

Title: Biomolecular structure modelling in CASP15 Competition

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CASP(Critical Assessment of Structure Prediction) competition provides amino-acid/nucleotide sequences for experimentally determined structures that haven't been published. Multiple groups from around the world then attempt to predict the structure from the given sequences. The predicted models are then assessed against the experimentally determined structure. CASP15 involved multiple categories of targets such as RNA structure modeling, Protein-Ligand Complexes, Oligomeric proteins and Antigen-Antibody docking. It consists of an automated server prediction and human modeling component. An array of tools and biological literature analysis was used for the human structure modeling component. Tools used included AlphaFold2 and AlphaFold-Multimer , PIPER, GLIDE and IFD from the Schrodinger Suite for antibody and ligand docking, ROSETTA FARFAR2 for RNA modeling, SAM and LZerD protein Docking for protein complex modeling. The poster would describe in detail the pipeline used for RNA structure modelling of G-quadruplexes as well as ligand docking methodologies used. It would also highlight the methods used to model large oligomeric complexes and briefly discuss the results obtained by the lab in the competition.