Nickel-Catalyzed C-3 Direct Arylation of Pyridinium Ions for the Synthesis of 1-Azafluorenes

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Supporting Information

Key to Abbreviated Terms:

$CDCl_3$ - Deuterated chloroform
DBU – 1,8-Diazabicycloundec-7-ene
DMSO- Dimethylsulfoxide
DMF- N,N-dimethylformamide
EtOAc - Ethyl Acetate
Hex - Hexanes
DMF - *N*,*N*-Dimethylformamide
Hex - Hexanes
Me-THF - 2-Methyl-Tetrahydrofuran
MTBE–Methyl-tert-butyl-ether
NaHMDS -Sodium hexamethyldisilazane

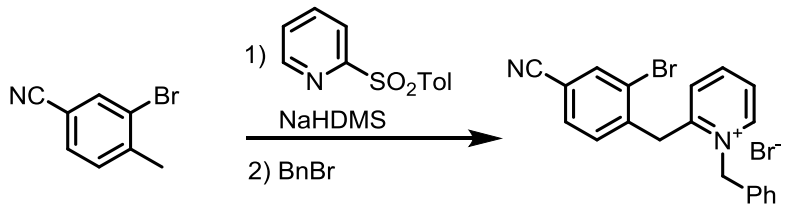
General Considerations:

General:
Unless stated otherwise, reactions were conducted under an atmosphere of nitrogen using standard Schlenk or glove box techniques. NMR Spectra (^{1}H, ^{13}C, ^{19}F) were performed at 298 K (unless otherwise specified) on either a Brüker Avance III Ultra Shield DPX-400 MHz NMR or Brüker Avance III Ultra Shield DRX 500 MHz NMR. ^{1}H-NMR Spectra obtained in $CDCl_3$ were referenced to residual non-deuterated chloroform (7.26 ppm) or DMSO (39.52 ppm) in the respective deuterated solvents. ^{13}C NMR Spectra obtained in $CDCl_3$ were referenced to chloroform (77.3 ppm). Reactions were monitored using a Waters Acquity UPLC, ^{1}H NMR, and/or by TLC on silica gel plates (60Å porosity, 250 μm thickness). Low-resolution mass spectra were obtained using Waters Xevo TDQ attached to a Waters Acquity UPLC**.** High resolution mass spectral data were acquired using an Agilent LC/MSD TOF (time-of-flight) mass spectrometer in an electrospray positive ionization mode *via* flow injection. TLC analysis was performed using hexanes/EtOAc as the eluent and visualized using UV light. Flash chromatography was accomplished using a Teledyne CombiFlash R_f (visualizing at 254 & 280 nm) with Silicycle SiliaSep Flash Cartridges (60Å porosity, 40-63 μm).

Chemicals:
Commercially obtained reagents were used as received. Deuterated NMR solvents ($CDCl_3$, DMSO) were purchased from Sigma Aldrich. $NiCl_2$(DME), and 1,10-phenanthroline. Ethyl acetate, and hexanes were purchased from Fischer. DMF and DBU were purchased from Sigma-Aldrich in a Sure-Seal bottle and degassed by sparging with nitrogen for 15 min prior to use.

Synthesis of Pyridinium Ions

General Procedure A

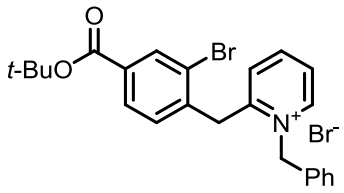


1-Benzyl-2-(4-cyano-2-bromobenzyl)pyridin-1-ium bromide, 4e-Br

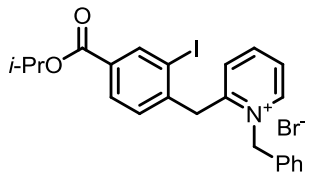
A round bottom flask containing 3-iodo-4-methylbenzonitrile (10.292 g, 52 mmol, 1.05 equiv) and 2-(phenylsulfonyl)pyridine (10.9g, 50 mmol, 1 equiv.) was purged with nitrogen. DMF (50

mL) was charged to the flask and the resulting slurry was stirred at room temperature for 30 minutes, then cooled to 10 °C. A solution of NaHMDS in THF (50 mL, 100 mmol, 2 equiv, 2M) was charged over 15 min while keeping the internal temperature below 20 °C. The reaction mixture was concentrated down under reduced pressure to remove THF, then water was added (30 mL). The organic layer was washed with 10% aq. $NaHCO_3$. The resulting mixture was extracted with Me-THF (100 mL). Combined organic layers were washed with water (30 mL) then concentrated. The resulting concentrated residue was dissolved in dry acetonitrile (30 mL) under nitrogen. Benzyl bromide (6.5 mL, 55 mmol, 1.1 equiv.) was then charged at room temperature and the reaction mixture was heated to 80 °C for about 12 h. The reaction mixture was cooled down to room temperature and was treated with EtOAc (10-20 mL). The slurry was stirred for 1 h at room temperature then filtered. The resulting solid was rinsed with EtOAc and dried under vacuum to afford the desired pyridinium salt **4e-Br** with 75% yield.

^{1}H NMR (DMSO, 400 MHz) δ ppm 9.53 (d, *J* = 6.3 Hz, 1H), 8.62 (t, *J* = 8.0 Hz, 1H), 8.27 (s, 1H), 8.24 (t, *J* = 6.7 Hz, 1H), 7.93 (d, *J* = 7.6 Hz, 1H), 7.58 (d, *J* = 7.8 Hz, 1H), 7.50 (d, *J* = 8.05 Hz, 1H), 7.47-7.35 (m, 5H), 6.25 (s, 2H), 4.81 (s, 2H); ^{13}C NMR (DMSO, 100 MHz) 155.0, 147.8, 147.0, 140.3, 136.7, 133.4, 133.2, 132.8, 129.7, 129.4, 129.2, 128.3, 127.1, 125.5, 117.6, 113.1, 60.9, 39.2; HRMS (ESI) m/z [M-Br]+ calcd for $C_{20}H_{16}BrN_2$: 363.0491, found: 363.0509.

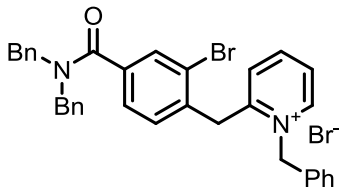


1-Benzyl-2-(2-bromo-4-(tert-butoxycarbonyl) benzyl) pyridin-1-ium bromide, 4b (59% yield) was prepared *via* General Procedure A. **5b** was obtained as a white solid. ^{1}H NMR (DMSO, 400 MHz) δ ppm 9.40 (d, *J* = 6.4 Hz, 1H), 8.55 (t, *J* = 7.8 Hz, 1H), 8.18 (t, *J* = 7.4 Hz, 1H), 8.07 (d, *J* = 1.6 Hz, 1H), 7.92 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.51 (d, *J* = 8.1 Hz, 1H), 7.48-7.37 (m, 4H), 7.36-7.32 (m, 2H), 6.15 (s, 2H), 4.70 (s, 2H), 1.54 (s, 9H); ^{13}C NMR (DMSO, 100 MHz) 163.7, 155.5, 147.8, 146.9, 139.1, 133.6, 133.4, 133.3, 133.1, 129.7, 129.5, 129.4, 129.0, 128.2, 127.0, 125.0, 82.2, 60.9, 39.0, 28.1; HRMS (ESI) m/z [M-Br]+ calcd for $C_{24}H_{25}BrN_2O_2$: 438.1063, found: 438.1084.

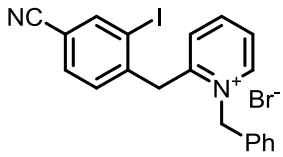


1-Benzyl-2-(2-bromo-4-(isopropoxy carbonyl) benzyl) pyridin-1-ium iodide, 4c (13% yield) was prepared *via* General Procedure A. **4c** was obtained as a white solid. ^{1}H NMR (DMSO, 400 MHz) δ ppm 9.41 (d, *J* = 6.3 Hz, 1H), 8.55 (t, *J* = 8.2 Hz, 1H), 8.37 (d, *J* = 1.6 Hz, 1H), 8.19 (t, *J* = 7.0 Hz, 1H), 7.96 (dd, *J* = 1.6, 7.9 Hz, 1H), 7.49-7.43 (m, 3H), 7.43-7.40 (m, 1H), 7.39-7.34 (m, 3H), 6.15 (s, 2H), 5.14 (sept, *J* = 6.1 Hz, 1H), 4.69 (s, 2H), 1.32 (d, *J* = 6.4 Hz, 6H); ^{13}C NMR (DMSO, 100 MHz) 164.0, 155.6, 147.8,

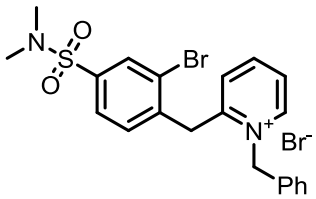
146.9, 142.9, 140.2, 133.2, 132.1, 131.8, 130.1, 129.8, 129.4, 129.2, 128.3, 127.0, 102.8, 69.3, 60.9, 43.4, 22.1; HRMS (ESI) m/z [M-Br]+ calcd for $C_{23}H_{23}INO_2$: 472.0768, found: 472.0767.



1-Benzyl-2-(2-bromo-4-(dibenzyl carbamoyl) benzyl) pyridin-1-ium bromide, 4d (69% yield) was prepared *via* General Procedure A. **4d** was obtained as a white solid. ^{1}H NMR (DMSO, 400 MHz) δ ppm 9.43 (d, *J* = 6.3 Hz, 1H), 8.58 (t, *J* = 8.4 Hz, 1H), 8.19 (t, *J* = 7.1 Hz, 1H), 7.75 (s, 1H), 7.51 (d, *J* = 8.1 Hz, 1H), 7.45 (d, *J* = 7.4 Hz, 1H), 7.43-7.26 (m, 15H), 7.21-7.15 (m, 2H), 6.16 (s, 2H), 4.66 (s, 2H), 4.61 (br s, 2H), 4.44 (br s, 2H); ^{13}C NMR (DMSO, 100 MHz) 169.6, 155.7, 147.7, 146.9, 138.2, 137.2, 136.9, 135.7, 133.3, 132.7, 132.4, 129.6, 129.3, 129.3 (2), 129.1, 128.2 (2), 128.0, 127.8, 127.4; 127.0, 126.9, 124.9, 60.9, 52.2, 47.8, 38.9; HRMS (ESI) m/z [M-Br]+ calcd for $C_{34}H_{30}BrN_2O$: 561.1536, found: 561.1559.

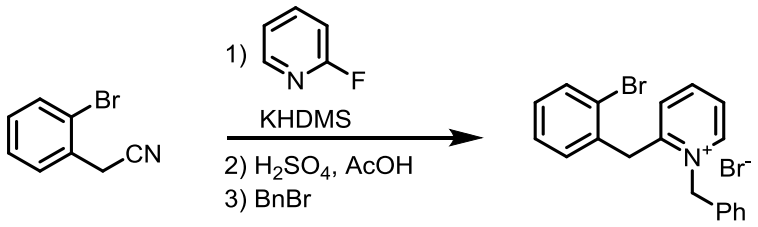


1-Benzyl-2-(4-cyano-2-iodobenzyl) pyridin-1-ium bromide, 4e-I (65% yield) was prepared *via* General Procedure A. **4e-I** was obtained as a white solid. ^{1}H NMR (DMSO, 400 MHz) δ ppm 9.43 (d, *J* = 6.2 Hz, 1H), 8.58 (t, *J* = 8.3 Hz, 1H), 8.42 (s, 1H), 8.21 (t, *J* = 7.2 Hz, 1H), 7.90 (d, *J* = 7.7 Hz, 1H), 7.48-7.34 (m, 7H), 6.16 (s, 2H), 4.72 (s, 2H); ^{13}C NMR (DMSO, 100 MHz) 155.3, 147.8, 146.9, 143.6, 142.9, 133.1 (2), 132.1, 129.8, 129.4, 128.3, 127.1, 117.5, 112.8, 13.7, 60.9, 43.5; HRMS (ESI) m/z [M-Br]+ calcd for $C_{20}H_{16}IN_2$: 411.0353, found: 411.0365.



1-Benzyl-2-(2-bromo-4-(N,N-dimethyl sulfamoyl)benzyl)pyridin-1-ium, **4f** (65% yield) was prepared *via* General Procedure A. **4f** was obtained as a white solid. ^{1}H NMR (DMSO, 400 MHz) δ ppm 9.46 (d, *J* = 6.3 Hz, 1H), 8.59 (t, *J* = 7.9 Hz, 1H), 8.21 (t, *J* = 7.0 Hz, 1H), 7.93 (s, 1H), 7.76 (d, *J* = 8.2 Hz, 1H), 7.57 (d, *J* = 8.1 Hz, 1H), 7.54 (d, *J* = 8.3 Hz, 1H), 7.45-7.33 (m, 5H), 6.19 (s, 2H), 4.77 (s, 2H), 2.66 (s, 6H); ^{13}C NMR (DMSO, 100 MHz) 155.1, 147.8, 147.0, 139.6, 136.6, 133.5, 133.2, 131.8, 129.7, 129.4, 128.3, 127.9, 127.1, 125.6, 61.0, 39.0, 38.1; HRMS (ESI) m/z [M-Br]+ calcd for $C_{21}H_{22}BrN_2O_2S$: 445.0580, found: 445.0585.

General Procedure B

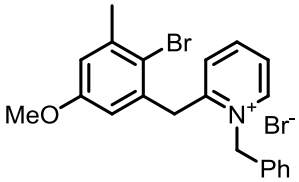


1-Benzyl-2-(2-bromobenzyl)pyridin-1-ium bromide, 4a A round bottom flask purged with nitrogen was charged with dry THF (2 mL). 2-bromophenylacetonitrile (3.9 g, 20 mmol, 1 equiv.) and 2-fluoropyridine (1.9 g, 20 mmol, 1 equiv.) were sequentially added to the flask. The resulting solution was then cooled to 10 °C. A solution of KHMDS in THF (20 mL, 2 equiv, 1M) was charged over 15 min while keeping the internal temperature below 20 °C. The reaction mixture was warmed to room temperature and stirred for about 5 h or until full consumption of the starting nitrile was observed by HPLC or UPLC. The reaction mixture was quenched with water (30 mL) and was diluted with Me-THF (50 mL) and 10% aq $NaHCO_3$ (15 mL). The reaction mixture was concentrated down under reduced pressure.

The resulting concentrated residue was dissolved in acetic acid (6 mL) and sulfuric acid (2 mL). The mixture was stirred for 15 h at 100 °C. Water (0.8 mL) was charged at 100 °C and allowed to stir for 3 h. The reaction mixture was neutralized using 25% aq. NaOH to pH = 14. The mixture was extracted with MTBE and solvent was evaporated.

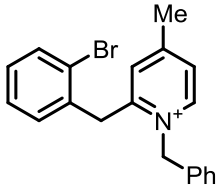
The resulting concentrated residue was dissolved in dry acetonitrile under nitrogen. Benzyl bromide (1.25g, 1.05 equiv) was then charged at room temperature and the reaction mixture was heated to 80 °C for about 12 h. The reaction mixture was cooled down to room temperature and was treated with EtOAc (or Me-THF). The slurry was stirred for 1 h at room temperature then filtered. The resulting solid was rinsed with EtOAc (or Me-THF) and dried under vacuum to afford the desired pyridinium salt **4a** with 50% yield.

^{1}H NMR (DMSO, 400 MHz) δ ppm 9.48 (d, *J* = 6.4 Hz, 1H), 8.60 (t, *J* = 7.7 Hz, 1H), 8.20 (t, *J* = 6.8 Hz, 1H), 7.70 (d, *J* = 8.1 Hz, 1H), 7.49-7.32 (m, 9H), 6.22 (s, 2H), 4.67 (s, 2H); ^{13}C NMR (DMSO, 100 MHz) 156.2, 147.6, 146.9, 134.3, 133.6, 133.4, 132.8, 130.8, 129.7, 129.4, 129.2, 128.7, 128.2, 126.8, 124.9, 60.8, 39.0; HRMS (ESI) m/z [M-Br]+ calcd for $C_{19}H_{17}BrN$: 338.0539, found: 338.0539.



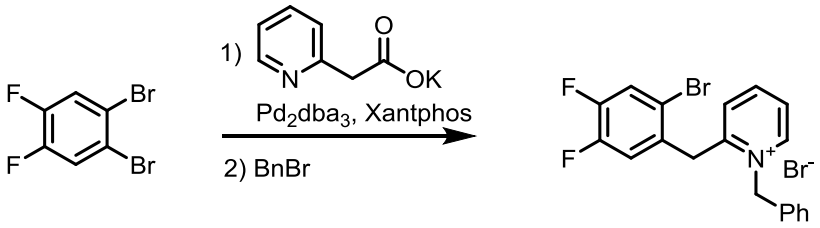
1-Benzyl-2-(2-bromo-5-methoxy-3-methyl-benzyl)-pyridin-1-ium bromide, **4h** (31% yield) was prepared *via* General Procedure B. **4h** was obtained as a white solid. ^{1}H NMR (DMSO, 400 MHz) δ ppm 9.29

(d, *J* = 6.2 Hz, 1H), 8.52 (t, *J* = 7.4 Hz, 1H), 8.14 (t, *J* = 7.1 Hz, 1H), 7.48-7.39 (m, 3H), 7.39-7.30 (m, 3H), 7.02 (d, *J* = 2.8 Hz, 1H), 6.80 (d, *J* = 2.8 Hz, 1H), 6.07 (s, 2H), 4.54 (s, 2H), 3.73 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (DMSO, 100 MHz) 158.5, 155.9, 147.0, 146.3, 139.9, 134.9, 132.8, 129.2, 129.0, 128.9, 128.2, 128.0, 127.6, 127.5, 126.5, 117.1, 116.1, 115.6, 60.3, 55.4, 23.4; HRMS (ESI) m/z [M-Br]+ calcd for $C_{21}H_{21}BrNO$: 382.0801, found: 382.0796.



1-Benzyl-2-(2-bromobenzyl)-4-methylpyridin-1-ium bromide, 4i (9% yield) was prepared *via* General Procedure B. **4i** was obtained as a white solid. ^{1}H NMR (DMSO, 400 MHz) δ ppm 9.15 (d, *J* = 6.5 Hz, 1H), 8.00 (d, *J* = 6.1 Hz, 1H), 7.69 (d, *J* = 7.8 Hz, 1H), 7.47-7.37 (m, 4H), 7.34 (d, *J* = 7.4 Hz, 1H), 7.32-7.26 (m, 3H), 7.22 (s, 1H), 5.98 (s, 2H), 4.52 (s, 2H), 4.81 (s, 2H), 253 (s, 3H); ^{13}C NMR (DMSO, 100 MHz) 160.3, 155.0, 146.6, 134.2, 133.7, 133.6, 132.5, 130.7, 129.7, 129.3, 129.1 (2), 128.0, 127.4, 124.8, 60.1, 38.7, 22.0; HRMS (ESI) m/z [M-Br]+ calcd for $C_{20}H_{19}BrN$: 352.0695, found: 352.0704.

Procedure C



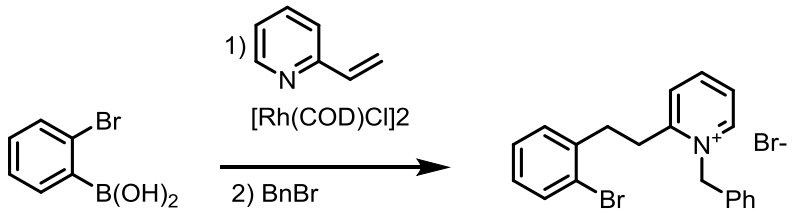
1-Benzyl-2-(2-bromo-4,5-difluorobenzyl)pyridin-1-ium bromide, 4g A reported protocol was followed: [1] A 10 ml oven-dried Schlenk tube was charged with $Pd_2(dba)_3$ (67 mg, 0.074 mmol, 2 mol%), Xantphos (127 mg, 0.221 mmol, 6 mol%), potassium pyridyl-2-acetate (0.644 g, 3.6 mmol, 1 equiv) and dibromo-4,5-difluorobenzene (1 g, 3.67 mmol, 1 equiv.). The tube was evacuated and filled with argon (this procedure was repeated three times). Then diglyme (6 mL) was added with a syringe under nitrogen. The tube was sealed with a screw cap, stirred at room temperature for 10 min, and connected to the Schlenk line which was full of argon, stirred in a preheated oil bath (150 °C) for 16 h. Upon completion of the reaction, the mixture was cooled to room temperature and diluted with EtOAc and passed through celite. The mixture was washed with water and layers separated. Solvent was evaporated under reduced pressure and the resulting concentrated residue (0.56 g) was dissolved in dry acetonitrile (1 mL) under nitrogen. Benzyl bromide (0.246 mL, 2 mmol, 1.05 equiv) was then charged at room temperature and the

[1] R. Shang, Z.-W. Yang, Y. Wang, S.-L. Zhang, L.Liu *J. Am. Chem. Soc*. **2010**, *132*, 14391–14393.

reaction mixture was heated to 75 °C for about 6 h. The reaction mixture was cooled down to room temperature and was treated with EtOAc. The slurry was stirred for 1 h at room temperature then filtered. The resulting solid was rinsed with EtOAc or Me-THF and dried under vacuum to afford the desired pyridinium **4g** with 12% yield.

^{1}H NMR (DMSO, 400 MHz) δ ppm 9.32 (d, *J* = 6.2 Hz, 1H), 8.56 (t, *J* = 7.8 Hz, 1H), 8.18 (t, J = 6.6 Hz, 1H), 7.96 (dd, *J* = 10.1, 8.0 Hz, 1H), 7.56-7.50 (m, 2H), 7.47-7.37 (m, 3H), 7.32 (d, *J* = 7.1 Hz, 2H), 6.11 (s, 2H), 4.60 (s, 2H); ^{13}C NMR (DMSO, 100 MHz) 155.4, 150.8, 150.7, 150.6 (2), 148.3, 148.2, 147.7, 146.9, 133.3, 132.0, 131.9 (3), 129.7, 129.4, 129.2, 128.2, 127.1, 122.8, 122.6, 121.3, 121.1, 119.2 (2), 119.1 (2), 60.9, 38.2; ^{19}F NMR (DMSO, 400 MHz) -136.2, -136.3, -137.9, -138.0; HRMS (ESI) m/z [M-Br]+ calcd for $C_{19}H_{15}BrF_2N$: 374.0350, found: 374.0341.

Procedure D



1-Benzyl-2-(2-bromophenethyl)pyridin-1-ium bromide, 4j A reported protocol was followed:[2] To a mixture of $[Rh(COD)Cl]_2$ (23 mg, 0.048 mmol, 2 mol %) in H_2O (11.5 mL, 0.2 M) at room temperature was successively added 2-bromophenylboronic acid (1.19 g, 5.94 mmol, 2.5 equiv.), Na_2CO_3 (0.504 g, 5.9 mmol, 2 equiv.) and 2-vinyl pyridine (0.250 g, 2.37 mmol, 1 equiv). The reaction mixture was heated at 80 °C for12 h. After cooling to room temperature the colored solution was poured into MTBE (50 mL) and the reaction flask was carefully rinsed with MTBE. The heterogeneous mixture was vigorously stirred at room temperature for 2 h. The two phases were separated, the aqueous phase was extracted with MTBE (3 x 30 mL), and the combined organic layers were dried over $MgSO_4$, filtered, and evaporated to dryness.

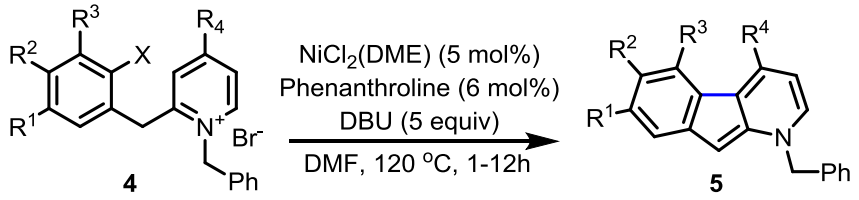
The resulting concentrated residue (0.368 g) was dissolved in dry acetonitrile (1 mL) under nitrogen. Benzyl bromide (0.2 mL, 1.65 mmol, 1.2 equiv.) was then charged at room temperature and the reaction mixture was heated to 80 °C for about 12 h. The reaction mixture was cooled down to room temperature and was treated with Me-THF (3 mL). The slurry was stirred for 1 h at room temperature then filtered. The resulting solid was rinsed with EtOAc or Me-THF and dried under vacuum to afford the desired pyridinium salt **4j** with 42% yield.

^{1}H NMR (DMSO, 500 MHz) δ ppm 9.31 (d, *J* = 5.7 Hz, 1H), 8.65 (t, *J* = 8.1 Hz, 1H), 8.16 (t, *J* = 6.2 Hz, 1H), 8.12 (d, *J* = 8.6 Hz, 1H), 7.57 (d, *J* = 7.6 Hz, 1H), 7.45-7.35 (m, 4H), 7.33 (t, *J* = 6.7

[2] M. Lautens, A. Roy, K. Fukuoka, K. Fagnou, B. Martın-Matute *J. Am. Chem. Soc.* **2001,** *123*, 5358-5359.

Hz, 1H), 7.27 (d, *J* =8.1 Hz, 2H), 7.19 (dt, *J* = 8.1, 1.7 Hz, 1 H), 6.12 (s, 2H), 3.38 (dd, J = 6.7, 8.8 Hz, 2H), 3.05 (dd, *J* = 6.7, 8.6 Hz, 2H); ^{13}C NMR (DMSO, 125 MHz) 157.0, 146.7, 146.1, 138.1, 133.8, 132.6, 130.9, 129.6, 129.3, 129.0, 128.8, 128.1, 127.2, 126.4, 123.7, 60.0, 33.6, 32.0; HRMS (ESI) m/z [M-Br]+ calcd for $C_{20}H_{19}BrN$: 352.0695, found: 352.0703.

General Procedure for the Synthesis of 1-Azafluorenes



In a glove-box, a reaction vial was charged with $NiCl_2$(DME) (10.4 mg, 0.048 mmol, 5 mol%) and 1,10-phenanthroline (10.2 mg, 0.057 mmol, 6 mol%) followed by nitrogen-sparged DMF (2.4 mL). The resulting suspension was stirred for 15-30 min at room temperature until solids dissolved and a light blue/turquoise solution is obtained. The starting pyridinium ion **4** (0.95 mmol, 1 equiv.) was added as one solid portion to the reaction mixture and the vial was sealed with a teflon-lined cap and brought out of the glove-box. Nitrogen-sparged DBU (0.7 mL, 4.77 mmol, 5 equiv) was charged to the reaction mixture and it was then heated to 120 °C for 1-12 hours or until complete conversion was observed by HPLC/UPLC.

Work-up procedure #1 (for polar substrates):[3] The reaction mixture was cooled down to 40 °C and water was charged over 15 min. The resulting slurry was cooled down to 15 °C and stirred at that temperature for 1 h. The desired 1-azafluorene precipitated/crystallized out and was isolated by filtration. The resulting cake was washed with additional water. The solid was then dried under vacuum to afford the desired 1-azafluorene derivative.[4]

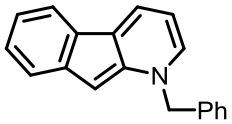
Note: If metallic impurities carry over in the crystallized material, they can be removed by dissolving the solid in EtOAc followed by a filtration on celite to remove insoluble impurities. Solvent was then evaporated under reduced pressure.

Work-up procedure #2 (for non-polar substrates):[3] The reaction mixture was cooled down to 25 °C and water was charged. The resulting mixture was extracted with EtOAc. Combined organic layers were washed with water and concentrated down under reduced pressure. The crude mixture was purified by flash chromatography using a short silica gel column with a fast gradient of 0-80% EtOAc in Hex. Solvent was evaporated and resulting solid dried under vacuum to afford desired 1-azafluorene derivative.[4]

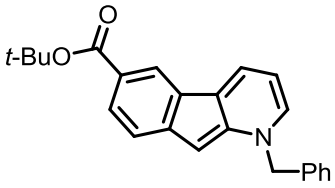
[3] In order to minimize decomposition of product (e.g. over-reduction), purification should be performed after completion of the reaction. Crude reaction mixtures cannot be stored and extended reaction times (≥2 days) lead to product decomposition.

[4] To extend the shelf-life of these compounds, they should be stored in an amber bottle under argon, in a fridge. Alternatively, the free base can be converted to the corresponding pyridinium ion by an aq. HBr treatment followed by isolation by filtration.

