

Supporting Information

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Chemical constituents of *Centaurea omphalotricha* Coss. & Durieu ex Batt. & Trab.

Soumia Mouffok¹, Hamada Haba*¹, Catherine Lavaud²,
Christophe Long³, Mohammed Benkhaled¹

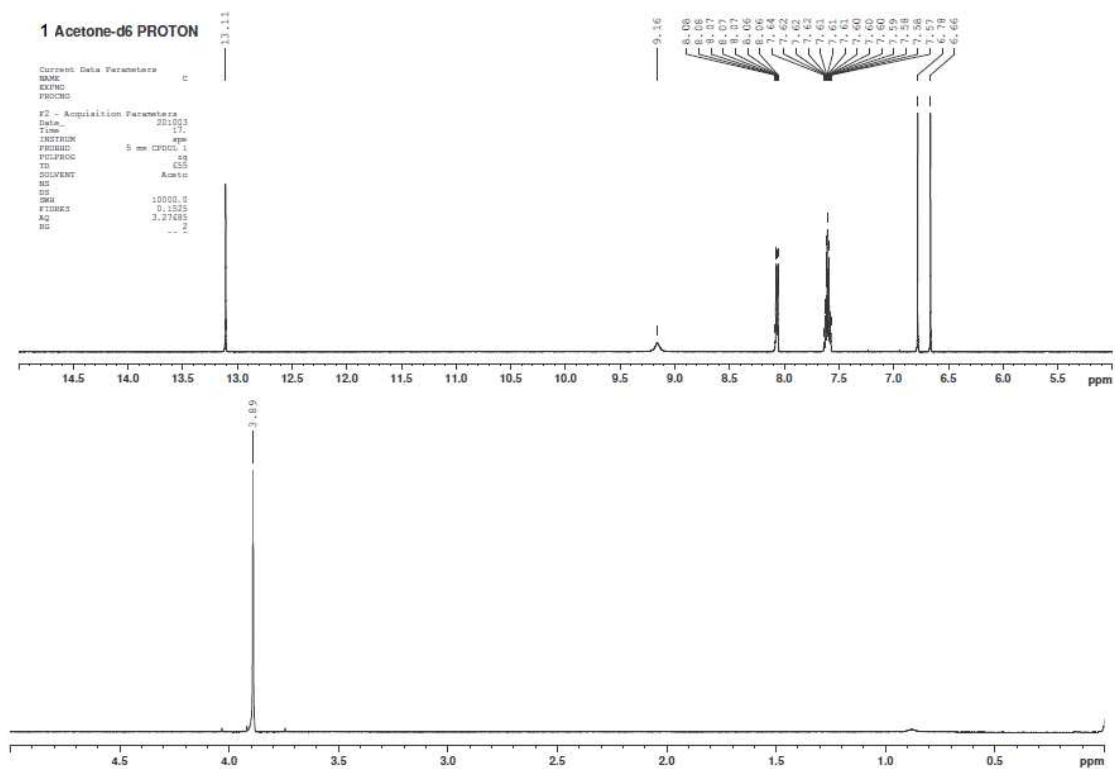
¹Laboratoire de Chimie et Chimie de l'Environnement (L.C.C.E), Département de
Chimie, Faculté des Sciences, Université de Batna, Batna 05000, Algeria

²Laboratoire de pharmacognosie, Institut de Chimie Moléculaire de Reims, CNRS
UMR 6229, BP 1039, 51097 Reims Cedex 2, France

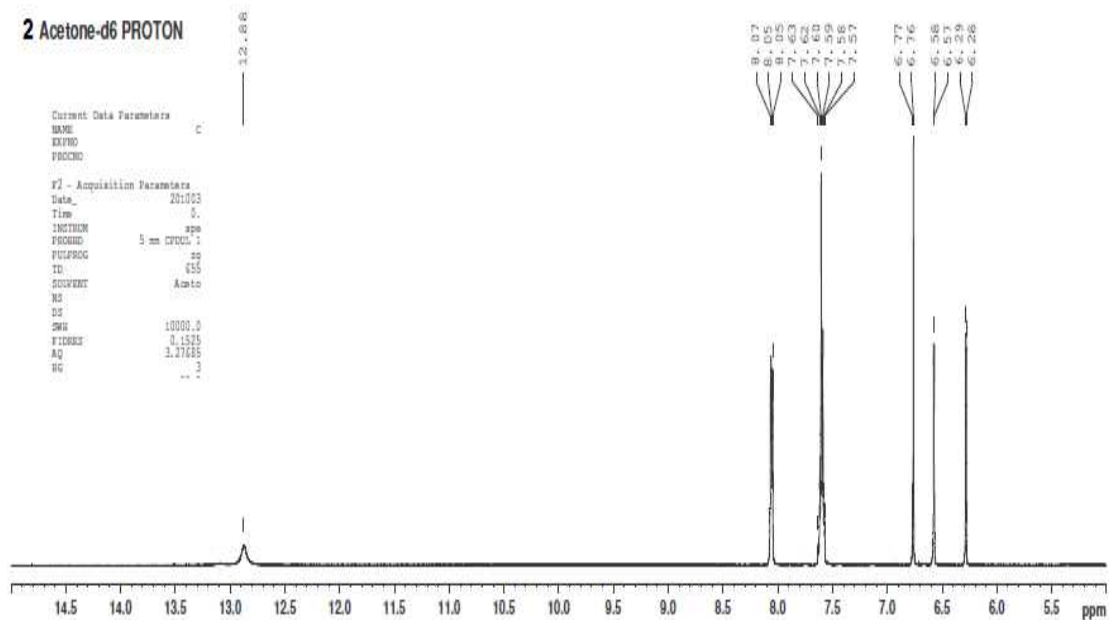
³Centre de Recherche sur les Substances Naturelles, UMS CNRS 2597, 3 rue des
Satellites, BP 94244, 31432 Toulouse, France

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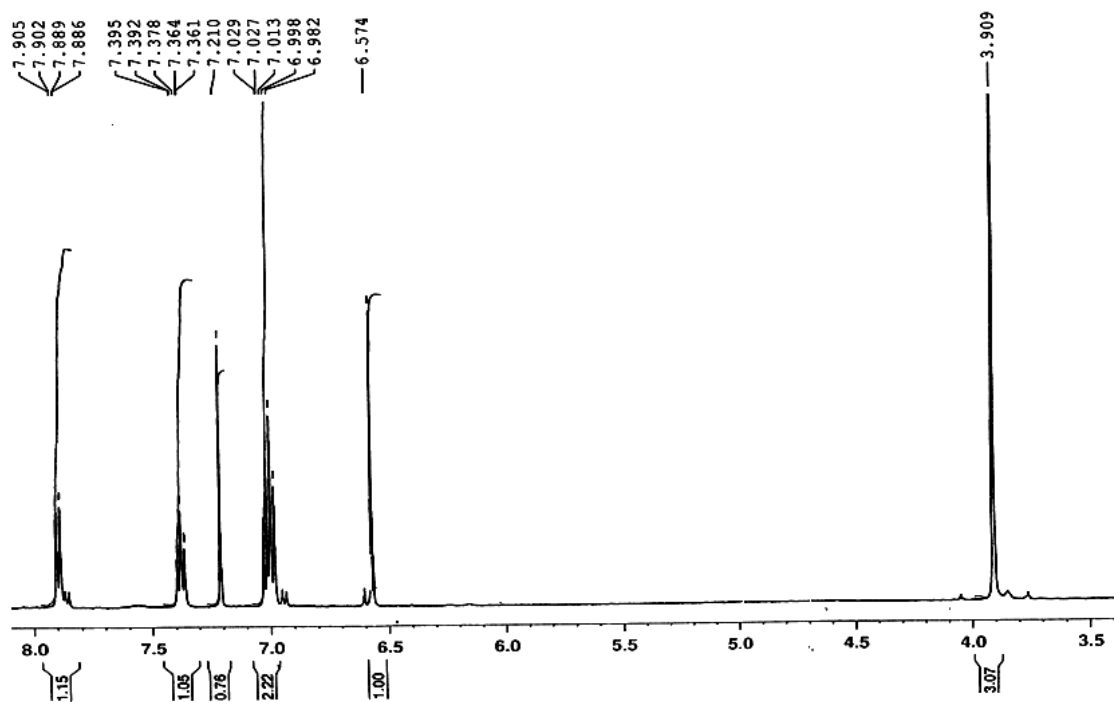
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S1: ^1H NMR spectrum of compound 1 (Oroxylin A)



S2: ^1H NMR spectrum of compound 2 (Chrysin)

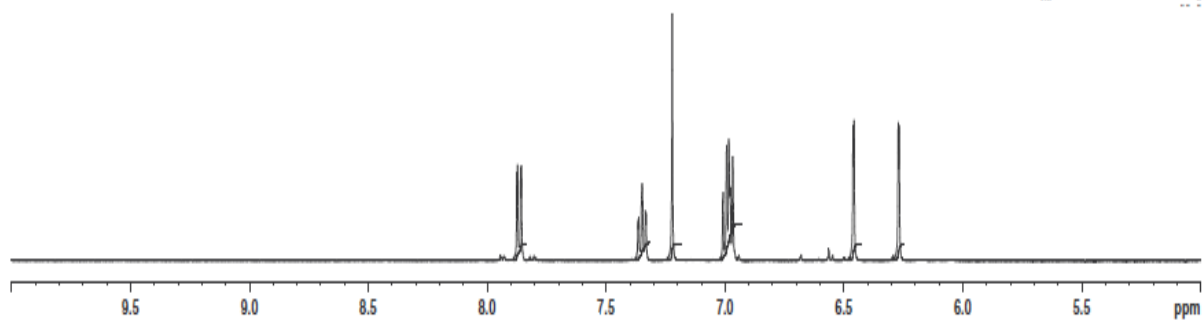


S3: ^1H NMR spectrum of compound 3 (Tenaxin II)

4 MeOD- CDCl_3 PROTON

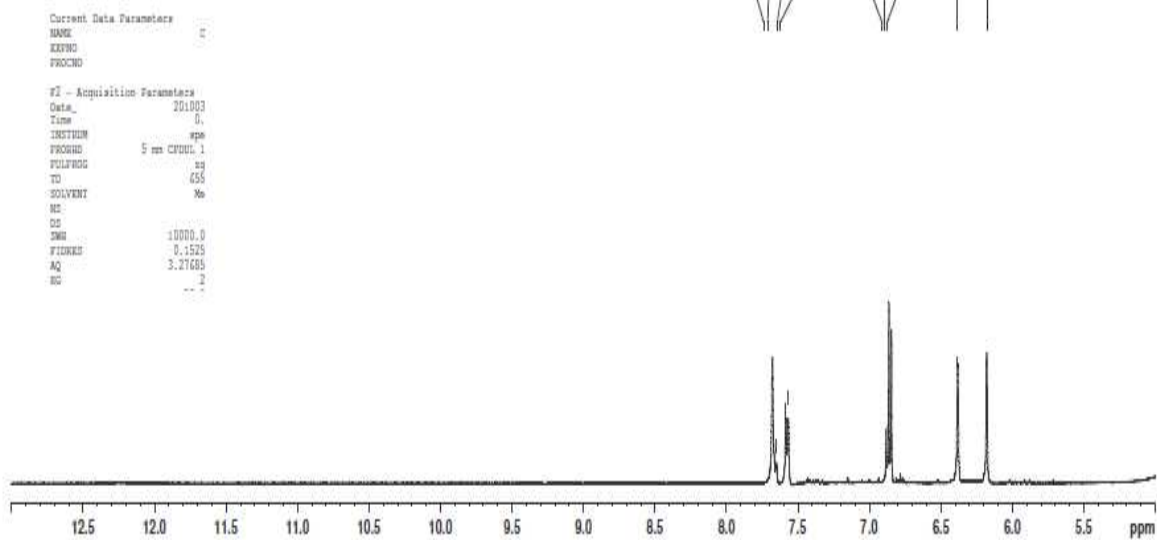
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PROCNO 1

