Supporting Information

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Secondary Metabolites from *Jacaranda mimosifolia* and *Kigelia africana* (*Bignoniaceae)* and their Anticandidal Activity

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Benzoic acid (**1**). Colorless needle crystal (MeOH); m. p. 122-124^{o}C; ^{1}H-NMR (600 MHz, CDCl3): δ 11.7 (1H,brs, COOH), 8.13 (2H, d, *J* = 8.0 Hz, H-3, H-7), 7.62 (1H, dd, *J* = 7.5 Hz, H-5), 7.47 (2H, dd, *J* = 7.5, 8.0 Hz, H-4, H-6). ^{13}C-NMR (125 MHz, CDCl3) δ: 172.3 (C-1), 129.1 (C-2), 130.1(C-3, C-7), 128.4 (C-4, C-6), 133.7 (C-5). The structure was confirmed by comparison with literature data [20].

1-Naphthaleneacetic acid, 5-carboxy-1,2,3,4,4a,7,8,8a-octahydro-1,2,4a-trimethyl-, [1S-(1α,2β,4aβ,8aα)] (**2**): White powder ; ^{1}H-NMR (600 MHz; $CDCl_3$): δ 0.88 (3H, t, J= 7; 0 Hz), 1.58 (2H, m), 1.26 (n'H, m), 1.26 (2H, m), 1.30 (2H, m), 2.28 (2H, t, J = 7 ; 0 Hz), 2.86 (2H, t, J = 7; 0Hz), 4.24 (2H, t, J = 7; 0 Hz), 6.76 (1H, d, J = 7; 0 Hz), 7.08 (1H, d, J = 7; 0 Hz); ^{13}C-NMR (125 MHz; $CDCl_3$): δ 174.0 (C-1), 154.3 (C-4'), 130.2 (C-1', 2', 6'), 115.5 (C-3', 5'), 65.1 (C-8'), 34.4 (C-2, 7'), 32.1 (C-5), 29.0 (C-4), 25.1 (C-3), 22.8 (C-6), 14.3 (C-7). The structure was confirmed by comparison with literature data [21].

Betulenic acid (**3**): White powder; m.p. 282º; ^{1}H-NMR (600MHz; DMSO-d6); δ 0.64, 0.76, 0.86, 0.92, 1.43, 1.64, 4.68 (1 H, *J* = 2 Hz), δ 4.58 (1H, *J* = 2; 1.5Hz), 1.64; ^{13}C-NMR (125 MHz; DMSO-d6); δ 177.69 (C-28), 150.77 (C-20), 110.09 (C-29), 77.27 (C-3), 55.87 (C-5), 55.35 (C-19), 50.38 (C-9), 48.9 9 (C-18), 47.07 (C-17), 42.46 (C-14), 40.55 (C-8), 38.95 (C-4), 38.06 (C-1), 37.18 (C-22), 37.06 (C-10), 36.79 (C-13), 34.37 (C-7), 32.16 (C-`16), 30.54 (C-21), 29.65 (C-15), 28.55 (C-2), 27.59 (C-23), 25.54 (C-13), 20.91 (C-11), 19.39 (C-30), 18.42 (C-6), 16.39 (C-26), 16.25 (C-25), 16.19 (C-24), 14.84 (C-27). The structure was confirmed by comparison with literature data [20].

Lupeol (**4**): White powder; m. p. 215°C–216°C. ^{1}H NMR (CDCl3, 600 MHz): δ 4.68, 4.56 (2H, s, H-29a, 29b), 3.16 (1H, dd, *J* = 4.76, 11.00 Hz, H-3), 0.75, 0.78, 0.82, 0.93, 0.95, 1.02, 1.25 (each 3H, s, Me × 7). 13C NMR (CDCl3, 100 MHz): δ 151.1 (C-20), 109.5 (C-29), 79.1 (C-3), 55.5 (C-5), 50.6 (C-9), 48.5 (C-18), 48.1 (C-19), 43.2 (C-17), 43.0 (C-14), 41.0 (C-8), 40.2 (C-22), 39.0 (C-13), 38.9 (C-4), 38.2 (C-1), 37.3 (C-10), 35.8 (C-16), 34.5 (C-7), 30.0 (C-21), 28.2 (C-23), 27.6 (C-15), 27.5 (C-12), 25.3 (C-2), 21.1 (C-11), 19.5 (C-30), 18.5 (C-6), 18.2 (C-28), 16.3 (C-25), 16.2 (C-26), 15.6 (C-24), 14.7 (C-27). The structure was confirmed by comparison with literature data [11].

