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标题: Functional Importance of Short-Range Binding and Long-Range Solvent Interactions in Helical Antifreeze Peptides
作者: Ebbinghaus, S (Ebbinghaus, Simon); Meister, K (Meister, Konrad); Prigozhin, MB (Prigozhin, Maxim B.); DeVries, AL (DeVries, Arthur L.); Havenith, M (Havenith, Martina); Dzubiella, J (Dzubiella, Joachim); Gruebele, M (Gruebele, Martin)
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摘要: Short-range ice binding and long-range solvent perturbation both have been implicated in the activity of antifreeze proteins and antifreeze glycoproteins. We study these two mechanisms for activity of winter flounder antifreeze peptide. Four mutants are characterized by freezing point hysteresis (activity), circular dichroism (secondary structure), Forster resonance energy transfer (end-to-end rigidity), molecular dynamics simulation (structure), and terahertz spectroscopy (long-range solvent perturbation). Our results show that the short-range model is sufficient to explain the activity of our mutants, but the long-range model provides a necessary condition for activity: the most active peptides in our data set all have an extended dynamical hydration shell. It appears that antifreeze proteins and antifreeze glycoproteins have reached different evolutionary solutions to the antifreeze problem, utilizing either a few precisely positioned OH groups or a large quantity of OH groups for ice binding, assisted by long-range solvent perturbation.
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地址: [Prigozhin, Maxim B.; Gruebele, Martin] Univ Illinois, Dept Chem, Urbana, IL USA
[Ebbinghaus, Simon; Meister, Konrad; Havenith, Martina] Ruhr Univ Bochum, Dept Phys Chem 2, Bochum, Germany
[DeVries, Arthur L.] Univ Illinois, Dept Anim Biol, Urbana, IL USA
[Gruebele, Martin] Univ Illinois, Dept Phys, Urbana, IL USA
Univ Illinois, Ctr Biophys & Computat Biol, Urbana, IL USA
[Dzubiella, Joachim] Humboldt Univ, Dept Phys, Berlin, Germany
Helmholtz Zentrum Berlin Mat & Energie, Berlin, Germany
通讯作者地址: Gruebele, M (通讯作者),Univ Illinois, Dept Chem, Urbana, IL USA.
电子邮件地址: gruebele@scs.illinois.edu
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