

# Biochemical Activities, *In Silico* Antifungal and Anticancer Activities of *J. Excisa*

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## Abstract

*Jatropha excisa* (family Euphorbiaceae) is an ornamental shrub that grows in subtropics and tropics regions. In the present work *J. excisa* flower oil has been extracted and conducted for phytochemical, antifungal and anticancer activities. The present experiment shows that *J. excisa* seed oil contains proteins, carbohydrates, fatty acids, terpenoids, tannins, cardiac glycosides, and saponins. The flower oil contains proteins, carbohydrates, fatty acids, phenols, cardiac glycosides, saponins and coumarins. The leaf ethanolic extract contains proteins, carbohydrates, phenols, terpenoids, cardiac glycosides and coumarins. The stem ethanolic extract contains carbohydrates, terpenoids, tannins, coumarins and flavonoids. The root ethanolic extract contains carbohydrates, phenols, tannins, coumarins and flavonoids. The *in silico* analysis shows gossipifan acid, gossipifan and gossypiline from *Jatropha* has good antifungal and anticancer activities.

## Keywords

Anticancer activities, biochemical activity, flower oil, *in silico* antifungal, *Jatropha*.

## INTRODUCTION

Drugs in barks, fruit bodies, seeds, flowers and other parts of the medicinal plants shows written documents that are preserved monuments from ancient times in healing several diseases [1]. Medicinal plants are commonly used in Sidda, Homeopathy, UNANI and Ayurveda systems of medicine [2].

The non-edible like *Jatropha* oils, residual like waste frying oils, coconut oil, corn oil, palm oil, olive oil, and other vegetable oils like acid oil from soybean soapstock are non-edible are used as fuels and are promoting a circular economy [3,4]. Different waste frying oil, raw materials like commercial sunflower and soybean oils, and acid oil from soybean soapstock, and pork fat are using to produce first- and second-generation biodiesel [5]. *Jatropha excisa* flower oil may promote as first- and second-generation biodiesel along with healthcare [6,7]. The present work on *Jatropha excisa* flower oil is applied for analysis of biochemical activities along with *in silico* anticancer and antifungal activities.

## MATERIALS AND METHODS

### Material Collection

Fresh seeds, flowers, root, stem and leaf of *J excisa* (Family: Euphorbiaceae) was collected and tested for Biochemical, antifungal and *in silico* anticancer activities.



Figure 1. *Jatropha excisa* seeds and flower

### Oil/Sample Extraction

The seeds and flowers of *J excisa* were air-dried and were used for oil extraction. Oil extraction machine was used for the extraction process of oil. Leaf ethanolic extract, Stem ethanolic extract, Root ethanolic extract, seed ethanolic waste, and Flower ethanolic waste (Figure 2).



Figure 2. Samples and extracts

### Phytochemical Screening

For Phytochemical screening, seven different sample were collected and perform biochemical tests from Seed oil, flower oil, leaf ethanolic extract, Stem ethanolic extract, Root ethanolic extract, seed ethanolic waste, and flower ethanolic waste.

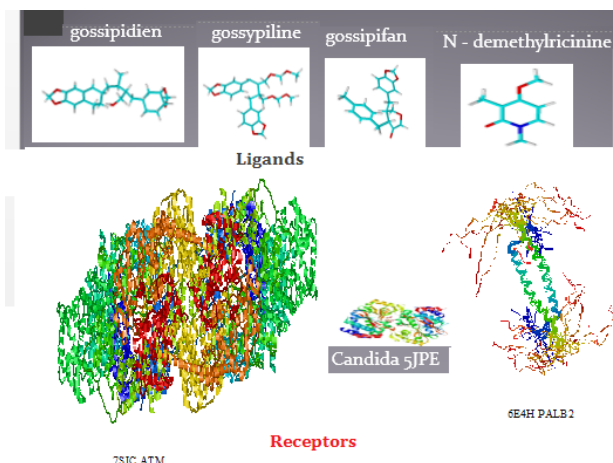
Protein, Cardiac glycosides, Carbohydrate, Phenols, Fattyacids, Tannins, Saponins, Terpenoids, Phlobatanins, Coumarin, Flavonoids and Quinone are analyzed in the present experimentation.

