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Selective Refinement and Molecular Dynamics Ranking Selection of Near-native Protein Structures JIONG ZHANG, JINGFEN ZHANG, DONG XU, YI SHANG, IOAN KOSZTIN, Univerisity of Missouri-Columbia — In recent years *in silico* protein structure prediction reached a level where a variety of servers can generate large pools of near-native structures. However, the identification and further refinement of the best structures from the pool of decoys remain problematic. To address these issues, we have developed a selective refinement protocol (SRP), and a molecular dynamics (MD) simulation based ranking method (MDR). In SRP the refinement of structures is accomplished by using the relax mode of the Rosetta software package, subject to specific constraints determined by the type and complexity of the target. The final best models are selected with MDR by testing their relative stability against gradual heating during all atom MD simulations. We have implemented the selective refinement protocol and the MDR method in Mufold-MD, our fully automated protein structure prediction server. Mufold-MD was one of the top servers in the CASP10 competition.

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