

Phytochemicals from *Anneslea fragrans* Wall. and Their Hepatoprotective and Anti-Inflammatory Activities

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The ¹³C NMR data of compounds 1-18

Compound **1**: White powder, C₃₀H₅₀O, HR-ESI-MS *m/z*: 427.3937 [M+H]⁺. ¹³C NMR (125 MHz, CDCl₃): δc 141.5 (C-5), 122.1 (C-6), 77.3 (C-3), 49.6 (C-10), 47.4 (C-8), 43.0 (C-18), 40.8 (C-4), 39.2 (C-14), 38.9 (C-16), 37.8 (C-13), 36.0 (C-22), 35.0 (C-21), 34.8 (C-9), 34.6 (C-11), 34.5 (C-29), 33.0 (C-19), 32.4 (C-30), 32.0 (C-15,28), 30.3 (C-12), 30.0 (C-17), 28.9 (C-23), 28.2 (C-20), 27.8 (C-2), 25.4 (C-24), 23.6 (C-7), 19.6 (C-27), 18.4 (C-26), 18.2 (C-1), 16.2 (C-25).

Compound **2**: White powder, C₃₀H₅₀O, HR-ESI-MS *m/z*: 427.3937 [M+H]⁺. ¹³C NMR (125 MHz, CDCl₃): δc 213.4 (C-3), 59.4 (C-5), 58.2 (C-9), 53.1 (C-6), 42.7 (C-8), 42.2 (C-18), 41.5 (C-14), 41.2 (C-13), 39.6 (C-10), 39.2 (C-4), 38.2 (C-1), 37.4 (C-22), 35.9 (C-19), 35.6 (C-29), 35.3 (C-11), 35.0 (C-30), 32.7 (C-17), 32.4 (C-21), 32.2 (C-15), 31.8 (C-12), 30.9 (C-16), 30.5 (C-20), 30.0 (C-23), 28.1 (C-2), 22.3 (C-24), 20.2 (C-28), 18.7 (C-27), 18.2 (C-25), 17.9 (C-7), 14.6 (C-26).

Compound **3**: White powder, C₃₀H₅₀O, HR-ESI-MS *m/z*: 425.3770 [M-H]⁺. ¹³C NMR (125 MHz, CDCl₃): δc 150.4 (C-20), 109.7 (C-29), 78.9 (C-3), 60.5 (C-28), 55.2 (C-5), 50.4 (C-9), 48.7 (C-18), 47.7 (C-17, C-19), 42.7 (C-14), 40.9 (C-8), 38.8 (C-4), 38.7 (C-1), 37.3 (C-13), 37.1 (C-10), 34.2 (C-7), 33.9 (C-22), 29.7 (C-21), 29.1 (C-16), 27.9 (C-23), 27.4 (C-2), 27.0 (C-15), 25.2 (C-12), 20.8 (C-11), 19.0 (C-30), 18.3 (C-6), 16.1 (C-26), 15.9 (C-25), 15.3 (C-24), 14.7 (C-27).

Compound **4**: White needle, C₃₀H₄₈O₅, HR-ESI-MS *m/z*: 487.3429 [M-H]⁺. ¹³C NMR (125 MHz, CDCl₃): δc 178.9 (C-28), 138.6 (C-13), 126.8 (C-12), 77.9 (C-3), 71.6 (C-19), 64.7 (C-2), 53.1 (C-18), 47.6 (C-5), 46.9 (C-9), 46.5 (C-17), 41.6 (C-1), 41.4 (C-14), 41.1 (C-20), 40.4 (C-8), 38.0 (C-4), 37.8 (C-22), 37.3 (C-10), 32.6 (C-7), 28.9 (C-23), 28.0 (C-15), 26.4 (C-21), 25.9 (C-29), 25.1 (C-16), 24.1 (C-27), 23.1 (C-11), 21.8 (C-30), 17.7 (C-6), 16.6 (C-26), 16.3 (C-24), 16.1 (C-25).

Compound **5**: White powder, C₃₀H₄₈O₄, HR-ESI-MS *m/z*: 471.3479 [M-H]⁺. ¹³C NMR (125 MHz, CDCl₃): δc 178.3 (C-28), 138.2 (C-13), 124.5 (C-12), 82.2 (C-3), 67.1 (C-2), 54.7 (C-18), 52.3 (C-5), 47.0 (C-17), 46.9 (C-9), 46.8 (C-1), 41.7 (C-14), 38.5 (C-8), 38.4 (C-19), 37.5 (C-20), 36.3 (C-22), 32.6 (C-4), 30.2 (C-10), 29.8 (C-23), 28.8 (C-7), 27.5 (C-21), 23.8 (C-15), 23.2 (C-27), 22.9 (C-16), 21.8 (C-30), 21.0 (C-11), 18.0 (C-6,30), 17.2 (C-26), 17.0 (C-29), 16.9 (C-25), 16.5 (C-24).

