



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

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J. Serb. Chem. Soc. 81 (3) (2016) 233–242

ANALYTICAL AND SPECTRAL DATA OF THE SYNTHESIZED COMPOUNDS

4-(Prop-2-yn-1-yl)thiomorpholine (2). Yellow oil; ¹H-NMR (500 MHz, CDCl₃, δ / ppm): 3.31 (2H, d, J = 2.4 Hz), 2.84–2.79 (8H, m), 2.26 (1H, t, J = 2.4 Hz); ESI-MS (m/z): 142 (M+H).

4-(Prop-2-yn-1-yl)thiomorpholine 1,1-dioxide (3). M.p.: 114–116 °C, ESI-MS (m/z): 174 (M+H).

4-((1-Heptyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine (4a). Yield: 75 %; yellow solid; m.p.: 48–50 °C; R_f (65 % ethyl acetate/n-hexane): 0.40; IR (KBr, cm⁻¹): 3019 (triazole ring), 1402, 1215, 1052, 757, 668; ¹H-NMR (500 MHz, CDCl₃, δ / ppm): 7.76 (1H, s, tri-H), 4.35 (2H, t, J = 7.32 Hz, N–N–CH₂–), 4.03 (2H, s, N–CH₂–tri), 3.20–3.10 (4H, m), 2.90–2.78 (4H, m), 1.90–1.80 (2H, m), 1.40–1.20 (8H, m), 0.87 (3H, t, J = 6.71 Hz); ¹³C-NMR (125 MHz, CDCl₃, δ / ppm): 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 (m/z): 283 (M+H).

4-((1-Octyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine (4b). Yield: 78 %; yellow solid; m.p.: 51–53 °C; R_f (65 vol.% ethyl acetate/n-hexane): 0.40; IR (KBr, cm⁻¹): 3019 (triazole ring), 2399, 1637, 1403, 1215, 1051, 928, 758, 669; ¹H-NMR (300 MHz, CDCl₃, δ / ppm): 7.44 (1H, s, tri-H), 4.30 (2H, t, J = 7.74 Hz, N–N–CH₂–), 3.68 (2H, s, N–CH₂–tri), 2.80–2.62 (8H, m), 1.90–1.80 (2H, m), 1.40–1.20 (10H, m), 0.84 (3H, t, J = 7.17 Hz); ¹³C-NMR (125 MHz, CDCl₃, δ / ppm): 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 (m/z): 297 (M+H).

4-((1-Decyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine (4c). Yield: 68 %; pale yellow solid; m.p.: 55–57 °C; R_f (65 vol. % ethyl acetate/n-hexane): 0.38; IR

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(KBr, cm^{-1}): 3019 (triazole ring), 2928, 2399, 1654, 1522, 1420, 1215, 1051, 928, 758, 669; $^1\text{H-NMR}$ (300 MHz, CDCl_3 , δ / ppm): 7.52 (1H, *s*, tri-H), 4.31 (2H, *t*, $J = 7.17$ Hz, N–N–CH₂–), 3.74 (2H, *s*, N–CH₂–tri), 2.80–2.60 (8H, *m*), 1.98–1.80 (2H, *m*), 1.40–1.20 (14H, *m*), 0.85 (3H, *t*, $J = 6.98$ Hz); $^{13}\text{C-NMR}$ (125 MHz, CDCl_3 , δ / ppm): 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 (*m/z*): 325 (M+H).

*4-((1-Tridecyl-1*H*-1,2,3-triazol-4-yl)methyl)thiomorpholine (4d).* Yield: 81 %; white solid; m.p.: 58–60 °C; R_f (65 vol. % ethyl acetate/*n*-hexane): 0.38; IR (KBr, cm^{-1}): 3021 (triazole ring), 2924, 2853, 1639, 1559, 1405, 1215, 1049, 928, 759, 669; $^1\text{H-NMR}$ (300 MHz, CDCl_3 , δ / ppm): 7.53 (1H, *s*, tri-H), 4.33 (2H, *t*, $J = 7.55$ Hz, N–N–CH₂–), 3.77 (2H, *s*, N–CH₂–tri), 2.95–2.60 (8H, *m*), 1.98–1.80 (2H, *m*), 1.40–1.18 (20H, *m*), 0.87 (3H, *t*, $J = 6.79$ Hz); $^{13}\text{C-NMR}$ (125 MHz, CDCl_3 , δ / ppm): 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 (*m/z*): 367 (M+H).

