

# Abstract

## **Biophysical and Biochemical Investigation on the Structure, Function and Dynamics of Biomolecules Under Physiologically Relevant Environments**

By

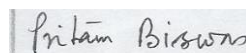
Pritam Biswas

Post Graduate and Research Department of Microbiology

Registration No. Ph.D./17/MCB/02

Essential dynamics is strongly correlated to biomolecular structure and function. The correlation between structure-dynamics of biomolecules is the key to understanding biomolecular function under different physiological environments. With time there has been an increase in demand for functional biomolecules by the biotechnology-industrial complex both in food, beverages as well as in the health care and pharmaceutical industries. However, a lack of understanding of the structure, function and dynamics of functional biomolecules under different physiologically relevant environments prevents our ability to utilize these biomolecules to their highest efficiency. Thus, exploring an in-depth structural, functional and dynamics study of the biomolecules under the different physiologically relevant environments are the motives of this thesis. Using a combined biophysical, biochemical and aided by various computational methods a correlation between structure-function and dynamics of biomolecules has been studied. In one set of work the influence of temperature on the structure, function and dynamics on a thermostable enzyme  $\beta$ -glucosidase (BGL) has been studied. Spectroscopic and computational studies confirmed the presence of four loop regions (LRs) acting as a gatekeeper to the incoming substrate. While, detailed studies of  $\alpha$ -Chymotrypsin (CHT) at different temperatures revealed the essential motions modulating the catalytic activity. Both spectroscopic and theoretical calculations aided in understanding the loop motions and corroborated with the CHT catalytic activity. Finally, a homeothermic enzyme  $\alpha$ -chymotrypsin was treated with a common covalent crosslinker formalin which resulted in reduced catalytic activity with increase in formalin concentration. Spectroscopic studies and computational calculations found remarkable change in molecular recognition of CHT and catalytic activity owing to residue modification by formalin. This study, will shed some light on the close relationship between structure-function-dynamics of biomolecules. Thus, opening up new avenues of research for the biotechnology-industrial complex to explore and also the possibility of engineering new enzymes.

Date: 5<sup>th</sup> December, 2021



-----  
Pritam Biswas