Supporting Information

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Cholinesterase Inhibition and Molecular Docking Studies of Sesquiterpene Coumarin Ethers from *Heptaptera cilicica*

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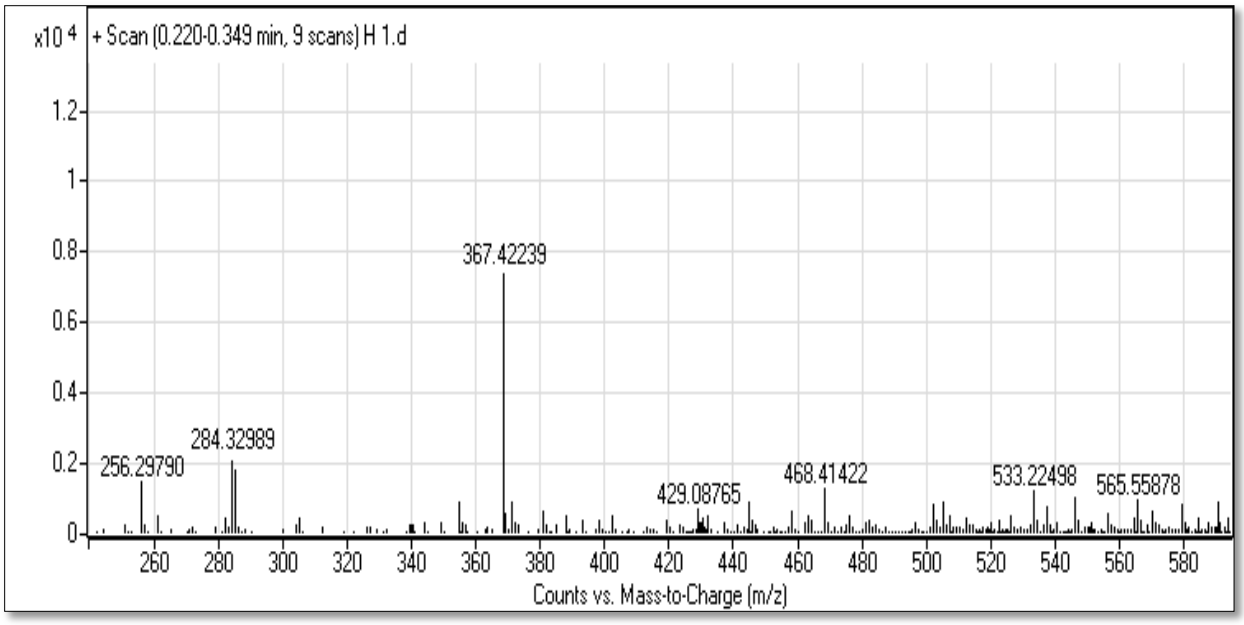
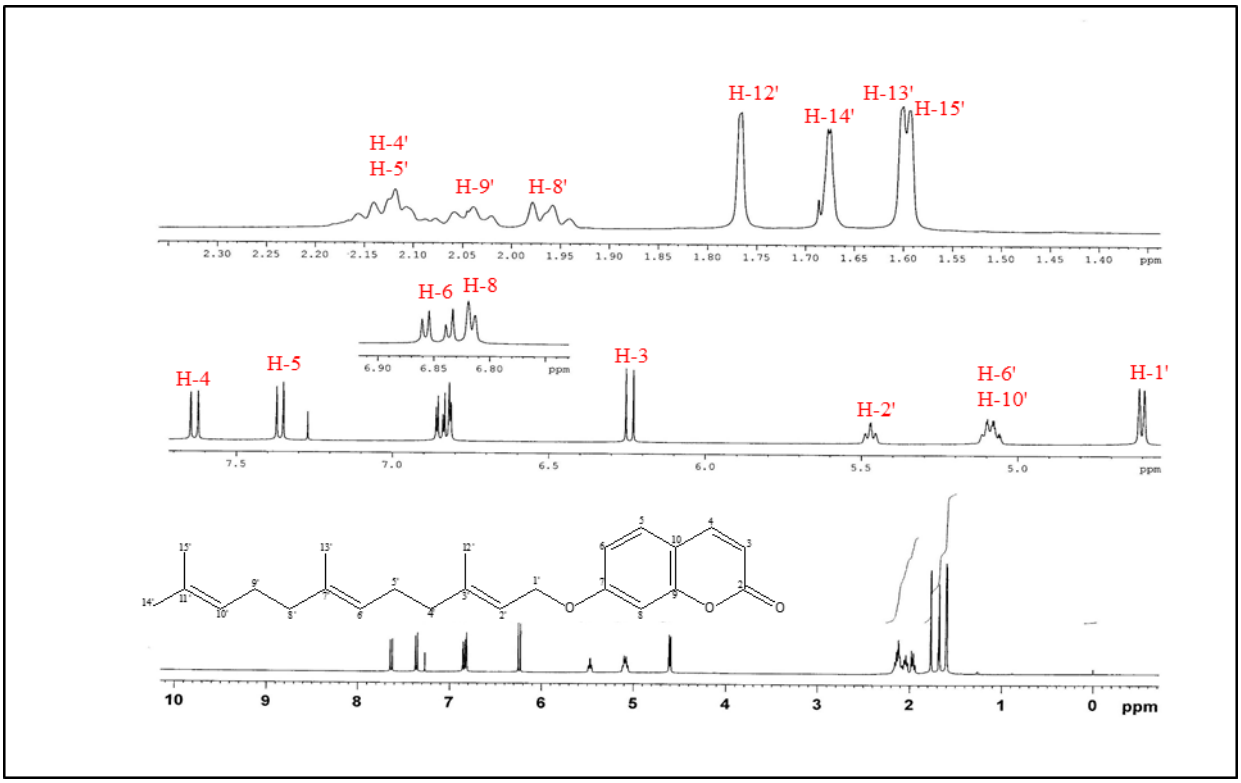
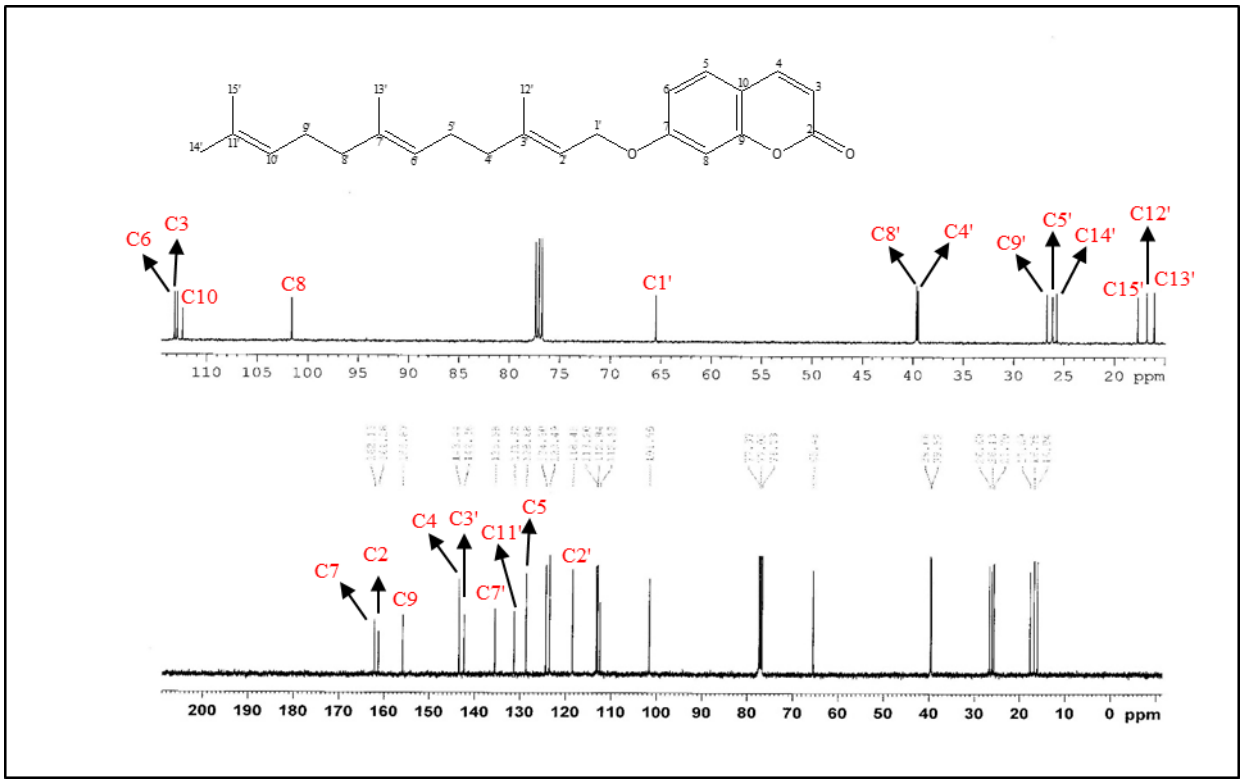


S1: HRESIMS Spectrum of Compound **1** (Umbelliprenin)

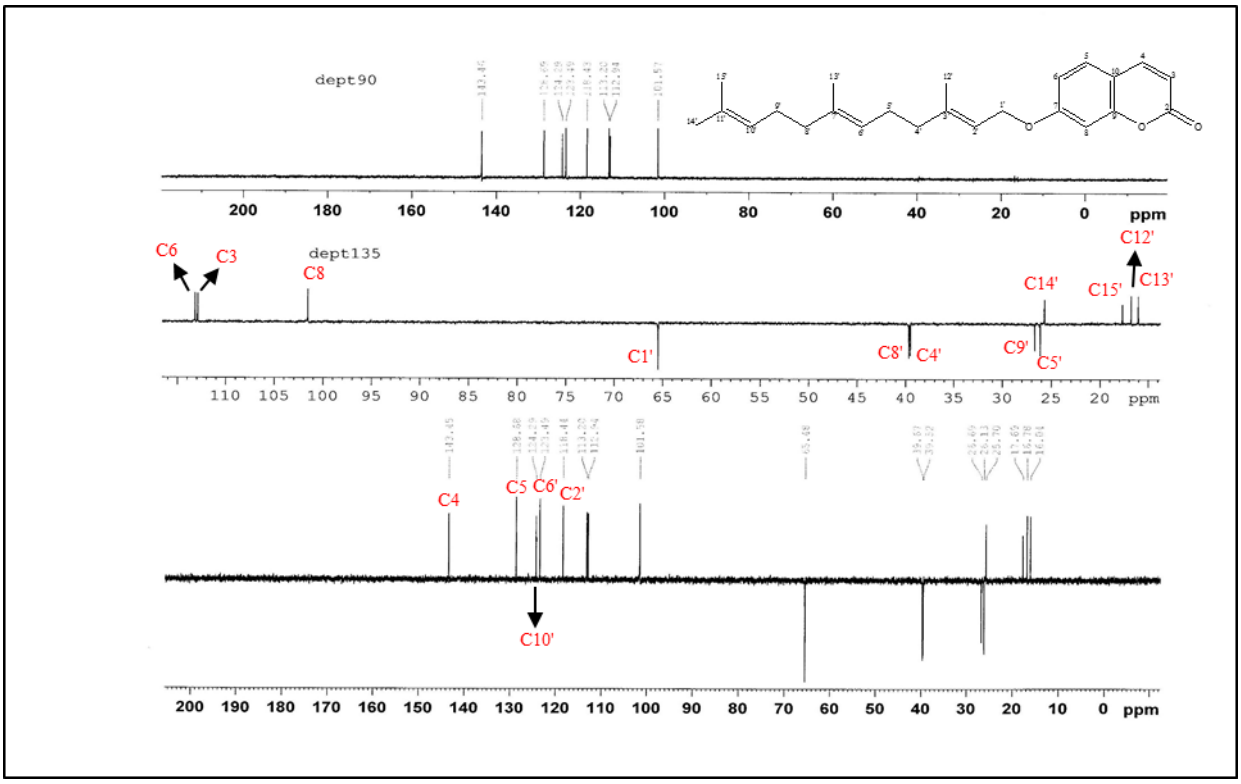


S2: ^{1}H-NMR (400 MHz, $CDCl_3$) Spectrum of Compound **1** (Umbelliprenin)

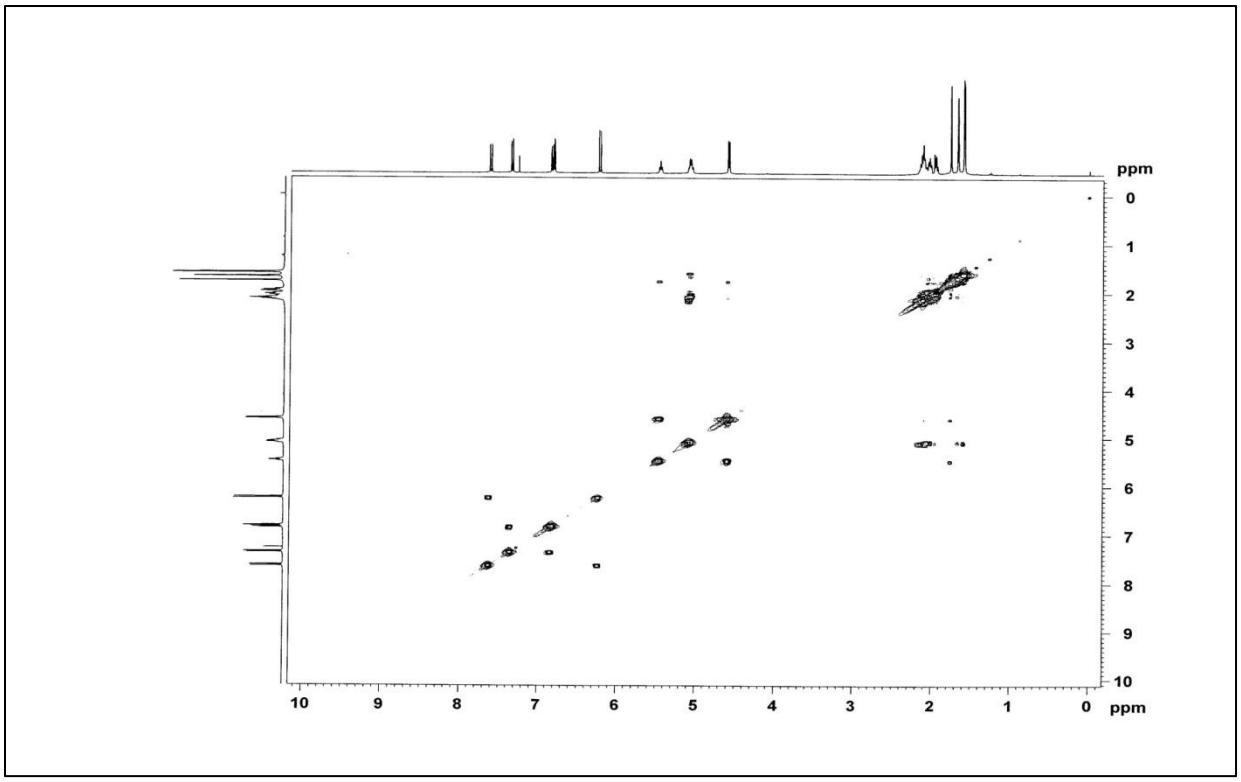
*Umbelliprenin (**1**):* White powder. ^{1}H-NMR ($CDCl_3$, 400 MHz), δ: 1.59 (3H, s, H-15'), 1.60 (3H, s, H-13'), 1.67 (3H, d, H-14'), 1.76 (3H, s, H-12'), 1.96 (2H, m, H-8'), 2.05 (2H, m, H-9'), 2.11 (2H, m, H-4'), 2.13 (2H, m, H-5'), 4.60 (2H, d, H-1'), 5.08 (1H, m, H-10'), 5.11 (1H, m, H-6'), 5.46 (1H, td, H-2'), 6.23 (1H, d, H-3), 6.81 (1H, d, H-8), 6.83 (1H, dd, H-6), 7.35 (1H, d, H-5), 7.62 (1H, d, H-4). ^{13}C-NMR ($CDCl_3$, 100 MHz), δ: 161.31 (C-2), 112.96 (C-3), 143.45 (C-4), 128.67 (C-5), 113.23 (C-6), 162.16 (C-7), 101.59 (C-8), 155.88 (C-9), 112.43 (C-10), 65.48 (C-1'), 118.42 (C-2'), 142.40 (C-3'), 39.52 (C-4'), 26.14 (C-5'), 123.49 (C-6'), 135.60 (C-7'), 39.67 (C-8'), 26.69 (C-9'), 124.29 (C-10'), 131.34 (C-11'), 16.78 (C-12'), 16.04 (C-13'), 25.70 (C-14'), 17.69 (C-15'). HRESIMS: *m/z* = 367.42239 $[M + H]^+$ (calcd for $C_{24}H_{30}O_3$, 366.4932) [8].



