

Supporting Information

Phytochemical Study and Antioxidant Evaluation of *Commelina erecta* (Commelinaceae) Stems

Estudo fitoquímico e avaliação antioxidante dos caules de *Commelina erecta* (Commelinaceae)

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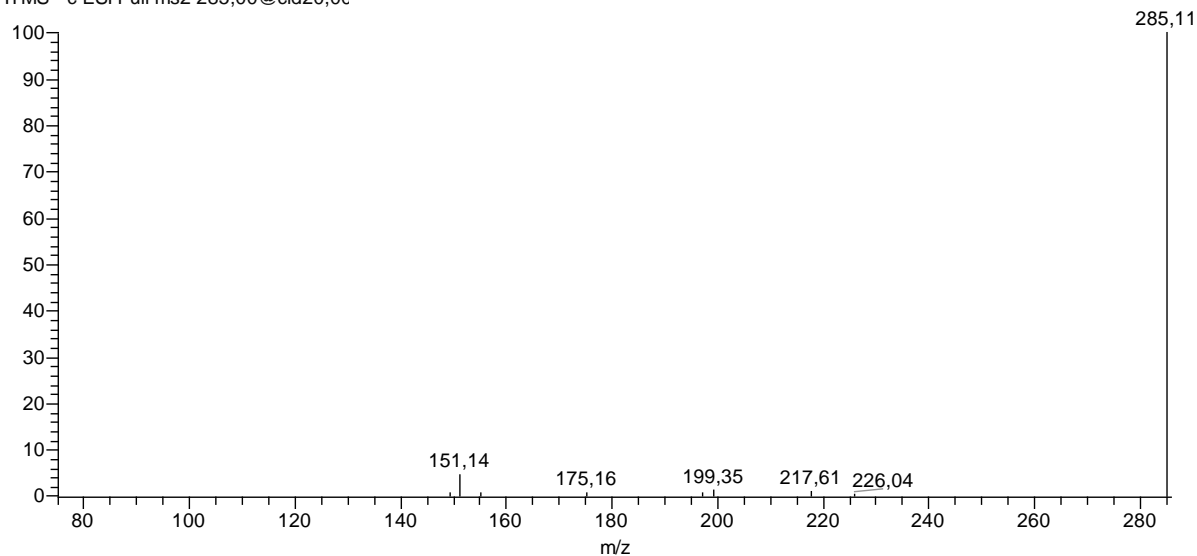
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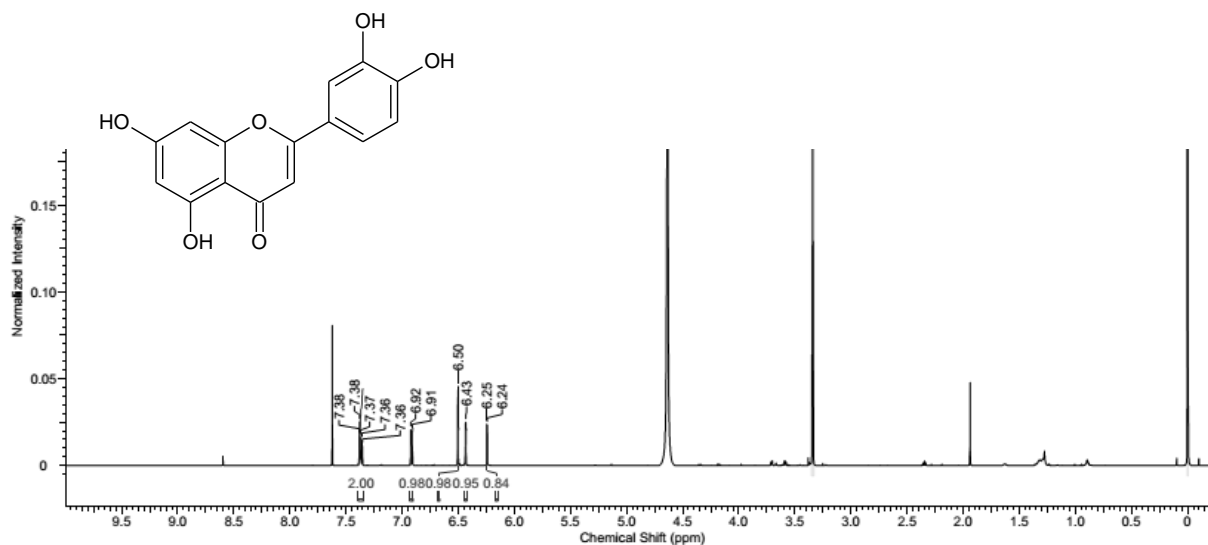
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fa jaque_130311125158 #276 RT: 3,42 AV: 1 NL: 2.23E3
T: ITMS - c ESI Full ms2 285,00@cid20,0c

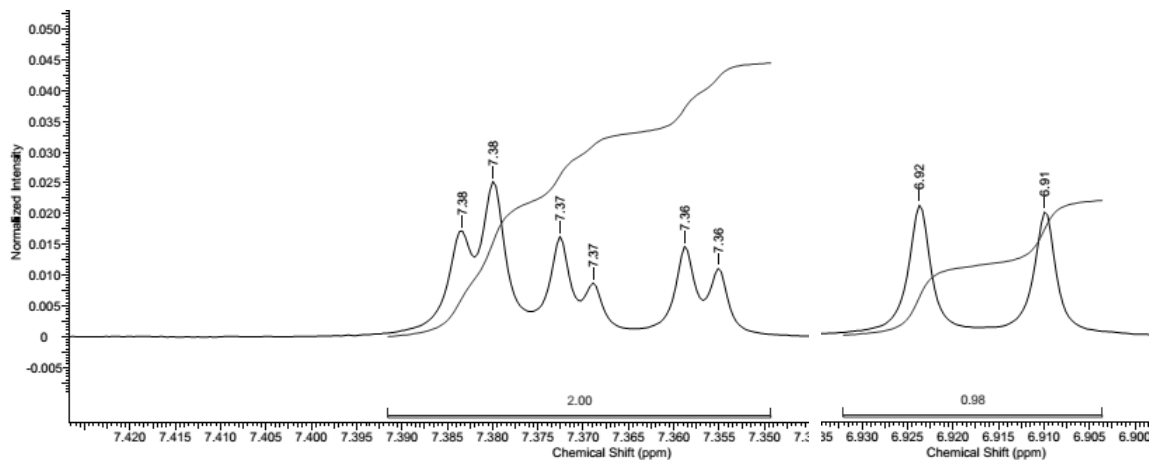


S1: MS Spectrum of Compound **1** (luteolin)

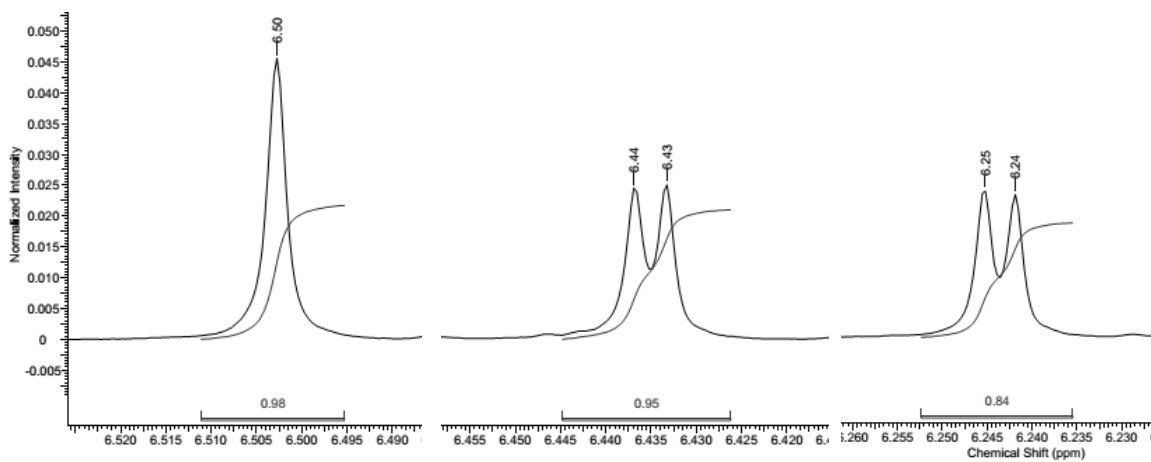


S2: ¹H-NMR (600 MHz, CDCl₃, CD₃OD) Spectrum of Compound **1** (luteolin)

