The Ultimate Software for NMR Analysis

NMR Workbook Suite

NMR Workbook Suite is more powerful than ever. Using its advanced features, you can feel confident about your analysis and experience a workflow that will save you time each and every day.

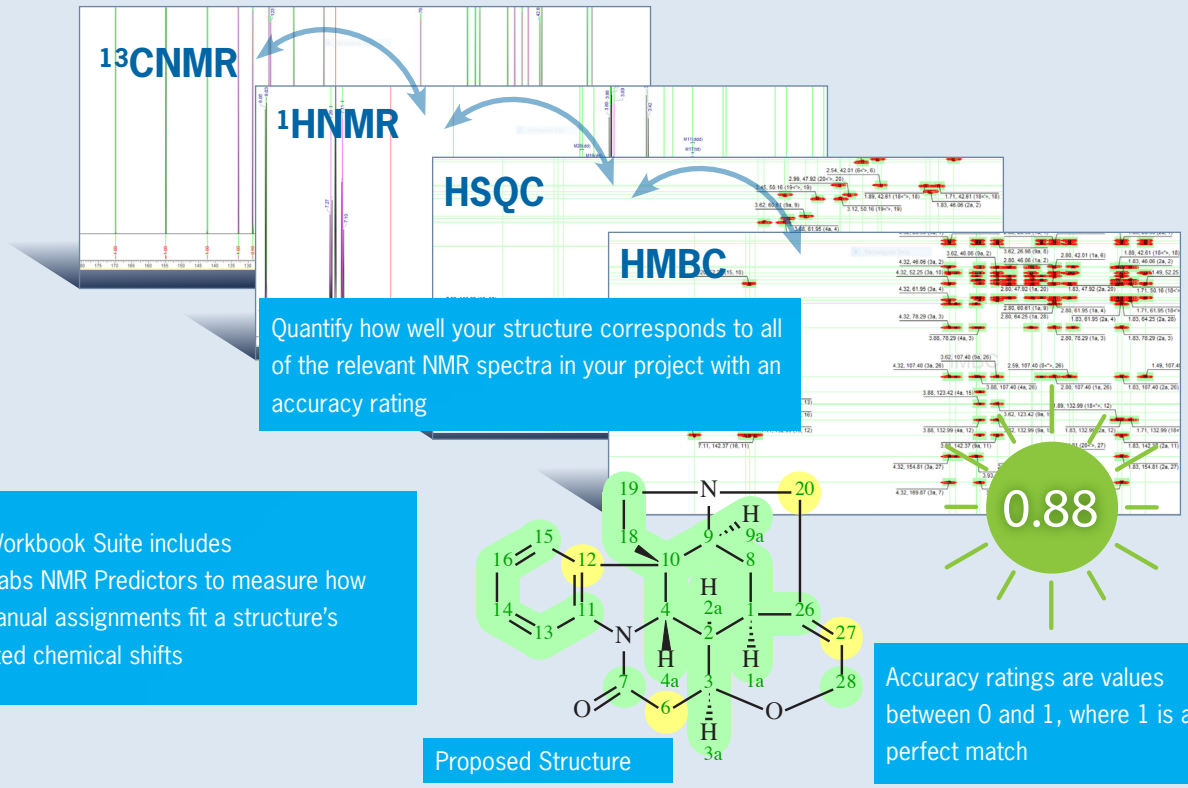
www.acdlabs.com/nmrworkbook

ACD/Labs®

ACD/NMR Workbook Suite provides advanced processing and interpretation tools so that you can deliver fast turnarounds on proof-of-structure reports. As part of the Spectrus Platform, the software radically simplifies workflows ensures reliable analysis and and makes the reporting process faster than ever before.

Analyze Multiple Spectra Quickly and Accurately

Simultaneously analyze and assign peaks across multiple data sets



Quantify how well your structure corresponds to all of the relevant NMR spectra in your project with an accuracy rating

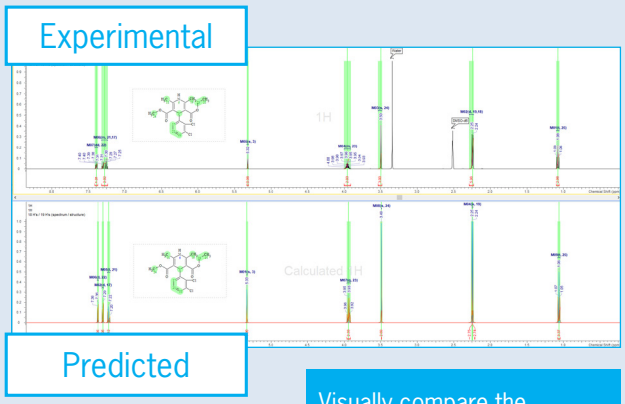
NMR Workbook Suite includes ACD/Labs NMR Predictors to measure how well manual assignments fit a structure's predicted chemical shifts

