CHEMOINFORMATIC STUDY ON SOME FUNGAL PECTINASES INHIBITORS

By

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B.Sc. Agric. Sc. (Agric.Biochem.), Faculty of Agric., Cairo Univ. 2008

M.Sc. Agric. Sc. (Agric.Biochem.), Faculty of Agric., Ain Shams Univ. 2014

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ABSTRACT

Rasha Abdel Kader Mohamed: Chemoinformatic Study on some Fungal Pectinases Inhibitors. Unpublished Ph.D. Thesis, Department of Biochemistry, Faculty of Agriculture, Ain Shams University, 2019.

Fusarium oxysporum f. sp. Lycopersici attacks tomato plants andcauses wilt disease. Fusarium Pathogenicity includes pectinases enzymes that enable the fungal penetration into the host cell wall.

The present study is focused on using Computational tools such as Auto-Dock program for screening of inhibitors of endo and exopolygalacturonase enzymes. It is based on a Lamarckian Genetic Algorithm (LGA) that estimates the binding energy and inhibition constant as parameters to select the best binding. The binding energy, Inhibition constant and amino acids interactions for the selected inhibitors were compared with that of the enzyme-substrate (sodium polygalacturonate). Allium species such as onion plant have been used widely as antimicrobial and antifungal plants. It contains 1 and 5 % of non-protein sulfur amino-acids, including S-E-prop-1-enyl-L-cysteine S-oxide, S-3-allylsulphinyl-L-alanine and S-methylcysteine sulfoxide which have satisfactory binding interactions and inhibition constant with endo and exopolygalacturonase. In the present study, these compounds were extracted from white onion bulb Giza 20 and detected in the onion extract LC/MS analysis. The Inhibitory effect of these compounds for endo and exopolygalacturonases enzymes were confirmed experimentally by determination of the enzyme activity in the presence and the absence of these compounds in onion extract. White onion extract has 45% inhibition percentage of the endo and exopolygalacturonases activity. The enzyme kinetic study showed an increase in the Km value with stable V-max value in presence of 7µg/µL of the onion extract. Also, the *In-vitro* experiment of inhibition of *F. oxysporum* growth in presence of 20% and 40% of onion extract

showed inhibition percentages of 47% and 53% respectively. Also, the *In-vivo* experiment of inhibition of *F. oxysporum* growth in presence of 10% ,20% and 40% of onion extract confirmed that presence inhibition percentage for onion extract The results concluded that onion extract inhibits Fusarium growth through inhibition of exo and endopolygalacturonases. The inhibitory effect of onion extract could be due to its contents of S-E-prop-1-enyl-L-cysteine S-oxide, S-3-allylsulphinyl-L-alanine, and S-methylcysteine sulphoxide. These compounds have excellent binding interactions and inhibition effects on both exo-and endo-polygalacturonases enzymes of *Fusarium oxysporumf. sp. Lycopersici.* In the present study, we strongly recommend usingthese compounds in the control of *Fusarium oxysporum f. sp. Lycopersici* infestation.

Keywords: Chemoinformatic, Auto-Dock program, *Fusarium oxysporum*, Pectinases, Endopolygalacturonase, Exopolygalacturonase, Onion extract

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