Synthesis, Characterization and Antibacterial Activity of Novel Pyridones

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Supplemental Materials

Table S1. Minimum-inhibitory concentrations (MIC, in µg/ ml) of synthesized pyridones

Compounds	Microorganisms			
	<i>Staphylococcus aureus</i> ATCC 29213	<i>β-Hemolytic Streptococcus</i> ATCC 2957	<i>Escherichia coli</i> 111	<i>Salmonella Enteritidis</i> ATCC 13076
4a	250	250	250	250
4b	250	250	250	250
4c	250	250	250	250
4d	250	250	250	250
4e	125	250	250	125
5a	250	250	125	250
5b	250	250	125	125
5c	250	250	125	125
5d	250	250	125	125
PEN	31.25	>250	1.95	0.98
CEF	31.25	15.63	31.25	62.25

PEN: Penicillin G **CEF:** Ceftriaxone

Figure S1. ORTEP drawing of the molecule **4b**. Thermal ellipsoids are shown at 50% probability level.

Figure S2. *H*-bonded dimers lie (dashed lines) along diagonal axis in the unit cell. $N1-H\cdots O3^a = 2.900(6)$ Å, $\angle(N3-H3\cdots O3^a) = 169^\circ$ (symmetry code $a = 1/2+x, 1/2-y, z$).

Spectral Data

Diethyl 2-(3-oxo-1,3-di(thiophen-2-yl)propyl)malonate (3a)

White solid; yield 82%; mp 58-60 °C; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.76 (d, $J = 4.0$ Hz, 1H), 7.62 (d, $J = 4.8$ Hz, 1H), 7.13-7.10 (m, 2H), 6.93 (d, $J = 3.2$ Hz, 1H), 6.86 (dd, $J = 4.8, 4.0$ Hz, 1H), 4.51 (q, $J = 7.4$ Hz, 1H), 4.26-4.16 (m, 2H), 4.07 (q, $J = 7.0$ Hz, 2H), 3.88 (d, $J = 8.8$ Hz, 1H), 3.49 (d, $J = 6.8$ Hz, 2H), 1.25 (t, $J = 7.0$ Hz, 3H), 1.90 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 190.0, 167.9, 167.5, 144.0, 143.2, 133.8, 132.1, 128.1, 126.5, 125.9, 124.2, 61.7, 61.5, 57.7, 43.8, 36.2, 14.0, 13.8; IR (KBr, cm^{-1}) 3112, 3073, 2991, 2938, 2904, 2871, 1747, 1725, 1660, 1517, 1419, 1290, 1245, 1213, 1166, 1051, 1027, 862, 723, 690, 538; Elemental analysis (%), Calcd for $\text{C}_{18}\text{H}_{20}\text{O}_5\text{S}_2$: C, 56.82; H, 5.30; S, 16.86; Found: C, 56.79; H, 5.27; S, 16.81.

Diethyl 2-(3-oxo-3-(thiophen-2-yl)-1-p-tolylpropyl)malonate (3b)

White solid; yield 84%; mp 67-70 °C; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.73 (d, $J = 3.6$ Hz, 1H), 7.54 (d, $J = 4.8$ Hz, 1H), 7.15 (d, $J = 8.0$ Hz, 2H), 7.07-7.02 (m, 3H), 4.22-4.10 (m, 3H), 3.95 (q, $J = 7.0$ Hz, 2H), 3.82 (d, $J = 10.0$ Hz, 1H), 3.45 (dd, $J = 16.0, 4.4$ Hz, 1H), 3.35 (dd, $J = 16.0, 9.2$ Hz, 1H), 2.23 (s, 3H), 1.23 (t, $J = 7.2$ Hz, 3H), 1.00 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 190.5, 168.3, 167.7, 144.1, 137.0, 136.6, 133.7, 132.1, 129.0 (2C), 128.1, 128.0 (2C), 61.6, 61.3, 57.5, 43.4, 40.8, 21.0, 14.0, 13.7; IR (KBr, cm^{-1}) 3104, 2981, 2904, 1725, 1662, 1517, 1419, 1259, 1230, 1162, 1027, 858, 728, 547; Elemental analysis (%), Calcd for $\text{C}_{21}\text{H}_{24}\text{O}_5\text{S}$: C, 64.93; H, 6.23; S, 8.25; Found: C, 64.89; H, 6.20; S, 8.21.

