Supporting Information

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Phytochemicals from the Bark of *Garcinia hombroniana* and Their Biological Activities

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Experimental Details

Extraction, Phytochemical Screening and Isolation

The air-dried 5.2 kg ground bark of *G. hombroniana* was successively extracted with Soxhlet extractor using *n*-hexane (*n*-C_6H_{14}), dichloromethane (DCM), chloroform ($CHCl_3$), ethyl acetate (EtOAc) and methanol (MeOH). These extracts along with the aqueous extracts (aqueous and aqueous-di) were screened for the detection of secondary metabolites such as terpenoids, phytosterols, phenolics, flavonoids, carbohydrates, reducing sugars, amino acids, proteins, alkaloids, phlobatannins and tannins, following the standard procedures of Indian Pharmacopoeia (1985) [1].

The dichloromethane extract (14.0 g) was subjected to silica gel (230-400 mesh, 900 g) column chromatography (CC), packed glass column (100 x 6 cm). Elution was carried out using *n*-C_6H_{14}, *n*-C_6H_{14}/EtOAc, EtOAc/MeOH in a polarity gradient manner (1:0 (1000 ml), 9:1 (750 ml), 8:2 (750 ml), 7:3 (500 ml), 6:4 (750 ml), 1:1 (1000 ml), 4:6 (750 ml), 3:7 (750 ml) and 2:8 (750 ml). A mixture of *n*-C_6H_{14}/EtOAc (10:0 to 0:10) was thoroughly used in the fractionation and separation, as this mixture was found to be the most suitable for the isolation of the components in preliminary TLC analysis of dichloromethane extract. A total of 35 fractions; D2FA1 to D2FA35 were collected. The fractions of similar TLC profiles were combined to fractions; D2FB1 to D2FB8.

Fraction, D2FB1 (~ 4.0 g) was rechromtatographed using silica gel and eluted with *n*-C_6H_{14}/EtOAc. A total of 25 sub-fractions; D2SFBa1 to DSFBa25 were collected. The sub-fractions; D2SFBa10-D2SFBa14 collected with *n*-C_6H_{14}/EtOAc (8.5:1.5) were found pure and yielded compound **1** (50.0 mg, 9.61 x 10^{-5}% of the dried bark). Fractions; D2SFBa17 to D2SFBa19 over repeated silica gel CC gave compound **14** (30.0 mg, 5.76 x 10^{-5}% of the dried bark) with *n*-C_6H_{14}/EtOAc (7:3).

Fraction, D2FB2 (~ 1.2 g) was subjected to silica gel CC and eluted with a mixture of *n*-C_6H_{14}/EtOAc to give 20 fractions; D2SFBb1 to D2SFBb20. Fractions D2SFBb4 to D2SFBb6 with *n*-C_6H_{14}/EtOAc (9:1) were found pure and afforded compound **2** with low yield (8.0 mg, 1.50 x 10^{-5}% of the dried bark). Fractions; D2SFBb17 to D2SFBb20 on silica gel CC gave compound **11** (12.0 mg, 2.30 x 10^{-5}% of the dried bark) with *n*-C_6H_{14}/$CHCl_3$ (7:3).

The fraction, D2FB3 (~ 200.0 mg) was fractionated on silica gel CC and conducted with *n*-C_6H_{14}/EtOAc. 13 sub fractions; D2SFBc1 to D2SFBc13 were collected in which D2SFBc5 to D2SFBc8 were semi-pure and rechromatographed on CC to isolate compound **3** (10.0 mg, 1.92 x 10^{-5}% of the dried bark) with *n*-C_6H_{14}/EtOAc (7.5:2.5) as white powder.

Fraction, D2FB4 (~ 3.0 g) was chromatographed on silica gel and eluted with a solvent blend of *n*-C_6H_{14}/EtOAc. A total of 40 sub-fractions; D2SFBd1 to D2SFBd40 were collected. Sub-fractions; D2SFBd9 to D2SFBd25 eluted with *n*-C_6H_{14}/EtOAc (8:2 to 0:1) were similar on TLC analysis, showing two prominent pink spots. These were combined and further subjected to silica gel CC separation, eluted with *n*-C_6H_{14}/EtOAc. 40 sub-fractions; D2SFBd-a1 to D2SFBd-a40 were collected. Sub-fractions; D2SFBda10 to D2SFBda14 with *n*-C_6H_{14}/EtOAc (1.5:8.5) afforded compound **4** (12.0 mg, 2.30 x 10^{-5}% of the dried bark) and sub fraction; D2SFBda32 eluted with *n*-C_6H_{14}/EtOAc (0:1) afforded compound **5** (10.0 mg, 1.92 x 10^{-5}% of the dried bark).

Fraction, D2FB7 (~ 1.6 g) was subjected to separation with silica gel CC and eluted with $CHCl_3$/EtOAc yielding fractions; D2SFBe1 to D2SFBe25. Fractions; D2SFBe6 to D2SFBe15 eluted with $CHCl_3$/EtOAc (3:7) yielded compound **6** (7.0 mg, 1.34 x 10^{-5}% of the dried bark) and **7** (8.0 mg, 1.53 x 10^{-5}% of the dried bark). Fractions; D2SFBe19 to D2SFBfe23 eluted with $CHCl_3$/EtOAc (4:6) gave compound **12** (10.0 mg, 1.92 x 10^{-5}%).

Fraction, D2FB8 (~ 1.2 g) fractionated with silica gel CC using *n*-C_6H_{14}/EtOAc and EtOAc/MeOH yielded sub-fractions; D2SFBf1 to D2SFBf35. Fractions; D2SF Bf10 to D2SFBf16 were found similar by TLC analysis with a prominent purple spot accompanying by other minor impurities. These fractions were combined and rechromatographed with *n*-C_6H_{14}/EtOAc. On elution with a solvent blend of 3:7 of *n*-C_6H_{14}/EtOAc, it gave a mixture of compounds **8** and **9** (30.0 mg, 5.76 x 10^{-5}%) while by eluting with EtOAc/MeOH (9.5:0.5), it afforded compound **13** (15.0 mg, 2.80 x 10^{-5}%).

Sub fraction, E2FA6 of ethyl acetate extract through silica gel CC with $CHCl_3$/MeOH (7:1) yielded a bright yellow compound **10** (12.0 mg, 2.30 x 10^{-5}%).

Biological Activities

The isolated compound (**1**-**14)** from different fractions of the dichloromethane and ethyl acetate extracts were investigated for their *in vitro* antioxidant and antibacterial potential. Antioxidant activities were evaluated using free radical scavenging of DPPH [2] and ABTS [3], and reducing power FRAP [2] assays. Antibacterial activities of the compounds **1**-**14** against two Gram positive (*Staphylococcus aureus* and *Bacillus subtilis*) and two Gram negative bacteria (*Pseudomonas aeruginosa* and *Escherichia coli*) were evaluated using Kirby-Bauer disc diffusion method [4] and dilution (minimum inhibitory concentration) method, described by Eloff (1998) [5].

Statistical Analyses

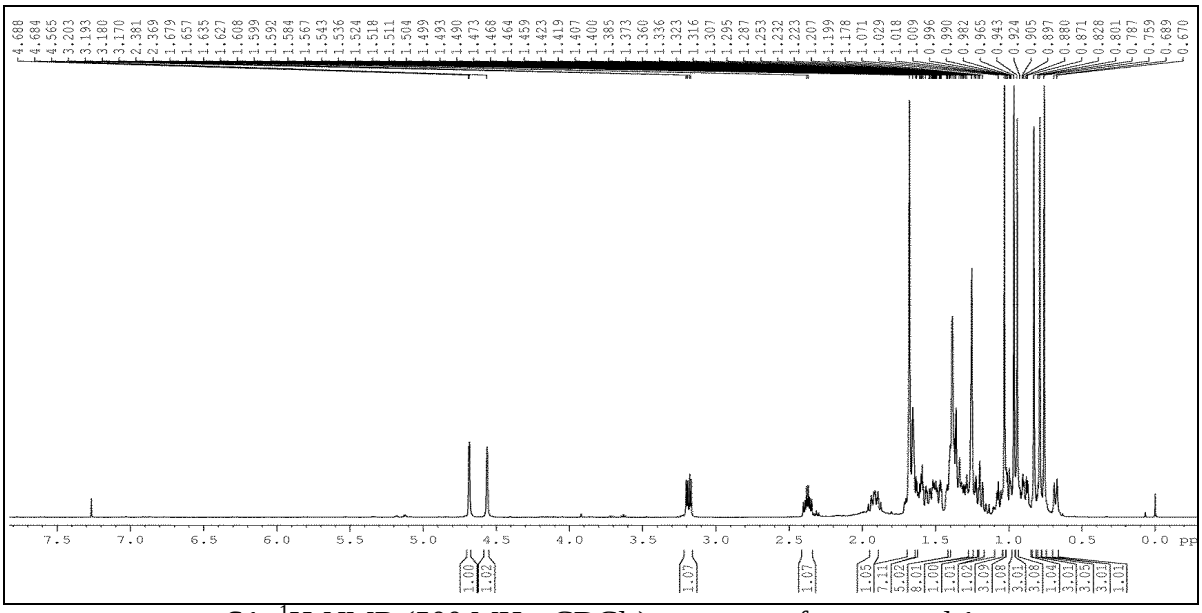
The data were reported in triplicates (n = 3). Significant differences between values were analyzed with one-way analysis of variance(ANOVA) using Tukey's HSD test at 95% confidence interval in SPSS (Statistical Package for Social Sciences) Software Version 20 (IBM, New York, USA). IC_{50} values were calculated with GraphPad Prism 6.02 (GraphPad Software Inc., La Jolla, USA).

Table S1. Phytochemical Screening of Bark Extracts of *G. hombroniana*

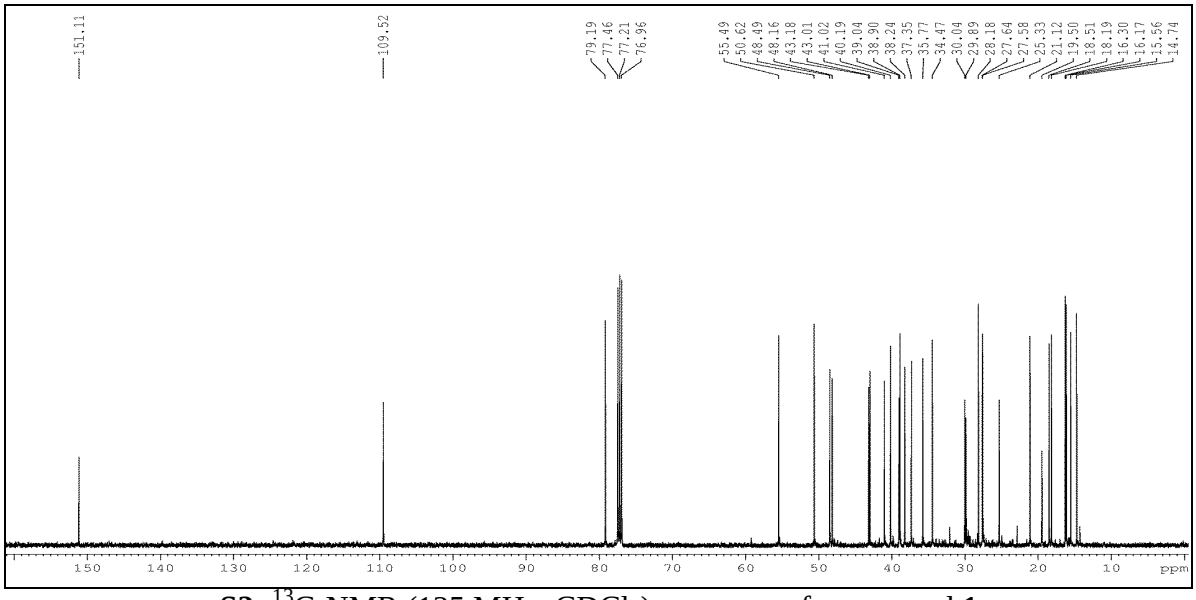
Extracts	*n*-hexane	Dichloromethane	Chloroform	E/acetate	Methanol	Aqueous	Aqueous-di
Carbohydrates	--	--	--	--	--	++	++
Glycosides	--	--	--	++	++	++	++
Proteins + Amino acids	--	--	--	--	--	---	--
Alkaloids	--	--	--	--	--	++	++
Terpenoids	++	++	++	--	--	--	--
Phytosterols	++	++	++	--	--	--	--
Phenolics	--	--	--	++	++	++	++
Flavonoids	--	--	--	++	++	++	++
Tannins	--	--	--	--	++	++	++
Phlobatannins	--	--	--	--	--	--	--

ND: not determined; ++: Present; --: Absent

Lupeol (**1**): white powder; mp 213-215 °C; molecular formula $C_{30}H_{50}O$; EI-MS *m/z*: 426.5 $[M]^+$; IR (KBr): 3360, 2944, 1638, 1453, 1379, 1043 and 880 cm^{-1}; ^{1}H-NMR ($CDCl_3$, 500 MHz): δ_H 4.68 (*d*, *J* = 2.0, 1H, H-29a), 4.56 (br. *s*, 1H, H-29a), 3.20 (*dd*, *J* = 11.5, 5.0 Hz, 1H, H-3), 2.40 (*m*, 1H, H-19), 1.95 (*m*, 1H, H-21), 1.68 (*m*, 1H, H-15a), 1.67 (*s*, 5H, H-1a, H-12a, Me-30), 1.66 (br. *m*, 2H, H-13), 1.60 (*m*, 1H, H-2a), 1.56 (*m*, 1H, H-2b), 1.52 (*m*, 1H, H-6a), 1.47 (*m*, 1H, H-16a), 1.42 (*m*, 1H, H-11), 1.40 (*m*, 2H, H-7), 1.38 (br. *m*, 1H, H-22a), 1.37 (*m*, 1H, H-16b), 1.36 (br. *m*, 1H, H-18), 1.32 (*m*, 1H, H-6b), 1.30 (*m*, 1H, H-21), 1.29 (br. *s*, 1H, H-9), 1.23 (*m*, 1H, H-11b), 1.20 (*s*, 1H, H-22b), 1.08 (*m*, 1H, H-12b),1.02 (*s*, 3H, Me-26), 1.01 (*m*, 1H, H-15a), 0.96 (*s*, 3H, Me-23), 0.94 (*s*, 3H, Me-27), 0.90 (*s*, 1H, H-1b), 0.82 (*s*, 3H, Me-25), 0.78 (*s*, 3H, Me-28), 0.75 (*s*, 3H, Me-24), 0.68 (*d*, *J* = 9.5 Hz, 1H, H-5); ^{13}C-NMR ($CDCl_3$, 125 MHz): δ_C 151.1 (C-20), 109.5 (C-29), 79.2 (C-3), 55.5 (C-5), 50.6 (C-9), 48.5 (C-18), 48.1 (C-19), 43.2 (C-17), 43.0 (C-14), 41.0 (C-8), 40.2 (C-22), 39.0 (C-4), 38.9 (C-1), 38.2 (C-13), 37.3 (C-10), 35.7 (C-16), 34.5 (C-7), 29.9 (C-21), 28.2 (C-23), 27.7 (C-15), 27.5 (C-2), 25.3 (C-12), 21.1 (C-11), 19.5 (C-30), 18.5 (C-6), 18.2 (C-28), 16.3 (C-25), 16.1 (C-26), 15.5 (C-24), 14.7 (C-27).