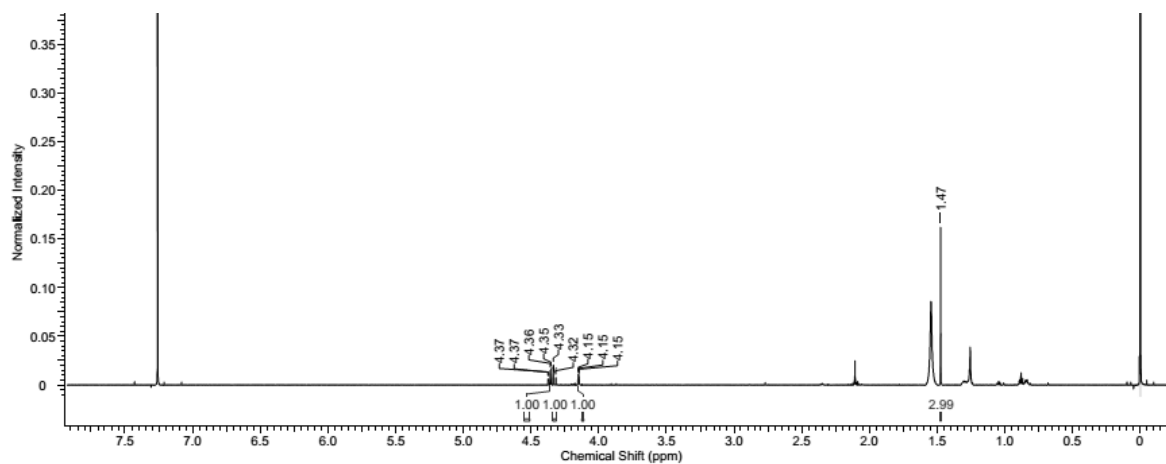
luteolin (1): yellow amorphous solid. ¹H NMR (600 MHz, CDCl₃, CD₃OD): δ (ppm) = 7.38 (d, J = 2.2 Hz, 1H, H-2'), 7.36 (dd, J = 8.2 and 2.2 Hz, 1H, H-6'), 6.92 (d, J = 8.2 Hz, 1H, H-5'), 6.24 (d, J = 2.2 Hz, 1H, H-6), 6.44 (d, J = 2.2 Hz, 1H, H-8), 6.50 (s, 1H, H-3); MS: m/z 285 [M-H]⁻ for formula C₁₅H₁₀O₆.



S3: $^1\text{H-NMR}$ Spectrum of Compound **1** (luteolin) (from 6.90 to 7.42 ppm)

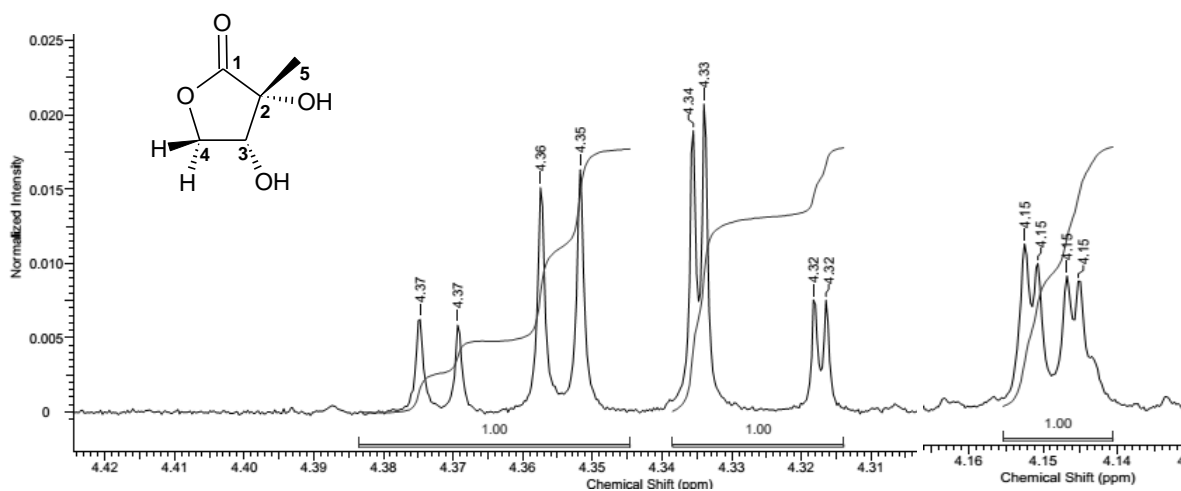


S4: $^1\text{H-NMR}$ Spectrum of Compound **1** (luteolin) (from 6.23 to 6.52 ppm)