Diethyl 2-(1-(4-methoxyphenyl)-3-oxo-3-(thiophen-2-yl)propyl)malonate (3c)

White solid; yield 82%; mp 79-82 °C; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.74 (d, J = 3.6 Hz, 1H), 7.57 (d, J = 4.8 Hz, 1H), 7.18 (d, J = 8.4 Hz, 2H), 7.08 (t, J = 4.4 Hz, 1H), 6.77 (d, J = 8.4 Hz, 2H), 4.23-4.16 (m, 2H), 4.12 (dt, J = 9.7, 4.6 Hz, 1H), 3.96 (q, J = 7.0 Hz, 2H), 3.79 (d, J = 10.0 Hz, 1H), 3.72 (s, 3H), 3.43 (dd, J = 16.0, 4.4 Hz, 1H), 3.33 (dd, J = 16.0, 9.6 Hz, 1H), 1.25 (t, J = 7.2 Hz, 3H), 1.02 (t, J = 7.2 Hz, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 190.5, 168.3, 167.7, 158.5, 144.1, 133.7, 132.1, 132.0, 129.2 (2C), 128.1, 113.7 (2C), 61.6, 61.3, 57.6, 55.1, 43.5, 40.5, 14.0, 13.8; IR (KBr, cm^{-1}) 3102, 2981, 2937, 2904, 2836, 1747, 1729, 1660, 1612, 1513, 1415, 1369, 1249, 1180, 1153, 1031, 858, 833, 728, 561; Elemental analysis (%), Calcd for $\text{C}_{21}\text{H}_{24}\text{O}_6\text{S}$: C, 62.36; H, 5.98; S, 7.93; Found: C, 62.32; H, 5.95; S, 7.90.

Diethyl 2-(3-(4-methoxyphenyl)-3-oxo-1-(thiophen-2-yl)propyl)malonate (3d)

Viscous oil; yield 86%; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.94 (d, J = 8.4 Hz, 2H), 7.13 (d, J = 4.8 Hz, 1H), 6.93 (bd, J = 6.8 Hz, 3H), 6.87 (d, J = 4.0 Hz, 1H), 4.54 (dd, J = 14.4, 7.0 Hz, 1H), 4.24-4.17 (m, 2H), 4.08 (q, J = 7.2 Hz, 2H), 3.89 (bd, 1H), 3.87 (s, 3H), 3.52 (d, J = 7.0 Hz, 2H), 1.26 (t, J = 7.0 Hz, 3H), 1.13 (t, J = 7.0 Hz, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 195.7, 168.1, 167.7, 163.5, 143.7, 130.4, 129.8, 126.5, 125.7, 124.1, 113.7, 61.6, 61.5, 57.9, 55.4, 42.8, 36.1, 14.0, 13.8; IR (KBr, cm^{-1}) 3108, 2981, 2935, 2840, 1747, 1731, 1675, 1600, 1575, 1509, 1419, 1369, 1307, 1259, 1172, 1029, 835, 703; Elemental analysis (%), Calcd for $\text{C}_{21}\text{H}_{24}\text{O}_6\text{S}$: C, 62.36; H, 5.98; S, 7.93; Found: C, 62.32; H, 5.97; S, 7.90.

