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Evaluation of Fixed Oil, Seed Extracts, of *Carum carvi* L

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Abstract: *Carum carvi* L. was used traditionally in different populations for many medical complains. The seeds are used for culinary purposes and medicinal treatment. The study was aimed to investigate the chemical composition of fixed oil of *Carum carvi* L. (seeds)**.** The oil was extraction by petroleum ether (60-80°C) using a Soxhlet apparatus. *Carum carvi* L. *seeds oil* showed 4.5% yield of fixed oil. The oil of *Carum carvi* L. seeds were Extract has been investigated by Fourier Transform Infrared Spectrophotometer (FTIR) and Gas Chromatography Mass Spectrometry (GC/MS) techniques Total of eight compounds were detected for petroleum ether oil extract. From the eight identified constituents, representing 100% of the oilthe most main abundant compounds detected were L-Fenchone (55.01%); p-Methoxy benzaldehyde (19.15%) and p-Methoxy allyl benzene (9.46%). *Carum carvi* L. seeds are rich sources of oils containing diverse group of phytochemicals.

Keywords: GC/MS, FT-IR, *Carum carvi* L (Seeds), Soxhlet Methods, L-Fenchone

1. Introduction

The value of natural products in the treatment of ailments is well-known. Amongst the various natural sources, plants are an important source of bioactive constituents. More than 1000 plant species are known for their anticancer potential. The use of plant compounds as prototypes of new drugs has a historical and economic importance. Some plants extracts were defined as effective in treating cancer, there action was attributed to additional or synergistic effect of compounds present in the extract. In consequence, the cytostatic effect of the extract observed in tumor cells seems to be more effective than the effect of isolated and biologically active compounds [1].

Carum carvi L. belonging to the family: Apiaceae, is one of the earliest cultivated herbs in Asia, Africa and Europe. In folk medicine, this plant is used as a carminative for stomach disorders, diarrhea, and colic, as well as particularly in veterinary medicine [2].

Caraway has a long history of use as a household remedy especially in the treatment of digestive complaints where its antispasmodic action soothes the digestive tract and its carminative action relieves bloating caused by windand improves the appetite [3], [4], [5]. It is often added to laxative medicines to prevent griping [4]. The seed is antiseptic, aromatic, anaesthetic, anodyne, antianxiety, diuretic, mildly expectorant, fungicidal, muscle relaxant, soporific, tonic, emmenagogue, expectorant, galactogogue and stimulant [3], [6]. It can be chewed raw for the almost immediate relief of indigestion and can also be made into infusions. The seed is also used in the treatment of bronchitis and are an ingredient of cough remedies, especially useful for children and for mothers for increasing breast milk. A tea made from the seeds is a pleasant stomachic and carminative, it has been used to treat flatulent colic [6], [7]. The seed is used in Tibetan medicine where it is considered to have an acrid taste and a heating potency. It is used to treat failing

vision and loss of appetite [8]. An essential oil from the seed is used in perfumery, for scenting soap, as a parasiticide etc. [9]. Also *C. carvi* are used in traditional Sudanese medicine and other folk medicines as a carminative, since it is effective against spasmodic gastrointestinal complaints, flatulence, irritable stomach, indigestion, lack of appetite, and dyspepsia in adults [10].