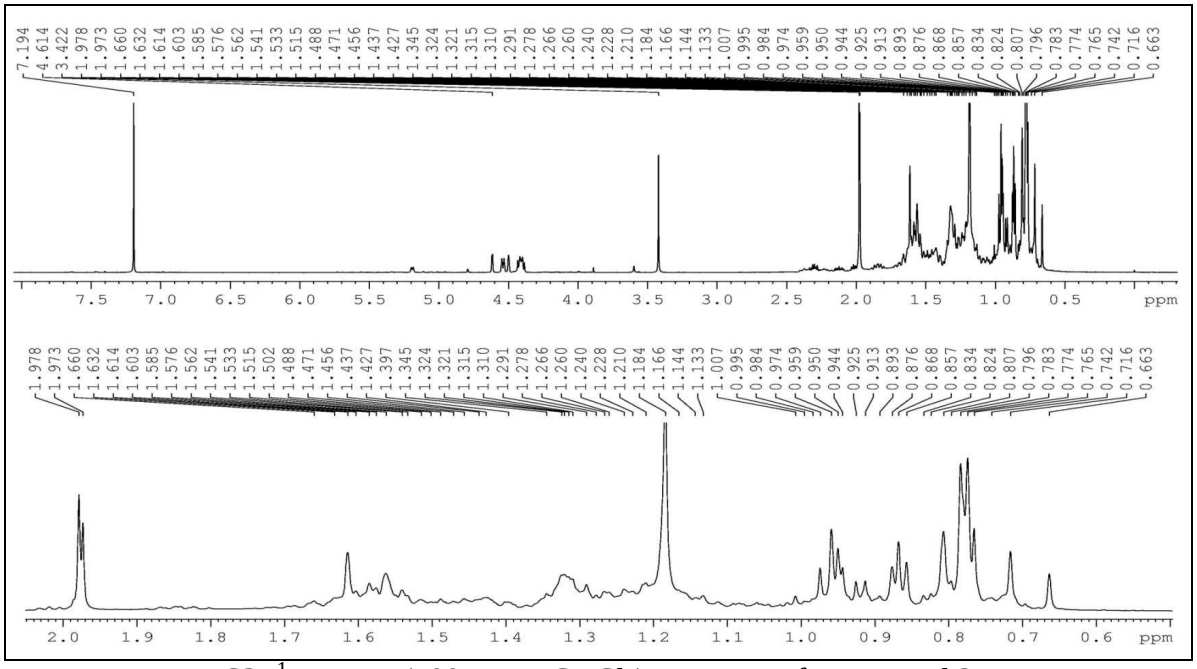


S1: ^{1}H-NMR (500 MHz, $CDCl_3$) spectrum of compound **1**

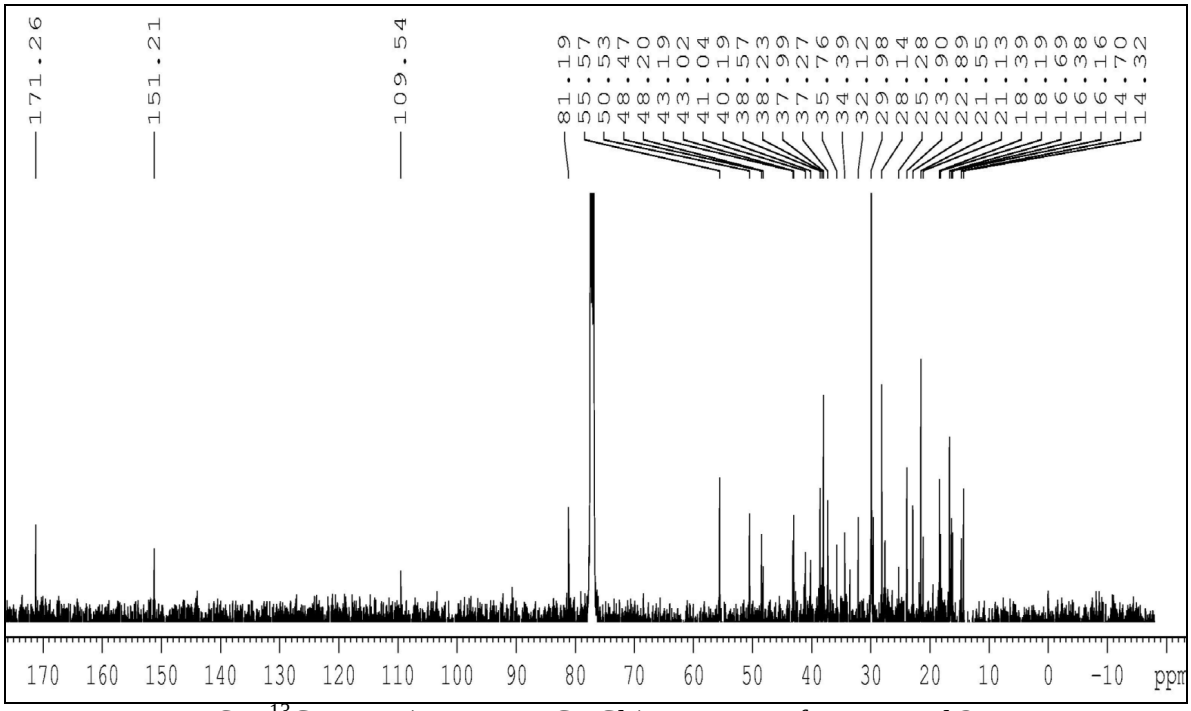


S2: ^{13}C-NMR (125 MHz, $CDCl_3$) spectrum of compound **1**

Lupeol acetate (**2**): white powder; mp 220-222 °C; molecular formula $C_{32}H_{52}O_3$ EI-MS *m/z*: 468.6 $[M]^+$; IR (KBr): 3360, 2946, 1638; 880 cm^{-1}; ^{1}H-NMR ($CDCl_3$, 500 MHz): δ_H 4.69 (*s*, 1H, H-29a), 4.57 (*s*, 1H, H-29a), 4.47 (*dd*, 1H, *J* = 4.4, 12.8 Hz, H-3), 2.33 (*dt*, *J* = 11.1, 5.6 Hz, 1H, H-19), 1.82-1.93 (*m*, 2H, H-21), 1.66 (*s*, 3H, H-30), 1.00 (*s*, 3H, H-26), 0.91 (*s*, 3H, H-27), 0.82 (*s*, 9H, H-23, H-24, H-25), 0.81 (*s*, 3H, H-28) 0.76 (*dd*, *J* = 10.8, 5.8 Hz, 1H, H-5); ^{13}C-NMR ($CDCl_3$, 125 MHz): δ_C 171.3 (C-1'), 151.1 (C-20), 109.5 (C-29), 81.2 (C-3), 55.5 (C-5), 50.6 (C-9), 48.5 (C-18), 48.1 (C-19), 43.2 (C-17), 43.0 (C-14), 41.0 (C-8), 40.2 (C-22), 39.0 (C-4), 38.9 (C-1), 38.2 (C-13), 37.3 (C-10), 35.7 (C-16), 34.5 (C-7), 29.9 (C-21), 28.1 (C-23, C-2'), 27.7 (C-15), 27.5 (C-2), 25.3 (C-12), 21.1 (C-11), 19.5 (C-30), 18.5 (C-6), 18.2 (C-28), 16.3 (C-25), 16.1 (C-26), 15.5 (C-24), 14.7 (C-27).

