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Decoding dynamic coiled-coils

How biomolecules reliably generate mechanical forces and torques in a fluctuating environment is an enduring problem of biological physics and molecular biology.

An unusual pair recently found to generate forces are the long membrane tethering protein early endosome antigen 1 (EEA1) — a 220 nm long coiled-coil protein — and the small GTPase Rab5*. Binding of the small GTPase to the end of the coiled-coil triggers long-range conformational changes to modulate the flexibility of EEA1, allowing it to sample conformations with a reduced end-to-end distance. However, what is the molecular basis for EEA1's multistability, and how is energy transmitted from top-to-bottom?

Here, I will discuss how an internal competition between unbalanced hydrophobic residues and electrostatic interactions can give rise to EEA1's dynamic behaviour. I will highlight our recent efforts to combine coarse-grained modelling and atomistic molecular dynamics simulations to explain the force generation mechanism of long coiled-coil proteins.

*Murray, D. and Jahnel, M. et al., An endosomal tether undergoes an entropic collapse to bring vesicles together. Nature (2016)

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