# A simple and convenient approach to the Kr€ohnke pyridine type synthesis of functionalised indol-3-yl pyridine derivatives using 3-cyanoacetyl indole

*Prakasam Thirumurugan, A. Nandakumar, D. Muralidharan and Paramasivan. T. Perumal.**

## Supplementary Data

Contents Page. No.

1. Spectral data compound **4a-t**

**4a**. *6-(1H-Indol-3-yl)-4-phenyl-2,2'-bipyridine-5-carbonitrile* (Table 2, entry 1)

Pale Yellow solid; mp 278-280 $^{o}$C; $R_f$ 0.33 (20% AcOEt/Petroleum ether); IR (KBr): 1143, 1212, 1367, 1437, 1533, 1569, 2215, 3334 cm$^{-1}$; $^{1}$H NMR (500 MHz, DMSO-d$_6$): δ 7.22 (s, 2H, Ar-*H*), 7.52-7.56 (m, 5H, Ar-*H*), 7.72 (s, 2H, Ar-*H*), 8.04 (s, 1H, Ar-*H*), 8.24 (s, 1H, Ar-*H*), 8.35 (s, 2H, Ar-*H*), 8.52 (d, 1H, *J* = 7.6 Hz Ar-*H*), 8.72 (s, 1H, Ar-*H*), 11.86 (brs, 1H, -N*H*); $^{13}$C NMR (125 MHz, DMSO-d$_6$)**:** δ 102.8, 112.1, 112.8, 116.3, 118.7, 120.9, 121.2, 121.6, 122.4, 125.3, 126.0, 128.6, 128.8, 128.9, 129.8, 136.3, 136.8, 137.8, 149.7, 153.9, 155.1, 157.1, 157.3; MS (EI): *m*/*z* 373.40 [M$^{+}$+H$^{+}$]; Anal. Calcd for $C_{25}H_{16}N_4$: C 80.63 H 4.33 N 15.04. Found: C 80.74 H 4.32 N 14.98.

**4b**. *6-(1H-Indol-3-yl)-4-(4-methylphenyl)-2,2'-bipyridine-5-carbonitrile* (Table 2, entry 2)

Light green solid; mp 276-278 $^{o}$C; $R_f$ 0.34 (20% AcOEt/Petroleum ether); IR (KBr): 1140, 1214, 1368, 1437, 1536, 2219, 3053 cm$^{-1}$; $^{1}$H NMR (500 MHz, DMSO-d$_6$): δ 2.36 (s, 3H, Ar-C*H*$_3$), 7.21 (q, 2H, *J* = 6.1 Hz, Ar-*H*), 7.33 (d, 2H, *J* = 7.6 Hz, Ar-*H*), 7.47-7.49 (m, 1H, Ar-*H*), 7.53 (d, 1H, *J* = 7.6 Hz, Ar-*H*), 7.59 (d, 2H, *J* = 7.6 Hz, Ar-*H*), 7.98 (t, 1H, *J* = 7.6 Hz, Ar-*H*), 8.21 (s, 1H, Ar-*H*), 8.34-8.38 (m, 2H, Ar-*H*), 8.50 (d, 1H, *J* = 7.6 Hz, Ar-*H*), 8.70 (s, 1H, Ar-*H*), 11.83 (brs, 1H, -N*H*); $^{13}$C NMR (75 MHz, DMSO-d$_6$)**:** δ 20.8, 102.7, 112.0, 112.7, 116.1, 118.8, 120.8, 121.2, 121.5, 122.3, 125.2, 126.0, 128.5, 128.7, 129.4, 133.9, 136.3, 137.7, 139.5, 149.6, 153.9, 155.0, 157.0, 157.4; MS (EI): *m*/*z* 387.33 [M$^{+}$+H$^{+}$]; Anal. Calcd for $C_{26}H_{18}N_4$: C 80.81 H 4.69 N 14.50. Found: C 80.72 H 4.81 N 14.56.

**4c**. *6-(1H-Indol-3-yl)-4-(3-methylphenyl)-2,2'-bipyridine-5-carbonitrile* (Table 2, entry 3)

Light green solid; mp 214-216 $^{o}$C; $R_f$ 0.34 (20% AcOEt/Petroleum ether); IR (KBr): 1129, 1218, 1376, 1439, 1539, 1627, 2219, 3256 cm$^{-1}$; $^{1}$H NMR (500 MHz, DMSO-d$_6$): δ 2.38 (s, 3H, Ar-

C*H*$_3$), 7.21 (q, 2H, *J* = 6.1 Hz, Ar-*H*), 7.33 (d, 1H, *J* = 6.9 Hz, Ar-*H*), 7.41-7.44 (t, 1H, *J* = 7.6 Hz, Ar-*H*), 7.50-7.54 (m, 4H, Ar-*H*), 8.00 (t, 1H, *J* = 7.6 Hz, Ar-*H*), 8.22 (s, 1H, Ar-*H*), 8.36-8.38 (m, 2H, Ar-*H*), 8.51 (d, 1H, *J* = 7.6 Hz, Ar-*H*), 8.71 (d, 1H, *J* = 4.6 Hz, Ar-*H*), 11.84 (brs, 1H, -N*H*); $^{13}$C NMR (125 MHz, DMSO-d$_6$)**:** δ 20.9, 102.7, 112.1., 112.8, 116.2, 118.7, 120.8, 121.2, 121.5, 122.4, 125.2, 125.8, 126.0, 128.6, 128.8, 129.0, 130.4, 136.4, 136.8, 137.6, 138.2, 149.6, 154.0, 155.2, 157.1, 157.4; MS (EI): *m*/*z* = 387.20 [$M^+$+$H^+$]; Anal. Calcd for $C_{26}H_{18}N_4$. C 80.81 H 4.69 N 14.50. Found: C 80.89 H 4.67 N 14.45.

**4d**. *6-(1H-Indol-3-yl)-4-(4-methoxyphenyl)-2,2'-bipyridine-5-carbonitrile* (Table 2, entry 4)

Light green solid; mp 254-256 $^o$C; $R_f$ 0.20 (20% AcOEt/Petroleum ether); IR (KBr): 1029, 1134, 1177, 1254, 1297, 1365, 1424, 1511, 1572, 1608, 2210, 3246 cm$^{-1}$; $^1$H NMR (500 MHz, DMSO-d$_6$): δ 3.81 (s, 3H, Ar-OC*H*$_3$), 7.08 (d, 2H, *J* = 8.4 Hz, Ar-*H*), 7.20-7.23 (m, 2H, Ar-*H*), 7.48-7.53 (m, 2H, Ar-*H*), 7.67 (d, 2H, *J* = 8.4 Hz, Ar-*H*), 8.00 (t, 1H, *J* = 9.2 Hz, Ar-*H*), 8.21 (s, 1H, Ar-*H*), 8.34-8.37 (m, 2H, Ar-*H*), 8.49 (d, 1H, *J* = 8.4 Hz, Ar-*H*), 8.71 (d, 1H, *J* = 4.6 Ar-*H*), 11.82 (brs, 1H, -N*H*); $^{13}$C NMR (125 MHz, DMSO-d$_6$): δ 55.3, 102.6, 112.1, 112.8, 114.2, 116.0, 119.0, 120.8, 121.2, 121.5, 122.3, 125.2, 126.0, 128.7, 128.9, 130.2, 136.3, 137.6, 149.6, 154.0, 156.9, 157.4, 157.6, 160.5; MS (EI): *m*/*z* 403.33 [$M^+$+$H^+$]; Anal. Calcd for $C_{26}H_{18}N_4O$: C 77.59 H 4.51 N 13.92. Found: C 80.48 H 4.52 N 13.88.

**4e**. *6-(1H-Indol-3-yl)-4-(3,4-methoxyphenyl)-2,2'-bipyridine-5-carbonitrile* (Table 2, entry 5)

Light green solid; mp 240-242 $^o$C; $R_f$ 0.10 (20% AcOEt/Petroleum ether); IR (KBr): 1023, 1141, 1254, 1438, 1516, 2206, 3312 cm$^{-1}$; $^1$H NMR (500 MHz, DMSO-d$_6$): δ 3.82 (s, 3H, Ar-OC*H*$_3$), 3.83 (s, 3H, Ar-OC*H*$_3$),7.13 (d, 2H, *J* = 8.4 Hz, Ar-*H*), 7.21-7.23 (m, 1H, Ar-*H*), 7.30-7.32 (m, 1H, Ar-*H*), 7.38 (d, 1H, *J* = 2.3 Hz, Ar-*H*), 7.52-7.54 (m, 2H, Ar-*H*), 8.00-8.07 (m, 1H, Ar-*H*), 8.27 (s, 1H, Ar-*H*), 8.35-8.37 (m, 2H, Ar-*H*), 8.52 (d, 1H, *J* = 7.6 Hz, Ar-*H*), 8.74 (d, 1H,

*J* = 4.6, Ar-*H*), 11.83 (brs, 1H, -N*H*); $^{13}$C NMR (125 MHz, DMSO-$d_6$): δ 55.5, 55.7, 102.9, 111.8, 112.1, 112.3, 112.8, 116.1, 119.0, 120.8, 121.1, 121.5, 121.6, 122.3, 125.2, 126.0, 128.8, 129.0, 136.3, 137.7, 148.6, 149.6, 150.2, 154.1, 154.9, 156.9, 157.4; MS (EI): *m*/*z* 433.20 [$M^+$+$H^+$]; Anal. Calcd for $C_{27}H_{20}N_4O_2$: C 74.98 H 4.66 N 12.95. Found: C 74.90 H 4.67 N 12.91.

**4f**. *6-(1H-Indol-3-yl)-4-(1-naphthyl)-2,2'-bipyridine-5-carbonitrile* (Table 2, entry 6)

Light green solid; mp 270-272 $^o$C; $R_f$ 0.29 (20% AcOEt/Petroleum ether); IR (KBr): 1129, 1234, 1359, 1430, 1533, 2215, 3055 cm$^{-1}$; $^1$H NMR (500 MHz, DMSO-$d_6$): δ 7.24-7.26 (m, 2H, Ar-*H*), 7.53-7.55 (m, 2H, Ar-*H*), 7.58 (t, 2H, *J* = 8.4 Hz, Ar-*H*) 7.65-7.69 (m, 3H, Ar-*H*), 8.06-8.12 (m, 3H, Ar-*H*), 8.26 (s, 1H, Ar-*H*), 8.36 (s, 1H, Ar-*H*), 8.47-8.49 (m, 1H, Ar-*H*), 8.60 (d, 1H, *J* = 8.4 Hz Ar-*H*), 8.69 (d, 1H, *J* = 4.6 Hz, Ar-*H*), 11.85 (brs, 1H, -N*H*); $^{13}$C NMR (125 MHz, DMSO-$d_6$): δ 104.8, 112.1, 112.7, 117.6, 118.1, 121.0, 121.3, 121.7, 122.5, 124.7, 125.3, 125.4, 126.0, 126.5, 127.1, 127.2, 128.6, 128.9, 129.6, 130.1, 133.2, 134.6, 136.4, 137.8, 149.7, 153.9, 154.5, 156.9, 157.1 ; MS (EI): *m*/*z* 423.40 [$M^+$+$H^+$]; Anal. Calcd for $C_{29}H_{18}N_4$: C 82.44 H 4.29 N 13.26. Found: C 82.49 H 4.28 N 13.22.

