

SUPPLEMENTARY INFORMATION

Manuscript title: Lupane triterpenes from the leaves of the tropical rain forest tree *Hopea odorata* Roxb. and their cytotoxic activities.

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Contents (S1 to S are the page numbers)

S1 – Title, authors and description of Supplementary information content.

S2-S3 – Evaluation of the cytotoxic activities of isolated lupanes: Experimental details and summary of results.

S4-S8 – Purification and identification of isolated compounds: Experimental with full physical and spectroscopic data for compounds **1-8**, including a complete assignment of ¹H and ¹³C NMR data for lupanes **6-8**.

S9-S35 – Original spectroscopic data:

S9 – MS (ESI-), ¹H, ¹³C and HSQC edit spectra of compound **1**.

S12 – MS (ESI-), ¹H and ¹³C spectra of compound **2**.

S14 – MS (ESI-), ¹H and ¹³C spectra of compound **3**.

S16 – MS (ESI+), ¹H and ¹³C spectra of compound **4**.

S18 – MS (ESI+), ¹H and ¹³C spectra of compound **5**.

S21 – MS (ESI-), ¹H, ¹³C, HSQC edit, HMBC and NOESY spectra of compound **6**.

S25 – MS (ESI+), ¹H, ¹³C, HSQC edit and NOESY spectra of compound **7**.

S28 – MS (ESI-), ¹H, ¹³C and HSQC edit spectra of compound **8**.

S30 – MS (EI), ¹H, ¹³C and HSQC edit spectra of compound **9**.

S34 – MS (EI), ¹H and ¹³C spectra of compound **10**.

Evaluation of the cytotoxic activities of isolated lupanes: Experimental details and summary of results.

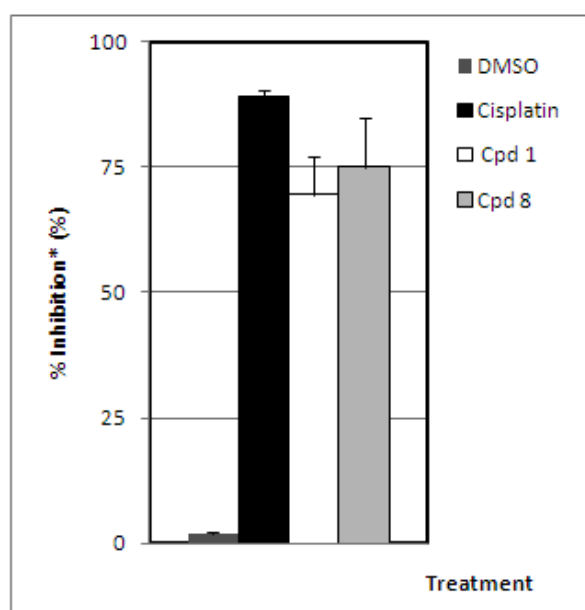
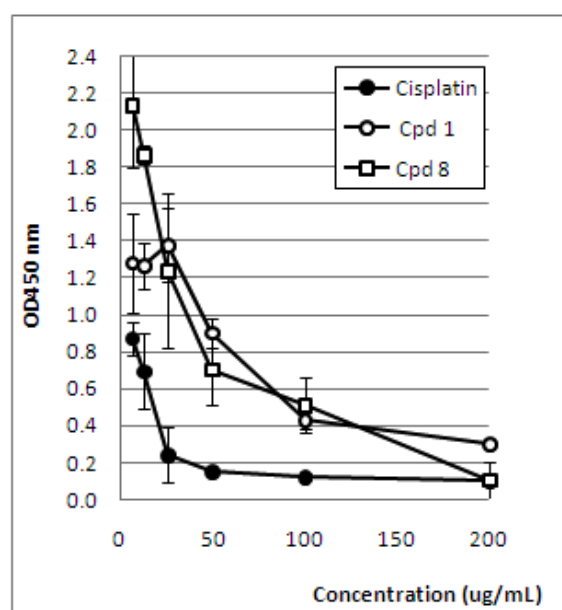
Materials. Dulbecco's Modified Eagle's Medium (DMEM), fetal bovine serum (FBS), penicillin, streptomycin, trypsin/EDTA were purchased from Invitrogen (Carlsbad, CA, USA), WST-1 solution were purchased from Roche Applied Science (Meylan Cedex, France).

In vitro cytotoxic assay. The cytotoxic effects of isolated lupanes on various human cancer cell lines were evaluated using WST-1 method, as previously described (Ishiyama et al., 1996; Tsai et al., 2011). Different human cancer cell lines (*i.e.* prostate cancer cell line (PC3), human breast adenocarcinoma cell line (MDA-MB-231), colorectal adenocarcinoma cell line (HT-29) and colorectal carcinoma cell line (HCT 116)), were selected and seeded onto 96-well plates at a cell density of 5,000 cells/well in 5% CO₂ incubator at 37°C. After 24 h incubation, cells were exposed to various concentrations of each compound **1** to **8** (3 wells for each dilution) for 24 hr. Then, the tetrazolium salt WST-1 solution was added and cultured for further 4 h. To determine the cell survival, Optical Density (OD) was measured with a Bio-Rad Coda microplate analyzer at a wavelength of 450 nm (reference wavelength: 600 nm). Cisplatin was used as a positive control. Results presented in Table 2 were expressed as IC₅₀, the concentration required for 50% inhibition cell growth of treated cells compared to untreated controls. Dose-response curves of the active lupane triterpenes against human cancer cell line compared to cisplatin were shown in Figure 4.

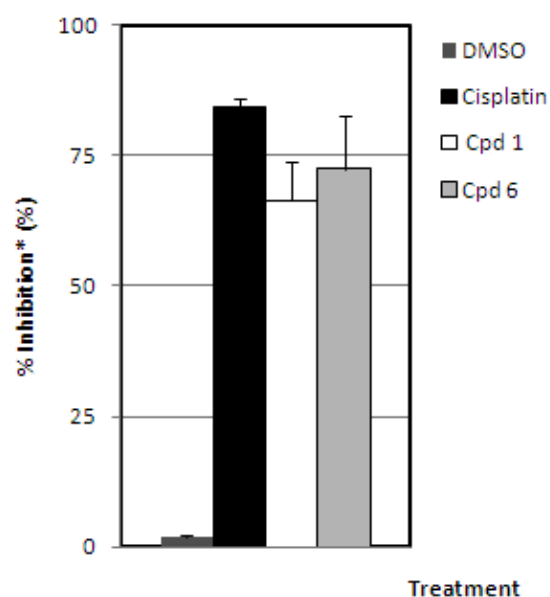
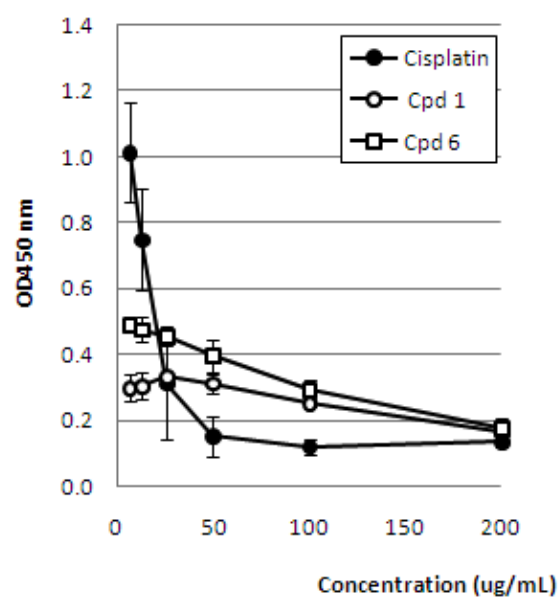
Statistical analysis: IC₅₀ are shown as mean $\pm$ standard deviation (SD) of triplicates from each independent experiment. Cell proliferation form WST-1 activities were analyzed using the student's t-test. P-values less than 0.05 were considered statistically significant.

Fig. 4 Dose-response curve and % growth inhibition at 200 μ g/mL of HCT116 cells to a 24-hour treatment with compounds **1** and **8** or cisplatin (positive control). (A); Dose-response curve and % growth inhibition at 200 μ g/mL of PC3 cells to a 24-hour treatment with compounds **1** and **6** or cisplatin (positive control). (B)

A) HCT116 cell line



B) PC3 cell line



Purification and identification of isolated compounds: Experimental with full physical and spectroscopic data for compounds **1-8**, including a complete assignment of ^1H and ^{13}C NMR data for lupanes **6-8**.

General methods

1D and 2D NMR spectra were recorded on Bruker AC300 (300 MHz) and Avance 400 (400 MHz). Chemical shifts are given in parts per million (ppm, δ) relative to solvent peaks as internal standards (δ : CDCl_3 : 7.27 ppm (^1H), 77.0 ppm (^{13}C)); coupling constants are given in hertz (Hz, J). IR spectra were recorded using Nicolet 510 FT-IR spectrophotometer as film on NaCl pellets. Optical rotations were measured on a Perkin-Elmer Model 341 polarimeter at 20°C. Mass spectra were determined on Thermo Finnigan LCQ Advantage (ESI-ion trap) for low resolution MS and LCT Premier Waters® (ESI-TOF) for high resolution measurement. GC/MS analyses for sesquiterpenes and fatty acid were carried out with a GC chromatograph Hewlett Pack 6890 GC coupled to a 5975 quadrupole MS. Rough fractionation was performed on MPLC (medium pressure liquid chromatography) BUCHI684 Fraction collector. Further separation was carried out on silica gel column chromatography (Silica gel 60A C.C. 20-45 μm chromagel SDS-CARLOERBA).

Betulonic acid (1) $\text{C}_{30}\text{H}_{46}\text{O}_3$; MW 454; white solid; $[\alpha]_{\text{D}}^{20} +12.2$ (CHCl_3 , $c=0.09$) ; IR (film) ν_{max} (cm^{-1}) 3500-2500 (br), 3066, 2917, 2849, 2863, 1703, 1694, 1462, 1377 and 757; ^1H and ^{13}C NMR (CDCl_3) data see Tables 1 and 2; MS (ESI-) m/z 453 $[\text{M-H}]^-$.

Betulinic acid (2) $\text{C}_{30}\text{H}_{48}\text{O}_3$; MW 456; colorless crystals; $[\alpha]_{\text{D}}^{20} +2.7^\circ$ (CHCl_3 , $c=0.075$) ; IR (film) ν_{max} (cm^{-1}) 3466-2500 (br), 3069, 2926, 2851 and 1687; ^1H NMR (δ_{H} , ppm, in CDCl_3) 0.70 (H5), 0.78 (H24), 0.82 (H25), 0.92 (H26), 0.96 (H23), 0.98 (H27), 1.71 (H30), 3.04 (H19), 3.21 (H3), 4.62, 4.75 (H29) ; ^{13}C NMR (δ_{C} , ppm, in CDCl_3) 38.7 (C1), 27.4 (C2), 79.0 (C-3), 38.8 (C4), 55.3 (C5), 18.3 (C6), 34.3 (C7), 40.7 (C8), 50.5 (C9), 37.2 (C10), 20.8 (C11), 25.5 (C12), 38.4 (C13), 42.4 (C14), 30.5 (C15), 32.1 (C16), 56.3 (C17), 49.2 (C18), 46.9 (C19), 150.4 (C20), 29.7 (C21), 37.1 (C22), 28.0

(C23), 15.4 (C24), 16.1 (C25), 16.1 (C26), 14.7 (C27), 180.5 (C28), 109.7 (C29), 19.4 (C30); MS (ES-) m/z 455 [M-H]⁻.

Epibetulinic acid (3) C₃₀H₄₈O₃; MW 456; white solid; $[\alpha]_D^{20}$ -3.3 (CHCl₃, c=0.09) ; IR (film) $\nu_{\max}$ (cm⁻¹) 3700-2500 (br), 3428, 3069, 2914, 2844, 1700, 1459, 1295 and 762; ¹H NMR (δ_H , ppm, in CDCl₃) 0.82 (H24), 0.84 (H25), 0.94 (H23+H26), 1.00 (H27), 1.70 (H30), 3.02 (H19), 3.40 (H3), 4.62, 4.75 (H29) ; ¹³C NMR (δ_C , ppm, in CDCl₃) 33.2 (C1), 25.4 (C2), 76.3 (C-3), 37.5 (C4), 49.0 (C5), 18.2 (C6), 34.2 (C7), 40.9 (C8), 50.3 (C9), 37.3 (C10), 20.7 (C11), 25.5 (C12), 38.4 (C13), 42.5 (C14), 30.6 (C15), 32.2 (C16), 56.4 (C17), 49.2 (C18), 46.9 (C19), 150.5 (C20), 29.6 (C21), 37.1 (C22), 28.3 (C23), 22.1 (C24), 15.9 (C25), 16.0 (C26), 14.8 (C27), 181.2 (C28), 109.7 (C29), 19.4 (C30); MS (ES-) m/z 455 [M-H]⁻.

28-hydroxylup-20(29)-en-3-one (Betulone) (4) C₃₀H₄₈O₂; MW 440; white solid; $[\alpha]_D^{20}$ +21.7 (CHCl₃, c=0.12) ; IR (film) $\nu_{\max}$ (cm⁻¹) 3435, 3065, 2917, 2847, 1705, 1463, 1376, 1025 and 757; ¹H NMR (δ_H , ppm, in CDCl₃) 0.93 (H25), 1.00 (H27), 1.03 (H24), 1.07 (H26), 1.08 (H23), 1.70 (H30), 3.36, 3.81 (H28), 4.59, 4.69 (H29) ; ¹³C NMR (δ_C , ppm, in CDCl₃) 39.6 (C1), 34.2 (C2), 218.3 (C3), 47.4 (C4), 54.9 (C5), 19.7 (C6), 33.5 (C7), 40.9 (C8), 49.7 (C9), 36.9 (C10), 21.4 (C11), 25.2 (C12), 37.4 (C13), 42.8 (C14), 27.0 (C15), 29.3 (C16), 47.8 (C17), 48.7 (C18), 47.8 (C19), 150.4 (C20), 29.6 (C21), 34.0 (C22), 26.6 (C23), 21.1 (C24), 15.8 (C25), 16.0 (C26), 14.7 (C27), 60.5 (C28), 109.8 (C29), 19.1 (C30); MS (ES+) m/z 463 [M+Na]⁺.

30-hydroxylup-20(29)-en-3-one (5) C₃₀H₄₈O₂; MW 440; white powder; $[\alpha]_D^{20}$ +14.4 (CHCl₃, c=0.18) ; IR (film) $\nu_{\max}$ (cm⁻¹) 3448, 3085, 2937, 2851 and 1705; ¹H and ¹³C NMR (CDCl₃) data see Tables 1 and 2; MS (ES+) m/z 463 [M+Na]⁺.

3,30-dioxo-lup-20,29-en-28-oic acid, (6) C₃₀H₄₄O₄; MW 468.3240; colorless crystals; $[\alpha]_D^{20}$ +30.6 (CHCl₃, c=0.11) ; IR (film) $\nu_{\max}$ (cm⁻¹) 3700-2500 (br), 3069, 2924, 2845, 1731, 1685, 1463 and 1276; ¹H and ¹³C NMR (CDCl₃) data see Tables 1 and 2; MS (ESI-) m/z 467 [M-H]⁻. HRMS (ESI-TOF) m/z (ESI-) : 467.3146 [M-H]⁻ (calcd for C₃₀H₄₃O₄ 467.3161)

28,30-dihydroxy-3-oxolup-20(29)-ene, (7) $C_{30}H_{48}O_3$; MW 456; green oil; $[\alpha]_D^{20} +3.0$ ($CHCl_3$, $c=0.33$) ; IR (film) ν_{max} (cm^{-1}) 3434, 1699 and 1456; 1H and ^{13}C NMR ($CDCl_3$) data see Tables 1 and 2; MS (ESI+) m/z 479 $[M+Na]^+$.

Messagenic acid G, (8) $C_{30}H_{46}O_4$; MW 470; amorphous solid; $[\alpha]_D^{20} +14.3$ ($CHCl_3$, $c=0.14$) ; IR (film) ν_{max} (cm^{-1}) 3700-2500 (br), 3074, 2938, 2864 and 1695; 1H and ^{13}C NMR ($CDCl_3$) data see Tables 1 and 2; MS (ESI-) m/z 469 $[M-H]^+$.

Table 1. ^1H NMR data (400 MHz) of **1**, **5**, **6**, **7**, **8** (in CDCl_3 , J in Hz, δ in ppm)

Position	1	5	6	7	8
	δ_{H}	δ_{H}	δ_{H}	δ_{H}	δ_{H}
1	1.38 (m), 1H 1.91 (m), 1H	1.38 (m), 1H 1.90 (m), 1H	1.37 (m), 1H 1.89 (m), 1H	1.38 (m), 1H 1.88 (m), 1H	1.39 (m), 1H 1.90 (m), 1H
2	2.42 (m), 1H 2.50 (m), 1H	2.43 (m), 1H 2.50 (m), 1H	2.41 (m), 1H 2.47 (m), 1H	2.42 (m), 1H 2.49 (m), 1H	2.43 (m), 1H 2.50 (m), 1H
3					
4					
5	1.35 (m), 1H	1.32 (m), 1H	1.31 (m), 1H	1.33 (m), 1H	1.33 (m), 1H
6	1.52 (m), 2H	1.47 (m), 2H	1.46 (m), 2H	1.47 (m), 2H	1.47 (m), 2H
7	1.44 (m), 2H	1.45 (m), 2H	1.43 (m), 2H	1.45 (m), 1H	1.43 (m), 2H
8					
9	1.38 (s), 1H	1.38 (m), 1H	1.35 (m), 1H	1.38 (m), 1H	1.38 (m), 1H
10					
11	1.34 (m), 1H 1.44 (m), 1H	1.28 (m), 1H 1.42 (m), 1H	1.31 (m), 1H 1.38 (m), 1H	1.27 (m), 1H 1.43 (m), 1H	1.32 (m), 1H 1.45 (m), 1H
12	1.06 (m), 1H 1.73 (m), 1H	1.13 (m), 1H 1.36 (m), 1H	0.91 (m), 1H 1.34 (m), 1H	1.02 (m), 1H 1.41 (m), 1H	1.48 (m), 1H
13	2.23 (m), 1H	1.68 (m), 1H	2.22 (m), 1H	1.67 (m), 1H	2.21 (m), 1H
14					
15	1.42 (m), 1H 1.99 (m), 1H	1.06 (m), 1H 1.71 (m), 1H	1.23 (m), 1H 1.55 (m), 1H	1.12 (m), 1H 1.73 (m), 1H	1.23 (m), 1H 1.54 (m), 1H
16	1.44 (m), 1H 2.28 (m), 1H	1.40 (m), 1H 1.52 (m), 1H	1.51 (m), 1H 2.32 (m), 1H	1.13 (m), 1H 1.90 (m), 1H	1.46 (m), 1H 2.31 (m), 1H
17					
18	1.64 (m), 1H	1.47 (m), 1H	2.02 (m), 1H	1.72 (m), 1H	1.77 (t, $J=11.5$), 1H
19	3.02 (td, $J=10.7$; 4.8), 1H	2.34 (td, $J=5.3$, 10.8), 1H	3.35 (td, $J=11.2$; 4.6), 1H	2.31 (m), 1H	2.90 (td, $J=11.0$, 4.5), 1H
20					
21	1.22 (m), 1H 1.54 (m), 1H	1.33 (m), 1H 2.08 (m), 1H	1.42 (m), 1H 2.16 (m), 1H	1.31 (m), 1H 1.96 (m), 1H	1.42 (m), 1H 2.11 (m), 1H
22	1.47 (m), 1H 1.99 (m), 1H	1.28 (m), 1H 1.40 (m), 1H	1.75 (m), 1H 2.00 (m), 1H	1.43 (m), 1H 2.12 (m), 1H	1.57 (m), 1H 1.98 (m), 1H
23	1.08 (s), 3H	1.08 (s), 3H	1.07 (s), 3H	1.07 (s), 3H	1.08 (s), 3H
24	1.03 (s), 3H	1.03 (s), 3H	1.01 (s), 3H	1.02 (s), 3H	1.02 (s), 3H
25	0.94 (s), 3H	0.93 (s), 3H	0.91 (s), 3H	0.92 (s), 3H	0.92 (s), 3H
26	0.99 (s), 3H	1.07 (s), 3H	0.96 (s), 3H	1.06 (s), 3H	0.97 (s), 3H
27	1.00 (s), 3H	0.96 (s), 3H	0.96 (s), 3H	0.99 (s), 3H	1.02 (s), 3H
28		0.80 (s), 3H		3.33 (d, $J=10.8$), 1H 3.80 (d, $J=10.8$), 1H	
29	4.62 (s), 1H 4.75 (s), 1H	4.91 (s), 1H 4.95 (s), 1H	5.93 (s), 1H 6.31 (s), 1H	4.91 (s), 1H 4.96 (s), 1H	4.94 (s), 1H 4.99 (s), 1H
30	1.70 (s), 3H	4.15 (br d, $J=14.3$), 1H 4.11 (br d, $J=14.3$), 1H	9.53 (s), 1H	4.12 (m), 2H	4.14 (m), 2H