Carum carvi L. seeds contain 1–9% essential oils consisting of more than 30 compounds. Carvone and limonene were account the main portions [11], [12]. However, the chemical groups isolated from the oils of the seeds of *Carum carvi* L. were included monoterpene hydrocarbons, oxygenated monoterpenes, oxygenated sesquiterpenes, saturated and unsaturated fatty acids, aldehydes, ketones and esters [13], [14]. The essential oil compounds were included (%) α-Pinene 0.3, Camphene 0.2, β-Pinene 0.1, β-Myrcene 0.1, Limonene 5.1, γ- Terpinene 12.6, β-Ocimene 0.1, *p*-Cymene 0.1, Terpinolene 0.1, limonene oxide 0.1, Camphor 0.2, Linalool 0.7, Linalyl acetate 0.3, Terpinene-4-ol 0.1, β- Caryophyllene, Dihydrocarvone 0.2, α-Terpineol 0.1, Germacrene-D 0.1, Carvone 70.1, β- Selinene 0.2, α- Farnesene 0.4, Citronellol 0.1, δ-Cadinene 0.3, γ-Cadinene 0.5, Cuminaldhyde 0.1, Nerol 0.2, Trans-carveol 0.1, Nonadecane 0.1, Spathulenol 0.3, Eugenol 0.2, Thymol 0.5 and Carvacrol 0.2 [20]. However, the same compounds with fluctuated percentages were recorded by other studies [15], [16], [17]. An aromatic compound, glucoside and a glucide were isolated from the water-soluble portion of the methanolic extract of caraway fruit (*Carum carvi* L.). Their structures were clarified as 2-methoxy-2-(4'- hydroxyphenyl) ethanol, junipediol A 2-O-beta-D-glucopyranoside and L-fucitol [18]. The flavonoid constituents of caraway were included quercetin-3-glucuronides, isoquercitrin, quercetin 3-0 caffeylglucoside, and kaempferol 3-glucoside [19]. Therefore, the study was aimed to investigate the chemical composition of fixed oil of *Carum carvi* L. (seeds)**.**

2. Materials and Methods

2.1. Plant Materials

The Caraway (*Carum carvi* L)*,* was collected from Khartoum central Sudan during September to October 2016, and the plant was kindly identified and authenticated by Medicinal and Aromatic Plants and Traditional Medicine Research Institute (MAPTMRI) in Khartoum, Sudan. Seeds were air-dried, under the shade, pulverized and stored prior to extraction. Shade with good ventilation and then ground finely in a mill and kept in the herbarium until oil extract preparation. Figure (1).

Figure 1. *Carum carvi L. Seeds.*

2.2. Extraction of Oil

Air-dried seeds of Caraway (*Carum carvi* L.)*,* was separately powdered and extracted with 1 L ofpetroleum ether (60-80°C) using a Soxhlet apparatus. This process of extraction was repeated for 6h, thepetroleum ether distilled out by distillation assembly, then concentrated by hot plate drying and air-drying at temperature of 40±2°C.

Yield % = (weigh of extract/weigh of sample) X 100

2.3. Fourier Transform Infrared Spectrophotometer (FTIR) Analysis

Principle: Fourier Transform Infrared Spectrophotometer (FTIR) is perhaps themost powerful tool for identifying the types of chemical bonds (functional groups) present in compounds. The wavelength of light absorbed is characteristic of the chemical bond as can be seen in the annotated spectrum. By interpreting the infrared absorption spectrum, the chemical bonds in a molecule can be determined.

Assay: Fixed oil was used for FTIR analysisusing KBr disk methodology. 1 mg of sample was encapsulated in 100 mg of KBr pellet in order to prepare translucent sample discs. The liquid sample of plant specimen was loaded in FTIR spectroscope (Shimadzu, IR Affinity 1, Japan), with a scan range from 400 to 4000 cm^{-1} with a resolution of 4 cm^{-1}. Each analysis was repeated ten times for the spectrum confirmation.

2.4. GC-MS Analysis

GC-MS technique was used in this study to identify the

phytocomponents present in the most active fractions. The tested extracts were analyzed by GC-MS using Shimadzu Mass Spectrometer-2010 series. 1 µL of sample was injected in GC-MS equipped with a split injector. The MS was operated in the electron ionization (EI) mode (70 eV). Helium was employed as the carrier gas and its flow rate was adjusted to 1.2 mL/min. The analytical column connected to the system was an Rtx-5 capillary column (length-30 m × 0.25 mm i. d., 0.25 µm film thickness). The column head pressure was adjusted to 93.9 kPa. Column temperature programmed from 110°C (7 min) to 200°C at 10°C/min and from 200-280°C at 5°C/min with hold time 0 and 9 min respectively. A solvent delay of 4.50 min was selected. The injector temperature was set at 250°C. The GC-MS interface was maintained at 280°C. The MS was operated in the ACQ mode scanning from m/z 40 to 550.0. In the full scan mode, EI mass spectra in the range of 40–550 (m/z) were recorded at electron energy of 70 eV. Compounds were identified by comparing mass spectra with library of the National Institute of Standard and Technology (NIST), USA/Wiley.

