

· Create a user-defined list of compound names and masses that may be present in the sample, and automatically add a label to the associated molecular ion peak

· Label metabolite components based on the mass(es) of the parent drug(s), and a pre-defined list of phase I and phase II transformations (included with the software)

· Label transformations from the parent compound(s) (e.g., neutral losses) with a user-defined table of modifications that may be saved and retrieved for different types of analyses

· Annotate chromatogram peaks with the mass of the protonated or de-protonated molecule

· Automatically attach chemical structures to components

· Use macros to automatically process several data files with different parent compounds in batch mode

Chromatographic Processing Features

· Accurately determine retention times of eluting compounds

· Deconvolute overlapping components

· Automatically calculate neutral losses for all components based on the difference between the (de)protonated molecule and possible fragment ions (PFI)

· Apply flexible data pre-smoothing and baseline correction to single ion chromatograms

· Extract high resolution mass chromatograms

· Apply a mass defect filter

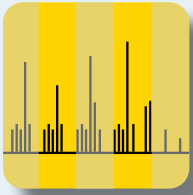· Apply an isotope pattern filter

Mass Spectral Processing Features

· Automatically assign $[M+H]^+$ or $[M-H]^-$, adduct ions, multimers, neutral losses, and possible fragment ions for each component

· Extract pure component spectra from overlapping components

· Automatically classify the quality of the data for extracted components as Good, Poor, or Requires Manual Review

· Calculate the average peak, peak top, and peak shoulder masses for the molecular ion and all other contributing ions within a component

· Evaluate the peak quality of extracted single ion peaks based on peak height, area, symmetry, full width half maximum, S/N, $^{12}C/^{13}C$, or a combination of parameters

· Evaluate the spectrum quality, apply pre-defined error limits for mass accuracy, $^{12}C/^{13}C$, %M ion, and isotope cluster analysis, or apply user-defined limits

· Automatically assign common adduct ions (Na, K, NH_3, and more)

  · Customize the list of possible adducts with a user-defined list

· Selectively search for proton and adduct multimers

· Automatically assign radical cations

Comparison Features

· Identify similarities and differences between two or more datasets:

  · Find unique peaks

  · Find differences between datasets based on user-defined differences in retention time or intensity

  · Find peaks common to the datasets

  · Apply Boolean comparison of peaks between datasets (present/not present)

  · Use isotope patterns to compare ion clusters between samples to confirm that similar components have similar spectral properties

· Calculate the relative differences between different components based on the contributing ions

· Compare components based on the contributing ion patterns using definable error tolerances

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ACD/Labs software is compatible with most major vendor files types and formats.

For more detailed information in the compatibility of specific MS vendor file formats, please visit our website.

www.acdlabs.com/msformats

Full List of Supported Formats

Vendor	Spectrum File
Agilent Technologies	*.ms, *.yep, *.wiff, *.bin
Applied Biosystems/MDS SCIEX	*.wiff
Bruker Daltonics	*.yep
Hitachi	*.msd; *.dad
JEOL (Japan)	*.jsp, *.jpf, *.jmc, *.spe
MasCom MASPEC II32 Data System	*.ms2
Matlab/Eigenvector Research	*.mat
National Institute of Standards and Technology	*.msp, *.sdf
Shimadzu Corporation	*.lcd, *.qgd, *.qld
Thermo	*.raw, *.dat, *.spc
Unidata	*.cdf, *.nc
Varian, Inc.	*.dat, *.xms, *.sms
Waters Corporation	_functns.inf, *.rpt
ASCII	*.txt
JCAMP	*.dx, *.jdx
netCDF	*.cdf, *.nc

ACD/IntelliTarget

Accurately find known compounds by screening LC/MS data.

ACD/IntelliTarget lets you quickly find compounds you already know about without manual data interpretation. Monitor samples analyzed by LC/MS and GC/MS for a list of expected compounds and be alerted if they are present or not even at trace levels, or when co-eluting with other compounds. Use ACD/IntelliTarget to evaluate samples for further analysis or to monitor specific compounds in your process.

Features

· Specify a list of known compounds by formula or monoisotopic mass
· Automatically assign [M+H]+ or [M-H]- for each component
· Extract and identify adducts with or without the exact formula
· Resolve overlapping peaks and co-eluting components
· Automate to analyze or monitor batches of samples

## Benefits

· Find known compounds quickly, even at low concentrations
· Reduce the time required for data interpretation
· Work with data from most major instrument vendors.

ACD/Labs software is compatible with most major vendor files types and formats.

For more detailed information in the compatibility of specific MS vendor file formats, please visit our website.

www.acdlabs.com/msformats
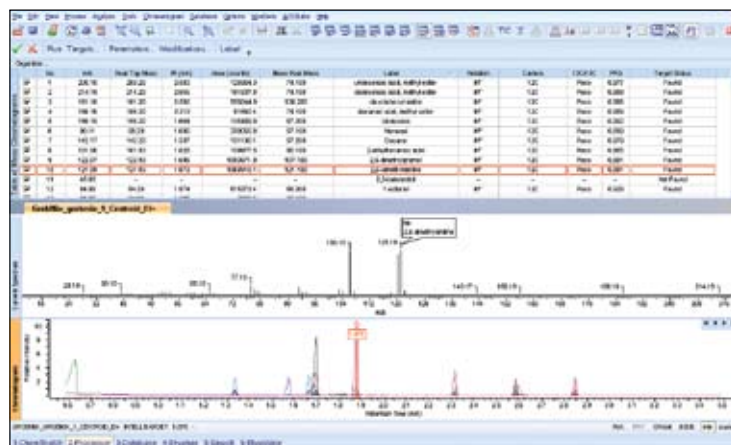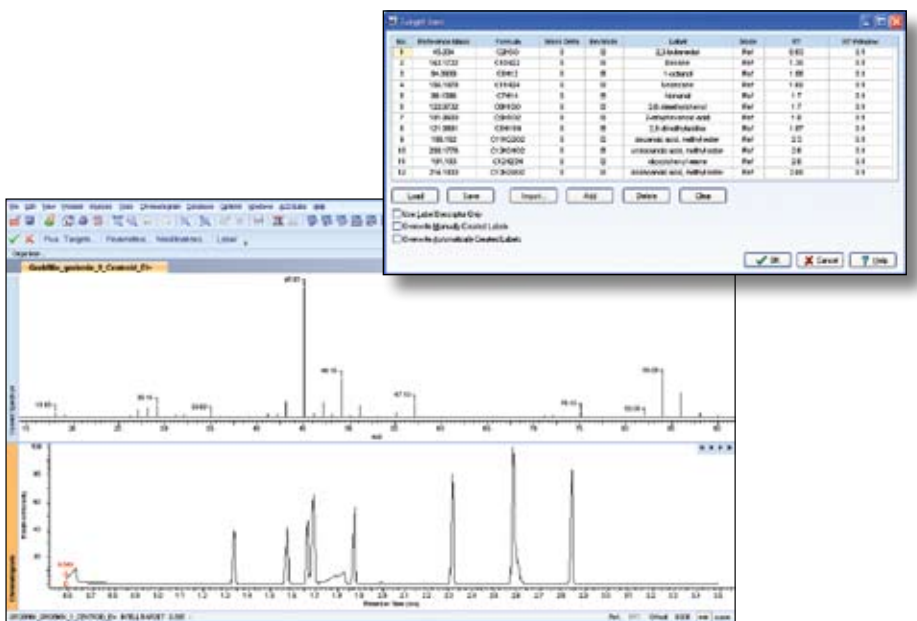
Full List of Processing Features

Compentization

· Identifies components present in the dataset at concentrations ranging from abundant to ultra-trace

· To limit the search, set thresholds based on peak intensity or a range of other parameters

· Results of componentization are presented in a concise and easy-to-read table of mass chromatograms

Deconvolution

· Once componentization is complete, all ions associated with the same component are grouped together in the table of mass chromatograms to more easily see the individual components present in the dataset

Automatically Assign Features

· For each component, $[M+H]^+$, $[M-H]^-$, and adduct ions are automatically assigned and labeled

· Predicted isotope peaks are shown for comparison with experimental peaks in the mass spectra

Reporting

· Generate a clear list of compounds labeled Found or Not Found

· Export the list to Microsoft® Excel®, convert to Adobe® PDF, or copy-and-paste into other programs

Compatibility

· Work with low or high resolution mass spectrometry data

· Compatible with various positive and negative ionization modes, including ESI, APCI, EI, CI

ACD/IntelliTarget helps identify the presence or absence of known compounds in much less time than manual data interpretation. Use it as a screening and monitoring tool, or as a preliminary step to further analysis by using ACD/IntelliXtract to extract unidentified components in a complicated sample.

Forensic Science

Save time by qualitatively screening samples before quantitative analysis to detect specific compounds and metabolites. ACD/IntelliTarget can be fully automated to accommodate high-throughput requirements for busy laboratories.

In forensic research, ACD/IntelliTarget and ACD/IntelliXtract are used to easily identify marker metabolites. ACD/IntelliTarget finds the compounds you know and ACD/IntelliXtract finds everything else.

Environmental Monitoring

Environmental protection legislation around the world is demanding more stringent monitoring of surface and ground waters. Reduce the cost and time required to monitor an array of herbicides, pesticides, and other controlled substances with ACD/IntelliTarget, either by pre-screening samples for analysis or with an automated solution that can handle higher volumes of samples.

ACD/IntelliTarget can also be used as a tool to assist in method development for new compounds, detecting them using only formula or mass, allowing you to find the retention time of new compounds without the laborious and time-consuming manual interpretation.

Water Analysis

ACD/IntelliTarget can be used by analytical staff or spectroscopy experts to quickly identify the presence of contaminants in emergency or complaint samples. Using a commercial database for comparison, ACD/IntelliTarget identifies, with a simple, easy-to-read tabular output, those compounds that are present in the sample. Once any known compounds have been confirmed or eliminated, ACD/IntelliXtract can be used to detect other, potentially harmful unknown compounds, indicating a need for further testing and identification.

Food Safety

Ensuring the quality of our food chain requires speed and accuracy in detecting the presence of antibiotics, hormones, pesticides, and other harmful compounds, ACD/IntelliTarget provides a rapid result, indicating either Found or Not Found, even at trace concentrations. Specify a list of compounds of interest or screen against a commercially available database. ACD/IntelliTarget can also be automated to handle high-throughput monitoring of samples.

Drug Discovery

Rapidly confirm the presence or absence of expected metabolites by screening samples with ACD/IntelliTarget. Follow up with extracting unknown or unexpected metabolites with ACD/IntelliXtract, resulting in a powerful combination of tools for metabolite identification.

Full List of Supported Formats

Vendor	Spectrum File
Agilent Technologies	*.ms, *.yep, *.wiff, *.bin
Applied Biosystems/MDS SCIEX	*.wiff
Bruker Daltonics	*.yep
Hitachi	*.msd; *.dad
JEOL (Japan)	*.jsp, *.jpf, *.jmc, *.spe
MasCom MASPEC II^{32} Data System	*.ms2
Matlab/Eigenvector Research	*.mat
National Institute of Standards and Technology	*.msp, *.sdf
Shimadzu Corporation	*.lcd, *.qgd, *.qld
Thermo	*.raw, *.dat, *.spc
Unidata	*.cdf, *.nc
Varian, Inc.	*.dat, *.xms, *.sms
Waters Corporation	_functns.inf, *.rpt
ASCII	*.txt
JCAMP	*.dx, *.jdx
netCDF	*.cdf, *.nc

ACD/MS Manager Suite

Process, store, and report MS, chromatography, and UV-Vis, data all with one package.

Multiple analytical techniques are often necessary for sample characterization or structure elucidation. Keeping data organized and correlated can be difficult and labor-intensive. Streamline the process of collecting and interpreting large amounts of analytical data by consolidating everything into a single interface.

ACD/MS Manager Suite allows you to work with MS, Chromatography and UV-IR data in a single interface, facilitating the use of hyphenated analytical techniques such as LC/MS and LC/UV. Use it to organize spectra and chromatograms related to the same chemical structure, store relevant metadata and create dynamic links between spectra and chromatographic peaks.

At a glance, see the relationship between experimental data and drill down into various levels of data directly from the experimental data point, allowing faster evaluation of experimental results.

Become even more efficient by searching the database by a variety of spectral, structure, and text-based queries for previously stored data, eliminating the need for redundant analysis. Share data, and create reports quickly and easily using report templates or your own report design.
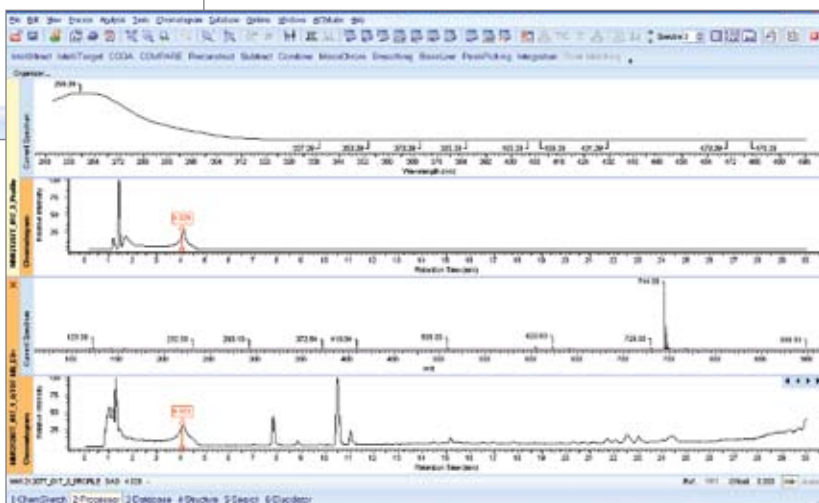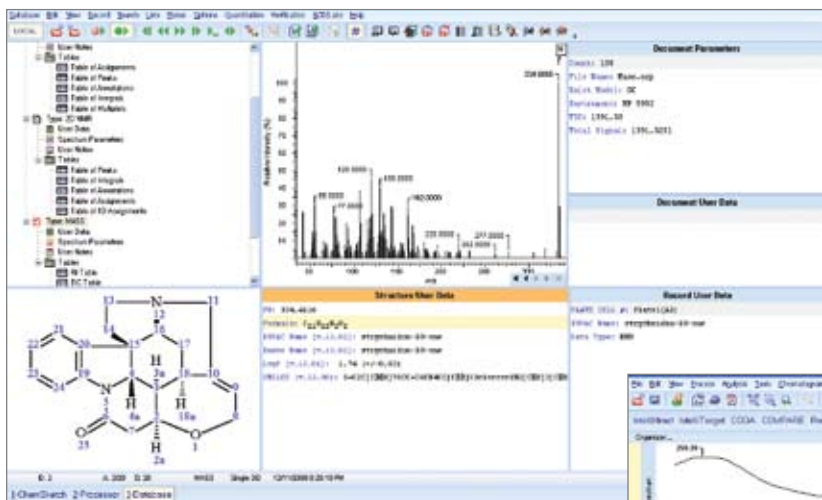
ACD/UV-IR Processor

Software for processing electronic, vibrational, or rotational transition spectroscopy data.

ACD/UV-IR Processor provides the ability to manipulate and manage optical spectra in a continuous range spanning the entire optical spectroscopy range from 1 cm^{-1} to 100,000 cm^{-1} (100 to 10,000,000 nm), encompassing the ultraviolet, visible, near-, middle- and far-infrared, and Raman techniques.

Features

· Process and interpret data from a variety of optical techniques, including:
  · Absorption
  · Reflectance
  · Fluorescence
  · Phosphorescence spectra
  · Circular dichroism (CD)
  · Spectroscopic ellipsometry
· Attach chemical structures to analytical spectra and assign peaks to chemical structural fragments
· Verify chemical structures with experimental spectra or review a list of characteristic fragments possibly present in an unknown structure

· Generate a list of functional groups from characteristic frequencies for over 1300 structural fragments (IR) and over 1100 structural fragments (Raman)
· Resolve the pure component spectra of mixtures with SIMPLISMA
· Automate repetitive processing tasks with macro commands that can be applied to a spectral series as well as to a single spectrum
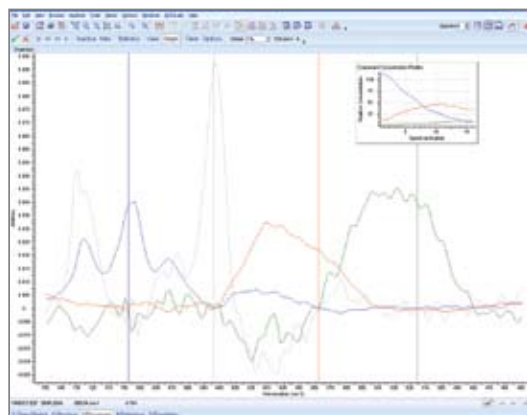
Benefits

· Uniformly process data for greater speed and consistency
· Correlate information from other analytical techniques by linking related data in a clear hierarchical system
· Confirm structure-to-spectrum correspondences with infrared or Raman verification algorithms

Posters

Simplify Structure-to-Spectrum Assignment and Annotation

Verify Structure-to-Spectrum Compatibility

Resolve pure components from a series of spectral mixtures and obtain corresponding concentration profiles with SIMPLISMA (SIMPLe-to-use Interactive Self-Modeling Mixture Analysis). This highly interactive curve-resolving algorithm extracts individual components without requiring *a priori* knowledge of the mixture composition.

Full List of Processing Features

- Import data files from most major vendor file formats, including single-scan, multi-scan, and hyphenated spectral data

- Load spectral data directly from an external application interface such as Waters, Empower or Dionex Chromeleon software

- Organize and compare multiple spectra in Tile, Full, or Overlay (series) modes

- Customize series display offsets for improved interpretation clarity and synchronize axes through multiple windows

- Specify x-axis orientation and define y-axis for spectral absorbance or reflectance to units of absorbance, transmittance, molar absorptivity, %reflectance, etc.

- Visualize contour maps and various associated 2D plots (integral, projection, slices, etc.) of hyphenated data with the ACD/Matrix feature

- Use fully interactive zooming features to focus on various spectral regions and automatically restrict spectral searches to these delimited x-axis regions

- Automatically save all the processing and analysis history (audit trail) with the full interpretation details

- Automate routine processing tasks and manipulate sizable collections of files with macro commands

- Create professional, high-quality reports in PDF, ACD/ChemSketch, or other formats

- Obtain the mean spectrum for a spectral series with the Average Spectrum command

- Interactively suppress noise from your spectroscopic data with flexible FFT or Savitzky-Golay smoothing algorithms

- Subtract a scaled spectrum from another spectrum; automatically subtract a component signal from a mixture spectrum

- Interactively convert a spectrum or series into its 1st, 2nd, 3rd, or 4th order derivatives

- Perform ATR (attenuated total reflectance) correction to remove the effect of varied penetration depth

- Deresolve a spectrum or enhance its resolution

- Interpolate an entire spectrum or series of spectra to another custom x-grid

- Attach chemical structure to the analytical spectrum

- Verify structure-spectra correspondence

- Review a list of characteristic fragments or functional groups possibly present in an unknown structure

- Link data from related techniques in a clear hierarchical system; active spectral data can be linked directly to a single data point or peak within a chromatogram, analytical curve, or another spectrum

- Generate a table of peaks automatically through the Auto or Peak by Peak picking modes

- Calculate peak areas, FWHH (full width at half-height), and asymmetry values where applicable

- Use the peak fit modeling capabilities to resolve overlapped spectral peaks as a sum of Gauss, Lorentz, Gauss+Lorentz, or asymmetric LogNormal functions

- Use SIMPLISMA to resolve and determine the pure component spectra of mixtures

Full List of Supported Formats

Vendor	Digital Format
Agilent Technologies	*.wav, *.uv
ASCII single, dual and multicolumn	*.txt; *.prn; *.csv; *.asc
Bruker	*.*
DeltaNu	*.spc
Dionex	Dionex Chromeleon †
Foss NIRSystems	*.da
JASCO Corporation	*.jws
JCAMP, JCAMP multispectra	*.dx; *.jdx
LabControl	*.uvd; *.irs
MATLAB DSO	*.mat †
Ocean Optics	*.*
PerkinElmer Instruments	*.sp
Shimadzu	*.irs
Thermo	*.spa; *.spg
Thermo Galactic	*.spc
Thermo Mattson	*.*
Varian	*.b*; *.d*
Waters Corporation	*.inf †

† Diode Array Detector (DAD) support for hyphenated data
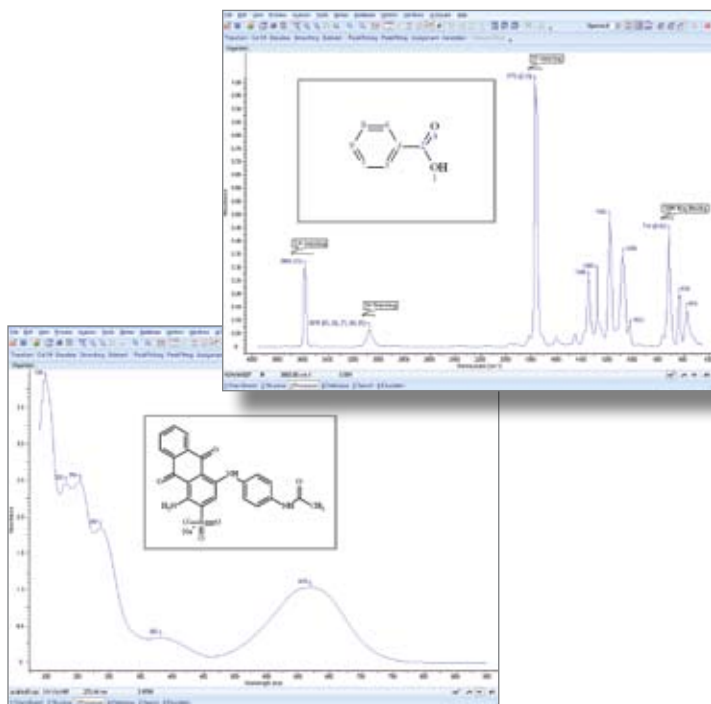
ACD/UV-IR Manager

Software for processing, interpretation, and storage of electronic,
vibrational, or rotational transition spectroscopy.

