

# Make Informed Decisions from Experimental Design to Data Interpretation

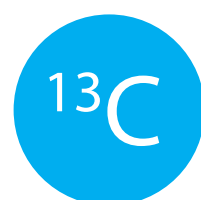
Predict Full 1D and 2D Spectra with Industry-Leading Accuracy



## Take Advantage of Comprehensive Databases and Sophisticated Algorithms



>2 million chemical shifts from over 250,000 structures



>5 million chemical shifts from over 380,000 structures



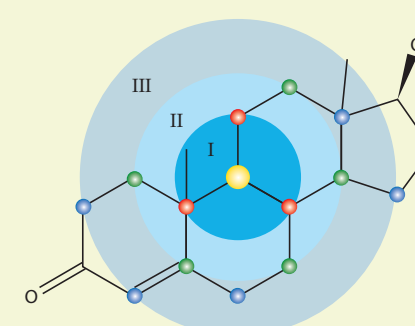
>24,000 chemical shifts from over 10,000 structures



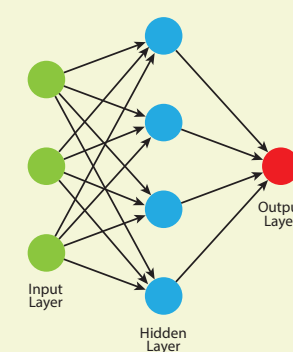
>56,000 chemical shifts from over 31,000 structures



>39,000 chemical shifts from over 32,000 structures



Hierarchical Organization of Spherical Environments (HOSE)



Artificial Neural Network

## See For Yourself How ACD/Labs' NMR Prediction Compares

Compared to other popular tools, ACD/Labs' NMR prediction algorithms provide more accurate <sup>13</sup>C chemical shifts of five natural products:

