In silico identification and evaluation of bioactive plant product constituents of *Glycyrrhiza inflata* using structure-based drug design and ADMET analysis on HSV- glycoprotein D

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Abstract:

Introduction

Viral infections remain a persistent global health burden, with limited therapeutic options often leading to drug resistance. Natural remedies, particularly phytochemicals, are emerging as valuable alternatives in antiviral research. *Glycyrrhiza inflata*, a traditional medicinal plant, contains bioactive compounds such as glycyrrhizin, Liquiritin which has been reported to exhibit antiviral effects. Herpes simplex virus utilizes glycoprotein D (gD) for host cell entry, making this protein a key molecular target for drug discovery.

Methods

Five phytoconstituents from *Glycyrrhiza inflata* were analysed using computational drug design techniques. Molecular docking was performed against HSV glycoprotein D (PDB ID: 5CVM) through AutoDock Vina, for ligand preparation where 2D structure design and energy minimization molecular visualization using Discovery studio BIOVIA to assess binding interactions. Additionally, ADMET analysis and toxicity prediction was conducted to evaluate pharmacokinetic suitability, including ADMET, and toxicity profiles as well as bioactivity evaluation using molinspiration.

Results

Docking simulations demonstrated that all selected plant constituents were able to interact with glycoprotein D, with Liquiritin (M5) showing the most favorable binding affinity and stable interactions. The ADMET evaluation further indicated good drug-likeness, acceptable oral bioavailability, and low predicted toxicity, highlighting as a promising therapeutic candidate.

Conclusion

The study provides computational evidence that *Glycyrrhiza inflata* phytochemicals, especially *glycyrrhizin*, may serve as potential inhibitors of HSV- glycoprotein D. These findings reinforce the significance of plant-derived molecules in antiviral drug discovery and demonstrate the utility of *in silico* tools for accelerating early-stage screening.

Keywords

Glycyrrhiza inflata, HSV, Glycoprotein D, Molecular docking, ADMET analysis

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