

Supporting Information

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Comparative Effects of Flavonoids from *Fructus Sophorae* on Rat Osteoblasts *in vitro*

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Table of Contents	Page
S1 : NMR and mass data and spectra of compound 1 (Genistein)	3
S2 : NMR and mass data and spectra of compound 2 (Genistin)	5
S3 : NMR and mass data and spectra of compound 3 (Sophoricoside)	6
S4 : NMR and mass data and spectra of compound 4 (Sophorabioside)	7
S5 : NMR and mass data and spectra of compound 5 (Biochanin A)	8
S6 :NMR and mass data and spectra of compound 6 (Sissotrin)	9
S7 :NMR and mass data and spectra of compound 7 (Oroboside)	10
S8 :NMR and mass data and spectra of compound 8 (Pratensein)	12
S9 :NMR and mass data and spectra of compound 9 (Prunetin)	13
S10 :NMR and mass data and spectra of compound 10 (3'-methylorobol)	14

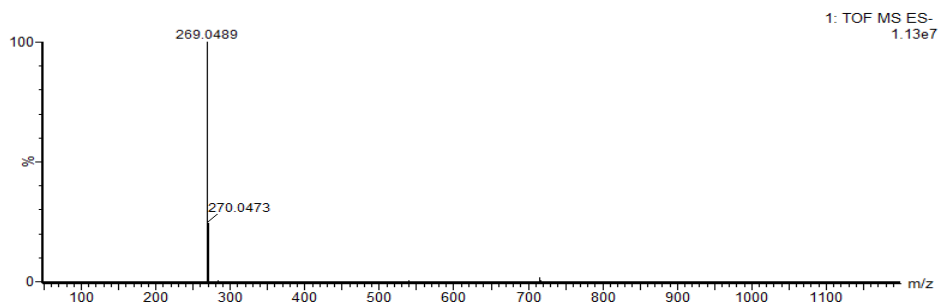
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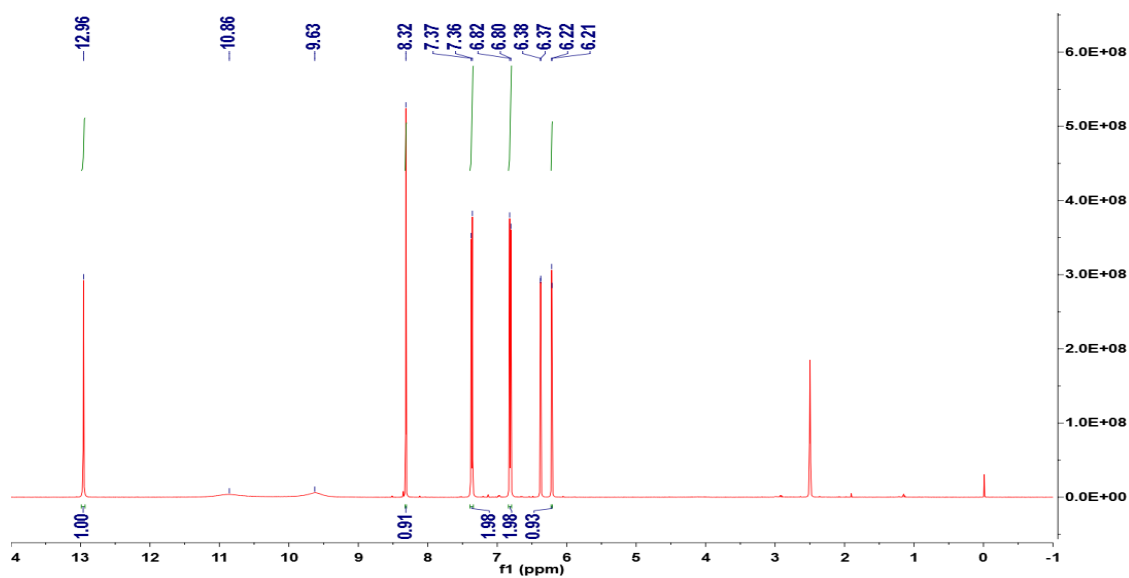
S11 :NMR and mass data and spectra of compound 11 (Dehydroferreirin)	15
S12 :NMR and mass data and spectra of compound 12 (Cajanin)	16
S13 :NMR and mass data and spectra of compound 13 (Tectoridin)	17
S14 :NMR and mass data and spectra of compound 14 (Ononin)	18
S15 :NMR and mass data and spectra of compound 15 (Kaempferol)	19
S16 :NMR and mass data and spectra of compound 16 (Sophoraflavonolside)	20
S17 :NMR and mass data and spectra of compound 17 (Nicotiflorin)	21
S18 :NMR and mass data and spectra of compound 18 (α -rhamnoisorobin)	22
S19 :NMR and mass data and spectra of compound 19 (Populnin)	23
S20 :NMR and mass data and spectra of compound 20 (Astragalin)	25
S21 :Mass data and spectra of compound 21 (Rutin)	26
S22 :NMR and mass data and spectra of compound 22 (Quercetin-3-O- β -D-sophoroside)	27
S23 :NMR and mass data and spectra of compound 23 (Quercitrin)	29
S24 :NMR and mass data and spectra of compound 24 (Isoquercitrin)	30
S25 :NMR and mass data and spectra of compound 25 (Thevetiaflavone)	31
S26 :NMR and mass data and spectra of compound 26 (Genkwanin)	33
S27 :NMR and mass data and spectra of compound 27 (Choerospondin)	34

S1 : NMR and mass data and spectra of compound 1 (Genistein)

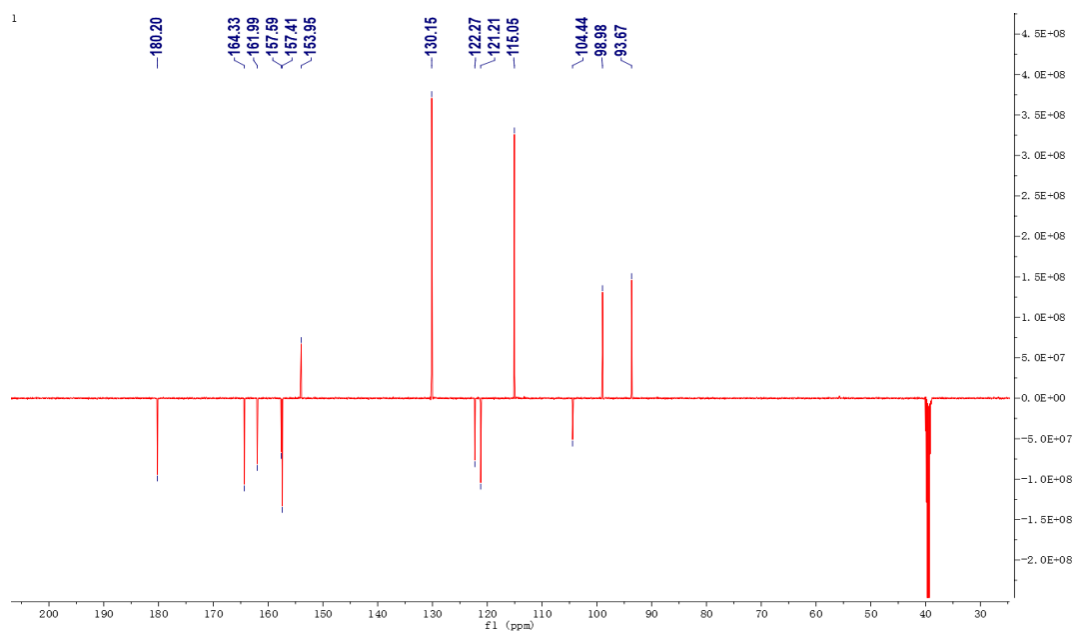
Q/TOF-MS (m/z): 269.0489 $[M-H]^-$, (calcd for $C_{15}H_{10}O_5$). 1H NMR (500 MHz, $DMSO-d_6$) δ : 12.96 (1H, s, 5-OH), 10.86 (1H, s, 7-OH), 9.63 (H, s, 4'-OH), 8.32 (1H, s, H-2), 7.37 (2H, d, $J = 8.6$ Hz, H-2', 6'), 6.82 (2H, d, $J = 8.6$ Hz, H-3', 5'), 6.38 (1H, d, $J = 2.1$ Hz, H-8), 6.22 (1H, d, $J = 2.1$ Hz, H-6); DEPTQSP (125 MHz, $DMSO-d_6$) δ : 153.95 (C-2), 121.21 (C-3), 180.20 (C-4), 157.59 (C-5), 98.98 (C-6), 164.33 (C-7), 93.67 (C-8), 157.41 (C-9), 104.44 (C-10), 122.27 (C-1'), 130.15 (C-2', 6'), 115.05 (C-3', 5'), 161.99 (C-4').



Compound 1: Q/TOF-MS spectra



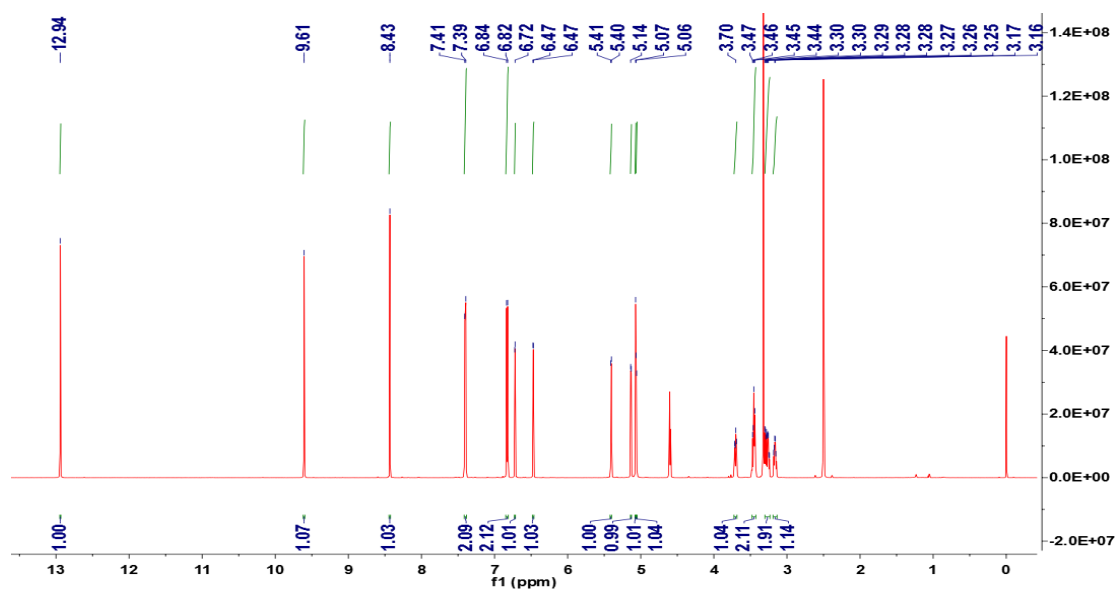
Compound 1: 1H -NMR spectra



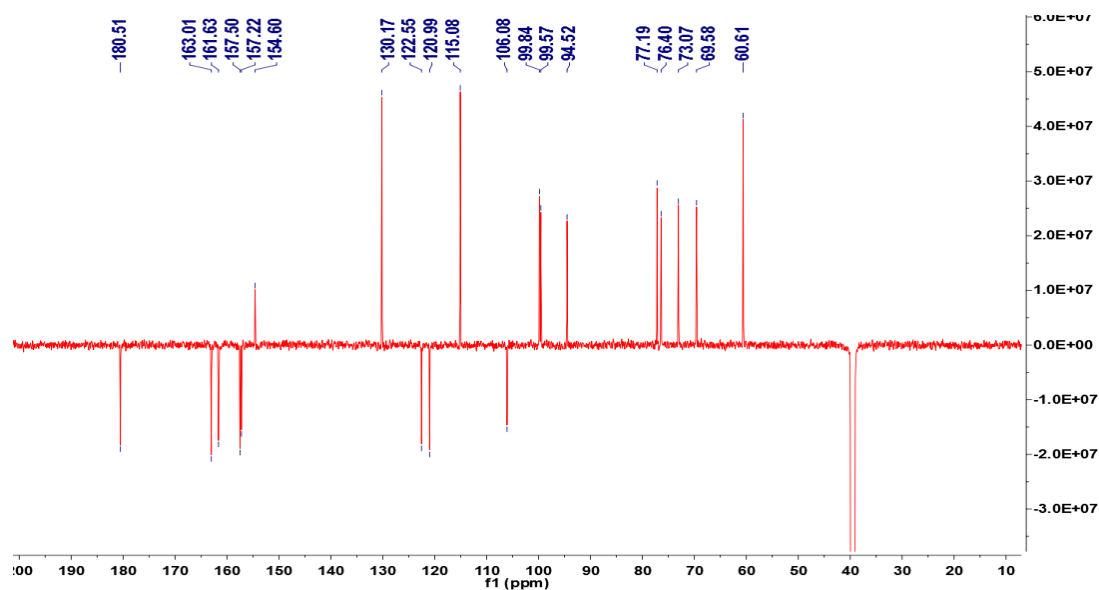
Compound 1: DEPTQSP spectra

S2 : NMR and mass data and spectra of compound 2 (Genistin)

ESI-MS (m/z) : 431.09 $[M-H]^-$ (calcd for $C_{21}H_{20}O_{10}$). 1H NMR (600 MHz, DMSO- d_6) δ : 12.94 (1H, s, 5-OH), 9.61 (H, s, 4'-OH), 8.43 (1H, s, H-2), 7.41 (2H, d, $J = 8.4$ Hz, H-2', 6'), 6.83 (2H, d, $J = 8.4$ Hz, H-3', 5'), 6.72 (1H, d, $J = 2.1$ Hz, H-8), 6.47 (1H, d, $J = 2.1$ Hz, H-6), 5.06 (d, $J = 7.0$ Hz, Glc-H-1''), 3.72-3.16 (m, 6H, Glc-H-2''-6''). DEPTQSP(125 MHz, DMSO- d_6) δ : 154.60 (C-2), 120.99 (C-3), 180.51 (C-4), 157.50 (C-5), 99.84 (C-6), 163.01 (C-7), 93.67 (C-8), 157.22 (C-9), 106.08 (C-10), 122.55 (C-1'), 130.17 (C-2', 6'), 115.08 (C-3', 5'), 161.63 (C-4'), 99.84 (C-1''), 73.07 (C-2''), 77.19 (C-3''), 69.58 (C-4''), 76.40 (C-5''), 60.61 (C-6'').