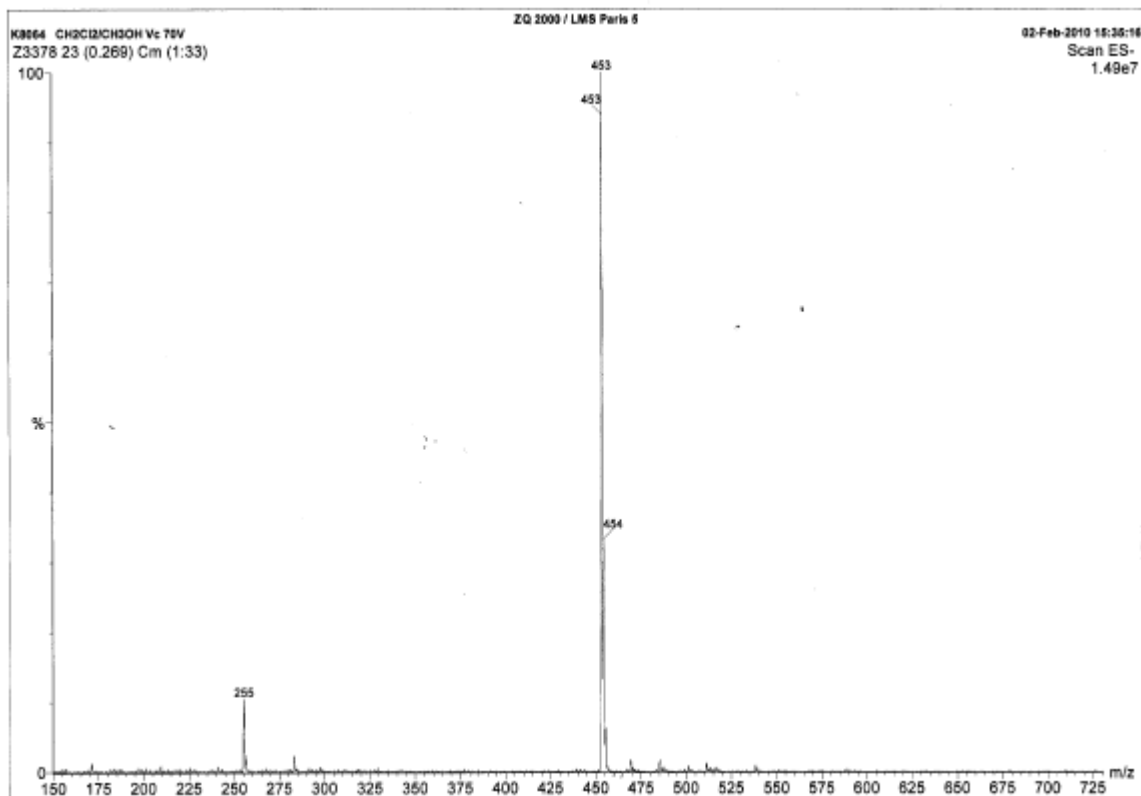
Table 2. ^{13}C NMR data (75 MHz) of **1**, **5**, **6**, **7**, **8** (in CDCl_3 , δ in ppm)

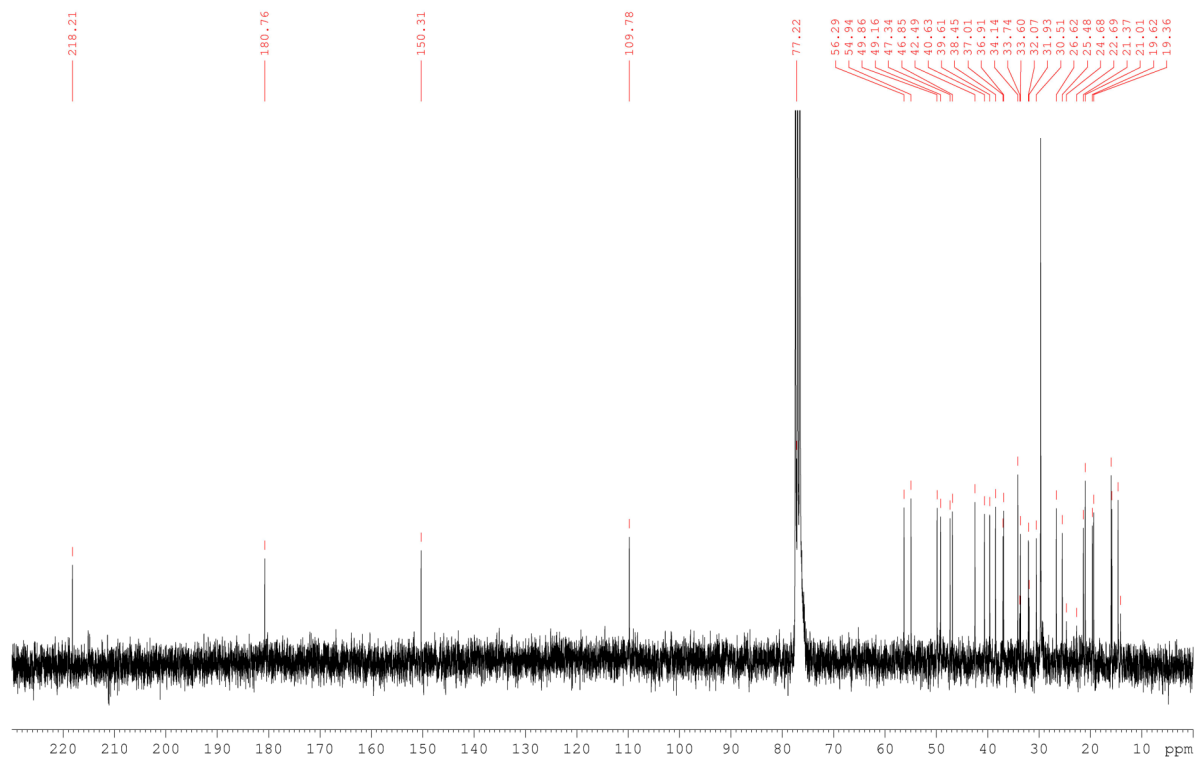
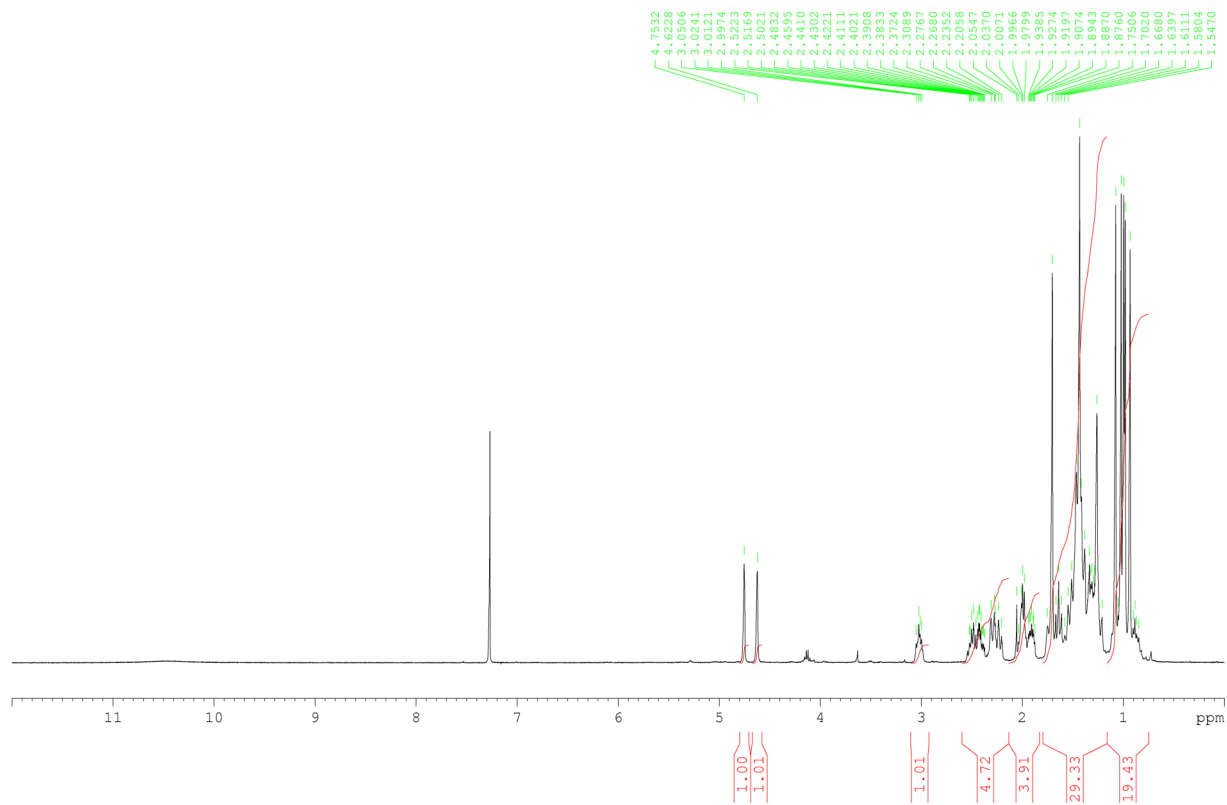
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	δ_{C}	δ_{C}	δ_{C}	δ_{C}	δ_{C}

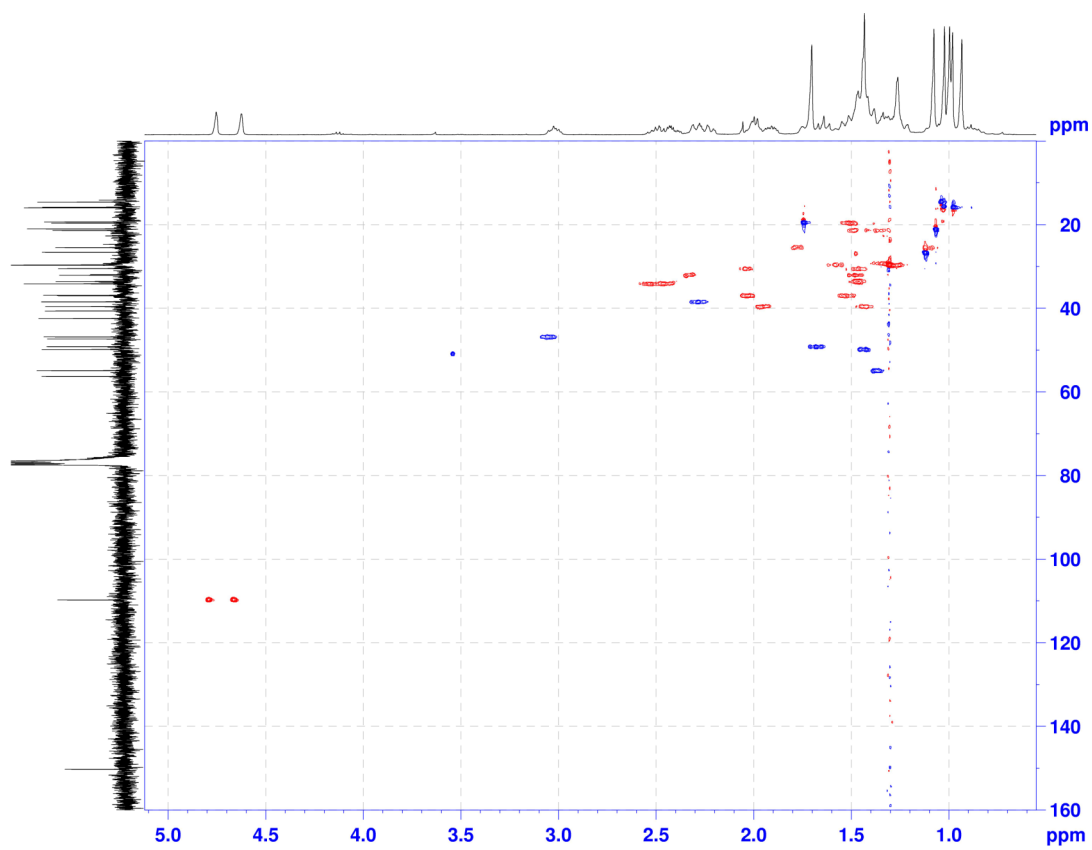
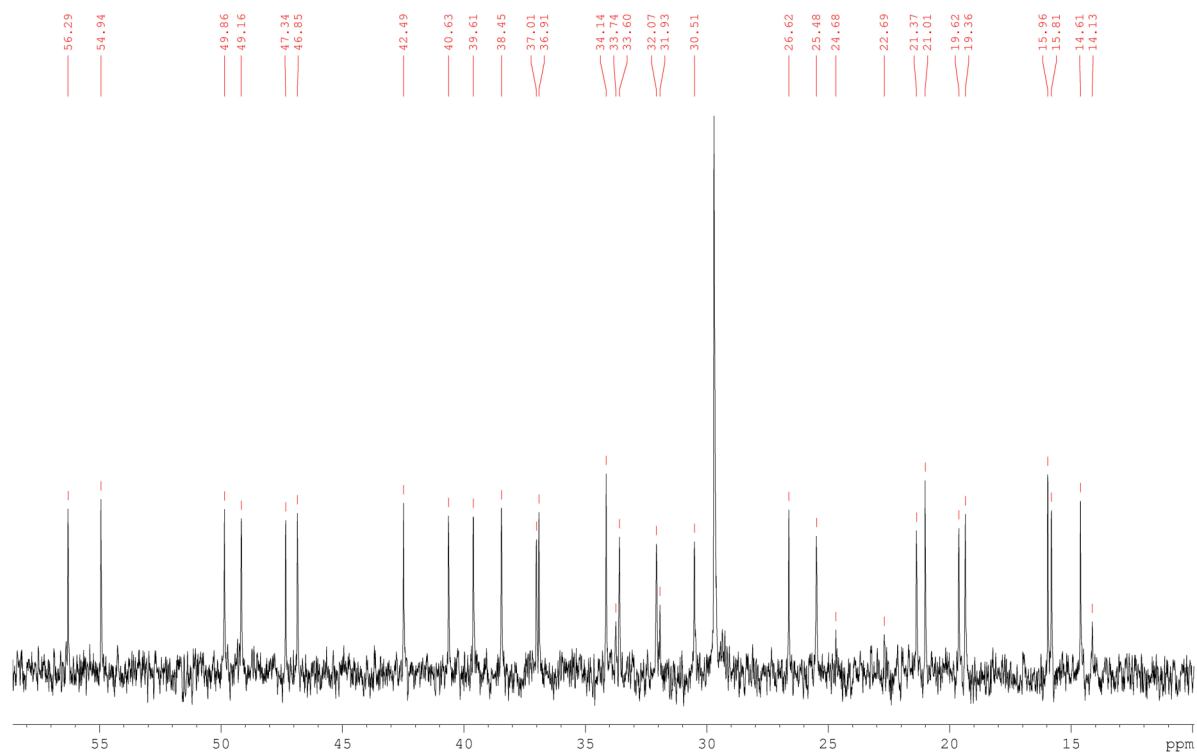
1	39.6	39.6	39.6	39.6	39.6
2	34.1	34.2	34.1	34.1	34.1
3	218.2	218.3	218.2	218.2	218.1
4	47.3	47.3	47.3	47.3	47.3
5	54.9	54.9	54.9	54.9	54.9
6	19.6	19.7	19.6	19.6	19.6
7	33.6	33.6	33.6	33.5	33.6
8	40.6	40.8	40.6	40.9	40.6
9	49.9	49.7	49.7	49.7	49.9
10	36.9	36.9	36.9	36.8	36.9
11	21.4	21.5	21.3	21.4	21.5
12	25.4	26.7	27.2	26.8	26.8
13	38.5	38.1	38.4	37.3	38.4
14	42.5	42.8	42.4	42.7	42.4
15	30.5	27.4	29.6	27.0	29.7
16	32.1	35.4	31.8	33.8	32.0
17	56.3	43.0	56.4	47.8	56.3
18	49.2	48.8	50.5	49.3	49.8
19	46.9	43.8	38.4	43.5	42.5
20	150.3	154.7	156.2	154.4	154.6
21	29.7	31.8	32.0	29.1	32.3
22	37.0	39.8	36.9	31.7	36.8
23	26.6	26.7	26.6	26.7	26.7
24	21.0	21.1	21.3	21.1	21.0
25	16.0	16.0	15.9	16.0	16.0
26	15.8	15.8	15.8	15.8	15.8
27	14.6	14.5	14.5	14.7	14.6
28	180.8	17.7	181.7	60.2	180.7
29	109.8	106.9	134.2	107.2	107.0
30	19.4	64.9	195.0	65.0	65.3

Original spectroscopic data:

