Supporting Information

for

Enantioselective Synthesis of α-(Hetero)aryl Piperidines Through Asymmetric Hydrogenation of Pyridinium Salts and Its Mechanistic Insights

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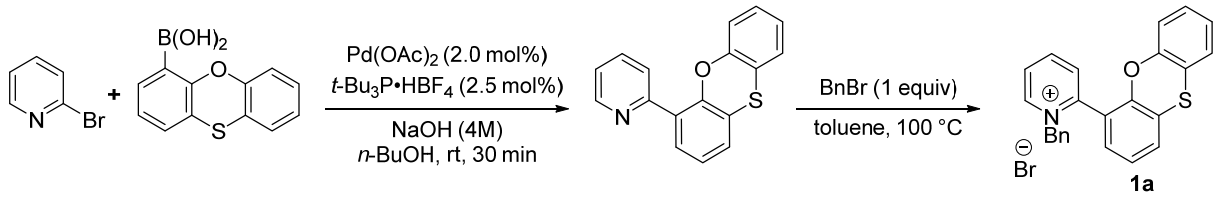
General Information

All reactions for the preparation of substrates and catalysts were performed in standard, dry glassware under an inert atmosphere of nitrogen or argon unless otherwise described. All starting materials and reagents were purchased from commercial sources and used as received unless otherwise noted. 2-(4-methyl-3-thienyl)pyridine, 2-(2,5-dimethyl-3-thienyl)pyridine, 2-(2-bromophenyl)pyridine, 2-(2,4-difluorophenyl)pyridine, 2-(2-(trifluoromethyl)phenyl)pyridine, 2-(2,4-dimethylphenyl)pyridine were purchased and used as received. Palladium catalysts and $[Ir(COD)Cl]_2$ were purchased from Aldrich or Strem and used as received. Ligand (*S*,*S*)-BoQPhos[1] and pyridinium salts **1h**[2] and **1r**[2] were prepared according to the reported procedures. ^1H and ^{13}C NMR spectra were recorded using 400 or 500 MHz spectrometers. Chemical shifts (δ) are given in ppm, and coupling constants (*J*) are given in Hz. The 7.26 resonance of residual $CHCl_3$ (or 0 ppm of TMS) for proton spectra and the 77.23 ppm resonance of $CDCl_3$ for carbon spectra were used as internal references. Chiral HPLC analyses (normal phase) were conducted on Waters Aquity SFC system or Agilent SFC system. UPLC-MS analyses were conducted on a Waters Acquity Ultra Performance LC system. Flash chromatography was performed on a Combi-Flash automated system with EMD 230-400 mesh silica gel columns. High resolution mass spectrometric data were obtained on an Agilent 6210 time-of-flight HPLC/MS spectrometer (ESI-TOF).

[1] B. Qu, L. P. Samankumara, J. Savoie, D. R. Fandrick, N. Haddad, X. Wei, S. Ma, H. Lee, S. Rodriguez, C. A. Busacca, N. K. Yee, J. J. Song, C. H. Senanayake, *J. Org. Chem*. **2014**, *79*, 993–1000.

[2] M. Chang, Y. Huang, S. Liu, Y. Chen, S. W. Krska, I. W. Davies, X. Zhang, *Angew. Chem., Int. Ed*. **2014**, *53*, 12761–12764.

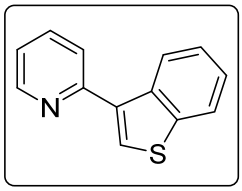
General procedure for the synthesis of pyridinium salts (except compounds **1f** and **1s**)



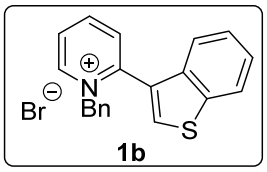
To a three-neck-flak under N_2 charge phenoxathiin-4-ylboronic acid (2.92 g, 12.0 mmol, 1.2 equiv), *n*-BuOH (15.0 mL) and 2-bromopyridine (1.58 g, 10.0 mmol). The mixture was sparged with Ar for 15 min; then degassed sodium hydroxide aqueous solution (5 mL, 4 M, 2.0 equiv) was slowly added. To this mixture add $Pd(OAc)_2$ (46 mg, 0.2 mmol) and tri-*tert*-butylphosphonium tetrafluoroborate (62 mg, 0.25 mmol). The resulting reaction mixture was stirred at room temperature for 0.5 – 4 h. The reaction progress was monitored by UPLC. Upon completion, the reaction was stopped with addition of water (10 mL). Crude mixture was extracted with ethyl acetate, dried over sodium sulfate, filtered, and concentrated. The crude mixture was submitted to silica gel chromatography (eluent: 20% ethyl acetate in hexanes) to afford the product 2-(phenoxathiin-4-yl)pyridine as pale yellow oil (2.72 g, 9.8 mmol, 98% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.73 (d, *J* = 4.6 Hz, 1H), 7.87-7.83 (m, 1H), 7.78 (dt, *J* = 7.7 Hz, 1.8 Hz, 1H), 7.61 (dd, *J* = 7.6 Hz, 1.6 Hz, 1H), 7.30-7.26 (m, 1H), 7.20-7.08 (m, 4H), 7.05-7.00 (m, 1H), 6.91 (dd, *J* = 8.1 Hz, 0.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 154.8, 152.4, 149.8, 149.7, 135.7, 130.2, 129.7, 127.7, 127.4, 126.9, 125.3, 124.8, 124.5, 122.2, 121.5, 121.2, 117.8.

To a solution of 2-(phenoxathiin-4-yl)pyridine (1.25 g, 4.5 mmol) in toluene (4.5 mL) was added benzyl bromide (765 mg, 4.5 mmol) in one portion, and the resulting mixture was heated at 100 °C for 14 h. Toluene was removed under reduced pressure, the product was purified by silica gel chromatography (eluent: DCM to 10% MeOH in DCM) to afford the product **1a** as pale brown solid (1.65 g, 3.46 mmol, 77% yield). ^{1}H NMR (500 MHz, DMSO-D_6) δ 9.53 (d, *J* = 6.1 Hz, 1H), 8.81 (t, *J* = 7.7 Hz, 1H), 8.38 (t, *J* = 6.6 Hz, 1H), 8.25 (d, *J* = 7.7 Hz, 1H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.46 (dd, *J* = 7.7 Hz, 0.9 Hz, 1H), 7.3 (d, *J* = 7.3 Hz, 1H), 7.23 (dd, *J* = 7.1 Hz, 2.1 Hz, 1H), 7.15-7.05 (m, 5H), 6.88 (d, *J* = 7.2 Hz, 2H), 6.63-6.60 (m, 1H), 5.81 (q, *J* = 13.3 Hz, 2H); ^{13}C NMR (125 MHz, DMSO-D_6) δ 151.0, 150.3, 148.4, 147.7, 146.9,

133.5, 132.2, 130.5, 129.1, 129.04, 128.96, 128.7, 128.5, 128.2, 127.3, 126.1, 125.6, 121.5, 121.1, 118.4, 118.3, 62.2. HRMS (ESI) $[M]^+$ m/z calcd for $[C_{24}H_{18}NOS]^+$ is 368.1104, found 368.1100.

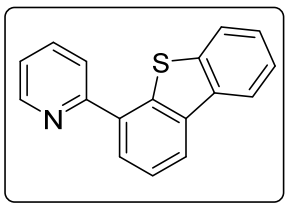


2-(benzo[b]thiophen-3-yl)pyridine: colorless oil, 2.06 g, 9.8 mmol, 98% yield (starting from 10.0 mmol 2-bromopyridine); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (d, *J* = 4.6 Hz, 1H), 8.45 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 7.5 Hz, 1H), 7.79-74 (m, 2H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.46-7.37 (m, 2H), 7.27-7.24 (m, 1H); ^{13}C NMR (100 Hz, $CDCl_3$) δ 154.6, 149.7, 140.9, 137.3, 136.7, 136.6, 126.4, 124.7, 124.6, 124.1, 122.7, 122.6, 122.0. HRMS (ESI) $[M+H]^+$ m/z calcd for $[C_{13}H_{10}NS]^+$ is 212.0528, found 212.0525.

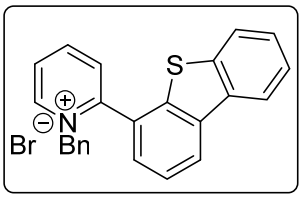


2-(benzo[b]thiophen-3-yl)-1-benzylpyridinium bromide (1b)

White solid, 1.12 g, 2.93 mmol, 64% yield (starting from 4.5 mmol 2-(benzo[b]thiophen-3-yl)pyridine); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.90 (d, *J* = 6.3 Hz, 1H), 8.72-8.67 (m, 1H), 8.27-8.23 (m, 2H), 7.95 (d, *J* = 8.1 Hz, 1H), 7.48-7.29 (m, 3H), 7.18-7.10 (m, 3H), 6.96-6.94 (m, 2H), 6.25 (br s, 1H), 5.97 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.4, 148.1, 145.9, 139.7, 136.7, 132.8, 132.5, 131.1, 129.3, 129.2, 128.5, 127.9, 126.0, 125.9, 123.1, 121.5, 62.8. HRMS (ESI) $[M]^+$ m/z calcd for $[C_{20}H_{16}NS]^+$ is 302.0998, found 302.0995.

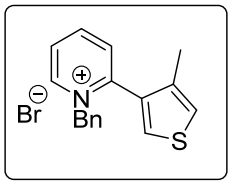


2-(dibenzo[b,d]thiophen-4-yl)pyridine: yellow solid, 1.93 mg, 7.4 mmol, 74% yield (starting from 10.0 mmol 2-bromopyridine); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.87 (d, *J* = 4.7 Hz, 1H), 8.25 (dd, *J* = 7.8, 1.1 Hz, 1H), 8.20-8.18 (m, 1H), 8.00 (d, *J* = 7.6 Hz, 1H), 7.97 (d, *J* = 8.3 Hz, 1H), 7.94-7.90 (m, 1H), 7.82 (dt, *J* = 7.6, 1.5 Hz, 1H), 7.59 (t, *J* = 7.7 Hz, 1H), 7.50-7.44 (m, 2H),7.30 (ddd, *J* = 4.9, 1.1 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.4, 148.7, 142.2, 137.9, 137.5, 134.9, 133.6, 129.9, 125.2, 124.8, 124.3, 122.7, 122.4, 122.3, 121.6, 121.1; HRMS (ESI) $[M+H]^+$ m/z calcd for $[C_{17}H_{12}NS]^+$ is 262.0685, found 262.0684.



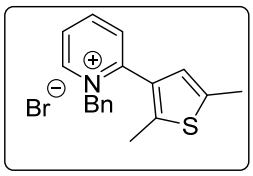
1-benzyl-2-(dibenzo[b,d]thiophen-4-yl)pyridinium bromide (1c)

Light brown foamy solid, 1.44 g, 3.3 mmol, 74% yield (starting from 4.5 mmol 2-(dibenzo[b,d]thiophen-4-yl)pyridine); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.99 (d, *J* = 6.2 Hz, 1H), 8.62 (td, *J* = 7.7, 1.4 Hz, 1H), 8.39 (dd, *J* = 8.0, 0.9 Hz, 1H), 8.29-8.13 (m, 1H), 8.01 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.86 (dd, *J* = 7.5, 1.2 Hz, 1H), 7.81 (m, 1H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.56 (m, 2H), 7.20-7.12 (m, 3H), 7.05 (m, 2H), 6.21 (d, *J* = 13.8 Hz, 1H), 6.00 (d, *J* = 13.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.7, 148.4, 145.9, 139.3, 138.8, 137.3, 134.9, 132.6, 130.2, 129.7, 129.5, 129.3, 128.7, 128.5, 128.3, 125.7, 124.7, 123.1, 122.5, 62.7; HRMS (ESI) $[M]^+$ m/z calcd for $[C_{24}H_{18}NS]^+$ is 352.1154, found 352.1151.



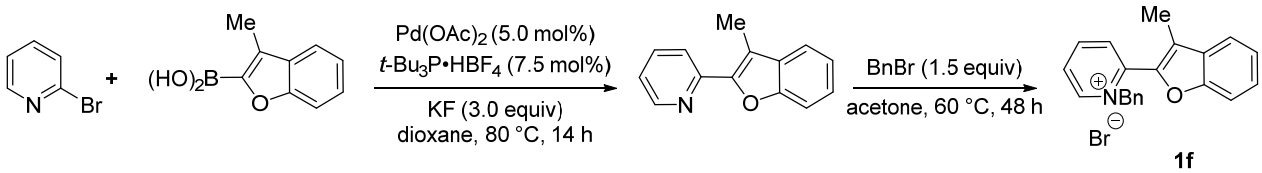
1-benzyl-2-(4-methylthiophen-3-yl)pyridinium bromide (1d)

Light red hygroscopic solid, 1.04 g, 3.02 mmol, 67% yield (starting from 4.5 mmol 2-(4-methylthiophen-3-yl)pyridine); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.03 (d, *J* = 6.0 Hz, 1H), 8.67 (t, *J* = 7.8 Hz, 1H), 8.23 (t, *J* = 7.5 Hz, 1H), 7.92 (d, *J* = 3.1 Hz, 1H), 7.77 (d, *J* = 7.8 Hz, 1H), 7.12-7.31 (m, 4H), 6.98-7.00 (m, 2H), 6.08 (s, 2H), 1.76 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.7, 148.4, 145.7, 136.4, 132.9, 131.6, 130.8, 129.8, 129.6, 129.4, 128.7, 127.9, 62.9, 14.3; HRMS (ESI) $[M]^+$ m/z calcd for $[C_{17}H_{16}NS]^+$ is 266.0998, found 266.0996.



1-benzyl-2-(2,5-dimethylthiophen-3-yl)pyridin-1-ium bromide (1e)

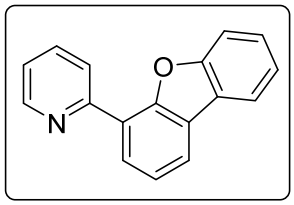
White solid, 1.34 g, 3.73 mmol, 83% yield (starting from 4.5 mmol 2-(2,5-dimethylthiophen-3-yl)pyridine); ^{1}H NMR ($CDCl_3$, 500 MHz) δ 10.08 (d, *J* = 5.0 Hz, 1H), 8.68 (t, *J* = 10.0 Hz, 1H), 8.20 (t, *J* = 10.0 Hz, 1H), 7.81 (d, *J* = 10.0, 1H), 7.31-7.24 (m, 3H), 7.01 (d, *J* = 5.0 Hz, 2H), 6.81 (s, 1H), 6.10 (br s, 2H), 2.49 (s, 3H), 1.90 (s, 3H); ^{13}C NMR ($CDCl_3$, 500 MHz) 151.4, 148.1, 146.0, 140.3, 139.7, 133.0, 130.8, 129.3, 129.1, 128.3, 127.6, 127.5, 124.8, 62.2, 15.1, 13.4. HRMS (ESI) $[M]^+$ m/z calcd for $[C_{18}H_{18}NS]^+$ is 280.1154, found 280.1152.



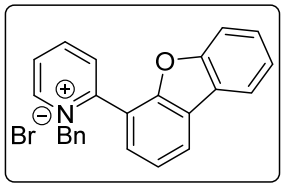
1f

To a three-neck-flak under N_2 charge (3-methylbenzofuran-2-yl)boronic acid (2.67 g, 15.2 mmol, 1.2 equiv), KF (2.2 g, 38.0 mmol, 3.0 equiv), degassed dioxane (50 mL), and 2-bromopyridine (2.0 g, 12.7 mmol, 1.0 equiv). The mixture was sparged with Ar for 15 min, before addition of tri-*tert*-butylphosphonium tetrafluoroborate (275 mg, 0.95 mmol) and $Pd(OAc)_2$ (142 mg, 0.63 mmol). The reaction mixture was stirred at 80 °C for 14 h and monitored by LC/MS. Upon completion, the reaction was diluted with water (40 mL). The crude mixture was extracted with ethyl acetate (60 mL x 2), dried over sodium sulfate, filtered, and concentrated. The crude mixture was submitted to silica gel chromatography (eluent: hexanes to 10% ethyl acetate in hexanes) to afford the product as pale yellow solid (1.14 g, 5.44 mmol, 43% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (d, J = 3.6 Hz, 1H), 7.87 (d, J = 6.8 Hz, 1H), 7.72 (td, J = 6.4, 1.2 Hz, 1H), 7.58 (d, J = 6.0 Hz, 1H), 7.50 (d, J = 6.4 Hz, 1H), 7.34-7.30 (m, 1H), 7.26-7.23 (m, 1H), 7.17-7.14 (m, 1H), 2.71 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.0, 151.4, 149.6, 149.1, 136.4, 131.2, 125.3, 122.6, 121.9, 121.0, 120.1, 115.9, 111.3, 9.7.

To a solution of 2-(3-methylbenzofuran-2-yl)pyridine (400 mg, 1.91 mmol, 1.0 equiv) in acetone (1.0 mL) was added benzyl bromide (0.34 mL, 2.87 mmol, 1.5 equiv), and the resulting mixture was heated at 60 °C for 48 h. The reaction was filtered and volatiles were removed under reduced pressure, the crude mixture was purified by silica gel chromatography (eluent: DCM to 10% MeOH in DCM) to afford the product (**1f**) as light yellow solid (602 mg, 1.58 mmol, 83% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.3 (d, J = 6.0 Hz, 1H), 8.77 (t, J = 8.0 Hz, 1H), 8.26 (t, J = 7.0 Hz, 1H), 8.09 (d, J = 7.6 Hz, 1H), 7.60-7.49 (m, 3H), 7.38 (t, J = 7.4 Hz, 1H), 7.24-7.20 (m, 1H), 7.17-7.09 (m, 4H), 6.32 (s, 2H), 2.21 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.4, 148.7, 146.7, 143.4, 139.8, 132.4, 131.5, 129.1, 128.7, 128.0, 127.9, 127.74, 127.71, 123.9, 123.0, 120.8, 111.5, 62.6, 8.7; HRMS (ESI) $[M]^+$ m/z calcd for $[C_{21}H_{18}NO]^+$ is 300.1383, found 300.1383.

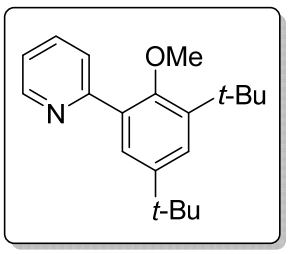


2-(dibenzo[b,d]furan-4-yl)pyridine: white solid, 1.70 g, 6.9 mmol, 69% yield (starting from 10.0 mmol 2-bromopyridine); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.79 (d, *J* = 4.4 Hz, 1H), 8.42 (d, *J* = 7.9 Hz, 1H), 8.28 (d, *J* = 7.8 Hz, 1H), 8.00 (t, *J* = 6.9 Hz, 2H), 7.87 (t, *J* = 6.9 Hz, 1H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.51-7.46 (m, 2H), 7.37 (t, *J* = 7.4 Hz, 1H), 7.30 (dd, *J* = 7.6, 5.3 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.3, 154.0, 153.9, 150.0, 136.8, 127.5, 125.3, 124.47, 124.46, 124.2, 123.5, 123.2, 122.6, 121.4, 120.9, 112.0; HRMS (ESI) $[M+H]^+$ m/z calcd for $[C_{17}H_{12}NO]^+$ is 246.0913, found 246.0913.

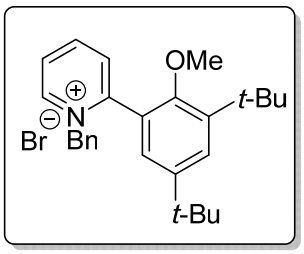


1-benzyl-2-(dibenzo[b,d]furan-4-yl)pyridinium bromide (1g)

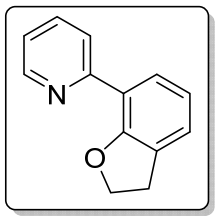
White solid, 1.33 g, 3.2 mmol, 71% yield (starting from 4.5 mmol 2-(dibenzo[b,d]furan-4-yl)pyridine); ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.26 (d, *J* = 6.0 Hz, 1H), 8.66 (t, *J* = 7.8 Hz, 1H), 8.29 (t, *J* = 6.9 Hz, 1H), 8.19 (d, *J* = 8.2 Hz, 1H), 8.01 (d, *J* = 7.8 Hz, 1H), 7.99 (d, *J* = 7.8 Hz, 1H), 7.61 (d, *J* = 7.6 Hz, 1H), 7.55-7.50 (m, 2H), 7.48 (m, 1H), 7.43 (t, *J* = 7.1 Hz, 1H), 7.09 (m, 3H), 6.94 (d, *J* = 6.9 Hz, 2H), 6.13 (br s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.4, 152.4, 151.2, 148.6, 145.9, 132.7, 131.2, 129.5, 129.2, 128.89, 128.86, 128.5, 128.2, 125.9, 124.7, 124.2, 124.0, 123.0, 121.4, 115.6, 112.3, 62.9; HRMS (ESI) $[M]^+$ m/z calcd for $[C_{24}H_{18}NO]^+$ is 336.1383, found 336.1379.



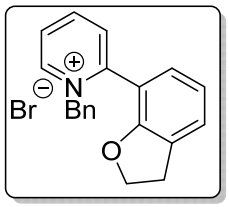
2-(3,5-di-tert-butyl-2-methoxyphenyl)pyridine: white solid, 2.68 g, 9.0 mmol, 90% yield (starting from 10.0 mmol 2-bromopyridine); ^{1}H NMR (400 Hz, $CDCl_3$) 8.73 (d, *J* = 3.7 Hz, 1H), 7.75-7.68 (m, 2H), 7.45 (d, *J* = 1.8 Hz, 1H), 7.39 (d, *J* = 1.84 Hz, 1H), 7.23-7.20 (m, 1H), 3.30 (s, 3H), 1.44 (s, 9H), 1.34 (s, 9H); ^{13}C NMR (100 Hz, $CDCl_3$) δ 158.4, 155.5, 149.7, 145.5, 141.9, 136.0, 133.3, 126.4, 124.8, 124.6, 121.6, 61.3, 35.3, 34.6, 31.5, 30.9. HRMS (ESI) $[M+H]^+$ m/z calcd for $[C_{20}H_{28}NO]^+$ is 298.2165, found 298.2163.



1-benzyl-2-(3,5-di-tert-butyl-2-methoxyphenyl)pyridinium bromide (1i) White solid, 1.52 g, 3.24 mmol, 72% yield (starting from 4.5 mmol 2-(3,5-di-tert-butyl-2-methoxyphenyl)pyridine); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.55 (d, *J* = 5.4 Hz, 1H), 8.84-8.80 (m, 1H), 8.31-8.27 (m, 1H), 7.86 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.60 (d, *J* = 2.44 Hz, 1H), 7.20-7.11 (m, 3H), 6.78 (d, *J* = 7.3 Hz, 1H), 6.73 (d, *J* = 2.44 Hz, 1H), 6.46 (d, *J* = 14.4 Hz, 1H), 5.73 (d, *J* = 14.4 Hz, 1H), 3.30 (s, 3H), 1.47 (s, 9H), 1.20 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.5, 153.9, 148.4, 147.8, 146.4, 143.9, 132.9, 130.8, 129.2, 128.9, 128.4, 128.3, 127.7, 126.3, 125.1, 62.7, 62.2, 35.6, 34.7, 31.2, 30.7. HRMS (ESI) $[M]^+$ m/z calcd for $[C_{27}H_{34}NO]^+$ is 388.2635, found 388.2631.

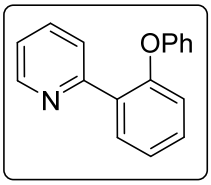


2-(2,3-dihydrobenzofuran-7-yl)pyridine: pale brown oil, 1.60 g, 8.1 mmol, 81% yield (starting from 10.0 mmol 2-bromopyridine); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.69 (m, 1H), 8.06 (d, *J* = 8.0 Hz, 1H), 7.91 (d, *J* =7.9 Hz, 1H), 7.71 (dt, *J* =7.8, 1.7 Hz, 1H), 7,23 (d, *J* =7.7 Hz, 1H), 7.17 (m, 1H), 6.98 (1H, *J* = 7.6 Hz, 1H), 4.67 (t, *J* = 8.7 Hz, 2H), 3.27 (t, *J* = 8.8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.8, 154.8, 149.4, 136.3, 128.1, 127.9, 125.5, 123.7, 122.2, 121.7, 120.9, 71.4, 29.4; HRMS (ESI) $[M+H]^+$ m/z calcd for $[C_{13}H_{12}NO]$+ is 198.0913, found 198.0912.

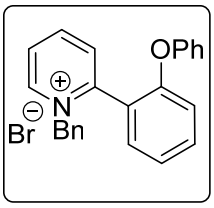


1-benzyl-2-(2,3-dihydrobenzofuran-7-yl)pyridin-1-ium bromide (1j)

Light brown hygroscopic solid, 773 mg, 2.1 mmol, 35% yield (starting from 6.0 mmol 2-(2,3-dihydrobenzofuran-7-yl)pyridine); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.13 (d, *J* = 5.9 Hz, 1H), 8.52 (td, *J* = 7.8, 1.2 Hz, 1H), 8.14 (t, *J* = 7.7 Hz, 1H), 7.82 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.45 (d, *J* = 7.9 Hz, 1H), 7.21-7.29 (m, 3H), 7.00-7.16 (m, 4H), 6.10 (s, 2H), 4.58 (t, *J* = 8.7 Hz, 2H), 3.33 (t, *J* = 8.7 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.0, 152.4, 147.9, 145.2, 133.0, 130.7, 129.3, 129.1, 128.9, 128.8, 128.8, 128.5, 127.5, 121.8, 113.3, 72.4, 62.2, 29.4; HRMS (ESI) $[M]^+$ m/z calcd for $[C_{20}H_{18}NO]^+$ is 287.1310, found 287.1309.

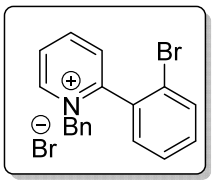


2-(2-phenoxyphenyl)pyridine: pale yellow oil, 2.40 g, 9.97 mmol, 97% yield (starting from 10.0 mmol 2-bromopyridine); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.67 (d, *J* = 4.5 Hz, 1H), 7.93 (d, *J* = 7.7 Hz, 1H), 7.83 (d, *J* = 8.1 Hz, 1H), 7.60 (dt, *J* = 7.7 Hz, 1.7 Hz, 1H), 7.36-7.31 (m, 1H), 7.28-7.22 (m, 3H), 7.16-7.12 (m, 1H), 7.04-6.98 (m, 2H), 6.95 (d, *J* = 8.1 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.5, 155.2, 154.1, 149.6, 135.9, 132.1, 131.5, 130.0, 129.7, 124.8, 124.3, 122.9, 122.0, 120.1, 118.2.



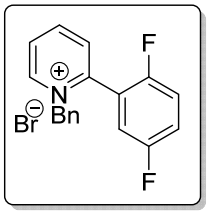
1-benzyl-2-(2-phenoxyphenyl)pyridin-1-ium bromide (1k)

Pale red solid, 1.34 g, 3.2 mmol, 71% yield (starting from 4.5 mmol 2-(2-phenoxyphenyl)pyridine); ^{1}H NMR (400 MHz, DMSO-D_6) δ 9.44 (d, *J* = 6.0 Hz, 1H), 8.73 (t, *J* = 7.4 Hz, 1H), 8.30-8.25 (m, 2H), 7.64-7.58 (m, 2H), 7.40-7.34 (m, 3H), 7.33-7.28 (m, 3H), 7.20 (t, *J* = 7.4 Hz, 1H), 6.96 (d, *J* = 7.4 Hz, 2H), 6.91 (d, *J* = 7.9 Hz, 2H), 6.84 (d, *J* = 8.4 Hz, 1H), 5.94 (d, *J* = 14.9 Hz, 1H), 5.84 (d, *J* = 14.9 Hz, 1H); ^{13}C NMR (125 MHz, DMSO-D_6) δ 154.93, 154.90, 152.3, 147.3, 146.8, 134.0, 133.8, 132.2, 131.4, 130.7, 129.3, 128.4, 128.3, 125.5, 123.8, 122.1, 121.4, 117.2, 61.9; HRMS (ESI) $[M]^+$ m/z calcd for $[C_{24}H_{20}NO]^+$ is 338.1545, found 338.1536.



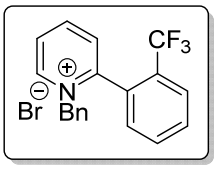
1-benzyl-2-(2-bromophenyl)pyridinium bromide (1l)

Ash color solid, 1.05 g, 2.6 mmol, 58% yield (starting from 4.5 mmol 2-(2-bromophenyl)pyridine); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.85 (d, *J* = 6.3 Hz, 1H), 8.71 (t, *J* = 8.2 Hz, 1H), 8.25 (m, 1H), 7.85 (d, *J* = 7.5 Hz, 1H), 7.74 (m, 2H), 7.52 (m, 2H), 7.35-7.23 (m, 3H), 7.11 (m, 2H), 5.94 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.8, 147.4, 146.1, 133.4, 133.2, 132.3, 132.0, 131.8, 130.9, 129.8, 129.52, 129.5, 129.4, 128.6, 128.3, 122.3, 62.7; HRMS (ESI) $[M]^+$ m/z calcd for $[C_{18}H_{15}NBr]^+$ is 324.0382, found 324.0380.



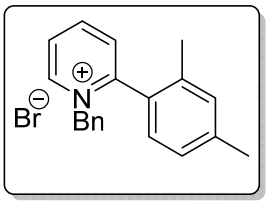
1-benzyl-2-(2,5-difluorophenyl)pyridinium bromide (1m)

White solid, 994 mg, 2.745 mmol, 61% yield (starting from 4.5 mmol 2-(2,5-difluorophenyl)pyridine); ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.88 (d, *J* = 6.0 Hz, 1H), 8.66 (t, *J* = 7.9 Hz, 1H), 8.27 (t, *J* = 6.9 Hz, 1H), 7.91 (d, *J* = 7.8 Hz, 1H), 7.61 (m, 1H), 7.35-7.30 (m, 4H), 7.22 (dt, *J* = 9.0, 3.8 Hz, 1H), 7.10 (d, *J* = 7.6 Hz, 2H), 6.07 (d, *J* = 14.3 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 159.7 (d, *J* = 2.2 Hz), 157.8 (d, *J* = 2.5 Hz), 155.9 (d, *J* = 2.5 Hz), 153.9 (d, *J* = 2.8 Hz), 148.7, 148.2, 146.2, 132.1, 131.1, 129.9, 129.6, 128.9, 128.8, 121.1 (dd, *J* = 24.4, 9.4 Hz), 120.4 (dd, *J* = 17.6, 8.8 Hz), 118.6 (dd, *J* = 26.4, 1.8 Hz), 118.4 (dd, *J* = 23.7, 8.4 Hz) 63.2; HRMS (ESI) $[M]^+$ m/z calcd for $[C_{18}H_{14}NF_2]^+$ is 282.1086, found 282.1089.



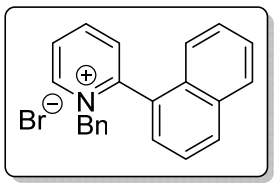
1-benzyl-2-(2-(trifluoromethyl)phenyl)pyridinium bromide (1n)

White solid, 1.10 g, 2.79 mmol, 62% yield (starting from 4.5 mmol 2-(2-(trifluoromethyl)phenyl)pyridine); ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.18 (d, *J* = 6.3 Hz, 1H), 8.50 (d, *J* = 7.7 Hz, 1H), 8.33 (d, *J* = 8.5 Hz, 1H), 8.10 (t, *J* = 7.3 Hz, 1H), 7.89 (d, *J* = 7.5 Hz, 1H), 7.81 (m, 3 H), 7.36 (m, 3H), 7.27 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 152.1, 146.5, 145.1, 133.2, 132.5, 131.9, 131.0, 130.1, 130.07, 130.04, 129.5, 128.9 (q, *J* = 2.1 Hz), 128.4 (q, *J* = 30.6 Hz), 127.0 (d, *J* = 4.7 Hz), 124.5 (q, *J* = 274.0 Hz), 63.0; HRMS (ESI) $[M]^+$ m/z calcd for $[C_{19}H_{15}F_3N]^+$ is 314.1151, found 314.1148.



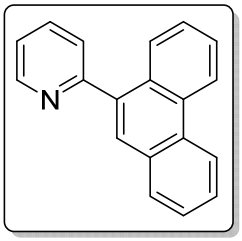
1-benzyl-2-(2-4-dimethylphenyl)pyridin-1-ium bromide (1o)

White solid, 1.45 g, 4.1 mmol, 91% yield (starting from 4.5 mmol 2-(2,4-dimethylphenyl)pyridine); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.17 (d, *J* = 6.0 Hz, 1H), 8.54 (t, *J* = 7.7 Hz, 1H), 8.18 (t, *J* = 6.9 Hz, 1H), 7.73 (d, *J* = 7.7 Hz, 1H), 7.31-7.38 (m, 5H), 7.16 (s, 1H), 7.03 (d, *J* = 7.4 Hz, 2H), 6.07 (d, *J* = 13.9 Hz, 1H), 5.98 (d, *J* = 13.9 Hz, 1H), 2.43 (s, 3H), 1.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.9, 148.3, 145.4, 142.4, 136.4, 132.7, 132.1, 130.2, 129.7, 129.4, 129.1, 128.0, 127.7, 127.6, 62.0, 21.6, 19.8; HRMS (ESI) $[M]^+$ m/z calcd for $[C_{20}H_{20}N]^+$ is 274.1590, found 274.1588.

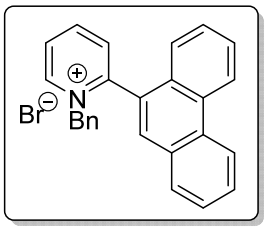


1-benzyl-2-(naphthalen-1-yl)pyridinium bromide (1p)

Pale brown solid, 0.93 g, 2.475 mmol, 55% yield (starting from 4.5 mmol 2-(naphthalen-1-yl)pyridine); ^{1}H NMR ($CDCl_3$, 500 mHz) δ 10.09 (d, *J* = 5.0 Hz, 1H), 8.75 (t, *J* = 10.0 Hz, 1H), 8.32 (t, *J* = 5.0 Hz, 1H), 8.12 (d, *J* = 5.0 Hz, 1H), 7.99 (d, *J* = 5.0 Hz, 1H), 7.94 (d, *J* = 10 Hz, 1H), 7.63-7.49 (m, 4H), 7.19-7.09 (m, 4H), 6.89 (d, *J* = 10.0 Hz, 2H), 5.93 (ABq, *J* = 10.0 Hz, $\Delta\upsilon_{AB}$ = 5.0 Hz, 2H); ^{13}C NMR ($CDCl_3$, 500 mHz) δ 154.6, 148.0, 145.9, 133.2, 132.6, 132.2, 131.0, 130.0, 129.4, 129.1, 129.0, 128.8, 128.0, 127.9, 127.4, 125.2, 123.7, 62.3. HRMS (ESI) $[M]^+$ m/z calcd for $[C_{22}H_{18}N]^+$ is 296.1434, found 296.1431.

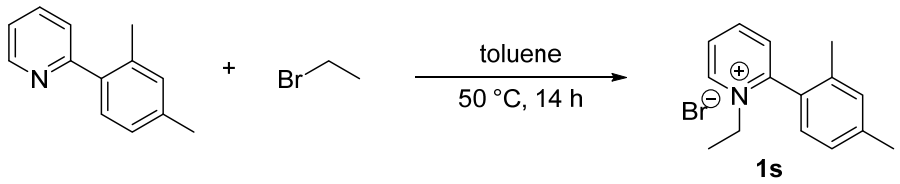


2-(phenanthren-9-yl) pyridine: white solid, 2.30 g, 9.0 mmol, 90% yield (starting from 10.0 mmol 2-bromopyridine); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.83 (m, 1H), 8.78 (d, *J* = 8.3 Hz, 1H), 8.73 (d, *J* = 7.7 Hz, 1H), 8.08 (d, *J* = 8.3 Hz, 1H), 7.94 (d, *J* = 8.3 Hz, 1H), 7.86 (m, 2H), 7.72-7.67 (m, 2H), 7.66 (m, 1H), 7.64-7.61 (m, 1H), 7.60-7.56 (m, 1H) 7.37 (ddd, *J* = 4.9,1.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.6, 149.8, 137.4, 136.7, 131.6, 131.0, 130.7, 130.5, 129.2, 128.3, 127.2, 127.0, 126.8, 125.3, 123.1, 122.8, 122.4; HRMS (ESI) $[M+H]^+$ m/z calcd for $[C_{19}H_{14}N]^+$ is 256.1121, found 256.1119.



1-benzyl-2-(phenanthren-9-yl)pyridinium bromide (1q)

White solid, 1.55 g, 3.645 mmol, 81% yield (starting from 4.5 mmol 2-(phenanthren-9-yl) pyridine); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.08 (dd, *J* = 6.4, 1.2 Hz, 1H), 8.80 (d, *J* = 8.2 Hz, 1H), 8.76 (d, *J* = 8.4 Hz, 1H), 8.67 (td, *J* = 7.8, 1.4 Hz, 1H), 8.33 (td, *J* = 7.8, 1.4 Hz, 1H), 7.96 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.93-7.89 (m, 2H), 7.83 (td, *J* = 7.3, 1.4 Hz, 1H), 7.75 (td, *J* = 7.3, 1.1 Hz, 1H), 7.70 (td, *J* = 7.0, 1.0 Hz, 1H), 7.58 (td, *J* = 7.0, 1.0 Hz, 1H), 7.22 (d, *J* = 8.2 Hz, 1H), 7.17 (m, 1H), 7.08 (m, 2H), 6.95 (m, 2H), 6.13 (d, *J* = 14.0 Hz, 1H), 5.77 (d, *J* = 15.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.8, 148.4, 145.8, 132.9, 131.4, 131.2, 130.9, 130.6, 130.0, 129.9, 129.6, 129.5, 129.3, 129.1, 128.7, 128.6, 128.4, 128.3, 128.1, 127.0, 125.1, 123.8, 123.6, 62.5; HRMS (ESI) $[M]^+$ m/z calcd for $[C_{26}H_{20}N]^+$ is 346.1590, found 346.1587.

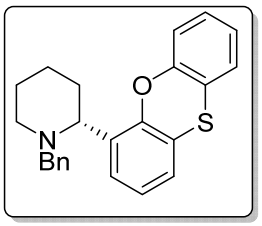


1s

To a solution of 2-(2,4-dimethylphenyl)pyridine (1.0 g, 5.74 mmol, 1.0 equiv) in toluene (5 mL) was added ethyl bromide (1.2 ml, 16.4 mmol, 3.0 equiv), and the resulting mixture was heated at 50 °C for 14 h. Precipitates were resulted. At end of the reaction, 5 ml EtOAc was added. The product was collected by filtration, dried to yield the desired product **1s** as white solid, 0.97 g, 3.5 mmol, 61% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.27 (d, *J* = 6.1 Hz, 1H), 8.59 (td, *J* = 7.9 Hz, 1H), 8.25 (t, *J* = 7.0 Hz, 1H), 7.74 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.20 (d, *J* = 10.6 Hz, 2H), 7.17 (s, 1H), 4.99 (dq, *J* = 7.4 Hz, 1H), 4.54 (dq, *J* = 7.4 Hz, 1H), 2.41 (s, 3H), 2.07 (s, 3H), 1.46 (t, *J* = 7.33 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 155.4, 147.8, 145.4, 142.4, 135.7, 132.2, 130.0, 128.7, 128.3, 127.84, 127.8, 54.2, 21.6, 20.0, 17.1; HRMS (ESI) $[M]^+$ m/z calcd for $[C_{15}H_{18}N]^+$ is 212.1434, found 212.1433.

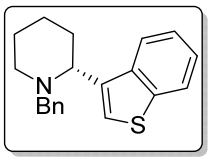
General procedure for the asymmetric hydrogenation of pyridinium salts

A high pressure steel autoclave (HEL 100 mL) hydrogenation vessel was taken into the glove box. Catalyst solution was prepared in a vial with $[Ir(COD)Cl]_2$ (1 mol%) and ligand (*S*,*S*)-MeOBoQPhos (3 mol%), and stir for 15 min in THF (5 mL). Then I_2 (5 mol%) was added and stir for 1-2 min. Pyridinium salt (1 mmol) was added to the hydrogenation vessel and degassed THF (15 mL). The catalyst solution was then transferred to the vessel and parafilmed before taking out of the glove box. The vessel was put onto the HEL hydrogenation autoclave reactor. The mixture was purged first purged with N_2 (3x) and then H_2 (3x) and stirred at the desired pressure and temperature for 20 h. Upon completion, the reactor was vented and purged with N_2 (2x). The mixture was added diethylamine (2 equiv). Percentage conversions and enantiomeric ratios were determined by chiral HPLC and SFC and the products were purified by silica gel (100% hexanes to 30% EtOAc/hexanes).



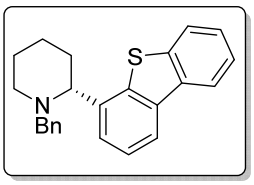
1-benzyl-2-(phenoxathiin-4-yl)piperidine (2a)

White solid, 343 mg, 0.92 mmol, 92% yield, er: 99.3:0.7; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.9 Hz, 1H), 7.25 (m, 4H), 7.21-7.15 (m, 3H), 7.10 (d, *J* = 7.9 Hz, 1H), 7.05 (t, *J* = 7.8 Hz, 2H), 7.01 (d, *J* = 7.5 Hz, 1H), 3.87 (d, *J* = 10.1 Hz, 1H), 3.80 (d, *J* = 13.3 Hz, 1H), 3.02 (d, *J* = 11.2 Hz, 1H), 2.90 (d, *J* = 13.3 Hz, 1H), 2.02 (d, *J* = 11.6 Hz, 1H), 1.86 (d, *J* = 13.6 Hz, 1H), 1.81 (d, *J* = 13.6 Hz, 1H), 1.68-1.59 (m, 2H),1.55-1.42 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.9, 150.1, 139.7, 134.8, 128.9, 128.2, 127.8, 127.1, 126.8, 126.7, 125.2, 124.9, 121.8, 120.8, 118.1, 60.5, 60.0, 53.7, 35.7, 26.2, 25.4; Enantiomeric ratio was determined by SFC: Chiralpack IC-3, 4.6 mm x 150 mm, temperature: 30 ºC, A: CO_2, B: denatured ethanol (contains 5% MeOH and 5% 2-propanol) with 0.2% of diethylamine; Isocratic: A/B:96.5/3.5, v/v, flow rate 3.0 mL/min. HRMS (ESI) $[M+H]^+$ m/z calcd for $[C_{24}H_{24}NOS]^+$ is 374.1573, found 374.1568.



2-(benzo[b]thiophen-3-yl)-1-benzylpiperidine (2b)

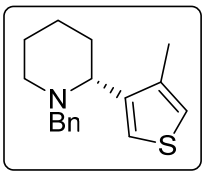
White solid, 272 mg, 0.89 mmol, 89% yield, er: 96.6:3.4; ^{1} H NMR (500 MHz, $CDCl_3$) δ 8.36 (d, *J* = 7.9 Hz, 1H), 7.84 (d, *J* = 7.9 Hz, 1H), 7.40 (m, 2H), 7.39 (m, 1H), 7.23-7.10 (m, 5H), 3.83 (d, *J* = 14.7 Hz, 1H), 3.59 (dd, *J* = 11.8, 2.7 Hz, 1H), 3.01 (m, 1H), 2.87 (d, *J* = 13.4 Hz, 1H), 2.04-1.90 (m, 2H), 1.86-1.78 (m, 2H), 1.68-1.61 (m, 2H), 1.43 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 141.4, 140.2, 139.8, 138.0, 129.0,128.2, 126.7, 124.5, 123.8, 123.0, 122.7, 64.6, 60.2, 53.8, 34.4, 26.2, 25.4; Enantiomeric ratio was determined by SFC: Lux Cellulose-3, 4.6 x 150 mm: 30 ºC, A: CO_2, B: denatured ethanol (contains 5% MeOH and 5% 2-propanol) with 0.2% of diethylamine; Isocratic: A/B:97/3, v/v, flow rate 3.0 mL/min. HRMS (ESI) $[M+H]^+$ m/z calcd for $[C_{20}H_{22}NS]^+$ is 308.1467, found 308.1465.



1-benzyl-2-(dibenzo[b,d]thiophen-4-yl)piperidine (2c)

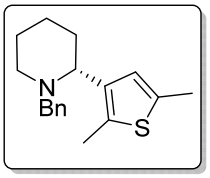
White solid, 332 mg, 0.93 mmol, 93% yield, er: 95.1:4.9; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (m, 1H), 8.05 (d, *J* = 7.6 Hz, 1H), 7.89 (d, *J* = 6.3, 1.9 Hz, 1H), 7.57 (d, *J* = 7.2 Hz, 1H), 7.46-7.41 (m, 3H), 7.30 (d, *J* = 7.3 Hz, 2H), 7.30 (t, *J* = 7.6 Hz, 2H), 7.30 (t, *J* = 7.1

Hz, 1H), 3.80 (d, *J* = 13.5 Hz, 1H), 3.45 (dd, *J* = 11.4, 2.8 Hz, 1H), 3.06 (m, 1H), 2.94 (d, *J* = 13.8 Hz, 1H), 1.99 (m, 2H), 1.83 (m, 2H), 1.73-1.62 (m, 2H), 1.47-1.37 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 140.4, 140.0, 139.1, 137.4, 136.7, 135.9, 129.4, 128.2, 126.8, 126.7, 125.6, 125.0, 124.3, 122.8, 121.6, 120.3, 68.9, 60.4, 53.3, 33.4, 26.0, 25.3; Enantiomeric ratio was determined by SFC: Chiracel OD-3, 4.6 x 150 mm: 30 ºC, A: CO_2, B: Methanol with 0.2% of diethylamine (DEA); Isocratic: A/B: 90/10, v/v, flow rate 3.0 mL/min. HRMS (ESI) $[M+H]^+$ m/z calcd for $[C_{24}H_{24}NS]^+$ is 358.1624, found 358.1622.



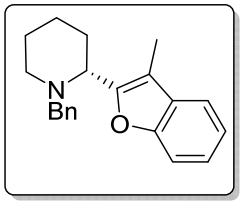
1-benzyl-2-(4-methylthiophen-3-yl)piperidine (2d)

Light brown solid, 192 mg, 0.71 mmol, 71% yield, er: 96.4:3.6; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.17-7.28 (m, 6H), 6.87 (m, 1H), 3.84 (d, *J* = 13.5 Hz, 1H), 3.24 (dd, *J* = 11.0, 2.9 Hz, 1H), 2.98 (d, *J* = 11.6 Hz, 1H), 2.87 (d, *J* = 13.4 Hz, 1H), 2.30 (s, 3H), 1.95-1.89 (m, 1H), 1.79-1.73 (m, 2H), 1.69-1.55 (m, 3H), 1.39-1.31 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 144.8, 139.7, 136.4, 128.7, 128.0, 126.5, 121.6, 121.3, 63.0, 59.5, 53.7, 35.1, 25.9, 25.2, 14.9; Enantiomeric ratio was determined by SFC: Chiracel OZ-3, 4.6 x 150 mm: 30 ºC, A: CO_2, B: denatured ethanol (contains 5% MeOH and 5% 2-propanol) with 0.2% of diethylamine (DEA); Isocratic: A/B: 99/1, v/v, flow rate 3.0 mL/min. HRMS (ESI) $[M+H]^+$ m/z calcd for $[C_{17}H_{22}NS]^+$ is 272.1467, found 272.1466.



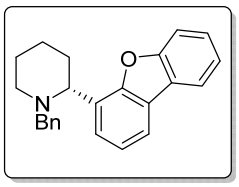
1-benzyl-2-(2,5-dimethylthiophen-3-yl)piperidine (2e)

Light yellow liquid, 237 mg, 0.83 mmol, 83% yield, er: 96.7:3.3; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.18 (m, 5H), 6.77 (s, 1H), 3.80 (d, *J* = 12.4 Hz, 1H), 3.13 (m, 1H), 2.92 (d, *J* = 13.3 Hz, 1H), 2.81 (d, *J* = 13.3 Hz, 1H), 2.40 (s, 3H), 2.35 (s, 3H), 1.88 (td, *J* = 11.4, 3.4 Hz, 1H), 1.77 (m, 1H), 1.68-150 (m, 4H), 1.34 (m 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 140.7, 140.0, 135.7, 129.0, 128.2, 126.7, 125.6, 62.0, 59.7, 53.8, 34.7, 26.2, 25.4, 15.5, 13.1; Enantiomeric ratio was determined by SFC: Chiralpack IC-3, 4.6 mm x 150 mm, temperature: 30 ºC, A: CO_2, B: denatured ethanol (contains 5% MeOH and 5% 2-propanol) with 0.2% of diethylamine (DEA); Isocratic: A/B: 96.5/3.5, v/v, flow rate 3.0 mL/min. HRMS (ESI) $[M+H]^+$ m/z calcd for $[C_{18}H_{24}NS]^+$ is 286.1624, found 286.1622.



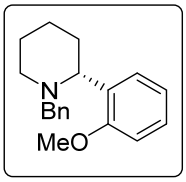
1-benzyl-2-(3-methylbenzofuran-2-yl)piperidine (2f)

White solid, 238 mg, 78% yield, er: 90.3:9.7; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49 (d, *J* = 8.0 Hz, 1H), 7.45 (d, *J* = 7.7 Hz, 1H), 7.26-7.16 (m, 7H), 3.80 (d, *J* = 13.1 Hz, 1H), 3.47 (dd, *J* = 11.4, 3.6 Hz, 1H), 3.07 (d, *J* = 13.4 Hz, 1H), 3.00 (m, 1H), 2.26 (s, 3H), 2.09-2.00 (m, 2H), 1.87-1.76 (m, 2H), 1.69-1.62 (m, 2H), 1.41-1.33 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 154.1, 154.0, 138.4, 130.1, 129.3, 128.0, 126.7, 123.6, 122.1, 118.9, 111.5, 111.2, 60.0, 59.6, 53.1, 31.9, 25.7, 24.5, 8.0; Enantiomeric ratio was determined by SFC: Lux Cel 1, 4.6 mm x 150 mm, temperature: 35 ºC, A: CO_2, B: MeOH with 0.1% of trimethylamine (TEA); Gradient: 1% B to 3% B in 3 min, to 50% B in 5 min, hold at 50%B for 1 min; flow rate 3.0 mL/min, BPR pressure: 150 bar; 254 nm UV detection. HRMS (ESI) $[M+H]^+$ m/z calcd for $[C_{21}H_{24}NO]^+$ is 306.1852, found 306.1850.



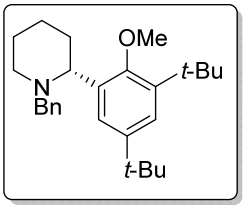
1-benzyl-2-(dibenzo[b,d]furan-4-yl)piperidine (2g)

White solid, 303 mg, 0.89 mmol, 89% yield, er: 90.3:9.7; ^{1} H NMR (500 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.6 Hz, 1H), 7.81 (dd, *J* = 7.9,1.2 Hz, 1H), 7.61 (d, *J* = 8.2 Hz, 1H), 7.46 (d, *J* = 7.7 Hz, 1H), 7.37-7.31(m, 2H), 7.28-7.22 (m, 5H), 7.18 (m, 1H), 3.95 (dd, *J* = 10.9, 2.9 Hz, 1H), 3.82 (d, *J* = 13.3 Hz, 1H), 3.05 (m, 1H), 2.93 (d, *J* = 13.3 Hz, 1H), 2.08 (m, 1H), 1.94 (m, 1H), 1.87-1.74 (m, 2H), 1.71-1.63 (m, 2H),1.55-1.42 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.9, 150.1, 139.7, 134.8, 128.9, 128.2, 127.8, 127.1, 126.8, 126.7, 125.2, 124.9, 121.8, 120.8, 118.1, 60.5, 60.0, 53.7, 35.7, 26.2, 25.4; Enantiomeric ratio was determined by SFC: Chiralpack IC-3, 4.6 mm x 150 mm, temperature: 30 ºC, A: CO_2, B: denatured ethanol (contains 5% MeOH and 5% 2-propanol) with 0.2% of diethylamine (DEA); Isocratic: A/B: 96.5/3.5, v/v, flow rate 3.0 mL/min. HRMS (ESI) $[M+H]^+$ m/z calcd for $[C_{24}H_{24}ON]^+$ is 342.1852, found 342.1850.



1-benzyl-2-(2-methoxyphenyl)piperidine (2h)

White solid, 256 mg, 0.91 mmol, 91% yield, er: 93.7:6.3; the compound data were in good accordance with the literature.[1] ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.9 Hz, 1H), 7.25 (m, 4H), 7.21-7.15 (m, 2H), 6.97 (t, *J* = 7.9 Hz, 1H), 6.86 (d, *J* = 8.4 Hz, 1H), 3.83 (s, 3H), 3.78 (d, *J* = 13.6 Hz, 1H), 3.69 (dd, *J* = 11.1, 2.6 Hz, 1H), 2.97 (m, 1H), 2.82 (d, *J* = 13.7 Hz, 1H), 1.96 (td, *J* = 11.5, 4.0 Hz, 1H), 1.76 (m, 3H), 1.61-1.58 (m, 2H), 1.48 (m, 2H), 1.38 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 140.2, 133.7, 129.9, 128.9, 128.6, 128.1, 127.9, 127.4, 126.6, 121.3, 110.8, 60.0, 59.8, 58.7, 53.9, 35.9, 26.3, 25.5; Enantiomeric ratio was determined by SFC: Chiralpack IC-3, 4.6 mm x 150 mm, temperature: 30 ºC, A: CO_2, B: denatured ethanol (contains 5% MeOH and 5% 2-propanol) with 0.2% of diethylamine (DEA); Isocratic: A/B: 96.5/3.5, v/v, flow rate 3.0 mL/min. HRMS (ESI) $[M+H]^+$ m/z calcd for $[C_{19}H_{24}NO]^+$ is 282.1852, found 282.1850.



1-benzyl-2-(3,5-di-tert-butyl-2-methoxyphenyl) piperidine (2i)

White solid, 350 mg, 0.89 mmol, 89% yield, er: 95.3:4.7; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 (d, *J* = 2.4 Hz, 1H), 7.27-7.22 (m, 4H), 7.20 (d, *J* = 2.4 Hz, 1H), 7.17 (m, 1H), 3.81 (s, 3H), 3.67 (d, *J* = 13.3 Hz, 1H) 3.56 (dd, *J* = 11.0, 2.2 Hz, 1H), 2.96 (d, *J* = 11.4 Hz, 1H), 2.76 (d, *J* = 13.3 Hz, 1H), 1.99 (m, 1H), 1.83 (m, 2H), 1.69-1.57 (m, 3H), 1.45 (m, 1H), 1.40 (s, 9H), 1.32 (m, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.6, 146.2, 141.6, 140.7, 138.2, 128.9, 128.1, 126.6, 123.8, 122.8, 62.9, 61.9, 59.7, 54.1, 36.6, 31.8, 31.5, 26.3, 25.8; Enantiomeric ratio was determined by SFC: Chiralcel OJ-3, 4.6 mm x 150 mm, temperature: 30 ºC, A: CO_2, B: denatured ethanol (contains 5% methanol and 5% 2-propanol) with 0.2% of diethylamine (DEA). Isocratic: A/B: 97/3, v/v, flow rate 3.0 mL/min. HRMS (ESI) $[M+H]^+$ m/z calcd for $[C_{27}H_{40}NO]^+$ is 394.3104, found 394.3098.

