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# Molecular docking of secondary metabolites in the Apocynaceae Plants family inhibit P-Glycoprotein in cancer treatment

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## Background

This study was performed to investigate the anti-cancer properties of the secondary metabolites of the plants of Apocynaceae family and their abilities to inhibit P-Glycoprotein (Pgp) drug resistance through molecular docking.

## Materials and Methods

The homology modeling of the crystal structure of Pgp (PDBID: 3G5U) was conducted by using the SWISS-MODEl ExPASy server. Upon drawing the Ramachandran plot, we saw that 98.4% of the residues were in the favored and allowed areas. Flexible docking study on Pgp by using a group of secondary metabolites, whose properties were demonstrated via the Way2Drug server, proved to be able to inhibit Pgp. As a result, Pgp was energy-minimized by applying UCSF Chimera software and docking by AutoDock Vina.

## Results

The result of the docking of the secondary metabolites in the plants of the Apocynaceae family has shown that steroid saponin and alkaloids ability to inhibit P-glycoprotein. Finally select the best poses, based on Gold score fitness function, Protein ligand hydrogen bond energy, Protein ligand Vander Waals energy and Ligand internal Vander Waals energy.

## Results

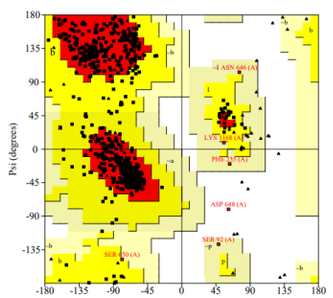
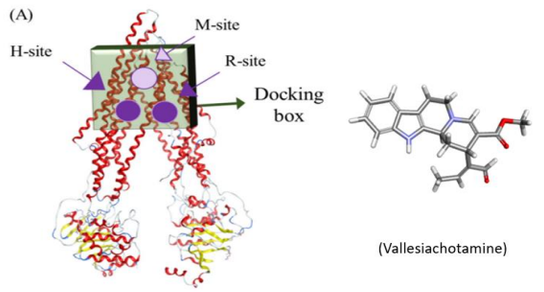
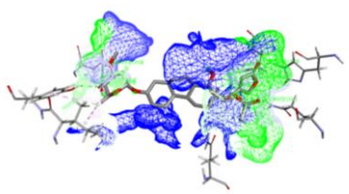



Figure (1): Ramachandran Plot




Figure(2): Active site Analysis and Ligand preparation



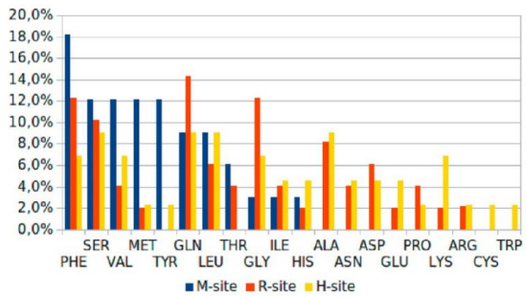
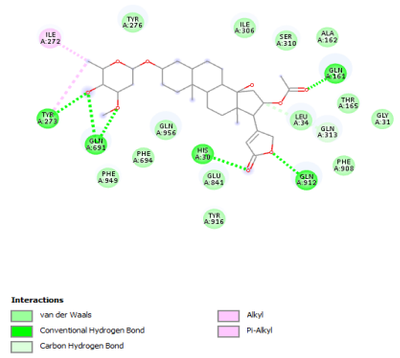



Figure (3): Residues Distribution Percentage for Each Site




Figure(4): Discovery studio Visualizer


Figure(5): Protein-Ligand interaction analysis

## Conclusion

We found that, secondary metabolites in the Apocynaceae Plants family ability to increase the chance of cancer treatment with reducing the dose of chemotherapy.

## References

Ricardo J. Ferreira, Maria-JoséU. Ferreira, and Daniel J. V. A. dos Santos. "Molecular Docking Characterizes Substrate-Binding Sites and Efflux." American Chemical Society (2013).

Keserű, Ákos Tarcsay & György M. "Homology modeling and binding site ." future science group (2011).

C. Tikhomiroff, M. Jolicoeur. "Screening of Catharanthus roseus secondary metabolites byhigh-performance liquid chromatography." Journal of Chromatography (2003).