Assessing the local structural quality of transmembrane protein models using statistical potentials (QMEANBrane)

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Motivation: Membrane proteins are an important class of biological macromolecules involved in many cellular key processes including signalling and transport. They account for one third of genes in the human genome and >50% of current drug targets. Despite their importance, experimental structural data are sparse, resulting in high expectations for computational modelling tools to help fill this gap. However, as many empirical methods have been trained on experimental structural data, which is biased towards soluble globular proteins, their accuracy for transmembrane proteins is often limited.

Results: We developed a local model quality estimation method for membrane proteins ('QMEAN-Brane') by combining statistical potentials trained on membrane protein structures with a per-residue weighting scheme. The increasing number of available experimental membrane protein structures allowed us to train membrane-specific statistical potentials that approach statistical saturation. We show that reliable local quality estimation of membrane protein models is possible, thereby extending local quality estimation to these biologically relevant molecules.

Availability and implementation: Source code and datasets are available on request.

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