Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Microwave-assisted *ortho*-alkylation of azine *N*-oxides with *N*-tosylhydrazones catalyzed by copper(I)iodide

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1. Experimental Section

All the chemicals were purchased from commercial sources and used as received. Solvents were dried according to literature procedure. All the reactions to make final products were done under microwave irradiation using CEM Discover system microwave power of 100 watts. All the products were purified by flash column chromatography on silica gel using 230-400 mesh. ^{1}H and ^{13}C NMR spectra were measured on a Bruker DPX-300 MHz spectrometer (^{1}H 300 MHz, ^{13}C 75MHz), using $CDCl_3$ and DMSO as the solvents with tetramethylsilane (TMS) as the internal standard at room temperature. Chemical shifts are given in δ (ppm) relative to TMS, the coupling constants (*J)* are given in Hz**.** High-resolution mass spectra were recorded with a Q-TOF instrument, using electrospray ionization (ESI) as the ionization method.

Experimental procedures:

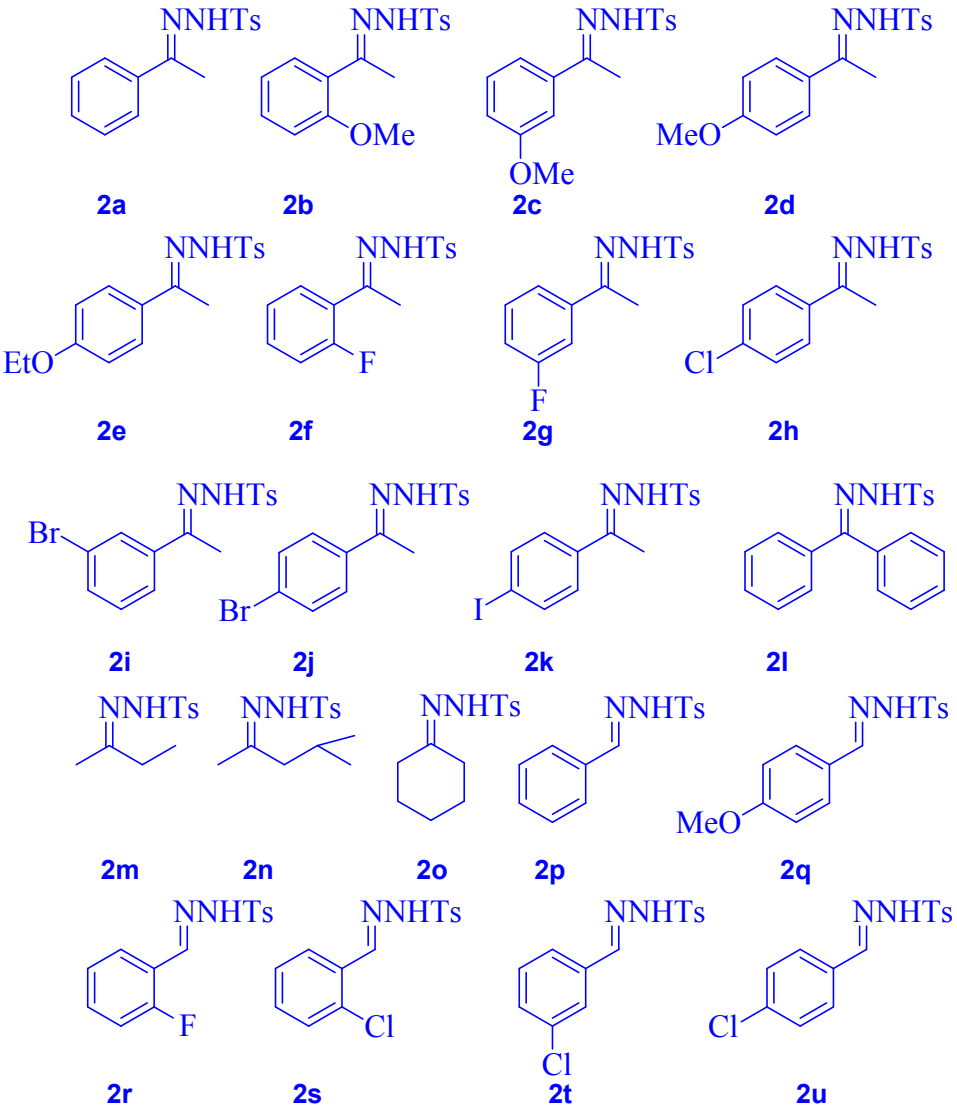
Preparation of tosylhydrazines

Hydrazine monohydrate (2.0 equiv.) was taken in one litre round bottom flask containing water and cooled to 0 ^{o}C. To this, a saturated solution of tosylchloride in THF was added dropwise at 0 ^{o}C. The reaction mixture was further stirred at 0 ^{o}C for 30 minutes. Progress of reaction was monitored through thin layer chromatography. The reaction mixture was extracted with dichloromethane and dried at low pressure to afford pure product.

General experimental procedure for preparation of tosylhydrazones:

The ketone or aldehyde (8.3 mmol) was added to the methanolic solution (24 mL) of *p*-toluenesulfonhydrazine (8.3 mmol) in 100 ml round bottom flask. The reaction mixture was refluxed for 0.5-2 h, and then allowed to cool to room temperature. The solvent was evaporated under reduced pressure. The crystalline product was washed thoroughly with 30 mL of hexane (4-5 times) and dried to afford pure product.

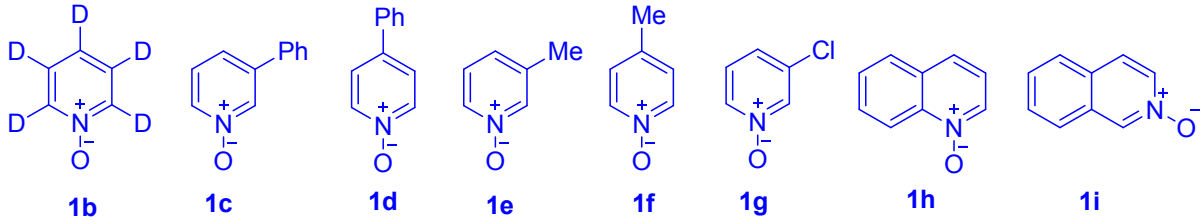
Hydrazones (2a – 2u) were synthesized using the above method:



General experimental procedure for preparation of *N*-Oxides:

Solution of nitrogenous compound (7.8 mmol) in dichloromethane was taken in 100 ml round bottom flask. To this solution 70% m-CPBA (1.0 equiv.) was added portion wise at 0 ^{o}C. The reaction mixture was stirred at room temperature for 12 h. The progress of reaction was monitored through TLC. The reaction mixture was diluted with dichloromethane, and 4.0 equiv. of K_2CO_3 was added and stirred for next 10 minutes. The desired product was purified by flash column chromatography using methanol-dichloromethane solvent.

***N*-Oxides (1b – 1i) were synthesized using the above method:**



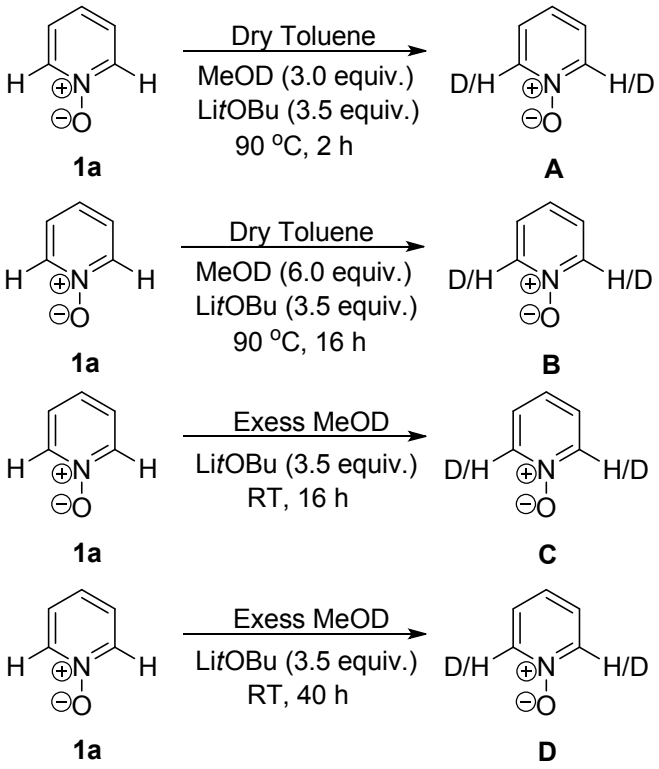
1b **1c** **1d** **1e** **1f** **1g** **1h** **1i**

General experimental procedure for *ortho*-alkylation of Pyridine *N*-Oxide and its derivatives (3a-3z, 3a', 3b'):

In an oven dried microwave tube, tosylhydrazone (1.1 mmol, 2.0 equiv.), LiO^{t}Bu (1.8 mmol, 3.5 equiv.), CuI (0.05 mmol, 0.1 equiv.) and Pyridine *N*-Oxide (0.53 mmol, 1.0 equiv.) were taken in dry toluene, and nitrogen was purged in the reaction mixture for 5-6 minutes. The contents were irradiated in *MW* at 100 °C for one hour. The solvent was removed on rota-evaporator at low pressure. The desired product was purified on flash column chromatography using 3% methanol-dichloromethane solvent. The coloured impurities was removed by passing through charcoal.

Experimental procedure for Deoxygenation of 2-(1-(3-methoxyphenyl)ethyl)pyridine1-oxide (3c) : Compound **3c** (0.22 mmol) and PBr_3 (0.26 mmol) were taken in round bottom flask in dry dichloromethane solvent and stirred for 1h. Solvent was evaporated on rotary evaporator at low pressure. The deoxygenated product (**5a**) was purified through flash column chromatography.

Deuterium exchange experiment: Deuterium exchange of **1a** was carried out under reported conditions,[1] and the product distribution was analysed by ^{1}HNMR spectra. The reaction was tried under varied reaction conditions involving change in amount of MeOD, time and temperature but in none of the cases, the reaction went to completion and a mixture of unreacted **1a** and its mono-deuterated or di-deuterated analogs (**A-D**) were obtained.



H^a: protons at 2,6-positions; H^b: protons at 3,5-positions; H^c: protons at 4-position.

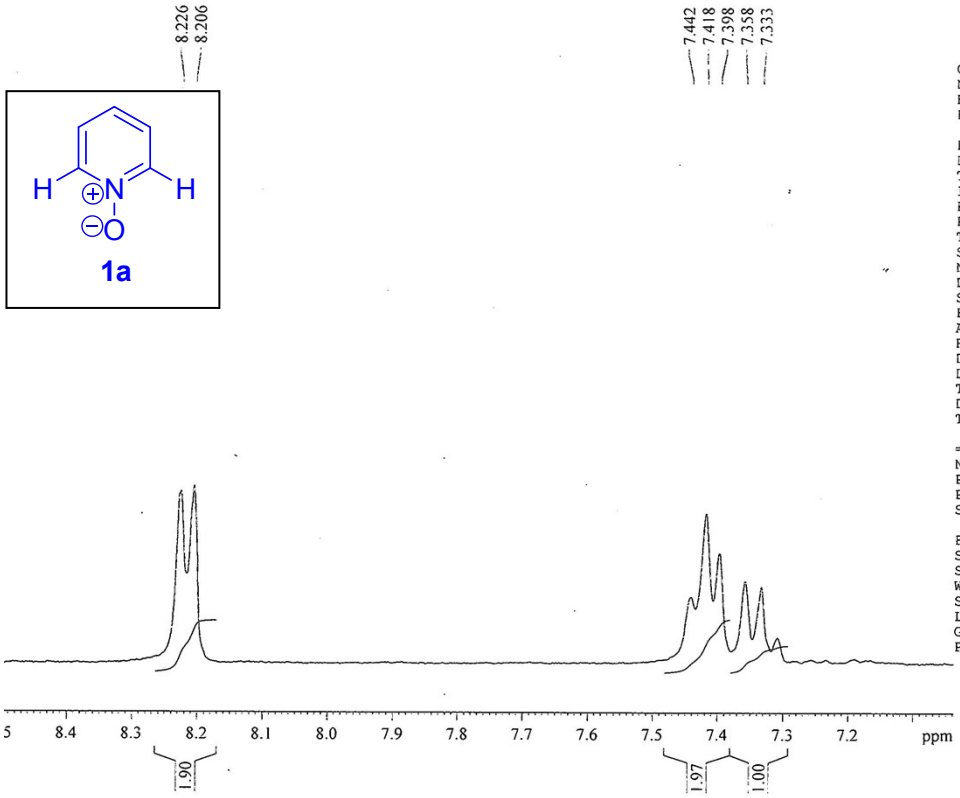
In **1a**, $H^a = 1.9$; $H^b = 1.97$; $H^c = 1$

In **A**, $H^a = 1.32$; $H^b = 2$; $H^c = 1$; In the presence of LiO*t*Bu, the decrease at H*a* indicates that the deuterium exchange only occurs at 2,6-positions.

In **B**, $H^a = 0.91$; $H^b = 2.31$; $H^c = 1$; This results indicate under the reaction conditions, deuterium exchange occurs preferentially at 2,6-positions.

In **C**, $H^a = 0.50$; $H^b = 2$; $H^c = 1$; This results indicate under the reaction conditions, deuterium exchange occurs preferentially at 2,6-positions.

In **D**, $H^a = 0.42$; $H^b = 2$; $H^c = 1$; This results indicate under the reaction conditions, deuterium exchange occurs preferentially at 2,6-positions.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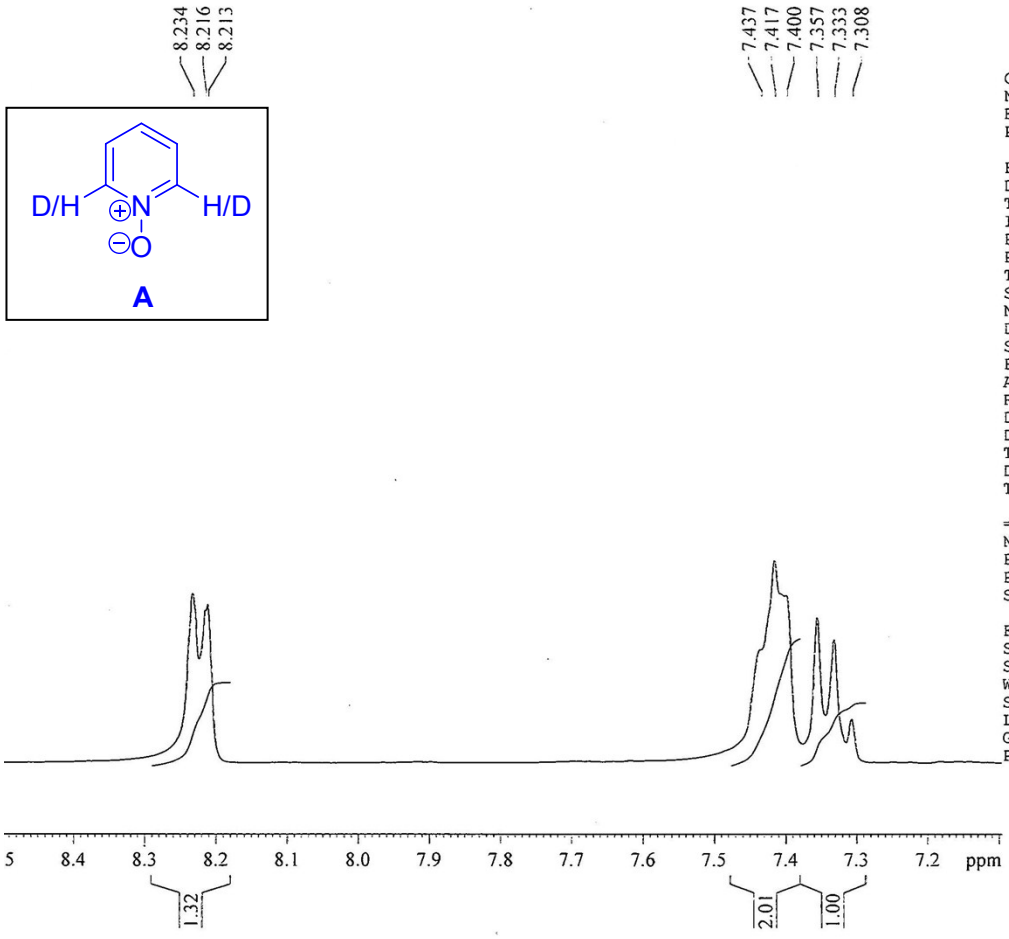
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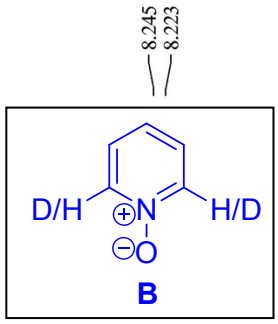


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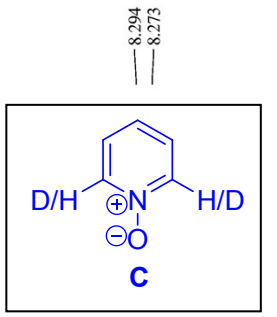


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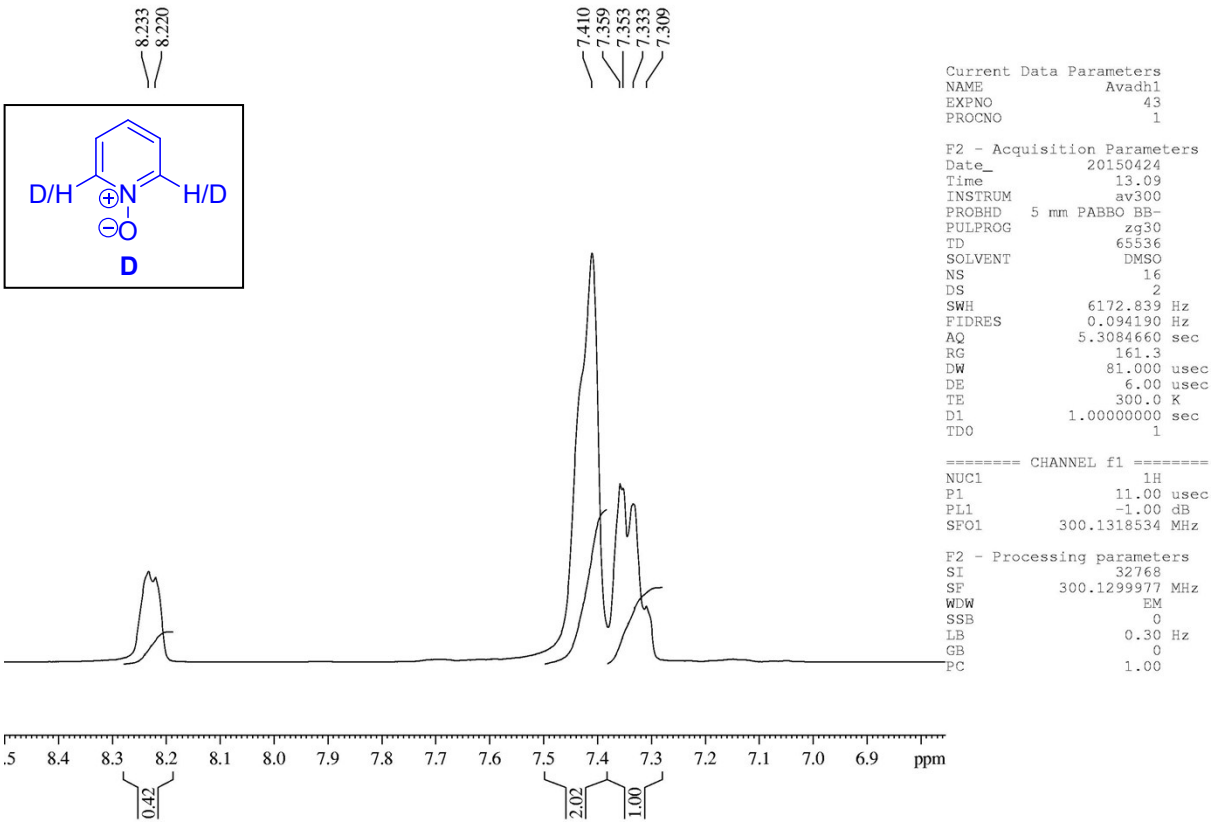


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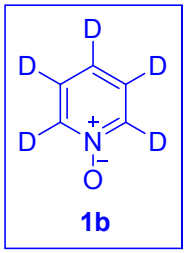
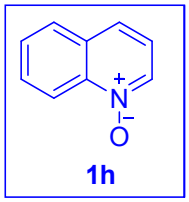
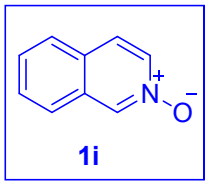


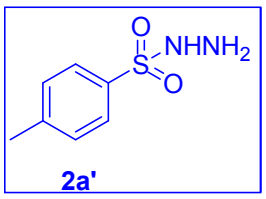
d^{5} pyridine 1-oxide (1b): Yellow solid, 593 mg, 76 %; ^{13}C NMR (75 MHz, $CDCl_3$) δ 139.33-139.57, 138.99-139.19, 138.62-138.79, 125.79-125.97, 125.64, 125.30-125.44.



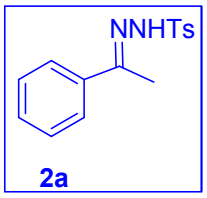
Quinoline 1-oxide (1h): Dark brown solid, 906 mg, 80 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.73 (d, *J* = 8.4 Hz, 1H), 8.55 (d, *J* = 6 Hz, 1H), 7.86 (d, J = 7.8 Hz, 1H), 7.75 (t, J = 4.5 Hz, 2H), 7.60-7.66 (m, 1H), 7.27-7.38 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 141.28, 135.66, 130.47, 130.41, 128.73, 128.13, 126.39, 120.92, 119.54.



Isoquinoline 1-oxide (1i): Dark brown solid, 974 mg, 86 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.80 (s, 1H), 8.14-8.17 (m, 1H), 7.79-7.82 (m, 1H), 7.73-7.76 (m, 1H), 7.66-7.70 (m, 1H), 7.58-7.65 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 136.18, 135.81, 129.10, 128.96, 128.77, 128.50, 126.20, 124.62, 123.86.

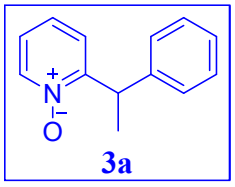


4-Methylbenzenesulfonohydrizide (2a'): White solid, ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.80 (d, J = 8.4 Hz, 2H), 7.36 (d, *J* = 8.4 Hz, 2H), 5.66 (s, 1H), 3.61 (s, 2H) 2.46 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 144.63, 133.20, 129.96, 128.28, 21.60.

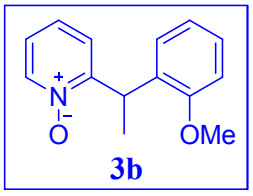


4-methyl-N'-(1-phenylethylidene)benzenesulfonohydrazide (2a): White crystalline solid, 1.92g, 80 %; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.16 (s, 1H), 7.94 (d, *J* = 8.1 Hz, 2H), 7.62-7.65 (m, 2H), 7.30-7.44 (m, 5H) 2.61 (s, 3H) 2.16 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 152.75, 144.18, 137.32, 135.43, 129.64, 129.57, 128.33, 128.14, 127.94, 126.31, 21.63, 13.53.

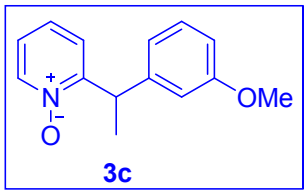
^{1}H and ^{13}C NMR data of *Ortho*-alkylation of pyridine N-Oxide (3a-3z, 3a', 3b', 4a-4d, 5a, 5b):



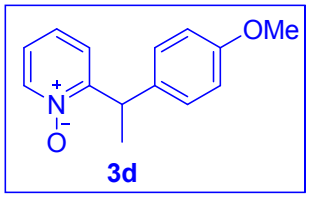
2-(1-phenylethyl)pyridine 1-oxide (3a): Sticky pale yellow solid, 59 mg, 70%; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.20 (d, *J* = 5.7 Hz, 1H), 7.23-7.28 (m, 4H), 7.18-7.21 (m, 1H), 7.13-7.17 (m, 1H), 7.03-7.11 (m, 2H), 4.99 (q, *J* = 7.2 Hz, 1H), 1.58 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.31, 141.19, 138.78, 127.60, 126.94, 125.84, 124.92, 123.45, 122.34, 37.20, 17.48; HRMS ESI: $[M+H]^+$, Calculated for $C_{13}H_{14}NO$ 200.1070; found 200.1069.



2-(1-(2-methoxyphenyl)ethyl)pyridine 1-oxide (3b): Sticky white solid, 87 mg, 90%; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.38 (d, *J* = 2.1 Hz, 1H), 7.16-7.28 (m, 4H), 7.04 (d, *J* = 7.5 Hz, 1H), 6.97 (t, *J* = 7.5 Hz, 1H), 6.85 (d, *J* = 8.7 Hz, 1H), 5.26 (q, J = 6.6 Hz, 1H), 3.69 (s, 3H), 1.62 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.27, 139.96, 130.33, 128.16, 127.78, 127.46, 124.28, 123.07, 120.55, 114.10, 110.83, 55.38, 33.10, 16.76; HRMS ESI: $[M+H]^+$, Calculated for $C_{14}H_{16}NO_2$ 230.1176; found 230.1175.

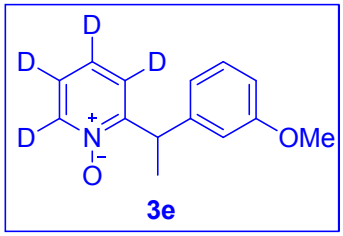


2-(1-(3-methoxyphenyl)ethyl)pyridine1-oxide (3c): Sticky dark brown solid, 84 mg, 87%; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.24 (d, *J* = 5.1Hz 1H), 7.23 (d, *J* = 8.1Hz 1H), 7.13-7.18 (m, 3H), 6.78-6.90 (m, 3H), 5.04 (q, J = 6.9 Hz, 1H), 3.78 (s, 3H), 1.64 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.81, 156.10, 143.96, 139.66, 129.55, 125.47, 124.49, 123.36, 120.30, 114.06, 112.01, 55.18, 38.21, 18.40; HRMS ESI: $[M+H]^+$, Calculated for $C_{14}H_{16}NO_2$ 230.1176; found 230.1176.



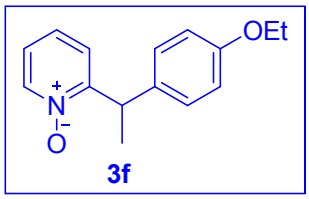
2-(1-(4-methoxyphenyl)ethyl)pyrizdine1-oxide (3d): Sticky dark brown solid, 89 mg, 92%; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.24 (d, *J* = 6Hz 1H), 7.17-7.26 (m, 3H), 7.13 (d, *J* = 6.9 Hz, 2H), 6.86 (d, *J* = 8.4 Hz, 2H), 4.97 (q, J = 7.2Hz, 1H), 3.78 (s, 3H), 1.62 (d, *J* = 7.5 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.48, 156.59, 139.79, 134.23, 128.97, 127.79,

126.10, 124.38, 123.35, 114.03, 55.26, 37.47, 18.61; HRMS ESI: $[M+H]^+$, Calculated for $C_{14}H_{16}NO_2$ 230.1176; found 230.1174.



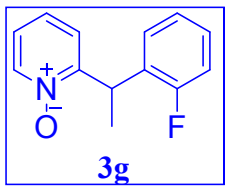
3e

2-(1-(3-methoxyphenyl)ethyl)d^4-pyridine1-oxide (3e): Sticky pale yellow solid, 86 mg, 88 %; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.25 (s, 1H), 7.23 (d, J = 7.8 Hz, 1H), 6.77-6.90 (m, 3H), 5.03 (q, J = 6.9 Hz, 1H), 3.78 (s, 3H), 1.64 (d, J = 6.9 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.82, 186.09, 143.87-153.92, 139.68, 129.55, 125.26-125.59, 123.81-124.47, 122.67-123.36, 120.30, 114.06, 112.03, 55.18, 38.20, 18.32-18.41; HRMS ESI: $[M+H]^+$, Calculated for $C_{14}H_{12}D_4NO_2$ 234.1427; found 234.1428.



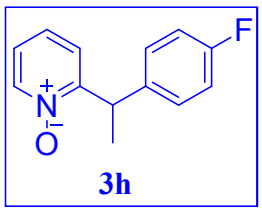
3f

2-(1-(4-ethoxyphenyl)ethyl)pyrizdine1-oxide (3f): Sticky dark brown solid, 70 mg, 68 %; **1**NMR (300 MHz, $CDCl_3$) δ 8.23 (d, J = 5.7 Hz, 1H), 7.21 (d, J = 8.7 Hz, 2H), 7.09-7.17(m, 3H), 6.85 (d, J = 8.7 Hz, 2H), 5.00 (q, J = 7.2 Hz, 1H), 4.01 (q, J = 7.2Hz, 2H), 1.63 (d, J = 7.2 Hz, 3H), 1040 (t, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.83, 156.78, 139.75, 134.13, 128.94, 125.48, 124.28, 123.12, 114.58, 63.42, 37.36, 18.47, 14.85; HRMS ESI: $[M+H]^+$, Calculated for $C_{15}H_{18}NO_2$ 244.1332; found 244.1323.



3g

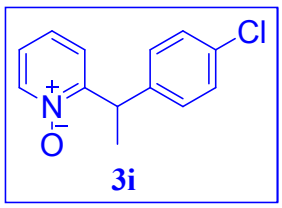
2-(1-(2-fluorophenyl)ethyl)pyridine 1-oxide (3g): Sticky brown solid, 78 mg , 86 %; **1**NMR (300 MHz, $CDCl_3$) δ 8.23 (d, J = 2.7 Hz 1H), 7.27-7.31 (m, 2H), 7.22 (m, 2H), 7.09-7.17 (m, 2H), 7.01 (t, J = 8.7 Hz, 1H), 5.14 (q, J = 6.6 Hz, 1H), 1.67 (d, J = 6.9 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.70, 159.43, 154.68, 139.73, 129.13-129.28, 128.47-128.58, 125.29, 124.10-124.28, 123.58, 115.81, 115.52, 33.45, 17.27; HRMS ESI: $[M+H]^+$, Calculated for $C_{13}H_{13}FNO$ 218.0976; found 218.0981.



3h

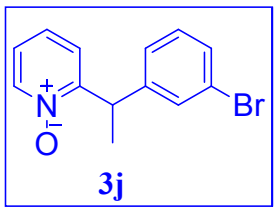
2-(1-(4-fluorophenyl)ethyl)pyridine 1-oxide (3h): Brown Sticky brown solid, 78 mg, 85 %; **1**NMR (300 MHz, $CDCl_3$) δ 8.22 (s, 1H), 7.23-7.26 (m, 2H), 7.14-7.17 (m, 3H), 6.70 (t, J = 8.7 Hz, 2H), 5.01 (d, J = 6.6 Hz, 1H), 1.63 (d, J = 6.9 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.35, 160.10, 156.05, 140.01, 137.74-137.78, 129.38-129.49, 126.94, 123.59-

124.30, 115.28-115.56, 37.63, 18.81; HRMS ESI: $[M+Na]^+$, Calculated for $C_{13}H_{13}FNNaO$ 240.0795; found 240.0795.



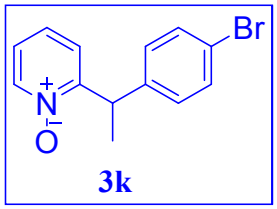
3i

2-(1-(4-chlorophenyl)ethyl)pyridine 1-oxide (3i): Sticky pale yellow solid, 74 mg, 75 %; ^{1}NMR (300 MHz, CDCl3) δ 8.23 (d, *J* = 5.7 Hz, 1H), 7.29-7.30 (m, 1H), 7.27 (s, 2H), 7.24 (s, 2H), 7.12-7.21 (m, 3H), 4.99 (q, *J* = 7.2 Hz, 1H), 1.63 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.70, 140.84, 139.94, 132.61, 129.23, 128.71, 125.59, 124.09, 123.51, 37.74, 18.68; HRMS ESI: $[M+Na]^+$, Calculated for $C_{13}H_{12}ClNNaO$ 256.0500; found 256.0496.



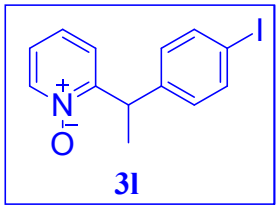
3j

2-(1-(3-bromophenyl)ethyl)pyridine 1-oxide (3j): Sticky pale yellow solid, 86 mg, 74 %; **1**NMR (300 MHz, $CDCl_3$) δ 8.20 (s, 1H), 7.24-7.29 (m, 4H), 7.16-7.21 (m, 3H), 5.01 (d, *J* = 5.1 Hz, 1H), 1.63 (d, *J* = 6.6 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.72, 140.87, 139.88, 132.57, 129.22, 129.03, 128.87, 128.70, 125.67, 124.04, 123.46, 37.72, 18.72; HRMS ESI: $[M+H]^+$, Calculated for $C_{13}H_{13}BrNO$ 278.0175; found 278.0174.



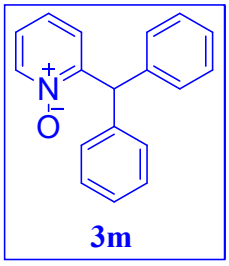
3k

2-(1-(4-bromophenyl)ethyl)pyridine 1-oxide (3k): Sticky brown solid, 89 mg, 76 %; **1**NMR (300 MHz, $CDCl_3$) δ 8.15 (d, *J* = 5.7 Hz, 1H), 7.33-7.37 (m, 2H), 7.04-7.10 (m, 5H), 4.90 (q, *J* = 6.9 Hz, 1H), 1.55 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.17, 141.38, 139.81, 131.66, 129.60, 125.53, 124.12, 123.57, 120.68, 37.82, 18.63; HRMS ESI: $[M+H]^+$, Calculated for $C_{13}H_{13}BrNO$ 278.0175; found 271.0176.



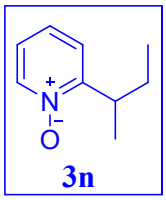
3l

2-(1-(4-iodophenyl)ethyl)pyridine 1-oxide (3l): Sticky dark brown solid, 94 mg, 69 %; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.20 (s, 1H), 7.63 (d, *J* = 7.8 Hz, 2H), 7.18 (s, 3H), 7.04 (d, *J* = 7.5 Hz, 2H), 4.98 (s, 1H), 1.61 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.36, 142.21, 140.16, 137.63, 129.93, 126.25, 123.94, 123.28, 92.16, 37.88, 18.72; HRMS ESI: $[M+Na]^+$, Calculated for $C_{13}H_{12}INNaO$ 347.9856; found 347.9856.

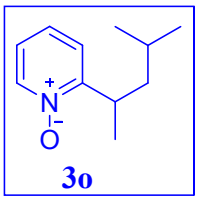


3m

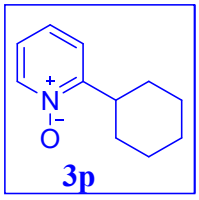
2-benzhydrylpyridine 1-oxide (3m): Sticky brown solid, 68 mg, 62 %; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.25 (s, 1H), 7.25-7.34 (m, 5H), 7.23 (s, 1H), 7.16 (s, 1H), 7.11 (d, *J* = 6.9 Hz, 4H), 6.98 (d, *J* = 6.3 Hz, 1H), 6.34 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.65, 140.28, 139.84, 129.24, 128.67, 128.28, 127.88, 127.41, 127.02, 126.84, 124.98, 124.88, 123.74, 50.41; HRMS ESI: $[M+H]^+$, Calculated for C18H16NO 262.1226; found 262.1227.



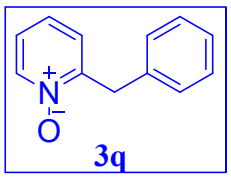
2-sec-butylpyridine 1-oxide (3n): Sticky dark brown solid, 47 mg, 74 %; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.19 (d, *J* = 6.3 Hz, 1H), 7.03-7.20 (m, 3H), 3.58-3.63 (m, 1H), 1.63-1.75 (m, 2H), 1.19 (d, *J* = 6.6 Hz, 3H), 0.86 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.08, 139.83, 125.62, 123.29, 122.88, 33.77, 27.33, 17.79, 11.55; HRMS ESI: $[M+H]^+$, Calculated for $C_9H_{14}NO$ 152.1070; found 152.1071.



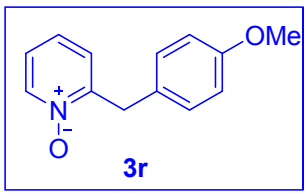
2-(4-methylpentan-2-yl)pyridine 1-oxide (3o): Sticky brown solid, 55 mg, 73 %; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.26 (d, *J* = 4.8 Hz, 1H), 7.11-7.27 (m, 3H), 3.84-3.89 (m, 1H), 1.54-1.67 (m, 2H), 1.37-1.44 (m, 1H), 1.26 (d, J= 6 Hz, 3H), 0.92-0.95 (m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.70, 139.88, 125.88, 123.31, 122.82, 44.25, 30.20, 25.83, 23.12, 22.29, 18.77; HRMS ESI: $[M+H]^+$, Calculated for $C_{11}H_{18}NO$ 180.1383; found 180.1382.



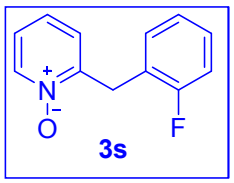
2-cyclohexylpyridine 1-oxide (3p): Sticky brown solid, 51 mg, 68 %; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.22 (s, 1H), 7.26 (d, *J* = 10.5 Hz, 1H), 7.15 (d, *J* = 10.8 Hz, 2H), 3.59 (d, *J* = 9.9 Hz, 1H), 2.06 (d, *J* = 12.6 Hz, 2H), 1.79-1.89 (m, 4H), 1.46-1.59 (m, 2H), 1.21-1.34 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.51, 139.81, 126.00, 123.01, 122.62, 37.00, 30.82, 26.30, 26.22; HRMS ESI: $[M+H]^+$, Calculated for $C_{11}H_{16}NO$ 178.1226; found 178.1225.



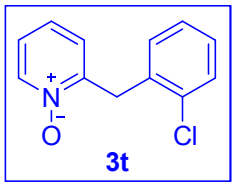
2-benzylpyridine 1-oxide (3q): Sticky brown solid, 67 mg, 86%; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.30 (t, *J* = 5.1 Hz, 1H), 7.25-7.30 (m, 2H), 7.18-7.23 (m, 3H), 7.10-7.13 (m, 2H), 6.88-6.91 (m, 1H), 4.20 (s, 2H), ^{13}C NMR (75 MHz, $CDCl_3$) δ 152.28, 139.62, 136.07, 129.71, 128.89, 127.12, 126.89, 125.99, 123.74, 36.52; HRMS ESI: $[M+Na]^+$, Calculated for $C_{12}H_{11}NNaO$ 208.0733; found 208.0735.



