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Research Article

Identification of Bioactive Phytometabolites in Essential Oil of African Marigold (*Tagetes erecta* L.) Using FT-IR & DART-MS Techniques

Sandeep Kumar Rajvanshi[1], Deepa H. Dwivedi[2] and Vikas Kumar[3]

[1]*Department of Agriculture, P.B.R Agriculture Degree College, Gaus Ganj, Hardoi- 241 305, Uttar Pradesh*
[2]*Department of Applied Plant Science (Horticulture), Babasaheb Bhimrao Ambedkar University, Vidya-Vihar Rae Bareli Road, Lucknow- 226 025, Uttar Pradesh*
[3]*Department of Agriculture, Dhampur- 246 761, Bijnor, Uttar Pradesh*

Abstract

Tagetes erecta L. belongs to family Asteraceae, most widely used as ornamental plant, has cosmetic as well as medicines values. Since oil extracted from its plant parts for secondary metabolites present in the plant such as alkaloids, steroids, tannins and phenolic compounds, flavonoids etc. Oil was extracted from flowers, as well as leaves marigold (*Tagetes erecta* L.) in fresh form and after processing by solvent extraction method using n-hexane as solvent. Samples were subjected to Fourier transform infrared spectroscopy (FT-IR) where spectra of samples have shown the presence of major functional groups *viz*., alkanes, aromatic, phenols, aliphatic, nitro compounds and amines, etc at wavelength of 3400 to 3480 cm^{-1} (alcohol & phenols), 2850 to 2990 cm^{-1} (alkanes), 1050 to 1200 cm^{-1} (aliphatic amines) and 720 to 890 cm^{-1} (aromatics). Presence of more number of peaks shows the presence of more number of bioactive compounds. These samples were further validated by DART Mass Spectrometry where peak at *m/z* 136 correspond to terpenoids, 151 (ketone), 169 (phenols), 183 (alcohol) etc. Presence of phenolic compound galic acid in the samples proves the antioxidant activity of the samples.

Keywords: *Bioactive compounds, Solvent extraction, African marigold, Tagetes oil, DART-MS and FT-IR*

Introduction

Tagetes erecta Linn belonging to family Asteraceae which is one of the largest and economically important family of flowering plants (Cronquist,1981), locally known as Gendaphul is a stout, profusely branched flowering herb. Different parts of this plant, including flower, are used in folk medicine to cure various diseases. Since the chief chemical constituents of *Tagetes erecta* are volatile oils, terpenoids and saponins (Lokesh, 2009 and Basavaraj, 2011). Effective therapeutic value occurs by the conbinations of plant metabolites like tannins, flavanoids, resins, gums, steroids, terpenes, and alkaloids etc. which have their own physiological and metabolic actions (Kadam, 2003 and Kiranmai, 2012). The essential oils extracted from leaves, stem, flowers etc. constitutes limonene, ocimene, valeric acid and tagetone which act as antibiotic, antiparasitic, antiseptic, antimicrobial, antispasmodic etc (Ester, 2011 and Mohammad, 2010). The essence or aromas of plants are due to volatile or essential oils, many of which have been valued since antiquity for their characteristic odors. Due to their antimicrobial, insecticidal, antifungal, and antibacterial activities, essential oils have been intensely screened and applied in the fields of pharmacology, medical and clinical micro-biology, phytopathology and food preservation (Daferera. *et al.*, 2000). The leaves of marigold are reported to be effective against piles, kidney troubles, muscular pain, ulcers, wound and earache.

***Corresponding Author:**
Sandeep Kumar Rajvanshi;
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Solvent extraction is a traditional method used for the isolation of metabolites from plant material. Analytes with medium to low volatility, effective for the aroma and quality of oil extracted from the plant material are extracted with this technique (Agarwal. *et al.,* 2012), which can be identified with the help of FTIR and further elucidated using DART-MS. Fourier Transform Infrared spectroscopy (FT-IR) is a high-resolution analytical technique to identify the chemical constituents and elucidate the structural compounds (Hussain. *et al.,* 2007).

The present study was planned with the hypothesis that generally *Tagetes minuta* (wild marigold) is used for extraction of oil and to study their phytochemicals but now a day's African marigold (*Tagetes erecta* L.) is a very important flower commonly grown as loose flower for use for religious purposes and for decoration in marriages. However, post harvest processing of Marigold for its oil, extracted from its flower as well as its plant parts may enhance value of the crop multifold since it is reported to be a rich source of biocolour, pigments and bioactive molecules which may be exploited in the food and pharmaceutical industry. Therefore this study was planned with the objective to identify the phytochemical properties of the essential oil extracted from *Tagetes erecta* L. a species commonly cultivated commercially for its ornamental rather than therapeutic applications.