*4-((1-Tetradecyl-1*H*-1,2,3-triazol-4-yl)methyl)thiomorpholine (4e).* Yield: 76 %; off-white solid; m.p.: 61–63 °C; R_f (65 vol. % ethyl acetate/*n*-hexane): 0.38; IR (KBr, cm^{-1}): 3019 (triazole ring), 2928, 2400, 1666, 1520, 1403, 1215, 1035, 928, 757, 669; $^1\text{H-NMR}$ (300 MHz, CDCl_3 , δ / ppm): 7.50 (1H, *s*, tri-H), 4.31 (2H, *t*, $J = 7.16$ Hz, N–N–CH₂–), 3.72 (2H, *s*, N–CH₂–tri), 2.85–2.65 (8H, *m*), 1.95–1.80 (2H, *m*), 1.41–1.18 (22H, *m*), 0.86 (3H, *t*, $J = 6.98$ Hz); $^{13}\text{C-NMR}$ (125 MHz, CDCl_3 , δ / ppm): 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 (*m/z*): 381 (M+H).

*4-((1-Pentadecyl-1*H*-1,2,3-triazol-4-yl)methyl)thiomorpholine (4f).* Yield: 84 %; off-white solid; m.p.: 65–67 °C; R_f (65 vol. % ethyl acetate /*n*-hexane): 0.37; IR (KBr, cm^{-1}): 3019 (triazole ring), 2927, 2855, 1403, 1215, 1051, 759, 668; $^1\text{H-NMR}$ (300 MHz, CDCl_3 , δ / ppm): 7.60 (1H, *s*, tri-H), 4.34 (2H, *t*, $J = 7.55$ Hz, N–N–CH₂–), 3.86 (2H, *s*, N–CH₂–tri), 3.05–2.62 (8H, *m*), 1.98–1.80 (2H, *m*), 1.40–1.18 (24H, *m*), 0.87 (3H, *t*, $J = 6.79$ Hz); $^{13}\text{C-NMR}$ (125 MHz, CDCl_3 , δ / ppm): 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 (*m/z*): 395 (M+H).

*4-((1-Heptadecyl-1*H*-1,2,3-triazol-4-yl)methyl)thiomorpholine (4g).* Yield: 74 %; off-white solid; m.p.: 68–70 °C; R_f (65 vol. % ethyl acetate/*n*-hexane): 0.37; IR (KBr, cm^{-1}): 3020 (triazole ring), 1639, 1405, 1216, 1038, 759, 668; $^1\text{H-NMR}$ (300 MHz, CDCl_3 , δ / ppm): 7.65 (1H, *s*, tri-H), 4.34 (2H, *t*, $J = 7.17$ Hz, N–N–CH₂–), 3.93 (2H, *s*, N–CH₂–tri), 3.05–2.80 (8H, *m*), 1.91–1.72 (2H, *m*), 1.48–1.10 (28H, *m*), 0.87 (3H, *t*, $J = 6.60$ Hz); $^{13}\text{C-NMR}$ (125 MHz, CDCl_3 , δ / ppm): 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 (*m/z*): 423 (M+H).

*4-((1-Hexyl-1*H*-1,2,3-triazol-4-yl)methyl)thiomorpholine (4h).* Yield: 75 %; yellow oil; R_f (65 vol. % ethyl acetate/*n*-hexane): 0.40; IR (KBr, cm^{-1}): 3019

(triazole ring), 1640, 1561, 1404, 928, 757, 668; $^1\text{H-NMR}$ (300 MHz, CDCl_3 , δ / ppm): 7.47 (1H, s, tri-H), 4.33 (2H, t, J = 7.74 Hz, N–N–CH₂–), 3.71 (2H, s, N–CH₂-tri), 2.82–2.64 (8H, m), 1.98–1.80 (2H, m), 1.40–1.20 (6H, m), 0.87 (3H, t, J = 7.17 Hz); $^{13}\text{C-NMR}$ (125 MHz, CDCl_3 , δ / ppm): 139.4, 124.4, 53.2, 51.9, 50.3, 31.2, 29.9, 28.3, 26.19, 22.2, 13.7; ESI-MS (m/z): 269 (M+H).

Ethyl 2-(4-(thiomorpholinomethyl)-1H-1,2,3-triazol-1-yl)acetate (4i). Yield: 75 %; pale yellow oil; R_f (65 vol. % ethyl acetate/n-hexane): 0.36; IR (KBr, cm⁻¹): 3019 (triazole ring), 1713, 1402, 1215, 1036, 928, 757, 669; $^1\text{H-NMR}$ (500 MHz, CDCl_3 , δ / ppm): 7.79 (1H, s, tri-H), 5.13 (2H, s, N–N–CH₂–CO–), 4.22 (2H, q, J = 7.09 and 7.09 Hz, O–CH₂–), 3.91 (2H, s, N–CH₂-tri), 3.01–2.91 (4H, m), 2.90–2.80 (4H, m), 1.25 (3H, t, J = 7.09 Hz); $^{13}\text{C-NMR}$ (75 MHz, CDCl_3 , δ / ppm): 165.9, 140.6, 126.1, 62.0, 53.2, 51.8, 50.6, 26.0, 13.6; ESI-MS (m/z): 271 (M+H).

