Supporting information

for

Iodine mediated intramolecular C2-amidative cyclization of indoles: A facile access to indole fused tetracycles

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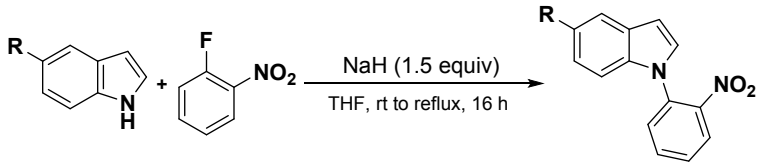
1. General considerations

All reactions were carried out in reaction tubes closed with stoppers and in LR grade solvents. All the solvents used for the reactions were obtained from Fischer Scientific, India Pvt. Ltd. Reactions were monitored by thin-layer chromatography (TLC) using Merck silica gel 60 F_{254} precoated plates (0.25 mm) and visualized by UV fluorescence quenching using appropriate mixture of ethyl acetate and hexanes. Silica gel (particle size: 100-200 mesh) was purchased from Avra synthesis Pvt. Ltd. India and used for column chromatography using hexanes and ethyl acetate mixture as eluent. Cs_2CO_3 was purchased from Sigma-Aldrich Company. Other reagents such as indole, iodine were purchased from Spectrochem India Pvt. Ltd., 2-fluoro nitrobenzene and 2-bromo nitrobenzene were obtained from Avra synthesis Pvt. Ltd. India. Various substituted indoles were obtained from Spectrochem India Pvt. Ltd and Alfa Aesar Company. All the reactions were carried out in temperature controlled IKA magnetic stirrers. ^1H and ^{13}C NMR spectra were recorded on a Bruker 400 instrument. ^1H NMR spectra were reported relative to Me_4Si (δ 0.0 ppm) or residual $CDCl_3$ (δ 7.26 ppm). ^{13}C NMR were reported relative to $CDCl_3$ (δ 77.16 ppm). FTIR spectra were recorded on a Nicolet 6700 spectrometer and were reported in frequency of absorption (cm^{-1}). High resolution mass spectra (HRMS) were recorded on Q-Tof Micro mass spectrometer. Melting points were measured either on a Toshniwal melting point apparatus or on a Kofler-Heizitschmikroskop apparatus. The melting points were uncorrected.

2. Experimental conditions

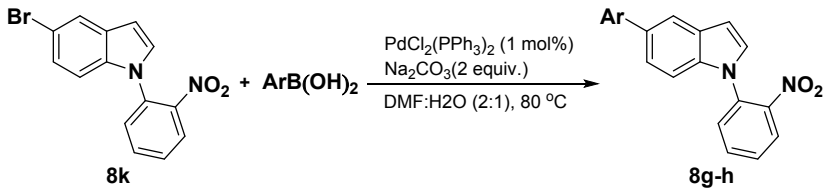
General Procedure for the preparation of compounds 8a-f, 8i and 8k[1]



8a-i

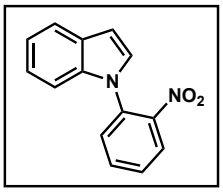
To a well stirred solution of indole (5 mmol) in dry THF maintained in ice bath, NaH (7.5 mmol) was added portion wise and is stirred at room temperature for 0.5 h. This was cooled using ice bath and 1-fluoro-2-nitrobenzene (6.5 mmol) was added slowly. The resulting reaction mixture was warmed to room temperature and was refluxed until the reaction was completed by TLC analysis. THF was removed by using rotary evaporator. Then the crude reaction was washed with water (2×15 mL) and extracted with ethyl acetate. Combined organic layers were dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was purified by column chromatography using hexanes/ethyl acetate as eluent to afford pure compound **8a-i**.

General Procedure for the preparation of compounds 8g and 8h

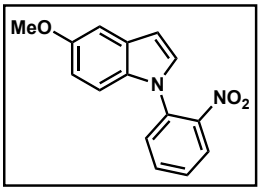


8k (1 mmol) was taken into a clean dry round bottomed flask, and $ArB(OH)_2$ (1.5 mmol), $PdCl_2(PPh_3)_2$ (0.1 mmol), K_2CO_3 (3 mmol) and 4 mL of DMF:H_2O (2:1) were added successively and the resulting reaction mixture was stirred at 80 °C. After the completion of reaction as monitored by TLC, reaction mixture was washed with water (2×15 mL) and extracted with ethyl acetate. Combined organic layers were dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was purified by column chromatography using hexanes/ethyl acetate as eluent to afford pure compound **8g-h**.

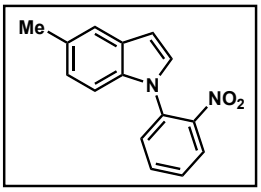
Spectral data for compounds 5a-i and 5k



1-(2-Nitrophenyl)-1*H*-indole (8a): Orange solid, mp 86-87 °C [lit. 85 °C][1]; R_f 0.46 (10% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz, ppm) δ 6.74 (dd, *J*=3.2, 0.8Hz, 1H), 7.12-7.22 (m, 4H), 7.55-7.62 (m, 2H), 7.67-7.71 (m, 1H), 7.74 (dt, *J*=7.8, 1.2Hz, 1H), 8.04 (dd, *J*=8.2,1.2Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 105.2, 109.6, 121.1, 121.5, 123.1, 125.6, 128.1, 128.5, 129.1, 129.9, 133.0, 133.8, 136.8, 146.5; FTIR (KBr) 3057, 1604, 1493, 1455, 1351 cm^{-1}.

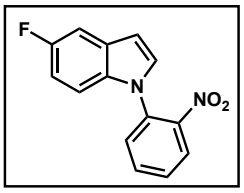


5-Methoxy-1-(2-nitrophenyl)-1*H*-indole (8b): Yellow solid, mp 75-77 °C; R_f 0.51 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.86 (s, 3H), 6.66 (dd, *J*=4, 0.8 Hz, 1H), 6.85 (dd, *J*=12, 2.4Hz, 1H), 7.04 (d, *J*=8.8 Hz, 1H), 7.12-7.15 (m, 2H), 7.52-7.60 (m, 2H), 7.72 (dd, *J*=8, 1.6 Hz, 1H), 8.01 (dd, *J*=8, 1.6Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 56.0, 103.3, 104.9, 110.4, 113.1, 125.6, 128.2, 128.6, 129.6, 129.7, 132.0, 133.1, 133.7, 146.3, 155.1; FTIR (KBr) 3110, 2938, 2834, 1607, 1528, 1492, 1447 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{15}H_{13}N_2O_3$: 269.0926; found: 269.0924.

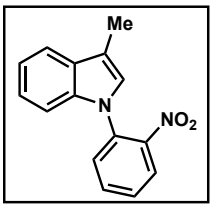


5-Methyl-1-(2-nitrophenyl)-1*H*-indole (8c): Yellow solid, mp 78-80 °C; R_f 0.45 (15% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.46 (s, 3H), 6.66 (d, *J*=7.6 Hz, 1H), 7.04 (s, 2H), 7.47 (s, 1H), 7.53-7.60 (m, 2H), 7.73 (dt, *J*=7.6, 1.6 Hz, 1H), 8.02 (dd, *J*=8, 1.6 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ21.5,

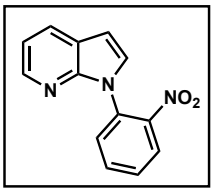
104.8, 109.3, 121.2, 124.7, 125.6, 128.1, 128.2, 129.4, 129.7, 130.4, 133.2, 133.7, 135.2; FTIR (KBr) 3104, 2919, 2863, 1605, 1529, 1495, 1468, 1348 cm^{-1}.



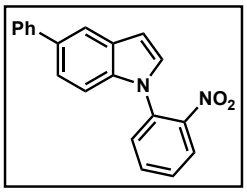
5-Fluoro-1-(2-nitrophenyl)-1*H*-indole (8d): Sticky orange solid, R_f 0.57 (20% ethyl acetate in hexanes); ^1H NMR ($CDCl_3$, 400 MHz) δ 6.69 (d, *J*=3.2 Hz, 1H), 6.94 (dt, *J*=9, 2.4 Hz, 1H), 7.01-7.06 (m, 1H), 7.20 (d, *J*=3.6 Hz, 1H), 7.32 (dd, *J*=9.2, 2.4 Hz, 1H), 7.56-7.62 m, 2H), 7.76 (dt, *J*=7.6, 1.6 Hz, 1H), 8.04 (dd, *J*=8, 1.2 Hz, 1H) ; ^{13}C NMR ($CDCl_3$, 100 MHz) δ 105.0, 105.1, 106.3, 106.5, 110.3, 110.4, 111.3, 111.5, 125.7, 128.8, 129.7, 129.9, 132.8, 133.9, 159.8; ^{19}F NMR (C_6F_6, 500 MHz) δ -126.68; FTIR (KBr) 3108, 1606, 1586, 1529, 1495, 1451, 1350 cm^{-1}.



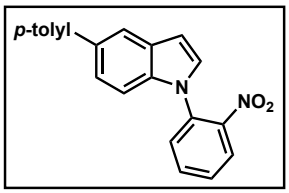
3-Methyl-1-(2-nitrophenyl)-1*H*-indole (8e)[6]: Dark orange sticky solid, R_f 0.45 (10% ethyl acetate in hexanes); ^1H NMR ($CDCl_3$, 400 MHz) δ 2.39 (d, *J*=1.2 Hz, 3H), 6.94 (d, *J*=1.2 Hz, 1H), 7.12-7.15 (m, 1H), 7.19-7.23 (m, 2H), 7.52 (dt, *J*=7.8, 1.6 Hz, 1H), 7.57 (dd, *J*=8, 1.2 Hz, 1H), 7.61-7.65 (m, 1H), 7.71 (dt, *J*=7.6, 1.6 Hz, 1H), 8.01 (dd, *J*=8.2, 1.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 9.7, 109.5, 114.6, 119.6, 120.6, 123.1, 125.4, 125.6, 127.9, 129.6, 129.8, 133.2, 133.6, 136.9, 146.2; FTIR (KBr) 3054, 2919, 2861, 1604, 1529, 1494, 1455, 1350 cm^{-1}.



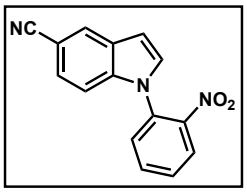
1-(2-Nitrophenyl)-1H-pyrrolo[2,3-*b*]pyridine (8f): Yellow solid, mp 86-88 °C [lit. 159 °C][7]; R_f 0.45 (30% ethyl acetate in hexanes); ^1H NMR ($CDCl_3$, 400 MHz) δ 6.70 (d, *J*=3.6 Hz, 1H), 7.12 (dd, *J*=7.6, 8 Hz, 1H), 7.36 (d, *J*=3.6 Hz, 1H), 7.59 (dd, *J*=8, 1.2 Hz, 1H), 7.52-7.58 (m, 1H), 7.74 (dt, *J*=7.6, 1.6 Hz), 7.96 (dd, *J*=12, 1.6 Hz, 1H), 8.09 (dd, *J*=8.2, 1.2 Hz, 1H), 8.27 (dd, *J*=4.8, 1.6 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 103.3, 115.9, 117.4, 121.2, 125.8, 127.7, 128.2, 129.3, 129.5, 131.7, 133.9, 144.1, 147.9; FTIR (KBr) 3053, 1600, 1423, 1355, 1279, 1156 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{13}H_{10}N_3O_2$: 240.0773; found: 240.0777.



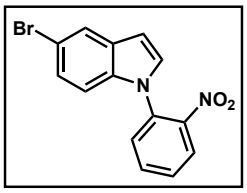
5-Phenyl-1-(2-nitrophenyl)-1*H*-indole (8g): Brown solid, mp 105-107 °C; R_f 0.52 (20% ethyl acetate in hexanes); ^1H NMR ($CDCl_3$, 400 MHz) δ 6.79 (dd, *J*=3.2, 0.8 Hz, 1H), 7.18-7.22 (m, 2H), 7.33 (tt, *J*=7.2, 1.2 Hz, 1H), 7.41-7.49 (m, 3H), 8.06 (dd, *J*=8.2, 1.2 Hz, 1H), 7.57-7.68 (m, 4H), 7.76 (dt, *J*=7.6, 1.2 Hz, 1H), 7.89 (d, *J*=1.6 Hz, 1H), 8.06 (dd, *J*=8.2, 1.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 105.5, 109.9, 120.0, 123.0, 125.7, 126.7, 127.6, 128.5, 128.7, 128.8, 129.6, 129.8, 133.0, 133.8, 134.7, 136.3, 142.2, 146.4; FTIR (KBr) 2918, 1604, 1529, 1462, 1346 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{20}H_{15}N_2O_2$: 315.1134; found: 315.1138.



5-(4-Methyl phenyl)-1-(2-nitrophenyl)-1*H*-indole (8h): Brown solid, mp 108-110 °C; R_f 0.52 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.41 (s, 3H), 6.78 (dd, J=3.4, 0.8 Hz Hz, 1H), 7.17-7.21 (m, 2H), 7.26 (d, J=7.6 Hz, 2H), 7.44 (dd, J=8.4, 1.6 Hz, 1H), 7.54 (d, J=8 Hz, 2H), 7.56-7.65 (m, 2H), 7.76 (dt, J=7.6, 1.2 Hz, 1H), 7.87 (d, J=1.6 Hz, 1H), 8.06 (dd, J=8.2, 1.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.2, 105.5, 109.8, 119.8, 122.9, 125.7, 127.4, 128.5, 128.7, 129.5, 129.6, 129.8, 133.0, 133.9, 134.7, 136.1, 13.6.4, 139.4, 146.3; FTIR (KBr) 2922, 2857, 1605, 1528, 1493, 1465, 1347, 1178 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{21}H_{17}N_2O_2$: 329.1290; found: 329.1215.

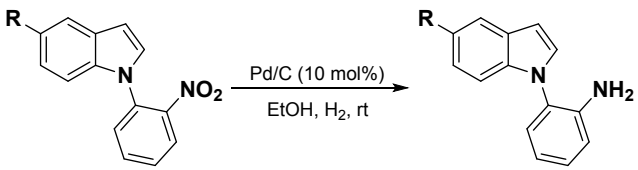


5-Cyano-1-(2-nitrophenyl)-1*H*-indole (8i): Yellow solid, mp 178-180 °C [lit. 186 °C][8]; R_f 0.45 (40% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.80 (dd, *J*=3.2, 0.8 Hz, 1H), 7.14 (d, *J*=8.4 Hz, 1H), 7.29 (d, *J*=3.2 Hz, 1H), 7.43 (d, *J*=8.4, 0.8 Hz, 1H), 7.58 (dd, *J*=8, 2 Hz, 1H), 7.68 (dt, *J*=7.8, 0.8 Hz, 1H), 7.81 (dt, *J*=8, 0.8 Hz, 1H), 8.11 (dd, *J*=8.2, 1.2 Hz, 1H), 8.04 (dd, *J*=1.4, 0.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 104.4, 105.5, 110.6, 120.3, 125.9, 126.0, 126.9, 128.8, 129.8, 130.1, 130.6, 131.8, 134.2, 138.6, 146.5; FTIR (KBr) 2221, 1604, 1529, 1490, 1344 cm^{-1}.



5-Bromo-1-(2-nitrophenyl)-1*H*-indole (8k): Orange solid, mp 148-150 °C; R_f 0.52 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.67 (dd, *J*=3.2, 0.8 Hz, 1H), 6.98 (d, *J*=8.8 Hz, 1H), 7.16 (d, *J*=3.2 Hz, 1H), 7.28 (dd, *J*=8.8, 2 Hz, 1H), 7.57 (dd, *J*=7.8, 1.6 Hz, 1H), 7.61 (dd, *J*=8, 1.6 Hz, 1H), 7.76 (dt, *J*=7.8, 1.6 Hz, 1H), 7.81 (d, *J*=1.6 Hz, 1H), 8.05 (dd, *J*=8.2, 1.6 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 104.6, 111.1, 114.3, 124.0, 125.8, 126.0, 129.0, 129.4, 130.0, 130.8, 132.5, 133.9, 135.7; FTIR (KBr) 3099, 1606, 1528, 1495, 1452, 1349, 1283 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{14}H_{10}N_2O_2Br$: 316.9926; found: 316.9935 (HRMS data for ^{79}Br isotope).

General Procedure for the preparation of compounds 9a-i[1]

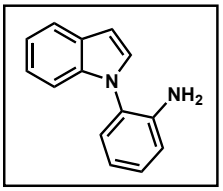


8a-i **9a-i**

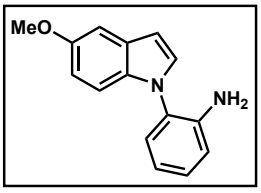
To a solution of compound **8** (4 mmol) in ethanol (8 mL), was added Pd/C (0.4 mmol). The resulting suspension was stirred under hydrogen pressure using hydrogen balloon until the completion of reaction.

The reaction mixture was filtered over celite and rinsed with DCM. The solvents were removed under vacuum and crude product was purified by column chromatography using hexanes/ethyl acetate as eluent to obtain pure product **9**.

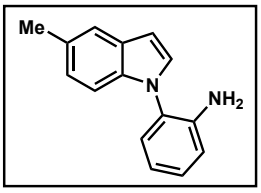
Spectral data for compounds 6a-i



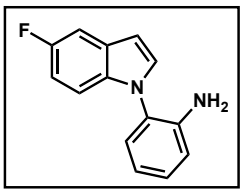
1-(2-Aminophenyl)-1*H*-indole[9] (9a): Orange viscous liquid, R_f 0.50 (10% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.53 (bs, 2H), 6.60 (d, J=3.2 Hz, 1H), 6.75-6.81 (m, 2H), 7.04-7.19 (m, 6H), 7.58-7.62 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 103.4, 110.9, 116.6, 119.0, 120.3, 121.1, 122.4, 125.3, 128.7, 128.8, 129.3, 136.6, 142.8; FTIR (KBr) 3463, 3372, 3050, 1617, 1508, 1460, 1261, 746 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{21}H_{13}N_2$: 209.1079; found: 209.1072.



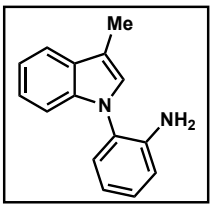
5-Methoxy-1-(2-aminophenyl)-1*H*-indole[9] (9b): White solid, mp 68-70 ^{o}C [lit. 66 ^{o}C][9]; R_f 0.50 (15% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.37 (bs, 2H), 3.78 (s, 3H), 6.52 (d, *J*=2.4 Hz, 1H), 6.74-6.83 (m, 3H), 6.96 (d, *J*=9.2Hz, 1H), 7.05-7.12 (m, 3H), 7.13-7.18 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 56.0, 102.8, 103.1, 111.6, 112.6, 116.7, 119.1, 125.5, 128.7, 129.2, 129.2, 129.3, 131.9, 142.7, 154.7; FTIR (KBr) 3464, 3370, 2995, 2941, 2831, 1617, 1583, 1506, 1472, 1451, 1340 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{15}H_{15}N_2O$: 239.1184; found: 239.1172.



