Electronic Supplementary Material (ESI) for Chemical Communications.

Ring-expanded *N*-Heterocyclic Carbenes as Ligands in Iron-Catalysed Cross-Coupling Reactions of Arylmagnesium Reagents and Aryl Chlorides

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Experimental Section

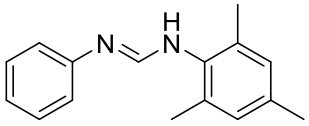
General Considerations. Unless otherwise noted, all operations were performed without taking precautions to exclude air and moisture, and all solvents and chemicals were used as received. All iron-catalyzed reactions were carried out under an argon atmosphere with dry solvents under anhydrous conditions, unless otherwise noted. THF was dried over alumina under N_2 using a Grubbs-type solvent purification system. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra were recorded at 298 K on a Bruker ACF 300, DRX-400 and AMX 500 spectrometer, and the chemical shifts (δ) were internally referenced to the residual solvent signals relative to tetramethylsilane. ESI mass spectra were measured using a Finnigan MAT LCQ spectrometer. Elemental analyses were performed on an ElementarVario Micro Cube elemental analyzer at the Department of Chemistry, National University of Singapore.

X-ray Diffraction Studies.

All single crystals were grown by slow evaporation of a saturated solution in dichloromethane and diethyl ether. CCDC 1584466−1584468 contain the supplementary crystallographic data for this paper. X-ray data were collected with a Bruker AXS SMART APEX diffractometer, using Mo- or Cu-K_α radiation with the SMART suite of Programs.[1] Data were processed and corrected for Lorentz and polarization effects with SAINT,[2] and for absorption effect with SADABS.[3] Structural solution and refinement were carried out with the SHELXTL suite of programs.[4] The structure was solved by direct methods to locate the heavy atoms, followed by difference maps for the light, non-hydrogen atoms. All non-hydrogen atoms were generally given anisotropic displacement parameters in the final

model. All H-atoms were put at calculated positions. A summary of the most important crystallographic data is given in Table S1.

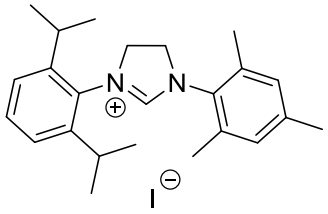
The formamidines were synthesized following literature.[5]



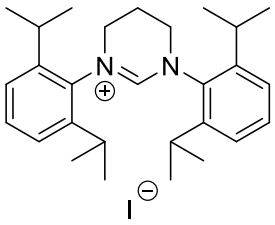
***N*-phenyl-*N'*-(2,4,6-trimethylphenyl)formamidine.** Acetic acid (43 μL, 0.05 mmol) was added to a round bottom flask charged with the aniline (15 mmol, 1.40 g) and triethyl orthoformate (3.75 mL, 22.5 mmol). The flask was fitted with a distillation head and was heated with stirring to 140 °C until ethanol (3.5 ml, 60 mmol) was collected by distillation. The resulting solution was cooled down to room temperature and subjected to vacuum distillation. The ethyl N-phenylformimidate (1.17g, 7.81 mmol) was collected after the excess triethyl orthoformate and acetic acid was distilled out. Mesidine (1.10 g, 7.81 mmol) was then added to the reaction mixture and heated at 160 °C for 1 h and 170 °C 1h. Upon cooling to room temperature, the solution solidified. The mixture was triturated with cold hexanes and the product collected as a white solid. Yield: 1.72 g, 4.94 mmol, 33% (based on aniline). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.85 (br-s, 1 H, NCHNH), 7.28 (t, ^{3}J(H,H) = 8 Hz, 2 H, Ar–H), 7.05 (t, ^{3}J(H,H) = 8 Hz, 1 H, Ar–H), 6.98 (br-s, 2 H, Ar–H), 6.91 (s, 2 H, Ar–H), 5.30 (br-s, 1 H, NH), 2.29 (s, 3 H, CH_3), 2.22 (s, 6 H, CH_3). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 151.8 (br, CH), 143.7, 143.3, 133.9, 131.5, 130.0, 129.5, 123.1, 117.7 (Ar–C), 21.4 (CH_3), 19.1 (CH_3). Anal. Calcd. for $C_{16}H_{18}N_2$: C, 80.63; H, 7.61; N, 11.75. Found: C, 80.19; H, 7.49; N, 11.93. MS (ESI): *m/z* 239 $[M + H]^+$.

General Procedure for the synthesis of the azolium bromide/iodide salts:[6] A mixture of

formamidine (5.00 mmol), K_2CO_3 (2.50 mmol), and 1.1 molar equiv. of the dibromoalkane in 30 mL of CH_3CN was heated under reflux and monitored by TLC. NaI (10.00 mmol) was added to reactions with low conversion and for the five membered ring salt, excess amount of dibromoethane (10 equiv.) was added to obtain better yield for the SIPrMes·HI. The solvent was removed by vacuum and CH_2Cl_2 (50 mL) was added. The resulting suspension was filtered through Celite and solvent was removed. Ethyl acetate (5 mL) was added to dissolve the residue, which upon stirring affords a suspension. The precipitate product was collected by filtration as white to yellowish solid. The tetrafluoroborate salts were synthesized by reacting the halide salts with 10 euqiv. $NaBF_4$ in water.

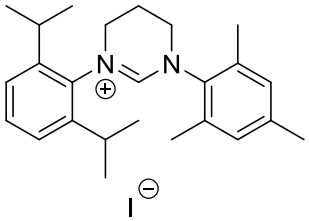


SIPrMes·HI. Yield: 13%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.14 (s, 1 H, NCHN), 7.50 (t, ^3J(H,H) = 8 Hz, 1 H, Ar–H), 7.30 (d, ^3J(H,H) = 8 Hz, 2 H, Ar–H), 7.03 (s, 2 H, Ar–H), 4.64 (br-s, 4 H, NCH_2), 3.01 (m, ^3J(H,H) = 7 Hz, 2 H, C*H*$(CH_3)_2$), 2.41 (s, 6 H, CH_3), 2.33 (s, 3 H, CH_3), 1.41 (d, ^3J(H,H) = 7 Hz, 6 H, CH(C*H*$_3)_2$), 1.29 (d, ^3J(H,H) = 7 Hz, 6 H, CH(C*H*$_3)_2$). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ 159.2 (NCHN), 146.9, 142.0, 135.5, 132.5, 131.1, 130.2, 129.7, 125.9 (Ar–C), 55.3, 53.2 (NCH_2), 29.9 (*C*H$(CH_3)_2$), 26.0, 24.6 (CH(*C*H$_3)_2$), 21.9 (CH_3), 18.8 (CH_3). No satisfactory elemental analysis result was obtained from multiple trials. MS (ESI): *m/z* 349 $[M - I]^+$.

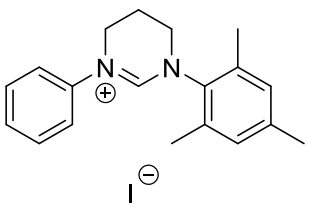


6Pr·HI. Yield: 65%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.57 (s, 1 H, NCHN), 7.44 (t, ^3J(H,H) = 8 Hz, 2 H, Ar–H), 7.26 (d, ^3J(H,H) = 8 Hz,

4 H, Ar–H), 4.20 (t, ^{3}J(H,H) = 4 Hz, 4 H, NCH_2), 3.02 (m, ^{3}J(H,H) = 7 Hz, 4 H, C*H*$(CH_3)_2$), 2.75 (br-s, 2 H, CH_2), 1.38 (d, ^{3}J(H,H) = 7 Hz, 12 H, CH(C*H*$_3)_2$), 1.24 (d, ^{3}J(H,H) = 7 Hz, 12 H, CH(C*H*$_3)_2$). $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$): δ 153.5 (NCHN), 146.1, 136.1, 131.8, 125.7 (Ar–C), 49.2 (NCH_2), 29.3 (*C*H$(CH_3)_2$), 25.4, 25.2 (CH(*C*$H_3)_2$), 19.8 (CH_2). Anal. Calcd. for $C_{28}H_{41}IN_2$: C, 63.15; H, 7.76; N, 5.26. Found: C, 63.14; H, 8.16; N, 5.69. MS (ESI): *m/z* 405 $[M - I]^+$.

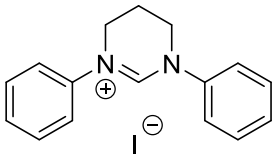


6PrMes·HI. Yield: 75%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.59 (s, 1 H, NCHN), 7.46 (t, ^{3}J(H,H) = 8 Hz, 1 H, Ar–H), 7.29 (d, ^{3}J(H,H) = 8 Hz, 2 H, Ar–H), 6.98 (s, 2 H, Ar–H), 4.24 (t, ^{3}J(H,H) = 5 Hz, 2 H, NCH_2), 4.18 (t, ^{3}J(H,H) = 5 Hz, 2 H, NCH_2), 3.03 (m, ^{3}J(H,H) = 7 Hz, 2 H, C*H*$(CH_3)_2$), 2.70 (m, 2 H, CH_2), 2.36 (s, 6 H, CH_3), 2.80 (s, 3 H, CH_3), 1.38 (d, ^{3}J(H,H) = 7 Hz, 6 H, CH(C*H*$_3)_2$), 1.23 (d, ^{3}J(H,H) = 7 Hz, 6 H, CH(C*H*$_3)_2$). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$): δ 153.9 (NCHN), 146.2, 141.3, 136.8, 136.3, 134.9, 131.9, 130.8, 125.7 (Ar–C), 49.1, 47.6 (NCH_2), 29.4 (*C*H$(CH_3)_2$), 25.5, 24.8 (CH(*C*$H_3)_2$), 21.6 (CH_3), 20.2 (CH_2), 18.5 (CH_3). Anal. Calcd. for $C_{25}H_{35}IN_2$: C, 61.22; H, 7.19; N, 5.71. Found: C, 61.61; H, 7.06; N, 5.89. MS (ESI): *m/z* 363 $[M - I]^+$.

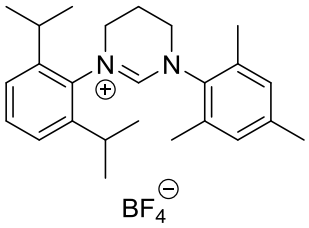


6MesPh·HI. Yield: 80%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93 (s, 1 H, NCHN), 7.56 (d, ^{3}J(H,H) = 8 Hz, 2 H, Ar–H), 7.47 (t, ^{3}J(H,H) = 8 Hz, 2 H, Ar–H), 7.39 (t, ^{3}J(H,H) = 8 Hz, 1 H, Ar–H), 6.96 (s, 2 H, Ar–H), 4.48 (t, ^{3}J(H,H) = 6 Hz, 2 H, NCH_2), 4.02 (t, ^{3}J(H,H) = 6 Hz, 2 H, NCH_2), 2.61 (m,

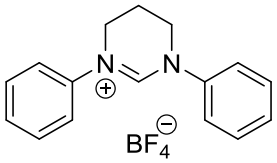
^{3}J(H,H) = 6 Hz, 2 H, CH_2), 2.38 (s, 6 H, CH_3), 2.28 (s, 3 H, CH_3). $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$): δ 153.0 (NCHN), 141.7, 141.2, 137.2, 135.2, 131.0, 130.9, 130.1, 124.0 (Ar–C), 48.1, 47.5 (NCH_2), 21.6 (CH_3), 20.3 (CH_2), 19.2 (CH_3). Anal. Calcd. for $C_{19}H_{23}IN_2$: C, 56.17; H, 6.71; N, 6.89. Found: C, 56.30; H, 5.42; N, 7.08. MS (ESI): *m/z* 279 $[M - I]^+$.



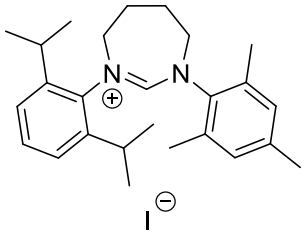
6Ph·HI. Yield: 51%. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.06 (s, 1 H, NCHN), 7.46 (t, ^{3}J(H,H) = 8 Hz, 1 H, Ar–H), 7.65 (d, ^{3}J(H,H) = 8 Hz, 4 H, Ar–H), 7.42–7.35 (m, 6 H, Ar–H), 4.21 (t, ^{3}J(H,H) = 6 Hz, 4 H, NCH_2), 2.60 (m, ^{3}J(H,H) = 6 Hz, 2 H, CH_2). $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$): δ 152.2 (NCHN), 142.0, 130.7, 129.8, 124.3 (Ar–C), 47.8 (NCH_2), 20.0 (CH_2). Anal. Calcd. for $C_{16}H_{17}IN_2$: C, 52.76; H, 4.70; N, 7.69. Found: C, 52.86; H,4.50; N, 7.56. MS (ESI): *m/z* 237 $[M - I]^+$.



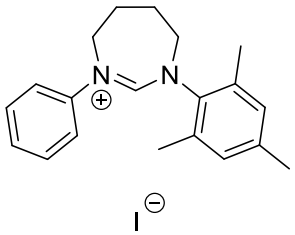
6PrMes·HBF$_4$. Yield: 68%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53 (s, 1 H, NCHN), 7.46 (t, ^{3}J(H,H) = 8 Hz, 1 H, Ar–H), 7.28 (d, ^{3}J(H,H) = 8 Hz, 2 H, Ar–H), 6.98 (s, 2 H, Ar–H), 4.00–3.96 (m, 4 H, NCH_2), 3.00 (m, ^{3}J(H,H) = 7 Hz, 2 H, C*H*$(CH_3)_2$), 2.64 (m, ^{3}J(H,H) = 6 Hz, 2 H, CH_2), 2.33 (s, 6 H, CH_3), 2.30 (s, 3 H, CH_3), 1.38 (d, ^{3}J(H,H) = 7 Hz, 6 H, CH(C*H*$_3)_2$), 1.23 (d, ^{3}J(H,H) = 7 Hz, 6 H, CH(C*H*$_3)_2$). $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$): δ 154.3 (NCHN), 146.3, 141.4, 137.0, 136.5, 135.1, 131.9, 130.8, 125.8 (Ar–C), 49.0, 47.1 (NCH_2), 29.4 (*C*H$(CH_3)_2$), 25.5, 24.6 (CH(*C*H$_3)_2$), 21.6 (CH_3), 19.9 (CH_2), 17.8 (CH_3). Anal. Calcd. for $C_{25}H_{35}BF_4N_2$: C, 66.67; H, 7.83; N, 6.22. Found: C, 66.57; H, 7.85; N, 6.17. MS (ESI): *m/z* 363 $[M - BF_4]^+$.



6Ph·HBF$_4$. Yield: 79%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.95 (s, 1 H, NCHN), 7.49–7.37 (m, 10 H, Ar–H), 4.02 (t, ^3J(H,H) = 6 Hz, 4 H, NCH_2), 2.48 (m, ^3J(H,H) = 6 Hz, 2 H, CH_2). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$): δ 152.2 (NCHN), 142.3, 130.9, 129.9, 124.1 (Ar–C), 47.3 (NCH_2), 20.0 (CH_2). Anal. Calcd. for $C_{16}H_{17}BF_4N_2$: C, 59.29; H, 5.29; N, 8.64. Found: C, 59.42; H, 5.14; N, 8.57. MS (ESI): *m/z* 237 $[M - BF_4]^+$.

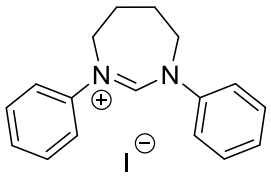


7PrMes·HI. Yield: 93%. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.41 (t, ^3J(H,H) = 8 Hz, 1 H, Ar–H), 7.26–7.24 (m, 3 H, NCHN and Ar–H), 6.95 (s, 2 H, Ar–H), 4.58–4.51 (m, 4 H, NCH_2), 3.18 (m, ^3J(H,H) = 7 Hz, 2 H, C*H*$(CH_3)_2$), 2.61 (br-s, 4 H, CH_2), 2.41 (s, 6 H, CH_3), 2.27 (s, 3 H, CH_3), 1.39 (d, ^3J(H,H) = 7 Hz, 6 H, CH(C*H*$_3)_2$), 1.23 (d, ^3J(H,H) = 7 Hz, 6 H, CH(C*H*$_3)_2$). $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$): δ 156.2 (NCHN), 145.5, 141.1, 140.0, 139.5, 134.3, 131.7, 131.0, 126.0 (Ar–C), 57.2, 55.9 (NCH_2), 29.5 (*C*H$(CH_3)_2$), 26.3, 25.6, 25.5, 24.9 (CH(*C*$H_3)_2$ and CH_2), 21.6 (CH_3), 18.8 (CH_3). Anal. Calcd. for $C_{26}H_{37}IN_2$: C, 61.90; H, 7.39; N, 5.55. Found: C, 61.78; H, 7.13; N, 5.69. MS (ESI): *m/z* 377 $[M - I]^+$.

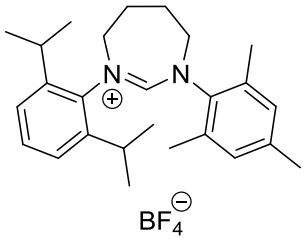


7MesPh·HI. Yield: 95%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.57 (d, ^3J(H,H) = 7 Hz, 2 H, Ar–H), 7.48 (s, 1 H, NCHN), 7.47–7.39 (m, 3 H, Ar–H), 6.93 (s, 2 H, Ar–H), 4.77 (t, ^3J(H,H) = 5 Hz, 2 H, NCH_2), 4.44 (t, ^3J(H,H) = 5 Hz, 2 H, NCH_2), 2.47–2.44 (m, 10 H, CH_2 and CH_3), 2.25 (s, 3 H, CH_3).

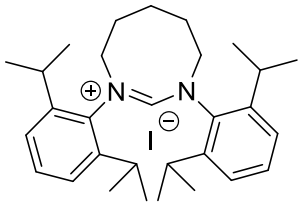
$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$): δ 157.7 (NCHN), 143.9, 140.8, 140.2, 134.5, 131.0, 130.9, 130.3, 125.4 (Ar–C), 56.5, 55.6 (NCH_2), 26.0, 25.9 (CH_2), 21.5 (CH_3), 19.5 (CH_3). Anal. Calcd. for $C_{20}H_{25}IN_2$: C, 57.15; H, 6.00; N, 6.66. Found: C, 57.25; H, 5.72; N, 7.04. MS (ESI): *m/z* 293 $[M - I]^+$.



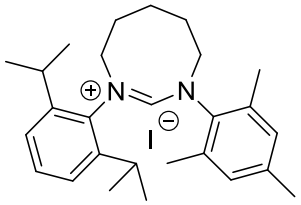
7Ph·HI. Yield: 66%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.73–7.72 (m, 5 H, NCHN and Ar–H), 7.42–7.38 (m, 6 H, Ar–H), 4.58 (br-s, 4 H, NCH_2), 2.44 (br-s, 4 H, CH_2). $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$): δ 157.2 (NCHN), 144.5, 130.8, 130.1, 125.6 (Ar–C), 56.4 (NCH_2), 25.8 (CH_2). Anal. Calcd. for $C_{17}H_{19}IN_2$: C, 53.98; H, 5.06; N, 7.41. Found: C, 53.94; H, 5.19; N, 7.38. MS (ESI): *m/z* 251 $[M - I]^+$.



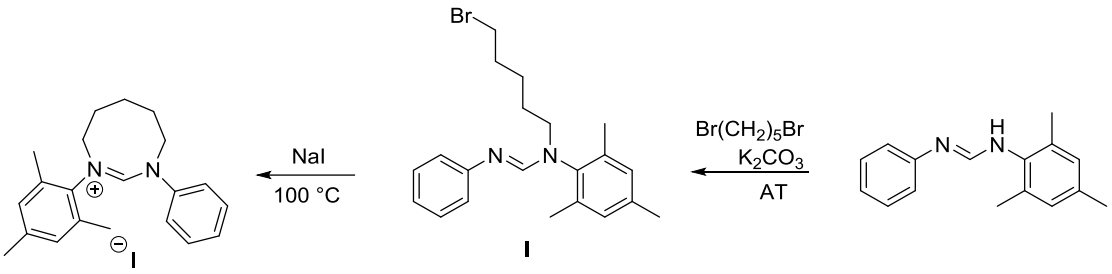
7PrMes·HBF$_4$. Yield: 89%. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.44 (t, ^{3}J(H,H) = 8 Hz, 1 H, Ar–H), 7.29–7.26 (m, 3 H, NCHN and Ar–H), 6.98 (s, 2 H, Ar–H), 4.32 (br-s, 4 H, NCH_2), 3.17 (m, ^{3}J(H,H) = 7 Hz, 2 H, C*H*$(CH_3)_2$), 2.56 (br-s, 4 H, CH_2), 2.39 (s, 6 H, CH_3), 2.29 (s, 3 H, CH_3), 1.41 (d, ^{3}J(H,H) = 7 Hz, 6 H, CH(C*H*$_3)_2$), 1.25 (d, ^{3}J(H,H) = 7 Hz, 6 H, CH(C*H*$_3)_2$). $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$): δ 158.5 (NCHN), 145.5, 141.2, 140.0, 139.6, 134.3, 131.7, 131.0, 126.0 (Ar–C), 56.9, 55.5 (NCH_2), 29.5 (*C*H$(CH_3)_2$), 26.1, 25.6, 25.4, 24.8 (CH(*C*H$_3)_2$ and CH_2), 21.6 (CH_3), 18.2 (CH_3). Anal. Calcd. for $C_{26}H_{37}BF_4N_2$: C, 67.25; H, 8.03; N, 6.03. Found: C, 67.43; H, 8.76; N, 6.06. MS (ESI): *m/z* 377 $[M - BF_4]^+$.



8Pr·HI. Yield: 56%. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.49 (s, 1 H, NCHN), 7.37 (t, ^{3}J(H,H) = 8 Hz, 2 H, Ar–H), 7.21 (d, ^{3}J(H,H) = 8 Hz, 4 H, Ar–H), 4.77 (br-s, 4 H, NCH_2), 3.22 (m, ^{3}J(H,H) = 7 Hz, 4 H, C*H*(CH_3)$_2$), 2.26 (m, ^{3}J(H,H) = 6 Hz, 4 H, CH_2), 2.12 (br-s, 2 H, CH_2), 1.34 (d, ^{3}J(H,H) = 7 Hz, 12 H, CH(C*H*$_3$)$_2$), 1.21 (d, ^{3}J(H,H) = 7 Hz, 12 H, CH(C*H*$_3$)$_2$). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 157.5 (NCHN), 145.2, 141.4, 131.3, 126.1 (Ar–C), 55.8 (NCH_2), 29.3 (*C*H(CH_3)$_2$), 28.2 (CH_2), 25.7, 25.4 (CH_3), 22.0 (CH_2). No satisfactory elemental analysis result was obtained from multiple trials. MS (ESI): *m/z* 433 $[M - I]^+$.



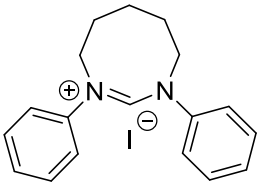
8PrMes·HI. Yield: 11%. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.42 (s, 1 H, NCHN), 7.37 (t, ^{3}J(H,H) = 8 Hz, 1 H, Ar–H), 7.21 (d, ^{3}J(H,H) = 8 Hz, 2 H, Ar–H), 6.91 (s, 2 H, Ar–H), 4.73 (br-s, 4 H, NCH_2), 3.24 (m, ^{3}J(H,H) = 7 Hz, 2 H, C*H*(CH_3)$_2$), 2.37 (s, 6 H, CH_3), 2.26 (br-s, 4 H, CH_2), 2.23 (s, 3 H, CH_3), 2.14 (br-s, 2 H, CH_2), 1.34 (d, ^{3}J(H,H) = 7 Hz, 6 H, CH(C*H*$_3$)$_2$), 1.18 (d, ^{3}J(H,H) = 7 Hz, 6 H, CH(C*H*$_3$)$_2$). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 158.0 (NCHN), 145.1, 142.2, 141.6, 140.8, 134.1, 131.3, 131.0, 126.1 (Ar–C), 55.4, 54.8 (NCH_2), 29.2 (*C*H(CH_3)$_2$), 28.7, 28.2 (CH_2), 25.5, 24.7 (CH_3), 21.7 (CH_2), 21.4 (CH_3), 19.1 (CH_3).. Anal. Calcd. for $C_{27}H_{39}IN_2$: C, 62.54; H, 7.58; N, 5.40. Found: C, 62.86; H, 7.13; N, 5.64. MS (ESI): *m/z* 391 $[M - I]^+$.



This salt was synthesized via a modified protocol. *N*-phenyl-*N'*-(2,4,6-trimethylphenyl)formamidine (500 mg, 2.10 mmol), K_2CO_3 (290 mg, 2.10 mmol) and 1,5-dibromopentane (376 μL, 2.76 mmol) were suspended in CH_3CN and stirred at 60 °C for two days before the solvent was removed in vacuum. CH_2Cl_2 (20 mL) was added to the residue and the suspension was filtered through Celite. The collected solution was concentrated to 2 mL and subjected to column chromatography (SiO_2, hexane/ethyl acetate, 50:1, Rf: 0.42, hexane/ethyl acetate, 4:1) to afford the product **I** as a colorless oil (246 mg, 0.64 mmol, 30%). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.54 (s, 1 H, NCHN), 7.29 (t, ^3J(H,H) = 8 Hz, 2 H, Ar–H), 7.05–7.04 (m, 3 H, Ar–H), 6.98 (s, 2 H, Ar–H), 3.77 (t, ^3J(H,H) = 8 Hz, 2 H, NCH_2), 3.43 (t, ^3J(H,H) = 7 Hz, 2 H, $BrCH_2$), 2.35 (s, 3 H, CH_3), 2,29 (s, 6 H, CH_3), 1.96–1.90 (m, 2 H, CH_2), 1.75–1.68 (m, 2 H, CH_2), 1.55–1.48 (m, 2 H, CH_2). $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$): δ 153.3 (NCHN), 152.3, 139.7, 138.0, 137.2, 130.1, 129.6, 123.3, 121.9 (Ar–C), 48.7 (NCH_2), 34.2 ($BrCH_2$), 33.1, 27.1, 26.5, 21.5, 19.1 (CH_2 and CH_3). MS (ESI): *m/z* 389 $[M + H]^+$.

8MesPh·HI. Compound **I** (200 mg, 0.52 mmol) was dissolved in CH_3CN (8 mL) in a sealed tube before NaI (233 mg, 1.55 mmol) was added. The mixture was heated at 100 °C overnight before the solvent was removed in vacuum. CH_2Cl_2 (20 mL) was added to the residue and the suspension was filtered through Celite. The collected solution was concentrated to 2 mL and dropwise added to diethyl ether (50 mL). Upon stirring, the product

precipitates as a red sticky solid (68 mg, 0.16 mmol, 30%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.75 (s, 1 H, NCHN), 7.57–7.45 (m, 5 H, Ar–H), 7.00 (s, 2 H, Ar–H), 4.75 (t, ^{3}J(H,H) = 6 Hz, 2 H, NCH_2), 4.45 (br-s, 2 H, NCH_2), 2.46 (s, 6 H, CH_3), 2.30–2.22 (m, 7 H, CH_2 and CH_3), 2.13–2.09 (m, 2 H, CH_2). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$): δ 157.6 (NCHN), 144.4, 142.1, 141.0, 134.0, 131.5, 131.3, 130.8, 125.8 (Ar–C), 54.8, 54.6 (NCH_2), 29.3, 28.4 (CH_2), 21.6, 21.4 (CH_3 and CH_2), 19.9 (CH_3). No satisfactory elemental analysis result was obtained from multiple trials. MS (ESI): *m/z* 307 $[M - I]^+$.



