



Universität
Basel

Research Project

Development of scoring functions for model quality estimation for membrane proteins

Project funded by own resources

Project title Development of scoring functions for model quality estimation for membrane proteins

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Organisation / Research unit

Departement Biozentrum / Bioinformatics (Schwede)

Project Website <http://swissmodel.expasy.org/qmean/>

Project start 01.01.2011

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Status Completed

Quality assessment of protein structures is an important part of experimental structure validation and plays a crucial role in protein structure prediction. Most current scoring functions are primarily designed to rank alternative models of the same sequence supporting model selection whereas the prediction of the absolute quality of an individual protein model has received little attention in the field. However, reliable absolute quality estimates are crucial to assess the suitability of a model for specific biomedical applications. We have developed a new absolute measure for the quality of protein models, which provides an estimate of the “degree of nativeness” of the structural features observed in a model and describes the likelihood that a given model is of comparable quality to experimental structures. Model quality scores for individual models are expressed as “Z-scores” in comparison to scores obtained for high-resolution crystal structures. We demonstrated the ability of the newly introduced QMEAN Z-score to detect experimentally solved protein structures containing significant errors, as well as to evaluate theoretical protein models.

The second part of the project aims at the development of potentials of mean force tailored for membrane protein models.

Financed by

Other funds

Add publication

Published results

156351, Benkert, Pascal; Tosatto, Silvio C E; Schwede, Torsten, Global and local model quality estimation at CASP8 using the scoring functions QMEAN and QMEANclust, 0887-3585, Proteins, Publication: JournalArticle (Originalarbeit in einer wissenschaftlichen Zeitschrift)

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156355, Benkert, Pascal; Schwede, Torsten; Tosatto, Silvio Ce, QMEANclust : estimation of protein model quality by combining a composite scoring function with structural density information, 1472-6807, BMC Structural Biology, Publication: JournalArticle (Originalarbeit in einer wissenschaftlichen Zeitschrift)

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749244, Benkert, Pascal; Biasini, Marco; Schwede, Torsten, Toward the estimation of the absolute quality of individual protein structure models, 1367-4803, Bioinformatics, Publication: JournalArticle (Originalarbeit in einer wissenschaftlichen Zeitschrift)

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2689815, Studer, Gabriel; Biasini, Marco; Schwede, Torsten, Assessing the local structural quality of transmembrane protein models using statistical potentials (QMEANBrane), 1367-4803, Bioinformatics, Publication: JournalArticle (Originalarbeit in einer wissenschaftlichen Zeitschrift)

Add documents

Specify cooperation partners

ID	Kreditinhaber	Kooperationspartner	Institution	Laufzeit - von	Laufzeit - bis
1533620	Schwede, Torsten	Tramontano, Anna	University of Rome	01.01.2009	31.12.2016
2355647	Schwede, Torsten	Kryshchak, Andriy	UC Davis Genome Center	01.01.2009	31.12.2021