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Title: **Molecular modeling of conformational space of the knot protein YibK**

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Abstract

Structurally, proteins follow entropy favorable layouts that have high stability while performing their function. Knots are typically not observed due the amount of energy needed to form this structure outweighed the stability of the protein. Despite this, there are several rare proteins whose polypeptide backbone form knotted configurations. YibK is one such protein with a trefoil knot (e.g., 3-1 knot) in its carboxy terminus. These proteins reveal interesting topographies with less entropy than if the protein were compressed. In the present work, we studied the main interactions involved in the folding pathway of YibK, based on molecular dynamics (MD) simulations and computational approaches for the calculation of ion-neutral collision cross section (CCS_{N2}). Briefly, a large pool of identity vectors was generated by MD simulations. Charge assignment was performed based on the scoring of the exposed residues, followed by energy optimization steps. In particular, the specific interactions involved in preserving the knotted structure of the protein were studied. The influence of the charge state was also assessed, as the increasing coulombic repulsion disrupts the structural integrity of the protein. Our results provide a better understanding on the interactions involved in the knotted nature of the protein.