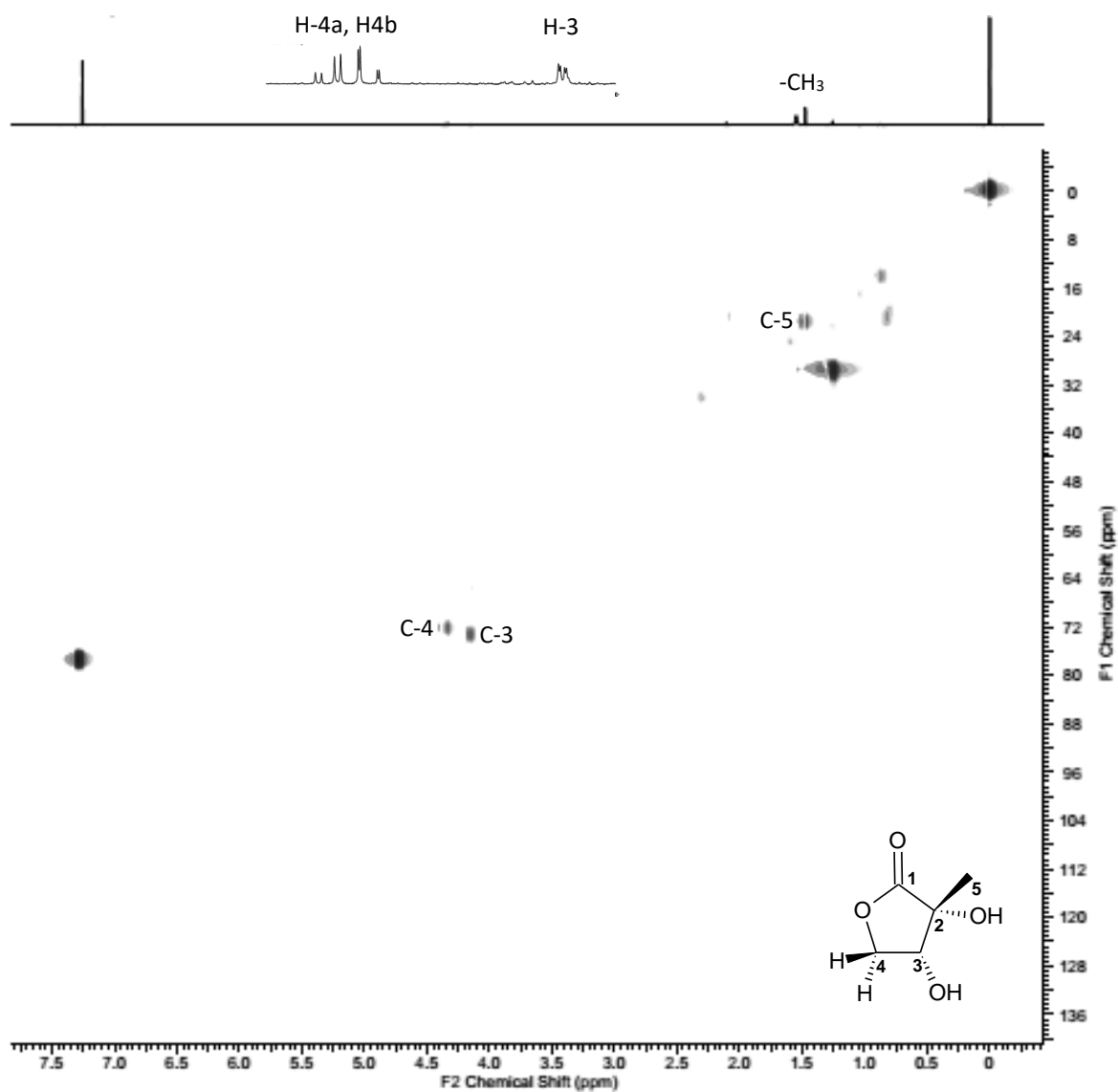


S5: $^1\text{H-NMR}$ (600 MHz, CDCl_3) Spectrum of Compound **2** (saccharinic acid lactone)

saccharinic acid lactone (2): $^1\text{H-NMR}$ (600 MHz, CDCl_3): δ (ppm) = 4.36 (dd, $J = 10.5$ and 3.4 Hz, 1H, H-4a), 4.33 (dd, $J = 10.5$ and 1.0 Hz, 1H, H-4b), 4.15 (dd, $J = 3.4$ and 1.0 Hz, 1H, H-3), 1.47 (s, 3H, CH_3 -5). $^{13}\text{C-NMR}$ (150 MHz, CDCl_3): δ (ppm) = 178.1 (C-1), 73.9 (C-3), 73.1 (C-2), 72.1 (C-4), 21.7 (C-5).

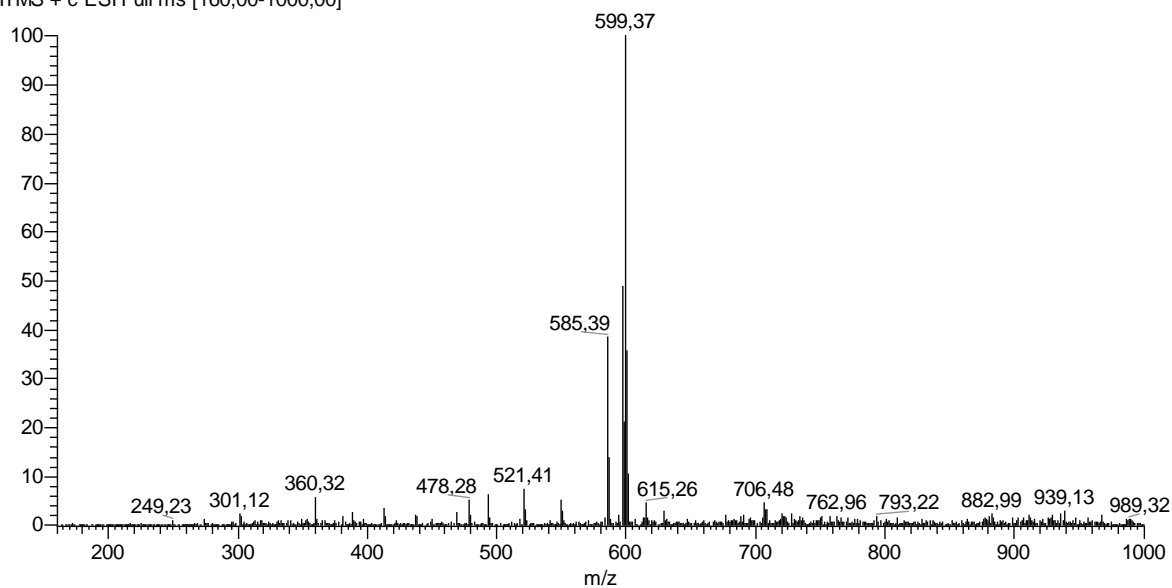


S6: $^1\text{H-NMR}$ Spectrum of Compound **2** (from 4.13 to 4.42 ppm)

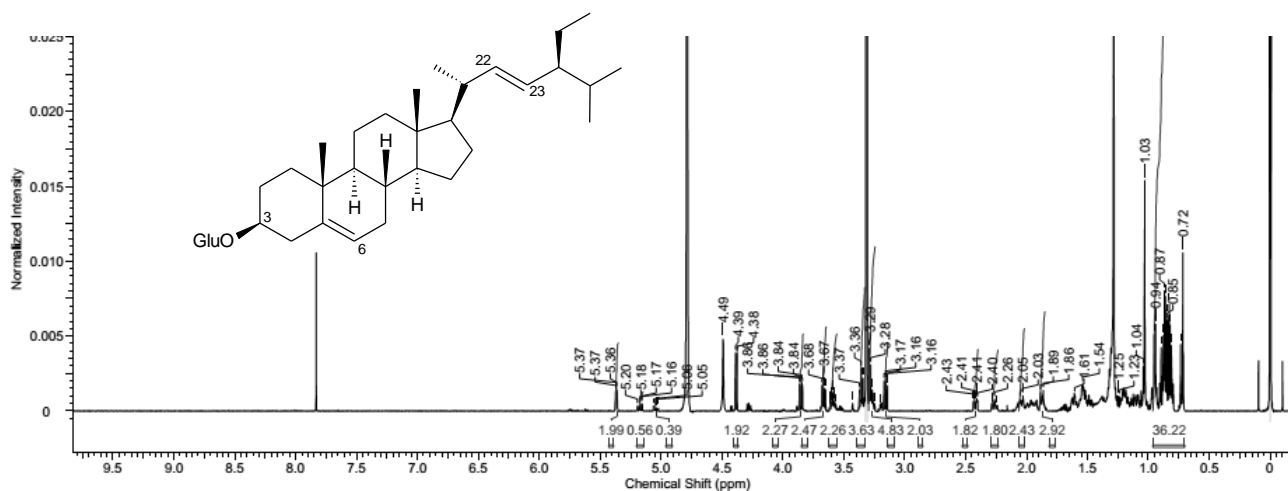


S7: HSQC (^1H 600 MHz, ^{13}C 150 MHz, CDCl_3) Spectrum of Compound 2 (saccharinic acid lactone)

jaqueeacc22_121129101220 #151 RT: 2,12 AV: 1 NL: 5,65E3
T: ITMS + c ESI Full ms [160,00-1000,00]

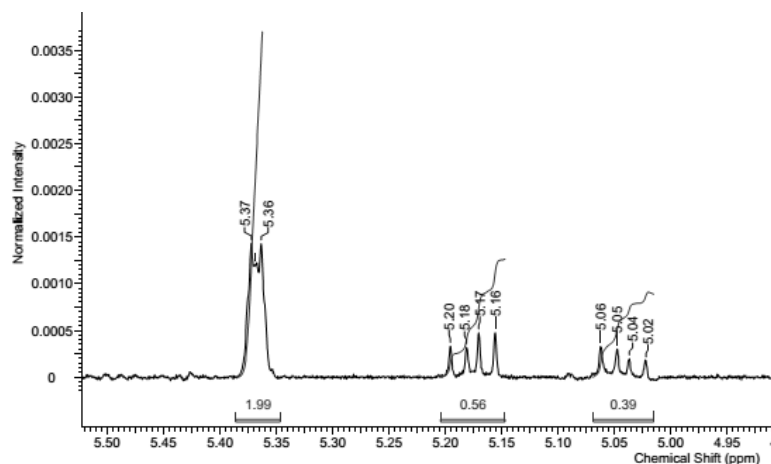


S8: MS Spectrum of Compounds **3**, **4**, **5** (sterol glucosides, sitosterol, stigmasterol, campesterol)