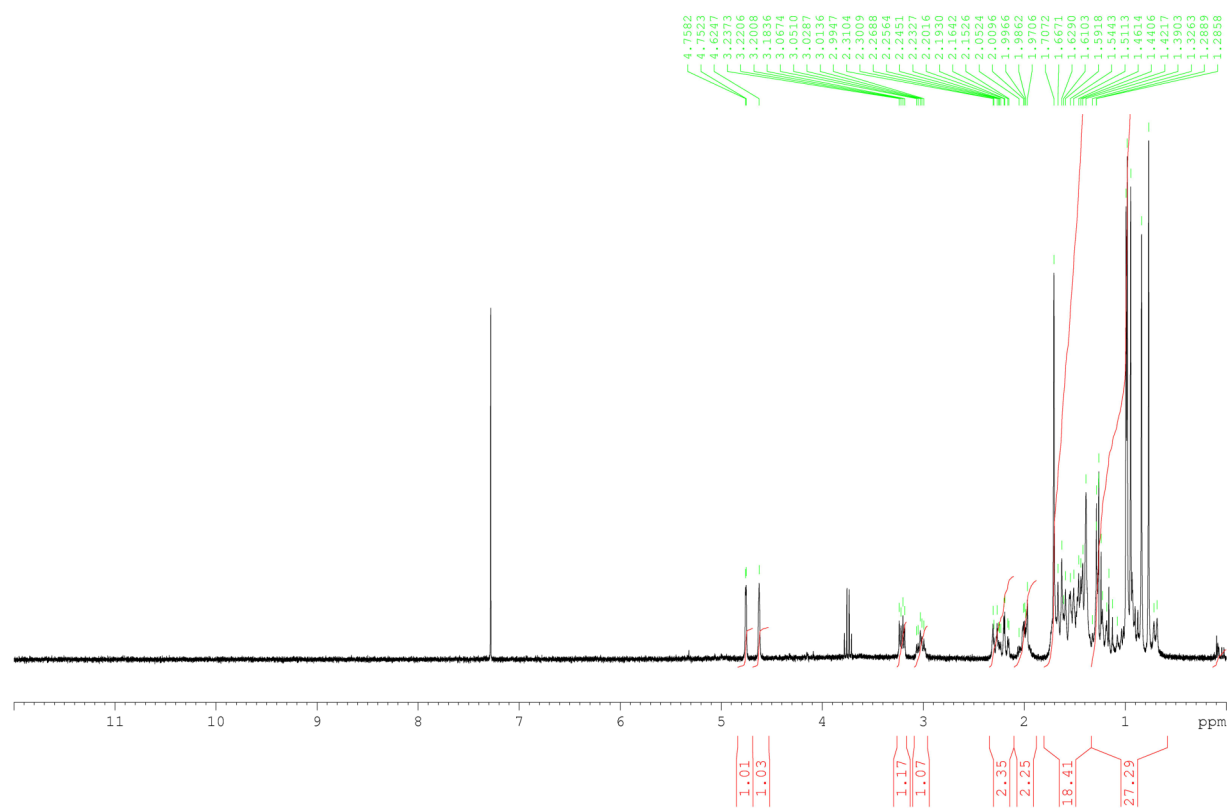
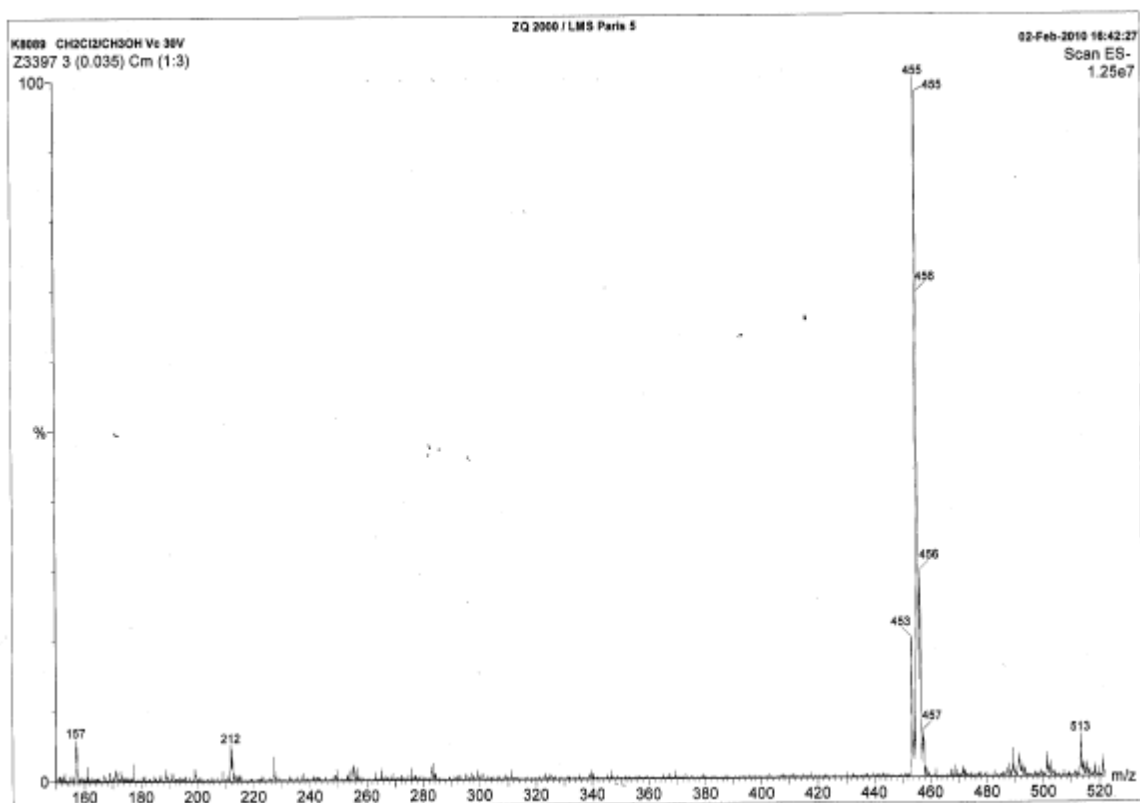
- Mass (ESI-: m/z 453 $[M-H]^-$) and NMR ($^1H+^{13}C$ +HSQC edit) spectra of betulonic acid ($C_{30}H_{46}O_3$; MW 454) (1):

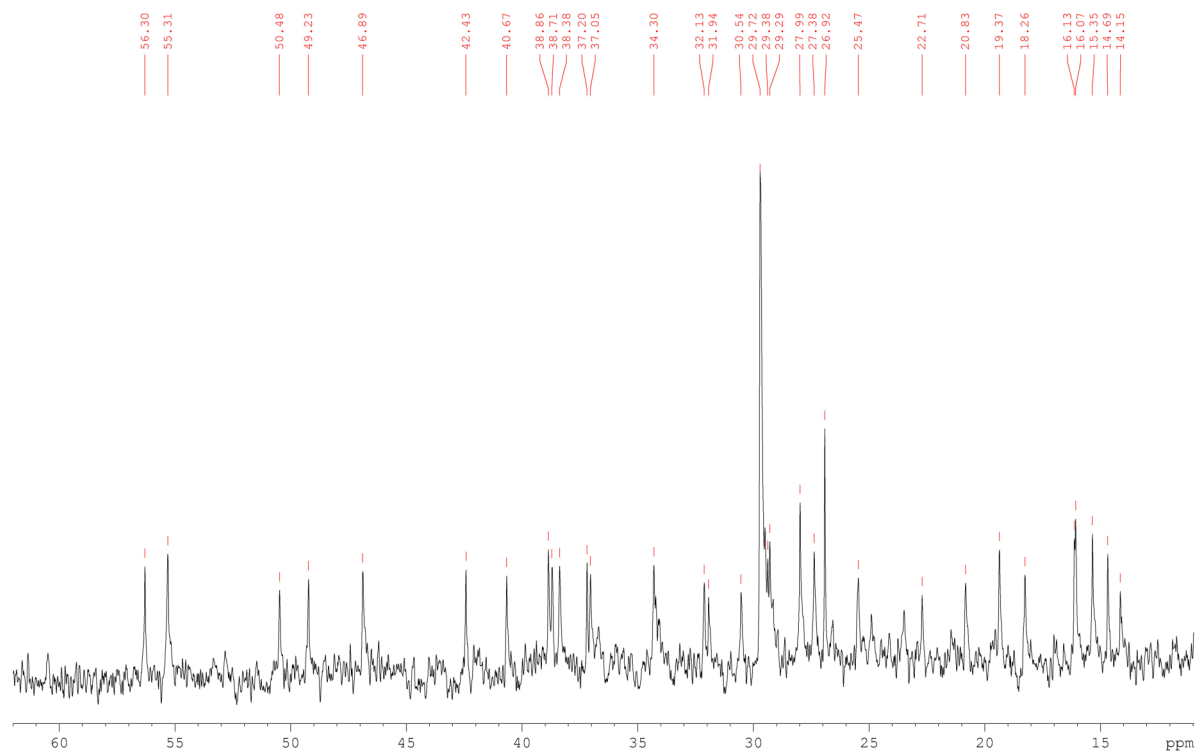
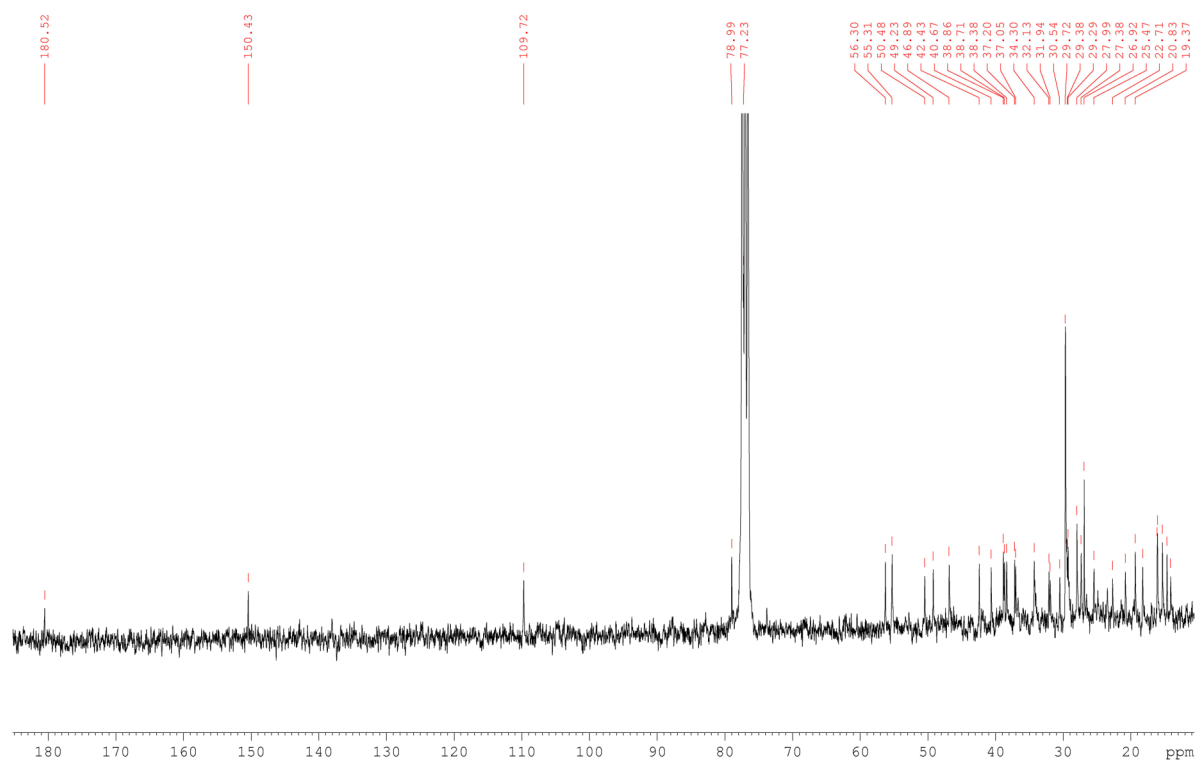




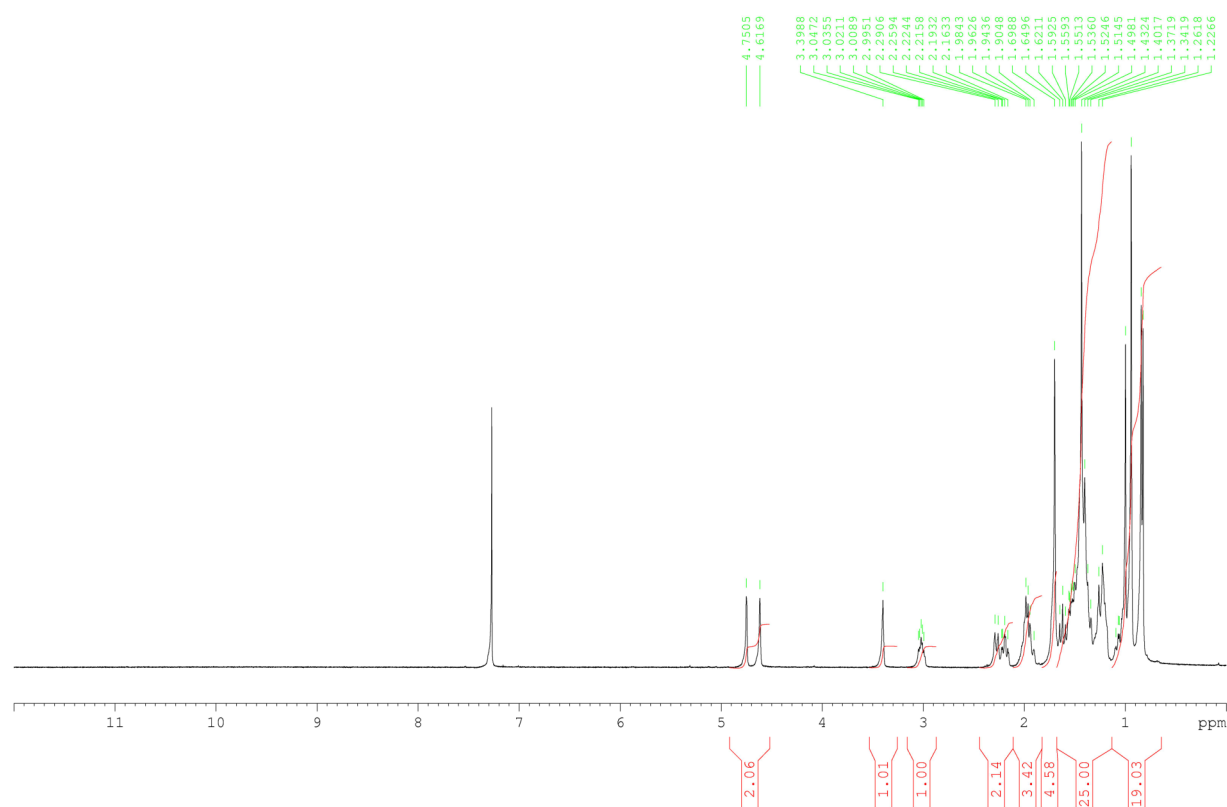
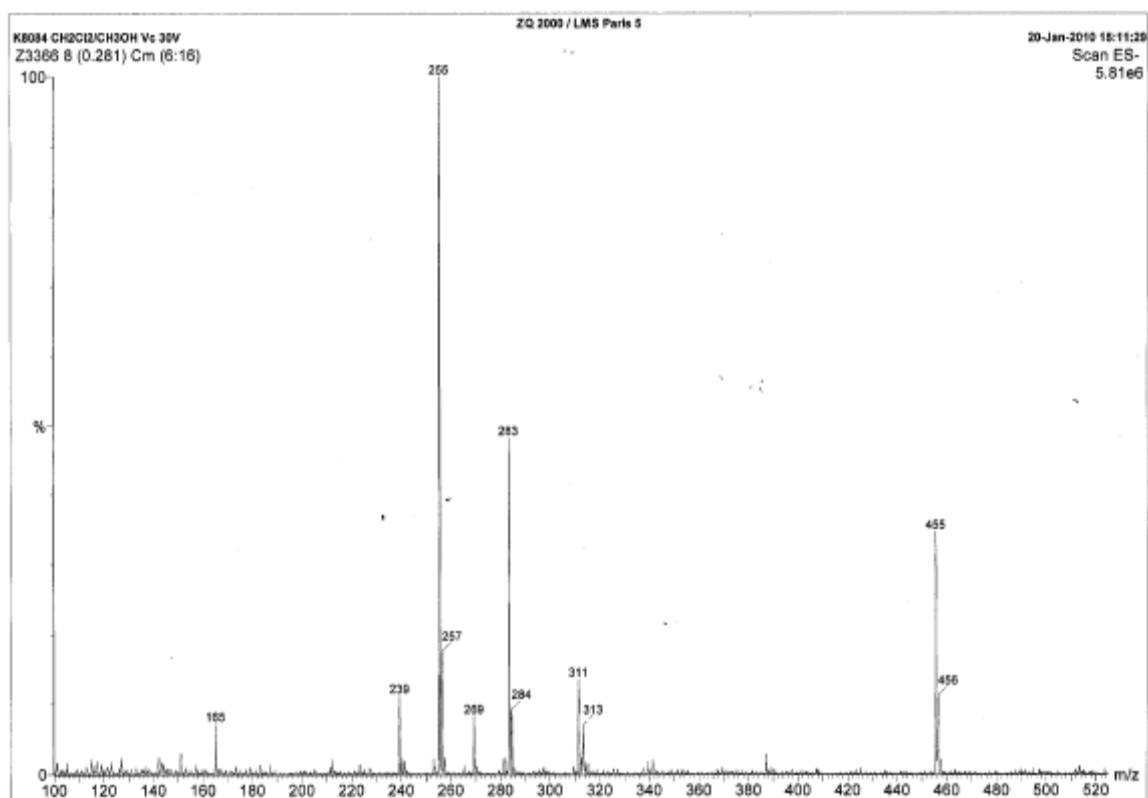


