S N BOSE NATIONAL CENTRE
FOR BASIC SCIENCES
Block JD, Sector III, Salt Lake, Kolkata 700 106

DEPARTMENTAL SEMINAR

Chemical, Biological & Macro-Molecular Sciences

02 November' 2021 11.00 AM ONLINE

SPEAKER

Prof. Nilashis Nandi, Professor, Kalyani University

TITLE OF THE TALK

A Tale of Two Sites

ABSTRACT

Accuracy of enzymatic reaction is often ensured by editing the erroneous product. Both synthesis and editing take place in the active sites. The active sites of bacterial aminoacyl tRNA synthetases (aaRS) are validated targets of antibiotics. The failure of eliminating the inhibitor is a way to halt the bacterial protein biosynthesis. We shall discuss the mechanism of binding of an approved drug, Mupirocin, in active site. The resistance development of Mupirocin is an impending dire threat. This inhibitor targets bacterial isoleucyl tRNA synthetase (IleRS). The present work is aimed at understanding the lacunae of knowledge concerning the active site conformational dynamics in IleRS in presence of inhibitor mupirocin. We have carried out classical molecular dynamics simulation and metadynamics simulations of the open state of IleRS from Staphylococcus aureus, the closed state tripartite complex bound with cognate adenylate and tRNA, the closed state tripartite complex bound with noncognate MRC, and the closed state tripartite complex bound with tRNA and MRC with mutated IleRS. The results reveal molecular details of the dynamics of mupirocin binding in the active site which has important bearing on development of IleRS inhibitors.

HOST FACULTY

Prof. Ranjit Biswas

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