

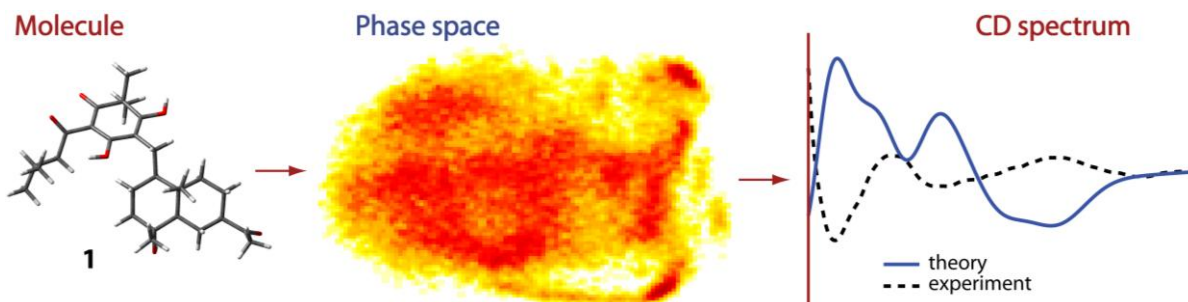
# Determining the stereochemistry and key excitations in the CD spectra of organic molecules by theoretical methods

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Circular dichroism (CD) spectroscopy is one of the most useful methods for the determination of the absolute configuration of optically active molecules, which represents one of the key aspects of molecular stereochemistry. However, since the CD spectrum strongly depends on the molecular flexibility of the involved chromophores, the interpretation of the experimental data is challenging. Hence, to properly assign the absolute configurations, theoretical methods need to be employed. In a recent study we have shown that a combination of replica exchange molecular dynamics, a clustering procedure, and TD-DFT methods can provide a general framework for the calculation of the CD spectra of flexible molecules [1]. We validate our methodology by finding excellent agreement with the experimental spectra of 3 novel terpenoid compounds of the rhodomyrtal family (such as **1**) for which we successfully determine the absolute configurations. We furthermore apply our method to flexible peptides and explore how the predominant amide and aromatic excitations shape the overall result.

[1] Z. Brkljača, K. Čondić-Jurkić, A.-S. Smith, D. M. Smith, *J. Chem. Theory Comput.* **2012**, *8*, 1694-1705.