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Computational Soft Matter and Interfaces

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Why are halophilic proteins rich in acidic amino acids?

Halophilic organisms live in high-salt environments and often accumulate large amounts of KCl in their cytoplasm. Cytoplasmic proteins stay stable and functional under these unusual conditions because of their unique amino acid composition. Their most noticeable compositional difference is their unusually high level of acidic amino acids. Using molecular dynamics simulations, we examined how this composition influences solvation, flexibility and stability at high KCl concentrations. We found that, while the level of hydration of halophilic and mesophilic proteins is equally robust to changes in KCl concentration, acidic amino acids in halophilic proteins may help stabilize the folded protein structure by forming cooperative interactions with cations. Surprisingly, the hydrophobic effect has minimal impact on protein flexibility, whereas electrostatic interactions influence flexibility based on salt concentration. These findings may aid enzyme design for sustainable molecule production in saline environments, conserving fresh-water resources.

