

Gas Chromatography-Mass Spectroscopy Determination of Chemical Composition of n- Hexane Extracts of *Morettiaphillaeana* (Del.) DC. Leaves from Sudan

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Abstract

The chemical composition of n-hexane extractable fractions of leaf of *Morettiaphillaeana* were analyzed by Gas chromatography-mass spectroscopy (GC/MS). The first fraction (n-Hexane) was dominated by aliphatic hydrocarbons (80.66%), fatty acids (9.00%) and esters (3.18%) as the main constituents, while the second and third fractions (n-Hexane) were dominated by alkanes (100%) for each fraction. Hydrocarbons (28.15%), alcohols (8.92%), ketones (7.35%) and aldehydes (7.35%) dominated the fourth fraction (ethyl acetate).

Key words - *Morettiaphillaeana*; chemical composition ; GC/MS; Leaves.

I. INTRODUCTION

Morettiaphillaeana (Del) DC (Brassicaceae) is one of two *Morettia* species which occur in [1]. It grows in the northern and central region of the country, where it is known by the popular name of "Gabshah". Its smell is characteristic. Stiff erect hispid herb. Leaves linear to lanceolate, hoary or hispid. Petals pinkish-white, slightly longer than the very hairy sepals. Fruit strongly curved. The plant is used by the Sudanese local people to nourish the sheep and chicken. It has also been used as an ingredient in local medicine for several elements [2]. Phytochemical studies conducted on the methanolic extract of the flowering aerial parts of *M. phillaeana* reported the presence of flavonoids [3], which revealed some in vitro antibacterial activity [4].

The objectives of the present work was to determine the chemical composition of n-hexane extractable fractions from *M. phillaeana* leaves.

II. EXPERIMENTAL

A. Plant material:

Leaves of *Morettiaphillaeana* were collected from a flowering plant during winter time in 2017 from University City Campus, Omdurman Islamic University

in the Omdurman south, Khartoum State, Central Sudan.

B. Extraction and fractionation

Two hundred grams of air-dried leaves were pulverized and extracted three times in n-hexane for a total of 24h. The extract was filtered and concentrated to dryness (yield 800 mg of extract). The dried extract was adsorbed in silica gel and later packed into a column of silica gel. The column was eluted with n-hexane as the mobile phase to yield F1-F3 and thereafter washing with ethyl acetate to give the fourth fraction (F4). After solvent evaporation, the fractions were re-suspended in n-hexane before analysis [5].

C. GC-MS analysis of the compound

The constituents of the n-hexane extract and fractions were characterized and identified by GC/MS. GC/MS analysis was performed on a Shimadzu GC/MS-QP2010A system in ET mode (70 eV) equipped with a split/splitters injector (250°C), at a split ratio of 5/50 using DB-5MS Column (30m x 0.25mm id, film thickness: 0.002E25, J and W Scientific, Folsom, CA, WA). Injection volume was 1 µl and electronic pressure programming was used to maintain a constant flame (0.67 ml/min) of the Helium carrier gas. The oven temperature was programmed from 150°C (4 min) to 320°C at a rate of 2°C/min and held at that temperature 200°C and interface temperature 250°C. The relative approach percentage of each compound was determined by area. Component identification was carried out using the NIST 147 and NIST 27 libraries.

III. RESULT AND DISCUSSION

The chemical composition of n-hexane extractable fractions from *Morettiaphillaeana* leaves were carried out. The extract was adsorbed in silica gel and later packed into a column of silica gel using vacuum liquid chromatography. The column was eluted with n-

hexane as the mobile phase to yield (Fr₁-Fr₃) and with ethyl acetate to give the fourth fraction (Fr₄).

A. GC/MS result of the Fraction 1

The GC/MS chromatogram of the fraction 1 (Figure 1) from n-hexane extract of *Morettiaphillaeana* revealed the presence of 35 compounds (Table 1). Six components were characterized representing 79.13% of total components. The most abundant compounds were Tetratetracontane (3(38.89%) , Pentatriacontane (13.97%) , Hexatriacontane (7(7.65%) , n-hexadecanoic acid (7.35) , Tetracosane (6.20%) and Dotriacontane (5.07).