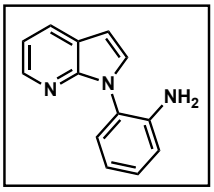
5-Methyl-1-(2-aminophenyl)-1*H*-indole[9] (9c): Brown viscous liquid, R_f 0.43 (10% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.47 (s, 3H), 3.68 (bs, 2H), 6.61 (dd, *J*=3.2, 0.8 Hz, 1H), 6.90 (dt, *J*=7.6, 1.6 Hz, 1H), 6.94 (dd, *J*=8, 1.2 Hz, 1H), 7.01-7.08 (m, 2H), 7.19 (d, *J*=3.2 Hz, 1H), 7.21 (dd, *J*=7.6, 1.6 Hz, 1H), 7.24-7.29 (m, 1H), 7.48 (s, 1H) ; ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.5, 103.0, 110.5, 117.1, 119.5, 120.8, 124.0, 125.9, 128.7, 128.8, 129.0, 129.2, 129.6, 135.0, 142.0; FTIR (KBr) 3464, 3373, 3030, 2919, 2859, 1618, 1508, 1470, 1369, 754 cm^{-1}.



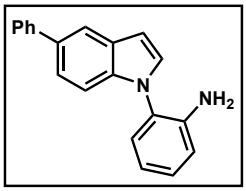
5-Fluoro-1-(2-aminophenyl)-1*H*-indole (9d): Brown viscous liquid, R_f 0.43 (10% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.62 (bs, 2H), 6.66 (dd, *J*=3, 0.8 Hz, 1H), 6.88-6.97 (m, 3H), 7.07 (1:1q, *J*=4.4 Hz, 1H), 7.21 (dd, *J*=7.8, 1.6 Hz, 1H), 7.25-7.31 (m, 2H), 7.34 (dd, *J*=9.6, 2.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 103.4, 105.7, 106.0, 110.6, 110.9, 111.5, 111.6, 117.0, 119.4, 125.3, 128.7, 129.5, 130.3, 133.2, 142.3, 157.2, 159.6; ^{19}F NMR (C_6F_6 , 500 MHz) δ -127.78; FTIR (KBr) 3472, 3380, 3101, 1619, 1584, 1508, 1470, 1370, 1276 cm^{-1}.



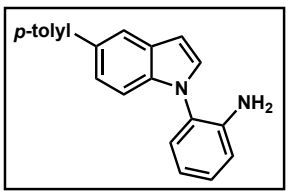
3-Methyl-1-(2-aminophenyl)-1*H*-indole (9e): Pale brown solid, mp 44-46 °C [lit. 43 °C][9]; R_f 0.53 (10% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.29 (d, *J*=1.2 Hz, 3H), 3.41 (bs, 2H), 6.71-6.77 (m, 2H), 6.88 (d, *J*=1.2 Hz, 1H), 7.00-7.14 (m, 5H), 7.52-7.55 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 9.7, 110.7, 112.5, 116.5, 118.8, 119.1, 119.6, 122.3, 125.4, 126.2, 128.7, 129.0, 129.1, 136.8, 142.9; FTIR (KBr) 3468, 3375, 3048, 2922, 2858, 1617, 1506, 1457, 1367, 1262 cm^{-1}.



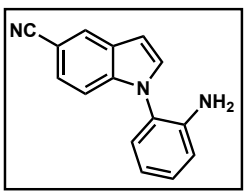
2-(1H-pyrrolo[2,3-*b*]pyridin-1-yl)aniline (9f): White solid, mp 104-106 °C; R_f 0.45 (30% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.74 (bs, 2H), 6.66 (d, *J*=3.6 Hz, 1H), 6.90 (dt, *J*=7.6, 1.6 Hz, 1H), 6.95 (dd, *J*=8, 1.2 Hz, 1H), 7.13 (dd, *J*=7.6 Hz, 1H), 7.18-7.25 (m, 2H), 7.34 (d, *J*=3.6 Hz, 1H), 8.00 (dd, *J*=7.6, 1.6 Hz, 1H), 8.34 (dd, *J*=4.8, 1.6 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 101.9, 116.5, 117.8, 119.5, 121.2, 125.3, 128.4, 129.2, 129.6, 129.7, 142.4, 143.7, 147.7; FTIR (KBr) 3329, 3216, 1624, 1510, 1423, 1319 cm^{-1}.



5-Phenyl-1-(2-aminophenyl)-1*H*-indole (9g): White solid, mp 92-94 °C [lit. 92 °C][9]; R_f 0.43 (15% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.21 (bs, 2H), 6.64 (d, *J*=3.8 Hz, 1H), 6.74-6.81 (m, 2H), 7.08-7.25 (m, 5H), 7.31-7.37 (m, 3H), 7.53-7.58 (m, 2H), 7.81 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 103.8, 111.1, 116.6, 118.9, 119.6, 122.2, 125.0, 126.5, 127.5, 128.7, 128.8, 129.2, 129.4, 129.4, 133.9, 136.0, 142.5, 143.0; FTIR (KBr) 3470, 3378, 3033, 1617, 1507, 1466, 1368, 1228 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{20}H_{17}N_2$: 285.1392; found: 285.1398.



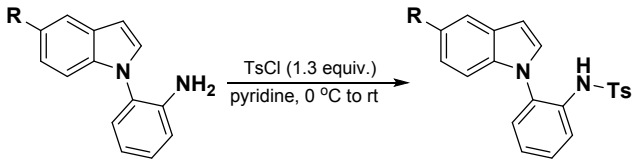
5-(4-Methyl phenyl)-1-(2-aminophenyl)-1*H*-indole (9h): Brown solid, mp 112-114 °C; R_f 0.43 (15% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.41 (s, 3H), 2.82 (bs, 2H), 6.87 -6.95 (m, 2H), 7.19-7.30 (m, 6H), 7.44 (dd, *J*=8.4, 1.6 Hz, 1H), 7.56 (d, *J*=8 Hz, 2H), 7.89 (d, *J*=1.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.2, 103.8, 111.1, 116.8, 119.2, 119.4, 122.2, 125.3, 127.4, 128.7, 129.2, 129.4, 129.5, 133.9, 136.0, 136.2, 139.6, 142.6; FTIR (KBr) 3467, 3376, 3026, 2921, 2855, 1617, 1507, 1467, 1369, 1227 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{21}H_{19}N_2$: 299.1548; found: 299.1551.



5-Cyano-1-(2-aminophenyl)-1*H*-indole (9i): Yellow solid, mp 126-128 °C; R_f 0.45 (30% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.50 (bs, 2H), 6.77 (dd, *J*=4, 0.8 Hz, 1H), 6.86-6.93 (m, 2H), 7.15-7.21 (m, 2H), 7.28-7.33 (m, 1H), 7.35 (d, *J*=3.2 Hz, 1H), 7.40 (dd, *J*=8.4, 0.8 Hz, 1H), 8.03 (d, *J*=0.8 Hz, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz) δ 103.5, 104.2, 111.8, 116.9, 119.2, 120.7, 123.9, 125.3, 126.7, 128.4, 128.5, 130.1, 131.1, 138.2, 142.7; FTIR (KBr) 3464, 3368, 3105, 3060, 2221, 1619, 1507, 1469, 1330 cm^{-1}.

General Procedure for the preparation of compounds 1a-i[2]



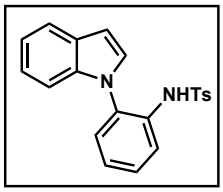
9a-i **1a-i**

To a solution of compound **9** (3.5 mmol) in 3 mL pyridine maintained at 0°C was added *p*-toluenesulfonyl chloride (4.6 mmol) and was stirred at room temperature for 4-5 h. Then the reaction mixture was washed with 10% HCl solution (2×15 mL) and extracted with ethyl acetate. Then the organic layer was washed with water (1×10 mL). Combined organic layers were dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was purified by column chromatography using hexanes/ethyl acetate as eluent to afford pure compound **1**.

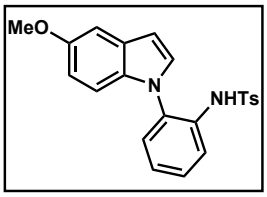
General Procedure for the preparation of compound 1j[3]

To a solution of compound **9a** (3.5 mmol) in 3 mL pyridine maintained at 0°C was added *p*-bromobenzenesulfonyl chloride (4.6 mmol) and was stirred at room temperature for 4-5 h. Then the reaction mixture is washed with 10% HCl solution (2×15 mL) and extracted with ethyl acetate. Then the organic layer was washed with water (1×10 mL). Combined organic layers were dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was purified by column chromatography using hexanes/ethyl acetate as eluent to afford pure compound **1j**.

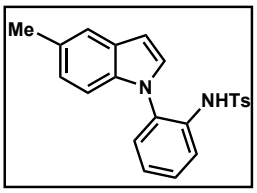
Spectral data for nitro compounds 1a-j



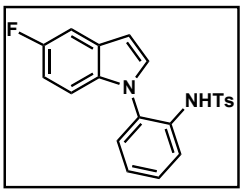
***N*-(2-(1H-indol-1-yl)phenyl)-4-methylbenzenesulfonamide (1a):** Pale brown solid, mp 112-114 °C; R_f 0.46 (15% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.39 (s, 3H), 6.31 (s, 1H), 6.62-6.68 (m, 3H), 7.09 (dt, *J*=7.2, 1.2 Hz, 1H), 7.12 (m, 5H), 7.12-7.22 (m, 3H), 7.88 (dd, *J*=8, 1.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 27.1, 104.7, 109.9, 121.0, 121.4, 121.9, 123.1, 125.6, 127.3, 128.0, 128.7, 128.9, 129.6, 129.8, 129.8, 134.0, 135.8, 136.9, 144.3; FTIR (KBr) 3352, 2923, 2856, 1595, 1505, 1458, 1340, 1162, 747 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{21}H_{19}N_2O_2S$: 363.1167; found: 363.1154.



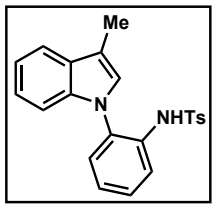
***N*-(2-(5-methoxy-1H-indol-1-yl)phenyl)-4-methylbenzenesulfonamide (1b):** Light brown solid, mp 128-130 ^{o}C; R_f 0.48 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.39 (s, 3H), 3.88 (s, 3H), 6.34 (s, 1H), 6.52 (d, *J*=8.8 Hz), 6.57 (dd, *J*=3.2, 0.8 Hz, 1H), 6.63 (d, *J*=3.2 Hz, 1H), 6.73 (dd, *J*=12, 2.4 Hz, 1H), 7.11-7.22 (m, 5H), 7.39-7.45 (m, 3H), 7.87 (dd, *J*=8, 1.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.7, 56.0, 102.9, 104.4, 110.7, 113.3, 121.7, 125.5, 127.3, 128.6, 128.8, 129.2, 129.5, 129.8, 129.9, 132.1, 133.9, 135.7, 144.3 155.1; FTIR (KBr) 3331, 2929, 2836, 1595, 1503, 1262, 1160 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{22}H_{21}N_2O_3$: 393.1273; found: 393.1273.



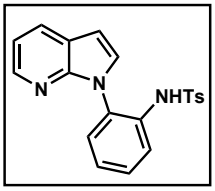
***N*-(2-(5-methyl-1H-indol-1-yl)phenyl)-4-methylbenzenesulfonamide (1c):** Pale brown gum, R_f 0.55 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.39 (s, 3H), 2.47 (s, 3H), 6.35 (s, 1H), 6.54-6.60 (m, 3H), 6.93 (dd, *J*=8.4, 1.6 Hz, 1H), 7.12-7.17 (m, 3H), 7.20 (dt, *J*=7.2, 1.6 Hz, 1H), 7.39-7.47 (m, 4H), 7.85 (dd, *J*=8, 1.2 Hz, 1H) ; ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.5, 21.7, 104.2, 109.6, 121.1, 121.9, 124.7, 125.6, 127.3, 128.1, 128.8, 129.0, 129.4, 129.7, 130.0, 130.0, 133.9, 135.3, 135.8, 144.2; FTIR (KBr) 3333, 3026, 2921, 2861, 1595, 1505, 1467, 1370 cm^{-1}.



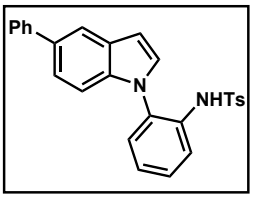
***N*-(2-(5-fluoro-1H-indol-1-yl)phenyl)-4-methylbenzenesulfonamide (1d):** White solid, mp 126-128 ^{o}C; R_f 0.48 (15% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.39 (s, 3H), 6.27 (s, 1H), 6.53 (dd, *J*=9.2, 8.8 Hz, 1H), 6.61 (d, *J*=3 Hz, 1H), 6.71 (d, *J*=3.2 Hz, 1H), 6.81 (dt, *J*=8, 2.4 Hz, 1H), 7.12-7.18 (m, 3H), 7.22 (dt, *J*=7.4, 1.2 Hz, 1H), 7.31 (dd, *J*=9.2, 2.4 Hz, 1H), 7.42 (d, *J*=8.4 Hz, 2H), 7.44-7.48 (m, 1H), 7.81 (dd, *J*=8.4, 1.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.7, 104.6, 104.7, 106.1, 106.4, 110.7, 110.8, 111.3, 111.6, 122.0, 125.6, 127.3, 128.9, 129.6, 129.8, 129.8, 134.0, 135.8, 144.4; ^{19}F NMR (C_6F_6, 500 MHz) δ -126.71; FTIR (KBr) 3337, 3066, 2924, 2859, 1593, 1503, 1468, 1357 cm^{-1}.



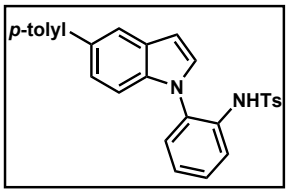
4-Methyl-*N*-(2-(3-methyl-1H-indol-1-yl)phenyl)benzenesulfonamide (1e): White solid, mp 136-138 ^{o}C; R_f 0.42 (15% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.32 (d, *J*=1.2 Hz, 1H), 2.41 (s, 3H), 6.31 (d, *J*=1.2 Hz, 1H), 6.35 (s, 1H), 7.07-7.12 (m, 1H), 7.13-7.23 (m, 5H), 7.38-7.45 (m, 3H), 7.61 (td, *J*=7.6, 0.4 Hz, 1H), 7.87 (dd, *J*=8, 1.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 9.7, 21.7, 109.7, 113.9, 119.5, 120.3, 122.2, 123.0, 125.6, 127.3, 128.8, 129.2, 129.3, 129.7, 130.1, 133.9, 135.9, 137.2, 144.2; FTIR (KBr) 3328, 3049, 2922, 2867, 1596, 1503, 1455, 1341, 1164, 745 cm^{-1}.



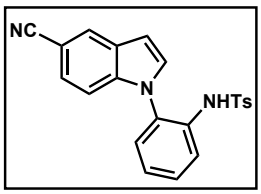
N-(2-(1H-pyrrolo[2,3-*b*]pyridin-1-yl)phenyl)-4-methylbenzenesulfonamide (1f): Pale brown solid, mp 80-82 °C; R_f 0.48 (30% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 2.23 (s, 3H), 6.39 (s, 1H), 6.62 (s, 1H), 6.81 (d, *J*=6.5 Hz, 2H), 6.90 (d, *J*=7 Hz, 2H), 7.05 (d, *J*=6.5 Hz, 1H), 7.14 (s, 1H), 7.25 (s, 1H), 7.35 (s, 1H), 7.69 (d, *J*=6.5 Hz, 1H), 7.93 (d, *J*=6 Hz, 1H), 8.31 (s, 1H), 9.20 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 21.5, 102.9, 117.0, 121.9, 126.2, 127.9, 128.4, 129.2, 129.3, 130.1, 130.6, 131.6, 134.0, 137.0, 142.9, 143.3, 146.6; FTIR (KBr) 3058, 2924, 2863, 1592, 1510, 1423, 1333, 1270 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{20}H_{18}N_3O_2S$: 364.1120; found: 364.1106.



4-Methyl-N-(2-(5-phenyl-1H-indol-1-yl)phenyl)benzenesulfonamide (1g): Pale brown solid, mp 150-152 °C; R_f 0.55 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.29 (s, 3H), 6.27 (s, 1H), 6.57-6.62 (m, 2H), 6.65 (d, *J*=8.4 Hz, 1H), 7.06 (d, *J*=8 Hz, 2H), 7.09-7.18 (m, 2H), 7.22-7.29 (m, 2H); 7.32-7.42 (m, 5H), 7.56 (d, *J*=8 Hz, 2H), 7.77-7.84 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.7, 105.1, 110.1, 119.1, 122.1, 122.9, 125.6, 126.8, 127.3, 127.5, 128.7, 128.9, 129.3, 129.7, 129.8, 129.8, 133.9, 134.7, 135.8, 136.4, 142.2, 144.3; FTIR (KBr) 3333, 3056, 2923, 2852, 1596, 1504, 1464, 1402, 1337 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{27}H_{23}N_2O_2S$: 439.1480; found: 439.1467.

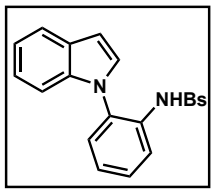


4-methyl-N-(2-(5-(p-tolyl)-1H-indol-1-yl)phenyl)benzenesulfonamide (1h): Pale brown solid, mp 194-196 °C; R_f 0.52 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.39 (s, 3H), 2.42 (s, 3H), 6.39 (s, 1H), 6.66-6.70 (m, 2H), 6.72 (d, *J*=8.4 Hz, 1H), 7.15 (d, *J*=8 Hz, 2H), 7.18-7.25 (m, 2H), 7.28 (d, *J*=7.6 Hz, 2H), 7.32 (dd, *J*=8.4, 1.2 Hz, 1H), 7.43-7.46 (m, 3H), 7.55 (td, *J*=8.4, 2 Hz, 2H), 7.86 (dd, *J*=1.6, 0.4 Hz, 1H), 7.89 (dd, *J*=8.2, 1.2, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.2, 21.7, 105.0, 110.1, 119.7, 122.0, 122.8, 125.6, 127.3, 127.4, 128.6, 128.9, 129.2, 129.6, 129.6, 129.8, 129.8, 133.9, 134.6, 135.8, 136.3, 136.4, 139.3, 144.3; FTIR (KBr) 3361, 2923, 2858, 1598, 1502, 1468, 1335, 1242 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{28}H_{25}N_2O_2S$: 453.1637; found: 453.1628.



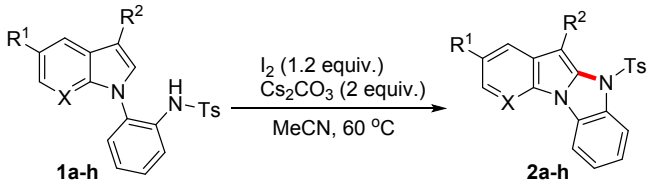
N-(2-(5-cyano-1H-indol-1-yl)phenyl)-4-methylbenzenesulfonamide (1i): White solid, mp 144-146 °C ; R_f 0.40 (40% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.40 (s, 3H), 6.20 (s, 1H), 6.67 (d, *J*=8.4 Hz, 1H), 6.74 (d, J=3.4 Hz, 1H), 6.84 (d, *J*=3.2 Hz, 1H), 7.12-7.19 (m, 3H), 7.42 (d, *J*=8.4 Hz, 2H), 7.49 (dt, *J*=8.2, 1.6 Hz, 1H), 7.86 (dd, *J*=8.4, 1.2 Hz, 1H), 8.01 (d, *J*=0.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.7, 104.3, 105.3, 111.0,120.3, 122.6, 125.9, 125.9, 126.9, 127.2, 128.4, 128.8,

129.8, 129.8, 130.4, 130.5, 133.9, 135.9, 138.6, 144.6; FTIR (KBr) 3397, 2925, 2857, 2221, 1597, 1500, 1467, 1357 cm^{-1}.



