Supplementary Materials for

Organoborohydride-Catalyzed Chichibabin-Type C4-Position Alkylation of Pyridines with Alkenes Assisted by Organoborane

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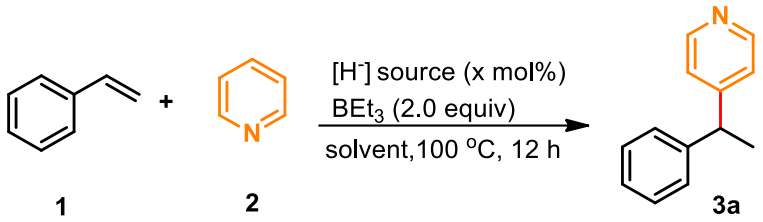
1. **Materials and Methods**

All reactions were performed under nitrogen atmosphere in flame dried flasks. Flash column chromatography was performed on silica gel 60 (particle size 300-400 mesh ASTM, purchased from Taizhou, China). ^{1}H, ^{13}C, ^{19}F, ^{31}B nuclear magnetic resonance (NMR) spectra were recorded with Bruker (600, 500 MHz) instruments. All ^{1}H NMR data are reported in δ units, parts per million (ppm), and were measured relative to the residual proton signal in the deuterated solvent at 7.26 ppm ($CDCl_3$). All ^{13}C NMR spectra are ^{1}H decoupled and reported in ppm relative to the solvent signal at 77.16 ppm ($CDCl_3$). High resolution mass spectra were obtained using a Bruck microtof. Melting points were measured on a Mel-Temp capillary melting point apparatus.

Unless otherwise stated, all commercially available compounds were purchased from Aldrich or Energy–Chemical Limited and used as supplied without further purification. Tetrahydrofuran, 1,4–dioxane, cyclohexane, toluene, methyl tertiary butyl ether was purified by distillation from sodium benzophenone ketyl immediately prior to use.

2. Optimization Studies for Selective Alkylation of Pyridines with styrenes

Table S1. Screening of the hydride sources and solvent[a]

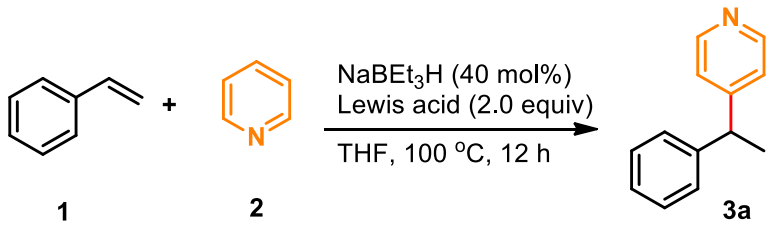


1 2 3a

Entry	Hydride source (x mol%)	Solvent	Yield (%)[b]
1	$LiBEt_3H$ (50)	THF	75
2	$NaBEt_3H$ (50)	THF	83
3	$NaBEt_3H$ (50)	THF	99[c]
4	$NaBEt_3H$ (40)	THF	90[d]
5	$NaBEt_3H$ (30)	THF	73[e]
6	$KBEt_3H$ (40)	THF	79
7	$LiB(^sC_4H_9)_3H$ (40)	THF	64
8	NaH (40)	THF	90
9	$LiAlH_4$ (40)	THF	34
10	-	THF	0
11	$NaBEt_3H$ (40)	THF	0[f]
12	$NaBEt_3H$ (40)	Toluene	74
13	$NaBEt_3H$ (40)	Dioxane	74
14	$NaBEt_3H$ (40)	MTBE	trace
15	$NaBEt_3H$ (40)	DEE	50
16	$NaBEt_3H$ (40)	2-CH_3-THF	21

[a] Reaction conditions: **1** (0.5 mmol), **2** (1.5 equiv), [H^-] source (50 mol%), BEt_3 (2.0 equiv), in 1 mL solvent at 100 °C. [b]Yield was determined by ^1H NMR with CH_2Br_2 as an internal standard. [c]**1** (1.5 equiv), **2** (0.5 mmol), $NaBEt_3H$ source (50 mol%). [d]**1** (1.5 equiv), **2** (0.5 mmol), $NaBEt_3H$ source (40 mol%). [e]**1** (1.5 equiv), **2** (0.5 mmol), $NaBEt_3H$ source (30 mol%). MTBE: methyl tertiary butyl ether; DEE: glycol dimethyl ether. [f]Without 2.0 equiv BEt_3.

Table S2. Screening of the Lewis acid[a]

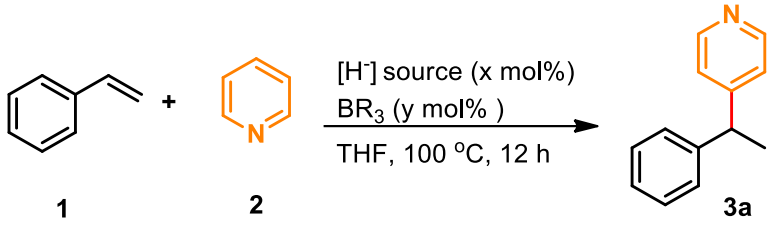


1 2 3a

Entry	Lewis acid	Yield (%)[b]
1	BEt_3	90
2	BEt_3	64[c]
3	BEt_3	90[d]
4	$B(^nC_4H_9)_3$	89
5	$B(OMe)_3$	trace
6	$B(O^iPr)_3$	20
7	BPh_3	trace
8	BCl_3	trace
9	$BF_3{\cdot}OEt_2$	0
10	$AlMe_3$	35
11	$Al(O^iPr)_3$	15

[a]Reaction conditions: **1** (1.5 equiv), **2** (0.5 mmol), $NaBEt_3H$ (50 mol%), Lewis acid (2.0 equiv) in 1 mL THF at 100 °C. [b]Yield was determined by ^1H NMR with CH_2Br_2 as an internal standard. [c]BEt_3 (1.5 equiv) as the additive. [d] BEt_3 (2.5 equiv) as the additive.

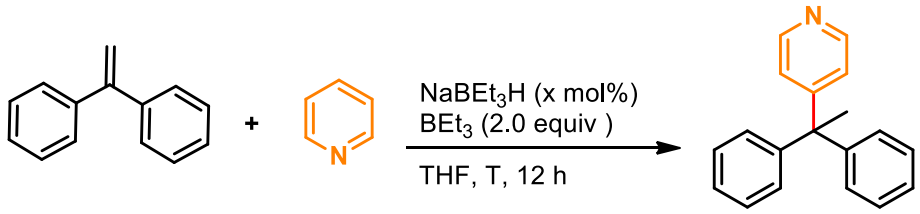
Table S3. Screening the loading of hydride catalyst and organoborane[a]



Entry	[H$^-$] source (x mol%)	BR_3 (y mol%)	Yield (%)[b]
1	$LiB(^sC_4H_9)_3H$ (50)	BEt_3 (200)	64
2	$LiB(^sC_4H_9)_3H$ (50)	$B(^nBu)_3$ (200)	94
3	$LiB(^sC_4H_9)_3H$ (50)	$B(^sBu)_3$ (200)	97
4	$LiB(^sC_4H_9)_3H$ (50)	$B(^sBu)_3$ (10)	90
5	$LiB(^sC_4H_9)_3H$ (20)	$B(^sBu)_3$ (10)	95

[a]Reaction conditions: **1** (1.5 equiv), **2** (0.5 mmol), [H$^-$] source (x mol%), BR_3 (y mol%), in 1 mL THF at 100 °C for 12 h. [b]Yield was determined by ^{1}H NMR with CH_2Br_2 as an internal standard.

Table S4. Optimization of the alkylation of pyridine with 1,1-diphenylethene[a]



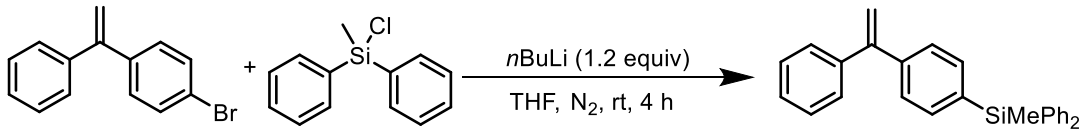
Entry	$NaBEt_3H$ (x mol%)	Temperature (°C)	Yield (%)[b]
1	40	100	97%
2	40	70	94%
3	30	70	93%
4	20	25	52%
5	30	25	80%[c]

[a]Reaction conditions: 1,1-diphenylethene (1.5 equiv), pyridine (0.5 mmol), $NaBEt_3H$, BEt_3 (2.0 equiv) in 1 mL THF for 12 h. [b]Isolated yield. [c]Reaction was performed for 48 h.

3. **Substrate preparation**

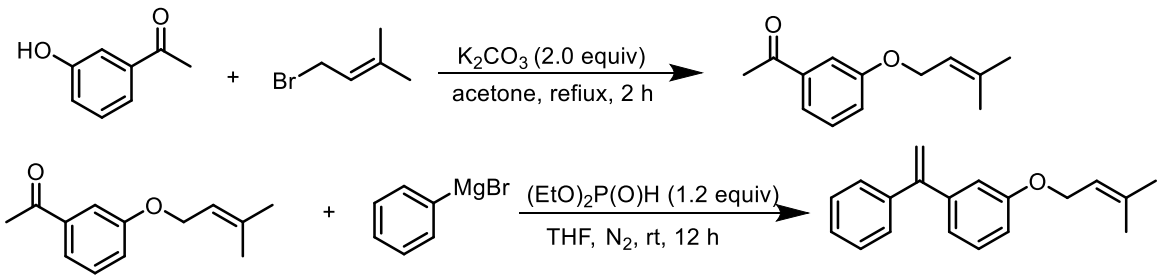
Alkenes **1d**,[1] **1e**,[2] **1k**,[3] **1l**,[4] **1ab**,[5] 3-phenylpyridine,[6] ethene-1,1-diyldibenzene,[6] 1-methoxy-4-(1-phenylvinyl)benzene,[7] 4,4,5,5-tetramethyl-2-(3-(1-phenylvinyl)phenyl)-1,3,2-dioxaborolane,[8] 2-chloro-1-methoxy-4-(1-phenylvinyl)benzene,[9] 2-(1-phenylvinyl)naphthalene[10] were synthesized according to procedures described in the literature. The other simple alkenes were commercially available and were used as received.

Synthesis of methyldiphenyl(4-(1-phenylvinyl)phenyl)silane:



To a solution of 1-bromo-3-(1-phenylvinyl)benzene (1.54 g, 6.0 mmol, 1.2 equiv) in 30 mL dried THF, the *n*BuLi (3.75 ml, 6.0 mmol, 1.2equiv) was dropwised with cooling and stirring in ice-salt bath. After half an hour, chloro(methyl)diphenylsilane (1.16 g, 5.0 mmol, 1.0equiv) was added. The reaction mixture was warmed up to room temperature (r. t.) and stirred for 4 hours. Water was added to the reaction mixture and the product is extracted three times with ether. The organic phases are combined, dried over sodium sulphate and evaporated under reduced pressure. The crude solid is then purified by flash column chromatography on silica gel (eluent: petroleum) to afford product (82%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.54 – 7.51 (m, 4H), 7.48 (d, *J* = 7.8 Hz, 2H), 7.42 – 7.39 (m, 2H), 7.36 – 7.31 (m, 11H), 5.48 (d, *J* = 18.6 Hz, 2H), 0.84 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 149.9, 142.3, 141.3, 136.1, 135.3, 135.1, 134.0, 129.4, 128.3, 128.1, 127.9, 127.7, 127.6, 114.7, -3.4.

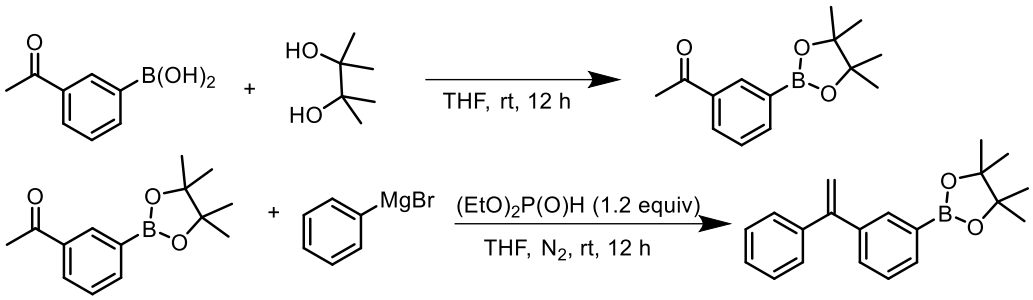
Synthesis of 1-((3-methylbut-2-en-1-yl)oxy)-3-(1-phenylvinyl)benzene:



1-(3-hydroxyphenyl)ethanone (0.68 g, 5.0 mmol, 1.0 equiv), 1-bromo-3-methylbut-2-ene (0.69 ml, 6.0 mmol, 1.2 equiv) and K_2CO_3 (1.38g, 10 mmol, 2.0 equiv) was mixture 10 mL acetone, the mixture was reflux for 2 hours to give the (*E*)-1-(3-((3-methylbut-1-en-1-yl)oxy)phenyl)ethanone. Then reacted with PhMgBr (1.0 M in THF, 6.0 mL, 6.0 mmol, 1.2 equiv), $(EtO)_2P(O)H$ (0.77 ml, 6.0 mmol, 1.2 equiv) at r.t. for 12 h. NH_4Cl solution is added

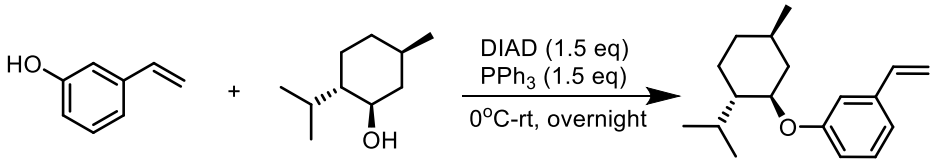
to the reaction mixture and the product extracted three times with ether. The organic phases are combined, dried over sodium sulphate and evaporated under reduced pressure. The crude solid is then purified by flash column chromatography on silica gel (eluent: petroleum) to afford product (67 %). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.28 –7.22 (m, 5H), 7.18 – 7.15 (m, 1H), 6.85 (d, *J* = 7.8 Hz, 1H), 6.81 – 6.80 (m, 2H), 5.41 – 5.37 (m, 3H), 4.41 (d, *J* = 7.2 Hz, 2H), 1.70 (s, 3H), 1.62 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 158.7, 150.0, 142.9, 141.4, 138.2, 129.1, 128.3, 128.1, 127.7, 120.8, 119.7, 114.7, 114.4, 113.9, 64.7, 25.9, 18.2.

Synthesis of 4,4,5,5-tetramethyl-2-(3-(1-phenylvinyl)phenyl)-1,3,2-dioxaborolane:



To a solution of (3-acetylphenyl)boronic acid (0.82 g, 5.0 mmol, 1.0 equiv) in THF 10.0 mL, pinacol (0.61 mL, 5.0 mmol, 1.0 equiv) was sequentially added at r.t. After being stirred for 12 h, the reaction mixture was diluted with EtOAc (10.0 mL) and quenched with H_2O (5.0 M). The organic layer was concentrated in vacuo to afford crude product. Then react with PhMgBr (1.0 M in THF, 6 mL, 6 mmol, 1.2 equiv), $(EtO)_2P(O)H$ (0.77 ml, 6.0 mmol, 1.2 equiv) at r.t. for 12 h. NH_4Cl solution is added to the reaction mixture and the product extracted three times with ether. The organic phases are combined, dried over sodium sulphate and evaporated under reduced pressure. The crude solid is then purified by flash column chromatography on silica gel (eluent: petroleum) to afford product (50 %). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.77 (s, 1H), 7.69 (d, *J* = 7.2 Hz, 1H), 7.29 – 7.21 (m, 7H), 5.38 (d, *J* = 10.2 Hz, 2H), 1.26 (s, 12H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 150.0, 141.5, 141.0, 134.3, 134.1, 131.4, 128.1, 128.1, 127.6, 127.5, 114.5, 83.8, 24.9.

Synthesis of 1-(((1R,2S,5R)-2-isopropyl-5-methylcyclohexyl)oxy)-3-vinylbenzene:



3-Vinylphenol (0.6 g, 5.0 mmol, 1.0 equiv), triphenylphosphine (1.92 g, 7.5 mmol, 1.5 equiv) and L-Menthol (1.17 g, 7.5 mmol, 1.5 equiv) are dissolved in dry THF. The solution is cooled at 0°C. DIAD (1.5 mL, 7.5 mmol, 1.5 equiv) is added slowly to the reaction mixture. The

solution is warmed up to r.t. and stirred overnight. Water is added to the reaction mixture and the product is extracted three times with ether. The organic phases are combined, dried over sodium sulphate and evaporated under reduced pressure. The crude solid is then purified by flash column chromatography on silica gel (eluent: petroleum) to afford product as a yellow oil (219 mg, 17 %). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.21 (t, *J* = 7.8 Hz, 1H), 6.96 (d, *J* = 7.2 Hz, 1H), 6.94 (s, 1H), 6.80 (dd, *J* = 7.8, 2.4 Hz, 1H), 6.70–6.65 (m, 1H), 5.73 (d, *J* = 18.0 Hz, 1H), 5.23 (d, *J* = 10.8 Hz, 1H), 4.65 – 4.64 (m, 1H), 2.10 (dq, *J* = 13.8, 3.0 Hz, 1H), 1.83–1.64 (m, 4H), 2.12–2.08 (m, 1H), 1.80–1.65 (m, 4H), 1.61–1.54 (m,1H),1.05–0.96 (m, 1H), 0.93 (d, *J* = 6.6 Hz, 3H), 0.87 (d, *J* = 6.6 Hz, 3H), 0.81 (d, *J* = 6.6 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 158.5, 139.0, 136.9, 129.5, 118.3, 114.9, 113.9, 113.6, 73.2, 47.8, 37.7, 35.0, 29.3, 26.2, 24.9, 22.3, 21.1.

4. Substrates scope

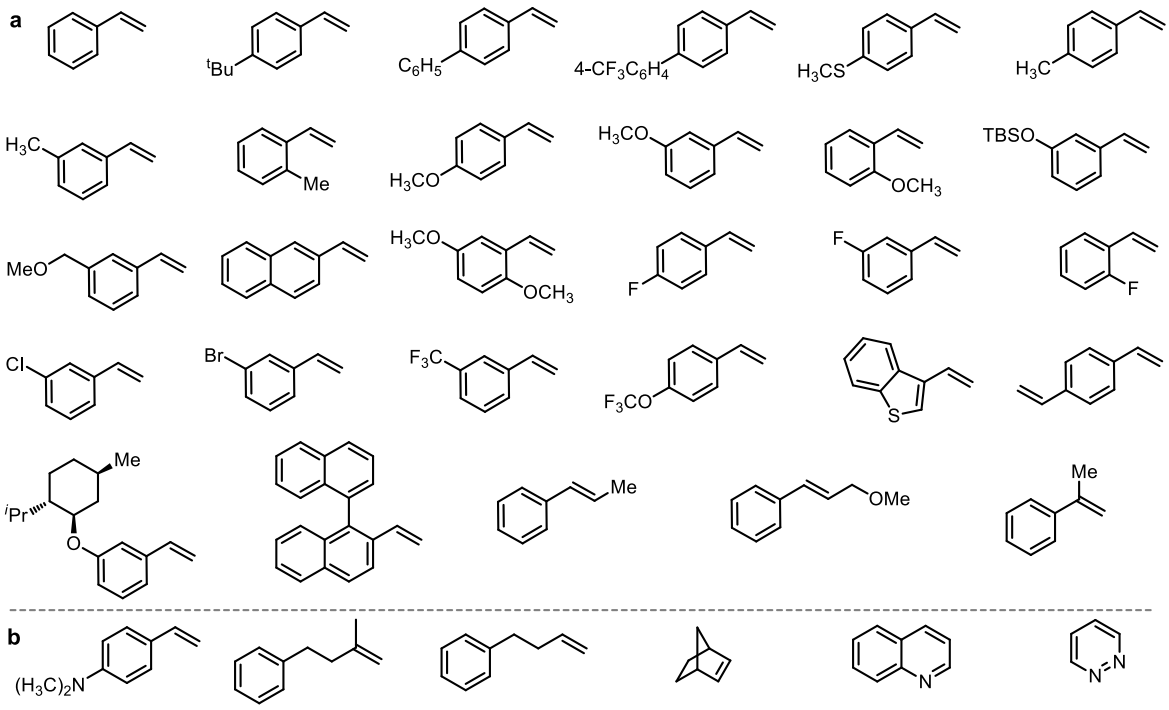
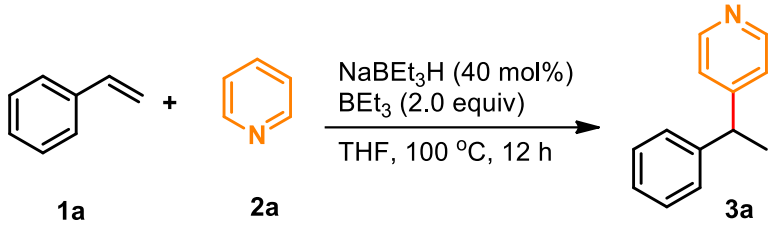


Figure. S1. The scope of the substrates. **a,** The valid substrate scope of alkenes. **b**, The invalid substrates of alkenes and heteroarenes.

5. Experimental procedures

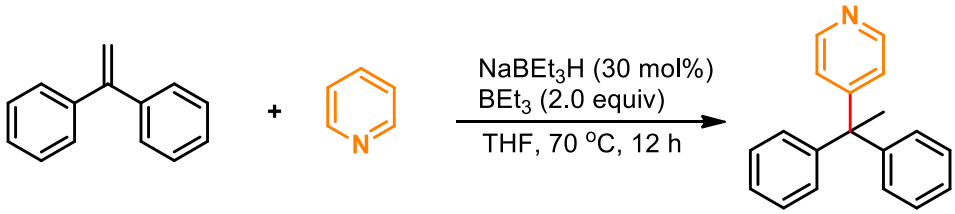
For the alkylation of pyridiens with styrenes (with 3a as an example):



1a 2a 3a

In a nitrogen-filled glove box, a screw-cap test tube was charged with styrene **1** (0.75 mmol, 1.5 equiv). Then, a solution of $NaBEt_3H$ in THF (1.0 M, 200 μL, 0.2 mmol) was added slowly by syringe. After addition of the pyridine **2** (40 μL, 0.5 mmol) and BEt_3 (1.0 M in THF, 1.0 mL, 1.0 mmol) and dry THF (1 mL), the test tube was sealed with a Teflon screw cap and removed from the glove box and then stirred at 100 °C for 12 h. After completion, the mixture was quenched by *sat.aq.* NH_4Cl solution, extracted with CH_2Cl_2 (3 × 5.0 mL), combined the organic phases, and dried over anhydrous $MgSO_4$. The solvents were evaporated under vacuum and the crude product was purified on silica gel column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1) to give the corresponding product **3**.