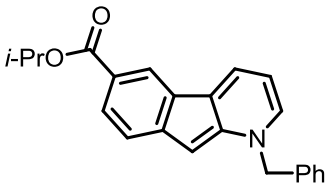
1-Azafluorene Product Data



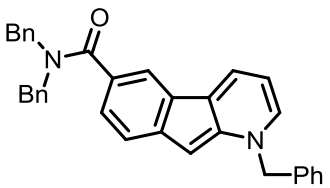
1-Benzyl-1H-indeno[2,1-b]pyridine, 5a (X=Br, 92% yield) was prepared *via* General Procedure and work-up procedure #2. **5a** was obtained as a deep purple solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ ppm 8.10 (d, *J* = 2.8 Hz, 1H), 8.05 (t, *J* = 3.8 Hz, 1H), 7.56 (t, J = 8.0 Hz, 1H), 7.39 (t, *J* = 7.7 Hz, 1H), 7.31 (d, J = 6.5 Hz, 1H), 7.29-7.22 (m, 3H), 7.17-7.09 (m, 2H), 6.38 (t, *J* = 6.5 Hz, 1H), 6.03 (s, 1H), 5.23 (s, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) 141.6, 138.7, 135.2, 129.0, 128.5, 127.5, 126.6, 124.9, 123.7, 120.6, 118.4, 117.5, 102.7, 85.3, 57.9; HRMS (ESI) m/z [M+H]+ calcd for $C_{19}H_{15}N$: 258.1277, found: 258.1277.



***tert*-Butyl 1-benzyl-1H-indeno[2,1-b]-pyridine-6-carboxylate, 5b** (X=Br, 81% yield) was prepared *via* General Procedure with work-up procedure #1. **5b** was obtained as a red solid. ^{1}H NMR (DMSO, 400 MHz) δ ppm 8.77 (s, 1H), 8.57 (d, *J* = 7.8 Hz, 1H), 8.25 (d, *J* = 6.0 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.50 (d, *J* = 7.8 Hz, 1H), 7.38-7.25 (m, 5H), 6.79 (t, *J* = 6.6 Hz, 1H), 6.26 (s, 1H), 5.60 (s, 2H), 1.59 (s, 9H); ^{13}C NMR (DMSO, 100 MHz) 166.9, 144.0, 141.1, 136.3, 136.1, 129.2, 128.4, 128.0, 127.9, 127.4, 126.8, 123.2, 122.6, 119.4, 117.5, 105.2, 86.7, 79.6, 57.9, 28.6; HRMS (ESI) m/z [M+H]+ calcd for $C_{24}H_{23}NO_2$: 358.1802, found: 358.1810.

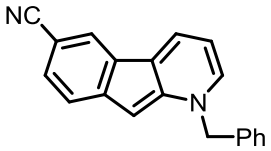


***isopropyl* 1-Benzyl-1H-indeno[2,1-b]pyridine-6-carboxylate, 5c** (X= I, 94% yield) was prepared *via* General Procedure with work-up procedure #1. **5c** was obtained as a red solid. ^{1}H NMR (DMSO, 400 MHz) δ ppm 8.77 (s, 1H), 8.62 (d, *J* = 7.4 Hz, 1H), 8.29 (d, *J* = 6.5 Hz, 1H), 7.87 (d, i = 8.4 Hz, 1H), 7.50 (d, *J* = 8.4 Hz, 1H), 7.36 (d, *J* = 3.8 Hz, 4H), 7.34-7.27 (m, 1H), 6.83 (t, *J* = 6.4 Hz, 1H), 6.27 (s, 1H), 5.63 (s, 2H), 5.15 (sept, J = 6.4 Hz, 1H), 1.34 (d, *J* = 6.1 Hz, 6H); ^{13}C NMR (DMSO, 100 MHz) 167.0, 144.1, 141.2, 136.2 (2), 129.2, 128.4, 128.1, 127.9, 127.4, 126.8, 123.3, 122.6, 118.1, 117.7, 105.3, 86.8, 67.3, 57.9, 22.4; HRMS (ESI) m/z [M+H]+ calcd for $C_{23}H_{21}NO_2$: 344.1645, found: 344.1651.

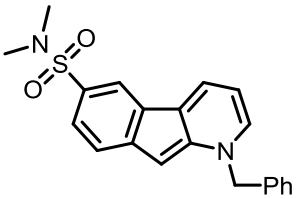


***N,N*,1-Tribenzyl-1H-indeno[2,1-b]pyridine-6-carboxamide, 5d** (X=Br, 95% yield) was prepared *via* General Procedure with work-up procedure #1. **5d** was obtained as a deep purple solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ ppm 8.35 (s, 1H), 8.08 (d, *J* = 6.4 Hz, 1H), 7.58

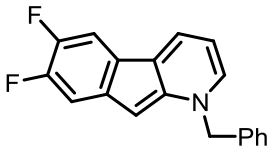
(d, *J* = 8.2 Hz, 1H), 7.50 (d, *J* = 8.2 Hz, 1H), 7.44 (d, *J* = 7.0 Hz, 1H), 7.38-7.21 (m, 9H), 7.19-7.15 (m, 3H), 6.48 (t, *J* = 6.4 Hz, 1H), 6.08 (s, 1H), 5.30 (s, 2H), 4.67 (br s, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) 174.1, 142.5, 140.2, 137.5, 134.8, 132.1, 132.0 (2), 131.9, 129.0, 128.7, 128.6, 128.5, 128.3, 128.1, 127.5, 127.4, 126.0, 125.5, 124.1, 122.9, 120.9, 120.6, 117.7, 103.8, 85.6, 58.1 ; HRMS (ESI) m/z [M+H]+ calcd for $C34H28N_2O$: 481.2274, found: 481.2292.



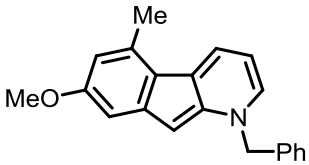
1-Benzyl-1H-indeno[2,1-b]pyridine-6-carbonitrile, 5e (X=Br, 77% yield' X=I, 80% yield) was prepared *via* General Procedure with work-up procedure #1. **5e** was obtained as deep purple solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ ppm 8.30 (s, 1H), 8.19 (d, *J* = 7.5 Hz, 1H), 7.57 (d, *J* = 6.7 Hz, 1H), 7.52 (s, 2H), 7.36-7.28 (m, 3H), 7.22-7.17 (m, 2H), 6.64 (t, *J* = 7.5 Hz, 1H), 6.17 (s, 1H), 5.37 (s, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) 143.6, 141.4, 134.3, 134.2, 129.2, 128.6 (2), 127.7, 127.5, 127.2, 125.4, 122.6, 122.1, 118.7, 105.1, 98.3, 86.8, 58.4; HRMS (ESI) m/z [M+H]+ calcd for $C_{20}H_{14}N_2$: 283.1230, found: 283.1236.



1-Benzyl-*N*,*N*-dimethyl-1H-indeno[2,1-b]pyridine-6-sulfonamide, 5f (X= Br, 95% yield) was prepared *via* General Procedure with work-up procedure #1. **5f** was obtained as red solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ ppm 8.57 (s, 1H), 8.35 (d, *J* = 6.9 Hz, 1H), 7.74 (d, *J* = 8.7 Hz, 1H), 7.64 (d, *J* = 7.4 Hz, 2H), 7.39-7.32 (m, 3H), 7.27-7.24 (m, 2H), 6.70 (t, *J* = 6.9 Hz, 1H), 6.24 (s, 1H), 5.47 (s, 2H), 2.7 (s, 6H); ^{13}C NMR (DMSO, 100 MHz) 143.2, 141.1, 136.8, 136.2, 129.3, 129.2, 128.4, 127.9, 126.7, 124.7, 122.1, 121.9, 121.2, 118.0, 105.6, 86.5, 58.0, 38.3; HRMS (ESI) m/z [M+H]+ calcd for $C_{21}H_{20}N_2O_2S$: 365.1318, found: 365.1321.

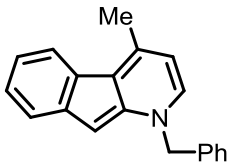


1-Benzyl-6,7-difluoro-1H-indeno[2,1-b]pyridine, 5g (X= Br, 51% yield) was prepared *via* General Procedure with work-up procedure #2. **5g** was obtained as deep purple solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ ppm 7.99 (d, J = 6.4 Hz, 1H), 7.74 (dd, *J* = 7.0, 10.2 Hz, 1H), 7.39 (d, *J* = 6.4 Hz, 1H), 7.29-7.22 (m, 3H), 7.22-7.13 (m, 3H), 6.41 (t, *J* = 5.7 Hz, 1H), 5.93 (s, 1H), 5.28 (s, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) 150.8, 150.7, 149.5, 148.4, 148.2, 145.3, 145.1, 142.9, 142.8, 138.2, 136.4, 136.3, 133.7, 131.9, 128.0, 127.3, 126.4, 124.5, 117.3, 117.2, 113.7, 113.5, 110.1, 109.9, 107.1 (2), 106.9 (2), 104.2, 104.0, 101.9, 83.3, 57.1; ^{19}F ($CDCl_3$, 400 MHz) -138.4, -138.5, -150.4, -150.5; HRMS (ESI) m/z [M+H]+ calcd for $C_{19}H_{13}F_2N$: 294.1089, found: 294.1096.



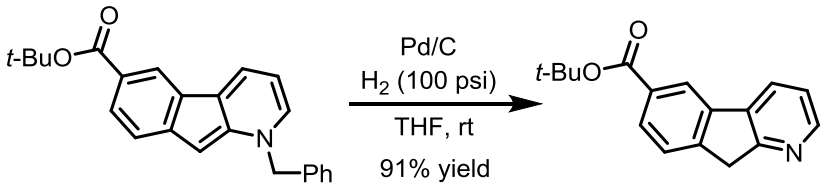
1-Benzyl-7-methoxy-5-methyl-1H-indeno[2,1-b]pyridine, 5h (X= Br, 48% yield) was prepared *via* General Procedure with work-up procedure #2. **5h** was obtained as a deep purple solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ ppm 8.05 (d, *J* = 7.7 Hz, 1H), 7.36 (d, *J* = 6.5 Hz,

1H), 7.35-7.29 (m, 3H), 7.24-7.19 (m, 2H), 6.94 (d, *J* = 2.8 Hz, 1H), 6.56 (d, *J* = 2.4 Hz, 1H), 6.47 (t, *J* = 6.9 Hz, 1H), 6.05 (s, 1H), 5.36 (s, 2H), 3.88 (s, 3H), 2.78 (s, 3H) ; ^{13}C NMR ($CDCl_3$, 100 MHz) 159.1, 148.3, 143.3, 135.3, 135.1, 130.8, 128.9, 128.8, 128.1, 127.3, 127.0, 125.6, 109.0, 103.3, 98.7, 85.8, 57.9, 55.3, 21.3; HRMS (ESI) m/z [M+H]+ calcd for $C_{21}H_{19}NO$: 302.1539, found: 302.1536.



1-Benzyl-4-methyl-1H-indeno[2,1-b]pyridine, 5i (X=Br, 75% yield) was prepared *via* General Procedure with work-up procedure #2. **5i** was obtained as a red solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ ppm 8.18 (d, *J* = 7.8 Hz, 1H), 7.60 (d, *J* = 7.3 Hz, 1H), 7.40-7.35 (m, 2H), 7.34-7.22 (m, 3H), 7.23-7.19 (m, 2H), 7.14 (t, *J* = 7.2 Hz, 2H), 6.31 (d, *J* = 6.4 Hz, 1H), 5.37 (s, 2H) 2.89 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) 149.8, 141.2, 135.4, 135.3, 132.1, 128.9, 128.1, 127.4, 125.5, 124.8, 123.8, 123.1, 118.4, 117.3, 107.2, 84.8, 57.7, 20.6; LRMS (ESI) m/z [M+H]+ calcd for $C_{20}H_{17}N$: 272.13, found: 272.09.

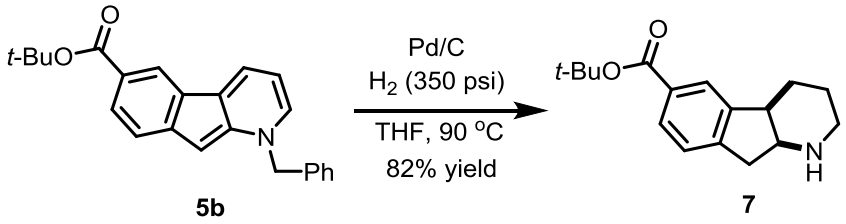
Procedures for Benzyl Hydrogenolysis and Pyridine Hydrogenation



5b **6**

***tert*-Butyl 9H-indeno[2,1-b]pyridine-6-carboxylate: 5b** (200 mg, 0.56 mmol) was added to a 10 mL vial followed by Pd/C (71.5 mg, 0.034 mmol, 10 mol % at 50% wet) and THF (2mL). The vial was placed into an Endeavor autoclave and was sealed. The mixture was purged with N_2 two times and H_2 two times and then pressurized to 100 psi H_2 and stir at RT for 2 h. The mixture was then vented, filtered and dried with Na_2SO_4. The product was purified on silica with 20% EtOAc in hexanes. The desired product **6** was obtained as a tan solid after drying under vacuum (136mg, 91% yield).

^{1}H NMR ($CDCl_3$, 500 Hz) δ 8.54 (d, *J* = 5.2 Hz, 1H), 8.39 (s, 1H), 8.08 (d, *J* = 7.7 Hz, 1H), 8.02 (d, *J* = 8.0 Hz, 1H), 7.63 (d, *J* = 8.0 Hz, 1H), 7.32 (dd, *J* = 7.7 Hz, 5.2 Hz, 1H), 4.05 (s, 2H), 1.64 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 165.7, 164.2, 147.7, 145.7, 139.3, 134.7, 131.3, 129.0, 127.8, 125.0, 122.0, 121.7, 81.3, 38.8, 28.2. HRMS (ESI) m/z [M+H]+ calcd for $C_{17}H_{17}NO_2$: 268.1332, found: 268.1338.

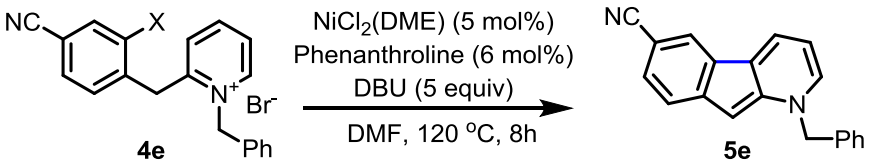


5b **7**

***tert*-Butyl 2,3,4,4a,9,9a hexahydro-1H-indeno[2,1-b]pyridine-6-carboxylate: 5b** (200mg, 0.56 mmol) was added to a 10 mL vial followed by Pd/C (71.5 mg, 0.034 mmol, 10 mol% at 50% wet) and THF (2 mL). The vial was placed into an Endeavor autoclave and sealed. The mixture was purged with N_2 two times and H_2 two times and then pressurized to 350 psi H_2 and heat to 90 °C and stir for 24 h. The mixture was then cooled to RT and vented. The mixture was filtered and dried with Na_2SO_4. The product was purified on silica with 15% MeOH in CH_2Cl_2. The desired product **7** was obtained as a white solid after drying under vacuum (125 mg, 82% yield).

^{1}H NMR ($CDCl_3$, 500 Hz) δ 7.80 (d, *J* = 8.0 Hz, 1H), 7.74 (s, 1H), 7.26 (d, *J* = 7.8 Hz, 1H), 3.97 (m, 1H), 3.35 (m, 1H), 3.16−3.19 (m, 2H), 3.06 (m, 1H), 2.94 (m, 1H), 1.95 (m, 2H), 1.64−1.72 (m, 2H), 1.52 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 165.6, 143.9, 142.2, 131.7, 129.3, 125.5, 124.2, 81.1, 56.9, 41.4, 41.3, 35.0, 28.2, 23.8, 19.0. HRMS (ESI) m/z [M+H]+ calcd for $C_{17}H_{23}NO_2$: 274.1802, found: 274.1792.

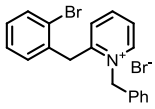
Glove-Box-Free Procedure for the Synthesis of 1-Azafluorenes



4e **5e**

A clean and inerted 100 mL reactor equipped with an overhead stirrer was charged with $NiCl_2$(DME) (148 mg, 0.675 mmol, 5 mol%) and 1,10-phenanthroline (146 mg, 0.810 mmol, 6 mol%). The reactor was sealed and 3 cycles of vacuum/nitrogen backfill were then performed. Nitrogen-sparged DMF (36 mL) was then charged to the reactor. The resulting suspension was stirred for about 30 min at room temperature until solids dissolved and a light blue/turquoise solution is obtained. The starting pyridinium ion **4e** (13.5 mmol, 1 equiv.) was added as one solid portion to the reaction mixture. The reactor was sealed and 2 cycles of vacuum/nitrogen backfill were then performed. Nitrogen-sparged DBU (10.1 mL, 67.5 mmol, 5 equiv) was charged to the reaction mixture and it was then heated to 120 °C for 8 hours or until complete conversion was observed by HPLC/UPLC. The reaction mixture was cooled down to 40 °C and water was charged over 15 min. The resulting slurry was cooled down to 15 °C and stirred at that temperature for 1 h. The desired 1-azafluorene **5e** precipitated/crystallized out and was isolated by filtration. The resulting cake was washed with additional water. The solid was then dried under vacuum to afford the desired 1-azafluorene derivative with 75-77% yield.

NMR Spectra of Synthesized Compounds

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PROCNO                       1

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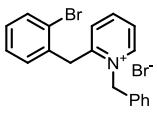


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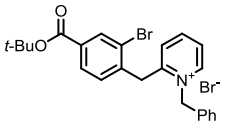


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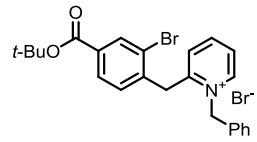
TE                298.0 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1327209 MHz
NUC1                   1H
P1                 15.00 usec
PLW1          10.50000000 W

F2 - Processing parameters
SI                 65536
SF            400.1300000 MHz
WDW                   EM
SSB       0
LB                 0.05 Hz
GB        0
PC                 1.00
```



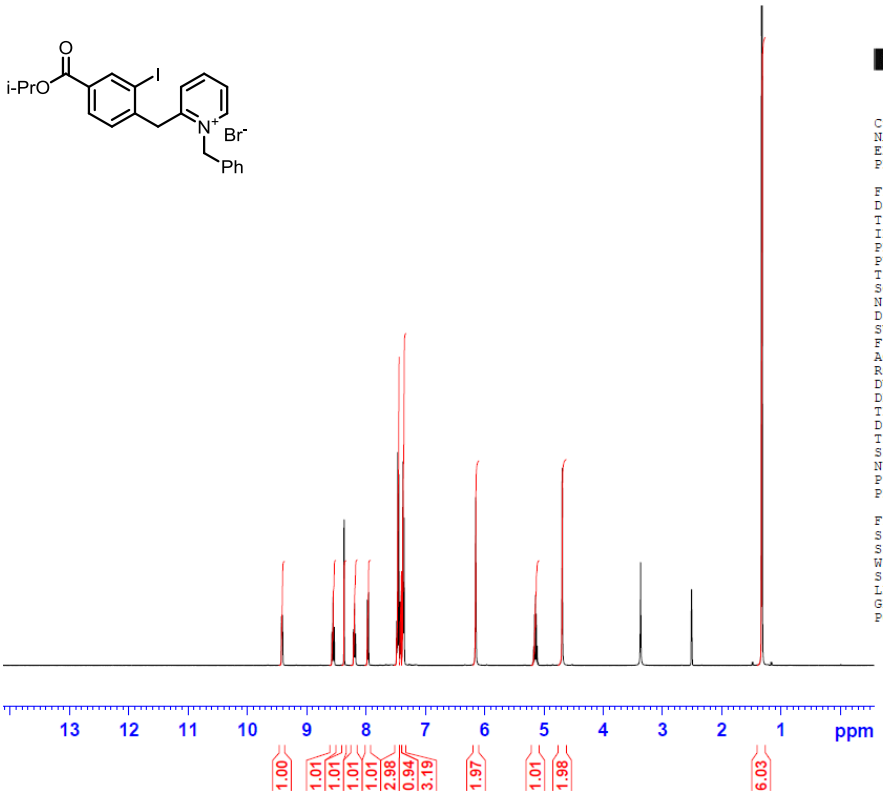

```
Current Data Parameters
NAME          102061-035
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151201
Time               12.02
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg
TD                 32768
SOLVENT             DMSO
NS                   320
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                  2050
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          100.6243395 MHz
NUC1                   13C
P1                 10.90 usec
PLW1          43.00000000 W

======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2              90.00 usec
PLW2          10.50000000 W
PLW12          0.29166999 W
PLW13          0.14670999 W

F2 - Processing parameters
SI                 65536
SF            100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

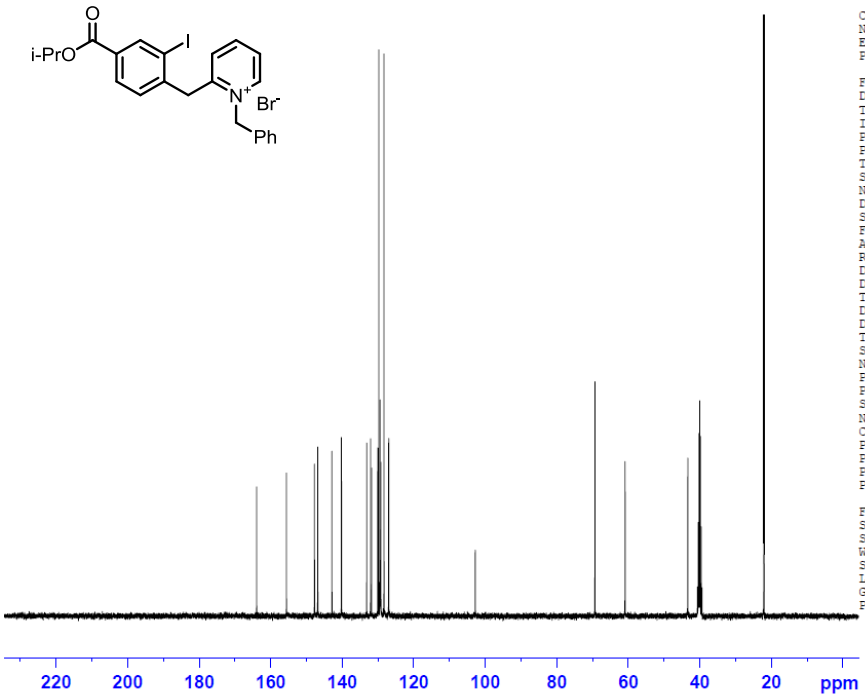


BRUKER

```
Current Data Parameters
NAME          102061-026
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151112
Time              16.26 h
INSTRUM            spect
PROBHD    Z104450_0178 (
PULPROG            zg10
TD                32768
SOLVENT            DMSO
NS                   32
DS                    4
SWH            5896.227 Hz
FIDRES         0.179939 Hz
AQ             2.7787263 sec
RG                  203
DW               84.800 usec
DE                6.50 usec
TE                298.0 K
D1           2.00000000 sec
TD0                    1
SFO1         400.1327209 MHz
NUC1                  1H
P1                14.00 usec
PLW1         12.05399990 W

F2 - Processing parameters
SI                 65536
SF           400.1300000 MHz
WDW                   EM
SSB       0
LB                 0.05 Hz
GB        0
PC                 1.00
```

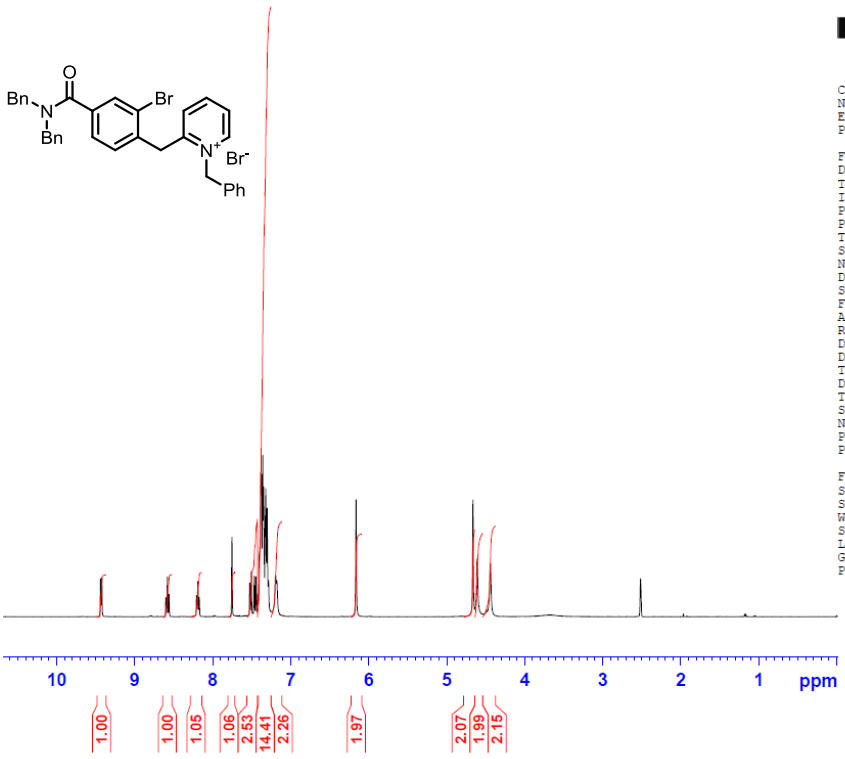


BRUKER

```
Current Data Parameters
NAME          102061-026
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151112
Time              16.39 h
INSTRUM            spect
PROBHD    Z104450_0178 (
PULPROG            zgpg
TD                32768
SOLVENT            DMSO
NS                  260
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG                  203
DW               20.800 usec
DE                6.50 usec
TE                300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         100.6243395 MHz
NUC1                  13C
P1                10.00 usec
PLW1         51.08800125 W
SFO2         400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         12.05399990 W
PLW12         0.30075201 W
PLW13         0.15073690 W

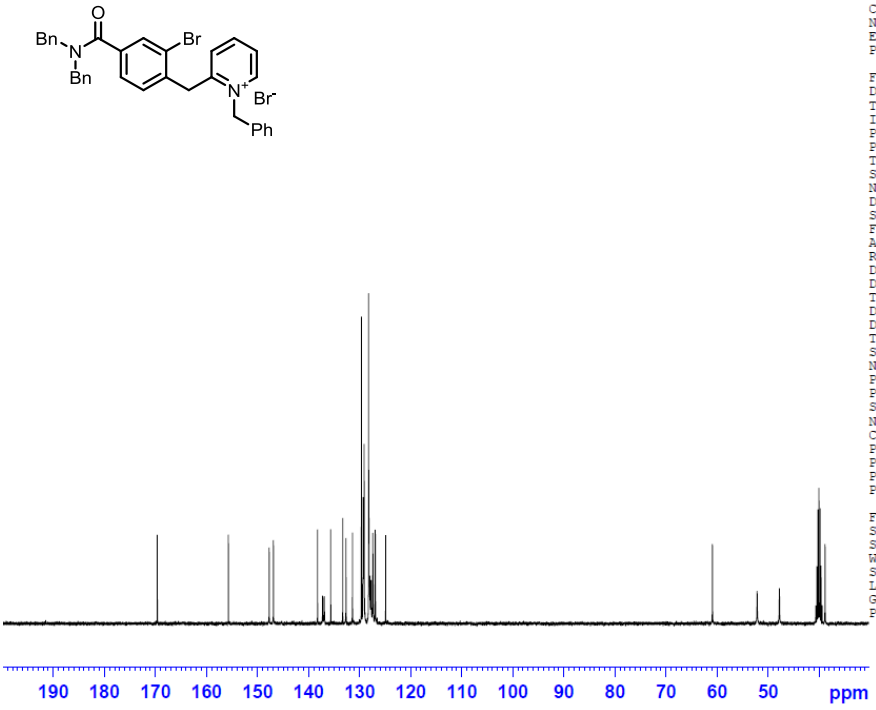
F2 - Processing parameters
SI                 65536
SF           100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```




```
Current Data Parameters
NAME          102061-033
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151111
Time              16.58 h
INSTRUM            spect
PROBHD   Z104450_0178 (
PULPROG             zg10
TD                 32768
SOLVENT             DMSO
NS                    32
DS                     4
SWH             5896.227 Hz
FIDRES          0.179939 Hz
AQ              2.7787263 sec
RG                   203
DW                84.800 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
TD0                    1
SFO1          400.1327209 MHz
NUC1                  1H
P1                14.00 usec
PLW1          12.05399990 W

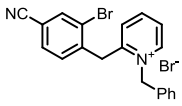
F2 - Processing parameters
SI                 65536
SF            400.1299980 MHz
WDW                   EM
SSB       0
LB                 0.05 Hz
GB        0
PC                 1.00
```




```
Current Data Parameters
NAME          102061-033
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151111
Time              17.11 h
INSTRUM            spect
PROBHD   Z104450_0178 (
PULPROG             zgpg
TD                 32768
SOLVENT             DMSO
NS                   260
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                   203
DW                20.800 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1          100.6243395 MHz
NUC1                  13C
P1                10.00 usec
PLW1          51.08800125 W
SFO2          400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2          12.05399990 W
PLW12          0.30075201 W
PLW13          0.15073690 W

