

Determining absolute configurations with vibrational CD spectroscopy

Vibrational Circular Dichroism (VCD) spectroscopy measures the small difference in the absorption of left- and right circular polarized infrared light by a chiral sample. It allows the unambiguous assignment of absolute configurations by comparison of experimental VCD spectra with computationally predicted spectra. Besides its unique sensitivity to chirality and absolute configurations, VCD spectroscopy is highly sensitive to even very subtle differences in structures, such as conformational changes induced by solute-solvent interactions.

In a brief section, this advanced module will introduce you first to some theoretical aspects like the CD effect in general, but also to computational aspects like conformational analysis. In a lab tour, you will learn about all important components of the spectrometer. Afterwards, in a more hands-on session, we will start a measurement together aiming to assign the absolute configuration of a simple chiral molecule. We will end the module by discussing potential links to your project, and maybe you even bring your own sample...