Ruthenium-catalyzed tandem annulation/arylation for the synthesis of unsymmetrical bis(heteroaryl)methanes

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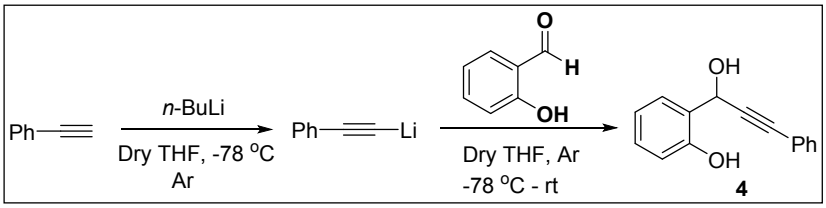
1. General information:

All reagents were purchased from commercial sources and used without further purification. ^{1}H NMR spectra were determined on 400 MHz spectrometer as solutions in $CDCl_3$. Chemical shifts are expressed in parts per million (δ) and the signals were reported as s (singlet), d (doublet), t (triplet), m (multiplet) and coupling constants (J) were given in Hz. $^{13}C\{^{1}H\}$ NMR spectra were recorded at 100 MHz in $CDCl_3$ solution. Chemical shifts as internal standard are referenced to $CDCl_3$ (δ = 7.26 for ^{1}H and δ = 77.16 for $^{13}C\{^{1}H\}$ NMR) as internal standard. TLC was done on silica gel coated glass slide. All solvents were dried and distilled before use. Commercially available solvents were freshly distilled before the reaction. All reactions involving moisture sensitive reactants were executed using oven dried glassware. All 2-substituted indoles were prepared by the reported method.[1]

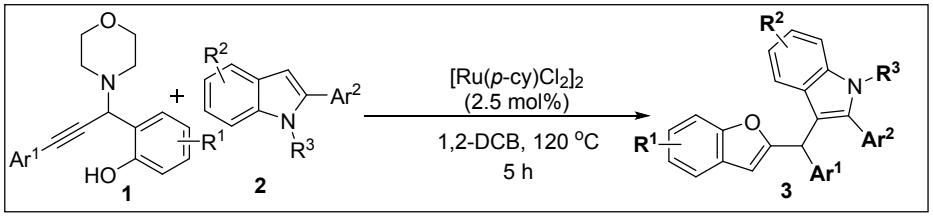
2. Experimental procedures:

2.1 Typical experimental procedure for the synthesis of compound 4:[2]



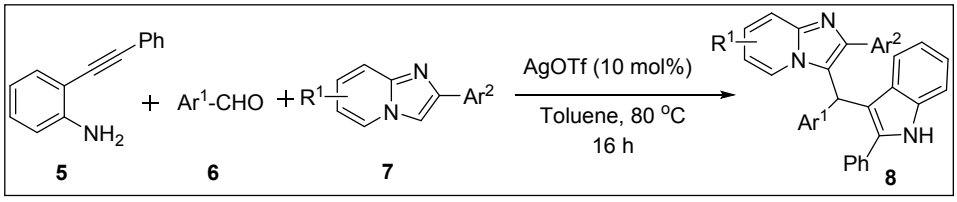
n-Butyl lithium (4 mL, 2.5 M in hexane) was added to a solution of phenylacetylene (1.12 g, 11 mmol) in dry THF (15 mL) at -78 °C under Ar atmosphere. The reaction mixture was allowed to stir at this temperature for 30 min. Salicylaldehyde (0.61 g, 5 mmol) in dry THF (5 mL) was then slowly added at -78 °C. The reaction mixture was naturally warmed to room temperature and kept stirring overnight. After quenched by 1(M) HCl solution, the reaction mixture was extracted with EtOAc. The organic layers were dried with anhydrous Na_2SO_4. The crude residue was obtained after evaporating the solvent in vacuum and was purified by column chromatography on silica gel using a mixture petroleum ether and ethyl acetate (90:10) as an eluting solvent to afford the pure product 2-(1-hydroxyprop-2-yn-1-yl)phenol (**4**) (750 mg, 67%) as a white solid.

2.2 Typical experimental procedure for the synthesized compounds (3aa-3ai):



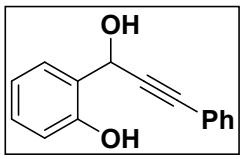
A mixture of 2-(1-morpholino-3-phenylprop-2-yn-1-yl)phenol (0.2 mmol, 58.6 mg) (**1a**) and 2-phenylindole (0.2 mmol, 38.6 mg) (**2a**) was taken in 1,2-DCB (2.0 ml) in an oven dried reaction tube. Then dichloro(*p*-cymene)ruthenium(II) dimer (2.5 mol%, 3 mg) was added to it and stirred at 120 °C for 5 h under open atmosphere. After completion of the reaction (TLC) the reaction was cooled to room temperature and extracted with dichloromethane. The organic phase was dried over anhydrous Na_2SO_4. The crude residue was obtained after evaporating the solvent in vacuum and was purified by column chromatography on silica gel using a mixture petroleum ether and ethyl acetate (94:6) as an eluting solvent to afford the pure product (**3aa**) (67 mg, 84%) as a white solid.

2. 2. Typical experimental procedure for the synthesized compounds (8a-8d):

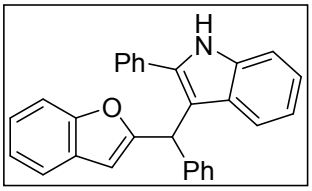


A mixture of 2-(phenylethynyl)aniline (0.1 mmol, 19.3 mg) (**5**), benzaldehyde (0.2 mmol, 21 mg) (**6**), and 7-methyl-2-phenylimidazo[1,2-*a*]pyridine (0.1 mmol, 20.8 mg) (**7**) was taken in an oven dried reaction tube in presence of silver trifluoromethanesulfonate (10 mol%, 5 mg) in toluene (2.0 mL) and stirred at 80 °C for 16 h under open atmosphere. After completion of the reaction (TLC) the reaction was cooled to room temperature and extracted with ethyl acetate. The organic phase was dried over anhydrous Na_2SO_4. The crude residue was obtained after evaporating the solvent in vacuum and was purified by column chromatography on silica gel using a mixture petroleum ether and ethyl acetate (76:24) as an eluting solvent to afford the pure product (**8a**) (62%, 60 mg) as a white solid.

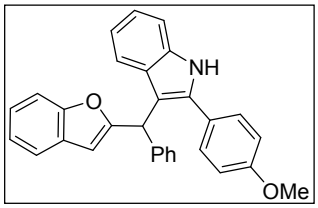
3. Characterization data for the synthesized products:



2-(1-Hydroxy-3-phenylprop-2-yn-1-yl)phenol (**4**): White solid (67%, 750 mg); R_f = 0.50 (PE : EA = 90 : 10); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38-7.33 (m, 3H), 7.24-7.18 (m, 3H), 7.15-7.10 (m, 1H), 6.83-6.79 (m, 2H), 5.80 (s, 1H), 3.33 (br s, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 155.1, 131.9, 130.2, 128.9, 128.4, 127.9, 124.8, 122.1, 120.4, 117.1, 88.1, 86.8, 64.2.

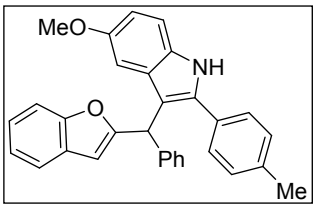


3-(Benzofuran-2-yl(phenyl)methyl)-2-phenyl-1*H*-indole (3aa): White solid (84%, 67 mg); R_f = 0.50 (PE : EA = 94 :6); M.p. 151-152 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00 (s, 1H), 7.45-7.40 (m, 3H), 7.39-7.30 (m, 5H), 7.28-7.17 (m, 6H), 7.16-7.09 (m, 3H), 6.92 (t, J = 7.6 Hz, 1H), 6.38 (s, 1H), 5.91 (s, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 160.2, 155.1, 141.5, 136.1, 136.0, 132.5, 128.9, 128.8, 128.7, 128.6, 128.4, 128.3, 128.1, 126.7, 123.5, 122.6, 122.2, 121.2, 120.6, 120.0, 112.0, 111.3, 111.0, 105.4, 42.5. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{29}H_{22}NO$: 400.1696; found: 400.1699.

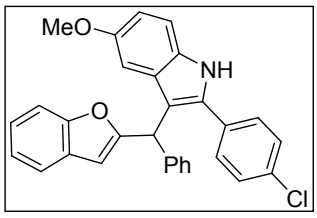


3-(Benzofuran-2-yl(phenyl)methyl)-2-(4-methoxyphenyl)-1*H*-indole (3ab): Brown gummy mass (76%, 65 mg); R_f = 0.55 (PE : EA = 93 : 7); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.11 (s, 1H), 7.46-7.41 (m, 3H), 7.38-7.31 (m, 3H), 7.29-7.26 (m, 4H), 7.20-7.11 (m, 4H), 6.98-6.91 (m, 3H), 6.40 (s, 1H), 5.89 (s, 1H), 3.84 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 160.3, 159.7, 155.1, 141.6, 136.08, 136.01, 130.0, 128.79, 128.70, 128.4, 128.2, 126.7, 126.1, 125.0, 123.5, 122.5,

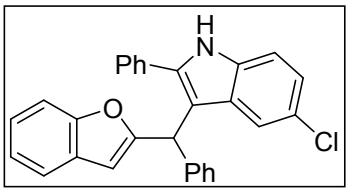
122.0, 121.0, 120.6, 119.9, 114.4, 111.3, 110.8, 105.4, 55.5, 42.6; Anal. Calcd for $C_{30}H_{23}NO_2$: C, 83.89; H, 5.40; N, 3.26%; Found: C, 84.11; H, 5.44; N, 3.21%.



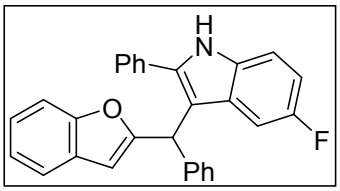
3-(Benzofuran-2-yl(phenyl)methyl)-5-methoxy-2-(*p*-tolyl)-1*H*-indole (**3ac**): Brown gummy mass (73%, 64 mg); R_f = 0.45 (PE : EA = 94 : 6); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02 (s, 1H), 7.46-7.44 (m, 1H), 7.39-7.37 (m, 3H), 7.29-7.22 (m, 8H), 7.21-7.17 (m, 2H), 6.80-6.77 (m, 1H), 6.72 (d, J = 2.4 Hz, 1H), 6.41 (s, 1H), 5.90 (s, 1H), 3.51 (s, 3H), 2.39 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 160.3, 155.1, 153.9, 141.6, 138.2, 136.9, 131.2, 129.8, 129.7, 128.77, 128.73, 128.4, 128.2, 127.8, 126.7, 123.6, 122.6, 120.6, 112.2, 111.7, 111.5, 111.3, 105.5, 102.8, 55.6, 42.6, 21.4; Anal. Calcd for $C_{31}H_{25}NO_2$: C, 83.95; H, 5.68; N, 3.16%; Found: C, 83.71; H, 5.62; N, 3.24%.



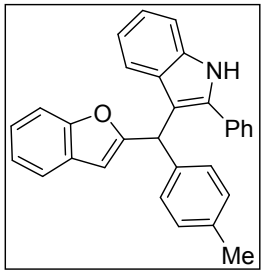
3-(Benzofuran-2-yl(phenyl)methyl)-2-(4-chlorophenyl)-5-methoxy-1*H*-indole (**3ad**): White solid (78%, 72 mg); R_f = 0.45 (PE : EA = 94 : 6); M.p. 177-178 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00 (s, 1H), 7.44-7.42 (m, 1H), 737-7.34 (m, 5H), 7.27-7.21 (m, 6H), 7.19-7.15 (m, 2H), 6.81-6.78 (m, 1H), 6.69 (s, 1H), 6.37 (s, 1H), 5.82 (s, 1H), 3.48 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 160.0, 155.1, 154.1, 141.3, 135.5, 134.3, 131.4, 131.2, 129.8, 129.2, 128.7, 128.6, 128.5, 128.2, 126.9, 123.7, 122.7, 120.7, 112.8, 112.4, 111.7, 111.3, 105.6, 102.7, 55.6, 42.6; Anal. Calcd for $C_{30}H_{22}ClNO_2$: C, 77.66; H, 4.78; N, 3.02%; Found: C, 77.47; H, 4.81; N, 3.08%.



3-(Benzofuran-2-yl(phenyl)methyl)-5-chloro-2-phenyl-1*H*-indole (3ae): Brown solid (75%, 64 mg); R_f = 0.40 (PE : EA = 95 : 5); M.p. 140-141 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.24 (s, 1H), 7.56-7.49 (m, 4H), 7.48-7.39 (m, 4H), 7.36-7.27 (m, 7H), 7.26-7.24 (m, 1H), 7.17-7.15 (m, 1H), 6.48 (s, 1H), 5.96 (s, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 159.6, 155.1, 141.0, 137.5, 134.5, 132.1, 129.1, 128.75, 128.71, 128.59, 128.57, 127.2, 126.9, 125.6, 123.7, 122.7, 120.8, 120.5, 119.6, 112.1, 112.0, 111.8, 111.3, 105.5, 42.3; Anal. Calcd for $C_{29}H_{20}ClNO$: C, 80.27; H, 4.65; N, 3.23%; Found: C, 80.42; H, 4.70; N, 3.19%.

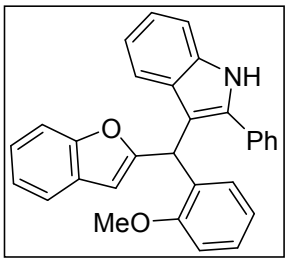


3-(Benzofuran-2-yl(phenyl)methyl)-5-fluoro-2-phenyl-1*H*-indole (**3af**): Brown gummy mass (74%, 61 mg); R_f = 0.50 (PE : EA = 93 : 7); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.15 (s, 1H), 7.50-7.39 (m, 6H), 7.38-7.36 (m, 1H), 7.29-7.22 (m, 6H), 7.20-7.16 (m, 2H), 7.01-6.98 (m, 1H), 6.91-6.86 (m, 1H), 6.40 (s, 1H), 5.89 (s, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 159.3 ($J_{C\text{-}F}$ = 85.0 Hz), 155.1, 141.1, 137.9, 132.7, 132.3, 129.1, 128.7, 128.68, 128.63, 128.5, 126.9, 123.7, 122.7, 120.8, 112.3 ($J_{C\text{-}F}$ = 5.0 Hz), 111.6, 111.5, 111.3, 110.9, 110.6, 106.2, 106.0, 105.4, 42.4; Anal. Calcd for $C_{29}H_{20}FNO$: C, 83.43; H, 4.83; N, 3.36%; Found: C, 83.22; H, 4.79; N, 3.43%.

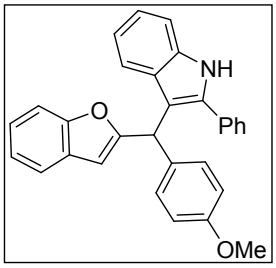


3-(Benzofuran-2-yl(*p*-tolyl)methyl)-2-phenyl-1*H*-indole (**3ba**): Brown gummy mass (81%, 66 mg); R_f = 0.55 (PE : EA = 95 : 5); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.14 (s, 1H), 7.53-7.51 (m, 2H), 7.47-7.42 (m, 3H), 7.41-7.37 (m, 4H), 7.20-7.14 (m, 5H), 7.09 (d, J = 8.0 Hz, 2H), 6.98-

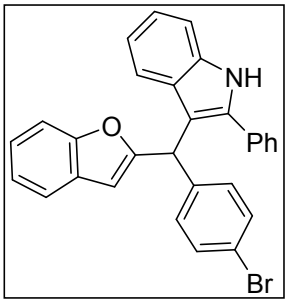
6.94 (m, 1H), 6.42 (s, 1H), 5.91 (s, 1H), 2.33 (s, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 160.5, 158.1, 138.4, 136.2, 136.1, 136.0, 132.7, 129.1, 128.9, 128.8, 128.7, 128.5, 128.3, 128.2, 123.5, 122.5, 122.2, 121.3, 120.6, 120.0, 112.2, 111.3, 110.9, 105.3, 42.2, 21.2; Anal. Calcd for $C_{30}H_{23}NO$: C, 87.14; H, 5.61; N, 3.39%; Found: C, 87.31; H, 5.58; N, 3.34%.



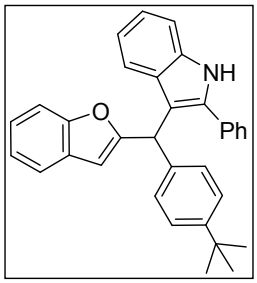
3-(Benzofuran-2-yl(2-methoxyphenyl)methyl)-2-phenyl-1*H*-indole (**3ca**): Brown gummy mass (72%, 61 mg); R_f = 0.45 (PE : EA = 94 : 6); ^1H NMR (400 MHz, $CDCl_3$): δ 8.14 (s, 1H), 7.49-7.47 (m, 2H), 7.44-7.40 (m, 4H), 7.39-7.33 (m, 4H), 7.23-7.20 (m, 1H), 7.17-7.12 (m, 3H), 6.96-6.92 (m, 1H), 6.90-6.84 (m, 2H), 6.34 (s, 1H), 6.26 (s, 1H), 3.59 (s, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 160.3, 157.1, 155.2, 136.1, 136.0, 133.2, 130.2, 130.0, 129.8, 128.9, 128.7, 128.6, 128.1, 128.0, 127.1, 123.3, 122.4, 122.0, 121.0, 120.5, 119.9, 111.7, 111.2, 110.9, 110.8, 105.1, 55.4, 41.5; Anal. Calcd for $C_{30}H_{23}NO_2$: C, 83.89; H, 5.40; N, 3.26%; Found: C, 83.69; H, 5.43; N, 3.33%.



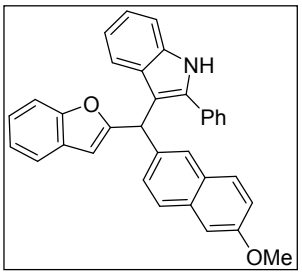
3-(Benzofuran-2-yl(4-methoxyphenyl)methyl)-2-phenyl-1*H*-indole (**3da**): Yellow solid (71%, 60 mg); R_f = 0.45 (PE : EA = 92 : 8); M.p. 196-197 °C; ^1H NMR (400 MHz, $CDCl_3$): δ 8.15 (s, 1H), 7.52-7.50 (m, 2H), 7.47-7.44 (m, 3H), 7.42-7.36 (m, 4H), 7.23-7.16 (m, 5H), 6.96 (t, J = 8.0 Hz, 1H), 6.82 (d, J = 8.8 Hz, 2H), 6.41 (s, 1H), 5.89 (s, 1H), 3.78 (s, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 160.6, 158.3, 155.1, 136.2, 135.9, 133.6, 132.7, 129.7, 128.9, 128.7, 128.4, 128.3, 128.2, 123.5, 122.5, 122.2, 121.2, 120.6, 120.0, 113.8, 112.3, 111.3, 110.9, 105.2, 55.3, 41.8; Anal. Calcd for $C_{30}H_{23}NO_2$: C, 83.89; H, 5.40; N, 3.26%; Found: C, 83.73; H, 5.35; N, 3.34%.



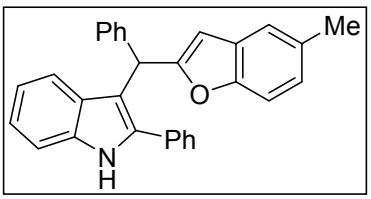
3-(Benzofuran-2-yl(4-bromophenyl)methyl)-2-phenyl-1*H*-indole (**3ea**): Brown gummy mass (61%, 58 mg); R_f = 0.50 (PE : EA = 93 : 7); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.19 (s, 1H), 7.50-7.46 (m, 4H), 7.45-7.37 (m, 5H), 7.31 (d, J = 8.0 Hz, 1H), 7.23-7.12 (m, 6H), 6.98-6.94 (m, 1H), 6.43 (s, 1H), 5.87 (s, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 159.4, 155.1, 140.6, 136.1, 132.5, 131.5, 130.4, 129.1, 128.7, 128.5, 128.2, 127.9, 127.2, 123.8, 122.7, 122.4, 121.1, 120.8, 120.6, 120.2, 111.5, 111.3, 111.0, 105.6, 42.0; Anal. Calcd for $C_{29}H_{20}BrNO$: C, 72.81; H, 4.21; N, 2.93%; Found: C, 73.01; H, 4.25; N, 2.87%.



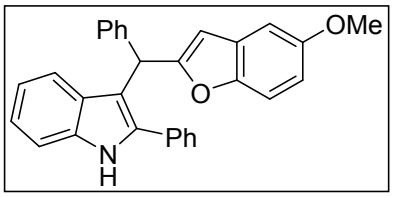
3-(Benzofuran-2-yl(4-(*tert*-butyl)phenyl)methyl)-2-phenyl-1*H*-indole (**3fa**): White solid (82%, 74 mg); R_f = 0.50 (PE : EA = 94 : 6); M.p. 186-187 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 (s, 1H), 7.54-7.52 (m, 2H), 7.47-7.37 (m, 7H), 7.30-7.28 (m, 2H), 7.24-7.15 (m, 5H), 6.97 (t, J = 8.0 Hz, 1H), 6.43 (s, 1H), 5.93 (s, 1H), 1.30 (s, 9H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 160.5, 155.1, 149.4, 138.3, 136.1, 136.0, 132.7, 129.1, 128.9, 128.8, 128.28, 128.23, 125.3, 125.2, 123.4, 122.5, 122.2, 121.4, 120.6, 119.9, 112.2, 111.3, 110.9, 105.2, 42.0, 34.5, 31.5; Anal. Calcd for $C_{33}H_{29}NO$: C, 87.00; H, 6.42; N, 3.07%; Found: C, 87.14; H, 6.36; N, 2.99%.



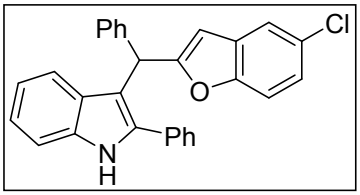
3-(Benzofuran-2-yl(6-methoxynaphthalen-2-yl)methyl)-2-phenyl-1*H*-indole (3ga): Brown gummy mass (76%, 72 mg); R_f = 0.45 (PE : EA = 93 : 7); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21 (s, 1H), 7.66-7.59 (m, 3H), 7.54-7.52 (m, 2H), 7.48-7.43 (m, 3H), 7.41-7.37 (m, 5H), 7.23-7.18 (m, 2H), 7.15-7.09 (m, 3H), 6.94-6.90 (m, 1H), 6.44 (s, 1H), 6.09 (s, 1H), 3.90 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 160.3, 157.6, 155.1, 136.8, 136.2, 136.1, 133.5, 132.6, 129.6, 129.0, 128.8, 128.7, 128.34, 128.30, 127.8, 127.2, 127.0, 126.8, 123.5, 122.6, 122.3, 121.2, 120.7, 120.0, 118.7, 112.0, 111.3, 110.9, 105.7, 105.5, 55.4, 42.5; Anal. Calcd for $C_{34}H_{25}NO_2$: C, 85.15; H, 5.25; N, 2.92%; Found: C, 85.36; H, 5.22; N, 2.97%.



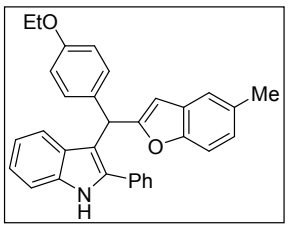
3-((5-Methylbenzofuran-2-yl)(phenyl)methyl)-2-phenyl-1*H*-indole (**3ia**): Brown gummy mass (85%, 70 mg); R_f = 0.50 (PE : EA = 95 : 5); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.09 (s, 1H), 7.49-7.46 (m, 2H), 7.43-7.39 (m, 2H), 7.38-7.32 (m, 3H), 7.25-7.21 (m, 7H), 7.15-7.11 (m, 1H), 7.00-6.97 (m, 1H), 6.94-6.91 (m, 1H), 6.32 (s, 1H), 5.90 (s, 1H), 2.39 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 160.3, 153.5, 141.6, 136.1, 132.6, 132.0, 129.0, 128.8, 128.74, 128.70, 128.4, 128.3, 128.2, 127.2, 126.7, 124.7, 122.2, 121.2, 120.5, 120.0, 112.1, 110.9, 110.8, 105.2, 42.5, 21.4; Anal. Calcd for $C_{30}H_{23}NO$: C, 87.14; H, 5.61; N, 3.39%; Found: C, 86.98; H, 5.66; N, 3.47%.



3-((5-Methoxybenzofuran-2-yl)(phenyl)methyl)-2-phenyl-1*H*-indole (**3ja**): Brown solid (83%, 71 mg); R_f = 0.50 (PE : EA = 92 : 8); M.p. 103-104 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.12 (s, 1H), 7.49-7.47 (m, 2H), 7.43-7.31 (m, 5H), 7.26-7.23 (m, 6H), 7.16-7.12 (m, 1H), 6.95-6.90 (m, 2H), 6.80-6.77 (m, 1H), 6.33 (s, 1H), 5.89 (s, 1H), 3.78 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 161.1, 155.8, 150.1, 141.5, 136.1, 132.6, 129.3, 129.0, 128.7, 128.6, 128.4, 128.3, 128.1, 127.2, 126.7, 122.3, 121.2, 120.0, 112.1, 112.0, 111.7, 111.0, 105.6, 103.5, 56.0, 42.6; Anal. Calcd for $C_{30}H_{23}NO_2$: C, 83.89; H, 5.40; N, 3.26%; Found: C, 84.07; H, 5.36; N, 3.18%.

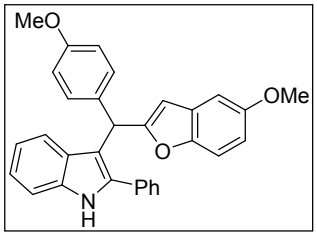


3-((5-Chlorobenzofuran-2-yl)(phenyl)methyl)-2-phenyl-1*H*-indole (**3ka**): White solid (71%, 61 mg); R_f = 0.45 (PE : EA = 93 : 7); M.p. 157-158 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.06 (s, 1H), 7.65-7.59 (m, 4H), 7.54-7.46 (m, 2H), 7.41-7.35 (m, 2H), 7.31-7.28 (m, 2H), 7.25-7.23 (m, 1H), 7.12-7.06 (m, 2H), 7.03-6.96 (m, 2H), 6.89-6.87 (m, 2H), 6.45 (s, 1H), 6.02 (s, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 158.1, 155.2, 135.7, 134.2, 132.4, 129.2, 129.1, 128.8, 128.7, 128.6, 128.48, 128.44, 127.8, 127.7, 127.2, 127.1, 125.6, 124.9, 122.6, 120.1, 112.1, 110.9, 110.5, 106.4, 41.0; Anal. Calcd for $C_{29}H_{20}ClNO$: C, 80.27; H, 4.65; N, 3.23%; Found: C, 80.21; H, 4.68; N, 3.29%.

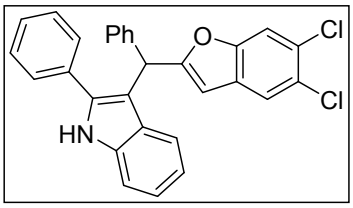


3-((4-Ethoxyphenyl)(5-methylbenzofuran-2-yl)methyl)-2-phenyl-1*H*-indole (3la): Brown gummy mass (76%, 69 mg); R_f = 0.45 (PE : EA = 95 : 5); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02

(s, 1H), 7.42-7.40 (m, 2H), 7.35-7.25 (m, 5H), 7.17-7.15 (m, 2H), 7.12-7.05 (m, 3H), 6.93-6.85 (m, 2H), 6.73-6.71 (m, 2H), 6.25 (s, 1H), 5.78 (s, 1H), 3.91 (q, J = 7.2 Hz, 2H), 2.33 (s, 3H), 1.31 (t, J = 7.2 Hz, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ 160.8, 157.7, 153.5, 136.2, 135.9, 133.6, 132.7, 131.9, 129.79, 129.70, 128.95, 128.90, 128.7, 128.2, 124.7, 122.2, 121.3, 120.5, 120.0, 114.4, 112.4, 110.9, 110.8, 105.0, 63.4, 41.8, 21.4, 15.0; Anal. Calcd for $C_{32}H_{27}NO_2$: C, 84.00; H, 5.95; N, 3.06%; Found: C, 84.19; H, 5.91; N, 3.14%.

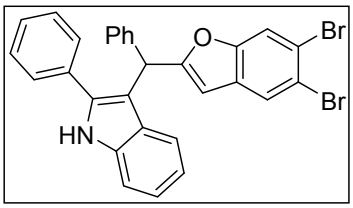


3-((5-Methoxybenzofuran-2-yl)(4-methoxyphenyl)methyl)-2-phenyl-1*H*-indole (3ma): Brown gummy mass (78%, 71 mg); R_f = 0.45 (PE : EA = 94 : 6); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.08 (s, 1H), 7.43-7.41 (m, 2H), 7.37-7.33 (m, 2H), 7.32-7.28 (m, 3H), 7.18-7.12 (m, 3H), 7.12-7.06 (m, 1H), 6.90-6.82 (m, 2H), 6.77-6.71 (m, 3H), 6.26 (s, 1H), 5.78 (s, 1H), 3.73 (s, 3H), 3.70 (s, 3H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ 161.5, 158.3, 155.8, 150.1, 136.2, 135.9, 133.7, 132.7, 129.8, 129.7, 129.3, 128.9, 128.7, 128.2, 127.2, 122.2, 121.2, 120.0, 113.8, 111.9, 111.6, 111.0, 105.4, 103.5, 56.0, 55.3, 41.8; Anal. Calcd for $C_{31}H_{25}NO_3$: C, 81.02; H, 5.48; N, 3.05%; Found: C, 81.24; H, 5.51; N, 2.96 %.