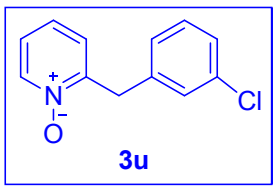
2-(4-methoxybenzyl)pyridine 1-oxide (3r): Sticky brown solid, 84 mg, 93 %; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.41 (d, *J* = 5.4 Hz, 1H), 8.02 (d, *J* = 8.1 Hz, 1H), 7.20 (d, *J* = 7.8 Hz, 4H), 6.89 (d, *J* = 7.8 Hz, 3H), 4.22 (s, 2H), 3.80 (s, 3H),; ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.71, 152.46, 139.46, 130.76, 128.15, 125.69, 123.41, 114.30, 113.48, 55.28, 35.67; HRMS ESI: $[M+Na]^+$, Calculated for $C_{13}H_{13}NNaO_2$ 238.0838; found 238.0847.



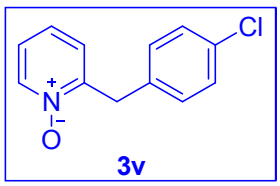
2-(2-fluorobenzyl)pyridine 1-oxide (3s): Sticky brown solid, 68 mg, 80 %; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.29 (s, 1H), 7.36 (t, J = 7.2 Hz, 1H), 7.08-7.16 (m, 4H), 7.02-7.05 (m, 2H), 4.28 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.01, 159.75, 150.33, 139.52, 132.16-132.21, 129.06-129.17, 125.62-125.70, 124.43-124.48, 123.78, 123.12-123.32, 115.37-115.66, 30.21-30.25; HRMS ESI: $[M+Na]^+$, Calculated for $C_{12}H_{10}FNNaO$ 226.0639; found 226.0644.



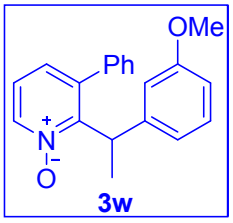
2-(2-chlorobenzyl)pyridine 1-oxide (3t): Sticky Pale yellow solid, 72 mg , 78 %; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.31(d, *J* = 6.3 Hz, 1H), 7.41-7.44 (m, 1H), 7.35-7.38 (m, 1H), 7.25-7.29 (m, 2H), 7.12-7.20 (m, 2H), 6.87-6.90 (m, 1H), 4.39 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 150.14, 139.45, 134.79, 134.19, 132.02, 129.78, 128.77, 127.24, 125.57, 125.47, 123.66, 34.54; HRMS ESI: $[M+H]^+$, Calculated for $C_{12}H_{11}ClNO$ 220.0524; found 220.0515.



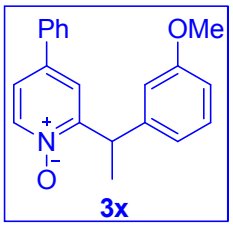
2-(3-chlorobenzyl)pyridine 1-oxide (3u): Sticky white solid , 70 mg, 76 %; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.30 (d, J = 2.7 Hz, 1H), 7.26-7.28 (m, 3H), 7.16-7.19 (m, 3H), 7.00 (t, J = 5.4 Hz, 1H), 4.24 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.81, 139.59, 138.39, 134.61, 130.04, 129.61, 127.83, 127.30, 125.86, 125.49, 123.88, 36.19; HRMS ESI: $[M+H]^+$, Calculated for $C_{12}H_{11}ClNO$ 220.0524; found 220.0523.



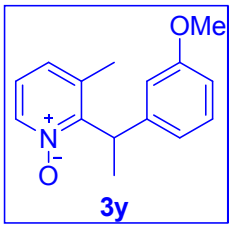
2-(4-chlorobenzyl)pyridine 1-oxide (3v): Sticky brown solid, 66 mg, 72 %; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.28 (d, *J* = 3 Hz, 1H), 7.30-7.40 (m, 3H), 7.25 (d, *J* = 8.4 Hz, 2H), 7.11-7.18 (m, 1H), 6.98-7.01 (m, 1H), 4.23 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.32, 139.55, 134.82, 132.96, 130.94, 128.96, 125.80, 125.62, 123.84, 35.92; HRMS ESI: $[M+Na]^+$, Calculated for $C_{12}H_{10}ClNNaO$ 242.0343; found 242.0341.



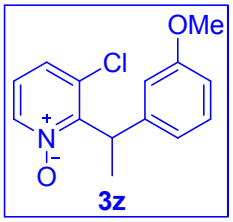
2-(1-(3-methoxyphenyl)ethyl)-3-phenylpyridine 1-oxide (3w): Sticky brown solid, 81 mg, 63 %; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.50 (s, 1H), 7.47 (t, *J* = 8.4 Hz, 6H), 7.20 (d, *J* = 7.2 Hz, 1H), 6.92 (t, *J* = 7.5 Hz, 3H), 6.80 (d, *J* = 7.8 Hz, 1H), 5.07 (d, *J* = 4.2 Hz, 1H), 3.80 (s, 3H), 1.68 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.82, 154.45, 144.03, 137.84, 135.32, 132.16, 132.03, 129.62, 129.29, 129.00, 126.82, 124.32, 120.32, 114.08, 112.01, 55.22, 38.08, 18.59; HRMS ESI: $[M+H]^+$, Calculated for $C_{20}H_{20}NO_2$ 306.1489; found 306.1487.



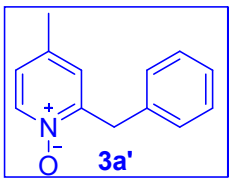
2-(1-(3-methoxyphenyl)ethyl)-4-phenylpyridine 1-oxide (3x): Sticky Brown solid, 105 mg, 82 %; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.28-7.39 (m, 8H), 7.14-7.18 (m, 1H), 6.81-6.85 (m, 2H), 6.70 (d, *J* = 7.5 Hz, 1H), 5.04 (s, 1H), 3.68 (s, 3H), 1.60 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.55, 159.82, 143.99, 139.83, 138.85, 136.58, 129.63, 129.19, 128.98, 126.61, 121.82, 120.99, 120.25, 114.10, 112.02, 55.22, 38.24, 18.78; HRMS ESI: $[M+H]^+$, Calculated for $C_{20}H_{20}NO_2$ 306.1489; found 306.1489.



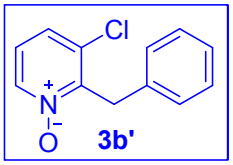
2-(1-(3-methoxyphenyl)ethyl)-3-methylpyridine 1-oxide (3y): Sticky brown solid, 86 mg, 84 %; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.13 (d, *J* = 17.1 Hz, 1H), 7.22 (d, *J* = 7.2 Hz, 1H), 7.02 (s, 2H), 6.88 (d, *J* = 7.2 Hz, 1H), 6.79 (t, J = 11.4 Hz, 3H), 5.01 (s, 1H), 3.78 (s, 3H), 2.25 (s, 3H), 1.62 (d, J = 6.6 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.75, 159.67, 144.28, 143.52, 129.50, 129.23, 120.22, 119.36, 113.96, 113.20, 111.89, 111.03, 55.16, 37.84, 18.58, 17.88; HRMS ESI: $[M+H]^+$, Calculated for $C_{15}H_{18}NO_2$ 224.1332; found 224.1335.



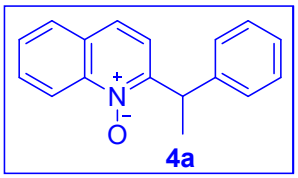
3-chloro-2-(1-(3-methoxyphenyl)ethyl)phenylpyridine 1-oxide (3z): Sticky brown solid, 95 mg, 86 %; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.13 (d, *J* = 5.7 Hz, 1H), 7.21 (t, *J* = 7.5 Hz, 2H), 7.06 (t, *J* = 6.9 Hz, 1H), 6.90 (d, *J* = 8.4 Hz, 2H), 6.77 (t, *J* = 9.9 Hz, 1H), 5.46 (s, 1H), 3.78 (s, 3H), 1.82 (d, J = 6.9 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.46, 153.80, 142.10, 138.92, 133.42, 129.00, 127.11, 122.93, 119.74, 113.61, 111.29, 55.16, 37.08, 13.40; HRMS ESI: $[M+Na]^+$, Calculated for $C_{14}H_{14}ClNNaO_2$ 286.0605; found 286.0604.



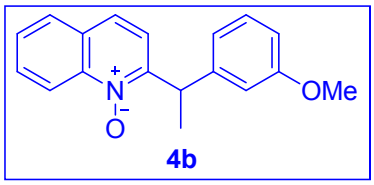
2-benzyl-4-methylpyridine 1-oxide (3a'): Sticky brown solid, 60 mg, 72 %; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.34 (s, 3H), 7.29 (s, 3H), 6.96 (s, 1H), 6.77 (s, 1H), 4.28 (s, 2H), 2.29 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 139.21, 136.57, 129.67, 128.83, 128.54, 128.13, 126.99, 125.91, 123.54, 36.25, 20.15; HRMS ESI: $[M+H]^+$, Calculated for $C_{13}H_{14}NO$ 200.1070; found 200.1073.



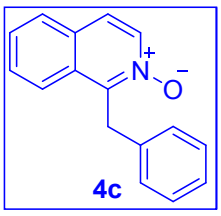
2-benzyl-3-chloropyridine 1-oxide (3b'): Sticky brown solid, 74 mg, 80 %; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.16 (s, 1H), 7.41 (s, 2H), 7.25 (s, 3H), 7.09 (s, 1H), 4.52 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 150.73, 138.69, 136.04, 133.41, 128.98, 128.51, 126.90, 122.86, 33.39; HRMS ESI: $[M+H]^+$, Calculated for $C_{12}H_{11}ClNO$ 220.0524; found 220.0527.



2-(1-phenylethyl)quinoline 1-oxide (4a): Sticky brown solid, 90 mg, 50 %; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.22 (s, 1H), 7.72-7.78 (m, 4H), 7.57 (d, J = 5.7 Hz, 2H), 7.41-7.52 (m, 3H), 6.97 (t, , J = 8.4 Hz 3H), 5.94 (s, 1H), 1.89 (d, J = 6.6 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.99, 159.75, 137.73, 136.98, 129.63, 128.73, 128.53, 128.42, 128.09, 127.67, 126.43, 124.24, 122.71, 115.38, 115.10, 34.81, 22.68, 21.48; HRMS ESI: $[M+H]^+$, Calculated for $C_{17}H_{16}NO$ 250.1226; found 250.1227.

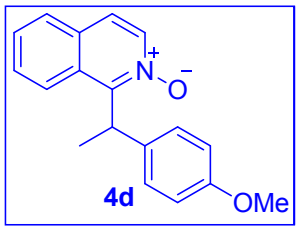


2-(1-(3-methoxyphenyl)ethyl)quinolone 1-oxide (4b): Sticky brown solid, 117 mg, 58 %; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.79 (s, 1H), 7.78 (d, J = 12.6 Hz, 2H), 7.63 (s, 2H), 6.91 (d, J = 15 Hz, 3H), 6.80 (s, 2H), 5.34 (s, 1H), 3.77 (s, 3H), 1.72 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.83, 143.15, 140.64, 138.26, 134.86, 129.39, 128.60, 128.41, 127.89, 126.96, 125.62, 124.31, 121.48, 119.38, 119.05, 113.04, 111.04, 54.17, 37.77, 21.67; HRMS ESI: $[M+H]^+$, Calculated for $C_{18}H_{18}NO_2$ 280.1332; found 280.1333.

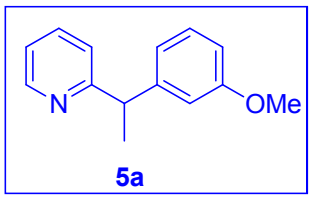


1-benzylisoquinoline 2-oxide (4c): Sticky brown solid, 48 mg, 58 %; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.24(S, 1H), 7.98 (d, J = 7.8 Hz, 1H), 7.77 (d, J = 7.5 Hz, 1H), 7.54-7.61 (m, 3H), 7.34 (d, J = 6.6 Hz, 2H), 7.17-7.26 (m, 3H), 4.82 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.75, 137.14,

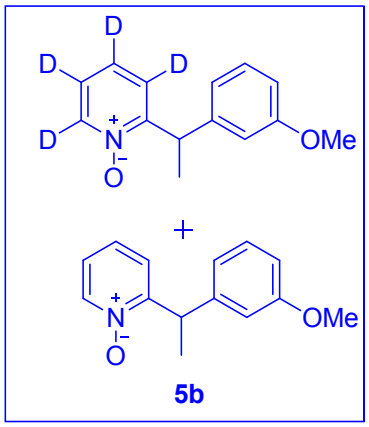
136.98, 129.84, 129.46, 129.24, 128.76, 128.73, 128.49, 127.48, 126.70, 124.25, 122.65, 89.38, 31.79; HRMS ESI: $[M+H]^+$, Calculated for $C_{16}H_{14}NO$ 236.1070; found 236.1068.



1-(1-(4-methoxyphenyl)ethyl)isoquinolone 2-oxide (4d): Sticky brown solid, 113 mg, 56 %; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.21 (s, 1H), 7.71 (d, *J* = 6 Hz, 2H), 7.54 (d, *J* = 6 Hz, 1H), 7.37-7.44 (m, 3H), 7.18 (t, *J* = 6 Hz, 2H), 6.84 (d, *J* = 9 Hz, 3H), 6.72 (d, *J* = 9 Hz, 2H), 6.05 (s, 1H), 3.72 (s, 3H), 1.84 (d, *J* = 6 Hz, 3H).; ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.02, 137.00, 134.28, 130.56, 130.21, 129.63, 128.99, 128.52, 128.02, 127.88, 127.56, 124.51, 122.48, 113.92, 55.24, 34.60, 15.68; HRMS ESI: $[M+Na]^+$, Calculated for $C_{18}H_{17}NNaO_2$ 302.1151; found 302.1156.

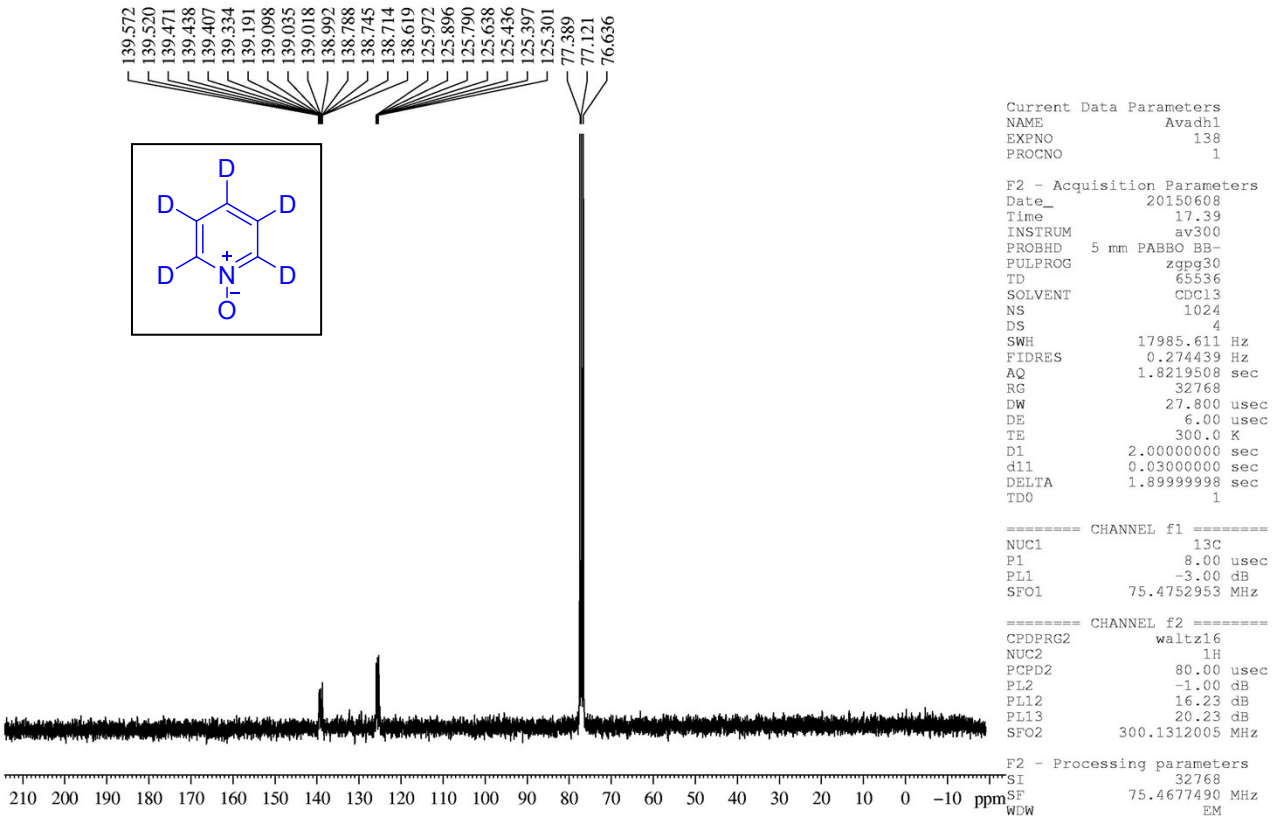


2-(1-(3-methoxyphenyl)pyridine (5a): Brown liquid, 1.0 g**,** 90 %; ^{1}NMR (300 MHz, $CDCl_3$) δ 8.48 (d, *J* = 4.2 Hz, 1H), 7.46-7.51 (m, 1H), 7.11-7.18 (m, 1H), 7.00-7.06 (m, 2H), 6.77-6.83 (m, 2H), 6.65-6.68 (m, 1H), 4.19 (q, *J* = 7.2 Hz, 1H), 3.70 (s, 3H), 1.62 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 164.92, 159.70, 149.11, 146.77, 136.38, 129.39, 122.10, 121.21, 120.12, 113.72, 111.47, 55.14, 47.42, 20.67; HRMS ESI: $[M+H]^+$, Calculated for $C_{14}H_{16}NO$ 214.1226; found 214.1234.

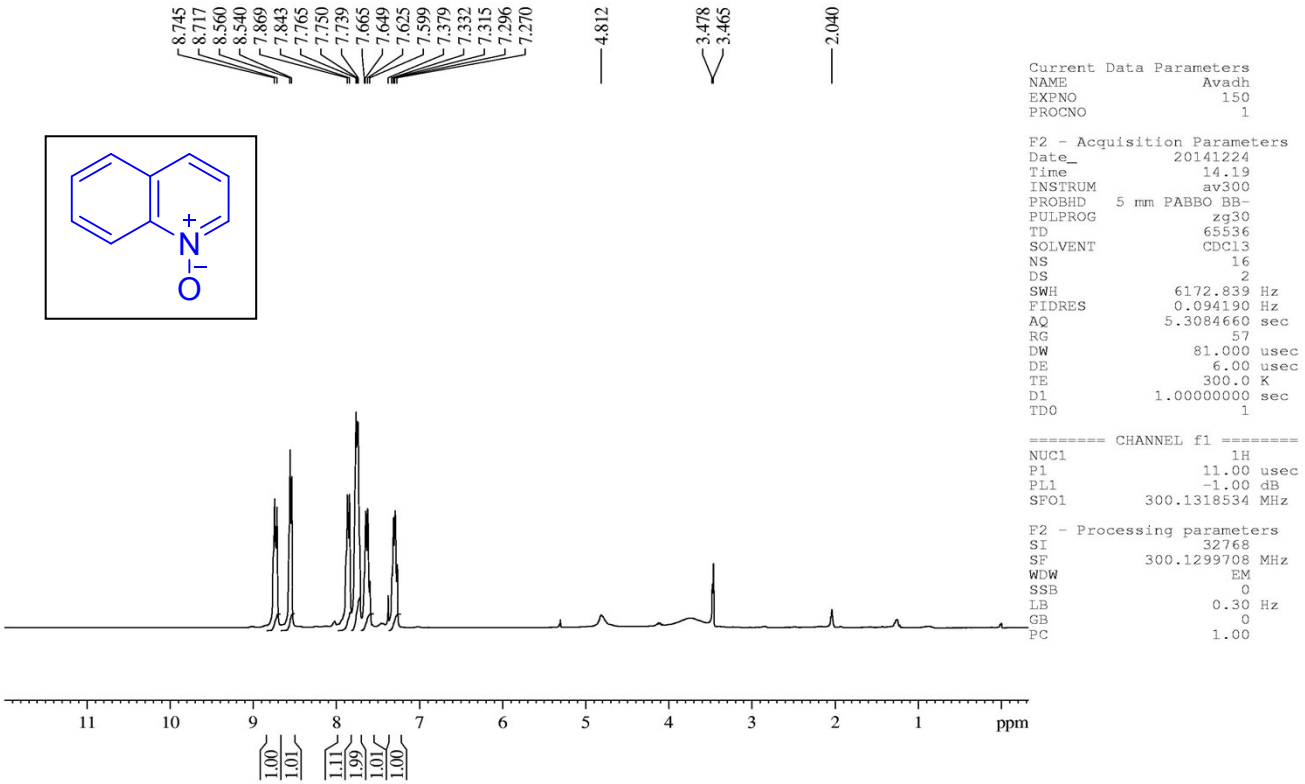


Mixture of 2-(1-(4-methoxyphenyl)ethyl)-pyridine1-oxide and 2-(1-(4-methoxyphenyl)ethyl)d^4-pyridine1-oxide (5b): Sticky dark brown solid, ^{1}NMR (300 MHz, $CDCl_3$) δ 8.22 (d, *J* = 2.4, Hz 1H), 7.22-7.24 (m, 1H), 7.14 (s, 2H), 6.84-6.90 (m, 3H), 6.79-6.80 (m, 1H), 5.06 (q, *J* = 2.7 Hz, 1H), 3.78 (s, 3H), 1.64 (d, *J* = 5.7Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.81, 156.15, 143.99, 139.71, 129.55, 125.42, 124.46, 123.32, 120.30, 114.06, 112.01, 55.18, 38.19, 18.41.

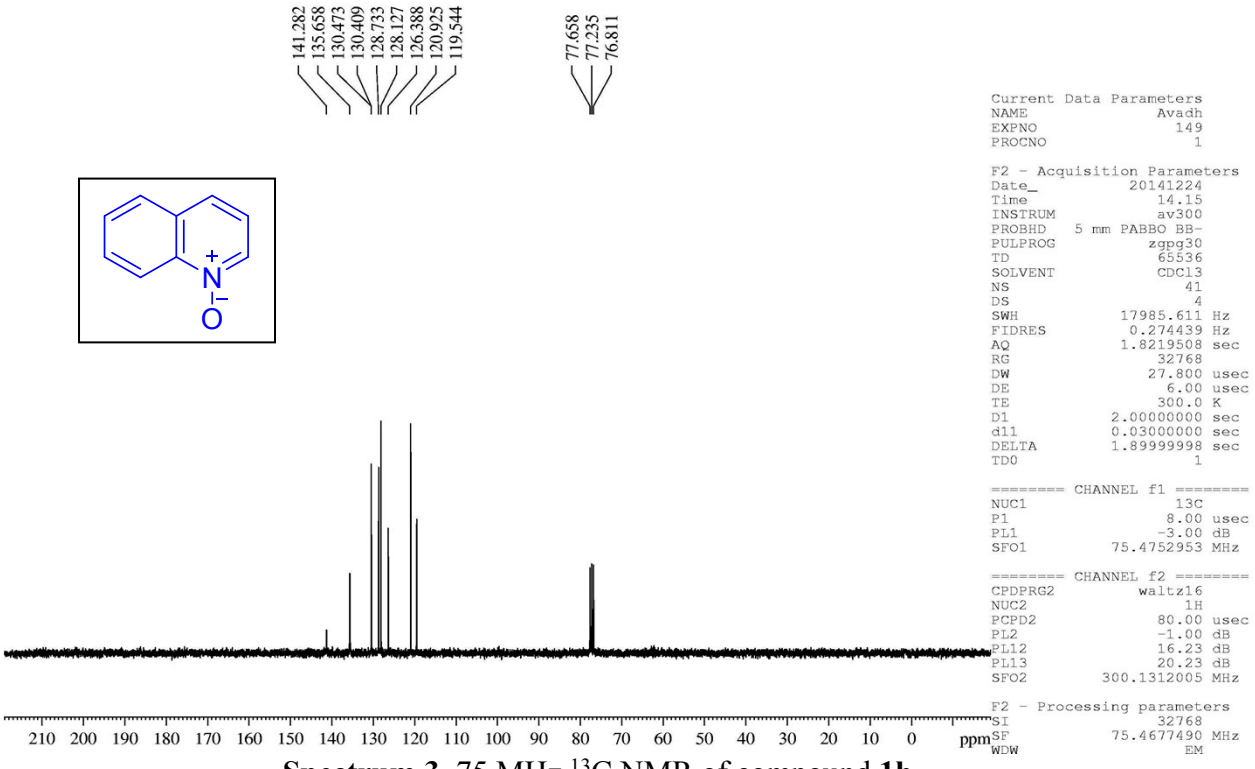
2. Copies of ^{1}H NMR, ^{13}C NMR:



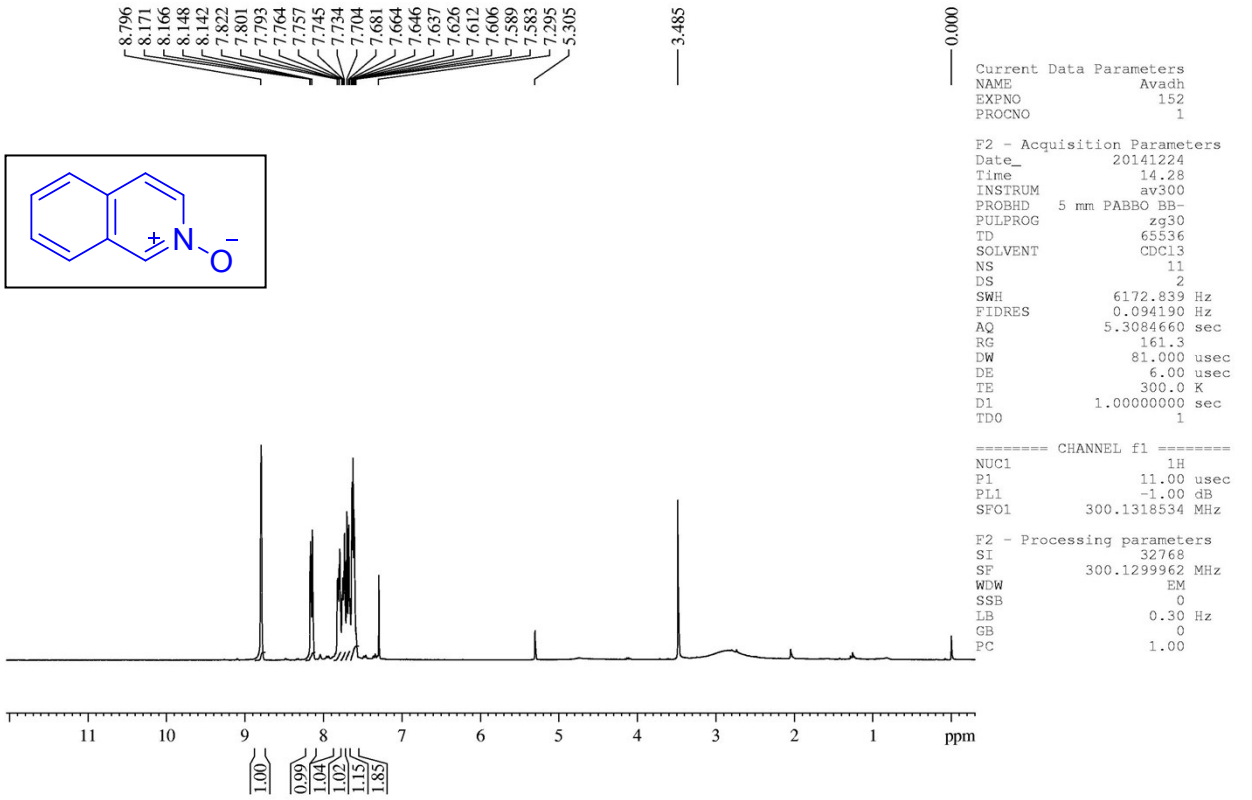
Spectrum 1. 75 MHz ^{13}C NMR of compound **1b**



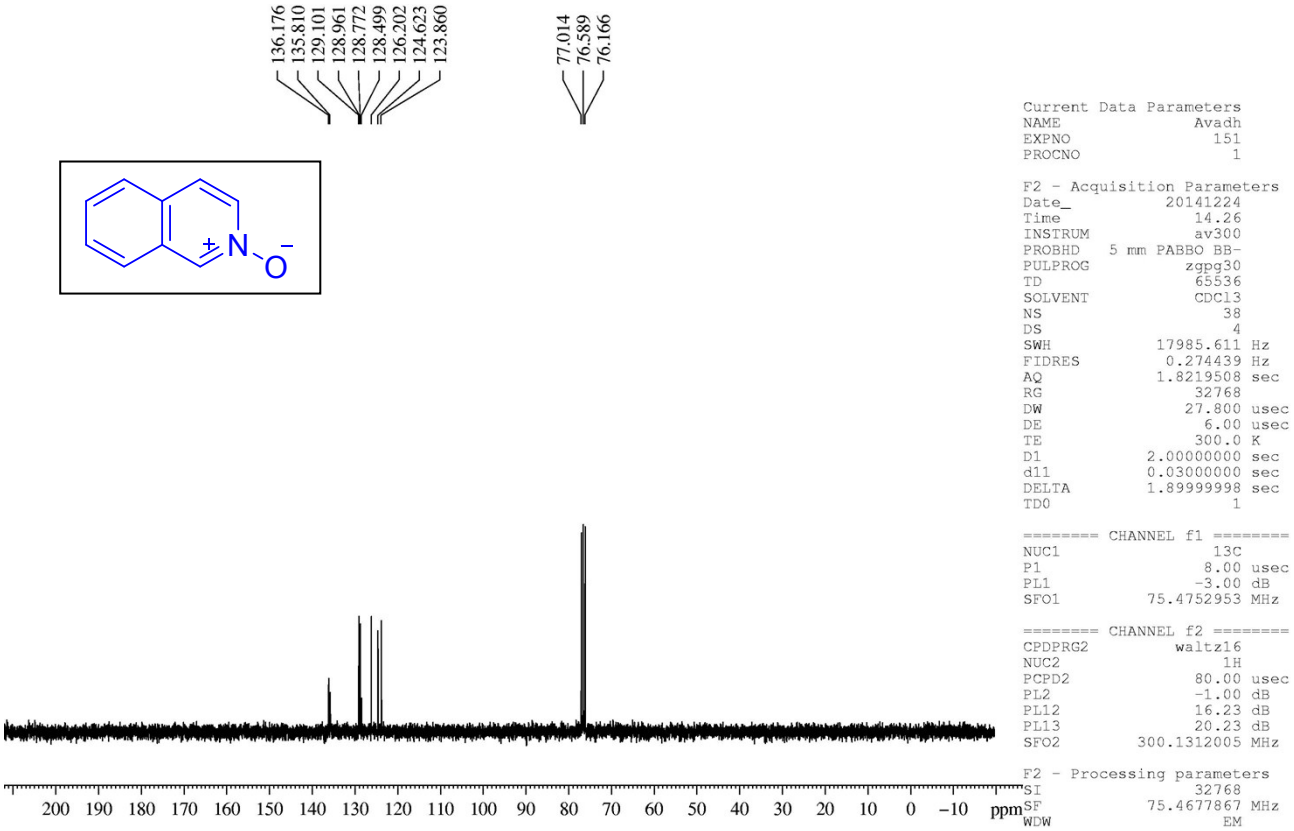
Spectrum 2. 300 MHz ^{1}H NMR of compound **1h**



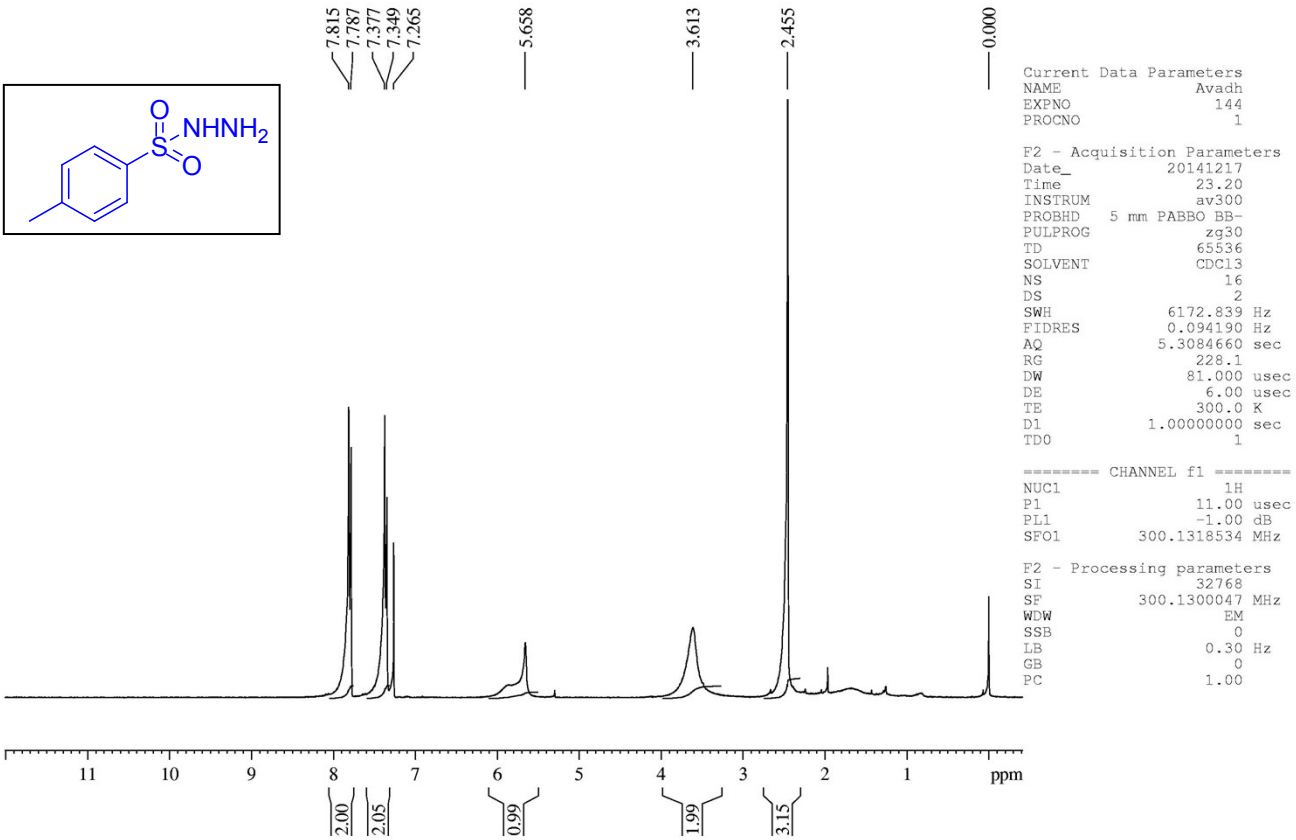
Spectrum 3. 75 MHz ^{13}C NMR of compound **1h**



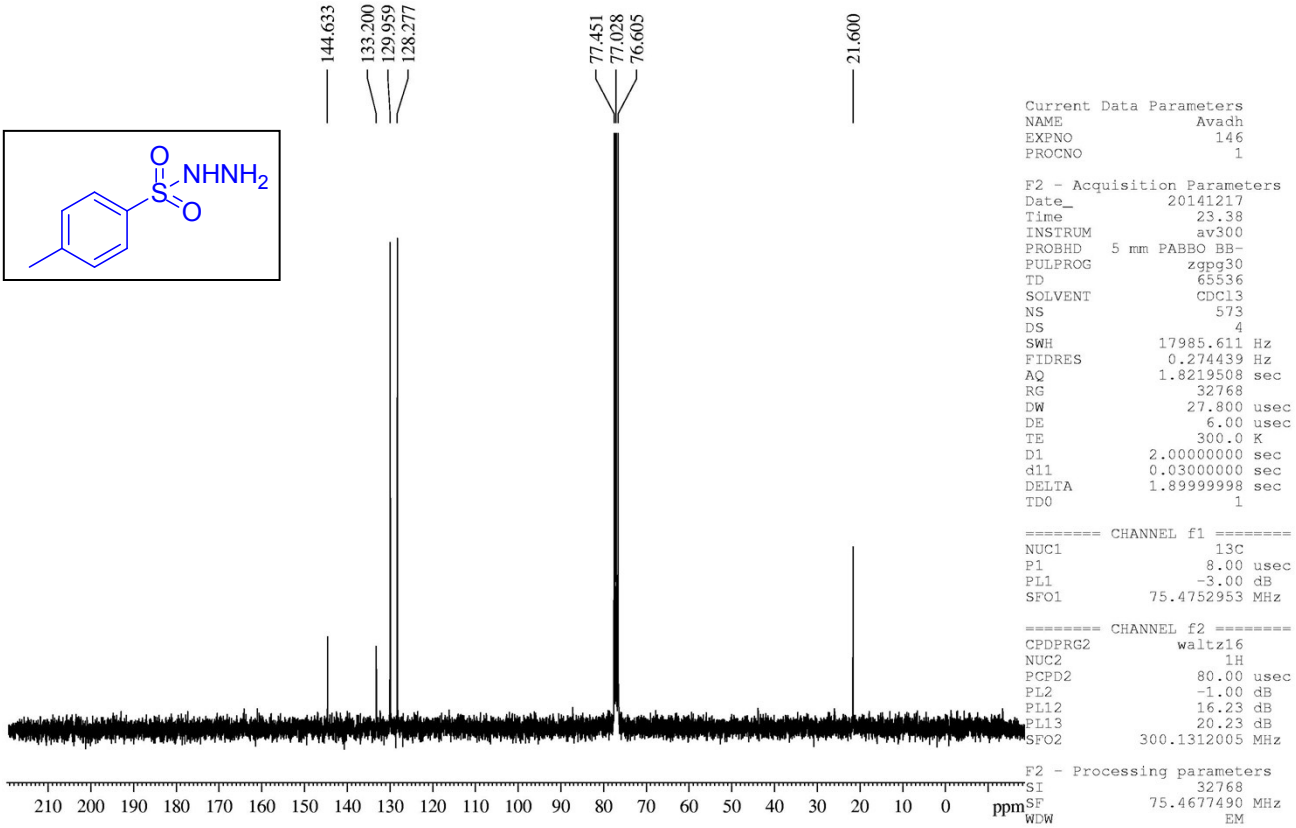
Spectrum 4. 300 MHz ^{1}H NMR of compound **1i**