B. GC/MS result of the Fraction 2

The GC/MS chromatogram (Figure 2) of the fraction 2 from n-hexane extract revealed the presence of 8 compounds (Table 2). Six compounds were characterized representing 99.47% of the total components. The most abundant compounds were Tetratetracontane (77.42%) , Tetracosane (9(9.77%) , Dotriacontane(7.67%) , Dodecane (1.22%) , Tetradecane (1.22%) and Heneicosane (1.17%).

C. GC/MS result of the Fraction 3

The GC/MS chromatogram (Figure 3) of the n-hexane extract (fraction 3) revealed the presence of 100% compound (table 3). Four components were characterized representing 100% of total compound. The most abundant components was Nonacosane (85.12).

D. GC/MS result of the Fraction 4

The GC/MS chromatogram (Figure 4) of the ethyl acetate fraction 4 from n-hexane extract revealed the presence of 45 compounds (Table 4). Six components were characterized representing 44.34% of the total components. The most abundant components were Docosylheptafluorobutyrate (1(11.83%) , n-hexadecanoic acid (9.16%) , Pentatriacontane (6(6.47%) , Cis,cis,cis-7,10,13-hexadecatrienal (6.39%) , PPhytol(5.55%) , and Hexatriacontane (4.94).

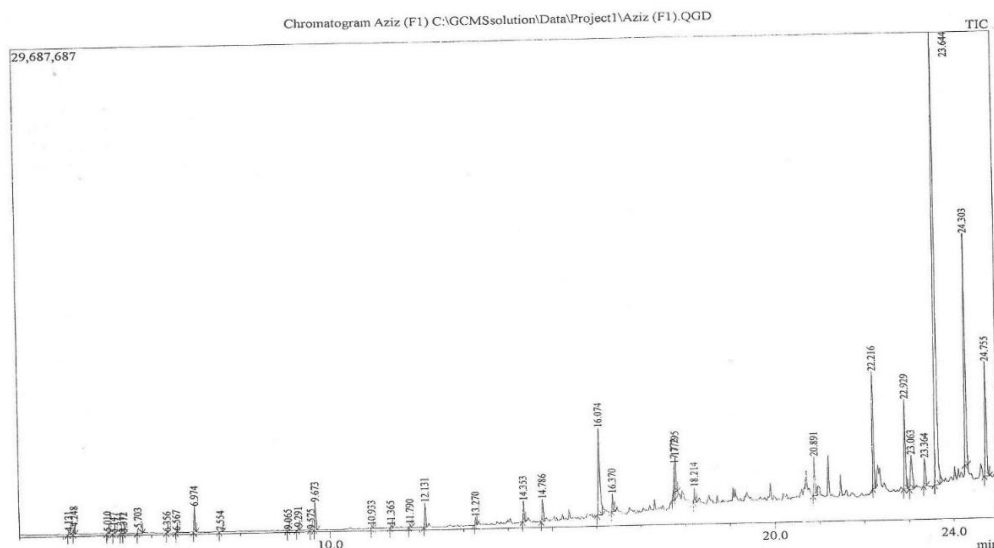


Fig. 1. GC/MS chromatogram of *M. phillaeana*-hexane fraction 1

Table 1
Composition of n-Hexane extract(fraction 1)