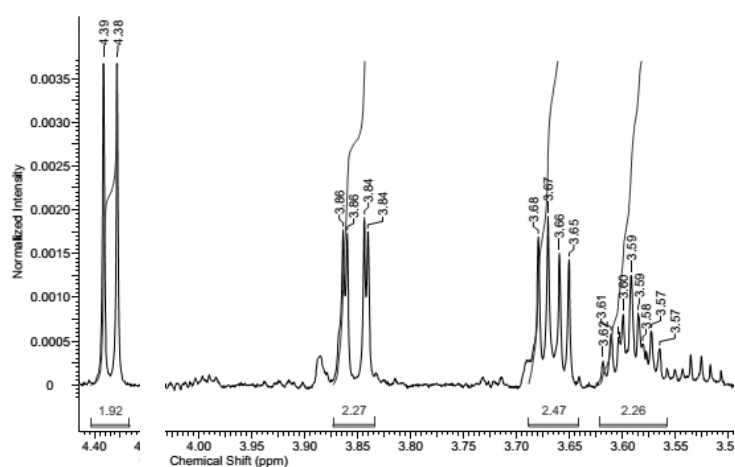


S9: $^1\text{H-NMR}$ (600 MHz, CD_3OD) Spectrum of Compounds **3**, **4**, **5** (sterol glucosides)

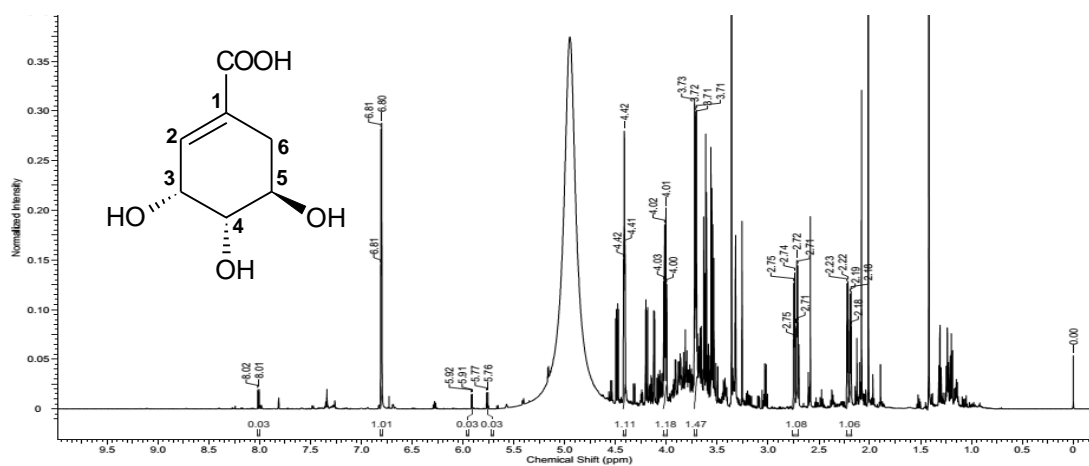
sterol glucosides, sitosterol (3), stigmasterol (4) campesterol (5): $^1\text{H-NMR}$ (600 MHz, CD_3OD): δ (ppm) = 5.37 (m, 1H, H-6), 5.17 (dd, $J = 15.1$ and 8.7 Hz, 1H, H-22), 5.04 (dd, $J = 15.1$ and 8.7 Hz, 1H, H-23), 3.59 (m, 1H, H-3), 4.38 (d, $J = 7.8$ Hz, 1H, H-1'), 3.85 (dd, $J = 12.0$ and 2.2 Hz, 1H, H-6'a), 3.66 (dd, $J = 12.0$ and 5.3 Hz, 1H, H-6'b), 3.36 (m, 1H, H-3'), 3.35 (m, 1H, H-2'), 3.27 (dd, $J = 5.3$ and 2.2 Hz, 1H, H-5'), 3.16 (m, 1H, H-4'). MS: m/z 599 $[\text{M}+\text{Na}]^+$ for formula $[\text{C}_{35}\text{H}_{60}\text{O}_6]$; m/z 597 $[\text{M}+\text{Na}]^+$ for formula $[\text{C}_{35}\text{H}_{58}\text{O}_6]$; m/z 585 $[\text{M}+\text{Na}]^+$ for formula $[\text{C}_{34}\text{H}_{58}\text{O}_6]$



S10: $^1\text{H-NMR}$ (600 MHz, CD_3OD) Spectrum of Compound **3**, **4**, **5** (from 4.95 to 5.50 ppm)

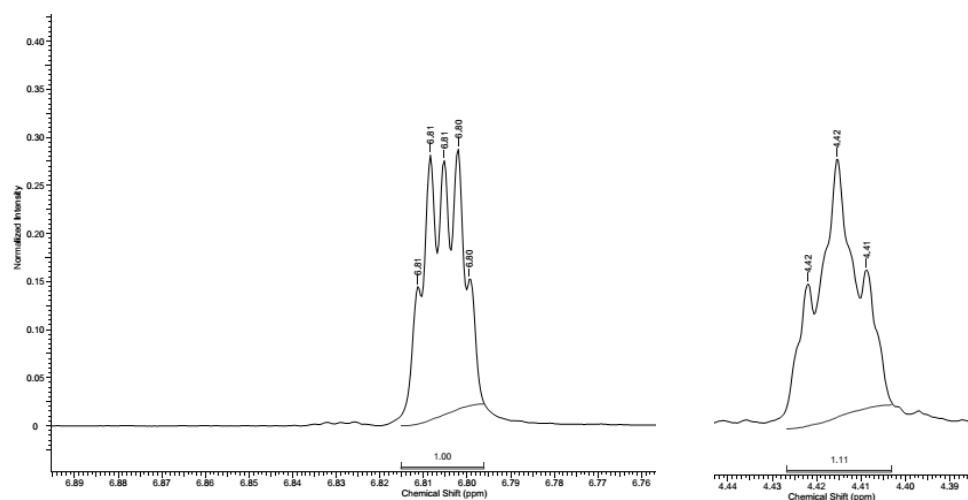


S11: $^1\text{H-NMR}$ (600 MHz, CD_3OD) Spectrum of Compound **3**, **4**, **5** (from 3.50 to 4.40 ppm)

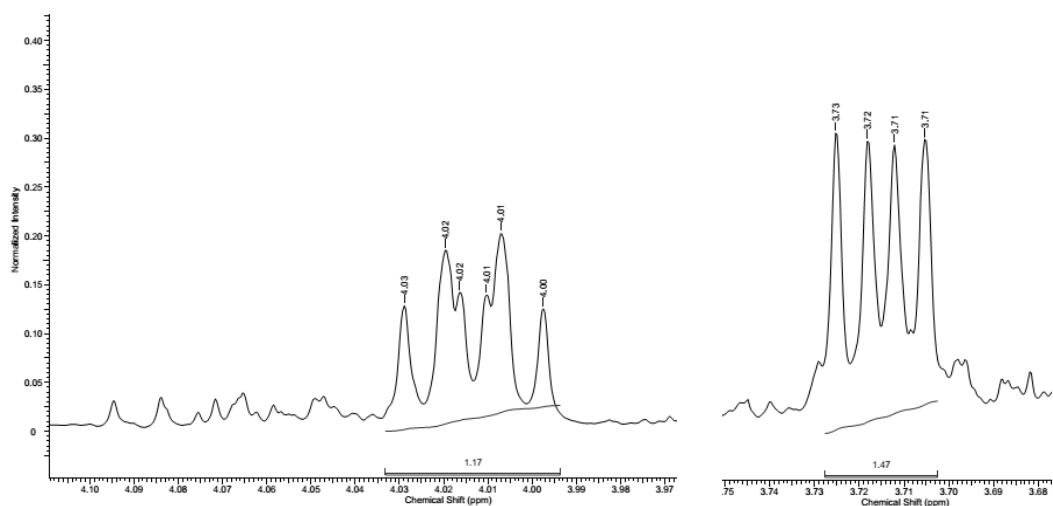


S12: $^1\text{H-NMR}$ (600 MHz, CD_3OD) Spectrum of Compound **6** (shikimic acid)

