Computational Studies of Antifreeze Peptides

Gandini E.[1,3], Sironi M.[1,2], Pieraccini S.[1,2]

[1]Dipartimento di Chimica, Università degli Studi di Milano, Via Golgi 19, 20133 Milano, Italy
[2]Istituto di Scienze e Tecnologie Chimiche “G. Natta” (SCITEC-CNR), CNR, and INSTM, UdR Milano, Via Golgi 19, 20133 Milano, Italy
[3]Contact: enrico.gandini@unimi.it

Antifreeze Proteins (AFPs) are a class of structurally diverse proteins that protect different organisms, e.g. polar fishes, from fatally freezing in icy environments. They are very attractive for potential practical applications, including food storage, cryopreservation, and anti-icing coatings. Efficient synthetic analogues of AFPs are highly desirable; three 12-residue analogues of Winter Flounder AFP (wfAFP) were successfully applied for the fabrication of anti-icing surfaces. Focus of the present work is the employment of computational techniques to elucidate the mechanism of action of such peptides.

To this aim, three kinds of simulation setups were devised, in order to observe and analyze different aspects of the antifreeze activity of the three wfAFP analogues at a molecular level. For control, a same lenght non-antifreeze peptide such as dodeca-Glycin (G12) was included in the study. Water molecules were described with TIP4P/Ice model, which is able to reproduce solvent properties near the freezing point.

Computational analysis are in good agreement with reported experimental results. The three simulation setups are able to realistically describe the properties of the antifreeze peptides at a molecular level, and to point out structural aspects of the ice-peptide interactions which will be useful for further optimization and engineering of AFP analogues.