

Supporting Information

Silver(I) Catalyzed Intramolecular Cyclization of N-(2-(alk-1-yn-1-yl))Tetrazoles leading to the formation of N-cyano-2-substituted Indoles under ambient conditions

Sangeetha Panaka,^{a, b} Rajiv Trivedi,^{a, b*} T. Sony,^c S. Prabhakar,^c L. Raju Chowhan^d

^a*Inorganic and Physical Chemistry Division, CSIR-Indian Institute of Chemical Technology, Hyderabad 500007, Telangana, India, trivedi@iict.res.in, Fax: +91-40-2716-0921; Tel: +91-40-2719-1667*

^b*Academy of Scientific and Innovative Research, AcSIR CSIR-IICT Campus, Hyderabad, 500007*

^c*Analytical Chemistry and Mass spectrometry Division, CSIR-Indian Institute of Chemical Technology, Hyderabad 500007, Telangana, India*

^d*School of Chemical Sciences, Central University of Gujarat, Sector 30, Gandhinagar, Gujarat - 382030, India*

Table of content:

1	Experimental data of compounds (4)	2- 13
----------	------------------------------------	-------

Experimental data for the compounds (4aa- 4ee)

1- N- cyano-2-Butyl-6-fluoro-1H-indole (4aa): Yield: 85%, colourless liquid, $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.43 (dd, $J = 8.8, 4.1$ Hz, 1H), 7.17 (dd, $J = 8.8, 2.4$ Hz, 1H), 7.04 (td, $J = 8.8, 2.4$ Hz, 1H), 6.32 (d, $J = 0.9$ Hz, 1H), 2.83 (t, $J = 7.7$ Hz, 2H), 1.76 (ddd, $J = 15.4, 8.5, 6.5$ Hz, 2H), 1.46 (dq, $J = 14.7, 7.4$ Hz, 2H), 0.98 (t, $J = 7.4$ Hz, 3H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 161.28, 158.90, 142.88, 133.05, 129.56, 129.46, 112.16, 111.96, 111.90, 111.87, 106.98, 106.74, 105.56, 105.53, 30.11, 26.67, 22.21, 13.73. $^{19}\text{F NMR}$ (375 MHz, CDCl_3): δ -119.13. **DEPT- 135 NMR (125 MHz, CDCl_3):** δ 112.13, 111.95, 111.92, 111.87, 106.95, 106.76, 105.55, 105.52, 31.45, 30.21, 30.10, 29.72, 29.29, 26.66, 22.20, 13.72. **IR DATA:** 3422.11, $\text{C}\equiv\text{N}$ - 2244.48, 2127.95, 1654.06, 1508.83, 1467.67, 1279.20, 1241.63, 1206.48, 1176.17, 1026.18, 1001.51, 825.32, 764.15, 628.07.

2. N- cyano-2-Cyclohexyl-6-fluoro-1H-indole (4ae): Yield: 92%, colourless liquid, $^1\text{H NMR}$ (500 MHz, CDCl_3): δ 7.36 (dd, $J = 8.8, 4.1$ Hz, 1H), 7.10 (dd, $J = 8.8, 2.4$ Hz, 1H), 6.97 (td, $J = 8.8, 2.4$ Hz, 1H), 6.21 (s, 1H), 2.76 – 2.69 (m, 1H), 2.07 (d, $J = 8.8$ Hz, 2H), 1.81 (dd, $J = 9.1, 3.4$ Hz, 2H), 1.74 – 1.69 (m, 2H), 1.43 – 1.36 (m, 5H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 161.28, 158.89, 147.97, 132.95, 129.50, 129.40, 112.17, 111.95, 111.90, 111.86, 107.09, 106.84, 103.58, 103.55, 36.52, 32.30, 26.04, 25.82. $^{19}\text{F NMR}$ (375 MHz, CDCl_3): δ -119.16. **DEPT- 135 (125 MHz, CDCl_3):** δ 111.09, 110.89, 110.81, 106.01, 105.82, 102.53, 102.50, 35.47, 31.24, 24.99, 24.78. **IR DATA:** 2930.54, 2855.40, $\text{C}\equiv\text{N}$ - 2241.75, 1738.37, 1622.10, 1599.61, 1472.08, 1449.87, 1385.25, 1341.41, 1292.60, 1263.58, 1243.09, 1210.74, 1182.58, 1124.51, 1149.18, 955.94, 858.58, 797.79, 730.46, 672.19, 602.33, 490.61, 437.12.

3.N- cyano-2-Cyclopentyl-6-fluoro-1H-indole (4af): Yield: 90%; colourless liquid; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.36 (dd, $J = 8.8, 4.2$ Hz, 1H), 7.10 (dd, $J = 8.8, 2.4$ Hz, 1H), 6.97 (td, $J = 9.0, 2.4$ Hz, 1H), 6.25 (d, $J = 0.8$ Hz, 1H), 3.66 (s, 2H), 2.21 – 2.12 (m, 2H), 1.77 (ddd, $J = 6.8, 5.8, 1.8$ Hz, 1H), 1.69 (tdd, $J = 8.5, 5.6, 3.1$ Hz, 4H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 161.28, 158.90, 147.33, 133.23, 129.41, 129.31, 112.14, 111.90, 111.81, 107.03, 106.79, 103.60, 43.47, 37.72, 32.23, 31.65, 30.95, 29.73, 25.23. $^{19}\text{F NMR}$ (470 MHz, CDCl_3): δ -119.20. **DEPT- 135 (100 MHz, CDCl_3):** δ 112.13, 111.87, 111.80, 107.03, 106.78, 103.59, 103.55, 37.72, 32.22, 29.73, 25.22. **IR DATA:** 2959.28, 2871.74, $\text{C}\equiv\text{N}$ - **2242.40**, 1727.58, 1622.56, 1599.92, 1472.95, 1452.43, 1378.36, 1337.75, 1266.26, 1216.00, 1183.87, 1128.13, 950.89, 859.92, 796.50, 730.72, 673.62, 602.53, 490.48, 464.39, 436.60.

