Supporting Information

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Secondary Metabolites from *Halostachys caspica* and Their Antimicrobial and Antioxidant Activities

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Betaine (**1**). Colorless crystal (MeOH); m.p. 294-296 °C; ESI-MS *m/z* 118 $[M+H]^+$; ^{1}H-NMR (MeOD, 500 MHz) δ (ppm), 3.27 (9H, s, 3×CH_3), 3.82 (2H, s, CH_2); ^{13}C-NMR (MeOD, 125 MHz) δ (ppm), 53.8 (3×CH_3), 67.3 (CH_2), 168.7 (C=O). The structure was confirmed by comparison with literature data [5].

Diphenylamine (**2**). Colorless crystal (EtOH); m.p. 53-54 °C; ESI-MS *m/z* 170 $[M+H]^+$; ^{1}H-NMR ($CDCl_3$, 500 MHz) δ (ppm), 5.70 (1H, s, H-N), 6.94 (2H, t, *J* = 7.0 Hz, H-4, 4'), 7.09 (4H, d, *J* = 8.0 Hz, H-2, 6, 2', 6'), 7.28 (4H, dd, *J* = 2.0, 8.5 Hz, H-3, 5, 3', 5'); ^{13}C-NMR ($CDCl_3$, 125 MHz) δ (ppm), 117.8 (C-2, 6, 2', 6'), 121.0 (C-4, 4'), 129.3 (C-3, 5, 3', 5'), 143.1 (C-1, 1'). The structure was confirmed by comparison with literature data [6].

Benzyl-O-β-D-glucopyranoside (**3**). White amorphous powder (MeOH); m.p. 120-121 °C; ESI-MS *m/z* 281 $[M+H]^+$; ^{1}H-NMR (MeOD, 300 MHz) δ (ppm), 4.34 (1H, d, *J* = 7.5 Hz, Glc H-1), 4.66 (1H, d, *J* = 11.8 Hz, H-1' a), 4.92 (1H, d, *J* = 11.8 Hz, H-1' b), 7.29 (1H, t, *J* = 7.0 Hz, H-4) , 7.34 (2H, t, *J* = 7.5 Hz, H-3, 5) , 7.41 (2H, d, *J* = 7.5, H-2, 6); ^{13}C-NMR (MeOD, 75 MHz) δ (ppm), 139.1 (C-1), 129.2 (C-2), 129.3 (C-3), 128.7 (C-4), 129.3 (C-5), 129.2 (C-6), 71.8 (C-1'), Glc: 103.3 (C-1), 75.2 (C-2), 78.0 (C-3), 71.8 (C-4), 78.1 (C-5), 62.9 (C-6). The structure was confirmed by comparison with literature data [7].

β-Sitosterol (**4**). White needle crystal ($CHCl_3$); m.p. 140-142 °C; ESI-MS *m/z* 415 $[M+H]^+$; ^{1}H-NMR ($CDCl_3$, 300 MHz) δ (ppm), 3.56 (1H, m, H-3), 5.36 (1H, d, *J* = 4.8 Hz, H-6), 0.70 (3H, m, H-18), 1.04 (3H, s, H-19), 0.94 (3H, s, H-21), 0.88 (3H, s, H-29), 0.81 (3H, s, H-26), 0.78 (3H, s, H-27). ^{13}C-NMR ($CDCl_3$, 75 MHz) δ (ppm), 37.5 (C-1), 31.3 (C-2), 71.8 (C-3), 39.7 (C-4), 140.5 (C-5), 122.0 (C-6), 32.2 (C-7), 32.3 (C-8), 50.3 (C-9), 37.0 (C-10), 21.2 (C-11), 39.9 (C-12), 42.3 (C-13), 56.9 (C-14), 24.4 (C-15), 28.4 (C-16), 56.1 (C-17), 12.0 (C-18), 20.1 (C-19), 36.4 (C-20), 19.7 (C-21), 33.9 (C-22), 26.0 (C-23), 46.2 (C-24), 29.1 (C-25), 19.0 (C-26), 21.0 (C-27), 23.0 (C-28), 12.3 (C-29). The structure was confirmed by comparison with literature data [8].