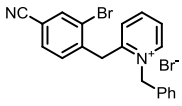
F2 - Processing parameters
SI                 65536
SF            100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

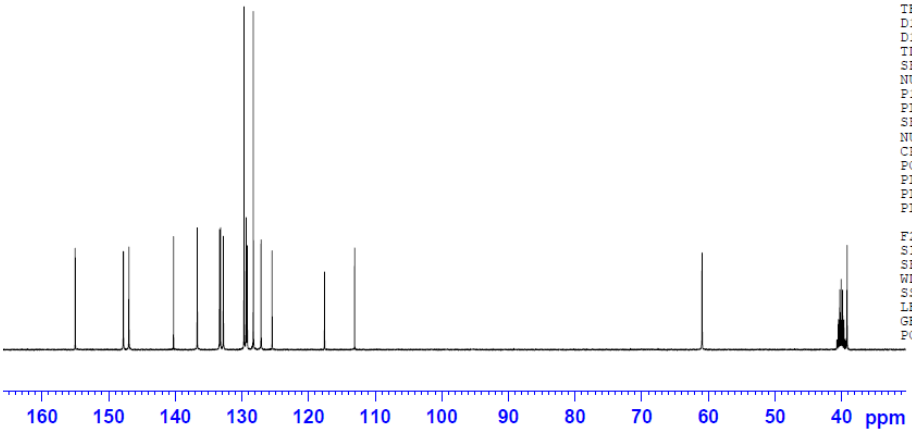



```
Current Data Parameters
NAME                  102900-016
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                  20151111
Time                      13.45 h
INSTRUM                   spect
PROBHD    Z104450_0178 (
PULPROG                    zg10
TD                        32768
SOLVENT                    DMSO
NS                           32
DS                            4
SWH                    5896.227 Hz
FIDRES                 0.179939 Hz
AQ                     2.7787263 sec
RG                          144
DW                        84.800 usec
DE                         6.50 usec
TE                        298.0 K
D1                     2.00000000 sec
TD0                            1
SFO1                 400.1327209 MHz
NUC1                         1H
P1                        14.00 usec
PLW1                12.05399990 W

F2 - Processing parameters
SI                         65536
SF                   400.1299887 MHz
WDW                           EM
SSB       0
LB                         0.05 Hz
GB        0
PC                         1.00
```

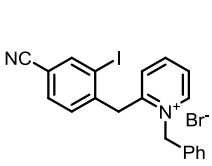





```
Current Data Parameters
NAME                  102900-016
EXPNO                          2
PROCNO                         1

F2 - Acquisition Parameters
Date_                  20151111
Time                      14.04 h
INSTRUM                   spect
PROBHD    Z104450_0178 (
PULPROG                    zgpg
TD                        32768
SOLVENT                    DMSO
NS                           365
DS                            4
SWH                   24038.461 Hz
FIDRES                 0.733596 Hz
AQ                     0.6815744 sec
RG                          203
DW                        20.800 usec
DE                         6.50 usec
TE                        298.0 K
D1                     2.00000000 sec
D11                    0.03000000 sec
TD0                            1
SFO1                100.6243395 MHz
NUC1                         13C
P1                        10.00 usec
PLW1                51.08800125 W
SFO2                400.1316005 MHz
NUC2                         1H
CPDPRG[2                waltz16
PCPD2                     90.00 usec
PLW2                12.05399990 W
PLW12                  0.30075201 W
PLW13                  0.15073690 W

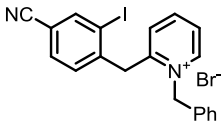
F2 - Processing parameters
SI                         65536
SF                  100.6127690 MHz
WDW                           EM
SSB       0
LB                         1.00 Hz
GB        0
PC                         1.40
```

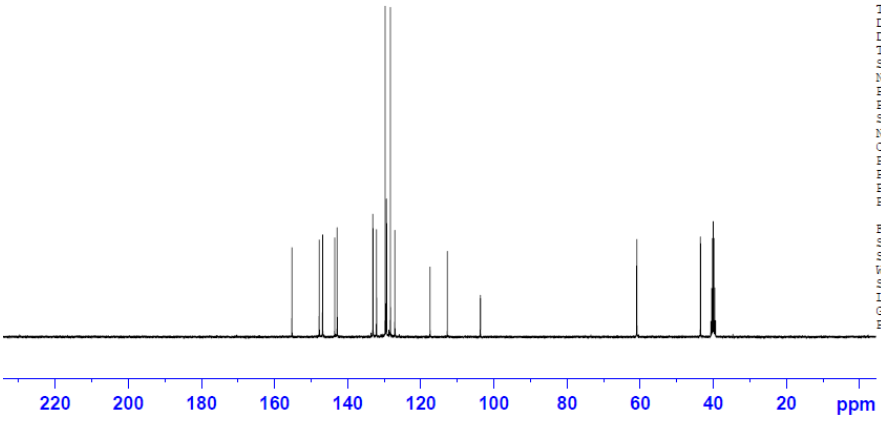



```
Current Data Parameters
NAME          102116-036
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_          20151111
Time              14.10 h
INSTRUM           spect
PROBHD   Z104450_0178 (
PULPROG           zg10
TD               32768
SOLVENT           DMSO
NS                  32
DS                   4
SWH            5896.227 Hz
FIDRES         0.179939 Hz
AQ             2.7787263 sec
RG                 203
DW              84.800 usec
DE               6.50 usec
TE              298.0 K
D1           2.00000000 sec
TD0                  1
SFO1       400.1327209 MHz
NUC1               1H
P1              14.00 usec
PLW1       12.05399990 W

F2 - Processing parameters
SI                65536
SF           400.1299956 MHz
WDW                EM
SSB       0
LB              0.05 Hz
GB        0
PC              1.00
```

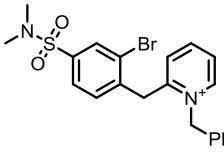





```
Current Data Parameters
NAME          102116-036
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_          20151111
Time              14.15 h
INSTRUM           spect
PROBHD   Z104450_0178 (
PULPROG           zgpg
TD               32768
SOLVENT           DMSO
NS                 480
DS                   4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG                 203
DW              20.800 usec
DE               6.50 usec
TE              298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1       100.6243395 MHz
NUC1              13C
P1              10.00 usec
PLW1       51.08800125 W
SFO2       400.1316005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2           90.00 usec
PLW2       12.05399990 W
PLW12       0.30075201 W
PLW13       0.15073690 W

F2 - Processing parameters
SI                65536
SF           100.6127690 MHz
WDW                EM
SSB       0
LB              1.00 Hz
GB        0
PC              1.40
```



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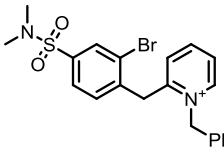
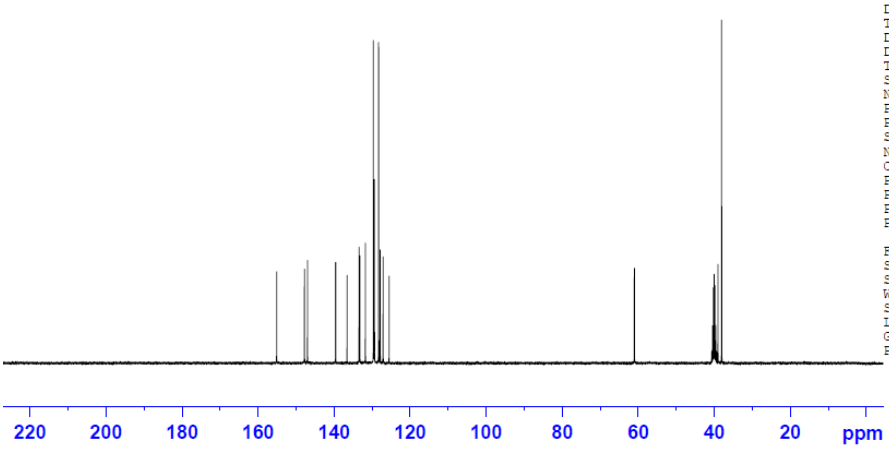
```
Current Data Parameters
NAME          103682-040
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151111
Time              16.38 h
INSTRUM            spect
PROBHD   Z104450_0178 (
PULPROG            zg10
TD                32768
SOLVENT            DMSO
NS                   32
DS                    4
SWH            5896.227 Hz
FIDRES         0.179939 Hz
AQ             2.7787263 sec
RG                  203
DW                84.800 usec
DE                 6.50 usec
TE                298.0 K
D1            2.00000000 sec
TD0                   1
SFO1         400.1327209 MHz
NUC1                 1H
P1                14.00 usec
PLW1         12.05399990 W

F2 - Processing parameters
SI                65536
SF           400.1300000 MHz
WDW                  EM
SSB       0
LB                0.05 Hz
GB        0
PC                1.00
```



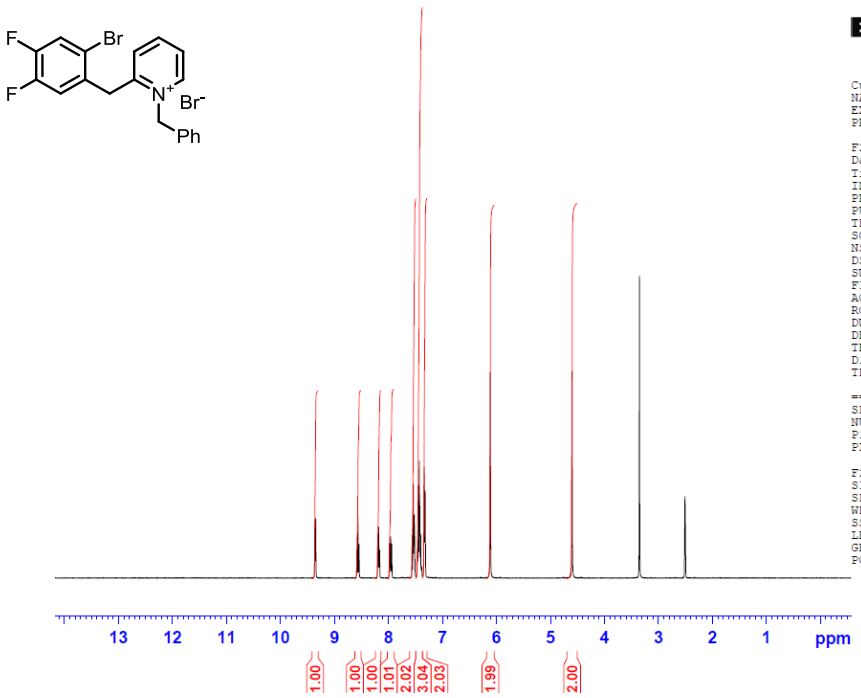


BRUKER

```
Current Data Parameters
NAME          103682-040
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151111
Time              16.52 h
INSTRUM            spect
PROBHD   Z104450_0178 (
PULPROG            zgpg
TD                32768
SOLVENT            DMSO
NS                  260
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG                  203
DW                20.800 usec
DE                 6.50 usec
TE                298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1         100.6243395 MHz
NUC1                 13C
P1                10.00 usec
PLW1         51.08800125 W
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         12.05399990 W
PLW12         0.30075201 W
PLW13         0.15073690 W

F2 - Processing parameters
SI                65536
SF           100.6127690 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



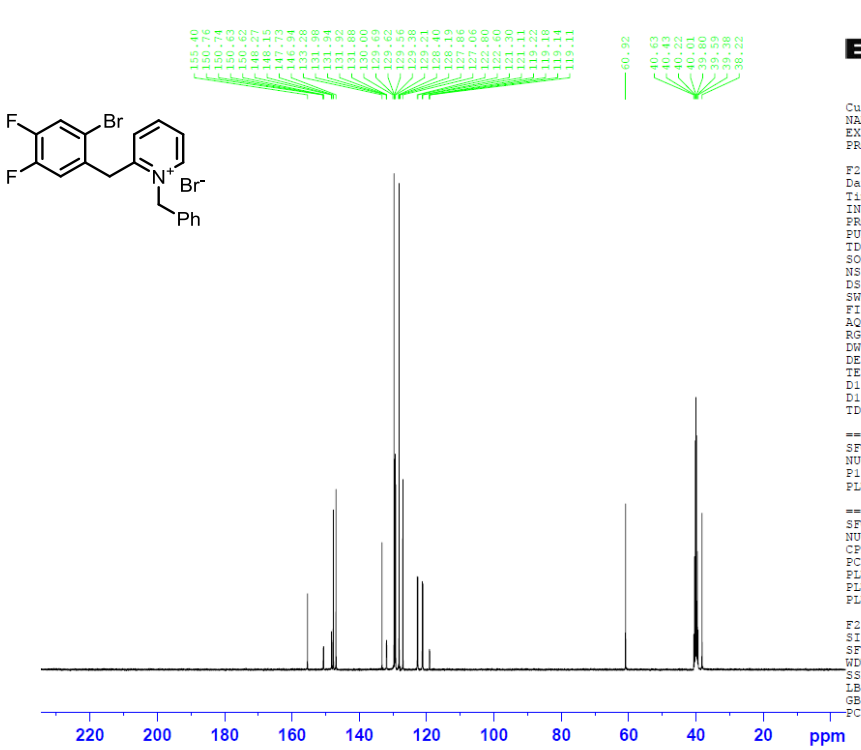
BRUKER

```
Current Data Parameters
NAME          103553-028
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_          20151215
Time              17.48
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg10
TD                32768
SOLVENT            DMSO
NS                   16
DS                    4
SWH            5896.227 Hz
FIDRES        0.179939 Hz
AQ            2.7787263 sec
RG                  456
DW               84.800 usec
DE                6.50 usec
TE               298.0 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1327209 MHz
NUC1                   1H
P1                15.00 usec
PLW1         10.50000000 W

F2 - Processing parameters
SI                 65536
SF            400.1300000 MHz
WDW                   EM
SSB          0
LB                0.05 Hz
GB           0
PC                1.00
```



BRUKER

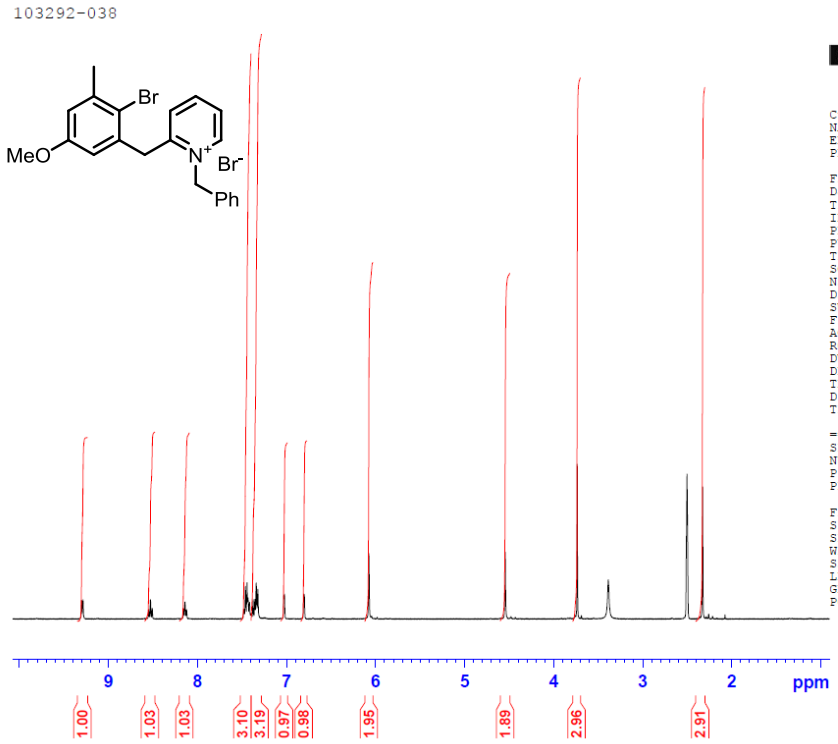
```
Current Data Parameters
NAME          103553-028
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_          20151215
Time              22.59
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg
TD                32768
SOLVENT            DMSO
NS                 5120
DS                    4
SWH           24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                 2050
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         100.6243395 MHz
NUC1                  13C
P1                10.90 usec
PLW1         43.00000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         10.50000000 W
PLW12         0.29166999 W
PLW13         0.14670999 W

F2 - Processing parameters
SI                 65536
SF            100.6127690 MHz
WDW                   EM
SSB          0
LB                1.00 Hz
GB           0
PC                1.40
```



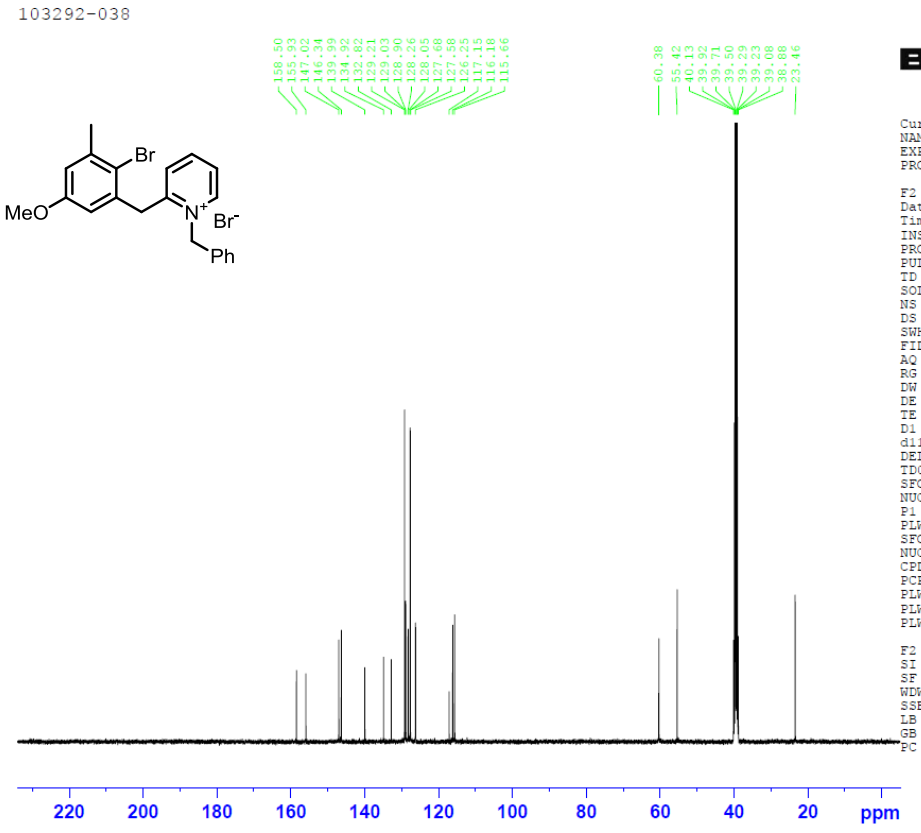
BRUKER

```
Current Data Parameters
NAME                 103292-038
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_               20151216
Time                   17.14
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg10
TD                    32768
SOLVENT                DMSO
NS                       16
DS                        4
SWH                5896.227 Hz
FIDRES            0.179939 Hz
AQ                2.7787263 sec
RG                      724
DW                 84.800 usec
DE                  6.50 usec
TE                  298.0 K
D1                2.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1            400.1327209 MHz
NUC1                      1H
P1                   15.00 usec
PLW1           10.50000000 W

F2 - Processing parameters
SI                    65536
SF              400.1300018 MHz
WDW                      EM
SSB          0
LB                  0.05 Hz
GB           0
PC                    1.00
```

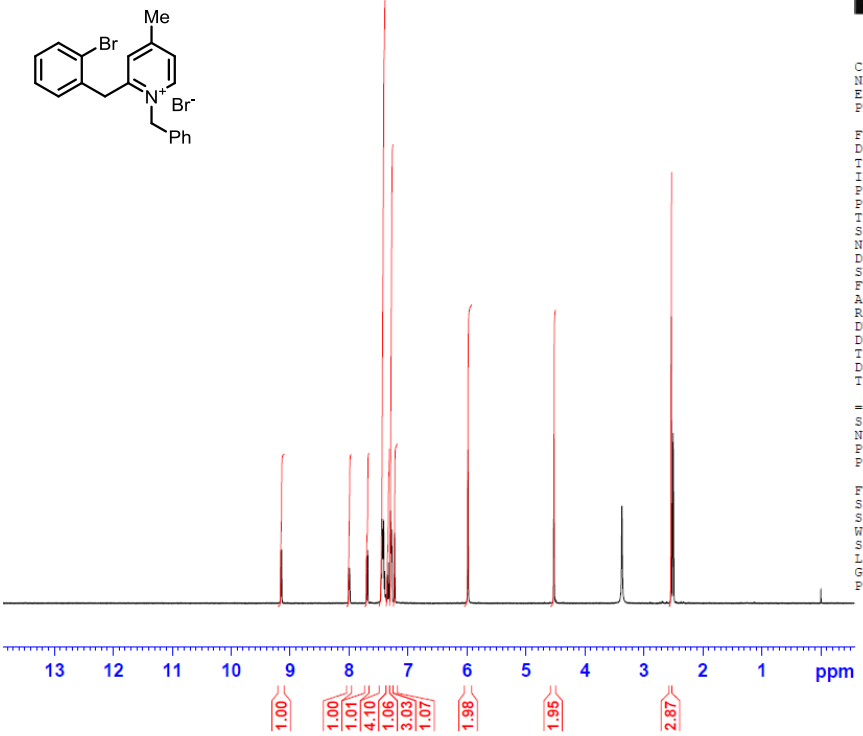


BRUKER

```
Current Data Parameters
NAME                 103292-038
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_               20141031
Time                   1.30
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zgpg
TD                    32768
SOLVENT                DMSO
NS                     5120
DS                        4
SWH               24038.461 Hz
FIDRES            0.733596 Hz
AQ                0.6815744 sec
RG                     2050
DW                 20.800 usec
DE                  6.50 usec
TE                  298.0 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                       1
SFO1            100.6243395 MHz
NUC1                     13C
P1                   10.10 usec
PLW1           -1.00000000 W
SFO2            400.1316005 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                90.00 usec
PLW2           -1.00000000 W
PLW12          -1.00000000 W
PLW13          -1.00000000 W

F2 - Processing parameters
SI                    65536
SF              100.6128193 MHz
WDW                      EM
SSB          0
LB                  1.00 Hz
GB           0
PC                    1.40
```

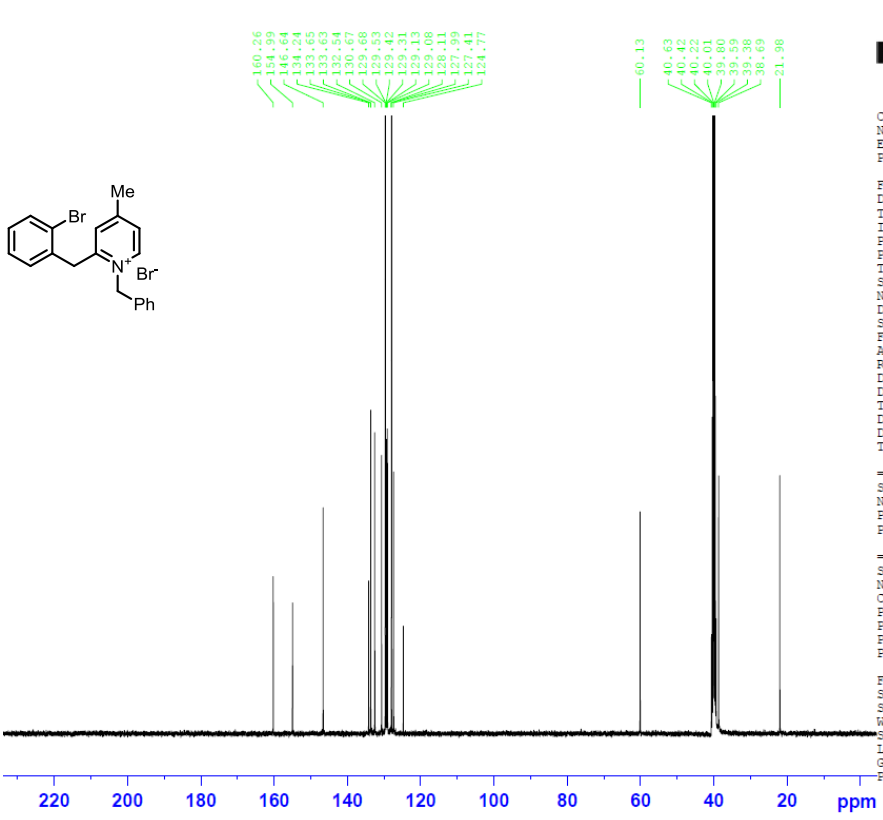



```
Current Data Parameters
NAME          103292-043
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_          20151216
Time              18.17
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg10
TD               32768
SOLVENT           DMSO
NS                  16
DS                   4
SWH           5896.227 Hz
FIDRES        0.179939 Hz
AQ            2.7787263 sec
RG                 645
DW              84.800 usec
DE               6.50 usec
TE              298.0 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        400.1327209 MHz
NUC1                   1H
P1                15.00 usec
PLW1        10.50000000 W

F2 - Processing parameters
SI                 65536
SF          400.1300012 MHz
WDW                   EM
SSB       0
LB                0.05 Hz
GB        0
PC                1.00
```



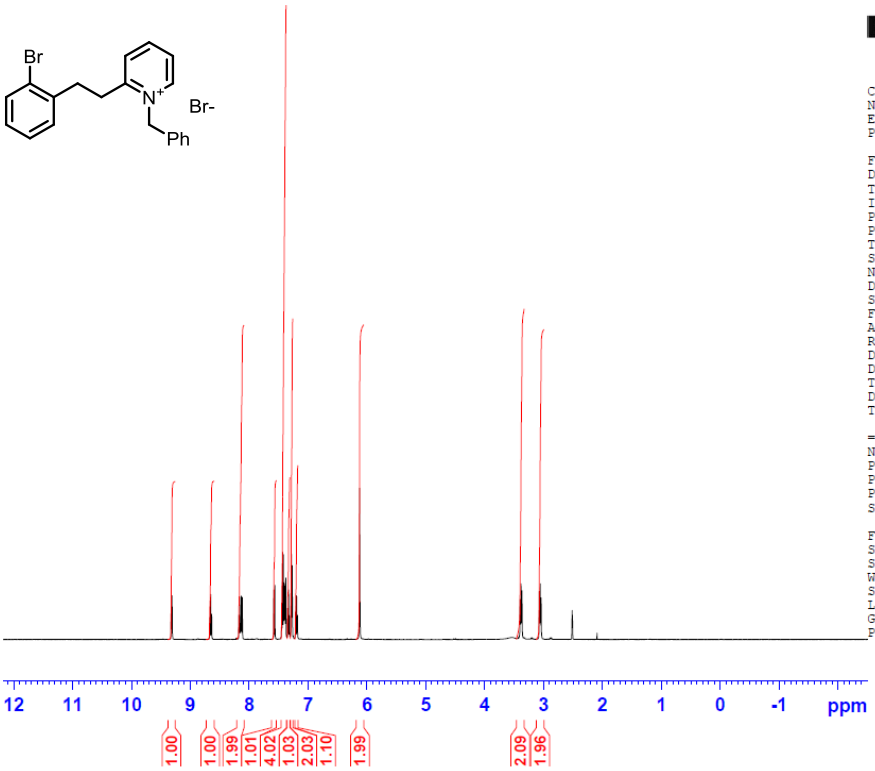

```
Current Data Parameters
NAME          103292-043
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_          20151217
Time               2.31
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg
TD               32768
SOLVENT           DMSO
NS                5120
DS                   4
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                2050
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        100.6243395 MHz
NUC1                   13C
P1                10.90 usec
PLW1        43.00000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2        10.50000000 W
PLW12        0.29166999 W
PLW13        0.14670999 W