Materials and Methods

Collection of Samples

Leaf and flower were collected from African marigold (*Tagetes erecta* L.) at full bloom stage from Horticulture Research Farm of the Department of Applied Plant Science (Horticulture), Babasaheb Bhimrao Ambedkar University, Lucknow, Uttar Pradesh in the early morning hours and 100g each flowers and leaf were used for further experiments. Additionally Fresh samples of both the flower and leaf was processed for 72 hours by air drying and stored in air tight containers for further study.

Solvent Extraction by Soxhlet Apparatus

100 g each of fresh and dry samples of both the flower and leaves of African marigold (*Tagetes erecta* L.) were subjected to solvent extraction for 3-4 hours at temperature 40-60^{0}C with the help of non- polar solvent n-hexane. The oil extracted was stored in small sealed tubes at low temperature for preliminary phytochemical screening through FT-IR and further elucidation through DART-MS analysis**.**

Preliminary Screening of Oil for Presence of Phytochemical Groups

The samples were tested for several phytochemicals using standard procedures (Mostafavi and Pezhhanfar, 2015) to identify the phytochemical groups present in the sample.

Identification of Phytometabolites by Fourier Transform Infrared Spectroscopy

This was subjected to further confirmation of presence of functional groups showing bioactivity in plant samples. Palettisation of extracted oil was done using KBr and was screened in Fourier transform infrared (FT-IR) spectroscope (Nicolet TM 6700, Thermo scientific: USA) over a range of wavelength from 400 to 4000 cm^{-1}, in University Scientific Instrumentation Centre, Babasaheb Bhimrao Ambedkar University, Vidya Vihar, Rae Bareli Road, Lucknow (U.P.) India. FT-IR spectroscopy was used to identify various types of chemical bonds in a molecule by producing an infrared absorption spectrum. The IR spectra were reported as % transmittance. The functional groups were determined by comparing the vibration frequencies in wave numbers of the sample spectrograph from library of the system and previous literature related to FT-IR studies.

Direct Analysis in Real Time (DART) Mass Spectrometry

Once the identification of presence of functional group present in the sample was performed by using FT-IR then further identification of particular compound present in the sample was tested by using the DART-MS. It was recorded on a JEOL AccuTOF LMS-T100LC Mass spectrometer having a

DART (Direct Analysis in Real Time) source. Samples were

Subjected as such in front of DART source. Dry Helium gas was used with 4 LPM flow rate for ionization at 350^{0}C. Data acquisition was from m/z 50.0 to 200.0. The orifice 1 was set at 28 V and spectra were collected. The compound of the oil was identified by comparison of their m/z value with those of a computer library and with data published in the literature.

Results and Discussion

The samples tested positive for the presence of terpenoids, flavonoids, alkaloids and coumarins. Negative results were found for the steroids, glycosides and saponins. (Table I)., The identification of the above compounds supports the use of these oils in traditional medicine as these compounds have valuable antifungal, antibacterial and anti-inflammatory properties (Hassanshshian. *et al.,* 2014; Gilani. *et al.,* 2005).

The FT-IR spectrum was used to identify and detect the characteristic peaks and functional groups of the active components based on the peak value in the region of infrared radiation. The results revealed the presence of different phytochemicals which are formed during the plants normal metabolic processes. (Fig 1 A, B, C and D). The bonds and the wave number (cm^{-1}) of prominent peaks obtained from spectra are elucidating in Table 2.

The extracts were subjected to FT-IR analysis and the functional groups of the components were separated based on their peak ratios. The results confirmed the presence of shows the presence of (O-H stretch) alcohol and phenol, (C-H) aromatic, (C-N) aliphatic amines, (C-H rock alkane, (N-H stretch) amides, (H-C=O: C-H Stretch) aldehydes,(N-O stretch) nitro compounds, (C=O) α, β-unsaturated aldehydes, ketones, (C-O stretch) carboxylic acid, which showed major peaks in fresh flower soxhlet extract (FFSE) sample at 3925.4cm^{-1}, 3869.3cm^{-1}, 3824.1cm^{-1}, 3752.3cm^{-1}, 3430.8cm^{-1}, 3009.5cm^{-1}, 2920.4cm^{-1}, 2852.1cm^{-1}, 2363.2cm^{-1}, 2037.2cm^{-1}, 1739.0cm^{-1}, 1715.2cm^{-1}, 1652.0cm^{-1}, 1545.7cm^{-1}, 1461.3cm^{-1}, 1377.3cm^{-1}, 1243.1cm^{-1}, 1167.1cm^{-1}. 1095.4cm^{-1}, 840.3cm^{-1}, 722.9cm^{-1}.and 582.4cm^{-1}. This was also observed in contrast to the study of (Rajvanshi. *et al.,* 2017).

