

## Evaluation of Multiple Methods for the Template-Based Modeling of Protein Structures

이상미, 장우대, 이상엽, 김현욱<sup>†</sup>

KAIST

(ehukim@kaist.ac.kr<sup>†</sup>)

Template-based modeling (TBM) is one of representative protein structure modeling approaches, and it is considered better than other approaches in terms of the ease of implementation and the quality of the resulting protein structure model. However, within TBM, it is still very challenging to select appropriate methods for pairwise alignments which is a critical initial step of TBM, and the quality of protein structure models to be built can be affected by the which model building program is used. To this end, total 13 alignment methods and two most popular model building programs for the TBM were evaluated with respect to the quality of their resulting structure models built using large-scale comprehensive datasets of soluble and membrane proteins. Overall, PSI-BLAST, a profile-based method, consistently performed the best although programs other than PSI-BLAST performed the best on a few occasions. Also, use of the two modeling building programs does not seem to heavily affect the model quality for the datasets considered except for few occasions. This study can provide useful guidelines to choose pairwise alignment methods and model building programs for more accurate TBM.