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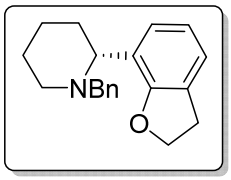
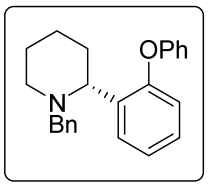
[1] M. Chang, Y. Huang, S. Liu, Y. Chen, S. W. Krska, I. W. Davies, X. Zhang, *Angew. Chem., Int. Ed*. **2014**, *53*, 12761–12764.



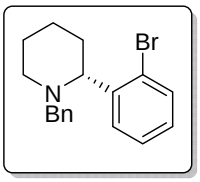
1-benzyl-2-(2,3-dihydrobenzofuran-7-yl)piperidine (2j)

White solid, 246 mg, 0.84 mmol, 84% yield, er: 94.5:5.5; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.9 Hz, 1H), 7.25 (m, 4H), 7.21-7.15 (m, 3H), 7.10 (d, *J* = 7.9 Hz, 1H), 7.05 (t, *J* = 7.8 Hz, 2H), 7.01 (d, *J* = 7.5 Hz, 1H), 3.87 (d, *J* = 10.1 Hz, 1H), 3.80 (d, *J* = 13.3 Hz, 1H), 3.02 (d, *J* = 11.2 Hz, 1H), 2.90 (d, *J* = 13.3 Hz, 1H), 2.02 (d, *J* = 11.6 Hz, 1H), 1.86 (d, *J* = 13.6 Hz, 1H), 1.81 (d, *J* = 13.6 Hz, 1H), 1.68-1.59 (m, 2H), 1.55-1.42 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.9, 150.1, 139.7, 134.8, 128.9, 128.2, 127.8, 127.1, 126.8, 126.7, 125.2, 124.9, 121.8, 120.8, 118.1, 60.5, 60.0, 53.7, 35.7, 26.2, 25.4; Enantiomeric ratio was determined by SFC: Lux Cellulose-3, 4.6 x 150 mm, temperature: 30 ºC, A: CO_2, B: MeOH contains 0.2% of diethylamine; Isocratic: A/B: 90/10, v/v, flow rate 3.0 mL/min. HRMS (ESI) $[M+H]^+$ m/z calcd for $[C_{20}H_{24}ON]^+$ is 294.1852, found 294.1850.



1-benzyl-2-(2-phenoxyphenyl)piperidine (2k)

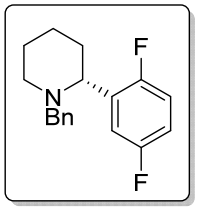
Colorless viscous liquid, 305 mg, 0.89 mmol, 89% yield, er: 93.7:6.3; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83-7.855 (m, 1H), 7.33-7.23 (m, 6H), 7.21-7.15 (m, 3H), 7.06 (t, *J* = 7.4 Hz, 1H), 6.94 (d, *J* = 7.9 Hz, 2H), 6.88 (m, 1H), 3.83 (d, *J* = 13.6 Hz, 1H), 3.64 (dd, *J* = 11.6, 2.9 Hz, 1H), 2.93 (d, *J* = 11.6 Hz, 1H), 2.76 (d, *J* = 13.6 Hz, 1H), 1.71-1.92 (m, 3H)1.51-1.58 (m, 3H), 1.24-1.36 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.5, 154.0, 140.1, 137.2, 129.8, 128.9, 128.7, 128.2, 127.7, 126.7, 124.7, 122.7, 120.0, 118.0, 60.7, 60.0, 53.6, 36.0, 26.2, 25.3; Enantiomeric ratio was determined by SFC: Chiralcel OJ-3, 4.6 mm x 150 mm, temperature: 30 ºC, A: CO_2, B: denatured ethanol (contains 5% methanol and 5% 2-propanol) with 0.2% of diethylamine (DEA). Isocratic: A/B: 97/3, v/v, flow rate 3.0 mL/min. HRMS (ESI) $[M+H]^+$ m/z calcd for $[C_{24}H_{26}ON]^+$ is 344.2009, found 344.2005.



1-benzyl-2-(2-bromophenyl)piperidine (2l)

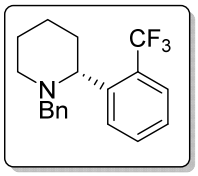
Light yellow solid, 304 mg, 0.92 mmol, 92% yield, er: 95.5:4.5; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.51(dd, *J* = 7.7, 0.9 Hz, 1H), 7.31 (m, 1H), 7.27-7.21 (m, 4H), 7.20 (m, 1H), 7.05 (m, 1H), 3.71 (d, *J* = 13.5 Hz, 1H), 3.67 (m, 1H), 2.98 (m, 1H), 2.89 (d, *J* = 13.7 Hz, 1H), 2.01 (dt, *J* = 11.8 Hz, 1H), 1.86 (m, 1H), 1.78 (m, 1H), 1.64-1.53 (m, 2H), 1.48-1.36 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.3, 139.6, 132.8, 129.1, 128.8, 128.28, 128.22, 128.0,

125.8, 123.8, 66.7, 59.8, 53.5, 35.3, 25.1, 25.2; Enantiomeric ratio was determined by HPLC: Kromasil 3-AmyCoat, 4.6 mm x 250 mm, temperature: 10 ºC, A: Heptane, B: ethanol denatured (contains 5% of IPA and 5% of methanol); Isocratic: A/B: 99/1, v/v, flow rate 3.0 mL/min. HRMS (ESI) $[M+H]^+$ m/z calcd for $[C_{18}H_{21}NBr]^+$ is 330.0852, found 330.0847.



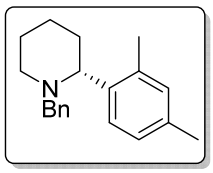
1-benzyl-2-(2,5-difluorophenyl)piperidine (2m)

White solid, 247 mg, 0.86 mmol, 86% yield, er: 94.7:5.3; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.41 (m, 1H), 7.30-7.23 (m, 4H), 7.23-7.18 (m, 1H), 6.96 (td, *J* = 9.0, 4.2 Hz, 1H), 6.85 (m, 1H), 3.74 (d, *J* = 13.8 Hz, 1H), 3.55 (d, *J* = 10.8 Hz, 1H), 2.97 (d, *J* = 11.5 Hz, 1H), 2.88 (d, *J* = 13.5 Hz, 1H), 1.96 (td, *J* = 11.5, 3.0 Hz, 1H), 1.83-1.75 (m, 2H), 1.64-1.47 (m, 3H), 1.43-1.31 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.5 (d, *J* = 2.0 Hz), 158.0 (d, *J* = 2.0 Hz), 157.6 (d, *J* = 2.5 Hz), 155.2 (d, *J* = 2.3 Hz), 139.2, 134.2 (dd, *J* = 15.3, 7.0 Hz), 128.6, 128.1, 126.7, 116.5 (dd, *J* = 26.0, 8.4 Hz), 114.8 (dd, *J* = 24.6, 4.9 Hz), 114.3 (dd, *J* = 24.4, 8.9 Hz), 59.9, 59.8, 53.3, 35.5, 22.8, 24.9; Enantiomeric ratio was determined by SFC: Chiralcel OJ-3, 4.6 mm x 150 mm, temperature: 30 ºC, A: CO_2, B: denatured ethanol (contains 5% methanol and 5% 2-propanol) with 0.2% of diethylamine (DEA). Isocratic: A/B: 97/3, v/v, flow rate 3.0 mL/min. HRMS (ESI) $[M]^+$ m/z calcd for $[C_{18}H_{20}NF_2]^+$ is 288.1558, found 288.1551.



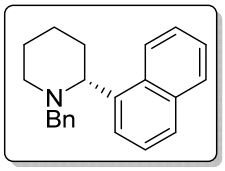
1-benzyl-2-(2-(trifluoromethyl)phenyl)piperidine (2n)

White solid, 281 mg, 0.88 mmol, 88% yield, er: 93.5:6.5; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.08 (d, *J* = 7.9 Hz, 1H), 7.59 (d, *J* = 7.9 Hz, 1H), 7.55 (t, *J* = 7.3 Hz, 1H), 7.30 (d, *J* = 7.9 Hz, 1H), 7.25 (m, 4H), 7.18 (m, 1H), 3.59 (m, 2H), 2.97 (m, 1H), 2.79 (d, *J* = 13.8 Hz, 1H), 1.96 (td, *J* = 11.7, 3.7 Hz, 1H), 1.82 (m, 2H), 1.65-1.47 (m, 3H), 1.46-1.36 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.0, 139.9, 132.2, 128.9, 128.6 (q, *J* = 29.6 Hz), 128.4, 128.0, 126.5, 125.3 (q, *J* = 6.0 Hz), 123.2 (q, *J* = 274.0 Hz), 64.1, 60.1, 53.4, 36.9, 26.1, 25.3; Enantiomeric ratio was determined by SFC: Chiralcel OD-3, 4.6 mm x 150 mm, temperature: 30 ºC, A: CO_2, B: denatured ethanol (contains 5% methanol and 5% 2-propanol). Isocratic: A/B: 99/1, v/v, flow rate 3.0 mL/min. HRMS (ESI) $[M+H]^+$ m/z calcd for $[C_{19}H_{21}NF_3]^+$ is 320.1621, found 320.1613.



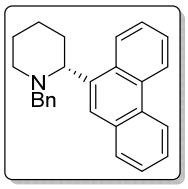
1-benzyl-2-(2,4-dimethylphenyl)piperidine (2o)

Light yellow viscous liquid, 245 mg, 0.88 mmol, 88% yield, er: 97.7:2.3; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.4 Hz, 1H), 7.28-7.22 (m, 4H), 7.20-7.16 (m, 1H), 7.03 (d, *J* = 7.6 Hz, 1H), 6.94 (s, 1H), 3.77 (d, *J* = 13.4 Hz, 1H), 3.32 (d, *J* = 11.2 Hz, 1H), 2.99 (d, *J* = 11.2 Hz, 1H), 2.78 (d, *J* = 13.4 Hz, 1H), 2.34 (s, 3H), 2.28 (s, 3H), 1.94 (td, *J* = 11.1,4.1 Hz, 1H), 1.75 (m, 2H), 1.62-1.52 (m, 3H), 1.41-1.31 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.5, 140.0, 135.7, 135.1, 131.2, 128.9, 128.1, 127.4, 127.2, 126.6, 64.1, 59.6, 53.9, 35.5, 26.3, 25.6, 21.1, 19.7; Enantiomeric ratio was determined by SFC: Chiralpack IC-3, 4.6 mm x 150 mm, temperature: 30 ºC, A: CO_2, B: ethanol (contains 5% methanol and 5% 2-propanol) with 0.2% of diethylamine); Isocratic: A/B:97/3, v/v, flow rate 3.0 mL/min. HRMS (ESI) $[M+H]^+$ m/z calcd for $[C_{20}H_{26}N]^+$ is 280.2060, found 280.2055.



1-benzyl-2-(naphthalen-1-yl)piperidine (2p)

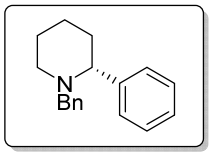
White solid, 247 mg, 0.82 mmol, 82% yield, ee: 94.2:5.8; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84 (d, *J* = 8.3 Hz, 1H), 7.72 (d, *J* = 8.4 Hz, 1H), 7.52 (t, *J* = 7.2 Hz, 1H), 7.46 (t, *J* = 7.2 Hz, 2H), 7.23 (m, 5H), 7.17 (m, 1H), 3.80 (d, *J* = 13.8 Hz, 1H), 3.08 (d, *J* = 13.8 Hz, 1H), 2.84 (d, *J* = 13.8 Hz, 1H), 2.08-1.80 (m, 4H), 1.74-1.54 (m, 3H), 1.51-1.40 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.2, 139.9, 134.4, 131.5, 128.9, 128.2,127.8, 126.7, 125.9, 125.6, 60.1, 54.0, 36.7, 36.2, 26.2, 25.4; Enantiomeric ratio was determined by SFC: Chiralcel OD-3, 4.6 mm x 150 mm, temperature: 30 ºC, A: CO_2, B: Methanol with 0.2% of diethylamine (DEA). Isocratic: A/B: 90/10, v/v, flow rate 3.0 mL/min. HRMS (ESI) $[M]^+$ m/z calcd for $[C_{22}H_{24}N]^+$ is 302.1903, found 302.1901.



1-benzyl-2-(phenanthren-9-yl)piperidine (2q)

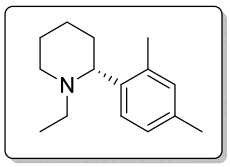
White solid, 312 mg, 0.89 mmol, 89% yield, er: 95.6:4.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (br s, 1H), 8.65 (d, *J* = 8.0 Hz, 1H), 8.25 (br s, 1H), 7.87 (br s, 1H), 7.66 (m, 2H), 7.58 (m, 2H), 7.58 (m, 2H), 7.33-7.09 (m, 4H), 4.14-3.55 (m, 2H), 3.11 (br s, 1H), 2.90 (br s, 1H), 2.21-1.97 (m, 1H), 1.85 (m, 2H), 1.74 (m, 3H), 1.49 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.5, 139.1, 132.1, 130.9, 130.5, 128.9, 128.5, 128.0, 126.6, 126.5, 126.3, 123.3, 122.4, 62.5,

60.5, 53.8, 36.1, 26.0, 25.5; Enantiomeric ratio was determined by SFC: Chiralcel OD-3, 4.6 mm x 150 mm, temperature: 30 ºC, A: CO_2, B: denatured ethanol (contains 5% methanol and 5% 2-propanol) with 0.2% of diethylamine (DEA). Isocratic: A/B: 75/25, v/v, flow rate 3.0 mL/min. HRMS (ESI) $[M+H]^+$ m/z calcd for $[C_{26}H_{26}N]^+$ is 352.2060, found 352.2056.



2-(2-phenyl)-1-benzylpiperidine (2r)

White solid, 228 mg, 0.91 mmol, 91% yield, er: 92.7:7.3; the compound data were in good accordance with the literature.[1] ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45 (d, *J* = 7.6 Hz, 2H), 7.32 (t, *J* = 7.7 Hz, 2H), 7.17-7.25 (m, 6H), 3.77 (d, *J* = 13.8 Hz, 1H), 3.11 (d, *J* = 11.3 Hz, 1H), 2.95-2.97 (m, 1H), 2.80 (d, *J* = 13.2 Hz, 1H), 1.90-1.95 (dt, *J* = 11.6, 3.4 Hz, 1H), 1.76-1.80 (m, 2H), 1.53-1.65 (m, 3H), 1.32-1.42 (m, 1H); ^{13}C NMR (500 MHz, $CDCl_3$): δ 145.7, 139.8, 128.7, 128.5, 128.0, 127.4, 126.8, 126.5, 69.2, 59.8, 53.4, 37.0, 26.0, 25.3, 25.3, 26.0; Enantiomeric ratio was determined by SFC: Lux Cel3, 4.6 mm x 150 mm, temperature: 35 ºC, A: CO_2, B: MeOH; Gradient: 1% B to 3% B in 3 min, to 50% B in 5 min, hold at 50% B for 1 min; flow rate 3.0 mL/min, BPR pressure: 150 bar; 220 nm UV detection.



2-(2,4-dimethylphenyl)-1-ethylpiperidine (2s)

Yellow liquid, 132 mg, 0.61 mmol, 61% yield, er: 99:1; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 (d, *J* = 7.9 Hz, 1H), 7.00 (d, *J* = 7.9 Hz, 1H), 6.92 (s, 1H), 3.22 (t, *J* = 10.8 Hz, 2H), 2.55 (hex, *J* = 7.2 Hz, 1H), 2.30 (s, 3H), 2.28 (s, 3H), 2.03 (dt, *J* = 12.0, 2.8 Hz, 1H), 1.94 (hex, *J* = 7.2 Hz, 1H), 1.79-1.63 (m, 4H), 1.52-1.45 (m, 1H), 1.37-1.31 (m, 1H), 0.90 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 140.4, 135.6, 135.0, 131.1, 127.2, 63.9, 53.1, 48.9, 35.5, 26.4, 25.6, 21.1, 19.6, 11.6; Enantiomeric ratio was determined by SFC: Chiralcel OZ-3, 4.6 mm x 150 mm, temperature: 40 ºC, A: CO_2, B: MeOH with 0.2% of diethylamine (DEA). Isocratic: A/B: 92/8, v/v, flow rate 3.0 mL/min; HRMS (ESI) $[M+H]^+$ m/z calcd for $[C_{15}H_{24}N]^+$ is 218.1903, found 218.1904.

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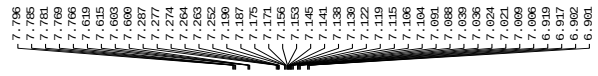
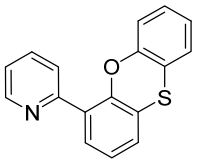
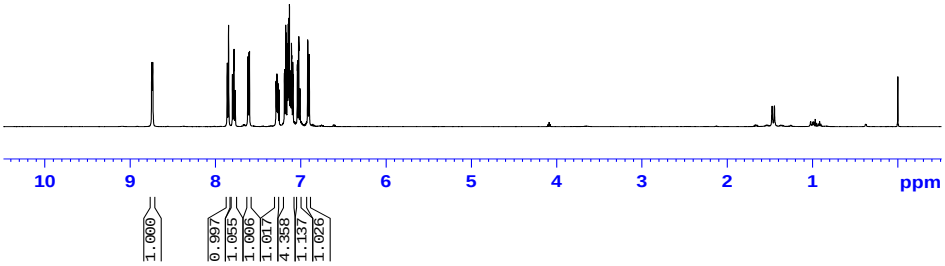
[1] M. Chang, Y. Huang, S. Liu, Y. Chen, S. W. Krska, I. W. Davies, X. Zhang, *Angew. Chem., Int. Ed*. **2014**, *53*, 12761–12764.





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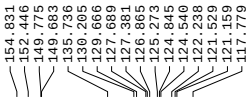

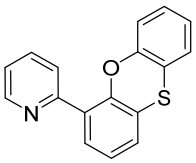

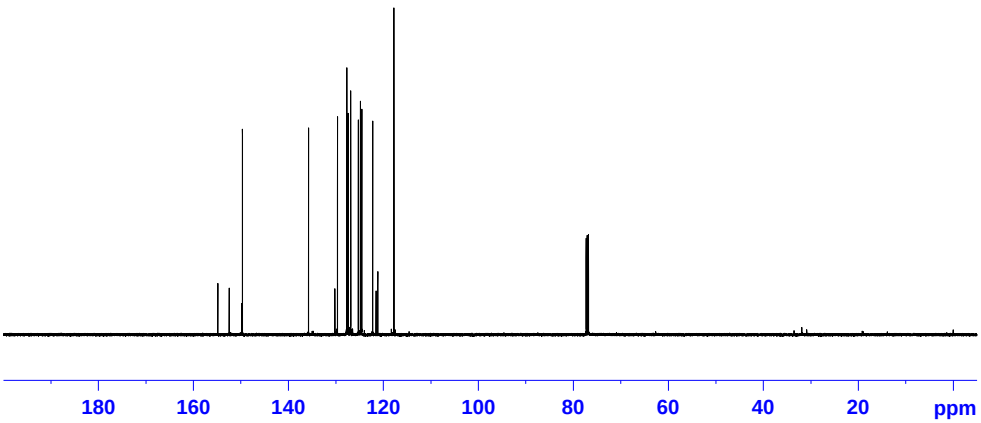


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NUC1                13C
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NUC2                1H
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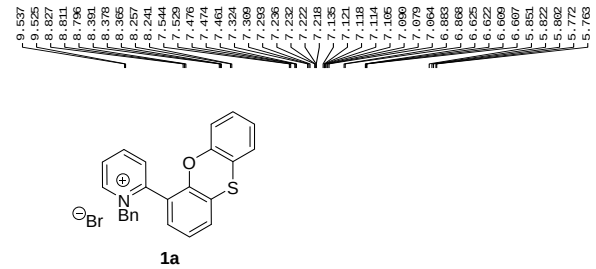

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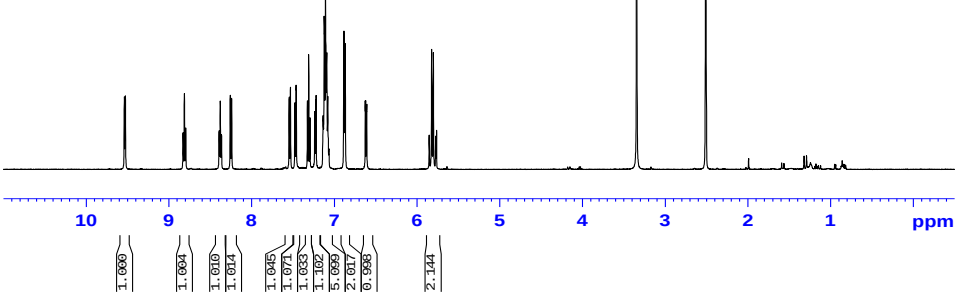

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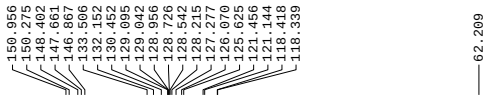

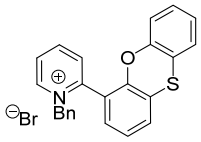

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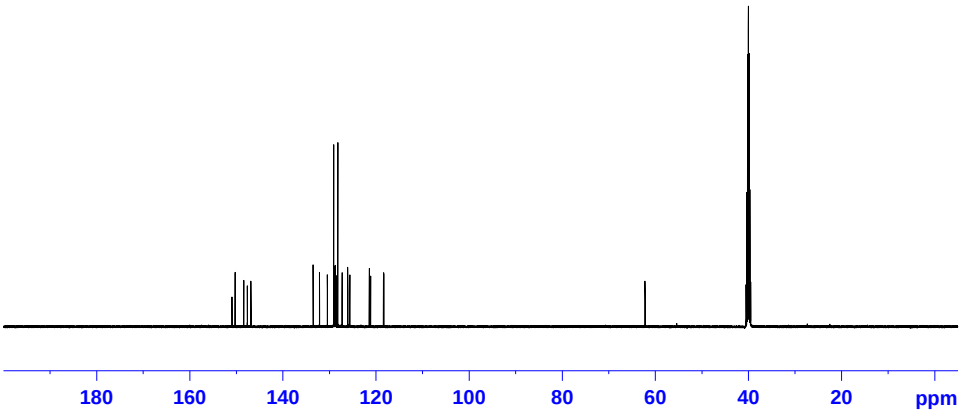

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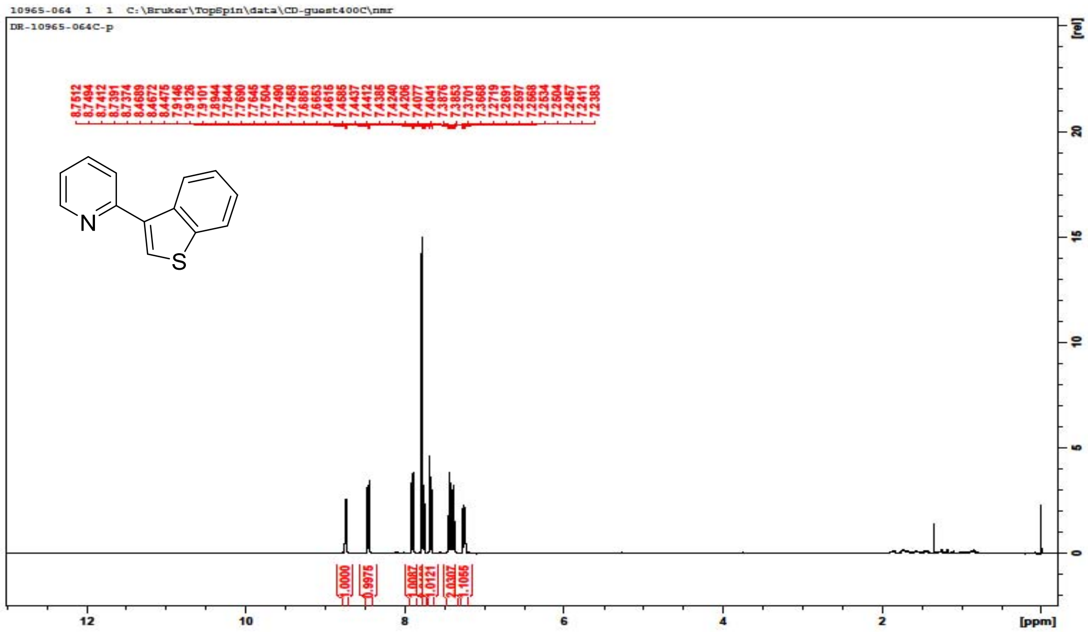
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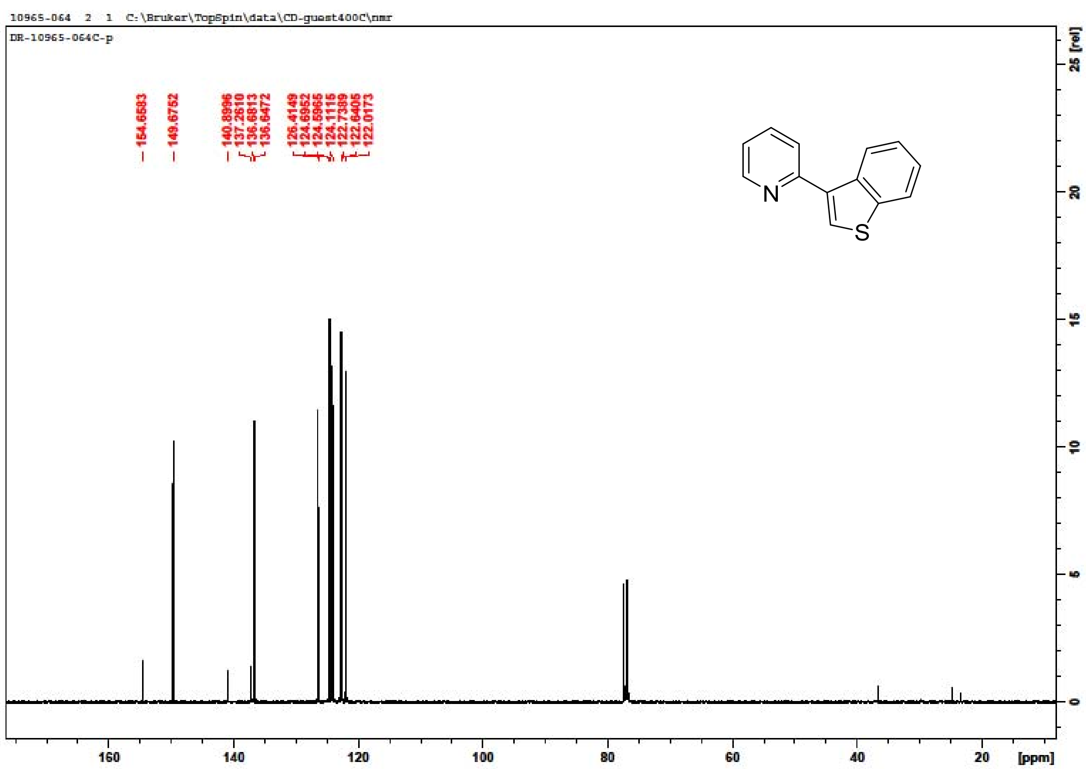
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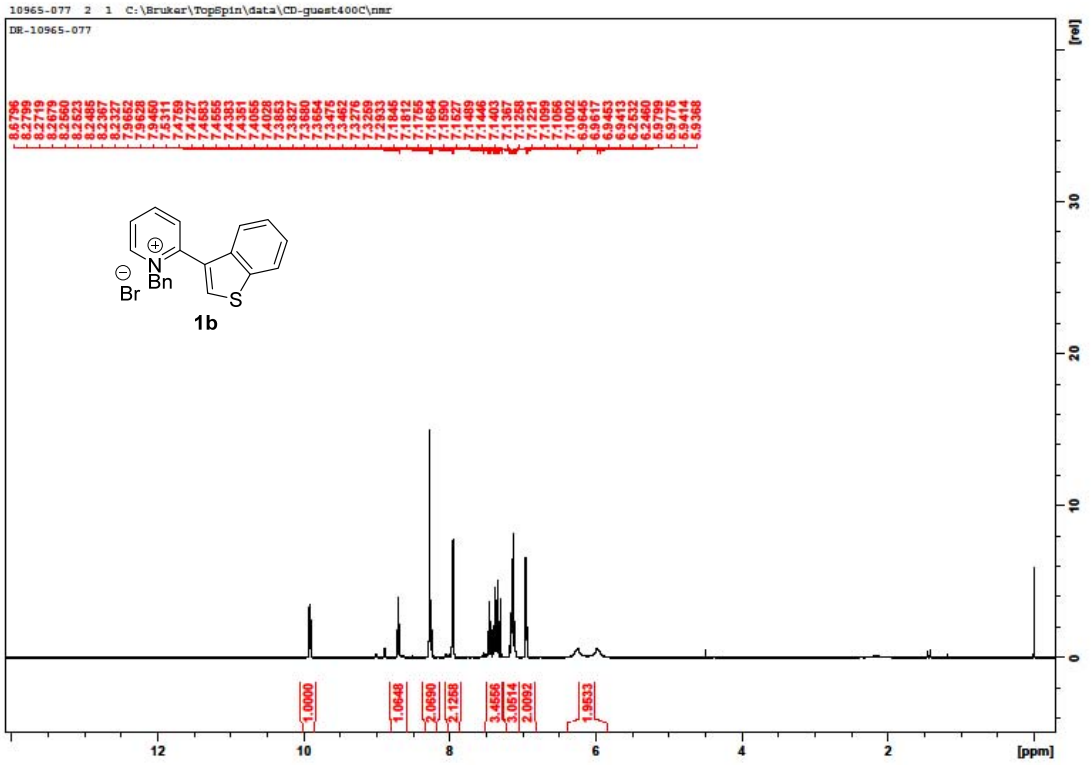
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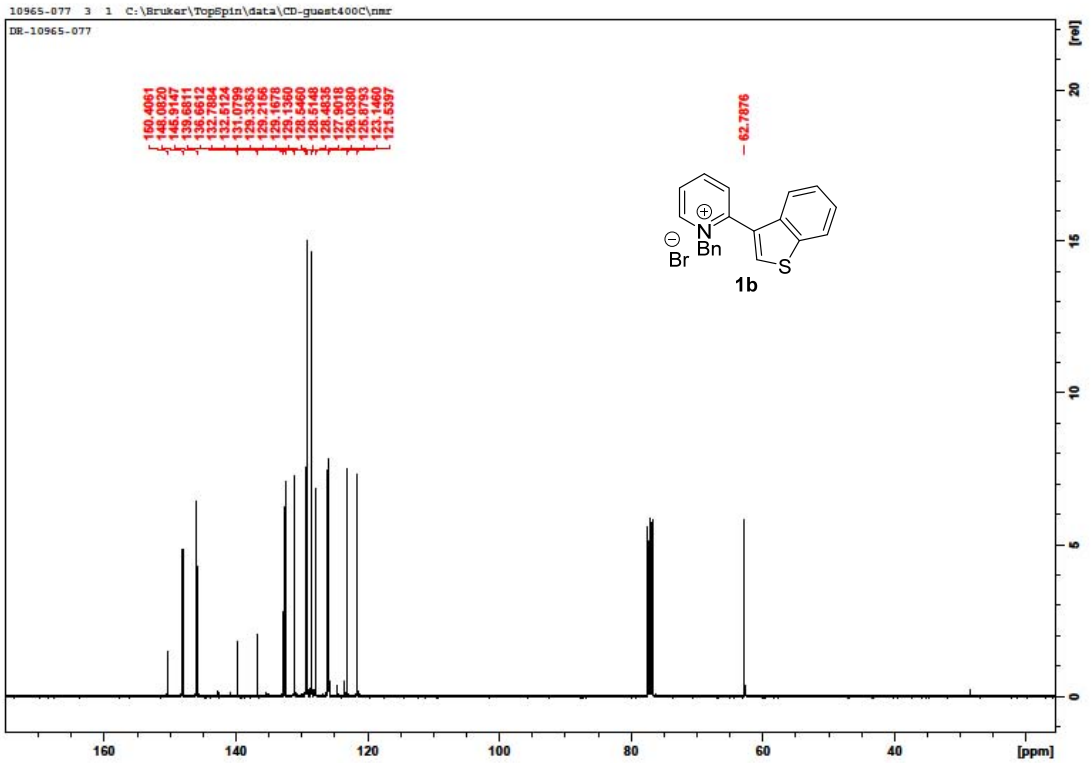
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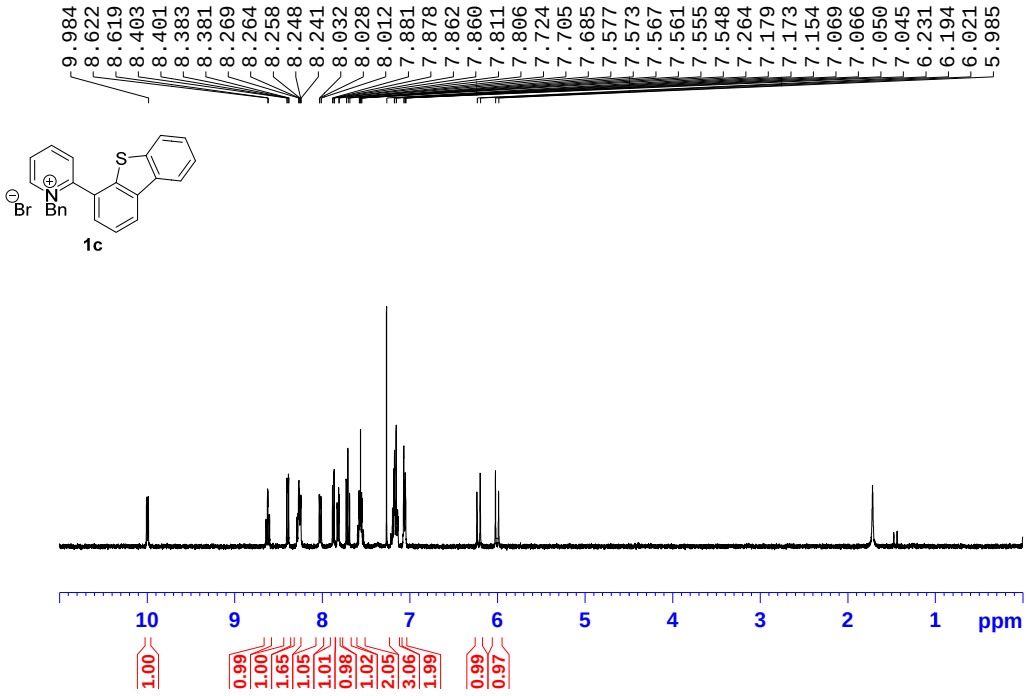


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TE                298.0 K
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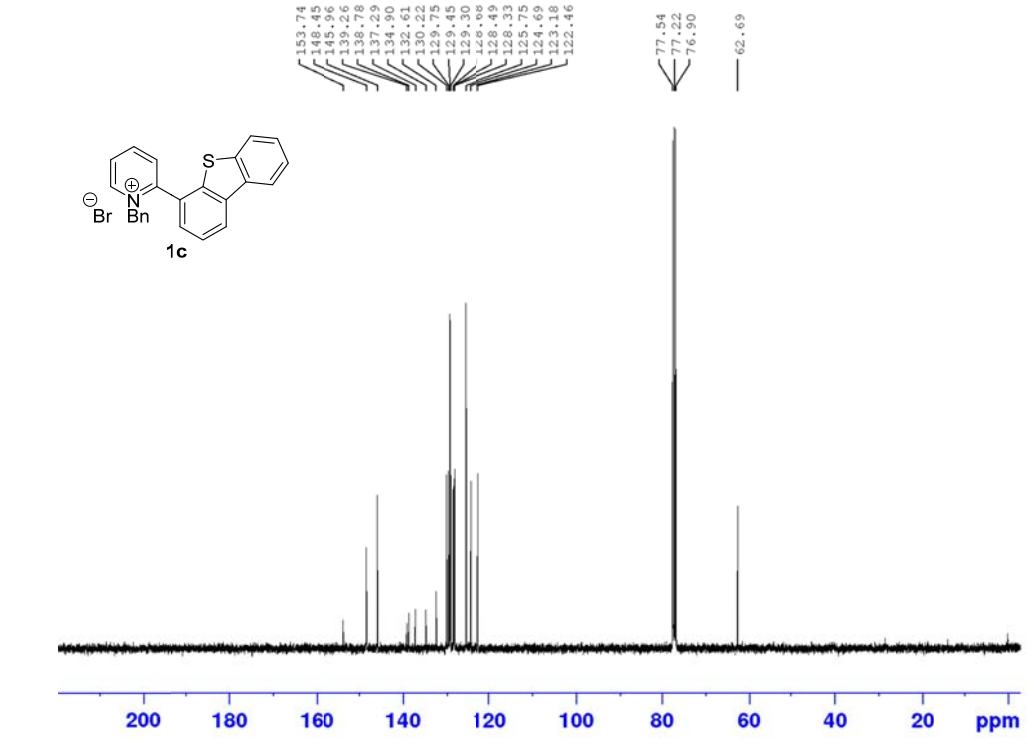


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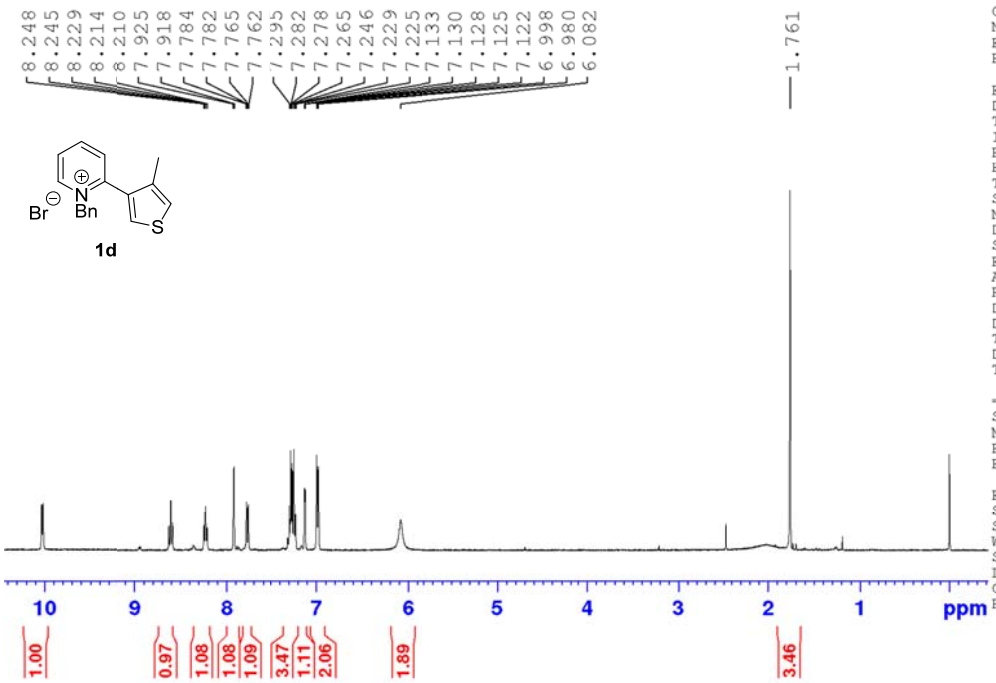


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TD0                    1

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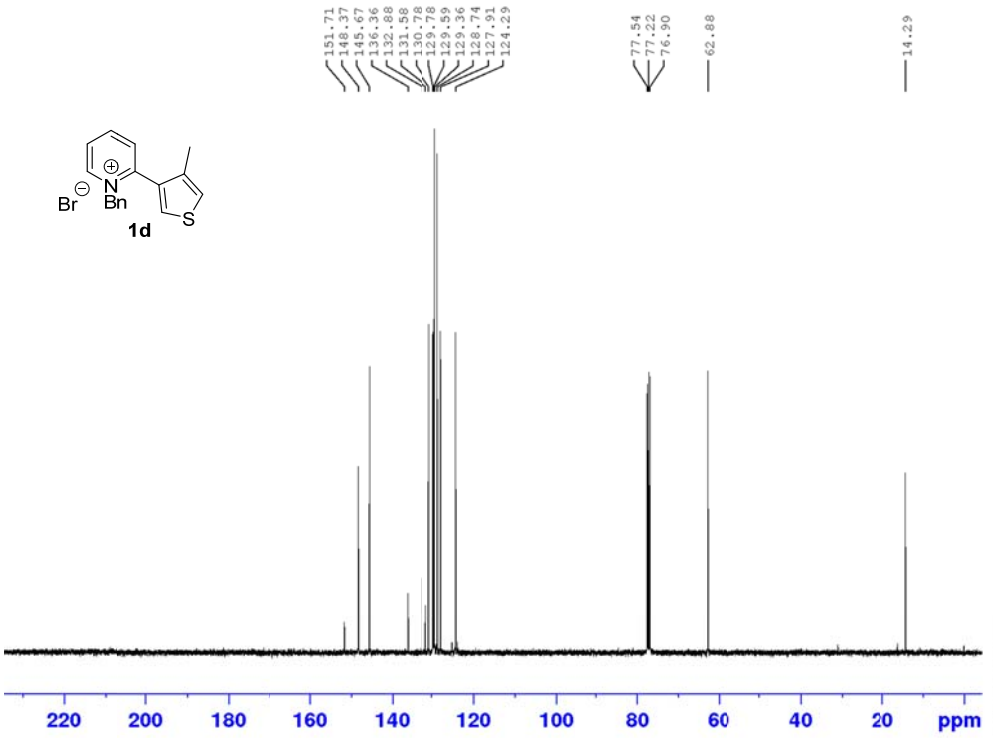
F2 - Processing parameters
SI                 65536
SF           400.1300013 MHz
WDW                   EM
SSB       0
LB                 0.05 Hz
GB        0
PC                 1.00
```



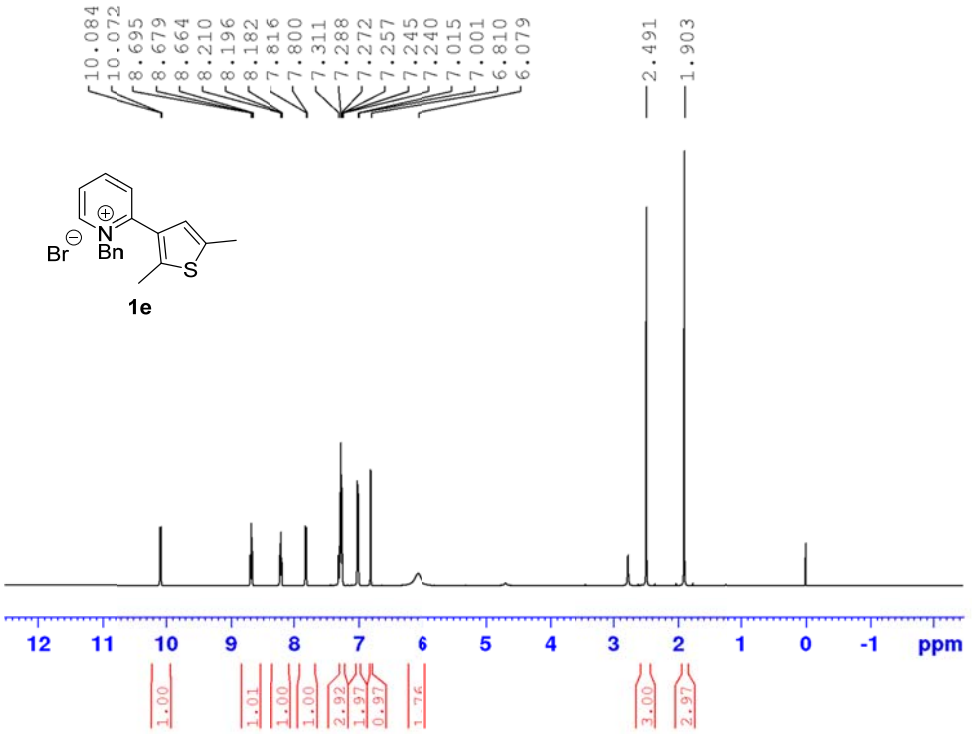

```
Current Data Parameters
NAME      sb_10945_103-2
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170525
Time               22.32
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg
TD                 32758
SOLVENT            CDCl3
NS                  4096
DS                     4
SWH            24038.451 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                  2050
DW                20.800 usec
DE                 6.50 usec
TE                298.0 K
D1             1.00000000 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           100.6127530 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

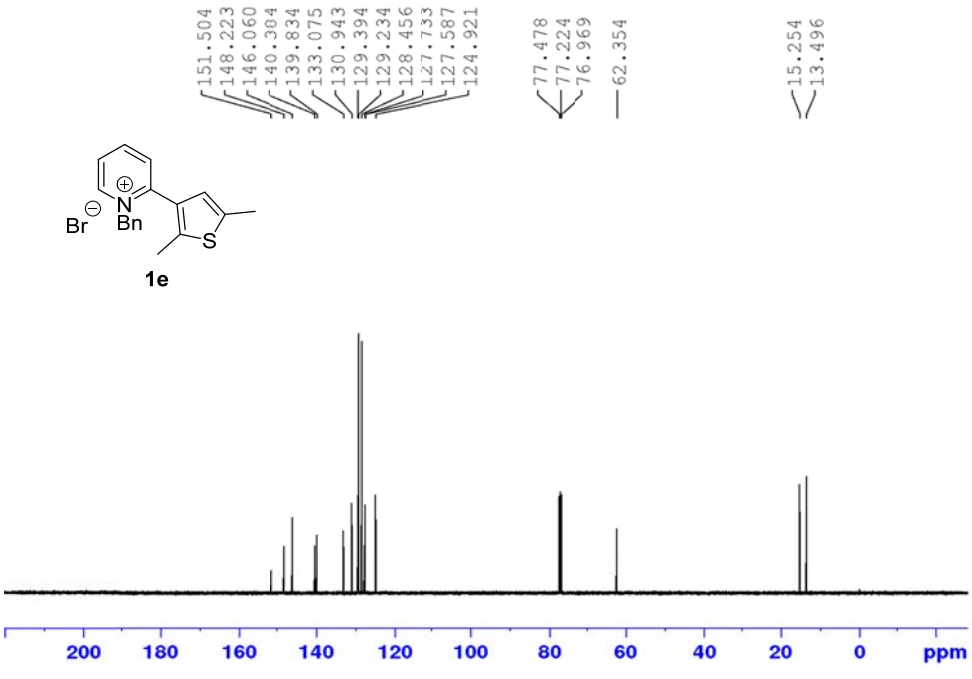



```
Current Data Parameters
NAME          10963-071
EXPNC                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170512
Time              12.02
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                  64
DS                   0
SWH           7500.000 Hz
FIDRES        0.228882 Hz
AQ            2.1845334 sec
RG                 256
DW            66.667 usec
DE             6.50 usec
TE              299.0 K
D1          1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        500.1325007 MHz
NUC1                1H
P1                11.75 usec
PLW1        18.39999962 W

F2 - Processing parameters
SI                16384
SF          500.1299867 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



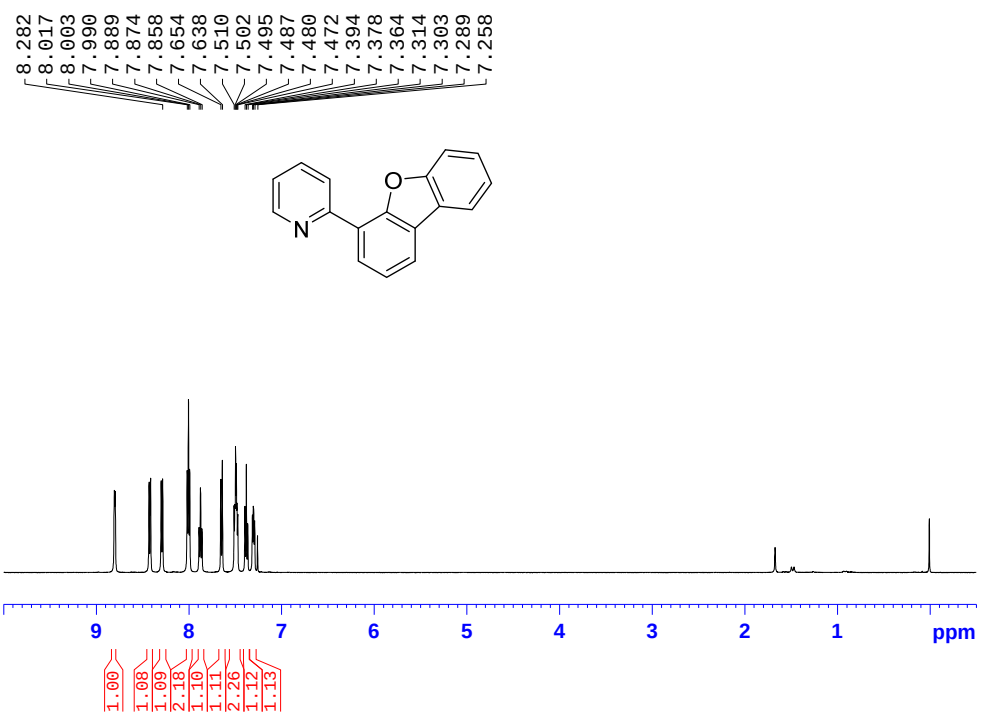

```
Current Data Parameters
NAME          10963-071
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20170512
Time              12.18
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg
TD              262144
SOLVENT          CDCl3
NS                 160
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
TD0                  1

======== CHANNEL f1 ========
SFO1        125.7698617 MHz
NUC1                13C
P1                 9.15 usec
PLW1       126.00000000 W

======== CHANNEL f2 ========
SFO2        500.1325007 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        18.39999962 W
PLW12        0.41056031 W
PLW13        0.20651031 W

F2 - Processing parameters
SI              131072
SF          125.7577760 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.40
```

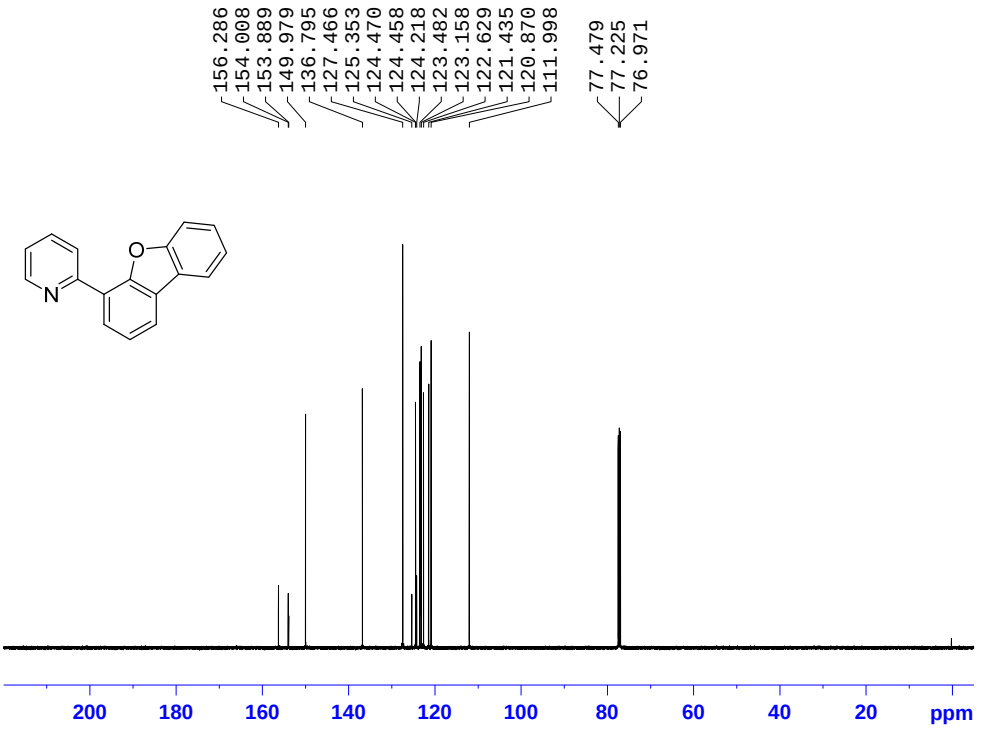



```
Current Data Parameters
NAME          10967-121
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170523
Time              17.04
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg10
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7500.000 Hz
FIDRES         0.228882 Hz
AQ           2.1845334 sec
RG                  362
DW               66.667 usec
DE                6.50 usec
TE               299.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        500.1325007 MHz
NUC1                  1H
P1                11.75 usec
PLW1        18.39999962 W

F2 - Processing parameters
SI                16384
SF          500.1300123 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



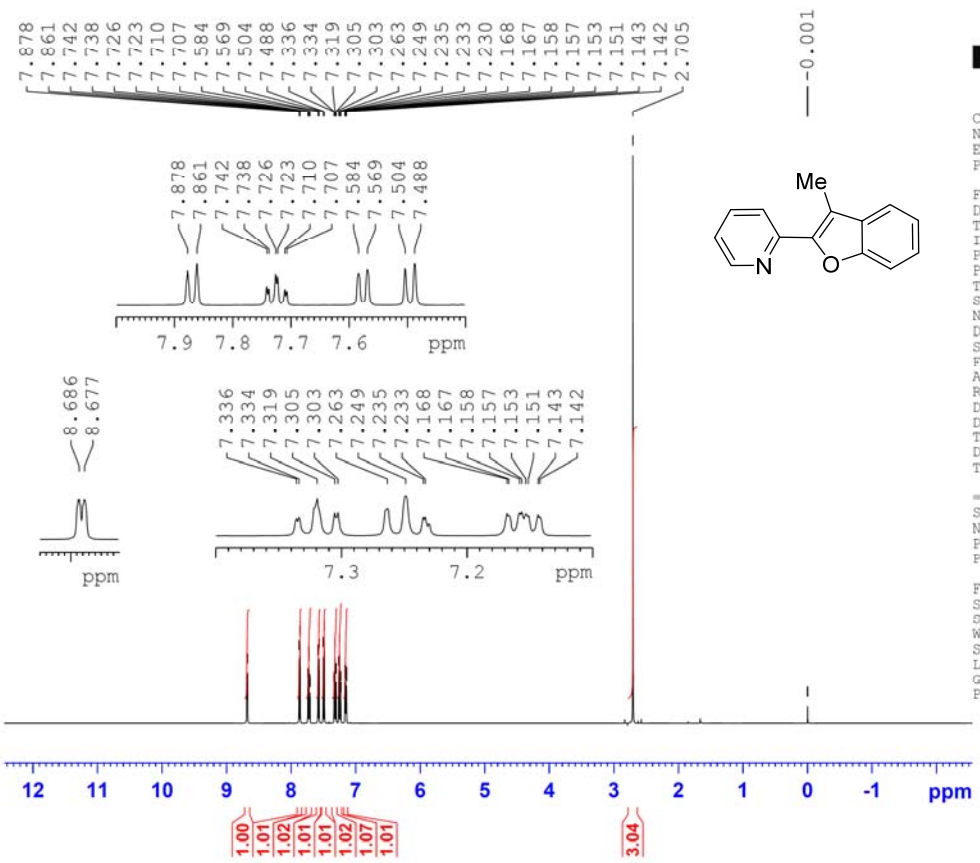

```
Current Data Parameters
NAME          10967-121
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20170523
Time              23.04
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg
TD               262144
SOLVENT           CDCl3
NS                 1200
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
TD0                   1

======== CHANNEL f1 ========
SFO1        125.7698617 MHz
NUC1                 13C
P1                9.75 usec
PLW1       126.00000000 W

======== CHANNEL f2 ========
SFO2        500.1325007 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        18.39999962 W
PLW12        0.41056001 W
PLW13        0.20651001 W

F2 - Processing parameters
SI               131072
SF          125.7577657 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.40
```