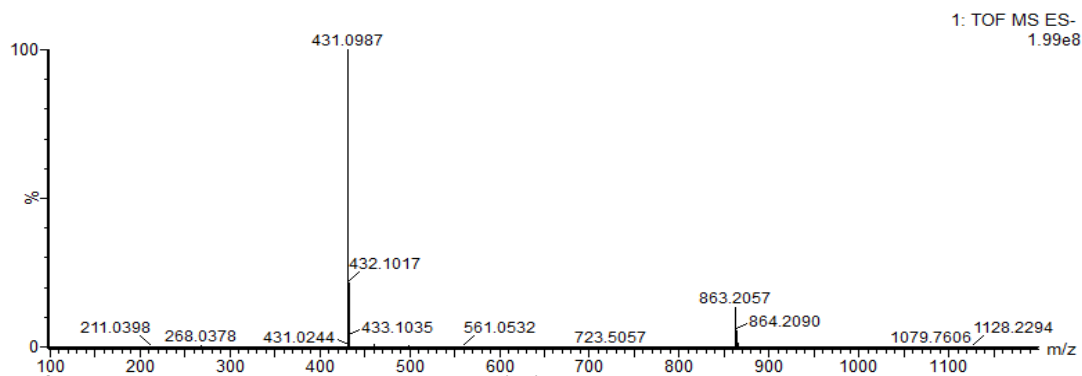
Compound 2: 1H -NMR spectra



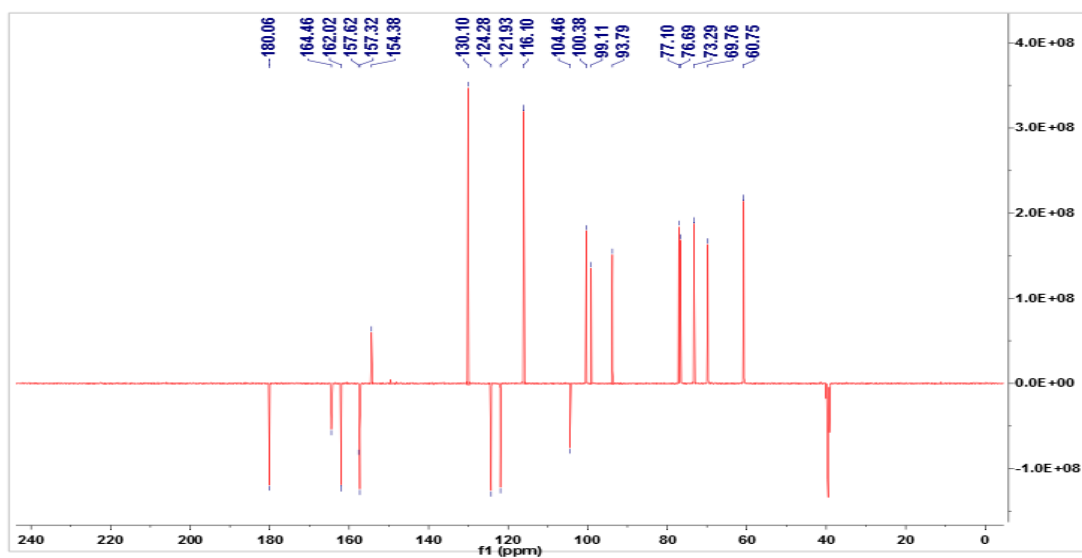
Compound 2: DEPTQSP spectra

S3 : NMR and mass data and spectra of compound 3 (Sophoricoside)

Q/TOF-MS (m/z) : 431.0987 [$M-H$]⁻ (calcd for $C_{21}H_{20}O_{10}$). DEPTQSP (125 MHz, DMSO- d_6) δ : 154.38 (C-2), 121.93 (C-3), 180.06 (C-4), 157.62 (C-5), 99.11 (C-6), 164.46 (C-7), 93.79 (C-8), 157.32 (C-9), 104.46 (C-10), 124.28 (C-1'), 130.10 (C-2', 6'), 116.10 (C-3', 5'), 162.02 (C-4'), 100.38 (C-1''), 73.29 (C-2''), 77.10 (C-3''), 69.76 (C-4''), 76.69 (C-5''), 60.75 (C-6'').



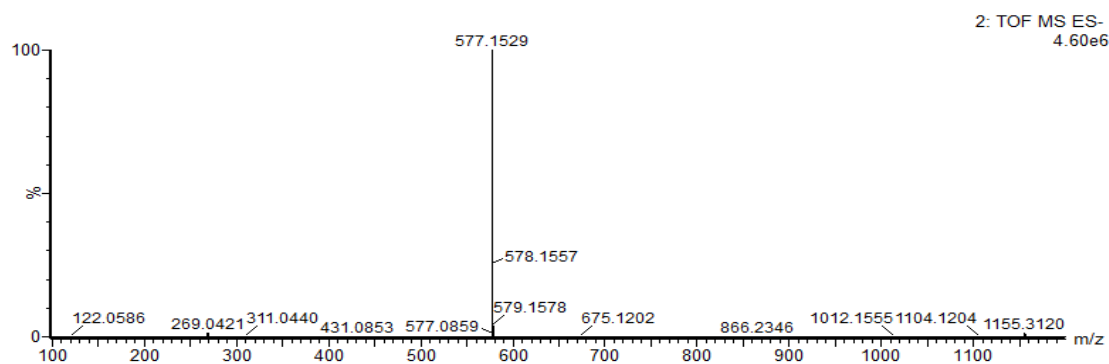
Compound 3: Q/TOF-MS spectra



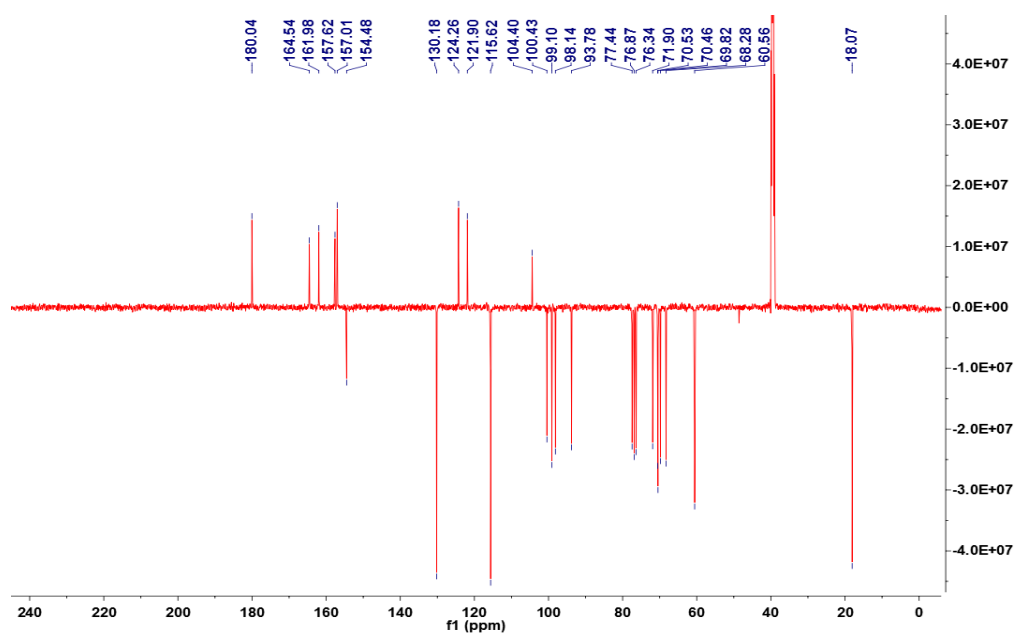
Compound 3: DEPTQSP spectra

S4 : NMR and mass data and spectra of compound 4 (Sophorabioside)

Q/TOF-MS (m/z): 577.1529 $[M-H]^-$ (calcd for $C_{27}H_{30}O_{14}$). DEPTQSP (125 MHz, DMSO- d_6) δ : 154.48 (C-2), 121.90 (C-3), 180.04 (C-4), 157.62 (C-5), 99.10 (C-6), 164.54 (C-7), 93.78 (C-8), 157.01 (C-9), 104.40 (C-10), 124.26 (C-1'), 130.18 (C-2', 6'), 115.62 (C-3', 5'), 161.98 (C-4'), 98.14 (C-1''), 76.87 (C-2''), 77.44 (C-3''), 69.82 (C-4''), 76.34 (C-5''), 60.56 (C-6''), 100.43 (C-1'''), 70.53 (C-2'''), 70.46 (C-3'''), 71.90 (C-4'''), 68.28 (C-5'''), 18.07 (C-6''').



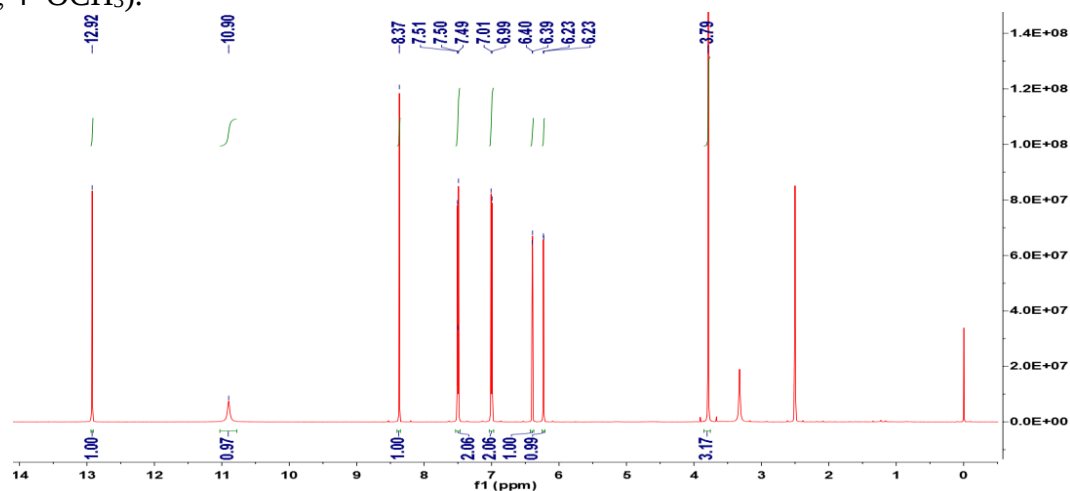
Compound 4: Q/TOF-MS spectra



Compound 4: DEPTQSP spectra

S5 : NMR and mass data and spectra of compound 5 (Biochanin A)

ESI-MS (m/z): 283.26 $[M-H]^-$ (calcd for $C_{16}H_{12}O_5$). 1H NMR (600 MHz, $DMSO-d_6$) δ : 12.92 (1H, s, OH), 10.90 (1H, s, OH), 8.37 (1H, s, H-2), 7.50 (2H, d, $J = 9.0$ Hz, H-2', 6'), 7.00 (2H, d, $J = 9.0$ Hz, H-3', 5'), 6.39 (1H, d, $J = 2.1$ Hz, H-6), 6.23 (1H, d, $J = 2.1$ Hz, H-8), 3.79 (3H, s, 4'-OCH₃).

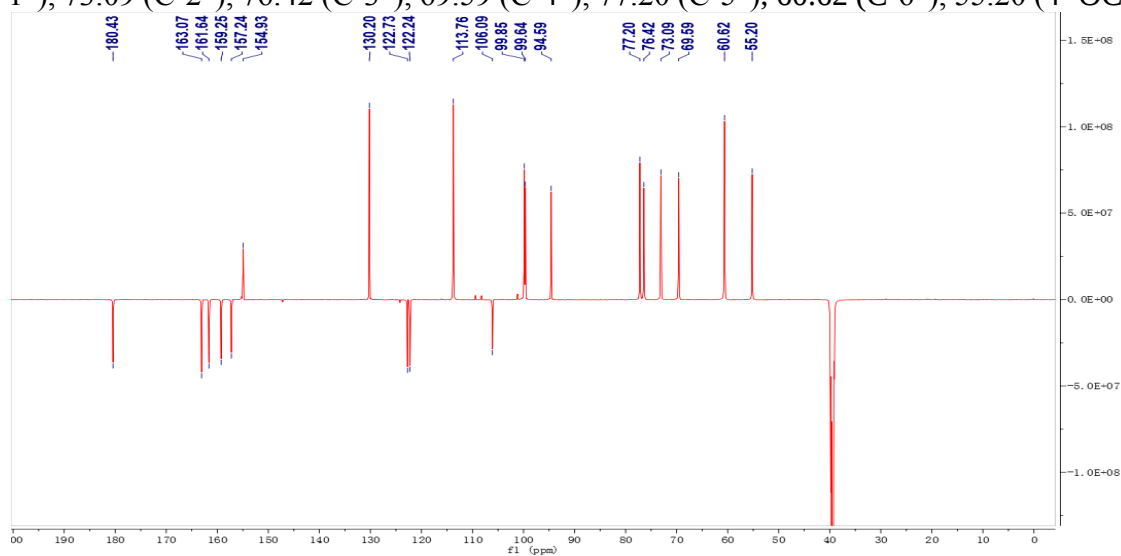


附图 12

Compound 5: 1H -NMR spectra

S6 :NMR and mass data and spectra of compound **6** (Sissotrin)