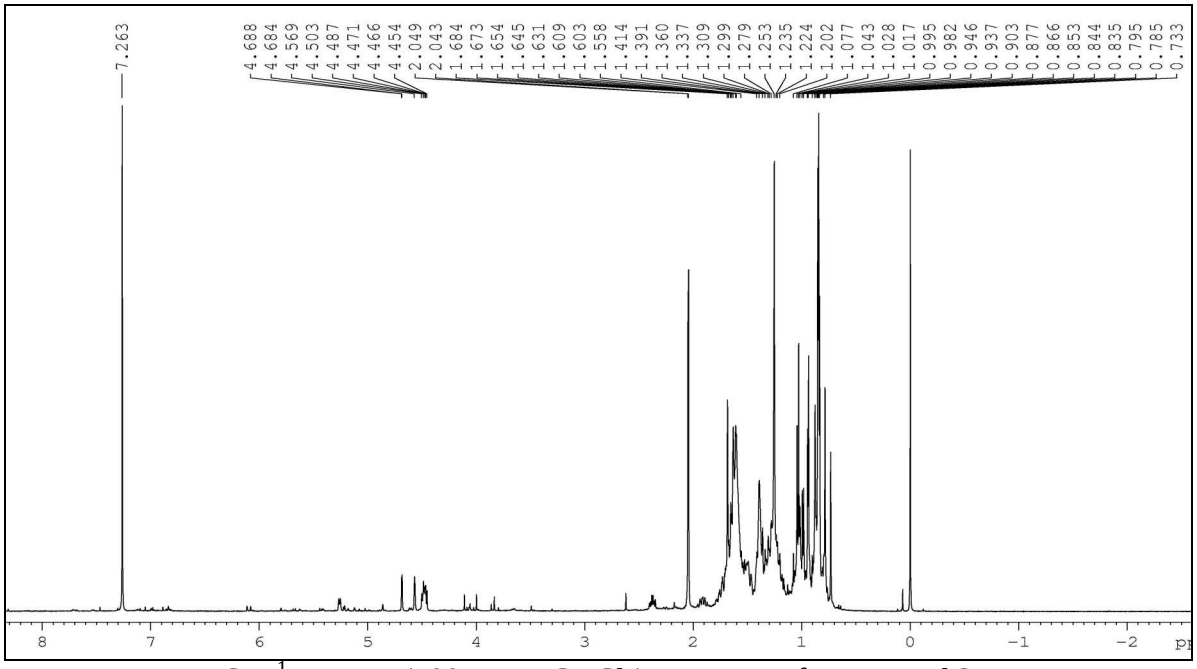


S3: ^{1}H-NMR (500 MHz, $CDCl_3$) spectrum of compound **2**

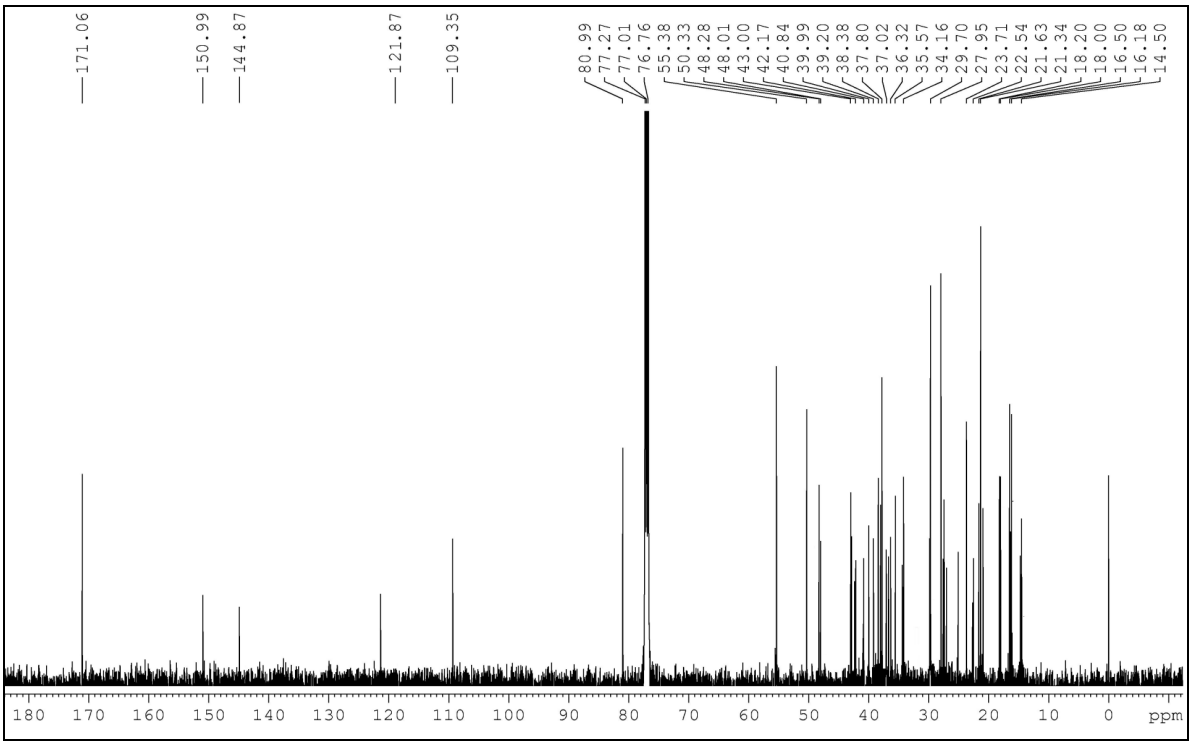


S4: ^{13}C-NMR (125 MHz, $CDCl_3$) spectrum of compound **2**

3β-acetoxy-12,20(29)-diene (**3**): white powder; mp 248-251 °C; molecular formula $C_{32}H_{50}O_3$ EI-MS *m/z*: 466.4 $[M]^+$; IR (KBr): 3389, 2975, 1651; 882 cm^{-1}; ^{1}H-NMR ($CDCl_3$, 500 MHz): δ_H 4.68 (*s*, 1H, H-29a), 4.56 (*s*, 1H, H-29a), 4.46 (*dd*, 1H, *J* = 12.0, 4.5 Hz, H-3), 2.03 (*t*, *J* = 11.5, 5.0 Hz, 1H, H-19), 1.67(*s*, 3H, H-30), 1.01 (*s*, 3H, H-26), 0.90 (*s*, 3H, H-27), 0.83 (*s*, 9H, H-23, H-24, H-25), 0.79 (*s*, 3H, H-28) 0.73 (*dd*, *J* = 10.2, 5.4 Hz, 1H, H-5); ^{13}C-NMR ($CDCl_3$, 125 MHz): δ_C 171.0 (C-1'), 150.9 (C-20), 109.3 (C-29), 80.9 (C-3), 55.3 (C-5), 50.3 (C-9), 48.2 (C-18), 48.0 (C-19), 43.0 (C-17), 42.1 (C-14), 40.8 (C-8), 39.9 (C-22), 39.2 (C-4), 38.3 (C-1), 144.8 (C-13), 37.0 (C-10), 35.5 (C-16), 34.1 (C-7), 29.7 (C-21), 27.9 (C-23, C-2'), 27.7 (C-15), 27.5 (C-2), 121.8 (C-12), 21.6 (C-11), 21.3 (C-30), 18.2 (C-6), 18.0 (C-28), 16.5 (C-25), 16.1 (C-26), 15.5 (C-24), 14.5 (C-27).

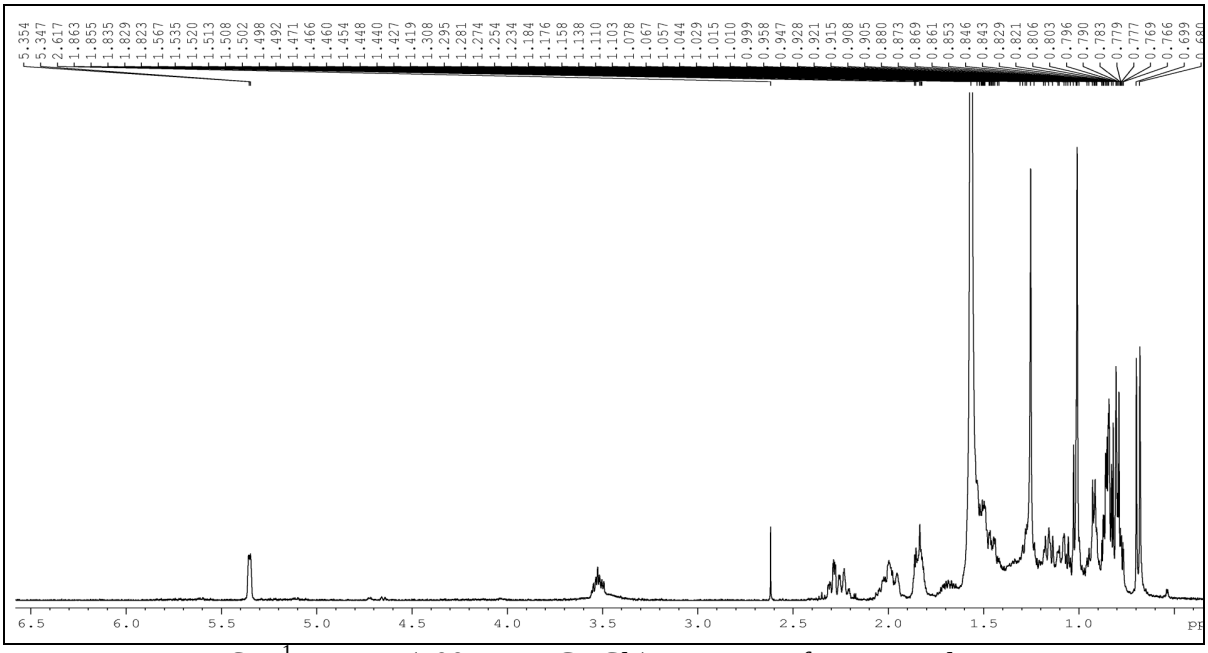


S5: ^{1}H-NMR (500 MHz, $CDCl_3$) spectrum of compound **3**

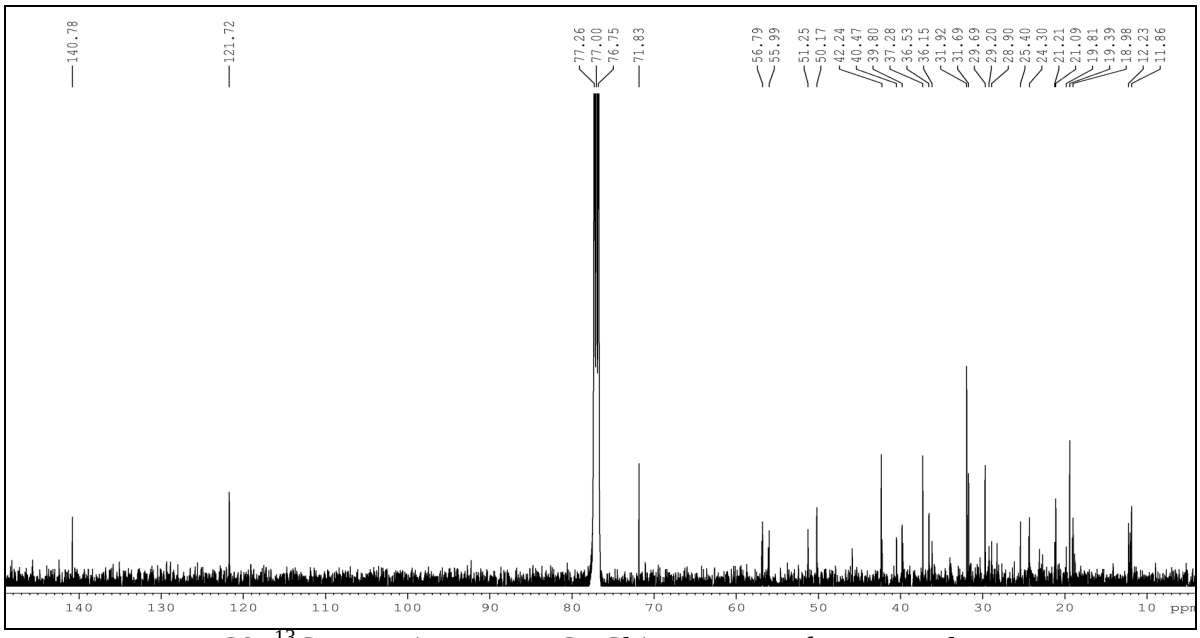


S6: ^{13}C-NMR (125 MHz, $CDCl_3$) spectrum of compound **3**

β-sitosterol (**4**): white crystals; mp 139-142 °C; molecular formula $C_{29}H_{50}O$; EI-MS *m/z*: 414.6 $[M]^+$; IR (KBr): 3390, 1646, 1452, 1178, 1133, 1041, 820 cm^{-1}; ^{1}H-NMR ($CDCl_3$, 500 MHz): δ_H 5.35 (*m*, 1H, H-6), 1.76 (*m*, 2H, H-22), 1.42 (*m*, 2H, H-23), 3.52 (*m*, 1H, H-3), 2.31-2.23 (*m*, 2H, H-4a, H-4b), 2.06-1.96 (*m*, 3H, H-20, H-7a, H-12a), 1.85-1.83 (*m*, 2H, H-1a, H-2a), 1.72 (*m*, 1H, H-16a), 1.56-1.50 (*m*, 8H, H-15a, H-28a, H-25, H-24, H-2b, H-7b, H-11a, H-11b), 1.47 (*m*, 1H, H-8), 1.29 (*m*, 1H, H-16b), 1.22 (*m*, 1H, H-28b), 1.17 (*dt*, 1H, H-12b), 1.10 (*m*, 1H, H-1b), 1.07 (*m*, 2H, H-14, H-15b), 1.03 (*d*, 3H, Me-21), 1.00 (*s*, 3H, Me-19), 0.95 (*m*, 1H, H-9), 0.85 (*d*, 3H, *J* = 6.5 Hz, Me-26), 0.80 (*s*, 3H, Me-29), 0.79 (*s*, 3H, Me-27), 0.69 (*s*, 3H, Me-18); ^{13}C-NMR ($CDCl_3$, 125 MHz): δ_C 140.7 (C-5), 36.1 (C-22), 28.9 (C-23), 121.7 (C-6), 71.8 (C-3), 56.7 (C-14), 55.9 (C-17), 51.2 (C-24), 50.1 (C-9), 42.3 (C-4, C-13), 40.4 (C-20), 39.8 (C-12), 37.2 (C-1), 36.5 (C-10), 31.9 (C-8), 31.6 (C-25), 29.6 (C-2, C-7), 29.2 (C-16), 25.4 (C-28), 24.3 (C-15), 21.2 C-21, C-26), 21.1 (C-11), 19.8 (C-27), 19.0 (C-19), 12.2 (C-18), 12.0 (C-29).