4-((1-Dodecyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine (4j). Yield: 79 %; off-white solid; m.p.: 54–56 °C; R_f (65 vol. % ethyl acetate/n-hexane): 0.38; IR (KBr, cm⁻¹): 3019 (triazole ring), 2928, 2400, 1666, 1520, 1403, 1215, 1035, 928, 757, 669; $^1\text{H-NMR}$ (300 MHz, CDCl_3 , δ / ppm): 7.52 (1H, s, tri-H), 4.33 (2H, t, J = 7.36 Hz, N–N–CH₂–), 3.74 (2H, s, N–CH₂-tri), 2.82–2.64 (8H, m), 1.97–1.80 (2H, m), 1.48–1.18 (18H, m), 0.87 (3H, t, J = 6.98 Hz); $^{13}\text{C-NMR}$ (125 MHz, CDCl_3 , δ / ppm): 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 (m/z): 353 (M+H).

4-((1-Heptyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine 1,1-dioxide (5a). Yield: 75 %; off-white solid; m.p.: 60–62 °C; R_f (70 vol. % ethyl acetate/n-hexane): 0.38; IR (KBr, cm⁻¹): 3018 (triazole ring), 1412, 1218, 1050, 750, 666; $^1\text{H-NMR}$ (500 MHz, CDCl_3 , δ / ppm): 7.79 (1H, s, tri-H), 4.36 (2H, t, J = 7.32 Hz, N–N–CH₂–), 4.05 (2H, s, N–CH₂-tri), 3.11–3.06 (4H, m), 2.86–2.81 (4H, m), 1.97–1.82 (2H, m), 1.48–1.22 (8H, m), 0.87 (3H, t, J = 6.98 Hz); ESI-MS (m/z): 315 (M+H).

4-((1-Octyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine 1,1-dioxide (5b). Yield: 78 %; white solid; m.p.: 61–63 °C; R_f (70 vol. % ethyl acetate/n-hexane): 0.38; IR (KBr, cm⁻¹): 3030 (triazole ring), 2412, 1638, 1413, 1221; $^1\text{H-NMR}$ (300 MHz, CDCl_3 , δ / ppm): 7.50 (1H, s, tri-H), 4.33 (2H, t, J = 7.74 Hz, N–N–CH₂–), 3.72 (2H, s, N–CH₂-tri), 3.09–3.04 (4H, m), 2.88–2.81 (4H, m), 1.98–1.80 (2H, m), 1.49–1.22 (10H, m), 0.87 (3H, t, J = 7.09 Hz); ESI-MS (m/z): 329 (M+H).

4-((1-Decyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine 1,1-dioxide (5c). Yield: 68 %; pale yellow solid; m.p.: 64–66 °C; R_f (70 vol. % ethyl acetate/n-hexane): 0.38; IR (KBr, cm⁻¹): 3033 (triazole ring), 2927, 2403, 1652, 1518, 1426, 1217; $^1\text{H-NMR}$ (300 MHz, CDCl_3 , δ / ppm): 7.56 (1H, s, tri-H), 4.33 (2H, t, J = 7.17 Hz, N–N–CH₂–), 3.75 (2H, s, N–CH₂-tri), 3.10–3.04 (4H, m), 2.87–

–2.83 (4H, *m*), 1.20–1.81 (2H, *m*), 1.46–1.22 (14H, *m*), 0.86 (3H, *t*, *J* = 7.55 Hz); ESI-MS (*m/z*): 357 (M+H).

4-((1-Tridecyl-1*H*-1,2,3-triazol-4-yl)methyl)thiomorpholine 1,1-dioxide (5d). Yield: 61 %; pale yellow solid; m.p.: 68–70 °C; *R_f* (70 vol. % ethyl acetate/*n*-hexane): 0.40; IR (KBr, cm^{−1}): 3026 (triazole ring), 2918, 2857, 1640, 1537, 1415, 1216; ¹H-NMR (300 MHz, CDCl₃, δ / ppm): 7.56 (1H, *s*, tri-H), 4.33 (2H, *t*, *J* = 7.74 Hz, N–N–CH₂–), 3.79 (2H, *s*, N–CH₂–tri), 3.10–3.04 (4H, *m*), 2.88–2.81 (4H, *m*), 1.96–1.81 (2H, *m*), 1.45–1.16 (20H, *m*), 0.86 (3H, *t*, *J* = 6.60 Hz); ESI-MS (*m/z*): 399 (M+H).