Proposed Structure

Accuracy ratings are values between 0 and 1, where 1 is a perfect match

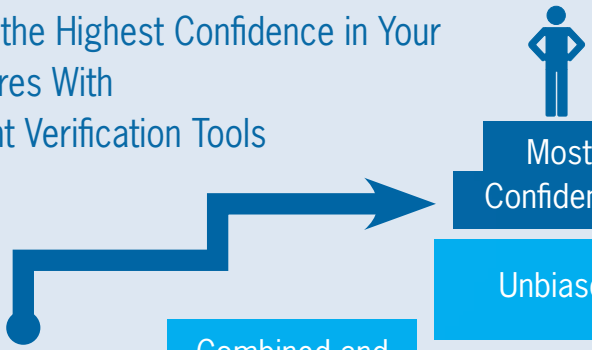
Industry Standard Spectral Prediction

Predict 1D and 2D spectra for small molecules, polymers, biomolecules, and mixtures.



Visually compare the experimental and the predicted NMR spectra

Ensure the Highest Confidence in Your Structures With Different Verification Tools



Single Molecule

Verify an individual structure using automated spectral searching and matching tools.

Combined and Concurrent

Verify your proposed structures against a select number of isomeric structures and/or user-defined alternative structures.

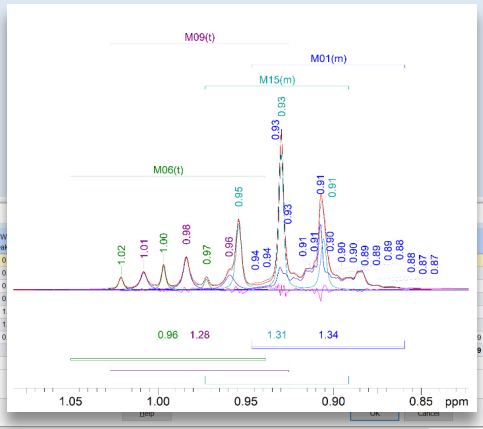
Most Confidence

Unbiased

Verify your proposed structure against all alternative structural and *cis/trans* isomers using a selection of NMR spectra that can support elucidations (i.e., ^{1}H, ^{13}C, HSQC, HMBC).

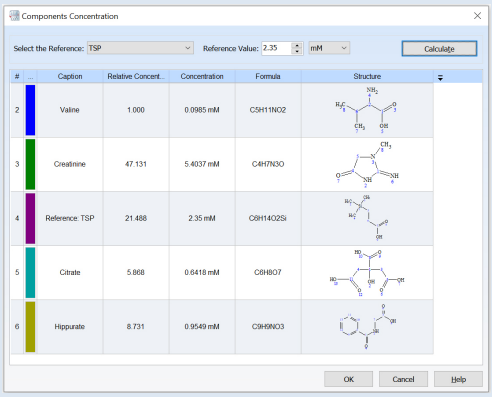
Streamline Your 1D NMR Mixture Analysis

Deconvolute, obtain kinetic information, and calculate relative and absolute concentrations from NMR data of highly complex mixtures (e.g. metabolomic or environmental samples) of known composition and variable component concentrations.



Easily analyze highly complex mixtures with strong multiplet overlaps

Automatically annotate the peaks and calculate the component areas using the normalized information of the target components



Display the concentrations calculated relative to the reference, formula, and structures of the components

Dereplication Has Never Been So Efficient

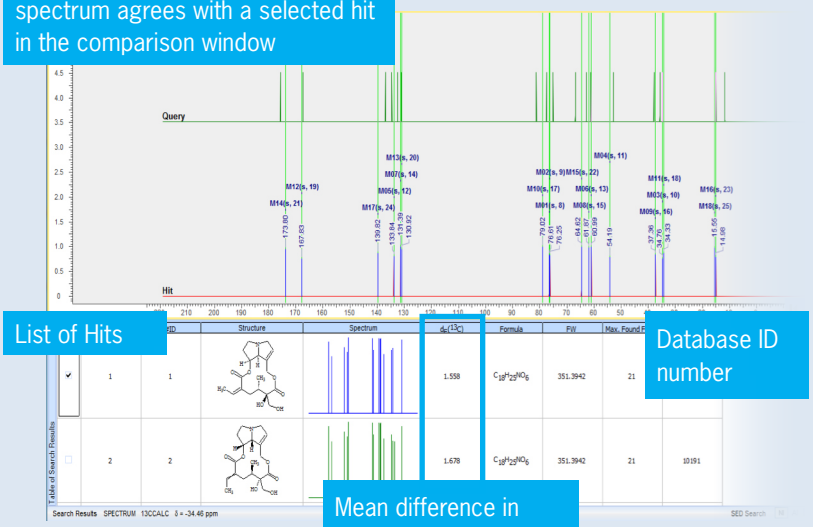
To simplify unknown compound identification/ dereplication, the Known Structure Search Add-On determines whether a compound's experimental ^{13}C resonances match the predicted signals of known structures.