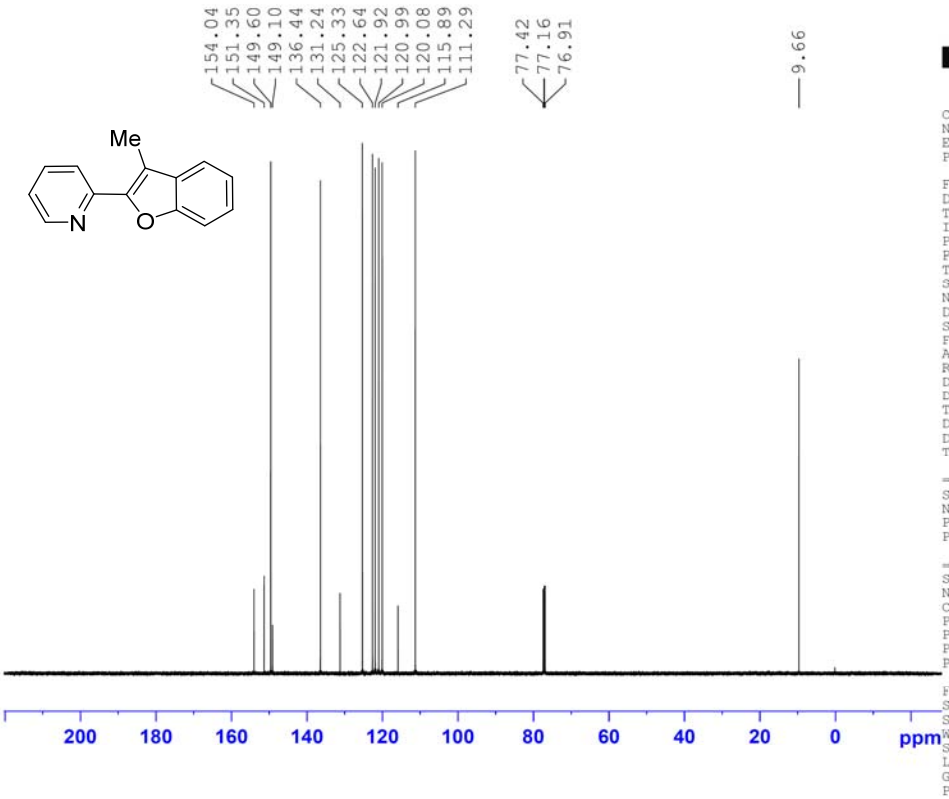



```
Current Data Parameters
NAME                  sr1-00274
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20171019
Time                      13.33
INSTRUM                   spect
PROBHD     5 mm PABBO BB-
PULPROG                   zg10
TD                       32768
SOLVENT                  CDCl3
NS                          16
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 ========
SFO1           500.1325007 MHz
NUC1                       1H
P1                      11.75 usec
PLW1          18.39999962 W

F2 - Processing parameters
SI                       16384
SF                500.1300268 MHz
WDW                         EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
```



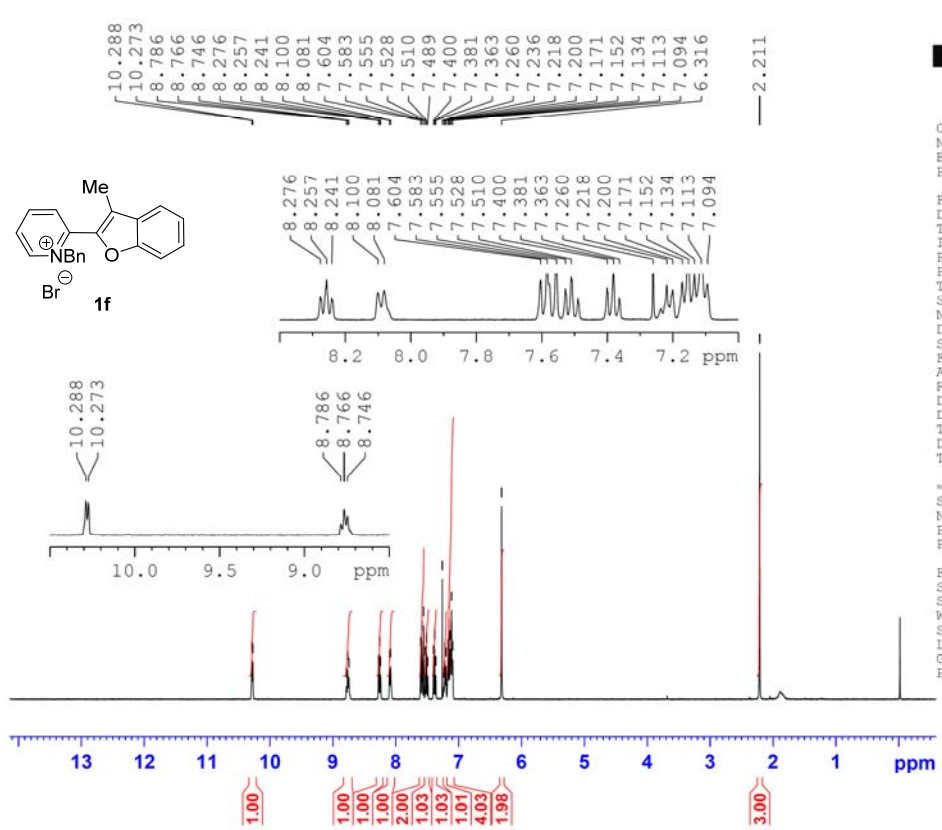

```
Current Data Parameters
NAME                  sr1-00274
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20171019
Time                      13.52
INSTRUM                   spect
PROBHD     5 mm PABBO BB-
PULPROG                   zgpg
TD                      262144
SOLVENT                  CDCl3
NS                          200
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
TD0                          1

======== CHANNEL f1 ========
SFO1           125.7698617 MHz
NUC1                       13C
P1                       9.75 usec
PLW1         126.00000000 W

======== CHANNEL f2 ========
SFO2           500.1325007 MHz
NUC2                       1H
CPDPRG[2             waltz16
PCPD2                 80.00 usec
PLW2          18.39999962 W
PLW12          0.41056001 W
PLW13          0.20651001 W

F2 - Processing parameters
SI                      131072
SF                125.7577784 MHz
WDW                         EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.40
```



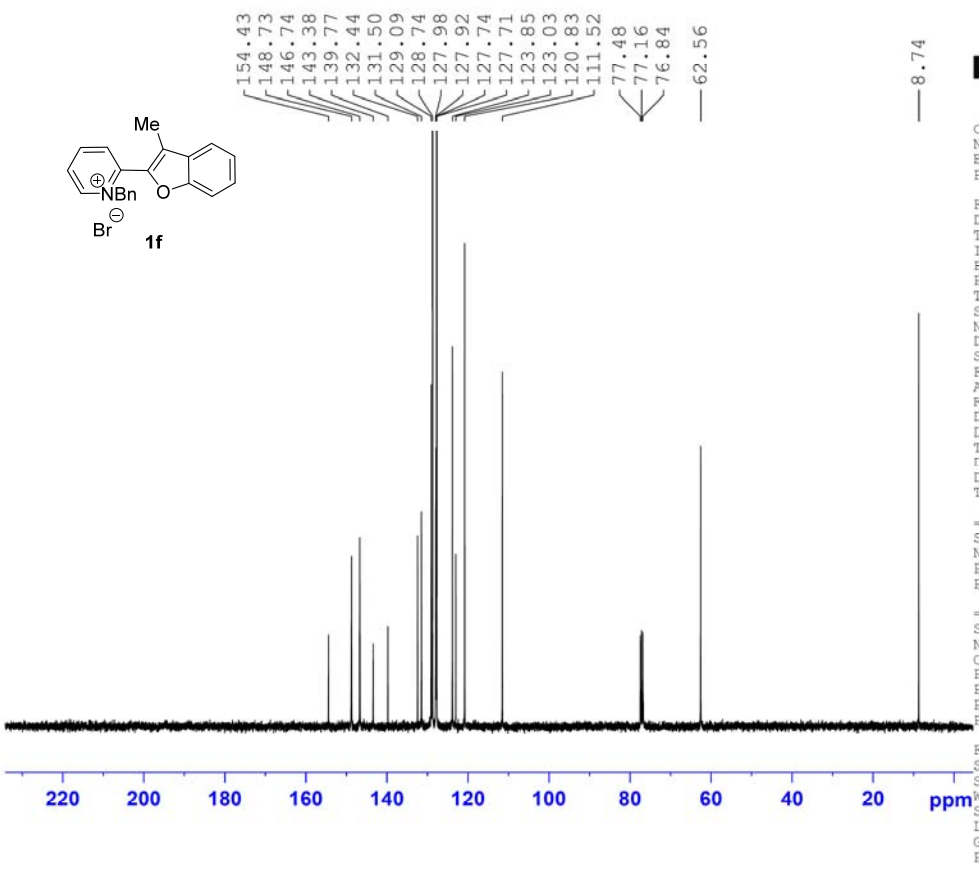
BRUKER

```
Current Data Parameters
NAME                 srl-00291
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_               20171227
Time                   15.21
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                       575
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                  400.1300101 MHz
WDW                         EM
SSB                  0
LB                       0.05 Hz
GB                   0
PC                       1.00
```



BRUKER

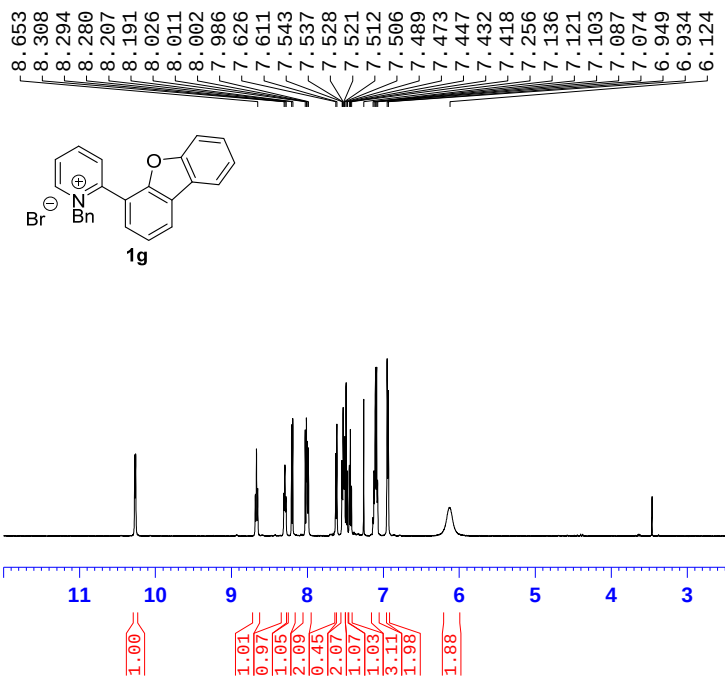
```
Current Data Parameters
NAME                 srl-00291
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_               20171201
Time                   18.17
INSTRUM                spect
PRODBD     5 mm PADDO BB-
PULPROG                 zgpg
TD                     32768
SOLVENT                CDCl3
NS                       200
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                  100.6127884 MHz
WDW                         EM
SSB                  0
LB                       1.00 Hz
GB                   0
PC                       1.40
```

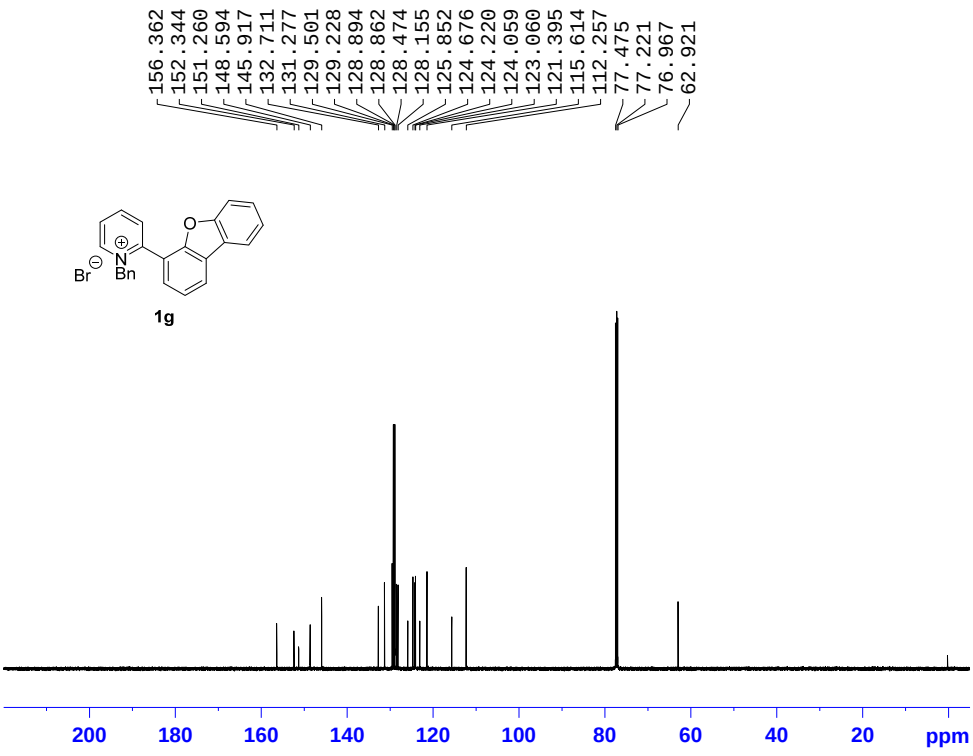



```
Current Data Parameters
NAME          10967-123
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170523
Time              17.08
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg10
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7500.000 Hz
FIDRES         0.228882 Hz
AQ            2.1845334 sec
RG                  456
DW               66.667 usec
DE                6.50 usec
TE               299.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        500.1325007 MHz
NUC1               1H
P1                11.75 usec
PLW1        18.39999962 W

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



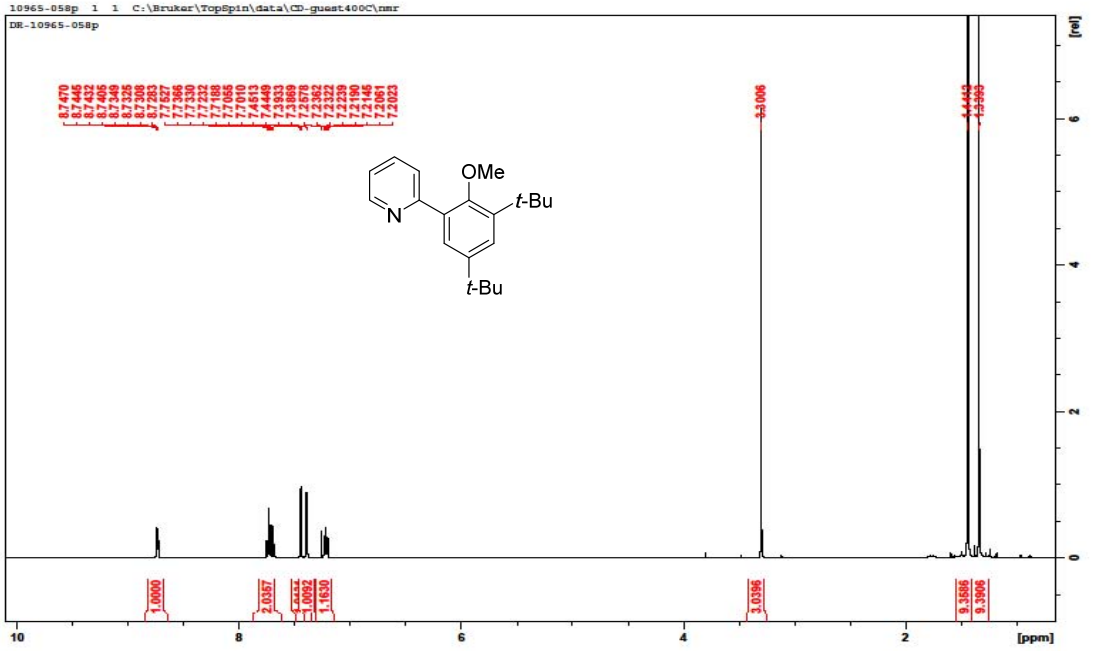

```
Current Data Parameters
NAME          10967-123
EXPNO                 2
PROCNO                1

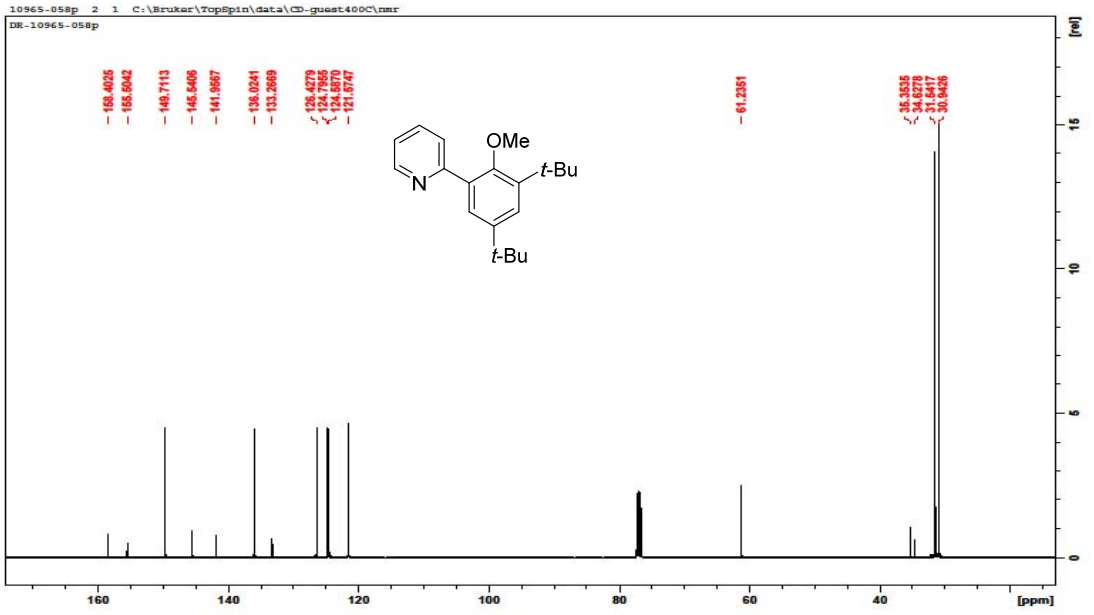
F2 - Acquisition Parameters
Date_          20170523
Time              21.15
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg
TD                262144
SOLVENT           CDCl3
NS                 1500
DS                    0
SWH           31250.000 Hz
FIDRES         0.119209 Hz
AQ            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
TD0                   1

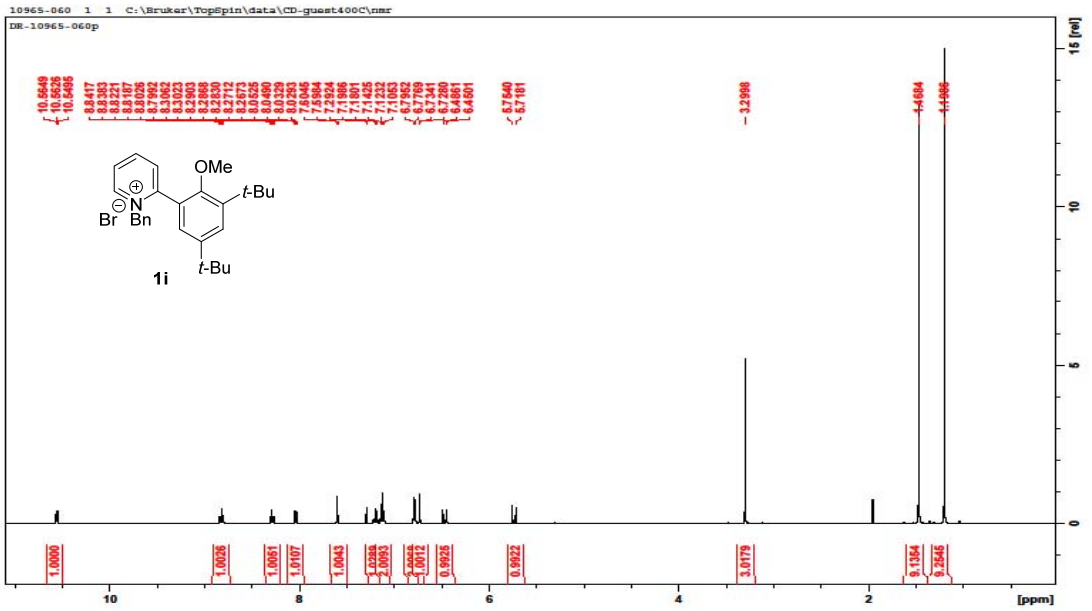
======== CHANNEL f1 ========
SFO1        125.7698617 MHz
NUC1               13C
P1                9.75 usec
PLW1       126.00000000 W

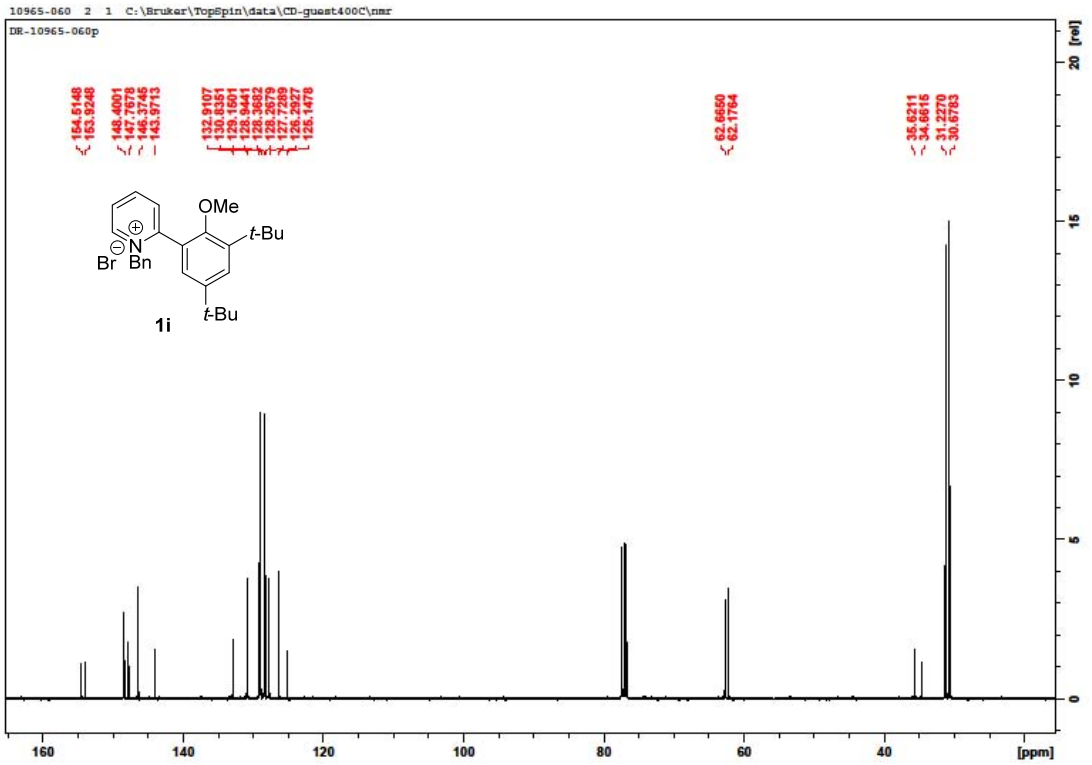
======== CHANNEL f2 ========
SFO2        500.1325007 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2            80.00 usec
PLW2        18.39999962 W
PLW12        0.41056001 W
PLW13        0.20651001 W

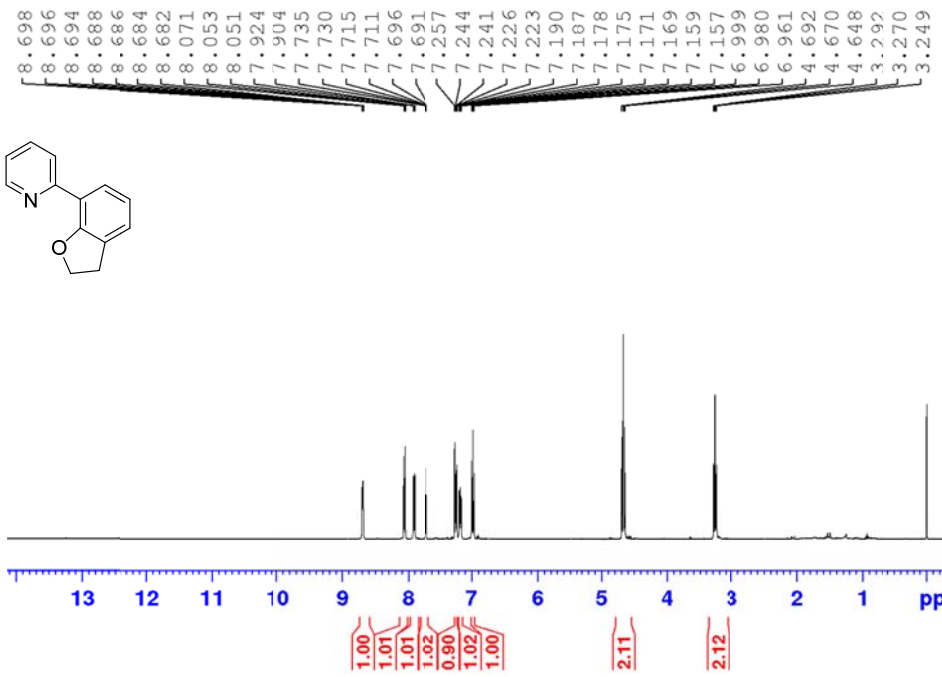
F2 - Processing parameters
SI                131072
SF          125.7577670 MHz
WDW                EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.40
```


10965-058p 1 1 C:\Bruker\TopSpin\data\CD-guest400C\nmr
DR-10965-058p
8.7470
8.7445
8.7432
8.7405
8.7348
8.7338
8.7308
8.7283
7.7527
7.7366
7.7330
7.7232
7.7188
7.7065
7.7010
7.6513
7.4449
7.3933
7.3869
7.2578
7.2362
7.2322
7.2239
7.2190
7.2145
7.2091
7.2023
3.3006
1.4443
1.3969
OMe
t-Bu
t-Bu
N
1.0000
2.0357
0.9999
1.0092
1.1630
3.0396
9.3586
9.3906
[rel]
[ppm]


10965-058p 2 1 C:\Bruker\TopSpin\data\CD-guest400C\nmr
DR-10965-058p
158.4025
155.5042
149.7113
145.5406
141.9667
136.0241
133.2669
126.4279
124.7945
124.6870
121.6747
61.2351
35.3535
34.6278
31.6417
30.9426
OMe
t-Bu
t-Bu
N
[rel]
[ppm]


10965-060 1 1 C:\Bruker\TopSpin\data\CD-guest400C\nmr
DR-10965-060p
OMe
t-Bu
Br Bn
t-Bu
1i
[ppm]


10965-060 2 1 C:\Bruker\TopSpin\data\CD-guest400C\nmr
DR-10965-060p
OMe
t-Bu
Br Bn
t-Bu
1i
[ppm]

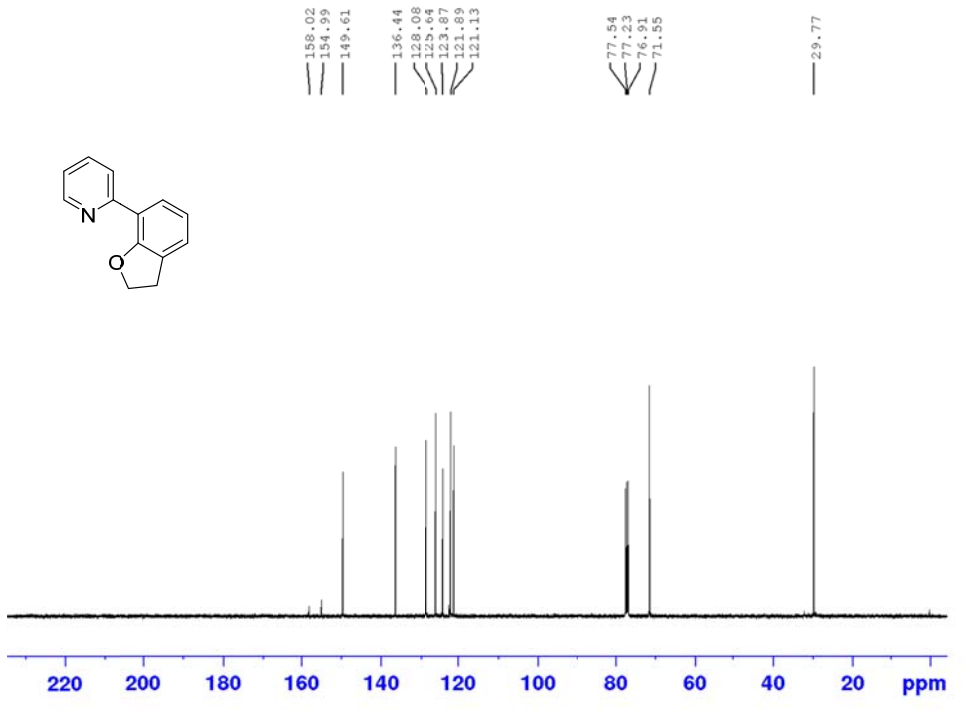



```
Current Data Parameters
NAME        sb_10945_116
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170525
Time               22.37
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                   575
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          400.1300109 MHz
WDW                   EM
SSB       0
LB                0.05 Hz
GB        0
PC                1.00
```



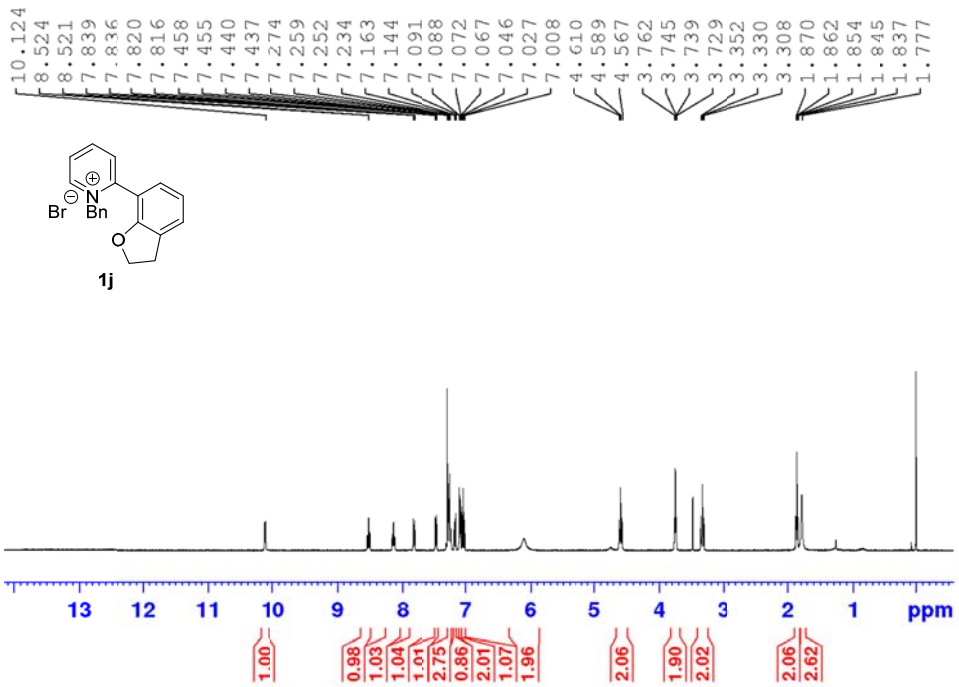

```
Current Data Parameters
NAME        sb_10945_116
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170526
Time               0.38
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg
TD                 32768
SOLVENT            CDCl3
NS                  4096
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           1.00000000 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          100.6127496 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

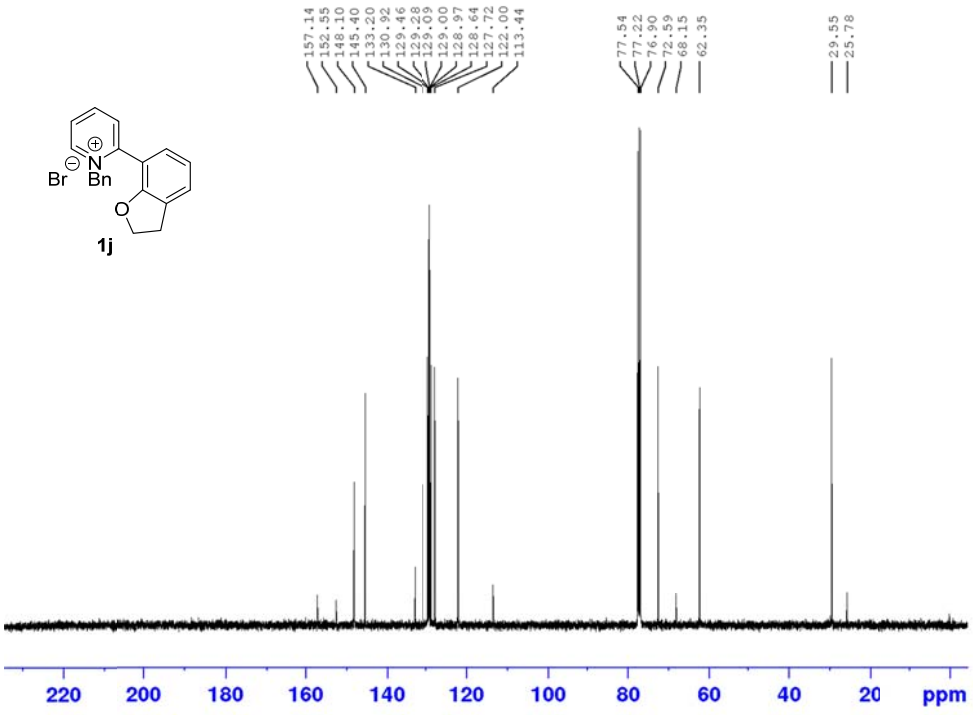



```
Current Data Parameters
NAME        sb_10945_119
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20170526
Time                0.43
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           400.1300045 MHz
WDW                  EM
SSB       0
LB                0.05 Hz
GB        0
PC                1.00
```



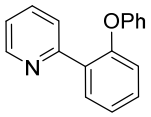

```
Current Data Parameters
NAME        sb_10945_119
EXPNO                 2
PROCNO                1

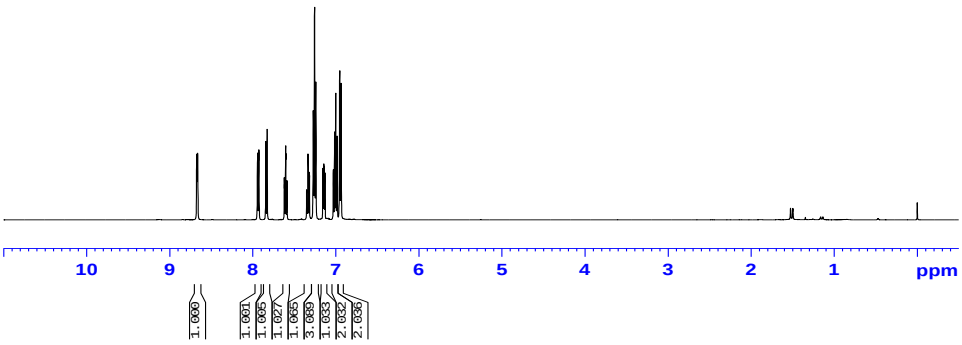
F2 - Acquisition Parameters
Date_           20170526
Time                2.44
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg
TD                 32768
SOLVENT            CDCl3
NS                  4096
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                  2050
DW                20.800 usec
DE                 6.50 usec
TE                298.0 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                   1

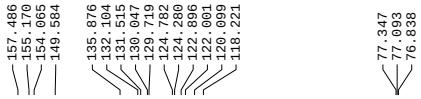
======== CHANNEL f1 ========
SFO1         100.6243395 MHz
NUC1                 13C
P1                10.90 usec
PLW1         43.00000000 W

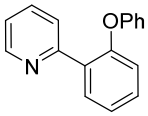
======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         10.50000000 W
PLW12         0.29166999 W
PLW13         0.14670999 W

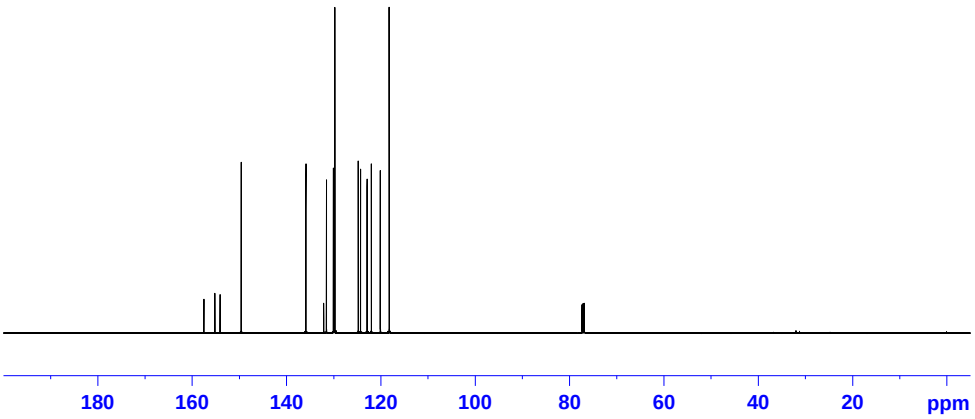
F2 - Processing parameters
SI                 65536
SF           100.6127511 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```












```
Current Data Parameters
NAME        ovz1-00025-d
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170105
Time               20.41
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            zg10
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7500.000 Hz
FIDRES        0.228882 Hz
AQ            2.1845334 sec
RG                  228
DW             66.667 usec
DE              6.50 usec
TE                299.0 K
D1          1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        500.1325007 MHz
NUC1                   1H
P1                 14.00 usec
PLW1        18.79999924 W

F2 - Processing parameters
SI                 16384
SF          500.1300223 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

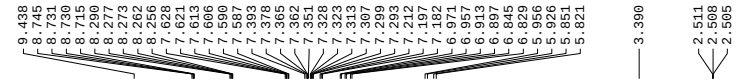
```
Current Data Parameters
NAME        ovz1-00025-d
EXPNO                  2
PROCNO                 1

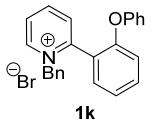
F2 - Acquisition Parameters
Date_           20170105
Time               22.12
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg
TD               262144
SOLVENT           CDCl3
NS                 1024
DS                    0
SWH           31250.000 Hz
FIDRES         0.119209 Hz
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
TD0                   1

======== CHANNEL f1 ========
SFO1        125.7698617 MHz
NUC1                  13C
P1                10.00 usec
PLW1        99.50000000 W

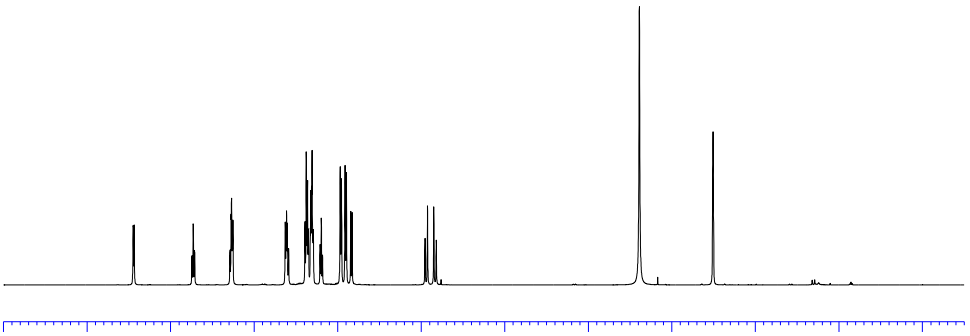
======== CHANNEL f2 ========
SFO2        500.1325007 MHz
NUC2                   1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        18.79999924 W
PLW12        0.57574999 W
PLW13        0.28960001 W

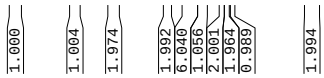
F2 - Processing parameters
SI                131072
SF          125.7577890 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.40
```

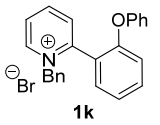




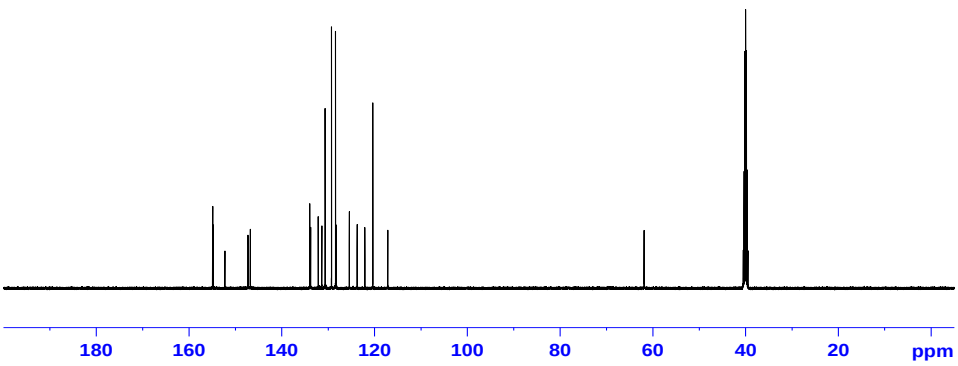
1k







1k



BRUKER

```
Current Data Parameters
NAME       ovz1-00028-d
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20170104
Time              20.37
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT            DMSO
NS                   16
DS                    0
SWH            7002.801 Hz
FIDRES        0.213709 Hz
AQ            2.3396351 sec
RG                  144
DW               71.400 usec
DE                6.50 usec
TE                299.1 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         500.1330008 MHz
NUC1                 1H
P1                14.00 usec
PLW1         18.79999924 W

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

BRUKER

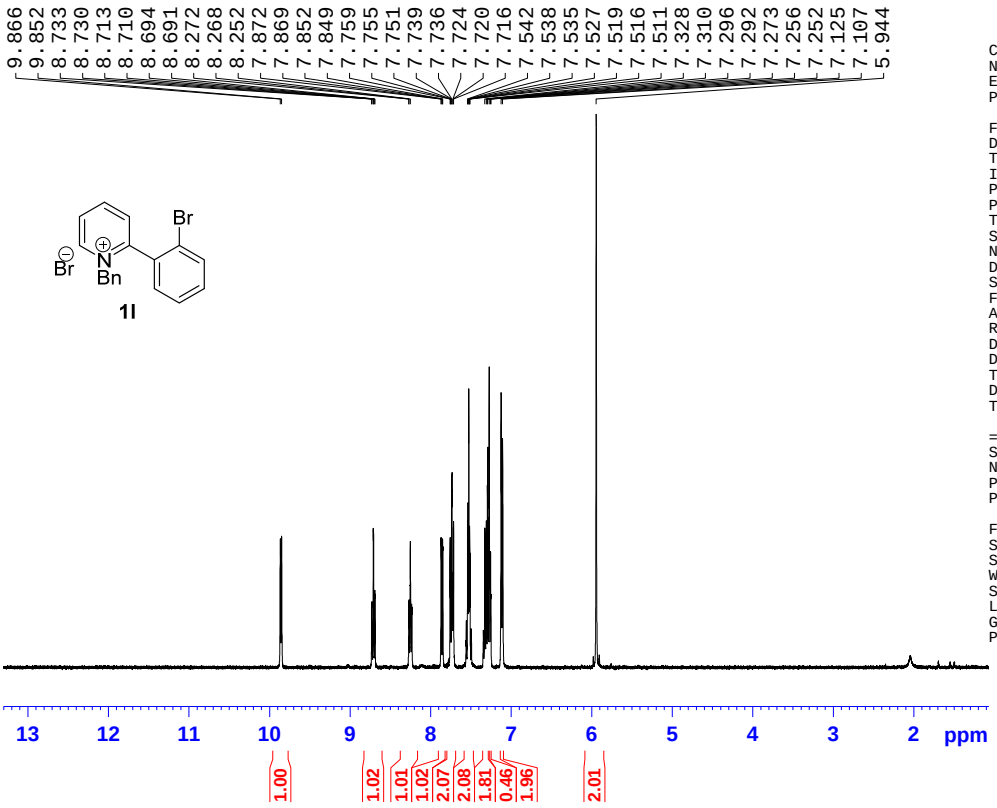
```
Current Data Parameters
NAME       ovz1-00028-d
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_           20170104
Time              22.07
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg
TD               262144
SOLVENT            DMSO
NS                 1024
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
TD0                   1

======== CHANNEL f1 ========
SFO1         125.7698617 MHz
NUC1                 13C
P1                10.00 usec
PLW1         99.50000000 W

======== CHANNEL f2 ========
SFO2         500.1325007 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         18.79999924 W
PLW12         0.57574999 W
PLW13         0.28960001 W

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

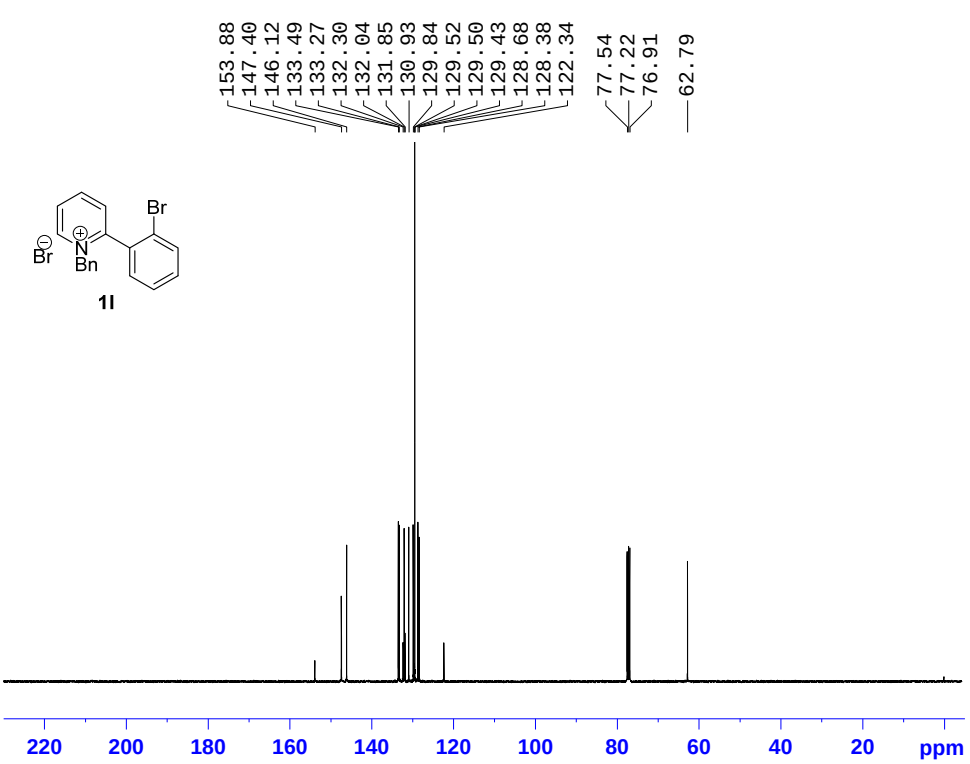



```
Current Data Parameters
NAME          10933-107
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20160902
Time               17.04
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                   406
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          400.1299958 MHz
WDW                   EM
SSB      0
LB                 0.05 Hz
GB       0
PC                 1.00
```



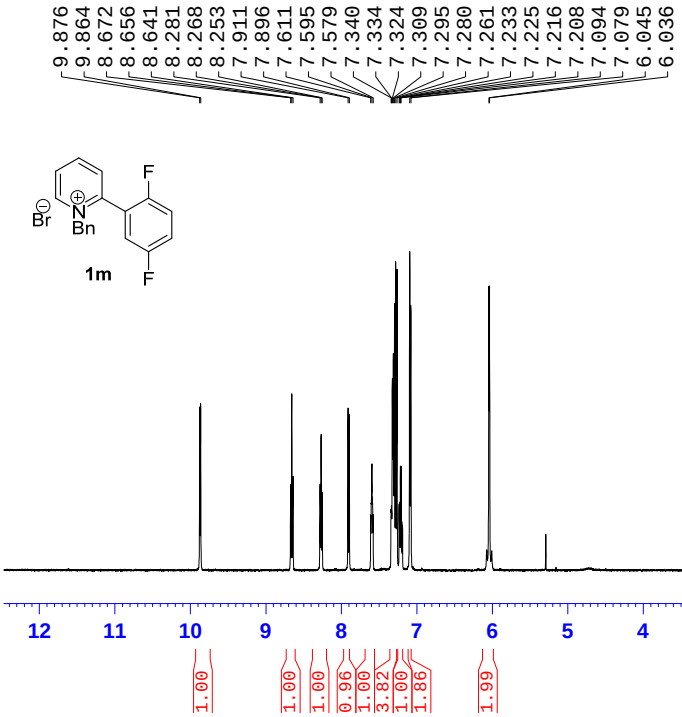

```
Current Data Parameters
NAME          10933-107
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_           20160902
Time               20.59
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg
TD                 32768
SOLVENT            CDCl3
NS                  2500
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          100.6127561 MHz
WDW                   EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.40
```

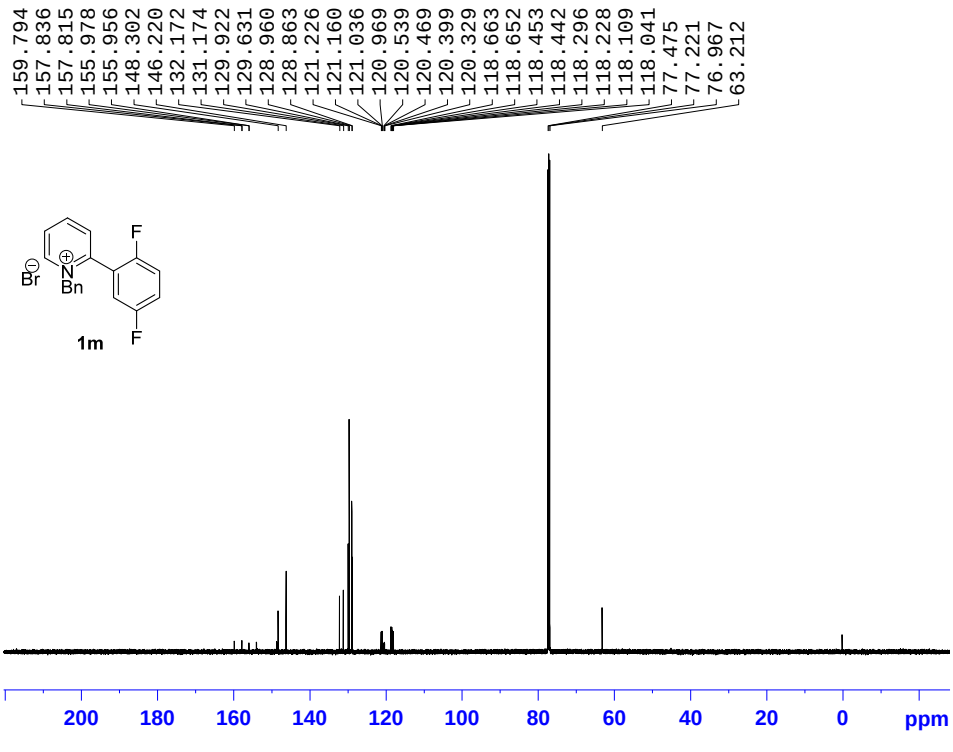



```
Current Data Parameters
NAME          10967-037
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20170106
Time               18.20
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg10
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             7500.000 Hz
FIDRES          0.228882 Hz
AQ             2.1845334 sec
RG                   812
DW                66.667 usec
DE                 6.50 usec
TE                299.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         500.1325007 MHz
NUC1                   1H
P1                 14.00 usec
PLW1         18.79999924 W

F2 - Processing parameters
SI                 16384
SF           500.1300120 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



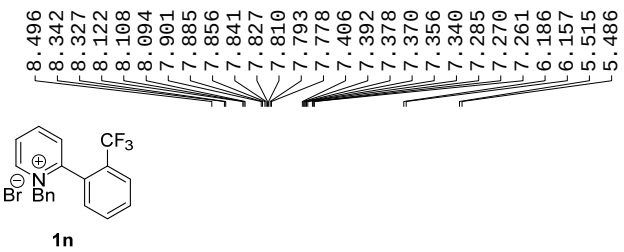

```
Current Data Parameters
NAME          10967-037
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20170107
Time               6.01
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg
TD                262144
SOLVENT            CDCl3
NS                  1500
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                299.1 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

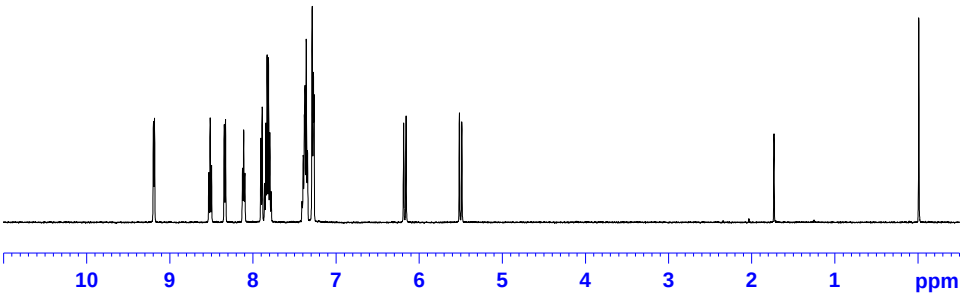
======== CHANNEL f1 ========
SFO1         125.7698617 MHz
NUC1                  13C
P1                 10.00 usec
PLW1         99.50000000 W

======== CHANNEL f2 ========
SFO2         500.1325007 MHz
NUC2                   1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         18.79999924 W
PLW12         0.57574999 W
PLW13         0.28960001 W

F2 - Processing parameters
SI                131072
SF           125.7577656 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.40
```



1n

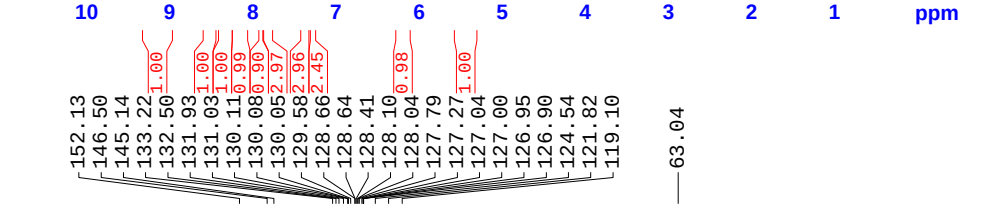



```
Current Data Parameters
NAME          10933-190
EXPNO                 1
PROCNO                1