3. Results and Discussion

Carum carvi L. oil has the low yield percentage with petroleum ether solvent shown in Table (1).

Table 1. *Yield percentageof Caraway (Carum carvi L.), oil.*

Name of plant	Part used	Weight of sample (g)	Volume of oil	Yield %
*Carum carvi*L	Seeds	500	22.5	4.5

3.1. FTIR Analysis

The FTIR spectrum was used to identify the functional groups of the chemical components present in the tested fractions based on the peak value in the region of infrared radiation. Fixed oil of *Carum carvi* L. its FTIR spectrum confirmed the presence of alkynes, alkenes, alkanes, carboxylic acids, esters, ethers, carbonyls, carboxylic acids, H–bonded alcohols and phenols and other compounds Shown in table (2) and Figure (2) show FT-IR spectra of *Carum carvi* L. fixed oil.

Table 2. *FT-IR spectral analysis of Caraway (Carum carvi L.), oil.*

NO	Frequancy CM^{-1}	Bond	Functional group
	719.47	O−H bending	Phenyl ring substitution bands
	756.12	C-H bending Out-of-plane	Alkenes
	912.36	C–O–H out-of-plane bending	Carboxylic acids
	962.51 993.37	Out-of-plane C–H bending	aliphatic hydrocarbons
	1039.67 1064.74	Aliphatic C–O stretching	Esters
	1099.46 1120.68	C–O–C stretching	Ethers
	1145.75	C-O stretch	alcohols, carboxylic acids, esters, ethers
	1247.99	C–H bending In-plane	aliphatic hydrocarbons
	1301.99	Aromatic C–O stretching	Phenols
	1357.93	Methyl symmetrical C–H bending	Alkanes
	1377.22	C–H bending	Alkanes
	1415.8	=C–H in-plane bending	Alkenes
	1444.73	C-C stretch (in-ring)	Aromatics
	1464.02	Methyl asymmetrical C–H bending	Alkanes
	1512.24	C–O–H in-plane bending	Carboxylic acids
	1585.54 1678.13	C=C stretch	Alkenes
	1710.92	C=O stretch	Aliphatic ketone
	1743.71	C=O stretch	Aliphatic aldehyde
	2852.81	C−H (med)	Aldehyde group
	2922.25 3005.2	C−H (m) stretching	Alkanes
	3061.13 3074.63	C−H (m) stretching	Aromatic rings
	3128.64 3192.3	C−H stretch	Aromatic
	3207.73	O–H stretch	Alcohols, phenol
	3250.16	O–H stretch	carboxylic acids
	3271.38	=C–H stretching	Alkynes
	3306.1	=C–H stretching	Alkynes
	3350.46 3381.33	O-H stretch	Carboxylicacids
	3400.62 3408.33 3427.62	O-H stretch	H-bonded alcohols, phenols