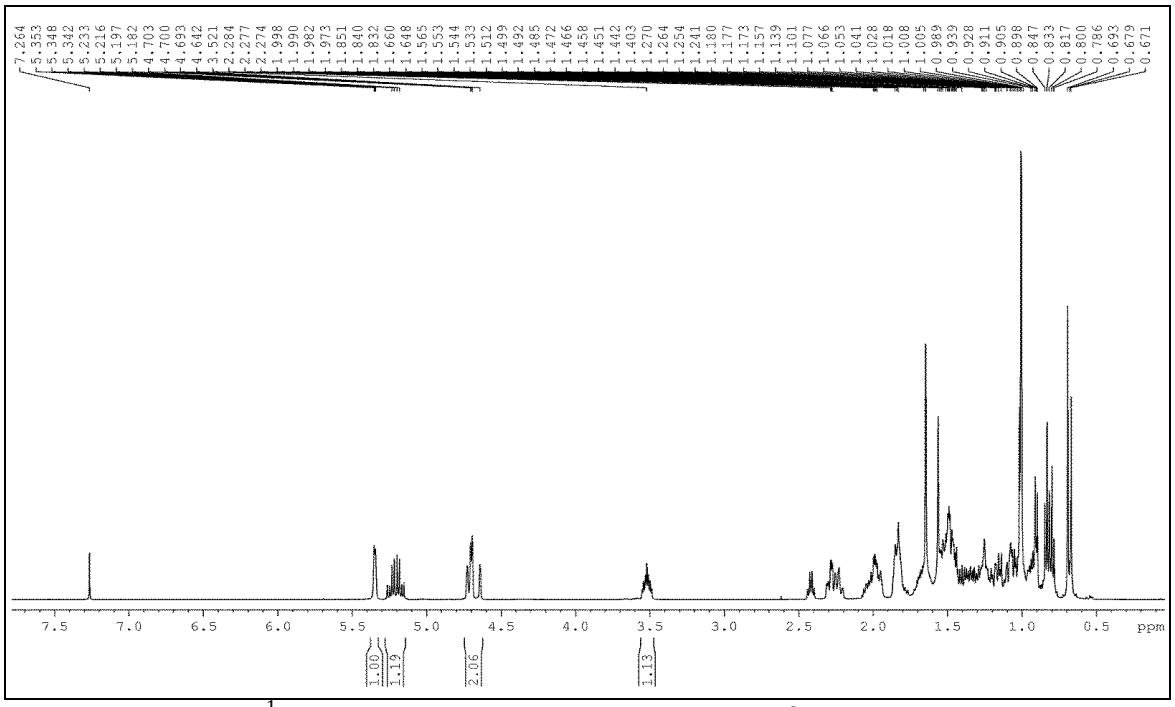


S7: ^{1}H-NMR (500 MHz, $CDCl_3$) spectrum of compound **4**

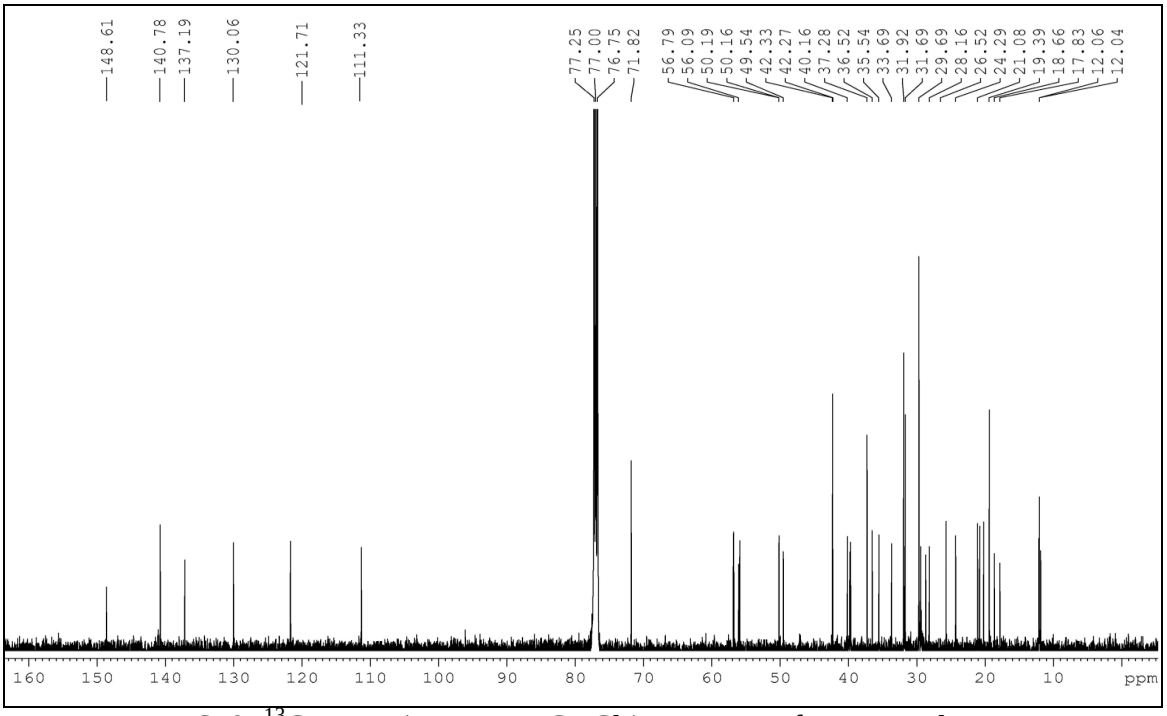


S8: ^{13}C-NMR (125 MHz, $CDCl_3$) spectrum of compound **4**

22-dehdroclerosterol (**5**): white solid; mp 157-160 °C; molecular formula $C_{29}H_{46}O$; EI-MS *m/z*: 410.4 $[M]^+$; IR (KBr): 3457, 1691, 1458, 1023 cm^{-1}; ^{1}H-NMR ($CDCl_3$, 500 MHz): δ_H 5.35 (br. *d*, *J* = 5.5 Hz, 1H, H-6), 5.23 (*m*, 1H, H-22), 5.19 (*m*, 1H, H-23), 4.70 (br. *s*, 1H, H-26a), 4.64 (br. *d*, *J* = 2.5 Hz, 1H, H-26b), 3.52 (*m*, 1H, H-3), 1.64 (*s*, 3H, H-27), 0.81 (*t*, *J* = 7.0 Hz, 3H, H-29), 0.67 (*s*, 3H, H-18); ^{13}C-NMR ($CDCl_3$, 125 MHz): δ_C 147.8 (C-25), 141.0 (C-5), 137.1 (C-22), 130.0 (C-23), 121.9 (C-6), 111.6 (C-27), 72.0 (C-3), 57.0 (C-14), 56.3 (C-17), 50.4 (C-9), 49.8 (C-24), 42.6 (C-13, 42.5 (4), 40.0 (C-12), 37.5 (C-1), 36.7 (C-10), 35.8 (C-20), 32.1 (C-7, C-8), 31.9 (C-2), 28.4 (C-16), 26.8 (C-28), 24.5 (C-15), 21.3 (C-11), 19.6 (C-19), 18.9 (C-21), 18.0 (C-26), 12.3 (C-18), 12.1 (C-29).

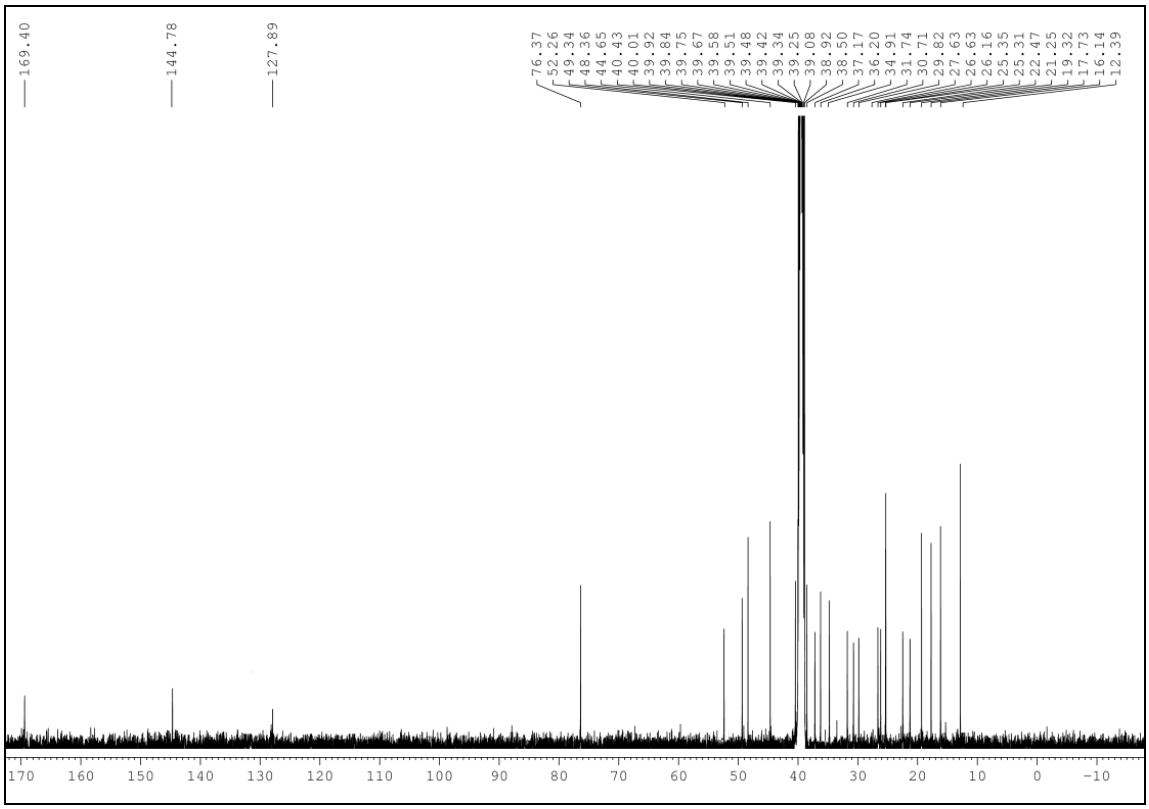


S9: ^{1}H-NMR (500 MHz, $CDCl_3$) spectrum of compound **5**



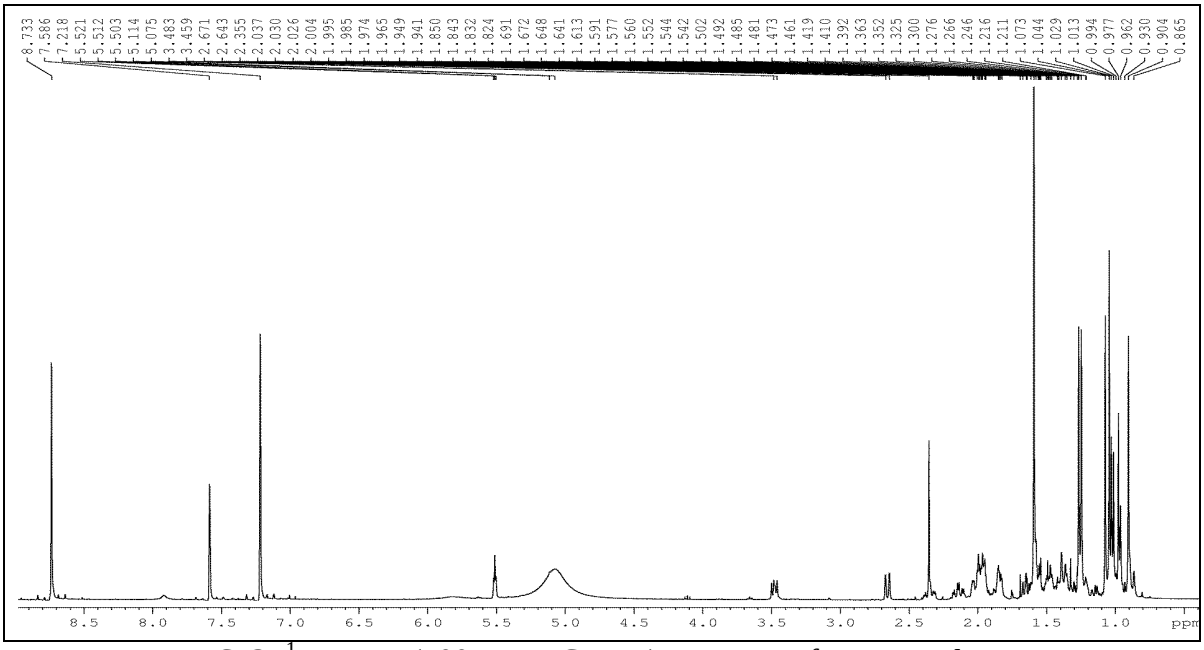
S10: ^{13}C-NMR (125 MHz, $CDCl_3$) spectrum of compound **5**

Magniferolic acid (**6**): white solid; molecular formula $C_{30}H_{48}O_3$; 214-216 °C; EI-MS *m/z*: 456.4 [M^+]; IR (KBr): 3437, 1693, 1443, 1048 cm^{-1}; ^{1}H-NMR (DMSO-d_6, 500 MHz): δ_H 6.67 (*t*, 1H, H-24), 3.41 (*overlapped*, 1H, H-3), 2.25 (*m*, 2H, H-23), 2.00 (*m*, 2H, H-11), 1.93 (*m*, 1H, H-2a), 1.89 (*m*,1H, H-1a), 1.86 (*s*, 3H, Me-27), 1.82 (*s*, 1H, H-5), 1.63 (*m*, 1H, H-2b), 1.59 (*m*, 5H, H-7a, H-12, H-17, H-22a), 1.55 (*m*, 1H, H-8), 1.52 *m*, 1H, H-6a), 1.43 (*m*, 1H, H-20), 1.30 (*m*, 3H, H-7b, H-15, H-16a), 1.18 (*m*, 1H, H-22b), 1.09 (*m*, 1H, H-16b), 1.02 (*m*, 1H, H-1b), 1.00 (*s*, 3H, Me-18), 0.94 (*s*, 3H, Me-28), 0.89 (s, 6H, Me-21, Me-30), 0.87 (*s*, 3H, Me-29), 0.75 (*m*, 1H, H-6b), 0.54 (*s*, 1H, H-19a), 0.42 (*d*, *J* = 3.0, 1H, H-19b); ^{13}C-NMR (DMSO-d_6, 125 MHz): δ_C 169.4 (C-26), 144.8 (C-24), 127.8 (C-25), 76.3 (C-3), 52.0 (C-17), 49.3 (C-14), 48.3 (C-8), 44.6 (C-13), 40.6 (C-5), 38.5 (C-4), 37.1 (C-20), 35.0 (C-15), 34.5 (C-22), 31.7 (C-12), 30.7 (C-19), 29.8 (C-2, C-16), 26.6 (C-1), 26.1 (C-10), 25.3 (C-7, C-11, C-23, C-28), 22.4 (C-29), 21.2 (C-6), 19.8 (C-9), 19.3 (C-30), 17.7 (C-18), 16.1 (C-21), 12.8 (C-27).