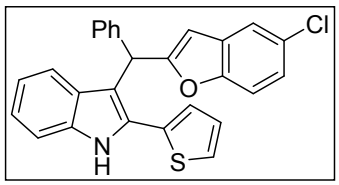


3-((5,6-Dichlorobenzofuran-2-yl)(phenyl)methyl)-2-phenyl-1*H*-indole (3na): Brown gummy mass (72%, 67 mg); R_f = 0.50 (PE : EA = 93 : 7); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17 (s, 1H), 7.50-7.48 (m, 2H), 7.43-7.41 (m, 2H), 7.39-7.34 (m, 3H), 7.28-7.26 (m, 3H), 7.24 (s, 2H), 7.19-7.14 (m, 2H), 7.11-7.09 (m, 1H), 6.99-6.94 (m, 1H), 6.39 (s, 1H), 5.96 (s, 1H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ 162.7, 156.7, 140.7, 136.4, 136.1, 132.5, 131.0, 129.1, 128.9, 128.8, 128.5,

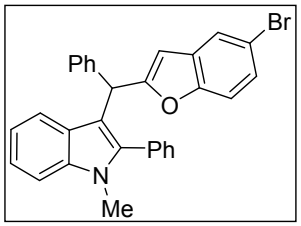
128.4, 127.9, 127.2, 126.9, 123.8, 122.4, 121.1, 120.7, 120.1, 119.8, 118.9, 111.0, 105.6, 42.4; Anal. Calcd for $C_{29}H_{19}Cl_2NO$: C, 74.37; H, 4.09; N, 2.99%; Found: C, 74.21; H, 4.03; N, 3.06%.



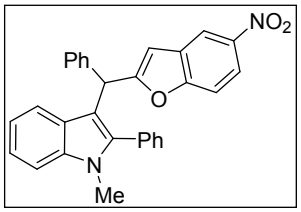
3-((5,6-Dibromobenzofuran-2-yl)(phenyl)methyl)-2-phenyl-1*H*-indole (3oa): Brown gummy mass (75%, 83 mg); R_f = 0.50 (PE : EA = 94 : 6); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.11 (s, 1H), 7.52-7.45 (m, 4H), 7.43-7.35 (m, 5H), 7.27-7.23 (m, 5H), 7.18-7.14 (m, 1H), 6.99-6.95 (m, 1H), 6.41 (s, 1H), 5.96 (s, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 162.5, 156.6, 140.6, 136.5, 136.1, 131.3, 129.19, 129.12, 128.9, 128.87, 128.84, 128.55, 128.52, 128.4, 127.8, 126.9, 122.5, 121.2, 120.1, 115.7, 111.3, 111.0, 105.6, 104.6, 42.3; Anal. Calcd for $C_{29}H_{19}Br_2NO$: C, 62.50; H, 3.44; N, 2.51%; Found: C, 62.22; H, 3.49; N, 2.57%.



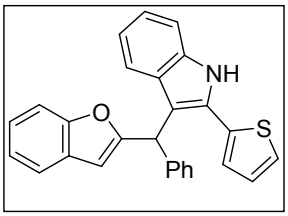
3-((5-Chlorobenzofuran-2-yl)(phenyl)methyl)-2-(thiophen-2-yl)-1*H*-indole (3ki): Brown gummy mass (77%, 67 mg); R_f = 0.45 (PE : EA = 94 : 6); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.16 (s, 1H), 7.39 (d, J = 2.0 Hz, 1H), 7.35-7.32 (m, 2H), 7.28 (d, J = 4.0 Hz, 4H), 7.23-7.16 (m, 3H), 7.14-7.10 (m, 3H), 7.08-7.06 (m, 1H), 6.93-6.89 (m, 1H), 6.30 (s, 1H), 6.05 (s, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 161.6, 153.5, 140.8, 136.1, 133.6, 130.0, 129.6, 128.9, 128.7, 128.6, 128.1, 128.0, 127.0, 126.4, 126.3, 123.8, 122.8, 120.9, 120.39, 120.32, 112.6, 112.2, 111.0, 105.1, 42.7; Anal. Calcd for $C_{27}H_{18}ClNOS$: C, 73.71; H, 4.12; N, 3.18%; Found: C, 73.54; H, 4.18; N, 3.11%.



3-((5-Bromobenzofuran-2-yl)(phenyl)methyl)-1-methyl-2-phenyl-1*H*-indole (**3pj**): Brown gummy mass (74%, 72 mg); R_f = 0.45 (PE : EA = 92 : 8); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38-7.36 (m, 4H), 7.21-7.05 (m, 7H), 6.88-6.86 (m, 3H), 6.76-6.72 (m, 3H), 6.18 (s, 1H), 5.51 (s, 1H), 3.38 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 158.2, 155.4, 138.2, 134.5, 133.6, 131.2, 131.1, 130.7, 130.4, 128.8, 128.74, 128.71, 128.6, 128.4, 128.0, 127.9, 127.7, 125.6, 122.1, 119.8, 114.1, 110.9, 109.6, 106.3, 41.1, 30.9; Anal. Calcd for $C_{30}H_{22}BrNO$: C, 73.18; H, 4.50; N, 2.84%; Found: C, 73.37; H, 4.45; N, 2.80%.

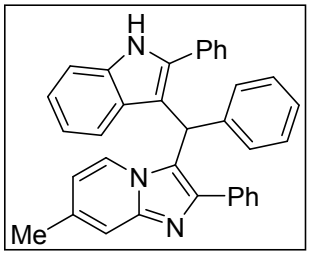


1-Methyl-3-((5-nitrobenzofuran-2-yl)(phenyl)methyl)-2-phenyl-1*H*-indole (**3qj**): Yellow solid (75%, 68 mg); R_f = 0.50 (PE : EA = 92 : 8); M.p. 175-176 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17-8.14 (m, 1H), 7.99 (s, 1H), 7.54-7.49 (m, 3H), 7.42 (d, J = 9.2 Hz, 1H), 7.31-7.17 (m, 4H), 7.07-7.01 (m, 5H), 6.90-6.87 (m, 2H), 6.42 (s, 1H), 5.67 (s, 1H), 3.53 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 161.1, 157.9, 143.3, 138.6, 137.4, 133.8, 133.0, 130.9, 130.7, 129.0, 128.8, 128.17, 128.10, 126.2, 125.8, 122.3, 121.1, 120.0, 118.6, 110.3, 109.8, 109.4, 108.2, 40.7, 31.0; Anal. Calcd for $C_{30}H_{22}N_2O_3$: C, 78.59; H, 4.84; N, 6.11%; Found: C, 78.75; H, 4.88; N, 6.16%.

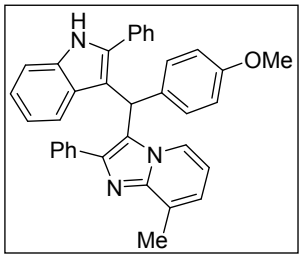


3-(Benzofuran-2-yl(phenyl)methyl)-2-(thiophen-2-yl)-1*H*-indole (**3ai**): Brown gummy mass (53%, 42 mg); R_f = 0.45 (PE : EA = 92 : 8); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.12 (s, 1H), 7.38-

7.36 (m, 1H), 7.31-7.27 (m, 3H), 7.21 (d, J = 6.4 Hz, 3H), 7.18-7.14 (m, 2H), 7.12-7.07 (m, 4H), 7.05-7.01 (m, 2H), 6.86-6.82 (m, 1H), 6.30 (s, 1H), 6.01 (s, 1H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 159.9, 155.1, 141.2, 136.2, 133.8, 129.5, 128.9, 128.7, 128.5, 128.2, 128.0, 126.8, 126.4, 126.2, 123.6, 122.7, 122.6, 121.1, 120.7, 120.3, 113.2, 111.3, 110.9, 105.5, 42.7; Anal. Calcd for $C_{27}H_{19}NOS$: C, 79.97; H, 4.72; N, 3.45%; Found: C, 79.73; H, 4.77; N, 3.56%.

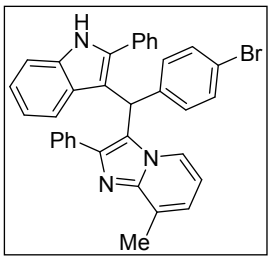


7-Methyl-2-phenyl-3-(phenyl(2-phenyl-1*H*-indol-3-yl)methyl)imidazo[1,2-*a*]pyridine (**8a**): White solid (62%, 60 mg); R_f = 0.55 (PE : EA = 76 : 24); M.p. 184-185 °C; ^1H NMR (400 MHz, $CDCl_3$): δ 8.37 (s, 1H), 7.51-7.48 (m, 2H), 7.39 (d, J = 7.2 Hz, 1H), 7.35 (d, J = 8.0 Hz, 1H), 7.24-7.16 (m, 8H), 7.14-7.06 (m, 3H), 7.02-7.01 (m, 4H), 6.91 (t, J = 8.0 Hz, 1H), 6.77 (d, J = 8.4 Hz, 1H), 6.46 (s, 1H), 6.15-6.13 (m, 1H), 2.26 (s, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 145.1, 143.8, 140.9, 137.0, 135.8, 135.2, 134.8, 134.5, 132.3, 128.88, 128.81, 128.4, 128.2, 128.1, 128.0, 127.2, 126.9, 126.1, 124.3, 122.2, 121.2, 120.4, 120.1, 115.6, 114.2, 111.2, 111.0, 39.3, 21.2; Anal. Calcd for $C_{35}H_{27}N_3$: C, 85.86; H, 5.56; N, 8.58%; Found: C, 86.01; H, 5.50; N, 8.49%.

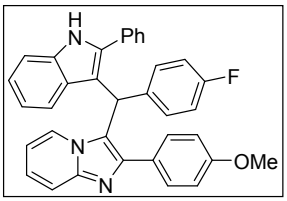


3-((4-Methoxyphenyl)(2-phenyl-1*H*-indol-3-yl)methyl)-8-methyl-2-phenylimidazo[1,2-*a*]pyridine (**8b**): White solid (82%, 85 mg); R_f = 0.45 (PE : EA = 78 : 22); M.p. 189-190 °C; ^1H NMR (400 MHz, $CDCl_3$): δ 8.30 (s, 1H), 7.50-7.47 (m, 2H), 7.41 (d, J = 6.8 Hz, 1H), 7.35 (d, J = 8.0 Hz, 1H), 7.20-7.13 (m, 4H), 7.10-7.06 (m, 1H), 7.04-6.99 (m, 6H), 6.94-6.90 (m, 1H), 6.85 (d, J = 8.0 Hz, 1H), 6.79-6.77 (m, 1H), 6.72 (d, J = 8.8 Hz, 2H), 6.39 (s, 1H), 6.24 (t, J = 6.8 Hz, 1H), 3.75 (s, 3H), 2.58 (s, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 171.2, 158.3, 144.9, 143.6,

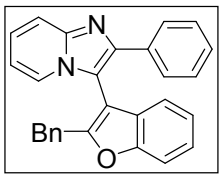
136.8, 135.9, 135.0, 132.9, 132.4, 129.8, 129.1, 128.4, 128.3, 128.05, 128.01, 127.7, 127.1, 126.9, 123.0, 122.4, 122.3, 122.0, 120.5, 119.9, 114.0, 111.4, 111.0, 55.2, 38.7, 17.2; Anal. Calcd for $C_{36}H_{29}N_3O$: C, 83.21; H, 5.63; N, 8.09%; Found: C, 83.03; H, 5.61; N, 8.16%.



3-((4-Bromophenyl)(2-phenyl-1*H*-indol-3-yl)methyl)-8-methyl-2-phenylimidazo[1,2-*a*]pyridine (8c): White solid (75%, 85 mg); R_f = 0.50 (PE : EA = 82 : 18); M.p. 196-197 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.43 (s, 1H), 7.46-7.43 (m, 2H), 7.35 (d, J = 8.0 Hz, 2H), 7.28 (d, J = 8.4 Hz, 2H), 7.19-7.15 (m, 4H), 7.11-7.07 (m, 1H), 7.04-7.00 (m, 4H), 6.96-6.92 (m, 3H), 6.85 (d, J = 8.0 Hz, 1H), 6.80 (d, J = 6.4 Hz, 1H), 6.35 (s, 1H), 6.26 (t, J = 6.8 Hz, 1H), 2.57 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 145.0, 143.9, 139.9, 137.0, 135.8, 134.9, 132.1, 131.7, 130.6, 129.1, 128.9, 128.6, 128.4, 128.2, 128.1, 128.0, 127.3, 127.1, 122.7, 122.4, 121.3, 120.7, 120.3, 120.2, 111.7, 111.1, 110.6, 39.1, 17.3; HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{35}H_{27}BrN_3$: 568.1383; found: 568.1384.



3-((4-Fluorophenyl)(2-phenyl-1*H*-indol-3-yl)methyl)-2-(4-methoxyphenyl)imidazo[1,2-*a*]pyridine (**8d**): Brown solid (81%, 84 mg); R_f = 0.55 (PE : EA = 77 : 23); M.p. 127-128 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.91 (s, 1H), 7.46-7.40 (m, 4H), 7.33 (d, J = 8.0 Hz, 1H), 7.15 (t, J = 7.6 Hz, 1H), 7.07-7.04 (m, 3H), 6.99-6.87 (m, 8H), 6.82 (d, J = 8.0 Hz, 1H), 6.74 (d, J = 8.8 Hz, 2H), 6.41 (s, 1H), 6.30 (t, J = 7.2 Hz, 1H), 3.75 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 161.7 ($J_{C\text{-}F}$ = 244 Hz), 159.1, 144.5, 144.0, 137.1, 136.5 ($J_{C\text{-}F}$ = 3.0 Hz), 135.9, 132.2, 130.38, 130.31, 130.1, 128.4, 128.1 ($J_{C\text{-}F}$ = 9.0 Hz), 128.0, 127.2, 124.8, 123.6, 122.2, 121.0, 120.19, 120.16, 117.0, 115.6 ($J_{C\text{-}F}$ = 21.0 Hz), 113.7, 111.5, 111.2, 110.7, 55.3, 38.8; Anal. Calcd for $C_{35}H_{26}FN_3O$: C, 80.29; H, 5.01; N, 8.03%; Found: C, 80.12; H, 5.04; N, 8.09%.



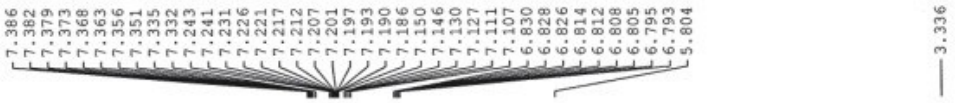
3-(2-Benzylbenzofuran-3-yl)-2-phenylimidazo[1,2-*a*]pyridine (11): White solid (54%, 43 mg); R_f = 0.50 (PE : EA = 75 : 25); M.p. 130-131 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76-7.72 (m, 3H), 7.63-7.61 (m, 1H), 7.56 (d, J = 8.4 Hz, 1H), 7.36-7.32 (m, 1H), 7.27-7.24 (m, 4H), 7.21-7.19 (m, 2H), 7.08-7.06 (m, 3H), 6.90-6.88 (m, 2H), 6.70-6.66 (m, 1H), 3.85-3.76 (m, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 157.3, 155.0, 145.8, 144.6, 136.2, 134.1, 128.7, 128.6, 128.4, 128.2, 127.9, 127.6, 126.7, 125.1, 124.7, 124.2, 123.5, 120.0, 117.7, 112.4, 111.8, 111.2, 105.8, 33.7. Anal. Calcd for $C_{28}H_{20}N_2O$: C, 83.98; H, 5.03; N, 7.00%; Found: C, 83.74; H, 5.06; N, 7.09%

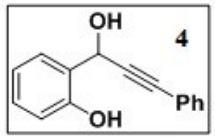
4. References:

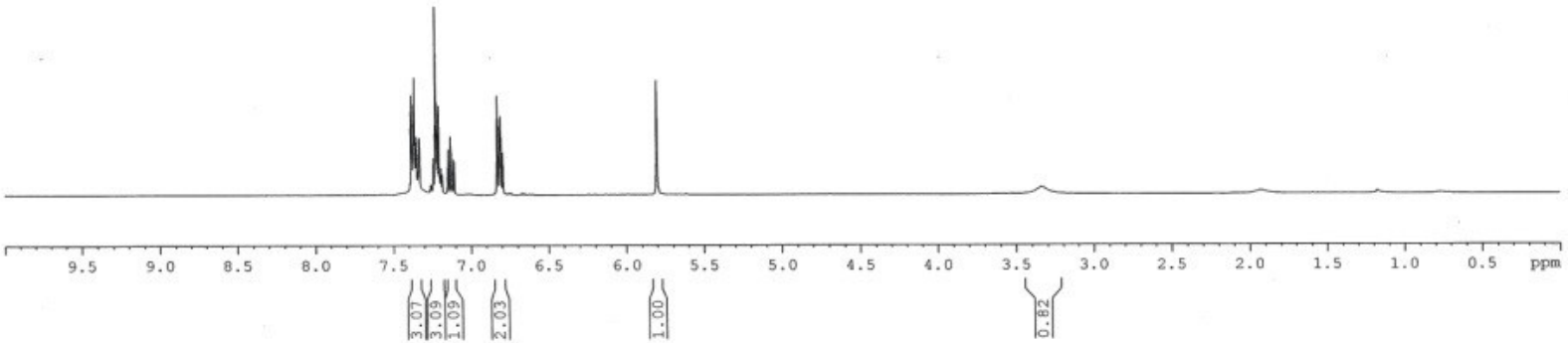
1) Y. Wei, I. Deb and N. Yoshikai, *J. Am. Chem. Soc.,* 2012, **134**, 9098.
2) M. Zheng, F. Wu, K. Chen and S. Zhu, *Org. Lett*., 2016, **18**, 3554.

5. NMR spectra for the synthesized products

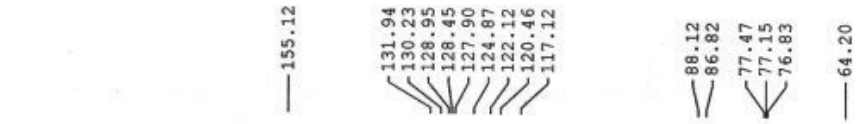
1H of VBSS-starting prop.

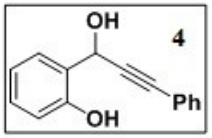


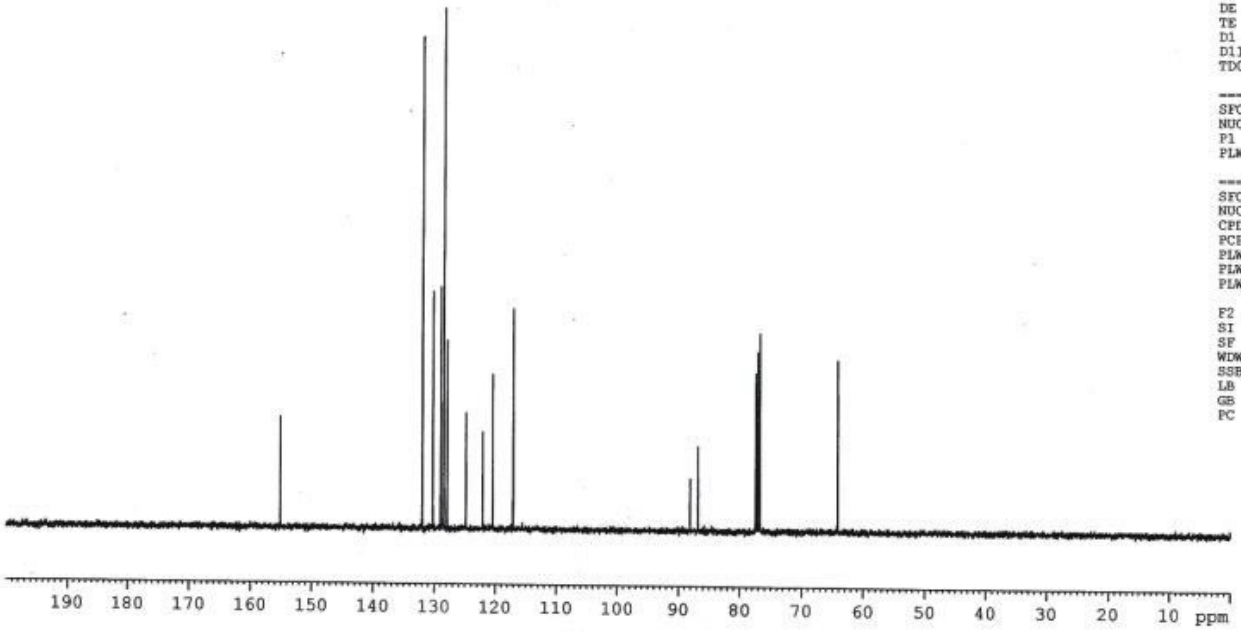




13C of vbSS-starti





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PROCNO                 1

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PULPROG          zgpg30
TD                32768
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FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG                62.69
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DE                6.50 usec
TE               300.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

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NUC1               13C
P1                8.90 usec
PLW1         54.00000000 W

======== CHANNEL f2 ========
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NUC2               1H
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PCPD2             90.00 usec
PLW2         12.00000000 W
PLW12         0.32231000 W
PLW13         0.16212000 W

F2 - Processing parameters
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WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
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1H of VBSS 135/44

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7.323
7.304
7.283
7.275
7.256
7.255
7.232
7.213
7.207
7.203
7.194
7.186
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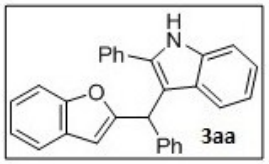
6.901
6.381
5.915



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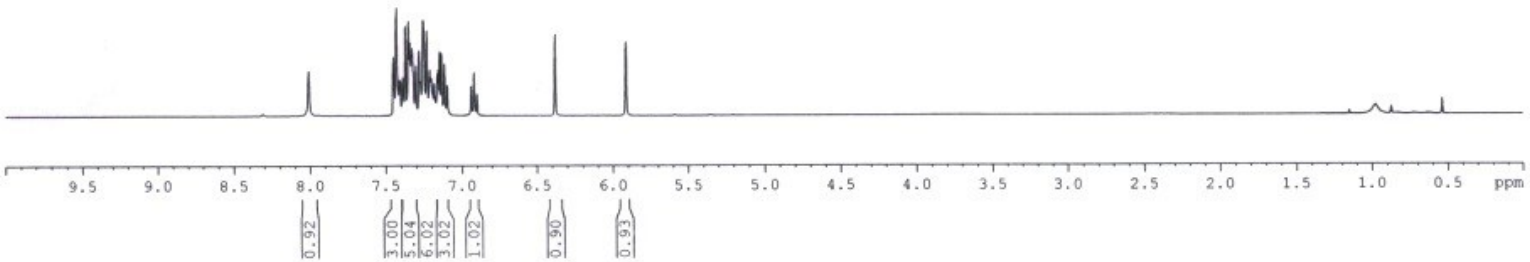
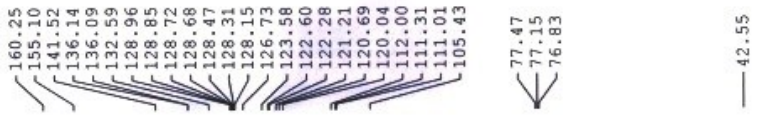
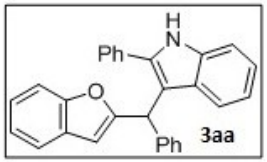
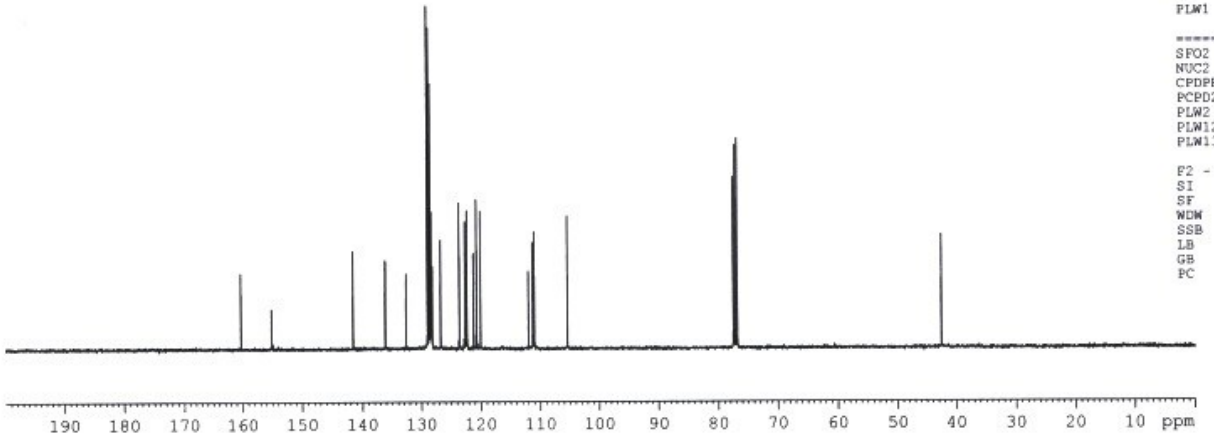


13C of VBSs 135/44





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EXPNO              180
PROCNO               1

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INSTRUM          spect
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PULPROG        zgpg30
TD               32768
SOLVENT          CDCl3
NS                 400
DS                   2
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG               37.83
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DE               6.50 usec
TE              294.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

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NUC1              13C
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======== CHANNEL f2 ========
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NUC2              1H
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PLW12        0.32231000 W
PLW13        0.16212000 W

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WDW                EM
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GB        0
PC               1.40
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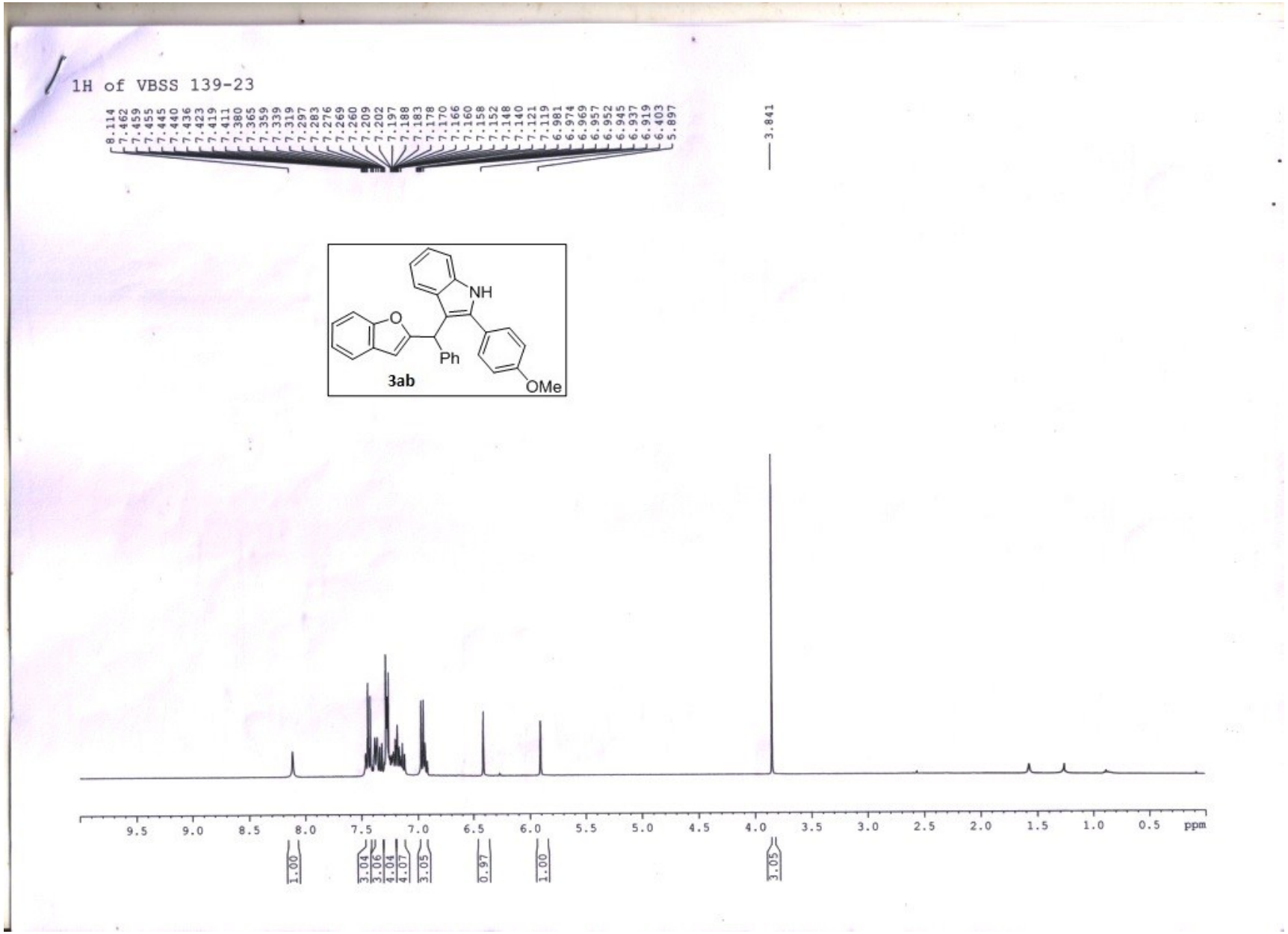
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7.297
7.283
7.276
7.269
7.260
7.209
7.202
7.197
7.188
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7.166
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7.119
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6.952
6.945
6.937
6.919
6.403
5.897
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Ph
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
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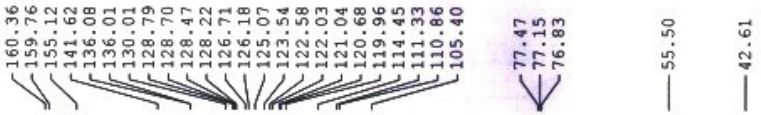
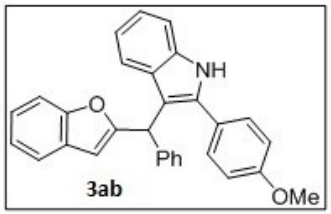
0.97
1.00
3.05

