Optimizing Your Analysis: The Many Ways NMR Predictors Can Be Applied

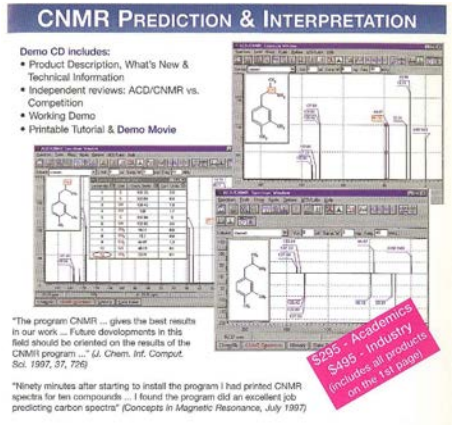
Grace Kennedy

ACD/Labs NMR Software Symposium

March 4th, 2018

ACD/Labs

Evolution of NMR Spectra Prediction



2002
1,700,000 ^{13}C shifts
1,200,000 ^{1}H shifts

2008
2,547,046 ^{13}C shifts
1,755,262 ^{1}H shifts

2017
3,295,442 ^{13}C shifts
2,401,629 ^{1}H shifts
369,210 C+H structures
49,081 ^{19}F shifts
37,911 ^{31}P shifts

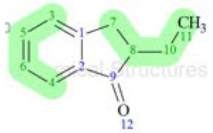
SpecManager Platform

Spectrus Platform

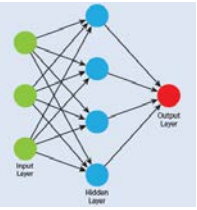
1994	1995	1998	2006	2008	2011	2017
ACD/CNMR	ACD/HNMR	ACD/XNMR ACD/2DNMR	Neural Network Predictions v. 1	Neural Network Predictions v. 2 Improved HNMR and CNMR algorithms New Incremental prediction schemes	ACD/Spectrus Spectrus Platform introduced	Predictions for mixtures, Biosequences, Pure Shift spectra. Full incorporation into Spectrus Platform

The Ways NMR Predictors Can Be Applied

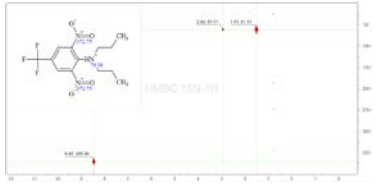
Enhance structure verification using NMR predictions



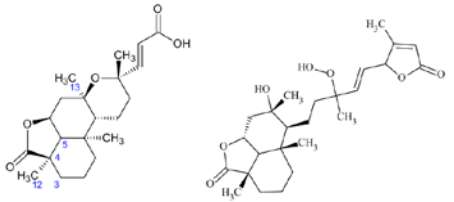
Improve NMR prediction accuracy through training



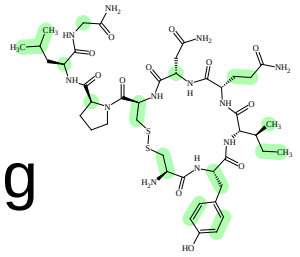
How you can use 2D NMR predictions to optimize instrument time



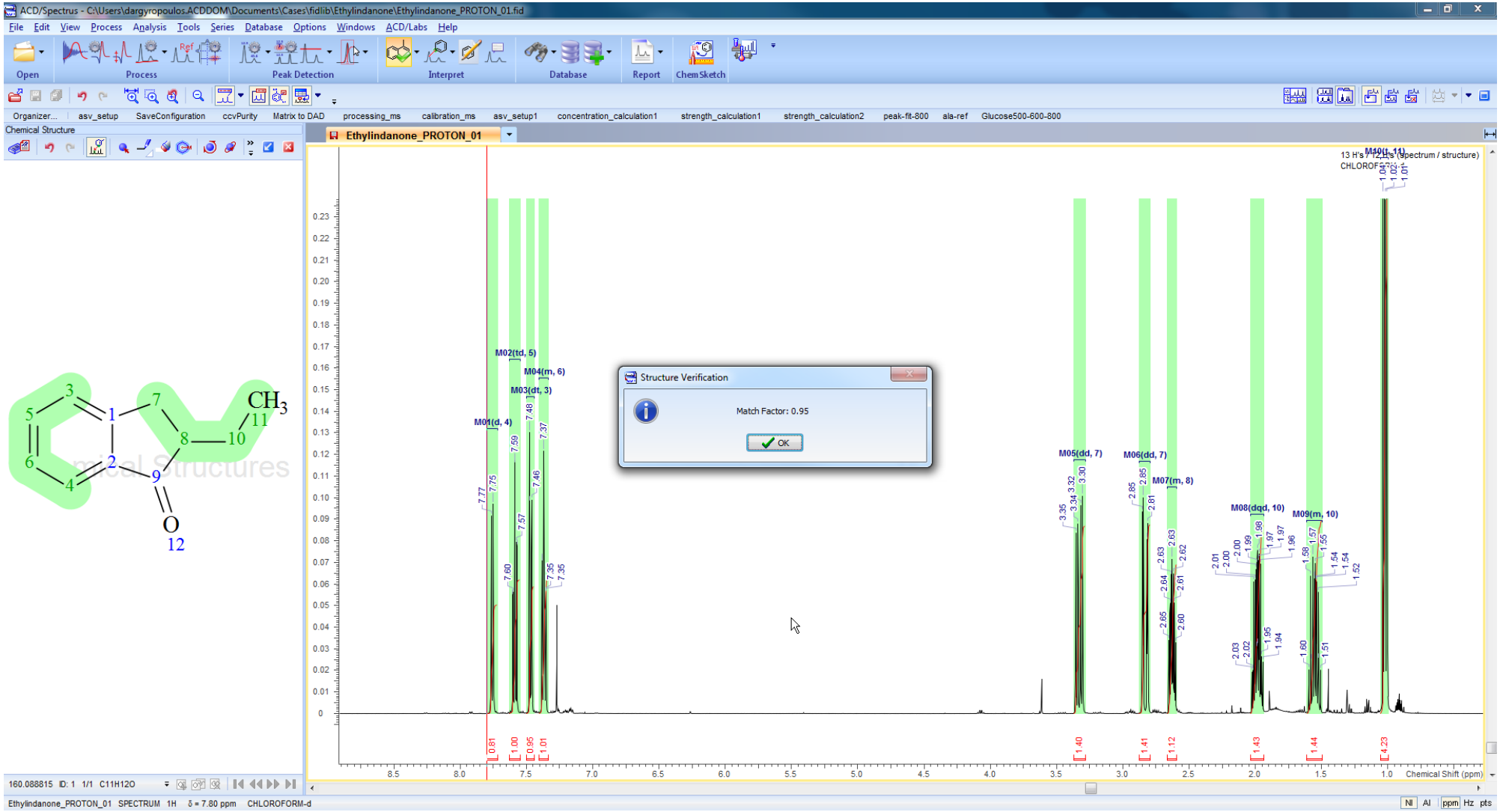
How to use the NMR predictors for analyzing mixtures and complex ^{1}H NMR spectra



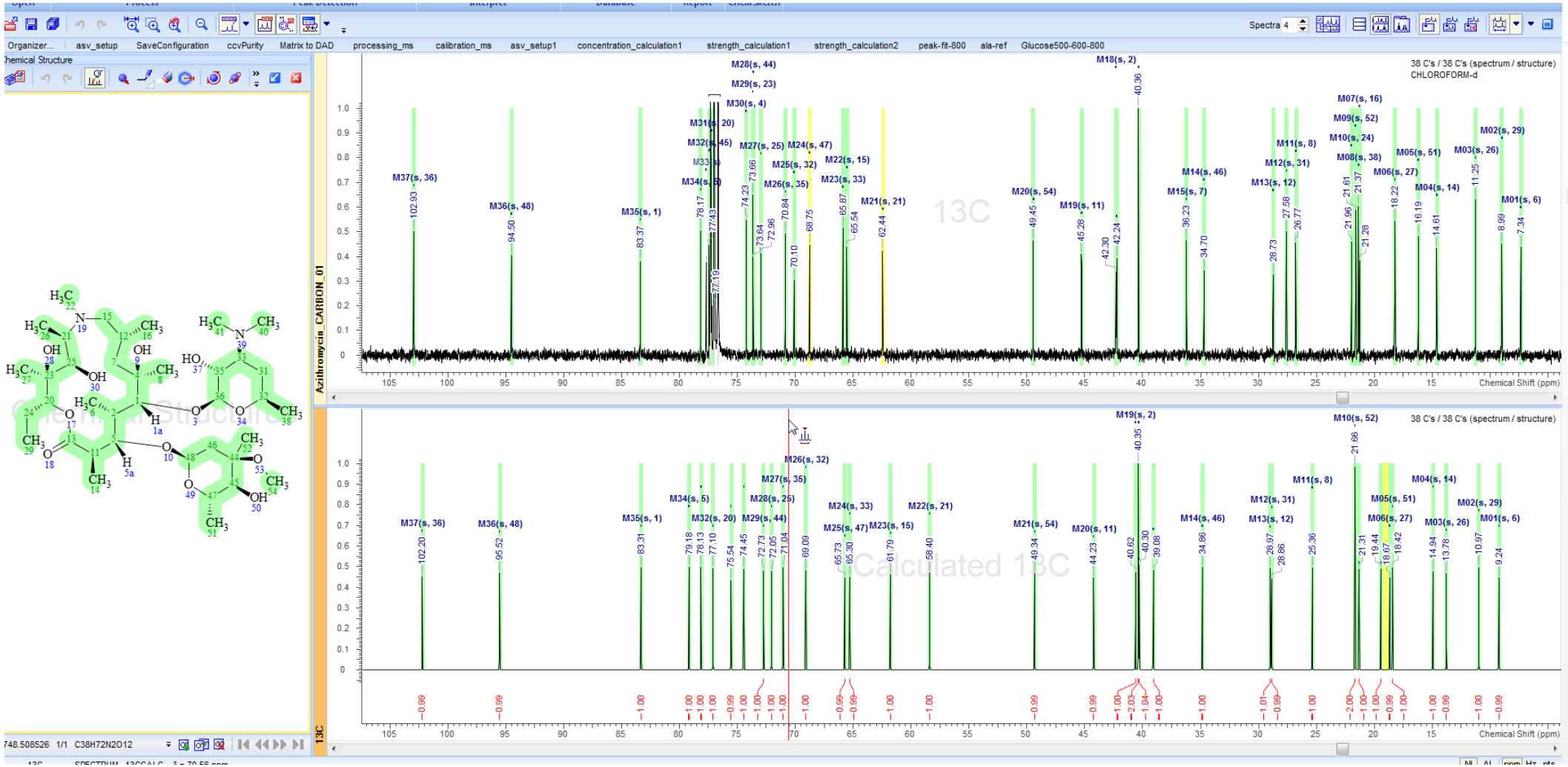
How to use the NMR predictors for biosequencing



