SUPPLEMENTARY MATERIAL TO

Synthesis and antimicrobial evaluation of some novel thiomorpholine derived 1, 4- disubstituted 1,2,3-triazoles

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ANALYTICAL AND SPECTRAL DATA OF THE SYNTHESIZED COMPOUNDS

4-(prop-2-yn-1-yl) thiomorpholine (**2**) Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.31 (d, *J*=2.4Hz, 2H), 2.84-2.79 (m, 8H), 2.26 (t, j=2.4 Hz, 1H); ESI-MS; 142 (M+H).

4-(prop-2-yn-1-yl) thiomorpholine 1,1-dioxide (**3**) M. P: 114-116^{o}C, ESI-MS; 174 (M+H).

4-((1-heptyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine (**4a**): Yellow solid; R_f 0.40 (65% ethyl acetate /n-hexane); Yield: 75 %; M.P: 48-50 ^{0}C; IR (KBr, cm^{-1}) ν_{max}: 3019(triazole ring), 1402, 1215, 1052, 757, 668 ; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.76 (s, 1H, tri-H), 4.35 (t, *J*= 7.32 Hz, 2H, N-N-*CH*$_2$-), 4.03 (s, 2H, N-*CH*$_2$-tri), 3.20-3.10 (m, 4H), 2.90-2.78 (m, 4H), 1.90-1.80 (m, 2H), 1.40-1.20 (m, 8H), 0.87 (t, *J*=6.71 Hz, 3H); **^{13}C** NMR (125 MHz, $CDCl_3$): δ 139.4,124.4, 53.2, 51.9, 50.3, 31.2 , 29.9, 28.3, 26.1, 25.8, 22.2, 13.7; ESI-MS; 283 (M+H).

4-((1-octyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine (**4b**): Yellow solid; R_f 0.40 (65% ethyl acetate /n-hexane); Yield: 78 %; M.P: 51-53 ^{0}C; IR (KBr, cm^{-1}) ν_{max}: 3019(triazole ring), 2399, 1637, 1403, 1215, 1051, 928, 758, 669 ; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.44 (s, 1H, tri-H), 4.30 (t, *J*= 7.74 Hz, 2H, N-N-*CH*$_2$-), 3.68 (s, 2H, N-*CH*$_2$-tri), 2.80-2.62 (m, 8H), 1.90-1.80 (m, 2H), 1.40-1.20 (m, 10H), 0.84 (t, *J*=7.17 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 143.8, 122.3, 54.5, 54.0, 50.2, 31.6 , 30.2, 28.9, 28.8, 27.7, 26.4, 22.5, 13.9; ESI-MS; 297 (M+H).

4-((1-decyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine (**4c**): Pale yellow solid; R_f 0.38 (65% ethyl acetate /n-hexane); Yield: 68 %; M.P : 55-57 ^{0}C; IR (KBr, cm^{-1}) ν_{max}: 3019(triazole ring), 2928, 2399, 1654, 1522, 1420, 1215,1051, 928, 758, 669 ; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.52 (s, 1H, tri-H), 4.31 (t, *J*= 7.17 Hz, 2H, N-N-*CH*$_2$-), 3.74 (s, 2H, N-*CH*$_2$-tri), 2.80-2.60 (m, 8H), 1.98-1.80 (m, 2H),1.40-1.20 (m, 14H), 0.85 (t, *J*=6.98 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 143.0, 122.8, 54.4, 53.8, 50.3, 31.7, 30.2, 29.3, 29.3, 29.1, 28.9, 27.4, 26.4, 22.5, 14.0; ESI-MS; 325 (M+H).

4-((1-tridecyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine (**4d**): White solid; R_f 0.38 (65% ethyl acetate /n-hexane); Yield: 81 %; M.P : 58-60 ^{0}C; IR (KBr, cm^{-1}) ν_{max}: 3021(triazole ring), 2924, 2853, 1639, 1559, 1405, 1215, 1049, 928, 759, 669 ; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.53 (s, 1H, tri-H), 4.33 (t, *J*= 7.55 Hz, 2H, N-N-*CH*$_2$-), 3.77 (s, 2H, N-*CH*$_2$-tri), 2.95-2.60 (m, 8H), 1.98-1.80 (m, 2H), 1.40.-1.18 (m, 20H), 0.87 (t, *J*=6.79 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 143.0, 122.8, 54.0, 53.3, 50.3, 31.7, 30.0, 29.4, 29.3, 29.2, 29.1, 28.8, 27.7, 26.3, 22.5, 13.9; ESI-MS; 367 (M+H).