4-((1-Tetradecyl-1*H*-1,2,3-triazol-4-yl)methyl)thiomorpholine 1,1-dioxide (5e). Yield: 66 %; off-white solid; m.p.: 69–72 °C; *R_f* (70 vol. % ethyl acetate/*n*-hexane): 0.39; IR (KBr, cm^{−1}): 3037 (triazole ring), 2941, 2388, 1668, 1534, 1417, 1215; ¹H-NMR (300 MHz, CDCl₃, δ / ppm): 7.56 (1H, *s*, tri-H), 4.36 (2H, *t*, *J* = 7.55 Hz, N–N–CH₂–), 3.74 (2H, *s*, N–CH₂–tri), 3.11–3.05 (4H, *m*), 2.87–2.80 (4H, *m*), 1.98–1.84 (2H, *m*), 1.47–1.20 (22H, *m*), 0.88 (3H, *t*, *J* = 6.98 Hz); ESI-MS (*m/z*): 413 (M+H).

4-((1-Pentadecyl-1*H*-1,2,3-triazol-4-yl)methyl)thiomorpholine 1,1-dioxide (5f). Yield: 64 %; pale yellow solid; m.p.: 77–79 °C; *R_f* (70 vol. % ethyl acetate/*n*-hexane): 0.37; IR (KBr, cm^{−1}): 3028 (triazole ring), 2920, 2860, 1413, 1218; ¹H-NMR (300 MHz, CDCl₃, δ / ppm): 7.65 (1H, *s*, tri-H), 4.36 (2H, *t*, *J* = 7.17 Hz, N–N–CH₂–), 3.88 (2H, *s*, N–CH₂–tri), 3.10–3.05 (4H, *m*), 2.86–2.80 (4H, *m*), 1.99–1.82 (2H, *m*), 1.48–1.19 (24H, *m*), 0.86 (3H, *t*, *J* = 6.60 Hz); ESI-MS (*m/z*): 427 (M+H).

4-((1-Heptadecyl-1*H*-1,2,3-triazol-4-yl)methyl)thiomorpholine 1,1-dioxide (5g). Yield: 74 %; off-white solid; m.p.: 73–75 °C; *R_f* (70 vol. % ethyl acetate/*n*-hexane): 0.38; IR (KBr, cm^{−1}): 3020 (triazole ring), 1639, 1405, 1216; ¹H-NMR (300 MHz, CDCl₃, δ / ppm): 7.70 (1H, *s*, tri-H), 4.37 (2H, *t*, *J* = 7.74 Hz, N–N–CH₂–), 3.94 (2H, *s*, N–CH₂–tri), 3.12–3.06 (4H, *m*), 2.88–2.81 (4H, *m*), 1.94–1.76 (2H, *m*), 1.52–1.18 (28H, *m*), 0.87 (3H, *t*, *J* = 6.79 Hz); ESI-MS (*m/z*): 455 (M+H).

4-((1-Hexyl-1*H*-1,2,3-triazol-4-yl)methyl)thiomorpholine 1,1-dioxide (5h). Yield: 70 %; yellow solid; m.p.: 68–70 °C; *R_f* (70 vol. % ethyl acetate/*n*-hexane): 0.36; IR (KBr, cm^{−1}): 3019 (triazole ring), 1644, 1567, 1414; ¹H-NMR (300 MHz, CDCl₃, δ / ppm): 7.49 (1H, *s*, tri-H), 4.38 (2H, *t*, *J* = 7.55 Hz, N–N–CH₂–), 3.74 (2H, *s*, N–CH₂–tri), 3.11–3.05 (4H, *m*), 2.86–2.80 (4H, *m*), 1.98–1.85 (2H, *m*), 1.45–1.22 (6H, *m*), 0.86 (3H, *t*, *J* = 6.98 Hz); ESI-MS (*m/z*): 301 (M+H).

Ethyl 2-(4-((1,1-dioxidothiomorpholino)methyl)-1*H*-1,2,3-triazol-1-yl)acetate (5i). Yield: 71 %; yellow oil; *R_f* (70 vol. % ethyl acetate/*n*-hexane): 0.39; IR (KBr, cm^{−1}): 3018 (triazole ring), 1715, 1412, 1218, 1033; ¹H-NMR (500 MHz, CDCl₃, δ / ppm): 7.80 (1H, *s*, tri-H), 5.14 (2H, *s*, N–N–CH₂–CO–), 4.25 (2H, *q*, *J* = 7.09 Hz, O–CH₂–), 3.94 (2H, *s*, N–CH₂–tri), 3.12–3.05 (4H, *m*), 2.88–2.81 (4H, *m*), 1.27 (3H, *t*, *J* = 7.09 Hz); ESI-MS (*m/z*): 303 (M+H).