For the alkylation of pyridiens with1,1-diaryl alkenes (with 4a as an example):



4a

In a nitrogen-filled glove box, a screw-cap test tube was charged with 1,1-dibenzylethene **1** (0.75 mmol, 1.5 equiv). Then, a solution of $NaBEt_3H$ in THF (1.0 M, 150 μL, 0.15 mmol) was added slowly by syringe. After addition of the pyridine **2** (40 μL, 0.5 mmol) and BEt_3 (1.0 M in THF, 1.0 mL, 1.0 mmol) and dry THF (1 mL), the test tube was sealed with a Teflon screw cap and removed from the glove box and then stirred at 70 °C for 12 h. After completion, the mixture was quenched by *sat.aq.* NH_4Cl solution, extracted with CH_2Cl_2 (3 × 5.0 mL), combined the organic phases, and dried over anhydrous $MgSO_4$. The solvents were evaporated under vacuum and the crude product was purified on silica gel column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1) to give the corresponding product **4**.

The procedure for gram-scale synthesis of 3a.

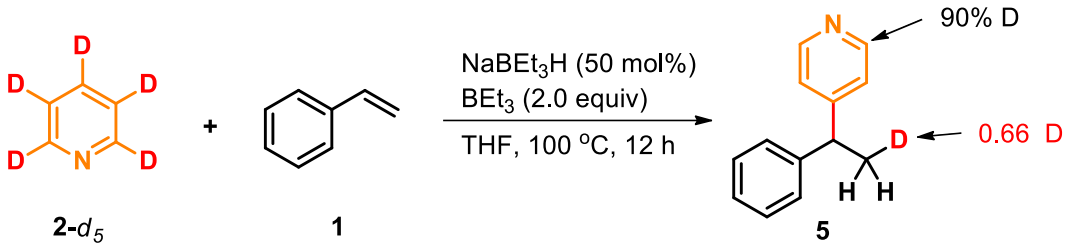
In a nitrogen-filled glove box, a screw-cap test tube was charged with styrene **2a** (9.75 mmol, 1.12 mL). Then, a solution of $NaBEt_3H$ in THF (1.0 M, 1.30 mL, 1.30 mmol) was added slowly by syringe. After addition of the pyridine (0.53 mL, 6.5 mmol) and BEt_3 (1.0 M in THF 0.65 mL,0.65 mmol) and dry THF (1 mL), the test tube was sealed with a Teflon screw cap and removed from the glove box and then stirred at 100 °C for 12 h. After completion, the mixture was quenched by *sat.aq*. NH_4Cl solution, extracted with CH_2Cl_2 (3 × 20.0 mL), combined the organic phases, and dried over anhydrous $MgSO_4$. The solvnts were evaporated under vacuum and the crude product was purified on silica gel column chromatography (eluent: petroleum/EtOAc/Et_3N = 4/1/1) to give the **3a** (1.056 g, 88%).

The procedure for gram-scale synthesis of 4a.

In a nirogen-filled glovebox, a flame-dried screw-cap reaction tube equipped with a magnetic stir bar was charged with ethene-1,1-diyldibenzene (1.3 ml, 7.5 mmol), Then, a solution of $NaBEt_3H$ in THF (1.0 M, 1.0 mL, 1.0 mmol) was added slowly by syringe. After addition of the pyridine (400 μL, 5.0 mmol) and BEt_3 (1.0 M in THF, 10 mL, 10 mmol) and dry THF (5.0 mL). the test tube was sealed with a Teflon screw cap and removed from the glove box and then stirred at r.t for 48 h. After completion, the mixture was quenched by *sat.aq*. NH_4Cl solution, extracted with CH_2Cl_2 (3 × 20.0 mL), combined the organic phases, and dried over anhydrous $MgSO_4$. The solvnts were evaporated under vacuum and the crude product was purified on silica gel column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1) to give the **4a** (1.002 g, 79%).

6. **Mechanistic study**

H/D Scrambling experiment



In a nitrogen-filled glove box, a screw-cap test tube was placed styrene (0.75mmol, 1.5equiv), a solution of $NaBEt_3H$ (1.0 M in THF, 200 μL, 0.2 mmol) and **2**-d_5 (40 μL, 0.5 mmol), then BEt_3 (1.0 M in THF, 1.0 mL, 1.0 mmol) was added slowly by syringe. After adding 1.0 mL dry THF, the test tube was sealed with a Teflon screw cap, removed from the glove box and stirred at 100 °C for 12 h. After completion, the mixture was quenched by *sat.aq.* NH_4Cl solution, extracted with CH_2Cl_2 (3 × 5.0 mL), combined the organic phases, and dried over anhydrous $MgSO_4$. The solvents were evaporated under vacuum and the crude product was purified on silica gel column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1) to give the product (Fig. S2).

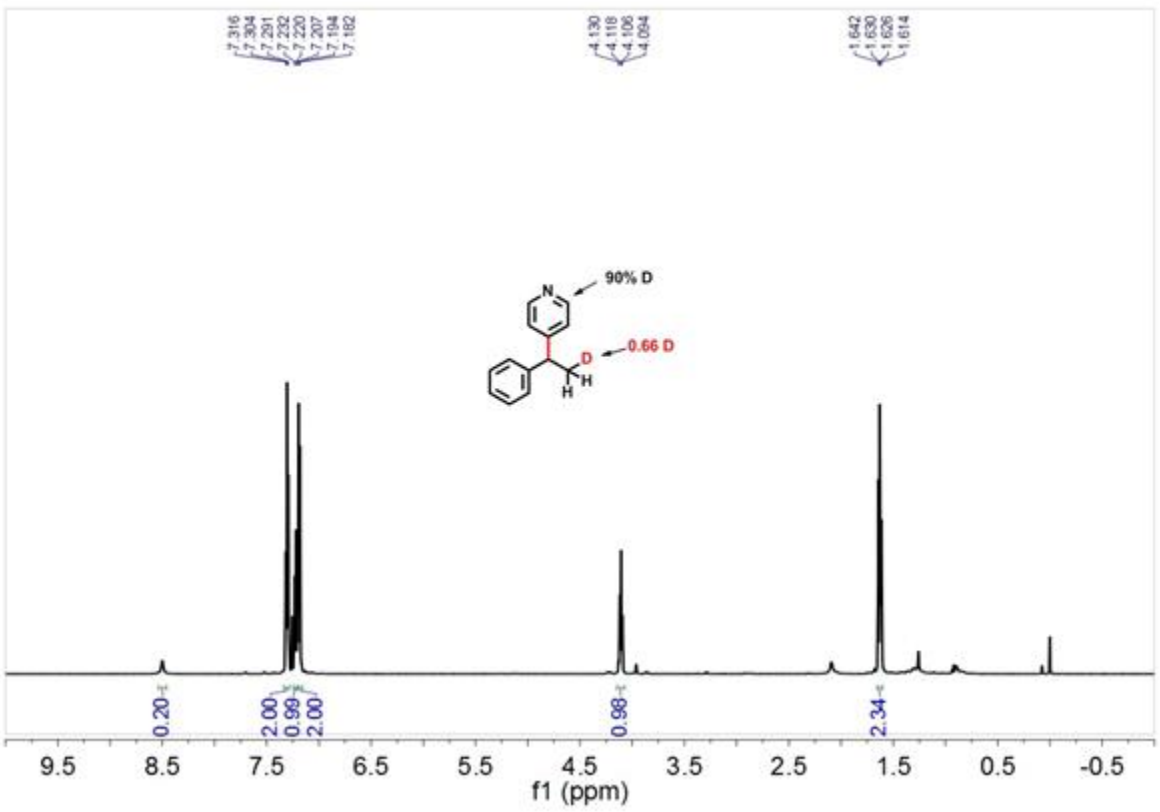
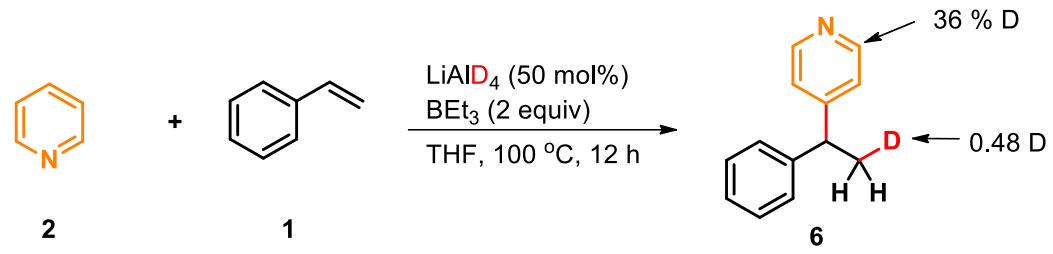


Figure. S2. The ^1H NMR spectrum of compound **5**.



In a nitrogen-filled glove box, a screw-cap test tube was placed styrene (0.75 mmol, 1.5equiv) and pyridine (40 μL, 0.5 mmol) in 1.0 mL dry THF, then BEt_3 (1.0 M in THF, 1.0 mL, 1.0 mmol) was added by syringe, followed by adding $LiAlD_4$ (0.01g, 0.25 mmol). Then, the test tube was sealed with a Teflon screw cap, removed from the glove box and stirred at 100 °C for 12 h. After completion, the mixture was quenched by *sat.aq.* NH_4Cl solution, extracted with CH_2Cl_2 (3 × 5.0 mL), combined the organic phases, and dried over anhydrous $MgSO_4$. The solvents were evaporated under vacuum and the crude product was purified on silica gel column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1) to give the **6** (Fig. S3).

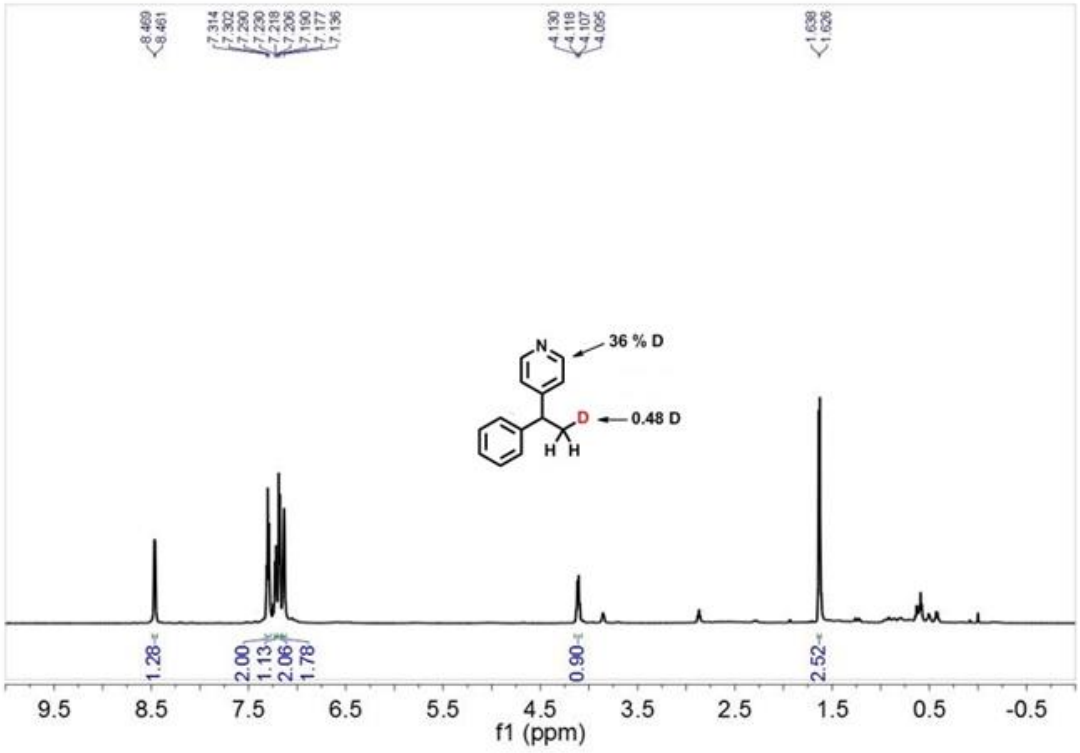
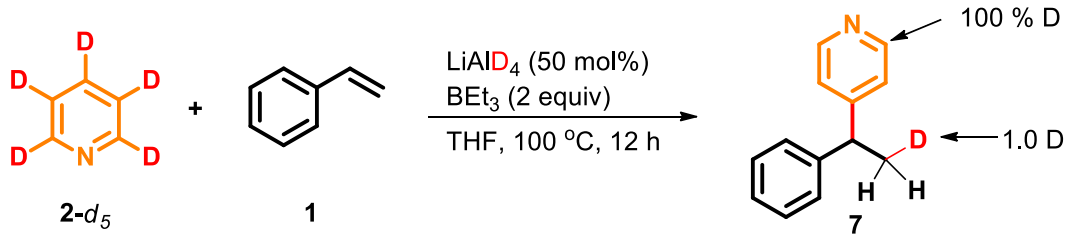


Figure. S3. The ^1H NMR spectrum of compound **6**.



In a nitrogen-filled glove box, a screw-cap test tube was placed styrene (0.75 mmol, 1.5equiv) and d_5-pyridine (40 μL, 0.5 mmol) in 1.0 mL dry THF, then the BEt_3 (1.0 M in THF, 1.0 mL, 1.0 mmol) was added slowly by syringe, followed by adding LiAlD4 (0.01 g, 0.25 mmol). Then the test tube was sealed with a Teflon screw cap, removed from the glove box and stirred at 100 °C for 12 h. After completion, the mixture was quenched by *sat.aq.* NH_4Cl solution, extracted with CH_2Cl_2 (3 × 5.0 mL), combined the organic phases, and dried over anhydrous $MgSO_4$. The solvents were evaporated under vacuum and the crude product was purified on silica gel column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1) to give the **7** (Fig. S4).

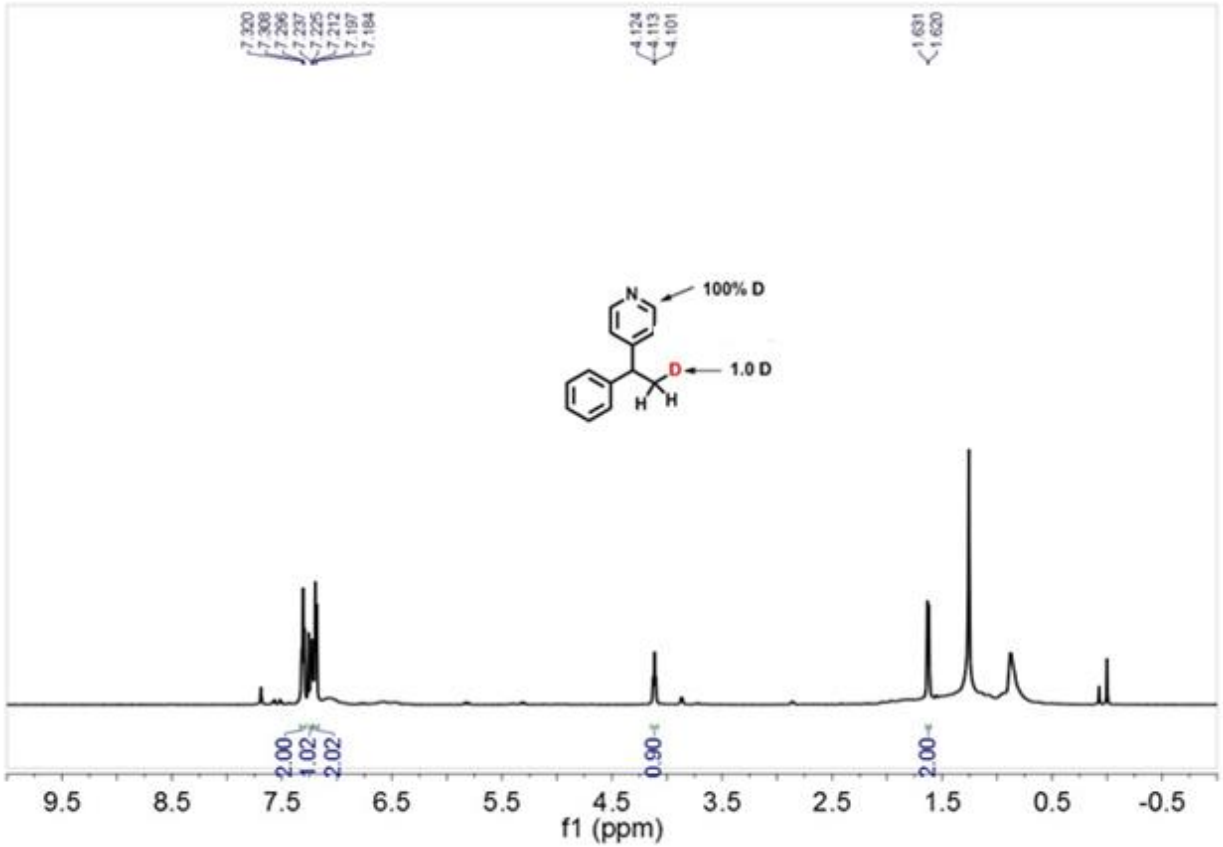
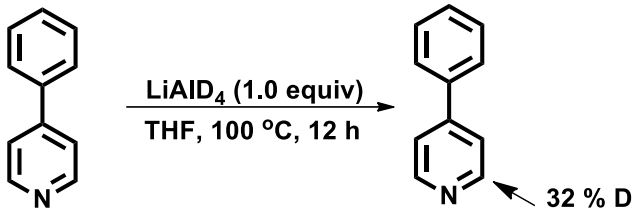


Figure. S4. The ^{1}H NMR spectrum of compound **7**.



In a nitrogen-filled glove box, a screw-cap test tube was placed 4-phenylpyridine (0.08 g, 0.5 mmol) in 1.0 mL dry THF, then LiAlD4 (0.02 g, 0.5 mmol) was added slowly. The test tube was sealed with a Teflon screw cap, removed from the glove box and stirred at 100 °C for 12 h. After completion, the mixture was quenched by *sat.aq.* NH_4Cl solution, extracted with CH_2Cl_2 (3 × 5.0 mL), combined the organic phases, and dried over anhydrous $MgSO_4$. The solvents were evaporated under vacuum and the crude product was purified on silica gel column chromatography (eluent: petroleum/EtOAc/Et_3N = 4/1/1) to give the product. From this ^1H NMR spectra, 32% D atom at the *ortho*-position of pyridine unit was observed (Fig. S5).

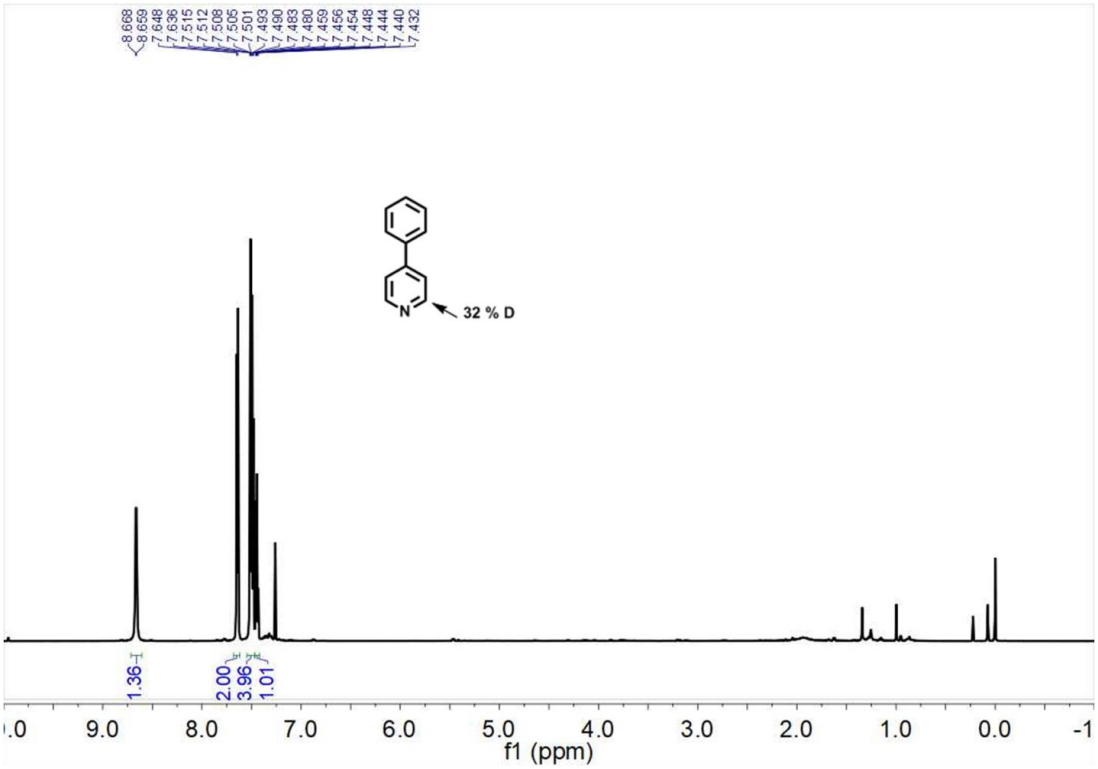


Figure. S5. The ^1H NMR spectra of the $LiAlD_4$ reacting with 4-phenylpyridine.

^{11}B NMR investigations.

1) $NaBEt_3H$

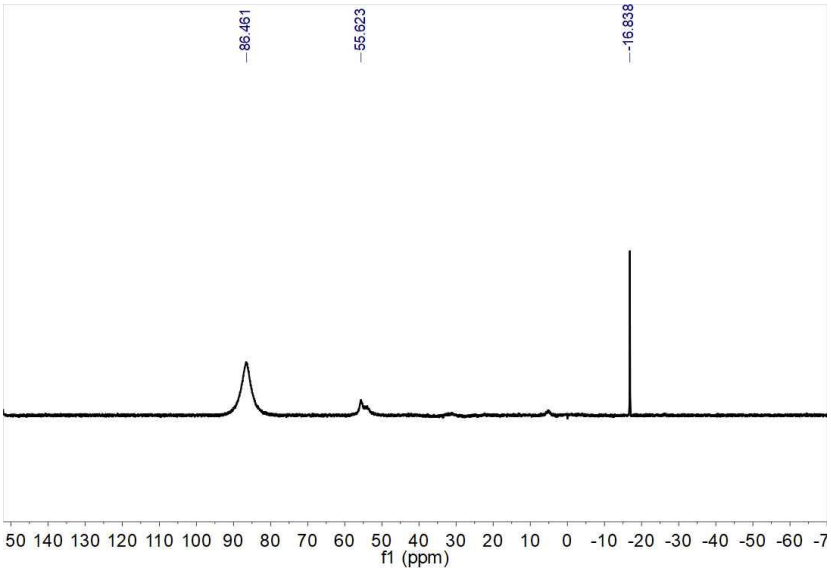


Figure. S6. The ^{11}B NMR spectra of $NaBEt_3H$ (1 M in THF)

As Fig S6, witnessed by ^{11}B NMR, two peaks were obtained in the solution of $NaBEt_3H$ (1. M in THF). This result indicates that a dissociation equilibrium existed in this $NaHBEt_3$ solution and were confirmed as BEt_3 (δ = 86.5 ppm) and tetraorganoborate anion $[BEt_3H]^-$ (δ = -16.8 ppm), respectively.

