Article

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Chemical Constituents, Insecticidal Activity, Herbicidal Potential and Soft Computing Analysis in *Foeniculum vulgare* Mill. (Fennel): A Bioherbicide

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Abstract. To develop an environment friendly natural herbicide is a new topic of interest in the agricultural era over the worldwide. Nowadays people are more concerned about their health in consideration to nutrition related problems for the better quality of life. The aim of present study is to examine the phytoconstituents and biological efficacy in the fennel seed collected from Tarai region in the Uttarakhand state. Chemical constituents, insecticidal activity and herbicidal potential in hexane, chloroform and methanol extract of fennel seed were evaluated. Soft computing analysis was done in terms of fuzzy-c-means clustering (FCM) and artificial neural network (ANN). FNL-120, FNL-125 and FNL-PM exhibits highest mortality rate in methanol and hexane extract of fennel against *Tribolium castaneum* and *S. oryzae*. Herbicidal activity in hexane, chloroform and methanol extract of fennel seed was analyzed by observing the seed germination inhibition potential in radish (*Raphanus sativus*) seeds. Methanol extract of FNL-PM have effective seed germination inhibition activity with IC_{50} =549.10 ±2.86 µg/ mL. Due to significant complexity of herbicidal activity (IC_{50} value) of fennel, having different concentrations of extract, traditional approaches to biological study struggle to provide meaningful outcomes. To rectify, the simulation data are intensify into an artificial neural network to evaluate the target responses. Fennel extract have higher seed germination inhibition potential can be used as a natural herbicide to control weed growth for the better yield of crop and a good initiative to develop sustainable management of weed.
Keywords: ANN; bioherbicide; *Foeniculum vulgare*; fuzzy-c-means clustering; insecticidal activity.

Resumen. Desarrollar un herbicida natural respetuoso con el medio ambiente es un tema de interés en la era agrícola mundial. Hoy en día, las personas se preocupan más por su salud que por los problemas nutricionales para una mejor calidad de vida. El objetivo del presente estudio es examinar los fitoconstituyentes y la eficacia biológica de las semillas de hinojo recolectadas en la región de Tarai, estado de Uttarakhand. Se evaluaron los componentes químicos, la actividad insecticida y el potencial herbicida de los extractos de hexano, cloroformo y metanólico de las semillas de hinojo. Se realizó un análisis computacional suave mediante agrupamiento difuso de c-medias (FCM) y redes neuronales artificiales (ANN). FNL-120, FNL-125 y FNL-PM presentaron la mayor tasa de mortalidad en extractos de hinojo con metanol y hexano contra Tribolium castaneum y S. oryzae. Se analizó la actividad herbicida de los extractos de hexano, cloroformo y metanólico de las semillas de hinojo observando el potencial de inhibición de la germinación de las semillas de rábano (Raphanus sativus). El extracto metanólico de FNL-PM presenta una actividad inhibidora eficaz de la germinación de las semillas con una CI50 de 549,10 ±2,86 µg/mL. Debido a la considerable complejidad de la actividad herbicida (CI50) del hinojo, con diferentes concentraciones de extracto, los enfoques tradicionales de estudios biológicos presentan dificultades para obtener resultados significativos. Para solucionar este problema, los datos de simulación se intensifican en una red neuronal artificial (RNA) para evaluar las respuestas

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objetivo. El extracto de hinojo, con un mayor potencial de inhibición de la germinación de las semillas, puede utilizarse como herbicida natural para controlar el crecimiento de malezas, lo que mejora el rendimiento del cultivo y constituye una buena iniciativa para el desarrollo de la gestión sostenible de malezas.
Palabras clave: RNA; bioherbicida; *Foeniculum vulgare*; agrupamiento de medias difusas; actividad insecticida.

Introduction

Medicinal herbs and spices are highly in demand in functional food and pharma industries due to favorable implementations [1]. Medicinal plants are known for their medicinal value due to rich in phytoconstituents [2]. Since ancient times medicinal plants are used for the specific ailments purpose [1]. Natural compounds obtained from plants are emphasizing due to their potentially used in medication purpose and possibly as natural herbicide [3]. Spices have property to isolate organically active compounds present in it [4]. Medicinal plants are good source of antioxidants and phytochemicals present in it represents various pharmacological activities [5]. Medicinal plants are good alternative to chemical drugs as they have hardly any side effects than synthetic drug [6]. Fennel is a cuisine spice of Apiaceae family, extensively cultivated in world's temperate and tropical areas [7]. Fennel seeds are known to be used for their antimicrobial, antispasmodic and anti-inflammatory property [8]. Methanol extract of fennel seed exhibits various phytochemicals such as terpenoids, saponins, tannins, phenols, glycosides, flavonoids and alkaloids [9]. A large range of bioactive components as well as polyphenols are observed in fennel [10]. Fennel is used in various purposes like cosmetics, food industry and medication [11]. Fennel seeds are rich source of antioxidants [12]. Fennel essential oil exhibits a good insecticidal effect even applied at low concentration [13]. Essential oils show a potent activity in insect and pest control [14]. ANN approach was used previously for the structure activity correlation [15]. ANN Characteristics were identified to be convenient for "data processing" in which the functional connection among input and output is essential and output hasn't been clearly described. As structure activity interactions are repeatedly non linear and complex, neural networks can calculated any type of analytical continuous function [16]. Herbicides are mainly used to destroy unwanted crops i.e. weeds in the agricultural land [17]. The present study emphasized chemical constituents, insecticidal effect and seed germination inhibition potential in hexane, chloroform and methanol extract of fennel seeds. Traditional approaches to the extraction study which involve a large number of parameters sometimes fail to infer meaningful experimental outcomes due to the error or uncertainty cause. To resolve this matter, present study assesses the capacity of soft computing methods such as artificial neural networks (ANN) and fuzzy c-means clustering (FCM) to predict the behavior of fennel seed extracts under different experimental conditions.