**4g**. *6-(1H-Indol-3-yl)-4-(4-chloroyphenyl)-2,2'-bipyridine-5-carbonitrile* (Table 2, entry 7)

Pale Yellow solid; mp 306-308 $^o$C; $R_f$ 0.35 (20% AcOEt/Petroleum ether); IR (KBr): 1089, 1140, 1221, 1364, 1433, 1535, 1713, 2218 cm$^{-1}$; $^1$H NMR (500 MHz, DMSO-$d_6$): δ 7.20-7.23 (m, 2H, Ar-*H*), 7.49-7.54 (m, 2H, Ar-*H*), 7.60 (d, 2H, *J* = 7.6 Hz, Ar-*H*), 7.73 (d, 2H, *J* = 7.6 Hz, Ar-*H*), 8.01 (t, 1H, *J* = 7.6 Hz, Ar-*H*), 8.21 (s, 1H, Ar-*H*), 8.34-8.37 (m, 2H, Ar-*H*), 8.50 (d, 1H, *J* = 8.4 Hz, Ar-*H*), 8.71 (d, 1H, *J* = 4.55 Hz, Ar-*H*), 11.84 (brs, 1H, -N*H*); $^{13}$C NMR (125 MHz, DMSO-$d_6$): 100.5, 110.0, 110.5, 114.0, 116.4, 118.8, 119.0, 119.3, 120.3, 123.1, 123.8, 126.7, 128.4, 132.6, 133.4, 134.2, 135.6, 147.5, 151.6, 155.0, 155.2; MS (EI): *m*/*z* 407.33 [$M^+$+$H^+$]; Anal. Calcd for $C_{25}H_{15}Cl\ N_4$: C 73.80 H 3.72 N 13.22. Found: C 73.70 H 3.71 N 13.72.

**4h**. *6-(1H-Indol-3-yl)-4-(4-bromophenyl)-2,2'-bipyridine-5-carbonitrile* (Table 2, entry 8)

Pale Yellow solid; mp 298-300 $^{o}$C; $R_f$ 0.33 (20% AcOEt/Petroleum ether); IR (KBr): 1010, 1140, 1212, 1435, 1535, 2217, 3332 cm$^{-1}$; $^{1}$H NMR (500 MHz, DMSO-d$_6$): δ 7.21-7.24 (m, 2H, Ar-*H*), 7.52-7.54 (m, 2H, Ar-*H*), 7.67 (d, 2H, *J* = 8.4 Hz, Ar-*H*), 7.74 (d, 2H, *J* = 8.4 Hz, Ar-*H*), 8.02 (t, 1H, *J* = 8.4 Hz, Ar-*H*), 8.21 (s, 1H, Ar-*H*), 8.34-8.37 (m, 2H, Ar-*H*), 8.50 (d, 1H, *J* = 8.4 Hz, Ar-*H*), 8.71 (d, 1H, *J* = 4.56 Hz, Ar-*H*), 11.84 (brs, 1H, -N*H*); $^{13}$C NMR (125 MHz, DMSO-d$_6$): δ 103.1, 112.6, 113.2, 116.5, 119.0, 121.4, 121.7, 122.0, 122.9, 124.0, 125.8, 126.5, 129.3, 131.3, 132.3, 136.4, 136.9, 138.2, 150.1, 154.2, 154.3, 157.7, 157.8; MS (EI): *m*/*z* 451.27 [M$^{+}$+H$^{+}$]; Anal. Calcd for $C_{25}H_{15}Br\ N_4$: C 66.53 H 3.35 N 12.41. Found: C 66.43 H 3.36 N 12.46.

**4i**. *6-(1H-Indol-3-yl)-4-(4-fluorophenyl)-2,2'-bipyridine-5-carbonitrile* (Table 2, entry 9)

Pale Yellow solid; mp 294-296 $^{o}$C; $R_f$ 0.28 (20% AcOEt/Petroleum ether); IR (KBr): 1142, 1437, 1537, 1575, 2218, 3337 cm$^{-1}$; $^{1}$H NMR (500 MHz, DMSO-d$_6$): δ 7.19-7.23 (m, 2H, Ar-*H*), 7.36 (t, 2H, *J* = 8.4 Hz, Ar-*H*), 7.50-7.54 (m, 2H, Ar-*H*), 7.76-7.78 (m, 2H, Ar-*H*), 8.00 (t, 1H, *J* = 8.4 Hz, Ar-*H*), 8.20 (s, 1H, Ar-*H*), 8.34-8.36 (m, 2H, Ar-*H*), 8.50 (d, 1H, *J* = 7.6 Hz, Ar-*H*), 8.70 (d, 1H, *J* = 3.8 Hz, Ar-*H*), 11.83 (brs, 1H, -N*H*); $^{13}$C NMR (125 MHz, DMSO-d$_6$): δ 102.8, 112.1, 112.7, 115.6, 115.9, 116.2, 118.6, 120.9, 121.2, 121.5, 122.4, 125.4, 126.0, 128.8, 130.9, 131.1, 133.2, 136.3, 137.6, 149.6, 153.8, 154.0, 157.1, 157.3, 161.7, 164.2; MS (EI): *m*/*z* 391.40 [M$^{+}$+H$^{+}$]; Anal. Calcd for $C_{25}H_{15}F\ N_4$: C 76.91 H 3.87 N 14.35. Found: C 79.80 H 3.88 N 14.40.

**4j**. *6-(1H-Indol-3-yl)-4-(3-nitrophenyl)-2,2'-bipyridine-5-carbonitrile* (Table 2, entry 10)

Yellow solid; mp 234-236 $^{o}$C; $R_f$ 0.20 (20% AcOEt/Petroleum ether); IR (KBr): 1098, 1236, 1349, 1433, 1531, 2216, 3386 cm$^{-1}$; $^{1}$H NMR (500 MHz, DMSO-d$_6$): δ 7.24-7.26 (m, 2H, Ar-*H*), 7.53-7.56 (m, 2H, Ar-*H*), 7.85 (t, 1H, *J* = 8.4 Hz, Ar-*H*), 8.08-8.10 (m, 1H, Ar-*H*), 8.22 (d, 1H, *J*

= 6.9 Hz, Ar-*H*), 8.32-8.39 (m, 4H, Ar-*H*), 8.54-8.60 (m, 2H, Ar-*H*), 8.75 (s, 1H, Ar-*H*), 11.87 (brs, 1H, -N*H*); $^{13}$C NMR (125 MHz, DMSO-$d_6$): δ 102.9, 112.2, 112.7, 116.4, 118.4, 121.0, 121.2, 121.6, 122.5, 123.6, 124.5, 125.4, 125.9, 129.0, 130.5, 135.4, 136.4, 137.8, 138.2, 147.9, 149.7, 152.8, 153.8, 157.3, 157.4; MS (EI): *m*/*z* 418.27 [$M^+$+$H^+$]; Anal. Calcd for $C_{25}H_{15}N_5O$: C 71.93 H 3.62 N 16.78. Found: C 71.80 H 3.63 N 16.73.

**4k**. *6-(1H-Indol-3-yl)-4-(4-Nitrophenyl)-2,2'-bipyridine-5-carbonitrile* (Table 2, entry 11)

Yellow solid; mp 308.-311 $^{o}$C; $R_f$ 0.20 (20% AcOEt/Petroleum ether); IR (KBr): 1248, 1378, 1435, 1548, 2212, 3389 cm$^{-1}$; $^1$H NMR (500 MHz, $CDCl_3$): δ 7.24-7.29 (m, 2H, Ar-*H*), 7.54-7.57 (m, 2H, -Ar-*H*), 8.07 (m, 2H, -Ar-*H*), 8.13 (d, 1H, *J* = 8.3 Hz -Ar-*H*), 8.31 (s, 1H, -Ar-*H*), 8.38-8.41 (m, 4H, -Ar-*H*), 8.59 (d, 1H, *J* = 8.1 Hz, -Ar-*H*), 8.78 (d, 1H, *J* = 4.7 Hz, -Ar-*H*), 11.97 (brs, 1H, -*NH*); $^{13}$C NMR (75 MHz, DMSO-d6): 102.7, 112.1, 112.6, 115.9, 118.1, 120.9, 121.1, 121.6, 122.4, 123.7, 125.3, 125.9, 128.9, 130.3, 136.4, 137.8, 143.1, 148.1, 149.7, 153.0, 153.7, 157.3, 157.4; MS (EI): *m*/*z* 418.40 [$M^+$+$H^+$]; Anal. Calcd for $C_{25}H_{15}N_5O$ C 71.93 H 3.62 N 16.78. Found: C 72.04 H 3.61 N 16.74.

**4l**. *6-(1H-Indol-3-yl)-4-(3-bromophenyl)-2,2'-bipyridine-5-carbonitrile* (Table 2, entry 12)

Pale Yellow solid; mp 235-238 $^{o}$C; $R_f$ 0.33 (20% AcOEt/Petroleum ether); IR (KBr): 1144, 1281, 1412, 1563, 1642 cm$^{-1}$; $^1$H NMR (500 MHz, $CDCl_3$): δ 7.22-7.24 (m, 2H, Ar-*H*), 7.52-7.54 (m, 3H, -Ar-*H*), 7.71-7.76 (m, 2H, -Ar-*H*), 7.95 (s, 1H, -Ar-*H*), 8.01-8.04 (m, 1H, -Ar-*H*), 8.22 (s, 1H, -Ar-*H*), 8.34-8.36 (m, 2H, -Ar-*H*), 8.51 (d, 1H, *J* = 6.9 Hz, -Ar-*H*), 8.71-8.73 (m, 1H, -Ar-*H*), 11.85 (brs, 1H, -*NH*); $^{13}$C NMR (75 MHz, DMSO-d6): 103.4, 112.7, 113.2, 116.8, 119.0, 121.5, 121.7, 122.1, 122.5, 125.9, 126.5, 128.4, 129.5, 131.5, 131.8, 136.4, 138.4, 139.6, 150.3, 153.9, 154.4, 157.8, 157.9; MS (EI): *m*/*z* 451.33 [$M^+$+$H^+$]; Anal. Calcd for $C_{25}H_{15}Br\ N_4$. C 66.53 H 3.35 N 12.41. Found: C 66.64 H 3.34 N 12.37.

