Accurately predict VCD and ECD spectra with Jaguar Spectroscopy

Perform accurate and rapid computational prediction of VCD and ECD spectra with Jaguar Spectroscopy. Benefit from the combined accuracy of conformational search by MacroModel, as well as fast calculations based on pseudospectral density functional theory and performed with Jaguar.

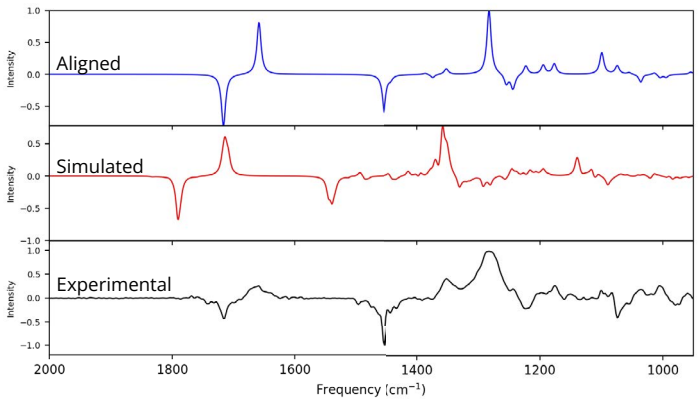
Determine stereoconfiguration without crystallizing the molecule or using X-ray spectroscopy.

Features

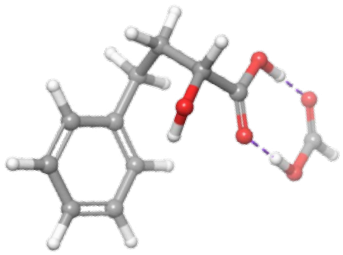
- **Fast VCD and ECD calculations** from a pseudospectral DFT implementation
- **Easy-to-use** graphical interface via Schrödinger's Maestro software
- **Highly accurate** conformational predictions from proprietary OPLS4 force field
- Availability of multiple conformational search options
- Support for water, chloroform, ethanol, methanol, DMSO, and acetonitrile solvents through an implicit solvent model
- Automated Boltzmann averaging and alignment of IR and VCD theoretical and experimental spectra

Automated VCD alignment simplifies assigning absolute stereoconfiguration

A simulation of the VCD spectrum of (*R*)-2-hydroxy-4-phenyl butyric acid ((*R*)-2H4PBA) was performed using Jaguar Spectroscopy at the B3LYP-D3/LACVP** level of theory in conjunction with an implicit chloroform solvation model and conformational search. (*R*)-2H4PBA was complexed with the formic acid in order to describe the effect of dimerization of (*R*)-2H4PBA in the non-polar solvent. The simulated spectrum is shown in red, the experimental spectrum (provided by BioTools) 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, 5, 1826–1838.



The model shows the lowest energy conformation of (*R*)-2H4PBA complexed with the formic acid in chloroform.



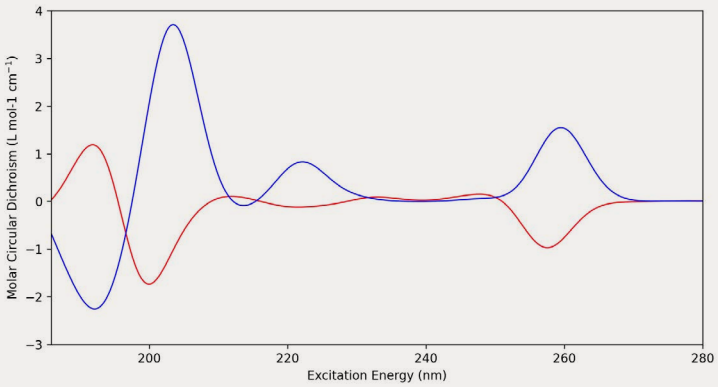
Schrödinger

ECD prediction confirms an unexpected experimental finding

A simulation of the ECD spectra of alkaloids penipyridones was performed using Jaguar Spectroscopy at the ωB97X-D/LACVP**++ level of theory, including conformational search, in methanol. 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. The results of the simulation confirm this unexpected experimental finding.

Same stereochemistry, opposite ECD spectra

Schrödinger simulation



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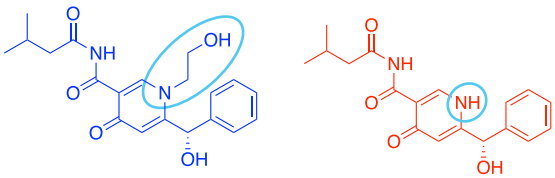
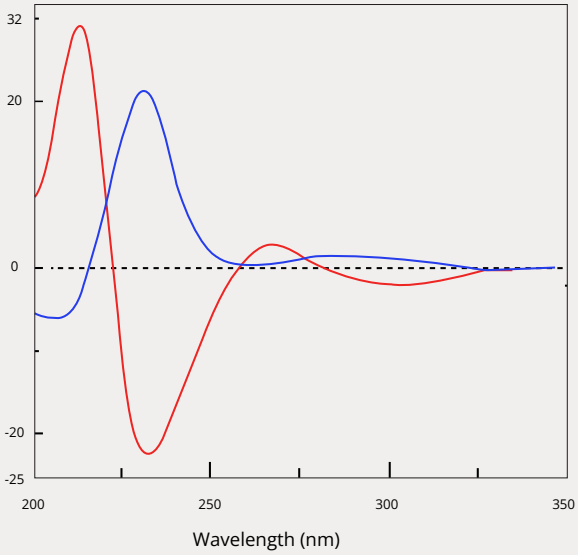


Experimental measurement



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