JETIR.ORG ISSN: 2349-5162 | ESTD Year : 2014 | Monthly Issue
JOURNAL OF EMERGING TECHNOLOGIES AND INNOVATIVE RESEARCH (JETIR)
An International Scholarly Open Access, Peer-reviewed, Refereed Journal

IN SILICO AND PHYTOCHEMICAL EVALUATION ANTIDEPRESSANT EFFECT OF QUERCETIN PRESENT IN THE WHOLE PLANT OF ETHANOLIC EXTRACT OF BRASSICA OLERACEA VAR. ITALICA

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ABSTRACT

Depression is a condition characterized by a lowering of the mood and dislike for movement that may distress an individual's thoughts, conduct, emotions, and comfort. The goal of this study was to use computational docking to investigate the antidepressant activity of quercetin. For this, the natural compound quercetin is isolated from the whole plant of *Brassica oleracea var.italica* (EEBO) were used as a ligand for molecular interaction. A small portion of the EEBO was subjected to the phytochemical test for the presence of alkaloids, flavonoids, terpenoids, phenols, tannins and saponins. In this study whole plant using EEBO showed abundant phytochemicals such as alkaloids, flavonoids, terpenoids, phenols, tannins, saponins, and secondary metabolites that can be used in the pharmaceutical industry for producing potent drugs.

Keywords: Depression, Docking, Broccoli, Ethanol, Phytochemical, Quercetin.

INTRODUCTION

World health organization (WHO) has estimated that approximately 80% of the world's population from developing countries mainly relies on traditional medicines for the primary healthcare.[1] Medicinal plants, either as an extract, pure compound or as a derivative, offer limitless opportunities for the discovery of new drugs. Plants in the family Brassicaceae are among the oldest cultivated plants. Evidence has been unearthed that indicates that a

Brassica vegetable was widely cultivated as early as 10,000 years ago.[2] Among plant foods with health benefits, crops from the family Brassicaceae have been the focus of numerous epidemiological and clinical studies[3] Cruciferous vegetables, those included into the Brassica genus, are good sources of a variety of nutrients and health promoting phytochemicals. It has been demonstrated that a high intake of Brassica vegetables reduces the risk of age-related chronic illnesses such as cardiovascular health and other degenerative diseases[4] and reduces the risk of several types of cancer.[5] Brassica oleracea var. Italica is popularly used as food and has many traditional claims for herbal medicine.[6]

Broccoli scientifically known as *"Brassica oleracea var. italica*", a Cruciferous green leaf Cole vegetable; is one such promising under exploited plant. This plant is native of Italy, but can be successfully grown in our country. [7] Broccoli is an edible green plant in the cabbage family whose large flowering head is eaten as a vegetable.[8] A small portion of the whole plant of EEBO was subjected to the phytochemical test for the presence of alkaloids, flavonoids, terpenoids, phenols, tannins and saponins.

Quercetin is a flavonol widely present in nature in the form of glycosides, is one of the main components of different traditional Chinese medicine.[9] Many studies have demonstrated that quercetin has a wide range of pharmacological effects such as anti-cancer, antibacterial, anti-oxidation and memory impairment improvement.[10] Recently, an increasing number of studies have focused on the treatment of depression with quercetin and its glycoside derivatives.[11] Based on Brassica oleracea var. Italica use in traditional practice and the literature references, the present study was undertaken to evaluate the comprehensive Phytochemicals and molecular docking of *Brassica oleracea var. Italica* and is reported here under.

Flavonoids are reported to have anti-inflammatory and anti-cancer activity, whereas tannins possess anti-inflammatory and anti-microbial activity[12]. Phenolic compounds are also present, which possess various physiological functions like anti-aging, anti-inflammation, anti-apoptosis, anti-carcinogenic, inhibition of angiogenesis and enhance-ment of endothelial function [13].

The purpose of this study was to analyze the antidepressant action of Quercetin (QU) by computational docking analysis studies(CDAS).The receptors for depression were obtained from PDB database (PDB ID: 1HOY, 5FUC , 1JL9). CDAS was performed for these three receptors using Pyrx, Pymol, Openbabel based on scoring functions. This study shows the hydrogen bond interaction and binding affinity of QU with CNS receptors. Hence the study shows that QU having similar binding affinity with receptors and thus shows that these drugs have anti-depressant acivity.

MATERIALS AND METHODS:

Collection and identification of plant materials

The whole plant of *Brassica oleracea var.italica* was collected in the month of September 2022 from the cultivated field in Ooty. The plant was authenticated from department of Botany, Christian College, Kattakada, Thiruvananthapuram.

Preparation of the plant extract

After shade drying, the whole plant of Brassica oleracea var. Italica were grinded through mechanical grinder and converted into coarse powder and then ethanolic extract of the plant was made through soxhlet extraction process using 200gm of the dry powder in 95% of ethanol for 48 hrs. After extraction, the extract was concentrated under electrical water bath temperature maintained at 25C° and then 40C° throughout the process and air dried. The dried powder obtained was 15gm (7.5%) on dry weigh basis which was calculated by using following equation: Percentage yield = Weight of dried extracts x 100 Weight of powder taken. The dry extract was placed in desiccator to avoid moisture and for further pharmacological studied.

