GC-MS Analysis of Bioactive Compounds Extracted from *Lantana camara* Linn.

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ABSTRACT

The phytochemical compounds analysis using GC-MS technique of L. camara revealed that the major compounds could be classified into phenols, triterpene essential oils, sterols, and miscellaneous. The results presented various solvents extracted hexane, EtOAc, and MeOH were 32 bioactive compounds. The hexane extraction yielded the highest number of compounds at 22, followed by Ethyl acetate with 16 compounds and methanol extraction with 6 compounds. The predominant compound in the ethyl acetate extract was 6S-2,3,8,8-Tetramethyltricyclo [5.2.2.0(1,6)] undec-2-ene (48.87%), while in the methanol extract, it was (+)-2-Bornanone (35.71%). Therefore, the choice of solvent significantly impacts the efficacy of phytochemical extraction, laying a foundation for further development of its therapeutic benefits, and evaluating their activities in living organisms or utilization.

Keywords: *Lantana camara*, phytochemical compounds, GC-MS technique

INTRODUCTION

Lantana camara L. belongs to the family Verbenaceae, known in Thai as "Phakakrong". The genus Lantana consists of 129 species. It is a widespread plant species, and most are native to subtropical and tropical regions of the world. Most is originated from South America (Ingawale G. S., and Goswami-Giri A. S., 2014). *Lantana camara* L. (Verbenaceae) is a rambling shrub with several flower colors viz. red, pink, white, yellow, and violet (Farzaei M. H.et al., 2015). It can grow up to 2–4 m in height under normal conditions but could climb up to 15 m in height with the support of surrounding vegetation (Day et al., 2003). *L. camara* have been widely used in traditional medicine for the treatment of malaria, ulcers, cancer, high blood pressure, tetanus, tumors, eczema, cuts, catarrhal infections, atoxy of abdominal viscera, chicken pox, measles, rheumatism, asthma, and fevers (Ghisalberti, 2000; Lenika et al., 2005; and Sathish et al., 2011). And their various biological activities such as hepatoprotective, leishmanicidal, anticancer, antibacterial, antioxidant, antimycobacterial, anti-inflammatory, nematicidal, and antiulcer have been reported (Begum et al., 2014; Qamar et al., 2005). It is an excellent provenance for several classes of bioactive natural products including triterpenoids, phenol, flavonoids, steroids, essential oil, saponin, iridoid glycosides, oligosaccharides, phenylpropanoid glycosides, and naphthoquinones (Sharma et al., 2007; Sousa et al., 2012). This study aims to explore the extraction of *L. camara* using statistical analysis of gas chromatography-mass spectrometry (GC-

MS) data, laying a foundation for further development of its therapeutic benefits, and evaluating their activities in living organisms or utilization.

OBJECTIVE

1. To study the solvent used in the extraction of Lantana camara Linn."

2. To study the chemical components of extracts from Lantana camara L. by GCMS technique.

MATERIALS AND METHODS

Plant material

The leaves of *L. camara* were collected from Sam Khok district, Pathum Thani province, in October 2022. A voucher specimen (Suwadee Chokchaisiri, No. 001) was deposited at the College of Allied Health Sciences Suan Sunandha Rajabhat University, Samut Songkhram Campus, Thailand.

Fig. 1. *Lantana camara* L. plant

Sample Extraction

The air-dried, powdered leaves of *L. camara* (1.19 kg) were extracted successively with n-hexane, EtOAc and MeOH at room temperature. The hexane, EtOAc and MeOH extracts were filtered and concentrated to dryness under reduced pressure. The hexane extract (22.47 g) EtOAc extract (77.83 g) and MeOH extract (85.41 g), respectively. Subsequently, they were analyzed using GC-MS.

Gas Chromatography-Mass Spectrometry (GC-MS) Analysis

The chemical composition of the samples was analyzed using a Shimadzu GCMS-QP2020 with an HP-5MS column (30 m x 0.25 mm ID x 0.25 mm), which is a non-polar fused silica capillary with a 5% phenyl-methylpolysiloxane stationary phase. The helium gas flow rate was set to 1.0 mL/min and 1 µL of the sample was injected in split mode with a split ratio of 1:20. The column temperature was programmed to start at 70°C for 2 minutes, then increase at a rate of 5°C/min to 200°C for 20 minutes, followed by an increase at a rate of 5°C/min to 230°C for 15

minutes, then an increase at a rate of 5°C/min to 250°C for 15 minutes, and finally an increase at a rate of 5°C/min to 320°C for 20 minutes. The ion source temperature was set to 250°C in Electron Impact Ionization (EI) mode. The total ion chromatogram (TIC) of each strain was generated in scan mode using a mass range of 35 to 500 amu (Atomic Mass Unit). The resulting spectra were compared to the NIST17.lib database (Yongram C. et al., 2019 and Palmieri S. et al., 2021).

