

Intramolecular Dynamics

Subjects: [Biochemistry & Molecular Biology](#)

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Intramolecular dynamics, within protein structure and dynamics, comprises the time-dependent internal motions and conformational transitions of atoms, residues, secondary-structure elements, loops, and domains within an individual protein molecule [\[1\]](#)[\[2\]](#). These motions arise from the protein's internal degrees of freedom and its conformational energy landscape, which permits the molecular structure to occupy an ensemble of interconverting conformational substates rather than a single invariant atomic configuration [\[1\]](#). Intramolecular motions span a broad temporal range, including rapid bond and side-chain fluctuations, backbone rearrangements, loop movements, collective structural fluctuations, and slower transitions involving larger protein regions or domains [\[2\]](#)[\[3\]](#). Their molecular description includes the amplitudes of internal displacement, populations of conformational states, rates of exchange between states, correlations among atomic motions, and the energetic barriers separating accessible configurations. The concept therefore represents the dynamic component of protein molecular structure expressed through internal conformational fluctuations and transitions over time across multiple spatial and temporal scales [\[1\]](#)[\[2\]](#)[\[3\]](#).

Protein dynamics

conformational ensemble

molecular motion

conformational exchange

▢ Protein Structure and Dynamics • ▢ Molecular Biology • ▢ Biochemistry, Genetics and Molecular Biology • ▢ Life Sciences

References

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3. Paul Schanda; Gilad Haran; NMR and Single-Molecule FRET Insights into Fast Protein Motions and Their Relation to Function. *Annu. Rev. Biophys.* **2024**, 53, 247-273. [CrossRef]

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