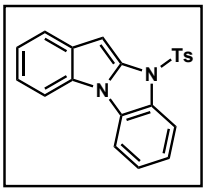
***N*-(2-(1H-indol-1-yl)phenyl)-4-bromobenzenesulfonamide (1j):** Pale brown solid, mp 126-128 °C; R_f 0.45 (15% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.27 (s, 1H), 6.52 (d, *J*=8.4 Hz, 1H), 6.60 (dd, *J*=11.2, 3.2 Hz, 2H), 7.04 (t, *J*=8 Hz, 1H), 7.08-7.15 (m, 2H), 7.16-7.24 (m, 3H), 7.31-7.42 (m, 3H), 7.60 (d, *J*=8 Hz, 1H), 7.79 (d, *J*=8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 105.0, 109.6, 121.1, 121.5, 122.8, 123.4, 126.3, 127.7, 128.5, 128.6, 128.6, 129.0, 129.7, 130.4, 132.4, 133.3, 136.8, 137.6; FTIR (KBr) 3326, 3061, 1595, 1577, 1506, 1459, 1398, 1343 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{20}H_{16}N_2O_2SBr$: 427.0116; found: 427.0113 (HRMS data for ^{79}Br isotope).

General procedure for iodine mediated intramolecular C2 amidative cyclization of compounds 1a-j



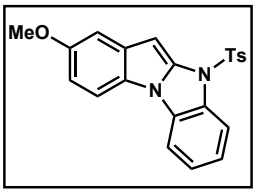
1 (0.5 mmol) was taken in a clean, dry reaction tube. To this iodine (0.3 mmol), Cs_2CO_3 (1.0 mmol) and acetonotrile (2 mL) were added. Reaction tube was stoppered and the resulting reaction mixture was stirred at 60 °C. After 4 h the second portion of iodine (0.3 mmol) was added and reaction was allowed to stir at 60 °C. Upon completion of reaction was monitored by TLC, then the solvent was removed under vacuum in rotary evaporator and DCM was added. The crude reaction mixture was washed with $Na_2S_2O_3$ solution (2 × 10 mL) and extracted with DCM. The organic layer was washed water (1 × 10 mL). Combined organic layers were concentrated using rotary evaporator and residue was purified by column chromatography on silica gel using hexanes/ethyl acetate as the eluent to afford pure product **2**.

Spectral data of compounds 2a-j

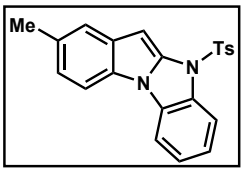


10-Tosyl-10H-benzo[4,5]imidazo[1,2-*a*]indole (2a): White solid, mp 148-150 °C; R_f 0.50 (15% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.28 (s, 3H), 6.57 (d, *J*=0.4 Hz, 1H), 7.22 (m, 3H), 7.33 (dt, J=8, 1.2 Hz, 1H), 7.59 (dd, *J*=1., 0.4 Hz, 1H), 7.68-7.72 (m, 2H), 7.79 (d, J=8.4 Hz, 2H), 8.04 (dd, J=8, 0.4 Hz, 1H) ; ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.7, 82.1, 110.5, 110.7, 115.1, 120.7, 121.2, 121.7, 123.1, 125.1, 127.0, 127.1,

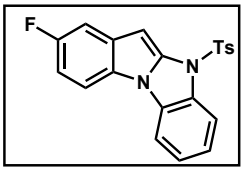
129.8, 130.0, 132.5, 133.6, 138.9, 145.7; FTIR (KBr) 2922, 2856, 1578, 1492, 1377, 1177, 1019cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{21}H_{17}N_2O_2S$: 361.1011; found: 361.0999.



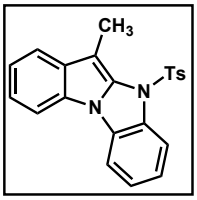
2-Methoxy-10-tosyl-10H-benzo[4,5]imidazo[1,2-*a*]indole (2b): Pale brown solid, mp 142-144 ^oC; R_f 0.51 (20% ethyl acetate in hexanes); ^1H NMR ($CDCl_3$, 400 MHz) δ 2.28 (s, 3H), 3.89 (s, 3H), 6.49 (s, 1H), 6.87 (dd, *J*=8.8 Hz, 1H), 7.13 (d, *J*=8 Hz, 2H), 7.17 (d, *J*=2.4 Hz, 1H), 7.22 (dt, *J*=8, 1.2 Hz, 1H), 7.31 (dt, *J*=7.6, 1.2 Hz, 1H), 7.52 (d, *J*=8 Hz, 1H), 7.56 (d, *J*=8.8 Hz, 1H), 7.79 (d, *J*=8.4 Hz, 2H), 8.02 (dd, *J*=8, 0.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.7, 56.0, 103.7, 110.0, 110.1, 111.3, 115.0, 122.1, 122.7, 125.1, 127.1, 128.3, 130.0, 133.3, 133.4, 133.7, 139.4, 145.7, 155.5; FTIR (KBr) 3065, 2924, 2854, 1598, 1577, 1490 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{22}H_{19}N_2O_3S$: 391.1116; found: 391.1102.



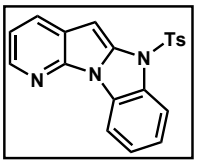
2-Methyl-10-tosyl-10H-benzo[4,5]imidazo[1,2-*a*]indole (2c): White solid, mp 155-158 ^oC; R_f 0.52 (15% ethyl acetate in hexanes); ^1H NMR ($CDCl_3$, 400 MHz) δ 2.27 (s, 3H), 2.49 (s, 3H), 6.48 (s, 1H), 7.06 (dd, *J*=8.4, 1.2 Hz, 1H), 7.12 (d, *J*=8 Hz, 2H), 7.22 (dt, *J*=8, 1.2 Hz, 1H), 7.31 (dt, *J*=7.8, 1.2 Hz, 1H), 7.49 (s, 1H), 7.53-7.58 (m, 2H), 7.78 (d, *J*=8.4 Hz, 2H), 8.02 (d, *J*=8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.7, 21.8, 81.7, 110.3, 115.1, 121.0, 122.1, 122.8, 125.1, 125.3, 127.1, 128.3, 129.9, 129.9, 131.2, 132.8, 133.5, 133.6, 139.0, 145.6; FTIR (KBr) 3061, 2923, 2858, 1600, 1575, 1495, 1457, 1377cm^{-1}.



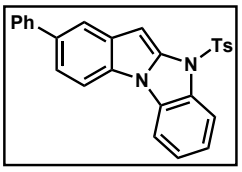
2-Fluoro-10-tosyl-10H-benzo[4,5]imidazo[1,2-*a*]indole (2d): Pale yellow solid, mp 162-165 ^oC; R_f 0.50 (15% ethyl acetate in hexanes); ^1H NMR ($CDCl_3$, 400 MHz) δ 2.29 (s, 3H), 6.53 (s, 1H), 6.97 (dt, *J*=9.2, 2.4 Hz, 1H), 7.15 (q, *J*=8.8 Hz, 3H), 7.31-7.37 (m, 2H), 7.56 (d, *J*=7.8 Hz, 1H), 7.59 (dd, *J*=8.8, 8.4 Hz, 1H), 7.80 (d, *J*=8.4 Hz, 2H), 8.04 (d, *J*=8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.7, 82.1, 106.4, 106.6, 108.5, 108.8, 110.2, 111.2, 111.3, 115.1, 123.2, 125.1, 127.1, 127.8, 128.3, 129.5, 130.0, 133.3, 145.9; ^{19}F NMR (C_6F_6, 500 MHz) δ -124.47; FTIR (KBr) 2923, 2855, 1568, 1489, 1466, 1458 cm^{-1}.



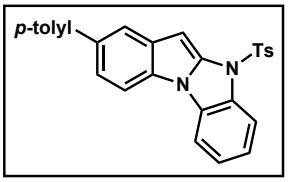
11-Methyl-10-tosyl-10H-benzo[4,5]imidazo[1,2-*a*]indole (2e): White solid, mp 158-160 ^oC; R_f 0.45 (10% ethyl acetate in hexanes); ^1H NMR ($CDCl_3$, 400 MHz) δ 2.14 (s, 3H), 2.60 (s, 3H), 6.93 (d, *J*=8 Hz, 2H), 7.10 (dt, *J*=8, 1.2 Hz, 1H), 7.16-7.24 (m, 3H), 7.35-7.42 (m, 3H), 7.49-7.55 (m, 1H), 7.57-7.62 (m, 1H), 8.01 (dd, *J*=8, 0.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 9.3, 21.6, 94.8, 109.8, 110.4, 117.6, 119.6, 121.1, 121.4, 122.5, 125.9, 126.8, 127.3, 129.7, 130.6, 133.6, 135.0, 145.1; FTIR (KBr) 3057, 2923, 2859, 1603, 1499, 1365, 1242, 1176 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{22}H_{19}N_2O_2S$: 375.1167; found: 375.1176.



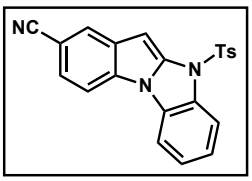
6-Tosyl-6H-benzo[4',5']imidazo[1',2':1,5]pyrrolo[2,3-*b*]pyridine (2f): White solid, mp 140-142 °C; R_f 0.48 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 2.29 (s, 3H), 6.51 (s, 1H), 7.15 (d, *J*=8 Hz, 2H), 7.21 (dd, *J*=8 Hz, 1H), 7.29 (dt, *J*=8, 1.5 Hz, 1H), 7.36 (dt, *J*=5, 1 Hz, 1H), 7.79 (d, *J*=8.5 Hz, 2H), 7.98 (dd, *J*=8, 1.5 Hz, 1H), 8.02 (d, *J*=7.5 Hz, 1H), 8.12 (d, *J*=8 Hz, 1H), 8.32 (dd, *J*=4.5, 1.5 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 21.7, 112.8, 114.8, 117.7, 124.0, 125.5, 127.1, 128.6, 128.8, 130.0, 133.4, 133.5, 139.0, 140.9, 146.0; FTIR (KBr) 3060, 2923, 2851, 1599, 1553, 1496, 1428 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{20}H_{16}N_3O_2S$: 362.0963; found: 362.0975.



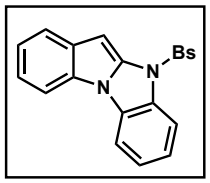
2-Phenyl-10-tosyl-10H-benzo[4,5]imidazo[1,2-*a*]indole (2g): White solid, mp 173-175 °C; R_f 0.41 (15% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.19, (s, 3H), 6.52 (s, 1H), 7.05 (d, *J*=8 Hz, 2H), 7.14-7.19 (m, 1H), 7.22-7.28 (m, 2H), 7.35-7.41 (m, 3H), 7.51 (d, *J*=8 Hz, 1H), 7.56-7.60 (m, 2H), 7.64 (d, *J*=8.4 Hz, 1H), 7.72 (d, *J*=8.4 Hz, 2H), 7.81 (d, *J*=1.2 Hz, 1H), 7.96 (d, *J*=8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.7, 110.5, 110.9, 115.1, 119.7, 120.4, 123.1, 125.2, 126.4, 126.8, 127.1, 127.6, 128.9, 129.7, 130.0, 133.1, 133.6, 135.3, 139.4, 142.3; FTIR (KBr) 3059, 2923, 2856, 1602, 1574, 1489, 1468 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{27}H_{21}N_2O_2S$: 437.1324; found: 437.1340.



2-(*p*-Tolyl)-10-tosyl-10H-benzo[4,5]imidazo[1,2-*a*]indole (2h): Light brown solid, mp 165-167 °C; R_f 0.43 (15% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.19 (s, 3H), 2.33 (s, 3H), 6.51 (s, 1H), 7.05 (d, *J*=8.4 Hz, 2H), 7.15-7.21 (m, 3H), 7.24 (dt, *J*=7.6, 1.2 Hz, 1H), 7.37 (dd, *J*=8.4, 2.0 Hz, 1H), 7.45-7.55 (m, 3H), 7.63 (d, *J*=8.4 Hz, 1H), 7.71 (d, *J*=8.4 Hz, 2H), 7.79 (d, *J*=1.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.2, 21.7, 82.3, 110.5, 110.8, 115.1, 119.5, 120.3, 123.1, 125.2, 126.3, 127.1, 127.4, 129.6, 129.7, 130.0, 133.0, 133.5, 133.5, 135.2, 136.5, 139.3, 145.7; FTIR (KBr) 3029, 2921, 2856, 1602, 1575, 1490, 1458, 1375, 1317 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{28}H_{23}N_2O_2S$: 451.1480; found: 451.1461.



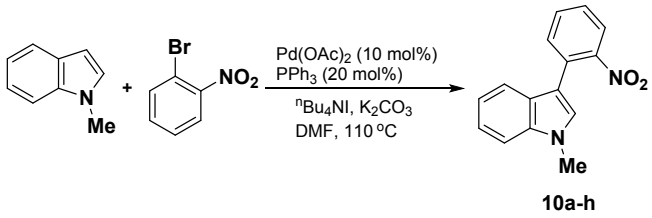
10-Tosyl-10H-benzo[4,5]imidazo[1,2-*a*]indole-2-carbonitrile (2i): Pale brown solid, mp 220-222 °C; R_f 0.50 (50% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.30 (s, 3H), 6.61 (s, 1H), 7.17 (d, *J*=8.4 Hz, 2H), 7.31-7.40 (m, 2H), 7.47 (dd, *J*=8.2, 1.2 Hz, 1H), 7.61-7.65 (m, 1H), 7.74 (d, *J*=8.4 Hz, 1H), 7.80 (d, *J*=8.4 Hz, 2H), 8.01 (d, *J*=1.2 Hz, 1H), 8.04-8.09 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.7, 82.1, 104.9, 111.1, 111.4, 115.2, 120.4, 123.6, 124.4, 125.3, 126.0, 127.1, 128.2, 128.7, 130.1, 132.2, 133.4, 133.6, 140.4, 146.2; FTIR (KBr) 2922, 2854, 2221, 1603, 1566, 1490, 1375 cm^{-1}.



10-((4-Bromophenyl)sulfonyl)-10H-benzo[4,5]imidazo[1,2-*a*]indole (2j): Pale green solid, mp 148-150 ^{o}C; R_f 0.46 (10% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.48 (s, 1H), 7.15-7.21 (m, 3H), 7.26 (dt, *J*=8, 0.8 Hz, 1H), 7.39 (d, *J*=8.8 Hz, 2H), 7.52 (d, *J*=8 Hz), 7.60-7.64 (m, 2H), 7.66 (d, *J*=8.8 Hz, 2H), 7.93 (d, *J*=8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.7, 82.1, 110.5, 110.7, 115.1, 120.7, 121.2, 121.7, 123.1, 125.1, 127.0, 127.1, 129.8, 130.0, 132.5, 133.6, 138.9, 145.7; FTIR (KBr) 3062, 1605, 1572, 1494, 1457, 1385 cm^{-1}; HRMS (m/z): $[M+H]^+$ calcd. for $C_{20}H_{14}N_2O_2SBr$: 424.9959; found:424.9980 (HRMS data for ^{79}Br isotope).

3. General procedure for the preparation of compounds 3a-h

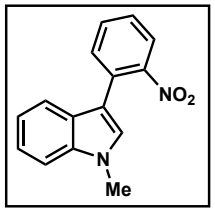
General procedure for the preparation of compounds 10a-h[4]



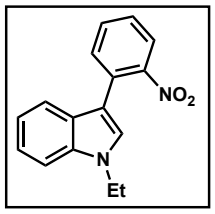
10a-h

N-alkylated indole (4 mmol), $Pd(OAc)_2$ (0.4 mmol), PPh_3 (0.3mmol), K_2CO_3 (12 mmol) and TBAB (0.8 mmol) were taken into an oven dried 50 mL round bottom flask. The flask was closed with septum, evacuated and back filled with N_2. To this dry DMF, 2-bromo-1-nitrobenzene was added under inert atmosphere at room temperature. The resulting reaction mixture was heated at 115 ^{o}C under N_2 atmosphere. After the completion of reaction, the reaction mixture was washed with water (2×15 mL) and extracted with ethyl acetate. Combined organic layers were dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was purified by column chromatography using hexanes/ethyl acetate as eluent to afford pure compound **10a-h**.

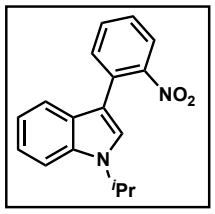
Spectral data for 3-aryl nitro compounds 10a-h



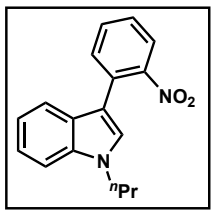
1-Methyl-3-(2-nitrophenyl)-1H-indole (10a): Yellow solid, mp 106-108 ^{o}C; R_f 0.43 (15% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.43 (s, 3H), 6.39 (s, 1H), 7.04 (dt, *J*=7.6, 0.8 Hz, 1H), 7.16 (t, *J*=7.2 Hz, 1H), 7.24 (d, *J*=8 Hz, 1H), 7.39 (d, *J*=7.6 Hz, 1H), 7.45 (dt, *J*=7.4, 1.2 Hz, 1H), 7.52 (d, *J*=8 Hz, 2H), 7.90 (d, *J*=8Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 30.7, 102.5, 109.6, 119.0, 120.0, 120.9, 122.3, 124.3, 126.9, 129.7, 132.7, 133.6, 135.8, 137.9, 149.8; FTIR (KBr) 3057, 2926, 2856, 1611, 1527, 1466, 1435, 1348 cm^{-1}.



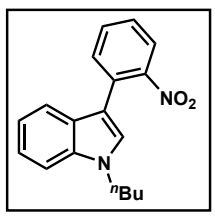
1-Ethyl-3-(2-nitrophenyl)-1H-indole (10b): Yellow solid, R_f 0.46 (15% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.43 (t, *J*=7.2 Hz, 3H), 4.13 (q, *J*=7.2 Hz, 2H), 7.03-7.10 (m, 1H), 7.16-7.22 (m, 2H), 7.29-7.34 (m, 2H), 7.44 (d, *J*=8 Hz, 1H), 7.51 (dt, *J*=7.6, 1.2 HZ, 1H), 7.58 (dd, *J*=7.8, 1.2 Hz, 1H), 7.72 (dd, *J*=8, 1.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 15.5, 41.3, 109.9, 111.0, 119.2, 120.0, 122.4, 124.1, 126.5, 126.9, 129.4, 129.7, 131.9, 132.6, 136.1; FTIR (KBr) 3057, 2928, 2878, 1609, 1525, 1464, 1352 cm^{-1}.