13C VBSS 139-23





3ab

```
Current Data Parameters
NAME      Dr.A.HAJRA 2017
EXPNO              802
PROCNO               1

F2 - Acquisition Parameters
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Time              12.52
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg
TD               32768
SOLVENT          CDCl3
NS                 640
DS                   2
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG               148.91
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DE                6.50 usec
TE               295.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

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NUC1               13C
P1                8.90 usec
PLW1       54.00000000 W

======== CHANNEL f2 ========
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NUC2               1H
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PCPD2            90.00 usec
PLW2       12.00000000 W
PLW12       0.32231000 W

F2 - Processing parameters
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LB                1.00 Hz
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PC                1.40
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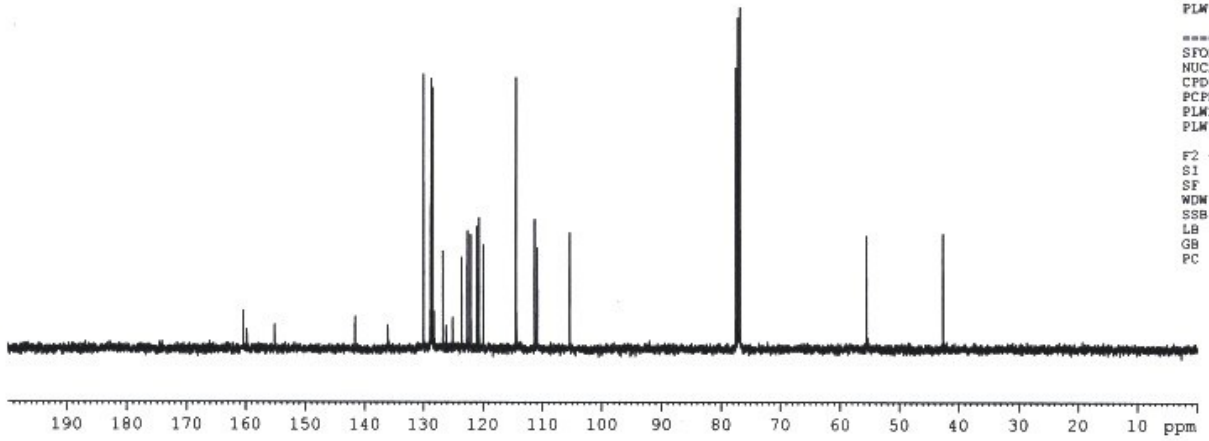
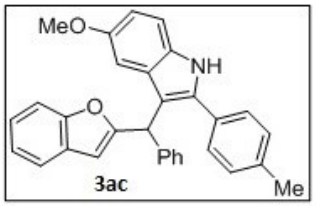
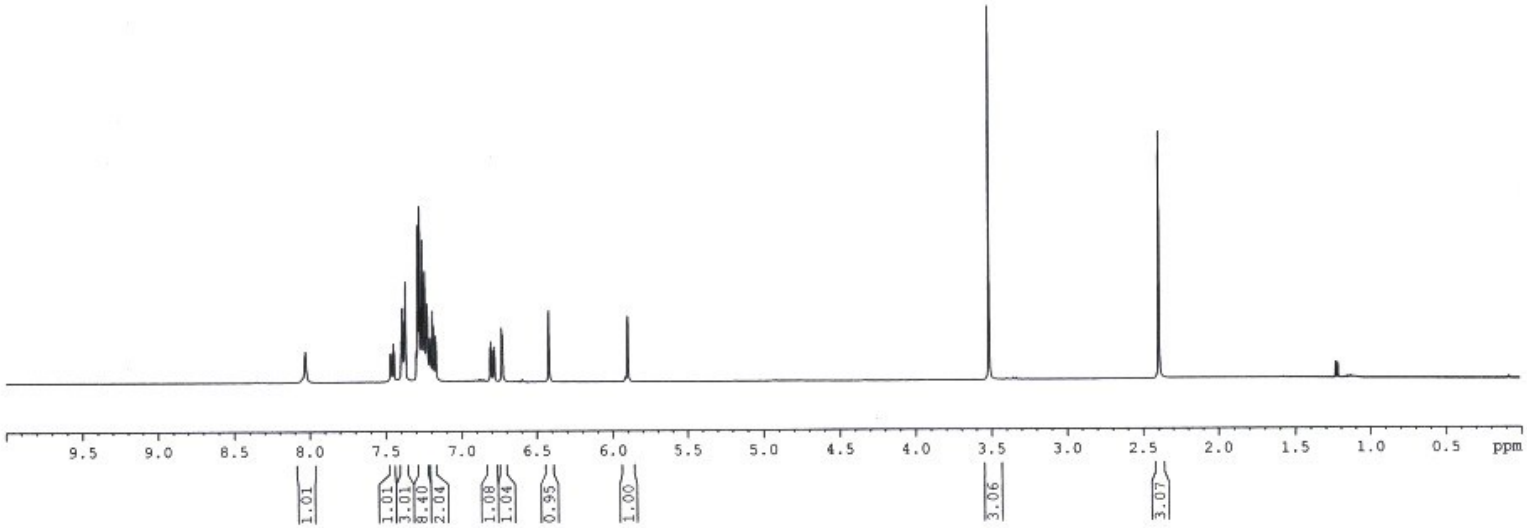


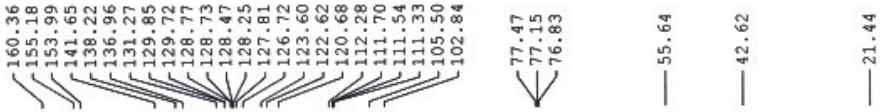
1H of VBSS-139/13

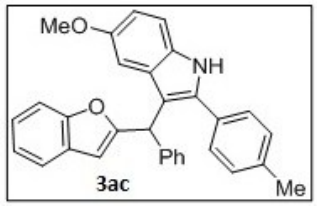


3ac



13C of VBSS 139 13





3ac


```
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EXPNO                 452
PROCNO                  1

F2 - Acquisition Parameters
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PULPROG         zgpg30
TD               32768
SOLVENT           CDCl3
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DS                    2
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG                 87.66
DW                20.800 usec
DE                 6.50 usec
TE                299.8 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6278588 MHz
NUC1                 13C
P1                  8.90 usec
PLW1        54.00000000 W

======== CHANNEL f2 ========
SFO2         400.1516006 MHz
NUC2                 1H
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PCPD2              90.00 usec
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PLW12        0.32231000 W
PLW13        0.16212000 W

F2 - Processing parameters
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WDW                   EM
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PC                 1.40
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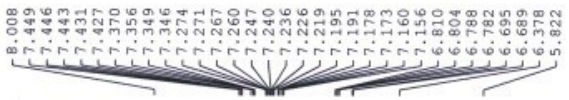
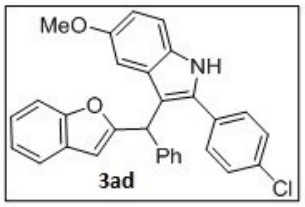
1H of VBSS 139-14





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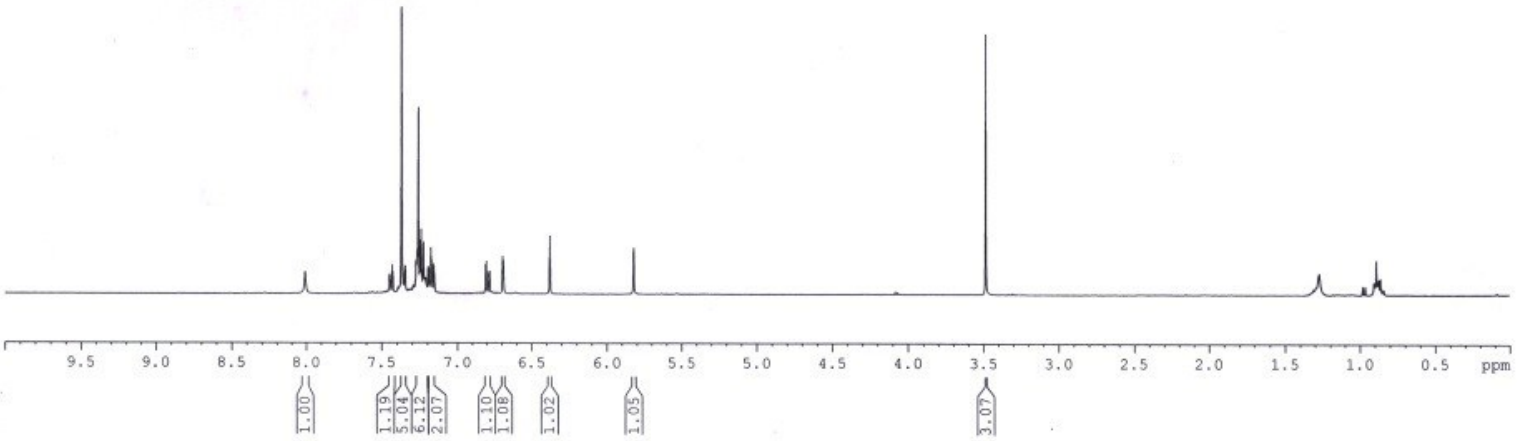

13C of vbss 139/14

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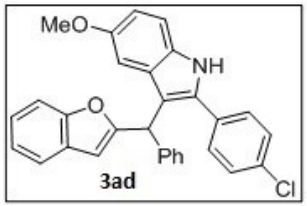
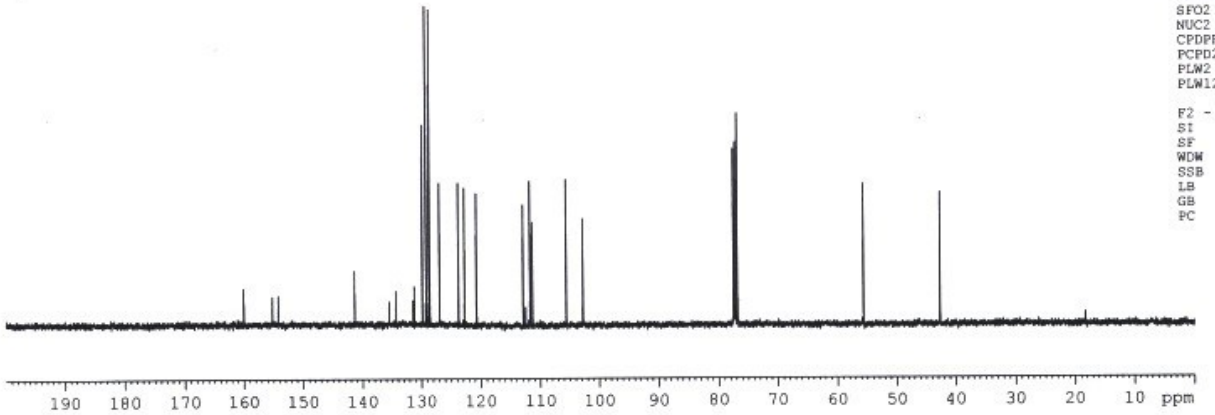


3ad



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EXPNO 470
PROCNO 1

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PULPROG zgpg
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FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 120.16
DW 20.800 usec
DE 6.50 usec
TE 301.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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P1 8.90 usec
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======== CHANNEL f2 ========
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NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W

F2 - Processing parameters
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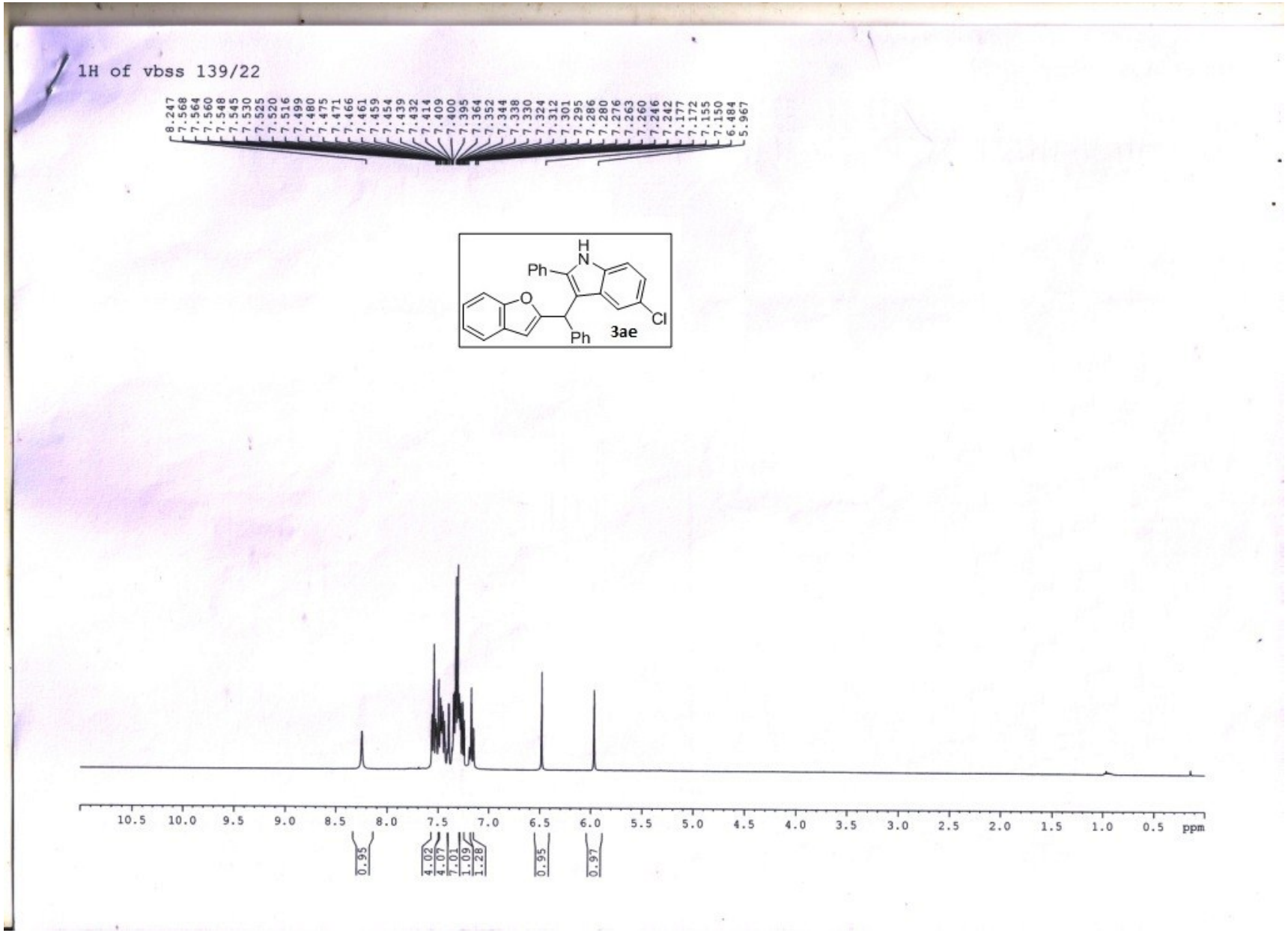
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Ph
O
Cl
Ph
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9.0
8.5
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1.0
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7.01
1.09
1.28
0.95
0.97

vbss 139/22

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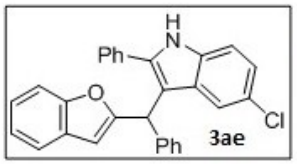
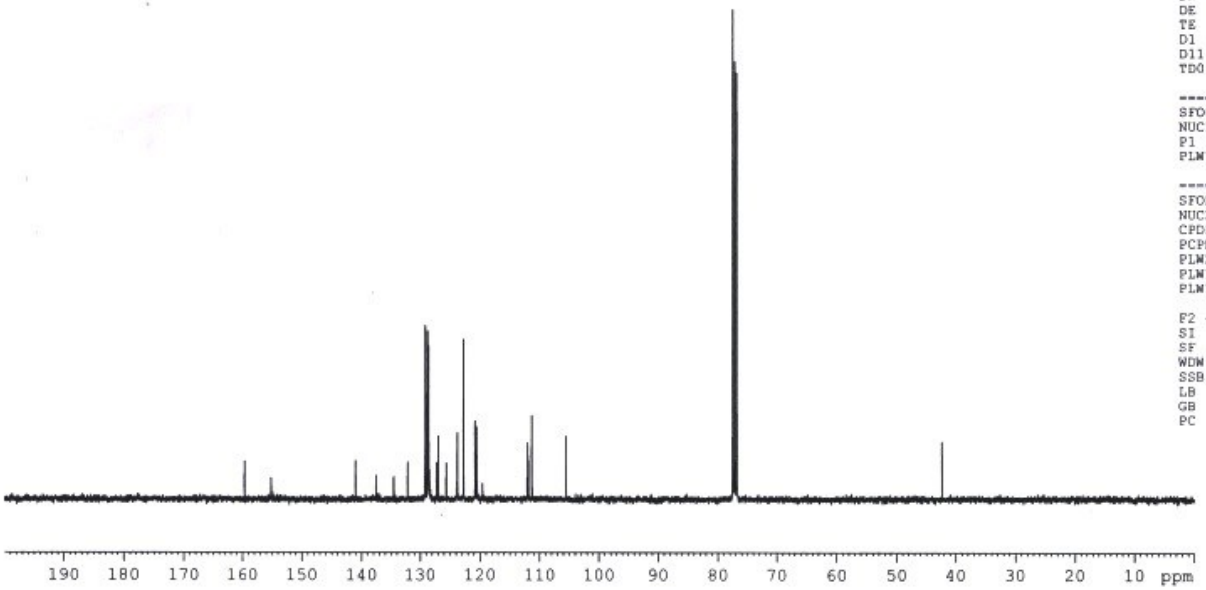
123.77
122.73
120.82
120.57
119.60
112.13
112.00
111.88
111.33
105.54

77.47
77.15
76.84

42.35





BRUKER

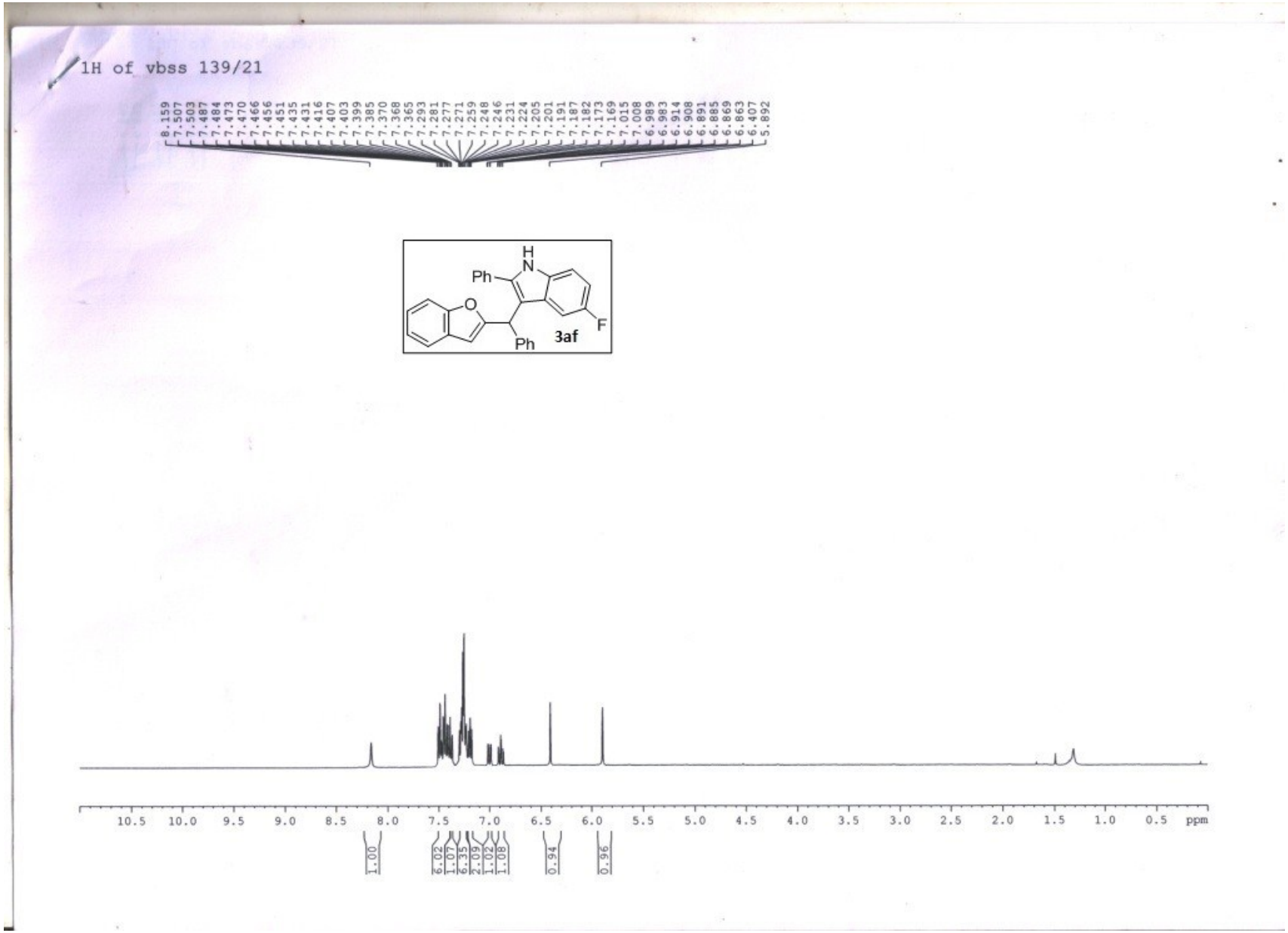
Current Data Parameters
NAME Dr.A.HAJRA 2017
EXPNO 728
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170504
Time 11.53
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 640
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 67.81
DW 20.800 usec
DE 6.50 usec
TE 297.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

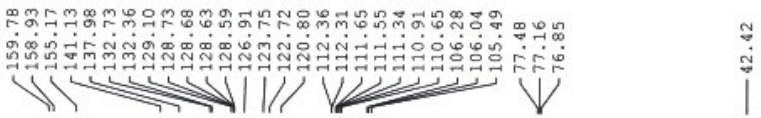
======== CHANNEL f1 ========
SFO1 100.6278588 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W

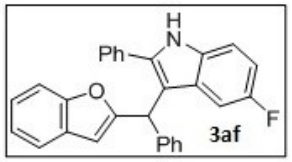
======== CHANNEL f2 ========
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W

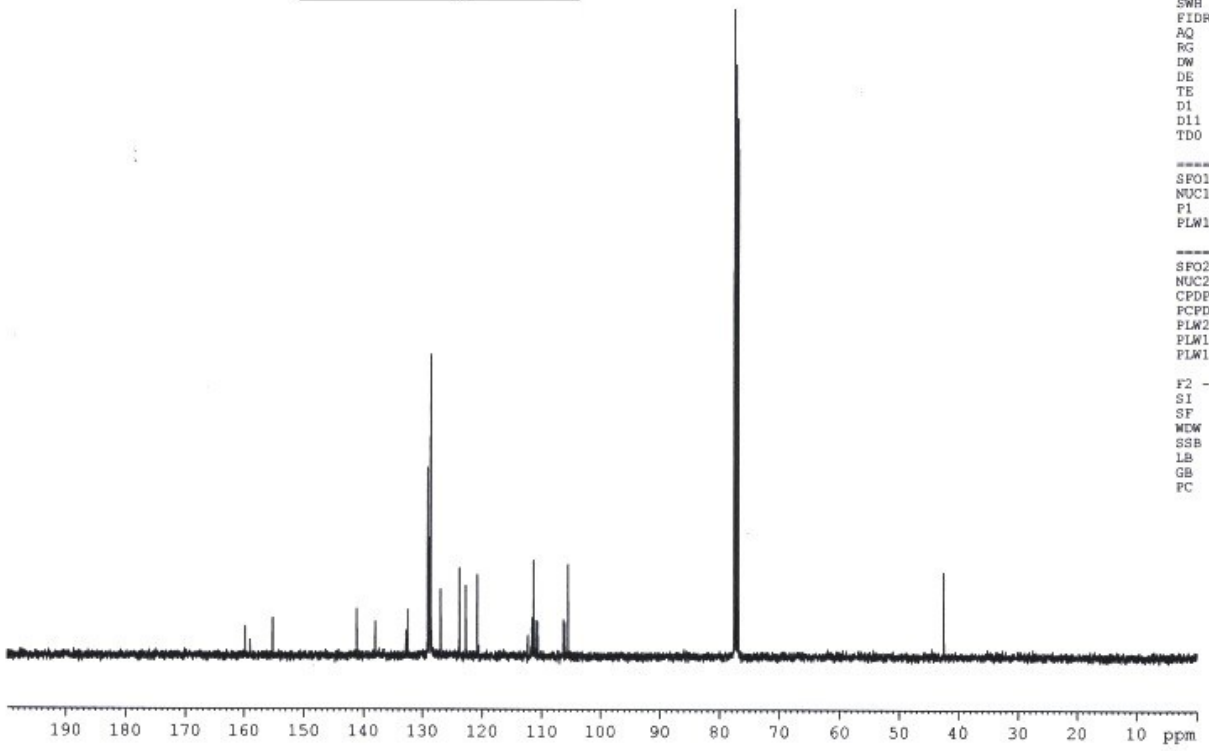
F2 - Processing parameters
SI 16384
SF 100.6177848 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


1H of vbss 139/21
8.159
7.507
7.503
7.487
7.484
7.473
7.470
7.466
7.456
7.451
7.435
7.431
7.416
7.407
7.403
7.399
7.385
7.370
7.368
7.365
7.293
7.281
7.277
7.271
7.259
7.248
7.246
7.231
7.224
7.205
7.201
7.191
7.187
7.182
7.173
7.169
7.015
7.008
6.989
6.983
6.914
6.908
6.891
6.885
6.869
6.863
6.407
5.892
H
N
Ph
O
F
Ph
3af
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.00
6.02
1.07
6.35
2.09
1.02
1.08
0.94
0.96

13C of vbss 139/21







BRUKER

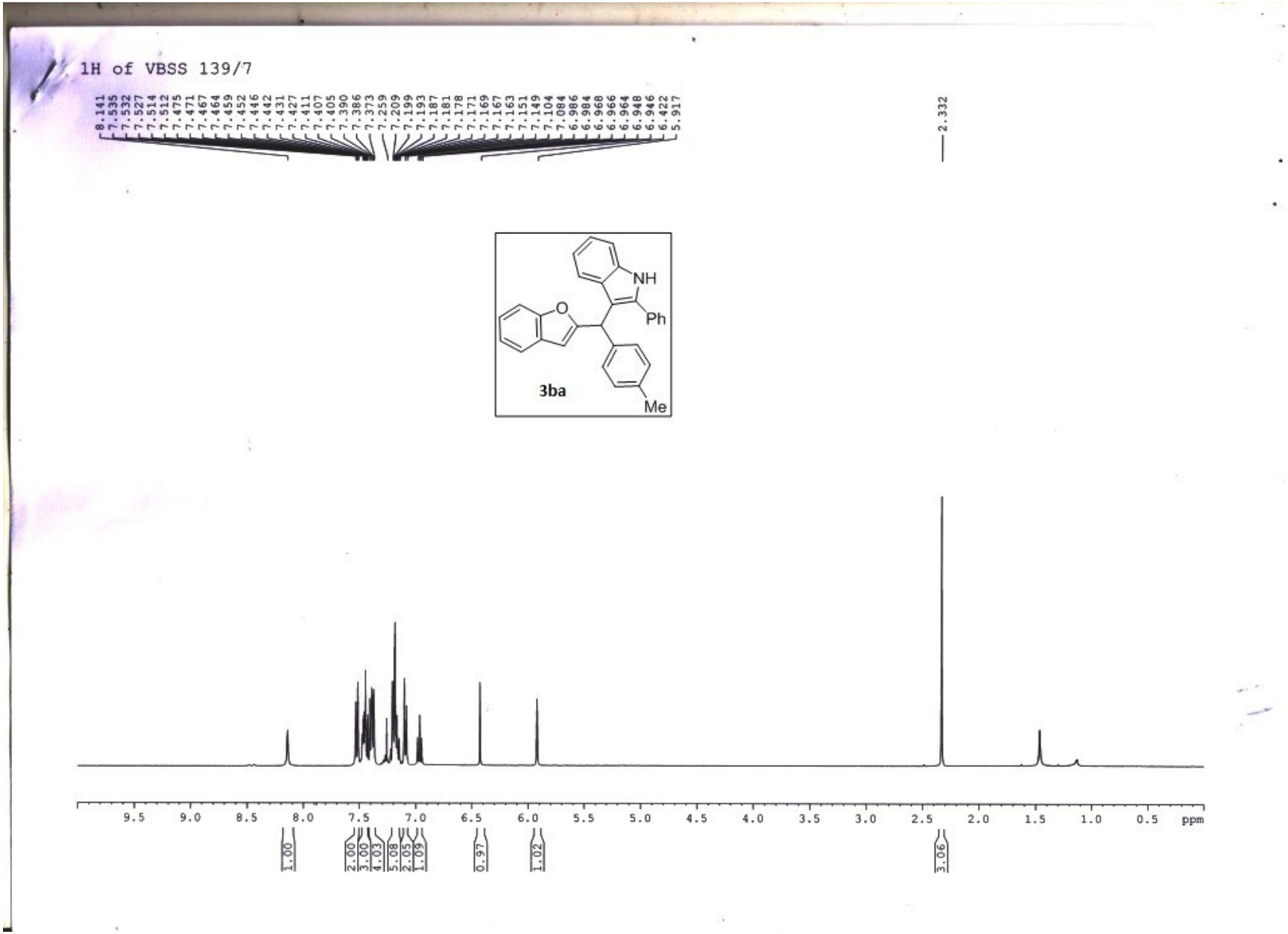
Current Data Parameters
NAME Dr.A.HAJRA 2017
EXPNO 716
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170503
Time 13.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 640
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 106.66
DW 20.800 usec
DE 6.50 usec
TE 298.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

