Efficacy of insect endogeneous cellulases for ligno-cellulosic biofuels deciphered using molecular docking studies

Sundaram Janarthanan¹, Ramanathan Nivetha¹, Sreeramulu Bhuvargavan¹, and Mani Meenakumari¹

¹University of Madras - Guindy Campus

January 11, 2023

Abstract

Cellulose, the substance that makes up most of a plant’s cell wall, is pondered to be one of the most abundant natural organic polymers on earth made up of glucose units linked by β-1, 4 glycosidic bonds. Insects possess cellulolytic system capable of producing variegate enzymes with multifarious specificities to break down complex lignocellulosic products. Astonishingly, endoglucanases, exoglucanase, and β-glycosidases act sequentially in a synergistic system to facilitate the breakdown of cellulose to utilizable energy source glucose. These extremely versatile enzymes are a better source in terms of environmental performance and overall energy efficiency. Pertaining to four main glycosyl hydrolase families (GHF), insect cellulases are distributed in all the insect orders explored up until now. In silico docking studies of endo-β-1,4-glucanase from 19 different insects belonging to six different orders identified that it possesses high affinity for all the six substrates, including CMC, cellulose, cellotriose, cellotetraose, cellopentose and cellohexaose. Additionally, β-glucosidase from nearly all the reported insect sources also showed considerable affinity towards cellobiose. Van der Waals, conventional hydrogen bonds, and carbon-hydrogen bonds stabilize the interaction between the enzyme and different substrates. Molecular dynamics simulations also held up the stability of various complexes. With lignocellulosic-based biofuels becoming a major focus of industrial and academic communities worldwide, this study can perhaps complement the propensity of insect cellulases for prospected applications.

Hosted file