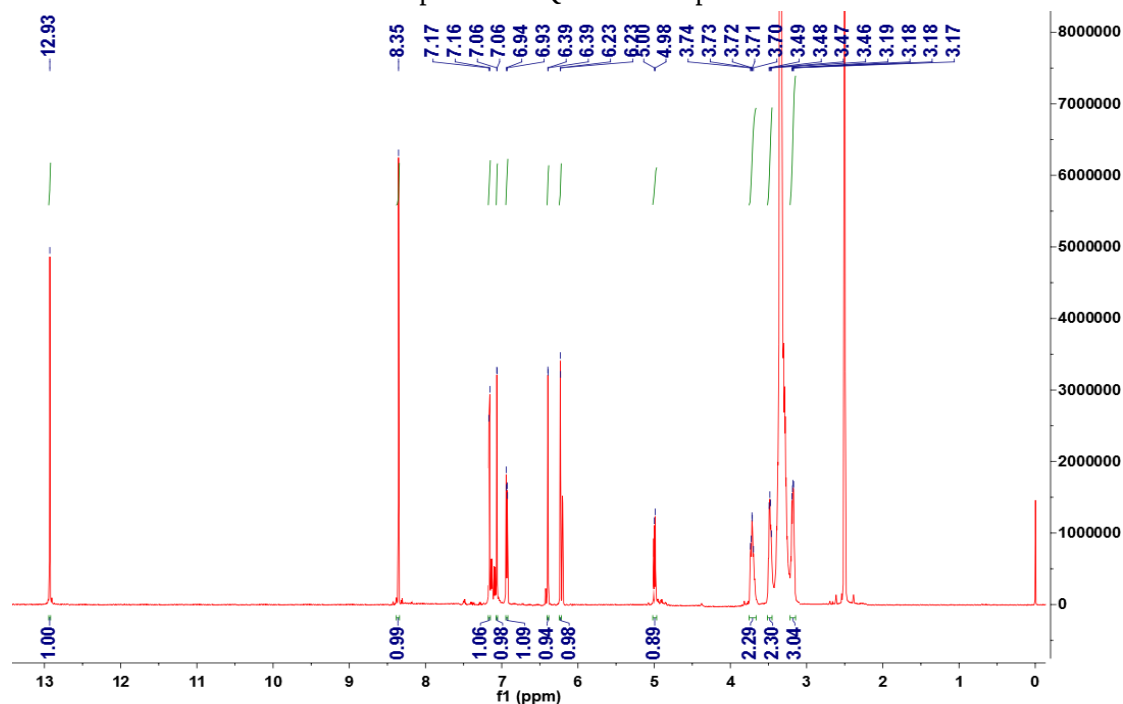
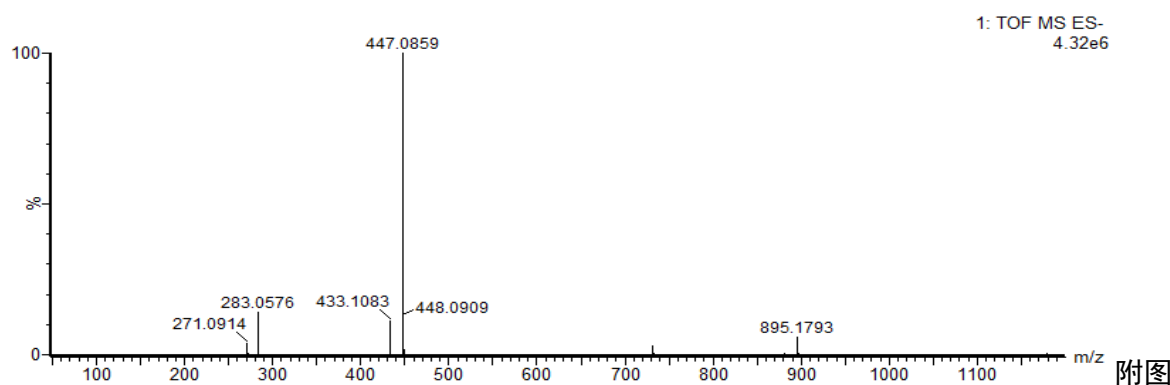
ESI-MS (m/z): 445 [M-H]⁻(calcd for C₂₂H₂₂O₁₀). DEPTQSP (150 MHz, DMSO-*d*₆) δ : 154.93 (C-2), 122.73 (C-3), 180.43 (C-4), 161.64 (C-5), 99.85 (C-6), 163.07 (C-7), 94.59 (C-8), 157.24 (C-9), 106.09 (C-10), 122.24 (C-1'), 130.20 (C-2', C-6'), 1.76 (C-3', C-5'), 159.25 (C-4'), 99.64 (C-1''), 73.09 (C-2''), 76.42 (C-3''), 69.59 (C-4''), 77.20 (C-5''), 60.62 (C-6''), 55.20 (4'-OCH₃).

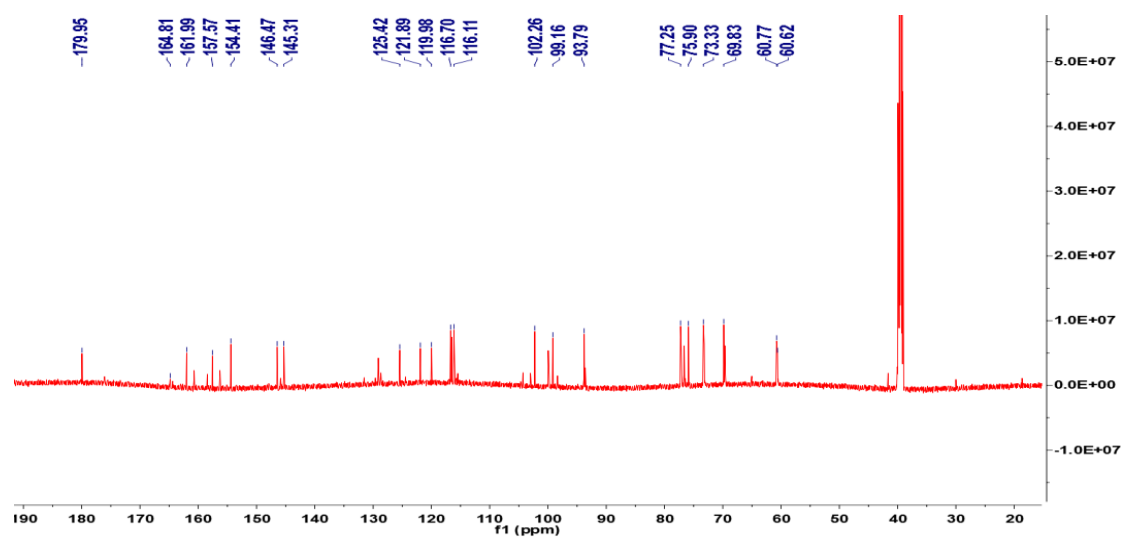


Compound **6**: DEPTQSP spectra

S7 :NMR and mass data and spectra of compound 7 (Oroboside)

Q/TOF-MS (m/z): 447.0859 [$M-H$]⁻, (calcd for $C_{21}H_{20}O_{11}$). 1H NMR (600 MHz, $DMSO-d_6$) δ : 12.93 (1H, s, 5-OH), 8.35 (1H, s, H-2), 7.16 (1H, d, $J = 8.4$ Hz, H-2'), 7.06 (1H, d, $J = 2.1$ Hz, H-5'), 6.93 (1H, dd, $J = 8.4, 2.1$ Hz, H-6'), 6.39 (1H, d, $J = 2.0$ Hz, H-8), 6.23 (1H, d, $J = 2.1$ Hz, H-6), 4.99 (1H, d, $J = 7.2$ Hz, H-1''), 3.71-3.47 (m, other sugar protons). ^{13}C -NMR (150 MHz, $DMSO-d_6$) δ : 179.95 (C-4), 164.81 (C-7), 161.99 (C-5), 157.57 (C-9), 154.41 (C-2), 146.47 (C-4'), 145.31 (C-3'), 125.42 (C-3), 121.89 (C-1'), 119.98 (C-6'), 116.70 (C-2'), 116.11 (C-5'), 104.28 (C-10), 102.26 (glc-C-1''), 99.16 (C-6), 93.79 (C-8), 77.25 (glc-C-3''), 75.90 (glc-C-5''), 73.33 (glc-C-2''), 69.83 (glc-C-4''), 60.77 (glc-C-6'').

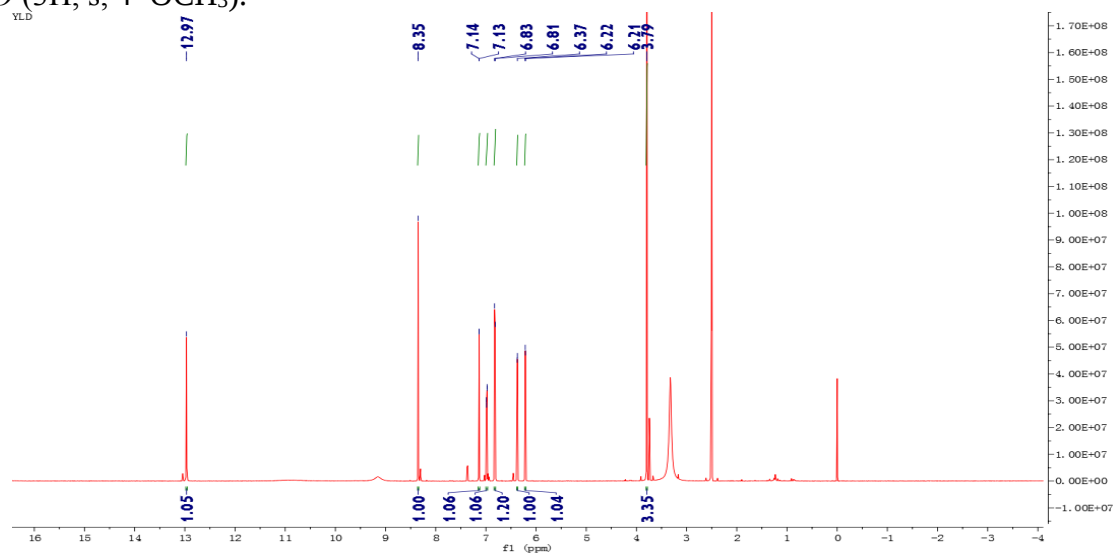




Compound 7: ^{13}C -NMR spectra

S8 :NMR and mass data and spectra of compound **8** (Pratensein)

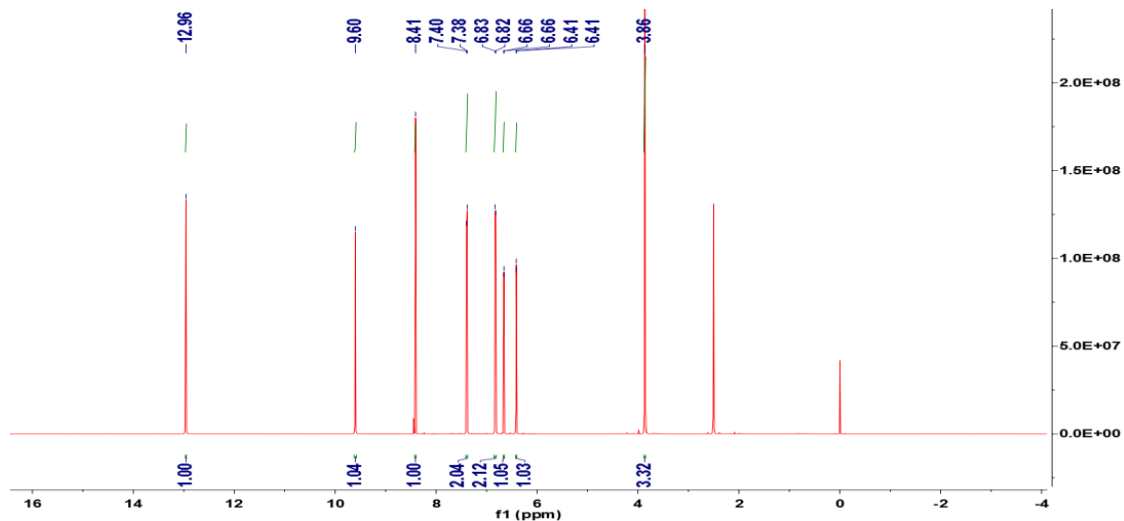
ESI-MS (m/z): 299.0530 [M-H]⁻(calcd for C₁₆H₁₂O₆). ¹H NMR (600 MHz, DMSO-*d*₆) δ : 12.97 (1H, s, OH), 8.35 (1H, s, H-2), 7.14 (1H, d, J = 2.1 Hz, H-2'), 6.98 (1H, dd, J = 8.4, 2.1 Hz, H-6'), 6.82 (1H, d, J = 8.4 Hz, H-5'), 6.37 (1H, d, J = 2.1 Hz, H-8), 6.21 (1H, d, J = 2.1 Hz, H-6), 3.79 (3H, s, 4'-OCH₃).



Compound **8**: ¹H-NMR spectra

S9 :NMR and mass data and spectra of compound **9** (Prunetin)

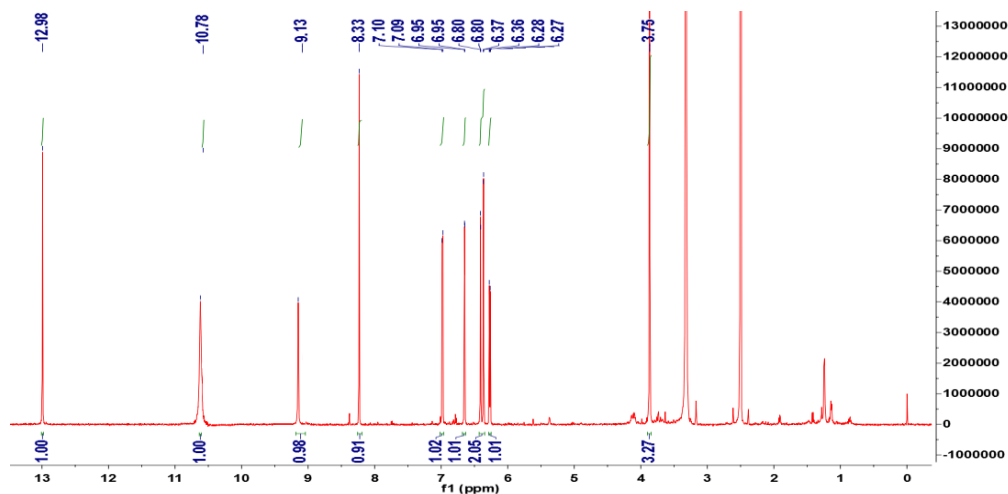
ESI-MS (m/z): 283.26 $[M-H]^-$, (calcd for $C_{16}H_{12}O_5$). 1H NMR (600 MHz, $DMSO-d_6$) δ : 12.96 (1H, s, 5-OH), 9.60 (H, s, 4'-OH), 8.41 (1H, s, H-2), 7.39 (2H, d, $J = 8.4$ Hz, H-2', 6'), 6.82 (2H, d, $J = 8.4$ Hz, H-3', 5'), 6.66 (1H, d, $J = 2.4$ Hz, H-8), 6.41 (1H, d, $J = 2.4$ Hz, H-6), 3.86 (3H, s, 7-OCH₃).



Compound **9**: 1H -NMR spectra

S10 :NMR and mass data and spectra of compound **10** (3'-methylorobol)

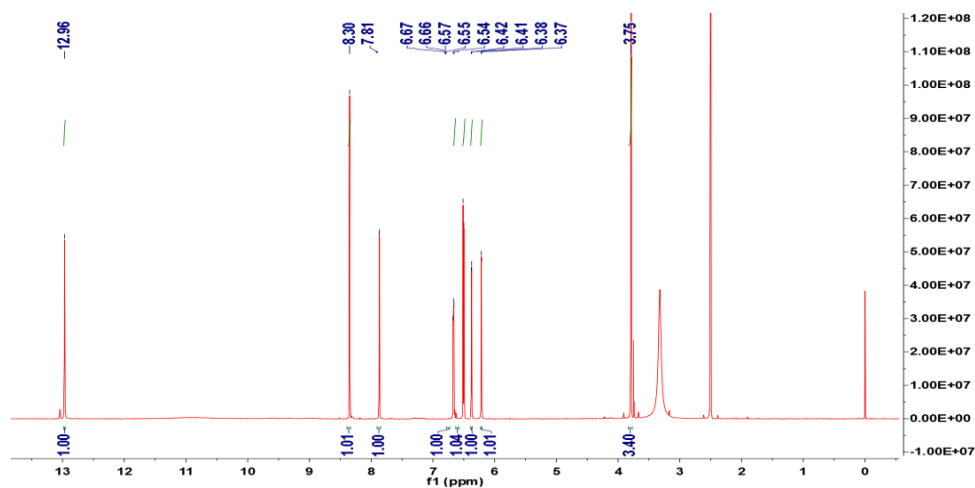
ESI-MS (m/z): 299.26 [M-H]⁻, (calcd for C₁₆H₁₂O₆). ¹H NMR (600 MHz, DMSO-*d*₆) δ 12.98 (1H, s, 5-OH), 10.78 (1H, s, 7-OH), 9.13 (1H, s, 4'-OH), 8.33 (1H, s, H-2), 7.10 (1H, d, J = 2.4 Hz, H-2'), 6.95 (1H, dd, J = 8.4, 2.4 Hz, H-6'), 6.80 (1H, d, J = 8.4 Hz, H-5'), 6.36 (1H, d, J = 2.4 Hz, H-8), 6.27 (1H, d, J = 2.4 Hz, H-6), 3.75 (3H, s, 3'-OCH₃).