4-((1-tetradecyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine (**4e**):Off white solid; R_f 0.38 (65% ethyl acetate /n-hexane); Yield: 76 %; M.P : 61-63 ^{0}C;IR (KBr, cm^{-1}) ν_{max}: 3019(triazole ring), 2928, 2400, 1666, 1520, 1403, 1215, 1035, 928, 757, 669; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.50 (s, 1H, tri-H), 4.31 (t, *J*= 7.16 Hz, 2H, N-N-*CH*$_2$-), 3.72 (s, 2H, N-*CH*$_2$-tri), 2.85-2.65 (m, 8H), 1.95-1.80 (m, 2H), 1.41.-1.18 (m, 22H), 0.86 (t, *J*=6.98 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 143.4, 122.6, 54.5, 53.9 , 50.3, 31.8 , 30.2, 29.6, 29.5, 29.5, 29.4, 29.3, 29.2, 28.9, 27.6, 26.4, 22.6, 14.0; ESI-MS; 381 (M+H).

4-((1-pentadecyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine (**4f**): Off white solid; R_f 0.37 (65% ethyl acetate /n-hexane); Yield:84%; M.P :65-67^{0}C; IR (KBr, cm^{-1}) ν_{max}: 3019(triazole ring), 2927, 2855,1403, 1215, 1051, 759, 668 ; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.60 (s, 1H, tri-H), 4.34 (t, *J*= 7.55 Hz, 2H, N-N-*CH*$_2$-), 3.86 (s, 2H, N-*CH*$_2$-tri), 3.05-2.62 (m, 8H), 1.98-1.80 (m, 2H), 1.40.-1.18 (m, 24H), 0.87 (t, *J*=6.79 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 143.0, 123.0, 54.4, 53.7 , 50.5, 32.0 , 30.3, 29.7, 29.6, 29.5, 29.4, 29.4, 29.0, 27.6, 26.6, 22.7, 14.2; ESI-MS; 395 (M+H).

4-((1-heptadecyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine (**4g**): Off white solid; R_f 0.37 (65% ethyl acetate /n-hexane); Yield: 74 %; M.P : 68-70 ^{0}C; IR (KBr, cm^{-1}) ν_{max}: 3020(triazole ring), 1639, 1405, 1216, 1038, 759, 668 ; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.65 (s, 1H, tri-H), 4.34 (t, *J*= 7.17 Hz, 2H, N-N-*CH*$_2$-), 3.93 (s, 2H, N-*CH*$_2$-tri), 3.05-2.80 (m, 8H), 1.91-1.72 (m, 2H), 1.48.-1.10 (m, 28H), 0.87 (t, *J*=6.60 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 141.0, 123.9, 53.9, 53.5 , 50.4, 31.8 , 30.1, 29.5, 29.4, 29.3, 29.2, 28.9, 27.5, 26.6, 26.4, 22.6, 21.0, 14.0; ESI-MS; 423 (M+H).

4-((1-hexyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine (**4h):** Yellow oil; R_f 0.40 (65% ethyl acetate /n-hexane); Yield: 75 %; IR (KBr, cm^{-1}) ν_{max}: 3019(triazole ring), 1640, 1561, 1404, 928, 757, 668; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.47 (s, 1H, tri-H), 4.33 (t, *J*= 7.74 Hz, 2H, N-N-*CH*$_2$-), 3.71 (s, 2H, N-*CH*$_2$-tri), 2.82-2.64 (m, 8H), 1.98-1.80 (m, 2H), 1.40-1.20 (m, 6H), 0.87 (t, *J*=7.17 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 139.4,124.4, 53.2, 51.9, 50.3, 31.2, 29.9, 28.3, 26.19, 22.2, 13.7; ESI-MS; 269 (M+H).

Ethyl 2-(4-(thiomorpholinomethyl)-1H-1,2,3-triazol-1-yl)acetate (**4i**): Light yellow oil ; R_f 0.36 (65% ethyl acetate /n-hexane); Yield: 75 %; IR (KBr, cm^{-1}) ν_{max}: 3019(triazole ring), 1713, 1402, 1215, 1036, 928, 757, 669 ; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.79 (s, 1H, tri-H), 5.13 (s, 2H, N-N-*CH*$_2$-CO-), 4.22 (q, *J*= 7.09 Hz, *J*=7.09 Hz, 2H,O-*CH*$_2$-), 3.91 (s, 2H, N-*CH*$_2$-tri), 3.01-2.91 (m, 4H), 2.90-2.80 (m, 4H), 1.25 (t, *J*=7.09 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 165.9, 140.6, 126.1, 62.0, 53.2, 51.8, 50.6, 26.0, 13.6; ESI-MS; 271 (M+H).

