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IMPACT OF NON-SPECIFIC INTERACTIONS OF INTRINSICALLY DISORDERED PROTEINS TO THE FORMATION OF TWO-COMPONENT CONDENSATES

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ABSTRACT

Recent application of sticker-and-spacer model has enabled the prediction of critical concentrations as a function of the molecular properties of the linker proteins [1]. In these molecular models, the intrinsically disordered linker molecule is parametrised using flexible spacers and stickers that bind to specific binding sites on Rubisco. While the model successfully described the condensation for linkers with three or more stickers, for linkers with two stickers the model severely overestimated the critical concentration. We hypothesise this is caused by (non-)specific interactions of the spacer strand with Rubisco. We have explored this mechanism using atomistic and coarse-grained molecular dynamics simulations using AMBER MD and CALVADOS, respectively.

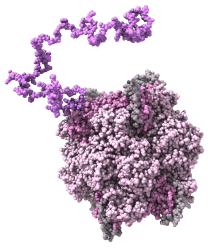

Figure 1: A molecular image of a (purple) and rubisco (light pink) protein

References

[1] Payne-Dwyer, A., Kumar, G., Barrett, J., Gherman, L.K., Hodgkinson, M., Plevin, M., Mackinder, L., Leake, M.C. and Schaefer, C., Predicting Rubisco-Linker Condensation from Titration in the Dilute Phase. *Physical Review Letters*, 132(21), p.218401, 2024.