8Ph·HI. Yield: 13%. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.91 (s, 1 H, NCHN), 7.59 (d, ^{3}J(H,H) = 8 Hz, 4 H, Ar–H), 7.47–7.41 (m, 6 H, Ar–H), 4.73 (br-s, 4 H, NCH_2), 2.19 (br-s, 4 H, CH_2), 2.01 (br-s, 2 H, CH_2). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ 156.7 (NCHN), 146.0, 131.1, 130.3, 125.6 (Ar–C), 56.6 (NCH_2), 28.8 (CH_2), 21.2 (CH_2). Anal. Calcd. for $C_{18}H_{21}IN_2$: C, 55.11; H, 5.40; N, 7.14. Found: C, 55.53; H, 5.51; N, 7.06. MS (ESI): *m/z* 265 $[M - I]^+$.

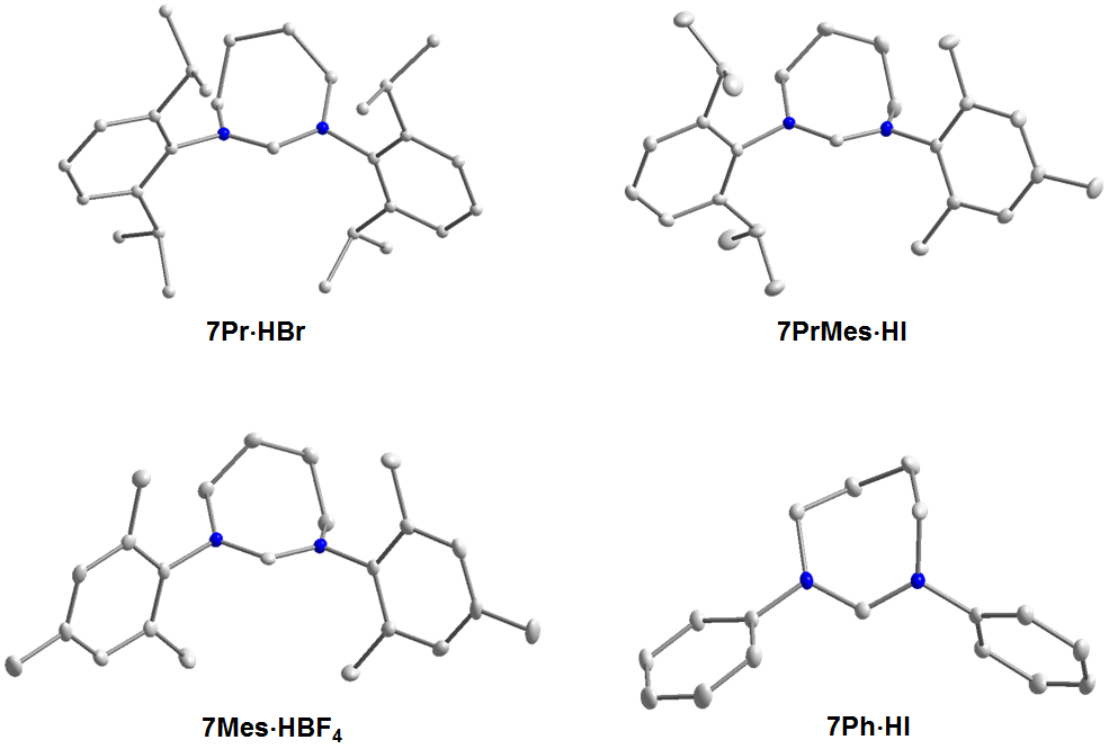


Figure S1. Molecular structures of **7Pr·HBr**,[7] **7PrMes·HI**, **7Mes·HBF$_4$** and **7Ph·HI**. Anions, hydrogen atoms and solvent molecules have been omitted for clarity. NCHN/Aryl dihedral angle, **7Pr·HBF$_4$**: 87°, 81°; **7PrMes·HI**: 87° (Dipp), 72° (Mes); **7Mes·HBF$_4$**: 83°, 75°; **7Ph·HI**: 60°, 58°.

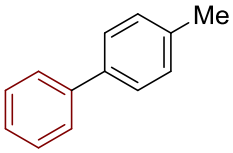
Table S1. Selected X-ray crystallographic data for the NHC·HX salts.

	7PrMes·HI	**7Mes·HBF$_4$**	**7Ph·HI**·0.5H$_2$O
formula	$C_{26}H_{37}IN_2$	$C_{23}H_{31}BF_4N_2$	$C_{17}H_{20}IN_2O_{0.5}$
fw	504.47	422.31	387.25
color, habit	colourless, prism frag	colourless, block	colourless, block
cryst size [mm]	0.23×0.41×0.46	0.34×0.21×0.19	0.33×0.26×0.19
temp [K]	100(2)	100(2)	100(2)
crystsyst	monoclinic	monoclinic	monoclinic
space group	*P*12(1)/n1	*P*21/c	*C*2
a[Å]	9.4821(7)	15.5061(6)	17.5096(8)
b [Å]	14.8496(8)	15.3089(8)	10.5339(5)
c [Å]	17.7290(12)	9.2595(4)	11.1338(6)
α [deg]	90.00	90.00	90.00
β [deg]	100.901(2)	90.915(2)	126.3150(10)
γ [deg]	90.00	90.00	90.00
V [Å^3]	2451.3(3)	2197.75(17)	1654.71(14)
Z	4	4	4
D_c [g cm^{-3}]	1.367	1.276	1.554
radiation used	Mo Kα	Mo Kα	Mo Kα
μ [mm^{-1}]	1.320	0.097	1.932
θ range [deg]	2.34–29.57	2.57–28.28	2.66–28.28
no. of unique data	37662	26959	47242
max., min. transmn	0.7550, 0.5800	0.7459, 0.6669	0.7466, 0.6848
final R indices	R_1 = 0.0222,	R_1 = 0.0556,	R1 = 0.0111,
[$I > 2\sigma(I)$]	wR_2 = 0.0611	wR_2 = 0.1259	wR2 = 0.0274
R indices (all data)	R_1 = 0.0239,	R_1 = 0.0829,	R1 = 0.0113,
	wR_2 = 0.0621	wR_2 = 0.1375	wR2 = 0.0274
goodness-of-fit	1.060	1.064	1.119
peak/hole [e Å^{-3}]	1.366/–0.839	0.351/–0.281	0.293/–0.375

General Procedure for Iron-catalyzed Biaryl Cross-coupling Reaction of Aryl Chlorides:

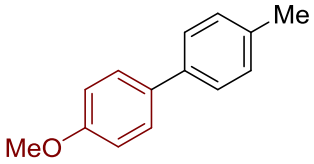
In a glovebox, $Fe(OTf)_2$ (5.3 mg, 0.015 mmol, 3 mol%), 7MesBr (18.7 mg, 0.045 mmol, 9 mol%) and NaO*t*Bu (4.3 mg, 0.045 mmol, 9 mol%) in THF (0.5 mL) were charged to a dried reaction tube. The mixture was allowed to stir at rt for 1 h before a solution of aryl chloride (0.5 mmol, 1.0 eq) and Grignard reagent (0.6 mmol, 1.2 eq) was added. The tube was sealed, taken out of the glovebox and stirred at 60 °C for 16h. The reaction progress was monitored by GC using dodecane as the internal standard. Once completed, the reaction mixture was quenched with saturated NH_4Cl and extracted with CH_2Cl_2 several times. The combined organic layers were dried over anhydrous $MgSO_4$, concentrated in vacuo and the resulting crude mixture was purified by silica gel column chromatography.

4-Methyl-1,1'-biphenyl (**3a**)[8]



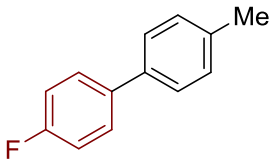
3a was prepared from chlorobenzene (56 mg, 0.5 mmol) and *p*-tolylmagnesium bromide (0.86 mL, 0.6 mmol, 0.70 M in THF). The crude mixture was purified by flash column chromatography (petroleum ether) to afford the desired product as white solid (79 mg, 94%).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.55 (m, 2H), 7.54 – 7.48 (m, 2H), 7.46 – 7.40 (m, 2H), 7.35 – 7.29 (m, 1H), 7.28 – 7.23 (m, 2H), 2.40 (s, 3H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 141.3, 138.5, 137.1, 129.6, 128.8, 127.1, 127.1, 126.9, 21.2.

4-Methoxy-4'-methyl-1,1'-biphenyl (**3b**) [3]



3b was prepared from 1-chloro-4-methoxybenzene (71 mg, 0.5 mmol) and *p*-tolylmagnesium (0. 86 mL, 0.6 mmol, 0.70 M in THF). The crude mixture was purified by flash column chromatography (5% Et_2O/petroleum ether) to afford the desired product as a white solid (98 mg, 99%).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 – 7.48 (m, 2H), 7.45 (d, *J* = 8.1 Hz, 2H), 7.22 (d, *J* = 7.7 Hz, 2H), 6.96 (d, *J* = 8.7 Hz, 2H), 3.85 (s, 3H), 2.38 (s, 3H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 159.1, 138.1, 136.4, 133.9, 129.5, 128.0, 126.7, 114.3, 55.4, 21.1.

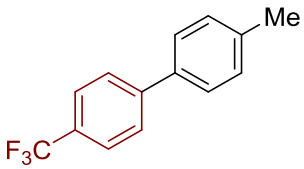
4-Fluoro-4'-methyl-1,1'-biphenyl (**3c**)[3]



3c was prepared from 1-chloro-4-fluorobenzene (65 mg, 0.5 mmol) and *p*-tolylmagnesium bromide (0. 86 mL, 0.6 mmol, 0.70 M in THF). The crude mixture was purified by flash column chromatography (petroleum ether) to afford the desired product as white solid (77 mg, 83%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 – 7.49 (m, 2H), 7.46 – 7.41 (m, 2H), 7.24 (d, *J* = 7.8 Hz, 2H), 7.10 (t, *J* = 8.7 Hz, 2H), 2.39 (s, 3H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 162.4 (d, *J* = 246.4 Hz), 137.5, 137.4 (d, *J* = 3.0 Hz), 137.1, 129.6, 128.5 (d, *J* = 8.1 Hz), 126.9, 115.6 (d, *J* = 21.2 Hz), 21.1.

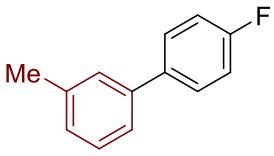
4-Methyl-4'-(trifluoromethyl)-1,1'-biphenyl (**3d**)[9]



3d was prepared from 1-chloro-4-(trifluoromethyl)benzene (90 mg, 0.5 mmol) and *p*-tolylmagnesium (0. 87 mL, 0.6 mmol, 0.69 M in THF). The crude mixture was purified by flash column chromatography (petroleum ether) to afford the desired product as a white solid (73 mg, 62%).

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.78 – 7.66 (m, 4H), 7.61 – 7.46 (m, 2H), 7.37 – 7.26 (m, 2H), 2.42 (s, 3H). ^{13}C{^{1}H} NMR (101 MHz, CD_2Cl_2) δ 145.0, 138.8, 137.0, 130.1, 129.1(q, *J*=32.3 Hz), 127.5, 127.4, 126.0(q, *J*=4.0 Hz),124.9 (d, *J*=272.7 Hz), 21.3.

4'-Fluoro-3-methyl-1,1'-biphenyl (**3e**)[10]

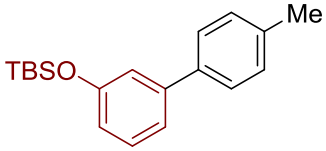


3e was prepared from 3-chlorotoluene (63 mg, 0.5 mmol) and (4-fluorophenyl)magnesium bromide (0.79 mL, 0.6 mmol, 0.76 M in THF). The crude mixture was purified by flash

column chromatography (petroleum ether) to afford the desired product as a white solid (90 mg, 96%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.48 (m, 2H), 7.34 (td, *J* = 7.0, 6.1, 2.9 Hz, 3H), 7.21 – 7.04 (m, 3H), 2.42 (s, 3H). ^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$) δ 162.5 (d, *J* = 247.5 Hz), 140.3, 138.5, 137.6 (d, *J* = 3.0 Hz), 128.8, 128.7 (d, *J* = 8.1 Hz), 128.1, 127.9, 124.2, 115.6 (d, *J* = 22.2 Hz), 21.6.

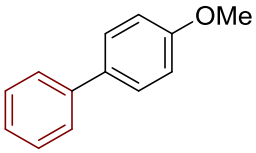
tert-Butyldimethyl((4'-methyl-[1,1'-biphenyl]-3-yl)oxy)silane (**3f**) [2]



3f was prepared from *tert*-butyl(3-chlorophenoxy)dimethylsilane (121 mg, 0.5 mmol), *p*-tolylmagnesium bromide (0. 86 mL, 0.6 mmol, 0.70 M in THF). The crude mixture was purified by flash column chromatography (petroleum ether) to afford the desired product as colourless oil (119 mg, 80%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.44 (m, 2H), 7.27 – 7.21 (m, 3H), 7.16 (ddd, *J* = 7.7, 1.8, 1.1 Hz, 1H), 7.05 (t, *J* = 2.1 Hz, 1H), 6.83 – 6.78 (m, 1H), 2.39 (s, 3H), 1.01 (s, 9H), 0.23 (s, 6H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 156.1, 142.7, 138.3, 137.2, 129.7, 129.5, 127.0, 120.1, 118.8, 118.7, 25.8, 21.2, 18.3, -4.2.

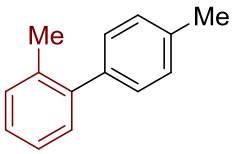
4-Methoxy-1,1'-biphenyl (**3g**) [3]



3g was prepared from chlorobenzene (56 mg, 0.5 mmol) and (4-methoxyphenyl)magnesium bromide (1.45 mL, 0.6 mmol, 0.41 M in THF). The crude mixture was purified by flash column chromatography (20% CH_2Cl_2/petroleum ether) to afford the desired product as white solid (83 mg, 90%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (td, *J* = 8.8, 8.1, 1.8 Hz, 4H), 7.41 (t, *J* = 7.7 Hz, 2H), 7.34 – 7.28 (m, 1H), 7.02 – 6.93 (m, 2H), 3.86 (s, 3H). ^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$) δ 159.3, 141.0, 133.9, 128.8, 128.2, 126.8, 126.7, 114.3, 55.4.

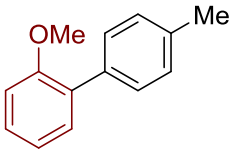
2,4'-Dimethyl-1,1'-biphenyl (**3h**)[2]



3h was prepared from 1-chloro-2-methylbenzene (63 mg, 0.5 mmol) and *p*-tolylmagnesium bromide (0. 86 mL, 0.6 mmol, 0.70 M in THF). The crude mixture was purified by flash column chromatography (petroleum ether) to afford the desired product as colourless oil (88 mg, 97%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (d, *J* = 6.5 Hz, 8H), 2.43 (s, 3H), 2.30 (s, 3H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 142.0, 139.2, 136.4, 135.5, 130.4, 129.9, 129.2, 128.9, 127.1, 125.8, 21.2, 20.6.

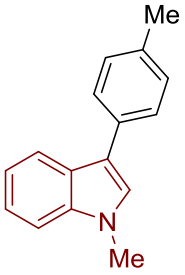
2-Methoxy-4'-methyl-1,1'-biphenyl (**3i**)[8]



3i was prepared from 2-chloroanisole (71 mg, 0.5 mmol) and *p*-tolylmagnesium bromide (0. 86 mL, 0.6 mmol, 0.70 M in THF). The crude mixture was purified by flash column chromatography (10% CH_2Cl_2/petroleum ether) to afford the desired product as white solid (88 mg, 88%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.39 (m, 2H), 7.31 (t, *J* = 7.2 Hz, 2H), 7.26 – 7.20 (m, 2H), 7.06 – 6.96 (m, 2H), 3.81 (s, 3H), 2.40 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.6, 136.6, 135.7, 130.9, 130.8, 129.5, 128.8, 128.4, 120.9, 111.3, 55.6, 21.3.

1-Methyl-3-(*p*-tolyl)-1*H*-indole (**3j**) [11]

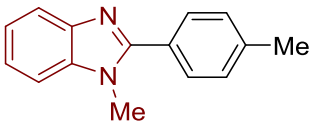


3j was prepared from 3-chloro-1-methyl-1*H*-indole (83 mg, 0.5 mmol) and *p*-tolylmagnesium bromide (0. 86 mL, 0.6 mmol, 0.70 M in THF), $Fe(OTf)_2$ (9 mg, 0.025 mmol, 5 mol%), 7MesBr (31 mg, 0.075 mmol, 15 mol%), NaO*t*Bu (7 mg, 0.075 mmol, 15 mol%) and 0.5 ml THF. The crude mixture was purified by flash column chromatography (5% dichloromethane/petroleum ether) to afford the desired product as colourless oil (91 mg,

82%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.55 (d, *J* = 7.9 Hz, 2H), 7.36 (dd, *J* = 8.3, 1.0 Hz, 1H), 7.31 – 7.23 (m, 3H), 7.22 – 7.13 (m, 2H), 3.84 (d, *J* = 0.7 Hz, 3H), 2.40 (s, 3H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 137.5, 135.3, 132.8, 129.5, 127.3, 126.3, 122.0, 120.0, 119.8, 116.8, 109.5, 32.8, 21.2.

1-Methyl-2-(*p*-tolyl)-1*H*-benzo[*d*]imidazole [12](**3k**)

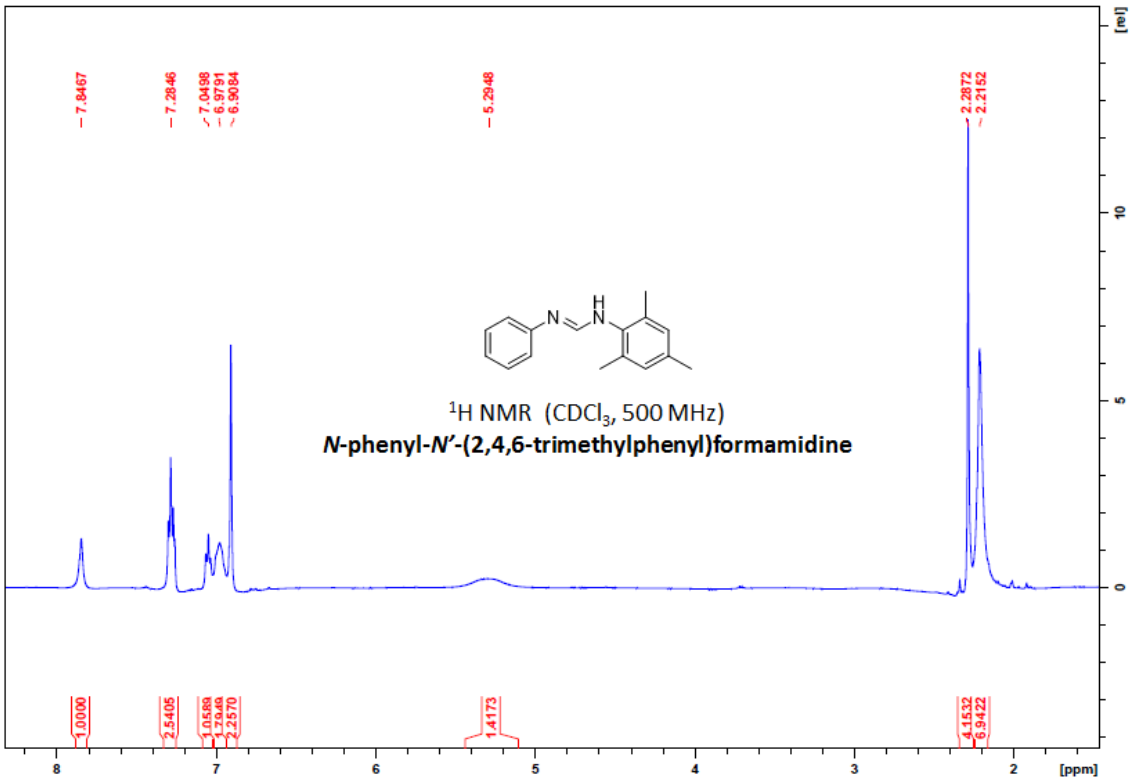


3k was prepared from 2-chloro-1-methyl-1*H*-benzo[*d*]imidazole (83.3 mg, 0.5 mmol) and *p*-tolylmagnesium bromide (0. 86 mL, 0.6 mmol, 0.70 M in THF). The crude mixture was purified by flash column chromatography (16% ethyl acetate/petroleum ether) to afford the desired product as white solid (79 mg, 71%).

^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 7.80 – 7.73 (m, 2H), 7.70 – 7.63 (m, 1H), 7.56 – 7.49 (m, 1H), 7.38 (d, *J* = 7.8 Hz, 2H), 7.33 – 7.20 (m, 2H), 3.92 (t, *J* = 0.8 Hz, 3H), 2.43 (s, 3H). ^{13}C NMR (101 MHz, $(CD_3)_2CO$) δ 154.4, 144.1, 140.4, 137.9, 130.2, 130.0, 128.8, 123.1, 122.7, 120.1, 110.9, 32.1, 21.4.

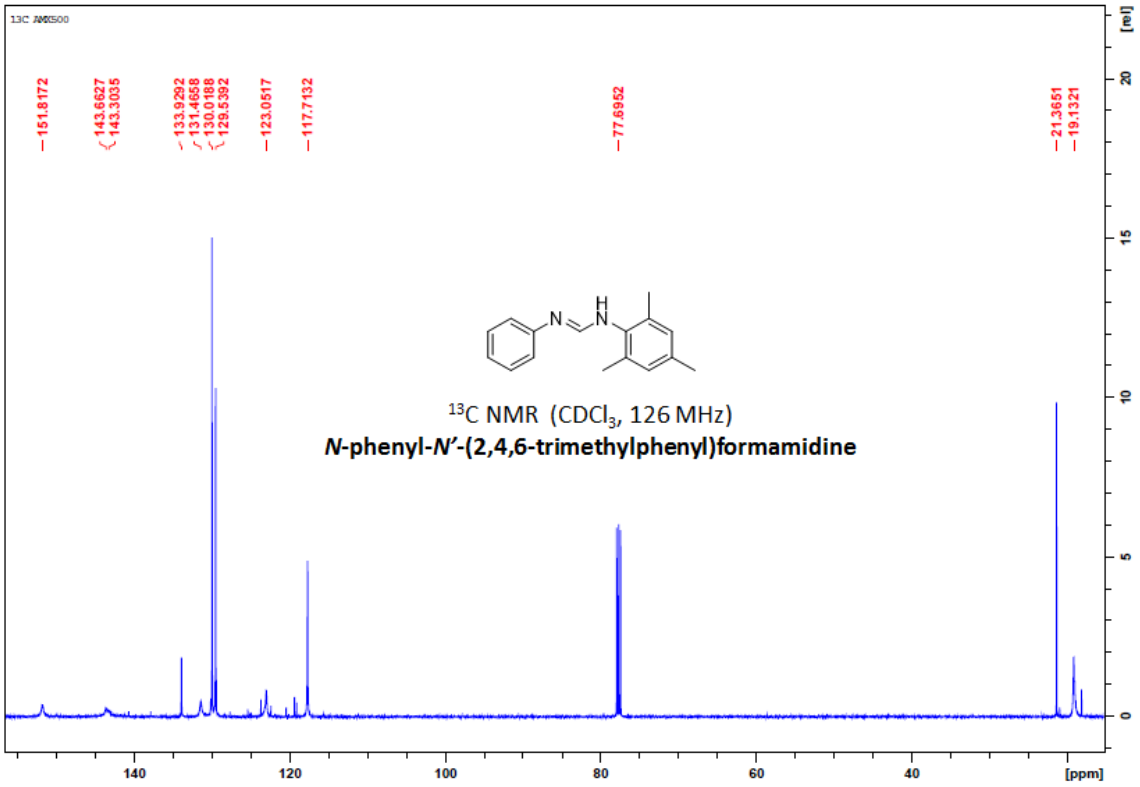
Table S2. Influence of NHCs' substituents and ring size on the formation of 3j (Table 2).