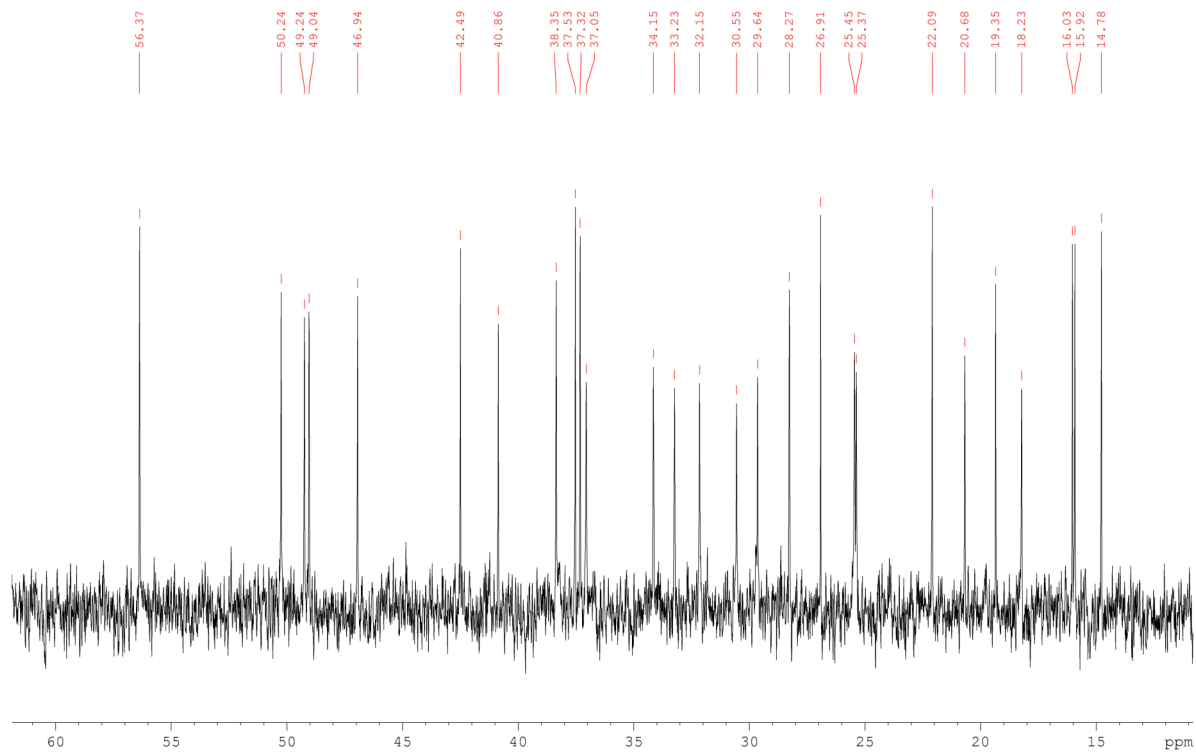
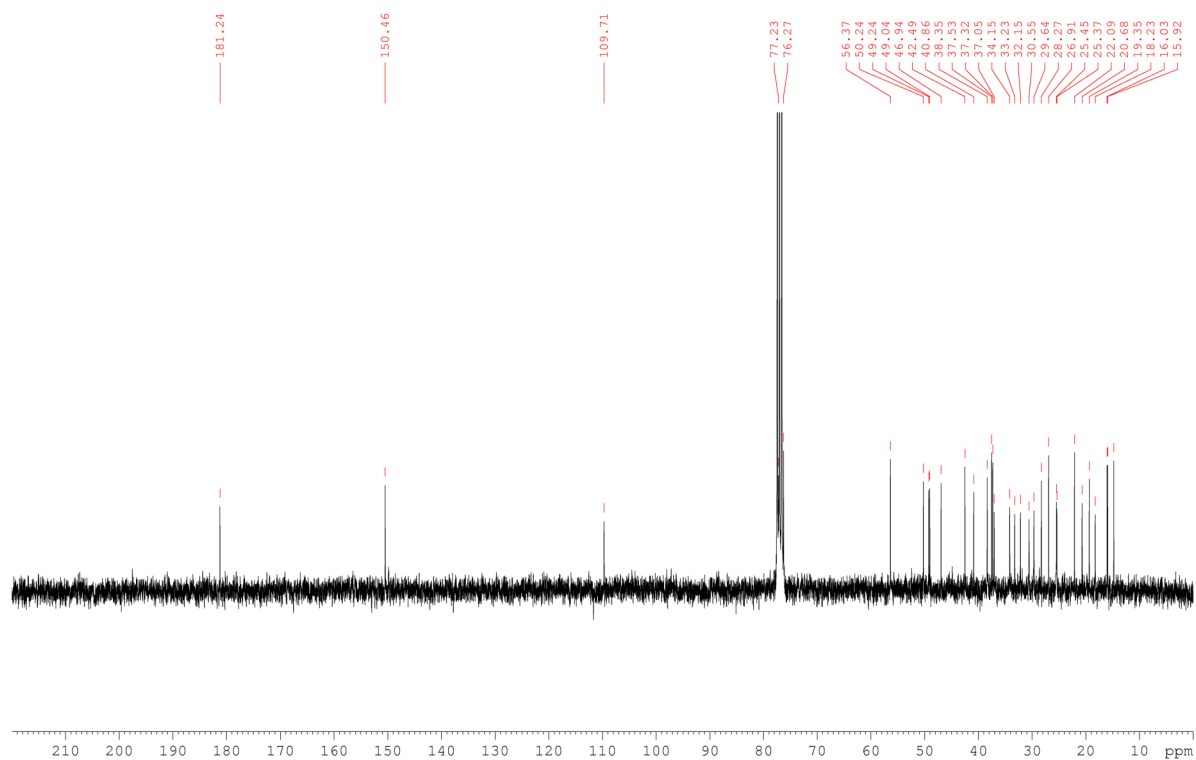
- Mass (ESI-: m/z 455 $[M-H]^-$) and NMR ($^1H+^{13}C$) spectra of betulinic acid ($C_{30}H_{48}O_3$; MW 456) (2):



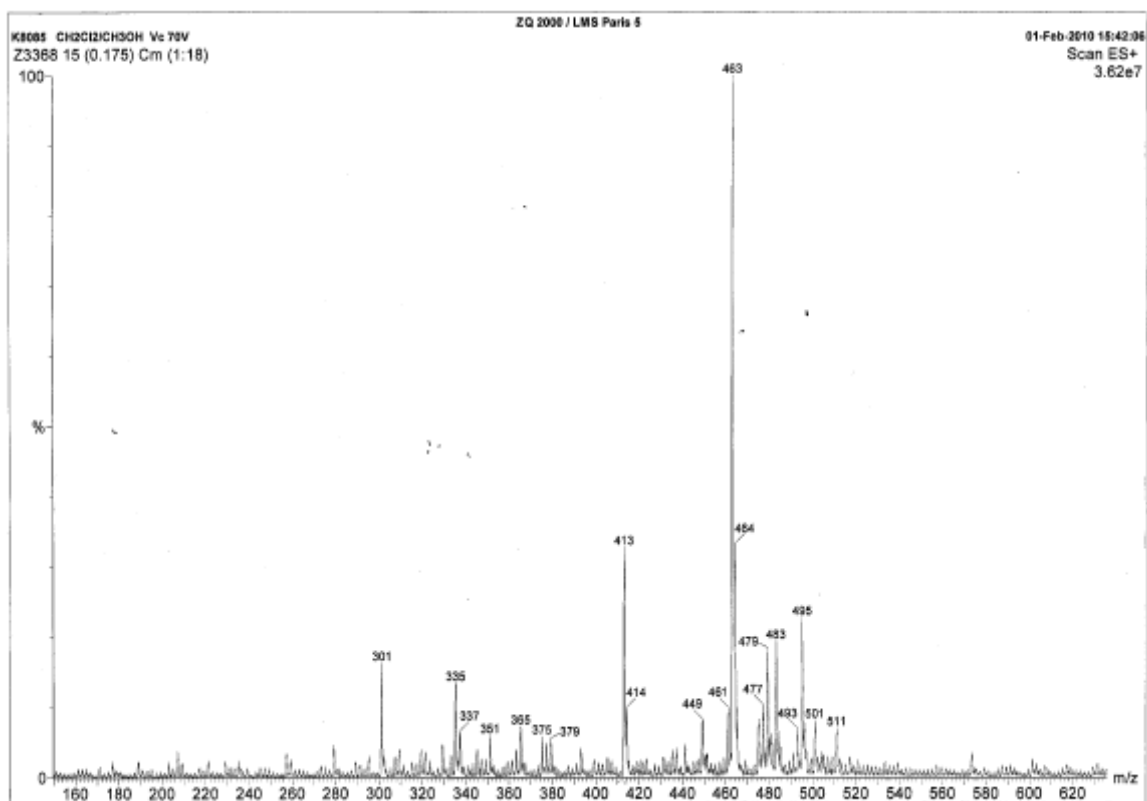


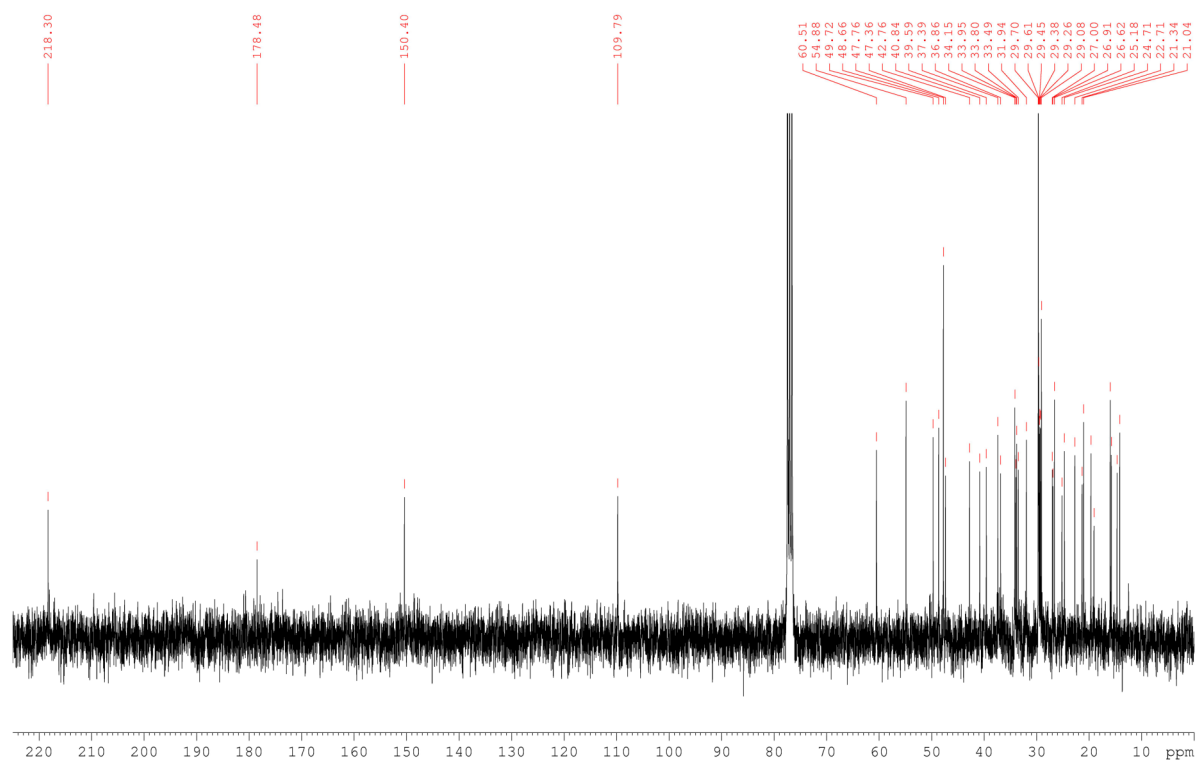
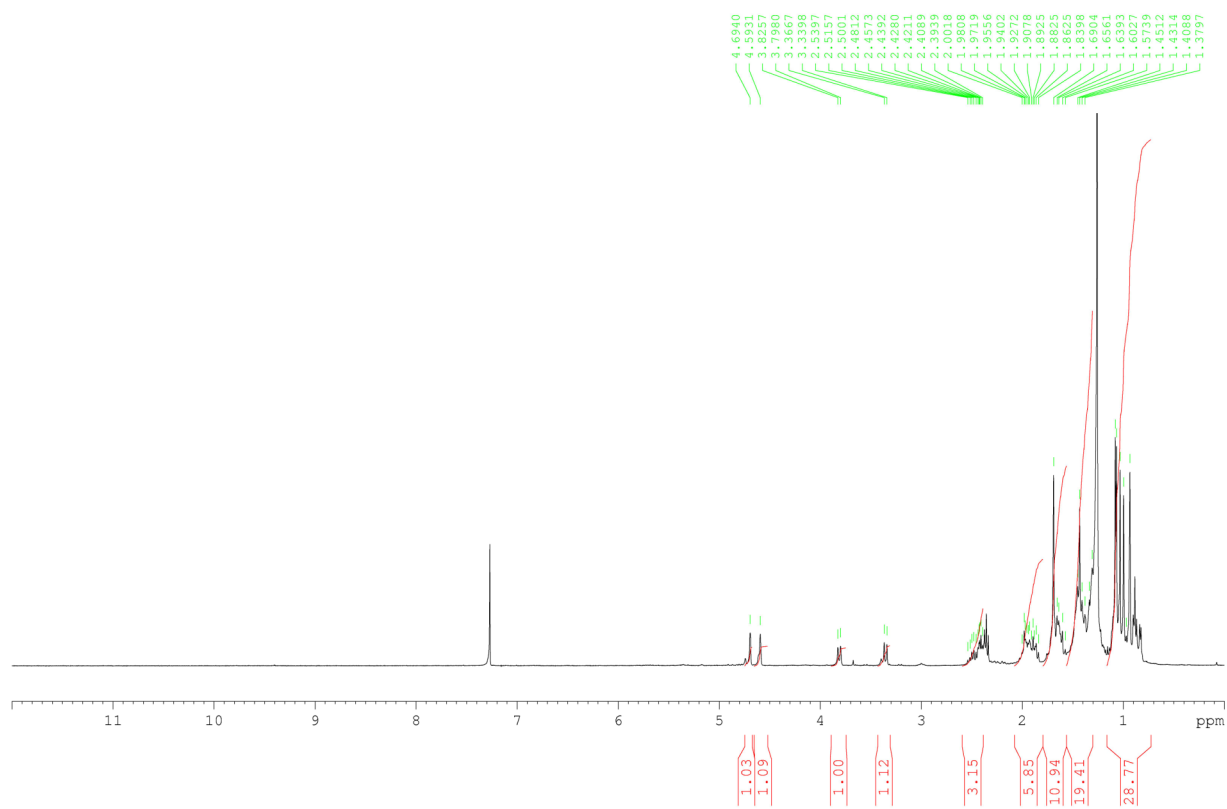
- Mass (ESI-: m/z 455 $[M-H]^-$) and NMR ($^1H+^{13}C$) spectra of epibetulinic acid ($C_{30}H_{48}O_3$; MW 456) (3):

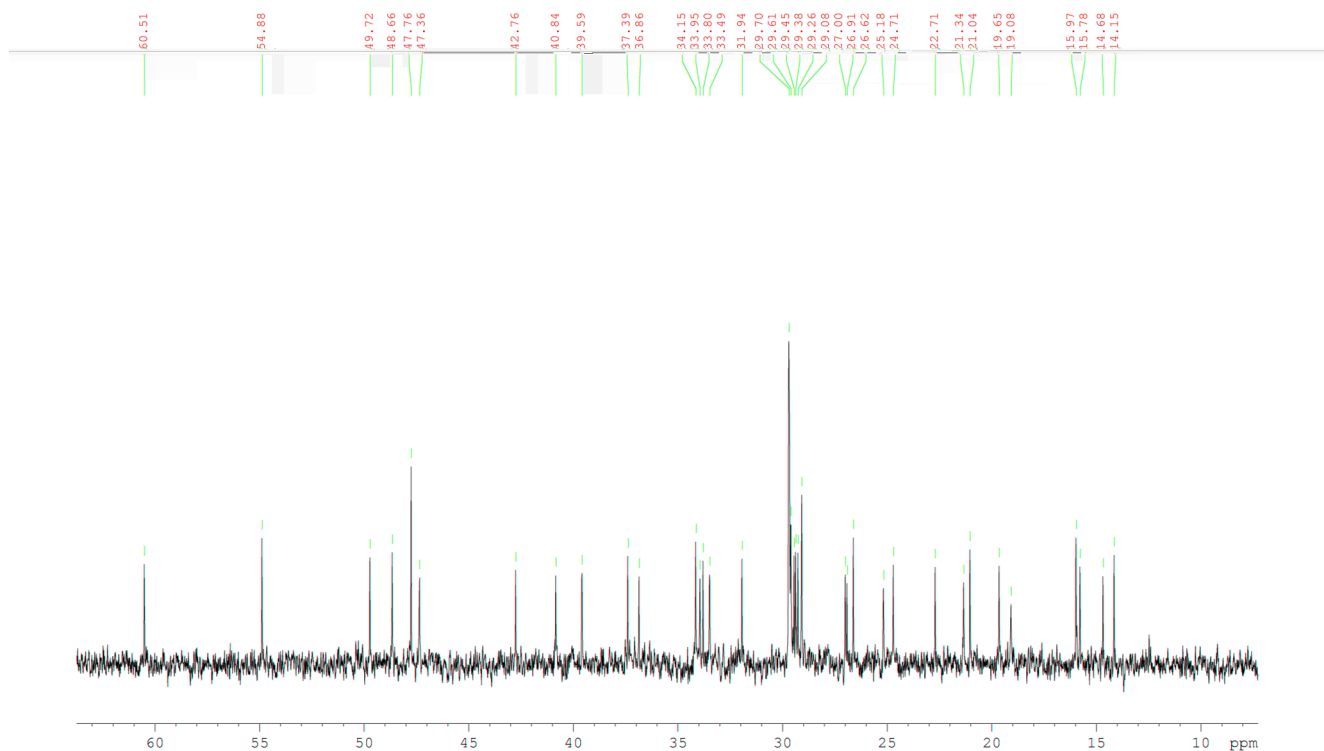




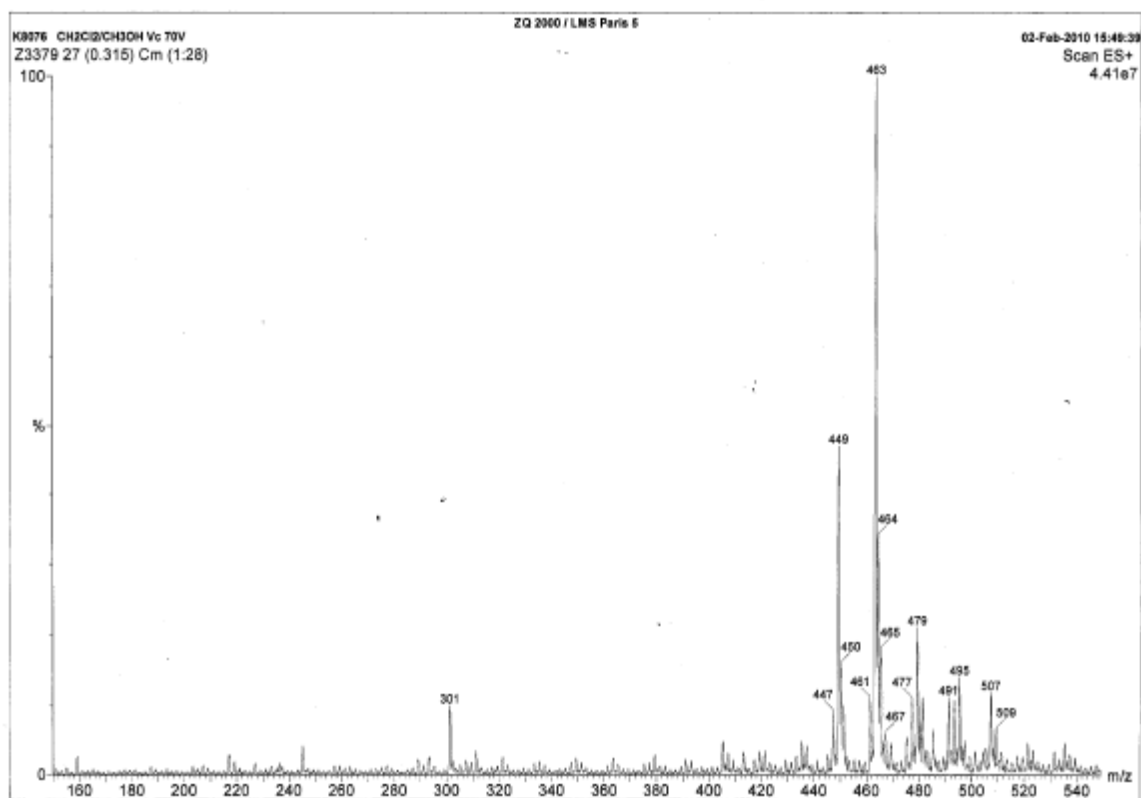
- Mass (ESI+: m/z 463 $[M+Na]^+$) and NMR (1H - ^{13}C) spectra of 28-hydroxylup-20(29)-en-3-one (= betulone) ($C_{30}H_{48}O_2$; MW 440) (4):

