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SUPPLEMENTARY MATERIAL TO

Synthesis and spectral characterization of novel 1,5-benzodiazepine oxime derivatives

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ANALYTICAL AND SPECTRAL DATA FOR THE SYNTHESIZED COMPOUNDS

*1,3,4,5-Tetrahydro-2*H-*1,5-benzodiazepin-2-one oxime* ***(1)***. Yield: 2.41 g, 68.1 %; cream-colored crystals, m.p.: 147–148 °C; Anal. Calcd. for $C_9H_{11}N_3O$ (*FW*: 177.20): C, 61.00; H, 6.26; N, 23.71 %. Found: C, 59.92; H, 6.14; N, 24.31 %; IR (cm^{-1}): 3388, 3262, 3060, 1665, 1491, 1447, 1435, 1407, 1299, 965, 765; ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 2.34 (2H, *m*, CH_2), 3.37 (2H, *m*, CH_2), 5.34 (1H, *brs*, NH), 6.57–6.92 (4H, *m*, Ar-H), 7.70 (1H, *s*, NH), 9.39 (1H, *s*, OH); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 29.3 (C-3), 46.2 (C-4), 118.8, 119.2, 121.6, 122.9 (C-9a), 128.5, 138.6 (C-5a), 150.7 (C-2).

*4-Methyl-1,3,4,5-tetrahydro-2*H-*1,5-benzodiazepin-2-one oxime* ***(2)***. Yield: 2.94 g, 78.4 %, cream-colored crystals; m.p.: 171–172 °C, Anal. Calcd. for $C_{10}H_{13}N_3O$ (*FW*:191.23): C, 62.81; H, 6.85; N, 21.97 %. Found: C, 62.64; H, 6.79; N, 22.08 %; IR (cm^{-1}): 3386, 3295, 3066, 1670, 1508, 1486, 1442, 1405, 1289, 976, 765; ^{1}H-NMR (300 MHz, DMSO-d_6, δ / ppm): 1.13 (3H, *d*, J = 6.3 Hz, CH_3), 2.01 (1H, *dd*, J = 6,9 Hz & J = 14.0 Hz, CH_2), 2.33 (1H, *dd*, J = 4,4 Hz & J = 14.1 Hz, CH_2), 3.62 (1H, *m*, CH), 4.91 (1H, *s*, NH), 6.65–6.93 (4H, *m*, Ar-H), 7.80 (1H, *brs*, NH), 9.32 (1H, *s*, OH); ^{13}C-NMR (75 MHz, DMSO-d_6, δ / ppm): 23.0 (CH_3), 34.8 (C-3), 52.8 (C-4), 119.9, 120.4, 121.0, 122.7, 130.7, 138.0, 148.9 (C-2).

*3-Methyl-1,3,4,5-tetrahydro-2*H-*1,5-benzodiazepin-2-one oxime* ***(3)***. Yield: 2.63 g, 68.8 %; cream-colored crystals; m.p.: 131–132°; Anal. Calcd. for $C_{10}H_{13}N_3O$ (*FW*: 191.23): C, 62.81; H, 6.85; N, 21.97 %. Found: C, 62.59; H, 6.74; N, 22.12 %; IR (cm^{-1}): 3350, 3176, 3048, 1660, 1497, 1460, 1424, 1411, 1299, 955, 767; ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 1.01 (3H, *d*, J = 7.0

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Hz, CH_3), 2.61 (1H, *m*, CH), 3.11 (1H, *dd*, J = 9.0 Hz & J = 11.5 Hz, CH_2), 3.37 (1H, *dd*, J = 3.3 Hz & J = 11.5 Hz, CH_2), 5.43 (1H, *brs*, NH), 6.54–6.91 (4H, *m*, Ar-H), 7.61 (1H, *s*, NH), 9.51 (1H, *s*, OH); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 14.6 (CH_3), 33.9 (C-3), 52.2 (C-4), 118.4, 118.5, 121.2, 122.5, 128.0, 138.5, 152.9 (C-2).