PHYTOCHEMICAL SCREENING TEST

Phytochemical analysis is useful to evaluate the therapeutic and physiological activities of a plant extract. A qualitative phytochemical screen is performed to determine the presence or absence of secondary plant metabolites.

A small portion of the ethanolic extract of ***Brassica oleracea var.Italica*** was subjected to the Phytochemical screening test using the standard methods (Evans, Trease GE , 1983; Harbourne,1998; and Shah M A, 2017) to conduct the test for the precence of alkaloids, flavonoids, terpinoids, phenols, tannins, and saponins.

Alkaloids Test

Mayer's test was used for the presence of an alkaloid; 0.5gm of EEBO was taken and diluted in 10ml of 1% HCL. The mixture was then boiled for 2 minutes on water bath and filtered. The filtrate was separated into portions. From the portion, 1ml was taken in a test tube and few drops of Mayer's reagent were added to the solution. Formation of the pale precipitate was considered the positive test for the presence of alkaloids.

Flavonoids Test

Hydrochloride test was used for the presence of flavonoid; 0.2 g of EEBO was dissolved in 2 ml of methanol and heated. A chip of magnesium metal was added to the mixture followed by the addition of a few drops of concentrated HCl. The occurrence of a red or orange coloration was indicative of the flavonoids.

Terpenoids Test

Salkowaski test was used to determine the presence of terpenoids in EEBO ; 2ml of chloroform was taken in a test tube, and then added 0.5gm of extract, mixed thoroughly. Add 3ml of concentrated Sulphur acid carefully to form a layer. A reddish-brown coloration showed the presence of terpenoids.

Phenols Test

The presence of phenols in EEBO was accessed by Ferric chloride test. An amount of 0.2gm of extracts was mixed with 1ml of absolute ethanol in a test tube, and then adds few drops of 10% ferric chloride solutions. The bluish colors formations showed the presence of phenols.

Tannins Test

Bromine water test for used to determine tannins. An amount of 0.1gm of EEBO was diluted in 5ml distilled water in a test tube, and then added few drops of 1% lead acetate solution. A red precipitate shows the presence of tannins.

Saponins Test

Foam test was used to determine the presence of saponins in EEBO ; 0.2gm of extract was takes in a test tube that contains 5ml distilled water, shacked vigorously. Formation of stable persistent for about 5 minutes indicates the presence of saponins.

DOCKING

The interaction between the ligand and protein were determined by using Autodock vina Pyrx virtual screening tool. The 3D structure of the compound was obtained from Pubchem, which contains information about the small molecule and their biological activities. Proteins are the macromolecule contains one or more aminoacid residues. The 3D structure of the protein were obtained from PDB (Protein data bank). Conversion of ligand from SDF to PDB format Openbabel-2.3.2/obgui.exe were used. pyMOL is a software used for the both purposes. pyMOL can produce high quality 3D images of proteins. This study shows the hydrogen bond interaction and binding affinity of QU with CNS receptors. When Quercetin docked with 3 receptors such as 1HOY,5FUC,1JL9 shows that their hydrogen bond interaction .

DRUG & RECEPTOR	NO.OF HYDROGRN BOND INTERACTIONS	BINDING AFFINITY(kcal/mol)
Quercetin & 1 HOY	4	-6.4
Quercetin & 5FUC	4	-6.9
Quercetin & 1JL9	4	-6.5

Table 1 number of hydrogen bond interaction and binding affinity of Quercetin with receptors

RESULT AND DISCUSSION

The phytochemicals screening on extract was done for the presence of alkaloids, flavonoids, terpenoids, phenols, tannins, saponins. The phytochemical analysis of EEBO showed the presence of several phytochemicals. The investigation showed positive results for secondary metabolites. Table 1 shows the interactions and binding affinity of QU with receptors such as 1HOY, 5FUC, 1JL9. Hence the study shows that QU having similar binding affinity with receptors and thus shows that these have anti-depressant acivity.