F2 - Processing parameters
SI                 65536
SF          100.6127690 MHz
WDW                   EM
SSB       0
LB             1.00 Hz
GB        0
PC                1.40
```

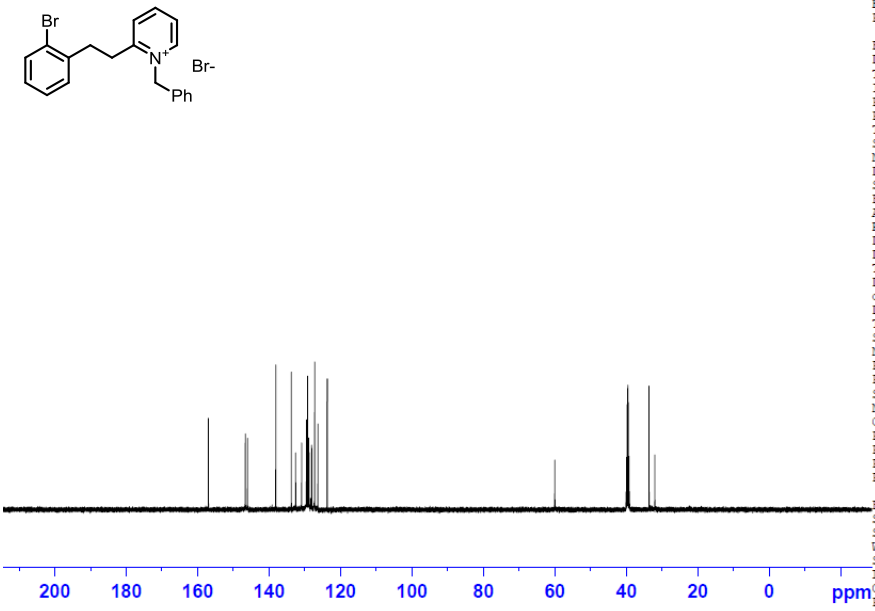



```
Current Data Parameters
NAME                  103210-096
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                 20151120
Time                      11.11
INSTRUM                   spect
PROBHD     5 mm PABBI 1H-
PULPROG                    zg10
TD                        32768
SOLVENT                    DMSO
NS                           32
DS                            0
SWH                    7500.000 Hz
FIDRES                 0.228882 Hz
AQ                     2.1845334 sec
RG                           144
DW                        66.667 usec
DE                         6.50 usec
TE                        299.0 K
D1                    1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                         8.00 usec
PL1                        3.00 dB
PL1W                14.98121262 W
SFO1                500.1325007 MHz

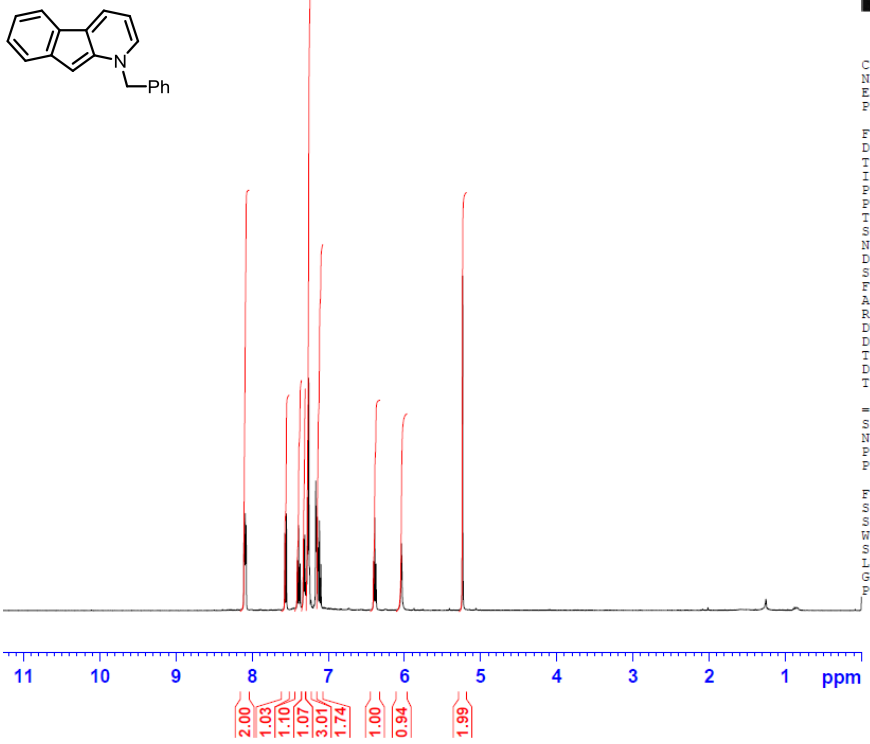
F2 - Processing parameters
SI                        16384
SF                  500.1300000 MHz
WDW                          EM
SSB                0
LB                         0.30 Hz
GB                 0
PC                         1.00
```




```
Current Data Parameters
NAME                  103210-096
EXPNO                          2
PROCNO                         1

F2 - Acquisition Parameters
Date_                 20151120
Time                      11.29
INSTRUM                   spect
PROBHD     5 mm PABBI 1H-
PULPROG                   zgpg
TD                       262144
SOLVENT                    DMSO
NS                          180
DS                            0
SWH                   31250.000 Hz
FIDRES                 0.119209 Hz
AQ                     4.1943040 sec
RG                          2050
DW                        16.000 usec
DE                         6.50 usec
TE                        299.0 K
D1                    1.00000000 sec
d11                   0.03000000 sec
DELTA                 0.89999998 sec
TD0                            1
SFO1                125.7698617 MHz
NUC1                         13C
P1                        15.75 usec
PLW1                 -1.00000000 W
SFO2                500.1325007 MHz
NUC2                          1H
CPDPRG[2                waltz16
PCPD2                     80.00 usec
PLW2                 -1.00000000 W
PLW12                -1.00000000 W
PLW13                -1.00000000 W

F2 - Processing parameters
SI                        131072
SF                  125.7578519 MHz
WDW                          EM
SSB                0
LB                         0.30 Hz
GB                 0
PC                         1.40
```

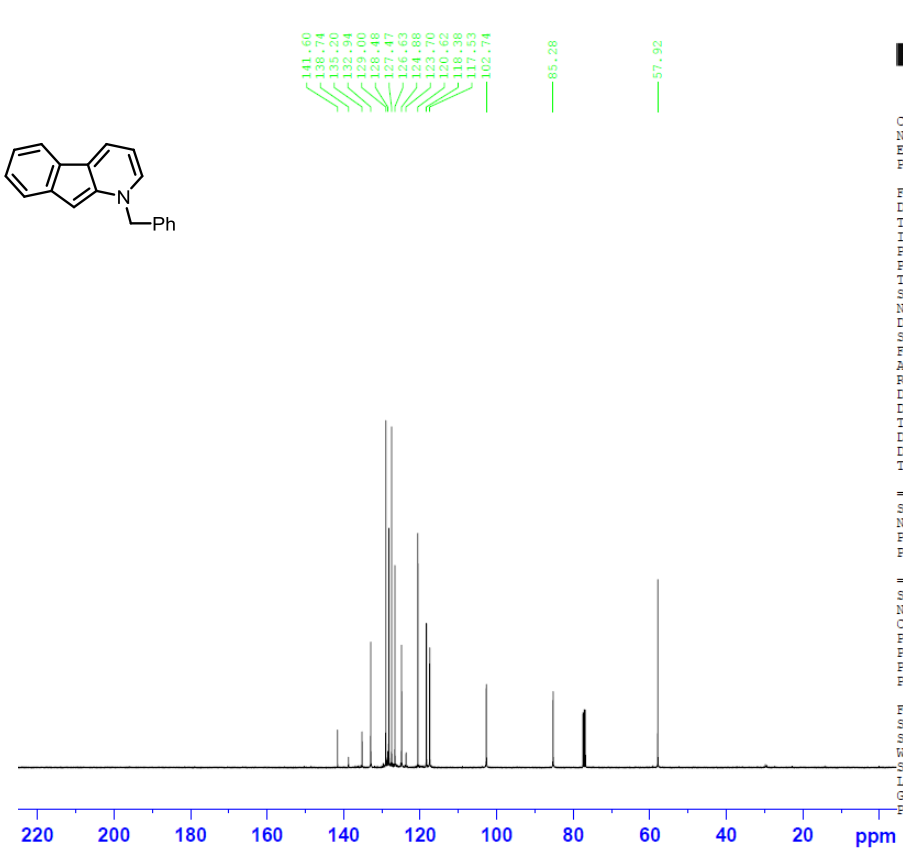



```
Current Data Parameters
NAME          103682-051
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151217
Time               17.40
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg10
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     4
SWH             5896.227 Hz
FIDRES          0.179939 Hz
AQ              2.7787263 sec
RG                   203
DW                84.800 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1327209 MHz
NUC1                  1H
P1                 15.00 usec
PLW1          10.50000000 W

F2 - Processing parameters
SI                 65536
SF            400.1300465 MHz
WDW                   EM
SSB       0
LB                 0.05 Hz
GB        0
PC                 1.00
```



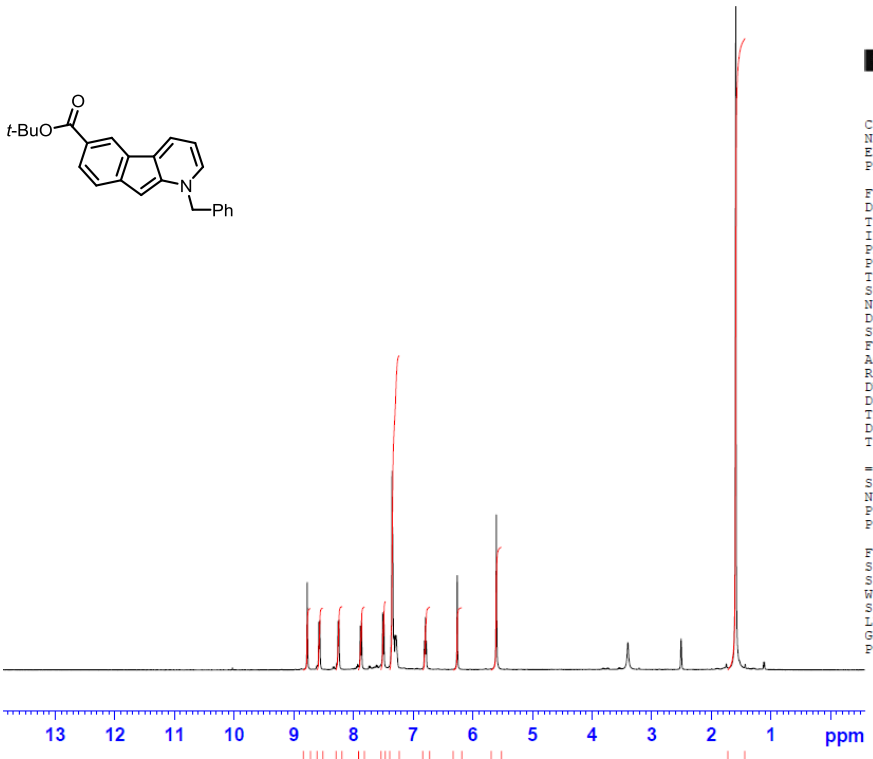

```
Current Data Parameters
NAME          103682-051
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151217
Time               23.44
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg
TD                 32768
SOLVENT            CDCl3
NS                  3000
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                  2050
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          100.6243395 MHz
NUC1                  13C
P1                10.90 usec
PLW1          43.00000000 W

======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2          10.50000000 W
PLW12          0.29166999 W
PLW13          0.14670999 W

F2 - Processing parameters
SI                 65536
SF            100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

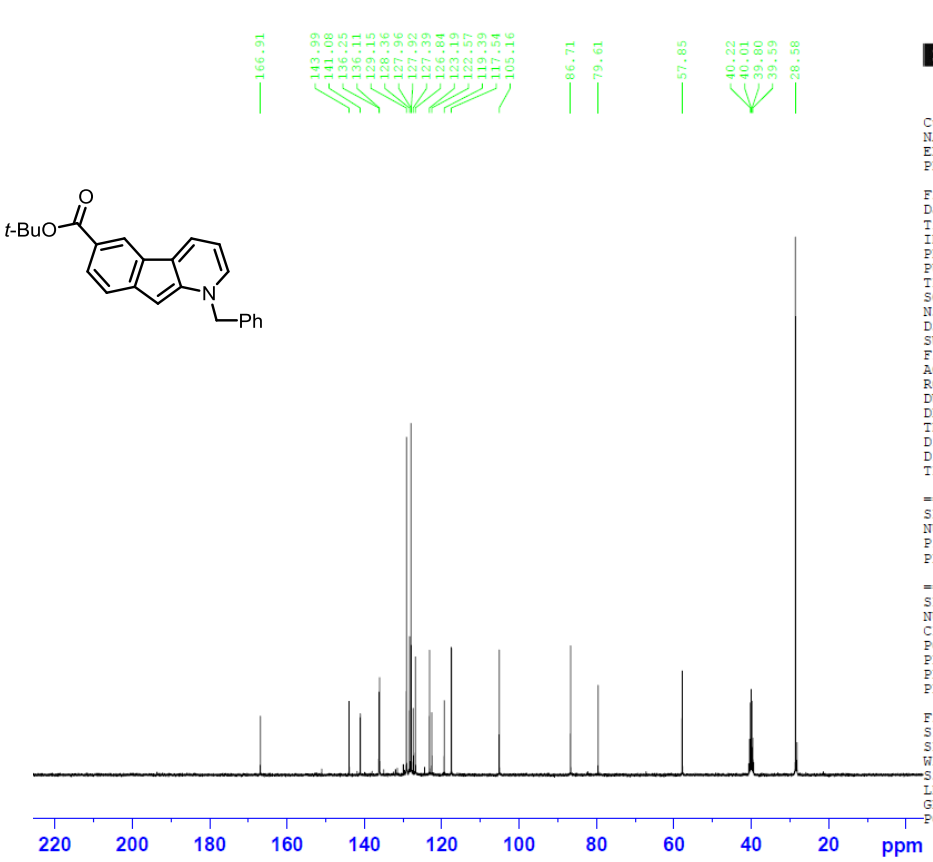



```
Current Data Parameters
NAME                  102061-036
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                  20151216
Time                       9.30
INSTRUM                   spect
PROBHD    5 mm PABBO BB-
PULPROG                    zg10
TD                        32768
SOLVENT                    DMSO
NS                           16
DS                            4
SWH                    5896.227 Hz
FIDRES                 0.179939 Hz
AQ                     2.7787263 sec
RG                           203
DW                        84.800 usec
DE                         6.50 usec
TE                        298.0 K
D1                     2.00000000 sec
TD0                            1

======== CHANNEL f1 ========
SFO1                 400.1327209 MHz
NUC1                         1H
P1                        15.00 usec
PLW1                10.50000000 W

F2 - Processing parameters
SI                         65536
SF                   400.1300000 MHz
WDW                           EM
SSB                0
LB                         0.05 Hz
GB                 0
PC                         1.00
```



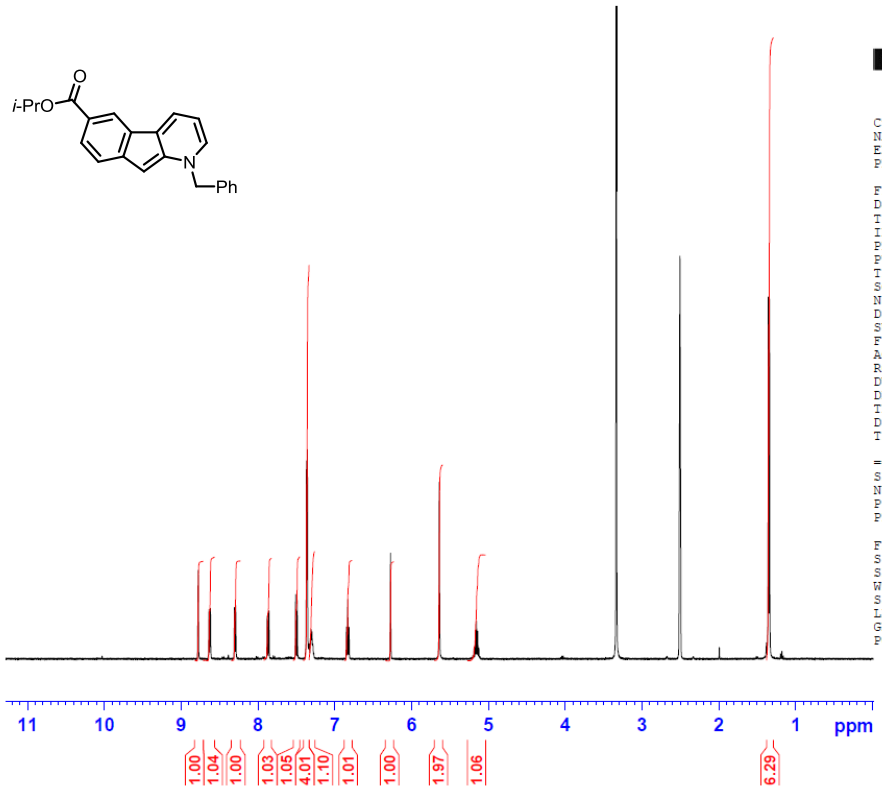

```
Current Data Parameters
NAME                  102061-036
EXPNO                          2
PROCNO                         1

F2 - Acquisition Parameters
Date_                  20151216
Time                       9.47
INSTRUM                   spect
PROBHD    5 mm PABBO BB-
PULPROG                    zgpg
TD                        32768
SOLVENT                    DMSO
NS                           320
DS                            4
SWH                   24038.461 Hz
FIDRES                 0.733596 Hz
AQ                     0.6815744 sec
RG                          2050
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                 100.6243395 MHz
NUC1                         13C
P1                        10.90 usec
PLW1                43.00000000 W

======== CHANNEL f2 ========
SFO2                 400.1316005 MHz
NUC2                         1H
CPDPRG[2                waltz16
PCPD2                     90.00 usec
PLW2                10.50000000 W
PLW12                0.29166999 W
PLW13                0.14670999 W

F2 - Processing parameters
SI                         65536
SF                   100.6127690 MHz
WDW                           EM
SSB                0
LB                         1.00 Hz
GB                 0
PC                         1.40
```



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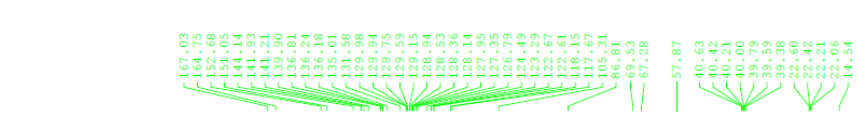
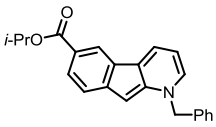
```
Current Data Parameters
NAME          103682-049
EXPNO                  1
PROCNO                 1

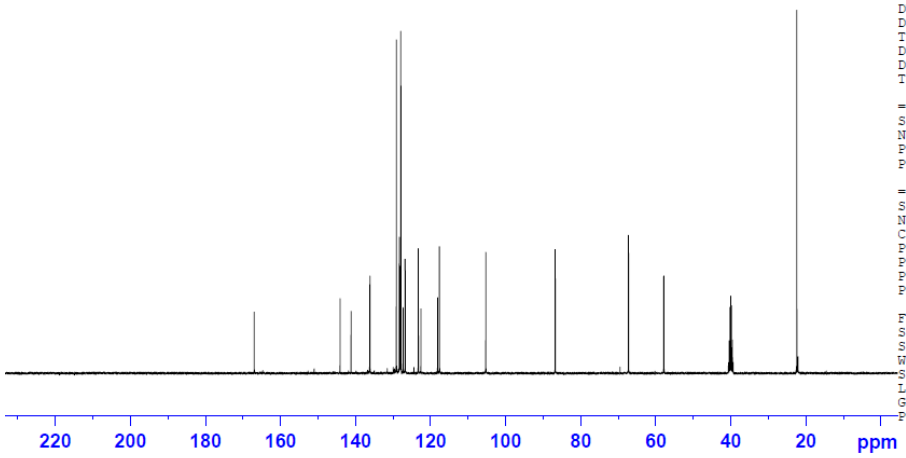
F2 - Acquisition Parameters
Date_           20151216
Time              10.10
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg10
TD                32768
SOLVENT            DMSO
NS                   32
DS                    4
SWH            5896.227 Hz
FIDRES         0.179939 Hz
AQ             2.7787263 sec
RG                  812
DW               84.800 usec
DE                6.50 usec
TE                298.0 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1327209 MHz
NUC1               1H
P1                15.00 usec
PLW1         10.50000000 W

F2 - Processing parameters
SI                 65536
SF           400.1300000 MHz
WDW                  EM
SSB       0
LB                0.05 Hz
GB        0
PC                1.00
```







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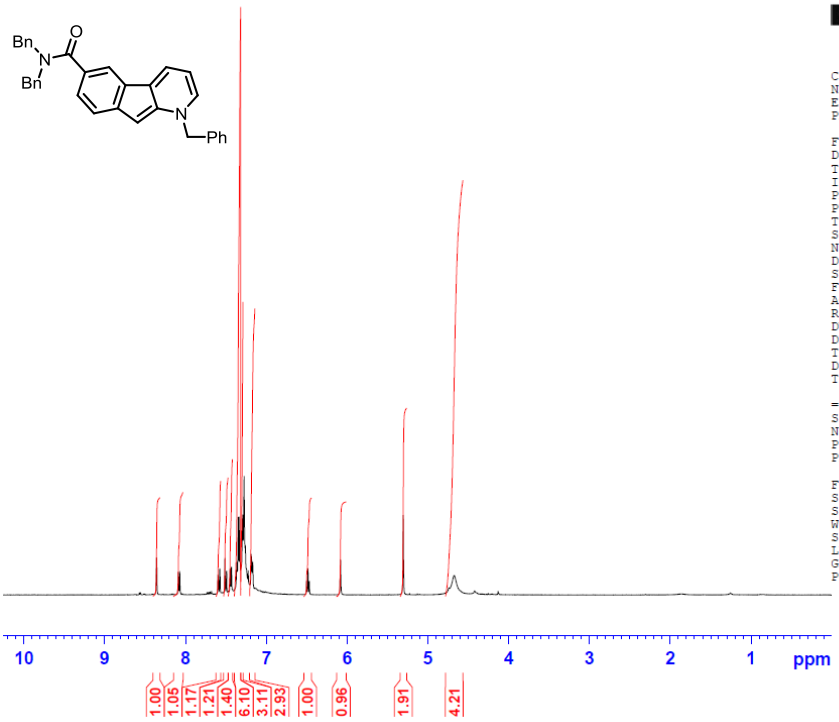
```
Current Data Parameters
NAME          103682-049
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151216
Time              11.24
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg
TD                32768
SOLVENT            DMSO
NS                   320
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG                 2050
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         100.6243395 MHz
NUC1               13C
P1                10.90 usec
PLW1         43.00000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         10.50000000 W
PLW12         0.29166999 W
PLW13         0.14670999 W

F2 - Processing parameters
SI                 65536
SF           100.6127690 MHz
WDW                  EM
SSB       0
LB             1.00 Hz
GB        0
PC                1.40
```

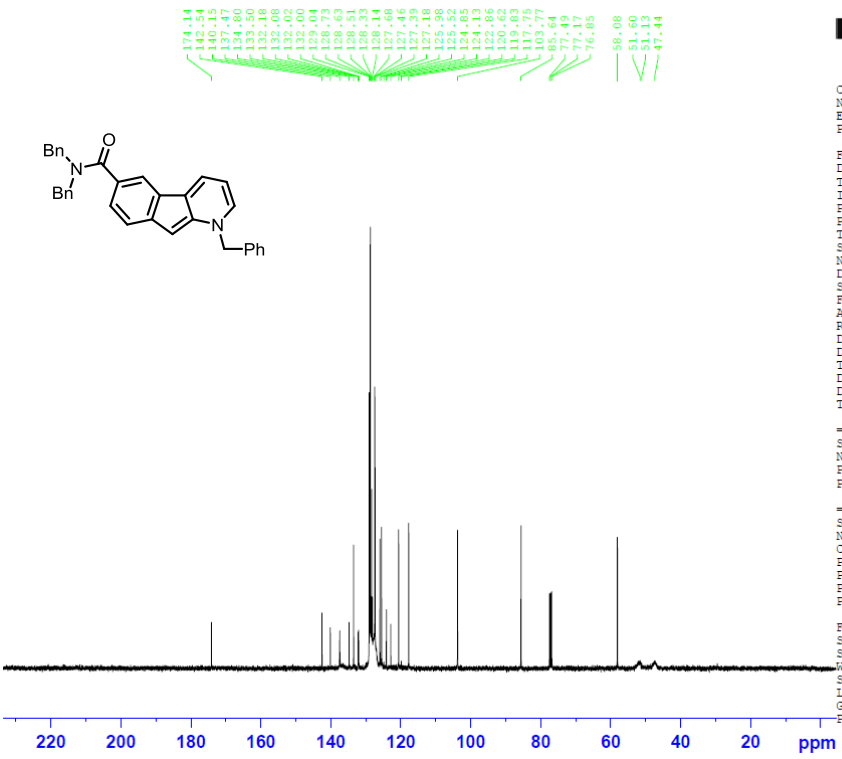



```
Current Data Parameters
NAME          102061-037
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_          20151217
Time              17.34
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg10
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    4
SWH            5896.227 Hz
FIDRES        0.179939 Hz
AQ            2.7787263 sec
RG                  203
DW               84.800 usec
DE                6.50 usec
TE               298.0 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1327209 MHz
NUC1                   1H
P1                  15.00 usec
PLW1         10.50000000 W

F2 - Processing parameters
SI                 65536
SF          400.1300240 MHz
WDW                   EM
SSB       0
LB                0.05 Hz
GB        0
PC                1.00
```



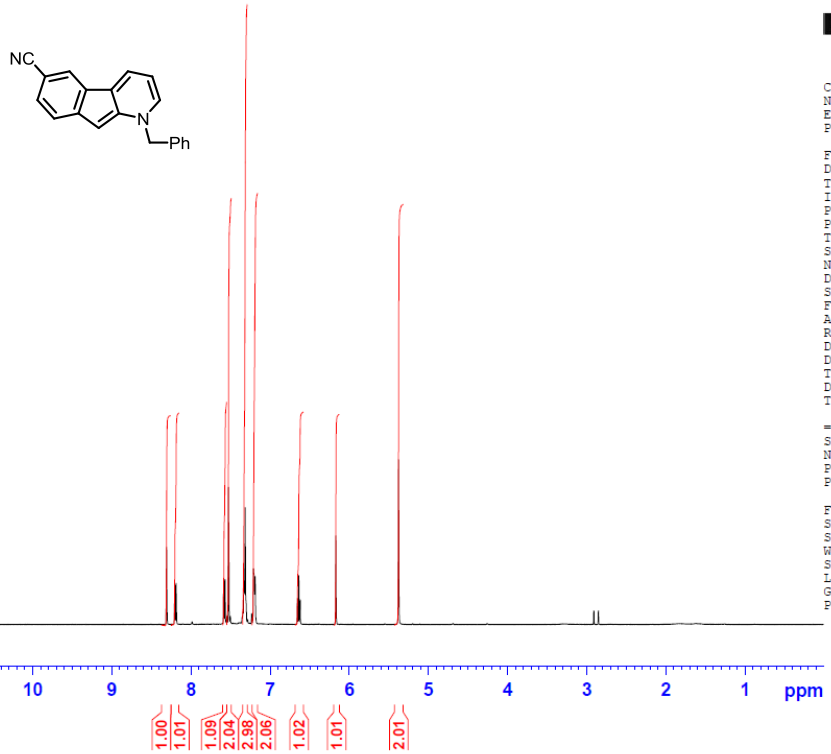

```
Current Data Parameters
NAME          102061-037
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_          20151215
Time              15.24
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg
TD                32768
SOLVENT           CDCl3
NS                  320
DS                    4
SWH           24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                 2050
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         100.6243395 MHz
NUC1                   13C
P1                  10.90 usec
PLW1         43.00000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2         10.50000000 W
PLW12         0.29166999 W
PLW13         0.14670999 W

F2 - Processing parameters
SI                 65536
SF          100.6127690 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



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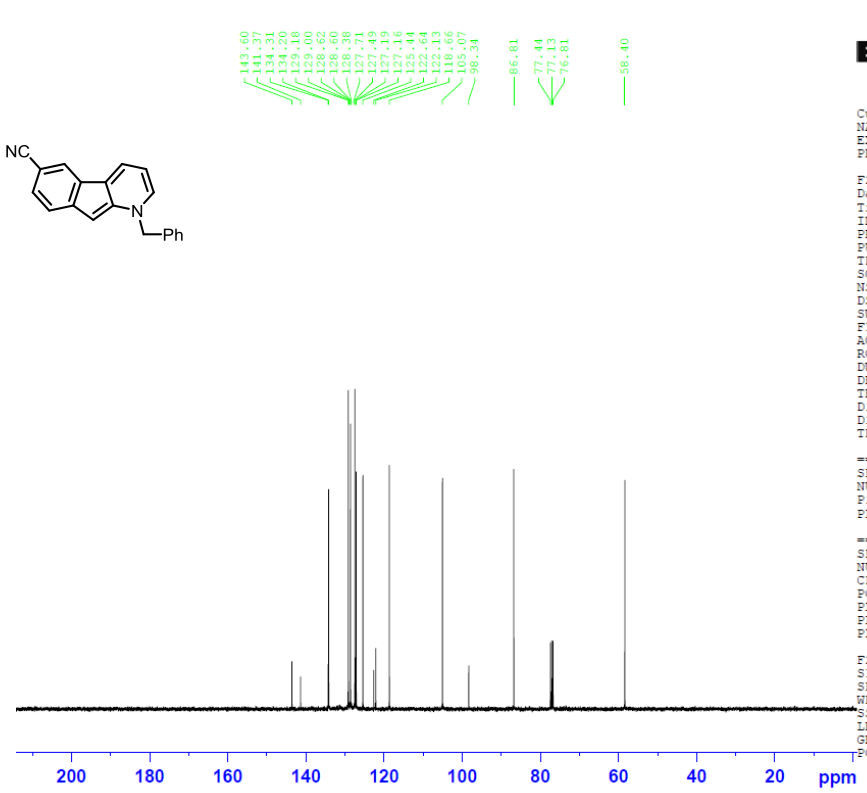
```
Current Data Parameters
NAME          103210-041
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151215
Time               14.40
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg10
TD                 32768
SOLVENT            CDCl3
NS                     4
DS                     4
SWH             5896.227 Hz
FIDRES          0.179939 Hz
AQ              2.7787263 sec
RG                   322
DW                84.800 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1327209 MHz
NUC1                   1H
P1                 15.00 usec
PLW1         10.50000000 W