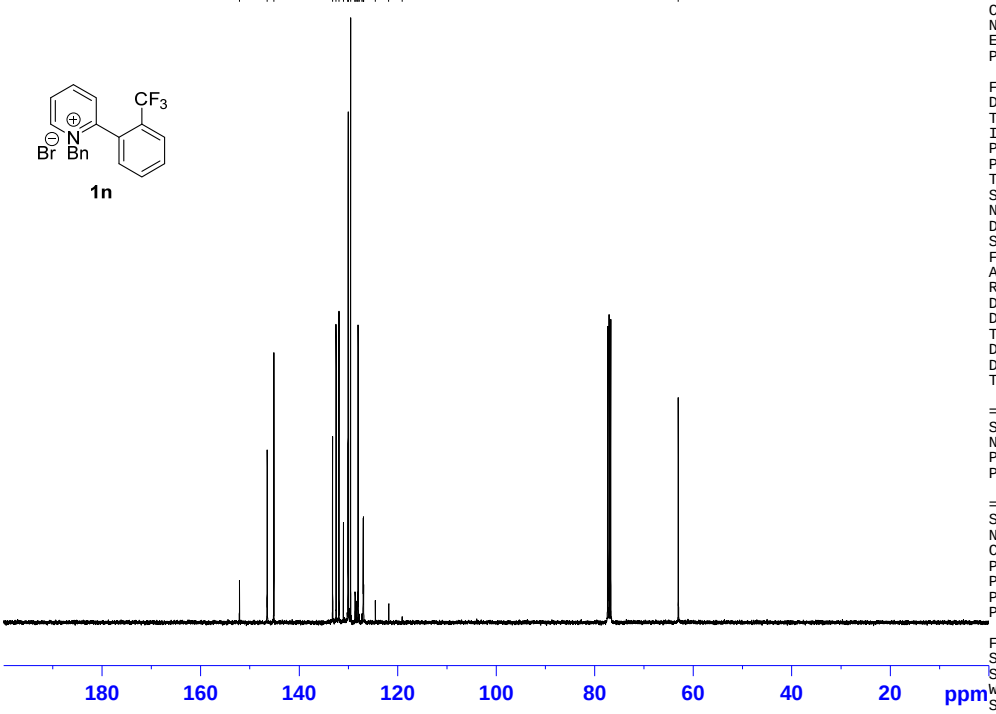
F2 - Acquisition Parameters
Date_          20161115
Time              16.47
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg10
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7500.000 Hz
FIDRES        0.228882 Hz
AQ            2.1845334 sec
RG                  812
DW               66.667 usec
DE                 6.50 usec
TE                298.9 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         500.1325007 MHz
NUC1                1H
P1                14.00 usec
PLW1         18.79999924 W

F2 - Processing parameters
SI                16384
SF           500.1300113 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



1n



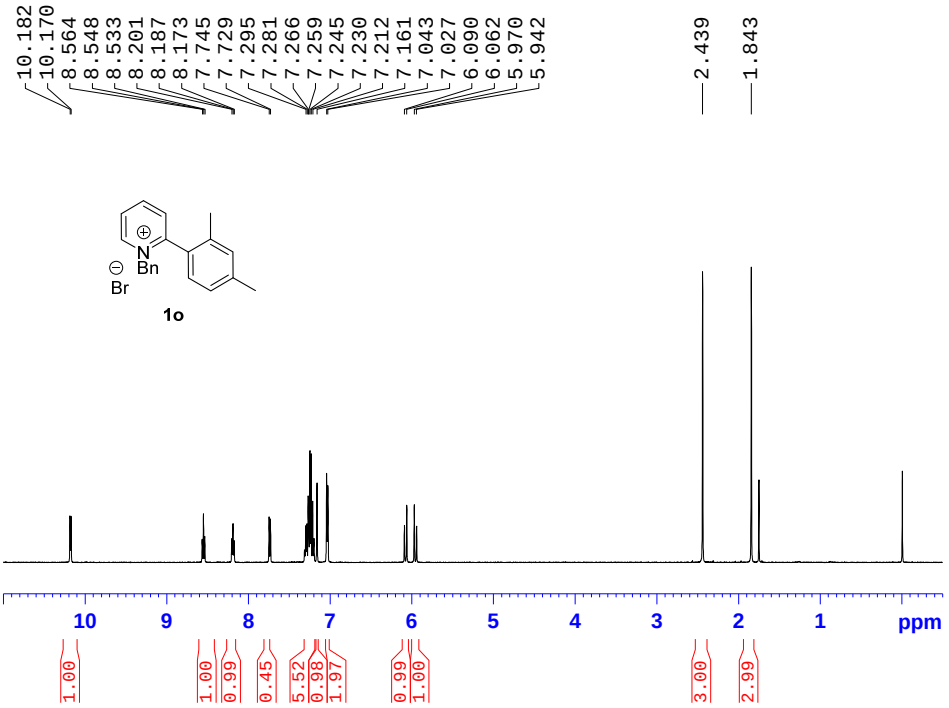

```
Current Data Parameters
NAME          10933-190-p
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20180206
Time              5.04
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg
TD                32768
SOLVENT           CDCl3
NS                 3072
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
```

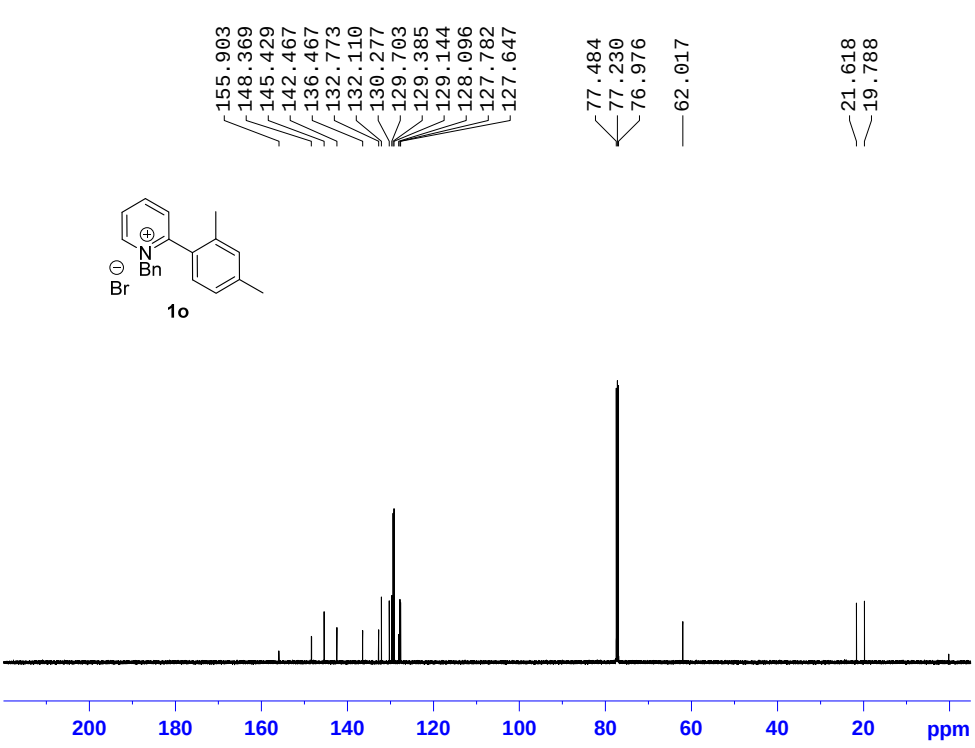



```
Current Data Parameters
NAME          10933-174
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20161109
Time              18.02
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg10
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7500.000 Hz
FIDRES         0.228882 Hz
AQ           2.1845334 sec
RG                  724
DW               66.667 usec
DE                6.50 usec
TE               299.0 K
D1          1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        500.1325007 MHz
NUC1                  1H
P1                14.00 usec
PLW1        18.79999924 W

F2 - Processing parameters
SI                16384
SF          500.1300080 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



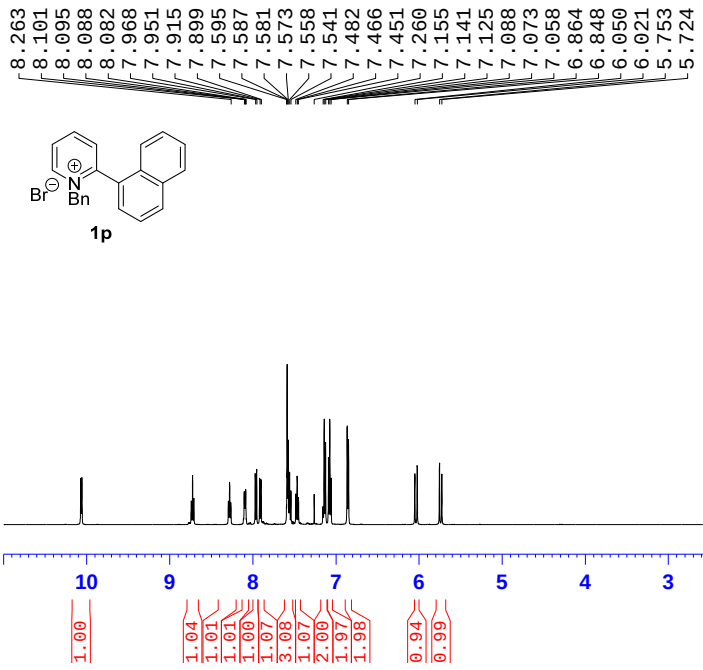

```
Current Data Parameters
NAME          10933-174
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20161109
Time              19.34
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg
TD               262144
SOLVENT           CDCl3
NS                 1024
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
TD0                   1

======== CHANNEL f1 ========
SFO1        125.7698617 MHz
NUC1                 13C
P1                10.00 usec
PLW1        99.50000000 W

======== CHANNEL f2 ========
SFO2        500.1325007 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        18.79999924 W
PLW12        0.57574999 W
PLW13        0.28960001 W

F2 - Processing parameters
SI               131072
SF          125.7577649 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.40
```

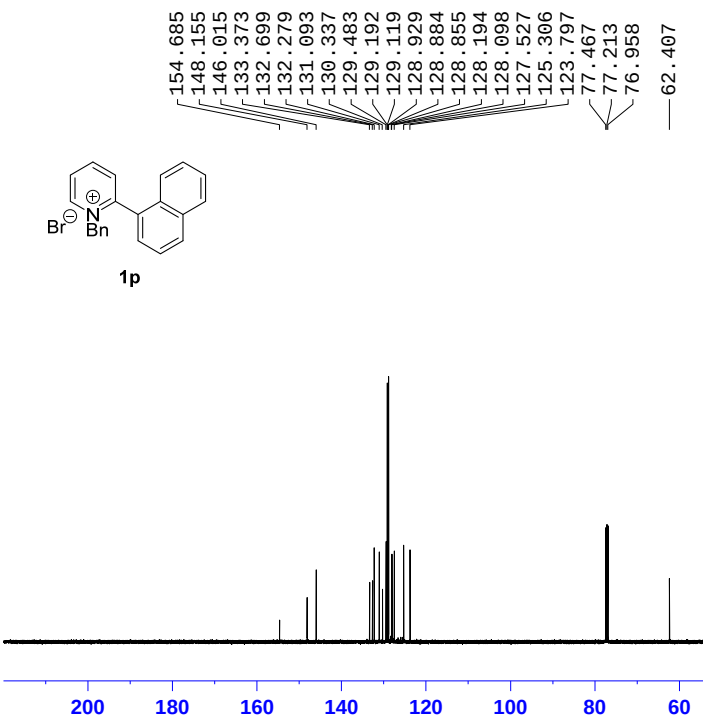



```
Current Data Parameters
NAME          10963-049
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170512
Time              11.40
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg10
TD                32768
SOLVENT           CDCl3
NS                   64
DS                    0
SWH            7500.000 Hz
FIDRES         0.228882 Hz
AQ             2.1845334 sec
RG                  287
DW               66.667 usec
DE                6.50 usec
TE               299.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        500.1325007 MHz
NUC1                1H
P1                11.75 usec
PLW1        18.39999962 W

F2 - Processing parameters
SI                16384
SF          500.1300118 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



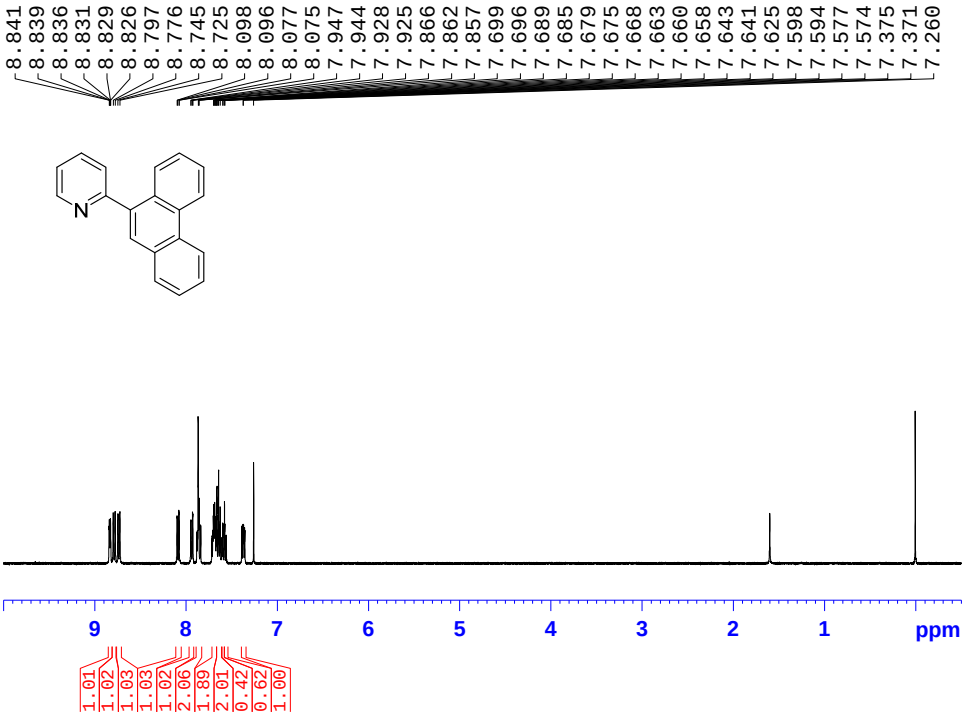

```
Current Data Parameters
NAME          10963-049
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20170512
Time              11.55
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg
TD               262144
SOLVENT           CDCl3
NS                  160
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
TD0                   1

======== CHANNEL f1 ========
SFO1        125.7698617 MHz
NUC1                13C
P1                 9.75 usec
PLW1       126.00000000 W

======== CHANNEL f2 ========
SFO2        500.1325007 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        18.39999962 W
PLW12        0.41056001 W
PLW13        0.20651001 W

F2 - Processing parameters
SI              131072
SF          125.7577751 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.40
```

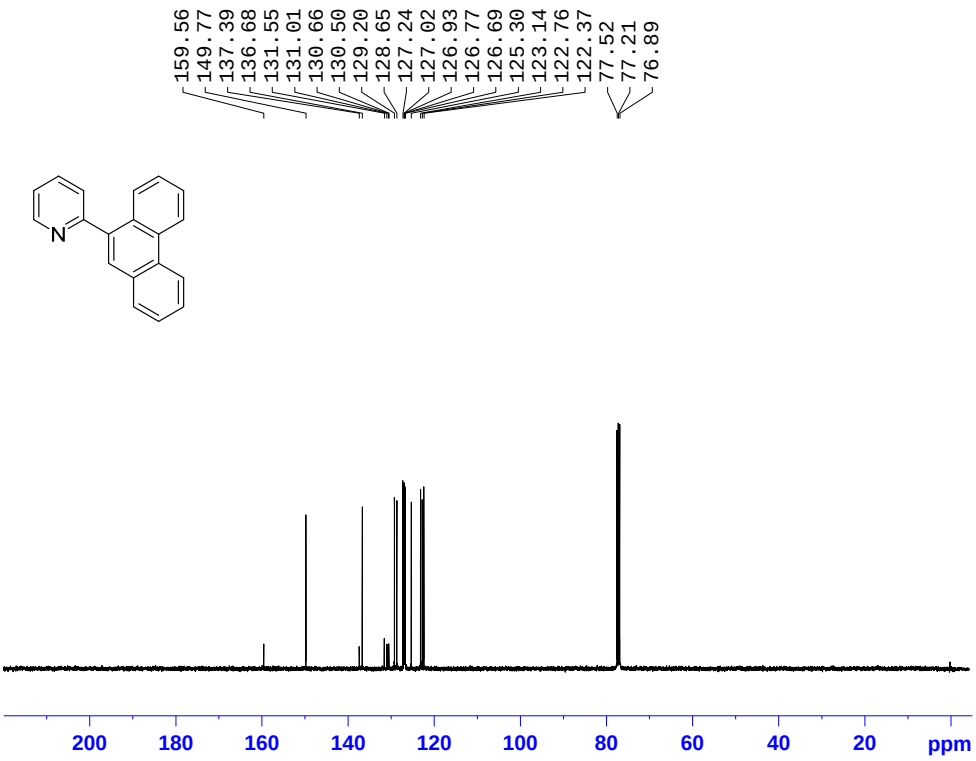



```
Current Data Parameters
NAME          10967-031
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170523
Time              16.55
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                  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          400.1300098 MHz
WDW                 EM
SSB       0
LB                0.05 Hz
GB        0
PC                1.00
```



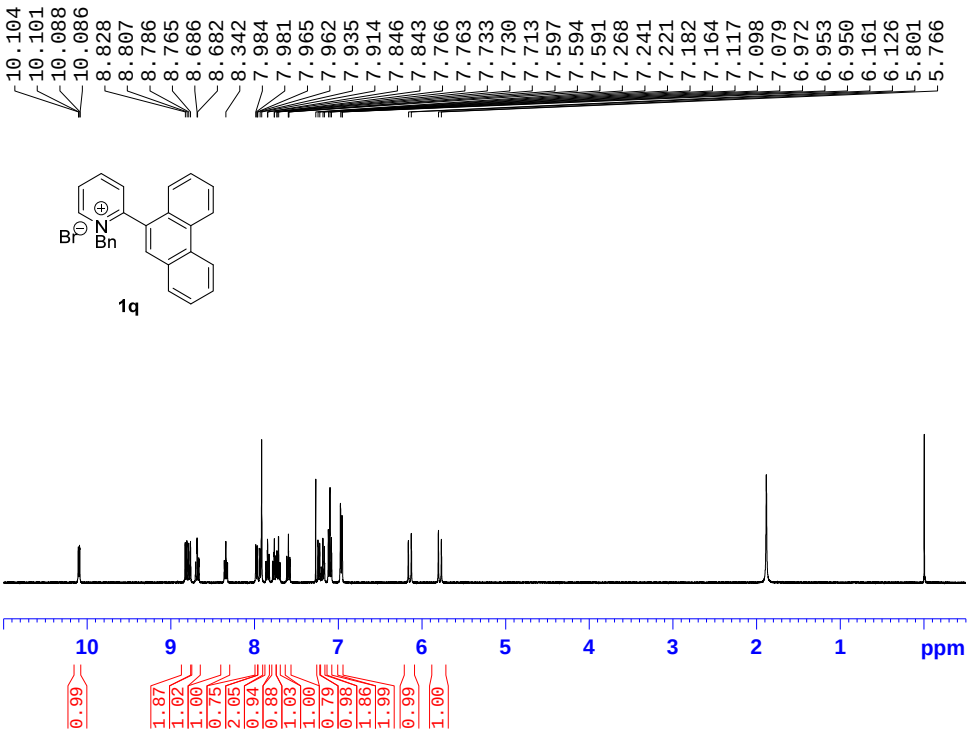

```
Current Data Parameters
NAME          10967-031
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20170523
Time              20.59
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg
TD                32768
SOLVENT           CDCl3
NS                 2500
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          100.6127509 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

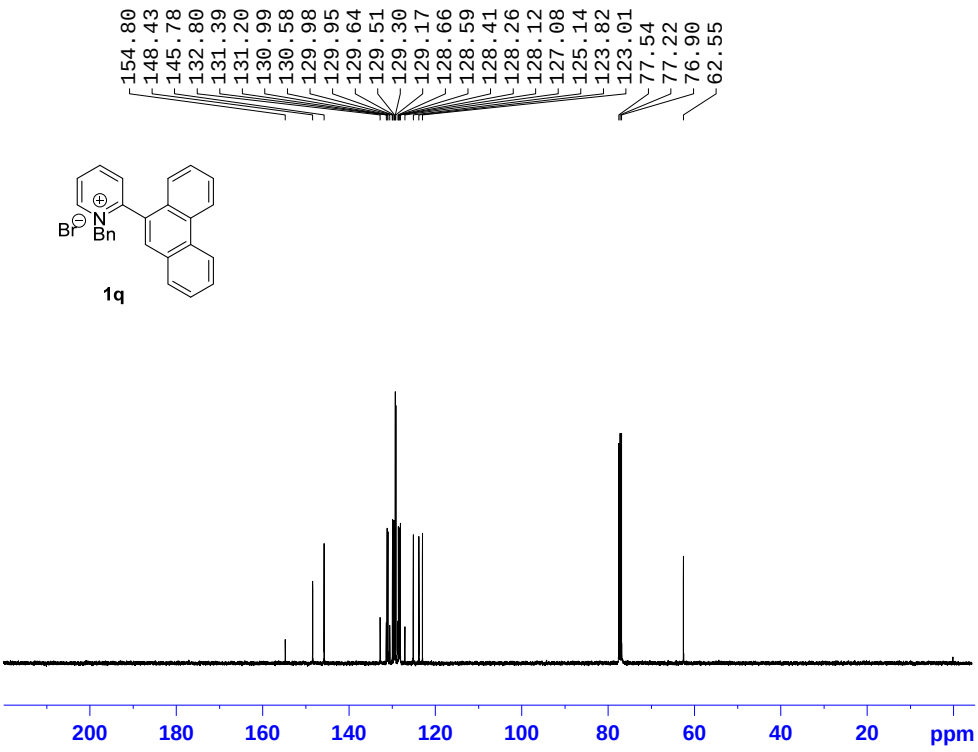



```
Current Data Parameters
NAME          10967-036
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170523
Time              16.59
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                  575
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          400.1300067 MHz
WDW                 EM
SSB       0
LB                0.05 Hz
GB        0
PC                1.00
```



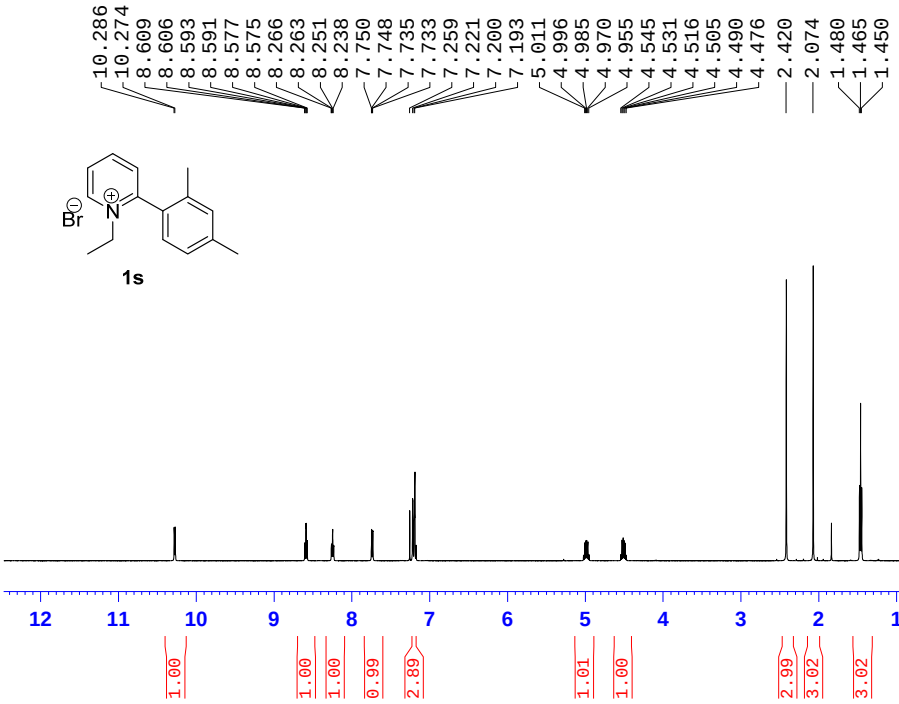

```
Current Data Parameters
NAME          10967-036
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20170523
Time              22.57
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg
TD                32768
SOLVENT           CDCl3
NS                 2500
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          100.6127524 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

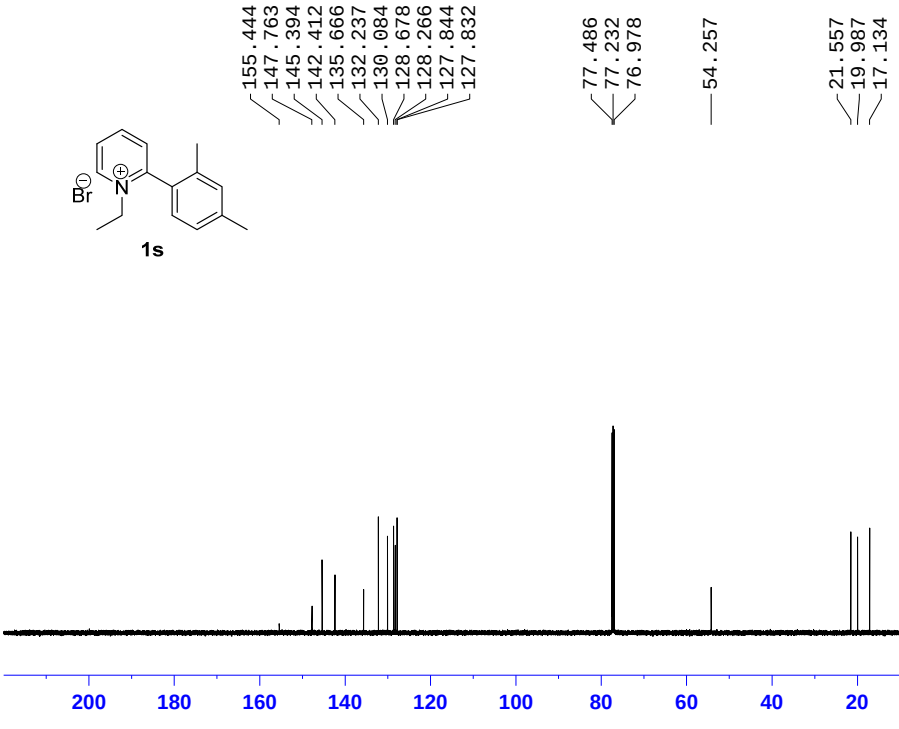



```
Current Data Parameters
NAME          10967-145
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170403
Time              10.38
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg10
TD               32768
SOLVENT          CDCl3
NS                  16
DS                   0
SWH           7500.000 Hz
FIDRES        0.228882 Hz
AQ            2.1845334 sec
RG                 456
DW              66.667 usec
DE               6.50 usec
TE              299.0 K
D1          1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        500.1325007 MHz
NUC1                1H
P1                11.75 usec
PLW1        18.39999962 W

F2 - Processing parameters
SI                16384
SF          500.1300114 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



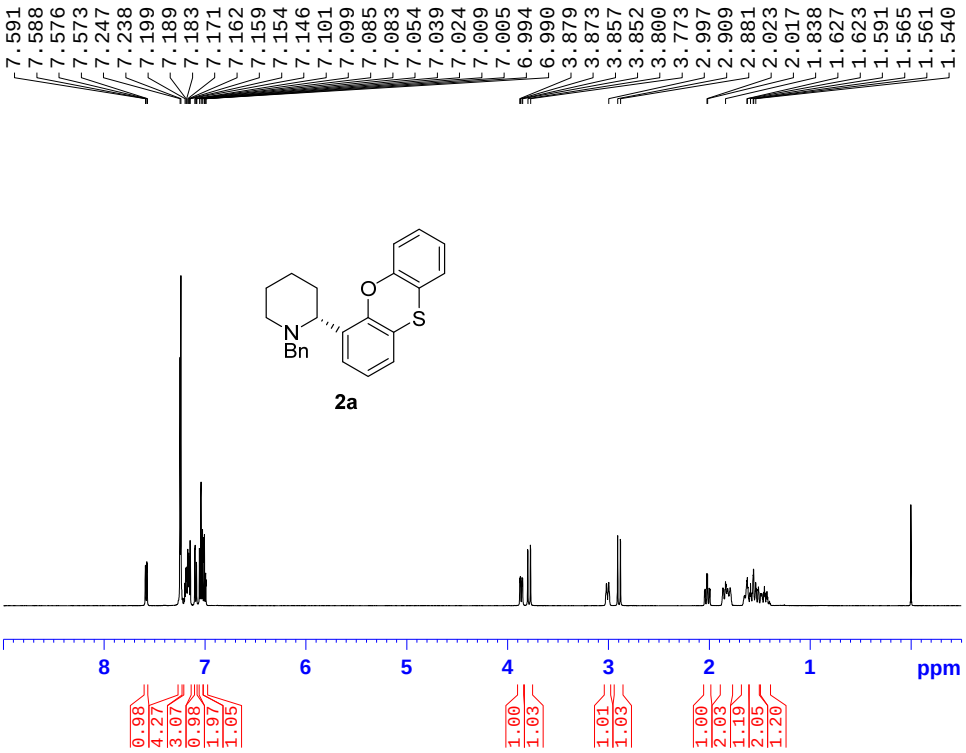

```
Current Data Parameters
NAME          10967-145
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20170403
Time              11.03
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg
TD              262144
SOLVENT          CDCl3
NS                 275
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
TD0                  1

======== CHANNEL f1 ========
SFO1        125.7698617 MHz
NUC1                13C
P1                 9.75 usec
PLW1       126.00000000 W

======== CHANNEL f2 ========
SFO2        500.1325007 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        18.39999962 W
PLW12        0.41056001 W
PLW13        0.20651001 W

F2 - Processing parameters
SI               131072
SF          125.7577663 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.40
```

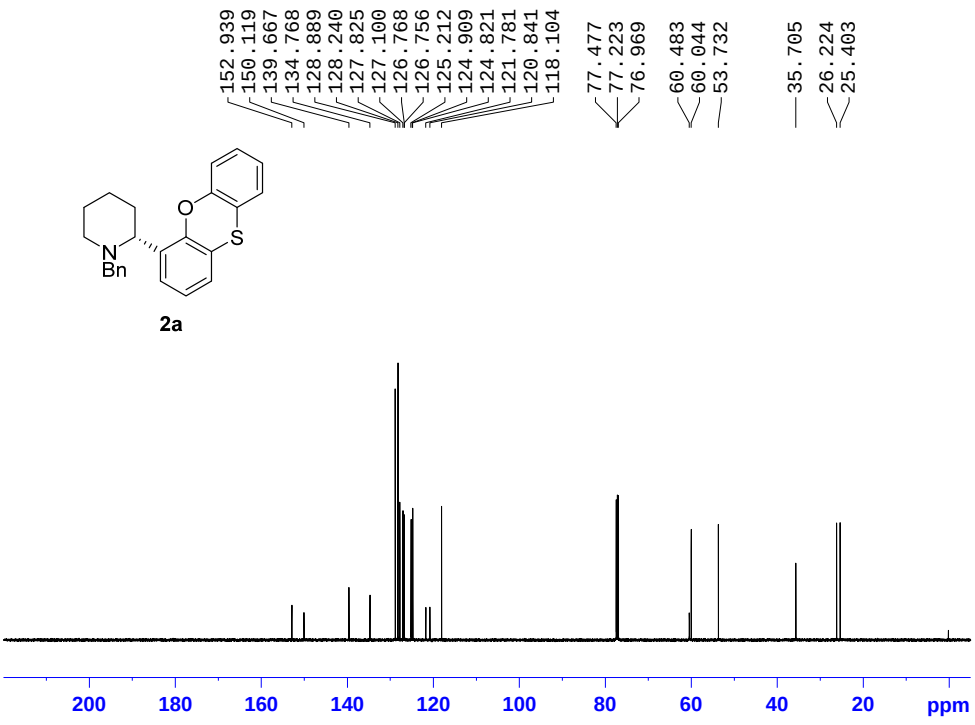



```
Current Data Parameters
NAME         10967-062-2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170412
Time              17.03
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg10
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7500.000 Hz
FIDRES         0.228882 Hz
AQ           2.1845334 sec
RG                  362
DW               66.667 usec
DE                6.50 usec
TE               299.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.1325007 MHz
NUC1                   1H
P1                 11.75 usec
PLW1        18.39999962 W

F2 - Processing parameters
SI                 16384
SF           500.1300159 MHz
WDW                   EM
SSB      0
LB                 0.30 Hz
GB       0
PC                 1.00
```



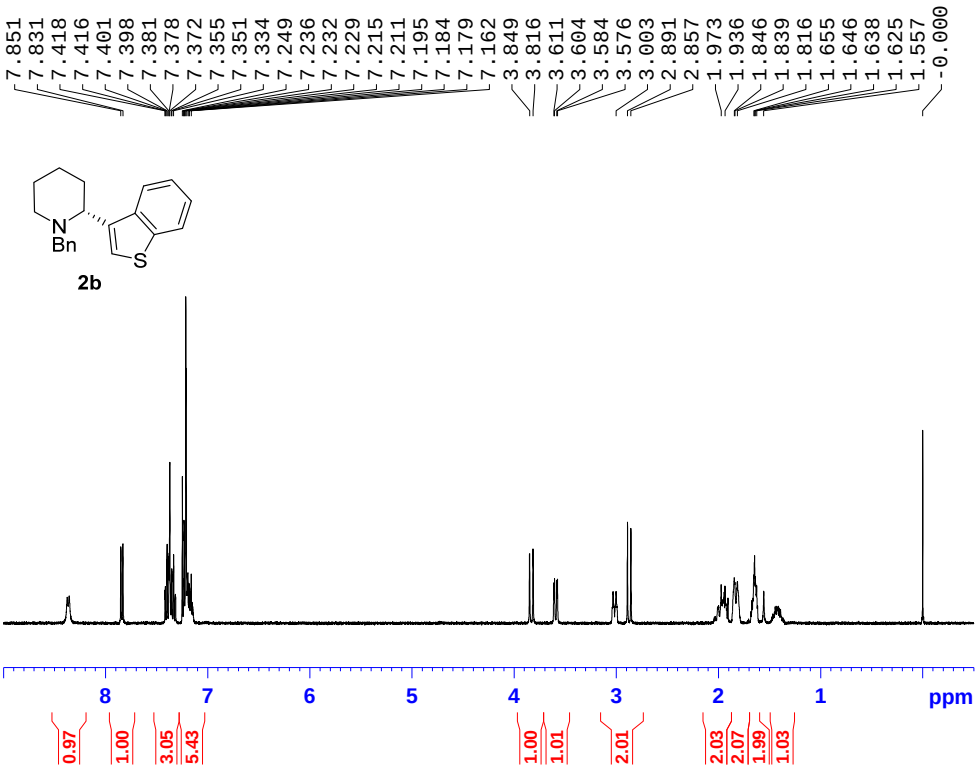

```
Current Data Parameters
NAME         10967-062-2
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170413
Time              0.03
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg
TD              262144
SOLVENT           CDCl3
NS                 1024
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
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7698617 MHz
NUC1                  13C
P1                 9.75 usec
PLW1       126.00000000 W

======== CHANNEL f2 ========
SFO2         500.1325007 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2             80.00 usec
PLW2        18.39999962 W
PLW12        0.41056001 W
PLW13        0.20651001 W

F2 - Processing parameters
SI                131072
SF           125.7577637 MHz
WDW                   EM
SSB      0
LB                 0.30 Hz
GB       0
PC                 1.40
```

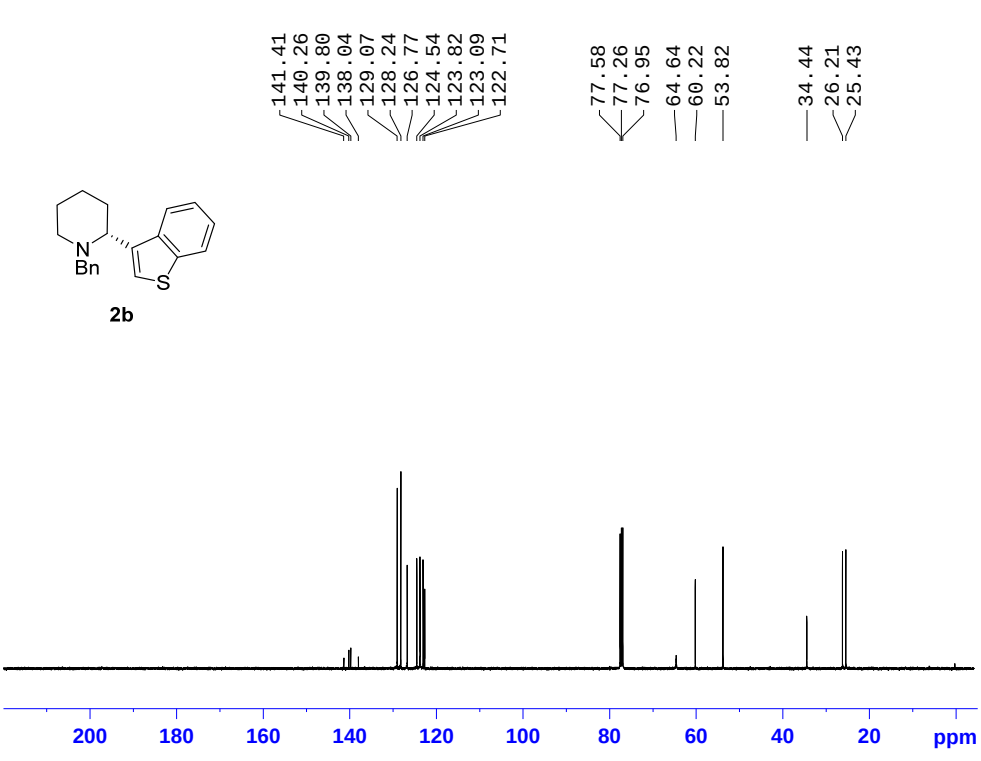



```
Current Data Parameters
NAME          10967-073
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170421
Time              17.39
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                  512
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           400.1300145 MHz
WDW                  EM
SSB       0
LB                0.05 Hz
GB        0
PC                1.00
```



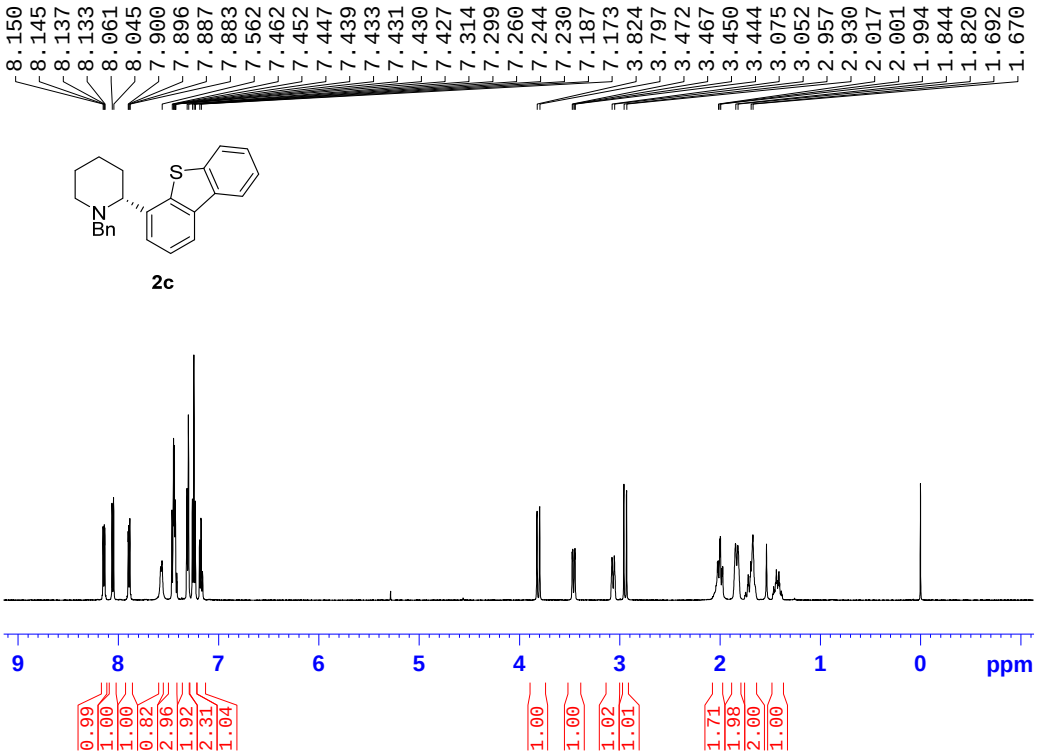

```
Current Data Parameters
NAME          10967-073
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20170422
Time               6.00
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg
TD                32768
SOLVENT           CDCl3
NS                 2500
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           100.6127450 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

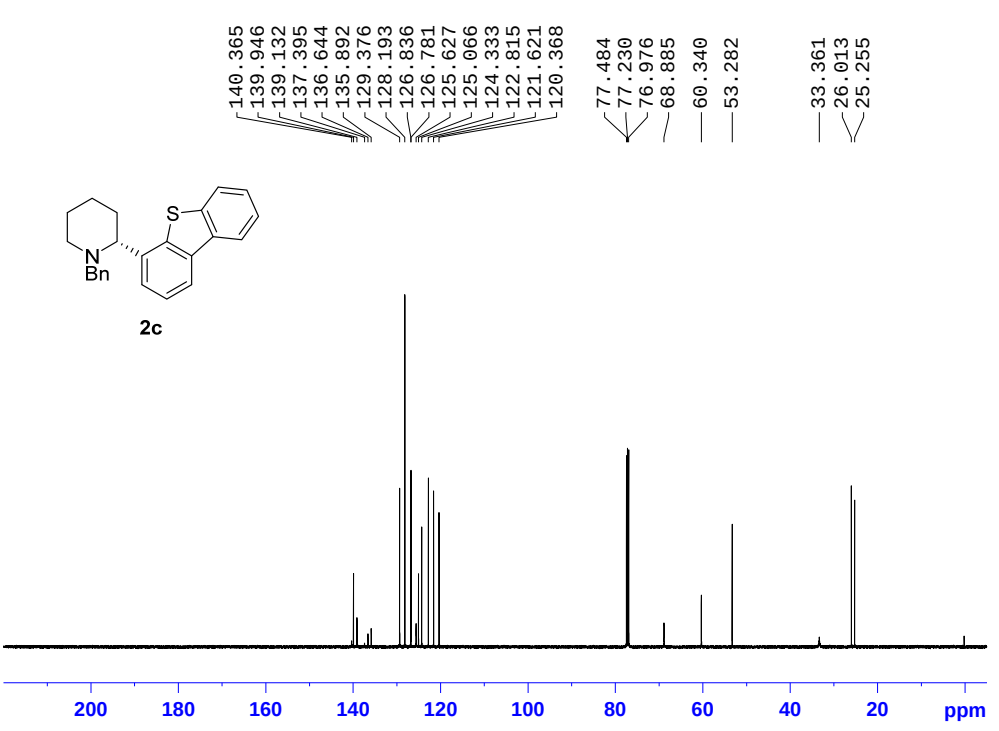



```
Current Data Parameters
NAME          10967-117
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170331
Time              16.25
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg10
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7500.000 Hz
FIDRES         0.228882 Hz
AQ             2.1845334 sec
RG                  362
DW               66.667 usec
DE                6.50 usec
TE                299.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        500.1325007 MHz
NUC1                1H
P1                11.75 usec
PLW1        18.39999962 W

F2 - Processing parameters
SI                16384
SF          500.1300190 MHz
WDW                  EM
SSB      0
LB                0.30 Hz
GB       0
PC                1.00
```



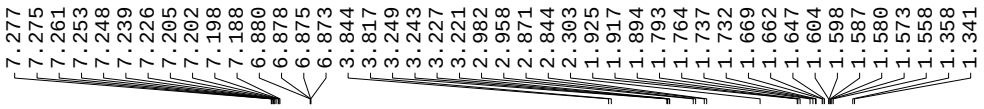

```
Current Data Parameters
NAME          10967-117
EXPNO                 2
PROCNO                1

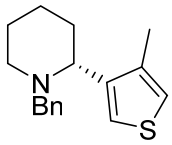
F2 - Acquisition Parameters
Date_          20170401
Time              1.32
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg
TD              262144
SOLVENT           CDCl3
NS                 2000
DS                    0
SWH           31250.000 Hz
FIDRES         0.119209 Hz
AQ             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
TD0                   1

======== CHANNEL f1 ========
SFO1        125.7698617 MHz
NUC1                13C
P1                9.75 usec
PLW1       126.00000000 W

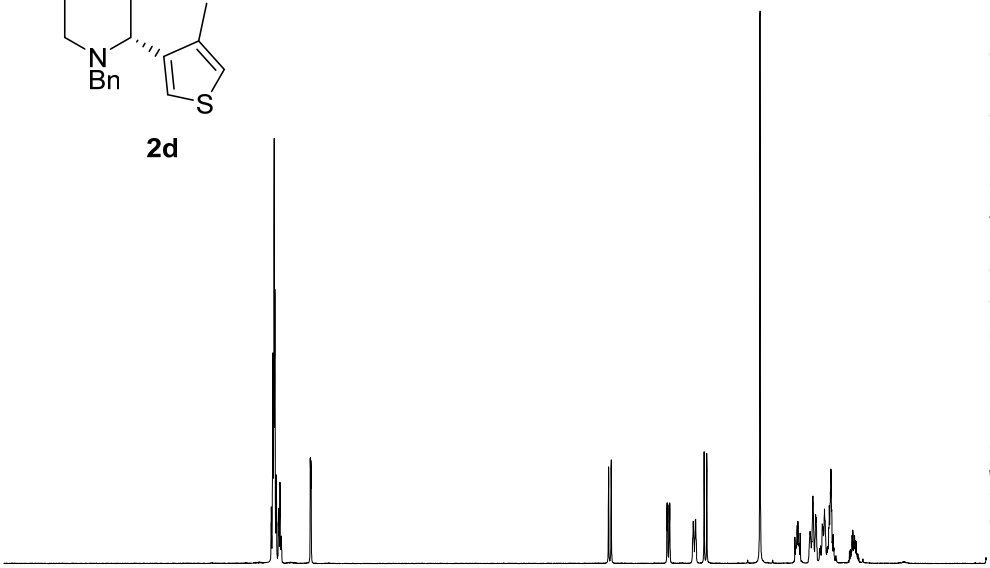
======== CHANNEL f2 ========
SFO2        500.1325007 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2            80.00 usec
PLW2        18.39999962 W
PLW12        0.41056001 W
PLW13        0.20651001 W

F2 - Processing parameters
SI              131072
SF          125.7577634 MHz
WDW                  EM
SSB      0
LB                0.30 Hz
GB       0
PC                1.40
```





2d

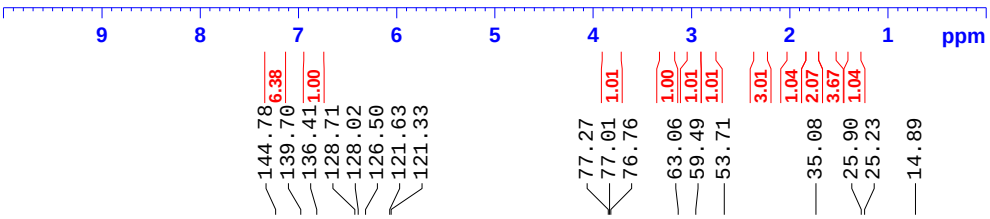


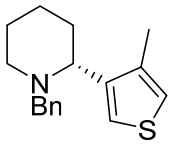
```
Current Data Parameters
NAME     bqu1-10967-080
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20171228
Time              10.08
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg10
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7500.000 Hz
FIDRES         0.228882 Hz
AQ           2.1845334 sec
RG                  406
DW               66.667 usec
DE                6.50 usec
TE                299.0 K
D1           1.00000000 sec
TD0                   1

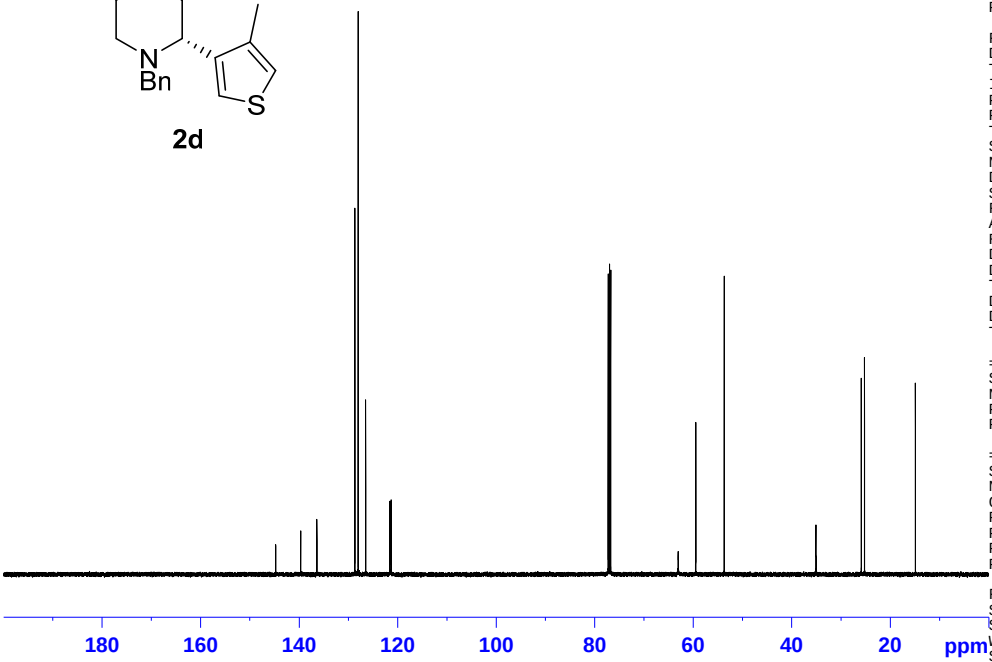
======== CHANNEL f1 ========
SFO1         500.1325007 MHz
NUC1                   1H
P1                14.00 usec
PLW1        16.00000000 W

F2 - Processing parameters
SI                 16384
SF           500.1300181 MHz
WDW                   EM
SSB      0
LB                0.30 Hz
GB       0
PC                1.00
```





2d



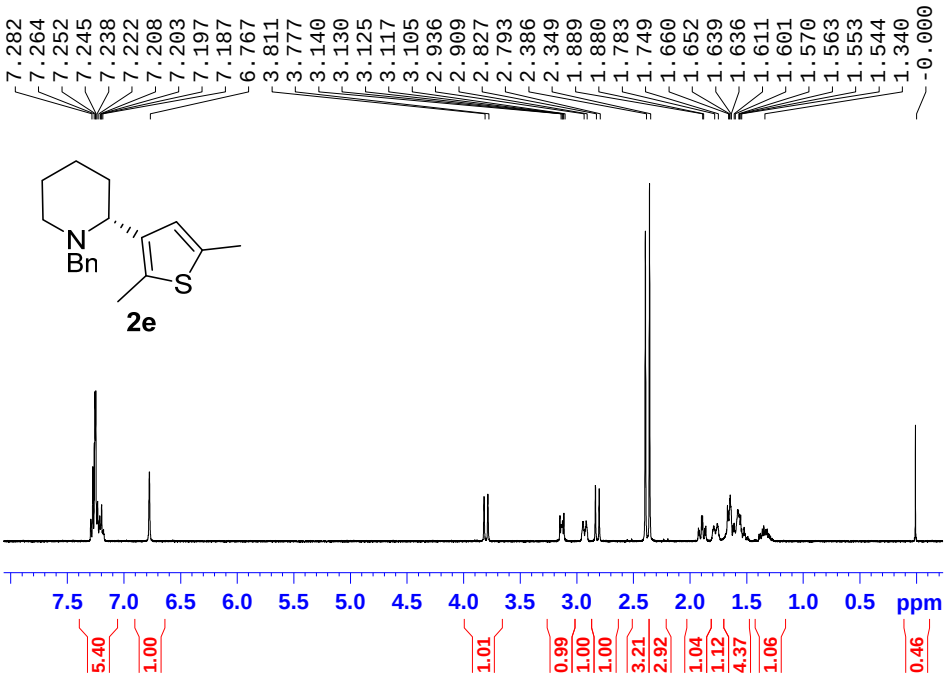

```
Current Data Parameters
NAME     bqu1-10967-080
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20171229
Time              0.17
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg
TD                262144
SOLVENT           CDCl3
NS                  1024
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
TD0                   1

======== CHANNEL f1 ========
SFO1         125.7698617 MHz
NUC1                  13C
P1                10.00 usec
PLW1        99.50000000 W

======== CHANNEL f2 ========
SFO2         500.1325007 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2             80.00 usec
PLW2        16.00000000 W
PLW12        0.49000001 W
PLW13        0.24647000 W

F2 - Processing parameters
SI                131072
SF           125.7577909 MHz
WDW                   EM
SSB      0
LB                0.30 Hz
GB       0
PC                1.40
```

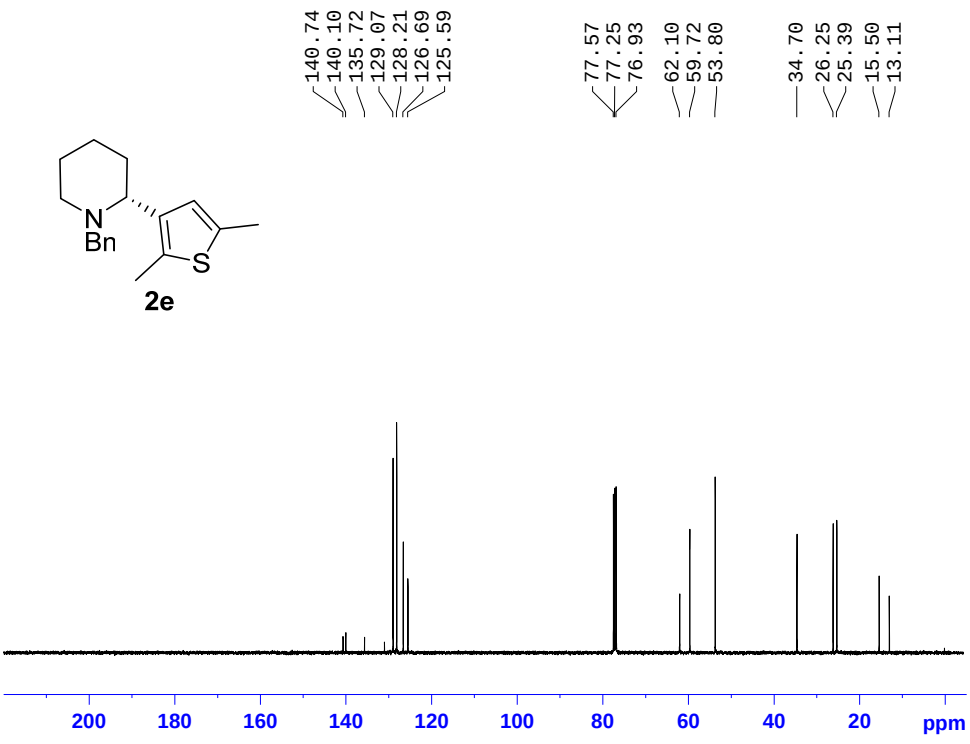



```
Current Data Parameters
NAME          10967-097
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170421
Time              17.43
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                  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          400.1300103 MHz
WDW                  EM
SSB       0
LB                0.05 Hz
GB        0
PC                1.00
```



