



SUPPLEMENTARY MATERIAL TO
**Synthesis and evaluation of some novel derivatives of
2-propoxybenzylideneisonicotinohydrazide for their
potential antimicrobial activity**

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ANALYTICAL AND SPECTRAL DATA OF THE SYNTHESIZED COMPOUNDS

N'-(2-Propoxybenzylidene)isonicotinohydrazide (**2a**). Yield 68 %; m.p. 201–204 °C; Anal. Calcd. for C₁₆H₁₇N₃O₂: C, 67.83; H, 6.05; N, 14.83 %. Found: C, 67.85; H, 6.09, N, 14.77 %; IR (KBr, cm⁻¹): 3264, 2948, 2859, 2839, 1667, 1655, 1557, 1125, 1075; ¹H-NMR (300 MHz, DMSO-*d*₆, δ / ppm): 11.98 (1H, *s*, –NH–N=), 8.86 (2H, *d*, *J* = 4.5 Hz, pyridine), 8.79 (1H, *s*, –N=C–H), 7.81 (2H, *d*, *J* = 4.2 Hz, pyridine), 7.73 (2H, *d*, *J* = 7.8 Hz, benzylidene), 7.37 (2H, *d*, *J* = 7.5 Hz, benzylidene), 3.89 (2H, *t*, *J* = 6.8 Hz, OCH₂), 1.69 (2H, *m*, CH₂), 1.18 (3H, *s*, CH₃); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 163.62, 157.49, 149.86, 143.19, 139.82, 131.67, 129.84, 122.62, 120.67, 117.34, 114.53, 72.81, 25.27, 12.37.

N'-(3-((Dimethylamino)methyl)-2-propoxybenzylidene)isonicotinohydrazide (**2b**). Anal. Calcd. for C₁₉H₂₄N₄O₂: C, 67.04; H, 7.11; N, 16.46 %. Found: C 67.17, H 7.10, N 16.34 %; IR (KBr, cm⁻¹): 3265, 2978, 2862, 2843, 1675, 1654, 1559, 1135, 1068; ¹H-NMR (300 MHz, DMSO-*d*₆, δ / ppm): 11.85 (1H, *s*, –NH–N=), 8.64 (2H, *d*, *J* = 4.2 Hz, pyridine), 8.51 (1H, *s*, –N=C–H), 7.77 (2H, *d*, *J* = 3.8 Hz, pyridine), 7.58 (2H, *d*, *J* = 3.2 Hz, benzylidene), 7.28 (1H, *t*, benzylidene), 3.85 (2H, *t*, *J* = 6.2 Hz, OCH₂), 3.62 (2H, *s*, Ar–CH₂–N), 2.21 (6H, *s*, N–(CH₃)₂),

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1.89 (2H, *m*, CH₂), 1.15 (3H, *t*, *J* = 9.3 Hz, CH₃); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 163.55, 157.51, 149.17, 143.45, 139.74, 132.17, 128.18, 122.53, 121.22, 120.44, 115.87, 72.47, 54.71, 46.22, 22.75, 12.87.

N'-(3-((Diethylamino)methyl)-2-propoxybenzylidene)isonicotinohydrazide (**2c**). Anal. Calcd. for C₂₁H₂₈N₄O₂: C, 68.45; H, 7.66; N, 15.21 %. Found: C, 68.35; H, 7.61; N, 15.36; IR (KBr, cm⁻¹): 3259, 2956, 2863, 2841, 1666, 1652, 1552, 1153, 1079; ¹H-NMR (300 MHz, DMSO-*d*₆, δ / ppm): 11.94 (1H, *s*, -NH-N=), 8.68 (2H, *d*, *J* = 4.5 Hz, pyridine), 8.54 (1H, *s*, -N=C-H), 7.64 (2H, *d*, *J* = 3.9 Hz, pyridine), 7.43 (2H, *d*, *J* = 3.2 Hz, benzylidene), 7.12 (1H, *t*, *J* = 7.8 Hz, benzylidene), 3.92 (2H, *t*, *J* = 6.5 Hz, OCH₂), 3.65 (2H, *s*, Ar-CH₂-N), 2.42 (4H, *m*, N-2(CH₂)), 1.89 (2H, *m*, CH₂), 1.08 (9H, *m*, 3CH₃); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 163.18, 157.29, 149.88, 143.26, 139.77, 132.23, 128.66, 122.55, 121.12, 120.52, 116.78, 72.59, 52.77, 48.18, 22.37, 13.76, 12.91.