ACD/UV-IR Manager provides the capability to manipulate and manage optical spectra in a continuous range spanning the entire optical spectroscopy range from 1 cm^{-1} to 100,000 cm^{-1} (100 to 10,000,000 nm), encompassing the ultraviolet, visible, near-, middle-, far-infrared, and raman techniques.

ACD/UV-IR Manager is designed to handle absorption, reflectance, fluorescence, and phosphorescence spectra, as well as other more specialized techniques like circular dichroism (CD) and spectroscopic ellipsometry. By offering an extensive toolset to treat different optical spectroscopy techniques within a single interface, ACD/UV-IR Manager provides a general solution for all your optical spectroscopy needs.

Features

· Import, process, interpret, and store single-scan, multi-scans, and hyphenated spectral data from many different file formats
· Attach chemical structures to analytical spectra and assign peaks to chemical structural fragments; verify chemical structures with experimental spectra or review a list of characteristic fragments possibly present in an unknown structure
· Resolve the pure component spectra of mixtures with SIMPLISMA
· Automate repetitive processing tasks with macro commands that can be applied to a spectral series as well as to a single spectrum
· Create a fully searchable database of spectra and related information

Benefits

· Uniformly process data for greater speed and consistency
· Organize spectra and information from various techniques and easily find it again
· Correlate information from other analytical techniques by linking related data in a clear hierarchical system
· Confirm structure-to-spectrum correspondences with infrared or Raman verification algorithms
· Standardize and validate data with custom data entry forms
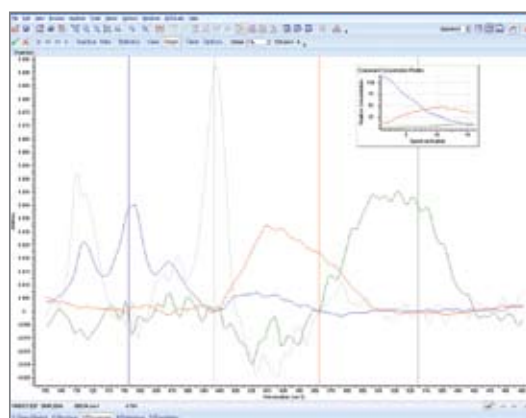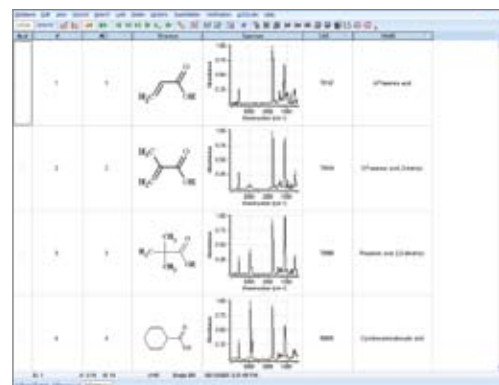
Resolve pure components from a series of spectral mixtures and obtain corresponding concentration profiles with SIMPLISMA (SIMPLe-to-use Interactive Self-Modeling Mixture Analysis). This highly interactive curve-resolving algorithm extracts individual components without requiring *a priori* knowledge of the mixture composition.

Full List of Processing Features

Processing Features

· Import data files from most major vendor file formats, including single-scan, multi-scan and hyphenated spectral data

· Load spectral data directly from an external application interface such as Waters, Empower or Dionex Chromeleon software

· Organize and compare multiple spectra in Tile, Full, or Overlay (series) modes

· Customize series display offsets for improved interpretation clarity and synchronize axes through multiple windows

· Specify x-axis orientation and define y-axis for spectral absorbance or reflectance to units of absorbance, transmittance, molar absorptivity, %reflectance, etc.

· Visualize contour maps and various associated 2D plots (integral, projection, slices, etc.) of hyphenated data with the ACD/Matrix feature

· Use fully interactive zooming features to focus on various spectral regions and automatically restrict spectral searches to these delimited x-axis regions

· Automatically save all the processing and analysis history (audit trail) with the full interpretation details.

· Automate routine processing tasks and manipulate sizable collections of files with macro commands

· Create professional, high-quality reports in PDF, ACD/ChemSketch, or other formats

· Obtain the mean spectrum for a spectral series with the Average Spectrum command

· Interactively suppress noise from your spectroscopic data with flexible FFT or Savitzky-Golay smoothing algorithms

· Subtract a scaled spectrum from another spectrum; automatically subtract a component signal from a mixture spectrum

· Interactively convert a spectrum or series into its 1st, 2nd, 3rd, or 4th order derivatives

· Perform ATR (attenuated total reflectance) correction to remove the effect of varied penetration depth

· Deresolve a spectrum or enhance its resolution

· Interpolate an entire spectrum or series of spectra to another custom x-grid

· Attach chemical structure to the analytical spectrum

· Verify structure-spectra correspondence

· Review a list of characteristic fragments or functional groups possibly present in an unknown structure

· Link data from related techniques in a clear hierarchical system; active spectral data can be linked directly to a single data point or peak within a chromatogram, analytical curve, or another spectrum

· Generate a Table of Peaks automatically through the Auto or Peak by Peak picking modes

· Calculate peak areas, FWHH (full width at half-height), and asymmetry values where applicable

· Use the peak fit modeling capabilities to resolve overlapped spectral peaks as a sum of Gauss, Lorentz, Gauss+Lorentz, or asymmetric LogNormal functions

· Use SIMPLISMA to resolve and determine the pure component spectra of mixtures

Databasing Features

· Update the database with the experimental spectra along with their chemical structures, analysis results (table of peaks, annotation) required by the user

· Replace user data fields systematically across an entire database list

· Select database records interactively in Tile or Table view

· Populate user databases with thousands of spectra in one step with the Group Macro batch processing tool

· Search by full spectrum or spectral regions, peaks, spectral parameters, chemical structure and substructure, formula, molecular weight, and user data text

· Merge spectral search results to a new database automatically and save the result to a specified location

· Perform spectral searches according to Euclidean distance, or squared or absolute difference methods

· Standardize data input to your corporate databases by means of the Data Forms Manager

· Store user-designed forms in the local forms library

Input/Output Formats

Vendor	Digital Format
Agilent Technologies	*.wav, *.uv
ASCII single, dual and multicolumn	*.*
Bruker	*.mat †
DeltaNu	*.spc
Dionex	Dionex Chromeleon †
Foss NIRSystems	*.da
JASCO Corporation	*.jws
JCAMP, JCAMP multispectra	*.txt; *.prn; *.csv; *.asc
LabControl	*.uvd; *.irs
MATLAB DSO	*.mat †
Ocean Optics	*.*
PerkinElmer Instruments	*.sp
Shimadzu	*.irs
Thermo Galactic	*.spc
Thermo Mattson	*.*
Thermo Nicolet	*.spa; *.spg
Varian	*.b*; *.d*
Waters Corporation	*.inf †

† Diode Array Detector (DAD) support for hyphenated data

ACD/IR & Raman Databases

Infrared and Raman Reference Spectra Databases for ACD/UV-IR Manager.

Fully searchable by a variety of structure, spectral and text-based queries.

Elsevier FT-Raman and FT-IR Polymer Database for ACD/Labs

This database includes pairs of IR and Raman spectra of 500 polymers and related materials.

For more information, visit:
www.acdlabs.com/libraries

NIST IR Database for ACD/Labs

This database contains gas-phase FT-IR absorption spectra and CAS registry numbers for over 5200 organic compounds compiled by both the National Institute of Standards and Technology (NIST) and the Environmental Protection Agency (EPA).

For more information, visit:
www.acdlabs.com/libraries

Coblentz Society Special Collections for ACD/Labs

The Coblentz Society Special Collection of over 9500 IR spectra were digitized by NIST.

For more information, visit:
www.acdlabs.com/libraries

FDM FT-IR Databases for ACD/Labs

FDM FT-IR Spectra of Polymers and Polymer Additives

This database references commonly used polymers such as cellulose, polyethylenes, nylons, and polymer additives including plasticizers, catalysts, stabilizers, etc.

For a complete list of materials, visit:
Polymer Chemical Name Index
www.acdlabs.com/ftir/polymers

FDM FT-IR Spectra of Surfactants

This spectral database contains detergents, wetting agents, emulsifiers, and surfactant materials formulated with oleates, palmitates, stearates, and many more. Many spectra include HLB (Hydrophilic Lipophilic Balance) values.

For a complete list of materials, visit:
Surfactant Chemical Name Index
www.acdlabs.com/ftir/surfactants

FDM FT-IR Spectra of Minerals and Inorganic Compounds

An expanded collection of over 130 spectra from minerals and over 120 spectra of inorganic materials.

For a complete list of materials and minerals, visit:
Minerals and Inorganic Chemical Name Index
www.acdlabs.com/ftir/minerals

FDM FT-IR Spectra of Organic Compounds

A high-quality collection of industrial chemical classes of spectra includes solvents, reagents, and organic chemicals. Chemical classes represented include acids, esters, alcohols, ketones, amides, and many more.

For a complete list of compounds, visit:
Organics Chemical Name Index
www.acdlabs.com/ftir/organic

FT-IR Spectra of Drugs / Canadian Forensic Spectra

These spectra represent both free and HCl-complexed forms of over-the-counter drugs, pharmaceuticals, controlled substances, intermediates, excipients, and fillers.

For a complete list of drugs, visit:
Drug Chemical Name Index
www.acdlabs.com/ftir/drugs

FDM Raman Databases for ACD/Labs

FDM Raman Spectra of Organic Compounds

This spectral database contains commonly utilized organic compounds generated from dispersive Raman spectroscopy between the range of 200 cm^{-1} to 2000 cm^{-1}. The collection includes small organic compounds, amino acids, dyes, OTCs, polymers, and some inorganic compounds.

For a complete list of compounds, visit:
Chemical Name Index
www.acdlabs.com/raman/organic

FDM Raman Spectra of Drugs

These spectra for drug substances found in the United States Pharmacopoeia (USP) provide a valuable reference across a wide range of scientific disciplines. The spectra were taken with a dispersive Raman instrument between 200 cm-1 to 2000 cm^{-1}.

For a complete list of drugs, visit:
Drug Chemical Name Index
www.acdlabs.com/raman/drugs

S.T. Japan FT-IR and Raman Databases for ACD/Labs

ATR/FTIR Aldrich-ICHEM Databases and Application Libraries

Over 25,000 high-quality attenuated total reflectance infrared spectra of organic and inorganic compounds, as well as some polymers and industrial chemical, are available in this comprehensive database compiled by ICHEM through samples from fine chemical manufacturers in Japan or by the Aldrich Chemical Company.

· ATR/FTIR Aldrich® Database (18,513 spectra)
· ATR/FTIR ICHEM Database (12,706 spectra)
· ATR/FTIR Aldrich-ICHEM Package Database
  (27,552 spectra)
    · ATR/FTIR Aldrich-ICHEM: Volume 1
    · ATR/FTIR Aldrich-ICHEM: Volume 2
    · ATR/FTIR Aldrich-ICHEM Database Supplement

For a full list of ATR/FTIR spectral databases and application-specific libraries, visit:
www.acdlabs.com/atr-ftir

SDBS FT-IR Spectra Databases and Application Libraries

The SDBS FT-IR database is one of the world's largest collections of over 50,000 spectra prepared from high-quality standards using KBr, Nujol, or Liquid Film and cross-validated by NMR and MS. The database includes polymers, plasticizers, and other commercial samples such as packaging materials.

· FTIR KBr Databases (21,140 spectra)
· FTIR KBr Databases (vol.1) (10,000 spectra)
· FTIR KBr Databases (vol.2) (11,140 spectra)
· FTIR Nujol Databases (20,571 spectra)
· FTIR Nujol Databases (vol.1) (10,000 spectra)
· FTIR Nujol Databases (vol.2) (10,571 spectra)
· FTIR SDBS Liquid Film Database (6718 spectra)

For a full list of FTIR spectra and application-specific libraries, visit:
www.acdlabs.com/ftirspectra

Raman ICHEM Database for ACD/Labs and Application Libraries

The Raman database is composed of 4000 spectra measured by the National Japanese Laboratory or obtained from the S.T. Japan ICHEM library. Like the SDBS FT-IR effort, the Raman databases were expertly obtained through rigorous methodology and use only the highest sample purity standards. The Raman database also includes polymers and commercial samples.

For a full list of Raman databases and application-specific libraries, visit:
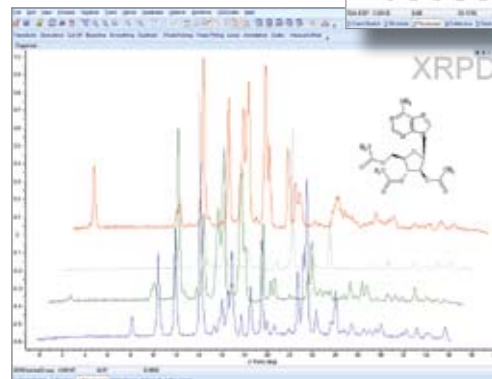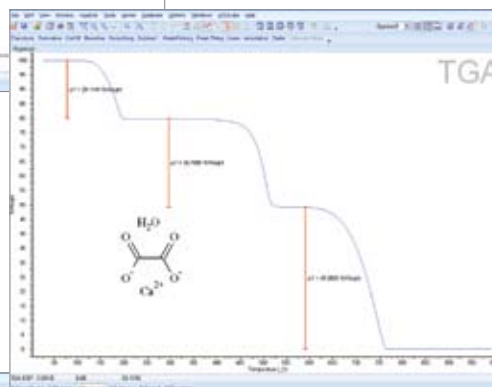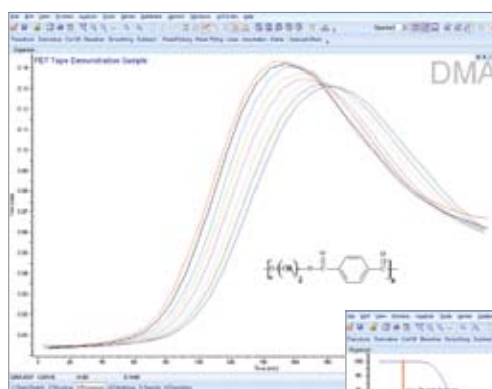www.acdlabs.com/ramanspectra

ACD/Curve Processor

Software for analytical curve processing, analysis, modeling, and visualization.

ACD/Curve Processor is a generic analysis tool designed to process and analyze experimental and calculated data generated from diverse analytical techniques. ACD/Curve Processor even handles data from hyphenated techniques such as TGA/FT-IR, kinetics followed by multi-channel detectors (e.g., DAD or FT-IR), and many other dual techniques.

Features

- Manage a wide range of analytical data, including:
  - EELS (Electron Energy Loss Spectra)
  - Thermal analysis (DSC, DTA, TGA)
  - DMA
  - Calorimetry
  - Titrimetric methods
  - Voltametric methods
  - X-ray methods (powder diffraction, fluorescence, and photoelectron)
  - ESR spectroscopy
  - Kinetics
- Advanced data modeling capabilities, including regression and curve-fitting
- Perform various x- and y-axis conversions and data manipulation
- Automate routine tasks with advanced macro processing tools

Benefits

- Work with data from many different techniques and data types
- Publish and present analysis and results quickly and easily

Full List of Processing Features

- Import data files from most major vendor file formats, including single-scan, multi-scan and hyphenated spectral data

- Review processing steps for your curve data with the History file (full audit trail)

- Attach chemical structures to your analytical curves

- Organize and compare multiple spectra in Tile, Full, or Overlay (series) modes

- Capture analytical curve interpretations from the analysts more fully through the use of multiple annotation layers

- Interactively zoom in on any part of the curve

- Create professional, high-quality reports in PDF and ACD/ChemSketch formats, and more

- Automate repetitious processing tasks with macro commands

- Perform various x- and y-axis conversions through standard mathematical operations with the transform tool

- Calculate derivatives from the 1st up to the 4th order derivative and overlay it above the curve for analysis, or permanently convert the curve to the given order

- Apply baseline correction to a curve or series of curves automatically

- Subtract a curve scaled by a given factor from another curve

- Interactively remove noise from the data with flexible FFT or Savitzky-Golay smoothing algorithms

- Standardize the apparent resolution of a curve to that of a lower or higher resolution instrument, or to produce uniformly spaced datasets

- Model spectrum or spectrum-like curves with a sum of analytic peak functions (Gauss, Lorentz, Gauss+Lorentz mix, LogNormal, Pearson VII)

- Pick the peaks and inflection points on the curve automatically or manually; these peak positions are automatically entered in a table of peaks

- Calculate peak areas and FWHH (full width at half-height)

- Create straight lines overlaying experimental curves manually or building linear regression on the selected part of the curve; move and rotate lines; find intersections of a pair of lines and the middle point of a line segment between two other lines

- Annotate curve regions, peaks, or characteristic points

- Fit the data with a straight line or polynomial, making use of a powerful and interactive regression tool

- Link data from related techniques in a clear hierarchical system

- Link live curve data to a single data point or peak within a chromatogram, spectrum, or another analytical curve

Full List of Supported Formats

Vendor	File Format
JCAMP	*.dx; *.jdx
ASCII single, dual and multi column	*.txt; *.prn; *.csv; *.asc
Galactic	*.spc
TA Instruments	*.*
PANalytical XRDML †	
Bruker DIFFRAC-AT	*.raw
Bruker DIFFRAC-PLUS	*.raw
Sirius Analytical Instruments	
STOE XRPD	*.raw

† Older Philips x-ray instrument data RD and UDF formats may be converted to the PANalytical XRDML formats with conversion software provided by PANalytical

ACD/Curve Manager

Software for analytical curve processing, modeling, databasing, and visualization.

Part of the SpecManager Family

ACD/Curve Manager is a generic analysis tool designed to process, analyze, and manage experimental and calculated data generated from diverse analytical techniques. It allows you to better organize and visualize any volume of data resulting from research efforts or high-throughput analytical analyses. ACD/Curve Manager even handles data from hyphenated techniques such as TGA/FT-IR, kinetics followed by multi-channel detectors (e.g., DAD or FT-IR), and many other dual techniques.

Features

· Manage a wide range of analytical data, including:
  · EELS (Electron Energy Loss Spectra)
  · Thermal analysis (DSC, DTA, TGA)
  · DMA
  · Calorimetry
  · Titrimetric methods
  · Voltametric methods
  · X-ray methods (powder diffraction, fluorescence, and photoelectron)
  · ESR spectroscopy
  · Kinetics
· Advanced data modeling capabilities, including regression and curve-fitting
· Perform various x- and y-axis conversions and data manipulation
· Automate routine tasks with advanced macro processing tools
· Create a fully searchable database of experimental data
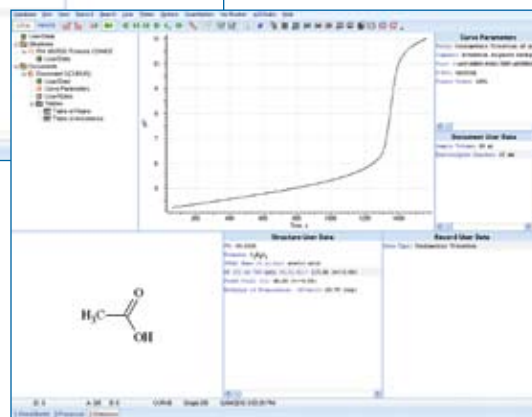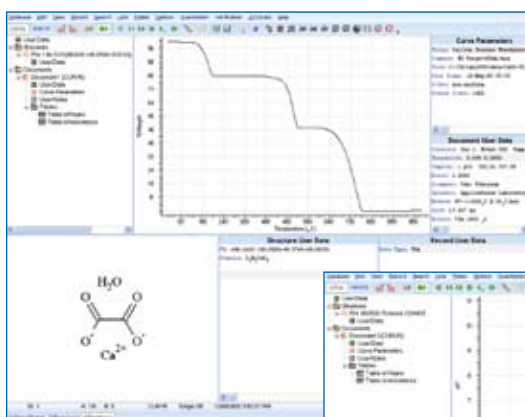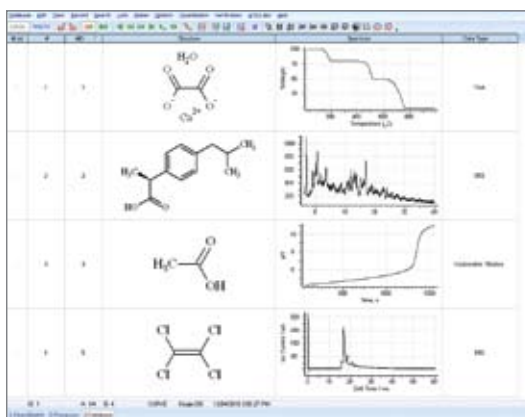
Benefits

· Organize and secure valuable experimental data
· Avoid redundant work by searching the database for existing information
· Bring together data from many different techniques and data types
· Publish and present analysis and results quickly and easily

Full List of Features

Processing Features

· Import data files from most major vendor file formats, including single-scan, multi-scan and hyphenated spectral data

· Review processing steps for your curve data with the History file (full audit trail)

· Attach chemical structures to your analytical curves

· Organize and compare multiple spectra in Tile, Full, or Overlay (series) modes

· Capture analytical curve interpretations from the analysts more fully through the use of multiple annotation layers

· Interactively zoom in on any part of the curve

· Create customized data entry dialog boxes with Data Forms Manager to facilitate data input

· Create professional, high-quality reports in PDF and ACD/ChemSketch formats, and more

· Automate repetitious processing tasks with macro commands

· Perform various x- and y-axis conversions through standard mathematical operations with the transform tool

· Calculate derivatives from the 1st up to the 4th order derivative and overlay it above the curve for analysis, or permanently convert the curve to the given order

· Apply baseline correction to a curve or series of curves automatically

· Subtract a curve scaled by a given factor from another curve

· Interactively remove noise from the data with flexible FFT or Savitzky-Golay smoothing algorithms

· Standardize the apparent resolution of a curve to that of a lower or higher resolution instrument, or to produce uniformly spaced datasets

· Model spectrum or spectrum-like curves with a sum of analytic peak functions (Gauss, Lorentz, Gauss+Lorentz mix, LogNormal, Pearson VII)

· Pick the peaks and inflection points on the curve automatically or manually; these peak positions are automatically entered in a table of peaks

· Calculate peak areas and FWHH (full width at half-height)

· Create straight lines overlaying experimental curves manually or building linear regression on the selected part of the curve; move and rotate lines; find intersections of a pair of lines and the middle point of a line segment between two other lines

· Annotate curve regions, peaks, or characteristic points

· Fit the data with a straight line or polynomial, making use of a powerful and interactive regression tool

· Link data from related techniques in a clear hierarchical system

· Link live curve data to a single data point or peak within a chromatogram, spectrum, or another analytical curve

Databasing Features

· Store experimental curves and associated data in a fully searchable database

· Search by parameter, chemical structure, structure similarity and substructure, peaks, formula, molecular weight, or user data

· Define up to 16,000 fully searchable user fields per curve record

· Data can be entered interactively, imported, or generated automatically by the software through a variety of ways

· Update the database of experimental curves with structures, tables of peaks, and any additional information required by the user

· Replace the user data field systematically across an entire database list

· Select database records interactively in Tile or Table view

· Store and display BMP, JPEG, GIF, and PNG image files with your analytical curve

· Standardize data input to your corporate databases by means of the Data Forms Manager

· Automate routine tasks with various pre-processing, macro automation, and well-plate navigation interfaces

Full List of Supported Formats

Vendor	File Format
JCAMP	*.dx; *.jdx
ASCII single, dual and multi column	*.txt; *.prn; *.csv; *.asc
Galactic	*.spc
TA Instruments	*.*
PANalytical XRDML†	
Bruker DIFFRAC-AT	*.raw
Bruker DIFFRAC-PLUS	*.raw
Sirius Analytical Instruments	
STOE XRPD	*.raw

† Older Philips x-Ray instrument data RD and UDF formats may be converted to the PANalytical XRDML formats with conversion software provided by PANalytical

ACD/ChromProcessor

Vendor-independent processing software for liquid and gas chromatography.