Material and methods

Collection and extraction of plant material

Fennel seeds were collected from Vegetable Research Centre (VRC), GBPUA&T Pantnagar, Uttarakhand India. These varieties of fennel were developed in Pantnagar Tarai region viz. FNL-116, FNL-117, FNL-118, FNL-119, FNL-120, FNL-121, FNL-123, FNL-124 FNL-125, FNL-126 and FNL-PM. Fennel seeds were shade dried and finely grounded to fine powder. Powder sample of fennel 10g were taken mixed in the ratio 1:5 with 50 ml of hexane, chloroform and methanol solvent respectively and left for 72 hours with periodically stirring. Further the mixture was centrifuged at 4000 rpm up to 10 minutes. The supernatant was carefully collected and allow concentrating using vacuum rotatory evaporator at 40˚C and stored in deep freezer for the further analysis.

Chemical constituents

Phytochemicals are the nutrient plant chemical that are produced by the primary or secondary metabolism. Phytochemicals have various therapeutic actions due to presence of phytoconstituents. Preliminary phytochemical screening is a qualitative method to check the availability of important phytoconstituents present in the plants. Present study are subjected to phytochemical test in fennel seeds to demonstrate the presence of alkaloids, glycosides, phenols, flavonoids, terpenoids, amino acids, proteins, carbohydrate, oils, fats and saponin presented in Table 1.

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Table 1. Phytochemical test in fennel seed.

Phytochemical Test	Test 1	Test 2
1. Alkaloid Test Each of three extracts of fennel was dissolved individually in dilute hydrochloric acid and filtered. Then the filtrates were separately treated with Wagner's and Hager's Reagent to test for the presence of alkaloids.	**Hager's test** In a 200µl of extract, add 200 µl of Hager's reagent (saturated picric acid solution). Yellow precipitate observed which indicates the presence of alkaloids.	**Wagner's test** 1 ml of extract was treated with Wagner's reagent (Iodine in a potassium iodide). Brown precipitate appears which indicates the positive test.
1. Terpenoid Test 2 ml of fennel extract was dissolved in 2 ml of $CHCl_3$ and evaporate to dryness. Then add 2 ml of conc. H_2SO_4 and heated for about 2 minutes. Grayish color indicates the presence of terpenoids.	Add each of three extracts with 5 ml of water in a test tube and shake vigorously for few minutes following process known as the Foam test.	-
2. Saponin Test	Add each of three extracts with 5 ml of water in a test tube and shake vigorously for few minutes following process known as the Foam test.	-
3. Carbohydrates Test All three extracts were dissolved individually in 5ml distilled water and then filtered. Further the filtrates were treated separately with Molisch's and Fehling's Reagent to test the presence of carbohydrates.	**Molisch's Test** Extracts were treated with a few drops of alcoholic solution of α-napthol and 2 ml of concentrated sulphuric acid. Appearence of violet colour at the junction indicates the presence of carbohydrates.	**Fehling's Test** Add few drops of dilute HCl followed by sodium hydroxide in each test solution. Then the solution was heated with Fehling solution A and Fehling solution B. Formation of a red precipitate showed the presence of reducing sugars.
4. Glycosides Test Each of the extracts was hydrolyzed with dil. HCl and then undergoing to test for glycosides by treating the extracts with modified Borntrager's Reagent and Legal's Reagent.	**Borntrager's Reagent Test** Extracts were treated with $FeCl_3$ solution and immersed into the boiling water for 5 minutes, cooled and shaken with an equal volume of benzene and then the resultant solution was treated with ammonia solution.	**Legal's Reagent Test** Extracts were treated with sodium nitroprusside in pyridine and methanol alkali solution.
5. Phytosterol test It was done by Solkowski's test.	**Solkowski's method** Extracts were treated with chloroform and filtered. The filtrates were then treated with few drops of conc.$H_2SO_4$and allowed to stand and brown and red colored ring in sulphuric acid layer give confirmatory test.	**Fats and Fixed oils Test** It was done by filter paper press test in which extracts were pressed in filter paper and results were observed.
6. Phenol Test	It was done by treating the extracts with 5 mL of $FeCl_3$ solution.	-