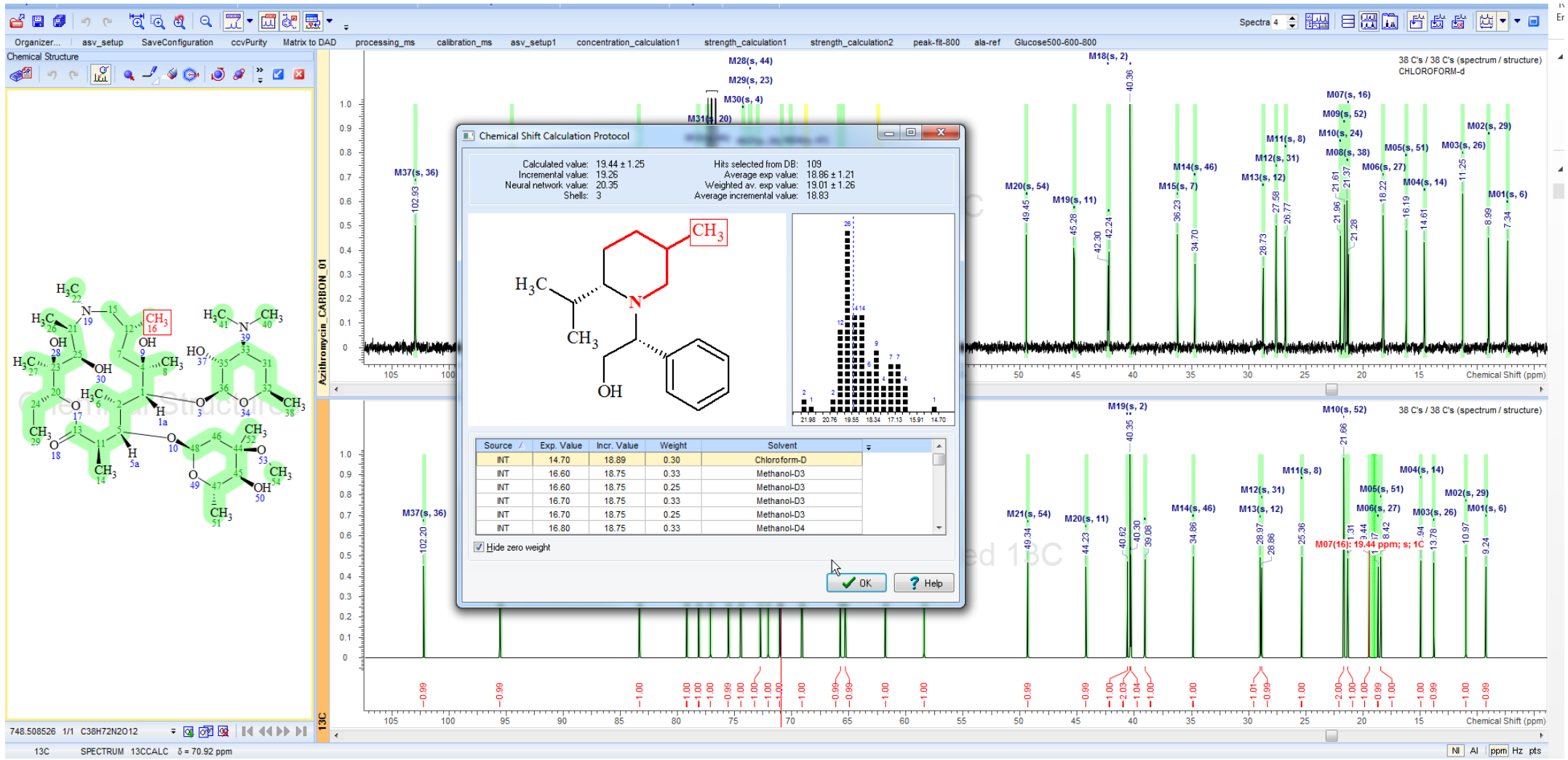
Enhance Verification with NMR Predictions



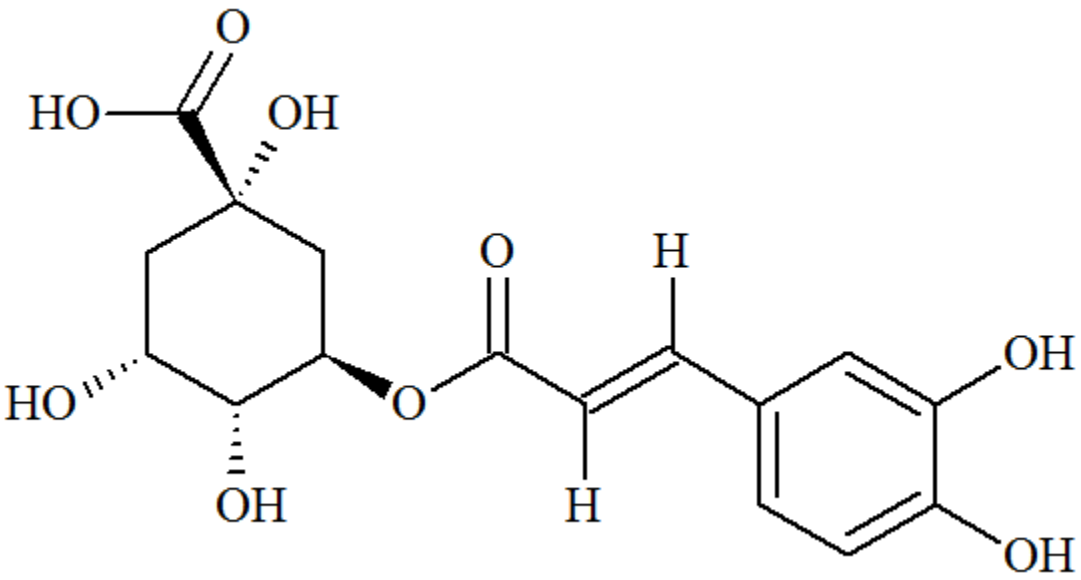
Enhance Verification with NMR Predictions



Enhance Verification with NMR Predictions



NMR Predictor Database Built from Literature



Formula: $C_{16}H_{18}O_9$

FW: 354.3087

Name: 3-(((2*E*)-3-(3,4-dihydroxyphenyl)prop-2-enoyl)oxy)-1,4,5-trihydroxycyclohexanecarboxylic acid

Trivial Name: chlorogenic acid

Ref1: J. Nat. Prod.,2004,v.67,p.1818(CNMR: Methanol-d_4; 125 MHz; 25 C; HNMR: Methanol-d_4; 500 MHz; 25 C)

Ref2: Chem. Pharm. Bull.,1988,v.36,p.87(HNMR: Acetone-d_6, Water-d_2; 200 MHz)

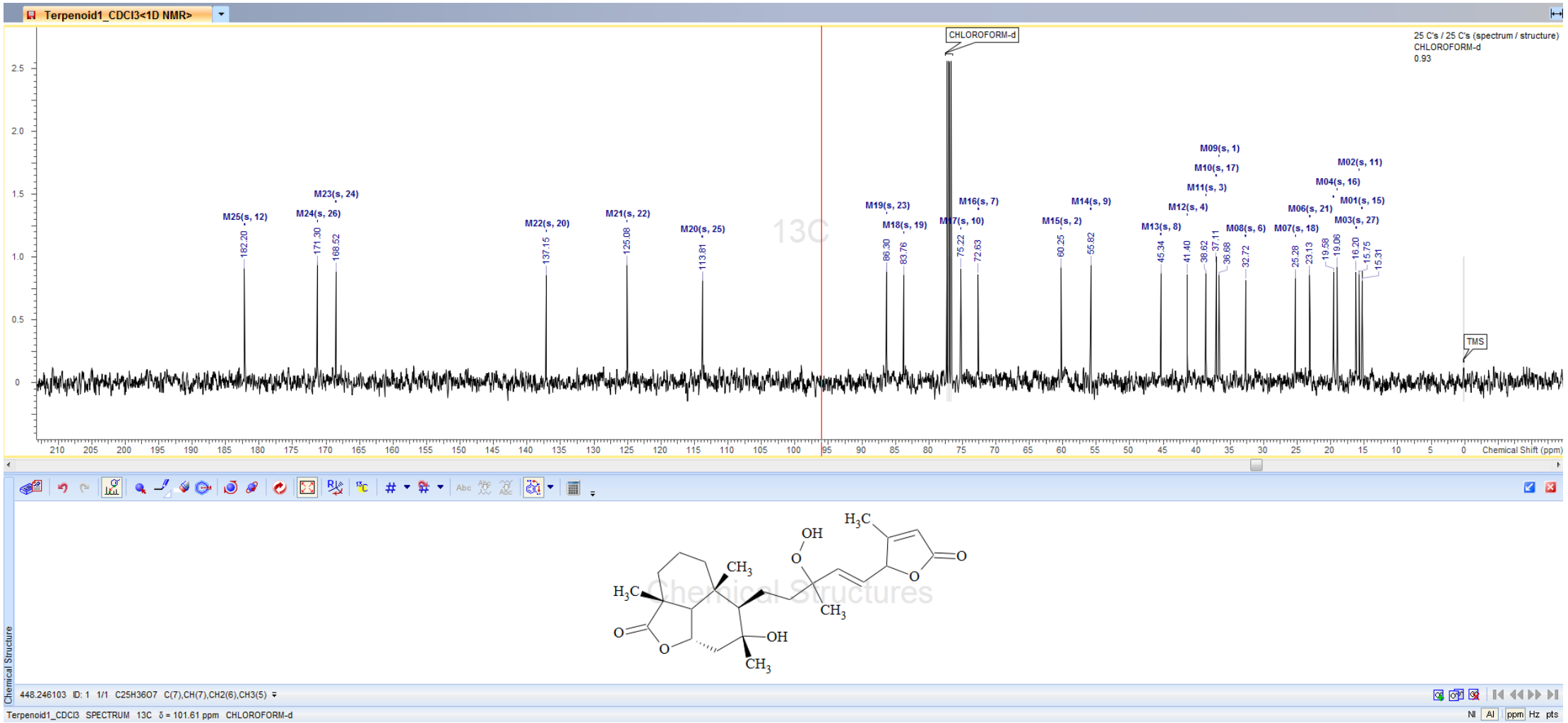
Ref3: J. Nat. Prod.,1999,v.62,p.405(CNMR: Methanol-d_4, Water-d_2; HETCOR, COLOC; 75 MHz)

Ref4: Chem. Pharm. Bull.,1988,v.36,p.807(CNMR: 100 MHz)