2) BEt_3

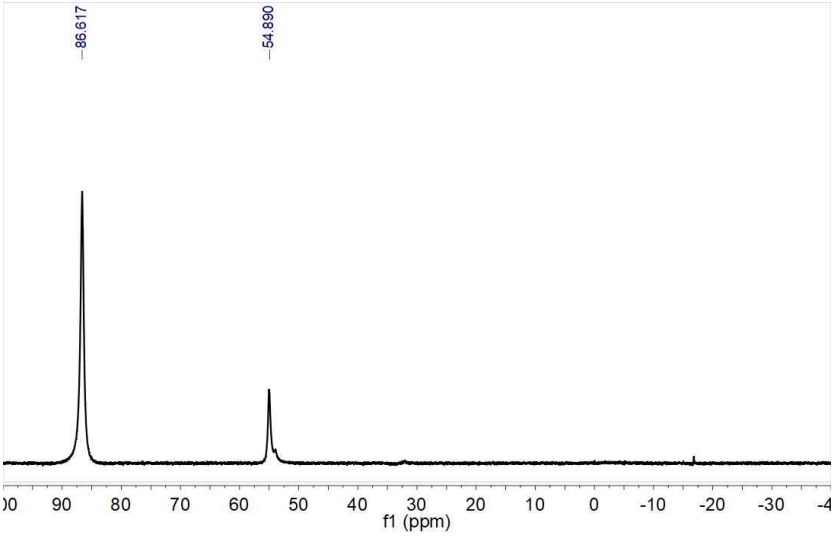


Figure. S7. The ^{11}B NMR spectra of BEt_3 (1 M in THF)

3) In a N_2-filled glovebox, a 15–mL oven dried Schlenk tube was charged with pyridine (40 μL, 0.5 mmol) and BEt_3 (1.0 mL, 1.0 mmol). Dry deuterated toluene (1.0 mL) was added and the mixture was reacted at 100 °C. After 10 min, the resulting was montiored by ^{11}B NMR (Fig.S8).

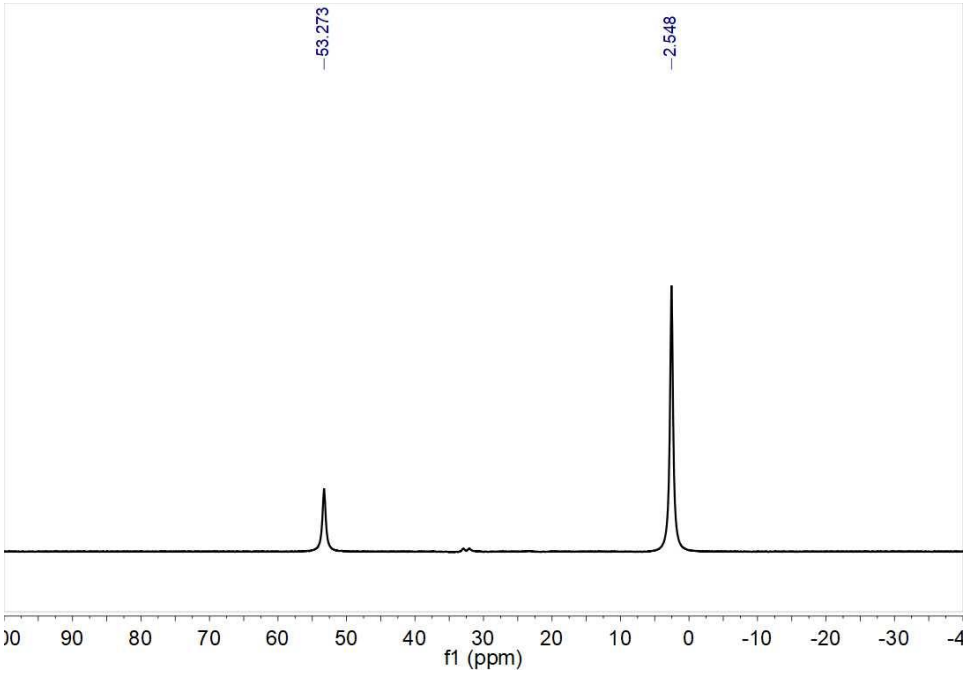


Figure. S8. The ^{11}B NMR spectra of pyridine with BEt_3

4）In a N_2-filled glovebox, a 15 mL oven dried Schlenk tube was charged with 4-fluorostyrene (60 μl, 0.5 mmol), $NaBEt_3H$ (1.0 M, 500μL, 0.5 mmol) was added slowly by syringe. Dry deuterated toluene (1.0 mL) was added and the mixture was reacted at 100 °C. After 10 min, the resulting was montiored by ^{11}B NMR (Fig. S9).

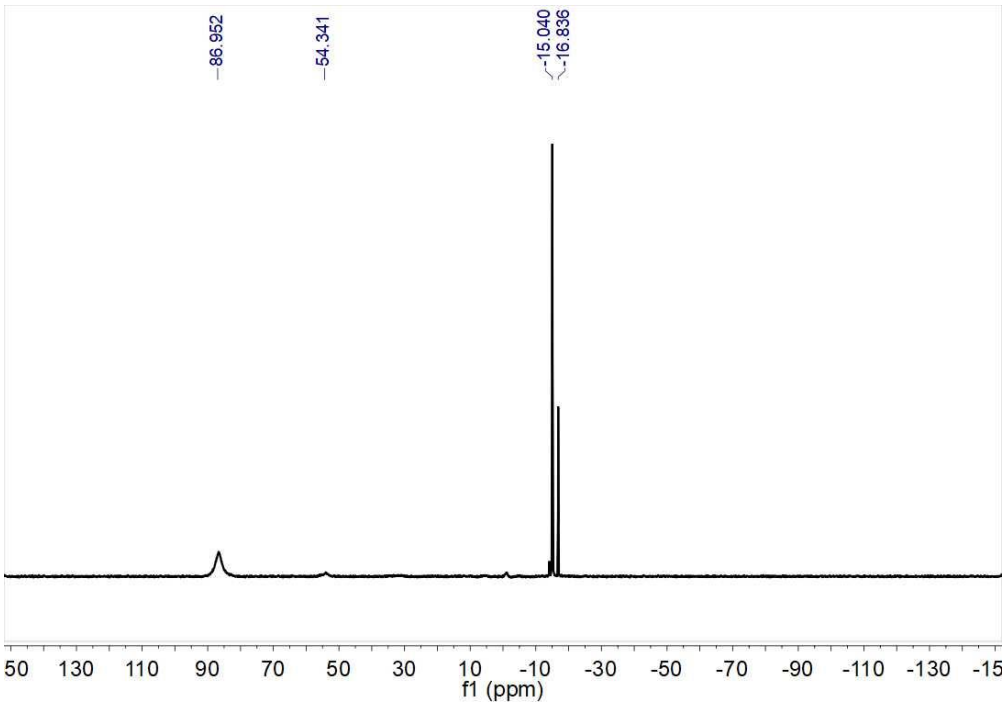


Figure. S9. The ^{11}B NMR spectra of 4-fluorostyrene with $NaBEt_3H$

5) In a N_2-filled glovebox, a 15 mL oven dried Schlenk tube was charged with 4-fluorostyrene (60 μl, 0.5 mmol), $NaBEt_3H$ (1.0 M, 500 μL, 0.5 mmol) was added slowly by syringe. After addition of the pyridine (40 μL, 0.5 mmol) and BEt_3 (1.0 mL, 1.0 mmol), dry deuterated toluene (1.0 mL) was added and the mixture was reacted at 100 °C. After 10 min, the resulting was montiored by ^{11}B NMR (Fig. S10).

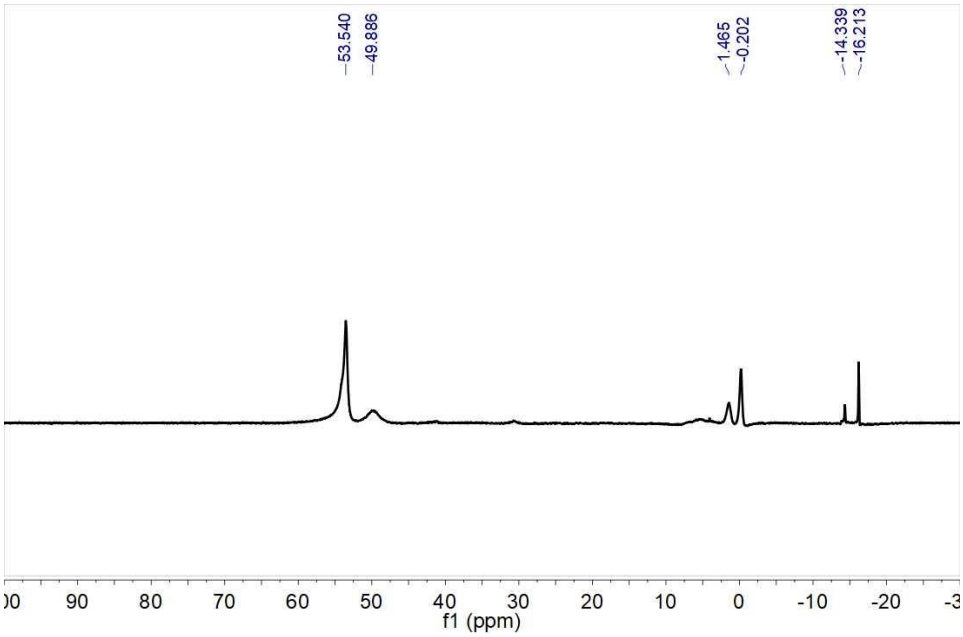
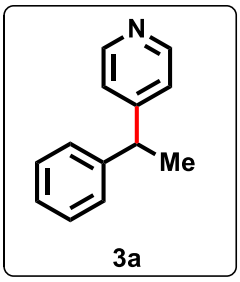


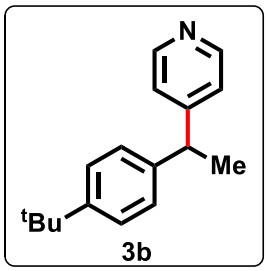
Figure. S10. The ^{11}B NMR spectra of 4-fluorostyrene, $NaBEt_3H$ and pyridine

7. Analytical data of new compounds



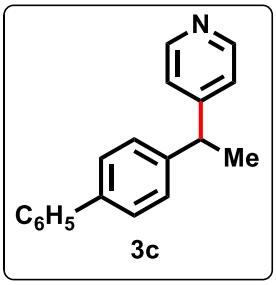
4-(1-phenylethyl)pyridine (3a)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1). Yellow oil (82.3 mg, 90%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.49 (d, *J* = 3.6 Hz, 2H), 7.32 – 7.30 (m, 2H), 7.23 – 7.21 (m, 1H), 7.19 – 7.18 (m, 2H), 7.13 (d, *J* = 5.4 Hz, 2H), 4.11 (q, *J* = 7.2 Hz, 1H), 1.64 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 155.0, 149.8, 144.3, 128.6, 127.6, 126.6, 122.9, 44.2, 21.0. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{13}H_{14}N$ ($[M + H]^+$): 184.1127; found: 184.1121.



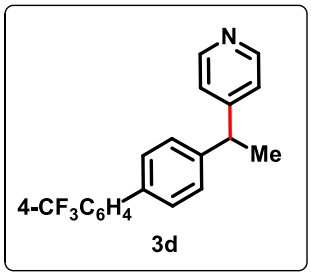
4-(1-(4-(tert-butyl)phenyl)ethyl)pyridine (3b)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1).Yellow oil (61.2 mg, 51%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.47 (d, *J* = 4.8 Hz, 2H), 7.32 (d, *J* = 8.4 Hz, 2H), 7.14 – 7.10 (m, 4H), 4.08 (q, *J* = 7.2 Hz, 1H), 1.62 (d, *J* = 7.2 Hz, 3H), 1.30 (s, 9H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 155.2, 149.7, 149.4, 141.2, 127.1, 125.4, 123.1, 43.7, 34.3, 31.3, 21.0. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{17}H_{22}N$ ($[M + H]^+$): 240.1747; found: 240.1740.



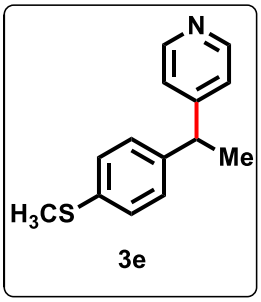
4-(1-([1,1'-biphenyl]-4-yl)ethyl)pyridine (3c)

Purified by flash column chromatography (eluent:petroleum/ EtOAc/Et_3N = 25/5/1) . Yellow oil (117.1 mg, 90%).**^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.51 (d, *J* = 5.4 Hz, 2H), 7.56 (d, J = 7.2 Hz, 2H), 7.53 (d, J = 8.4 Hz, 2H), 7.41 (t, *J* = 7.8 Hz, 2H), 7.32 (t, *J* = 7.2 Hz, 1H), 7.26 – 7.22 (m, 2H), 7.16 (d, J = 5.4 Hz, 2H), 4.14 (q, *J* = 7.2 Hz, 1H), 1.66 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 154.9, 149.8, 143.4, 140.6, 139.5, 128.7, 128.0, 127.3, 127.2, 127.0, 122.9, 43.9, 21.0. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{19}H_{18}N$($[M+H]^+$):260.1434; found: 260.1443.



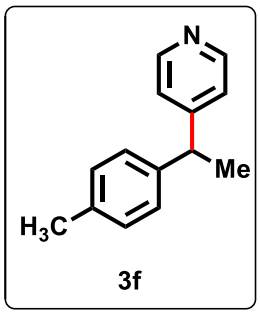
4-(1-(4'-(trifluoromethyl)-[1,1'-biphenyl]-4-yl)ethyl)pyridine(3d)

Purified by flash column chromatography (eluent: petroleum/ EtOAc/Et3N =20/5/1). Yellow oil (114.8 mg, 70%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.41 (d, *J* = 6.0 Hz, 2H), 7.40 (d, *J* = 8.4 Hz, 2H), 7.28 – 7.22 (m, 2H), 7.16 (d, *J* = 8.4 Hz, 3H), 7.05 (d, *J* = 6.0 Hz, 2H), 6.90 (t, *J* = 7.8 Hz, 1H), 4.04 (q, *J* = 7.2 Hz, 1H), 1.56 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 154.7, 150.0, 144.6, 144.2, 138.1, 129.3 (q, J = 32.6 Hz), 128.3, 127.5, 127.3, 125.7 (q, J = 3.8 Hz), 124.3 (q, J = 270.0 Hz), 122.9, 44.0, 21.0. **^{19}F NMR** (564 MHz; $CDCl_3$) δ 62.4. Mass Spectrometry: HRMS (ESI-TOF) (m/z): Calcd for $C_{20}H_{17}F_3N$ ($[M + H]^+$):328.1308; found: 328.1316.



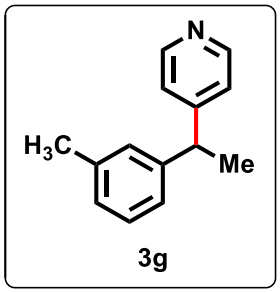
4-(1-(4-(methylthio)phenyl)ethyl)pyridine (3e)

Purified by flash column chromatography (eluent:petroleum/ EtOAc/ = 3/1). Yellow oil (93.2 mg, 81%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.47 (d, *J* = 6.0 Hz, 2H), 7.22 – 7.16 (m, 2H), 7.10 (d, *J* =7.8 Hz, 4H), 4.05 (q, *J* = 7.2 Hz, 1H), 2.43 (s, 3H), 1.59 (d, *J* = 7.2, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 154.7, 149.6, 141.1, 136.4, 127.9, 126.7, 122.7, 43.5, 20.8, 15.7. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{14}H_{16}NS$ ($[M + H]^+$): 230.0998; found: 230.1000.



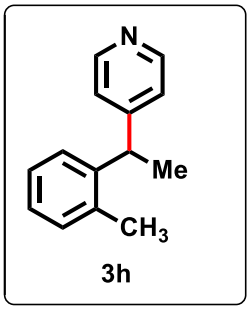
4-(1-(p-tolyl)ethyl)pyridine (3f)

Purified by flash column chromatography (eluent:petroleum/ EtOAc/Et_3N = 25/5/1). Yellow oil (40.6 mg, 41%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.49 (s, 2H), 7.13 – 7.11(m, 4H), 7.08 (d, *J* = 8.4 Hz, 2H), 4.07 (q, *J* = 7.2 Hz, 1H), 2.32 (s, 3H), 1.61 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 155.3, 149.7, 141.4, 136.2, 129.3, 127.4, 123.0, 43.8, 21.1, 20.9. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{14}H_{16}N$ ($[M +H]^+$): 198.1277; found: 198.1286.



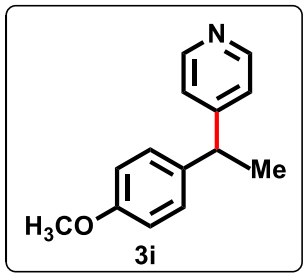
4-(1-(m-tolyl)ethyl)pyridine (3g)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1) Yellow oil (93.1 mg, 94%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.49 (s, 2H), 7.20 (t, *J* = 7.8 Hz, 1H), 7.13 (d, *J* = 5.4 Hz, 2H), 7.04 (d, *J* = 7.2 Hz, 1H), 6.99 (d, *J* = 5.4 Hz, 2H), 4.07 (q, *J* = 7.2 Hz, 1H), 2.32 (s, 3H), 1.62 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 155.2, 149.8, 144.4, 138.3, 128.5, 128.4, 127.4, 124.6, 123.0, 44.2, 21.5, 21.1. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{14}H_{16}N$ ($[M + H]^+$): 198.1277; found: 198.1287.



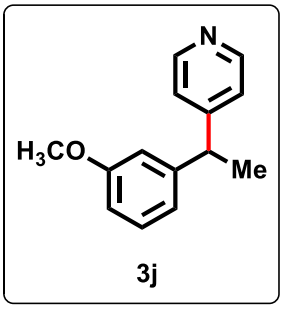
4-(1-(o-tolyl)ethyl)pyridine (3h)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1) Yellow oil (88.1 mg, 89%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.46 (d, *J* = 4.8 Hz, 2H), 7.22 –7.21 (m, 2H), 7.16 – 7.15 (m, 2H), 7.06 (d, *J* = 5.4 Hz, 2H), 4.28 (q, *J* = 7.2 Hz, 1H), 2.20 (s, 3H), 1.60 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 155.1, 149.8, 142.0, 135.9, 130.5, 126.6, 126.6, 126.2, 122.9, 40.4, 21.2, 19.6. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{14}H_{16}N$ ($[M + H]^+$): 198.1277; found: 198.1283.



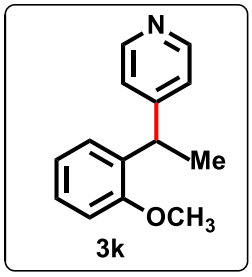
4-(1-(4-methoxyphenyl)ethyl)pyridine (3i)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et3N = 3/1/1). Yellow oil (19.7 mg, 18%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.54 (s, 2H), 7.15 (s, 2H), 7.11 (d, J = 8.4 Hz, 2H), 4.07 (q, *J* = 7.2 Hz, 1H), 3.78 (s, 3H), 1.61 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 158.3, 155.7, 149.5, 136.4, 128.6, 123. 2, 114.0, 55.3, 43.4, 21.2. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for C16H18N ([M + H]+): 214.1226; found: 214.1246.



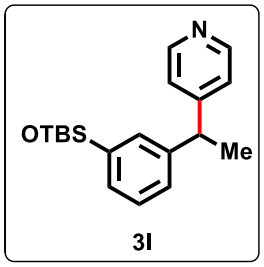
4-(1-(3-methoxyphenyl)ethyl)pyridine (3j)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 3/1/1). Yellow oil (97.3 mg, 91%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.49 (s, 2H), 7.22 (t, *J* = 7.8 Hz, 1H), 7.13 (d, *J* = 4.8 Hz, 2H), 6.79 – 6.75 (m, 2H), 6.73 (s, 1H), 4.08 (q, *J* = 7.2 Hz, 1H), 3.77 (s, 3H), 1.62 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 159.8, 154.9, 149.8, 146.0, 129.6, 123.0, 120.05, 113.9, 111.5, 55.2, 44.2, 21.0. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{14}H_{16}NO$ ([M + H]$^+$): 214.1226; found: 214.1236.



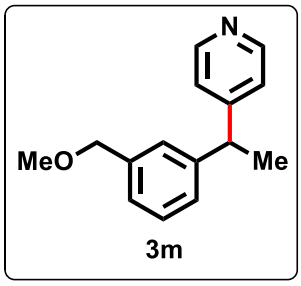
4-(1-(2-methoxyphenyl)ethyl)pyridine (3k)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et3N = 3/1/1). Yellow oil (69.6 mg, 65%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.44 (s, 2H), 7.20 (t, *J* = 7.8 Hz, 1H), 7.15 (d, *J* = 7.8 Hz, 1H), 7.11 (d, *J* = 6.0 Hz, 2H), 6.92 (t, *J* = 7.2 Hz, 1H), 6.83 (d, *J* = 7.8 Hz, 1H), 4.49 (q, *J* = 7.2 Hz, 1H), 3.71 (s, 3H), 1.56 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 156.7, 155.4, 149.3, 132.6, 127.6, 127.4, 122.8, 120.5, 110.5, 55.1, 37.1, 19.8. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for C16H18N ([M + H]+): 214.1226; found: 214.1238.



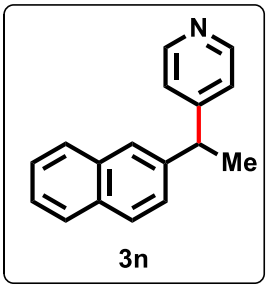
4-(1-(3-((tert-butyldimethylsilyl)oxy)phenyl)ethyl)pyridine (3l)

Purified by flash column chromatography(eluent: petroleum/EtOAc/Et_3N = 20/5/1). Green oil (128.9 mg, 82%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.29 (d, *J* = 6.0 Hz, 2H), 6.96 (t, *J* = 7.8 Hz, 1H), 6.93 (d, *J* = 6.0 Hz, 2H), 6.59 (d, *J* = 7.8 Hz, 1H), 6.51 (d, *J* = 7.8 Hz, 1H), 6.47 (s, 1H), 3.86 (q, *J* = 7.2 Hz, 1H), 1.41 (d, *J* = 7.2 Hz, 3H), 0.77 (s, 9H), -0.03 (s, 6H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 155.7, 155.0, 149.5, 145.8, 129.4, 122.8, 120.5, 119.4, 118.1, 43.9, 25.6, 20.8, 18.1, -4.5. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{19}H_{28}NOSi$ ([M +H]$^+$): 314.1935; found: 314.1994.



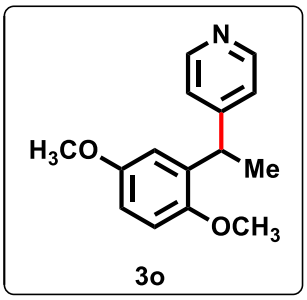
4-(1-(3-(methoxymethyl)phenyl)ethyl)pyridine (3m)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 20/5/1). Yellow oil (62.7 mg, 55%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.49 (s, 2H), 7.29 (t, *J* = 7.2 Hz, 1H), 7.20 – 7.17 (m, 2H), 7.14 – 7.11 (m, 3H), 4.42 (s, 2H), 4.12 (q, *J* = 7.2 Hz, 1H), 3.38 (s, 3H), 1.64 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 155.0, 149.7, 144.5, 138.6, 128.7, 126.9, 126.0, 123.0, 74.6, 58.2, 44.2, 21.0. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{15}H_{18}NO$ ([M +H]$^+$): 228.1383; found: 228.1390.