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Phytochemical Test	Test 1	Test 2
7. Tannin Test	It was done by gelatin test method in which extracts were treated with 5 mL of 1 % gelatin solution containing NaCl and results were observed.	-
8. Flavonoid Test It was done by lead acetate test and shinoda test.	**Lead Acetate Test** Extracts were treated with 5 mL of lead acetate solution and yellow precipitate indicates the presence of flavonoid.	**Shinoda Test** Few fragments of magnesium ribbon and 5 mL of concentrated HCl were added to the alcoholic solution of the extracts and results were observed.
9. Proteins and Amino Acids Test It was done by Xanthoproteic test and Biuret test.	**Xanthoproteic Test** Extracts were treated with 2 drops of concentrated HNO_3 and observed.	**Biuret Test** Extracts were treated with 1 ml of 10 % sodium hydroxide solution and heated. Now add a drop of 0.7 % copper sulphate solution, violet color indicates the presence of proteins.

Insecticidal activity
Single dose contact effects assay
A stock solution of 100 mg/mL of hexane, chloroform and methanol extract of *F. vulgare* was prepared in sterilized distilled water [18]. Ten insects of *Tribolium castaneum* and *S. oryzae* were placed in each separate sterilized petriplates of 9 cm diameter filled with 1 g of wheat. Lined the Whatman filter paper No.10 in each petriplates and poured the test solution in those petriplates. Sterilized distilled water was taken as control (1 µL/insect). For each replication 10 insects were used and each experiment was repeated three times. Arrange petriplates in the random manner. Now petriplates were kept in the incubator at 27 ºC. The numbers of dead insects was recorded after 24 h % mortality rate was calculated.

Herbicidal activity
To evaluate the herbicidal potential in hexane, chloroform and methanol extracts of *F. vulgare* seeds in terms of seed germination inhibition activity were tested on *Raphanus sativus* seed using procedure Sahu and Devkota, 2013 [19].

Preparation of test solution
Stock solution of 10,000 ppm was prepared for hexane, chloroform and methanol extracts in sterilized distilled water. Four concentration 200 ppm, 400 ppm, 600 ppm and 800 ppm respectively used for testing seed germination inhibition activity. Pendimethalin (3 mL/L) was used as standard.

Germination bioassay
Firstly seeds of *Raphanus sativus* were sterilized using 5% hypochlorite solution up to 15 seconds. Ten seeds of *Raphanus sativus* were placed in each sterilized petriplates of 9 cm diameter. Lined the Whatman filter paper No.10 in each petriplates and poured the test solution of different concentration (200-800 µg/mL) in those petriplates. Sterilized distilled water was taken as control. Each treatment was replicated three times and petriplates arranged in random manner. Now petriplates were kept in the incubator at 25 ºC. After 5 days, the number of germinated seeds was counted for each concentration, and % germination inhibition values were calculated.

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Soft computing method

This section evaluates the capability of soft computing techniques like fuzzy-c-means clustering (FCM) and artificial neural network (ANN) to fore see the behavior of an extracts of fennel seeds with various experimental parameters. The FCM is utilized to cluster analysis of all concentrations of hexane, chloroform and methanol extracts of fennel seeds. The data obtained by simulation is used to train the artificial neural network. Thereafter ANN is used to precisely estimate the values of all concentrations in hexane, chloroform and methanol extracts of fennel seeds. The prediction performance of the ANN is analyzed with the help of mean absolute percentage error (MAPE)."

Fuzzy c-means clustering (FCM)

FCM is done in python programming language in Intel^R core (TM), i5-103 5GI CPU @1.00Ghz on 64 bit windows with 8GB RAM.

Fuzzy c-means (FCM) clustering algorithm was developed by Bezdek 1981[20].

Suppose $X = \{x_1, x_2, ..., x_n\}$ is the set of data points which have to partition into $2 \le c \le n$ clusters. In FCM process, dataset is partitioned into *c* clusters with minimizing the sum squared error (SSE) with respect to data point and grades of the cluster.

$$SSE = \sum_{i=1}^{n}\sum_{j=1}^{c} u_{ij}^{p} d^{2}\left(x_i, v_j\right)$$

where u_{ij} is the degree of belongingness of each data point $\left(x_i\right)$ to each cluster $(j = 1, 2, ..., 3)$ and center of the clusters $\left(v_j\right)$. $p > 1$ is parameter of fuzziness and $d\left(x_i, v_j\right)$ denotes Euclidean distance between data point x_i and cluster center v_j. The constraints for membership grades are given as

$$0 \le u_{ij} \le 1; \quad 0 \le \sum_{n=1}^{c} u_{ij} \le n; \quad \sum_{j=1}^{c} u_{ij} = 1$$

Minimization of SSE ensures each data point belongs to the cluster whose center is nearest to it and it also makes well separated clusters. To apply FCM, first we have to specify the optimal number of clusters(*c*). For this we take number of clusters is equal to number extracts which is 3.