RESULTS AND DISCUSSION

In our ongoing research aimed at elucidating the constituents of *Lantana camara* L. (Verbenaceae), this study embarks on a comprehensive phytochemical investigation. Utilizing Gas Chromatography-Mass Spectrometry (GCMS), we analyze the extract to identify and characterize a total of 34 compounds. Among them are Cyclopentasiloxane (**1**), (+)-2-Bornanone (**2**), Cyclohexasiloxane (**3**), Caryophyllene (**4**), (S,1Z,6Z)-8-Isopropyl-1-methyl-5-methylenecy (**5**), Germacrene D (**6**), Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-4a (**7**), 1H-Cycloprop[e]azulen-7-ol (**8**), Caryophylleneoxide (**9**), Phytol (**10**), Squalene (**11**), Dotriacontane (**12**), Vitamin E (**13**), Tetrapentacontane (**14**), Stigmasterol (**15**), 28-Norolean-17-en-3-one (**16**), Tetrapentacontane (**17**), γ-Sitostenone (**18**), Phytyl stearate (**19**), Phytyllinoleate (**20**), Trichloromethane (**21**), Cyclotetrasiloxane (**22**), Cycloheptasiloxane (**23**), Hexadecanoicacid (**24**), 2-Hexadecen-1-ol (**25**), β-Sitosterol acetate (**26**), Caryopalpha.-Tocopherol-.beta.-D-mannoside (**27**) , 6S-2,3,8,8-Tetramethyltricyclo[5.2.2.0 (1,6)]undec-2-ene (**28**), 6S-2,3,8,8 Tetramethyltricyclo[5.2.2.0(1,6)]undec-2-ene (**29**), Acetyl betulinaldehyde (**30**), Stigmasta-5,22-dien-3-ol (**31**), Stigmast-5-en-3-ol (**32**), 6S-2,3,8,8-Tetramethyltricyclo[5.2.2.0(1,6)]undec-2-ene (**33**), 1,2,2-trichloro-1,1-difluoroethane (**34**), respectively.

Table 1 and **Figure 2** present the 22 compounds extracted from *L. camara.* with the hexane solvent. The main compounds identified based on relative contents were Vitamin E (12.57%), Squalene (7.86%), 1H-Cycloprop[e]azulen-7-ol (7.62%), Phytol (6.03%), and Caryophyllene oxide (5.93%). Most of the compounds extracted with hexane were phenol and triterpene similarly, previous data showed the existence of phenol and triterpene in *L. camara* (Sharma et al., 2007; Sousa et al., 2012). In the *L. camara* extract using the EtOAc solvent, 16 compounds were identified, as shown in **Table 2** and **Figure 3**. The main compounds identified based on the relative contents were 6S-2,3,8,8-Tetramethyltricyclo [5.2.2.0(1,6)] undec-2-ene (48.87%), 2-Hexadecen-1-ol (15.61%), and Stigmast-5-en-3-ol (12.18%). Most of the compounds extracted with EtOAc were essential oils and sterols. Additionally, the in vitro antioxidant and antimicrobial potential has been evaluated (Hidayathulla S. et al., 2018; Patra A. et al., 2010). **Table 3** and **Figure 4** display the 6 compounds identified in the *L. camara* extract using the MeOH solvent. The predominant compounds, based on their relative contents, were (+)-2-Bornanone (35.71%), Cyclohexasiloxane (22.56%), Cyclopentasiloxane (18.03%), and 1,2,2-trichloro-1,1-difluoro-ethane (16.91%). The majority of the compounds extracted with MeOH were essential oils. Essential oils serve as a rich source of various bioactive compounds known for their antioxidative and

antimicrobial properties. Furthermore, certain essential oils have been utilized for medicinal purposes (Tongnuanchan P. and Benjakul S., 2014).

Table 1. Phytochemical compounds of the hexane extract of *L. camara*.

