Supplementary materials:

Text S1: Compound 1 [pentacos-7-ene]: (500 mg) white waxy substance; R_f: 0.69 and 0.85 by using solvent systems (100% Light petroleum) and (Light petroleum: CH_2Cl_2 90:10), ^{1}H-NMR ($CDCl_3$, 400 MHz) spectral analyses were carried out by: JEOL at 500 MHz and Bruker at 400 MHz and chemical shifts were given in ppm with the TMS as internal standard: δ_H 5.32 (2H, br. s, H-7, H-8), 0.91(6H, t, H-1,25, *J*= 7.2 Hz), 1.00-1.30 (42H, m, H2-6 and H9-24); EI-MS that carried out on Jeol JMS-AX 500, 70 ev. displayed *m/z* (% relative abundance) as follow: 351 (M^++H, 1), 350 (M^+, 0.05), 322.28 (M^++H-C_2H_5,1.5), 308 (322-CH_2, 0.5), 295 (1.5), 294 (322-C_2H_4, 0.3), 280 (322-C_3H_6, 0.1), 266 (322-C_4H_8, 0.07), 252 (322-C_5H_{10}, 0.1), 211 (1.6), 183 (2.2), 155 (2.3), 127 (3.4), 125 (23), 111 (42), 97 (65), 85 (87),71 (100).

Text S2: Compound 2 [Nonatriacontanoic acid]: (100 mg) white crystalline scales; R_f: 0.55 & 0.73 using solvent systems (Light petroleum:CH_2Cl_2 75:25) & (100% CH_2Cl_2); ^{1}H-NMR ($CDCl_3$, 400 MHz):δ_H 2.33 (2H, t, H-2, *J*=8.0Hz), 1.63 (2H, m, H-3), 1.25 (66H, m, H-4-36), 1.25 (2H, m, H-37), 1.56 (2H, m, H-38), 0.86 (3H,t, H-39), ^{13}C-NMR ($CDCL_3$, 100MH_Z); δ_C176.94 (COOH), 33.64 (C-2), 32.08 (C-3), 29.85 (C-4 : C-36), 24.87 (C-37), 22.84 (C-38), 14.26 (C-39); EI-MS *m/z* (% relative abundance): 578 (M^+,1.62), 577 (3.83), 563 (M^+-CH_3, 1.84), 549 (M^+-C_2H_5, 1.02), 534 (M^+-COO, 1.16), 520 (534- CH_2, 1.02), 506 (534-C_2H_4, 0.06), 396 (5.59), 313 (32.81), 236 (47.94), 98 (91.02), 83 (82.21), 57 (C_4H_9,100.00).

Text S3: Compound 3 [Melissic acid (Triacontanoic acid)]: (400 mg) white amorphous substance; R_f: 0.53 [CH_2CL_2: MeOH (9.8: 0.2)], R_f: 0.50, 0.64 by using solvent systems (Light petroleum:CH_2Cl_2 75:25) & (100% CH_2Cl_2); ^{1}H-NMR ($CDCl_3$, 400 MHz): δ_H 2.35 (2H, t, H-2, *J* = 8.0 Hz), 1.67 (2H, m, H-3), 1.65 (2H, m, H-4), 1.63 (2H, m, H-5, H-6), 1.60 (2H, m, H-7), 1.55

(2H, m, H-8), 1.25 (38H, m, H-9-27), 1.25 (2H, m, H-28), 1.25 (2H, m, H-29), 0.89 (3H, t, H-30, J = 8.0 Hz), ^{13}C-NMR ($CDCL_3$, 100MH_Z); δ_C176.82 (C=O), 33.65 (C-2), 24.89 (C-3), 29.22 (C-4), 29.39 (C-5, C-6), 29.51 (C-7), 29.59 (C-8),29.85 (C-9 – C-27), 32.08 (C-28), 22.84 (C-29), 14.27 (C-30), 51.05 (C-O); EI-MS *m/z* (% relative abundance): 453.21 (M^++H, 0.5), 452 (M^+, 4.17), 424 (M^++H-C_2H_5,13.13), 408 (M^++H- COOH, 0.5), 396 (424-C_2H_4, 71.90), 354 (396-C_3H_6, 9.63), 353 (38.15), 297 (354-C_4H_8+H, 32.87), 278 (10.42),187 (7.86), 129 (61.82), 97 (58.93), 71 (63.26), 57 (100), 45 (77.19).

Text S4: Compound 4 [Cerotic acid (Hexacosanoic acid**)**]:(100 mg) white granules; R_f: 0.42, 0.54 by using solvent system (Light petroleum:CH_2Cl_2 75:25) & (100% CH_2Cl_2); ^{1}H-NMR ($CDCl_3$, 400 MHz): δ_H 2.36 (2H, t, H-2, J = 8.0 Hz), 1.63 (2H, m, H-3), 1.25 (40H, m, H-4-24), 1.25 (2H, m, H-25), 0.86 (3H, t, H-26, J = 8.0 Hz), ^{13}C-NMR ($CDCL_3$, 100MH_Z); δ_C177.3 (C=O), 36.28 (C-2), 24.87 (C-3), 29.59 (C-4 – C-24), 22.85 (C-25), 14.27 (C-26), 51.05 (C-O) ; EI-MS *m/z* (% relative abundance): 396 (M^+,100), 381 (M^+-CH_3, 15.65), 354 (3.64], 288 (12.22), 255 (16.98), 213 (8.54), 161 (8.66),147(32.06), 95(25.53), 85(31.77) , 69(27.64), 57 (34.32).

Text S5: Compound 5 [Palmitic acid]: (200 mg) white crystalline scales; m.p. 63-64 ºC; R_f 0.22 & 0.40 using solvent systems (Light petroleum:CH_2Cl_2 75:25 & (100% CH_2Cl_2); ^{1}H-NMR ($CDCl_3$, 400 MHz):δ_H 2.33 (2H, t, H-2, J = 8.0 Hz), 1.63 (2H, m, H-3), 1.25 (20H, m, H-4-13), 1.25 (2H, m, H-14), 1.56 (2H, m, H-15), 0.88 (3H, t, H-16, J = 8.0 Hz), ^{13}C-NMR ($CDCL_3$, 100MH_Z); δ_C 176.94 (C=O), 33.64 (C-2), 32.08 (C-3), 29.85 (C-4 - C-13), 24.87 (C-14), 22.84 (C-15), 14.26 (C-16); EI-MS *m/z* (relative abundance %): 256 (M^+, 2.08), 227 (M^+-C_2H_5, 1.14), 213 (M^+-C_3H_6+H, 2.62), 185 (2.84), 149 (7.25), 129 (7.80), 121 (9.61), 97 (11.27), 83 (16.02), 69 (72.17) and 40 (100).

Text S6: Compound 6 [Lupeol palmiteolate]: (200 mg) white needles; m.p. 110-112 °C, R_f 0.78 & 0.85 by using solvent system (CH_2Cl_2:MeOH 99:1) & (CH_2Cl_2:MeOH 98:2).^{1}H-NMR ($CDCl_3$, 400 MHz): δ_H 4.26 (1H,dd, H-3, *J* = 6.0, 12.0 Hz), 5.8 (1H,m, H-9`), 5.01 (1H,m, H-10`), 4.69, 4.57 (2H,s, H-29a ,H-29b), 2.39 , 2.41 (2H, t, H-2`, *J* = 7.2 Hz), 2.31 (1H ,t, H-19, *J* = 1.8 Hz), 1.68 (3H, s, H-30), 1.57 (2H, m, H-3`), 0.94 (3H, s, H-23), 0.89 (3H, s, H-24), 0.83 (3H, s, H-25), 0.79 (3H, s, H-26), 0.76 (3H, s, H-27), 0.76 (3H, t, H-16`), ^{13}C-NMR ($CDCL_3$, 100MH_Z); δ_C 38.89 (C-1), 23.90 (C-2), 79.17 (C-3), 37.33 (C-4), 55.45 (C-5),18.15 (C-6) , 34.44 (C-7), 40.99 (C-8), 50.60 (C-9), 38.21 (C-10), 21.08 (C-11), 25.30 (C-12), 38.21 (C-13), 42.99 (C-14), 27.57 (C-15), 35.74 (C-16), 43.16 (C-17), 48.46 (C-18), 48.14 (C-19), 151.14 (C-20), 29.85 (C-21), 40.16 (C-22), 28.14 (C-23), 16.27 (C-24), 16.13 (C-25), 15.52 (C-26), 15.50 (C-27), 18.47 (C-28),109.47 (C-29),19.31 (C-30),167.91 (C=O), 32.08 (C-1`), 25.30 (C-2`), 29.08 (C-3`), 29.51 (C-4`-C-8`), 131.03 (C-9`), 132.61 (C-10`), 30.51 (C-11`), 22.84 (C-12`), 33.97 (C-13`), 23.14 (C-14`), 22.84 (C-15`), 21.08 (C-16`); EI-MS *m/z* (relative abundance %): 662 [M^+,0.83], 647 (M^+-CH_3, 0.5), 426 [M^+- palmiteolic acid,13.27], 411(9.53), 316 (7.06), 267 (7.17), 239 (10.95), 219 (19.97), 218 (77.01), 189 (73.36), 147 (43.69), 135 (70.01), 109 (85.65), 95 (100), 81 (84.14), 69 (81.63), 54 (61.05).

Text S7: Compound 7 [Lupeol acetate]: (500 mg) white needles; m.p: 216-218 °C and R_f values 0.43 and 0.55 by using solvent systems (CH_2Cl_2:MeOH 99:1) & (CH_2Cl_2:MeOH 98:2);^{1}H-NMR ($CDCl_3$, 400 MHz): δ_H 4.46 (1H, m ,H-3), 4.68, 4.56 (2H, s, H-29b ,H-29a, respectively), 2.05 (3H, s, CH_3OCO), 2.04 (1H, m, H-19), 1.68 (3H, s, H-30), 1.03 (3H, s, H-25), 0.94 (3H, s, H-28), 0.85 (3H, s, H-23), 0.84 (3H, s, H-24), 0.83 (3H, s, H-26), 0.79 (3H, s, H-27), ^{13}C-NMR ($CDCL_3$, 100MH_Z); δ_C 38.62 (C-1), 21.56 (C-2), 81.13 (C-3), 38.20 (C-4), 55.54 (C-5), 18.36 (C-6), 34.37 (C-7), 41 (C-8), 50.50 (C-9), 37.3 (C-10), 21.10 (C-11), 23.85 (C-12), 36.95 (C-13), 42.98 (C-14),

25.26 (C-15), 35.73 (C-16), 43.16 (C-17), 48.44 (C-18), 48.19 (C-19), 151.13 (C-20), 29.99 (C-21), 40.15 (C-22), 27.59 (C-23), 16.89 (C-24), 16.65 (C-25), 16.34 (C-26), 14.66 (C-27), 18.16 (C-28),109.51 (C-29), 19.45 (C-30),171.18 (C=O), 28.19 (CH_3 of acetyl group); EI-MS *m/z* (relative abundance %): 468[M^+,7.33], 426 [M^+-acetate, 2.1] , 393(5.27), 257(3.96), 229(5.27), 218(100), 203(57.32), 189(49.82),147 (15.91), 121(22.55), 107 (24.29), 81 (32.94), 69 (43.28) and 43 (59.46).

