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ProTSAV+: A meta-server for identification and scoring of protein tertiary structures

Ankita Singh[1, 2], Rahul Kaushik[1], Himani Kuntal[2] and B Jayaram[1]
[1]Indian Institute of Technology Delhi, India
[2]Banasthali University, India

Statement of the Problem: Protein structure quality assessment is among the most important challenges in the field of structural biology. Recent methodological advancements in protein structure prediction approaches have created an immediate necessity for highly efficient quality assessment methods for discriminating good model structures. Better quality predicted protein structures may help in further biological function assignment and in structure based drug discovery.

Methodology & Theoretical Orientation: The ProTSAV+ meta-server integrates 11 individual approaches of quality assessment and provides the user with a single quality score in case of individual model structure and ranking in case of multiple decoy structures. The ProTSAV+ performs weight, age based combination of some of the widely used and thoroughly validated freely/on request available tools. These tools mainly embed various structural and energetic features individually or in combination like accessible surface area, non-covalent interactions, residues based contact potentials, etc.

Findings: The specificity and sensitivity of meta-server is 88% and 91%, respectively for good quality model structures and the same goes to 100% and 98%, respectively for experimental structures. The updated version of the meta-server is fielded in recently concluded CASP12 protein structure prediction experiment under 'QA category' and performed among some of the leading QA participants. For instance, the meta-server ranked among top 20 participants in 22 targets out of 40 publically released target.

Conclusion & Significance: The server overcomes the limitations of any single method and is seen to be robust in helping in improved quality assessment.

Biography

Ankita Singh is currently pursuing PhD from Indian Institute of Technology Delhi, India. Her research interests centers around the development of protein structural database for malarial parasites and advancing the quality assessment methodologies. She has her expertise in scoring and assessing the predicted protein tertiary structures with different parameters to select best predicted model.

ankita@scfbio-iitd.res.in

Notes:

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