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PHYTOCHEMICAL STUDY OF *CALENDULA OFFICINALIS* PLANT BY USED GC-MS AND FTIR TECHNIQUES

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Abstract

The study showed to search the phytochemical compounds of *Calendula officinalis* L. Using GC-MS (Gas chromatography-Mass spectrum) and FTIR (Fourier transform infrared spectrophotometer) techniques. The detection of phytochemical compound depended on peak area, chemical formula, molecular weight, structural formula and RT (min). The results of the FTIR established the occurrence of many numbers of functional groups in flowers. Functional groups were alkyl halides, alcohols, phenols, carboxylic acids, alkanes, and aliphatic amines.

Key words : Calendula officinalis, GC-MS,FTIR, phytochemical.

Introduction

Calendula officinalis is belonging to the family Asteraceae . It is generally well-known as pot marigold, English marigold. It is used as medicinal plant. The flower is yellow or orange colored which are used as food, dye, spice, tea, ointment or cream in cosmetics (Chakraborthy, 2010). The plant is an annual, seldom biennial. It raises to between 30 to 50 cm tall, The root is tap, long (about 20 cm) and many tinny secondary roots. The stem is branched, angular, erect, downy or higher, containing of an epicalyx of abundant narrow-lanceolate sepals, which are tightly covered on both margins with glandular hairs (Tyler, 1994; Parente, *et al.,* 2011).

Chemically *C. officinalis* possesses different biological active components such as terpene, carotenoids, glycoside, flavonoids, saponins, phenolic acids, lipids, etc. Various parts of plant such as leaves, flowers have been described to own therapeutic activity (Muley, *et al.,* 2009). Advanced analytical techniques have been used to separate different chemical components such as isorhamnetin, rutin, quercetin glucoside, which are biologically active as well as used in food and cosmetic industry (Albulescu, *et al.,* 2004).

Gas chromatography–mass spectrometry is an analytical technique which collect the types of mass spectrometry and gas-chromatography to recognize diverse materials inside a test sample. The applications of GC-MS included fire investigation; drug detection; environmental analysis and identification of unidentified samples (David, *et al.,* 2011)

Fourier transform infrared (FTIR) spectroscopy is technique used in chemical investigation (identification of substances). It is based on the measure the vibration of a molecule by IR radiation at a specific range of wavelength within chemical functional groups and generate a spectrum biochemical of the sample (David and Mauer, 2010). The aim of study to detected of phytochemicals in *C. officinalis* by used GC-MS and FTIR techniques.

Materials and Methods

Preparation the plant material

The plant collected from plantation Hilla city, during March to May (2018), the flowers was dried in shade at room temperature. It was grinded and keeped in airtight flask to prevent the humidity effect and then stored at room temperature until further use.

Plant extract preparation

The flowers (dried and powdered) are extract with solvent methanol-water solvent [1:1 V/V] and the phytochemical compound were detected by using GC-MS and FTIR (Ekpenyong, 2012).

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Result and Discussion

GC-MS analysis of methanol- watery extract of flowers of *Calendula officinalis L* revealed the existence of 37 compounds. The name of phytochemical compound,chemical formula, molecular weight,structural formula, and RT(min) were as shown in (table & fig. 1). The spectrum profile of GC-MS revealed the existence of thirty major peaks and the components corresponding to the peaks were determined as follows. The first peak was determined to be Hydroxyacetic Acid Hydrazide at

Table 1: GC-MS analysis of *Calendula officinalis* L. Flowers methanol- watery extract.

