Learning by teaching: the theoretical-computational characterization of the trp-cage miniprotein
(an experiment made by the students of the Biological Physical Chemistry course)

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In this contribution, we present the results of an experiment based on active learning[1], a form of learning in which teaching strives to involve students in the learning process more directly than in other methods.
Starting from a long molecular dynamics trajectory of the trp-cage small protein made available to the students, we started to discuss in the class about the possible ways to describe such a system. First, the trajectory has been analysed by visual inspection and several folding/unfolding events have been found.
Then, we explored which structural observables can be used to describe such structural transitions. To this end, we calculated several structural-based properties such as the gyration radius, the end-to-end distance, the number of h-bonds and many others. Such an analysis pointed out that not all the observables are able to discriminate between the folded and the unfolded conformations and, thus some of them have been selected to model the thermodynamics and the kinetics of the trp-cage folding behaviour. The main results of this cooperative research driven by students are presented and discussed against available literature data[2,3,4].

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