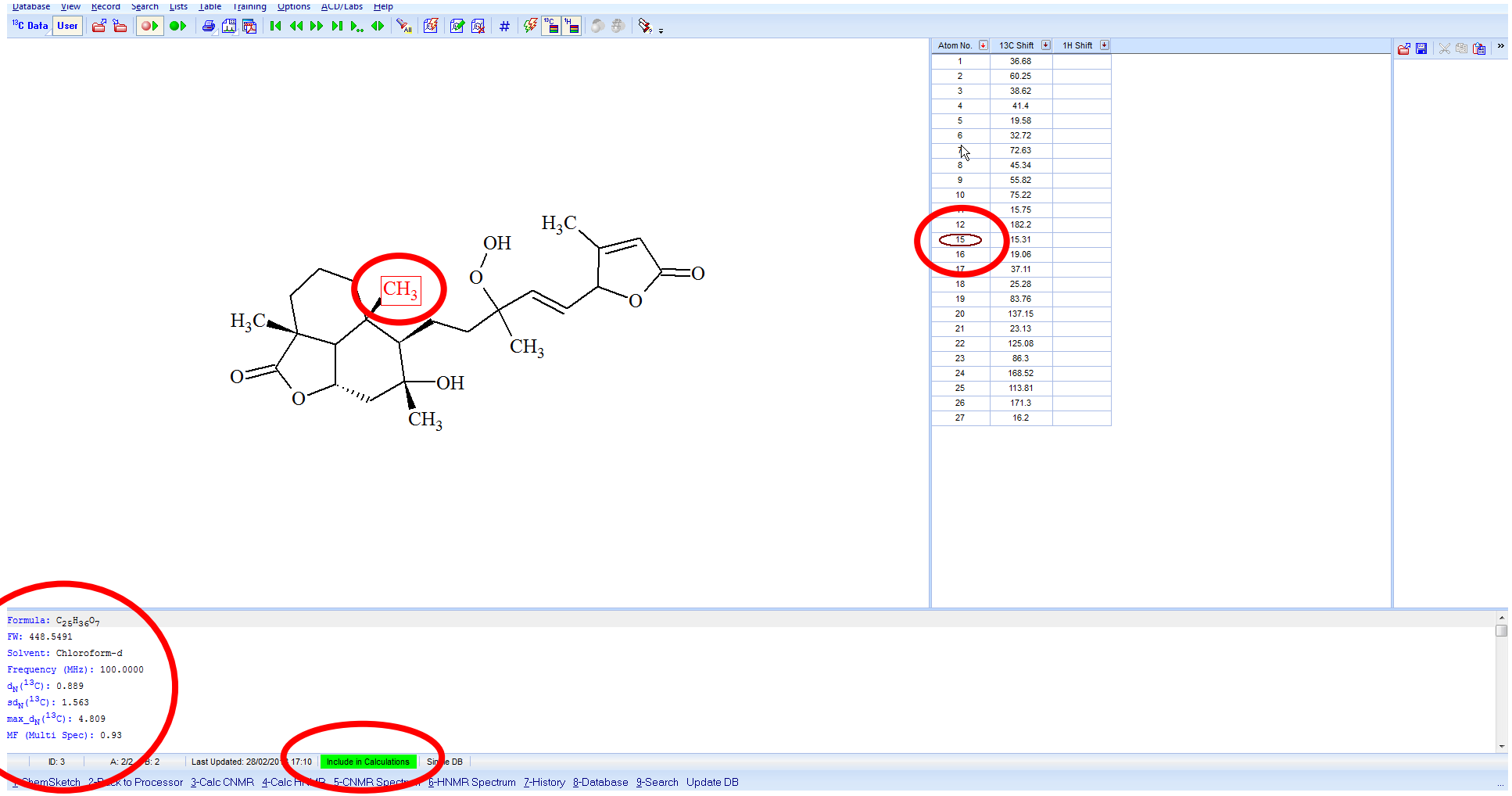
Database Statistics

	Structures	Shifts	Coupling Constants
C+H NMR Database	369,210	4,973,786	998,168
CNMR Database	240,361	3,295,442	132,792
HNMR Database	260,342	2,401,629	908,473
NNMR Database	10,216	24,277	5,077
FNMR Database	26,069	49,081	57,662
PNMR Database	31,102	37,911	42,364

