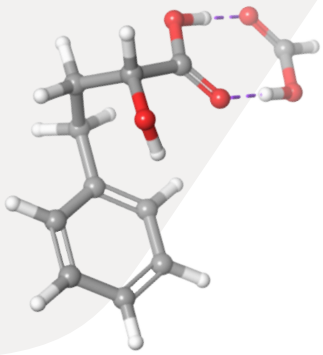
VCD/IR, ECD/UV-vis, and NMR spectra prediction with Jaguar Spectroscopy

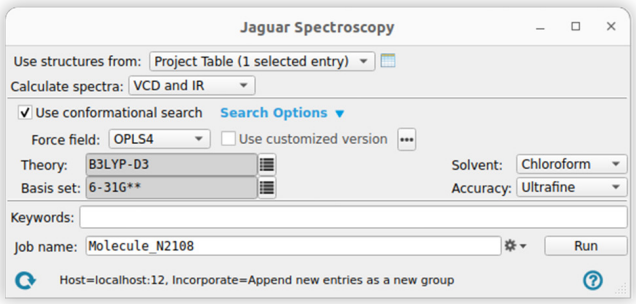


Perform accurate and rapid computational prediction of VCD/IR, ECD/UV-vis, and NMR spectra with Schrödinger's new product, Jaguar Spectroscopy. Benefit from the combined accuracy of conformational search by MacroModel, as well as fast pseudospectral density functional (DFT) theory calculations performed with Jaguar.

Use VCD and ECD spectra predictions in Jaguar Spectroscopy to determine stereo configuration without crystallizing your molecule or using X-ray spectroscopy. Additionally, Jaguar Spectroscopy enables you to use computationally predicted NMR spectra for structure determination, assignment of experimental NMR signals, and to gain greater insight into conformational effects.

Features

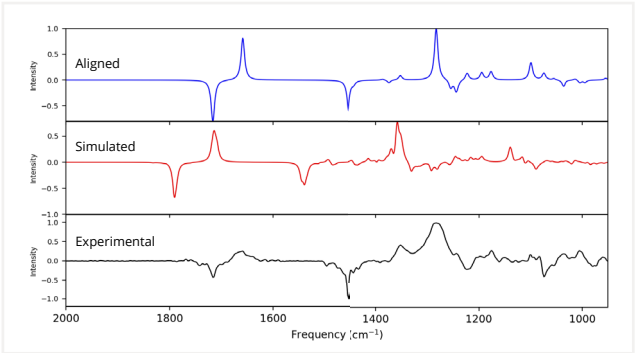
- Fast VCD/IR, ECD/UV-vis, and NMR calculations with a pseudospectral DFT implementation
- Automated Boltzmann averaging of VCD/IR, ECD/UV-vis, and NMR spectra, as well as alignment of VCD/IR theoretical and experimental spectra
- Support for water, chloroform, ethanol, methanol, DMSO, and acetonitrile solvents through an implicit solvent model in VCD/IR and ECD/UV-vis spectra modeling
- Simulated NMR spectra of isotopes ^{1}H, ^{13}C, ^{15}N, ^{19}F, and ^{31}P and support of partly deuterated compounds
- Highly accurate, automated conformational search with proprietary OPLS4 force field
- Needleman-Wunsch and scaling algorithms for automated alignment of theoretical and experimental VCD/IR spectra



Jaguar Spectroscopy panel available from Maestro GUI

Automated VCD alignment simplifies assigning absolute stereo-configuration

A simulation of the VCD spectrum of (*R*)-2-hydroxy-4-phenyl butyric acid [(*R*)-2H4PBA] was performed by the Jaguar Spectroscopy VCD workflow at the B3LYP-D3/LACVP** level of theory in conjunction with an implicit chloroform solvation model and conformational search. (*R*)-2H4PBA was complexed with formic acid in order to describe the effect of dimerization of (*R*)-2H4PBA in the non-polar solvent.



The model (image on top) shows the lowest energy conformation of (*R*)-2H4PBA complexed with formic acid in chloroform.
The simulated spectrum of (*R*)-2H4PBA complexed with formic acid in chloroform is shown in red, the experimental spectrum (provided by BioTools Inc.) is in black, and the automatically aligned spectrum is in blue. The alignment was performed by an algorithm from Böselt et al., *J. Chem. Inf. Model*. 2019, 59,1826–1838.

