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Fast loop modeling for protein structures[1] JIONG ZHANG, SON NGUYEN, YI SHANG, DONG XU, IOAN KOSZTIN, University of Missouri —
X-ray crystallography is the main method for determining 3D protein structures. In many cases, however, flexible loop regions of proteins cannot be resolved by this approach. This leads to incomplete structures in the protein data bank, preventing further computational study and analysis of these proteins. For instance, all-atom molecular dynamics (MD) simulation studies of structure-function relationship require complete protein structures. To address this shortcoming, we have developed and implemented an efficient computational method for building missing protein loops. The method is database driven and uses deep learning and multi-dimensional scaling algorithms. We have implemented the method as a simple stand-alone program, which can also be used as a plugin in existing molecular modeling software, e.g., VMD. The quality and stability of the generated structures are assessed and tested via energy scoring functions and by equilibrium MD simulations. The proposed method can also be used in template-based protein structure prediction.

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