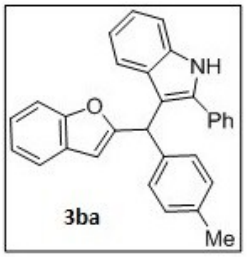
======== CHANNEL f1 ========
SFO1 100.6278588 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W

======== CHANNEL f2 ========
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W

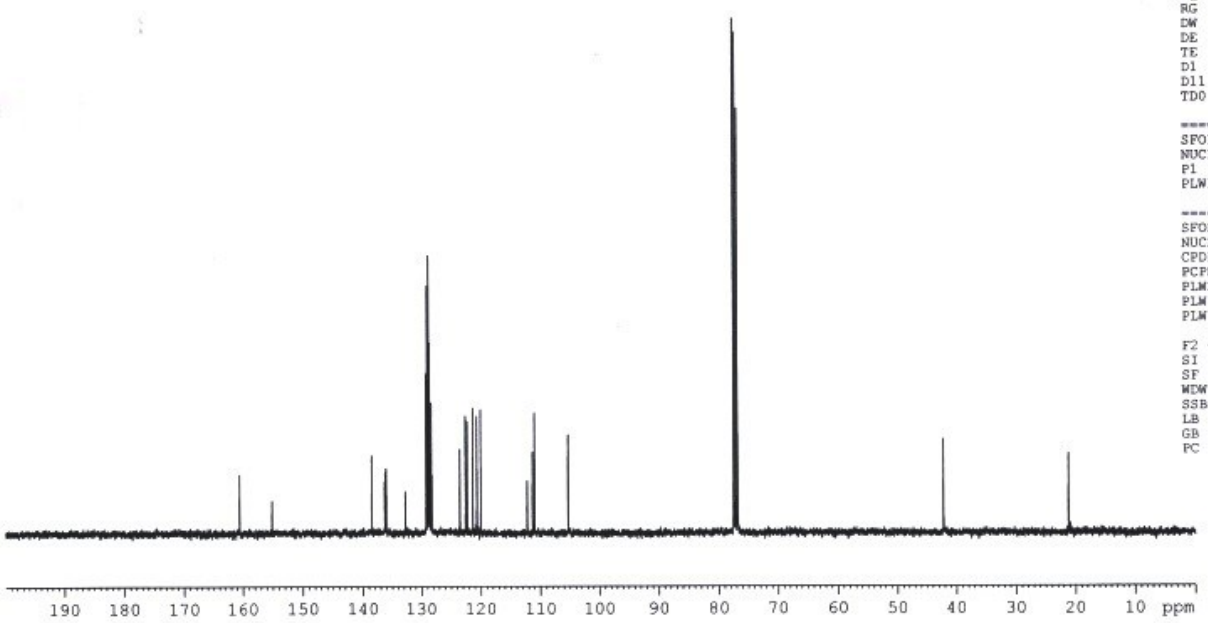
F2 - Processing parameters
SI 16384
SF 100.6177839 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


1H of VBSS 139/7
8.141
7.535
7.532
7.527
7.514
7.512
7.475
7.471
7.467
7.464
7.459
7.452
7.446
7.442
7.431
7.427
7.411
7.407
7.405
7.390
7.386
7.373
7.259
7.209
7.199
7.193
7.187
7.181
7.178
7.171
7.169
7.167
7.163
7.151
7.149
7.104
7.084
6.986
6.984
6.968
6.966
6.964
6.948
6.946
6.422
5.917
2.332
NH
Ph
O
Me
3ba
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.00
2.00
3.00
4.03
5.08
2.05
1.09
0.97
1.02
3.06

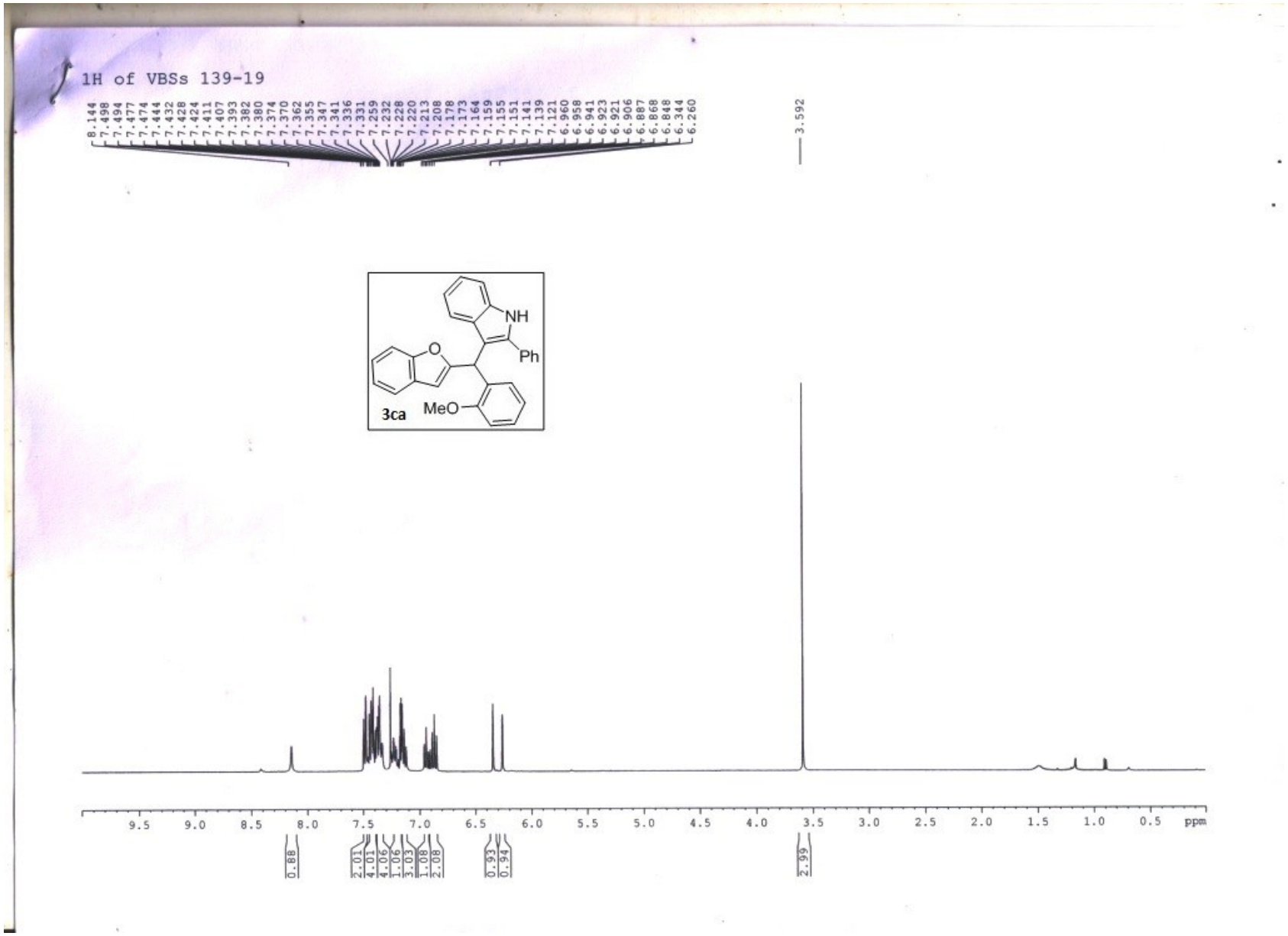
13C of VBSS-139/7



3ba

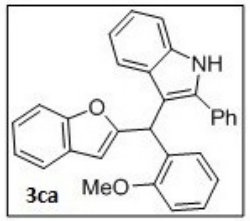



```
Current Data Parameters
NAME      Dr.A.HAJRA 2017
EXPNO              250
PROCNO               1

F2 - Acquisition Parameters
Date_          20170214
Time             16.48
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG        zgpg30
TD             32768
SOLVENT        CDCl3
NS               420
DS                 2
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG               77.59
DW              20.800 usec
DE               6.50 usec
TE              296.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                1

======== CHANNEL f1 ========
SFO1        100.6278588 MHz
NUC1              13C
P1               8.90 usec
PLW1        54.00000000 W

======== CHANNEL f2 ========
SFO2        400.1516006 MHz
NUC2              1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2        12.00000000 W
PLW12        0.32231000 W
PLW13        0.16212000 W

F2 - Processing parameters
SI               16384
SF          100.6177872 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

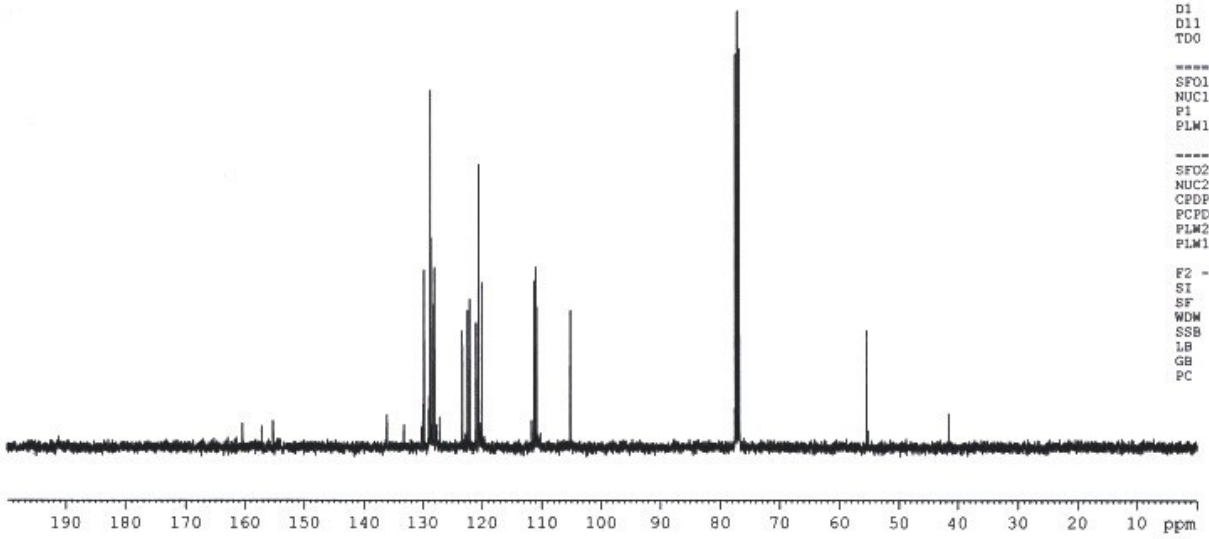

1H of VBSs 139-19
8.144
7.498
7.494
7.477
7.474
7.444
7.432
7.428
7.424
7.411
7.407
7.393
7.382
7.380
7.374
7.370
7.362
7.355
7.347
7.341
7.336
7.331
7.259
7.232
7.228
7.220
7.213
7.208
7.178
7.173
7.164
7.159
7.155
7.151
7.141
7.139
7.121
6.960
6.958
6.941
6.923
6.921
6.906
6.887
6.868
6.848
6.344
6.260
3.592
NH
Ph
O
MeO
3ca
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.88
2.01
4.01
4.06
1.06
3.03
1.08
2.08
0.93
0.94
2.99

VBSS 139-19

160.39
157.11
155.22
136.13
136.09
133.21
130.21
130.00
129.81
128.92
128.74
128.66
128.17
128.04
127.18
123.33
122.44
122.05
121.00
120.55
119.99
111.72
111.29
110.94
110.88
105.19
77.47
77.15
76.83
55.44
41.54

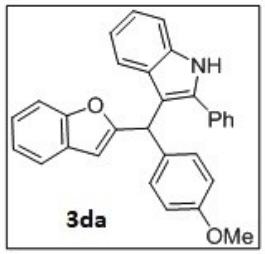


3ca

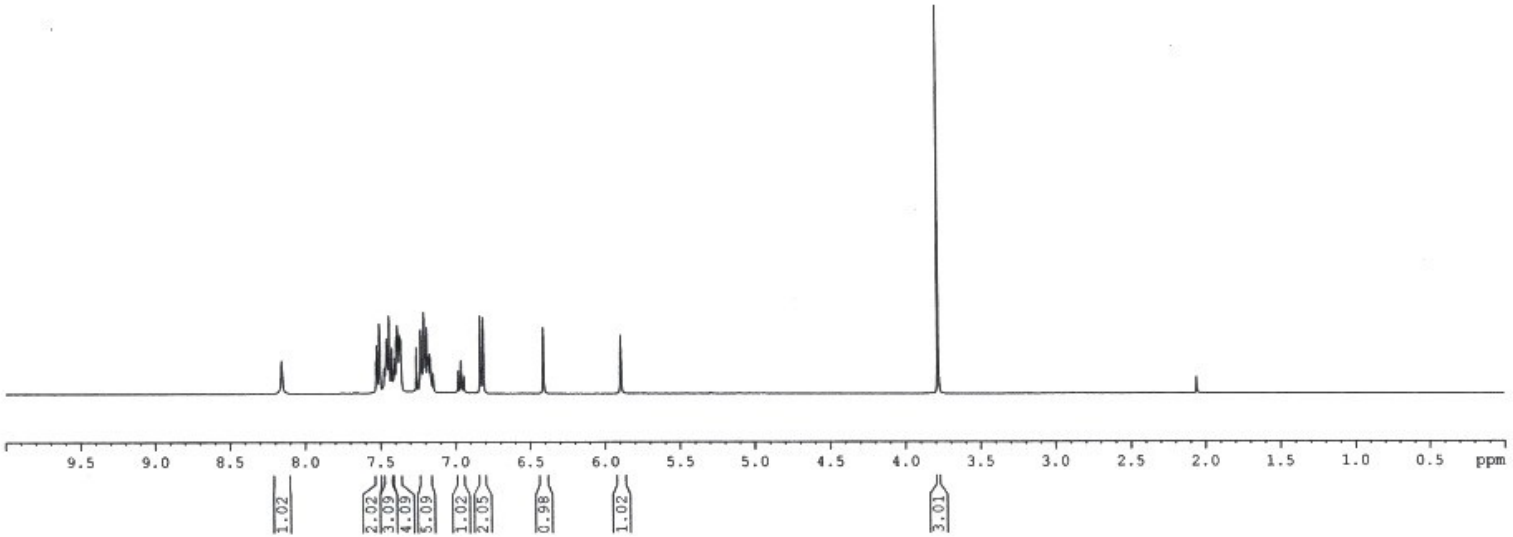



```
Current Data Parameters
NAME      Dr.A.HAJRA 2017
EXPNO              638
PROCNO               1

F2 - Acquisition Parameters
Date_          20170422
Time               7.14
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg
TD              32768
SOLVENT          CDCl3
NS                 640
DS                   2
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG               186.42
DW               20.800 usec
DE                6.50 usec
TE               300.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6278588 MHz
NUC1              13C
P1                8.90 usec
PLW1       54.00000000 W

======== CHANNEL f2 ========
SFO2        400.1516006 MHz
NUC2              1H
CPDPRG[2       waltz16
PCPD2            90.00 usec
PLW2       12.00000000 W
PLW12       0.32231000 W

F2 - Processing parameters
SI                16384
SF          100.6177814 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

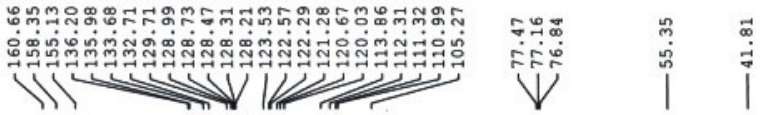
1H of VBSS 139/8

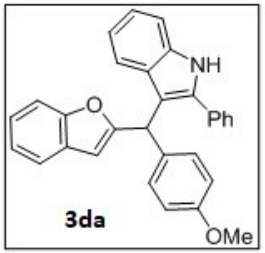


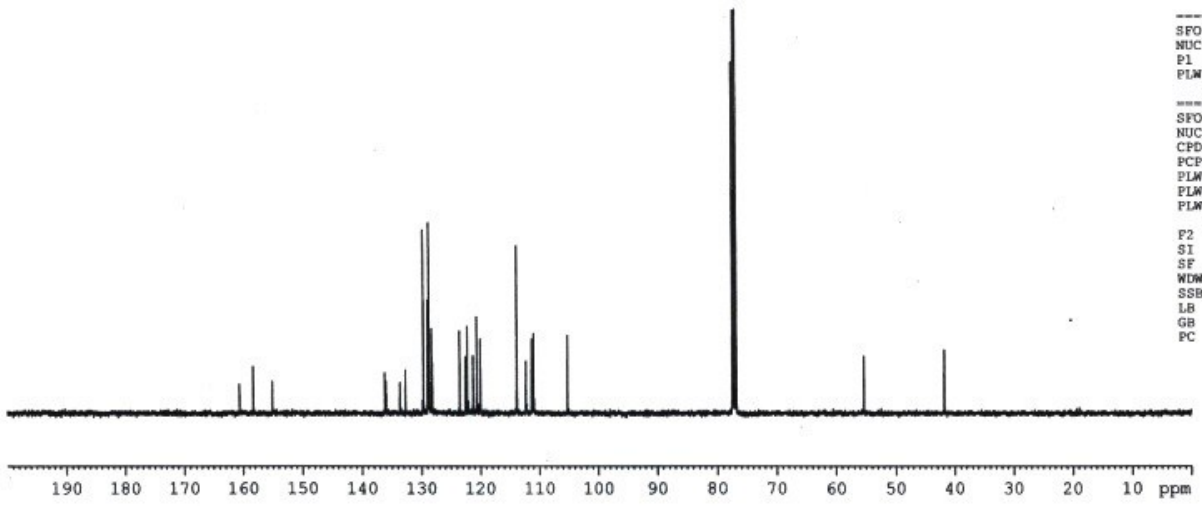
3da



13C of VBSS 139/8

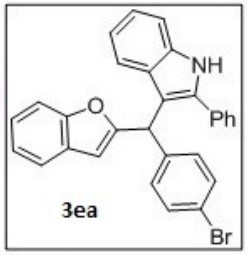


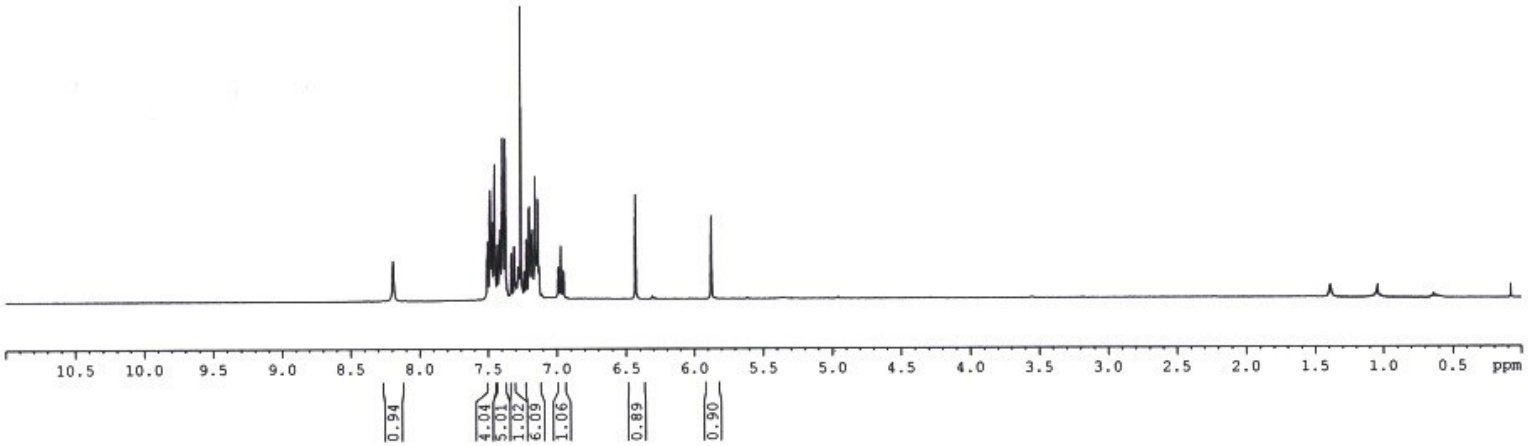




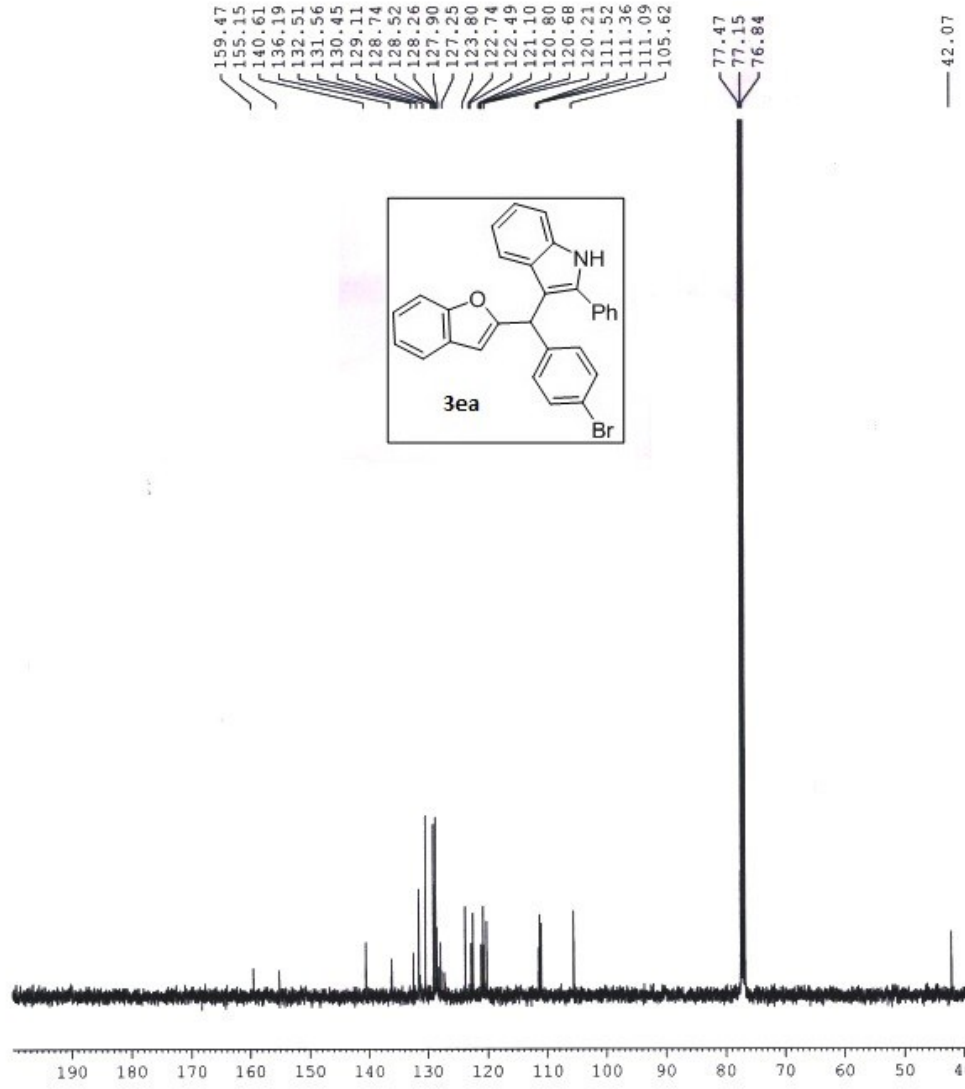

```
Current Data Parameters
NAME      Dr.A.HAJRA 2018
EXPNO              520
PROCNO               1

F2 - Acquisition Parameters
Date_          20180718
Time             09.45
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG        zgpg30
TD               32768
SOLVENT          CDCl3
NS                 420
DS                   2
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG               54.28
DW              20.800 usec
DE               6.50 usec
TE              297.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1       100.6278588 MHz
NUC1              13C
P1                8.90 usec
PLW1      54.00000000 W

======== CHANNEL f2 ========
SFO2       400.1516006 MHz
NUC2              1H
CPDPRG[2       waltz16
PCPD2            90.00 usec
PLW2      12.00000000 W
PLW12      0.32231000 W
PLW13      0.16212000 W

F2 - Processing parameters
SI               16384
SF         100.6177868 MHz
WDW                EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
```