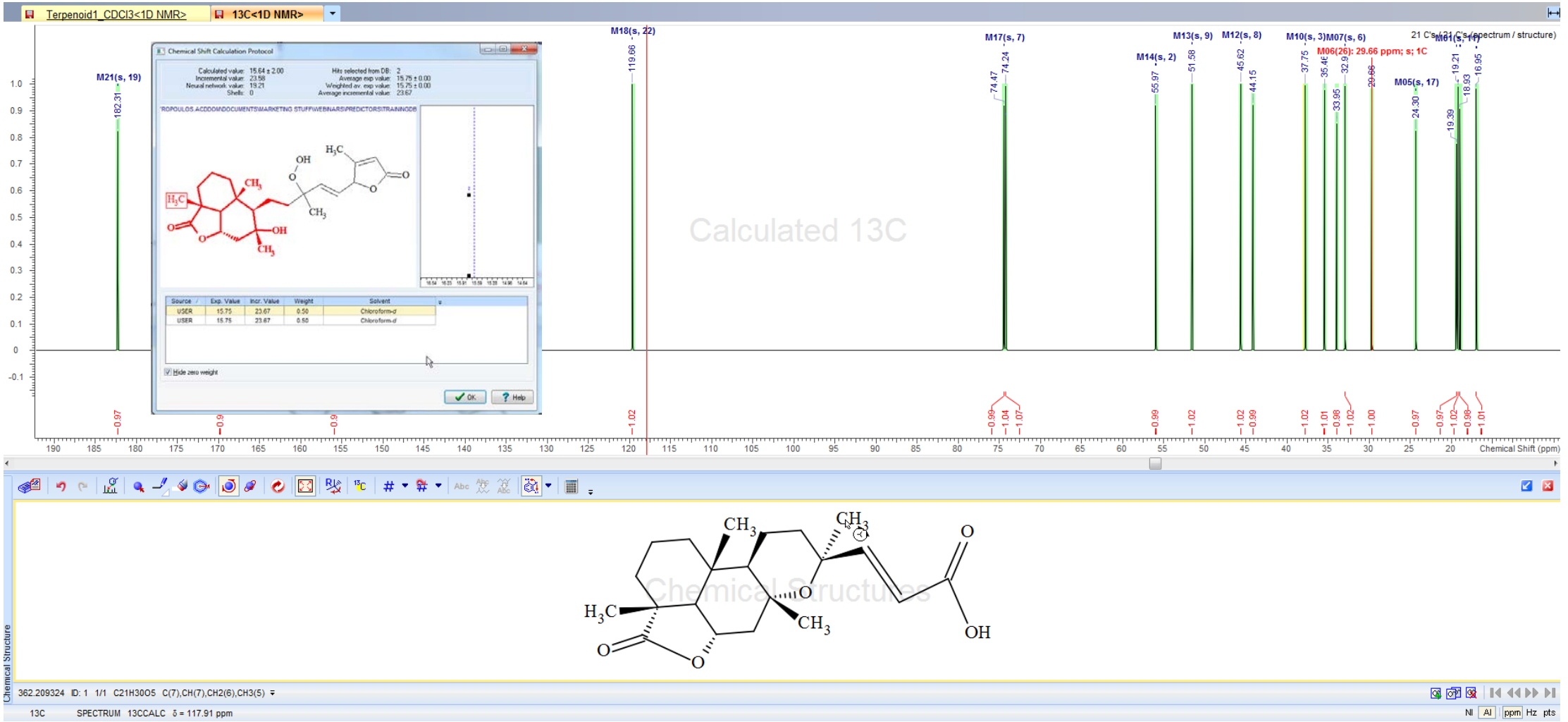
Training the NMR Predictor Database



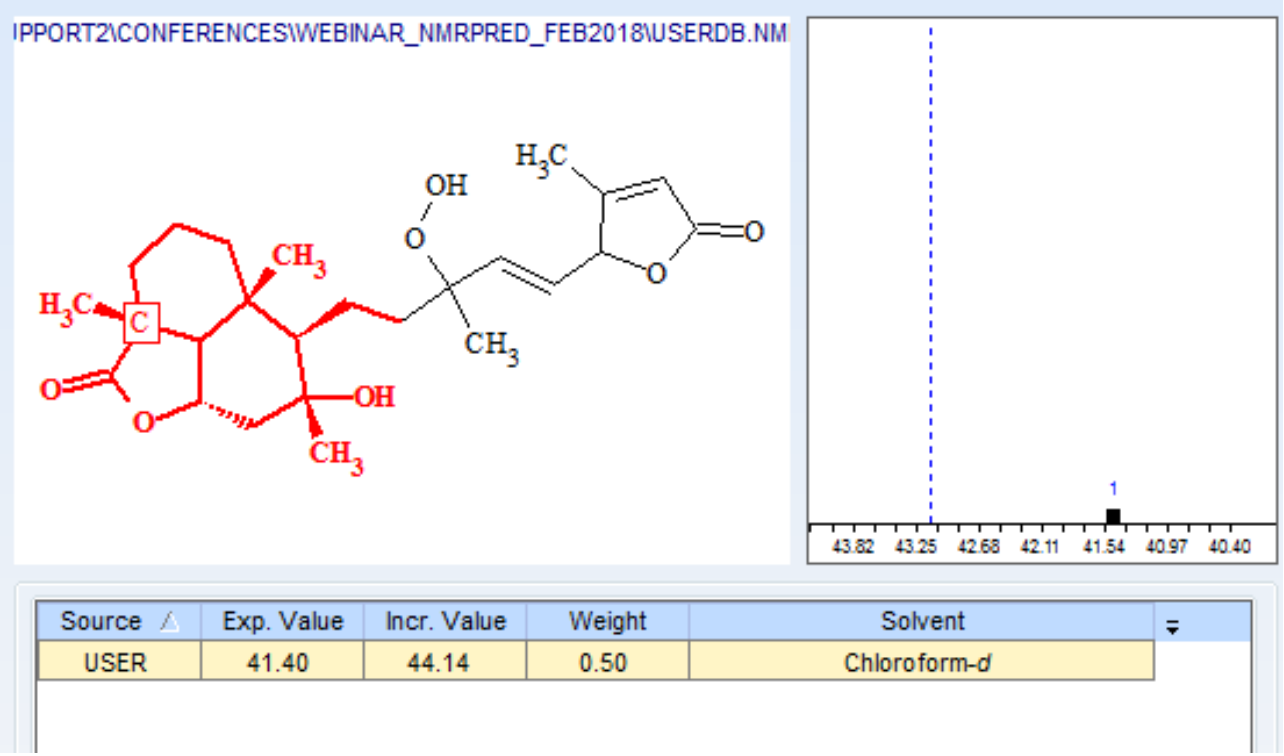
Training the NMR Predictor Database



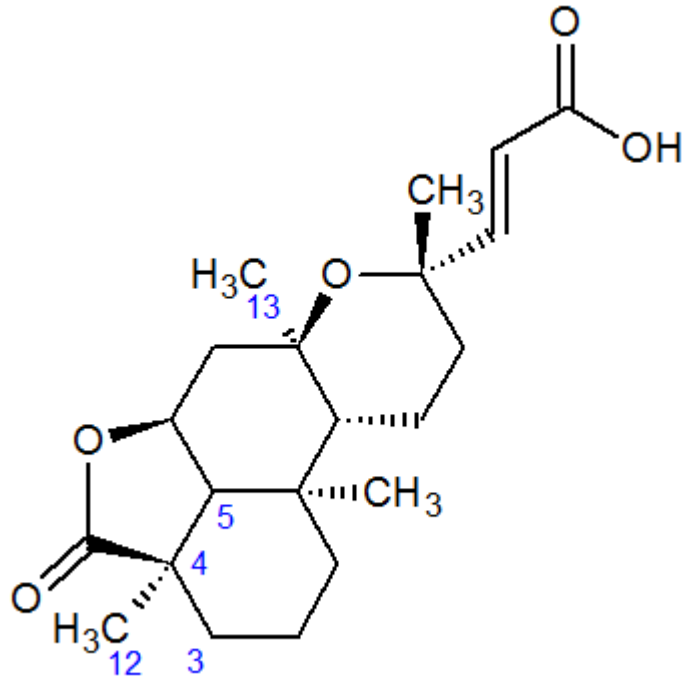
Training the NMR Predictor Database



Accurately Predict Novel Compounds



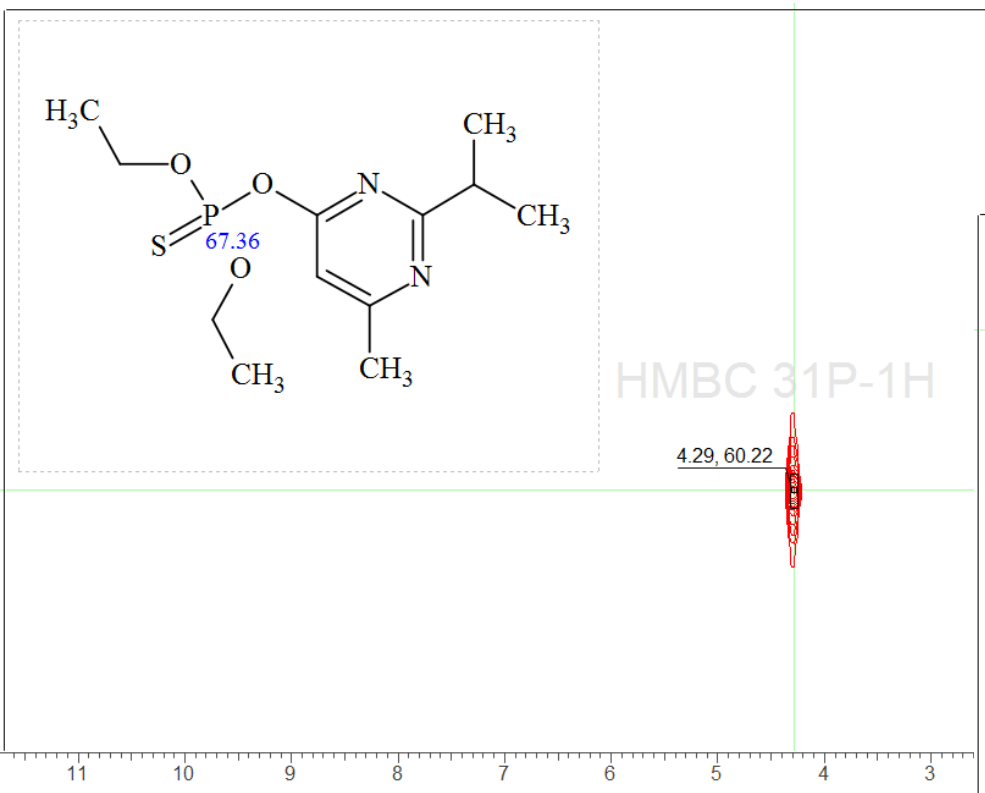
Source	Exp. Value	Incr. Value	Weight	Solvent
USER	41.40	44.14	0.50	Chloroform-*d*

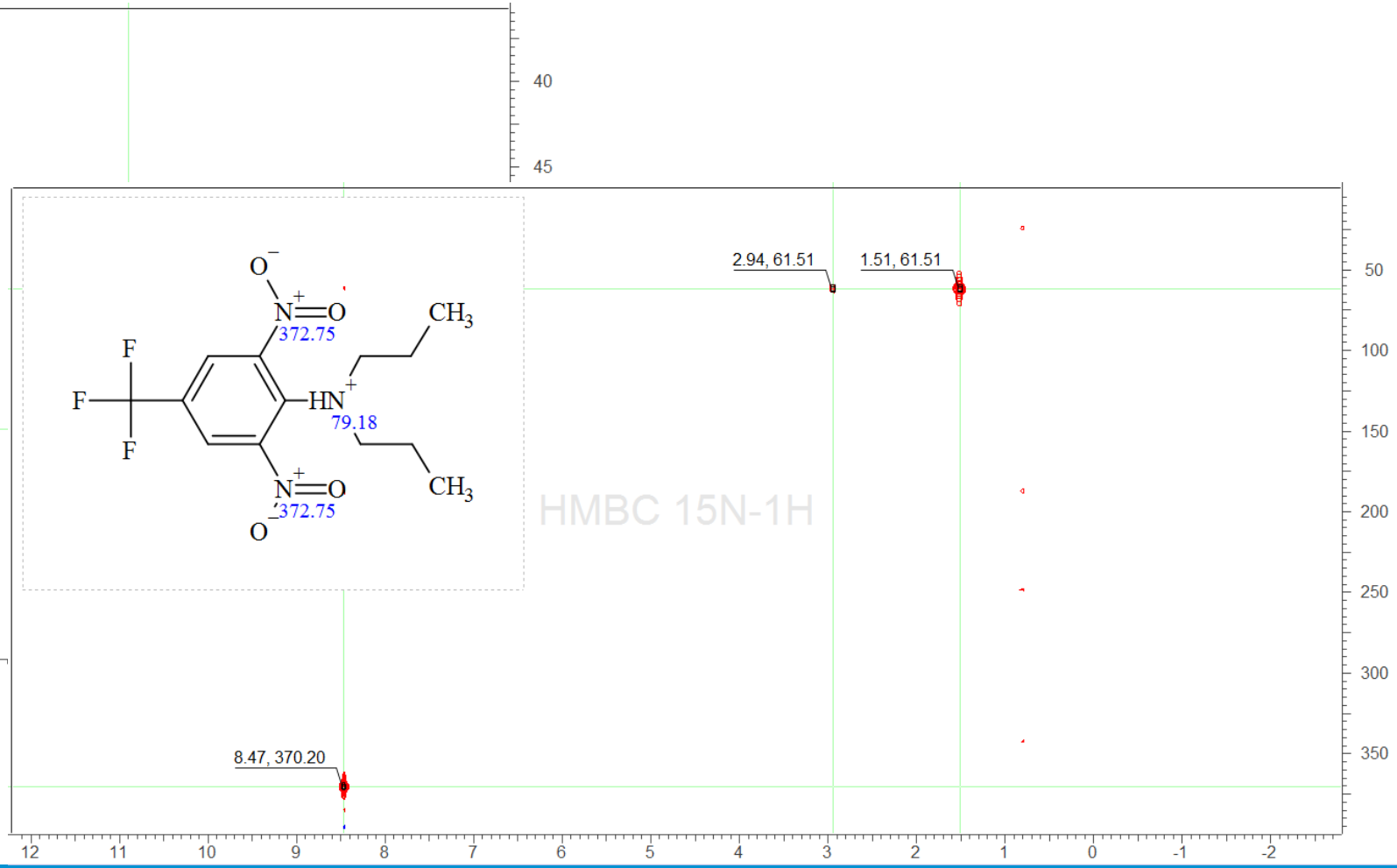


J. Nat. Prod., 2010, v. 73, 10, 1601–1605

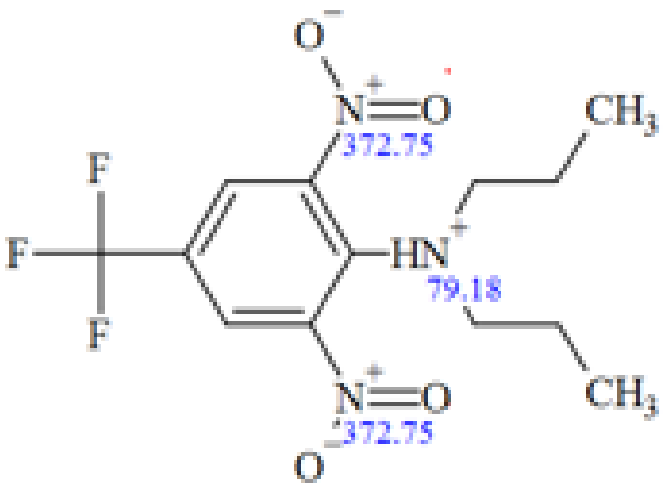
^{15}N, ^{19}F, ^{31}P NMR Prediction

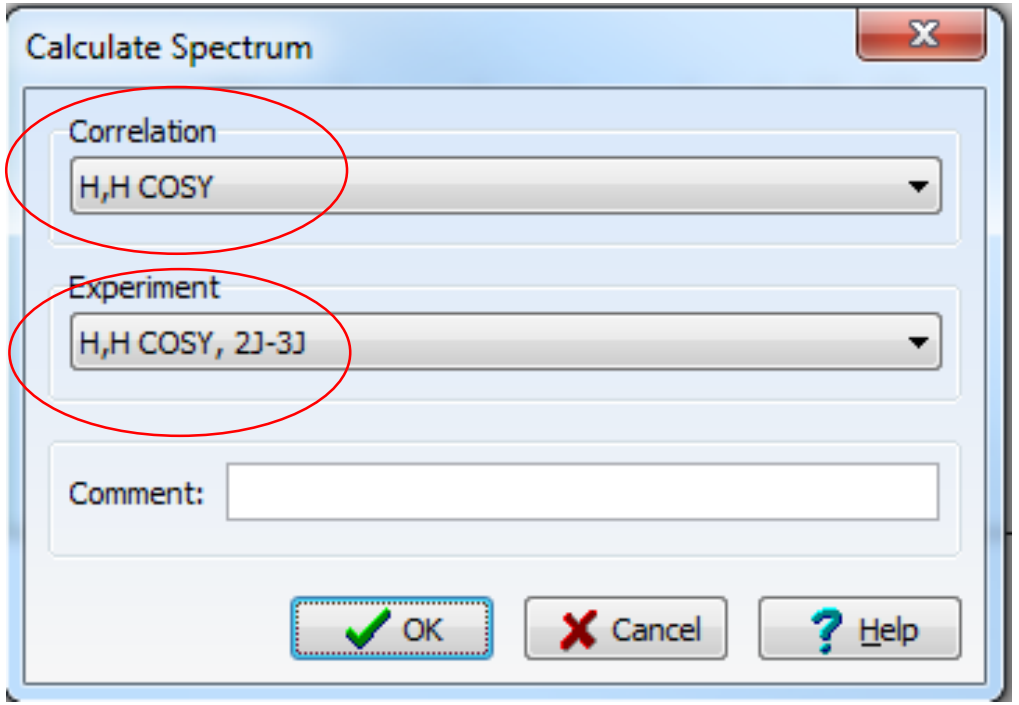
- Determine spectral widths based on expected chemical shifts



