SUPPLEMENTARY MATERIAL TO

**Design, synthesis and antimycobacterial evaluation of some new azaheterocycles with 4,7-phenanthroline skeleton. Part VI**

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PHYSICAL AND SPECTRAL DATA FOR THE PREPARED COMPOUNDS

*4-(2-(4-Tolyl)-2-oxoethyl)-4,7-phenanthrolin-4-ium bromide (****1****).* Beige powder; Yield: 67%; m.p. 246-248 °C; Anal. Calcd. for C21H17BrN2O: C, 64.13; H, 4.36; N, 7.12%. Found: C, 64.10, H, 4,30; N, 7.20; IR (KBr, cm-1): 2968 (C-H stretching), 1672 (-C=O stretching) , 1503 (-C=C- and –C=N- stretching of aromatic ring); 1H-NMR (500 MHz, DMSO-*d6*, *δ* / ppm): 2.48 (3H, *s*, CH3), 7.14 (2H, *s*, 15-H), 7.52 (2H, *d*, *J* = 8.5 Hz, 2xH-phenyl), 8.06 (1H, *dd*, *J* = 8.5, 4.5 Hz, 9-H), 8.08 (2H, *d*, *J* = 8.5 Hz, 2xH-phenyl), 8.58 (2H, *m*, 2-H, 6-H), 8.63 (1H, *d*, *J* = 10.0 Hz, 5-H), 9.27 (1H, *ad*, *J* = 4.0 Hz, 10-H ), 9.60 (2H, *m*, 1-H, 8-H), 10.31 (1H, *ad*, *J* = 8.5 Hz, 3-H); 13C-NMR (125 MHz, DMSO-*d6*, *δ* / ppm): 21.4 (CH3), 63.9 (C15), 129.6 (2xCH-phenyl), 120.5 (C6), 123.4 (C2), 123.9 (C14), 124.5 (C9), 127.9 (C13), 128.8 (2xCH-phenyl), 131.1 (Cq-phenyl), 133.0 (C8), 138.2 (C5), 139.5 (C110), 143.1 (C3), 145.6 (Cq-phenyl), 146.2 (C12), 149.3 (C1), 153.3 (C10), 190.2 (CO).

*4-(2-(4-Methoxyphenyl)-2-oxoethyl)-4,7-phenanthrolin-4-ium bromide (****2****).*Beige powder; Yield: 94%; m.p. 253-255°C; Anal. Calcd. for C21H17BrN2O2: C, 61.63; H, 4.19; N, 6.84%. Found: C, 61.64, H, 4,10; N, 6.90%; IR (KBr, cm-1): 2940 (C-H stretching), 1684 (-C=O stretching), 1599 (-C=C- and –C=N- stretching of aromatic ring), 1238, 1179 (-C-O- stretching); 1H-NMR (500 MHz, DMSO-*d6*, *δ* / ppm): 3.93 (3H, *s*, OCH3), 7.07 (2H, *s*, 15-H), 7.23 (2H, *d*, *J* = 8.5 Hz, 2xH-phenyl), 8.06 (1H, *dd*, *J* = 8.5, 4.0 Hz, 9-H), 8.15 (2H, *d*, *J* = 8.5 Hz, 2xH-phenyl), 8.57 (2H, *m*, 2-H, 5-H), 8.64 (1H, *d*, *J* = 10.0 Hz, 6-H), 9.28 (1H, *ad*, *J* = 4.0 Hz, 10-H ), 9.54 (1H, *ad*, *J* = 6.0 Hz, 1-H), 9.60 (1H, *ad*, *J* = 4.0 Hz, 8-H), 10.30 (1H, *ad*, *J* = 8.5 Hz, 3-H); 13C-NMR (125 MHz, DMSO-*d6*, *δ* / ppm): 55.9 (OCH3), 63.7 (C15), 114.4 (2xCH-phenyl), 120.5 (C6), 123.4 (C2), 123.9 (C14), 124.5 (C9), 126.4 (Cq-phenyl), 127.9 (C13), 131.2 (2xCH-phenyl), 132.9 (C8), 138.3 (C5), 139.5 (C11), 143.0 (C)3, 146.2 (C12), 149.3 (C1), 153.4 (C10), 164.5 (Cq-phenyl), 188.8 (CO).