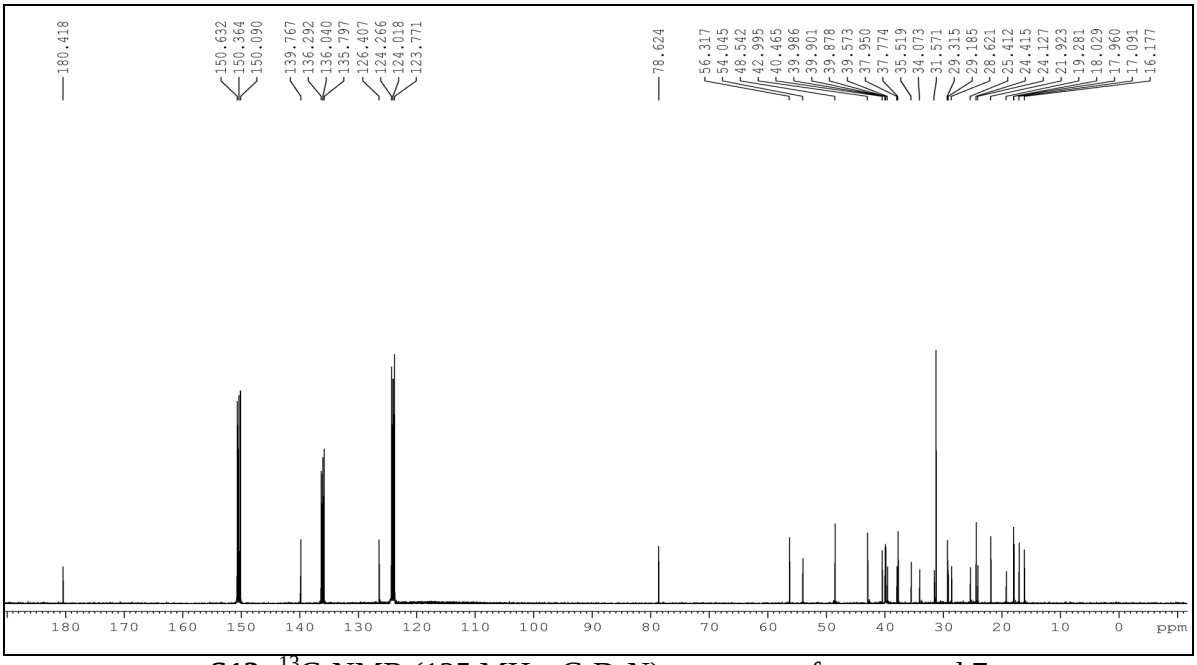


S11: ^{13}C-NMR (125 MHz, DMSO-d_6) spectrum of compound **6**

Ursolic acid (**7**): white solid; molecular formula $C_{30}H_{48}O_3$; 238-240 °C; EI-MS *m/z*: 456.4 $[M]^+$; IR (KBr): 3440, 2912, 2874, 1696, 1452, 1041 cm^{-1}; ^{1}H-NMR (C_5D_5N, 500 MHz): δ_H 5.46 (*t*, *J* = 5.2, 1H, H-12), 3.42 (*dd*, *J* = 10.5, 4.0, 1H, H-3), 2.61 (*d*, *J* = 11.0, 2H, H-18), 2.35 (*m*, 1H, H-15b), 2.13 (*m*, 1H, H-16a), 2.00 (*m*, 1H, H-16b), 1.97 (*m*, 2,H H-22), 1.95 (*m*, 2H, H-11), 1.83 (*m*, 2H, H-2), 1.64 (*m*, 1H, H-9), 1.57 (*m*, 3H, H-7a, H-6a, H-1b), 1.47 (*m*, 2H, H-19, H-21b), 1.40 (*m*, 1H, H-21a), 1.37 (*m*, 2H, H-6b, H-7b), 1.24 (*m*, 6H, Me-23, Me-27), 1.23 (*m*, 1H, H-15a), 1.06 (*m*, 4H, H-20, H-26), 1.04 (*m*, 3H, H-24), 1.01 (*m*, 4H, H-1a, H-29), 0.95 (*d*, *J* = 6.5, 3H, H-30), 0.89 (*s*, 3H, Me-25), 0.87 (*s*, 1H, Me-5); ^{13}C-NMR ($CDCl_3$, 125 MHz): δ_C 180.7 (C-28), 138.8 (C-13), 125.5 (C-12), 78.9 (C-3), 55.9 (C-5), 53.4 (C-18), 48.7 (C-9, C-17), 42.4 (C-14), 40.2 (C-4), 39.7 (C-20, C-8), 39.5 (C-19), 38.8 (C-1), 37.4 (C-10), 37.2 (C-22), 33.5 (C-7), 30.8 (C-21), 28.1 (C-2, C-15), 27.8 (C-23), 24.5 (C-16), 23.4 (C-11), 23.1 (C-27), 20.6 C-30), 18.6 (C-6), 16.8 (C-26), 16.0 (C-29), 15.0 (C-25).



S12: ^{1}H-NMR (500 MHz, C_5D_5N) spectrum of compound **7**



S13: ^{13}C-NMR (125 MHz, C_5D_5N) spectrum of compound **7**

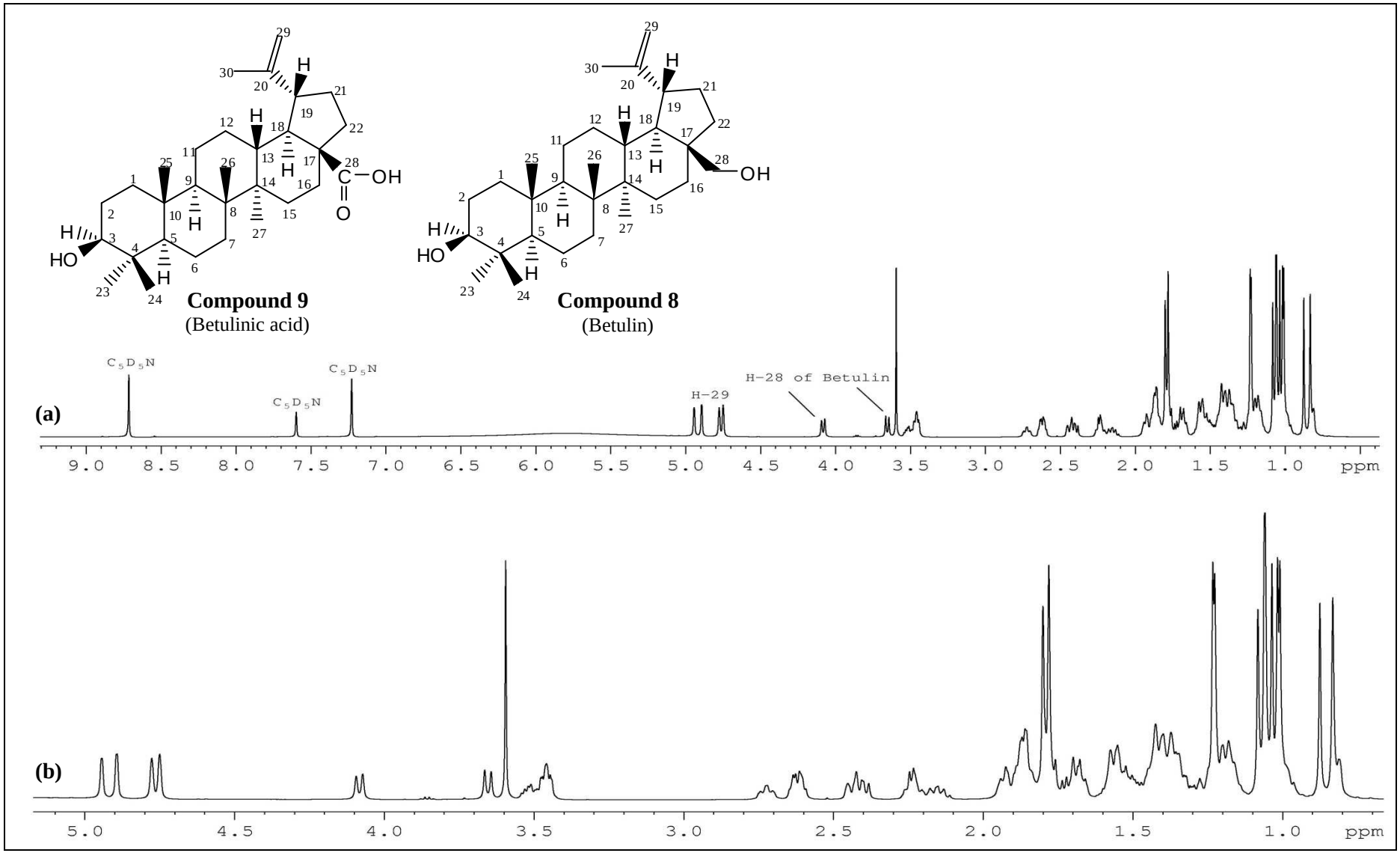
Betulin (**8**) and *Betulinic acid* (**9**): see Tables **S2** and **S3**, and Figures **S14-S16** for ^{1}H and ^{13}C-NMR data

Table S2. Comparison of ^{1}H-NMR Data of Compounds **8** and **9** (mixture), Betulinic acid [14] and Betulin [15]

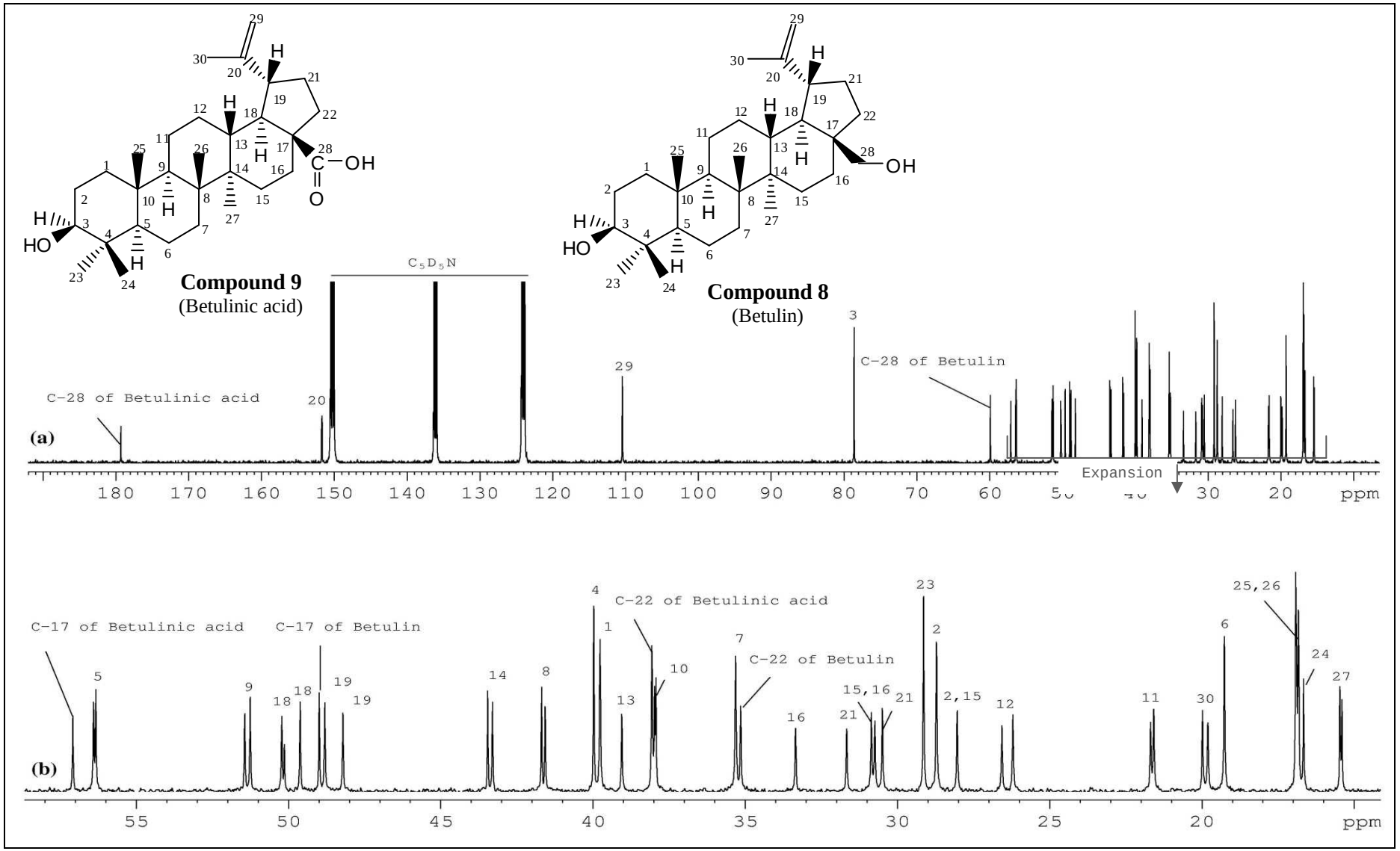
Proton No.	δ_H in ppm (multiplicity, *J* in Hz)					
	8 and **9** (mixture) (C_5D_5N, 500 MHz)		Betulinic acid[a] (C_5D_5N, 700 MHz)		Betulin[b] ($CDCl_3$, 600 MHz)	
	Ha	Hb	Ha	Hb	Ha	Hb
1	1.73-1.65 (*m*)	1.00 (*s*)	1.67 (br. *d*, 12.9)	0.99 (*m*)	1.65 (*dd*, 12.6, 3.6)	0.89 (*dd*, 12.6, 3.2)
2	1.87-1.85 (*m*)	-	1.85 (*m*)	-	1.58 (*m*)	-
3	3.47-3.44 (*m*)	-	3.45 (*t*, 7.2)	-	3.18 (*dd*, 8.0, 3.2)	-
5	0.81 (overlapped *s*)	-	0.82 (*m*)	-	0.68 (br. *d*, 18.0)	-
6	1.57-1.55 (*m*)	1.39-1.37 (*m*)	1.56 (*m*)	1.38 (*m*)	1.50 (*m*)	1.38 (*m*)
7	1.39-1.37 (*m*)	1.19-1.16 (*m*)	1.56 (*m*)	1.38 (*m*)	1.37 (*m*)	-
9	1.39-1.37 (*m*)	-	1.38 (*m*)	-	1.29 (*m*)	-
11	1.42 (br. *s*)	1.19-1.16 (*m*)	1.43 (*m*)	1.21 (*m*)	1.40 (*m*)	1.19 (*m*)
12	1.94-1.92 (*m*)	1.19-1.16 (*m*)	1.94 (*m*)	1.21 (*m*)	1.62 (*m*)	1.05 (*m*)
13	2.74-2.70 (*m*)	-	2.74 (*m*)	-	1.63 (*m*)	-
15	1.87-1.85 (*m*)	1.27 (br. *s*)	1.88 (*m*)	1.26 (*m*)	1.69 (*m*)	1.08
16	2.63-2.59 (*m*)	1.57-1.55 (*m*)	2.63 (*m*)	1.55 (*m*)	1.89 (*m*)	1.28 (*m*)
18	1.73-1.65 (*m*)	-	1.77 (*t*, 11.5)	-	1.58 (*m*)	-
19	3.54-3.51 (*m*)	-	3.52 (*m*)	-	2.36 (*m*)	-
21	2.26-2.23 (*m*)	1.53-1.47 (*m*)	2.24 (*m*)	1.53 (*m*)	1.98 (*m*)	1.29 (*m*)
22	2.26-2.23 (*m*)	1.57-1.55 (*m*)	2.25 (*m*)	1.57 (*m*)	1.85 (*m*)	1.04 (*m*)
23	1.23 (*s*), 1.22 (*s*)	-	1.22 (*s*)	-	0.92 (*s*)	-
24	1.01 (*s*), 1.00 (*s*)	-	1.00 (*s*)	-	0.74 (*s*)	-
25	0.83 (*s*)	-	0.83 (*s*)	-	0.79 (*s*)	-
26	1.05 (*s*, 6 H)	-	1.06 (*s*)	-	0.99 (*s*)	-
27	1.08 (3 H)	-	1.07 (*s*)	-	0.94 (*s*)	-
28	4.09 (*d*, 10.5)	3.66 (*d*, 11.0)	-	-	3.75 (*d*, 9.0)	3.30 (*dd*, 9.0)
29	4.94 (*d*, 13.0)	4.77 (*d*, 13.0)	4.95 (*s*)	4.77 (*s*)	4.65 (br. *s*)	4.55 (br. *s*)
30	1.78 (*s*), 1.80 (*s*)	-	1.79 (*s*)	-	1.68 (*s*)	-