### To perform antifungal activity by zone method

The experimentation on antifungal activity by zone method was conducted based on protocol given by Kaladhar et al., 2023 [8].

### **In silico docking activity**

The oil extract collected from plants *Jatropha* has been searched further compounds based on previous research based on the search result, the selected compound has been absorbed as gossipidien acid, gossipifan, gossypiline and n – demethyl ricinine. Few *Jatropha* seed compounds has been design as 3D molecule in mol format using chemSketch software (Figure 3).



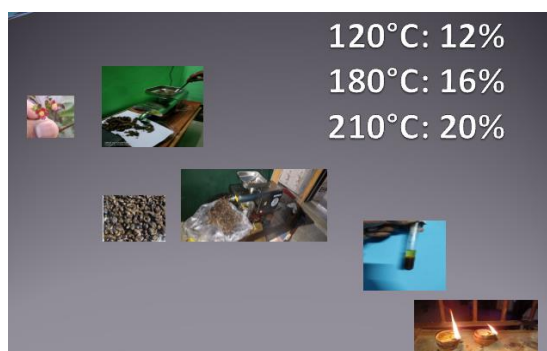
**Figure 3.** Molecules in present study

### **RESULTS AND DISCUSSION**

Previous experimentation on *Jatropha curcus* oil has promising antifungal effect on organisms like *Aspergillus niger* and *Penicillium glabrum* [9]. The *Jatropha* oil is commonly using in India to cure skin disease [10]. The compounds like jatrophone, spruceanol and jatropha-trione has shown antitumor effects [11].

### **Phytochemical activity**

The Phytochemical screening of seven different sample were tested for Seed oil, Flower oil (Figure 4). Leaf ethanolic extract, stem ethanolic extract, root ethanolic extract, seed ethanolic waste, and flower ethanolic waste has been also analysed for phytochemical activity (Table 1).



**Figure 4.** Process of oil extraction and % oil extracted

### **Test for Proteins**

About 2 ml of the concerned sample mixed with 2 ml of Biuret reagent has showed appearance of violet color ring that indicates the presence of protein (Figure 5).



**Figure 5.** Protein identification

### **Test for Carbohydrate**

About 2 ml of concerned sample mixed with 2 drops of Molisch's reagent and 2 ml of Conc. H<sub>2</sub>SO<sub>4</sub> (drop by drop from the sides of the test tube), a reddish violet color ring appearance at the junction of two layers indicates the presence of carbohydrates (Figure 6).



**Figure 6.** Carbohydrate identification

### **Test for fattyacid**

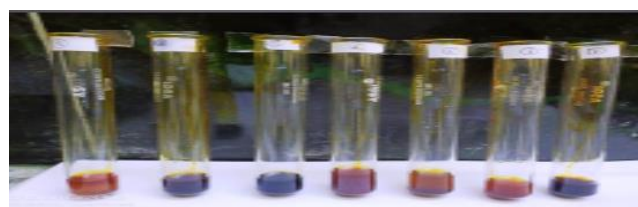
About 0.5 ml of concerned sample, add 5 ml of ether and allowed for evaporation on a filter paper and dried. The development of transparency on the filter paper indicates the presence of fattyacids (Figure 7).



**Figure 7.** Fatty acid identification

### **Test for Phenol**

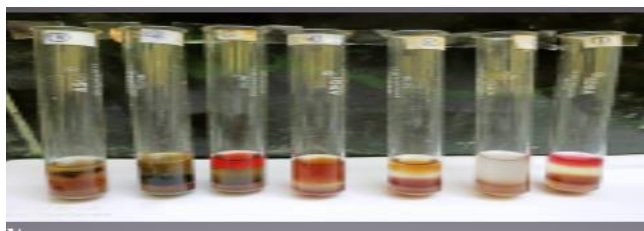
When 2 ml of concerned sample mixed with 3ml of ethanol and a pinch of FeCl<sub>3</sub>, formation of greenish yellow color solution shows the presence of phenols (Figure 8).



