tRMSF: a protein flexibility analysis in molecular dynamics as a function of both time and residue

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Molecular dynamics (MD) simulations may be considered as an important tool to investigate protein behavior as a low cost atomic resolution technique. It has a remarkable ability to provide information about the motions of specific amino acid residues and so provide structural insights into its roles on numerous biological processes, such as enzyme catalysis and allosteric modulation, antigen-antibody interactions and gene regulation. Among the several analysis strategies employed to interpret the behavior of a given protein in MD, one of the most common is the root mean square fluctuation (RMSF), which supply a global perspective of the protein flexibility, at a residue level, as an average over the entire simulation, so lacking time resolution. Other strategies, as the root mean square deviation (RMSD), provide a description of the protein flexibility and conformational change as an average over all amino acid residues, at each instant of the simulation, so lacking residue resolution. In this context, our group had developed a combined strategy, named tRMSF (temporal RMSF), able to describe the protein dynamics at time and residue levels in a single contour plot. This approach was applied in several systems, as melittin, p17, antithrombin, SufU, EGF-like domain, CD59, hsCD2$_{105}$, and α-hCG, allowing us to obtain a picture of each protein dynamics, equilibration and periodicity of movements within MD trajectories, supporting the identification of possible regions involved in sensible biological events.

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