The dry flower Soxhlet extract (DFSE) sample which shows the existence of 16 peaks primarily at the frequency 2957.9cm^{-1}, 2923.8cm^{-1}, 2862.7cm^{-1}, 2733.4cm^{-1}, 2674.1cm^{-1}, 1461.7cm^{-1}, 1379.2cm^{-1}, 1342.6cm^{-1}, 1296.8cm^{-1}, 1247.5cm^{-1}, 1135.8cm^{-1}, 1060.9cm^{-1}, 887.3 cm^{-1}, 797.8cm^{-1} 758.2cm^{-1} and 724.5cm^{-1}. The peak at 2957.9cm^{-1}, 2923.8cm^{-1}, 2862.7cm^{-1}, 1461.7cm^{-1}, 1379.2cm^{-1} and 724.5cm^{-1}. Depending on the fingerprint characters of the peaks positions, shape and intensities, the fundamental components may be identified (Chen. *et al*., 2001).

In Dry leaf Soxhlet extract (DLSE) sample total 14 peaks was obtained which was 3471.1cm^{-1}, 3009.8cm^{-1}, 2921.0cm^{-1}, 2852.7cm^{-1}, 2396.4cm^{-1}, 1735.2cm^{-1}, 1635.0cm^{-1}, 1458.5cm^{-1}, 1366.8cm^{-1}, 1231.5cm^{-1}, 1093.7cm^{-1}, 835.4cm^{-1} 728.7cm^{-1} and 592.9cm^{-1}.

The minimum number of peaks was obtained in the fresh flower Soxhlet extract sample (FFSE) which shows peaks 3458.2cm^{-1}, 2923.6cm^{-1} ,2853.8cm^{-1}, 1734.4cm^{-1}, 1461.9cm^{-1}, 1374.3cm^{-1}, 1245.6cm^{-1}, 1174.7cm^{-1}, 1112.5cm^{-1}, 980.1cm^{-1} and 724.1cm^{-1}.. Biochemical screening of *Tagetes patula* and *Tagetes erecta* leaf and flower extracts have indicated the presence of alkaloids, flavonoids, steroids, tannins and phenolic compounds as the major secondary metabolites. Many of these compounds have been reported to have various bioactive properties on living organisms including bacteristatic or bactericidal action (Barnabas. *et al*., 1988; Harborne. *et al*., 1988).

The phytometabolites component present in solvent extracted essential oil from various samples of African marigold was subjected to DART-MS and correlates the results obtained by FTIR spectroscopy. A representative DART-MS spectrogram and various constituent phytometabolites of samples were given in Fig: 2 A, B, C and D & Table 3, 4, 5 and 6. The constituents were identified by matching their mass spectra with those recorded in literature.

In fresh flower soxhlet extract (FFSE) sample, the peak at *m/z* 114.11 could be due to n-Heptanal or 2-Heptanone having relative intensity (R.I % 1.8), the peak at *m/z* 123.14 best match with the compound p-Methylanisol, 4-Ethylphenol (R.I % 1.8).The peak at *m/z* 135.14 could be due to terpinolene, thujene, sabinene, α-terpinolene, α pinene, β-ocimene, limonene (R.I % 2.3). However, they have the same molecular formula; a distinction could not be easily made.). Besides this, the peak of other terpenes was observed at *m/z*, 139.17, 149.11, and 151.13 corresponding to Tran-pinane, Cis pinane (R.I % 1.6), Piperitenone, Ocimenone, umbellulone, verbenone (R.I % 6.2) and, tagetone (R.I % 40.8) respectively. The peak at *m/z*, 153.19 could be due to Linalool, fenchol, Terpinen-4-ol (R.I % 7.4). The peak at *m/z* 165.11 was best match with the compound Furomyrcenol (R.I % 2.5). The peak at *m/z* 167.12 could be due to Trans Dihydrocarvone epoxide, a-Campholenic acid (R.I % 6.1). Besides this, the peak of observed at *m/z*, 169.15, 173.18 , and 180.20 corresponding to Galic acid (R.I % 2.5), Trans Linalool oxide (furanoid), 3,7-Dimethyl-3,7-dihydroxyoct-1-ene (R.I % 0.4) and TransPinocarvyl formate (R.I % 0.3) respectively. The peak at *m/z*, 183.12 could be due to annitol (R.I % 4). The peak at *m/z* 185.14 best match with the compound 3,4-Dihydroxy-5-methoxybenzoic acid (R.I % 0.3) and the peak at *m/z* 201.18 best match with the compound Aromadendra1- (10),4(15)-diene (R.I % 2.0).