1H of VBSS 139/12

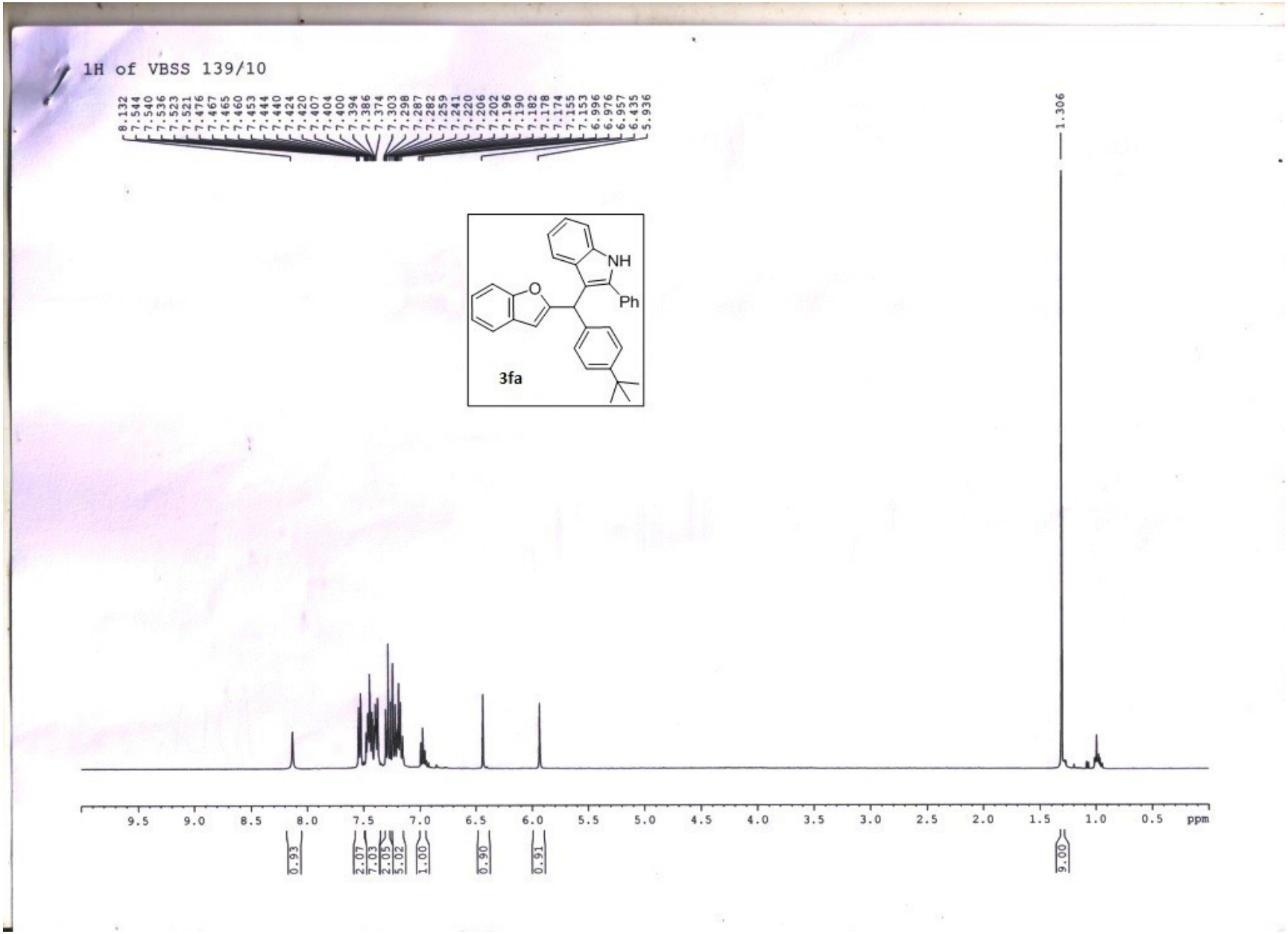




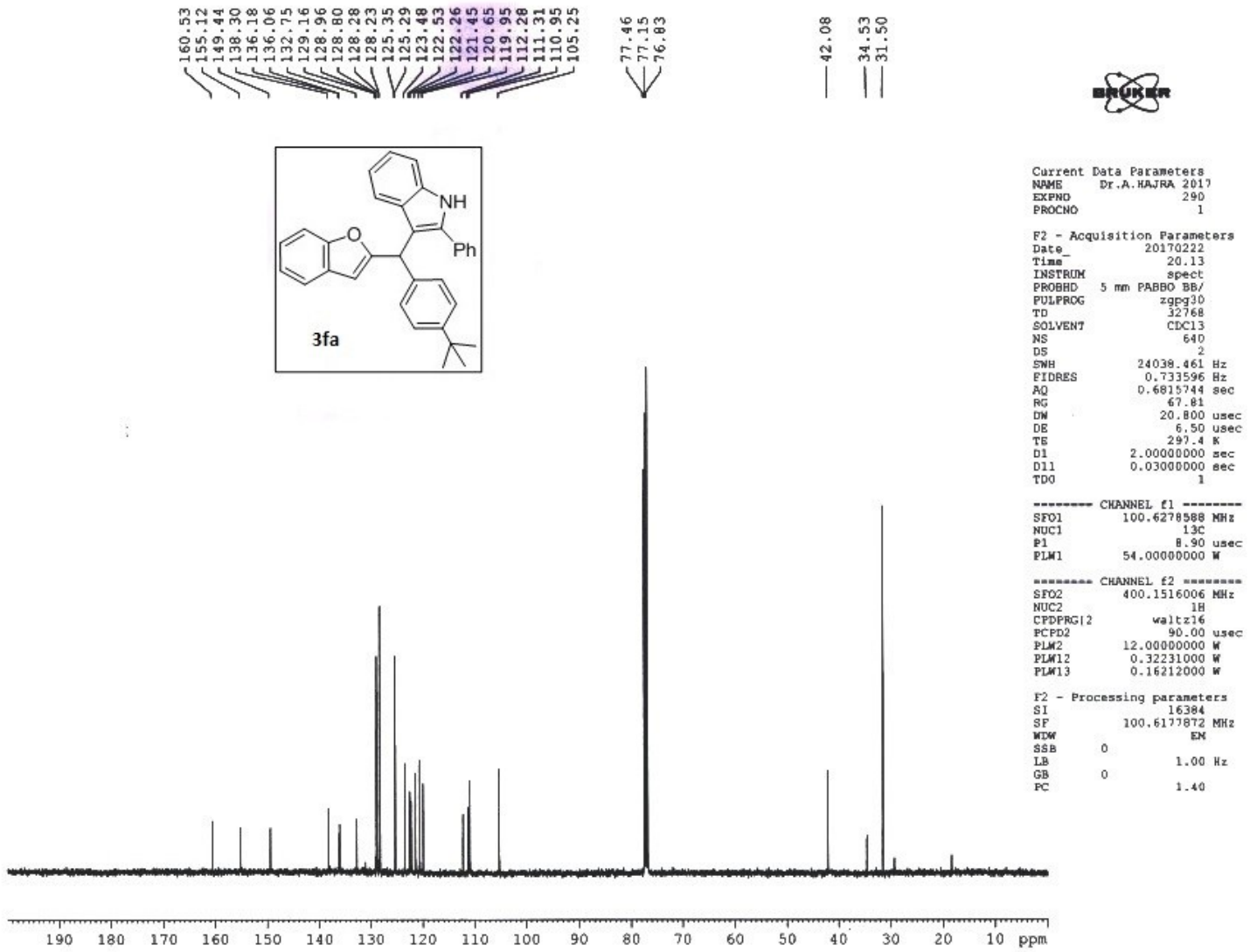
13C of VBSS-139/12




```
Current Data Parameters
NAME      Dr.A.HAJRA 2017
EXPNO              395
PROCNO               1

F2 - Acquisition Parameters
Date_         20170306
Time             12.29
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG       zgpg30
TD             32768
SOLVENT         CDCl3
NS                640
DS                  2
SWH         24038.461 Hz
FIDRES       0.733596 Hz
AQ           0.6815744 sec
RG               77.59
DW              20.800 usec
DE               6.50 usec
TE              297.6 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                 1

======== CHANNEL f1 ========
SFO1       100.6278588 MHz
NUC1              13C
P1               8.90 usec
PLW1       54.00000000 W

======== CHANNEL f2 ========
SFO2       400.1516006 MHz
NUC2              1H
CPDPRG[2       waltz16
PCPD2            90.00 usec
PLW2       12.00000000 W
PLW12       0.32231000 W
PLW13       0.16212000 W

F2 - Processing parameters
SI              16384
SF         100.6177844 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

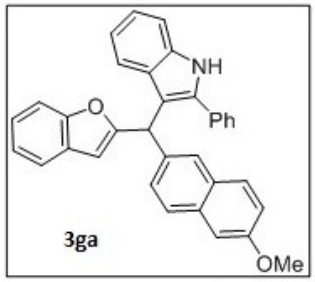

1H of VBSS 139/10
8.132
7.544
7.540
7.536
7.523
7.521
7.476
7.467
7.465
7.460
7.453
7.444
7.440
7.424
7.420
7.407
7.404
7.400
7.394
7.386
7.374
7.303
7.298
7.287
7.282
7.259
7.241
7.220
7.206
7.202
7.196
7.190
7.182
7.178
7.174
7.155
7.153
6.996
6.976
6.957
6.435
5.936
1.306
NH
O
Ph
3fa
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.93
2.07
7.03
2.05
5.02
1.00
0.90
0.91
9.00

13C of VBSS 139/10

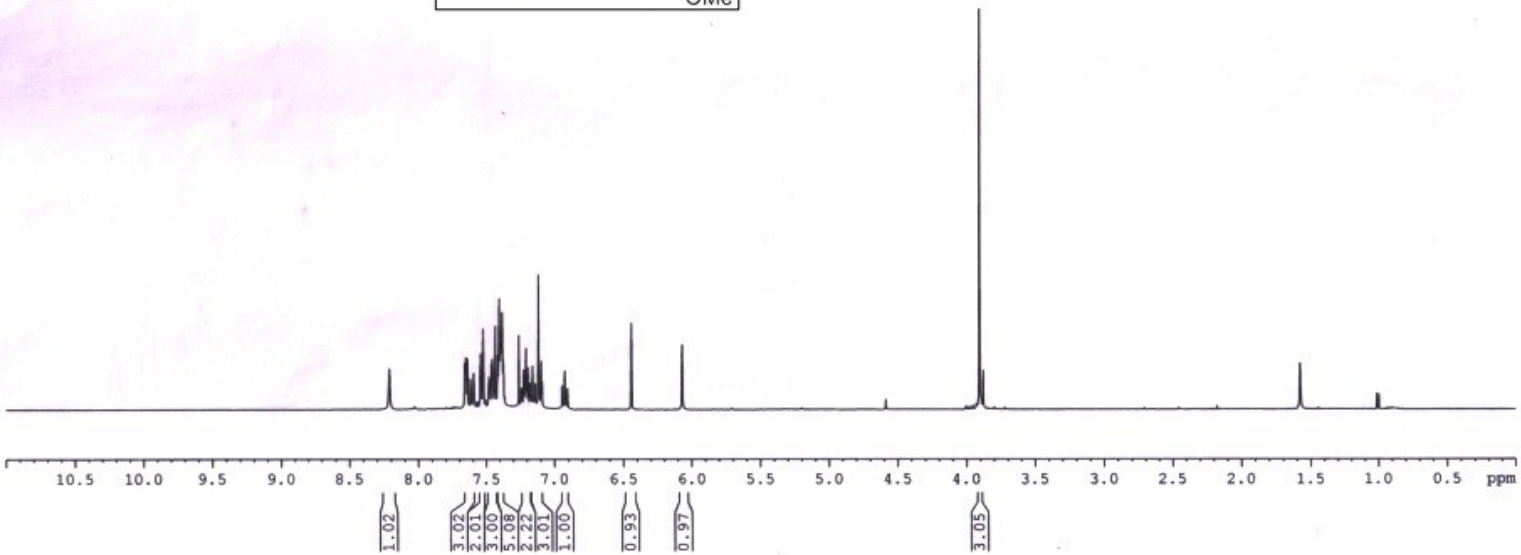


1H of VBSS 139/9

8.212 7.662 7.653 7.641 7.620 7.616 7.596 7.546 7.543 7.525 7.523 7.481 7.478 7.474 7.464 7.458 7.453 7.435 7.431 7.416 7.405 7.400 7.395 7.392 7.384 7.383 7.374 7.259 7.238 7.224 7.220 7.212 7.206 7.201 7.193 7.189 7.159 7.141 7.139 7.116 7.096 6.944 6.942 6.925 6.923 6.907 6.905 6.443 6.069 — 3.906

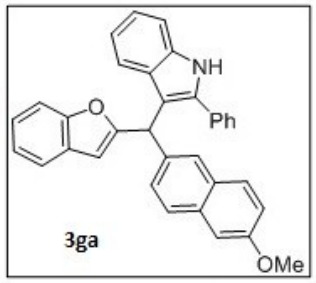


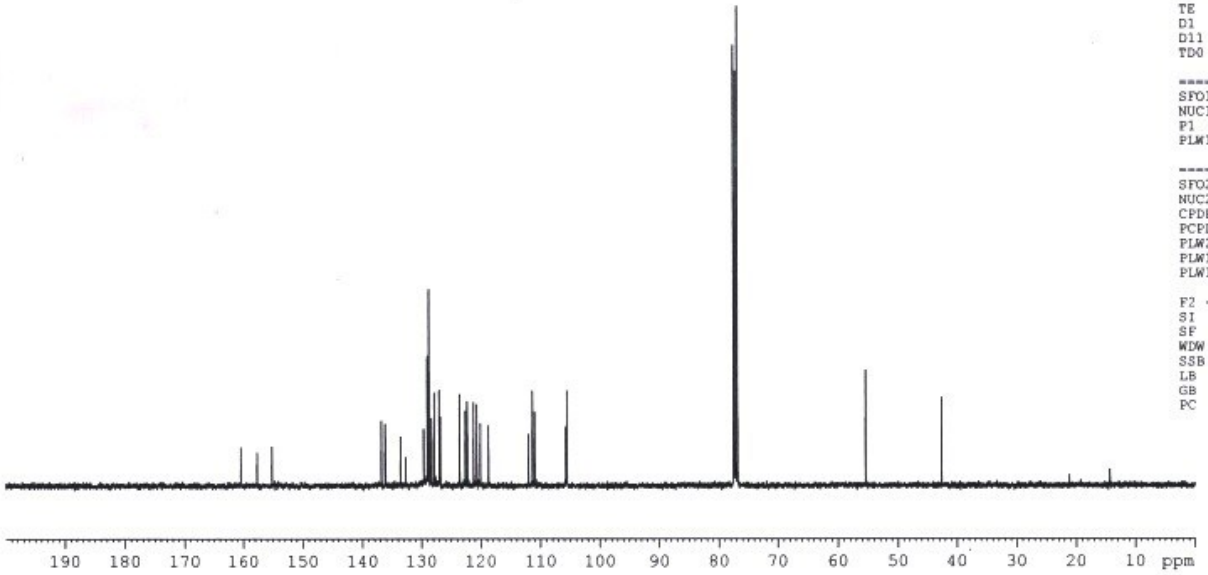
3ga



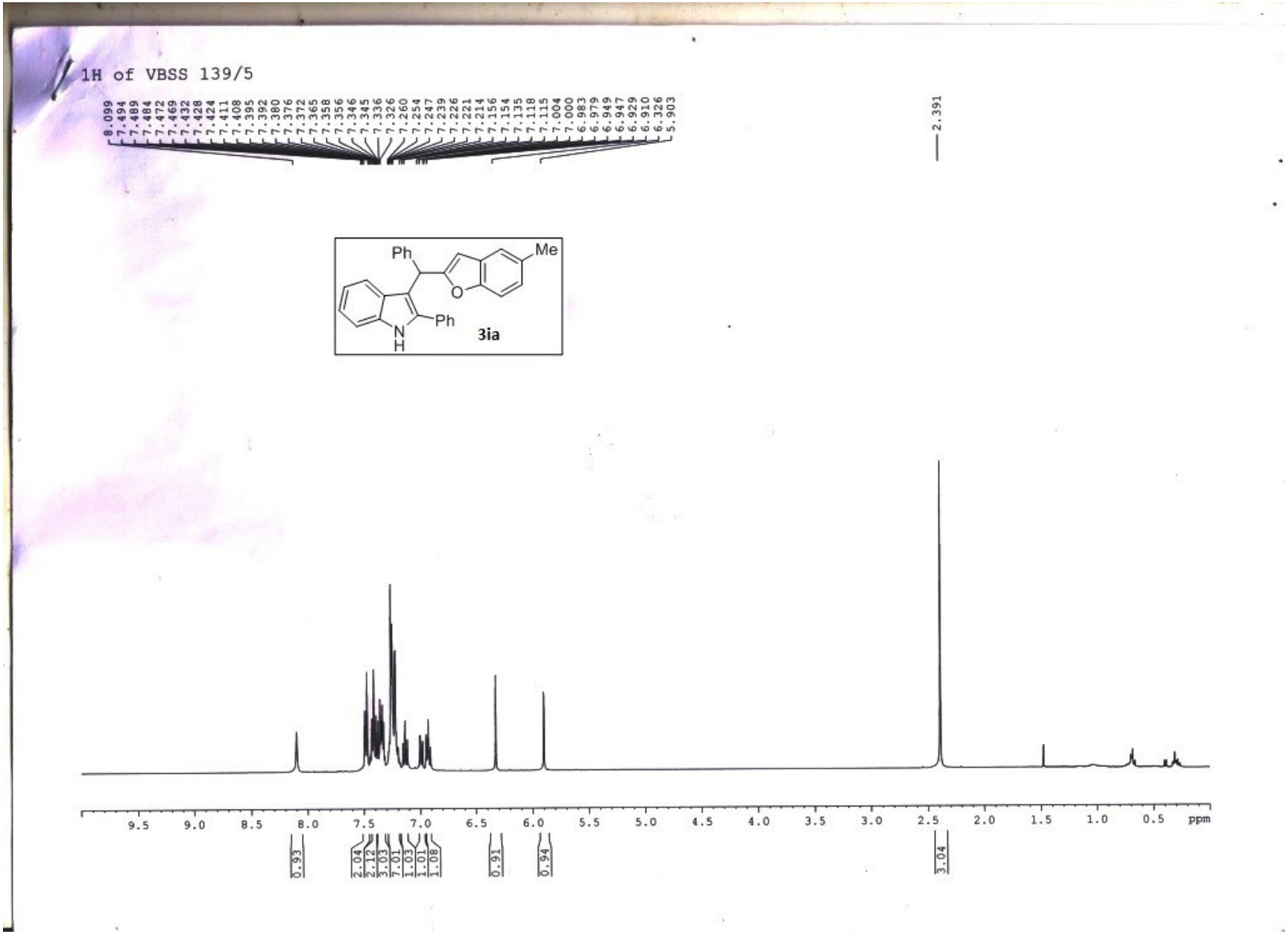
13C of VBSS 139/9

160.38
157.68
155.16
136.81
136.20
136.14
133.56
132.68
129.63
129.00
128.80
128.74
128.34
128.30
127.83
127.26
127.00
126.82
123.59
122.61
122.31
121.24
120.71
120.09
118.77
112.02
111.37
110.99
105.73
105.55
77.47
77.15
76.84
55.42
42.59

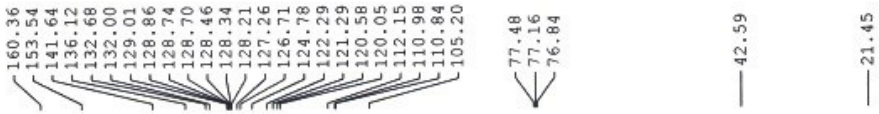


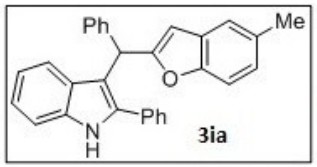



```
Current Data Parameters
NAME      Dr.A.HAJRA 2017
EXPNO              286
PROCNO               1

F2 - Acquisition Parameters
Date_          20170222
Time             14.46
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG        zgpg30
TD              32768
SOLVENT          CDCl3
NS                 640
DS                   2
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG               186.42
DW               20.800 usec
DE                6.50 usec
TE               297.0 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1       100.6278588 MHz
NUC1              13C
P1                8.90 usec
PLW1      54.00000000 W

======== CHANNEL f2 ========
SFO2       400.1516006 MHz
NUC2              1H
CPDPRG[2       waltz16
PCPD2            90.00 usec
PLW2      12.00000000 W
PLW12      0.32231000 W
PLW13      0.16212000 W

F2 - Processing parameters
SI               16384
SF         100.6177880 MHz
WDW                EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
```


1H of VBSS 139/5
8.099
7.494
7.489
7.484
7.472
7.469
7.432
7.428
7.424
7.411
7.408
7.395
7.392
7.380
7.376
7.372
7.365
7.358
7.356
7.346
7.345
7.336
7.326
7.260
7.254
7.247
7.239
7.226
7.221
7.214
7.156
7.154
7.135
7.118
7.115
7.004
7.000
6.983
6.979
6.949
6.947
6.929
6.910
6.326
5.903
2.391
Ph
Me
O
Ph
N
H
3ia
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.93
2.04
2.12
3.03
7.01
1.03
1.01
1.08
0.91
0.94
3.04

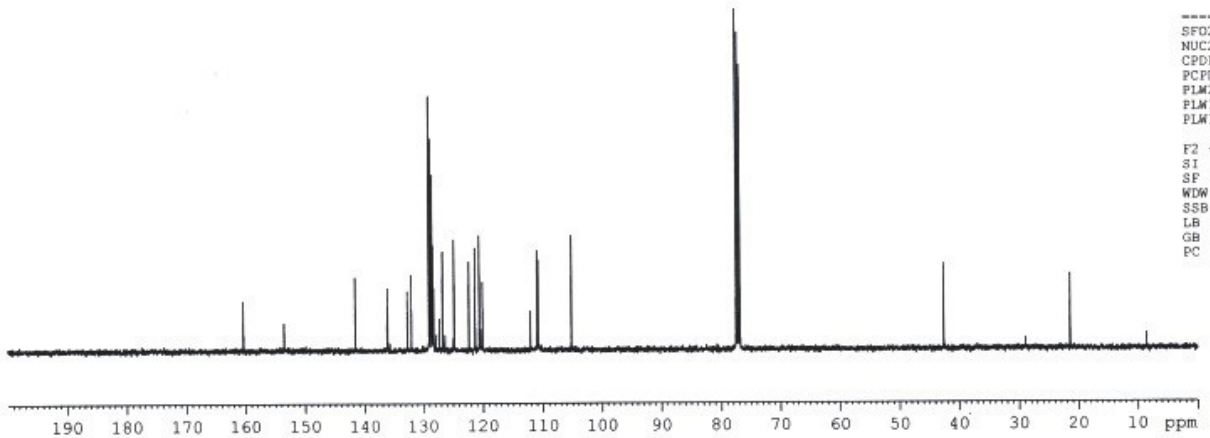
13C of VBSS-139/5

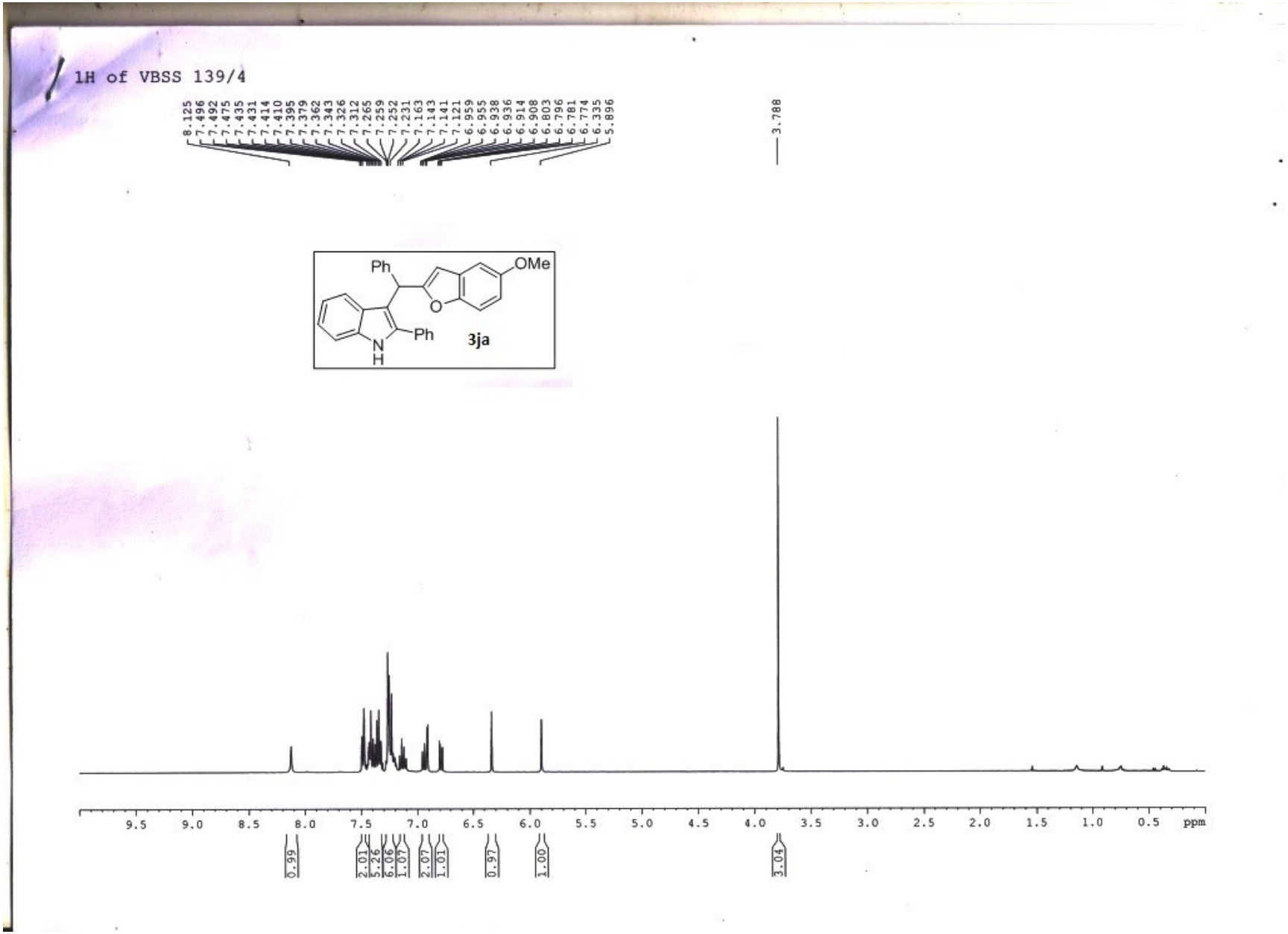




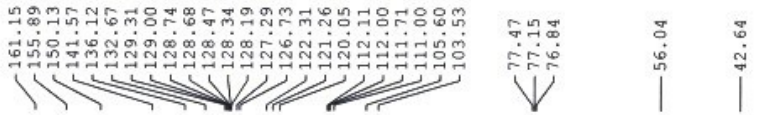
3ia

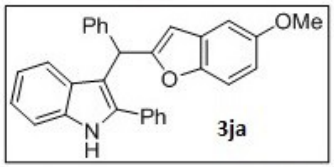
```
Current Data Parameters
NAME      Dr.A.HAJRA 2017
EXPNO              258
PROCNO               1

F2 - Acquisition Parameters
Date_          20170215
Time             18.46
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG        zgpg30
TD              32768
SOLVENT          CDCl3
NS                 420
DS                   2
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG               77.59
DW              20.800 usec
DE               6.50 usec
TE              296.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1       100.6278588 MHz
NUC1              13C
P1               8.90 usec
PLW1       54.00000000 W

======== CHANNEL f2 ========
SFO2       400.1516006 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2       12.00000000 W
PLW12       0.32231000 W
PLW13       0.16212000 W

F2 - Processing parameters
SI               16384
SF         100.6177885 MHz
WDW                EM
SSB      0
LB               1.00 Hz
GB       0
PC               1.40
```

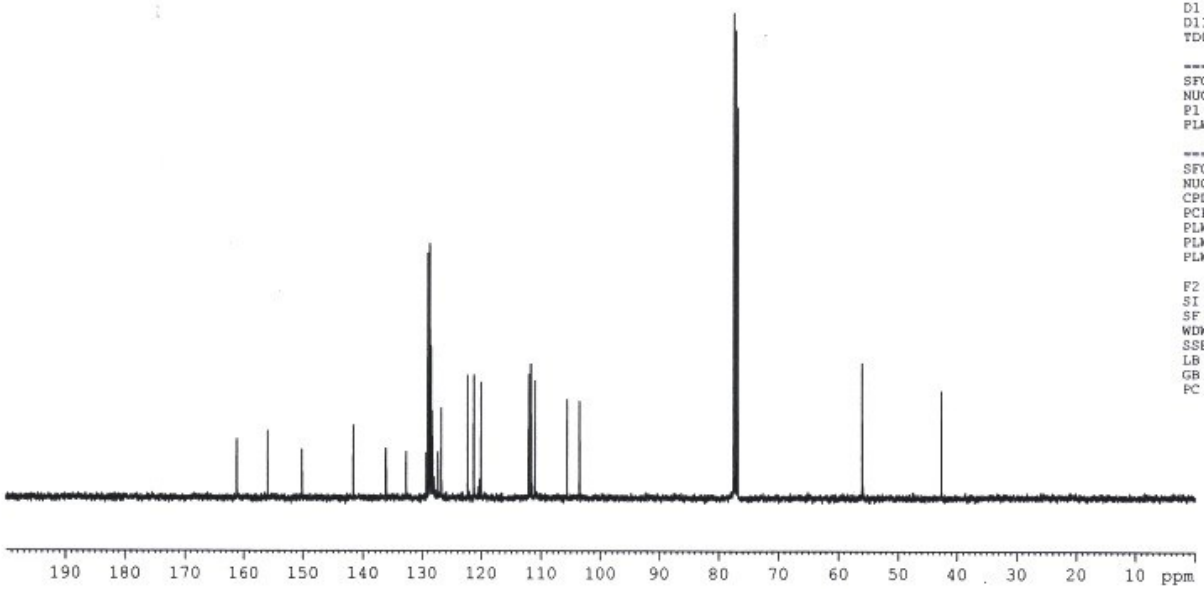



1H of VBSS 139/4
8.125
7.496
7.492
7.475
7.435
7.431
7.414
7.410
7.395
7.379
7.362
7.343
7.326
7.312
7.265
7.259
7.252
7.231
7.163
7.143
7.141
7.121
6.959
6.955
6.938
6.936
6.914
6.908
6.803
6.796
6.781
6.774
6.335
5.896
3.788
Ph
OMe
O
Ph
N
H
3ja
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.99
2.01
5.26
6.06
1.07
2.07
1.01
0.97
1.00
3.04

VBSS-13974



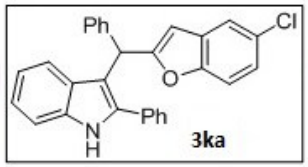




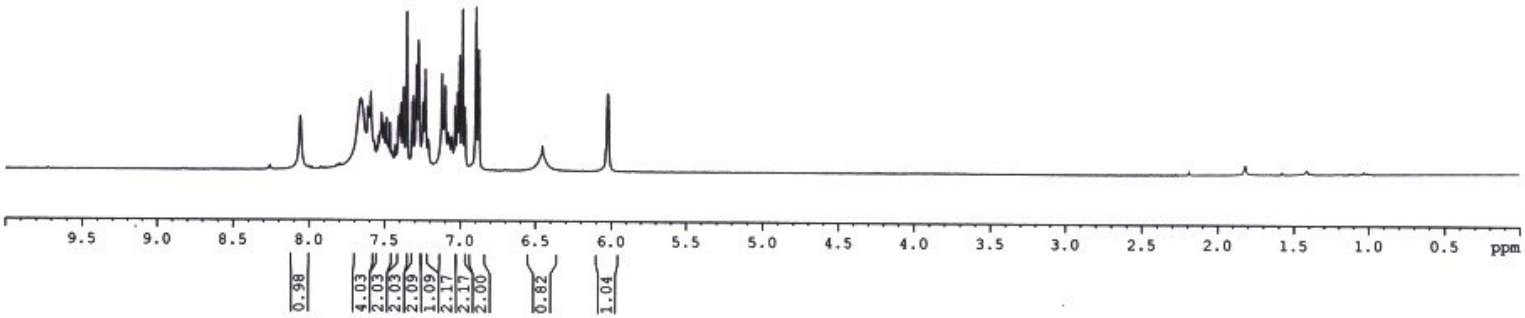

```
Current Data Parameters
NAME      Dr.A.HAJRA 2017
EXPNO              246
PROCNO               1

F2 - Acquisition Parameters
Date_          20170213
Time              20.13
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD              32768
SOLVENT           CDCl3
NS                  420
DS                    2
SWH           24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                186.42
DW               20.800 usec
DE                6.50 usec
TE               298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6278588 MHz
NUC1              13C
P1                8.90 usec
PLW1       54.00000000 W

======== CHANNEL f2 ========
SFO2        400.1516006 MHz
NUC2              1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2       12.00000000 W
PLW12       0.32231000 W
PLW13       0.16212000 W

F2 - Processing parameters
SI               16384
SF          100.6177873 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

1H of VBSS-139-2-chloro

8.061
7.659
7.613
7.606
7.593
7.542
7.523
7.518
7.509
7.506
7.489
7.467
7.410
7.402
7.394
7.390
7.377
7.357
7.318
7.313
7.297
7.291
7.280
7.250
7.238
7.233
7.124
7.103
7.085
7.078
7.065
7.061
7.039
7.021
7.008
6.989
6.972
6.968
6.898
6.881
6.877
6.454
6.025