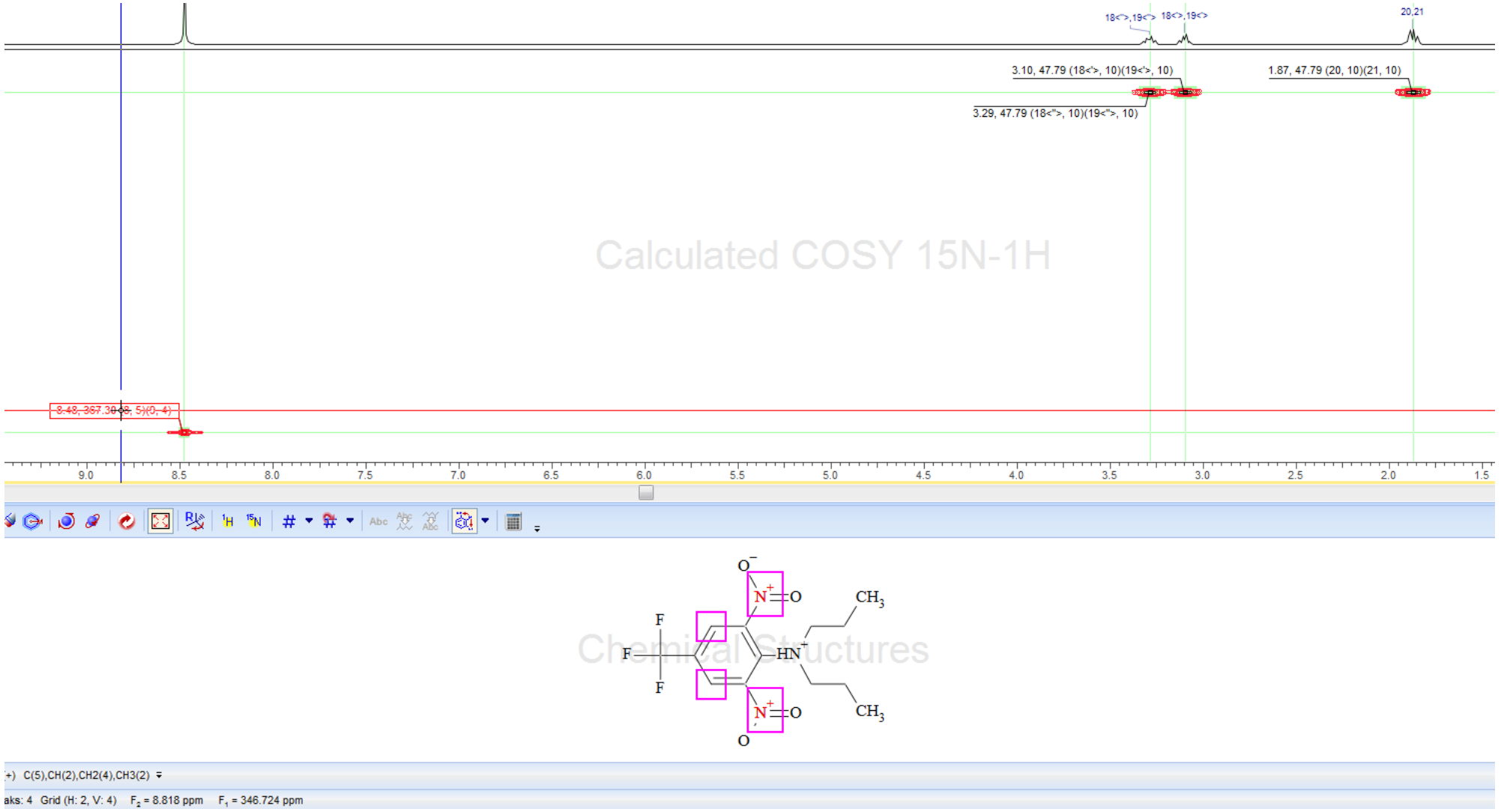


Optimize Instrument Time with 2D NMR Predictions

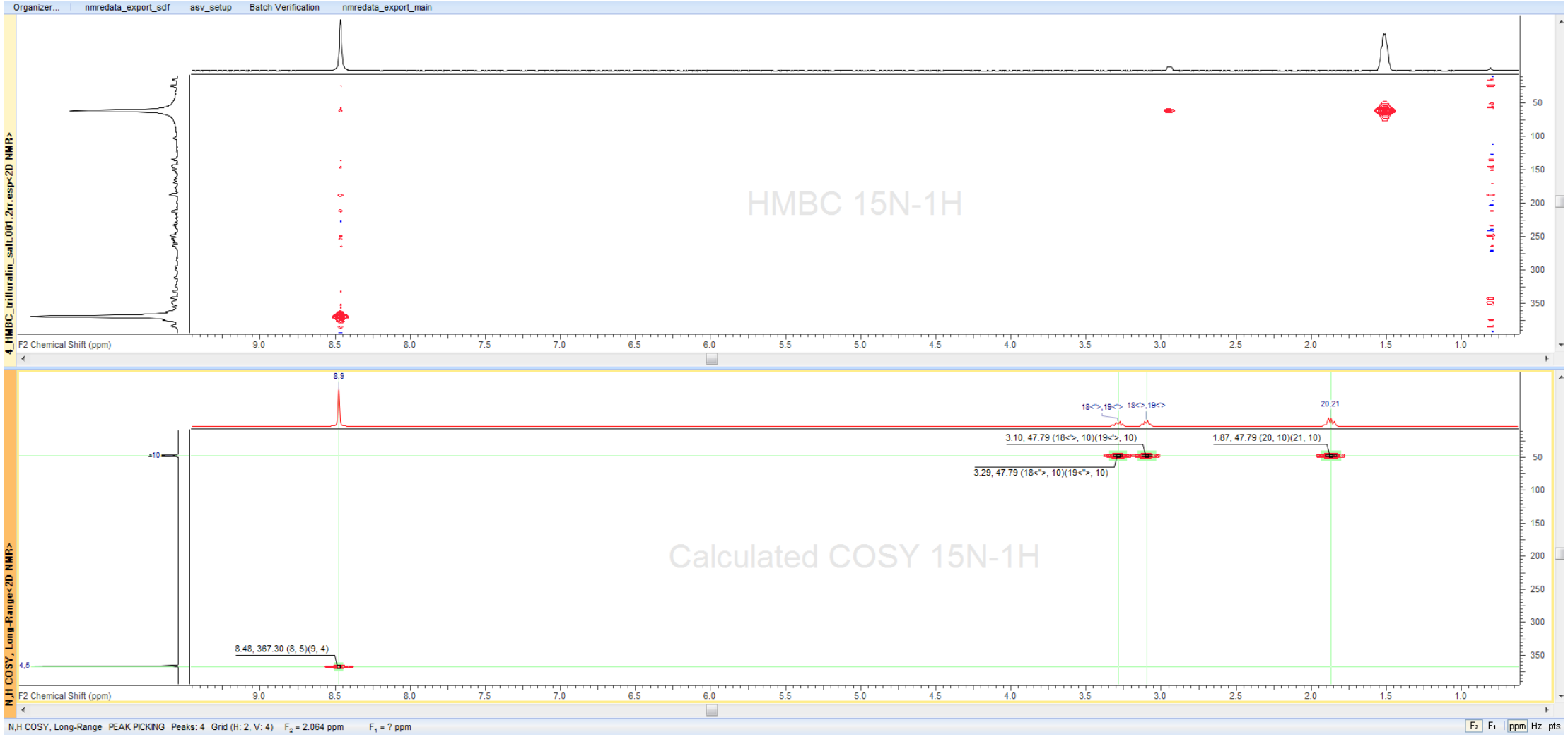




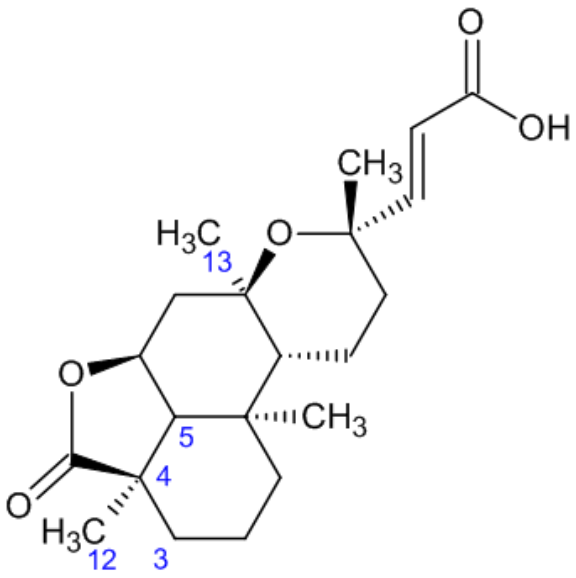
Optimize Instrument Time with 2D NMR Predictions

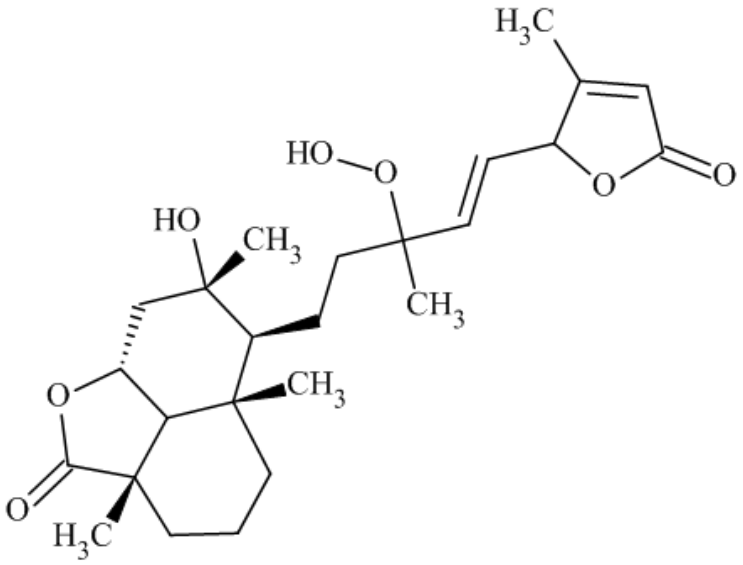


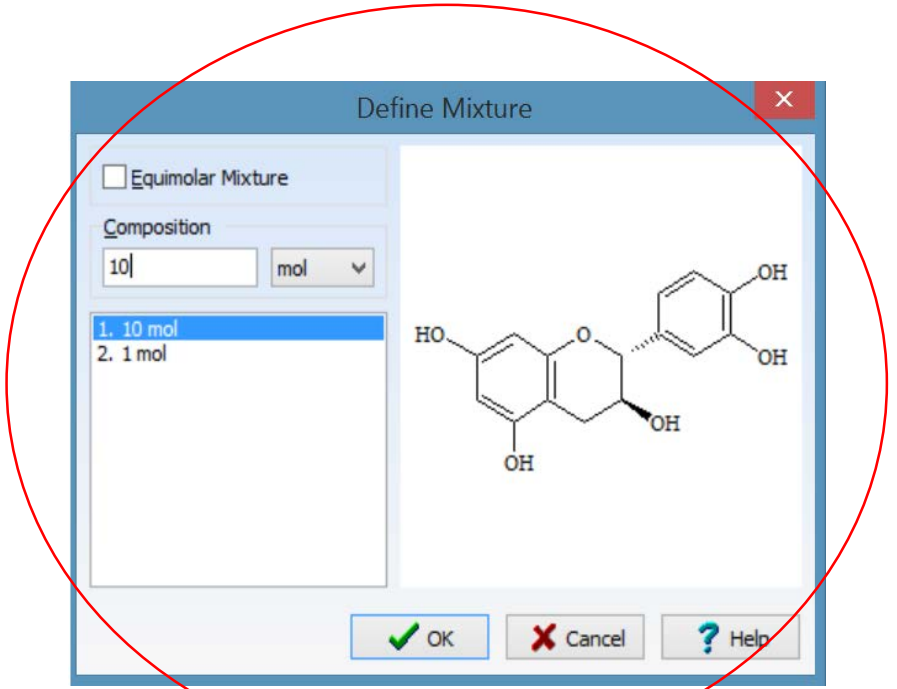
Optimize Instrument Time with 2D NMR Predictions