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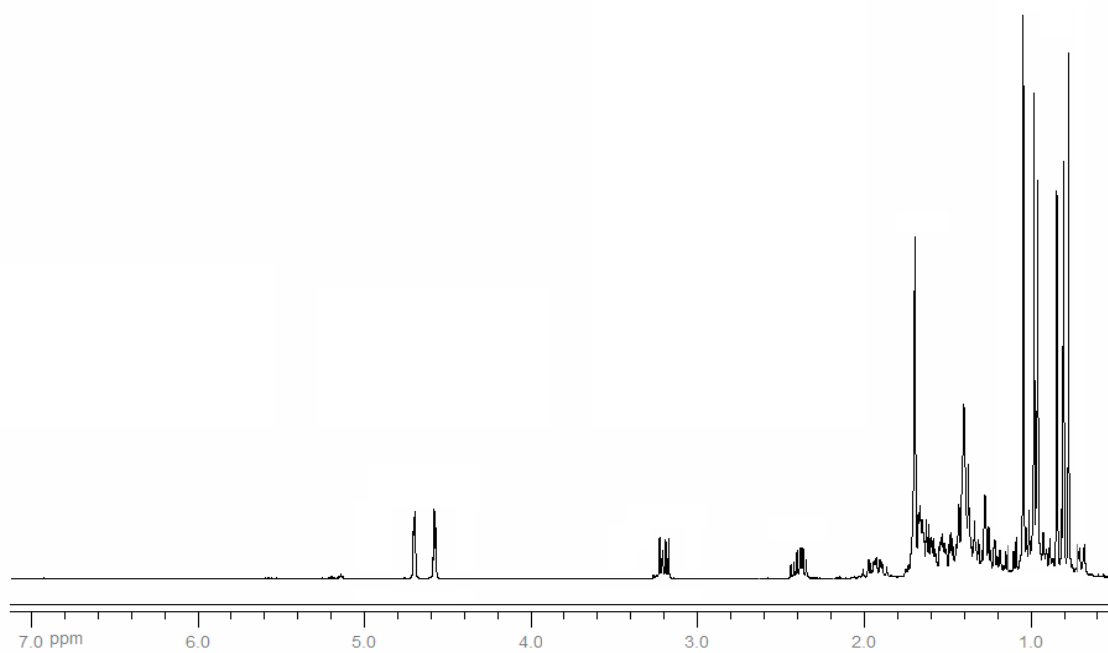


S4: ^1H NMR spectrum of compound 4 (5,7,2'-trihydroxyflavone)

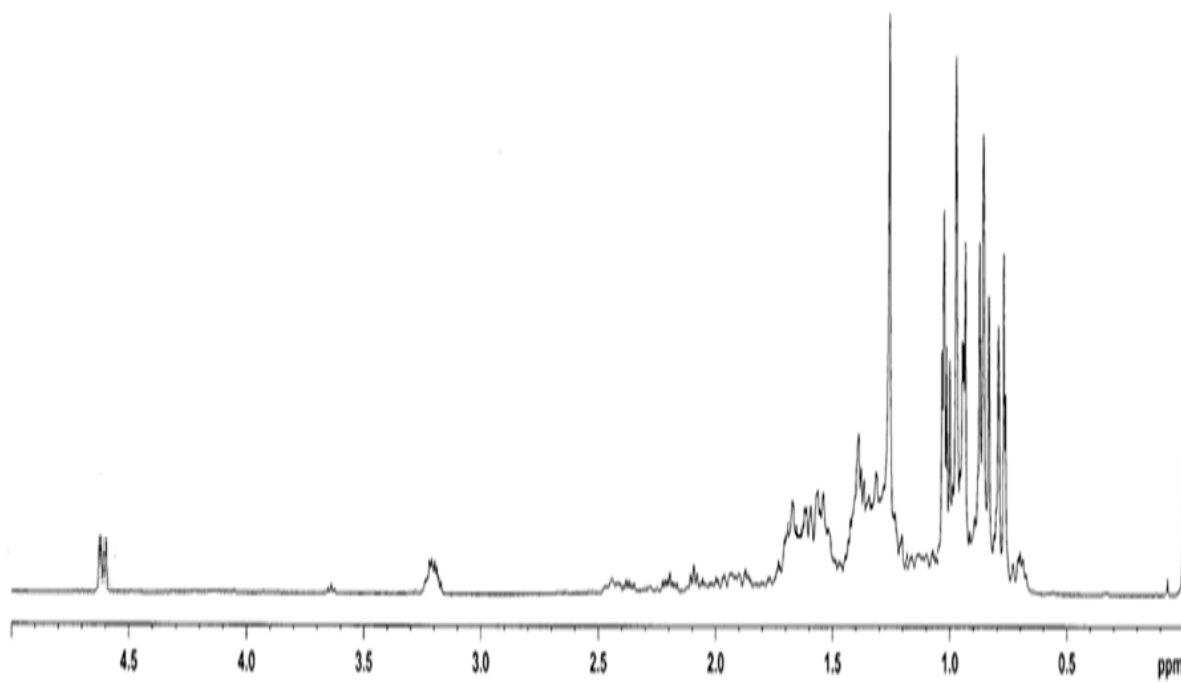
5 MeOD PROTON



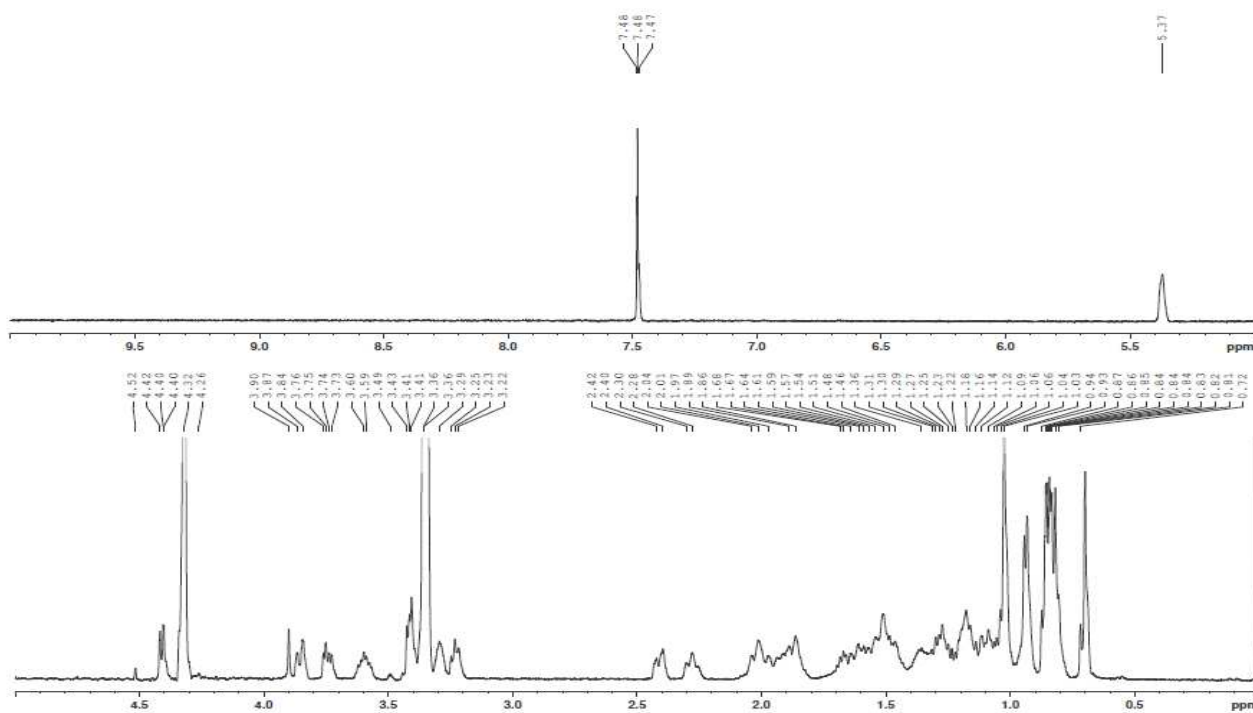
S5: ¹H NMR spectrum of compound 5 (Quercetin)



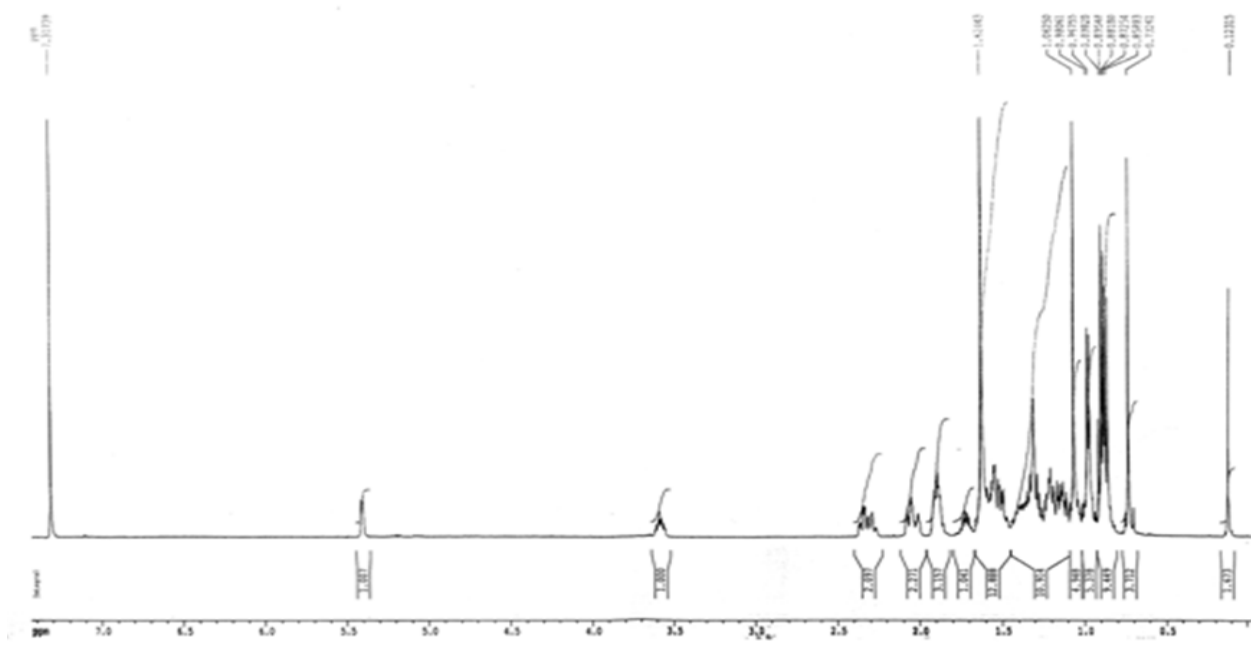
S6: ¹H NMR spectrum of compound 6 (Lupeol)



