Identifying Ice-Philic Patches to Inform the Ice Binding Sites of Antifreeze Proteins

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Creatures living in cold environment have developed unique strategies to survive. One of their tactics is to evolve antifreeze proteins (AFPs) which lower the freezing temperature by binding to ice. AFPs bind to ice through specific regions on their surface known as ice binding sites (IBS). Each AFP has its own IBS which binds to specific ice planes. Identifying IBS is crucial for understanding how AFPs bind to ice. Here, we use specialized molecular simulation wherein an external potential is used to stimulate ice formation in the AFP hydration shell. We find that the most ice-philic AFP regions, which ice nucleate most readily in response to the external potential, display a strong correspondence with the experimentally-determined IBS (using site-directed mutagenesis). In addition to identifying the IBS, our specialized simulations also shed light on ice polymorph and facet that optimally binds the AFP IBS.