F2 - Processing parameters
SI                 65536
SF           400.1300200 MHz
WDW                   EM
SSB       0
LB                 0.05 Hz
GB        0
PC                 1.00
```



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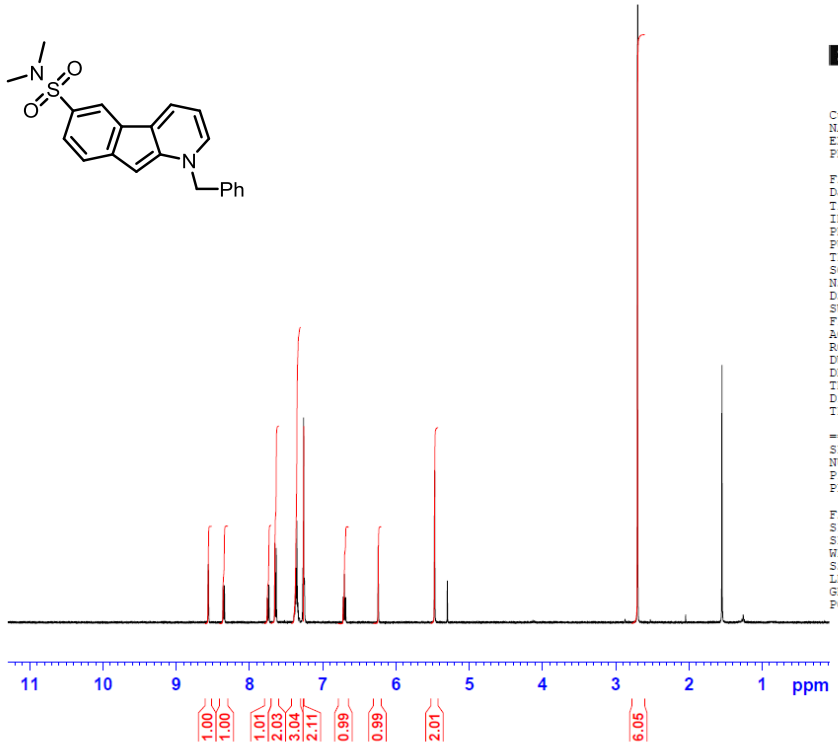
```
Current Data Parameters
NAME          103210-041
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151215
Time               14.58
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg
TD                 32768
SOLVENT            CDCl3
NS                   320
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                  2050
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         100.6243395 MHz
NUC1                  13C
P1                 10.90 usec
PLW1         43.00000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2              90.00 usec
PLW2         10.50000000 W
PLW12         0.29166999 W
PLW13         0.14670999 W

F2 - Processing parameters
SI                 65536
SF           100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



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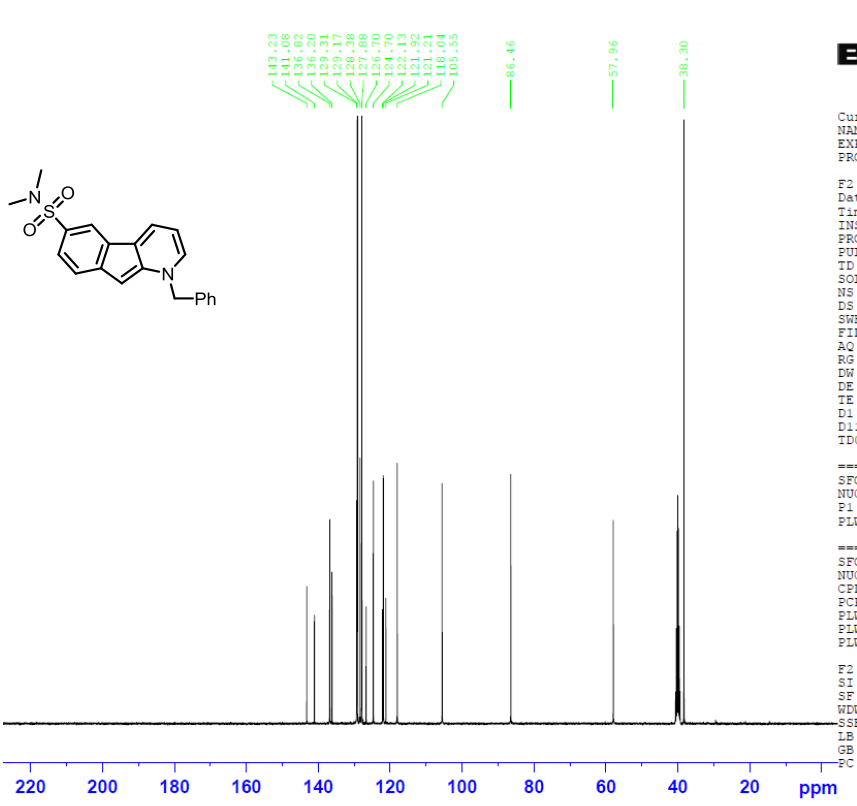
```
Current Data Parameters
NAME          103682-050
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151217
Time               11.01
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg10
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     4
SWH            5896.227 Hz
FIDRES        0.179939 Hz
AQ            2.7787263 sec
RG                  1150
DW                84.800 usec
DE                 6.50 usec
TE                298.0 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1327209 MHz
NUC1                   1H
P1                 15.00 usec
PLW1        10.50000000 W

F2 - Processing parameters
SI                 65536
SF           400.1300099 MHz
WDW                   EM
SSB       0
LB                 0.05 Hz
GB        0
PC                 1.00
```



BRUKER

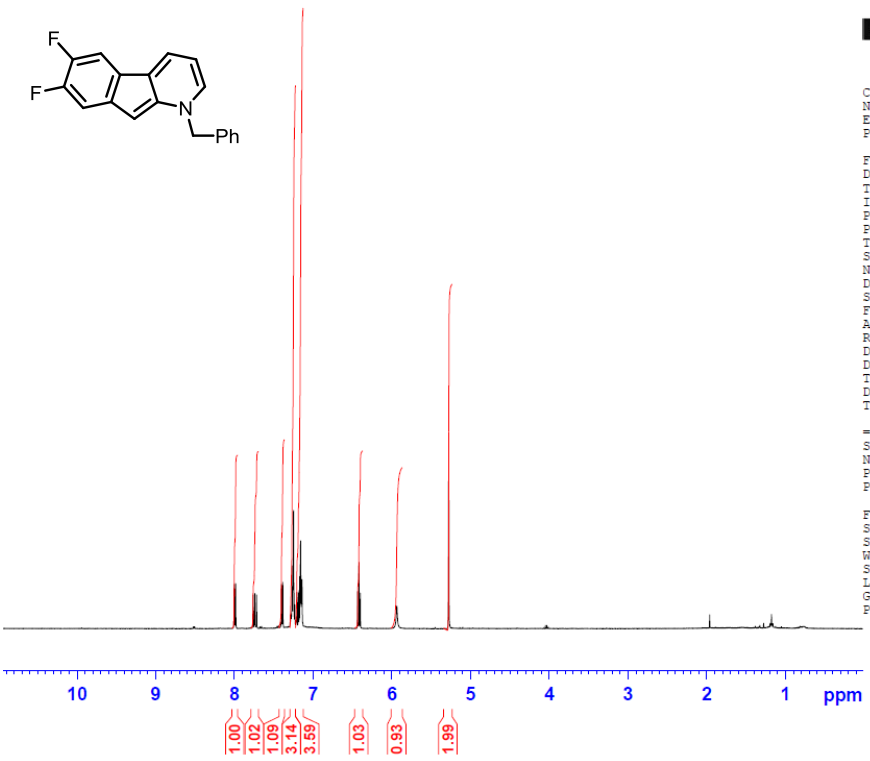
```
Current Data Parameters
NAME          103682-050
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151218
Time               2.05
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg
TD                 32768
SOLVENT             DMSO
NS                  3000
DS                     4
SWH           24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                  2050
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         100.6243395 MHz
NUC1                  13C
P1                 10.90 usec
PLW1        43.00000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2        10.50000000 W
PLW12        0.29166999 W
PLW13        0.14670999 W

F2 - Processing parameters
SI                 65536
SF           100.6127690 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



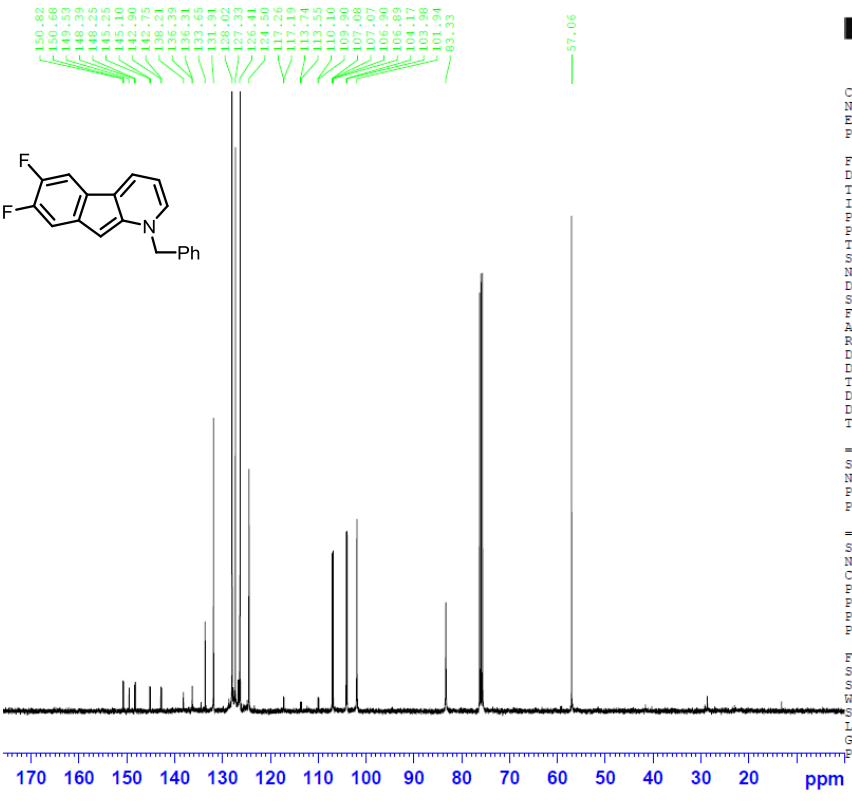
BRUKER

```
Current Data Parameters
NAME          103682-054
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151221
Time               14.22
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg10
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     4
SWH             5896.227 Hz
FIDRES          0.179939 Hz
AQ              2.7787263 sec
RG                   645
DW                84.800 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1327209 MHz
NUC1                  1H
P1                15.00 usec
PLW1          10.50000000 W

F2 - Processing parameters
SI                 65536
SF            400.1300456 MHz
WDW                   EM
SSB       0
LB                 0.05 Hz
GB        0
PC                 1.00
```



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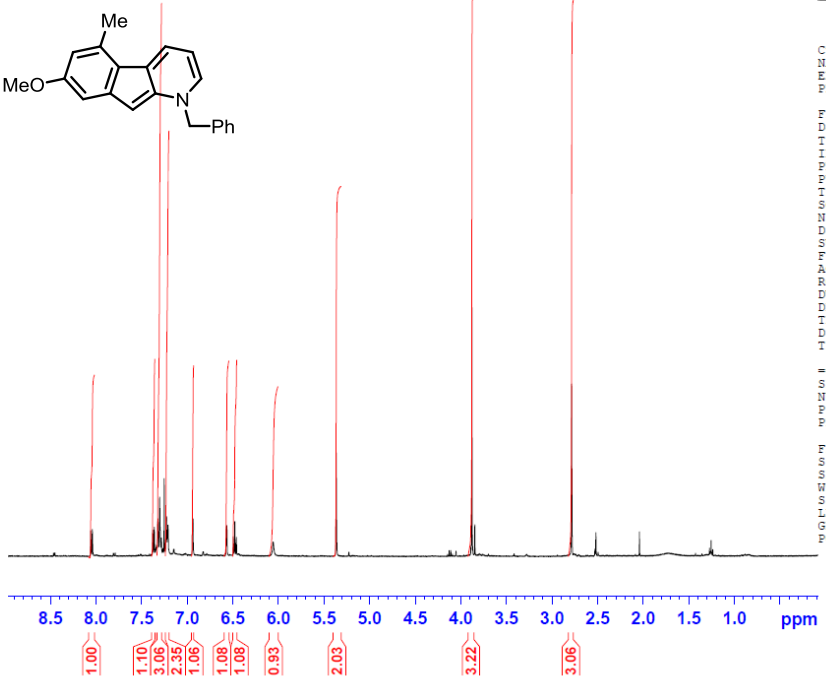
```
Current Data Parameters
NAME          103682-054
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151222
Time               1.56
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg
TD                 32768
SOLVENT            CDCl3
NS                  9000
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                  2050
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          100.6243395 MHz
NUC1                  13C
P1                10.90 usec
PLW1          43.00000000 W

======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          10.50000000 W
PLW12          0.29166999 W
PLW13          0.14670999 W

F2 - Processing parameters
SI                 65536
SF            100.6128742 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

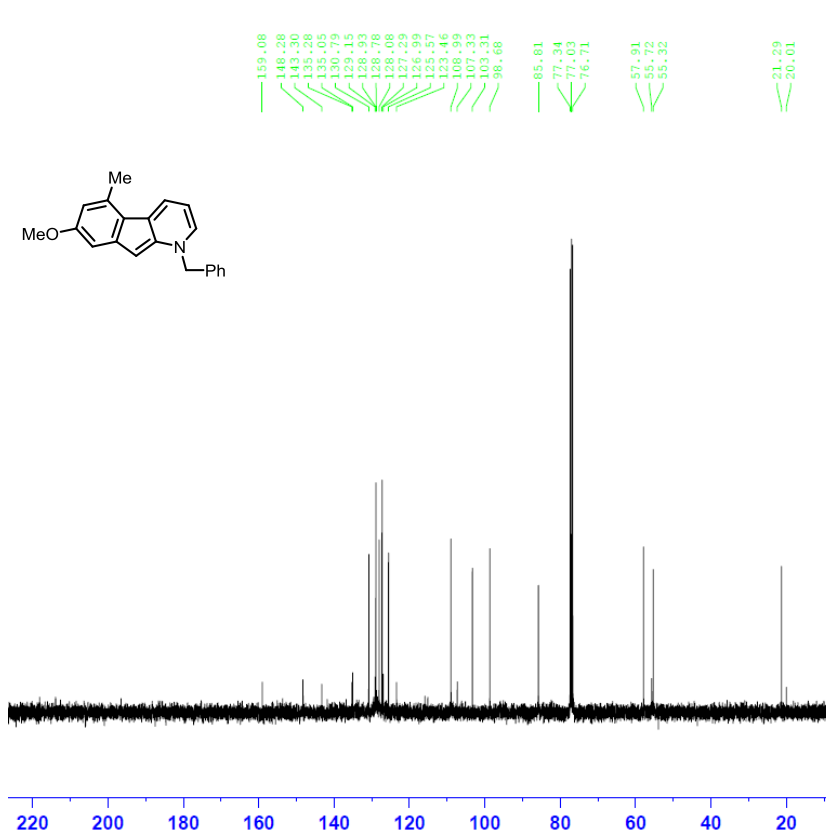



```
Current Data Parameters
NAME          103682-053
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151221
Time              13.53
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg10
TD               32768
SOLVENT          CDCl3
NS                  16
DS                   4
SWH           5896.227 Hz
FIDRES        0.179939 Hz
AQ           2.7787263 sec
RG                 812
DW              84.800 usec
DE               6.50 usec
TE              298.0 K
D1           2.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        400.1327209 MHz
NUC1               1H
P1              15.00 usec
PLW1        10.50000000 W

F2 - Processing parameters
SI               65536
SF          400.1300126 MHz
WDW                EM
SSB       0
LB              0.05 Hz
GB        0
PC              1.00
```



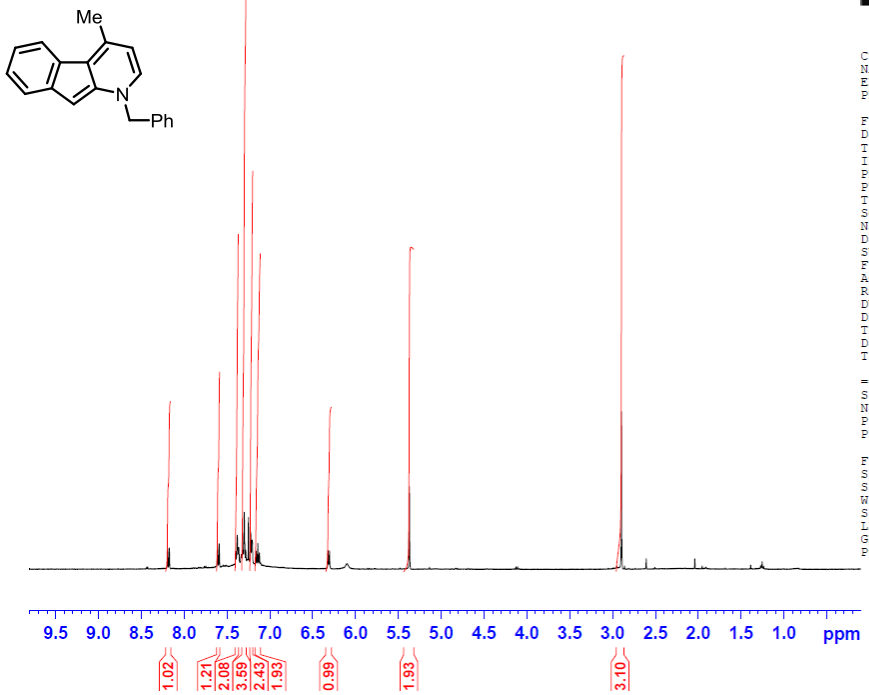

```
Current Data Parameters
NAME          103682-053
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151222
Time               9.43
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg
TD               32768
SOLVENT          CDCl3
NS                 700
DS                   4
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ           0.6815744 sec
RG                2050
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        100.6243395 MHz
NUC1               13C
P1              10.90 usec
PLW1        43.00000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2            90.00 usec
PLW2        10.50000000 W
PLW12        0.29166999 W
PLW13        0.14670999 W

F2 - Processing parameters
SI               65536
SF          100.6127690 MHz
WDW                EM
SSB       0
LB              1.00 Hz
GB        0
PC              1.40
```

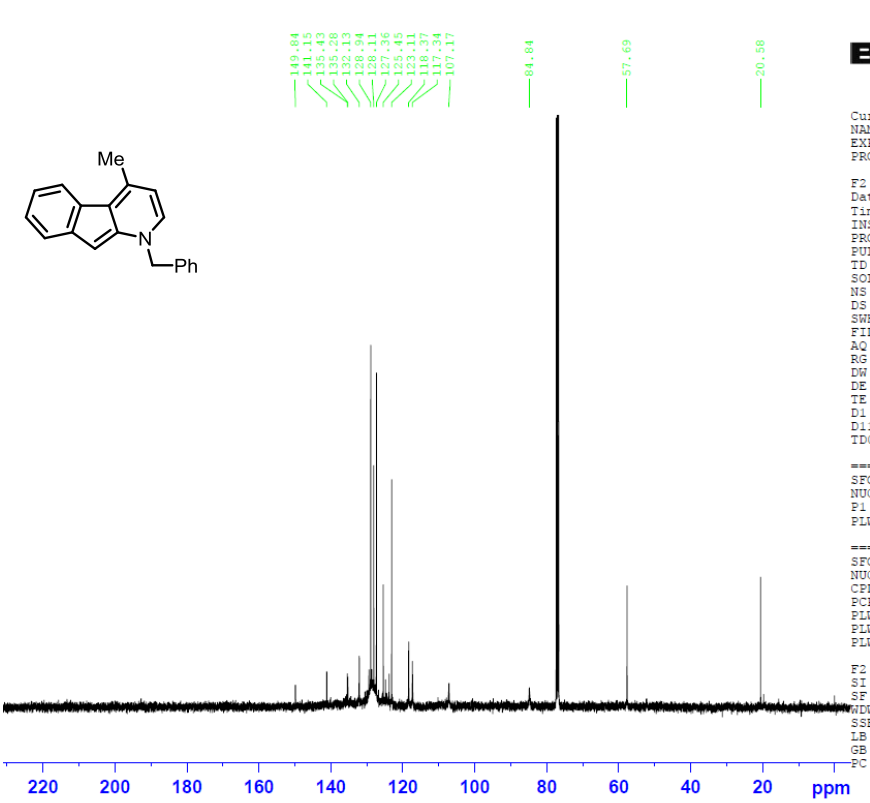



```
Current Data Parameters
NAME          103682-052
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151218
Time              15.59
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg10
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    4
SWH            5896.227 Hz
FIDRES         0.179939 Hz
AQ             2.7787263 sec
RG                  645
DW               84.800 usec
DE                6.50 usec
TE                298.0 K
D1            2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.1327209 MHz
NUC1                 1H
P1                15.00 usec
PLW1         10.50000000 W

F2 - Processing parameters
SI                65536
SF           400.1300138 MHz
WDW                  EM
SSB       0
LB                0.05 Hz
GB        0
PC                1.00
```



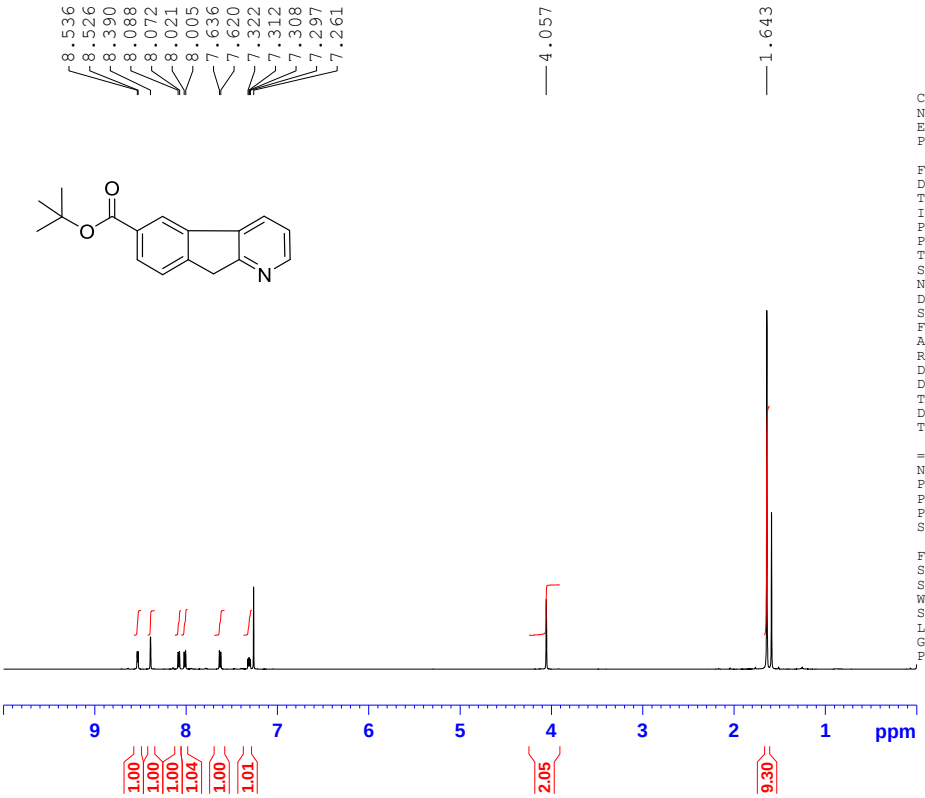

```
Current Data Parameters
NAME          103682-052
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151219
Time                2.10
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg
TD                32768
SOLVENT           CDCl3
NS                 4000
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG                 2050
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         100.6243395 MHz
NUC1                 13C
P1                10.90 usec
PLW1         43.00000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         10.50000000 W
PLW12         0.29166999 W
PLW13         0.14670999 W

F2 - Processing parameters
SI                65536
SF           100.6127690 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

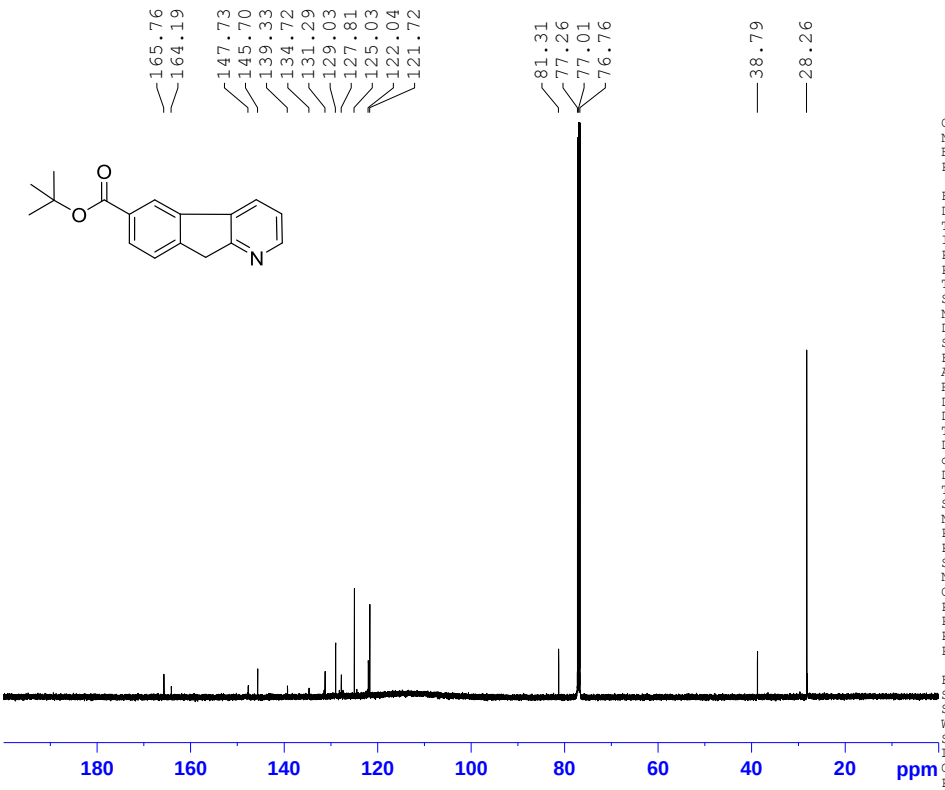



```
Current Data Parameters
NAME      103687-039-p-2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151110
Time              19.11
INSTRUM           spect
PROBHD   5 mm PABBI 1H-
PULPROG          q_zg10
TD                32768
SOLVENT           CDCl3
NS                  128
DS                    0
SWH            9014.423 Hz
FIDRES         0.275098 Hz
AQ            1.8175317 sec
RG                 1620
DW               55.467 usec
DE                6.50 usec
TE                299.0 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                 8.00 usec
PL1                3.00 dB
PL1W        14.98121262 W
SFO1       500.1334009 MHz