Compound **10**: ¹H-NMR spectra

S11 :NMR and mass data and spectra of compound **11** (Dehydroferreirin)

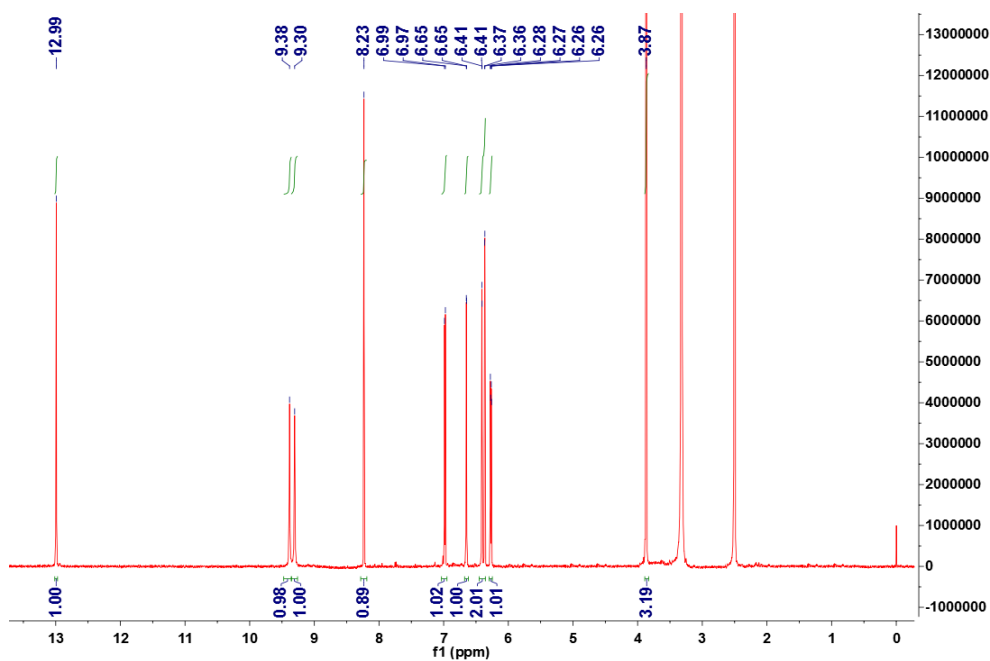
ESI-MS (m/z): 299.06 $[M-H]^-$ (calcd for $C_{16}H_{12}O_6$). 1H NMR (600 MHz, $DMSO-d_6$) δ : 12.96 (1H, s, 5-OH), 8.30 (1H, s, H-2), 7.81 (1H, d, $J = 8.4$ Hz, H-6'), 6.66 (1H, d, $J = 2.4$ Hz, H-8), 6.55 (1H, dd, $J = 2.4, 8.4$ Hz, H-5'), 6.42 (1H, d, $J = 2.4$ Hz, H-6), 6.38 (1H, d, $J = 2.4$ Hz, H-3'), 3.75 (3H, s, 4'-OCH₃).



Compound **11**: 1H -NMR spectra

S12 :NMR and mass data and spectra of compound **12** (Cajanine)

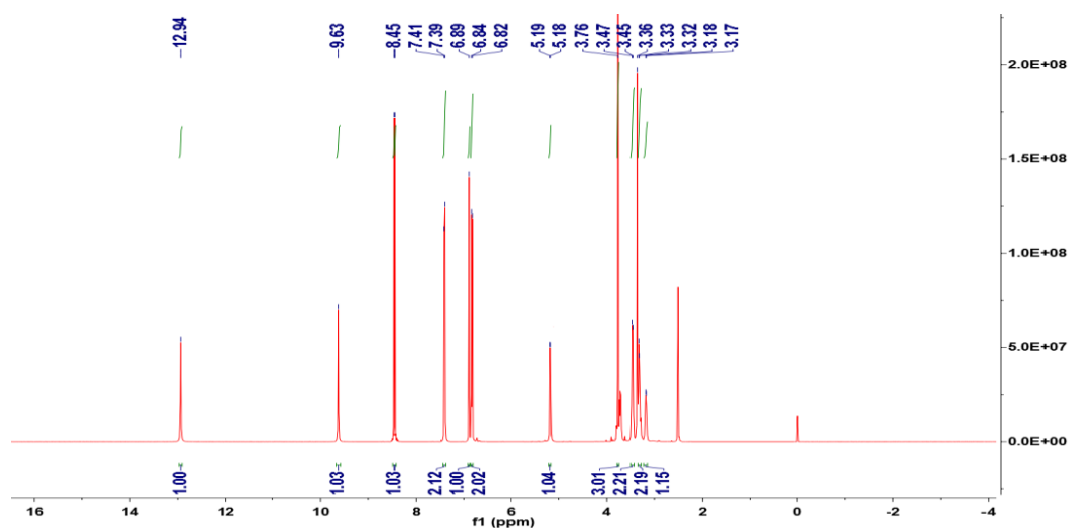
ESI-MS (m/z): 299.06 [M-H]⁻(calcd for C₁₆H₁₂O₆). ¹H NMR (600 MHz, DMSO-*d*₆) δ : 12.99 (1H, s, OH), 9.38 (1H, s, 4'-OH), 9.30 (1H, s, 2'-OH), 8.23 (1H, s, H-2), 6.98 (1H, d, J = 8.4 Hz, H-6'), 6.65 (1H, d, J = 2.1 Hz, H-8), 6.42 (1H, d, J = 2.4 Hz, H-6), 6.38 (1H, d, J = 2.4 Hz, H-3'), 6.27 (1H, dd, J = 8.4, 2.4 Hz, H-5'), 3.87 (3H, s, 7'-OCH₃).



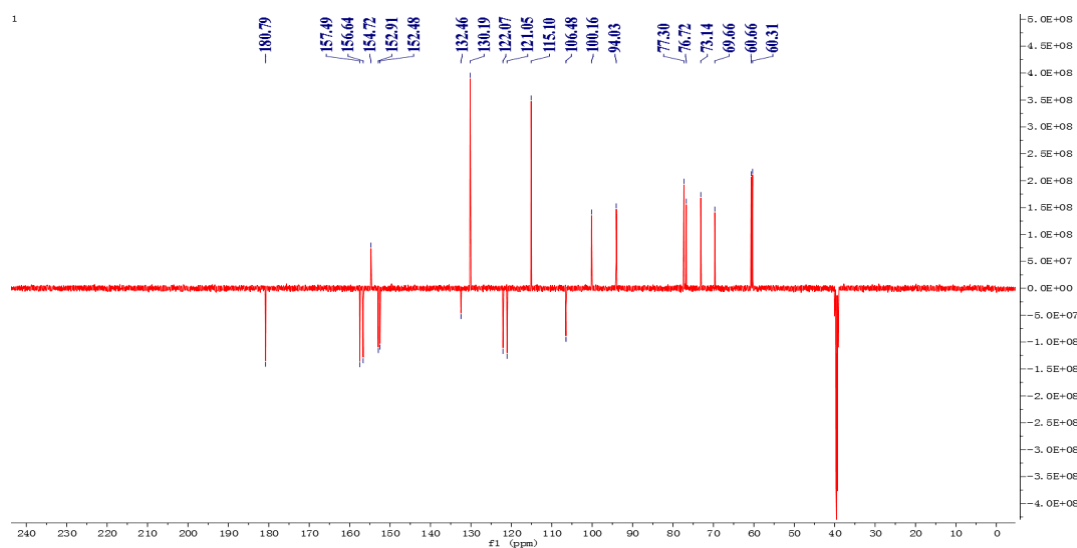
Compound **12**: ¹H-NMR spectra

S13: NMR and mass data and spectra of compound **13** (Tectoridin)

ESI-MS (m/z): 461[M-H]⁻, (calcd for C₂₂H₂₂O₁₁). ¹H NMR (500 MHz, DMSO-*d*₆) δ : 12.94 (1H, s, 5-OH), 9.63 (1H, s, 4'-OH), 8.45 (1H, s, H-2), 7.40 (2H, d, J = 8.6 Hz, H-2',6'), 6.89 (1H, s, H-8), 6.83 (2H, d, J = 8.6 Hz, H-3',5'), 3.76 (3H, s, 6-OCH₃), 5.18 (1H, d, J =4.5 Hz, H-1''), 3.17-3.47 (m, other sugar protons); DEPTQSP (125 MHz, DMSO-*d*₆) δ : 180.79 (C-4), 157.49 (C-4'), 156.64 (C-7), 154.72 (C-9), 152.91 (C-2), 152.48 (C-5), 132.46 (C-6), 130.19 (C-2', 6'), 122.07 (C-1'), 121.05 (C-3), 115.10 (C-3', 5'), 106.48 (C-10), 94.03 (C-8), 60.31 (6-OCH₃), 100.16 (C-1''), 73.14 (C-2''), 77.30 (C-3''), 69.66 (C-4''), 76.72 (C-5''), 60.66 (C-6'').



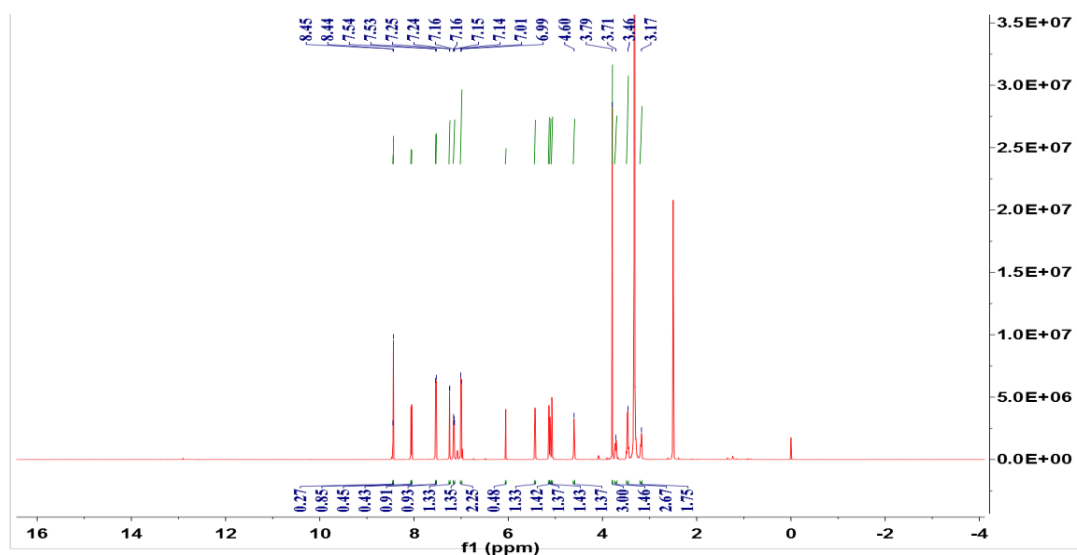
Compound **13**: ¹H-NMR spectra



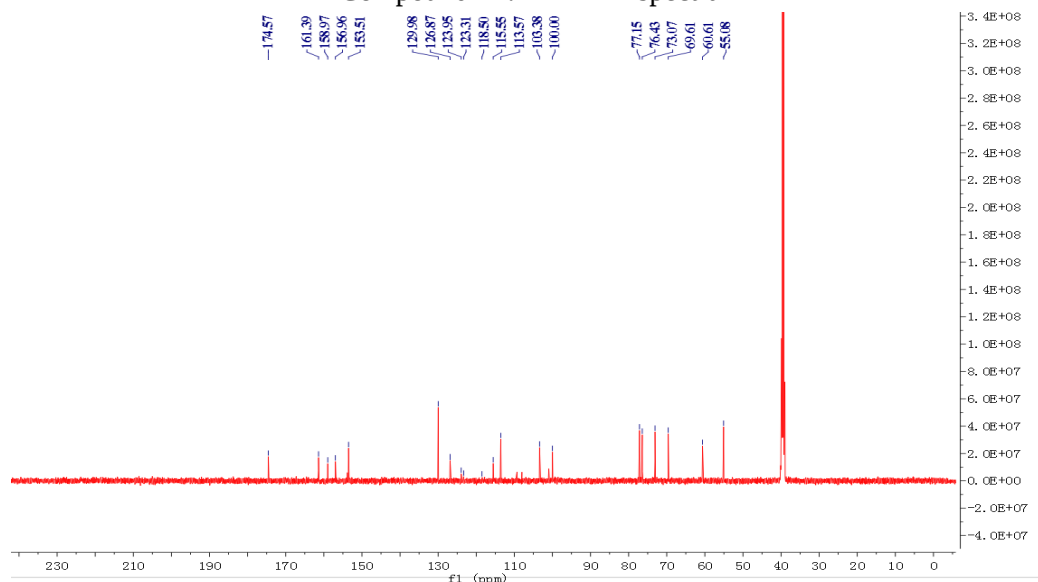
Compound **13**: DEPTQSP spectra

S14 :NMR and mass data and spectra of compound 14 (Ononin)

ESI-MS (m/z): 429 $[M-H]^-$, (calcd for $C_{22}H_{22}O_9$). 1H NMR (600 MHz, $DMSO-d_6$) δ 8.44 (1H, s, H-2), 8.06 (1H, d, $J=9.0$ Hz, H-5), 7.53 (2H, d, $J=8.7$ Hz, H-2', 6'), 7.24 (1H, d, $J=2.1$ Hz, H-8), 7.15 (1H, dd, $J=9.0, 2.1$ Hz, H-6), 7.00 (2H, d, $J=8.7$ Hz, H-3', 5'), 3.79 (3H, s, 4'-OCH₃), 5.11 (1H, d, $J=7.3$ Hz, H-1''), 3.17-3.46 (m, other sugar protons); DEPTQSP (150 MHz, $DMSO-d_6$) δ : 174.80 (C-4), 161.53 (C-7), 159.12 (C-4'), 157.14 (C-9), 153.75 (C-2), 130.18 (C-2', 6'), 127.07 (C-5), 124.07 (C-3), 123.47 (C-1'), 118.53 (C-10), 115.74 (C-6), 113.73 (C-3', 5'), 103.49 (C-8), 100.05 (glc-C-1''), 77.27 (C-5''), 76.53 (C-3''), 73.20 (C-2''), 69.71 (C-4''), 60.72 (C-6''), 55.23 (4'-OCH₃).