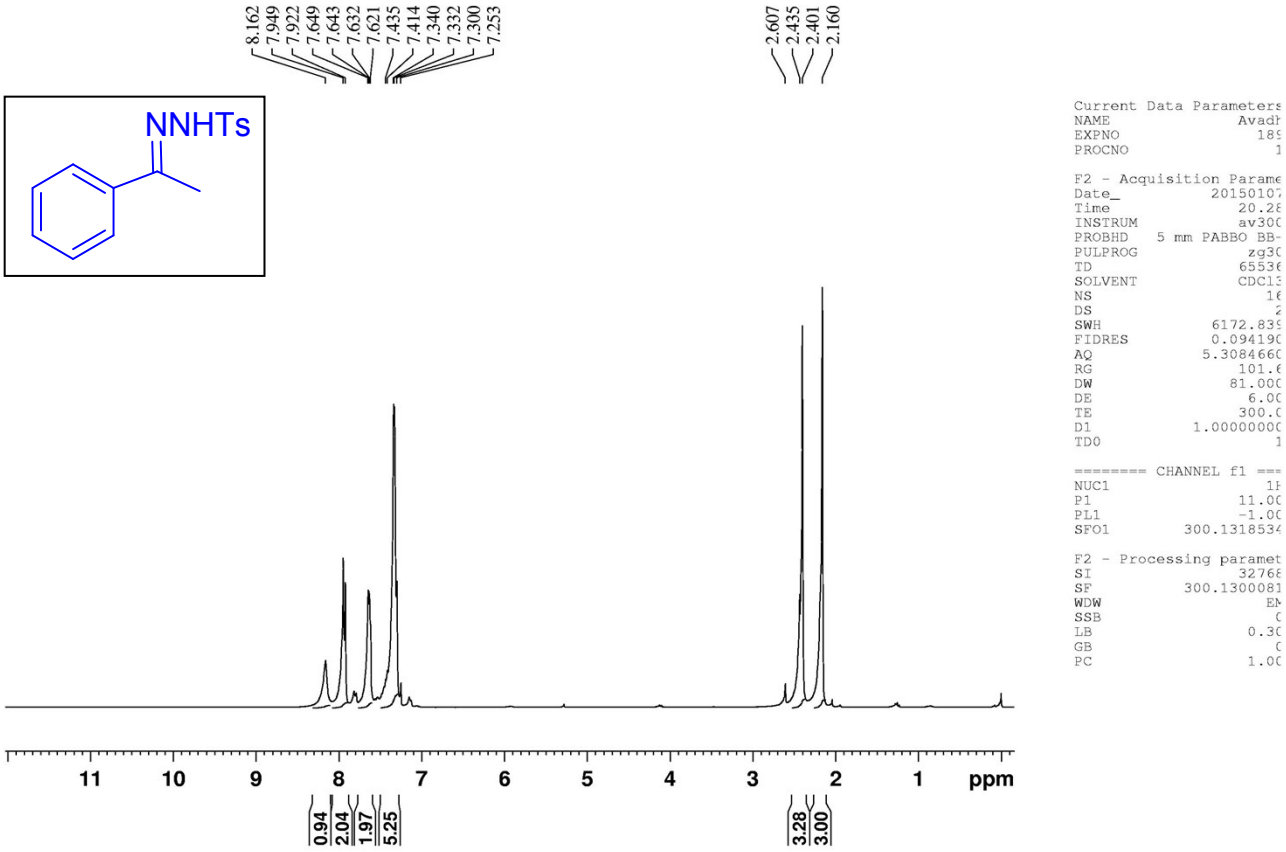
Spectrum 5. 75 MHz ^{13}C NMR of compound **1i**



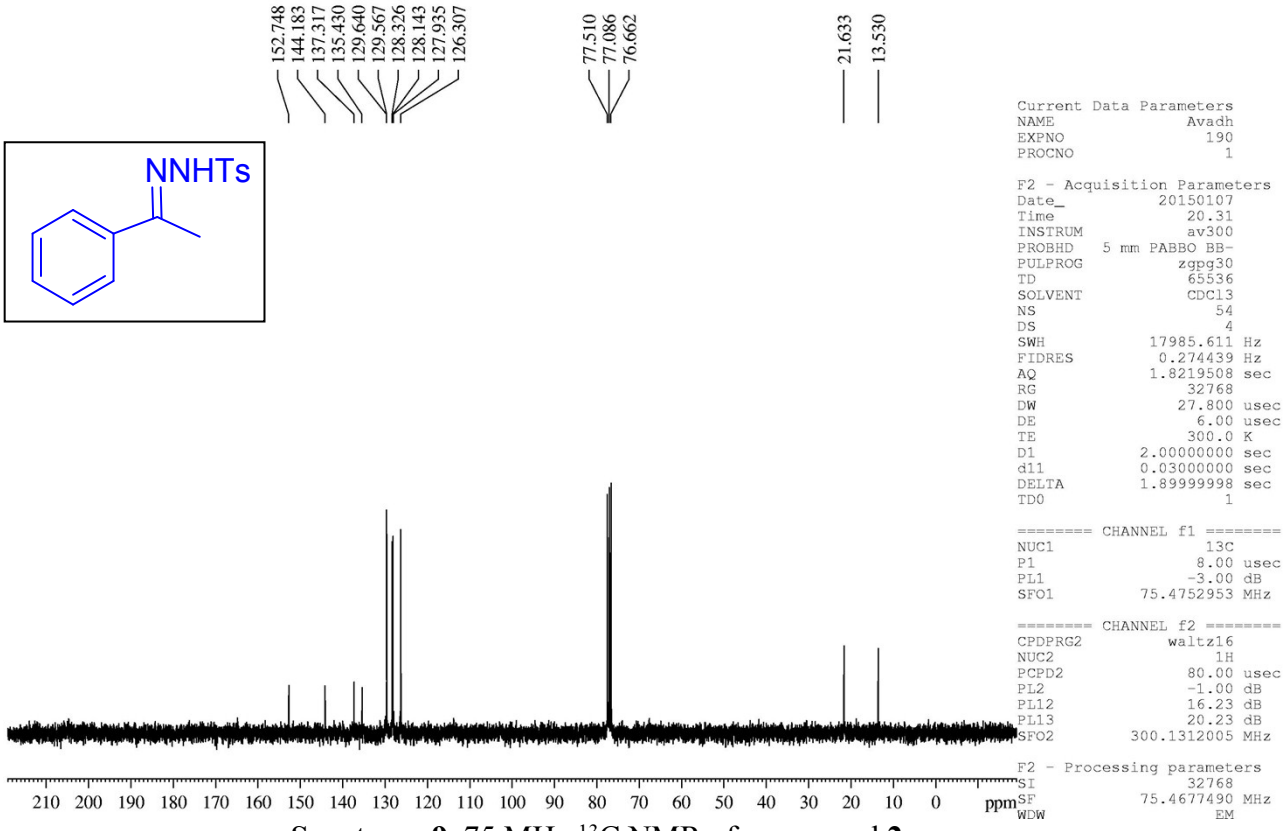
Spectrum 6. 300 MHz ^{1}H NMR of compound **2a'**



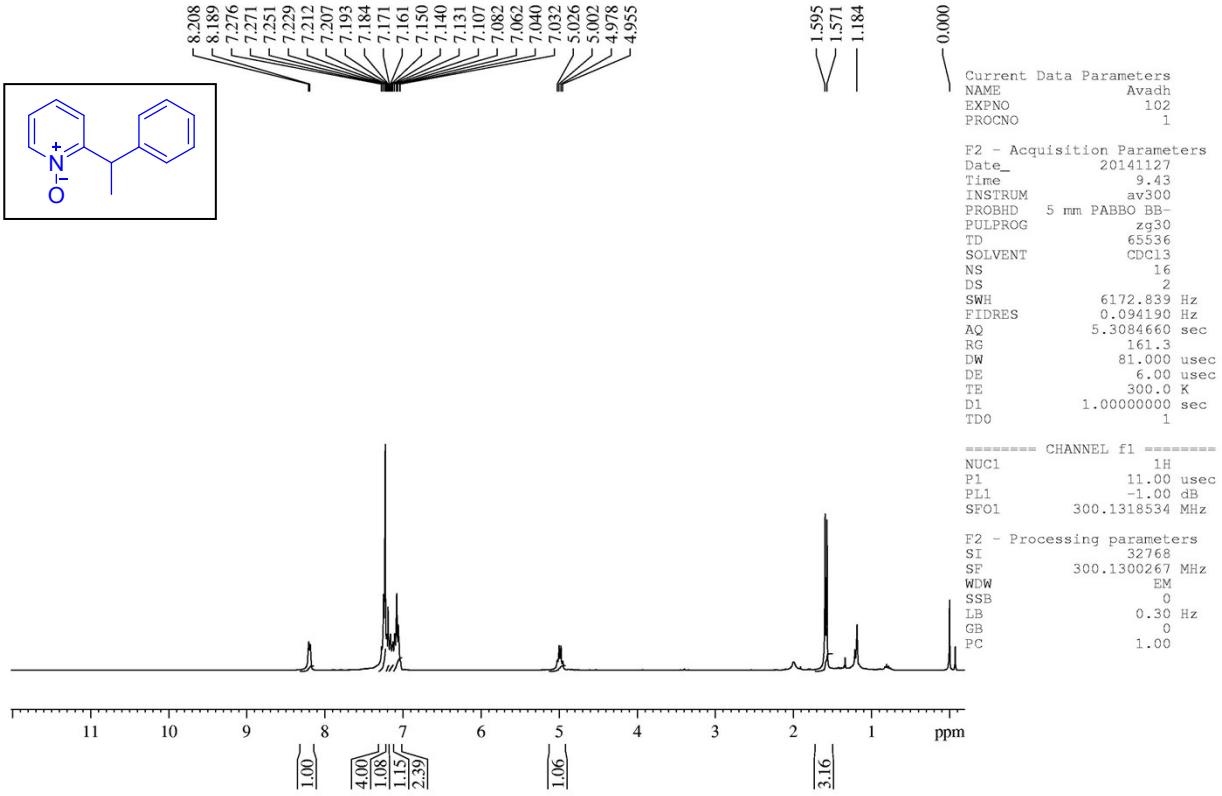
Spectrum 7. 75 MHz ^{13}C NMR of compound **2a'**



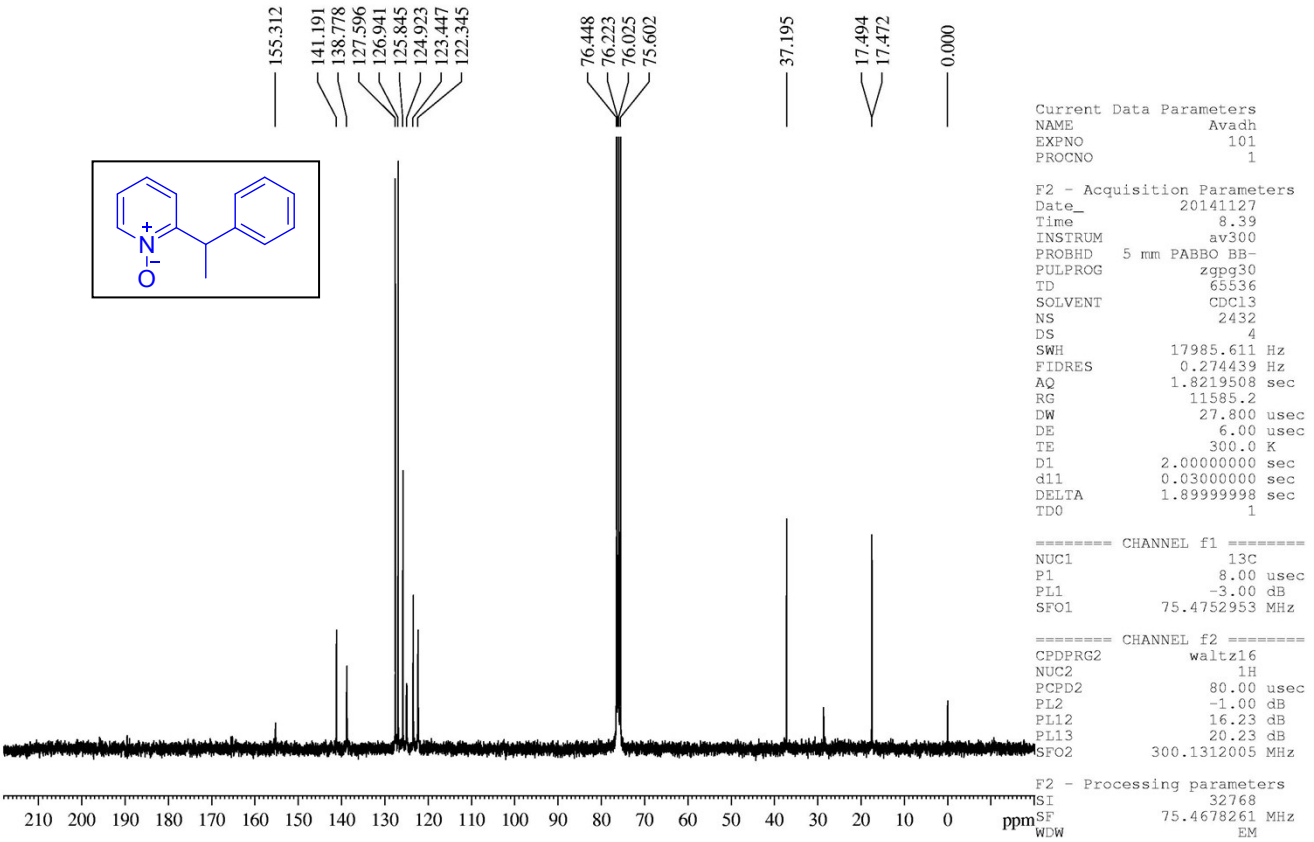
Spectrum 8. 300 MHz ^{1}H NMR of compound **2a**



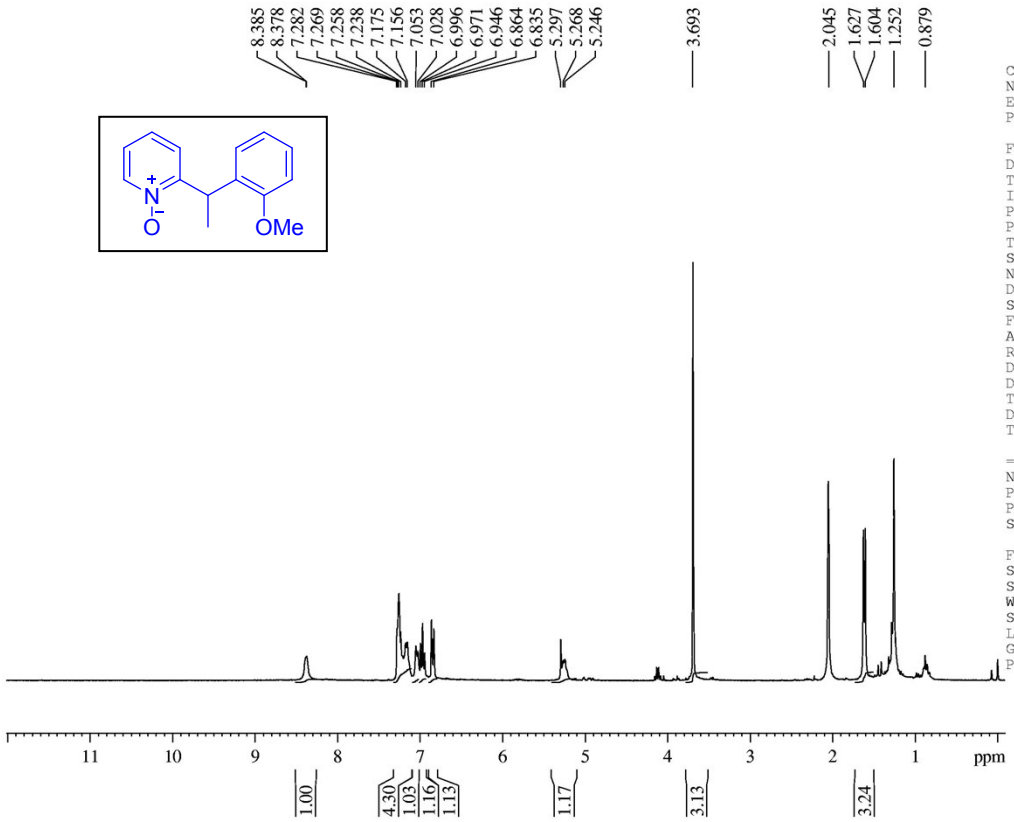
Spectrum 9. 75 MHz ^{13}C NMR of compound **2a**



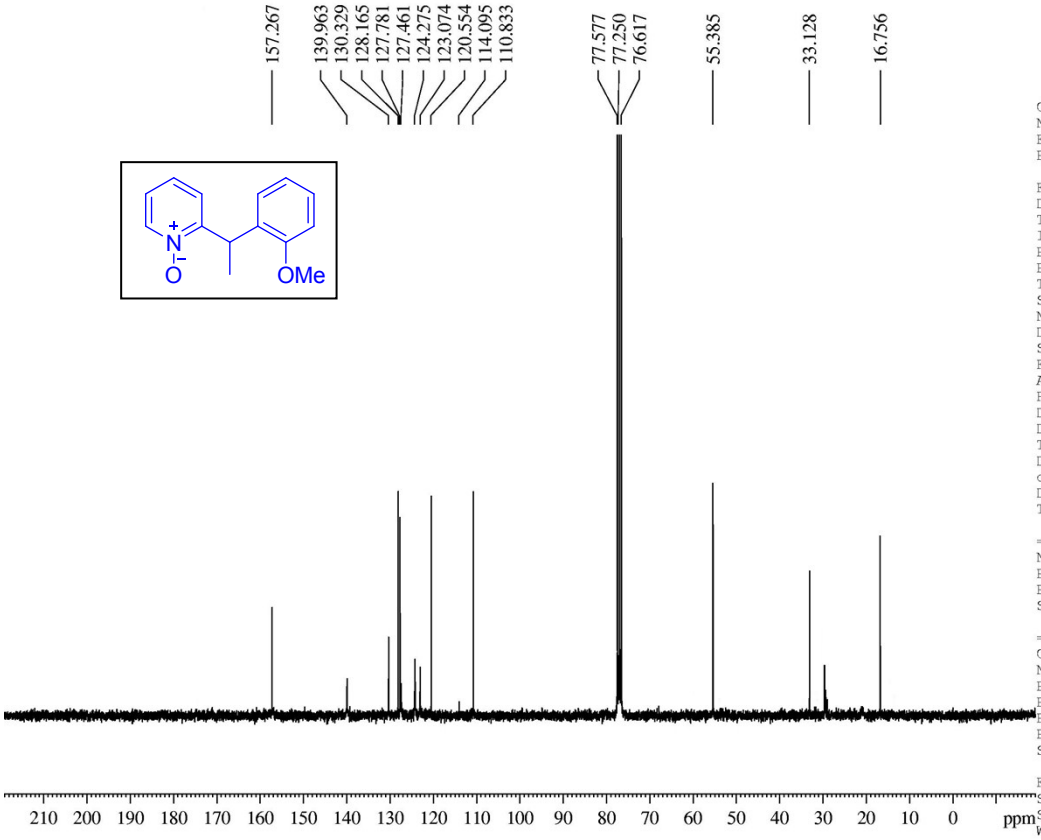
Spectrum 10. 300 MHz ^{1}H NMR of compound **3a**



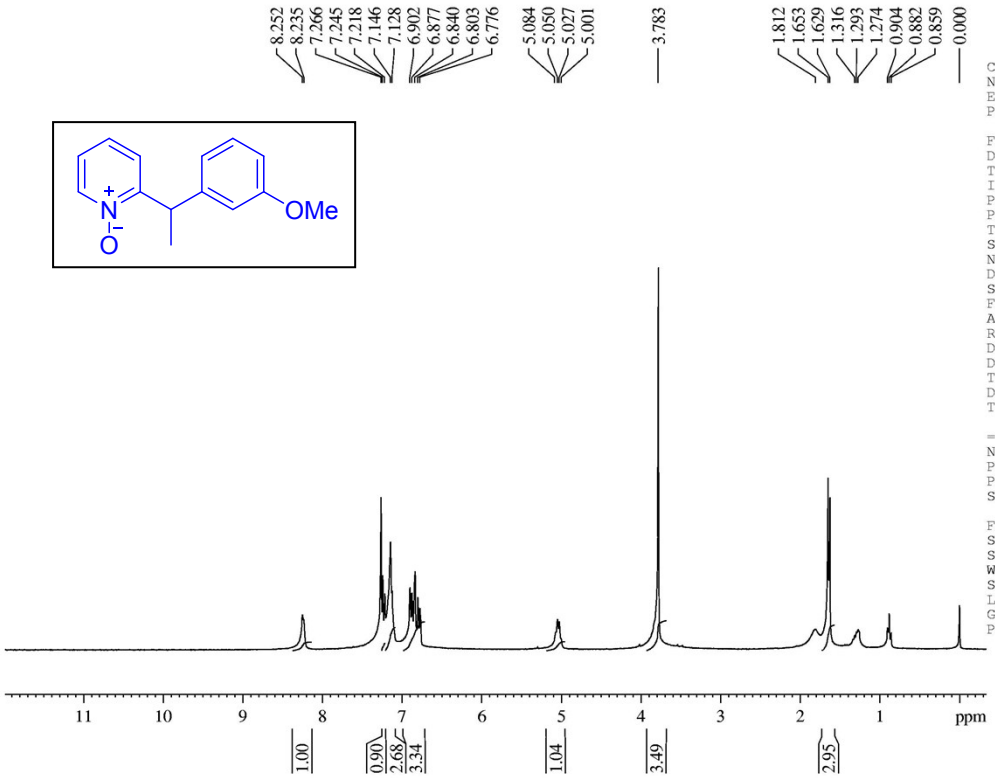
Spectrum 11. 75 MHz ^{13}C NMR of compound **3a**



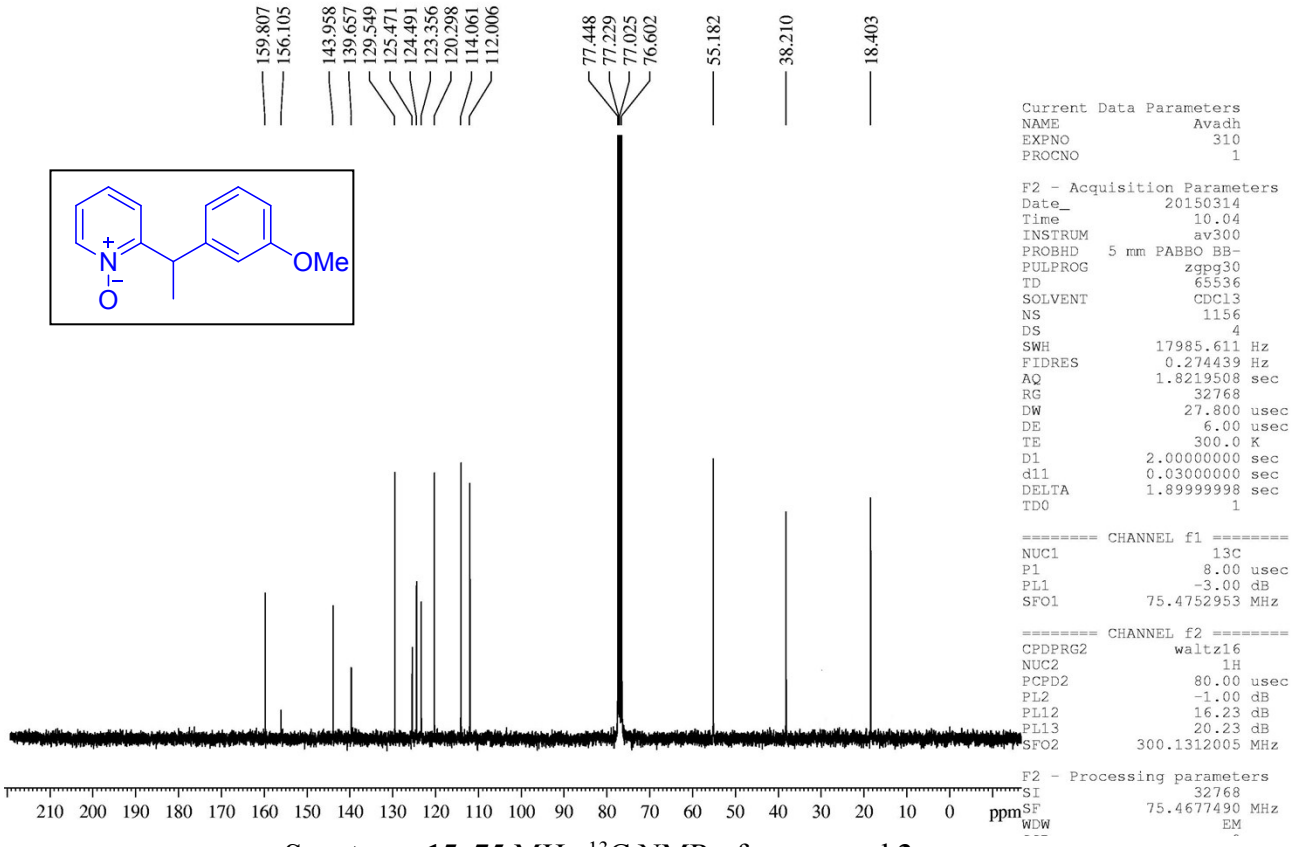
Spectrum 12. 300 MHz ^{1}H NMR of compound **3b**



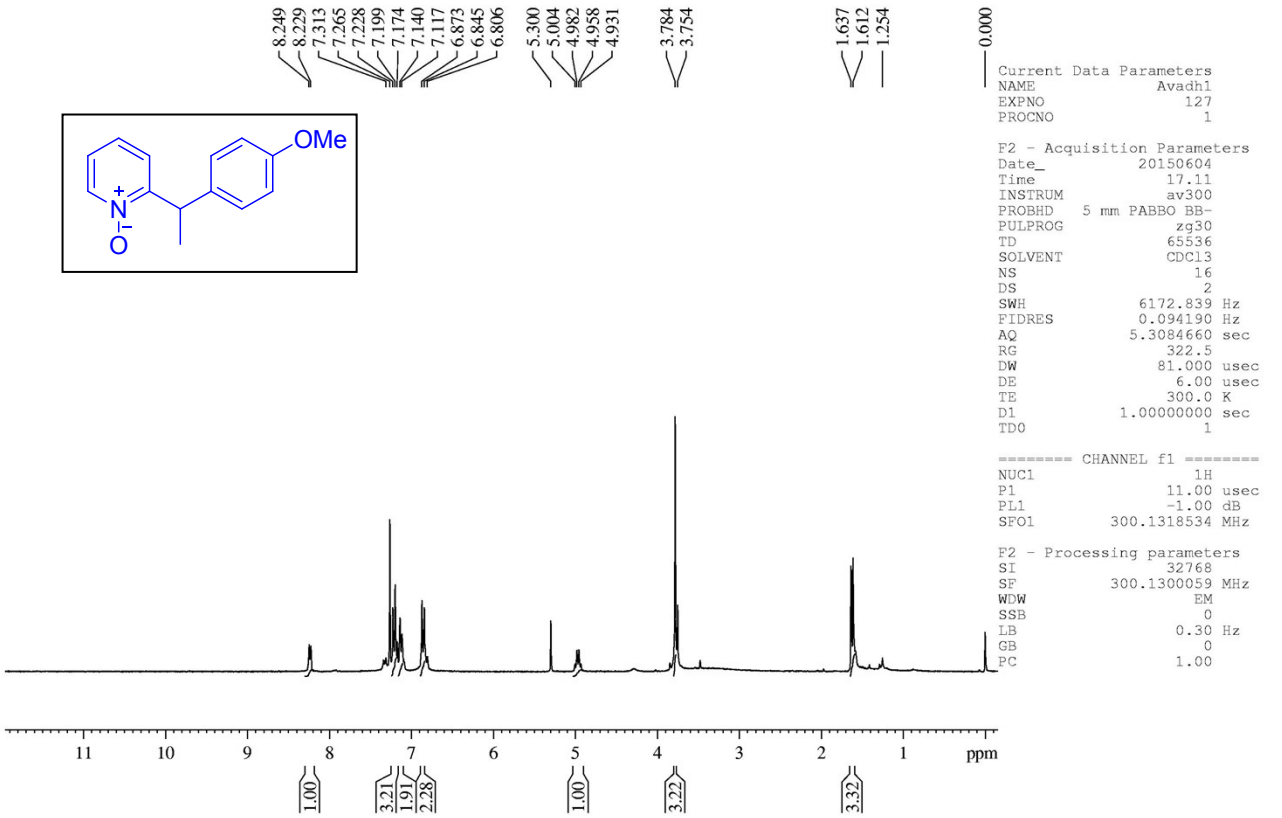
Spectrum 13. 75 MHz ^{13}C NMR of compound **3b**



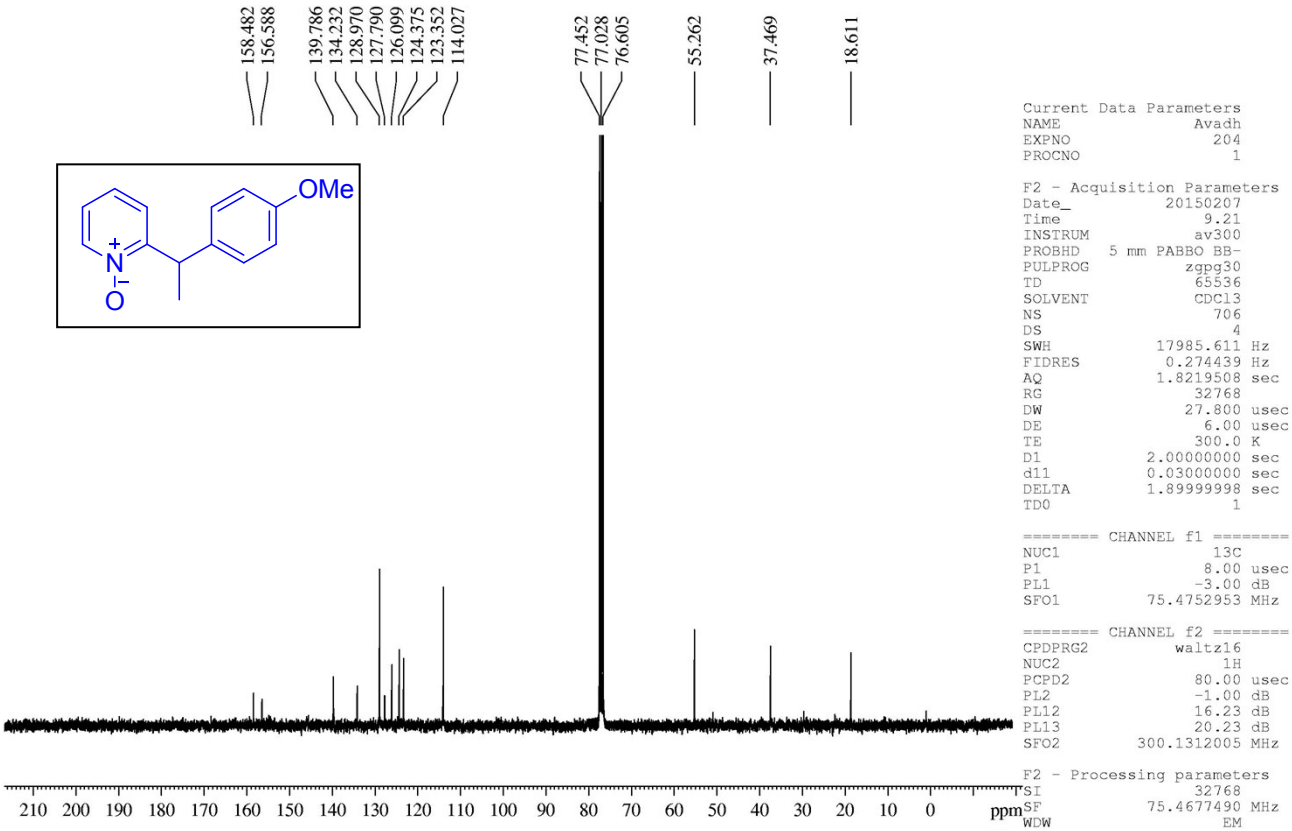
Spectrum 14. 300 MHz ^{1}H NMR of compound **3c**



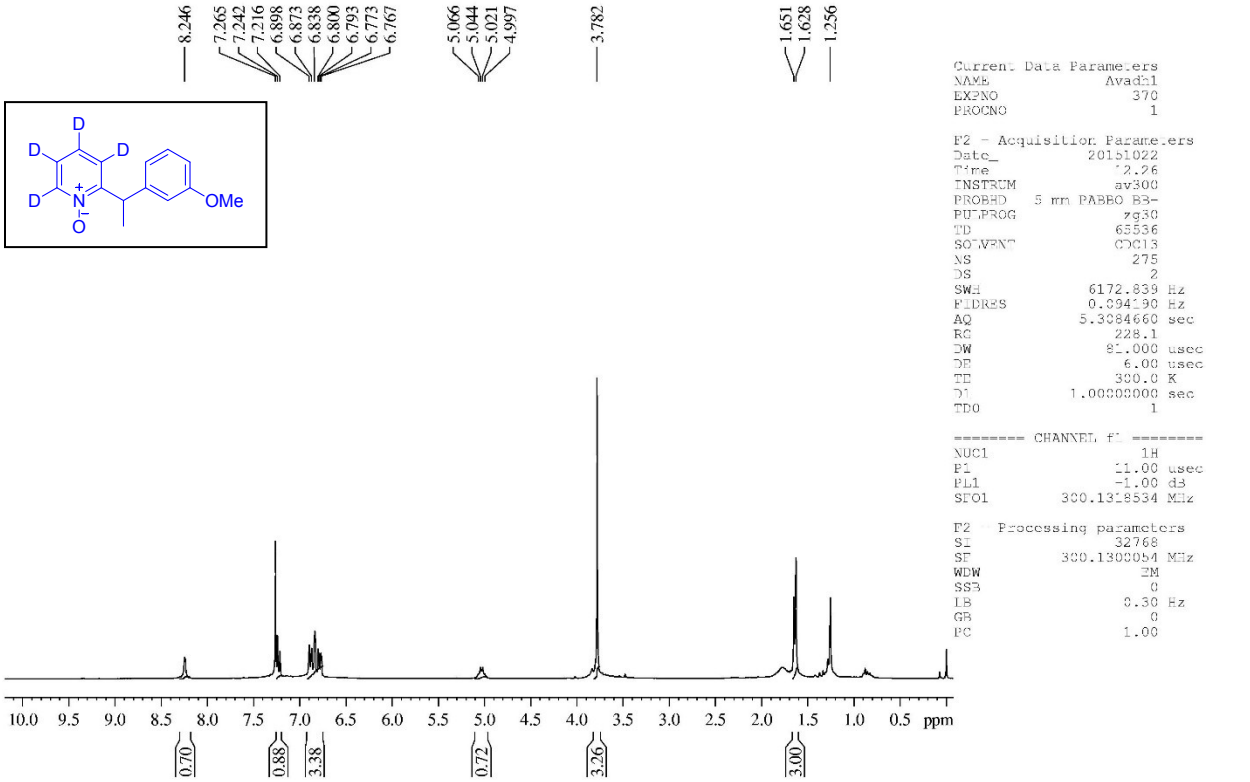
Spectrum 15. 75 MHz ^{13}C NMR of compound **3c**



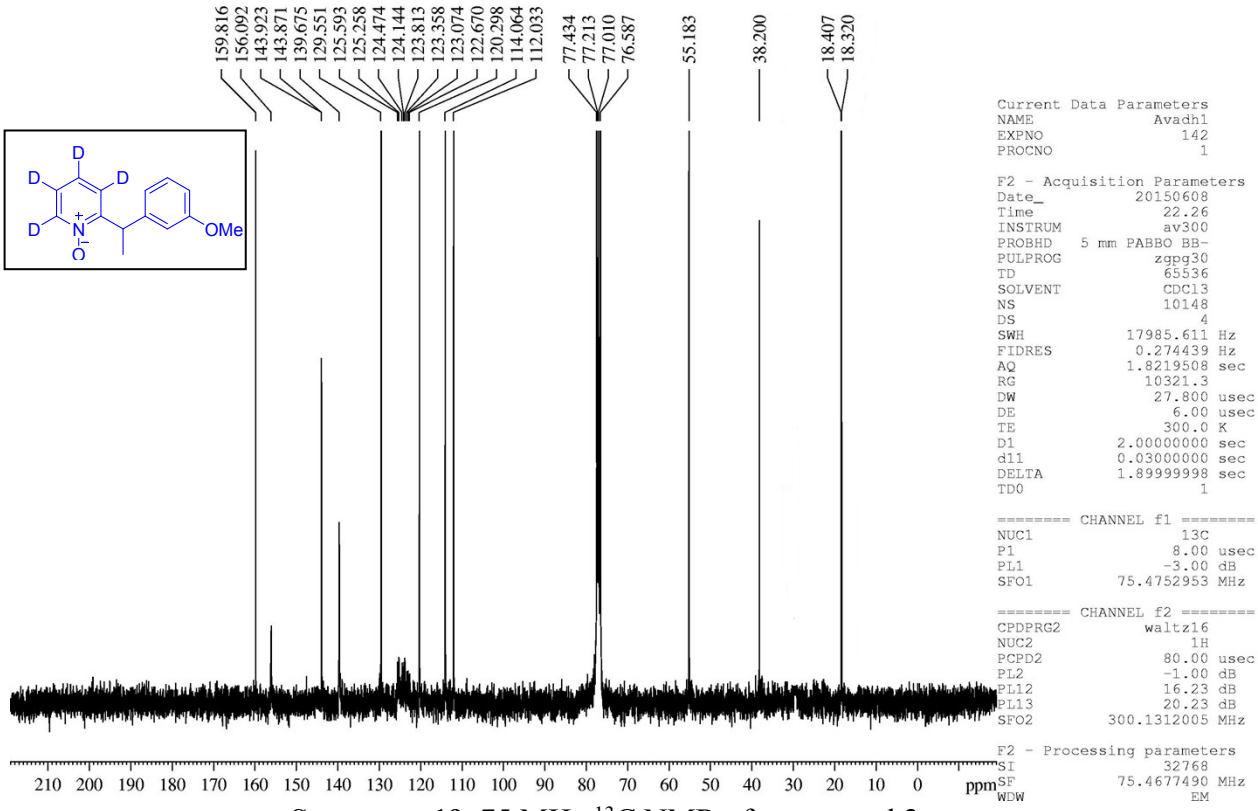
Spectrum 16. 300 MHz ^{1}H NMR of compound **3d**