Entry	NHC.HX	3i (%)
1	**7Mes.HBr**	5
2	**7MesPh.HI**	2
3	**7Ph.HI**	1
4	**6PrMes.HI**	4
5	**6Mes.HBr**	29
6	**6Ph.HI**	0



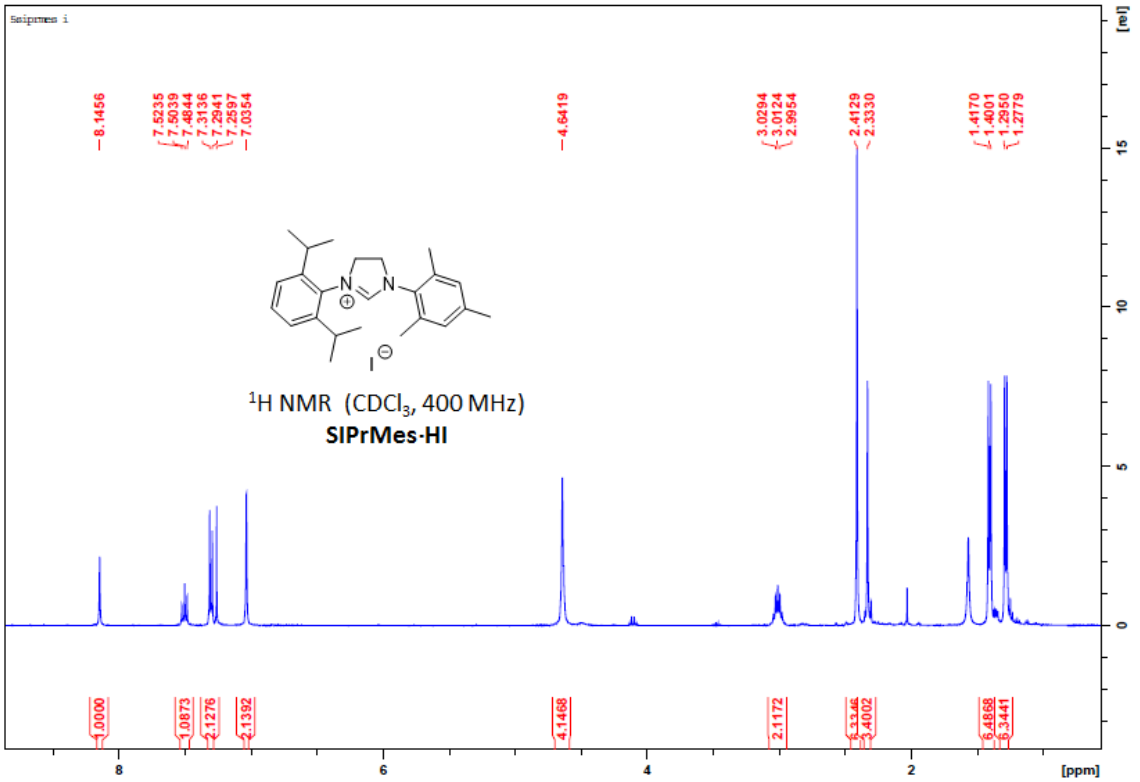
^{1}H NMR ($CDCl_3$, 500 MHz)

***N*-phenyl-*N'*-(2,4,6-trimethylphenyl)formamidine**

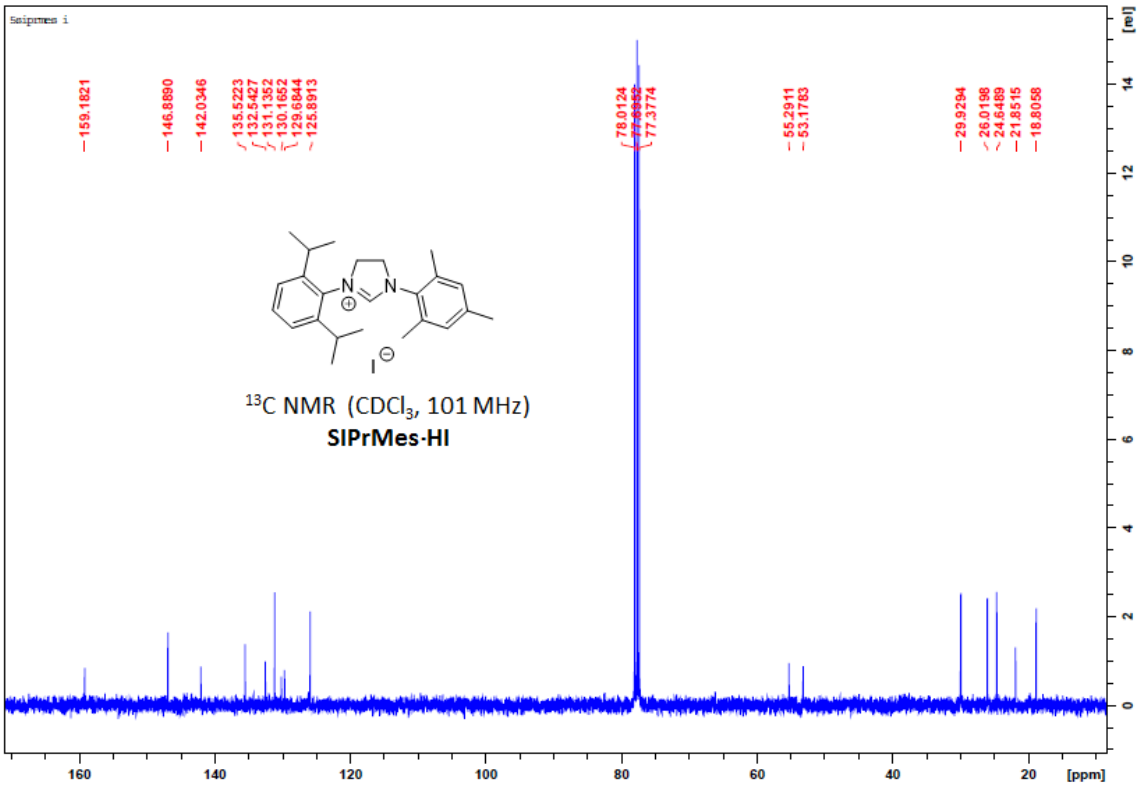


^{13}C NMR ($CDCl_3$, 126 MHz)

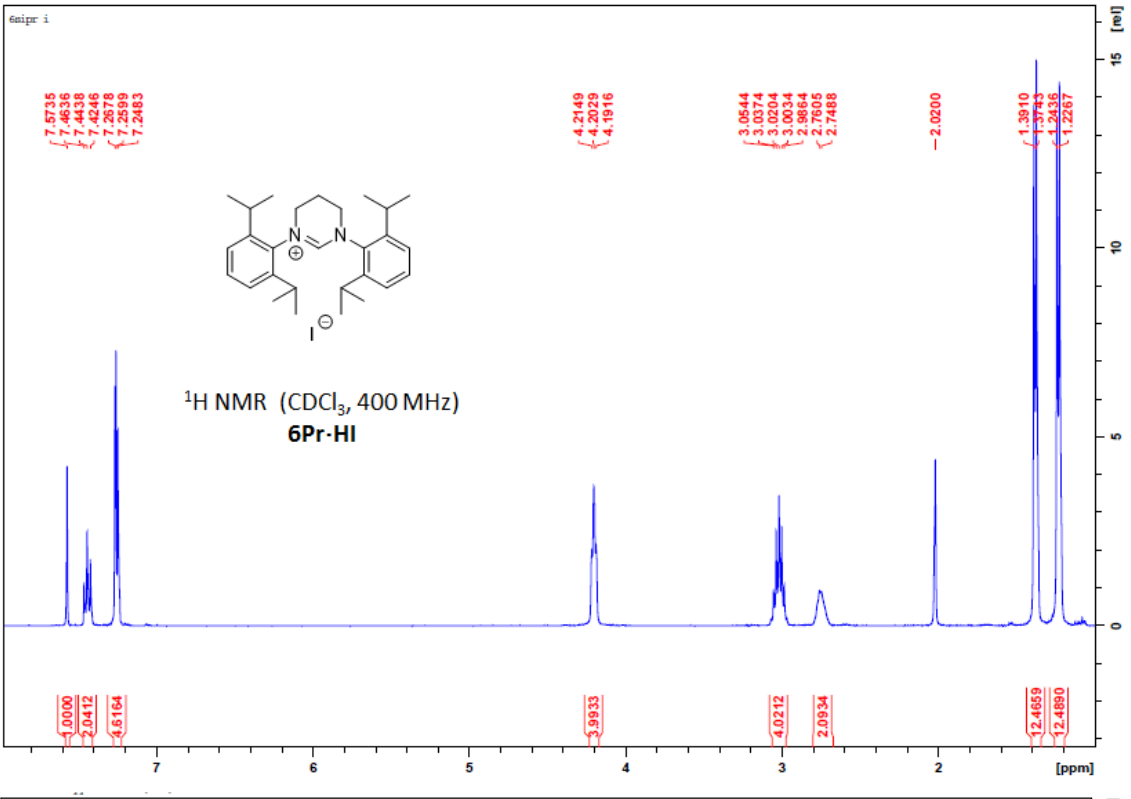
***N*-phenyl-*N'*-(2,4,6-trimethylphenyl)formamidine**



^{1}H NMR ($CDCl_3$, 400 MHz)
SIPrMes·HI

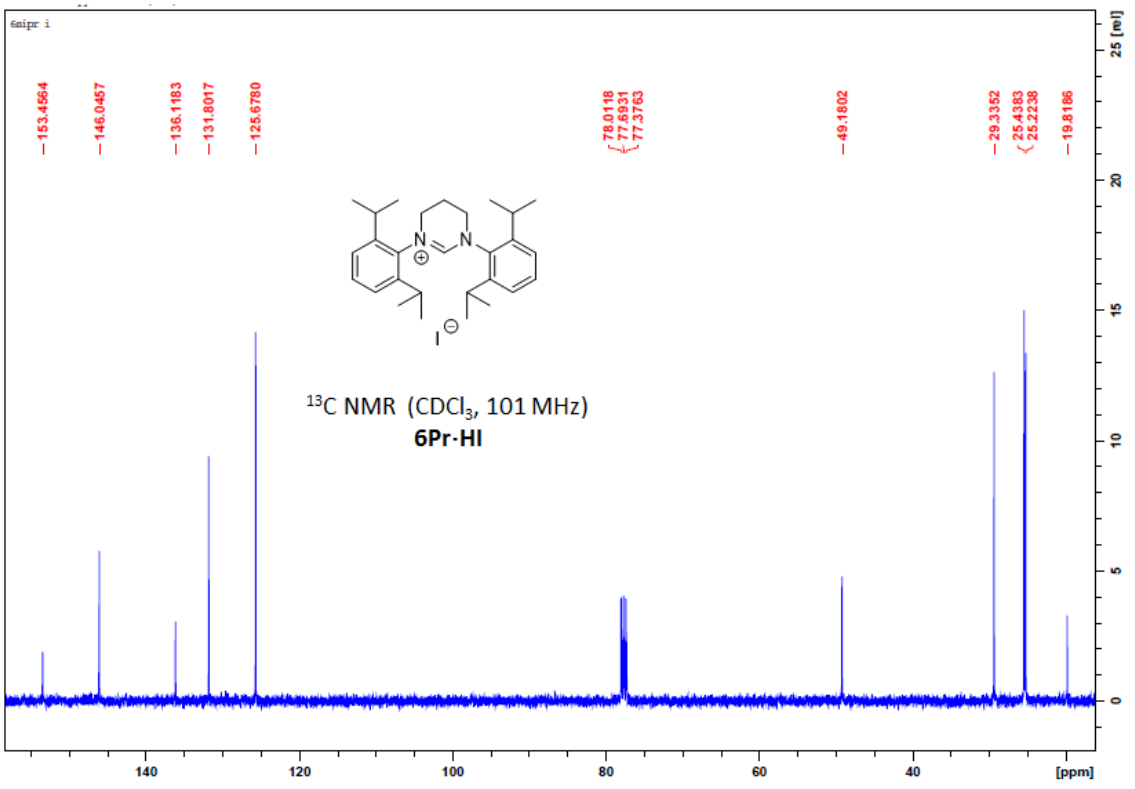


^{13}C NMR ($CDCl_3$, 101 MHz)
SIPrMes·HI



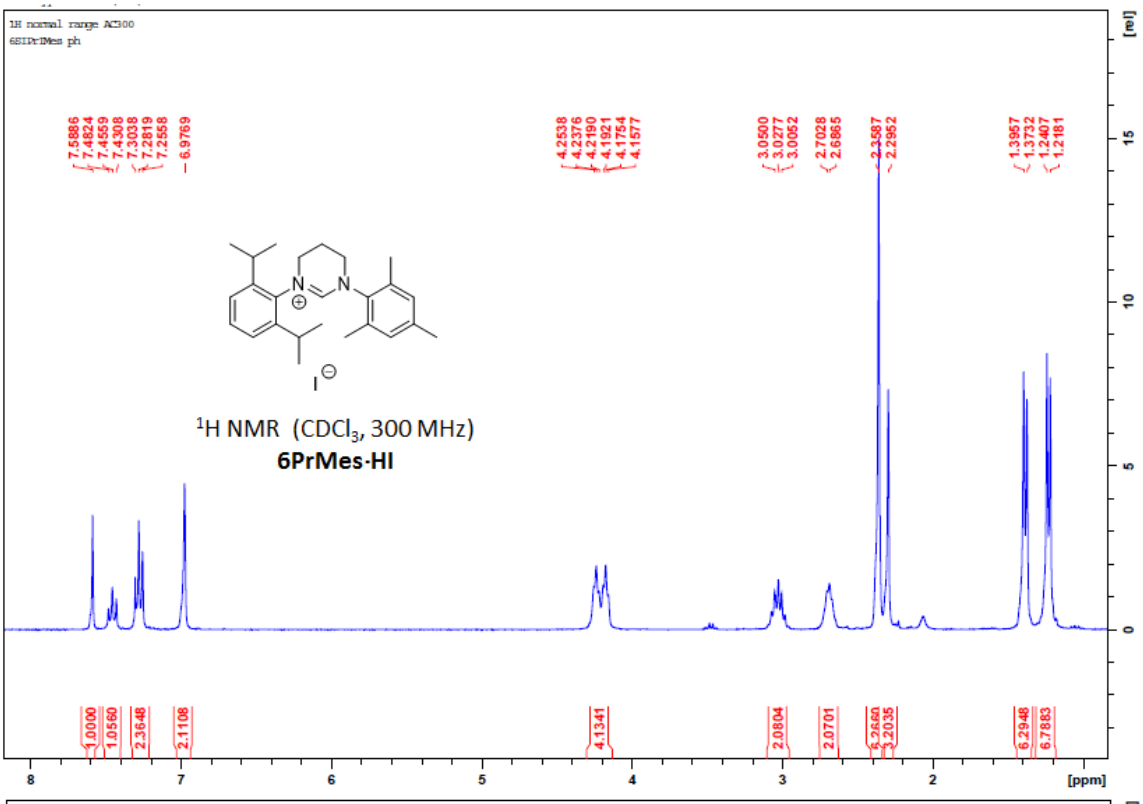
^{1}H NMR ($CDCl_3$, 400 MHz)

6Pr·HI



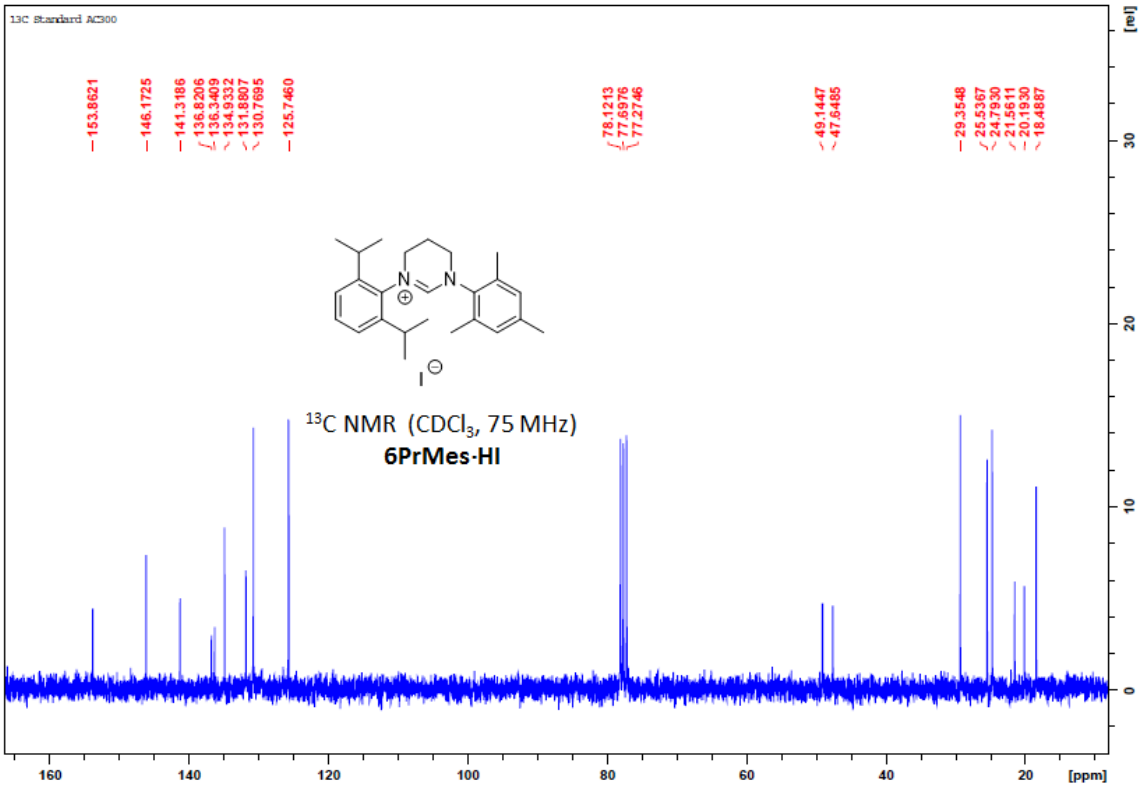
^{13}C NMR ($CDCl_3$, 101 MHz)

6Pr·HI



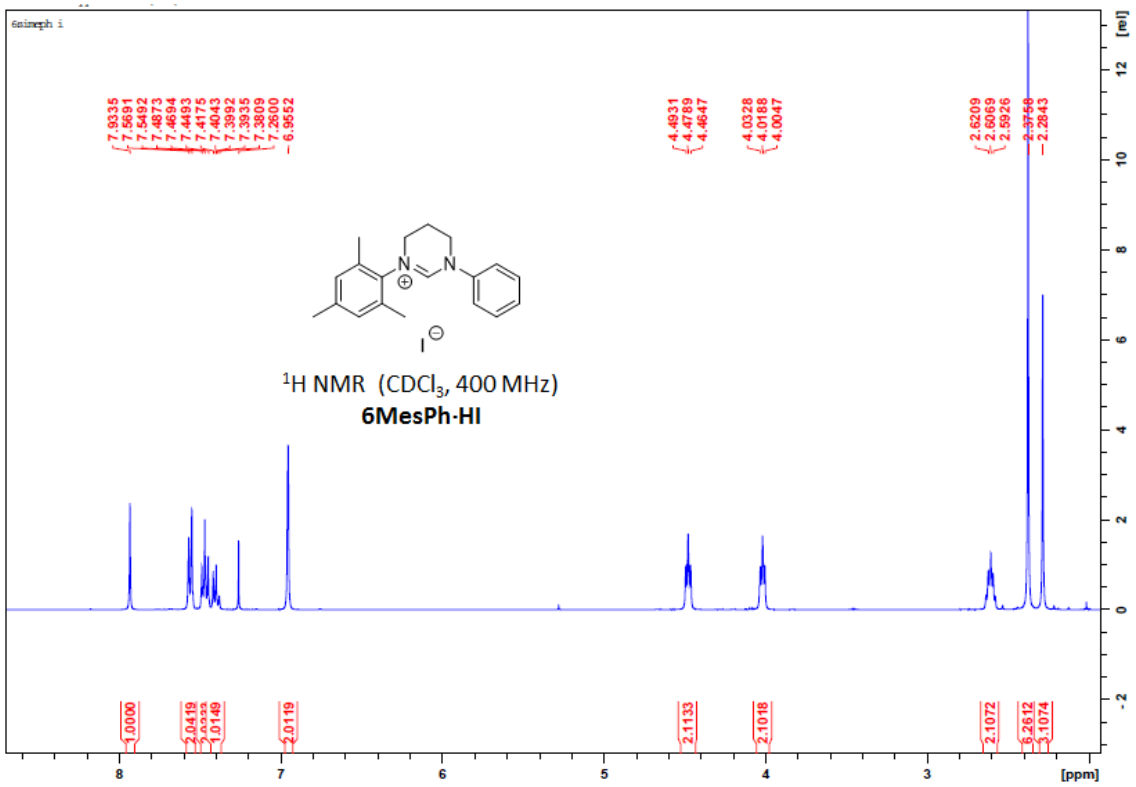
^{1}H NMR ($CDCl_3$, 300 MHz)

6PrMes·HI



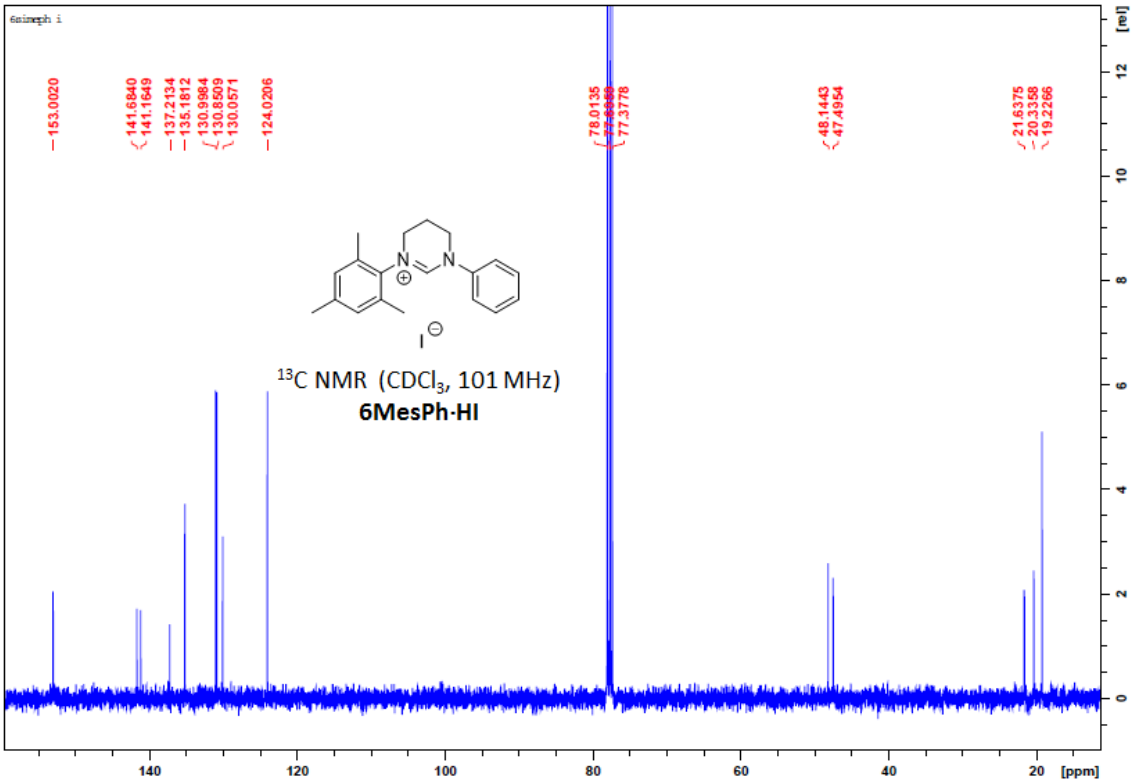
^{13}C NMR ($CDCl_3$, 75 MHz)

6PrMes·HI



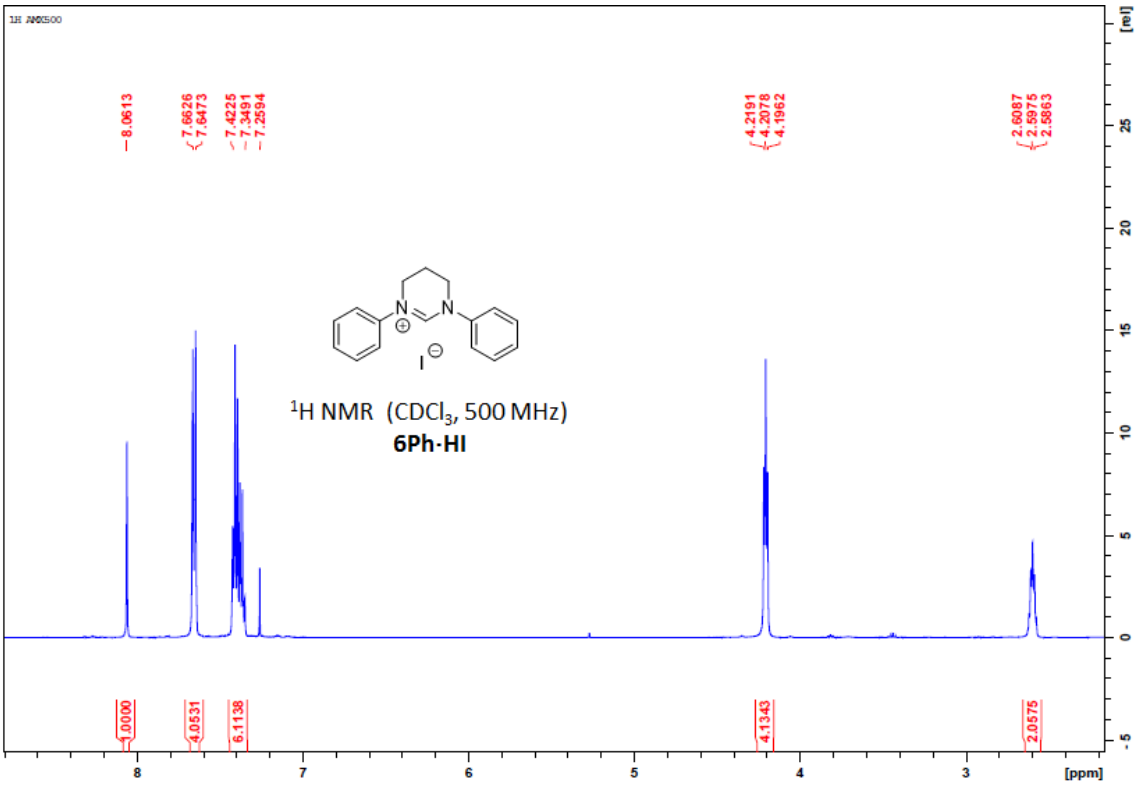
^{1}H NMR ($CDCl_3$, 400 MHz)

6MesPh·HI

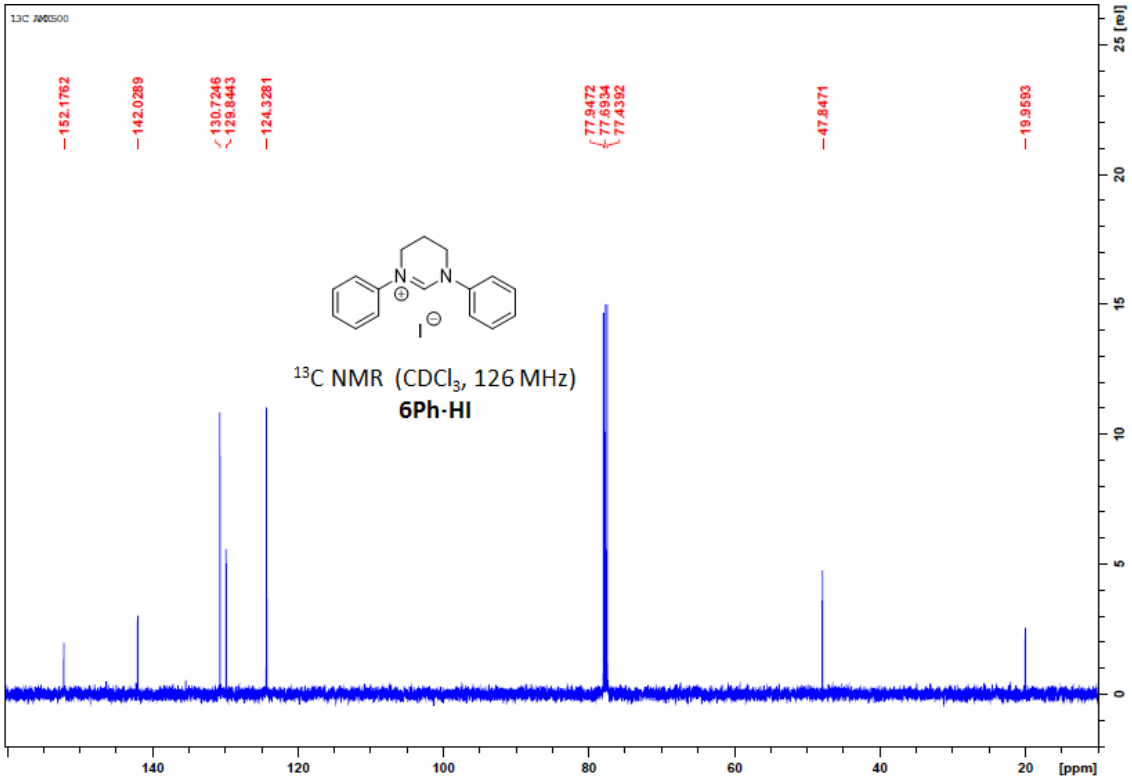


^{13}C NMR ($CDCl_3$, 101 MHz)