Artificial neural network (ANN)

The MATLAB software [21] was employed to computational analysis using artificial neural networks (ANN). Before extended learning network, the input and output vector data were allow standardizing among 0.1 to 0.9. The lowest and highest values of sigmoidal transfer function are 0 and 1, respectively. In the original data file, maximum and minimum output values normalizing between 0.1 and 0.9. The possibility of random connections can be achieved simply repeating the computations, but with the dependent variables scrambled. With this scrambling, any interrelation between the descriptors and the dependent variable is demolished. No model should efficiently perform better than chance. The obtained findings are compared to the ANN results to demonstrate that the actual results were obtained through the disclosure of relationships instead by accidental correlations.

Statistical analysis

All the experiments were conducted in triplicates and results were analyzed as Mean ± SD. Statistical analysis was performed using software SPSS 20 by applying Tukey's test for the significant result. Correlation was performed using R studio (Version 4.2.2, 2022-10-31) in Intel® core (TM), i5-103 5GI CPU @1.00Ghz on 64 bit windows with 8 GB RAM.

Results

Hexane, chloroform and methanol extracts of fennel is undertaken to evaluate the qualitative analysis of phytochemicals are presented in table 2.

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Table 2. Phytochemicals preset in fennel seed extract.

Phytoconstituents	Extract	FNL-116	FNL-117	FNL-118	FNL-119	FNL-120	FNL-121	FNL-123	FNL-124	FNL-125	FNL-126	FNL-PM
Alkaloids	Hexane	+	-	-	+	+	+	-	-	+	+	+
	Chloroform	-	-	-	+	-	-	-	-	+	-	-
	Methanol	+	+	+	+	+	+	+	+	+	+	+
Terpenoids	Hexane	+	+	+	+	+	+	+	+	+	+	+
	Chloroform	-	-	-	-	-	-	-	-	-	-	-
	Methanol	+	+	+	+	+	+	+	+	+	+	+
Glycosides	Hexane	+	+	+	+	+	+	+	+	+	+	+
	Chloroform	+	+	+	+	+	+	+	+	+	+	+
	Methanol	+	+	+	+	+	+	+	+	+	+	+
Phenols	Hexane	+	+	+	+	+	+	+	+	+	+	+
	Chloroform	+	+	+	+	+	+	+	+	+	+	+
	Methanol	+	+	+	+	+	+	+	+	+	+	+
Flavonoids	Hexane	-	-	-	-	-	-	-	-	-	-	-
	Chloroform	+	+	+	+	+	+	+	+	+	+	+
	Methanol	+	+	+	+	+	+	+	+	+	+	+
Tannins	Hexane	+	+	+	+	+	+	+	+	+	+	+
	Chloroform	+	+	+	+	+	+	+	+	+	+	+
	Methanol	++	++	++	++	++	++	++	++	++	++	++

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Phytoconstituents	Extract	FNL-116	FNL-117	FNL-118	FNL-119	FNL-120	FNL-121	FNL-123	FNL-124	FNL-125	FNL-126	FNL-PM
Phytosterols	Hexane	+	+	+	+	+	+	+	+	+	+	+
	Chloroform	+	+	+	+	+	+	+	+	+	+	+
	Methanol	+	+	+	+	+	+	+	+	+	+	+
Protein and amino acids	Hexane	+	+	+	+	+	+	+	+	+	+	+
	Chloroform	+	+	+	+	+	+	+	+	+	+	+
	Methanol	+	+	+	+	+	+	+	+	+	+	+
Carbohydrates	Hexane	+	+	+	+	+	+	+	+	+	+	+
	Chloroform	+	+	+	+	+	+	+	+	+	+	+
	Methanol	++	++	++	++	++	++	++	++	++	++	++
Fixed oil and fat	Hexane	+	+	+	+	+	+	+	+	+	+	+
	Chloroform	-	-	-	-	-	-	-	-	-	-	-
	Methanol	+	+	+	+	+	+	+	+	+	+	+
Saponins	Hexane	+	+	+	+	+	+	+	+	+	+	+
	Chloroform	+	+	+	+	+	+	+	+	+	+	+
	Methanol	+	+	+	+	+	+	+	+	+	+	+

"+"=slightly present, "++"=moderately present, "-"= absent

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Insecticidal activity

Insecticidal activity observed in terms of mortality rate in hexane, chloroform and methanol extract of fennel seeds presented in table 3.