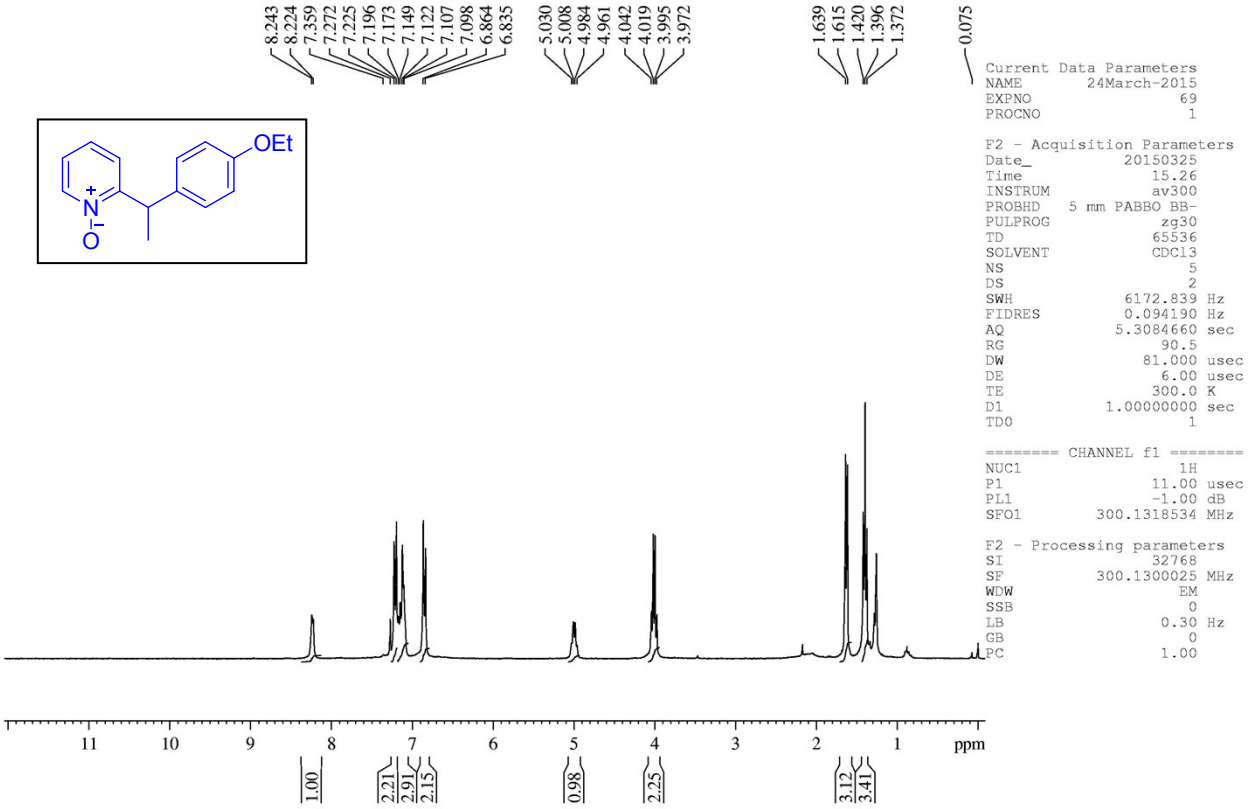
Spectrum 17. 75 MHz ^{13}C NMR of compound **3d**



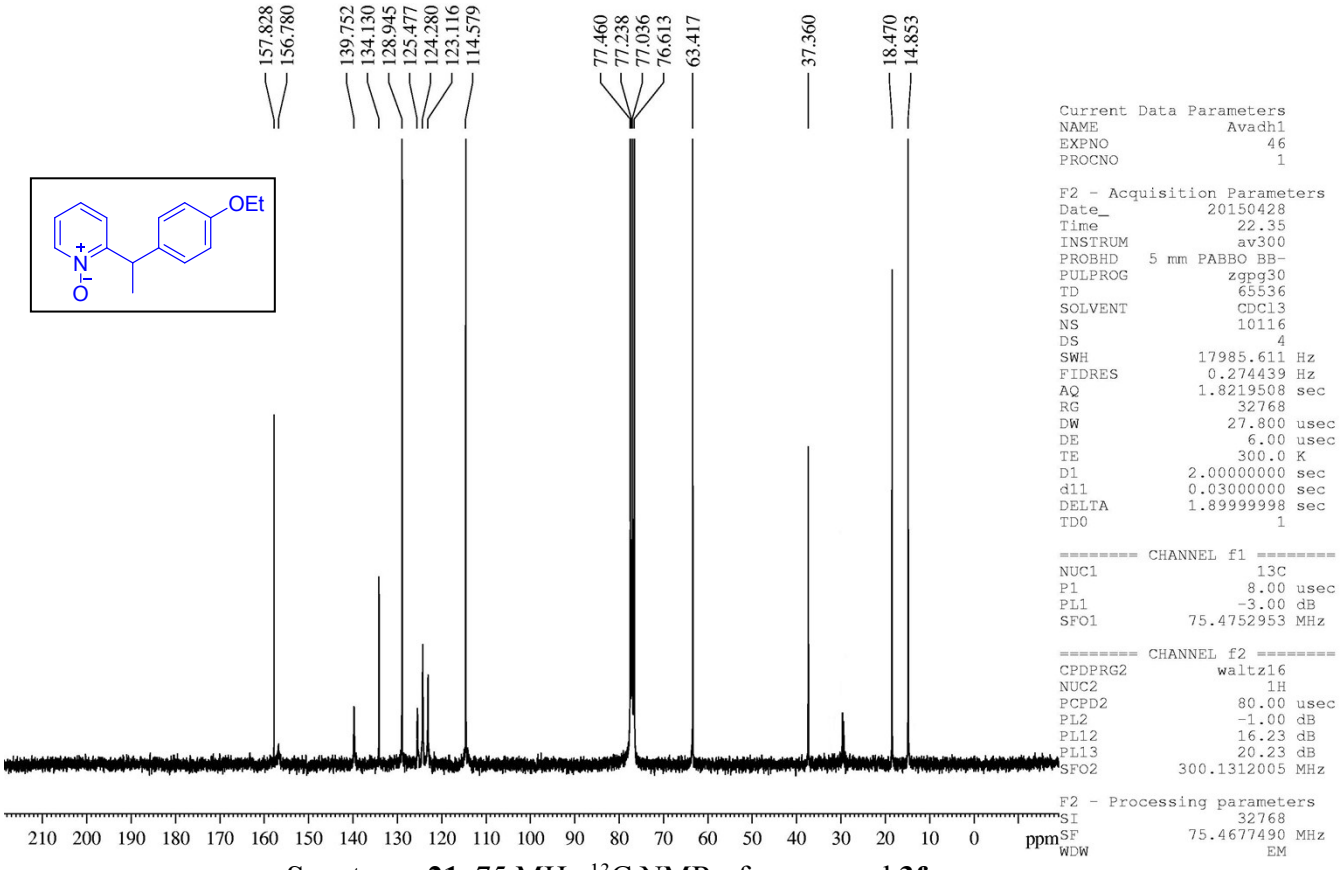
Spectrum 18. 300 MHz ^{1}H NMR of compound **3e**



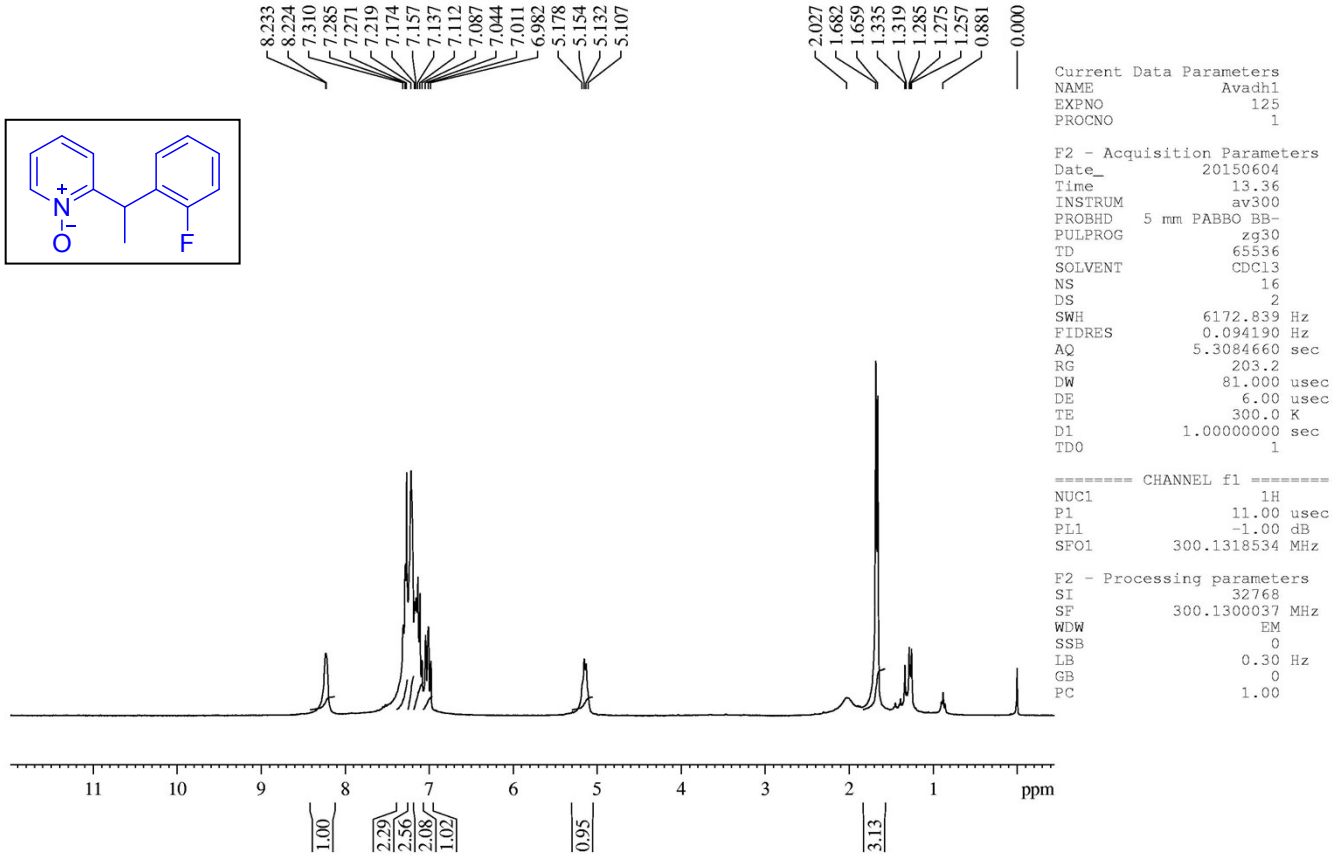
Spectrum 19. 75 MHz ^{13}C NMR of compound **3e**



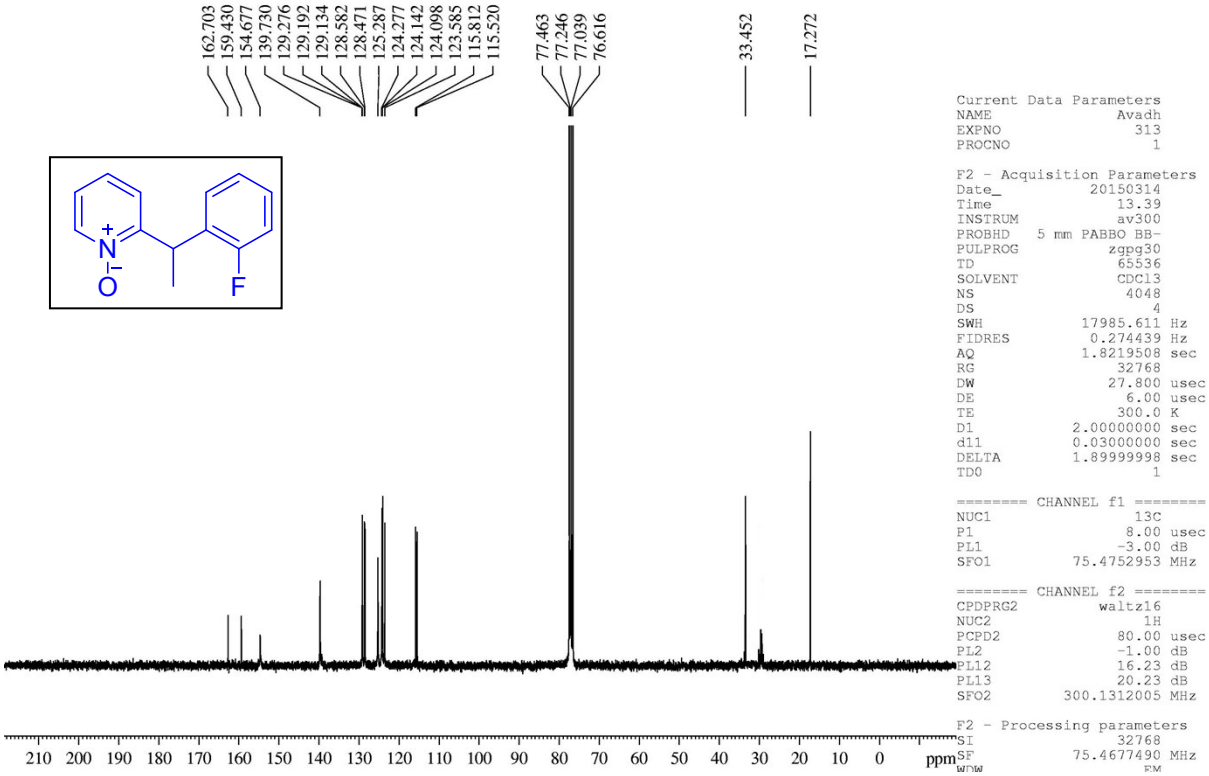
Spectrum 20. 300 MHz ^{1}H NMR of compound **3f**



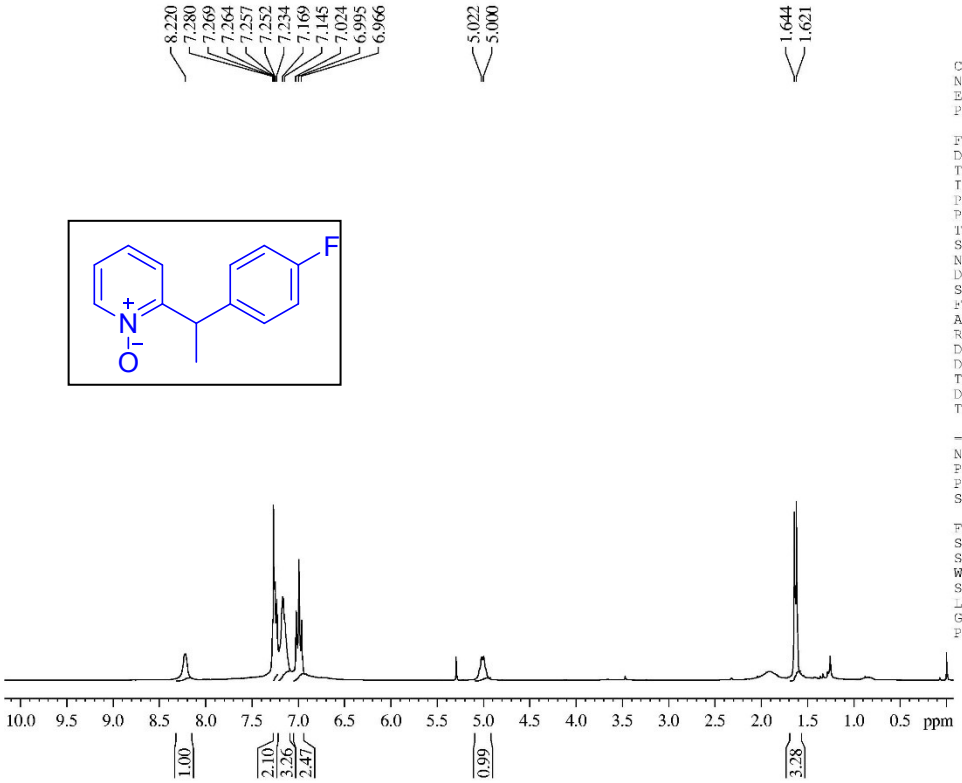
Spectrum 21. 75 MHz ^{13}C NMR of compound **3f**



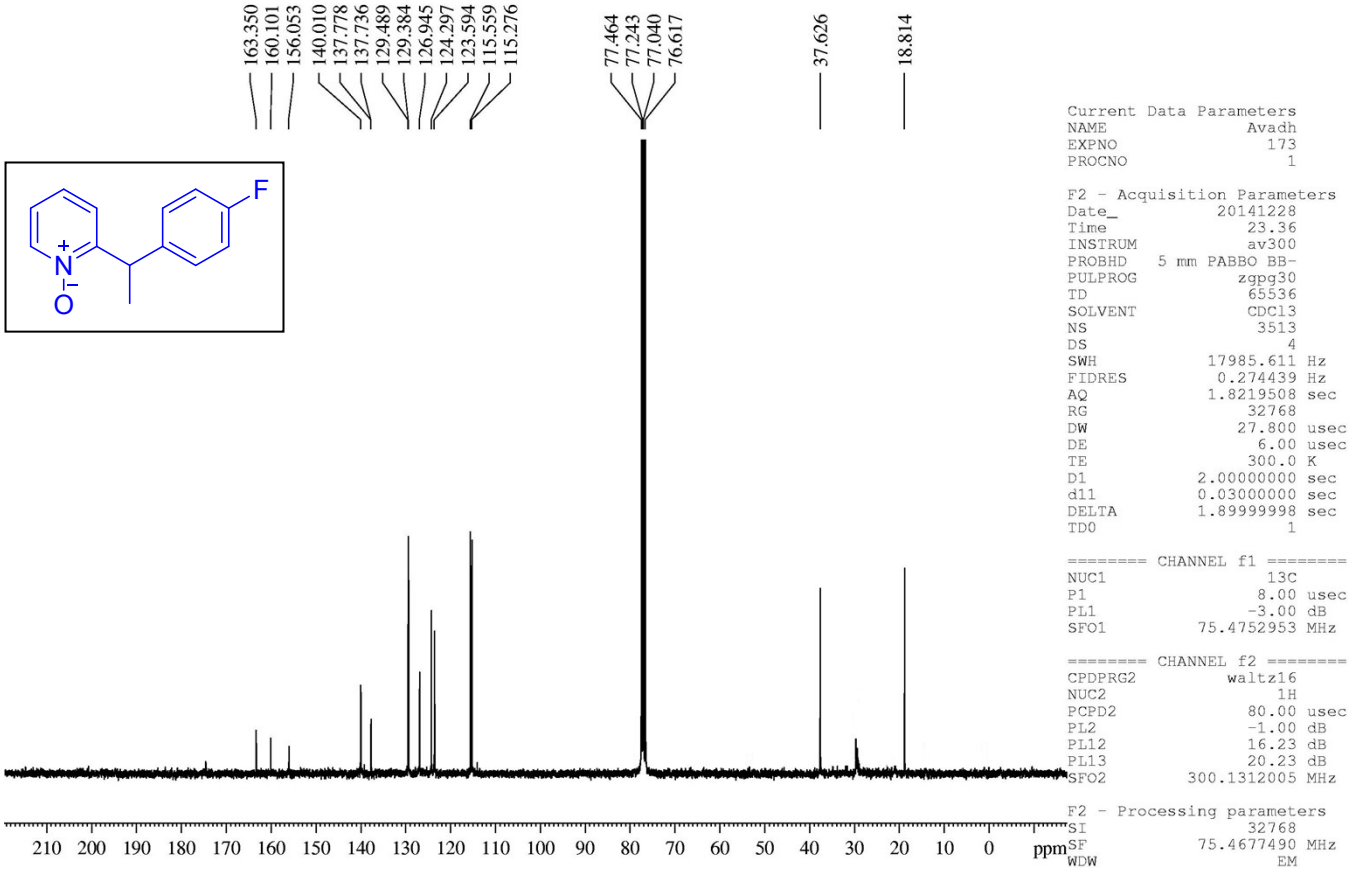
Spectrum 22. 300 MHz ^{1}H NMR of compound **3g**



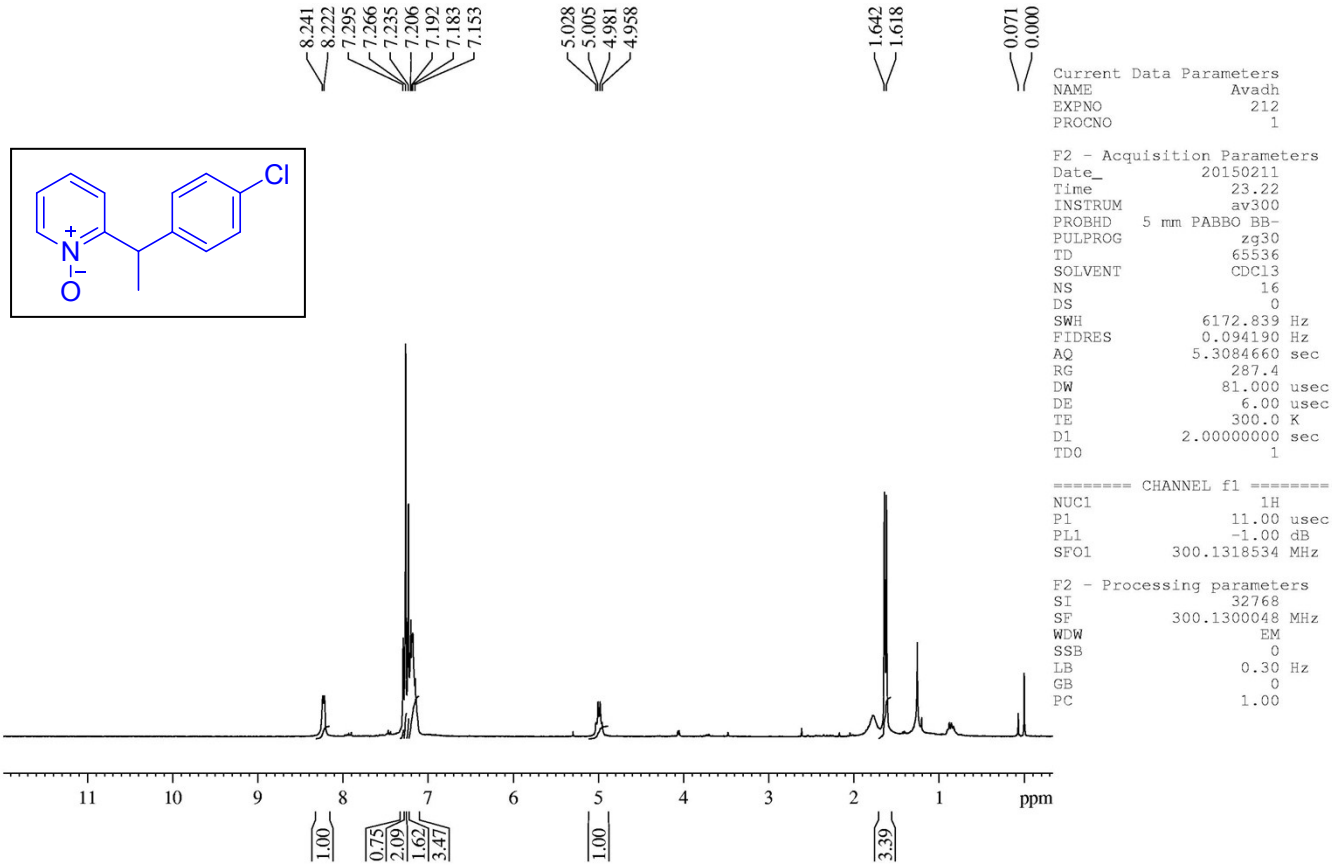
Spectrum 23. 75 MHz ^{13}C NMR of compound **3g**



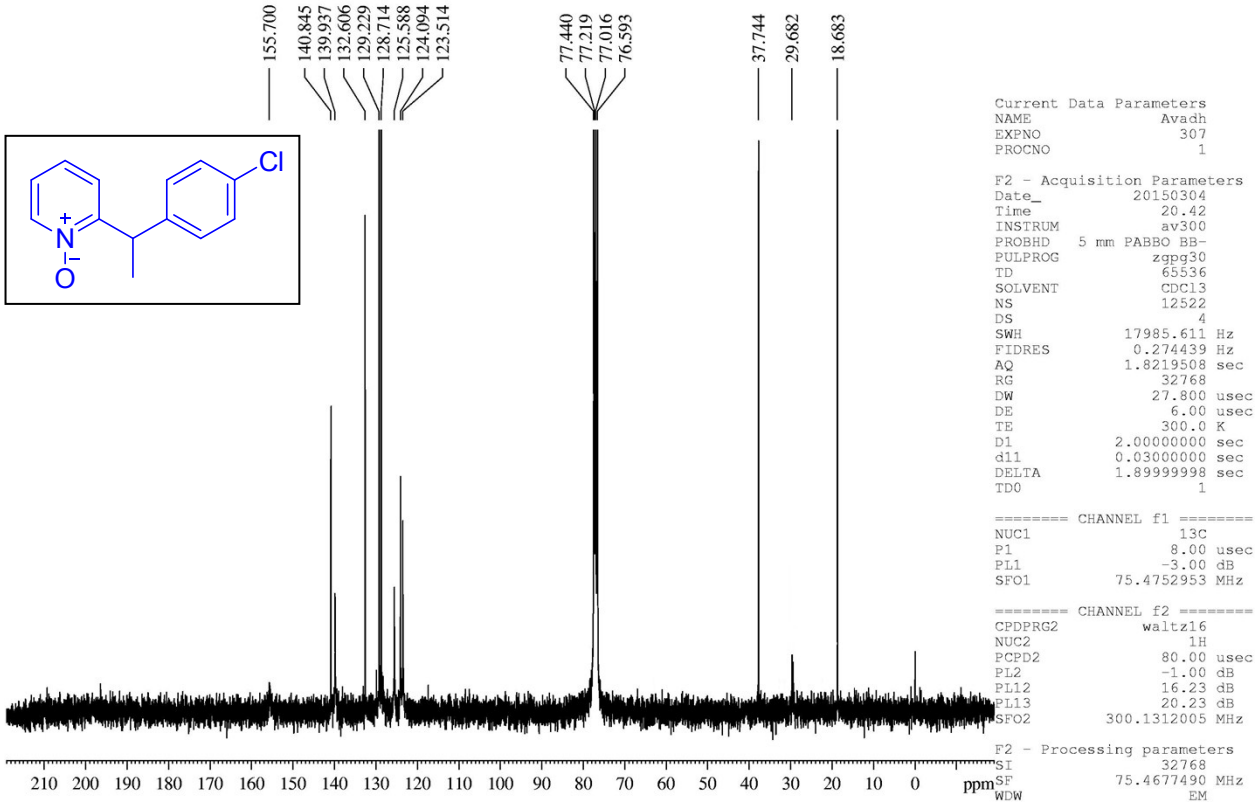
Spectrum 24. 300 MHz ^{1}H NMR of compound **3h**



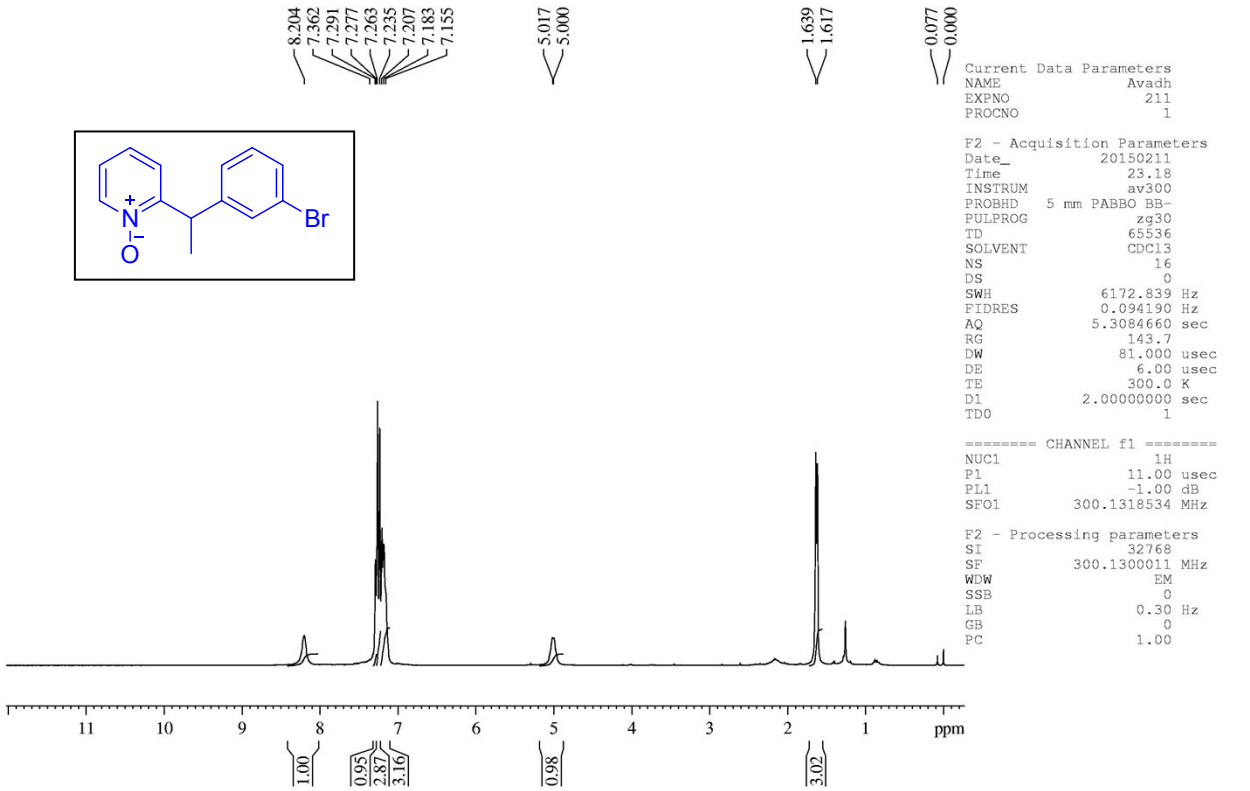
Spectrum 25. 75 MHz ^{13}C NMR of compound **3h**



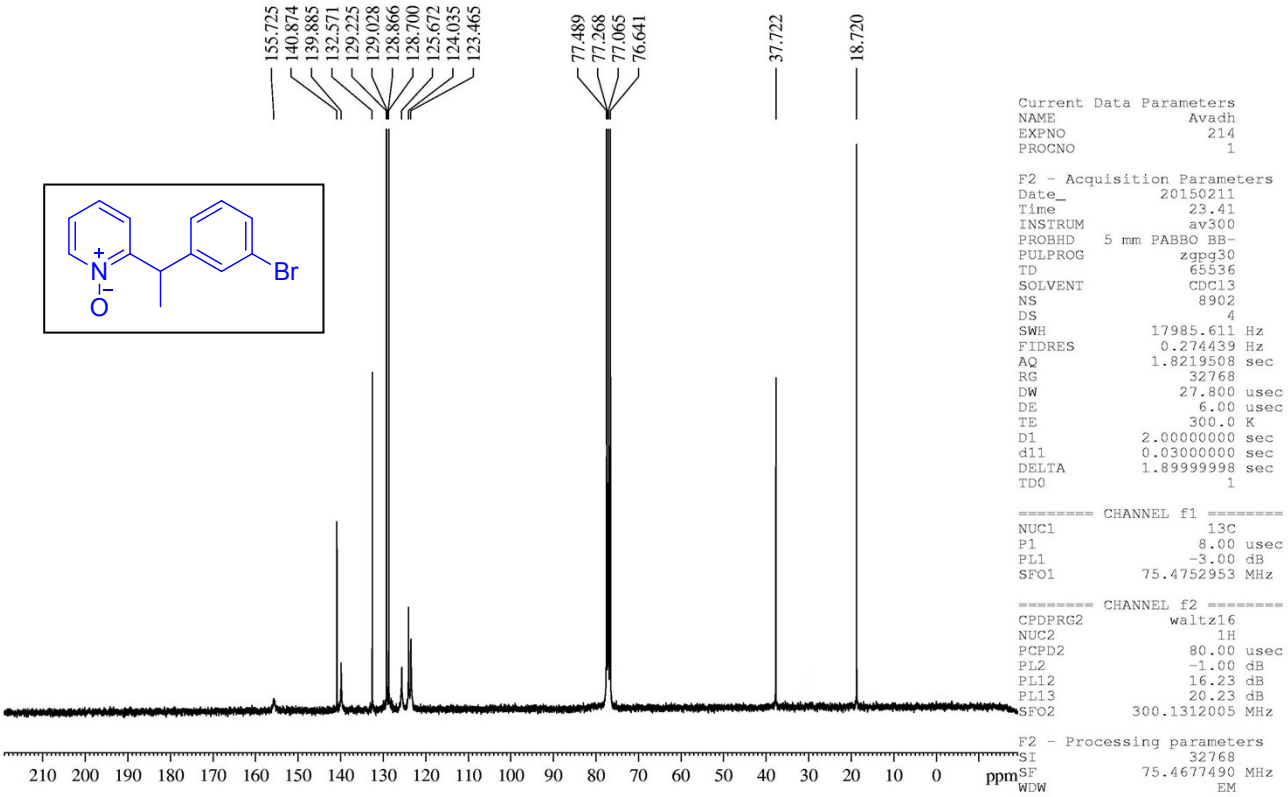
Spectrum 26. 300 MHz ^{1}H NMR of compound **3i**



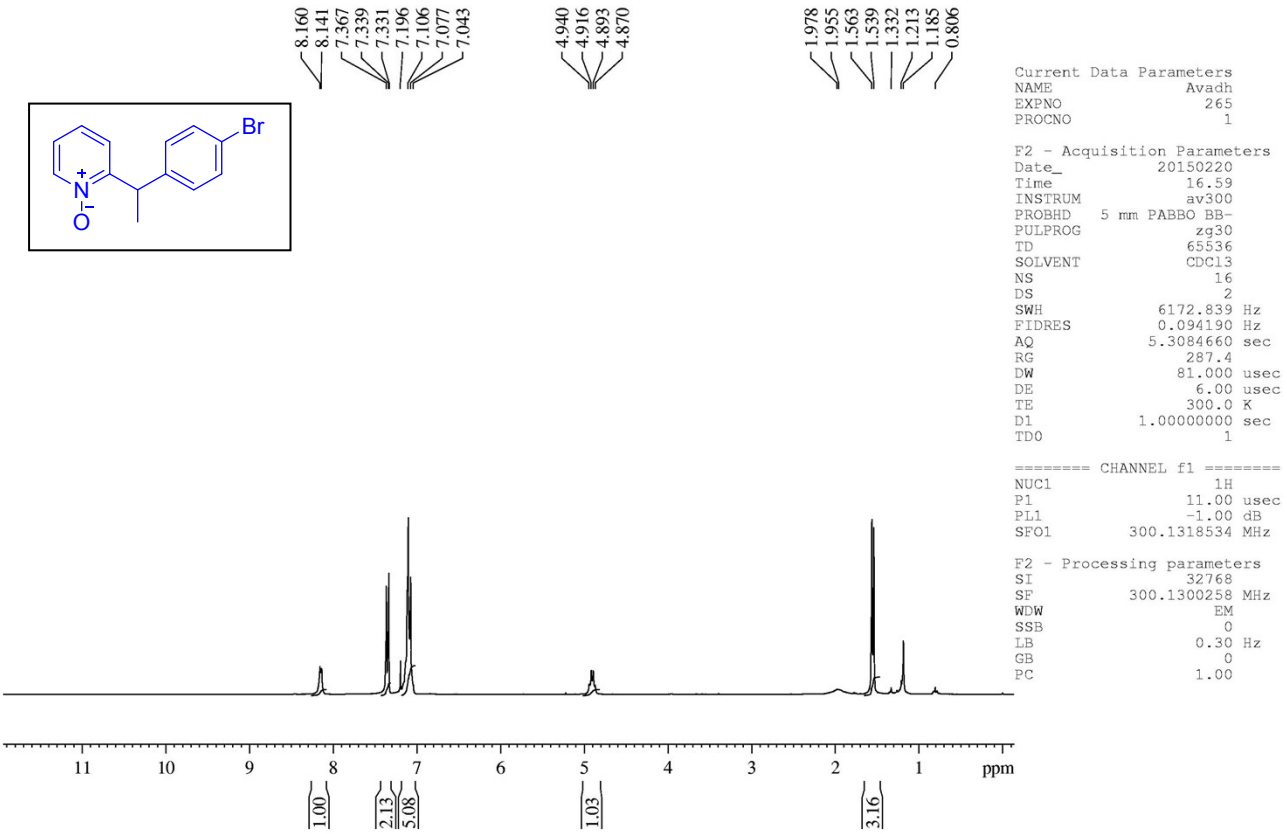
Spectrum 27. 75 MHz ^{13}C NMR of compound **3i**



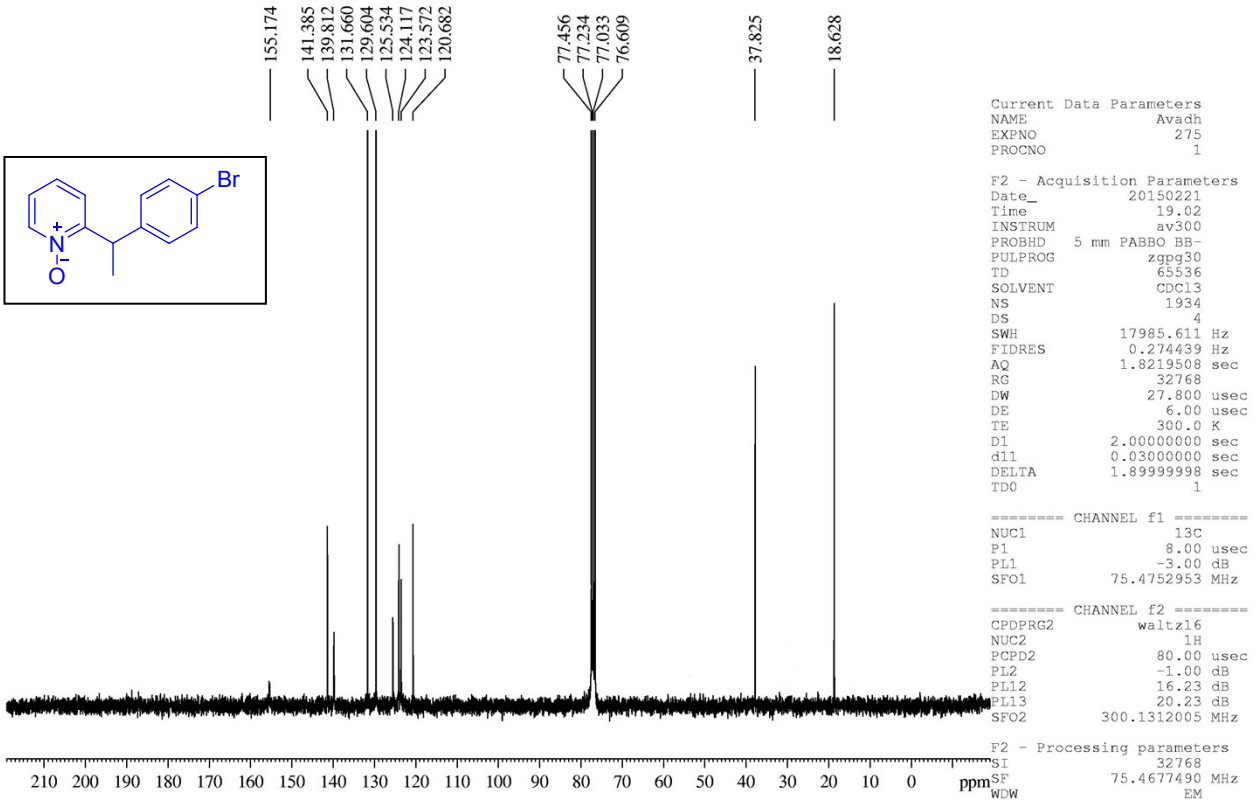
Spectrum 28. 300 MHz ^{1}H NMR of compound **3j**