**4m**. *6-(1H-Indol-3-yl)-4-(2-bromophenyl)-2,2'-bipyridine-5-carbonitrile* (Table 2, entry 13)

Pale Yellow solid; mp 302-305 $^{o}$C; $R_f$ 0.33 (20% AcOEt/Petroleum ether); IR (KBr): 1245, 1432, 1548, 1598, 2221, 3025, 3349 cm$^{-1}$; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.26-7.29 (m, 2H, Ar-*H*), 7.50 (t, 1H, *J* = 7.7 Hz, -Ar-*H*), 7.57-7.62 (m, 4H, -Ar-*H*), 7.86 (d, 1H, *J* = 8.0 Hz, -Ar-*H*), 8.08 (t, 1H, *J* = 7.6 Hz, -Ar-*H*), 8.19 (s, 1H, -Ar-*H*), 8.46-8.48 (m, 2H, -Ar-*H*), 8.58 (d, 1H, *J* = 8.4 Hz, -Ar-*H*), 8.76 (d, 1H, *J* = 4.0 Hz, -Ar-*H*), 11.89 (brs, 1H, -*NH*); $^{13}$C NMR (75 MHz, DMSO-d6): 103.9, 112.2, 112.5, 116.4, 117.8, 121.1, 121.3, 121.6, 122.5, 125.4, 125.9, 128.1, 128.8, 130.7, 131.4, 132.9, 136.5, 137.8, 137.9, 149.8, 153.8, 154.8, 156.8, 157.3; MS (EI): *m*/*z* 451.20 [$M^+$+$H^+$]; Anal. Calcd for $C_{25}H_{15}Br\ N_4$. C 66.53 H 3.35 N 12.41. Found: C 66.64 H 3.34 N 12.37

**4n**. *6-(1H-Indol-3-yl)-4-(2-chloroyphenyl)-2,2'-bipyridine-5-carbonitrile* (Table 2, entry 14)

Pale Yellow solid; mp 314-316-$^{o}$C; $R_f$ 0.35 (20% AcOEt/Petroleum ether); IR (KBr): 1278, 1345, 1478, 1547, 2226, 3096, 3458 cm$^{-1}$; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.27-7.29 (m, 2H, Ar-*H*), 7.56-7.59 (m, 4H, -Ar-*H*), 7.66 (d, 1H, *J* = 7.6 Hz, -Ar-*H*), 7.73 (d, 1H, *J* = 7.6 Hz, -Ar-*H*), 8.13 (t, 1H, *J* = 7.6 Hz, -Ar-*H*), 8.22 (s, 1H, -Ar-*H*), 8.39 (s, 1H, -Ar-*H*), 8.45-8.47 (m, 1H, -Ar-*H*), 8.60 (d, 1H, *J* = 8.4 Hz, -Ar-*H*), 8.77 (d, 1H, *J* = 4.5 Hz, -Ar-*H*), 11.89 (brs, 1H, -N*H*); $^{13}$C NMR (75 MHz, DMSO-d6): 104.1. 112.2, 112.4, 116.7, 117.8, 121.1, 121.2, 121.7, 122.4, 125.4, 125.8, 127.6, 128.7, 129.8, 130.8, 131.3, 131.4, 135.8, 136.5, 137.9, 149.8, 153.2, 153.8, 156.8, 157.3 ; MS (EI): *m*/*z* 407.40 [$M^+$+$H^+$]; $C_{25}H_{15}Cl\ N_4$. Anal. Calcd for $C_{24}H_{15}Cl\ N_4$. C 73.80 H 3.72 N 13.22. Found: C 73.92 H 3.71 N 13.26.

**4o**. *6-(1H-Indol-3-yl)-4-(2-furyl)-2,2'-bipyridine-5-carbonitrile* (Table 2, entry 15)

Pale Yellow solid; mp 248-251 $^{o}$C; $R_f$ 0.16 (20% AcOEt/Petroleum ether); IR (KBr): 1124, 1452, 1568, 1623, 2258, 3256, 3425 cm$^{-1}$; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 6.86-6.88 (m, 1H, Ar-*H*),

7.21-7.26 (m, 2H, -Ar-*H*), 7.57-7.62 (m, 2H, -Ar-*H*), 7.66 (d, 1H, *J* = 3.6 Hz, -Ar-*H*), 8.05-8.08 (m, 2H, -Ar-*H*), 8.33 (d, 1H, *J* = 8.0 Hz, -Ar-*H*), 8.37 (d, 1H, *J* = 2.9 Hz, -Ar-*H*), 8.53 (d, 1H, *J* = 8.4 Hz, -Ar-*H*), 8.66 (s, 1H, -Ar-*H*), 8.81 (d, 1H, *J* = 4.5 Hz, -Ar-*H*), 11.86 (brs, 1H, -N*H*); $^{13}$C NMR (75 MHz, DMSO-d6): 98.2, 111.1, 112.1, 11.2.5, 113.1, 114.1, 119.0, 120.8, 121.2, 121.4, 122.4, 125.3, 126.1, 128.9, 136.3, 137.6, 141.4, 146.1, 148.0, 149.5, 153.7, 157.3, 158.0; MS (EI): *m*/*z* 363.20 [$M^+$+$H^+$]; Anal. Calcd for $C_{23}H_{14}N_4O$. C 76.23 H 3.89 N 15.46. Found: C 76.33 H 3.88 N 15.42.

**4p**. *4,6-di-1H-indol-3-yl-2,2'-bipyridine-5-carbonitrile* (Table 2, entry 16)

Pale Yellow solid; mp 282-285 $^o$C; $R_f$ 0.64 (40% AcOEt/Petroleum ether); IR (KBr): 1246, 1491, 1546, 2219, 3342 cm$^{-1}$; $^1$H NMR (500 MHz, $CDCl_3$): δ 6.77 (t, 1H, *J* = 7.6 Hz, -Ar-*H*), 7.06-7.09 (m, 3H, Ar-*H*), 7.21-7.24 (m, 2H, -Ar-*H*), 7.47-7.49 (m, 2H, -Ar-*H*), 7.65 (s, 1H, -Ar-*H*), 8.15-8.19 (m, 2H, -Ar-*H*), 8.24 (s, 1H, -Ar-*H*), 8.37 (d, 1H, *J* = 3.9 Hz, -Ar-*H*), 8.50-8.52 (m, 1H, -Ar-*H*), 8.57 (d, 1H, *J* = 8.4 Hz, -Ar-*H*), 11.31 (brs, 1H, -N*H*), 11.67 (brs, 1H, -N*H*); $^{13}$C NMR (75 MHz, DMSO-d6): 103.8, 112.8, 113.4, 113.8 114.1, 119.6, 121.4, 122.4, 122.8, 123.3, 123.8, 126.0, 126.4,128.6, 129.1, 129.3, 130.2, 133.2, 136.2, 136.4, 137.4, 137.6, 156.1, 158.9, 162.9; MS (EI): *m*/*z*. 412.40 [$M^+$+$H^+$]; Anal. Calcd for $C_{27}H_{17}N_5$. C 78.81 H 4.16 N. 17.02. Found: C 78.78 H 4.15 N 16.98.

**4q**. *6'-(1H-indol-3-yl)-2,2':4',4''-terpyridine-5'-carbonitrile* (Table 2, entry 17)

Pale Yellow solid; mp 312-315 $^o$C; $R_f$ 0.42 (40% AcOEt/Petroleum ether); IR (KBr): 1245, 1347, 1564, 1623, 2203, 3241 cm$^{-1}$; $^1$H NMR (500 MHz, $CDCl_3$): δ 7.21-7.24 (m, 2H, Ar-*H*), 7.53-7.56 (m, 2H, -Ar-*H*), 7.71-7.73 (m, 2H, -Ar-*H*), 8.05 (s, 1H, -Ar-*H*), 8.23 (s, 1H, -Ar-*H*), 8.36-8.38 (m, 2H, -Ar-*H*), 8.51-8.52 (m, 1H, -Ar-*H*), 8.73-8.77 (m, 3H, -Ar-*H*), 11.88 (brs, 1H, -N*H*); $^{13}$C NMR (75 MHz, DMSO-d6): 102.9, 112.8, 113.1, 116.4, 118.7, 121.6, 121.7, 122.2,

123.8, 126.0, 126.5, 129.5, 136.9, 138.4, 144.8, 150.3, 150.7, 153.1, 154.2, 157.8, 158.0, 163.0; MS (EI): *m*/*z* 374.40 [$M^+$+$H^+$]; Anal. Calcd for $C_{24}H_{15}N_5$. C 77.20 H 4.05 N 18.76. Found: C 77.07 H 4.06 N 18.79.

**4r**. *6'-(1H-indol-3-yl)-2,2':4',3''-terpyridine-5'-carbonitrile* (Table 2, entry 18)

Pale Yellow solid; mp 282-285 $^oC$; $R_f$ 0.42 (40% AcOEt/Petroleum ether); IR (KBr): 1186, 1254, 1325, 1542, 1612, 2256, 3241 $cm^{-1}$; $^1H$ NMR (500 MHz, $CDCl_3$): δ 7.21-7.24 (m, 2H, Ar-*H*), 7.52-7.54 (m, 2H, -Ar-*H*), 7.60-7.63 (m, 1H, -Ar-*H*), 8.06 (t, 1H, *J* = 3.9 Hz, -Ar-*H*), 8.17 (d, 1H, *J* = 7.7 Hz, -Ar-*H*), 8.28 (s, 1H, -Ar-*H*), 8.36-8.37 (m, 2H, -Ar-*H*), 8.53 (d, 1H, *J* = 7.7 Hz, -Ar-*H*), 8.73-8.77 (m, 2H, -Ar-*H*), 8.92-8.94 (m, 1H, -Ar-*H*), 11.87 (brs, 1H, -N*H*); $^{13}C$ NMR (75 MHz, DMSO-d6): 103.6, 112.8, 113.2, 116.9, 119.0, 121.5, 121.7, 122.2, 123.1, 124.3, 126.0, 126.5, 129.5, 137.0, 138.4, 149.4, 150.3, 151.2, 152.5, 154.3, 157.9; MS (EI): *m*/*z* 374.33 [$M^+$+$H^+$]; Anal. Calcd for $C_{24}H_{15}N_5$. C 77.20 H 4.05 N 18.76. Found: C 77.07 H 4.06 N 18.79.