Table 3. % Mortality rate in fennel seeds.

S. No.	Fennel	Extract	% Mortality± SD	
			Tribolium castaneum	*S. oryzae*
1	FNL-116	Hexane	10.22±0.1[a]	11.02±0.5 [a]
		Chloroform	21.05±0.21 [c]	13.02±0.31 [b]
		Methanol	22.1±0.51 [a]	12.22±0.23 [a]
2	FNL-117	Hexane	12.15±0.24 [a]	21.32±0.41 [bc]
		Chloroform	11.21±0.4 [ab]	18.41±0.12 [d]
		Methanol	30.31±0.31 [b]	21.13±0.24 [b]
3	FNL-118	Hexane	33.21±0.34 [c]	25.13±0.17 [cd]
		Chloroform	44.23±0.32 [e]	21.05±0.14 [d]
		Methanol	58.12±0.22 [d]	45.1±0.31 [f]
4	FNL-119	Hexane	20.41±0.13 [b]	31.12±0.03 [e]
		Chloroform	48.21±0.15 [g]	35.13±0.4 [g]
		Methanol	47.21±0.06 [c]	41.22±0.7 [e]
5	FNL-120	Hexane	21.22±0.3 [b]	26.33±0.41[d]
		Chloroform	20.31±0.17 [c]	24.12±0.31 [e]
		Methanol	78.24±0.16 [g]	54.21±0.17 [h]
6	FNL-121	Hexane	66.24±0.13 [f]	39.12±0.6 [g]
		Chloroform	46.31±0.05 [f]	30.6±0.08 [f]
		Methanol	69.22±0.11 [f]	47.22±0.25 [f]
7	FNL-123	Hexane	31.11±0.41 [c]	23.1±0.22 [c]
		Chloroform	12.41±0.23 [b]	10.22±0.05 [a]
		Methanol	54.13±0.33 [d]	39.12±0.13 [e]
8	FNL-124	Hexane	20.31±0.21 [b]	34.12±0.24 [f]
		Chloroform	10.25±0.15 [a]	15.21±0.31 [c]
		Methanol	66.23±0.17 [ef]	52.11±0.06 [h]

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S. No.	Fennel	Extract	% Mortality± SD	
			Tribolium castaneum	*S. oryzae*
9	FNL-125	Hexane	67.14±0.01 [f]	42.1±0.04 [g]
		Chloroform	53.21±0.31 [h]	30.11±0.11 [f]
		Methanol	75.12±0.12 [g]	36.02±0.09 [d]
10	FNL-126	Hexane	22.41±0.24 [b]	19.21±0.22 [b]
		Chloroform	38.22±0.17 [d]	34.2±0.07 [g]
		Methanol	62.31±0.07 [e]	41.31±0.12 [e]
11	FNL-PM	Hexane	45.23±0.12 [d]	31.24±0.03 [ef]
		Chloroform	46.08±0.15 [f]	39.15±0.07 [h]
		Methanol	84.26±0.09 [h]	31.22±0.5 [c]
12	Control		0±0.00	0±0.00

Values are mean of three replicates±SD. Within a column, mean value followed by same letter are significantly not different according to Tukey's test ($p < 0.005$).

Herbicidal activity

Mean percent seed germination inhibition results were presented in table 4 and respective IC_{50} value presented in table 5.

Table 4. Seed germination inhibition activity in fennel seed.

S. No.	Fennel	Extract	% seed germination inhibition			
			200 µg/mL	400 µg/mL	600 µg/mL	800 µg/mL
1	FNL-116	Hexane	18.33±7.63[a]	31.66±2.88[b]	38.33±7.63[c]	40.00±10.00[d]
		Chloroform	26.66±15.27[c]	33.33±1.15[c]	36.66±15.27[c]	43.33±11.54[d]
		Methanol	15.00±8.66 [a]	20.00±10.00[b]	30.00±10.00[b]	36.66±5.77[c]
2	FNL-117	Hexane	16.66±5.77[a]	20.00±10.00[b]	41.66±10.40[d]	43.33±11.54[d]
		Chloroform	20.00±10.00[b]	26.66±15.27[b]	46.66±5.77[d]	53.01±10.00[e]
		Methanol	20.00±10.00[b]	23.33±11.54[b]	28.33±10.40[b]	43.33±5.77[e]
3	FNL-118	Hexane	13.33±11.54[b]	23.33±5.77[b]	30.70±16.00[c]	60.00±10.00[f]
		Chloroform	18.33±7.63[a]	25.00±13.27[b]	30.00±10.00[c]	40.00±10.00[d]
		Methanol	18.63±7.63[a]	30.00±10.00[b]	36.66±5.77[d]	46.66±5.77[e]