Text S8: Compound 8 [*β*-sitosterol]:(500 mg) colorless crystals; m.p. 136-140ºC; R_f 0.65 and 0.83 using solvent systems (CH_2Cl_2:MeOH 95:5) & (CH_2Cl_2:MeOH 85:15),^{1}H-NMR ($CDCl_3$, 400 MHz): δ_H 3.52 (1H, m, H-3), 5.34 (1H, t, H-6) *J*=5.2 H_Z), 1.03 (3H, s, H-18), 0.91 (3H, d, *J* = 8.0 Hz, H-21), 0.89 (3H, t, *J* = 7.2 Hz, H-24), 0.84 (3H, t, *J* = 7.2 Hz, H-29), 0.82 (3H, d, *J* = 7.2 Hz, H-27), 0.80 (3H, d, *J* = 7.2 Hz, H-26), 0.68 (3H, s, H-19), 0.68 (2H, m, H-28), ^{13}C-NMR ($CDCL_3$, 100MH_Z); δ_C 37.41 (C-1), 31.82 (C-2), 71.97 (C-3),42.46 (C-4), 140.91 (C-5), 121.88 (C-6),, 32.06 (C-7, C-8), 50.29 (C-9), 36.66 (C-10) , 21.24 (C-11), 39.93 (C-12), 42.47 (C-13), 56.92 (C-14), 26.22 (C-15), 28.40 (C-16), 56.21 (C-17), 36.30 (C-18), 19.18 (C-19), 34.10 (C-20), 24.46 (C-21), 45.99 (C-22), 23.22 (C-23), 12.13 (C-24), 29.30 (C-25), 19.97 (C-26), 19.55 (C-27), 18.93 (C-28), 12.01 (C-29); EI-MS *m/z* (relative abundance %): 414 (M^+, 59.88%) , 396 (M^+-H_2O, 32.87), 381 (M^+-H_2O-CH_3, 28.23%), 329 (91.62%), 303 (90.25%), 273 (59.75%), 255 (59.65%), 213 (49.10%), 145(62.34%), 107(87.64%), 105(72.50%), 79(66.87%), 55(74.61%) and 43(100%).

Text S9: Compound 9 [*β*-sitosterol-3-O-β-D-glucopyranoside]: (2 g) white powder; R_f values 0.33 & 0.48 by using solvent systems (CH_2Cl_2: MeOH 95:5) & (CH_2Cl_2: MeOH 85:15); ^{1}H-NMR ($CDCl_3$, 400 MHz): δ_H 5.34 (1H, m, H-6) *J*=5.2 H_Z), 4.44 (2H, dd, *J*= 2.5, 11.77, H-6′), 4.22 (1H, m, H-1′), 3.64 (1H, m, H-3), 2.36 (2H, m, H-4) *J*=5.2 H_Z), 2.13 (2H, m, H-15), 1.95 (1H, m, H-14), 1.81 (2H, m, H7), 1.64 (4H, m, H-2, H-12), 1.64 (1H, m, H-25), 1.48 (2H, m, H-11), 1.43

(1H, m, H-20), 1.30 (4H, m, H-1, H-28), 1.30 (1H, m, H-8), 1.24 (4H, m, H-16, H-23), 1.16 (1H, m, 17), 0.66 (3H, s, H-18), 0.92 (3H, s, H-19), 0.96 (3H, m, H-21), 0.90 (1H, m, H-24), 0.97 (3H, t, J = 7.2 Hz, H-29), 0.90 (3H, d, J = 8 Hz, H-27), 0.83 (3H, d, J = 8 Hz, H-26), 0.84 (1H, m, H-9), 2.91-3.36 (sugar protons; ESI-MS in positive mode MS *m/z* (relative abundance %): 577 (M^+ +1, 100.00) and 415 (M^++H - 162, 16.23).

Text S10: Identification of phenolic acids and phenolic acid glycosides:

Compounds 1 and **3** showed molecular ion peaks at *m/z* 137, and 153 $[M-H]^+$ and base peak fragments at *m/z* 93 [M-H-COO] and 109 were suggested to be hydroxybenzoic acid and protocatecheic acid, respectively.[1] In addition, **compound 6** was identified as coumaric acid from MS^1 at *m/z* 163 $[M-H]^+$ and MS^2 at *m/z* 119 due to loss of carboxylic group.[2] Finally, **compound 22** exhibited $[M-H]^-$ at *m/z* 301 and MS^2 base peak fragment ion at *m/z* 139 (100%) in addition to fragments at *m/z* 256 (35%) and 228 (30%), comparing these results with those previously published data, compound **22** was identified as ellagic acid.[2] All the above compounds were identified for the first time in *M. macroura*.

The molecular ion $[M-H]^+$ of **compound 23** was observed at *m/z* 355, and the base peak at *m/z* 193.3 was detected due to the loss of glucoside unit (162 amu) in the MS^2 spectrum. Hence, this compound was identified as ferulic acid-*O*-glucoside.[2] Additionally, **compound 29** showed a molecular ion peak at *m/z* 329 $[M-H]^+$, MS^2 at *m/z* 287 attributed to $[M-H-COCH_3]$, which suggested to be phloracetophenone-4-*O*-glucoside,[3] and it was isolated as a pure compound in the current work. However, To our knowledge, ferulic acid-O-glucoside and phloracetophenone-4-*O*-glucoside, were identified for the first time in the family Moraceae.

Text S11: Identification of other phenolic compounds

Compound 4 showed a molecular ion peak at *m/z* 339 $[M-H]^+$ and fragment ion at *m/z* 177 (loss of 163 amu), besides other diagnostic peaks for morachalcone A at *m/z* 175, 161, 135, 109.[4] Moreover, compound **47** showed a molecular ion peak at *m/z* 391 $[M+H]^+$ and significant MS^2 fragment ion at *m/z* 279 that attributed to dibutyl phthalate, 167 corresponding to phthalic acid and base peak at *m/z* 149, this compound was suggested to be bis (2-ethyl hexyl) phthalate,[5] which was isolated as a pure compound in this work. All compounds are the first report in *M. macroura*, while bis (2-ethyl hexyl) phthalate is identified for the first time in the family Moraceae.

Text S12: Identification of flavonoid aglycones

The deprotonated molecular ion at *m/z* 301 was detected for compounds **25** and **26**, where, **peak 25** which showed MS^2 fragmentation at *m/z* 179, 151, and 121, was suggested to be quercetin. However, MS^2 fragment ions at *m/z* 256, 151, 107 were matched with morin (**26**). [2] Thus, these compounds were identified for the first time in *M. macroura*.

Text S13: Identification of flavonoid *O*- and C-glycosides:

Five peaks **5, 10, 15,** and **24** at R_t 6.27, 7.62, 8.53, 8.96, and 12.17 min, respectively, showed the same molecular ion peak at *m/z* 431 $[M-H]^-$. Where peaks **5, 15** were identified as apigenin-*O*-glucoside and its isomer depending upon MS^2 fragmentation that gave a base peak at *m/z* 269 by the loss of glucosyl residue (162 amu). [6] While MS^2 of compound **10** gave fragment ions at *m/z* 269.0 [M-H-162], 341 $[M^+-H-90]$, and 311 $[M^+-H-120]$ that are characteristic features for mono-*C*-glucoside flavonoid. Moreover, the absence of fragment at [M-H-18] indicated the presence of 8-C- glucoside; therefore, peak **10** was confirmed to be apigenin-8-C-glucoside. [7] Additionally, compound **24** was suggested to be kaempferol-*O*-rhamnoside (afzelin) through MS^2 fragment ions at *m/z* 285**,** 284 [Loss of sugar moiety], 255, 227. [8] Moreover, compounds **8, 16, 17,** and **20,** displayed at retention time 7.26, 8.71, 9.24, 9.24, and 11.14 min, respectively, have the same [M-

H]$^-$ at *m/z* 447 with different MS^2 fragmentation patterns. Where, MS^2 of compound 8 exhibited fragment ions at *m/z* 285 due to loss of glucosyl moiety (162 amu), 257, and 242.5, [6] hence it was identified as luteolin-7-O-glucoside**.** Furthermore, compound **16** showed MS^2 fragment ion at *m/z* 285 (100%) and 284; therefore, this compound was confirmed to be kaempferol-3-*O*-glucoside. [2] Also, compound 17 showed MS^2 fragment ion at *m/z* 301 [M-H-rham] and 343 [M-H-104] for [aglycone + 41], which is a characteristic feature of mono-*C*-rhamnoside flavonoid. Moreover, the absence of fragment at [M-H-18] indicated the presence of 8-C- rhamnoside , [7] so it was identified as quercetin-8-C-rhamnoside. However, compound **20** was identified as quercetin-3-*O*-rhamnoside (quercitrin), depending on the MS^2 fragmentation pattern with characteristic ions at *m/z* 301 and 255. [9] **Compound 18** (R_t, 10.95 min) was suggested to be hesperidin which was confirmed by the [M+H] ion at *m/z* 611 and MS^2 fragments at *m/z* 303 [M-H-rutinosyl moiety, 308 amu]. [10] In addition, three **compounds**, **11**, **13,** and **14,** have the same molecular ion peak at *m/z* 463 [M-H] $^+$**, compound 11** was identified as morin-3-*O*-glucoside from MS^2 fragmentation that showed fragment ions at *m/z* 301, 257**. Compound 13** was identified as quercetin-3-*O*-glucoside from MS^2 that showed a base peak at *m/z* 301, indicating the loss of glucose moiety leaving quercetin aglycone. [2]Additionally, compound **14** was suggested to be quercetin-3-O-galactoside (Hyperoside) according to MS^2 fragmentation that displayed ion at *m/z* 301. [11] In addition, compound 38 was identified as chrysoeriol-uronic acid according to the molecular ion peak at *m/z* 475 [M-H]$^-$ and MS^2 base peak fragment ion at *m/z* 299 [Chrysoeriol aglycone]. [6] **Compound 39 was** identified as naringenin-7-*O*- glucoside, [12] with a molecular ion peak at *m/z* 433 [M-H] $^+$ and MS^2 at *m/z* 271, indicating naringenin moiety. Finally, compound **53** showed a molecular ion peak at *m*/*z* 535 [M+H]$^-$ along with MS^2 data which showed the loss of 218 amu for acetyl glucuronide from the fragment signal at *m/z* 317 [Isorhamnetin aglycone+H] $^+$ and 153**,** [13] so this compound

suggested to be isorhamnetin 3-*O*-acetyl glucuronide. All compounds are the first report in *M. macroura* and the family Moraceae.

Text S14: Identification of prenylated flavonoids:

Compound 34, displayed at R_t 17.83 min, was suggested to be albanin A, which was confirmed by $[M+H]^-$ ion at *m/z* 355 and MS^2 fragment ions at *m/z* 299, 69. [14] Finally, **compound 55** at R_t 24.95 min was suggested to be euchrenone a7 from MS^1 at *m/z* 339 $[M-H]^+$ and MS^2 fragment ion at *m/z* 163 (100%). [15] These prenylated flavonoids were identified for the first time in *M. macroura*.

Text S15: Identification of flavonoid derivatives

Compound 7 was identified as naringenin derivatives from MS^1 at *m/z* 463 $[M-H]^+$ and MS^2 at *m/z* 270.7, indicating naringenin moiety). [7] **Also, compound 38** that detected at at *m/z* 475 $[M-H]^+$ together with a base peak at *m/z* 299 was identified as Chrysoeriol-uronic acid. [6]Moreover, **compound 51** (R_t – 24.14 min) exhibited molecular ion peak at *m/z* 607 $[M+H]^+$ and gave base peak fragment ion in MS^2 at *m/z* 286, indicating the presence of kaempferol aglycone moiety. Therefore, it was tentatively assigned as australisine A. [16]Thus, all compounds were identified for the first time in *M. macroura*.

Text S16: Identification of tannin compounds

Compounds 27 and **28** were suggested to be gallocatechin glycoside and epigallocatechin glycoside, [2] respectively, based on MS^1 at *m/z* 467 $[M-H]^+$ and MS^2 fragments at *m/z* 305 due to loss of glycosyl moiety. Thus, these compounds represent the first report in the family Moraceae.

Text S17: Identification of coumarin compounds

Coumarin compounds were detected in the plant under investigation at different retention times as in compound **2** that identified as aesculin depending upon MS^1 at *m/z* 339 $[M-H]^+$ and MS^2 at *m/z* 177, which attributed to cleavage of glycosidic linkage and loss of glycosyl moiety. [2] In

addition, **compound 9** that displayed MS^1 at *m/z* 355 $[M+H]^+$ and MS^2 at *m/z* 193 due to loss of 162 amu was identified as scopolin. [17]Also, **compound 33,** which detected *m/z* 355 $[M+H]^+$ with MS^2 fragment ion at *m/z* 203 (loss of side chain,152), was identified as epoxybergamottin. [18]All compounds are the first report in *M. macroura*.