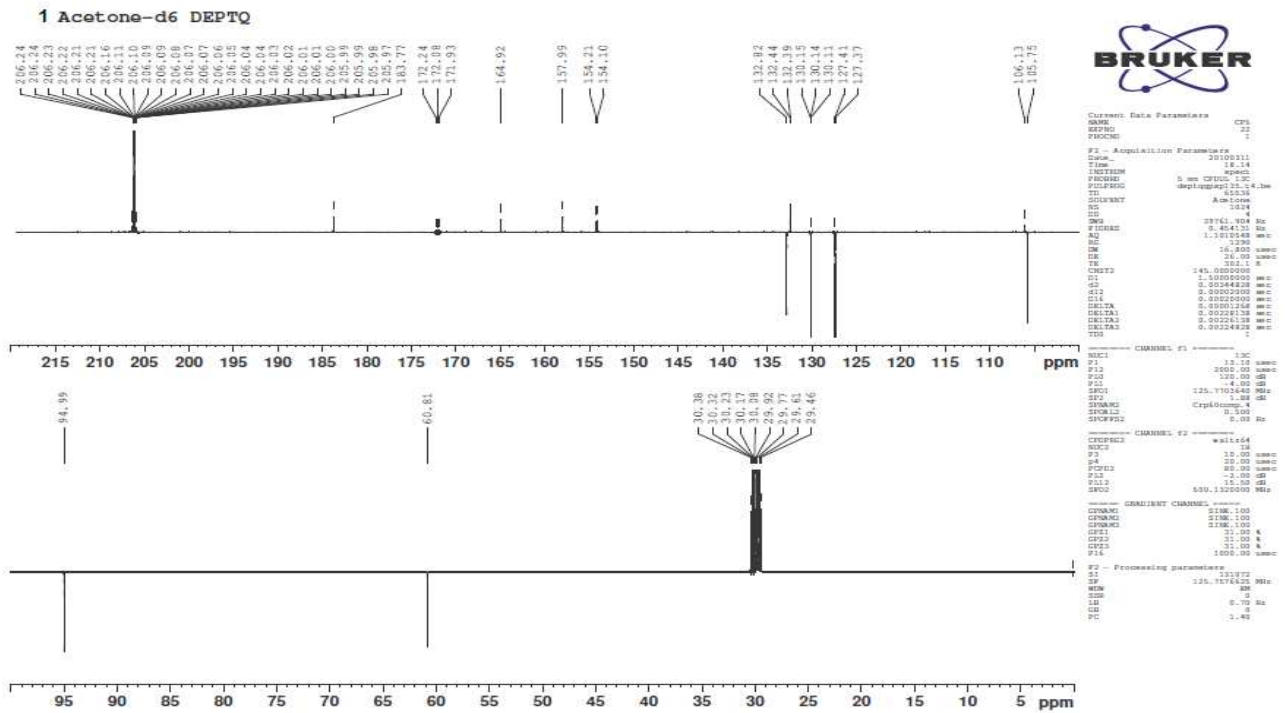
S7: ^1H NMR spectrum of compound 7 (Taraxasterol)



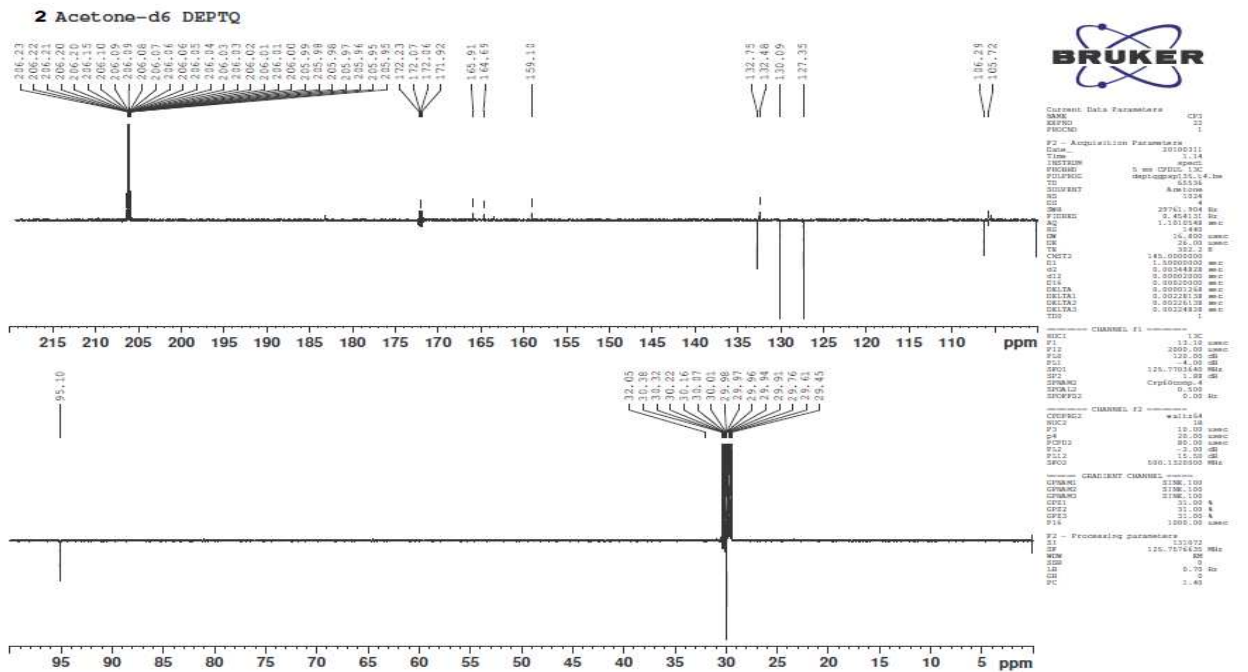
S8: ^1H NMR spectrum of compound 8 (Daucosterol)



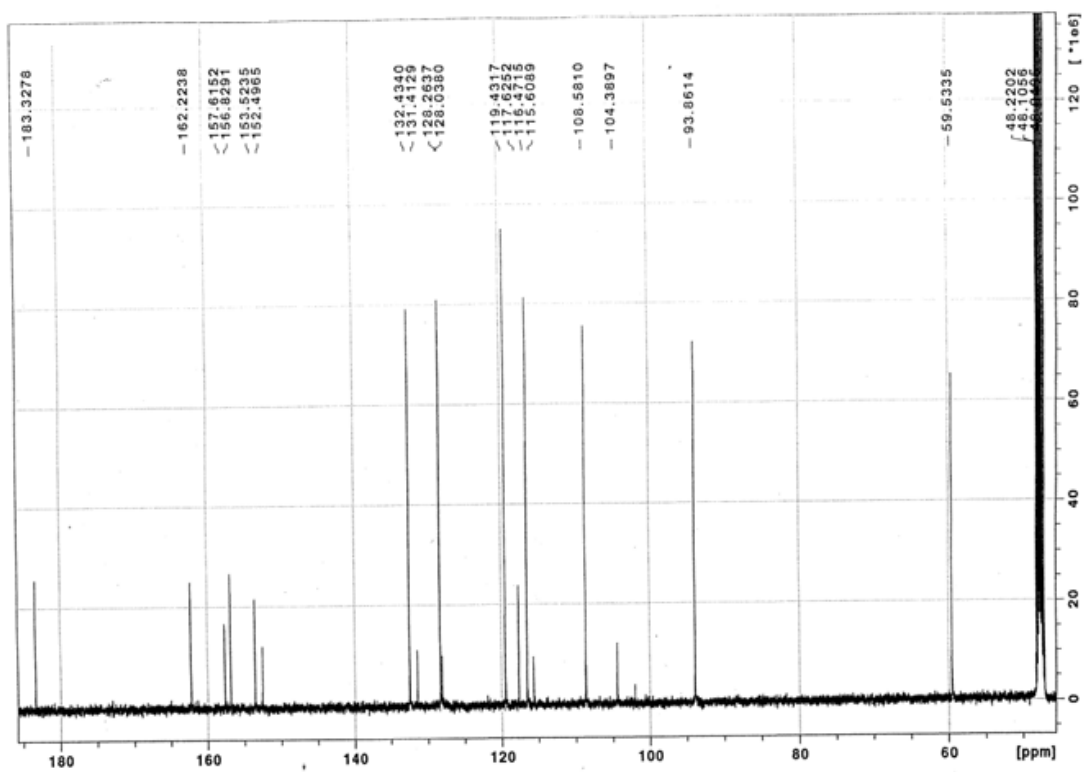
S9: ^1H NMR spectrum of compound 9 (β -sitosterol)



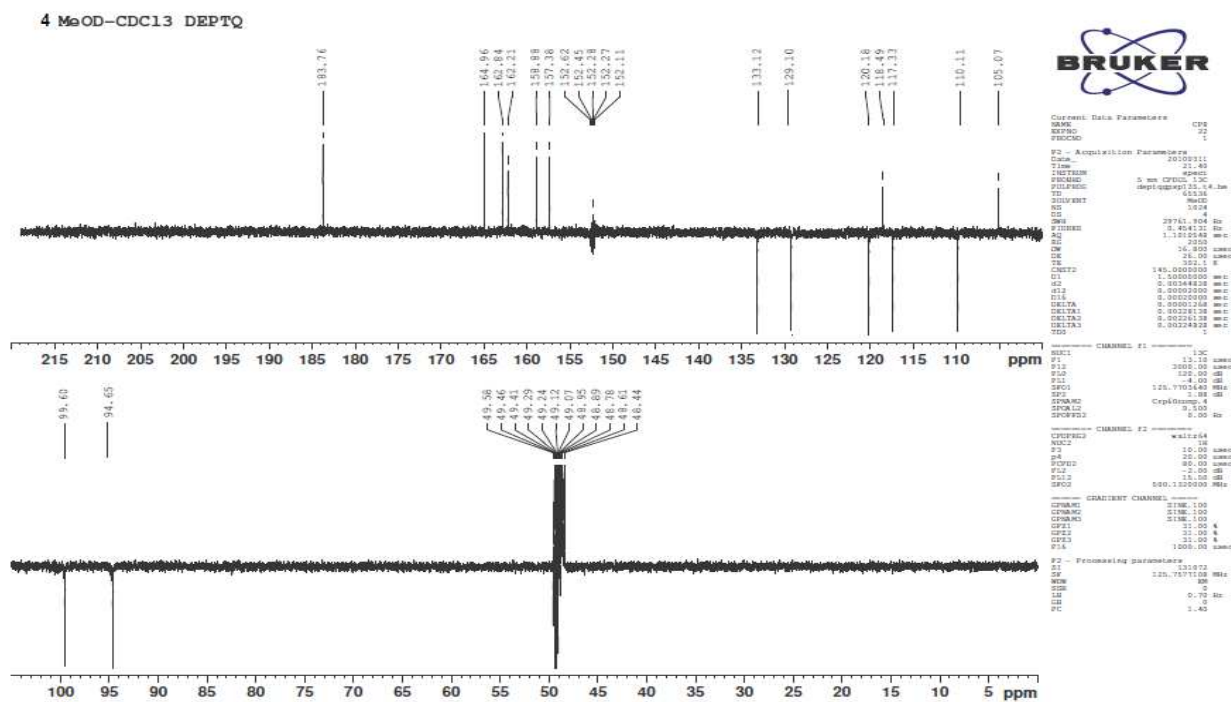
S10: ^{13}C NMR spectrum of compound 1 (Oroxilin 1)

