

INHIBITORY ACTIVITIES OF SYZYGIIUM CORDATUM (WATER BERRY) AGAINST PEPTIC ULCER: MOLECULAR DOCKING

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28-29 September, 2022

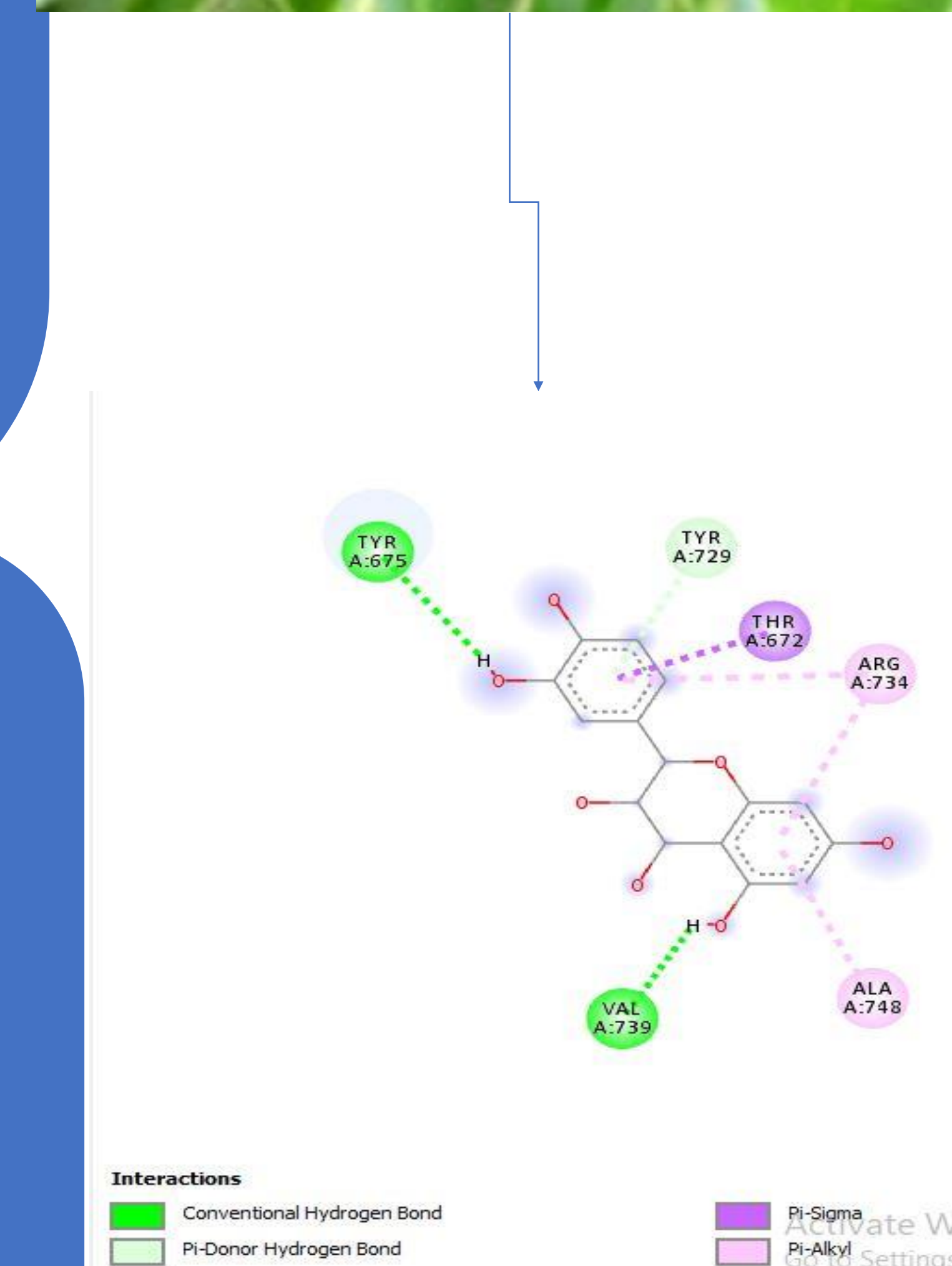


INTRODUCTION

- An ulcer is a painful sore that is slow to heal and sometimes recurs. Ulcers aren't uncommon. How they appear and corresponding symptoms depend on what caused them and where they occur on your body.
- *Helicobacter pylori* are a Gram-negative bacterium that chronically infects the stomachs of > 50% of the human population. *H. pylori* infection is a significant risk factor for the development of peptic ulcer disease, gastric adenocarcinoma, and gastric lymphoma (Marshall BJ, Warren JR (1984), Suerbaum S, Michetti P (2002)).
- *Helicobacter pylori* are a Gram-negative bacterium that chronically infects the stomachs of > 50% of the human population. *H. pylori* infection is a significant risk factor for the development of peptic ulcer disease, gastric adenocarcinoma, and gastric lymphoma (Marshall BJ, Warren JR (1984), Suerbaum S, Michetti P (2002)).
 - In silico study, plant metabolites showed interaction between protodioscin (secondary metabolites of *Asparagus racemosus*) and interferon- γ (virulent factor of gastric ulcer) during molecular docking. All the residues of interferon- γ exhibited hydrophobic interactions with plant metabolites. These interactions helps in understanding the plant secondary metabolites vis a vis will open a new door in the research field of new drug discovery and designing for the ulcer treatment.
- *Syzygium cordatum* Hochst. exKrauss (family Myrtaceae) is a valuable herbal medicine in east, west and southern Africa and it is included in the monographic guide of the most valuable herbal medicines in South Africa (Van Wyk, B.-E.; Van Oudtshoorn, B.; Gericke, N (2013). According to van Wyk, *S. cordatum* bark and leaf has commercial potential as remedy for respiratory ailments and stomach complaints.

METHODOLOGY

- ✓ Forty Compounds were selected from leafs of *Syzygium cordatum* from the reported literatures and they were used as ligands for their probable inhibitory against Ulcer toxin p5 domain, while two clinical drugs (Cimetidine and Omeprazole) were used as standard drugs.