4. N- cyano-6-Fluoro-2-phenyl-1H-indole (4ah): Yield: 95%; white solid, m.p. 152-155 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.74 – 7.70 (m, 1H), 7.58 – 7.47 (m, 2H), 7.29 (dd, $J = 8.6, 2.4$ Hz, 1H), 7.14 (td, $J = 8.9, 2.5$ Hz, 1H), 6.74 (d, $J = 0.7$ Hz, 1H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 161.51, 159.11, 141.42, 134.34, 129.92, 129.60, 129.49, 129.22, 128.77, 127.64, 113.33, 113.07, 112.62, 112.53, 107.50, 107.25, 107.18, 106.93, 106.89. $^{19}\text{F NMR}$ (470 MHz, CDCl_3): δ -118.20. **DEPT- 135(100 MHz, CDCl_3):** δ 129.91, 129.21, 127.63, 113.32, 113.06, 112.62, 112.52, 107.49, 107.25, 106.92, 106.88. **IR DATA:** 3451.40, 3139.48, 2920.87, 2853.64, $\text{C}\equiv\text{N}$ - **2216.41**, 1747.33, 1593.12, 1505.30, 1457.77, 1385.64, 1222.77, 1160.31, 1081.45, 954.86, 876.36, 832.28, 798.13, 758.49, 724.16, 525.15, 490.17, 409.10.

5. N- cyano-6-Fluoro-2-phenethyl-1H-indole (4aj): Yield: 92%; white solid, m.p. 162-164 °C; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.34 (dd, $J = 8.8, 4.1$ Hz, 1H), 7.22 (t, $J = 7.4$ Hz, 2H), 7.17 – 7.12 (m, 3H), 7.07 (dd, $J = 8.8, 2.4$ Hz, 1H), 6.96 (td, $J = 8.8, 2.4$ Hz, 1H), 6.22 – 6.20 (m, 1H), 3.09 – 3.03 (m, 2H), 3.01 – 2.95 (m, 2H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 161.31, 158.92, 141.66, 139.73, 133.04, 129.43, 129.33, 128.71, 128.39, 126.67, 112.44, 112.18, 112.05, 111.95, 107.16, 106.91, 106.62, 106.15, 106.12, 34.36, 29.76, 28.90. $^{19}\text{F NMR}$ (375 MHz, CDCl_3): δ -118.84. **DEPT-135 (125 MHz, CDCl_3):** δ 128.72, 128.40, 126.68, 112.40, 112.19, 112.03,

111.95, 107.13, 106.94, 106.14, 106.11, 34.34, 28.89. **IR DATA:**3060.53, 3028.13, 2926.17, 2855.64, **C≡N-** **2240.54**, 1765.82, 1599.67, 1574.20, 1495.24, 1457.39, 1376.20, 1334.88, 1243.14, 1200.77, 1175.72, 1051.70, 932.58, 805.86, 744.50, 698.87, 593.44, 486.81, 427.87.

6. N- cyano-6-Fluoro-2-(2-(trifluoromethyl)phenyl)-1H-indole (4al): Yield: 76%; sticky white solid; **¹H NMR (400 MHz, CDCl₃):** δ 7.80 (d, *J* = 7.1 Hz, 1H), 7.68 – 7.57 (m, 3H), 7.55 – 7.47 (m, 2H), 7.28 – 7.22 (m, 1H), 7.12 (td, *J* = 8.9, 2.5 Hz, 1H), 6.65 (s, 1H). **¹³C NMR (100 MHz, CDCl₃):**δ 142.74, 133.72, 133.64, 133.50, 130.21, 129.82, 129.73, 125.29, 125.18, 124.60, 121.64, 116.48, 116.18, 115.96, 111.60, 107.21, 77.36, 77.04, 76.72. **¹⁹F NMR (470 MHz, CDCl₃):** δ 117.58, -118.69. **IR DATA:**3423.65, 3084.95, 2922.44, **C≡N-** **2242.31**, 1584.39, 1356.90, 1165.15, 1063.10, 793.59, 689.63, 480.02.

7. N- cyano-2-(4-Chlorophenyl)-6-fluoro-1H-indole (4am): Yield: 75%; sticky white solid; **¹H NMR (400 MHz, CDCl₃):** δ 7.68 – 7.64 (m, 1H), 7.57 (dd, *J* = 8.8, 3.9 Hz, 1H), 7.53 – 7.49 (m, 1H), 7.30 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.16 (td, *J* = 8.9, 2.4 Hz, 1H), 6.75 (s, 1H). **¹³C NMR (100 MHz, CDCl₃):** δ 161.56, 140.14, 137.95, 136.17, 134.32, 132.82, 129.93, 129.55, 128.85, 127.20, 120.31, 113.68, 113.42, 112.69, 112.60, 107.60, 107.35, 107.00. **¹⁹F NMR (375 MHz, CDCl₃):** δ -117.89. **DEPT- 135 (125 MHz, CDCl₃):** δ 127.71, 127.30, 126.13, 121.79, 111.32, 108.44, 77.23, 31.64, 29.68, 21.45. **IR DATA:**3415.95, 2921.29, 2853.78, **C≡N-** **2238.73**, 1763.88, 1453.77, 1370.87, 1338.15, 1302.99, 1242.97, 1170.93, 1089.11, 818.26, 730.41, 482.29, 438.50.