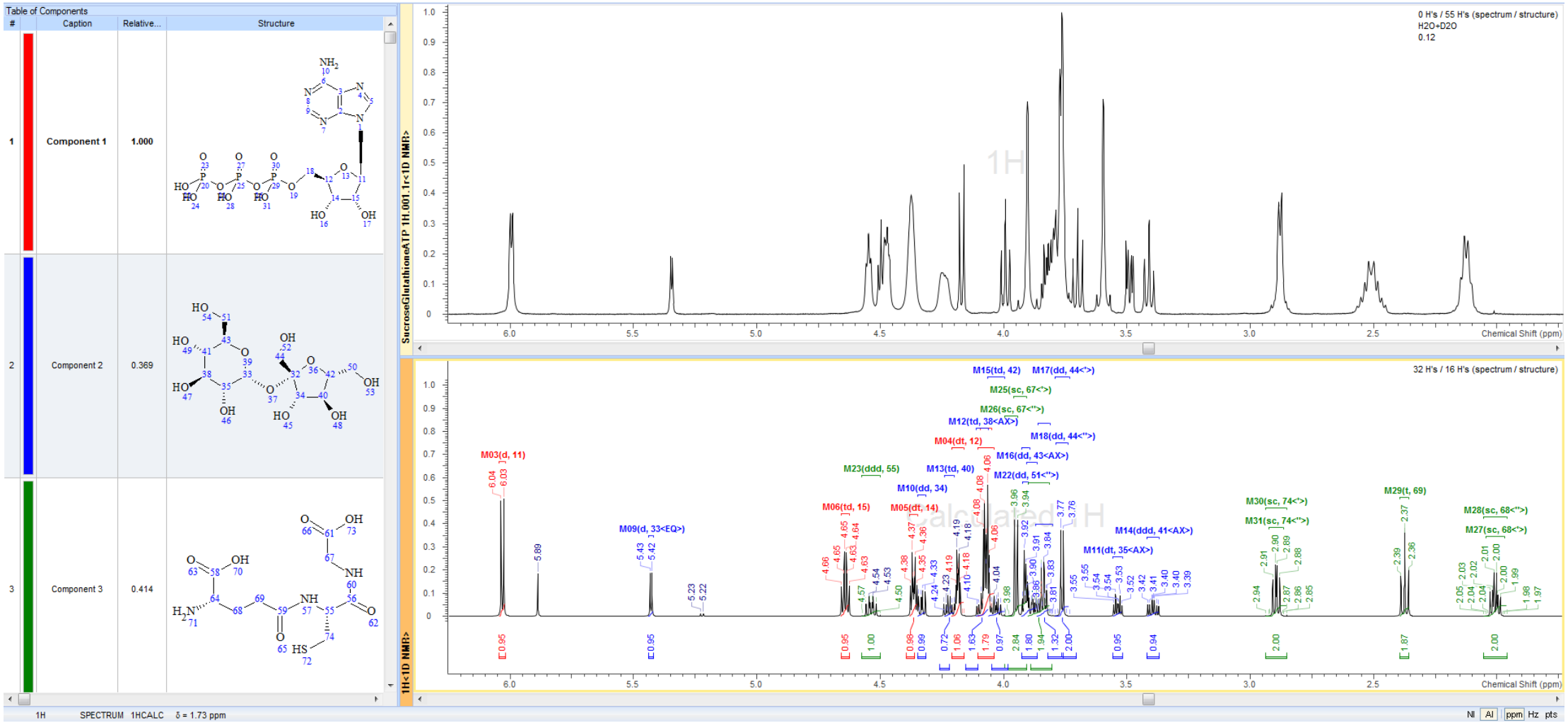
Predicting NMR for Mixtures







Predicting Spectra of Mixtures



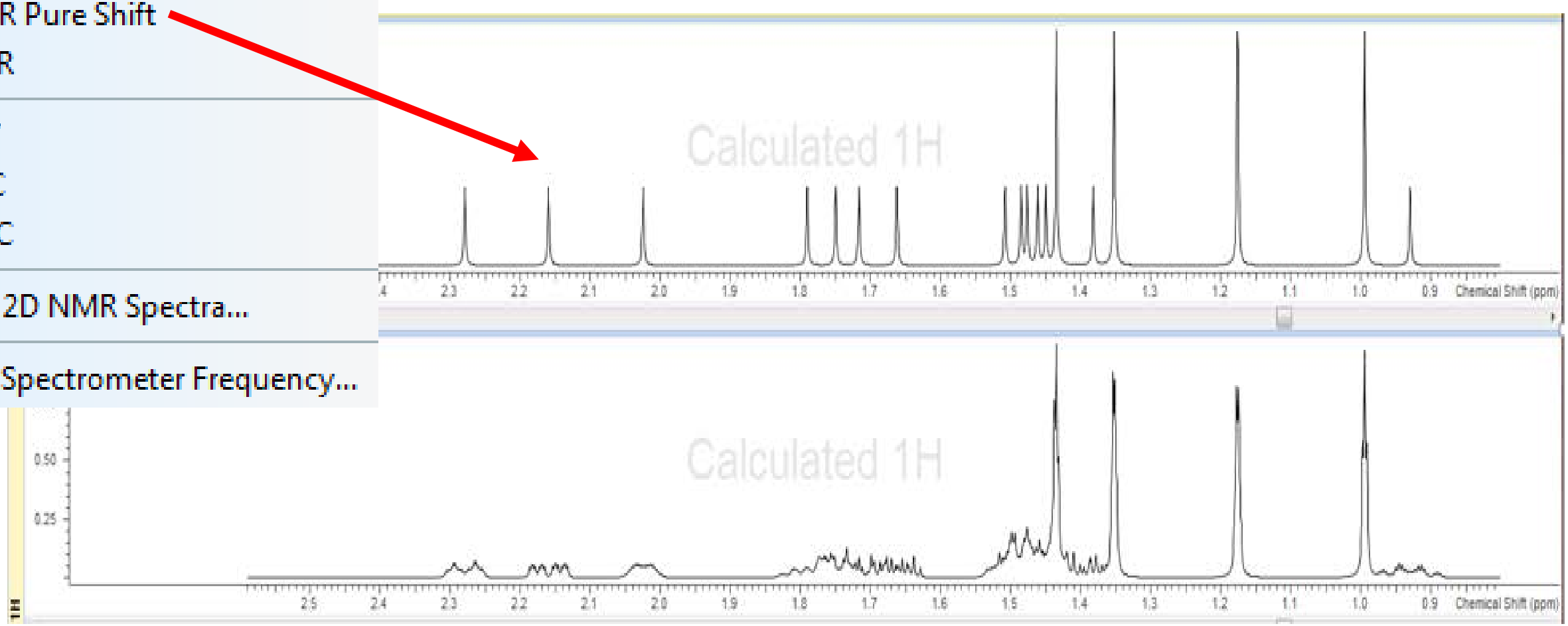
Pure Shift ^{1}H Prediction Capabilities

HNMR
HNMR Pure Shift
CNMR

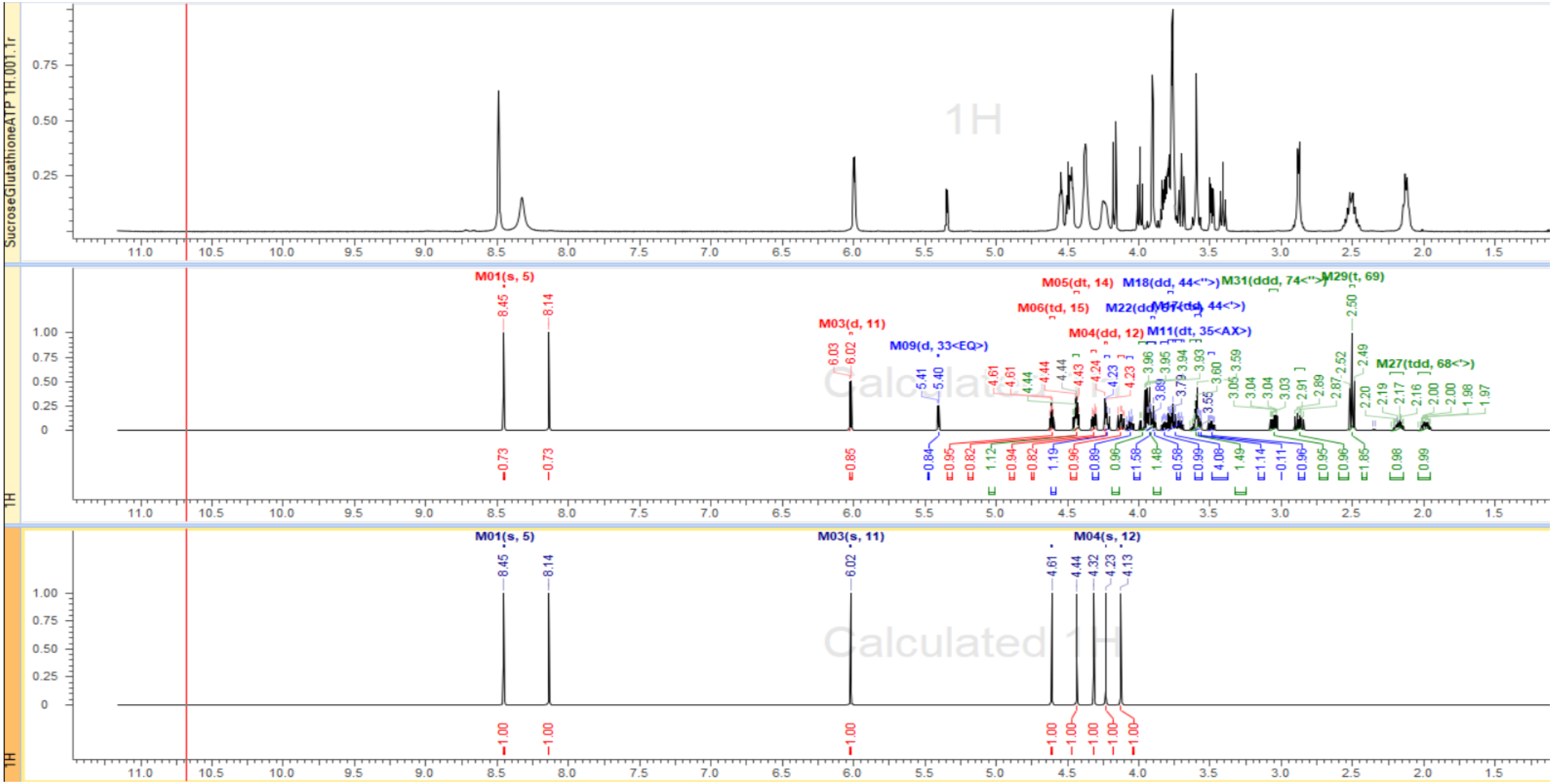
COSY
HSQC
HMBC

More 2D NMR Spectra...