ACD/ChromProcessor enables convenient importing, processing, and reporting of chromatography data from various vendors in one interface.

ACD/ChromProcessor allows you to get out of the lab and to work up data on any computer, with tools to help visualize the results more easily.

Features

· Advanced functions for processing, including peak picking, noise removal, baseline correction, smoothing and many more
· Deconvolution algorithm for single chromatograms
· Enhanced data visualization and interpretation displays data as a Contour Map, Dual Plots, Map and Plots, and Aligned Plots
· Process or reprocess data away from the instrument
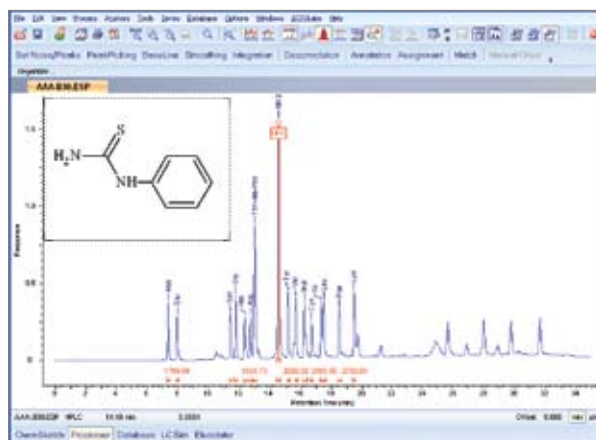
Benefits

· Bring together data from different instruments for standardized processing
· Reduce instrument downtime required for data processing
· Visualize data in a variety of ways to facilitate interpretation and comparison

Compare and Contrast Columns

ACD/Column Selector is a tool, developed in collaboration with Mel Euerby (HiChrom) and Patrik Petersson (Astra Zeneca) and available through ACD/ChemSketch, that allows you to search a knowledgebase of the most commonly used columns to locate those with the properties best-suited to the separation at hand. The Column Selector database contains information for 228 characterized columns, along with results for more than 4800 systematic experiments.[1]

Download ACD/Column Selector from our website.
www.acdlabs.com/download

[1] Euerby, MR; Petersson, P. "Chromatographic classification and comparison of commercially available reversed-phase liquid chromatographic columns using principal component analysis." *J. Chromatogr.* A, 994: 13−36, 2003.

Full List of Features

Processing

· Import chromatographic data from Waters Millennium[32], Empower, and Empower 2; Dionex Chromeleon 6, PerkinElmer TotalChrom 6.1, and Turbochrom 4, Agilent ChemStation; NetCDF (AIA); and ASCII formats

· Import LC/UV (PDA, DAD) records associated with chromatography data from Agilent ChemStation, Waters MassLynx, Waters Empower, and Dionex Chromeleon 6

· Perform peak picking, smoothing, baseline correction, peak integration, and peak deconvolution on single chromatograms

· Perform peak picking and baseline correction for LC/UV datasets

· Import or export structures from or to an SDfile; the files can contain compound names and retention times

· Manually assign chemical structures to peaks on your chromatogram

· Automatically assign chemical structures from an SDfile to labeled chromatogram peaks

· Attach multiple structures to a co-eluting peak

· Automate standard processing steps with a macro program

· Record all processing actions into the Audit Trail; transfer the Audit Trail to create a macro program to apply to subsequent datasets

· Display a series of chromatograms on a single plot with structures, peak data, and annotations

· Export chromatographic data to ACD/Labs Spectrum, NetCDF, and ASCII formats

Reporting

· Produce professional reports with one chromatogram or a series, structure assignments, method parameters, peak tables, annotations, and more

· Add a table to your reports that contains chemical structures and peak data

· Create custom templates with your company logo for consistency in the appearance of reports

· Save reports as Adobe PDF files

· Print reports according to built-in or customized templates

· Transfer reports to other applications such as Microsoft Word

Compatible Data Formats

Digital Format	Import	Export
ACD/Labs Spectrum (*.esp)	✓	✓
ASCII (*.txt; *.prn; *.csv; *.asc)	✓	✓
NetCDF (*.cdf, *.nc)	✓	✓
Agilent (HP) ChemStation (*.ms, *.ch, *.uv) [1,2]	✓	
Waters® Millennium® 32 [1]	✓	
Waters Empower™ and Empower 2 [1]	✓	
Dionex® Chromeleon® 6 [1]	✓	
PerkinElmer® TotalChrom™ [1]	✓	
PerkinElmer Turbochrom™ 4 (*.rax)	✓	
MATLAB® DSO (*.mat) [1]	✓	✓
Shimadzu Corporation (*.lcd)	✓	✓
Waters Corporation MassLynx (_functns.inf) [1]	✓	✓

[1] Support for hyphenated data involving Diode Array Detector (DAD)
[2] Valid license of MS software also required to import MS data

Free Resource for Chromatographers:

ACD/Labs Public Chromatography Applications Database contains over 6300 HPLC, GC, and CE separations from 19 column vendors. For more, visit:
www.acdlabs.com/chromappsdb_public

ACD/ChromManager

Advanced software for processing and managing HPLC, LC/UV (DAD or PDA), GC, and CE separations.

Part of the SpecManager Family

ACD/ChromManager is designed to process, database, and manage chromatographic separations, including HPLC, LC/UV (DAD or PDA), GC, and CE. Apply a complete array of processing tools to raw chromatographic data, assign structures to peaks, provide method information, then store chromatograms and methods in a database. Retrieve separation methods from your database through a variety of search options using method parameters, chemical structure, substructure, and structural similarity.

Features

· Process LC, GC, and hyphenated data*
  such as LC/UV, LC/MS, or LC/IR
· Create a database of chromatographic
  information, and search it by structure
  and text-based queries
· Attach chemical structures to peaks
· Apply multiple processing steps to
  batches of samples automatically
· Create customized data forms
  and reports
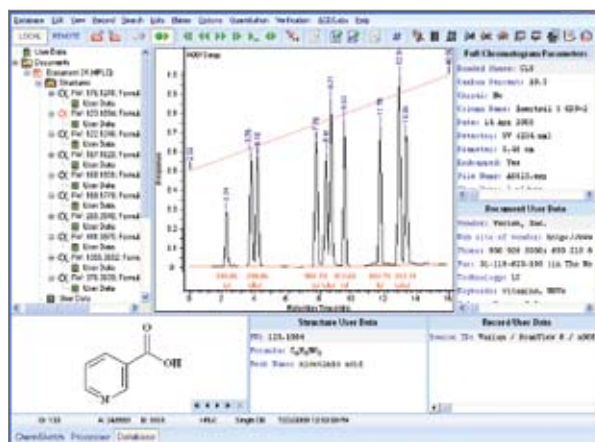
Benefits

· Collect data from different instruments
  and vendors in a central location and
  single data format
· Capture or enter chromatographic
  data systematically to ensure
  consistency and standardized
  treatment of data

Industry Application

Rapid Chiral Method Selection

The ACD/Chromatography Applications Database included with ACD/ChromManager contains experimental data for over 8100 real-life applications covering HPLC, GC, and CE methods. Each application is provided with instrument and column parameters, solvent and buffer information, chemical structure assignments, and reference sources. The database is fully searchable with ACD/ChromManager.

* Processing of LC/MS and LC/IR data requires additional
  ACD/SpecManager modules

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Chiral Applications Databases for ACD/ChromManager

ChirBase, ChirBase/GC, and ChirBase/CE for ACD/Labs are chiral applications databases that allow chromatographers to locate separation methods for similar compounds as a starting point for method development.

All three of the ChirBase databases can be searched by structure, structure similarity, and substructure similarity.

ChirBase/LC and ChirBase/GC can also be searched by a variety of experimental conditions and separation parameters. Complete method or analyte information is provided with each entry along with references.

ChirBase/LC for ACD/Labs contains method information for over 100,000 HPLC experiments, including data for 30,000 unique structures linked to over 1400 unique chiral selectors.

ChirBase/GC for ACD/Labs contains method information from over 24,000 experiments for more than 8000 unique structures.

ChirBase/CE for ACD/Labs contains information from over 8000 experiments for more than 2000 unique structures.

Full List of Features

Processing

· Import chromatographic data from Waters Millennium[32], Empower, and Empower 2; Dionex Chromeleon 6, PerkinElmer TotalChrom 6.1, and Turbochrom 4, Agilent ChemStation, NetCDF (AIA), and ASCII formats

· Import LC/UV (PDA, DAD) records associated with chromatography data from Agilent ChemStation, Waters MassLynx, Waters Empower, and Dionex Chromeleon 6

· Perform peak picking, smoothing, baseline correction, peak integration, and peak deconvolution on single chromatograms

· Perform peak picking and baseline correction for LC/UV datasets

· Import or export files from or to an SDfile; the files can contain compound names and retention times

· Manually assign chemical structures to peaks on your chromatogram

· Automatically assign chemical structures from an SDfile to labeled chromatogram peaks

· Attach multiple structures to a co-eluting peak

· Automate standard processing steps with a macro program

· Record all processing actions into the audit trail; transfer the audit trail to create a macro program to apply to subsequent data sets

· Display a series of chromatograms on a single plot with structures, peak data and annotations

· Export chromatographic data to ACD/Labs Spectrum, NetCDF, and ASCII formats

Reporting

· Produce professional reports with one chromatogram or a series, structure assignments, method parameters, peak tables, annotations, and more

· Add a table to your report that contains chemical structures and peak data

· Create custom templates with your company logo for consistency in the appearance of reports

· Save reports as Adobe PDF files

· Print reports according to built-in or customized templates

· Transfer reports to other applications such as Microsoft Word

Databasing

· Search databases by chromatographic parameters, peak information, method parameters, chemical structure, chemical substructure fragments, and user-defined data

· View database records separately, as a table, in tile view, or as a custom layout

· Search by structural similarity when retrieving stored chromatographic applications

· Search by "remembering" results of different searches and then intersecting, merging, or subtracting the result sets from each other

· Search through multiple databases simultaneously

· Apply passwords for viewing and modifying database records

Compatible Data Formats

Digital Format	Import	Export
ACD/Labs Spectrum (*.esp)	✓	✓
ASCII (*.txt; *.prn; *.csv; *.asc)	✓	✓
NetCDF (*.cdf, *.nc)	✓	✓
Agilent (HP) ChemStation (*.ms, *.ch, *.uv) [1,2]	✓	
Waters® Millennium® 32 [1]	✓	
Waters Empower™ and Empower 2 [1]	✓	
Dionex® Chromeleon® 6 [1]	✓	
PerkinElmer® TotalChrom™ [1]	✓	
PerkinElmer Turbochrom™ 4 (*.rax)	✓	
MATLAB® DSO (*.mat) [1]	✓	✓
Shimadzu Corporation (*.lcd)	✓	✓
Waters Corporation MassLynx (_functns.inf) [1]	✓	✓

[1] Support for hyphenated data involving Diode Array Detector (DAD)
[2] Valid license of MS software also required to import MS data

Analytical & Chemical Knowledge Management

ACD/Labs offers desktop and enterprise solutions to help manage the vast quantities of knowledge produced in R&D. Our software for chemical and analytical knowledge management provides a single unified interface for viewing data for various analytical techniques as well as a unified storage facility that is searchable by structure and spectral data. We also offer integration into existing knowledge management systems.

Table of Contents/Knowledge Management

ACD/SpecManager

Software for processing, interpreting, storing, retrieving, and reporting of data and spectra from multiple analytical techniques.

With ACD/SpecManager, create an analytical knowledgebase including spectra, chromatograms, and metadata from a variety of analytical techniques, including NMR, MS, UV-Vis, IR, Raman, chromatography, and more. Use technique-specific modules for analytical data processing, assimilating different types of chemical data from structure, spectra, and instrumental parameters. Then store experimental results in a fully searchable database that simplifies access and stimulates collaboration. View and further manipulate data from your own or commercially available databases, create reports, and much more.

ACD/SpecManager consists of several technique-specific modules for NMR, MS, UV-IR, chromatography, and other analytical techniques such as XRPD, kinetics, and titrimetry. Use the modules independently within ACD/SpecManager or in any combination to achieve efficient analytical knowledge management.

While ACD/SpecManager allows databases of proprietary experimental data to be built, searched, and viewed, several commercial databases for NMR, IR, Raman, and chromatography are also available for use with ACD/SpecManager.

Features

- Import data files from multiple analytical techniques and most vendor file formats
- Process data away from the instrument with technique-specific processing tools
- Create fully searchable databases of experimental spectra, chromatograms, and related data
- Automate routine processing tasks with macros
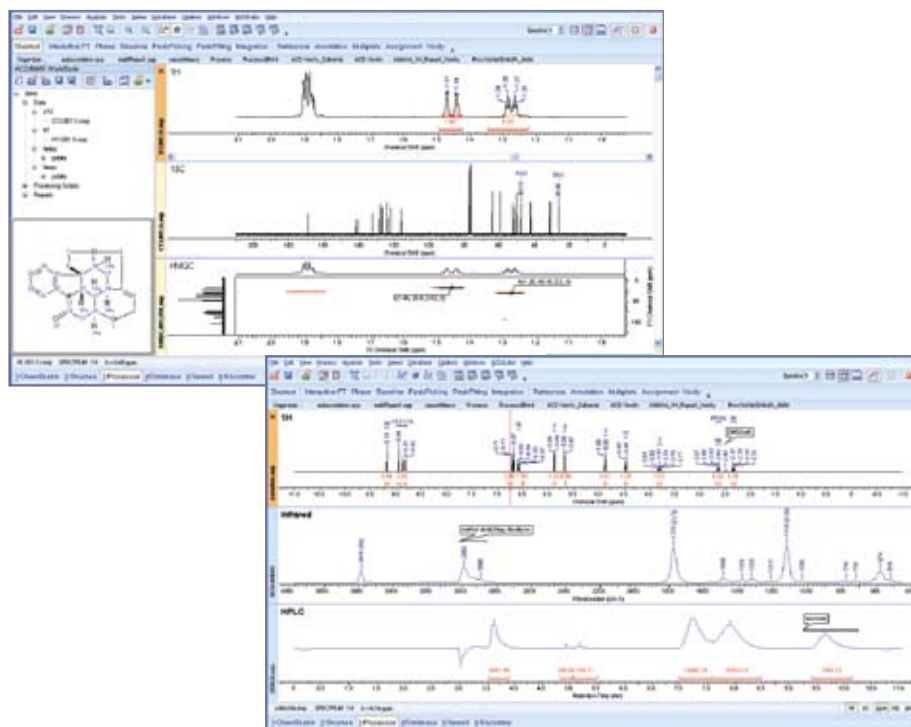
Benefits

- Visualize data in different ways to enhance understanding and interpretation
- Communicate results and make decisions more quickly
- Centralized repository to safeguard and leverage analytical knowledge
- Standardize treatment of data and ensure proper data entry
- Chemical structure intelligence highlights the relationship between structure and analytical data

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Full list of databasing features common to all ACD/SpecManager modules.

- Browse through multiple database records in Table view or Tile view and sort by different columns

- Store and manage experimental spectra and chromatograms in the same database

- Attach chemical structures (organic, inorganic, organometallic, generic (Markush), isotopically labeled, and polymers) to spectra, chromatograms, and curves

- Link individual spectral or chromatographic peaks to their related NMR, Mass, and IR spectra

- Establish up to 16,000 fully searchable user-defined fields per database record

- Find trends and correlations in the data with the Graph tool, which lets you plot a set of database values that you are interested in

- Store and display images (BMP, JPEG, GIF, PNG) directly in the database screen form

- Protect the database from being viewed or modified with two available password restricted levels

- Apply electronic signatures to spectra and database records

- Include hyperlinks to external pathnames, files, or URLs in any record user data fields:
  - Include links to a text file, Microsoft Word document, or Excel spreadsheet containing notes, plots, assay results, or reaction conditions

- Create links to spectral or plot files from third-party programs

- Establish links to image files such as well-plate or microscopy images

- Link to WAV and AVI files

- Insert links to other databases (e.g., an ACD/ChemFolder database)

- Merge databases together using appropriate duplication options and data entry controls

- Calculate certain chemical properties directly from your ACD/SpecManager database

- Search databases by a variety of structural, spectral, and text-based parameters:
  - Look for whole or partial analytical spectrum or curve regions
  - Perform peak searches according to exact positions or ranges and with various associated peak characteristics such as full width, half height, intensity, and multiplicity
  - Search multiple data fields simultaneously
  - Query multiple databases at the same time
  - Search by structure similarity (by the Tanimoto, Cosine, Dice, Hamming distance, and Euclidean distance algorithms), substructure, and Markush structure
  - Find different relevant tautomeric forms for a structure or target specific stereoisomers
  - Perform structure similarity searches
  - Manipulate sets of search results as lists (merge, intersect, subtract, and subtract+duplicate the two lists to restrict or expand search results)

- Manage high-throughput screening results
  - Load crystallization conditions, spectra, well plate images, and structural and property information
  - Directly support various microtitre results using 96 or 384 well-plates
  - Use the virtual plate mode to browse through the entire database content

- Automate time-consuming and repetitive tasks:
  - Use macros and other programming tools to help automatically import data and associate it with the appropriate spectrum, chromatogram, or curve
  - Remap data fields from third-party file formats and values in user data fields
  - Standardize data input with Database Forms Manager

- Create customizable reports including spectra, drawings, properties, tables, parameters, chemical structures, your company logo, and more; copy them to Microsoft Word or save as an Adobe PDF.

- Create report templates for one-click reporting
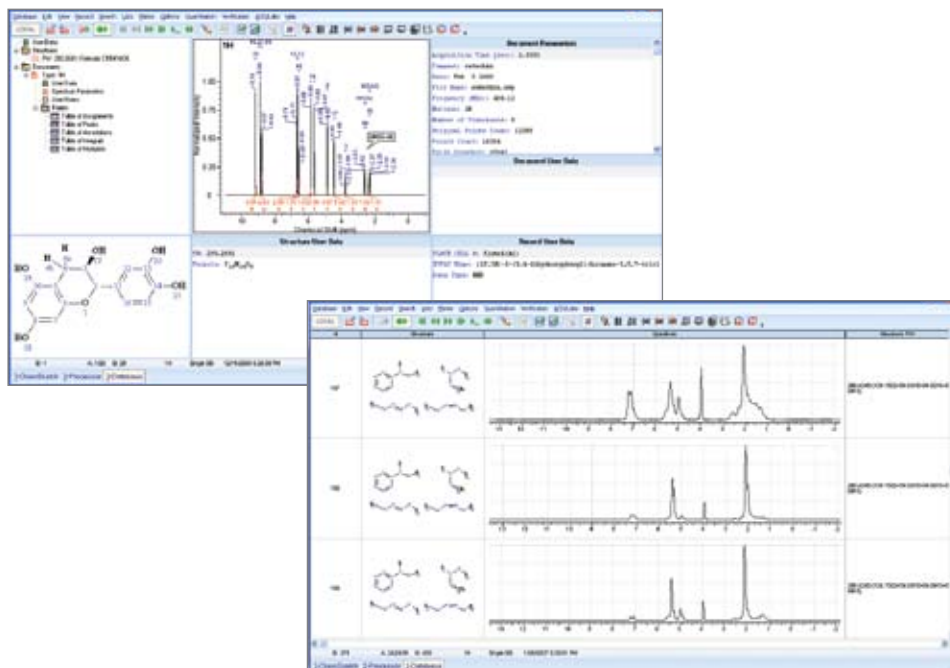
ACD/ChemFolder

Knowledge management software for chemical structures, properties, experimental data, and more.

ACD/ChemFolder allows you to create and manage databases containing thousands of chemical structures and data, reactions, reports, and other supporting material as a means of harmonizing chemical knowledge. ACD/ChemFolder is flexible and easily customized to meet the specific needs of individuals and groups.

ACD/ChemFolder can be configured with additional features such as the ability to predict physicochemical properties ($logD$, $logP$, pK_a, aqueous and DMSO solubility), predict ADME and Tox properties, generate systematic nomenclature based on chemical structure, and allow database information to be shared over the Internet.

