

# Modeling of intrinsically disordered proteins in a crowded environment

## Student Project

January 2021

### Project description

Intrinsically Disordered Proteins (IDPs) are proteins lacking a tertiary structure whose inherent flexibility has been found to exhibit unique biological advantages. The cellular environment is very crowded, and these conditions are more likely to affect disordered proteins than folded ones.

In this work we study the coupling between the ionization and the conformational properties of two IDPs, histatin-5 and  $\beta$ -amyloid 42, in the presence of Bovine Serum Albumin (BSA) as crowding agent, using the modeling package ESPResSo (<https://espressomd.org/wordpress/>).

The disordered and crowder proteins are described using coarse-grained models. Both ionization properties (global and specific aminoacid charge, binding capacity) and radius of gyration ( $R_g$ ) will be analyzed in a range of pH and salt concentrations.

Throughout this project, the student will prepare the simulation input files, start the simulations and analyse the results. The student will receive close guidance and training but will have the opportunity to work independently.

**Qualifications:** Interest in the project and in learning.

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