**4s**. 4-(1*H*-imidazol-2-yl)-6-(1*H*-indol-3-yl)-2,2'-bipyridine-5-carbonitrile (Table 2, entry 19)

Pale Yellow solid; mp 245-248 $^oC$; $R_f$ 0.36 (40% AcOEt/Petroleum ether); IR (KBr): 1014, 1139, 1476, 1526, 1600, 2203, 3391 $cm^{-1}$; $^1H$ NMR (500 MHz, $CDCl_3$): δ 7.21-7.24 (m, 3H, Ar-*H*), 7.32-7.34 (m, 1H, -Ar-*H*), 7.49 (d, 1H, *J* = 7.6 Hz, -Ar-*H*), 7.68 (s, 1H, -Ar-*H*), 7.72 (d, 1H, *J* = 8.4 Hz, -Ar-*H*), 8.03 (s, 1H, -Ar-*H*), 8.17-8.20 (m, 2H, -Ar-*H*), 8.53 (d, 1H, *J* = 3.9 Hz, -Ar-*H*), 8.72-8.73 (m, 1H, -Ar-*H*), 11.87 (brs, 1H, -N*H*), 12.04 (brs, 1H, -N*H*); $^{13}C$ NMR (75 MHz, DMSO-d6): 101.2, 112.4, 113.3, 114.6, 119.8, 121.1, 122.4, 122.7, 124.2, 126.2, 128.2, 130.4, 136.7, 137.8, 149.2, 152.6, 152.9, 157.6, 163.1; MS (EI): *m*/*z* 363.33 [$M^+$+$H^+$]; Anal. Calcd for $C_{22}H_{14}N_6$. C 72.92 H 3.89 N 23.19. Found: C 72.81 H 3.90 N 23.25.

**4t**. *6-(1H-indol-3-yl)-4-(2-thienyl)-2,2'-bipyridine-5-carbonitrile* (Table 2, entry 20)

Pale Yellow solid; mp 245-248 $^{o}$C; $R_f$ 0.30 (40% AcOEt/Petroleum ether); IR (KBr): 1042, 1238, 1425, 1534, 2220, 3365 cm$^{-1}$; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.19-7.23 (m, 2H, Ar-*H*), 7.28-7.30 (m, 1H, -Ar-*H*), 7.49-7.53 (m, 2H, -Ar-*H*), 7.89-7.91 (m, 2H, -Ar-*H*), 8.00-8.02 (m, 1H, -Ar-*H*), 8.30-8.33 (m, 3H, -Ar-*H*), 8.46 (d, 1H, *J* = 7.6 Hz, -Ar-*H*), 8.72 (d, 1H, *J* = 3.9 Hz, -Ar-*H*), 11.84 (brs, 1H, -N*H*); $^{13}$C NMR (75 MHz, DMSO-d6): 101.2, 112.6, 113.2, 115.6, 119.7, 121.5, 121.7, 122.0, 122.9, 125.9, 126.6, 129.3, 129.5, 130.4, 130.4, 130.9, 136.9, 138.0, 138.3, 147.2, 150.2, 154.2, 156.2, 157.8, 158.6, 160.3, 162.9; MS (EI): *m/z*. 379.27 [$M^+$+$H^+$]; Anal. Calcd for $C_{23}H_{14}N_4S$. C 72.99 H 3.73 N 14.80. Found: C 73.10 H 3.72 N 14.76.

2. Spectral data compound **5**

**5**. *4-(2,4-Dichlorophenyl)-6-(1H-indol-3-yl)-1,4-dihydro-2,2'-bipyridine-5-carbonitrile*

Yellow solid; mp 212-214 $^{o}$C; $R_f$ 0.23 (20% AcOEt/Petroleum ether); IR (KBr): 1046, 1100, 1432, 1432, 1465, 1561, 1593, 2188, 3385 cm$^{-1}$; $^{1}$H NMR (500 MHz, DMSO-$d_6$): δ 5.06 (d, 1H, *J* = 5.35 Hz, dihydropyridyl, Ar-*H* ), 5.83 (d, 1H, *J* = 5.35 Hz, dihydropyridyl, Ar-*H* ), 7.14 (t, 1H, *J* = 7.6 Hz, Ar-*H*), 7.19 (t, 1H, *J* = 7.6 Hz, Ar-*H*), 7.34-7.37 (m, 1H, Ar-*H*), 7.48-7.52 (m, 2H, Ar-*H*), 7.56 (d, 1H, *J* = 8.4 Hz, Ar-*H*), 7.63 (d, 1H, *J* = 2.3 Hz), 7.72 (d, 1H, *J* = 7.6 Hz, Ar-*H*), 7.80-7.83 (m, 1H, Ar-*H*), 7.87 (d, 1H, *J* = 8.4 Hz, Ar-*H*), 7.95 (d, 1H, *J* = 3.1 Hz, Ar-*H*), 8.54 (d, 1H, *J* = 4.6 Hz, Ar-*H*), 8.64 (brs, 1H, N*H*), 11.83 (brs, 1H, -N*H*); $^{13}$C NMR (125 MHz, DMSO-$d_6$)**:** δ 74.5, 100.6, 107.8, 112.5, 119.2, 119.3, 120.4, 121.6, 122.2, 123.7, 124.6, 127.6, 128.3, 128.9, 132.0, 132.4, 133.5, 136.2, 137.3, 141.6, 146.2, 148.4, 149.4; MS (EI): *m/z* 443.32 [$M^+$+$H^+$]; Anal. Calcd for $C_{25}H_{16}Cl_2N_4$: C 67.73 H 3.64 N 12.64. Found: C 67.89 H 3.62 N 12.60.

3. Spectral data compound **6**

**6**. *6-(1H-Indol-3-yl)-4-(2,4-dichlorophenyl)-2,2'-bipyridine-5-carbonitrile*

Pale Yellow solid; mp 268-270 $^{o}$C; $R_f$ 0.33 (20% AcOEt/Petroleum ether); IR (KBr): 1080, 1390, 1428, 1447, 1480, 1533, 2229, 3312 cm$^{-1}$; $^{1}$H NMR (500 MHz, DMSO-d$_6$): δ 7.23-7.25 (m, 2H, Ar-*H*), 7.53-7.68 (m, 4H, Ar-*H*), 7.89 (s, 1H, Ar-*H*), 8.07 (t, 1H, *J* = 6.9 Hz, Ar-*H*), 8.19 (s, 1H, Ar-*H*), 8.35-8.42 (m, 2H, Ar-*H*), 8.55 (d, 1H, *J* = 7.6 Hz, Ar-*H*), 8.72 (d, 1H, *J* = 3.8 Hz, Ar-*H*), 11.89 (brs, 1H, -N*H*); $^{13}$C NMR (125 MHz, DMSO-d$_6$): δ 104.4, 112.7, 113.0, 117.2, 118.2, 121.6, 121.7, 122.2, 123.1, 126.0, 126.3, 128.4, 129.3, 129.9, 132.7, 133.0, 135.2, 135.6, 136.9, 138.4, 150.3, 152.6, 154.2, 157.3, 157.9; MS (EI): *m*/*z* 441.33 [M$^{+}$+H$^{+}$]; Anal. Calcd for $C_{25}H_{14}Cl_2N_4$: C 68.04 H 3.20 N 12.70. Found: C 68.15 H 3.19 N 12.66.

4. Spectral data compound **8**

**8**. *Phenyl-1,4-bis(6-(1H-indol-3-yl)-2,2'-bipyridine-5-carbonitrile)*

Light brown solid; mp 220-223 $^{o}$C; $R_f$ 0.87 (60% AcOEt/Petroleum ether); IR (KBr): 1152, 1438, 1638, 2248, 3222 cm$^{-1}$; $^{1}$H NMR (500 MHz, DMSO-d$_6$): δ 7.23-7.26 (m, 5H, Ar-*H*), 7.54-7.58 (m, 5H, Ar-*H*), 8.03-8.11 (m, 3H, Ar-*H*), 8.08-8.11 (m, 2H, Ar-*H*), 8.37-8.41 (m, 5H, Ar-*H*),8.56 (d, 2H, *J* = 7.6 Hz, Ar-*H*), 8.76-8.80 (m, 2H, Ar-*H*), 11.88 (brs, 2H, -N*H*); $^{13}$C NMR (125 MHz, DMSO-d$_6$): δ 102.6, 111.8, 112.8, 116.3, 120.5, 121.0, 121.4, 122.1, 124.9, 125.9, 128.4, 128.8, 129.4, 130.2, 136.3, 137.3, 138.0, 149.3, 154.0, 157.3; MS (EI): *m*/*z* 667.40 [M$^{+}$+H$^{+}$]; Anal. Calcd for $C_{44}H_{26}N_8$: C 79.29 H 3.93 N 16.81. Found: C 79.19 H 3.92 N 16.85.

5. Spectral data compound **10a-g**

**10a**. *6,6'-Bis-(1H-indol-3-yl)-4-4'-diphenyl-[2,2']bipyridinyl-5,5'dicarbonitrile*. (Table 3, entry 1)

Yellow solid; mp >350 $^{o}$C; $R_f$ 0.78 (40% AcOEt/Petroleum ether); IR (KBr): 1070, 1171, 1323, 1573, 1637, 2236, 3377, 3420 cm$^{-1}$; $^{1}$H NMR (500 MHz, DMSO-d$_6$): δ 7.11 (t, 3H, *J* = 8.4 Hz, Ar-*H*), 7.20 (t, 3H, *J* = 7.6 Hz, Ar-*H*), 7.51 (t, 2H, *J* = 8.4 Hz, Ar-*H*), 7.58-7.63 (m, 5H, Ar-*H,* Ar-*H*), 7.80 (d, 4H, *J* = 6.8 Hz, Ar-*H*), 8.39-8.45 (m, 5H, Ar-*H*), 11.87 (brs, 2H, -N*H*); $^{13}$C NMR (125 MHz, DMSO-d$_6$): δ 104.1, 112.7, 113.5, 118.0, 118.8, 121.1, 121.8, 123.0, 126.7, 129.1, 129.3, 129.4, 130.4, 137.1, 137.4, 156.0, 156.6, 158.1; MS (EI): 589.53 *m*/*z* [M$^{+}$+H$^{+}$]; Anal. Calcd for $C_{40}H_{24}N_6$: C 81.61 H 4.11 N 14.28. Found: C 81.54 H 4.13 N 14.33.

**10b**. *6,6'-Bis-(1H-indol-3-yl)-4-4'-di-4-methylphenyl-[2,2']bipyridinyl-5,5'dicarbonitrile* (Table 3, entry 2)

Yellow solid; mp 258-260 $^{o}$ C; $R_f$ 0..63 (40% AcOEt/Petroleum ether); IR (KBr): 1141, 1236, 1431, 1526, 2376, 3402 cm$^{-1}$; $^{1}$H NMR (500 MHz, DMSO-d$_6$): δ 2.38 (s, 6H, Ar-C*H$_3$*), 7.10 (t, 3H, *J* = 7.6 Hz, Ar-*H*), 7.20 (t, 3H, *J* = 7.6 Hz, Ar-*H*), 7.35 (d, 3H, *J* = 7.6 Hz, Ar-*H*), 7.51 (d, 3H, *J* = 7.6 Hz, Ar-*H*), 7.64 (d, 2H, *J* = 7.6 Hz, Ar-*H*), 8.36 (t, 6H, *J* = 7.6 Hz, Ar-*H*), 11.86 (brs, 2H, -N*H*); $^{13}$C NMR (125 MHz, DMSO-d$_6$): δ 21.3, 102.6, 111.8, 117.9, 121.1, 121.9, 122.9, 126.7, 127.2, 127.8, 127.9, 128.0, 129.3, 129.4, 134.5, 137.1, 140.3, 155.9, 156.5, 158.1; MS (EI): *m*/*z* 617.53 [M$^{+}$+H$^{+}$]; Anal. Calcd for $C_{42}H_{28}N_6$: C 81.80 H 4.58 N 13.63. Found: C 81.70 H 4.59 N 13.67.