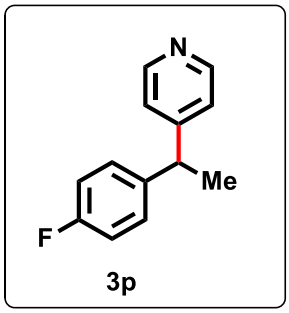
4-(1-(naphthalen-2-yl)ethyl)pyridine (3n)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1). Yellow solid (117.1 mg, 73%). m.p. 111 – 113 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.51 (s, 2H), 7.78 (d, *J* = 8.4 Hz, 2H), 7.74 (d, *J* = 8.4 Hz, 1H), 7.86 (s, 1H), 7.47 – 7.41 (m, 2H), 7.23 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.15 (s, 2H), 4.24 (q, *J* = 7.2 Hz, 1H), 1.70 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 154.8, 149.8, 141.7, 133.4, 132.2, 128.2, 127.6, 127.5, 126.3, 126.1, 125.7, 125.6, 123.1, 44.2, 20.9. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{17}H_{16}N$ ($[M + H]^+$): 234.1277; found: 234.1274.



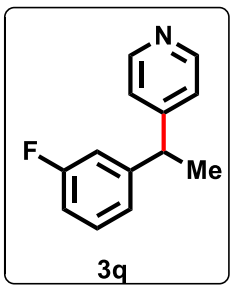
4-(1-(2,5-dimethoxyphenyl)ethyl)pyridine (3o)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 15/5/1). Yellow oil (101.1 mg, 83%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.45 (s, 2H), 7.12 (d, *J* = 4.8 Hz, 2H), 6.77 – 6.71 (m, 3H), 4.47 (*J* = 7.2 Hz, 1H), 3.73 (s, 3H), 3.66 (s, 3H), 1.55 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 155.1, 153.5, 151.0, 149.3, 133.9, 122.8, 114.5, 111.4, 110.9, 55.7, 55.4, 37.1, 19.7. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{15}H_{18}NO_2$ ($[M + H]^+$): 244.1332; found: 244.1332.



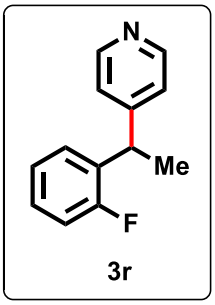
4-(1-(4-fluorophenyl)ethyl)pyridine (3p)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1). Yellow oil (82.8 mg, 82%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.48 (d, *J* = 6.0 Hz, 2H), 7.14 (dd, *J* = 8.4, 5.4 Hz, 2H), 7.10 (d, *J* = 6.0 Hz, 2H), 6.98 (t, *J* = 8.4Hz, 2H), 4.09 (q, *J* = 7.2 Hz, 1H), 1.60 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 161.4 (d, *J* = 243.6 Hz), 155.0, 149.7, 140.0, 129.0 (d, *J* = 8.0 Hz), 122.9, 115.4 (d, *J* = 24.0 Hz), 43.7, 21.2. **^{19}F NMR** (564 MHz; $CDCl_3$) δ -116.23. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{13}H_{13F}N$ ($[M + H]^+$): 202.1027; found: 202.1036.



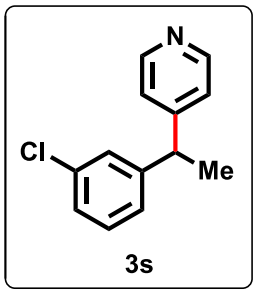
4-(1-(3-fluorophenyl)ethyl)pyridine (3q)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1). Yellow oil (80.8 mg, 80%).**^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.51 (d, *J* = 3.0 Hz, 2H), 7.28 – 7.24 (m, 1H), 7.11 (d, *J* = 5.4 Hz, 2H), 6.97 (d, *J* = 7.8 Hz, 1H), 6.93 – 6.88 (m, 2H), 4.10 (q, *J* = 7.2 Hz, 1H), 1.62 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 162.9 (d, *J* = 244.5 Hz), 154.2, 149.9, 146.9 (d, *J* = 6.9 Hz), 130.0 (d, *J* = 8.4Hz), 123.2, 122.8, 114.5 (d, *J* = 21.0 Hz), 113.5 (d, *J* = 21.0 Hz), 43.9, 20.8. **^{19}F NMR** (564 MHz; $CDCl_3$) *δ* - 60.67. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{13}H_{13}FN$ ($[M + H]^+$): 202.1027; found: 202.1036.



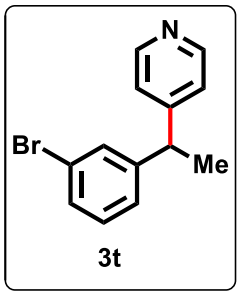
4-(1-(2-fluorophenyl)ethyl)pyridine (3r)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1). Yellow oil (87.9 mg, 87%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.48 (d, *J* = 4.8 Hz, 2H), 7.19 (t, *J* = 7.2 Hz, 2H), 7.13 (d, *J* = 4.8 Hz, 2H), 7.09 (t, *J* = 7.8 Hz, 1H), 7.01– 6.98 (m, 1H), 4.41 (q, *J* = 7.2 Hz, 1H), 1.61 (d, *J* = 7.8Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 160.5 (d, *J* = 244.5 Hz) , 154.0, 149.7, 131.3 (d, *J* = 14.4 Hz), 128.4, 128.3 (d, *J* =4.7 Hz), 124.2 (d, *J* = 3.7Hz), 122.8, 115.6 (d, *J* = 22.0 Hz), 37.2, 19.8.**^{19}F NMR** (564 MHz; $CDCl_3$) δ -117.32 – -117.36 (m). Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{13}H_{13}FN$ ($[M + H]^+$): 202.1027; found: 202.1035.



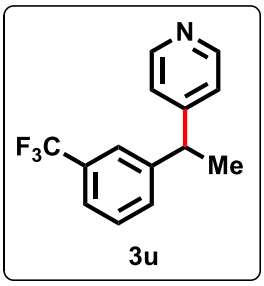
4-(1-(3-chlorophenyl)ethyl)pyridine (3s)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1). Yellow oil (86.1 mg, 79%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.53 (s, 2H), 7.27 – 7.18 (m, 3H), 7.12 (d, *J* = 4.2 Hz, 2H), 7.06 (d, *J* = 7.2 Hz, 1H), 4.08 (q, *J* = 7.2 Hz, 1H), 1.62 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 154.1, 149.9, 146.4, 134.4, 129.9, 127.7, 126.8, 125.8, 122.9, 43.9, 20.8. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{13}H_{13}ClN$ ($[M + H]^+$): 218.0731; found: 218.0740.



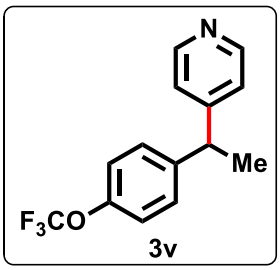
4-(1-(3-bromophenyl)ethyl)pyridine (3t)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1). Yellow oil (107.4 mg, 82%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.50 (d, *J* = 4.2 Hz, 2H), 7.36 – 7.34 (m, 2H), 7.16 (t, *J* = 7.8 Hz, 1H), 7.10 (d, *J* = 6.0 Hz, 3H), 4.07 (q, *J* = 7.2 Hz, 1H), 1.61 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 154.1, 149.9, 146.7, 130.6, 130.2, 129.8, 126.3, 122.9, 122.7, 43.9, 20.9. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{13}H_{13}BrN$ ($[M +H]^+$): 262.022; found: 262.0235.



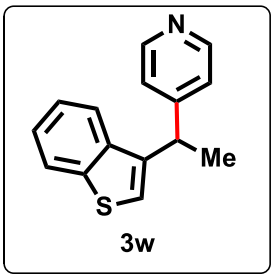
4-(1-(3-(trifluoromethyl)phenyl)ethyl)pyridine (3u)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1). Yellow oil (50.4 mg, 40%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.54 (s, 2H), 7.50 (d, *J* = 7.8 Hz, 1H), 7.47 (s, 1H), 7.43 (t, *J* = 7.8 Hz, 1H), 7.36 (d, *J* = 7.8 Hz, 1H), 7.13 (d, *J* = 3.6 Hz, 2H), 4.18 (q, *J* = 7.2 Hz, 1H), 1.66 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 153.9, 150.0, 145.3, 131.1, 130.8 (q, *J* = 31.8 Hz), 129.9, 124.2 (q, *J* = 3.8 Hz), 124.0 (q, *J* = 270.6 Hz), 123.6 (q, *J* = 3.8 Hz), 122.9, 44.0, 20.9. **^{19}F NMR** (564 MHz; $CDCl_3$) δ -62.9. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{14}H_{13}F_3N$ ($[M + H]^+$): 252.0995; found: 252.1003.



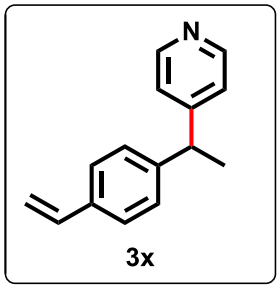
4-(1-(4-(trifluoromethoxy)phenyl)ethyl)pyridine (3v)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 20/5/1). Yellow oil (101.8 mg, 76%).**^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.52 (s, 2H), 7.21 (d, *J* = 8.4 Hz, 2H), 7.15 (d, *J* = 8.4 Hz, 2H), 7.12 (d, *J* = 4.8 Hz, 2H), 4.13 (q, *J* = 7.2 Hz, 1H), 1.64 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 154.4, 149.9, 147.9, 143.1, 128.9, 122.9, 121.3 (q, *J* = 255.3 Hz), 121.1, 43.6, 21.1. **^{19}F NMR** (564 MHz; $CDCl_3$) δ -57.9. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{14}H_{13}F_3NO$ ($[M + H]^+$): 268.0994; found: 268.0951.



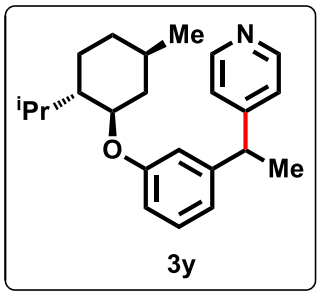
4-(1-(benzo[b]thiophen-3-yl)ethyl)pyridine (3w)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 15/5/1). Yellow oil (86.2 mg, 72%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.47 (d, *J* = 5.4 Hz, 2H), 7.84 (d, *J* = 7.8 Hz, 1H), 7.45 (d, *J* = 7.8 Hz, 1H), 7.31 – 7.28 (m, 1H), 7.25 – 7.23 (m, 2H), 7.12 (d, *J* = 6.0 Hz, 2H), 4.40 (d, *J* = 7.2 Hz, 1H), 1.71 (d, *J* = 7.2 Hz, 3H).**^{13}C NMR** (150 MHz, $CDCl_3$) δ 154.1, 150.0, 140.6, 138.4, 138.0, 124.4, 123.9, 122.9, 122.6, 122.2, 122.0, 38.8, 21.5. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{15}H_{14}NS$ ($[M + H]^+$): 240.0841; found: 240.0844.



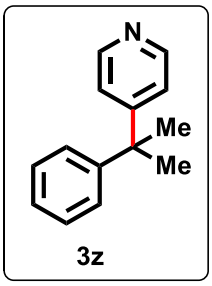
4-(1-(4-vinylphenyl)ethyl)pyridine (3x)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 15/5/1). Brown oil (53.2 mg, 51%).**^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.49 (d, *J* = 4.8 Hz, 2H), 7.35 (d, *J* = 7.8 Hz, 2H), 7.15 (d, *J* =7.8 Hz, 2H), 7.12 (d, *J* = 4.8 Hz, 2H), 6.68 (dd, *J* = 10.8, 7.8 Hz, 1H), 5.71 (d, *J* = 17.4 Hz, 1H), 5.22 (d, *J* = 10.8 Hz, 1H), 4.10 (q, *J* = 7.2 Hz, 1H), 1.63 (d, *J* = 7.2 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 154.9, 149.8, 144.0, 136.3, 136.0, 127.7, 126.4, 122.9, 113.7, 43.9, 20.9. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{15}H_{16}N$ ($[M + H]^+$): 209.1236; found: 209.1240.



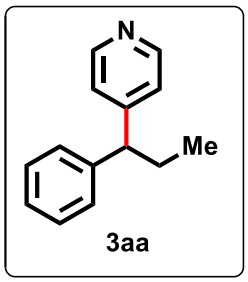
4-(1-(3-(((1R,2S,5R)-2-isopropyl-5-methylcyclohexyl)oxy)phenyl)ethyl)pyridine (3y)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1). Yellow oil (81.2 mg, 48%).**^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.49 (d, *J* = 6.0 Hz, 2H), 7.19 (t, *J* = 8.4 Hz, 1H), 7.14 (d, *J* = 6.0 Hz, 2H), 6.77 – 6.75(m, 1H), 6.73 – 6.71 (m, 2H), 4.58 (s, 1H), 4.06 (q, *J* = 7.2 Hz, 1H), 2.06 – 2.02 (m, 1H), 1.78 – 1.64 (m, 4H), 1.62 (d, *J* = 7.2 Hz, 3H), 1.58 – 1.52 (m, 1H), 1.04 – 1.01(m, 1H), 0.98 – 0.93 (m, 2H), 0.91 (d, *J* = 7.2 Hz, 3H), 0.85 – 0.83 (m, 3H), 0.80 (d, *J* = 6.6 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 158.5, 155.1, 149.7, 145.85, 129.5, 123.0, 119.4, 115.7, 113.25, 73.3, 47.8, 44.2, 37.7, 35.0, 29.2, 26.1, 24.75, 22.25, 21.0, 20.85. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{23}H_{32}NO$ ($[M +H]^+$): 338.2478; found: 338.2490.



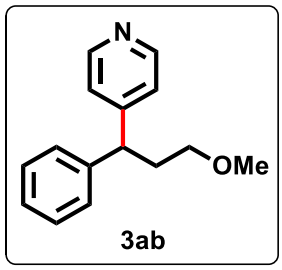
4-(2-phenylpropan-2-yl)pyridine (3z)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1). Brown oil (81.2 mg, 48%)..**^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.48 (d, *J* = 7.2 Hz, 2H), 7.30 – 7.27 (m, 2H), 7.21 – 7.19 (m, 3H), 7.13 (d, *J* = 7.8 Hz, 2H), 1.67 (s, 3H). **^{13}C NMR** (150MHz, $CDCl_3$) δ 159.5, 149.5, 148.6, 128.2, 126.6, 126.2, 122.1, 42.8, 29.9. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{14}H_{16}N$ ($[M + H]^+$): 198.1277; found:198.1280.



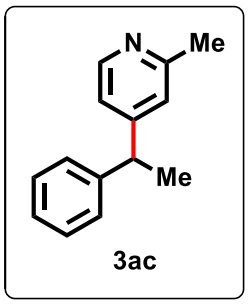
4-(1-phenylpropyl)pyridine (3aa)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1). Yellow oil (68.3 mg, 69%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.51 (s, 2H), 7.29 (t, *J* = 7.8 Hz, 2H), 7.22 – 7.19 (m, 3H), 7.15 (d, *J* = 3.6 Hz, 2H), 3.76 (t, *J* = 7.8 Hz, 1H), 2.09 – 2.06 (m, 2H), 0.90 (t, *J* = 7.8 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 153.9, 149.8, 143.1, 128.6, 127.9, 126.6, 123.3, 52.6, 27.9, 12.5. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{14}H_{16}N$ ($[M + H]^+$): 198.1277; found:198.1285.



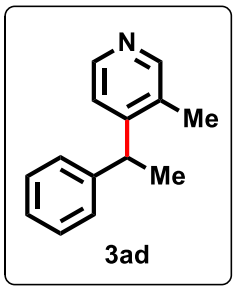
4-(3-methoxy-1-phenylpropyl)pyridine (3ab)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 20/5/1). Yellow oil (82.1 mg, 72%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.50 (s, 2H), 7.30 (t, *J* = 7.2 Hz, 2H), 7.22 (d, *J* = 6.6 Hz, 3H), 7.18 (s, 2H), 4.13 (t, *J* = 7.8 Hz, 1H), 3.27 (s, 5H), 2.29 (q, *J* = 7.2 Hz, 2H)**. ^{13}C NMR (**150 MHz, $CDCl_3$**)** δ 153.6, 149.5, 142.4, 128.6, 127.8, 126.7, 123.3, 69.9, 58.5, 46.5, 34.4. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{15}H_{18}NO$ ($[M + H]^+$): 228.1383; found: 228.1392.



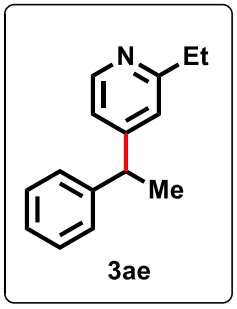
2-methyl-4-(1-phenylethyl)pyridine (3ac)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1). Yellow oil (72.3 mg, 73%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.36 (d, *J* = 5.4 Hz, 1H), 7.29 (t, *J* = 7.8 Hz, 2H), 7.22 – 7.18 (m, 3H), 6.99 (s, 1H), 6.93 (d, *J* = 4.8 Hz, 1H), 4.06 (q, *J* = 7.2 Hz, 1H), 2.50 (s, 3H), 1.61 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 158.2, 155.3, 149.0, 144.5, 128.5, 127.5, 126.4, 122.4, 120.0, 44.1, 24.3, 20.9. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{14}H_{16}N$ ($[M + H]^+$): 198.1277; found: 198.1284.8.



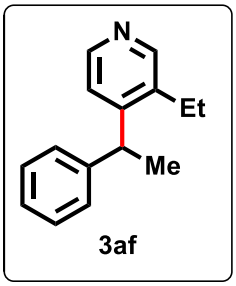
3-methyl-4-(1-phenylethyl)pyridine (3ad)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1). Yellow oil (86.1mg, 87%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.43 (s, 1H), 8.35 (s, 1H), 7.27 (t, *J* = 7.8 Hz, 2H), 7.19 (t, *J* = 7.2 Hz, 2H), 7.12 (d, *J* = 7.8 Hz, 2H), 4.25 (q, *J* = 7.2 Hz, 1H), 2.19 (s, 3H), 1.60 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 153.0, 150.5, 147.4, 144.1, 131.8, 128.6, 127.6, 126.5, 121.6, 40.8, 21.3, 16.5. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{14}H_{16}N$ ($[M +H]^+$): 198.1277; found: 198.1272.



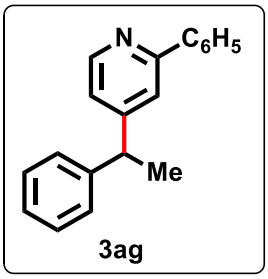
2-ethyl-4-(1-phenylethyl)pyridine (3ae)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1). Yellow oil (60.8 mg, 57%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.40 (d, *J* = 5.0 Hz, 1H), 7.30 (t, *J* = 7.8 Hz, 2H), 7.22 – 7.19 (m, 3H), 7.00 (s, 1H), 6.94 (d, *J* = 4.8 Hz, 1H), 4.08 (q, *J* = 7.2 Hz, 1H), 2.77 (q, *J* = 7.2 Hz, 2H), 1.63 (d, *J* = 7.2 Hz, 3H), 1.28 (t, *J* = 7.8 Hz, 3H).**^{13}C NMR** (150 MHz, $CDCl_3$) δ 163.5, 155.4, 149.1, 144.6, 128.5, 127.6, 126.5, 121.2, 120.2, 44.3, 31.3, 21.1, 13.9. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{15}H_{18}N$ ($[M + H]^+$): 212.1434; found: 212.1440.



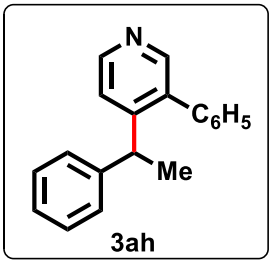
3-ethyl-4-(1-phenylethyl)pyridine (3af)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1). Yellow oil (92.3 mg, 87%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.39 (s, 2H), 7.27 (t, *J* = 7.8 Hz, 2H), 7.20 – 7.17 (m, 1H), 7.15 – 7.12 (m, 3H), 4.36 (q, *J* = 7.2 Hz, 1H), 2.70 – 2.58 (m, 2H), 1.60 (d, *J* = 7.2 Hz, 3H), 1.15 (t, *J* = 7.8 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 152.2, 150.2, 147.6, 144.7, 137.0, 128.6, 127.6, 126.4, 121.9, 39.8, 23.1, 21.8, 15.2. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{15}H_{18}N$ ($[M + H]^+$): 212.1434; found: 212.1447.



2-phenyl-4-(1-phenylethyl)pyridine (3ag)

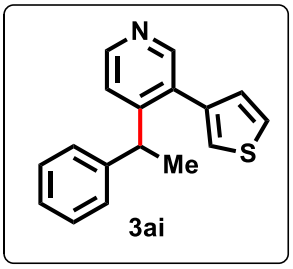
Purified by flash column chromatography (eluent:petroleum/EtOAc/Et_3N = 20/5/1). Brown oil (85.8 mg, 66%).**^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.51 (d, *J* = 5.4 Hz, 2H), 7.56 (d, *J* = 7.2 Hz, 2H), 7.53 (d, *J* = 8.4 Hz, 2H), 7.41 (t, *J* = 7.8 Hz, 2H), 7.32 (t, *J* = 7.2 Hz, 1H), 7.25 (d, *J* = 7.8 Hz, 2H), 7.16 (d, *J* = 5.4 Hz, 2H), 4.14 (q, *J* = 7.2 Hz, 1H), 1.66 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 157.7, 155.9, 149.8, 144.5, 139.6, 128.9, 128.7, 127.6, 127.0, 126.7, 121.5, 120.0, 44.5, 21.2. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{19}H_{18}N$ ($[M + H]^+$): 260.1434; found: 260.1437.



3-phenyl-4-(1-phenylethyl)pyridine (3ah)

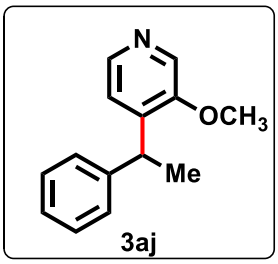
Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1). Brown oil (93.6 mg, 72%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.52 (s, 1H), δ 8.44 (s, 1H), 7.41 – 7.40 (m, 3H), 7.24 – 7.21 (m, 5H), 7.16 (t, *J* = 7.2 Hz, 1H), 7.02 (d, *J* = 7.2 Hz, 2H), 4.29 (q, *J* = 7.2 Hz, 1H), 1.53 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 152.7, 150.3, 148.8, 144.5, 137.8, 137.4, 129.5, 128.4, 128.3, 127.7, 127.4, 126.3, 122.2, 39.9, 21.5. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{19}H_{18}N$ ($[M +H]^+$): 260.1434; found: 260.1441.

4-(1-phenylethyl)-3-(thiophen-3-yl)pyridine (3ai)



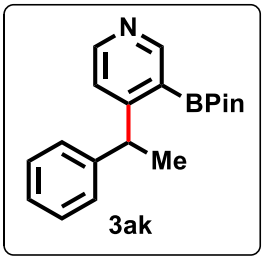
Purified by flash column chromatography(eluent:petroleum/EtOAc/Et_3N = 3/1/1). Yellow oil (71.8 mg, 54%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.50 (d, *J* = 4.8 Hz, 1H), 8.48 (s, 1H), 7.37 – 7.36 (m, 1H), 7.25 – 7.21(m, 3H), 7.18 – 7.15 (m, 1H), 7.10 (s, 1H), 7.03 (d, *J* = 7.8 Hz, 2H), 7.00 (d, *J* = 4.8 Hz, 1H), 4.35 (q, *J* = 7.2 Hz, 1H), 1.55 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 152.9, 150.6, 149.0, 144.7, 137.9, 132.5, 128.9, 128.5, 127.5, 126.4, 125.8, 124.0, 122.3, 40.3, 21.7. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{17}H_{16}NS$ ($[M + H]^+$):266.0998; found: 266.1008.