4-((1-dodecyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine (**4j**) : Off white solid; R_f 0.38 (65% ethyl acetate /n-hexane); Yield: 79 %; M.P: 54-56 ^{0}C; IR (KBr, cm^{-1}) ν_{max}: 3019(triazole ring), 2928, 2400,1666, 1520, 1403, 1215, 1035, 928, 757, 669 : ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.52 (s, 1H, tri-H), 4.33 (t, *J*= 7.36 Hz, 2H, N-N-*CH*$_2$-), 3.74 (s, 2H, N-*CH*$_2$-tri), 2.82-2.64 (m, 8H), 1.97-1.80 (m, 2H),1.48-1.18 (m, 18H), 0.87 (t, *J*=6.98 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 143.2, 122.7, 54.3, 53.5, 50.4, 31.8 , 30.2, 29.5, 29.4, 29.3, 29.2, 28.9, 27.8, 27.6, 26.4, 22.6, 14.0; ESI-MS; 353 (M+H).

4-((1-heptyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine 1,1-dioxide (**5a**): Off white solid; R_f 0.38 (70% ethyl acetate /n-hexane); Yield: 75 %; m.p: 60-62 ^{0}C; IR (KBr, cm^{-1}) ν_{max}: 3018 (triazole ring), 1412, 1218, 1050, 750, 666 ; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.79 (s, 1H, tri-H), 4.36 (t, *J*= 7.32 Hz, 2H, N-N-*CH*$_2$-),4.05 (s, 2H, N-*CH*$_2$-tri), 3.11 – 3.06 (m, 4H), 2.86 – 2.81 (m, 4H), 1.97-1.82 (m, 2H), 1.48-1.22 (m, 8H), 0.87 (t, *J*=6.98 Hz, 3H); ESI-MS; 315 (M+H).

4-((1-octyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine 1,1-dioxide (**5b**): white solid; R_f 0.38 (70% ethyl acetate /n-hexane); Yield: 78 %; M.P: 61-63 ^{0}C; IR (KBr, cm^{-1}) ν_{max}: 3030(triazole ring), 2412, 1638, 1413, 1221; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.50 (s, 1H, tri-H), 4.33 (t, *J*= 7.74 Hz, 2H, N-N-*CH*$_2$-), 3.72 (s, 2H, N-*CH*$_2$-tri), 3.09 – 3.04 (m, 4H), 2.88 – 2.81 (m, 4H), 1.98-1.80 (m, 2H), 1.49-1.22 (m, 10H), 0.87 (t, *J*=7.09 Hz, 3H); ESI-MS; 329 (M+H).

4-((1-decyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine 1,1-dioxide (**5c**): Pale yellow solid; R_f 0.38 (70% ethyl acetate /n-hexane); Yield: 68 %; M.P : 64-66 ^{0}C; IR (KBr, cm^{-1}) ν_{max}: 3033 (triazole ring), 2927, 2403, 1652, 1518, 1426, 1217; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.56 (s, 1H, tri-H), 4.33 (t, *J*= 7.17 Hz, 2H, N-N-*CH*$_2$-), 3.75 (s, 2H, N-*CH*$_2$-tri), 3.10 – 3.04 (m, 4H), 2.87 – 2.83 (m, 4H), 1.20-1.81 (m, 2H),1.46-1.22 (m, 14H), 0.86 (t, *J*= 7.55 Hz, 3H); ESI-MS; 357 (M+H).

4-((1-tridecyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine1,1-dioxide (**5d**): Pale yellow solid; R_f 0.40 (70% ethyl acetate /n-hexane); Yield: 61 %; m.p : 68-70 ^{0}C; IR (KBr, cm^{-1}) ν_{max}: 3026 (triazole ring), 2918, 2857, 1640, 1537, 1415, 1216; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.56 (s, 1H, tri-H), 4.33 (t, *J*= 7.74 Hz, 2H, N-N-*CH*$_2$-), 3.79 (s, 2H, N-*CH*$_2$-tri), 3.10 – 3.04 (m, 4H), 2.88 –

2.81 (m, 4H), 1.96-1.81 (m, 2H), 1.45.-1.16 (m, 20H), 0.86 (t, *J*=6.60 Hz, 3H); ESI-MS; 399 (M+H).

