IBP2022 Oral Presentation Abstract

Probing the structure-function relationships of a bacterial ice nucleation protein guided by its AlphaFold model

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Bacterial ice nucleation proteins (INPs) are efficient nucleators of ice crystals at high sub-zero temperatures. Despite the ubiquity of ice-nucleating bacteria and their apparent role in frost damage and atmospheric precipitation, relatively little is known about the structure of INPs and the mechanism through which they trigger ice formation. *Pseudomonas borealis* ice nucleation protein (*Pb*INP) has a central domain comprised of 65 tandem 16-residue repeats flanked by N- and C-terminal domains. The central domain features highly conserved peptide motifs common to IBPs that we propose organize water molecules to initiate ice nucleation. The public release of DeepMind's AlphaFold has enabled rapid generation of protein structure models using artificial intelligence. Analysis of the AlphaFold model of *Pb*INP supports features of previous models for the solenoid region while suggesting structures for the solenoid caps and an N-terminal domain. Examining the impact of truncations and mutations on ice nucleation temperatures has validated many aspects of the AlphaFold model. The new model suggests additional sets of mutations to probe the structure-function relationships in INPs.