



Hydnora africana Derived Phytochemicals against Acetaldehyde Dehydrogenase of *Aeromonas hydrophila* Causing Septicemia

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Authors' contributions

This work was carried out in collaboration among all authors. All authors read and approved the final manuscript.

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ABSTRACT

For drug discovery it takes approximately 6 years to expose in the market and for commercial uses. There are different procedure to get success in the drug discovery like preliminary phytochemical analysis, structural elucidation of the bioactive compound, preclinical test and clinical test etc. So to optimize the time for invention of new drug molecule, computer aided drug designing and molecular docking analysis is being used as one of the highly effective methodology. The phytochemical extraction of *Hydnora africana* plant was reported to inhibit the growth of *Aeromonas hydrophila* which cause Septicemia. "Biovia Discovery Studio" molecular docking methods give us opportunity to identify the effective molecule against the microbes. "High positive values of -CDOCKER energy and -CDOCKER interaction energy" recommended that flavone can effectively deactivate the acetaldehyde dehydrogenase enzyme thereby interrupting the life cycle of the organism.

Keywords: *Flavon; Hydnora africana; Aeromonas hydrophila; Septicemia.*

1. INTRODUCTION

In Indian plant biology, they mentioned identification of different plants, herb, tree, lower

plants etc., importance in various vedic rituals, medicinal and their utilization to mankind. Nature directly or indirectly provides us lots of valuable things that are as blessings to all forms of life.

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From the beginning nature has been taking into account as major source medicine [1]. The secondary metabolites, the non-nutritive component of the plant is corporeal factor for the medicinal properties of the plant and it can be extracted from every part of the plant which shows all the anti-microbial action including anti bacterial, anti fungal, anti diabetic, anti oxidant, anti cancer etc. [2]. So in this modern era the valuable medicinal plants are playing the key role in eradicating the possible diseases of human being. Many people rely on the use of traditional medicine the minimum or no side effect [3].

Recently *Hydnora africana* is being focused due to its many medicinal properties. This plant is an achlorophyllous, parasite on the roots of family euphorbeaceae, belongs to family hydnoaceae. Recent study have found on the isolation and structural elucidation of phytoconstituents present in *Hydnora africana* plant. In traditional medicine, it is also indicated that the root of *Hydnora* species, tuber, fruits, leaves and fruit pulp (such as potato) is used for the treatment of infectious diseases [4]. Alkaloid-A, Saponins, Flavone, Tannic acid, and Steroid-U are the main phytochemicals that are found in this plant. The present study will reveal the structure of the bioactive compound of the plant which is the responsible for curing disease like blood poisoning.

2. MATERIALS AND METHODS

2.1 Software Used

All the operations were carried out in Discovery studio module of Biovia 2020 software (Dassault Systemes of France). Biovia 2020 discovery studio is one of the user-friendly software. Its user interface is quite easy to carry out the molecular docking. The software utilizes machine learning techniques to predict the level of molecular interaction between the receptor (enzyme) and Ligand (Phytochemicals).

2.2 Methodology

2.2.1 List of phytochemicals

Phytochemicals are these condary metabolites produced by plants as are sponse to flight or fight mechanism against the irpredators. Phytochemicals are generally bio-active compounds which can affect animal biochemistry and metabolism. Hence they are widely examined to prove the irability towards our health

benefits. It becomes important forus to include the minour foods, as potential nutritionally active ingredients. Published works showed that *Hydnora africana* contains Alkaloid-A, saponins, Tannic acid, steroid-U, Flavone. It has already been established that *Hydnora africana* plant belonging to Euphorbiaceae family has potential to help controlling Septicemia. This work is focused on identification of the particular phytochemical responsible for inhibiting and controlling of Septicemia.

2.2.2 Enzyme found in *Aeromonas hydrophila*

Based on previous published papers it has been known that Septicemia caused due to *Aeromonas hydrophila* .infestation [3,5]. For the survival of apathogeninits host there are involved certain metabolic pathways. These metabolic pathways require certain enzyme sasitsco-factor to function properly . Brenda enzyme data base has proved useful to identify and list different enzymes found in *Aeromonas hydrophila* [6]. It has been found that acetaldehyde dehydrogenase (protein data base code 51UU) is involved in Flavone biosynthesis metabolism. This metabolism proves to be very crucial for the pathogenthus blocking or inhibiting that path way results in death of the particular microbe.