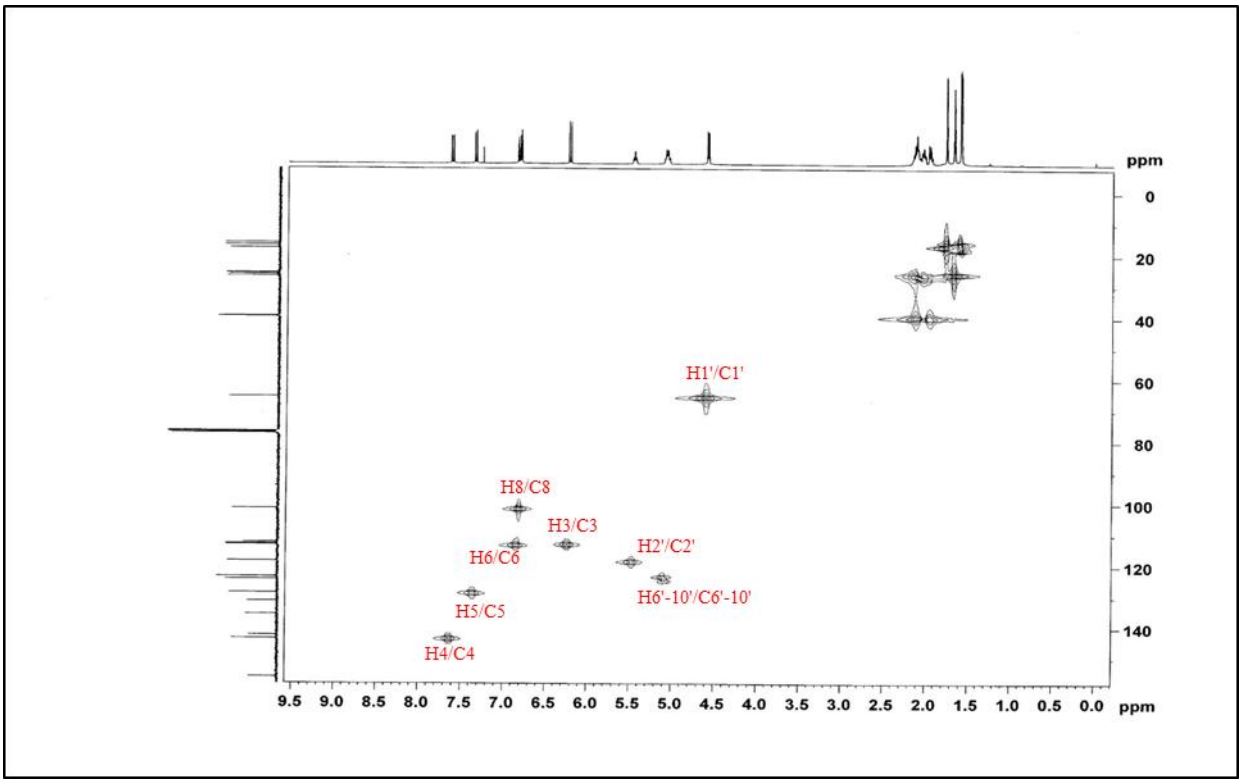
S3: ^{13}C-NMR (100 MHz, $CDCl_3$) Spectrum of Compound **1** (Umbelliprenin)



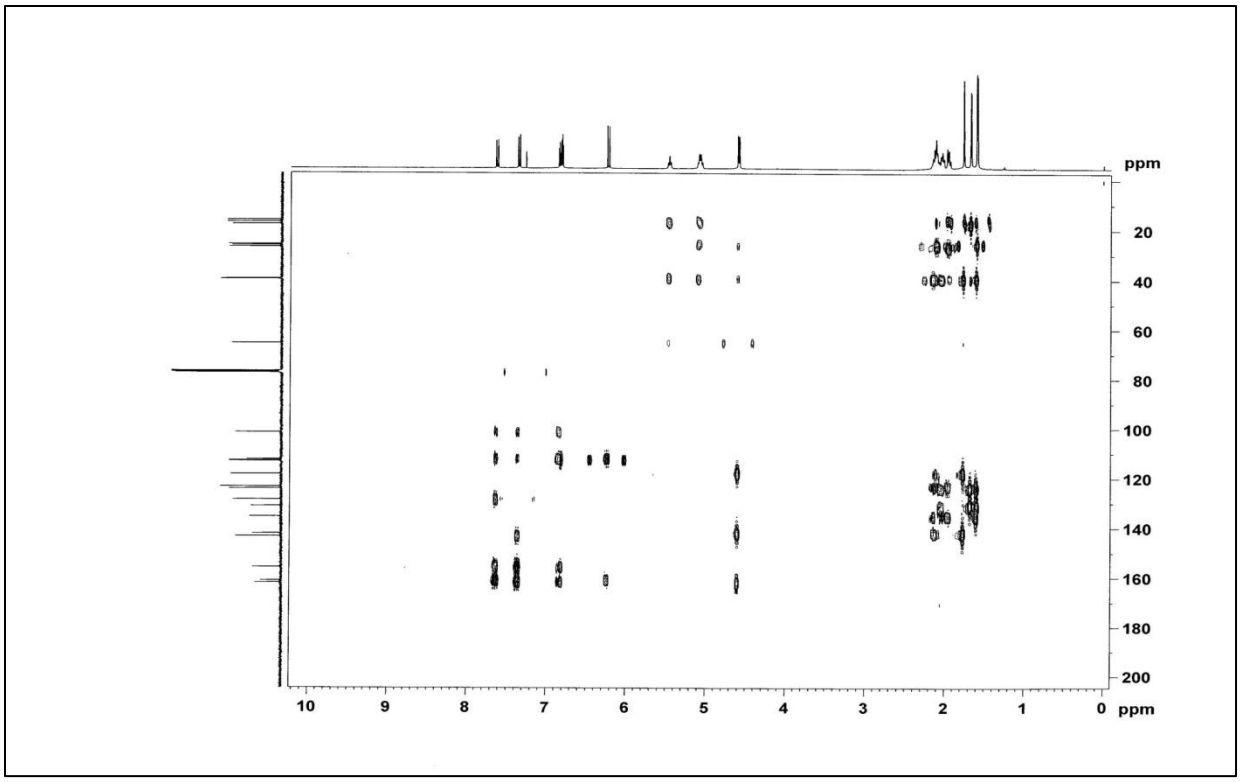
S4: DEPT (100 MHz, $CDCl_3$) Spectrum of Compound **1** (Umbelliprenin)



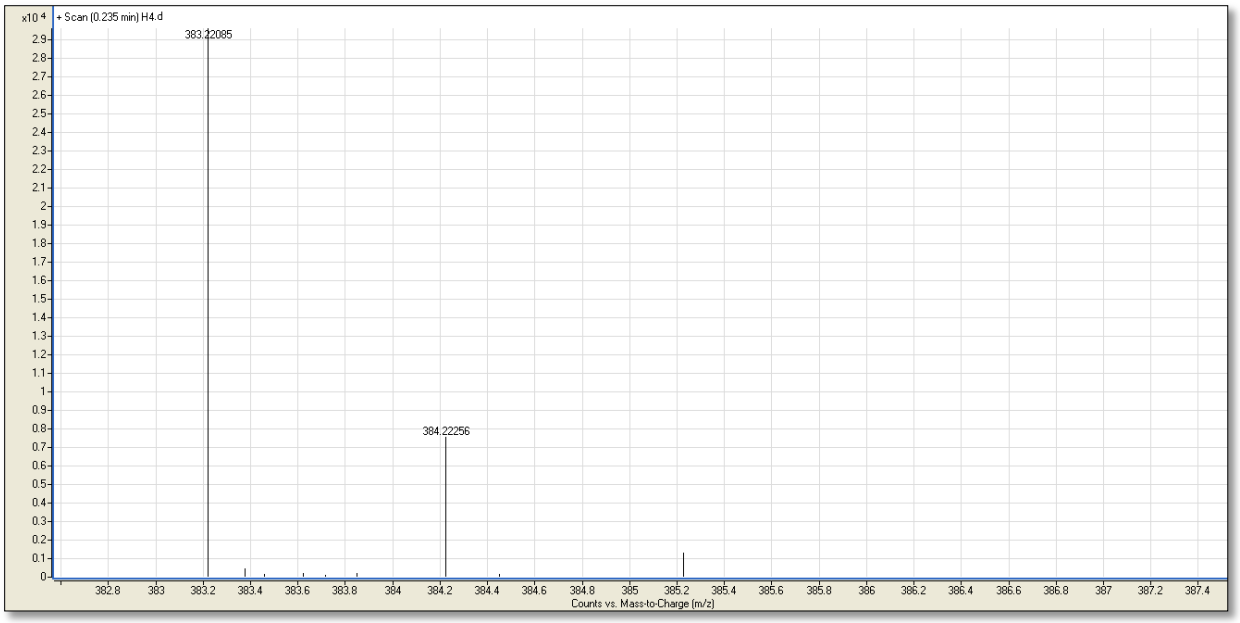
S5: COSY (400 MHz) Spectrum of Compound **1** (Umbelliprenin)



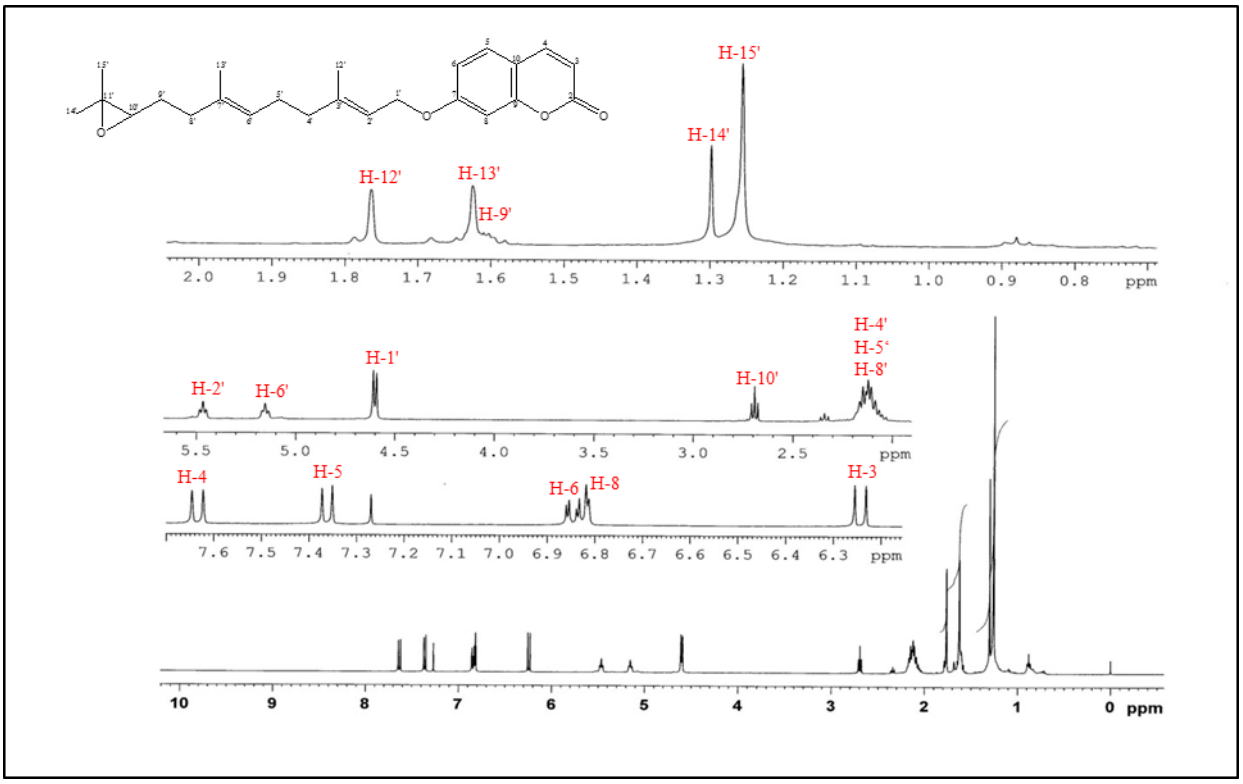
S6: HMQC Spectrum of Compound **1** (Umbelliprenin)



S7: HMBC Spectrum of Compound **1** (Umbelliprenin)