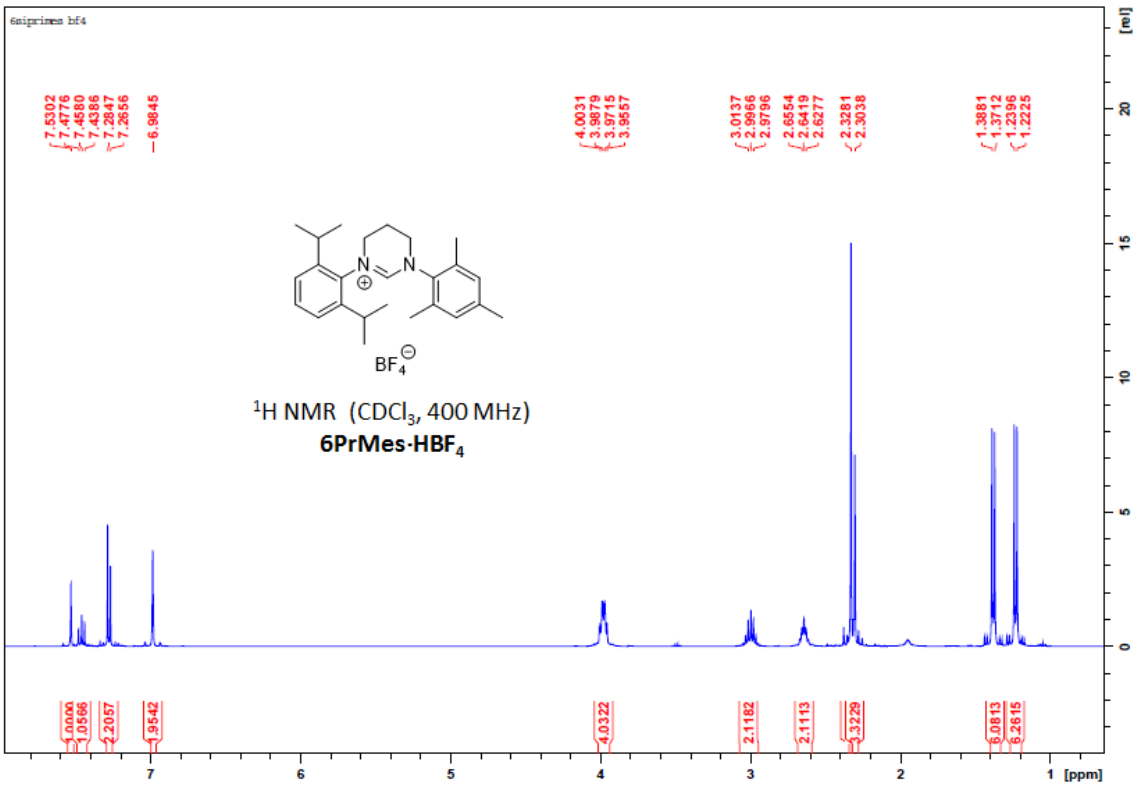
6MesPh·HI



^{1}H NMR ($CDCl_3$, 500 MHz)
6Ph·HI

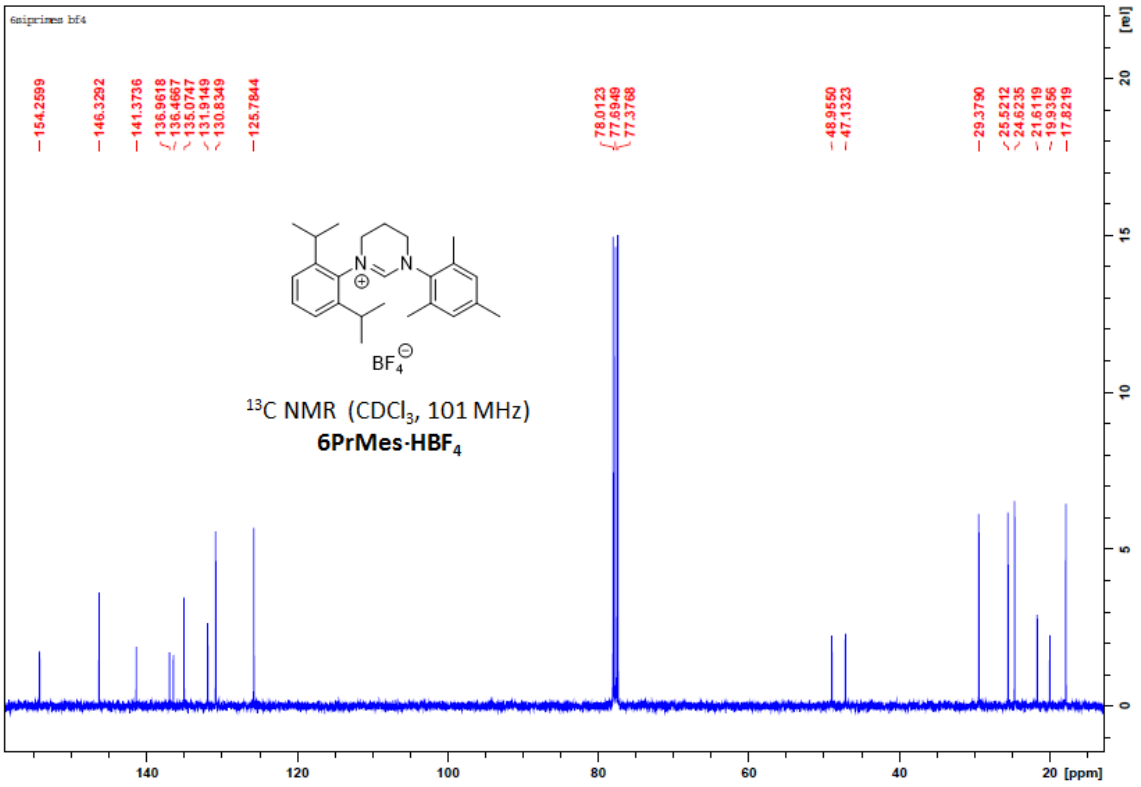


^{13}C NMR ($CDCl_3$, 126 MHz)
6Ph·HI



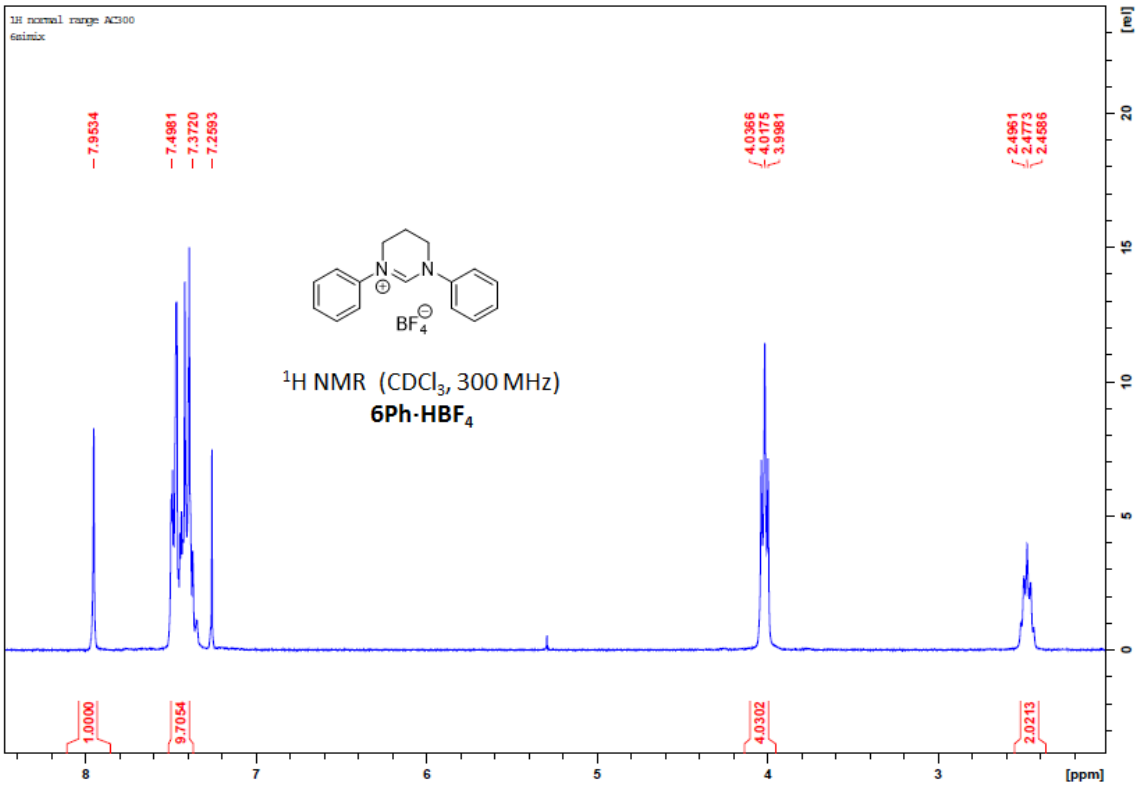
^{1}H NMR ($CDCl_3$, 400 MHz)

6PrMes·HBF$_4$



^{13}C NMR ($CDCl_3$, 101 MHz)

6PrMes·HBF$_4$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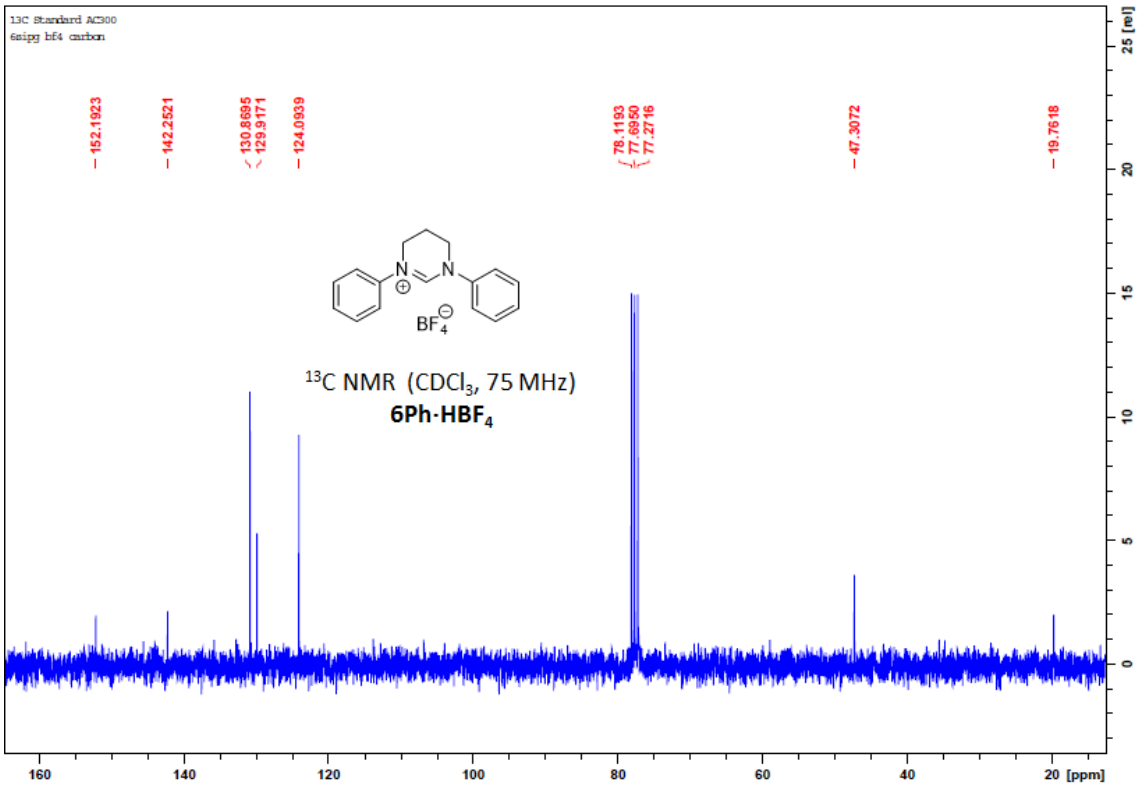
7.4981
7.3720
7.2593
4.0366
4.0175
3.9981
2.4961
2.4773
2.4586
1.0000
9.7054
4.0302
2.0213
[rel]
[ppm]
BF4
1H NMR (CDCl3, 300 MHz)
6Ph·HBF4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6sipg bf4 carbon
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142.2521
130.8695
129.9171
124.0939
78.1193
77.6950
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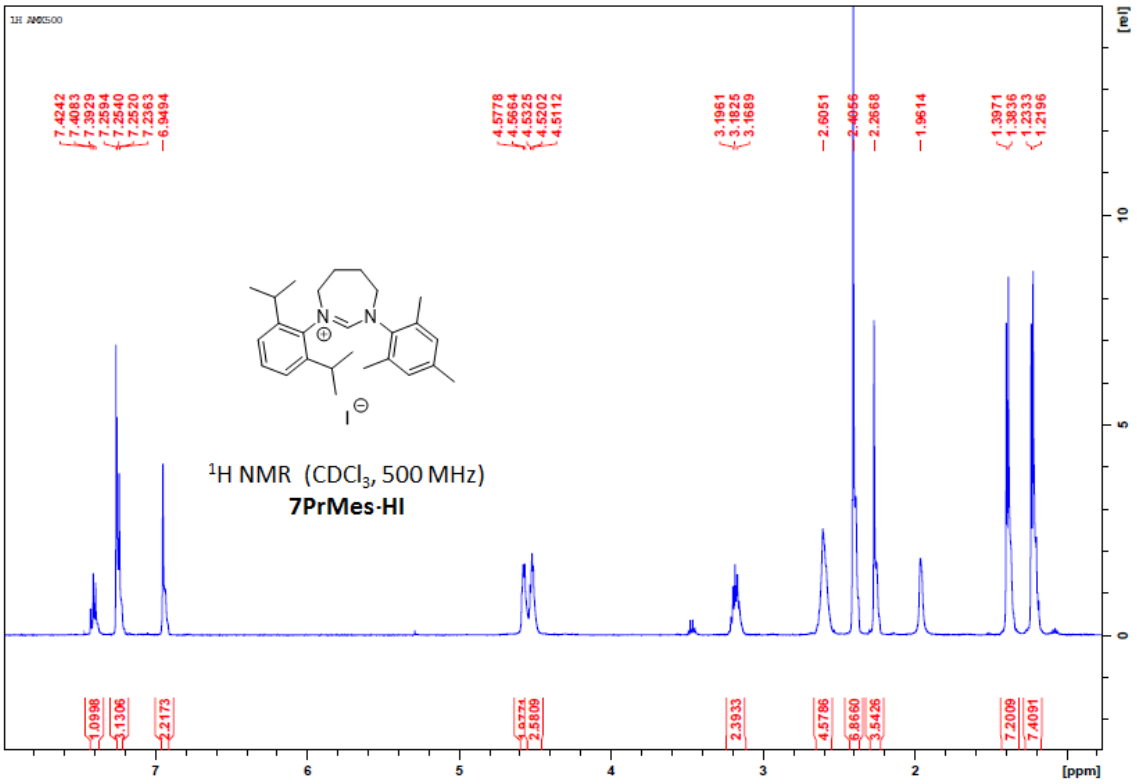
47.3072
19.7618
[rel]
[ppm]
BF4
13C NMR (CDCl3, 75 MHz)
6Ph·HBF4


1H AM500
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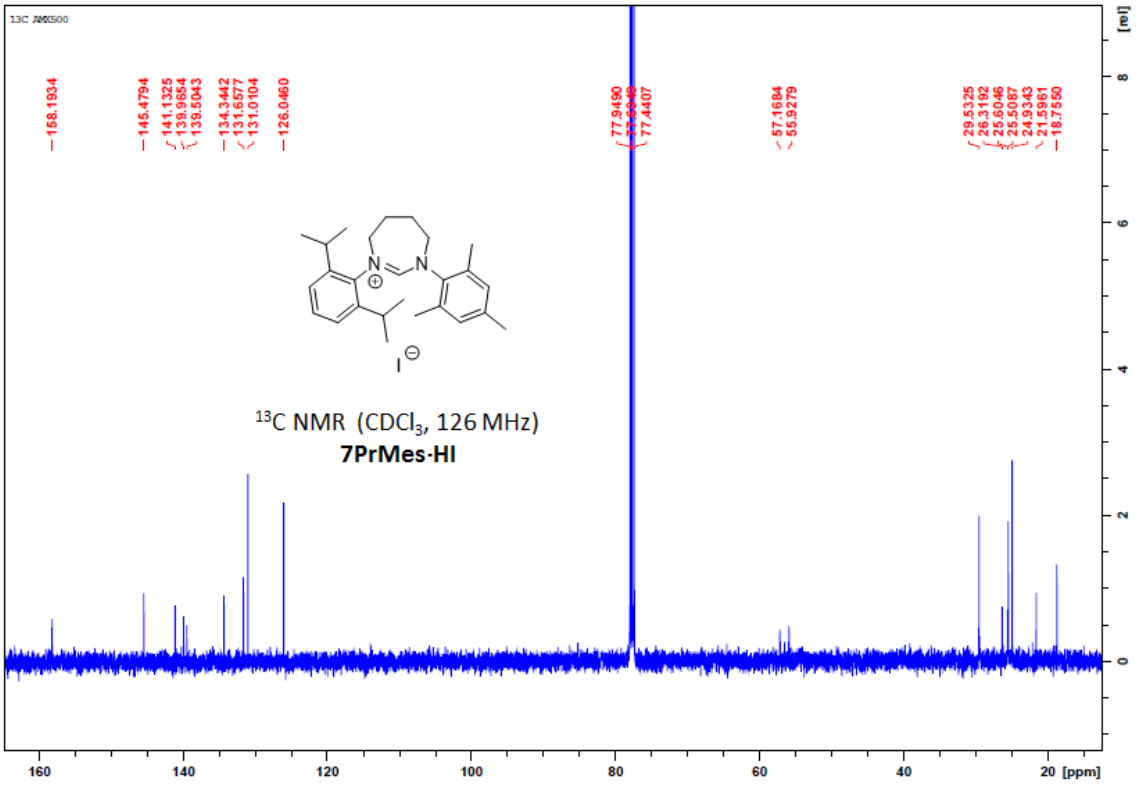
7.4083
7.3929
7.2594
7.2540
7.2520
7.2363
6.9494
4.5778
4.5664
4.5325
4.5202
4.5112
3.1961
3.1825
3.1689
2.6051
2.4956
2.2668
1.9614
1.3971
1.3836
1.2333
1.2196
[rel]
1.0998
3.1306
2.2173
1.6374
2.5809
2.3933
4.5786
6.8660
3.5426
7.2009
7.4091
[ppm]
^{1}H NMR (CDCl$_3$, 500 MHz)
7PrMes·HI


13C AM500
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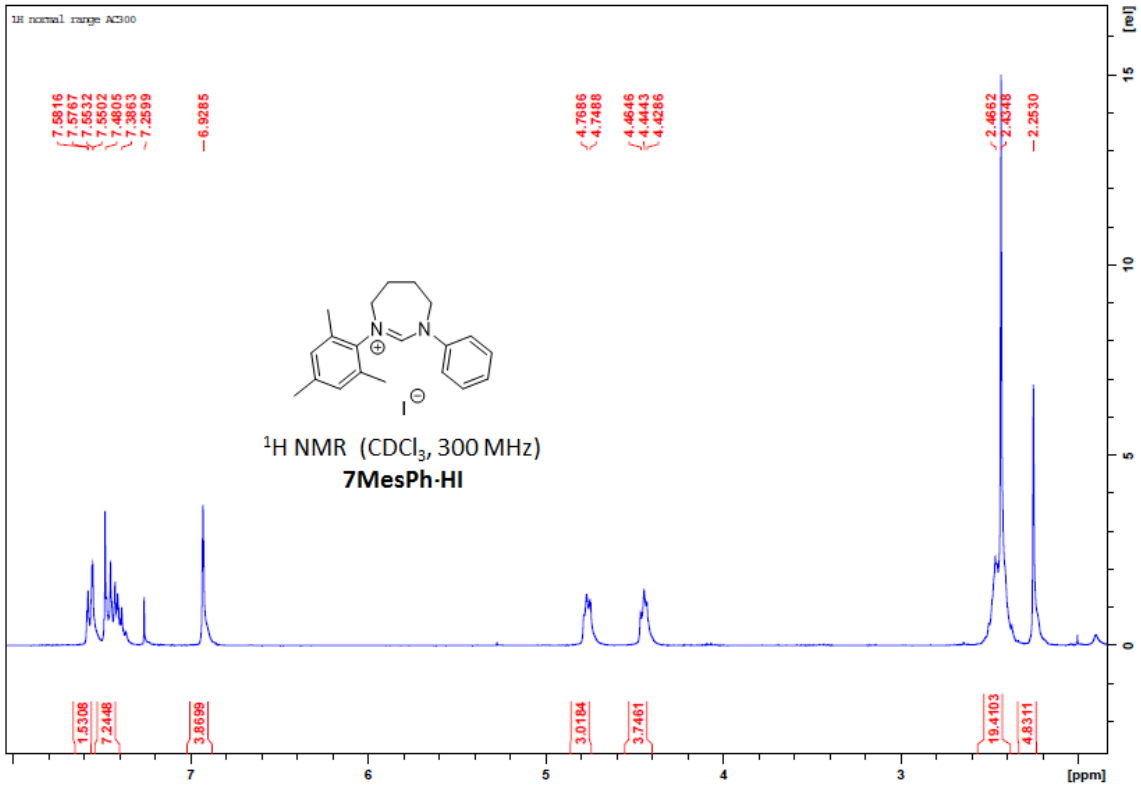
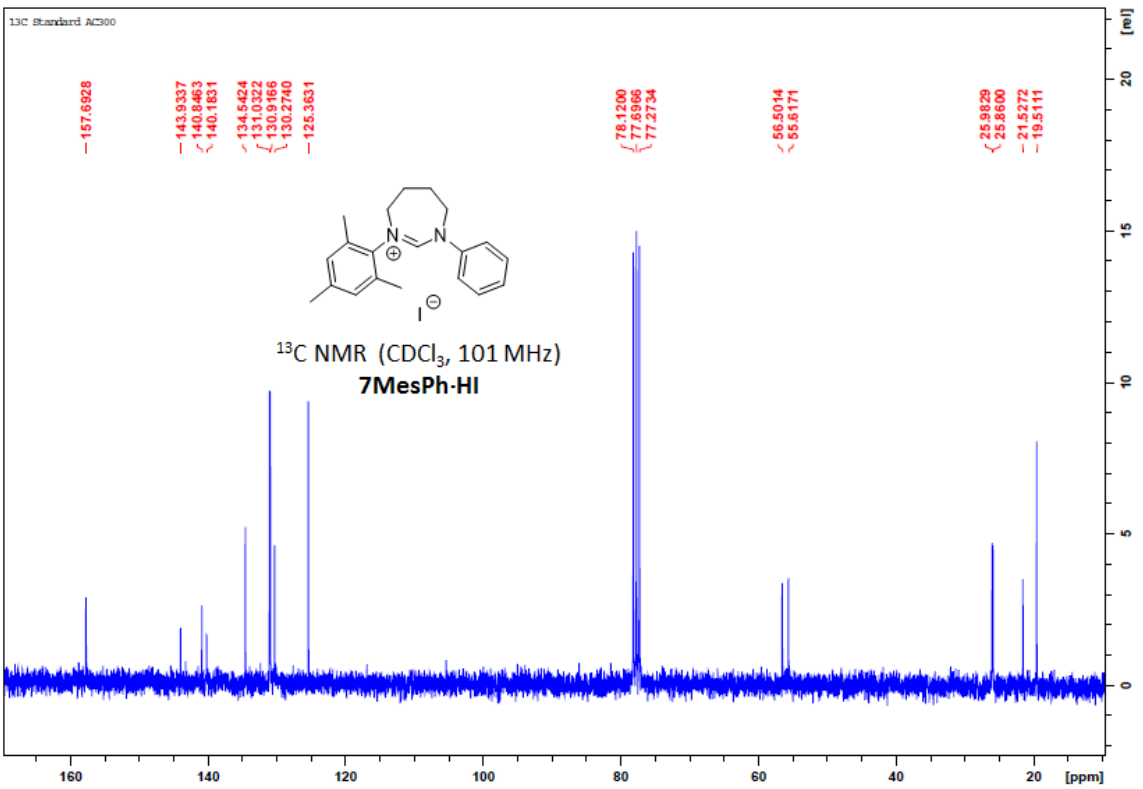
145.4794
141.1325
139.9654
139.5043
134.3442
131.6577
131.0104
126.0460
77.9490
77.4407
57.1684
55.9279
29.5325
26.3192
25.6046
25.5087
24.9343
21.5961
18.7550
[rel]
[ppm]
^{13}C NMR (CDCl$_3$, 126 MHz)
7PrMes·HI



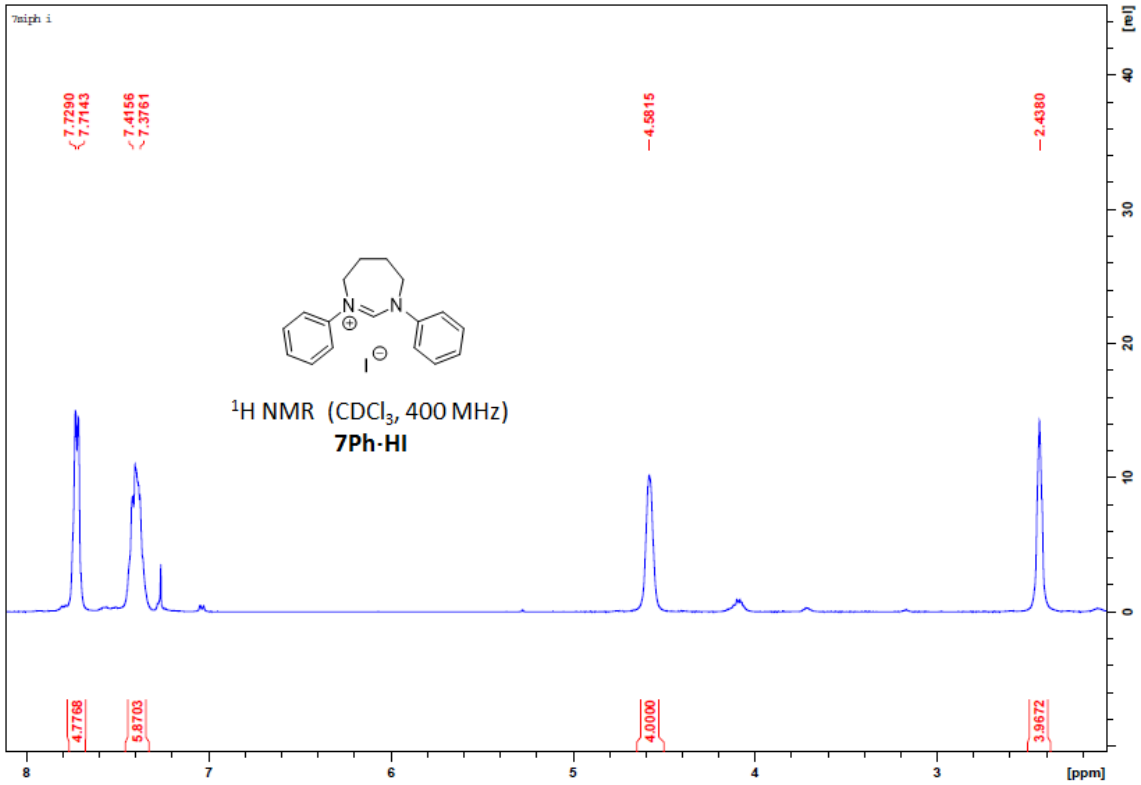
^{1}H NMR ($CDCl_3$, 300 MHz)

7MesPh·HI

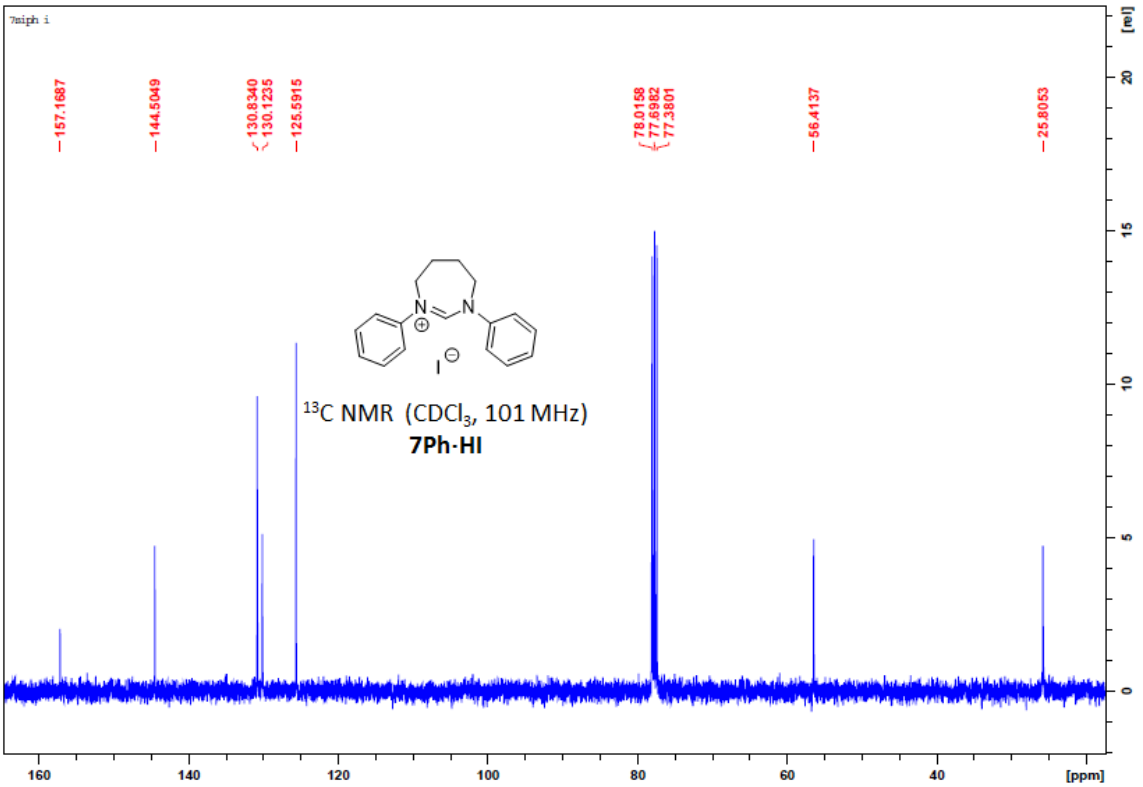


^{13}C NMR ($CDCl_3$, 101 MHz)