Text S18: Identification of anthocyanin derivatives compounds:

Compound 12 showed a molecular ion peak at *m/z* 449 $[M+H]^+$ with MS^2 fragment ion at *m/z* 287 due to loss of glycoside; it has been suggested to be cyanidin-3-*O* glucoside. [1]Additionally, **compound 19** showed a molecular ion peak at *m/z* 610 $[M+H]^+$ and characteristic MS^2 fragment at *m/z* 317.5 due to loss of two molecules of rhamnose (292 amu), 256.8, 151.2, which suggested to be petunidin dirhamnoside. [19] Furthermore, **compound 36** which detected at *m/z* 591 $[M-H]^+$ with MS^2 at *m/z* 287 due to cyanidin moiety, was identified as cyanidin cinnamoyl glucuronide. [20] Also, **compound 42** that identified as malvidin diglucuronide showed MS^1 at *m/z* 683 $[M+H]^+$ and MS^2 at *m/z* 331 attributed to loss of two moieties of glucuronic acid (352 amu). [21]**Compound 44** was identified as cyanidin derivative from MS^1 at *m/z* 683 $[M+H]^+$ and MS^2 at *m/z* 597 (loss of 86), 435 (loss of glucose), 287. [22]Moreover, **compound 48** exhibited protonated molecular ion at *m/z* 593 $[M+H]^+$ with MS^2 at *m/z* 287 due to loss of rutinose, was identified as cyanidin-3-*O*-rutinoside from **Jin *et al.* (2017)**. [1]Additionally, **compound 54** was confirmed as petunidin 3-*O*-acetyl glucuronide based on MS^1 at *m/z* 535 $[M+H]^+$ and MS^2 at *m/z* 317 due to loss of 218 amu attributed to loss of acetyl group and glucuronic moiety (42, 176 amu), 153. [23]Moreover, malvidin-3-*O*-acetyl glucoside was designated for **compound 57** based on molecular ion at *m/z* 535 $[M+H]^+$ and MS^2 at *m/z* 331 due to loss of 204 amu. [24]In addition, **compound 58** that showed a molecular ion at *m/z* 683 $[M+H]^+$ with MS^2 at *m/z* 597 (loss of 86 malonyl moiety), 435 (loss of glucose), 287.7 was proposed to be cyanidin-3-*O*-malonyl glucoside derivative. [25]Also, cyanidin-3-O-

malonyl glucoside was suggested for **compound 59** depending on MS^1 at *m/z* 535 [M+H] and MS^2 at *m/z* 287**. Compound 61** concluded to be cyanidin-3-*O*-hexosyl hexoside according to MS^1 at *m/z* 611 $[M+H]^+$ and MS^2 at *m/z* 449 (loss of glucose). [1]Finally, **compound 62** showed a molecular ion peak at *m/z* 475 $[M-H]^+$ along with MS^2 ions at *m/z* 429 (loss of 46), 299.8 (loss of 176), hence identified as peonidin-3-*O*-glucuronide. [26]All anthocyanin compounds identified for the first time in *M. macroura*.

Text S19: Identification of fatty acids:

Cerotic acid (hexacosanoic acid) was designated for compound **21** according to protonated molecular ion at *m/z* 397 $[M+H]^+$ and MS^2 at *m/z* 351$[M^+-COOH]$. [27]Cerotic acid was isolated as a pure compound from the plant species under investigation **(Compound 4**). However, compound **32** was identified as nonatriacontanoic acid which displayed MS^1 at *m/z* 579 $[M+H]^+$ and it was isolated as a pure compound in the current work **(Compound 2**). [28]Moreover, compound **35** was suggested to be hydroxy octadecatrienoic acid based on MS^1 at *m/z* 293 $[M-H]^+$ and MS^2 at *m/z* 220.8 $[M^+-CH_2-CH_2-COOH]$**.** [29]Furthermore, compound **43** was identified as melissic acid (triacontanoic acid) depending upon MS^1 at *m/z* 451 $[M-H]^+$ and MS^2 fragmentation at *m/z* 249.8, 390.5 $[M^+-COOH-CH_3]$, 406.7 $[M^+-COOH]$, 435.1 $[M^+-H-CH_3]$, [30]and it was isolated as a pure compound in our work **(Compound 3**). **Compound 45** showed a molecular ion peak at *m/z* 255 $[M-H]^+$ which suggested to be palmitic acid, [28]and it was isolated as a pure compound in the current work **(Compound 5**). Oleic acid was designated for compound **46** which showed a molecular ion peak at *m/z* 281 $[M-H]^+$. [28]Finally, compound **52** was proposed to be octadecanoic acid according to MS^1 at *m/z* 283 $[M-H]^+$ and MS^2 at *m/z* 239 [M-H-COO]. All compounds identified for the first time in *M. macroura*. Nonatriacontanoic, hydroxyl octadecatrienoic and melissic acids are first report in Moraceae family**.**

Text S20: Identification of fatty acids derivatives

Compound 41 suggested to be palmitic acid ester based on MS^1 at *m/z* 475 $[M-H]^+$ besides MS^2 fragment ion at *m/z* 255**.** [28]Also, compound **50** was identified as oleic acid ester which displayed molecular ion at *m/z* 395 $[M-H]^+$ and MS^2 at *m/z* 281. [28]All these fatty acid esters are identified for the first time in *M. macroura*.

Identification of steroid and triterpenoid compounds

Compound 40 that exhibited a molecular ion peak at *m/z* 381 $[M+H]^-$ with distinctive fragment ions at *m/z* 318, 163, 139, 71, 69, was identified as brasicasteol**.** [31]Also, **compound 56** which showed a molecular ion at *m/z* 414 $[M+H]^-$ along with characteristic fragment ion at *m/z* 254.9 was identified as *β*-sitosterol. Moreover, 24-Methylene ergosta-5-en-3*β*-Ol was designated as compound **63** which showed MS^1 at *m/z* 398 and MS^2 at *m/z* 381 $[M-H_2O+H]^+$, 281 $[M-C_7H_{13}-H_2O-2H]^+$. [31]Also, compound **64** showed a molecular ion peak at *m/z* 455 $[M-H]^-$ which suggested to be oleanolic acid.[28]All compounds identified for the first time in *M. macroura*. Cholesterol, brasicasteol and 24-Methylene ergosta-5-en-3*β*-Ol were reported for the first time in family Moraceae.

Text S21: Identification of steroid and triterpenoid derivatives

β-sitosterol-3-*O*-D-glucoside, [32]was assigned for compound **30**, based on deprotonated molecular ion at *m/z* 575 $[M-H]^-$ and it was isolated as a pure compound in this work (**Compound 10)**. Finally compounds **31 and 60** were identified as lupeol acetate and lupeol palmiteolate**,** [33]based on MS^1 at *m/z* 467 $[M-H]^-$ and 663$[M+H]^-$ and both compounds were isolated in pure form during the current study and designated as (**Compound 7**) and **(Compound 6)**, respectively. All compounds identified for first time in *M. macroura.*

Text S22: Identification of hydrocarbons and sugars

Compound 49 was identified as pentacos-7-ene, [34]from MS^1 at *m/z* 349 $[M-H]^-$ and it was isolated as a pure compound in the current work and is identified for the first time in family Moraceae.

In conclusion, the major compounds in DCM-L fraction are cyanidin-3-*O*-malonyl glucoside and its derivatives, cyanidin rutinoside, chlorogenic acid, quercetin-*O*-glucoside, kaempferol-*O*-glucoside, 24-Methylene-ergosta-5-en-3*β*-Ol, isorhamnetin-3-*O*-acetyl glucuronide, bis (2-ethyl hexyl) phthalate and morin-*O*-*β*-glucoside. On the other side, cyanidin-3-*O*-malonyl glucoside, melissic acid, phloracetophenone-4-*O*-glucoside, 24-methylene-ergosta-5-en-3*β*-Ol, cerotic acid, and bis (2-ethyl hexyl) phthalate are the most abundant constituents in DCM-S fraction. The major flavonoids that present in the DCM -L and absent in the DCM-S are quercetin-*O*-glucoside, kaempferol-*O*-glucoside, morin-*O*-*β*-glucoside, naringenin derivatives, apigenin-8-C-glucoside, luteolin-7-*O*-glucoside, quercetin-8-C-rhamnoside, and quercetin-3-*O*-*β*-rhamnoside. These results agree with **Jin et al. (2015),** [35]and could give insights into the possible potentials of these fractions as an anti-depressant and cardioprotective against ISO induced post-MI depression rat model.

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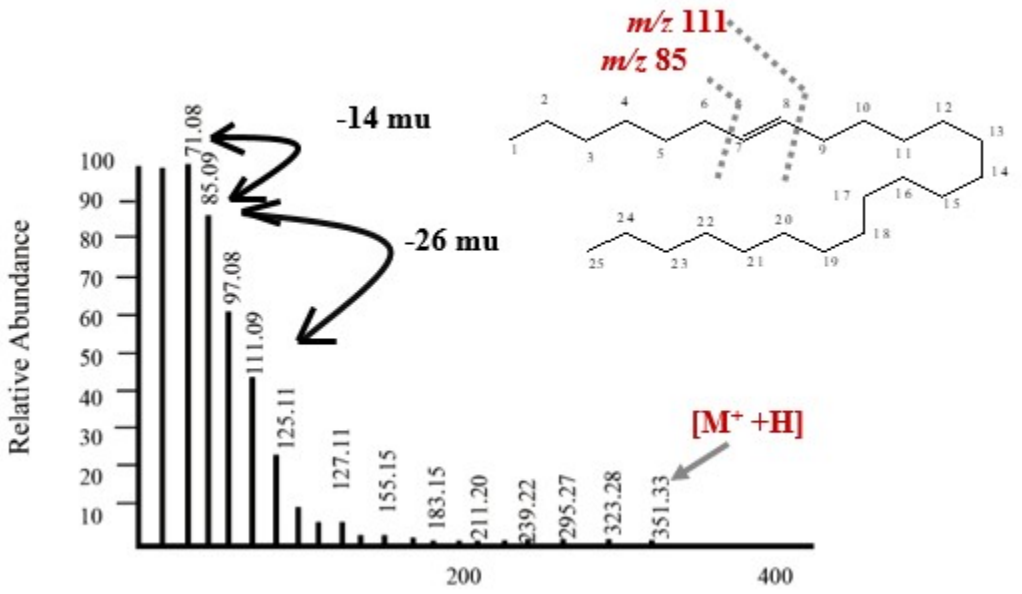


Figure (S1): EI-MS spectrum of compound "1".

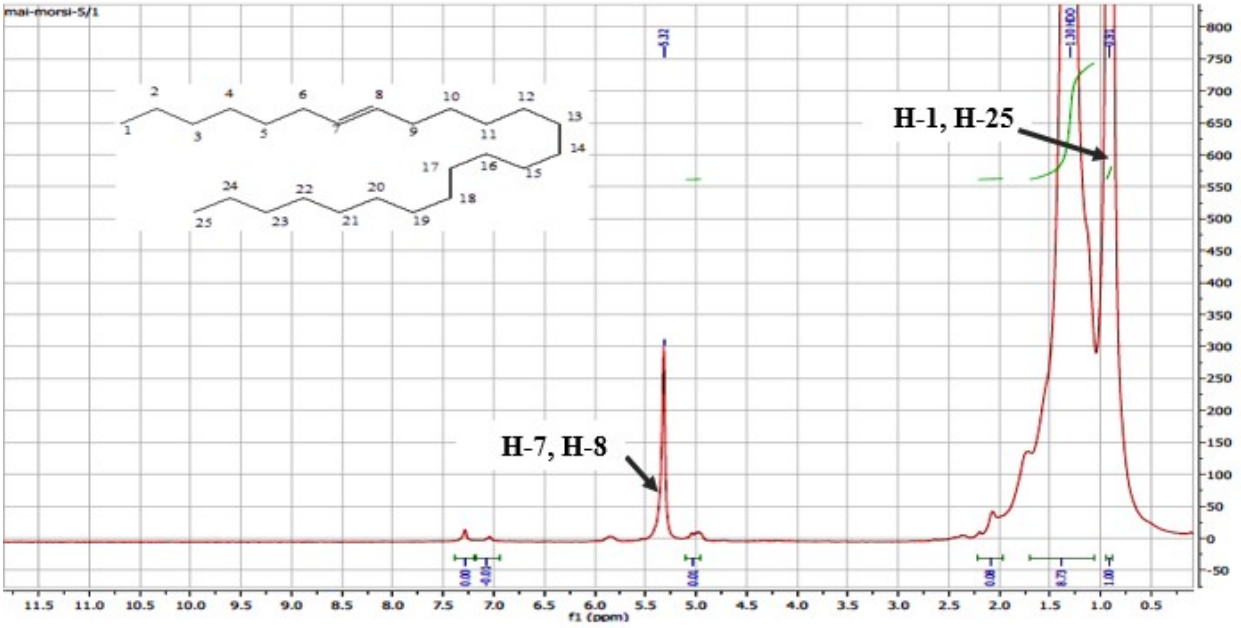


Figure (S2): ^{1}H-NMR spectrum of compound "1".