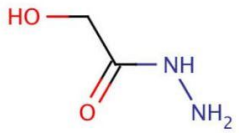
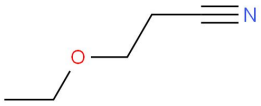
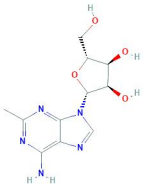
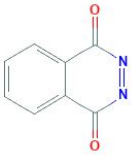
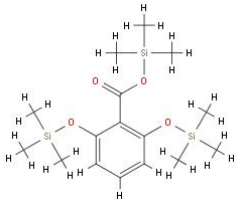
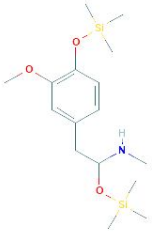
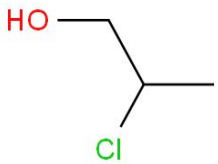
Chemical structure	Molecular Weight g/mol	RT (min)	Area	Chemical Formula	Phytochemical Name	No.
	90.08	9.616	4.89	$C_2H_6N_2O_2$	Hydroxyacetic Acid Hydrazide	1
	99.133	9.616	4.89	C_5H_9NO	3-Ethoxy-propanenitrile	2
	281.272	9.616	4.89	$C_{11}H_{15}N_5O_4$	2-Methyl, Adenosin	3
	160.132	10.331	3.89		Phthalazine-1,4-dione	4
	370.664	10.331	3.89		Benzoicacid, 2,6-bis[(trimethylsilyl) ester	5
	341.598	10.331	3.89	$C_{16}H_{31}NO_3Si_2$	etanephrine bis(trimethylsilyl) ether	6
	94.540	10.979	1.46	C_3H_7	2-Chloro-1-Propanol	8

Table 1 continued ....

Table 1 continued ....

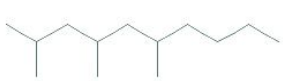
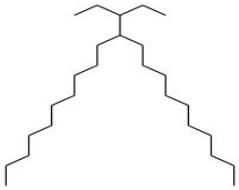
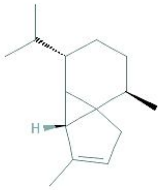
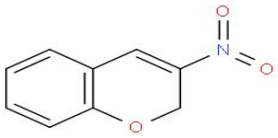
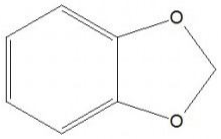
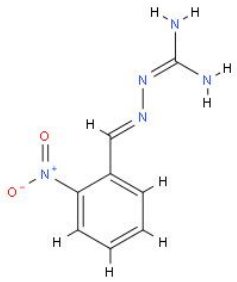
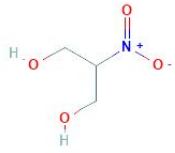
	184.367	16.017	1.12	$C_{13}H_2$	2,4,6-trimethyldecane	9
	172.312	16.017	1.12	$C_{11}H_{24}O$	Hexyl pentyl ether	10
	366.71	16.017	1.12	C26H54	Heneicosane, 11-(1-ethylpropyl)	11
	204.357	17.960	1.77	$C_{15}H_{24}$	Alpha-Cubebene	12
	204.357	19.033	2.33	$C_{15}H_{24}$	beta.-Copaene	13
	177.157	20.648	1.16	$C_9H_7NO_3$	3-Nitro-2H-chromene	14
	122.12	20.648	1.16	$C_7H_6O_2$	2H-benzo[d]1,3 dioxolane	15
	207.189	21.238	1.00	$C_8H_9N_5$	Benzaldehyde, 2-nitro-, diaminomethylid enhydrazone	16
	121.092	21.238	1.00	$C_3H_7NO_4$	2-Nitropropane-1,3-diol	17

Table 1 continued ....

Table 1 continued ....