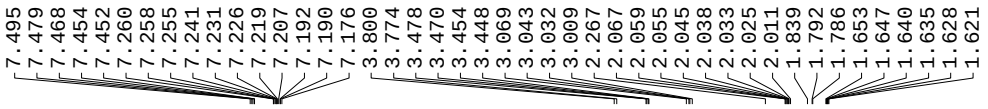

```
Current Data Parameters
NAME          10967-097
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20170422
Time              20.59
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg
TD                32768
SOLVENT           CDCl3
NS                 2500
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

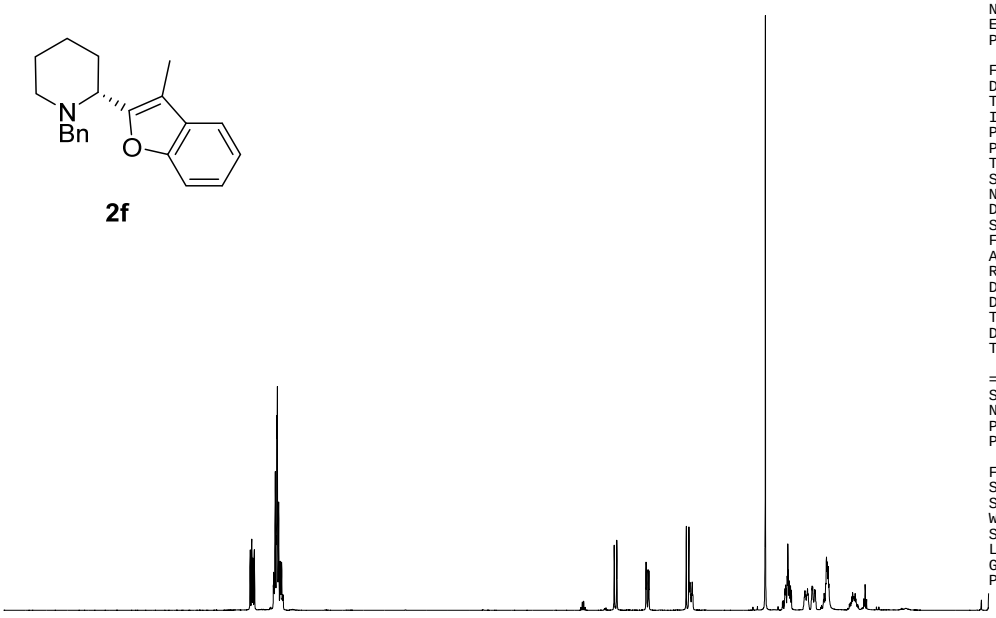
======== CHANNEL f1 ========
SFO1        100.6243395 MHz
NUC1                13C
P1                10.90 usec
PLW1        43.00000000 W

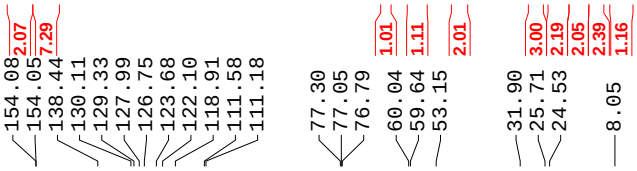
======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        10.50000000 W
PLW12        0.29166999 W
PLW13        0.14670999 W

F2 - Processing parameters
SI                65536
SF          100.6127464 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



2f



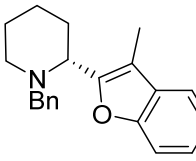



```
Current Data Parameters
NAME         bqu1-00183b
EXPNO                  1
PROCNO                 1

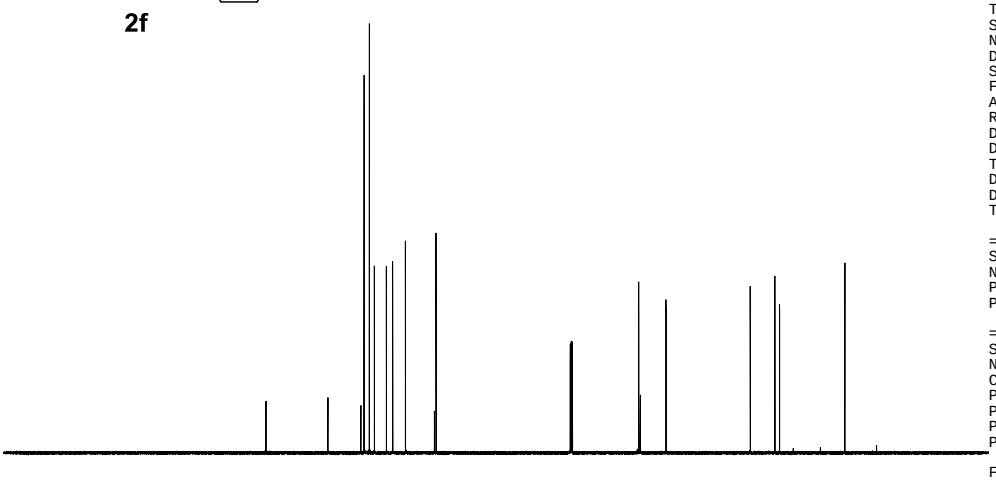
F2 - Acquisition Parameters
Date_           20171222
Time              17.05
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg10
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7500.000 Hz
FIDRES         0.228882 Hz
AQ           2.1845334 sec
RG                  322
DW               66.667 usec
DE                6.50 usec
TE                299.0 K
D1          1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         500.1325007 MHz
NUC1                 1H
P1                14.00 usec
PLW1        16.00000000 W

F2 - Processing parameters
SI                16384
SF           500.1300214 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



2f



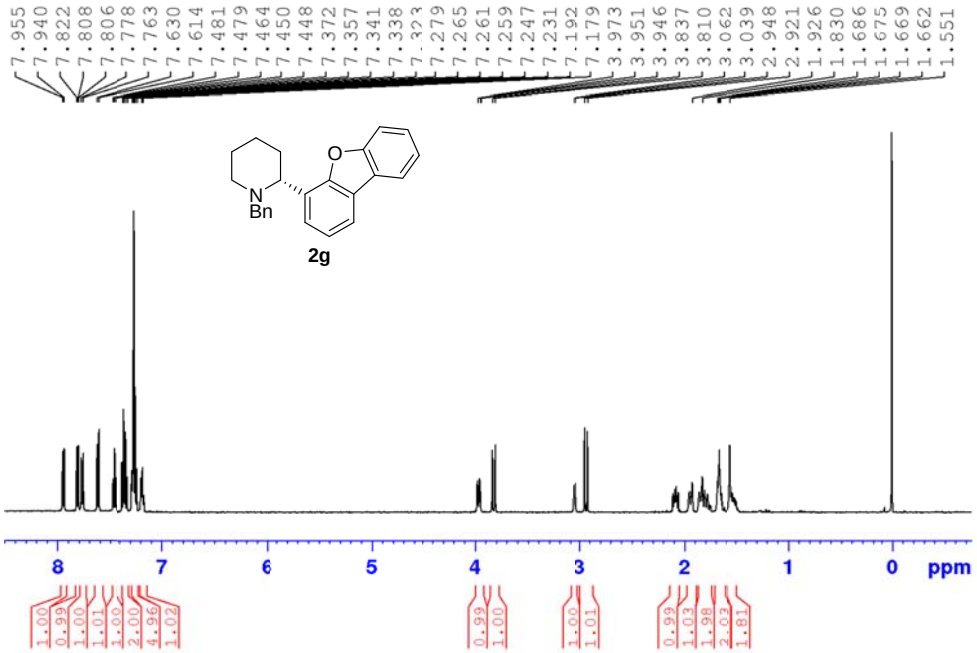

```
Current Data Parameters
NAME         bqu1-00183b
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171222
Time              19.48
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg
TD               262144
SOLVENT           CDCl3
NS                  512
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
TD0                   1

======== CHANNEL f1 ========
SFO1         125.7698617 MHz
NUC1                 13C
P1                10.00 usec
PLW1        99.50000000 W

======== CHANNEL f2 ========
SFO2         500.1325007 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        16.00000000 W
PLW12        0.49000001 W
PLW13        0.24647000 W

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

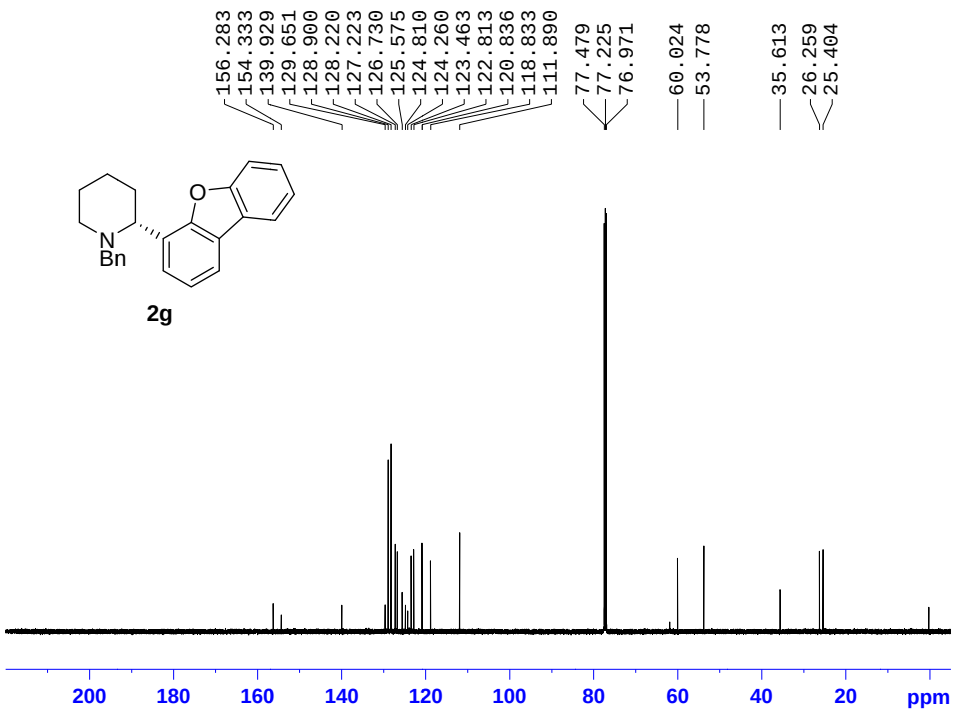



```
Current Data Parameters
NAME           10967-135
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170412
Time               17.12
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg10
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             7500.000 Hz
FIDRES          0.228882 Hz
AQ              2.1845334 sec
RG                   5.2
DW                66.667 usec
DE                 6.50 usec
TE                299.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          500.1325007 MHz
NUC1                   1H
P1                 11.75 usec
PLW1          18.39999952 W

F2 - Processing parameters
SI                 16384
SF            500.1300115 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



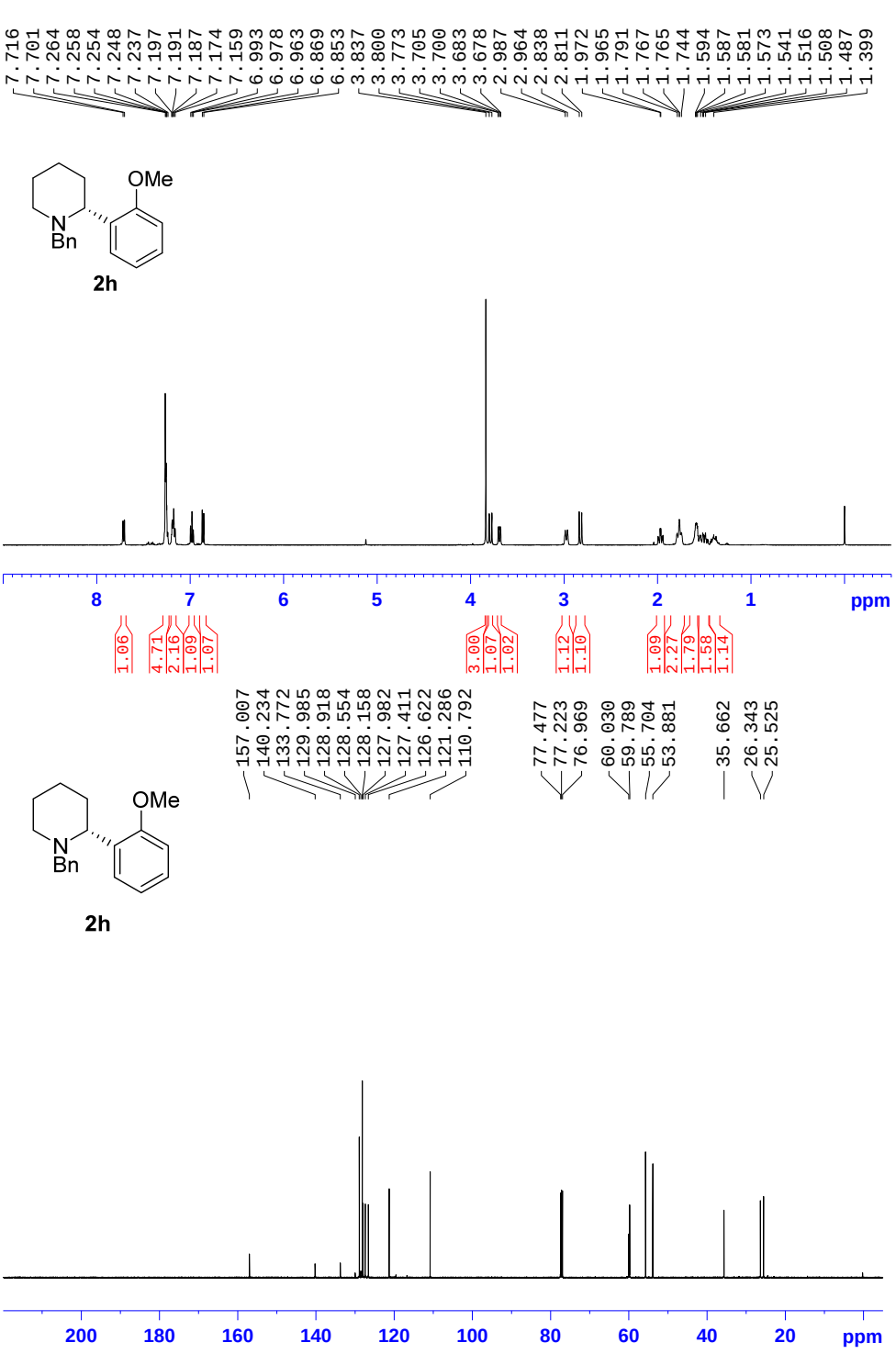

```
Current Data Parameters
NAME           10967-135
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170413
Time                4.34
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg
TD                262144
SOLVENT            CDCl3
NS                   1500
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
TD0                    1

======== CHANNEL f1 ========
SFO1          125.7698617 MHz
NUC1                  13C
P1                 9.75 usec
PLW1       126.00000000 W

======== CHANNEL f2 ========
SFO2          500.1325007 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2             80.00 usec
PLW2          18.39999962 W
PLW12          0.41056001 W
PLW13          0.20651001 W

F2 - Processing parameters
SI                131072
SF            125.7577622 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.40
```




```
Current Data Parameters
NAME          10967-185
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20170509
Time              16.25
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg10
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7500.000 Hz
FIDRES         0.228882 Hz
AQ           2.1845334 sec
RG                  322
DW               66.667 usec
DE                6.50 usec
TE               299.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        500.1325007 MHz
NUC1                  1H
P1                11.75 usec
PLW1        18.39999962 W

F2 - Processing parameters
SI                16384
SF          500.1300174 MHz
WDW                  EM
SSB      0
LB                0.30 Hz
GB       0
PC                1.00
```

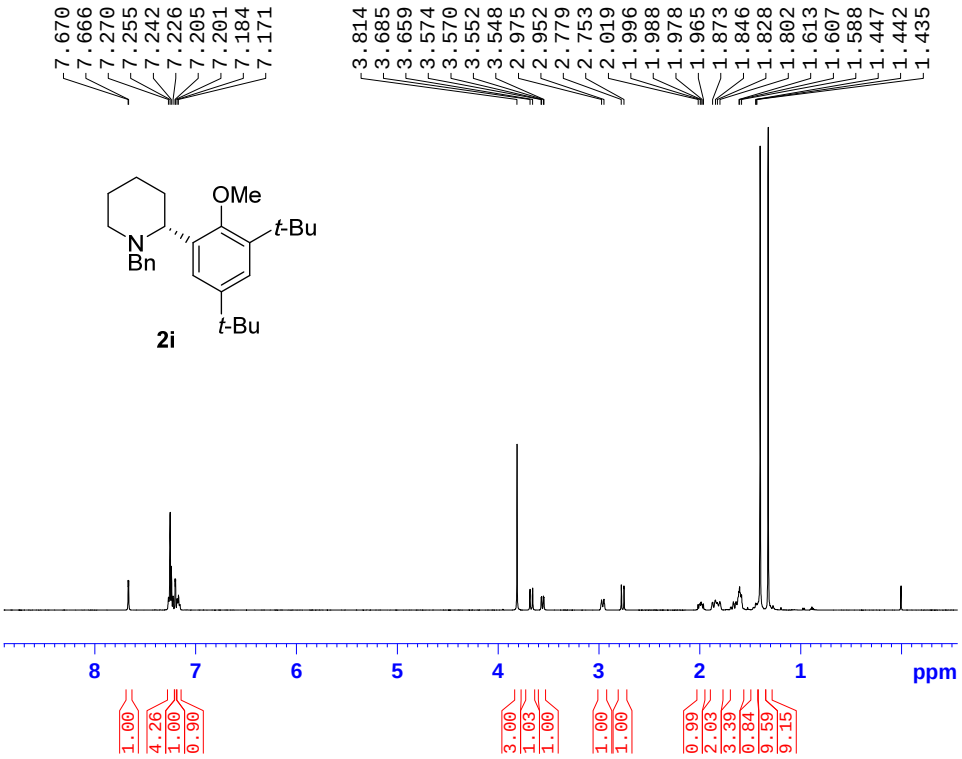
```
Current Data Parameters
NAME          10967-185
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20170429
Time              1.20
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg
TD               262144
SOLVENT           CDCl3
NS                 2500
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
TD0                   1

======== CHANNEL f1 ========
SFO1        125.7698617 MHz
NUC1                 13C
P1                 9.75 usec
PLW1       126.00000000 W

======== CHANNEL f2 ========
SFO2        500.1325007 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        18.39999962 W
PLW12        0.41056001 W
PLW13        0.20651001 W

F2 - Processing parameters
SI                65536
SF          125.7577645 MHz
WDW                  EM
SSB      0
LB                0.30 Hz
GB       0
PC                1.40
```

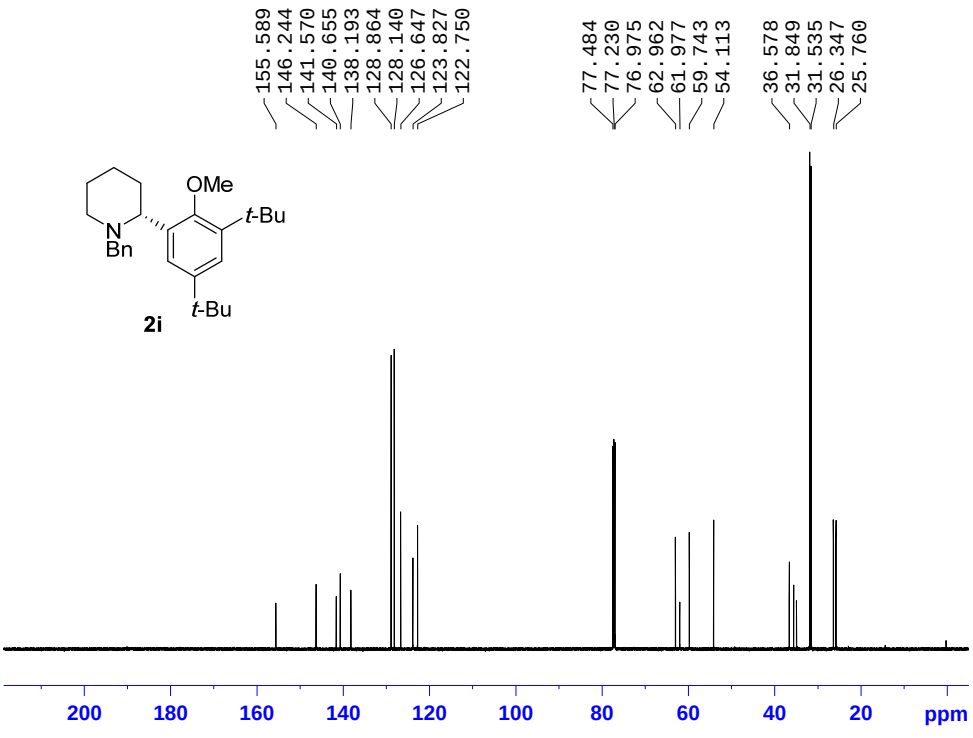



```
Current Data Parameters
NAME          10967-042
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170106
Time              18.11
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg10
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7500.000 Hz
FIDRES         0.228882 Hz
AQ             2.1845334 sec
RG                  322
DW               66.667 usec
DE                6.50 usec
TE                299.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         500.1325007 MHz
NUC1                1H
P1                14.00 usec
PLW1         18.79999924 W

F2 - Processing parameters
SI                16384
SF           500.1300152 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



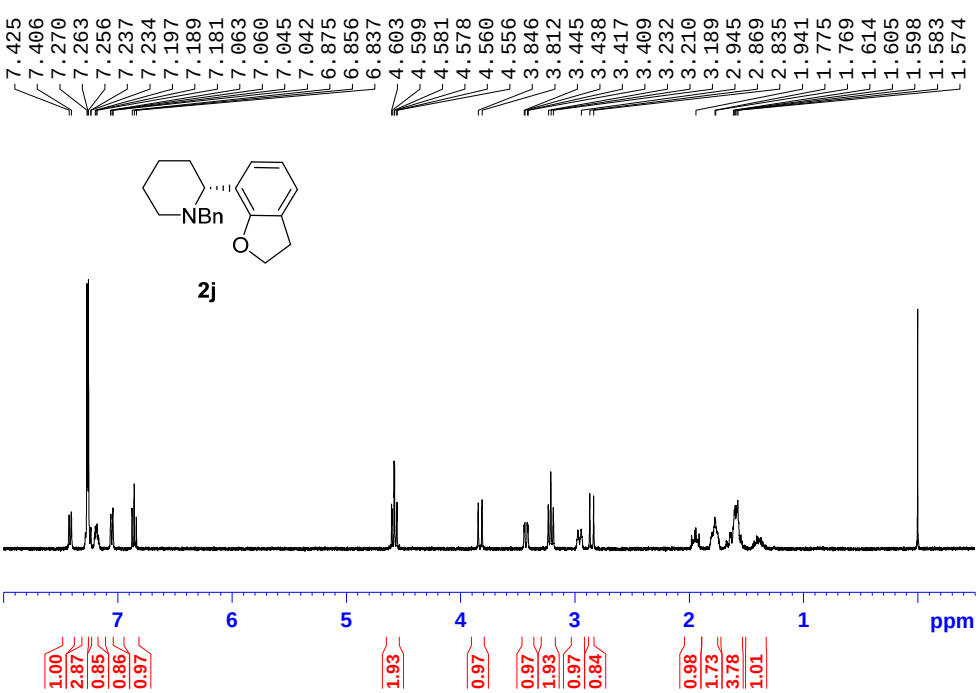

```
Current Data Parameters
NAME          10967-042
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20170107
Time              1.30
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg
TD              262144
SOLVENT           CDCl3
NS                 1250
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
TD0                   1

======== CHANNEL f1 ========
SFO1         125.7698617 MHz
NUC1                13C
P1                10.00 usec
PLW1         99.50000000 W

======== CHANNEL f2 ========
SFO2         500.1325007 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         18.79999924 W
PLW12         0.57574999 W
PLW13         0.28960001 W

F2 - Processing parameters
SI                131072
SF           125.7577627 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.40
```

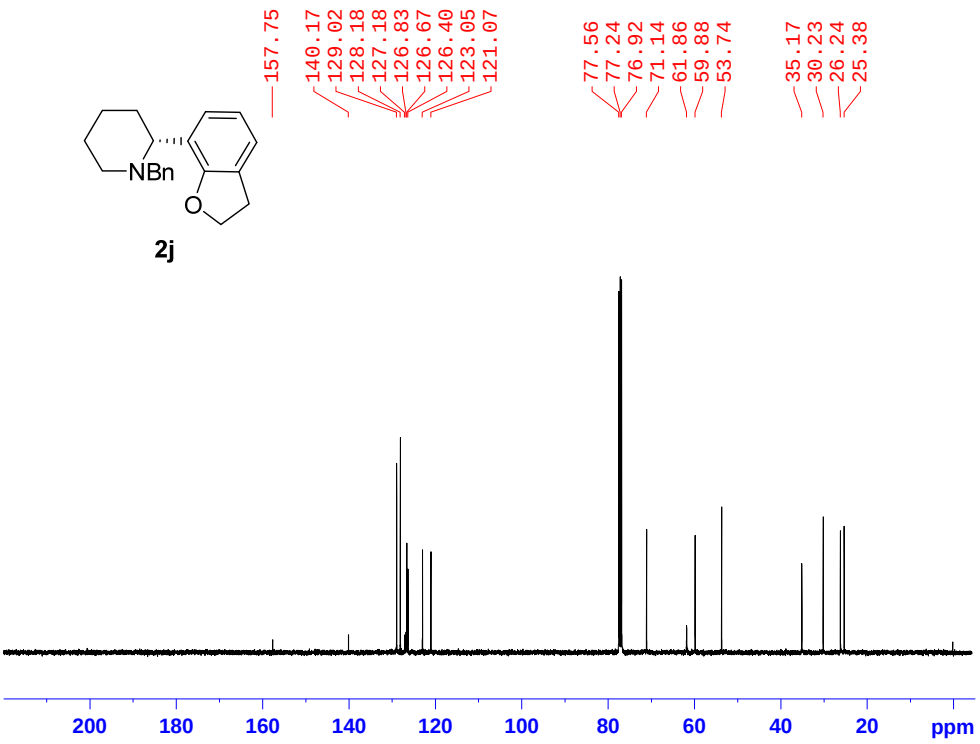



```
Current Data Parameters
NAME           10967-120
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170421
Time               17.21
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                   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           400.1300116 MHz
WDW                   EM
SSB       0
LB                0.05 Hz
GB        0
PC                1.00
```



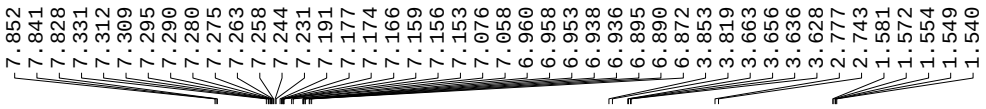

```
Current Data Parameters
NAME           10967-120
EXPNO                  2
PROCNO                 1

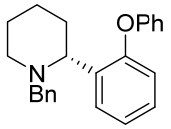
F2 - Acquisition Parameters
Date_           20170421
Time               22.07
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg
TD                 32768
SOLVENT            CDCl3
NS                  4000
DS                     4
SWH            24038.461 Hz
FIDRES          0.733596 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

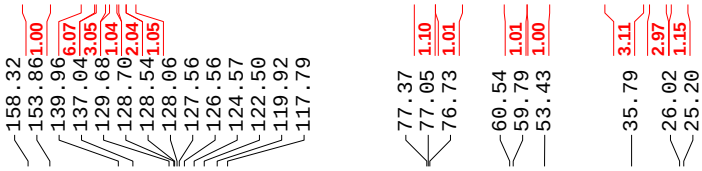
======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2         10.50000000 W
PLW12         0.29166999 W
PLW13         0.14670999 W

F2 - Processing parameters
SI                 65536
SF           100.6127468 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```





2k

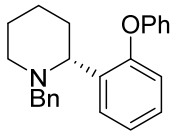



```
Current Data Parameters
NAME         10967-056-p
EXPNO                  1
PROCNO                 1

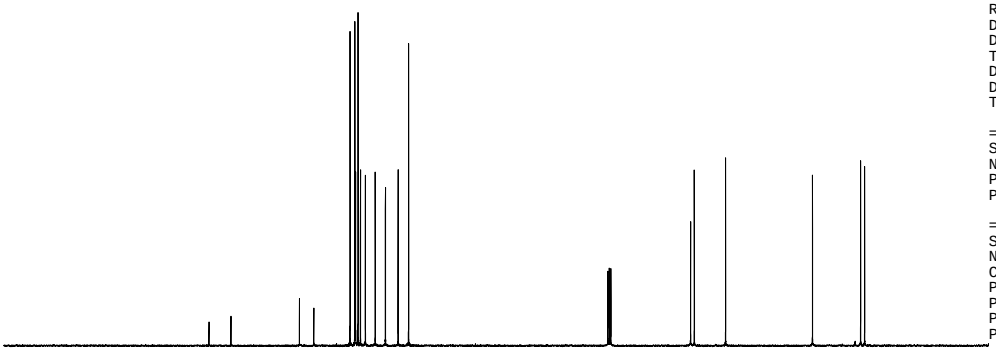
F2 - Acquisition Parameters
Date_           20180205
Time               18.37
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg10
TD                 32768
SOLVENT            CDCl3
NS                     4
DS                     4
SWH             5896.227 Hz
FIDRES          0.179939 Hz
AQ            2.7787263 sec
RG                   203
DW                84.800 usec
DE                 6.50 usec
TE                298.0 K
D1           2.00000000 sec
TD0                    1

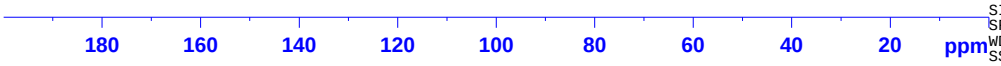
======== CHANNEL f1 ========
SFO1         400.1327209 MHz
NUC1                   1H
P1                 15.00 usec
PLW1        10.50000000 W

F2 - Processing parameters
SI                 65536
SF           400.1300211 MHz
WDW                   EM
SSB      0
LB                 0.05 Hz
GB       0
PC                 1.00
```



2k





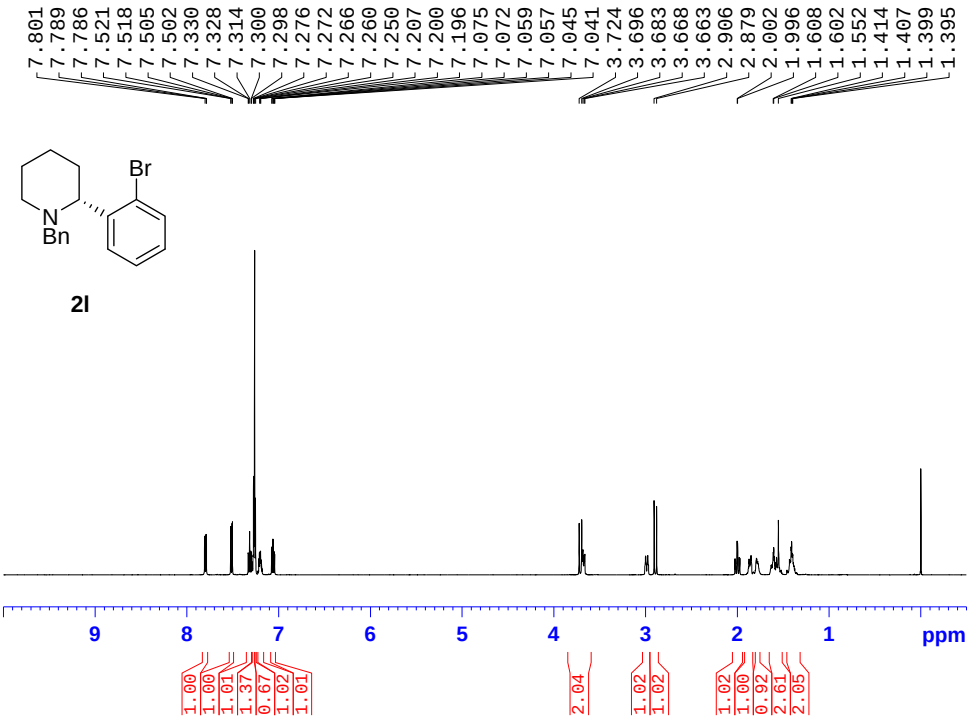

```
Current Data Parameters
NAME         10967-056-p
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180205
Time               20.39
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg
TD                 32768
SOLVENT            CDCl3
NS                  2560
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
```

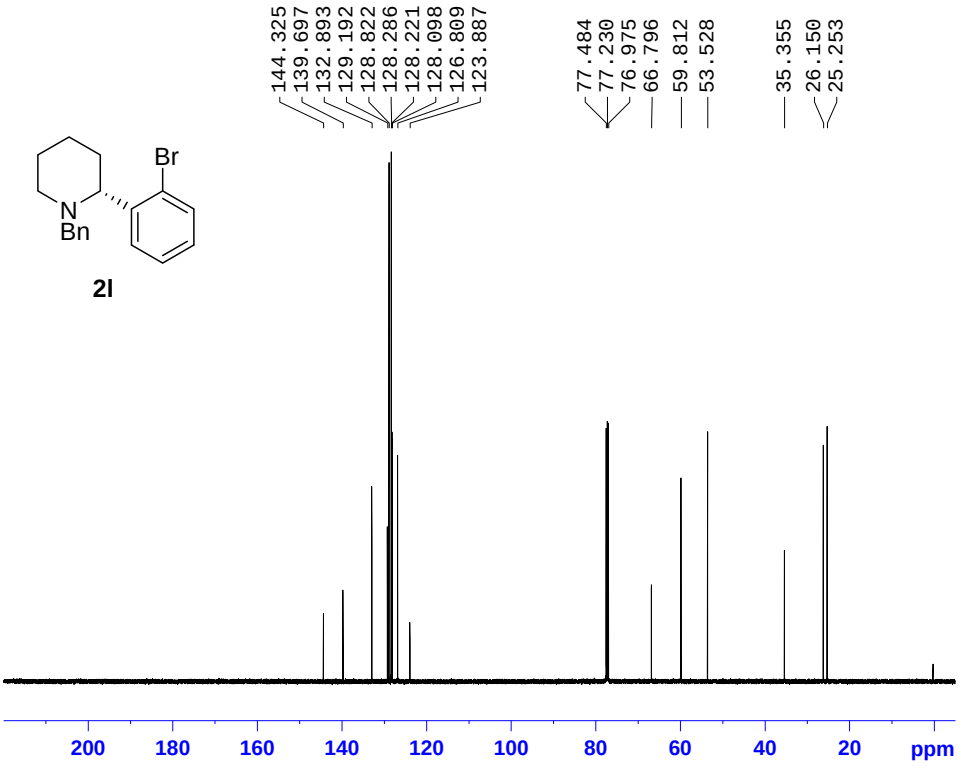



```
Current Data Parameters
NAME          10933-112
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20160915
Time              17.13
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg10
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7500.000 Hz
FIDRES         0.228882 Hz
AQ            2.1845334 sec
RG                  512
DW               66.667 usec
DE                6.50 usec
TE               299.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         500.1325007 MHz
NUC1                1H
P1                14.00 usec
PLW1         18.79999924 W

F2 - Processing parameters
SI                16384
SF           500.1300164 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



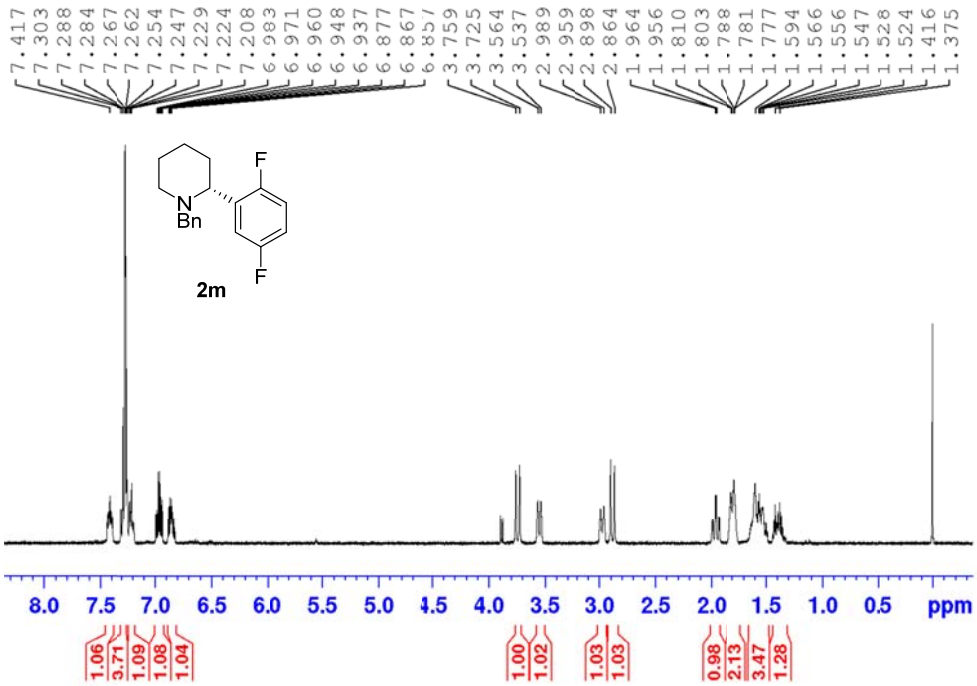

```
Current Data Parameters
NAME          10933-112
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20160915
Time              20.33
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg
TD               262144
SOLVENT           CDCl3
NS                 1024
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               298.9 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         125.7698617 MHz
NUC1                13C
P1                10.00 usec
PLW1         99.50000000 W

======== CHANNEL f2 ========
SFO2         500.1325007 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         18.79999924 W
PLW12         0.57574999 W
PLW13         0.28960001 W

F2 - Processing parameters
SI               131072
SF           125.7577628 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.40
```

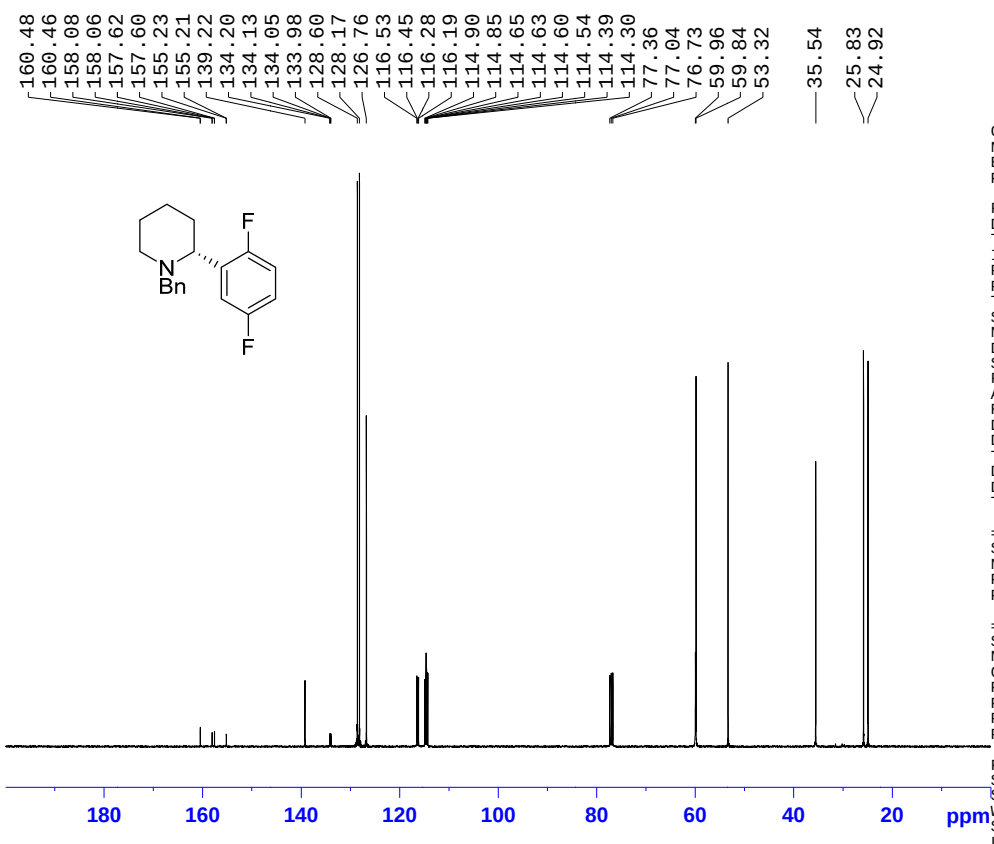



```
Current Data Parameters
NAME            10967-055
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_          20170421
Time              17.48
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD                32768
SOLVENT           CDCl3
NS                    4
DS                    4
SWH            5896.227 Hz
FIDRES          0.179939 Hz
AQ             2.7787263 sec
RG                  512
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           400.1300125 MHz
WDW                   EM
SSB       0
LB                 0.05 Hz
GB        0
PC                 1.00
```



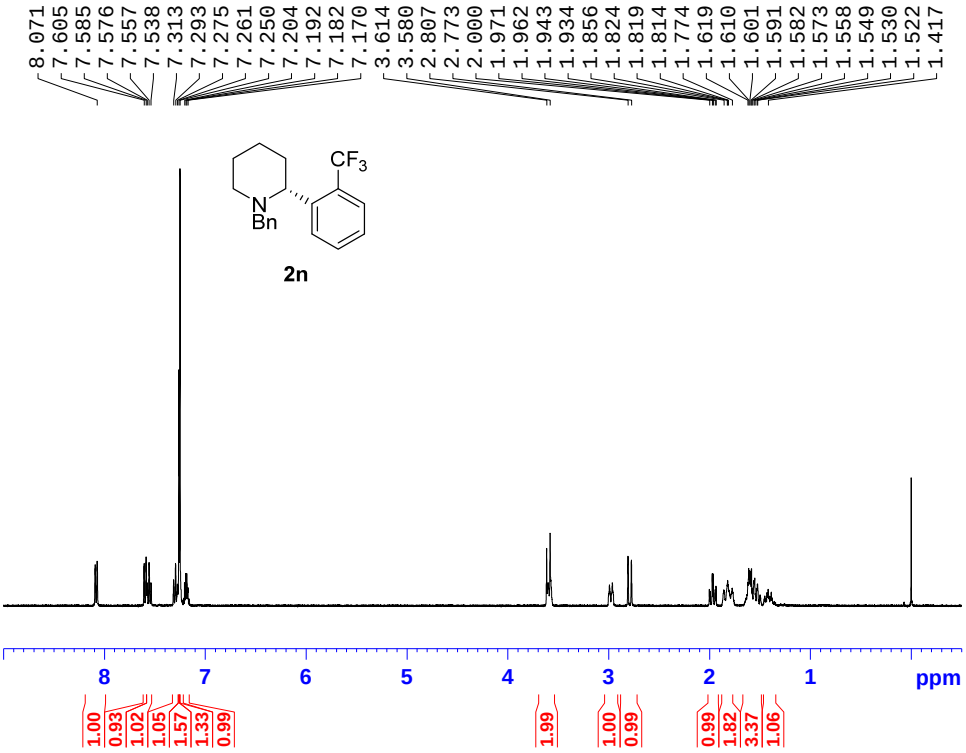

```
Current Data Parameters
NAME        10967-055-pp
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_          20180207
Time              21.04
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg
TD                32768
SOLVENT           CDCl3
NS                 2560
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
```

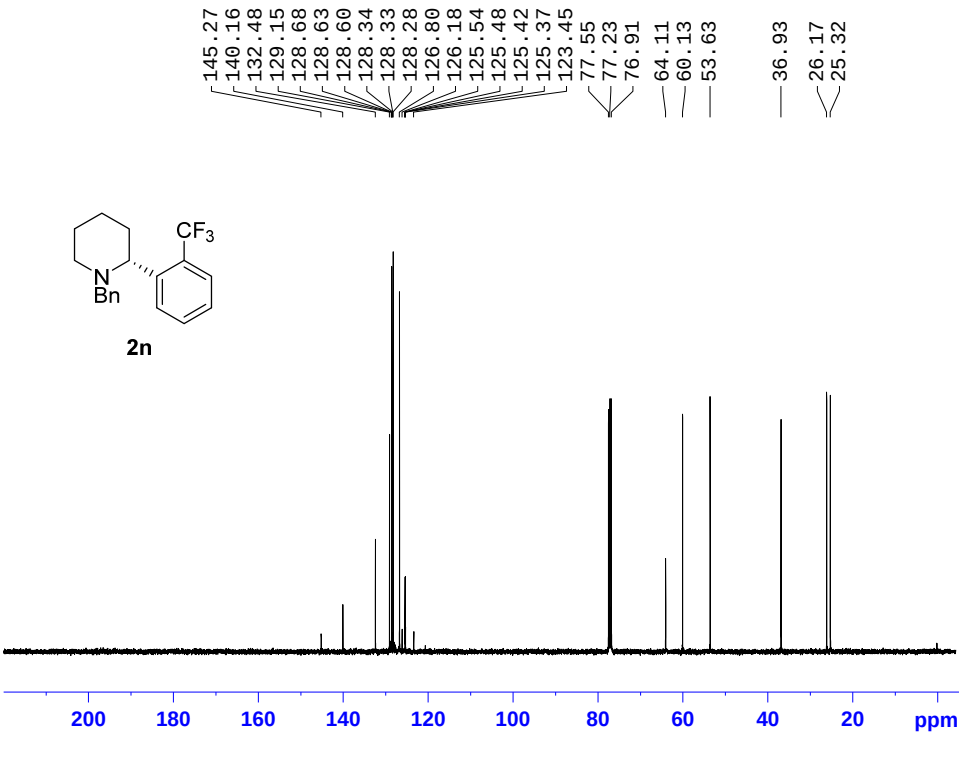



```
Current Data Parameters
NAME          10967-004
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170421
Time              17.30
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                  575
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          400.1300137 MHz
WDW                  EM
SSB       0
LB                0.05 Hz
GB        0
PC                1.00
```



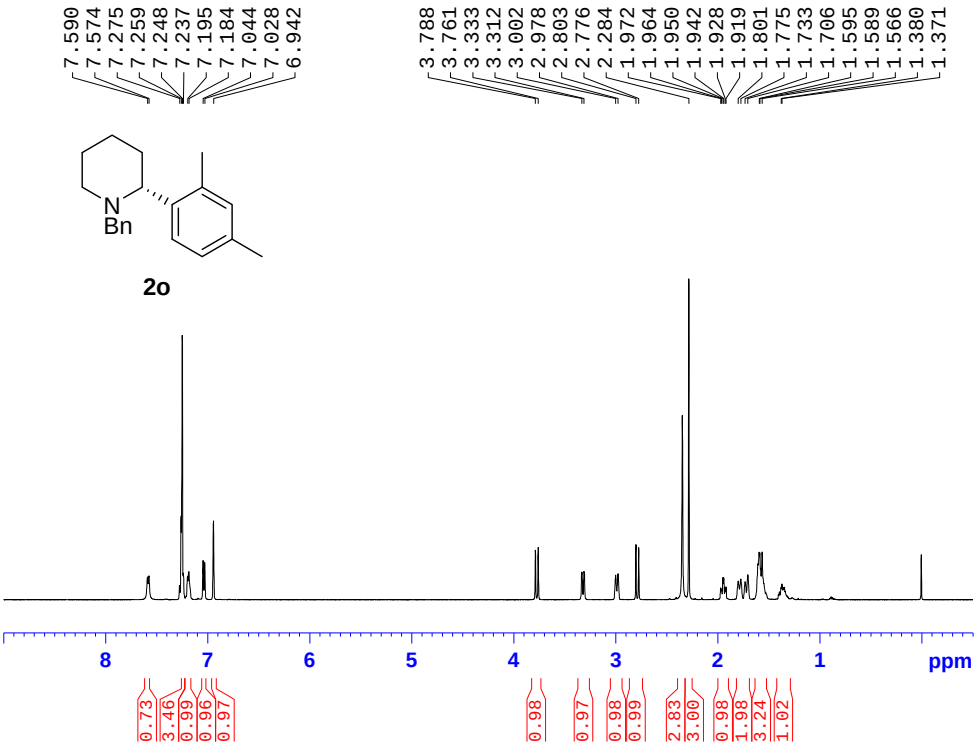

```
Current Data Parameters
NAME          10967-004
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20170422
Time              2.03
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg
TD                32768
SOLVENT           CDCl3
NS                 2500
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          100.6127477 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

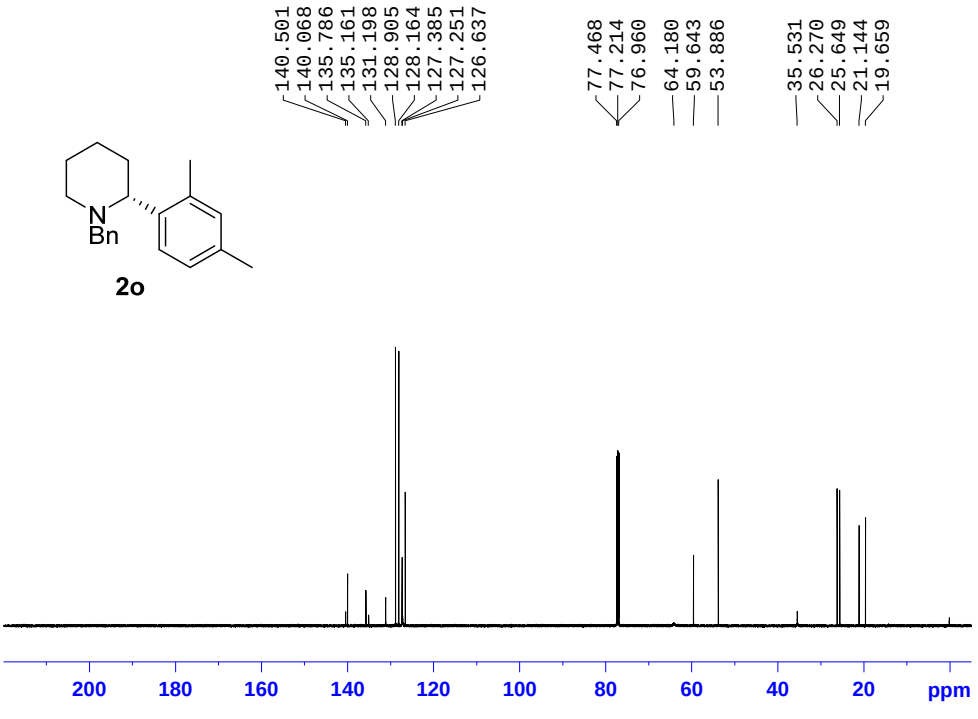



```
Current Data Parameters
NAME          10933-177
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20161110
Time               2.25
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg10
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7500.000 Hz
FIDRES         0.228882 Hz
AQ           2.1845334 sec
RG                  406
DW               66.667 usec
DE                6.50 usec
TE                299.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         500.1325007 MHz
NUC1                1H
P1                14.00 usec
PLW1         18.79999924 W

F2 - Processing parameters
SI                16384
SF           500.1300157 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



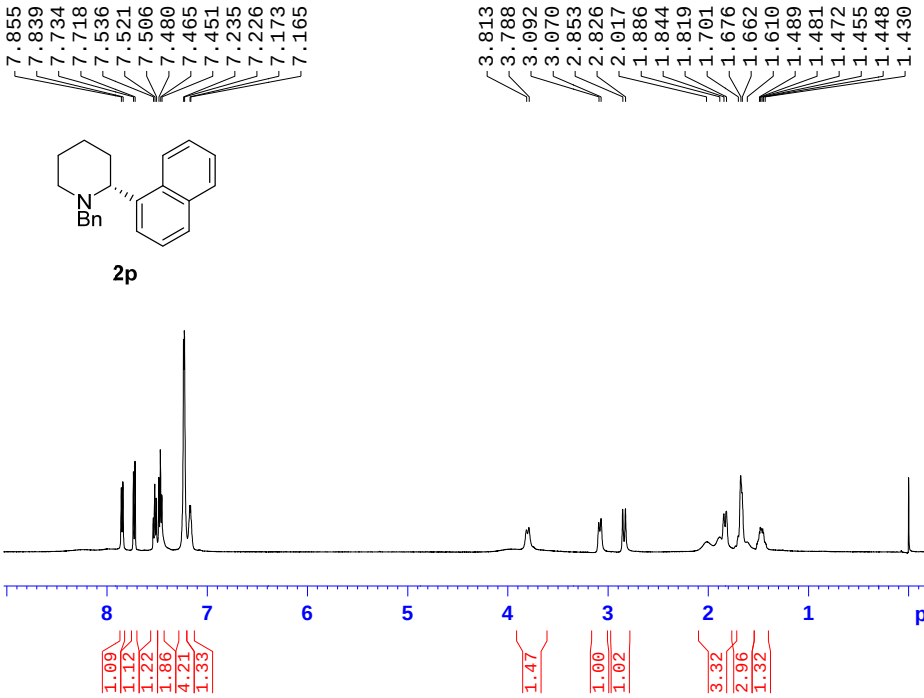

```
Current Data Parameters
NAME          10933-177
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20161110
Time               4.38
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg
TD               262144
SOLVENT           CDCl3
NS                 1500
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                299.1 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         125.7698617 MHz
NUC1                13C
P1                10.00 usec
PLW1         99.50000000 W

======== CHANNEL f2 ========
SFO2         500.1325007 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         18.79999924 W
PLW12         0.57574999 W
PLW13         0.28960001 W

F2 - Processing parameters
SI               131072
SF           125.7577653 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.40
```

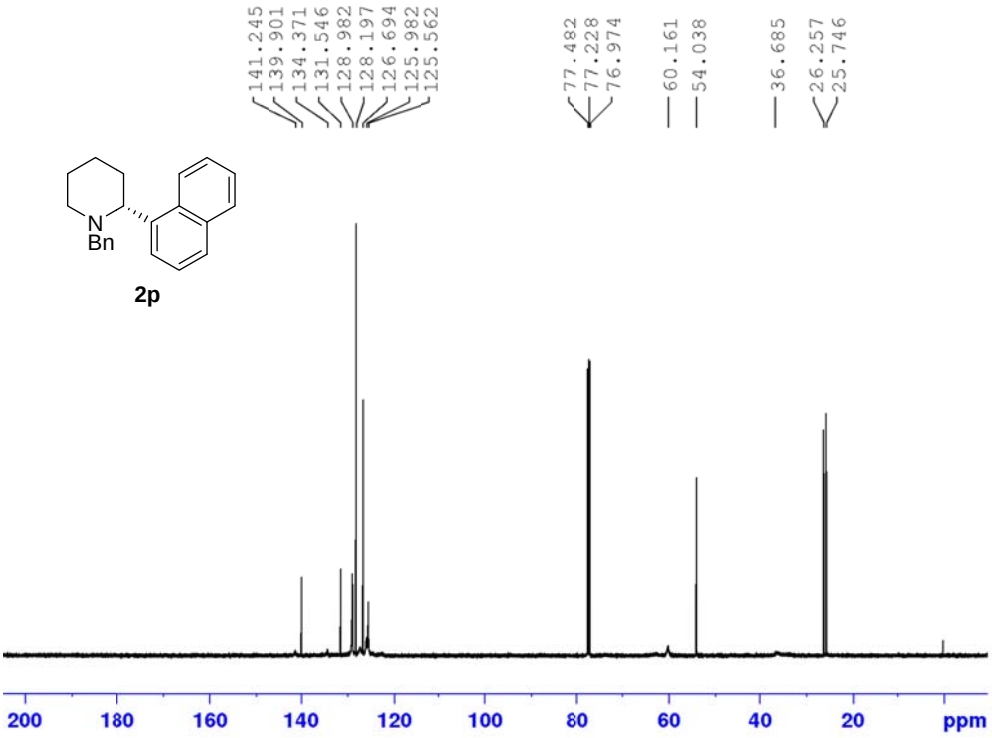