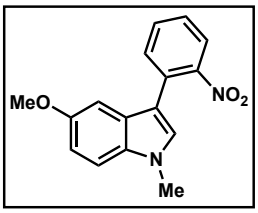
1-Isopropyl-3-(2-nitrophenyl)-1H-indole (10c): Yellow semi solid; R_f 0.43 (15% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.58 (d, *J*=6.8 Hz, 6H), 4.72 (septet, *J*=6.8 Hz, 1H), 7.15 (dt, *J*=7.8, 1.2 Hz, 1H), 7.27 (dt, *J*=7.4, 1.2 Hz, 1H), 7.39 (s, 1H), 7.40-7.46 (m, 2H), 7.53 (td, *J*=7.6, 1.2 Hz, 1H), 7.60 (dt, *J*=7.6, 1.2 Hz, 1H), 7.67 (dd, *J*=7.6, 1.2 Hz, 1H), 7.81 (dd, *J*=12.2, 1.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 22.9, 47.5, 110.1, 111.0, 119.2, 120.4, 122.2, 123.3, 124.2, 126.8, 126.9, 129.6, 132.0, 132.6, 135.9, 149.8; FTIR (KBr) 3050, 2973, 2927, 1608, 1523, 1461, 1403, 1361 cm^{-1}.



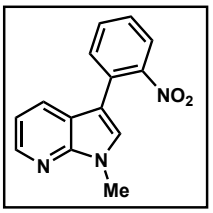
3-(2-nitrophenyl)-1-propyl-1H-indole (10d): Orange semi solid; R_f 0.45 (15% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 0.88 (t, *J*=7.2 Hz, 3H), 1.83 (sextet, *J*=7.2 Hz, 2H), 4.05 (t, *J*=7.2 Hz, 2H), 7.07 (dt, *J*=7.4, 1.2 Hz, 1H), 7.16-7.21 (m, 2H), 7.29-7.35 (m, 2H), 7.45 (d, *J*=8.0 Hz, 1H), 7.52 (dt, *J*=8.0, 1.2 Hz, 1H), 7.59 (dd, *J*=7.8, 1.2 Hz, 1H), 7.73 (dd, *J*=8.4, 1.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 11.6, 23.5, 48.4, 110.1, 110.7, 119.2, 120.3, 122.3, 124.1, 126.9, 127.3, 129.3, 131.9, 132.5, 133.6, 136.3, 149.9; FTIR (KBr) 3058, 2965, 2931, 2877, 1608, 1527, 1465, 1353 cm^{-1}.



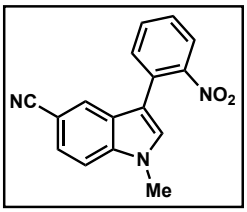
1-butyl-3-(2-nitrophenyl)-1H-indole (10e): Orange semi solid, R_f 0.46 (15% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 0.96 (t, *J*=7.6 Hz, 3H), 1.38 (sextet, *J*=7.2 Hz, 2H), 1.86 (quintet, *J*=7.2 Hz, 2H), 4.16 (t, *J*=7.2 Hz, 2H), 7.15 (t, *J*=8.0 Hz, 1H), 7.24-7.29 (m, 2H), 7.38-7.43 (m, 2H), 7.53 (d, *J*=8.0 Hz, 1H), 7.60 (dt, *J*=7.6, 1.2 Hz, 1H), 7.67 (dd, *J*=7.8, 1.2 Hz, 1H), 7.81 (dd, *J*=8.0, 1.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 13.8, 20.3, 32.3, 46.5, 110.1, 110.7, 119.2, 120.4, 122.3, 124.1, 126.9, 127.3, 128.0, 129.3, 132.0, 132.5, 136.3, 149.9; FTIR (KBr) 3058, 2958, 2869, 1609, 1527, 1465, 1357 cm^{-1}.



5-Methoxy-1-methyl-3-(2-nitrophenyl)-1H-indole (10f): Yellow solid, R_f 0.43 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.69 (s, 3H), 3.71 (s, 3H), 6.81-6.86 (m, 2H), 7.07 (s, 1H), 7.15(d, *J*=9.6 Hz, 1H), 7.30 (dt, *J*=7.2, 1.6 Hz, 1H), 7.43-7.53 (m, 2H), 7.71 (dd, J=8, 1.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 33.2, 55.1, 100.8, 110.7, 112.9, 124.1, 124.9, 126.8, 128.5, 129.2, 131.0, 132.0, 132.4, 133.5, 149.8, 155.0; FTIR (KBr) 3067, 2928, 2857, 1612, 1572, 1525, 1489, 1457, 1428, 1350, 1261 cm^{-1}.

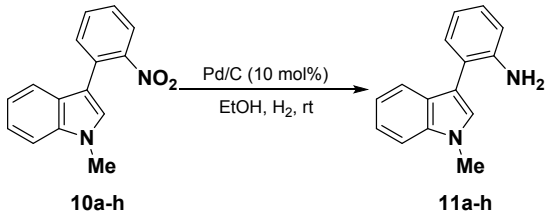


1-Methyl-3-(2-nitrophenyl)-1H-pyrrolo[2,3-*b*]pyridine (10g): Yellow solid, R_f 0.43 (30% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 4.02 (s, 3H), 7.15 (dd, *J*=8.0, 7.6 Hz, 1H), 7.38 (s, 1H), 7.47-7.50 (m, 1H), 7.55-759 (m, 1H), 7.61-7.64 (m, 1H), 7.83-7.89 (m, 2H), 8.40 (dd, *J*=4.8, 1.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 32.0, 110.1, 116.5, 119.8, 124.4, 125.8, 127.7, 127.8, 128.2, 128.4, 132.3, 132.5, 143.0, 149.8; FTIR (KBr) 3061, 2924, 2857, 1607, 1525, 1453, 1407, 1351 cm^{-1}.



1-Methyl-3-(2-nitrophenyl)-1H-indole-5-carbonitrile (10h): Yellow solid, mp 144-146 ^{o}C; R_f 0.45 (30% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.88 (s, 3H), 7.31 (s, 1H), 7.42(d, *J*=8.8 Hz, 1H), 7.48-7.52 (m, 2H), 7.57 (dd, *J*=7.8, 1.6 Hz, 1H), 7.65 (dd, *J*=7.4, 1.6 Hz, 1H), 7.84, (d, *J*=1.4 Hz, 1H), 7.86 (dd, *J*=8, 1.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 33.4, 103.7, 110.8, 112.1, 120.5, 124.3, 124.9, 125.4, 126.9, 128.1, 130.2, 130.6, 132.4, 132.6, 133.6, 138.4; FTIR (KBr) 2925, 2859, 2220, 1613, 1526, 1484, 1351 cm^{-1}.

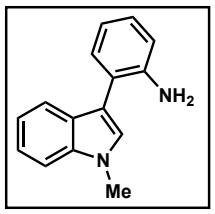
General procedure for the preparation of compounds 11a-h



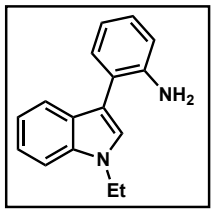
10a-h **11a-h**

To a solution of compound **10** (3 mmol) in ethanol (6 mL), was added Pd/C (0.3 mmol). The resulting suspension was stirred under hydrogen pressure using hydrogen balloon until the completion of reaction. The reaction mixture was filtered over celite and rinsed with DCM. The solvent was removed under vacuum and crude product was purified by column chromatography using hexanes/ethyl acetate as eluent to obtain pure product **11**.

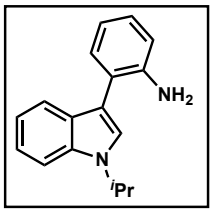
Spectral data for 3-aryl amino compounds 11a-h



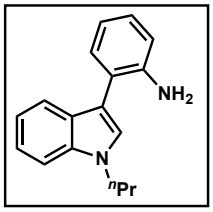
2-(1-Methyl-1H-indol-3-yl)aniline (11a): Brown solid, mp 138-140 ^{o}C; R_f 0.46 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.91 (s, 3H), 3.71 (bs, 2H), 6.87-6.98 (m, 2H), 7.22-7.32 (m, 3H), 7.34-7.44 (m, 2H), 7.48 (d, *J*=8 Hz, 1H), 7.74 (td, *J*=8, 0.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 32.9, 109.5, 113.3, 115.4, 118.4, 119.6, 120.5, 120.7, 122.1, 127.0, 127.7, 127.8, 131.3, 137.1, 144.7; FTIR (KBr) 3458, 3370, 3048, 2931, 2821, 1612, 1547, 1482, 1375, 746 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{15}H_{15}N_2$: 223.1235; found: 223.1240.



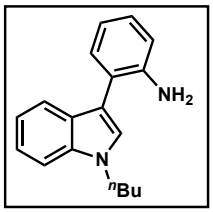
2-(1-Ethyl-1H-indol-3-yl)aniline (11b): Brown sticky solid, R_f 0.50 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.44 (t, *J*=7.2 Hz, 3H), 3.08(bs, 2H), 4.15 (q, *J*=7.2 Hz, 2H), 6.76 (t, *J*=7.6 Hz, 2H), 7.07 (q, *J*=8 Hz, 2H), 7.18 (s, 2H), 7.23 (d, *J*=7.6 Hz, 1H), 7.33 (d, *J*=8.4 Hz, 1H), 7.55 (d, *J*=8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 15.6, 41.2, 109.6, 113.4, 115.7, 118.7, 119.7, 120.7, 121.1, 122.0, 126.0, 127.2, 127.9, 131.4, 136.3, 144.4; FTIR (KBr) 3459, 3371, 3050, 2975, 2931, 2880, 1612, 1546, 1458, 1365 cm^{-1}.



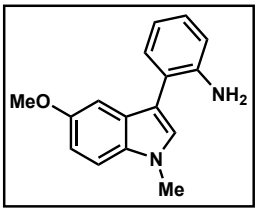
2-(1-Isopropyl-1H-indol-3-yl)aniline (11c): Colourless semi solid; R_f 0.45 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.58 (d, *J*=6.8 Hz, 6H), 4.75 (septet, *J*=6.8 Hz, 1H), 6.82-6.87 (m, 2H), 7.16 (dq, *J*=7.6, 1.2 Hz, 2H), 7.27 (dt, *J*=7.8, 1.2 Hz, 1H), 7.31-7.34 (m, 1H), 7.45 (d, *J*=8.4 Hz, 1H), 7.64 (d, *J*=8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 23.0, 47.3, 109.8, 113.5, 115.4, 118.5, 119.6, 120.6, 121.0, 121.8, 122.7, 127.0, 127.8, 131.3, 136.0, 144.7; FTIR (KBr) 3463, 3370, 3050, 2973, 2927, 1612, 1546, 1461, 1365, 1249 cm^{-1};



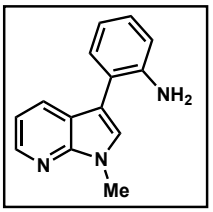
2-(1-propyl-1H-indol-3-yl)aniline (11d): Pale Brown semi solid; R_f 0.46 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 0.89 (t, *J*=7.2 Hz, 3H), 1.84 (sextet, *J*=7.2 Hz, 2H), 3.69-3.92 (bs, 2H), 4.05 (t, *J*=7.2 Hz, 2H), 6.71-6.79 (m, 2H), 7.07 (dq, *J*=8.0, 1.2 Hz, 2H), 7.15-7.21 (m, 2H), 7.23 (dd, *J*=7.6, 1.6 Hz, 1H), 7.32 (d, *J*=8 Hz, 1H), 7.55 (d, *J*=8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 11.8, 23.7, 48.2, 109.8, 113.1, 115.5, 118.4, 119.6, 120.6, 120.8, 121.9, 126.9, 127.0, 127.8, 131.3, 136.4, 144.7; FTIR (KBr) 3459, 3370, 3050, 2962, 2873, 1612, 1546, 1461 cm^{-1};



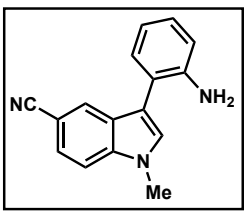
2-(1-butyl-1H-indol-3-yl)aniline (11e): Pale Brown semi solid; R_f 0.44 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 0.88 (t, *J*=7.6 Hz, 3H), 1.31 (sextet, *J*=7.6 Hz, 2H), 1.73-1.84 (m, 2H), 3.77 (bs, 2H), 4.09 (t, *J*=7.2 Hz, 2H), 6.76(dt, *J*=8.0, 1.2 Hz, 2H), 7.04-7.11 (m, 2H), 7.15-7.21 (m, 2H), 7.23 (dd, *J*=7.4, 1.2 Hz, 1H), 7.33 (d, *J*=8.0 Hz, 1H), 7.55 (d, *J*=8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 13.9, 20.4, 32.4, 46.3, 109.8, 113.1, 115.5, 118.4, 119.5, 120.6, 121.9, 126.8, 127.0, 127.8, 131.3, 136.4, 144.7; FTIR (KBr) 3459, 3370, 3050, 2954, 2869, 1612, 1546, 1461 cm^{-1};



2-(5-Methoxy-1-methyl-1H-indol-3-yl)aniline (11f): Brown solid, mp 118-120 ^{o}C; R_f 0.50 (25% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.93 (s, 6H), 3.37 (bs, 2H), 6.96 (t, *J*=8 Hz, 2H), 7.06 (dd, *J*=7, 2 Hz, 1H), 7.17 (d, *J*=2.5 Hz, 1H), 7.23-7.33 (m, 2H), 7.36-7.43 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 33.1, 56.1, 101.9, 110.4, 112.6, 112.8, 115.5, 118.5, 120.9, 127.8, 128.3, 128.9, 131.2, 132.5, 144.7, 154.4; FTIR (KBr) 3456, 3370, 3053, 2926, 2836, 1613, 1488, 1452, 1368, 753 cm^{-1}.

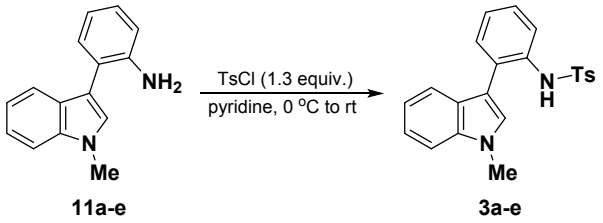


2-(1-Methyl-1H-pyrrolo[2,3-*b*]pyridin-3-yl)aniline (11g): Pale brown solid, mp 136-138 ^{o}C; R_f 0.45 (40% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.49 (bs, 2H), 3.97 (s, 3H), 6.81-6.87 (m, 2H), 7.10 (dd, *J*=8 Hz, 1H), 7.17 (dt, *J*=7.6, 1.6 Hz, 1H), 7.26 (dd, *J*=7.6, 1.6 Hz, 1 H), 7.33 (s, H), 7.97 (d, *J*=8 Hz, 1H), 8.38 (dd, *J*=4.6, 1.6 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 31.5, 112.0, 115.6, 115.8, 118.6, 119.5, 119.9, 127.6, 128.2, 129.0, 131.1, 143.3, 144.7, 147.9; FTIR (KBr) 3419, 3303, 2924, 1622, 1490, 1459, 1345 cm^{-1}.



3-(2-Aminophenyl)-1-methyl-1H-indole-5-carbonitrile (11h): Brown solid, mp 166-168 ^{o}C; R_f 0.45 (40% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.43 (bs, 2H), 3.88 (s, 3H), 6.86 (t, *J*=8 Hz, 2H), 7.21 (q, *J*=7.6 Hz, 2H), 7.30 (s, 1H), 7.41 (d, *J*=8.4 Hz, 1H), 7.49 (d, *J*=8.8 Hz, 1H), 7.98 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 33.3, 102.9, 110.5, 114.6, 115.9, 118.9, 119.1, 120.8, 125.0, 126.4, 126.9, 128.6, 129.8, 131.3, 138.6; FTIR (KBr) 3421, 3367, 3063, 2923, 2217, 1616, 1487, 1449, 1379 cm^{-1}.

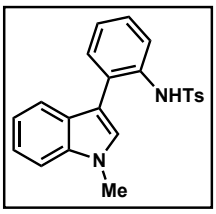
General Procedure for the preparation of compounds 3a-h



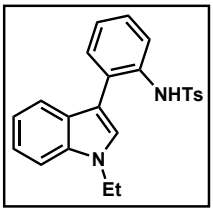
11a-e **3a-e**

To a solution of compound **11** (2.5 mmol) in 3 mL pyridine maintained at 0 °C was added *p*-toluenesulfonyl chloride (3.3 mmol) and was stirred at room temperature for 4-5 h. Then the reaction mixture was washed with 10% HCl solution (2×15 mL) and extracted with ethyl acetate. Then the organic layer was washed with water (1×10 mL). Combined organic layers were dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was purified by column chromatography using hexanes/ethyl acetate as eluent to afford pure compound **3**.

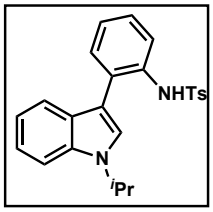
Spectral data for compounds 3a-h



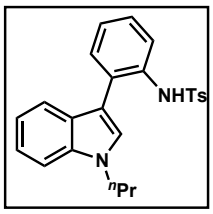
4-methyl-*N*-(2-(1-methyl-1H-indol-3-yl)phenyl)benzenesulfonamide (3a): White solid, mp 148-150 °C; R_f 0.43 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.29 (s, 3H), 3.72 (s, 3H), 6.59 (s, 1H), 6.84 (s, 1H), 6.97-7.07 (m, 5H), 7.14-7.25 (m, 3H), 7.28 (d, *J*=8.4 Hz, 1H), 7.37 (d, *J*=8.4 Hz, 2H), 7.63 (dd, *J*=8.2, 1.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.7, 33.1, 109.7, 110.9, 119.4, 120.3, 120.4, 122.7, 124.6, 126.1, 127.0, 127.3, 127.5, 128.2, 129.5, 131.7, 135.3, 136.5, 137.1, 143.7; FTIR (KBr) 3057, 2926, 2856, 1611, 1527, 1466, 1435, 1348 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{22}H_{21}N_2O_2S$: 377.1324; found: 377.1326.



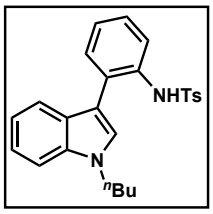
4-Methyl-*N*-(2-(1-ethyl-1H-indol-3-yl)phenyl)benzenesulfonamide (3b): White solid, mp 92-94 °C; R_f 0.43 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.51 (t, *J*=7.2 Hz, 3H), 2.37 (s, 3H), 4.19 (q, *J*=7.2 Hz, 2H), 6.75 (s, 1H), 6.91 (s, 1H), 7.05-7.10 (m, 1H), 7.10-7.16 (m, 4H), 7.22-7.35 (m, 3H), 7.47 (td, *J*=8.4, 2 Hz, 2H), 7.50 (d, *J*=8 Hz, 1H), 7.72 (dd, *J*=8.2, 1.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 15.7, 21.8, 41.3, 109.9, 111.0, 119.6, 120.4, 120.5, 122.7, 124.7, 125.8, 126.3, 127.2, 127.4, 128.2, 129.7, 131.8, 135.3, 136.3, 136.5, 143.8; FTIR (KBr) 3455, 3053, 2977, 2925, 2852, 1642, 1549, 1464, 1397, 1334 cm^{-1}.