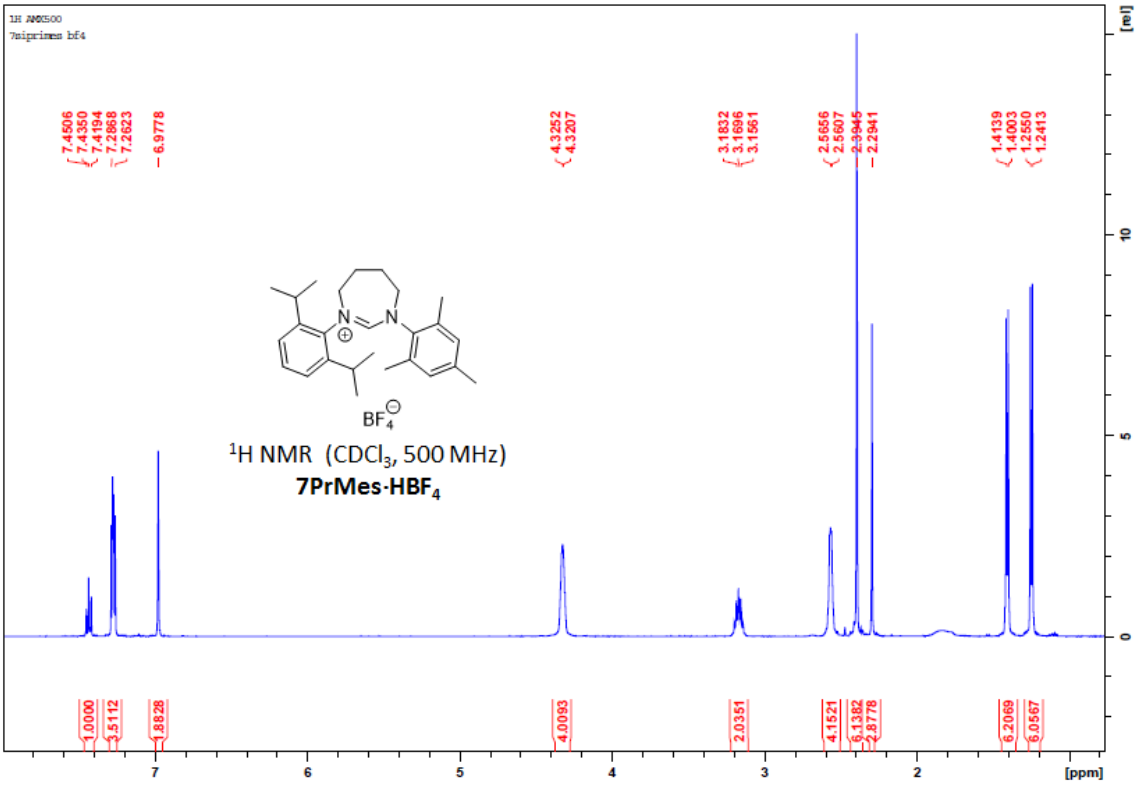
7MesPh·HI



^{1}H NMR ($CDCl_3$, 400 MHz)
7Ph·HI

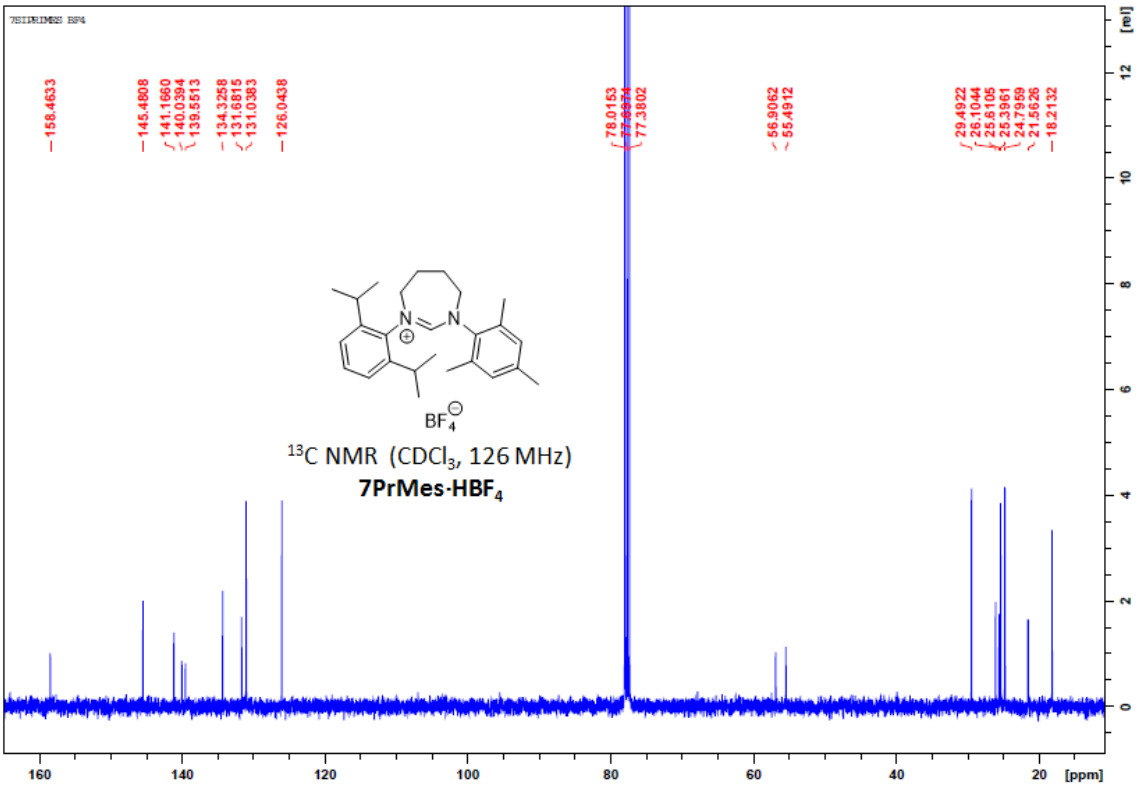


^{13}C NMR ($CDCl_3$, 101 MHz)
7Ph·HI



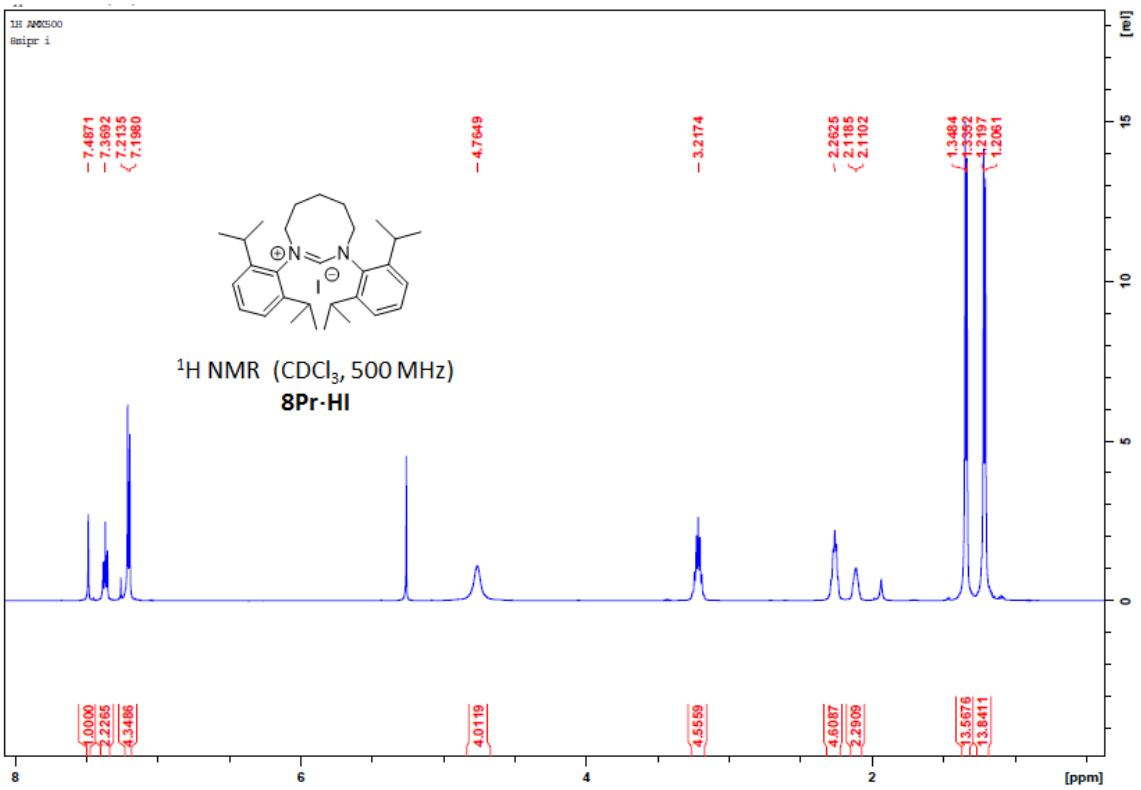
^{1}H NMR ($CDCl_3$, 500 MHz)

7PrMes·HBF$_4$



^{13}C NMR ($CDCl_3$, 126 MHz)

7PrMes·HBF$_4$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8mipr i
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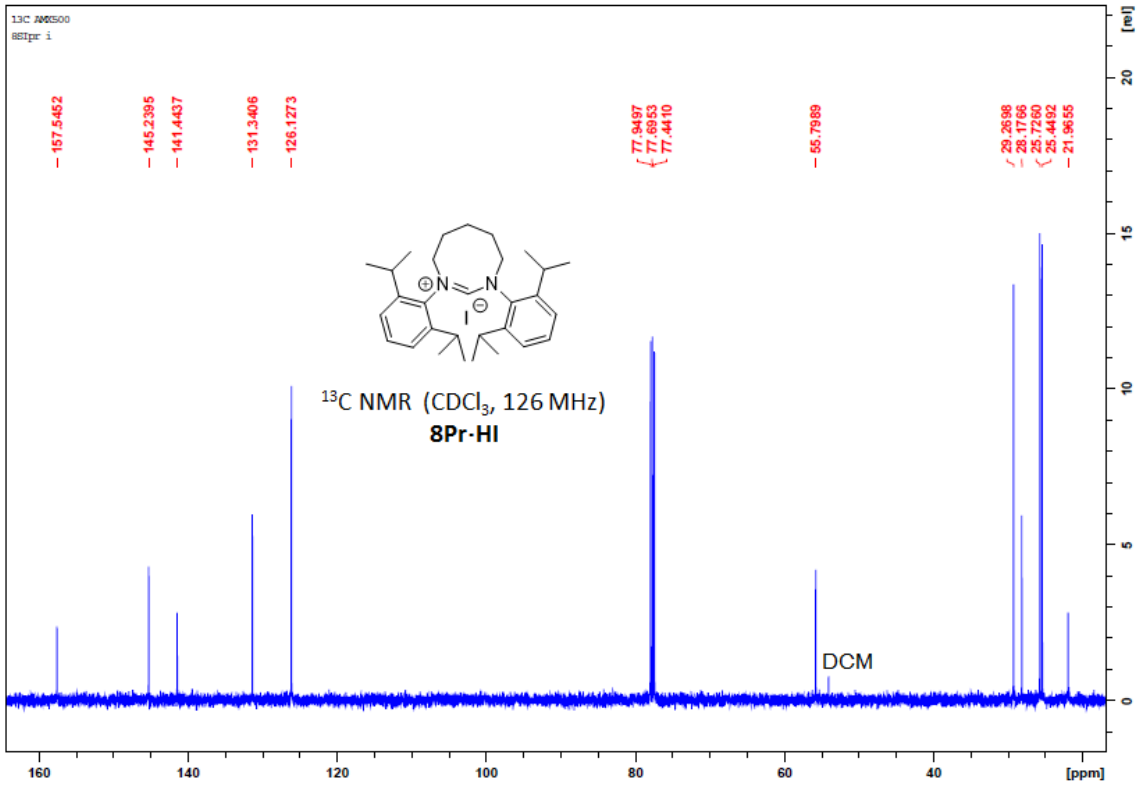
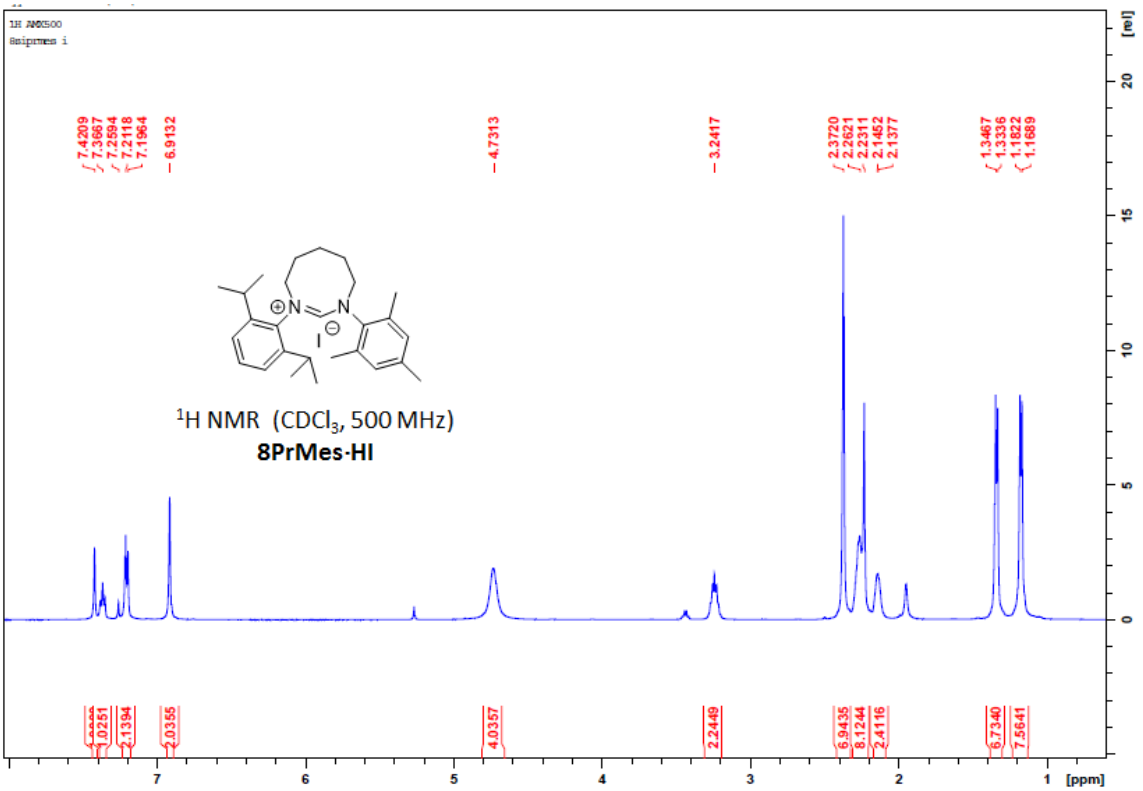
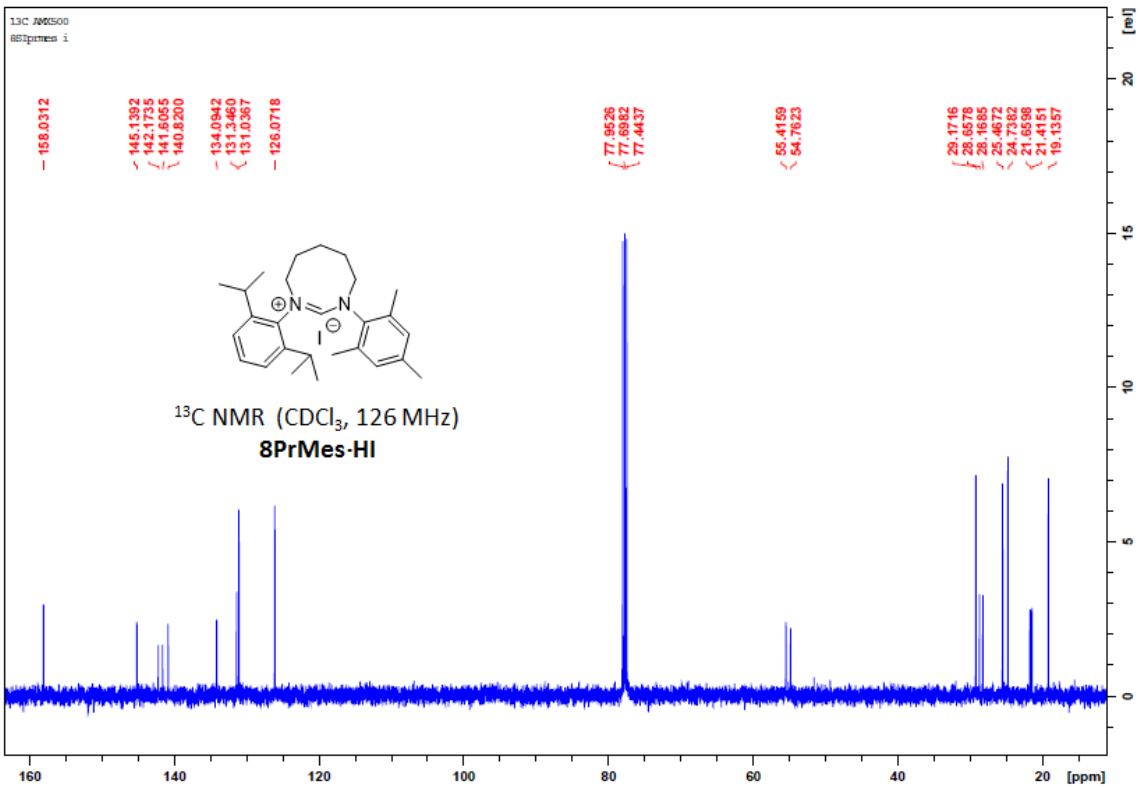
7.3692
7.2135
7.1980
4.7649
3.2174
2.2625
2.1185
2.1102
1.3484
1.3352
1.2197
1.2061
1.0000
2.2265
3.3486
4.0119
4.5559
4.6087
2.2909
13.5676
13.8411
[rel]
[ppm]
^{1}H NMR (CDCl$_3$, 500 MHz)
8Pr·HI


13C AM500
8SIpr i
157.5452
145.2395
141.4437
131.3406
126.1273
77.9497
77.6953
77.4410
55.7989
29.2698
28.1766
25.7260
25.4492
21.9655
DCM
[rel]
[ppm]
^{13}C NMR (CDCl$_3$, 126 MHz)
8Pr·HI



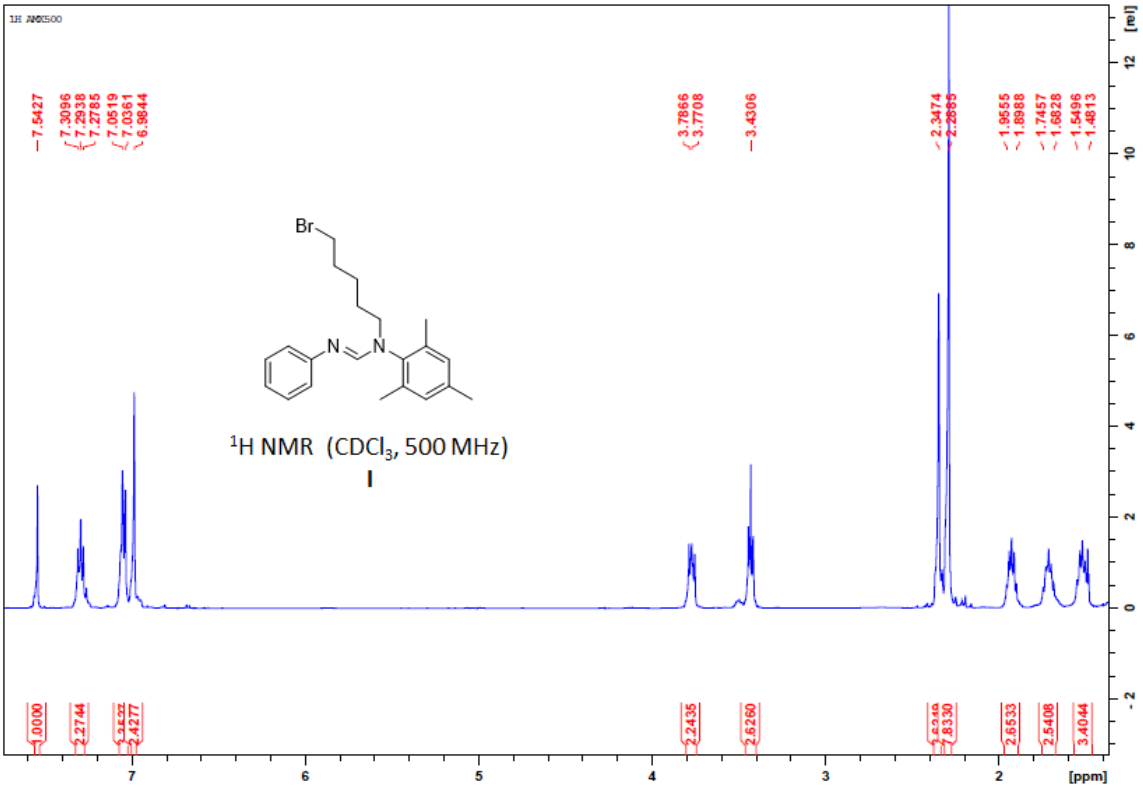
^{1}H NMR ($CDCl_3$, 500 MHz)

8PrMes·HI



^{13}C NMR ($CDCl_3$, 126 MHz)

8PrMes·HI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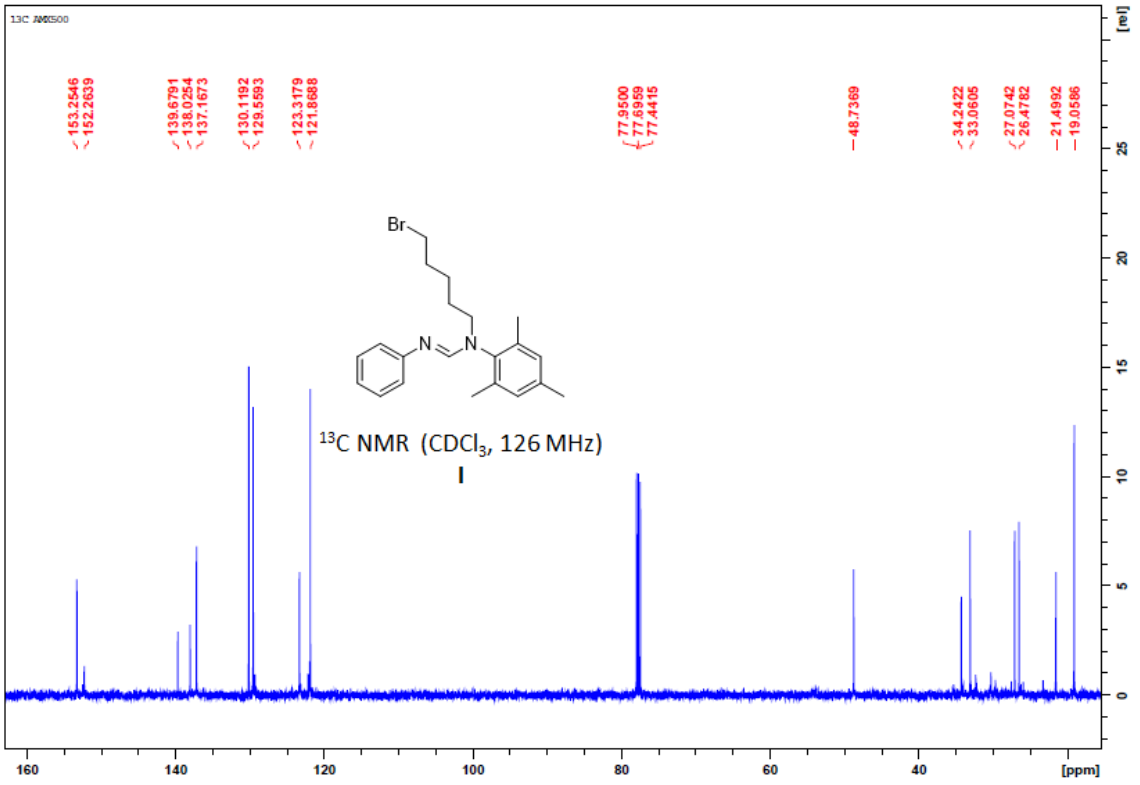
7.3096
7.2938
7.2785
7.0519
7.0361
6.9844
3.7866
3.7708
3.4306
2.3474
2.2885
1.9555
1.8988
1.7457
1.6828
1.5496
1.4813
Br
N
N
1H NMR (CDCl3, 500 MHz)
I
1.0000
2.2744
2.4277
2.2435
2.6260
7.8330
2.6533
2.5406
3.4044
[ppm]
[m]