Diethyl 2-(3-(furan-2-yl)-3-oxo-1-(thiophen-2-yl)propyl)malonate (3e)

White solid; yield 79%; mp 76-79 °C; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.35 (m, 1H), 7.17 (d, J = 3.6 Hz, 1H), 7.09 (d, J = 5.2 Hz, 1H), 6.90 (d, J = 3.2 Hz, 1H), 6.82 (t, J = 4.2 Hz, 1H), 6.48 (t, J = 1.8 Hz, 1H), 4.47 (dt, J = 8.8, 4.8 Hz, 1H), 4.22-4.13 (m, 2H), 4.03 (q, J = 7.0 Hz, 2H), 3.84 (d, J = 8.8 Hz, 1H), 3.43 (dd, J = 16.6, 9.0 Hz, 1H), 3.34 (dd, J = 16.6, 5.0 Hz, 1H), 1.22 (t, J = 7.0 Hz, 3H), 1.09 (t, J = 7.0 Hz, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 186.1, 167.8, 167.5, 152.4, 146.5, 143.2, 126.5, 125.8, 124.2, 117.4, 112.2, 61.6, 61.5, 57.8, 42.9, 35.7, 13.9, 13.8; IR (KBr, cm^{-1}): 3126, 3095, 2994, 2929, 1747, 1725, 1670, 1562, 1471, 1403, 1290, 1247, 1218, 1168, 1039, 1027, 914, 850, 771, 690, 595; Elemental analysis (%), Calcd for $\text{C}_{18}\text{H}_{20}\text{O}_6\text{S}$: C, 59.33; H, 5.53; S, 8.80; Found: C, 59.30; H, 5.51; S, 8.78.

rel-(3R,4S)-Ethyl 2-oxo-4,6-di(thiophen-2-yl)-1,2,3,4-tetrahydropyridine-3-carboxylate (4a)

Colorless crystal; yield 85%; mp 140-143 °C; ¹H-NMR (400 MHz, CDCl₃) δ 9.00 (s, 1H), 7.32 (d, *J* = 3.2 Hz, 1H), 7.27 (d, *J* = 5.2 Hz, 1H), 7.23 (d, *J* = 4.4 Hz, 1H), 7.04 (t, *J* = 4.2 Hz, 1H), 6.98 (d, *J* = 3.6 Hz, 1H), 6.96 (d, *J* = 3.6 Hz, 1H), 5.66 (d, *J* = 2.8 Hz, 1H), 4.67 (dd, *J* = 9.6, 4.0 Hz, 1H), 4.28-4.17 (m, 2H), 3.76 (d, *J* = 9.6 Hz, 1H), 1.24 (t, *J* = 7.2 Hz, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 168.2, 167.2, 143.6, 136.9, 131.5, 127.7, 127.0, 125.7, 125.1, 124.7, 124.2, 104.7, 61.7, 56.0, 37.2, 14.1; IR (KBr, cm⁻¹) 3205, 3108, 3068, 2973, 2933, 1743, 1679, 1648, 1477, 1375, 1249, 1145, 1031, 842, 759, 703, 692; Elemental analysis (%), Calcd for C₁₆H₁₅NO₃S₂: C, 57.64; H, 4.53; N, 4.20; S, 19.23; Found: C, 57.59; H, 4.44; N, 4.10; S, 19.11; GC/MS (m/z)(%) 261 (M⁺, 100), 200 (34.69), 110 (63.94), 45 (34.36).

rel-(3R,4S)-Ethyl 2-oxo-6-(thiophen-2-yl)-4-p-tolyl-1,2,3,4-tetrahydropyridine-3-carboxylate (4b)