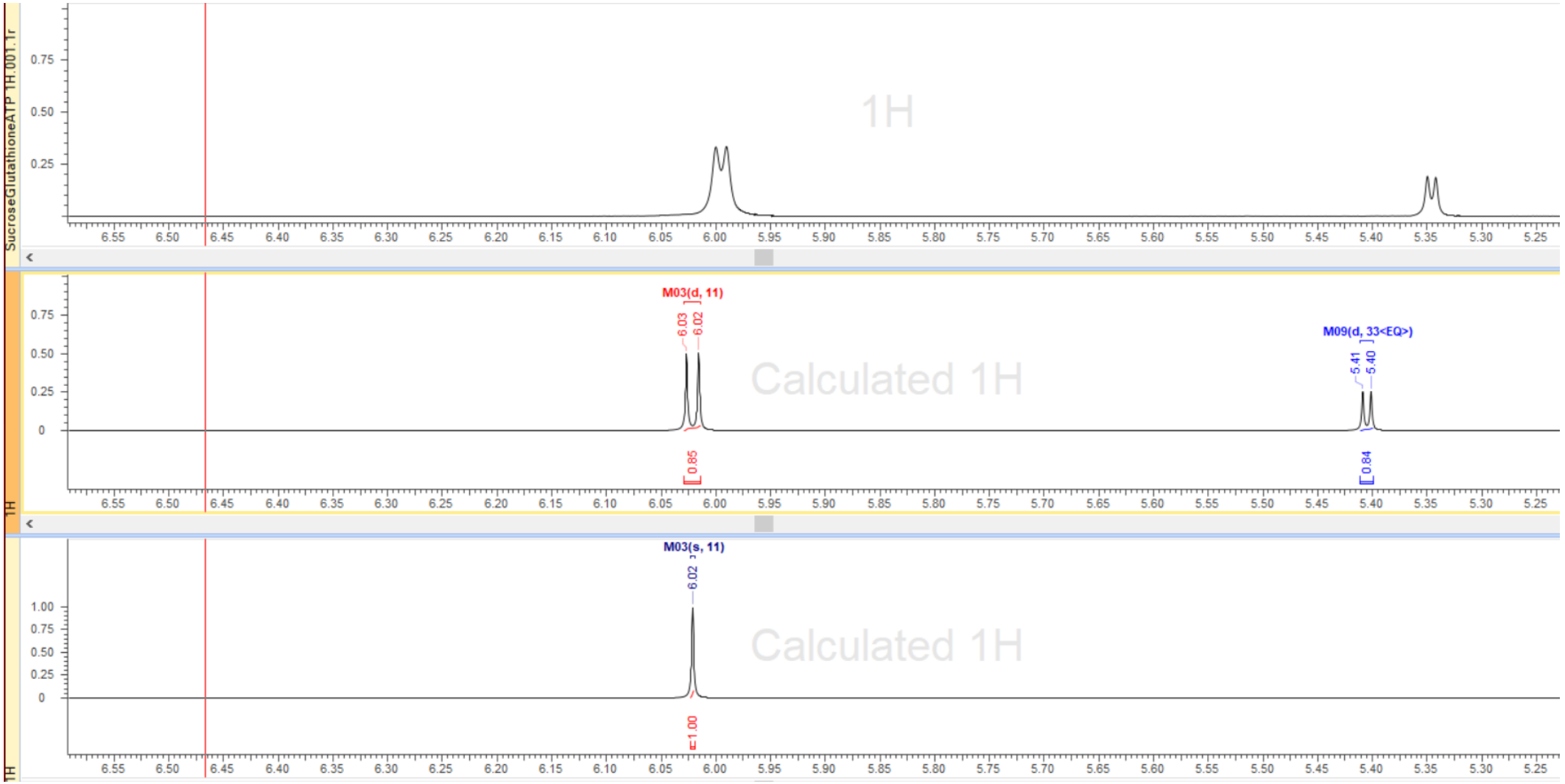
NMR Spectrometer Frequency...



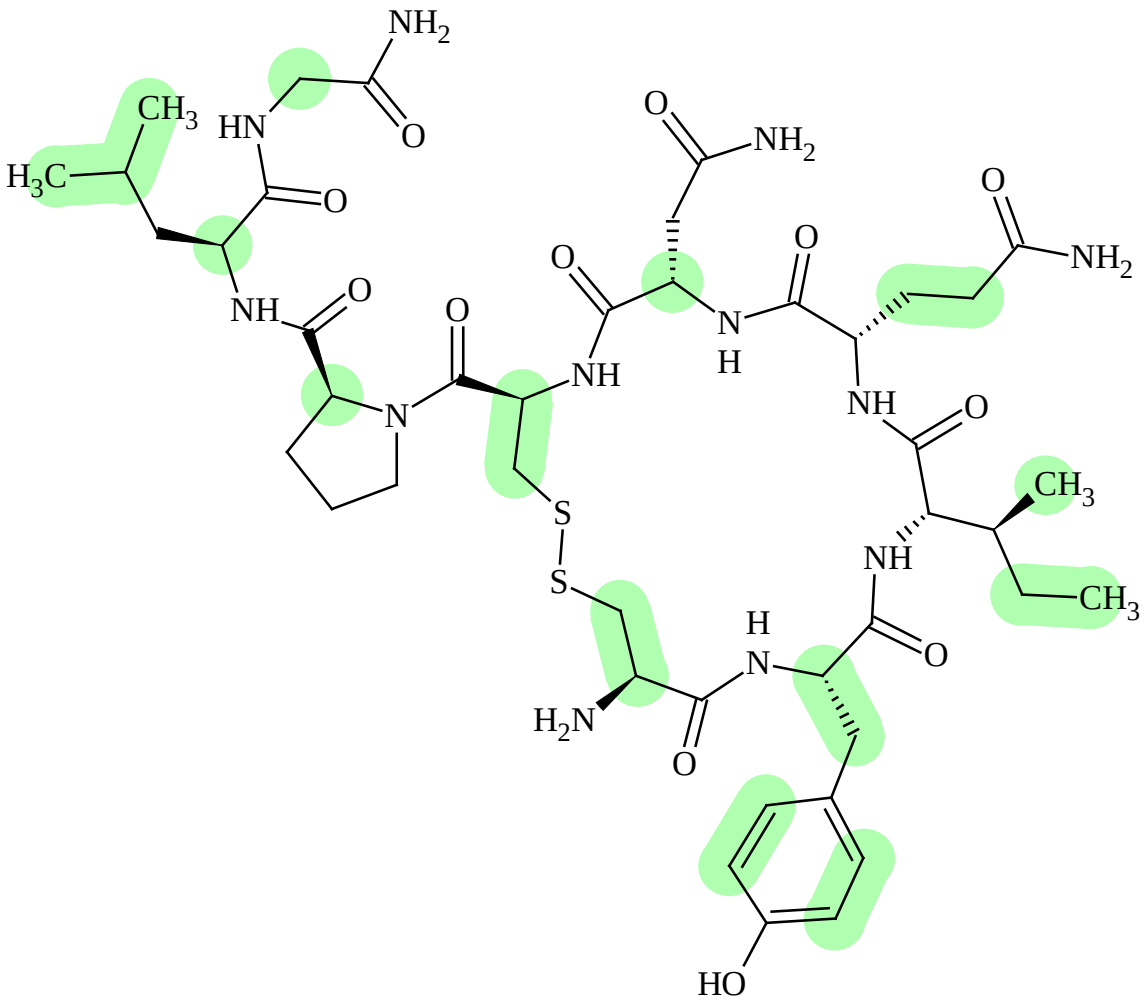
Pure Component Spectrum Simulation from any Mixture Spectrum