3-methoxy-4-(1-phenylethyl)pyridine (3aj)



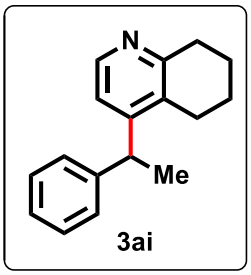
Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 3/1/1). Yellow oil (70.6 mg, 66%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.20 (d, *J* = 6.6 Hz, 2H), 7.29 – 7.26 (m, 2H), 7.22 – 7.18 (m, *J* = 3H), 7.05 (d, *J* = 4.8 Hz, 1H), 4.53 (q, *J* = 7.2 Hz, 1H), 3.87 (s, 3H), 1.57 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 153.2, 144.4, 143.2, 142.9, 133.3, 128.4, 127.7, 126.3, 122.1, 56.1, 37.1, 20.2. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{14}H_{16}NO$ ($[M + H]^+$): 214.1226; found: 214.1236.

4-(1-phenylethyl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridine (3ak)

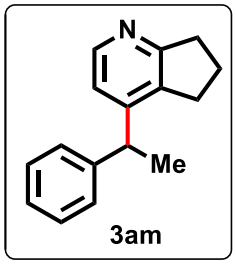


Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 2/1/1). Yellow oil (71.1 mg, 46%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.86 (s, 1H), 8.52 (d, *J* = 4.8 Hz, 1H), 7.27 – 7.25 (m, 2H), 7.21 – 7.16 (m, 3H), 7.09 (d, *J* = 4.8 Hz, 1H), 4.99 (q, *J* = 7.2 Hz, 1H), 1.59 (d, *J* = 7.2 Hz, 3H), 1.31 (d, *J* = 7.8 Hz, 12H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 161.8, 156.3, 151.7, 145.3, 128.2, 127.9, 126.1, 121.9, 83.9, 41.7, 24.8, 24.7, 21.7. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{19}H_{25}BNO_2$ ($[M +H]^+$): 309.2009; found: 309.2019.

4-(1-phenylethyl)-5,6,7,8-tetrahydroquinoline (3ai)

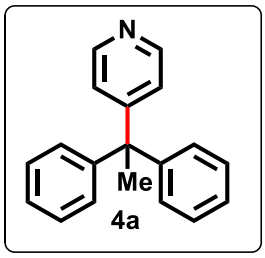


Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 3/1/1). Yellow oil (61.9 mg, 52%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.34(d, *J* = 4.8 Hz, 1H), 7.26 (t, *J* = 7.2 Hz, 2H), 7.18 (t, *J* = 7.2 Hz, 1H), 7.11 (d, *J* = 7.8 Hz, 2H), 7.03 (d, *J* = 5.4 Hz, 1H), 4.25 (q, *J* = 7.2 Hz, 1H), 2.92 – 2.91 (m, 2H), 2.78 – 2.73 (m, 1H), 2.50 – 2.45 (m, 1H), 1.78 – 1.73 (m, 4H), 1.57 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 157.3, 152.6, 146.5, 144.5, 130.4, 128.5, 127.6, 126.2, 119.4, 39.9, 33.2, 25.4, 22.8, 22.6, 21.7.Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{17}H_{20}N$ ($[M + H]^+$): 238.1590; found: 238.1600.



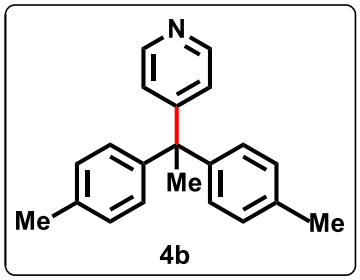
4-(1-phenylethyl)-6,7-dihydro-5H-cyclopenta[b]pyridine (3am)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 3/1/1). Yellow oil (66.9 mg, 59%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.33 (s, 1H), 7.26 (t, *J* = 7.2 Hz, 2H), 7.19 – 7.14 (m, 3H), 6.96 (d, *J* = 4.2 Hz, 1H), 4.12 (q, *J* = 7.2 Hz, 1H), 2.99 – 2.96 (m, 2H), 2.85 – 2.80 (m, 1H), 2.67 – 2.62 (m, 1H), 2.06 – 2.00 (m, 2H), 1.59 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 165.5, 150.4, 148.0, 144.2, 135.5, 128.5, 127.6, 126.4, 119.0, 42.1, 34.4, 29.3, 22.5, 20.7. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{16}H_{18}N$ ($[M + H]^+$): 224.1434; found: 224.1442.



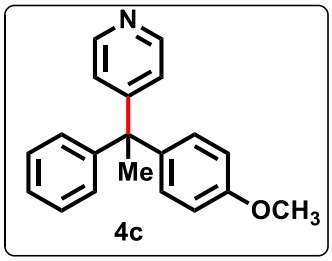
4-(1,1-diphenylethyl)pyridine (4a)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 4/1/1). White solid (120.9 mg, 93%). m.p. 84 – 85 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.50 (s, 2H), 7.27 (t, *J* = 7.2 Hz, 4H), 7.23 (t, *J* = 7.2 Hz, 2H), 7.07 (d, *J* = 7.8 Hz, 4H), 7.03 (d, *J* = 5.4 Hz, 2H), 2.16 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 157.9, 149.5, 147.2, 128.4, 128.1, 126.4, 123.8, 52.3, 29.7. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{19}H_{18}N$ ($[M + H]^+$): 260.1434.; found: 260.1442



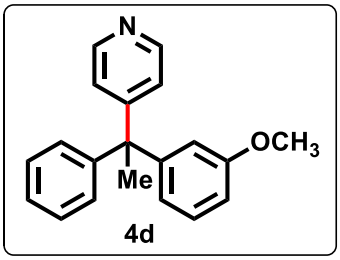
4-(1,1-di-p-tolylethyl)pyridine (4b)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 4/1/1). Yellow oil (108.9 mg, 75%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.48 (d, *J* = 4.8 Hz, 2H), 7.08 (d, *J* = 7.8 Hz, 4H), 7.03 (d, *J* = 5.4 Hz, 2H), 6.95 (d, *J* = 8.4 Hz, 4H), 2.33 (s, 6H), 2.12 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 158.3, 149.4, 144.5, 136.0, 128.8, 128.4, 123.8, 51.7, 29.8, 20.9. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{21}H_{22}N$ ($[M + H]^+$): 288.1742; found: 288.1747.



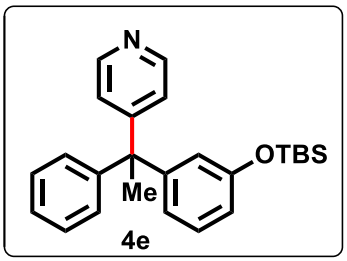
4-(1-(4-methoxyphenyl)-1-phenylethyl)pyridine (4c)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 3/1/1). Yellow oil (130.5 mg, 90%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.50 (s, 2H), 7.29 – 7.25 (m, 2H), 7.22 (t, *J* = 7.2 Hz, 1H), 7.06 (d, *J* = 7.2 Hz, 2H), 7.03 (d, *J* = 4.8 Hz, 2H), 6.98 (d, *J* = 8.4 Hz, 2H), 6.81 (d, *J* = 9.0 Hz, 3H), 3.78 (s, 3H), 2.14 (s, 3H).**^{13}C NMR** (150 MHz, $CDCl_3$) δ 158.2, 157.9, 149.4, 147.5, 139.3, 129.5, 128.4, 128.0, 126.4, 123.8, 113.4, 55.2, 51.7, 29.8. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{20}H_{20}NO$ ($[M + H]^+$): 290.1539; found: 290.1545.



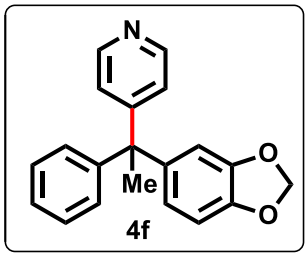
4-(1-(3-methoxyphenyl)-1-phenylethyl)pyridine (4d)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 3/1/1). Yellow oil (140.6 mg, 97%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.58 (s, 2H), 7.30 – 7.20 (m, 4H), 7.07 (d, *J* = 7.2 Hz,3H), 6.80 – 6.77 (m,1H), 6.67 – 6.65 (m, 1H), 6.62 –6.61 (m, 1H),3.72 (s, 3H), 2.15 (s, 3H).**^{13}C NMR** (150 MHz, $CDCl_3$) δ 159.4, 157.8, 148.9, 147.1, 129.0, 128.5, 128.1, 126.5, 121.2, 115.3, 111.1, 55.2, 52.4, 29.7. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{20}H_{20}NO$ ($[M + H]^+$): 290.1539; found: 290.1546.



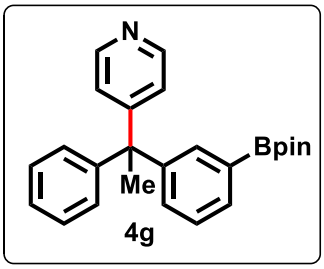
4-(1-(3-((tert-butyldimethylsilyl)oxy)phenyl)-1-phenylethyl)pyridine (4e)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 3/1/1). Yellow oil (175.5 mg, 90%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.49 (d, *J* = 6.0 Hz, 2H), 7.28 (t, *J* = 7.8 Hz, 2H), 7.22 (t, *J* = 7.2 Hz, 1H), 7.14 (t, *J* = 7.8 Hz, 1H), 7.07 (d, *J* = 7.8 Hz, 2H), 7.03 (d, *J* = 6.0 Hz, 2H), 6.73 (d, *J* = 7.8 Hz, 1H), 6.68 (d, *J* = 7.8 Hz, 1H), 6.49 (s, 1H), 2.14 (s, 3H), 0.91 (s, 9H), 0.07 (s, 6H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 157.8, 155.4, 149.5, 148.7, 147.3, 129.0, 128.4, 128.1, 126.4, 123.8, 121.3, 120.7, 118.2, 52.2, 29.6, 25.6, 18.2, -4.5. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{25}H_{32}NOSi$ ($[M + H]^+$): 390.2248; found: 390.2253.



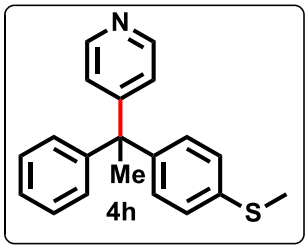
4-(1-(benzo[d][1,3]dioxol-5-yl)-1-phenylethyl)pyridine (4f)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 25/5/1). Yellow oil (135.2 mg, 89%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.49 (d, *J* = 5.4 Hz, 2H), 7.29 – 7.27 (m, 2H), 7.23 (t, *J* = 7.2 Hz, 1H), 7.07 (d, *J* = 7.8 Hz, 2H), 7.03 (d, *J* = 6.0 Hz, 2H), 6.70 (d, *J* = 7.8 Hz, 1H), 6.58 (d, *J* = 1.8 Hz, 1H), 6.49 (dd, *J* = 8.4, 2.4 Hz, 1H), 5.93 (s, 2H), 2.12 (s, 3H).**^{13}C NMR** (150 MHz, $CDCl_3$) δ 158.0, 149.5, 147.5, 147.25, 146.0, 141.25, 128.4, 128.1, 126.5, 123.7, 121.7, 109.3, 107.5, 101.0, 52.1, 30.0. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{20}H_{18}NO_2$ ($[M + H]^+$): 304.1332.; found: 304.1340.



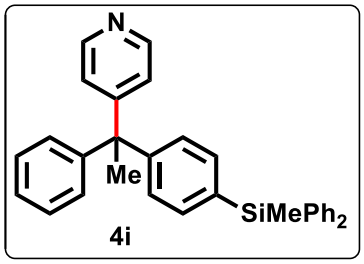
4-(1-phenyl-1-(3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)ethyl)pyridine (4g)

Purified by flash column chromatography (eluent: petroleum/EtOAc = 2/1). Yellow oil (84.9 mg, 44%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.50 (d, *J* = 6.0 Hz, 2H), 7.71 – 7.68 (m, 1H), 7.30 – 7.22 (m, 5H), 7.08 – 7.03 (m,5H), 2.17 (s, 3H), 1.31 (s, 12H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 158.6, 149.0, 147.3, 146.3, 133.9, 133.1, 132.0, 128.6, 128.2, 127.5, 126.5, 124.1, 83.8, 52.5, 29.9, 24.9. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{25}H_{29}BNO_2$ ($[M + H]^+$): 386.2239; found: 386.2249.



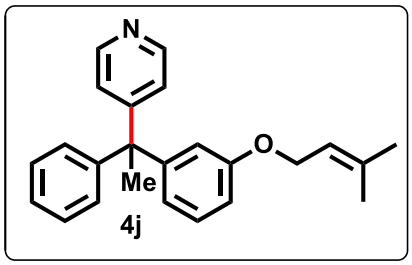
4-(1-(4-(methylthio)phenyl)-1-phenylethyl)pyridine (4h)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 3/1/1). Yellow oil (107.1 mg, 71%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.48 (d, *J* = 5.4 Hz, 2H), 7.29 – 7.26 (m, 2H), 7.22 (t, *J* = 7.2 Hz, 1H), 7.16 (d, *J* = 8.4 Hz, 2H), 7.06 (d, *J* = 7.8 Hz, 2H), 7.02 (d, *J* = 6.0 Hz, 2H), 6.98 (d, *J* = 8.4 Hz, 2H), 2.45 (s, 3H), 2.13 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 157.7, 149.5, 147.0, 144.0, 136.5, 128.9, 128.3, 128.1, 126.4, 126.0, 123.7, 51.9, 29.6, 15.6. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{20}H_{20}NS$ ($[M + H]^+$): 306.1237; found: 306.1239.



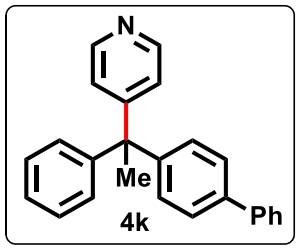
4-(1-(4-(methyldiphenylsilyl)phenyl)-1-phenylethyl)pyridine (4i)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 3/1/1). Yellow solid (143.6 mg, 63%). m.p. 174 – 177 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.49 (s, 2H), 7.51 (d, *J* = 7.8 Hz, 4H), 7.43 (d, *J* = 7.8 Hz, 2H), 7.39 – 7.32 (m, 6H), 7.27 (t, *J* = 7.2 Hz,2H), 7.21 (t, *J* = 7.2 Hz, 1H), 7.07 – 7.02 (m, 6H), 2.14 (s, 3H), 0.82 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 157.7, 149.5, 148.3, 147.1, 136.0, 135.2, 135.1, 134.1, 129.4, 128.5, 128.1, 127.9, 127.8, 126.5, 123.9, 52.4, 29.6, -3.4. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{33}H_{30}NSi$ ($[M + H]^+$): 456.2134; found: 456.2137.



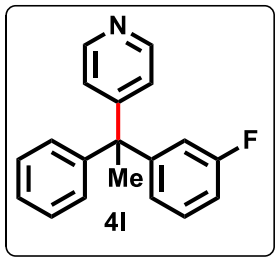
4-(1-(3-((3-methylbut-2-en-1-yl)oxy)phenyl)-1-phenylethyl)pyridine (4j)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 3/1/1). Yellow oil (80.9mg, 47%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.51 (s, 2H), 7.30 – 7.25 (m, 2H), 7.25 – 7.17 (m, 2H), 7.07 (d, *J* = 7.2 Hz, 2H), 7.04 (d, *J* = 4.8 Hz, 2H), 6.79 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.66 – 6.63 (m, 2H), 5.42 (t, *J* = 6.6 Hz, 1H), 4.42 (d, *J* = 7.2 Hz, 2H), 2.14 (s, 3H), 1.76 (s, 3H), 1.68 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 158.6, 157.9, 149.5, 148.9, 147.1, 138.2, 129.0, 128.5, 128.1, 126.5, 123.9, 121.0, 119.6, 116.0, 111.9, 64.6, 52.4, 29.7, 25.8, 18.1.Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{24}H_{26}NO$ ($[M + H]^+$): 344.1942; found: 344.1950.



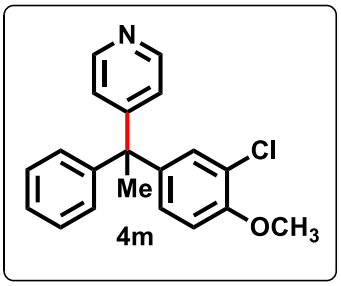
4-(1-([1,1'-biphenyl]-4-yl)-1-phenylethyl)pyridine (4k)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 3/1/1). Yellow solid (151.2 mg, 91%). m.p. 141 – 143 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.51 (s, 2H), 7.57 (d, *J* = 7.8 Hz, 2H), 7.51 (d, *J* = 8.4 Hz, 2H), 7.41 (t, *J* = 7.2 Hz, 2H), 7.33 – 7.24 (m, 4H), 7.12 (dd, *J* = 15.0, 7.8 Hz, 4H), 7.06 (d, *J* = 5.4 Hz, 2H), 2.18 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 157.8, 149.5, 147.1, 146.3, 140.4, 139.2, 128.9, 128.7, 128.6, 128.1, 127.3, 126.9, 126.7, 126.5, 123.8, 52.1, 29.7. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{25}H_{22}N$ ($[M + H]^+$): 336.1741; found: 3361747.



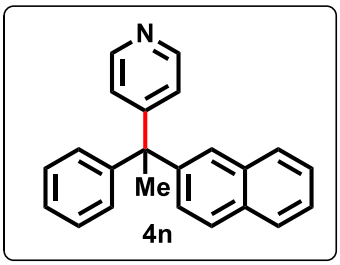
4-(1-(3-fluorophenyl)-1-phenylethyl)pyridine (4l)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 3/1/1). Yellow oil (63.5 mg, 45%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.52 (d, *J* = 4.8 Hz, 2H), 7.32 – 7.30 (m, 2H), 7.27 – 7.24 (m, 2H), 7.07 – 7.05 (m, 2H), 7.02 – 7.01 (m, 2H), 6.97 – 6.93 (m, 1H), 6.85 (d, *J* = 7.8 Hz, 1H), 6.78 (dt, *J* = 10.8, 2.4 Hz, 1H), 2.16 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 162.7 (d, *J* = 203.4 Hz), 157.2, 150.0, 149.7, 146.6, 129.5 (d, *J* =8.2 Hz), 128.4, 128.3, 126.7, 124.3 (d, *J* = 2.7 Hz), 123.7, 115.7 (d, *J* = 21.0 Hz), 113.3 (d, *J* = 20.9 Hz), 52.3, 29.7. Mass Spectrometry:**HRMS** (ESI-TOF) (m/z): Calcd for $C_{19}H_{17}FN$ ($[M + H]^+$): 278.1340; found: 278.1346.



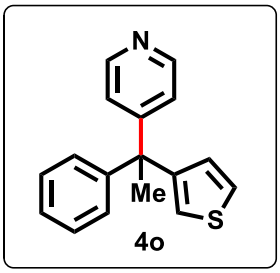
4-(1-(3-chloro-4-methoxyphenyl)-1-phenylethyl)pyridine (4m)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 3/1/1). Yellow oil (145.8 mg, 90%). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.79 (s, 2H), 7.29 (t, *J* = 7.2 Hz, 2H), 7.26 – 7.23 (m, 2H), 7.14 – 7.11 (m, 2H), 7.05 (d, *J* = 7.8 Hz,2H), 6.88 (dd, *J* = 8.4, 1.8 Hz, 1H), 6.83 (d, *J* = 8.4 Hz, 1H), 3.88 (s, 1H), 2.13 (s, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 157.4, 153.5, 149.3, 146.8, 140.4, 130.2, 128.3, 128.2, 127.9, 126.6, 122.2, 111.4, 56.1, 51.7, 29.7. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{20}H_{19}ClNO$ ($[M + H]^+$): 324.1138; found: 324.1150.



4-(1-(naphthalen-2-yl)-1-phenylethyl)pyridine (4n)

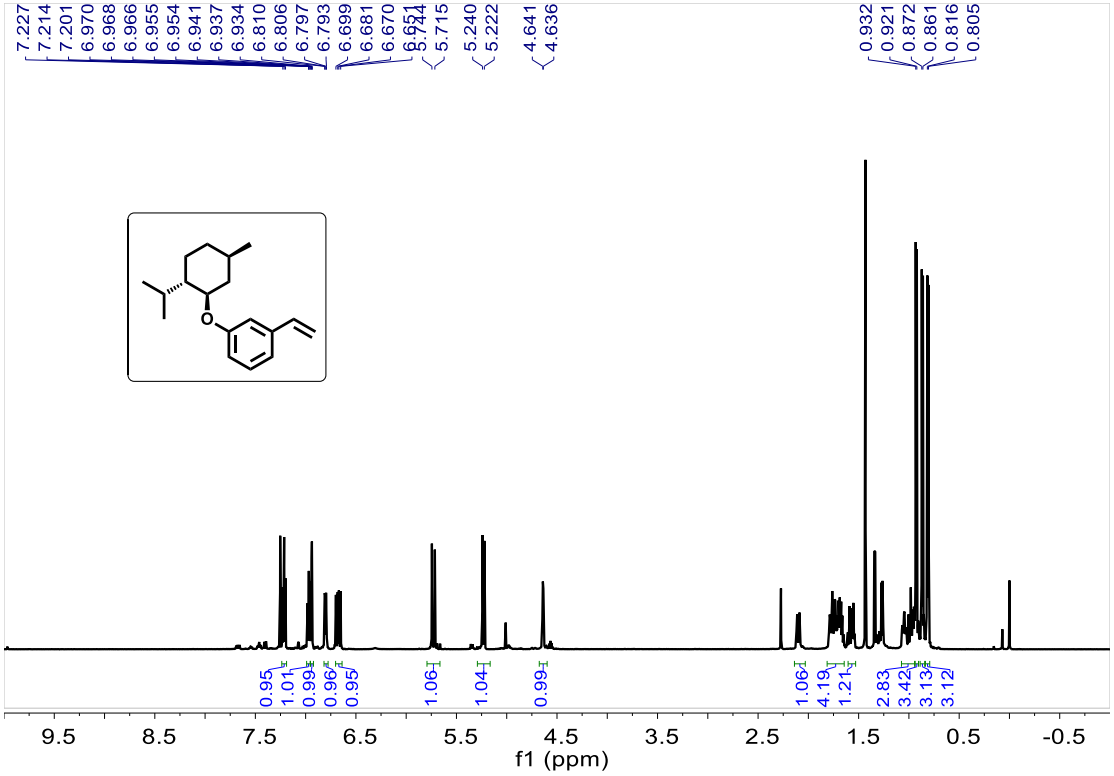
Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 3/1/1). Yellow solid (130.2 mg, 84%). m.p. 96 – 97 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.51 (d, *J* = 5.4 Hz, 2H), 7.79 (d, *J* = 7.8 Hz, 1H), 7.74 (d, *J* = 8.4 Hz, 1H), 7.67 (d, *J* = 8.4 Hz, 1H), 7.46 – 7.41 (m, 3H), 7.30 – 7.24 (m, 4H), 7.11 (d, *J* = 7.8 Hz, 2H), 7.07 (d, *J* = 5.4 Hz, 2H), 2.24 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 157.6, 149.6, 147.0, 144.6, 132.9, 131.9, 128.6, 128.2, 128.1, 127.7, 127.3, 127.0, 126.8, 126.5, 126.1, 126.0, 123.9, 52.5, 29.7. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{23}H_{20}N$ ($[M + H]^+$): 310.1588; found: 310.1590.