**10c**. *6,6'-Bis-(1H-indol-3-yl)-4-4'-di-3-methylphenyl-[2, 2']bipyridinyl-5,5'dicarbonitrile* (Table 3, entry 3)

Yellow solid; mp 298-300 °C; $R_f$ 0.63 (40% AcOEt/Petroleum ether); IR (KBr): 1170, 1448, 1506, 1573, 1638, 2232, 3460 $cm^{-1}$; $^1H$ NMR (500 MHz, DMSO-$d_6$): δ 2.41 (s, 6H, Ar-C*H*$_3$), 7.11 (t, 3H, *J* = 7.6 Hz, Ar-*H*), 7.21 (t, 2H, *J* = 7.6 Hz, Ar-*H*), 7.38 (d, 2H, *J* = 7.6 Hz, Ar-*H*), 7.46 (t, 2H, *J* = 8.4 Hz, Ar-*H*), 7.52 (d, 2H, *J* = 7.6 Hz, Ar-*H*), 7.57-7.59 (m, 3H, Ar-*H*), 8.08 (s, 1H, Ar-*H*), 8.39-8.42 (m, 5H, Ar-*H*), 11.89 (brs, 2H, -N*H*); $^{13}C$ NMR (125 MHz, DMSO-$d_6$): δ 21.4, 102.6, 112.1, 117.9, 119.8, 121.3, 121.8, 123.1, 126.8, 127.4, 127.9, 128.3, 129.6, 129.9, 134.9, 137.8, 140.5, 154.9, 156.8, 159.8; MS (EI): *m*/*z* 617.40 [$M^+$+$H^+$]; Anal. Calcd for $C_{42}H_{28}N_6$: C 81.80 H 4.58 N 13.63. Found: C 81.87 H 4.57 N 13.57.

**10d**. *6,6'-Bis-(1H-indol-3-yl)-4-4'-di-4-methoxyphenyl-[2,2']bipyridinyl-5,5'dicarbonitrile* (Table 3, entry 4)

Yellow solid; mp >350 °C; $R_f$ 0.12 (20% AcOEt/Petroleum ether); IR (KBr): 1027, 1251, 1428, 1529, 1609, 2392, 3416 $cm^{-1}$; $^1H$ NMR (500 MHz, DMSO-$d_6$): δ 3.85 (s, 6H, Ar-*OCH*$_3$), 7.15-7.24 (m, 8H, Ar-*H*), 7.52 (d, 2H, *J* = 8.4 Hz, Ar-*H*), 7.79 (d, 4H, *J* = 8.4 Hz), 8.40-8.44 (m, 6H, Ar-*H*), 11.87 (brs, 2H, -N*H*); $^{13}C$ NMR (125 MHz, DMSO-$d_6$): δ 56.0, 103.7, 112.6, 113.5, 115.0, 117.8, 119.1, 121.1, 121.9, 122.9, 126.7, 129.3, 129.5, 130.6, 137.1, 155.5, 156.5, 158.1, 161.4; MS (EI): *m*/*z* 649.47 [$M^+$+$H^+$]; Anal. Calcd for $C_{42}H_{28}N_6O_2$: C 77.76 H 4.35 N 12.95. Found: C 77.65 H 4.36 N 13.00.

**10e**. *6,6'-Bis-(1H-indol-3-yl)-4-4'-di-3,4-dimethoxyphenyl-[2,2']bipyridinyl-5,5'dicarbonitrile* (Table 3, entry 5)

Yellow solid; mp >350 °C; $R_f$ 0.29 (40% AcOEt/Petroleum ether); IR (KBr): 1026, 1139, 1264, 1478, 1512, 1582, 2184, 3313, 3414 $cm^{-1}$; $^1H$ NMR (500 MHz, DMSO-$d_6$): δ 3.75 (s, 6H, Ar-OC*H*$_3$), 3.77 (s, 6H, Ar-OC*H*$_3$), 6.89 (d, 1H, *J* = 8.4 Hz, Ar-*H*), 6.94-6.98 (m, 5H, Ar-*H*), 7.11 (d, 2H, *J* = 7.6 Hz, Ar-*H*), 7.16 (t, 2H, *J* = 7.6 Hz, Ar-*H*), 7.42-7.48 (m, 2H, Ar-*H*), 7.51-7.65 (m,

3H, Ar-*H*), 7.81 (d, 1H, *J = 3.8 Hz,* Ar-*H*), 7.95 (s, 1H, Ar-*H*), 8.08 (s, 1H, Ar-*H*), 11.72 (brs, 2H, -N*H*); $^{13}$C NMR (125 MHz, DMSO-$d_6$): δ 55.5, 55.7, 104.2, 112.7, 113.8, 117.9, 119.6, 120.7, 122.0, 122.6, 124.4, 125.3, 126.8, 127.7, 128.1, 129.4, 134.8, 136.8, 152.4, 152.8, 155.6; MS (EI): *m*/*z* 709.47 [$M^+$+$H^+$]; Anal. Calcd for $C_{44}H_{32}N_6O_4$: C 74.56 H 4.55 N 11.86. Found: C 74.42 H 4.57 N 11.90.

**10f**. *6,6'-Bis-(1H-indol-3-yl)-4-4'-di-4-chlorophenyl-[2,2']bipyridinyl-5,5'dicarbonitrile* (Table 3, entry 6)

Yellow solid; mp >350 $^o$C; $R_f$ 0.74 (40% AcOEt/Petroleum ether); IR (KBr): 1078, 1259, 1445, 1589, 1645, 2378, 3349 cm$^{-1}$; $^1$H NMR (500 MHz, DMSO-$d_6$): δ 7.08-7.14 (m, 6H, Ar-*H*), 7.18-7.22 (m, 2H, Ar-*H*), 7.54 (d, 2H, *J* = 7.7 Hz, Ar-*H*), 7.82 (d, 2H, *J* = 8.4 Hz), 8.01 (m, 2H, Ar-*H*), 8.40-8.44 (m, 6H, Ar-*H*), 11.75 (brs, 2H, -N*H*); $^{13}$C NMR (125 MHz, DMSO-$d_6$): δ 103.8, 112.7, 113.8, 115.3, 118.1, 119.2, 121.2, 122.0, 123.2, 126.9, 128.6, 129.4, 129.8, 131.5, 137.3, 157.2, 159.1, 160.1, 162.2; MS (EI): *m*/*z* 658.40 [$M^+$+$H^+$]; Anal. Calcd for $C_{40}H_{22}Cl_2N_6$: C 73.06 H 3.37 N 12.78. Found: C 73.40 H 3.36 N 12.74.

**10g**. *6,6'-Bis-(1H-indol-3-yl)-4-4'-di-4-bromophenyl-[2,2']bipyridinyl-5,5'dicarbonitrile* (Table 3, entry 7)

Yellow solid; mp >350 $^o$C; $R_f$ 0.68 (40% AcOEt/Petroleum ether); IR (KBr): 1121, 1286, 1356, 1578, 1628, 2345, 3442 cm$^{-1}$; $^1$H NMR (500 MHz, DMSO-$d_6$): δ 7.06-7.16 (m, 8H, Ar-*H*), 7.44 (d, 2H, *J* = 7.7 Hz, Ar-*H*), 7.78 (d, 2H, *J* = 8.4 Hz), 7.94 (m, 2H, Ar-*H*), 8.36-8.39 (m, 6H, Ar-*H*), 11.23 (brs, 2H, -N*H*); $^{13}$C NMR (125 MHz, DMSO-$d_6$): δ 102.9, 112.6, 113.5, 115.5, 118.2, 119.5, 121.4, 121.9, 123.4, 126.7, 128.7, 129.6, 128.4, 130.8, 137.6, 156.7, 158.5, 159.5, 161.2; MS (EI): *m*/*z* 747.20 [$M^+$+$H^+$]; Anal. Calcd for $C_{40}H_{22}Br_2N_6$: C 64.36 H 2.97 N 11.26. Found: C 64.48 H 2.98 N 11.30.

6. Spectral data compound **12a-f**

**12a**. *7,7,7',7'-Tetramethyl-4,4'-diphenyl-4,6,7,8,4',6',7',8'-octahydro-1H,1H-[2,2']biquinolinyl-5,5'-dione* (Table 4, entry 1)

Yellow solid; mp 293-296 $^{o}$C; $R_f$ 0.81 (40% AcOEt/Petroleum ether); IR (KBr): 1126, 1314, 1384, 1485, 1587, 2934, 3340 cm$^{-1}$; $^{1}$H NMR (500 MHz, DMSO-d$_6$): δ 0.86 (s, 6H, -C*H*$_3$), 0.94 (s, 6H, -C*H*$_3$), 1.88 (Abq, 4H, *J* = 8.2 Hz, -C*H*), 2.35 (s, 4H, -C*H*$_2$), 4.42 (d, 2H, *J* = 5.3 Hz, dihydropyridyl-C*H*), 5.26 (d, 2H, *J* = 5.3 Hz, dihydropyridyl-C=C*H*), 7.05 (m, 2H, Ar-*H*), 7.13 (d, 4H, *J* = 7.6 Hz, Ar-*H*), 7.18 (m, 4H, Ar-*H*), 8.15 (brs, 2H, -*NH*); $^{13}$C NMR (125 MHz, DMSO-d$_6$): δ 27.6, 29.2, 29.6, 32.6, 38.2, 41.8, 50.8, 107.2, 117.1, 119.3, 127.6,128.2, 128.5, 128.8, 128.9, 129.2, 129.8, 131.6, 133.5, 136.2, 141.3, 143.2, 144.8, 150.2, 158.2, 162.2, 183.1, 195.2; MS (ESI LCQ-MS): *m*/*z* 505.47 [M$^+$+H$^+$]. Anal. Calcd for $C_{34}H_{36}N_2O_2$: C 80.92 H 7.19 N 5.55. Found: C 80.81 H 7.22 N 5.52.