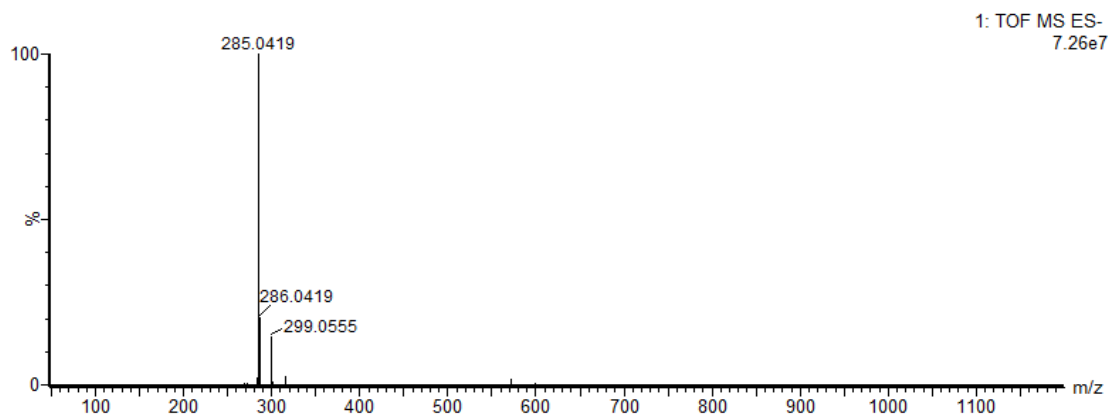
Compound 14: 1H -NMR spectra



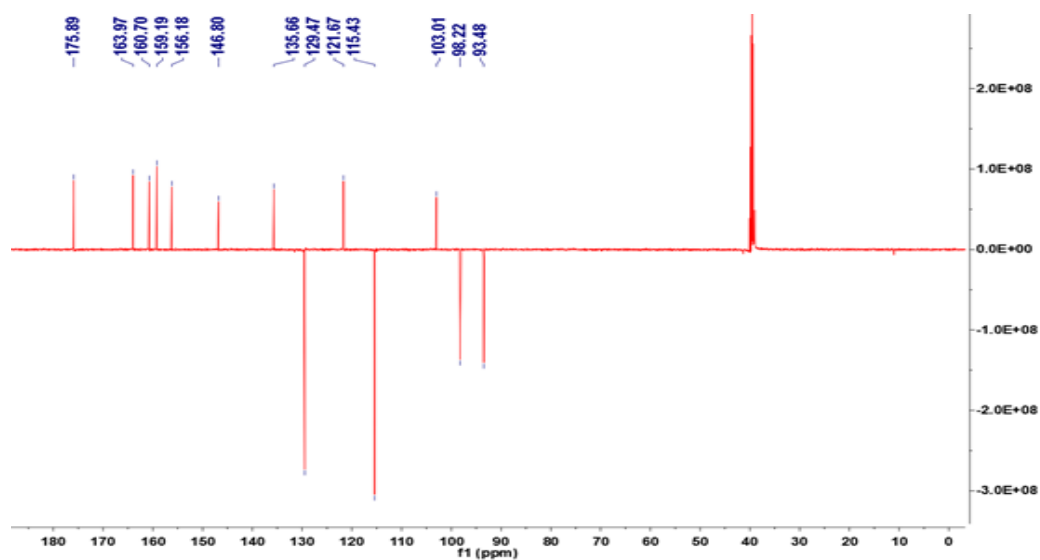
Compound 14: ^{13}C -NMR spectra

S15 :NMR and mass data and spectra of compound 15 (Kaempferol)

Q/TOF-MS (m/z): 285.0419 [$M-H$]⁻, (calcd for $C_{15}H_{10}O_6$). DEPTQSP (125 MHz, DMSO- d_6) δ : 146.80 (C-2), 135.66 (C-3), 175.89 (C-4), 160.70 (C-5), 98.22 (C-6), 163.97 (C-7), 93.48 (C-8), 156.18 (C-9), 103.02 (C-10), 121.67 (C-1'), 129.47 (C-2', 6'), 115.43 (C-3', 5'), 159.19 (C-4').



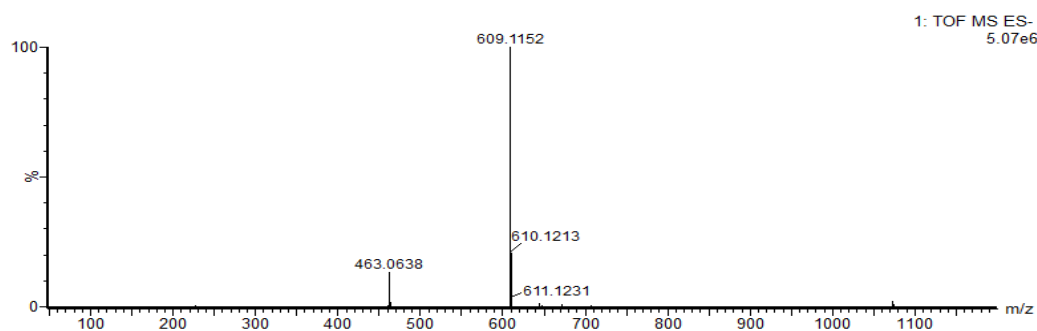
Compound 15: Q/TOF-MS spectra



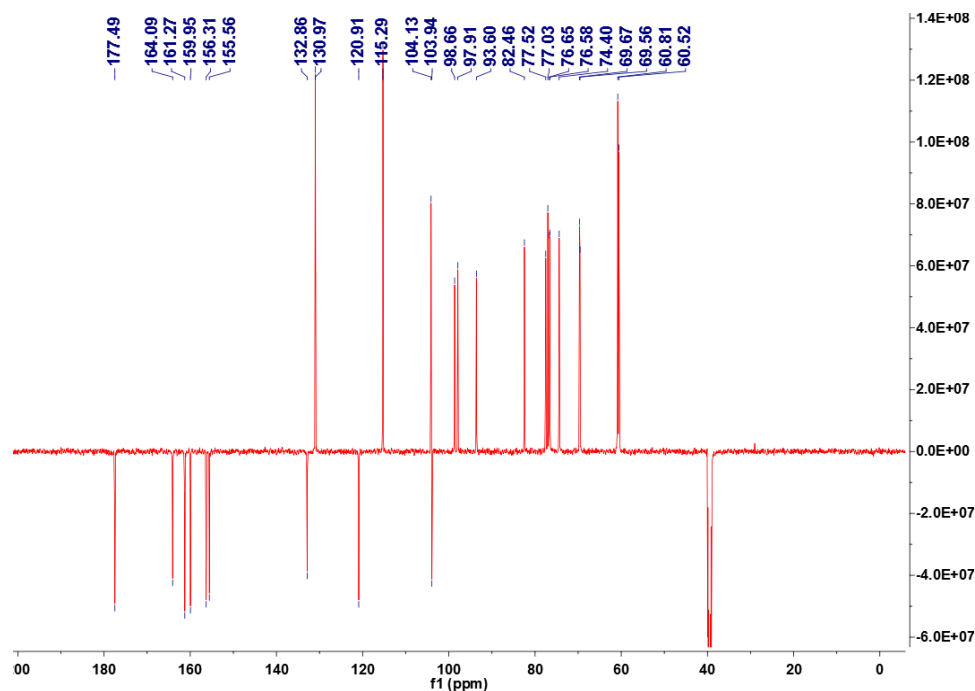
Compound 15: DEPTQSP spectra

S16 :NMR and mass data and spectra of compound 16 (Sophoraflavonolside)

Q/TOF-MS (m/z): 609.1152 [$M-H$]⁻, (calcd for $C_{27}H_{30}O_{16}$). DEPTQSP (125 MHz, DMSO- d_6) δ : 156.31 (C-2), 132.86 (C-3), 177.49 (C-4), 161.27 (C-5), 98.66 (C-6), 164.09 (C-7), 93.60 (C-8), 155.56 (C-9), 103.94 (C-10), 120.91 (C-1'), 0.97 (C-2', 6'), 115.29 (C-3', 5'), 159.95 (C-4'), 97.91 (C-1''), 82.46 (C-2''), 77.52 (C-3''), 69.67 (C-4''), 77.03 (C-5''), 60.81 (C-6''), 104. (C-1'''), 74.40 (C-2'''), 76.65 (C-3'''), 69.56 (C-4'''), 76.58 (C-5'''), 60.52 (C-6''').



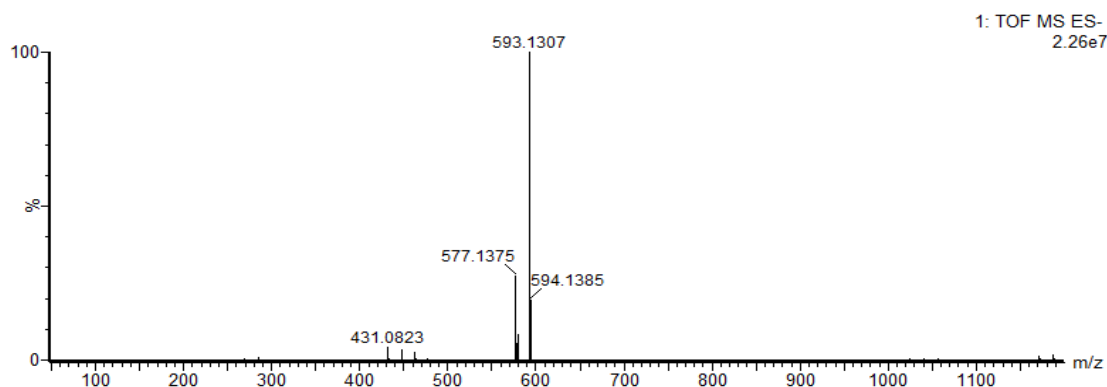
Compound 16: Q/TOF-MS spectra



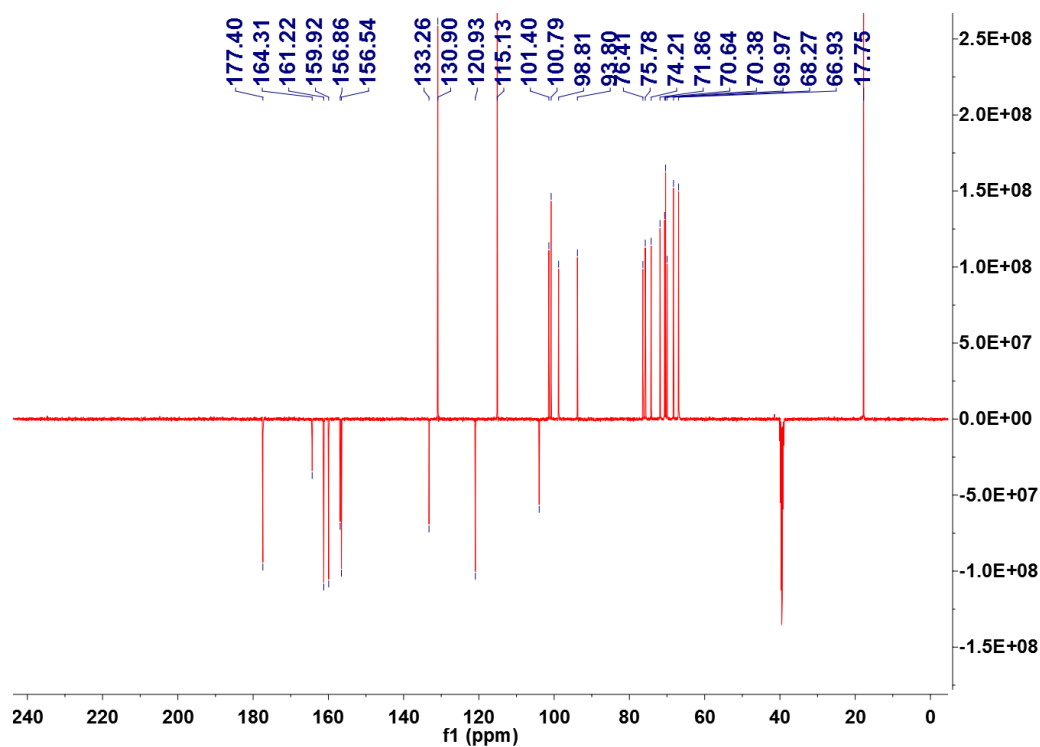
Compound 16: DEPTQSP spectra

S17 :NMR and mass data and spectra of compound **17** (Nicotiflorin)

Q/TOF-MS (m/z): 593.1307 [M-H]⁻, (calcd for C₂₇H₃₀O₁₅). DEPTQSP (125 MHz, DMSO-d₆) δ : 156.86 (C-2), 133.26 (C-3), 177.40 (C-4), 161.22 (C-5), 98.81 (C-6), 164.31 (C-7), 93.80 (C-8), 156.54 (C-9), 103.97 (C-10), 120.93 (C-1'), 130.90 (C-2', C-6'), 115.13 (C-3', C-5'), 159.92 (C-4'), 101.40 (C-1''), 74.21 (C-2''), 76.41 (C-3''), 70.64 (C-4''), 75.78 (C-5''), 66.93 (C-6''), 100.79 (C-1'''), 71.86 (C-2'''), 69.97 (C-3'''), 70.38 (C-4'''), 68.27 (C-5'''), 17.75 (C-6''').