**Figure 8.** Phenol identification

### **Test for Terpenoid**

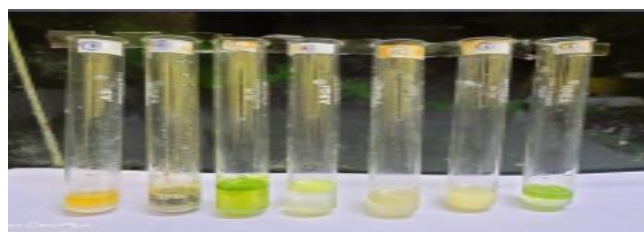
When 2 ml of concerned sample added with 2 ml of chloroform and 3 ml of Conc. H<sub>2</sub>SO<sub>4</sub>, the formation of a monolayer of reddish brown coloration in the solution indicates presence of terpenoids (Figure 9).



**Figure 9.** Terpenoid identification

**Test for Tannins**

When 5 ml of concerned sample added with few drops of 1% of lead acetate, formation of yellow colored precipitate in the test tube shows the presence of tannins (Figure 10).



**Figure 10.** Tannin identification

**Test for Phlobatnin**

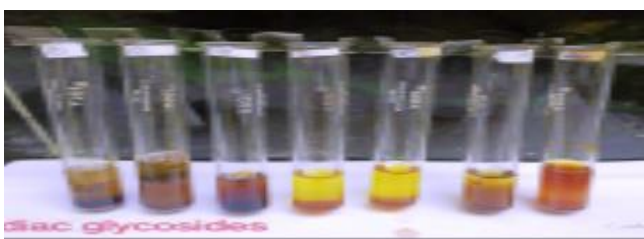
When 2 ml of concerned sample is added with 1% aqueous HCl and boiled for few minutes, a red colored precipitate formed or deposited in the test tube indicates presence of phlobatnins (Figure 10).



**Figure 11.** Phlobatnin identification

**Test for Cardiac glycosides**

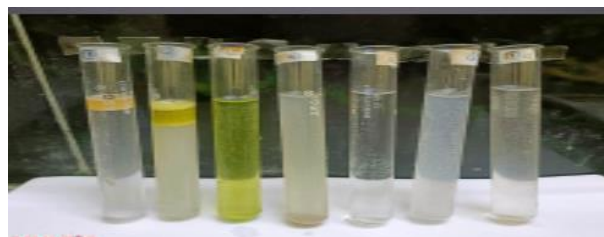
When 5 ml of concerned sample is added with 2 ml of glacial acetic acid, one drop of ferric chloride solution and 1ml of Conc. H<sub>2</sub>SO<sub>4</sub>, a violet ring appearing under the brown ring indicates and a greenish ring might form further indicates presence of cardiac glycosides (Figure 12).



**Figure 12.** Cardiac glycosides identification

**Test for Saponin**

When 5 ml of concerned sample mixed with 20 ml of distilled water and kept in waterbath at 80°C for 15 minutes, development of 1cm layer of foam in the test tube observed presence of saponins (Figure 13).



**Figure 13.** Saponin identification

**Test for Coumarin**

When 3 ml of 10% NaOH added with 2 ml of concerned sample, an yellow color solution formation in test tube indicates the presence of coumarins.



**Figure 14.** Coumarin identification

**Test for Flavonoid**

When 2ml of concerned sample added with 5 ml of dilute ammonia solution and a few drops of Conc. H<sub>2</sub>SO<sub>4</sub>, a yellow colored solution produced that confirmed the presence of flavonoids (Figure 15).



**Figure 15.** Flavonoid identification

**Test for Quinone**

When 2 ml of concerned sample added with 3 ml of Conc. HC, a green color solution formation indicates the presence of Quinone's (Figure 16).