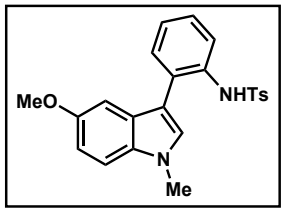
N-(2-(1-isopropyl-1H-indol-3-yl)phenyl)-4-methylbenzenesulfonamide(3c): White solid, mp 120-122 ^{o}C; R_f 0.45 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.55 (d, *J*=6.8 Hz, 6H), 2.38 (s, 3H), 4.71 (septet, *J*=6.8 Hz, 1H), 6.86 (s, 1H), 6.89 (s, 1H), 7.07 (dt, *J*=7.2, 0.8 Hz, 1H), 7.11-7.17 (m, 4H), 7.24-7.29 (m, 2H), 7.32 (dt, *J*=7.6, 1.6 Hz, 1H), 7.43 (d, *J*=8.4 Hz, 1H), 7.49 (td, *J*=8.0, 1.6, Hz, 2H), 7.75 (dd, *J*=8.4, 0.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.7, 23.0, 47.4, 110.0, 111.0, 119.5, 120.2, 120.3, 122.4, 122.5, 124.6, 126.3, 127.1, 127.3, 128.1, 129.6, 131.7, 135.2, 135.9, 136.4, 143.8; FTIR (KBr) 3316, 3054, 2977, 2927, 1600, 1546, 1461, 1160 cm^{-1};



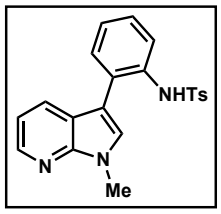
4-methyl-N-(2-(1-propyl-1H-indol-3-yl)phenyl)benzenesulfonamide (3d): Pale brown semi solid; R_f 0.43 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 0.98 (t, *J*=7.2 Hz, 3H), 1.90 (sextet, *J*=7.2 Hz, 2H), 2.37 (s, 3H), 4.09 (t, *J*=7.2 Hz, 2H), 6.72(s, 1H), 6.92 (s, 1H), 7.07 (dt, *J*=7.4 1.2 Hz, 1H), 7.11-7.17 (m, 4H), 7.24-7.34 (m, 3H), 7.39 (d, *J*=8.4 Hz, 1H), 7.47 (d, *J*=8.4 Hz, 2H), 7.73 (dd, *J*=8.2, 1.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 11.8, 21.7, 23.6, 48.3, 110.0, 110.7, 119.5, 120.2, 120.3, 122.5, 124.6, 126.1, 126.6, 127.1, 127.3, 128.1, 129.6, 131.7, 135.2, 136.4, 136.4, 143.8; FTIR (KBr) 3320, 3054, 2965, 2877, 1600, 1550, 1465, 1334, 1160 cm^{-1};



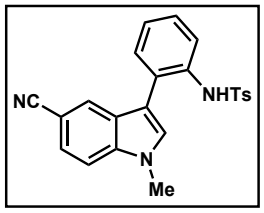
N-(2-(1-butyl-1H-indol-3-yl)phenyl)-4-methylbenzenesulfonamide (3e): colour less semi solid; R_f 0.45 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 0.99 (t, *J*=7.6 Hz, 3H), 1.39 (sextet, *J*=7.6 Hz, 2H), 1.85 (quintet, J=7.6 Hz, 2H), 2.37 (s, 3H), 4.12 (t, *J*=7.2 Hz, 2H), 6.71(s, 1H), 6.92 (s, 1H), 7.07 (dt, *J*=6.8, 0.8 Hz, 1H), 7.10-7.17 (m, 4H), 7.24-7.31 (m, 3H), 7.39 (d, *J*=8.4 Hz, 1H), 7.47 (d, *J*=8.0 Hz, 2H), 7.73 (dd, *J*=8.2, 1.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 13.9, 20.4, 21.7, 32.3, 46.4, 109.9, 110.7, 119.5, 120.2, 120.3, 122.5, 124.6, 126.1, 126.5, 127.0, 127.3, 128.1, 129.6, 131.7, 135.2, 136.4, 143.8; FTIR (KBr) 3320, 3054, 2958, 2869, 1600, 1550, 1465, 1160 cm^{-1};



***N*-(2-(5-Methoxy-1-methyl-1H-indol-3-yl)phenyl)-4-methylbenzenesulfonamide (3f):** Pale Brown solid, mp 144-146 ^{o}C; R_f 0.55 (30% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.37 (s, 3H), 3.76 (s, 3H), 3.78 (s, 3H), 6.60-6.63 (m, 2H), 6.92-6.97 (m, 2H), 7.10-7.16 (m, 3H), 7.22-7.29 (m, 3H), 7.60 (dd, *J*=8.4 Hz, 2H), 7.67 (dd, *J*=8.2, 0.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.7, 33.3, 56.1, 100.9, 110.4, 110.7, 113.3, 120.6, 124.8, 126.4, 127.4, 128.0, 128.2, 129.6, 130.1, 131.6, 132.5, 135.3, 136.6, 143.8, 155.0; FTIR (KBr) 3315, 3060, 2926, 2838, 1608, 1548, 1487, 1334 cm^{-1}.



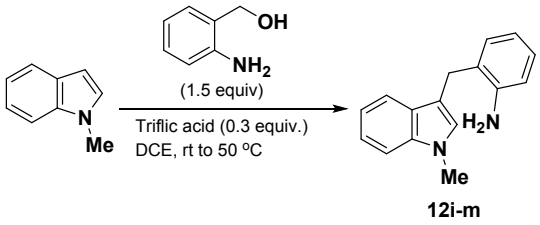
4-Methyl-*N*-(2-(1-methyl-1H-pyrrolo[2,3-*b*]pyridin-3-yl)phenyl)benzenesulfonamide (3g): Pale yellow solid, mp 182-184 ^{o}C; R_f 0.50 (50% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.37 (s, 3H), 3.94 (s, 3H), 6.86 (s, 2H), 7.02-7.10 (m, 1H), 7.13 (d, *J*=8 Hz, 1H), 7.17 (d, *J*=7.2 Hz, 1H), 7.22 (dd, *J*=7.6, 1.6 Hz, 1H), 7.33 (t, *J*=7.6 Hz, 1H), 7.44-7.55 (m, 3H), 7.68 (d, *J*=8.4 Hz, 1H), 8.39 (d, *J*=4.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.7, 31.9, 116.2, 121.4, 125.0, 125.5, 127.2, 127.3, 128.0, 128.5, 128.6, 129.6, 131.5, 135.7, 136.6, 143.2, 143.9; FTIR (KBr) 3326, 3060, 2925, 2856, 1599, 1491, 1461, 1342, 1161 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{21}H_{20}N_3O_2S$: 378.1276; found: 378.1276.



***N*-(2-(5-cyano-1-methyl-1H-indol-3-yl)phenyl)-4-methylbenzenesulfonamide (3h):** Pale brown solid, mp 186-188 ^{o}C; R_f 0.47 (40% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.40 (s, 3H), 3.87 (s, 3H), 6.78 (s, 1H), 6.96 (s, 1H), 7.12-7.18 (m, 4H), 7.24 (d, *J*=0.8Hz, 1H), 7.33-7.38 (m, 1H), 7.39-7.46 (m, 3H), 7.48 (dd, *J*=8.4, 1.6 Hz, 1H), 7.74 (d, *J*=8Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.7, 33.4, 103.4, 110.7, 112.0, 120.4, 120.7, 124.4, 124.9, 125.1, 125.5, 127.2, 127.2, 129.0, 129.7, 130.0, 131.7, 135.3, 136.0, 138.5, 144.4; FTIR (KBr) 3328, 2925, 2219, 1610, 1486, 1395, 1333 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{23}H_{20}N_3O_2S$: 402.1276; found: 402.1283.

General Procedure for the preparation of compounds 3i-m[5]

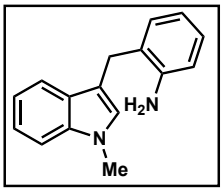
General Procedure for the preparation of compounds 12i-m



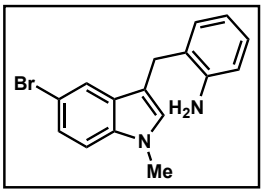
12i-m

To the solution of *N*-methyl indole (5 mmol) in DCE was added 2-aminobenzyl alcohol (7.5 mmol) and TFA (1.5 mmol) at room temperature. The resulting reaction mixture was stirred at 50 ^{o}C. After the completion of the reaction, the reaction was quenched with the $NaHCO_3$ and extracted with DCM. This was washed with brine solution and organic layers were dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was purified by column chromatography using hexanes/ethyl acetate as an eluent to afford pure compound **12**.

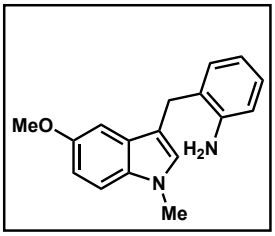
Spectral data for compounds 12i-m



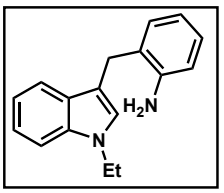
2-((1-Methyl-1H-indol-3-yl)methyl)aniline (12i): Light brown sticky solid, R_f 0.43 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.41 (bs, 2H), 3.55 (s, 3H), 3.89 (s, 3H), 6.54-6.58 (m, 2H), 6.66 (dt, = 7.6, 1.2 hz, 1h), 6.96-7.02 (m, 2H), 7.06 (dd, *J*=7.6, 1.2 Hz, 1H), 7.12 (dd, *J*=8, 1.2 Hz, 1H), 7.16-7.19 (m, 1H), 7.47 (td, *J*=7.6, 1.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 28.1, 32.7, 109.3, 112.2, 115.9, 11.8, 119.0, 119., 121.8, 125.6, 127.1, 127.4, 127.9, 130.5, 137.4, 144.8; FTIR (KBr) 3443, 3057, 2962, 1621, 1483, 1370 cm^{-1}.



2-((5-bromo-1-methyl-1H-indol-3-yl)methyl)aniline (12j): white solid, mp 118-120 ^{o}C R_f 0.53 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz, ppm) δ 3.57 (s, 3H), 3.90 (s, 2H), 6.59 (s, 1H), 6.74 (q, *J*= 8 Hz, 2H), 7.00-7.08 (m, 3H), 7.16-7.22 (m, 1H), 7.60 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm) δ 27.7, 32.9, 110.8, 111.4, 112.5, 118.4, 121.8, 122.0, 124.6, 127.7, 128.0, 128.7, 129.5, 130.5, 136.0, 140.1; FTIR (KBr) 3441, 3371, 3060, 2920, 2851, 1619, 1585, 1493, 1476, 1456, 1375, 1247 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{16}H_{16}N_2Br$: 315.0497; found: 315.0523 (HRMS data for ^{79}Br isotope).

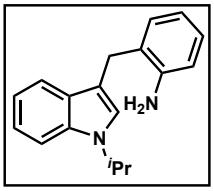


2-((5-Methoxy-1-methyl-1H-indol-3-yl)methyl)aniline (12k): brown oil, R_f 0.43 (25% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.66 (s, 3H), 3.82 (s, 3H), 4.01 (s, 2H), 6.66 (s, 1H), 6.81 (q, *J*=8.4 Hz, 2H), 6.88 (dd, *J*=8.8, 2.4 hz, 1H), 6.99 (d, *J*=2 Hz, 1H), 7.1 (dt, *J*=7.6, 1.2 Hz, 1H), 7.15-7.21 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 28.2, 32.9, 56.0, 101.0, 111.3, 112.1, 116.9, 120.0, 126.7, 127.5, 127.9, 128.1, 130.5, 132.8, 143.2, 153.9; FTIR (KBr) 3443, 3365, 3051, 2924, 2832, 1620, 1580, 1491, 1455, 1428, 1262 cm^{-1}.



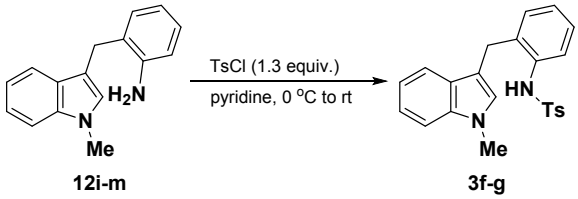
2-((1-ethyl-1H-indol-3-yl)methyl)aniline (12l): Light brown oil, R_f 0.52 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz, ppm) δ 1.28 (t, *J*=7.2 Hz, 3H), 3.63 (bs, 2H), 3.92 (s, 2H), 3.96 (q, *J*=7.2 Hz, 2H), 6.60 (d, *J*=8.0 Hz, 1H), 6.65 (s, 1H), 6.68 (dt, *J*=7.2, 1.2 Hz, 1H), 6.94-7.02 (m, 2H), 7.04-7.14 (m, 2H), 7.21 (d, *J*= 8.4 Hz, 1H), 7.47 (d, *J*= 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm) δ 15.5, 28.2, 40.8, 109.4, 112.2, 115.9, 118.8, 118.9, 119.3, 121.6, 125.4, 125.6,

127.4, 128.0, 130.5, 136.4, 144.7; FTIR (KBr) 3444, 3366, 3048, 2975, 2930, 2882, 1619, 1583, 1494, 1459, 1334, 1277 cm^{-1};



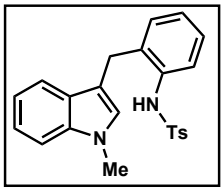
2-((1-isopropyl-1H-indol-3-yl)methyl)aniline (12m): Light brown semi solid, R_f 0.48 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.48 (6H, d, *J*=6.83 Hz), 3.42-3.43 (br s, 2H), 4.64 (sep, *J*=6.8 Hz, 1H), 6.69 (dd, *J*=7.8, 1.2 Hz, 1H), 6.78 (dt, *J*=7.8, 1.2 Hz, 1H), 6.90 (s, 1H), 7.07-7.14 (m, 2H), 7.16-7.25 (m, 2H), 7.37 (d, *J*=8.4 Hz, 1H), 7.57 (d, *J*=8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 22.9, 28.5, 47.1, 109.6, 112.2, 115.9, 118.7, 119.0, 119.4, 121.6, 121.9, 125.6, 127.4, 128.0, 130.6, 136.2, 145.0; FTIR (KBr) 3444, 3367, 3043, 2969, 2923, 1616, 1416, 1357 cm^{-1}.

General Procedure for the preparation of compounds 3i-m:

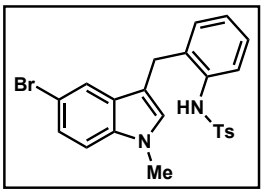


To a solution of compound **12** (2.5 mmol) in 3 mL pyridine maintained at 0 °C was added *p*-toluenesulfonyl chloride (3.3 mmol) and was stirred at room temperature for 4-5 h. Then the reaction mixture is washed with 10% HCl solution (2×15 mL) and extracted with ethyl acetate. Then the organic layer was washed with water (1×10 mL). Combined organic layers were dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was purified by column chromatography using hexanes/ethyl acetate as an eluent to afford pure compound **3i-m**.

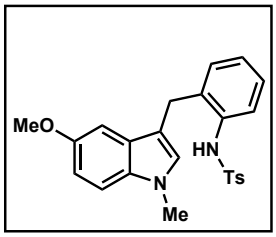
Spectral data for compounds 3i-m



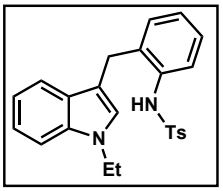
4-Methyl-*N*-(2-((1-methyl-1H-indol-3-yl)methyl)phenyl)benzenesulfonamide (3i): Pale yellow solid, mp 198-200 °C [lit. 203 °C][5]; R_f 0.50 (25% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.40 (s, 3H), 3.67 (s, 2H), 3.72 (s, 3H), 6.58-6.63 (m, 2H), 7.04 (dt, *J*=7.4, 1.2 Hz, 1H), 7.11-7.18 (m, 3H), 7.20-7.27 (m, 4H), 7.28-7.32 (m, 1H), 7.43-7.49 (m, 3H) ; ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.7, 28.6, 32.9, 109.6, 111.3, 119.1, 119.4, 122.3, 124.3, 124.3, 126.1, 127.0, 127.2, 127.4, 127.7, 126.7, 130.7, 133.1, 135.4, 136.9, 137.7cm^{-1}; FTIR (KBr) 3431, 2923, 1636, 1480, 1378 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{23}H_{23}N_2O_2S$: 391.1480; found: 391.1480.



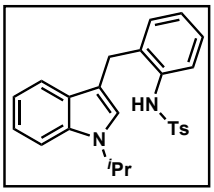
N-(2-((5-bromo-1-methyl-1H-indol-3-yl)methyl)phenyl)-4-methylbenzenesulfonamide (3j): white solid, mp 158-160°C [lit. 157 °C][5];R*f* 0.52 (30% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz, ppm) δ 2.42 (s, 3H), 3.59 (s, 2H), 3.68 (s, 3H), 6.49 (bs, 1H), 6.58 (s, 1H), 7.13-7.18 (m, 3H), 7.20 (d, *J*=8.0 Hz, 2H), 7.22-7.27 (m, 1H), 7.28-7.32 (m, 2H), 7.47 (d, *J*=8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm) δ 21.7, 28.1, 33.0, 111.1, 111.1, 112.7, 121.7, 124.9, 125.1, 126.4, 127.1, 127.9, 128.2, 129.0, 130.6, 132.9, 135.2, 136.2, 136.9, 144.0; FTIR (KBr) 3282, 3064, 2921, 1598, 1491, 1476, 1455, 1377, 1291, 1120 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{23}H_{21}N_2O_2NaSBr$: 491.0405; found: 491.0427 (HRMS data for ^{79}Br isotope). .



***N*-(2-((5-Methoxy-1-methyl-1H-indol-3-yl)methyl)phenyl)-4-methylbenzenesulfonamide (3k):** Pale pink solid, mp 120-122 °C [lit. 123 °C][5]; R_f 0.41 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.28 (s, 3H), 3.56 (s, 5H), 3.64 (s, 3H), 6.48 (s, 1H), 6.57 (d, *J*=2.4 Hz, 1H), 6.61 (s, 1H), 7.01-7.15 (m, 6H), 7.32-7.37 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.6, 28.6, 33.0, 56.0, 101.1, 110.3, 110.5, 112.3, 1240, 125.9, 127.1, 127.6, 127.6, 127.6, 130.0, 130.6, 133.0, 133.0, 135.4, 136.8, 143.7, 154.0; FTIR (KBr) 3285, 3068, 2926, 2836, 1491, 1455, 1428 cm^{-1}.