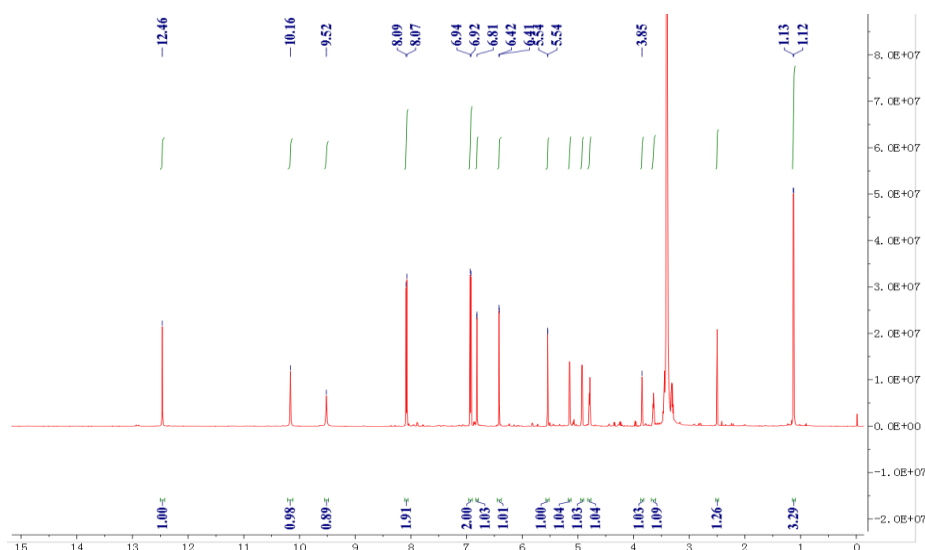
Compound **17**: Q/TOF-MS spectra



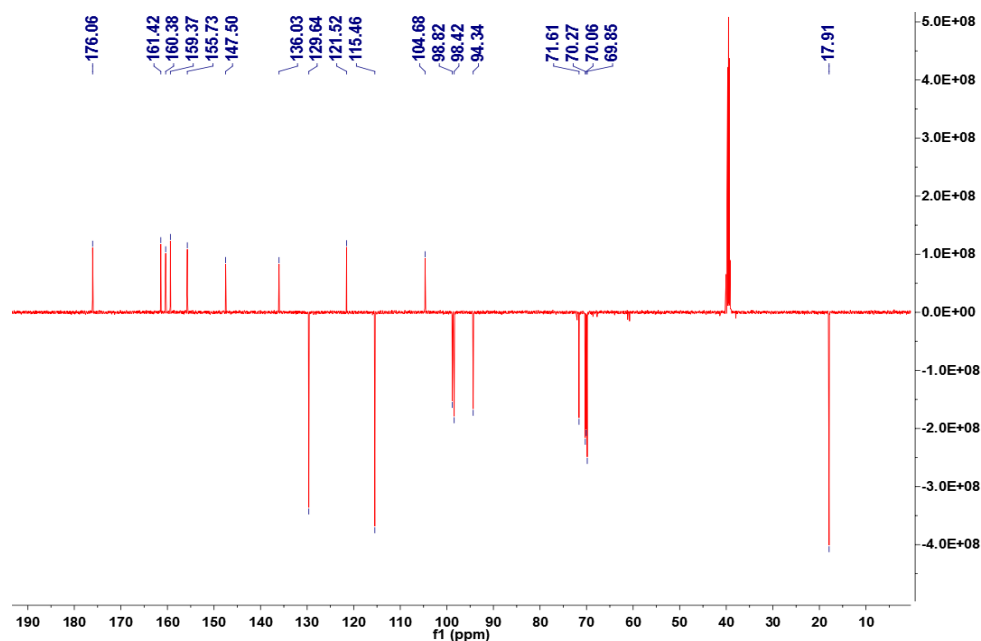
Compound **17**: DEPTQSP spectra

S18 :NMR and mass data and spectra of compound **18** (α -rhamnoisorbin)

ESI-MS (m/z): 431 $[M-H]^-$ (calcd for $C_{21}H_{20}O_{10}$). 1H NMR (600 MHz, $DMSO-d_6$) δ : 12.46 (1H, s, 5-OH), 10.16 (1H, s, 3-OH), 9.52 (1H, s, 4'-OH), 8.08 (2H, d, $J = 8.9$ Hz, H-2', H-6'), 6.93 (2H, d, $J = 8.9$ Hz, H-3', H-5'), 6.81 (1H, d, $J = 2.1$ Hz, H-8), 6.41 (1H, d, $J = 2.1$ Hz, H-6), 5.54 (1H, d, $J = 1.4$ Hz, H-1''), 3.85 (1H, s, H-5''), 1.13 (3H, d, $J = 6.2$ Hz, 5''C-H₃); DEPTQSP (150 MHz, $DMSO-d_6$) δ : 176.06 (C-4), 161.42 (C-7), 160.38 (C-5), 159.37 (C-4'), 155.73 (C-9), 147.50 (C-2), 136.03 (C-3), 129.64 (C-2', C-6'), 121.52 (C-1'), 115.46 (C-3', C-5'), 104.68 (C-10), 98.82 (C-6), 98.42 (C-1''), 94.34 (C-8), 71.61 (C-4''), 70.27 (C-3''), 70.06 (C-2''), 69.85 (C-5''), 17.91 (C-6'').



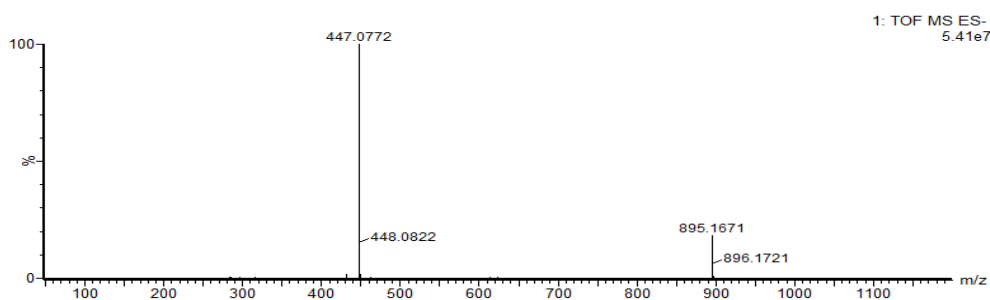
Compound **18**: 1H -NMR spectra



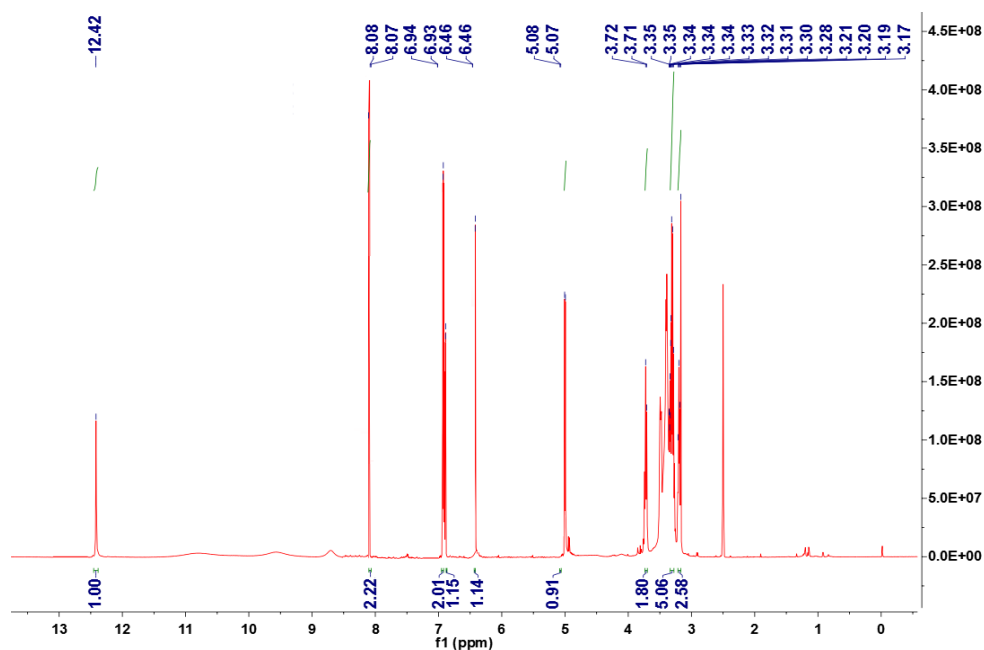
Compound **18**: DEPTQSP spectra

S19 :NMR and mass data and spectra of compound 19 (Populnin)

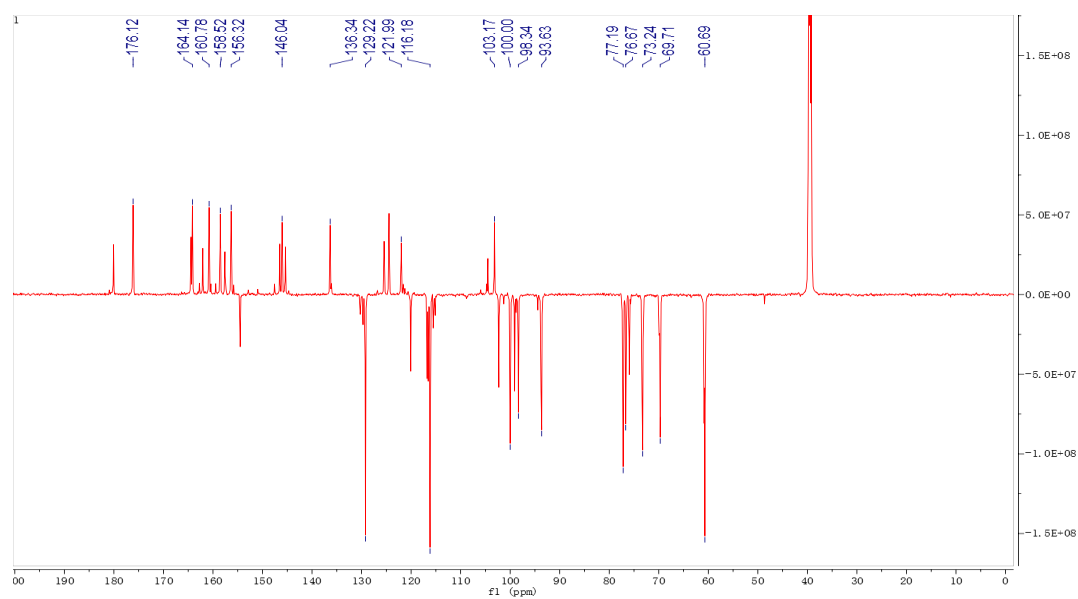
Q/TOF-MS (m/z): 447.0772 [$M-H$]⁻, (calcd for $C_{21}H_{20}O_{11}$). 1H NMR (600 MHz, $DMSO-d_6$) δ : 12.42 (1H, s, 5-OH), 8.07 (2H, d, $J = 8.9$ Hz, H-2', 6'), 6.93 (2H, d, $J = 8.4$ Hz, H-3', 5'), 6.80 (1H, d, $J = 2.1$ Hz, H-8), 6.46 (1H, d, $J = 2.0$ Hz, H-6), 5.07 (1H, d, $J = 7.5$ Hz, H-1''), 3.20-3.72 (m, other sugar protons); DEPTQSP (150 MHz, $DMSO-d_6$) δ : 147.58 (C-2), 136.34 (C-3), 176.12 (C-4), 160.78 (C-5), 98.34 (C-6), 162.05 (C-7), 93.63 (C-8), 155.81 (C-9), 103.17 (C-10), 121.99 (C-1'), 129.22 (C-2', 6'), 116.18 (C-3', 5'), 159.44 (C-4'), 100.00 (C-1''), 73.24 (C-2''), 77.19 (C-3''), 69.71 (C-4''), 76.67 (C-5''), 60.69 (C-6'').



Compound **19**: Q/TOF-MS spectra



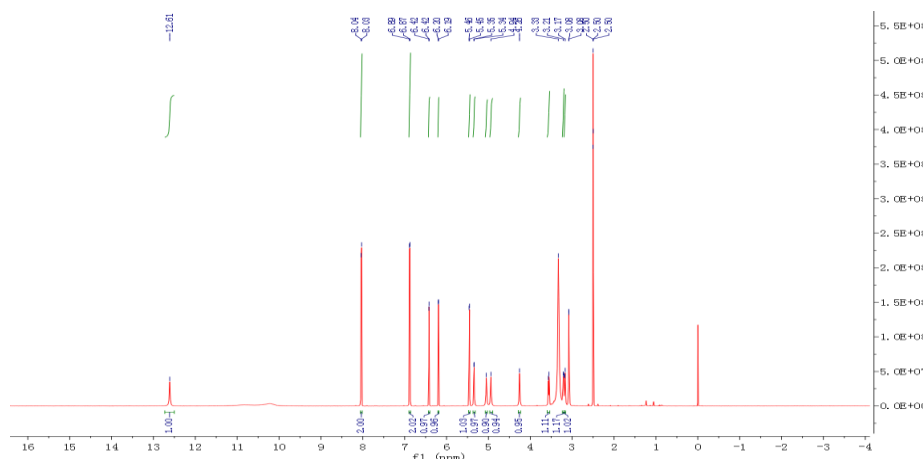
Compound **19**: 1H -NMR spectra



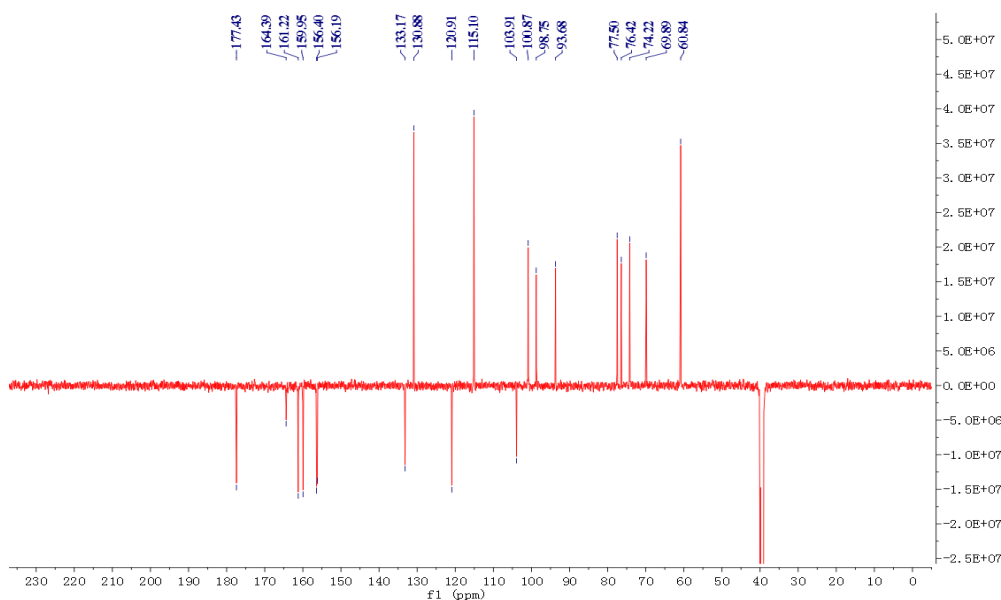
Compound **19**: DEPTQSP spectra

S20 :NMR and mass data and spectra of compound 20 (Astragalin)

Q/TOF-MS (m/z): 471 [M-H]⁻, (calcd for C₂₁H₂₀O₁₀). ¹H NMR (600 MHz, DMSO-*d*₆) δ 12.61 (1H, s, 5-OH), 8.04 (2H, d, J = 8.8 Hz, H-2', 6'), 6.88 (2H, d, J = 8.8 Hz, H-3', 5'), 6.42 (1H, d, J = 1.8 Hz, H-8), 6.19 (1H, d, J = 1.8 Hz, H-6), 5.46 (1H, d, J = 7.6 Hz, H-1''), 103.91 (C-10), 100.86 (C-1''), 77.50 (C-5''), 76.42 (C-3''), 74.21 (C-2''), 69.89 (C-4''), 60.83 (C-6'').