4-((1-tetradecyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine1,1-dioxide (**5e**): Off white solid; R_f 0.39 (70% ethyl acetate /n-hexane); Yield: 66 %; m.p : 69-72 ^{0}C;IR (KBr, cm^{-1}) ν_{max}: 3037 (triazole ring), 2941, 2388, 1668, 1534, 1417, 1215; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.56 (s, 1H, tri-H), 4.36 (t, *J*= 7.55 Hz, 2H, N-N-*CH*$_2$-), 3.74 (s, 2H, N-*CH*$_2$-tri), 3.11 – 3.05 (m, 4H), 2.87 – 2.80 (m, 4H), 1.98-1.84 (m, 2H), 1.47.-1.20 (m, 22H), 0.88 (t, *J*=6.98 Hz, 3H); ESI-MS; 413 (M+H).

4-((1-pentadecyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine1,1-dioxide (**5f**): Pale yellow solid; R_f 0.37 (70% ethyl acetate /n-hexane); Yield:64%; m.p: 77-79 ^{0}C; IR (KBr, cm^{-1}) ν_{max}: 3028 (triazole ring), 2920, 2860,1413, 1218; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.65 (s, 1H, tri-H), 4.36 (t, *J*= 7.17 Hz, 2H, N-N-*CH*$_2$-), 3.88 (s, 2H, N-*CH*$_2$-tri), 3.10 – 3.05 (m, 4H), 2.86 – 2.80 (m, 4H), 1.99-1.82 (m, 2H), 1.48-1.19 (m, 24H), 0.86 (t, *J*=6.60 Hz, 3H); ESI-MS; 427 (M+H).

4-((1-heptadecyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine 1,1-dioxide (**5g**): Off white solid; R_f 0.38 (70% ethyl acetate /n-hexane); Yield: 74 %; m.p : 73-75 ^{0}C; IR (KBr, cm^{-1}) ν_{max}: 3020 (triazole ring), 1639, 1405, 1216; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.70 (s, 1H, tri-H), 4.37 (t, *J*= 7.74 Hz, 2H, N-N-*CH*$_2$-), 3.94 (s, 2H, N-*CH*$_2$-tri), 3.12 – 3.06 (m, 4H), 2.88 – 2.81 (m, 4H), 1.94-1.76 (m, 2H), 1.52.-1.18 (m, 28H), 0.87 (t, *J*=6.79 Hz, 3H); ESI-MS; 455 (M+H).

4-((1-hexyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine 1,1-dioxide (**5h):** Yellow solid; R_f 0.36 (70% ethyl acetate /n-hexane); Yield: 70 %; m.p : 68-70 ^{0}C; IR (KBr, cm^{-1}) ν_{max}: 3019(triazole ring), 1644, 1567, 1414; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.49 (s, 1H, tri-H), 4.38 (t, *J*= 7.55 Hz, 2H, N-N-*CH*$_2$-), 3.74 (s, 2H, N-*CH*$_2$-tri), 3.11 – 3.05 (m, 4H), 2.86 – 2.80(m, 4H), 1.98-1.85 (m, 2H), 1.45-1.22 (m, 6H), 0.86 (t, *J*=6.98 Hz, 3H); ESI-MS; 301 (M+H).

Ethyl 2-(4-((1,1-dioxidothiomorpholino)methyl)-1H-1,2,3-triazol-1-yl)acetate (**5i):** yellow oil ; R_f 0.39 (70% ethyl acetate /n-hexane); Yield: 71 %; IR (KBr, cm^{-1}) ν_{max}: 3018(triazole ring), 1715, 1412, 1218, 1033; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.80 (s, 1H, tri-H), 5.14 (s, 2H, N-N-*CH*$_2$-CO-), 4.25(q, *J*= 7.09 Hz, *J*=7.09 Hz, 2H,O-*CH*$_2$-), 3.94 (s, 2H, N-*CH*$_2$-tri), 3.12 – 3.05 (m, 4H), 2.88 – 2.81 (m, 4H), 1.27 (t, *J*=7.09 Hz, 3H); ESI-MS; 303 (M+H)

4-((1-dodecyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine1,1-dioxide (**5j**) : White solid; R_f 0.37 (70% ethyl acetate /n-hexane); Yield: 67 %; m.p: 64-66 ^{0}C; IR (KBr, cm^{-1}) ν_{max}: 3020(triazole ring), 2929, 2418,1669, 1522, 1413, 1218, 1045: ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.54 (s, 1H, tri-H), 4.34 (t, *J*= 7.36 Hz, 2H, N-N-*CH*$_2$-), 3.75 (s, 2H, N-*CH*$_2$-tri), 3.10 – 3.05 (m, 4H), 2.86 – 2.80 (m, 4H),, 1.96-1.84 (m, 2H),1.44-1.16 (m, 18H), 0.86 (t, *J*=7.17 Hz, 3H); ESI-MS; 385 (M+H).