8. N- cyano-6-Fluoro-2-(4-hydroxyphenyl)-1H-indole (4ao): Yield: 87%; white solid, m.p. 142-144 °C; **¹H NMR (300 MHz, CDCl₃+DMSO):** δ 9.54 (s, 1H), 7.61 – 7.49 (m, 3H), 7.27 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.10 (td, *J* = 9.0, 2.4 Hz, 1H), 6.98 (d, *J* = 8.8 Hz, 2H), 6.64 (s, 1H) **¹³C NMR (75 MHz, CDCl₃+DMSO):** δ 166.46, 164.00, 163.27, 146.67, 138.72, 134.70, 134.56, 133.83, 124.32, 121.02, 117.26, 117.08, 116.95, 112.11, 111.94, 111.61, 110.13. **¹⁹F NMR (375**

MHz, CDCl₃): δ -118.77. **DEPT- 135 NMR (125 MHz, CDCl₃):** δ 128.97, 116.17, 112.33, 112.19, 112.11, 107.01, 106.81, 105.22. **IR DATA:**2925.19, 2853.93, **C \equiv N-** 2244.57, 1725.89, 1610.89, 1509.16, 1464.70, 1375.22, 1280.19, 1126.37, 1072.98, 797.63, 742.52

9. N- cyano-6-Fluoro-2-(hydroxymethyl)-1H-indole (4ap): Yield: 81%; sticky white solid; **¹H NMR (400 MHz, CDCl₃):** δ 7.96 (dd, J = 8.9, 4.6 Hz, 1H), 7.24 (dd, J = 9.3, 2.4 Hz, 1H), 7.06 (td, J = 9.1, 2.5 Hz, 1H), 6.31 (s, 1H), 5.35 (d, J = 1.5 Hz, 2H). **¹³C NMR (100 MHz, CDCl₃):** δ 160.61, 158.24, 152.03, 138.98, 135.15, 126.72, 113.56, 113.47, 111.55, 111.29, 106.73, 106.49, 96.02, 95.98, 66.90, 31.96, 29.73, 22.72, 14.15. **IR DATA:**2969.41, 2928.99, **C \equiv N-** 2240.68, 1735.84, 1595.98, 1570.28, 1459.42, 1366.65, 1330.04, 1278.09, 1173.79, 1123.20, 930.23, 808.08,744.21, 660.43, 488.30, 444.67.

10. N- cyano-2-Butyl-1H-indole (4ba): Yield: 95%; liquid; **¹H NMR (400 MHz, CDCl₃):** δ 7.38 (d, J = 8.4 Hz, 2H), 7.17 (dt, J = 14.9, 7.2 Hz, 2H), 6.22 (s, 1H), 2.70 (t, J = 7.7 Hz, 2H), 1.64 (dt, J = 15.4, 7.6 Hz, 2H), 1.40 – 1.29 (m, 2H), 0.87 (t, J = 7.4 Hz, 3H). **¹³C NMR (75 MHz, CDCl₃):** δ 140.85, 136.87, 128.57, 124.15, 123.97, 120.97, 111.03, 107.00, 105.57, 30.17, 29.78, 26.52, 22.24, 13.79. **DEPT-135 NMR (125 MHz, CDCl₃):** δ 124.15, 123.97, 120.95, 111.08, 105.59, 30.20, 26.53, 22.21, 13.75. **IR DATA:**3057.68, 2868.08, **C \equiv N-** 2241.12, 1726.09, 1458.87, 1375.64, 1335.48, 1197.98, 806.38, 590.61.

11. N- cyano-2-Hexyl-1H-indole (4bb): Yield: 92%; liquid; **¹H NMR (500 MHz, CDCl₃):** δ 7.54 – 7.48 (m, 2H), 7.31 (td, J = 7.7, 1.2 Hz, 1H), 7.28 – 7.24 (m, 1H), 6.35 (d, J = 0.9 Hz, 1H), 2.83 (dd, J = 11.4, 4.0 Hz, 2H), 1.77 (dd, J = 15.3, 7.7 Hz, 2H), 1.43 (tt, J = 9.0, 6.1 Hz, 2H), 1.35 – 1.31 (m, 4H), 0.92 – 0.87 (m, 3H). **¹³C NMR (100 MHz, CDCl₃):** δ 140.94, 136.90, 128.59, 124.15, 123.97, 120.96, 111.08, 107.01, 105.58, 60.43, 31.47, 29.74, 28.78, 28.10, 26.84, 22.56, 21.08, 14.23, 14.07. **DEPT- 135 NMR (100 MHz, CDCl₃):** δ 124.15, 123.96, 120.95, 111.08, 105.57, 31.46, 29.73, 28.78, 28.09, 26.83, 22.56, 14.07. **IR DATA:**3418.17, 2929.09,

2858.18, **C≡N-** 2241.08, 1724.88, 1574.76, 1458.67, 1373.40, 1335.83, 1201.47, 1013.56, 929.80, 804.86, 743.66, 591.73, 485.16, 429.11.