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S. No.	Fennel	Extract	% seed germination inhibition			
			200 µg/mL	400 µg/mL	600 µg/mL	800 µg/mL
4	FNL-119	Hexane	23.33±11.54^{b}	36.66±15.27^{c}	40.00±10.00^{d}	63.53±15.27^{f}
		Chloroform	28.33±2.88^{b}	40.00±10.00^{d}	45.00±8.66^{d}	56.66±5.77^{e}
		Methanol	21.66±10.40^{b}	28.63±7.63^{b}	31.66±2.88^{e}	40.00±10.00^{d}
5	FNL-120	Hexane	15.33±13.22^{a}	25.00±10.00^{b}	36.66±15.27^{b}	48.33±15.27^{e}
		Chloroform	33.33±5.77^{c}	43.33±5.77^{d}	50.00±10.00^{e}	60.00±10.00^{f}
		Methanol	16.66±7.63^{a}	33.33±5.77^{c}	35.00±8.66^{c}	41.66±2.88^{d}
6	FNL-121	Hexane	20.00±10.00^{a}	30.00±10.00^{c}	35.00±13.22^{c}	46.66±5.27^{d}
		Chloroform	40.00±10.00^{d}	46.66±5.77^{d}	53.33±5.77^{e}	63.33±15.27^{f}
		Methanol	30.00±10.00^{c}	40.00±10.00^{d}	43.33±5.77^{d}	60.00±10.00^{f}
7	FNL-123	Hexane	26.66±5.77^{b}	33.33±5.77^{c}	43.33±5.77^{d}	66.66±15.27^{g}
		Chloroform	15.00±5.33^{a}	26.66±15.27^{b}	30.00±10.00^{c}	33.33±11.54^{c}
		Methanol	26.66±15.27^{b}	38.33±7.63^{b}	53.16±10.00^{e}	70.00±10.00^{h}
8	FNL-124	Hexane	21.66±7.63^{b}	28.33±10.40^{b}	45.00±13.22^{d}	56.66±5.77^{e}
		Chloroform	21.66±10.40^{b}	30.00±10.00^{b}	33.33±5.77^{c}	38.33±10.40^{c}
		Methanol	23.33±10.40^{b}	26.66±11.54^{b}	33.33±15.27^{d}	50.00±10.00^{e}
9	FNL-125	Hexane	25.00±8.66^{b}	26.66±15.27^{b}	33.33±5.77^{c}	41.66±12.58^{d}
		Chloroform	16.66±15.27^{a}	23.33±15.27^{b}	35.00±13.22^{c}	36.66±12.58^{d}
		Methanol	20.00±5.00^{b}	21.66±10.40^{b}	38.33±2.88^{c}	45.00±5.00 ^{d}
10	FNL-126	Hexane	26.66±5.77^{b}	31.66±7.63^{c}	46.66±15.77^{e}	55.00±13.22^{e}
		Chloroform	27.5±6.61^{b}	36.66±5.77^{c}	40.00±10.00^{d}	56.66±11.54^{e}
		Methanol	17.5±11.45^{a}	28.33±7.33^{b}	35.83±5.20^{c}	42.5±2.5^{d}
11	FNL-PM	Hexane	11.66±10.40^{a}	20.00±10.00^{b}	31.66±14.43^{c}	36.33±15.27^{c}
		Chloroform	31.66±7.63^{c}	38.33±7.63^{d}	31.66±7.63^{c}	46.66±5.77^{d}
		Methanol	36.66±5.77^{c}	43.33±5.77^{d}	53.33±5.77^{e}	66.66±11.54^{g}
12	Pendimethalin		100.00±00^{a}	100.00±00^{a}	100.00±00^{a}	100.00±00^{a}

Values are mean of three replicates±SD. Within a column, mean value followed by same letter are significantly not different according to Tukey's test ($p < 0.005$).

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Table 5. IC_{50} value for seed germination inhibition activity in fennel.

S. No.	Fennel	Extract	Seed germination inhibition IC_{50} value (µg/mL)
1	FNL-116	Hexane	841.85±1.30[b]
		Chloroform	807.10±0.60[b]
		Methanol	1021.17±6.81[b]
2	FNL-117	Hexane	946.07±1.03[b]
		Chloroform	724.35±2.53[b]
		Methanol	817.21±2.52[b]
3	FNL-118	Hexane	769.68±0.50[b]
		Chloroform	940.42±1.20[b]
		Methanol	802.25±2.66[b]
4	FNL-119	Hexane	639.20±0.64[ab]
		Chloroform	640±1.34[ab]
		Methanol	896.14±1.34[ab]
5	FNL-120	Hexane	815.06±0.66[ab]
		Chloroform	589.42±1.07[ab]
		Methanol	845.67±1.33[ab]
6	FNL-121	Hexane	806.99±1.19[ab]
		Chloroform	559.41±1.86[ab]
		Methanol	626.67±1.34[ab]
7	FNL-123	Hexane	614.01±0.56[ab]
		Chloroform	1023.17±7.08[ab]
		Methanol	563.98±1.50[ab]
8	FNL-124	Hexane	682.59±1.89[b]
		Chloroform	894.13±3.16[b]
		Methanol	796.20±0.581[b]
9	FNL-125	Hexane	870.33±0.89[b]
		Chloroform	949.03±1.43[b]
		Methanol	837.16±0.24[b]

