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BhageerathH+: A software suite for tertiary structure prediction of globular proteins

Rahul Kaushik^{1, 2}, Ankita Singh¹, Shashank Shekhar¹ and B Jayaram^{1, 2, 3} ¹Supercomputing Facility for Bioinformatics & Computational Biology IIT Delhi, India ²Kusuma School of Biological Sciences IIT Delhi, India ³Indian Institute of Technology Delhi, India

The constantly widening gap between known protein sequences and experimentally solved structures, the need for structures of novel protein drug targets to benefit in structure based drug discovery have raised the necessity for developing highly reliable protein structure prediction approaches. Over the past two decades, chronological assessments of improvements in structure prediction methodologies have been accounted via CASP experiments. The success of prediction methodologies has assisted the scientific community to explore the experimentally unsolved proteins more efficiently at their structural level. In the recently concluded CASP12 experiment, we tested BhageerathH+ software suite which delivers a reliable structure for the protein from sequence information. BhageerathH+ primarily comprises three major steps namely structure generation for conformational sampling, structure scoring for selecting the best conformations and structure refinement and side chain optimization for quality improvement. The sampled conformations are scored and ranked with an improved version of ProTSAV (ProTSAV+) for selecting top 50 conformations. The selected conformations are further processed with molecular dynamics based refinement and side chain optimization for enhancing their structural quality and re-ranked with ProTSAV+ for selecting top 5 conformations. The methodology was automated and fielded in the recently concluded CASP12 experiment under TS category as BhageerathH+ server and ranked jointly at 1st position for low resolution structures (under 7Å), 4th for medium resolution structures (under 5Å) and 8th for low resolution structures (under 7Å).

Biography

Rahul Kaushik has been working in the field of protein structure prediction as a Doctoral student for last five years and his thrust area of research work mainly focuses on development of new algorithms for improvement in protein structure prediction. He has contributed to development of other algorithms namely NCL Align, SD Index, ProTSAV, RM2TS and BhageerathH.

rahul@scfbio-iitd.res.in

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