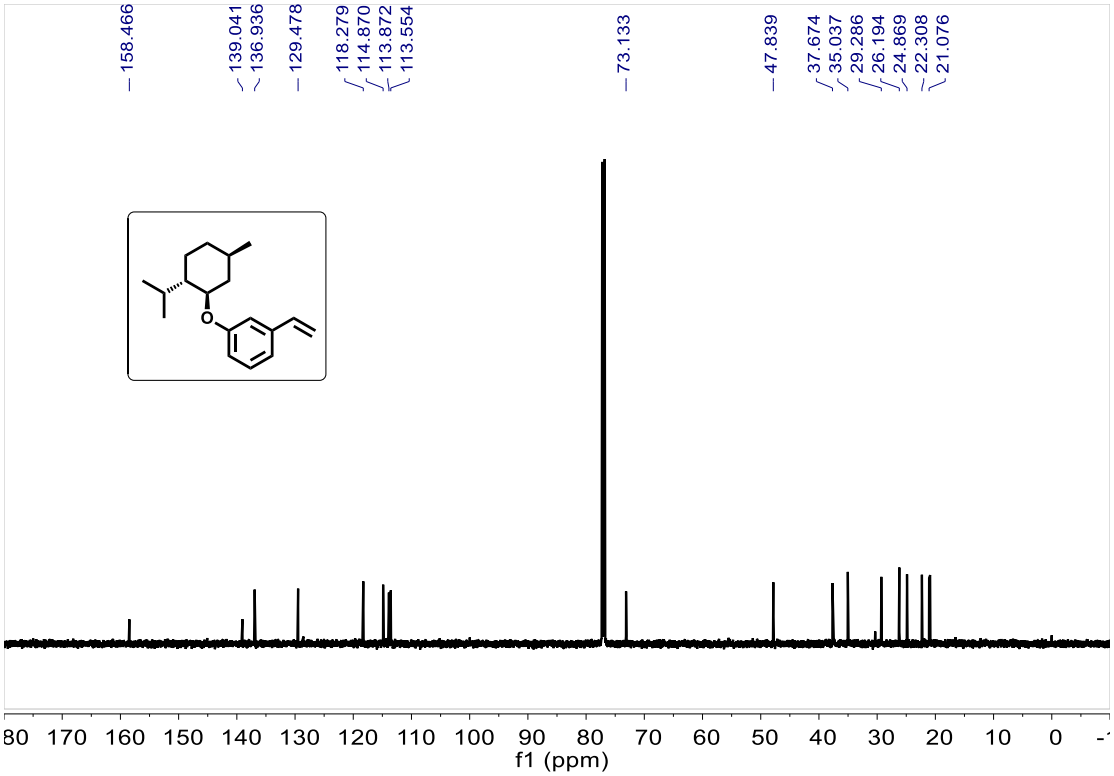


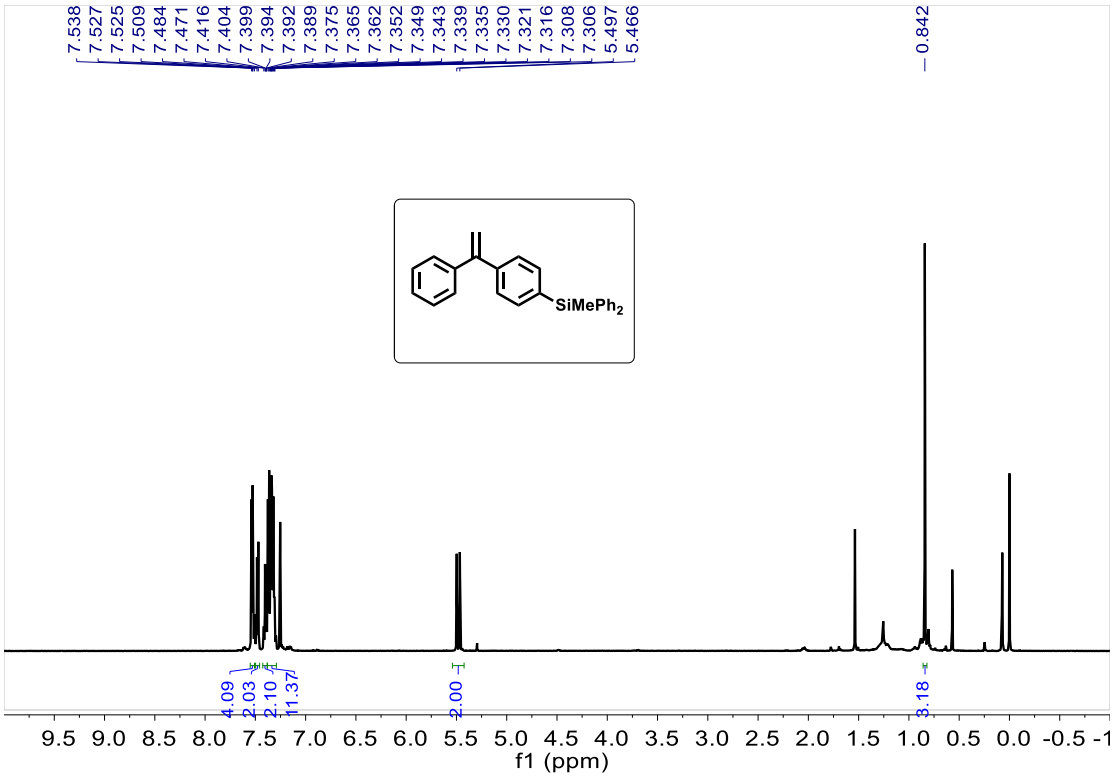
4-(1-phenyl-1-(thiophen-3-yl)ethyl)pyridine (4o)

Purified by flash column chromatography (eluent: petroleum/EtOAc/Et_3N = 3/1/1). Yellow solid (103.6 mg, 78%). m.p. 87 – 90 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.50 (d, *J* = 5.4 Hz, 2H), 7.30 – 7.27 (m, 3H), 7.23 (t, *J* = 7.2 Hz, 1H), 7.09 (d, *J* = 7.8 Hz, 2H), 7.04 (d, *J* = 5.4 Hz, 2H), 6.85 (d, *J* = 5.4 Hz, 1H), 6.70 (d, *J* = 7.8 Hz, 1H), 2.12 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 157.6, 149.6, 148.3, 147.0, 128.1, 128.0, 126.6, 125.6, 123.3, 122.4,50.0, 29.4. Mass Spectrometry: **HRMS** (ESI-TOF) (m/z): Calcd for $C_{17}H_{16}NS$ ($[M + H]^+$): 266.0998; found: 266.1007.

8. ^{1}H, ^{13}C and ^{19}F Spectra of New Compounds



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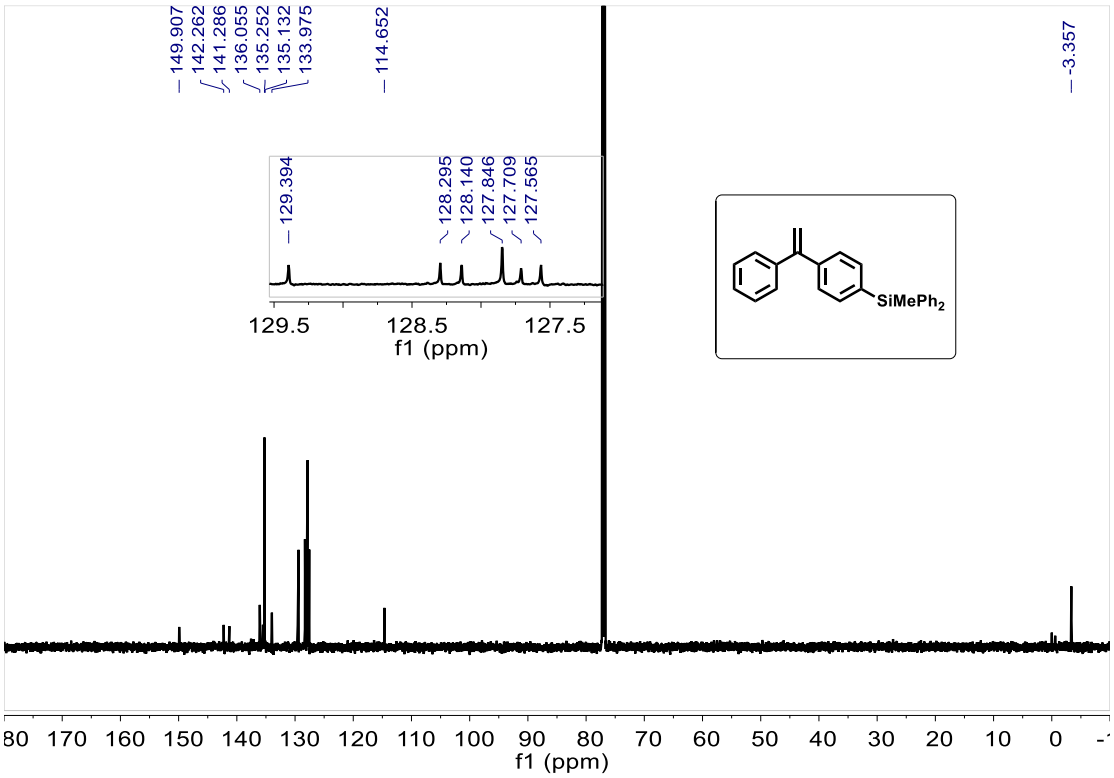
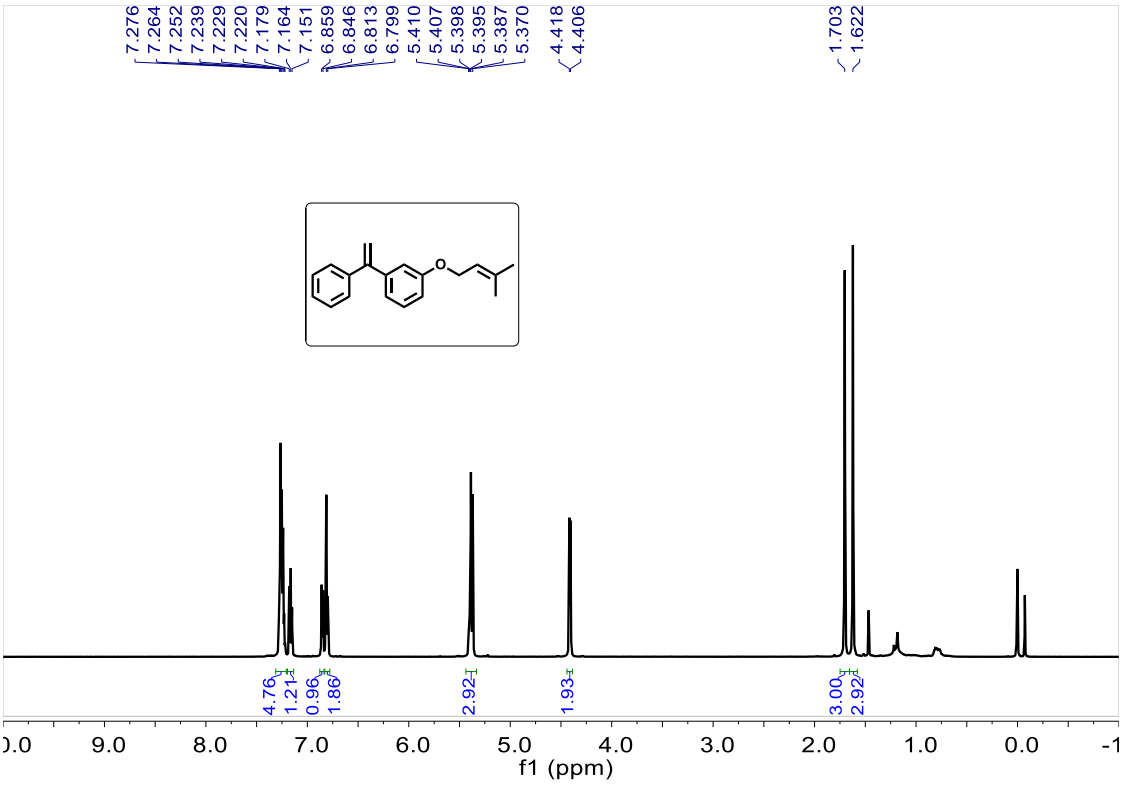
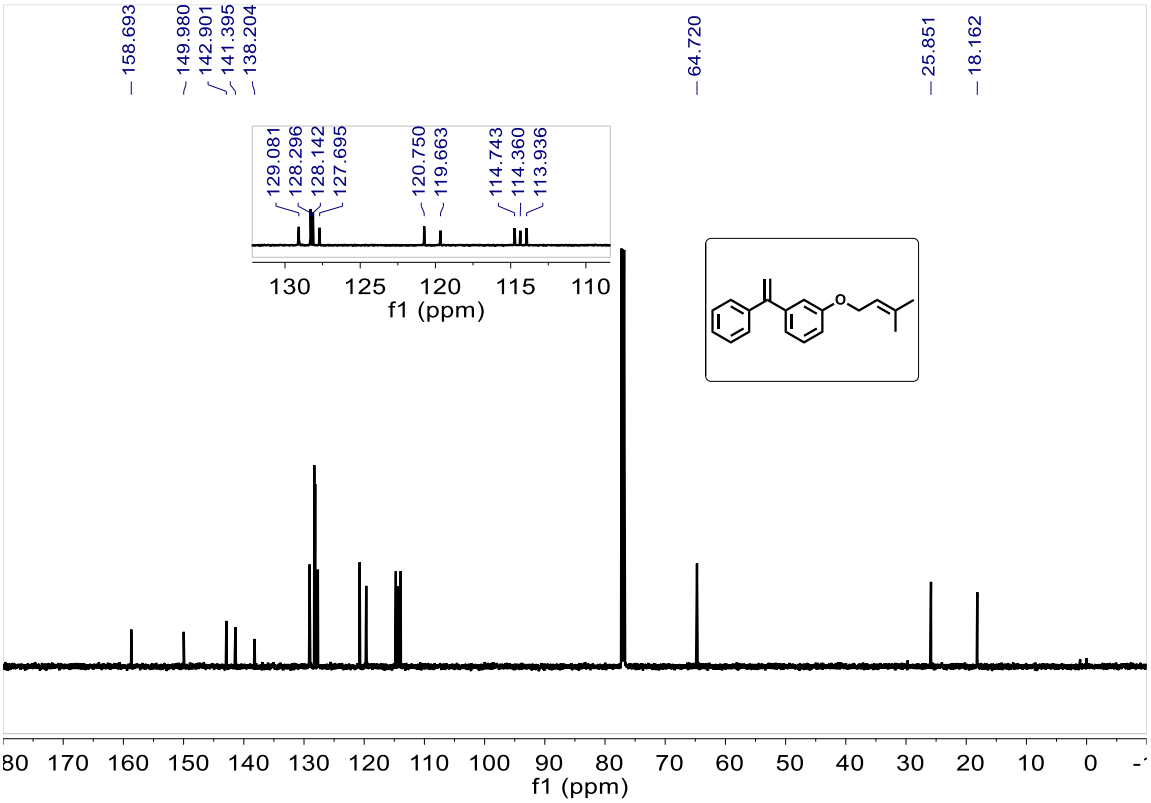
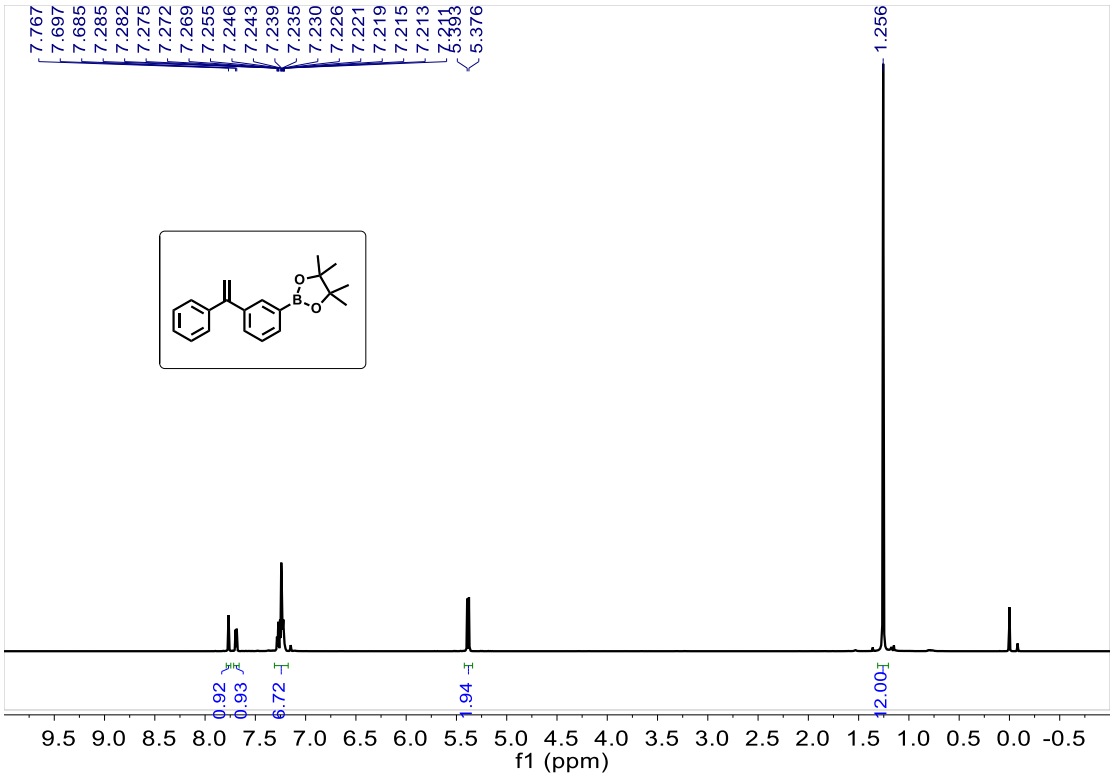
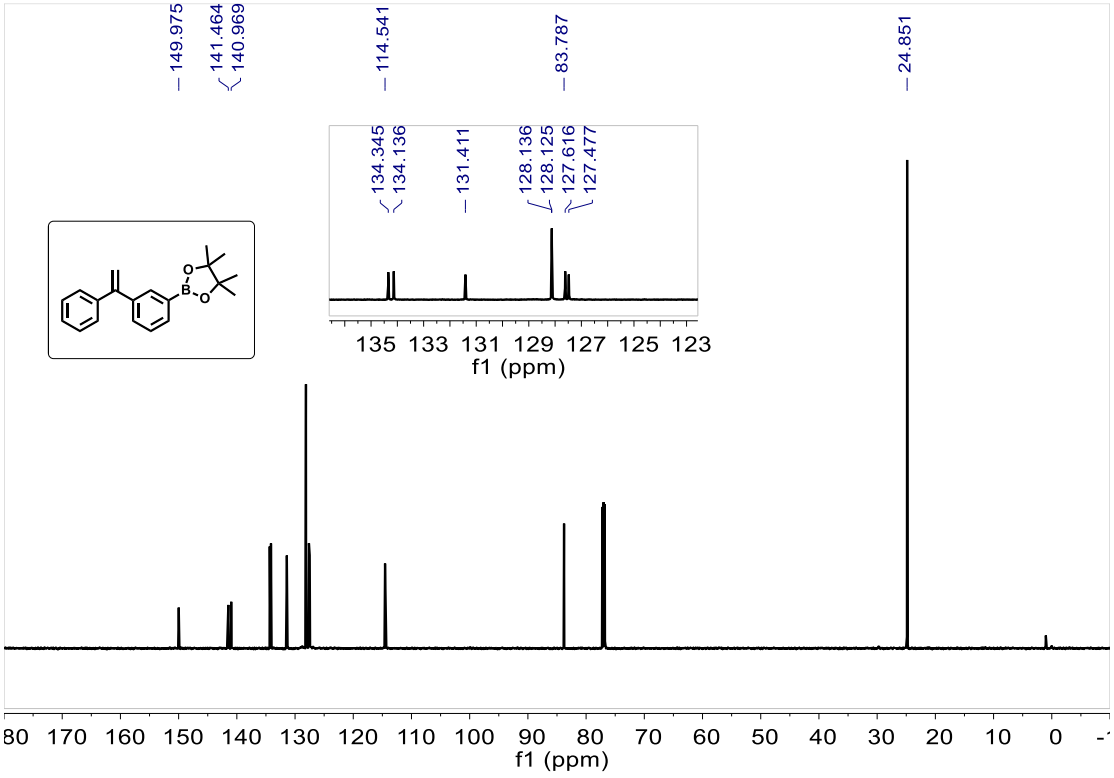
7.527
7.525
7.509
7.484
7.471
7.416
7.404
7.399
7.394
7.392
7.389
7.375
7.365
7.362
7.352
7.349
7.343
7.339
7.335
7.330
7.321
7.316
7.308
7.306
5.497
5.466
0.842
SiMePh2
4.09
2.03
2.10
11.37
2.00
3.18
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


149.907
142.262
141.286
136.055
135.252
135.132
133.975
114.652
-3.357
129.394
128.295
128.140
127.846
127.709
127.565
129.5
128.5
127.5
f1 (ppm)
SiMePh2
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.276
7.264
7.252
7.239
7.229
7.220
7.179
7.164
7.151
6.859
6.846
6.813
6.799
5.410
5.407
5.398
5.395
5.387
5.370
4.418
4.406
1.703
1.622
4.76
1.21
0.96
1.86
2.92
1.93
3.00
2.92
f1 (ppm)


158.693
149.980
142.901
141.395
138.204
64.720
25.851
18.162
129.081
128.296
128.142
127.695
120.750
119.663
114.743
114.360
113.936
f1 (ppm)
f1 (ppm)