```
Current Data Parameters
NAME         10967-099-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170404
Time              21.03
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg10
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7500.000 Hz
FIDRES         0.228882 Hz
AQ           2.1845334 sec
RG                  287
DW               66.667 usec
DE                6.50 usec
TE               299.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.1325007 MHz
NUC1                   1H
P1                 11.75 usec
PLW1         18.39999962 W

F2 - Processing parameters
SI                 16384
SF           500.1300230 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



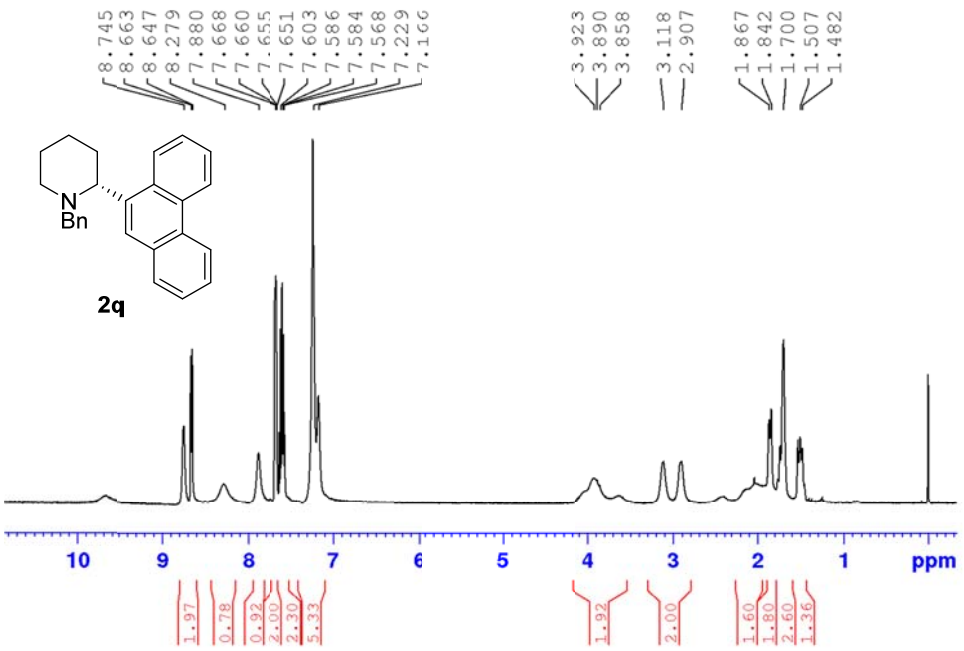

```
Current Data Parameters
NAME         10967-099-1
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170405
Time      0
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg
TD               262144
SOLVENT           CDCl3
NS                 2000
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
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7698617 MHz
NUC1                  13C
P1                 9.75 usec
PLW1        126.00000000 W

======== CHANNEL f2 ========
SFO2         500.1325007 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         18.39999952 W
PLW12         0.41056001 W
PLW13         0.20651001 W

F2 - Processing parameters
SI                131072
SF           125.7577645 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.40
```

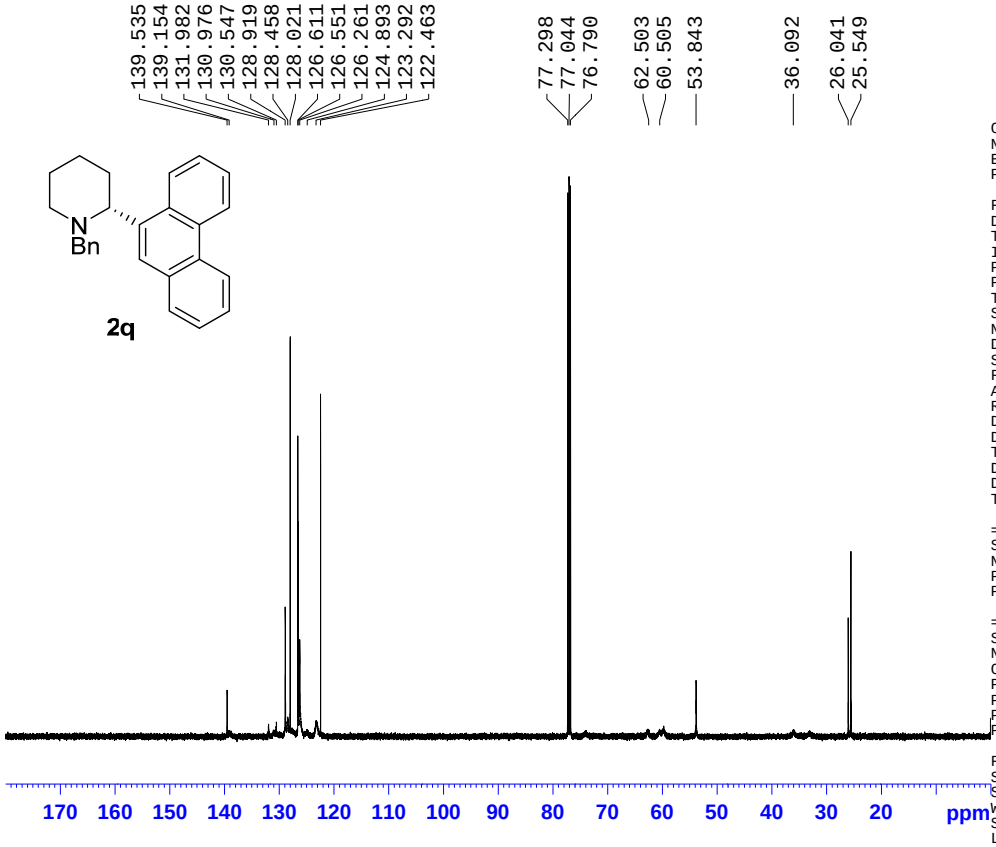



```
Current Data Parameters
NAME           10967-052
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_          20170113
Time               16.29
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH          7500.000 Hz
FIDRES       0.228882 Hz
AQ           2.1845334 sec
RG                  362
DW           66.667 usec
DE            6.50 usec
TE               299.0 K
D1          1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1       500.1325007 MHz
NUC1               1H
P1              14.00 usec
PLW1       18.79999924 W

F2 - Processing parameters
SI                 16384
SF         500.1300257 MHz
WDW                EM
SSB       0
LB              0.30 Hz
GB        0
PC                 1.00
```



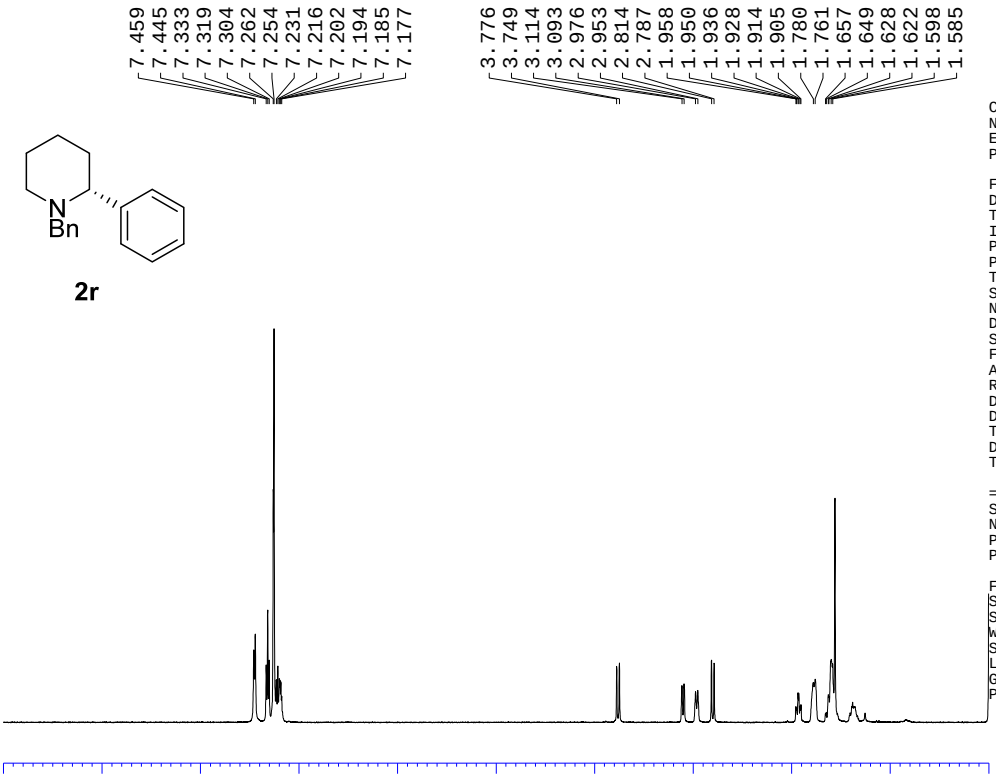

```
Current Data Parameters
NAME           10967-052
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_          20170114
Time               16.34
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg
TD               262144
SOLVENT           CDCl3
NS                 1500
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
TD0                    1

======== CHANNEL f1 ========
SFO1       125.7698617 MHz
NUC1               13C
P1              10.00 usec
PLW1        99.50000000 W

======== CHANNEL f2 ========
SFO2       500.1325007 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2           80.00 usec
PLW2       18.79999924 W
PLW12       0.57574999 W
PLW13       0.28960001 W

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

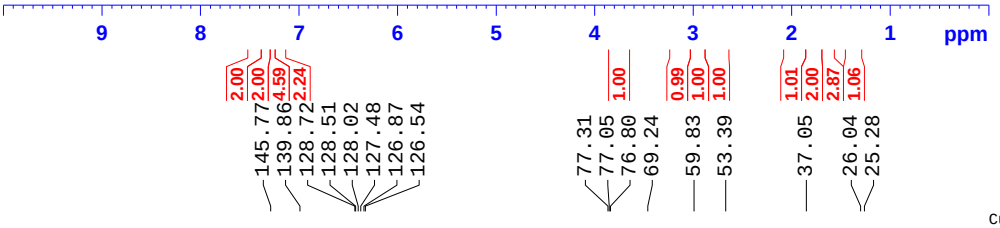


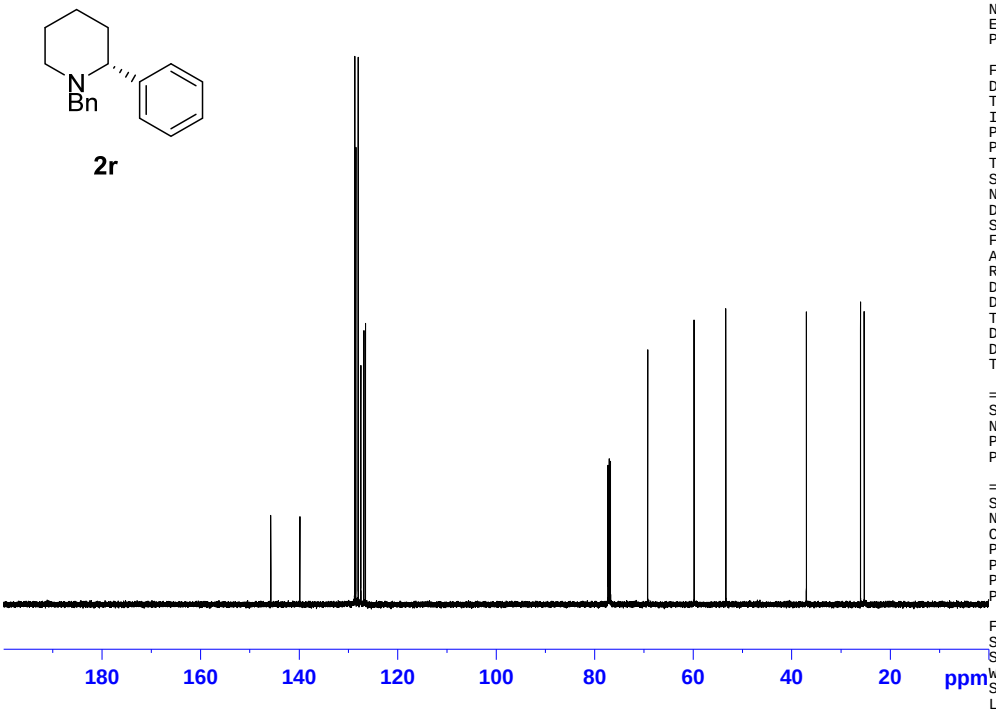

```
Current Data Parameters
NAME     bqu1-10967-170
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20180201
Time              14.28
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg10
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7500.000 Hz
FIDRES         0.228882 Hz
AQ           2.1845334 sec
RG                  645
DW                66.667 usec
DE                 6.50 usec
TE                299.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         500.1325007 MHz
NUC1                 1H
P1                14.00 usec
PLW1         16.00000000 W

F2 - Processing parameters
SI                16384
SF           500.1300143 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```





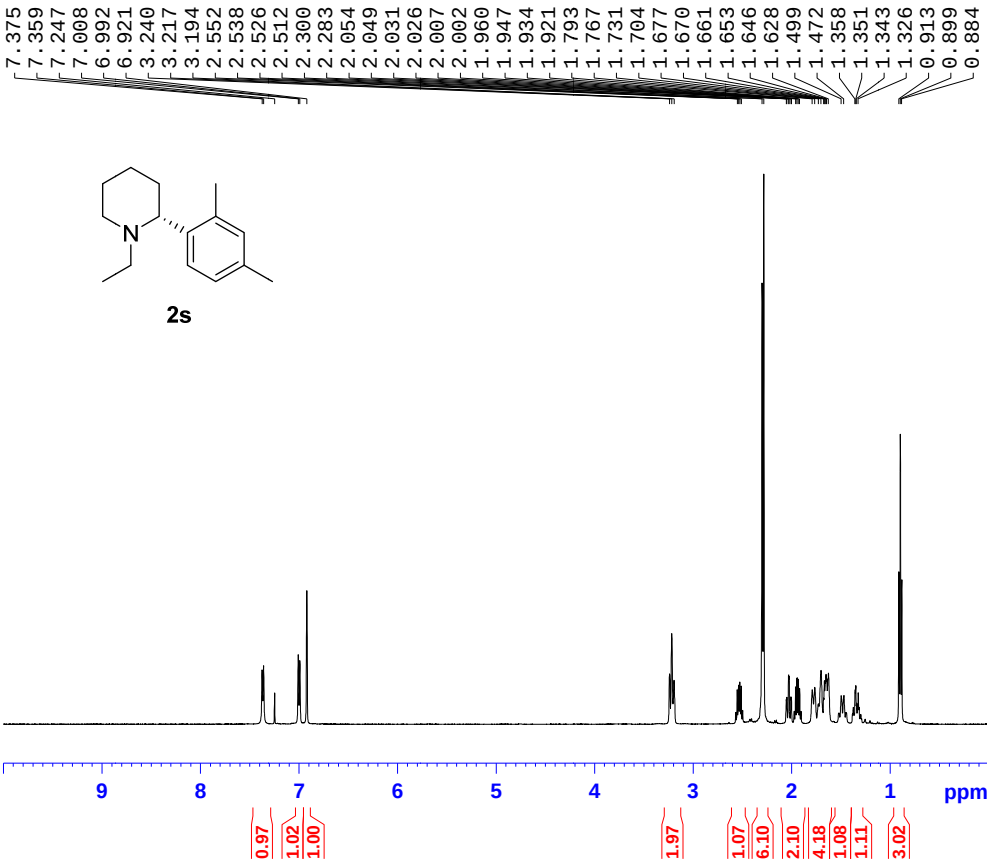

```
Current Data Parameters
NAME     bqu1-10967-170
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20180201
Time              14.58
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg
TD               262144
SOLVENT           CDCl3
NS                  256
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
TD0                   1

======== CHANNEL f1 ========
SFO1         125.7698617 MHz
NUC1                 13C
P1                10.00 usec
PLW1         99.50000000 W

======== CHANNEL f2 ========
SFO2         500.1325007 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         16.00000000 W
PLW12         0.49000001 W
PLW13         0.24647000 W

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

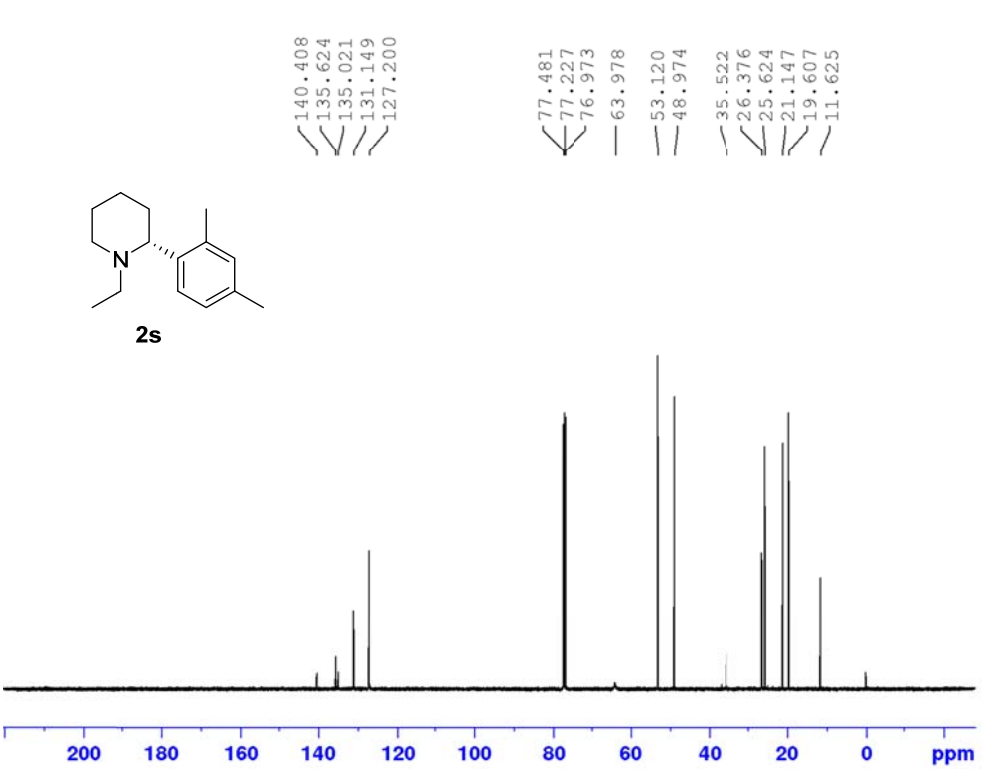



```
Current Data Parameters
NAME       bqu1-35793-4
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20171219
Time               17.21
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg10
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             7500.000 Hz
FIDRES          0.228882 Hz
AQ            2.1845334 sec
RG                   228
DW                66.667 usec
DE                 6.50 usec
TE                299.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.1325007 MHz
NUC1                   1H
P1                 14.00 usec
PLW1        16.00000000 W

F2 - Processing parameters
SI                 16384
SF           500.1300182 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```




```
Current Data Parameters
NAME          10967-151
EXPNO                 2
PROCNO                1

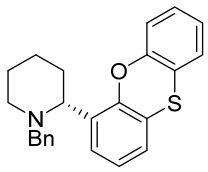
F2 - Acquisition Parameters
Date_           20170413
Time               2.19
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg
TD                262144
SOLVENT            CDCl3
NS                  1500
DS                     0
SWH            31250.000 Hz
FIDRES          0.119209 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
TD0                    1

======== CHANNEL f1 ========
SFO1        125.7698617 MHz
NUC1                  13C
P1                 9.75 usec
PLW1       126.00000000 W

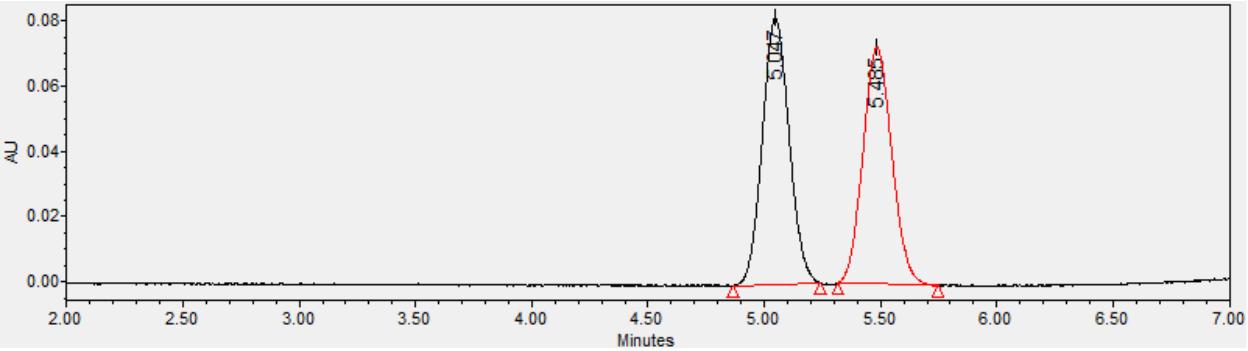
======== CHANNEL f2 ========
SFO2         500.1325007 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2        18.39999952 W
PLW12        0.41056001 W
PLW13        0.20651001 W

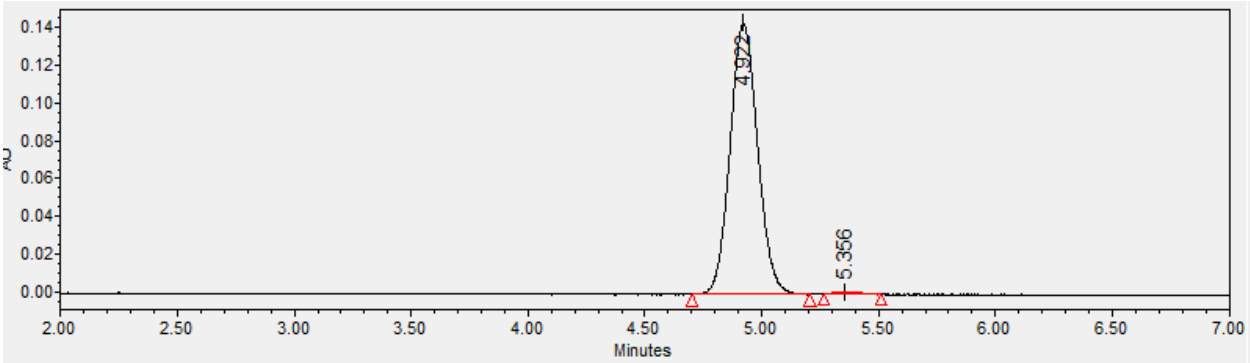
F2 - Processing parameters
SI                131072
SF           125.7577630 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.40
```

HPLC Spectra:



2a





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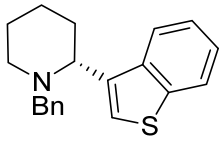
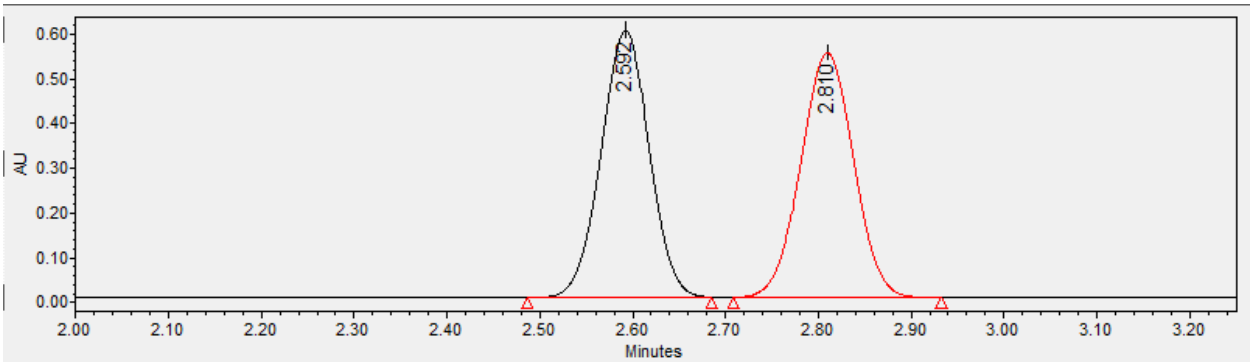
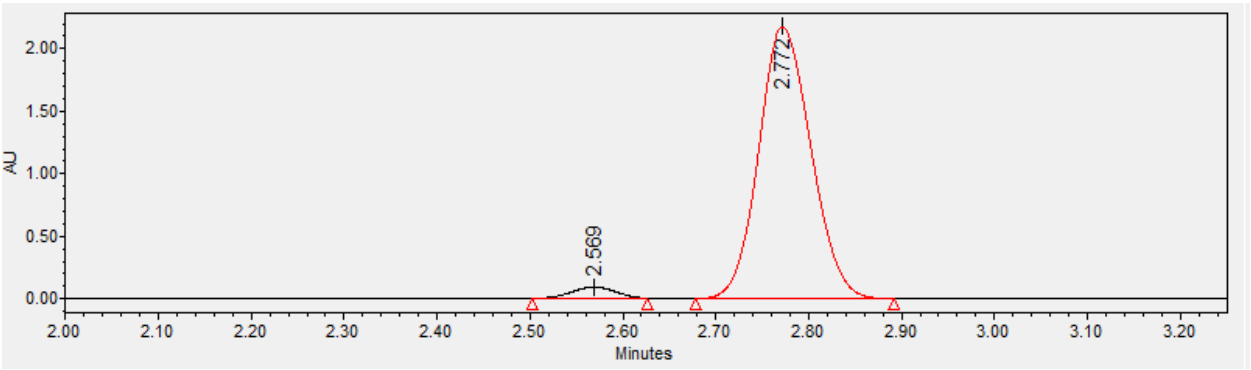
1	4.922	1170432	99.31	142769
2	5.356	8166	0.69	1268

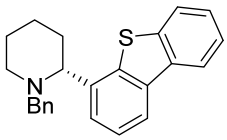


2b

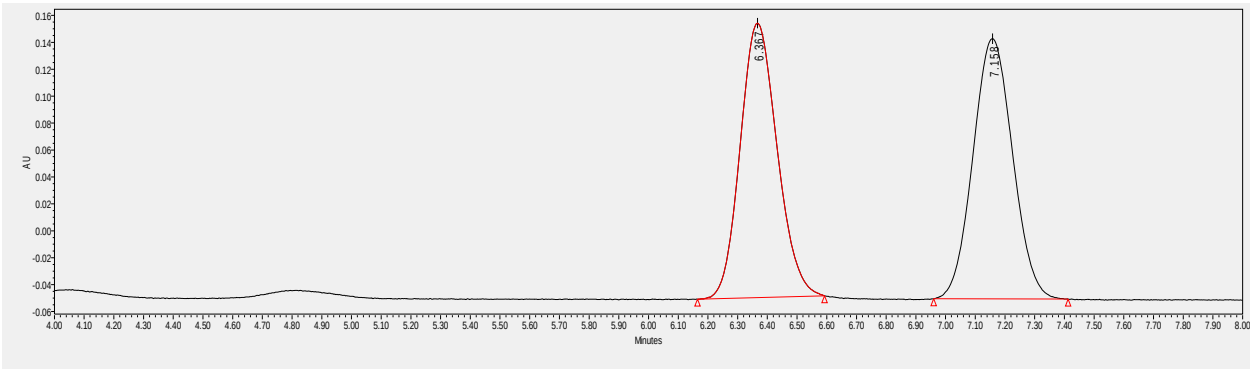


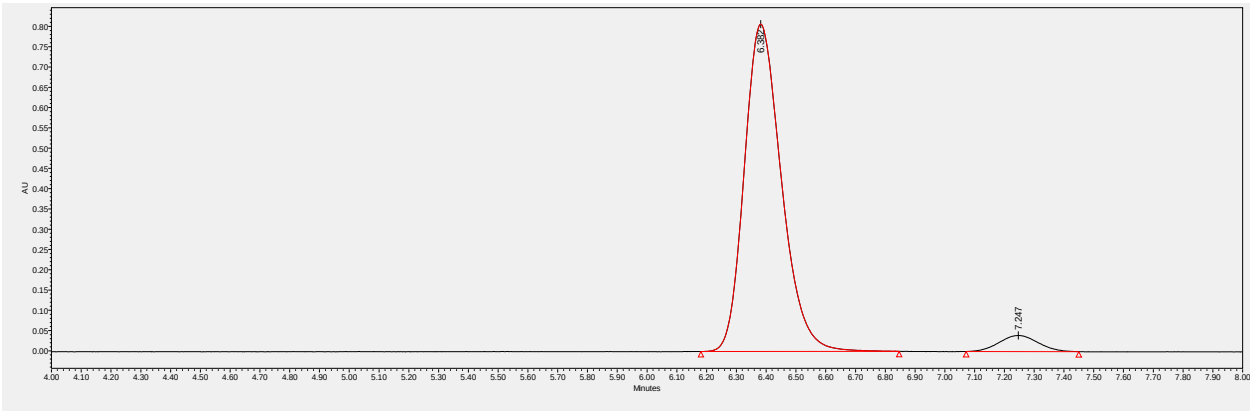


	RT	Area	% Area	Height
1	2.569	301912	3.41	91273
2	2.772	8549875	96.59	2171814

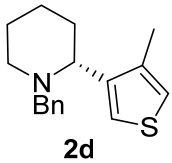


2c



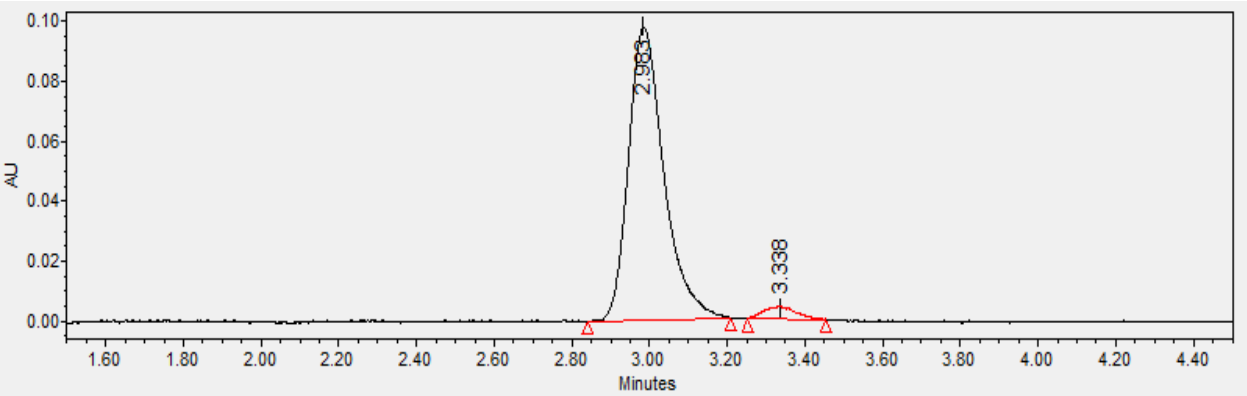


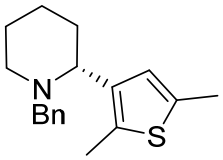
	RT	Area	% Area	Height
1	6.382	6986628	95.08	807349
2	7.247	361667	4.92	39736


N
Bn
S

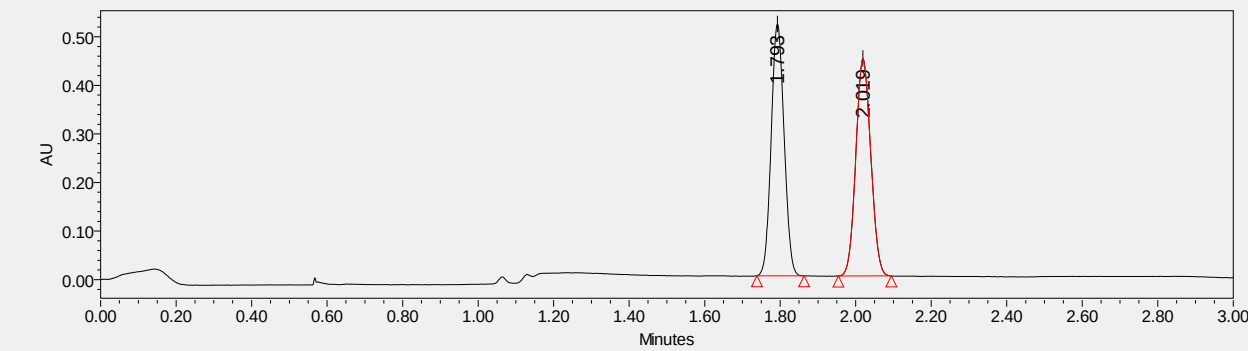
2d

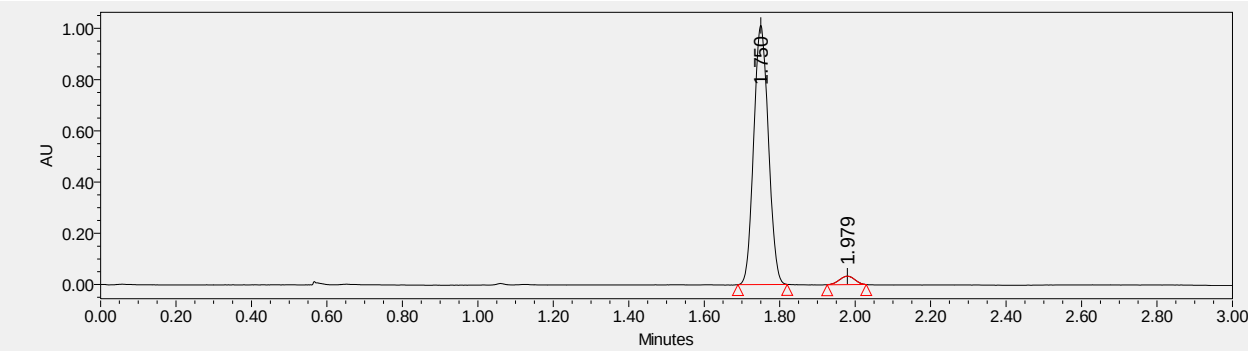
96.4:3.6 er


0.10
0.08
0.06
0.04
0.02
0.00
AU
2.983
3.338
1.60
1.80
2.00
2.20
2.40
2.60
2.80
3.00
3.20
3.40
3.60
3.80
4.00
4.20
4.40
Minutes

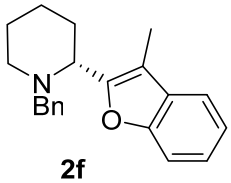


2e

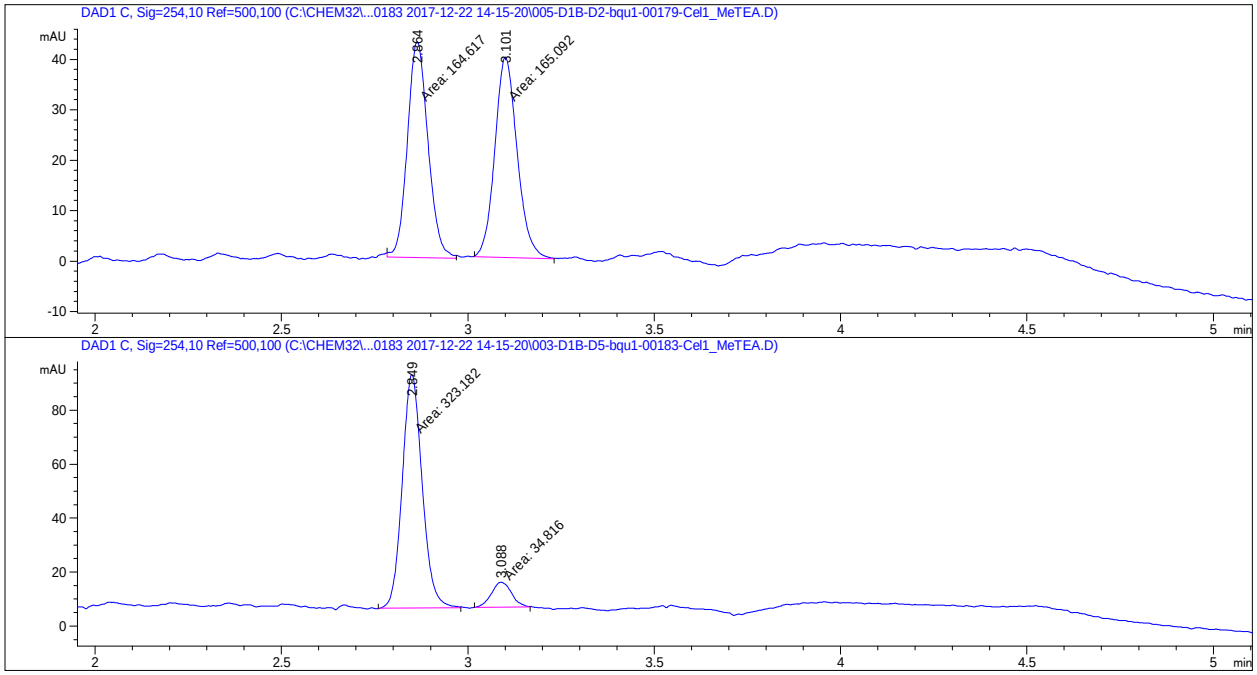




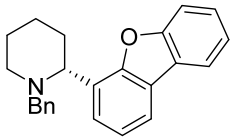
	RT	Area	% Area	Height
1	1.750	2635222	96.70	973469
2	1.979	89900	3.30	31745



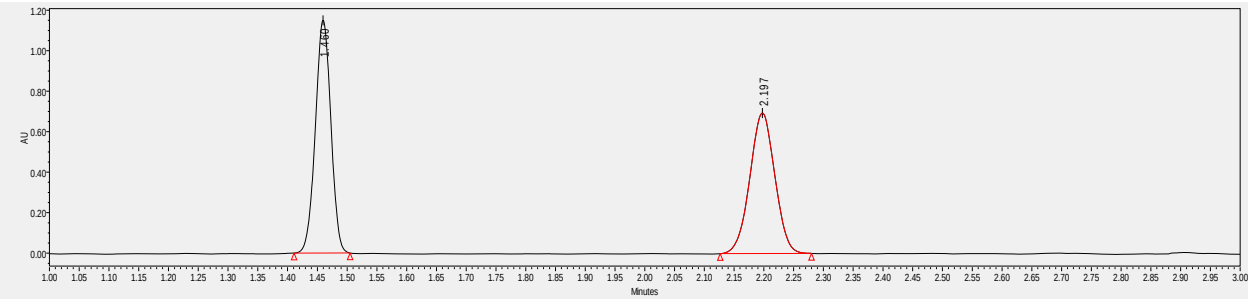
2f

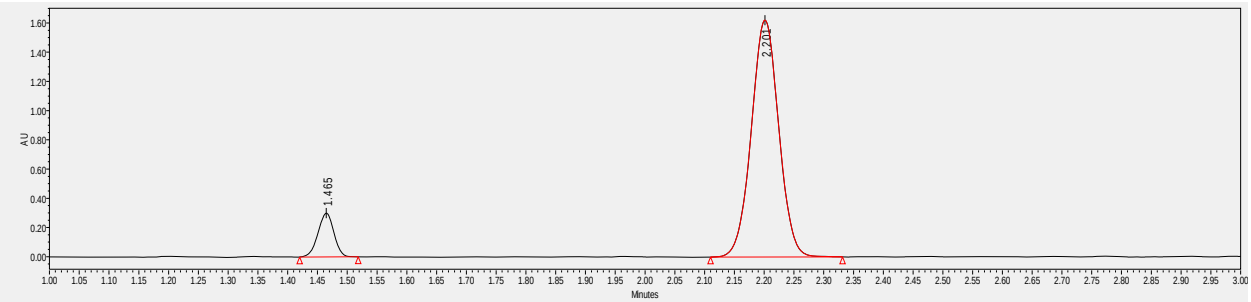


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.849	MM	0.0621	323.18152	86.66904	90.2748
2	3.088	MM	0.0627	34.81601	9.25409	9.7252

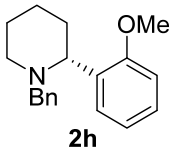


2g

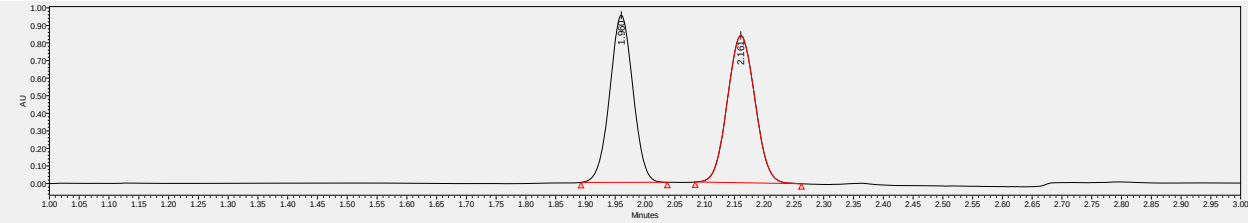


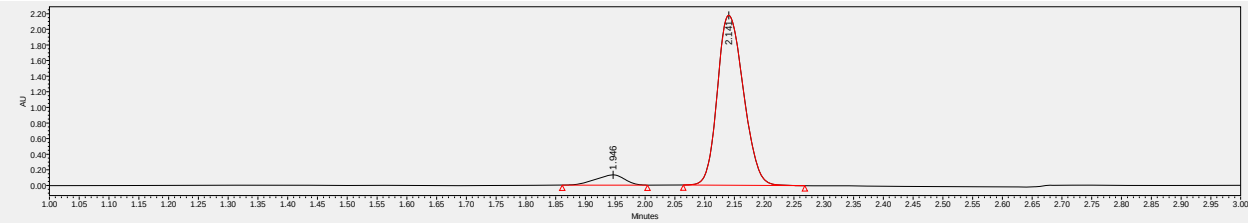


	RT	Area	% Area	Height
1	1.465	556314	9.71	300047
2	2.201	5172635	90.29	1621413



2h





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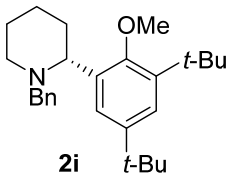
2	2.141	6622939	93.69	2176127



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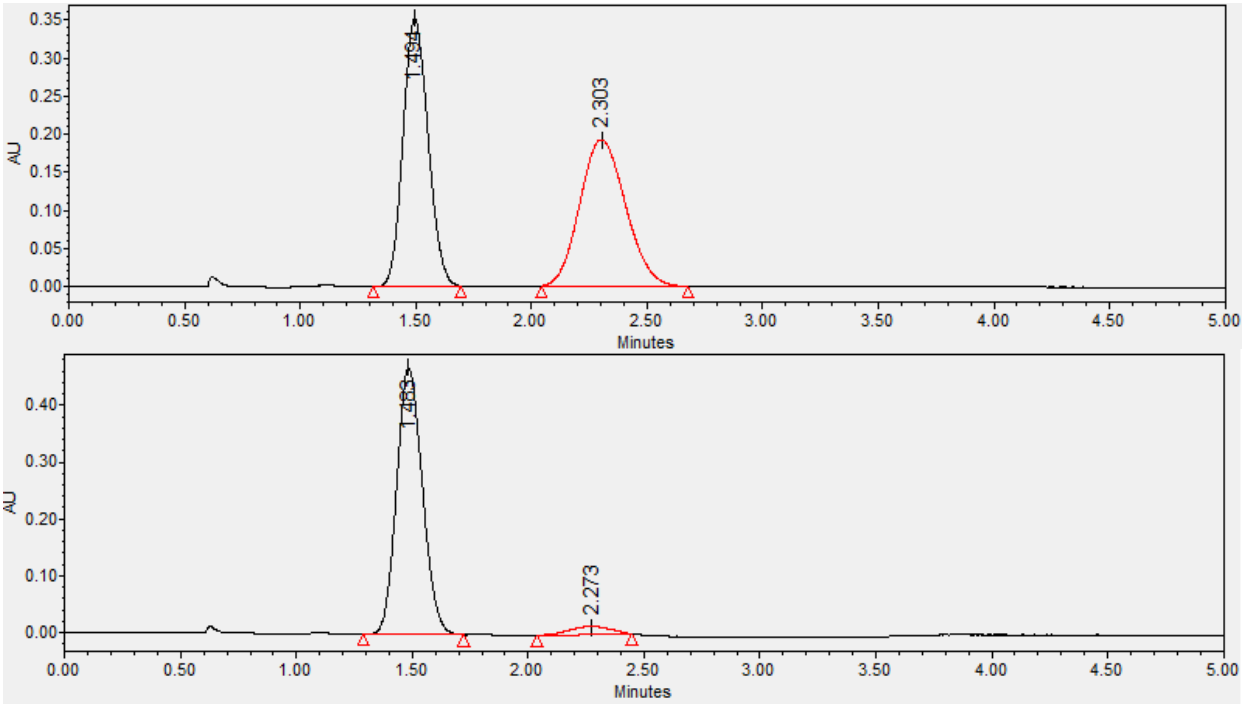

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1	1.483	3621779	95.27	468227
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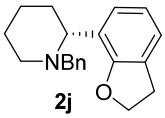

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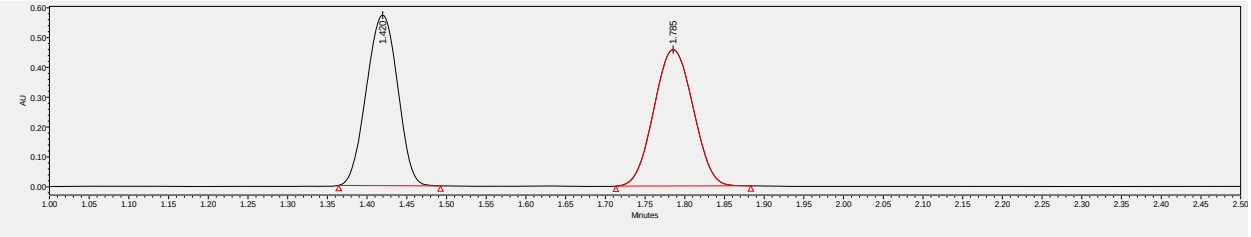

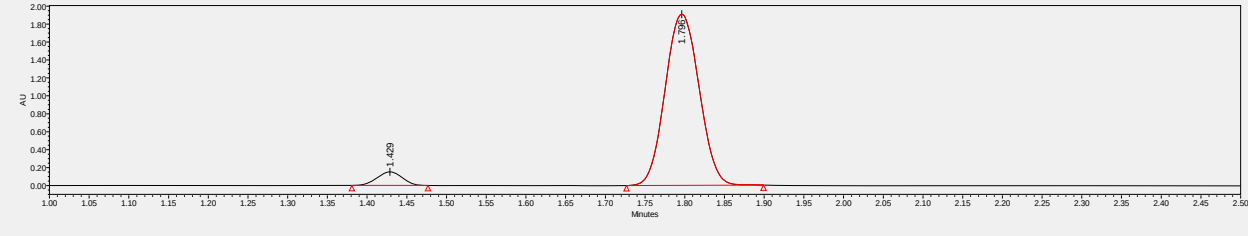

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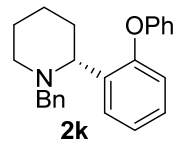
1	1.429	333888	5.55	151696
2	1.796	5679565	94.45	1908871



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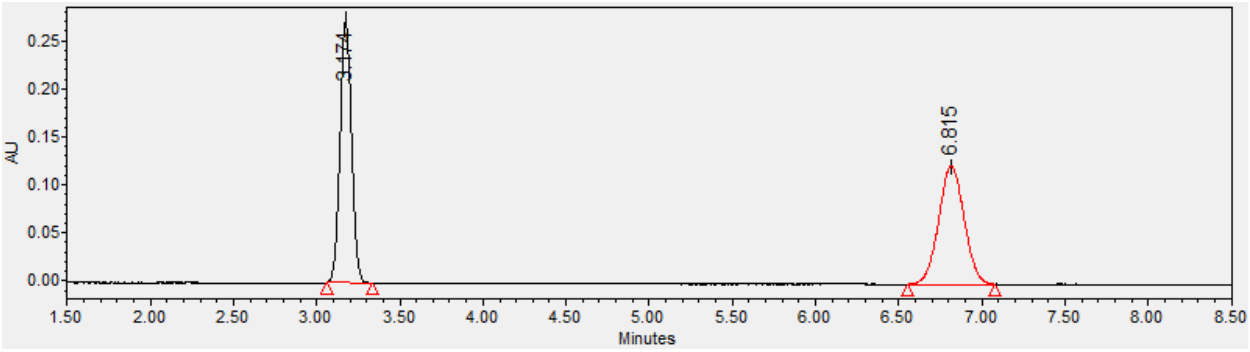

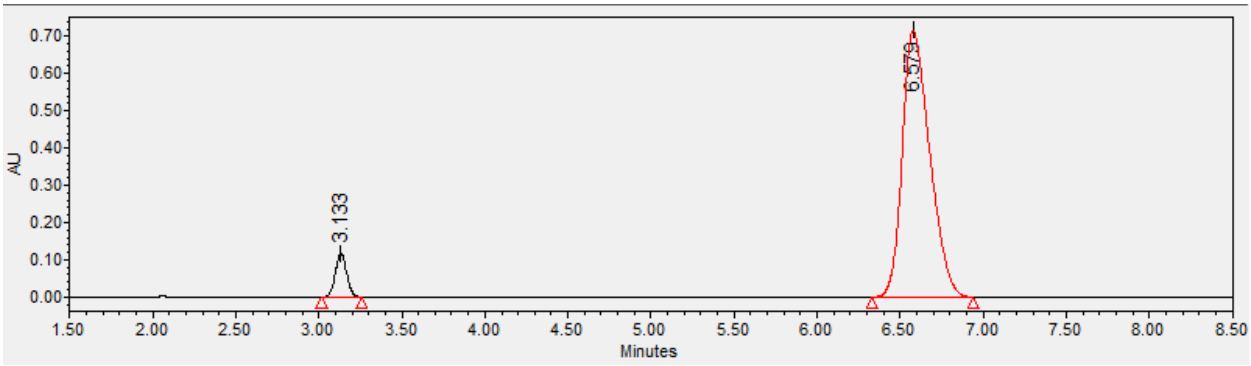

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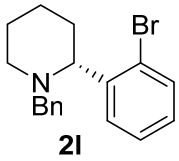
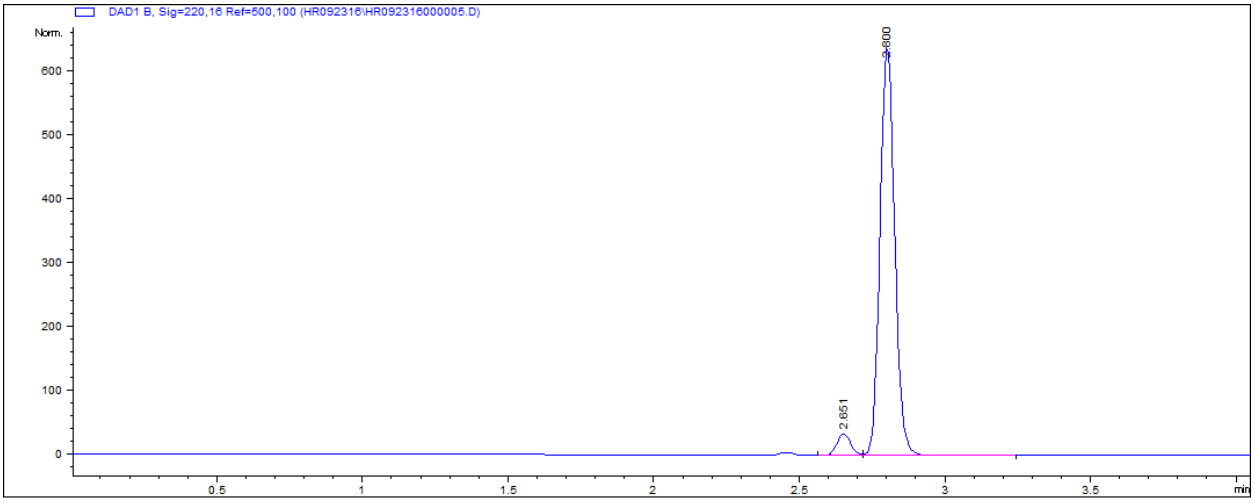

Br
N
Bn

2l

95.5:4.5 er


DAD1 B, Sig=220,16 Ref=500,100 (HR092316\HR092316000005.D)
Norm.
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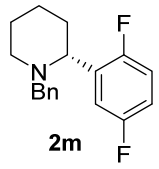
1
1.5
2
2.5
3
3.5
min



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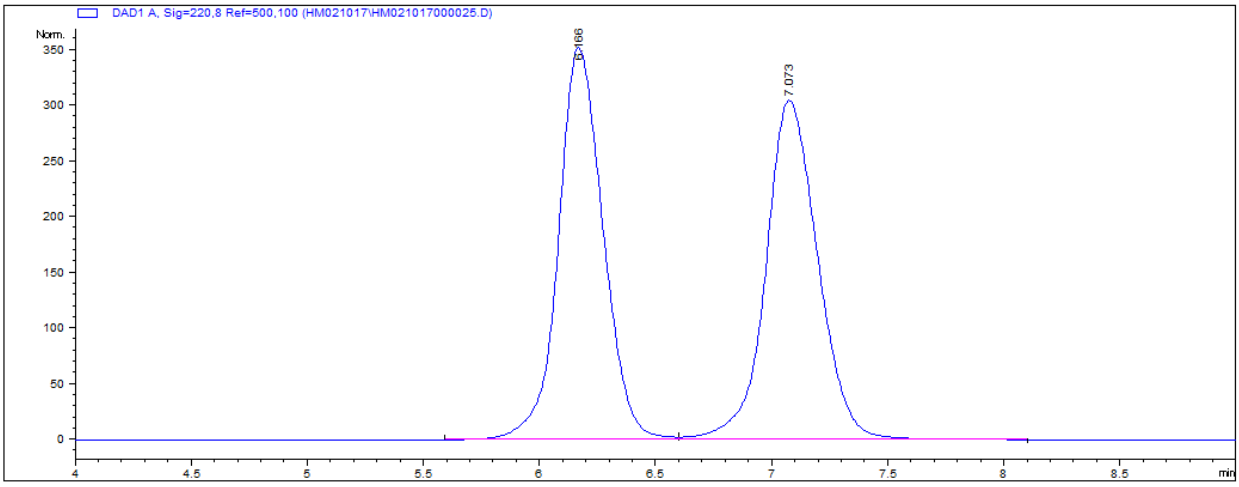
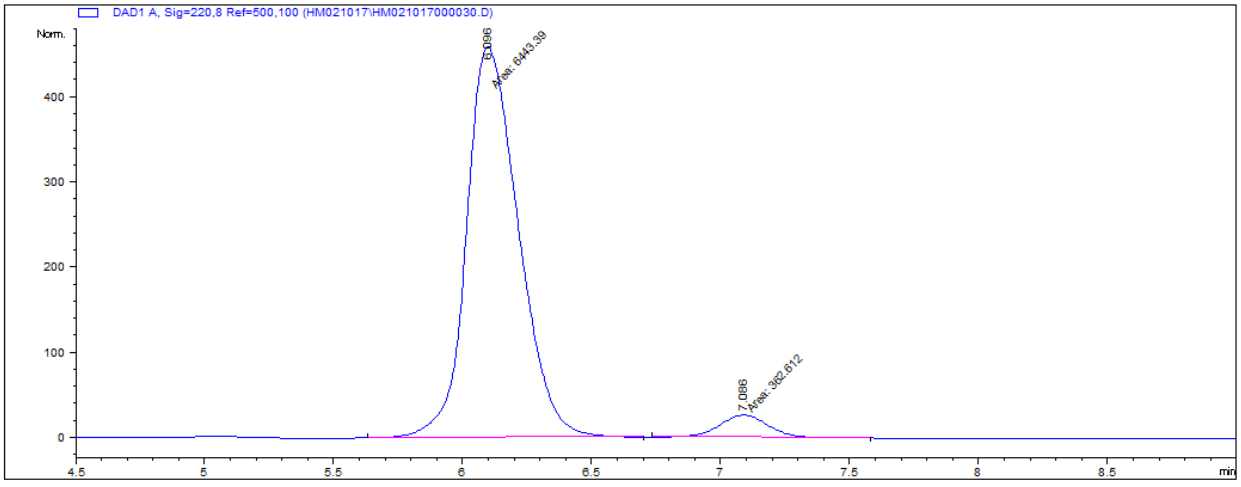
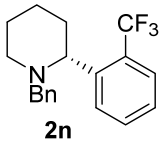




