

Computational studies on eukaryotic transmembrane β -barrel proteins

Ahmed F. Roumia¹, Margarita C. Theodoropoulou¹, Konstantinos D. Tsirigos², Pantelis G. Bagos¹

¹Department of Computer Science and Biomedical Informatics, University of Thessaly, 35100 Lamia, Greece.

²Department of Bio and Health Informatics, Technical University of Denmark, Kgs Lyngby, Denmark
Email of Corresponding author: pbagos@compngen.org

Abstract

Transmembrane β -barrel proteins perform multiple cellular functions such as passive transport of ions and allowing the flux of molecules. Also, they act as enzymes, transporters, receptors and virulence factors. Even though, in the last few years, several families of eukaryotic β -barrel outer membrane proteins (OMPs) have been discovered, the computational characterization of these families is far from complete. The PFAM database includes only very few characteristic profiles for these families and, in most cases, the profile Hidden Markov Models were trained using both prokaryotic and eukaryotic proteins. Here, we present, for the first time, a comprehensive computational analysis of eukaryotic transmembrane β -barrels. Ten characteristic pHMMs were built that can discriminate eukaryotic β -barrels from other classes of β -barrel proteins (globular and bacterial) and are, also, capable of discriminating between mitochondrial and chloroplastic ones. Specifically, we built six new pHMMs for the chloroplastic β -barrel families not included in the PFAM database and, also, updated the profile for MDM10 family (PF12519) and divided the porin family (PF01459) into two separated families VDAC and TOM40. We hope that all the pHMMs presented here will be used for the detection and characterization of eukaryotic OMPs in newly discovered proteomes.