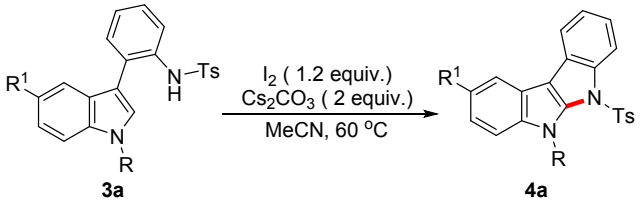
4-methyl-N-(2-((1-ethyl-1H-indol-3-yl)methyl)phenyl)benzenesulfonamide (3l): White solid, mp 192-194 °C; R_f 0.46 (15% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz, ppm) δ 1.42 (t, *J*=7.2 Hz, 3H), 2.39 (s, 3H), 3.68 (s, 2H), 4.11 (q, *J*=7.2 Hz, 2H), 6.66 (bs, 1H), 6.71 (s, 1H), 7.02 (t, *J*= 7.2 Hz, 1H), 7.14 (d, *J*= 8.8 Hz, 3H), 7.19-7.25 (m, 4H), 7.33 (d, *J*=8.4 Hz, 1H), 7.41 (d, *J*=8.4 Hz, 2H), 7.45 (d, *J*=8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm) δ 15.6, 21.7, 28.8, 41.1, 109.7, 111.4, 119.3, 122.2, 123.9, 125.3, 125.9, 127.1, 127.1, 127.5, 127.7, 129.7, 130.7, 132.7, 135.5, 136.7, 136.8, 143.8; FTIR (KBr) 3266, 2925, 2855, 1597, 1577, 1483, 1459, 1375, 1329, 1159 cm^{-1};



4-Methyl-*N*-(2-((1-isopropyl-1H-indol-3-yl)methyl)phenyl)benzenesulfonamide (3m): Pale brown semi solid, R_f 0.43 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ1.50 (d, *J*=6.8 Hz, 6H), 2.38 (s, 3H), 3.72 (s, 2H), 4.64 (sep, *J*=6.8 Hz, 1H), 6.75 (s, 1H), 6.88 (s, 1H), 7.00 (dt, *J*=7.6, 0.8 Hz, 1H), 7.09-7.15 (m, 3H), 7.17 (d, *J*=8.0 Hz, 1H), 7.19-7.26 (m, 3H), 7.37 (d, *J*=8.4 Hz, 3H), 7.42 (dd, J=7.8, 1.2 Hz, 1H); ^{13}C

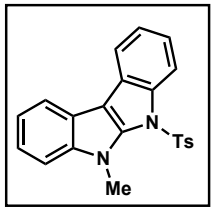
NMR ($CDCl_3$, 100 MHz) δ 21.7, 22.9, 29.1, 47.2, 109.9, 111.3, 119.3, 119.4, 121.9, 122.1, 123.5, 125.7, 127.1, 127.4, 127.7, 129.6, 130.7, 132.4, 135.6, 136.5, 136.7, 143.7; FTIR (KBr) 3274, 3050, 2973, 1596, 1465, 1334 cm^{-1}.

General procedure for iodine mediated intramolecular C2 amidative cyclization of compounds 3a-h

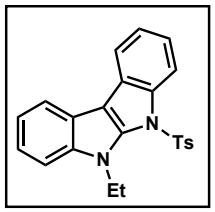


3 (0.5 mmol) was taken in a clean and dry reaction tube. To this iodine (0.6 mmol), Cs_2CO_3 (1.0 mmol) and acetonotrile (2 mL) was added. Reaction tube is stoppered and the resulting reaction mixture was stirred at 60 °C. After 4 h the second portion of iodine (0.3 mmol) was added and reaction was allowed to stir at 60 °C. Upon completion of reaction as monitored by TLC, solvent was removed under vacuum in rotary evaporator and DCM was added. The crude reaction mixture was washed with saturated $Na_2S_2O_3$ solution (2 × 10 mL) and extracted with DCM. The organic layer was washed water (1 × 10 mL). Combined organic layers were concentrated using rotary evaporator and residue is purified by column chromatography on silica gel using hexanes/ethyl acetate as an eluent to afford pure product **4**.

Spectral data for compounds 4a-j

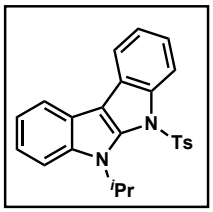


5-Methyl-6-tosyl-5,6-dihydroindolo[2,3-*b*]indole (4a)[10]: White solid, mp 164-166 °C [lit. 162 °C][10]; R_f 0.56 (10% ethyl acetate in hexanes); ^1H NMR ($CDCl_3$, 400 MHz) δ 2.11 (s, 3H), 4.13 (s, 3H), 6.86 (d, *J*=8.4 Hz, 2H), 7.11 (dt, *J*=7.6, 1.2 Hz, 1H), 7.15-7.30 (m, 5H), 7.41 (d, *J*=8 Hz, 1H), 7.50 (dd, *J*=7.6, 0.8 Hz, 1H), 7.71 (d, *J*=7.6 Hz, 1H), 8.07 (dd, *J*=8.4, 0.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.6, 34.0, 111.0, 118.0, 118.5, 119.5, 120.5, 121.0, 122.3, 122.4, 125.6, 127.0, 129.4, 132.5, 140.7, 141.7, 143.0, 145.0; FTIR (KBr) 3057, 2923, 2853, 1600, 1528, 1505, 1436, 1396, 1368, 1175 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{22}H_{19}N_2O_2S$: 375.1167; found: 375.1166.

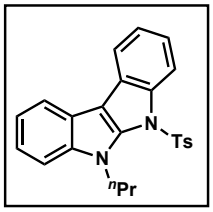


5-Ethyl-6-tosyl-5,6-dihydroindolo[2,3-*b*]indole (4b): Pale brown solid, mp 156-158 °C; R_f 0.55 (10% ethyl acetate in hexanes); ^1H NMR ($CDCl_3$, 400 MHz) δ 1.48 (t, *J*=7.2 Hz, 3H), 2.11 (s, 3H), 4.70 (q, *J*=7.2 Hz, 2H), 6.86 (d, *J*=8.4 Hz, 2H), 7.11 (dt, *J*=7.6, 1.2 Hz, 1H), 7.15-7.21 (m, 2H), 7.21-7.29 (m, 3H), 7.45 (d, *J*=8 Hz, 1H), 7.49 (td, *J*=7.6, 0.8 Hz, 1H), 7.72dd, *J*=7.4, 0.8 Hz, 1H), 8.07 (dd, *J*=8.2, 0.8 Hz, 1H); ^{13}C

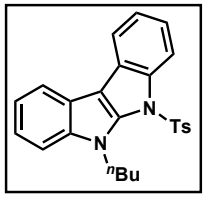
NMR ($CDCl_3$, 100 MHz) δ 15.0, 21.6, 41.8, 109.6, 111.3, 117.9, 118.4, 119.6, 120.9, 122.3, 125.6, 127.0, 127.3, 129.4, 132.5, 140.8, 141.0, 142.5, 144.9; FTIR (KBr) 3056, 2926, 2859, 1604, 1515, 1453, 1370, 1251, 1176 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{23}H_{21}N_2O_2S$: 389.1324; found: 389.1313.



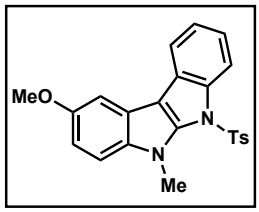
5-Isopropyl-6-tosyl-5,6-dihydroindolo[2,3-b]indole (4c): White solid, mp 148-150 °C; R_f 0.53 (10% ethyl acetate in hexanes); ^1H NMR ($CDCl_3$, 400 MHz) δ 1.74 (d, *J*=7.2 Hz, 6H), 2.17 (s, 3H), 5.64 (septet, *J*=7.2 Hz, 1H), 6.88 (s, 1H), 6.89 (d, *J*=8 Hz 2H), 7.15-7.22 (m, 3H), 7.23-7.29 (m, 3H), 7.49 (dd, *J*=7.6, 0.8 Hz, 1H), 7.73-7.79 (m, 2H), 8.11 (d, *J*=8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.6, 21.7, 51.8, 114.5, 118.3, 118.8, 120.0, 120.7, 121.6, 122.1, 122.3, 125.9, 127.2, 128.1, 129.1, 131.3, 139.4, 141.4, 143.7, 144.8; FTIR (KBr) 3058, 2973, 2927, 2854, 1604, 1531, 1504, 1457, 1172 cm^{-1};



5-propyl-6-tosyl-5,6-dihydroindolo[2,3-b]indole (4d): Pale brown semi solid; R_f 0.55 (10% ethyl acetate in hexanes); ^1H NMR ($CDCl_3$, 400 MHz) δ 0.94 (t, *J*=7.6 Hz, 3H), 2.01 (sextet, *J*=7.6 Hz, 2H), 2.19 (s, 3H), 4.69 (t, *J*=7.6 Hz, 2H), 6.93 (d, *J*=8.0 Hz, 2H), 7.19 (dt, *J*=8.4, 1.2 Hz, 1H), 7.21-7.29 (m, 2H), 7.30-7.35 (m, 3H), 7.52 (d, *J*=8.0 Hz, 1H), 7.58 (dd, *J*=3.6, 0.8 Hz, 1H), 7.80 (d, *J*=7.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 11.4, 21.6, 22.9, 48.2, 109.5, 111.4, 117.9, 118.4, 119.5, 120.6, 120.8, 122.1, 122.4, 125.5, 126.9, 127.3, 129.3, 132.3, 140.7, 141.2, 142.5, 144.9; FTIR (KBr) 3058, 2965, 2927, 2865, 1604, 1511, 1454, 1176 cm^{-1};

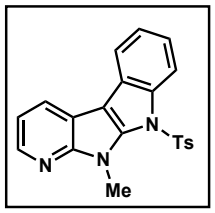


5-butyl-6-tosyl-5,6-dihydroindolo[2,3-b]indole (4e): White solid, mp 137-139 °C; R_f 0.52 (10% ethyl acetate in hexanes); ^1H NMR ($CDCl_3$, 400 MHz) δ 0.96 (t, *J*=7.6 Hz, 3H), 1.35 (sextet, *J*=7.6 Hz, 2H), 1.94 (quintet, *J*=7.6 Hz, 2H) 2.19 (s, 3H), 4.74 (t, *J*=7.6 Hz, 2H), 6.94 (d, *J*=8.0 Hz, 2H), 7.19 (dt, *J*=8.0, 1.2 Hz, 1H), 7.23-7.29 (m, 2H), 7.32 (d, *J*=8.4 Hz, 3H), 7.52 (d, *J*=8.4 Hz, 1H), 7.58 (d, *J*=7.6 Hz, 1H), 7.80 (d, *J*=7.6 Hz, 1H), 8.16 (d, *J*=8.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 14.0, 20.2, 21.6, 31.6, 46.5, 109.5, 111.4, 118.0, 118.4, 119.5, 120.7, 120.8, 122.1, 122.4, 125.6, 126.9, 127.3, 129.3, 132.3, 140.7, 141.1, 142.5, 144.9; FTIR (KBr) 3058, 2965, 2927, 2865, 1604, 1511, 1457, 1373, 1176 cm^{-1};

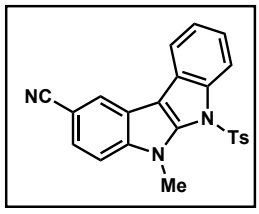


2-Methoxy-5-methyl-6-tosyl-5,6-dihydroindolo[2,3-*b*]indole (4f): Pale green solid, mp 162-164 °C; R_f 0.43 (15% ethyl acetate in hexanes); ^1H NMR ($CDCl_3$, 400 MHz) δ 2.11 (s, 3H), 3.82 (s, 3H), 4.08 (s, 3H), 6.83-6.92 (m, 3H), 7.10 (dt, *J*=8.4, 1.2 Hz, 1H), 7.15-7.21 (m, 2H), 7.23 (d, *J*=8.4 Hz, 2H), 7.28 (d, *J*=8.8 Hz, 1H), 7.47 (d, *J*=7.4 Hz, 1H), 8.05 (d, *J*=8.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100

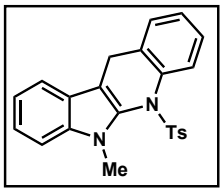
MHz) δ 21.6, 34.0, 56.1, 102.5, 108.8, 111.3, 111.6, 117.9, 118.3, 120.9, 122.2, 125.6, 127.0, 127.3, 129.4, 132.5, 136.7, 140.5, 143.5, 144.9, 155.1; FTIR (KBr) 3060, 2927, 2845, 1623, 1527, 1466, 1433, 1369, 1177 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{23}H_{21}N_2O_3S$: 405.1273; found: 405.1264.



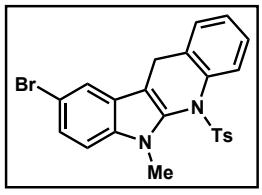
10-Methyl-9-tosyl-9,10-dihydropyrido[3',2':4,5]pyrrolo[2,3-*b*]indole (4g): White solid, mp 160-162 °C; R_f 0.46 (20% ethyl acetate in hexanes); ^1H NMR ($CDCl_3$, 400 MHz) δ 2.21 (s, 3H), 4.33 (s, 3H), 6.98 (d, *J*=8.4 Hz, 2H), 7.20(dd, *J*=7.6 Hz, 1H), 7.22-7.27 (m, 1H), 7.31 (t, *J*=8.4 Hz, 1H), 7.39 (d, *J*=8.4 Hz, 2H), 7.58 (d, *J*=7.6 Hz, 1H), 8.05 (dd, *J*=7.6, 0.8 Hz, 1H), 8.22 (d, *J*=8.4 Hz, 1H), 8.40 (dd, *J*=4.8, 1.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.6, 32.5, 106.1, 113.9, 117.0, 117.6, 118.5, 122.9, 125.6, 126.6, 126.9, 127.0, 129.6, 132.9, 139.9, 142.4, 145.2, 151.5; FTIR (KBr) 3056, 2926, 1609, 1514, 1435 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{21}H_{12}N_3O_2S$: 376.1120; found: 376.1131.



5-Methyl-6-tosyl-5,6-dihydroindolo[2,3-*b*]indole-2-carbonitrile (4h): White solid, mp 223-225 °C; R_f 0.43 (20% ethyl acetate in hexanes); ^1H NMR ($CDCl_3$, 400 MHz ppm) δ 2.13 (s, 3H), 4.16 (s, 3H), 6.89 (d, *J*=8 Hz, 2H), 7.15-7.28 (m, 4H), 7.42-7.52 (m, 3H), 8.00 (s, 1H), 8.08 (d, *J*=8Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.7, 34.4, 104.2, 109.2, 111.7, 118.0, 118.9, 120.2, 120.5, 124.5, 125.4, 126.0, 126.2, 127.0, 129.6, 132.4, 140.8, 143.0, 144.2, 145.5; FTIR (KBr) 2923, 2855, 2217, 1614, 1515, 1466, 1439, 1169 cm^{-1}.



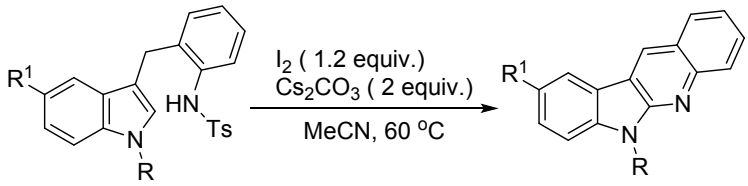
6-Methyl-5-tosyl-6,11-dihydro-5H-indolo[2,3-*b*]quinoline (4i): Pale red solid, mp 97-99 °C; R_f 0.46 (10% ethyl acetate in hexanes); ^1H NMR ($CDCl_3$, 400 MHz) δ 2.21 (d, *J*=18.6 Hz, 1H), 2.27 (s, 3H), 3.41 (d, *J*=18.6 Hz, 1H), 3.86 (s, 3H), 6.89 (s, 3H), 6.93 (d, *J*=8.4 Hz, 1H), 7.03 (dt, *J*=7.2, 0.8 Hz, 1H), 7.11 (dt, *J*=7.6, 1.2 Hz, 1H), 7.15-7.25 (m, 2h), 7.28 (d, *J*=8.4 Hz, 1H), 7.32 (dd, *J*=7.6, 0.8 Hz, 1H), 7.77 (dd, *J*=8, 1.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.8, 25.3, 30.8, 106.2, 110.0, 118.2, 119.6, 122.1, 124.1, 126.6, 127.3, 128.2, 128.7, 128.9, 129.1, 131.7, 133.5, 136.3, 136.4, 138.2, 144.8; FTIR (KBr) 3054, 2925, 2855, 1636, 1608, 1516, 1483, 1428 cm^{-1}; HRMS (*m*/*z*): $[M+H]^+$ calcd. for $C_{23}H_{21}N_2O_2S$: 389.1324; found: 389.1327.



9-bromo-6-methyl-5-tosyl-6,11-dihydro-5H-indolo[2,3-b]quinoline (4j): White solid, mp 154-156 °C; R_f 0.52 (10% ethyl acetate in hexanes); ^1H NMR ($CDCl_3$, 400 MHz, ppm) δ 2.23 (d, *J*=18.4 Hz, 1H), 2.38 (s, 3H), 3.44 (d, *J*=18.4 Hz, 1H), 3.93 (s, 3H), 6.93 (d, *J*= 8.4 Hz, 2H), 7.02 (d, *J*=8.0 Hz, 3H), 7.21-7.26 (m, 2H), 7.30-7.36 (m, 2H), 7.53 (d, *J*=0.8 Hz, 1H), 7.85 (dd, *J*= 8, 0.8

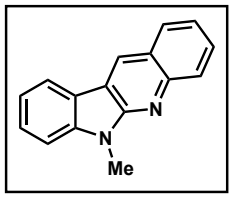
Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm) δ 21.8, 25.1, 31.0, 105.8, 111.6, 112.9, 120.8, 124.9, 125.6, 126.3, 126.8, 127.5, 128.2, 128.7, 128.8, 129.3, 131.5, 135.0, 135.9, 138.0, 145.1; FTIR (KBr) 3060, 2953, 2853, 1606, 1596, 1567, 1491, 1468, 1362, 1280 cm^{-1}; HRMS (m/z): $[M+Na]^+$ calcd. for $C_{23}H_{19}N_2O_2NaSBr$: 489.0248; found: 489.0219 (HRMS data for ^{79}Br isotope).

General procedure for iodine mediated intramolecular domino cyclization-detosylation-aromatization reaction of compounds 3i-m

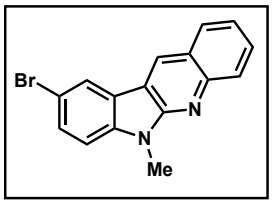


3i-m **5a-e**

3 (0.5 mmol) was taken in a clean and dry reaction tube. To this iodine (0.6 mmol), Cs_2CO_3 (1.0 mmol) and acetonotrile (2 mL) were added. The reaction tube was stoppered and the resulting reaction mixture was stirred at 60 °C. After 4 h the second portion of iodine (0.3 mmol) was added and reaction is allowed to stir at 60 °C. Upon completion of reaction as monitored by TLC, solvent was removed under vacuum in rotary evaporator and DCM was added. The crude reaction mixture was washed with saturated $Na_2S_2O_3$ solution (2 × 10 mL) and extracted with DCM. The organic layer was washed with water (1 × 10 mL). Combined organic layers were concentrated using rotary evaporator and residue is purified by column chromatography on silica gel using hexanes/ethyl acetate as an eluent to afford pure product **5**.