Ursolic acid (**5**): White powder; m.p. 284-286°C; ^{1}H-NMR (600MHz; pyridine-d5,) δ 5.51 (1H, t-like, H-12), 3.47 (1H, dd, J = 9.0, 7.2 Hz,H-3), 2.65 (1H, d, J = 11.1 Hz, H-18), 1.26 (3H, s, H-23), 1.25(3H, s, H-27), 1.07 (3H, s, H-26), 1.04 (3H, s, H-24), 1.03(3H, d, *J* = 6.3 Hz, H-30), 0.98 (3H, d, *J* = 5.4 Hz, H-29), 0.91(3H, s, H-25); ^{13}C-NMR (pyridine-d5, 125 MHz) δ 180.3 (C-28), 139.6 (C-13), 126.0 (C-12), 78.5(C-3), 56.2 (C-5), 53.9 (C-18), 48.4(C-9), 42.9 (C-17), 40.0 (C-14), 39.9 (C-19), 39.8 (C-20 , C-4), 39.7(C-8), 39.5 (C-1), 37.8(C-13), 37.7 (C-10), 34.0(C-7), 31.4 (C-21), 29.2 (C-23), 29.1 (C-15), 28.5 (C-2), 25.3(C-16), 24.3(C-27), 24.0(C-11), 21.8 (C-30), 19.2 (C-6), 17.9 (C-26), 17.8 (C-29), 17.0 (C-24), 16.1 (C-25). The structure was confirmed by comparison with literature data [22].

Nonacosanoic acid, 2-(4-hydroxyphenyl) ethyl ester (**11**): White powder, EIMS m/z 558 [M]+, (calc.for $C_{37}H_{66}O_3$). ^{1}H NMR (600 MHz; $CDCl_3$) : δ_H 7.08 (1H,d, *J* = 7.0 Hz, H-2ʹ, H-6ʹ), 6.76 (1H, d, *J* = 7.0 Hz, H-3ʹ, H-5ʹ), 4.24 (2H, t, *J* = 7.0 Hz, H-8ʹ), 2.86 (2H, t, *J* = 7.0 Hz, H-7ʹ), 2.28 (2H, t, *J* = 7.0 Hz, H-2), 1.58 (2H, m, H-3), 1.30 (2H, m, H-6), 1.26 (2H, m, H-4, H-5), 0.88 (3H, t, *J* = 7.0 Hz, H-7). ^{13}C NMR (125 MHz; $CDCl_3$,): δ_C 14.3 (C-7), 22.8 (C-6), 25.1 (C-3), 29.0 (C-4), 32.1 (C-5), 34.4 (C-2, C-7ʹ), 65.1 (C-8ʹ), 115.5 (C-3ʹ, C-5ʹ), 130.2 (C-1ʹ, C-2ʹ, C-6ʹ),154.3 (C-4ʹ), 174.0 (C-1). The structure was confirmed by comparison with literature data [28].

Oleanolic acid (14): White powder: EIMS m/z 456 [M]+ (calc. for C30H48O3). 1 H-NMR (600 MHz, $CDCl_3$): δ 5.24 (1H, t , *J* =3.6 Hz, H-12), 3.21 (1H, dd, *J* =10.2; 4.4 Hz, H-3), 2.82 (1H, dd, *J* =12.7; 4.3 Hz, H-18), 0.96 (3H, s, Me-23), 0.78 (3H, s, Me-24), 0.84 (3H, s, Me-25), 0.76 (3H, s, Me-26), 1.25 (3H, s, Me-27), 0.87 (3H, s, Me-29), 0.93 (3H, s, Me-30). 13C-NMR (125 MHz, CDCl3): δ 38.6 (C-1), 26.7 (C-2), 78.5 (C-3), 39.2 (C-4), 55.5 (C-5), 18.3 (C-6), 32.6 (C-7), 39.6 (C-8), 48.1 (C-9), 37.0 (C-10), 22.7 (C-11), 122.4 (C-12), 144.1 (C-13), 42.0 (C-14), 27.7 (C-15), 22.8 (C-16), 46.7 (C-17), 41.5 (C-18), 46.1 (C-19), 30.4 (C-20), 33.7 (C-21), 32.3 (C-22), 28.8 (C-23), 14.7 (C-24), 15.1 (C-25), 16.5 (C-26), 25.2 (C-27), 180.4 (C-28), 32.8 (C-29), 23.3 (C-30). The structure was confirmed by comparison with literature data [22].