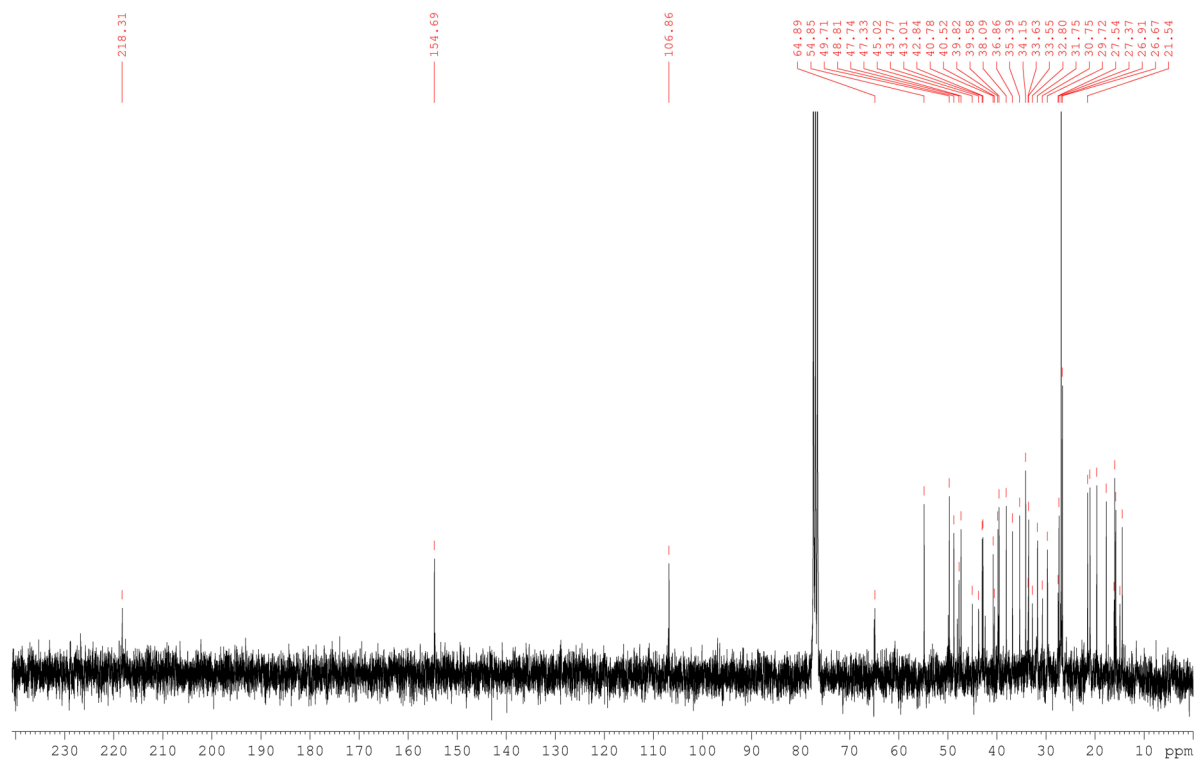
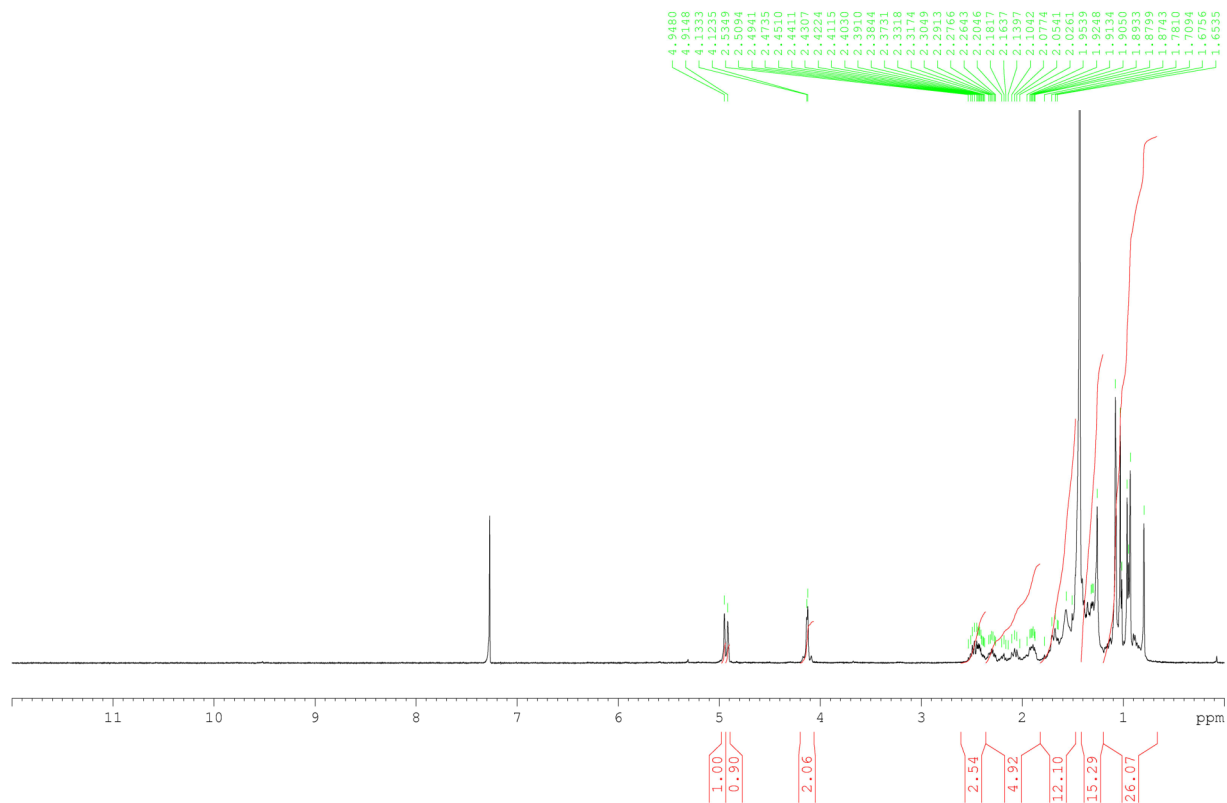


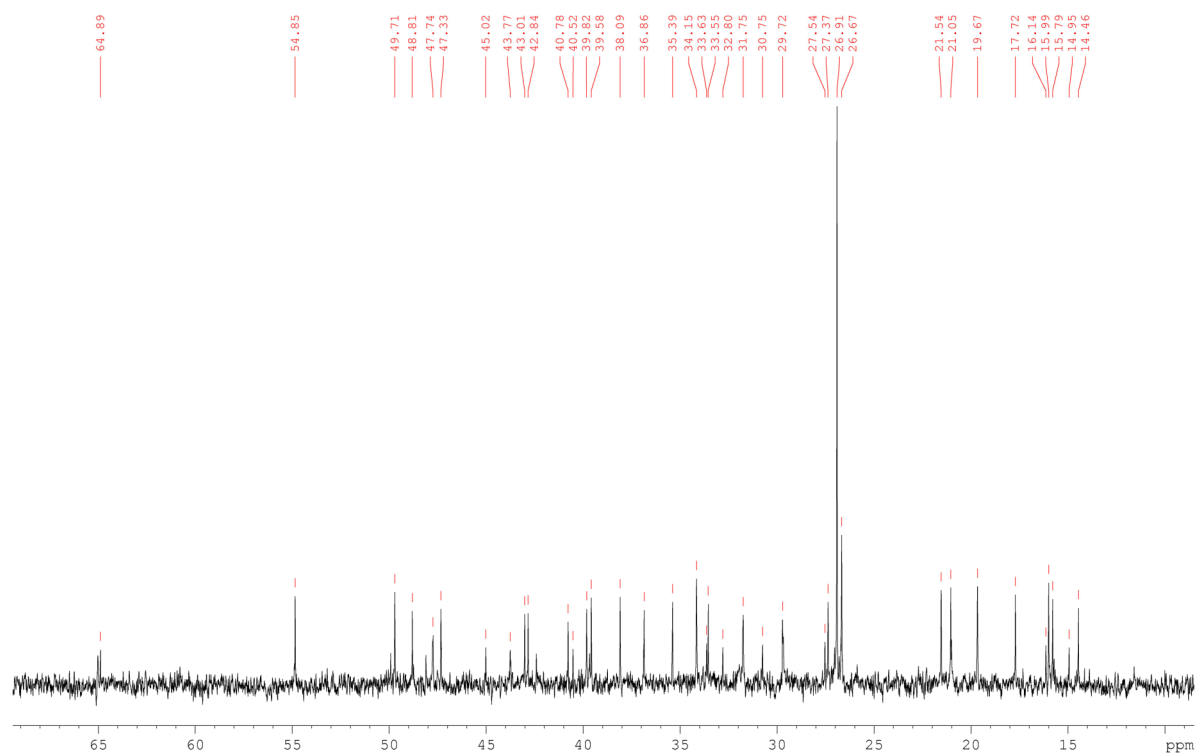




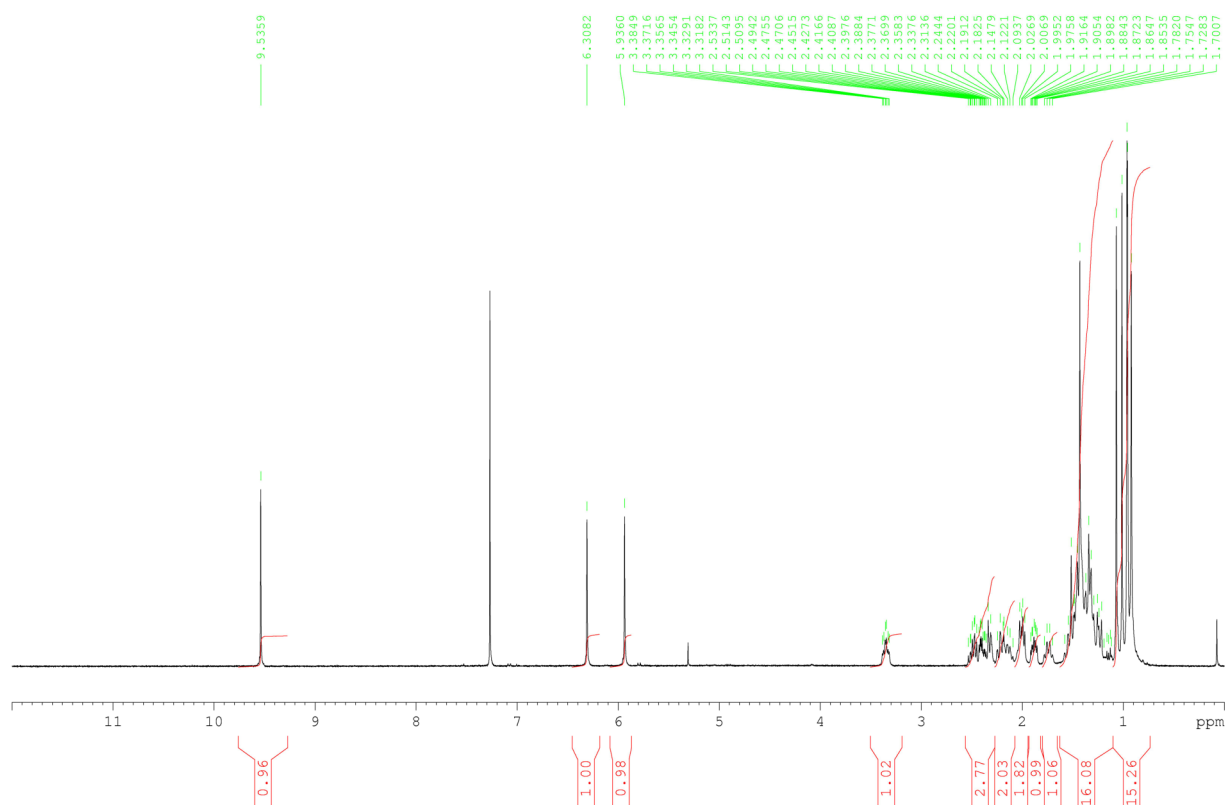
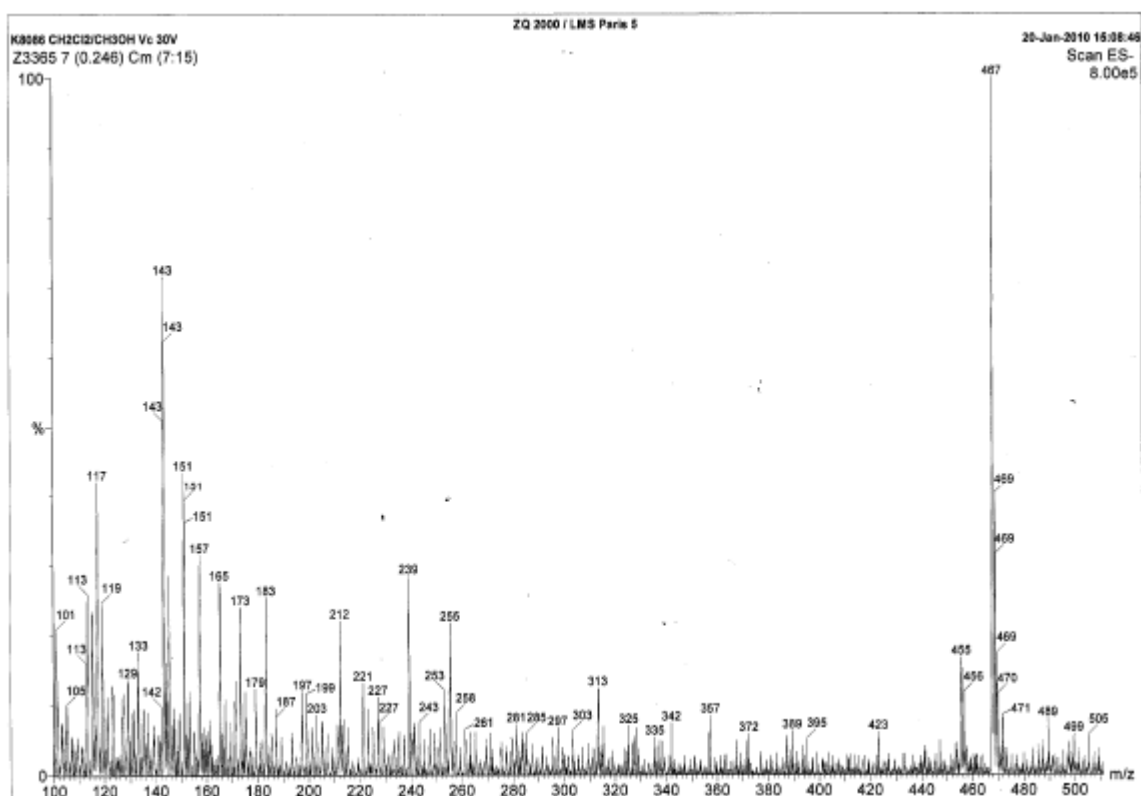
- Mass (ESI+: m/z 463 $[M+Na]^+$) and NMR (1H - ^{13}C) spectra of 30-hydroxy-3-lup-20(29)-ene ($C_{30}H_{48}O_2$; MW 440) (5):

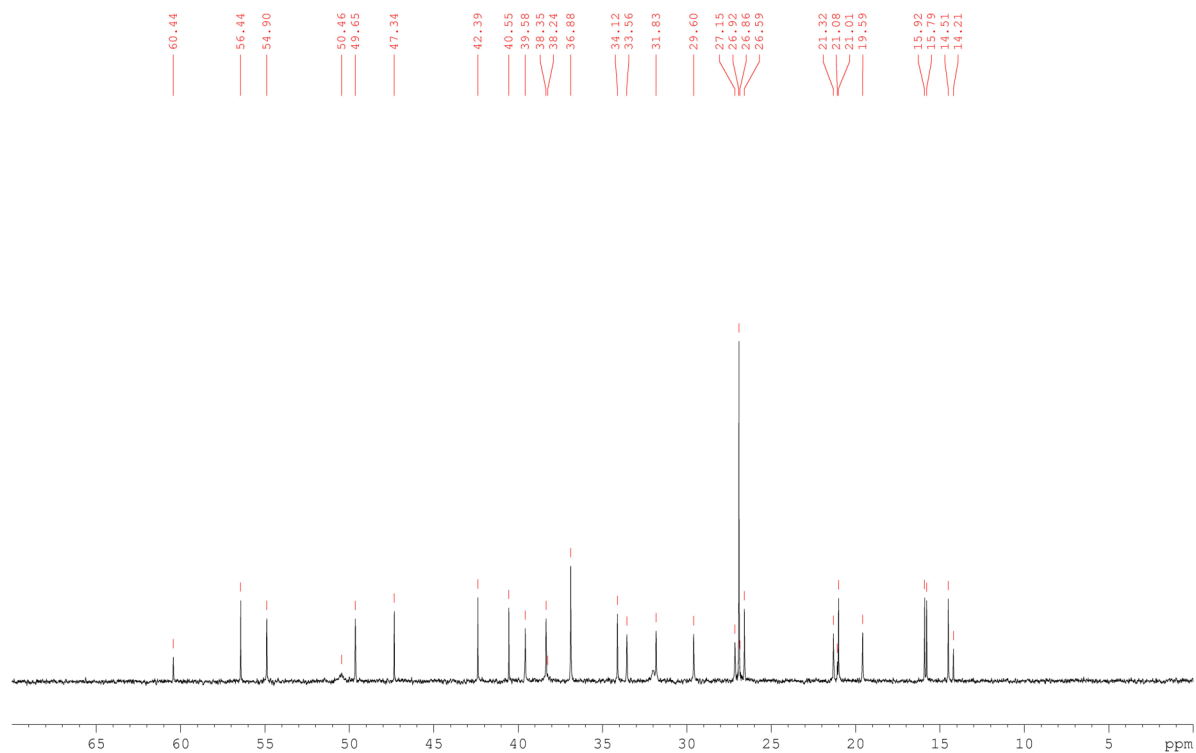
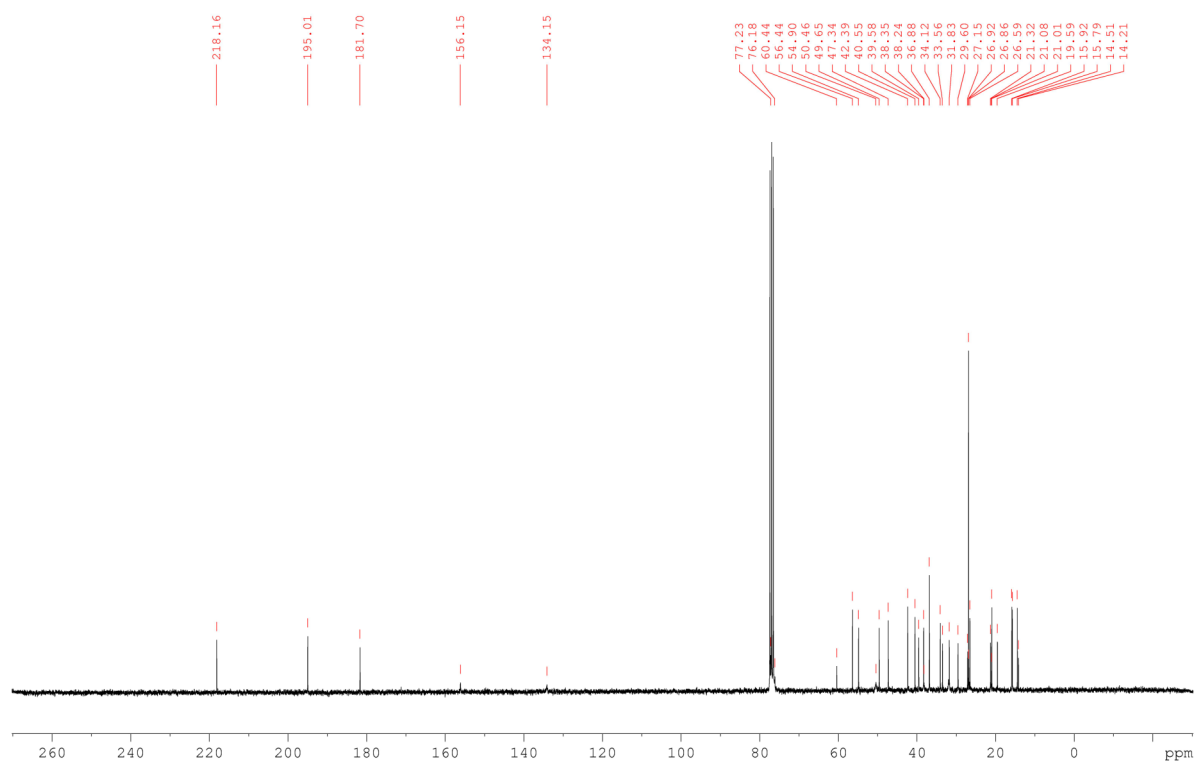