13C AM500
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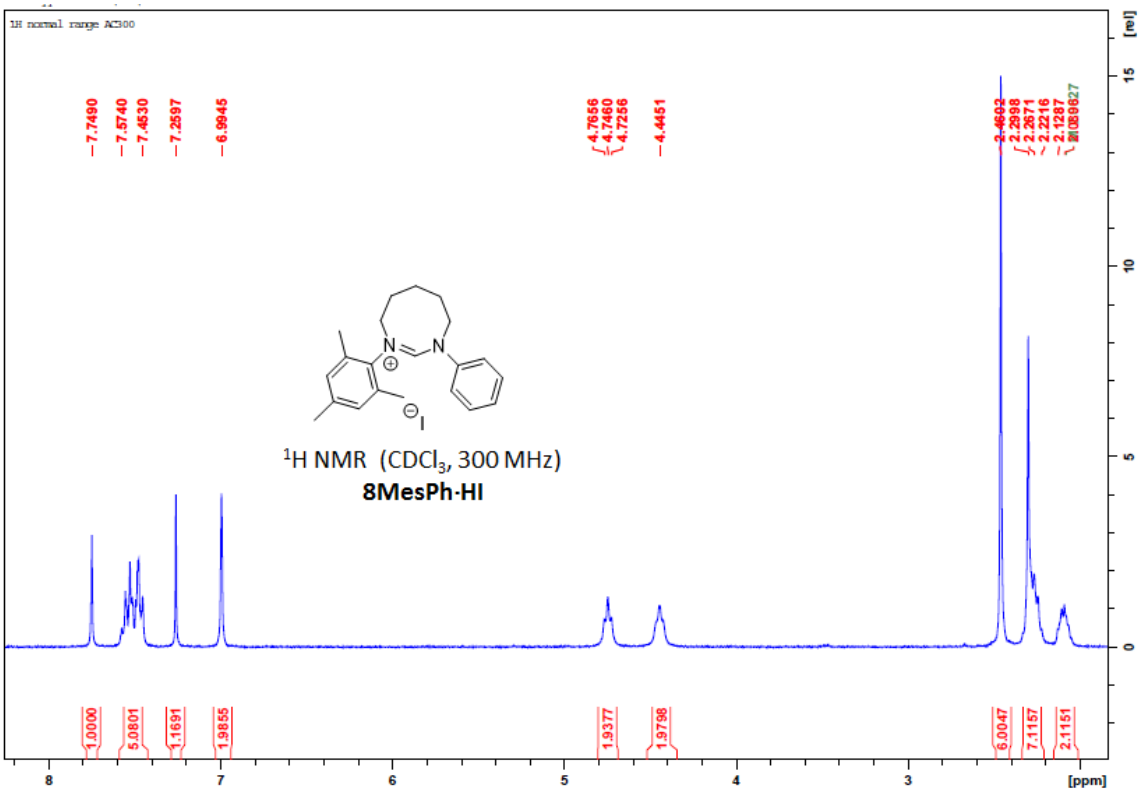
152.2639
139.6791
138.0254
137.1673
130.1192
129.5593
123.3179
121.8688
77.9500
77.6959
77.4415
48.7369
34.2422
33.0605
27.0742
26.4782
21.4992
19.0586
Br
N
N
13C NMR (CDCl3, 126 MHz)
I
[ppm]
[m]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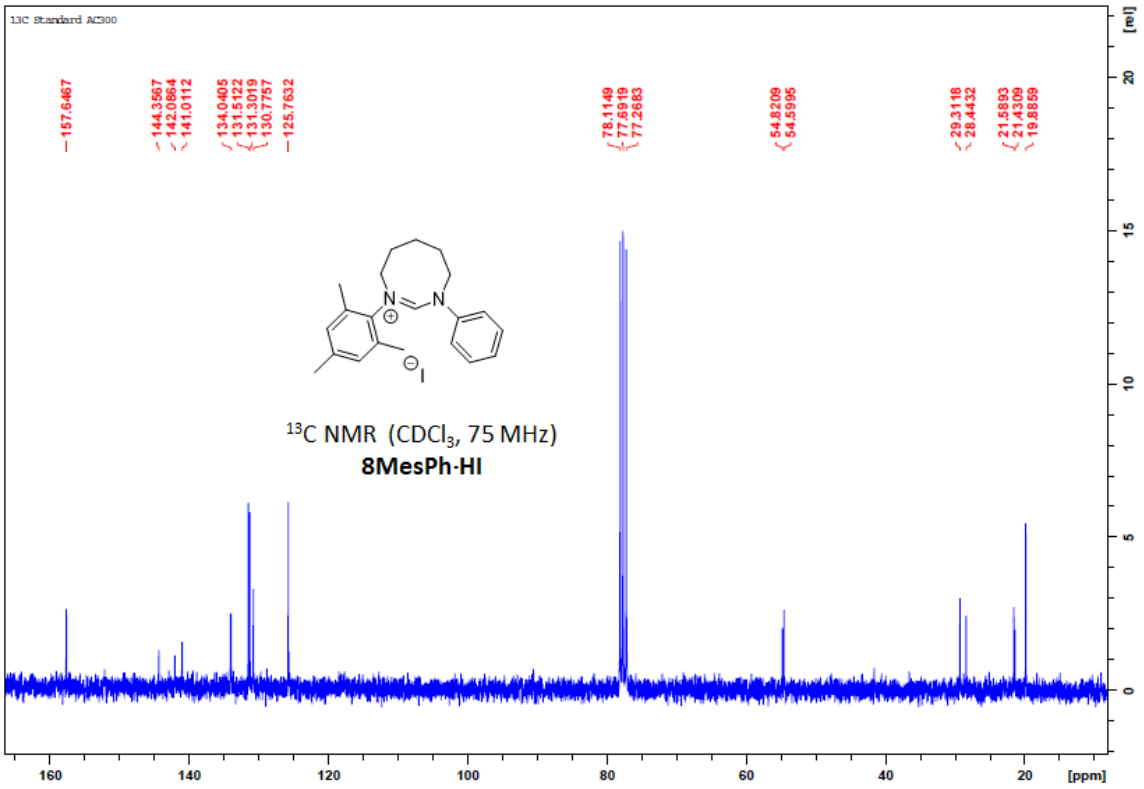
7.4530
7.2597
6.9945
4.7656
4.7460
4.7256
4.4451
2.4603
2.2998
2.2671
2.2216
2.1287
2.0069
1.0000
5.0801
1.1691
1.9855
1.9377
1.9798
6.0047
7.1157
2.1151
[rel]
[ppm]
^{1}H NMR (CDCl$_3$, 300 MHz)
8MesPh·HI


13C Standard AC300
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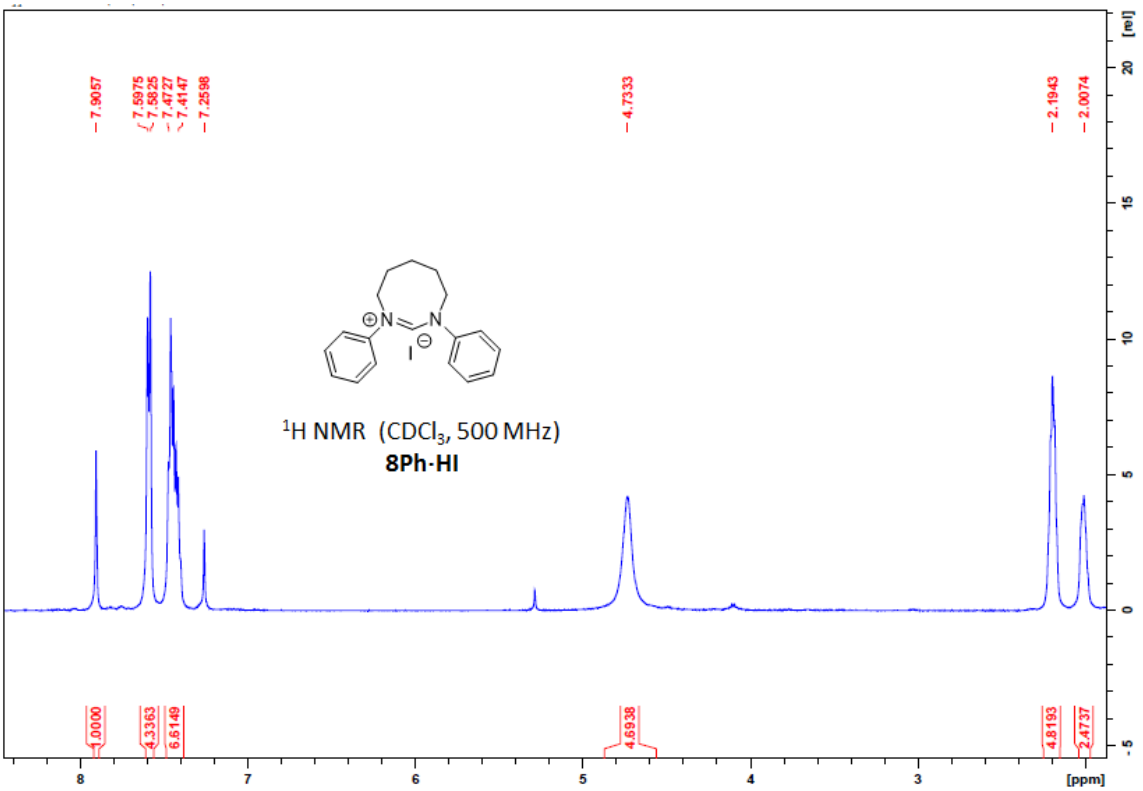
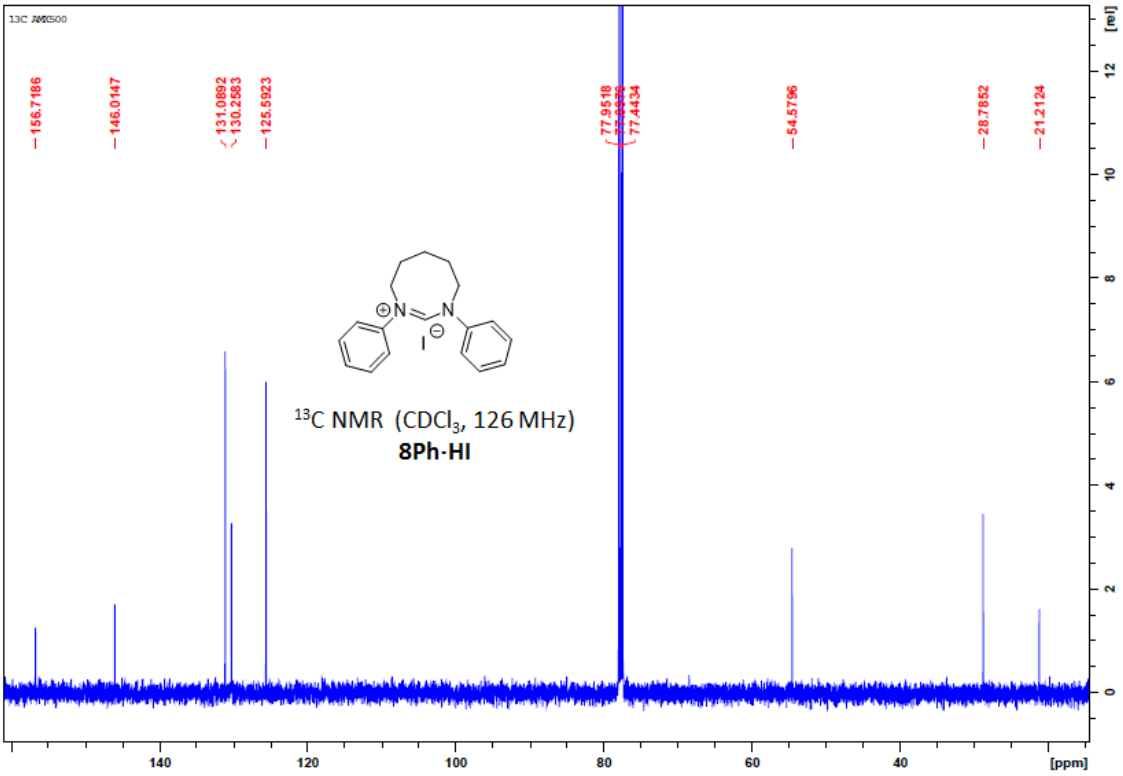
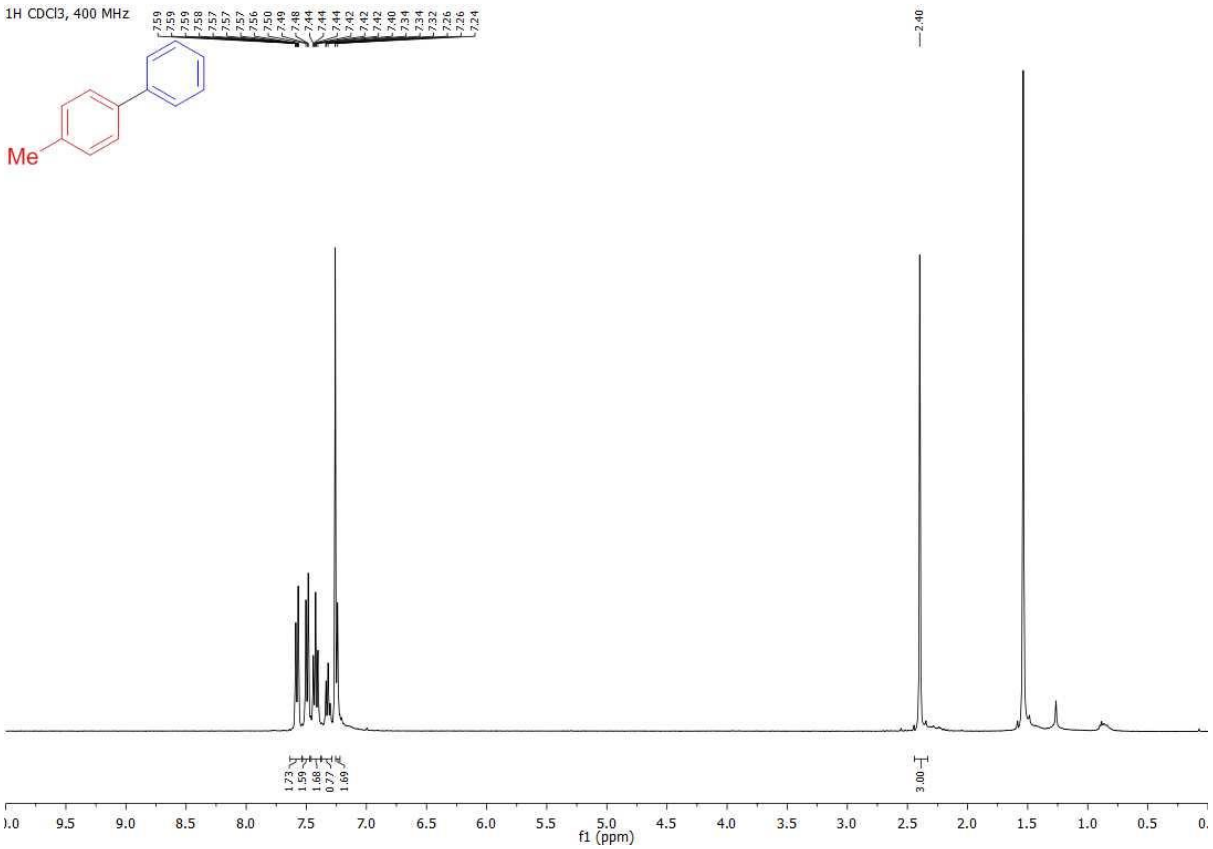
144.3567
142.0864
141.0112
134.0405
131.5122
131.3019
130.7757
125.7632
78.1149
77.6919
77.2683
54.8209
54.5995
29.3118
28.4432
21.5893
21.4309
19.8859
[rel]
[ppm]
^{13}C NMR (CDCl$_3$, 75 MHz)
8MesPh·HI



