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KEYNOTE 5 - Neutron Spin Echo Spectroscopy: Protein internal dynamics, forces and friction

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The biological function of proteins is often related to large-scale domain motions, which are induced or suppressed by the binding of a substrate or due to cosolvents. Domain motions can be related to soft hinges, flexible linker regions or -as in the case of intrinsic unfolded proteins- be native to the unfolded protein structure. These large-scale domain motions in solution cannot be observed by X-ray crystallography or NMR spectroscopy. Small angle scattering by X-rays or neutrons in combination with neutron spin echo spectroscopy (NSE) in solution can be used to observe configurational changes and equilibrium dynamics between functional domains on 1-100 nanosecond timescale.

I present here examples for different types of motions related to the structure of proteins and bioconjugates. Thermal unfolded Ribonuclease A shows polymer like dynamics despite the 4 disulfide bonds restricting the degrees of freedom. Phosphoglycerate kinase shows a clear hinge motion between the main domains. PEGylation seems not to influence domain motion but adds additional internal dynamics in the protein-polymer complex. Immunoglobulin 1 (IGG1) presents a strong dynamics due to the short linkers connecting the Fc with the Fab domains.

Relevant forces and friction will be discussed in terms of the Ornstein-Uhlenbeck process.

References

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- (2) Ciepluch K., Radulescu, A., Hoffmann I., Raba, A., Allgaier, J., Richter D., Biehl R., in review
- (3) Stingaciu, L. R.; Ivanova, O.; Ohl, M.; Biehl, R.; Richter, D. *Sci. Rep.* 2016, 6, 22148.

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