**12b**. *7,7,7',7'-Tetramethyl-4,4'-bis(4-methylphenyl)-4,6,7,8,4',6',7',8'-octahydro-1H,1H-[2,2']biquinolinyl-5,5'-dione* (Table 4, entry 2)

Yellow solid; mp 185-187 $^{o}$C; $R_f$ 0.84 (40% AcOEt/Petroleum ether); IR (KBr): 1057, 1128, 1386, 1490, 1588, 2935, 3320 cm$^{-1}$; $^{1}$H NMR (500 MHz, DMSO-d$_6$): δ 0.91 (s, 6H, -C*H*$_3$), 0.97 (s, 6H, -C*H*$_3$), 1.93 (Abq, 4H, *J* = 8.6 Hz, -C*H*), 2.19 (s, 6H, Ar-C*H*$_3$), 2.29 (s, 4H, -C*H*$_2$), 4.58 (d, 2H, *J* = 6.1 Hz, dihydropyridyl-C*H*), 6.63 (d, 2H, *J* = 4.5 Hz, dihydropyridyl-C=C*H*), 7.18 (m, 4H, Ar-*H*), 7.67 (d, 4H, *J* = 7.6 Hz, Ar-*H*), 8.55 (brs, 2H, -*NH*); $^{13}$C NMR (125 MHz, $CDCl_3$): δ 21.0, 21.5, 27.5, 29.2, 29.6, 32.6, 38.1, 41.7, 50.7, 107.3, 117.1, 119.4, 127.9, 128.5, 128.8, 128.9, 129.3, 129.7, 131.7, 133.7, 136.3, 141.5, 143.3, 144.9, 150.2, 183.2, 195.3; MS

(ESI LCQ-MS): *m*/*z* 533.47 [$M^+$+$H^+$]. Anal. Calcd for $C_{36}H_{40}N_2O_2$: C 81.17 H 7.57 N 5.26. Found: C 80.28 H 7.52 N 5.23.

**12c**. *7,7,7',7'-Tetramethyl-4,4'-bis(4-methoxyphenyl)-4,6,7,8,4',6',7',8'-octahydro-1H,1H-[2,2']biquinolinyl-5,5'-dione* (Table 4, entry 3)

Yellow solid; mp 226-228 $^oC$; $R_f$ 0.6 (40% AcOEt/Petroleum ether); IR (KBr): 1176, 1257, 1445, 1562, 3014, 3129 $cm^{-1}$; $^1H$ NMR (500 MHz, DMSO-$d_6$): δ 1.02 (s, 6H, -C$H_3$), 1.08 (s, 6H, -C$H_3$), 2.15 (Abq, 4H, *J* = 8.1 Hz, -C*H*), 2.36 (s, 4H, -C$H_2$), 3.75 (s, 6H, Ar-OC$H_3$), 4.78 (d, 2H, *J* = 5.6 Hz, dihydropyridyl-C*H*), 6.24 (m, 2H, dihydropyridyl-C=C*H*), 6.81 (m, 4H, Ar-*H*), 6.88 (m, 2H, Ar-*H*), 7.50 (m, 2H, Ar-*H*) 8.55 (brs, 2H, -*NH*); $^{13}C$ NMR (125 MHz, $CDCl_3$): δ 27.5, 28.3, 29.2, 29.7, 32.6, 37.6, 41.7, 50.7, 55.2, 55.4, 107.4, 113.6, 113.9, 114.4, 115.7, 119.0, 127.2, 129.1, 129.5, 130.4, 133.7, 138.6, 144.6, 150.1, 158.4, 161.9, 183.1, 195.3; MS (ESI LCQ-MS): *m*/*z* 565.20 [$M^+$+$H^+$]. Anal. Calcd for $C_{36}H_{40}N_2O_4$: C 76.57 H 7.14 N 4.96. Found: C 76.66 H 7.17 N 4.98.

**12d**. *7,7,7',7'-Tetramethyl-4,4'-bis(4-chlorophenyl)-4,6,7,8,4',6',7',8'-octahydro-1H,1H-[2,2']biquinolinyl-5,5'-dione* (Table 4, entry 4)

Yellow solid; mp 286-289 $^oC$; $R_f$ 0.81 (40% AcOEt/Petroleum ether); IR (KBr): 1319, 1384, 1484, 1590, 2928, 3352 $cm^{-1}$; $^1H$ NMR (500 MHz, DMSO-$d_6$): δ 0.85 (s, 6H, -C$H_3$), 0.95 (s, 6H, -C$H_3$), 1.89 (Abq, 4H, *J* = 9.2 Hz, -C*H*), 2.35 (s, 4H, -C$H_2$), 4.46 (d, 2H, *J* = 4.6 Hz, dihydropyridyl-C*H*), 5.52 (d, 2H, *J* = 4.6 Hz, dihydropyridyl-C=C*H*), 7.14 (m, 4H, *J* = 8.4 Hz, Ar-*H*), 7.25 (d, 4H, *J* = 8.4 Hz, Ar-*H*), 8.22 (brs, 2H, -*NH*); $^{13}C$ NMR (125 MHz, DMSO-$d_6$): δ 27.3, 28.1, 29.0, 29.5, 32.4, 37.4, 41.5, 50.8, 55.1, 55.3, 107.2, 113.4, 113.8, 114.2, 115.5, 119.1, 127.1, 129.2, 129.4, 130.5, 133.5, 138.5, 144.5, 150.2, 158.2, 161.7, 183.3, 195.4; MS (ESI

LCQ-MS): *m*/*z* 573.20 [$M^+$+$H^+$]. Anal. Calcd for $C_{34}H_{34}Cl_2N_2O_2$: C 71.20 H 5.98 N 4.88. Found: C 71.28 H 5.95 N 4.87.

**12e**. *7,7,7',7'-Tetramethyl-4,4'-bis(3,4-dimethoxyphenyl)-4,6,7,8,4',6',7',8'-octahydro-1H,1H-[2,2']biquinolinyl-5,5'-dione* (Table 4, entry 5)

Yellow solid; mp 211-214 $^oC$; $R_f$ 0.35 (40% AcOEt/Petroleum ether); IR (KBr): 1345, 1212, 1496, 1575, 2945, 3345 $cm^{-1}$; $^1H$ NMR (500 MHz, DMSO-$d_6$): δ 1.07 (s, 6H, -C$H_3$), 1.12 (s, 6H, -C$H_3$), 2.12 (Abq, 4H, *J* = 8.6 Hz, -C*H*), 2.31 (s, 4H, -C$H_2$), 3.68 (s, 6H, Ar-OC$H_3$), 3.73 (s, 6H, Ar-OC$H_3$), 4.76 (d, 2H, *J* = 5.6 Hz, dihydropyridyl-C*H*), 6.21 (m, 2H, dihydropyridyl-C=C*H*), 6.85 (m, 2H, Ar-*H*), 6.94 (m, 2H, Ar-*H*), 7.56 (m, 2H, Ar-*H*) 8.59 (brs, 2H, -N*H*); $^{13}C$ NMR (125 MHz, $CDCl_3$): δ 27.8, 28.6, 29.4, 29.9, 32.8, 37.7, 42.3, 51.5,55.8, 56.1, 56.2, 56.8, 108.1, 113.8, 114.0, 114.6, 115.8, 119.1, 127.2, 129.3, 129.7, 130.7, 133.9, 138.9, 144.5, 150.4, 159.3, 162.4, 184.5, 196.5; MS (ESI LCQ-MS): *m*/*z* 625.40 [$M^+$+$H^+$]. Anal. Calcd for $C_{38}H_{44}N_2O_6$: C 73.05 H 7.10 N 4.48. Found: C 73.18 H 7.16 N 4.52.

**12f**. *7,7,7',7'-Tetramethyl-4,4'-bis(4-bromophenyl)-4,6,7,8,4',6',7',8'-octahydro-1H,1H-[2,2']biquinolinyl-5,5'-dione* (Table 4, entry 6)

Yellow solid; mp 282-284 $^oC$; $R_f$ 0.79 (40% AcOEt/Petroleum ether); IR (KBr): 1189, 1259, 1426, 1559, 2975, 3189 $cm^{-1}$; $^1H$ NMR (500 MHz, DMSO-$d_6$): δ .89 (s, 6H, -C$H_3$), .95 (s, 6H, -C$H_3$), 2.08 (Abq, 4H, *J* = 8.1 Hz, -C*H*), 2.32 (s, 4H, -C$H_2$), 4.91 (d, 2H, *J* = 5.6 Hz, dihydropyridyl-C*H*), 6. 21 (m, 2H, dihydropyridyl-C=C*H*), 7.08-7.12 (m, 2H, Ar-*H*), 7.18-7.22 (m, 4H, Ar-*H*), 7.48 (m, 2H, Ar-*H*) 8.47 (brs, 2H, -N*H*); $^{13}C$ NMR (125 MHz, $CDCl_3$): δ 26.8, 27.2, 29.1, 29.7, 32.4, 37.3, 41.5, 50.3, 107.1, 112.7, 113.5, 114.1, 115.3, 118.3, 126.3, 128.6.6, 129.9, 130.7, 133.3, 138.3, 144.1, 149.8, 157.2, 160.5, 182.9, 194.3; MS (ESI LCQ-MS): *m*/*z*

663.28 [$M^+$+$H^+$]. Anal. Calcd for $C_{34}H_{34}Br_2N_2O_4$: C 61.64 H 5.17 N 4.23. Found: C 61.75 H 5.15 N 4.21.

7. Spectral data compound **14a-j**

**14a**. *6-(2-furyl)-2-(1H-indol-3-yl)-4-(4-methylphenyl)-3-carbonitrile* (Table 5, entry 1)

Pale Yellow solid; mp 199-202 $^oC$; $R_f$ 0.77 (40% AcOEt/Petroleum ether); IR (KBr): 1019, 1191, 1249, 1446, 1536, 2236, 3286 $cm^{-1}$; $^1H$ NMR (500 MHz, DMSO-$d_6$): δ 2.38 (s, 3H, Ar-C*H*$_3$), 6.74-6.76 (m, 1H, Ar-*H*), 7.20-7.22 (m, 2H, Ar-*H*), 7.36 (d, 2H, *J* = 7.6 Hz, Ar-*H*), 7.41 (d, 1H, *J* = 3.8 Hz, Ar-*H*), 7.50-7.52 (m, 1H, Ar-*H*), 7.58 (s, 1H, Ar-*H*), 7.61 (d, 2H, *J* = 7.6 Hz, Ar-*H*),7.98 (s, 1H, Ar-*H*), 8.38 (d, 1H, *J* = 3.1 Hz, Ar-*H*), 8.45-8.47 (m, 1H, Ar-*H*), 11.81 (brs, 1H, -N*H*); $^{13}C$ NMR (125 MHz, DMSO-$d_6$)**:** δ 21.4, 100.8, 112.9, 113.2, 113.5, 114.3, 121.4, 122.4, 122.9, 126.7, 129.2, 129.9, 134.4, 136.9, 140.1, 146.5, 150.4, 152.8, 155.5, 158.1; MS (EI): *m*/*z* 376.40 [$M^+$+$H^+$]; Anal. Calcd for $C_{25}H_{17}N_3O$: C 79.98 H 4.56 N 11.19. Found: C 79.90 H 4.57 N 11.22.