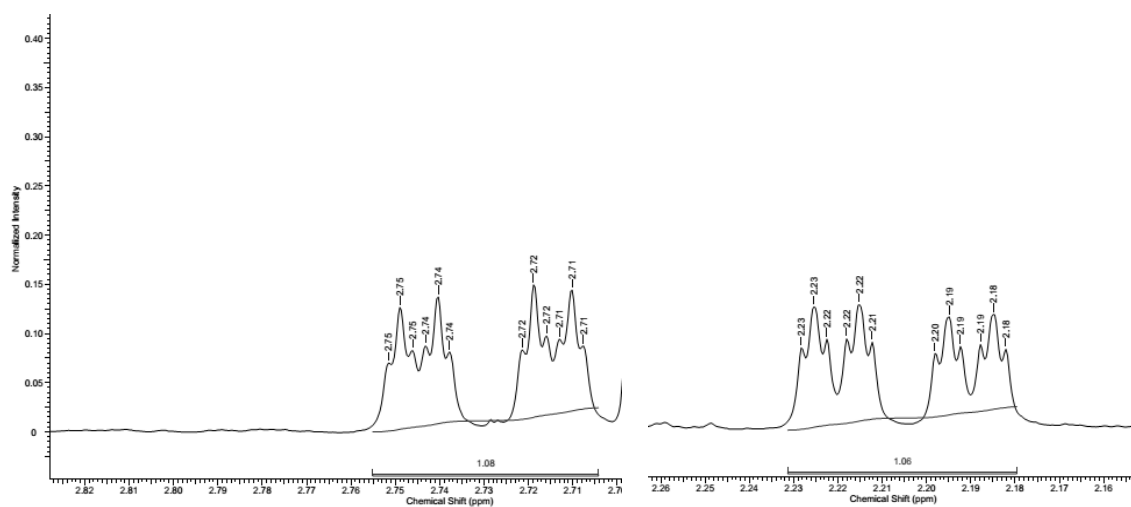
shikimic acid (**6**): $^1\text{H-NMR}$ (600 MHz, CD_3OD): δ (ppm) = 6.81 (ddd, J = 3.7, 1.7 and 1.6 Hz, 1H, H-2), 4.41 (dddd, J = 4.7, 3.7, 1.7 and 1.6 Hz, 1H, H-3), 3.72 (dd, J = 7.7 and 4.2 Hz, 1H, H-4), 4.01 (ddd, J = 7.7, 6.1 and 5.1 Hz, 1H, H-5), 2.72 (dddd, J = 18.1, 5.1, 1.6 and 1.6 Hz, 1H, H-6a), 2.20 (dddd, J = 18.1, 6.1, 1.7 and 1.7 Hz, 1H, H-6b). $^{13}\text{C-NMR}$ (150 MHz, CD_3OD): δ (ppm) = 170.3 (COOH), 131.3 (C-1), 138.6 (C-2), 67.4 (C-3), 73.1 (C-4), 68.4 (C-5), 32.0 (C-6).



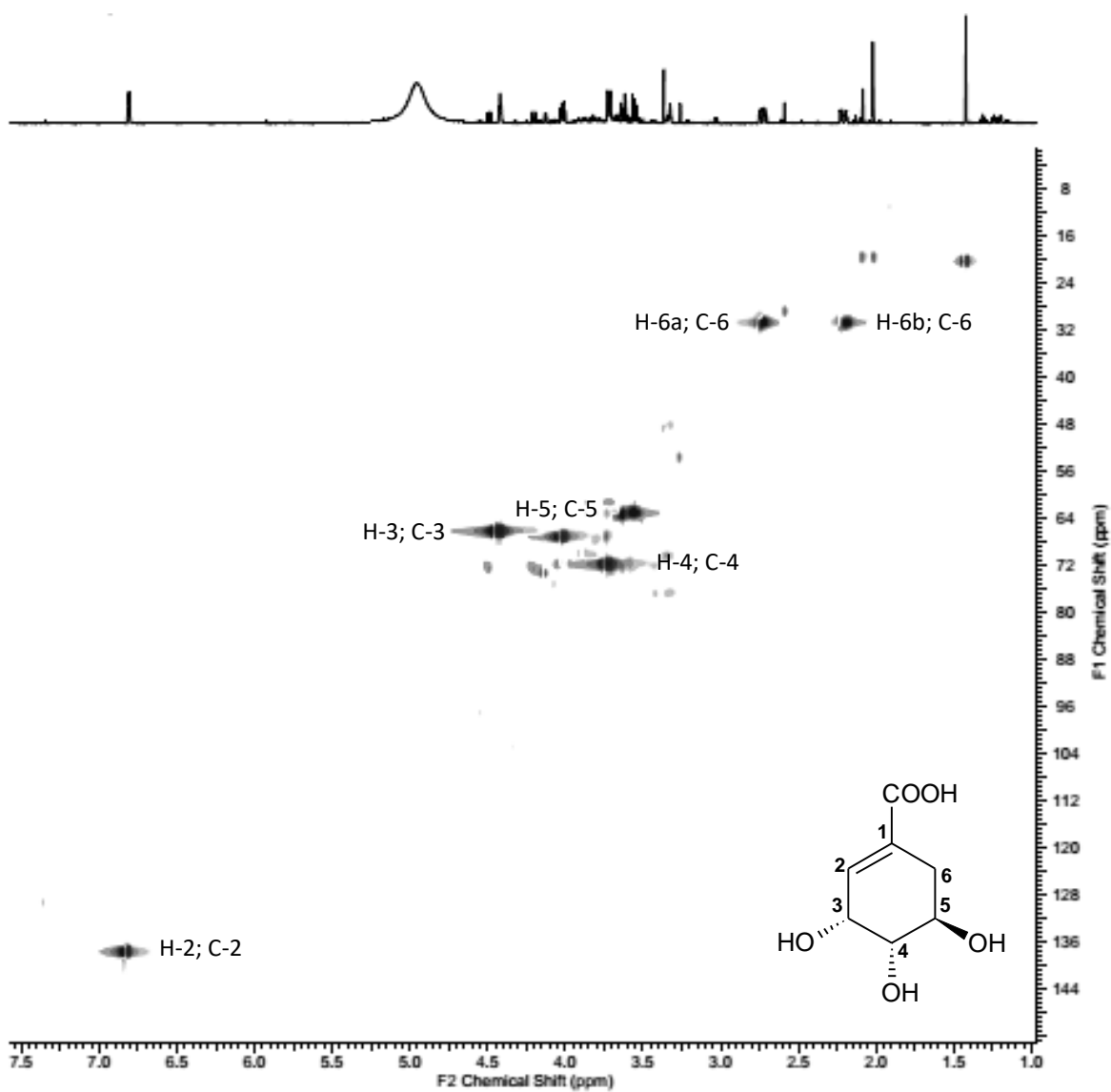
S13: $^1\text{H-NMR}$ (600 MHz, CD_3OD) Spectrum of Compound **6** (from 6.76 to 6.89, 4.39 to 4.44 ppm)