N'-(3-((Dipropylamino)methyl)-2-propoxybenzylidene)isonicotinohydrazide (**2d**). Anal. Calcd. for C₂₃H₃₂N₄O₂: C, 69.97; H, 8.13; N, 14.13 %. Found: C, 69.95; H, 8.10; N, 14.18 %; IR (KBr, cm⁻¹): 3259, 2956, 2863, 2841, 1666, 1652, 1552, 1152, 1079; ¹H-NMR (300 MHz, DMSO-*d*₆, δ / ppm): 11.79 (1H, *s*, -NH-N=), 8.78 (2H, *d*, *J* = 4.1 Hz, pyridine), 8.47 (1H, *s*, -N=C-H), 7.98 (2H, *d*, *J* = 3.8 Hz, pyridine), 7.35 (2H, *d*, *J* = 3.1 Hz, benzylidene), 7.17 (1H, *t*, *J* = 7.5 Hz, benzylidene), 3.92 (2H, *t*, *J* = 6.9 Hz, OCH₂), 3.68 (2H, *s*, Ar-CH₂-N), 2.54 (4H, *t*, N-2(CH₂)), 1.68 (6H, *m*, 3CH₂), 1.07 (9H, *m*, 3CH₃); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 163.19, 157.38, 149.74, 143.19, 139.85, 132.17, 128.47, 122.48, 121.78, 119.89, 116.45, 72.23, 55.89, 51.73, 23.77, 21.75, 13.18, 12.89.

N'-(3-((Dibutylamino)methyl)-2-propoxybenzylidene)isonicotinohydrazide (**2e**). Anal. Calcd. for C₂₅H₃₆N₄O₂: C, 70.72; H, 8.55; N, 13.20 %. Found: C, 70.68; H, 8.64; N, 13.15 %; IR (KBr, cm⁻¹): 3269, 2967, 2858, 2843, 1663, 1658, 1561, 1174, 1058. ¹H-NMR (300 MHz, DMSO-*d*₆, δ / ppm): 11.85 (1H, *s*, -NH-N=), 8.72 (2H, *d*, *J* = 4.1 Hz, pyridine), 8.39 (1H, *s*, -N=C-H), 7.74 (2H, *d*, *J* = 3.9 Hz, pyridine), 7.31 (2H, *d*, *J* = 3.2 Hz, benzylidene), 7.15 (1H, *t*, *J* = 7.9 Hz, benzylidene), 3.49 (2H, *t*, *J* = 5.9 Hz, OCH₂), 3.62 (2H, *s*, Ar-CH₂-N), 2.35 (4H, *t*, N-2(CH₂)), 1.66 (10 H, *m*, 5CH₂), 1.04 (9H, *t*, 3CH₃); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 163.14, 157.45, 149.54, 146.18, 143.27, 139.81, 131.93, 128.35, 122.85, 121.87, 120.74, 116.87, 72.38, 55.18, 52.81, 32.85, 20.25, 21.77, 14.18, 12.92.

N'-(3-((Diphenylamino)methyl)-2-propoxybenzylidene)isonicotinohydrazide (**2f**). Anal. Calcd. for C₂₉H₂₈N₄O₂: C, 74.98; H, 6.08; N, 12.06 %. Found: C, 74.91; H, 6.18; N, 12.03 %; IR (KBr, cm⁻¹): 3255, 2956, 2861, 2845, 1669, 1649, 1558, 1155, 1062; ¹H-NMR (300 MHz, DMSO-*d*₆, δ / ppm): 11.92 (1H, *s*, -NH-N=), 8.68 (2H, *d*, *J* = 4.2 Hz, pyridine), 8.27 (1H, *s*, -N=C-H), 7.59 (2H, *d*, *J* = 3.7 Hz, pyridine), 7.25–6.78 (13H, *m*, benzylidene), 3.84 (2H, *t*, *J* = 6.5 Hz,

OCH₂), 3.69 (2H, *s*, Ar-CH₂-N), 1.64 (2H, *m*, CH₂), 1.04 (9H, *t*, 3CH₃); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 163.69, 155.28, 149.74, 143.29, 139.84, 129.75, 127.88, 122.76, 119.75, 118.72, 117.95, 116.84, 72.44, 45.59, 23.79, 12.76.

