World Academy of Science, Engineering and Technology
International Journal of Biotechnology and Bioengineering
Vol:10, No:04, 2016

Quantitative Structure Activity Relationship and Insilco Docking of Substituted 1,3,4-Oxadiazole Derivatives as Potential Glucosamine-6-Phosphate Synthase Inhibitors

Authors : Suman Bala, Sunil Kamboj, Vipin Saini

Abstract : Quantitative Structure Activity Relationship (QSAR) analysis has been developed to relate antifungal activity of novel substituted 1,3,4-oxadiazole against Candida albicans and Aspergillus niger using computer assisted multiple regression analysis. The study has shown the better relationship between antifungal activities with respect to various descriptors established by multiple regression analysis. The analysis has shown statistically significant correlation with R² values 0.932 and 0.782 against Candida albicans and Aspergillus niger respectively. These derivatives were further subjected to molecular docking studies to investigate the interactions between the target compounds and amino acid residues present in the active site of glucosamine-6-phosphate synthase. All the synthesized compounds have better docking score as compared to standard fluconazole. Our results could be used for the further design as well as development of optimal and potential antifungal agents.

Keywords : 1,3,4-oxadiazole, QSAR, multiple linear regression, docking, glucosamine-6-phosphate synthase
Conference Title : ICBBPE 2016 : International Conference on Bioscience, Biochemical and Pharmaceutical Engineering
Conference Location : Los Angeles, United States
Conference Dates : April 05-06, 2016