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S. No.	Fennel	Extract	Seed germination inhibition IC_{50} value (μg/mL)
10	FNL-126	Hexane	665.75±0.79^{ab}
		Chloroform	691.73±1.33^{ab}
		Methanol	854.66±1.44^{ab}
11	FNL-PM	Hexane	1021.15±5.75^{ab}
		Chloroform	771.25±1.98^{b}
		Methanol	549.10±2.86^{ab}
12	Pendimethalin		369.52±2.62^{a}

Values are mean of three replicates±SD. Within a column, mean value followed by same letter are significantly not different according to Tukey's test ($p < 0.005$).

FCM is done in MATLAB programming language in Intel^{R} core (TM), i5-103 5GI CPU @1.00Ghz on 64 bit windows with 8GBRAM. To apply FCM, first we have to specify the optimal number of clusters(*c*). For this we take number of clusters is equal to number extracts which is 3. FCM cluster analysis was implemented on all concentrations of hexane, chloroform and methanol extracts of fennel seeds including IC_{50} values shown in Fig. 1 and Table 6 represent 3 clusters groups of fennel seeds and their respective cluster centers.

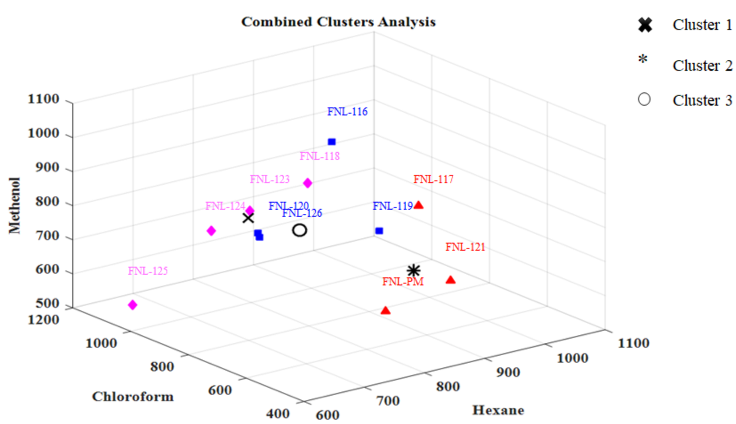

Fig. 1. Combined Cluster analysis in hexane, chloroform and methanol extract of fennel seeds.

Table 6. Cluster centre in hexane, chloroform and methanol extract of fennel.

Cluster center	IC_{50} (μg/mL)			Cluster group
	Hexane	Chloroform	Methanol	
1	941.67	731.69	626.07	FNL-116, FNL-119, FNL-120, FNL-126
2	758.22	923.47	791.18	FNL-117, FNL-121, FNL-PM
3	720.66	665.74	861.58	FNL-118, FNL-123, FNL-124, FNL-125

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Computational neural network ANN was implanted using MATLAB 2020. A sigmoid function acts as an initiation function in feed forward neural network. The input and output values were standardized between 0.1 and 0.9 before learning network was employed. ANN was used to predict the IC_{50} values of the fennel as well as part of evaluation of the ANN's prediction ability [22]. The ANN calculated value for the herbicidal activity in fennel presented in Table 7. The mean absolute percentage error (MAPE) of fennel extract using ANN was shown in Table 8. A correlation study between insecticidal and herbicidal activity in fennel seed are presented in Fig. 2.

Table 7. IC_{50} value in fennel seed extract using ANN.

Fennel	**Hexane Extract**		**Chloroform Extract**		**Methanol Extract**	
	IC_{50} (µg/mL) Experimental	**IC_{50} (µg/ mL) Predicted (ANN)**	**IC_{50} (µg/ mL) Experimental**	**IC_{50} (µg/ mL) Predicted (ANN)**	**IC_{50} (µg/ mL) Experimental**	**IC_{50} (µg/ mL) Predicted (ANN)**
FNL-116	841.85	836.79	807.1	800.71	1021.17	1006.1
FNL-117	946.07	938.83	724.35	719.94	817.21	808.53
FNL-118	769.68	766.13	940.42	930.85	802.25	794.04
FNL-119	639.2	638.38	640	637.61	896.14	884.99
FNL-120	815.06	810.56	589.42	588.23	845.67	836.1
FNL-121	806.99	802.66	549.41	549.18	626.67	623.95
FNL-123	614.01	613.71	1023.17	1011.62	563.98	563.22
FNL-124	682.59	680.86	894.13	885.66	796.2	788.18
FNL-125	870	864.35	949	939.22	837	827.7
FNL-126	665.75	664.37	691.73	688.1	854.66	844.81
FNL-PM	1021.15	1012.34	771.25	765.72	549.1	548.81

Table 8. Mean absolute percentage error (MAPE) of fennel extract using ANN.