ACD/Labs



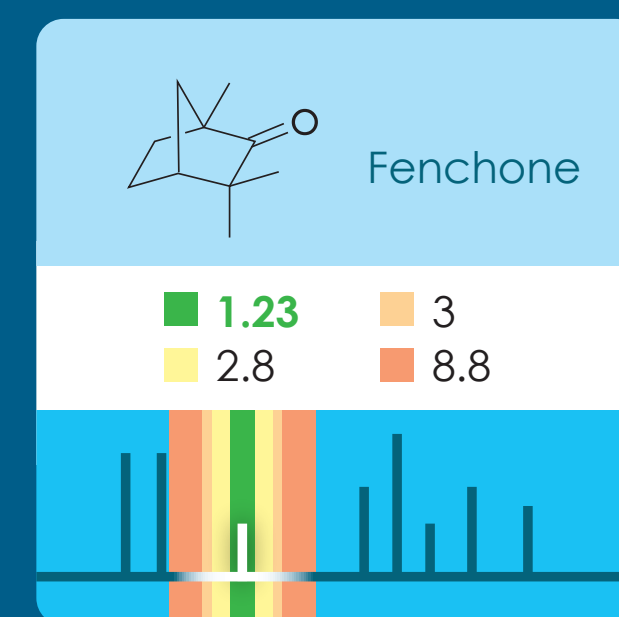
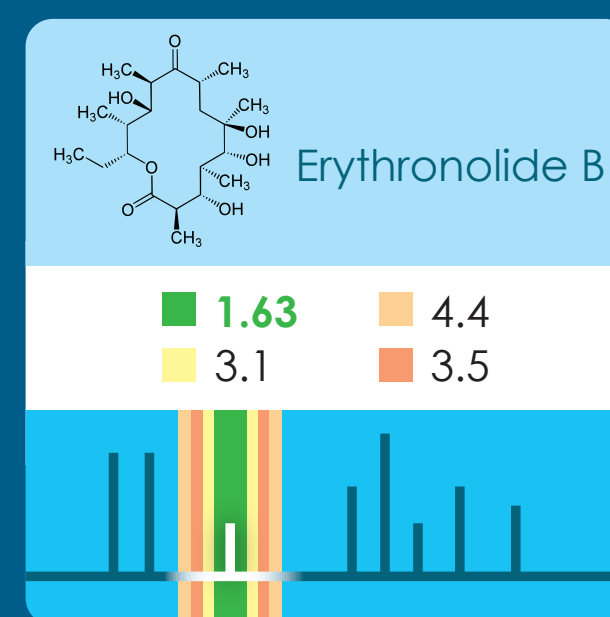
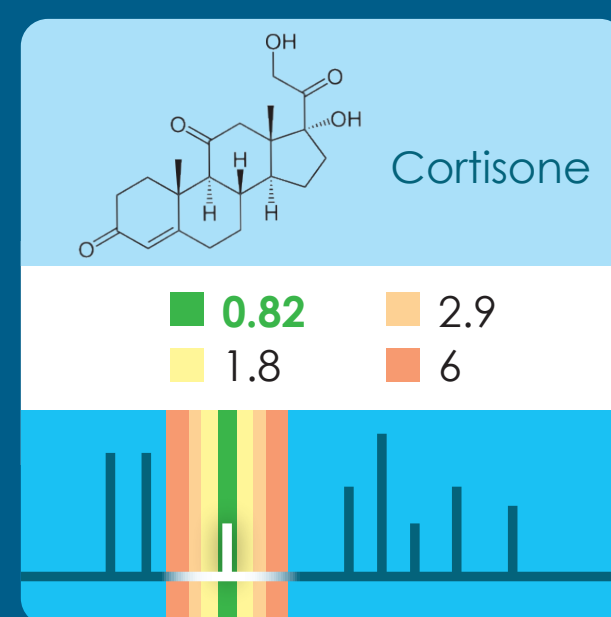
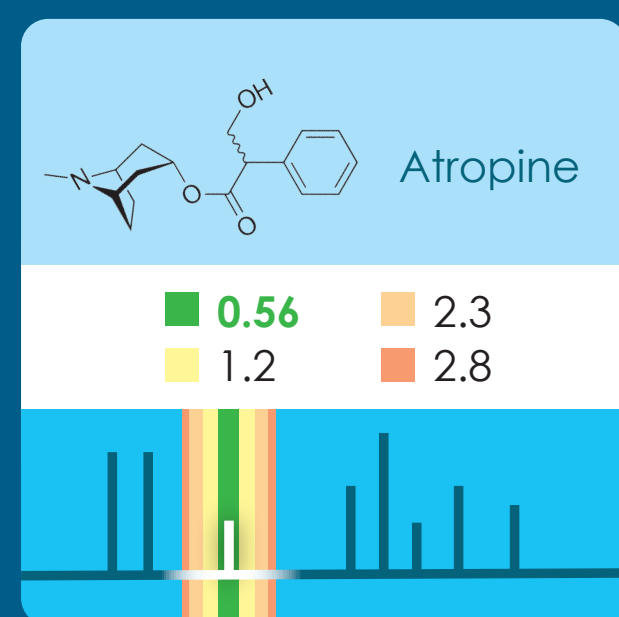
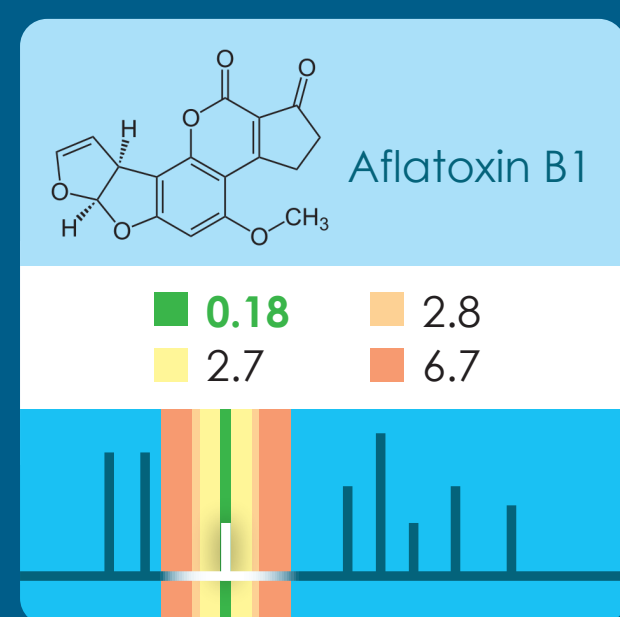
Mnova



DFT177

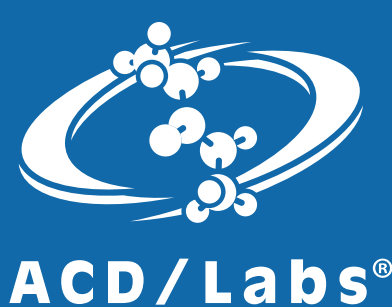


ChemDraw



ACD/Labs values obtained from ACD/CNMR Predictors v. 2016.2. Data presented by Burkhard Kirste, Freie Universität Berlin, 38<sup>th</sup> FGNMR Meeting, Sept. 2016, Dusseldorf.

Contact us to request a demonstration of our industry-leading NMR prediction capabilities.



[www.acdlabs.com/NMRPredictors](http://www.acdlabs.com/NMRPredictors)

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