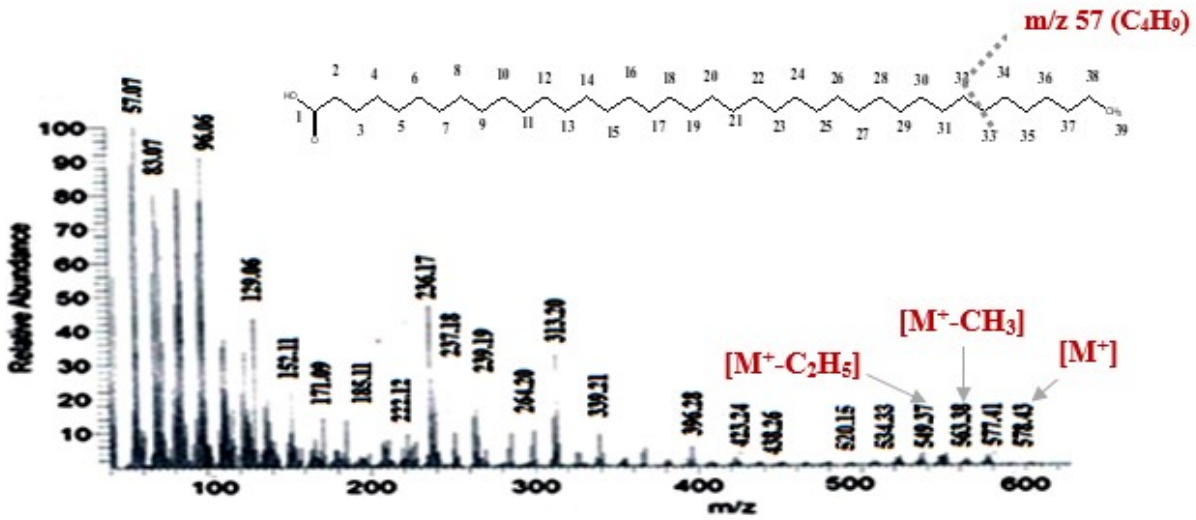


Figure (S3): EI-MS spectrum of compound "2".

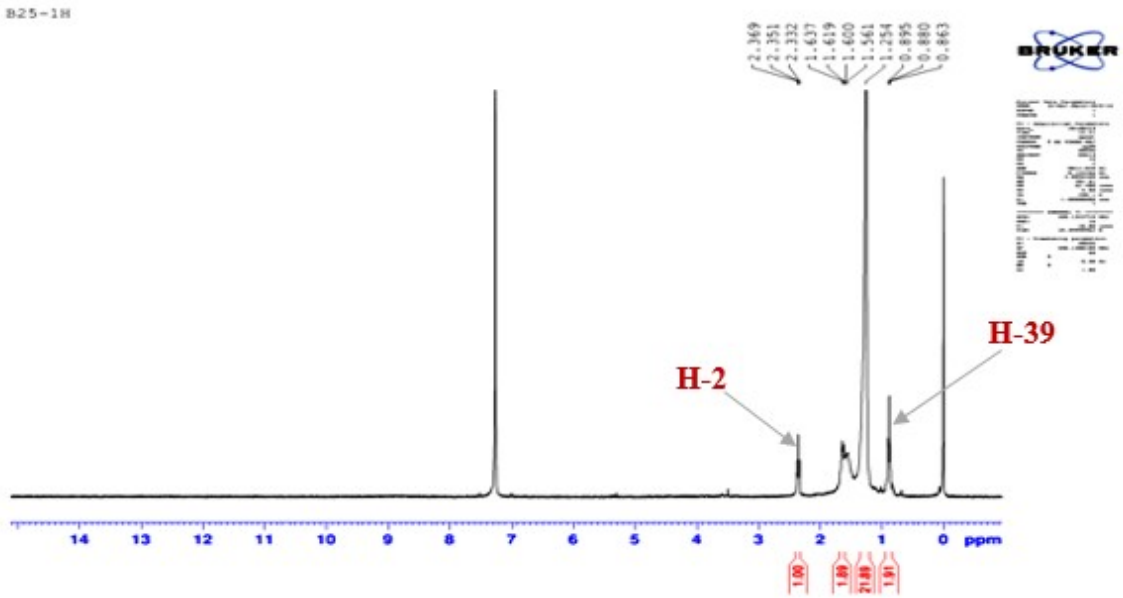


Figure (S4): ^{1}H-NMR spectrum of compound "2".

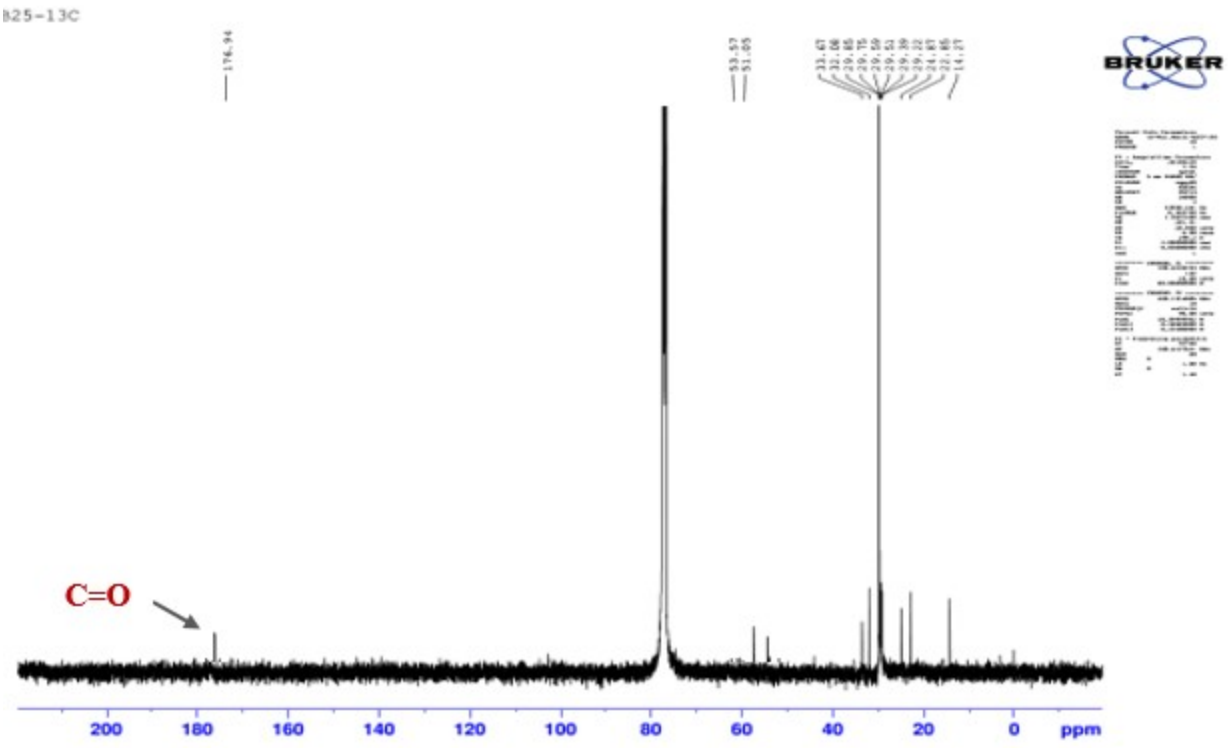


Figure (S5): ^{13}C-NMR spectrum of compound "2".

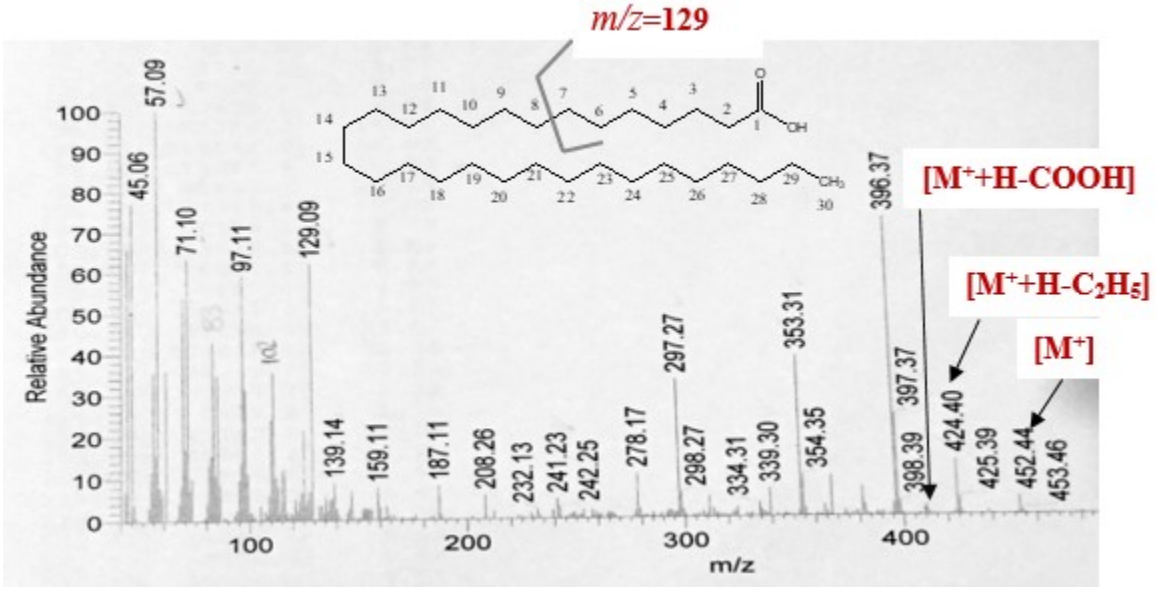


Figure (S6): EI-MS spectrum of compound "3".

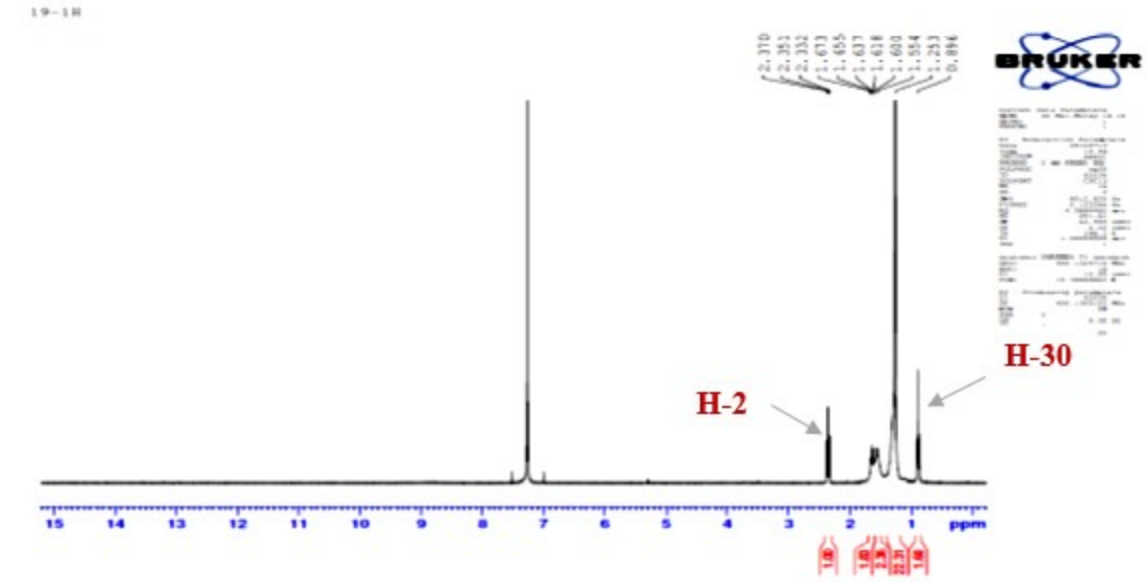


Figure (S7): ^{1}H-NMR spectrum of compound “3”.