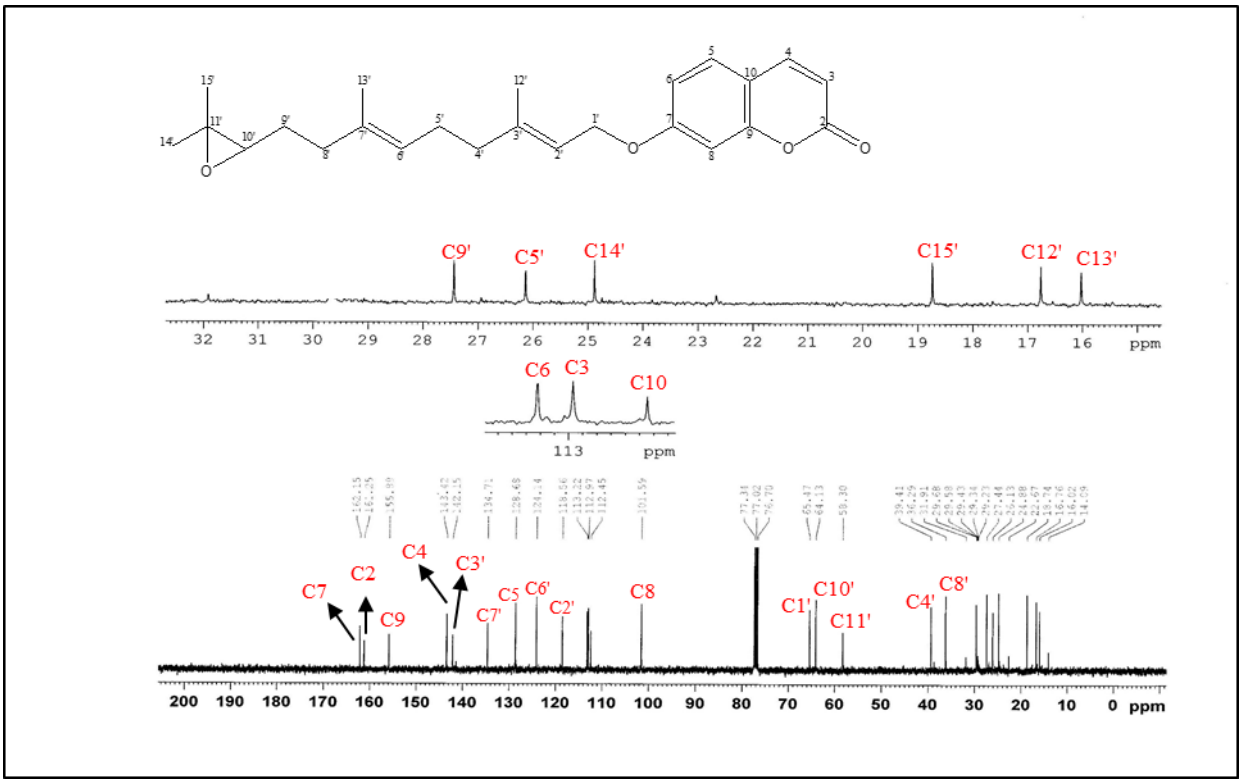


S8: HRESIMS Spectrum of Compound **2** (Umbelliprenin-10′,11′-monoepoxide)

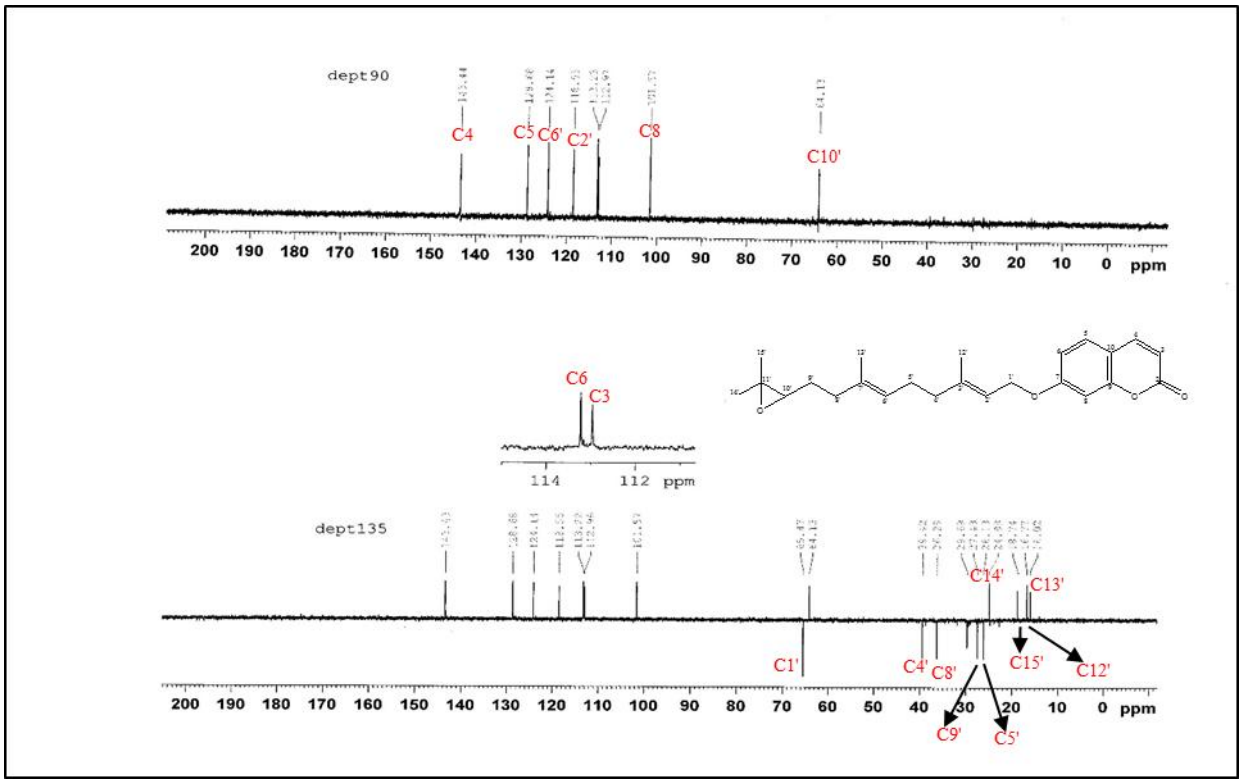


S9: ^{1}H-NMR (400 MHz, $CDCl_3$) Spectrum of Compound **2** (Umbelliprenin-10′,11′-monoepoxide)

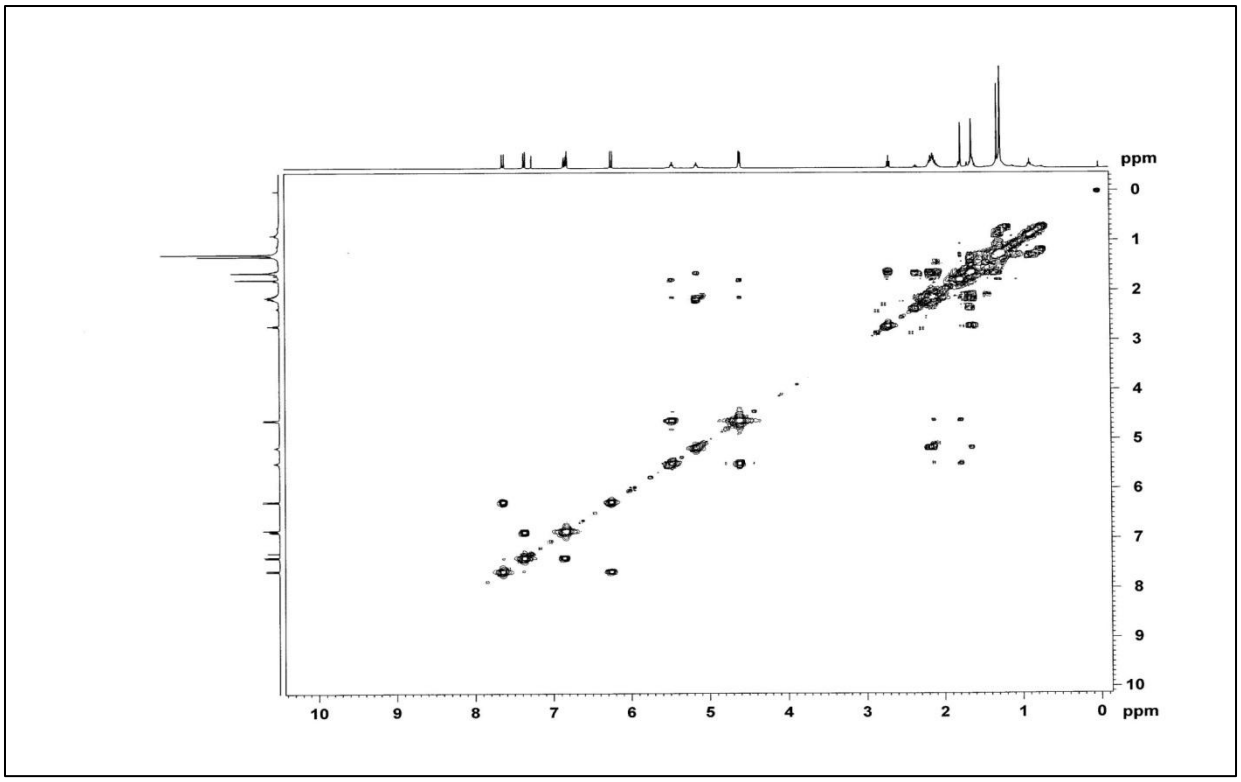
*Umbelliprenin-10',11'-monoepoxide (**2**):* White powder. ^{1}H-NMR ($CDCl_3$, 400 MHz), δ: 1.25 (3H, s, H-15'), 1.29 (3H, s, H-14'), 1.61 (2H, m, H-9'), 1.62 (3H, s, H-13'), 1.76 (3H, s, H-12'), 2.10 (2H, m, H-8'), 2.12 (2H, m, H-4'), 2.13 (2H, m, H-5'), 2.69 (1H, t, H-10'), 4.60 (2H, d, H-1'), 5.15 (1H, m, H-6'), 5.46 (1H, t, H-2'), 6.24 (1H, d, H-3), 6.81 (1H, d, H-8), 6.84 (1H, dd, H-6), 7.36 (1H, d, H-5), 7.63 (1H, d, H-4). ^{13}C-NMR ($CDCl_3$, 100 MHz), δ: 161.25 (C-2), 112.97 (C-3), 143.42 (C-4), 128.68 (C-5), 113.22 (C-6), 162.15 (C-7), 101.59 (C-8), 155.89 (C-9), 112.45 (C-10), 65.47 (C-1'), 118.56 (C-2'), 142.15 (C-3'), 39.41 (C-4'), 26.13 (C-5'), 124.14 (C-6'), 134.71 (C-7'), 36.29 (C-8'), 27.44 (C-9'), 64.13 (C-10'), 58.30 (C-11'), 16.76 (C-12'), 16.02 (C-13'), 24.88 (C-14'), 18.74 (C-15'). HRESIMS: *m/z* = 383.22085 $[M + H]^+$ (calcd for $C_{24}H_{30}O_4$, 382.4926) [9].



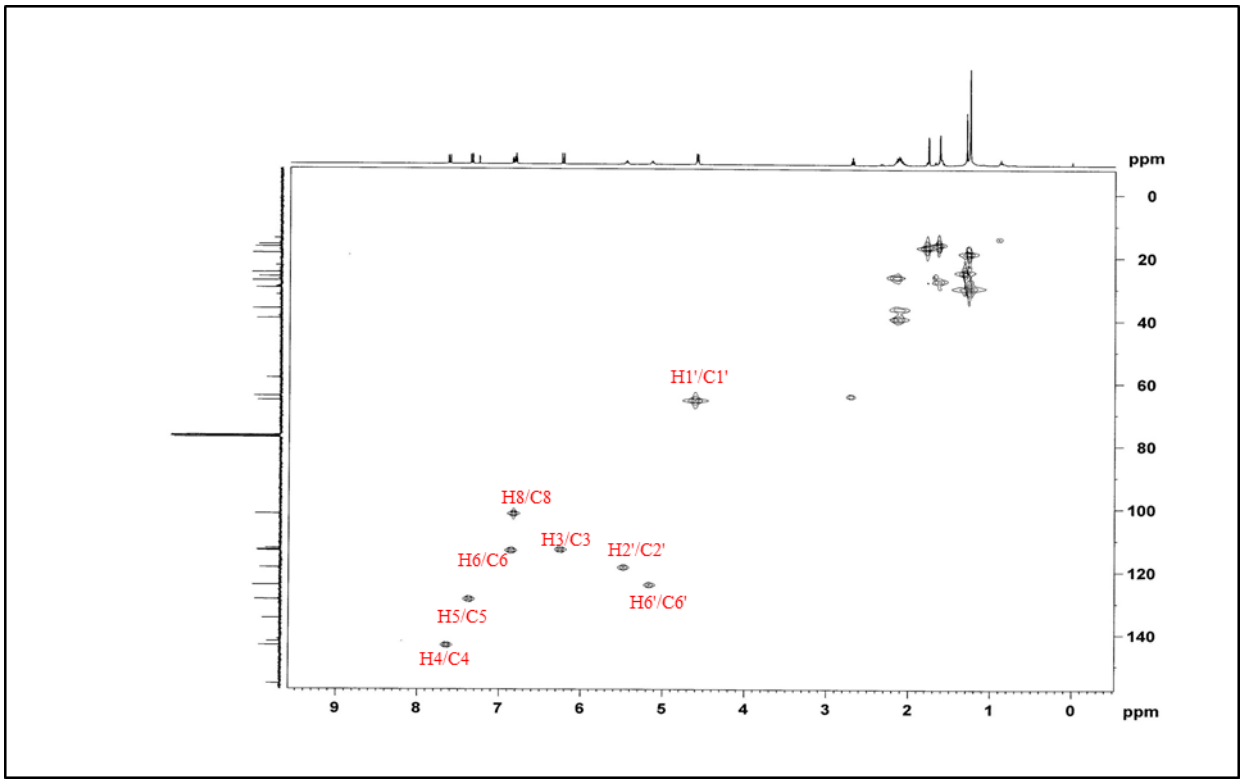
S10: ^{13}C-NMR (100 MHz, $CDCl_3$) Spectrum of Compound **2** (Umbelliprenin-10′,11′-monoepoxide)