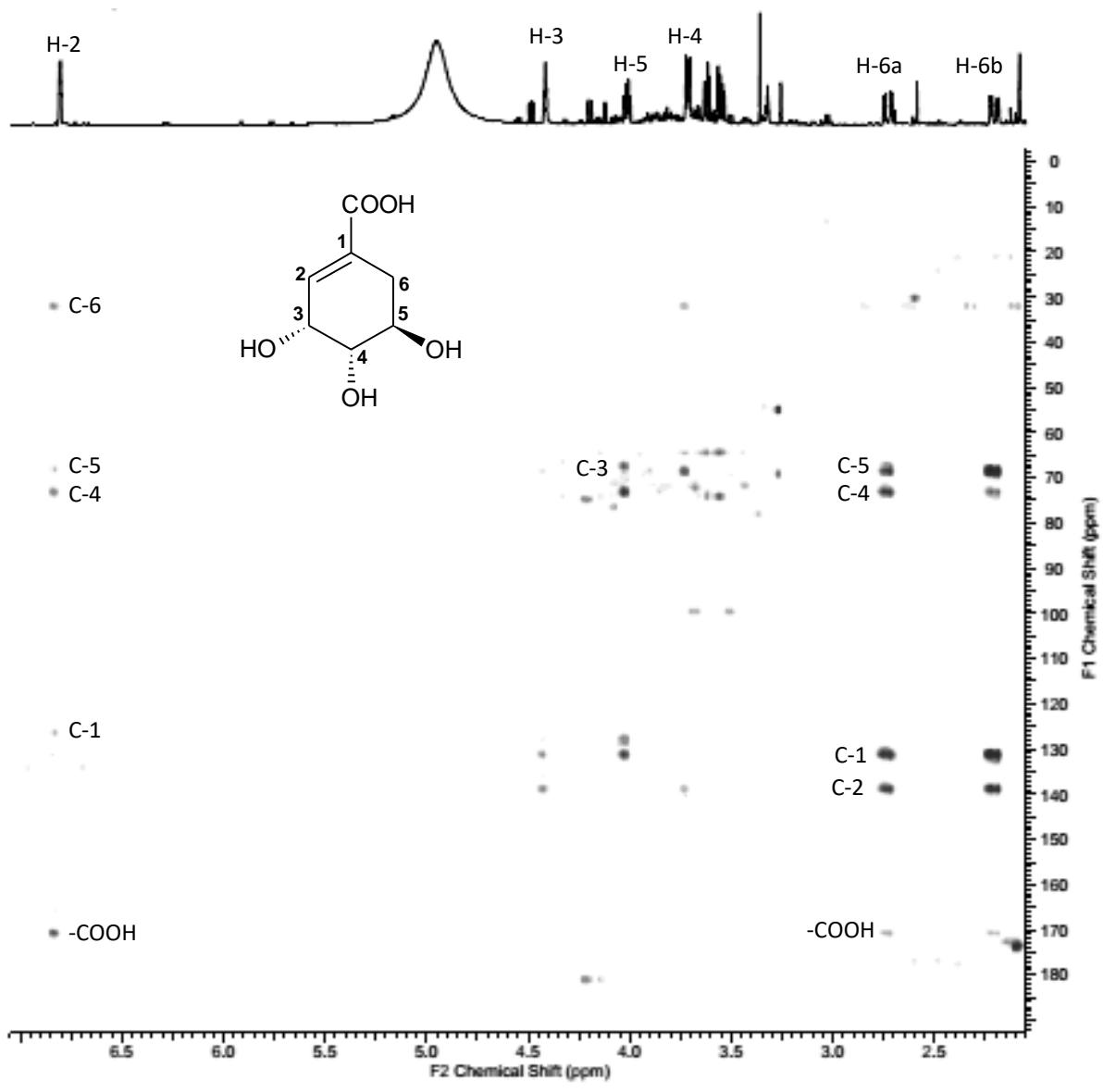
S14: $^1\text{H-NMR}$ (600 MHz, CD_3OD) Spectrum of Compound **6** (from 3.97 to 4.10, 3.68 to 3.75 ppm)



S15: $^1\text{H-NMR}$ (600 MHz, CD_3OD) Spectrum of Compound **6** (from 2.70 to 2.80, 2.16 to 2.26 ppm)