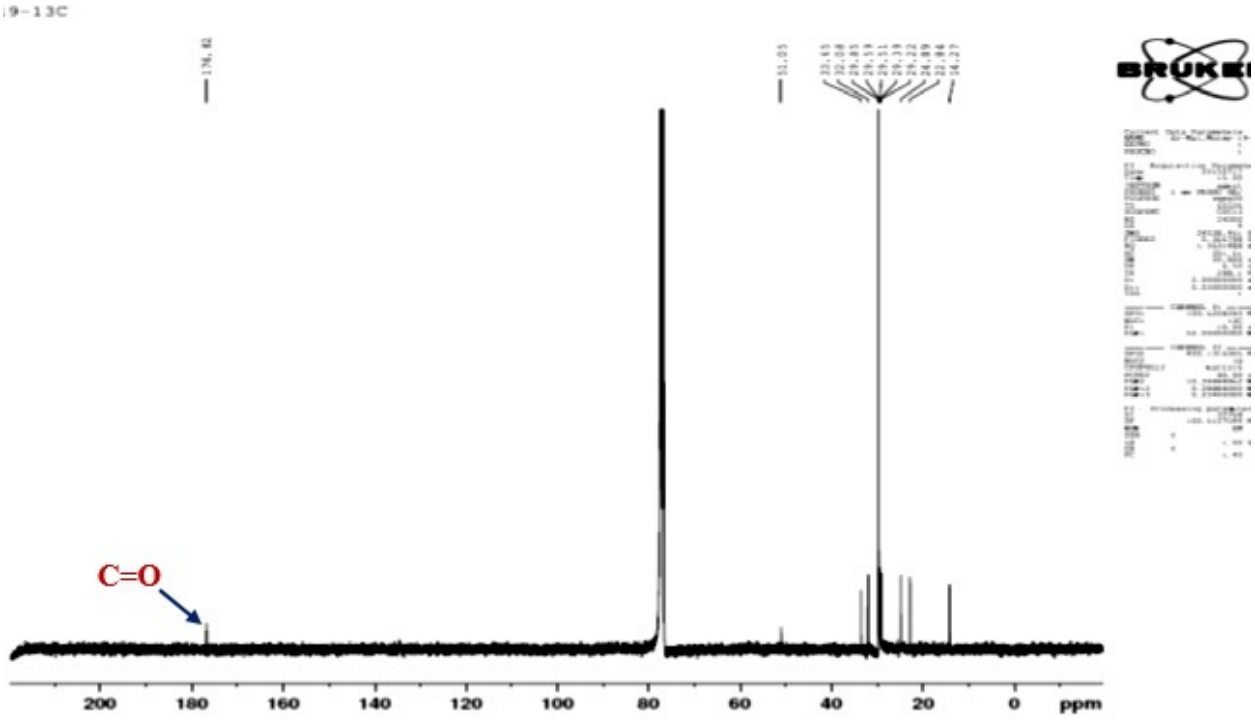


Figure (S8): ^{13}C-NMR spectrum of compound “3”.

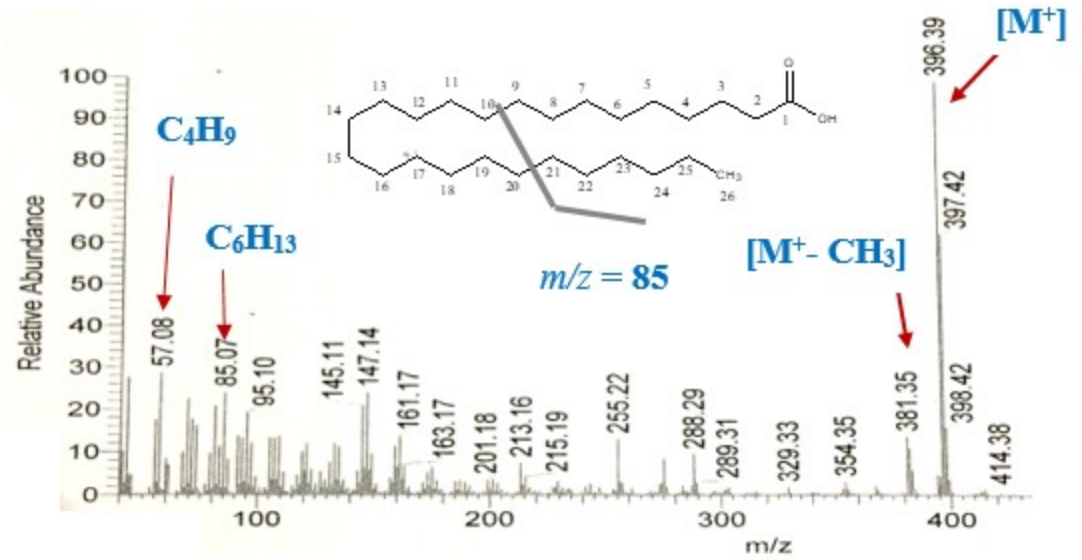


Figure (S9): EI-MS spectrum of compound "4".

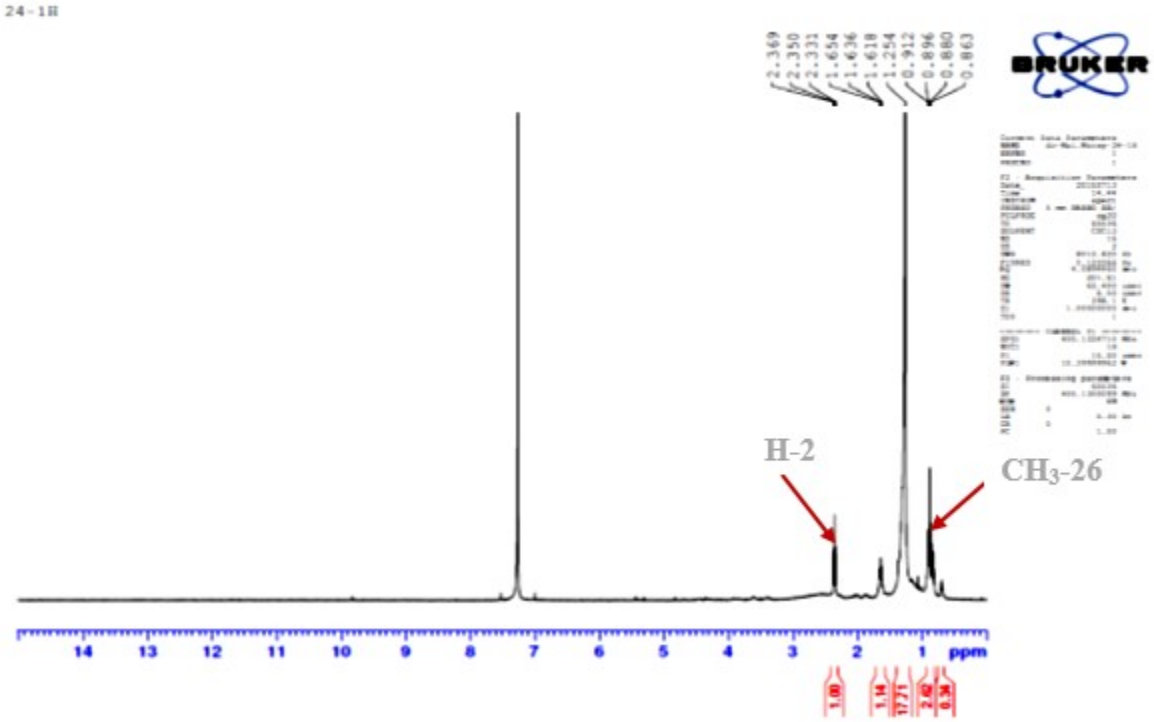


Figure (S10): ^{1}H-NMR spectrum of compound "4".

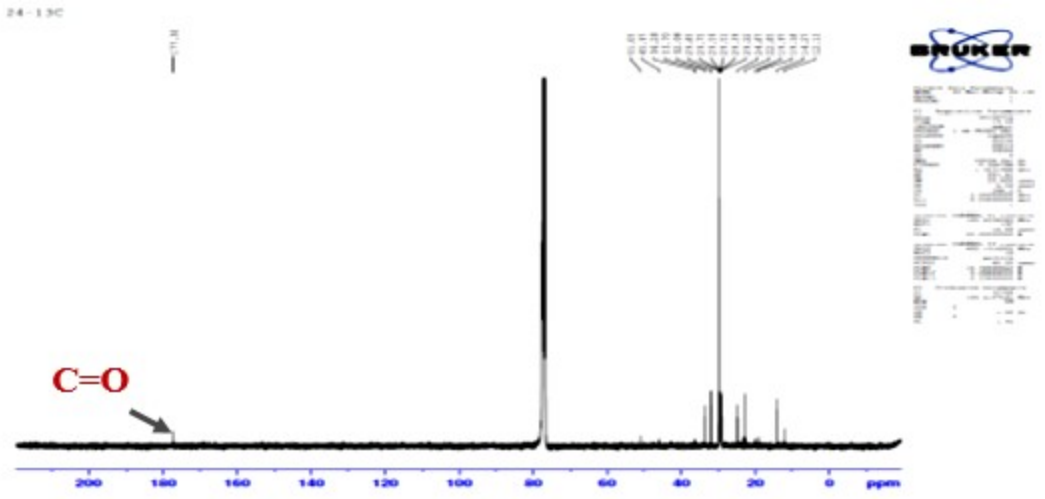


Figure (S11): ^{13}C-NMR spectrum of compound "4".

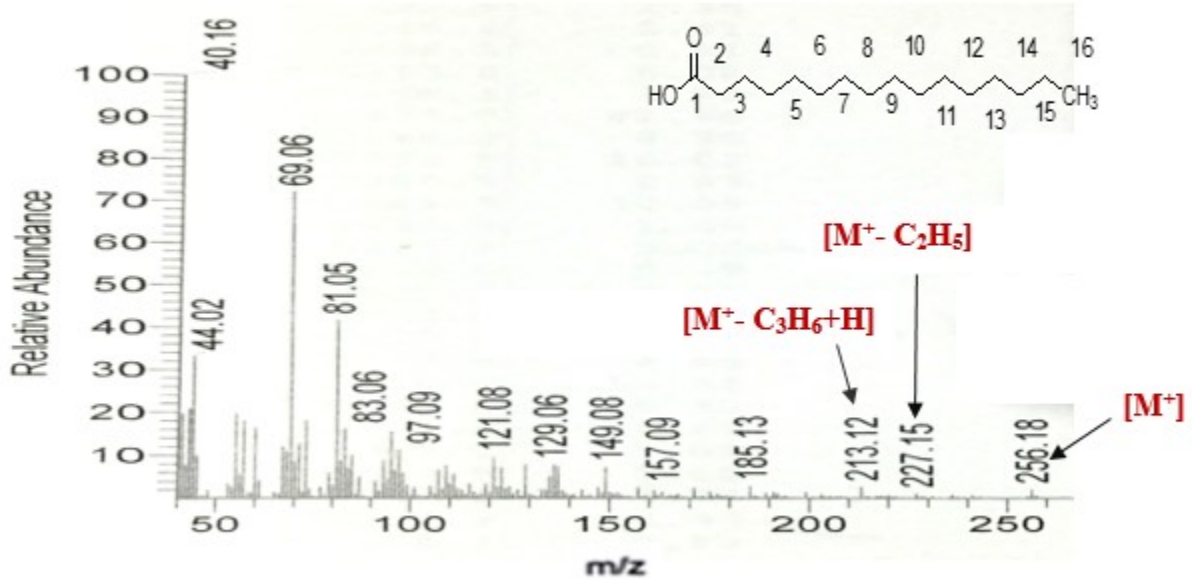


Figure (S12): EI-MS spectrum of compound "5".

