武汉物数所理论交叉学术交流系列报告

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分子动力学方法用于细胞膜环境中胰岛淀粉性多肽(IAPP)聚合机制的研究

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频标楼四楼报告厅

Brief Introduction of the Speaker:

Dr. Mojie Duan

2004 B.S(Physics), Huazhong Univ. of Sci. and Tech.
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Dr. Duan's research interests include: Computational simulation study and analysis of biological complex system; Protein-protein, Protein-membrane, protein-drug and protein-nucleic acid interaction; Protein design and computer-aided drug discovery; Enhanced sampling methodology development; Application of dimensionality reduction methods in the analysis of large-scale data.

Abstract: The amyloid fibrils formed by islet amyloid polypeptide (IAPP) are associated with type II diabetes. However, the aggregation and toxicity mechanisms of IAPP remain unclear. One of the proposed mechanisms of the toxicity of IAPP is that it causes membrane damage. Besides, it has been revealed that IAPP variants with single mutations significantly differ with the wild-type IAPP in the aggregation rates and the toxicity. By using the molecular dynamics simulation technology, we studied the dynamic properties of monomeric IAPP variants and IAPP aggregates in the membrane environment. We discovered the structure differences of wild type IAPP and its mutants. Based on the simulation results, we proposed a model to explain the early stage of IAPP fibril formation. In addition, the effects of cholesterols to the IAPP fibrils formation were also studied. Our simulation results would provide useful insights in the development of novel drugs to the therapy of type II diabetes.

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