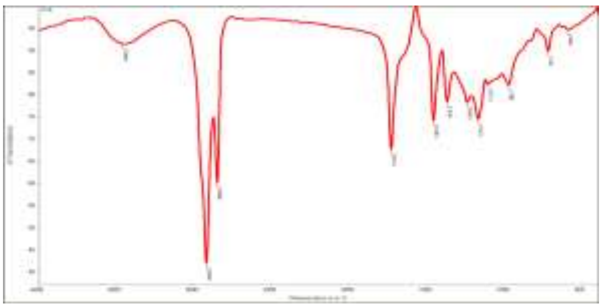
In dry flower soxhlet extract (DFSE) sample, the peak at *m/z* 114.11 could be due to n-Heptanal or 2 Heptanone having relative intensity (R.I % 5.8), the peak at *m/z* 123.14 best match with the compound p-Methylanisol, 4-Ethylphenol (R.I % 3.7). The peak at *m/z* 135.14 could be due to Terpinolene, Thujene, sabinene, α-terpinolene, α pinene, β-ocimene, limonene (R.I % 3.8). Besides this, the peak observed at *m/z*, 139.17 , 149.12, and 151.13 corresponding to Tran-pinane, Cis pinnae (R.I % 2.2), Piperitenone, Ocimenone, umbellulone, verbenone (R.I % 7.9) and tagetone (R.I % 52) respectively. The peak at *m/z*, 153.15 could be due to Linalool, fenchol, Terpinen-4-ol (R.I % 14). The peak at *m/z* 165.12 was best match with the compound Furomyrcenol (R.I % 4.3). The peak at *m/z* 167.13 could be due to Trans Dihydrocarvone epoxide, a-Campholenic acid (R.I % 12). Besides this, the peak of observed at *m/z*, 169.15 and 180.13 corresponding to Galic acid (R.I % 6), and TransPinocarvyl formate (R.I % 0.3) respectively. The peak at *m/z*, 183.12 could be due to annitol (R.I % 7.9). The peak at *m/z* 185.15 best match with the compound 3,4-Dihydroxy-5-methoxybenzoic acid (R.I % 0.3) .The peak at *m/z* 193.18 and201.19 was best match with the compound Trans sabinyl acetate (R.I % 0.3) and 6-ethoxy-2,4-dimethylquinoline (RI % 2.4).

In fresh leaves soxhlet extract (FLSE) sample, the major peaks with higher relative intensity at *m/z* 173 which could be due to Trans Linalool oxide (furanoid), having relative intensity (R.I % 3.5), the peak at *m/z* 218.25 best match with the compound Hydroxytremetone (R.I % 12.5). The peak at *m/z* 246.26 could be due to Avocadynofuran, Amberone (R.I % 11). Besides this, the peak observed at *m/z*, 262.28, 274.32, and 302.36 corresponding to 4b-Acetoxygymnomitr3 (15)-ene (R.I % 10), 2-Acetoxyfuranoelemene (R.I % 97.5) and (Z)-Nuciferyl 2-methylbutyrate (R.I % 32) respectively. The peak at *m/z*, 318.34 could be due to flavonoid compound Quercetagetin (R.I % 95). The peak at *m/z* 319.34 was best match with the compound 4b, 5b-Diacetoxygymnomitr-3(15)-ene (R.I % 20). The peak at *m/z* 346.37 could be due to 11-b-Hydroxykauren-15yl- acetate (R.I % 30). Besides this, the peak of observed at *m/z*, 362.38 and 374.42 corresponding to catalpol (R.I % 33.5), and Geniposidic acid (R.I % 14) respectively. The peak at *m/z*, 418.43 could be due to Kaempferol-3-O-α-L-arabinoside (R.I % 3.5). The peak at *m/z* 429.42 was best match with the compound 37β-hydroxysitosterol R.I % 6.0).

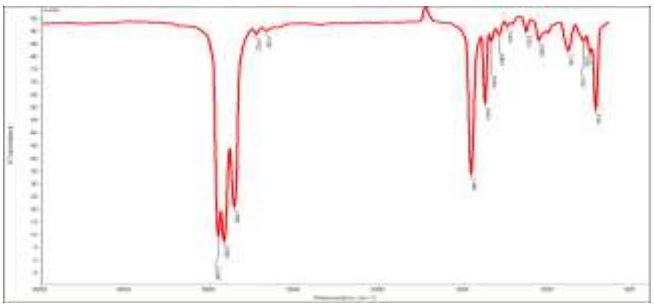
In dry leaves soxhlet extract (DLSE) sample, the major peaks with higher relative intensity at *m/z* 114.11 which could be due to 2-Heptanone having relative intensity (R.I % 3.0), the peak at *m/z* 136.04 best match with the Terpinolene, thujene, sabinene, α-terpinolene, α pinene, β-ocimene, limonene (R.I % 8.0). The peak at *m/z* 143.12 could be due to 2, 3, 5-Trimethylvalerolactone (R.I % 2.1). Besides this, the peak observed at *m/z*, 151.14 , 157.11 , and 169.16 corresponding to piperonal, verbenone, thymol, carvone, carvacrol_ (R.I % 3.4), Menthol, Dihydro-linalool (R.I % 6.0) and Galic acid (R.I % 3.4) respectively. The peak at *m/z*, 173.13 could be due to Trans Linalool oxide (furanoid), (R.I % 4.1). The peak at *m/z* 183.12 was best match with the compound manifold (R.I % 3.4). The peak at *m/z* 190.17 could be due to 8, 9-Dehydrothymol acetate (R.I % 8.5). Besides this, the peak of observed at *m/z*, 193.16 and 197.15 corresponding to Trans Sabinyl acetate (R.I % 2.5), and Lavandulyl acetate (R.I % 4.5) respectively. The peak at *m/z*, 218.25 could be due to lemnalone or taylorione (R.I % 15.0). The peak at *m/z* 225.18 was best match with the compound g-Tetradecanolide R.I % 3.4).