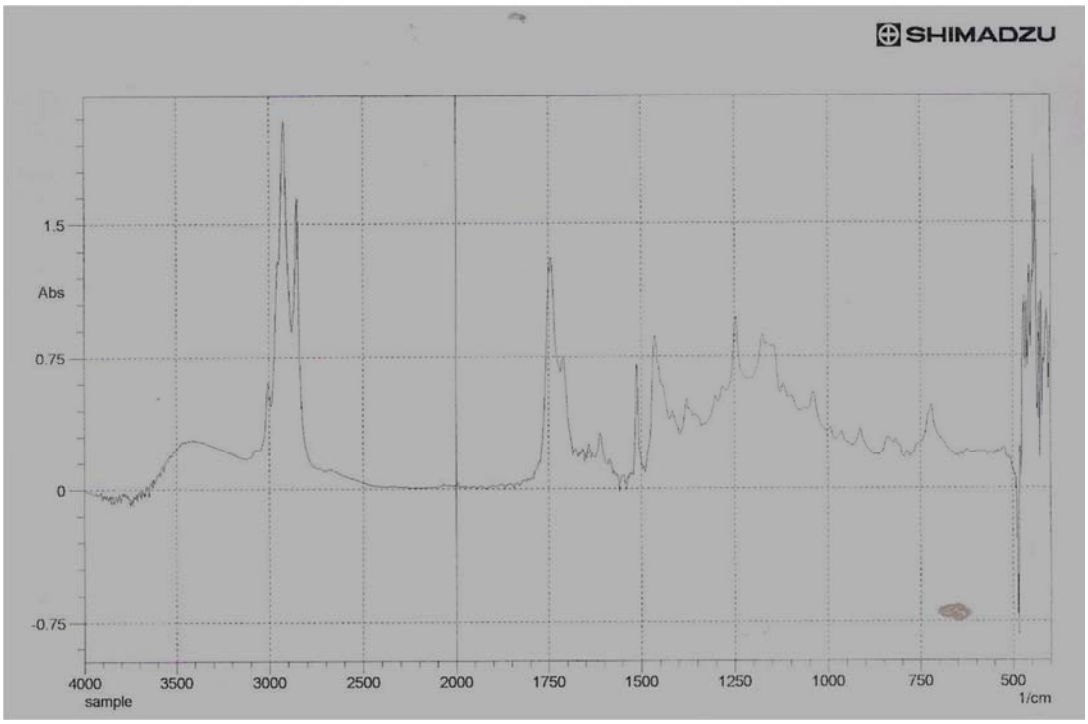

Figure 2. *Show FT-IR spectra of Carum carvi L. fixed oil.*

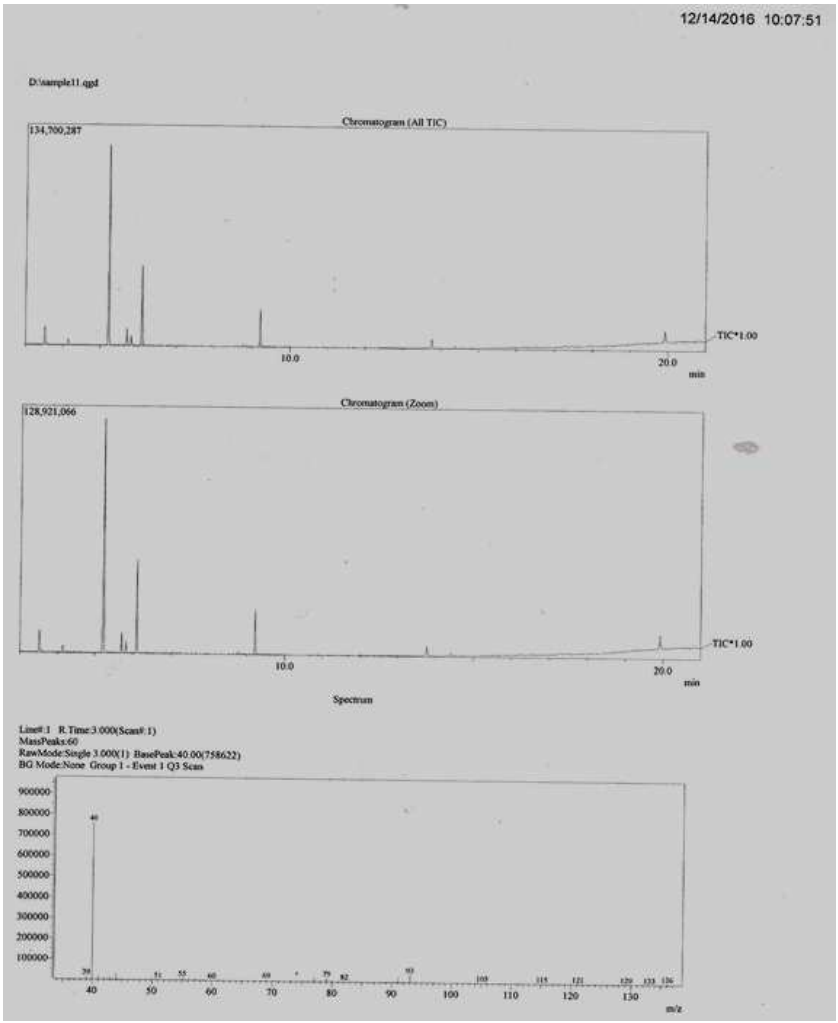

Figure 3. *GC-MS chromatogram of Caraway (Carum carvi L.), oil.*

3.2. GC-MS Analysis

The results pertaining to GC-MS analysis lead to the identification of number of compounds. These compounds were identified through mass spectrometry attached with GC. The mass spectrometer analyzes the compounds eluted at different times to identify the nature and structure of these compounds. Interpretation of mass spectrum GC–MS was conducted using the database of National Institute of Standards and Technology (NIST). The name, molecular weight and structure