

## Supporting Information

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### Isolation, Identification and Antiproliferative Activity of Triterpenes from the Genus *Monotheca* A. DC.

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*Lupeol (1)*: White amorphous solid; melting point 215°C, EI-MS *m/z* (rel. abundance): 426 (52) [M]<sup>+</sup>, 411 (20), 393 (8), 218 (42), 207 (80), 189 (100), 139 (74). HREI-MS *m/z*: 426.3820 (calcd. for C<sub>30</sub>H<sub>50</sub>O, 426.3861). <sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD),  $\delta$  ppm = 4.20 and 4.21 (2H, br, 1H each, H-29), 3.30 (1H, *dd*, *J* = 9.4, 4.6 Hz, H-3), 0.74, 0.81, 0.85, 0.89, 0.91, 0.97, 1.06 (3H, 7s, 7 Me); <sup>13</sup>C NMR (100 MHz, CD<sub>3</sub>OD)  $\delta$  ppm = 150.7 (C-20), 109.7 (C-29), 79.2 (C-3), 55.2 (C-5), 50.3 (C-9), 48.3 (C-18), 47.8 (C-19), 43.2 (C-17), 42.7 (C-14), 40.7 (C-8), 39.9 (C-22), 38.6 (C-4), 38.2 (C-1), 38.0 (C-13), 37.3 (C-10), 35.9 (C-16), 35.0 (C-7), 29.7 (C-21), 28.4 (C-22), 28.2 (C-23), 27.9 (C-2), 27.2 (C-15), 25.3 (C-12), 21.1 (C-11), 19.3 (C-30), 18.4 (C-6), 18.2 (C-28), 15.8 (C-25), 15.5 (C-26), 15.3 (C-27), 15.1 (C-24). All data were in agreement with the published data [7].

*Lupeol acetate (2)*: White greasy substance; melting point 214-216°C; EI-MS *m/z* (rel. abundance): 468.2 (36) [M]<sup>+</sup>, 453 (18), 427 (8), 408 (10), 357 (14), 249 (22), 218 (46), 189 (100), 135 (44), 95 (46). HREI-MS *m/z*: 468.3960 (calcd. for C<sub>32</sub>H<sub>52</sub>O<sub>2</sub>, 468.3961). <sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD),  $\delta$  ppm = 4.47 and 4.44 (2H, br, 1H each, H-29), 4.03 (1H, *dd*, *J* = 9.8, 4.3 Hz, H-3), 0.76, 0.81, 0.83, 0.86, 0.92, 1.01, 1.31 (3H, 7s, 7 Me) and 2.32 (3H, *s*, CH<sub>3</sub>COO). <sup>13</sup>C NMR (100 MHz, CD<sub>3</sub>OD)  $\delta$  ppm = 172.2 (C-1'), 150.2 (C-20), 110.5 (C-29), 81.1 (C-3), 50.7 (C-9), 48.7 (C-18), 48.4 (C-19), 38.5 (C-1), 22.7 (C-2), 37.2 (C-4), 55.3 (C-5), 18.3 (C-6), 34.8 (C-7), 41.2 (C-8), 40.1 (C-22), 37.2 (C-10), 21.2 (C-11), 24.6 (C-12), 37.2 (C-13), 43.0 (C-14), 26.4 (C-15), 35.8 (C-16), 43.1 (C-17), 29.9 (C-21), 28.2 (C-23), 20.4 (C-2'), 19.3 (C-30), 16.1 (C-24), 16.3 (C-25), 15.4 (C-26), 14.2 (C-27), 14.8 (C-28). All data were in agreement with the published data [8].

*Betulic acid (3)*: White amorphous powder; melting point 217-219°C; EI-MS *m/z* (rel. abundance): 442 [M]<sup>+</sup> (6), 411 (6), 384 (8), 207 (30), 203 (74), 183 (34), 57 (100). HREI-MS *m/z*: 442.3819 calcd. for molecular formula C<sub>30</sub>H<sub>50</sub>O<sub>2</sub>; <sup>1</sup>H NMR (500 MHz, CD<sub>3</sub>OD),  $\delta$  ppm = 4.46 and 4.92 (*br s*, 1H each, H-29), 3.40 and 3.71 (2H, *d*, *J* = 11.2 Hz, H-28), 3.25 (*dd*, *J* = 11.4, 5.2 Hz, H-3), 0.83 (H<sub>3</sub>-24), 0.84 (H<sub>3</sub>-25), 0.86 (H<sub>3</sub>-23), 0.87 (H<sub>3</sub>-26), 1.02 (H<sub>3</sub>-27), 1.04 (H<sub>3</sub>-30) (3H, 6s, 6 Me); <sup>13</sup>C NMR (125 MHz, CD<sub>3</sub>OD)  $\delta$  ppm = 150.8 (C-20), 109.8 (C-29), 79.1 (C-3), 60.4 (C-28), 38.4 (C-1), 55.3 (C-5), 50.6 (C-9), 48.6 (C-19), 46.6 (C-17), 42.5 (C-18), 42.8 (C-14), 27.5 (C-2), 39.2 (C-4), 37.5 (C-13), 36.2 (C-22), 30.2 (C-21), 18.4 (C-6), 34.3 (C-7), 39.5 (C-8), 37.2 (C-10), 21.0 (C-11), 24.2 (C-12), 27.2 (C-15), 30.3 (C-16), 28.1 (C-23), 19.1 (C-30), 16.1 (C-25), 16.2 (C-26), 15.2 (C-24), 14.8 (C-27). All data were in agreement with the published data [9].