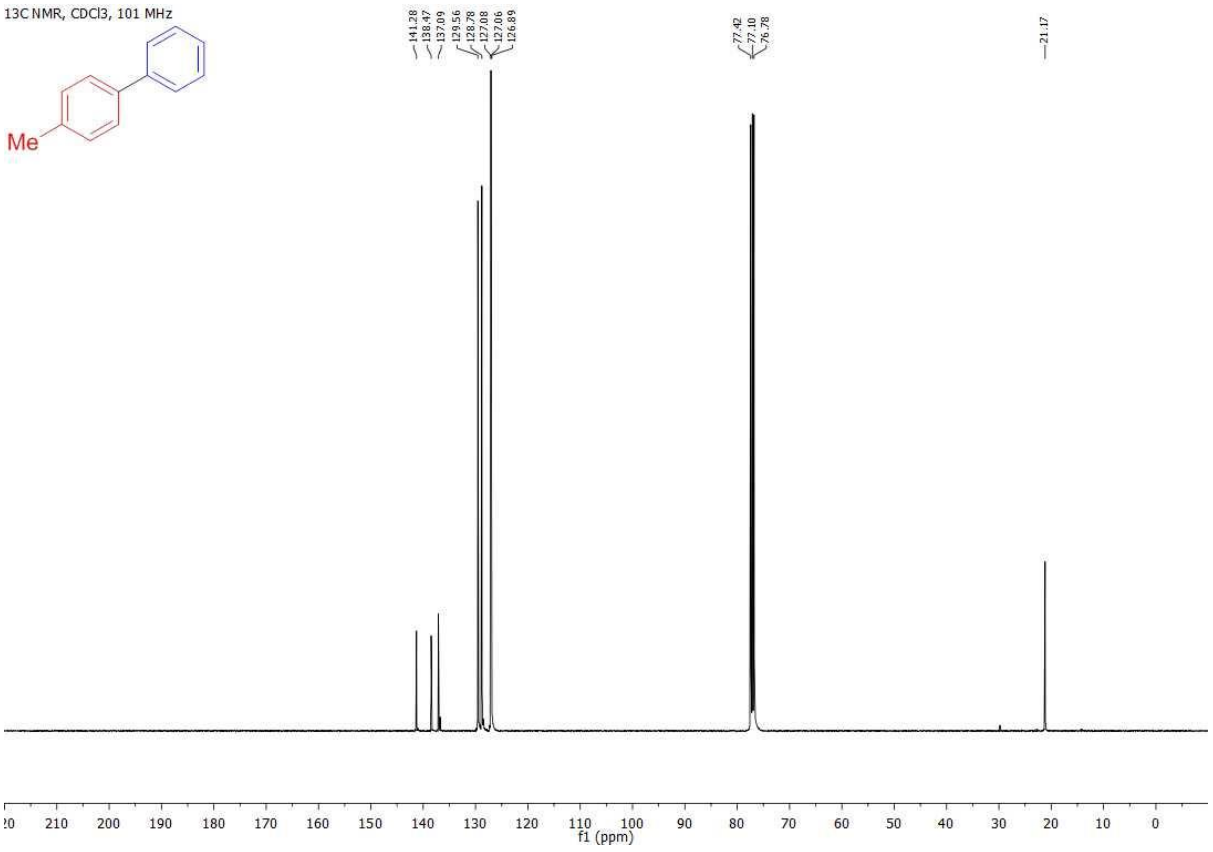
^{1}H NMR (CDCl$_3$, 500 MHz)
8Ph·HI



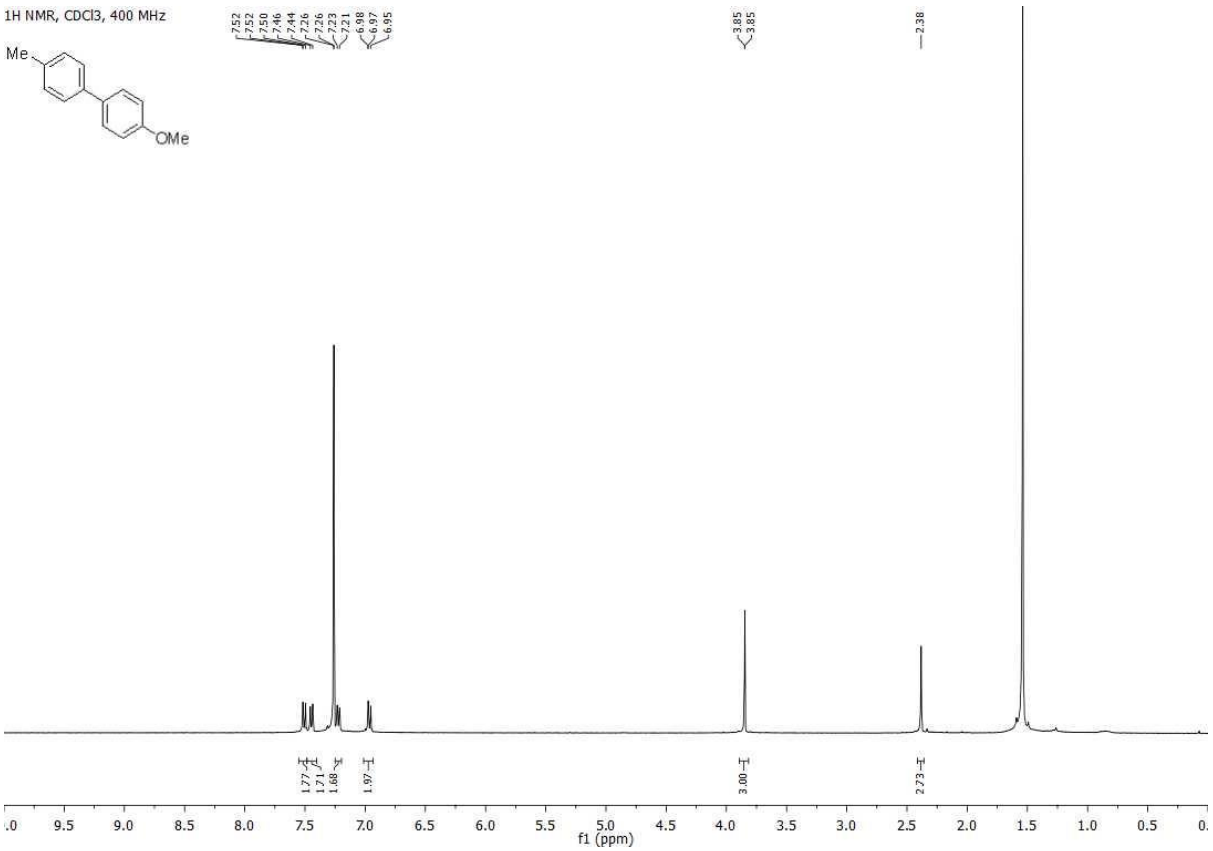
^{13}C NMR (CDCl$_3$, 126 MHz)
8Ph·HI



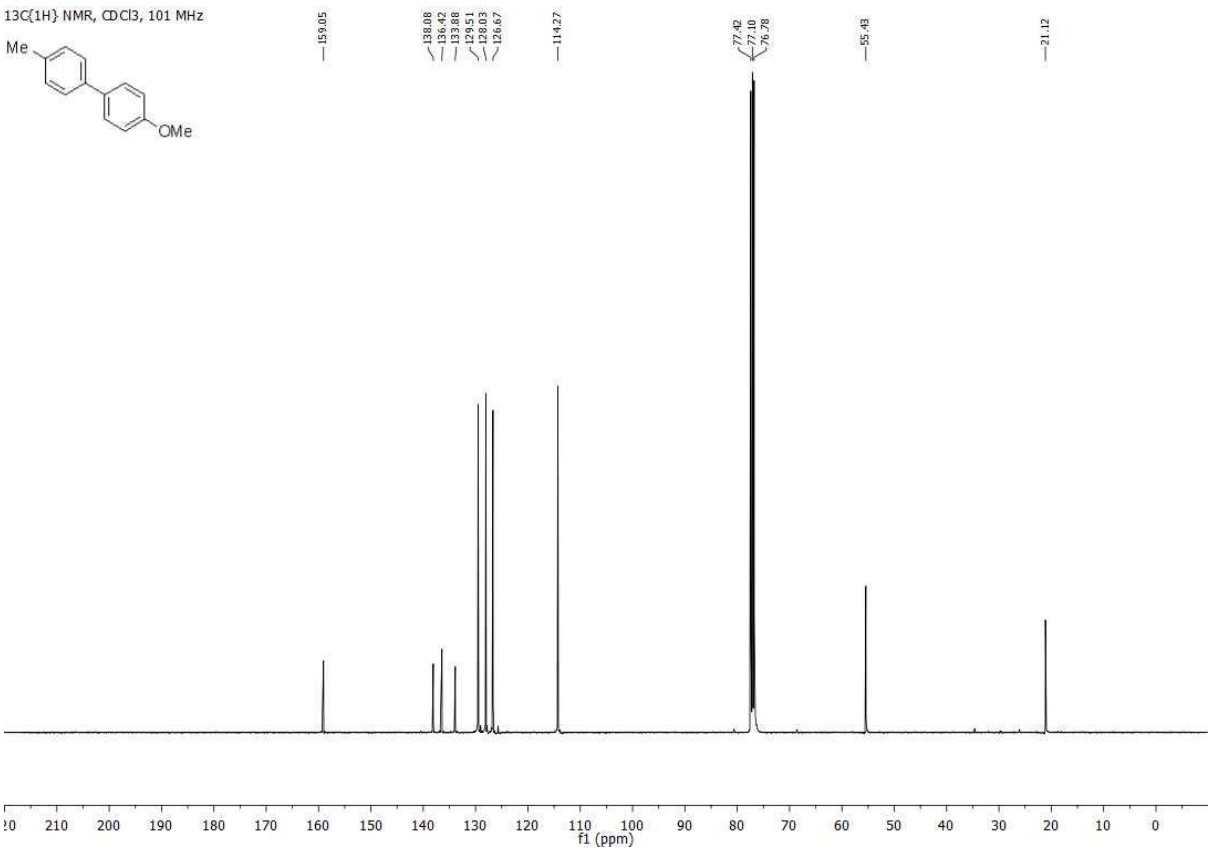
^{1}H Spectra of **3a**



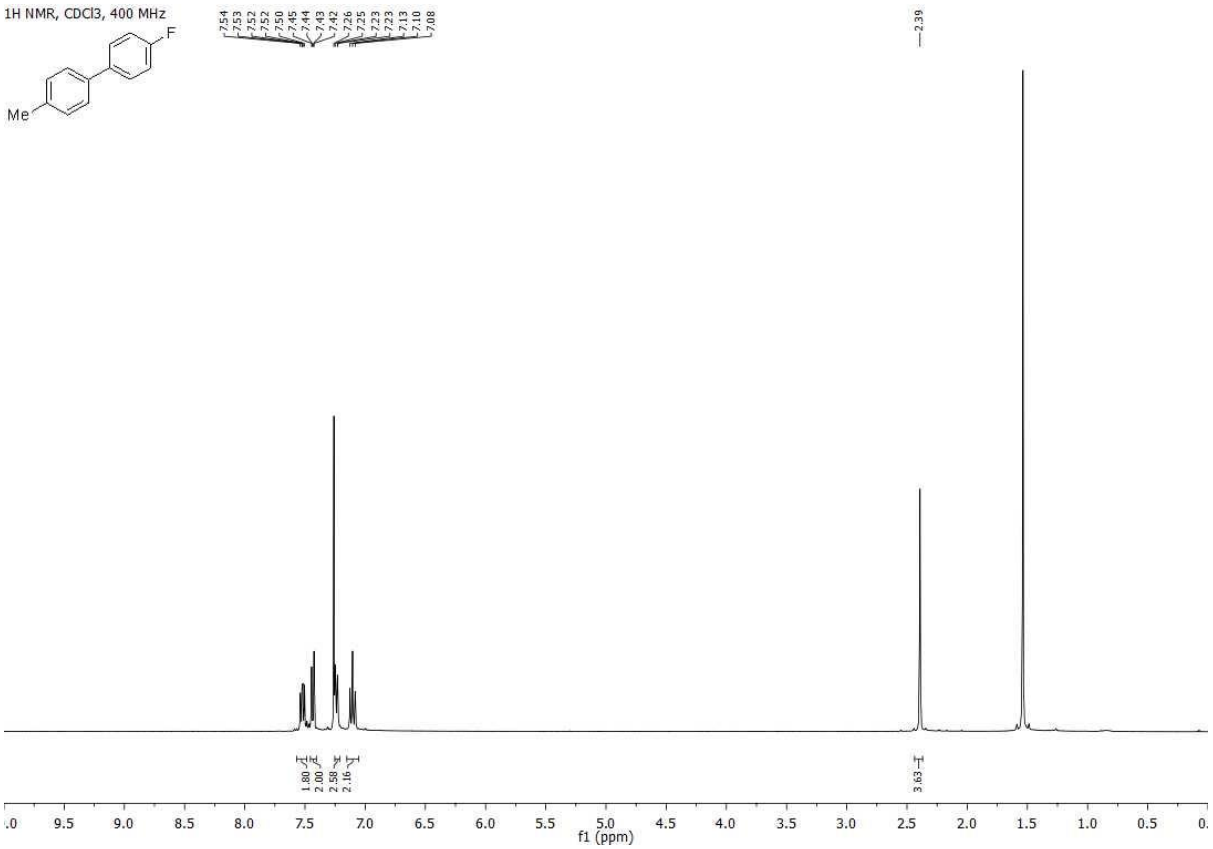
^{13}C Spectra of **3a**



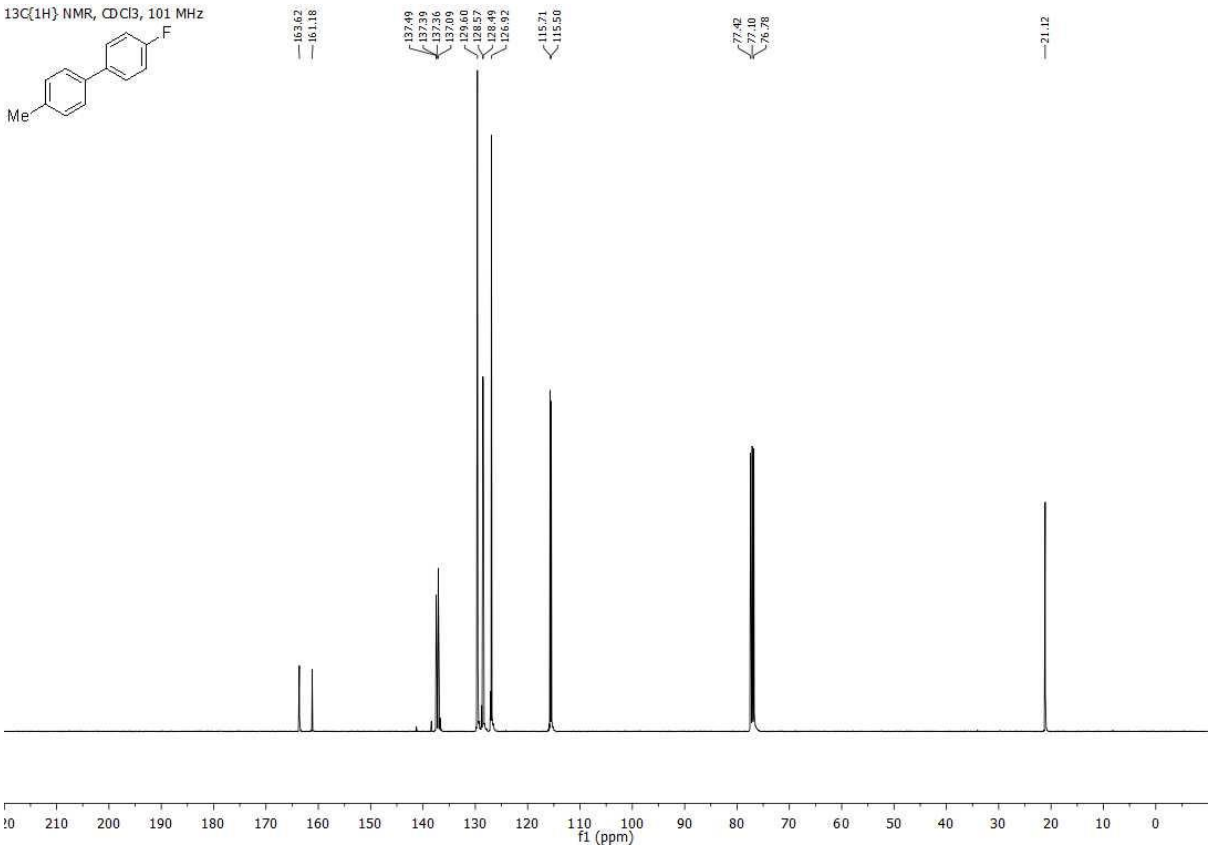
^{1}H Spectra of **3b**



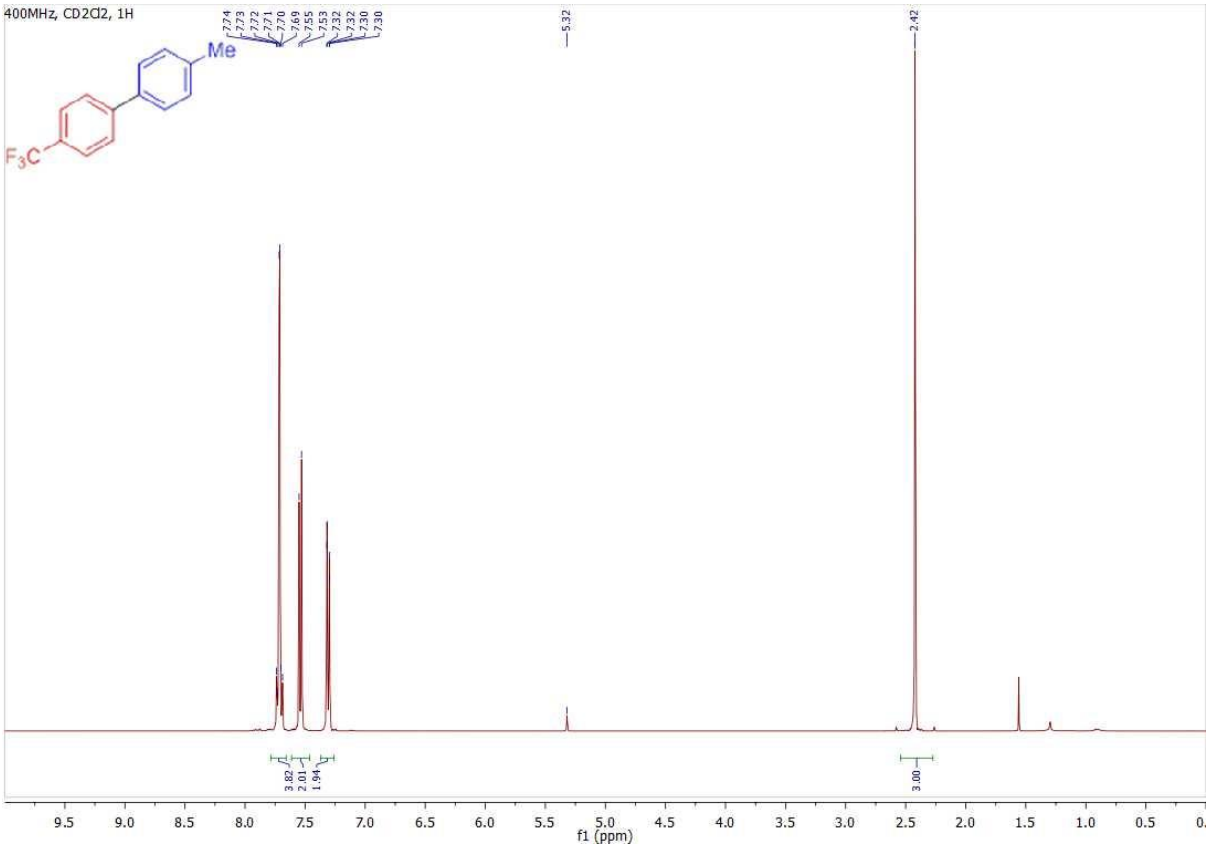
^{13}C Spectra of **3b**



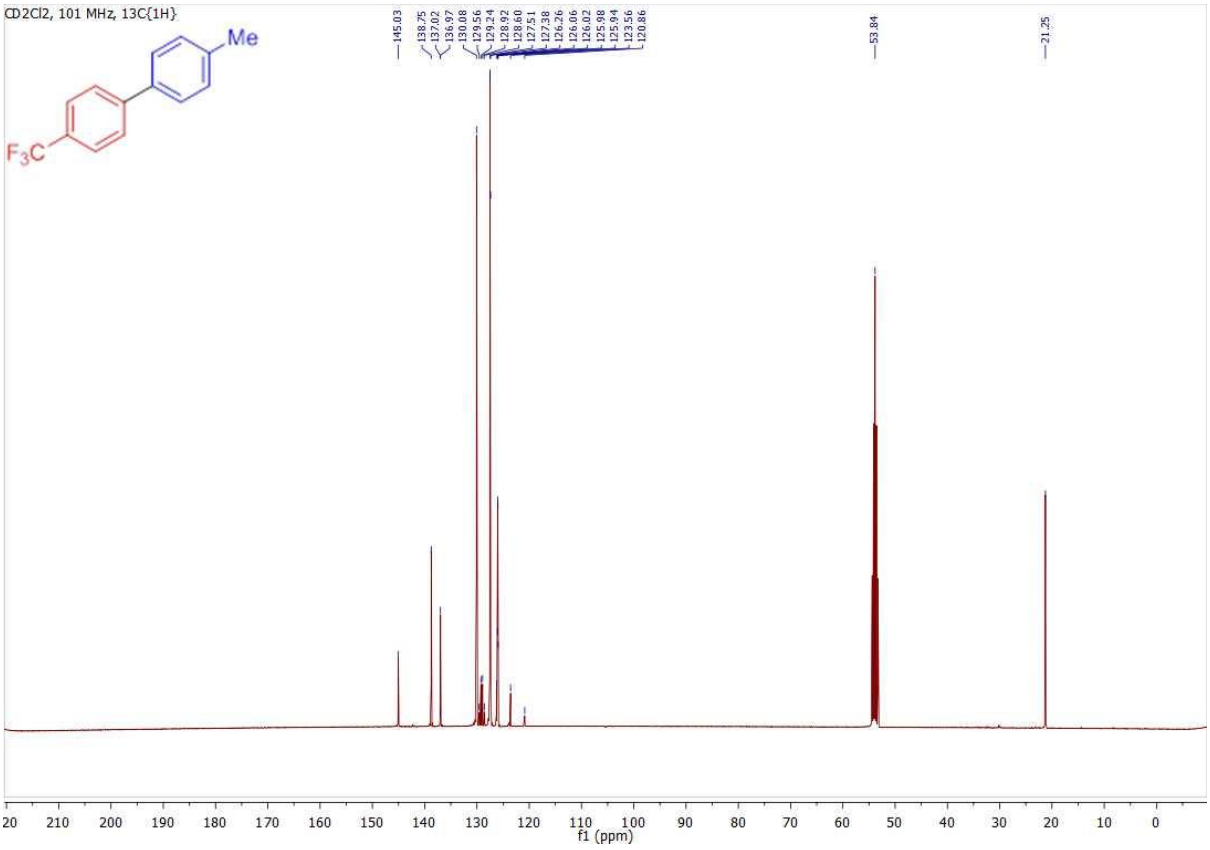
^{1}H Spectra of **3c**



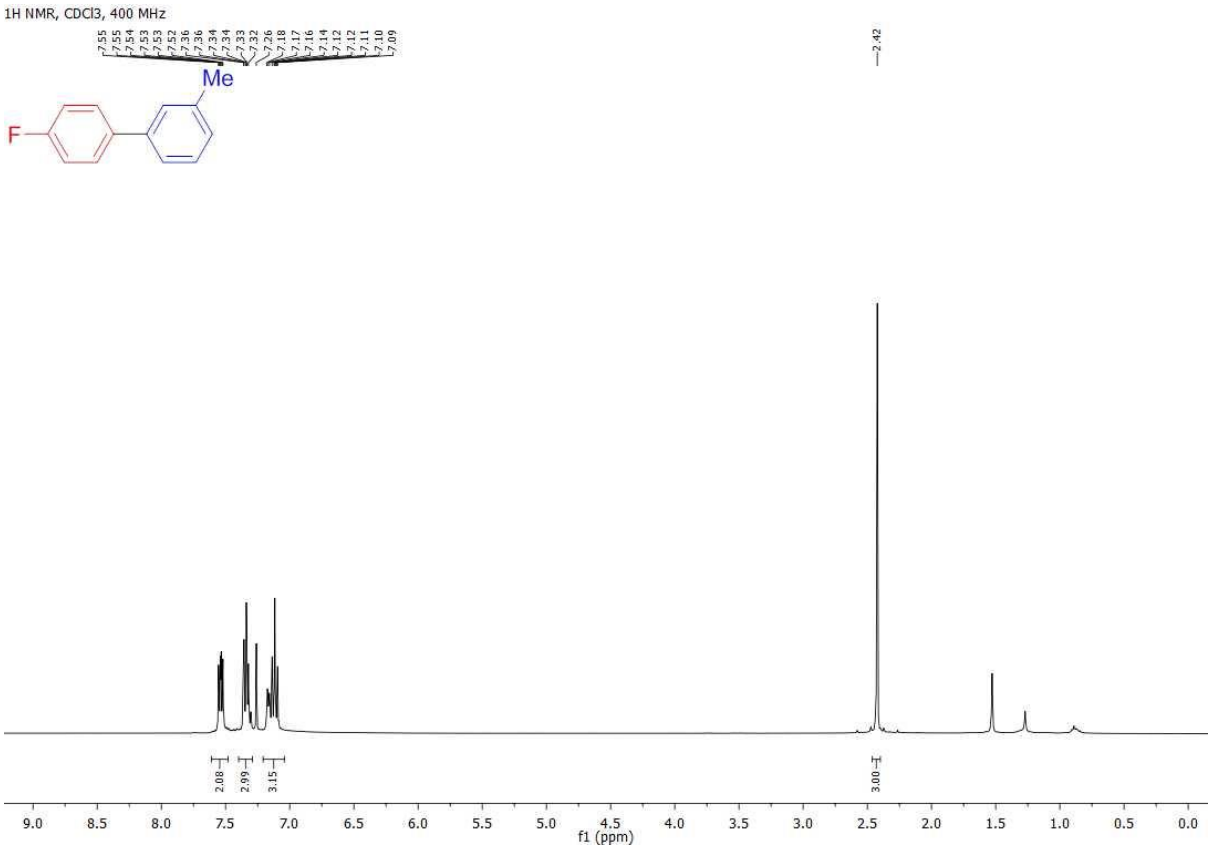
^{13}C Spectra of **3c**



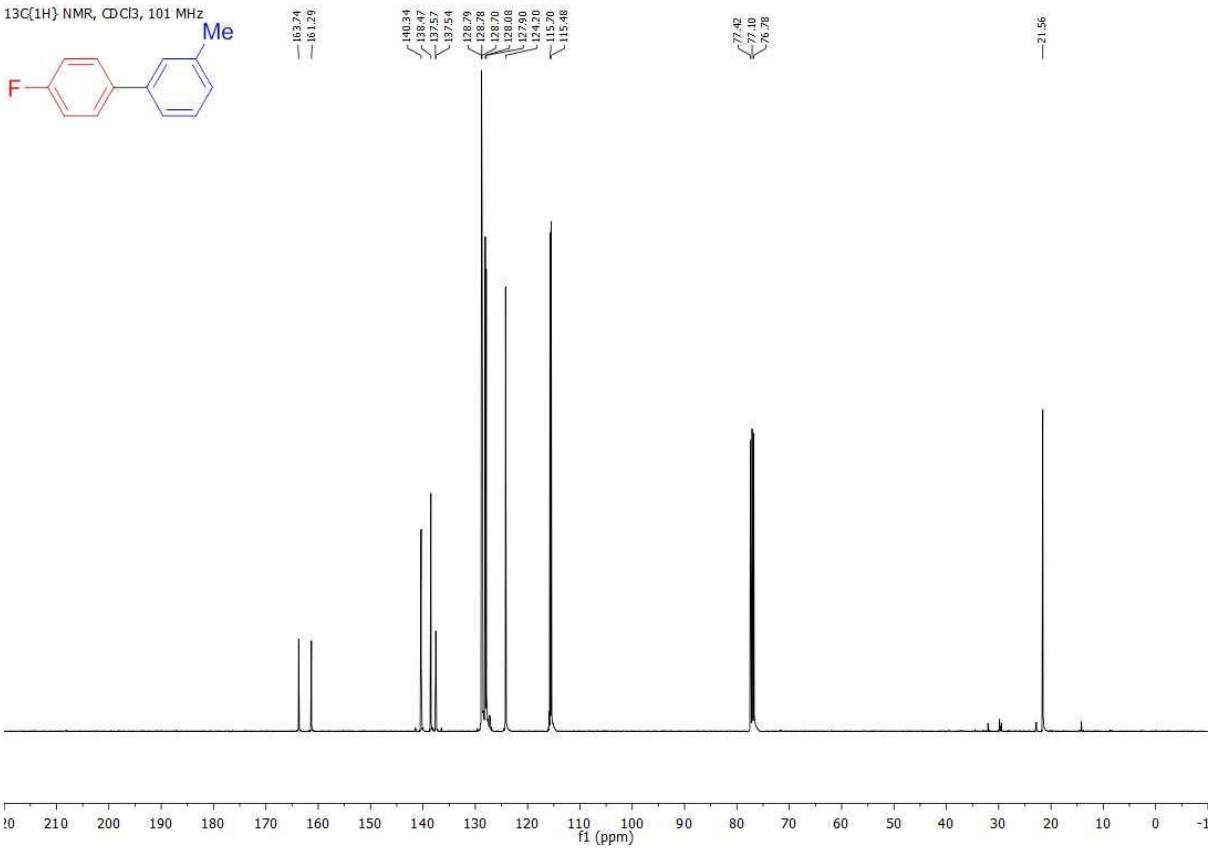
^{1}H Spectra of **3d**



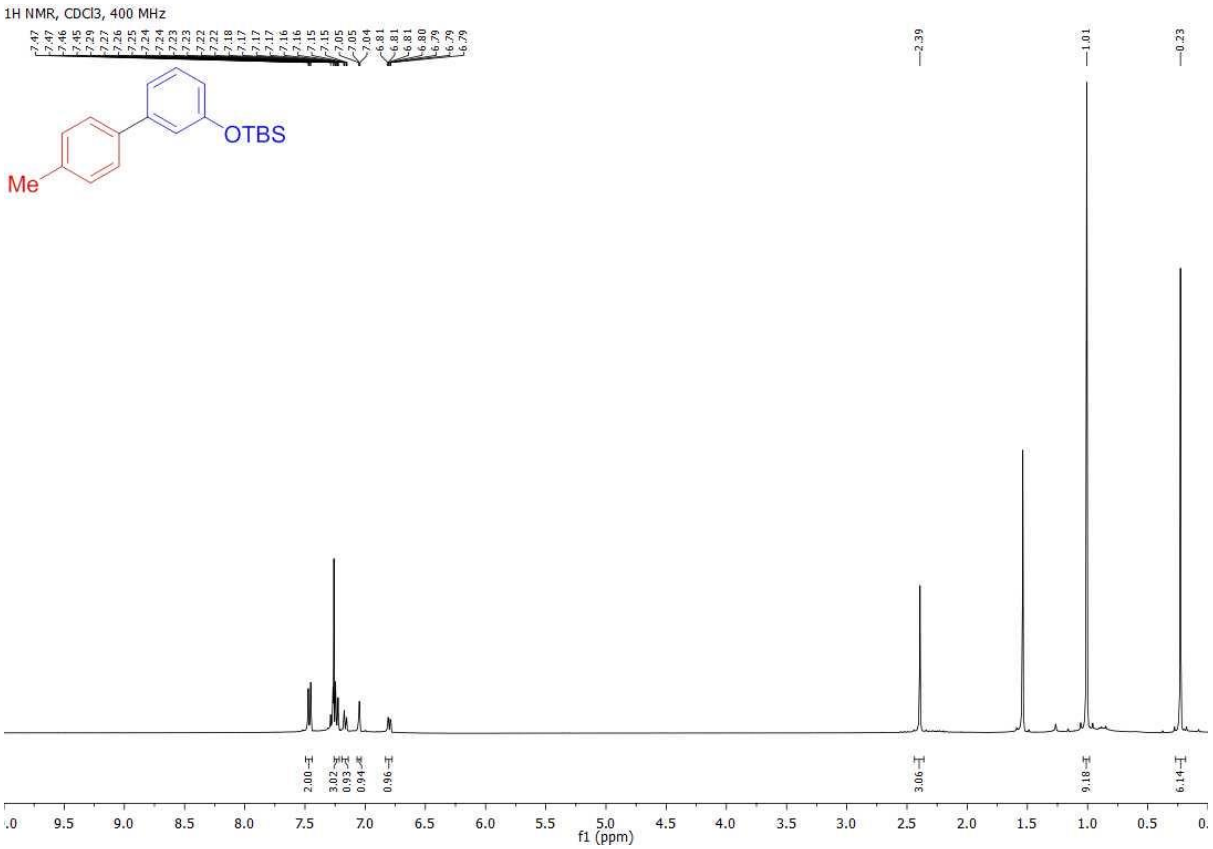
^{13}C Spectra of **3d**



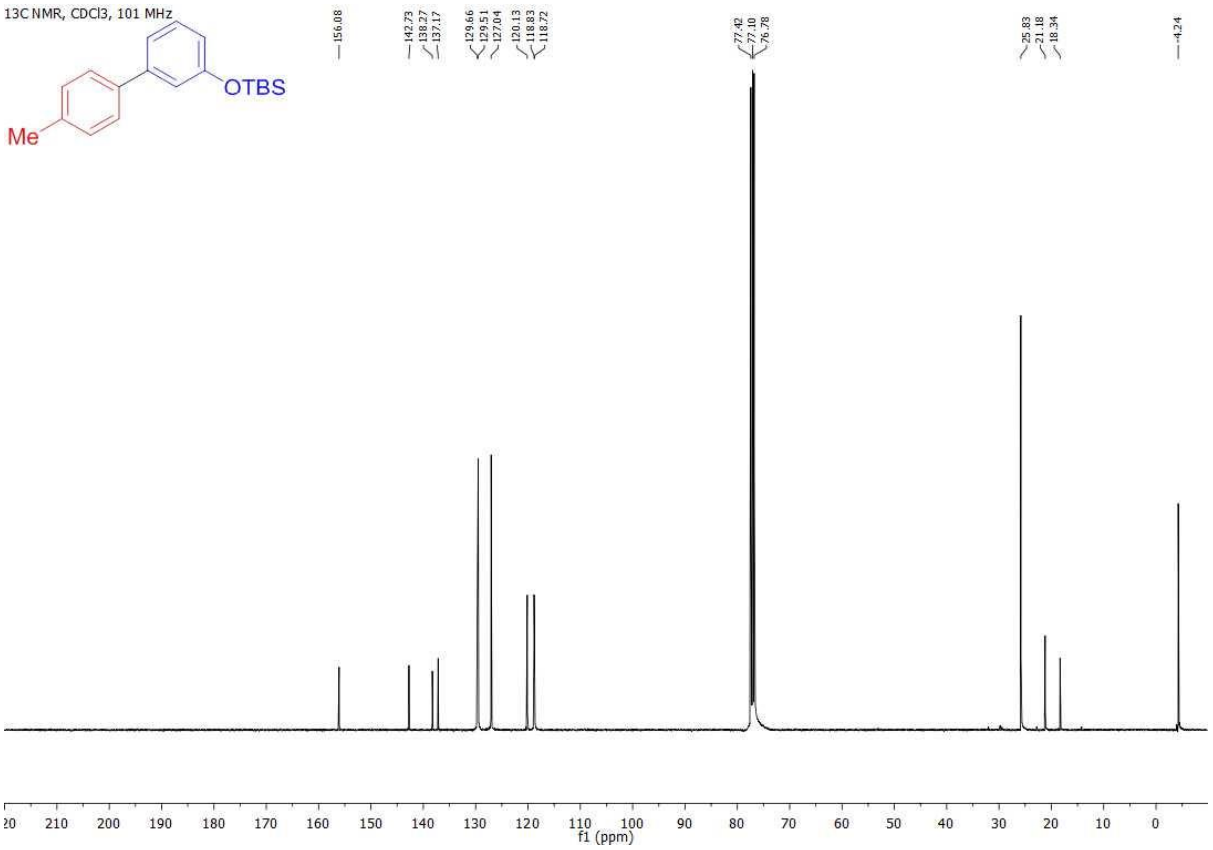
^{1}H Spectra of **3e**



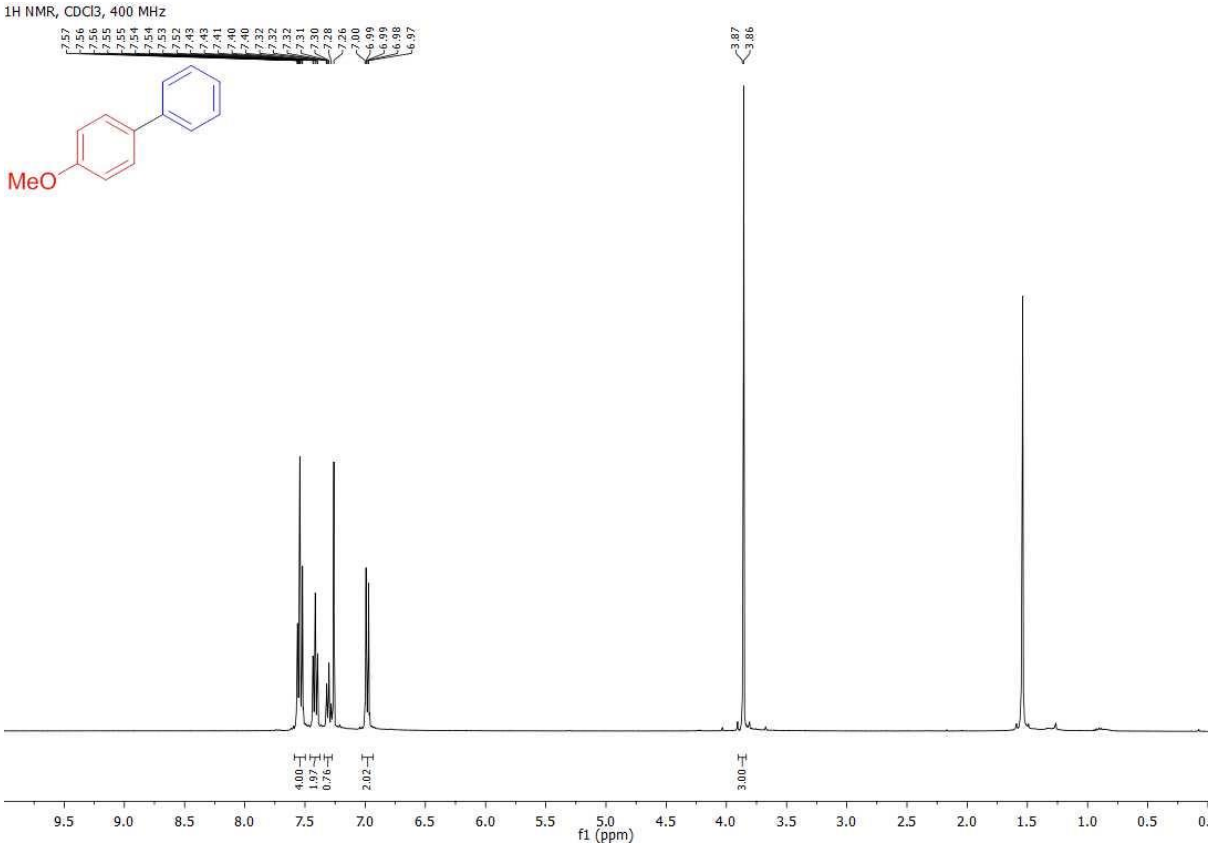