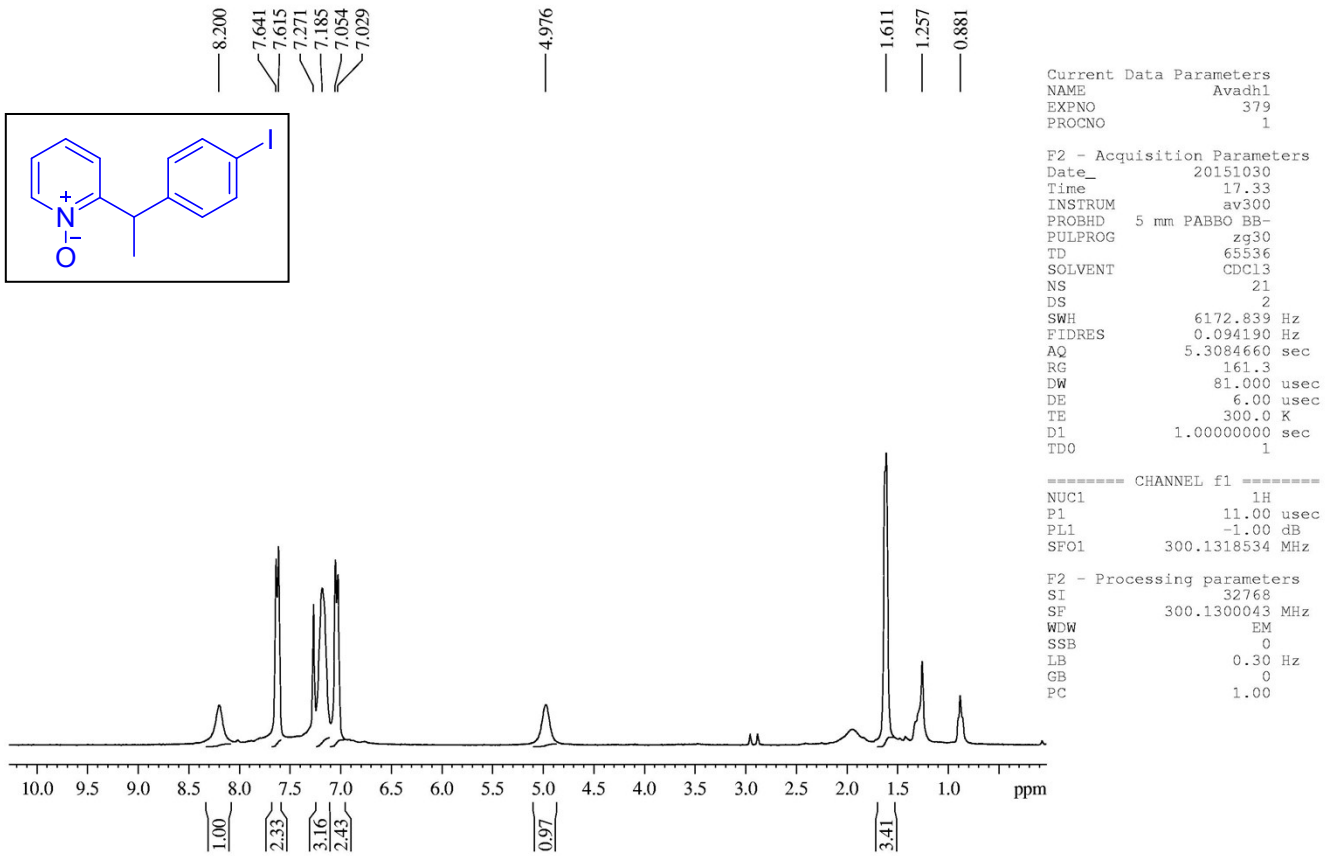
Spectrum 29. 75 MHz ^{13}C NMR of compound **3j**



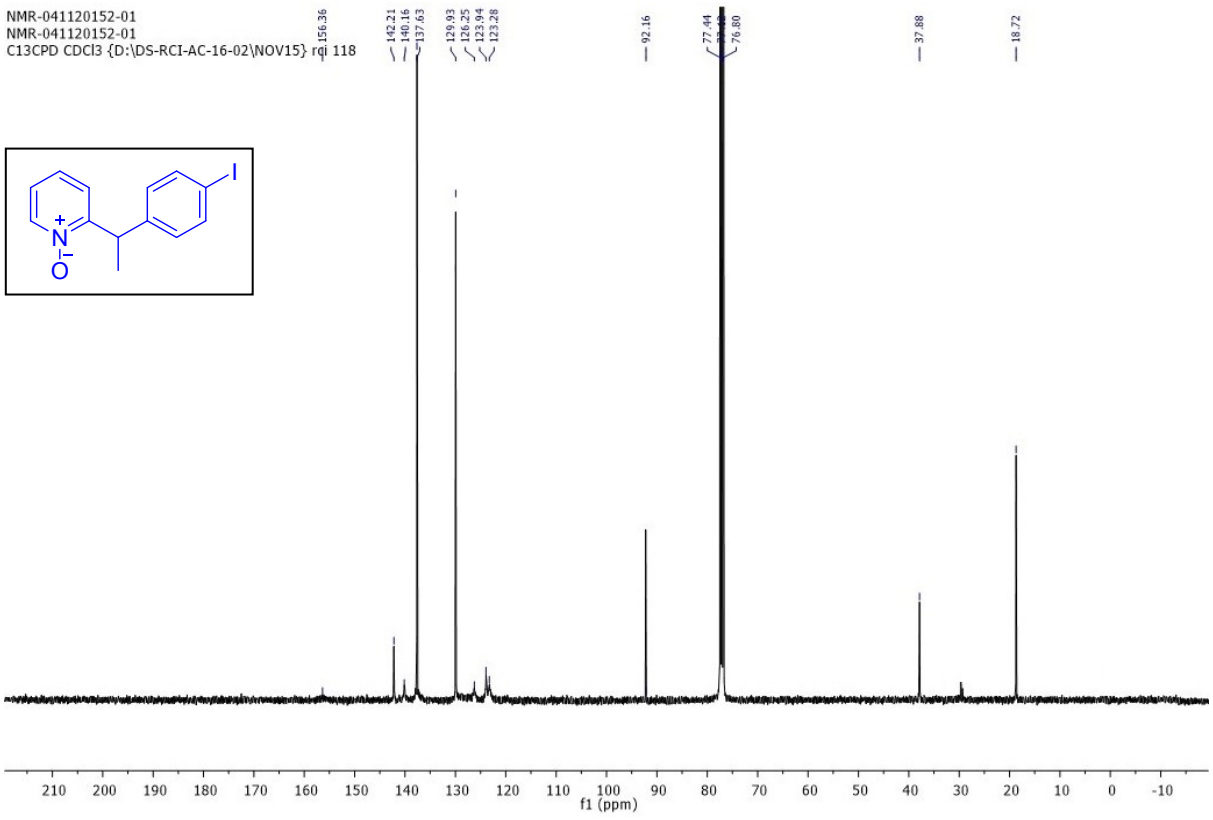
Spectrum 30. 300 MHz ^{1}H NMR of compound **3k**



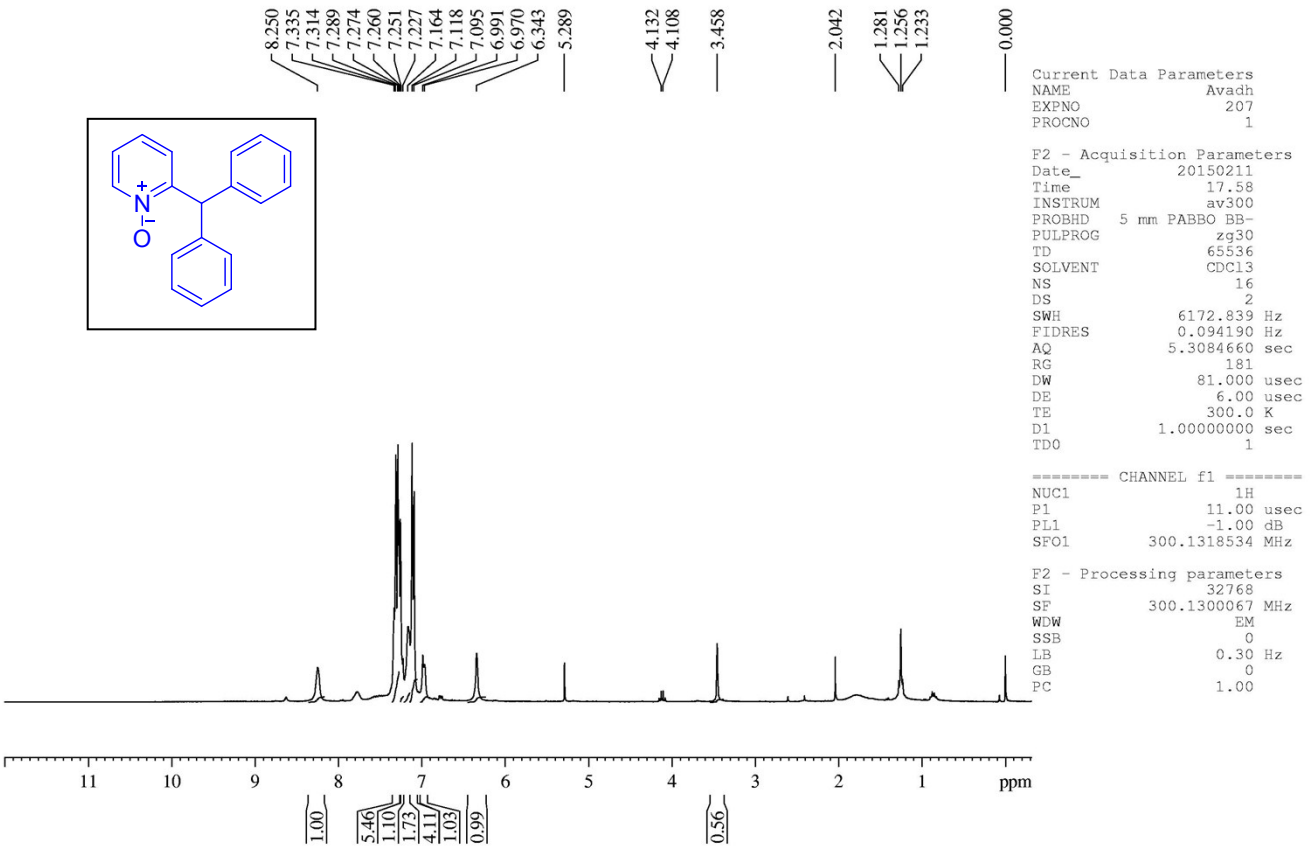
Spectrum 31. 75 MHz ^{13}C NMR of compound **3k**



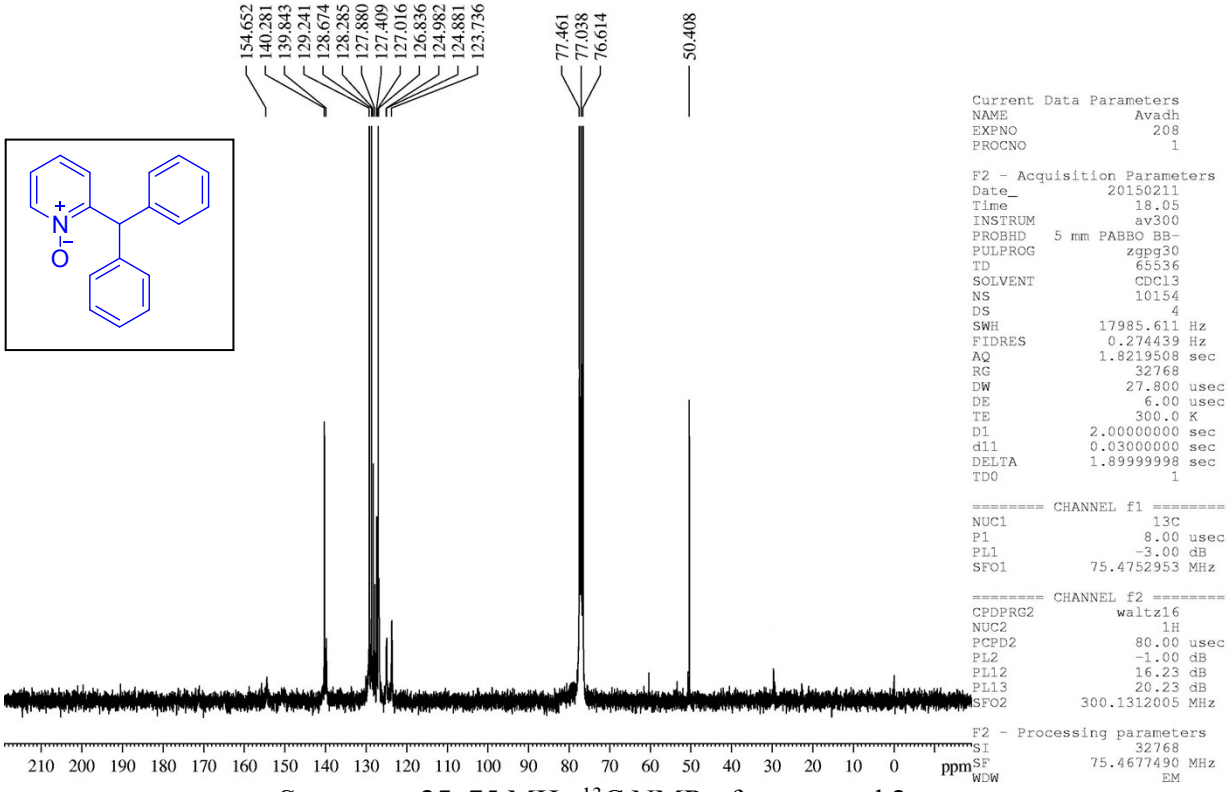
Spectrum 32. 300 MHz ^{1}H NMR of compound **3l**



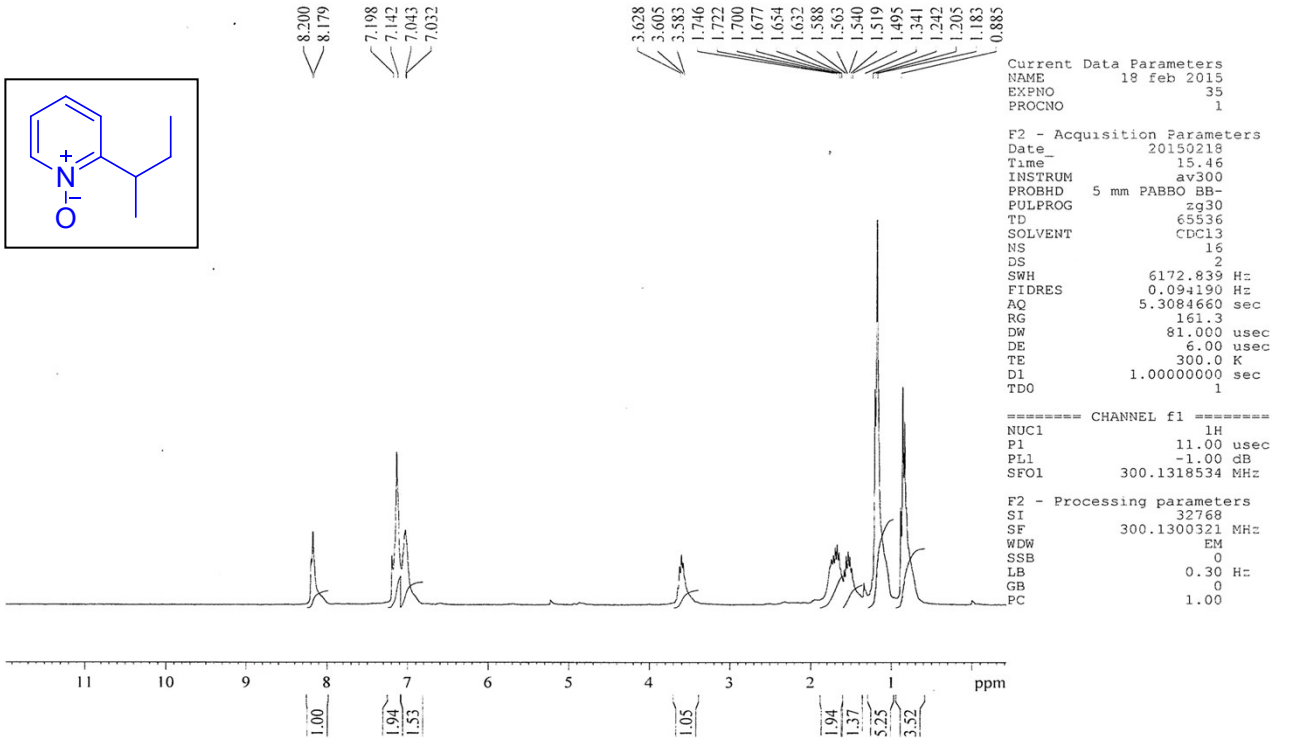
Spectrum 33. 100 MHz ^{13}C NMR of compound **3l**



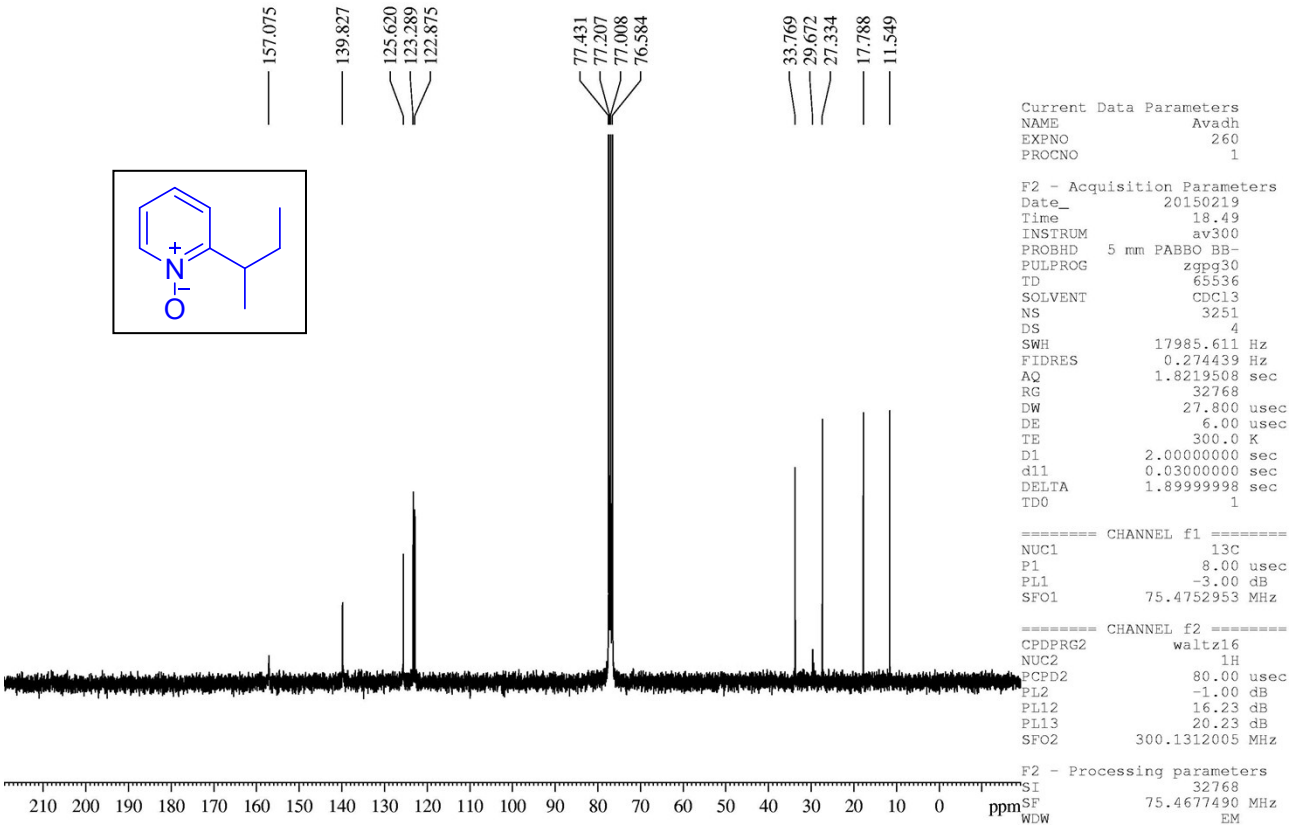
Spectrum 34. 300 MHz ^{1}H NMR of compound **3m**



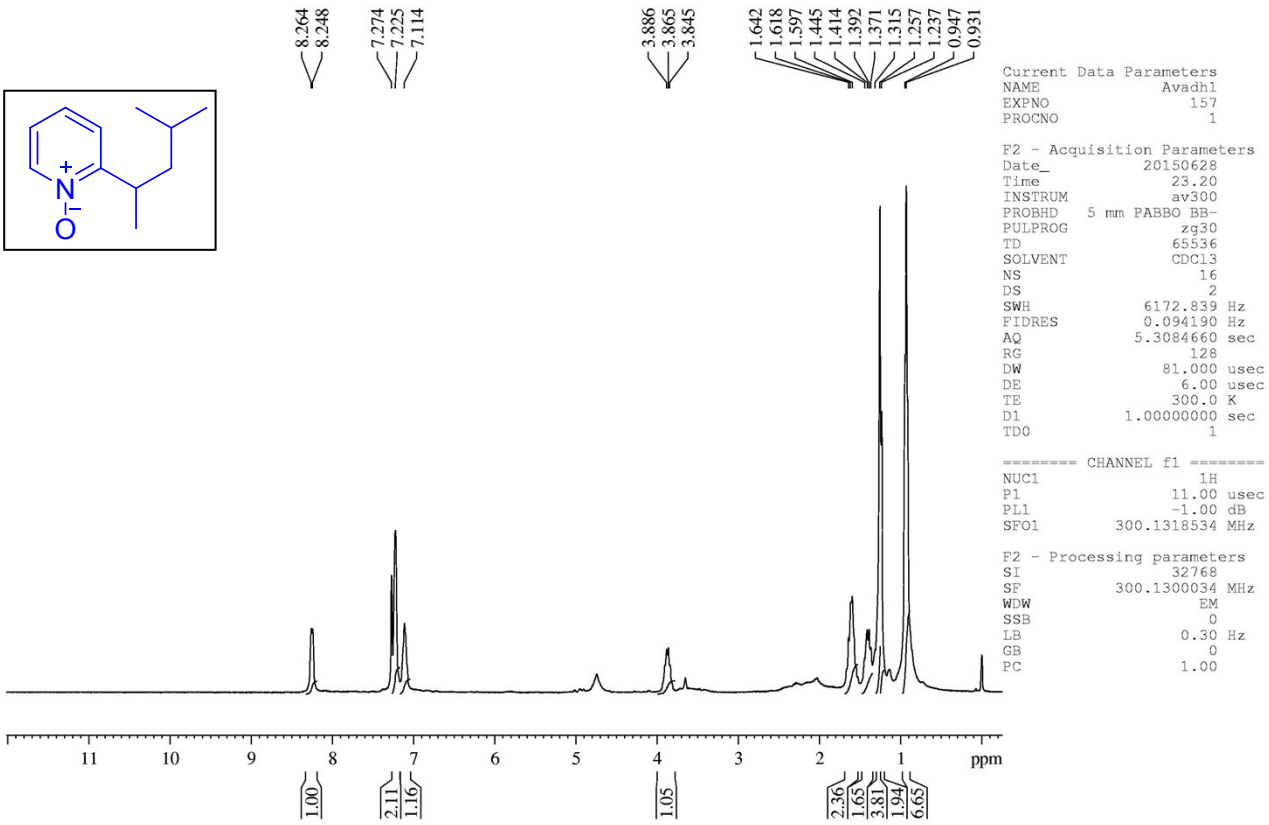
Spectrum 35. 75 MHz ^{13}C NMR of compound **3m**



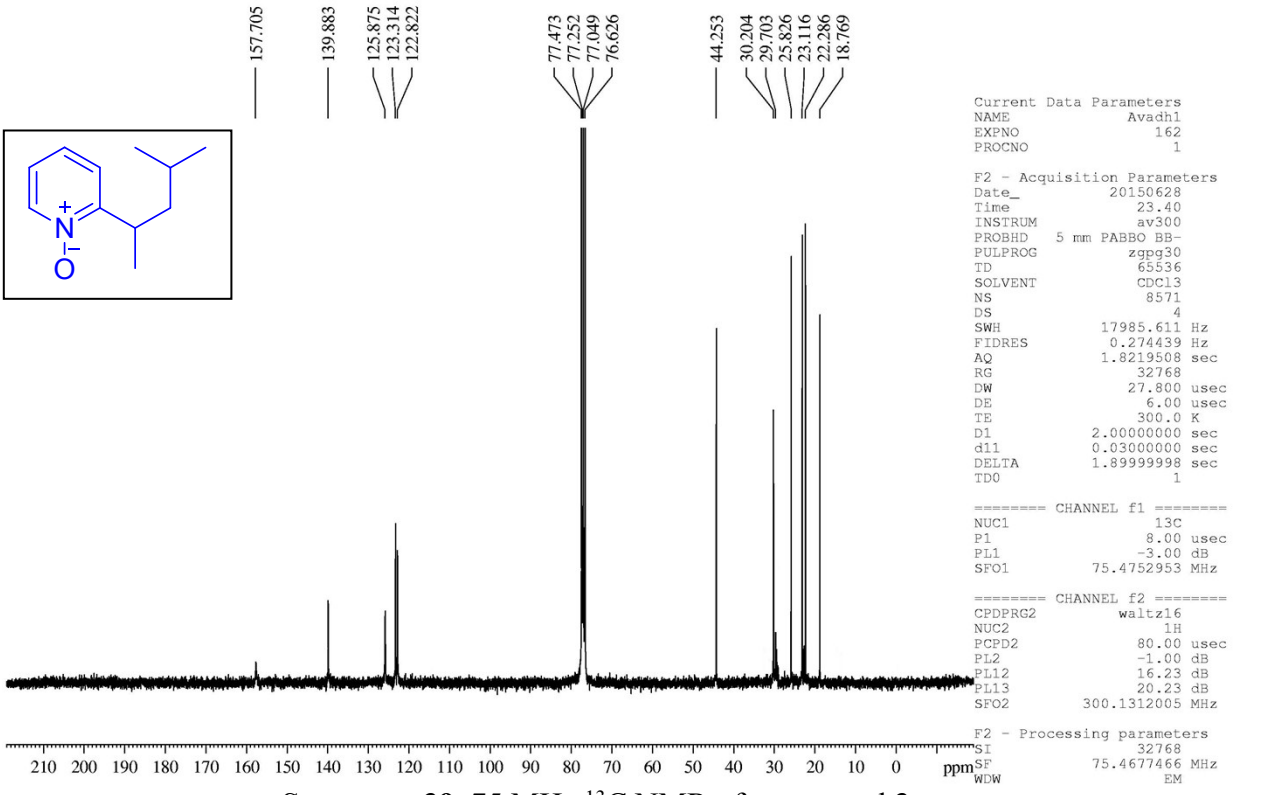
Spectrum 36. 300 MHz ^{1}H NMR of compound **3n**



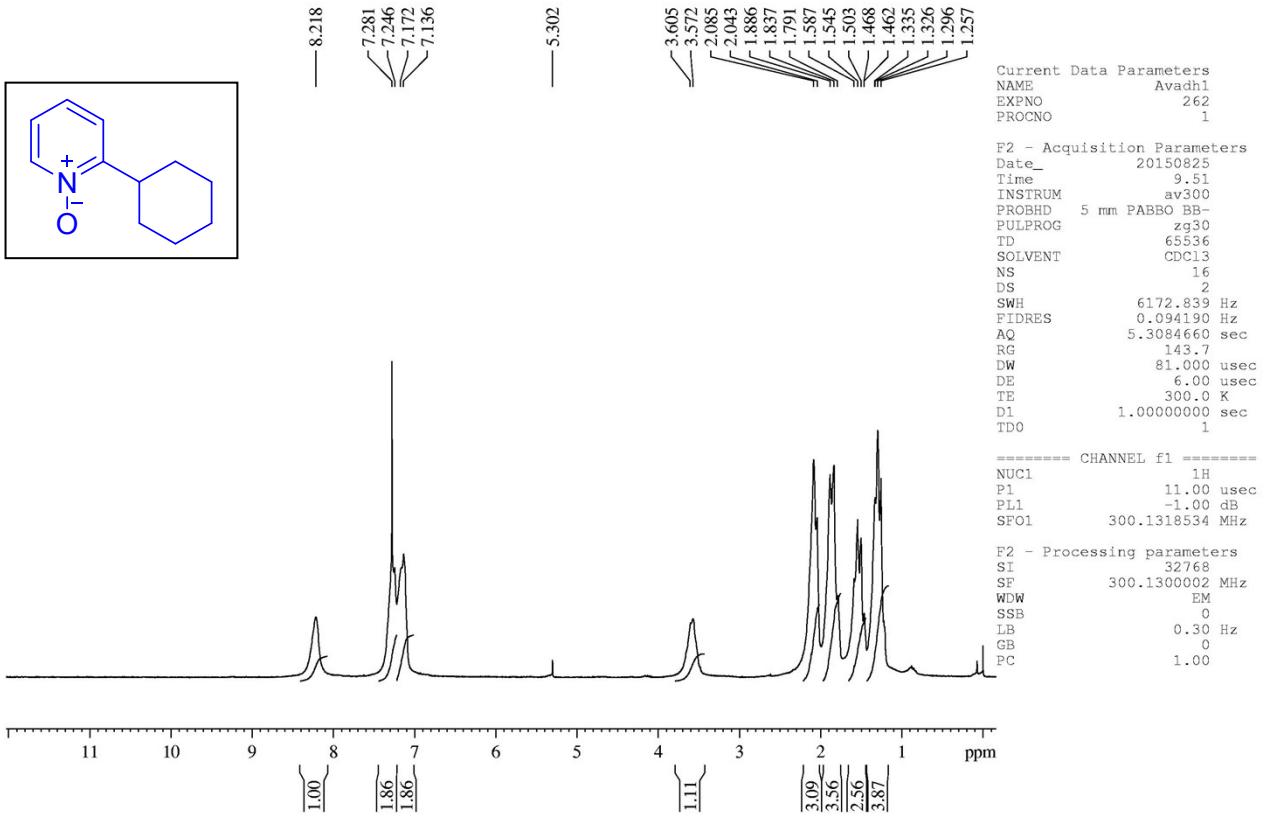
Spectrum 37. 75 MHz ^{13}C NMR of compound **3n**



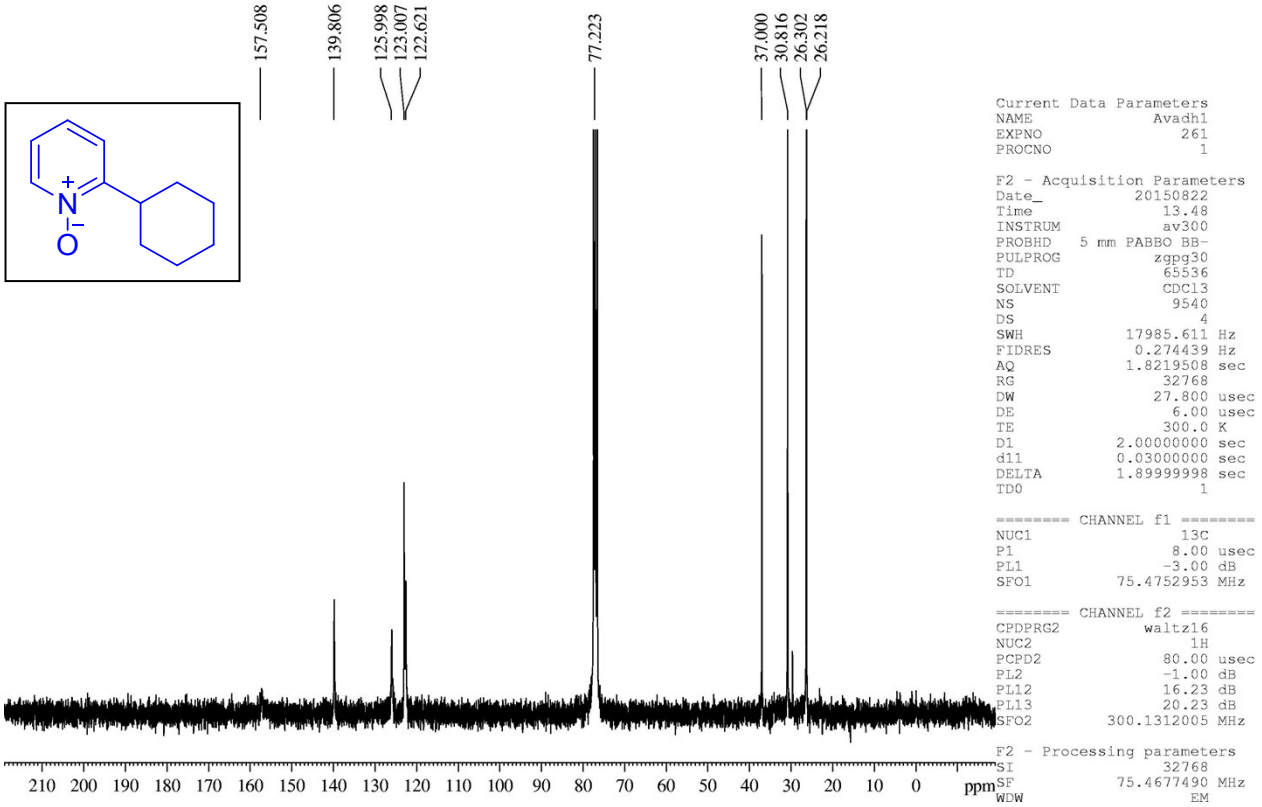
Spectrum 38. 300 MHz ^{1}H NMR of compound **3o**



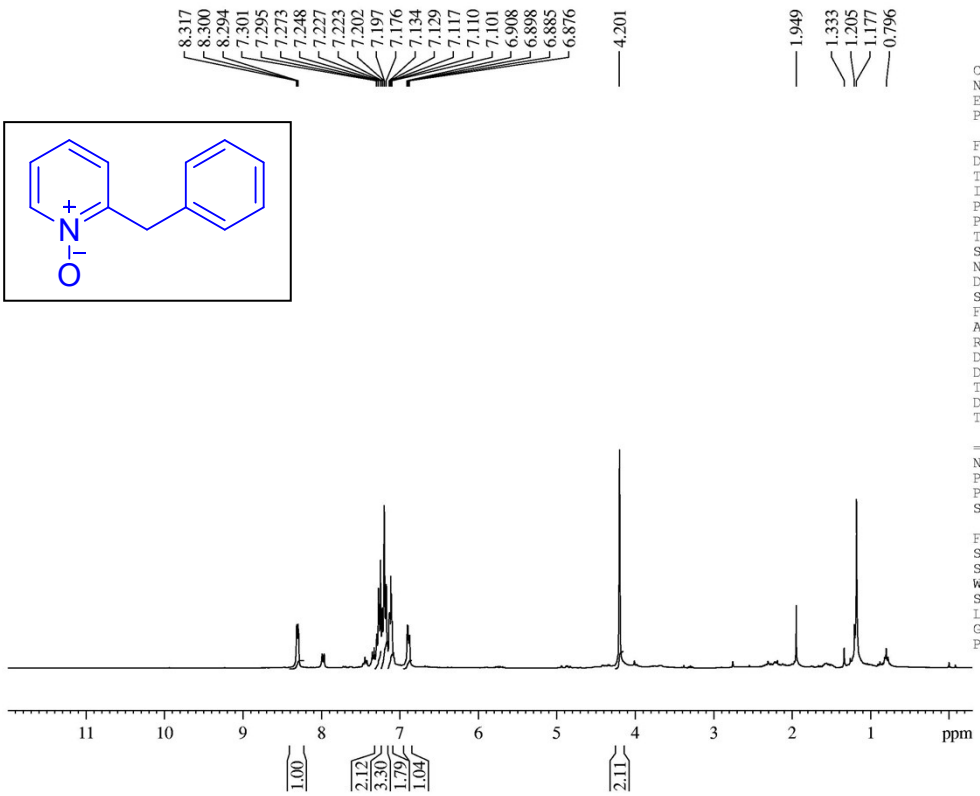
Spectrum 39. 75 MHz ^{13}C NMR of compound **3o**