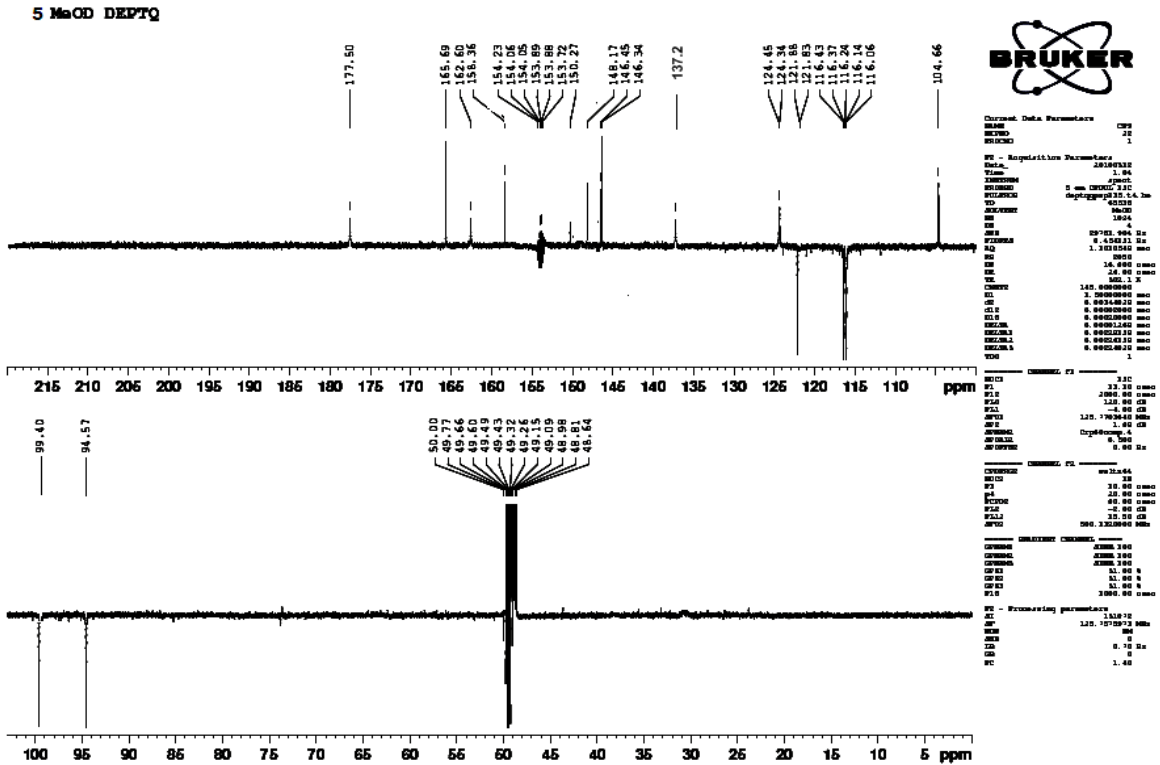


S11: ^{13}C NMR spectrum of compound 2 (Chrysin)

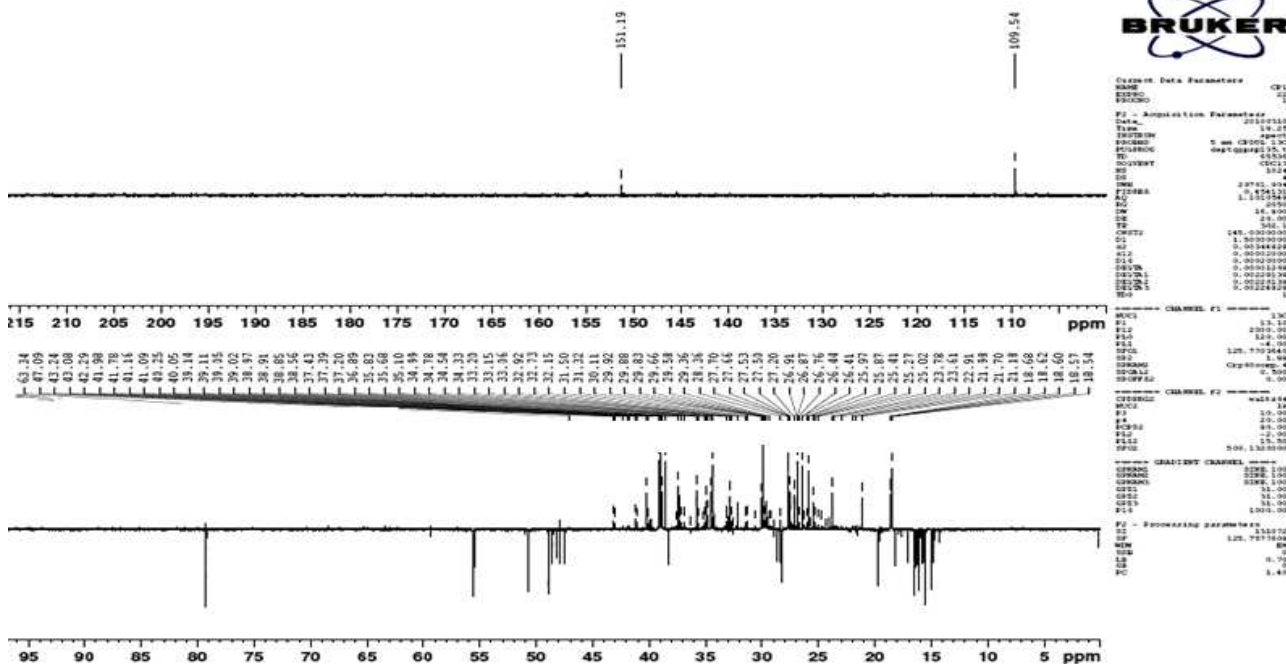


S12: ^{13}C NMR spectrum of compound 3 (Tenaxin II)