2.2.3 Molecular docking

Molecular docking method has been used to identify the phytochemical from the plant extract, which act as a ligand and form a strong covalent bond with the fungal protein to successfully inhibit the microbe. The Discovery studio module of Biovia software was used for identifying molecular interaction and molecular docking was performed. First step involves collection of list of phytochemicals present in *Hydnora africana* from various research papers. Second step involves own loading the sdf files for the phytochemicals found in the *Hydnora africana* plant from various websites like PubChem, MollInstinctsetc. The protein data base code of 51UU enzyme was identified from the RCSB-PDB website. The active site of the enzyme was identified via "receptor cavity" protocol found under "receptor-ligand interaction" menu. Molecular docking was done using the CDOCKER protocol of Biovia software under "receptor-ligand interaction". The enzyme molecule was treated as the receptor molecule and the phytochemical was treated as the ligand. The "-CDOCKER_ENERGY" and "-CDOCKER_INTERACTION_ENERGY" were used as indicator for the quality of molecular docking. The high positive value of those

Table 1. Results of C docking of phytochemicals with acetaldehyde dehydrogenase (receptor)

Sl. no.	Ligand	-CDOCKER energy	- CDOCKER interaction energy	Difference between - C DOCKER interaction energy and - C DOCKER energy	Remarks
1	Flavone	10.7996	27.0472	16.2476	Maximum inhibition in microbial enzyme
2	Steroid-U	-71.1543	10.1824	-60.9719	
3	Alkaloid-A	-82.099	17.3961	-64.7029	
4	Tannic acid	Failed	Failed	NA	
5	Saponins	Failed	Failed	NA	

indicators presented a good interaction between the ligand and the receptor. Thus, the interactions with high values might indicate the major phytochemical responsible for curing the disease.

3. RESULTS AND DISCUSSION

CDOCKER energy was calculated based on the internal ligand strain energy and receptor-ligand interaction energy. -CDOCKER interaction signifies the energy of the non bonded interaction that exists between the protein and the ligand. The criteria for best interaction was chosen based on a) high positive value of -CDOCKER energy and b) small difference between - CDOCKER energy and -CDOCKER interaction energy [5,7]. Table 1 shows that acetaldehyde dehydrogenase-Flavone interaction has the highest positive value of -CDOCKER energy 16.2476 between-CDOCKER interaction energy and-CDOCKER energy. Thus the results indicated that flavone can effectively deactivate the acetaldehyde dehydrogenase enzyme there by interrupting the biological cycle of *Aeromonas hydrophila*. Higher positive values for indicated that it was the most active ingredient against *Aeromonas hydrophila*. On the other hand, Alkaloid-A and Steroid-U can deactivate the enzyme to a small extent (negative-CDOCKER energy but positive-CDOCKER interaction energy). Thus, the key phytochemicals preventing Septicemia by *Aeromonas hydrophila* is Flavone.

4. CONCLUSIONS

It was previously known that *Hydnora africana* plant has medicinal action against Septicemia,

caused by *Aeromonas hydrophila*. This study was carried out to provide the theoretical basis of this observation. Molecular docking operation was executed to identify the phytochemical (Alkaloid-A, Saponins, flavones, steroid-u, tannic acid) by using Discovery studio module of Biovia software, which can have a major interaction with the dynamic enzyme (acetaldehyde dehydrogenase) of the microbe. It was found that flavones can form strong bond with the enzyme successfully inhibiting the metabolic cycle of the microbe. Alkaloid-A, steroid-U, saponins, tannic acid were found to be not much effective in deactivating the enzyme of the microbe as they fail to maintain stability. Thus, this study could explain that the presence of flavone provided the medicinal values to flavone against Septicemia caused by *Aeromonas hydrophila*.

DISCLAIMER

The products used for this research are commonly and predominantly use products in our area of research and country. There is absolutely no conflict of interest between the authors and producers of the products because we do not intend to use these products as an avenue for any litigation but for the advancement of knowledge. Also, the research was not funded by the producing company rather it was funded by personal efforts of the authors.

CONSENT

It is not applicable.

ETHICAL APPROVAL

It is not applicable.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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