of the components of the test materials were ascertained, the components identified by the GC-MS are illustrated in tables (3). and Figure (3) show GC-MS spectra of *Carum carvi* L. fixed oil.

Themass spectrographs of the identified constituents are given in Figure 4 to 11 the relative amount of individual components wascalculated based on GC peak areas.

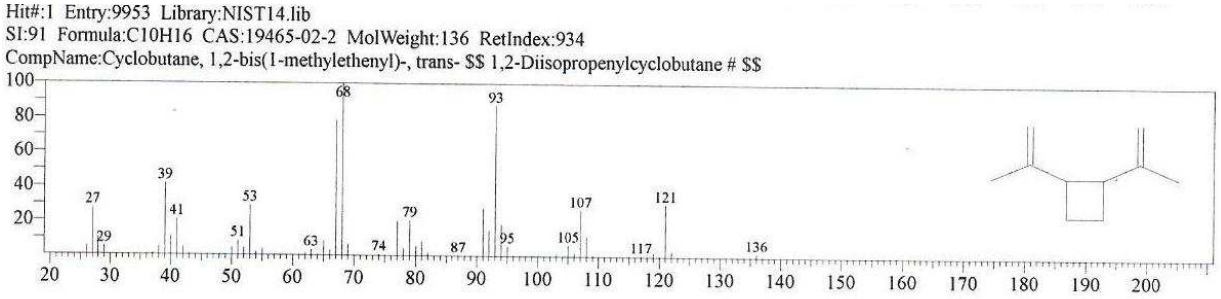

Figure 4. *Mass profile of Peak at R. Timt 3.517 min; A GC- MS of peak eluted at R. Time 3.517 min; 1, 2-Diisopropenylcyclobutane.*

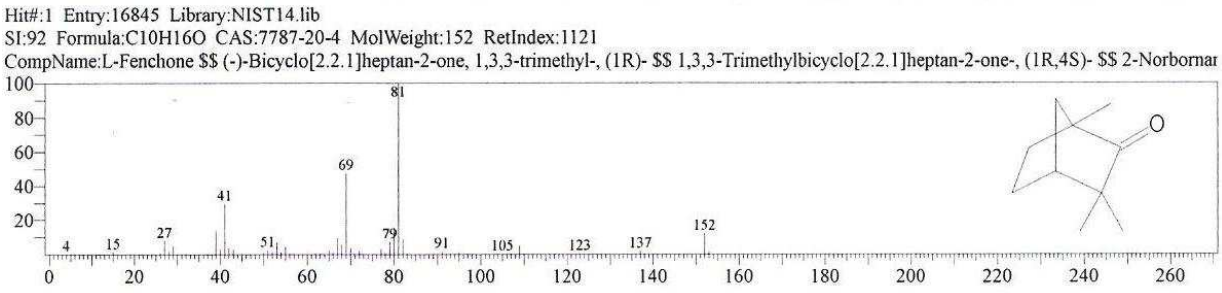

Figure 5. *Mass profile of Peak at R. Time 4.142 min; A GC- MS of peak eluted at R. Time 4.142 min; L-Fenchone.*