Table 1: Preliminary phytochemical screening of various samples of essential oil of *Tagetes erecta* L. extracted by solvent extraction method

Phytochemical Tests	Fresh Flower	Observation	Dry Flower	Observation	Fresh Leaf	Observation	Dry Leaf	Observation
Terpinoids	+	Red brown color	+	Red brown color	+	Red brown color	+	Red brown color
Steroids	-	No Change	-	No Change	-	No Change	-	No Change
Flavonoid	+	Yellow colour	+	Yellow colour	+	Yellow colour	+	Yellow colour
Alkaloid	+	Green colour	+	Green colour	+	Green colour	+	Green colour
Quinones	+	Red colour	+	Red colour	-	No Change	+	Red colour
Glycosides	-	No Change	-	No Change	-	No Change	-	No Change
Phenols	+	Green colour	+	Green colour	-	No Change	-	No Change
Triterpinoids	-	No Change	+	Blue green colour	-	No Change	-	No Change
Coumanins	+	Yellow colour	+	Yellow colour	+	Yellow colour	+	Yellow colour
Tannin	-	No Change	+	Blue colour	-	No Change	-	No Change
Saponin	--	No Change	-	No Change	-	No Change	-	No Change



(A)



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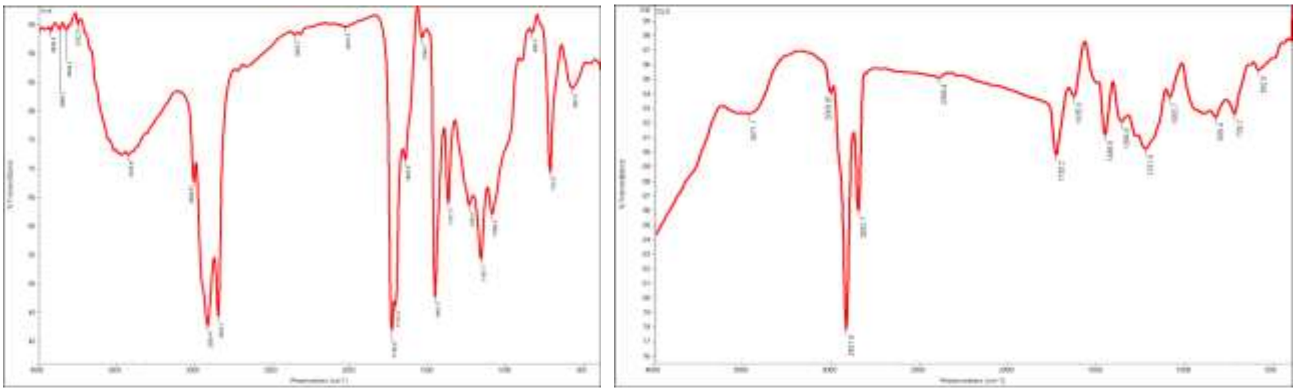


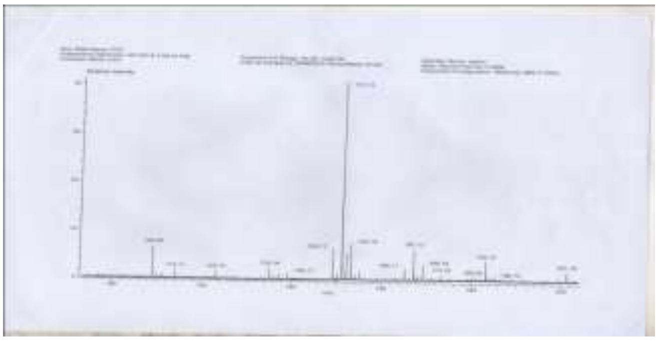
(C) (D)

Fig 1: FT-IR Transmittance spectrum of solvent extracted essential oil from fresh flowers (A) and dry flowers (B) fresh leaves (C) and dry leaves (D) of African marigold (*Tagetes erecta* L.)

Table 2: FTIR analysis of solvent extracted essential oil of various samples from African marigold (*Tagetes erecta* L.)

