Computational Investigations on Target-Site Searching and Recognition Mechanism by Thymine DNA Glycosylase during DNA Repair Process

SPEAKER: Lin-Tai Da, Shanghai Jiao Tong University
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VENUE: Room 264, Geography Building, Zhongbei Campus

HOST: Fei Xia, East China Normal University

ABSTRACT OF THE TALK

DNA glycosylase, as one member of the DNA repair machineries, plays an essential role in correcting mismatched/damaged DNA base pair by cleaving the N-glycosidic bond between the sugar and target base through the base excision repair (BER) pathways. Efficient corrections of these DNA lesions are critical for maintaining genome integrity and preventing premature aging and cancer. The target-site searching and recognition mechanism by DNA glycosylase, however, remains unknown and experimental characterization of the above process is still challenging due to the limited spatiotemporal resolutions. In this work, by employing high performance computing, combined with Markov state model construction based on extensive all-atom molecular dynamics (MD) simulations, we revealed the key intermediates of thymine DNA glycosylase (TDG) involved in the target-searching process and obtained associated kinetic properties.

BIOGRAPHY

Dr. Lin-Tai Da obtained his Ph.D. degree from Peking University in 2010. Then, he conducted postdoc research at Hong Kong University of Science and Technology and Florida State University, respectively. In 2017, he joined the Shanghai Center for Systems Biomedicine, Shanghai Jiao Tong University as a Principle Investigator.