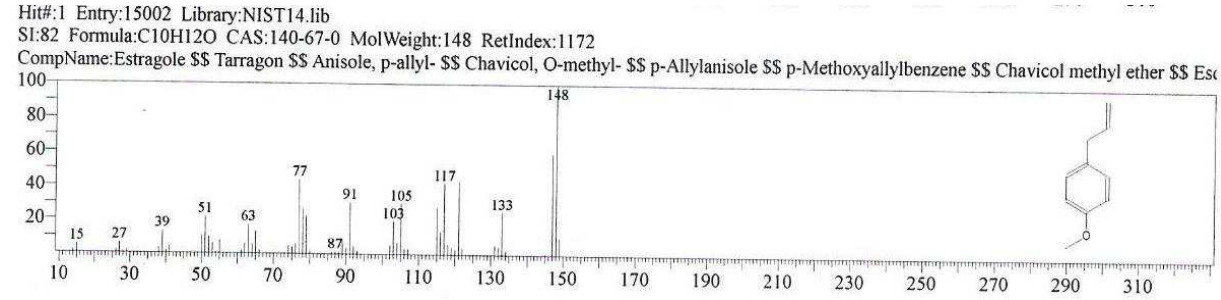

Figure 6. *Mass profile of Peak at R. Time 5.225 min; A GC- MS of peak eluted at R. Time 5.225 min; Tarragon.*

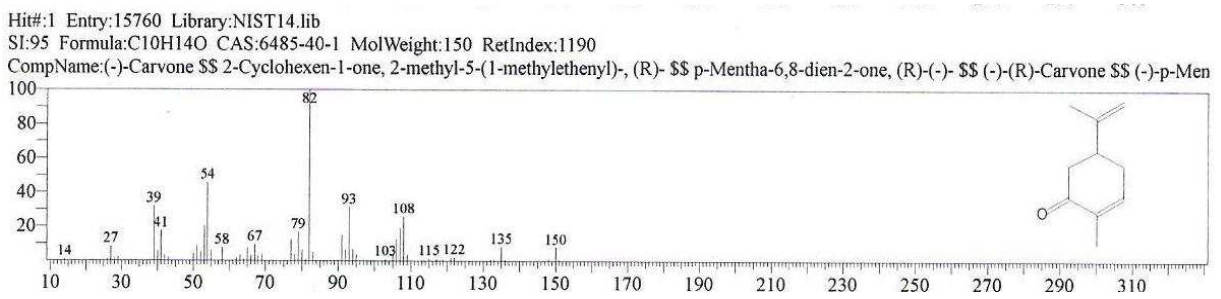

Figure 7. *Mass profile of Peak at R. Time 5.708 min; A GC- MS of peak eluted at R. Time 5.708 min; R-Carvone.*

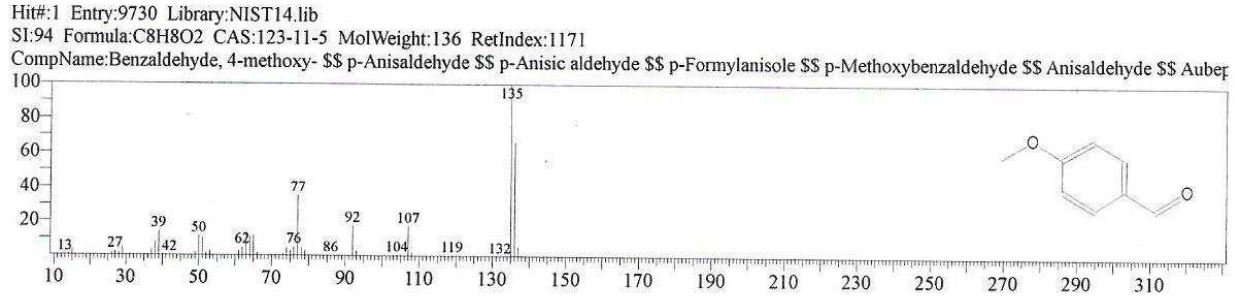

Figure 8. *Mass profile of Peak at R. Time 5.825 min; A GC- MS of peak eluted at R. Time 5.825 min; P-Methoxy benzaldehyde.*