*4-((1-Dodecyl-1H-1,2,3-triazol-4-yl)methyl)thiomorpholine 1,1-dioxide (**5j**).*

Yield: 67 %; white solid; m.p.: 64–66 °C; R_f (70 vol. % ethyl acetate/n-hexane): 0.37; IR (KBr, cm⁻¹): 3020 (triazole ring), 2929, 2418, 1669, 1522, 1413, 1218, 1045; ¹H-NMR (300 MHz, CDCl₃, δ / ppm): 7.54 (1H, s, tri-H), 4.34 (2H, t, J = 7.36 Hz, N–N–CH₂–), 3.75 (2H, s, N–CH₂–tri), 3.10–3.05 (4H, m), 2.86–2.80 (4H, m), 1.96–1.84 (2H, m), 1.44–1.16 (18H, m), 0.86 (3H, t, J = 7.17 Hz); ESI-MS (*m/z*): 385 (M+H).

TABLE S-I. *In vitro* antibacterial activity data for compounds **4a–j** and **5a–j** as MIC / µg mL⁻¹

Compound	<i>B. subtilis</i>	<i>S. aureus</i>	<i>S. epidermidis</i>	<i>E. coli</i>	<i>P. aeruginosa</i>	<i>K. pneumoniae</i>
4a	>150	75	2.34	>150	2.34	9.37
4b	>150	2.34	1.17	>150	>150	2.34
4c	>150	>150	2.34	>150	>150	>150
4d	>150	>150	>150	>150	>150	>150
4e	>150	>150	>150	>150	>150	>150
4f	>150	>150	>150	>150	>150	>150
4g	>150	>150	1.17	>150	>150	4.68
4h	>150	>150	>150	>150	>150	>150
4i	>150	>150	>150	>150	>150	>150
4j	>150	>150	>150	>150	>150	>150
5a	>150	2.34	2.34	>150	9.37	>150
5b	2.34	4.68	>150	>150	>150	>150
5c	>150	>150	>150	>150	>150	>150
5d	>150	>150	>150	>150	4.68	>150
5e	9.37	75	>150	>150	>150	>150
5f	>150	>150	>150	>150	>150	>150
5g	>150	>150	>150	>150	>150	>150
5h	>150	>150	>150	>150	>150	>150
5i	>150	>150	>150	>150	>150	>150
5j	2.34	>150	9.37	>150	>150	>150
Penicillin	1.56	1.56	3.12	12.5	12.5	6.25
Streptomycin	6.25	6.25	3.12	6.25	1.56	3.12

TABLE S-II. *In vitro* antifungal activity data for compounds **4a–j** and **5a–j** as zone of inhibition (mm) measured at 100 and 150 µg mL⁻¹

Compound	<i>C. albicans</i>		<i>S. cerevisiae</i>		<i>A. niger</i>		<i>A. flavus</i>	
	100 µg	150 µg	100 µg	150 µg	100 µg	150 µg	100 µg	150 µg
4a	0	0	0	0	0	0	0	0
4b	0	0	0	0	0	0	0	0
4c	10	13	0	0	10	14	9	12
4d	0	0	0	0	0	0	0	0
4e	9	12	0	0	15	16	10	13
4f	8	11	0	0	12	14	0	0
4g	0	0	0	0	0	0	0	0
4h	0	0	0	0	0	0	0	0
4i	0	0	0	0	0	0	0	0

TABLE S-II. Continued

Compound	<i>C. albicans</i>		<i>S. cerevisiae</i>		<i>A. niger</i>		<i>A. flavus</i>	
	100 µg	150 µg	100 µg	150 µg	100 µg	150 µg	100 µg	150 µg
4j	10	13	0	0	10	14	0	0
5a	0	0	0	0	0	0	0	0
5b	0	0	0	0	0	0	0	0
5c	8	10	0	0	10	12	0	0
5d	10	12	0	0	10	13	0	0
5e	0	0	0	0	0	0	0	0
5f	0	0	0	0	0	0	0	0
5g	11	13	0	0	0	0	8	11
5h	0	0	0	0	0	0	0	0
5i	0	0	0	0	0	0	0	0
5j	10	14	0	0	12	15	10	13
Amphotericin B	23.5		22		25		25	