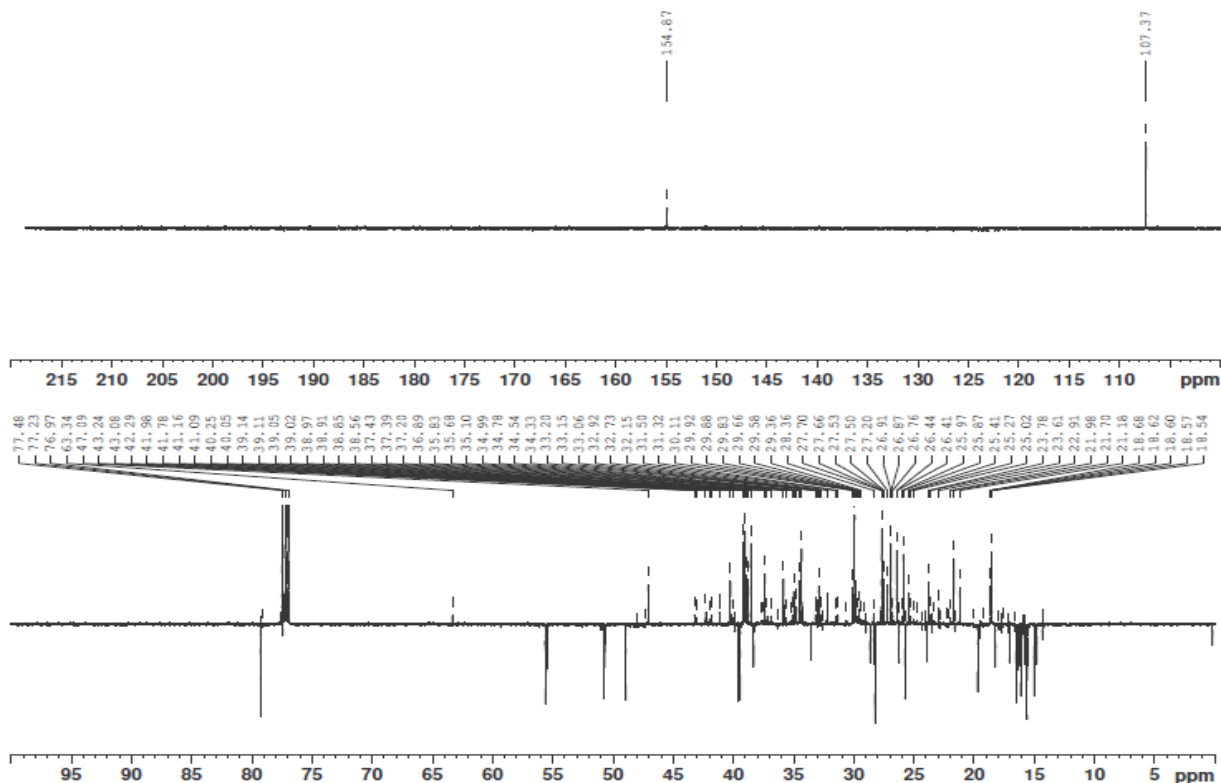




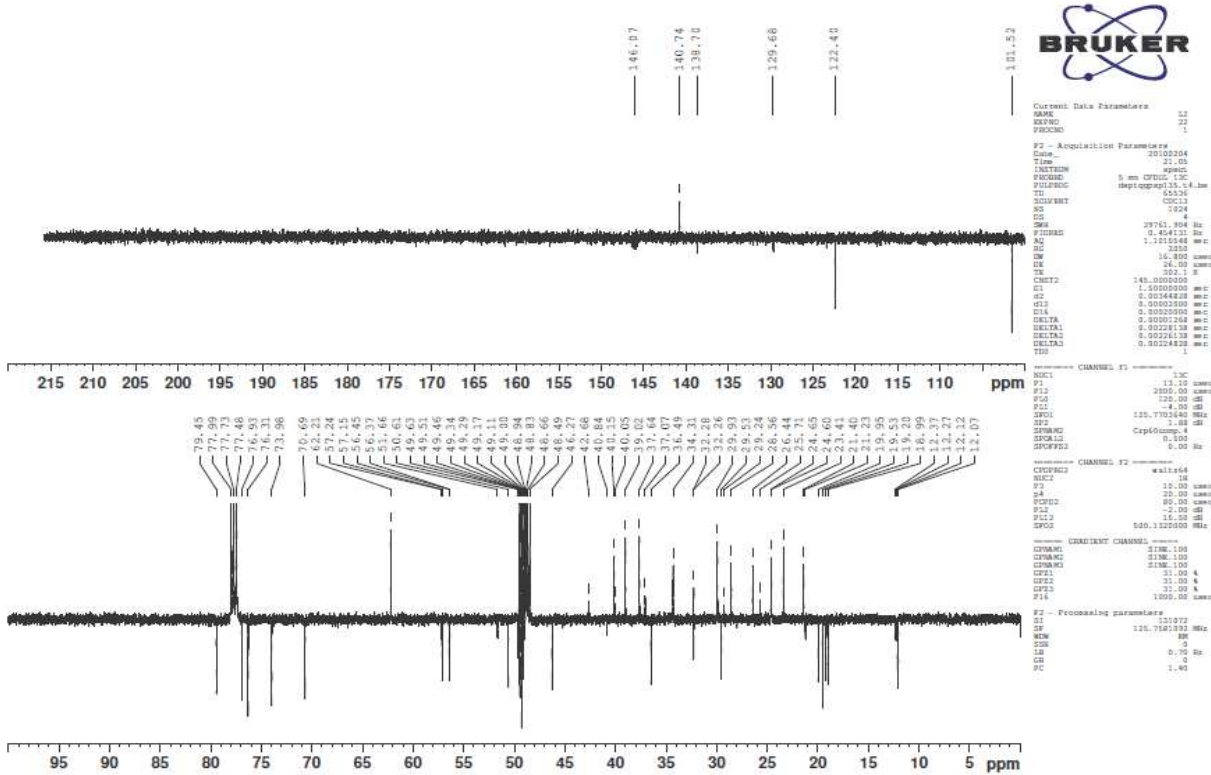
S14: ^{13}C NMR spectrum of compound 5 (Quercetin)



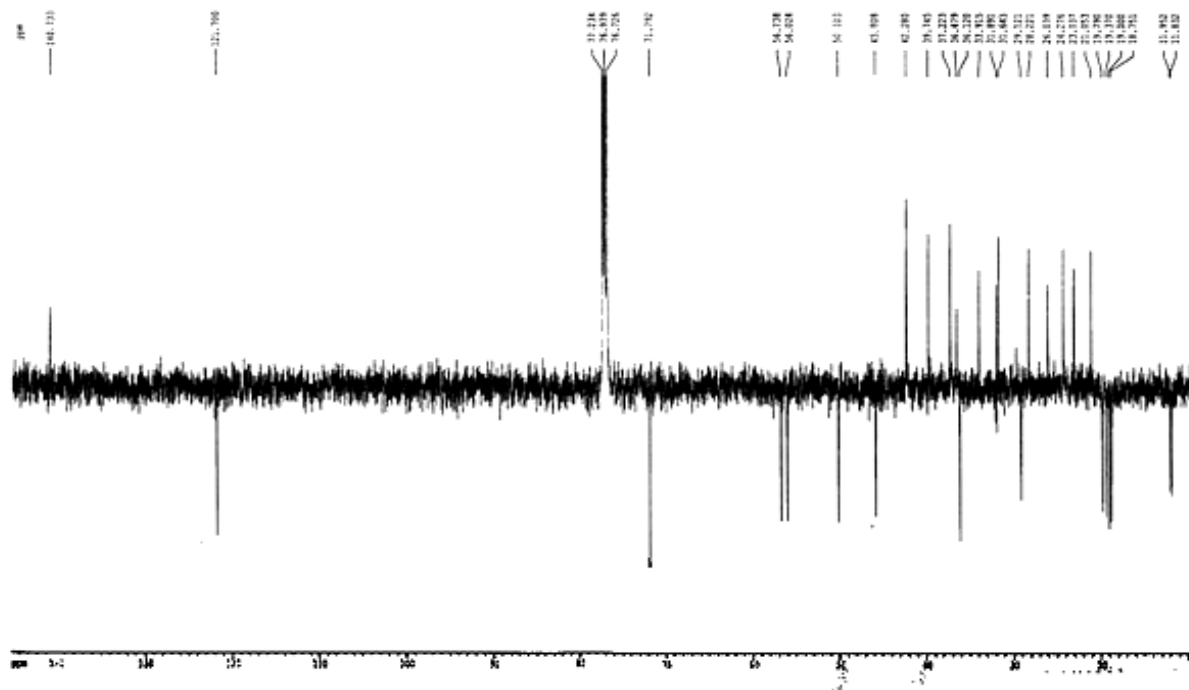
S15: ^{13}C NMR spectrum of compound 6 (Lupeol)



S16: ^{13}C NMR spectrum of compound 7 (Taraxasterol)



S17: ^{13}C NMR spectrum of compound 8 (Daucosterol)



S18: ^{13}C NMR spectrum of compound 9 (β -sitosterol)

Mass Spectrum List Report

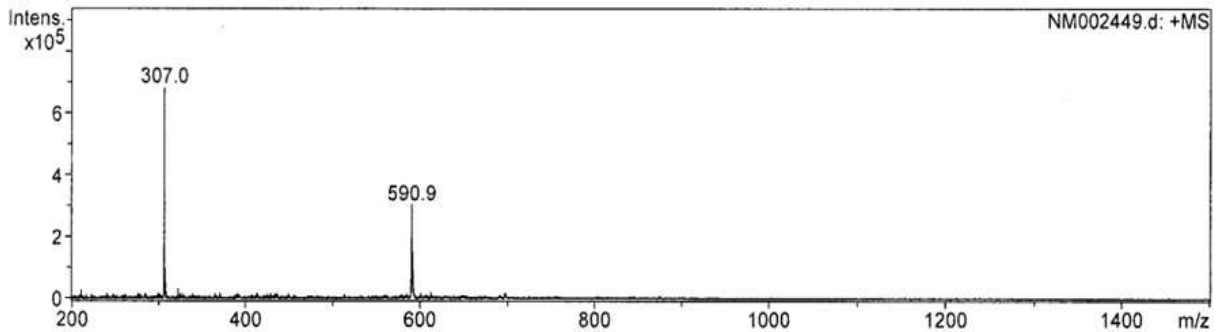
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Comment

Acquisition Date 03/10/10 15:17:51
Operator LONG Christophe
Instrument Esquire-LC_00088

Acquisition Parameter

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S19: ESI-MS (positive mode) of compound 1 (Oroxylin A)

Mass Spectrum List Report

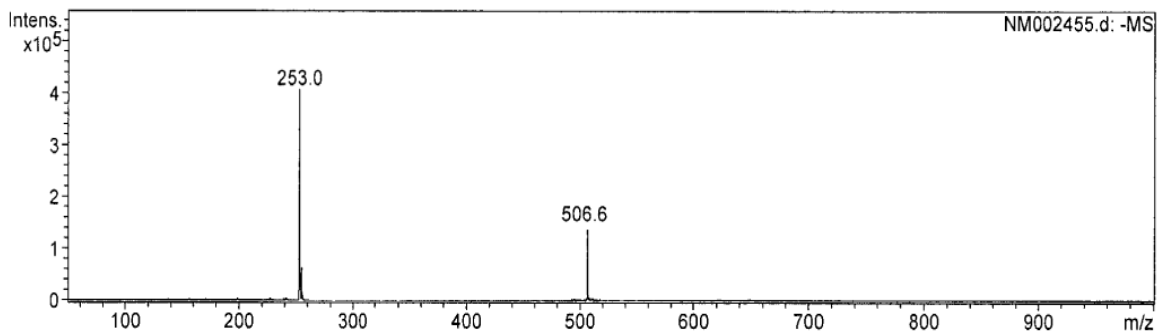
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Analysis Name NM002455.d
Method infusion.MS
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Comment

Acquisition Date 03/10/10 15:27:17
Operator LONG Christophe
Instrument Esquire-LC_00088

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Negative	Alternating Ion Polarity	n/a
Mass Range Mode	Std/Normal	Scan Begin	50.00 m/z	Scan End	1000.00 m/z
Capillary Exit	-96.0 Volt	Skim 1	-26.1 Volt	Trap Drive	38.3
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S20: ESI-MS (negative mode) of compound 2 (Chrysin)

Mass Spectrum List Report

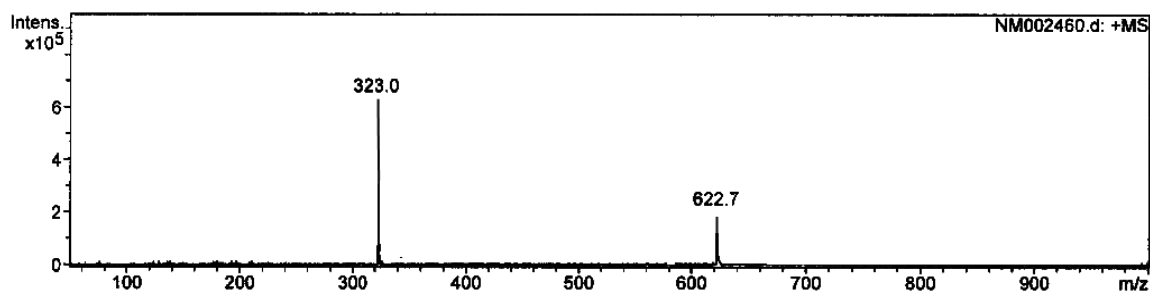
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Method infusion.MS
Sample Name 3
Comment

Acquisition Date 03/10/10 15:32:57
Operator LONG Christophe
Instrument Esquire-LC_00088

Acquisition Parameter

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Mass Range Mode	Std/Normal	Scan Begin	50.00 m/z	Scan End	1000.00 m/z
Capillary Exit	90.8 Volt	Skim 1	22.1 Volt	Trap Drive	34.9
Accumulation Time	737 μ s	Averages	10 Spectra	Auto MS/MS	Off



S21: ESI-MS (positive mode) of compound 3 (Tenaxin II)