S. No.	Frequency (Cm^{-1})	Fresh Flower	Dry Flower	Fresh Leave	Dry Leave	Bond	Functional Group
1.	3480-3400	3458.2	-	3430.8	3471.1	O-H stretch	alcohols, phenols
2.	3390-3300	-	-	-	-	N-H Stretch	1*, 2* amines, amides
3.	2990-2950	-	2957.9	-	-	C-H Stretch	alkanes
4.	3050-3000	-	-	3009.5	3009.8	=C-H stretch	aromatic
5.	2950-2900	2923.6	2923.8	2920.4	2921.0	C-H Stretch	alkanes
6.	2880-2850	2853.8	2862.7	2852.1	2852.7	C-H Stretch	alkanes
7.	2750-2700	-	2733.4	-	-	H-C=O: C-H Stretch	aldehydes
8.	2690-2650	-	2674.1	-	-	H-C=O: C-H Stretch	aldehydes
9.	2400-2350	-	-	2363.2	2396.4	-	-
10.	2050-2000		-	2037.2		-	-
11.	1750-1700	1734.4	-	1739.0 1715.2	1735.2	C=O Stretch	α, β- unsaturated aldehydes, ketones
12.	1690-1650	-	-	1652.0	-	C=O Stretch	Carbonyls (general)
13.	1650-1600	-	-	-	1635.0	N-H Bend	1* amines
14.	1550-1500	-	-	1545.7	-	N-O asymmetric stretch	Nitro compounds
15.	1490-1450	1461.9	1461.7	1461.3	1458.5	C-H bend	alkanes
16.	1390-1350	1374.3	1379.2	1377.3	1366.8	C-H rock	alkanes
17.	1350-1300	-	1342.6		-	N-O Symmetric stretch	Nitro compounds
18.	1300-1250	-	1296.8		-	C-O Stretch	carboxylic acid
19.	1250-1200	1245.6	1247.5	1243.1	1231.5	C-O stretch	carboxylic acid
20.	1200-1150	1174.7	1135.8	1167.1	-	C-N Stretch	Aliphatic amines
21.	1150-1050	1112.5	1060.9	1095.4	1093.7	C-N Stretch	Aliphatic amines
22.	1050-900	980.1	-	-	-	C-N Stretch	Aliphatic amines
23.	890-850	-	887.3	840.3	-	C-H "oop"	aromatic
24.	850-800	-	-	-	835.4	C-H Bend	aromatic

						(para)	
25.	800-760	-	797.8	-		C-H "oop"	aromatic
26.	760-720	-	758.2	722.9	728.7	C-H Bend (ortho)	aromatics
27.	720-700	724.1	724.5	-	-	C-H rock	alkanes
28.	600-550	-	-	582.4	592.9	C-Br stretch	Alkyl halides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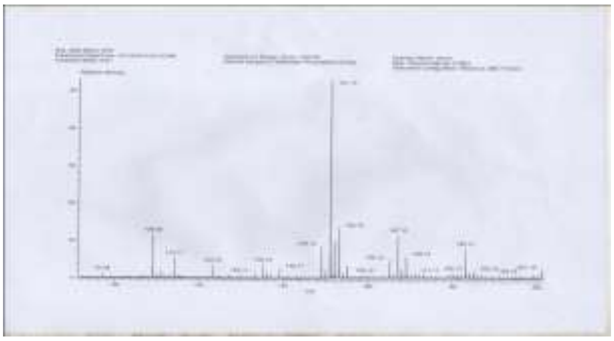
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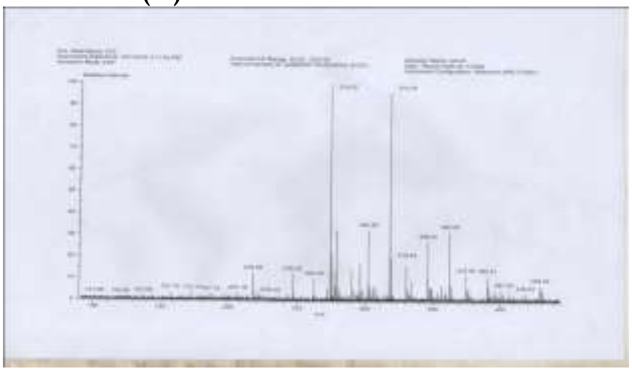
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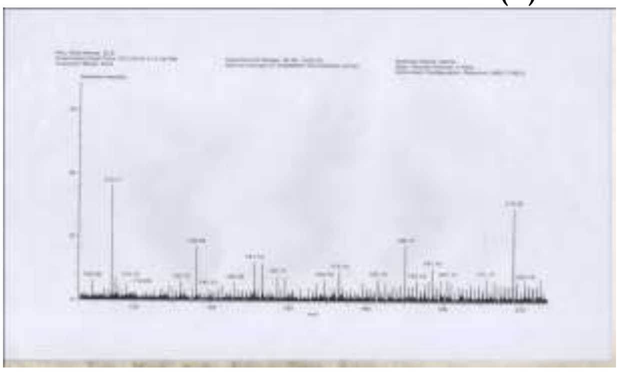
(D)

Fig 2: DART-MS of solvent extracted essential oil from fresh flowers (A) and dry flowers (B) fresh leaves (C) and dry leaves (D) of African marigold (*Tagetes erecta* L.)

Table 3: Exact mass data from the DART–MS of soxhlet extracted essential oil from fresh flowers of African marigold (*Tagetes erecta* L.)