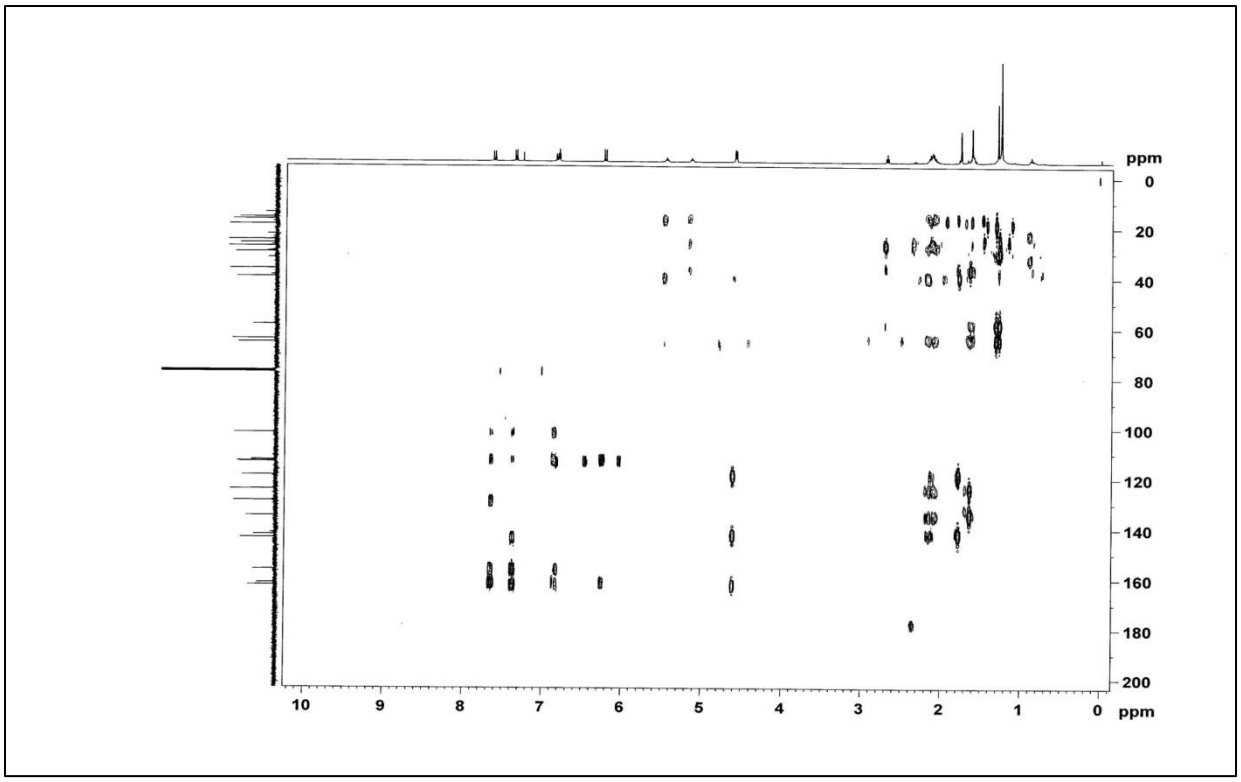
S11: DEPT (100 MHz, $CDCl_3$) Spectrum of Compound **2** (Umbelliprenin-10′,11′-monoepoxide)



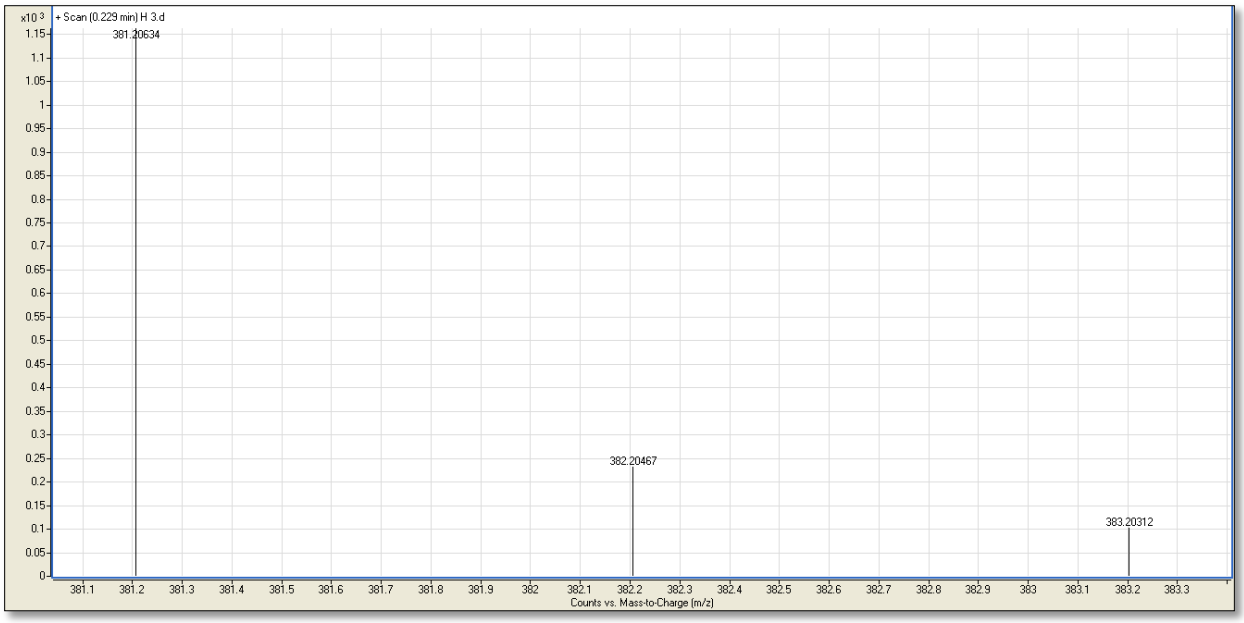
S12: COSY Spectrum of Compound **2** (Umbelliprenin-10′,11′-monoepoxide)



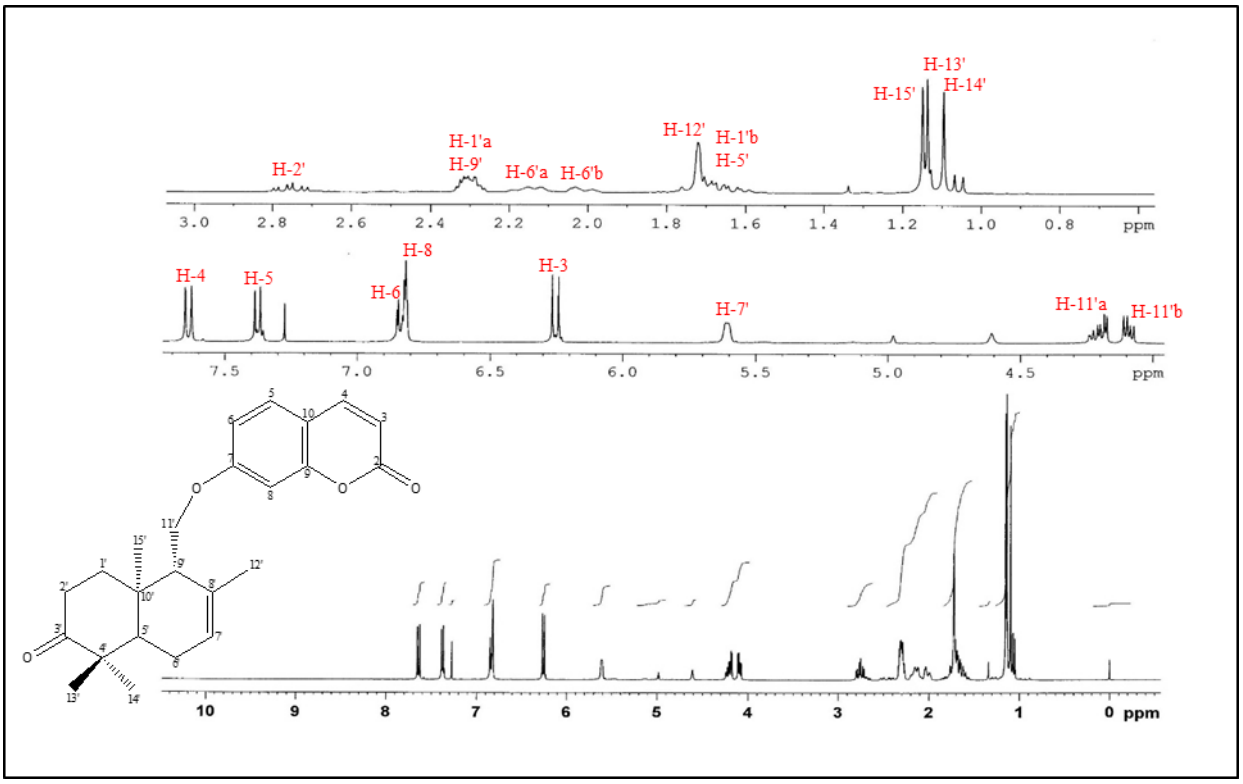
S13: HMQC Spectrum of Compound **2** (Umbelliprenin-10′,11′-monoepoxide)



S14: HMBC Spectrum of Compound **2** (Umbelliprenin-10′,11′-monoepoxide)

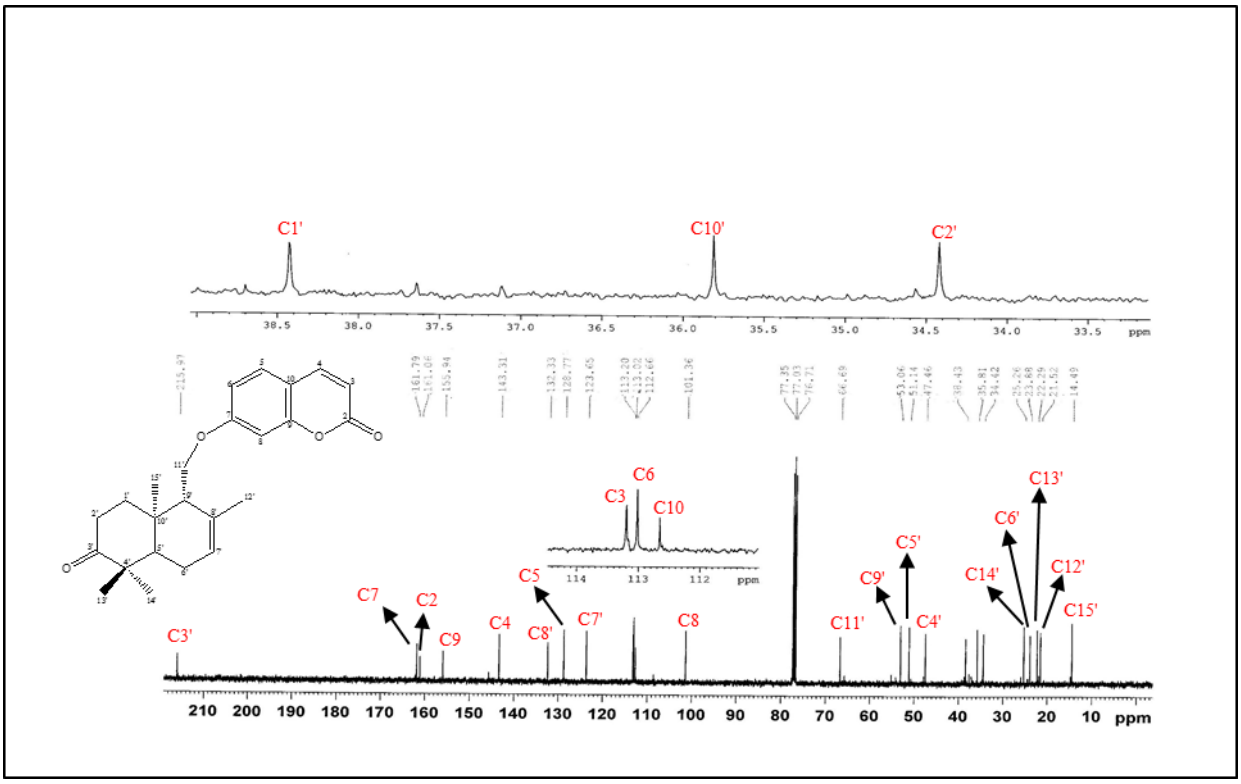


S15: HRESIMS Spectrum of Compound **3** (Conferone)

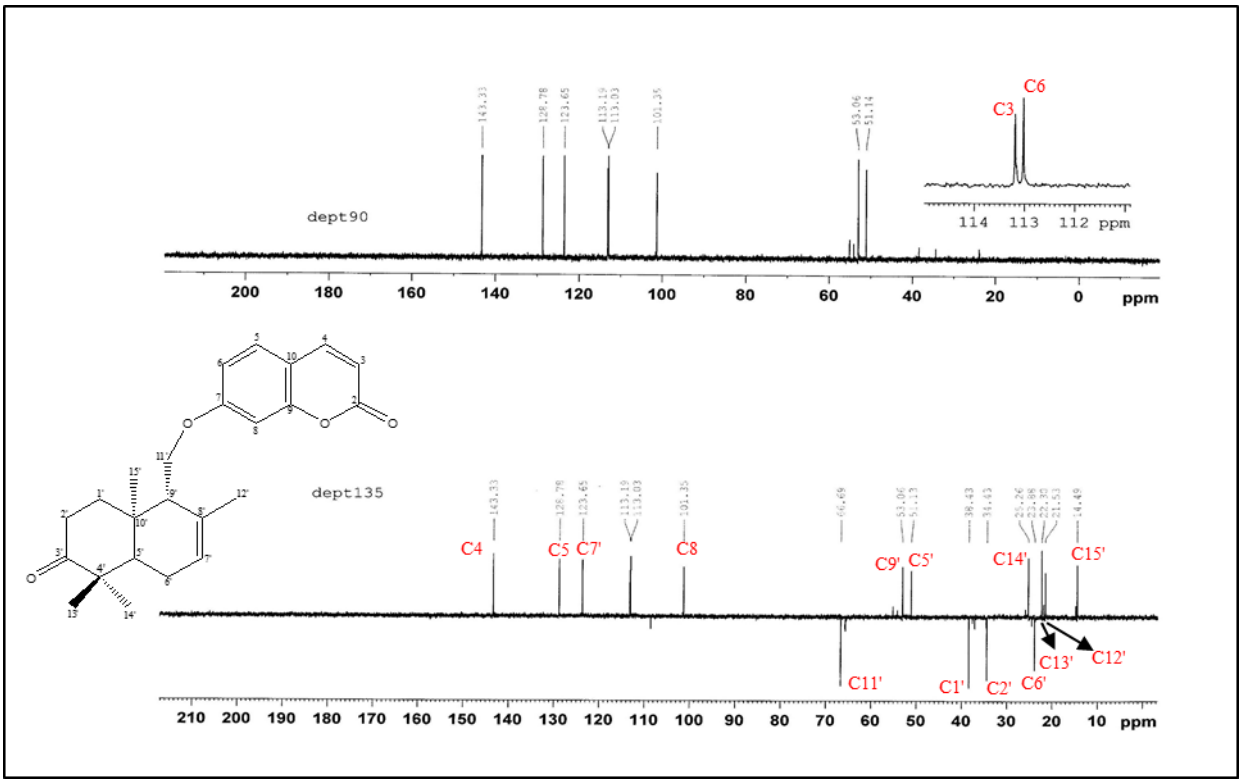


S16: ^{1}H-NMR (400 MHz, $CDCl_3$) Spectrum of Compound **3** (Conferone)