Mass Spectrum List Report

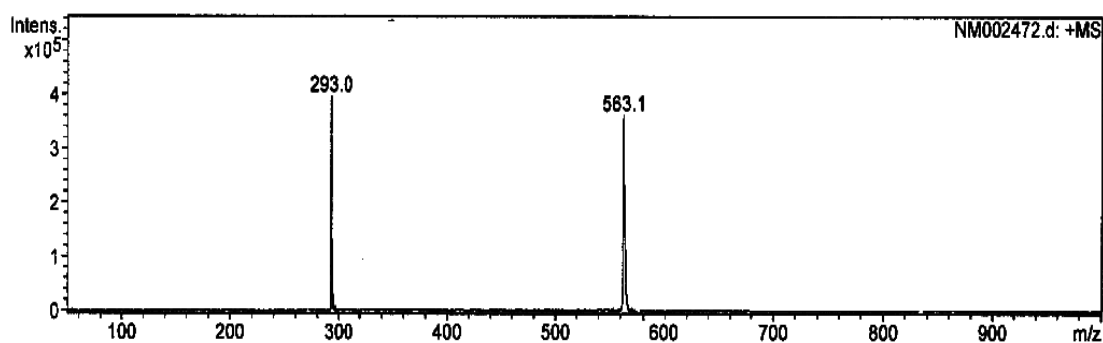
Analysis Info

Analysis Name NM002472.d
Method infusion.MS
Sample Name 4
Comment

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Operator LONG Christophe
Instrument Esquire-LC_00088

Acquisition Parameter

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Capillary Exit	116.8 Volt	Skim 1	40.8 Volt	Trap Drive	34.9
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S22: ESI-MS (positive mode) of compound 4 (5,7,2'-trihydroxyflavone)

Mass Spectrum List Report

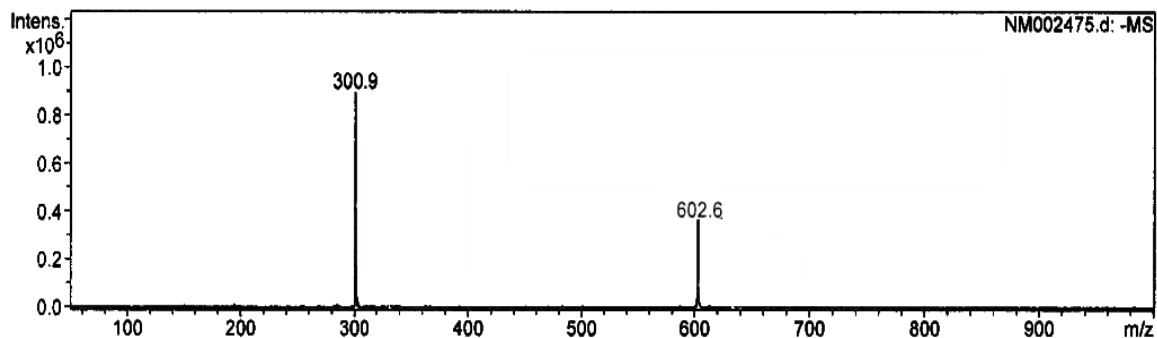
Analysis Info

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Method infusion.MS
Sample Name 5
Comment

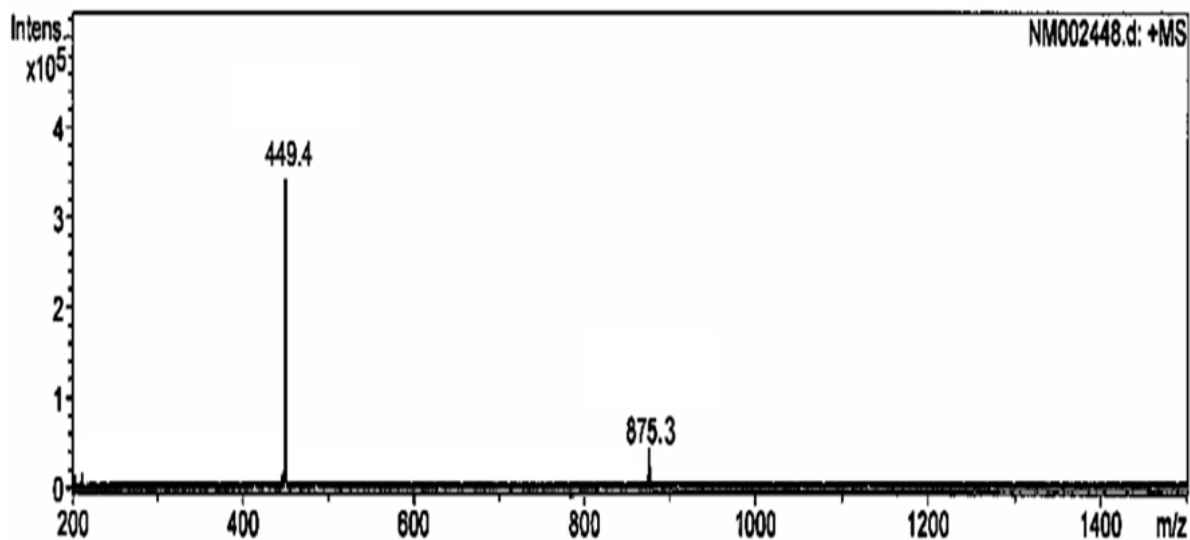
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Operator LONG Christophe
Instrument Esquire-LC_00088

Acquisition Parameter

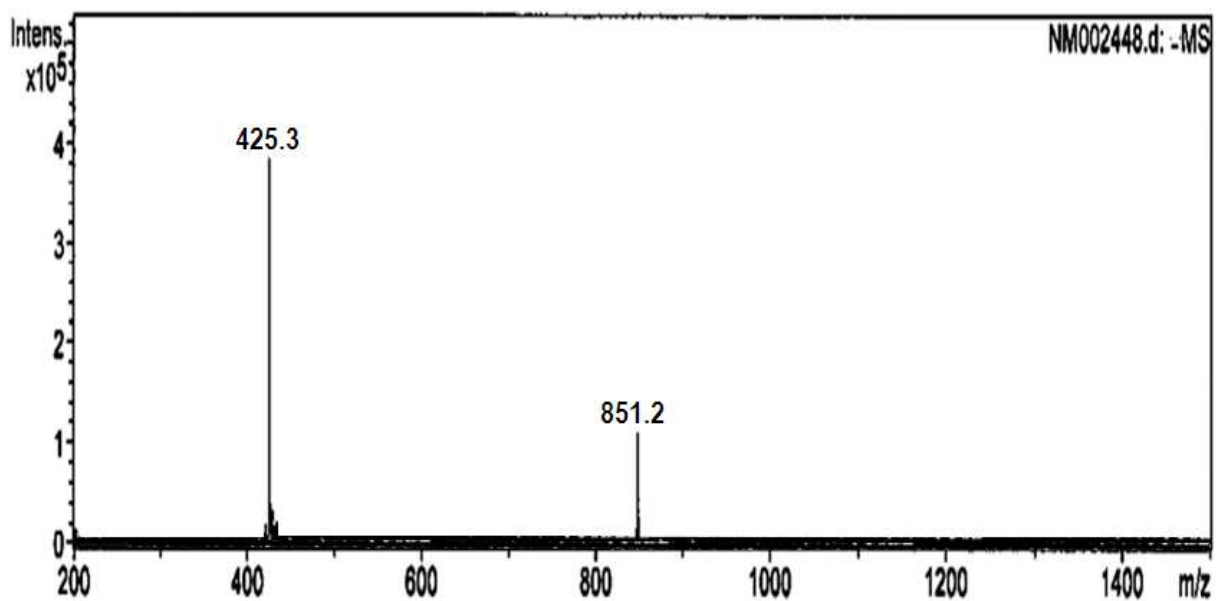
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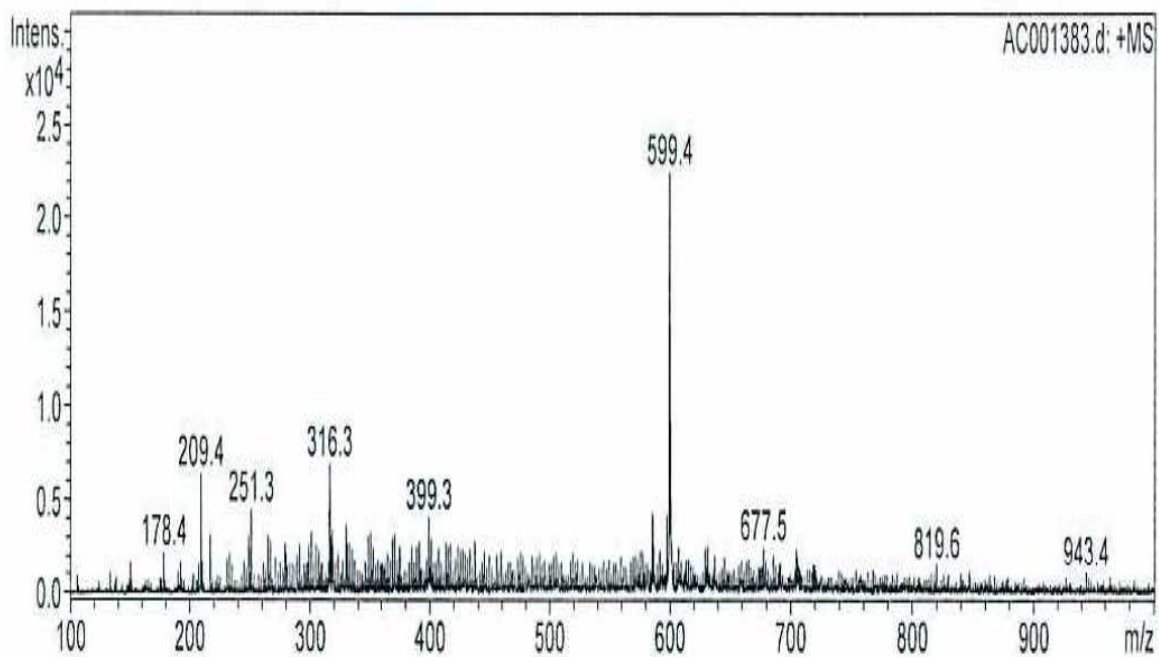
S23: ESI-MS (negative mode) of compound 5 (Quercetin)



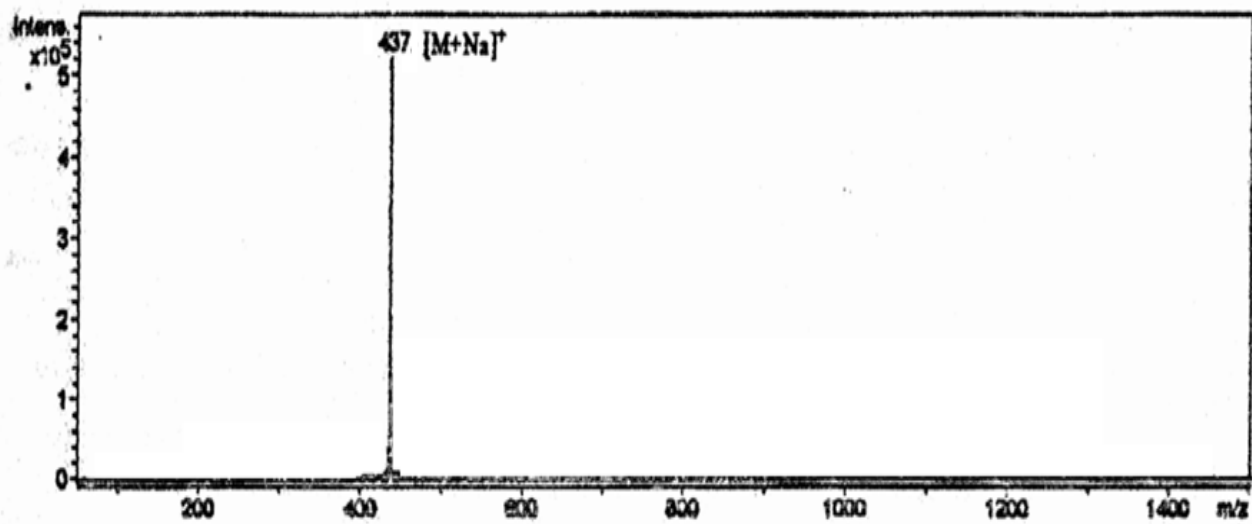
S24: ESI-MS (positive mode) of compound 6 (Lupeol)