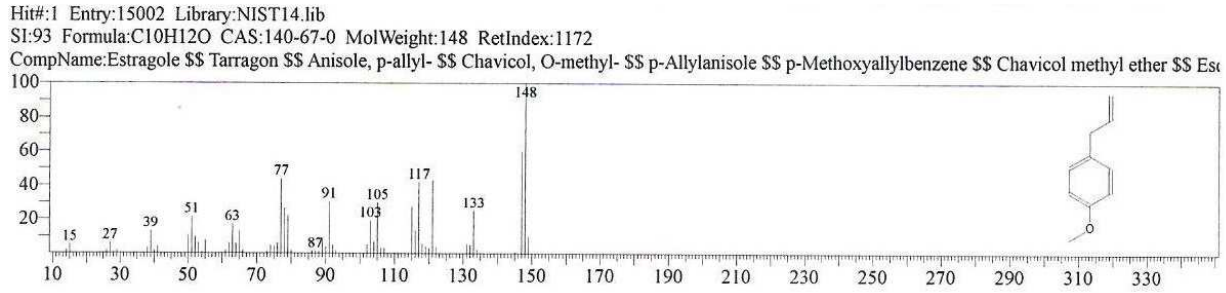

Figure 9. *Mass profile of Peak at Rt 6.108 min; A GC- MS of peak eluted at Rt 6.108 min; P-Methoxy allyl benzene.*

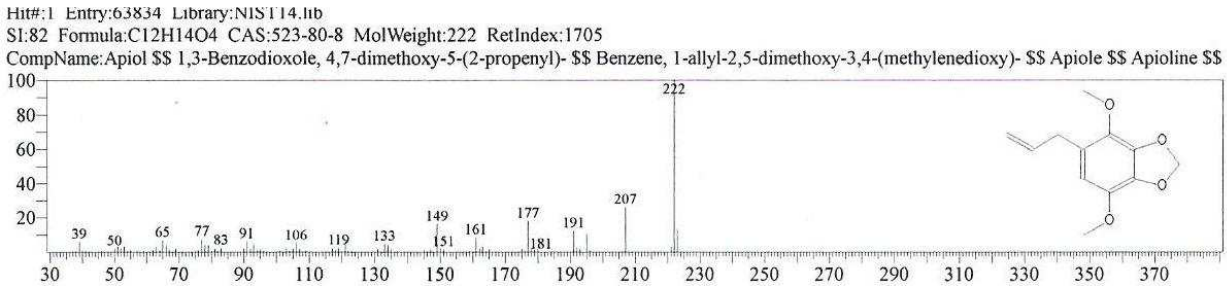

Figure 10. *Mass profile of Peak at R. Time 9.217 min; A GC- MS of peak eluted at R. Time 9.217 min; Apioline.*

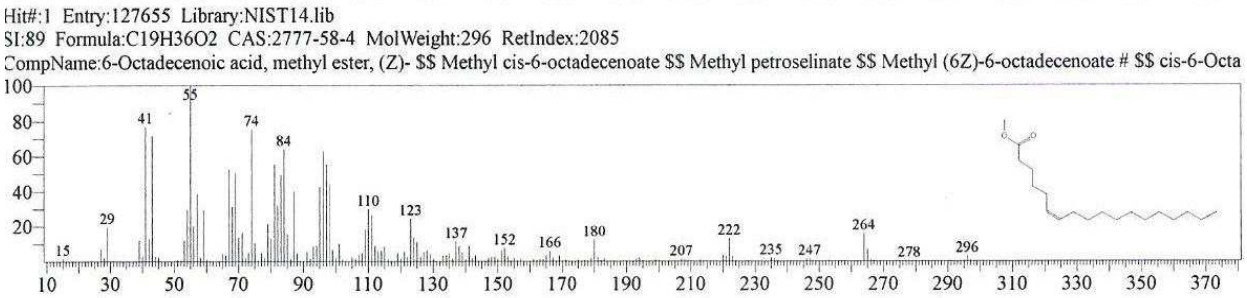

Figure 11. *Mass profile of Peak at R. Time 13.676 min; A GC- MS of peak eluted at R. Time 13.676 min; Methyl petroselinate.*