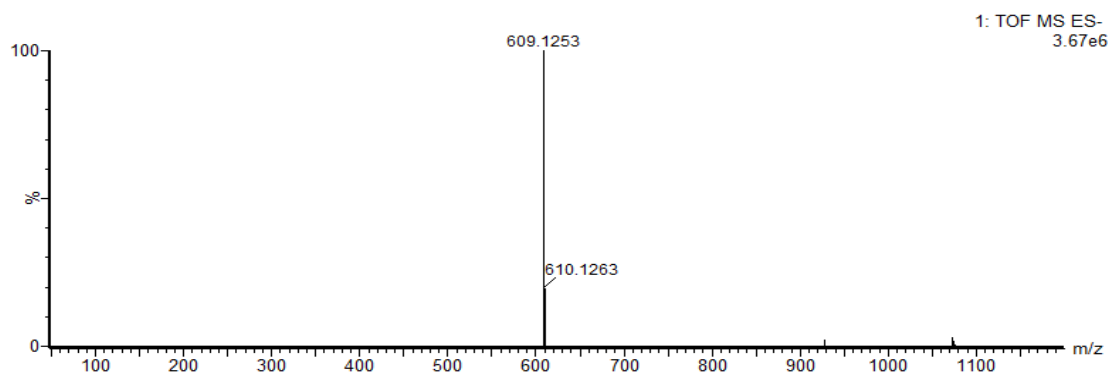
Compound 20: ¹H-NMR spectra



Compound 20: DEPTQSP spectra

S21 :Mass data and spectra of compound 21 (Rutin)

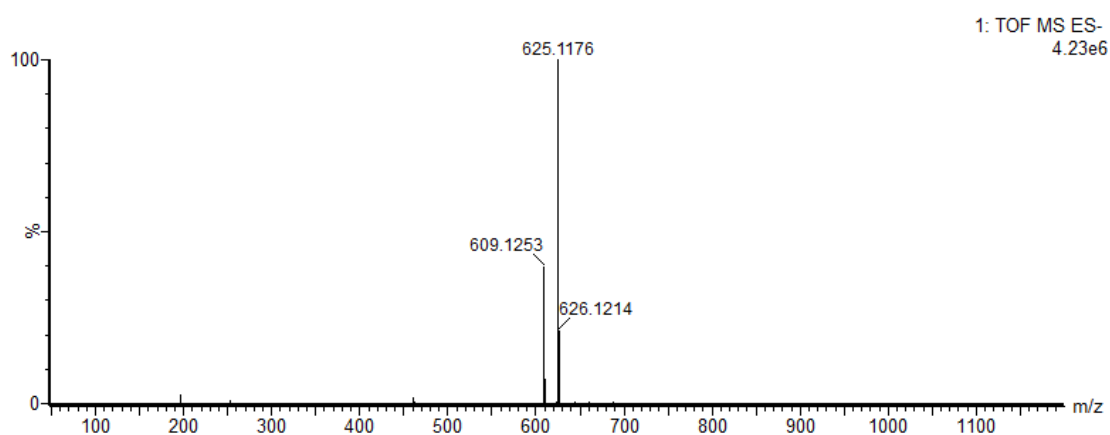
Q/TOF-MS (m/z): 609.1253 $[M-H]^-$, (calcd for $C_{27}H_{30}O_{17}$). Using TLC method to compare the compound **21** with rutin control samples. The results showed that under three different expansion systems, the R_F values these two samples were consistent. Combined with Q/TOF-MS result, the compound was identified as rutin.



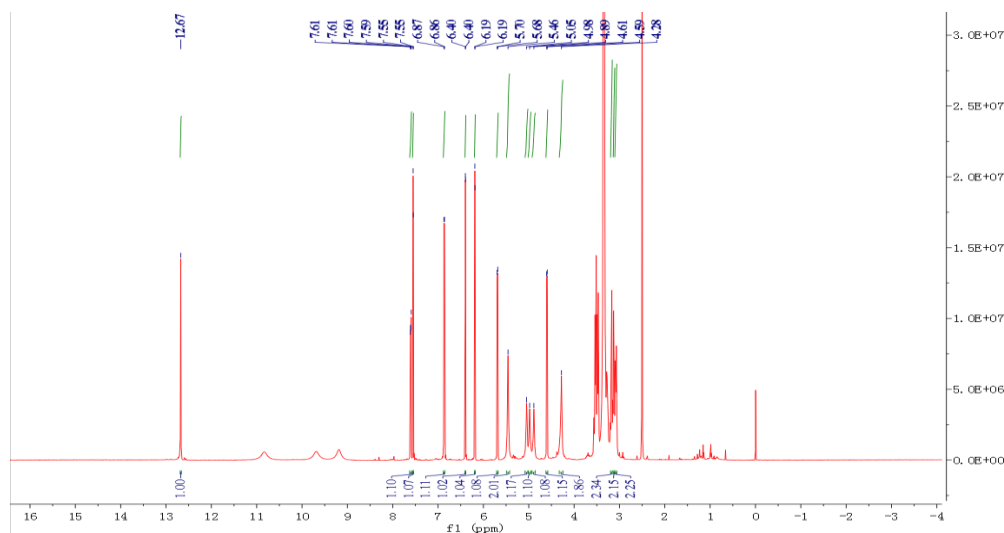
Compound **21**: Q/TOF-MS spectra

S22 :NMR and mass data and spectra of compound 22 (Quercetin-3-O- β -D-sophoroside)

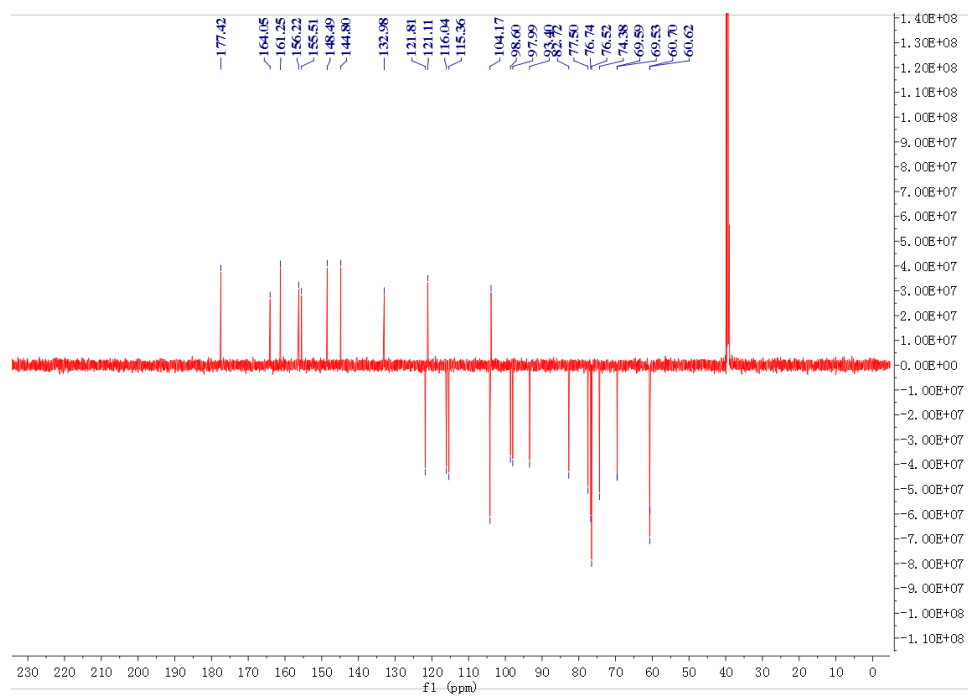
Q/TOF-MS (m/z): 625.1176 [$M-H$]⁻, (calcd for C₂₇H₃₀O₁₇), ¹H NMR (500 MHz, DMSO-*d*₆) δ : 12.67 (1H, s, 5-OH), 10.84 (1H, s, 7-OH), 9.69 (1H, s, 4'-OH), 9.19 (1H, s, 3'-OH), 7.60 (1H, dd, J = 8.5, 2.2 Hz, H-6'), 7.55 (1H, d, J = 2.2 Hz, H-2'), 6.87 (1H, d, J = 8.5 Hz, H-5'), 6.40 (1H, d, J = 2.0 Hz, H-8), 6.19 (1H, d, J = 2.0 Hz, H-6), 5.69 (1H, d, J = 7.5 Hz, H-1''), 4.60 (1H, d, J = 7.8 Hz, H-1'''), 3.58-3.04 (m, other sugar protons); DEPTQSP (125 MHz, DMSO-*d*₆) δ : 177.42 (C-4), 164.05 (C-7), 161.25 (C-5), 156.22 (C-2), 155.51 (C-9), 148.49 (C-4'), 144.80 (C-3'), 132.98 (C-3), 121.81 (C-6'), 121.11 (C-1'), 116.04 (C-5'), 115.36 (C-2'), 103.89 (C-10), 104.17 (C-1''), 98.60 (C-1'''), 97.99 (C-6), 93.40 (C-8), 82.72 (C-2''), 77.50 (C-5'''), 76.74 (C-3'''), 76.52 (C-5''), 76.52 (C-3''), 74.38 (C-2''), 69.59 (C-4''), 69.53 (C-4'''), 60.70 (C-6''), 60.62 (C-6''').



Compound 22: Q/TOF-MS spectra



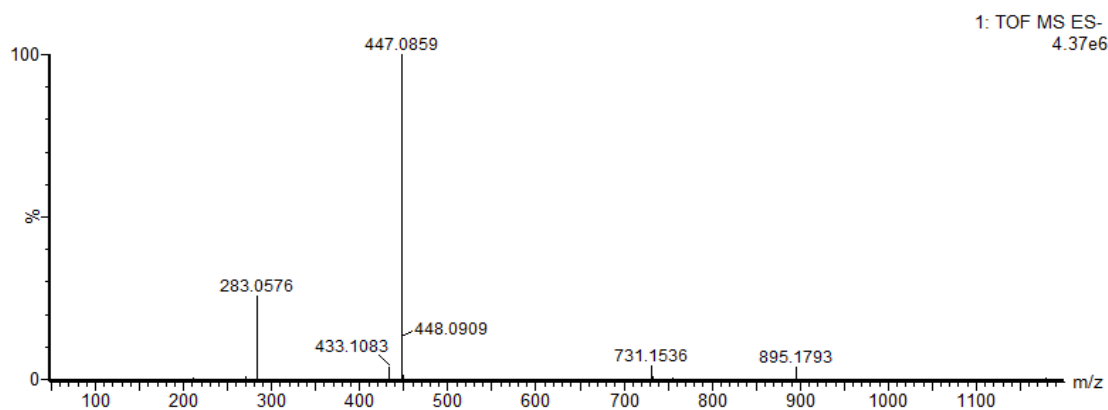
Compound 22: ¹H-NMR spectra



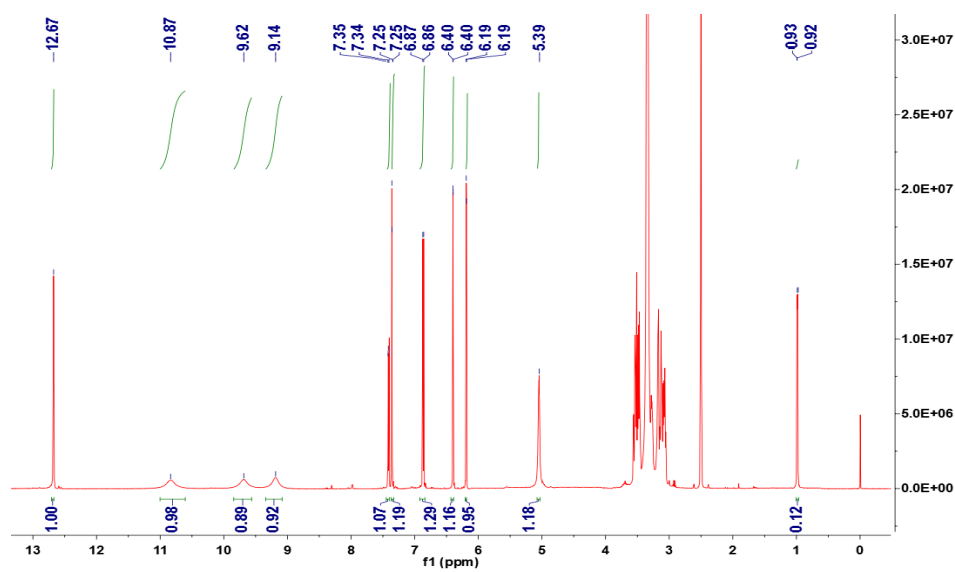
Compound 22: DEPTQSP spectra

S23 :NMR and mass data and spectra of compound 23 (Quercitrin)

Q/TOF-MS (m/z): 447.0859 [$M-H$]⁻, (calcd for $C_{21}H_{20}O_{11}$). 1H NMR (500 MHz, $DMSO-d_6$) δ : 12.67 (1H, s, 5-OH), 10.87 (1H, s, 7-OH), 9.62 (1H, s, 4'-OH), 9.14 (1H, s, 3'-OH), 7.35 (1H, d, $J = 2.2$ Hz, H-2'), 7.25 (1H, dd, $J = 8.5, 2.0$ Hz, H-6'), 6.87 (1H, d, $J = 8.5$ Hz, H-5'), 6.40 (1H, d, $J = 2.0$ Hz, H-8), 6.19 (1H, d, $J = 2.0$ Hz, H-6), 5.39 (1H, brs, H-1''), 0.92 (3H, d, $J = 6.2$ Hz, CH_3-5'').



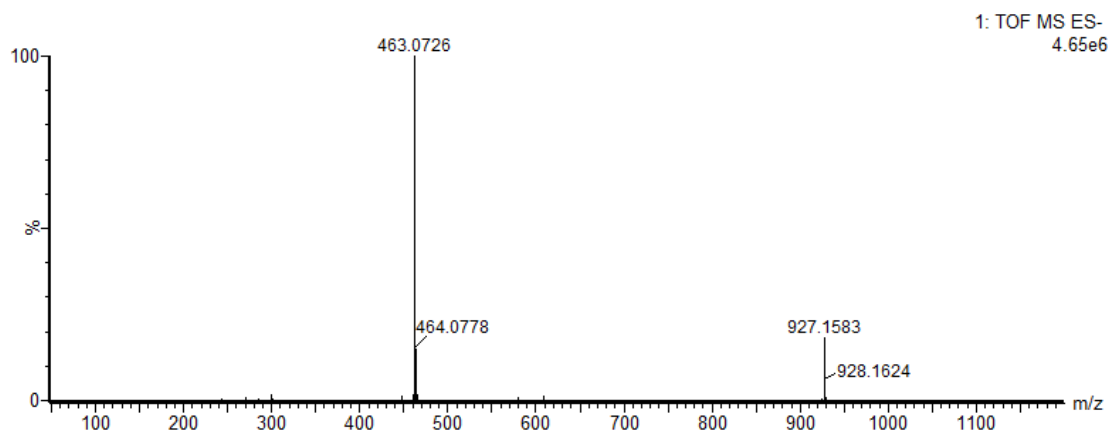
Compound 23: Q/TOF-MS spectra



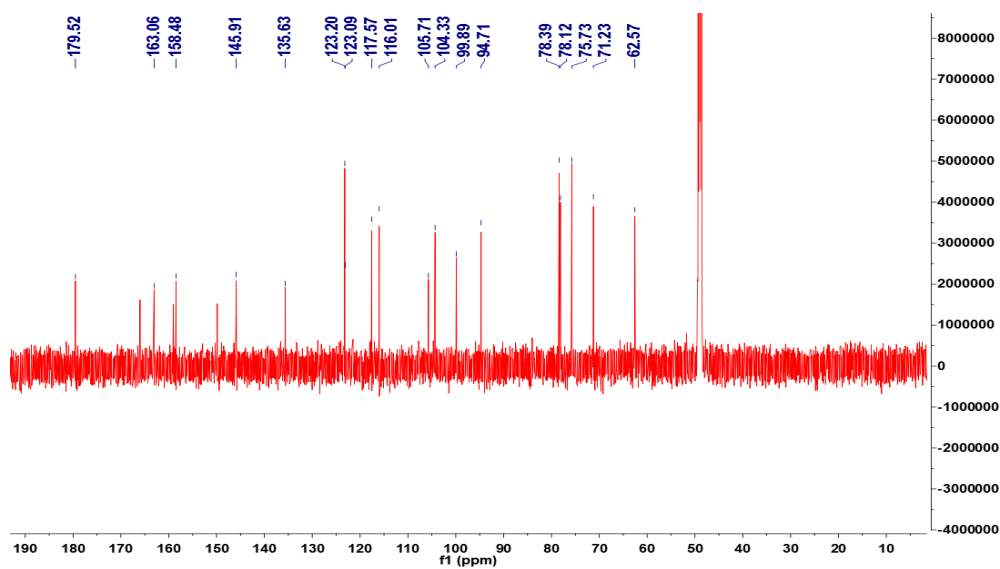
Compound 23: 1H -NMR spectra

S24 :NMR and mass data and spectra of compound 24 (Isoquercitrin)

ESI-MS m/z : 463 $[M-H]^-$, ^{13}C NMR (150 MHz, CD_3OD) δ 179.52 (C-4), 166.00 (C-5), 163.06 (C-7), 159.05 (C-2), 158.48 (C-9), 149.85 (C-4'), 145.91 (C-3'), 135.63 (C-3), 123.20 (C-1'), 123.09 (C-6'), 117.57 (C-5'), 116.01 (C-2'), 105.71 (C-10), 104.33 (Glc-C-1''), 99.89 (C-6), 94.71 (C-8), 78.39 (Glc-C-4''), 78.12 (Glc-C-3''), 75.73 (Glc-C-2''), 71.23 (Glc-C-4''), 62.57 (Glc-C-6'').