*4-(2-(4-Nitrophenyl))-2-oxoethyl)-4,7-phenanthrolin-4-ium bromide (****3****).*Beige powder; Yield: 91%; m.p. 235-237°C; Anal. Calcd. for C20H14BrN3O3: C, 56.62; H, 3.33; N,9.90%. Found: C, 56.70, H, 3,20; N, 9.97%; IR (KBr, cm-1): 3034 (aromatic C-H stretching), 2893 (C-H stretching), 1698 (-C=O stretching), 1520 (N-O stretching), 1504 (-C=C- and –C=N- stretching of aromatic ring), 1344 (N-O stretching); 1H-NMR (500 MHz, DMSO-*d6*, *δ* / ppm): 7.20 (2H, *s*, 15-H), 8.06 (1H, *dd*, *J* = 8.5, 4.5 Hz, 9-H), 7.40 (2H, *d*, *J* = 8.5 Hz, 2xH-phenyl), 8.53 (2H, *d*,  *J* = 8.5 Hz, 2xH-phenyl), 8.59 (1H, *dd*, *J* = 8.5, 6.0 Hz, 2-H), 8.64 (1H, *d*, *J* = 10.0 Hz, 6-H), 8.73 (1H, *d*, *J* = 10.0 Hz, 5-H), 9.28 (1H, *ad*, *J* = 3.0 Hz, 10-H ), 9.58 (1H, *ad*, *J* = 6.0 Hz, 1-H), 9.61(1H, *ad*, *J* = 8.5 Hz, 8-H), 10.33 (1H, *ad*, *J* = 8.5 Hz, 3-H); 13C-NMR (125 MHz, DMSO-*d6*, *δ* / ppm): 64.3 (C15), 120.7 (C6), 123.4 (C2), 123.9 (C14), 124.5 (C9), 128.0 (C13), 124.0 (2xCH-phenyl), 130.2 (2xCH-phenyl), 133.0 (C8), 138.2 (C5), 138.3 (Cq-phenyl), 139.6 (C11), 143.4 (C3), 146.2 (C12), 149.3 (C1), 150.7 (C-NO2), 153.4 (C10), 190.1 (CO).

*4-(2-(4-Chlorophenyl)-2-oxoethyl)-4,7-phenanthrolin-4-ium bromide (****4****).*Beige powder; Yield: 74%; m.p. 242-244°C;Anal. Calcd. for C20H14BrClN2O: C, 58.07; H, 3.41; N, 6.77%. Found: C, 58.10, H, 3,29; N, 6.87%; IR (KBr, cm-1): 2951 (C-H stretching), 1688 (-C=O stretching), 1588, 1504 (-C=C- and –C=N- stretching of aromatic ring); 1H-NMR (500 MHz, DMSO-*d6*, *δ* / ppm): 7.12 (2H, *s*, 15-H), 7.81 (2H, *d*, *J* = 8.5 Hz, 2xH-phenyl), 8.06 (1H, *dd*, *J* = 8.5, 4.0 Hz, 9-H), 8.18 (2H, *d*, *J* = 8.5 Hz, 2xH-phenyl), 8.57 (1H, *dd*, *J* = 8.5, 6.0 Hz, 2-H), 8.63 (1H, *d*, *J* = 10.0 Hz, 6-H), 8.65 (1H, *d*, *J* = 10.0 Hz, 5-H), 9.28 (1H, *dd*, *J* = 4.0, 1.0 Hz, 10-H), 9.56 (1H, *ad*, *J* = 6.0 Hz, 1-H), 9.60 (1H, *ad*, *J* = 4.0 Hz, 8-,), 10.31 (1H, *ad*, *J* = 8.5 Hz, 3-H); 13C-NMR (125 MHz, DMSO-*d6*, *δ* / ppm): 64.0 (C15), 120.6 (C6), 123.4 (C2), 123.9 (C14), 124.5 (C9), 128.0 (C13), 129.2 (2xCH-phenyl), 130.6 (2xCH-phenyl), 132.4 (Cq-phenyl), 133.0 (C8), 138.3 (C5), 139.6 (C11), 139.7 (Cq-phenyl), 143.2 (C3), 146.2 (C12), 149.3 (C1), 153.4 (C10), 189.9 (CO).

