

Preface

Cellulase is an industrial enzyme which has significant applications in biofuel production and cellulosic waste management. Cellulase 7a from *Trichoderma reesei* is the most efficient enzyme in biohydrolysis of cellulose. In order to improve its thermostability it can be engineered by many approaches, such as hydrophobic interactions, aromatic interactions, hydrogen bonds, ion pairs, and disulfide bridge creation. In this study, introduction of disulfide bonds into the enzyme was chosen as an approach to achieve this aim. According to disulfide by design software, potential residues for creating disulfide bonds were identified. Accordingly, nine residues are mutated to cysteine, and as a result, five disulfide bridges were created. In order to study conformational stability of all the mutated proteins, molecular dynamic simulation was run for 20,000 ps by using GROMACS software. Root-mean-square deviation (RMSD), Root-mean-square fluctuation (RMSF), and Radius of gyration calculations were used for analysis the results. From the result it can be concluded that disulfide bridges can improve the stability of the protein if they are introduced in specific sites. In addition, more disulfide bridges make the protein more stable by increasing the compactness.

In Silico Engineering of Disulphide Bonds to Produce
Stable Cellulase

Barati, B.; Sadegh Amiri, I.

2015, VIII, 48 p. 34 illus., 30 illus. in color., Softcover

ISBN: 978-981-287-431-3