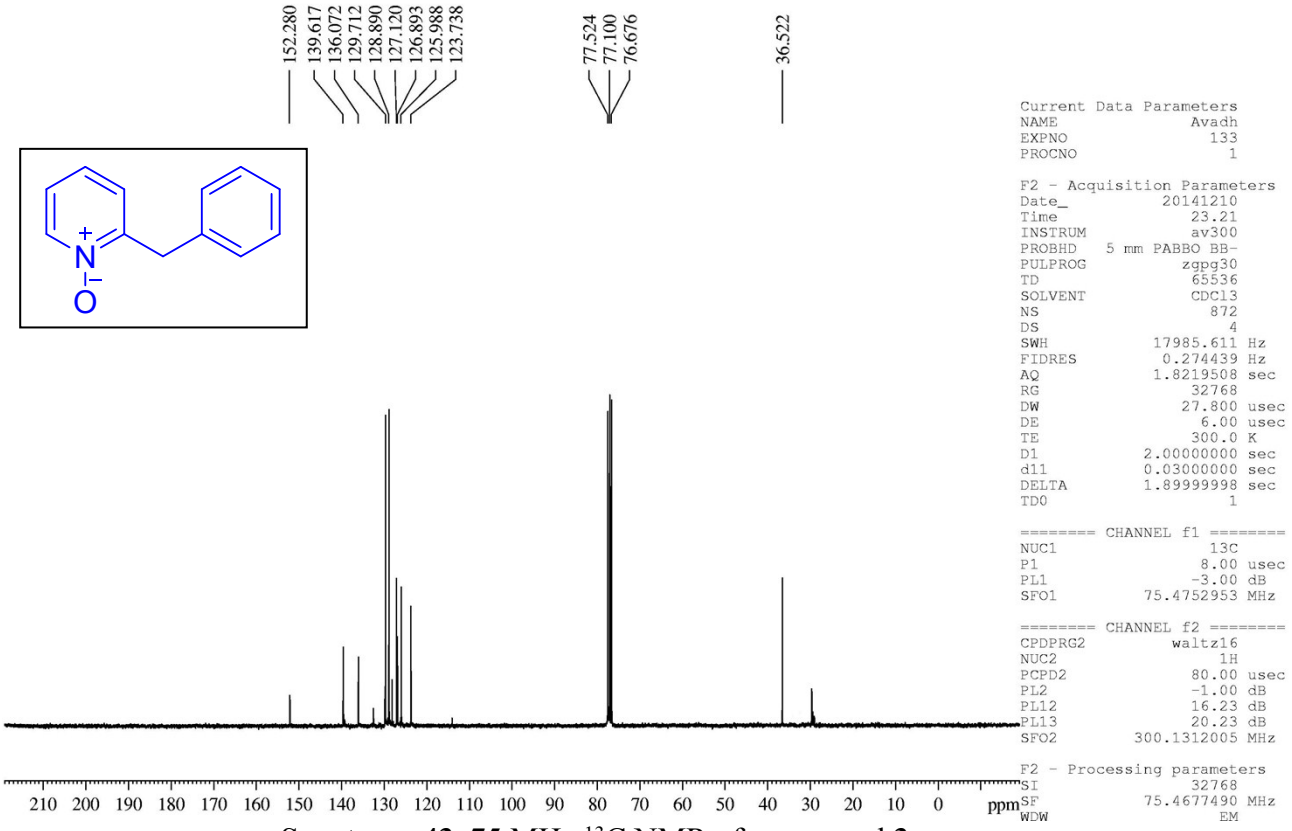
Spectrum 40. 300 MHz ^{1}H NMR of compound **3p**



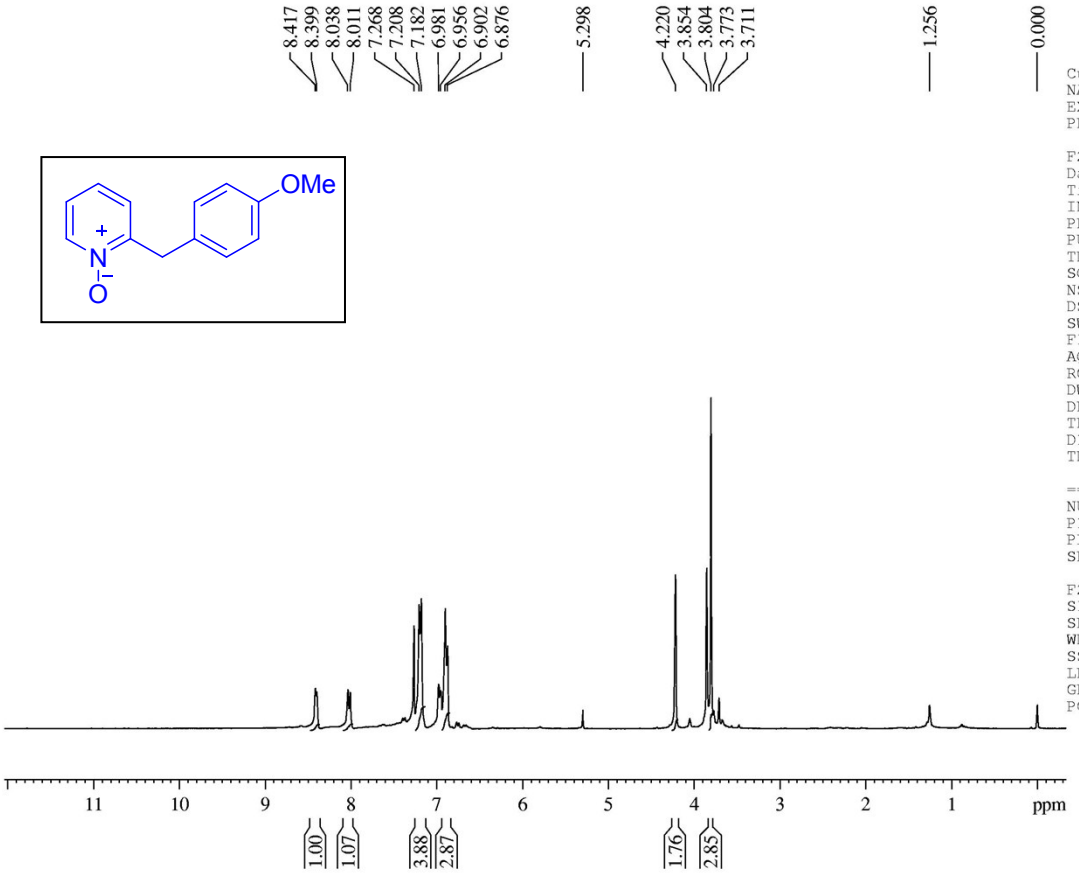
Spectrum 41. 75 MHz ^{13}C NMR of compound **3p**



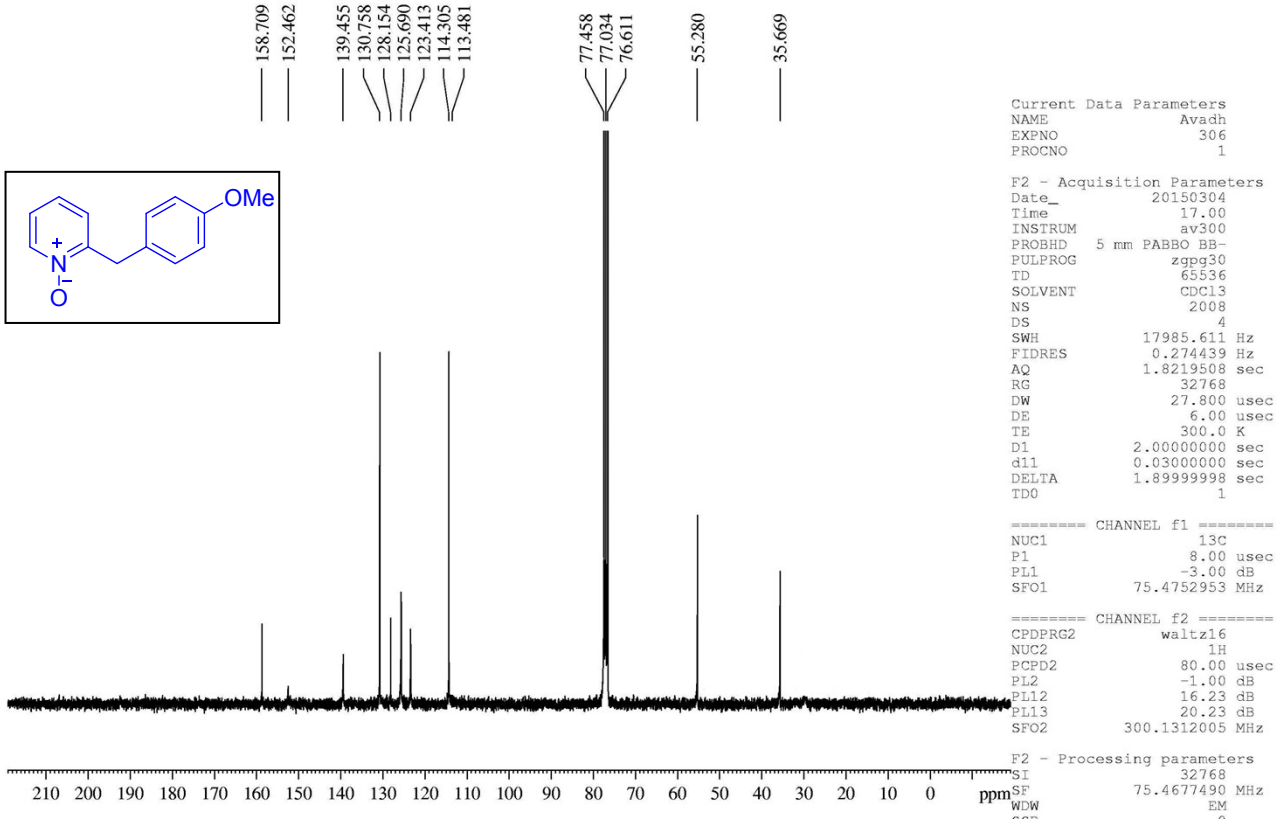
Spectrum 42. 300 MHz ^{1}H NMR of compound **3q**



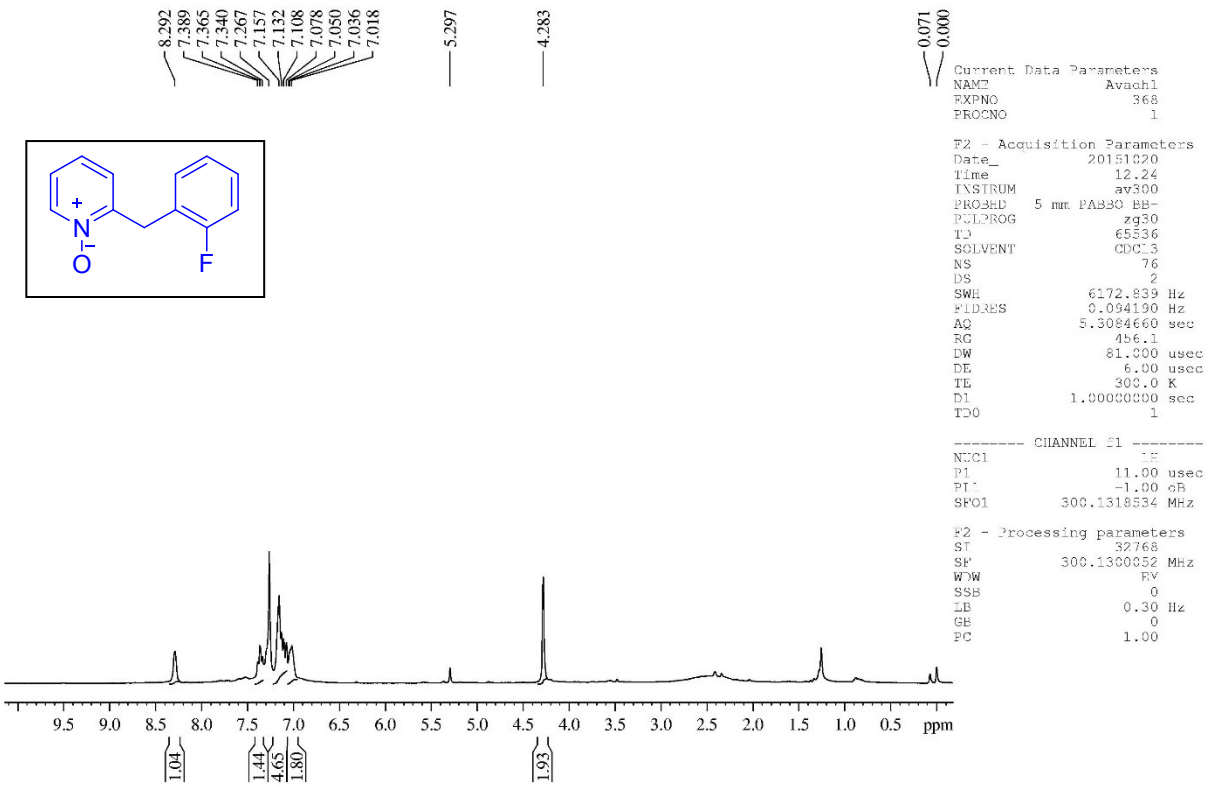
Spectrum 43. 75 MHz ^{13}C NMR of compound **3q**



Spectrum 44. 300 MHz ^{1}H NMR of compound **3r**



Spectrum 45. 75 MHz ^{13}C NMR of compound **3r**



Spectrum 46. 300 MHz ^{1}H NMR of compound **3s**

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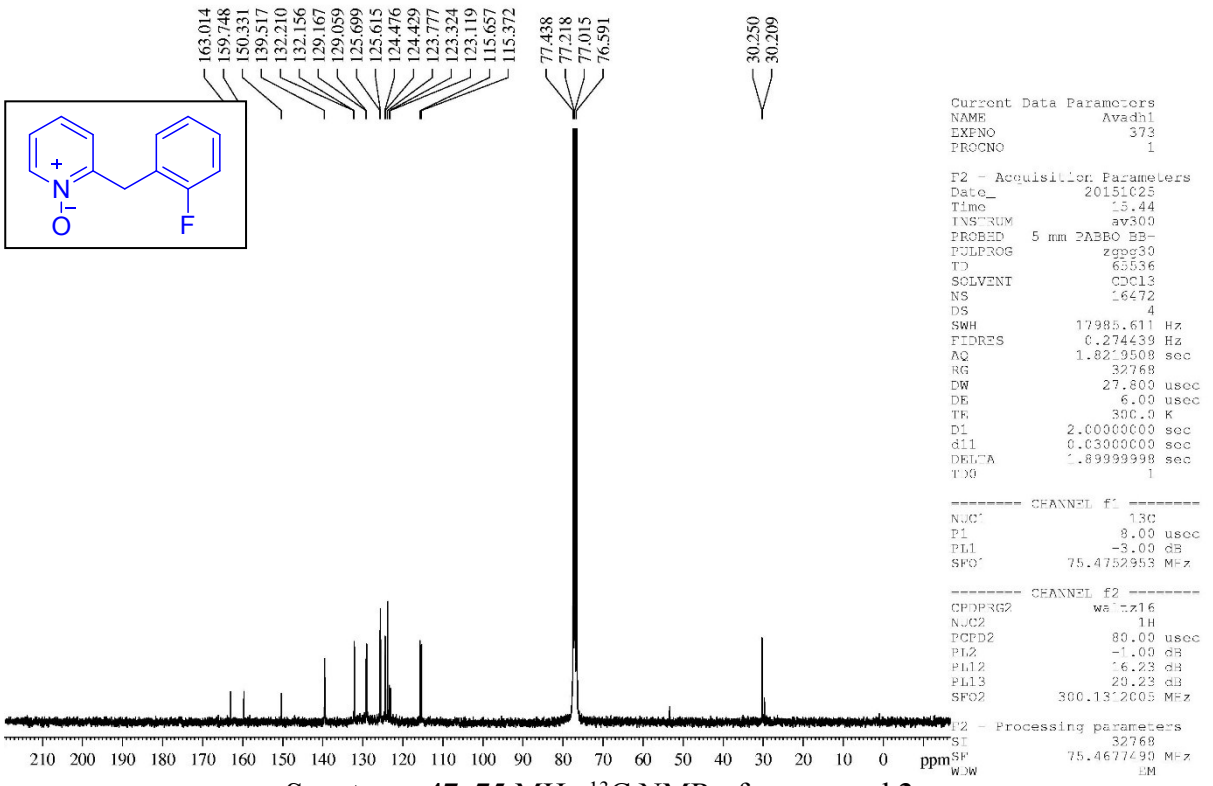

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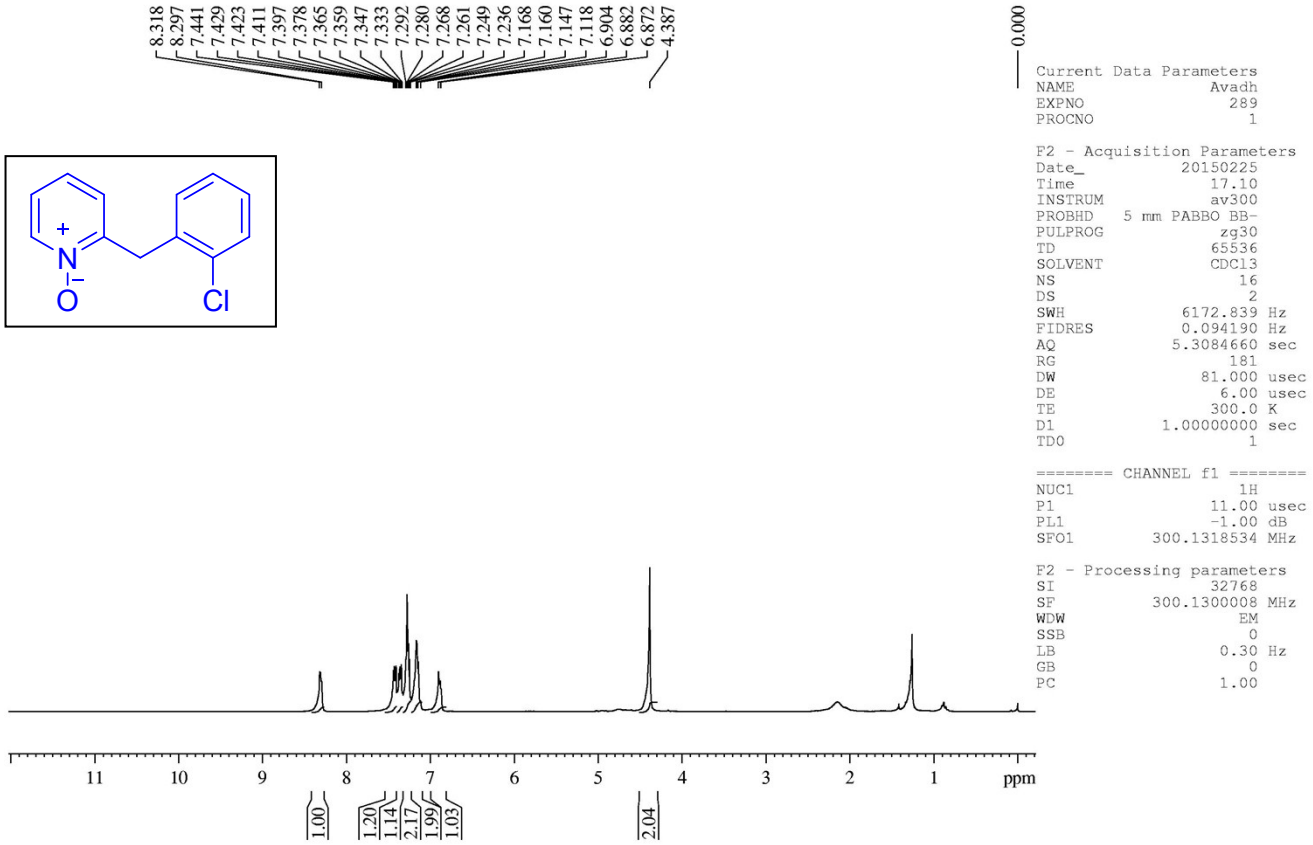
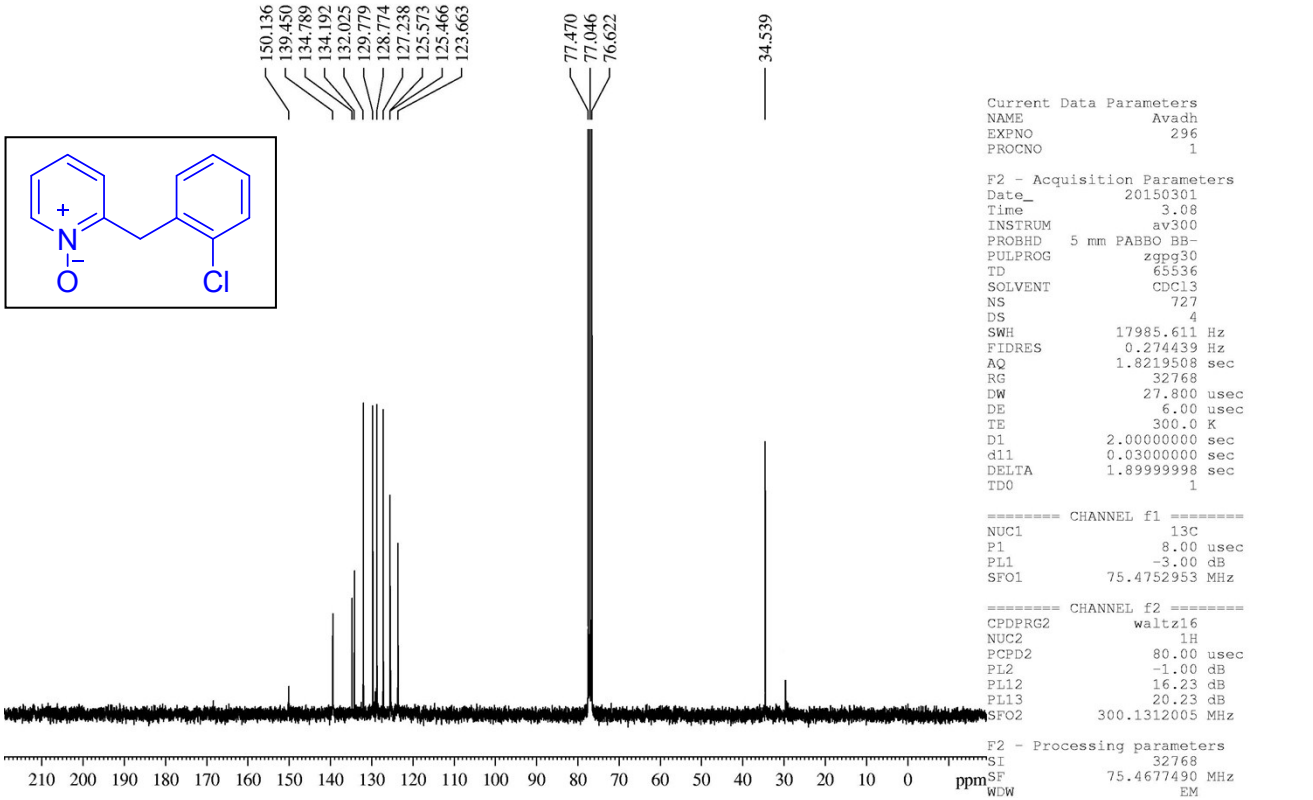
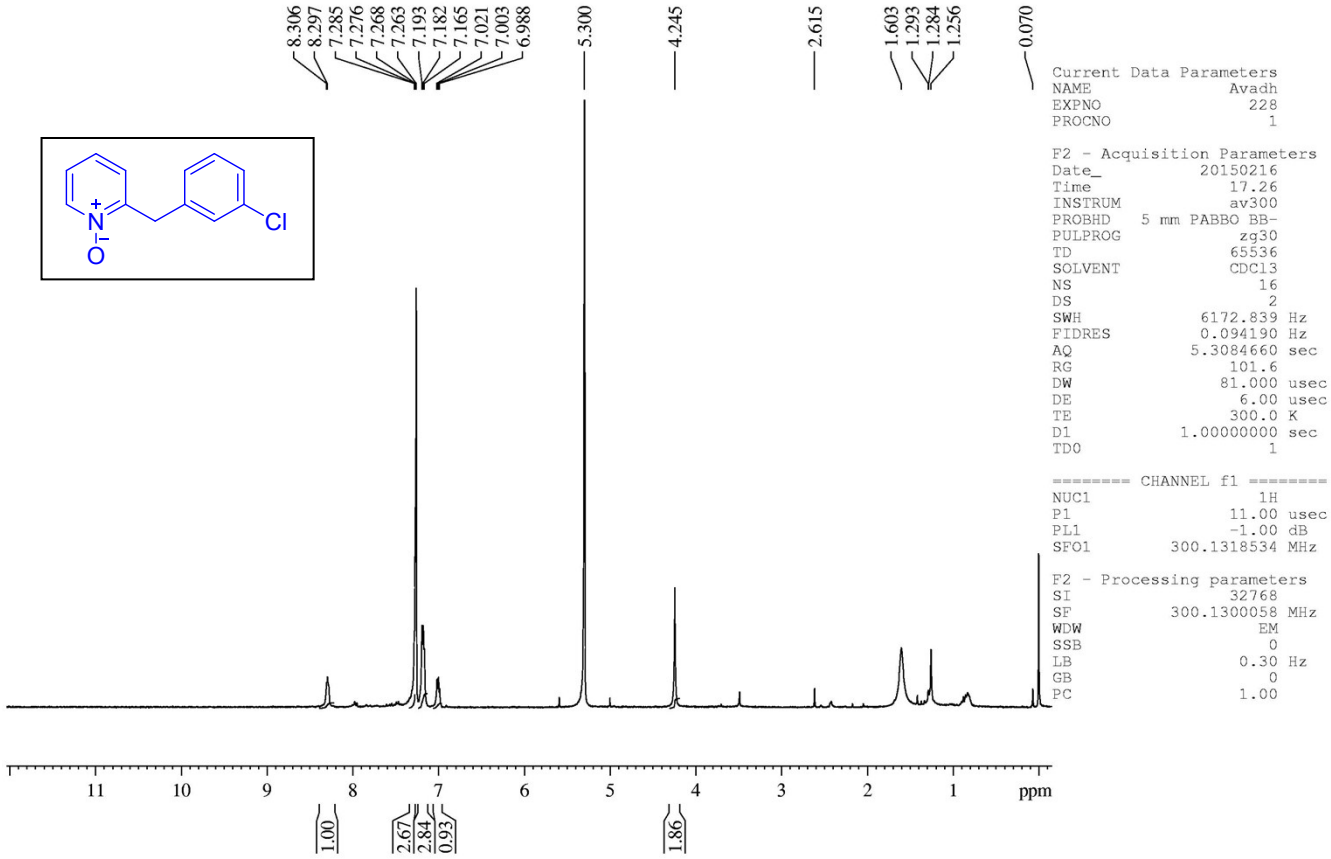


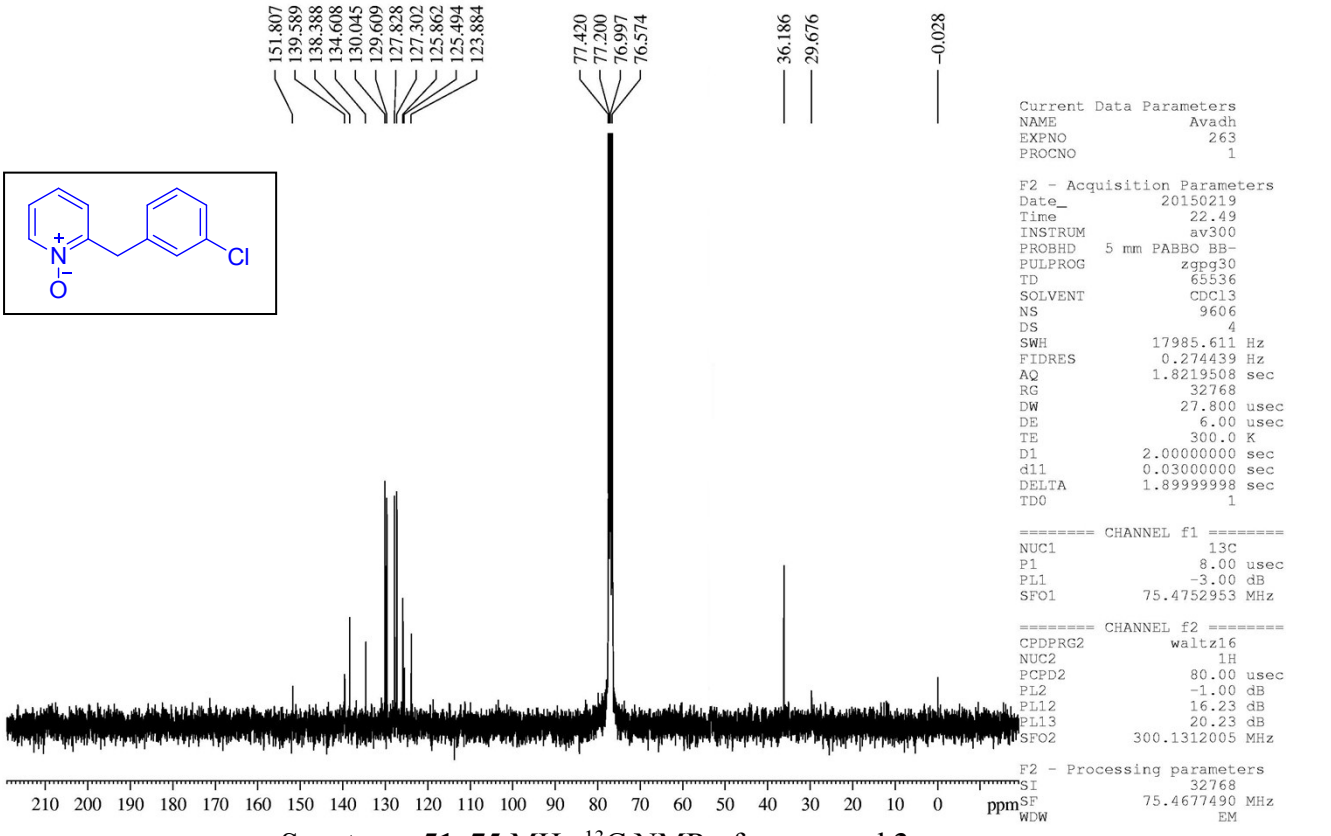
Spectrum 48. 300 MHz ^{1}H NMR of compound **3t**



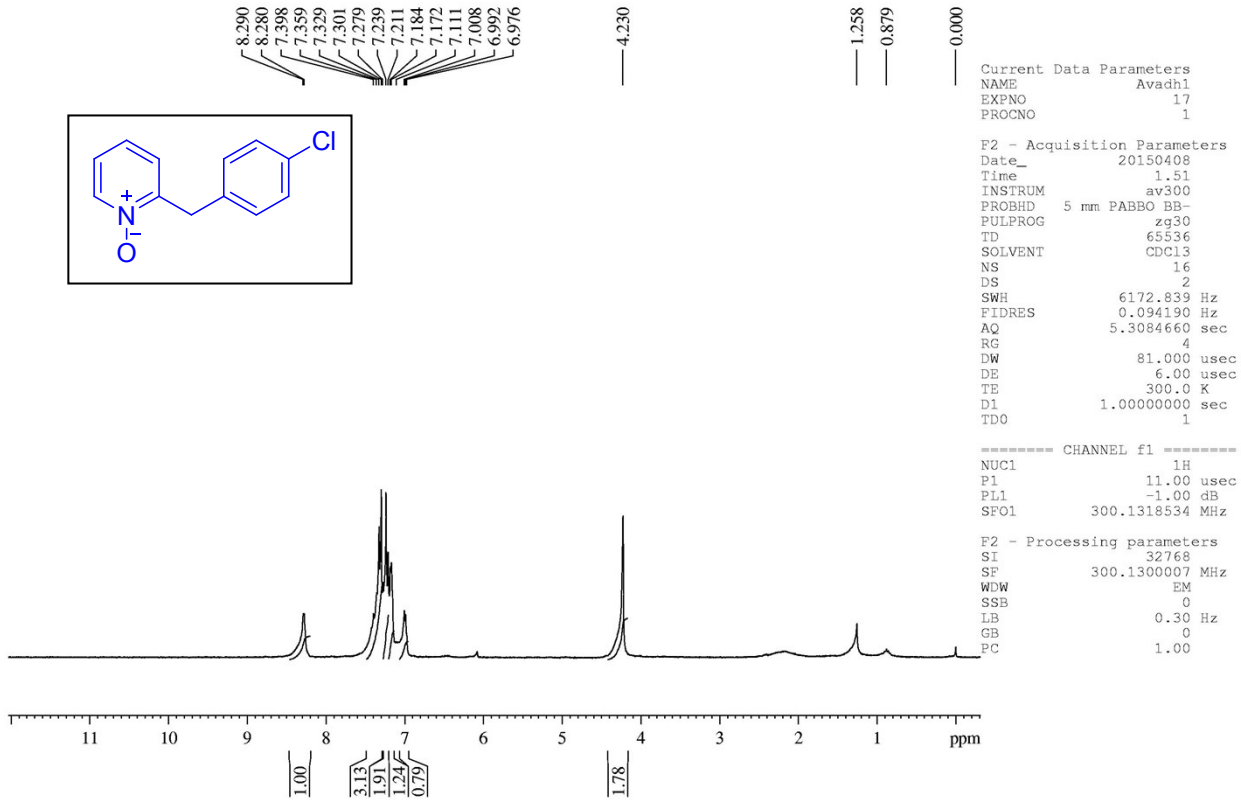
Spectrum 49. 75 MHz ^{13}C NMR of compound **3t**



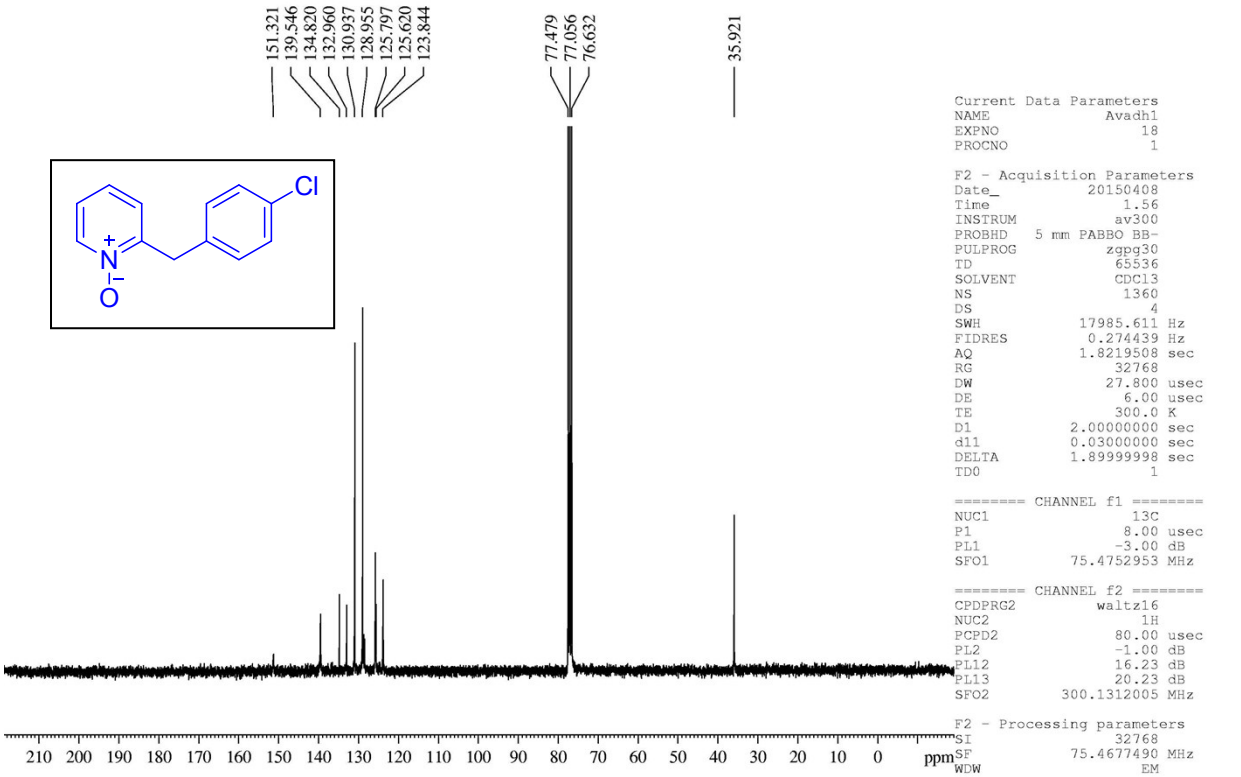
Spectrum 50. 300 MHz ^{1}H NMR of compound **3u**



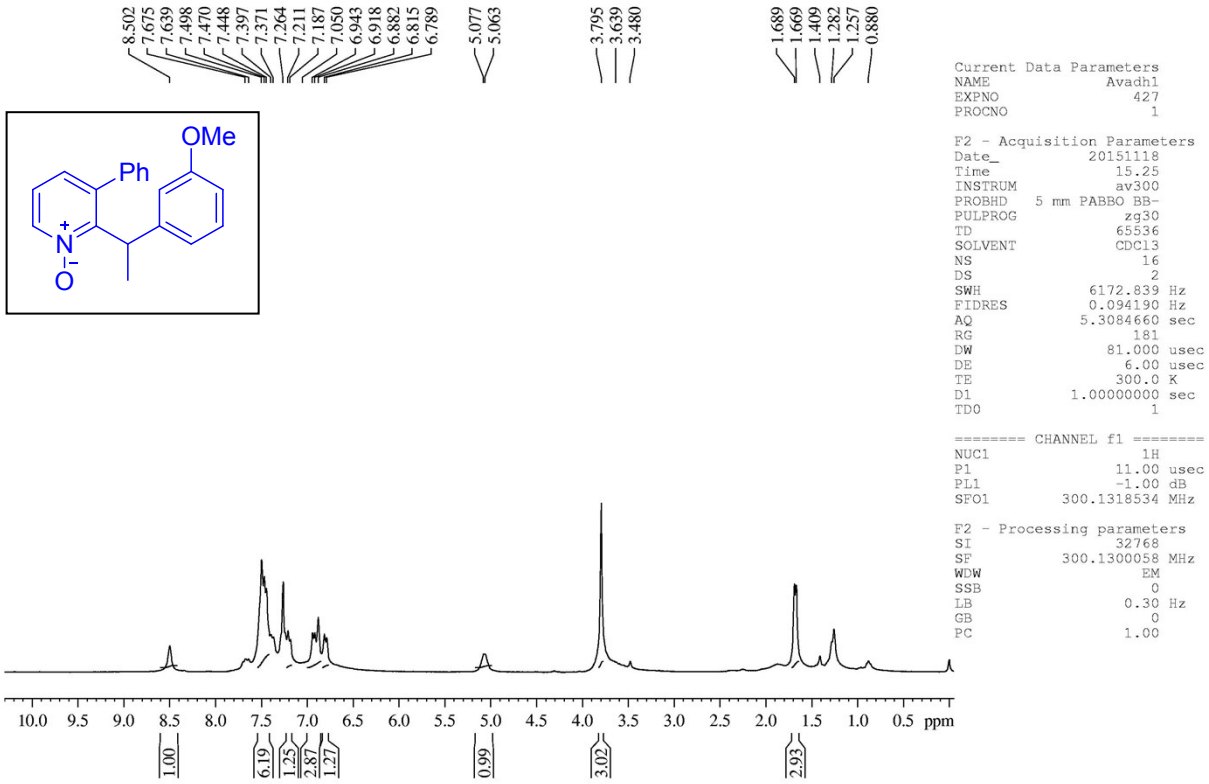
Spectrum 51. 75 MHz ^{13}C NMR of compound **3u**