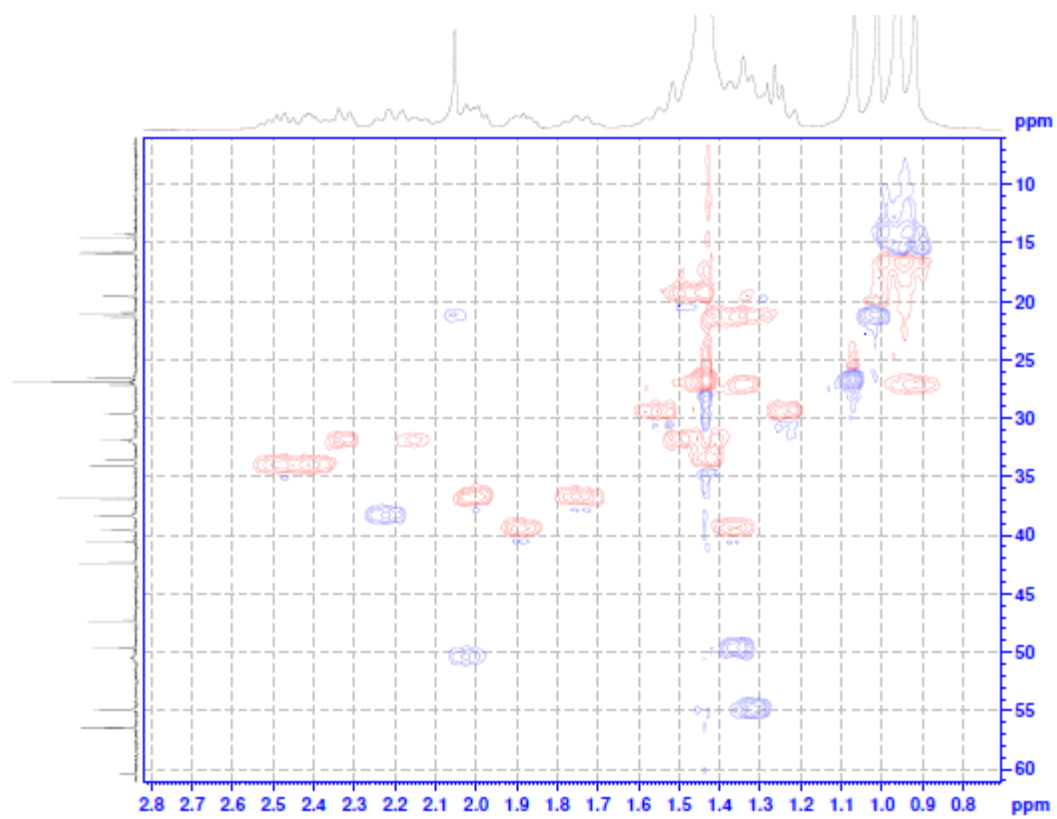
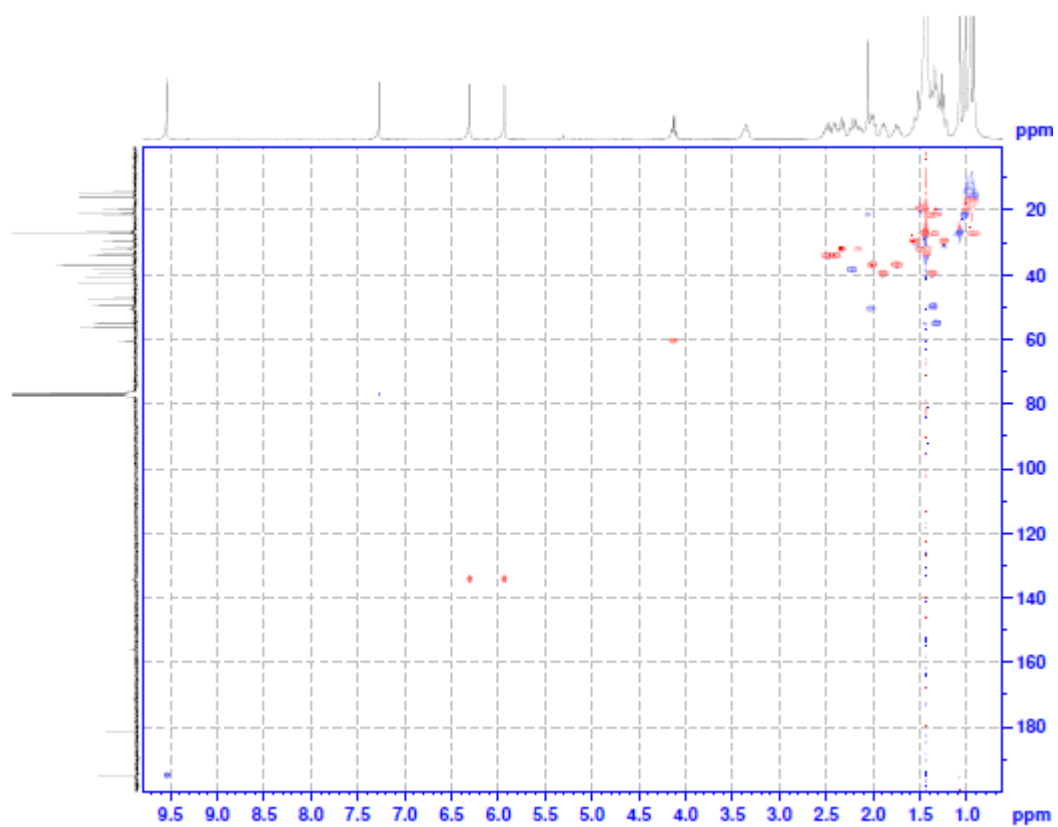


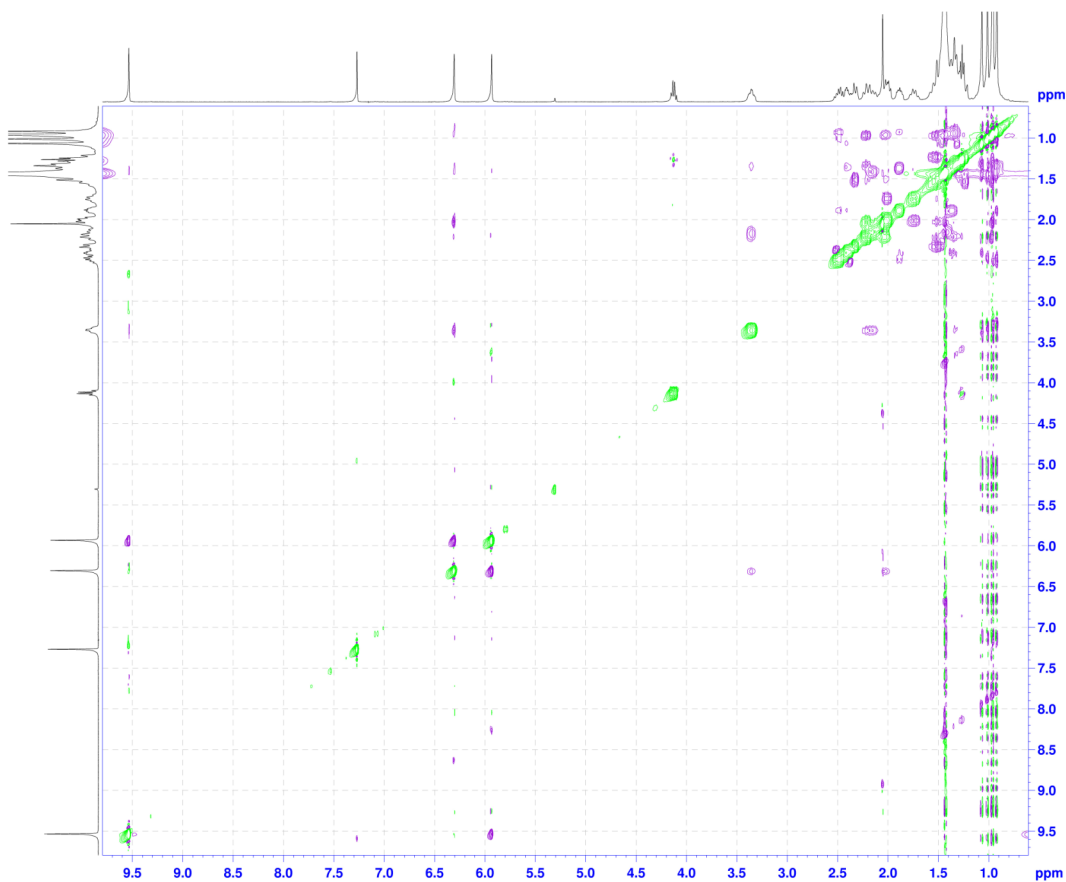
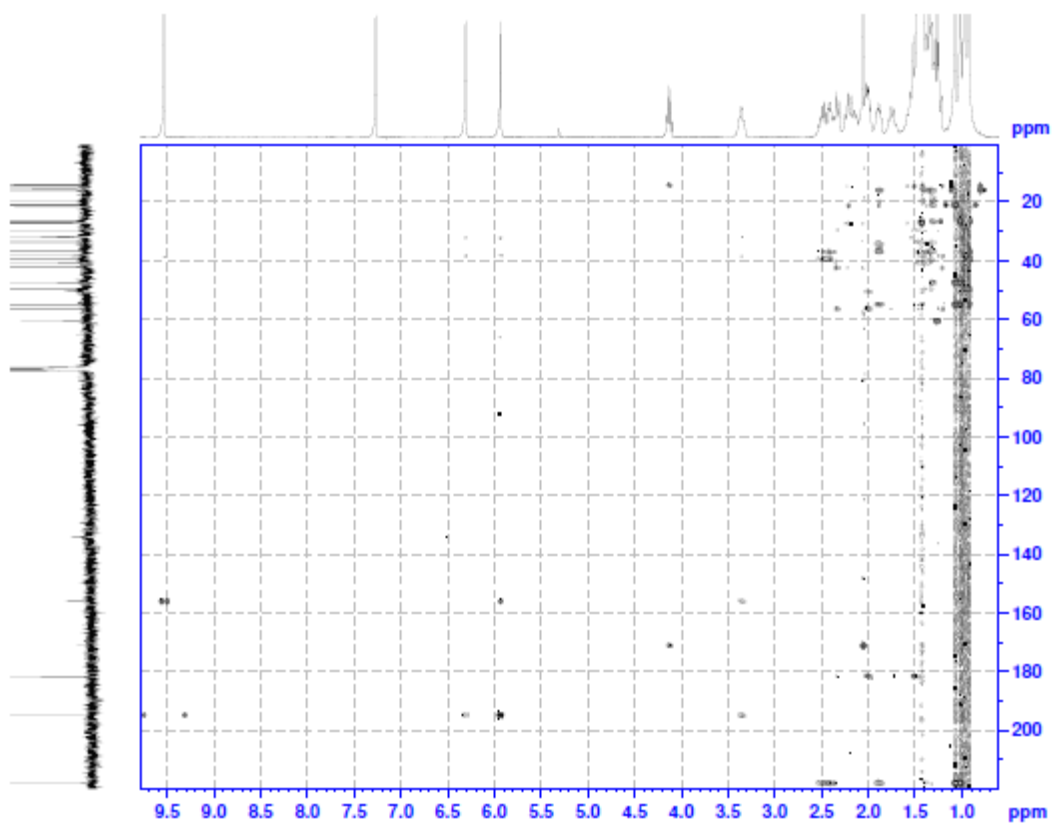


- Mass (ESI-: m/z 467 $[M-H]^-$) and NMR (1H + ^{13}C + HSQC edit + HMBC + NOESY) spectra of 3,30-dioxolup-20(29)-en-28-oic acid ($C_{30}H_{44}O_4$; MW 468) (6):









Current Data Parameters
 NAME 1-xc-malai-bo-ald-02
 EXPNO 4
 PROCNO 1

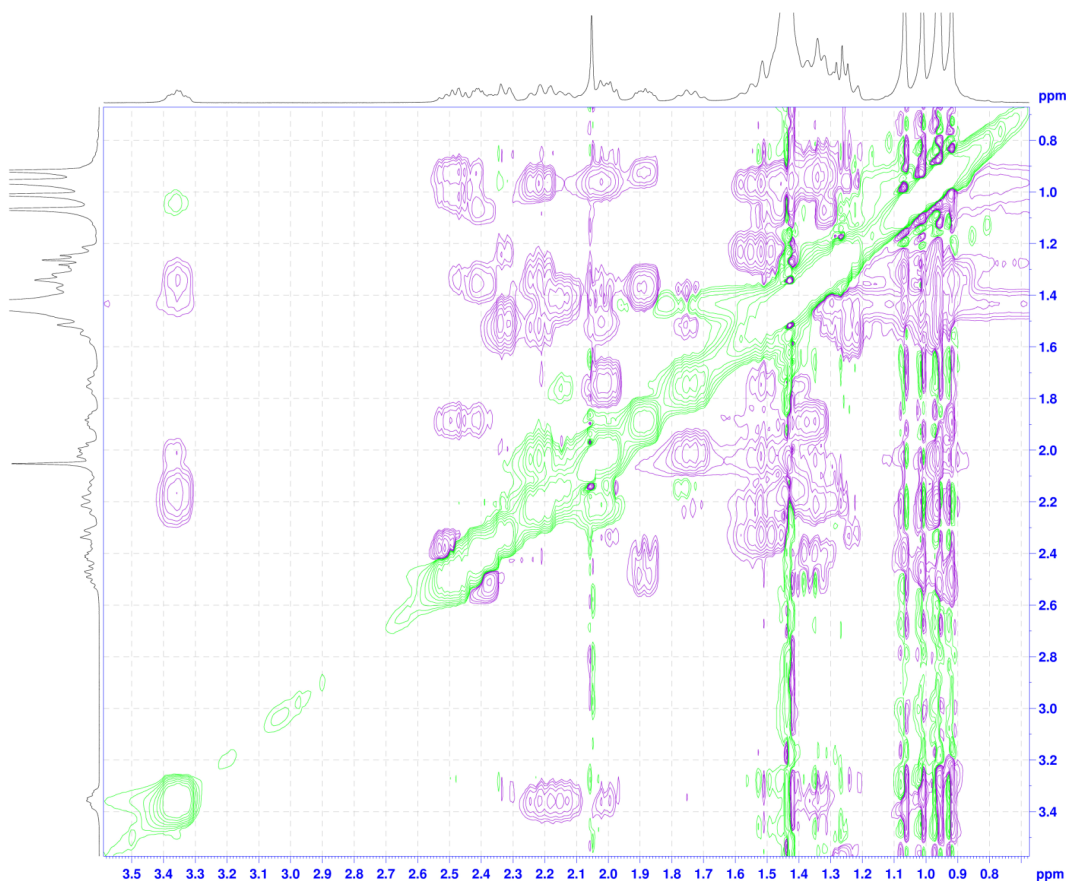
F2 - Acquisition Parameters
 Date_ 20100126
 Time 17.39
 INSTRUM spect
 PROBRD 5 mm Multinucl
 PULPROG noesyph
 TD 2048
 SOLVENT CDCl3
 NS 64
 DS 16
 SWH 3676.471 Hz
 FIDRES 1.795152 Hz
 AQ 0.2785760 sec
 RG 64
 DE 7.00 usec
 DW 136.000 usec
 TE 295.2 K
 d0 0.00012862 sec
 D1 2.00000000 sec
 D8 0.69999999 sec
 IN0 0.00027200 sec
 STICNT 128

===== CHANNEL f1 =====
 NUC1 1H
 P1 5.80 usec
 PL1 -1.00 dB
 SFO1 400.1320965 MHz

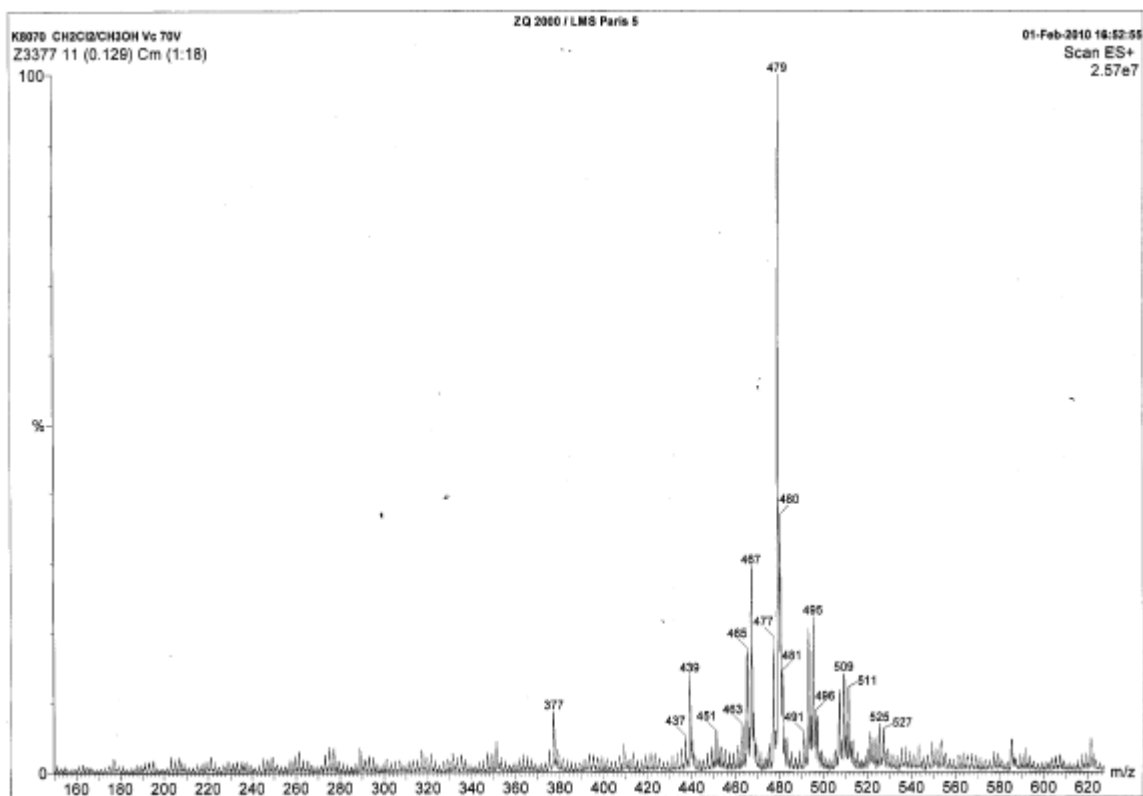
F1 - Acquisition parameters
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 FIDRES 14.361214 Hz
 SW 9.188 ppm
 FMODE States-TPPI