12. N- cyano-2-Isopropyl-1H-indole (4bc): Yield: 86%; liquid, **¹H NMR (500 MHz, CDCl₃):** δ 7.54 – 7.49 (m, 2H), 7.32 (td, *J* = 7.7, 1.1 Hz, 1H), 7.29 – 7.24 (m, 1H), 6.35 (s, 1H), 3.18 (dtd, *J* = 13.7, 6.8, 0.7 Hz, 1H), 1.42 (s, 3H), 1.41 (s, 3H). **¹³C NMR (125 MHz, CDCl₃):** δ 146.94, 137.01, 128.39, 124.26, 123.99, 121.11, 111.06, 107.09, 103.46, 29.74, 26.92, 21.79. **DEPT- 135 NMR (125 MHz, CDCl₃):** δ 124.25, 123.98, 121.10, 111.05, 103.46, 29.73, 26.91, 21.78. **IR DATA:** 3132.99, 2971.67, 2929.15, 2872.29, **C≡N-** 2237.76, 1725.28, 1612.01, 1582.36, 1506.02, 1466.64, 1389.55, 1319.38, 1275.89, 1182.58, 1118.09, 1087.56, 1023.63, 993.66, 952.01, 873.41, 823.91, 665.38, 625.08, 577.17, 536.74, 491.33.

13. N- cyano-2-Cyclohexyl-1H-indole (4be): Yield: 95%; liquid; **¹H NMR (400 MHz, CDCl₃):** δ 7.46 – 7.40 (m, 2H), 7.24 (td, *J* = 7.7, 1.3 Hz, 1H), 7.20 – 7.15 (m, 1H), 6.24 (s, 1H), 2.77 – 2.69 (m, 1H), 2.11 – 2.05 (m, 2H), 1.80 (dd, *J* = 9.0, 3.5 Hz, 2H), 1.43 – 1.35 (m, 4H), 1.24 – 1.15 (m, 2H). **¹³C NMR (100 MHz, CDCl₃):** δ 146.04, 136.80, 128.51, 124.17, 123.95, 121.08, 111.06, 107.11, 103.58, 36.37, 32.38, 29.75, 26.10, 25.89. **DEPT- 135 NMR (125 MHz, CDCl₃):** δ 111.09, 110.89, 110.81, 106.01, 105.82, 102.53, 102.50, 35.47, 31.24, 24.99, 24.78. **IR DATA:** 2929.35, 2854.91, **C≡N-** 2239.74, 1740.20, 1568.88, 1456.12, 1382.99, 1334.38, 1277.22, 1200.71, 1174.92, 1013.37, 806.29, 743.28, 487.33, 441.63.

14. N- cyano-2-Cyclopentyl-1H-indole (4bf): Yield: 91%; liquid; **¹H NMR (400 MHz, CDCl₃):** δ 7.38 – 7.28 (m, 1H), 7.20 (d, *J* = 8.0 Hz, 1H), 7.00 (t, *J* = 7.6 Hz, 1H), 6.50 (s, 1H), 2.72 – 2.58 (m, 1H), 1.92 (dd, *J* = 9.5, 3.5 Hz, 1H), 1.79 – 1.71 (m, 1H), 1.56 (ddd, *J* = 9.4, 7.8, 3.4 Hz, 2H), 1.38 (dd, *J* = 10.9, 5.2 Hz, 2H). **¹³C NMR (125 MHz, CDCl₃):** δ 145.34, 137.09, 128.42, 124.15, 123.96, 121.02, 111.00, 107.27, 103.61, 37.61, 32.25, 29.75, 25.24. **DEPT-135 NMR (100 MHz, CDCl₃):** δ 124.15, 123.95, 121.02, 110.99, 103.61, 37.60, 32.25, 25.23. **IR**

DATA:2956.16, 2923.09, 2853.43, **C≡N-** **2241.59**, 1765.07, 1455.93, 1490.11, 1403.07, 1374.98, 1338.88, 1305.37, 1242.86, 1169.62, 1090.02, 966.50, 820.06, 732.65, 483.48, 444.86

15. N- cyano-2-Cyclopropyl-1H-indole(4bg): Yield: 91%; liquid, **¹H NMR (400 MHz, CDCl₃):** δ = 7.45 – 7.39 (m, 1H), 7.25 (td, J = 7.7, 1.3 Hz, 1H), 7.20 – 7.16 (m, 1H), 6.12 (t, J = 0.9 Hz, 1H), 1.95 (dq, J = 8.3, 5.1, 1.1 Hz, 1H), 1.04 (dd, J = 8.4, 2.0 Hz, 1H), 0.78 (dd, J = 5.0, 1.9 Hz, 1H). **¹³C NMR (125 MHz, CDCl₃):** δ 143.02, 137.02, 128.31, 124.26, 123.99, 121.08, 111.01, 107.08, 103.75, 29.74, 7.24. **DEPT-25 NMR (75 MHz, CDCl₃):** δ 165.19, 162.77, 132.28, 130.42, 130.26, 118.00, 116.63, 113.70, 112.38, 96.51, 94.71, 63.00, 62.03, 36.65, 31.59, 30.71, 30.46, 29.61, 25.46, 25.30, 19.91, 19.78, 18.79. **IR DATA:**2957.50, 2925.56, 2854.78, **C≡N-** **2242.62**, 1739.34, 1622.60, 1599.90, 1472.62, 1377.55, 1338.15, 1262.60, 1216.20, 1184.19, 1127.94, 1101.36, 1024.21, 952.37, 859.83, 797.77, 728.84, 602.57, 490.33, 464.65, 436.89.