**Figure 16.** Quinone identification

**Table 1.** Biochemical activity on *Jatropha excisa* oil

S.No	Biochemical compound	Seed oil	Flower oil	Leaf extract	Stem extract	Root extract	Seed waste	Flower waste
1.	Protein	+	+	+	-	-	-	+
2.	Carbohydrate	+	+	+	+	+	+	+
3.	Fattyacid	+	+	-	-	-	-	-
4.	Phenol	-	+	+	-	+	-	+
5.	Terpenoid	+	-	+	+	-	-	+
6.	Tannin	+	-	-	+	+	+	-
7.	Phlobatinin	-	-	-	-	-	-	+
8.	Cardiac glycosides	+	+	+	-	-	+	+
9.	Saponin	+	+	-	-	-	-	-
10.	Coumarin	-	+	+	+	+	+	+
11.	Flavonoid	-	-	-	+	+	-	+
12.	Quinone	-	-	-	-	-	-	-

Note: + means PRESENT; - means Absent

**Test for Quinone**

When 2 ml of concerned sample was added with 3 ml of Conc. HCl, green color solution formation indicates the presence of quinones (Figure 17).



**Figure 17.** Quinone identification

**Antifungal activity**

The ethanolic extract of flower oil (12mm) has shown good activity compared with petroleum ether (11mm) with *Candida albicans*. The ethanolic seed oil (13mm) has shown good activity petroleum ether extract of flower oil (11mm) with *Candida albicans* (Table 2).

**Table 2.** Antifungal activity

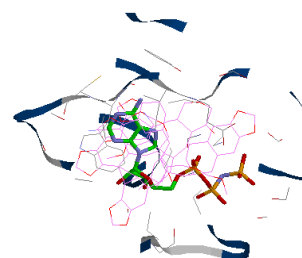
Microorganism	Sample (zone in mm)				Standard
	Oil Flower		Oil Seed		
	E	PE	E	PE	Fluconazole
<i>Candida albicans</i>	12	11	13	11	20

**In silico docking activity**

The *in silico* docking studies of gossipidien acid, gossipifan, gossypiline and n – demethylricinine from *Jatropha* species was analysed against *Candida* protein (5JPE). Gossypiline (-124 kcal/mol) has shown good activity followed by Gossipifan (-118.4kcal/mol) and Gossipidien (-108.7kcal/mol).

**Table 3.** *in silico* antifungal and anticancer activity

COMPOUND NAME	Fungi (Candida)	Cancer (ATM)	Cancer (PALB2)
Gossipidien	-108.7	-93.22	-94.41
Gossipifan	-118.4	-98.37	-87.91
Gossypiline	-124	-108.74	-106.44
N - demethylricinine	-77	-66.74	-64.26



**Figure 18.** Interaction profile of ATM with selected molecules

The *in silico* docking studies of gossipidien acid, gossipifan, gossypiline and n – demethylricinine from *Jatropha* species was analysed against omcprotein (ATM) (7SIC). Gossypiline (-108.74 kcal/mol) has shown good activity followed by Gossipifan (-98.37 kcal/mol) and Gossipidien (-93.22 kcal/mol) (Table 3 and Figure 18).

The *in silico* docking studies of gossipidien acid, gossipifan, gossypiline and n – demethylricinine from *Jatropha* species was analysed against omcprotein (PALB2) (6E4H). Gossypiline (-106.44 kcal/mol) has shown good activity followed by Gossipidien (-94.41 kcal/mol) and Gossipifan (-87.91 kcal/mol).

N – demethylricinine has not shown good interaction antifungal or anticancer activity.

### CONCLUSION

The search for plants with several medicinal properties continue to focus on scientific studies on plants, particularly on ethanobotanical significance, for a complete range of biochemical and biological activities that range from antifungal to anticancer properties. The present experiment shows that *J. excisa* seed oil contains proteins, carbohydrates, fatty acids, terpenoids, tannins, cardiac glycosides, and saponins. The flower oil contains proteins, carbohydrates, fatty acids, phenols, cardiac glycosides, saponins and coumarins. The leaf ethanolic extract contains proteins, carbohydrates, phenols, terpenoids, cardiac glycosides and coumarins. The stem ethanolic extract contains carbohydrates, terpenoids, tannins, coumarins and flavonoids. The root ethanolic extract contains carbohydrates, phenols, tannins, coumarins and flavonoids. The study also shown anti-candida activity and *in silico* anticancer activity with Seed and flower oil.

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### Conflict of interest

There is no conflict of interest.

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