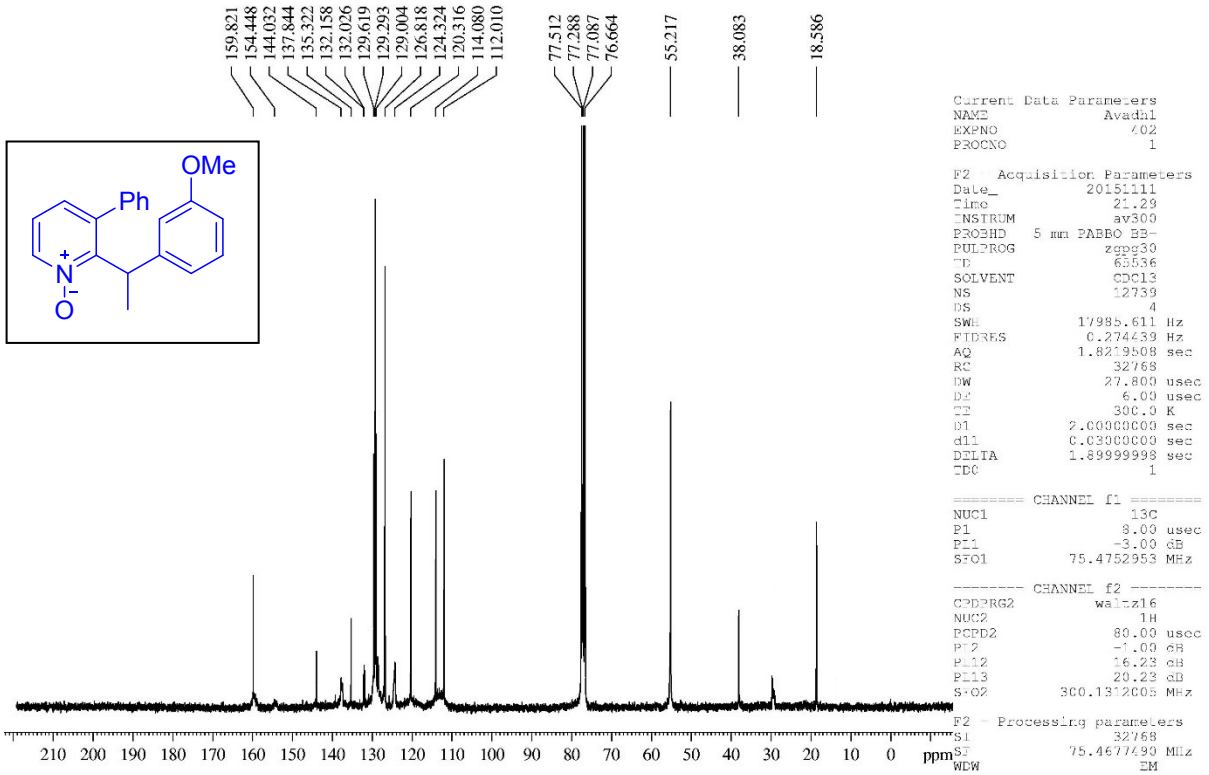
Spectrum 52. 300 MHz ^{1}H NMR of compound **3v**



Spectrum 53. 75 MHz ^{13}C NMR of compound **3v**



Spectrum 54. 300 MHz ^{1}H NMR of compound **3w**



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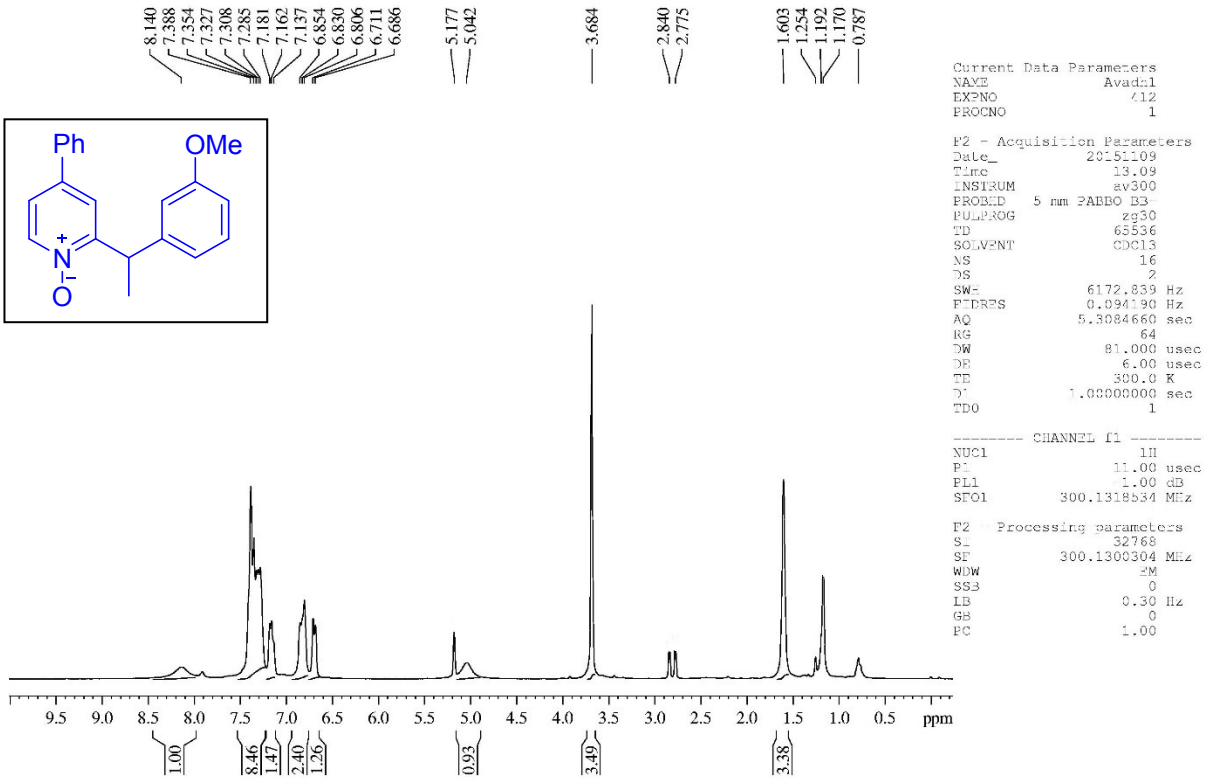
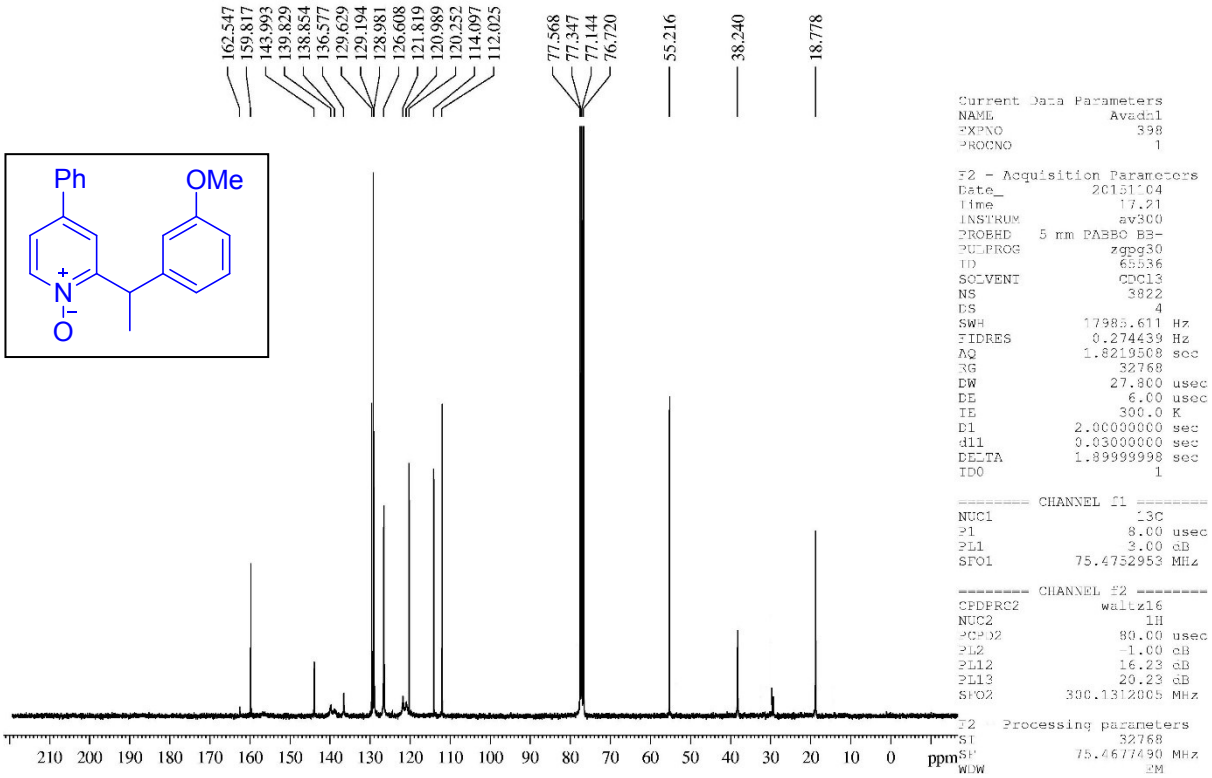
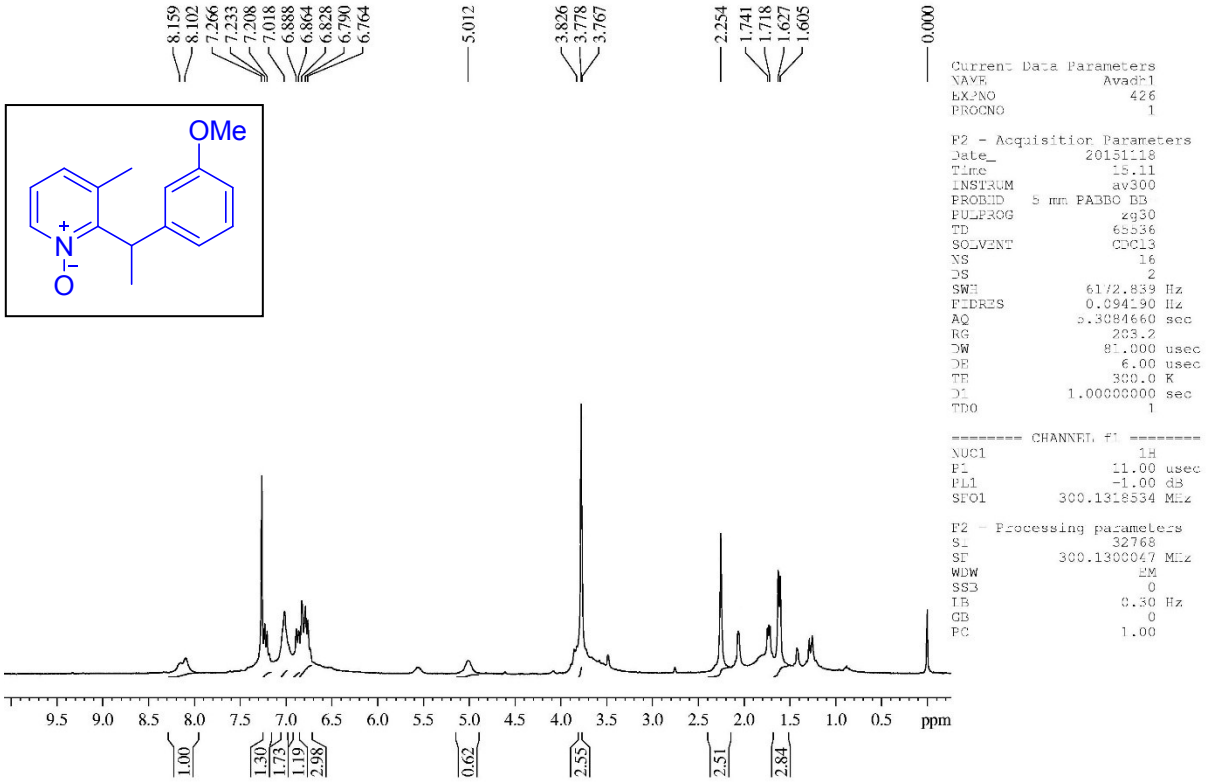


Spectrum 56. 300 MHz ^{1}H NMR of compound **3x**



Spectrum 57. 75 MHz ^{13}C NMR of compound **3x**



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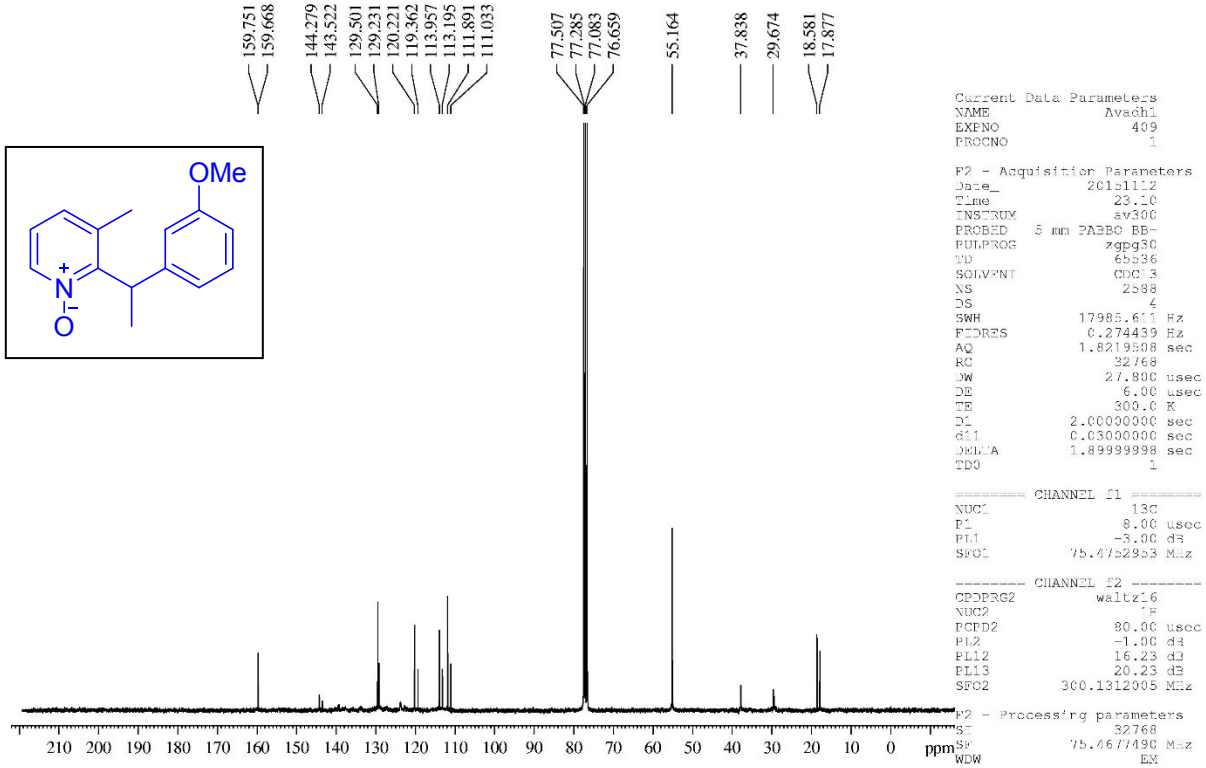

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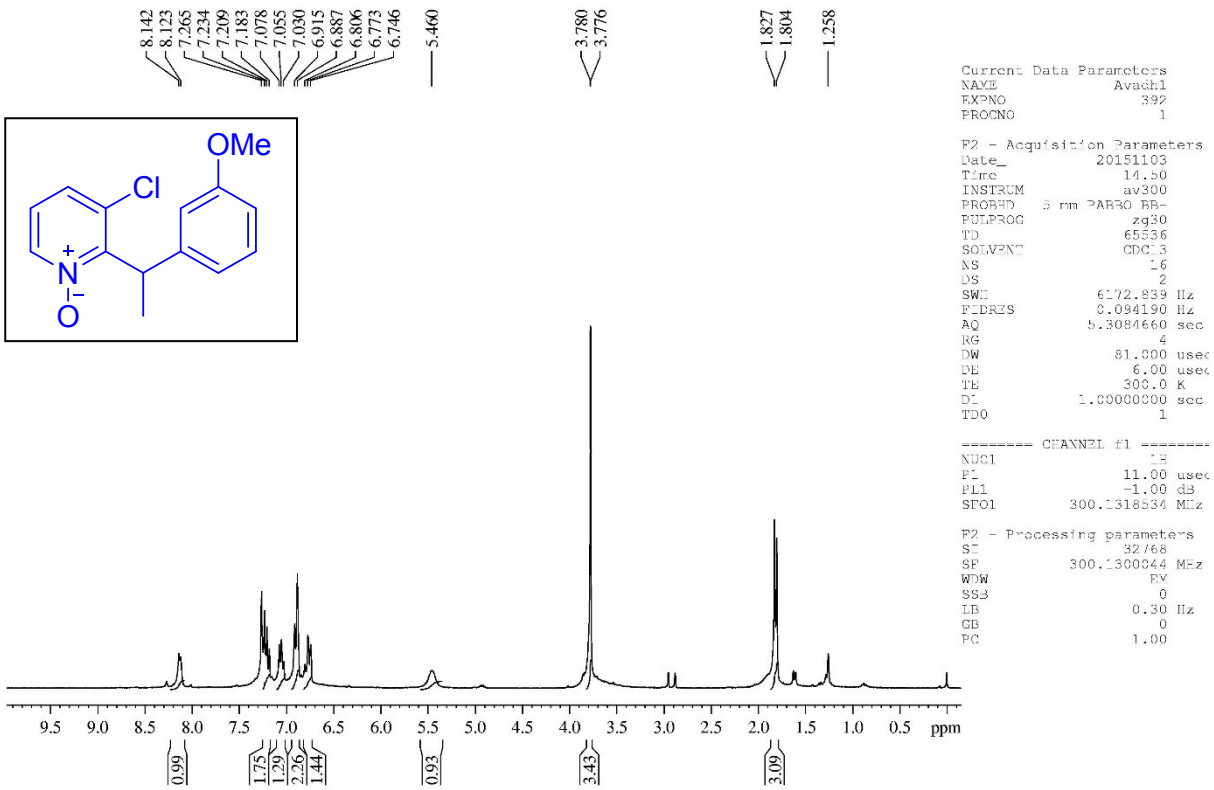

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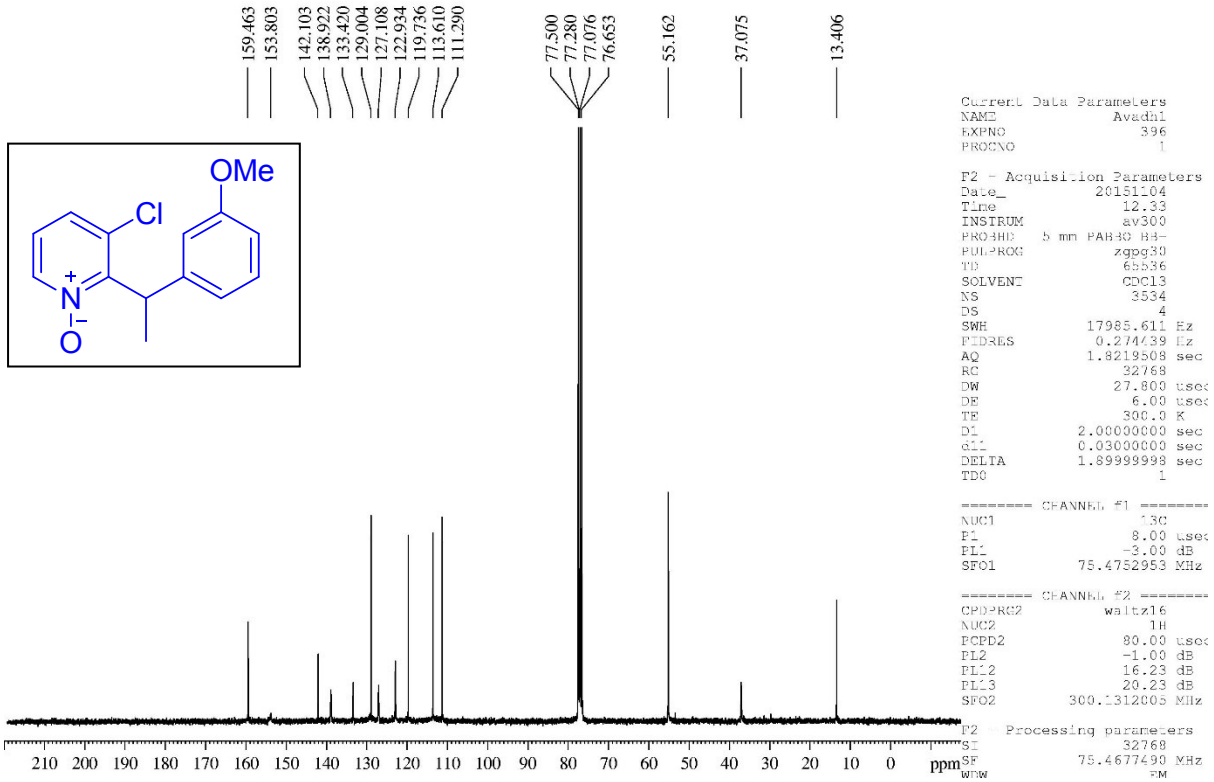

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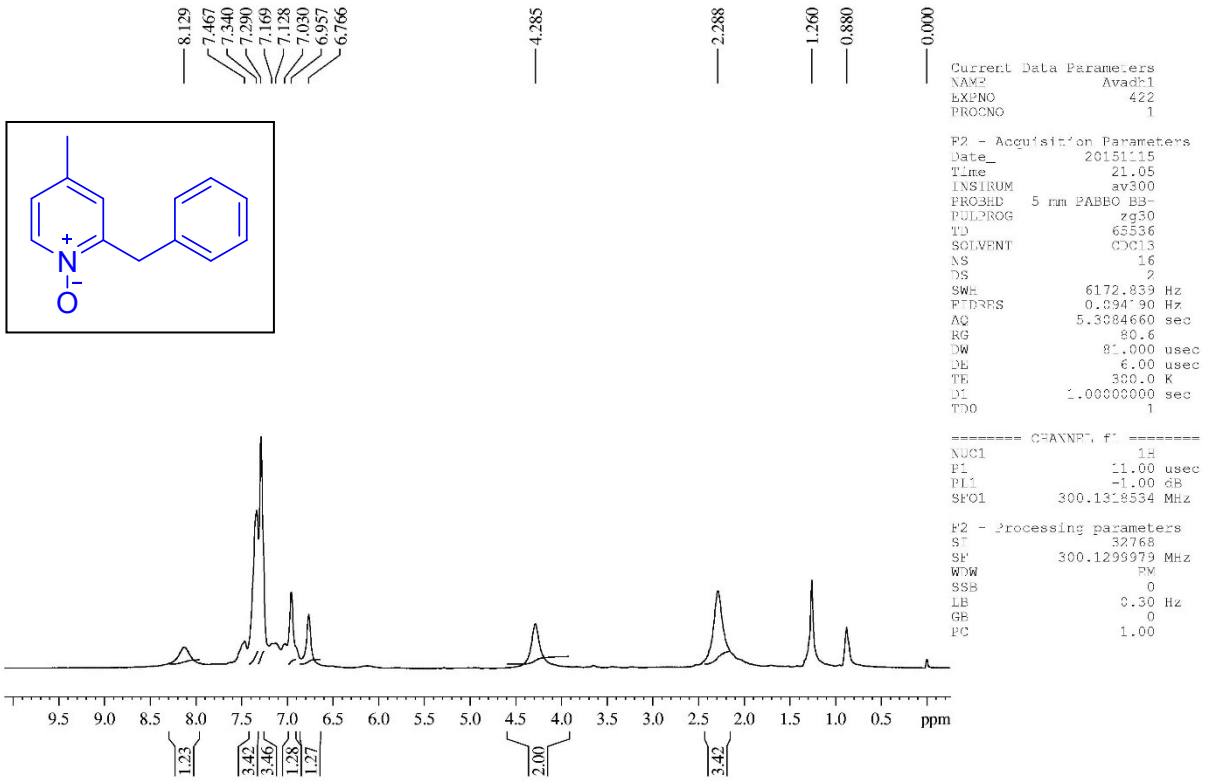

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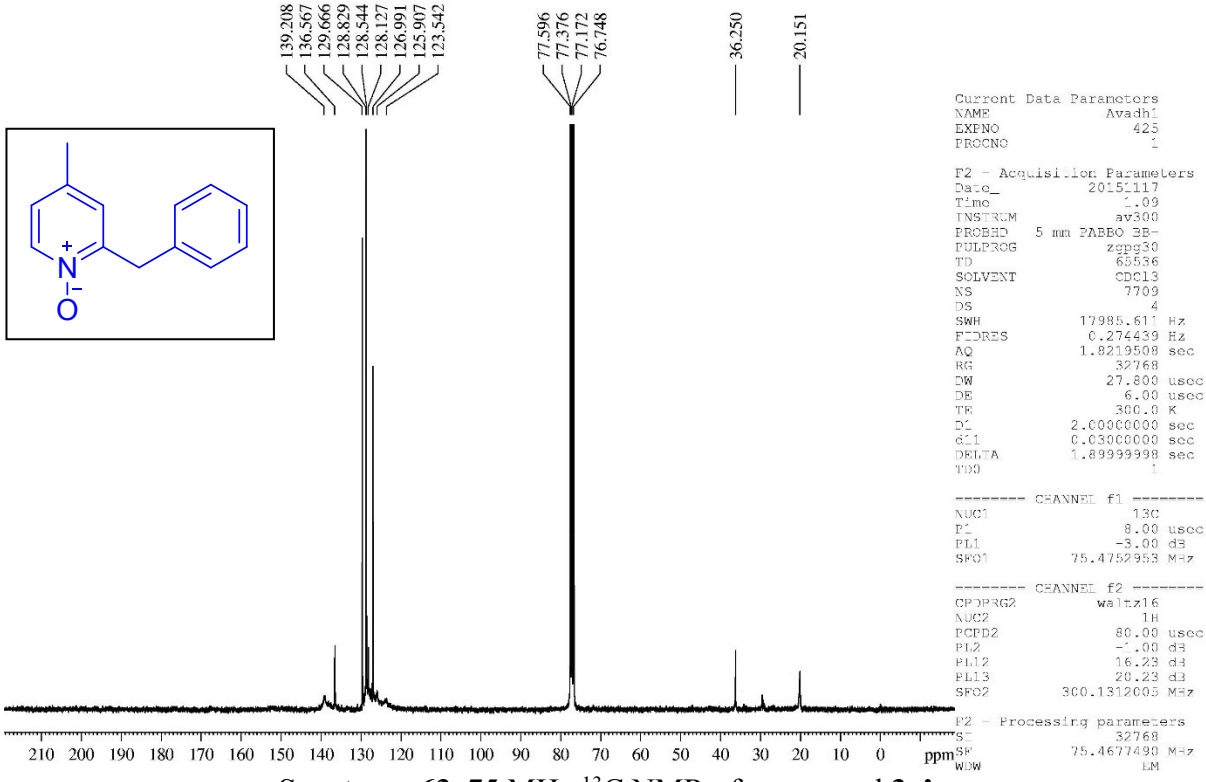

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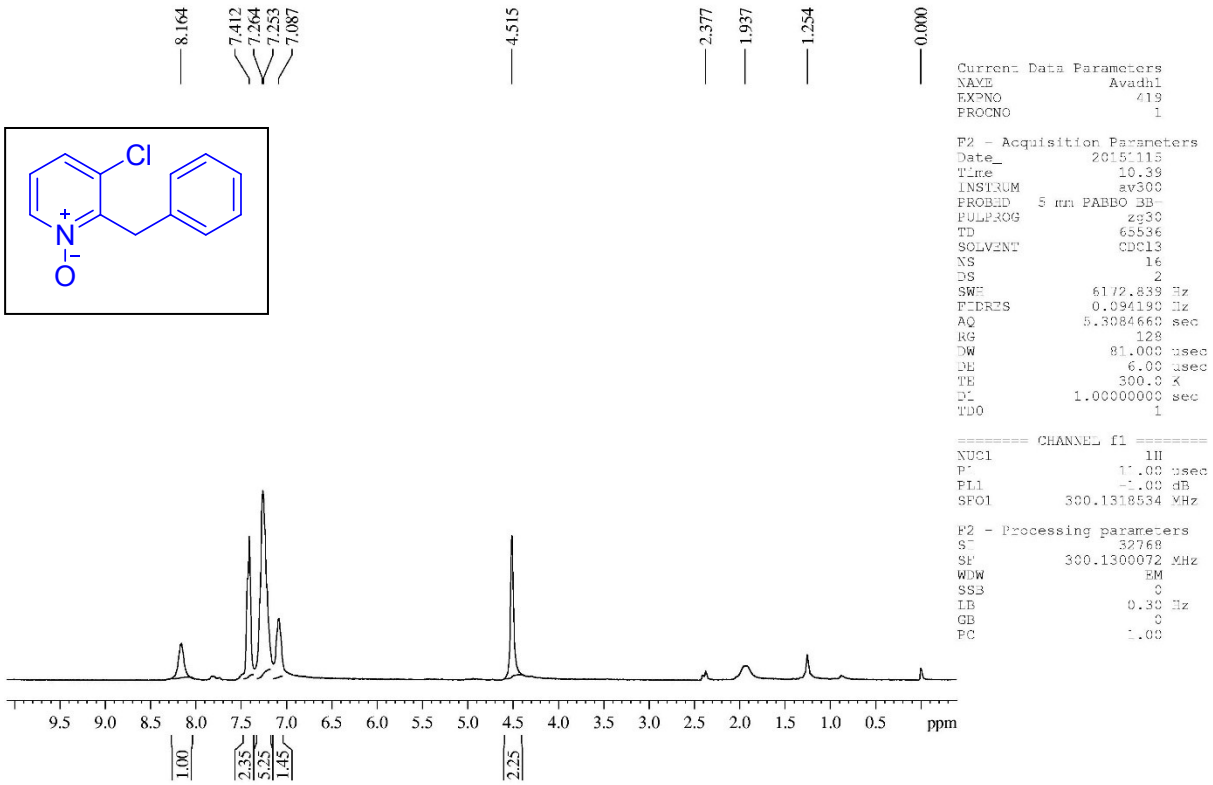
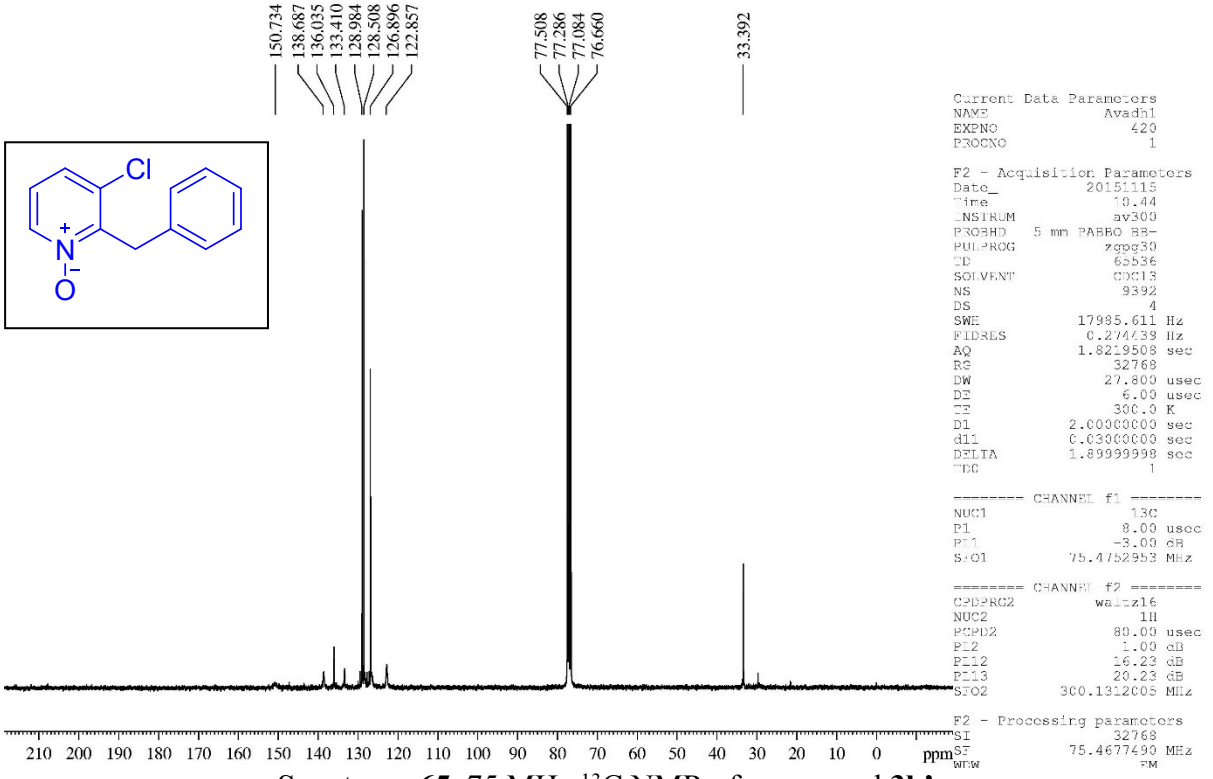
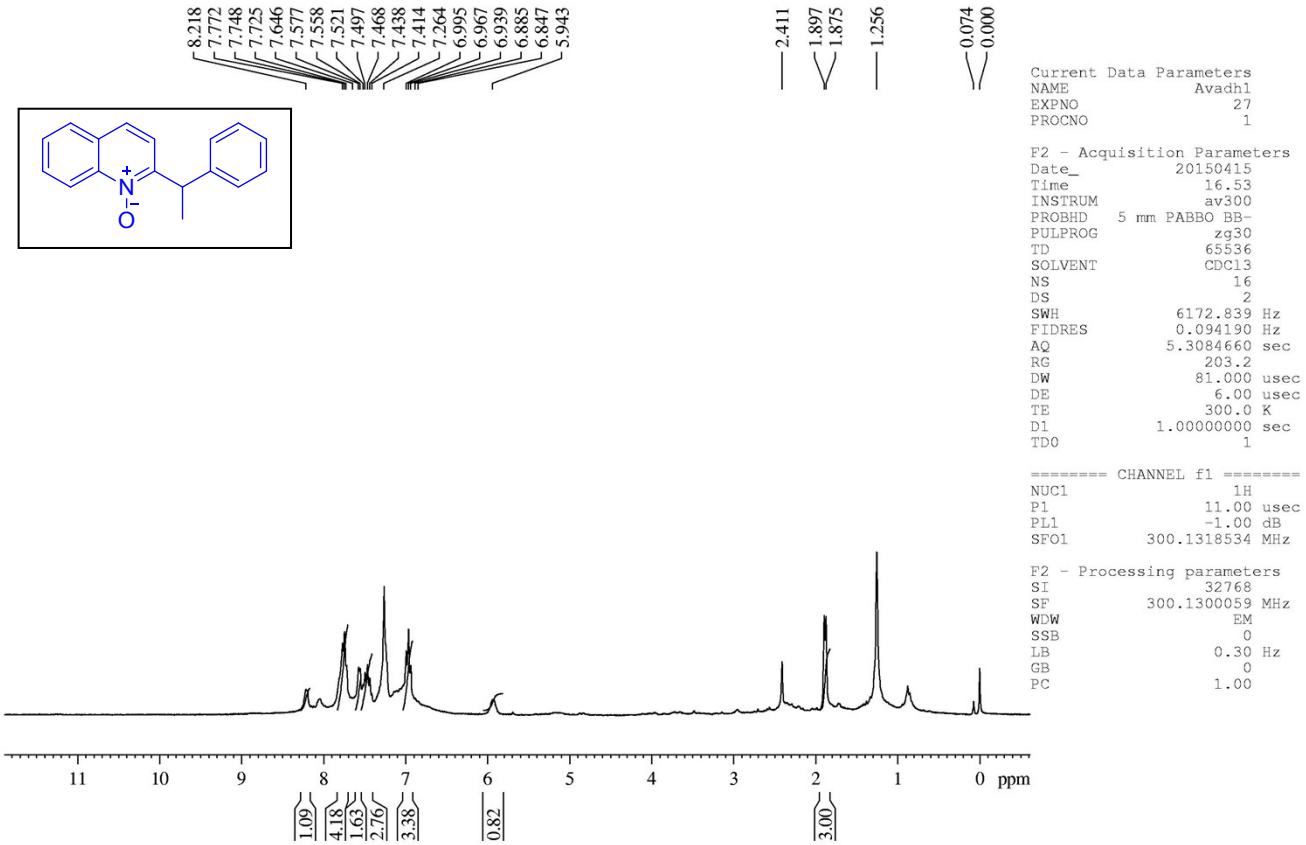


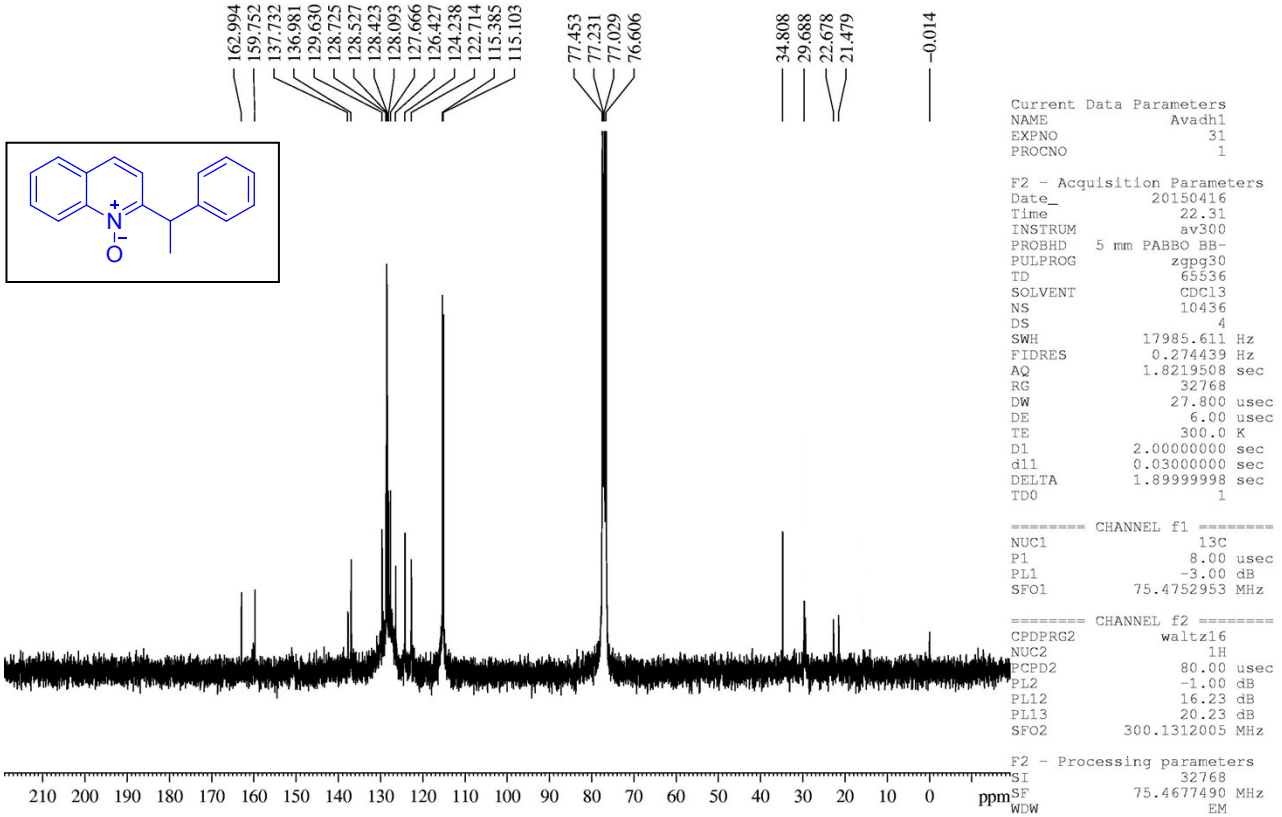
Spectrum 64. 300 MHz ^{1}H NMR of compound **3b'**



