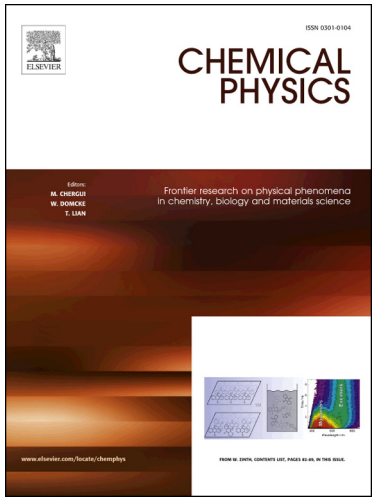


# Water rotation barriers on protein molecular surfaces

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# Water rotation barriers on protein molecular surfaces *

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***Abstract*** The experimental characterization of hindered-rotation barriers and mapping the energetic heterogeneity of water molecules bound to the molecular "surface" of proteins is critical for understanding the functional interaction of proteins with their environment. Here, we show how to achieve this goal by an original wide-line NMR procedure, which is based on the spectral motional narrowing phenomenon following the melting (thawing) process of interfacial ice. The procedure highlights the differences between globular and intrinsically disordered proteins and it enables to delineate the effect of solvent on protein structure, making a distinction between point mutants, monomeric and oligomeric states, and characterizing the molecular interactions taking part in different cellular processes. We put this unique experimental approach introducing novel physical quantities and quantifying the heterogeneous distribution of motional activation energy of water in the interfacial landscape into a historical perspective, demonstrating its utility through a variety of globular and disordered proteins.

## *1 Introduction*

Understanding protein function at the molecular level is one of the best proxies to understanding life itself. Proteins are the workhorses of living systems, being involved in countless types of activities and interactions orchestrating the action of other types of molecules: partner proteins, substrates and other macromolecules, which collectively make up a living cell. For a long time, a dominant approach to deciphering protein function has been to solve 3D structures, primarily by X-ray crystallography, as witnessed by more than 100,000