3ka

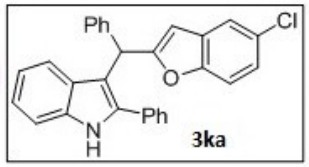


13C of VBSS-139-2

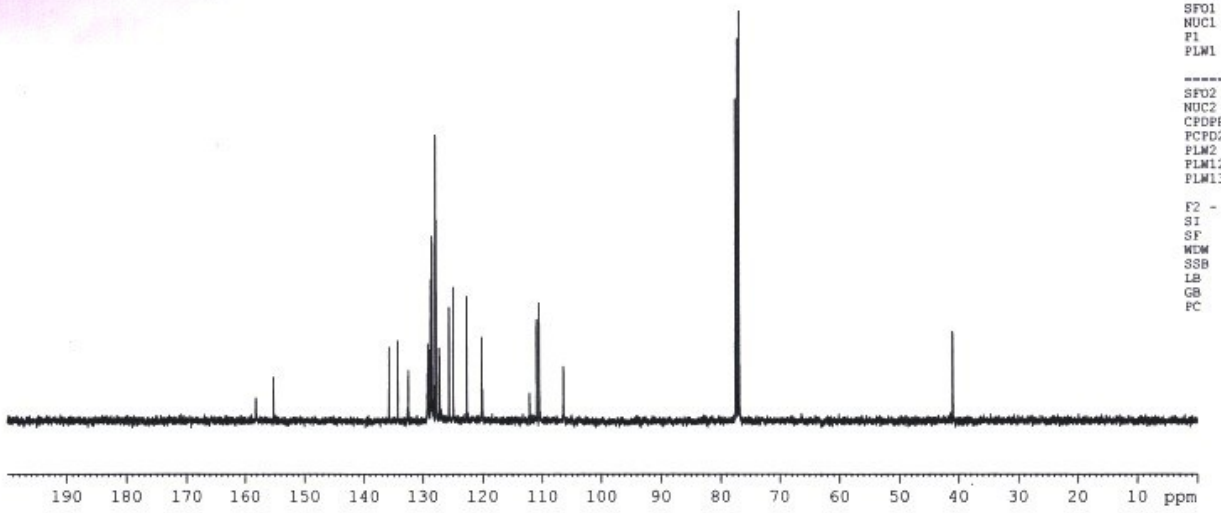
158.19
155.22
135.75
134.26
132.47
129.21
129.11
128.86
128.72
128.66
128.48
128.44
127.89
127.79
127.28
127.17
125.63
124.93
122.63
120.14
112.17
110.96
110.52
106.44

77.47
77.16
76.84

41.03

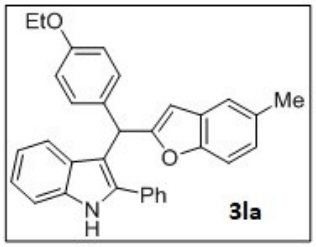


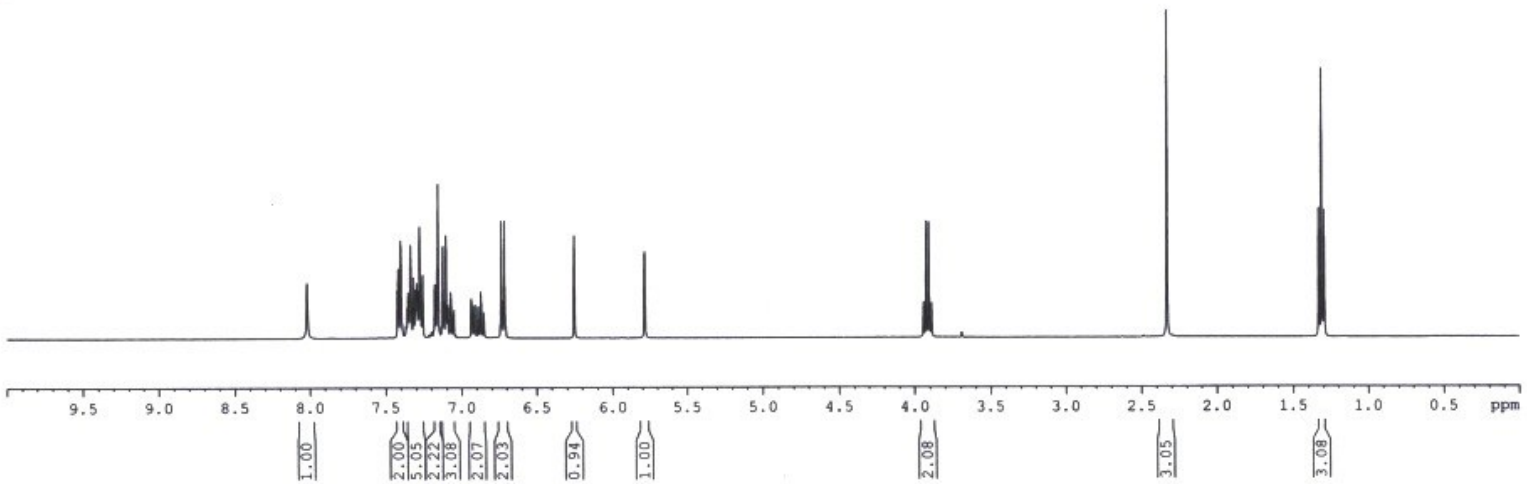
3ka




```
Current Data Parameters
NAME      Dr. A HAJRA 2018-2nd
EXPNO                  295
PROCNO                   1

F2 - Acquisition Parameters
Date_           20180414
Time                13.00
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 32768
SOLVENT             CDCl3
NS                    320
DS                      2
SWH             24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                  57.28
DW                20.800 usec
DE                 6.50 usec
TE                298.3 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          100.6278588 MHz
NUC1                  13C
P1                   8.90 usec
PLW1          54.00000000 W

======== CHANNEL f2 ========
SFO2          400.1516006 MHz
NUC2                  1H
CPDPRG[2           waltz16
PCPD2                90.00 usec
PLW2          12.00000000 W
PLW12          0.32231000 W
PLW13          0.16212000 W

F2 - Processing parameters
SI                    16384
SF            100.6177882 MHz
WDW                     EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

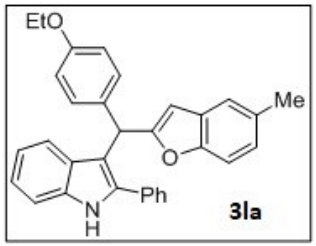
1H of vbSS-139-Me/OEt



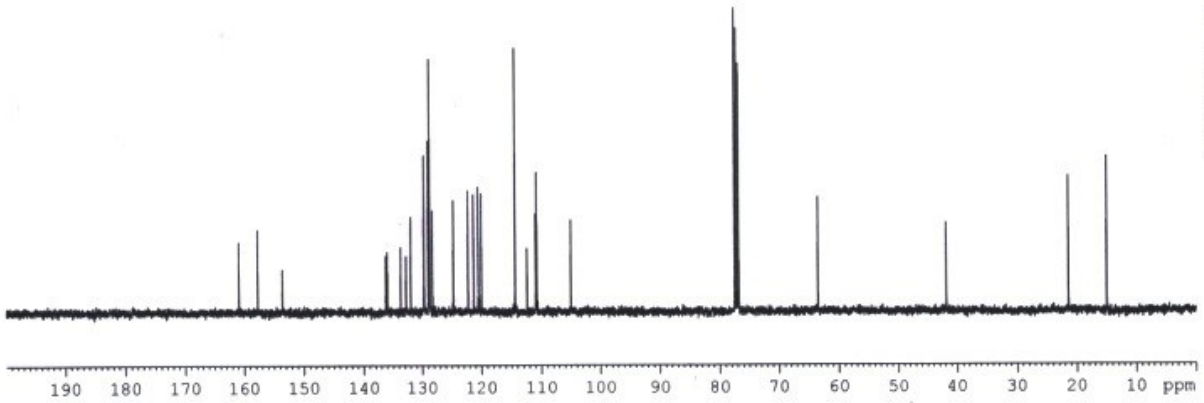


13C of vbSS-139-Me/OEt

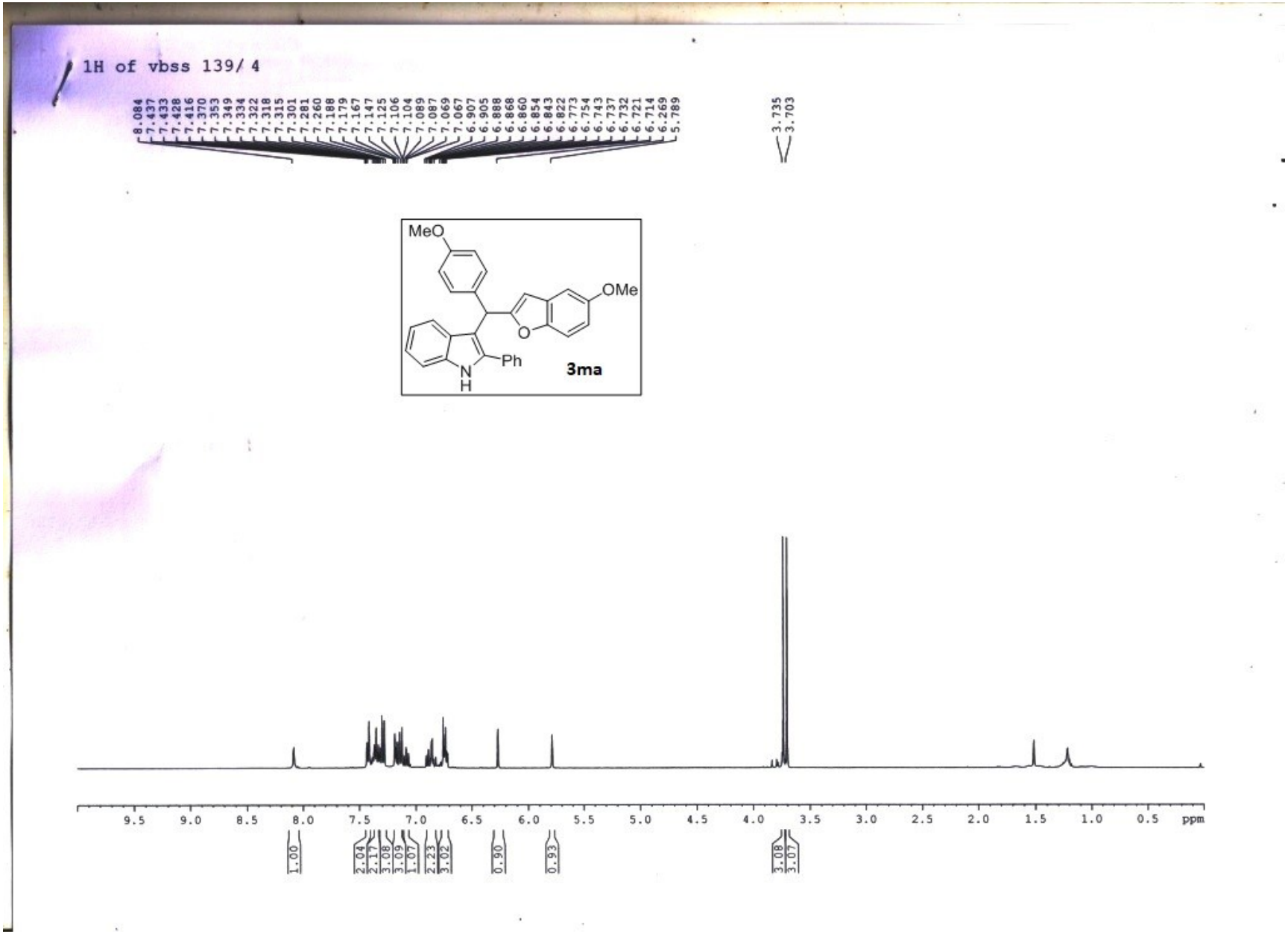
160.84
157.72
153.55
136.20
135.95
133.66
132.75
131.94
129.79
129.70
128.95
128.90
128.73
128.26
124.71
122.24
121.31
120.55
120.01
114.40
112.41
110.98
110.81
105.01
77.47
77.16
76.84
63.49
41.86
21.42
15.00

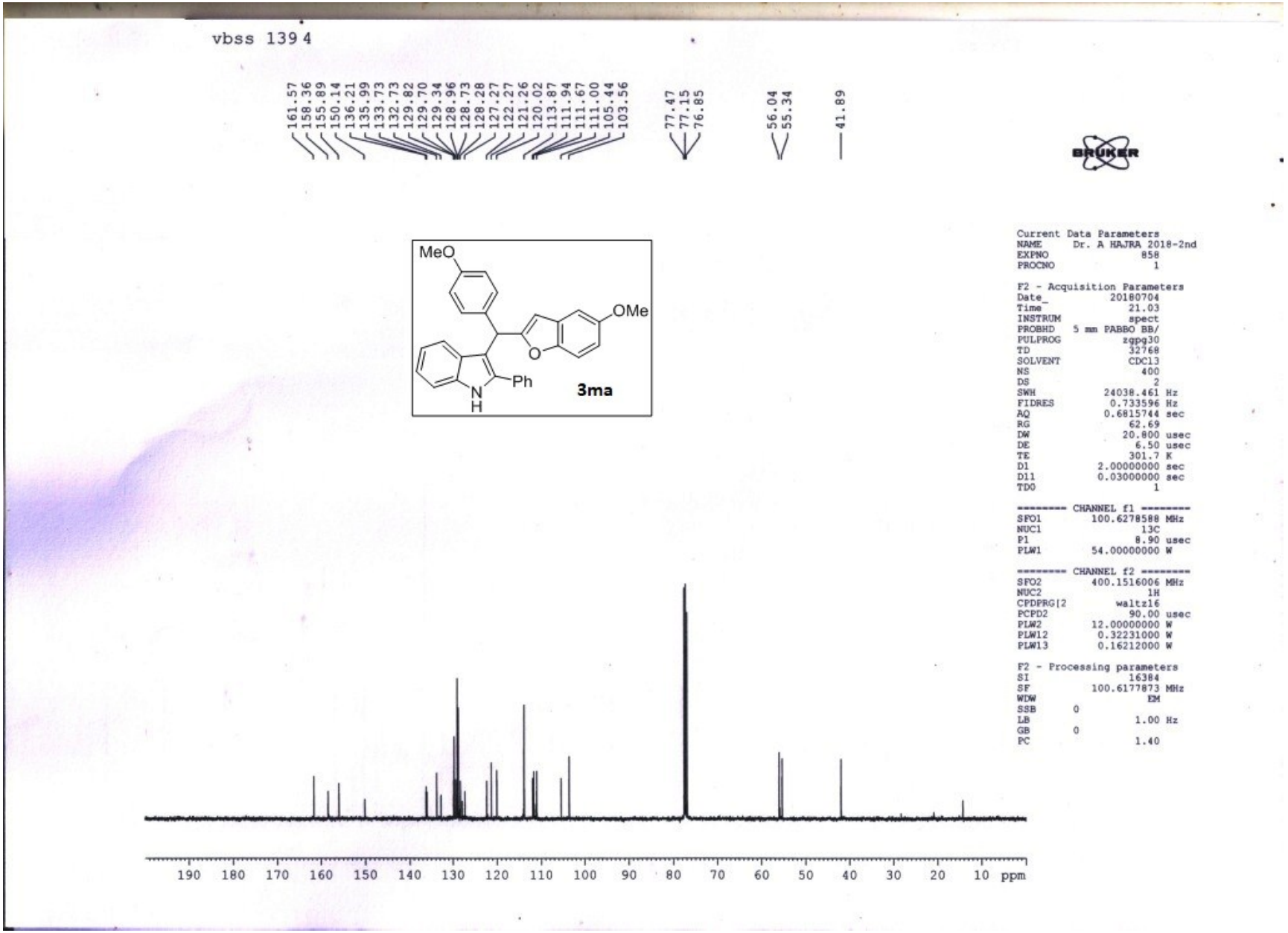


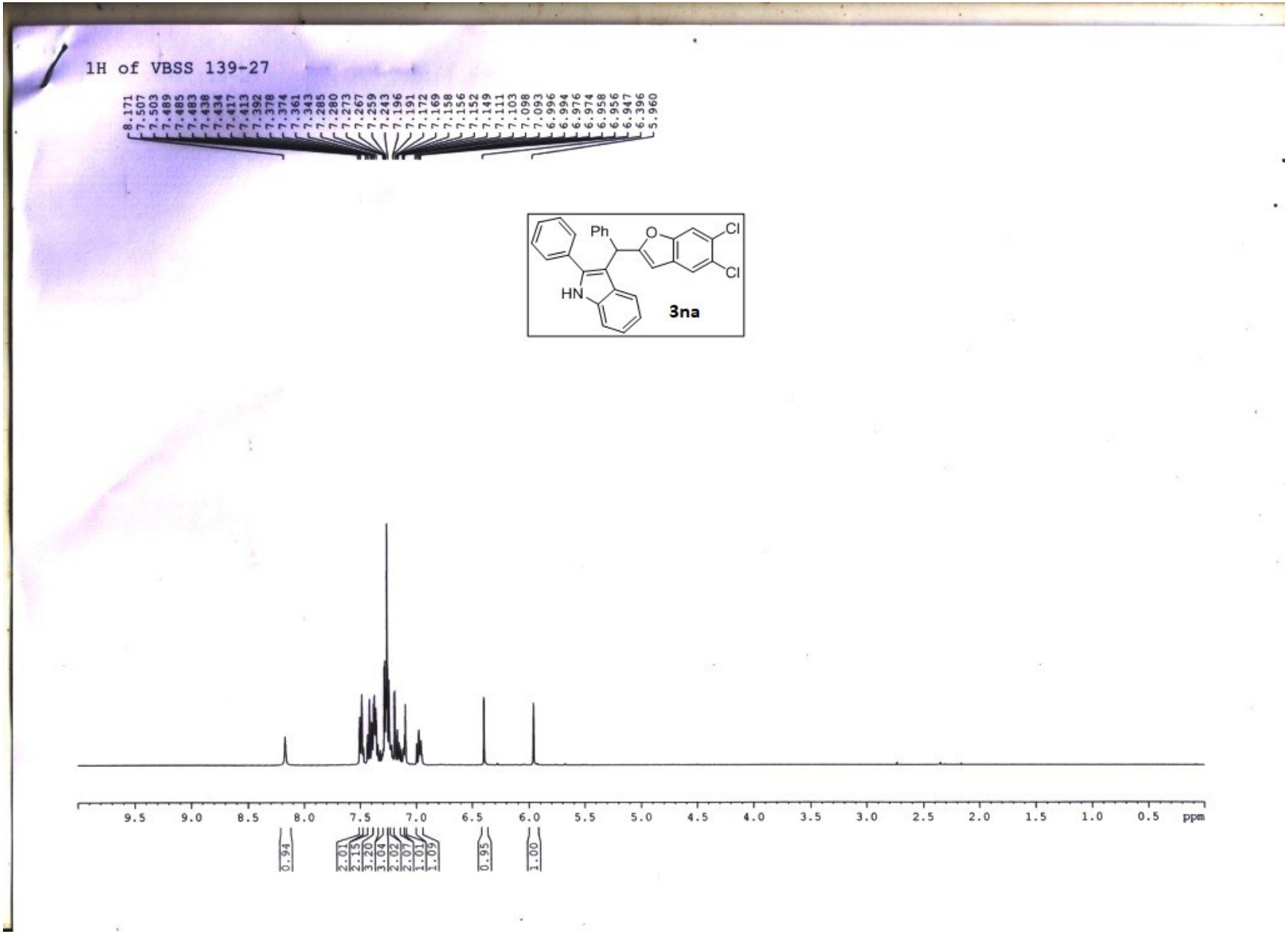
3la




```
Current Data Parameters
NAME      Dr. A HAJRA 2018-2nd
EXPNO                  854
PROCNO                   1

F2 - Acquisition Parameters
Date_              20180704
Time                  9.30
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 32768
SOLVENT             CDCl3
NS                    106
DS                      2
SWH             24038.461 Hz
FIDRES           0.733596 Hz
AQ               0.6815744 sec
RG                   67.81
DW                 20.800 usec
DE                  6.50 usec
TE                 299.6 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         100.6278588 MHz
NUC1                   13C
P1                    8.90 usec
PLW1         54.00000000 W

======== CHANNEL f2 ========
SFO2         400.1516006 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2                90.00 usec
PLW2         12.00000000 W
PLW12         0.32231000 W
PLW13         0.16212000 W

F2 - Processing parameters
SI                    16384
SF           100.6177887 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```


1H of vbss 139/ 4
8.084
7.437
7.433
7.428
7.416
7.370
7.353
7.349
7.334
7.322
7.318
7.315
7.301
7.281
7.260
7.188
7.179
7.167
7.147
7.125
7.106
7.104
7.089
7.087
7.069
7.067
6.907
6.905
6.888
6.868
6.860
6.854
6.843
6.822
6.773
6.754
6.743
6.737
6.732
6.721
6.714
6.269
5.789
3.735
3.703
MeO
OMe
O
Ph
N
H
3ma
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.00
2.04
2.17
3.08
3.09
1.07
2.23
3.02
0.90
0.93
3.08
3.07


vbss 139 4
161.57
158.36
155.89
150.14
136.21
135.99
133.73
132.73
129.82
129.70
129.34
128.96
128.73
128.28
127.27
122.27
121.26
120.02
113.87
111.94
111.67
111.00
105.44
103.56
77.47
77.15
76.85
56.04
55.34
41.89
BRUKER
MeO
OMe
O
Ph
N
H
3ma
Current Data Parameters
NAME Dr. A HAJRA 2018-2nd
EXPNO 858
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180704
Time 21.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 400
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 62.69
DW 20.800 usec
DE 6.50 usec
TE 301.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6278588 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
======== CHANNEL f2 ========
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W
F2 - Processing parameters
SI 16384
SF 100.6177873 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

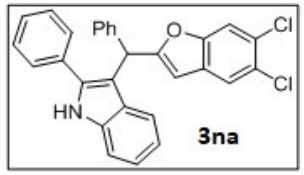

1H of VBSS 139-27
8.171
7.507
7.503
7.489
7.485
7.483
7.438
7.434
7.417
7.413
7.392
7.378
7.374
7.361
7.343
7.285
7.280
7.273
7.267
7.259
7.243
7.196
7.191
7.172
7.169
7.158
7.156
7.152
7.149
7.111
7.103
7.098
7.093
6.996
6.994
6.976
6.974
6.958
6.956
6.947
6.396
5.960
Ph
O
Cl
Cl
HN
3na
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.94
2.01
2.15
3.20
3.04
2.02
2.07
1.01
1.09
0.95
1.00

13C VBSS 139-27

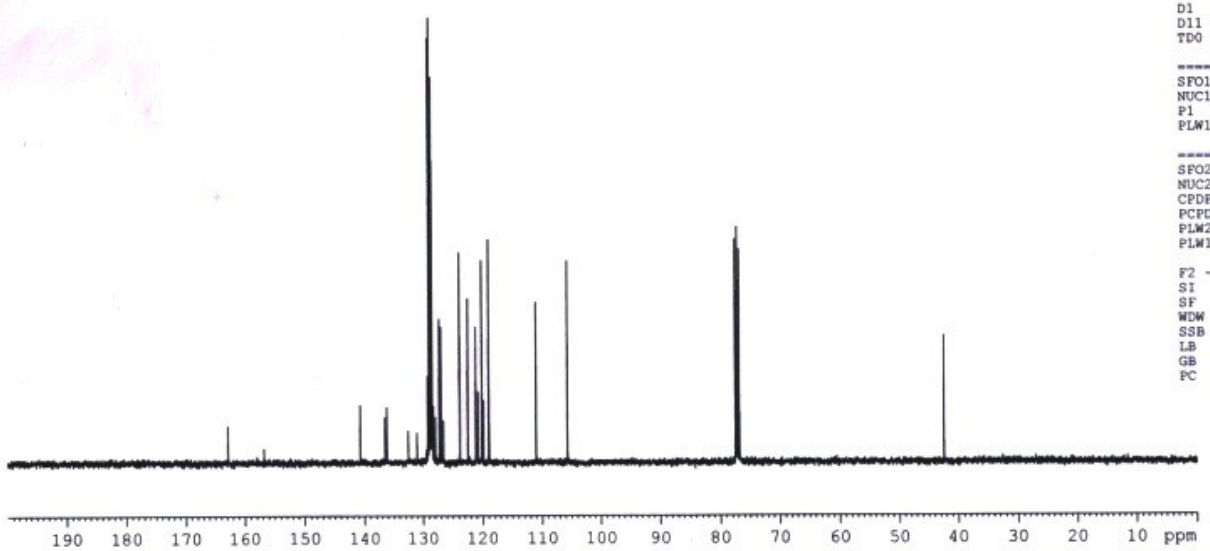
162.78
156.77
140.72
136.47
136.18
132.53
131.04
129.19
128.98
128.83
128.56
128.47
127.93
127.23
126.95
123.83
122.44
121.12
120.77
120.12
119.86
118.97
111.06
105.69

77.47
77.15
76.83

42.43



3na



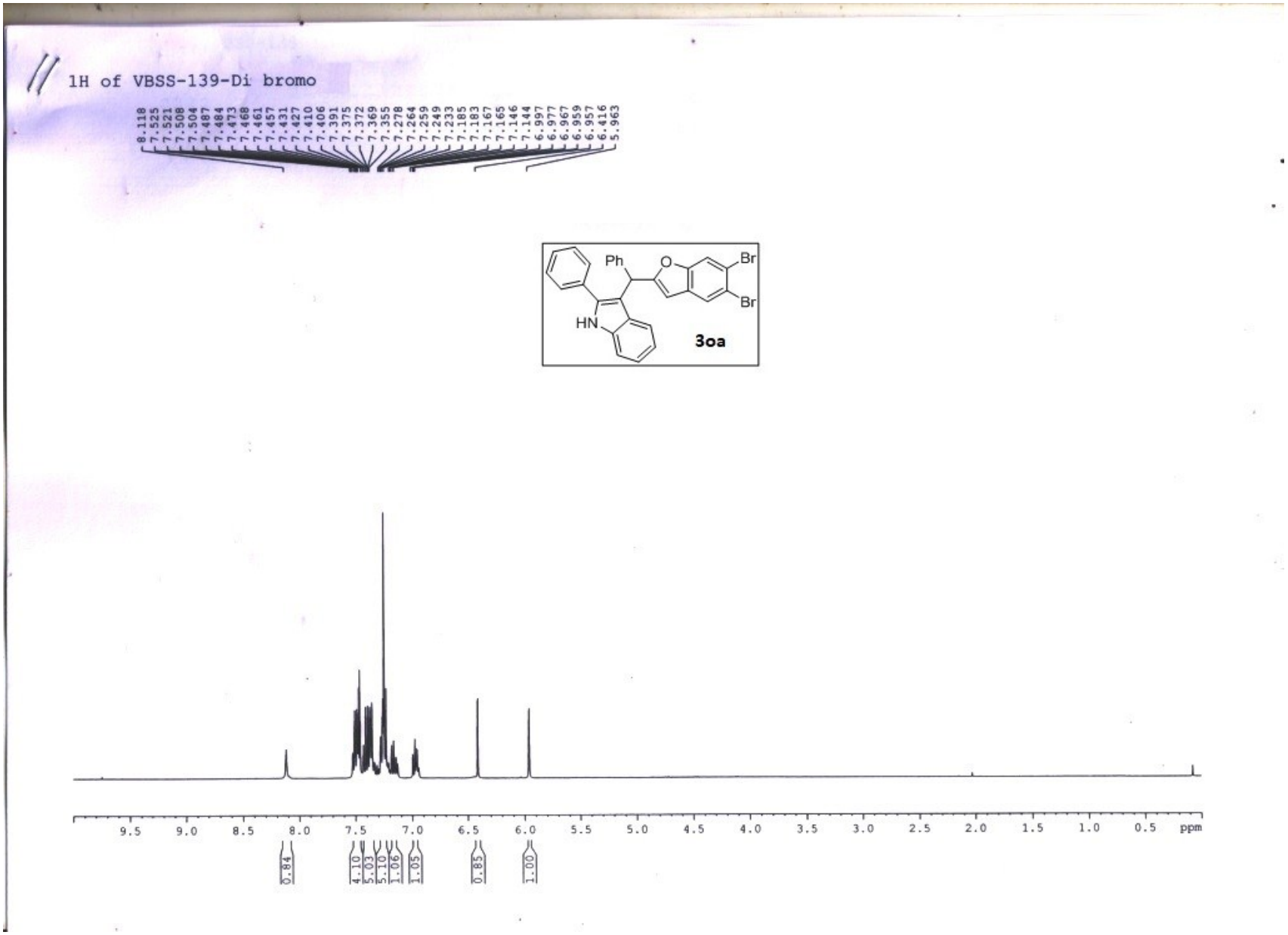
Current Data Parameters
NAME Dr.A.HAJRA 2017
EXPNO 828
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170519
Time 12.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 640
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 77.59
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

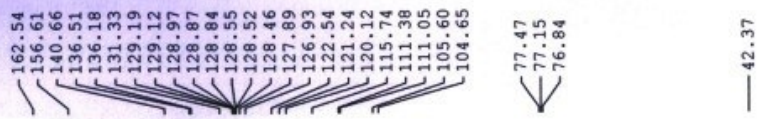
======== CHANNEL f1 ========
SFO1 100.6278588 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W

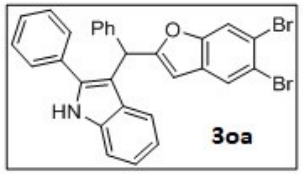
======== CHANNEL f2 ========
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W