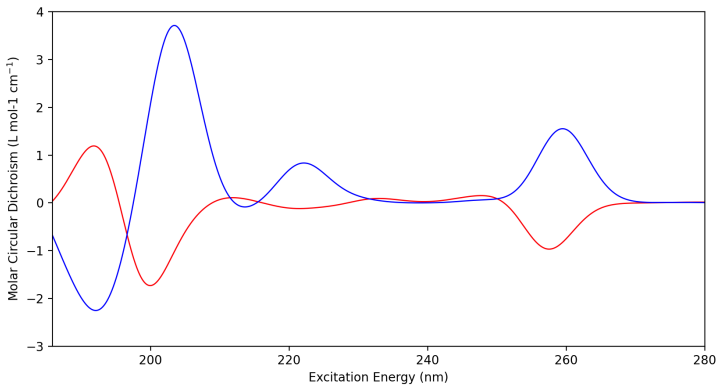
Schrödinger

ECD prediction confirms an unexpected experimental result

According to H. Zhou et al., *J. Nat. Prod.* 2016, 79, 1783−1790, a small structural change not directly affecting the stereocenter of one penipyridone alkaloid leads to an “almost opposite” ECD spectrum. This unexpected effect was reproduced by a Jaguar Spectroscopy simulation of the ECD spectra at the ωB97X-D/LACVP**++ level of theory, including conformational search, in methanol.

Same stereochemistry, opposite ECD spectra

Schrödinger simulation



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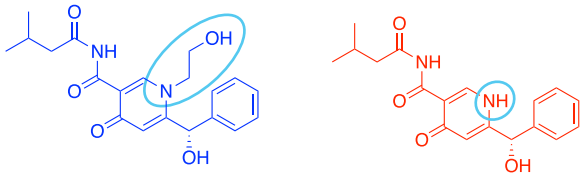
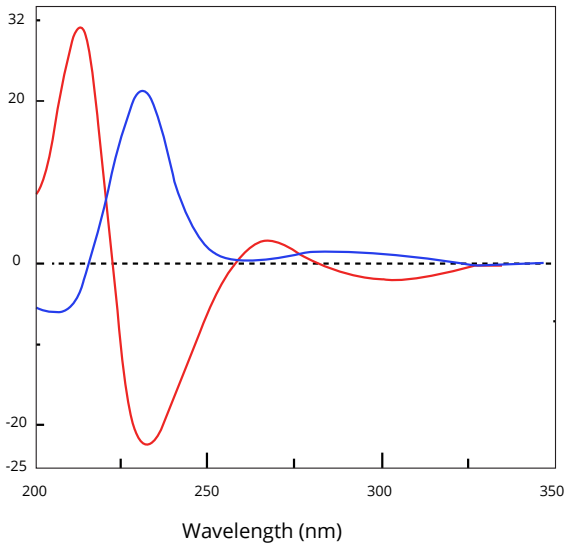


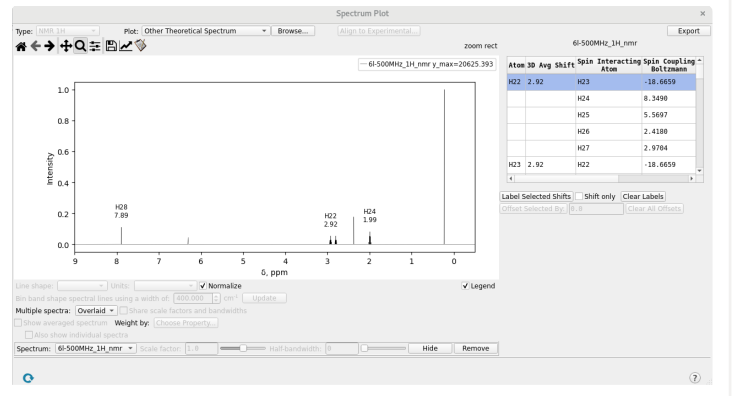
Experimental measurement

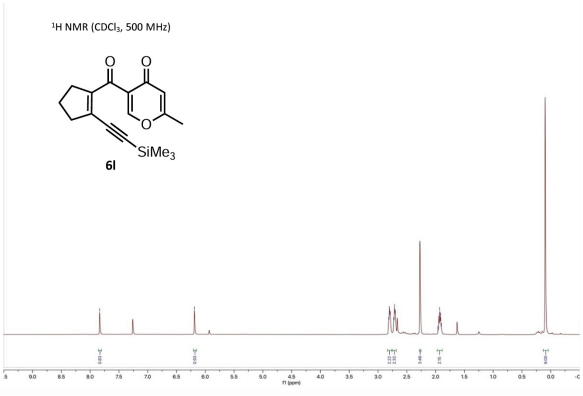


Reprinted (adapted) with permission from H. Zhou et al., *J. Nat. Prod.* 2016, 79, 1783−1790. Copyright 2016 American Chemical Society.

Computed ^{1}H NMR spectrum agrees well with experimental data

A Jaguar Spectroscopy-computed (B3LYP-D3/6-31G** in implicit chloroform solvent), conformationally averaged ^{1}H spectrum of an organic compound from E. L. Perera et al., *J. Org. Chem.* 2024, 89, 4496-4502 is shown in the Spectrum Plot panel alongside the experimental spectrum. The predicted spectrum matches the experimental one both qualitatively and quantitatively, better than an empirical NMR simulation model (not shown).