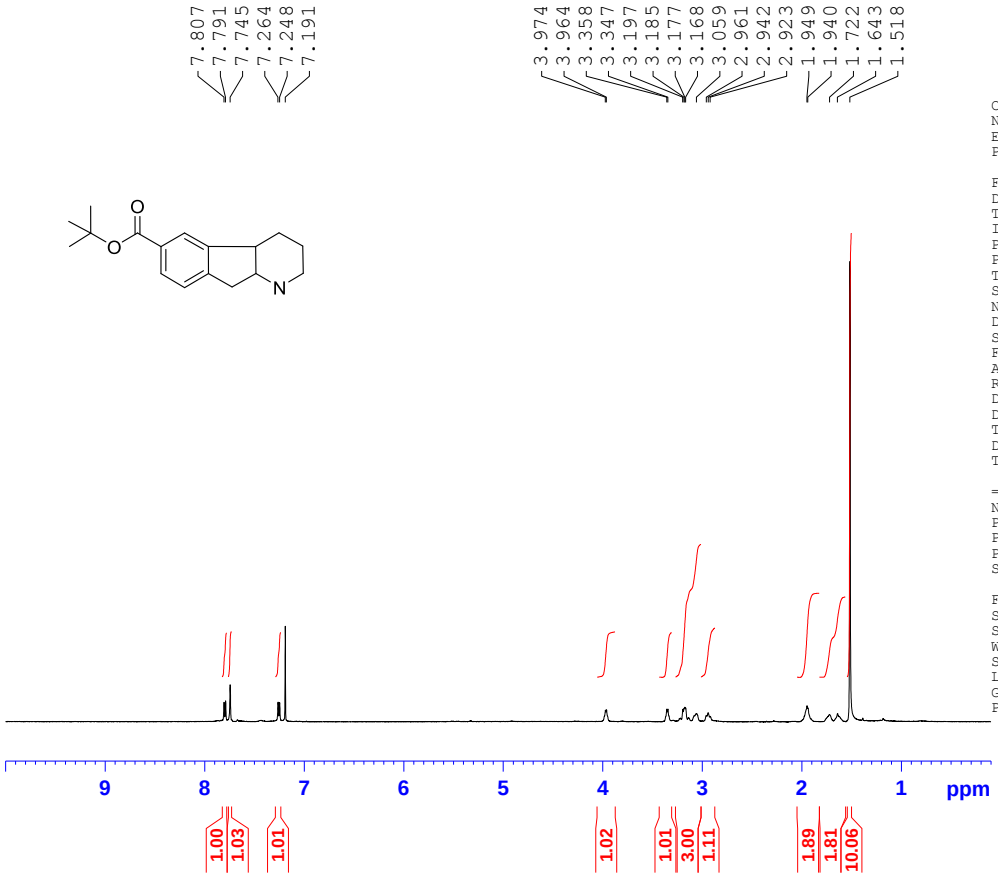
F2 - Processing parameters
SI                16384
SF         500.1300132 MHz
WDW                  EM
SSB       0
LB              0.30 Hz
GB        0
PC              1.00
```




```
Current Data Parameters
NAME      103687-039f1-c
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20151114
Time              11.12
INSTRUM           spect
PROBHD   5 mm PABBI 1H-
PULPROG           zgpg
TD              262144
SOLVENT           CDCl3
NS                11264
DS                    0
SWH           31250.000 Hz
FIDRES         0.119209 Hz
AQ            4.1943040 sec
RG                 2050
DW               16.000 usec
DE                6.50 usec
TE                299.0 K
D1           1.00000000 sec
d11          0.03000000 sec
DELTA        0.89999998 sec
TD0                   1
SFO1       125.7698617 MHz
NUC1                 13C
P1                15.75 usec
PLW1        -1.00000000 W
SFO2       500.1325007 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        -1.00000000 W
PLW12       -1.00000000 W
PLW13       -1.00000000 W

F2 - Processing parameters
SI                131072
SF         125.7577890 MHz
WDW                  EM
SSB       0
LB              0.30 Hz
GB        0
PC              1.40
```

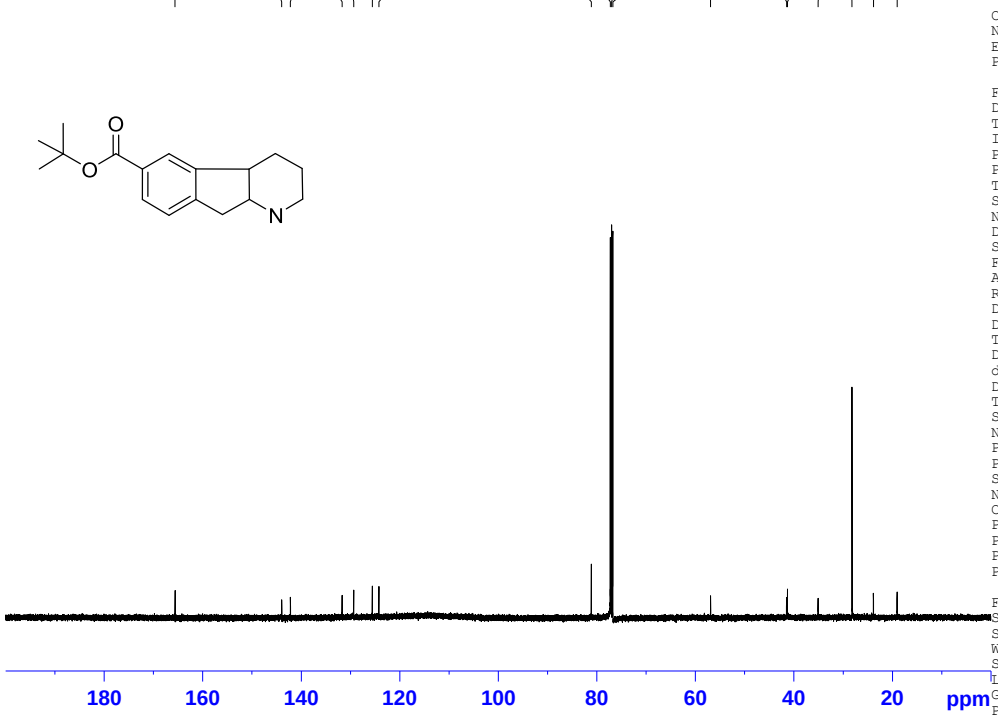



```
Current Data Parameters
NAME      103687-039-f2
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20151111
Time              11.55
INSTRUM           spect
PROBHD   5 mm PABBI 1H-
PULPROG            zg10
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7500.000 Hz
FIDRES         0.228882 Hz
AQ           2.1845334 sec
RG                 1030
DW               66.667 usec
DE                6.50 usec
TE                299.0 K
D1          1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                8.00 usec
PL1               3.00 dB
PL1W       14.98121262 W
SFO1      500.1325007 MHz

F2 - Processing parameters
SI                16384
SF         500.1300482 MHz
WDW                  EM
SSB       0
LB              0.30 Hz
GB        0
PC              1.00
```




```
Current Data Parameters
NAME     103687-039-f2-c
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20151114
Time              18.45
INSTRUM           spect
PROBHD   5 mm PABBI 1H-
PULPROG            zgpg
TD               262144
SOLVENT           CDCl3
NS                 5120
DS                    0
SWH           31250.000 Hz
FIDRES         0.119209 Hz
AQ            4.1943040 sec
RG                 2050
DW               16.000 usec
DE                6.50 usec
TE                299.0 K
D1          1.00000000 sec
d11         0.03000000 sec
DELTA       0.89999998 sec
TD0                   1
SFO1      125.7698617 MHz
NUC1                 13C
P1               15.75 usec
PLW1       -1.00000000 W
SFO2      500.1325007 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2            80.00 usec
PLW2       -1.00000000 W
PLW12      -1.00000000 W
PLW13      -1.00000000 W