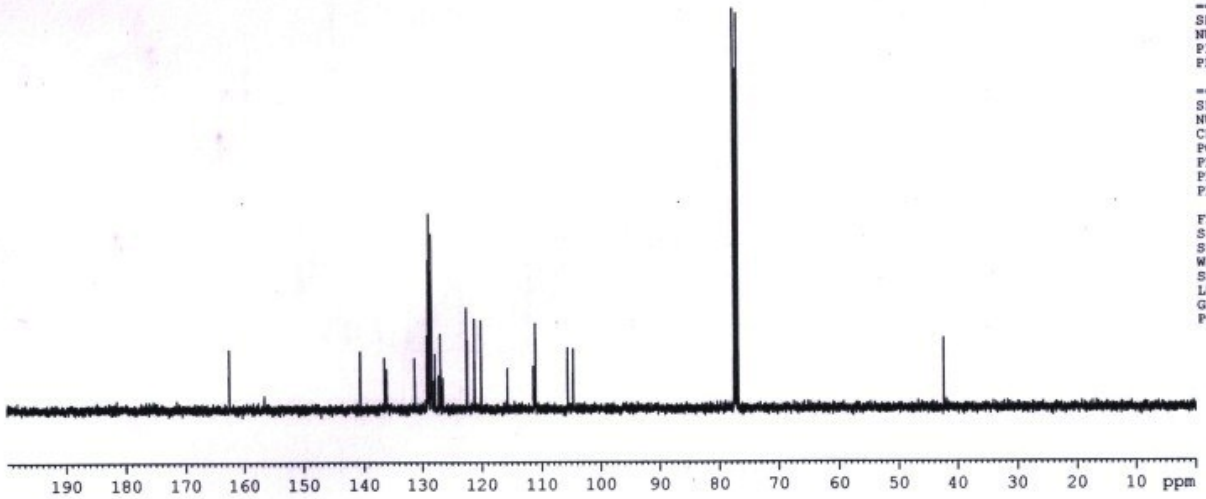
F2 - Processing parameters
SI 16384
SF 100.6177858 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


1H of VBSS-139-Di bromo
8.118
7.525
7.521
7.508
7.504
7.487
7.484
7.473
7.468
7.461
7.457
7.431
7.427
7.410
7.406
7.391
7.375
7.372
7.369
7.355
7.278
7.264
7.259
7.249
7.233
7.185
7.183
7.167
7.165
7.146
7.144
6.997
6.977
6.967
6.959
6.957
6.416
5.963
Ph
O
Br
Br
HN
3oa
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.84
4.10
5.03
5.10
1.06
1.05
0.85
1.00

13C of VBSS-139-dil



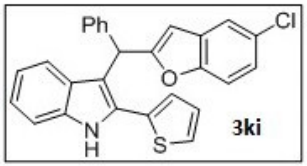




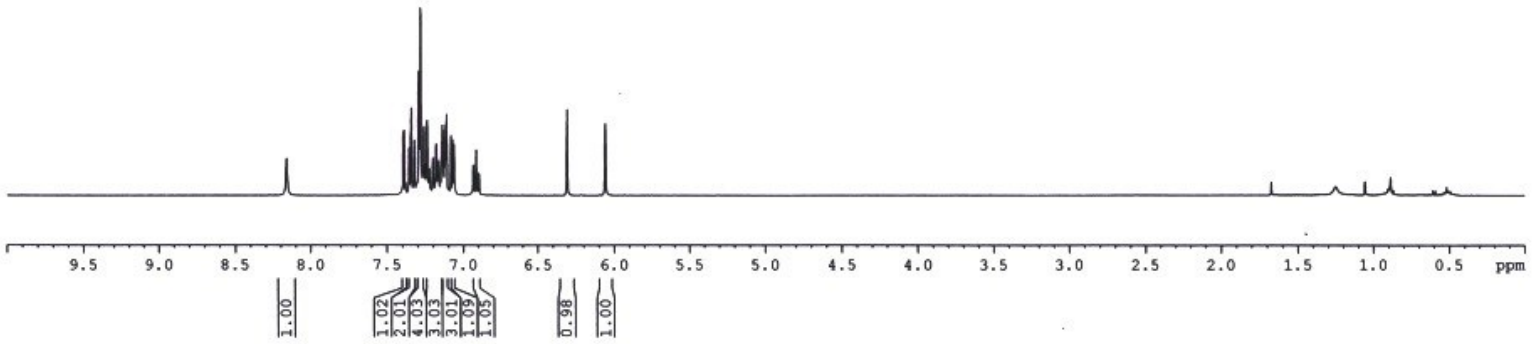

```
Current Data Parameters
NAME      Dr. A HAJRA 2018-2nd
EXPNO                 836
PROCNO                  1

F2 - Acquisition Parameters
Date_              20180701
Time                  9.14
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                     196
DS                       2
SWH              24038.461 Hz
FIDRES           0.733596 Hz
AQ               0.6815744 sec
RG                   62.69
DW                  20.800 usec
DE                   6.50 usec
TE                  300.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         100.6278588 MHz
NUC1                 13C
P1                  8.90 usec
PLW1         54.00000000 W

======== CHANNEL f2 ========
SFO2         400.1516006 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2         12.00000000 W
PLW12         0.32231000 W
PLW13         0.16212000 W

F2 - Processing parameters
SI                   16384
SF           100.6177865 MHz
WDW                    EM
SSB      0
LB                   1.00 Hz
GB       0
PC                   1.40
```

1H of VBSS 139-29

8.161
7.395
7.390
7.358
7.355
7.342
7.322
7.292
7.282
7.260
7.238
7.222
7.201
7.180
7.171
7.167
7.164
7.162
7.146
7.144
7.140
7.135
7.126
7.123
7.118
7.112
7.109
7.084
7.075
7.071
7.062
6.934
6.914
6.896
6.894
6.307
6.059



3ki

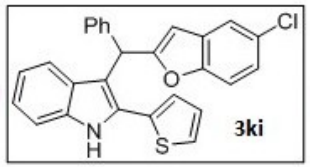


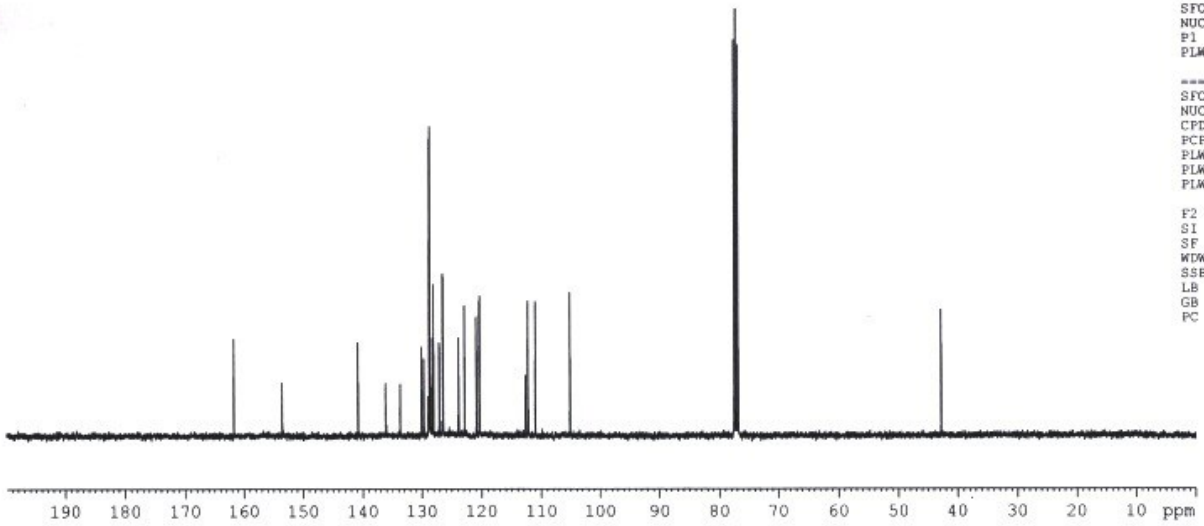
13C of VBSS 139-29

161.69
153.52
140.80
136.16
133.66
130.03
129.65
128.91
128.72
128.63
128.17
128.00
127.03
126.47
126.38
123.84
122.84
120.90
120.39
120.32
112.69
112.28
111.03
105.14

77.47
77.15
76.84

42.77





Current Data Parameters
NAME Dr.A.HAJRA 2017
EXPNO 889
PROCNO 1

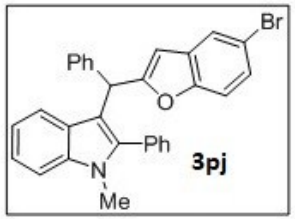
F2 - Acquisition Parameters
Date_ 20170527
Time 10.43
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 340
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 62.69
DW 20.800 usec
DE 6.50 usec
TE 294.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

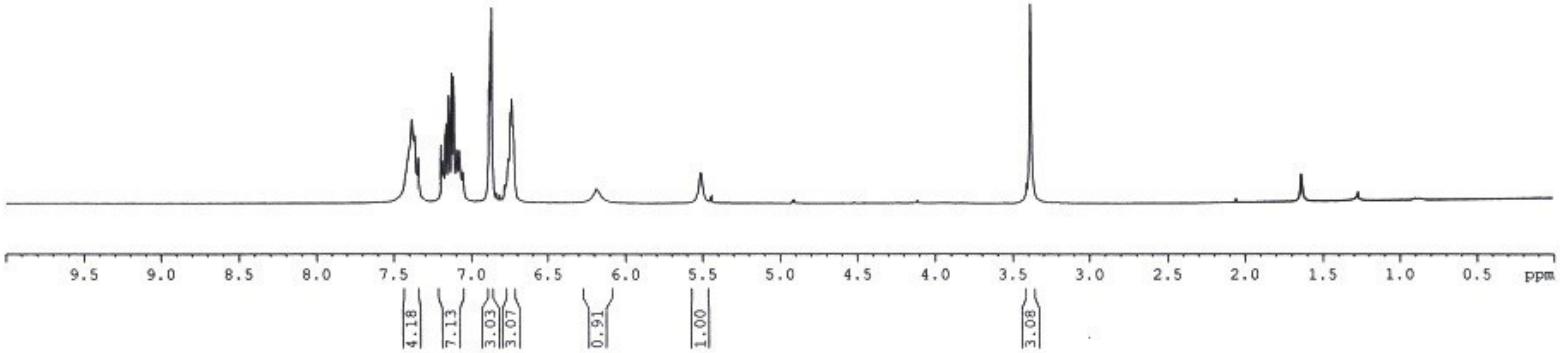
======== CHANNEL f1 ========
SFO1 100.6278588 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W

======== CHANNEL f2 ========
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W

F2 - Processing parameters
SI 16384
SF 100.6177901 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1H of VBSS-139-36





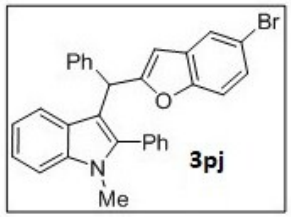
13C of VBss-139-36

158.21
155.40
138.29
134.53
133.67
131.28
131.14
130.79
130.45
128.83
128.74
128.71
128.61
128.41
128.01
127.94
127.75
125.69
122.11
119.88
114.17
110.95
109.61
106.34

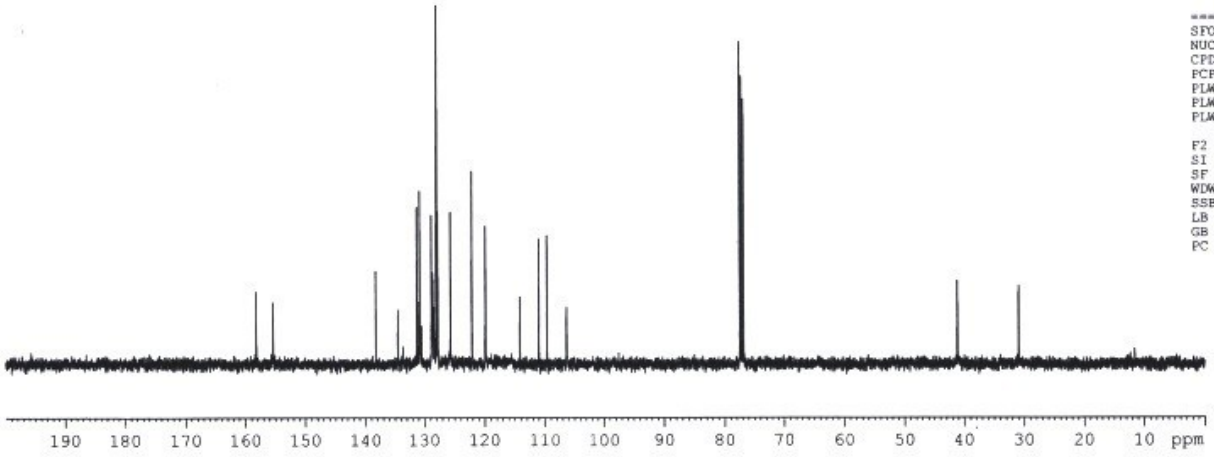
77.47
77.16
76.84

41.18

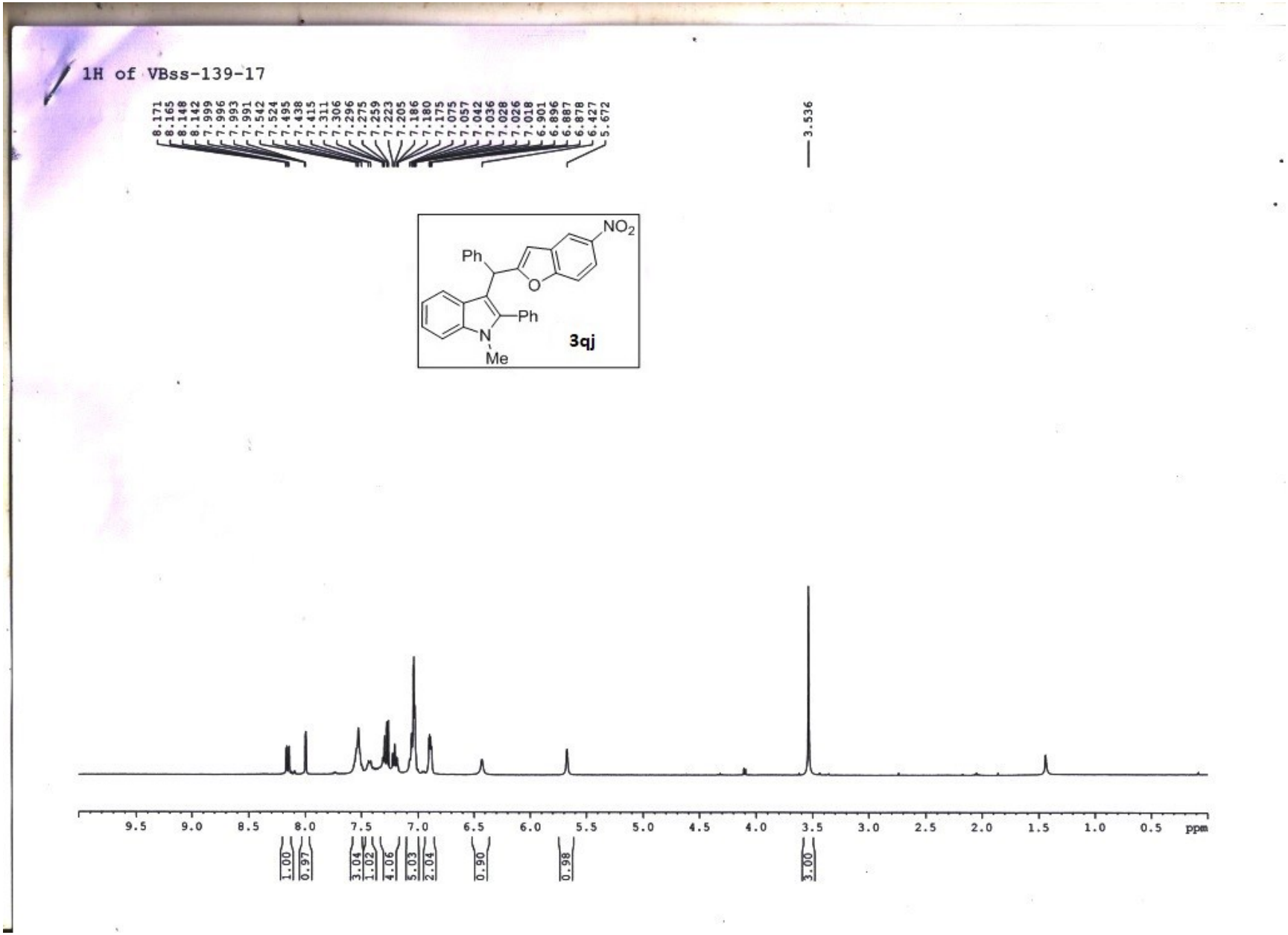
30.93



3pj




```
Current Data Parameters
NAME      Dr. A HAJRA 2018-2nd
EXPNO                  358
PROCNO                   1

F2 - Acquisition Parameters
Date_           20180424
Time              18.32
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD               32768
SOLVENT          CDCl3
NS                  44
DS                   2
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG                77.59
DW               20.800 usec
DE                6.50 usec
TE              299.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6278588 MHz
NUC1               13C
P1                8.90 usec
PLW1         54.00000000 W

======== CHANNEL f2 ========
SFO2        400.1516006 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         12.00000000 W
PLW12         0.32231000 W
PLW13         0.16212000 W

F2 - Processing parameters
SI                16384
SF          100.6177937 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```


1H of VBss-139-17
8.171
8.165
8.148
8.142
7.999
7.996
7.993
7.991
7.542
7.524
7.495
7.438
7.415
7.311
7.306
7.296
7.275
7.259
7.223
7.205
7.186
7.180
7.175
7.075
7.057
7.042
7.036
7.028
7.026
7.018
6.901
6.896
6.887
6.878
6.427
5.672
3.536
NO2
Ph
O
Ph
N
Me
3qj
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.00
0.97
3.04
1.02
4.06
5.03
2.04
0.90
0.98
3.00

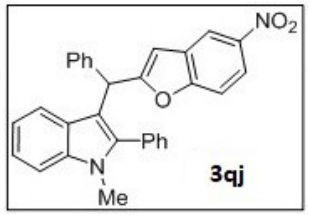
13C of VBSS-139-17

161.14
157.95
143.31
138.61
137.45
133.85
133.04
130.97
130.79
129.08
128.80
128.17
128.10
126.29
125.83
122.31
121.16
120.08
118.61
110.34
109.82
109.41
108.25

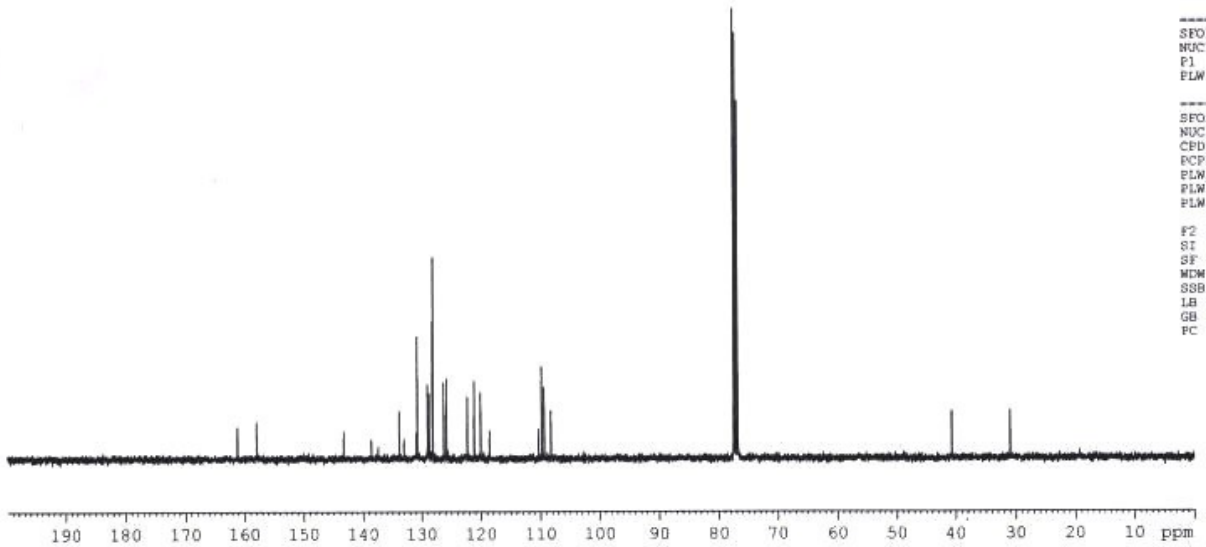
77.47
77.15
76.84

40.70

31.00

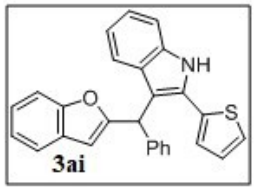



```
Current Data Parameters
NAME      Dr. A HAJRA 2018-2nd
EXPNO              320
PROCNO               1

F2 - Acquisition Parameters
Date_          20180420
Time               20.00
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  420
DS                    2
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG                93.46
DW               20.800 usec
DE                6.50 usec
TE               300.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6278588 MHz
NUC1               13C
P1                8.90 usec
PLW1         54.00000000 W

======== CHANNEL f2 ========
SFO2         400.1516006 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         12.00000000 W
PLW12         0.32231000 W
PLW13         0.16212000 W

F2 - Processing parameters
SI                16384
SF           100.6177844 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

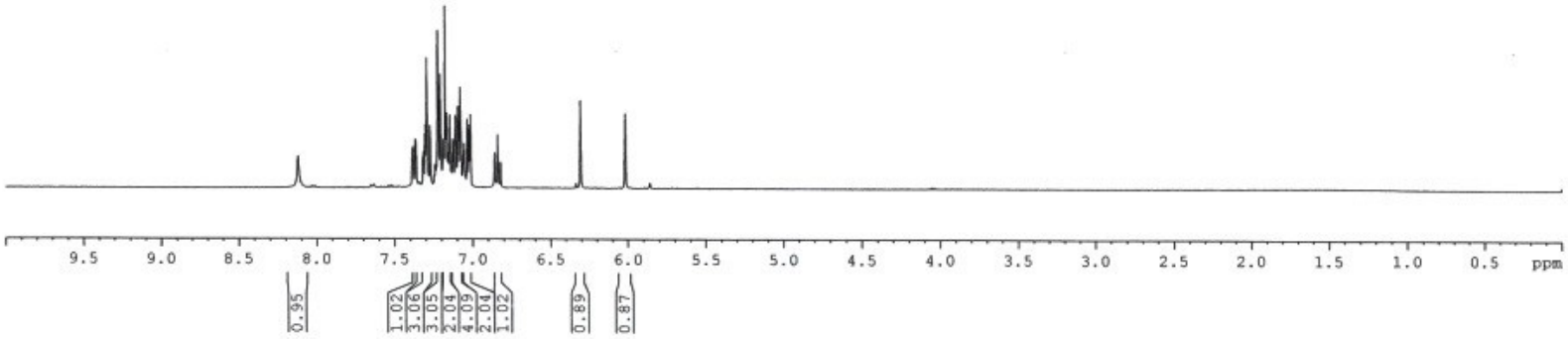


1H of vbss-139-rev-2

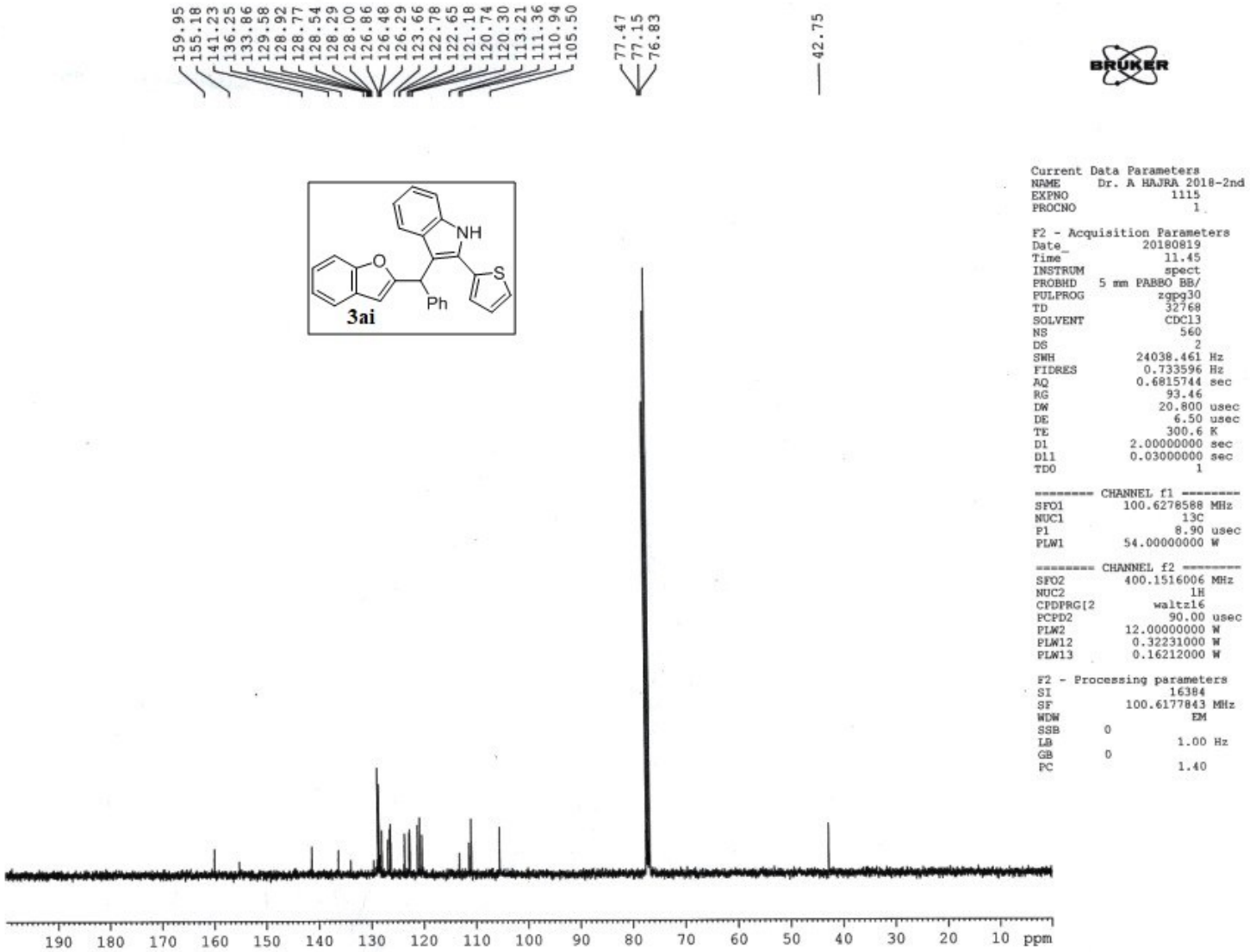
8.121
7.388
7.386
7.370
7.366
7.318
7.308
7.305
7.295
7.293
7.275
7.224
7.208
7.189
7.178
7.168
7.148
7.129
7.124
7.113
7.111
7.109
7.105
7.095
7.091
7.088
7.082
7.079
7.058
7.056
7.035
7.026
7.022
7.013
6.861
6.841
6.839
6.823
6.821
6.307
6.018