7.767
7.697
7.685
7.285
7.282
7.275
7.272
7.269
7.255
7.246
7.243
7.239
7.235
7.230
7.226
7.221
7.219
7.215
7.213
5.393
5.376
1.256
0.92
0.93
6.72
1.94
12.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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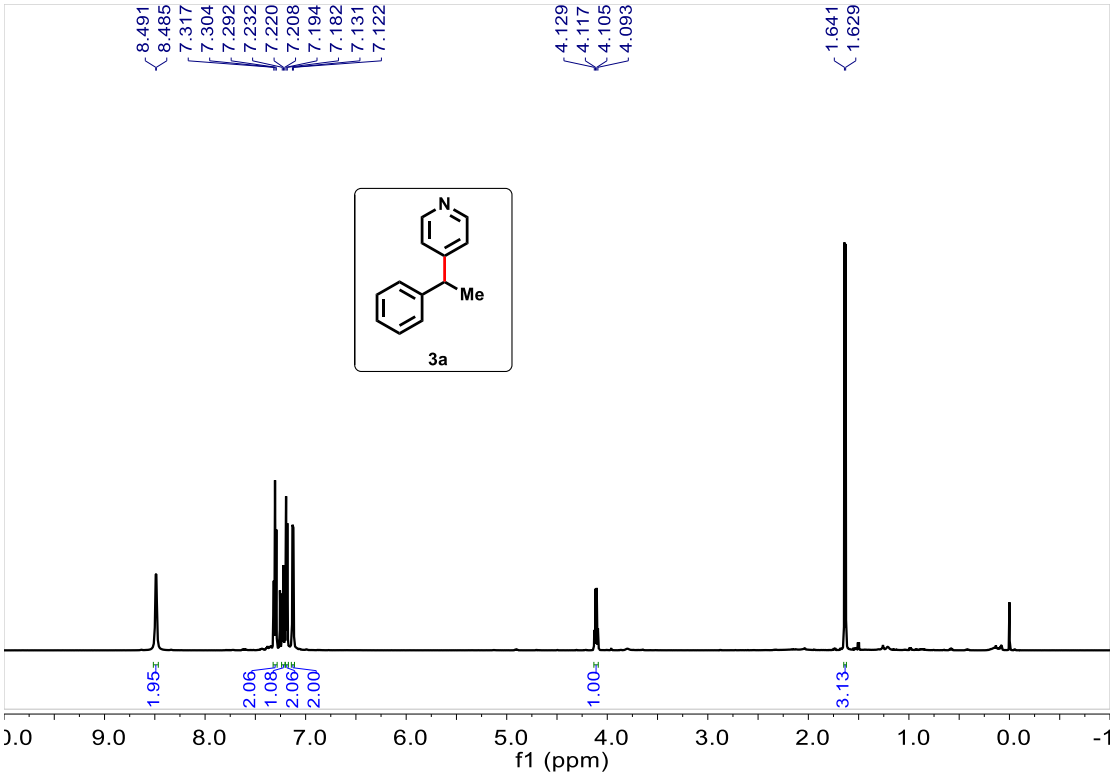
141.464
140.969
114.541
83.787
24.851
134.345
134.136
131.411
128.136
128.125
127.616
127.477
135 133 131 129 127 125 123
f1 (ppm)
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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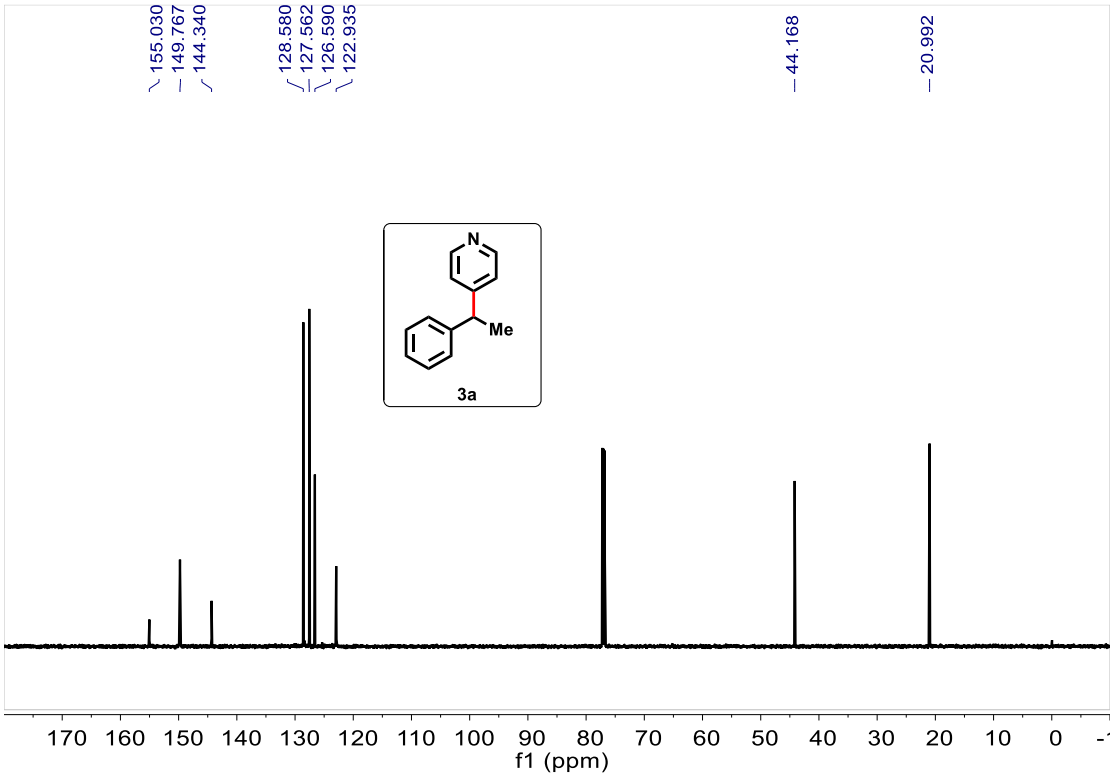
8.485
7.317
7.304
7.292
7.232
7.220
7.208
7.194
7.182
7.131
7.122
4.129
4.117
4.105
4.093
1.641
1.629
N
Me
3a
1.95
2.06
1.08
2.06
2.00
1.00
3.13
f1 (ppm)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144.340
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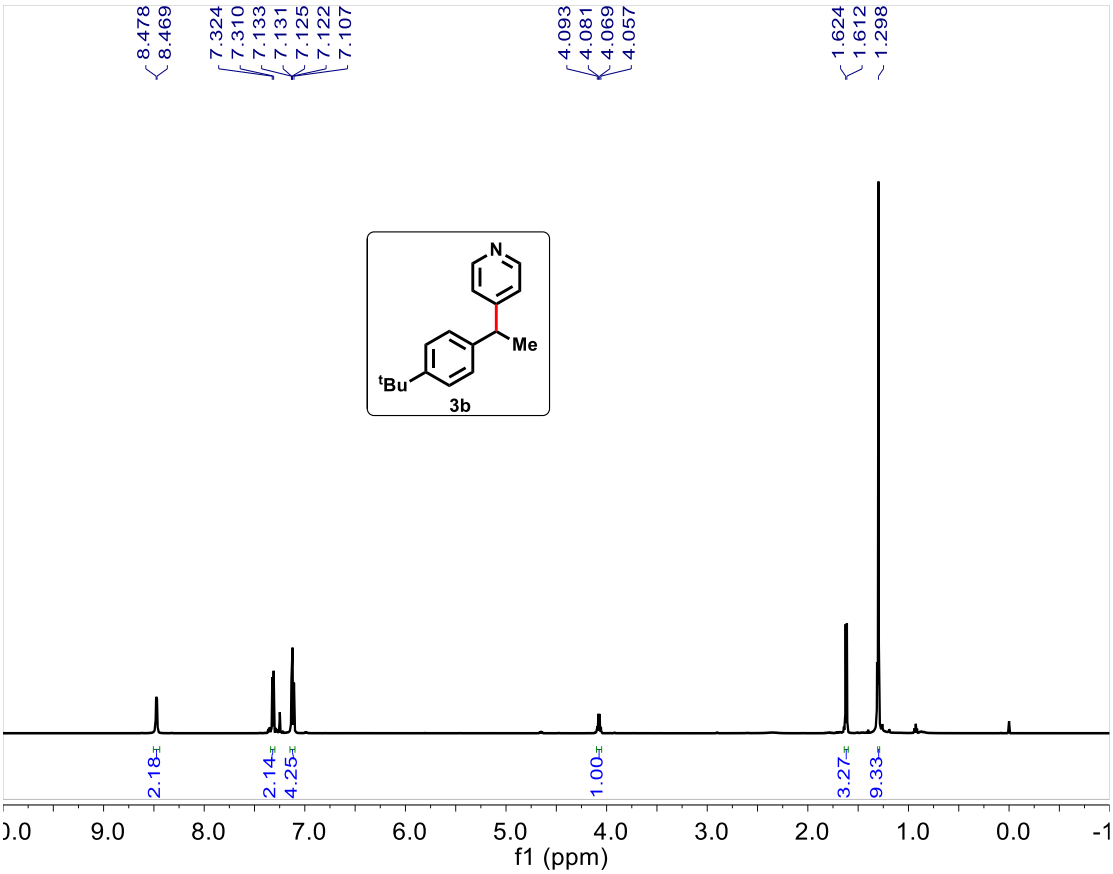
126.590
122.935
44.168
20.992
N
Me
3a
f1 (ppm)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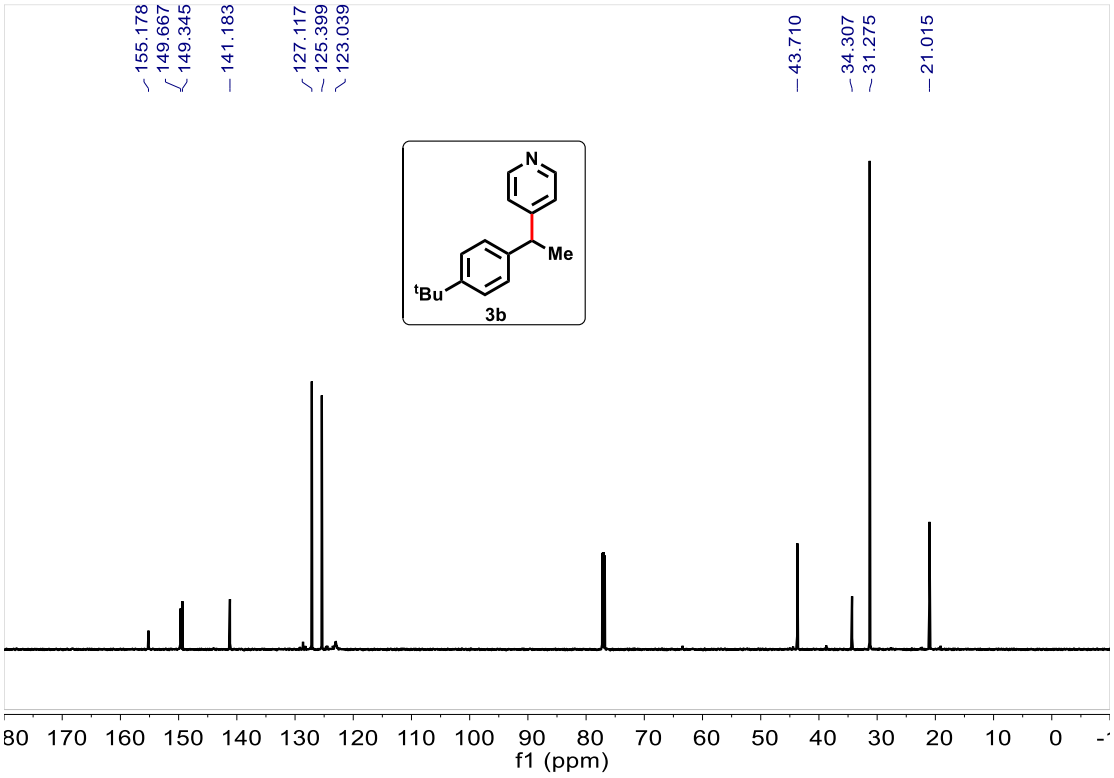
8.469
7.324
7.310
7.133
7.131
7.125
7.122
7.107
4.093
4.081
4.069
4.057
1.624
1.612
1.298
N
Me
tBu
3b
2.18
2.14
4.25
1.00
3.27
9.33
f1 (ppm)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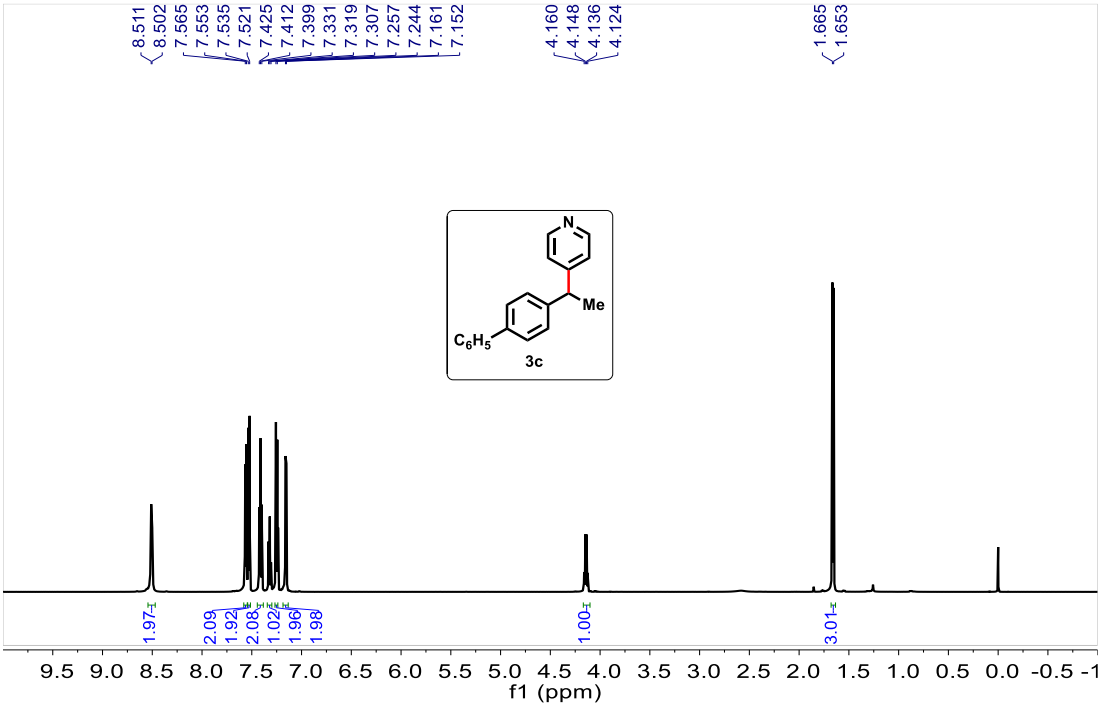
149.667
149.345
141.183
127.117
125.399
123.039
43.710
34.307
31.275
21.015
N
Me
tBu
3b
f1 (ppm)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8.502
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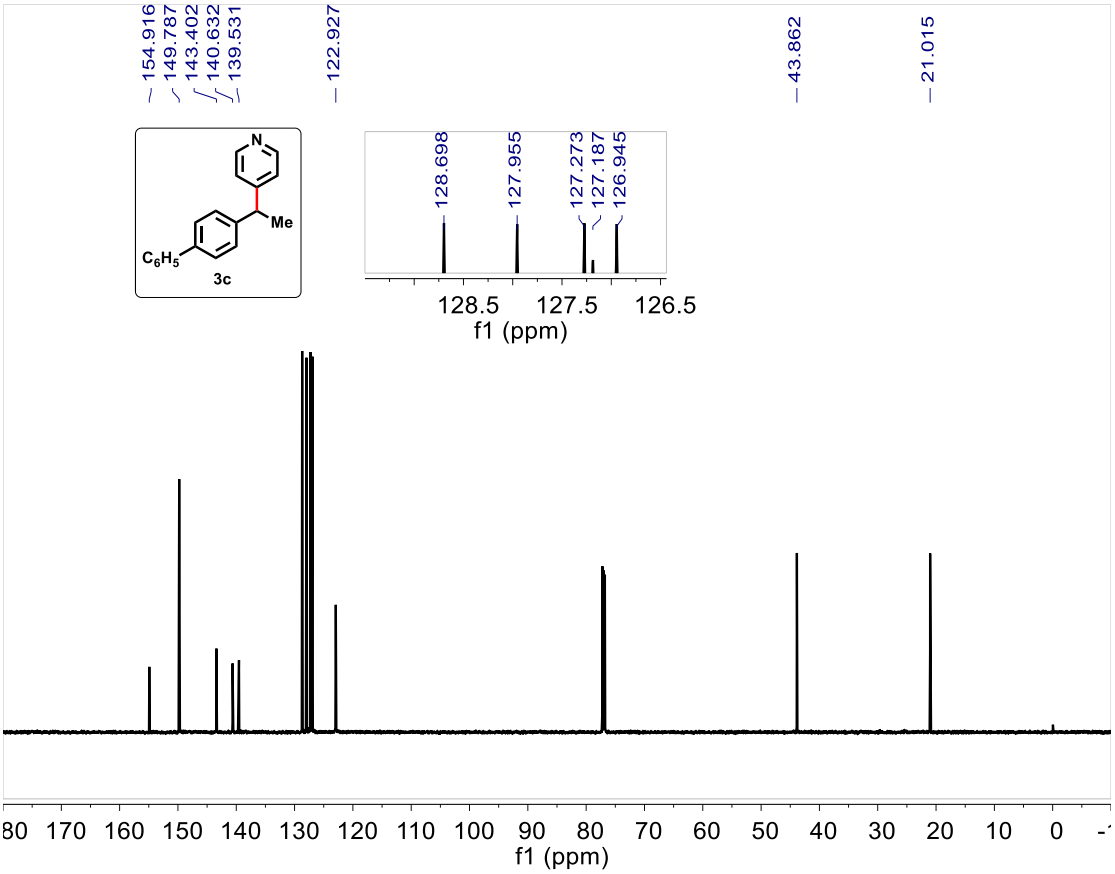
7.553
7.535
7.521
7.425
7.412
7.399
7.331
7.319
7.307
7.257
7.244
7.161
7.152
4.160
4.148
4.136
4.124
1.665
1.653
N
Me
C6H5
3c
1.97
2.09
1.92
2.08
1.02
1.96
1.98
1.00
3.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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143.402
140.632
139.531
122.927
43.862
21.015
N
Me
C6H5
3c
128.698
127.955
127.273
127.187
126.945
128.5 127.5 126.5
f1 (ppm)
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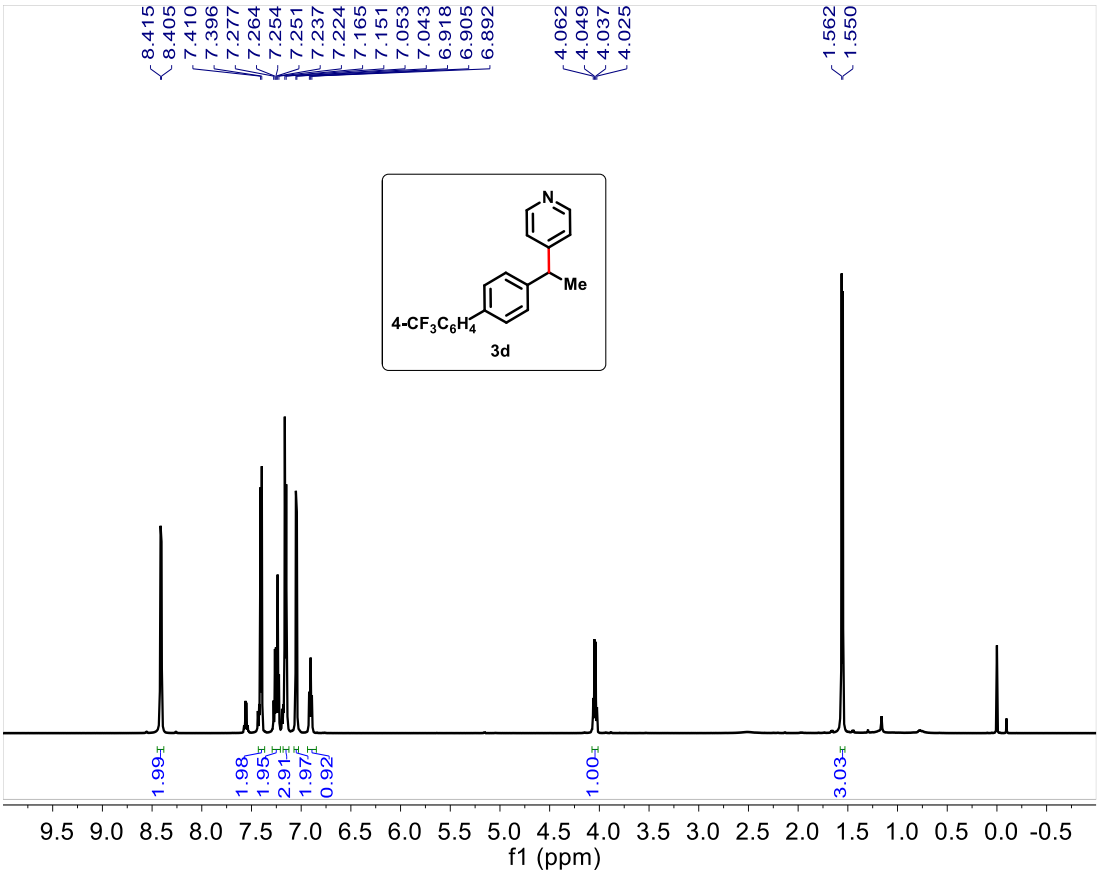
f1 (ppm)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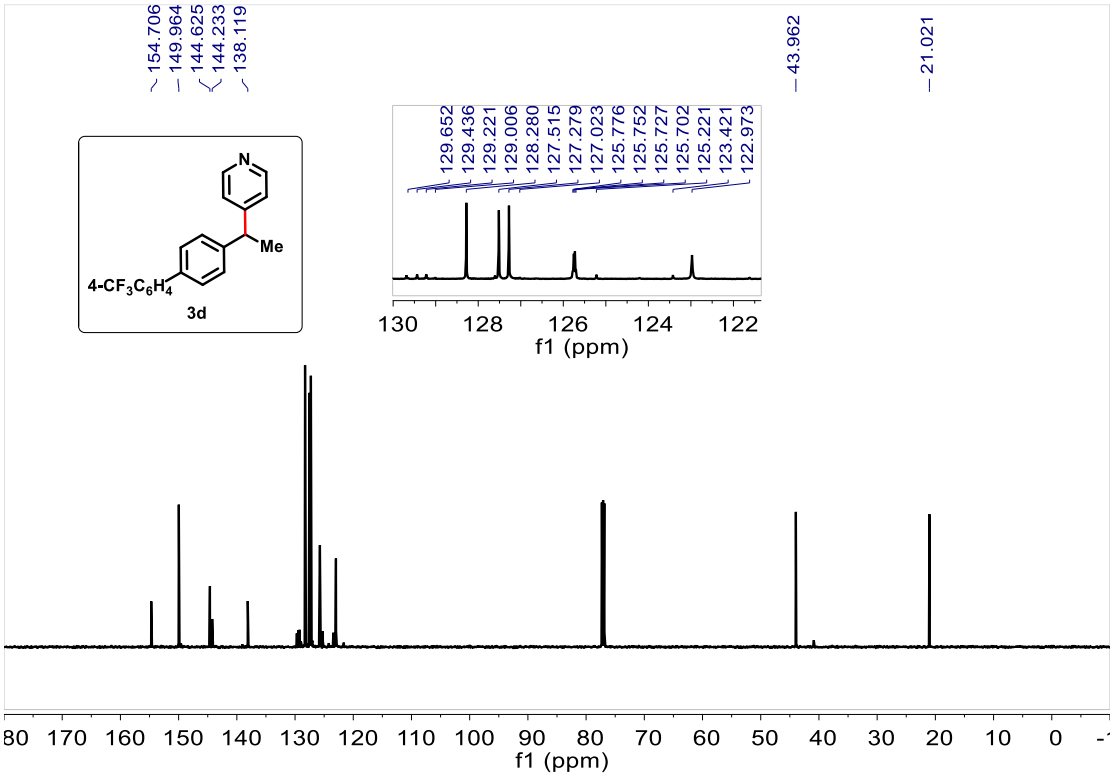
7.410
7.396
7.277
7.264
7.254
7.251
7.237
7.224
7.165
7.151
7.053
7.043
6.918
6.905
6.892
4.062
4.049
4.037
4.025
1.562
1.550
N
Me
4-CF3C6H4
3d
1.99
1.98
1.95
2.91
1.97
0.92
1.00
3.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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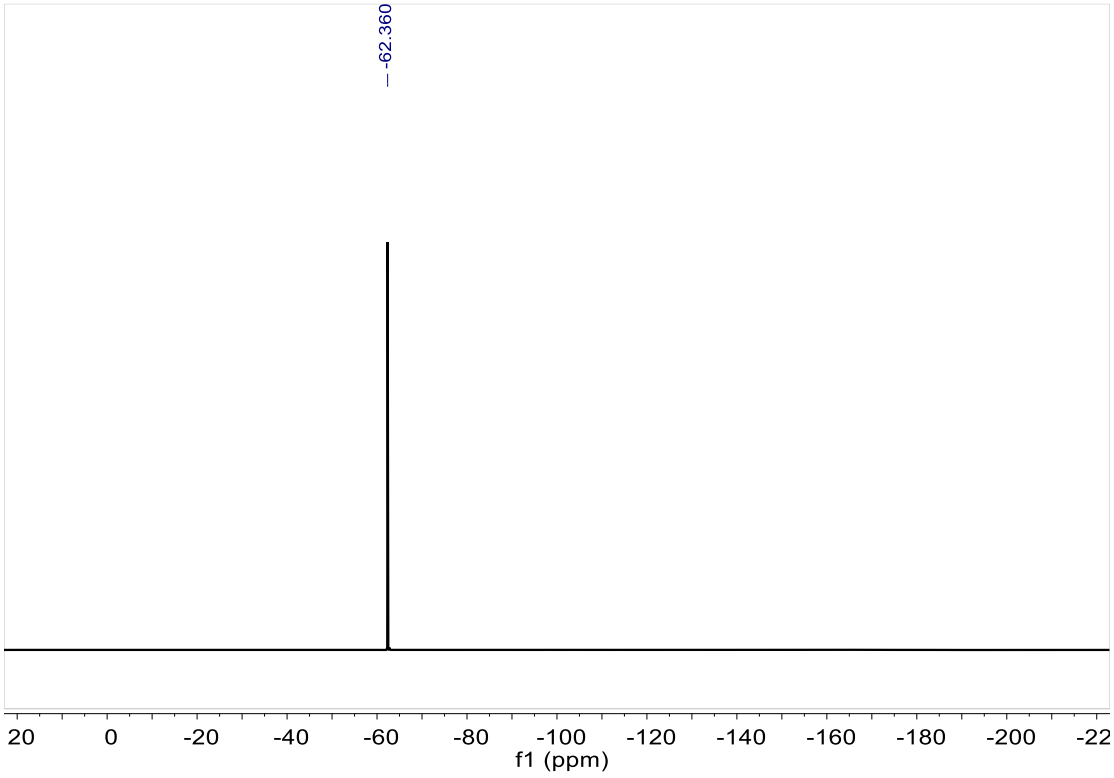
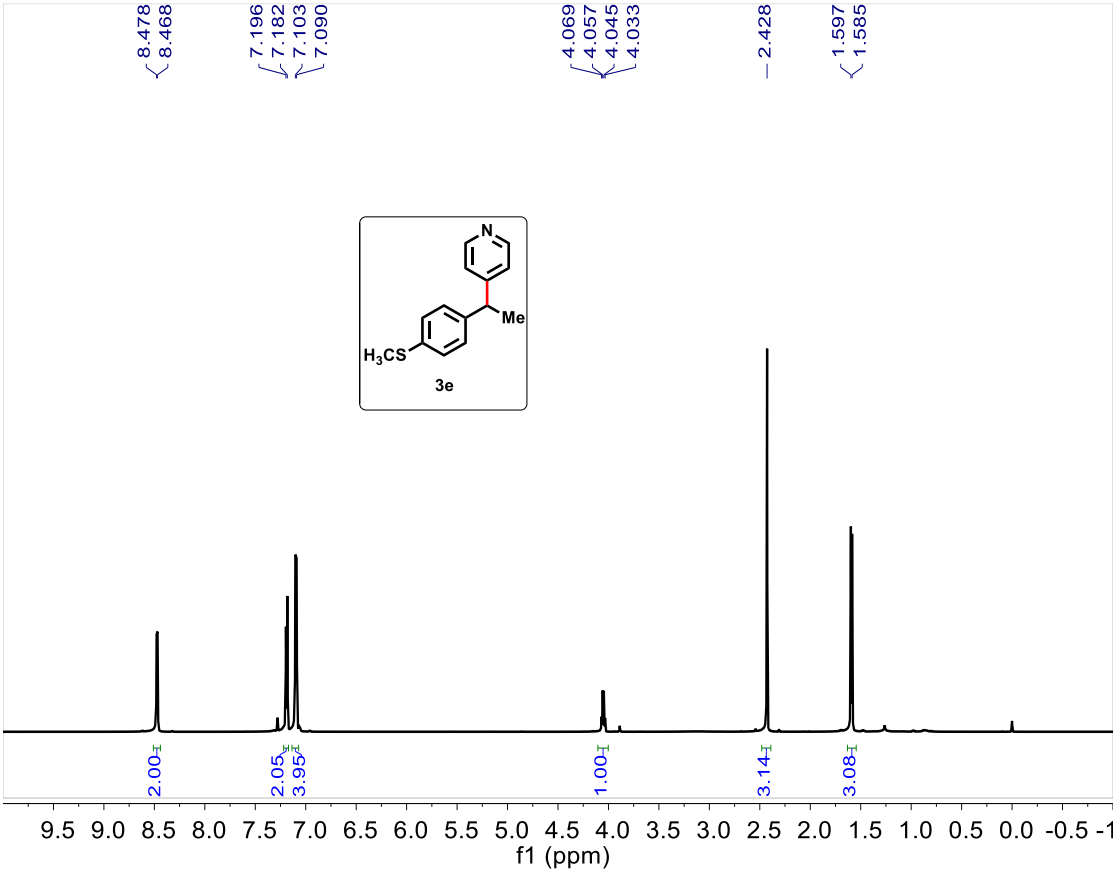
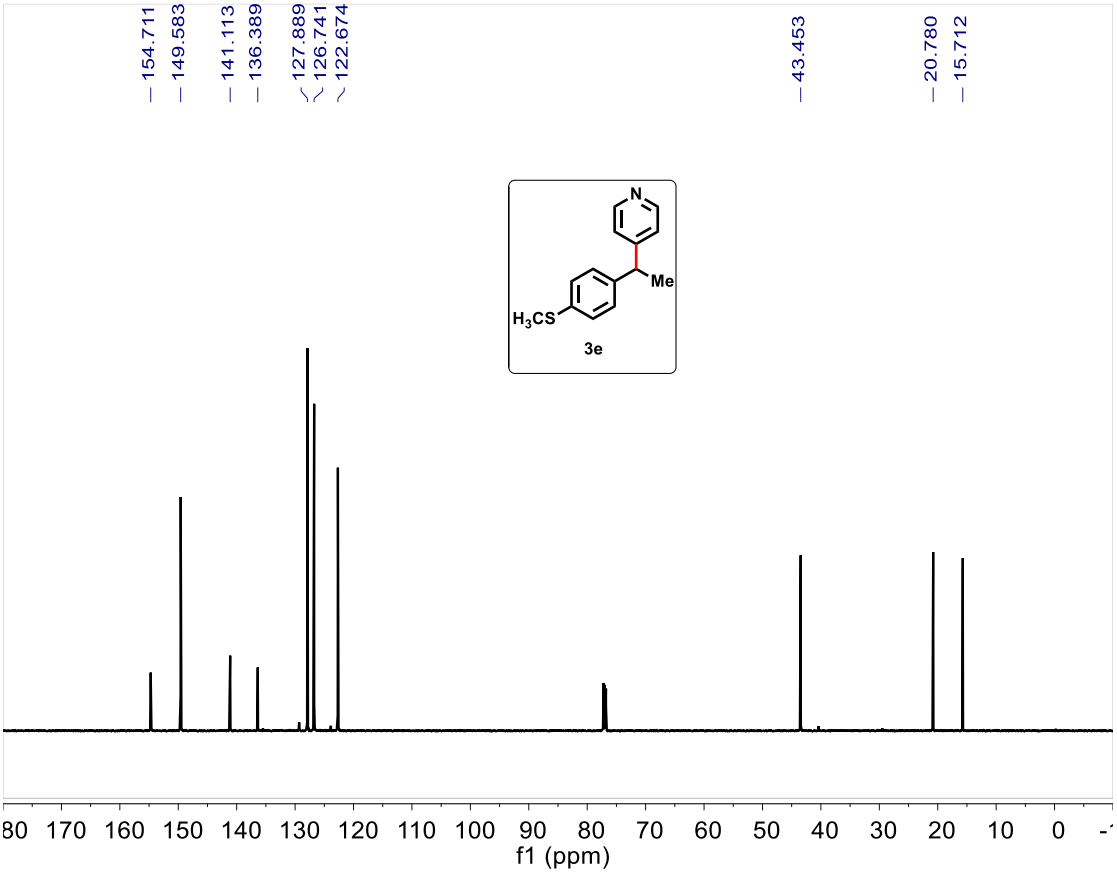
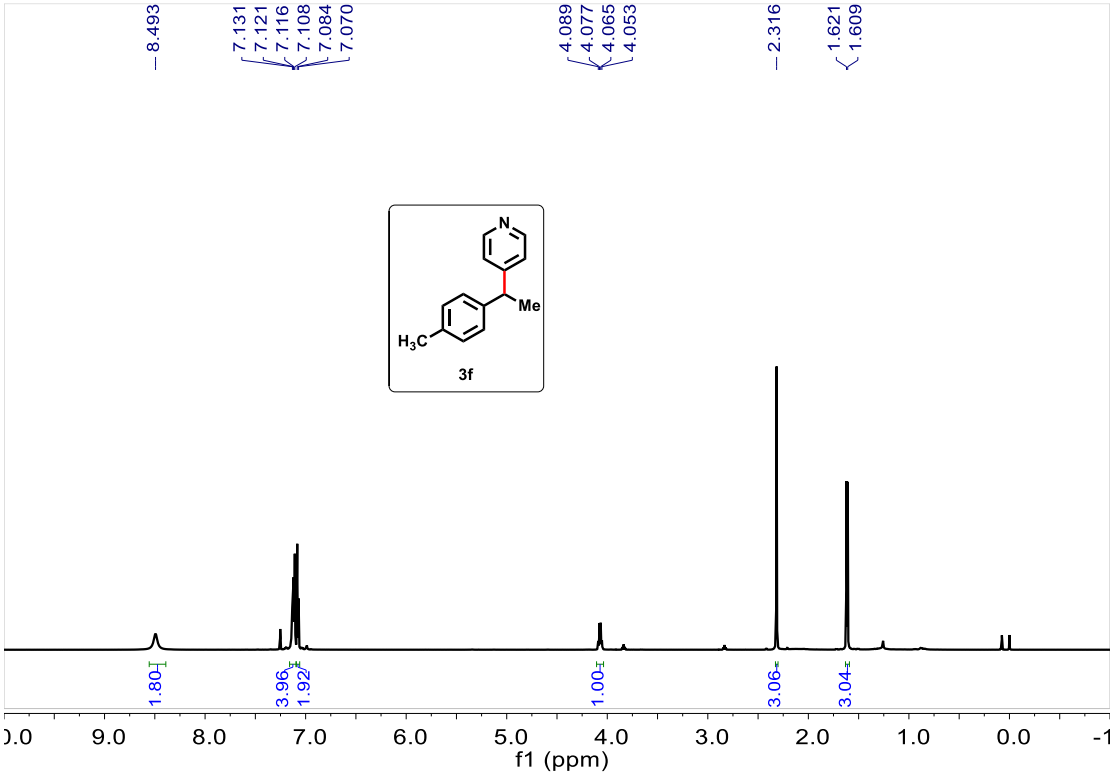
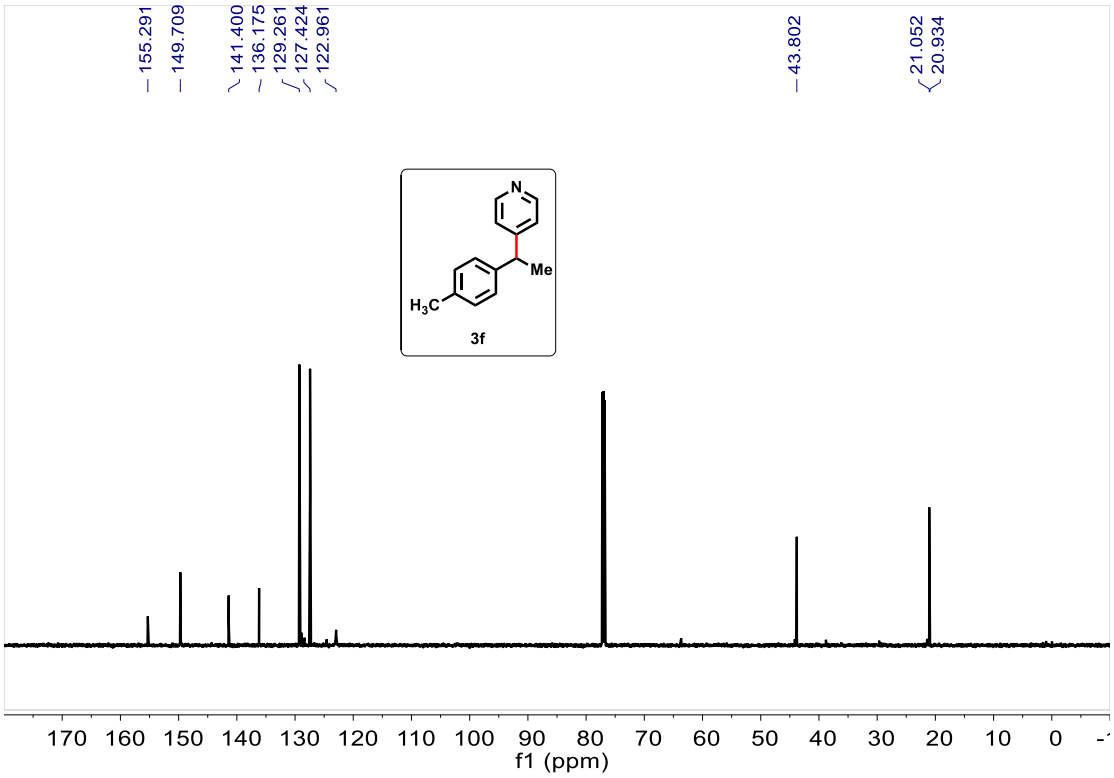
144.233
138.119
43.962
21.021
129.652
129.436
129.221
129.006
128.280
127.515
127.279
127.023
125.776
125.752
125.727
125.702
125.221
123.421
122.973
N
Me
4-CF3C6H4
3d
130 128 126 124 122
f1 (ppm)
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