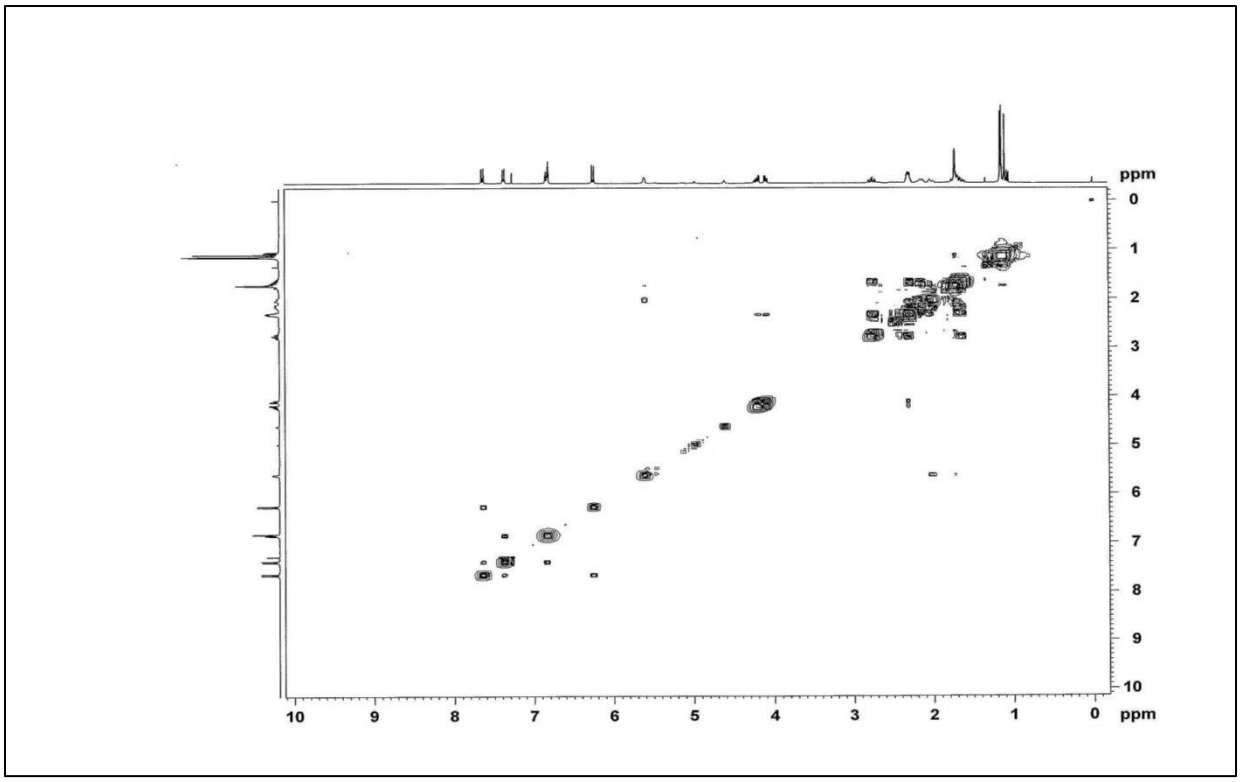
*Conferone (**3**):* White powder. ^{1}H-NMR ($CDCl_3$, 400 MHz), δ: 1.09 (3H, s, H-14'), 1.13 (3H, s, H-13'), 1.15 (3H, s, H-15'), 1.64 (1H, m, H-1'b), 1.68 (1H, m, H-5'), 1.72 (3H, s, H-12'), 2.01 (1H, m, H-6'b), 2.19 (1H, m, H-6'a), 2.30 (1H, m, H-1'a), 2.31 (1H, m, H-9'), 2.75 (2H, m, H-2'), 4.09 (1H, dd, H-11'b), 4.19 (1H, dd, H-11'a), 5.60 (1H, bs, H-7'), 6.25 (1H, d, H-3), 6.82 (1H, d, H-8), 6.84 (1H, dd, H-6), 7.37 (1H, d, H-5), 7.63 (1H, d, H-4). ^{13}C-NMR ($CDCl_3$, 100 MHz), δ: 161.06 (C-2), 113.20 (C-3), 143.31 (C-4), 128.77 (C-5), 113.02 (C-6), 161.79 (C-7), 101.36 (C-8), 155.94 (C-9), 112.66 (C-10), 38.43 (C-1'), 34.42 (C-2'), 215.97 (C-3'), 47.46 (C-4'), 51.14 (C-5'), 23.88 (C-6'), 123.65 (C-7'), 132.33 (C-8'), 53.06 (C-9'), 35.81 (C-10'), 66.69 (C-11'), 21.52 (C-12'), 22.29 (C-13'), 25.26 (C-14'), 14.49 (C-15'). HRESIMS: *m/z* = 381.20634 $[M + H]^+$ (calcd for $C_{24}H_{28}O_4$, 380.4767) [10].



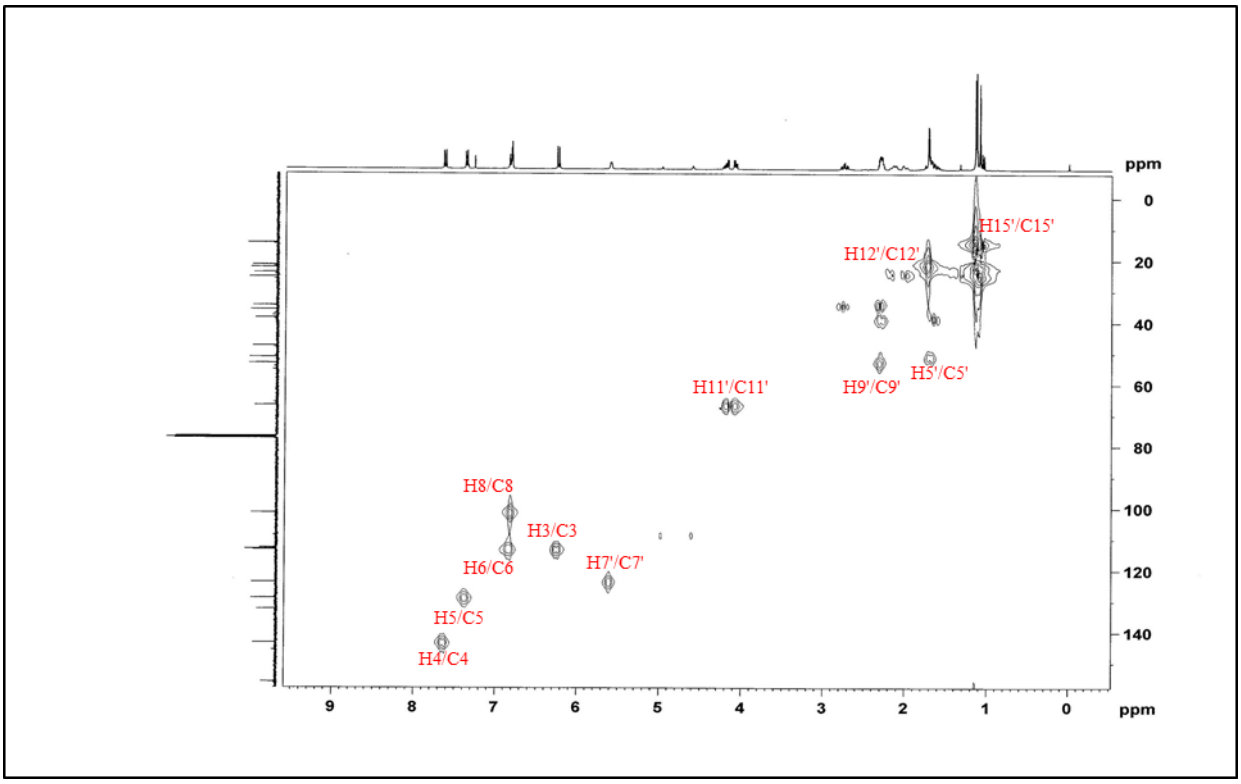
S17: ^{13}C-NMR (100 MHz, $CDCl_3$) Spectrum of Compound **3** (Conferone)



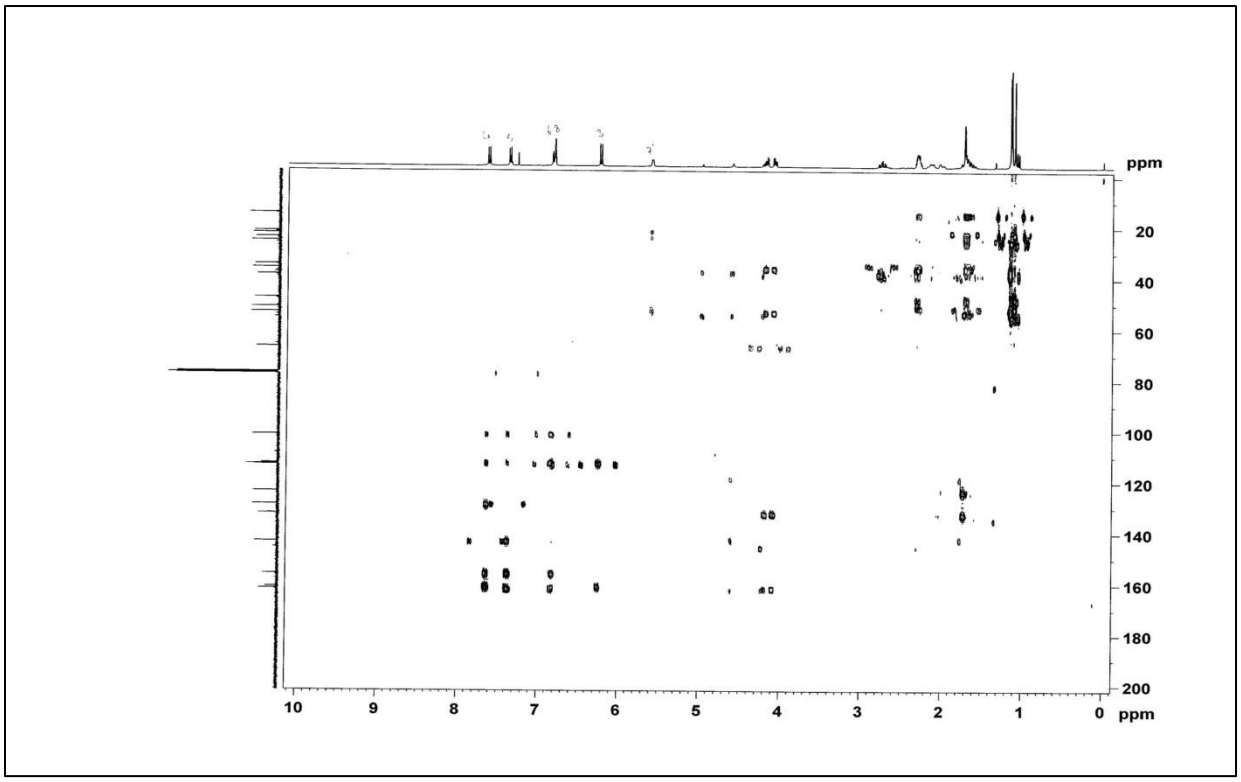
S18: DEPT (100 MHz, $CDCl_3$) Spectrum of Compound **3** (Conferone)



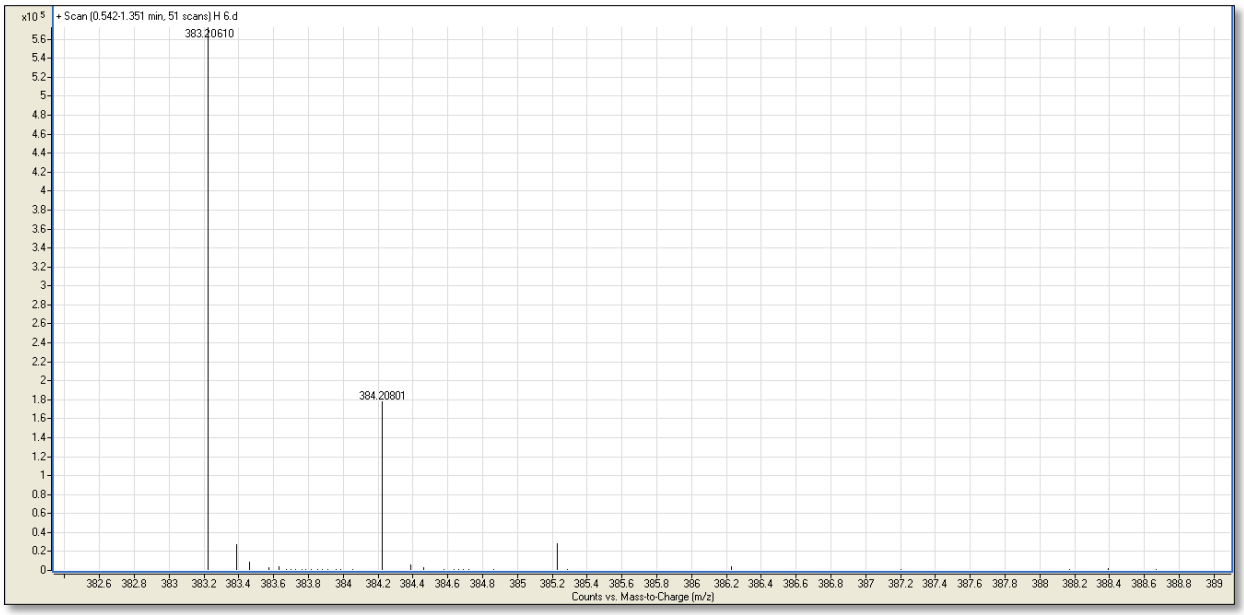
S19: COSY Spectrum of Compound **3** (Conferone)