#	RT	Compound	Formula	Area%
1	4.131	1-Butene,4-isothicyanato	C ₅ H ₇ NS	0.18
2	4.248	Undecan	C ₁₁ H ₂₄	0.28

3	5.010	2-Octene,2-methyl-6-methylene	C ₁₀ H ₁₈	0.07
4	5.147	Cyclopropanecarboxaldehyde, 2-mehtyl-2-	C ₁₁ H ₁₈ O	0.02
5	5.311	Citral	C ₁₀ H ₁₆ O	0.03
6	5.372	Benzathiol,2-methyl	C ₇ H ₈ S	0.03
7	5.703	1-Butanol,3-methyl-,acetate	C ₇ H ₁₄ O ₂	0.56
8	6.356	Undecane,5-methyl	C ₁₂ H ₂₆	0.02
9	6.567	Undecane,3-methyl	C ₁₂ H ₂₆	0.07
10	6.974	Dodecane	C ₁₂ H ₂₆	1.11
11	7.554	Benothiazola	C ₇ H ₅ NS	0.06
12	9.065	Oxalic acid, 6-ethyloct-3-ylisoheptyl ester	C ₁₈ H ₃₄ O ₄	0.04
13	9.291	2-Bromododecane	C ₁₂ H ₂₅ Br	0.14
14	9.575	3-Hexadecene,(Z)-	C ₁₆ H ₃₂	0.02
15	9.673	Tetradecane	C ₁₄ H ₃₀	1.29
16	10.933	Octadecane	C ₁₈ H ₃₈	0.13
17	11.365	2,6,10-Dodecatrial-1-ol,3,7,11-trimethyl-	C ₁₅ H ₂₆ O	0.11
18	11.790	Pentadecane,3-methyl	C ₁₆ H ₃₄	0.15
19	12.131	Heptadecane	C ₁₇ H ₃₆	1.14
20	13.270	Nonadecane	C ₁₉ H ₄₀	0.39
21	14.353	Heneicosane	C ₂₁ H ₄₄	1.02
22	14.786	3,7,11,15-tetramethyl-2-hexadecene-1-ol	C ₂₀ H ₄₀ O	1.25
23	16.074	n-Hexadecanoic acid	C ₁₆ H ₃₂ O ₂	7.35
24	16.370	Eicosane	C ₂₀ H ₄₂	0.88
25	17.772	7-Tetradecenal,(Z)	C ₁₄ H ₂₆ O	2.23

26	17.795	9,12,15-Octadecatrienoic acid ,(Z,Z,Z)-	C ₁₈ H ₃₀ O ₂	1.65
27	18.214	Docosane	C ₂₂ H ₄₆	0.78
28	20.891	Hexadecanoicacid,2-hydroxy-1-(hydroxy)ethyl ester	C ₁₉ H ₃₈ O ₄	2.58
29	22.216	Tetracosane	C ₂₄ H ₅₀	6.20
30	22.929	Dotriacontane	C ₃₂ H ₆₆	5.07
31	23.063	Vitamin E	C ₂₉ H ₅₀ O ₂	3.11
32	23.364	Tetratriacontane	C ₃₄ H ₇₀	1.53
33	23.644	Tetratetracontane	C ₄₄ H ₉₀	38.89
34	24.303	Pentatriacontane	C ₃₅ H ₇₂	13.97
35	24.755	Hexatrioctane	C ₃₆ H ₇₄	7.65