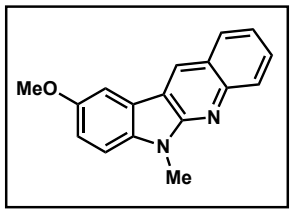


6-Methyl-6H-indolo[2,3-*b*]quinoline (5a): Pale yellow solid, mp 83-87 °C; R_f 0.42 (10% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 4.02 (s, 3H), 7.32 (d, *J*=7.2 Hz, 1H), 7.41 (d, *J*=8 Hz, 1H), 7.47 (dt, *J*=7, 1 Hz, 1H), 7.57-7.62 (m, 1H), 7.71-7.76 (m, 1H), 8.00 (d, *J*=8 Hz, 1H), 8.14 (d, *J*=7.5 Hz, 1H), 8.22 (d, *J*=8.5 Hz, 1H), 8.70 (s, 1H) ; ^{13}C NMR ($CDCl_3$, 125 MHz) δ 28.2, 109.0, 118.6, 120.4, 120.4, 121.6, 123.3, 124.0, 127.0, 128.1, 128.4, 128.7, 129.4, 142.9, 146.0, 152.3; FTIR (KBr) 3053, 2928, 1607, 1579, 1483, 1430 cm^{-1}.

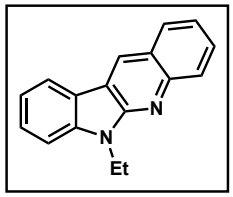


9-bromo-6-methyl-6H-indolo[2,3-*b*]quinoline (5b): Yellow solid, mp 132-134 °C; R_f 0.46 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz, ppm) δ 3.86 (s, 3H), 7.07 (1:1 q, *J*=7.2 Hz, 1H), 7.14-7.19 (m, 1H), 7.39 (t, *J*= 7.2 Hz, 1H), 7.56 (dd, *J*= 8.4, 2.4 Hz, 1H), 7.65 (dt, *J*=

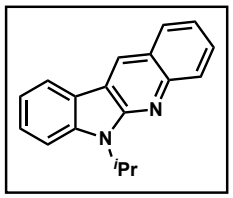
7.6, 1.2 Hz, 1H), 7.89 (d, *J*= 8.0 Hz, 1H), 8.07 (d, *J*=8.8 Hz, 1H), 8.11 (s, 1H), 8.52 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm) δ 28.1, 110.3, 112.9, 117.2, 122.2, 123.5, 124.1, 124.3, 127.4, 127.8, 128.2, 128.4, 128.8, 129.6, 130.9, 141.5; FTIR (KBr) 2923, 2852, 1603, 1572, 1477, 1458, 1325, 1254 cm^{-1}; HRMS (m/z): $[M+H]^+$ calcd. For $C_{16}H_{12}N_2Br$: 311.0184; found: 311.0172 (HRMS data for ^{79}Br isotope).



9-Methoxy-6-methyl-6H-indolo[2,3-*b*]quinoline (5c): Yellow solid, mp 110-112 °C; R_f 0.46 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.95 (s, 3H), 3.96 (s, 3H), 7.20 (dd, *J*=8.6, 2.4 Hz, 1H), 7.31 (d, *J*=8.8 Hz, 1H), 7.44 (dd, *J*=7.4, 1.2 Hz, 1H), 7.66 (d, *J*=2.4 Hz, 1H), 7.71 (dt, *J*=7.6, 1.6 Hz, 1H), 7.98 (dd, *J*=8.4, 1.2 Hz, 1H), 8.15 (d, *J*=8.4 Hz, 1H), 8.66 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 28.0, 56.3, 105.7, 109.5, 116.3, 118.5, 120.9, 122.9, 123.9, 127.4, 127.7, 127.8, 128.3, 128.7, 129.1, 137.7, 154.5; FTIR (KBr) 3055, 2927, 2855, 1615, 1576, 1392, 1285 cm^{-1}.



6-ethyl-6H-indolo[2,3-*b*]quinoline (5d): White solid, mp 93-95 °C; R_f 0.56 (10% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 1.52 (t, *J*=7.2 Hz, 3H), 4.61 (q, *J*=7.2 Hz, 2H), 7.30 (dt, *J*= 7.2, 0.8 Hz, 1H), 7.42-7.49 (m, 2H), 7.58 (dt, *J*= 7.6, 1.2 Hz, 1H), 7.73 (dt, *J*= 7.6, 1.6 Hz, 1H), 8.00 (dd, *J*= 8.2, 1.6 Hz, 1H), 8.17 (t, *J*= 8.4 Hz, 2H), 8.71 (s, 1H) ; ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 13.8, 36.4, 109.0, 118.5, 120.0, 120.7, 121.7, 123.0, 124.2, 127.5, 127.8, 128.2, 128.6, 129.0, 142.0, 146.7, 152.1; FTIR (KBr) 3056, 2926, 2853, 1605, 1571, 1481, 1450, 1349, 1229 cm^{-1};

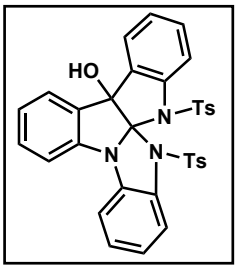


6-Isopropyl-6H-indolo[2,3-*b*]quinoline (5e): Pale orange solid, mp 98-100 °C; R_f 0.54 (10% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 1.66 (d, *J*=7.0 Hz, 6H), 5.56 (septet, *J*=7.0 Hz, 1H), 7.17 (t, *J*=7.5 Hz, 1H), 7.34 (t, *J*=8 Hz, 1H), 7.43 (t, *J*=7.5 Hz, 1H), 7.49 (d, *J*=8.5 Hz, 1H), 7.60 (t, *J*=7.5 Hz, 1H), 7.88 (d, *J*=8.5 Hz, 1H), 8.02 (d, *J*=8.5 Hz, 1H), 8.59 (s, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 21.0, 44.9, 110.7, 118.3, 119.5, 121.1, 121.5, 122.7, 124.1, 127.0, 127.2, 127.6, 128.3, 128.7, 141.3, 146.8, 152.3; FTIR (KBr) 3058, 2969, 2854, 1604, 1569, 1461, 1365, 1234 cm^{-1}.

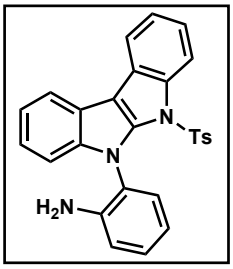
General procedure for iodine mediated intramolecular competitive experiment:

6a (0.5 mmol) was taken in a clean and dry reaction tube. To this iodine (0.6 mmol), Cs_2CO_3 (1.0 mmol) and acetonotrile (2 mL) were added. The reaction tube was stoppered and the resulting reaction

mixture was stirred at 60 °C. After 4 h the second portion of iodine (0.3 mmol) was added and reaction is allowed to stir at 60 °C. Upon completion of reaction as monitored by TLC, solvent was removed under vacuum in rotary evaporator and DCM was added. The crude reaction mixture was washed with saturated $Na_2S_2O_3$ solution (2 × 10 mL) and extracted with DCM. The organic layer was washed with water (1 × 10 mL). Combined organic layers were concentrated using rotary evaporator and residue is purified by column chromatography on silica gel using hexanes/ethyl acetate as an eluent to afford pure products **7a** and **7b**.



14,15-ditosyl-15H-benzo[4,5]imidazo[1,2-*a*]indolo[2,3-*b*]indol-(14H)-ol (7a): White solid, mp 198-200 °C; R_f 0.41 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 2.21 (s, 3H), 2.45 (s, 3H), 6.61 (d, *J*=7.6 Hz, 1H), 6.93 (d, *J*=8 Hz, 2H), 6.96 (dd, *J*=7.4, 1.2 Hz, 1H), 7.02 (dt, *J*=7.6, 1.6 Hz, 1H), 7.07-7.10 (m, 2H), 7.27 (d, *J*=8.0 Hz, 3H), 7.39 (d, *J*=8 Hz, 4H), 7.71 (dd, *J*=8, 1.6 Hz, 1H), 7.77 (dd, *J*=7.6, 1.2 Hz, 1H), 7.83 (d, *J*=8.0 Hz, 1H), 7.87 (d, *J*=8.8 Hz, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 21.4, 21.9, 87.5, 110.8, 111.9, 113.6, 113.7, 123.2, 123.4, 123.7, 124.6, 125.1, 125.3, 126.1, 128.0, 129.0, 129.8, 129.9, 132.6, 132.8, 134.4, 135.3, 138.9, 141.3, 143.5, 144.4, 145.2; FTIR (KBr) 3061, 2923, 2857, 1597, 1487, 1169 cm^{-1};



2-(6-tosylindolo[2,3-b]indol-5(6H)-yl)aniline (7b): Pale yellow solid, mp 105-107 °C; R_f 0.56 (20% ethyl acetate in hexanes); ^{1}H NMR ($CDCl_3$, 500 MHz, ppm) δ 2.24 (s, 3H), 6.89 (t, *J*=7.6 Hz, 1H), 7.12-7.20 (m, 2H), 7.23-7.27 (m, 1H), 7.28-7.32 (m, 2H), 7.33-7.40 (m, 2H), 7.46 (d, *J*=8.4 Hz, 2H), 7.76 (d, *J*= 7.2 Hz, 1H), 7.89 (d, *J*=7.6 Hz, 1H), 8.21 (d, *J*= 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125 MHz, ppm) δ 21.6, 112.4, 116.8, 116.9, 118.8, 118.9, 119.3, 120.9, 121.9, 122.8, 122.8, 125.1, 126.0, 127.1, 129.1, 129.5, 129.8, 134.0, 139.9, 141.6, 141.7, 143.9, 144.9; FTIR (KBr) 3472, 3382, 3056, 2925, 2857, 1615, 1509, 1456, 1375, 1262 cm^{-1};

Crystal data for compound 7a

Table 1. Crystal data and structure refinement for **7a**.

Identification code	**7a**
Empirical formula	C35 H28 Cl3 N3 O5 S2
Formula weight	741.07
Temperature	296(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 10.1831(2) A alpha = 90 deg.
	b = 17.6304(4) A beta = 92.2453(11) deg.
	c = 18.6382(5) A gamma = 90 deg.
Volume	3343.59(13) A^3
Z, Calculated density	4, 1.472 Mg/m^3
Absorption coefficient	0.447 mm^-1
F(000)	1528
Crystal size	0.350 x 0.250 x 0.250 mm
Theta range for data collection	1.590 to 25.000 deg.
Limiting indices	-12<=h<=12, -20<=k<=18, -22<=l<=22
Reflections collected / unique	26328 / 5880 [R(int) = 0.0276]
Completeness to theta = 25.000	100.0 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5880 / 0 / 436
Goodness-of-fit on F^2	1.023
Final R indices [I>2sigma(I)]	R1 = 0.0495, wR2 = 0.1330

R indices (all data) R1 = 0.0715, wR2 = 0.1514

Extinction coefficient n/a

Largest diff. peak and hole 0.495 and -0.485 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **7a**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	2960(3)	3370(2)	10259(2)	62(1)
C(2)	3468(4)	4066(3)	10038(2)	75(1)
C(3)	2769(4)	4557(2)	9599(2)	73(1)
C(4)	1523(4)	4366(2)	9352(2)	61(1)
C(5)	1006(3)	3675(2)	9548(2)	47(1)
C(6)	-315(3)	3348(2)	9332(2)	42(1)
C(7)	-418(3)	2619(2)	9828(2)	38(1)
C(8)	1705(3)	3185(2)	9998(2)	45(1)
C(9)	-366(3)	2989(2)	8598(2)	41(1)
C(10)	-250(3)	3336(2)	7941(2)	52(1)
C(11)	-393(3)	2903(2)	7324(2)	58(1)
C(12)	-598(3)	2132(2)	7371(2)	59(1)

C(13)	-709(3)	1772(2)	8028(2)	50(1)
C(14)	-623(3)	2223(2)	8638(2)	40(1)
C(15)	-1886(3)	1611(2)	9603(2)	44(1)
C(16)	-2530(4)	976(2)	9336(2)	63(1)
C(17)	-3624(4)	729(3)	9695(3)	80(1)
C(18)	-4035(4)	1098(3)	10295(2)	79(1)
C(19)	-3390(3)	1726(2)	10563(2)	63(1)
C(20)	-2307(3)	1975(2)	10214(2)	45(1)
C(21)	-964(3)	2763(2)	11806(2)	48(1)
C(22)	-1804(3)	2431(2)	12280(2)	62(1)
C(23)	-1309(3)	2145(2)	12922(2)	64(1)
C(24)	19(3)	2201(2)	13112(2)	54(1)
C(25)	839(3)	2516(2)	12616(2)	59(1)
C(26)	365(3)	2792(2)	11972(2)	55(1)
C(27)	560(4)	1957(3)	13838(2)	73(1)
C(28)	1909(3)	1206(2)	9608(2)	47(1)
C(29)	1179(3)	591(2)	9364(2)	62(1)
C(30)	1549(4)	199(2)	8760(2)	71(1)
C(31)	2616(4)	418(2)	8391(2)	67(1)
C(32)	3326(4)	1030(2)	8633(2)	76(1)
C(33)	2992(4)	1426(2)	9238(2)	68(1)
C(34)	3004(5)	-13(3)	7726(3)	109(2)
C(35)	2951(4)	5262(2)	2013(2)	75(1)
Cl(1)	1795(1)	4553(1)	1919(1)	118(1)
Cl(2)	3098(2)	5614(1)	2872(1)	111(1)

Cl(3)	4498(1)	4916(1)	1762(1)	107(1)
N(1)	-763(2)	1986(1)	9358(1)	38(1)
N(2)	-1469(2)	2608(1)	10347(1)	44(1)
N(3)	918(2)	2541(1)	10168(1)	42(1)
O(1)	-1382(2)	3878(1)	9368(1)	51(1)
O(2)	-728(3)	3813(1)	10856(1)	63(1)
O(3)	-2951(2)	3343(2)	11105(1)	68(1)
O(4)	2675(2)	1823(2)	10805(1)	71(1)
O(5)	424(2)	1297(1)	10697(1)	62(1)
S(1)	-1590(1)	3203(1)	11020(1)	51(1)
S(2)	1493(1)	1688(1)	10393(1)	51(1)

Table 3. Bond lengths [A] and angles [deg] for **7a**.

C(1)-C(8)	1.388(4)
C(1)-C(2)	1.400(6)
C(1)-H(1)	0.9300
C(2)-C(3)	1.371(6)
C(2)-H(2)	0.9300
C(3)-C(4)	1.375(5)
C(3)-H(3)	0.9300
C(4)-C(5)	1.381(5)
C(4)-H(4)	0.9300

C(5)-C(8)	1.383(5)
C(5)-C(6)	1.504(4)
C(6)-O(1)	1.436(4)
C(6)-C(9)	1.507(4)
C(6)-C(7)	1.590(4)
C(7)-N(1)	1.452(4)
C(7)-N(2)	1.472(4)
C(7)-N(3)	1.485(4)
C(8)-N(3)	1.432(4)
C(9)-C(14)	1.377(4)
C(9)-C(10)	1.378(4)
C(10)-C(11)	1.383(5)
C(10)-H(10)	0.9300
C(11)-C(12)	1.378(5)
C(11)-H(11)	0.9300
C(12)-C(13)	1.389(5)
C(12)-H(12)	0.9300
C(13)-C(14)	1.388(4)
C(13)-H(13)	0.9300
C(14)-N(1)	1.418(4)
C(15)-C(16)	1.379(5)
C(15)-C(20)	1.389(4)
C(15)-N(1)	1.412(4)
C(16)-C(17)	1.391(5)
C(16)-H(16)	0.9300

C(17)-C(18)	1.373(6)
C(17)-H(17)	0.9300
C(18)-C(19)	1.371(5)
C(18)-H(18)	0.9300
C(19)-C(20)	1.374(4)
C(19)-H(19)	0.9300
C(20)-N(2)	1.421(4)
C(21)-C(26)	1.377(4)
C(21)-C(22)	1.384(4)
C(21)-S(1)	1.756(3)
C(22)-C(23)	1.376(5)
C(22)-H(22)	0.9300
C(23)-C(24)	1.388(5)
C(23)-H(23)	0.9300
C(24)-C(25)	1.386(5)
C(24)-C(27)	1.504(5)
C(25)-C(26)	1.366(5)
C(25)-H(25)	0.9300
C(26)-H(26)	0.9300
C(27)-H(27A)	0.9600
C(27)-H(27B)	0.9600
C(27)-H(27C)	0.9600
C(28)-C(33)	1.378(4)
C(28)-C(29)	1.382(5)
C(28)-S(2)	1.758(3)

C(29)-C(30)	1.384(5)
C(29)-H(29)	0.9300
C(30)-C(31)	1.365(5)
C(30)-H(30)	0.9300
C(31)-C(32)	1.366(6)
C(31)-C(34)	1.518(6)
C(32)-C(33)	1.381(5)
C(32)-H(32)	0.9300
C(33)-H(33)	0.9300
C(34)-H(34A)	0.9600
C(34)-H(34B)	0.9600
C(34)-H(34C)	0.9600
C(35)-Cl(2)	1.719(4)
C(35)-Cl(1)	1.721(4)
C(35)-Cl(3)	1.770(5)
C(35)-H(35)	0.9800
N(2)-S(1)	1.644(3)
N(3)-S(2)	1.662(3)
O(1)-H(1A)	0.8200
O(2)-S(1)	1.428(2)
O(3)-S(1)	1.422(2)
O(4)-S(2)	1.422(2)
O(5)-S(2)	1.425(2)

C(8)-C(1)-C(2)	116.7(4)

C(8)-C(1)-H(1)	121.7
C(2)-C(1)-H(1)	121.7
C(3)-C(2)-C(1)	122.7(4)
C(3)-C(2)-H(2)	118.7
C(1)-C(2)-H(2)	118.7
C(2)-C(3)-C(4)	119.7(4)
C(2)-C(3)-H(3)	120.2
C(4)-C(3)-H(3)	120.2
C(3)-C(4)-C(5)	118.9(4)
C(3)-C(4)-H(4)	120.5
C(5)-C(4)-H(4)	120.5
C(4)-C(5)-C(8)	121.3(3)
C(4)-C(5)-C(6)	127.8(3)
C(8)-C(5)-C(6)	110.9(3)
O(1)-C(6)-C(5)	114.2(2)
O(1)-C(6)-C(9)	108.4(2)
C(5)-C(6)-C(9)	113.7(2)
O(1)-C(6)-C(7)	115.6(2)
C(5)-C(6)-C(7)	103.5(2)
C(9)-C(6)-C(7)	100.7(2)
N(1)-C(7)-N(2)	102.8(2)
N(1)-C(7)-N(3)	112.5(2)
N(2)-C(7)-N(3)	113.3(2)
N(1)-C(7)-C(6)	107.0(2)
N(2)-C(7)-C(6)	117.3(2)

