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What can biologists learn from statistical mechanics: conformational averaging in structural biophysics

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One of the central preoccupations of all of molecular biology is studying the connection between the structure of biomolecules (proteins, DNA, carbohydrates, lipids) and their function. However, most biomolecular structures are determined on the basis of highly time- and ensemble-averaged experimental observables. From X-ray crystallography to nuclear magnetic resonance to circular dichroism, most techniques in structural biophysics deal with large ensembles of identical biomolecules and operate on time-scales that are much longer than the relevant relaxation times. Given that biomolecules fluctuate, change structure and can correctly be described only on the level of ensembles, it is important to ask how representative and ultimately useful are the idealized averages coming from the experiment? Can it be that sometimes experiments filter and amplify certain aspects of molecular structure at the expense of others? Finally, is it possible that sometimes experiment, due to averaging, produces structural motifs that are not microscopically persistent or even relevant? In this talk, I will discuss some recent progress in addressing these issues, and demonstrate the utility of molecular dynamics simulations in such attempts.

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