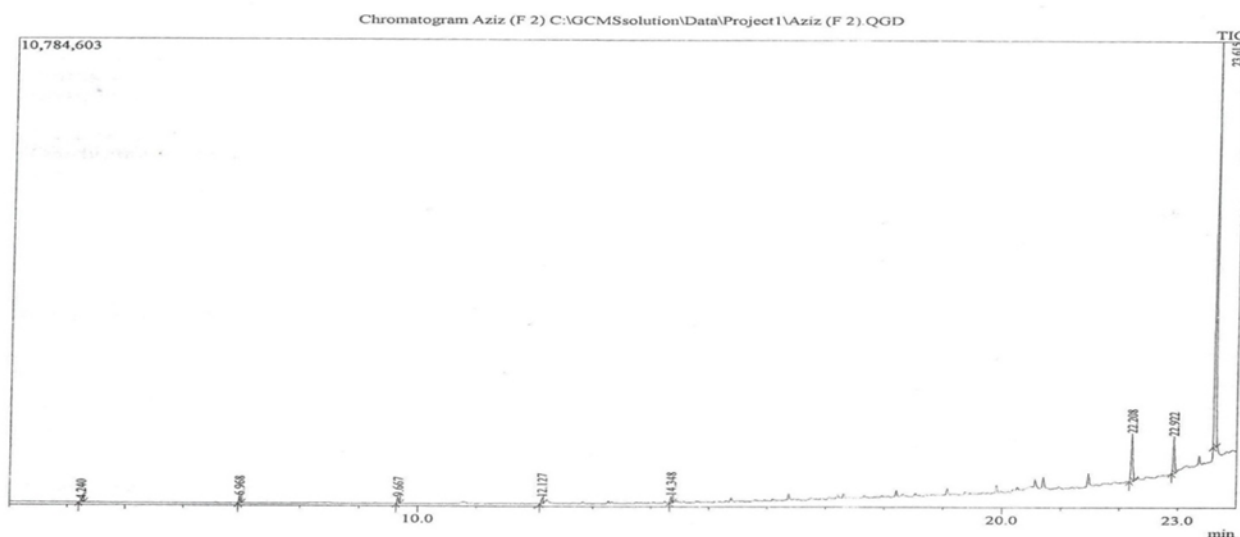


Fig. 2. GC/MS chromatogram of n-hexane fraction 2 from *Morettiaphillaeana*

Table 2
Composition of n-Hexane extract (fraction 2)

#	RT	Compound	Formula	Area%
1	4.240	Undecane	C ₁₁ H ₂₄	0.43
2	6.968	Dodecane	C ₁₂ H ₂₆	1.22
3	9.667	Tetradecane	C ₁₄ H ₃₀	1.22
4	12.127	Heptadecane	C ₁₇ H ₃₆	1.10

5	14.348	Heneicosane	C ₂₁ H ₄₄	1.17
6	22.208	Tetracosane	C ₂₄ H ₅₀	9.77
7	22.922	Dotriacontane	C ₃₂ H ₆₆	7.67
8	23.615	Tetratetracontane	C ₄₄ H ₉₀	77.42

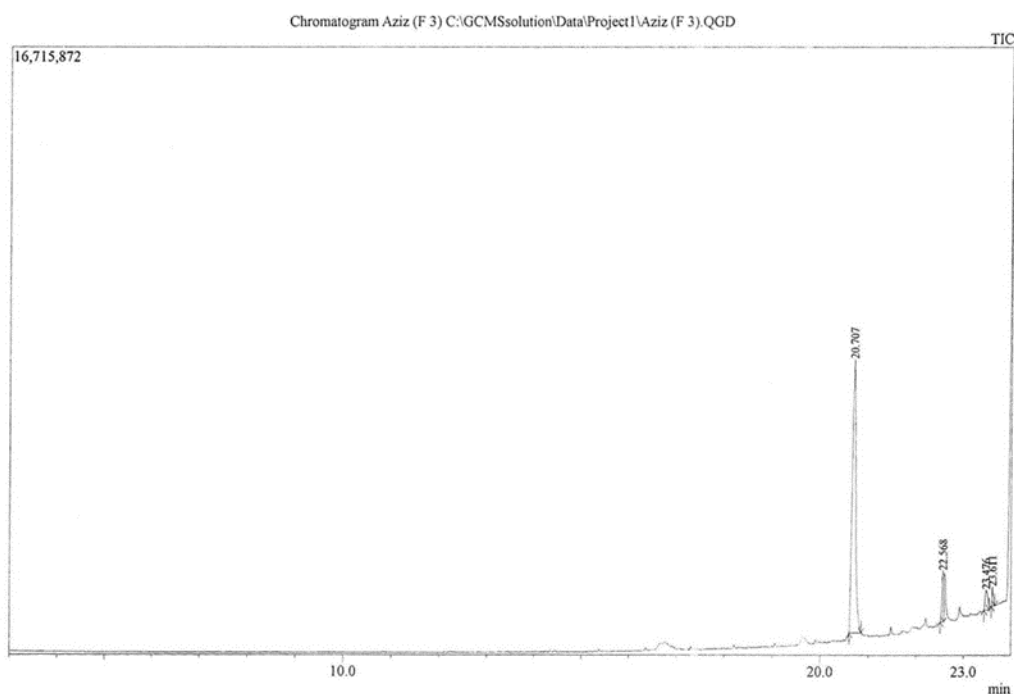


Fig. 3.GC/MS chromatogram of n-hexane fraction 3 from Morettiaphillaeana

Table 3
n-Hexane extract (fraction 3)

