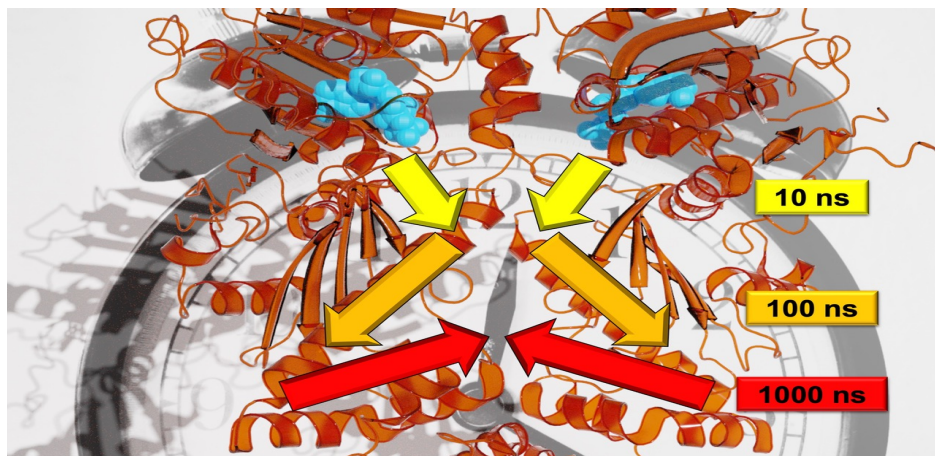




Learning the signaling pathways of proteins

To achieve their biological function, proteins need to communicate over long distances, enclosing hundreds to thousands of atoms in between. Despite ongoing effort, the mechanism of this signaling process is only poorly understood. Using the recently proposed computational approach Mosaic [1], the task is to identify networks of inter-residue contacts (such as hydrogen bonds) in the multi-domain protein Hsp90, which mediate the long-range signal transport. Studied by a cooperation between Chemists and Physicists in Freiburg, Hsp90 is one of the most promising targets for anti-cancer drugs in our body [2].



Useful information

[1] Correlation-based feature selection to identify functional dynamics in proteins
G. Diez, D. Nagel and G. Stock, *J. Chem. Theory Comput.* 18, 5079 (2022)

[2] Hierarchical dynamics in allostery following ATP hydrolysis monitored by single molecule FRET measurements and MD simulations
S. Wolf et al., *Chem. Sci.*, 1–10 (2021)

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