No.	Identified Name	Rt* (min)	Peak area (%)
3	Cyclopentasiloxane	15.294	1.23
4	(+)-2-Bornanone	15.782	2.90
5	Cyclohexasiloxane	23.146	1.60
6	Caryophyllene	27.219	4.13
7	(S,1Z,6Z)-8-Isopropyl-1-methyl-5-methylenecy	27.568	1.37
8	Germacrene D	29.129	1.58
9	Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-4a	29.605	2.90
10	1H-Cycloprop[e]azulen-7-ol	32.474	7.62
11	Caryophyllene oxide	32.650	5.93
12	Phytol	53.868	6.03
13	Squalene	75.986	7.86
14	Dotriacontane	81.923	5.04
15	Vitamin E	82.222	12.57
16	Tetrapentacontane	83.113	1.82
17	Stigmasterol	84.102	2.66
18	28-Norolean-17-en-3-one	85.572	3.47
19	Tetrapentacontane	85.999	2.52
20	γ-Sitostenone	86.845	3.13
21	Phytyl stearate	88.219	5.74
22	Phytyllinoleate	90.732	2.11

Table 2. Phytochemical compounds of the EtOAc extract of *L. camara*.

No.	Identified Name	Rt* (min)	Peak area (%)
1	Trichloromethane	3.023	0.45
2	Cyclotetrasiloxane	10.435	0.47
3	Cyclopentasiloxane	15.298	2.45
4	(+)-2-Bornanone	15.777	5.73
5	Cyclohexasiloxane	23.155	4.52
6	Caryophyllene	27.230	0.47
7	Cycloheptasiloxane	28.781	0.67
8	Hexadecanoicacid	50.140	0.85

No.	Identified Name	Rt* (min)	Peak area (%)
9	2-Hexadecen-1-ol	58.581	15.61
10	β-Sitosterol acetate	81.410	0.57
11	Caryopalpha.-Tocopherol-.beta.-D-mannoside	82.239	0.81
12	6S-2,3,8,8-Tetramethyltricyclo[5.2.2.0(1,6)]undec-2-ene	84.348	4.03
13	6S-2,3,8,8-Tetramethyltricyclo[5.2.2.0(1,6)]undec-2-ene	85.015	26.80
14	Acetyl betulinaldehyde	85.552	3.17
15	Stigmasta-5,22-dien-3-ol	85.873	1.17
16	Stigmast-5-en-3-ol	86.719	12.18
17	γ-Sitostenone	86.873	3.90
18	6S-2,3,8,8-Tetramethyltricyclo[5.2.2.0(1,6)]undec-2-ene	89.722	18.04

Table 3. Phytochemical compounds of the MeOH extract of *L. camara*.

No.	Identified Name	Rt* (min)	Peak area (%)
1	1,2,2-trichloro-1,1-difluoro-ethane	3.028	16.91
2	Cyclotetrasiloxane	10.435	1.57
3	Cyclopentasiloxane	15.300	18.03
4	(+)-2-Bornanone	15.785	35.71
5	Cyclohexasiloxane	23.158	22.56
6	Cycloheptasiloxane	28.782	5.23

Rt*: the retention time (RT) of a single compound. The time it takes for the compound to go through the column is affected by its length, temperature, and the flow rate of carrier gas.

