DYNAMICS OF BIOLOGICAL WATER:
A COMPUTATIONAL APPROACH

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1. INTRODUCTION

Investigating the biochemical and physicochemical properties of water, in particular that localized to a biomolecule surface, is essential for understanding biological and medical phenomena.1

Contradictions between different reports (both experimental and theoretical) concerning the dynamics of water surrounding biomolecules have been the object of a continuous debate.2 Thus, some of them state that this special water is affected to a small extent (2-4-fold slowdown when compared with bulk water) while some others report an ultra-slow component of the solvation dynamics (2-3 orders of magnitude larger than neat water).

3. Multiple time scales: MACROSCOPIC VIEW

C(t) = Average number of water molecules that still remains, at a distance < 0.4 nm of the protein, after a time t. C(t) = equivalent calculation for bulk water.

\[ C(t) = \frac{1}{N} \sum_{i=1}^{N} \exp \left( -\frac{t}{\tau_{water}} \right) \]

\[ \tau \text{(biological water)} \approx 2\tau \text{(bulk water)} \]

\[ \tau \text{(experimental)} = 10-100 \text{ ps} \approx \tau \text{(simulation)} \]

A value of \( \beta = 0.48(1) \) indicates significant temporal disorder (multiple time scales).

4. Multiple time scales: MESOSCOPIC VIEW

Water at the Protein Interface:
Scale Free behaviour

5. Multiple time scales: MICROSCOPIC VIEW

Atom of reference:
N (amine group) at the non-polar Tryptophan 44 residue of the protein inhibitor Barstar.

Ultra-Slow (nanosecond scale) and Ultra-Fast (femtosecond scale) Water at the Protein Interface

6. CONCLUDING SKETCH

When macroscopic data are considered (global/averaged view), the dynamics of the hydration water at the biological interface would be affected only to a small extent (2-4-fold slowdown when compared with neat water). This is due to the reduced number of very slow solvent molecules in such an interface.

However if microscopic data are taken into account, the hydration water dynamics would exhibit a slow component neatly smaller than that of the bulk water (2-3 orders of magnitude).

That hydration water can be regarded as a scale free system.