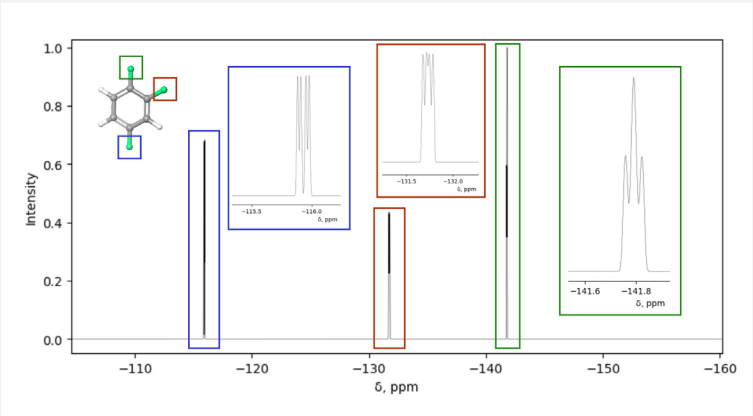


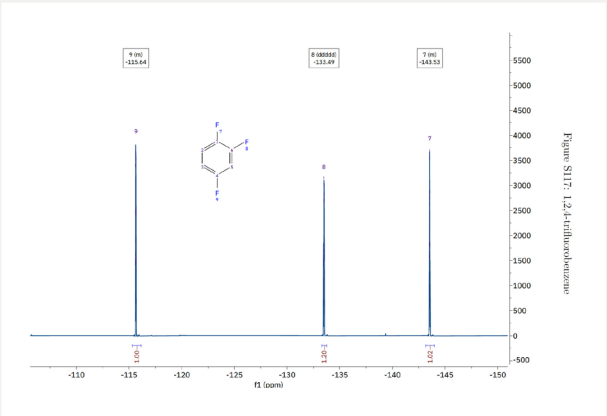


Reprinted (adapted) with permission from E. L. Perera et al., *J. Org. Chem.* 2024, 89, 4496-4502.

Exceptional detail in predicted fine structure due to F-F and F-H interactions in a ^{19}F NMR Spectrum

Jaguar Spectroscopy-predicted (PBE0/6-31+G*) ^{19}F NMR spectrum of 1,2,4-trifluorobenzene shows complex splitting patterns due to strong long-distance F-F interactions and weak F-H interactions. The theoretical spectrum is in excellent agreement with the experimental spectrum taken from J. R. Gathier, S. A. Mabury, *Environ. Sci. Technol.* 2023, 57, 8760-8767.

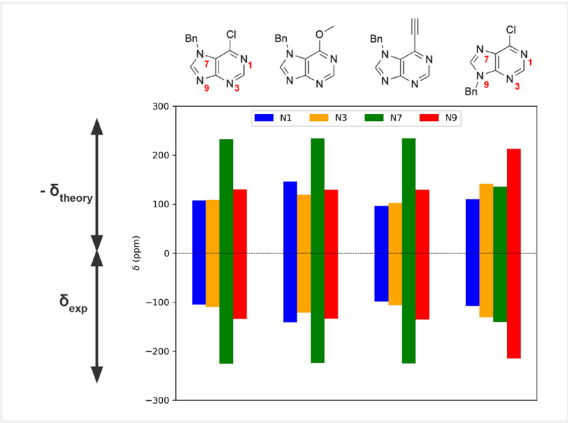




Reprinted (adapted) with permission from J. R. Gathier, S. A. Mabury, *Environ. Sci. Technol.* 2023, 57, 8760-8767.

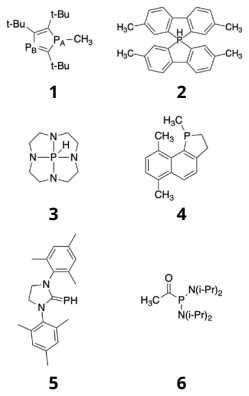
Accurate prediction of ^{15}N NMR chemical shifts of substituted purines

The chemical shifts of nitrogen atoms are accurately predicted in this simulation of ^{15}N NMR spectra of several purine compounds. The excellent match between theoretical calculations (PBE0/6-31+G*) and experiment (as reported in H. Andersson et al., *Annu. Rep. NMR Spectrosc.* 2010, 86, 73-210) is illustrated by nearly perfect "mirror reflections" of the chemical shift values. The agreement is very good despite the difference in the treatment of solvent (DFT calculations in vacuum projected to chloroform vs. experiment in DMSO-d_6).



Theory: B3LYP/6-311G*/gas phase

Compound	δ_{Jag} (ppm)	δ_{exp} [a] (ppm)
1	P(A): 44.8 P(B): 326.3	P(A): 39.6 P(B): 297.6
2	-117.0	-110
3	-60.4	-54.5
4	-0.4	-10.2
5	-117.2	-127.2
6	63.7	63.5



Accurate prediction of ^{31}P NMR chemical shifts of diverse P-containing molecules

The chemical shifts of phosphorus atoms depend strongly on the local environment (the experimental values measured in nonpolar solvents are from W. H. Hersh, T.-Y. Chan. *Beilstein J. Org. Chem*. 2023, 19, 36–56). The trends are very well reproduced by Jaguar Spectroscopy (B3LYP/6-311G*/gas phase and projected to chloroform via an automated parameterization).

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