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Abstract

Methods for the Refinement of Protein Structure 3D Models

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Abstract:
The refinement of predicted 3D protein models is crucial in bringing them closer towards experimental accuracy for further computational studies. Refinement approaches can be divided into two main stages: The sampling and scoring stages. Sampling strategies, such as the popular Molecular Dynamics (MD)-based protocols, aim to generate improved 3D models. However, generating 3D models that are closer to the native structure than the initial model remains challenging, as structural deviations from the native basin can be encountered due to force-field inaccuracies. Therefore, different restraint strategies have been applied in order to avoid deviations away from the native structure. For example, the accurate prediction of local errors and/or contacts in the initial models can be used to guide restraints. MD-based protocols, using physics-based force fields and smart restraints, have made significant progress towards a more consistent refinement of 3D models. The scoring stage, including energy functions and Model Quality Assessment Programs (MQAPs) are also used to discriminate near-native conformations from non-native conformations. Nevertheless, there are often very small differences among generated 3D models in refinement pipelines, which makes model discrimination and selection problematic. For this reason, the identification of the most native-like conformations remains a major challenge.

Biography:
Recep Adiyaman is faculty at School of Biological Sciences, University of Reading, Reading RG6 6AS, UK.

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