S. No.	Molecular Weight	Measured Mass	Molicular Formula	Relative Intensity (%)	Remarks
1.	109	109.08	-	6.3	-
2.	114	114.11	$C_7H_{14}O$	1.8	n-Heptanal, 2Heptanone
3.	123	123.14	$C_8H_{10}O$	1.8	p-Methylanisol, 4-Ethylphenol
4.	135	135.14	$C_{10}H_{16}$	2.3	Terpinolene, Thujene, sabinene, α-terpinolene, α pinene, β-ocimene, limonene
6.	139	139.17	$C_{10}H_{18}$	1.6	Tran-pinane, Cis pinane
7.	149	149.11	$C_{10}H_{14}O$	6.2	Piperitenone, Ocimenone, umbellulone,verbenone
8.	151	151.13	$C_{10}H_{18}0$	40.8	Tagetone
9.	153	153.19	$C_{10}H_{18}O$	7.4	Linalool, fenchol, Terpinen-4-ol
10.	165	165.11	$C_{10}H_{14}O_2$	2.5	Furomyrcenol
11.	167	167.12	$C_{10}H_{16}O_2$	6.1	Trans Dihydrocarvone epoxide, a-Campholenic acid
12.	169	169.15	$C_7H_6O_5$	2.5	Galic acid

13.	173	173.18	$C_{10}H_{20}O_2$	0.4	Trans Linalooloxide (furanoid), 3,7-Dimethyl-3,7-dihydroxyoct-1-ene
14.	180	180.20	$C_{11}H_{16}O_2$	0.3	TransPinocarvyl formate
15.	183	183.12	$C_6H_{14}O_6$	4.0	Mannitol
16.	185	185.14	$C_8H_8O_5$	0.3	3,4-Dihydroxy-5-methoxybenzoic acid
17	201	201.18	$C_{15}H_{22}$	2.0	Aromadendra1- (10),4(15)-diene

Table 4: Exact mass data from the DART –MS of soxhlet extracted essential oil from dry flowers of African marigold (*Tagetes erecta* L.)

S. No.	Molecular Weight	Measured Mass	Molicular Formula	Relative Intensity (%)	Remarks
1.	97	97.08	-	0.5	-
2.	109	109.08	-	11.8	-
3.	114	114.11	$C_7H_{14}O$	5.8	2-Heptanone
4.	123	123.14	$C_8H_{10}O$	3.7	p-Methylanisol, 4-Ethylphenol
6.	133	133.11	-	0.3	-
7.	135	135.14	$C_{10}H_{16}$	3.8	Terpinolene, Thujene, sabinene, α-terpinolene, α pinene, β-ocimene, limonene
8.	139	139.17	$C_{10}H_{18}$	2.2	Tran-pinane, Cis pinane
9.	149	149.12	$C_{10}H_{14}O$	7.9	Piperitenone, Ocimenone, umbellulone
10.	151	151.13	$C_{10}H_{14}0$	52.0	Tagetone
11.	153	153.15	$C_{10}H_{18}O$	14.0	Linalool, fenchol, Terpinen-4-ol
12.	159	159.14	$C_{10}H_{22}O$	0.3	1-Decanol
13.	165	165.12	$C_{10}H_{14}O_2$	4.3	Furomyrcenol
14.	167	167.13	$C_{10}H_{16}O_2$	12.0	Trans Dihydrocarvone epoxide, a-Campholenic acid
15.	169	169.15	$C_7H_6O_5$	6.0	Galic acid
16.	171	171.17	-	0.2	-
17.	180	180.13	$C_{11}H_{16}O_2$	0.3	TransPinocarvyl formate
18.	183	183.13	$C_6H_{14}O_6$	7.9	Mannitol
19.	185	185.15	$C_8H_8O_5$	0.3	3,4-Dihydroxy-5-methoxybenzoic acid
20.	193	193.18	$C_{12}H_{16}O_2$	0.3	Trans Sabinyl acetate
21.	201	201.19	$C_{13}H_{15}NO$	2.4	6-ethoxy-2,4-dimethylquinoline

Table 5: Exact mass data from the DART –MS of soxhlet extracted essential oil from fresh leaves of African marigold (*Tagetes erecta* L.)