4-Hydroxy-3-methoxy benzoic acid (**5**). White amorphous powder (MeOH); m.p. 210-212 °C; EI-MS *m/z* 168 $[M]^+$; ^{1}H-NMR (MeOD, 300 MHz) δ (ppm), 7.55 (1H, s, H-6), 7.55 (1H, s, H-2), 6.79 (1H, d, *J* = 7.6 Hz, H-5), 3.87 (3H, s, OCH_3-3); 13C-NMR (MeOD, 75 MHz) δ (ppm), 169.2 (COOH), 113.2 (C-1), 115.0 (C-2), 147.7 (C-3), 152.5 (C-4), 122.7 (C-5), 124.9(C-6), 56.2 (OCH_3). The structure was confirmed by comparison with literature data [9].

4-Hydroxy benzoic acid (**6**). White amorphous powder (MeOH); m.p. 213-214 °C; EI-MS *m/z* 138 $[M]^+$; ^{1}H-NMR (acetone-d_6, 500 MHz) δ (ppm), 7.91 (2H, d, *J* = 9.0 Hz, H-2 and H-6), 6.90 (2H, d, *J* = 7.0 Hz, H-3 and H-5); ^{13}C-NMR (acetone-d_6, 125 MHz) δ (ppm), 169.2 (COOH), 121.7 (C-1), 132.2 (C-2 and C-6), 115.9 (C-3 and C-5), 162.5 (C-4). The structure was confirmed by comparison with literature data [10].

2-Hydroxy benzoic acid (**7**). Colorless crystal (acetone); m.p.157-158 °C; ^{1}H-NMR (acetone-d_6, 500 MHz) δ (ppm), 6.95 (1H, d, *J* = 9.0 Hz, H-3), 7.52 (1H, m, H-4), 6.93 (1H, t, *J* = 9.0 Hz, H-5), 7.88 (1H, dd, *J* = 9.0, 1.5 Hz, H-6); ^{13}C-NMR (acetone-d_6, 125 MHz) δ (ppm), 113.1 (C-1), 162.9 (C-2), 118.0 (C-3), 136.7 (C-4), 119.9 (C-5), 131.2 (C-6), 172.7 (C-7). The structure was confirmed by comparison with literature data [11].

4-Hydroxy-3,5-dimethoxy benzoic acid (**8**). White needle crystal (MeOH); m.p.204-207 °C; ESI-MS *m/z* 199 $[M+H]^+$, 197 $[M-H]^-$; ^{1}H-NMR (MeOD, 500 MHz) δ (ppm), 9.30 (1H, s, OH-4), 7.32 (2H, s, H-2 and H-6), 3.89 (6H, s, OCH_3-3 and OCH_3-5); ^{13}C-NMR (MeOD, 125 MHz) δ (ppm), 122.0 (C-1), 108.4 (C-2), 148.9 (C-3), 141.8 (C-4), 148.9 (C-5), 170.0 (C=O), 56.1 (OCH_3-3 and OCH_3-5). The structure was confirmed by comparison with literature data [12].

3,4-Dihydroxy benzeneacrylic acid (**9**). Yellow powder (MeOH); m.p. 195-196 °C; ESI-MS *m/z* 203 $[M+Na]^+$; ^{1}H-NMR (DMSO-d_6, 500 MHz) δ (ppm), 12.22 (1H, br s, COOH), 9.62 (1H, br s, OH-4), 9.23 (1H, br s, OH-3), 7.41 (1H, d, *J* = 15.8 Hz, H-7), 7.06 (1H, s, H-2), 6.77(1H, d, H-5), 6.94 (1H, dd, *J* = 2.1, 8.2 Hz, H-6), 6.20 (1H, d, *J* = 15.8 Hz, H-8); ^{13}C-NMR (DMSO-d_6, 125 MHz) δ (ppm), 126.3 (C-1), 116.3 (C-2), 145.7 (C-3), 148.9 (C-4), 115.9 (C-5), 115.4 (C-6), 145.0 (C-7), 121.9 (C-8), 168.4 (C-9). The structure was confirmed by comparison with literature data [13,14].