S25: ESI-MS (negative mode) of compound 7 (Taraxasterol)



S26: ESI-MS (positive mode) of compound 8 (Daucosterol)



S27: ESI-MS (positive mode) of compound 9 (β -sitosterol)

Spectroscopic data of 1-9

Oroxylin A (1): Slightly yellow Crystals; MP. 219 °C; UV (AlCl₃+MeOH): λ_{\max} (log ϵ): 339 (1.75), 283 (3.26); IR ν_{\max} (KBr): = 3406, 1656, 3090, 1600, 1571, 1500 cm⁻¹; ¹H NMR (500 MHz, Acetone-d₆): δ (ppm) = 3.89 (3H, s, OCH₃), 6.67 (1H, s, H-8), 6.79 (1H, s, H-3), 7.58 (2H, m, H-3', H-5'), 7.61 (1H, m, H-4'), 8.07 (2H, dd, J = 8.1; 1.8 Hz, H-2', H-6'), 9.16 (1H, s, OH), 13.11 (1H, s, OH); ¹³C NMR (125MHz, Acetone-d₆): δ (ppm) = 60.8 (CH₃, OMe), 95.0 (CH, C-8), 105.8 (CH, C-3), 106.1 (C, C-10), 127.4 (CH, C-2', C-6'), 130.1 (CH, C-3', C-5'), 132.4 (C, C-1' and C-6), 132.8 (CH, C-4'), 154.1 (C, C-5), 154.2 (C, C-9), 158.0 (C, C-7), 164.9 (C, C-2), 183.8 (C, C-4); ESI-MS: m/z 307.0 [M+Na]⁺, 590.9 [2M+Na]⁺ for formula C₁₆H₁₂O₅.

Chrysin (2): Slightly yellow Crystals; MP. 206 °C; UV (AlCl₃+MeOH): λ_{\max} (log ϵ): 389 (0.07), 276(0.71); IR ν_{\max} (KBr): = 3406, 1656, 3090, 1600, 1571, 1500 cm⁻¹; ¹H NMR (500 MHz, Acetone-d₆): δ (ppm) = 6.28 (1H, d, J = 1,9 Hz, H-6), 6.57 (1H, d, J = 1,9 Hz, H-8), 6.76 (1H, s, H-3), 7.58 (2H, m, H-3', H-5'), 7.60 (1H, m, H-4'), 8.05 (2H, dd, J = 8.1; 1.8 Hz, H-2', H-6'), 12.88 (1H, sl, OH); ¹³C NMR (125MHz, Acetone-d₆): δ (ppm) = 95.1 (CH, C-8), 100.0 (CH, C-6), 105.7 (C, C-10), 106.3 (CH, C-3), 127.4 (CH, C-2', C-6'), 130.1(CH, C-3' and C-5'), 132.5 (C, C-1'), 132.8 (CH, C-4'), 159.1 (C, C-9), 163.1(C, C-5), 164.7 (C, C-2), 165.9 (C, C-7), 183.1 (C, C-4); ESI-MS: m/z 253.0 [M-H]⁻, 506.6 [2M-H]⁻ for formula C₁₅H₁₀O₄.

Tenaxin II (3): Slightly yellow Crystals; MP. 271 °C; UV (AlCl₃ + MeOH): λ_{\max} (log ϵ): 376 (0.18), 282(2.29); IR ν_{\max} (KBr): = 3468, 3144, 1664 cm⁻¹; ¹H NMR (500 MHz, CD₃OD): δ (ppm) = 3.91 (3H, s, OCH₃), 6.57 (1H, s, H-8), 6.99 (1H, dd, J = 8.3; 1.3 Hz, H-3'), 7.03 (1H, td, J = 8.3; 1.3 Hz, H-5'), 7.21 (1H, s, H-3), 7.38 (1H, td, J = 8.3; 1.3 Hz, H-4'), 7.89 (1H, dd, J = 8.3; 1.3 Hz, H-6'); ¹³C NMR (125MHz, CD₃OD): δ (ppm) = 59.5 (CH₃, OMe), 93.9 (CH, C-8), 104.4 (C, C-10), 108.6 (CH, C-3), 116.5 (CH, C-3'), 117.6 (C, C-1'), 119.4 (CH, C-5'), 128.3 (CH, C-6'), 131.4 (C, C-6), 132.4 (CH, C-4'), 152.5 (C, C-5), 153.5 (C, C-9), 156.8 (C, C-2'), 157.6 (C, C-7), 162.2 (C, C-2), 183.3 (C, C-4); ESI-MS: m/z 323.0 [M+Na]⁺, 622.7 [2M+Na]⁺ for formula C₁₆H₁₂O₆.

5,7,2'-trihydroxyflavone (4): White powder; MP. 258 °C; UV (AlCl₃ + MeOH): λ_{\max} (log ϵ): 389 (0.5), 276 (2.05); IR ν_{\max} (KBr): = 3315, 1656, 3074, 1617, 1571, 1500 cm⁻¹; ¹H NMR (500 MHz, CD₃OD-CDCl₃): δ (ppm) = 6.27 (1H, d, J = 2.0 Hz, H-6), 6.46 (1H, d, J

= 2.0 Hz, H-8), 6.89 (1H, dd, $J = 8.2$; 1.2 Hz, H-3'), 7.01 (1H, td, $J = 8.2$; 1.2 Hz, H-5'), 7.22 (1H, s, H-3), 7.35 (1H, td, $J = 8.2$; 1.2 Hz, H-4'), 7.86 (1H, dd, $J = 8.2$; 1.2 Hz, H-6'); ^{13}C NMR (125 MHz, $\text{CD}_3\text{OD}-\text{CDCl}_3$): δ (ppm) = 94.7 (CH, C-8), 99.6 (CH, C-6), 105.1 (C, C-10), 110.1 (CH, C-3), 117.3 (CH, C-3'), 118.5 (C, C-1'), 120.2 (CH, C-5'), 129.1 (CH, C-6'), 133.1 (CH, C-4'), 157.4 (C, C-2'), 158.9 (C, C-9), 162.2 (C, C-5), 162.8 (C, C-2), 165.0 (C, C-7), 183.8 (C, C-4); ESI-MS: m/z 293.0 $[\text{M}+\text{Na}]^+$, 563.1 $[2\text{M}+\text{Na}]^+$ for formula $\text{C}_{15}\text{H}_{10}\text{O}_4$.

Quercetin (5): Slightly yellow powder; MP. 316 °C; UV ($\text{AlCl}_3+\text{MeOH}$): λ_{max} (log ϵ): 484 (2.86), 272(2.79); IR ν_{max} (KBr): = 3500, 1662, 1614, 1512 cm^{-1} ; ^1H NMR (500 MHz, MeOD): δ (ppm) = 6.18 (1H, *d*, $J = 2.0$ Hz, H-6), 6.39 (1H, *d*, $J = 2.0$ Hz, H-8), 6.88 (1H, *d*, $J = 8.3$ Hz, H-5'), 7.62 (1H, *dd*, $J = 8.3$; 2.1 Hz, H-6'), 7.74 (1H, *d*, $J = 2.1$ Hz, H-2'), ^{13}C NMR (125MHz, MeOD): δ (ppm) = 94.6 (CH, C-8), 99.4 (CH, C-6), 104.7 (C, C-10), 116.1 (CH, C-2', C-5'), 121.8 (CH, C-6'), 124.3 (C, C-1'), 137.2 (C, C-3), 146.3 (C, C-3'), 148.2 (C, C-2), 150.3 (C, C-4'), 158.4 (C, C-9), 162.6 (C, C-5), 165.7 (C, C-7), 177.5 (C, C-4); ESI-MS: m/z 300.9 $[\text{M}-\text{H}]^-$, 602.6 $[2\text{M}-\text{H}]^-$ for formula $\text{C}_{15}\text{H}_{10}\text{O}_7$.

Lupeol (6): White powder; MP. 215 °C; : $[\alpha]_{\text{D}} = +26,4$ ($c = 0.4$, CHCl_3); ^1H NMR (500 MHz, CDCl_3): δ (ppm) = 0.69 (1H, *m*, H-5), 0.77 (1H, *s*, H-24), 0.80 (1H, *s*, H-28), 0.84 (1H, *s*, H-25), 0.94 (1H, *m*, H-1b), 0.96 (1H, *m*, H-15b), 0.96 (1H, *s*, H-27), 0.97 (1H, *s*, H-23), 1.04 (1H, *s*, H-26), 1.10 (1H, *m*, H-12b), 1.19 (1H, *m*, H-22), 1.27 (1H, *m*, H-21), 1.29 (1H, *m*, H-11b), 1.30 (1H, *m*, H-9), 1.38 (1H, *m*, H-7), 1.39 (1H, *m*, H-6b), 1.39 (1H, *m*, H-18), 1.43 (1H, *m*, H-11a), 1.48 (1H, *m*, H-16), 1.52 (1H, *m*, H-6a), 1.61 (1H, *m*, H-15a), 1.61 (1H, *m*, H-2), 1.62 (1H, *m*, H-13), 1.64 (1H, *m*, H-1a), 1.70 (1H, *m*, H-12a), 1.70 (1H, *sl*, H-30), 2.38 (1H, *m*, H-19), 3.18 (1H, *dd*, $J = 11.0$; 5.3 Hz, H-3), 4.56 (1H, *sl*, H-29b), 4.68 (1H, *sl*, H-29a); ^{13}C NMR (125MHz, CDCl_3): δ (ppm) = 14.8 (CH_3 , C-27), 15.6 (CH_3 , C-24), 16.1 (CH_3 , C-26), 16.2 (CH_3 , C-25), 18.1 (CH_3 , C-28), 19.0 (CH_2 , C-6), 19.8 (CH_3 , C-30), 21.2 (CH_2 , C-11), 25.3 (CH_2 , C-12), 27.2 (CH_2 , C-15), 27.5 (CH_2 , C-2), 28.4 (CH_3 , C-23), 30.1 (CH_2 , C-21), 34.2 (CH_2 , C-7), 35.9 (CH_2 , C-16), 37.2 (C, C-10), 38.5 (CH, C-13), 38.7 (CH_2 , C-1), 39.8 (C, C-4), 40.3 (CH_2 , C-22), 41.1 (C, C-8), 42.8 (C, C-14), 43.2 (C, C-17), 47.8 (CH, C-19), 48.5 (CH, C-18), 50.9 (CH, C-9), 55.5 (CH, C-5), 79.3 (CH, C-3), 109.5 (CH_2 , C-29), 151.2 (C, C-20); ESI-MS: m/z 449.4 $[\text{M}+\text{Na}]^+$, 875.3 $[2\text{M}+\text{Na}]^+$ for formula $\text{C}_{30}\text{H}_{50}\text{O}$.