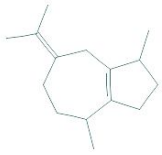
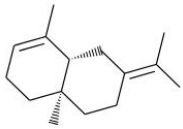
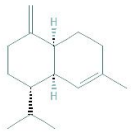
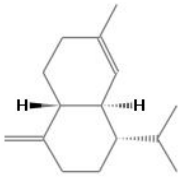
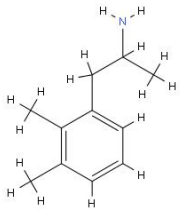
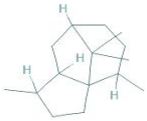
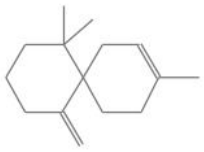
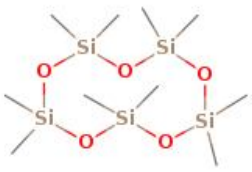
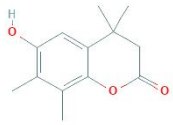
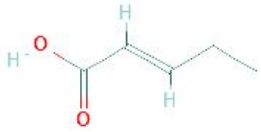
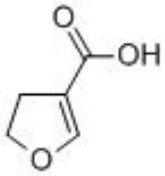
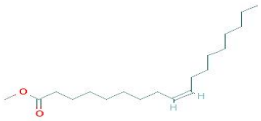
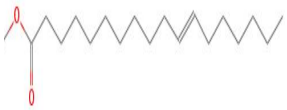
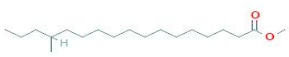
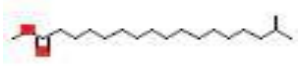
	204.357	21.750	1.47	$C_{15}H_{24}$	Beta-Guaiene	18
	204.35	21.750	1.47	$C_{15}H_{24}$	Selina-3,7(11)-diene	19
	204.357	22.311	4.13	$C_{15}H_{24}$	gamma-Muurolene	20
	204.3511	22.311	4.13	$C_{15}H_{24}$	Naphthalene, 1,2,3,4, 4a, 5,6,8a-octahydro-7-methyl-4-methylene-1-(1-methylethyl)-, (1α,4aβ,8aα)-	21
	204.3511	22.543	3.45	$C_{15}H_{24}$	Naphthalene, 1,2,4a,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-	22
	163.259	25.975	0.99	$C_{11}H_{17}$	2,3-Dimethylamphetamine	23
	206.373	25.975	0.99	$C_{15}H_{26}$	1H-3a,7-Methanoazulene, octahydro-1,4,9,9-tetramethyl-	24
	204.3511	25.975	0.99	$C_{15}H_{24}$	Spiro[5.5]undec-2-ene, 3,7,7-trimethyl-11-methylene-, (-)-	25
	370.7697	26.372	1.17	$C_{10}H_{30}O_5Si_5$	Cyclopentasiloxane, decamethyl-	26

Table 1 continued ....

Table 1 continued ....

	220.268	26.826	2.69	$C_{13}H_{16}O_3$	6-Hydroxy-4, 4,7,8-tetramethyl-3H-chromen-2-one	27
	100.117	28.392	1.27	$C_5H_8O_2$	2-Pentenoic acid	28
	114.1	28.392	1.27	$C_5H_6O_3$	4,5-Dihydro-furan-3-carboxylic acid	29
	270.4507	32.888	28.83	$C_{17}H_{34}O_2$	$C_{17}H_{34}O_2$	30
	270.457	36.330	31.36	$C_{17}H_{34}O_2$	Pentadecanoic acid, 14-methyl-, methyl ester	31
	296.495	36.330	31.36	$C_{19}H_{36}O_2$	Methyl(Z)-9-octadecenoate	32
	296.4879	36.330	31.36	$C_{19}H_{36}O_2$	11-Octadecenoic acid, methyl ester	33
	296.4879	36.330	31.36	$C_{19}H_{36}O_2$	9-Octadecenoic acid, methyl ester, (E)-	34
	298.511	36.804	5.05	$C_{19}H_{38}O_2$	Heptadecanoic acid, 14-methyl-, methyl ester	35
	298.5102	36,804	5.05	$C_{19}H_{38}O_2$	methyl16-methyl heptadecanoate	36
	298.511	36,804	5.05	$C_{19}H_{38}O_2$	Methyl Stearat	37

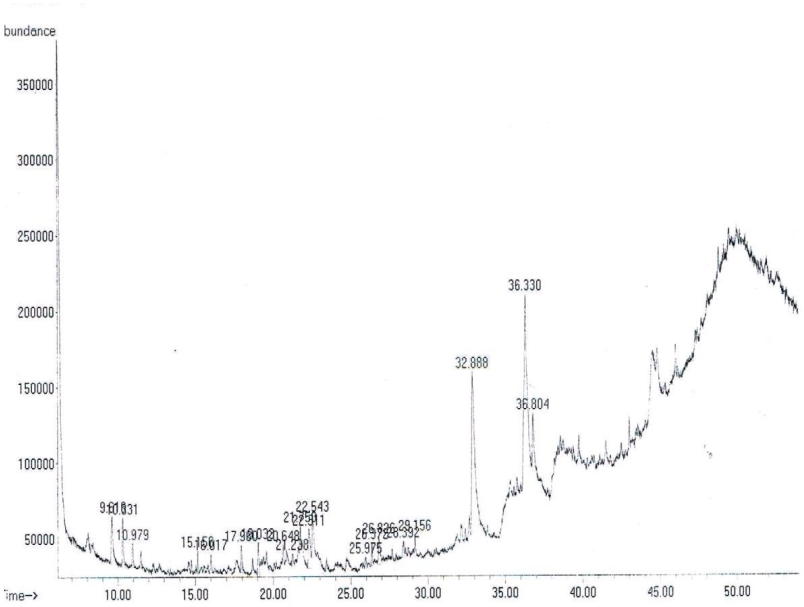


Fig. 1 : GC-MS analysis of *Calendula officinalis* L. Flowers methanol- watery extract

