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Protein-protein recognition mechanism through interfacial hydrogen-bonded water chains

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Protein-protein recognition through the hydrogen-bonded chains of interfacial water is a less explored mechanism due to the technical challenges involved in the analyses, and the role of waters in forming a stable protein-protein complex is often elusive. It is still unclear whether and how the hydrogen-bonded interfacial-water chains contribute to triggering or participating in the recognition process, especially when the interacting proteins are about to encounter to form a complex, but are still distinctly separated. In this work, we used the trajectories generated by curvilinear-path umbrella sampling approach to extract some conformations from the physical paths of unbinding. We analyzed the water-interface formed between interacting proteins and systematically characterized the hydrogen-bonded water molecules through a newly developed procedure. The revealed hydrogen-bonded water molecules are used for shortest-path network analysis. The presence of significant clusters in the mid of the interface and overall robustness of the connectivity between the interacting proteins through hydrogen-bonded water-chains suggest that these waters play a crucial role in bridging the interacting proteins, much before they encounter. This work proposes a highly generalized approach to characterize interfacial waters for protein-protein recognition.

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