β-friedelinol (**15**): White powder: EIMS m/z 428 [M]+ (calc. for $C_{30}H_{52}O$). ^{1}H NMR (600 MHz; pyiridine-d5): δ 5.42 (3-OH), 4.00 (1H, sl, H-3), 2.17, (1H, dq, *J* = 13.20, 2.90 Hz, H_a-2), 1.93 (1H, qd, *J* = 12.80, 3.10 Hz, H_a-1), 1.92 (1H, qd, *J* = 13.10; 3.30 Hz, H_a-7), 1.86 (1H, dt, *J* = 12.60; 3.00 Hz, H_a-6), 1.69 (1H, tdd, *J* = 13.20; 4.00, 3.50Hz, H_b-2), 1.59 (1H, m, H-18), 1.58 (1H, m, H_a-16), 1.53 (1H, m, H_b-7), 1.52 (1H, m, H_b-1, H_a-21), 1.51(1H, m, H_a-22), 1.49 (1H,m, H_a-11), 1.48 (1H, m, H_a-15), 1.44 (1H, m, H_a-19), 1.37 (1H, m, H_b-16), 1.36 (1H, m, H-8), 1.32 (1H, m, H-12), 1.31 (1H, m, H-4, H_b-21), 1.31 (1H, s, H-24), 1.30 (1H, m, H_b-15), 1.27 (1H, m, H_b-19), 1.21 (1H,m, H_b-11), 1.21(3H, s, H-28), 1.19 (3H, d, J = 7.2Hz; H-23), 1.08 (3H, s, H-30), 1.06 (1H, m, H_b-6), 1.06 (3H, s, H-27), 1.03 (1H, m, H-10), 1.02 (3H, s, H-29), 1.01 (3H, s, H-26), 0.95 (1H, dd, *J* = 11.00; 2.60 Hz, H_b-22), 0.95 (3H, s, H-25). ^{13}C NMR (125 MHz; pyiridine-d5,): δ 17.1 (C-1), 37.1 (C-2), 71.9 (C-3), 50.5(C-4), 39.1 (C-5), 42.8 (C-6), 17.1(C-7), 54.0 (C-8), 37.9 (C-9), 62.4 (C-10), 36.5 (C-11), 31.4 (C-12), 39.1 (C-13), 40.5 (C-14), 33.0 (C-15), 36.9 (C-16), 30.7 (C-17), 43.6 (C-18), 36.0 (C-19), 28.8 (C-20), 33.6 (C-21), 39.9 (C-22), 13.0 (C-23), 17.5 (C-24), 19.1 (C-25), 20.8 (C-26), 19.3 (C-27), 33.0 (C-28), 35.5 (C-29), 32.5 (C-30). The structure was confirmed by comparison with literature data [31].