S. No.	Molecular Weight	Measured Mass	Molicular Formula	Relative Intensity (%)	Remarks
1.	101	101.08	$C_6H_{12}O$	1.0	Hex-5-en-1-ol, Hex-5-en-3-ol, (Z)-Hex-3-en-1-ol
2.	120	120.08	C_8H_8O	1.0	Phenylacetaldehyde
3.	137	137.09	$C_8H_{10}O_2$	1.0	2-Methyl5propionylfuran, 1,3Dimethoxybenzene
4.	157	157.15	$C_{10}H_{20}O$	3.5	Dihydrolinalool

6.	173	173.14	$C_{10}H_{20}O_2$	3.5	Trans Linalooloxide (furanoid), 3,7-Dimethyl-3,7-dihydroxyoct-1-ene
7.	187	187.14	$C_{11}H_{22}O_2$	2.0	Methyl decanoate. n-Heptyl butanoate
8.	207	207.19	$C_{13}H_{20}O_2$	3.0	Trans and Cis Carvyl propionate
9.	218	218.25	$C_{15}H_{24}O_3$	12.5	Hydroxytremetone
10.	219	219.24	$C_{15}H_{24}O$	1.0	Caryophyllene oxide, Spathulenol
11.	246	246.26	$C_{17}H_{26}O$	11	Avocadynofuran, Amberone
12.	262	262.28	$C_{17}H_{26}O_2$	10	4b-Acetoxygymnomitr3(15)-ene
13.	274	274.32	$C_{17}H_{22}O_3$	97.5	2-Acetoxyfuranoelemene
14.	302	302.36	$C_{20}H_{30}O_2$	32	(Z)-Nuciferyl 2-methylbutyrate
15.	318	318.34	$C_{15}H_{10}$	95	Quercetagetin
16.	319	319.34	$C_{19}H_{28}O_4$	20	4b,5b-Diacetoxygymnomitr-3(15)-ene
17.	346	346.37	$C_{22}H_{34}O_3$	30	11-b-Hydroxykauren-15-a-yl-acetate
18.	362	362.38	$C_{15}H_{22}O_{10}$	33.5	Catalpol
19.	374	374.42	$C_{16}H_{22}O_{10}$	14	Geniposidic acid
20.	390	390.41	$C_{17}H_{26}O_{10}$	13	Loganin
21.	391	391.33	$C_{24}H_{25}NO_4$	5.0	Flavoxate
22.	418	418.43	$C_{20}H_{18}$	3.5	Kaempferol-3-O-α-L-arabinoside
23.	429	429.42	$C_{29}H_{50}O_2$	6.0	7β-hydroxysitosterol

Table 6: Exact mass data from the DART –MS of soxhlet extracted essential oil from dry leaves of African marigold (*Tagetes erecta* L.)

S. No.	Molecular Weight	Measured Mass	Molicular Formula	Relative Intensity (%)	Remarks
1.	109	109.08	C_7H8_O	18	o-Cresol
2.	114	114.11	$C_7H_{14}O$	3.0	2-Heptanone
3.	115	115.10	$C_7H_{16}O$	3.2	2-Heptanol, 3-Heptanol
4.	118	118.09	C_8H_7N	2.2	Indole
6.	132	132.12	$C_6H_{12}O_3$	2.4	Methyl 2-hydroxyisopentanoate
7.	136	136.04	$C_{10}H_{16}$	8.0	Terpinolene, Thujene, sabinene, α-terpinolene, α pinene, β-ocimene, limonene
8.	143	143.12	$C_8H_{14}O_2$	2.1	2,3,5-Trimethylvalerolactone
9.	146	146.09	$C_{11}H_{14}$	3.0	Desmarestene
10.	151	151.14	$C_{10}H_{14}0$	3.4	, verbenone, thymol, carvone, carvacrol_
11.	157	157.11	$C_{10}H_{20}O$	6.0	Menthol, Dihydrolinalool
12.	169	169.16	$C_7H_6O_5$	3.4	Galic acid
13.	173	173.13	$C_{10}H_{20}O_2$	4.1	Trans Linalooloxide (furanoid), 3,7-Dimethyl-3,7-dihydroxyoct-1-ene
14.	183	183.12	$C_6H_{14}O_6$	3.4	Mannitol
15.	190	190.17	$C_{12}H_{14}O_2$	8.5	8,9-Dehydrothymol acetate

16.	193	193.16	$C_{12}H_{16}O_2$	2.5	Trans Sabinyl acetate
17.	197	197.15	$C_{12}H_{20}O_5$	4.5	Lavandulyl acetate
18.	201	201.17	$C_{13}H_{15}NO$	4.0	6-ethoxy-2,4-dimethylquinoline
19.	211	211.17	$C_{12}H_{20}O_3$	4.0	5-Acetoxylinalool,
20.	218	218.25	$C_{15}H_{22}O$	15.0	Lemnalone, Taylorione
21.	225	225.18	$C_{14}H_{26}O_2$	3.4	g-Tetradecanolide

Conclusion

The present study concludes that the phytochemical screening of the *Tagetes erecta* proved to contain flavonoid, terpenoids, alkaloid, quinones, phenols and coumarins bioactive compounds which are of medicinal value and have a definite physiological action on the human body. The oil extracted from the fresh leaves from *Tagetes erecta* L. by Soxhlet apparatus shows the more bioactive compounds compare to other samples. It shows that the plant *T. erecta* is an important source of many pharmacologically and medicinally important phyto-constituents. There is huge scope for research; the plant could be further exploited in future as a source of useful phyto-chemical compound for the pharma industry.

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