#	RT	Compound	Formula	Area%
1		Nonacosane	C ₂₉ H ₆₀	85.12
2		5-ethyl-5-methylnondecane	C ₂₂ H ₄₆	7.87
3		Tetratricontane	C ₃₄ H ₇₀	4.83
4		Tetratetracontane	C ₄₄ H ₉₀	2.18

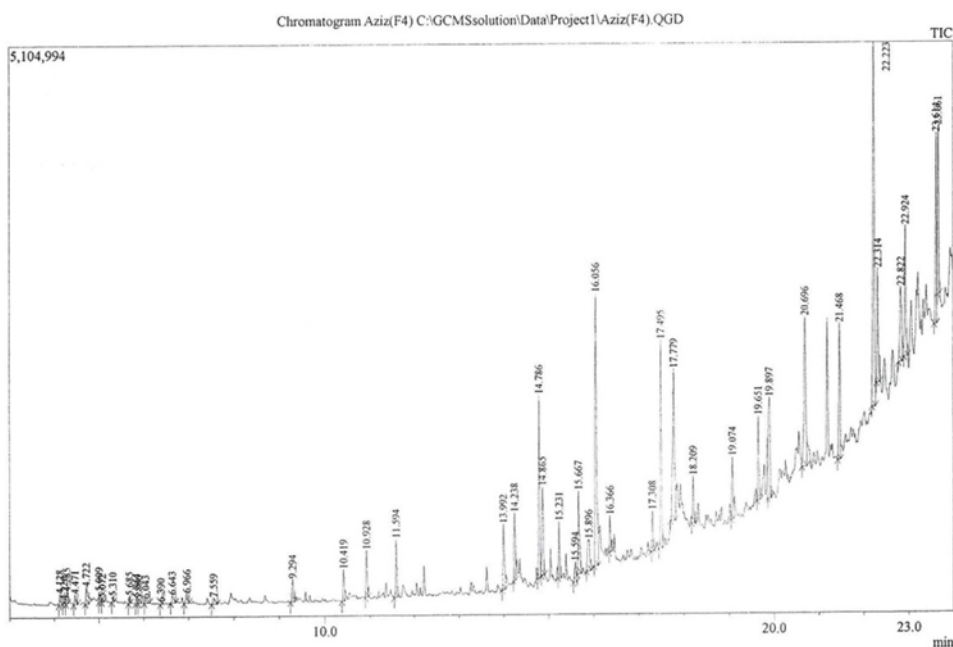


Fig. 4. GC/MS chromatogram of n-hexane fraction 4 from *morettiaphillaeana*

Table 4
Ethyl acetate fraction 4 from n-hexane extract of *M.phillaeana*

#	RT	Compound	Formula	Area%
1	4.128	5-Hepten-2-one,6methyl-	C ₈ H ₁₄ O	0.40
2	4.220	3-Undecyne	C ₁₂ H ₂₂	0.06
3	4.285	2,4-Heptadienal	C ₇ H ₁₀ O	0.34
4	4.471	1,4-Hexadiene,3-ethyl-	C ₈ H ₁₄	0.38
5	4.722	D-Limonene	C ₁₀ H ₁₆	0.74
6	5.009	1,5-Heptadiene,2,3,6-trimethyl	C ₁₀ H ₁₈	0.21
7	5.072	Benzene,1,2-diethyl-	C ₁₀ H ₁₄	0.08
8	5.310	Cyclopropanecarboxaldehyde2-methyl-2-(4-		0.12