*Oleanolic acid (4)*: White powder; melting point 304-306°C; EI-MS *m/z* (rel. abundance): 456 [M]<sup>+</sup> (2), 410 (8), 248 (100), 203 (56), 133 (42); HR-EI-MS *m/z*: 456.3671 (calcd. for C<sub>30</sub>H<sub>48</sub>O<sub>3</sub>, 456.3603); <sup>1</sup>H NMR (500 MHz, CD<sub>3</sub>OD),  $\delta$  ppm = 5.18 (1H, *br s*, H-12), 3.14 (1H, *dd*, *J* = 10, 5.5 Hz, H-3), 1.19 (3H, *s*), 1.02 (3H, *s*), 0.92 (3H, *s*), 0.88 (3H, *s*), 0.80 (3H, *s*), 0.74 (3H, *s*) and 0.71 (3H, *s*); <sup>13</sup>C NMR (125 MHz, CD<sub>3</sub>OD)  $\delta$  ppm = 180.8 (C-28),

145.8 (C-13), 124.4 (C-12), 78.2 (C-3), 55.9 (C-5), 48.5 (C-9), 47.2 (C-17), 46.6 (C-19), 42.5 (C-18), 42.4 (C-14), 39.4 (C-4), 38.8 (C-1), 33.8 (C-29), 33.3 (C-7), 40.1 (C-8), 37.1 (C-10), 31.4 (C-20); 34.8 (C-21), 33.1 (C-22), 29.8 (C-23), 24.1 (C-11), 28.8 (C-15), 28.2 (C-2), 26.8 (C-27), 24.2 (C-16), 23.6 (C-30), 19.1 (C-6), 17.2 (C-26), 16.4 (C-24), 16.1 (C-25). All data were in agreement with the published data [10].

*β*-Amyrin (5): White amorphous solid; melting point 196-198°C; EI-MS  $m/z$  (rel. abundance): 426 [M]<sup>+</sup> (18), 408 (6), 393 (6), 248 (92), 219 (26), 203 (90), 203 (90), 133 (100), 119 (50), 43 (90). HREI-MS  $m/z$ : 426.3534 (calcd. for C<sub>30</sub>H<sub>50</sub>O, 426.3860); <sup>1</sup>H NMR (500 MHz, CD<sub>3</sub>OD),  $\delta$  ppm = 5.22 (1H, *br s*, H-12), 3.61 (1H, *dd*,  $J = 8, 4.4$  Hz, H-3), 0.80 (3H, *s*), 0.84 (3H, *s*), 0.88 (3H, *s*), 0.95 (3H, *s*), 1.12 (3H, *s*), 1.34 (3H, *s*), 1.01 (3H, *s*) and 1.11 (3H, *s*); <sup>13</sup>C NMR (125 MHz, CD<sub>3</sub>OD)  $\delta$  ppm = 145.6 (C-13), 121.4 (C-12), 78.8 (C-3), 47.2 (C-18), 46.6 (C-19), 37.8 (C-1), 28.1 (C-2), 38.4 (C-4), 55.6 (C-5), 18.8 (C-6), 33.1 (C-7), 38.2 (C-8), 47.8 (C-9), 37.2 (C-10), 23.4 (C-11), 41.2 (C-14), 26.8 (C-15), 27.3 (C-16), 32.2 (C-17), 31.1 (C-20); 34.2 (C-21), 37.3 (C-22), 28.9 (C-23), 15.5 (C-24), 15.6 (C-25), 16.7 (C-26), 26.4 (C-27), 28.8 (C-28), 33.4 (C-29), 23.8 (C-30). All data were in agreement with the published data [11].