16. N- cyano-2-Phenyl-1H-indole (4bh): Yield: 80%; sticky white solid; **¹H NMR (400 MHz, CDCl₃):** δ 7.74 (dt, J = 3.5, 1.9 Hz, 2H), 7.64 (dd, J = 8.0, 3.1 Hz, 2H), 7.56 – 7.47 (m, 3H), 7.45 – 7.39 (m, 1H), 7.35 (dd, J = 11.0, 4.2 Hz, 1H), 6.79 (s, 1H). **¹³C NMR (100 MHz, CDCl₃):** δ 132.53, 129.23, 128.47, 121.83, 109.28, 81.58, 73.94, 29.75. **DEPT- 135 NMR (125 MHz, CDCl₃):** δ 132.52, 129.23, 128.46, 77.23, 29.74. **IR DATA:**3449.63, 2989.63, **C≡N-** **2241.87**, 1763.96, 1453.91, 1376.59, 1242.83, 1055.19, 751.11, 630.65.

17. N- cyano-2-(4-(tert-Butyl)phenyl)-1H-indole (4bi): Yield: 84%; sticky white solid; **¹H NMR (400 MHz, CDCl₃):** δ 7.70 – 7.65 (m, 2H), 7.64 – 7.60 (m, 2H), 7.56 – 7.52 (m, 2H), 7.43 – 7.37 (m, 1H), 7.36 – 7.31 (m, 1H), 6.74 (d, J = 0.7 Hz, 1H), 1.37 (s, 9H). **¹³C NMR (125 MHz, CDCl₃):** δ 152.92, 139.76, 138.11, 128.78, 128.32, 127.34, 126.23, 126.13, 124.96, 124.43, 121.50, 111.55, 110.18, 107.58, 106.62, 34.90, 31.24, 29.74, 29.40. **DEPT- 135 NMR (125 MHz, CDCl₃):** δ 129.47, 128.31, 127.34, 126.12, 124.96, 124.43, 121.50, 111.54, 106.61, 31.95,

31.23, 29.73, 29.39, 22.72. **IR DATA:**3062.17, 2960.97, 2865.86, **C≡N-** **2240.49**, 1723.79, 1600.33, 1501.15, 1459.66, 1399.06, 1364.58, 136.12, 1305.45, 1268.62, 1199.22, 1173.87, 1111.23, 1090.29, 1019.17, 951.46, 835.57, 751.98, 700.29, 563.84, 494.03.

18. N- cyano-2-Phenethyl-1H-indole (4bj): Yield: 90%; white solid, m.p. 161-164°C; **¹H NMR (500 MHz, CDCl₃):** δ 7.56 – 7.49 (m, 2H), 7.36 – 7.29 (m, 3H), 7.28 (dd, *J* = 7.6, 0.9 Hz, 1H), 7.24 (dt, *J* = 6.9, 2.9 Hz, 3H), 6.35 (d, *J* = 0.8 Hz, 1H), 3.21 – 3.14 (m, 2H), 3.12 – 3.06 (m, 2H). **¹³C NMR (100 MHz, CDCl₃):** δ 139.93, 139.69, 136.90, 128.67, 128.41, 126.58, 124.40, 124.06, 121.13, 111.15, 106.92, 106.19, 34.48, 28.80. **DEPT- 135 NMR (125 MHz, CDCl₃):** δ 128.66, 128.41, 126.57, 124.39, 124.05, 121.13, 111.14, 106.18, 34.46, 28.80. **IR DATA:**3446.71, 2924.55, **C≡N-** **2239.95**, 1895.74, 1501.85, 1453.14, 1339.39, 816.13, 738.42, 440.89.

19. N- cyano-2-(4-Fluorophenyl)-1H-indole (4bk): Yield: 86%; white solid, m.p. 168-170 °C; **¹H NMR (400 MHz, CDCl₃):** δ 7.70 (ddd, *J* = 7.0, 5.1, 2.5 Hz, 2H), 7.61 (d, *J* = 8.8 Hz, 2H), 7.44 – 7.38 (m, 1H), 7.37 – 7.31 (m, 1H), 7.24 – 7.16 (m, 2H), 6.73 (s, 1H). **¹³C NMR (75 MHz, CDCl₃):** δ 165.15, 161.83, 138.55, 138.04, 129.72, 129.61, 128.53, 125.29, 124.59, 121.64, 116.50, 116.21, 111.58, 107.20. **¹⁹F NMR (375 MHz, CDCl₃):** δ -110.60. **DEPT- 135 NMR (125 MHz, CDCl₃):** δ 129.70, 129.64, 125.29, 124.59, 121.64, 116.45, 116.28, 111.58, 107.20. **IR DATA:**3448.34, 2924.73, 2853.41, **C≡N-** **2240.34**, 1895.84, 1597.61, 1566.38, 1502.23, 1453.45, 1409.86, 1339.66, 1301.87, 1235.24, 1160.99, 1099.05, 1035.18, 927.96, 840.38, 816.02, 738.64, 666.93, 641.56, 601.48, 543.42, 513.48, 487.29, 442.99.

20. N- cyano-2-(4-(Trifluoromethyl)phenyl)-1H-indole (4bl): Yield: 71%; sticky white solid; **¹H NMR (500 MHz, CDCl₃):** δ 7.87 (d, *J* = 7.7 Hz, 1H), 7.71 (t, *J* = 7.5 Hz, 1H), 7.63 (ddd, *J* = 13.8, 12.8, 7.7 Hz, 4H), 7.48 – 7.44 (m, 1H), 7.40 – 7.36 (m, 1H), 6.76 (s, 1H). **¹³C NMR (100 MHz, CDCl₃):** δ 132.75, 131.88, 130.33, 126.79, 125.59, 124.47, 121.96, 111.51, 110.48. **¹⁹F**

NMR (470 MHz, CDCl₃): δ -58.50. **DEPT- 135 NMR (100 MHz, CDCl₃):** δ 132.74, 131.87, 130.32, 125.59, 124.47, 121.96, 111.50. **IR DATA:**3448.20, 2923.52, **C \equiv N- 2237.91**, 1763.48, 1665.23, 1463.63, 1377.51, 1242.94, 1055.39, 810.81, 622.49.