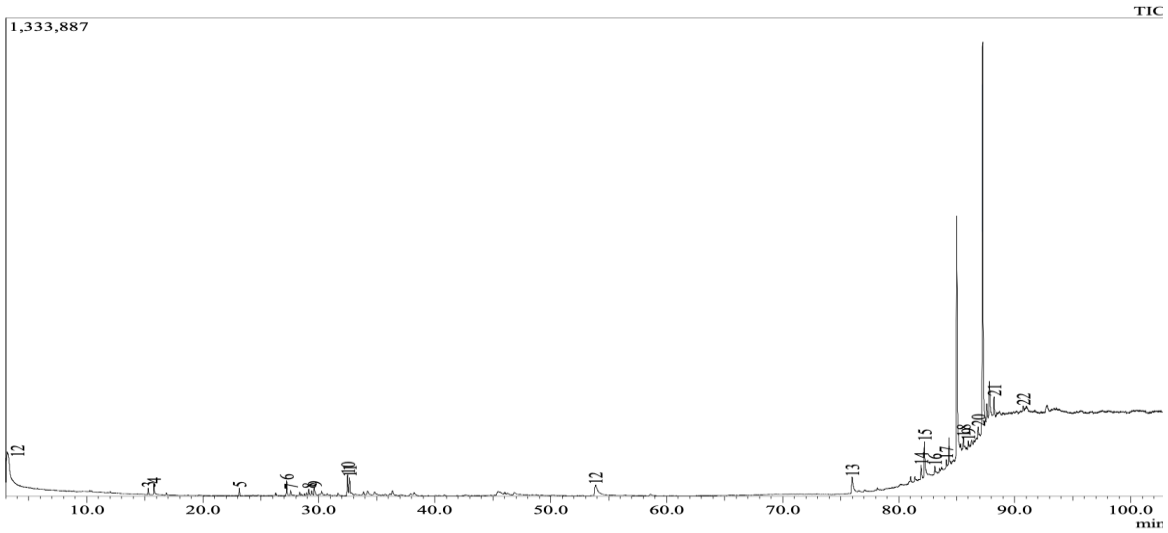

Figure 2. GC–MS chromatograms of the hexane extract of *L. camara*.