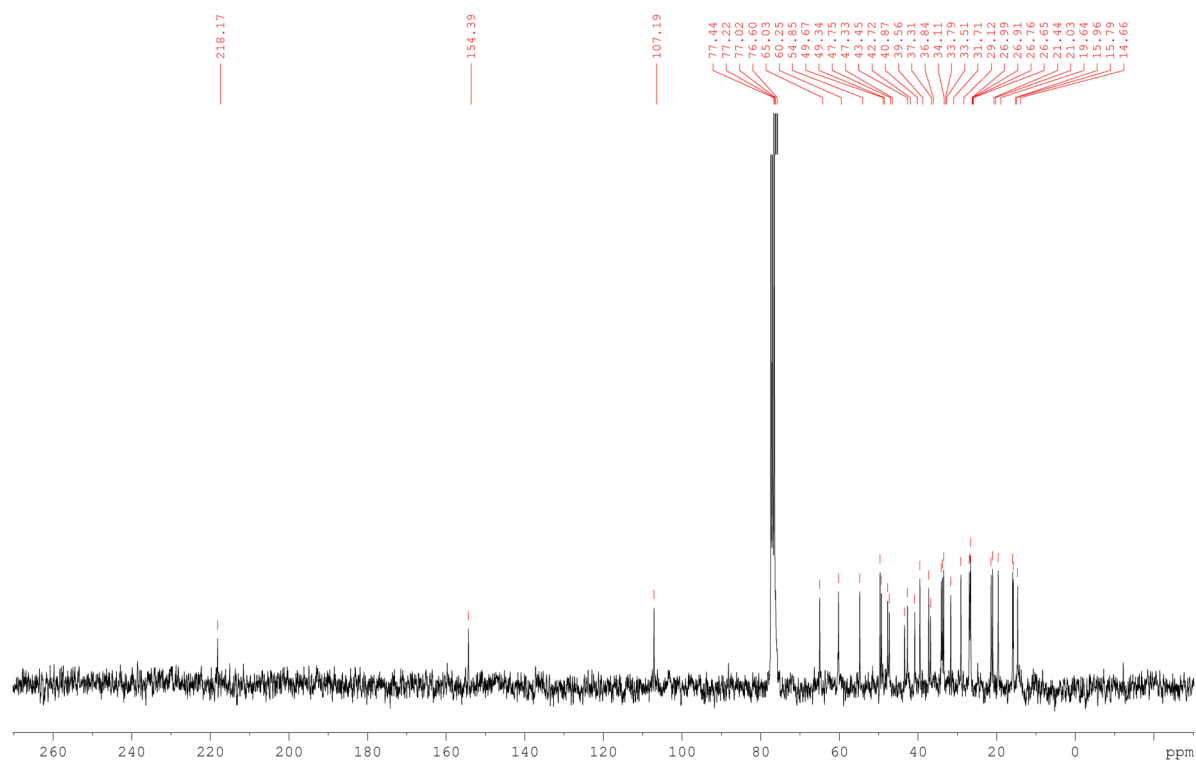
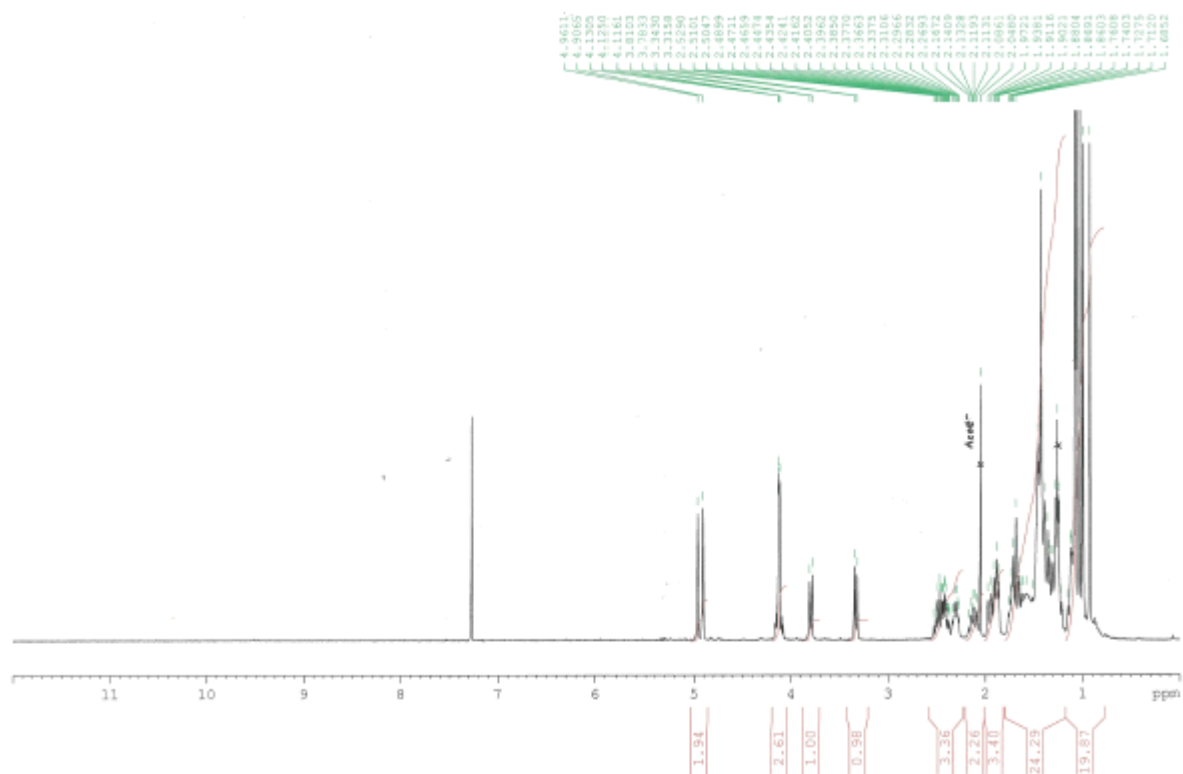
F2 - Processing parameters
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 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

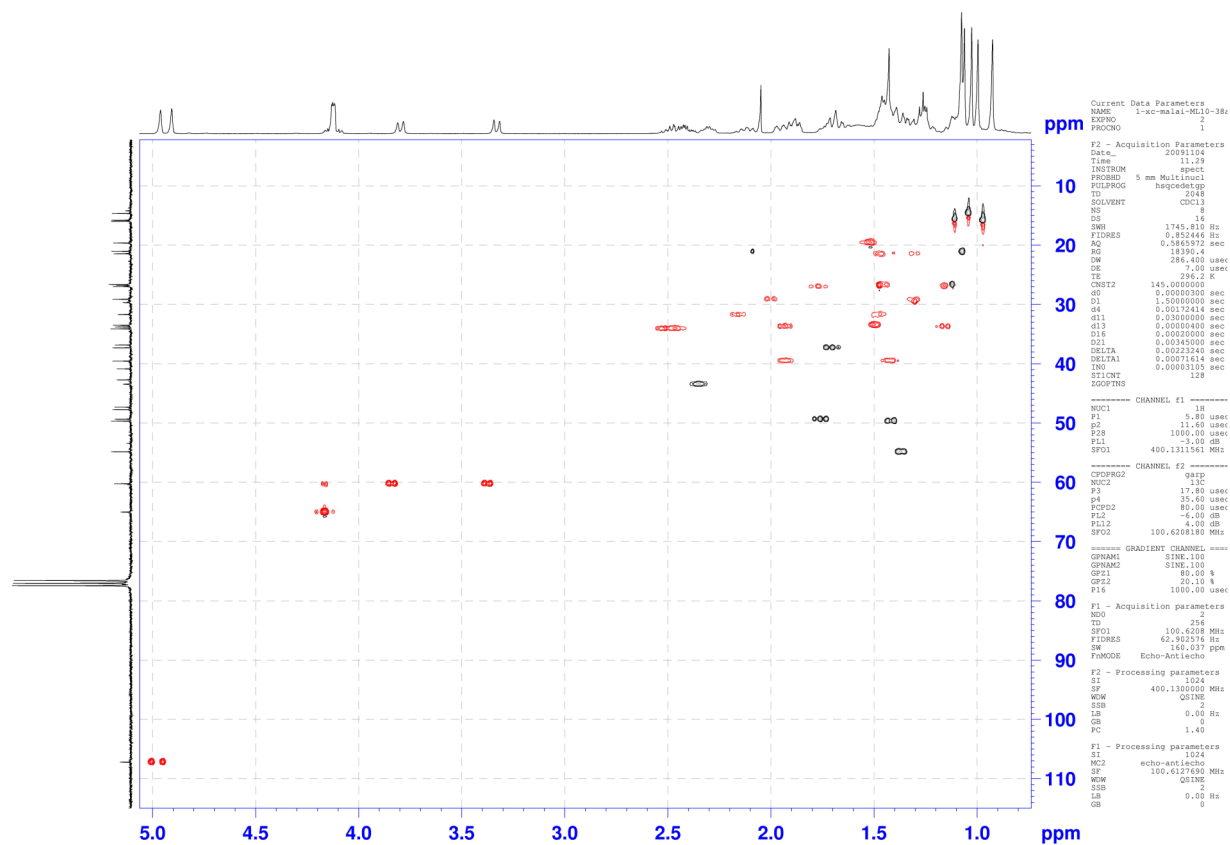
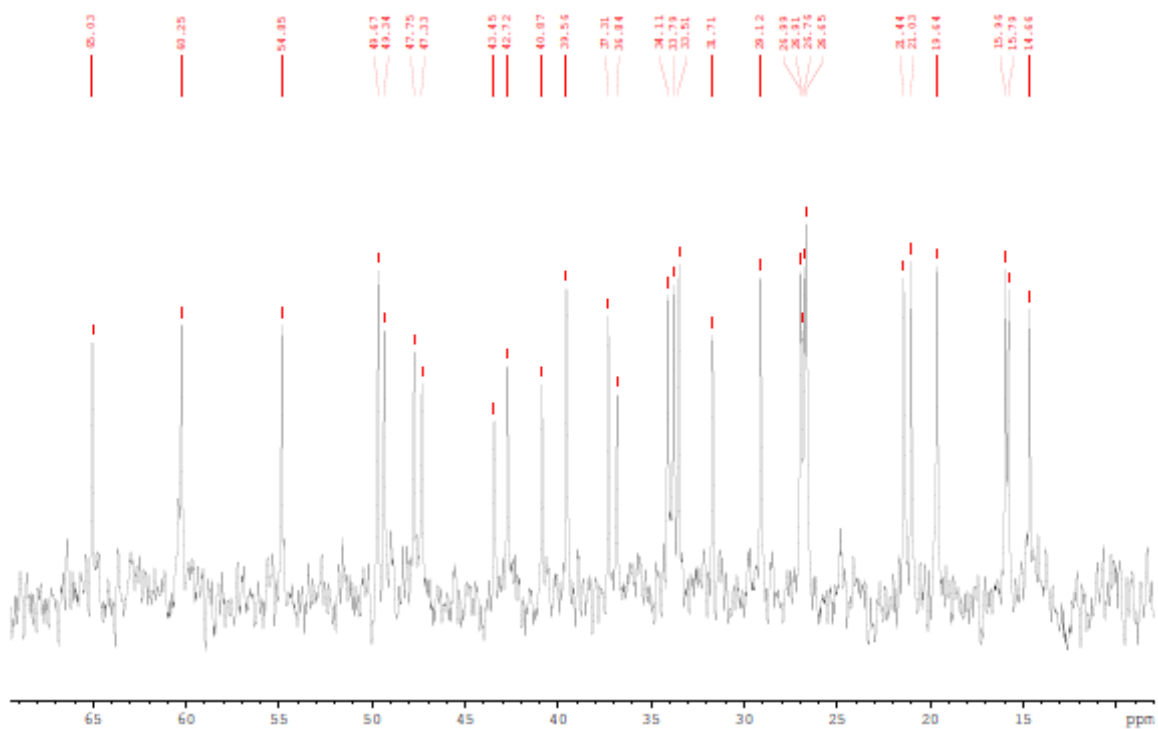
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 WDW QSINE
 SSB 0
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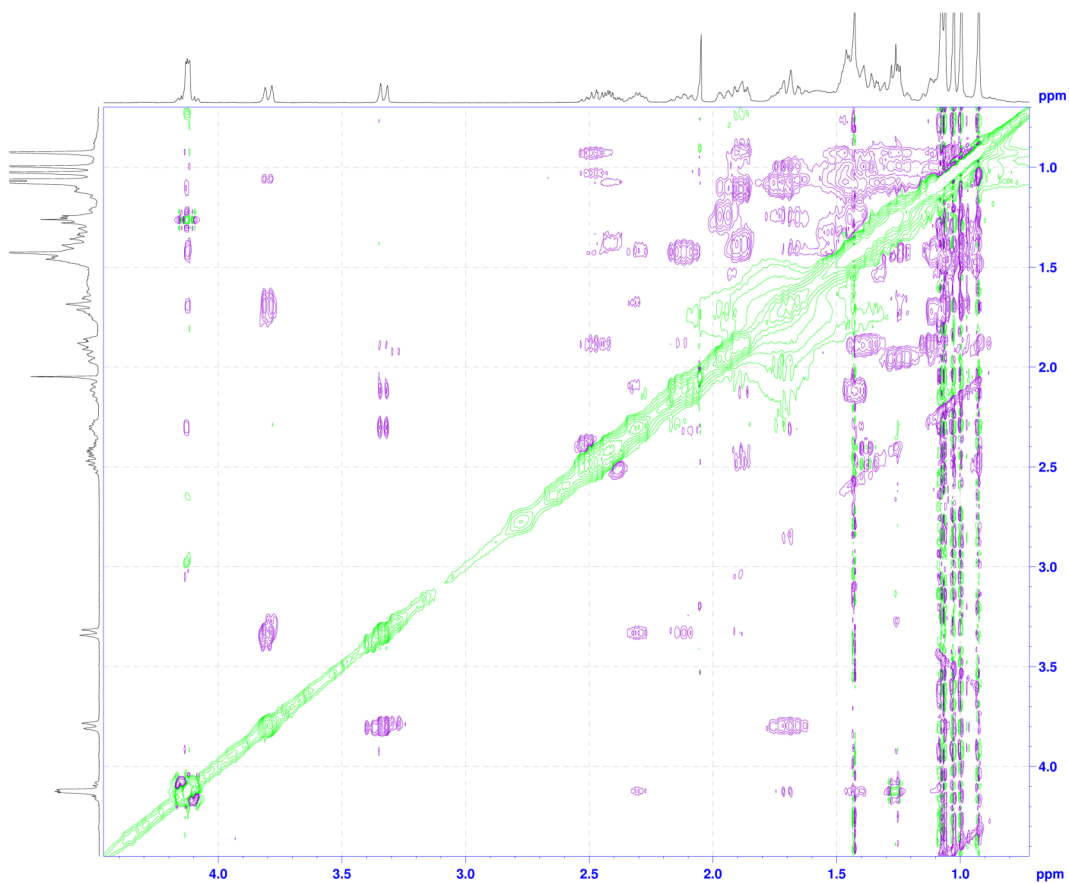


- Mass (ESI+: m/z 479 $[M+Na]^+$) and NMR ($^1H + ^{13}C$ + HSQC edit + NOESY) spectra of 28,30-dihydroxy-3-oxolup-20(29)-ene ($C_{30}H_{48}O_3$; MW 456) (7):