Table S3. Comparison of ^{13}C-NMR Data of Compounds **8** and **9** (mixture), Betulinic acid [14] and Betulin [15]

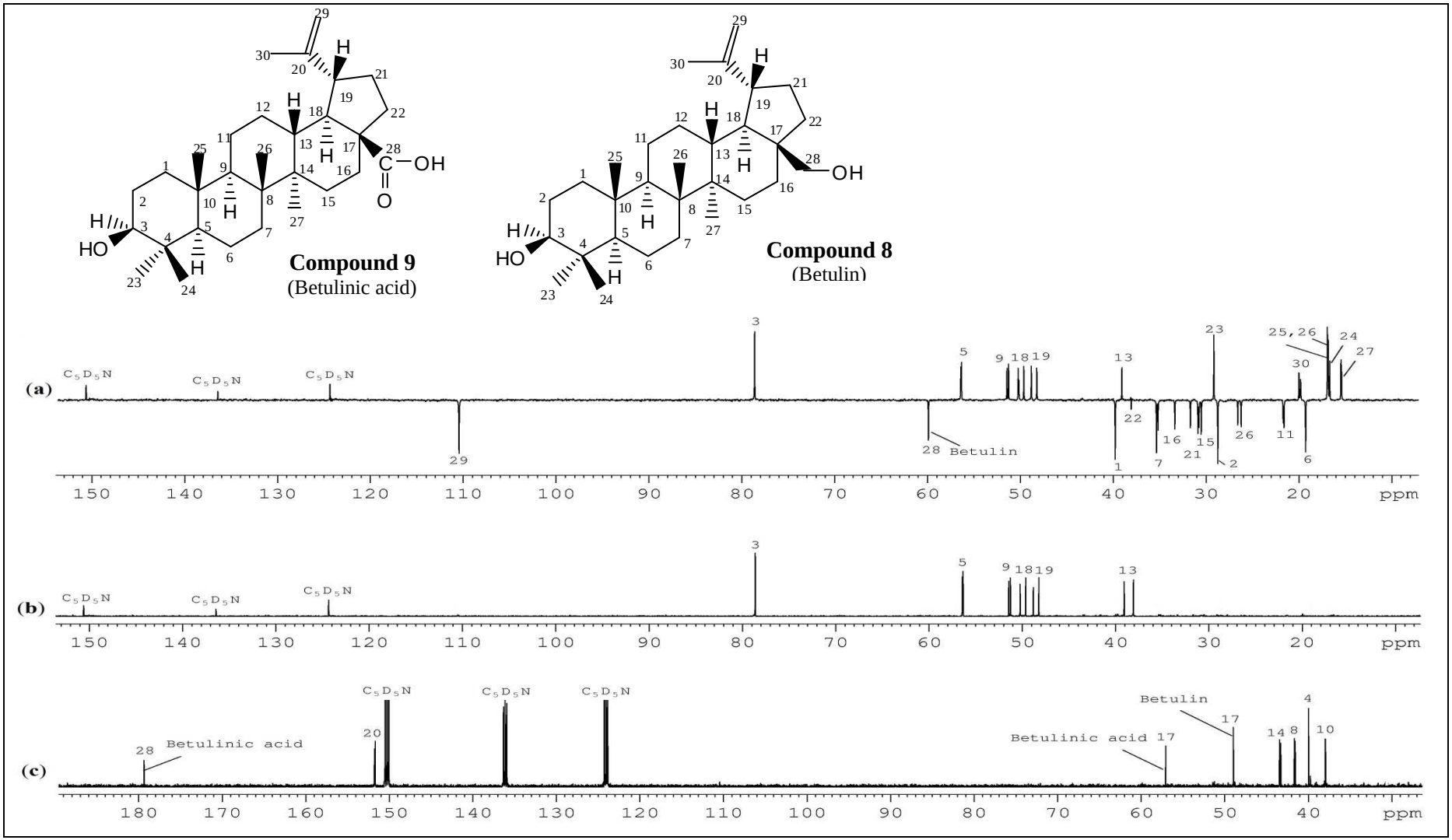
S. No.	**8** and **9** (mixture)		Betulinic acid[a]	Betulin[b] ($CDCl_3$, 150 MHz)	S. No.	**8** and **9** (mixture)		Betulinic acid[a]	Betulin[b] ($CDCl_3$, 150 MHz)
	δ_C	C-Type	δ_C	δ_C		δ_C	C-Type	δ_C	δ_C
1	179.3	C	178.82 (C-28)	-	26	37.98	C	37.55 (C-10)	-
2	151.75	C	151.32 (C-20)	-	27	37.93	C	-	37.1 (C-10)
3	151.66	C	-	150.3 (C-20)	28	35.32	CH_2	34.86 (C-7)	-
4	110.4	CH_2	109.92 (C-29)	109.7 (C-29)	29	35.15	CH_2	-	34.2 (C-7)
5	78.60	CH	78.14 (C-3)	78.8 (C-3)	30	33.35	CH_2	32.89 (C-16)	33.9 (C-22)
6	59.88	CH_2	-	60.8 (C-28)	31	31.67	CH_2	31.24 (C-21)	-
7	57.0	C	56.64 (C-17)	-	32	30.86	CH_2	30.29 (C-15)	-
8	56.40	CH	55.15 (C-5)	-	33	30.74	CH_2	-	29.1 (C-16)
9	56.32	CH	-	55.2 (C-5)	34	30.49	CH_2	-	29.7 (C-21)
10	51.43	CH	50.99 (C-9)	-	35	29.14	CH_3	28.67 (C-23)	27.9 (C-23)
11	51.25	CH	-	50.3 (C-9)	36	28.72	CH_2	28.32 (C-2)	
12	50.21	CH	49.80 (C-18)	-	37	28.04	CH_2	-	27.0 (C-2, 15)
13	49.61	CH	-	48.7 (C-18)	38	26.57	CH_2	26.15 (C-12)	-
14	48.98	C	-	47.74 (C-17)	39	26.21	CH_2	-	25.1 (C-12)
15	48.80	CH	47.78 (C-19)		40	21.68	CH_2	21.68 (C-11)	
16	48.20	CH	-	47.77 (C-19)	41	21.58	CH_2	-	20.8 (C-11)
17	43.46	C	42.87 (C-14)		42	19.98	CH_3	19.50 (C-30)	
18	43.30	C	-	42.6 (C-14)	43	19.80	CH_3	-	19.0 (C-30)
19	41.69	C	41.14 (C-8)		44	19.26	CH_2	18.81 (C-6)	18.2 (C-6)
20	41.57	C	-	40.8 (C-8)	45	16.91	CH_3	16.43 (C-25, 26)	-
21	39.98	C	39.53 (C-4)	38.8 (C-4)	46	16.83	CH_3	-	16.0 (C-25)
22	39.77	CH_2	39.31 (C-1)	38.6 (C-1)	47	16.66	CH_3	16.33 (C-24)	15.3 (C-24) 15.9 (C-26)
23	39.05	CH	38.65 (C-13)	-	48	15.45	CH_3	14.93 (C-27)	
24	38.07	CH	-	37.2 (C-13)	49	15.4	CH_3	-	14.7 (C-27)
25	38.05	CH	37.57 (C-22)	-				-	



S14 : ^{1}H-NMR (500 MHz, C_5D_5N) (**a**) full and (**b**) expanded spectra of compounds **8** and **9** (mixture)

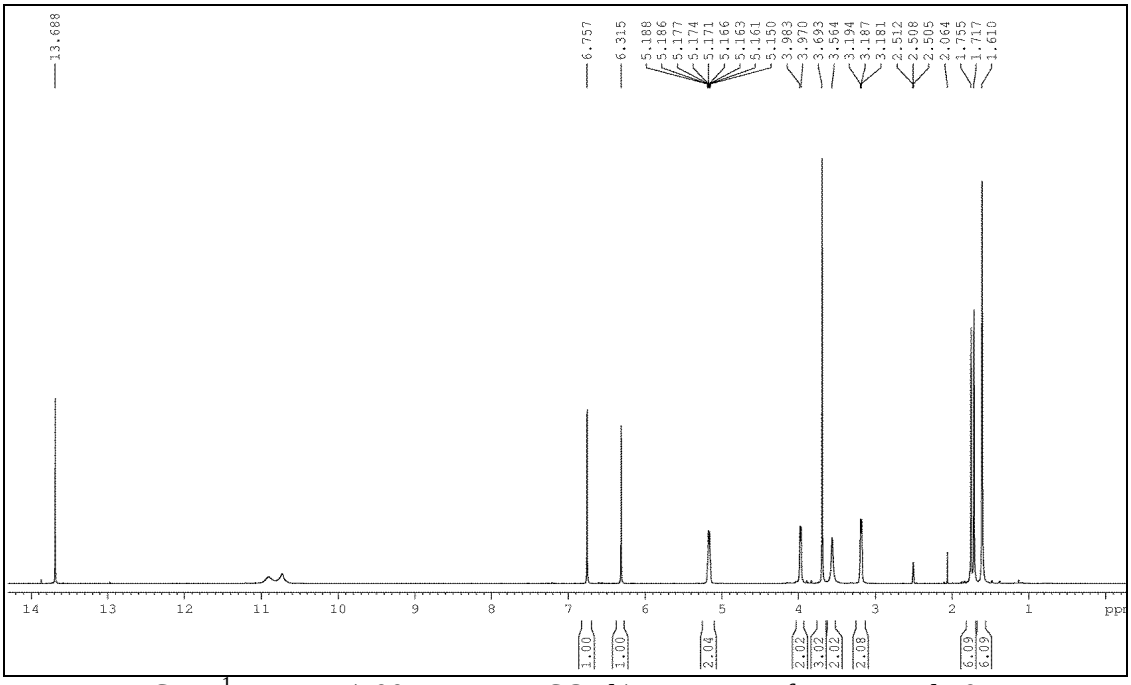


S15 : ^{13}C-NMR (125 MHz, C_5D_5N) (**a**) full and (**b**) expanded spectra of compounds **8** and **9** (mixture)

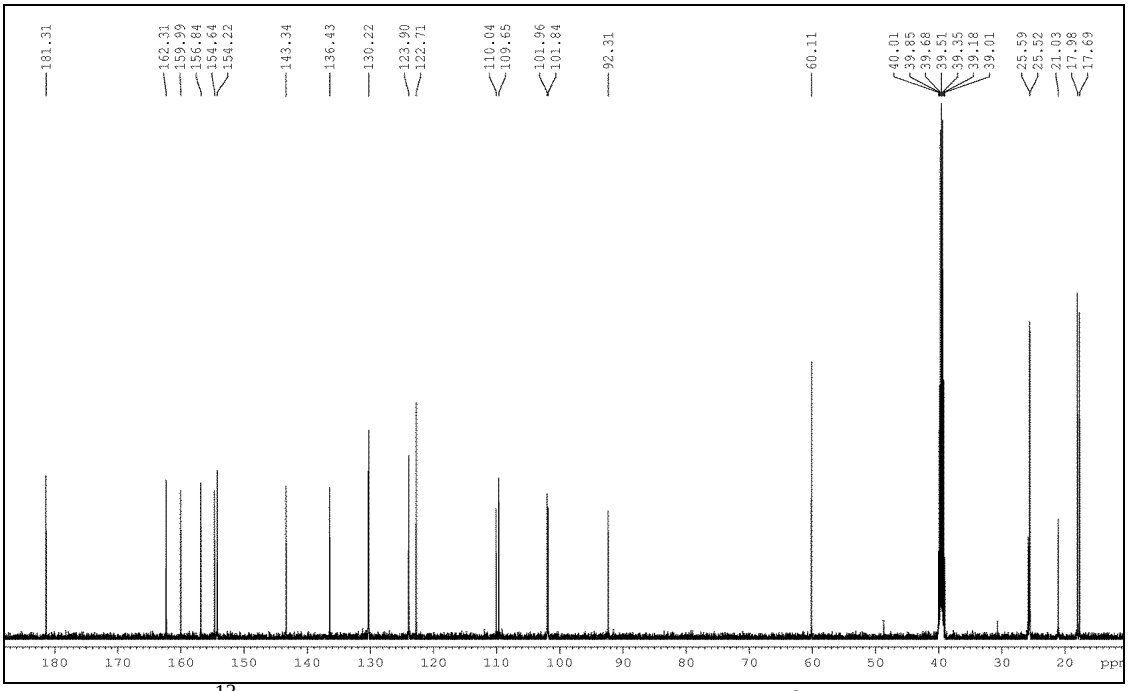


S16 : DEPT (**a**) 135, (**b**) 90 and (**c**) Q-NMR (125 MHz, C_5D_5N) spectra of compounds **8** and **9** (mixture)

1,3,6-trihydroxy-7-methoxy-2,8-(3-methyl-2-butenyl)xanthone (**10**): bright yellow solid; molecular formula $C_{24}H_{26}O_6$; mp 181-183 °C; EI-MS *m/z*: 409.4 $[M]^+$; UV λ_{max} nm: 206, 243, 316; IR (KBr): 3425, 1608 cm^{-1}; ^{1}H-NMR (DMSO-d_6, 500 MHz): δ_H 13.6 (*s*, 1H, 1-OH), 6.75 (*s*, 1H, H-5), 6.31 (*s*, 1H, H-4), 5.18 (*t*, *J* = 6.0 Hz, 2H, H-12, H-17), 3.98 (*dd*, *J* =18.0, 10.0 Hz, 2H, H-11), 3.69 (*s*, 3H, 7-OMe), 3.19 (*d*, *J* = 6.0 Hz, 2H, H-16), 1.75 (*s*, 3H, Me-14), 1.71 (*s*, 3H, Me-15), 1.61 (*s*, 3H, H-19), 1.61 (*s*, 3H, Me-20); ^{13}C-NMR (DMSO-d_6, 125 MHz): δ_C 181.3 (C-9), 162.3 (C-3), 159.9 (C-1), 156.8 (C-6), 154.6 (C-10a), 154.2 (C-4a), 143.3 (C-7), 136.4 (C-8), 130.2 (C-13), 130.2 (C-18), 123.9 (C-17), 122.7 (C-12), 110.0 (C-8a), 109.6 (C-2), 101.9 (C-9a), 101.9 (C-5), 92.3 (C-4), 60.1 (C-21), 25.5 (C-14), 25.5 (C-16), 25.0 (C-19), 21.0 (C-11), 17.9 (C-20), 17.6 (C-15).