S. No.	**Extract**	**MAPE**
1	Hexane	0.46
2	Chloroform	0.67
3	Methanol	0.89

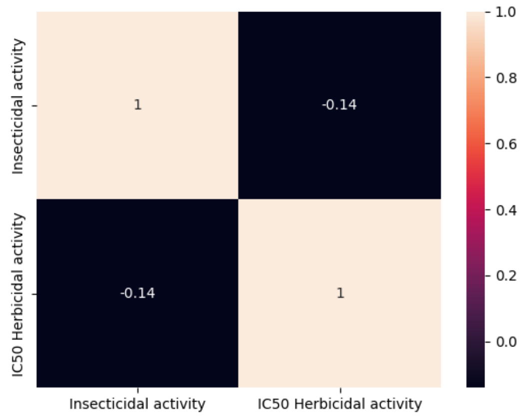

Fig. 2. Correlation study between insecticidal and herbicidal activity in fennel seed.

Correlation study depicts a significant correlation in biological activities of fennel seeds.

Discussion

Secondary metabolites such as terpenoids, phenol, alkaloids, tannins, flavonoids, protein, amino acid, carbohydrates, oil, fat and saponins were analysed in fennel. Methanol extract of fennel seed exhibits higher phytoconstituents than hexane and chloroform extract. Alkaloid was the most abundant phytochemical present in fennel seed [23]. Flavonoids, terpenoids and glycosides are present in methanol extract of fennel seeds [24].. Previous study depicted Fennel seed have promising amount of phytoconstituents in terms of flavonoid content and phenolic content in hexane, chloroform and methanol extract [25]. Trans-anethole, d-arabitol, trans-sinapyl alcohol, floctafenine, palmitic acid are the major chemical compounds observed in fennel seed extract [26]. Maximum insecticidal activity was found in methanol followed by hexane and chloroform extract of fennel. The mortality rate of *Tribolium castaneum* observed in methanol extract in ranged 10.22-84.26 % highest in FNL-120, FNL-125 and FNL-PM was 78.24 ± 0.16, 75.12 ± 0.12 and 84.26 ± 0.09, respectively. *S. oryzae* mortality rate was observed highest in methanol extract in ranged 11.02-54.21 %. Mainly terpenoids, terpenes are responsible for the pesticidal activity [27]. Previous study revealed fennel essential oil caused larval mortality in *C. quiquefasciatus* ranged in between 28-38µg/mL [28]. The mortality rate for the fennel against *Callosobruchus maculates* observed in ranged 5-70 µg/ml for different concentrations [29]. Seed germination inhibition found to be increased with increase in extract concentration. Results showed methanol extract have potent seed germination inhibition potential followed by chloroform and hexane extract. In hexane extract, higher inhibition activity found in FNL-123 (IC_{50}=614.01 ± 0.56 µg/mL). In chloroform extract, higher inhibition activity in FNL-121 (IC_{50}=559.41 ± 1.86 µg/ mL). Higher seed germination inhibition observed in methanol extract of FNL-PM (IC_{50}=549.10 ± 2.86µg/ mL). Fennel essential oil strongly inhibits the seed germination activity [30]. It is observed that using 1000 µl/l fennel essential oil is better to control weed growth [31]. Fuzzy-c-means clustering depicts the cluster of fennel seeds are promising for the future study with potent biological activity. ANN results demonstrated the good prediction ability for the herbicidal activity in fennel seeds. Future perspective research may be focused on the other soft computing techniques i.e. machine learning, artificial intelligence, evolutionary computation and fuzzy prediction method.

Conclusions

The present study concludes fennel seed are rich in phytoconstituent like alkaloid, terpenoid, flavonoid, fats, oils, tannin, saponin etc. These fennel seeds could be effectively used for the medication purpose in pharma

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industries. In conclusion, the insecticidal and herbicidal activities of fennel seed extracts offer valuable alternatives for sustainable agriculture, reducing dependence on synthetic chemicals and promoting environmentally friendly practices in the commercial production of crops. Results concluded the FCM method was help to develop a new crop with efficient results on clustering in fennel. Computational method shows the efficient data analysis. Comparison of experimental and predicted ANN data values, ANN has good predictive power. Using fennel seed extracts as a natural herbicide can offer an alternative to chemical herbicides. Fennel seed extracts can be incorporated into organic farming practices, supporting farmers in obtaining organic certifications and meeting consumer preferences for pesticide-free produce. Ongoing research into the properties of fennel seeds and their extracts may lead to the development of more effective and targeted insecticidal and herbicidal solutions. This continuous innovation can drive the commercial viability of fennel seed extracts in agriculture.

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