Colorless crystal; yield 88%; mp 186-189 °C; ¹H-NMR (400 MHz, CDCl₃) δ 8.77 (s, 1H), 7.26 (bt, *J* = 5.6 Hz, 2H), 7.21 (d, *J* = 8.4 Hz, 2H), 7.16 (d, *J* = 8.4 Hz, 2H), 7.04 (dd, *J* = 5.0, 3.8 Hz, 1H), 5.57 (d, *J* = 2.8 Hz, 1H), 4.34 (dd, *J* = 10.4, 4.0 Hz, 1H), 4.23-4.12 (m, 2H), 3.71 (d, *J* = 10.8 Hz, 1H), 2.35 (s, 3H), 1.19 (t, *J* = 7.2 Hz, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 168.6, 167.6, 137.5, 137.2 (2C), 131.2, 129.6 (2C), 127.7, 127.5 (2C), 125.4, 123.7, 105.8, 61.5, 55.5, 41.6, 21.0, 14.0; IR (KBr, cm⁻¹) 3193, 3099, 2977, 2904, 2863, 1737, 1673, 1650, 1511, 1473, 1371, 1263, 1160, 1029, 811, 707; Elemental analysis (%), Calcd for C₁₉H₁₉NO₃S: C, 66.84; H, 5.61; N, 4.10; S, 9.39; Found: C, 66.79; H, 5.57; N, 4.04; S, 9.34; GC/MS (m/z)(%) 269 (M⁺, 100), 164 (64.55), 110 (66.90), 91 (38.81).

rel-(3R,4S)-Ethyl 4-(4-methoxyphenyl)-2-oxo-6-(thiophen-2-yl)-1,2,3,4-tetrahydropyridine-3-carboxylate (4c)

Colorless crystal; yield 91%; mp 194-197 °C; ¹H-NMR (400 MHz, CDCl₃) δ 8.56 (s, 1H), 7.29-7.22 (m, 4H), 7.03 (dd, *J* = 4.8, 4.0 Hz, 1H), 6.88 (d, *J* = 8.8 Hz, 2H), 5.56 (bd, *J* = 2.4 Hz, 1H), 4.32 (dd, *J* = 10.6, 3.8 Hz, 1H), 4.23-4.12 (m, 2H), 3.81 (s, 3H), 3.68 (d, *J* = 10.8 Hz, 1H), 1.19 (t, *J* = 7.2 Hz, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 168.6, 167.4, 158.9, 137.2, 132.5, 131.2, 128.7 (2C), 127.7, 125.4, 123.7, 114.2 (2C), 105.9, 61.5, 55.7, 55.3, 41.3, 14.1; IR (KBr, cm⁻¹) 3191, 3118, 3099, 2979, 2929, 2830, 1739, 1673, 1644, 1511, 1471, 1371, 1249, 1151, 1039, 827, 715, 549; Elemental analysis (%), Calcd for C₁₉H₁₉NO₄S: C, 63.85;

H, 5.36; N, 3.92; S, 8.97; Found: C, 63.78; H, 5.29; N, 3.87; S, 8.91; GC/MS (m/z)(%) 285 (M^+ , 100), 256 (39.07), 121 (67.73), 110 (58.49).

rel-(3R,4S)-Ethyl 6-(4-methoxyphenyl)-2-oxo-4-(thiophen-2-yl)-1,2,3,4-tetrahydropyridine-3-carboxylate (4d)

Colorless crystal; yield 89%; mp 135-138 °C; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.86 (s, 1H), 7.42 (d, $J = 8.4$ Hz, 2H), 7.22 (bd, $J = 4.8$ Hz, 1H), 6.98-6.92 (m, 4H), 5.51 (bd, $J = 4.0$ Hz, 1H), 4.65 (dd, $J = 9.0, 4.2$ Hz, 1H), 4.28-4.15 (m, 2H), 3.84 (s, 3H), 3.74 (d, $J = 9.2$ Hz, 1H), 1.23 (t, $J = 7.0$ Hz, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 168.4, 166.8, 160.4, 144.1, 136.6 (2C), 127.0, 126.6 (2C), 125.0, 124.6, 114.3 (2C), 104.0, 61.7, 56.1, 55.4, 37.3, 14.1; IR (KBr, cm^{-1}) 3203, 3102, 2973, 2933, 2838, 1737, 1681, 1650, 1606, 1515, 1378, 1292, 1245, 1147, 1027, 823, 769, 701, 514; Elemental analysis (%), Calcd for $\text{C}_{19}\text{H}_{19}\text{NO}_4\text{S}$: C, 63.85; H, 5.36; N, 3.92; S, 8.97; Found: C, 63.80; H, 5.30; N, 3.85; S, 8.92; GC/MS (m/z)(%) 285 (M^+ , 100), 188 (56.47), 134 (61.77), 91 (27.81).