Features

- Highly flexible search capabilities with an extensive range of basic and advanced search capabilities including structure similarity, sub-structure, and text-based parameters
- Create databases of up to 512,000 records, each with up to 16,000 data fields
- Advanced reaction mapping tools let you create multi-step reaction schema, biotransformation pathways, and metabolic pathways
- Customized forms for data entry
- Automatic calculation of predicted molecular properties for structures in database records and reaction schema

Benefits

- Capture and protect chemical data for more efficient research
- Visualize sets of interconnected chemical relationships more easily
- Reduce time spent searching for data
- Standardize data collection and reporting

Full List of Features

Database Records

· Create structure, reaction, and property databases of up to 512,000 records or a maximum 2 GB database file size

· Define up to 16,000 data fields for one record and easily browse them in a scrollable list

· Each record can be provided with:

   · Chemical structures, reactions, or graphics from ACD/ChemSketch

   · User- defined data fields

   · Free-form text notes

   · Complex multi-step reaction schemes (maps)

· Import data from many file formats

· Create calculated user data fields using mathematical and logical operations on data in other fields

· Include links (URL) to external documents

Data Entry and Manipulation

· Standardize data entry forms with mandatory fields, drop-down lists, or check-boxes set to your specifications

· Set criteria to validate data input on forms

· Merge, intersect, or compare your ACD/ChemFolder databases.

· Customize and extend the functionality of your database with the add-on organizer

· Manipulate sets of search results as lists that correspond to a subset of the database matching the search criteria

· Group and analyze your data using advanced graphic presentation and statistical analysis

Searching

General Search Features

· Search multiple data fields simultaneously

· Save complex search queries for applying the same search in other databases

· Store your search history and set search history files as macro buttons on the toolbar

· Use the audit trail feature (Search History) for complex searches; keeps information about performed searches and is used to perform similar searches in other ChemFolder databases

· Query multiple databases at the same time

Structure-based Searches

· Search by molecular structure, substructure, and Markush structure using query atoms and bonds

· Find different relevant tautomeric forms for a structure or target specific stereoisomers

· Search for reactions, subreactions, reactants, and products

· Limit structure searches to parent (reactants) or Metabolites (Products) compounds

· Perform structure similarity searches by the Tanimoto, Cosine, Dice, Hamming distance, and Euclidean distance algorithms

· Flexible stereo search options allow you to selectively search by configuration of chiral centers and double bonds

Non-structure Searches

· Easily find text or numerical values in user data fields or structural parameters

· Search by empirical chemical formula

· Search by specific formula weight or range

Reaction Mapping

· Manually or automatically create reaction maps for complex chemical processes and multi-step reactions

· Store single and multi-step chemical reactions (e.g., metabolic biotransformation data or mass fragmentation pathways)

· Define structures with special Markush fragments with mass or formula difference values

· Keep complete notes and information for the overall synthesis of each component in a single record

· Automatically calculate and store quantities of reactant, product, solvent, and catalyst

· Create lists of common solvents, catalysts, and reagents with their molecular formulae, formula weights, names, densities, and concentrations

· Highlight created, broken, and changed bonds in different colors

Reporting

· Print reports directly from the screen form, export to Adobe PDF, or create *.sk2 files

· Display a single record of reactions in a dedicated reaction table that facilitates reaction management manipulations. Calculate, add, and store synthesis data for each reaction component

· Browse through multiple database records in Table view and sort by columns to reveal hidden trends

· Scan through records in Tile view to highlight characteristic chemical structure information and selected names and properties

· Create custom data layouts for the database window to present only the information you need

· Create 2D barcodes containing structure information

View a complete list of supported formats on our website:
www.acdlabs.com/cfformats

Supported Formats for Import/Export

Format Name	File Extension	Input	Output
ACD/Labs ChemFolder Database file	*.cfd	✓	✓
ACD/Labs Database ID List File	*.lst	✓	✓
MDL SDfile	.sdf	✓	✓
MDL RDfile	*.rdf	✓	✓
MDL molfire	*.mol	✓	✓
MDL RXNfile	*.rxn	✓	✓
SMILES string	*.txt	✓	✓
ChemSketch drawing	*.sk2	✓	✓
Images	*.gif, *.tif, *.wmf, etc.	✓	✓
Tables	*.txt, *.sdf		✓

ACD/Labs Enterprise Software

ACD/Labs' enterprise solutions enable the automation of data analysis, reporting, storage, and the creation of searchable repositories of live laboratory data that can be viewed and accessed worldwide. Get access to the information generated in R&D through desktop software that provides full analysis, processing, and updating capabilities through web-based applications.

ACD/SpecManager Enterprise and ACD/ChemFolder Enterprise extend our desktop tools to diverse work groups in different departments or across geographic locations. Our enterprise-level solutions allow fast and flexible access to information, enabling truly effective collaborative research. Our server and desktop tools have scripting capabilities for pulling and manipulating data from other services that provide access via web services.

Features

- Industry-standard three-tier (client, server, and database) architecture[†]
- Supports Oracle and PostGreSQL databases[†]
- Web service interface for access to data stored in local databases, and capabilities to integrate with and retrieve information from ELN, LIMS, archives, and other external systems
- Ability to fully automate analytical data processing and analysis, database access, report generation, and other processes
- Security permissions for read/write access and administrative controls
- Flexible licensing to fit your needs, including single or multi-seats, floating licenses, or network

[†]ACD/ SpecManager DB currently offers two-tier database on Oracle platform only
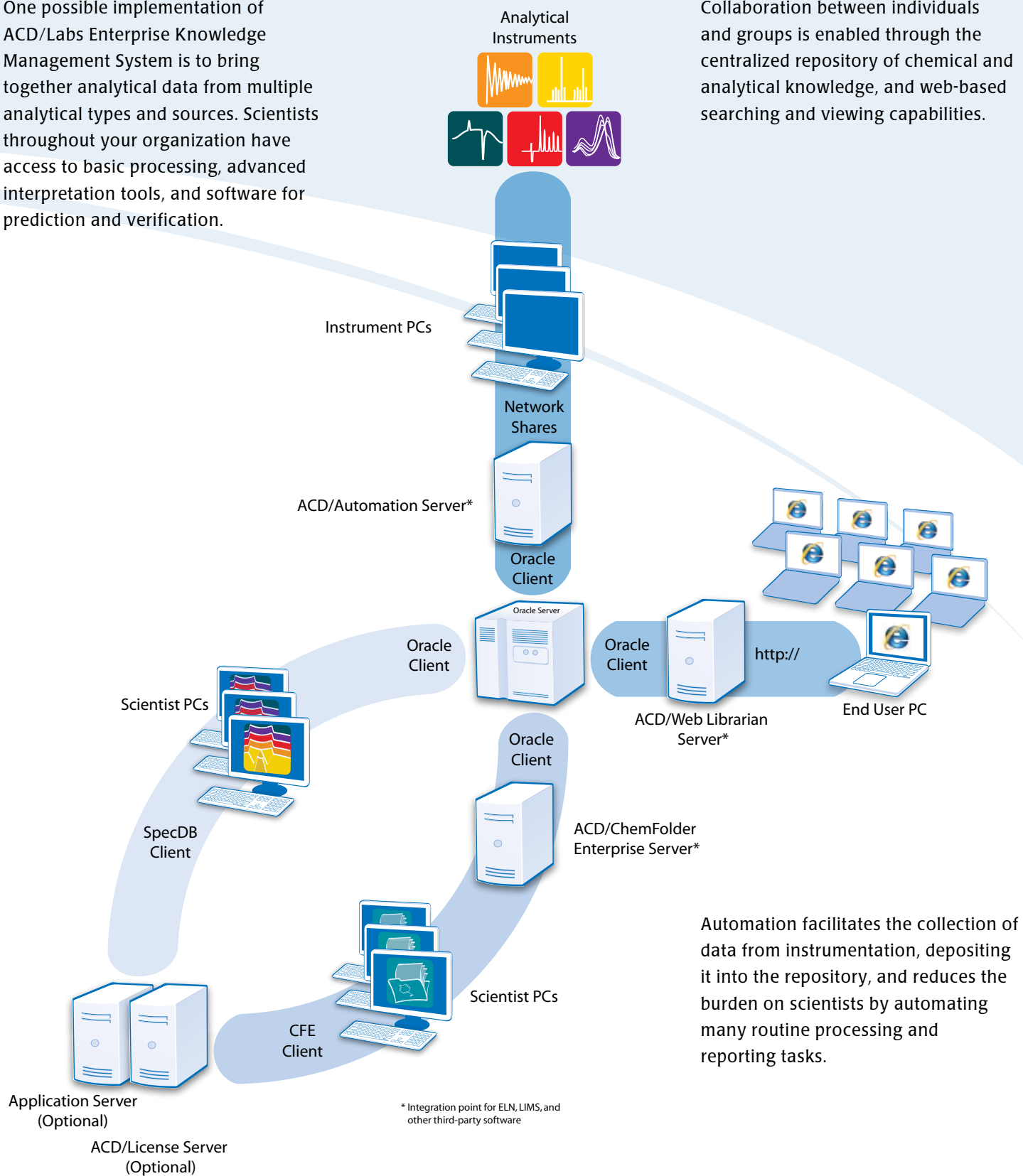
Benefits

- Connect multiple users locally or across geographic locations quickly and easily
- Standardize processes across your entire organization with data analysis and workflow automation
- Integrate with multiple external systems and provide a unified view of related data through the ACD/Labs interface
- Centralize knowledge management to promote better decision-making
- Retain and protect intellectual property

ACD/Labs Professional Services

Our Professional Services Team can assist or perform deployments of routine or custom installations, provide advanced technical training and support, and enable connection between various software platforms. Use their experience and expertise to get the most from your software.

One possible implementation of ACD/Labs Enterprise Knowledge Management System is to bring together analytical data from multiple analytical types and sources. Scientists throughout your organization have access to basic processing, advanced interpretation tools, and software for prediction and verification.

Collaboration between individuals and groups is enabled through the centralized repository of chemical and analytical knowledge, and web-based searching and viewing capabilities.

Analytical Instruments

Instrument PCs

Network Shares

ACD/Automation Server*

Oracle Client

Oracle Client

Oracle Server

Oracle Client

http://

ACD/Web Librarian Server*

End User PC

Scientist PCs

SpecDB Client

Oracle Client

ACD/ChemFolder Enterprise Server*

Scientist PCs

CFE Client

Application Server (Optional)

ACD/License Server (Optional)

Automation facilitates the collection of data from instrumentation, depositing it into the repository, and reduces the burden on scientists by automating many routine processing and reporting tasks.

* Integration point for ELN, LIMS, and other third-party software
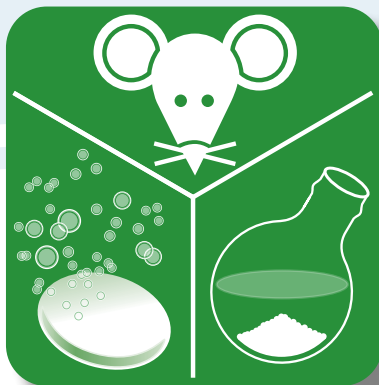
Physicochemical & ADMET Prediction

ACD/Labs' suite of predictors for PhysChem, ADME, and Tox provide a complete array of tools for the prediction of molecular physical properties from structure. The ability to easily train the models with in-house experimental data allows for the inclusion of novel chemical space in many modules. The value of predictions has also been extended to include a tool for property-based structure design.

Table of Contents/Physicochemical & ADMET Prediction
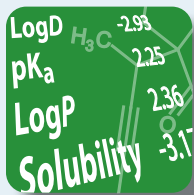
ACD/PhysChem Suite

Software for the fast and reliable prediction of physicochemical properties from chemical structure.

ACD/PhysChem Suite is a suite of comprehensive tools for the prediction of basic physicochemical properties. Predict pK_a, $\log P$, $\log D$, aqueous solubility, and an array of molecular properties in seconds, within one interface, and from chemical structure. Our fragment-based models offer unsurpassed accuracy and cover a good breadth of chemical space, giving you instant insight into the properties and behavior of your compounds.

Physicochemical and molecular properties available in ACD/PhysChem Suite:

Aqueous Solubility	Index of Refraction	pK_a	Freely Rotatable Bonds
Adsorption Coefficient (Koc)	$\log D$	Polar Surface Area	Molecular Weight
Boiling Point	$\log P$	Polarizability	Surface Tension
Bio-Concentration Factor	Molar Refractivity	Rule-of-5	Density
H-Bond Donors and Acceptors	Molar Volume	Sigma	Parachor

Features

· Predict $\log P$, $\log D$, pK_a, aqueous solubility, and boiling point from structure; results are provided with calculation error or reliability index
· Consider the pH dependence of aqueous solubility and lipophilicity ($\log D$) across the full pH range (pH 0−14)
· Graphically view and identify structures of ionic species and their distribution in aqueous solubility, $\log D$, and pK_a profiles

· Train the models with your own experimental data to extend chemical space coverage (the applicability domain) and improve prediction accuracy for proprietary compounds
· Search the highly curated reference databases to quickly look up publicly available data around the chemical space of interest
· Run calculations for thousands of compounds quickly and efficiently with our PhysChem Batch software

Benefits

· Anticipate the characteristics of your compounds prior to acquiring or synthesizing samples
· Take a realistic look at the behavior of electrolytes and non-electrolytes
· Save time on in-house model development by training prediction algorithms
· Enhance in-house development of more complex parameters by plugging in ACD/Labs predictions

Application Note

The Importance of Training Predictors

Poster

The Rule-of-5 Revisited−Applying Log*D* in Place of Log*P* in Drug-Likeness Filters
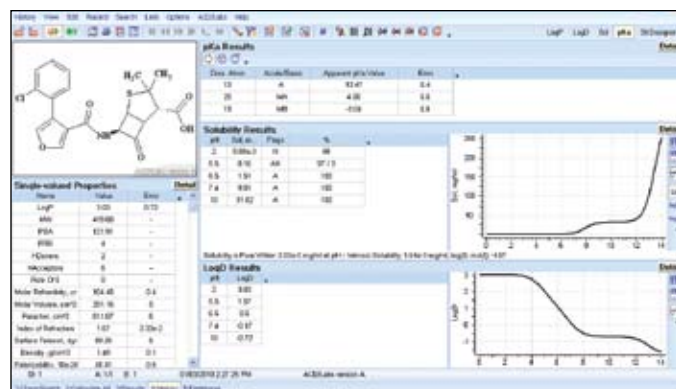
Full List of Features

pK$_a$

· Calculate accurate acid-base ionization constants (pKa values) under 25°C and zero ionic strength in aqueous solutions for organic structures; the specific constants calculated are:

  · Apparent
  · Approximate
  · Exact microscopic
  · Single

· Calculations are provided with 95% confidence intervals and a detailed report on how it has been carried out (including Hammett-type equation(s), substituent constants, and literature references where available or with Reliability Index (RI) of the calculation and display of the five most similar structures for each ionizable site in the training set)

· View tabular/graphical representations of net charge vs. pH with a breakdown of % ionic species at any given pH

· Train the model with experimental values to improve predictions for proprietary chemical space

Log*P*

· Calculate the octanol-water partition coefficient for a wide range of neutral compounds under standard conditions at 25 °C

· Calculations are provided with 95% confidence intervals or reliability Index (RI)

· Review bioconcentration factor (BCF) and the adsorption coefficient (Koc)

· Evaluate Rule-of-5 compliance

· Train the model with experimental values to improve predictions for proprietary chemical space

Log*D*

· Calculate the distribution coefficient (log*D*) at any pH (pH 0−14) with or without ion-pair partitioning

· View results in tabular/graphical form with % ionic species at given pH values

· Calculate the % dominant form in aqueous and organic phases

· Calculate BCF and Koc at any given pH

· Train the model with experimental values to improve predictions for proprietary chemical space

Aqueous Solubility

· Calculate pH dependent aqueous solubility, intrinsic solubility, and solubility of the chemical dissolved in pure (unbuffered) water at 25°C and zero ionic strength

· View results in tabular/graphical form as a function of pH with references to experimental research

· View tabular/graphical representation of % ionic species at given pH values

· View and select appropriate tautomeric forms

· Include melting point data for solids

· Train the model with experimental values to improve predictions for proprietary chemical space

Boiling Point

· Predict the vapor pressure of organic compounds as a function of temperature, boiling point temperature, or pressure

· Estimate boiling point at atmospheric pressure

· Calculate enthalpy of vaporization at 760 mmHg

· Calculate flash point

Sigma

· Calculate the Hammett electronic substituent constant (sigma) for selected fragments of a molecule or substituents

· Calculate only inductive and resonance sigma constants (option)

Batch

· Batch versions of all physicochemical and molecular properties in ACD/PhysChem Suite are available for those working with thousands or tens of thousands of compounds at a time with minimal operator intervention

· Available for Microsoft Windows and Linux platforms, and runs from the Windows command line

· No inherent limit to the number of database records that can be handled

· Train the models with experimental data to improve predictions for proprietary chemical space

· Plug ACD/PhysChem Batch into Pipeline Pilot
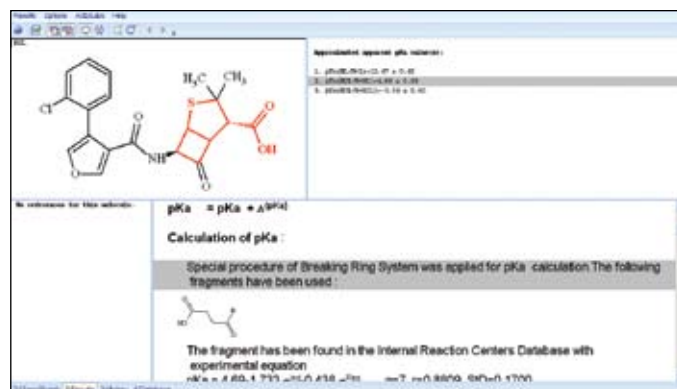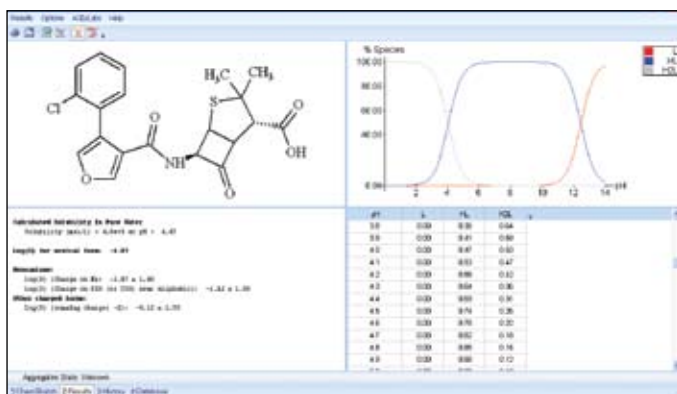
ACD/Structure Design Suite

Software for the optimization of chemical structures with regard to physicochemical property endpoints.

ACD/Structure Design Suite (SDS) is a tool to help chemists optimize the physicochemical properties of their compounds. The software suggests alternative substituents (at one or more sites on the molecule) to drive the property of choice in the desired direction. SDS will help you investigate diverse substituents to adjust aqueous solubility, lipophilicity (log$P$ or log$D$), or change the ionization profile (pK_a) of your molecule. Automatic enumeration of results provides a list of alternative structures for you to consider. You can also calculate the full property profile for enumerated structures and analyze results to make more informed decisions about future synthetic endeavors.

Features

· Use the optimization wizard to guide you through SDS's workflow
· Consider an array of possibilities for structure optimization using the diverse substituent database, which is comprised of approximately 30,000 neutral, acidic, basic, and heterocyclic groups
· Enumerate structures with single/ multiple substitutions
· Import up to 1000 compounds for fast and accurate prediction of log$P$, log$D$, aqueous solubility, and pK_a, along with an array of molecular properties (including density, molar volume, Rule-of-5 violations, and more)
· Analyze results using graphing tools to select structures with the most balanced property profile
· Train prediction models with in-house data to accommodate novel chemistry

Benefits

· Identify novel substituents without significantly changing topology, electronics, or other desired characteristics of the lead
· Explore property-based structure optimization
· Plan future synthetic work around well-balanced analogs, and molecules that comply with property restrictions
· Ease literature searches in new chemical space with fast and accurate naming of new suggested analogs

Application Note

Structural Optimization of Leads to Improve ADME Properties
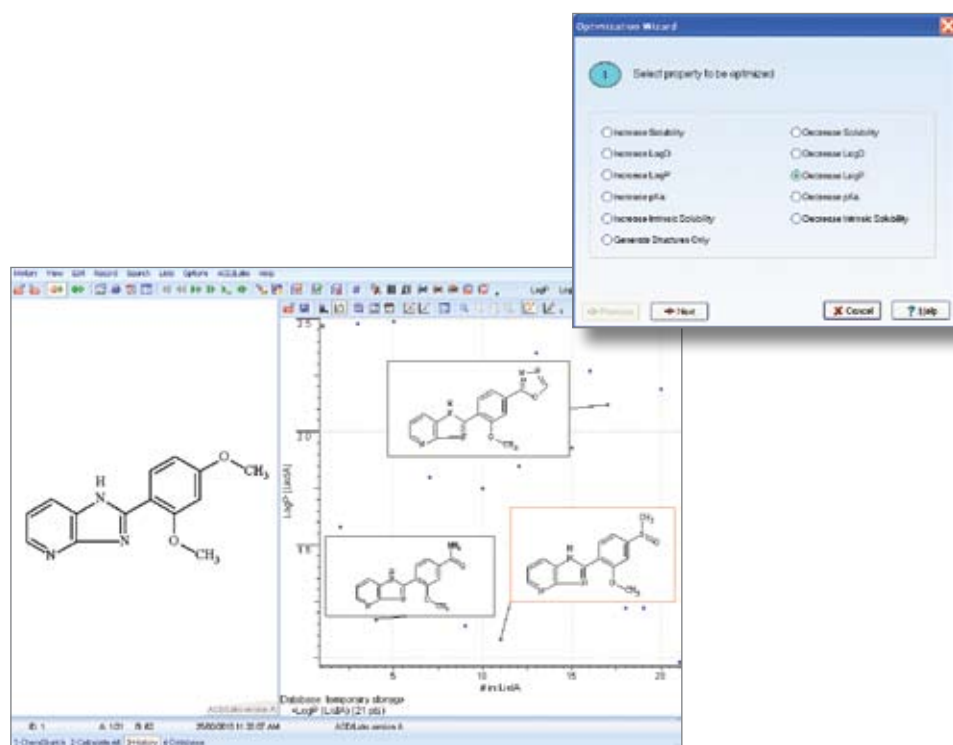
ACD/Structure Design Suite Workflow
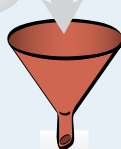
29,520 * **Substituents**

Filter substituent database

Accelerate property calculation and evaluation steps, for example, by:
- Formula weight (FW)
- Structural similarity to the substituent to be modified
- Substructure
- Ring type (aromatic, heterocyclic)

*The workflow detailed here illustrates the database for ACD/Structure Design Suite v12.0

< 2000 Substituents

Submit your structure and select the PhysChem property for optimization
- Decrease solubility
- Increase solubility
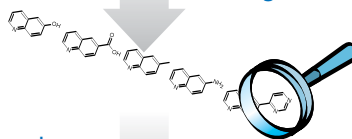- Decrease ionization

Lead Compound

Select fragment/substituent to be modified and follow the optimization wizard prompts
- Select substituent type
- Add further restrictions to focus results (e.g., restrict FW of final analogs)
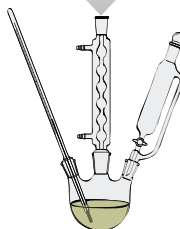
Auto-generate analog structures

Evaluate analogs and choose the best candidates for synthesis

Incorporate your own models and measurements

Expert users can apply their own models and algorithms to calculate topological descriptors, physicochemical properties, or other parameters using scripting tools. These models can then be incorporated into the optimization process.