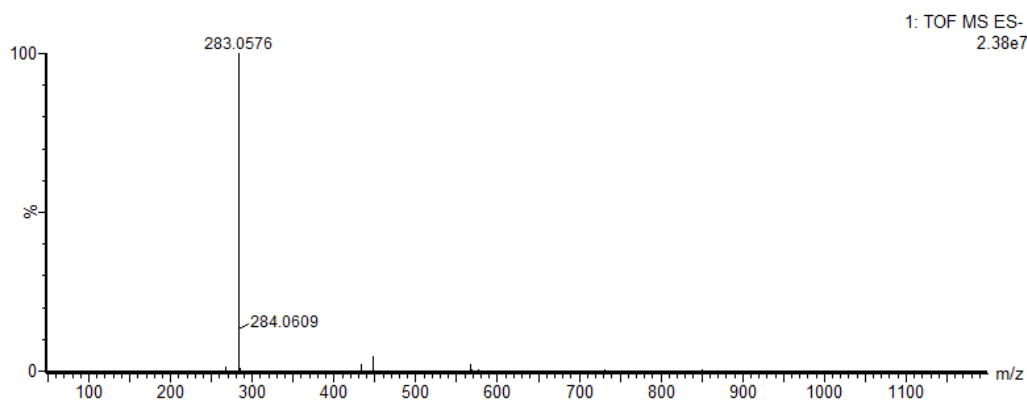
Compound 24: Q/TOF-MS spectra



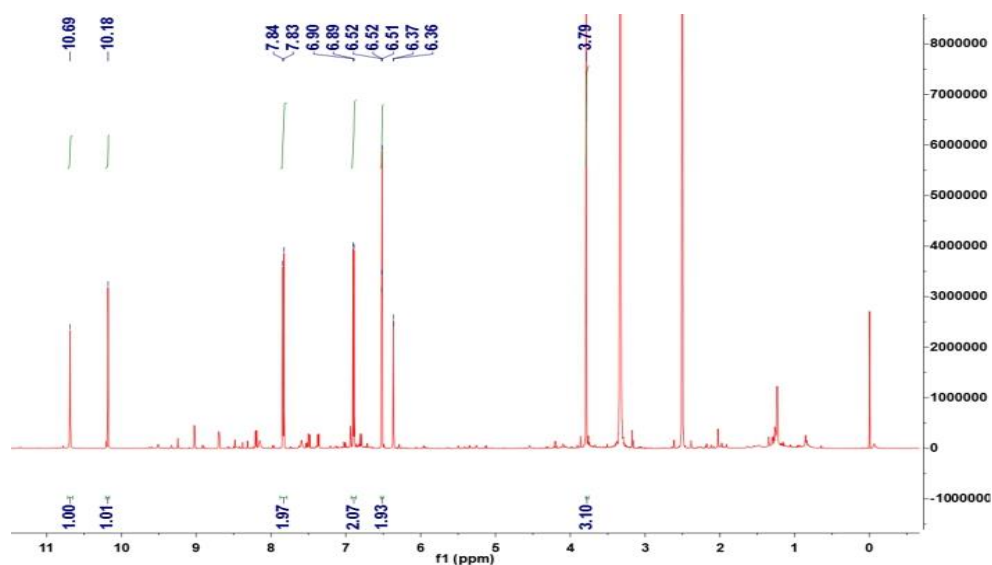
Compound 24: ^1H -NMR spectra

S25 :NMR and mass data and spectra of compound 25 (Thevetiaflavone)

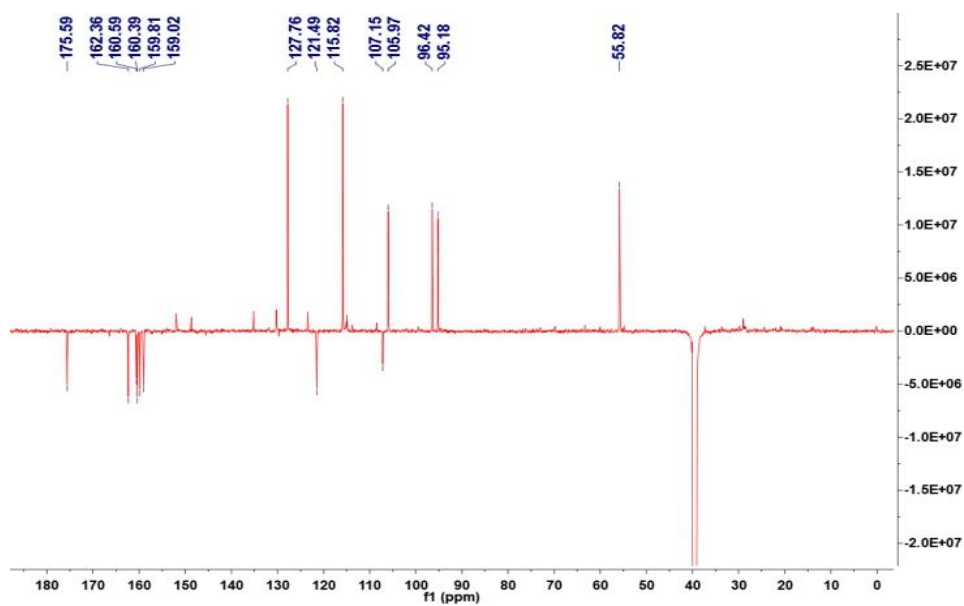
Q/TOF-MS (m/z): 283.0576 $[M-H]^-$, (calcd for $C_{16}H_{12}O_5$). 1H NMR (600 MHz, $DMSO-d_6$) δ : 10.69 (1H, s, 4'-OH), 10.18 (1H, s, 7-OH), 7.83 (2H, d, $J = 8.4$ Hz, H-2', 6'), 6.89 (2H, d, $J = 8.4$ Hz, H-3', 5'), 6.52 (1H, d, $J = 1.8$ Hz, H-8), 6.51 (1H, s, H-3), 6.36 (1H, d, $J = 1.8$ Hz, H-6), 3.79 (3H, s, 5-OCH₃). DEPTQSP (150 MHz, $DMSO-d_6$) δ : 175.59 (C-4), 162.36 (C-7), 160.59 (C-4'), 160.39 (C-2), 159.81 (C-5), 159.02 (C-9), 127.76 (C-2',6'), 121.49 (C-1'), 115.82 (C-3', 5'), 107.15 (C-3), 105.97 (C-10), 96.42 (C-6), 95.18 (C-8), 55.82 (5-OCH₃).



Compound 25: Q/TOF-MS spectra



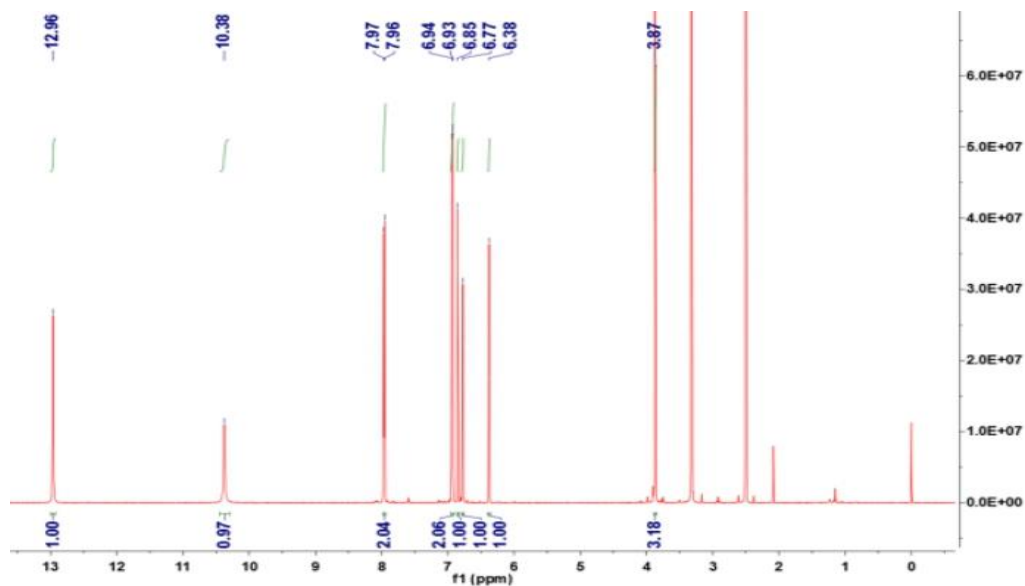
Compound 25: 1H -NMR spectra



Compound 25: DEPTQSP spectra

S26 :NMR and mass data and spectra of compound **26** (Genkwanin)

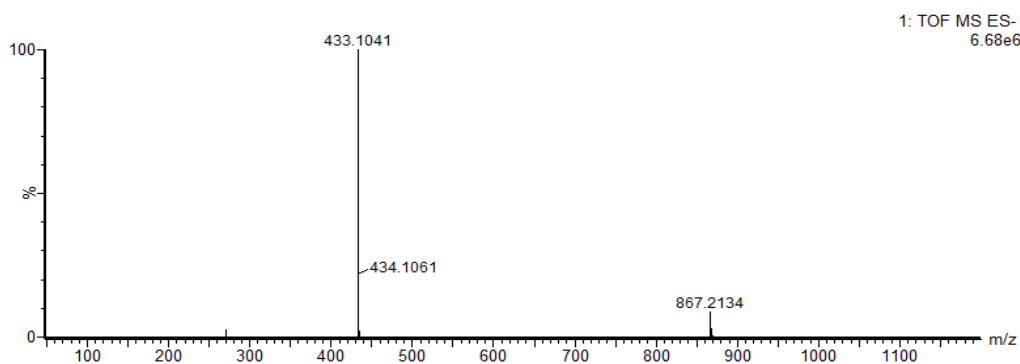
ESI-MS (m/z): 305 [M-H]⁻, (calcd for C₁₆H₁₂O₅). ¹H NMR (600 MHz, DMSO-*d*₆) δ 12.96 (1H, s, 5-OH), 10.38 (1H, s, 4'-OH), 7.96 (2H, d, J = 8.2 Hz, H-2', 6'), 6.93 (2H, d, J = 8.6 Hz, H-3', 5'), 6.85 (1H, s, H-8), 6.77 (1H, s, H-6), 6.38 (1H, s, H-3), 3.87 (3H, s, 7-OCH₃).



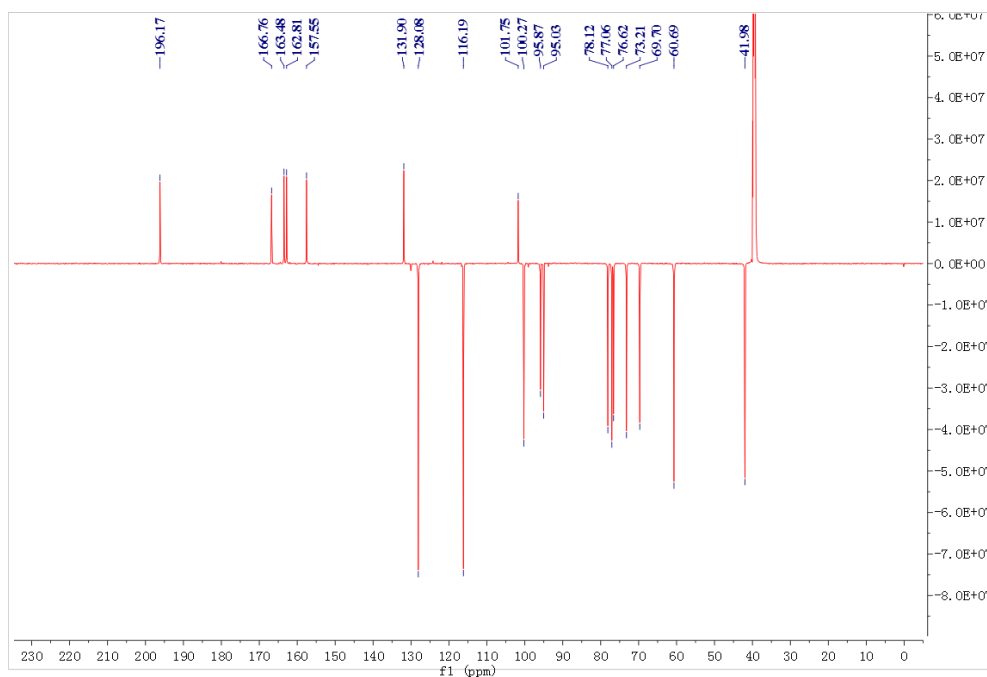
Compound **26**: ¹H-NMR spectra

S27 :NMR and mass data and spectra of compound 27 (Choerospondin)

Q/TOF-MS (m/z): 433.1041 [$M-H$]⁻, (calcd for $C_{21}H_{22}O_{10}$). DEPTQSP (150 MHz, $DMSO-d_6$) δ : 78.12 (C-2), 41.98 (C-3), 196.17 (C-4), 163.48 (C-5), 95.87 (C-6), 166.76 (C-7), 95.03 (C-8), 162.81 (C-9), 101.75 (C-10), 131.90 (C-1'), 128.08 (C-2', 6'), 116.19 (C-3', 5'), 157.55 (C-4'), 100.27 (C-1''), 73.21 (C-2''), 77.06 (C-3''), 69.70 (C-4''), 76.62 (C-5''), 60.69 (C-6'').



Compound 27: Q/TOF-MS spectra



Compound 27: DEPTQSP spectra