3-(Piperidin-1-ylmethyl)-N'-(2-propoxybenzylidene)isonicotinohydrazide (2g).
Anal. Calcd. for C₂₂H₂₈N₄O₂: C, 69.45; H, 7.42; N, 14.73 %. Found: C, 69.48; H, 7.47; N, 14.65 %; IR (KBr, cm⁻¹): 3268, 2968, 2862, 2843, 1667, 1644, 1569, 1168, 1072; ¹H-NMR (300 MHz, DMSO-*d*₆, δ / ppm): 11.89 (1H, *s*, -NH-N=), 8.64 (2H, *d*, *J* = 4.5 Hz, pyridine), 8.21 (1H, *s*, -N=C-H), 7.46 (2H, *d*, *J* = 4.2 Hz, pyridine), 7.54 (2H, *d*, *J* = 3.2 Hz, benzylidene), 7.18 (1H, *t*, *J* = 7.6 Hz, benzylidene), 3.85 (2H, *t*, *J* = 6.8 Hz, OCH₂), 3.62 (2H, *s*, Ar-CH₂-N), 2.62 (4H, *t*, N-2(CH₂), 1.74 (2H, *m*, CH₂), 1.52 (6H, *m*, 3CH₂), 1.06 (3H, *t*, *J* = 7.6 Hz, CH₃); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 163.19, 157.28, 149.74, 146.73, 143.39, 139.48, 131.76, 128.39, 122.83, 121.55, 121.18, 120.29, 116.77, 72.42, 55.79, 52.34, 26.63, 24.37, 22.18, 12.44.

N'-(2-Propoxy-3-(pyrrolidin-1-ylmethyl)benzylidene)isonicotinohydrazide (2h).
Anal. Calcd. for C₂₁H₂₆N₄O₂: C, 68.83; H, 7.15; N, 15.29 %. Found: C, 68.71; H, 7.18; N, 15.38 %; IR (KBr, cm⁻¹): 3269, 2958, 2862, 2844, 1669, 1642, 1572, 1167, 1075; ¹H-NMR (300 MHz, DMSO-*d*₆, δ / ppm): 11.83 (1H, *s*, -NH-N=), 8.68 (2H, *d*, *J* = 4.3 Hz, pyridine), 8.43 (1H, *s*, -N=C-H), 7.85 (2H, *d*, *J* = 3.9 Hz, pyridine), 7.59 (2H, *d*, *J* = 3.2 Hz, benzylidene), 7.19 (1H, *t*, *J* = 7.6 Hz, benzylidene), 3.91 (2H, *t*, *J* = 6.9 Hz, OCH₂), 3.58 (2H, *s*, Ar-CH₂-N), 2.31 (4H, *t*, N-2(CH₂), pyrrolidine), 1.68–1.55 (6H, *m*, 3CH₂), 1.05 (3H, *t*, *J* = 9.3 Hz, CH₃); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 163.55, 157.38, 149.69, 143.23, 139.27, 131.87, 128.39, 122.77, 121.57, 120.26, 116.76, 72.84, 58.89, 52.84, 26.67, 23.58, 12.76.

3-(Morpholinomethyl)-N'-(2-propoxybenzylidene)isonicotinohydrazide (2i).
Anal. Calcd. for C₂₁H₂₆N₄O₃: C, 65.95; H, 6.85; N, 14.65 %. Found: C, 65.85; H, 6.88; N, 14.72 %; IR (KBr, cm⁻¹): 3273, 2973, 2861, 2845, 1676, 1641, 1581, 1154, 1068; ¹H-NMR (300 MHz, DMSO-*d*₆, δ / ppm): 11.92 (1H, *s*, -NH-N=), 8.85 (2H, *d*, *J* = 4.2 Hz, pyridine), 8.46 (1H, *s*, -N=C-H), 7.79 (2H, *d*, *J* = 3.8 Hz, pyridine), 7.38 (2H, *d*, *J* = 3.1 Hz, benzylidene), 7.19 (1H, *t*, *J* = 7.5 Hz, benzylidene), 3.94 (2H, *t*, *J* = 6.3 Hz, OCH₂), 3.55 (2H, *s*, Ar-CH₂-N), 3.45 (4H, *t*, O-2(CH₂), morpholine), 2.31 (4H, *t*, N-2(CH₂), morpholine), 1.65 (2H, *m*, CH₂), 1.08 (3H, *t*, *J* = 8.9 Hz, CH₃); ¹³C-NMR (100 MHz, DMSO-*d*₆, δ / ppm): 163.81, 157.18, 149.81, 143.39, 139.75, 131.68, 128.39, 122.15, 121.59, 120.38, 116.78, 72.81, 67.47, 54.27, 52.66, 23.45, 12.35.