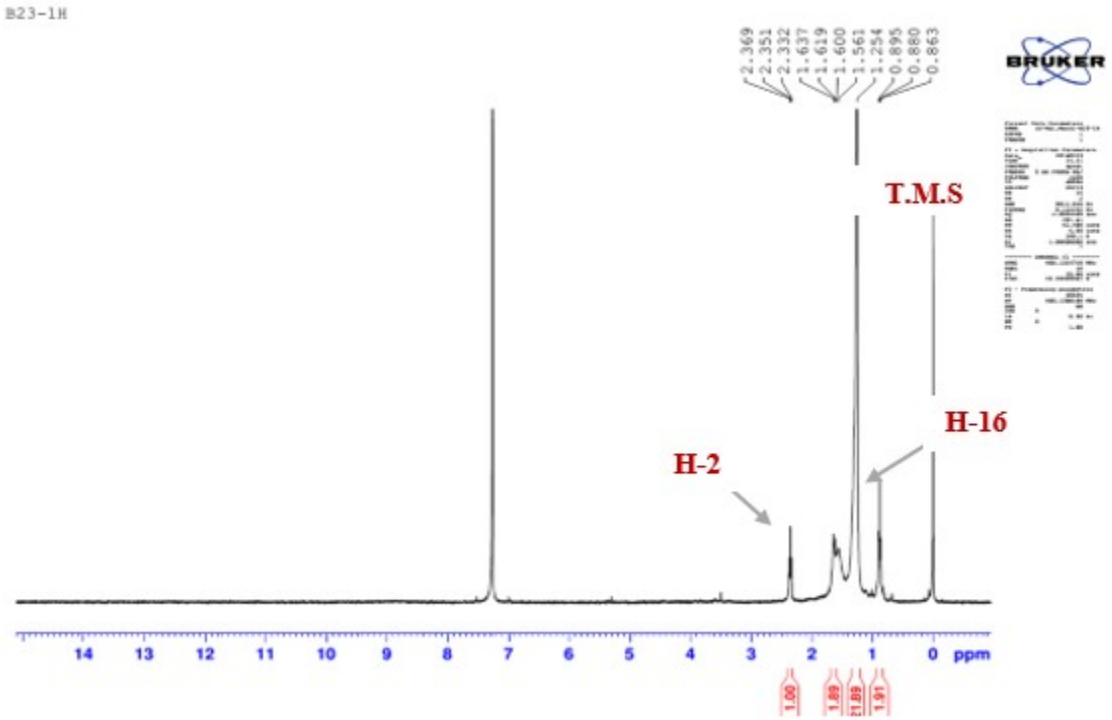


Figure (S13): ^{1}H-NMR spectrum of compound "5".

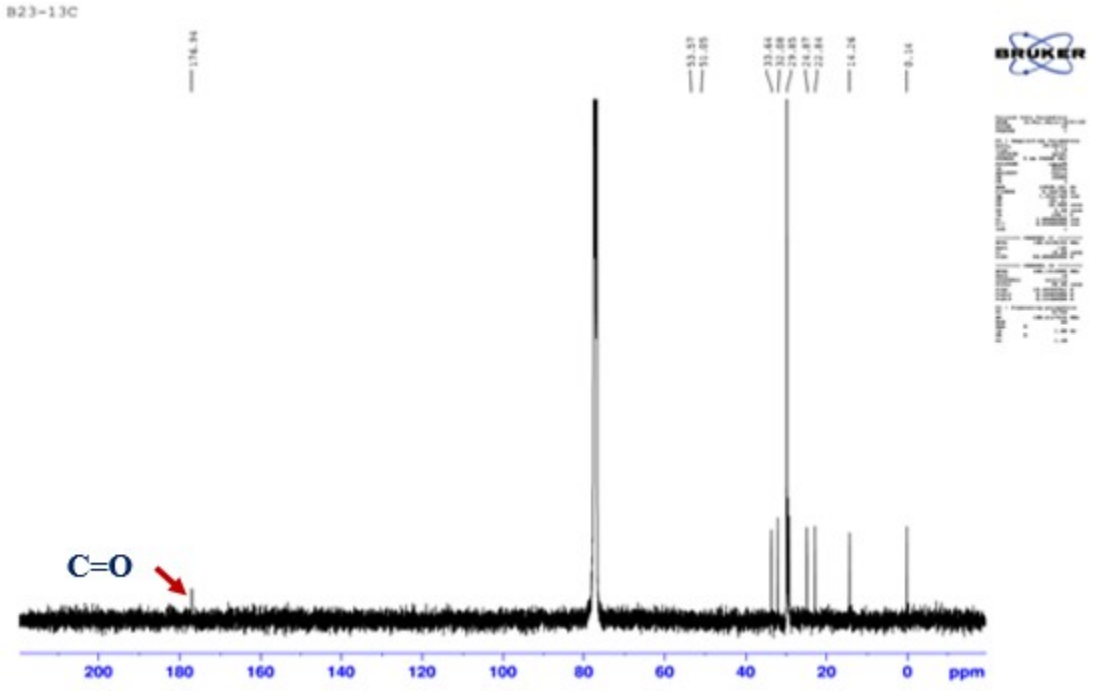


Figure (S14): ^{13}C-NMR spectrum of compound "5".

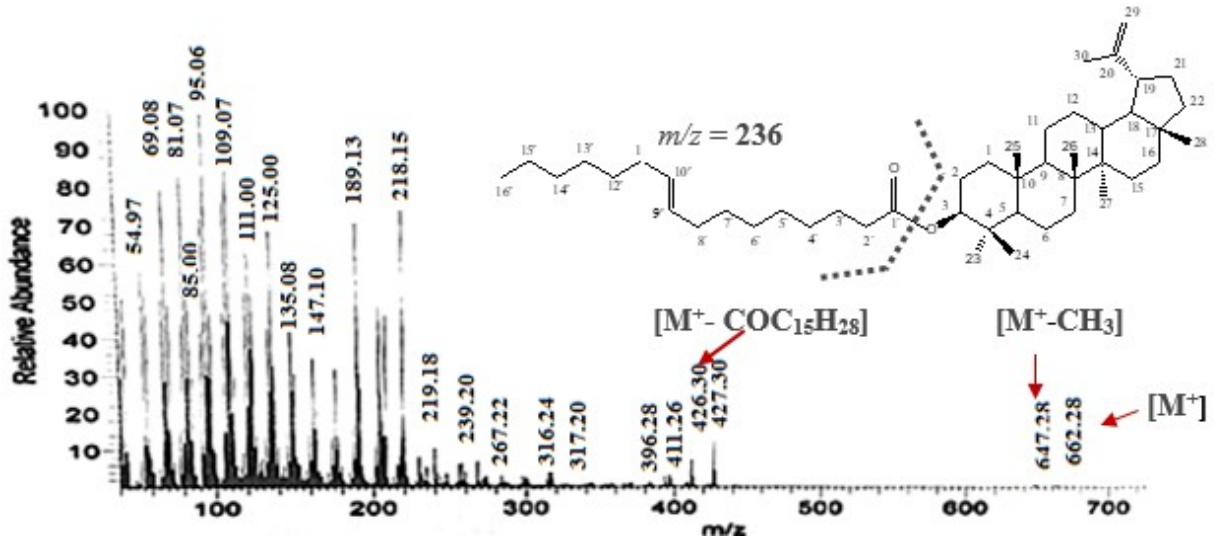


Figure (S15): EI-MS spectrum of compound "6".

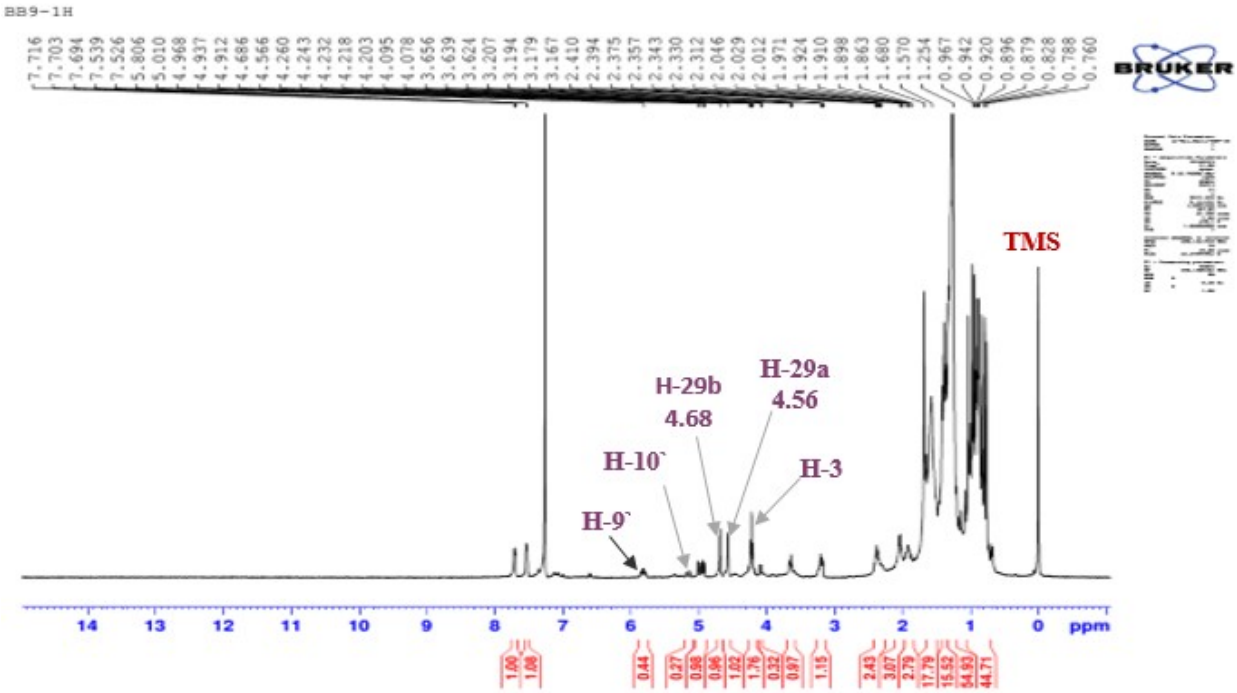


Figure (S16): ^{1}H-NMR spectrum of compound "6".