Employ our training tools to extend the accuracy of prediction of log$P$, log$D$, pK$_a$, and solubility to their proprietary chemistry using in-house experimental data.

Create your own database of substituents for use with the application.

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ACD/DMSO Solubility

Software for the prediction of solubility in DMSO solution.

ACD/DMSO Solubility predicts the probability that an organic compound will be soluble in DMSO solution.

Features

- Predict solubility in DMSO from structure at greater or less than 20 mM concentration, with reliability index
- View up to five of the most similar structures in the training set
- Batch module facilitates the calculation of large compound collections
- Train the model with your own experimental data to extend chemical space coverage (the applicability domain) and improve prediction accuracy for proprietary compounds

Benefits

- Identify the compounds that may cause erratic results in compound screening and biological assays
- Eliminate compounds from your project that will not allow the use of standard testing protocols
- Add your data to the model to easily build a customized model based on your chemical space

Import/Export

- Import SDfile or SMILES
- Export to SDfile, or copy and paste into Microsoft Excel

Training & Reference Databases

- The internal training set of ACD/DMSO Solubility contains data from more than 15,500 compounds
- The software also provides a reference database of more than 22,200 compounds

ACD/ADME Suite

Software for the prediction of ADME properties from chemical structure.

ACD/ADME Suite is a collection of software modules that provide predictions relating to the pharmacokinetic profiling of compounds, specifically their absorption, distribution, metabolism, and excretion properties. Predictions are based on a combination of expert knowledge, scientific intuition, and QSAR modeling.

Features

· From simple structure input (name, 2D structure, or SMILES string), obtain predicted values with a reliability index
· See a display of up to five similar compounds from within the training set with literature data and references
· Perform calculations of large compound collections with batch modules
· Access the related database in certain modules that are fully searchable by a variety of parameters
· Train select models with in-house data to better reflect proprietary chemical space and improve prediction accuracy

Customize ADME Suite to suit your needs from the following prediction modules:

P-gp Specificity Trainable	Oral Bioavailability	P450 Inhibitors Trainable	P450 Regioselectivity
Oral Bioavailability	Passive Absorption	Blood-Brain Barrier Permeation	Absolv
Distribution Trainable	Maximum Recommended Daily Dose	PK Explorer	

Benefits

· Reduce attrition rates with early *in silico* ADME profiling
· Focus research efforts on molecules that meet property requirements
· Investigate the influence of changing interrelated properties to gain a deeper understanding of your compounds
· Reduce the need for expensive, labor-intensive assays

Application Note

The Importance of Training Predictors

Full List of Features

P-gp Specificity
· Knowledge-based models classify compounds as P-gp substrates or non-substrates, as well as P-gp inhibitors or non-inhibitors; classification is made according to a set of rules based on the compound's physicochemical properties (ionization, molecular size), biological class, etc.
· The statistical models, employing a fragment-based approach, calculate probability for a compound to be a P-gp substrate or inhibitor
· A reference database of over 2300 compounds is provided with P-gp specificity data and literature references

P450 Inhibitors
· Calculates the probability of a compound being an inhibitor of the five major drug metabolizing enzymes—CYP3A4, CYP2D6, CYP2C9, CYP2C19, and CYP1A2 (general inhibition K_i < 50 μM and specific inhibition < 10 μM)
· Displays experimental values for similar compounds for each isoform in the database
· Trainable module

P450 Substrates
· Calculates the probability of a compound being a substrate of the five major drug metabolizing enzymes—CYP3A4, CYP2D6, CYP2C9, CYP2C19, and CYP1A2 (K_i ≤ 50μM)
· Displays experimental values for similar compounds for each isoform in the database
· Trainable module

P450 Regioselectivity
· Predicts sites susceptible to metabolism by human liver microsomes on a compound
· Predicts sites likely to be metabolized by each of the five major isoforms of CYP450—CYP3A4, CYP2D6, CYP2C9, CYP2C19, and CYP1A2
· Graphically highlights metabolic hotspots
· Proposes associated biotransformation reactions
· Displays experimental values for similar compounds in the database

Oral Bioavailability
· Compounds are evaluated accounting for the influence of solubility, acid stability, passive absorption, first pass metabolism, P-gp efflux, and active transport. Results are given in a simple traffic-lights imitation (red=problematic, amber=suspect, green=acceptable)

· A searchable reference database is provided with oral bioavailability data for over 700 compounds

Passive Absorption
· Predicts the limiting effects of lipophilicity and ionization constant on the following absorption-related properties:
   · Maximum achievable human intestinal absorption (HIA)
   · Jejunum permeability
   · Caco-2 permeability
   · Absorption rate
· Estimates relative contributions of different transport routes for %HIA and Caco-2 permeability predictions
· User-defined data can be added to improve prediction accuracy for proprietary chemical space (e.g., experimental log$P$ and pK_a data can be used to improve prediction of intestinal permeation rates) experimental conditions (pH, stirring rate); can be defined in the case of Caco-2 permeability prediction
· A fully searchable absorption database is provided with experimental data and literature references

Blood Brain Barrier Permeation
· Provides reliable and easily interpreted predictions of passive BBB permeation rate (expressed as LogPS constants)
· Calculates steady-state distribution ratio between brain tissue and plasma (LogBB) and unbound (i.e., pharmacologically active) fraction of drug in brain tissue
· Provides a unified interface for the evaluation of various parameters related to drug transfer across BBB and gives a qualitative estimate of whether brain uptake of the analyzed compound is sufficient for CNS activity
· User-defined data (e.g., experimental log$P$ and pK_a data) can be entered to improve prediction accuracy for proprietary chemical space
· Values of the main physicochemical determinants (log$P$, pK_a, hydrogen bonding, molecular size) may also be altered to simulate the influence of these properties on BBB transport potential
· Special alerts are provided for compounds likely to undergo BBB transport by mechanisms other than passive diffusion

Absolv
· Absolv calculates solvation-associated properties from Abraham-type equations and predicts calculation parameters necessary for these calculations:
   · H-bonding acidity and basicity (A, B, and BO)
   · Partitioning coefficient between gaseous phase and hexadecane (L)
   · Polarity/polarizability (S)
   · Excessive molar refraction (E)
   · McGowan volume (V)
· Individual atom contributions are color-mapped onto molecules for visual display
· Various solvent-solvent or gas-solvent partition coefficients can be calculated from predefined Abraham-type equations or custom equations using Abraham solvation parameters
· An extensive reference database of over 5000 compounds is provided, with referenced literature values of Abraham solvation parameters

Distribution
· Predictions are provided for the following:
   · Plasma protein bound fraction - trainable
   · Equilibrium binding constant to human serum albumin (logK_a^{HSA}) - trainable
   · Apparent volume of distribution for a compound dissolved in blood plasma (Vd)
   · Predictions of the extent of plasma protein binding and logK_a^{HSA} constants are supported by reliability estimation (calculated Reliability Index values)
· Binding properties are derived from automatic calculation of underlying physicochemical properties (e.g., lipophilicity, ionization, and fragmental descriptors a brief, general description of the compound's likely binding behavior in plasma is provided

PK Explorer
· Explore the interdependence of oral bioavailability, drug plasma levels, and dose
· Alter the values of key physicochemical determinants (log$P$, pK_a) and derived parameters (absorption and elimination rates) to investigate their effect on pharmacokinetics of the drug; the effect of first-pass metabolism may be also included in the simulation
· Simulate the drug-plasma concentration vs. time curve

ACD/Tox Suite

Software for the prediction of basic toxicity endpoints from chemical structure.

ACD/Tox Suite is a collection of software modules that predict probabilities for basic toxicity endpoints. Predictions are made from chemical structure and based upon large validated databases and QSAR models along with expert knowledge of organic chemistry and toxicology.
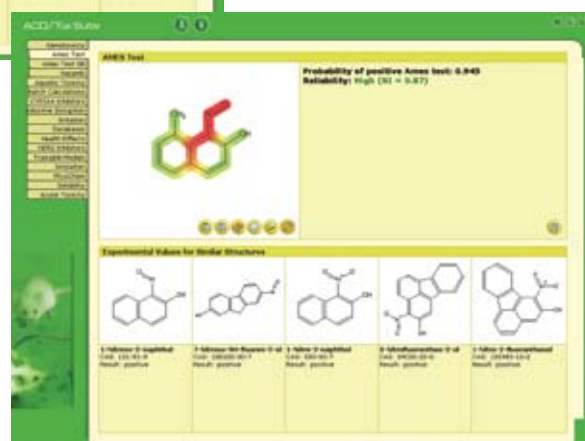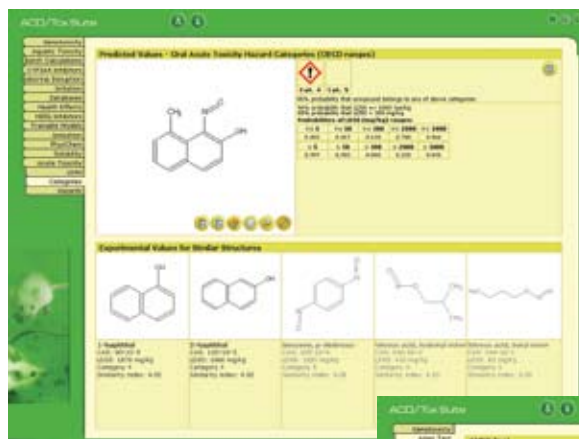
Features

· From simple structure input (name, 2D structure, or SMILES string), obtain predicted values with a reliability index
· See a display of up to five similar compounds from within the training set with literature data and references
· Perform calculations of large compound collections with batch modules
· Access the related database in certain modules that are fully searchable by a variety of parameters
· Train select models with in-house data to better reflect proprietary chemical space and improve prediction accuracy

Benefits

· Reduce attrition rates with early *in silico* toxicity screening
· Provide timely information to direct new compound synthesis
· Focus animal testing requirements
· Gain a clearer understanding of the toxicity profile of your compounds

Customize Tox Suite to suit your needs from the following prediction modules:

hERG Inhibition Trainable	P450 Inhibitors Trainable	Genotoxicity Trainable	Acute Toxicity (Rodent LD$_{50}$)
Aquatic Toxicity	Health Effects	Irritation	Endocrine System Disruption

Full List of Features

hERG Inhibition
· Predicts the probability of hERG channel inhibition at clinically relevant concentrations ($IC_{50} < 10 \mu M$)
· Estimates the reliability of prediction and displays experimental values for similar compounds in the database
· Trainable with data from in-house protocols

P450 Inhibition
· Calculates the probability of a compound being an inhibitor of several cytochrome P450 isoforms (3A4, 2D6, 2C9, 2C19, 1A2) with $IC_{50} < 50 \mu M$ and $IC_{50} < 10 \mu M$
· Estimates the reliability of predictions and displays experimental values for similar compounds in the database
· Trainable with in-house experimental data

Genotoxicity
· Calculates the probability of a positive Ames test
· Visually identifies structural fragments/substructures that are known to be involved in genotoxic activity; provides a visual display of the distribution of experimental data for compounds possessing selected hazardous fragments in various bacterial strains; displays experimental confirmation of observed effects with or without metabolic activation
· Provides a fully searchable Ames test database with critically evaluated and standardized experimental genotoxicity data for approximately 5500 compounds
· Trainable with in-house experimental data

Acute Toxicity (Rodent LD_{50})
· Predicts potential toxicity (LD_{50}) in two species (mouse and rat) for various administration routes (intraperitoneal, intravenous, subcutaneous, and oral administrations)
· Predictions are based on a combination of expert knowledge of various basal and extra-cellular effects (e.g., inhibition of cholinesterase and ATP synthesis, CNS and PNS disruption), and C-SAR/QSAR analysis of over 100,000 compounds
· Predictions are provided with reliability estimations (reliability index)
· Hazardous fragments (toxicophores) are visually identified on the molecule structure
· Compounds are classified into one of five toxicity categories (as defined by the OECD) for guidance in labeling

Aquatic Toxicity
· This module provides calculated LC_{50} values (mg/L) for fathead minnows (Pimephales promelas) and water fleas (Daphnia magna) with reliability indices for predictions

Health Effects
· Calculates the probability of a compound to cause organ-specific health effects
· Structural features contributing to adverse health effects are identified on the molecule with highlighting and color mapping (red=associated with toxic action, green=unrelated to health effects under investigation)

Irritation
· Calculates the probability for a chemical to cause moderate to severe irritation to the eye and skin of a rabbit at a standard dose (100 mg and 500 mg as per standard Draize test)
· Applicable rules by which the compound has been identified as an irritant are provided, along with highlighting of corresponding structural fragments

Endocrine System Disruption
· Compounds are classified into one of three classes (strong binding, weak binding, or no binding) for relative binding affinity to the ER
· Probabilities of overall binding combining specific and non-specific ($\log RBA > -3$) and strong binding ($\log RBA > 0$) are provided
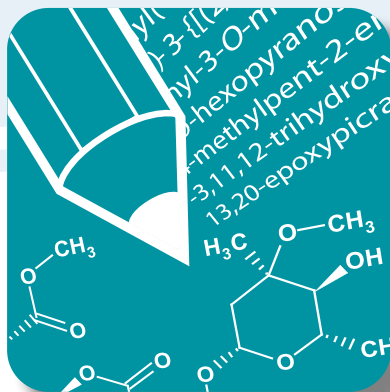
Chemical Drawing & Nomenclature

ACD/Labs' chemical structure drawing and nomenclature tools offer advanced features and unparalleled accuracy in representing virtually any molecule graphically or according to a variety of nomenclature conventions. ACD/ChemSketch and ACD/Name are used by professionals around the world for research, education, publication, and securing intellectual property rights.

Table of Contents/Chemical Drawing & Nomenclature
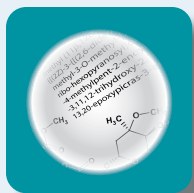
ACD/Name

Generate chemical nomenclature from structure.

ACD/Name generates chemical names according to IUPAC and CAS Index rules, converts names back to structures, and can easily handle challenging areas of nomenclature, such as biological molecules, organometallics, and polymers. Derivative rule reports and links back to the relevant nomenclature recommendations permit a greater insight and understanding of the nomenclature process and the generated name.

ACD/Name Chemist Version is also available. Designed for synthetic chemists, it provides names according to standard IUPAC rules and offers structure-to-name functionality.

Features

· Generate nomenclature for chemical structures from IUPAC and CAS Index rules
· Generate chemical structures from systematic names
· Generate InChI and SMILES strings
· Obtain derivative rules reports and view IUPAC recommendations for each name
· Generate single names or batches for libraries

Benefits

· Reliable and accurate to ensure high-quality names for publications, presentations, and patenting
· Quickly generate names for a single compound in a matter of seconds
· Gain a deeper understanding into how nomenclature is derived for your compounds

Multilingual Add-On

While ACD/Name already provides IUPAC rules in English, German and French, the multilingual add-on allows name generation in seven additional languages:

    Danish
    Dutch
    Italian
    Finnish
    Portuguese
    Spanish
    Swedish

Chemical Nomenclature Service

For particularly challenging nomenclature problems, ACD/Labs experts are available to provide systematic names for individual structures for a fee.

"...the quality of names that are generated from ACD/Name is second to none..."

Prof. G. A. Eller,
University of Vienna

Full List of Features

Structure to Name

- Generate accurate systematic names according to IUPAC recommendations and CAS Index rules
- Generate chemically accurate structures from chemical names with the Name-to-Structure module
- Assign stereodescriptors and numbering to atoms, and review stereo protocol that displays a hierarchical graph created for each atom with a stereodescriptor
- Review the full text of basic IUPAC nomenclature recommendations with examples
- Dynamically display for easy manual examination the nomenclature rules used to name the particular structure
- Set up nomenclature preferences and language (IUPAC naming only)

- Draw the molecular structure or set of structures for naming using ACD/ChemSketch
- Create InChI identifiers, generate structures from InChI labels, and interpret SMILES strings
- Import up to 99 structures from SDfiles and automatically name them
- Export structures and names as SDfiles

Name to Structure

- Generate chemical structures from the following name types:
  - Systematic names of most classes of general organic compounds
  - Derivatives of more than 180 basic natural product parent structures
  - Semi-systematic and trivial names of common organic compounds

- Systematic names of some coordination compounds and polymers
- Incorrect names that do not strictly follow organic nomenclature rules
- Report warnings about ambiguous names or generate several possible structures
- Accept chemical names both in uninverted and inverted forms (Index names) in formatted and unformatted text
- Designate stereo configuration of chiral centers and double bonds
- Assign numbers to atoms in the structure

Disclaimer: Index naming algorithms have been developed by ACD/Labs alone and CAS makes no warranty or guarantee about its effectiveness or accuracy. If you require chemical substance names for reporting to regulatory agencies, names should be manually checked or obtained directly from CAS.

(3β,25R)-spirost-5-en-3-yl β-D-glucopyranoside
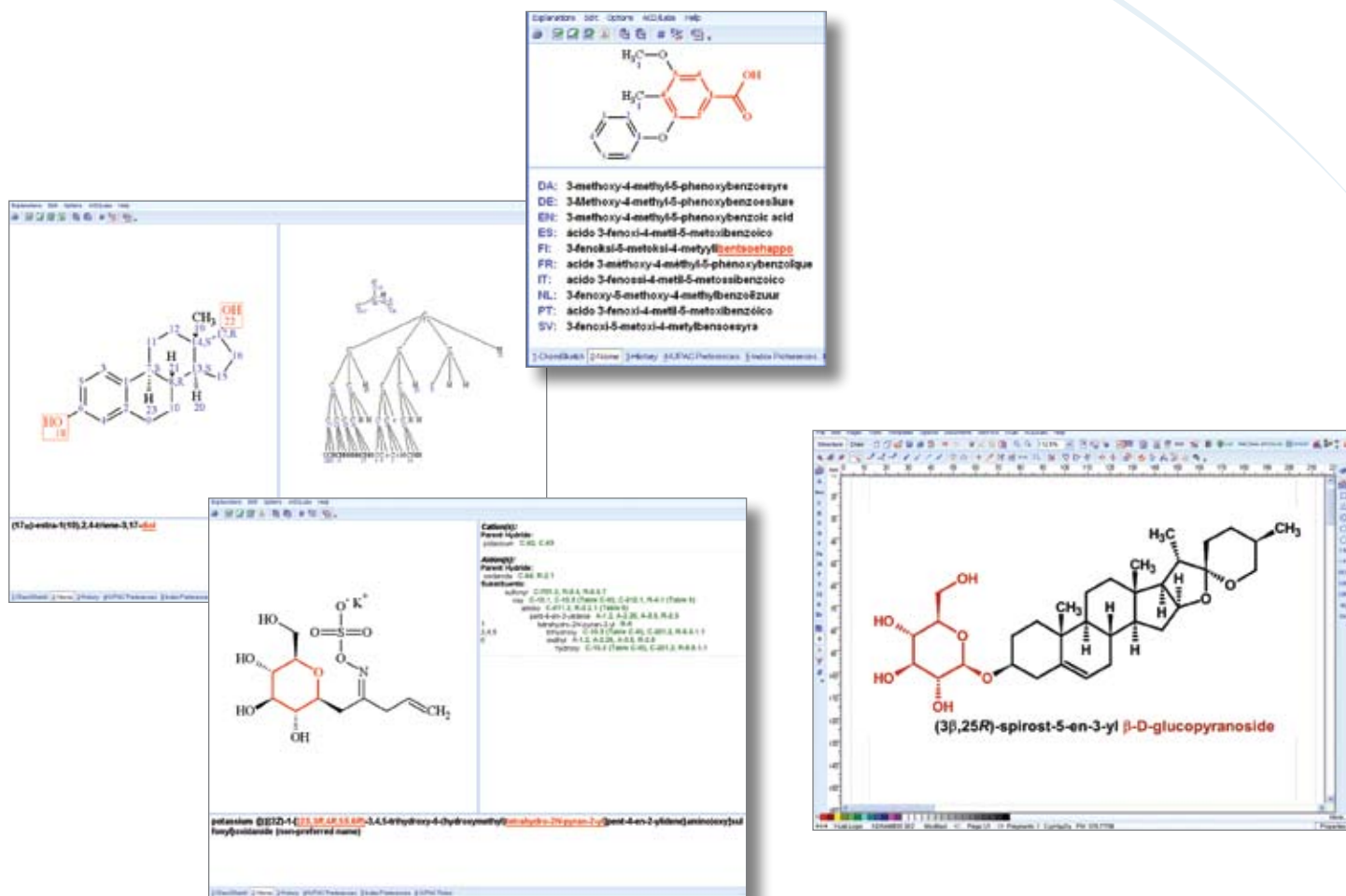
ACD/ChemSketch

A complete software package for drawing chemical structures.

ACD/ChemSketch is a chemically intelligent drawing interface that allows you to draw almost any chemical structure including organics, organometallics, polymers, and Markush structures. Use it to produce professional-looking structures and diagrams for reports and publications.

ACD/ChemSketch also provides a tool that allows you to check other tautomeric forms for your drawn structure.

