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An artificial neural network model to predict structure-based protein–protein free energy of binding from rosetta-calculated properties

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The prediction of the free energy (ΔG) of binding for protein–protein complexes is of general scientific interest as it has a variety of applications in the fields of molecular and chemical biology, materials science, and biotechnology. Despite its centrality in understanding protein association phenomena and protein engineering, the ΔG of binding is a daunting quantity to obtain theoretically. In this work, we devise a novel Artificial Neural Network (ANN) model to predict the ΔG of binding for a given three-dimensional structure of a protein– protein complex with Rosetta-calculated properties. Our model was tested using two data sets, and it presented a root-mean-square error ranging from 1.67 kcal mol-1 to 2.45 kcal mol-1, showing a better performance compared to the available state-of-the-art tools. Validation of the model for a variety of protein–protein complexes is showcased.

Biography

Experience on computational science, machine learning research, quantum computing, and computational/theoretical chemistry. Currently professor at CESAR School of undergraduate, master and doctoral computer science program, coordinator of Natural Computing and Computational Natural Science Research group and Quantum Application in Technology and Software at CESAR School.