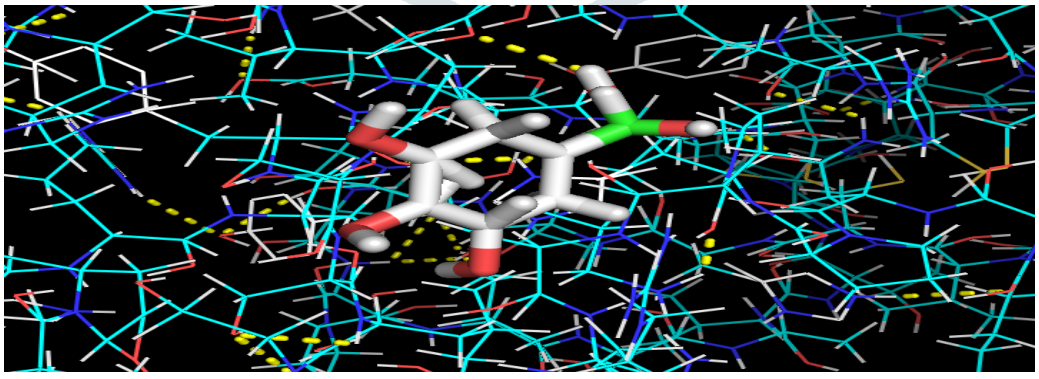

Figure 1 Quercetin with 1HOY

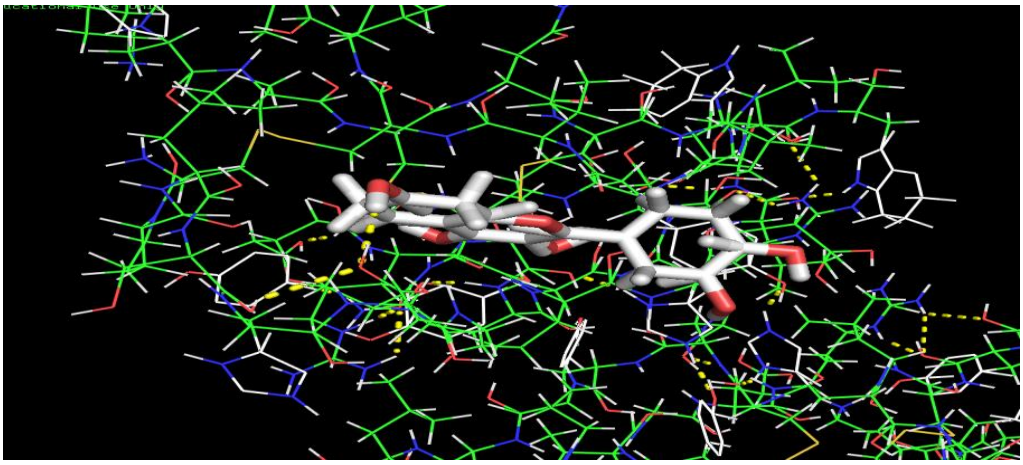

Figure 2 Quercetin with 5FUC

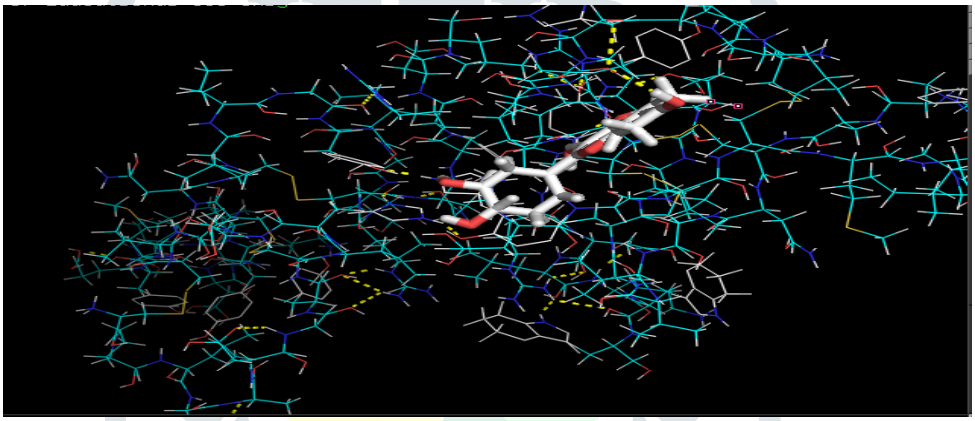

Figure 3 Quercetin with 1JL9

SL.NO	CHEMICAL COMPOUNDS	TEST NAME	OBSERVATIONS	RESULTS
1	Alkaloids	Mayer's test	Pale precipitate formed	Present
2	Flavonoids	Hydrochloride test	Orange color formed	Present
3	Terpinoids	Salkowaski test	Reddish brown color	Present
4	Phenols	Ferric chloride test	Bluish color formed	Present
5	Tannins	Bromine water test	Red precipitate	Present
6	Saponins	Foam test	stable persistent	Present

Table 2: Result of Phytochemical screening test

CONCLUSION

The present study of the whole plant using EEBO showed abundant Phytochemicals such as alkaloids, flavonoids, terpenoids, phenols, tannins, saponins, and secondary metabolites that can be used in the pharmaceutical industry for producing potent drugs. The investigation revealed that the QU have a potential role in anti-depression activity. It is established through CDAS (Computational Docking Analysis Studies), using the most predominant anti-depressive brain level receptors & found to be most effective in binding with 1HOY, 5FUC, 1JL9 receptors. The study results of the above plant give a basis for its use in antidepression activity. Further invivo and invitro studies are required to prove the antidepressant activity.

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