Spectrum 65. 75 MHz ^{13}C NMR of compound **3b'**



Spectrum 66. 300 MHz ^{1}H NMR of compound **4a**



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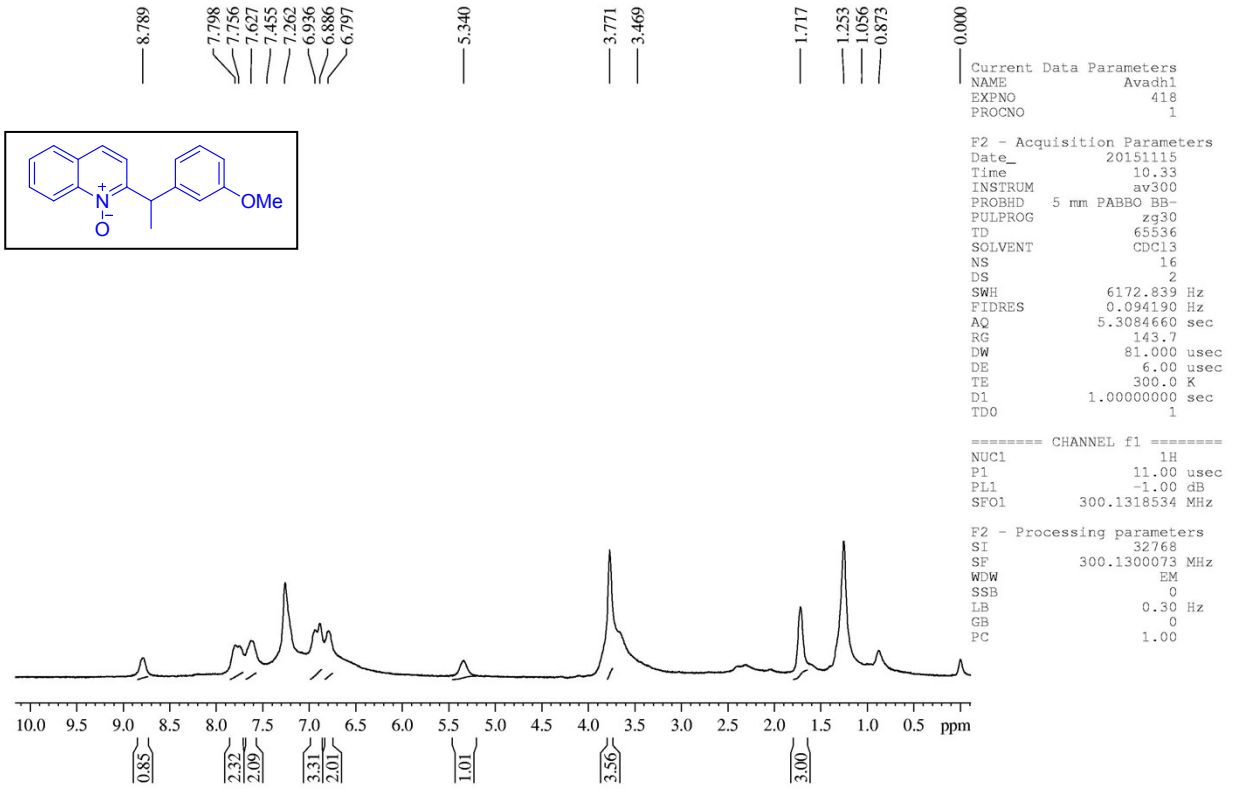
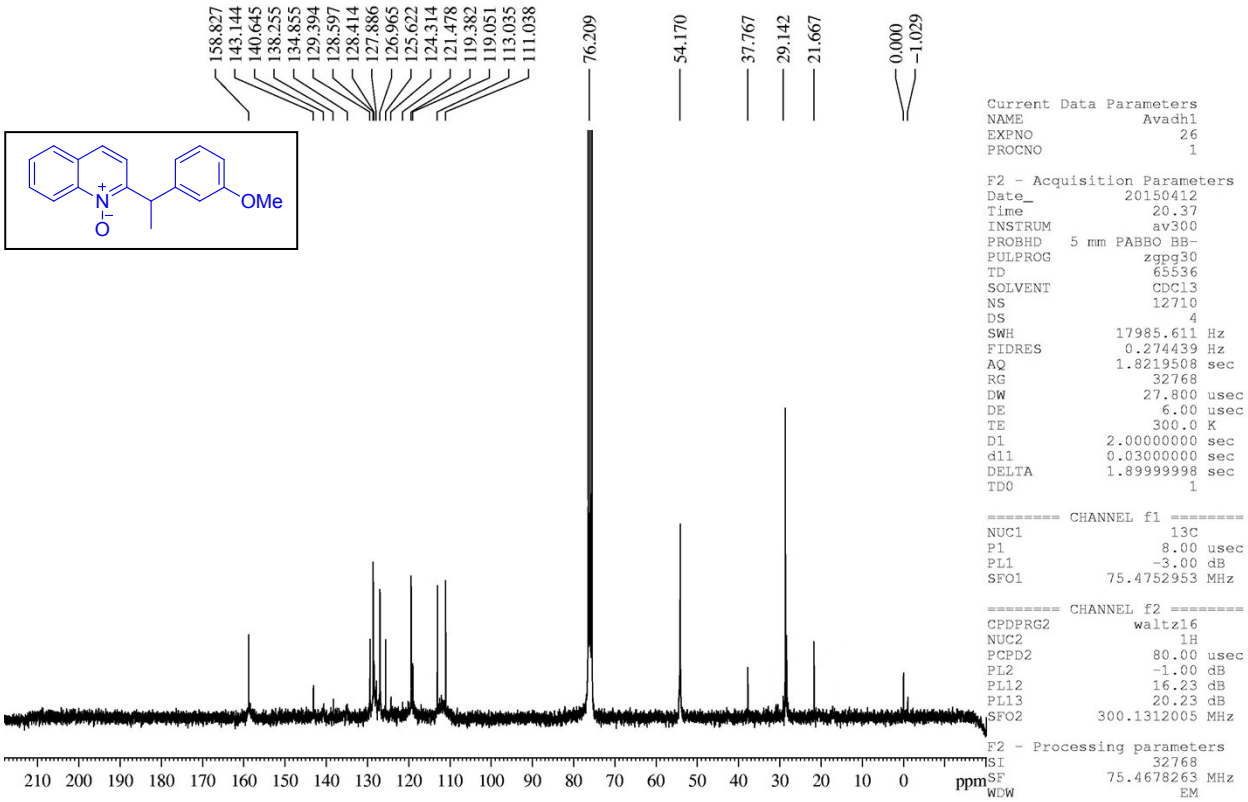
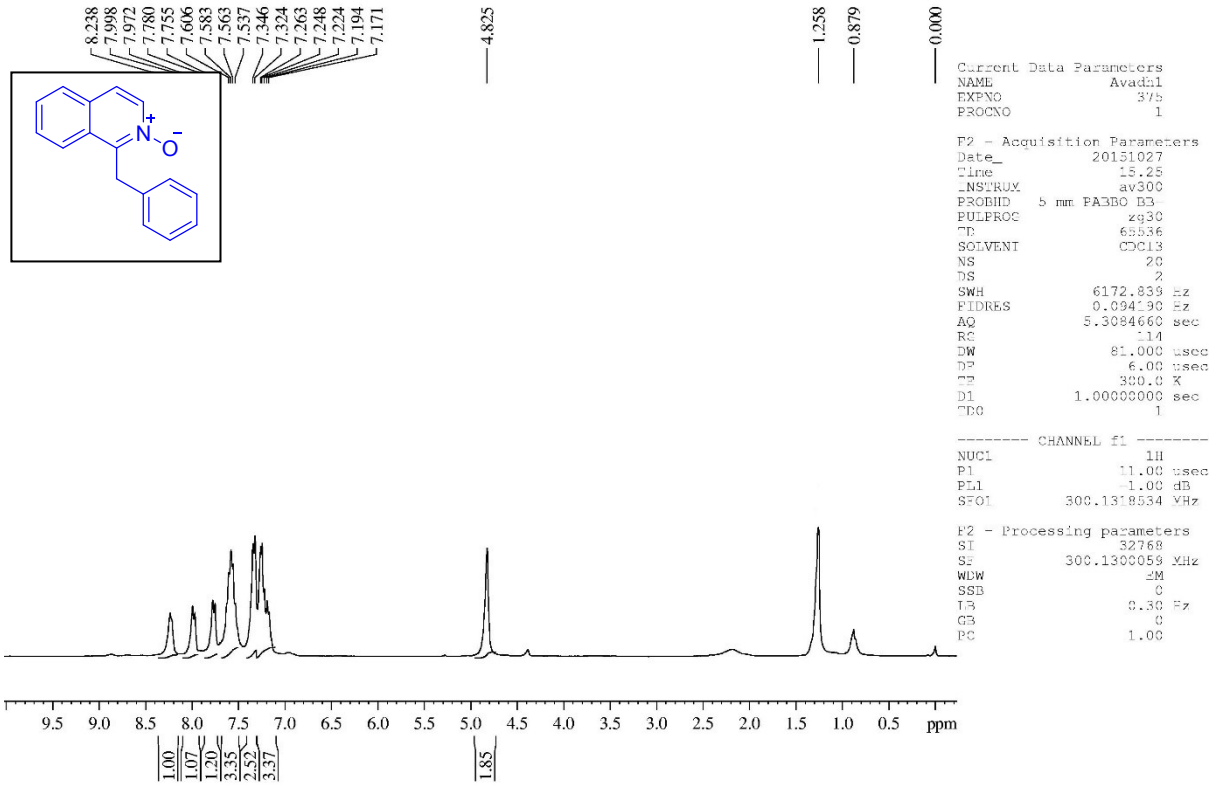


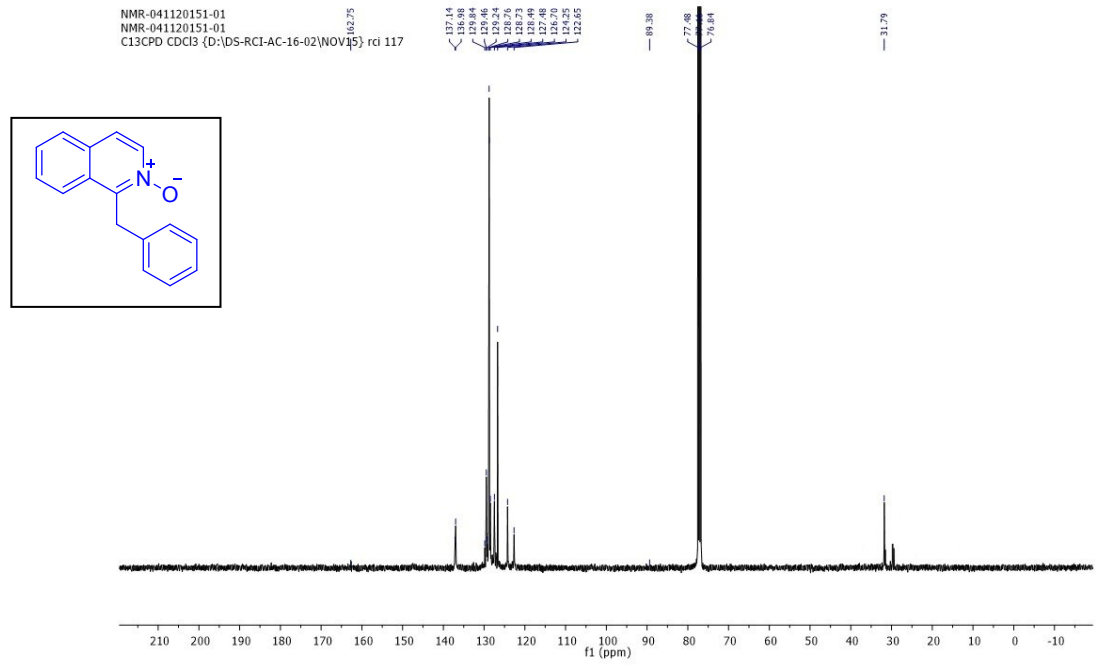
Spectrum 68. 300 MHz ^{1}H NMR of compound **4b**



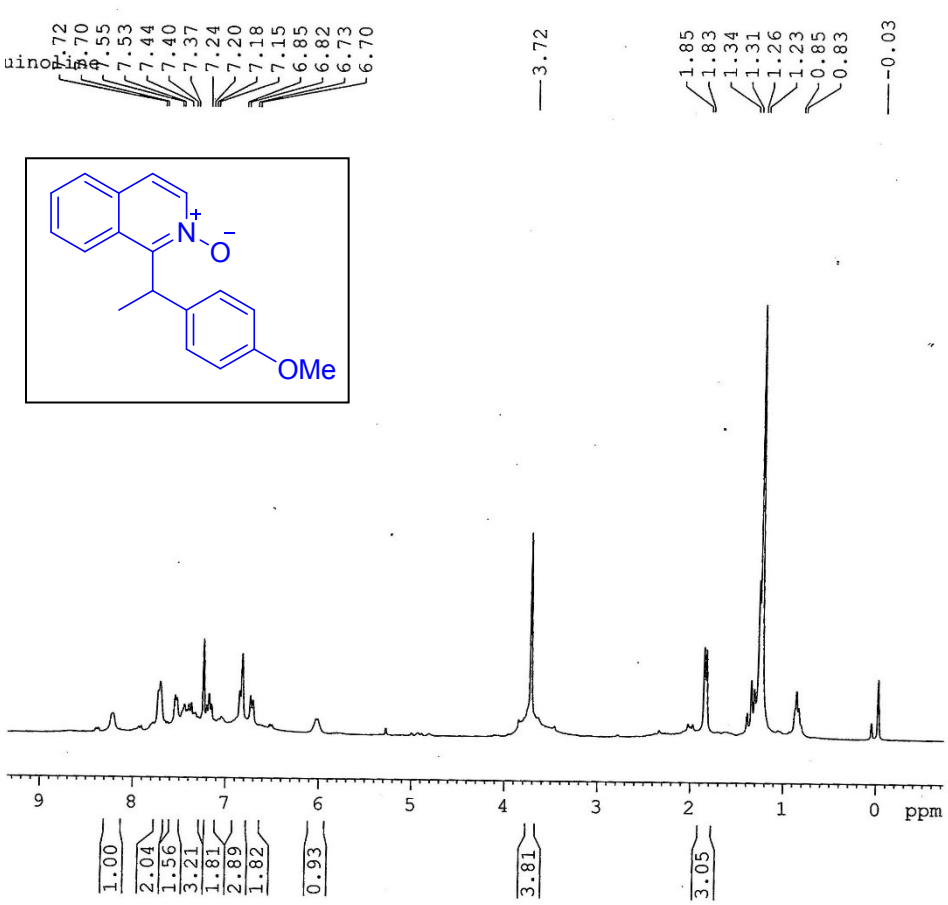
Spectrum 69. 75 MHz ^{13}C NMR of compound **4b**

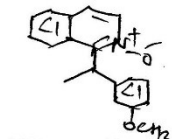


Spectrum 70. 300 MHz ^{1}H NMR of compound **4c**



Spectrum 71. 75 MHz ^{13}C NMR of compound **4c**





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TE                     12759.0 K
D1                  1.00000000 sec
TD0                            1

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PL1                    0.00 dB
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SFO1               300.1312005 MHz
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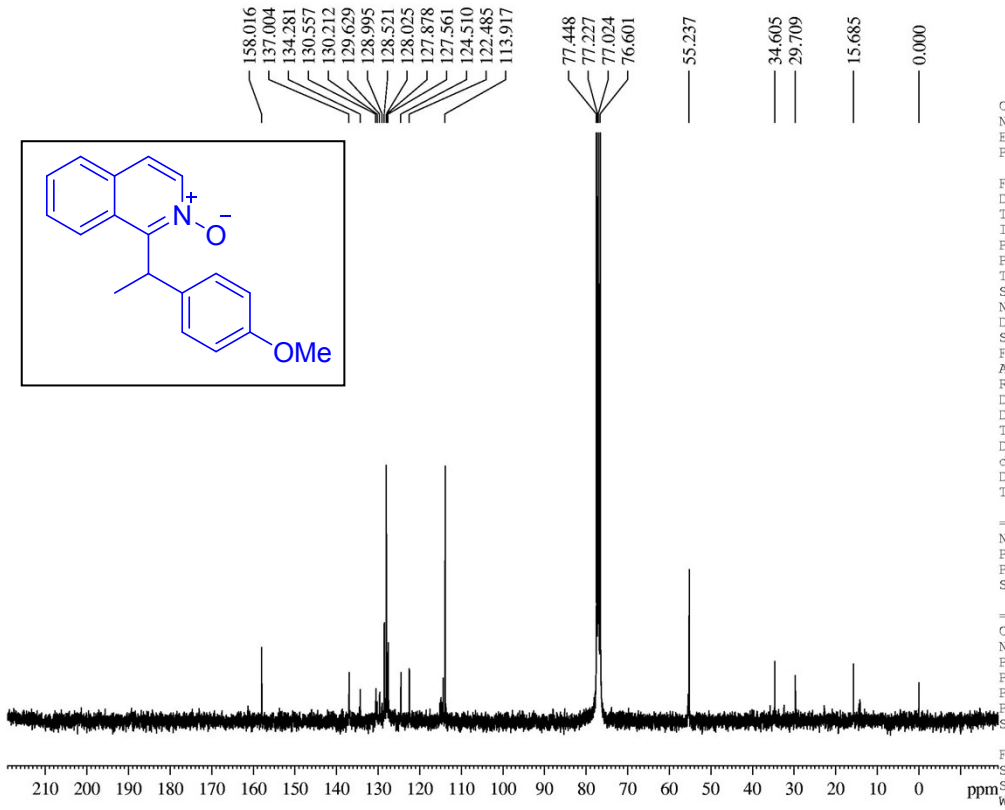
Spectrum 72. 300 MHz ^{1}H NMR of compound **4d**

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DE                     6.00 usec
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D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
TD0                          1

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PL1                   -3.00 dB
SFO1               75.4752953 MHz

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PL13                   20.23 dB
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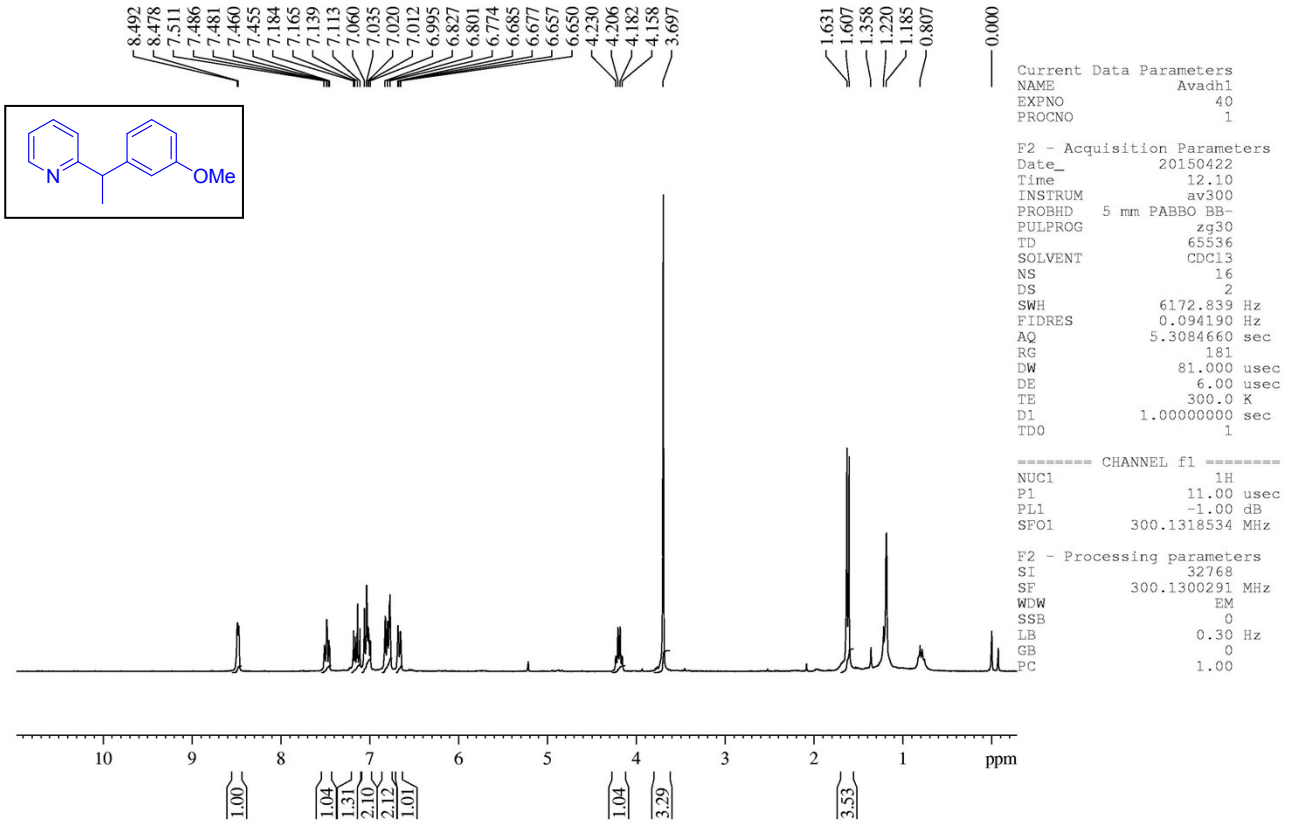
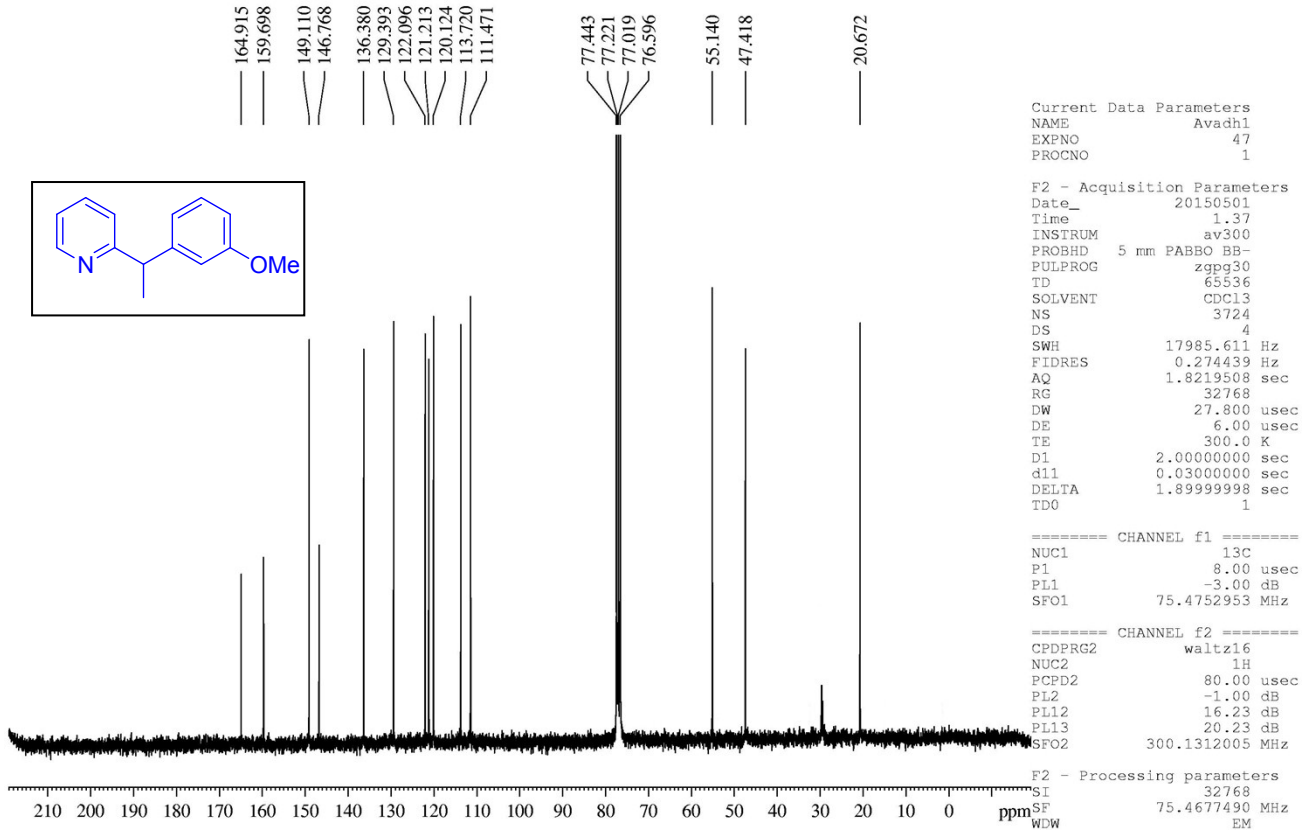
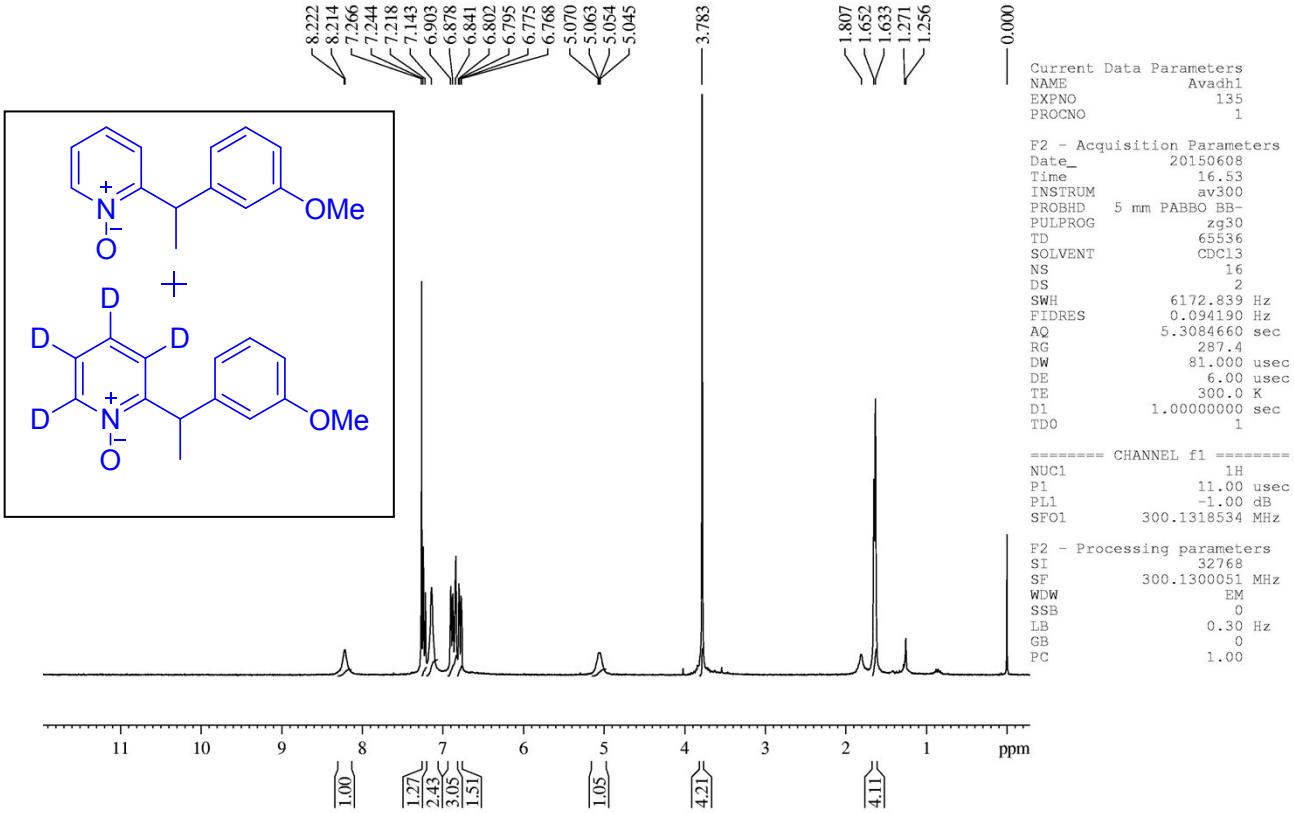
Spectrum 73. 75 MHz ^{13}C NMR of compound **4d**



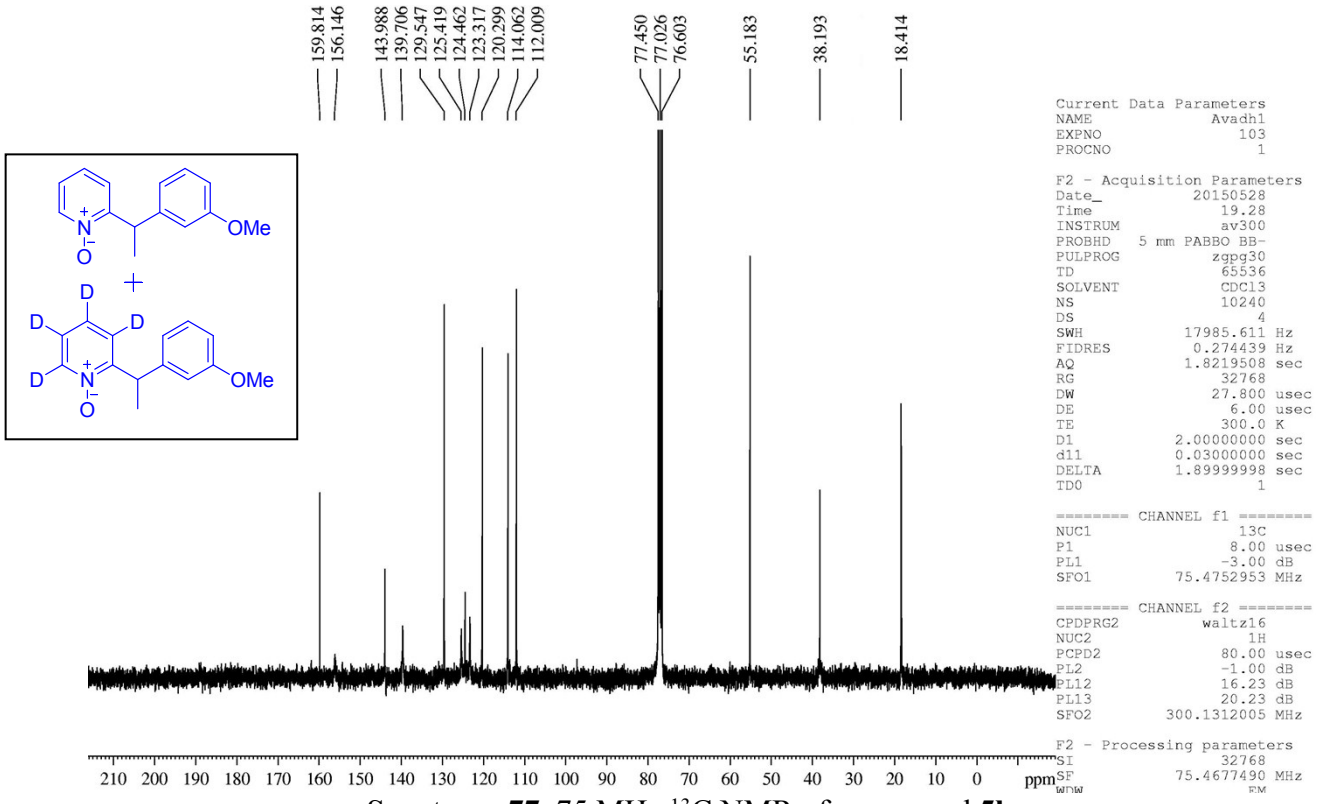
Spectrum 74. 300 MHz ^{1}H NMR of compound **5a**



Spectrum 75. 75 MHz ^{13}C NMR of compound **5a**



Spectrum 76. 300 MHz ^{1}H NMR of compound **5b**



Spectrum 77. 75 MHz ^{13}C NMR of compound **5b**

3. Single-Crystal X-Ray experimental details:

Data Collection and Refinement

X-ray intensity data measurements of compound 3r was carried out on a Bruker SMART Apex2 CCD diffractometer with graphite-monochromatized (MoKα= 0.71073 Å) radiation at 150(2) K. The X-ray generator was operated at 50 kV and 30 mA. A preliminary set of cell constants and an orientation matrix were calculated from three sets of 36 frames (12 frames from each set). The optimized strategy used for data collection consisted of one φ and four ω scan sets, with 0.5° steps in φ or ω; completeness achieved was100% with redundancy 3.98. Data were collected with a frame time of 15 sec keeping the sample-to-detector distance fixed at 5.00 cm. A total of 1552 frames were collected. The X-ray data collection was monitored by APEX2 program (Bruker, 2006).[2] All the data were corrected for Lorentzian, polarization and absorption effects using SAINT and SADABS programs (Apex2, Bruker, 2006). SHELX-97 was used for structure solution and full matrix least-squares refinement on F2.[3]All the hydrogen atoms were placed in geometrically idealized positionand constrained to ride on their parent atoms. Further information on the crystal structure determination (excluding structure factors) has been given as table S1 and also deposited in the Cambridge Crystallographic Data Centre as supplementary publications no. 1417856. Copies of the data can be obtained free of charge upon application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: (+44) 1223-336-033. e-mail: deposit@ccdc.cam.ac.uk) or via internet.

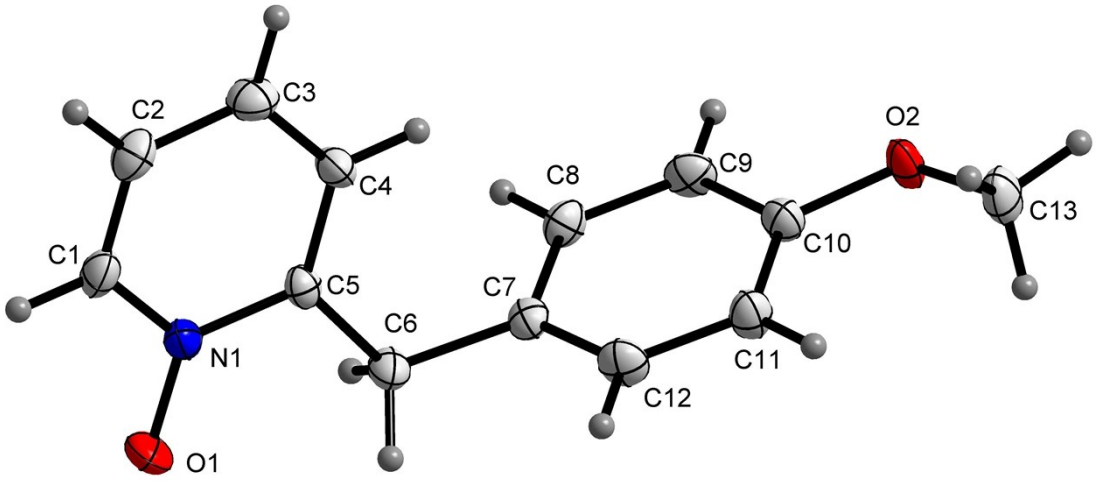


Figure S1. Single crystal X-ray structure of **c**ompound **3r** shown in capped stick model.

Table S1. Crystallographic refinement data for compound **3r**

Property	**Data 3r**
Empirical Formula	$C_{13}H_{13}NO_2$
Formula Weight	215.24
Crystal System	Orthorhombic
Space group	Pbca
a (Å)	13.273 (4)
b (Å)	8.870 (3)
c (Å)	18.749 (6)
α, β, γ (°)	90, 90, 90
V (Å^3)	2207.4 (12)
Z	8
Density (calc)	1.295
F(000)	912
μ (mm^{-1})	0.088
Crystal Size [mm]	0.35 x 0.33 x 0.29
Temperature (K)	298(2)
Radiation / λ	Mo*K*\α / 0.71073
θ Min/Max [°]	0.967/0.978
h, k, l	15; 10; 22
Tot.,UniqData, R(int)	8808, 1908, 0.1058
Obs. data [I > 2.0 σ(I)]	1281
Nref, Npar	1908, 146
R1, wR2, S	0.0951, 0.1831, 1.199
Min. - Max. resd. dens. [e/ Å^3]	-0.173, 0.202
CCDC	1417856

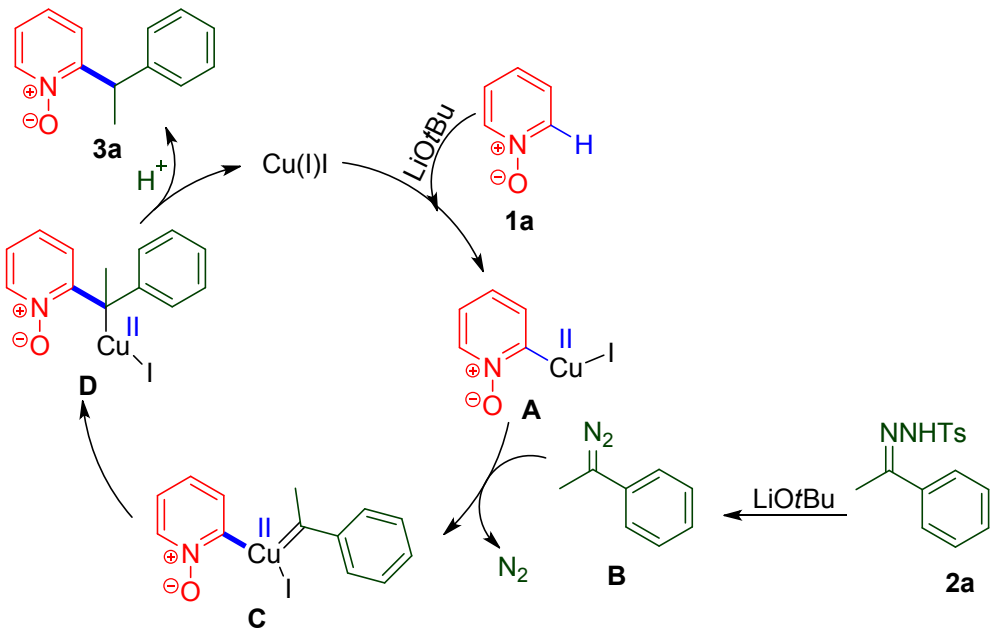


Figure S2. Plausible Mechanism

References:

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