N(3)-C(7)-C(6)	104.1(2)
C(5)-C(8)-C(1)	120.7(3)
C(5)-C(8)-N(3)	110.5(3)
C(1)-C(8)-N(3)	128.6(3)
C(14)-C(9)-C(10)	120.5(3)
C(14)-C(9)-C(6)	111.3(3)
C(10)-C(9)-C(6)	128.2(3)
C(9)-C(10)-C(11)	118.9(3)
C(9)-C(10)-H(10)	120.5
C(11)-C(10)-H(10)	120.5
C(12)-C(11)-C(10)	120.2(3)
C(12)-C(11)-H(11)	119.9
C(10)-C(11)-H(11)	119.9
C(11)-C(12)-C(13)	121.7(3)
C(11)-C(12)-H(12)	119.2
C(13)-C(12)-H(12)	119.2
C(14)-C(13)-C(12)	117.1(3)
C(14)-C(13)-H(13)	121.5
C(12)-C(13)-H(13)	121.5
C(9)-C(14)-C(13)	121.5(3)
C(9)-C(14)-N(1)	111.5(2)
C(13)-C(14)-N(1)	126.9(3)
C(16)-C(15)-C(20)	120.9(3)
C(16)-C(15)-N(1)	130.0(3)
C(20)-C(15)-N(1)	109.2(3)

C(15)-C(16)-C(17)	117.3(4)
C(15)-C(16)-H(16)	121.4
C(17)-C(16)-H(16)	121.4
C(18)-C(17)-C(16)	121.3(4)
C(18)-C(17)-H(17)	119.4
C(16)-C(17)-H(17)	119.4
C(19)-C(18)-C(17)	121.4(4)
C(19)-C(18)-H(18)	119.3
C(17)-C(18)-H(18)	119.3
C(18)-C(19)-C(20)	117.9(4)
C(18)-C(19)-H(19)	121.1
C(20)-C(19)-H(19)	121.1
C(19)-C(20)-C(15)	121.3(3)
C(19)-C(20)-N(2)	131.0(3)
C(15)-C(20)-N(2)	107.7(2)
C(26)-C(21)-C(22)	120.0(3)
C(26)-C(21)-S(1)	119.5(2)
C(22)-C(21)-S(1)	120.4(3)
C(23)-C(22)-C(21)	119.7(3)
C(23)-C(22)-H(22)	120.1
C(21)-C(22)-H(22)	120.1
C(22)-C(23)-C(24)	121.0(3)
C(22)-C(23)-H(23)	119.5
C(24)-C(23)-H(23)	119.5
C(25)-C(24)-C(23)	117.8(3)

C(25)-C(24)-C(27)	120.3(3)
C(23)-C(24)-C(27)	121.9(3)
C(26)-C(25)-C(24)	121.8(3)
C(26)-C(25)-H(25)	119.1
C(24)-C(25)-H(25)	119.1
C(25)-C(26)-C(21)	119.6(3)
C(25)-C(26)-H(26)	120.2
C(21)-C(26)-H(26)	120.2
C(24)-C(27)-H(27A)	109.5
C(24)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(24)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(33)-C(28)-C(29)	119.1(3)
C(33)-C(28)-S(2)	120.2(3)
C(29)-C(28)-S(2)	120.6(3)
C(28)-C(29)-C(30)	119.9(3)
C(28)-C(29)-H(29)	120.0
C(30)-C(29)-H(29)	120.0
C(31)-C(30)-C(29)	121.1(4)
C(31)-C(30)-H(30)	119.4
C(29)-C(30)-H(30)	119.4
C(30)-C(31)-C(32)	118.5(4)
C(30)-C(31)-C(34)	120.6(4)

C(32)-C(31)-C(34)	120.9(4)
C(31)-C(32)-C(33)	121.7(4)
C(31)-C(32)-H(32)	119.2
C(33)-C(32)-H(32)	119.2
C(28)-C(33)-C(32)	119.6(4)
C(28)-C(33)-H(33)	120.2
C(32)-C(33)-H(33)	120.2
C(31)-C(34)-H(34A)	109.5
C(31)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(31)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
Cl(2)-C(35)-Cl(1)	113.1(3)
Cl(2)-C(35)-Cl(3)	108.9(2)
Cl(1)-C(35)-Cl(3)	109.6(2)
Cl(2)-C(35)-H(35)	108.4
Cl(1)-C(35)-H(35)	108.4
Cl(3)-C(35)-H(35)	108.4
C(15)-N(1)-C(14)	123.8(2)
C(15)-N(1)-C(7)	110.2(2)
C(14)-N(1)-C(7)	108.2(2)
C(20)-N(2)-C(7)	110.0(2)
C(20)-N(2)-S(1)	124.9(2)
C(7)-N(2)-S(1)	124.91(19)

C(8)-N(3)-C(7)	110.1(2)
C(8)-N(3)-S(2)	125.3(2)
C(7)-N(3)-S(2)	119.97(19)
C(6)-O(1)-H(1A)	109.5
O(3)-S(1)-O(2)	120.19(16)
O(3)-S(1)-N(2)	107.33(14)
O(2)-S(1)-N(2)	104.60(13)
O(3)-S(1)-C(21)	107.95(15)
O(2)-S(1)-C(21)	107.73(15)
N(2)-S(1)-C(21)	108.59(15)
O(4)-S(2)-O(5)	120.67(15)
O(4)-S(2)-N(3)	105.43(15)
O(5)-S(2)-N(3)	105.71(14)
O(4)-S(2)-C(28)	107.76(16)
O(5)-S(2)-C(28)	108.08(16)
N(3)-S(2)-C(28)	108.71(13)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **7a**.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	51(2)	83(3)	52(2)	-14(2)	0(2)	-14(2)
C(2)	58(2)	89(3)	79(3)	-31(2)	14(2)	-37(2)
C(3)	78(3)	64(3)	79(3)	-11(2)	21(2)	-29(2)
C(4)	68(2)	52(2)	64(2)	-4(2)	15(2)	-17(2)
C(5)	50(2)	49(2)	41(2)	-6(1)	8(1)	-12(2)
C(6)	43(2)	44(2)	39(2)	2(1)	4(1)	-2(1)
C(7)	40(2)	42(2)	32(1)	-1(1)	3(1)	-4(1)
C(8)	42(2)	55(2)	39(2)	-9(1)	6(1)	-12(1)
C(9)	38(2)	50(2)	35(2)	2(1)	2(1)	0(1)
C(10)	51(2)	61(2)	44(2)	11(2)	9(1)	-2(2)
C(11)	49(2)	90(3)	35(2)	9(2)	9(1)	4(2)
C(12)	53(2)	86(3)	37(2)	-11(2)	1(1)	4(2)
C(13)	51(2)	59(2)	41(2)	-9(2)	-1(1)	3(2)
C(14)	35(1)	51(2)	34(2)	0(1)	-1(1)	0(1)
C(15)	43(2)	43(2)	46(2)	5(1)	-3(1)	-7(1)
C(16)	67(2)	57(2)	63(2)	-6(2)	-3(2)	-16(2)
C(17)	70(2)	74(3)	96(3)	1(2)	-3(2)	-39(2)
C(18)	62(2)	91(3)	84(3)	3(2)	12(2)	-33(2)
C(19)	54(2)	79(3)	59(2)	2(2)	13(2)	-16(2)
C(20)	42(2)	50(2)	44(2)	3(1)	2(1)	-7(1)
C(21)	45(2)	59(2)	39(2)	-8(2)	7(1)	-7(2)

C(22)	42(2)	92(3)	52(2)	2(2)	7(2)	-14(2)
C(23)	58(2)	85(3)	48(2)	7(2)	10(2)	-15(2)
C(24)	55(2)	57(2)	49(2)	-8(2)	7(2)	1(2)
C(25)	41(2)	79(3)	57(2)	-13(2)	6(2)	-4(2)
C(26)	48(2)	73(2)	45(2)	-10(2)	13(2)	-14(2)
C(27)	71(2)	91(3)	58(2)	2(2)	-2(2)	9(2)
C(28)	44(2)	49(2)	49(2)	11(2)	0(1)	4(1)
C(29)	57(2)	51(2)	80(3)	11(2)	9(2)	-7(2)
C(30)	69(2)	51(2)	93(3)	-14(2)	3(2)	-1(2)
C(31)	64(2)	58(2)	78(3)	-5(2)	7(2)	9(2)
C(32)	70(2)	76(3)	86(3)	-8(2)	30(2)	-11(2)
C(33)	60(2)	65(2)	79(3)	-7(2)	15(2)	-17(2)
C(34)	108(4)	105(4)	116(4)	-44(3)	30(3)	10(3)
C(35)	91(3)	63(2)	70(3)	12(2)	-15(2)	-9(2)
Cl(1)	97(1)	79(1)	177(2)	-19(1)	-3(1)	-24(1)
Cl(2)	171(1)	86(1)	73(1)	-13(1)	-16(1)	9(1)
Cl(3)	97(1)	118(1)	105(1)	3(1)	5(1)	-3(1)
N(1)	41(1)	41(1)	33(1)	-1(1)	1(1)	-5(1)
N(2)	46(1)	49(2)	38(1)	-4(1)	8(1)	-9(1)
N(3)	40(1)	50(2)	37(1)	0(1)	-2(1)	-6(1)
O(1)	54(1)	53(1)	47(1)	4(1)	2(1)	4(1)
O(2)	88(2)	49(1)	52(1)	-8(1)	14(1)	-11(1)
O(3)	60(1)	86(2)	59(2)	-4(1)	13(1)	17(1)
O(4)	60(1)	96(2)	54(2)	10(1)	-22(1)	1(1)
O(5)	65(1)	72(2)	49(1)	24(1)	6(1)	-4(1)

S(1)	57(1)	55(1)	42(1)	-5(1)	11(1)	0(1)
S(2)	50(1)	64(1)	39(1)	12(1)	-5(1)	0(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **7a**.

	x	y	z	U(eq)
H(1)	3439	3047	10564	75
H(2)	4313	4201	10196	90
H(3)	3137	5018	9469	88
H(4)	1036	4696	9057	73
H(10)	-77	3853	7913	62
H(11)	-352	3133	6876	69
H(12)	-663	1846	6952	70
H(13)	-836	1250	8058	60
H(16)	-2245	724	8933	75
H(17)	-4085	306	9526	96
H(18)	-4767	918	10525	94
H(19)	-3677	1976	10968	76
H(22)	-2700	2401	12165	74

H(23)	-1873	1910	13234	76
H(25)	1737	2541	12726	71
H(26)	937	2997	11647	66
H(27A)	376	2340	14186	110
H(27B)	1494	1888	13820	110
H(27C)	157	1489	13971	110
H(29)	440	440	9605	75
H(30)	1062	-220	8604	85
H(32)	4054	1184	8384	92
H(33)	3494	1839	9396	82
H(34A)	2693	-526	7752	164
H(34B)	3944	-14	7700	164
H(34C)	2621	228	7306	164
H(35)	2692	5678	1689	90
H(1A)	-1256	4158	9715	77

Table 6. Torsion angles [deg] for **7a**.

C(8)-C(1)-C(2)-C(3)	1.3(6)
C(1)-C(2)-C(3)-C(4)	-0.8(6)
C(2)-C(3)-C(4)-C(5)	-0.6(6)
C(3)-C(4)-C(5)-C(8)	1.5(5)
C(3)-C(4)-C(5)-C(6)	-179.0(3)

C(4)-C(5)-C(6)-O(1)	-44.4(4)
C(8)-C(5)-C(6)-O(1)	135.2(3)
C(4)-C(5)-C(6)-C(9)	80.8(4)
C(8)-C(5)-C(6)-C(9)	-99.6(3)
C(4)-C(5)-C(6)-C(7)	-170.9(3)
C(8)-C(5)-C(6)-C(7)	8.7(3)
O(1)-C(6)-C(7)-N(1)	105.8(3)
C(5)-C(6)-C(7)-N(1)	-128.6(2)
C(9)-C(6)-C(7)-N(1)	-10.8(3)
O(1)-C(6)-C(7)-N(2)	-8.9(4)
C(5)-C(6)-C(7)-N(2)	116.7(3)
C(9)-C(6)-C(7)-N(2)	-125.5(2)
O(1)-C(6)-C(7)-N(3)	-134.9(2)
C(5)-C(6)-C(7)-N(3)	-9.3(3)
C(9)-C(6)-C(7)-N(3)	108.5(2)
C(4)-C(5)-C(8)-C(1)	-1.0(5)
C(6)-C(5)-C(8)-C(1)	179.4(3)
C(4)-C(5)-C(8)-N(3)	175.1(3)
C(6)-C(5)-C(8)-N(3)	-4.5(3)
C(2)-C(1)-C(8)-C(5)	-0.4(5)
C(2)-C(1)-C(8)-N(3)	-175.7(3)
O(1)-C(6)-C(9)-C(14)	-115.0(3)
C(5)-C(6)-C(9)-C(14)	116.8(3)
C(7)-C(6)-C(9)-C(14)	6.7(3)
O(1)-C(6)-C(9)-C(10)	61.9(4)

C(5)-C(6)-C(9)-C(10)	-66.3(4)
C(7)-C(6)-C(9)-C(10)	-176.3(3)
C(14)-C(9)-C(10)-C(11)	0.0(4)
C(6)-C(9)-C(10)-C(11)	-176.7(3)
C(9)-C(10)-C(11)-C(12)	-2.5(5)
C(10)-C(11)-C(12)-C(13)	2.1(5)
C(11)-C(12)-C(13)-C(14)	0.8(5)
C(10)-C(9)-C(14)-C(13)	3.1(4)
C(6)-C(9)-C(14)-C(13)	-179.7(3)
C(10)-C(9)-C(14)-N(1)	-177.4(3)
C(6)-C(9)-C(14)-N(1)	-0.2(3)
C(12)-C(13)-C(14)-C(9)	-3.5(4)
C(12)-C(13)-C(14)-N(1)	177.1(3)
C(20)-C(15)-C(16)-C(17)	1.2(5)
N(1)-C(15)-C(16)-C(17)	179.7(3)
C(15)-C(16)-C(17)-C(18)	-0.7(6)
C(16)-C(17)-C(18)-C(19)	0.3(7)
C(17)-C(18)-C(19)-C(20)	-0.5(6)
C(18)-C(19)-C(20)-C(15)	1.0(5)
C(18)-C(19)-C(20)-N(2)	178.1(4)
C(16)-C(15)-C(20)-C(19)	-1.4(5)
N(1)-C(15)-C(20)-C(19)	179.8(3)
C(16)-C(15)-C(20)-N(2)	-179.1(3)
N(1)-C(15)-C(20)-N(2)	2.1(3)
C(26)-C(21)-C(22)-C(23)	1.4(6)

S(1)-C(21)-C(22)-C(23)	-174.6(3)
C(21)-C(22)-C(23)-C(24)	1.7(6)
C(22)-C(23)-C(24)-C(25)	-3.5(6)
C(22)-C(23)-C(24)-C(27)	174.2(4)
C(23)-C(24)-C(25)-C(26)	2.4(5)
C(27)-C(24)-C(25)-C(26)	-175.4(4)
C(24)-C(25)-C(26)-C(21)	0.5(5)
C(22)-C(21)-C(26)-C(25)	-2.4(5)
S(1)-C(21)-C(26)-C(25)	173.5(3)
C(33)-C(28)-C(29)-C(30)	0.7(5)
S(2)-C(28)-C(29)-C(30)	-177.5(3)
C(28)-C(29)-C(30)-C(31)	-1.1(6)
C(29)-C(30)-C(31)-C(32)	0.6(6)
C(29)-C(30)-C(31)-C(34)	-179.5(4)
C(30)-C(31)-C(32)-C(33)	0.2(7)
C(34)-C(31)-C(32)-C(33)	-179.7(5)
C(29)-C(28)-C(33)-C(32)	0.1(6)
S(2)-C(28)-C(33)-C(32)	178.3(3)
C(31)-C(32)-C(33)-C(28)	-0.6(7)
C(16)-C(15)-N(1)-C(14)	51.5(5)
C(20)-C(15)-N(1)-C(14)	-129.8(3)
C(16)-C(15)-N(1)-C(7)	-178.1(3)
C(20)-C(15)-N(1)-C(7)	0.5(3)
C(9)-C(14)-N(1)-C(15)	123.8(3)
C(13)-C(14)-N(1)-C(15)	-56.7(4)

C(9)-C(14)-N(1)-C(7)	-7.3(3)
C(13)-C(14)-N(1)-C(7)	172.1(3)
N(2)-C(7)-N(1)-C(15)	-2.7(3)
N(3)-C(7)-N(1)-C(15)	119.5(2)
C(6)-C(7)-N(1)-C(15)	-126.9(2)
N(2)-C(7)-N(1)-C(14)	135.4(2)
N(3)-C(7)-N(1)-C(14)	-102.3(3)
C(6)-C(7)-N(1)-C(14)	11.3(3)
C(19)-C(20)-N(2)-C(7)	178.7(3)
C(15)-C(20)-N(2)-C(7)	-3.9(3)
C(19)-C(20)-N(2)-S(1)	3.0(5)
C(15)-C(20)-N(2)-S(1)	-179.6(2)
N(1)-C(7)-N(2)-C(20)	4.0(3)
N(3)-C(7)-N(2)-C(20)	-117.6(3)
C(6)-C(7)-N(2)-C(20)	121.0(3)
N(1)-C(7)-N(2)-S(1)	179.7(2)
N(3)-C(7)-N(2)-S(1)	58.0(3)
C(6)-C(7)-N(2)-S(1)	-63.3(3)
C(5)-C(8)-N(3)-C(7)	-2.1(3)
C(1)-C(8)-N(3)-C(7)	173.5(3)
C(5)-C(8)-N(3)-S(2)	153.6(2)
C(1)-C(8)-N(3)-S(2)	-30.8(4)
N(1)-C(7)-N(3)-C(8)	122.7(2)
N(2)-C(7)-N(3)-C(8)	-121.2(3)
C(6)-C(7)-N(3)-C(8)	7.3(3)

N(1)-C(7)-N(3)-S(2)	-34.5(3)
N(2)-C(7)-N(3)-S(2)	81.6(3)
C(6)-C(7)-N(3)-S(2)	-149.92(19)
C(20)-N(2)-S(1)-O(3)	-40.5(3)
C(7)-N(2)-S(1)-O(3)	144.5(2)
C(20)-N(2)-S(1)-O(2)	-169.2(3)
C(7)-N(2)-S(1)-O(2)	15.8(3)
C(20)-N(2)-S(1)-C(21)	76.0(3)
C(7)-N(2)-S(1)-C(21)	-99.0(3)
C(26)-C(21)-S(1)-O(3)	-158.5(3)
C(22)-C(21)-S(1)-O(3)	17.5(3)
C(26)-C(21)-S(1)-O(2)	-27.3(3)
C(22)-C(21)-S(1)-O(2)	148.7(3)
C(26)-C(21)-S(1)-N(2)	85.5(3)
C(22)-C(21)-S(1)-N(2)	-98.6(3)
C(8)-N(3)-S(2)-O(4)	35.9(3)
C(7)-N(3)-S(2)-O(4)	-170.6(2)
C(8)-N(3)-S(2)-O(5)	164.7(2)
C(7)-N(3)-S(2)-O(5)	-41.7(2)
C(8)-N(3)-S(2)-C(28)	-79.4(3)
C(7)-N(3)-S(2)-C(28)	74.1(2)
C(33)-C(28)-S(2)-O(4)	-42.4(3)
C(29)-C(28)-S(2)-O(4)	135.8(3)
C(33)-C(28)-S(2)-O(5)	-174.3(3)
C(29)-C(28)-S(2)-O(5)	3.9(3)

C(33)-C(28)-S(2)-N(3)	71.4(3)
C(29)-C(28)-S(2)-N(3)	-110.4(3)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for **7a** [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

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