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# Improved 3D Structure Prediction of Beta-Barrel Membrane Proteins by Using Evolutionary Coupling Constraints, Reduced State Space and an Empirical Potential Function

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**Abstract :** Beta-barrel membrane proteins are found in the outer membrane of gram-negative bacteria, mitochondria, and chloroplasts. They carry out diverse biological functions, including pore formation, membrane anchoring, enzyme activity, and bacterial virulence. In addition, beta-barrel membrane proteins increasingly serve as scaffolds for bacterial surface display and nanopore-based DNA sequencing. Due to difficulties in experimental structure determination, they are sparsely represented in the protein structure databank and computational methods can help to understand their biophysical principles. We have developed a novel computational method to predict the 3D structure of beta-barrel membrane proteins using evolutionary coupling (EC) constraints and a reduced state space. Combined with an empirical potential function, we can successfully predict strand register at > 80% accuracy for a set of 49 non-homologous proteins with known structures. This is a significant improvement from previous results using EC alone (44%) and using empirical potential function alone (73%). Our method is general and can be applied to genome-wide structural prediction.

**Keywords :** beta-barrel membrane proteins, structure prediction, evolutionary constraints, reduced state space
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