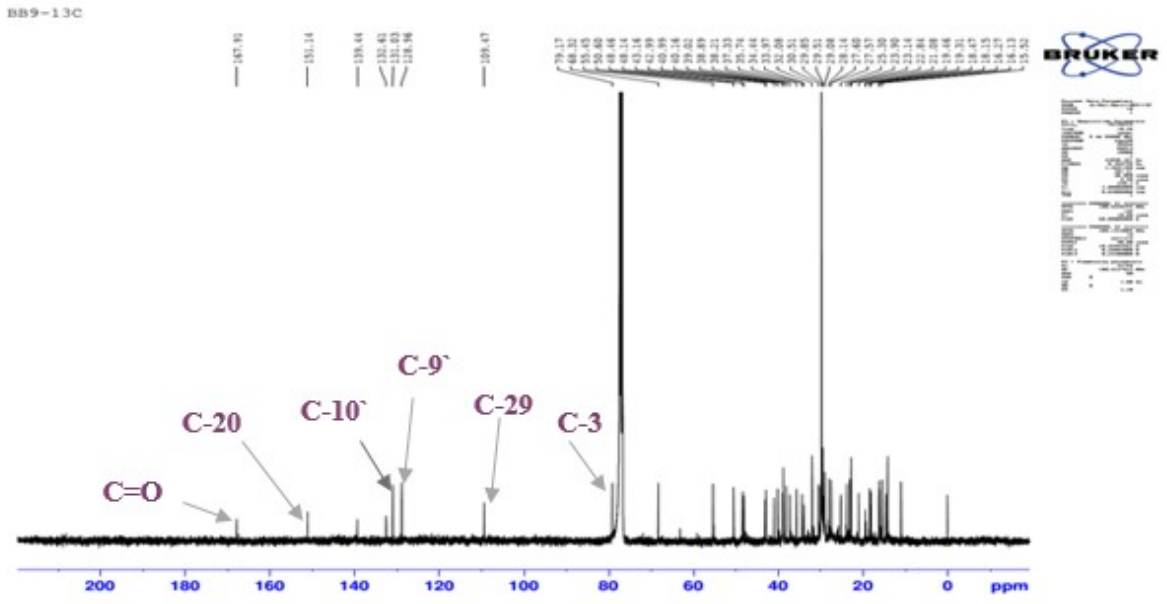


Figure (S17): ^{13}C-NMR spectrum of compound "6".

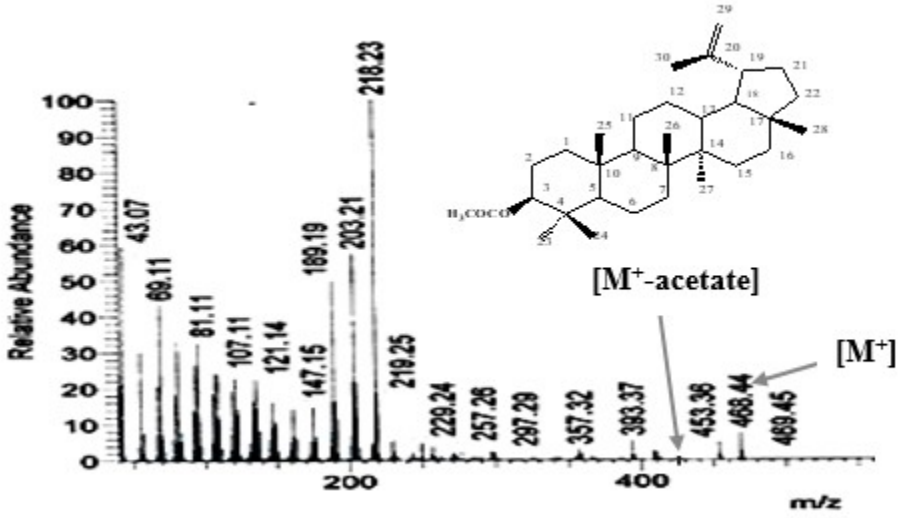


Figure (S18): EI-MS spectrum of compound "7".

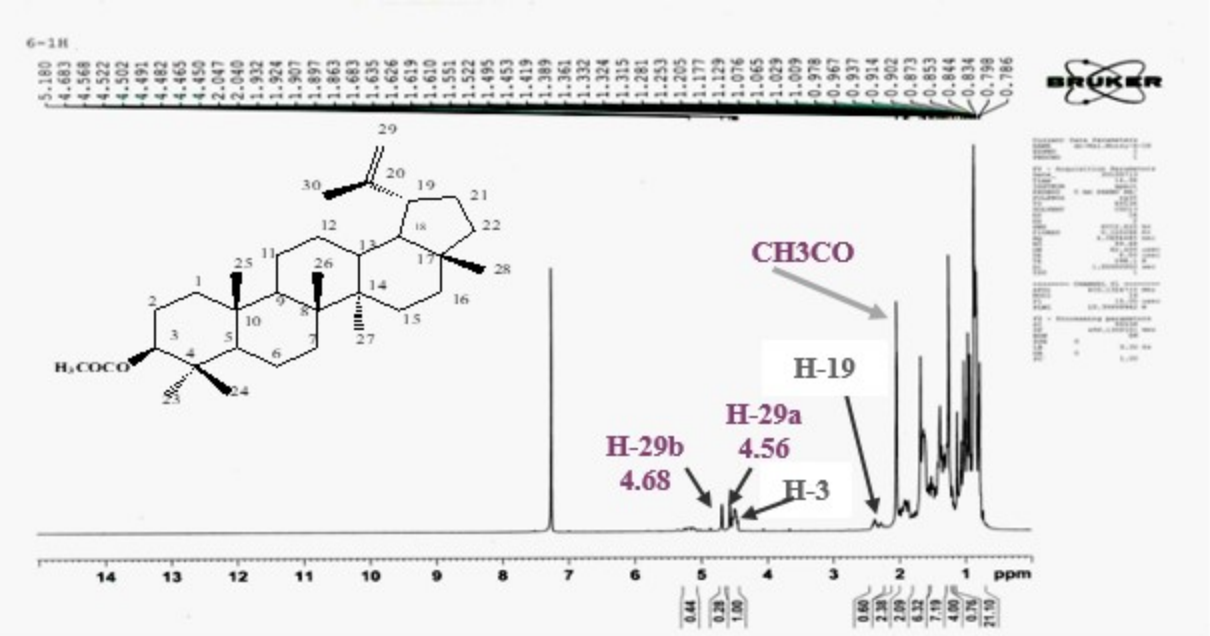


Figure (S19): ^{1}H-NMR spectrum of compound "7".

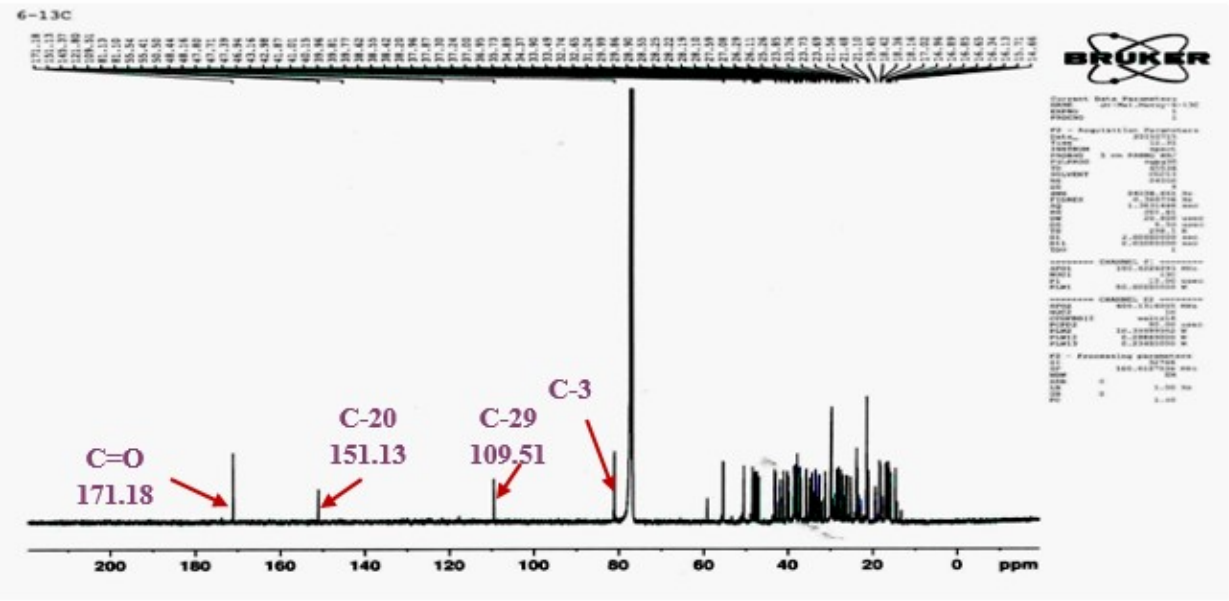


Figure (S20): ^{13}C-NMR spectrum of compound "7".

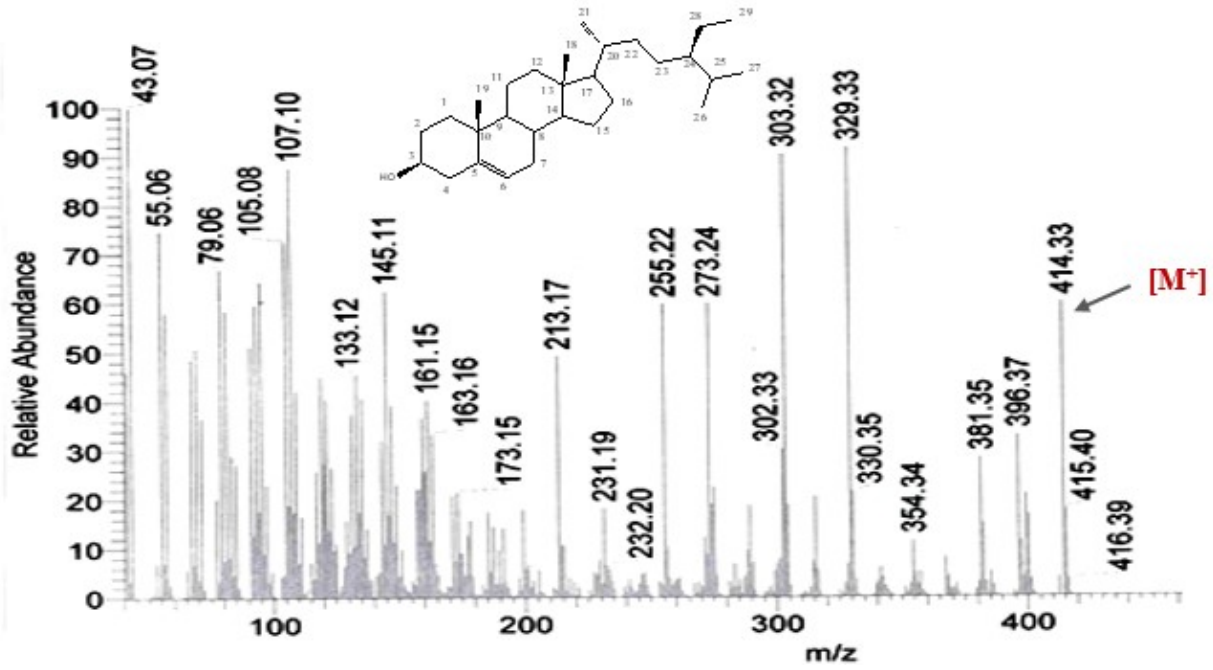


Figure (S21): EI-MS spectrum of compound "8".