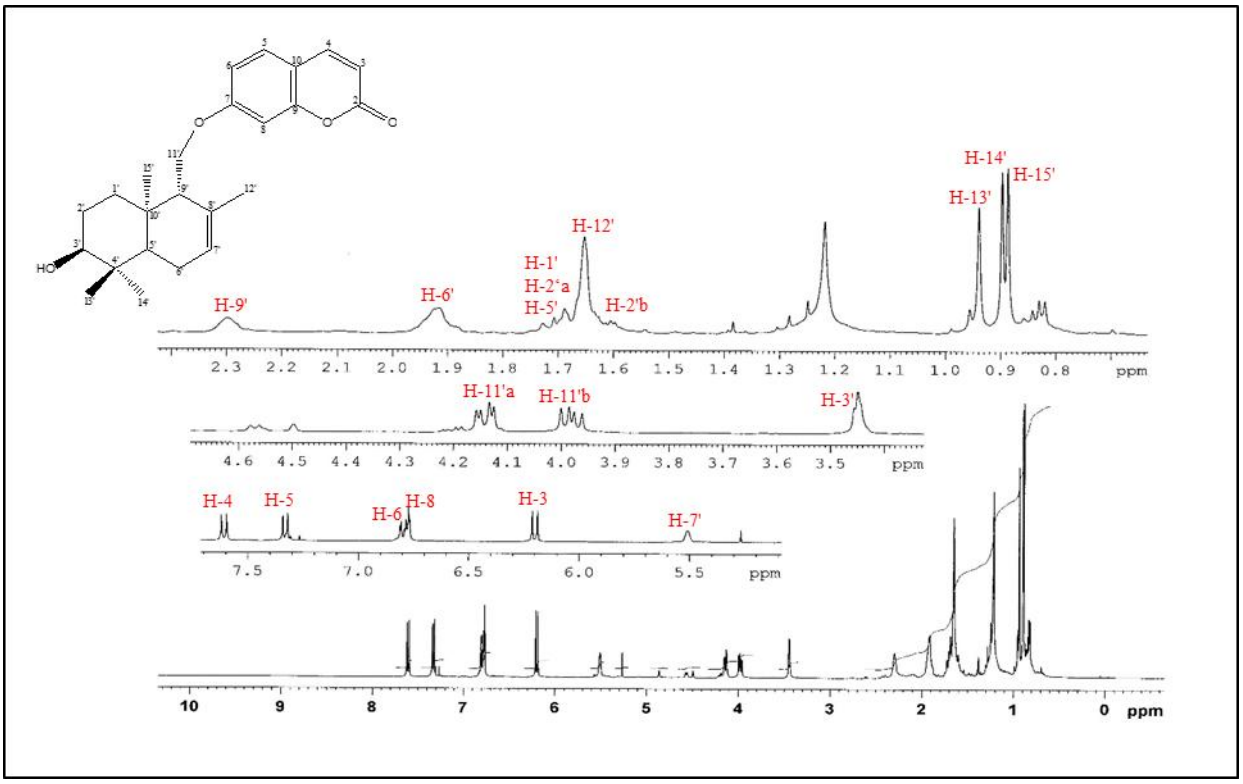
S20: HMQC Spectrum of Compound **3** (Conferone)



S21: HMBC Spectrum of Compound **3** (Conferone)

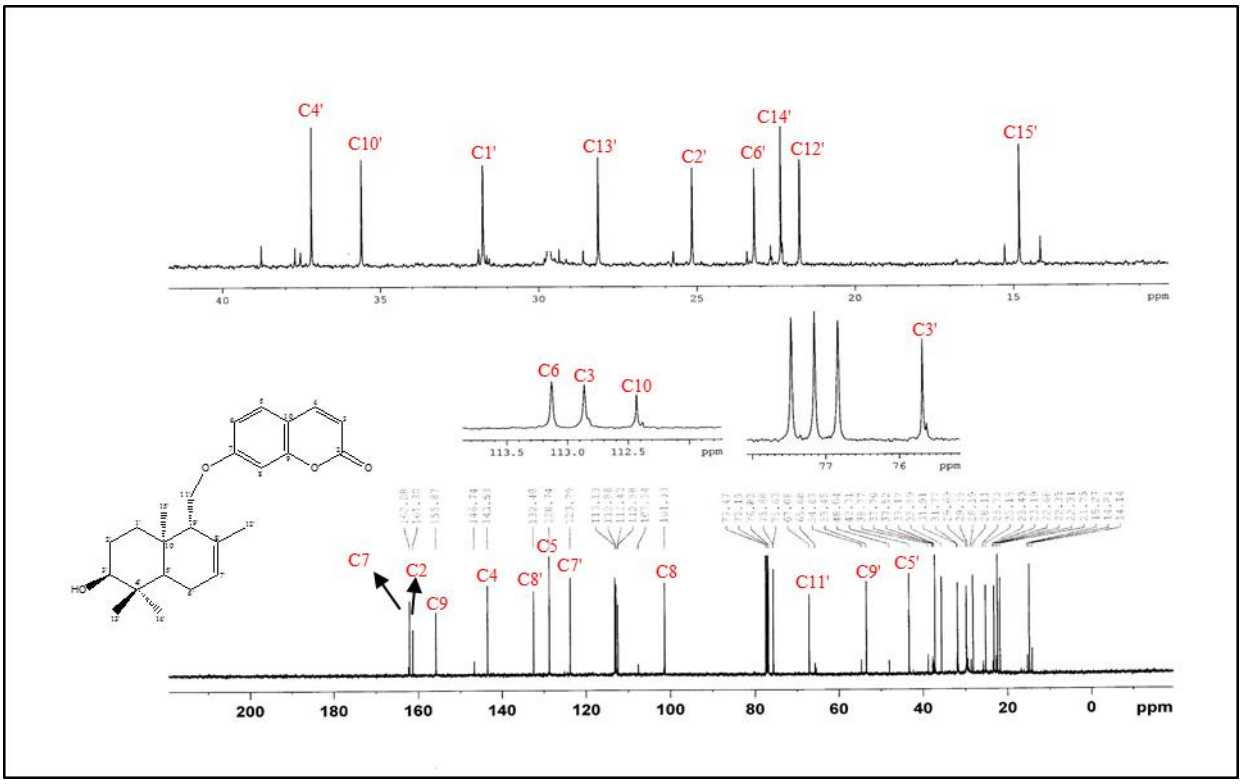


S22: HRESIMS Spectrum of Compound **4** (Mogoltacin)

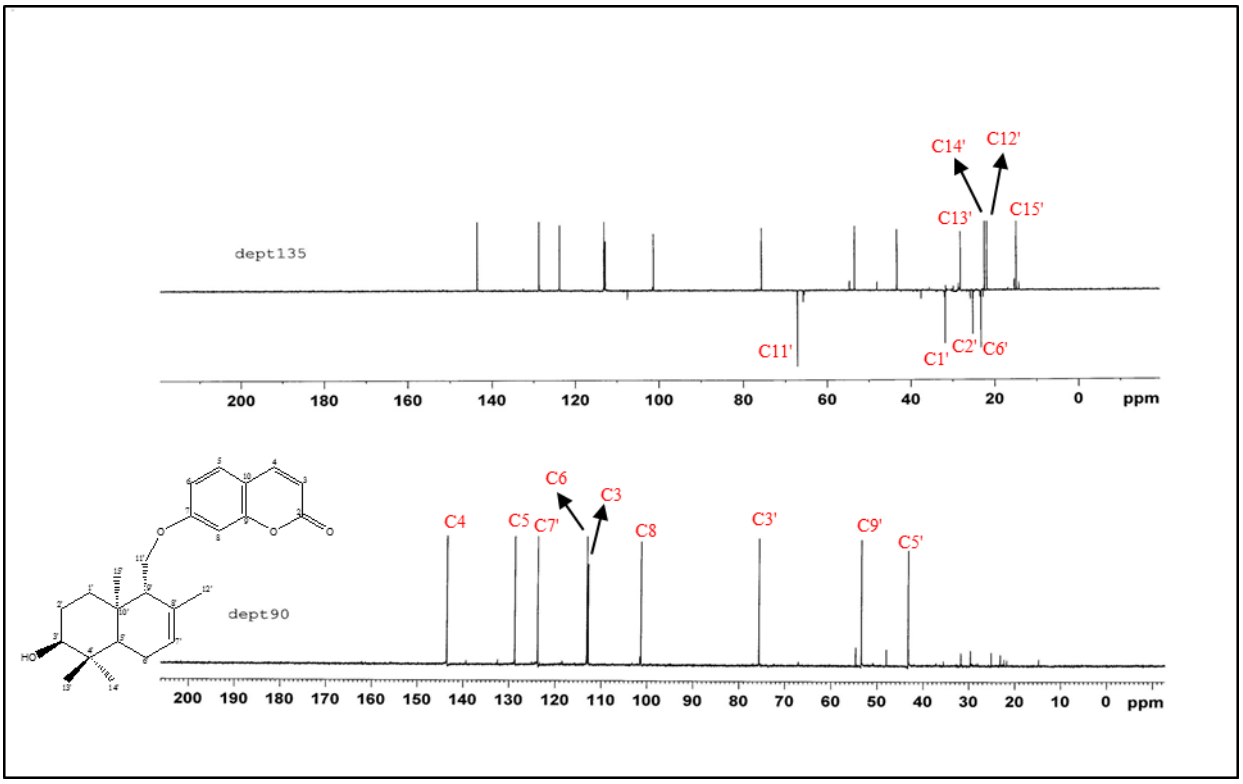


S23: ^{1}H-NMR (400 MHz, $CDCl_3$) Spectrum of Compound **4** (Mogoltacin)

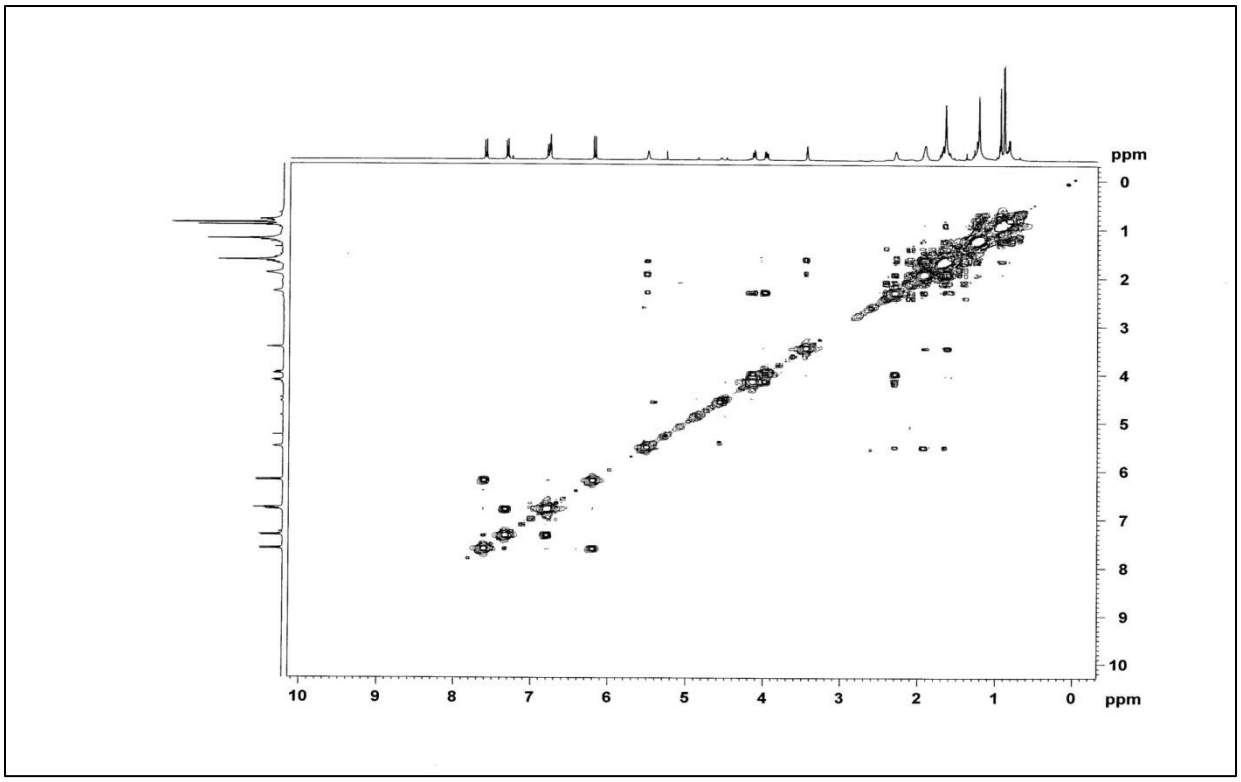
*Mogoltacin (**4**):* White powder. ^{1}H-NMR ($CDCl_3$, 400 MHz), δ: 0.88 (3H, s, H-15'), 0.89 (3H, s, H-14'), 0.93 (3H, s, H-13'), 1.60 (1H, m, H-2'b), 1.65 (3H, m, H-1', H-2'a), 1.65 (3H, s, H-12'), 1.70 (1H, m, H-5'), 1.93 (2H, m, H-6'), 2.29 (1H, bs, H-9'), 3.45 (1H, bs, H-3'), 3.98 (1H, dd, H-11'b), 4.13 (1H, dd, H-11'a), 5.50 (1H, bs, H-7'), 6.20 (1H, d, H-3), 6.77 (1H, d, H-8), 6.79 (1H, dd, H-6), 7.33 (1H, d, H-5), 7.61 (1H, d, H-4). ^{13}C-NMR ($CDCl_3$, 100 MHz), δ: 161.30 (C-2), 112.86 (C-3), 143.53 (C-4), 128.74 (C-5), 113.13 (C-6), 162.08 (C-7), 101.33 (C-8), 155.87 (C-9), 112.43 (C-10), 31.77 (C-1'), 25.15 (C-2'), 75.68 (C-3'), 37.17 (C-4'), 43.31 (C-5'), 23.19 (C-6'), 123.79 (C-7'), 132.48 (C-8'), 53.45 (C-9'), 35.59 (C-10'), 67.08 (C-11'), 21.75 (C-12'), 28.11 (C-13'), 22.35 (C-14'), 14.81 (C-15'). HRESIMS: *m/z* = 383.20610 $[M + H]^+$ (calcd for $C_{24}H_{30}O_4$, 382.4926) [10].