21. N- cyano-2-(4-Chlorophenyl)-1H-indole (4bm): Yield: 76%; sticky white solid; **¹H NMR (500 MHz, CDCl₃):** δ 7.69 – 7.65 (m, 2H), 7.65 – 7.62 (m, 2H), 7.51 – 7.48 (m, 2H), 7.45 – 7.41 (m, 1H), 7.35 (td, J = 7.6, 0.9 Hz, 1H), 6.79 (d, J = 0.7 Hz, 1H). **¹³C NMR (125 MHz, CDCl₃):** δ 138.36, 138.17, 135.81, 129.47, 128.83, 127.55, 125.48, 124.66, 121.72, 111.63, 107.57, 107.24, 31.96, 29.73, 29.40, 27.33, 22.73, 14.15. **IR DATA:**3450.38, 2925.28, 2854.67, **C \equiv N- 2240.35**, 1736.17, 1461.61, 1372.23, 1242.77, 1183.16, 1051.29, 965.78, 864.17, 821.00, 793.89, 727.71, 483.90.

22. N- cyano-2-(4-Methoxyphenyl)-1H-indole ((4bn): Yield: 88%; white solid, m.p. 148-150 °C; **¹H NMR (400 MHz, CDCl₃):** δ 7.69 – 7.64 (m, 2H), 7.63 – 7.58 (m, 2H), 7.41 – 7.36 (m, 1H), 7.34 – 7.30 (m, 1H), 7.05 – 7.02 (m, 2H), 6.68 (d, J = 0.7 Hz, 1H), 3.88 (s, 3H). **¹³C NMR (125 MHz, CDCl₃):** δ 160.71, 139.65, 137.95, 129.11, 128.84, 124.79, 124.41, 121.57, 121.36, 114.61, 111.50, 106.06, 55.47, 29.73. **DEPT- 135 NMR (100 MHz, CDCl₃):** δ 129.11, 124.79, 124.41, 121.36, 114.60, 111.49, 106.06, 77.24, 55.46, 29.73. **IR DATA:**3436.30, 3067.75, 2924.10, 2851.19, **C \equiv N- 2238.62**, 1615.37, 1505.04, 1450.96, 1347.42, 1303.76, 1247.75, 1172.91, 1023.40, 814.89, 726.75, 638.72, 604.45, 557.06, 481.07, 428.81.

23. N- cyano-2-(4-Hydroxyphenyl)-1H-indole (4bo): Yield: 83%; liquid, sticky white solid; **¹H NMR (500 MHz, CDCl₃):** δ 7.60 (dd, J = 7.5, 4.4 Hz, 4H), 7.41 – 7.37 (m, 1H), 7.33 (t, J = 7.9 Hz, 1H), 6.99 (d, J = 8.5 Hz, 2H), 6.67 (s, 1H). **¹³C NMR (100 MHz, CDCl₃):** δ 131.63, 129.32, 124.76, 124.42, 121.36, 116.16, 111.49, 106.00, 77.36, 77.04, 76.72, 44.32, 42.21, 40.55, 32.78, 29.81, 20.88. **DEPT- 135 NMR (125 MHz, CDCl₃):** δ 131.64, 129.32, 126.18, 124.99, 124.76,

121.36, 116.15, 115.98, 111.48, 106.00, 98.53, 77.24, 42.21, 29.83, 20.88. **IR DATA:**3353.41, 2925.13, 2855.85, **C≡N-** **2242.95**, 1667.42, 1610.48, 1504.90,1453.28, 1337.81, 1274.23, 1236.68, 1173.91, 1108.96, 838.76, 808.84, 745.49, 522.16, 491.60, 430.47.

24. N- cyano-2-(Hydroxymethyl)-1H-indole (4bp): Yield: 78%; sticky white solid; **¹H NMR (400 MHz, CDCl₃):** δ 8.03 (d, *J* = 8.0 Hz, 1H), 7.59 (d, *J* = 7.8 Hz, 1H), 7.37 – 7.27 (m, 2H), 6.34 (d, *J* = 0.7 Hz, 1H), 5.36 (d, *J* = 1.5 Hz, 2H). **¹³C NMR (125 MHz, CDCl₃):** δ 152.35, 137.28, 134.36, 130.23, 123.99, 123.30, 122.90, 121.39, 121.10, 112.69, 96.04, 66.97, 31.96, 31.47, 30.22, 29.73, 29.39, 22.73, 14.15. **DEPT- 135 NMR (125 MHz, CDCl₃):** δ 124.48, 123.99, 123.30, 122.90, 121.39, 121.09, 112.77, 96.04, 95.37, 77.24, 66.96, 66.08, 62.16, 31.95, 31.46, 30.22, 29.72, 29.39, 22.72, 14.15. **IR DATA:**3132.99, 2971.67, 2929.15, 2872.29, **C≡N-** **2237.76**, 1725.28, 1612.01, 1582.36, 1506.02, 1466.64, 1389.55, 1319.38, 1275.89, 1182.58, 1118.09, 1087.56, 1023.63, 993.66, 952.01, 873.41, 823.91, 665.38, 625.08, 577.17, 536.74, 491.33.