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Pomolic acid (**16**): white powder; ^{1}H-NMR (600 MHz; C_5D_5N) δ 5.64 (1H, t, *J* = 3.20 Hz, H-12), 3.46 (1H, dd, *J* = 11.1; 4.5 Hz, H-3), 3.16 (1H, td, *J* = 13.3; 4.6 Hz, H_a-16), 3.08 (1H, s, H-18), 2.37 (1H, m, H_a-15), 2.20 (2H, m, H_a-22), 2.12 (2H, m, H_a-21), 2.10 (1H, m, H_a-11, H_b-16, H_b-22), 2.06 (1H, m, H_b-11),1.92 (1H, m, H_a-2), 1.88 (1H, m, H-9), 1.85 (1H, m, H_b-2), 1.78 (1H, m, H_a-7), 1.76 (3H, s, H-27), 1.75 (1H, m, H_b-15), 1.61 (1H, m, H_a-6), 1.60 (1H, m, H_a-1), 1.53 (1H, m, H-20), 1.48 (3H, s, H-29), 1.43 (1H, m, H_b-6,7), 1.37 (1H, m, H_b-21), 1.26 (3H, s, H-23), 1.15 (3H, s, H-26), 1.14 (3H, d, J = 4.5Hz, H-30), 1.05 (3H, s, H-24), 0.95 (3H, s, H-25). ^{13}C-NMR (125 MHz; C_5D_5N,) δ 39.5 (C-1), 28.6 (C-2), 78.7 (C-3), 39.9 (C-4), 56.3 (C- 5), 19.4 (C-6), 34.1 (C-7), 40.8 (C-8), 48.3 (C-9), 37.8 (C-10), 24.5 (C-11), 128.5 (C-12), 140.4 (C-13), 42.6 (C-14), 29.8 (C-15), 26.9 (C-16), 48.8 (C-17), 55.1 (C-18), 73.2 (C-19), 42.8 (C-20), 27.4 (C-21), 39.0 (C-22), 17.0 (C-23), 29.3 (C-24), 16.0 (C-25), 17.2 (C- 26), 25.2 (C-27), 181.1 (C-28), 27.6 (C-29), 17.4 (C-30). The structure was confirmed by comparison with literature data [32].

Anticandidal assessment

The different Compounds were prepared by weighing 2 mg, dissolving them in 1 mL of DMSO 10 % for a final concentration of 2 mg/mL. 500 mg of Nystatin (Novadina Pharmaceutical Ltd) was dissolved in 250 mL of DMSO 10 % for a concentration of 2 mg/mL. After preparation, the different stock solutions were sterilized by heating at 60 °C for 30 minutes.

Four *Candida albicans* strains ATCCL26, ATCC12C, ATCCP37039, and ATCCP37037 were obtained from BEI Resources, NAID, and NIH. The disc-diffusion method was used to determine the inhibition zones of the tested compounds against the standard *C. albicans* strains. The plates containing Mueller-Hinton agar were spread with 0.1 mL of the inoculum. Discs (6 mm diameter) were deposited on agar plates using sterilized pincers with 10 µL of the compound. The plates inoculated with different yeasts strains were incubated at 37 °C up to 48 hours and diameter

of any resultant zone of inhibition was measured. The zones of inhibition of more than 6 mm on all the strains were considered to be sensitive. Nystatin was used as the positive control.

The Minimum Inhibitory Concentration (MIC) and the Minimum Fungicidal Concentrations (MFC) was determined according to National Committee for Clinical laboratory Standards (NCCLS) M27-A3 microdilution method using (12 x 8 wells) microtitre plates. In the well of the first line (1-12), 100 µL of culture medium Mueller Hinton broth was introduced and 100 µL in the other well of the plates. Later on, 100 µL of stock solution of crude extracts and compounds were added to the first well. The medium and compound in the first well were mixed before transferring 100 µL of the resultant mixture to the well of the second line. Serial two-fold dilutions of the test samples were made and 20 µL of inoculum 2.5×10^4 CFU/mL, were introduced in the entire well containing the test substances except the column of blank which constitute the sterility control. The concentration range was 0.01 to 0.83 mg/mL for compounds. In each microtiter plate, a column with broad-spectrum antibiotic (Nystatin) with the concentration range from 0.013 mg/mL to 2 mg/mL was used as positive control. After an incubation period at 37 °C for 48 hours, turbidity was observed as indication of growth. Thus the lowest concentration inhibiting the growth of yeast was considered as the Minimum Inhibitory Concentration (MIC).

The MFC was determined by transferring 25 µL aliquots of the clear wells into 100 µL of freshly prepared broth medium and incubated at 37 °C for 48 hours. The MFC was considered as the lowest concentration of test sample which did not produce turbidity, indicating no microbial growth. All tests were performed in triplicates. The results obtained were expressed in average ± standard deviation.