F2 - Processing parameters
SI                131072
SF         125.7577890 MHz
WDW                  EM
SSB       0
LB              0.30 Hz
GB        0
PC              1.40
```

Computational Studies

Full Reference of Gaussian09:

Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T.Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

All optimizations were performed using spin-unrestricted broken-symmetry DFT at the UB3LYP[5]/6-31G(d) level (with the guess=mix keyword as implemented in Gaussian09) in the gas phase. Vibrational frequencies were computed at the same level to obtain thermal corrections (at 298 K) and to characterize the stationary points as transition states (one and only one imaginary frequency) or minima (zero imaginary frequencies). Single point energy calculations in solvent [nitromethane(ε=36.562)] were performed on optimized geometries using the SMD[6]-solvation model which resembles the dielectric of experimental solvent used (dimethylformamide ε=37.219) using the UM06[7] functional with the 6-311+G(d,p) basis set.

[5] (a) Becke, A. D. J. Chem. Phys. **1993**, *98*, 1372-1377. (b) Becke, A. D. J. Chem. Phys.**1993**, *98*, 5648-5652. (c) Lee, C.; Yang, W.; Parr, R. G. Phys. Rev. B. **1988**, *37*, 785-789. (d) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. J. Phys. Chem. **1994**, *98*, 11623-11627.

[6] Marenich, A. V.; Cramer, C. J.; Thrular, D. G. *I. Phys. Chem. B,* **2009**, *113*, 6378-6396.

[7] Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc*., **2008**, *120*, 215-41

Figure 1:

A^0 : Ni(pyridine)COD

Zero-point correction= 0.341621 (Hartree/Particle)
Thermal correction to Energy= 0.359621
Thermal correction to Enthalpy= 0.360565
Thermal correction to Gibbs Free Energy= 0.295892
Sum of electronic and zero-point Energies= -2315.290386
Sum of electronic and thermal Energies= -2315.272386
Sum of electronic and thermal Enthalpies= -2315.271442
Sum of electronic and thermal Free Energies= -2315.336115

Single point energy (electronic) = -2315.2749059 (nitromethane)

Ni	-1.31200100	2.51441700	0.01532300
C	-2.87279500	2.54923200	-1.32235300
C	-3.33959900	2.23367600	-0.04272400
C	-1.42877800	4.55982700	-0.02071600
C	-4.07216900	3.21169100	0.87210900
C	-1.71213100	4.09688300	1.26719500
H	-2.73069200	1.72193700	-2.01785200
H	-4.61851100	3.94786400	0.27242000
H	-3.51577500	1.17819800	0.16354100
H	-0.41709300	4.92576300	-0.19470100
H	-4.83691400	2.67248500	1.44432700
H	-0.90866600	4.14645500	2.00219900
C	-2.94408200	3.92231600	-1.96694600
H	-2.29134300	3.91214100	-2.84948500
H	-3.95641100	4.13271800	-2.34921100
C	-2.48186600	5.05085100	-1.00981100
H	-3.33931600	5.46689500	-0.46955100
H	-2.07161200	5.88204400	-1.59609900
C	-3.10338300	3.92389300	1.84987700
H	-3.01032000	3.32148900	2.76261300
H	-3.52481700	4.88980800	2.17344000
C	0.51621100	0.47451000	0.70088400
C	1.08967000	-0.61518800	1.38643500
C	0.46103100	-1.14968000	2.49365700
H	2.02705400	-1.03698500	1.03922000
C	-1.27882000	0.47814500	2.20524200
C	-0.76143400	-0.58446400	2.91522300
H	0.89829000	-1.98909000	3.02588300
H	-2.21872800	0.93675900	2.49621500
H	-1.29370600	-0.96927500	3.77920500
C	1.08891100	1.10777800	-0.46593700
C	2.31299900	0.74042600	-1.06010600
C	0.80818500	2.78469700	-2.07666400
C	2.77343600	1.41058100	-2.17624500
H	2.89553300	-0.07003500	-0.63495700
C	1.99554600	2.46504100	-2.70034600
H	0.18384700	3.59156400	-2.44770100
H	3.71581700	1.13198200	-2.63818200
H	2.31459400	3.02102800	-3.57609400
N	-0.67823800	1.02590300	1.11837600
N	0.33132600	2.13939000	-0.98226000

A^0 : substrate

Zero-point correction= 0.216387 (Hartree/Particle)
Thermal correction to Energy= 0.229486
Thermal correction to Enthalpy= 0.230430
Thermal correction to Gibbs Free Energy= 0.175458
Sum of electronic and zero-point Energies= -3128.816865
Sum of electronic and thermal Energies= -3128.803767
Sum of electronic and thermal Enthalpies= -3128.802823
Sum of electronic and thermal Free Energies= -3128.857795

Single point energy (electronic) = -3131.0640104 (nitromethane)

C	1.69648200	-2.70614800	0.81118300
C	1.87242700	-3.13771200	-1.90098600
C	0.87280700	-3.75380900	0.23902000
H	1.59290400	-2.52633000	1.87334700
H	1.88716000	-3.36106900	-2.96205600
Br	2.56290200	-5.11549300	2.90651800
C	2.64235400	-2.16368700	-1.35091100
H	3.30421300	-1.57514700	-1.97448900
N	1.01757600	-3.91706400	-1.15911400
C	0.24605700	-4.95482600	-1.82463000
H	0.54477500	-5.01328800	-2.87246200
H	0.42564000	-5.92250900	-1.34200200
H	-0.82872000	-4.73972600	-1.77378500
C	-0.01940400	-4.51947000	0.94777300
H	-0.72978900	-5.13454600	0.40732200
C	-0.23372500	-4.49171700	2.40146700
C	-1.55129600	-4.31695700	2.88436500
C	0.75131800	-4.69936700	3.38980400
C	-1.86071900	-4.31164700	4.23937000
H	-2.34067700	-4.16759800	2.15183600
C	0.46269000	-4.67441700	4.75503000
C	-0.84671200	-4.47658300	5.18607000
H	-2.88964500	-4.16668800	4.55779500
H	1.26308900	-4.83412300	5.46958500
H	-1.07003000	-4.46547600	6.24913700
C	2.53579000	-1.94622700	0.06049900
H	3.11901300	-1.15946200	0.53082500

COD

Zero-point correction= 0.181167 (Hartree/Particle)
Thermal correction to Energy= 0.188586
Thermal correction to Enthalpy= 0.189531
Thermal correction to Gibbs Free Energy= 0.149675
Sum of electronic and zero-point Energies= -311.849240
Sum of electronic and thermal Energies= -311.841820
Sum of electronic and thermal Enthalpies= -311.840876
Sum of electronic and thermal Free Energies= -311.880731 H

Single point energy (electronic) = -311.8611887 (nitromethane)

C	-3.85791700	2.58046000	0.96343400
C	-3.81755900	3.31795100	2.07996100
C	-1.84153900	4.68974000	-0.34794600
C	-3.62937100	4.81228000	2.23648500
C	-1.40708000	5.03781500	0.86950900
H	-3.99882800	1.50680800	1.10073700
H	-4.23174500	5.37072600	1.51561000
H	-3.90763600	2.77251300	3.01999100
H	-1.07594600	4.56714400	-1.11485600
H	-4.00981500	5.10434700	3.22327800
H	-0.33080800	5.18823000	0.97182800
C	-3.74278100	2.97664300	-0.48796600
H	-3.06788900	2.25687200	-0.97494500
H	-4.72032800	2.82054000	-0.97263100
C	-3.25254600	4.40294200	-0.81668900
H	-3.96168100	5.13874400	-0.42925100
H	-3.28106800	4.51508700	-1.90773000
C	-2.15738800	5.27177000	2.15753400
H	-1.59541200	4.77642500	2.96341100
H	-2.11197300	6.34607700	2.39955500

A

Zero-point correction= 0.376928 (Hartree/Particle)
Thermal correction to Energy= 0.401586
Thermal correction to Enthalpy= 0.402530
Thermal correction to Gibbs Free Energy= 0.319374
Sum of electronic and zero-point Energies= -5132.231330
Sum of electronic and thermal Energies= -5132.206673
Sum of electronic and thermal Enthalpies= -5132.205729
Sum of electronic and thermal Free Energies= -5132.288885

Single point energy (electronic) = -5134.4644507 (nitromethane)

C	-2.62018100	2.13645800	1.28977800
C	-0.98694600	2.05521700	2.94784700
C	-1.90426900	2.40419800	3.93162200
C	-3.23535000	2.61811600	3.56722500
C	-3.59452700	2.47809000	2.22936200
C	-2.86241600	1.97243600	-0.15546800
C	-1.86246300	1.38335300	-2.17576600
C	-3.02437500	1.67245500	-2.88284700
C	-4.14721000	2.12134100	-2.18489900
C	-4.05929200	2.28211600	-0.80467700
H	0.05348600	1.85813100	3.18041000
H	-1.57803800	2.50169000	4.96197800
H	-3.98054200	2.88372700	4.31087200
H	-4.62472500	2.62286100	1.92216000
H	-0.94793100	1.06361300	-2.66569000
H	-3.04142300	1.55053800	-3.96108200
H	-5.07003000	2.35704100	-2.70650000
H	-4.90749800	2.65771000	-0.24249400
N	-1.32053400	1.92380800	1.64930300
N	-1.77773300	1.50463000	-0.83673400
Ni	-0.25474700	1.16243600	0.26534400
C	1.55005500	0.73260800	0.77550200
C	1.18756600	-2.06232200	0.66215600
C	1.97127000	-0.10937300	1.86465000
H	2.09358800	1.67445300	0.67260600
C	1.74972200	-1.46021500	1.82233700
H	0.95476500	-3.12336800	0.68991800
H	2.49019000	0.33715200	2.71169200
H	2.02440500	-2.09378200	2.66267800
Br	1.74758300	0.91355100	-2.20913600
C	0.91289200	-1.35734400	-0.50246700
C	1.05390300	0.09164700	-0.45139100
C	0.39837800	-1.98431700	-1.71679200
H	-0.29587700	-1.37115900	-2.27763700
C	0.75933200	-3.20243900	-2.23907300
C	1.84366400	-4.03340700	-1.74964700
C	2.16135600	-5.23056600	-2.30663500
H	2.42732000	-3.63263200	-0.93099100
C	0.42266100	-4.94723700	-3.92135000
C	1.41294200	-5.73090000	-3.42414700
H	3.00054600	-5.80221400	-1.91958800
H	-0.17137400	-5.23944600	-4.78068300
H	1.63151700	-6.68862700	-3.88081700
C	-0.97420300	-2.94952600	-3.98591600
H	-0.59399200	-1.99610600	-4.37321700
H	-1.41366500	-3.51585000	-4.80913300
H	-1.75164500	-2.73108400	-3.24300900
N	0.09467100	-3.72613200	-3.38271500

A-TS

Zero-point correction= 0.375185 (Hartree/Particle)
Thermal correction to Energy= 0.399607
Thermal correction to Enthalpy= 0.400552
Thermal correction to Gibbs Free Energy= 0.317713
Sum of electronic and zero-point Energies= -5132.220386
Sum of electronic and thermal Energies= -5132.195963
Sum of electronic and thermal Enthalpies= -5132.195019
Sum of electronic and thermal Free Energies= -5132.277858

Single point energy (electronic) = -5134.4413639 (nitromethane)

C	-2.12981100	2.55653500	1.01460100
C	-0.39576500	2.69805300	2.56582300
C	-1.07361900	3.65136200	3.30878300
C	-2.34098200	4.06651100	2.88176300
C	-2.86843100	3.51066500	1.72326600
C	-2.57892800	1.89552900	-0.21539700
C	-2.11012000	0.18084700	-1.71996600
C	-3.20796900	0.50864300	-2.50313300
C	-4.01823400	1.58319500	-2.12013500
C	-3.69429000	2.28529600	-0.96629100
H	0.58685800	2.34561500	2.85930500
H	-0.61698000	4.06170600	4.20365500
H	-2.90396100	4.80495200	3.44440800
H	-3.85454600	3.80115900	1.37692100
H	-1.44828400	-0.64074200	-1.97497700
H	-3.42097400	-0.06505300	-3.39966100
H	-4.87906500	1.87208400	-2.71588000
H	-4.28742900	3.14056000	-0.66042100
N	-0.89678000	2.14594200	1.43930700
N	-1.79766500	0.83980200	-0.58565400
Ni	-0.17859300	0.65209500	0.47818100
C	1.18117600	-0.42382800	1.52254500
C	0.13462000	-3.02357300	1.20788200
C	1.03389100	-1.29092500	2.64589000
H	2.01885400	0.26939500	1.54915900
C	0.47519600	-2.54245900	2.49438900
H	-0.26916500	-4.02963500	1.11080400
H	1.44323100	-0.99235300	3.60959600
H	0.36145800	-3.20139600	3.35134900
Br	1.62612800	0.40417500	-1.33742300
C	0.26636400	-2.26614400	0.04296100
C	0.64593100	-0.91186600	0.26698300
C	-0.16635000	-2.84166800	-1.25150200
H	-1.17930200	-3.22997900	-1.26344000
C	0.65522900	-3.08296900	-2.32266200
C	2.08089900	-2.81142700	-2.33304500
C	2.86624100	-3.08450500	-3.40583800
H	2.50155200	-2.38827400	-1.43088100
C	0.97217600	-3.93531400	-4.59099800
C	2.30087400	-3.66100100	-4.59117600
H	3.93115100	-2.87365000	-3.36393900
H	0.46881600	-4.38149800	-5.44189100
H	2.90233400	-3.88298100	-5.46448500
C	-1.25074600	-4.00953700	-3.58736000
H	-1.86653900	-3.11997600	-3.40410200
H	-1.47876700	-4.40416200	-4.57903500
H	-1.51469400	-4.76396900	-2.83518200
N	0.15906100	-3.67288300	-3.51204000

B

Zero-point correction= 0.378257 (Hartree/Particle)
Thermal correction to Energy= 0.402903
Thermal correction to Enthalpy= 0.403848
Thermal correction to Gibbs Free Energy= 0.321533
Sum of electronic and zero-point Energies= -5132.295835
Sum of electronic and thermal Energies= -5132.271189
Sum of electronic and thermal Enthalpies= -5132.270245
Sum of electronic and thermal Free Energies= -5132.352560

Single point energy (electronic) = -5134.5190127 (nitromethane)

C	-2.74906100	0.27800800	1.57920000
C	-0.61754900	1.17702400	1.77836400
C	-0.97668900	2.29929400	1.03797300
C	-2.27874700	2.39889300	0.55070500
C	-3.17876100	1.37418300	0.82724400
C	-3.59369300	-0.86622900	1.94814500
C	-3.62552800	-2.95587300	2.96231700
C	-5.00051800	-3.06330400	2.79099400
C	-5.69229600	-2.02750100	2.16580200
C	-4.97384900	-0.91452700	1.74297300
H	0.37439900	1.04506300	2.19737500
H	-0.24247200	3.07596800	0.85131000
H	-2.59069400	3.25793200	-0.03610600
H	-4.19569100	1.42252700	0.45459000
H	-3.05304900	-3.74110600	3.43634300
H	-5.51118300	-3.95153400	3.14773700
H	-6.76700800	-2.07836000	2.01943800
H	-5.48183100	-0.08079500	1.27172300
N	-1.47963900	0.18216300	2.04604500
N	-2.91474000	-1.88611600	2.54790500
Ni	-1.06154200	-1.57812200	2.86112000
C	0.82977600	-2.49218100	0.46801600
C	-0.06393000	-2.19241100	-2.12329900
C	-0.33660600	-3.25545000	0.06355500
H	1.20509700	-2.66640600	1.46715300
H	-0.46063700	-2.13611800	-3.13155300
Br	0.94189400	-0.91479100	3.74734400
C	1.00288400	-1.45803800	-1.71852900
H	1.49094800	-0.78140800	-2.41002700
N	-0.72236200	-3.07051500	-1.29276100

C	-1.85909200	-3.81442200	-1.80213300
H	-2.06482700	-3.50713200	-2.82929900
H	-1.66317300	-4.89430600	-1.78875800
H	-2.74566700	-3.62481600	-1.18290500
C	-1.00432800	-4.13406500	0.87698300
H	-1.73162100	-4.80015000	0.42339100
C	-0.75894300	-4.38858100	2.31292300
C	-0.67647200	-5.74156400	2.71313000
C	-0.71565300	-3.37506100	3.30838300
C	-0.53764700	-6.10716400	4.04782500
H	-0.72064300	-6.51268300	1.94540600
C	-0.54488900	-3.76949400	4.64534700
C	-0.46686200	-5.11122500	5.02410600
H	-0.47581300	-7.15793700	4.32202300
H	-0.48379900	-3.00699000	5.41743200
H	-0.34981200	-5.37531900	6.07298400
C	1.46963300	-1.63841800	-0.37221500
H	2.35329200	-1.10825700	-0.02807900

B-TS

Zero-point correction= 0.377821 (Hartree/Particle)
Thermal correction to Energy= 0.401442
Thermal correction to Enthalpy= 0.402387
Thermal correction to Gibbs Free Energy= 0.324425
Sum of electronic and zero-point Energies= -5132.242048
Sum of electronic and thermal Energies= -5132.218427
Sum of electronic and thermal Enthalpies= -5132.217483
Sum of electronic and thermal Free Energies= -5132.295445

Single point energy (electronic) = -5134.471906 (nitromethane)

C	0.28834700	2.73322100	-0.88486600
C	0.69607800	4.05252000	-0.65170100
C	1.77016400	4.32946100	0.19847600
C	2.47779600	3.27664400	0.77571200
C	2.08595300	1.94792300	0.54670600
C	0.90859200	1.67249200	-0.20936700
H	-0.56849300	2.53529900	-1.51985500
H	0.15108300	4.86489400	-1.12601400
H	2.07724100	5.35646700	0.37992900
H	3.37064700	3.47255200	1.36578900
C	2.88010500	0.79774200	0.93914600
H	3.65277500	0.85459600	1.69733200
C	2.54897100	-0.31739900	0.24056500
C	1.53923100	-0.11310200	-0.83377200
C	0.63837500	-1.17752700	-1.12760600
H	1.88906700	0.47821700	-1.67797500
C	2.17124500	-2.67161500	0.07886100
C	1.03018400	-2.49834300	-0.62030300
H	2.52180500	-3.65051900	0.38823000
H	0.45092800	-3.37655900	-0.88110300
C	4.07173900	-1.82878400	1.40583800
H	3.75233700	-1.57379800	2.42796200
H	4.37817300	-2.87692300	1.38150700
H	4.93571900	-1.20694100	1.14965800
N	3.00742900	-1.61547000	0.44237900
Br	-2.20901100	0.59923900	-1.71115900
C	-2.11236300	-1.18659100	1.90064700
C	-2.03830600	-2.34332000	-0.10660400
C	-3.07583900	-2.07199000	2.40351400
C	-2.98371800	-3.25885500	0.32873900
H	-1.65120700	-2.38237000	-1.11372600
C	-3.50554700	-3.13107800	1.61847900
H	-3.50280500	-1.91164800	3.38657600
H	-3.31295900	-4.04664400	-0.34046700
H	-4.25152700	-3.82657600	1.99120600
C	-1.68522600	0.03086600	2.59081900
C	-2.06213200	0.35512200	3.89946900
C	-1.71531400	1.59140400	4.42625400
H	-2.62448900	-0.35477200	4.49510700
C	-0.64627100	2.08543500	2.33531200
C	-1.01232400	2.48273900	3.61470600
H	-1.99840300	1.85879000	5.43997000
H	-0.09863600	2.75584400	1.68951700
H	-0.74372100	3.47518500	3.96110400
N	-1.56735100	-1.34570100	0.66870000
N	-0.93933800	0.87387700	1.82318400
Ni	-0.36799600	0.07869400	0.06926200
H	0.15643200	-1.15486400	-2.10197800

A’

Zero-point correction= 0.375566 (Hartree/Particle)
Thermal correction to Energy= 0.400257
Thermal correction to Enthalpy= 0.401201
Thermal correction to Gibbs Free Energy= 0.320140
Sum of electronic and zero-point Energies= -5132.246187
Sum of electronic and thermal Energies= -5132.221497
Sum of electronic and thermal Enthalpies= -5132.220552
Sum of electronic and thermal Free Energies= -5132.301614

Single point energy (electronic) = -5134.4607011 (nitromethane)

C	-3.02806900	-2.12853700	-1.39104000
C	-2.57762500	-2.46179600	0.89384300
C	-1.45073400	-3.21449300	0.62764100
C	-1.10061800	-3.43743100	-0.72509100
C	-1.88416300	-2.89467400	-1.72022400
C	-3.91052200	-1.50954600	-2.33981300
C	-5.91100500	-0.30017300	-2.61806500
C	-5.78096900	-0.27760800	-3.98929400
C	-4.64164200	-0.89581200	-4.56793000
C	-3.71983700	-1.50032100	-3.74212900
H	-2.87713900	-2.24340200	1.91589600
H	-0.85398900	-3.61169800	1.44182100
H	-0.22610900	-4.03033100	-0.97840400
H	-1.63435900	-3.06441900	-2.76247500
H	-6.76488400	0.16222500	-2.12926300
H	-6.53934200	0.19878900	-4.60193500
H	-4.49586700	-0.88914300	-5.64427400
H	-2.83506700	-1.96520900	-4.16570900
N	-3.36319400	-1.92253600	-0.06274500
N	-5.02454100	-0.89323500	-1.78125800
Ni	-5.02279200	-0.90945700	0.18076200
C	-8.71882500	-1.42154700	2.92083600
C	-7.61061600	-1.09141000	2.14740900
C	-7.33309500	0.20322800	1.68389400
C	-8.28751700	1.18041300	2.03159000
C	-9.41680000	0.88180300	2.78950000
C	-9.63349400	-0.42055700	3.24534500
H	-8.87219900	-2.44446000	3.24805300
H	-8.11856600	2.19995900	1.69391800
H	-10.12578700	1.66872700	3.03221700
H	-10.50940300	-0.66206200	3.84046400
Br	-6.40299800	-2.51378200	1.63843600
C	-6.15223400	0.55960700	0.85250700
H	-6.39669200	1.33216100	0.12722300
C	-4.82494000	0.64587500	1.43417600
C	-4.52140500	0.21909300	2.79793400
C	-3.29670900	0.39848900	3.35869800
H	-5.30682400	-0.28411400	3.34935300
C	-2.62757700	1.70731800	1.47049200
C	-2.27909500	1.11349100	2.64270600
H	-3.09911600	0.03451000	4.36350100
H	-1.93609800	2.32990800	0.91239800
H	-1.27660700	1.23304900	3.03534300
N	-3.88492400	1.60711800	0.92815800
C	-4.19802000	2.36284500	-0.27542300
H	-3.32295100	2.94646100	-0.56696800
H	-4.46615200	1.69307000	-1.10002200
H	-5.03063100	3.05455300	-0.09793300

A’-TS

Zero-point correction= 0.374111 (Hartree/Particle)
Thermal correction to Energy= 0.398749
Thermal correction to Enthalpy= 0.399693
Thermal correction to Gibbs Free Energy= 0.318381
Sum of electronic and zero-point Energies= -5132.222163
Sum of electronic and thermal Energies= -5132.197525
Sum of electronic and thermal Enthalpies= -5132.196581
Sum of electronic and thermal Free Energies= -5132.277893

Single point energy (electronic) = -5134.4407267 (nitromethane)

C	-2.98256800	-2.08816700	-1.30660400
C	-2.68954700	-2.60914300	0.94702900
C	-1.51034900	-3.29533800	0.69259100
C	-1.06984800	-3.39686500	-0.63536600
C	-1.81064600	-2.79232900	-1.63804100
C	-3.83527800	-1.40400900	-2.27654700
C	-5.85652400	-0.27739200	-2.58903800
C	-5.66556000	-0.18985400	-3.96029100
C	-4.48189000	-0.71729100	-4.50085200
C	-3.56735000	-1.32409400	-3.65485000
H	-3.08090200	-2.50854300	1.95417400
H	-0.95595000	-3.74513400	1.50939700
H	-0.16313800	-3.94329200	-0.87868700
H	-1.49266500	-2.87088700	-2.67189800
H	-6.74786300	0.12608900	-2.11732000
H	-6.41727100	0.27816700	-4.58693300
H	-4.28433000	-0.65626100	-5.56708700
H	-2.64848400	-1.73711900	-4.05641400
N	-3.41450900	-2.01289800	-0.01402200
N	-4.97585200	-0.85734900	-1.75333000
Ni	-5.17081000	-1.08050100	0.22772000
C	-8.67225400	-1.27031600	3.23325400
C	-7.58560200	-0.98396700	2.42936300
C	-7.39053700	0.22283100	1.75869400
C	-8.39642000	1.19394300	1.94939100
C	-9.50507800	0.94782500	2.76029900
C	-9.64525700	-0.27943500	3.41448400
H	-8.77340100	-2.24333900	3.70908900
H	-8.29513300	2.15938100	1.45442500
H	-10.26205900	1.71857600	2.88247400
H	-10.50886800	-0.46947700	4.04847400
Br	-6.30231600	-2.75655100	1.50844900
C	-6.22600400	0.51372400	0.87209300
H	-6.48224900	1.21856200	0.08413300
C	-4.88594500	0.61889500	1.37138500
C	-4.49208500	0.13913400	2.69084900
C	-3.22056100	0.26692700	3.15392100
H	-5.25480100	-0.36021400	3.27664100
C	-2.65473600	1.59107400	1.24153800
C	-2.23821300	0.96043500	2.37132900
H	-2.95434500	-0.13028900	4.12984400
H	-1.98840200	2.20018000	0.63955800
H	-1.20346900	1.03528900	2.68403200
N	-3.95770100	1.54674200	0.80483000
C	-4.35211600	2.37756900	-0.32066700
H	-3.51689500	3.02497400	-0.59443900
H	-4.62641600	1.77036000	-1.19080600
H	-5.20693600	3.00865400	-0.05184100

NiBr(pyr)

Zero-point correction= 0.160253 (Hartree/Particle)
Thermal correction to Energy= 0.172550
Thermal correction to Enthalpy= 0.173494
Thermal correction to Gibbs Free Energy= 0.117685
Sum of electronic and zero-point Energies= -4575.184258
Sum of electronic and thermal Energies= -4575.171961
Sum of electronic and thermal Enthalpies= -4575.171017
Sum of electronic and thermal Free Energies= -4575.226827

Single point energy (electronic) = -4577.4855185 (nitromethane)

C	-3.58462900	-2.57578300	-2.50220000
C	-2.60659000	-0.61698100	-1.68096000
C	-2.39007000	-0.12817200	-2.96041800
C	-2.79488900	-0.90867200	-4.05209700
C	-3.39517400	-2.13879600	-3.82019000
C	-4.19805000	-3.84235900	-2.10580600
C	-4.81154000	-5.16259900	-0.27107700
C	-5.30990100	-6.15420800	-1.09398400
C	-5.24873800	-5.97948400	-2.48722100
C	-4.68741700	-4.81227200	-2.98720400
H	-2.31603600	-0.05855400	-0.79635200
H	-1.91752200	0.83823700	-3.09967500
H	-2.64248300	-0.55836100	-5.06861400
H	-3.71510400	-2.75632800	-4.65246900
H	-4.83809700	-5.25445500	0.81020800
H	-5.73960300	-7.04980500	-0.65738000
H	-5.63163500	-6.73975000	-3.16054900
H	-4.62749000	-4.65132400	-4.05849300
N	-3.18774700	-1.80807900	-1.44438800
N	-4.25965500	-4.01638600	-0.74312500
Ni	-3.55436900	-2.60198000	0.28286200
Br	-3.13339600	-1.76968200	2.31974400

B': radical-substrate-open

Zero-point correction= 0.213531 (Hartree/Particle)
Thermal correction to Energy= 0.225181
Thermal correction to Enthalpy= 0.226126
Thermal correction to Gibbs Free Energy= 0.174563
Sum of electronic and zero-point Energies= -557.035608
Sum of electronic and thermal Energies= -557.023958
Sum of electronic and thermal Enthalpies= -557.023013
Sum of electronic and thermal Free Energies= -557.074576

Single point energy (electronic) = -556.9676734 (nitromethane)

C	-0.60909000	3.33114600	1.09959500
C	-0.04854800	4.47229500	1.69871200
C	1.25723300	4.40094000	2.19309700
C	1.99902300	3.22626600	2.09933400
C	1.47574900	2.04591600	1.50190500
C	0.17061700	2.20321000	1.03628700
H	-1.62210000	3.34884300	0.70375300
H	-0.62408600	5.39137400	1.77384300
H	1.70583900	5.27459400	2.65940800
H	3.01424500	3.19878000	2.49267700
C	2.30057900	0.85214200	1.43428500
H	3.28416800	0.97922000	1.86942000
C	1.97060800	-0.36978000	0.89342700
C	0.69890300	-0.68524800	0.27756600
C	0.42142500	-1.90876700	-0.24607900
H	-0.03686300	0.11141000	0.25072800
C	2.59966300	-2.66990100	0.37172500
C	1.40170000	-2.95098200	-0.20467700
H	3.39454100	-3.40410600	0.44331900
H	1.21196300	-3.93600100	-0.61343200
C	4.20864400	-1.23279600	1.50561600
H	4.10933800	-0.95625400	2.56205800
H	4.79050400	-2.15272300	1.43203500
H	4.74506600	-0.42856000	0.98809700
N	2.89906500	-1.44168200	0.90714300
H	-0.54839800	-2.09693800	-0.69834200

B'-TS

Zero-point correction= 0.211984 (Hartree/Particle)
Thermal correction to Energy= 0.222899
Thermal correction to Enthalpy= 0.223843
Thermal correction to Gibbs Free Energy= 0.174750
Sum of electronic and zero-point Energies= -557.019146
Sum of electronic and thermal Energies= -557.008231
Sum of electronic and thermal Enthalpies= -557.007287
Sum of electronic and thermal Free Energies= -557.056380

Single point energy (electronic) = -556.948519 (nitromethane)

C	-0.60909000	3.33114600	1.09959500
C	-0.04854800	4.47229500	1.69871200
C	1.25723300	4.40094000	2.19309700
C	1.99902300	3.22626600	2.09933400
C	1.47574900	2.04591600	1.50190500
C	0.17061700	2.20321000	1.03628700
H	-1.62210000	3.34884300	0.70375300
H	-0.62408600	5.39137400	1.77384300
H	1.70583900	5.27459400	2.65940800
H	3.01424500	3.19878000	2.49267700
C	2.30057900	0.85214200	1.43428500
H	3.28416800	0.97922000	1.86942000
C	1.97060800	-0.36978000	0.89342700
C	0.69890300	-0.68524800	0.27756600
C	0.42142500	-1.90876700	-0.24607900

H	-0.03686300	0.11141000	0.25072800
C	2.59966300	-2.66990100	0.37172500
C	1.40170000	-2.95098200	-0.20467700
H	3.39454100	-3.40410600	0.44331900
H	1.21196300	-3.93600100	-0.61343200
C	4.20864400	-1.23279600	1.50561600
H	4.10933800	-0.95625400	2.56205800
H	4.79050400	-2.15272300	1.43203500
H	4.74506600	-0.42856000	0.98809700
N	2.89906500	-1.44168200	0.90714300
H	-0.54839800	-2.09693800	-0.69834200

B1-(cyclized product)

Zero-point correction= 0.214022 (Hartree/Particle)
Thermal correction to Energy= 0.224968
Thermal correction to Enthalpy= 0.225912
Thermal correction to Gibbs Free Energy= 0.177057
Sum of electronic and zero-point Energies= -557.088423
Sum of electronic and thermal Energies= -557.077477
Sum of electronic and thermal Enthalpies= -557.076532
Sum of electronic and thermal Free Energies= -557.125388
Single point energy (electronic) = -557.0214977 (nitromethane)

C	-1.41841800	-4.67019200	1.59288300
C	-0.09480500	-2.39921800	2.62287200
C	-1.50402800	-4.26686600	3.05723100
H	-2.25093200	-4.15682700	1.06689200
H	0.26951300	-1.44583700	2.98389800
C	0.41194300	-3.02328500	1.47842200
H	1.25388300	-2.54830400	0.98178400
N	-1.05568500	-3.01378100	3.41974000
C	-1.24654400	-2.56928400	4.79214400
H	-1.01087400	-1.50483400	4.86348800
H	-2.29035300	-2.71961200	5.08333300
H	-0.60341400	-3.12396000	5.49005400
C	-2.18255500	-6.45270200	2.97324700
C	-2.62830400	-7.74225800	3.27852300
C	-1.77914600	-6.14052500	1.65160100
C	-2.65685100	-8.70570900	2.26530500
H	-2.94259400	-7.99671900	4.28788800
C	-1.82082000	-7.09630200	0.64923500
C	-2.25610100	-8.39284800	0.96340800
H	-2.99595000	-9.71292500	2.49473500
H	-1.51697600	-6.85357200	-0.36685400
H	-2.28221300	-9.15591600	0.19025900
C	-0.12538300	-4.19619200	0.98513900
H	0.29739100	-4.70722100	0.12651500
C	-2.00035900	-5.27945000	3.82075100
H	-2.16722500	-5.26311100	4.89147700

B'-TS-Br

Zero-point correction= 0.372598 (Hartree/Particle)
Thermal correction to Energy= 0.396743
Thermal correction to Enthalpy= 0.397688
Thermal correction to Gibbs Free Energy= 0.317244
Sum of electronic and zero-point Energies= -5132.232586
Sum of electronic and thermal Energies= -5132.208440
Sum of electronic and thermal Enthalpies= -5132.207496
Sum of electronic and thermal Free Energies= -5132.287940

Single point energy (electronic) = -5134.4538916 (nitromethane)

C	0.21610400	2.98074100	-0.19229500
C	0.92218200	4.18972400	-0.15615200
C	2.23769200	4.20375600	0.31550800
C	2.85644700	3.01020500	0.67938300
C	2.16601000	1.78075700	0.60743800
C	0.80096300	1.79165400	0.25175000
H	-0.80757400	2.96454500	-0.55861600
H	0.44445300	5.10933400	-0.48587800
H	2.79236700	5.13798600	0.36731700
H	3.90278600	3.01176000	0.98110600
C	2.88125700	0.52750500	0.77088900
H	3.89835500	0.58312300	1.14184400
C	2.40622800	-0.63543200	0.22788000
C	1.07922200	-0.78021300	-0.39624100
C	0.91521400	-1.77018200	-1.32703600
H	-0.11165300	0.15330600	-0.96777600
C	2.99219900	-2.79516700	-0.72463200
C	1.90385500	-2.78696400	-1.53714300
H	3.74022700	-3.58071500	-0.74719900
H	1.76048800	-3.57368700	-2.26874200
C	4.43617400	-1.83372900	0.98661200
H	4.21616800	-1.53266400	2.01588200
H	4.83837900	-2.84927700	0.98915100
H	5.19691800	-1.15103000	0.58393800
N	3.21645600	-1.80173400	0.19558800
C	-2.44620100	-0.89243400	1.97097800
C	-1.55681600	-2.49808600	0.56551300
C	-3.54153100	-1.71081600	2.26156600
C	-2.60405200	-3.37690000	0.82295300
H	-0.74853900	-2.77057000	-0.09925100
C	-3.62618200	-2.96904700	1.67615400
H	-4.32188800	-1.36833000	2.93088800
H	-2.61345000	-4.35358400	0.35097600
H	-4.47135900	-3.61730900	1.88747800
C	-2.21866800	0.41922900	2.59776000
C	-2.99190500	0.91832500	3.64948000
C	-2.64543000	2.12931700	4.23830400
H	-3.84508700	0.35953400	4.01520700
C	-0.80332900	2.25481500	2.70814400
C	-1.52087900	2.80212700	3.76631900
H	-3.23460300	2.52991600	5.05787500
H	0.06916900	2.75015200	2.30579200
H	-1.19462900	3.73996600	4.20295700
N	-1.47326400	-1.27509100	1.10792400
N	-1.14484200	1.09609500	2.11412600
Ni	-0.24224500	0.25441000	0.56788800
H	-0.00349000	-1.79938500	-1.90904600
Br	-1.79120500	0.39541100	-1.81798200

B'-TS-HBr

Zero-point correction= 0.372831 (Hartree/Particle)
Thermal correction to Energy= 0.397340
Thermal correction to Enthalpy= 0.398284
Thermal correction to Gibbs Free Energy= 0.316910
Sum of electronic and zero-point Energies= -5132.246753
Sum of electronic and thermal Energies= -5132.222244
Sum of electronic and thermal Enthalpies= -5132.221300
Sum of electronic and thermal Free Energies= -5132.302674

Single point energy (electronic) = -5134.466805 (nitromethane)

C	0.78829300	2.81062400	-0.64195500
C	1.57157200	3.96892300	-0.54283600
C	2.83319500	3.89118700	0.05138000
C	3.33183600	2.65543200	0.45722500
C	2.57593300	1.47442300	0.30142100
C	1.23595800	1.57485400	-0.15918700
H	-0.20425500	2.88187400	-1.08477900
H	1.19153600	4.91815900	-0.91364700
H	3.44445800	4.78418300	0.16250200
H	4.34528700	2.58494400	0.84964200
C	3.22258100	0.17798200	0.44569700
H	4.23672300	0.16678500	0.83040800
C	2.70770700	-0.90454400	-0.22218200
C	1.36583900	-0.87268900	-0.81261300
C	1.11823000	-1.69105700	-1.87933300