25. N- cyano-6-Methyl 2-(1H-indol-2-yl)acetate (4bq): Yield: 74%; sticky white solid; **¹H NMR (400 MHz, CDCl₃):** δ 7.60 (ddd, *J* = 5.9, 5.3, 2.8 Hz, 2H), 7.44 (ddd, *J* = 8.4, 7.3, 1.1 Hz, 1H), 7.36 – 7.30 (m, 1H), 6.74 (d, *J* = 0.5 Hz, 1H), 5.30 (s, 2H), 2.14 (s, 3H). **¹³C NMR (100 MHz, CDCl₃):** δ 170.31, 155.34, 133.69, 127.47, 125.91, 124.41, 122.13, 111.46, 110.59, 59.13, 57.12, 29.72, 27.04, 20.69. **DEPT- 135 NMR (125 MHz, CDCl₃):** δ 125.92, 124.42, 122.13, 111.47, 110.59, 57.13, 52.22, 29.73, 20.69. **IR DATA:**3474.84, 2924.49, 2853.53, **C≡N-** **2243.43**, 1746.39, 1605.74, 1455.49, 1370.39, 1334.12, 1220.86, 1172.74, 1143.84, 1104.49, 1025.60, 970.35, 818.53, 746.44, 602.89, 536.92, 482.72, 423.01.

26. N- cyano-6-Methyl-2-pentyl-1H-indole (4cd): Yield: 86%; liquid; **¹H NMR (400 MHz, CDCl₃):** δ 7.39 (d, *J* = 8.3 Hz, 1H), 7.29 (d, *J* = 0.7 Hz, 1H), 7.13 (dt, *J* = 8.7, 1.9 Hz, 1H), 6.27 (d, *J* = 0.9 Hz, 1H), 2.86 – 2.79 (m, 2H), 2.43 (s, 3H), 1.75 (ddd, *J* = 15.3, 8.5, 6.5 Hz, 2H), 1.45

(dq, $J = 14.7, 7.4$ Hz, 3H), 1.01 – 0.95 (m, 4H). ^{13}C NMR (100 MHz, CDCl_3): δ 140.97, 133.62, 125.40, 120.93, 110.71, 105.36, 30.21, 29.73, 26.57, 22.21, 21.40, 13.75. DEPT- 135 NMR (125 MHz, CDCl_3): δ 127.94, 125.39, 120.92, 110.70, 105.35, 77.23, 31.46, 30.21, 29.72, 26.56, 22.20, 21.40, 13.74. IR DATA:3449.16, 2926.10, $\text{C}\equiv\text{N}$ - 2238.99, 1729.83, 1468.63, 1219.29, 771.67, 403.78.

27. N- cyano-6-Methyl-2-phenyl-1H-indole (4ch): Yield: 92%; white solid, m.p. 152-155 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.74 – 7.70 (m, 1H), 7.52 – 7.47 (m, 2H), 7.45 (ddd, $J = 7.4, 3.6, 1.4$ Hz, 1H), 7.41 – 7.39 (m, 1H), 7.25 – 7.19 (m, 1H), 6.69 (d, $J = 0.7$ Hz, 1H), 2.47 (s, 3H). ^{13}C NMR (125 MHz, CDCl_3): δ 139.66, 136.40, 134.21, 129.48, 129.25, 129.11, 128.85, 127.54, 126.53, 121.51, 111.20, 107.68, 106.93, 21.46. DEPT- 135 NMR (100 MHz, CDCl_3): δ 129.48, 129.10, 127.54, 126.52, 121.51, 111.20, 106.92, 21.45. IR DATA:3420.44, 2923.97, 2853.16, $\text{C}\equiv\text{N}$ - 2243.30, 1723.53, 1621.88, 1593.76, 1466.86, 1444.51, 1361.59, 1338.74, 1278.38, 1206.88, 1160.86, 1123.11, 1072.46, 1045.27, 1024.36, 949.83, 916.54, 862.17, 844.51, 796.98, 757.44, 727.68, 683.89, 642.44, 598.82, 474.64, 435.33.

28. N- cyano-6-Methyl-2-(4-(trifluoromethyl)phenyl)-1H-indole (4cl): Yield: 76%; sticky white solid; ^1H NMR (400 MHz, CDCl_3): δ 7.86 (d, $J = 8.2$ Hz, 1H), 7.77 (d, $J = 8.3$ Hz, 1H), 7.56 – 7.51 (m, 1H), 7.44 (s, 1H), 7.29 (dd, $J = 4.2, 1.9$ Hz, 1H), 6.81 (s, 1H), 2.49 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3): δ 134.59, 127.71, 127.31, 126.13, 121.79, 111.33, 108.45, 31.65, 29.69, 21.45. ^{19}F NMR (375 MHz, CDCl_3): δ -62.85. IR DATA:3444.96, 3123.08, 2925.21, 2856.38, $\text{C}\equiv\text{N}$ - 2239.99, 1729.92, 1598.51, 1462.31, 1401.02, 1361.34, 1333.30, 1270.48, 1206.11, 1166.02, 1120.71, 1088.31, 1036.80, 1011.79, 953.19, 866.42, 821.83, 792.18, 723.95, 679.57, 635.08, 589.72, 482.92, 444.46, 403.44.