- ✓ The structures of these ligands and standard drugs were obtained from a drug bank called PubChem, (<https://pubchem.ncbi.nlm.nih.gov>). AND were converted to 3-dimensional (3D) structures in PDB format for the efficient virtual screening exercise employing SMILES Online Translator (<https://cactus.nci.nih.gov/translate>) then later minimized to acquire lowest energy and most stable conformer before docking.
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- ✓ The target receptor *Helicobacter pylori* vacuolating toxin p55 domain was downloaded from a protein data bank and then extends to a vigorous treatment to remove unwanted atoms and all water molecules that comes with the protein using Discovery Studio.
- ✓ After all atoms and complexes including water molecules attached with the protein (2ZQ3) were detached using Biovia Discovery Studio 4.5, Pyrx-virtual screening tool (Autodock Vina and Open babel,) was employed for the docking process



RESULTS AND DISCUSSION

- From the molecular docking analysis, the results obtained shows that out of the forty (40) screened phytochemicals, only few of them have a reasonable number of ligands among the docked phytochemicals such as Leucocyanidin (-8 kcal/mol), Ledol (-7.5 kcal/mol), Leucodelphinidin (-7.2 kcal/mol), Isoaromadendrene epoxide (-7.0 kcal/mol), Cedol (-7.0 kcal/mol), Caffeic acid (-6.7 kcal/mol), Naphthalene (-6.6 kcal/mol), Hydrazine-2-propenyl (-6.4 kcal/mol), 2(4H)-benzofuranone (-6.2 kcal/mol), Azulene (-6.1 kcal/mol) among others have better binding affinities after been docked with target receptor the *Helicobacter pylori* vacuolating toxin p55 domain (PDB ID:2QV3) using Pyrx-virtual screening tools (Autodock tool, Autodock vina and Open babel). Visualizing was done using Pymol and Biosvia discovery studio(2019).
- Considering the other analysis done, Drug likeness of Lipinski rule of five only two(2): Leucocyanidin(1) and Leucodelphinidin(1) violated 1 of the Lipinski rule of five while the other eight(8) adhered with all the rule of five, therefore the ten (10) phytochemicals can be considered for further processing into potential therapeutic agent.