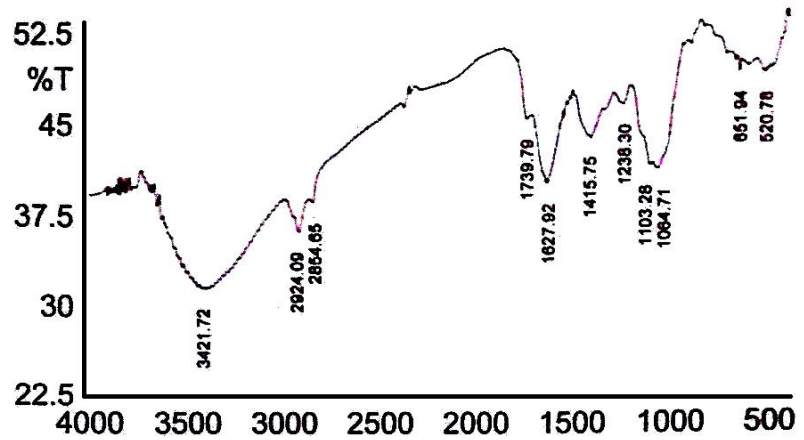


Fig. 2 : FT- IR peak *Calendula officinalis* L. Flowers methanol- watery extract.

Table 2: FT- IR peak *Calendula officinalis* L. Flowers methanol- watery extract.

Peak area	Bond	Functional group
520.78	C-Br stretch	Alkyl halides
651.94	C-Br stretch	Alkyl halides
1064.71	C-N stretch	Aliphatic amin
1103.28	C-N stretch	Aliphatic amin
1238.30	C-H wag (-CH2X)	Alkyl halides
1415.75	C-H bend	Alkanes
1627.92	N-H bend	Amines
1739.79	C=O stretch	Ketones, saturated aliphatic
2854.65	C-H stretch	Alkanes
2924.09	O-H	Carboxylic acid
3421.72	O-H Alkanes , H- bonded	Alcohols , phenols

RT 9.616. The second peaks indicated to be Phthalazine-1,4-dione at RT 10.331 (Fig.1). The next peaks were measured to, Metanephrine bis (trimethylsilyl) ether; 2-Chloro-1Propanol; 2,4,6- trimethyldecane; Hexyl pentyl ether; Alpha-Cubebene; beta.-Copaene 3-; Nitro-2H-chromene; Beta-Guaiene; gamma-Muurolene; Spiro [5.5] undec-2-ene, 3,7,7-trimethyl-11-methylene-(-)- **;** Cyclopentasiloxane, decamethyl-; 6-Hydroxy-4,4,7,8-tetramethyl-3H-chromen-2-one; 2-Pentenoic acid**;** 4,5-Dihydro - furan-3- carboxylic acid; Hexadecanoic acid, methyl ester**;** Pentadecanoic acid, 14-methyl-,methyl ester**;** Methyl(Z)-9-octadecenoate**;**11-Octadecenoic acid, methyl ester**;** 9-Octadecenoic acid, methyl ester, (E)-**;** Heptadecanoic acid, 14-methyl-methyl ester; Methyl16-methylheptadecanoate and Methyl Stearate**.** FT-IR analysis of flowers proved presence of alkyl halides, alcohols phenols, saturated amine and aliphatic amine (Table & Fig. 2) which have property of antimicrobial and antioxidiant.

Conclusion

C. officinalis is a natural plant of Iraq. Thus the GC-MS analysis of flowers methanol-watery extract showed a highly complex profile contain thirty seven components. it contain phytochemicals which may be you useful for many herbal formulation such as antibacterial and antifungal and others.

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