#	Time	Area	Height	Width	Area%	Symmetry
1	6.096	6443.4	459	0.234	94.672	0.7
2	7.086	362.6	26.5	0.2279	5.328	0.928



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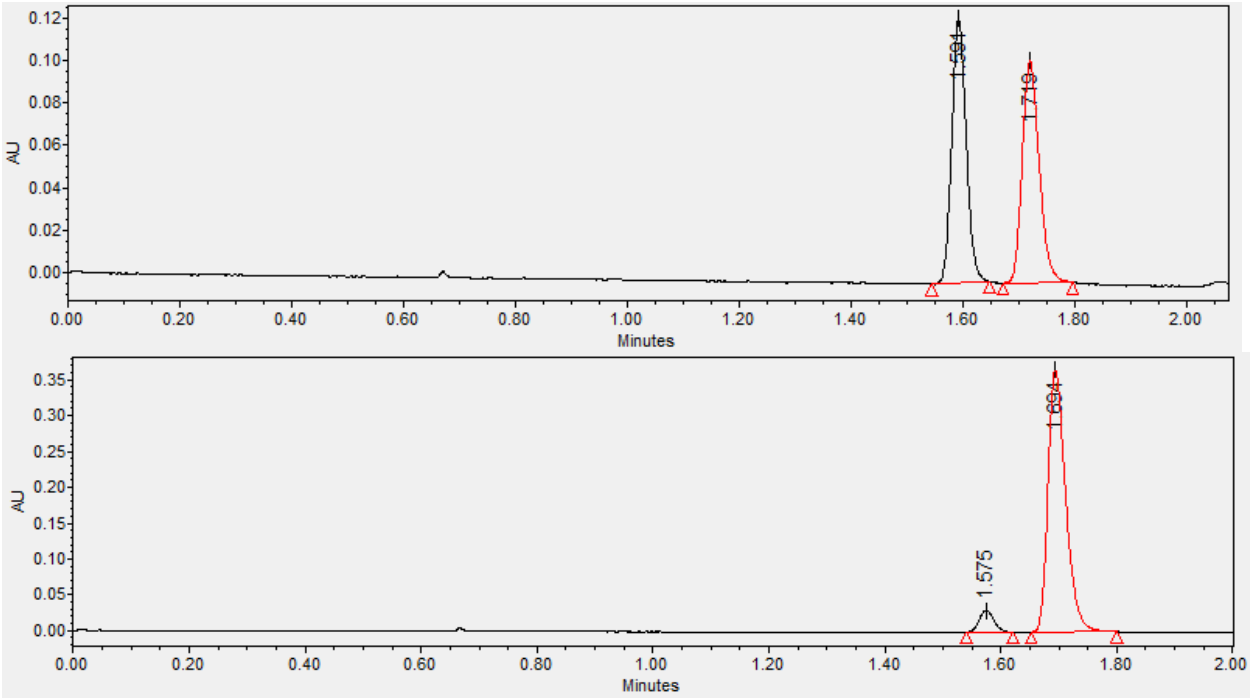

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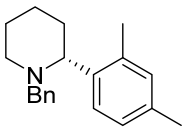
1	1.575	54068	6.53	30567
2	1.694	773491	93.47	365132



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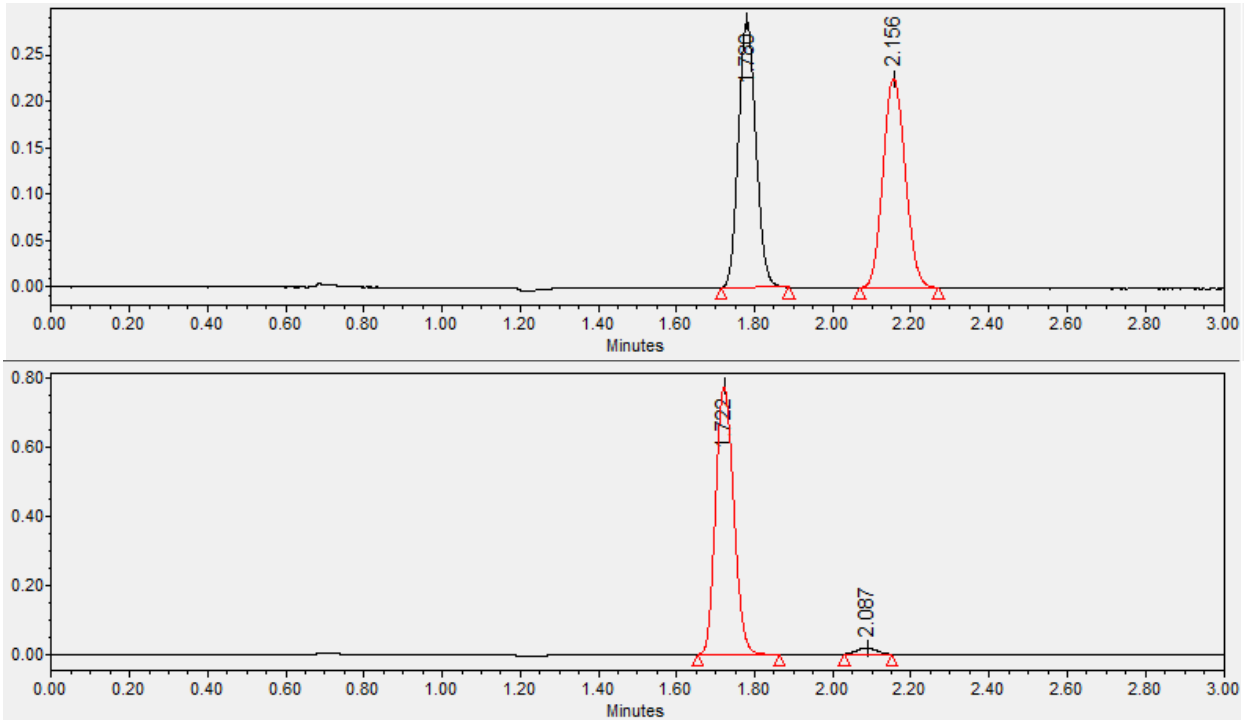

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1	1.722	2480156	97.66	771624
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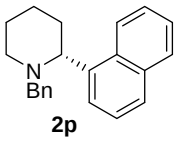

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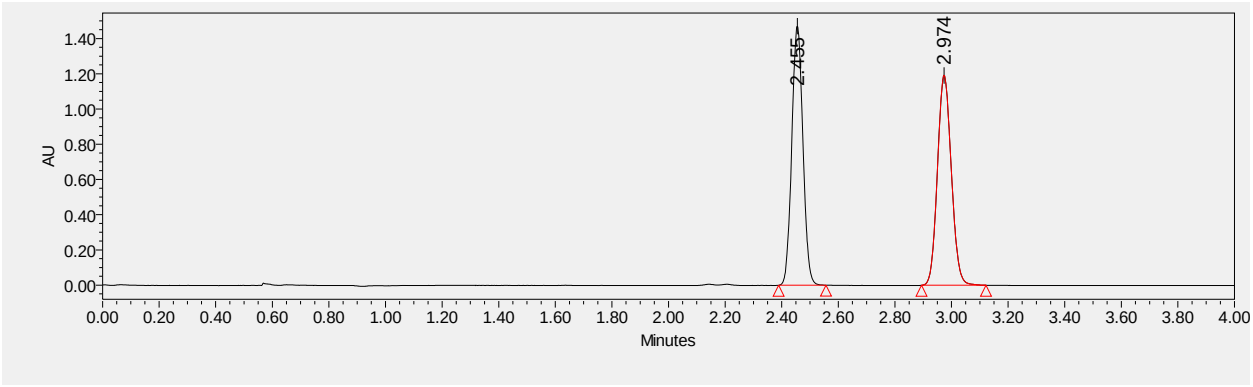

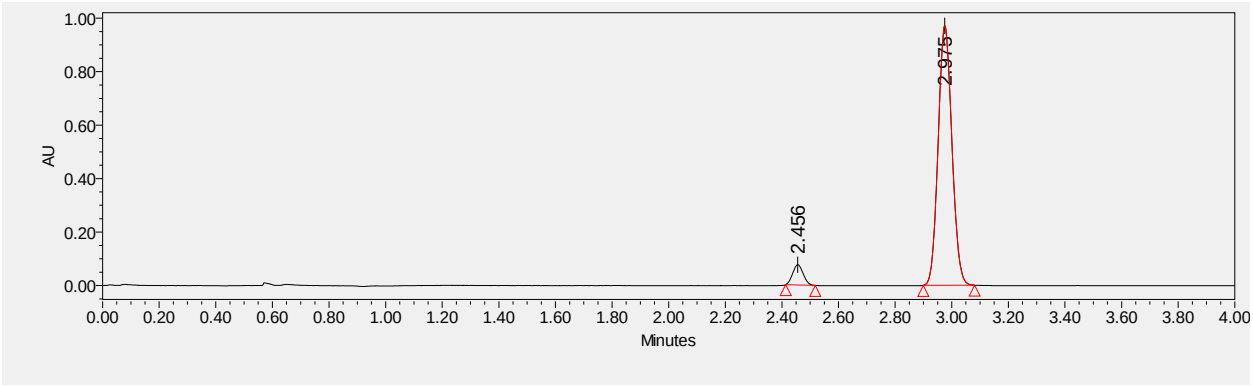

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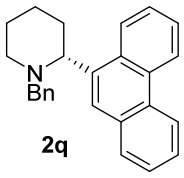
1	2.456	203030	5.82	77365
2	2.975	3282748	94.18	971211



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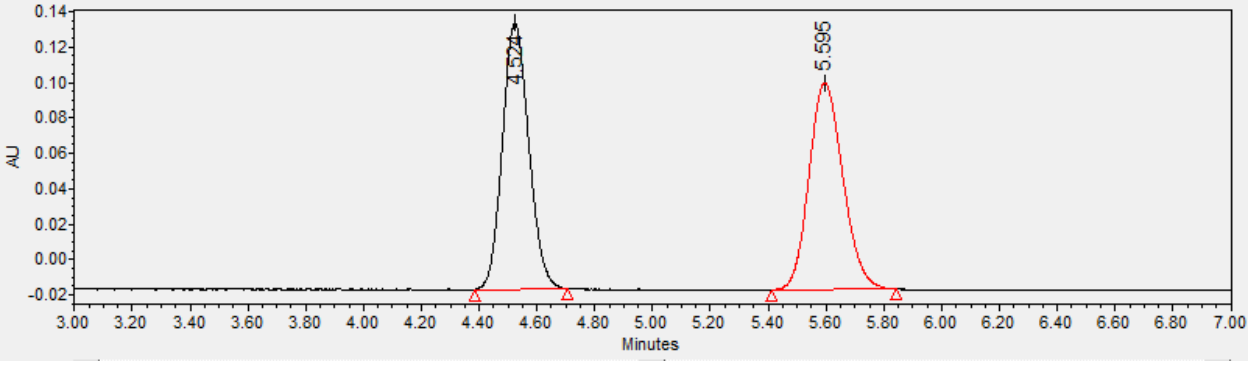
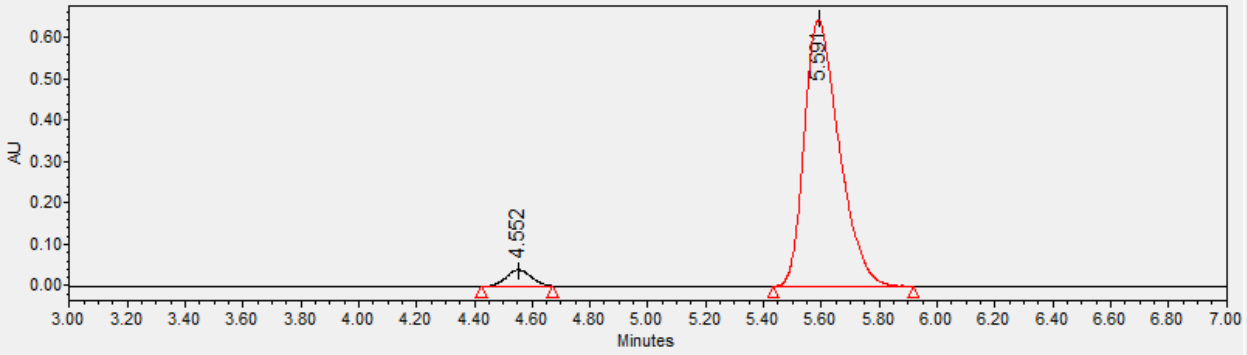
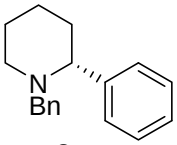




	RT	Area	% Area	Height
1	4.552	319546	4.42	50819
2	5.590	6913569	95.58	823284



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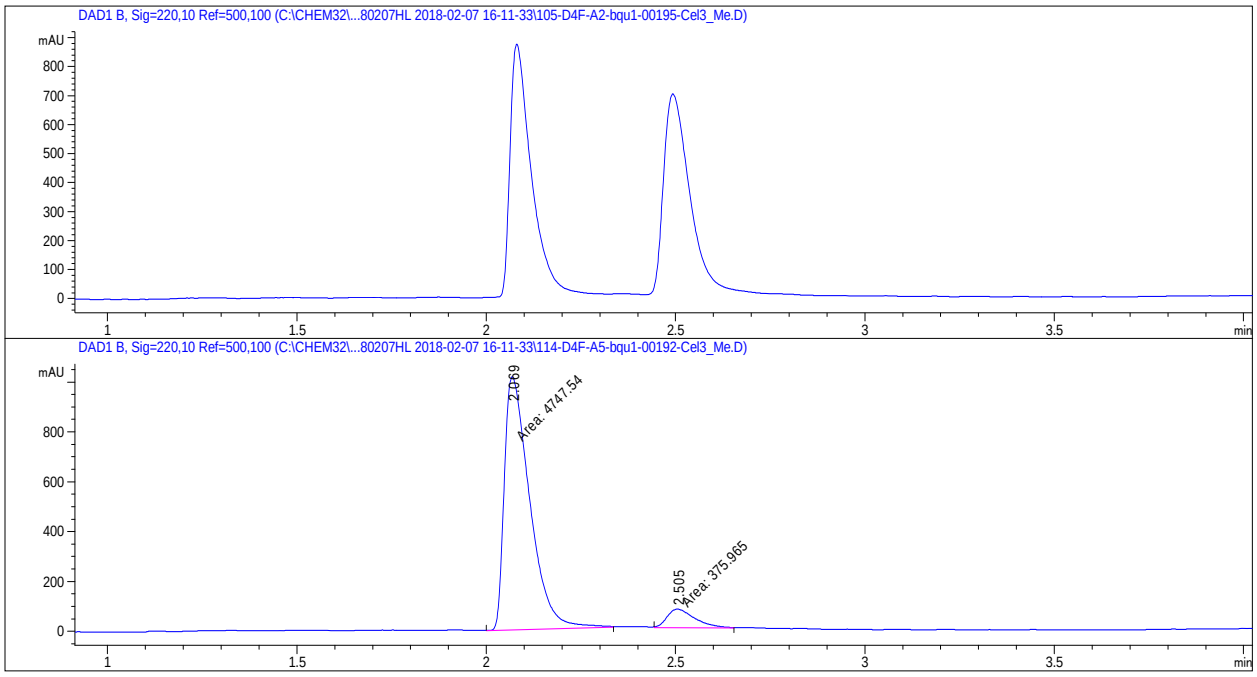
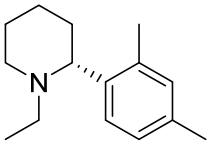


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.069	MM	0.0779	4747.54297	1015.71893	92.6620
2	2.505	MM	0.0845	375.96524	74.12060	7.3380



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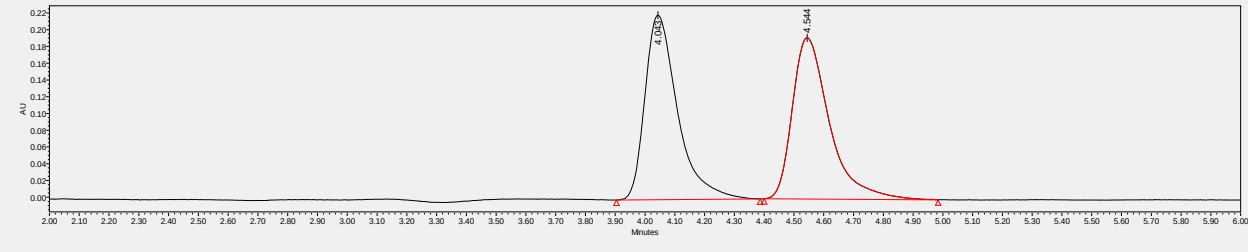
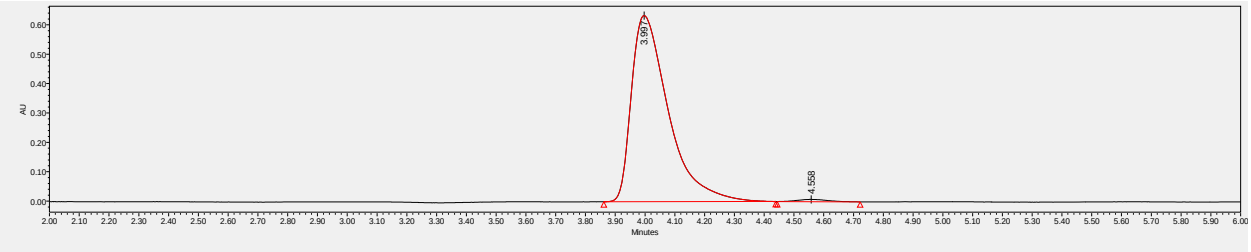
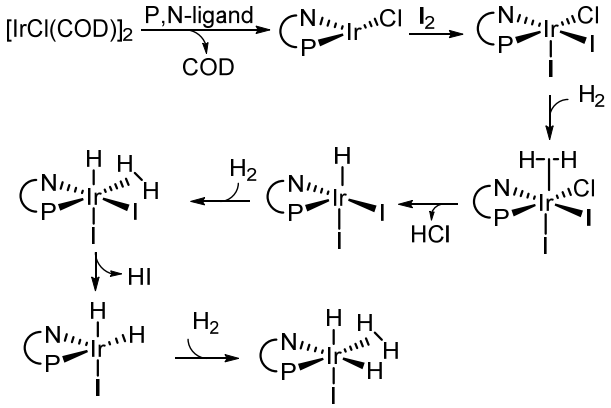




	RT	Area	% Area	Height
1	3.997	5454632	99.01	633510
2	4.558	54288	0.99	7757

Proposed Generation of the Ir-H Species[1]



[1] Saidi O., Williams J.M.J. (2011) Iridium-Catalyzed Hydrogen Transfer Reactions. In: Andersson P. (eds) Iridium Catalysis. Topics in Organometallic Chemistry, vol 34. Springer, Berlin, Heidelberg

Details of Computational Studies

Optimizations of intermediates and transition states were performed using Gaussian 09[1] software with spin-restricted DFT using PBE[2] functional and split basis set (6-31G(d) for C, P, N, O, H and LANL2DZ for Ir and I) in the gas phase. For all species, vibrational frequencies were also computed at the specified level of theory to obtain thermal Gibbs Free Energy 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 were performed on optimized geometries in THF solvent using the PCM[3]-solvation model, PBE functional including Grimme dispersion correction D2[4], and split basis set (6-311+G(d,p) for C, P, N, O, H; LANL2DZ for I and LANL2DZ (f) for Ir).[5] Obtained single-point energies were converted to the enthalpies and Gibbs free energies using corrections from gas-phase frequency analysis. Extensive conformational analysis of the transition states and intermediates was performed manually.

Example of the input file specifying basis set used in single-point:

```
# rpbepbe/gen pseudo=read extrabasis scrf=(iefpcm,solvent=TetraHydroFuran) empiricaldispersion=GD2

Title Card Required
0 1
COORDINATES

C H P O N 0
6-311G(d,p)
****
Ir I 0
Lanl2dz
****
Ir 0
F 1 1.0
0.938 1.0
****
Ir I 0
Lanl2dz
```

S2. Coordinates and thermochemical data for computed intermediates and transition states

[1] Gaussian 09, Revision D.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, 2013.

[2] Perdew, J. P., Burke, K., Ernzerhof, M. *Phys. Rev. Lett.,* **1996***, 77,* 3865*;* [2] Perdew, J. P., Burke, K., Ernzerhof, M. *Phys. Rev. Lett.,* **1997***, 78,* 1396*;*

[3] Tomasi, J., Mennucci,B., Cammi, R. *Chem. Rev.*, **2005**, *105*, 2999.

[4] Grimme, S. *J. Comp. Chem.*, **2006**, *27*, 1787.

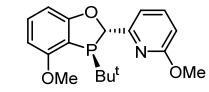
[5] Hopmann, K. H. *Organometallics*, **2016**, *35*, 3795.

S2. Coordinates and thermochemical data for computed intermediates and transition states

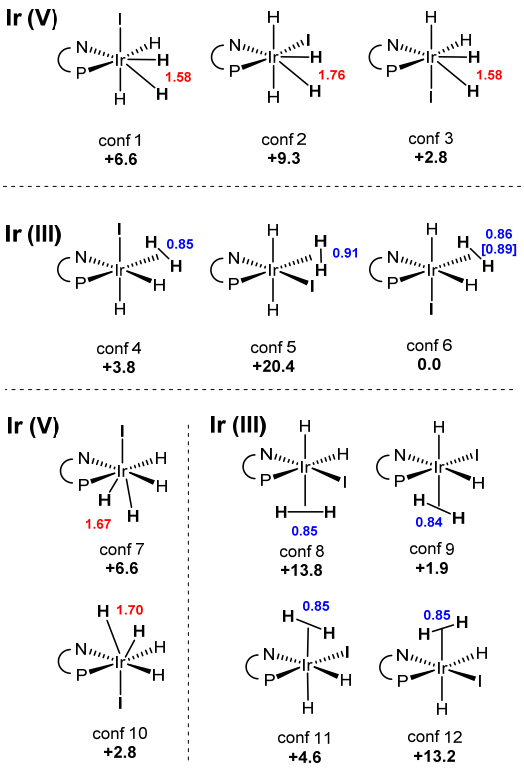
Conformational analysis of Ir complexes.

Multiple isomers were considered for the starting Ir-H_2 complex. Out of the analyzed isomers, lowest energy one was chosen for further computational study of the mechanism.

Starting $LIrIH_2(H)_2$ complexes



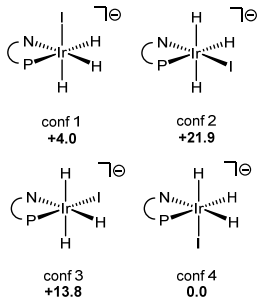
Conformational analysis:
pbe-d2/
C,N,H,O,P:6-31G(d),
Ir,I:lanl2dz;



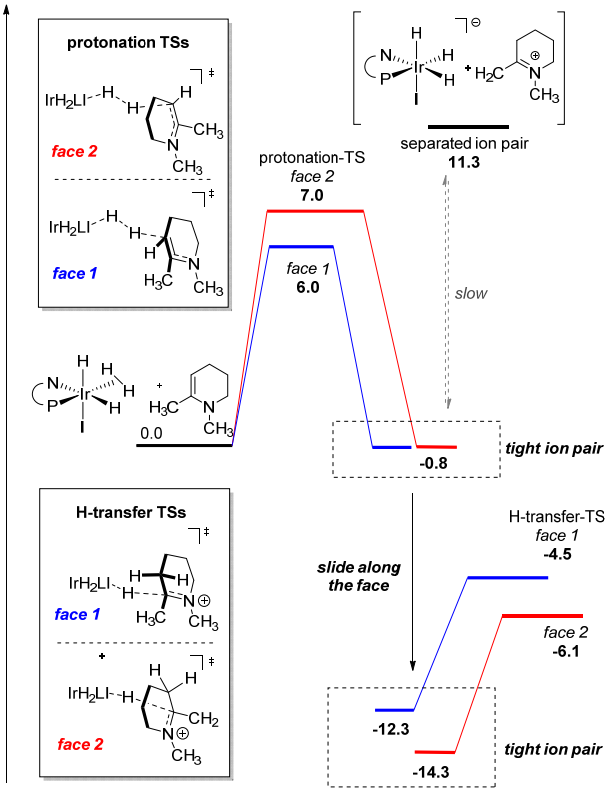
Similar analysis was performed for post-protonation Ir intermediates:

Pre-protonation $LIrIH_3$ complexes

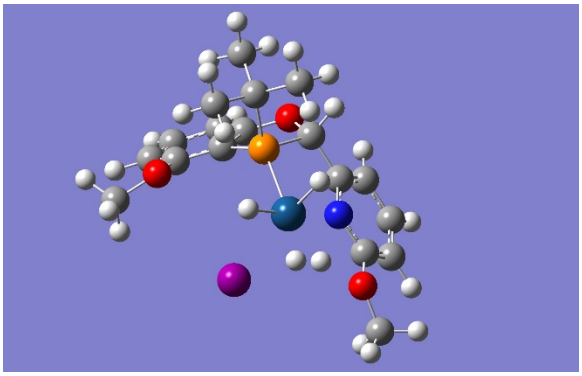
Ir (III) anions



Reaction diagram:



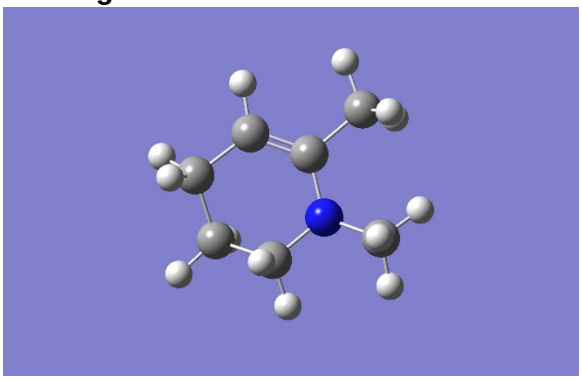
Starting Ir(III)-complex



Zero-point correction= 0.396543
(Hartree/Particle)
Thermal correction to Energy= 0.425064
Thermal correction to Enthalpy= 0.426009
Thermal correction to Gibbs Free Energy= 0.336782
Sum of electronic and zero-point Energies= -1437.703797
Sum of electronic and thermal Energies= -1437.675276
Sum of electronic and thermal Enthalpies= -1437.674332
Sum of electronic and thermal Free Energies= -1437.763559
Electronic energy -1438.50247257

C	-3.32377400	1.40751500	2.22031700
C	-2.72620600	1.08262300	0.98590800
C	-2.08573700	-0.16534700	0.84108500
C	-2.07550500	-1.07076800	1.91608900
C	-2.69170400	-0.78090500	3.13895600
C	-3.30413000	0.47298900	3.26779700
H	-3.80509000	2.37655000	2.36690600
H	-2.66666100	-1.50312800	3.95819500
H	-3.77815300	0.73739800	4.21867600
O	-2.74037500	1.87498900	-0.11870200
C	-3.00967900	3.26793400	0.06623600
H	-2.30732100	3.69950200	0.80049600
H	-2.84045100	3.73136500	-0.91538500
H	-4.05630400	3.44113300	0.38101700
O	-1.44465800	-2.28544700	1.72108000
C	-0.57562100	-2.23629700	0.56762300
P	-1.13850400	-0.82694200	-0.55956800
C	-2.40075500	-1.55791500	-1.78001400
C	-2.90674000	-0.39813400	-2.66163500
H	-3.66111500	-0.78497800	-3.37183400
H	-3.37181400	0.40033900	-2.06050800
H	-2.07964500	0.04690300	-3.23881600
C	-3.57049600	-2.19272100	-1.00351500
H	-4.28333800	-2.63140700	-1.72563200
H	-3.23850300	-3.00114600	-0.32851800
H	-4.11310700	-1.44753900	-0.39960600
C	-1.71054900	-2.61633000	-2.65863300
H	-0.85960800	-2.18962900	-3.21333900
H	-1.34442400	-3.47843900	-2.07263900
H	-2.44274000	-3.00493800	-3.39043400
C	0.86745100	-2.03220000	1.01648300
C	1.31872700	-2.69642000	2.16245200
C	2.64276900	-2.51295300	2.57245500
H	0.62328600	-3.32464400	2.72243700
C	2.95650900	-1.05259600	0.68091900
C	3.48033300	-1.68625800	1.82297400
H	3.02371300	-3.01272800	3.46832200
N	1.66464100	-1.20618500	0.28677600
Ir	0.76283000	0.05538800	-1.32026000
O	3.67714800	-0.24409700	-0.12303100
C	4.93878100	0.23763100	0.35333200
H	5.68121600	-0.57800200	0.42999800
H	4.81900900	0.74176100	1.32790900
H	5.27169300	0.96618700	-0.39809300
H	0.77888500	-1.10512500	-2.43696400
I	0.98568500	2.28989100	0.44094500
H	-0.04857100	0.94883400	-2.37245900
H	4.51909700	-1.52790300	2.11688900
H	-0.67253000	-3.21161100	0.05851100
H	1.96571100	0.95751300	-2.28038800
H	2.45368600	0.38937500	-1.85648400

Starting enamine

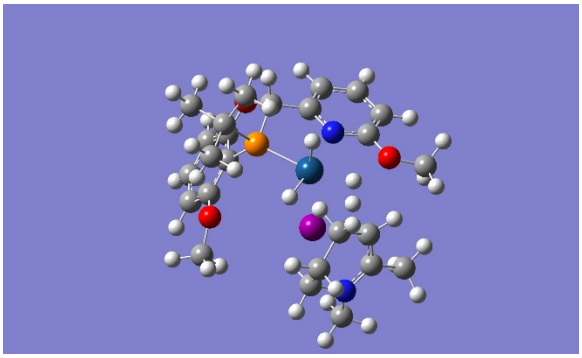


Zero-point correction= 0.186832
(Hartree/Particle)
Thermal correction to Energy= 0.195270
Thermal correction to Enthalpy= 0.196214
Thermal correction to Gibbs Free Energy= 0.154477
Sum of electronic and zero-point Energies= -328.668570
Sum of electronic and thermal Energies= -328.660132
Sum of electronic and thermal Enthalpies= -328.659188
Sum of electronic and thermal Free Energies= -328.700925
Electronic energy -328.95956467

C	-1.95618900	0.79054300	0.21618800
C	-1.89591100	-0.62419900	-0.38054400
H	-2.34868400	0.75115500	1.25435700
C	-0.66765300	-1.36998500	0.14663100
H	-1.82153900	-0.55968100	-1.48116900
H	-0.61891600	-2.38859700	-0.28120000
C	1.88630100	1.43595400	-0.14656400
H	2.58514500	1.17090800	0.66838600
H	1.72934900	2.52476300	-0.11116500
H	-0.74769200	-1.48520700	1.25362900
H	-2.80689900	-1.20174800	-0.14394200
H	-2.68341700	1.40477200	-0.34945200
N	0.57064800	-0.67540200	-0.21089000
C	1.76219300	-1.42650000	0.15656500

H	1.90828100	-1.51571500	1.25829300
H	2.66465600	-0.96761200	-0.27405000
H	2.39329300	1.19788100	-1.10037100
H	1.67815200	-2.44795200	-0.25367300
C	0.55967000	0.72472300	-0.03109700
C	-0.58975000	1.42449600	0.17162800
H	-0.51823300	2.51465400	0.23974500

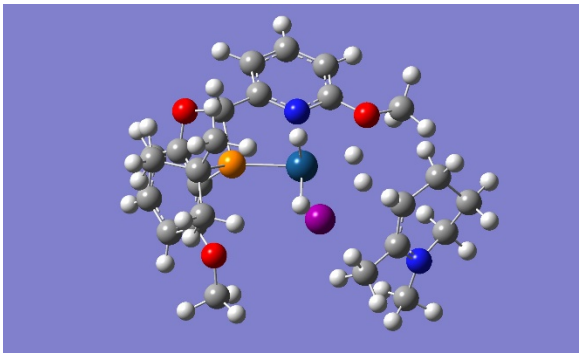
Protonation TS_face2



Zero-point correction= 0.583568
(Hartree/Particle)
Thermal correction to Energy= 0.621617
Thermal correction to Enthalpy= 0.622561
Thermal correction to Gibbs Free Energy= 0.511987
Sum of electronic and zero-point Energies= -1766.367063
Sum of electronic and thermal Energies= -1766.329015
Sum of electronic and thermal Enthalpies= -1766.328070
Sum of electronic and thermal Free Energies= -1766.438644
Electronic energy -1767.47146025

C	4.03919700	-0.00758600	1.37482400
H	2.51385200	0.51929900	1.08465300
C	-3.12509600	-2.43844100	-2.50985100
C	-2.36709200	-2.20373000	-1.34574800
C	-2.66221600	-1.08462100	-0.54201800
C	-3.71104600	-0.22629300	-0.91156000
C	-4.49654900	-0.45560700	-2.04879600
C	-4.17825400	-1.56896100	-2.83711300
H	-2.90396700	-3.29009500	-3.15678100
H	-5.30537200	0.23038500	-2.31146200
H	-4.76230000	-1.76453300	-3.74249300
O	-1.36067200	-3.01068000	-0.90157500
C	-0.75587500	-3.89047800	-1.84908000
H	-0.41128300	-3.32638500	-2.73383600
H	0.11176600	-4.32607000	-1.33283600
H	-1.44465500	-4.70163200	-2.15456600
O	-3.96009100	0.86296300	-0.10012900
C	-2.84879000	1.11299000	0.79433300
P	-1.78163000	-0.44430500	0.92041900
C	-2.46830000	-1.42348200	2.40606000
C	-1.64719900	-2.72502300	2.50170700
H	-2.01492300	-3.32912500	3.35259200
H	-1.73340500	-3.32912300	1.58325100
H	-0.57975400	-2.50124400	2.66458800
C	-3.96108300	-1.74457800	2.20305200
H	-4.34015800	-2.28111700	3.09289700
H	-4.57353200	-0.83417900	2.07582300
H	-4.12507200	-2.38795500	1.32317400
C	-2.27681000	-0.59739100	3.69132800
H	-1.22118700	-0.31686500	3.83846600
H	-2.88180600	0.32742200	3.69217700
H	-2.60250800	-1.20124000	4.55893500
C	-2.03407600	2.29971300	0.29063600
C	-2.71659400	3.40242600	-0.23758600
C	-1.98157600	4.50620900	-0.67733400
H	-3.80548400	3.36830800	-0.31072400
C	0.02487400	3.33999200	-0.02246800
C	-0.59104000	4.48506600	-0.56206700
H	-2.48438600	5.38081000	-1.10166200
N	-0.67640900	2.24795700	0.38391600
Ir	0.31730400	0.30521500	0.92879100
O	1.35913100	3.21879400	0.14236300
C	2.19788100	4.23463300	-0.40697200
H	2.04586100	5.20725200	0.09793800
H	2.03124000	4.34555700	-1.49364000
H	3.22553500	3.88870300	-0.22874500
H	1.82842000	1.12973700	1.19134500
H	0.21080600	0.51139000	2.51705300
I	0.89939900	-0.02190100	-1.86032400
H	0.91976500	-1.13588000	1.26546800
H	0.00718400	5.33661900	-0.88970800
H	-3.28977900	1.36539900	1.77542000
H	4.34866700	0.94634300	1.81903300
C	4.45490900	-0.21276400	0.05629000
C	4.91156500	0.95793500	-0.77735200
H	4.19418100	1.15675900	-1.59325900
H	4.97815100	1.85782300	-0.14670300
H	5.90639400	0.78350300	-1.22569000
C	3.79303800	-2.54716900	0.21647900
H	2.69211600	-2.48752000	0.10496200
H	4.13347600	-3.49172100	-0.24400100
C	4.19153800	-2.49338800	1.69406900
H	3.73429900	-3.34817700	2.22223900
H	5.28884100	-2.60915000	1.76778400
C	4.46232700	-1.61905300	-1.98031700
H	3.46690200	-1.43744400	-2.43551400
H	5.19217700	-0.93167100	-2.43238100
H	4.78409600	-2.65101100	-2.19940500
N	4.41109400	-1.44405900	-0.53300600
C	3.75784000	-1.15910700	2.32166500
H	4.29370900	-1.00124700	3.27575400
H	2.67681600	-1.19178200	2.56912600

Protonation TS_face1

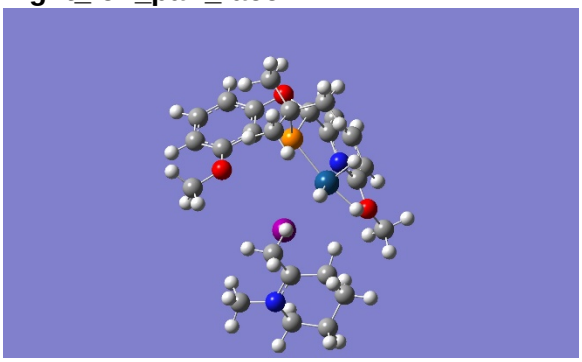


Zero-point correction= 0.582944
(Hartree/Particle)

Thermal correction to Energy= 0.621009
Thermal correction to Enthalpy= 0.621953
Thermal correction to Gibbs Free Energy= 0.510804
Sum of electronic and zero-point Energies= -1766.367554
Sum of electronic and thermal Energies= -1766.329488
Sum of electronic and thermal Enthalpies= -1766.328544
Sum of electronic and thermal Free Energies= -1766.439693
Electronic energy -1767.47198523

C	3.84043000	-0.44106800	1.65363400
C	4.68075000	0.80247500	1.41330300
C	3.93117000	-1.56796300	0.82943900
C	5.71675300	0.55333400	0.30667400
H	4.03009000	1.65987900	1.14125100
C	5.09730800	-0.24683300	-0.84227500
H	6.56986200	-0.02057200	0.71272800
H	5.84941600	-0.44962200	-1.62522700
H	4.25896700	0.31003600	-1.31400200
H	6.12171500	1.50281700	-0.08676600
H	5.19505700	1.09866500	2.34592900
N	4.59139200	-1.53844200	-0.36648200
H	2.38143700	0.07720800	1.27845800
C	-3.68588400	-1.91667500	-2.47386500
C	-2.82699600	-1.82697000	-1.35904900
C	-2.91335800	-0.70588400	-0.50824000
C	-3.86876000	0.28976400	-0.77669100
C	-4.75205400	0.20720800	-1.86050200
C	-4.63494300	-0.90691400	-2.70156500
H	-3.62386200	-2.76476500	-3.15897800
H	-5.48188000	0.99965300	-2.04290300
H	-5.29776500	-0.99199700	-3.56906600
O	-1.91365000	-2.77209100	-1.00387300
C	-1.58869100	-3.77675300	-1.96357800
H	-1.24738900	-3.32044700	-2.90970200
H	-0.76303100	-4.35034800	-1.51965600
H	-2.44596300	-4.45087000	-2.15453600
O	-3.92678500	1.36522800	0.08957700
C	-2.70392500	1.45538900	0.85838300
P	-1.89759100	-0.25458900	0.94453400
C	-2.71338300	-1.15751100	2.41306800
C	-2.19184500	-2.60972700	2.39189300
H	-2.63024500	-3.16619400	3.24184800
H	-2.46536700	-3.13115000	1.45970700
H	-1.09329800	-2.63652100	2.48714300
C	-4.24832500	-1.14340500	2.28674800
H	-4.68736200	-1.67127200	3.15382800
H	-4.65712500	-0.11821800	2.27471600
H	-4.58764100	-1.65460000	1.37085200
C	-2.28378100	-0.47691700	3.72475900
H	-1.18784000	-0.47281300	3.83459500
H	-2.63725700	0.56784000	3.79172400
H	-2.72278500	-1.02945300	4.57665400
C	-1.76187800	2.45608900	0.19425700
C	-2.30897000	3.59729600	-0.40516600
C	-1.45350400	4.51184500	-1.02537700
H	-3.39180600	3.73557200	-0.39512500
C	0.39823000	3.10136100	-0.39439900
C	-0.07982000	4.26786500	-1.02179800
H	-1.85051200	5.41059400	-1.50761300
N	-0.42553800	2.19550700	0.19770000
Ir	0.29466600	0.22063000	0.98029200
O	1.70626400	2.78031200	-0.31762300
C	2.62448600	3.51384300	-1.12774200
H	2.69953600	4.57116200	-0.81046200
H	2.34112100	3.45605800	-2.19373000
H	3.59622400	3.02199800	-0.98036800
H	1.84974400	0.89832400	1.23032500
H	0.12466700	0.65610300	2.51637200
I	0.98828200	-0.55118300	-1.69451300
H	0.67666600	-1.23017300	1.53773100
H	0.61140500	4.96588600	-1.49668100
H	-2.98773400	1.81123700	1.86448700
H	3.52562200	-0.64231300	2.68447300
C	4.37782400	-2.53683600	-1.40841500
H	4.22702200	-3.53313800	-0.96981100
H	3.49307200	-2.27882700	-2.02524300
H	5.27382300	-2.57542800	-2.05115100
C	3.21398500	-2.83259700	1.21929300
H	2.35705900	-3.00832400	0.54345400
H	3.87710000	-3.71558600	1.18289000
H	2.81837200	-2.73693300	2.24056700

Tight_ion_pair_face2

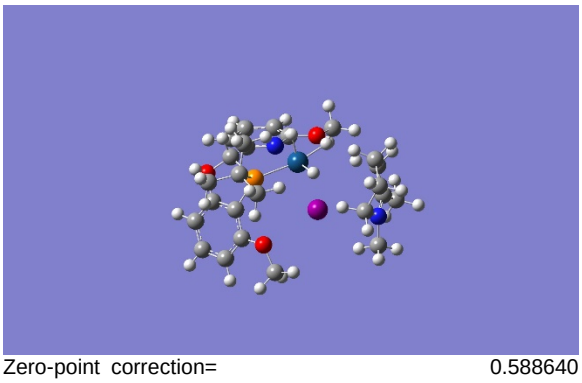


Zero-point correction= 0.587043 (Hartree/Particle)
Thermal correction to Energy= 0.625711
Thermal correction to Enthalpy= 0.626655
Thermal correction to Gibbs Free Energy= 0.512994
Sum of electronic and zero-point Energies= -1766.372436
Sum of electronic and thermal Energies= -1766.333767
Sum of electronic and thermal Enthalpies= -1766.332823
Sum of electronic and thermal Free Energies= -1766.446484
Electronic energy -1767.48503753

C	4.11646300	0.43600800	0.99853200
H	3.05289800	0.83729400	0.87161400
C	-3.06239700	-2.56441000	-2.56301800
C	-2.26170600	-2.29250000	-1.43531900
C	-2.60698400	-1.23803100	-0.56829900
C	-3.77097800	-0.49484800	-0.83293000
C	-4.60075400	-0.76355300	-1.93064000
C	-4.21992500	-1.80183500	-2.78946000
H	-2.79850800	-3.36617100	-3.25624700
H	-5.49654300	-0.16279400	-2.10665200
H	-4.83752900	-2.02452600	-3.66602200
O	-1.15904000	-3.02065200	-1.08194000
C	-0.57754400	-3.85722700	-2.07601000

H	-0.32581900	-3.27563200	-2.98154800
H	0.34674700	-4.25013000	-1.62748500
H	-1.23936200	-4.70417800	-2.34366800
O	-4.09357500	0.51504200	0.04941600
C	-2.93930700	0.86639100	0.85558100
P	-1.70958600	-0.57668300	0.89483100
C	-2.30269200	-1.69321300	2.33450900
C	-1.38055500	-2.92992600	2.33196700
H	-1.65434000	-3.59635500	3.17239500
H	-1.46848500	-3.50159800	1.39282700
H	-0.32635400	-2.62693000	2.45153500
C	-3.77087000	-2.12418100	2.17307200
H	-4.07089400	-2.74261300	3.04050300
H	-4.45512700	-1.25933200	2.12424400
H	-3.92233800	-2.72423800	1.26057400
C	-2.11919000	-0.92918600	3.65844000
H	-1.08238700	-0.57475200	3.77533300
H	-2.78990400	-0.05429800	3.73467300
H	-2.36168000	-1.60224600	4.50292700
C	-2.29041500	2.12169400	0.28069500
C	-3.12370800	3.12668700	-0.22876800
C	-2.54850200	4.29018500	-0.74356200
H	-4.20418300	2.96973700	-0.22645500
C	-0.38367200	3.36779500	-0.20526600
C	-1.15872400	4.42002500	-0.72932100
H	-3.17223000	5.09237200	-1.15062200
N	-0.93001400	2.22177300	0.28996000
Ir	0.29300600	0.50584700	1.00448900
O	0.96431100	3.39918900	-0.14620800
C	1.63159700	4.50552600	-0.74522200
H	1.39522500	5.45679800	-0.23071900
H	1.38554700	4.59496500	-1.81975200
H	2.70411500	4.29136200	-0.63399200
H	1.60602100	1.44449000	1.34863000
H	0.01710800	0.84726100	2.53907100
I	1.19765700	0.02907700	-1.71956800
H	1.14420500	-0.72844100	1.57810700
H	-0.68144600	5.31921900	-1.12197000
H	-3.31864400	1.08035300	1.87051600
H	4.75364100	1.33372000	1.07286200
C	4.39772600	-0.24497500	-0.28230700
C	4.92123700	0.56641800	-1.43568500
H	4.40359400	0.33785300	-2.37758500
H	4.78003100	1.63615400	-1.22576800
H	6.00722300	0.38185300	-1.56516300
C	3.71127300	-2.33650200	0.73398100
H	2.61795000	-2.16776500	0.77508400
H	3.90380700	-3.39972000	0.52040400
C	4.39301400	-1.89090700	2.02791700
H	4.02525300	-2.51537200	2.85969000
H	5.47972800	-2.07630500	1.93374000
C	4.26471800	-2.21179100	-1.71329900
H	3.30655300	-1.97430200	-2.22408200
H	5.11092500	-1.85651200	-2.31890600
H	4.35943600	-3.29726200	-1.56940500
N	4.24668800	-1.55698600	-0.40459200
C	4.10676000	-0.40757400	2.29491100
H	4.84536700	-0.00505600	3.00884700
H	3.10747400	-0.30054600	2.75073600

Tight_ion_pair_face1

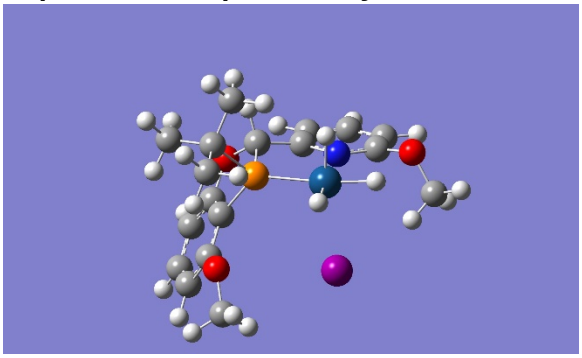


Zero-point correction= 0.588640 (Hartree/Particle)
Thermal correction to Energy= 0.626646
Thermal correction to Enthalpy= 0.627590
Thermal correction to Gibbs Free Energy= 0.516710
Sum of electronic and zero-point Energies= -1766.376683
Sum of electronic and thermal Energies= -1766.338676
Sum of electronic and thermal Enthalpies= -1766.337732
Sum of electronic and thermal Free Energies= -1766.448612
Electronic energy -1767.48875168

C	3.84547900	-0.18666200	1.44753900
C	4.66520200	0.91232100	0.76904900
C	3.61220100	-1.41904400	0.61278800
C	5.85175200	0.30300400	0.01711800
H	4.00510200	1.44754300	0.06217900
C	5.35707600	-0.75646300	-0.96553100
H	6.56253900	-0.16147700	0.72684000
H	6.20223900	-1.27629700	-1.44675600
H	4.73725000	-0.28794000	-1.76062300
H	6.41153400	1.06905400	-0.54828900
H	5.00501400	1.64391800	1.52199700
N	4.52261200	-1.78509900	-0.31327700
H	2.85364000	0.19704900	1.75984200
C	-2.67689100	-3.01945200	-2.39193400
C	-2.10703100	-2.51403600	-1.20590000
C	-2.54474300	-1.27929500	-0.68555500
C	-3.56436800	-0.58543800	-1.36120800
C	-4.16088300	-1.07444700	-2.53299200
C	-3.69556600	-2.29514800	-3.03381900
H	-2.34238100	-3.96837600	-2.81672100
H	-4.95034800	-0.50521400	-3.02997300
H	-4.13193400	-2.69834200	-3.95377300
O	-1.14754600	-3.16485400	-0.47599700
C	-0.60232500	-4.35826100	-1.02344900
H	-0.13205500	-4.17341000	-2.00790600
H	0.16450100	-4.69007000	-0.30751400
H	-1.36840100	-5.15127400	-1.12736000
O	-3.99729600	0.60286200	-0.81489600
C	-3.04852500	1.08653700	0.17219300
P	-1.95673800	-0.33821000	0.78570800
C	-2.95148700	-1.10882600	2.23248100
C	-2.14635700	-2.33887000	2.69909800
H	-2.65080300	-2.80599700	3.56676100
H	-2.05965300	-3.09610600	1.90177700

H	-1.12777700	-2.04375200	3.00335500
C	-4.37168300	-1.52770800	1.81629900
H	-4.90388500	-1.94713900	2.69141900
H	-4.96488400	-0.67526500	1.44124600
H	-4.35492700	-2.29910200	1.02842700
C	-3.01642900	-0.08362000	3.37955200
H	-2.00894300	0.24961400	3.67683700
H	-3.60668000	0.81116800	3.11005100
H	-3.50842000	-0.54861200	4.25509200
C	-2.21379500	2.20603800	-0.44186300
C	-2.84820400	3.11476700	-1.30006900
C	-2.10536400	4.15873500	-1.85486400
H	-3.90699600	2.97621200	-1.52782700
C	-0.17900800	3.32114700	-0.66557900
C	-0.75159900	4.27156700	-1.53230800
H	-2.57221000	4.88248800	-2.53051200
N	-0.88890500	2.28947600	-0.12598400
Ir	0.03903500	0.72767800	1.15641600
O	1.11826000	3.34077300	-0.29546200
C	1.96595200	4.32586200	-0.87854900
H	1.65187700	5.35178200	-0.60712700
H	2.00144400	4.22877200	-1.97995900
H	2.96381600	4.12989000	-0.46132600
H	1.31653400	1.65647300	1.58172300
H	-0.54325100	1.38795100	2.48084300
I	1.52982900	-0.31020200	-1.09284600
H	0.65627100	-0.33810100	2.19014900
H	-0.14726000	5.07899900	-1.94909500
H	-3.64590800	1.49561700	1.00634900
H	4.35395200	-0.53995300	2.37218000
C	4.28855100	-2.98023400	-1.12430800
H	4.15474800	-3.86647400	-0.48725300
H	3.38267800	-2.83260000	-1.74742000
H	5.15848500	-3.14553400	-1.77626200
C	2.71795900	-2.45696100	1.23552100
H	1.86538000	-1.94279600	1.70891500
H	2.31705800	-3.18218300	0.51491500
H	3.28430100	-3.00177400	2.01937800

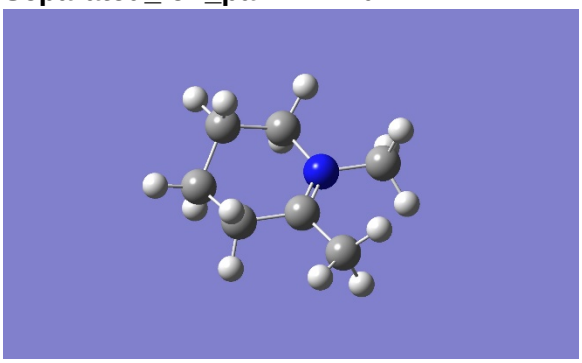
Separated_ion_pair: catalyst



Zero-point correction= 0.385723 (Hartree/Particle)
Thermal correction to Energy= 0.413947
Thermal correction to Enthalpy= 0.414891
Thermal correction to Gibbs Free Energy= 0.325728
Sum of electronic and zero-point Energies= -1437.180357
Sum of electronic and thermal Energies= -1437.152133
Sum of electronic and thermal Enthalpies= -1437.151189
Sum of electronic and thermal Free Energies= -1437.240353
Electronic energy -1438.02310071

H	2.38998400	0.64905800	-1.78625500
Ir	0.93560200	0.12178600	-1.26163800
I	0.78149400	2.42153500	0.52195300
C	-3.57725600	1.24297400	2.02546700
C	-2.90450300	0.93084500	0.82502500
C	-2.18518700	-0.27371300	0.71566100
C	-2.16005000	-1.14986600	1.81317300
C	-2.84958700	-0.88205800	3.00531200
C	-3.54793700	0.33030300	3.09142900
H	-4.12060400	2.18556400	2.12922200
H	-2.80480300	-1.58689200	3.84017500
H	-4.07526800	0.57964200	4.01940700
O	-2.93951300	1.71380200	-0.29656700
C	-3.10859000	3.11746200	-0.11110200
H	-4.12980800	3.37054300	0.24077300
H	-2.34548800	3.50364600	0.58824900
H	-2.94630100	3.56626500	-1.10193800
O	-1.42262100	-2.30769000	1.68576100
C	-0.50745000	-2.21056400	0.55798500
P	-1.03477700	-0.81621200	-0.62207100
C	-2.21038900	-1.70259600	-1.86027200
C	-1.37811900	-2.70067000	-2.68534700
H	-1.99582100	-3.10361000	-3.51216800
H	-0.48562900	-2.21136800	-3.11036100
H	-1.03877600	-3.56153900	-2.07976700
C	-2.74341600	-0.59883600	-2.79651000
H	-3.38861300	-1.04949700	-3.57730700
H	-3.33522800	0.15142500	-2.24534100
H	-1.90684400	-0.07212000	-3.28666900
C	-3.37734300	-2.42798400	-1.17147000
H	-4.00432200	-2.93860400	-1.92965500
H	-3.02732000	-3.19404800	-0.45613700
H	-4.02097200	-1.72424700	-0.61727300
C	0.91712300	-1.99966200	1.06177600
C	1.32134600	-2.68662500	2.21290400
C	2.64794100	-2.59388700	2.64894500
H	0.57936600	-3.28052700	2.75265300
C	3.06445600	-1.16793200	0.73693100
C	3.53349500	-1.83732700	1.87986300
H	2.98552700	-3.11735200	3.54993000
N	1.75967000	-1.19143500	0.33916800
O	3.97231000	-0.53703500	-0.05308700
C	4.33246900	0.80095800	0.34128700
H	4.80547300	0.79640400	1.34514400
H	3.44720700	1.46063400	0.33534700
H	5.06183000	1.14238100	-0.40859900
H	4.59558700	-1.75388800	2.12722400
H	-0.55307300	-3.18873100	0.04429100
H	1.18438400	-0.93938100	-2.43765500
H	0.38945800	1.08303200	-2.41891800

