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Predicting protein-peptide interactions from scratch[1] CHENGFEI YAN, XIANJIN XU, XIAOQIN ZOU, University of Missouri, ZOU LAB TEAM
— Protein-peptide interactions play an important role in many cellular processes. The ability to predict protein-peptide complex structures is valuable for mechanistic investigation and therapeutic development. Due to the high flexibility of peptides and lack of templates for homologous modeling, predicting protein-peptide complex structures is extremely challenging. Recently, we have developed a novel docking framework for protein-peptide structure prediction. Specifically, given the sequence of a peptide and a 3D structure of the protein, initial conformations of the peptide are built through protein threading. Then, the peptide is globally and flexibly docked onto the protein using a novel iterative approach. Finally, the sampled modes are scored and ranked by a statistical potential-based energy scoring function that was derived for protein-peptide interactions from statistical mechanics principles. Our docking methodology has been tested on the Peptidb database and compared with other protein-peptide docking methods. Systematic analysis shows significantly improved results compared to the performances of the existing methods. Our method is computationally efficient and suitable for large-scale applications.

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Chengfei Yan
University of Missouri

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