29. N- cyano-2-(Hydroxymethyl)-6-methyl-1H-indole (4cp): Yield: 70%; sticky white solid; **¹H NMR (500 MHz, CDCl₃):** δ 7.89 (d, *J* = 8.2 Hz, 1H), 7.37 (s, 1H), 7.15 (dd, *J* = 7.5, 6.4 Hz, 1H), 6.25 (d, *J* = 0.5 Hz, 1H), 5.34 (d, *J* = 1.5 Hz, 2H), 2.46 (s, 3H). **¹³C NMR (100 MHz, CDCl₃):** δ 137.38, 132.44, 128.45, 124.73, 120.95, 112.22, 95.71, 66.94, 29.73, 21.60, 14.15. **IR DATA:**3325.24, 2923.22, 2854.75, , **C≡N-** **2241.65**, 1784.62, 1709.99, 1597.33, 1461.70, 1393.50, 1287.30, 1216.50, 1181.52, 1077.34, 1026.48, 967.12, 873.62, 802.77, 747.47, 430.07.

30. N- cyano-2-Butyl-6-chloro-1H-indole (4da): Yield: 82%; liquid, **¹H NMR (500 MHz, CDCl₃):** δ 7.46 (d, *J* = 0.8 Hz, 1H), 7.34 (d, *J* = 8.3 Hz, 1H), 7.19 – 7.16 (m, 1H), 6.26 (d, *J* = 0.9 Hz, 1H), 2.79 – 2.74 (m, 2H), 1.69 (dt, *J* = 15.4, 4.6 Hz, 2H), 1.40 (dt, *J* = 14.9, 7.4 Hz, 2H), 0.91 (t, *J* = 7.4 Hz, 3H). **¹³C NMR (100 MHz, CDCl₃):** δ 155.01, 141.67, 130.22, 127.12, 124.72, 121.72, 111.47, 105.30, 30.09, 29.73, 26.53, 22.20, 13.73. **DEPT- 135 NMR (100 MHz, CDCl₃):** δ 124.16, 123.94, 121.07, 111.06, 103.57, 36.36, 32.38, 26.09, 25.88. **IR DATA:**3448.79, 2960.89, 2929.07, 2858.73, **C≡N-** **2239.52**, 1764.05, 1706.47, 1597.89, 1565.84, 1463.83, 1430.77, 1380.47, 1359.39, 1323.52, 1291.71, 1245.50, 1197.51, 1055.71, 946.24, 852.91, 826.60,776.95, 736.94, 588.18, 483.09, 428.23.

31.N-cyano-2-butyl-5-chloro-1H-indole(4ea):Yield: 85%; sticky white solid;**¹H NMR (500 MHz, CDCl₃):** δ 7.46 (s, 1H), 7.41 (d, *J* = 8.6 Hz, 1H), 7.26 (dd, *J* = 8.4, 1.9 Hz, 1H), 6.29 (s, 1H), 2.82 (t, *J* = 7.7 Hz, 2H), 1.75 (dt, *J* = 15.3, 7.6 Hz, 2H), 1.50 – 1.41 (m, 2H), 0.98 (t, *J* = 7.4 Hz, 3H). **¹³C NMR (100 MHz, CDCl₃):** δ 142.57, 135.18, 129.76, 129.72, 124.34, 120.67, 112.00, 106.44, 105.01, 30.06, 26.59, 22.22, 13.73.**IR DATA:**3421.71, 2959.46, 2931.22, 2867.87, **C≡N-** **2242.89**, 1742.42, 1592.09, 1455.34,1139.78, 1065.14,869.70, 735.65, 693.55, 485.77.

32.N-cyano-5-chloro-2-cyclohexyl-1H-indole(4ee): Yield: 89%; sticky white solid;**¹H NMR (400 MHz, CDCl₃) :** δ 7.48 (d, *J* = 1.8 Hz, 1H), 7.43 (d, *J* = 8.6 Hz, 1H), 7.28 (dd, *J* = 8.6, 2.0 Hz, 1H), 6.27 (s, 1H), 2.81 (td, *J* = 7.8, 4.1 Hz, 1H), 2.21 – 2.08 (m, 3H), 1.92 – 1.83 (m, 3H), 1.46 (dd, *J* = 12.7, 8.5 Hz, 5H), 1.33 – 1.24 (m, 4H). **¹³C NMR (100 MHz, CDCl₃):** δ 147.65,

135.12, 129.71, 124.37, 120.81, 112.04, 106.59, 103.08, 36.44, 32.27, 26.02, 25.80.**IR DATA:**3422.42, 3078.95, 2929.93, 2852.79, **C≡N-2242.50**, 1862.56,1734.98, 1582.86, 1564.08, 1447.78, 1377.15, 1348.34, 1325.10, 1269.54, 1177.76, 1146.87, 1107.82, 1060.64, 931.75, 889.28, 866.22, 842.94, 797.67, 717.14, 659.27, 635.52, 585.53, 489.64, 444.64, 422.40

33. N- Cyano-5-chloro-2-phenyl-1H-indole(4eh): Yield: 91%; sticky white solid;**¹H NMR (500 MHz, CDCl₃):** δ 7.74 – 7.71 (m, 1H), 7.61 (d, *J* = 1.9 Hz, 1H), 7.57 – 7.49 (m, 2H), 7.37 (dd, *J* = 8.6, 2.0 Hz, 1H), 6.72 (s, 1H). **¹³C NMR (100 MHz, CDCl₃):** δ 141.10, 136.48, 130.28, 129.98, 129.80, 129.23, 128.63, 127.67, 125.40, 121.28, 112.62, 106.94, 106.38.**IR DATA:**3449.53, 2924.39, 2855.34, **C≡N-2242.20**, 1730.73, 1583.96, 1449.10, 1356.74, 1303.68, 1163.78, 1062.18, 918.63, 864.07, 792.66, 757.56, 730.42, 689.30, 639.65, 580.95, 480.59, 448.02