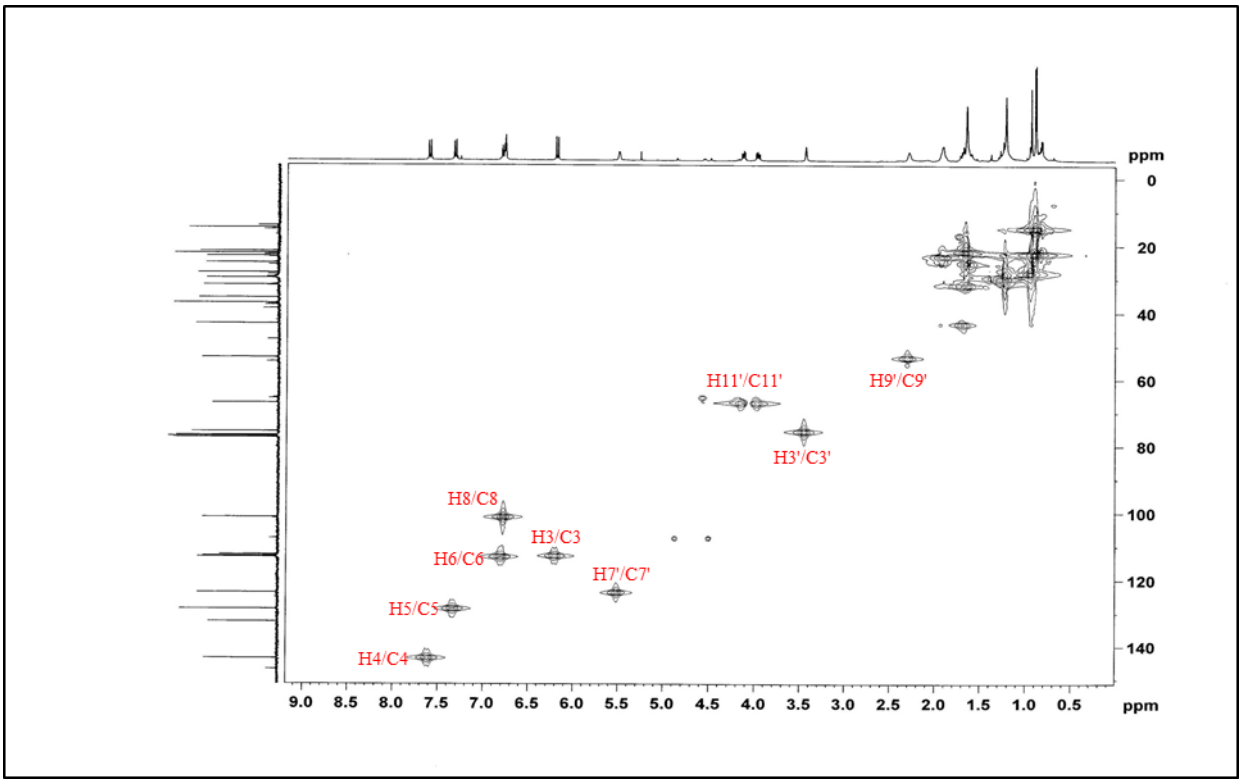
S24: ^{13}C-NMR (100 MHz, $CDCl_3$) Spectrum of Compound **4** (Mogoltacin)



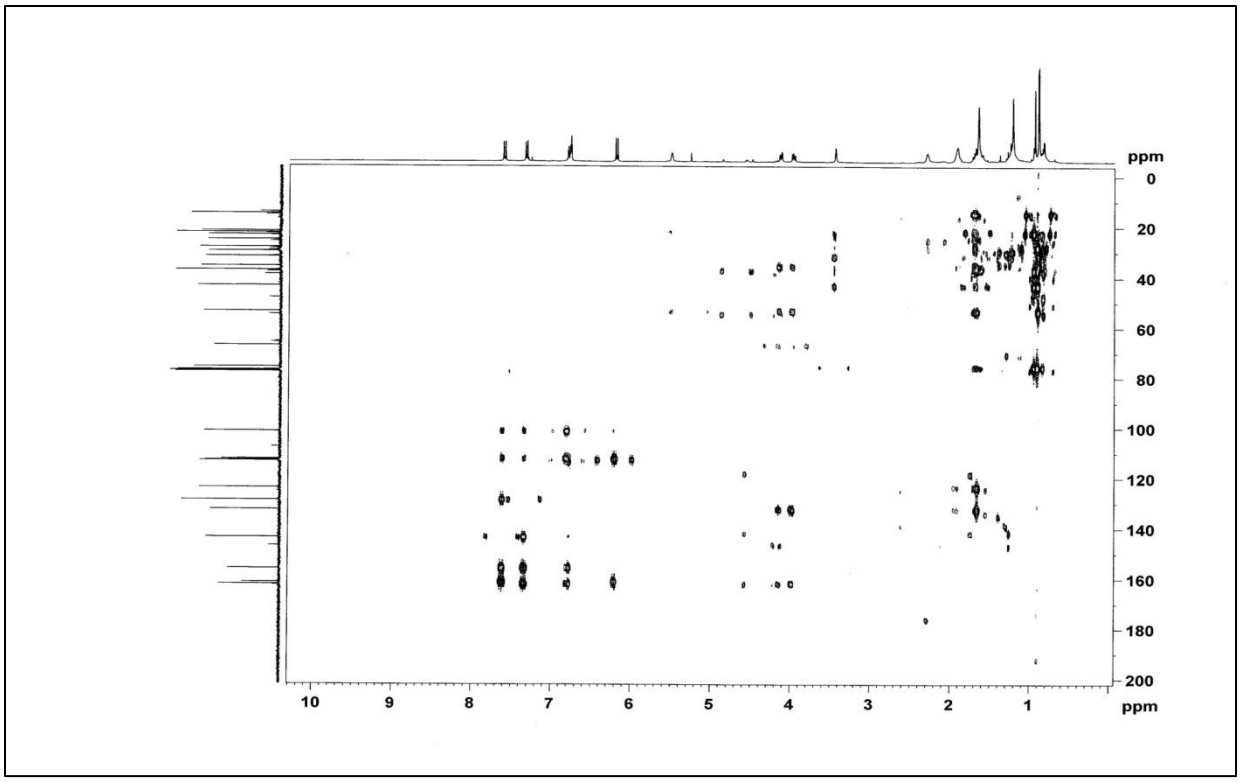
S25: DEPT (100 MHz, $CDCl_3$) Spectrum of Compound **4** (Mogoltacin)



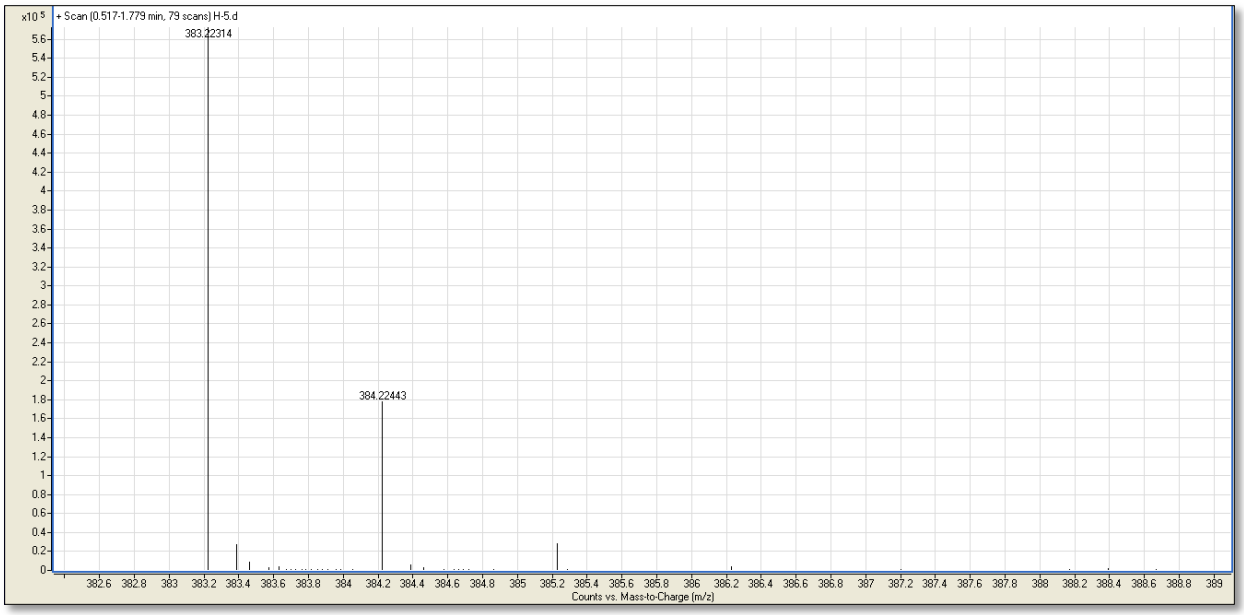
S26: COSY Spectrum of Compound **4** (Mogoltacin)



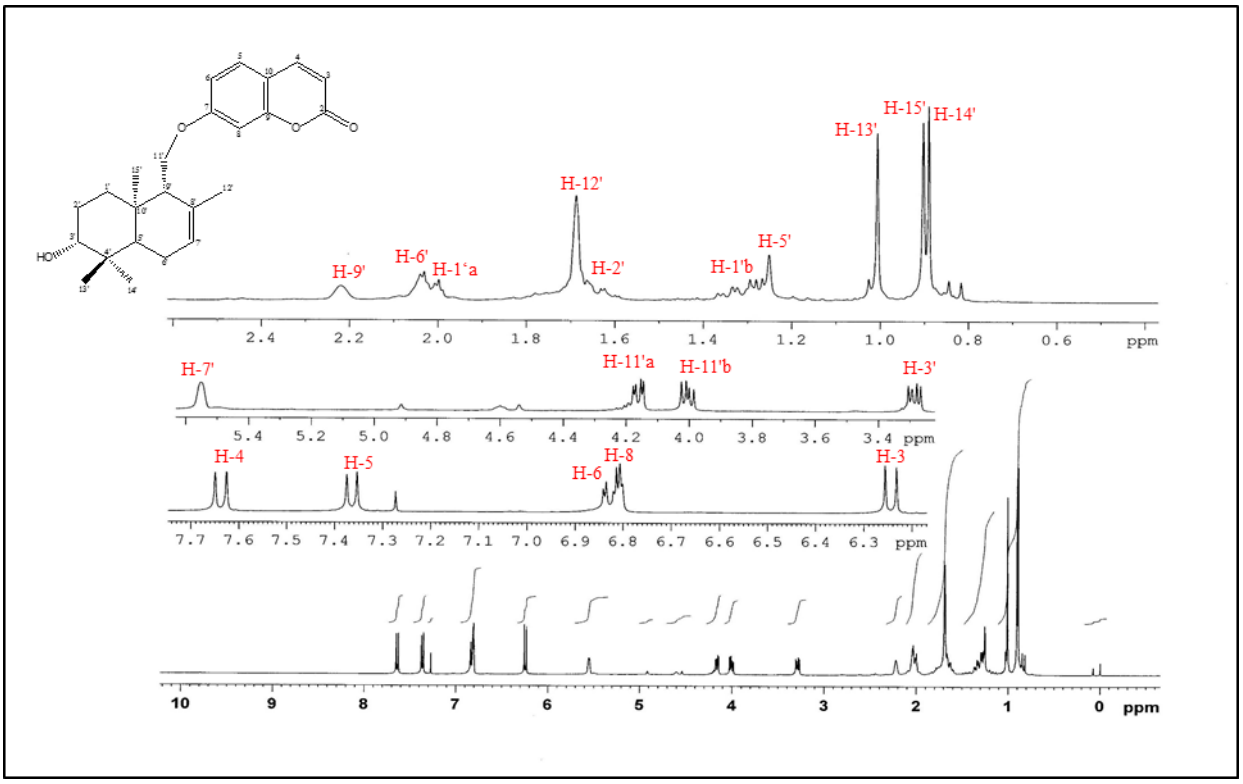
S27: HMQC Spectrum of Compound **4** (Mogoltacin)



S28: HMBC Spectrum of Compound **4** (Mogoltacin)

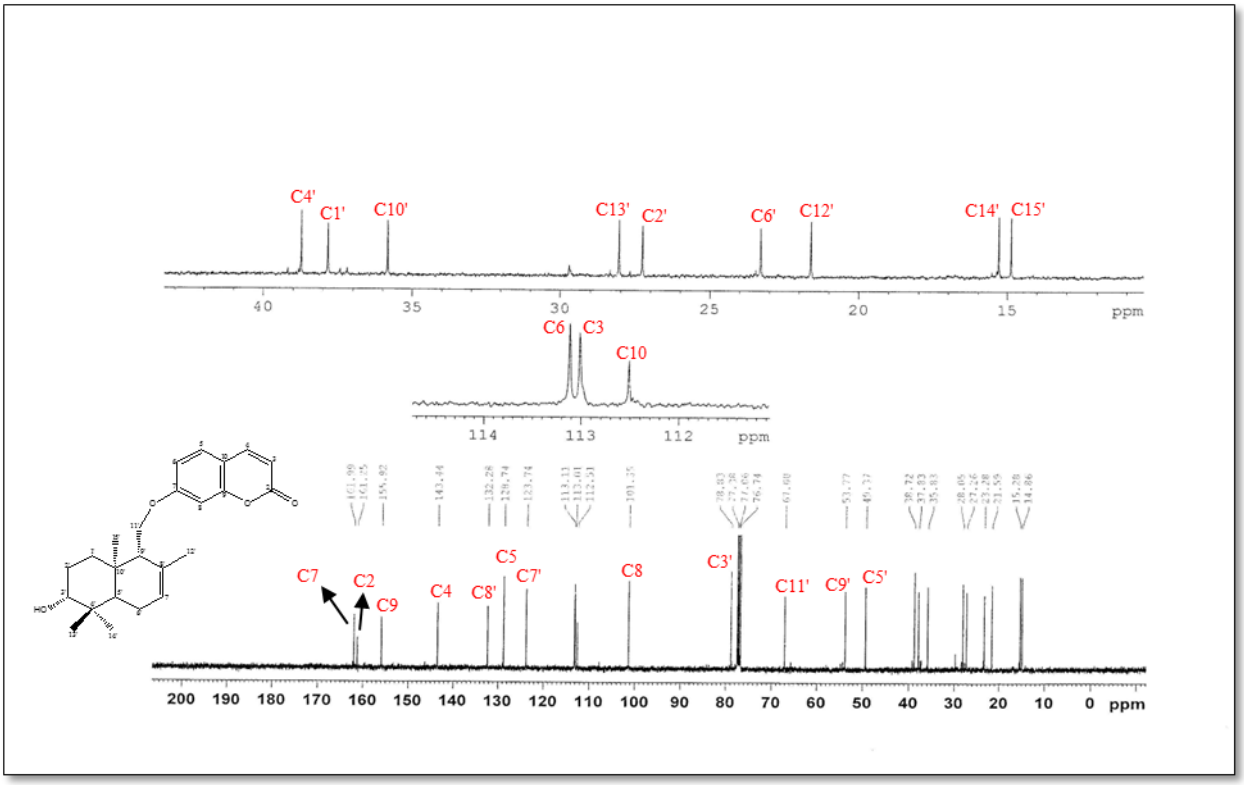


S29: HRESIMS Spectrum of Compound **5** (Feselol)

