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Disulfide Bonds Modulate Dynamics of Catalytic site in Native State of Pseudomonas Aeruginosa Elastase

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Pseudomonas aeruginosa Elastase (PAE) is a Thermolysin like protease (TLP) containing two disulfide bonds. A disulfide bond is located between Cys30-Cys57 which connects two β -strands within the N-terminal domain, while another disulfide bond, Cys270-Cys297, is located close to the end of C-terminal domain and connects two α -helices. Previous experimental studies have demonstrated the role of disulfide bonds in enzyme stability and activity. In this study a series of short time molecular dynamics simulations were performed in the native and disulfide bond broken states at 298 and 333 °K. Results revealed that removal of the disulfide bonds in the native state cause a significant change in dynamics of stability determinant loop. Moreover, flexibility and correlation of motions significantly altered within the active site region in low as well as high temperatures. These results suggest that disulfide bonds are crucial for structural stability and activity tuning of PAE in the native state by adjusting force distribution in structure.

Keywords: Disulfide Bonds, Molecular Dynamics Simulation, Stability Determinant Loop, Correlation of Motions.

administered with non-steroidal anti inflammatory agents. one of these enzymes is Strain-dependent extracellular metalloproteases which secreted by varied *S.marcescens* strains and has been purified and characterized by some scholars. This metalloprotease (serrapeptidase) is an important pharmaceutical agent. Serrapeptidase is useful for a wide range of inflammatory conditions. It is an effective drug for the treatment of breast engorgement. serrapeptidase relieve swelling and pain after surgery buccal, swelling, after maxillary sinus antrotomy. Enzyme may be effective to break down atherosclerotic plaques and fibrin on the inside of the arteries. In general, this major metalloprotease (SMP) has been detected in various strains of *S. marcescens* which is now manufactured for commercial exploitation because of its economic importance. In this research, the first, protease gene encoding a zinc-metalloprotease from the red-pigmented *Serratia marcescens* ZF03, which is isolated from hot-spring waters has been sequenced and reported to the GenBank. This fragment encodes an extracellular zinc-metalloendopeptidase with a molecular weight of approximately 50 kDa. This metalloprotease purified by ammonium sulphate precipitation, dialysis and DEAE-Sepharose chromatography and characterized. Proteolytic activity was determined by skim milk agar medium and zymography. Protease activity was optimum at temperature 50-55 °C and a range of pH 8-10. The effects of various compounds on protease activity and Kinetic parameters were determined. Considering high expression of metalloprotease and proteolytic activity, this protease can be used in the pharmaceutical Industries.

Keywords: Metalloprotease, *Serratia marcescens*, Extracellular protease, Characterization, Pharmaceutical.

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Purification and Characterizations of 50-kDa Extracellular Metalloprotease from Serratia Marcescens ZF03

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Proteolytic enzymes have been widely used in management of enzyme deficiencies and therapeutic applications. These enzymes are co-

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Structural Changes of Ribonucleoprotein ,LMG160, in the Presence of Sodium Chloride

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Low mobility group (LMG) proteins have been studied less intensively as they are very heterogeneous with low solubility. A fraction of these proteins named LMG160 (160 kDa) has been isolated from rat liver in pure form and characterized as a ribonucleoprotein (RNP) which detected in RNP-containing nuclear matrix of hepatocytes. In this study, we have investigated the effect of sodium chloride on the structure of