This add-on uses ACD/Labs' leading proprietary NMR prediction neural network algorithms.

- Access a database of ~100 million known structures collected from open chemistry databases (e.g. PubChem) with predicted ^{13}C NMR signals
- Rapidly search using any combination of 1D (^{13}C NMR) or 2D (^{1}H-^{13}C HSQC and ^{1}H-^{13}C HMBC) signal entries within a project

Available as an add-on for Spectrus Processor and NMR Workbook and included in Structure Elucidator.

Visualize how well your query spectrum agrees with a selected hit in the comparison window



List of Hits

Database ID number

Mean difference in experimental and predicted chemical shifts

Process All Your Other Analytical Data Too!

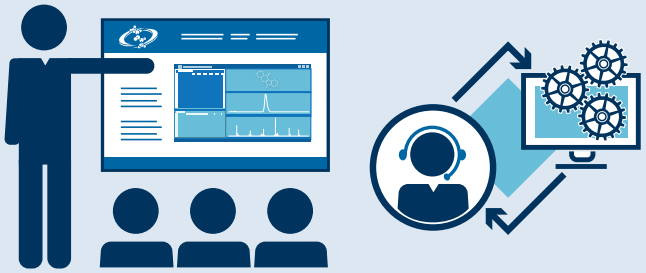
NMR Workbook Suite comes with general processing tools for LC/UV/MS, IR, Raman and other analytical techniques. Most major instrument formats are supported.

Maximize Your Software Capabilities With Minimal Learning Time

We're equipped to help you.

We offer training courses led by our Technical and Scientific Services Staff both on-site and on-line.

Our software comes with excellent technical support from experienced professionals.



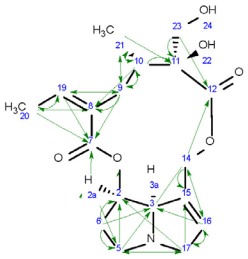
"ACD/Labs couldn't have a better sales and support staff. They are one of the main reasons to go with ACD/Labs."

Quickly Create Customized Reports

Generate comprehensive reports of your NMR analyses and pre-formatted multiplet reports in one click. Export to Microsoft Word, Excel, PowerPoint, Adobe PDF, and ChemSketch.

#	Atom#	C Label	C Shift	XHn	H Label	H Shift
1	21	M01	11.702	CH3	H 1	0.884
2	20	M02	15.062	CH3	H 4	1.864
3	6	M03	34.769	CH2	H 5	2.144
4	6	M03	34.769	CH2	H 7	2.416
5	10	M04	35.664	CH	H 2	1.712
6						
7						
8						
9						
10						
11						
12						
13						
14						
15						
16						
17						
18	11	M12	81.348	C		
19	15	M13	131.252	C		

Organize chemical shifts, assignments, and coupling constants in an automatically generated table

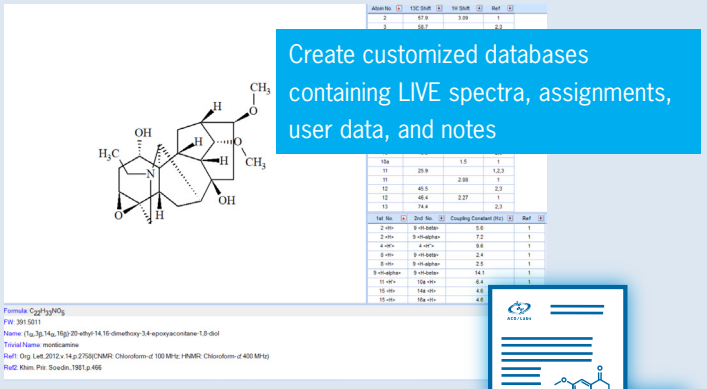


Easily visualize 2D Correlations between nuclei

^{1}H NMR (600 MHz, CHLOROFORM-*d*) δ ppm 0.88 (d, *J*=6.70 Hz, 3 1.74 (m, 1 H) 1.80 (m, 1 H) 1.86 (dd, *J*=7.05, 1.55 Hz, 2 H) 2.10 - 2.20 (m, 1 H) 2.56 (dd, *J*=15.68, 2 (ddd, *J*=15.68, Hz, 1 H) 3.96 (br d, *J*=2.23 Hz, 1 H) 5.03 (t, *J*=3.18 Hz, 1 H) 5.53 (d, *J*=11.08 Hz, 1 H) 5.75 (qd, *J*=7.07, 1.12 Hz, 1 H) 6.24 (d, *J*=1.55 Hz, 1 H)

Automatically generate formatted Multiplet Reports

Never Lose Data



Create customized databases containing LIVE spectra, assignments, user data, and notes

Easily search your own and commercial databases using structure, spectral, and text based parameters

For easy data sharing, entries can be uploaded to both local and remote servers

Learn more and request a demo at: www.acdlabs.com/nmrworkbook

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