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COMPREHENSIVE ANALYSIS OF THE CATALYTIC AND STRUCTURAL PROPERTIES OF A MU-CLASS GLUTATHIONE S-TRANSFERASE FROM *FASCIOLA GIGANTICA*

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Glutathione S-transferases (GSTs) play an important role in the detoxification of xenobiotics. They catalyze the nucleophilic addition of glutathione (GSH) to nonpolar compounds, rendering the products water-soluble. Fascioliasis is a neglected tropical disease caused by the food-borne trematodes *Fasciola hepatica* and *Fasciola gigantica*. These parasites infect mammals through ingestion of aquatic plants or contaminated water having encysted metacercaria. GST plays important roles in maintaining the cellular homeostasis, protection against oxidative stress and detoxification of xenobiotics thereby helping in survival. In the present study, we have investigated the catalytic and structural properties of a mu-class GST from the liver *Fasciola gigantica* (FgGST1). This will help in understanding the structure-function relationship of GSTs in these flukes. The gst1 gene was amplified, cloned in pET23a vector and overexpressed in BL21(DE3) cells. The purified recombinant FgGST1 formed a homodimer and composed of ~25 kDa subunit. Kinetic analysis revealed that FgGST1 displays broad substrate specificity and shows high GSH conjugation activity towards 1-chloro-2,4-dinitrobenzene, 4-nitroquinoline-1-oxide, trans-4-phenyl-3-butene-2-one and peroxidase activity towards trans-2-nonenal and hexa-2,4-dienal. The FgGST1 was highly sensitive to inhibition by Cibacron blue. The cofactor(GSH) and inhibitor(Cibacron blue) were docked against FgGST1 and binding sites were identified. The molecular dynamics studies and principal component analysis indicated the stability of the systems and the collective motions, respectively. Unfolding studies suggest that FgGST1 is a highly cooperative molecule because, during GdnHCl-induced denaturation, a simultaneous unfolding of the protein without stabilization of any partially folded intermediate is observed. The protein is stabilized with a conformational free energy of about 10±0.3 kcal mol−1.

BIOGRAPHY

Jupitara Kalita is a PhD student in the Department of Biochemistry, NEHU, Shillong. She has completed her MSc in Biochemistry in the year 2014. Her research interest concerns the structure, function, folding and stability of GSTs in infectious liver flukes. Her thesis centers around understanding the structure-function relationship of GSTs. This includes biochemical and biophysical characterization of the proteins. Other than this, she is also working in a project which deals with interactions of mRNA export factors (proteins) and nuclear pores.

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