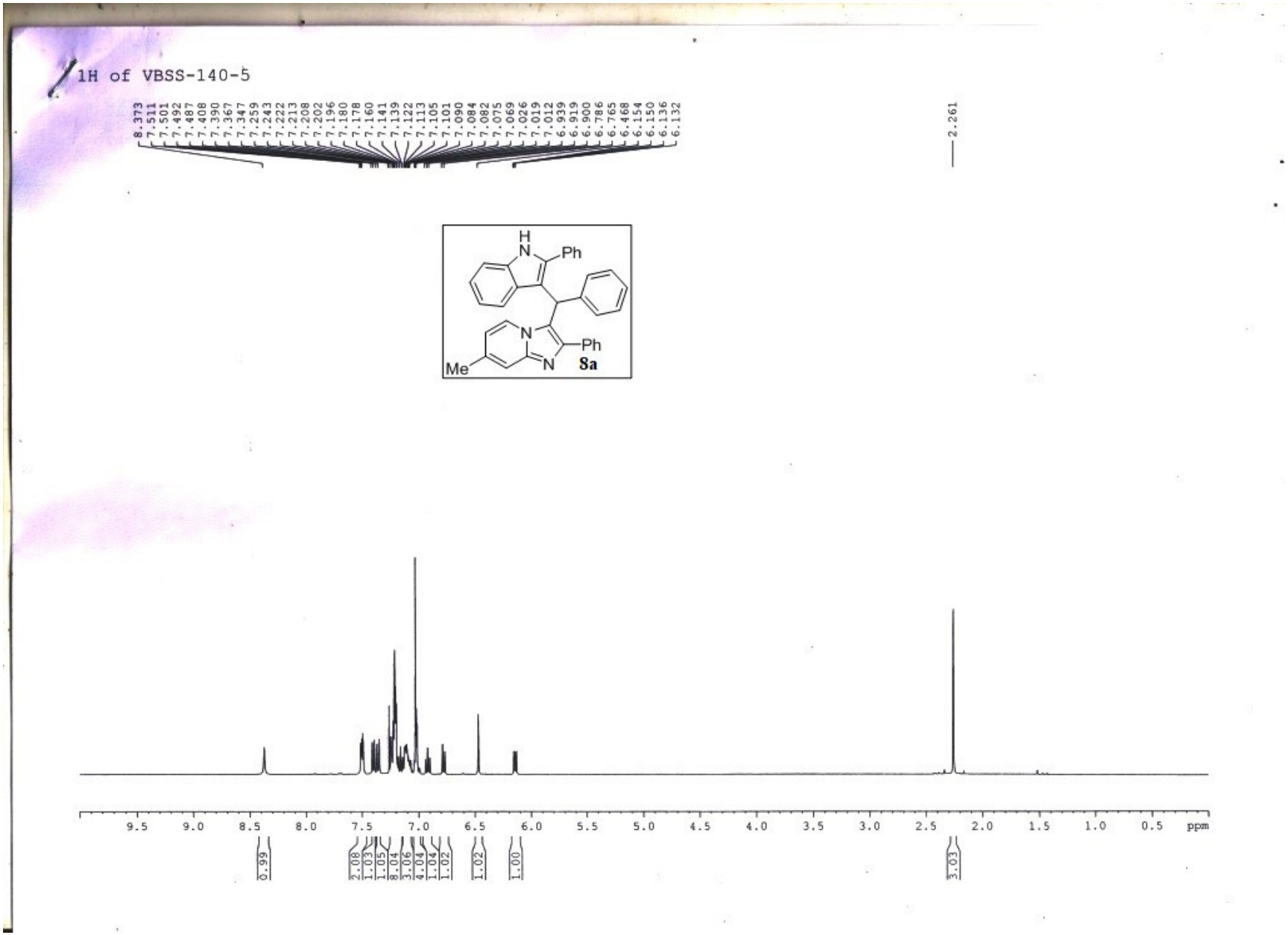
3ai



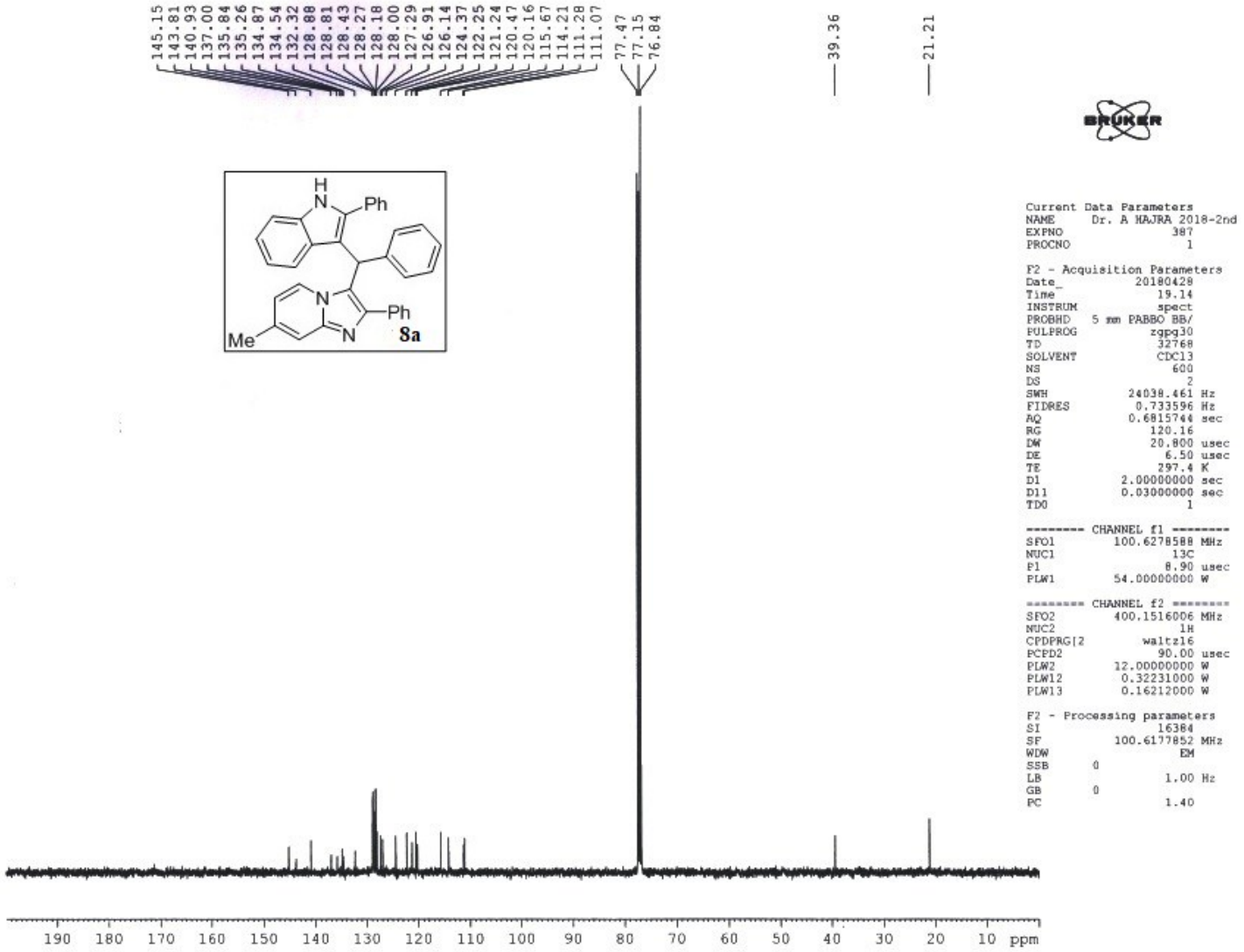
13C of vbSS-139-re



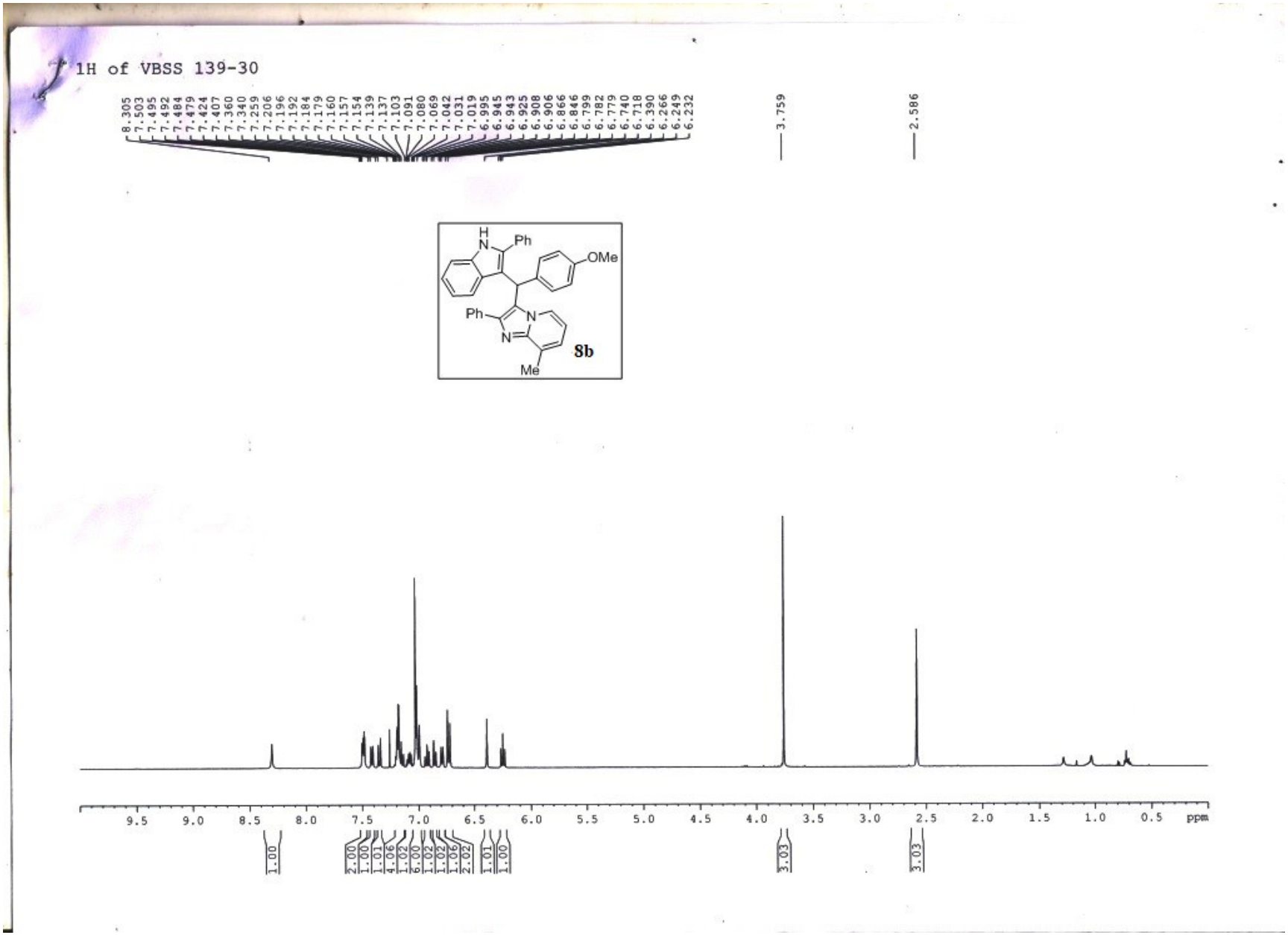

```
Current Data Parameters
NAME      Dr. A HAJRA 2018-2nd
EXPNO              1115
PROCNO                1

F2 - Acquisition Parameters
Date_          20180819
Time              11.45
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               32768
SOLVENT          CDCl3
NS                 560
DS                   2
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                93.46
DW               20.800 usec
DE                6.50 usec
TE               300.6 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6278588 MHz
NUC1               13C
P1                8.90 usec
PLW1       54.00000000 W

======== CHANNEL f2 ========
SFO2        400.1516006 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2       12.00000000 W
PLW12       0.32231000 W
PLW13       0.16212000 W

F2 - Processing parameters
SI                16384
SF          100.6177843 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```


1H of VBSS-140-5
8.373
7.511
7.501
7.492
7.487
7.408
7.390
7.367
7.347
7.259
7.243
7.222
7.213
7.208
7.202
7.196
7.180
7.178
7.160
7.141
7.139
7.122
7.113
7.105
7.101
7.090
7.084
7.082
7.075
7.069
7.026
7.019
7.012
6.939
6.919
6.900
6.786
6.765
6.468
6.154
6.150
6.136
6.132
2.261
H
N
Ph
N
Ph
Me
N
8a
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.99
2.08
1.03
1.05
8.04
3.06
4.04
1.04
1.02
1.02
1.00
3.03

13C of vbSS-140-5

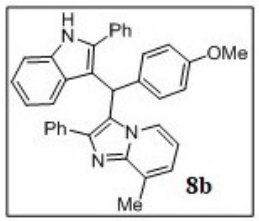



```
Current Data Parameters
NAME      Dr. A HAJRA 2018-2nd
EXPNO                  387
PROCNO                   1

F2 - Acquisition Parameters
Date_              20180428
Time                 19.14
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                     600
DS                       2
SWH              24038.461 Hz
FIDRES           0.733596 Hz
AQ               0.6815744 sec
RG                   120.16
DW                   20.800 usec
DE                    6.50 usec
TE                   297.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          100.6278588 MHz
NUC1                   13C
P1                    8.90 usec
PLW1         54.00000000 W

======== CHANNEL f2 ========
SFO2          400.1516006 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2                90.00 usec
PLW2         12.00000000 W
PLW12         0.32231000 W
PLW13         0.16212000 W

F2 - Processing parameters
SI                   16384
SF            100.6177852 MHz
WDW                    EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

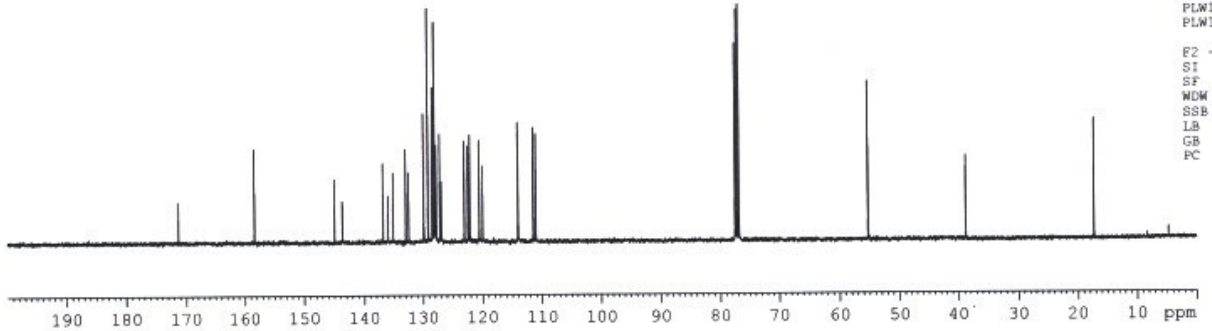

1H of VBSS 139-30
8.305
7.503
7.495
7.492
7.484
7.479
7.424
7.407
7.360
7.340
7.259
7.206
7.196
7.192
7.184
7.179
7.160
7.157
7.154
7.139
7.137
7.103
7.091
7.080
7.069
7.042
7.031
7.019
6.995
6.945
6.943
6.925
6.908
6.906
6.866
6.846
6.799
6.782
6.779
6.740
6.718
6.390
6.266
6.249
6.232
3.759
2.586
H
N
Ph
OMe
Ph
N
N
Me
8b
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.00
2.00
1.00
1.01
4.06
1.02
6.00
1.02
1.02
1.06
2.02
1.01
1.00
3.03
3.03

13C of VBSSS 139-3

171.27
158.37
144.95
143.63
136.80
135.96
135.09
132.94
132.43
129.87
129.14
128.46
128.38
128.05
128.01
127.75
127.13
126.90
123.03
122.44
122.38
122.07
120.53
119.95
114.05
111.48
111.05
77.48
77.16
76.84
55.26
38.76
17.29

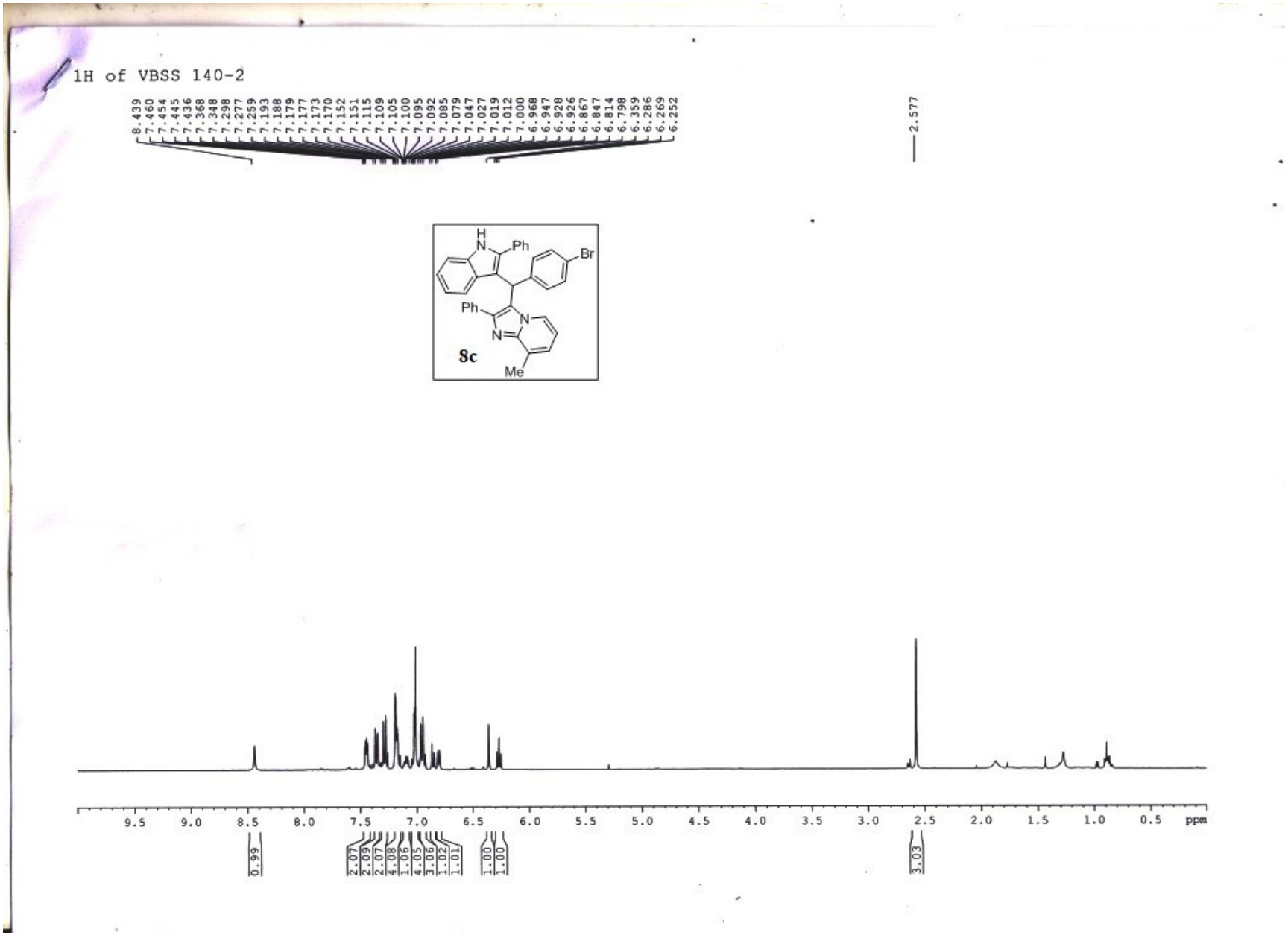


8b

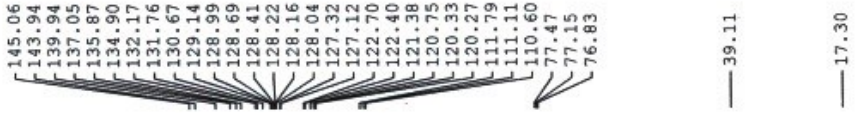


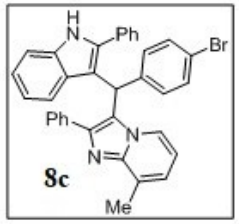
BRUKER

```
Current Data Parameters
NAME      Dr.A.HAJRA 2017
EXPNO              925
PROCNO               1

F2 - Acquisition Parameters
Date_         20170601
Time             12.25
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG        zgpg30
TD              32768
SOLVENT         CDCl3
NS                512
DS                  2
SWH         24038.461 Hz
FIDRES       0.733596 Hz
AQ           0.6815744 sec
RG               67.81
DW              20.800 usec
DE               6.50 usec
TE              298.9 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                 1

======== CHANNEL f1 ========
SFO1       100.6278588 MHz
NUC1              13C
P1               8.90 usec
PLW1      54.00000000 W

======== CHANNEL f2 ========
SFO2       400.1516006 MHz
NUC2              1H
CPDPRG[2       waltz16
PCPD2           90.00 usec
PLW2      12.00000000 W
PLW12      0.32231000 W
PLW13      0.16212000 W

F2 - Processing parameters
SI               16384
SF         100.6177880 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

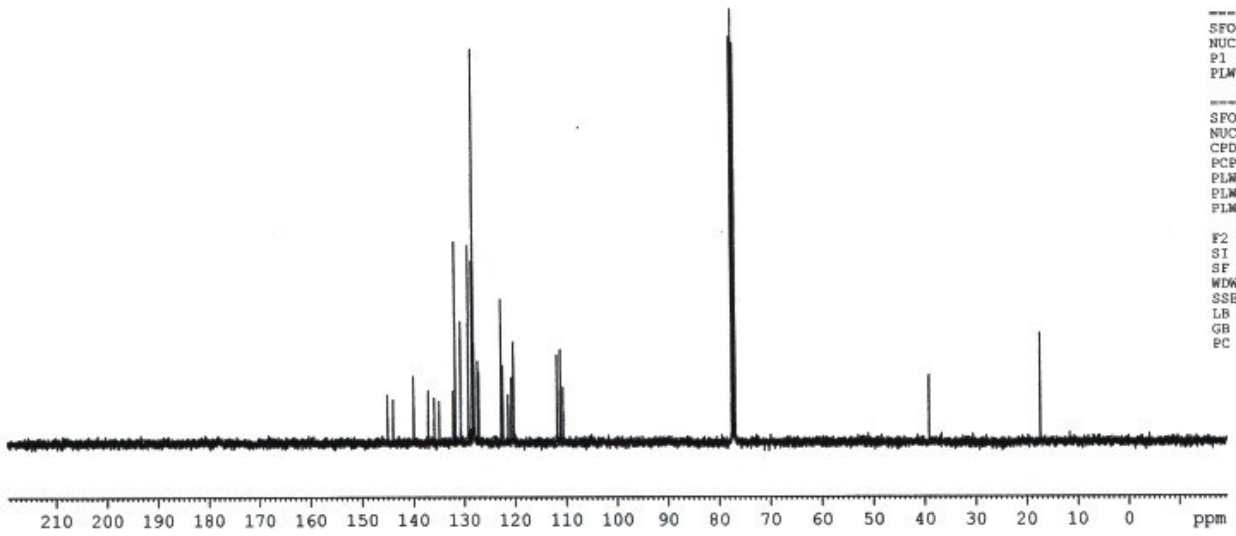

1H of VBSS 140-2
8.439
7.460
7.454
7.445
7.436
7.368
7.348
7.298
7.277
7.259
7.193
7.188
7.179
7.177
7.173
7.170
7.152
7.151
7.115
7.109
7.105
7.100
7.095
7.092
7.085
7.079
7.047
7.027
7.019
7.012
7.000
6.968
6.947
6.928
6.926
6.867
6.847
6.814
6.798
6.359
6.286
6.269
6.252
2.577
Ph
Br
Ph
N
N
8c
Me
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.99
2.07
2.09
2.07
4.08
1.06
4.05
3.06
1.02
1.01
1.00
1.00
3.03

13C of VBSS 140-2



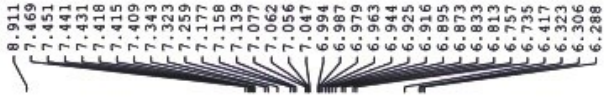


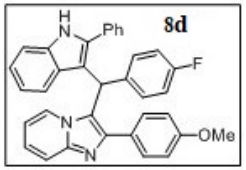
8c

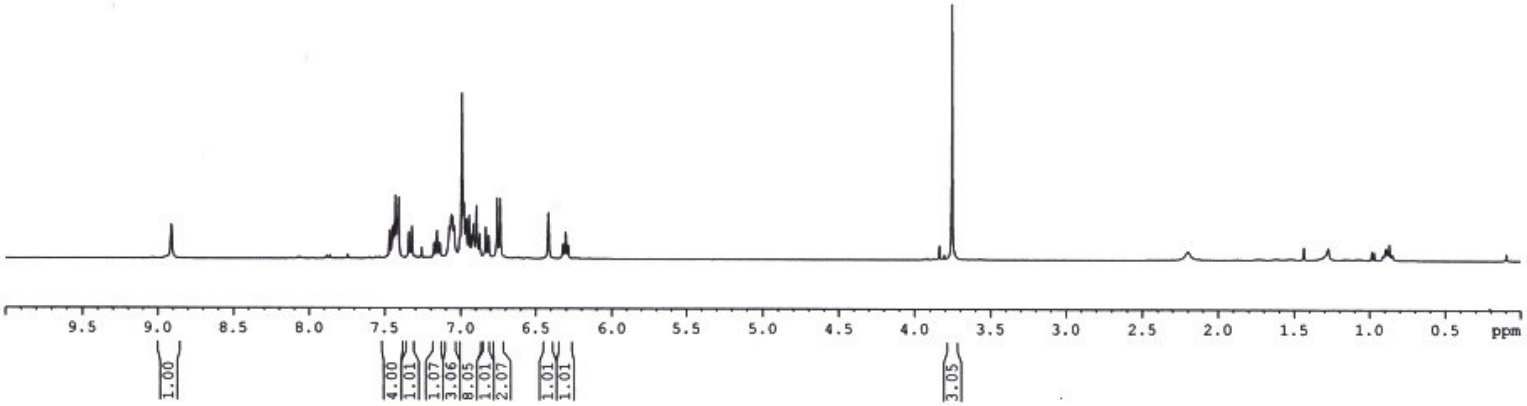



```
Current Data Parameters
NAME      Dr.A.HAJRA 2018
EXPNO                318
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180704
Time              21.24
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  256
DS                    2
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG                57.60
DW                20.800 usec
DE                 6.50 usec
TE                298.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6278588 MHz
NUC1               13C
P1                8.90 usec
PLW1       54.00000000 W

======== CHANNEL f2 ========
SFO2        400.1516006 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2       12.00000000 W
PLW12       0.32231000 W
PLW13       0.16212000 W

F2 - Processing parameters
SI                16384
SF          100.6177858 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

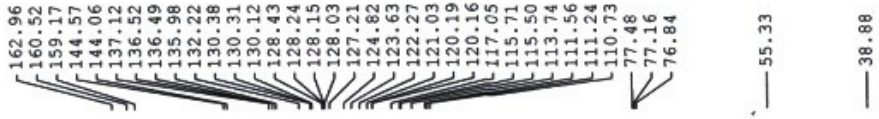
1H of of VBSS-140-6

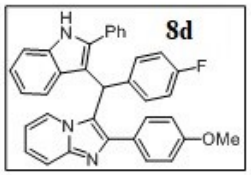




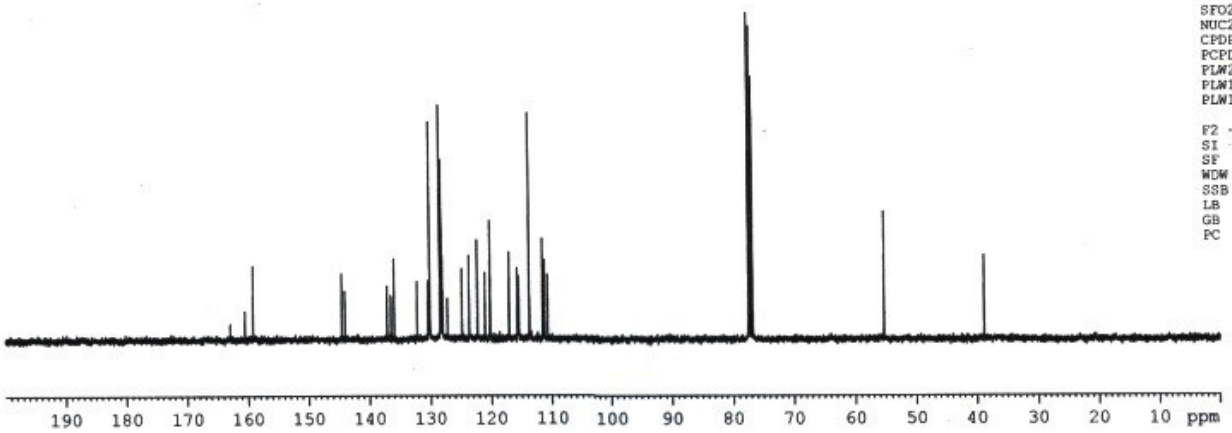


13C of VBSS-140-6

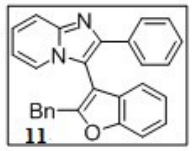




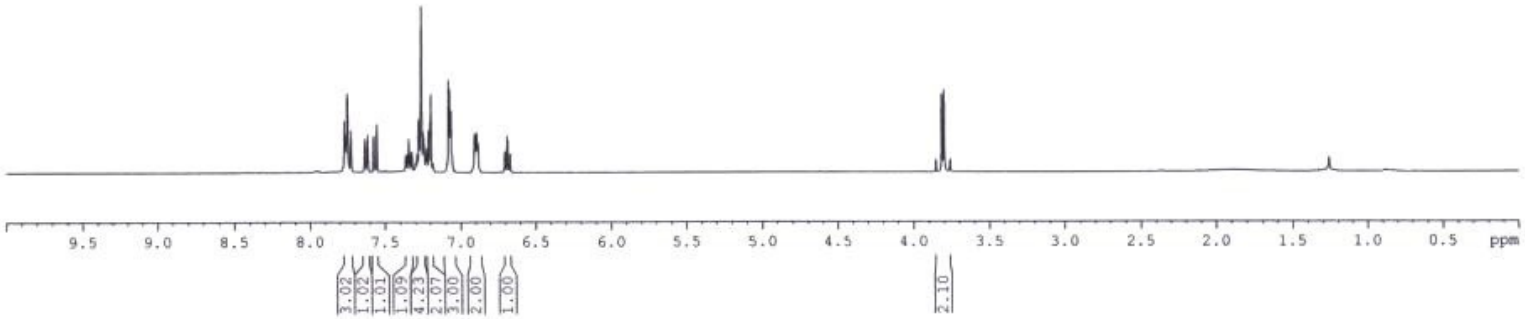

```
Current Data Parameters
NAME      Dr.A.HAJRA 2018
EXPNO              320
PROCNO               1

F2 - Acquisition Parameters
Date_          20180705
Time             08.07
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG        zgpg30
TD               32768
SOLVENT          CDCl3
NS                 320
DS                   2
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                87.23
DW               20.800 usec
DE                6.50 usec
TE               299.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1       100.6278588 MHz
NUC1              13C
P1                8.90 usec
PLW1      54.00000000 W

======== CHANNEL f2 ========
SFO2       400.1516006 MHz
NUC2              1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2      12.00000000 W
PLW12      0.32231000 W
PLW13      0.16212000 W

F2 - Processing parameters
SI                16384
SF         100.6177882 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```



1H of vbSS-139-10

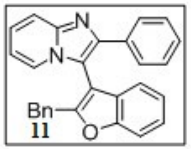


11



13C of VBSS-139-10

157.34
155.08
145.89
144.62
136.22
134.13
128.76
128.66
128.48
128.23
127.90
127.64
126.72
125.14
124.72
124.21
123.51
120.02
117.72
112.43
111.82
111.26
105.88
77.47
77.15
76.83
33.73




```
Current Data Parameters
NAME      Dr. A HAJRA 2018-2nd
EXPNO                  651
PROCNO                   1

F2 - Acquisition Parameters
Date_              20180521
Time                 10.50
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG              zgpg30
TD                    32768
SOLVENT               CDCl3
NS                      456
DS                        2
SWH                24038.461 Hz
FIDRES              0.733596 Hz
AQ                  0.6815744 sec
RG                     148.91
DW                     20.800 usec
DE                      6.50 usec
TE                     300.5 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1             100.6278588 MHz
NUC1                     13C
P1                      8.90 usec
PLW1             54.00000000 W

======== CHANNEL f2 ========
SFO2             400.1516006 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                  90.00 usec
PLW2             12.00000000 W
PLW12             0.32231000 W
PLW13             0.16212000 W

F2 - Processing parameters
SI                       16384
SF               100.6177843 MHz
WDW                         EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```