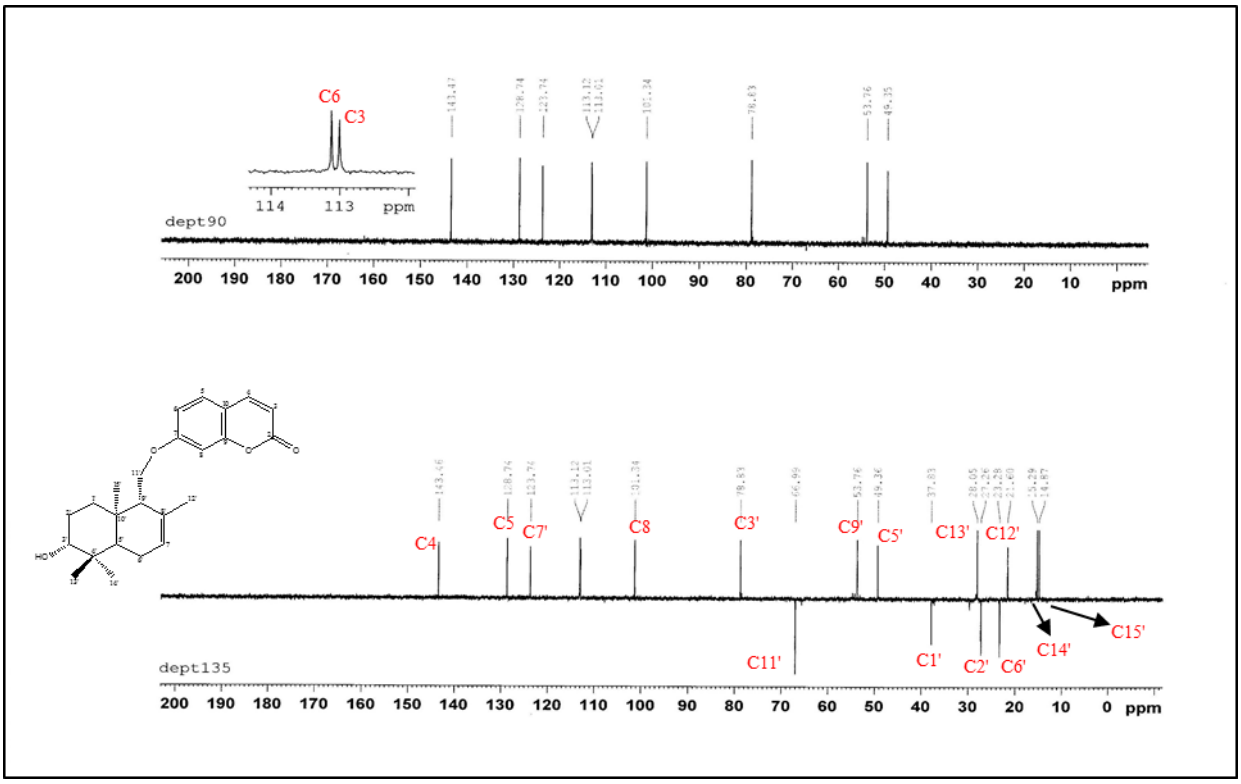


S30: ^{1}H-NMR (400 MHz, $CDCl_3$) Spectrum of Compound **5** (Feselol)

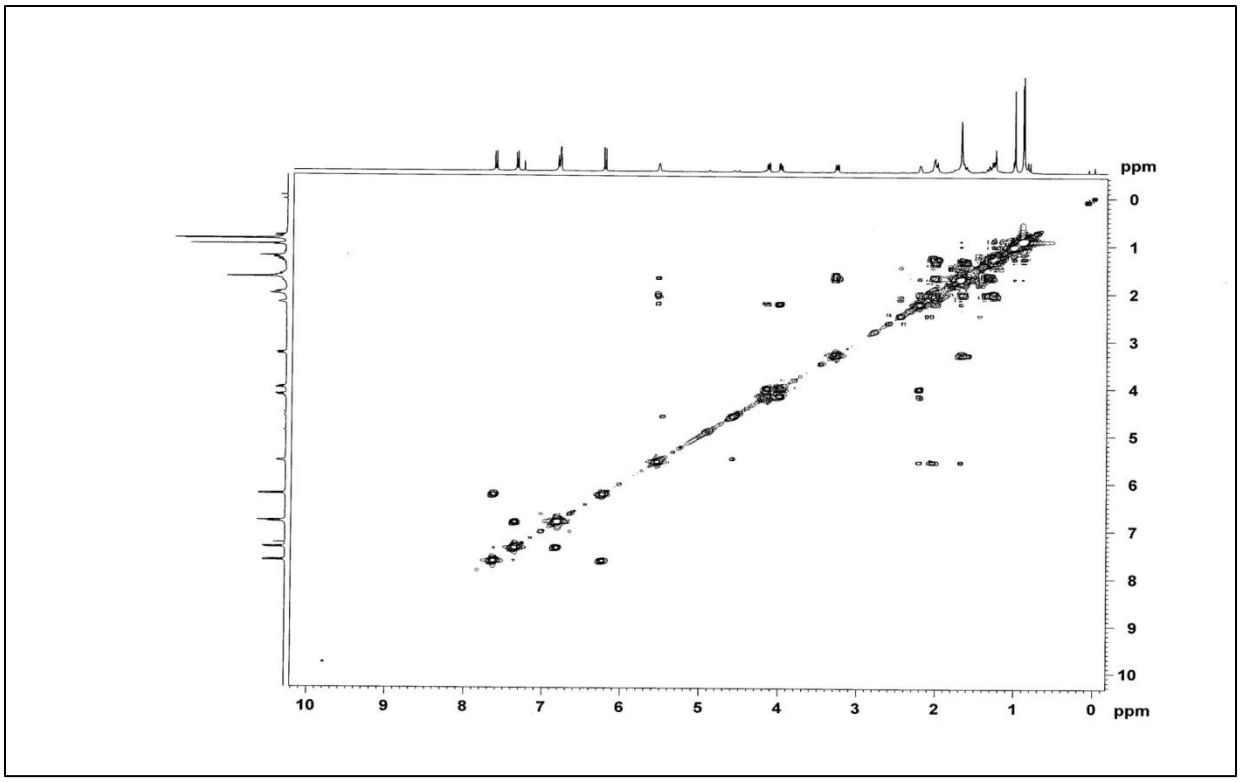
*Feselol (**5**):* White powder. ^{1}H-NMR ($CDCl_3$, 400 MHz), δ: 0.89 (3H, s, H-14'), 0.90 (3H, s, H-15'), 1.00 (3H, s, H-13'), 1.28 (1H, dd, H-5'), 1.34 (1H, dd, H-1'b), 1.67 (2H, m, H-2'), 1.68 (3H, s, H-12'), 2.02 (1H, dd, H-1'a), 2.03 (2H, m, H-6'), 2.21 (1H, bs, H-9'), 3.28 (1H, dd, H-3'), 4.00 (1H, dd, H-11'b), 4.16 (1H, dd, H-11'a), 5.55 (1H, bs, H-7'), 6.24 (1H, d, H-3), 6.80 (1H, d, H-8), 6.83 (1H, dd, H-6), 7.36 (1H, d, H-5), 7.61 (1H, d, H-4). ^{13}C-NMR ($CDCl_3$, 100 MHz), δ: 161.25 (C-2), 113.01(C-3), 143.44 (C-4), 128.74 (C-5), 113.11 (C-6), 161.99 (C-7), 101.35 (C-8), 155.92 (C-9), 112.51 (C-10), 37.83 (C-1'), 27.26 (C-2'), 78.83 (C-3'), 38.72 (C-4'), 49.37 (C-5'), 23.28 (C-6'), 123.74 (C-7'), 132.28 (C-8'), 53.77 (C-9'), 35.83 (C-10'), 67.00 (C-11'), 21.59 (C-12'), 28.05 (C-13'), 15.28 (C-14'), 14.86 (C-15'). HRESIMS: *m/z* = 383.22314 $[M + H]^+$ (calcd for $C_{24}H_{30}O_4$, 382.4926) [10].



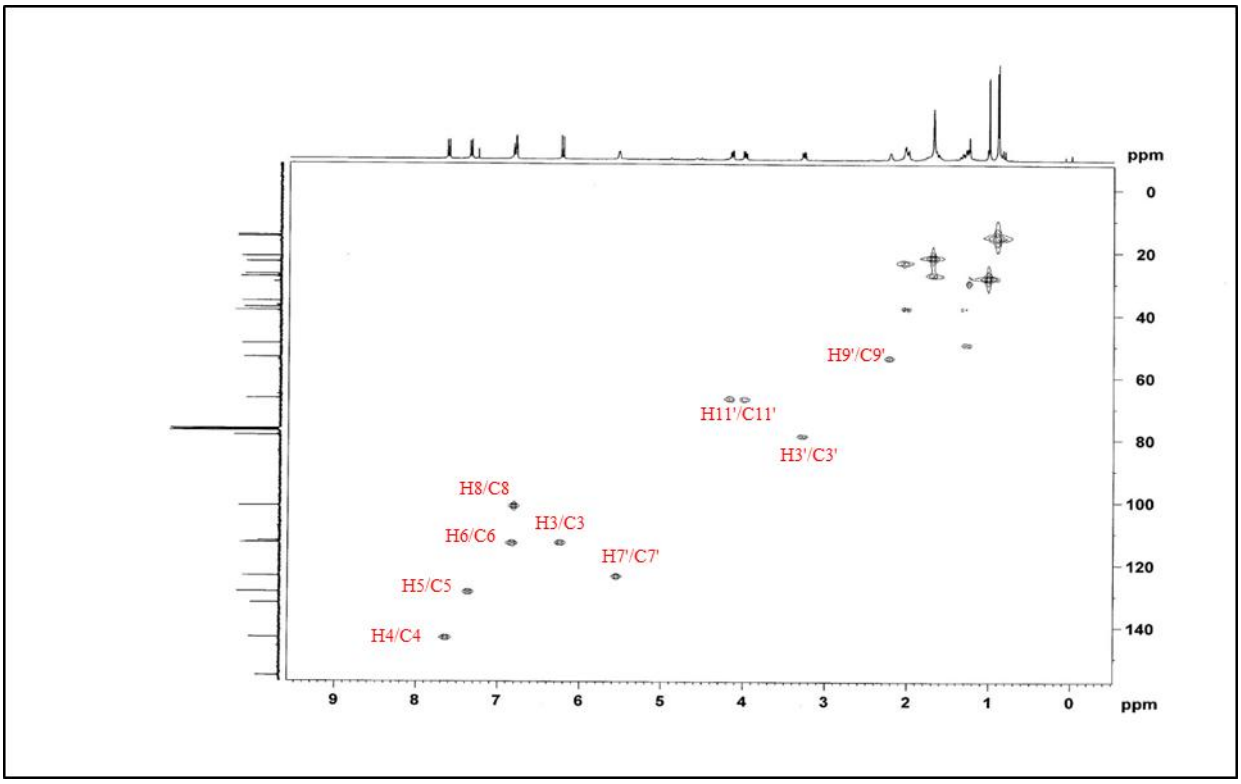
S31: ^{13}C-NMR (100 MHz, $CDCl_3$) Spectrum of Compound **5** (Feselol)



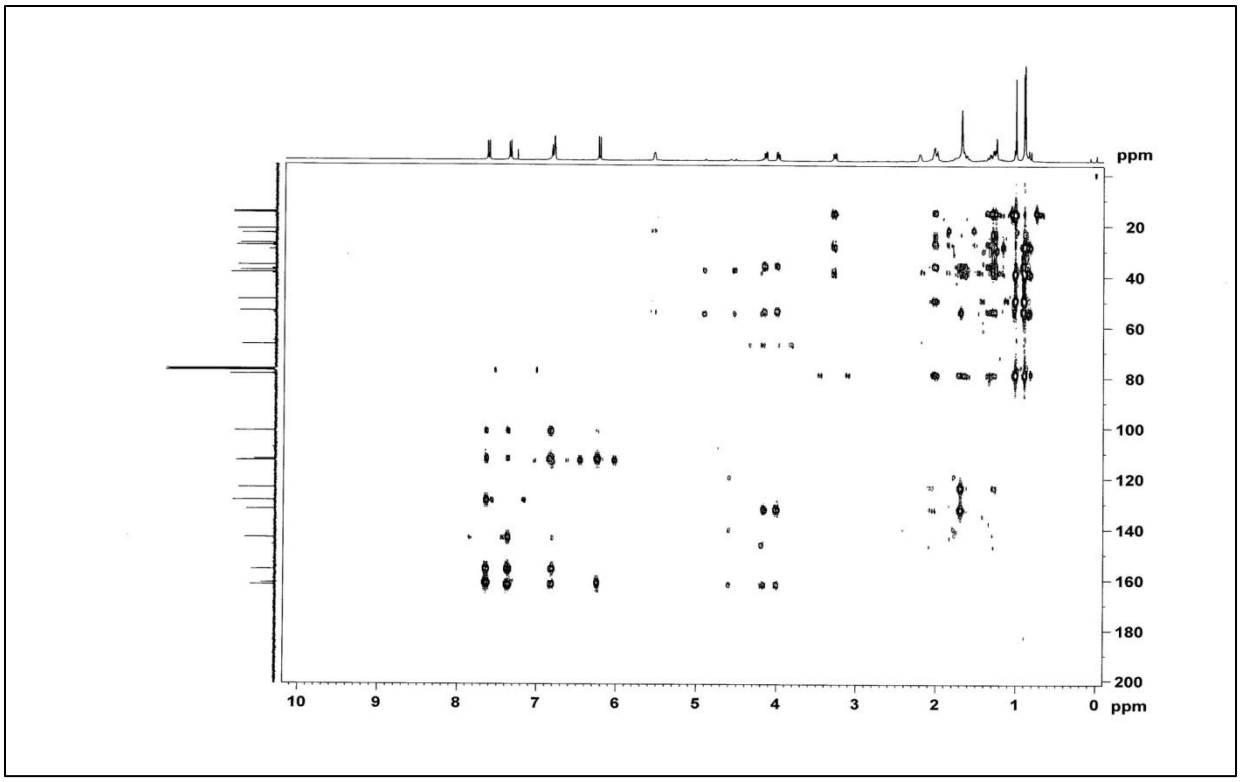
S32: DEPT (100 MHz, $CDCl_3$) Spectrum of Compound **5** (Feselol)



S33: COSY Spectrum of Compound **5** (Feselol)



S34: HMQC Spectrum of Compound **5** (Feselol)



S35: HMBC Spectrum of Compound **5** (Feselol)