<https://s3.amazonaws.com/academia.edu.documents/30804839/TopPredII.pdf?response-content-disposition=inline%3B%20filename%3DCABIOS_APPLICATIONS_NOTES.pdf&X-Amz-Algorithm=AWS4-HMAC-SHA256&X-Amz-Credential=AKIAIWOWYYGZ2Y53UL3A%2F20190914%2Fus-east-1%2Fs3%2Faws4_request&X-Amz-Date=20190914T133314Z&X-Amz-Expires=3600&X-Amz-SignedHeaders=host&X-Amz-Signature=9484da90ac950aebef08ad763cacb392acb031482c38bf5a0f0880398256c06e>

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TopPred II: an improved software for membrane protein structure predictions Manuel G.CIaros1 , Gunnar von Heijne2

The prediction of membrane protein structure begins with the construction of a hydrophobicity profile (Figure 1A) which serves to identify 'certain' and 'putative' transmembrane segments (Figure IB). This is accomplished using a trapezoid sliding window (a more detailed description of the method is given in (von Heijne, 1992)) which is more realistic than a simple rectangular window. Although several hydrophobicity scales are provided with the program, the GES one (Engelman et al., 1986) is recommended. Transmembrane domains are considered as 'certain' or 'putative' according to the 'Upper Cutoff and 'Lower Cutoff parameters. Once the transmembrane segments have been identified, the topologies (Figure 1C) are predicted differently for eukaryotic and prokaryotic proteins. For prokaryotic proteins, the number of positively charged residues (including the free N-terminal amino group) at inter-transmembrane segments of each structure is counted. Segments longer than the 'Critical Length' parameter [60 residues, (Andersson and von Heijne, 1993)] are not considered (von Heijne and Gavel, 1988), but the first N-terminal loop segment is always taken into account regardless of its length (von Heijne, unpublished results). The best topology is then predicted by application of the 'positive-inside' rule (von Heijne, 1986). In the case of eukaryotic proteins, three different criteria are used to determine the topology (Sipos and von Heijne, 1993). The first is, as for prokaryotic proteins, the difference in positively charged residues between the two sides of the membrane. The second criterion considered is the net charge difference (Arg, Lys, Glu, Asp) between the 15 N-terminal and the 15 C-terminal residues flanking the most N-terminal transmembrane segment (Hartman et al., 1989). Finally, the overall amino acid composition of loops longer than 60 residues is analysed by the compositional distance method (Nakashima and Nishikawa, 1992). The program also has an option in which the unfavorable free energy of membrane insertion of charged residues in the transmembrane segments can be reduced by means of the 'Charge-pair Energy' parameter if they can form i,i+3 and i,i + 4 charge-pairs.

**2.**

**Transmembrane Topology Prediction Methods: A Re-assessment and Improvement by a Consensus Method Using a Dataset of Experimentally-Characterized Transmembrane Topologies**

**Article type:**Research Article

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**Abstract:**We selected 10 transmembrane (TM) prediction methods (KKD, TMpred, TopPred II, DAS, TMAP, MEMSAT 2, SOSUI, PRED-TMR2, TMHMM 2.0 and HMMTOP 2.0) and re-assessed its prediction performance using a reliable dataset with 122 entries of experimentally-characterized TM topologies.  Then, we improved prediction performance by a consensus prediction method.  Prediction performance during re-assessment and consensus prediction were based on four attributes: (i) the number of transmembrane segments (TMSs), (ii) the number of TMSs plus TMS-position, (iii) N-tail location and (iv) TM topology.  We noted that hidden Markov model-based methods dominate over other methods by individual prediction performance for all four attributes.  In addition, all top-performing methods generally were model-based.  Among prokaryotic sequences, HMMTOP 2.0 solely topped among other methods with prediction accuracies ranging from 64% to 86% across all attributes.  However, among eukaryotic sequences, prediction performance for all the attributes was relatively poor compared with prokaryotic ones.  On the other hand, our results showed that our proposed consensus prediction method significantly improved prediction performance by, at least, an additional nine percentage points particularly among prokaryotic sequences for the number of TMS (84%), number of TMS and position (80%), and TM topology attributes (74%).  Although our consensus prediction method improved also the prediction performance among eukaryotic sequences, the obtained accuracies for all attributes were relatively lower than that obtained by prokaryotic counterparts particularly for TM topology.

**Keywords:**consensus prediction, prediction performance assessment, transmembrane proteins, transmembrane protein database, transmembrane topology prediction

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