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Comparative study of three benchmark protein structure prediction techniques for the prediction of epidermal growth factor receptor (EGFR) family protein structures

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Background: Epidermal Growth Factor receptor (EGFR) family is a group of four highly conserved trans-membrane tyrosine kinase receptors (EGFR, ErbB2/HER2, ErbB3/HER3 and ErbB4/HER4) involved in fate decision of many pivotal biological processes. Several mutations on EGFR have been associated to number of human cancers making it one of the most sought after target for cancer therapeutics. However despite its therapeutic importance, its full length structural behavior is still illusive. Therefore to utilize and exploit this magic drug target, it is imperative to decipher its structure.

Methodology: The present work was carried out by a comparison of three benchmark techniques of protein structure prediction viz. Homology modeling, threading and ab-initio. Homology modeling was carried out exhaustively using single as well as multiple template modeling with all the combinations possible with homologs having e-value 0; Threading was done using HHpred online server while ITASSER was utilized for ab-initio structure prediction. Further, the structures were energy minimized iteratively 10 times with evaluation of the structure being done at each step using SAVES server and superimposition of experimentally determined partial structures.

Result: Despite homology modeling being the best technique, which exploits the added advantage of longer template knowledge, threading proved to be the best technique for predicting EGFR family structures followed by Homology modeling and ab-initio.

Conclusion: This study is indicative that even after advancement of biological and computer sciences, a huge lacuna still remains in development of automated and accurate protein structure prediction tools, which can only be tackled using human expertise and intervention. However, this anomaly may also be attributed to some hidden technical and biological biasness which still needs to be explored.

Biography

Saurav B Saha joined the Department of Computational biology and Bioinformatics, Sam Higginbotom Institute of Agriculture, Technology & Sciences - Deemed University in the year 2011 as Assistant Professor. Before joining the institution, he has served in both academia and corporate in different capacities viz., Assistant Professor and In-charge (Bioinformatics) at Shoolini Univesity and as Bioinformatician in LabIndia Pvt. Ltd. (Applied Biosystems Wing). He underwent his under graduation (BTech Biotechnology) and Post graduation (MTech Bioinformatics) from Sam Higginbotom Institute of Agriculture, Technology & Sciences - Deemed University (formerly Allahabad Agricultural Institute). His research focuses to understand different robustness machinery in biological systems, development of novel drugs pertaining to menacingly dreadful infectious diseases and facilitation of life science research through development of databases, algorithms and softwares.

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