Taraxasterol (7): White powder; MP. 226 °C; : $[\alpha]_{\text{D}} = +95$ ($c = 0.36$, CHCl_3); ^1H NMR (500 MHz, CDCl_3): δ (ppm) = 0.70 (1H, *m*, H-5), 0.77 (1H, *s*, H-24), 0.84 (1H, *s*, H-25), 0.86 (1H, *s*, H-28), 0.93 (1H, *s*, H-27), 0.96 (1H, *m*, H-1b), 0.96 (1H, *m*, H-18), 0.97 (1H, *m*, H-15b), 0.98 (1H, *s*, H-23), 1.01 (1H, *d*, $J = 7.1$ Hz, H-29), 1.02 (1H, *s*, H-26),

1.13 (1H, *m*, H-12b), 1.17 (1H, *m*, H-16b), 1.23 (1H, *m*, H-16a), 1.27 (1H, *m*, H-11b), 1.32 (1H, *sl*, H-9), 1.37 (1H, *m*, H-22), 1.38 (1H, *m*, H-6b), 1.39 (1H, *m*, H-7), 1.53 (1H, *m*, H-6a), 1.54 (1H, *m*, H-11a), 1.59 (1H, *m*, H-13), 1.61 (1H, *m*, H-2), 1.68 (1H, *m*, H-12a), 1.68 (1H, *m*, H-15a), 1.71 (1H, *m*, H-1a), 2.08 (1H, *quint*, $J = 6.8$ Hz, H-19), 2.19 (1H, *m*, H-21b), 2.43 (1H, *m*, H-21a), 3.20 (1H, *m*, H-3), 4.60 (1H, *sl*, H-30b), 4.62 (1H, *sl*, H-30a); ^{13}C NMR (125MHz, CDCl_3): δ (ppm) = 14.8 (CH_3 , C-27), 15.4 (CH_3 , C-24), 15.9 (CH_3 , C-26), 16.3 (CH_3 , C-25), 18.5 (CH_2 , C-6), 19.6 (CH_3 , C-28), 21.2 (CH_2 , C-11), 25.6 (CH_3 , C-29), 25.9 (CH_2 , C-21), 26.4 (CH_2 , C-12), 26.9 (CH_2 , C-15), 28.2 (CH_3 , C-23), 34.2 (CH_2 , C-7), 34.5 (C, C-17), 37.1 (C, C-10), 37.4 (CH_2 , C-2), 38.3 (CH_2 , C-16), 38.8 (CH_2 , C-1), 38.9 (C, C-4), 38.9 (CH_2 , C-22), 39.2 (CH, C-13), 39.6 (CH, C-19), 40.3 (C, C-8), 42.0 (C, C-14), 48.7 (CH, C-18), 50.5 (CH, C-9), 55.5 (CH, C-5), 79.0 (CH, C-3), 107.4 (CH_2 , C-30), 154.9 (C, C-20); ESI-MS: m/z 425.3 $[\text{M}-\text{H}]^-$, 851.2 $[2\text{M}-\text{H}]^-$ for formula $\text{C}_{30}\text{H}_{50}\text{O}$.

Daucosterol (**8**): White powder; MP. 285 °C; : $[\alpha]_{\text{D}} = -41.5$ ($c = 0.4$, MeOH); ^1H NMR (500 MHz, $\text{CDCl}_3 + \text{CD}_3\text{OD}$): δ (ppm) = 0.70 (1H, *s*, H-18), 0.83 (1H, *d*, $J = 6.9$ Hz, H-27), 0.85 (1H, *t*, $J = 7.4$ Hz, H-29), 0.93 (1H, *m*, H-24), 0.94 (1H, *d*, $J = 5.3$ Hz, H-26), 0.95 (1H, *d*, $J = 5.1$ Hz, H-21), 0.96 (1H, *m*, H-9), 1.02 (1H, *m*, H-11b), 1.03 (1H, *s*, H-19), 1.03 (1H, *m*, H-14), 1.04 (1H, *m*, H-22b), 1.08 (1H, *m*, H-1b), 1.11 (1H, *m*, H-15b), 1.14 (1H, *m*, H-17), 1.17 (1H, *m*, H-12b), 1.19 (1H, *m*, H-23), 1.26 (1H, *m*, H-28), 1.29 (1H, *m*, H-16b), 1.34 (1H, *m*, H-22a), 1.37 (1H, *m*, H-20), 1.45 (1H, *m*, H-11a), 1.47 (1H, *m*, H-7), 1.59 (1H, *m*, H-15a), 1.62 (1H, *m*, H-2b), 1.68 (1H, *m*, H-25), 1.84 (1H, *m*, H-16a), 1.88 (1H, *m*, H-1a), 1.91 (1H, *m*, H-2a), 1.97 (1H, *m*, H-8), 2.01 (1H, *m*, H-12a), 2.28 (1H, *tl*, $J = 10.0$ Hz, H-4b), 2.42 (1H, *dm*, $J = 10.0$ Hz, H-4a), 3.23 (1H, *t*, $J = 7.9$ Hz, H-2'), 3.29 (1H, *m*, H-5'), 3.42 (1H, *t*, $J = 7.9$ Hz, H-3'), 3.42 (1H, *m*, H-4'), 3.59 (1H, *m*, H-3), 3.75 (1H, *dd*, $J = 10.0; 5.0$ Hz, H-6'b), 3.84 (1H, *dl*, $J = 10.0$ Hz, H-6'a), 4.41 (1H, *d*, $J = 7.9$ Hz, H-1'), 5.37 (1H, *d*, $J = 5.0$ Hz, H-6); ^{13}C NMR (125MHz, $\text{CDCl}_3 + \text{CD}_3\text{OD}$): δ (ppm) = 12.1 (CH_3 , C-18), 12.3 (CH_3 , C-29), 18.9 (CH_3 , C-21), 19.2 (CH_3 , C-27), 19.5 (CH_3 , C-19), 19.9 (CH_3 , C-26), 21.2 (CH_2 , C-11), 23.4 (CH_2 , C-28), 24.6 (CH_2 , C-15), 26.4 (CH_2 , C-23), 28.6 (CH_2 , C-16), 29.5 (CH, C-25), 29.9 (CH_2 , C-2), 32.3 (CH_2 , C-7), 32.3 (CH, C-8), 34.3 (CH_2 , C-22), 36.5 (CH, C-20), 37.1 (C, C-10), 37.6 (CH_2 , C-1), 39.0 (CH_2 , C-4), 40.8 (CH_2 , C-12), 42.7 (C, C-13), 46.2 (CH, C-24), 50.6 (CH, C-9), 56.4 (CH, C-17), 57.2 (CH, C-14), 62.2 (CH_2 , C-6'), 70.7 (CH, C-4'), 74.0 (CH, C-2'), 76.3 (CH, C-5'), 76.9 (CH, C-3'), 79.5 (CH, C-3), 101.5 (CH, C-1'), 122.4 (CH, C-6), 140.7 (C, C-5); ESI-MS: m/z 599.4 $[\text{M}+\text{Na}]^+$ for formula $\text{C}_{35}\text{H}_{60}\text{O}$.

β-sitosterol (9): White powder; MP. 136 °C; : $[\alpha]_D = -30$ ($c = 0.8$, CHCl_3); ^1H NMR (500 MHz, CDCl_3): δ (ppm) = 0.74 (1H, *s*, H-18), 0.87 (1H, *d*, $J = 6.9$ Hz, H-27), 0.88 (1H, *d*, $J = 6.9$ Hz, H-26), 0.89 (1H, *t*, $J = 7.4$ Hz, H-29), 0.93 (1H, *d*, $J = 6.5$ Hz, H-21), 0.97 (1H, *m*, H-24), 0.98 (1H, *m*, H-9), 1.04 (1H, *m*, H-14), 1.06 (1H, *s*, H-19), 1.07 (1H, *m*, H-22b), 1.11 (1H, *tm*, $J = 11.2$ Hz, H-15b), 1.13 (1H, *m*, H-1b), 1.16 (1H, *t*, $J = 10.0$ Hz, H-17), 1.21 (1H, *m*, H-23), 1.21 (1H, *m*, H-12b), 1.30 (1H, *m*, H-16b), 1.31 (1H, *m*, H-28), 1.36 (1H, *m*, H-22a), 1.40 (1H, *m*, H-20), 1.50 (1H, *qd*, $J = 10.8$; 4.6 Hz, H-11b), 1.50 (1H, *m*, H-7), 1.55 (1H, *m*, H-11a), 1.56 (1H, *m*, H-2b), 1.63 (1H, *m*, H-15a), 1.71 (1H, *m*, H-25), 1.88 (1H, *m*, H-2a), 1.89 (1H, *m*, H-16a), 1.90 (1H, *m*, H-1a), 2.03 (1H, *td*, $J = 12.1$; 2.4 Hz, H-8), 2.06 (1H, *dt*, $J = 12.8$; 3.6 Hz, H-12a), 2.30 (1H, *td*, $J = 11.0$; 2.0 Hz, H-4b), 2.34 (1H, *ddd*, $J = 13.0$; 5.0; 2.0 Hz, H-4a), 3.58 (1H, *tt*, $J = 11.3$; 5.3 Hz, H-3), 5.40 (1H, *dd*, $J = 5.2$; 2.3 Hz, H-6); ^{13}C NMR (125MHz, CDCl_3): δ (ppm) = 11.8 (CH_3 , C-18), 12.0 (CH_3 , C-29), 18.8 (CH_3 , C-21), 19.0 (CH_3 , C-27), 19.4 (CH_3 , C-19), 19.8 (CH_3 , C-26), 21.1 (CH_2 , C-11), 23.0 (CH_2 , C-28), 24.3 (CH_2 , C-15), 26.0 (CH_2 , C-23), 28.2 (CH_2 , C-16), 29.1 (CH , C-25), 31.6 (CH_2 , C-2), 31.8 (CH , C-8), 31.9 (CH_2 , C-7), 33.9 (CH_2 , C-22), 36.1 (CH , C-20), 36.5 (C, C-10), 37.2 (CH_2 , C-1), 39.7 (CH_2 , C-12), 42.3 (CH_2 , C-4), 42.3 (C, C-13), 45.8 (CH , C-24), 50.1 (CH , C-9), 56.0 (CH , C-17), 56.7 (CH , C-14), 71.8 (CH , C-3), 121.7 (CH , C-6), 140.7 (C, C-5); ESI-MS: m/z 437 $[\text{M}+\text{Na}]^+$ for formula $\text{C}_{29}\text{H}_{50}\text{O}$.