rel-(3R,4S)-Ethyl 6-(furan-2-yl)-2-oxo-4-(thiophen-2-yl)-1,2,3,4-tetrahydropyridine-3-carboxylate (4e)

Viscous oil; yield 75%; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.57 (s, 1H), 7.44 (d, $J = 0.8$ Hz, 1H), 7.23 (dd, $J = 4.8, 0.8$ Hz, 1H), 6.98-6.94 (m, 2H), 6.67 (d, $J = 3.2$ Hz, 1H), 6.46 (dd, $J = 3.2, 2.0$ Hz, 1H), 5.78 (bd, $J = 4.0$ Hz, 1H), 4.69 (dd, $J = 9.4, 4.2$ Hz, 1H), 4.28-4.19 (m, 2H), 3.75 (d, $J = 9.6$ Hz, 1H), 1.24 (t, $J = 7.2$ Hz, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 168.2, 166.6, 147.0, 143.7, 142.9, 128.1, 126.9, 125.0, 124.7, 111.6, 106.7, 102.9, 61.8, 56.1, 37.0, 14.0; IR (KBr, cm^{-1}) 3226, 3116, 2979, 2935, 2871, 1735, 1683, 1496, 1373, 1263, 1157, 1024, 740, 703; Elemental analysis (%), Calcd for $\text{C}_{16}\text{H}_{15}\text{NO}_4\text{S}_2$: C, 60.55; H, 4.76; N, 4.41; S, 10.10; Found: C, 60.47; H, 4.68; N, 4.35; S, 10.03; GC/MS (m/z)(%) 245 (M^+ , 100), 216 (33.94), 148 (25.63), 94 (32.15).

4,6-Di(thiophen-2-yl)-3,4-dihydropyridin-2(1H)-one (5a)

Brown crystal; yield 58%; mp 172-175 °C; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.67 (s, 1H), 7.30 (d, $J = 5.2$ Hz, 1H), 7.22 (d, $J = 4.8$ Hz, 1H), 7.20 (d, $J = 3.6$ Hz, 1H), 7.07 (dd, $J = 4.8, 4.0$ Hz, 1H), 7.00-6.95 (m, 2H), 5.69 (bd, $J = 4.4$ Hz, 1H), 4.27-4.21 (m, 1H), 2.98 (dd, $J = 16.0, 6.8$ Hz, 1H), 2.83 (dd, $J = 16.0, 8.4$ Hz, 1H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 169.9, 145.8, 137.6, 131.6, 127.7, 127.0, 125.6, 124.1, 123.9, 123.4, 105.6, 39.4, 33.7; IR (KBr, cm^{-1}) 3210, 3097, 2958, 2927, 2854, 1725, 1679, 1646, 1463, 1378, 1297, 973, 786, 721, 698; Elemental analysis (%), Calcd for $\text{C}_{13}\text{H}_{11}\text{NOS}_2$: C, 59.74; H, 4.24; N, 5.36; S, 24.54; Found:

C, 59.66; H, 4.09; N, 5.30; S, 24.45; GC/MS (m/z)(%) 261 (M^+ , 100), 200 (34.20), 110 (63.13), 45 (32.90).

6-(Thiophen-2-yl)-4-p-tolyl-3,4-dihydropyridin-2(1H)-one (5b)