RECOMMENDATION

However, the significance of performing other analysis such as bioactivities, ADMET properties, Hit/Lead optimization, Molecular Dynamics, Meta-Dynamics (free energy calculation), and *In vivo* biochemical assay to further validate our outcome is highly recognized and recommended, but time constraint and some other factors restricted our scope.

REFERENCES

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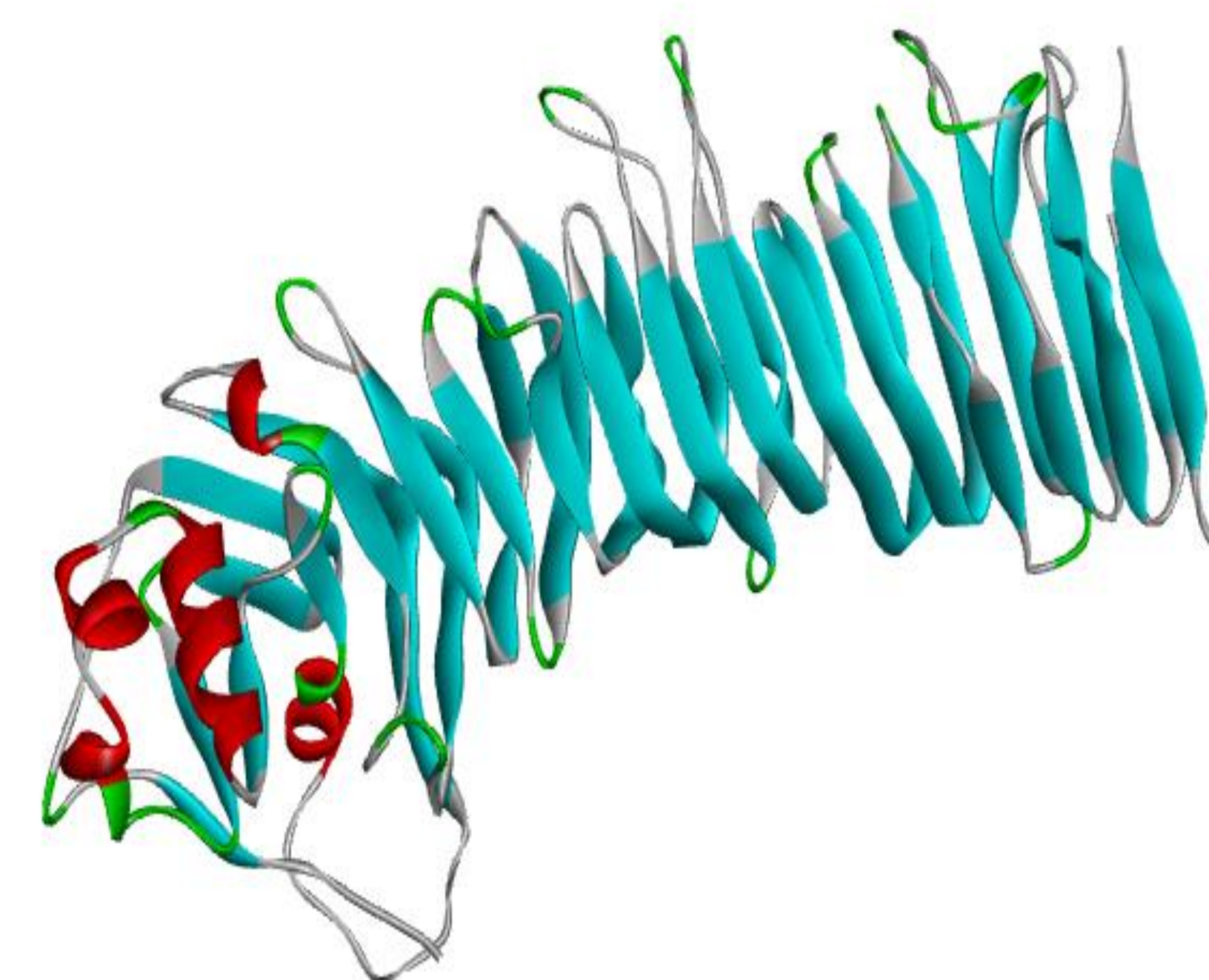


Figure 2: 3-Dimensional (3D) structure of *Helicobacter pylori* vacuolating toxin p55 domain