**14b**. *4-(4-chlorophenyl)-6-(2-furyl)-2-(1H-indol-3-yl)-3-carbonitrile* (Table 5, entry 2)

Pale Yellow solid; mp 236-239 $^oC$; $R_f$ 0.89 (20% AcOEt/Petroleum ether); IR (KBr): 1016, 1141, 1230, 1429, 1483, 1530, 1599, 2206, 3377 $cm^{-1}$; $^1H$ NMR (500 MHz, DMSO-$d_6$): δ 6.74-6.76 (m, 1H, Ar-*H*), 7.20-7.23 (m, 2H, Ar-*H*), 7.40 (d, 1H, *J* = 7.6 Hz, Ar-*H*), 7.50-7.52 (m, 1H, Ar-*H*), 7.57 (s, 1H, Ar-*H*), 7.59 (d, 2H, *J* = 8.9 Hz, Ar-*H*), 7.72 (d, 2H, *J* = 8.5 Hz, Ar-*H*),7.97 (s, 1H, Ar-*H*), 8.37 (d, 1H, *J* = 3.1 Hz, Ar-*H*), 8.46-8.48 (m, 1H, Ar-*H*), 11.82 (brs, 1H, -N*H*); $^{13}C$ NMR (125 MHz, DMSO-$d_6$)**:** δ 100.7, 112.6, 113.1, 113.2, 113.5, 114.4, 119.3, 121.4, 122.4, 123.0, 126.6, 129.2, 129.3, 131.2, 135.3, 136.0, 136.9, 146.6, 150.5, 152.7, 154.2, 158.0; MS

(EI): *m*/*z* 395.40 [$M^+$+$H^+$]; Anal. Calcd for $C_{24}H_{14}ClN_3O$: C 79.98 H 4.56 N 11.19. Found: C 79.90 H 4.57 N 11.22.

**14c.** *6-(2-furyl)-2-(1H-indol-3-yl)-4-(3-nitrophenyl)-3-carbonitrile* (Table 5, entry 3)

Pale Yellow solid; mp 151-153 $^oC$; $R_f$ 0.75 (40% AcOEt/Petroleum ether); IR (KBr): 1233, 1347, 1531, 2213, 3062, 3339 $cm^{-1}$; $^1H$ NMR (500 MHz, DMSO-$d_6$): δ 6.76-6.78 (m, 1H, Ar-*H*), 7.20-7.23 (m, 2H, Ar-*H*), 7.45 (d, 1H, *J* = 3.1 Hz, Ar-*H*), 7.50-7.52 (m, 1H, Ar-*H*), 7.71 (s, 1H, Ar-*H*), 7.84 (t, 1H, *J* = 7.6 Hz, Ar-*H*), 8.00 (s, 1H, Ar-*H*), 8.19 (d, 1H, *J* = 8.4 Hz, Ar-*H*), 8.38-8.40 (m, 2H, Ar-*H*), 8.47-8.49 (m, 1H, Ar-*H*), 8.58 (s, 1H, Ar-*H*), 11.84 (brs, 1H, -N*H*); $^{13}C$ NMR (125 MHz, DMSO-$d_6$)**:** δ 100.8, 112.6, 113.4, 113.6, 114.7, 119.2, 121.5, 122.3, 123.0, 124.3, 125.0, 126.6, 129.4, 130.9, 136.1, 136.9, 138.6, 146.8, 148.4, 150.6, 152.6, 153.1, 158.0, 163.2; MS (EI): *m*/*z* 407.13 [$M^+$+$H^+$]; Anal. Calcd for $C_{24}H_{14}N_4O_3$: C 70.93 H 3.47 N 13.79. Found: C 70.83 H 3.46 N 13.82.

**14d** *4-(4-fluorophenyl)-6-(2-furyl)-2-(1H-indol-3-yl)-3-carbonitrile* (Table 5, entry 4)

Pale Yellow solid; mp 145-148 $^oC$; $R_f$ 0.84 (40% AcOEt/Petroleum ether); IR (KBr): 1143, 1428, 1528, 1598, 2206, 3377 $cm^{-1}$; $^1H$ NMR (500 MHz, DMSO-$d_6$): δ 6.74-6.75 (m, 1H, Ar-*H*), 7.21-7.23 (m, 2H, Ar-*H*), 7.37-7.41 (m, 3H, Ar-*H*), 7.50-7.52 (m, 1H, Ar-*H*), 7.56 (s, 1H, Ar-*H*), 7.75-7.78 (m, 2H, Ar-*H*), 7.96 (s, 1H, Ar-*H*), 8.37 (d, 1H, *J* = 3.1 Hz, Ar-*H*), 8.47-8.49 (m, 1H, Ar-*H*), 11.82 (brs, 1H, -N*H*); $^{13}C$ NMR (125 MHz, DMSO-$d_6$)**:** δ 100.8, 112.6, 113.0, 113.1, 113.5, 114.5, 116.2, 116.4, 119.4, 121.4, 122.4, 123.0, 126.7, 129.3, 131.6, 131.7, 133.6, 136.9, 146.6,150.4, 152.7, 154.4, 158.0; MS (EI): *m*/*z* 380.20 [$M^+$+$H^+$]; Anal. Calcd for $C_{24}H_{14}BrN_3O$: C 65.47 H 3.20 N 9.54. Found: C 65.54 H 3.21 N 9.57.

**14e.** *4-(4-bromophenyl)-6-(2-furyl)-2-(1H-indol-3-yl)-3-carbonitrile* (Table 5, entry 5)

Pale Yellow solid; mp 172-174 $^{o}$C; $R_f$ 0.74 (40% AcOEt/Petroleum ether); IR (KBr): 1146, 1235, 1426, 1426, 1476, 1526, 1628, 2206, 3233 cm$^{-1}$; $^{1}$H NMR (500 MHz, DMSO-d$_6$): δ 6.74-6.76 (m, 1H, Ar-*H*), 7.19-7.22 (m, 2H, Ar-*H*), 7.40 (d, 1H, *J* =3.1 Hz, Ar-*H*), 7.49-7.51 (m, 1H, Ar-*H*), 7.58 (s, 1H, Ar-*H*), 7.65 (d, 2H, *J* = 8.4 Hz, Ar-*H*), 7.74 (d, 2H, *J* = 8.4 Hz, Ar-*H*), 7.97 (s, 1H, Ar-*H*), 8.36 (d, 1H, *J* = 3.1 Hz, Ar-*H*), 8.45-8.47 (m, 1H, Ar-*H*), 11.82 (brs, 1H, -N*H*); $^{13}$C NMR (125 MHz, DMSO-d$_6$)**:** δ 100.6, 112.6, 113.1, 113.2, 113.6, 114.2, 119.3, 121.5, 122.4, 123.0, 124.0, 126.6, 129.3, 131.4, 132.3, 136.4, 136.8, 146.6, 150.5, 152.6, 154.3, 158.0, 163.0; MS (EI): *m*/*z* 440.20 [M$^{+}$+H$^{+}$]; Anal. Calcd for $C_{24}H_{14}BrN_3O$: C 65.47 H 3.20 N 9.54. Found: C 65.54 H 3.21 N 9.57.

**14f.** *4-(3-bromophenyl)-6-(2-furyl)-2-(1H-indol-3-yl)*-3-carbonitrile (Table 5, entry 6)

Pale Yellow solid; mp 145-148 $^{o}$C; $R_f$ 0.74 (20% AcOEt/Petroleum ether); IR (KBr): 1265, 1378, 1576, 1636, 2241, 3326 cm$^{-1}$; $^{1}$H NMR (500 MHz, DMSO-d$_6$): δ 6.76-6.78 (m, 1H, Ar-*H*), 7.21-7.24 (m, 2H, Ar-*H*), 7.51-7.54 (m, 2H, Ar-*H*), 7.68 (d, 1H, *J* = 7.6 Hz, Ar-*H*), 7.74-7.77 (m, 2H, Ar-*H*), 7.83 (s, 1H, Ar-*H*), 8.02 (s, 1H, Ar-*H*), 8.34 (m, 2H, Ar-*H*), 8.45-8.47 (m, 1H, Ar-*H*), 11.89 (brs, 1H, -N*H*); $^{13}$C NMR (125 MHz, DMSO-d$_6$)**:** δ 102.4, 112.3, 112.8, 113.1, 113.7, 114.4, 119.2, 121.3, 122.5, 123.2, 124.3, 126.8, 129.6, 131.8, 132.6, 136.7, 137.2, 147.3, 151.6, 153.4, 155.6, 159.4, 163.5; MS (EI): *m*/*z* 440.32 [M$^{+}$+H$^{+}$]; Anal. Calcd for $C_{24}H_{14}BrN_3O$: C 65.47 H 3.20 N 9.54. Found: C 65.36 H 3.22 N 9.52.

**14g** *6-(2-furyl)-2-(1H-indol-3-yl)-4,4'-bipyridine-3-carbonitrile* (Table 5, entry 7)

Pale Yellow solid; mp 235-238 $^{o}$C; $R_f$ 0.61 (20% AcOEt/Petroleum ether); IR (KBr): 1238, 1326, 1452, 1547, 2241, 3216 cm$^{-1}$; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 6.68-6.70 (m, 2H, Ar-*H*), 6.74-6.75 (m, 1H, Ar-*H*), 6.95-6.98 (m, 2H, Ar-*H*), 7.23-7.26 (m, 2H, -Ar-*H*), 7.60 (s, 1H, -Ar-*H*), 7.99 (s, 1H, -Ar-*H*), 8.14-8.19 (m, 3H, -Ar-*H*), 8.34 (d, 1H, *J* = 3.9 Hz, -Ar-*H*), 12.17 (brs, 1H, -N*H*); $^{13}$C

NMR (75 MHz, DMSO-d6): 101.4, 112.9, 113.1, 113.2, 113.5, 114.6, 118.8, 121.5, 122.4, 122.8, 123.2, 124.2, 126.5, 129.3, 133.1, 136.0, 137.4, 146.6, 150.8, 151.2, 158.2; MS (EI): *m*/*z* 363.40 [$M^+$+$H^+$]; Anal. Calcd for $C_{23}H_{14}N_4O$. C 76.23 H 3.89 N 15.46. Found: C 76.12 H 3.90 N 15.50.