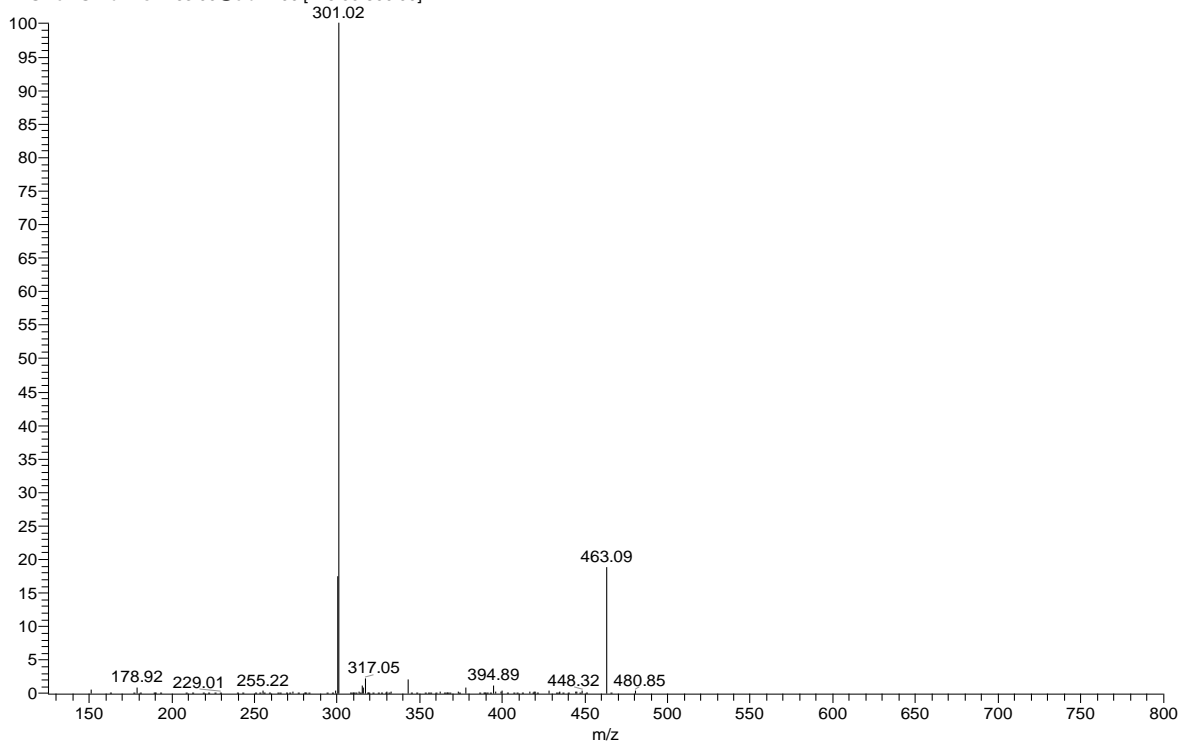


S16: HSQC (^1H 600 MHz, ^{13}C 150 MHz, CD_3OD) Spectrum of Compound **6**



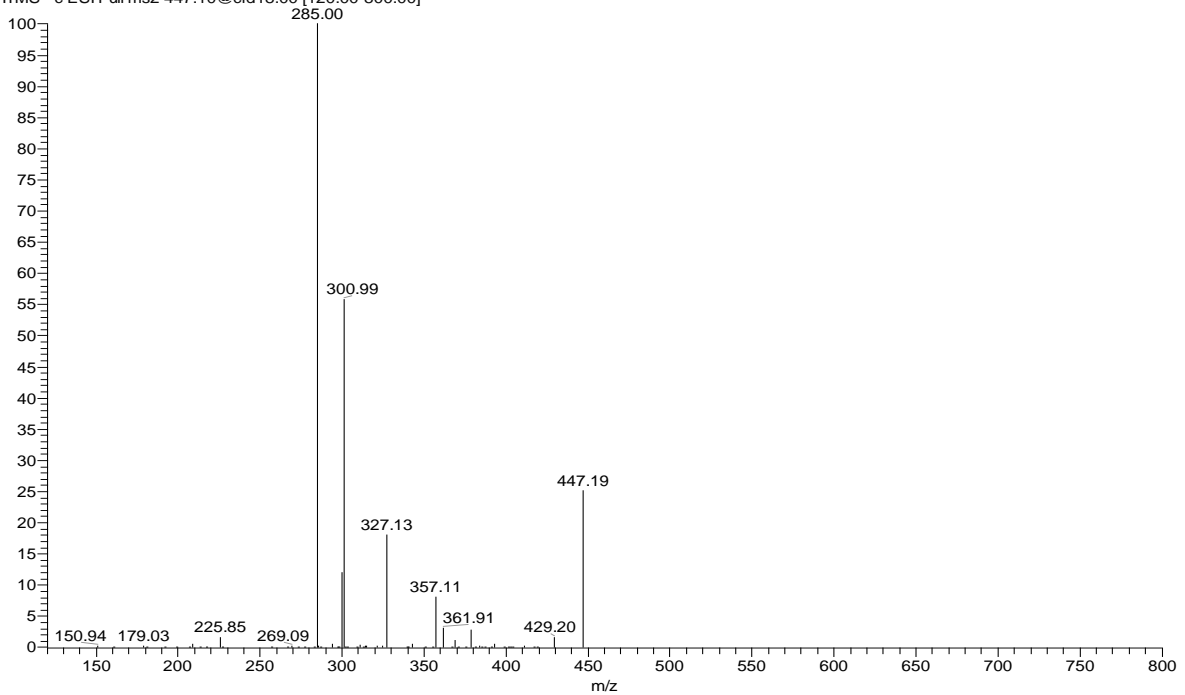
S17: HMBC (¹H 600 MHz, ¹³C 150 MHz, CD₃OD) Spectrum of Compound 6

eccc9_140212145639 #891 RT: 2.92 AV: 1 NL: 4.17E3
T: ITMS - c ESI Full ms2 463.00@cid17.00 [125.00-800.00]

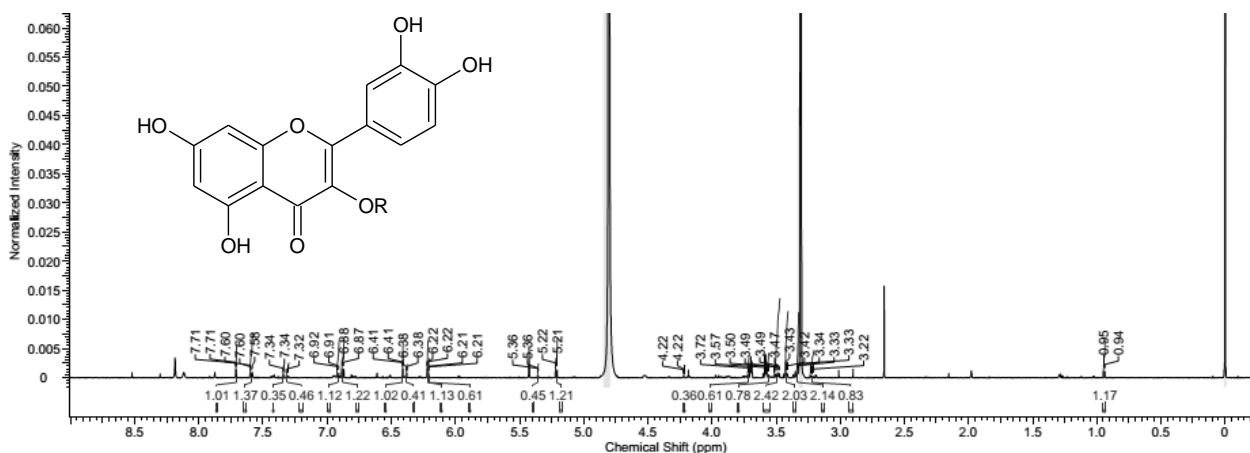


S18: MS Spectrum of Compound 7 (isoquercitrin)

eccc9_140212145639 #683 RT: 2.14 AV: 1 NL: 1.29E4
T: ITMS - c ESI Full ms2 447.10@cid18.00 [120.00-800.00]



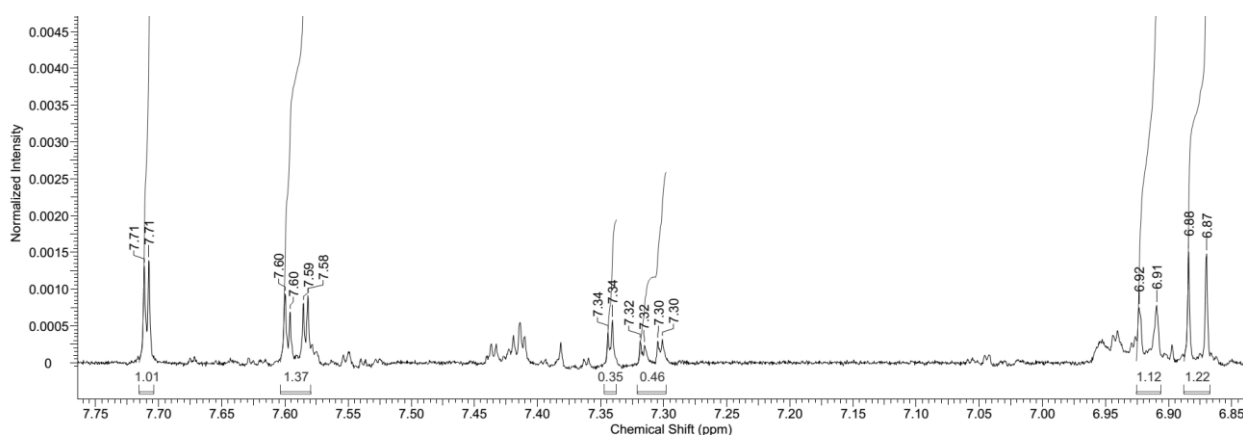
S19: MS Spectrum of Compound 8 (quercitrin)



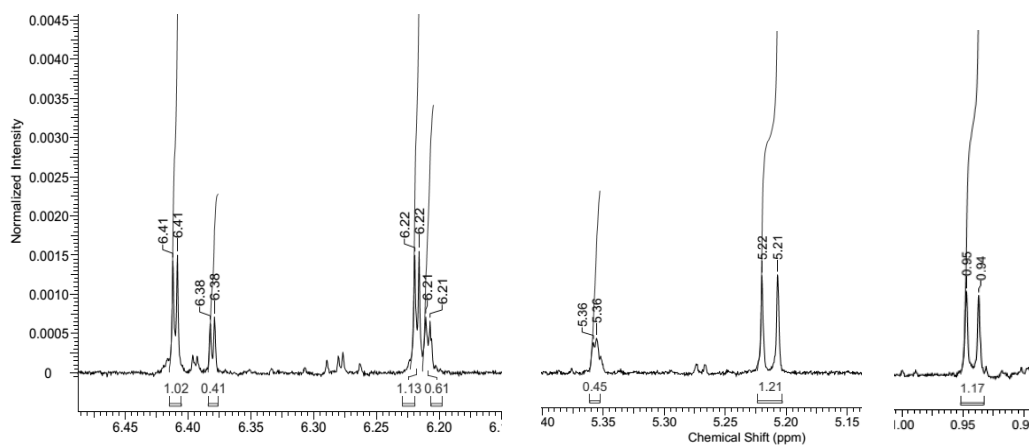
S20: $^1\text{H-NMR}$ (600 MHz, CD_3OD) Spectrum of Compounds **7** and **8** (isoquercitrin and quercitrin)