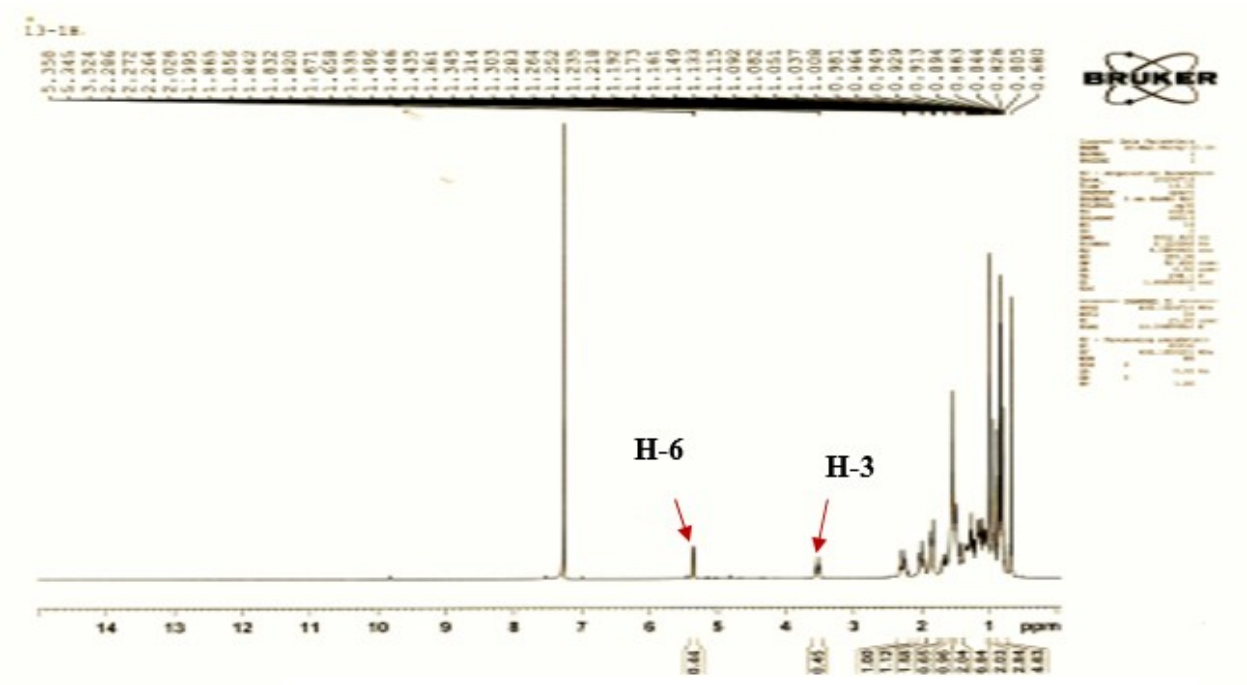


Figure (S22): ^{1}H-NMR spectrum of compound "8".

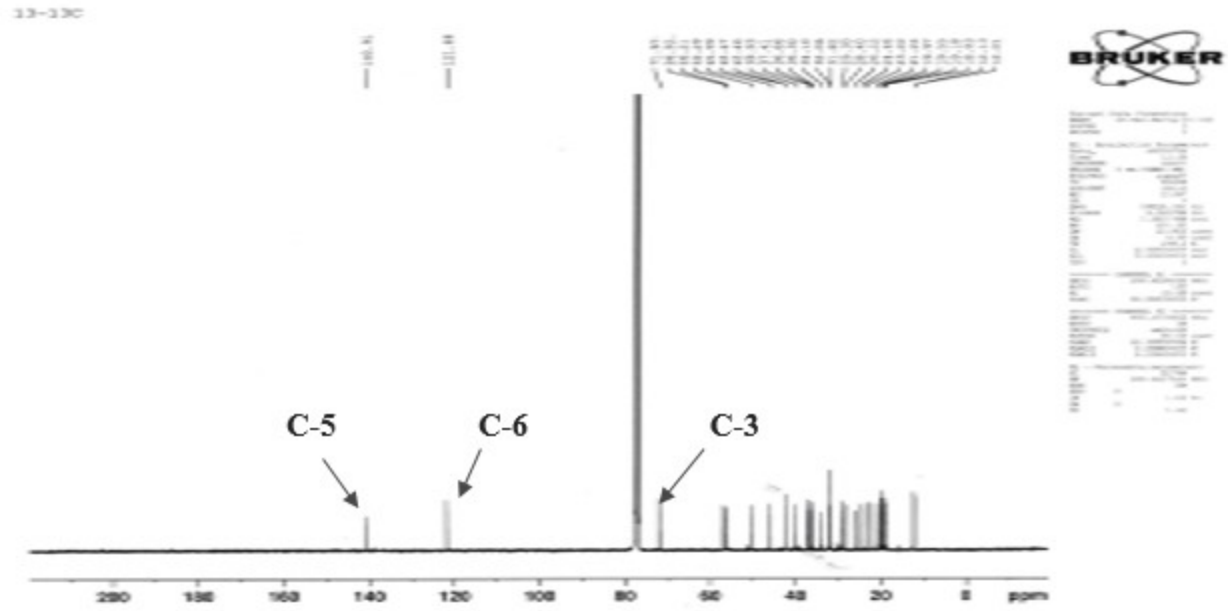


Figure (S23): ^{13}C-NMR spectrum of compound "8".

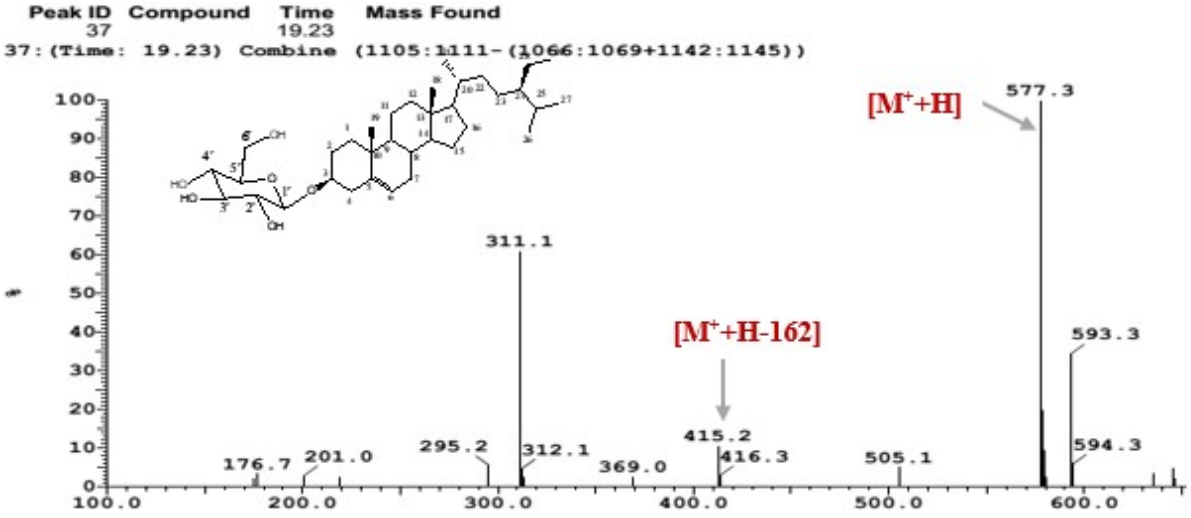


Figure (S24): ESI-MS spectrum (positive mode) of compound "9".

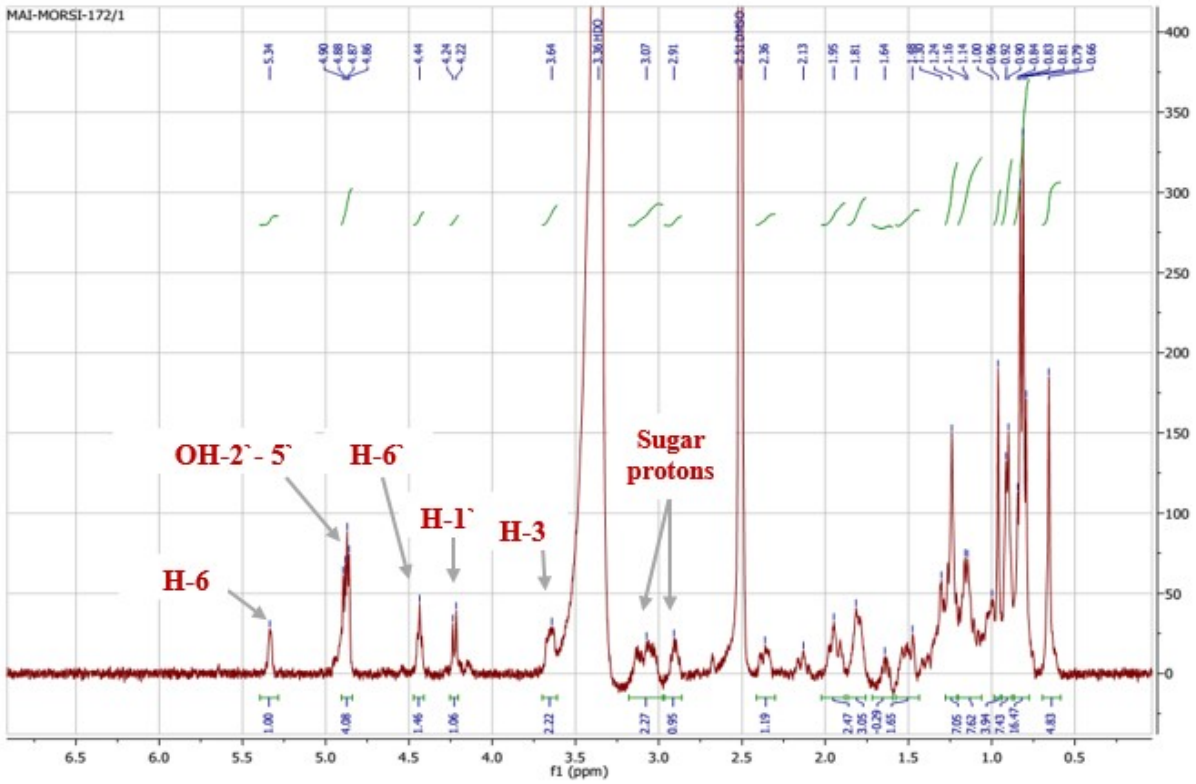
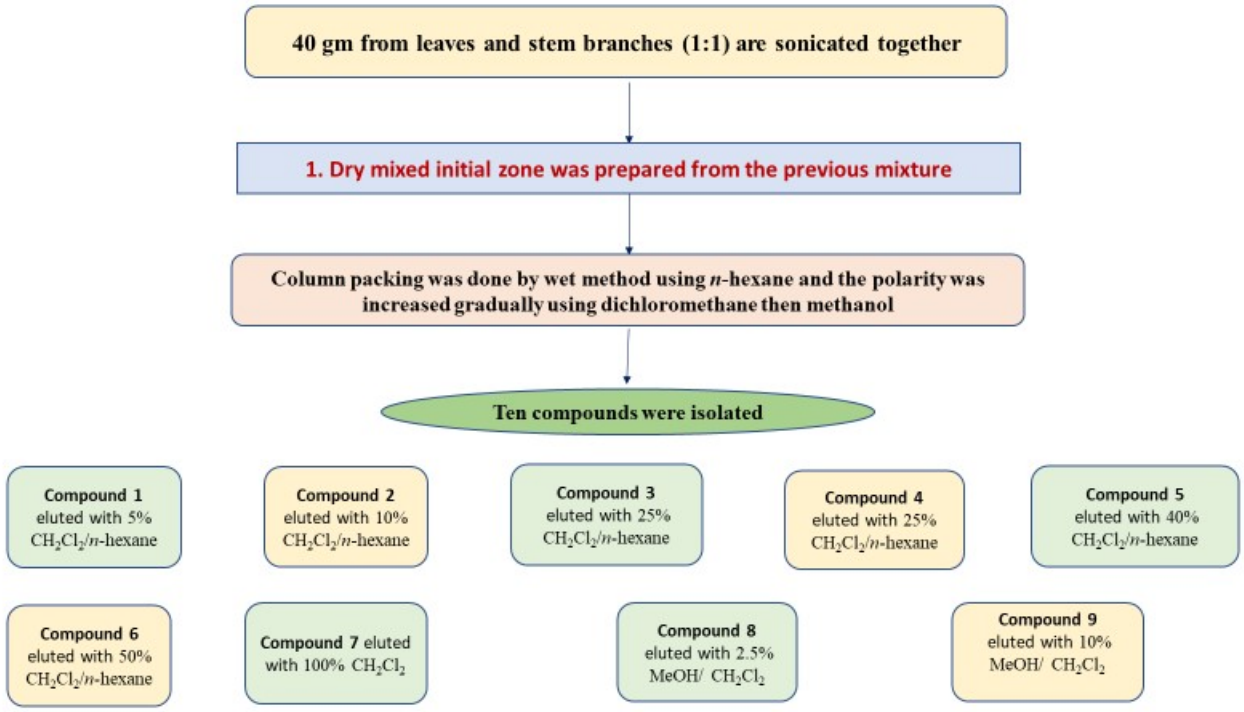


Figure (S25): ^{1}H-NMR spectrum of compound "9".



Scheme S1: Column chromatography for isolation of secondary metabolites from DCM fractions mixture of *M. macroura* leaves and stem branches.