H	-0.69835900	0.44286000	-1.24725600
C	3.15885600	-2.90562400	-1.50521200
C	2.05584600	-2.71040500	-2.27379400
H	3.86047800	-3.71640000	-1.67062400
H	1.85350100	-3.37239200	-3.10876300
C	4.71330800	-2.25657500	0.26716400
H	4.55484300	-2.11149900	1.34090800
H	5.08884100	-3.26805700	0.09567200
H	5.46988300	-1.53300100	-0.06769200
N	3.45872100	-2.07966100	-0.44321100
C	-2.08679700	-1.10910300	1.52328400
C	-0.91680000	-2.72188800	0.34362500
C	-3.05732700	-2.04358800	1.89257600
C	-1.83796700	-3.70914200	0.68190400

H	-0.05655000	-2.94295900	-0.27533800
C	-2.93595500	-3.36144700	1.46343700
H	-3.90068400	-1.74789900	2.50515400
H	-1.69054300	-4.72413200	0.32828400
H	-3.68317300	-4.09939600	1.73992900
C	-2.09083100	0.29392100	1.97583600
C	-3.02884500	0.81496100	2.87010000
C	-2.91381800	2.13742700	3.28721800
H	-3.83638500	0.19671800	3.24393600
C	-0.95850200	2.31446800	1.91204300
C	-1.85303500	2.89832700	2.80542100
H	-3.63550500	2.55805000	3.98125700
H	-0.12623800	2.87208100	1.50174700
H	-1.71062900	3.93059100	3.10701000
N	-1.03167300	-1.44418900	0.73867200
N	-1.07107700	1.04495800	1.48876700
Ni	0.12752000	0.10830700	0.17598300
H	0.16878200	-1.62355300	-2.40820700
Br	-1.99405500	0.58620800	-2.12471300

B’-TS-RE

Zero-point correction= 0.374609 (Hartree/Particle)
Thermal correction to Energy= 0.398532
Thermal correction to Enthalpy= 0.399476
Thermal correction to Gibbs Free Energy= 0.319008
Sum of electronic and zero-point Energies= -5131.833760
Sum of electronic and thermal Energies= -5131.809837
Sum of electronic and thermal Enthalpies= -5131.808893
Sum of electronic and thermal Free Energies= -5131.889361

Single point energy (electronic) = -5134.4517488 (nitromethane)

C	0.77586900	2.46274600	-1.31655100
C	1.40621000	3.69142200	-1.11257900
C	2.47656900	3.79822800	-0.19818200
C	2.96905100	2.66406700	0.44715600
C	2.38912700	1.40190400	0.20110300
C	1.19038900	1.31453600	-0.59762600
H	-0.07730500	2.39254800	-1.98465400
H	1.06019800	4.57144400	-1.64711700
H	2.94470400	4.76334900	-0.02576300
H	3.84231900	2.73715800	1.09097600
C	3.00489400	0.12354200	0.48489200
H	3.91698100	0.03451700	1.06066800
C	2.49624800	-0.85467700	-0.34936300
C	1.25924400	-0.47448000	-1.08230500
C	1.05538100	-1.08974900	-2.31702800
H	-1.09160400	0.30926600	-1.05113700
C	2.78897100	-2.72167600	-1.83880900
C	1.84146500	-2.21278200	-2.69861800
H	3.34247600	-3.63067900	-2.03472800
H	1.64579400	-2.72661600	-3.63256200
C	4.19999600	-2.54633600	0.18291600
H	3.89938300	-2.54095300	1.23470800
H	4.47259400	-3.56195200	-0.10873400
H	5.07280700	-1.89169500	0.06721000
N	3.08983600	-2.07763900	-0.65180500
C	-2.03390700	-1.17456600	1.69164700
C	-1.08214500	-2.69457800	0.17399000
C	-2.88431900	-2.16712700	2.18913700
C	-1.90671400	-3.72431200	0.62756500
H	-0.37518700	-2.83379300	-0.63503200
C	-2.81678700	-3.45671800	1.65545300
H	-3.60013700	-1.93903800	2.96903700
H	-1.84051700	-4.70786300	0.17837600
H	-3.47328300	-4.23517500	2.02788000
C	-2.04389400	0.23738700	2.12305700
C	-2.87269500	0.76488500	3.11825700
C	-2.81994000	2.13443400	3.39345000
H	-3.55422600	0.12654100	3.66681300
C	-1.13586300	2.36065600	1.68935800
C	-1.94444000	2.94618000	2.66518800
H	-3.45835000	2.56023500	4.15956500
H	-0.44634200	2.93702800	1.08464900
H	-1.88861800	4.01313500	2.84369300
N	-1.13112200	-1.45374100	0.70394300
N	-1.17701300	1.03609800	1.43455300
Ni	-0.07576600	0.08931500	0.07340200
H	0.23402700	-0.77216600	-2.95147300
Br	-2.53936600	0.53224300	-1.93993200

B’-TSa

Zero-point correction= 0.373924 (Hartree/Particle)
Thermal correction to Energy= 0.398650
Thermal correction to Enthalpy= 0.399594
Thermal correction to Gibbs Free Energy= 0.317062
Sum of electronic and zero-point Energies= -5132.224297
Sum of electronic and thermal Energies= -5132.199571
Sum of electronic and thermal Enthalpies= -5132.198627
Sum of electronic and thermal Free Energies= -5132.281159

Single point energy (electronic) = -5134.442664 (nitromethane)

C	-3.27581300	-1.69922100	-1.76993700
C	-2.02332700	-1.94087900	0.20312700
C	-0.82860800	-1.91990800	-0.48754000
C	-0.86197200	-1.76177400	-1.89048900
C	-2.08668100	-1.65452500	-2.52328400
C	-4.61594500	-1.64363900	-2.31629200
C	-6.89892300	-1.76865800	-1.78747800
C	-7.26840400	-1.66086400	-3.11370900
C	-6.25608300	-1.52270300	-4.08645900
C	-4.93405900	-1.51629700	-3.68304000
H	-2.05216300	-2.06395400	1.28241200
H	0.10970100	-2.03114000	0.04586000
H	0.05822300	-1.73587500	-2.46644400
H	-2.13431600	-1.54684600	-3.60202600
H	-7.63706000	-1.88605600	-0.99909400
H	-8.31699900	-1.69057500	-3.39041000
H	-6.50938500	-1.43014000	-5.13838800
H	-4.14071100	-1.41894700	-4.41693700
N	-3.23181000	-1.82340400	-0.39664000
N	-5.61167300	-1.75456400	-1.37331700
Ni	-4.99141100	-1.77500500	0.48759300
C	-7.90003300	0.25111400	4.12134300
C	-6.76899200	0.23655900	3.34024500
C	-6.74909800	0.19086000	1.94648100
C	-8.00167500	0.24958300	1.30933000
C	-9.17600900	0.32834700	2.06188900
C	-9.13798000	0.32669100	3.45841500
H	-7.85098400	0.24395700	5.20782200
H	-8.05369900	0.22933300	0.22223100
H	-10.13399200	0.37993600	1.55072400
H	-10.05856300	0.39277300	4.03337900
Br	-5.64838100	-3.33250100	2.10725400
C	-5.44177700	0.13727300	1.25169800
H	-5.39192400	0.71539600	0.33158900
C	-4.37156200	0.25719100	2.16801300
C	-4.54385600	-0.28589600	3.50490000
C	-3.64359200	0.05845400	4.50907300
H	-5.10326500	-1.21477300	3.58119300
C	-2.34398900	1.30668600	2.92771300
C	-2.54960600	0.90125000	4.22121300
H	-3.74943300	-0.37719000	5.49796300
H	-1.48725600	1.89522400	2.62390400
H	-1.82784500	1.17467400	4.98270700
N	-3.22741100	0.99084600	1.92139000
C	-3.02356700	1.57311800	0.59319800
H	-2.02963300	2.01963100	0.54984600
H	-3.09962400	0.79708900	-0.17023500
H	-3.77640900	2.34498200	0.39907800

C-syn-RE

Zero-point correction= 0.374200 (Hartree/Particle)
Thermal correction to Energy= 0.398159
Thermal correction to Enthalpy= 0.399103
Thermal correction to Gibbs Free Energy= 0.319188
Sum of electronic and zero-point Energies= -5132.278609
Sum of electronic and thermal Energies= -5132.254650
Sum of electronic and thermal Enthalpies= -5132.253706
Sum of electronic and thermal Free Energies= -5132.333622

Single point energy (electronic) = -5134.5031565 (nitromethane)

C	-2.99373900	-3.04204700	-2.36245200
C	-1.37845200	-1.53927800	-1.60294900
C	-1.31643700	-0.90869600	-2.83556200
C	-2.13411900	-1.37192300	-3.87188000
C	-2.98501200	-2.44083800	-3.62747800
C	-3.87238900	-4.14656500	-1.96641600
C	-4.57332700	-5.45600100	-0.17361200
C	-5.45333100	-6.16659700	-0.97687400
C	-5.53804800	-5.84590300	-2.33547700
C	-4.73814100	-4.82464700	-2.83217900
H	-0.79438700	-1.19984200	-0.75600000
H	-0.64965300	-0.06457600	-2.97623500
H	-2.11730900	-0.89619500	-4.84777400
H	-3.65205100	-2.79774600	-4.40409400
H	-4.47372600	-5.67299500	0.88352900
H	-6.05895900	-6.95556100	-0.54340700
H	-6.21498200	-6.38274500	-2.99306800
H	-4.78111500	-4.55875600	-3.88276700
N	-2.17458600	-2.59951100	-1.36760900
N	-3.78953300	-4.46522300	-0.64395300
Ni	-2.49355700	-3.37730200	0.35240000
C	-1.35635900	-4.48949300	1.73926800
C	-0.29441400	-2.14654600	2.87878600
C	-1.37342800	-4.24288300	3.21597600
H	-2.83917800	-4.01484300	1.61587700
H	0.02455900	-1.22692900	3.35422000
Br	-3.50558100	-1.41750900	1.36244500
C	0.00871600	-2.44476000	1.58723600
H	0.62261500	-1.74950400	1.02527300
N	-1.01027800	-3.00381200	3.68985400
C	-1.19298600	-2.71846800	5.10466300
H	-0.94671700	-1.67312200	5.29724800
H	-2.23726000	-2.89336200	5.38146000
H	-0.55013400	-3.36073900	5.72154300
C	-1.78742200	-6.46550100	2.92337100
C	-2.02878300	-7.83701300	3.09186800
C	-1.51949300	-5.95830800	1.61956500
C	-1.98508500	-8.67700200	1.97983200
H	-2.23553700	-8.24259900	4.07933500
C	-1.49004200	-6.80483600	0.51508600
C	-1.71258900	-8.17226000	0.69948400
H	-2.16439100	-9.74193300	2.10744200
H	-1.29719500	-6.40994600	-0.47984000
H	-1.67783400	-8.84567800	-0.15245200
C	-0.56060900	-3.60080300	0.93726500
H	-0.07309000	-3.98960600	0.04562800
C	-1.70122000	-5.38909100	3.89021900
H	-1.79029400	-5.50809600	4.96238300

C-*anti*

Zero-point correction= 0.379656 (Hartree/Particle)
Thermal correction to Energy= 0.403444
Thermal correction to Enthalpy= 0.404388
Thermal correction to Gibbs Free Energy= 0.325032
Sum of electronic and zero-point Energies= -5132.301956
Sum of electronic and thermal Energies= -5132.278169
Sum of electronic and thermal Enthalpies= -5132.277225
Sum of electronic and thermal Free Energies= -5132.356581

Single point energy (electronic) = -5134.5337764 (nitromethane)

C	-3.23034800	-3.24239900	-2.64362000
C	-1.63506800	-1.56705500	-2.44021900
C	-1.37894500	-1.58905000	-3.80697700
C	-2.05959200	-2.50102100	-4.61115800
C	-3.00425700	-3.33200400	-4.01717200
C	-4.29556500	-3.96024900	-1.93397900
C	-5.55253100	-3.97491800	0.01724300
C	-6.31069500	-5.05131100	-0.43303100
C	-6.02692100	-5.60481300	-1.68142900
C	-5.00470600	-5.04868300	-2.44465000
H	-1.12109200	-0.88024700	-1.77809400
H	-0.65314100	-0.89823800	-4.22369900
H	-1.87801800	-2.54980700	-5.68060200
H	-3.58767100	-4.02112100	-4.61739500
H	-5.72187100	-3.50081900	0.97823600
H	-7.10623900	-5.44522200	0.19099100
H	-6.58839800	-6.45632300	-2.05434400
H	-4.75016000	-5.46472300	-3.41325200
N	-2.52328100	-2.38744300	-1.84995900
N	-4.56092000	-3.43506400	-0.71171100
Ni	-3.08740200	-2.27632500	-0.04410700
C	-0.39537800	-3.14907800	0.60085000
C	0.58010600	-0.62815800	-0.09638800
C	0.58112700	-2.96856500	-0.54558400
H	0.22253100	-3.20968000	1.51562600
H	1.12882000	0.29991000	-0.22278100
Br	-4.24924600	-1.51578900	1.79636300
C	-0.60261400	-0.69229800	0.55575700
H	-1.00766800	0.23081800	0.96203400
N	1.21389400	-1.75253200	-0.66564000
C	2.22409300	-1.57395600	-1.69007800
H	2.74452600	-0.62645100	-1.52706100
H	2.95378200	-2.38822200	-1.63204600
H	1.79449700	-1.57003600	-2.70510900
C	-0.24884200	-5.09038300	-0.77426100
C	-0.53726400	-6.39365700	-1.19248100
C	-0.94435200	-4.53271600	0.32810000
C	-1.51532800	-7.12384600	-0.50859100
H	-0.00812300	-6.83725600	-2.03305300
C	-1.90203200	-5.26850600	1.01224600
C	-2.19456200	-6.57229100	0.58196700
H	-1.74530700	-8.13811600	-0.82717500
H	-2.42689900	-4.83907200	1.86269000
H	-2.94753700	-7.15690600	1.10387900
C	-1.34951400	-1.94831900	0.80138500
H	-1.65492800	-1.94455500	1.84933800
C	0.68636300	-4.09997800	-1.29763200
H	1.31873500	-4.24796700	-2.16555500

C-*syn*

Zero-point correction= 0.377304 (Hartree/Particle)
Thermal correction to Energy= 0.401838
Thermal correction to Enthalpy= 0.402782
Thermal correction to Gibbs Free Energy= 0.319872
Sum of electronic and zero-point Energies= -5132.296393
Sum of electronic and thermal Energies= -5132.271858
Sum of electronic and thermal Enthalpies= -5132.270914
Sum of electronic and thermal Free Energies= -5132.353825

Single point energy (electronic) = -5134.5202606 (nitromethane)

C	-3.80282800	-2.52266100	-2.92429300
C	-2.51688100	-0.59458800	-2.70714600
C	-2.92978900	-0.12664000	-3.94925300
C	-3.82006800	-0.89876900	-4.69854100
C	-4.26757500	-2.10807400	-4.17706600
C	-4.20882500	-3.76415300	-2.24479100
C	-3.95177000	-5.04833800	-0.32613000
C	-4.91593800	-5.95671500	-0.74377600
C	-5.53772800	-5.75665700	-1.97765100
C	-5.18118100	-4.64379700	-2.73071500
H	-1.86159400	-0.02401000	-2.05812800
H	-2.56677500	0.82862100	-4.31396500
H	-4.16623800	-0.56104800	-5.67091000
H	-4.96791200	-2.71842200	-4.73637200
H	-3.44838200	-5.16740700	0.62606800
H	-5.17121600	-6.79999400	-0.11062400
H	-6.29321100	-6.44702000	-2.34026200
H	-5.66257400	-4.45329500	-3.68338900
N	-2.92910200	-1.77272100	-2.20836300
N	-3.58222500	-3.97684400	-1.05304700
Ni	-2.28111500	-2.58195600	-0.53039100
C	-0.21795500	-3.09842500	1.64028100
C	0.86910000	-3.04217100	-0.97182000
C	1.26763300	-3.03328700	1.36293100
H	-0.54551800	-2.05094500	1.74851200
H	1.31008800	-2.90045300	-1.95268400
Br	-2.29606600	-0.57637000	0.70895800
C	-0.36428500	-3.64348600	-0.79613300
H	-0.74168100	-4.21274400	-1.64338200
N	1.68067700	-2.67465000	0.09055500
C	3.08477300	-2.37609900	-0.14212100
H	3.20324700	-1.94301200	-1.13828800

H	3.42968400	-1.65049600	0.60005100
H	3.71008800	-3.27784400	-0.06882700
C	1.07729400	-3.80828600	3.50388200
C	1.31489700	-4.28963300	4.79465700
C	-0.25036100	-3.71537600	3.01485200
C	0.22697200	-4.68359900	5.57988800
H	2.32817200	-4.36273400	5.18313000
C	-1.32536900	-4.09295300	3.80553200
C	-1.08102900	-4.58972300	5.09425500
H	0.40127700	-5.06532400	6.58308500
H	-2.34346000	-3.99703100	3.43468400
H	-1.91374500	-4.89686300	5.72174800
C	-1.02530700	-3.71680200	0.49353900
H	-1.47337200	-4.68333600	0.73462800
C	1.99834800	-3.37304200	2.45848300
H	3.07904100	-3.38107700	2.54658600

C-*syn*-*TS*

Zero-point correction= 0.374635 (Hartree/Particle)
Thermal correction to Energy= 0.399323
Thermal correction to Enthalpy= 0.400267
Thermal correction to Gibbs Free Energy= 0.315847
Sum of electronic and zero-point Energies= -5132.280626
Sum of electronic and thermal Energies= -5132.255939
Sum of electronic and thermal Enthalpies= -5132.254995
Sum of electronic and thermal Free Energies= -5132.339415
Single point energy (electronic) = -5134.5142473 (nitromethane)

C	-3.43410600	-2.83626100	-2.57766700
C	-1.99049800	-1.13341000	-1.87470900
C	-1.66716400	-0.79750500	-3.17824200
C	-2.26973000	-1.51428700	-4.22449300
C	-3.15819800	-2.53455000	-3.91987700
C	-4.33323100	-3.88944500	-2.11446300
C	-5.23347000	-4.92346000	-0.21536500
C	-5.94924300	-5.82070100	-0.98458300
C	-5.85826800	-5.73876400	-2.38494200
C	-5.04676700	-4.76376700	-2.94563000
H	-1.57261400	-0.60139300	-1.02517000
H	-0.96915200	0.00942400	-3.37442300
H	-2.04787400	-1.27279500	-5.25965800
H	-3.63853400	-3.09510800	-4.71455600
H	-5.28406800	-4.93810900	0.86890200
H	-6.56945900	-6.56883700	-0.50237300
H	-6.41345600	-6.42360400	-3.01833600
H	-4.96262900	-4.67825400	-4.02390000
N	-2.84457600	-2.12955800	-1.56537400
N	-4.43036100	-3.97023700	-0.74641800
Ni	-3.50960900	-2.58644500	0.19680800
C	-1.79602300	-4.43881700	1.82755600
C	-0.62106100	-2.12127700	2.94459200
C	-1.43826800	-4.32519900	3.29851000
H	-2.85440000	-4.10298700	1.74376500
H	-0.34895200	-1.17912000	3.40155400
Br	-4.08688700	-1.23950100	1.93662600
C	-0.45042500	-2.38055000	1.58244000
H	0.07911200	-1.63494300	0.99516800
N	-1.12180400	-3.08417900	3.80546600
C	-0.98494400	-2.91904400	5.24447700
H	-0.94289200	-1.85387200	5.48138700
H	-1.85327100	-3.35645800	5.74539300
H	-0.07521100	-3.40673900	5.62203700
C	-1.68033600	-6.56321800	2.88565500
C	-1.73617800	-7.95726800	2.98004500
C	-1.81436500	-5.93676300	1.62106600
C	-1.91046500	-8.70860800	1.81349900
H	-1.63674600	-8.45244300	3.94296700
C	-1.99608600	-6.68658500	0.46967000
C	-2.03610600	-8.08610300	0.56836600
H	-1.94646100	-9.79349000	1.87714600
H	-2.10092100	-6.20310500	-0.49890500
H	-2.16413200	-8.68727200	-0.32778600
C	-0.94401900	-3.52672900	0.98426200
H	-0.71406200	-3.78453300	-0.04392200
C	-1.44978400	-5.54595300	3.90356700
H	-1.24491900	-5.75482500	4.94699900

C-*anti*-*TS*

Zero-point correction= 0.374770 (Hartree/Particle)
Thermal correction to Energy= 0.399426
Thermal correction to Enthalpy= 0.400370
Thermal correction to Gibbs Free Energy= 0.315679
Sum of electronic and zero-point Energies= -5132.282079
Sum of electronic and thermal Energies= -5132.257423
Sum of electronic and thermal Enthalpies= -5132.256479
Sum of electronic and thermal Free Energies= -5132.341170

Single point energy (electronic) = -5134.5167917 (nitromethane)

C	-3.54083400	-2.40657700	-2.31287200
C	-2.71403300	-0.32344200	-1.62898400
C	-2.61687300	0.12082200	-2.93362900
C	-3.01398400	-0.73808800	-3.97412100
C	-3.48024200	-2.00466800	-3.65352000
C	-3.97408900	-3.72040900	-1.84439600
C	-4.27775400	-5.04216500	0.06324400
C	-4.64460300	-6.14159200	-0.69559700
C	-4.69625400	-6.00659800	-2.09068000
C	-4.36021200	-4.78901400	-2.66546200
H	-2.43770100	0.30800300	-0.78979500
H	-2.24600700	1.11987500	-3.13789100
H	-2.96101700	-0.41688900	-5.00971500
H	-3.79782500	-2.68349600	-4.43807200
H	-4.22906500	-5.09102900	1.14589800
H	-4.87283300	-7.08082800	-0.20462200
H	-4.98958100	-6.84400700	-2.71686200
H	-4.38766800	-4.66674800	-3.74300700
N	-3.15922000	-1.55984900	-1.29958700
N	-3.94969700	-3.85382200	-0.48255800
Ni	-3.49333200	-2.23152400	0.44512500
C	-0.49842100	-5.25313200	1.83805700
C	-0.29420100	-2.47370300	2.26794400
C	-1.16625800	-4.55046300	3.01045700
H	0.52023200	-5.54467600	2.17151600
H	-0.09595800	-1.44086600	2.52241200
Br	-4.09968700	-1.33219000	2.42962200
C	-0.16823600	-2.97227700	0.96575000
H	0.09392600	-2.26702500	0.18169500
N	-0.78527400	-3.25941900	3.29949800
C	-1.28197700	-2.62217700	4.51624500
H	-0.67842400	-1.73473200	4.72264200
H	-2.32877900	-2.32113300	4.39738300
H	-1.18153000	-3.31894400	5.35301100
C	-2.21001600	-6.58057900	2.82568500
C	-3.04331900	-7.69341300	2.98587900
C	-1.30995100	-6.52753900	1.73104500
C	-2.97139800	-8.73377500	2.05280200
H	-3.73695000	-7.75147500	3.82116500
C	-1.23610100	-7.56584100	0.81693200
C	-2.08039700	-8.67623800	0.97666200
H	-3.61409300	-9.60293600	2.17159500
H	-0.53882400	-7.52550300	-0.01723000
H	-2.03681200	-9.49547500	0.26401500
C	-0.35740400	-4.31074200	0.67290300
H	-0.29580400	-4.69278200	-0.34066300
C	-2.10218000	-5.34917000	3.59831300
H	-2.72846000	-5.09518600	4.44495000

D (Ni(pry)HBr)

Zero-point correction= 0.169807 (Hartree/Particle)
Thermal correction to Energy= 0.181994
Thermal correction to Enthalpy= 0.182939
Thermal correction to Gibbs Free Energy= 0.129653
Sum of electronic and zero-point Energies= -4575.754681
Sum of electronic and thermal Energies= -4575.742494
Sum of electronic and thermal Enthalpies= -4575.741550
Sum of electronic and thermal Free Energies= -4575.794835

Single point energy (electronic) = -4578.0625319 (nitromethane)

C	-3.31935500	-3.52772100	-2.09561400
C	-1.48895000	-2.10569600	-2.22972700
C	-1.28601500	-2.42718300	-3.56812900
C	-2.14490800	-3.33816100	-4.18237300
C	-3.17634800	-3.89681000	-3.43566400
C	-4.35610000	-4.03444000	-1.18877100
C	-5.18834000	-3.91038200	0.98562300
C	-6.18909900	-4.82803200	0.69745300
C	-6.27077900	-5.36660700	-0.58741400
C	-5.34019000	-4.96080100	-1.53759000
H	-0.85968000	-1.40415900	-1.69193800
H	-0.46794500	-1.96692400	-4.11202600
H	-2.01530400	-3.61031600	-5.22565500
H	-3.85869300	-4.60756500	-3.88818600
H	-5.08707000	-3.46810400	1.96659200
H	-6.89096300	-5.11196800	1.47451000
H	-7.04167000	-6.08654000	-0.84415600
H	-5.37628800	-5.36063600	-2.54461300
N	-2.48202400	-2.63911600	-1.50117000
N	-4.27672600	-3.50734900	0.07041000
Ni	-2.91799600	-2.29561200	0.37821200
H	-3.34112800	-2.11569100	1.76176100
Br	-1.25781400	-0.81503700	0.75430500

D (product)

Zero-point correction= 0.204936 (Hartree/Particle)
Thermal correction to Energy= 0.215355
Thermal correction to Enthalpy= 0.216299
Thermal correction to Gibbs Free Energy= 0.169182
Sum of electronic and zero-point Energies= -556.544883
Sum of electronic and thermal Energies= -556.534464
Sum of electronic and thermal Enthalpies= -556.533520
Sum of electronic and thermal Free Energies= -556.580637

Single point energy (electronic) = -556.4688763 (nitromethane)

C	-1.05342600	-4.15876700	1.58266800
C	-0.93901700	-2.20116900	3.54761100
C	-1.61404700	-4.40082400	2.91655700
H	-0.91815500	-1.46846100	4.34635300
C	-0.40847700	-1.95300400	2.30662800
H	0.04934400	-0.98992600	2.11325900
N	-1.53115200	-3.39231700	3.86079000
C	-2.08967700	-3.64011700	5.18317800
H	-1.94763200	-2.76124600	5.81420000
H	-3.15991800	-3.86063000	5.10055000
H	-1.59268700	-4.50236400	5.64184100
C	-1.96032700	-6.28552900	1.70749600
C	-2.31104000	-7.55848500	1.22942300
C	-1.28644000	-5.37264400	0.83260000
C	-1.99609600	-7.90285300	-0.08174900
H	-2.82272400	-8.26819100	1.87538000
C	-0.97800200	-5.73581400	-0.48272600
C	-1.33412100	-7.00214100	-0.93738500
H	-2.26652100	-8.88813200	-0.45434400
H	-0.46653300	-5.03957000	-1.14419600
H	-1.10125500	-7.29877300	-1.95638800
C	-0.46552500	-2.95436300	1.29768600
H	-0.04406200	-2.75383300	0.31587500
C	-2.15542800	-5.66398700	2.99804100
H	-2.63761300	-6.12331300	3.85087400

Figure 2

A^2 (cationic substrate)

Zero-point correction= 0.231039 (Hartree/Particle)
Thermal correction to Energy= 0.244034
Thermal correction to Enthalpy= 0.244978
Thermal correction to Gibbs Free Energy= 0.189897
Sum of electronic and zero-point Energies= -3129.226666
Sum of electronic and thermal Energies= -3129.213671
Sum of electronic and thermal Enthalpies= -3129.212727
Sum of electronic and thermal Free Energies= -3129.267808

Single point energy (electronic) = -3131.5446423 (nitromethane)

C	1.50147400	-0.01500400	0.56781300
C	0.41407800	-2.49998700	1.22540300
C	1.53819600	-0.46849800	1.88782300
H	1.91581200	0.95074100	0.30066600
C	0.99473000	-1.70977700	2.21773900
H	-0.02091000	-3.46126300	1.48812200
H	1.98870600	0.15548900	2.65349000
H	1.01578200	-2.06145800	3.24432900
Br	0.87717200	-0.16607900	-2.21418000
C	0.36485700	-2.06983500	-0.10703800
C	0.91938400	-0.81782100	-0.40812600
C	0.68736900	-3.50542000	-2.17335000
C	1.91859500	-4.01429700	-1.75686100
C	2.79948500	-4.59512200	-2.66040200
H	2.17098000	-3.93322200	-0.70591200
C	1.22179900	-4.15561700	-4.39607400
C	2.44357400	-4.66330500	-4.01004700
H	3.75227400	-4.98831800	-2.32015700
H	0.88559800	-4.17394300	-5.42496700
H	3.09738400	-5.10148300	-4.75522400
C	-0.91505300	-3.04711000	-4.00818300
H	-0.92410500	-1.96881900	-3.83512800
H	-0.97725100	-3.24710100	-5.07657200
H	-1.75606200	-3.52508500	-3.50434200
N	0.36522600	-3.59818300	-3.49752600
C	-0.29470000	-2.92152900	-1.17374100
H	-1.05813700	-2.33094800	-1.68216200
H	-0.81550900	-3.76171100	-0.69449100

A'^2 (complex)

Zero-point correction= 0.391818 (Hartree/Particle)
Thermal correction to Energy= 0.416303
Thermal correction to Enthalpy= 0.417247
Thermal correction to Gibbs Free Energy= 0.335271
Sum of electronic and zero-point Energies= -5132.661858
Sum of electronic and thermal Energies= -5132.637373
Sum of electronic and thermal Enthalpies= -5132.636429
Sum of electronic and thermal Free Energies= -5132.718405

Single point energy (electronic) = -5134.9437371 (nitromethane)

C	-2.48567200	2.43959000	1.23364100
C	-0.78058400	2.15404800	2.79156500
C	-1.47553100	2.88151400	3.75310600
C	-2.72934100	3.39627100	3.42702100
C	-3.24111700	3.17015100	2.15053000
C	-2.89392800	2.15134500	-0.15699300
C	-2.25006200	1.08617200	-2.12477000
C	-3.35377800	1.58624900	-2.80841000
C	-4.26407100	2.38775900	-2.12050600
C	-4.02367900	2.68208400	-0.77994700
H	0.19190600	1.72170900	2.99776200
H	-1.03849100	3.03551800	4.73380400
H	-3.30271300	3.96378700	4.15329100
H	-4.21801900	3.55396200	1.87913600
H	-1.48337600	0.49396200	-2.61303000
H	-3.48730500	1.35636300	-3.86022700
H	-5.13672900	2.79472300	-2.62171200
H	-4.69976600	3.33058200	-0.23444200
N	-1.26349800	1.93512200	1.55687600
N	-2.02863000	1.33710100	-0.82266700
Ni	-0.53471500	0.76043900	0.22316100
C	1.24721400	0.15507400	0.62620300
C	0.57075800	-2.53783800	1.10741200
C	1.70869100	-0.52662500	1.80001400
H	1.85807600	0.99762800	0.29559000
C	1.32483000	-1.81498700	2.07260300
H	0.26758000	-3.55878500	1.33643400
H	2.39085000	-0.01155500	2.47393200
H	1.63321200	-2.31015300	2.98830500
C	0.23183500	-2.00154300	-0.11835000
C	0.49387500	-0.60734100	-0.38693200
C	0.63032800	-3.50632700	-2.11167200
C	1.82148800	-4.03856600	-1.60831400
C	2.73809900	-4.66785100	-2.43615700

H	2.01459600	-3.91854100	-0.54939500
C	1.28576900	-4.24437000	-4.27741200
C	2.46596100	-4.77011900	-3.80421900
H	3.65828300	-5.07128200	-2.02539800
H	1.01317800	-4.28034500	-5.32434500
H	3.15337700	-5.24527400	-4.49426300
C	-0.81501600	-3.03787400	-4.05996900
H	-0.74357900	-1.95616600	-3.92085800
H	-0.82477100	-3.27704200	-5.12226900
H	-1.71783100	-3.43500900	-3.59490800
N	0.38798900	-3.64410100	-3.44822800
Br	1.12527200	-0.35205700	-2.42986400
C	-0.39957000	-2.88123700	-1.18001900
H	-1.14135500	-2.31625900	-1.74308000
H	-0.93216900	-3.71282600	-0.69610100

A^2-TS

Zero-point correction= 0.390368 (Hartree/Particle)
Thermal correction to Energy= 0.414892
Thermal correction to Enthalpy= 0.415836
Thermal correction to Gibbs Free Energy= 0.333231
Sum of electronic and zero-point Energies= -5132.649858
Sum of electronic and thermal Energies= -5132.625335
Sum of electronic and thermal Enthalpies= -5132.624391
Sum of electronic and thermal Free Energies= -5132.706995

Single point energy (electronic) = -5134.933981 (nitromethane)

C	0.15903600	-0.00797500	0.05300200
C	0.09418800	0.34927300	2.35413500
C	1.48159300	0.35531300	2.44030200
C	2.22429600	0.18519400	1.27178100
C	1.55451700	0.00124600	0.06456200
C	-0.67667200	-0.24311200	-1.14041500
C	-2.86957900	-0.45680800	-1.89182600
C	-2.44097200	-0.81040100	-3.16754900
C	-1.07291200	-0.86709900	-3.42877400
C	-0.17936500	-0.59511300	-2.39592700
H	-0.52688200	0.48765600	3.23245100
H	1.96282100	0.49284300	3.40239500
H	3.30937400	0.19319900	1.29881900
H	2.11389000	-0.13108400	-0.85438500
H	-3.91253800	-0.48606700	-1.59584400
H	-3.17214400	-1.05057400	-3.93195400
H	-0.70451500	-1.14331000	-4.41186900
H	0.88872100	-0.67462400	-2.56240300
N	-0.55980000	0.17398300	1.19274800
N	-2.01311900	-0.14684000	-0.90477600
Ni	-2.44900700	0.41174500	0.87839300
C	-3.59307100	1.04983000	2.49815200
C	-5.14282100	3.20924300	1.66575800
C	-3.84914300	2.11336900	3.38612100
H	-3.26962500	0.09905400	2.92703300
C	-4.60494400	3.19772200	2.96340300
H	-5.74078400	4.06710300	1.35893600
H	-3.53142500	2.04684800	4.42374500
H	-4.82060800	4.01687200	3.64227600
Br	-4.91960200	-1.39534100	0.64886800
C	-4.90123800	2.17838100	0.75744900
C	-4.05068600	1.12994500	1.14868100
C	-7.01230100	2.03844800	-0.59322700
C	-7.56515900	0.83672500	-0.13916000
C	-8.94105100	0.67195200	-0.06445000
H	-6.87807000	0.03689300	0.14931400
C	-9.21373200	2.89500500	-0.88946200
C	-9.78269900	1.72460100	-0.44204600
H	-9.35444700	-0.26876100	0.28597700
H	-9.80479700	3.74615600	-1.20237000
H	-10.86271800	1.64358400	-0.39502300
C	-7.34286500	4.33328500	-1.49043800
H	-6.80360500	4.16693300	-2.42471300
H	-8.18746100	4.99422000	-1.67888100
H	-6.68314300	4.79873300	-0.75772300
N	-7.85975600	3.04516900	-0.96708800
C	-5.50847300	2.20984400	-0.64126500
H	-5.10232000	1.37157200	-1.21311600
H	-5.22360400	3.12178100	-1.17014300

B^2

Zero-point correction= 0.393276 (Hartree/Particle)
Thermal correction to Energy= 0.417712
Thermal correction to Enthalpy= 0.418657
Thermal correction to Gibbs Free Energy= 0.337125
Sum of electronic and zero-point Energies= -5132.732906
Sum of electronic and thermal Energies= -5132.708470
Sum of electronic and thermal Enthalpies= -5132.707526
Sum of electronic and thermal Free Energies= -5132.789057

Single point energy (electronic) = -5135.0029377 (nitromethane)

C	0.17445300	-0.07849900	-0.17562400
C	-0.02616400	-0.02825600	1.20564000
C	1.07121400	-0.02660000	2.06812900
C	2.35612300	-0.02680200	1.52736100
C	2.55385400	-0.02850400	0.13618200
C	1.45991700	-0.10463600	-0.74771900
H	-0.70075900	-0.10820500	-0.82242700
H	-1.03610300	-0.01014600	1.60722000
H	0.93052300	-0.02430900	3.14516300
H	3.21852400	-0.02101300	2.19335700
C	4.47385400	1.51958300	-0.49930500
C	4.01563900	2.53432700	0.34634600
C	4.54899300	3.81266300	0.29155100
H	3.21136900	2.29466200	1.02988600
C	5.99912600	3.08078000	-1.45169400
C	5.56312700	4.09421700	-0.62962600
H	6.77175000	3.22765900	-2.19551000
H	6.00601300	5.07959000	-0.71532200
C	5.94138800	0.82454700	-2.35849700
H	5.11875300	0.63613400	-3.05410100
H	6.79659000	1.23229500	-2.89557700
H	6.24044100	-0.09344300	-1.85224200
N	5.47832900	1.82608800	-1.37330400
Br	2.32512500	1.76136500	-2.89587400
C	0.67966600	-1.90258000	-4.81987200
C	1.11948500	0.26188600	-5.53338300
C	0.23868100	-2.26762400	-6.09287200
C	0.69593000	-0.03196100	-6.82636600
H	1.47989100	1.24626200	-5.25844800
C	0.24600600	-1.31859300	-7.11174500
H	-0.11531900	-3.27296700	-6.28799600
H	0.71902700	0.74154300	-7.58634100
H	-0.09733500	-1.58187400	-8.10740600
C	0.72086300	-2.81043900	-3.66324800
C	0.43977600	-4.17519900	-3.73512400
C	0.53357600	-4.95855600	-2.58902400
H	0.15868700	-4.62432700	-4.68015300
C	1.17550900	-2.98253100	-1.39092000
C	0.91398500	-4.34809100	-1.39690100
H	0.31825100	-6.02161500	-2.63039900
H	1.45968200	-2.47437900	-0.48032600
H	1.00700100	-4.91166500	-0.47496100
N	1.11573800	-0.64724100	-4.54341400
N	1.08177200	-2.20993200	-2.49265100
Ni	1.49437500	-0.34986000	-2.61754200
H	4.17554300	4.58780800	0.95329500
C	3.96694000	0.08930100	-0.40762200
H	4.67665300	-0.45798500	0.23374800
H	4.00622700	-0.37396200	-1.39403700

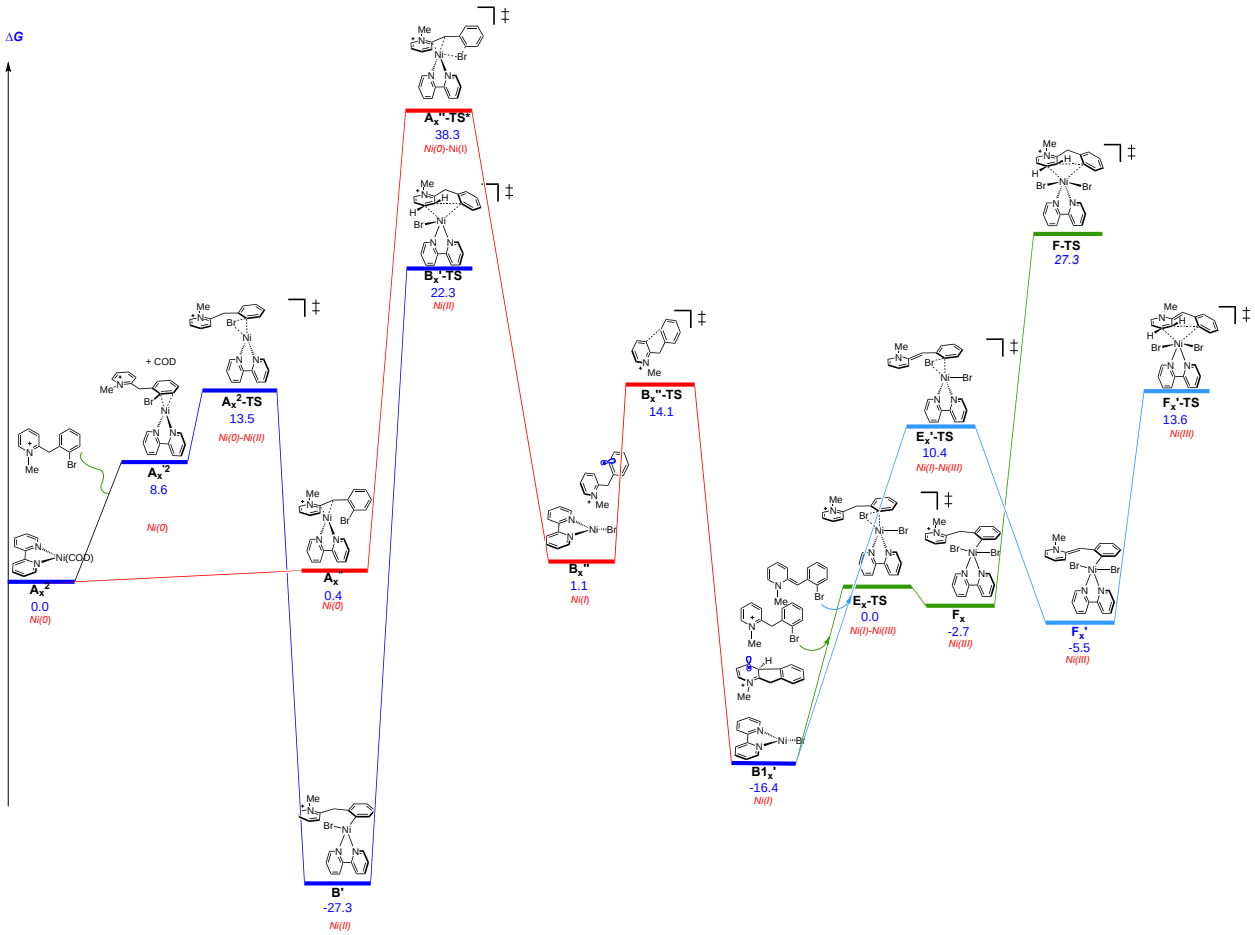


Figure S1. Cyclization Pathways Commencing from Cationic pyridine substrate.[a] [a] Free energies are given in kcal/mol for calculations with *UM06/6-311+G(d,p)-SMD-nitromethane//UB3LYP/6-31G(d)-gas. * Denotes that structure has geometric constraints about bond-breaking/forming.*