

## Quantifying molecular chirality through enhanced sampling methods

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When examining complex problems, such as the folding of polymers, accurate descriptions of the system degrees of freedom help us to rationalize the results. Oftentimes collective variables (CVs), derived through some chemical intuition about the process of interest, serve this purpose. When disclosing chiral free energy surfaces, finding these CVs become the most difficult part of the investigation. In these regards, the chirality index introduced in (Pietropaolo et al., *Proteins* 2008, 70, 667) enable to quantify molecular chirality. Recently it was exploited to explore complex molecular free-energy landscape, introducing it as a metrics in the path collective variables (PCVs) framework. A picture of the methods used to calculate the free energy will be discussed together with recent application to biopolymers. The use of this chirality index to reconstruct the free energy surface of the chirality inversion of a stacked helical polymer will be presented.

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