Compound **6**: White powder, C₃₁H₆₄O, HR-ESI-MS *m/z*: 453.3428 [M+H]⁺. ¹³C NMR (125 MHz, CDCl₃): δc 63.1 (1-CH₂OH), 22.6-32.8 (2~30-CH₂), 14.1 (31-CH₃).

Compound **7**: Yellow needle crystal, C₂₁H₂₄O₉, HR-ESI-MS *m/z*: 419.1348 [M-H]⁺. ¹³C NMR (125 MHz, DMSO-*d*₆): δ_c 204.4 (C-7'), 163.5 (C-2'), 163.3 (C-4'), 155.4 (C-4), 132.6 (C-6'), 130.9 (C-1), 129.2 (C-2,6), 115.0 (C-3,5), 114.4 (C-1'), 108.3 (C-5'), 103.4 (C-1''), 99.6 (C-3'), 77.1 (C-5''), 76.4 (C-3''), 73.0 (C-2''), 69.5 (C-4''), 62.3 (C-6''), 39.9 (C-α), 28.9 (C-β).

Compound **8**: Yellow oil, C₁₅H₁₄O₅, HR-ESI-MS *m/z*: 274.0769 [M]. ¹³C NMR (125 MHz, DMSO-*d*₆): δ_c 203.9 (C-7'), 164.7 (C-2'), 164.2 (C-4'), 145.0 (C-3), 143.3 (C-4), 133.1 (C-6'), 131.7 (C-1), 118.9 (C-6), 115.8 (C-2), 115.4 (C-5), 112.5 (C-1'), 108.1 (C-5'), 102.4 (C-3'), 39.5 (C-α), 29.2 (C-β).

Compound **9**: Yellow crystal, C₁₅H₁₄O₄, HR-ESI-MS *m/z*: 258.0818 [M]. ¹³C NMR (125 MHz, DMSO-*d*₆): δ_c 203.8 (C-7'), 164.8 (C-2'), 164.2 (C-4'), 155.5 (C-4), 133.1 (C-6'), 131.0 (C-1), 129.2 (C-2,6), 115.1 (C-3,5), 112.5 (C-1'), 108.1 (C-5'), 102.4 (C-3'), 38.6 (C-α), 29.1 (C-β).

Compound **10**: Yellow powder, C₂₂H₂₆O₁₀, HR-ESI-MS *m/z*: 449.1463 [M-H]⁺. ¹³C NMR (125 MHz, DMSO-*d*₆): δ_c 198.8 (C-7'), 162.6 (C-4'), 158.7 (C-2'), 147.3 (C-3), 144.3 (C-4), 132.5 (C-1), 131.7 (C-6'), 120.3 (C-1'), 119.6 (C-6), 115.2 (C-5), 112.3 (C-2), 109.3 (C-5'), 102.0 (C-3'), 100.6 (C-1''), 77.1 (C-3''), 76.6 (C-5''), 73.4 (C-2''), 69.5 (C-4''), 62.7 (C-6''), 55.5 (3-OCH₃), 44.6 (C-α), 29.6 (C-β).

Compound **11**: White crystals, C₂₂H₂₆O₁₀, HR-ESI-MS *m/z*: 451.1885 [M+H]⁺. ¹³C NMR (125 MHz, DMSO-*d*₆): δ_c 204.5 (C-7'), 163.5 (C-2'), 163.3 (C-4'), 147.4 (C-3), 144.6 (C-4), 132.6 (C-6'), 131.6 (C-1), 120.4 (C-6), 115.2 (C-5), 114.5 (C-1'), 112.6 (C-2), 108.3 (C-5'), 103.3 (C-1''), 99.5 (C-3'), 77.0 (C-5''), 76.3 (C-3''), 73.0 (C-2''), 69.5 (C-4''), 60.5 (C-6''), 55.5 (3-OCH₃), 39.5 (C-α), 29.4 (C-β).

Compound **12**: Yellow crystal, C₂₁H₂₂O₁₀, HR-ESI-MS *m/z*: 433.1139 [M-H]⁺. ¹³C NMR (125 MHz, DMSO-*d*₆): δ_c 192.0 (C-7'), 165.0 (C-2'), 163.5 (C-4'), 149.1 (C-3), 145.6 (C-α), 145.5 (C-4), 132.4 (C-6'), 126.1 (C-1), 122.6 (C-6), 117.3 (C-β), 116.0 (C-5), 115.7 (C-2), 114.8 (C-1'), 108.2 (C-5'), 103.4 (C-3'), 101.6 (C-1''), 77.1 (C-3''), 76.4 (C-5''), 73.1 (C-2''), 69.6 (C-4''), 60.6 (C-6'').

