

March 15-16 2018
Barcelona, SpainWei Liu et al., Biochem Mol Biol J, Volume 4
DOI: 10.21767/2471-8084-C1-009

MPGA: A MIXED ALGORITHM OF MATCHING PURSUIT AND GENETIC ALGORITHM FOR STRUCTURE CHARACTERIZATION OF LARGE INTRINSICALLY DISORDERED PROTEINS

Wei Liu¹, Xiao Liu¹, Guanhua Zhu², Lanyuan Lu² and Daiwen Yang¹¹National University of Singapore, Singapore²Nanyang Technological University, Singapore

Structure characterization of intrinsically disordered proteins (IDPs) remains a key obstacle in understanding their functional mechanism. Due to the highly dynamic feature of IDPs, structure ensembles instead of static unique structures are often derived from experimental data. Several state-of-art computational methods have been developed to select an optimal ensemble from a pre-generated structure pool. For a large IDP, we usually need a large structure pool to sample the possible conformational space and a big structure ensemble to describe its dynamic feature. In such a case, the search space becomes too big to be adequately explored by conventional algorithms, causing the decline of their optimization performance. We developed a matching pursuit genetic algorithm (MPGA), which takes advantages both from

matching pursuit (MP) to reduce the search space and from genetic algorithm (GA) to free the requirement on the constraint types for structure determination. The MPGA method was tested in a structure ensemble selection from a large pool (>200 k) of an IDP with 306 amino acids. By comparing with conventional GA, MPGA demonstrated both higher calculation speed and better optimization result.

Biography

Wei Liu has completed his PhD from Nanyang Technology University, Singapore. He is a research fellow of National University of Singapore, Singapore.

dbslw@nus.edu.sg