**14h**. *6-(2-furyl)-2-(1H-indol-3-yl)-4,3'-bipyridine-3-carbonitrile* (Table 5, entry 8)

Pale Yellow solid; mp 215-218 $^oC$; $R_f$ 0.61 (20% AcOEt/Petroleum ether); IR (KBr): 1238, 1326, 1452, 1547, 2241, 3216 $cm^{-1}$; $^1H$ NMR (500 MHz, $CDCl_3$): δ 6.76 (s, 1H, Ar-*H*), 7.21-7.23 (m, 2H, Ar-*H*), 7.43-7.45 (m, 1H, Ar-*H*), 7.51-7.60 (m, 2H, -Ar-*H*), 7.68.-7.70 (m, 1H, -Ar-*H*), 7.99 (s, 1H, -Ar-*H*), 8.15-8.17 (m, 1H, -Ar-*H*), 8.37-8.39 (m, 1H, -Ar-*H*), 8.48-8.49 (m, 1H, -Ar-*H*), 8.73 (d, 1H, *J* = 4.6 Hz, -Ar-*H*), 8.73 (s, 1H, -Ar-*H*), 11.89 (brs, 1H, -N*H*); $^{13}C$ NMR (75 MHz, DMSO-d6): 100.9, 112.6, 113.0, 113.3, 113.5, 114.6, 119.3, 121.5, 122.4, 123.0, 124.2, 126.6, 129.3, 133.2, 136.9, 137.0, 146.7, 149.5, 150.6, 151.2, 152.3, 152.6, 158.0; MS (EI): *m*/*z* 363.27 [$M^+$+$H^+$]; Anal. Calcd for $C_{23}H_{14}N_4O$. C 76.23 H 3.89 N 15.46. Found: C 76.33 H 3.88 N 15.42.

**14i**. *6-(2-furyl)-2-(1H-indol-3-yl)-4-(2-thienyl) -3-carbonitrile* (Table 5, entry 9)

Pale Yellow solid; mp 226-228 $^oC$; $R_f$ 0.36 (20% AcOEt/Petroleum ether); IR (KBr): 1014, 1139, 1228, 1421, 1529, 1602, 2265, 3342 $cm^{-1}$; $^1H$ NMR (500 MHz, $CDCl_3$): δ 6.71-6.73 (m, 1H, Ar-*H*), 7.18-7.26 (m, 3H, Ar-*H*), 7.34-7.36 (m, 1H, Ar-*H*), 7.49 (d, 1H, *J* = 7.6 Hz, -Ar-*H*), 7.59 (s, 1H, -Ar-*H*), 7.86-7.94 (m, 3H, -Ar-*H*), 8.35-8.40 (m, 2H, -Ar-*H*), 11.82 (brs, 1H, -N*H*); $^{13}C$ NMR (75 MHz, DMSO-d6): 98.9, 112.6, 113.0, 113.1, 113.2, 113.5, 119.8, 121.4, 122.3, 123.0, 126.7, 129.1, 129.4, 130.5, 130.8, 136.8, 137.7, 146.6, 147.1, 150.6, 152.5, 158.8; MS (EI): *m*/*z* 363.20 [$M^+$+$H^+$]; Anal. Calcd for $C_{22}H_{13}N3_4OS$. C 71.92 H 3.57 N 11.44. Found: C 71.82 H 3.56 N 11.48.

**14j**. 6-(2-furyl)-2,4-di-1*H*-indol-3-yl-3-carbonitrile (Table 5, entry 10)

Pale Yellow solid; mp 210 $^{o}$C; $R_f$ 0.29 (20% AcOEt/Petroleum ether); IR (KBr): 1114, 1264, 1442, 1612, 2246, 3248 cm$^{-1}$; $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.20-7.26 (m, 2H, Ar-*H*), 7.51-7.56 (m, 3H, -Ar-*H*), 7.85-7.89 (m, 2H, -Ar-*H*), 7.85 (s, 1H, -Ar-*H*), 8.19-8.21 (m, 2H, -Ar-*H*), 8.36 (s, 1H, -Ar-*H*), 8.51-8.52 (m, 1H, -Ar-*H*), 8.73-8.77 (m, 2H, -Ar-*H*), 11.76 (brs, 1H, -N*H*), 12.11 (brs, 1H, -N*H*); $^{13}$C NMR (75 MHz, DMSO-d6): 102.4, 110.9, 112.3, 112.8, 113.3, 113.8, 114.2, 119.1, 121.4, 121.8, 122.1, 122.4, 124.0, 126.4, 128.4, 128.9, 129.4, 130.4, 131.1, 131.8, 136.1, 136.8, 152.6, 156.4, 160.2; MS (EI): *m*/*z* 401.20 [$M^+$+$H^+$]; Anal. Calcd for $C_{26}H_{16}N_4O$. C 77.99 H 4.03 N 13.99. Found: C 77.89 H 4.04 N 13.96.

8. Spectral data compound 1**5**

**15.** *4-(2,4-dichlorophenyl)-6-(2-furyl)-2-(1H-indol-3-yl)-1,4-dihydropyridine-3-carbonitrile*

Pale Yellow solid; mp 185-188 $^{o}$C; $R_f$ 0.6 (40% AcOEt/Petroleum ether); IR (KBr): 1018, 1155, 1223, 1499, 1599, 2189, 3295, 3358 cm$^{-1}$; $^{1}$H NMR (500 MHz, DMSO-$d_6$): δ 4.95 (d, 1H, *J* = 5.4 Hz, dihydropydinyl -C*H*), 5.28 (d, 1H, *J* = 6.1 Hz, dihydropydinyl -C*H*), 6.51 (m, 1H, Ar-*H*) 6.87 (d, 1H, *J* = 3.1 Hz, Ar-*H*), 7.10-7.18 (m, 2H, Ar-*H*), 7.46 (d, 1H, *J* = 8.4 Hz, Ar-*H*), 7.53 (s, 1H, Ar-*H*), 7.56 (d, 1H, *J* = 7.6 Hz, Ar-*H*), 7.63-7.65 (m, 2H, Ar-*H*), 7.84 (d, 2H, *J* = 3.1 Hz, Ar-*H*), 8.96 (brs, 1H, -N*H*), 11.72 (brs, 1H, -N*H*); $^{13}$C NMR (125 MHz, DMSO-$d_6$)**:** δ 76.1, 97.8, 108.0, 108.5, 112.0, 112.7, 120.4, 120.6, 122.2, 122.5, 125.8, 128.3, 128.7, 128.9, 129.5, 132.1, 132.5, 132.8, 136.6, 142.2, 143.8, 147.6, 148.0; MS (EI): *m*/*z* 432.20 [$M^+$+$H^+$]; Anal. Calcd for $C_{24}H_{15}Cl_2N_3O$: C 66.68 H 3.50 N 9.72. Found: C 66.60 H 3.51 N 9.73.

9. Spectral data compound 1**6**

**16.** 4-(2,4-dichlorophenyl)-6-(2-furyl)-2-(1*H*-indol-3-yl)nicotinonitrile

Yellow solid; mp 268-271 $^{o}$C; $R_f$ 0.77 (40% AcOEt/Petroleum ether); IR (KBr): 1143, 1231, 1475, 15333, 1600, 2217, 3358 cm$^{-1}$; $^{1}$H NMR (500 MHz, DMSO-$d_6$): δ 6.76-6.77 (m, 1H, Ar-

*H*), 7.22-7.24 (m, 2H, Ar-*H*), 7.45 (d, 1H, *J* = 7.6 Hz, Ar-*H*), 7.51-7.53 (m, 1H, Ar-*H*), 7.59-7.65 (m, 3H, Ar-*H*), 7.87 (d, 1H, *J* = 1.5 Hz, Ar-*H*), 8.00 (s, 1H, Ar-*H*), 8.37 (d, 1H, *J* = 3.1 Hz, Ar-*H*), 8.52-8.54 (m, 1H, Ar-*H*), 11.86 (brs, 1H, -N*H*); $^{13}$C NMR (125 MHz, DMSO-$d_6$)**:** δ 101.8, 112.7, 112.9, 113.5, 113.6, 114.9, 118.4, 121.6, 122.5, 123.1, 126.5, 128.4, 129.2, 129.8, 132.8, 133.2, 135.2, 135.6, 136.9, 146.9, 150.6, 152.4, 152.5, 157.4; MS (EI): *m*/*z* 430.20 [$M^+$+$H^+$]; Anal. Calcd for $C_{24}H_{13}ClN_3O$: C 66.99 H 3.05 N 9.77. Found: C 67.08 H 3.04 N 9.74.

10. Crystallographic data for compound **4h**

The single-crystal growth was carried out in ethanol at room temperature.

$C_{25}H_{15}BrN_4$

Mr = 451.32

Orthorhombic, Pbca

a = 14.7393 (4) A °

b = 10.7465 (3) A °

c = 25.4251 (7) A °

V = 4027.23 (19) A ° 3

Z = 8

Mo *K*α radiation

μ = 2.06 $mm^{-}1$

T = 293 (2) K

0.29 X 0.26 X 0.22 mm

Data collection

Bruker Kappa APEXII areadetector

diffractometer

Absorption correction: multi-scan

(SADABS; Sheldrick, 2001)

Tmin = 0.556, Tmax = 0.635

47903 measured reflections

5545 independent reflections

3138 reflections with I > 2σ(I)

Rint = 0.057

Refinement

R[F2 > 2σ(F2)] = 0.040

wR(F2) = 0.120

S = 0.99

5545 reflections

272 parameters

11. Crystallographic data for compound **5**

The single-crystal growth was carried out in ethanol at room temperature.

$C_{25}H_{16}Cl_2N_4$

Mr = 443.32

Triclinic, P1

a = 8.0158 (9) A ° b = 10.0261 (12) A ° c = 14.3653 (17) A °

α = 72.260 (6) ° β= 79.420 (6) ° γ = 78.224 (6) °

V = 1067.3 (2) A ° 3

Z = 2

Mo *K*α radiation

μ = 0.33 $mm^{-1}$

T = 298 (2) K

0.35 X 0.32 X 0.28 mm

Data collection

Bruker APEXII CCD area-detector

diffractometer

Absorption correction: multi-scan

(SADABS; Sheldrick, 2001)

Tmin = 0.895, Tmax = 0.915

12383 measured reflections

3707 independent reflections

3172 reflections with I > 2_(I)

Rint = 0.023

Refinement

R[F2 > 2_(F2)] = 0.044

wR(F2) = 0.140

S = 1.08

12. Crystallographic data for compound **6**

The single-crystal growth was carried out in ethanol at room temperature.

$C_{25}H_{14}Cl_2N_4$

Mr = 441.30

Monoclinic, $P2_1$=c

a = 10.0307 (12) A °

b = 22.446 (3) A °

c = 17.932 (3) A °

β = 90.991 (4) °

V = 4036.7 (10) A ° 3

Z = 8

Mo Kα radiation

μ = 0.34 mm_1

T = 293 K

0.30 X 0.25 X 0.20 mm

Data collection

Bruker Kappa APEXII areadetector

diffractometer

Absorption correction: multi-scan

(SADABS; Sheldrick, 2001)

Tmin = 0.902, Tmax = 0.934

38628 measured reflections

7874 independent reflections

5586 reflections with I > 2σ(I)

Rint = 0.038

Refinement

R[F2 > 2σ(F2)] = 0.043

wR(F2) = 0.141

S = 1.06

7874 reflections

567 parameters