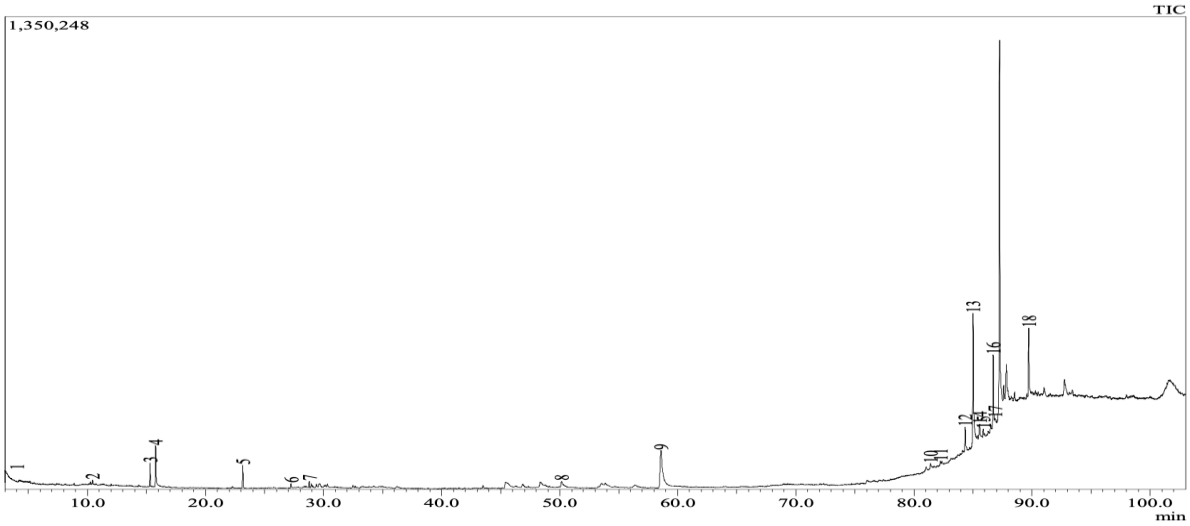

Figure 3. GC–MS chromatograms of the EtOAc extract of *L. camara.*

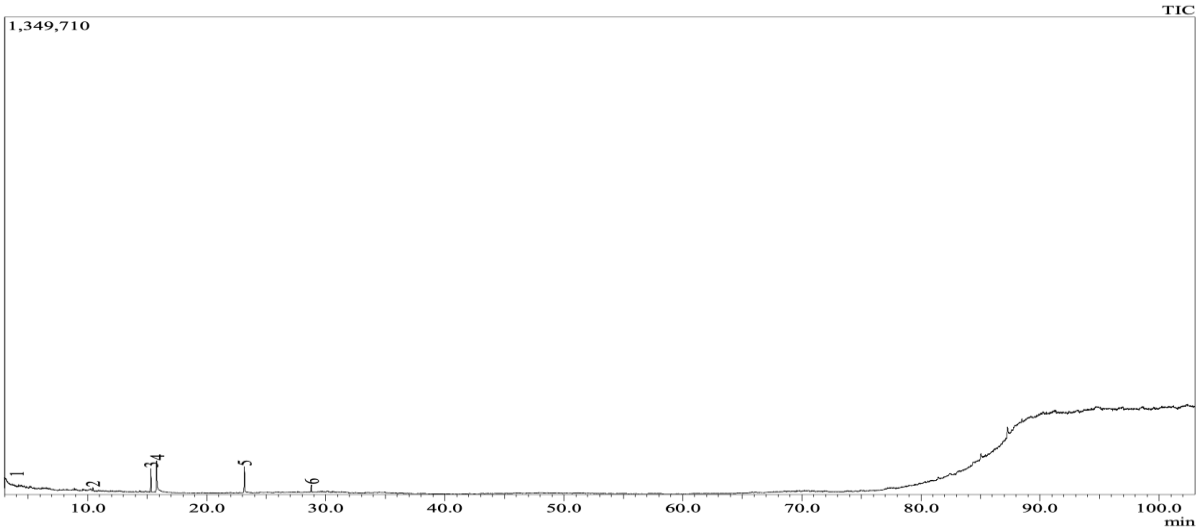

Figure 4. GC–MS chromatograms of the MeOH extract of *L. camara.*

3.1 Comparison between Extraction Percentage of the Phytochemical Compounds Using Different Solvents

The chemical composition analysis using GCMS technique of *L. camara.* revealed that the major compounds could be classified into phenols, triterpene essential oils, sterols, and miscellaneous compounds. The results presented in **Table 4** demonstrate that various solvents extracted a total of 32 bioactive compounds. Hexane extraction yielded the highest number of compounds, totaling 22, followed by ethyl acetate with 16 compounds and methanol extraction with 6 compounds. The predominant compound in the ethyl acetate extract was 6S-2,3,8,8-Tetramethyltricyclo [5.2.2.0(1,6)] undec-2-ene (48.87%), while in the methanol extract, it was (+)-2-Bornanone (35.71%). These findings underscore the significant impact of solvent selection on the efficacy of phytochemical extraction, emphasizing the importance of careful consideration in assay design.

Table 4. Comparison of phytochemical compounds of *L. camara* extracted with various solvents.

No.	Identified Name	Peak area (%)		
		Hexane extract	EtOAc extract	MeOH extract
3	Cyclopentasiloxane	1.23	2.45	18.03
4	(+)-2-Bornanone	2.90	5.73	35.71
5	Cyclohexasiloxane	1.60	4.52	22.56
6	Caryophyllene	4.13	0.47	-
7	(S,1Z,6Z)-8-Isopropyl-1-methyl-5-methylenecy	1.37	-	-
8	Germacrene D	1.58	-	-
9	Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-4a	2.90	-	-
10	1H-Cycloprop[e]azulen-7-ol	7.62	-	-
11	Caryophylleneoxide	5.93	-	-
12	Phytol	6.03	-	-
13	Squalene	7.86	-	-
14	Dotriacontane	5.04	-	-
15	Vitamin E	12.57	-	-
16	Tetrapentacontane	1.82	-	-
17	Stigmasterol	2.66	-	-
18	28-Norolean-17-en-3-one	3.47	-	-
19	Tetrapentacontane	2.52	-	-
20	γ-Sitostenone	3.13	3.90	-
21	Phytyl stearate	5.74	-	-
22	Phytyllinoleate	2.11	-	-
23	Trichloromethane	-	0.45	-
24	Cyclotetrasiloxane	-	0.47	1.57
25	Cycloheptasiloxane	-	0.67	5.23
26	Hexadecanoicacid	-	0.85	-
27	2-Hexadecen-1-ol	-	15.61	-
28	β-Sitosterol acetate	-	0.57	-
29	Caryopalpha.-Tocopherol-.beta.-D-mannoside	-	0.81	-
30	Acetyl betulinaldehyde	-	3.17	-
31	Stigmasta-5,22-dien-3-ol	-	1.17	-
32	Stigmast-5-en-3-ol	-	12.18	-
33	6S-2,3,8,8-Tetramethyltricyclo[5.2.2.0(1,6)]undec-2-ene	-	48.87	-
34	1,2,2-trichloro-1,1-difluoroethane	-	-	16.91

CONCLUSIONS

This study explored solvents with different polarities for extracting phytochemical compounds from *L. camara.* The solvents used included hexane, ethyl acetate, and methanol. Results revealed that the hexane extract contained the highest number of phytochemical compounds, with a total of 22 distinct compounds identified. This was followed by the ethyl acetate extract, which had 16 compounds, and the methanol extract, which had 6 compounds. The majority of the compounds extracted with EtOAc were 6S-2,3,8,8-Tetramethyltricyclo [5.2.2.0(1,6)] undec-2-ene (48.87%), and with methanol, it was (+)-2-Bornanone (35.71%). Hence, the choice of extraction solvents significantly influences the efficiency of phytochemical compound extraction. Furthermore, *L. camara* is a rich source of antioxidants, essential oils, and sterols. Therefore, it is feasible to separate, isolate, and characterize all the phytoconstituents present in L. camara to discover novel drugs, explore their therapeutic benefits, and evaluate their activities in living organisms.

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