Brown crystal; yield 65%; mp 143-146 °C; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.46 (s, 1H), 7.28 (d, $J = 2.8$ Hz, 1H), 7.26 (d, $J = 4.8$ Hz, 1H), 7.21 (d, $J = 8.2$ Hz, 2H), 7.18 (d, $J = 8.2$ Hz, 2H), 7.06 (dd, $J = 5.0, 3.8$ Hz, 1H), 5.62 (d, $J = 3.6$ Hz, 1H), 3.97-3.90 (m, 1H), 2.88 (dd, $J = 16.3, 7.2$ Hz, 1H), 2.72 (dd, $J = 16.3, 10.2$ Hz, 1H), 2.37 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 171.1, 139.7, 137.9, 136.7, 131.6, 129.6 (2C), 127.7, 127.0 (2C), 125.1, 123.3, 106.4, 39.1, 38.2, 21.0; IR (KBr, cm^{-1}) 3197, 3104, 2998, 2935, 2842, 1681, 1644, 1509, 1473, 1369, 1249, 935, 815, 715, 505; Elemental analysis (%), Calcd for $\text{C}_{16}\text{H}_{15}\text{NOS}$: C, 71.34; H, 5.61; N, 5.20; S, 11.90; Found: C, 71.27; H, 5.55; N, 5.13; S, 11.79; GC/MS (m/z)(%) 269 (M^+ , 100), 164 (65.58), 110 (65.20), 91 (37.42).

4-(4-Methoxyphenyl)-6-(thiophen-2-yl)-3,4-dihydropyridin-2(1H)-one (5c)

Brown crystal; yield 68%; mp 123-126 °C; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.90 (s, 1H), 7.27 (d, $J = 4.8$ Hz, 1H), 7.22 (d, $J = 8.6$ Hz, 2H), 7.21-7.20 (m, 1H), 7.06 (dd, $J = 4.8, 3.6$ Hz, 1H), 6.90 (d, $J = 8.6$ Hz, 2H), 5.61 (d, $J = 3.6$ Hz, 1H), 3.95-3.89 (m, 1H), 3.82 (s, 3H), 2.87 (dd, $J = 16.1, 7.0$ Hz, 1H), 2.70 (dd, $J = 16.1, 10.0$ Hz, 1H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 170.6, 158.6, 137.9, 134.7, 131.4, 128.1 (2C), 127.7, 125.2, 123.1, 114.3 (2C), 106.6, 55.3, 39.2, 37.8; IR (KBr, cm^{-1}) 3205, 3097, 2991, 2902, 2829, 1679, 1644, 1610, 1511, 1461, 1365, 1247, 1035, 823, 701; Elemental analysis (%), Calcd for $\text{C}_{16}\text{H}_{15}\text{NO}_2\text{S}$: C, 67.34; H, 5.30; N, 4.91; S, 11.24; Found: C, 67.26; H, 5.23; N, 4.88; S, 11.16; GC/MS (m/z)(%) 285 (M^+ , 100), 256 (39.48), 121 (72.17), 110 (63.07).

6-(4-Methoxyphenyl)-4-(thiophen-2-yl)-3,4-dihydropyridin-2(1H)-one (5d)

Brown crystal; yield 62%; mp 122-125 °C; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.41 (bd, $J = 8.8$ Hz, 3H), 7.21 (d, $J = 4.0$ Hz, 1H), 7.00-6.92 (m, 4H), 5.53 (d, $J = 3.6$ Hz, 1H), 4.23 (dd, $J = 11.6, 8.0$ Hz, 1H), 3.85 (s, 3H), 2.96 (dd, $J = 16.0, 6.8$ Hz, 1H), 2.81 (dd, $J = 16.0, 8.4$ Hz, 1H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 170.3, 160.3, 146.5, 136.8, 127.2, 126.9, 126.5 (2C), 123.9, 123.7, 114.3 (2C), 104.7, 55.3, 39.4, 33.7; IR (KBr, cm^{-1}) 3193, 3097, 3014, 2956, 2931, 2832, 1673, 1644, 1610, 1513, 1371, 1286, 1240, 1029, 829, 767, 721; Elemental analysis (%), Calcd for $\text{C}_{16}\text{H}_{15}\text{NO}_2\text{S}$: C, 67.34; H, 5.30; N, 4.91; S, 11.24; Found: C, 67.22; H, 5.24; N, 4.84; S, 11.18; GC/MS (m/z)(%) 285 (M^+ , 100), 188 (55.29), 134 (59.10), 91 (26.23).