*4-(2-(3-Methoxyphenyl)-2-oxoethyl)-4,7-phenanthrolin-4-ium bromide (****5****).*Beige powder; Yield: 74%; m.p. 208-210°C;Anal. Calcd. for C21H17BrN2O2: C, 61.63; H, 4.19; N, 6.84%; Found: C, 61.60, H, 4,12; N, 6.92%; IR (KBr, cm-1): 3006 (aromatic C-H stretching), 2964 (C-H stretching), 1684 (-C=O stretching), 1599, 1573 (-C=C- and –C=N- stretching of aromatic ring), 1238, 1179 (C-O stretching); 1H-NMR (500 MHz, DMSO-*d6*, *δ* / ppm): 3.89 (3H, *s*, OMe), 7.18 (2H, *s*, 15-H), 7.41 (1H, *dd*, *J* = 8.50, 2.0 Hz, H-phenyl), 7.64 (2H, *m*, 2xH-phenyl), 7.78 (1H, *ad*, *J* = 7.5 Hz, H-phenyl), 8.05 (1H, *dd*, *J* = 8.5, 4.0 Hz, 9-H), 8.56-8.65 (3H, *m*, 2-H, 5-H, 6-H), 9.27 (1H, *ad*, *J* = 3.5 Hz, 10-H ), 9.54 (2H, *ad*, 1-H, 8-H), 10.32 (1H, *ad*, *J* = 8.5 Hz, 3-H); 13C-NMR (125 MHz, DMSO-*d6*, *δ* / ppm): 55.7 (OCH3), 64.2 (C15), 113.2 (CH-phenyl), 120.5 (C6), 120.8 (CH-phenyl), 121.2 (CH-phenyl), 123.5 (C2), 123.8 (C14), 124.5 (C9), 127.9 (C13), 130.3 (CH-phenyl), 133.0 (Cq-phenyl), 134.9 (C8), 138.2 (C5), 139.4 (C11), 143.2 (C3), 146.1 (C12), 149.2 (C1), 153.3 (C10), 159.5 (Cq-phenyl), 190.6 (CO).

*4-(2-Amino-2-oxoethyl)-4,7-phenanthrolin-4-ium iodide (****6****).* Yellow powder; Yield: 84%; m.p. 264-266°C; Anal. Calcd. for C14H12IN3O: C, 46.05; H, 3.31; N, 11.51%; Found: C, 46.10, H, 3,29; N, 11.59%; IR (KBr, cm-1): 3351, 3167 (N-H stretching), 1673 (-C=O stretching), 1502 (-C=C- and –C=N- stretching of aromatic ring); 1H-NMR (500 MHz, DMSO-*d6*, *δ* / ppm): 5.27 (2H, *s*, 15-H), 7.89 (1H, *s*, -NH), 8.02(1H, *dd*, *J* = 8.5, 3.5Hz, 9-H), 8.21 (1H, *s*, -NH), 8.44(1H, *d*, *J* = 10.0 Hz, 5-H), 8.50 (1H, *dd*, *J* = 8.5, 6.5 Hz, 2-H), 8.70 (1H, *d*, *J* = 10.0 Hz, 6-H), 9.25 (1H, *ad*, *J* = 3.5 Hz, 10-H ), 9.54 (1H, *ad*, *J* = 8.5 Hz, 8-H), 9.57 (1H, *ad*, *J* = 6.0 Hz, 1-H),10.22 (1H, *ad*, *J* = 8.5 Hz, 3-H); 13C-NMR (125 MHz, DMSO-*d6*, *δ* / ppm): 59.5 (C15), 119.9 (C6), 123.2 (C2), 123.8 (C14), 124.5 (C9), 127.8 (C13), 132.9 (C8), 138.3 (C5), 139.1 (C11), 142.8 (C3), 146.1 (C12), 149.4 (C1), 153.3 (C10), 165.8 (CO).