		methyl-3-pentyl)	$C_{11}H_{18}O$	
9	5.685	Nonanal	$C_9H_{18}O$	0.17
10	5.844	3,4-Dimethylcyclohexanal	$C_8H_{16}O$	0.13
11	5.886	tricyclo[3.2.2.0]nonane-2-carboxylic acid	$C_{10}H_{14}O_2$	0.12
12	6.043	Benzylisocynate	C_8H_7NO	0.18
13	6.390	bicyclo[3.1.0]hexan-3-ol,4-methyl-1-(1-methylethyl)	$C_{10}H_{18}O$	0.04
14	6.643	1-propanone,1-phenyl	$C_9H_{10}O$	0.41
15	6.966	3,6-Undecandione	$C_{11}H_{20}O_2$	0.42
16	7.559	Benzothiazola	C_7H_5NS	0.34
17	9.294	Naphthalene,1,2,3,4-tetrahydro-1,1,6-trimethyl	$C_{13}H_{18}$	0.74
18	10.419	5,9-Udecadien-2-one,6,10-dimethyl-	$C_{13}H_{22}O$	0.88
19	10.928	Trans-.beta.-Ionone	$C_{13}H_{20}O$	1.17
20	11.594	2(4H)-Benzofuranone,5,6,7,7a-tetrahydro-4,4,7a-trimethyl	$C_{11}H_{16}O_2$	1.52
21	13.992	Tetradecanoic acid	$C_{14}H_{28}O_2$	2.19
22	14.238	1,4-Naphthalenedione,2,3,6-trimethyl	$C_{13}H_{12}O_2$	1.96

23	14.786	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	C ₂₀ H ₄₀ O	4.78
24	14.865	2-Pentadecanone,6,10,14-trimethyl	C ₁₈ H ₃₆ O	2.86
25	15.231	Phytol,acetate	C ₂₂ H ₄₂ O ₂	1.42
26	15.594	Trans-Geranylgeraniol	C ₂₀ H ₃₄ O	0.75
27	15.667	5,9,13-Peptadecatrien-2-one ,6,10,14-trimethyl	C ₁₈ H ₃₀ O	2.79
28	15.896	9,12,15-Octadecatrienoic acid (Z,Z,Z)	C ₁₈ H ₃₀ O ₂	1.73
29	16.056	n-Hexadecanoic acid	C ₁₆ H ₃₂ O ₂	9.16
30	16.366	Heneicosane	C ₂₁ H ₄₄	0.80
31	17.308	Hexacosane	C ₂₆ H ₅₄	0.95
32	17.495	Phytol	C ₂₀ H ₄₀ O	5.55
33	17.779	Cis,cis,cis-7,10,13-Hexadecatrienal	C ₁₆ H ₂₆ O	6.39
34	18.209	Dodcosane	C ₂₂ H ₄₆	1.17
35	19.074	Eicosane	C ₂₀ H ₄₂	1.61
36	19.651	4,8,12,16-Tetramethylheptadecan-4-olide	C ₂₁ H ₄₀ O ₂	2.21
37	19.897	Tetracosane	C ₂₄ H ₅₀	3.90
38	20.696	Pentatriacontane	C ₃₅ H ₇₂	6.47

39	21.468	Tritricontane	$C_{33}H_{68}$	3.87
40	22.223	Docosylheptafluorobutyrate	$C_{26}H_{45}F_7O_2$	11.83
41	22.314	4,4-((p-phenylene)diisopropylidene) diphenol	$C_{24}H_{26}O_2$	3.17
42	22.822	Gamma.-sitosterol	$C_{29}H_{50}O$	3.15
43	22.924	Tetraricontane	$C_{34}H_{70}$	3.79
44	23.614	Hexatriacontane	$C_{36}H_{74}$	4.94
45	23.661	1-heptacosanol	$C_{27}H_{56}O$	4.10

Table 5
Comparison between the major constituents in fractions 1-4 from Morettiaphillaeana