Features

· Draw and view structures in 2D or render in 3D to view from any angle
· Draw reactions and reaction schemes, and calculate reactant quantities
· Generate structures from InChI and SMILES strings
· Generate IUPAC systematic names for molecules of up to 50 atoms and 3 ring structures
· Predict log$P$ for individual structures
· Search for structures in the built-in dictionary of over 165,000 systematic, trivial, and trade names
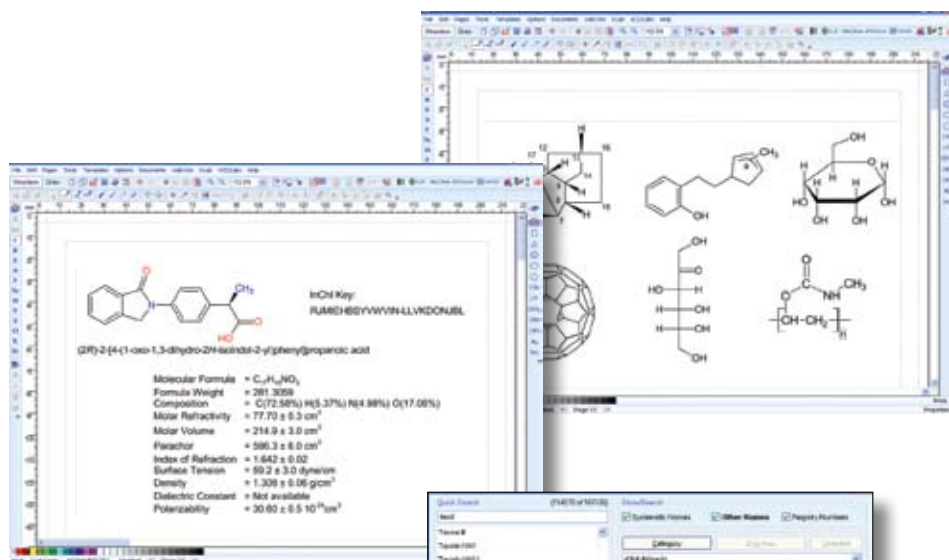
Benefits

· Visualize chemical structures in 2D or 3D to gain more insight into spatial configurations, and relationships to molecular properties
· Create professional reports, working with structures, text, and graphics simultaneously

ACD/ChemSketch also allows you to check other tautomeric forms for your drawn structure. Consideration of tautomeric forms is very important for structure searching, predictions (such as physicochemical properties, i.e., pK_a), and interpretation (i.e., of NMR, MS, and other analytical data).

"ACD/ChemSketch... fits our enterprise environment perfectly, and provides an excellent drawing suite for our users."

Gideon Richter
IT Director

"I was able to start using it as soon as it booted up without looking at the user manuals/ instructions. It seamlessly integrates with other MS Office programs... the automatic update feature for MS Word is efficient."

Attorney, Birch,
Stewart, Kolasch, & Birch, LLP

Full List of Features

Drawing

- Click and drag between two atoms to quickly create bonds
- Create chemical structures from InChl and SMILES codes
- Draw Markush structures (generic view), structures with delocalization, and polymers
- Create special Markush structures with added or removed mass or fragments to describe metabolic and mass-spectral transformations
- Depict reactions by drawing, importing, mapping atom-atom transformation, and editing reaction conditions
- Adjust the position of hydrogens near each atom
- Apply powerful 3D and 2D rotation, and move/resize features
- Create 3D models from 2D structures with the geometry optimization button

Structure Searching

- Search for chemical structures in various file formats throughout your computer's file systems (SK2; MOL; SDF; SKC; CHM; CDX; RXN; Adobe PDF; Microsoft Office DOC, XLS, PPT; and ACD/Labs databases CUD, HUD, CFD, NDB, ND5, INT)
- Search Microsoft Word documents with structures created in ChemDraw or Symyx (MDL) ISIS
- Search using full or partial structures

Chemistry

- Choose from a wide range of special bond types, including aromatic, delocalized, undefined single and double stereo, quadruple, and coordination bonds
- Automatically assign hydrogen atoms and charges to fill valence
- Instantly display chemical formula, molecular weight, percentage composition, and estimated macroscopic properties such as molar refractivity, refractive index, molar volume, density, and parachor

- Look up elements on the expanded periodic table of elements, which includes physical properties, NMR properties, isotope composition, and images of elements in their natural form
- Draw reactions and complex chemical schemes with manual or automatic mapping
- Calculate quantities for chemical reactions and solutions
- View all the suggested tautomeric forms for your structure

Reporting

- Create professional chemistry-related reports and presentations
- Export your ChemSketch files to Adobe Acrobat PDF
- Cut-and-paste structures and chemical information directly into Windows applications and maintain OLE links
- Convert your work into HTML

- Create templates for generating reports from other ACD/Labs products, defined by rules or company standards

Convenient Interface Design

- Customize toolbars
- Customize display properties such as atom numbering, chemical symbols, and valence
- Send ChemSketch SK2 files or PDF documents as an e-mail attachment directly from the ACD/ChemSketch interface
- Work with structures, text, and graphics simultaneously
- Save and load object styles

Disclaimer: Index naming algorithms have been developed by ACD/Labs alone and CAS makes no warranty or guarantee about its effectiveness or accuracy. If you require chemical substance names for reporting to regulatory agencies, names should be manually checked or obtained directly from CAS.

Supported Formats for Import/Export

Format Name	File Extension
ACD/Labs	*.sk2
Adobe Acrobat (output only)	*.pdf
Symyx	*.mol, *.sdf, *.rxn
ChemDraw	*.cdx
Excel (output only)	*.xls, *.xlsx
ISIS Sketch	*.skx
InChi	
SMILES	
Chemical Markup Language (output only)	*.cml
GIF image format	*.gif
PNG image format	*.png
JPG image format	*.jpg
Windows Bitmap	*.bmp, *.dib
Paintbrush (output only)	*.pcx
TIFF Bitmap (output only)	*.tif
HTML (output only)	*.html
Windows Metafile	*.wmf
ChemSketch 1.0 (input only)	*.mst, *.rtp

Some file formats require the installation of ChemBasic Goodies, a separate download and installation for freeware users.

Input structures from unsupported formats by opening the file with another program and pasting it into ACD/ChemSketch as an OLE object.

Elucidation & Identification

ACD/Labs offers a variety of software packages that enable elucidation and identification using one or many analytical techniques. Advanced algorithms for structure elucidation, sample deconvolution, and spectral matching, combined with the ability to leverage prior experimental data, result in effective tools that reduce time spent on compound identification.

Table of Contents/Elucidation & Identification
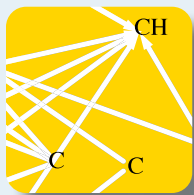
ACD/Structure Elucidator

Software to help resolve unknown structures from experimental data.

ACD/Structure Elucidator is a complete software package to help in the elucidation of unknown structures. It allows you to incorporate data from various analytical techniques (Chrom, UV-IR, MS, and NMR) to assist in the elucidation. The software follows the steps you might take manually when carrying out an elucidation, providing results in an unbiased fashion. Either use the software for full elucidation, entering all analytical data and using it to guide the software to provide all viable structures that fit the data, or enter a proposed structure and let the software predict the 1D and 2D NMR spectra and propose alternative structures.

Features

· Vendor-neutral analytical data processing for NMR, MS, UV-IR, Chrom, and MS
· Dereplication of known compounds— search the internal library of 2 million structural fragments
· Computer-assisted structure elucidation (CASE) using NMR, MS, UV-IR, and chromatography data
· NMRSync automatically synchronizes peak picking and assignment across all spectra for a particular dataset
· Structure evaluation automatically compares predicted and experimental NMR spectra to generate a factor
· Database experimental spectra, chemical structures, and analysis results along with user data and notes
· Determine relative stereochemistry— optimize structures in 3D and determine stereochemistry with NOESY and ROESY data

Benefits

· Resolve structures faster and more efficiently by collectively applying all your analytical data
· Generate a complete set of structures that fit the experimental data provided
· View viable alternatives to a proposed structure based on predicted NMR spectra for your compound

Dereplication of Known Compounds

The internal library of ACD/Structure Elucidator contains over 2 million structural fragments from approximately 410,000 compounds. Searching this extensive database before getting stuck in an elucidation will save time in the identification of known fragments that are consistent with the analytical data.
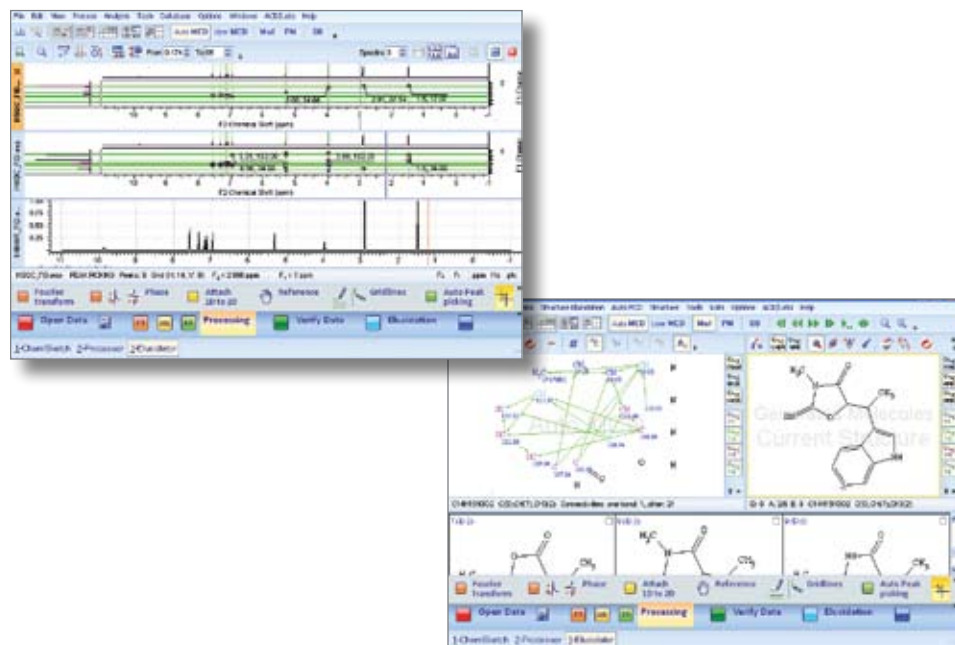
Application Note

Verifying Structural Hypotheses: Finding Alternative Candidate Structures from Elucidations

Journal Publication

Computer-Assisted Methods for Molecular Structure Elucidation: Realizing a Spectroscopist's Dream

Full List of Features

Spectral Data Import

· Import raw or processed NMR, UV/IR, and MS data directly into ACD/Structure Elucidator

· Enter compositional information such as MS data, known molecular formula, etc.

· Automatically generate a mass value from MS data (when available)

· Automatically generate molecular formula from MS data and NMR spectral information

· Use DEPT-edited NMR spectra to automatically determine ^{13}C multiplicity

· Create Good or Bad lists to provide the software with any structural knowledge that may be known prior to elucidation (e.g., include or exclude known structure fragments, functional groups, ring sizes, etc.)

Database Searching *(Dereplication Stage)*

· Automatically search ACD/Structure Elucidator's internal library of over 410,000 compounds from the spectral data provided

· If no structures are found in the initial database search, the software can search through its internal library of over 2,000,000 structural fragments. Any found structural fragments can be used in the ensuing elucidation process or can be used for substructure searches in in-house or commercial libraries

Structure Elucidation
(Compound Generation Phase)

· Generate a 2D connectivity map molecular connectivity diagram (MCD) and then draw in carbonyl, carboxyl, or other obvious features from IR knowledge or synthetic pathways; the MCD is a map of atoms and correlations between atoms that is automatically built by the software from 2D NMR spectral inputs and is used as a starting point for structure generation

· The MCD can be viewed and edited within the software; different bond correlations are denoted in color

· Edit the MCD to draw forbidden and obligatory bonds based on your own knowledge of the chemical structure and substance

Structure Identification
(Compound Evaluation Phase)

· Following structure elucidation, the software compiles all possible structures based on the provided spectral, MF, and mass data, along with their correspondence with the proposed MCD

· View the generated structures in a Tile, Table, or O ne Record mode

· Calculate the deviation statistic for each proposed structure; the deviation statistic is a value that determines agreement between the experimental ^{13}C NMR data and predicted ^{13}C NMR data−the lower the match, the better the correspondence the proposed structure has with the experimental data

· Sort the generated structures based on the deviation statistic to determine which compounds best match the experimental 1D and 2D NMR data provided

· Interactively select only the chemically relevant structures from the proposed list and create a new list of structures in Table or Tile mode

· Automatically remove any structures from consideration based on a deviation statistic threshold

· If proposed structures have several stereoisomers, the software can use NOESY and ROESY data to determine the relative stereochemistry of the proposed compounds

Databasing Features

· Update the database with the experimental spectra along with their chemical structures, analysis results (table of peaks, annotation), and any miscellaneous information copied to User Data and Notes

· Populate user databases with thousands of spectra in one step with the group macro batch processing tool

· Search by full spectrum or spectral regions, peaks, spectral parameters, chemical structure and substructure, formula, molecular weight, and user data text

· Perform spectrum searches according to Euclidean distance, or squared or absolute difference methods; the search hits will be ranked by HQI (Hit Quality Index)

· Control data that is entered into your corporate databases with Data Forms Manager

· Manage remote databases through a local or global network with an Oracle-based SQL client-server system

Supported Formats for Import/Export

· View the full list of input formats for NMR, MS, and UV/IR on the Manager product pages

· ACD/Labs software will also handle standard file formats such as ASCII, netCDF, JCAMP, etc.

· ACD/Structure Elucidator includes full processing for all the analytical techniques that can be used in elucidation. See individual manager product pages−ACD/ NMR Workbook, ACDMS Manager, ACD/UV-IR Manager, and ACD/Chrom Manager−to read about the full processing features for each technique
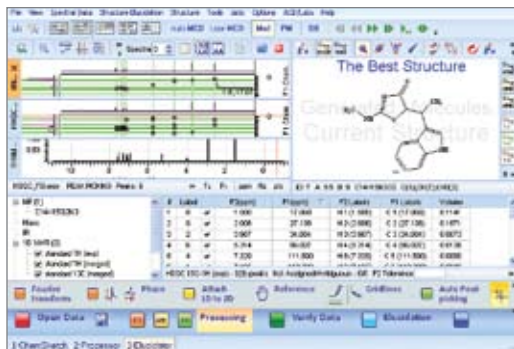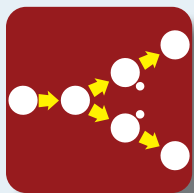
ACD/Metabolite ID Suite

**A package of software modules that facilitate metabolism studies.**

ACD/Metabolite ID Suite contains tools for faster computer-assisted data analysis and extraction of metabolites, efficient data management, and effective reporting, establishing a connection between chemical structure and chemical data that enhances your understanding of the overall process. ACD/Labs software is vendor-neutral, enabling data from major instrument vendors to be processed and stored in a unified format.

Features

· Advanced data processing for chromatographic, IR, Raman, and MS data, including deconvolution with ACD/IntelliXtract
· Automatic assignment of ions and fragments to spectral peaks
· Map fragmentation pathways in seconds
· Create biotransformation maps of metabolites
· Store metabolite structures and analytical data in a fully searchable database

Benefits

· Unify chemical and analytical knowledge in a single platform
· Miss fewer trace metabolite components
· Save time interpreting the fragmentation of proposed structures
· Leverage prior knowledge by searching databases of analytical and chemical data
· Produce better-quality reports with less tedium and effort
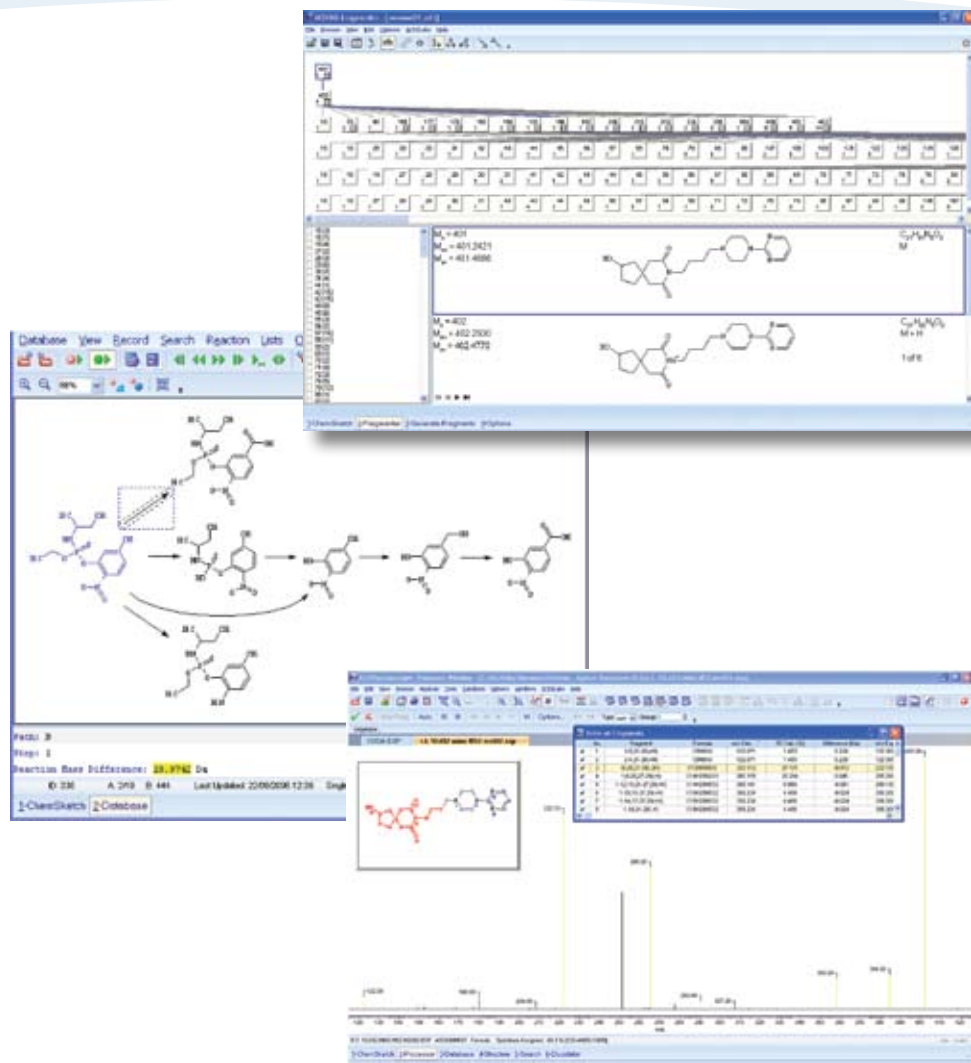
Additional Resources

Universal MS data processing and databasing with ACD/MS Manager.

Deconvolution of complicated LC/MS data with ACD/IntelliXtract.

MS fragment prediction based on chemical structure with ACD/MS Fragmenter.

Reaction and structure databasing with ACD/ChemFolder.

Universal MS data processing and databasing with ACD/ChromManager.

Universal MS data processing and databasing with ACD/UV-IR Manager.

ACD/IXCR

Intelligent compound recognition using component detection software and spectral matching capabilities.

Reduce the time spent on manual interpretation, searching and validation of GC/MS spectra by using ACD/IXCR to conduct rapid, non-targeted analysis of water, wastewater, and other environmental samples.

ACD/IXCR is a suite of software tools with flexible options for screening quality control samples or for deformulation of mixtures, and is user friendly to both analysts and experienced spectroscopists. ACD/Labs software is vendor-neutral and supports a variety of GC/MS file formats from most major instrument vendors.

Extract

ACD/IXCR uses component detection algorithms (CODA) to reduce noise and background signals, eliminating the need for time consuming manual interpretation and reducing the potential for error. CODA helps to ensure that mass chromatograms containing analyte peaks are retained while those attributed to noise are filtered out.

Search

Tables of known compounds can be imported (for example, EPA 8270 compounds) into the Ion Presence™ table to quickly identify components with known retention times that are present in your samples. Processed sample data is then searched against the NIST database for similar spectral patterns. The results are summarized in a clear and concise report, identifying compound names and a match score to measure the quality of the match.

Compare

Compare full scan data of samples against standards or blanks to quickly determine the differences, or subtract spectra to highlight features that are not the same. Even use semi-quantitative analyses to help focus further study of certain compounds.

Automate

ACD/IXCR offers the ability to perform intelligent compound recognition on batches of samples or to automate the CODA and search steps, increasing efficiency and throughput.

Report

Results are presented in an easy-to-read tabular display and can be automatically exported to Microsoft Excel or converted to PDF. Analysts and spectroscopists can drill down into the search data to see details of the reference spectrum for greater insight into the IXCR results.

Retain the Results

Save experimental spectra in a fully searchable database to enable faster identification in the future. Stored spectra can be easily accessed for reference and auditing, or to integrate results into an existing LIMS. Search by spectrum, partial spectrum, structure, sub-structure and a variety of text-based queries.

Secondary Verification

ACD/IXCR can also provide a secondary check on whether the compound has been properly identified by confirming the correlation of peak assignments with experimental data. Simply attach a chemical structure (drawn in ACD/ChemSketch or obtained from the NIST library) to the experimental spectrum and the built-in AutoAssigment function generates a table of fragments. A quality index score indicates whether peak intensities in the spectrum are consistent with isotope abundances expected for the predicted assignments, providing a means of verifying the proposed structure.
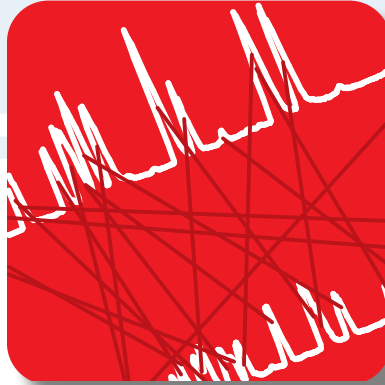
Chromatographic Optimization & Method Development

Save time and develop better separation methods with tools that facilitate the use of quality by design (QbD) principles to help eliminate much of the trial-and-error normally associated with optimization and method development.

# Table of Contents/Chromatographic Optimization & Method Development

ACD/LC & GC Simulator

Software to predict retention times and help
optimize LC and GC methods.

ACD/LC and GC Simulator help you to optimize concentration gradient, temperature,
and resolution of your separation during method development. Using either a database
of experimental chromatograms or calculations of physicochemical properties such
as boiling point, log$P$, log$D$, and pK$_a$, ACD/LC and GC Simulator models hypothetical
chromatograms and predicts optimal separation conditions and retention times for
your compounds.

