

PAID DIPLOMA / MASTER'S THESIS

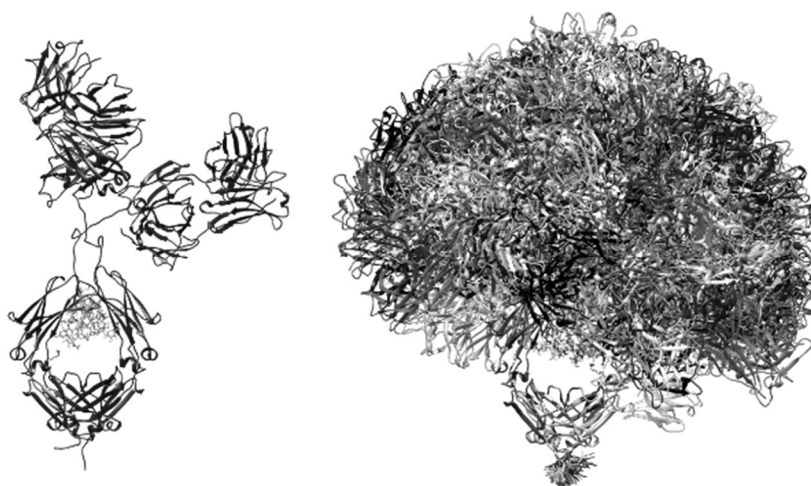
CONFORMER GENERATION OF FLEXIBLE MULTI-DOMAIN PROTEINS – TOWARDS MORE REALISTIC MODELS OF SOLUTION STRUCTURES

Ref. No. DA197

To dedicated students of Chemistry, Physics or related.

Objective

With tools such as alphafold or RoseTTAFold it is now possible to reliably predict the structures of globular/single domain proteins, based on their amino acid sequences. An equally reliable prediction of the solution structures of multi-domain proteins has not been achieved yet. This project tries to make progress in this direction by designing and testing algorithms for the generation and analysis of large conformational ensembles of such proteins in-silico, using as test-case IGG3. An existing pipeline, specific for IGG1/2/4 antibody conformational sampling, will be modified and extended. The result will be validated using data from small angle x-ray scattering (SAXS) experiments. (<https://pubmed.ncbi.nlm.nih.gov/7417493/>), and coarse grained MD simulation.



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