No	Compound	Fr1	Fr2	Fr3	Fr4
1	Tetratetracontane	38.89	77.42	2.18	
2	Pentatriacontane	13.97			6.47
3	Hexatriacontane	7.65			4.94
4	n-hexadecanoic acid	7.35			9.16
5	Tetracosane	6.20	9.77		
6	Dotricontane	5.07	7.67		
7	Dodecane	1.11	1.22		1.17
8	Tetradecane	1.29	1.22		
9	Heneicosane	1.02	1.17		0.80
10	Nonacosane			85.12	
11	5-ethyl-5-methylnonadecane			7.87	
12	Tetratriacontane	1.53		4.83	3.79

13	Docosylheptaflourobutyrate				11.83
14	Cis,cis,cis-7,10,13-hexadecatrienal				6.39
15	Phytol				5.55

The fraction (F1) was found to be dominated by alkanes (80.57%) with tetraetracontane (38.89%) and pentacontane (13.97%) as main constituents, other compounds identified in the fraction were hexatriacontane, tetracosane, dotriacontane and n-hexadecanoic acid.

The second fraction (F2) was dominated by alkanes (100%) with tetraetracontane (77.42%), tetracosane (9.77%) and dotriacontane (7.67%) as the main compounds. Undecane, dodecane, tetradecane, heptadecane, and heneicosane was also observed in this fraction.

The fraction (F3) contain a high portion of nonacosane (85.12%). The other preminent Compounds were 5-ethyl-5-methyl-nonadecane (7.87%) and tetracontane.

The fourth (F4) was dominated by Docosylheptaflourobutyrate (11.83%), nhexadecanoic acid (9.16) and pentatriacontane (6.47). the presence of diterpene Phytol (table 11) in this fraction is worth nothing. phytol was reported to be toxic and lethal [6]. Hexadecanoic acid has been reported to induce apoptosis in hepatocytes [7].

Fraction 1 obtained from n-hexane extract of *Morettiaphillaeana* leaves contain eleven class of compounds including hydrocarbons (alkanes (80.57%), alkenes (0.02%) and alkyne (0.07%)), fatty acid (9.00%) , alcohols (1.36%), aldehydes (2.28%) , tocopherols (3.11%) , halide (0.14%) , amide (0.18%), aromatic compound (0.09%) and ester (3.18%). Fraction 2 and fraction 3 obtained from n-hexane extract of *Morettiaphillaeana* leaves contain alkanes (100%) for each fraction. Fraction 4 obtained from n-hexane extract of *Morettiaphillaeana* leaves contain eight class of compound including hydrocarbons (alkanes (27.5%), alkyne (0.65%)) alcohols (8.92%) , aldehydes (7.15%) , ketones (7.35%) , fatty acid (14.62%) , phytosterol (5.55%) , aromatic compound (8.4%) , terpenes (1.91%), carbohydrates (2.21%) and diterpenes (6.3%).

IV. CONCLUSION

Morettiaphillaeana was characterized by presence of alkanes composition C₄₄, C₄₀, C₃₅, C₂₈ and

C₂₅. Long chain n-alkanes (C₂₁-C₃₇) are among the most long-lived and

R widely terrestrial plants biomarkers n-Alkane distributions have been used for a variety of purpose in paleoclimatology and paleoecology as well as chemotaxonomy.

The constituents of n-hexane extractable fractions of leaves of *Morettiaphillaeana* were also analyzed by GC/MS. The first fraction (n-hexane) revealed 35 compounds, second fraction revealed (n-hexane) 8 compounds, third fraction (n-hexane) revealed 4 compounds, and fourth fraction (ethyl acetate) revealed 45 compounds. Hydrocarbons are the most high rate compounds in all fractions. Higher percentage of hydrocarbons was found in the *Morettiaphillaeana* n-hexane extract which might be used in fuel industry, Some compounds found in *Morettiaphillaeana* leaves are toxic such as phytol, it requires cautions.

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