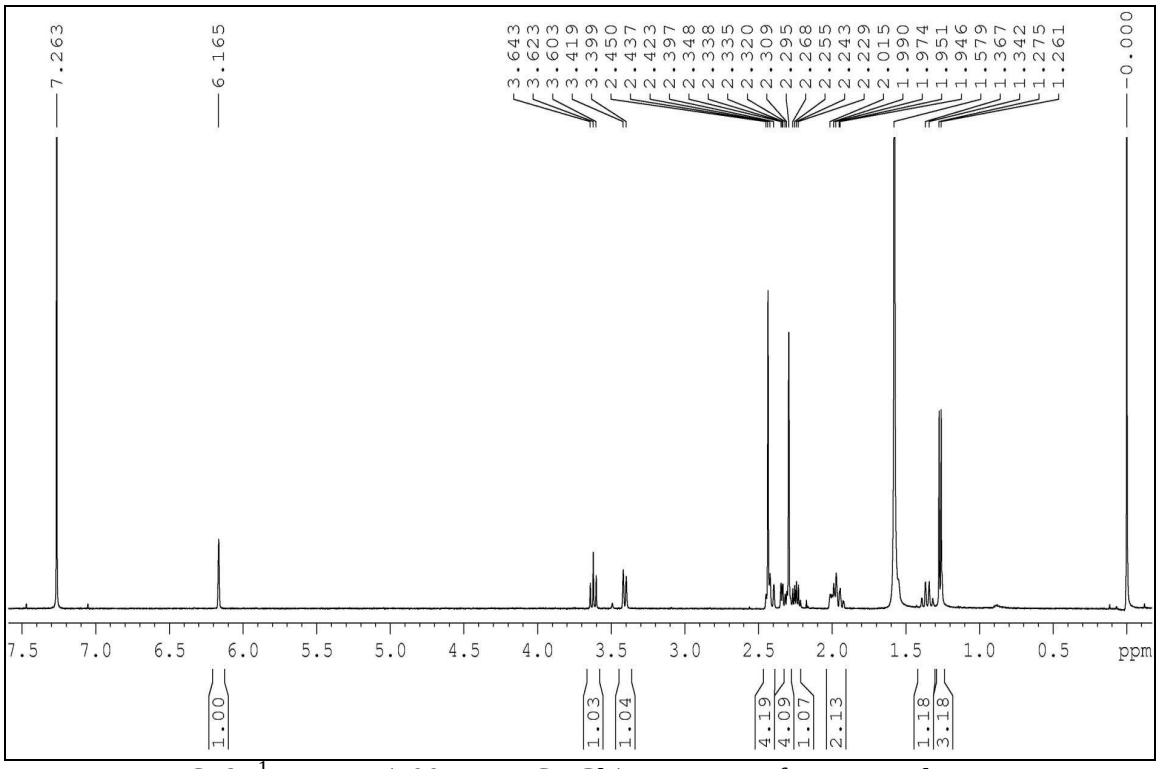


S17: ^{1}H-NMR (500 MHz, DMSO-d_6) spectrum of compound **10**

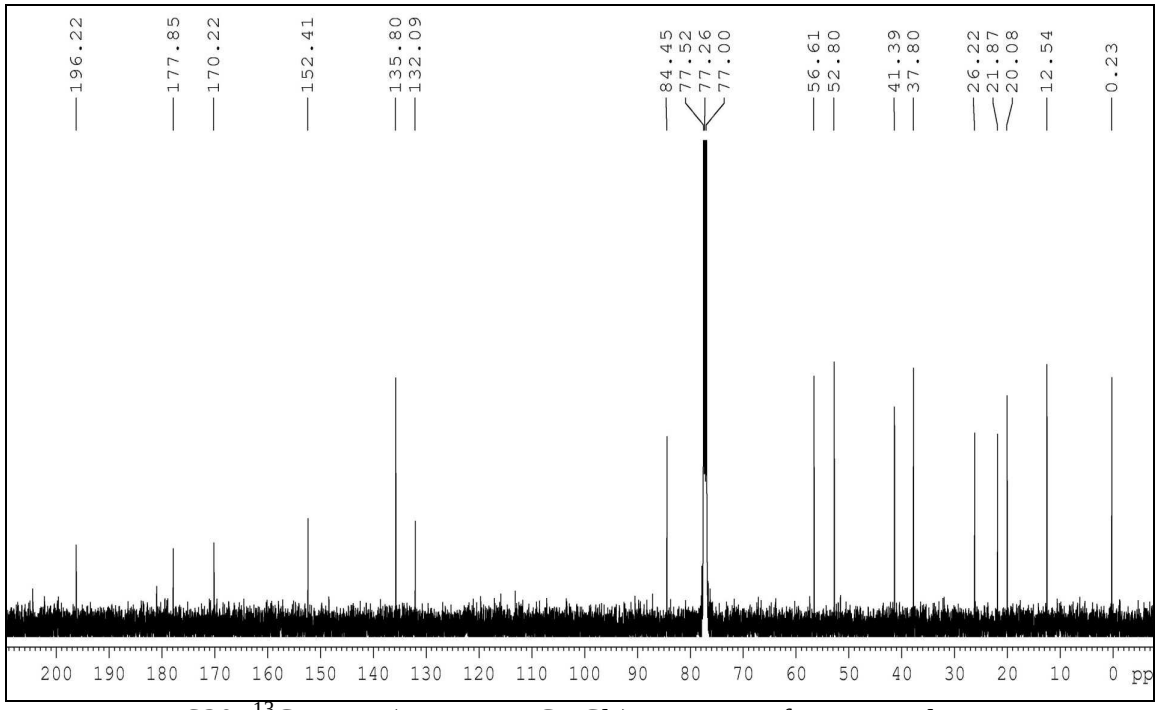


S18: ^{13}C-NMR (125 MHz, DMSO-d_6) spectrum of compound **10**

Leucodin (**11**): white solid; 205-207 °C; molecular formula $C_{15}H_{18}O_3$ (calcd. for 246.302); EI-MS *m*/*z* : 246.2 $[M]^+$; IR (KBr): 3436, 1737 cm^{-1}; ^{1}H-NMR ($CDCl_3$, 500 MHz): δ_H 6.16 (*s*, 1H, H-3), 3.41 (*d*, *J* = 1.0 Hz, 1H, H-5), 3.64-3.60 (*m*, 1H, H-6), 2.0-1.92 (*m*, 1H, H-7), 2.00, 1.39-1.31 (*m*, 1H, H-8), 2.43, 2.29 (*s*, 2H, H-9), 2.25-2.23 (*m*, 1H, H-11), 1.27 (*m*, 3H, H-13), 2.43 (*s*, 3H-14), 2.34 (*s*, 3H, H-15). ^{13}C-NMR ($CDCl_3$, 125 MHz): δ_C 196.2 (C-2), 177.8 (C-12), 170.2 (C-4), 152.4 (C-10), 135.8 (C-3), 132.0 (C-1), 84.4 (C-6), 56.6 (C-7), 52.8 (C-5), 41.3 (C-11), 37.8 (C-9), 26.8 (C-8), 21.8 (C-15), 20.0 (C-14), 12.5 (C-13).

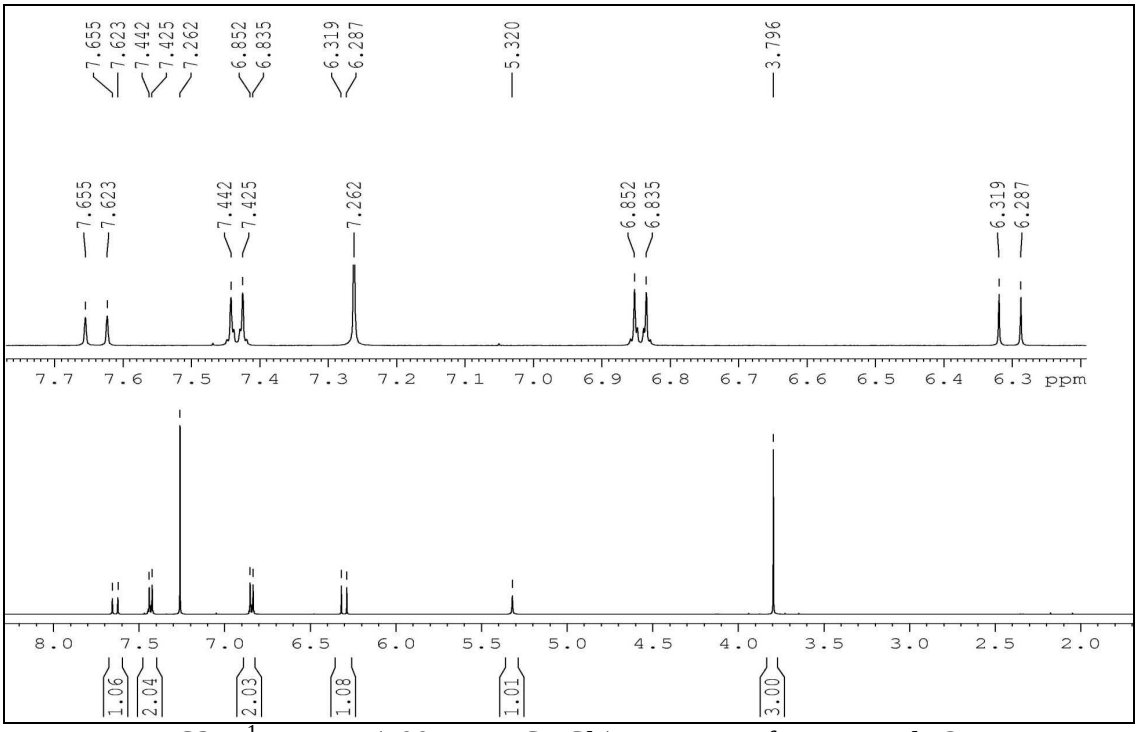


S19: ^{1}H-NMR (500 MHz, $CDCl_3$) spectrum of compound **11**

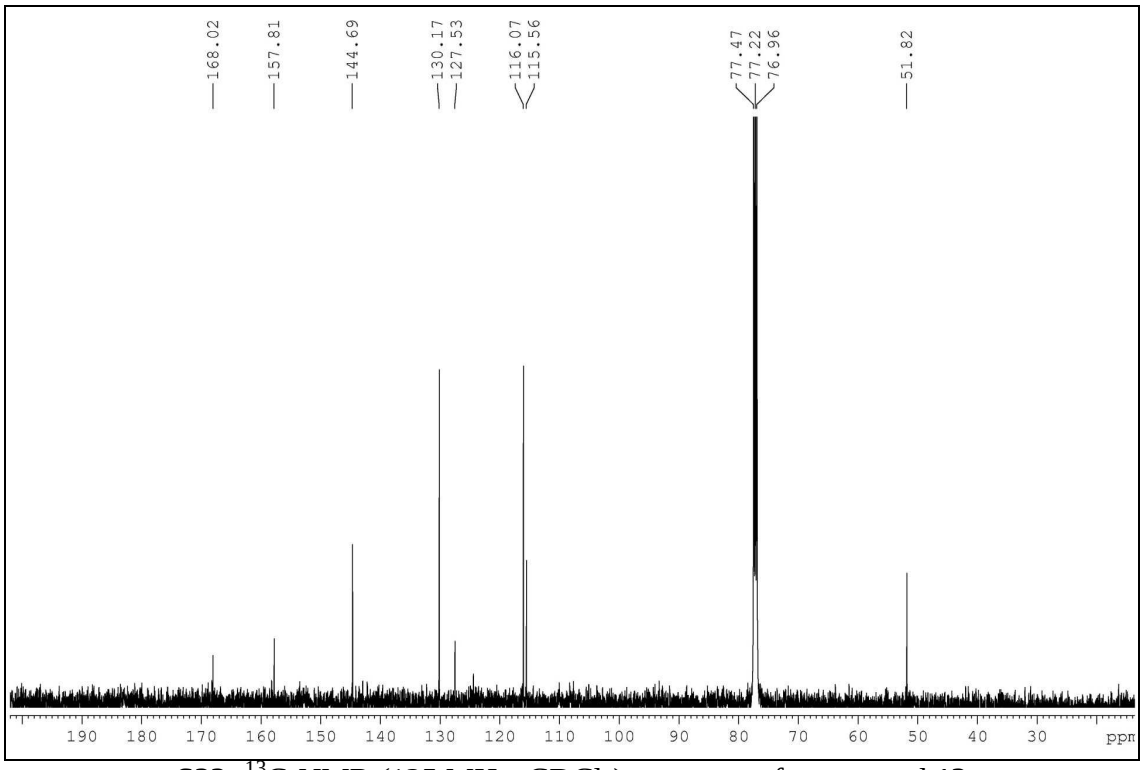


S20: ^{13}C-NMR (125 MHz, $CDCl_3$) spectrum of compound **11**

p-hydroxycinnamate (**12**): yellow solid; mp 140-142 °C; molecular formula $C_{10}H_{10}O_3$ (calcd. for 178.18); ^{1}H-NMR ($CDCl_3$, 500 MHz): δ_H 7.65 (*d*, *J* = 16.0 Hz, 1H, H-3), 7.44 (*d*, *J* = 8.5, 2H, H-2', 6'), 6.85 (*d*, *J* = 8.5, 1H, H-3', 5'), 6.31 (*d*, *J* = 16.0 Hz, 1H, H-2), 3.79 (*s*, 3H, OMe); ^{13}C-NMR ($CDCl_3$, 125 MHz): δ_C 168.0 (C-1), 157.8 (C-4'), 144.6 (C-3), 130.1 (C-2', 6'), 127.5 (C-1'), 116.0 (C-3', 5'), 115.5 (C-2), 51.8 (C-1").

