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Whole Protein Native Fitness Potentials ESHEL FARAGGI, Research and Information Systems, LLC; IUPUI Biochem. and Mol. Bio. Dept.; NCH/OSU Battelle Center for Mathematical Medicine, ANDRZEJ KLOCZKOWSKI, Battelle Center for Mathematical Medicine, NCH/OSU, Columbus, Ohio, USA — Protein structure prediction can be separated into two tasks: sample the configuration space of the protein chain, and assign a fitness between these hypothetical models and the native structure of the protein. One of the more promising developments in this area is that of knowledge based energy functions. However, standard approaches using pair-wise interactions have shown shortcomings demonstrated by the superiority of multi-body-potentials. These shortcomings are due to residue pair-wise interaction being dependent on other residues along the chain. We developed a method that uses whole protein information filtered through machine learners to score protein models based on their likeness to native structures. For all models we calculated parameters associated with the distance to the solvent and with distances between residues. These parameters, in addition to energy estimates obtained by using a four-body-potential, DFIRE, and RWPlus were used as training for machine learners to predict the fitness of the models. Testing on CASP 9 targets showed that our method is superior to DFIRE, RWPlus, and the four-body potential, which are considered standards in the field.

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