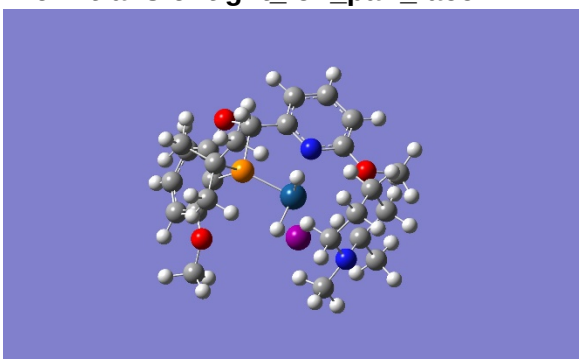
Separated_ion_pair: iminium



Zero-point correction= 0.199954 (Hartree/Particle)
Thermal correction to Energy= 0.208728
Thermal correction to Enthalpy= 0.209672
Thermal correction to Gibbs Free Energy= 0.166975
Sum of electronic and zero-point Energies= -329.059334
Sum of electronic and thermal Energies= -329.050560
Sum of electronic and thermal Enthalpies= -329.049616
Sum of electronic and thermal Free Energies= -329.092314
Electronic energy -329.42231158

C	0.67388600	1.47488400	0.00270500
C	1.94409800	0.68479800	-0.32568000
C	1.89179700	-0.66992100	0.38564000
H	2.02286100	0.53666100	-1.41779900
C	0.66320400	-1.44673100	-0.06875900
H	1.86286200	-0.52939600	1.48161100
H	0.46739200	-2.31788600	0.57884400
C	-1.88989500	1.43628200	0.11385700
H	-2.41018200	1.43665900	-0.86305800
H	-1.69316400	2.48521400	0.37954900
H	0.77195900	-1.82064200	-1.10337600
H	2.78451000	-1.27719700	0.16367500
H	2.82969500	1.26237500	-0.01769200
N	-0.58874900	-0.62983500	-0.04733600
C	-1.82240300	-1.43932700	-0.08545800
H	-1.63007900	-2.32756000	-0.70511300
H	-2.65516200	-0.87313500	-0.51979800
H	0.51549600	2.31965700	-0.69529000
H	0.74393800	1.95569400	1.00153500
H	-2.57853800	1.00494100	0.85857300
H	-2.08192100	-1.76640700	0.93560700
C	-0.59875800	0.67999200	0.02004300

Pre-H transfer tight_ion_pair_face2

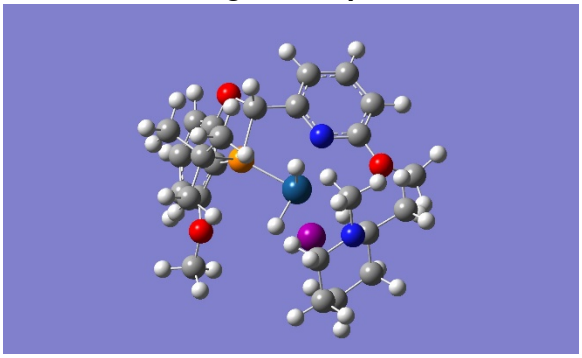


Zero-point correction= 0.590645 (Hartree/Particle)
Thermal correction to Energy= 0.628625
Thermal correction to Enthalpy= 0.629569
Thermal correction to Gibbs Free Energy= 0.518803
Sum of electronic and zero-point Energies= -1766.401211
Sum of electronic and thermal Energies= -1766.363232
Sum of electronic and thermal Enthalpies= -1766.362287
Sum of electronic and thermal Free Energies= -1766.473054
Electronic energy -1767.51239308

C	-3.68498300	-2.57740800	-0.94857300
C	-3.69605400	-0.57332600	0.44969800
C	-4.55869000	-1.91853400	-2.01963800
H	-2.60787000	-2.47242300	-1.22453000
C	-4.32360100	-0.40402100	-2.03111200
H	-5.62178500	-2.13333100	-1.79992100
H	-5.00058000	0.09715600	-2.74727300
C	-3.95579200	-0.00362200	1.84575000
H	-3.96951400	1.09632900	1.80014200
H	-3.16612900	-0.27785400	2.56255600
H	-3.28728000	-0.19450900	-2.35974000
H	-4.32826600	-2.36467500	-3.00433800
H	-3.90718900	-3.65812400	-0.88593900
H	-2.56340900	-0.34410200	0.20499900
Ir	-0.52325900	-0.20326400	-0.22431800
I	-0.08561900	0.51217100	2.45839900
C	4.49400200	-0.89109700	1.80531700
C	3.32097000	-1.23124300	1.10366500
C	2.95392900	-0.47785000	-0.03110700
C	3.76033500	0.59702900	-0.44128700
C	4.94393500	0.93597500	0.22699600
C	5.28631500	0.17715300	1.35328700
H	4.79277500	-1.44735000	2.69621300
H	5.55168000	1.77715800	-0.11452100
H	6.19656700	0.42900400	1.90725500
O	2.49648500	-2.26650000	1.42124300
C	2.61855900	-2.83532100	2.72673100
H	3.57891000	-3.37160500	2.84920000
H	2.51484100	-2.05436500	3.50009500
H	1.78741700	-3.54884400	2.81422100
O	3.35724900	1.31745000	-1.54796400
C	1.97971700	1.03436900	-1.89240800
P	1.45314300	-0.57842100	-1.05099200
C	1.74507700	-1.96514000	-2.32588800
C	0.84240900	-1.73161700	-3.55052500

H	0.96577700	-2.57621400	-4.25365200
H	-0.22011300	-1.67196200	-3.26383000
H	1.10408100	-0.80899600	-4.09952400
C	1.36861300	-3.29861100	-1.65034500
H	1.53029200	-4.12741000	-2.36483800
H	1.97957800	-3.48920800	-0.75255200
H	0.30869900	-3.29761000	-1.34658400
C	3.22548300	-1.97536500	-2.75309500
H	3.37583700	-2.76682300	-3.51048000
H	3.53963400	-1.01771900	-3.20490500
H	3.89493600	-2.18528500	-1.90319400
C	1.08948400	2.19586900	-1.46276000
C	1.53691600	3.50222600	-1.69315600
C	0.72457400	4.57221500	-1.30688500
H	2.51710000	3.65887500	-2.14835900
C	-0.89543500	2.96822700	-0.52420500
C	-0.51382800	4.30965500	-0.71953300
H	1.04831800	5.60550700	-1.46529200
N	-0.10519400	1.92167500	-0.87072800
O	-2.07468900	2.59218500	0.01731400
C	-2.88941900	3.62213900	0.58711700
H	-3.25026600	4.32605900	-0.18571800
H	-2.33915600	4.17023000	1.37210300
H	-3.74722900	3.10394200	1.03534900
H	-1.16865200	5.12741100	-0.41560700
H	1.94764000	0.93285300	-2.99196700
H	-1.09615100	-0.64986600	-1.65813400
H	-0.68006900	-1.71545300	0.25558300
H	-4.93734000	-0.34858700	2.21723300
C	-3.28135700	-2.78618900	1.43122900
H	-3.63428700	-2.47045100	2.42455300
H	-3.55340600	-3.84679700	1.29475700
H	-2.17220500	-2.69595500	1.40893000
N	-3.92130700	-1.99927600	0.38015000
C	-4.51993600	0.16566800	-0.62271500
H	-4.23929200	1.23190400	-0.59922800
H	-5.58648500	0.09268600	-0.33089300

Pre-H transfer tight_ion_pair_face1

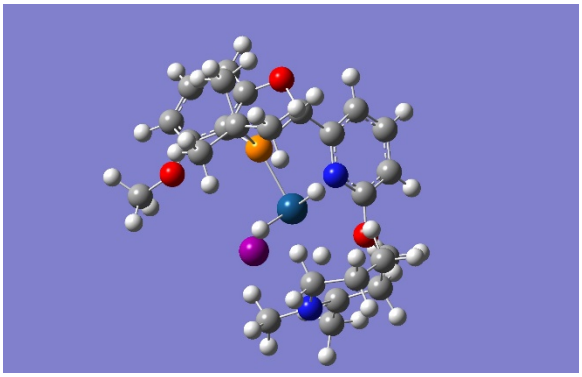


Zero-point correction= 0.591060 (Hartree/Particle)
Thermal correction to Energy= 0.628885
Thermal correction to Enthalpy= 0.629829
Thermal correction to Gibbs Free Energy= 0.519757
Sum of electronic and zero-point Energies= -1766.399592
Sum of electronic and thermal Energies= -1766.361766
Sum of electronic and thermal Enthalpies= -1766.360822
Sum of electronic and thermal Free Energies= -1766.470894
Electronic energy -1767.51018231

C	-4.20536400	-0.44995000	1.13911900
C	-3.79120200	-1.86467600	1.55319300
C	-3.82966200	-0.10066000	-0.31240700
C	-4.29012500	-2.88237300	0.52232700
H	-2.68842700	-1.90491500	1.62338200
C	-3.81097200	-2.48881900	-0.87645200
H	-5.39658300	-2.92011300	0.52614700
H	-4.22377700	-3.18009800	-1.63406100
C	-4.39527600	1.27280900	-0.69660900
H	-3.90565800	1.70739600	-1.58139400
H	-4.25297100	1.97430100	0.13904000
H	-2.69823500	-2.56313200	-0.92652800
H	-3.92520700	-3.89899400	0.75693900
H	-4.18579900	-2.09399100	2.55973200
N	-4.24288000	-1.13250000	-1.24050500
C	-3.96321100	-0.84183900	-2.64070900
H	-2.87104200	-0.71236700	-2.83234600
H	-4.48325200	0.07351600	-2.96375000
H	-3.72451600	0.29120300	1.80207200
H	-2.65597800	-0.00469100	-0.33933200
H	-5.30330400	-0.33032400	1.23610500
Ir	-0.53731600	-0.11066800	-0.37194800
I	-0.41167300	0.41488000	2.39030900
C	4.29857500	-1.00266400	2.08085000
C	3.13783300	-1.30044700	1.33855200
C	2.90157400	-0.61710300	0.12646300
C	3.83359100	0.33342900	-0.32606800
C	5.00761000	0.62129100	0.38052100
C	5.21341400	-0.05764500	1.58862400
H	4.49414900	-1.50105300	3.03263800
H	5.71336200	1.36516000	0.00336900
H	6.11266200	0.15952400	2.17438200
O	2.21163000	-2.23354900	1.68329700
C	2.23292100	-2.73765300	3.02049000
H	3.14021100	-3.34198200	3.21154200
H	2.16209300	-1.91201300	3.74985300
H	1.34108100	-3.37344700	3.10605300
O	3.56597800	0.97493100	-1.52147800
C	2.16804900	0.84118100	-1.87209400
P	1.46586000	-0.68388400	-0.99251700
C	1.74953600	-2.17204800	-2.14521200
C	0.90302700	-2.00217500	-3.41948700
H	1.06036400	-2.88079500	-4.07231800
H	-0.17091500	-1.93147300	-3.18465400
H	1.18715700	-1.10621000	-4.00006300
C	1.29866700	-3.43673100	-1.38744700
H	1.45689400	-4.32105800	-2.03274800
H	1.86822600	-3.58080700	-0.45459300
H	0.22876100	-3.37895400	-1.12742300
C	3.24364000	-2.27079600	-2.51146500
H	3.38746600	-3.12187200	-3.20256000
H	3.61434600	-1.36228300	-3.01744100
H	3.87321800	-2.44570200	-1.62391400
C	1.41585100	2.09752500	-1.43897000
C	2.03325800	3.34322900	-1.60201900
C	1.36647300	4.49198800	-1.16277700
H	3.03234000	3.39075800	-2.03996500
C	-0.45574200	3.08061100	-0.45964900
C	0.10436700	4.36648100	-0.58119400
H	1.82525500	5.47949900	-1.27283500
N	0.18657800	1.95857000	-0.87056700

O	-1.67429400	2.83998300	0.06570600
C	-2.19859500	3.81176300	0.97876000
H	-2.53519700	4.72480400	0.45328100
H	-1.44742100	4.06004000	1.74767800
H	-3.05864000	3.32739600	1.45988000
H	-0.44308800	5.24374300	-0.23160700
H	2.12783100	0.72737200	-2.96954900
H	-0.95437500	-0.40361100	-1.89617400
H	-0.93012300	-1.61168500	-0.00539000
H	-5.47908400	1.18290900	-0.89098900
H	-4.32954200	-1.67678000	-3.26181000

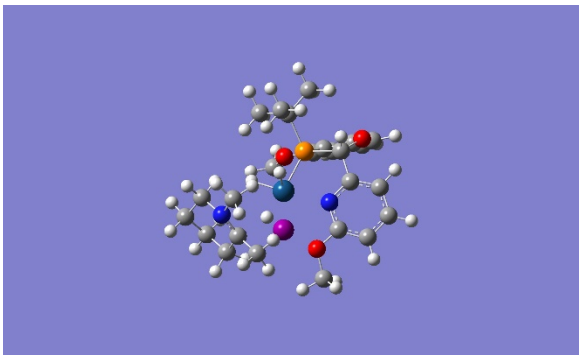
H_transfer_TS_face2



Zero-point correction= 0.586834 (Hartree/Particle)
Thermal correction to Energy= 0.624449
Thermal correction to Enthalpy= 0.625393
Thermal correction to Gibbs Free Energy= 0.515463
Sum of electronic and zero-point Energies= -1766.387264
Sum of electronic and thermal Energies= -1766.349649
Sum of electronic and thermal Enthalpies= -1766.348705
Sum of electronic and thermal Free Energies= -1766.458635
Electronic energy -1767.49602994

C	-3.89672400	-2.37000000	-1.07380600
C	-3.97672900	-0.35784300	0.30918200
C	-4.69568700	-1.66985000	-2.17258700
H	-2.81233800	-2.37009900	-1.31897600
C	-4.32670300	-0.18362600	-2.22103700
H	-5.77872400	-1.79162600	-1.97912800
H	-4.92153000	0.34909400	-2.98378500
C	-4.02962500	0.28373000	1.66899900
H	-4.23016700	1.35857900	1.55686900
H	-3.07226800	0.16830200	2.21685100
H	-3.25943000	-0.07669900	-2.48613400
H	-4.47893900	-2.16665700	-3.13464700
H	-4.22719400	-3.41559400	-0.95165300
H	-2.42456600	-0.09475100	-0.02797400
Ir	-0.61014400	-0.26291800	-0.30842700
I	-0.27645800	0.10399300	2.49629300
C	4.71516100	-0.41748200	1.73558700
C	3.52305500	-0.89873800	1.15551900
C	3.04609300	-0.31473600	-0.03629400
C	3.79098400	0.71353800	-0.64107100
C	4.99440900	1.18514100	-0.10100100
C	5.43219400	0.60774100	1.09797000
H	5.08910300	-0.83980900	2.67072900
H	5.54672600	1.98792900	-0.59552500
H	6.35907900	0.96800500	1.55661700
O	2.78940000	-1.93709200	1.64402200
C	3.02462900	-2.34601700	2.99103800
H	4.02625900	-2.80262200	3.11037400
H	2.90946000	-1.49375900	3.68363400
H	2.25089100	-3.09507600	3.20935800
O	3.30508700	1.24298400	-1.82199000
C	1.90023200	0.92080500	-1.97148700
P	1.49960900	-0.63167900	-0.96834700
C	1.92495600	-2.11228900	-2.09895800
C	0.92662600	-2.15349300	-3.26973600
H	1.13676300	-3.04347300	-3.89249000
H	-0.11110800	-2.21223000	-2.90481800
H	1.00782700	-1.26581800	-3.92289200
C	1.76149500	-3.38503800	-1.24246000
H	1.97719000	-4.27487400	-1.86413700
H	2.44804300	-3.38922400	-0.37979600
H	0.73202000	-3.46843000	-0.85505200
C	3.36465100	-2.01411100	-2.63594500
H	3.56782100	-2.88150500	-3.29189200
H	3.52822600	-1.09799300	-3.22966400
H	4.10644300	-2.02513300	-1.82054700
C	1.06668700	2.10596400	-1.48871700
C	1.53105100	3.39557800	-1.77825000
C	0.79955200	4.49761500	-1.33090500
H	2.46735600	3.51013100	-2.32791000
C	-0.77433500	2.95396500	-0.34754200
C	-0.37118600	4.27872000	-0.60444000
H	1.13404100	5.51788200	-1.54315800
N	-0.07584500	1.87025700	-0.78120000
O	-1.89533800	2.65086000	0.34865000
C	-2.48534200	3.70540800	1.11273400
H	-2.98067900	4.45408200	0.46524000
H	-1.73395000	4.20181500	1.75182900
H	-3.23523000	3.22216600	1.75298900
H	-0.96574100	5.11972700	-0.24453700
H	1.72672500	0.74907000	-3.04854500
H	-1.04883400	-0.50881500	-1.83551600
H	-0.91442600	-1.80641100	-0.02818900
H	-4.84561100	-0.15381700	2.27378500
C	-3.50039800	-2.50176900	1.35062100
H	-3.92018300	-2.16369600	2.30855100
H	-3.77128400	-3.55770200	1.19717800
H	-2.39772200	-2.39175100	1.38316200
N	-4.03487700	-1.71216700	0.23848600
C	-4.54817800	0.44633600	-0.84542600
H	-4.10770800	1.45460500	-0.79390800
H	-5.63644400	0.55647400	-0.64410300

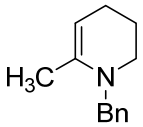
H_transfer_TS_face1



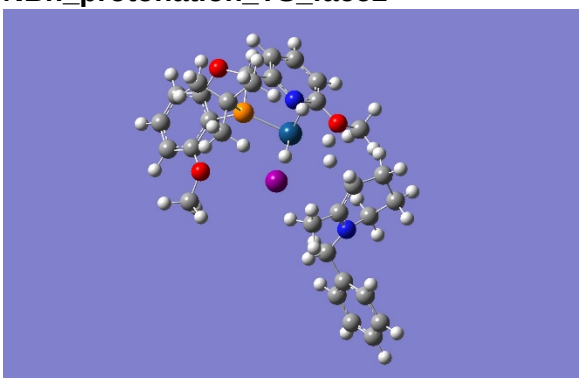
Lowest energy structure was located by sequential relaxed PES scans. This allowed to identify the minimum energy conformation. However, optimization of obtained TS structure proved to be unsuccessful with various algorithms, grid sizes and step sizes. This suggests very shallow PES around TS. Located structure satisfies single negative frequency analysis.

Zero-point correction= 0.586974 (Hartree/Particle)
Thermal correction to Energy= 0.624652
Thermal correction to Enthalpy= 0.625596
Thermal correction to Gibbs Free Energy= 0.516526
Sum of electronic and zero-point Energies= -1766.383180
Sum of electronic and thermal Energies= -1766.345502
Sum of electronic and thermal Enthalpies= -1766.344558
Sum of electronic and thermal Free Energies= -1766.453628
Electronic energy -1767.49439253

C	-4.13519600	-0.40881200	1.16406200
C	-3.77594100	-1.85035700	1.53141900
C	-4.02332300	-0.07577300	-0.30681100
C	-4.36833300	-2.82754700	0.51360900
H	-2.67494600	-1.93540200	1.54281200
C	-3.89597300	-2.45329600	-0.88948500
H	-5.47508400	-2.80996500	0.54674800
H	-4.37582500	-3.08772900	-1.65437200
C	-4.41963600	1.33487200	-0.68985000
H	-3.86142300	1.71502800	-1.55631500
H	-4.22114100	2.00627800	0.15578500
H	-2.79446400	-2.56986100	-0.97174400
H	-4.05211100	-3.86423900	0.72514400
H	-4.13194900	-2.07201400	2.55232400
N	-4.21618700	-1.05392400	-1.22666200
C	-4.06728400	-0.72839600	-2.64366700
H	-3.00702000	-0.47162100	-2.85096600
H	-4.71229600	0.11733100	-2.92388700
H	-3.47519600	0.28663500	1.71683600
H	-2.28601700	0.24549600	-0.38707100
H	-5.18159300	-0.17436500	1.45872400
Ir	-0.61415800	-0.13287200	-0.45644200
I	-0.49224700	0.24482600	2.36599800
C	4.43518700	-0.84571800	2.05232800
C	3.26126100	-1.18625500	1.34868300
C	2.97036900	-0.53747000	0.13086300
C	3.87328300	0.41608500	-0.37155400
C	5.06065000	0.74759300	0.29399200
C	5.31551800	0.10610000	1.51310300
H	4.66917800	-1.31895700	3.00848800
H	5.74015600	1.49494100	-0.12299500
H	6.22566500	0.35740800	2.06788200
O	2.37433800	-2.14234700	1.74088200
C	2.44641700	-2.60754900	3.08801100
H	3.37364400	-3.18442000	3.27107600
H	2.37658900	-1.76498400	3.79833600
H	1.57343500	-3.26181400	3.21841900
O	3.55954500	1.01407600	-1.57837800
C	2.14697300	0.85226400	-1.85905400
P	1.50010000	-0.67954600	-0.95336000
C	1.88668200	-2.16952300	-2.08436200
C	1.00730400	-2.08269700	-3.34441300
H	1.19119700	-2.97219900	-3.97609600
H	-0.06174600	-2.04908900	-3.08038000
H	1.23597400	-1.19038000	-3.95469000
C	1.51892900	-3.43800900	-1.28734300
H	1.70624300	-4.33121300	-1.91331900
H	2.11666400	-3.52867000	-0.36535600
H	0.45396000	-3.42662000	-1.00022700
C	3.37451000	-2.20381300	-2.47991600
H	3.55315400	-3.06704100	-3.14848200
H	3.68592700	-1.29141500	-3.01728600
H	4.02847300	-2.31674500	-1.59969400
C	1.40034000	2.09629800	-1.38130800
C	2.03256200	3.33998100	-1.50750000
C	1.38633300	4.48307000	-1.02976600
H	3.03033100	3.38417900	-1.94825000
C	-0.44826400	3.06890400	-0.35690900
C	0.12803800	4.35049400	-0.44217000
H	1.85636400	5.46820900	-1.11115400
N	0.16864200	1.94748700	-0.81441800
O	-1.66800100	2.84663000	0.18001000
C	-2.15777600	3.81678100	1.10895400
H	-2.48800700	4.74436600	0.60298600
H	-1.39316300	4.04819700	1.87052500
H	-3.01841100	3.34369200	1.60242900
H	-0.40533000	5.22245100	-0.05909900
H	2.05138400	0.74094500	-2.95337700
H	-0.95606200	-0.34424900	-2.01504300
H	-1.06688600	-1.64363800	-0.19939900
H	-5.50426500	1.36812900	-0.91456100
H	-4.35768100	-1.60329500	-3.24428000



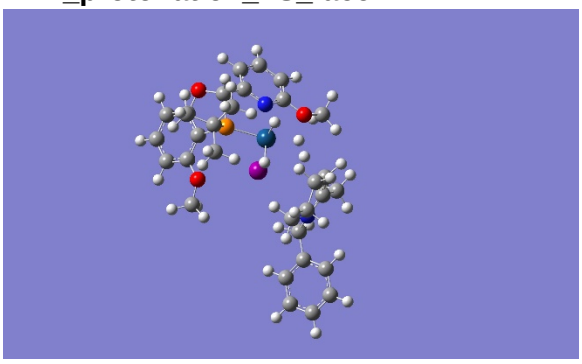
NBn_protonation_TS_face1



Zero-point correction= 0.662159 (Hartree/Particle)
Thermal correction to Energy= 0.704769
Thermal correction to Enthalpy= 0.705713
Thermal correction to Gibbs Free Energy= 0.582563
Sum of electronic and zero-point Energies= -1997.037945
Sum of electronic and thermal Energies= -1996.995335
Sum of electronic and thermal Enthalpies= -1996.994391
Sum of electronic and thermal Free Energies= -1997.117541
Electronic energy -1998.29069634

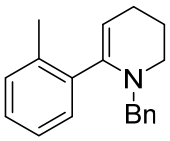
C	2.59165600	1.29292700	2.25592300
C	3.10381300	2.66750000	1.85223300
C	3.16867500	0.11200700	1.77239100
C	4.38713400	2.54744200	1.01635400
H	2.32564700	3.21408000	1.27914300
C	4.27071200	1.39079100	0.02234900
H	5.25351600	2.35498400	1.67559700
H	5.19713200	1.28391100	-0.56613600
H	3.43120900	1.55440500	-0.68672100
H	4.59896700	3.48238700	0.46757100
H	3.29809800	3.27669100	2.75378600
N	4.04054700	0.11935300	0.71918100
H	1.19906100	1.24969000	1.54052600
C	-3.35176900	-3.45928400	-1.93334800
C	-2.81910300	-2.77629600	-0.82078000
C	-3.30533300	-1.49310900	-0.49660800
C	-4.33817100	-0.93624800	-1.27125000
C	-4.90432800	-1.60903500	-2.36155200
C	-4.38521700	-2.87051300	-2.67943200
H	-2.97284200	-4.44396100	-2.21484600
H	-5.70350000	-1.14475900	-2.94435600
H	-4.79259500	-3.41403700	-3.53833800
O	-1.87089400	-3.28271700	0.01537900
C	-1.11406800	-4.40453300	-0.43834200
H	-0.63889300	-4.18779300	-1.41148500
H	-0.33345000	-4.55738600	0.31992500
H	-1.73858400	-5.31567800	-0.51359200
O	-4.80550600	0.31165300	-0.90642400
C	-3.84772600	0.97686900	-0.04939900
P	-2.76004500	-0.31946400	0.79821600
C	-3.69625400	-0.84792200	2.37434800
C	-2.88732100	-1.99676100	3.01188700
H	-3.39837700	-2.33372700	3.93348100
H	-2.79421700	-2.85930800	2.33135700
H	-1.87114500	-1.66153300	3.27844800
C	-5.12130600	-1.32575300	2.03711300
H	-5.63742100	-1.61059300	2.97304100
H	-5.72290800	-0.53934400	1.54880200
H	-5.11201600	-2.20615400	1.37396600
C	-3.75468700	0.34151000	3.34950400
H	-2.74645200	0.71198700	3.59416500
H	-4.34199600	1.18701500	2.94793400
H	-4.24673700	0.01481200	4.28498800
C	-3.00232400	1.93129100	-0.88679600
C	-3.62576400	2.64586700	-1.91729800
C	-2.86166800	3.52288600	-2.69092800
H	-4.68931400	2.48720600	-2.10572700
C	-0.94557400	2.91786600	-1.35597600
C	-1.50262400	3.66757200	-2.40977200
H	-3.31786200	4.09323100	-3.50606900
N	-1.67559100	2.04888400	-0.60554400
Ir	-0.77459000	0.71804900	0.95261500
O	0.35193400	2.99662800	-0.99237400
C	1.23446700	3.74856200	-1.82464700
H	0.96892100	4.82251100	-1.83995500
H	1.24680200	3.34818800	-2.85437800
H	2.22958300	3.62826800	-1.37422500
H	0.50773200	1.83622500	1.14213500
H	-1.37235200	1.58143900	2.16600500
I	0.64022600	-0.69688400	-1.10549900
H	-0.23860600	-0.28749600	2.07700200
H	-0.88259400	4.34613300	-2.99726400
H	-4.43149600	1.54798700	0.69402900
H	2.12354800	1.20817300	3.24370900
C	4.35108300	-1.07122300	-0.07753500
H	4.01480500	-1.96025500	0.47707000
H	3.74356000	-1.04958600	-1.00622000
C	2.75634900	-1.20661100	2.37104600
H	2.08013000	-1.73918700	1.67640500
H	3.62245600	-1.85402600	2.59557100
H	2.20235900	-1.03319700	3.30486400
C	5.82994300	-1.20169600	-0.40521000
C	6.81482800	-0.99707900	0.58027500
C	6.23466400	-1.57404900	-1.69956300
C	8.17247700	-1.16666300	0.27840400
H	6.50767700	-0.69246600	1.58727900
C	7.59268800	-1.75143000	-2.00279100
H	5.47520500	-1.72597900	-2.47547800
C	8.56571300	-1.54743300	-1.01424200
H	8.92722500	-1.00248000	1.05501300
H	7.89035400	-2.04056500	-3.01629100
H	9.62679200	-1.67970500	-1.25011800

NBn_protonation_TS_face2



Zero-point correction= 0.663030
(Hartree/Particle)
Thermal correction to Energy= 0.705644
Thermal correction to Enthalpy= 0.706588
Thermal correction to Gibbs Free Energy= 0.583017
Sum of electronic and zero-point Energies= -1997.037126
Sum of electronic and thermal Energies= -1996.994512
Sum of electronic and thermal Enthalpies= -1996.993568
Sum of electronic and thermal Free Energies= -1997.117139
Electronic energy -1998.29035967

C	2.63180900	2.10159900	1.79042300
H	1.14970900	1.88569200	1.19473700
C	-2.49572800	-3.75428200	-2.04283300
C	-2.01198700	-3.02366600	-0.93902400
C	-2.77869800	-1.96054600	-0.42175600
C	-4.02391900	-1.66433800	-1.00170800
C	-4.53900100	-2.39559200	-2.07996100
C	-3.74919600	-3.43421900	-2.58932000
H	-1.90879400	-4.56895000	-2.47202700
H	-5.51017800	-2.13909000	-2.50990600
H	-4.11571100	-4.01227500	-3.44404700
O	-0.84584500	-3.28871700	-0.28522900
C	0.11450300	-4.11058200	-0.94747600
H	0.36577600	-3.69505800	-1.93957300
H	1.00822200	-4.09090000	-0.30777600
H	-0.24057300	-5.15425000	-1.04994900
O	-4.75078200	-0.62502900	-0.45498900
C	-3.90905200	0.21016100	0.37456800
P	-2.37822600	-0.76879000	0.90446500
C	-2.85109600	-1.64999800	2.53118700
C	-1.63202700	-2.49517300	2.95202300
H	-1.85993400	-3.02021800	3.89886800
H	-1.37549600	-3.24892500	2.18926300
H	-0.74912000	-1.85332500	3.10887000
C	-4.08364000	-2.55084200	2.32730100
H	-4.34977000	-3.02459400	3.29075900
H	-4.96433600	-1.98321500	1.97858300
H	-3.88837100	-3.35308900	1.59710300
C	-3.14390500	-0.59540700	3.61374600
H	-2.28791000	0.08299000	3.75846400
H	-4.03236800	0.01690000	3.37593800
H	-3.34801800	-1.11031200	4.57115500
C	-3.51365400	1.46509200	-0.39651400
C	-4.46299500	2.06479600	-1.23317400
C	-4.11232800	3.22063500	-1.93572600
H	-5.44811900	1.60509400	-1.33417100
C	-1.93280000	3.09504800	-0.91186500
C	-2.83260200	3.75235300	-1.77208300
H	-4.82930800	3.70932400	-2.60277600
N	-2.25309500	1.95640300	-0.24138500
Ir	-0.73538300	0.74190000	0.88057500
O	-0.67988200	3.53403700	-0.66858000
C	-0.16072900	4.57311800	-1.49839800
H	-0.68909500	5.53137000	-1.33463900
H	-0.21264000	4.29083100	-2.56520700
H	0.89126100	4.68291700	-1.20030700
H	0.27812600	2.14665200	1.00872800
H	-1.22289800	1.24582100	2.32583700
I	0.50004600	0.04725500	-1.61113200
H	0.27478000	-0.21701200	1.66290200
H	-2.53297200	4.65788500	-2.30186600
H	-4.51596100	0.49261100	1.25313200
H	2.50268200	3.17966800	1.94501400
C	3.37201600	1.74986000	0.65657100
C	3.59797600	2.77111900	-0.43143400
H	3.00537300	2.52607100	-1.33116500
H	3.28336400	3.76376500	-0.07432700
H	4.66148800	2.83659100	-0.72306100
C	3.51987300	-0.54061000	1.48208100
H	2.51829800	-0.94666100	1.23924300
H	4.26066500	-1.35152400	1.37812200
C	3.54654800	0.03992300	2.89776200
H	3.30400100	-0.75918600	3.61965200
H	4.57477400	0.38182800	3.12005000
C	4.33446800	-0.03631400	-0.79540000
H	3.59408800	-0.76750000	-1.17771800
H	4.34485400	0.78192800	-1.53147000
N	3.85653500	0.48694600	0.48348700
C	2.55909700	1.21182600	3.01787200
H	2.78513200	1.80442500	3.92334700
H	1.52809100	0.82281200	3.14321900
C	5.71778900	-0.66593600	-0.71134700
C	6.01697200	-1.80772500	-1.47638300
C	6.73037700	-0.10071600	0.08630000
C	7.30280300	-2.36683300	-1.45644200
H	5.23204400	-2.26092300	-2.09335200
C	8.01429700	-0.66192300	0.11415300
H	6.49916500	0.77885100	0.69770500
C	8.30574300	-1.79548700	-0.65988000
H	7.51835900	-3.25662500	-2.05749700
H	8.79069000	-0.21255300	0.74265800
H	9.30856700	-2.23461500	-0.63769900



NBn_*o*Ph_protonation_TS_face1

Zero-point correction= 0.740010
(Hartree/Particle)
Thermal correction to Energy= 0.787921
Thermal correction to Enthalpy= 0.788865
Thermal correction to Gibbs Free Energy= 0.653299
Sum of electronic and zero-point Energies= -2227.710262
Sum of electronic and thermal Energies= -2227.662350

Sum of electronic and thermal Enthalpies= -2227.661406
Sum of electronic and thermal Free Energies= -2227.796972
Electronic energy -2229.11318139

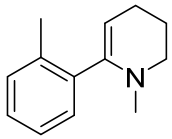
C	-2.44089300	0.55573600	-2.24705600
C	-2.76405800	2.02479100	-2.49502700
C	-3.06612400	-0.17011400	-1.22144200
C	-3.82792500	2.52910000	-1.50702200
H	-1.84144300	2.63538500	-2.41028700
C	-3.60444400	1.92006400	-0.11988200
H	-4.83748100	2.24168000	-1.85453100
H	-4.36993800	2.26910700	0.59224900
H	-2.60400600	2.18476600	0.28406300
H	-3.81427400	3.63088100	-1.43031000
H	-3.12218000	2.15847200	-3.53281600
N	-3.69388100	0.45542200	-0.18347800
H	-0.96972000	0.68156700	-1.73021300
C	3.32361200	-2.00657600	3.54091800
C	2.75166300	-1.94696200	2.25392700
C	3.38672900	-1.18910300	1.24893500
C	4.58445000	-0.51672100	1.54797900
C	5.18593600	-0.58523400	2.81119300
C	4.53010700	-1.33470000	3.79591800
H	2.84001600	-2.57176400	4.34040600
H	6.11660900	-0.04905300	3.01165600
H	4.96483900	-1.39287400	4.79927200
O	1.61563800	-2.60341300	1.88146900
C	0.76041900	-3.08198200	2.91911700
H	0.48108400	-2.26033200	3.60223000
H	-0.14185400	-3.45224900	2.41106500
H	1.22705000	-3.91042200	3.48608200
O	5.17414500	0.21582000	0.53635400
C	4.23102300	0.46060900	-0.53387400
P	2.85477300	-0.83318900	-0.46285600
C	3.46560300	-2.31558400	-1.49454600
C	2.42817100	-3.44361800	-1.31583400
H	2.74042200	-4.32206500	-1.91156600
H	2.33931200	-3.75443500	-0.26158900
H	1.43099500	-3.12379600	-1.66228000
C	4.85265400	-2.78670000	-1.01806200
H	5.17843600	-3.64043500	-1.64122300
H	5.61791100	-1.99564400	-1.10773200
H	4.83371300	-3.12163500	0.03207200
C	3.52762500	-1.90529000	-2.97678400
H	2.54695700	-1.55774300	-3.33822200
H	4.26423300	-1.10244800	-3.16069100
H	3.83634400	-2.77996000	-3.57943000
C	3.66052800	1.87023900	-0.40568400
C	4.51684100	2.90278600	-0.00290800
C	4.01309900	4.20277900	0.08682600
H	5.55309800	2.66675600	0.24704900
C	1.87667800	3.34830700	-0.63536600
C	2.67722500	4.43753700	-0.24095800
H	4.65444600	5.03114900	0.40367000
N	2.34767000	2.07448500	-0.70204100
Ir	1.01473700	0.29169300	-1.07393800
O	0.57804600	3.46773800	-0.98461400
C	-0.04739700	4.73916000	-0.81156000
H	0.40280600	5.50865700	-1.46670300
H	-0.00006100	5.06904100	0.24205100
H	-1.09696300	4.58661300	-1.10013100
H	-0.18986900	1.30482100	-1.74947000
H	1.45315000	0.14560900	-2.60880400
I	-0.12256100	0.68870500	1.53628600
H	0.19587100	-1.05595100	-1.31633200
H	2.26031600	5.44425400	-0.18618900
H	4.79905300	0.37838000	-1.47788800
H	-2.14358300	-0.04312100	-3.11650900
C	-4.06445900	-0.21344100	1.06906700
H	-3.99171700	-1.29975700	0.90151800
H	-3.31080900	0.04459800	1.84116200
C	-3.01082700	-1.66797100	-1.25683900
C	-2.06739500	-2.35402300	-0.46433000
C	-3.86842900	-2.38899400	-2.12784600
C	-1.96551400	-3.75023600	-0.53056000
H	-1.40083300	-1.77706100	0.18678500
C	-3.75503200	-3.79139500	-2.16486800
C	-2.81372100	-4.47163500	-1.38105800
H	-1.21707000	-4.26878700	0.07830600
H	-4.42089100	-4.35684900	-2.82724200
H	-2.74509400	-5.56334700	-1.43658400
C	-4.87801100	-1.69009100	-3.01102300
H	-4.38822900	-1.18509600	-3.86336400
H	-5.60521300	-2.40944600	-3.42264500
H	-5.43741800	-0.91013600	-2.46547100
C	-5.46084900	0.14673700	1.54706600
C	-6.57826500	-0.02075000	0.70620500
C	-5.66449100	0.62117600	2.85509100
C	-7.86814000	0.27499500	1.16446000
H	-6.42961000	-0.38849300	-0.31542300
C	-6.95599500	0.91325900	3.31953900
H	-4.79986500	0.76090900	3.51441300
C	-8.06116900	0.74156000	2.47479800
H	-8.72745300	0.13686400	0.49949700
H	-7.09631500	1.28154300	4.34127800
H	-9.06991300	0.97111200	2.83364700

NBn_oPh_protonation_TS_face2

Zero-point correction= 0.740675 (Hartree/Particle)
Thermal correction to Energy= 0.788634
Thermal correction to Enthalpy= 0.789578
Thermal correction to Gibbs Free Energy= 0.654230
Sum of electronic and zero-point Energies= -2227.711923
Sum of electronic and thermal Energies= -2227.663965
Sum of electronic and thermal Enthalpies= -2227.663021
Sum of electronic and thermal Free Energies= -2227.798368
Electronic energy -2229.11185550

C	2.54703600	1.13995400	2.05010300
H	1.08025100	1.27391000	1.37727000
C	-3.56628700	-3.23048700	-2.35682900
C	-2.98137400	-2.71362000	-1.18355400
C	-3.53888700	-1.56877900	-0.57807000
C	-4.68028800	-0.97707800	-1.14558400
C	-5.29606000	-1.49124900	-2.29430700
C	-4.71315300	-2.61805600	-2.88742800
H	-3.13976600	-4.10338500	-2.85545300
H	-6.18179900	-1.00652700	-2.71178200
H	-5.15980100	-3.03235100	-3.79734100
O	-1.90866900	-3.26354100	-0.54728400
C	-1.10876900	-4.18986500	-1.28165400

H	-0.74989300	-3.73168900	-2.22030700
H	-0.24968800	-4.41507700	-0.63394800
H	-1.65954800	-5.12547000	-1.49784800
O	-5.20200300	0.13601000	-0.51743900
C	-4.24431400	0.70473500	0.40810000
P	-2.94846900	-0.60140600	0.85328100
C	-3.62548900	-1.50663300	2.38966800
C	-2.62637500	-2.63399800	2.71973400
H	-2.97814900	-3.18527900	3.61214600
H	-2.52764400	-3.34762900	1.88515500
H	-1.62718400	-2.21944100	2.93371100
C	-5.02008600	-2.09532000	2.10593700
H	-5.39299300	-2.59707800	3.01842000
H	-5.75533800	-1.31998000	1.82702500
H	-4.99160600	-2.84219000	1.29570900
C	-3.69733900	-0.52137800	3.57021100
H	-2.71481900	-0.06778100	3.77707200
H	-4.42256900	0.29413000	3.39666500
H	-4.02890100	-1.06703500	4.47347000
C	-3.59611400	1.93312100	-0.22054200
C	-4.40654700	2.81625400	-0.94477000
C	-3.82933800	3.95804500	-1.50601800
H	-5.46680300	2.58619600	-1.06784000
C	-1.71306800	3.25320700	-0.58743800
C	-2.46568000	4.18996900	-1.32216500
H	-4.43435100	4.66675900	-2.08009700
N	-2.26074500	2.13190100	-0.04651900
Ir	-1.03561700	0.53445900	0.95990800
O	-0.39155100	3.37879900	-0.35018000
C	0.28622800	4.50528200	-0.91066800
H	-0.10453600	5.45569400	-0.50120900
H	0.20475900	4.51244800	-2.01318700
H	1.33965900	4.38067600	-0.62649200
H	0.27226400	1.67530700	1.21087500
H	-1.43909100	1.02143000	2.43568900
I	0.06660600	-0.22619900	-1.57169000
H	-0.25758300	-0.66159400	1.67687100
H	-1.98976700	5.07479700	-1.74685300
H	-4.81669000	1.00849900	1.30282200
H	2.61571900	2.20009100	2.32361800
C	3.30851300	0.76977700	0.93418100
C	2.83946500	-1.56440900	1.41527500
H	1.79226500	-1.65178100	1.06481400
H	3.35002700	-2.52336700	1.22802000
C	2.89127500	-1.20109900	2.90205800
H	2.40774200	-2.00347000	3.48574200
H	3.95079700	-1.16037600	3.21715000
C	3.94100000	-0.96676500	-0.73553200
H	3.03556800	-1.22980200	-1.32198600
H	4.40074100	-0.09788800	-1.23338600
N	3.52070400	-0.53939000	0.60577000
C	2.20756400	0.15202700	3.15461900
H	2.52997100	0.56206900	4.12987600
H	1.10882800	0.01593000	3.21540900
C	3.90563900	1.84392500	0.07309100
C	3.23579200	2.26156800	-1.09466600
C	5.12627100	2.46092100	0.45269100
C	3.76831100	3.28331900	-1.89414400
H	2.29725000	1.76422700	-1.37194300
C	5.64092400	3.48239700	-0.36789300
C	4.97495800	3.89556900	-1.52954200
H	3.24287300	3.58892400	-2.80523300
H	6.58680700	3.95916600	-0.08536200
H	5.40322500	4.69011500	-2.14995500
C	5.86508400	2.04986600	1.70647800
H	5.32567200	2.36951000	2.61641400
H	5.97398400	0.95355200	1.77734400
H	6.87170000	2.49817400	1.73599200
C	4.92024000	-2.12687600	-0.71852900
C	4.67163600	-3.27180200	-1.49636700
C	6.10711200	-2.06765700	0.03772800
C	5.59090700	-4.33113100	-1.52895400
H	3.74705800	-3.32853200	-2.08242200
C	7.02372700	-3.12639300	0.01331700
H	6.30789000	-1.18181400	0.65132300
C	6.76912000	-4.26156100	-0.77283500
H	5.38174300	-5.21464300	-2.14135900
H	7.94259400	-3.06514700	0.60631700
H	7.48680000	-5.08835200	-0.79325700



NMe_oPh_protonation_TS_face1

Zero-point correction= 0.661021 (Hartree/Particle)
Thermal correction to Energy= 0.704228
Thermal correction to Enthalpy= 0.705172
Thermal correction to Gibbs Free Energy= 0.582303
Sum of electronic and zero-point Energies= -1997.039925
Sum of electronic and thermal Energies= -1996.996718
Sum of electronic and thermal Enthalpies= -1996.995774
Sum of electronic and thermal Free Energies= -1997.118643
Electronic energy -1998.29463566

C	-3.41336200	0.94810700	-1.20894400
C	-3.62922600	2.45582000	-1.28859500
C	-3.86720500	0.20676000	-0.10794500
C	-4.42437100	2.96520300	-0.07577100
H	-2.65326200	2.97984900	-1.35355800
C	-3.98299500	2.24214400	1.20121200
H	-5.50407400	2.77965100	-0.22500900
H	-4.56174600	2.59365500	2.07323700
H	-2.90592500	2.41376000	1.41383000
H	-4.29958400	4.05482600	0.05685400
H	-4.16995600	2.70667600	-2.21976700
N	-4.20526900	0.79925800	1.07270200
H	-1.84081700	0.92588300	-1.06452700
C	3.36214500	-2.55183300	2.68495000
C	2.52555500	-2.30113700	1.57865500
C	2.95815600	-1.41504200	0.57099200
C	4.21962600	-0.80589400	0.68489000
C	5.07883900	-1.06074300	1.76155600
C	4.62250400	-1.93625500	2.75509300
H	3.04068400	-3.22085600	3.48580800
H	6.05343200	-0.57043100	1.82133400
H	5.26313500	-2.14253300	3.61886400
O	1.30819400	-2.88189000	1.38057900
C	0.69758000	-3.53473700	2.49336700
H	0.61753900	-2.84805000	3.35474000
H	-0.31179900	-3.81055500	2.15570900

H	1.25076400	-4.44822400	2.78538600
O	4.60504100	0.05420700	-0.32549500
C	3.46143000	0.45881400	-1.11562000
P	2.08185200	-0.81795900	-0.91680800
C	2.38868700	-2.15350600	-2.24381700
C	1.33935300	-3.26111800	-2.01423200
H	1.47408200	-4.05364100	-2.77431800
H	1.43983900	-3.71820300	-1.01570100
H	0.31595700	-2.86027100	-2.10470200
C	3.81024400	-2.73347900	-2.12120400
H	3.96161600	-3.49243300	-2.91129500
H	4.58994000	-1.96154000	-2.24401000
H	3.96866100	-3.22225200	-1.14601800
C	2.18851700	-1.53520000	-3.63921600
H	1.18242300	-1.09993400	-3.74706700
H	2.92954200	-0.74555300	-3.85937100
H	2.31307900	-2.32502600	-4.40350700
C	2.99145600	1.83932700	-0.66490900
C	3.95835400	2.78970900	-0.31395900
C	3.54174600	4.05740600	0.09958000
H	5.01373400	2.51258200	-0.34989700
C	1.26299600	3.33882400	-0.23070800
C	2.17689100	4.34396300	0.14029300
H	4.27189300	4.82048800	0.38675600
N	1.65486400	2.09571900	-0.61790300
Ir	0.20492900	0.40512100	-0.95773500
O	-0.07565000	3.51817200	-0.24020700
C	-0.58974700	4.71598100	0.34179800
H	-0.28012900	5.61382500	-0.22571400
H	-0.27613700	4.80889300	1.39706100
H	-1.68306900	4.61652600	0.29158900
H	-1.06173500	1.51722600	-1.24738800
H	0.31531700	0.47537000	-2.55499900
I	-0.34492600	0.45140500	1.86867700
H	-0.70536000	-0.87838700	-1.22698300
H	1.82515800	5.32637300	0.45842400
H	3.80466600	0.50656700	-2.16432500
H	-3.39281100	0.39453200	-2.15552400
C	-4.32234400	0.06477100	2.32789800
H	-4.59072900	-0.98163300	2.12834100
H	-3.36063000	0.08692800	2.87893900
H	-5.10944500	0.52910300	2.94744600
C	-4.01303400	-1.28137400	-0.22494800
C	-2.91922600	-2.12117800	0.05757900
C	-5.24959900	-1.83325400	-0.65046600
C	-3.03974200	-3.51086800	-0.08603600
H	-1.97518200	-1.67211900	0.38455400
C	-5.34635200	-3.23086000	-0.77830100
C	-4.25566900	-4.06760000	-0.50294900
H	-2.17810300	-4.15375300	0.12481900
H	-6.29766000	-3.66624900	-1.10597800
H	-4.35875000	-5.15210900	-0.61714000
C	-6.43755600	-0.95019100	-0.95881900
H	-6.76046800	-0.37565800	-0.07172500
H	-6.19407600	-0.20945900	-1.74145600
H	-7.29607100	-1.54739700	-1.30703400

NMe_oPh_protonation_TS_face2

Zero-point correction= 0.661941 (Hartree/Particle)
Thermal correction to Energy= 0.705089
Thermal correction to Enthalpy= 0.706034
Thermal correction to Gibbs Free Energy= 0.583538
Sum of electronic and zero-point Energies= -1997.041358
Sum of electronic and thermal Energies= -1996.998210
Sum of electronic and thermal Enthalpies= -1996.997266
Sum of electronic and thermal Free Energies= -1997.119761
Electronic energy -1998.29323846

C	-3.26942500	-0.90046700	-1.64952700
H	-1.89448300	-0.08796400	-1.27312600
C	4.08190300	-1.50072100	2.91117100
C	3.31867700	-1.58534000	1.72943200
C	3.43708800	-0.57344000	0.75492200
C	4.32907500	0.49031400	0.97330400
C	5.11907800	0.57968400	2.12673900
C	4.97116000	-0.42843200	3.08747400
H	3.99252800	-2.26261600	3.68835900
H	5.80178100	1.42121300	2.26638400
H	5.56115900	-0.37775200	4.00854100
O	2.47459900	-2.61251100	1.42687700
C	2.04470100	-3.44851000	2.50120100
H	1.58948700	-2.84217300	3.30423500
H	1.28361900	-4.11395900	2.06980800
H	2.87663600	-4.05707900	2.90503800
O	4.42401400	1.45635400	-0.00852500
C	3.30535300	1.37683100	-0.92350400
P	2.51638200	-0.33745700	-0.80406400
C	3.41979700	-1.41631700	-2.09179300
C	2.85127500	-2.84464200	-1.96497900
H	3.36124700	-3.50616400	-2.69052800
H	3.00197800	-3.25646900	-0.95334000
H	1.76978400	-2.85721500	-2.18040000
C	4.93749800	-1.42045800	-1.82841300
H	5.43814000	-2.02358400	-2.60873000
H	5.37134200	-0.40544900	-1.85925300
H	5.18161300	-1.86232000	-0.84853800
C	3.13045300	-0.87118700	-3.50222500
H	2.04780800	-0.81881500	-3.70010900
H	3.55794800	0.13546800	-3.66086200
H	3.59184600	-1.54374300	-4.24937600
C	2.29673100	2.47514600	-0.60341800
C	2.78133300	3.74461200	-0.26515600
C	1.86851900	4.77268500	-0.01711700
H	3.85960400	3.89960800	-0.19095500
C	0.09021600	3.20698900	-0.47096800
C	0.50289100	4.51019600	-0.13179900
H	2.21411500	5.77497100	0.25458900
N	0.96776300	2.18987800	-0.68407500
Ir	0.33159700	0.05076800	-0.97705700
O	-1.20212700	2.84996200	-0.62131000
C	-2.20597400	3.83391300	-0.36296000
H	-2.13478900	4.67860800	-1.07355800
H	-2.13788200	4.21151000	0.67385700
H	-3.16354200	3.31279400	-0.49559100
H	-1.29168800	0.59358200	-1.34463000
H	0.48142500	0.11495300	-2.57493700
I	-0.35532400	-0.10753100	1.79810800
H	-0.00182100	-1.49814100	-1.16974600
H	-0.23087700	5.29789800	0.04420200
H	3.71639000	1.54607600	-1.93496900
H	-3.70464300	-0.07379100	-2.22401500
C	-3.81145900	-1.08289600	-0.37226600
C	-2.62301800	-3.19106700	-0.17639200

H	-1.58715000	-2.85432500	0.02470900
H	-2.78923000	-4.13753500	0.36815500
C	-2.85120800	-3.38037900	-1.67971000
H	-2.15849600	-4.15318200	-2.05549600
H	-3.87965300	-3.75661800	-1.83539700
C	-3.78152900	-2.26235300	1.81061700
H	-2.86956200	-1.94886000	2.35856100
H	-4.61055100	-1.60007300	2.09621900
H	-4.03770200	-3.29894800	2.09054200
N	-3.56103100	-2.20035100	0.36962200
C	-2.65395800	-2.05201600	-2.42797000
H	-3.11864000	-2.11289100	-3.42964400
H	-1.57285100	-1.86669500	-2.59143400
C	-4.71011400	-0.02766600	0.20135600
C	-4.17214300	0.99932500	1.00095100
C	-6.09996400	-0.05513300	-0.08588500
C	-5.00236200	2.00563800	1.51705100
H	-3.09831400	0.98781400	1.22796600
C	-6.91105900	0.96562700	0.44338000
C	-6.37503900	1.98974400	1.23627600
H	-4.57377900	2.79252700	2.14707900
H	-7.98567600	0.95128700	0.22712600
H	-7.03183400	2.76909700	1.63750600
C	-6.70415000	-1.15251900	-0.93231000
H	-6.27406500	-1.15986900	-1.94979500
H	-6.50704500	-2.15057100	-0.50183200
H	-7.79576300	-1.02883400	-1.02203800

Tunneling Probability

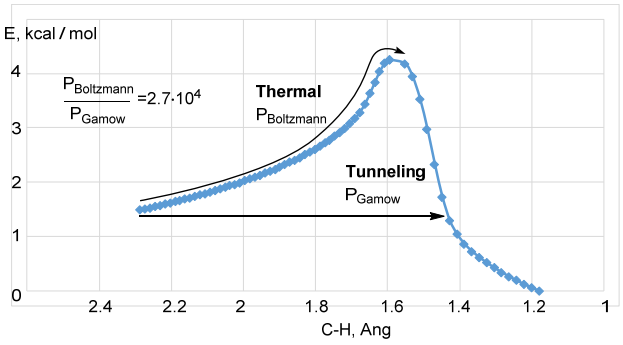
Probability of the particle to acquire enough energy to go over the barrier:

$$P_{Boltzmann} = \exp\left(-\frac{E_{act}}{RT}\right)$$

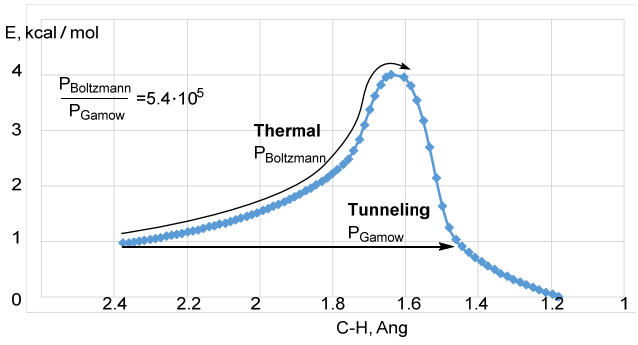
Probability of the particle to go through the barrier[6]:

$$P_{Gamow} = \exp\left(-\frac{2S}{\hbar}\right); S = \int_a^b \sqrt{2m(E - E_0)}dx$$

Where x is reaction coordinate;
Protonation molecular vibration can be associated with migration of proton; Mapping corresponding IRC curves in corresponding coordinates we get the width and shape of the barrier; Using triangular approximation of the barrier shape $E(x)$ we can estimate P_{Gamow}; At reaction temperature tunneling is unlikely to contribute significantly to the mechanism of proton transfer;



Face 1



Face 2

[6] Skodje, R. T., Truhlar, D. G., Garrett., B. C. *J. Phys. Chem.*, **1981**, *85*, 3019.