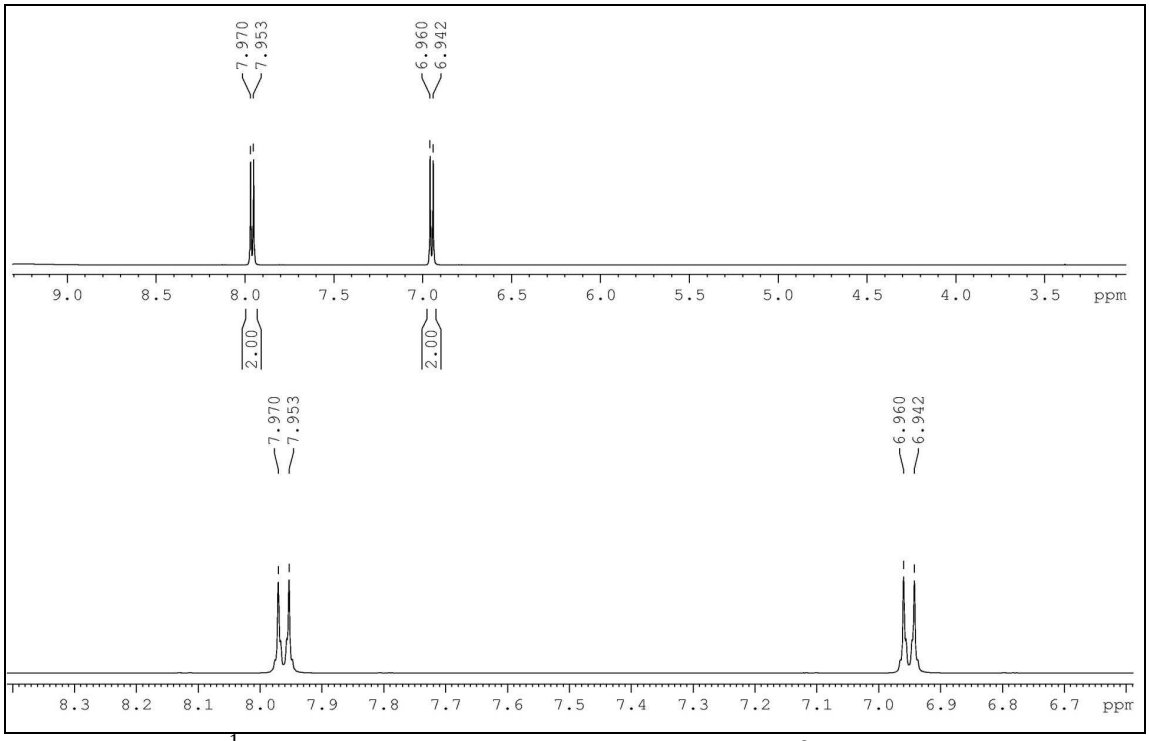


S21: ^{1}H-NMR (500 MHz, $CDCl_3$) spectrum of compound **12**

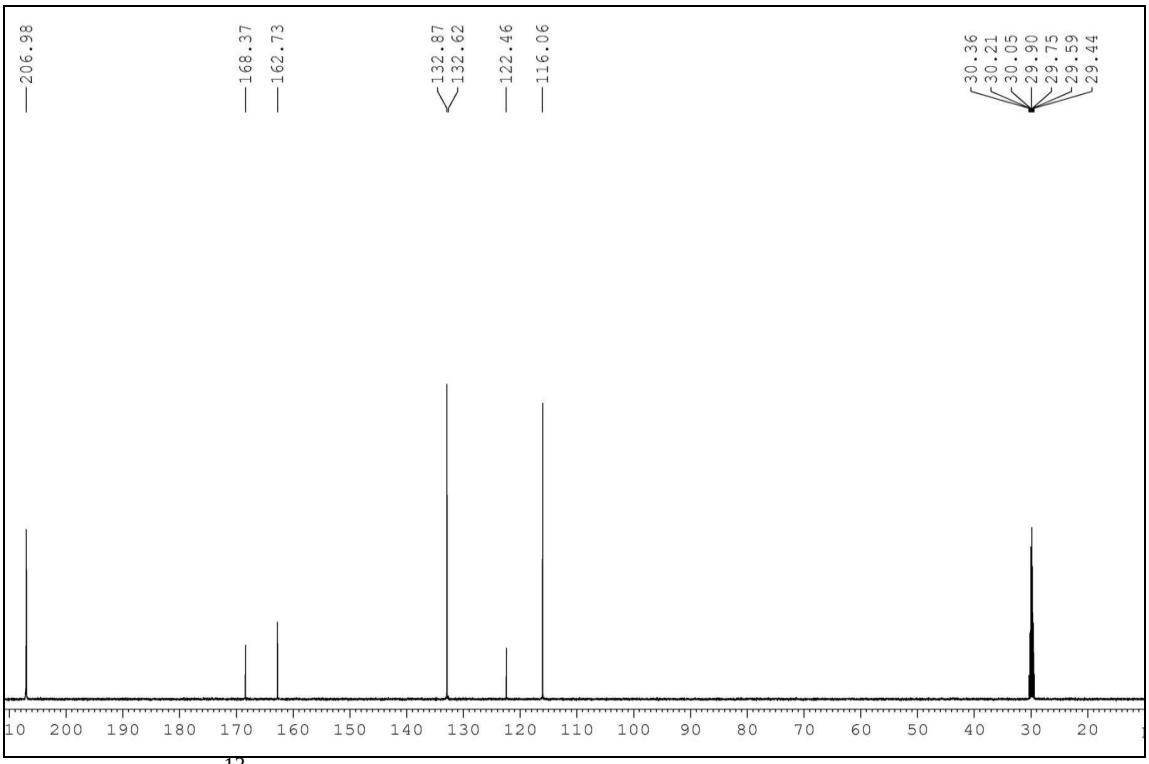


S22: ^{13}C-NMR (125 MHz, $CDCl_3$) spectrum of compound **12**

p-hydroxybenzoic acid (**13**): obtained as yellow solid. ^{1}H and ^{13}C-NMR: see Figures **S23** and **S24**.

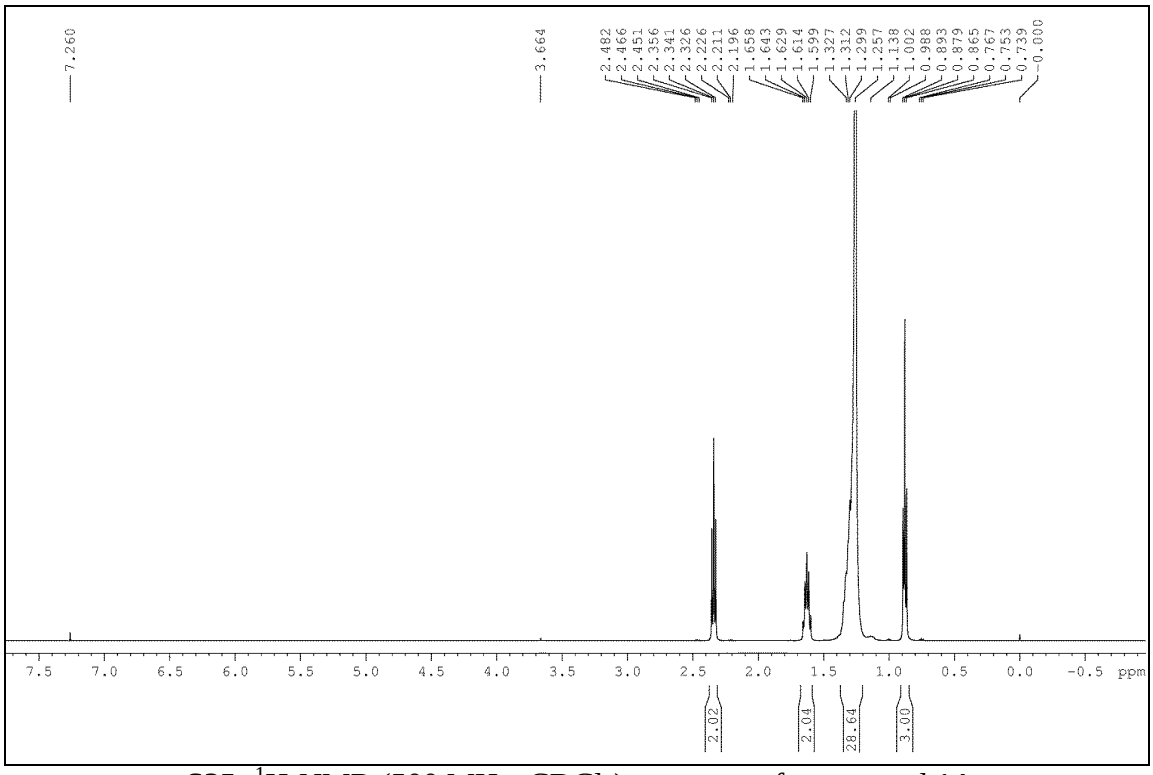


S23: ^{1}H-NMR (500 MHz, CD_3OCD_3) spectrum of compound **13**

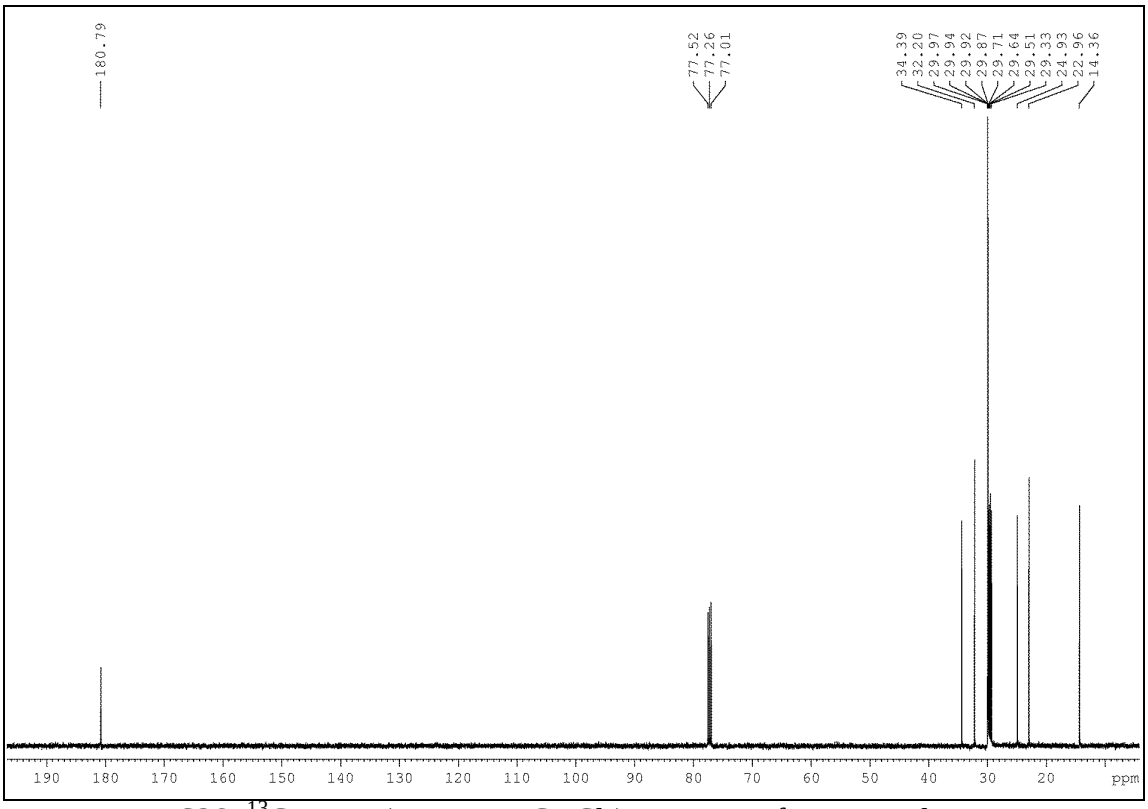


S24: ^{13}C-NMR (125 MHz, CD_3OCD_3) spectrum of compound **13**

Stearic acid (**14**): obtained as white crystals; ^{1}H and ^{13}C-NMR: see Figures **S25** and **S26**.



S25: ^{1}H-NMR (500 MHz, $CDCl_3$) spectrum of compound **14**



S26: ^{13}C-NMR (125 MHz, $CDCl_3$) spectrum of compound **14**

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