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Molecular Modelling and Docking Studies of Potent and Selective Aminocoumarin Derivatives as Dipeptidyl Peptidase -4 (Dpp – Iv) Inhibitors and Anticancer Agents

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Objectives

In an effort to identify new anticancer agents molecular docking studies and anticancer activity of potent and selective aminocoumarin derivatives as dipeptidyl peptidase -4 inhibitors, has become an attractive target for the treatment of cancer since it was shown clinically to inhibit dipeptidyl peptidase – 4 (DPP-IV). A novel derivative of aminocoumarin was selected from the literature for anticancer activity as dipeptidyl peptidase – 4 (DPP-IV) inhibitors.

Methods & Materials

in-silico studies using molecular docking methodology. The all selected compounds were sketched and energy minimized using Chem Draw ultra and Chem 3D ultra respectively. Further, the compounds were docked into dipeptidyl peptidase – 4 (2G5T) using Molegro Virtual Docker Platform. thirty three compounds were docked into the active site of dipeptidyl peptidase – 4 (DPP-IV) inhibitors cavity and all of them found to have similar binding interactions of a co-crystallized ligand with cyanopyrrolidine (c5-pro-pro) inhibitor 21ag. The binding interaction information derived from these molecules will be useful in future anticancer agent design.

Conclusion

From the docking study, it was observed that ligands bind to the electrostatic, hydrophobic clamp formed by the residues His 156, Gly 546, Arg 125, Ser 209, Glu 205, His 710, Val 662, Val 711, Arg 669, Tyr 666 and Tyr 631 which play an important role for dipeptidyl peptidase – 4 (DPP-IV). The binding affinity, grid calculation and RMSD percentage lower and upper parameters were calculated. Hence, the observable data indicated that, above compounds can serve as good leads for further modification and optimization in the of treatment of cancer.

Article Information

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