Table 3. *GC-MS spectral analysis of Caraway (Carum carvi L.), oil.*

Peak no.	R. Time	Compound name	Molecular Formula	Mass	Area	Area%	Height
1.	3.517	1,2-Diisopropenylcyclobutane	$C_{10}H_{16}$	136	14966811	3.99	10901148
2.	4.142	L-Fenchone	$C_{10}H_{16}O$	152	206376292	55.01	122068324
3.	5.225	Tarragon	$C_{10}H_{12}O$	148	15079830	4.02	10449149
4.	5.708	R-Carvone	$C_{10}H_{14}O$	150	9928045	2.65	5971587
5.	5.825	P-Methoxy benzaldehyde	$C_8H_8O_2$	136	71846445	19.15	48773817
6.	6.108	P-Methoxy allyl benzene	$C_{10}H_{12}O$	148	35502972	9.46	23183764
7.	9.217	Apioline	$C_{12}H_{14}O_4$	222	8796641	2.34	4815244
8.	13.767	Methyl petroselinate	$C_{19}H_{36}O_2$	296	12652486	3.37	6113308
					375149522	100.00	232276341

Most drugs bind to appropriate receptor molecules to exert their pharmacological actions, which inherently related chemical structure of that drug. Any changes in the functional groups in a drug molecule can render significant changes in the activity and toxicity. This phenomenon is the basis of any structure–activity-relationship (SAR) study [21]. In the current study various functional groups were observed in the selected plants fractions. These functional groups are most likely responsible for all chemical and biological characteristics of these fractions. The functional group diversity showed in the test leads to many different in biological activity and the Nutritional properties. IR spectrum was a clue in choosing the compounds suggested from the GC-MS library, (compounds with certin functional groups which were not confirmed by FTIR were excluded). No conflict was observed between these spectroscopic techniques.

Results obtained from gas chromatography mass detector showed the presence of high number of active constituents in all tested fractions. This could give a clue to a wide medicinal activity they may possess. The spectrum of petroleum ether oil of *Carum carvi* L. shown in Table (3). A total of eight compounds which found in extracted sample were. L-Fenchone (55.01%), P-Methoxy benzaldehyde (19.15%), P-Methoxy allyl benzene (9.46%), Tarragon (4.02%), 1, 2-Diisopropenylcyclobutane (3.99%), Methyl petroselinate (3.37%), R-Carvone (2.65%), Apioline (2.34%).

In the review; Caraway seeds contain a several components. Thirty chemical has been reported in *C. carvi*, which is 97.58% of the total oil. The major phytochemicals of *C. carvi* essential oil were 37.98% (R)-carvone, 26.55% D-limonene, 5.21% [-pinene, 5.01% cis-carveol and 4.67% -myrcene [23]. The essential oil of *C. carvi* was also characterized by high contents of oxygenated monoterpenes (62.17%), monoterpenes (36.08%) and sesquiterpenes (0.41%), saturated and unsaturated fatty acids, ketones, aldehydes and esters. [22], [17].

The study of the terpene 6 (L-Fenchone) can be a better skin penetration enhancer than other terpenes used in this study to increase the transport of a protein in a transdermal formulation.

4. Conclusion

According to the results obtained in this study, the following general conclusion can be derived

a) Sudanese *Carum carvi* L. seeds are rich sources of oils containing diverse group of phytochemicals.
b) The fixed oil of *Carum carvi* L. btained by soxhlate method was extracted using petroleum ether (60-80) solvent and the yield of oil (4.5%).
c) GC-MS analysis of *Carum carvi* L. revealed the presence of well-known chemical compound in the sample.
d) According to GC-MS, *Carum carvi* L. oil seeds is rich sources of L-Fenchone compound (55.01%) and p-Methoxy benzaldehyde compound (19.15%).

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