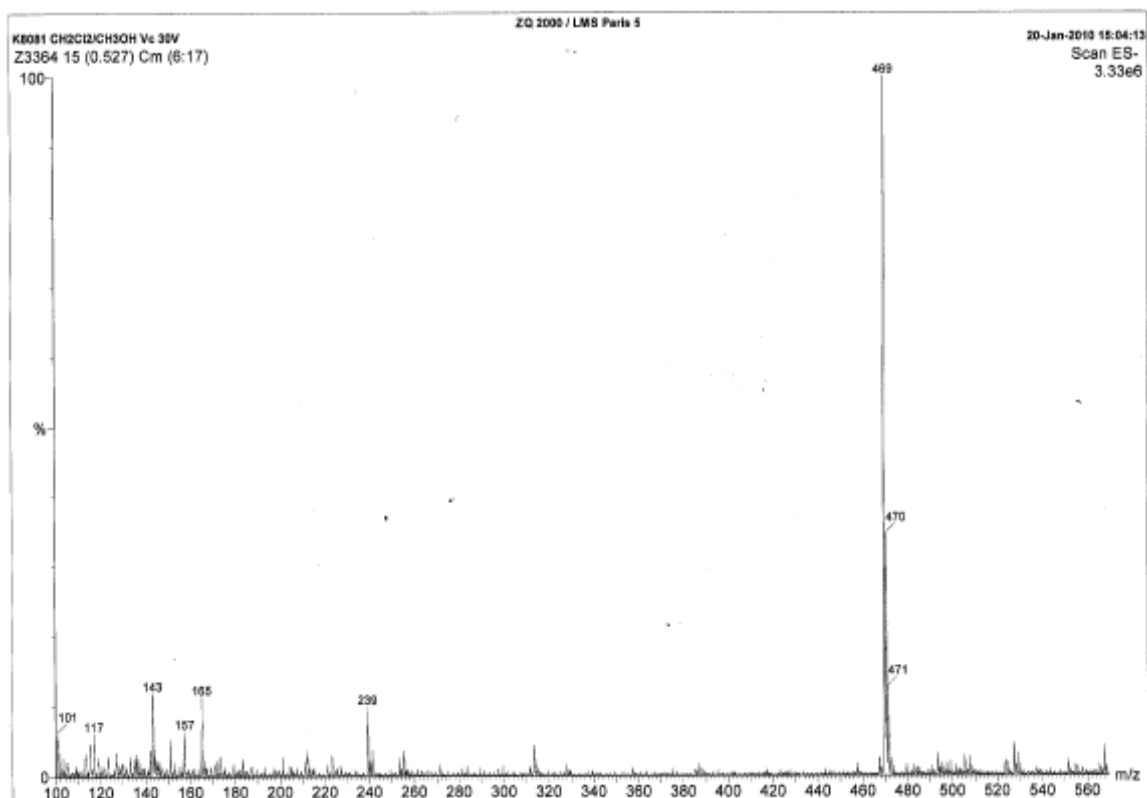


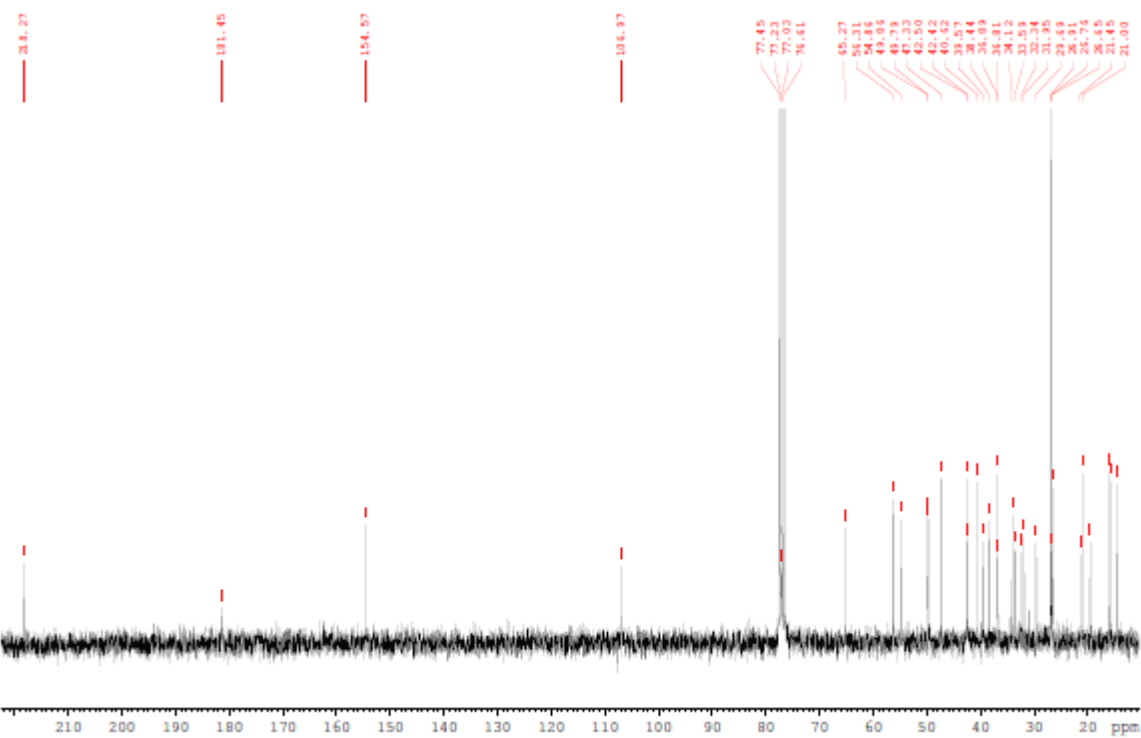


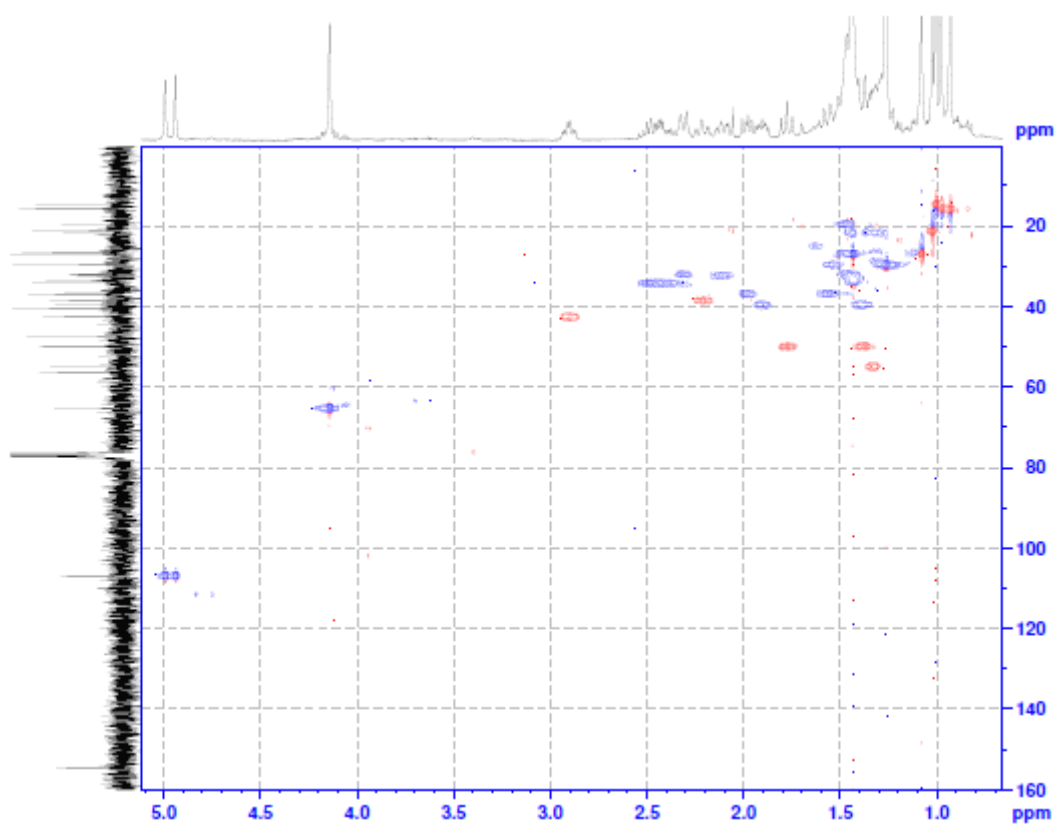
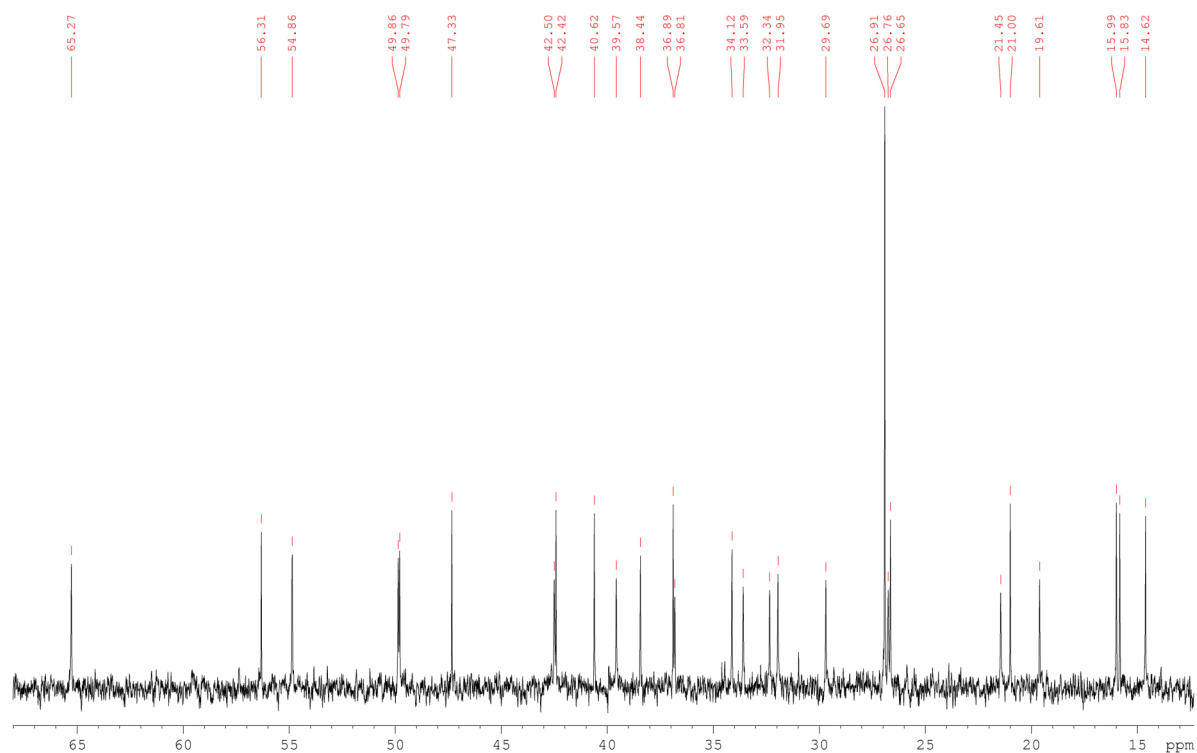




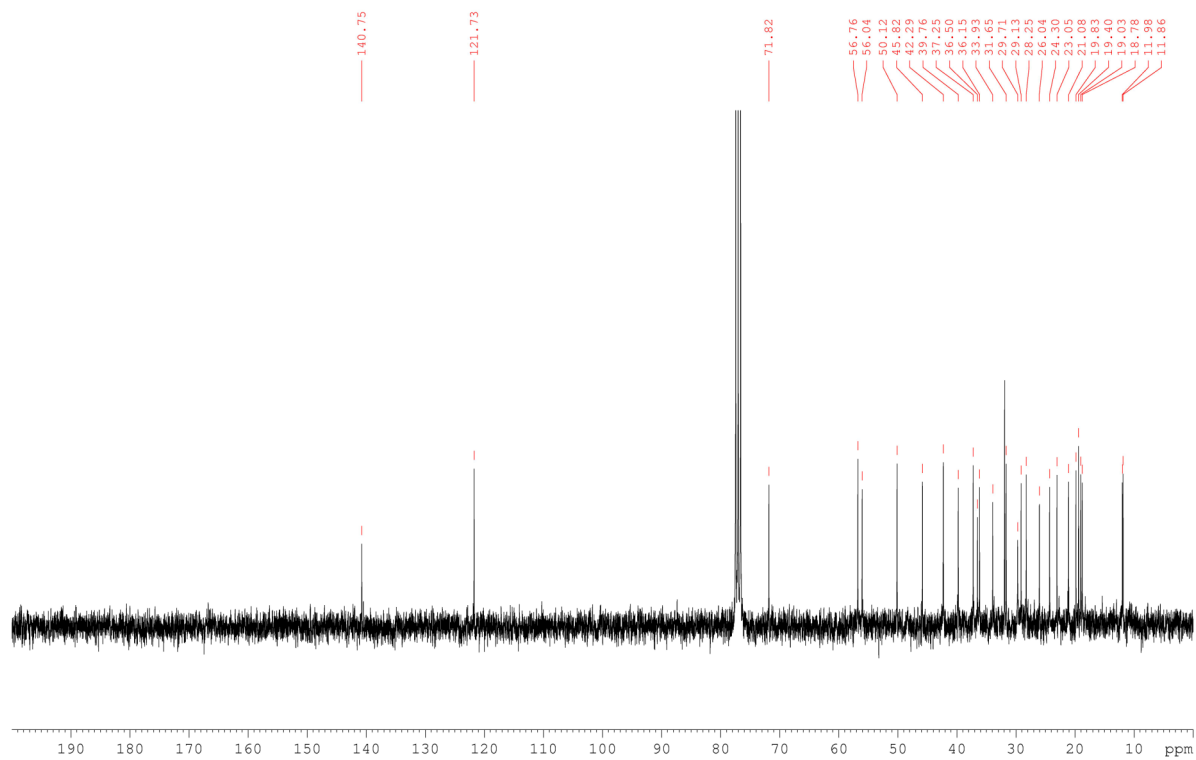
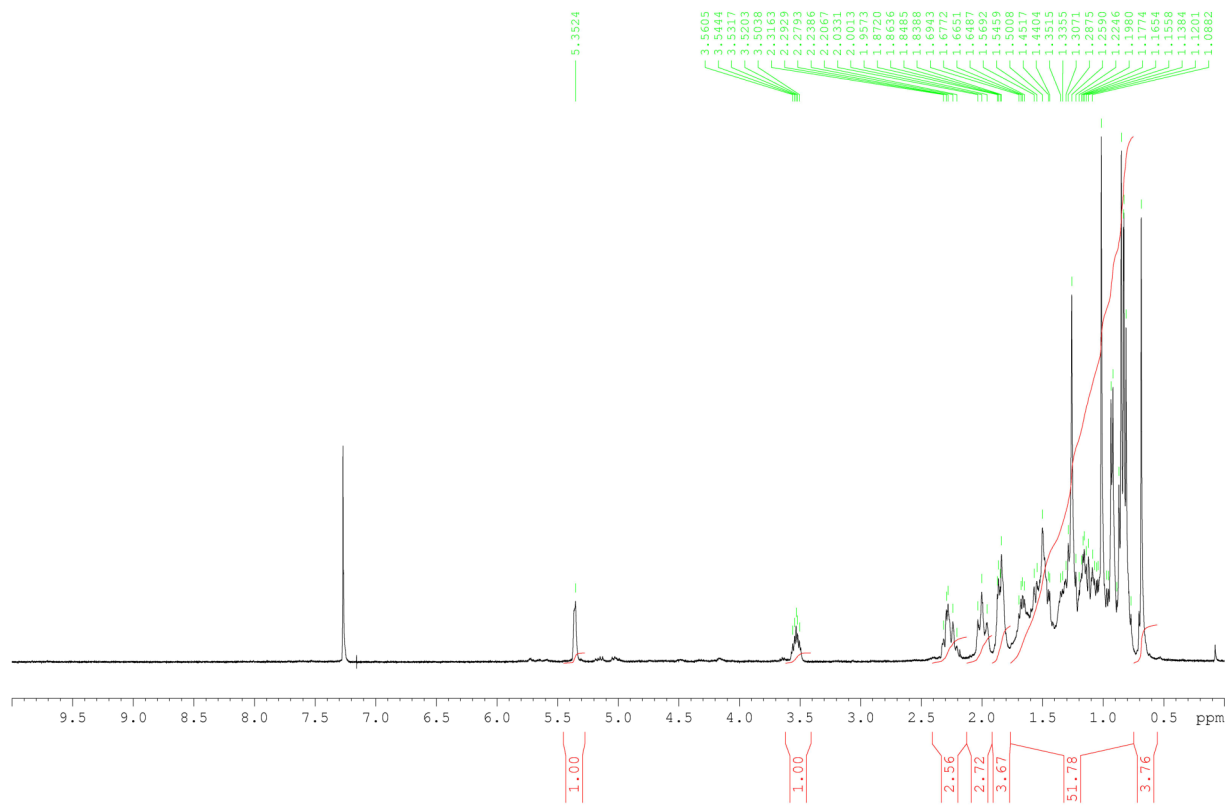
- Mass (ESI-: m/z 469 $[M-H]^-$) and NMR ($^1H + ^{13}C + HSQC$ edit) spectra of Messagenic acid G ($C_{30}H_{46}O_4$; MW 470) (8):

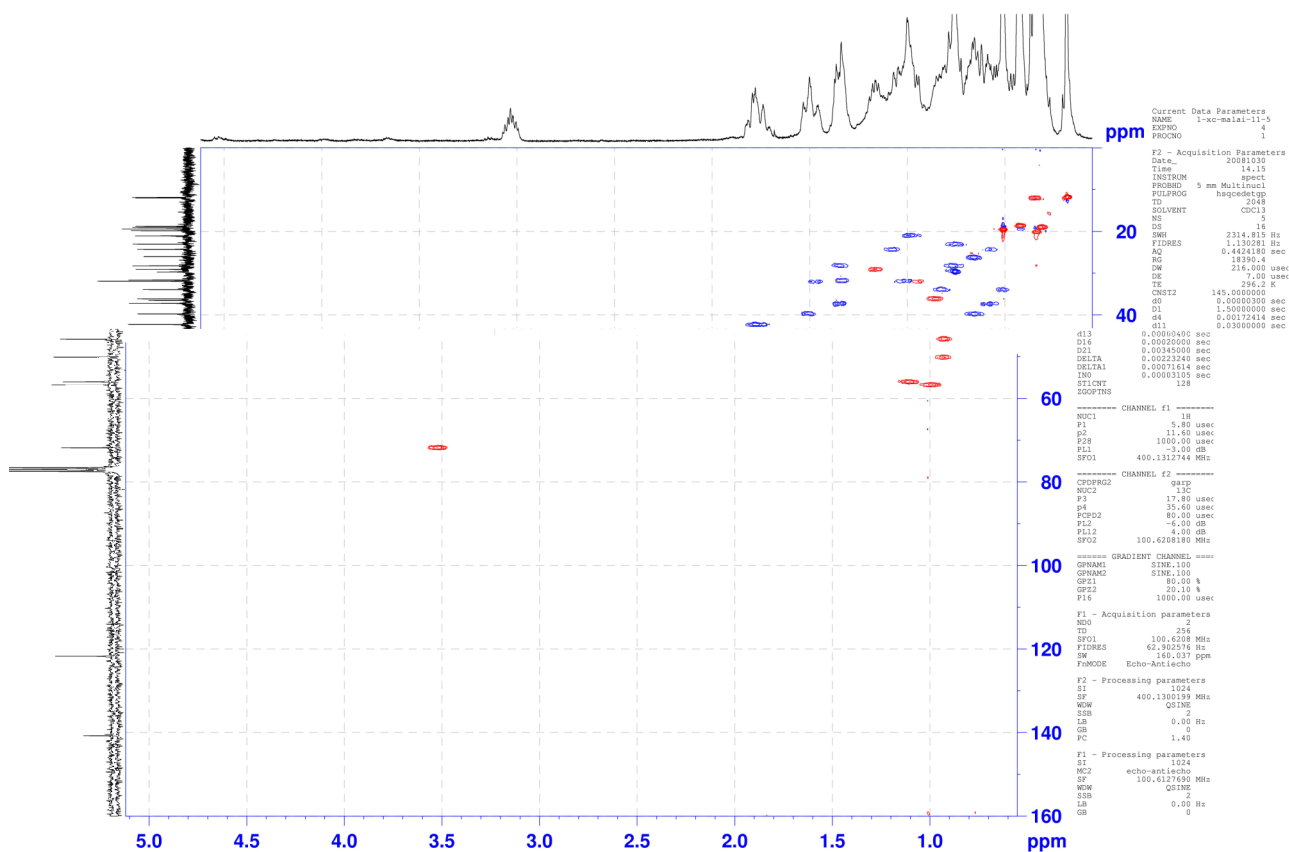




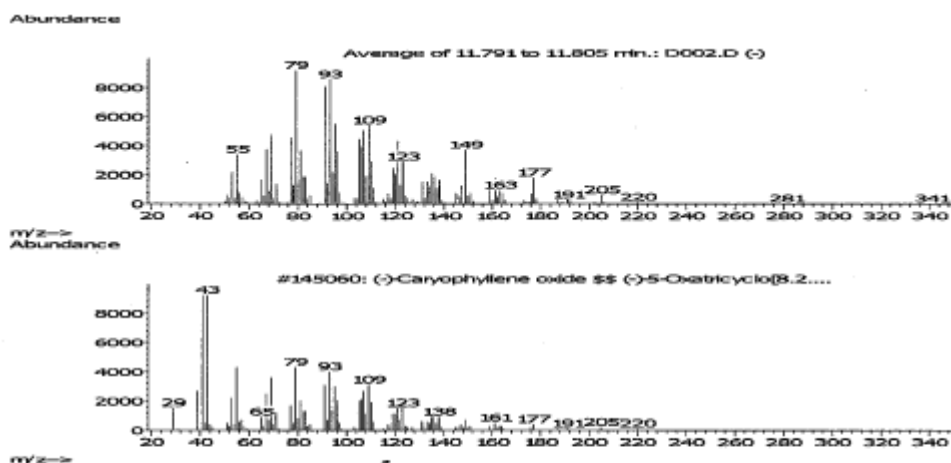


- Mass (EI: m/z 414 $[M]^+$) and NMR (¹H+¹³C+HSQC edit) spectra of β-sitosterol (C₂₉H₅₀O) (9):





- Mass (EI: m/z 220 $[M]^+$) and NMR ($^1\text{H}+^{13}\text{C}$) spectra of β -caryophyllene oxide ($\text{C}_{15}\text{H}_{24}\text{O}$; MW 220) (10):



Match Quality 92

Name (-)-Caryophyllene oxide \$\$ (-)-5-Oxatricyclo[8.2.0(4,6)]dodecane, 12-trimethyl-9-methylene-, [1R-(1R*,4R*,6R*,10S*)]- (CAS) \$\$ (-)-.beta.-Caryophyllene epoxide \$\$
 Caryophyllene oxide \$\$ (-)-caryophyllene oxide \$\$ 5-Oxatricyclo[8.2.0(4,6)]dodecane, 4,1
 CAS Number 001139-30-6
 Molecular Formula $\text{C}_{15}\text{H}_{24}\text{O}$
 Molecular Weight 220.18

