Molecular Docking of DEP B enzyme with DON mycotoxin chemotype (15ADON): In-silico analysis

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Abstract

Deoxynivalenol (DON), which is secreted by fusarium molds, is one of the most common mycotoxin in cereal grains and thus poses a significant risk on human health and productivity of farm animals . Although, DON cannot be controlled by common methods such as mycotoxin-binding absorbents, numerous studies have reported that enzymatic transformation seems to be the most promising method for detoxification of DON and its chemotypes . Therefore, the aim of present study was to investigate the interaction between DEP-A (DON deactivators enzyme) with DON mycotoxin chemotypes such as 15-acetyl-deoxynivalenol (15ADON) through molecular docking. The three-dimensional structure of DEP-A was predicted by SWISS MODEL server. The accuracy of the predicted structure was estimated by ERRAT and Z-score. Then, the stability of this structure was evaluated in molecular dynamic conditions with GROMACS (5.1.2) software. After that, the root mean square deviation (RMSD) curve of enzymes was drawn with Grace software. H-DOCK online server was used to docking of DEP-A with 15ADON. The results showed that, ERRAT and Z-score of predicted DEP-A structure were 91% and -8.65, respectability, which is within acceptable range. The calculation of the root mean square deviation (RMSD) verifies that the system is in an equilibrated structure during 100 ns simulation. Moreover, the results of molecular docking demonstrated that DEP-A enzymes bind to active site of 15ADON with relatively strong binding energy (-157.90). Finally, it is suggested that using DEP-A enzyme is an effective detoxification method through changing the molecular structure of 15ADON, however, laboratory studies are needed in the future.

Keywords: DEP-A, Mycotoxin, 15ADON, GROMACS, Molecular Docking