

# **Calcium Ion Implicitly Modulates the Adsorption Ability of Ion-Dependent Type II Antifreeze Proteins on Ice/Water Interface: A Structural Insight**

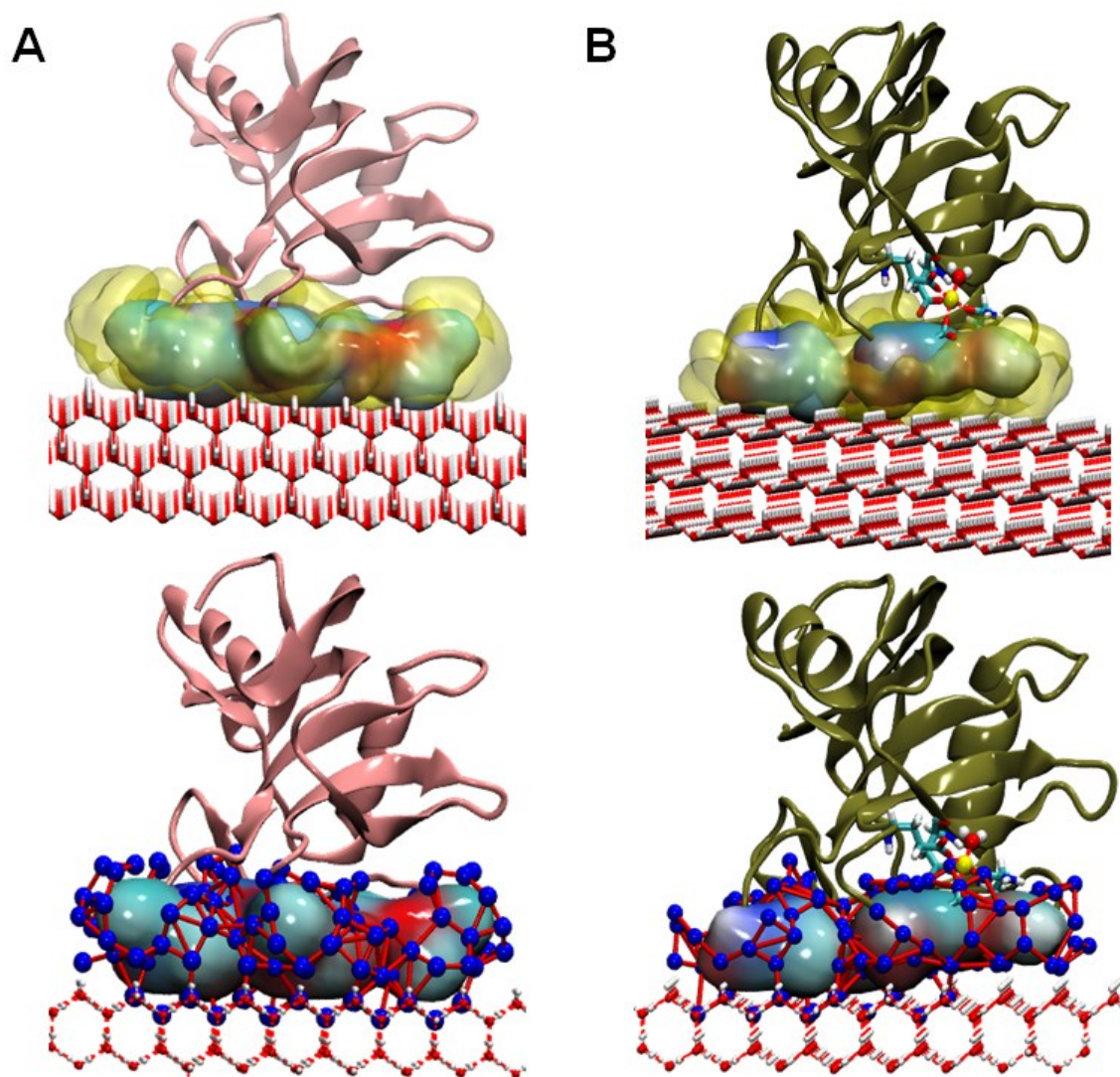
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**Fig. S1:** (A) Structure of the apo Type II AFP adsorbed on the prism plane corresponds to the PMF minimum is shown. Upper panel: The protein is rendered in pink cartoon, ice is shown as sticks and the IBS is rendered in surface representation. The hydration layer around the IBS is shown in transparent yellow surface. Lower panel: Detailed hydration layer water structure of the AFP-ice adsorbed complex is shown. The water layer that anchors AFP on the ice surface is shown as blue ball and hydrogen bonds between them is shown as red line. IBS is shown on surface representation and the top layer of the prism plane adjacent to the IBS is also shown in stick mode. (B) Structure of the Zn<sup>2+</sup> coordinated AFP adsorbed on the prism plane corresponds

to the PMF minimum is shown. Upper panel: The protein is rendered in green cartoon, ice is shown as sticks and the IBS is rendered in surface representation. The hydration layer around the IBS is shown in transparent yellow surface and bound zinc is shown as yellow ball. Lower panel: Detailed hydration layer water structure of the AFP-ice adsorbed complex is shown. The water layer that anchors AFP on the ice surface is shown as blue ball and hydrogen bonds between them is shown as red line. IBS is shown on surface representation and the top layer of the prism plane adjacent to the IBS is also shown in stick mode.