Features

· Optimize your gradient, solvent
  concentration, temperature, pH,
  and more
· Predict retention times for new
  compounds under existing methods
· Automatically match peaks between
  LC/UV (DAD, PDA) datasets based on
  spectral similarity
· Visualize the effect of changing your
  method conditions with predicted
  chromatograms
· Process raw chromatographic
  data from many different vendor
  instruments
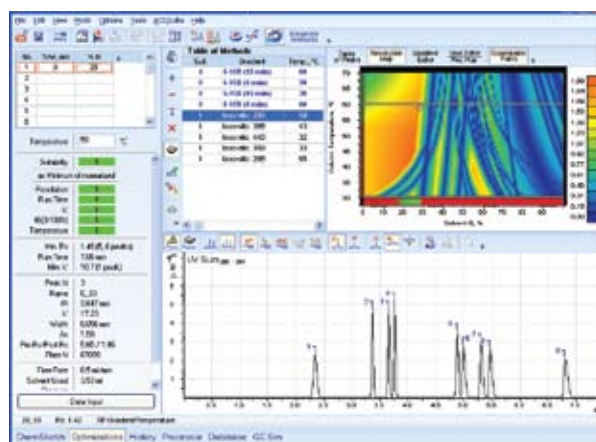
Benefits

· Quickly optimize methods in less time
  and with fewer injections
· Eliminate manual peak matching
  between runs
· Database experimental data for use in
  future method development

Movie

**See a video highlighting some of LC
Simulator's features**

Technical Note

Gradient Temperature Optimization

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LC Features

- Calculate pK_a values from structure for your compounds
- Optimize the chromatographic separation of complex chemical mixtures by the following parameters:
  - Solvent concentration
  - Gradient elution program
  - Temperature
  - User's parameters
- Automatically match peaks between LC/UV (DAD, PDA) datasets using the UV Mutual Automated Peak Matching algorithm (UV-MAP)
  - Compare UV spectra for the same peak from different injections and overlay the resulting spectra for easy comparison
- Optimize the chromatographic separation of complex matrices using 2D optimization modes:
  - RP Isocratic/Temperature
  - Gradient/Temperature
  - RP isocratic/pH
  - Gradient/pH
  - User parameters
- Select optimal experimental chromatographic conditions using the Suitability Map, which is available for 1D and 2D Optimization modes with Suitable and Minimal Resolution, Robustness, Suitable and Maximal Run Time, Suitable and Minimal k', and Column Stability
- Calculate the calibration equation for your column using experimental data
- Set the virtual pH to determine optimum separation conditions and review a modeled separation under any pH

GC Features

- Recalculate the hypothetical GC simulation at any pressure value within the 0–7600 mmHg range
- Predict retention times for new compounds using a known GC column and the experimentally available retention times for a number of chemical compounds (three or more)
- Use experimental log$P$/log$D$ data to correlate log$P$ and retention time values for calculation of the prediction equation

- Simulate retention times in several ways:
  1. Optimize the temperature gradient using two experimental chromatograms for the same compounds under different conditions
  2. Calculate retention times for new compounds on the basis of the experimental retention times of related compounds and physicochemical properties
  3. Predict the retention times for new compounds under new conditions by combining the temperature optimization and predicting mechanisms

Processing

- Import chromatographic data from Waters Millennium[32], Empower, and Empower 2, Dionex Chromeleon 6, PerkinElmer TotalChrom 6.1, and Turbochrom 4, Agilent ChemStation, NetCDF (AIA), and ASCII formats
- Import LC/UV (PDA, DAD) records associated with chromatography data from Agilent ChemStation, Waters MassLynx, Waters Empower, and Dionex Chromeleon 6

- Perform peak picking, smoothing, baseline correction, peak integration, and peak deconvolution on single chromatograms
- Perform peak picking and baseline correction for LC/UV datasets
- Import or export structures from or to an SDfile; the files can contain compound names and retention times
- Manually assign chemical structures to peaks on your chromatogram
- Automatically assign chemical structures from an SDfile to labeled chromatogram peaks
- Attach multiple structures to a co-eluting peak
- Automate standard processing steps with a macro program
- Record all processing actions into the Audit Trail; transfer the audit trail to create a macro program to apply to subsequent datasets
- Display a series of chromatograms on a single plot with structures, peak data, and annotations
- Export chromatographic data to ACD/Labs Spectrum, NetCDF, and ASCII formats

Compatible Data Formats

Digital Format	Import	Export
ACD/Labs Spectrum (*.esp)	✓	✓
ASCII (*.txt; *.prn; *.csv; *.asc)	✓	✓
NetCDF (*.cdf, *.nc)	✓	✓
Agilent (HP) ChemStation (*.ms, *.ch, *.uv) [1,2]	✓	
Waters® Millennium® [32] [1]	✓	
Waters Empower™ and Empower 2 [1]	✓	
Dionex® Chromeleon® 6 [1]	✓	
PerkinElmer® TotalChrom™ [1]	✓	
PerkinElmer Turbochrom™ 4 (*.rax)	✓	
MATLAB® DSO (*.mat) [1]	✓	✓
Shimadzu Corporation (*.lcd)	✓	✓
Waters Corporation MassLynx (_functns.inf) [1]	✓	✓

[1] Support for hyphenated data involving Diode Array Detector (DAD)
[2] Valid license of MS software also required to import MS data

ACD/ChromGenius

Software for method selection based on chemical structure.

ACD/ChromGenius predicts retention times and chromatograms based on the structures of the compounds to be separated, and allows you to select the best generic separation method for your sample prior to injection. ACD/ChromGenius reduces the number of screening experiments needed by helping you determine which methods will work and which will fail before you perform a single separation or sample preparation.

Features

- Predict retention times and chromatograms of samples based on chemical structure
- Set restrictions on separation conditions and parameters to focus results
- Display a color-coded summary of method suitability, predicted chromatograms, and more
- Train ACD/ChromGenius predictions with your own structures and experimental data
- Automate ACD/ChromGenius to rapidly screen lists of samples
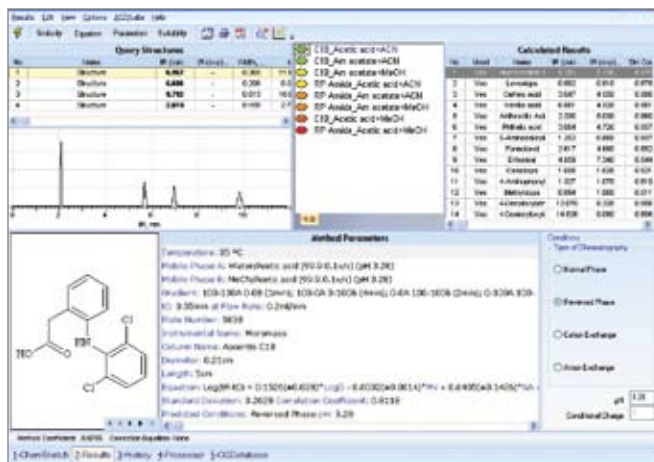
Benefits

- Increase sample throughput by speeding method selection
- Achieve enhanced separation quality and increased accuracy
- Reduce iterative experiments and instrument downtime

Poster

Building a Global Chromatography Knowledgebase for Method Development Prediction

Industry Application

Screening Method Simulation at NLS

ACD/ChromGenius uses a knowledgebase of experimental structures and retention times as a basis to predict retention times and chromatograms for new compounds using ACD/Labs' physicochemical prediction algorithms.

Draw or import the chemical structure of compounds to be separated and ACD/ChromGenius simulates the separation for different separation methods available in the knowledgebase. In just a few seconds, the methods are ranked according to suitability, and displayed with a simulated chromatogram and a table of predicted retention times.

Full List of Features

· Import databases from ACD/ChromManager

· Build new databases from your own set of standard methods by pushing data directly from ACD/Method Development Suite, ACD/AutoChrom, and other vendor file formats

· Use an existing database of retention times and structures for sets of generic methods:

  · SupelcoAscentis database of 250 structures and retention times for a set of 8 LC/MS-compatible methods

  · Thermo Electron database of 70 structures and retention times for a set of 10 LC/MS-compartible methods

· Specs database of retention times for thousands of structures

· Predict chromatographic retention times on the basis of physicochemical properties such as $logP$, $logD$, and pK_a

· View predicted chromatograms

· View tables of predicted retention times, peak width, k1

· View the compounds used to build separation models

· Display a graph of retention prediction accuracy

· Import and export SDfiles

· Target conditions and elution time to increase solvent volatility and decrease solvent evaporation time

· Predict method suitability for single compounds or lists of samples

· Generate a report containing the best generic method for each sample to import to your chromatography data system

Boost Prediction Accuracy with Absolv Parameters

Depending on the application or when the compounds under investigation fall outside of the chemical space covered by your experimental database, you may want greater accuracy than can be achieved with ACD/ChromGenius alone. The ACD/ChromGenius Absolv add-on increases the accuracy of predicted retention times using Abraham solvation parameters calculated from chemical structure. The parameters are then incorporated into the prediction algorithm, resulting in greater accuracy.

Compatible Data Formats

Digital Format	Import	Export
ACD/Labs Spectrum (*.esp)	✓	✓
ASCII (*.txt; *.prn; *.csv; *.asc)	✓	✓
NetCDF (*.cdf, *.nc)	✓	✓
Agilent (HP) ChemStation (*.ms, *.ch, *.uv) [1,2]	✓	
Waters® Millennium® 32 [1]	✓	
Waters Empower™ and Empower 2 [1]	✓	
Dionex® Chromeleon® 6 [1]	✓	
PerkinElmer® TotalChrom™ [1]	✓	
PerkinElmer Turbochrom™ 4 (*.rax)	✓	
MATLAB® DSO (*.mat) [1]	✓	✓
Shimadzu Corporation (*.lcd)	✓	✓
Waters Corporation MassLynx (_functns.inf) [1]	✓	✓

[1] Support for hyphenated data involving Diode Array Detector (DAD)
[2] Valid license of MS software also required to import MS data

ACD/AutoChrom MDS

Method development software for chromatography.

ACD/AutoChrom Method Development Suite (MDS) combines instrument control for LC/MS and LC/UV systems with software for logical method development. Define your project and your goals, and AutoChrom will execute the experiments, guide you through data processing and interpretation, and help you select the next experiment to perform. Develop better, more robust methods in less time than you ever could before.
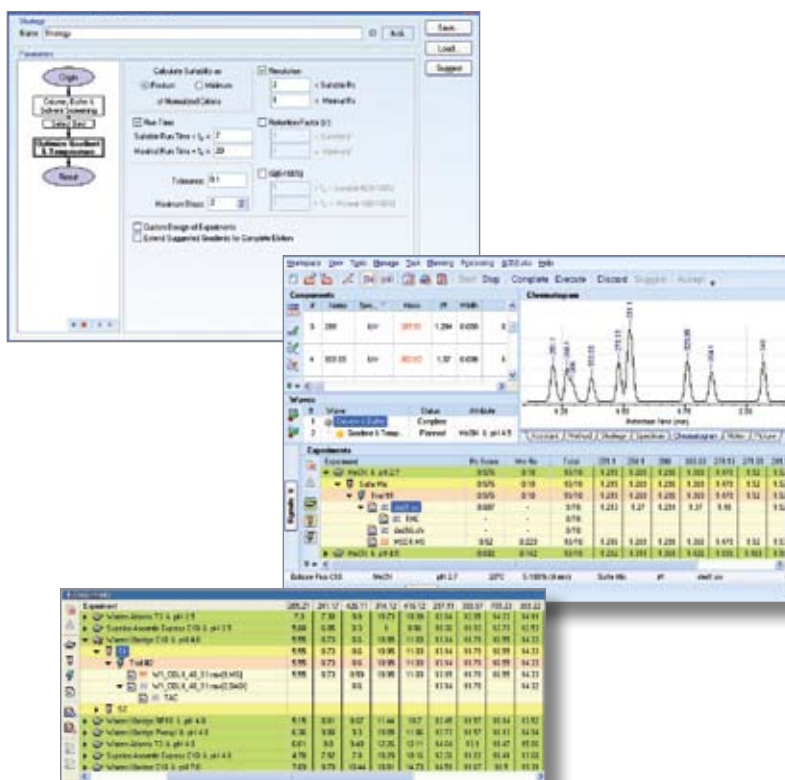
Features

· Automatic peak tracking between runs helps you find all relevant components
· Instrument control through Agilent ChemStation or Waters® Empower™ 2 software
· Method Development Assistant suggests the next experiment to run
· Store new methods in a fully searchable database
· Run in Automated or Manual modes

With instrument control (Automated mode) or without (Manual mode), ACD/AutoChrom MDS significantly reduces the time it takes to develop new methods. From selecting a better starting point to intelligent optimization, you will get better methods faster.

Benefits

· Find a better starting point for method development
· Develop more robust methods in less time
· Reduce the need for manual data interpretation
· Manage projects more efficiently and protect valuable research data

Industry Application

Rapid Chiral Method Selection

Poster

Efficient Chiral Screening in Support of Medicinal Chemistry

Full List of Features

Method Selection & Optimization

· Search the built-in ACD/Chromatography applications database or a database of your own methods for a suitable starting point

· Predict retention times so that archived separations can be evaluated and modified before the first injection

· Optimize for pH based solely on a nalyte structure; accurate structure-based pK_a prediction algorithms are incorporated into ACD/LC Simulator

· Design your method development strategy and AutoChrom will automatically generate method sequences for:
  · Agilent ChemStation
  · Waters® Empower™ 2 Software

· Specify success criteria for your method

· Create flexible method development strategies to optimize method development variables

· Update and refine strategies over the course of a project

· Design experimental waves to optimize method variables

· Select the best result of screening experiments:
  · Column selection
  · Mobile phase selection
  · Buffer selection

· Optimize:
  · Gradient
  · Temperature
  · Combined gradient and temperature

Data Interpretation

· Import LC/UV (PDA, DAD) records associated with chromatography data from most major instrument vendors

· Process and collate many types of chromatographic data, including:
  · LC/MS
  · LC/UV (PDA, DAD)
  · Single UV wavelength chromatograms

· Perform peak picking, smoothing, baseline correction, peak integration, and peak deconvolution on single chromatograms

· Import or export structures from or to an SDfile; the files can contain compound names and retention times

· Manually assign chemical structures to peaks on your chromatogram via ACD/ChemSketch or from the table of peaks

· Automatically match peaks between injections or between runs based on spectral similarity for LC/UV and LC/MS datasets

· Peak labels and structures are copied from one dataset to the next; if no peak labels exist, ACD/AutoChrom MDS assigns a label to both datasets

Project Management

· Manage your project using the dashboard overview

· Dig down into the original data when necessary to review or reprocess

· View a collapsible Table of Peaks that summarizes your injections

· Manage and summarize composite samples, and visualize composite chromatograms

· Store your experimental data and ACD/LC Simulator predictions in one place to quickly understand the rationale behind your experiments

· View chromatograms and UV spectra or mass spectra alongside your peak tables

· Reconcile peaks across detectors or across samples

· Automatically update all related files with chemical structures

· Ignore irrelevant peaks without deleting the information from the dataset

Databasing

· Build a database of in-house methods complete with method parameters, chromatograms, and chemical structures

· Share your databases within your organization to build a company-wide repository of chromatographic knowledge

· Retrieve previous separation methods from the ACD/Chromatography applications database or your own database of separations:
  · Perform a simple structure, substructure, or structure similarity search of the database to retrieve methods for compounds similar to those in your sample
  · Perform a chromatographic smart search to not only retrieve separations of similar compounds, but also to estimate the retention times and evaluate the suitability of the found separations for your novel compounds
  · Additionally, search the databases by method parameters or other user data

Additional Resources

ACD/AutoChrom MDS uses the powerful component extraction and peak tracking capabilities of ACD/IntelliXtract to help do the dirty work of matching chromatographic components between runs. Learn more about how ACD/IntelliXtract works.

View a complete list of hardware compatibility on our website:
www.acdlabs.com/autochrom_hardware

Agilent Technologies

Systems	1100 LC systems
	1200 LC systems
	1200 RRLC systems
Detectors	G1946 LC/MSD
	G1956 LC/MSD
	6100 MS Series

Waters — THE SCIENCE OF WHAT'S POSSIBLE.™

Systems	ACQUITY UPLC
	Alliance LC
	Alliance 3100
Detectors	ACQUITY SQD MS
	ACQUITY TDQ MS
	W3100 MS
	2996 PDA
	2998 PDA

Automation & Integration

ACD/Labs software offers flexible, customizable software solutions that streamline and improve the efficiency of your operation through automation, and innovative products that facilitate the movement of data and results. Add the ability to integrate with in-house or other vendor software to further enhance the capabilities of your organization.

Table of Contents/Automation & Integration

ACD/Analytical Automation Suite

Software to streamline analytical operations.

ACD/Analytical Automation Suite is a flexible, customizable collection of software modules for processing, interpretation, and storage of an array of optical and chromatographic techniques, which are configured to meet your organization's specific needs. The Suite is adaptable to various pharmaceutical research environments and addresses a number of industry challenges such as alleviating the bottlenecks of high-throughput qualitative analysis, management of data from multiple analytical techniques and instrument vendors, and the timely delivery of reports to the desktops of users and decision-makers via desktop, LIMS, or web-based applications.

Features

· Flexible and customizable
· Integrate multiple analytical techniques and vendor instrumentation
· Connect to ELN, LIMS, or deploy web-based dissemination of results
· Track workflow and sample submission
· Standardize and automate processing, data interpretation, and storage of spectral and chromatographic results

Brochure for IT professionals

Download

Benefits

· Increase efficiency and streamline processes
· Protect and leverage analytical knowledge
· Reduce high-throughput bottlenecks
· Advance research faster by integrating results into your decision-making

Customize ACD/Analytical Automation Suite with only the modules you need from the complete range of ACD/Labs' vendor-neutral analytical products, including:
· 1D and 2D NMR
· MS
· UV-Vis, IR, Raman
· Chromatography
· XRPD, TGA, DSC, EPR, IMS, Physisorption, Potentiometry, Kinetics and more
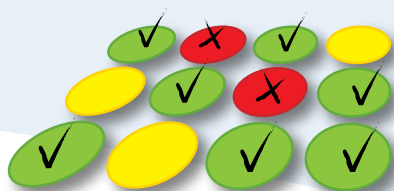
Resources

The flexibility of ACD/Analytical Automation Suite makes it adaptable to a variety of applications in research settings.

Automated Structure Verification by NMR

Using 1D and 2D NMR spectra and their corresponding proposed chemical structures, it is possible to unambiguously confirm structure-spectrum match for 75−90% of the samples, leaving the remaining for manual evaluation by the user. This results in extensive time savings when compared to standard spectral evaluation processes.

Application Note

### Automated Structure Verification

Purity Assessment by LC/MS

Before screening compound libraries, make sure you have the compounds you think you have. Advanced LC/MS deconvolution algorithms use all available chromatographic and MS information to automatically reduce the number of false positive compound identifications by LC/MS and help identify impurities.

Application Note

Compound Recognition and Identification using LC/MS
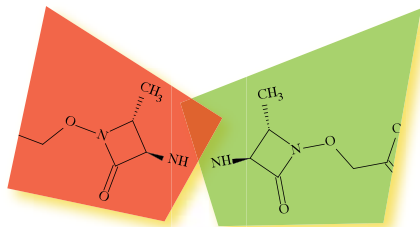
Method Selection in HT Chromatography

Automatic method selection has been shown to increase throughput of chiral sample purification in support of medicinal chemistry groups. Diverse instrument data was automatically combined with chemical structures and metadata, generating a knowledgebase of thousands of separations per month. The process has since been used in laboratories doing achiral purity control. Select, don't screen, to find the right method.

Application Note

Rapid Method Selection for Chromatography

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ACD/Web Librarian

View and search local and remote databases via the web.

