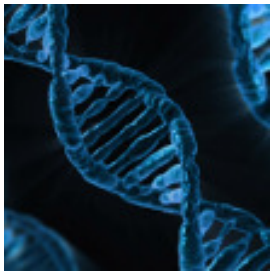

Contribution ID: **49** Type: **Poster**

A computational and experimental investigation of the structural properties of Keif, the intrinsically disordered N-terminus part of MgtA

A recent study by Subramani et al. (*eLife*, 2016) implied that the N-terminus of the magnesium transporter A (MgtA) protein (from hereon called Keif) is intrinsically disordered, but the advantage of this disordered feature to the function of the protein is still unknown. Thus, in this study, the structure of the Keif peptide part have been investigated by using both atomisic molecular dynamics (MD) and coarse-grained Monte Carlo (MC) simulations, as well as different experimental techniques such as circular dichroism (CD, ongoing) and small-angle X-ray scattering (SAXS). Early predictions of the structure of Keif suggested that even though it is disordered, its average shape should still be quite globular. However, it was quickly discovered through both simulations and experiments that Keif in fact adopts extended conformations instead. In addition to these bulk studies at different ionic strengths, the effect of divalent ions will also be examined. Future work in this study might also include investigation of the surface and membrane interactions, as well as analysis of the protein dynamics.

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Session Classification: Dynamics of Intrinsically Disordered Proteins

Track Classification: Dynamics of intrinsically disordered proteins