3-(Piperazin-1-ylmethyl)-N'-(2-propoxybenzylidene)isonicotinohydrazide (2j).
Anal. Calcd. for C₂₁H₂₇N₅O₂: C, 66.12; H, 7.13; N, 18.36 %. Found: C, 66.24; H, 7.05; N 18.32 %; IR (KBr, cm⁻¹): 3274, 2977, 2862, 2842, 1675, 1643, 1579, 1164, 1038; ¹H-NMR (300 MHz, DMSO-*d*₆, δ / ppm): 11.89 (1H, *s*, -NH-N=),

8.72 (2H, *d*, $J = 4.1$ Hz, pyridine), 8.35 (1H, *s*, $-\text{N}=\text{C}-\text{H}$), 7.69 (2H, *d*, $J = 3.7$ Hz, pyridine), 7.69 (2H, *d*, $J = 3.2$ Hz, benzylidene), 7.19 (1H, *t*, $J = 7.5$ Hz, benzylidene), 4.12 (1H, *s*, NH, D_2O exchangeable), 3.89 (2H, *m*, OCH_2), 3.65 (2H, *s*, $\text{Ar}-\text{CH}_2-\text{N}$), 2.68–2.48 (8H, *m*, 4CH_2 , piperazine), 1.68 (2H, *m*, CH_2), 1.05 (3H, *t*, $J = 8.8$ Hz, CH_3); ^{13}C -NMR (100 MHz, $\text{DMSO}-d_6$, δ / ppm): 163.58, 157.46, 149.12, 143.38, 139.48, 131.75, 128.35, 122.45, 121.62, 120.65, 116.58, 72.26, 55.69, 52.27, 47.35, 25.18, 12.18.

3-((4-Methylpiperazin-1-yl)methyl)- N' -(2-propoxybenzylidene)isonicotinohydrazide (**2k**). Anal. Calcd. for $\text{C}_{22}\text{H}_{29}\text{N}_5\text{O}_2$: C, 66.81; H, 7.39; N, 17.71 %. Found: C, 66.73; H, 7.43; N, 17.75 %. IR (KBr, cm^{-1}): 3269, 2946, 2852, 2835, 1674, 1659, 1552, 1129, 1078; ^1H -NMR (300 MHz, $\text{DMSO}-d_6$, δ / ppm): 11.95 (1H, *s*, $-\text{NH}-\text{N}=\text{C}$), 8.65 (2H, *d*, $J = 4.2$ Hz, pyridine), 8.24 (1H, *s*, $-\text{N}=\text{C}-\text{H}$), 7.83 (2H, *d*, $J = 3.7$ Hz, pyridine), 7.77 (2H, *d*, $J = 3.2$ Hz, benzylidene), 7.15 (1H, *t*, $J = 7.3$ Hz, benzylidene), 3.91 (2H, *t*, $J = 6.5$ Hz, OCH_2), 3.65 (2H, *s*, $\text{Ar}-\text{CH}_2-\text{N}$), 2.45 (8H, *m*, 4CH_2 , piperazine), 2.18 (3H, *s*, NCH_3 , piperazine), 1.84 (2H, *m*, CH_2), 1.05 (3H, *t*, $J = 9.1$ Hz, CH_3); ^{13}C -NMR (100 MHz, $\text{DMSO}-d_6$, δ / ppm): 163.91, 157.58, 149.51, 143.48, 139.64, 132.23, 128.25, 122.59, 121.29, 120.49, 115.75, 72.19, 55.18, 51.25, 49.37, 43.29, 23.18, 12.74.