Systematic and comparative evaluation of methods for template-based modeling of protein structures

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Modeling protein structures is critical for understanding protein functions in various biological and biotechnological studies. Template-based modeling (TBM) can generate high-accuracy structural models using structural information of homologous proteins. However, it still remains as a challenge to select appropriate software programs for pairwise alignments, which is a critical initial step of the TBM and heavily affects the quality of protein structure models to be built. Here, pairwise alignment methods for TBM are compared with respect to the quality of structure models built using these methods. This comparative study is conducted using comprehensive datasets of soluble and membrane proteins. Overall, PSI-BLAST consistently shows high performance across the datasets and model evaluation metrics used. [This work was supported by the Technology Development Program to Solve Climate Changes on Systems Metabolic Engineering for Biorefineries (NRF-2012M1A2A2026556 and NRF-2012M1A2A2026557) and the Bio & Medical Technology Development Program (NRF-2018M3A9F3079664) from the Ministry of Science and ICT (MSIT) through the National Research Foundation (NRF) of Korea].