*4-(Cyanomethyl)-4,7-phenanthrolin-4-ium bromide (****7****).*Beige powder; Yield: 58%; m.p. 214-216°C; Anal. Calcd. for C14H10BrN3: C, 56.02; H, 3.36; N, 14.00%; Found: C, 56.10, H, 3,29; N, 14.09%; IR (KBr, cm-1): 3056 (aromatic C-H stretching), 2201 (C≡N stretching), 1619 (-C=O stretching); 1H-NMR (500 MHz, DMSO-*d6*, *δ* / ppm): 6.58 (2H, *s*, 15-H), 8.08 (1H, *dd*, *J* = 8.5, 4.0 Hz, 9-H), 8.55 (1H, *dd*, *J* = 8.5, 6.0 Hz, 2-H), 8.80 (1H, *d*, *J* = 10.0 Hz, 5-H), 8.83 (1H, *d*, *J* = 10.0 Hz, 6-H), 9.31 (1H, *ad*, *J* = 4.5 Hz, 10-H), 9.59 (1H, *ad*, *J* = 8.5 Hz, 8-H), 9.70 (1H, *ad*, *J* = 6.0 Hz, 1-H), 10.32 (1H, *ad*, *J* = 8.5 Hz, 3-H); 13C-NMR (125 MHz, DMSO-*d6*, *δ* / ppm): 45.6 (C15), 114.0 (CN), 119.4 (C6), 123.7 (C2), 124.1 (C14), 124.8 (C9), 128.4 (C13), 133.0 (C8), 138.1 (C5), 139.2 (C11), 144.3 (C3), 146.2 (C12), 149.5 (C1), 153.6 (C10).

*4-(2-Methoxy-2-oxoethyl)-4,7-phenanthrolin-4-ium bromide (****8****).*Beigepowder;Yield: 71%; m.p. 169-170°C; *Anal.* Calcd. for C15H13BrN2O2: C, 54.07; H, 3.93; N, 8.41%; Found: C, 54.10, H, 3,89; N, 8.49%; IR (KBr, cm-1): 3033 (aromatic C-H stretching), 2977 (C-H stretching), 1745 (ester C=O stretching), 1704 (ketone C=O stretching), 1235 (-C-O- stretching); 1H-NMR (500 MHz, DMSO-*d6*, *δ* / ppm): 3.81 (3H, *s*, CH3), 6.35 (2H, *s*, 15-H), 8.04 (1H, *dd*, *J* = 8.5, 4.0 Hz, 9-H), 8.55 (1H, *dd*, *J* = 8.5, 6.0 Hz, 2-H), 8.65 (1H, *d*, *J* = 10.0 Hz, 5-H), 8.68 (1H, *d*, *J* = 10.0 Hz, 6-H), 9.26 (1H, *dd*, *J* = 4.0, 1.0 Hz, 10-H), 9.58 (1H, *ad*, *J* = 8.5 Hz, 8-H), 9.66 (1H, *ad*, *J* = 5.5 Hz, 1-H), 10.31 (1H, *ad*, *J* = 8.5 Hz, 3-H); 13C-NMR (125 MHz, DMSO-*d6*, *δ* / ppm): 53.3 (CH3), 58.1 (C15), 120.3 (C6), 123.4 (C2), 123.8 (C14), 124.5 (C9), 127.9 (C13), 133.0 (C8), 138.4 (C5), 139.1 (C11), 143.6 (C3), 146.1 (C12), 149.5 (C10, 153.4 (C100, 166.6 (C=O).