Compound **13**: White powder, C₂₁H₂₀O₁₁, HR-ESI-MS *m/z*: 447.2132 [M-H]⁺. ¹³C NMR (125 MHz, DMSO-*d*₆): δ_c 178.2 (C-4), 166.4 (C-7), 161.8 (C-5), 158.8 (C-4'), 157.7 (C-9), 148.4 (C-2), 135.1 (C-3), 129.2 (C-2',6'), 122.9 (C-1'), 115.8 (C-3',5'), 109.6 (C-6), 102.3 (C-10), 94.0 (C-8), 81.6 (C-5''), 78.9 (C-3''), 75.7 (C-1''), 74.1 (C-2''), 71.5 (C-4''), 62.2 (C-6'').

Compound **14**: Yellow oil, C₂₁H₂₀O₁₁, HR-ESI-MS *m/z*: 447.0933 [M-H]⁺. ¹³C NMR (125 MHz, DMSO-*d*₆): δ_c 177.7 (C-4), 164.2 (C-7), 161.3 (C-5), 157.3 (C-9), 156.4 (C-2), 148.4 (C-4'), 145.2 (C-3'), 134.2 (C-3), 121.1 (C-6'), 120.7 (C-1'), 115.6 (C-5'), 115.4 (C-2'), 104 (C-10), 101.8 (C-1''), 98.7 (C-6), 93.6 (C-8), 71.1 (C-2''), 70.6 (C-3''), 70.3 (C-4''), 70.1 (C-5''), 17.5 (C-6'').

Compound **15**: Yellow powder, C₂₁H₂₀O₁₂, HR-ESI-MS *m/z*: 463.0897 [M-H]⁺. ¹³C NMR (125 MHz, DMSO-*d*₆): δ_c 177.6 (C-4), 164.1 (C-7), 161.2 (C-5), 156.3 (C-2), 156.2 (C-9), 148.5 (C-4'), 144.8 (C-3'), 133.4 (C-3), 122.1 (C-6'), 121.1 (C-1'), 115.9 (C-5'), 115.1 (C-2'), 103.8 (C-10), 101.8 (C-1''), 98.7 (C-6), 93.5 (C-8), 75.8 (C-5''), 73.1 (C-3''), 71.2 (C-2''), 67.9 (C-4''), 60.1 (C-6'').

Compound **16**: Yellow powder, C₁₅H₁₀O₅, HR-ESI-MS *m/z*: 269.0455 [M-H]⁺. ¹³C NMR (125 MHz, DMSO-*d*₆): δ_c 181.2 (C-3), 167.4 (C-6), 166.1 (C-8), 148.1 (C-4'), 148.6 (C-2), 145.5 (C-3'), 125.7 (C-4), 124.5 (C-6'), 123.4 (C-1'), 117.9 (C-2'), 116.5 (C-5'), 116.1 (C-9), 114.1 (C-10), 113.9 (C-7), 98.3 (C-5).

Compound **17**: Yellow powder, C₁₅H₂₀O₈, HR-ESI-MS *m/z*: 327.1139 [M-H]⁺. ¹³C NMR (125 MHz, DMSO-*d*₆): δ_c 203.3 (C-7), 163.5 (C-2), 163.4 (C-4), 132.8 (C-6), 121.7 (C-1), 108.3 (C-5), 103.4 (C-3), 99.6 (C-1'), 77.1 (C-3'), 76.4 (C-5'), 73.1 (C-2'), 69.5 (C-4'), 67.4 (C-6'), 58.1 (4-OCH₃), 38.1 (C-8).

Compound **18**: White powder, C₃₁H₃₈O₁₁, HR-ESI-MS *m/z*: 585.2344 [M-H]⁺. ¹³C NMR (125 MHz, DMSO-*d*₆): δ_c 152.6 (C-3',C-5'), 146.8 (C-3''), 145.4 (C-4''), 145.3 (C-3), 147.4 (C-4), 136.9 (C-1), 138.7 (C-1'), 135.3 (C-4'), 132.9 (C-1''), 128.9 (C-5), 119.2 (C-6''), 116.4 (C-6), 114.6 (C-5''), 112.5 (C-2), 111.0 (C-2''), 103.3 (C-2',6'), 87.1 (C-8''), 86.7 (C-7'), 71.5 (C-7''), 62.8 (C-9'), 60.2 (C-9''), 56.0 (3-OCH₃), 55.7 (3',5'-OCH₃), 55.5 (3''-OCH₃), 53.3 (C-8'), 34.7 (C-8), 31.5 (C-7), 62.3 (C-9).