^{13}C Spectra of **3e**



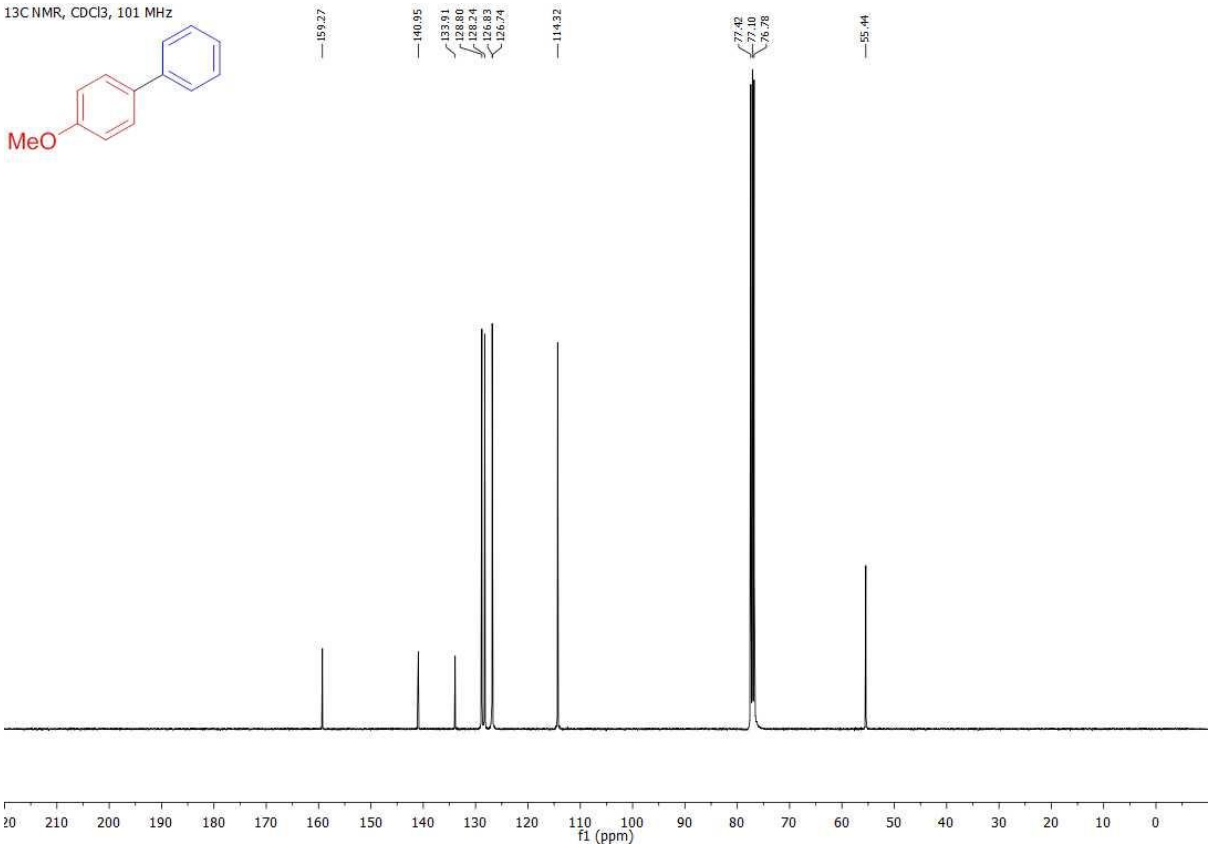
^{1}H Spectra of **3f**



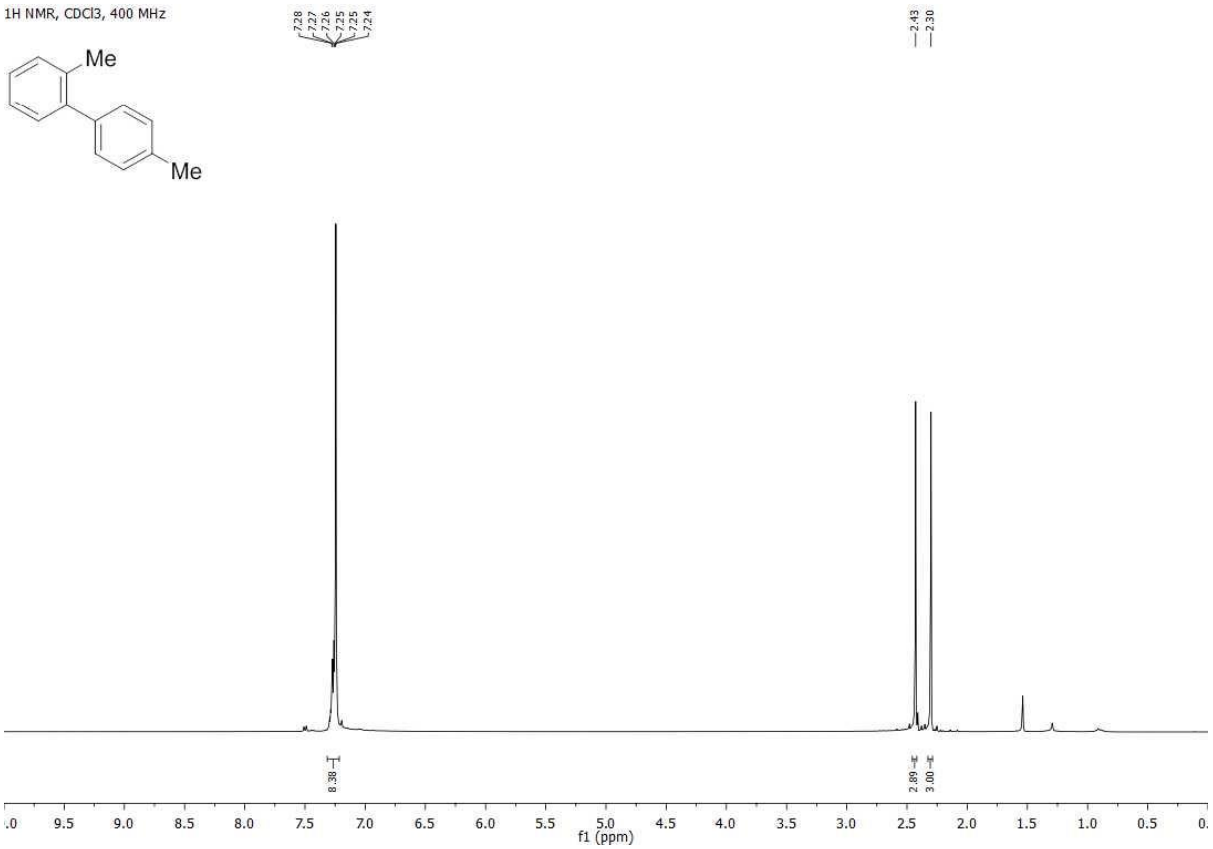
^{13}C Spectra of **3f**



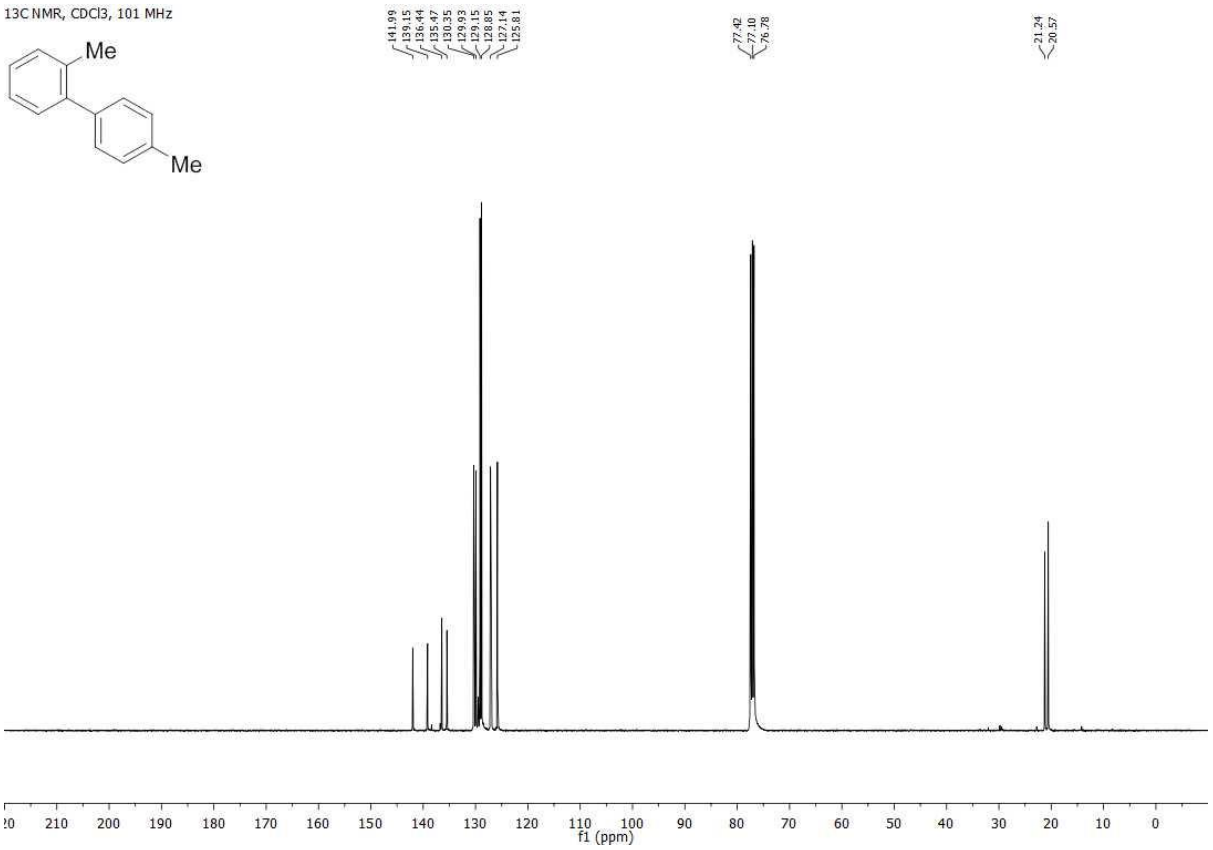
^{1}H Spectra of **3g**



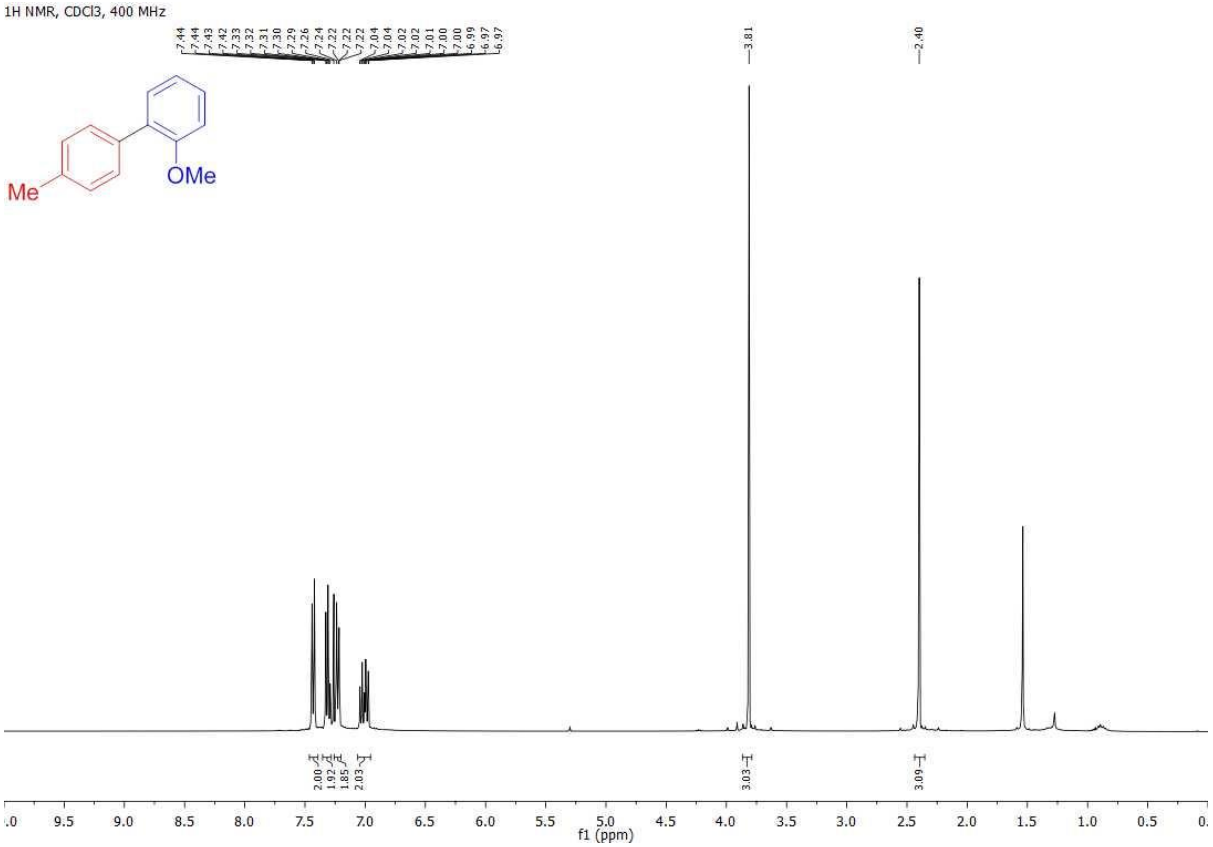
^{13}C Spectra of **3g**



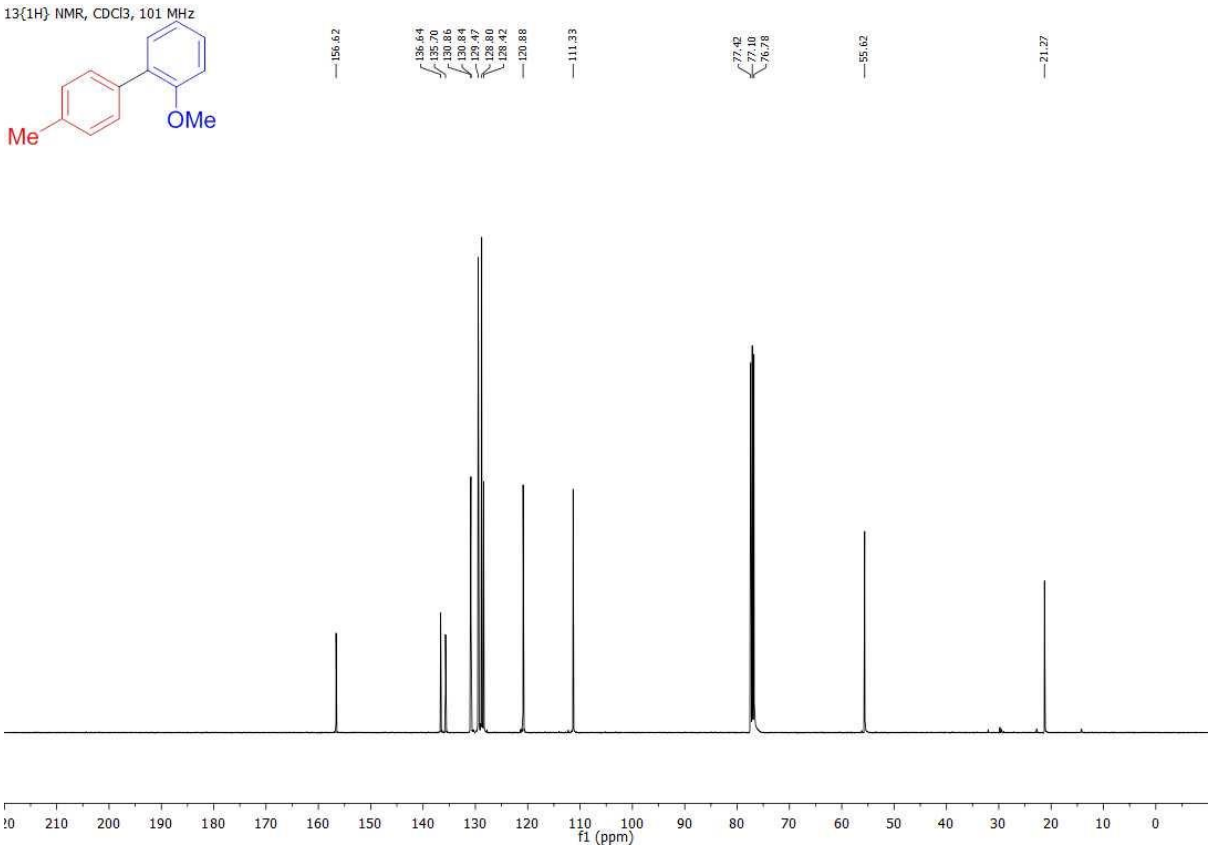
^{1}H Spectra of **3h**



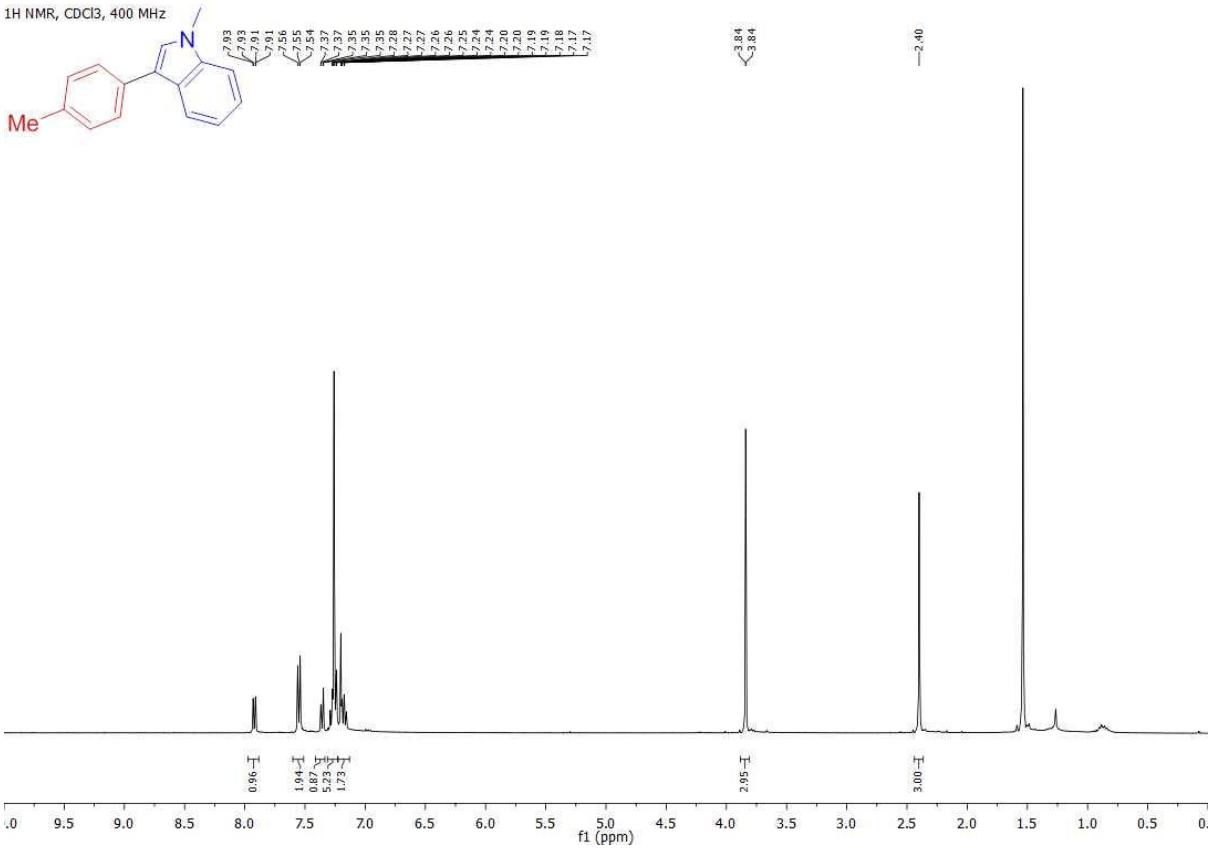
^{13}C Spectra of **3h**



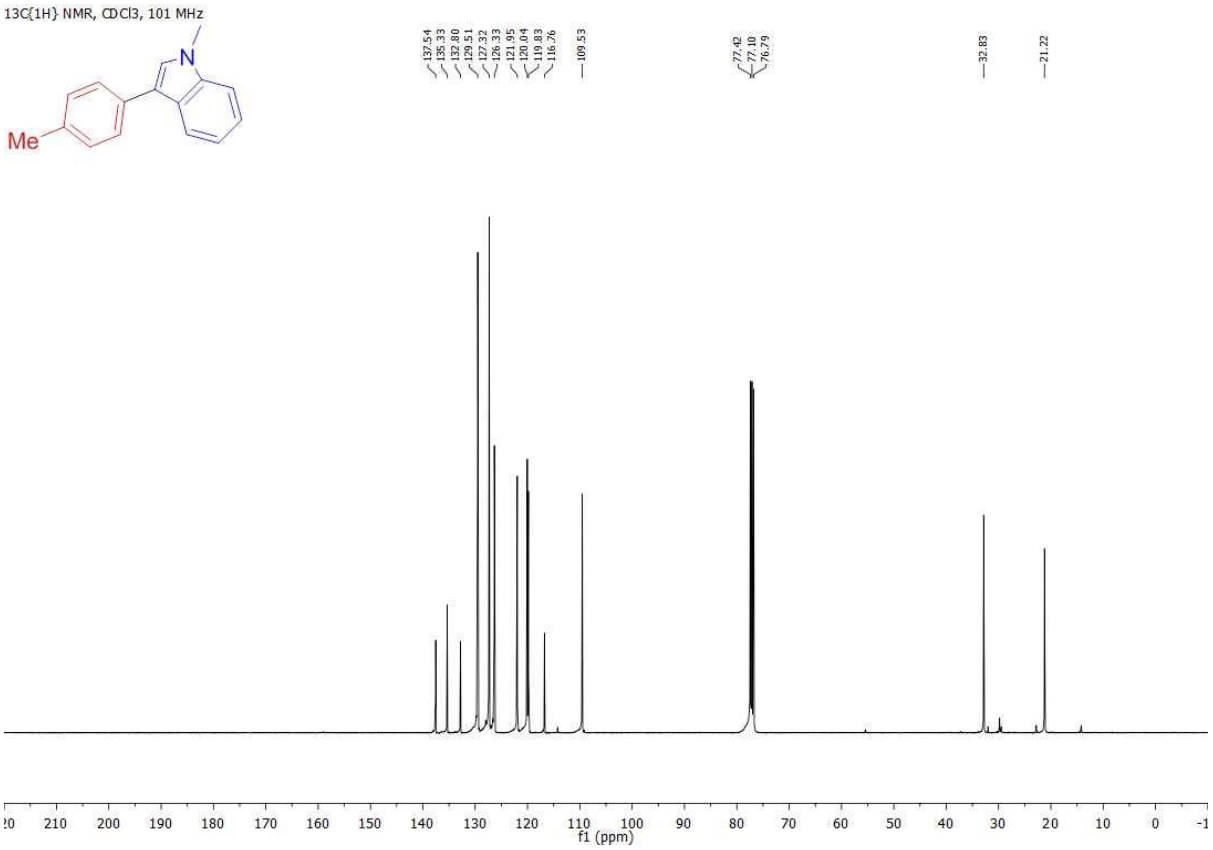
^{1}H Spectra of **3i**



^{13}C Spectra of **3i**



^{1}H Spectra of **3k**



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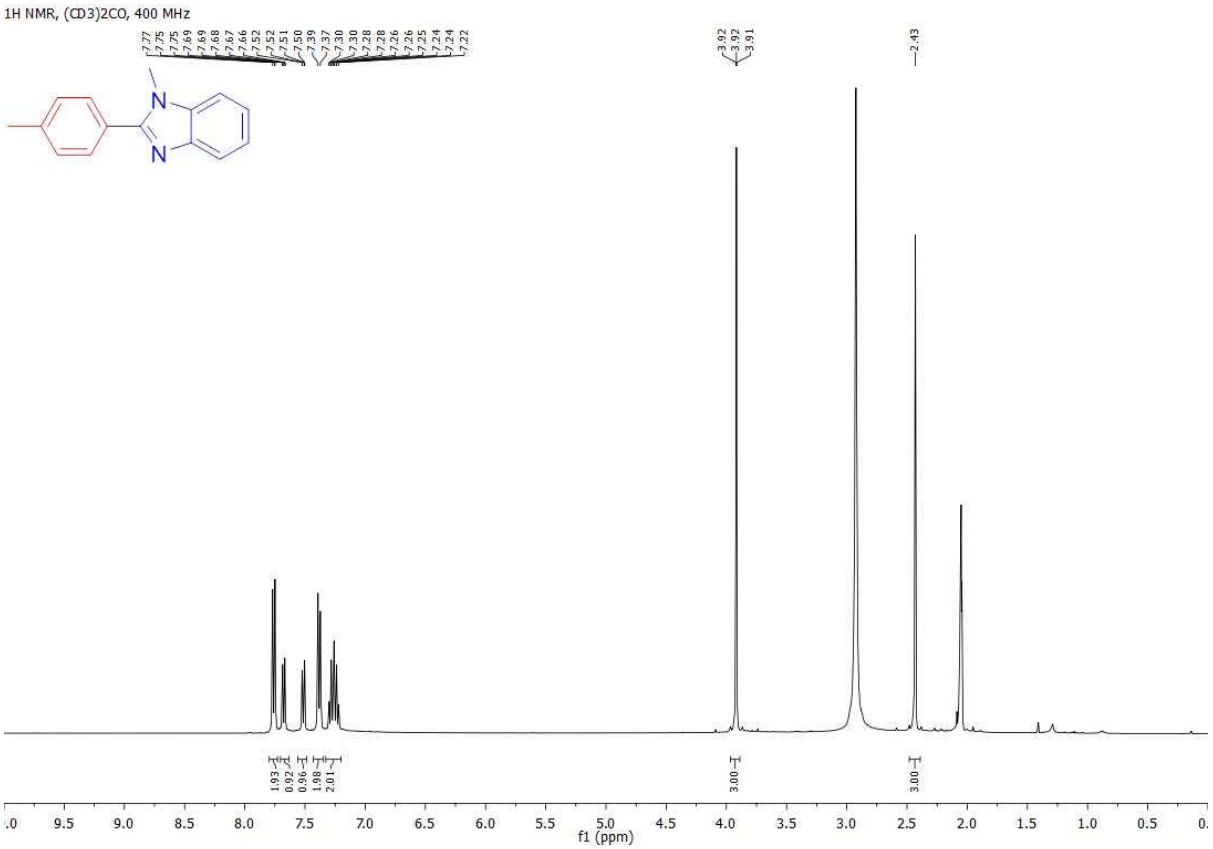

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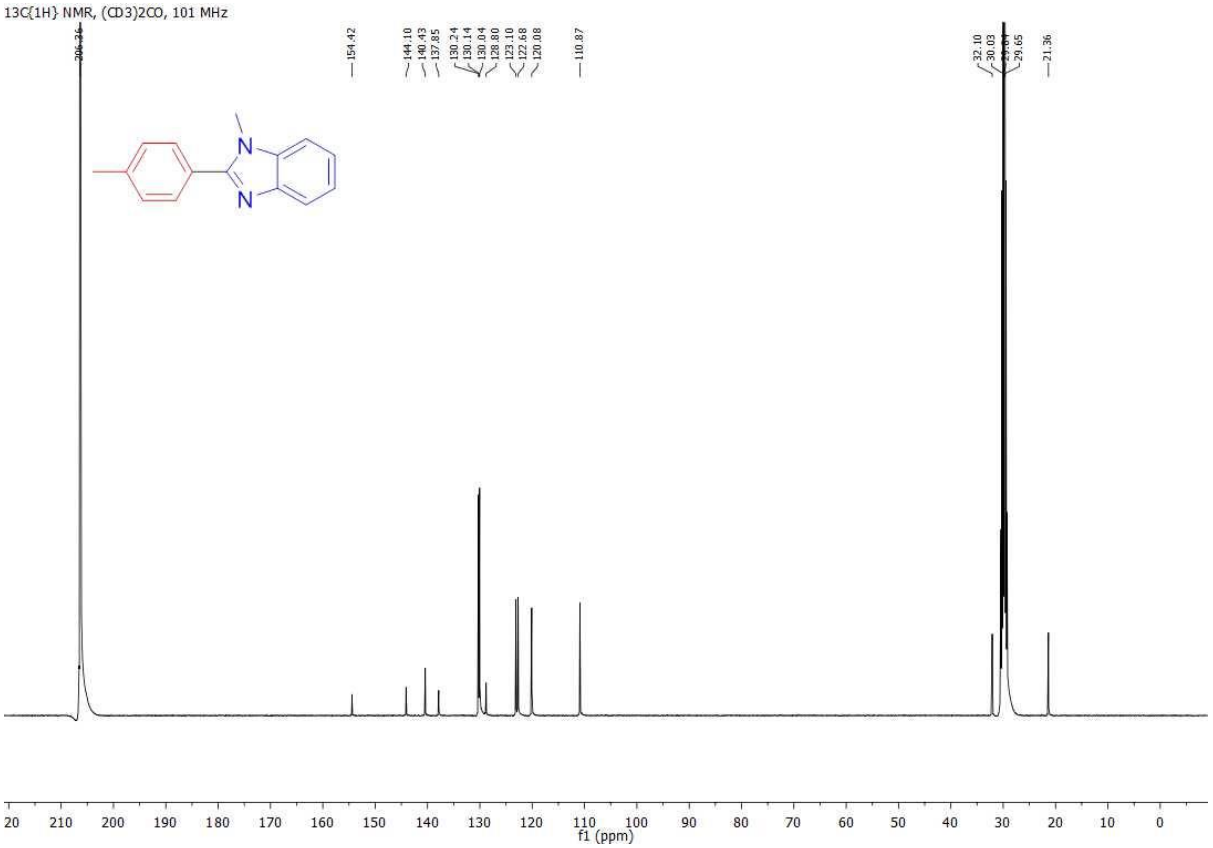

^{13}C Spectra of **3l**

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