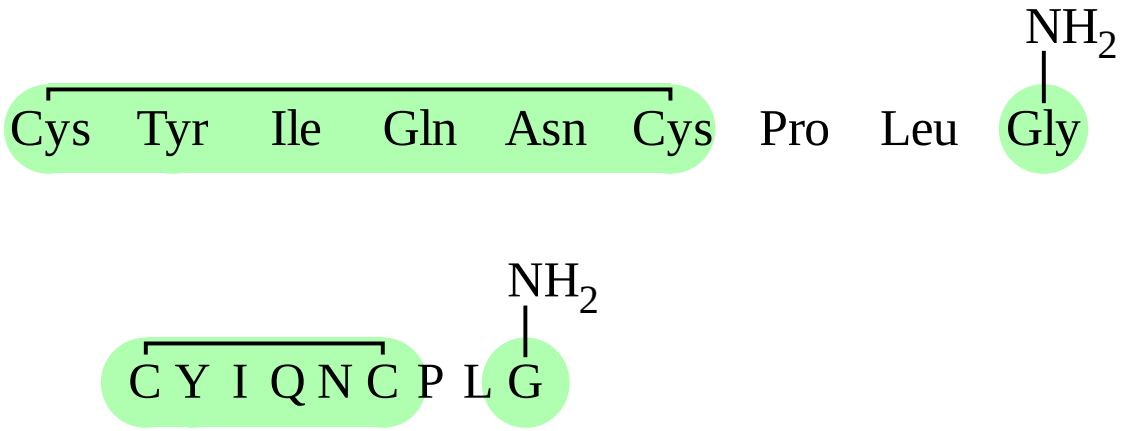


Pure Component Spectrum Simulation from any Mixture Spectrum

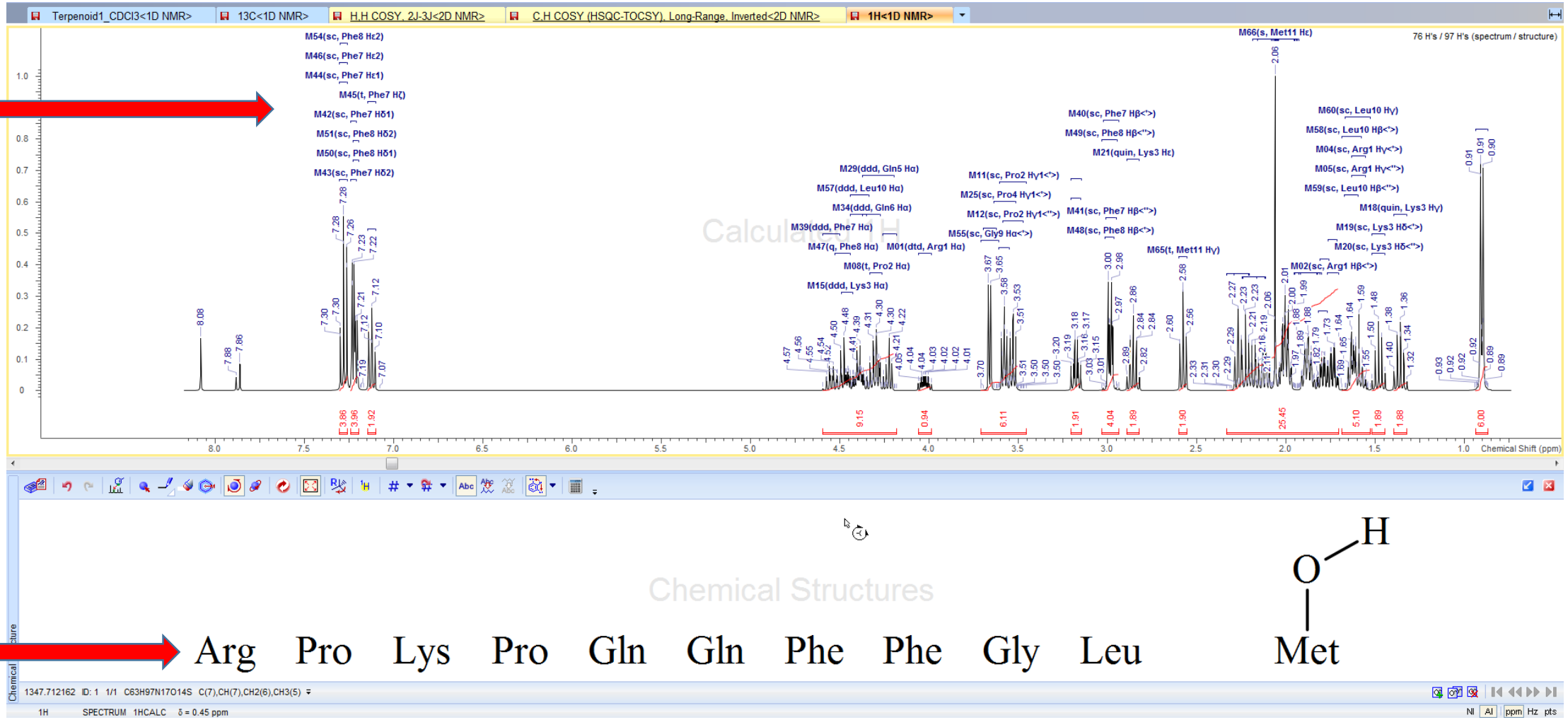


Easily Predict NMR Spectra for Peptides

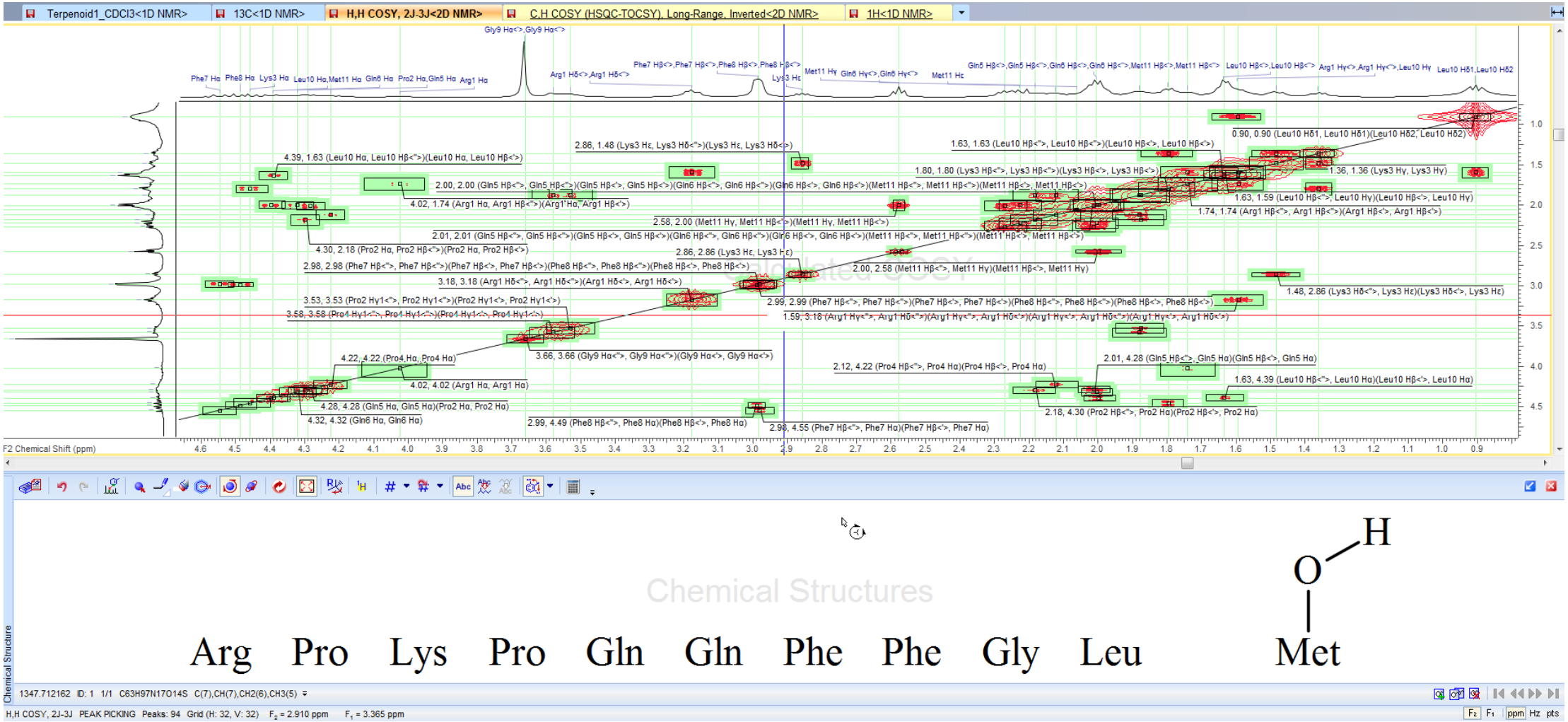




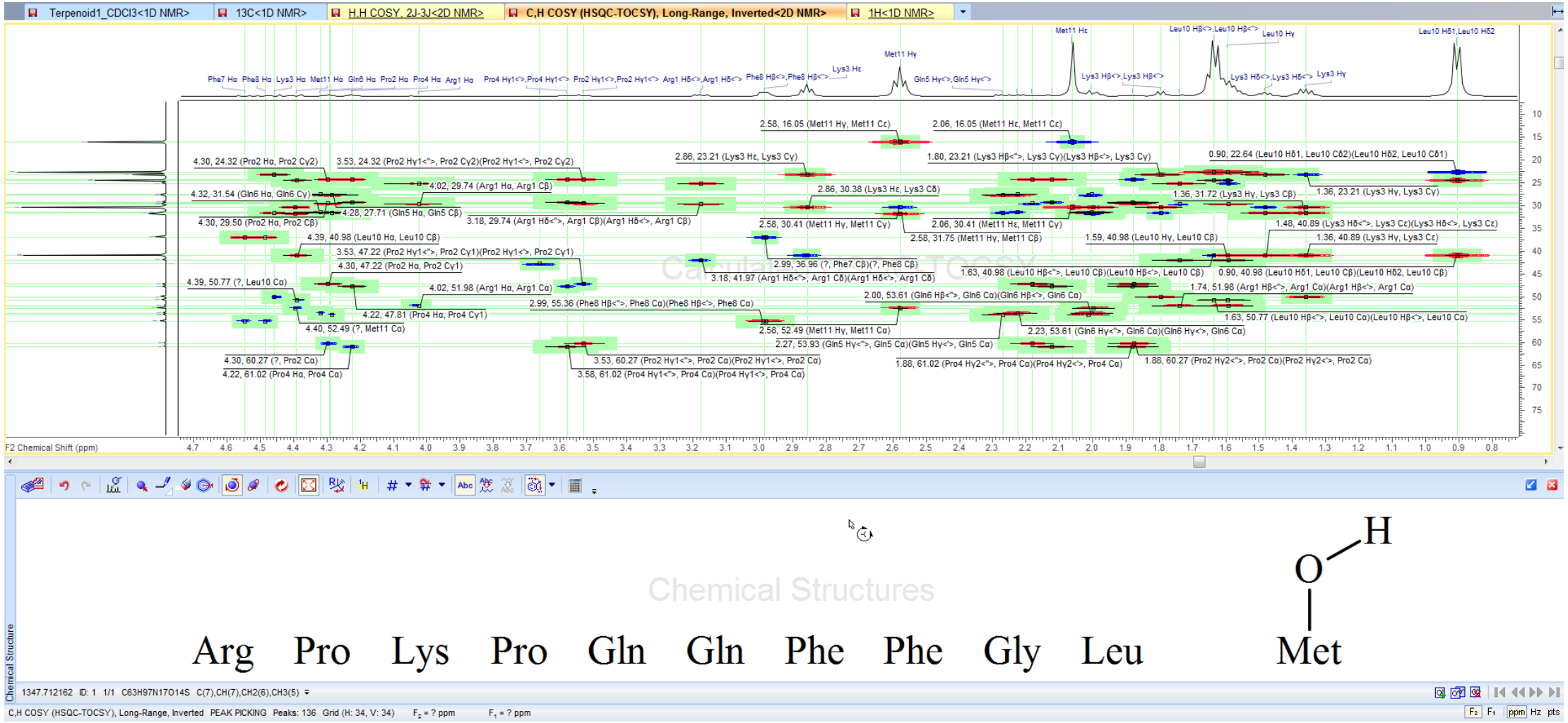
Predicting ^{1}H spectrum of Substance-P



Predicting the ^{1}H-^{1}H COSY spectrum of Substance-P



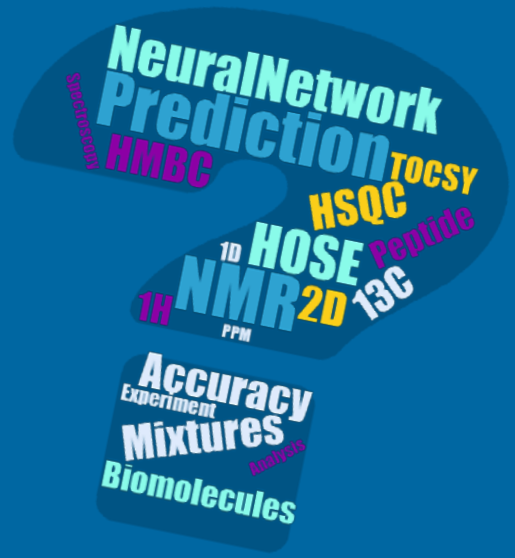
Predicting the ^{1}H-{^{13}C} HSQC-TOCSY spectrum of Substance P



Concluding Remarks

- Today we discussed the following ways of applying NMR predictions:
  - Using1D Predictors (^{1}H, ^{13}C, ^{15}N, ^{19}F, and ^{31}P), and 2D Predictors (^{1}H, ^{13}C, and ^{15}N) to facilitate structure verification and increase confidence in results
  - Training the NMR Predictors to increase confidence and accurately predict for novel compounds
  - Using 2D NMR predictions for complex mixture analysis and for planning experiments
  - Streamlining the NMR analysis for peptides and complex ^{1}H NMR spectra

Questions?



Grace Kennedy
Grace.Kennedy@ACDLabs.com
o: (416) 368-3435 x 239
www.ACDLabs.com

ACD/Labs

Connect with Us