isoquercitrin (7): $^1\text{H-NMR}$ (600 MHz, CD_3OD): δ (ppm) = 6.22 (d, $J = 2.1$ Hz, 1H, H-6), 6.41 (d, $J = 2.1$ Hz, 1H, H-8), 7.70 (d, $J = 2.2$ Hz, 1H, H-2'), 6.87 (d, $J = 8.5$ Hz, 1H, H-5'), 7.59 (dd, $J = 8.5$ and 2.2 Hz, 1H, H-6'), 5.21 (d, $J = 7.7$ Hz, 1H, H-1''), 3.49 (dd, $J = 9.0$ and 7.7 Hz, 1H, H-2''), 3.43 (t, $J = 9.0$ Hz, 1H, H-3''), 3.35 (t, $J = 9.6$ and 9.0 Hz, 1H, H-4''), 3.22 (ddd, $J = 9.6$, 5.3 and 2.5 Hz, 1H, H-1''), 3.72 (d, $J = 2.5$ Hz, 1H, H-6''a), 3.56 (d, $J = 5.3$ Hz, 1H, H-6''b). $^{13}\text{C-NMR}$ (CD_3OD , 150 MHz): δ (ppm) = 159.4 (C-2), 163.1 (C-5), 100.0 (C-6), 166.2 (C-7), 94.8 (C-8), 158.5 (C-9), 105.8 (C-10), 123.1 (C-1'), 117.7 (C-2'), 149.9 (C-3'), 146.2 (C-4'), 116.2 (C-5'), 123.2 (C-6'), 104.5 (C-1''), 75.8 (C-2''), 78.2 (C-3''), 71.4 (C-4''), 78.6 (C-5''), 62.3 (C-6''); MS: m/z 463 [M-H] $^-$ for formula $\text{C}_{21}\text{H}_{20}\text{O}_{12}$.

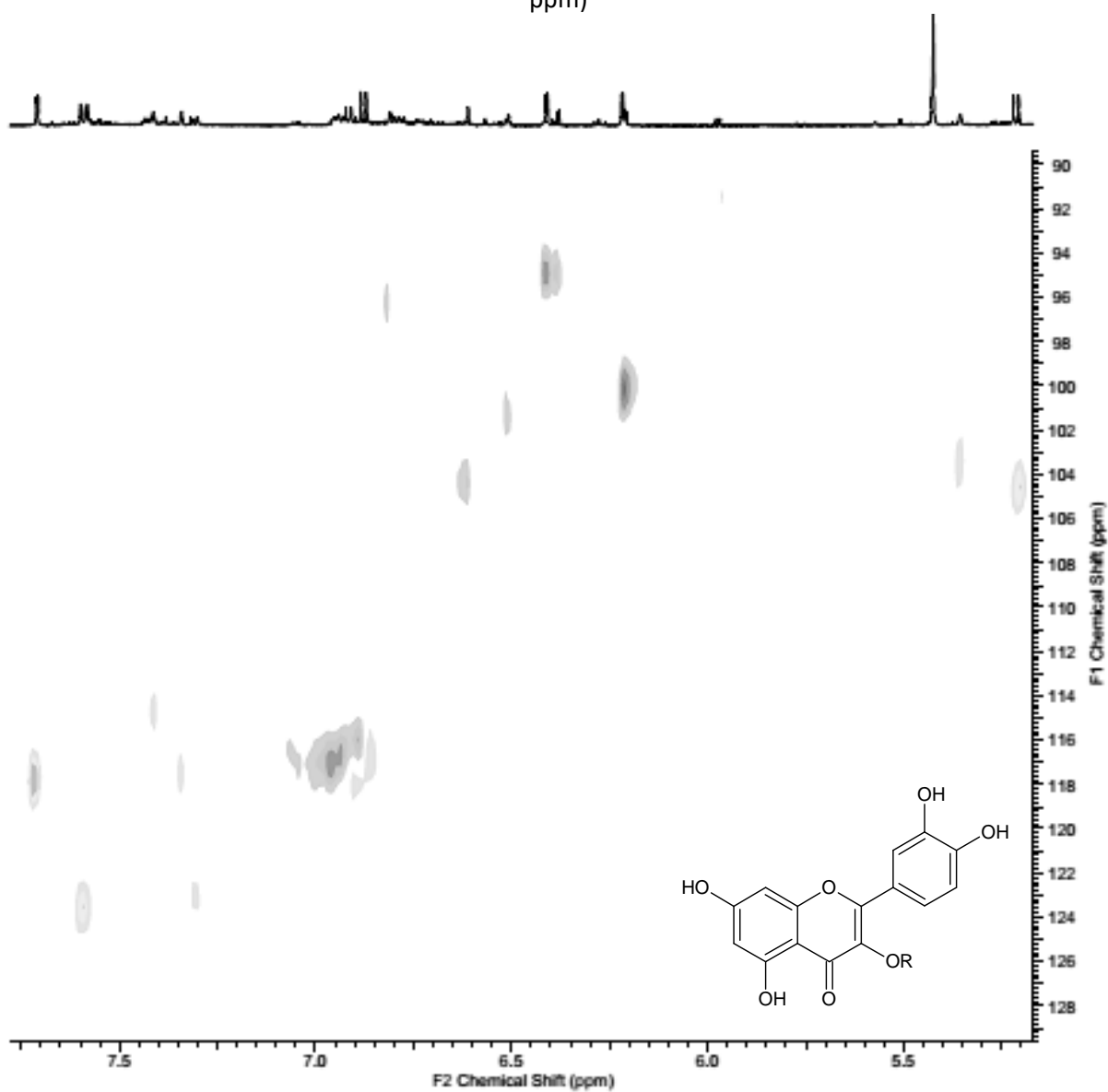
quercitrin (8): $^1\text{H-NMR}$ (600 MHz, CD_3OD): δ (ppm) = 6.21 (d, $J = 2.1$ Hz, 1H, H-6), 6.38 (d, $J = 2.1$ Hz, 1H, H-8), 7.34 (d, $J = 2.1$ Hz, 1H, H-2'), 6.92 (d, $J = 8.3$ Hz, 1H, H-5'), 7.31 (dd, $J = 8.3$ and 2.1 Hz, 1H, H-6'), 5.36 (d, $J = 1.5$ Hz, 1H, H-1''), 0.94 (d, $J = 6.1$ Hz, 1H, H-6''). $^{13}\text{C-NMR}$ (150 MHz, CD_3OD): δ (ppm) 163.0 (C-5), 100.0 (C-6), 94.8 (C-8), 105.5 (C-10), 117.0 (C-2'), 147.7 (C-3'), 150.2 (C-4'), 116.1 (C-5'), 122.9 (C-6'), 103.7 (C-1''), 17.7 (C-6'') other overlapping signals; MS: m/z 447 [M-H] $^-$ for formula $\text{C}_{21}\text{H}_{20}\text{O}_{11}$.



S21: $^1\text{H-NMR}$ (600 MHz, CD_3OD) Spectrum of Compounds **7** and **8** (6.85 to 7.75 ppm)



S22: ^1H -NMR (600 MHz, CD_3OD) Spectrum of Compounds **7** and **8** (6.15 to 6.45, 5.15 to 5.40, 0.90 to 1.00 ppm)



S23: HSQC (^1H 600 MHz, ^{13}C 150 MHz, CD_3OD) Spectrum of Compound **7** and **8**