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3D-QSAR, Homology modelling and docking studies of phthalimide derivatives as α-glucosidase inhibitors

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In view of the biological importance, some substituted Phthalimide derivatives having different activities like Anti-HIV and hypoglycemic agents, were engaged in further structural development studies of α-glucosidase inhibitors. A set of 17 compounds of Phthalimide was subjected to three dimensional quantitative structure activity relationship analysis using k nearest neighbour molecular field analysis method to design 4,5,6,7-substituted phthalimide derivative as novel α-glucosidase inhibitors. The 3D-QSAR model was developed using 11 compounds (training set) and its predictive ability was assessed using a test set of 6 compounds. The highly predictive 3D-QSAR models by KNN method for molecular field analysis (MFA) have cross-validated coefficient q2 value was 0.9451, Predicted r^2 value was 0.9610. The results have showed that phthalimide group are necessary for activity and halogen group in phthalimide nucleus enhanced the biological activity. Homology modeling showed Enzyme, α-glucosidase had highest amino acid sequence identity with the amino acid sequence of sulfolobus sulfataricus α-glucosidase Mal-A PDB ID 2G3M (F-chain). GRIP batch Docking indicated ligands were bind in the ATP pocket in cavity number four by requiring minimum energy score (between -40 to -60) and Pi-stacking, Hydrophobic interaction, VDW interaction with TRP618 was found to be crucial for selectivity among other α-glucosidase. The results of 3D-QSAR & docking studies validated each other. The combination of both methodologies provided a powerful tool directed to the design of novel and selective 2G3MF receptor inhibitors. All the Molecular Modeling studies were completed by the using of software V-LIFE MDS 3.0.

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