ACD/Web Librarian allows users to search and view information stored in ACD/ChemFolder, ACD/SpecManager, or ACD/SpecManager Enterprise databases in a convenient web browser interface. Data is displayed in a virtual centralized repository that is accessible to authorized members of the organization to browse, review, use, and report. ACD/Web Librarian is an efficient and cost-effective way to make analytical and chemical information available to those who need it, when they need it, whether across the lab or across the globe.
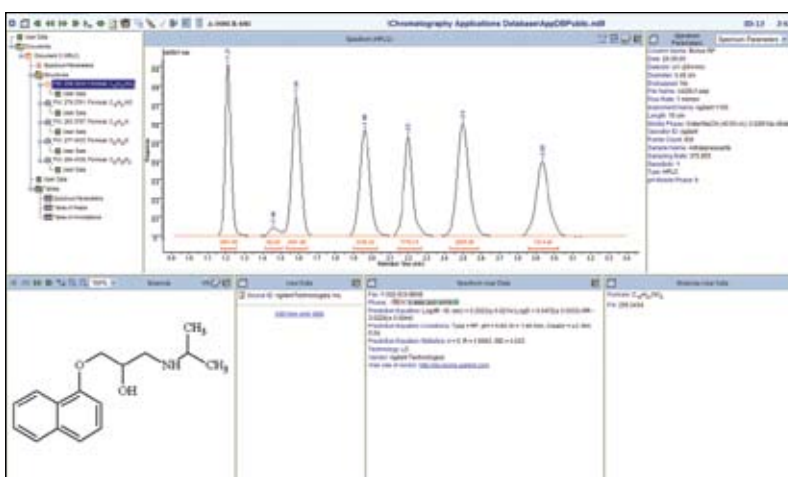
Features

· Search databases by a variety of parameters, including:
  · Exact structure/reaction
  · Substructure/subreaction
  · User data
  · Spectrum or chromatogram parameters
· Create restrictions on access to sensitive data, create user groups, and monitor client connections
· Export and save spectra and structures from the database
· Pass record data to other ACD/Labs products for further processing or reporting
· Generate reports including spectra, structures, reactions, and all accompanying information in Microsoft Word (DOC), Adobe Acrobat (PDF), ACD/ChemSketch (SK2), and HTML formats

Benefits

· Facilitate collaboration by allowing shared information across organizations
· Efficient delivery of results to decision-makers
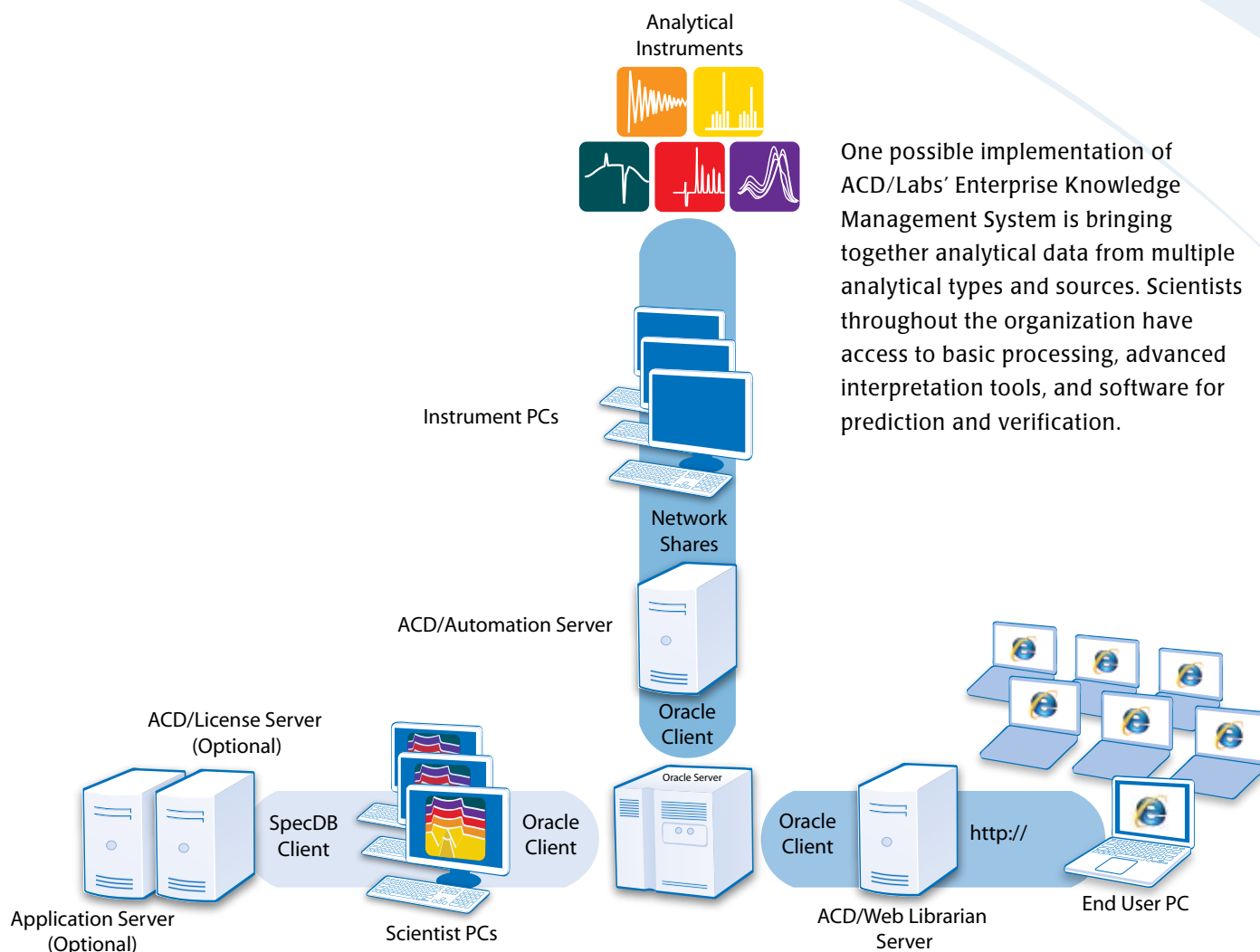· Safe, secure, and cost-effective

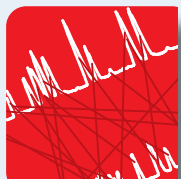ACD/Web Librarian can be customized to enable searching and viewing within your own web interface.

ACD/Web Librarian Web Services provides a platform-independent XML (eXtensible Markup Language) web service using SOAP (Simple Object Access Protocol) over HTTP (HyperText Transfer Protocol) that runs under Microsoft Internet Information Services (IIS).

Full List of Features

- Navigate through the network and locate plain files and databases using a browser

- Browse databases in One Record, Tile, or Table viewing modes

- Search through databases by a variety of parameters, including exact structure/reaction, substructure/subreaction, user data, spectrum or chromatogram parameters, similar spectrum/subspectrum, multiplets, record ID, and many others

- Create a special list of filters/subfilters that are available either to all users or for your work only, and that define search conditions for all/current databases or a particular data type

- Search data on the basis of scanned barcode information or put barcodes containing partial record information into your report

- Use the ACD/Web Librarian searching/viewing facilities from other ACD/Labs desktop programs (ACD/ChemSketch, ACD/SpecManager, etc.)

- View spectra and structures in scalable pop-up windows and copy them as images to the Windows clipboard

- Customize the database view

- Manipulate record lists (e.g., merge, intersect, or subtract them)

- Pass record data to a corresponding ACD/Labs Processor

- Export spectra in the following formats:
  - ESP
  - JCAMP
  - ASCII

- Export/save structures or reaction schemes in the following formats:
  - Symyx (MDL) molfile (MOL)
  - Symyx (MDL) rxnfiles (RXN)
  - ACD/ChemSketch (SK2)
  - CambridgeSoft ChemDraw (CHM, CDX)

- Generate reports, including spectra, structures, reactions, and all accompanying information in Microsoft Word (DOC), Adobe Acrobat (PDF), ACD/ChemSketch (SK2), and HTML formats

- Use the template reporting facility to create reports in PDF and SK2 formats

- Export the current dataset to an SDfile

- Add files/databases from Web Librarian, and backup and assign arbitrary attributes to them while integrating with ACD/Documents Manager

- E-mail record links to colleagues within your organization to allow them to instantly view specific information; use your Address Book to quickly search for e-mail addresses

- Organize automatic data processing by creating a flexible workflow of your own design on the basis of integration with ACD/Workflow Manager

Analytical Instruments

One possible implementation of ACD/Labs' Enterprise Knowledge Management System is bringing together analytical data from multiple analytical types and sources. Scientists throughout the organization have access to basic processing, advanced interpretation tools, and software for prediction and verification.

Instrument PCs

Network Shares

ACD/Automation Server

Oracle Client

Oracle Server

ACD/License Server (Optional)

SpecDB Client

Oracle Client

Oracle Client

http://

Application Server (Optional)

Scientist PCs

ACD/Web Librarian Server

End User PC

ACD/Automation Server

Software to automate and standardize data handling.

ACD/Automation Server coordinates the flow of analytical knowledge between instruments, databases, and people by automatically performing certain routine tasks such as data processing, storage, and reporting. Flexible and customizable, ACD/Automation Server can be configured to match your specific needs, making workflows more efficient and productive.
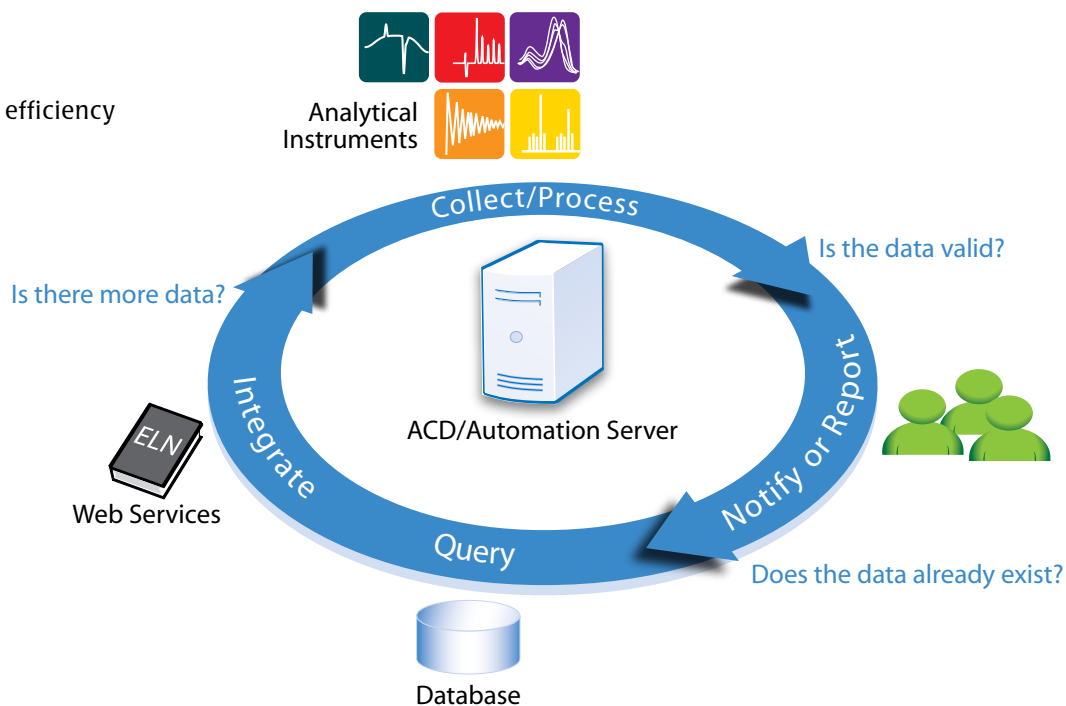
Features

· Extensive instrumentation type and raw data compatibility
· File handling capabilities to move, copy, delete, import, export, rename, and more
· Custom scripting and application development interface
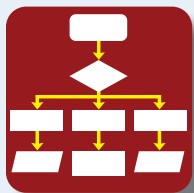· Generate reports and populate databases automatically

ACD/Automation Server can be used to build a bigger and better system for data collection, storage and reporting, recognizing instrument and data types, and executing a series of predefined processing tasks through integration with the ACD/SpecManager portfolio of analytical data handling products.

Data processed through ACD/Automation server can be reported and the data stored in a central database, which can then be searched and viewed to produce additional reports. A range of options are available to view, manipulate, and report data via other ACD/Labs desktop or web-based tools.

Benefits

· Improve the quality of data with standardized treatment
· Streamline processes
· Customizable
· Increase productivity and efficiency
· Customizable interface

Analytical Instruments

Collect/Process

Is the data valid?

Is there more data?

Integrate

ACD/Automation Server

Notify or Report

ELN

Web Services

Query

Does the data already exist?

Database

94

ACD/Workflow Manager

Design custom workflows to manage analytical processes.

ACD/Workflow Manager works with other ACD/Labs products such as ACD/SpecManager to automate the collection, processing, and reporting of data, and to monitor the movement of samples throughout a particular process. Each workflow is treated as a project managed by ACD/Workflow Manager from start to finish.

Features

· User-friendly interface for creating and editing workflow diagrams
· Create forms for documenting sample information during the execution of the workflow
· Define alerts and notifications at critical stages
· Automatically report results upon completion of the process

Benefits

· Design the workflow for a range of applications such as sample tracking, quality control, or data consolidation and storage
· Quicker, more efficient movement of samples throughout the laboratory
· Improve and speed up decision-making with notifications and alerts
· Consistent treatment of samples and data

To discuss how ACD/Workflow Manager can help automate routine processes in your organization, contact an ACD/Labs representative.

www.acdlabs.com/contact
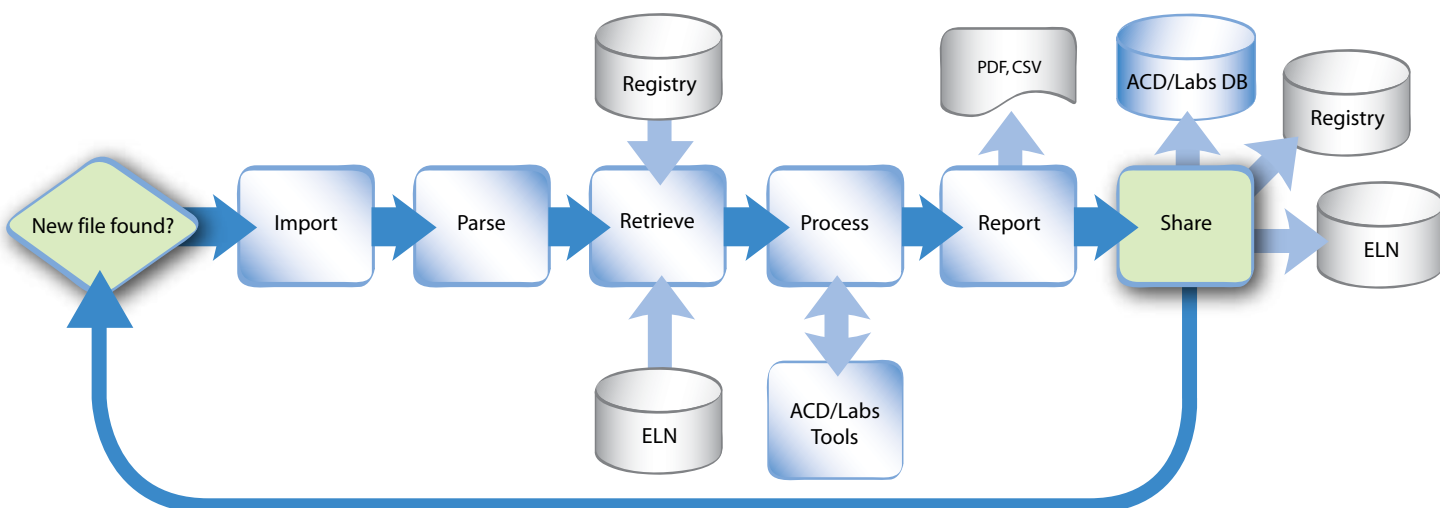
Applied Biosystems LightSight™

Elucidate metabolite structures

AB SCIEX

Learn more about your metabolites quickly using automated fragment prediction and automatic spectral assignment with ACD/Labs MS Software and LightSight™.

Gaining a better understanding of the relationship between the structure and spectrum of a parent drug molecule can have a positive impact on the ability to elucidate the structures of resulting metabolites. Automated fragment prediction with ACD/MS Fragmenter and spectral assignment with ACD/MS Processor, which is accessible from within the LightSight environment, offer effective ways to help visualize this relationship and elucidate metabolite structures more easily.

Assign Fragments To Experimental Spectra

· ACD/MS Processor automatically assigns structure fragments to experimental spectra pushed directly from LightSight
· Use the assigned spectrum to identify possible sites of metabolic modification, reviewing common fragment ions and common neutral losses flagged by LightSight
· Evaluate possible metabolite structures to see which one is the best match for your experimental spectrum

Predict Fragments from Structure

· Predict mass fragmentation according to different ionization techniques and polarity
· Review possible fragment ion structures and fragmentation pathways
· Create fragmentation pathway reports with one click

Track Partially Elucidated Structures with Markush Representations

When it is not possible to fully elucidate structures with MS data only, ACD/Labs' shaded Markush representations allow you to unambiguously communicate which regions of the structure were modified.

Application Note

Automatic MS/MS Fragment Assignment for the Structural Elucidation of Metabolites
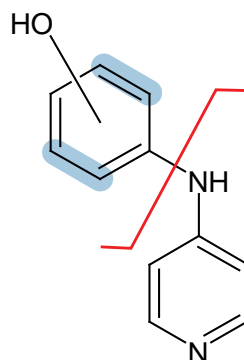
ACD/Labs Batch Integration with Pipeline Pilot

Apply ACD/Labs' predictions seamlessly in your Pipeline Pilot workflows.

accelrys®

If you already own Pipeline Pilot and ACD/Labs batch products for ACD/PhysChem Suite, ACD/Name, ACD/ADME Suite, and ACD/Tox Suite, all you need to integrate your software tools is a free integration component from ACD/Labs. Then, based on calculation options specified prior to execution of the protocol, you can apply our algorithms in your workflows and make your software work harder for you.

ACD/Name generates accurate systematic names for almost any organic structure in accordance with IUPAC and CAS rules, and generates structures from systematic names, SMILES, and InChI™ (and vice versa).

ACD/PhysChem Suite calculates properties such as boiling point, log$P$, log$D$ (at a given pH or pH range), pK_a, sigma, and aqueous solubility (at a given pH or pH range).

ACD/ADME Suite's various modules predict ADME parameters such as passive absorption, bioavailability, interactions with CYP450 enzymes, and blood brain barrier permeation.

ACD/Tox Suite predicts various toxicity endpoints such as hERG inhibition, genotoxicity, and endocrine system disruption from structure.

How has it been applied?

Implementation of this integration at Boehringer Ingelheim (Canada), Ltd., moves molecules from different sources for calculation of physicochemical property data using ACD/PhysChem Suite algorithms within Pipeline Pilot. Results are then pushed into other programs for further analysis where necessary. All of this occurs in an automated fashion, providing chemists with one simple tool to analyze and prioritize molecules based on various properties and parameters.

To take advantage of this powerful integration in your research, simply log in and then request the integration component below. An ACD/Labs Account Manager will then contact you to ensure license compatibility before providing a download link for the integration component.

To request Integration of ACD/Labs Batch software, visit our website and log in.

ACD/Labs Calculator Add-ins for Symyx Draw
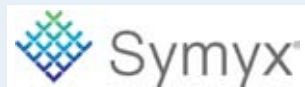
Get accurate predictions of molecular properties, chemical names, and spectroscopic parameters from ACD/Labs' predictive tools without leaving the Symyx Draw environment. Simple add-ins allow you to seamlessly integrate Symyx Draw with the ACD/Labs PhysChem, Name, and NMR modules you already use.

ACD/PhysChemSuite calculates properties such as $\log P$, $\log D$, pK_a, solubility, bioconcentration factor, absorption coefficient, and boiling point.

ACD/Labs NMR Predictors calculates ^{1}H, ^{12}C, and 2D NMR spectra, chemical shifts, and coupling constants for the compounds, based on their chemical structure.

ACD/Name generates accurate systematic names for almost any organic structure in accordance with IUPAC and CAS index type rules, and converts names to structures.

Use ACD/Labs' Predictive Power in Two Modes:

Calculator Mode
Run ACD/Labs programs in the background while using Symyx Draw to see predicted physiochemical properties, generate chemical names, or predict NMR chemical shifts and coupling constants, without leaving the Symyx Draw interface.

Application Mode
Step out of Symyx Draw to use ACD/Labs' predictors and nomenclature tools in their own environment. Chemical structures drawn in Symyx Draw are automatically transferred to the selected ACD/Labs program, allowing you to review details of how the calculation was made or to further search ACD/Labs databases.

The ACD/Labs calculator add-ins for Symyx Draw are currently only compatible with versions 2 and 3 of Symyx Draw.

Integration is possible only with valid licenses for any or all of the following: ACD/Name, ACD/HNMR Predictor, ACD/CNMR Predictor, ACD/2D NMR Predictor, or any ACD/Labs PhysChem predictor.

> To request the free ACD/Labs calculator add-in for
> Symyx Draw, go to our website:
> www.acdlabs.com/symyxdraw

ACD/Labs Extension for ChemDraw

CambridgeSoft ®
www.cambridgesoft.com

The ACD/Labs Extension for ChemDraw allows you to use CambridgeSoft ChemDraw™ as the interface for the ACD/Labs software you already use to predict NMR spectra, calculate physicochemical properties and search ACD/Labs databases.*

Predict CNMR, HNMR, XNMR, and 2D NMR spectra with ACD/Labs NMR Predictors.

Calculate pK_a, log$P$, log$D$, solubility, bioconcentration factor, adsorption coefficient, and boiling point with ACD/Labs PhysChem Suite.

Predict macroscopic properties such as molar volume, parachor, index of refraction, surface tension, density, dielectric constant, and polarizability with the free tools included in the extension.

Generate IUPAC and Index names either through integration with ACD/Name (commercial version) or using the free IUPAC naming feature (for molecules of up to 50 atoms and 3 ring structures) present in the extension.

Search through ACD/Labs databases (ACD/ChemFolder, spectral and physicochemical databases, and ACD/Dictionary), and view the results in either the ChemDraw interface or switch back to the ACD/Labs interface.

* Valid licenses for the appropriate ACD/Labs product are required to use the extension. The ACD/Labs Extension for ChemDraw is compatible with ChemDraw for Windows version 5 and later.

ACD/Labs Integration Components

ACD/Labs ActiveX controls give you the flexibility to bring chemical structure handling and spectral processing capabilities to your PC-based applications. They can be easily embedded into custom applications written in a variety of programming environments that support ActiveX technology: C++, Delphi, Basic, or web-related languages.

ACD/MolX

- Display chemical structures and other drawn images—the following formats are supported:
  - ACD/ChemSketch Document (*.sk2)
  - Molfile (*.mol) or molfile contents (as text strings in molfile format)
  - Rxnfile (*.rxn) or rxnfile contents (as text strings in rxnfile format)
  - SDfile (*.sdf)
  - ISIS/Draw Sketch File (*.skc)
  - CambridgeSoft ChemDraw Sketch File (*.cdx, *.chm)
- Set the display preferences to control the colors, sizes, and fonts of atomic symbols, and size, color, and thickness of bonds
- Calculate various physicochemical properties and generate the chemical names (depending on installed ACD/Labs modules) for the currently displayed chemical structure
- Display results in a dialog box or output them to a text file
- Activate registered ACD/Labs programs and use them to calculate available properties for the currently displayed chemical structure, or search the ACD/Labs databases (spectral, physicochemical, ChemFolder, or Dictionary)

ACD/SpecX

View analytical data from files in many formats. All of the NMR, MS, UV-Vis, IR, Raman, Curve, and Chromatography filters acceptable by ACD/SpecManager are available. Files can be local, on the network, or from FTP or HTTP addresses.

- Set the display preferences for each spectral technique; choose the colors and fonts for axis labels, grid, peaks, integrals, multiplets, assignments, and annotations
- Use Zoom In/Zoom Out tools
- Display tables of peaks, assignments, annotations, etc. in dialog boxes
- Coordinate with ACD/MolX so that scrolling through a table of assignments or fragments will display and highlight the assigned chemical structure.

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Worldwide Offices & Distributors

ACD/Labs has distributors in many countries throughout Europe, Asia, and Africa. Direct sales are available for North America, UK, France, Germany, and a number of countries in the Asia-Pacific region.

Please review the list of distributors at www.acdlabs.com/distributors, or contact ACD/Labs and we will put you in touch with the appropriate distributor.