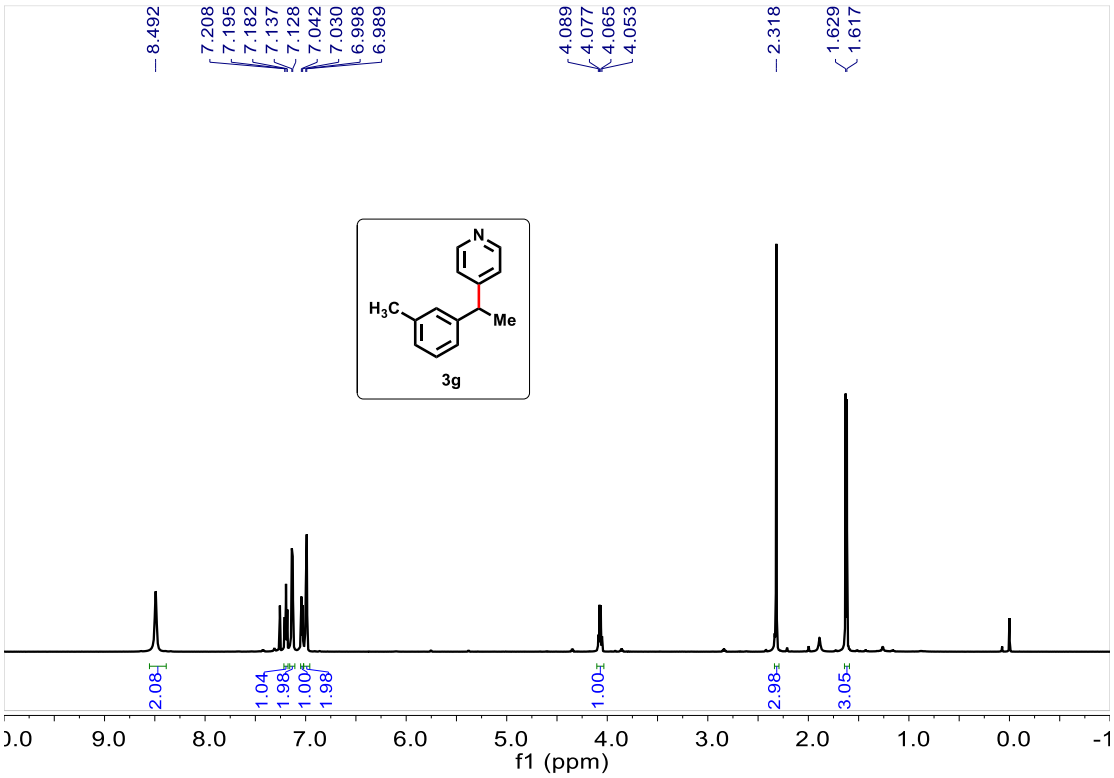

-62.360
20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -22
f1 (ppm)

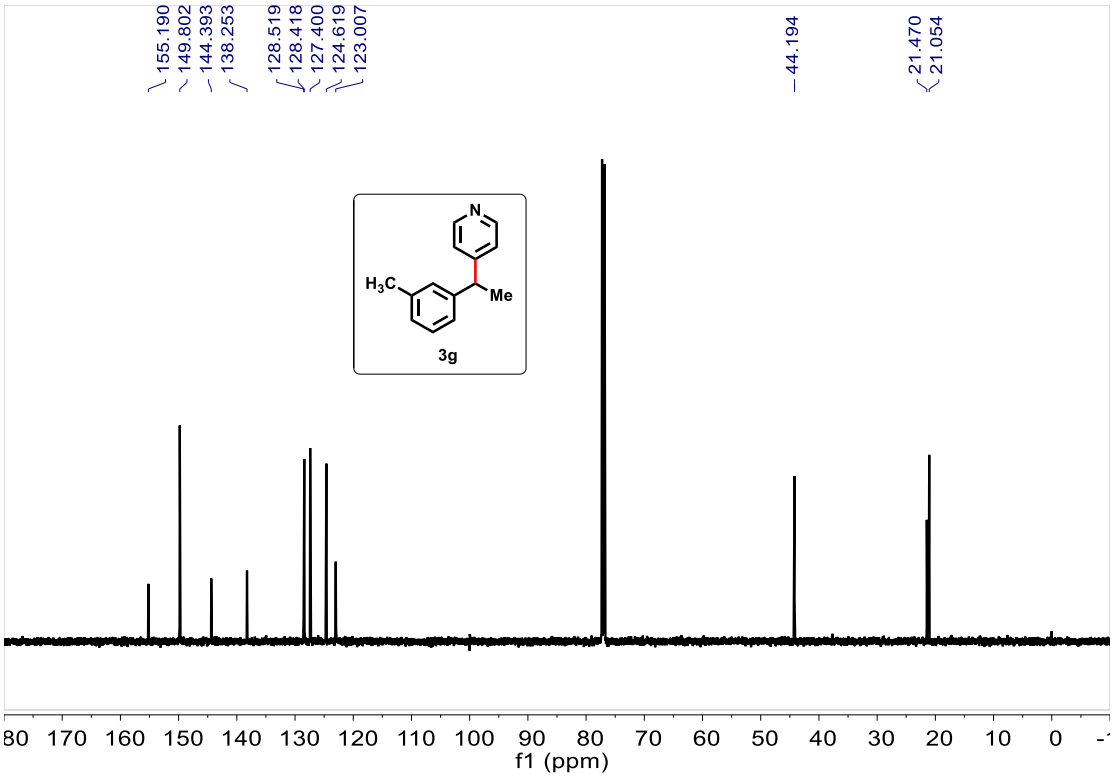

8.478
8.468
7.196
7.182
7.103
7.090
4.069
4.057
4.045
4.033
2.428
1.597
1.585
N
Me
H3CS
3e
2.00
2.05
3.95
1.00
3.14
3.08
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

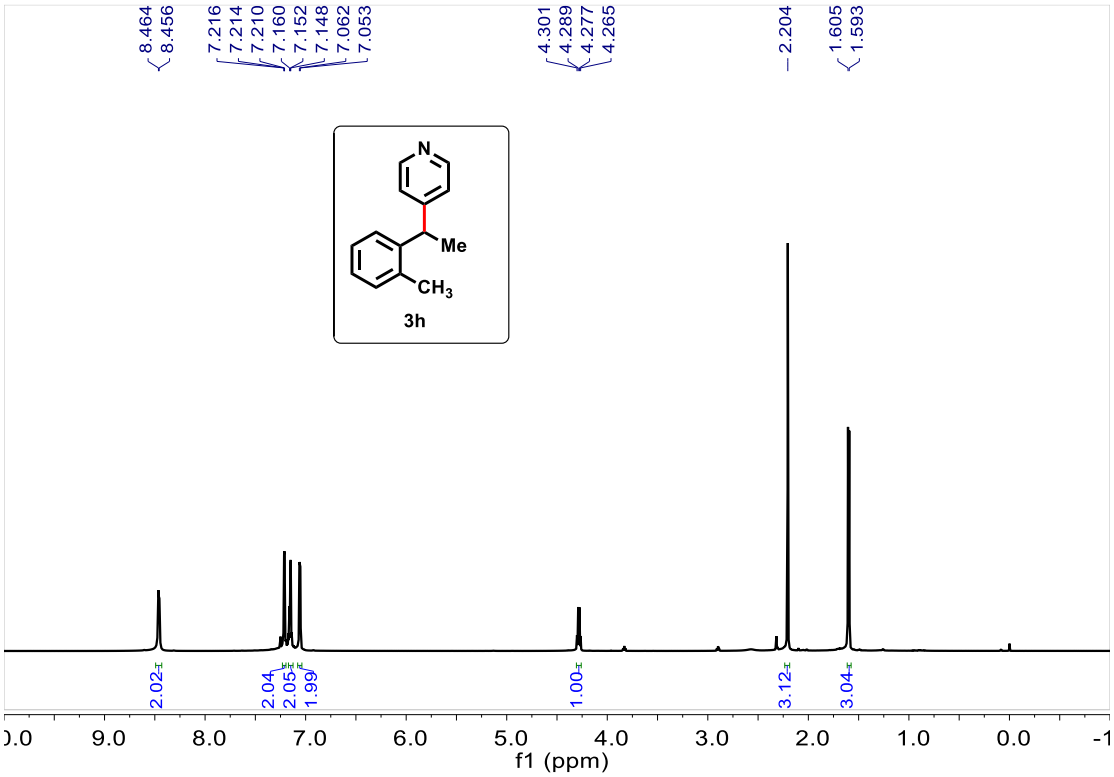

154.711
149.583
141.113
136.389
127.889
126.741
122.674
43.453
20.780
15.712
N
Me
H3CS
3e
f1 (ppm)

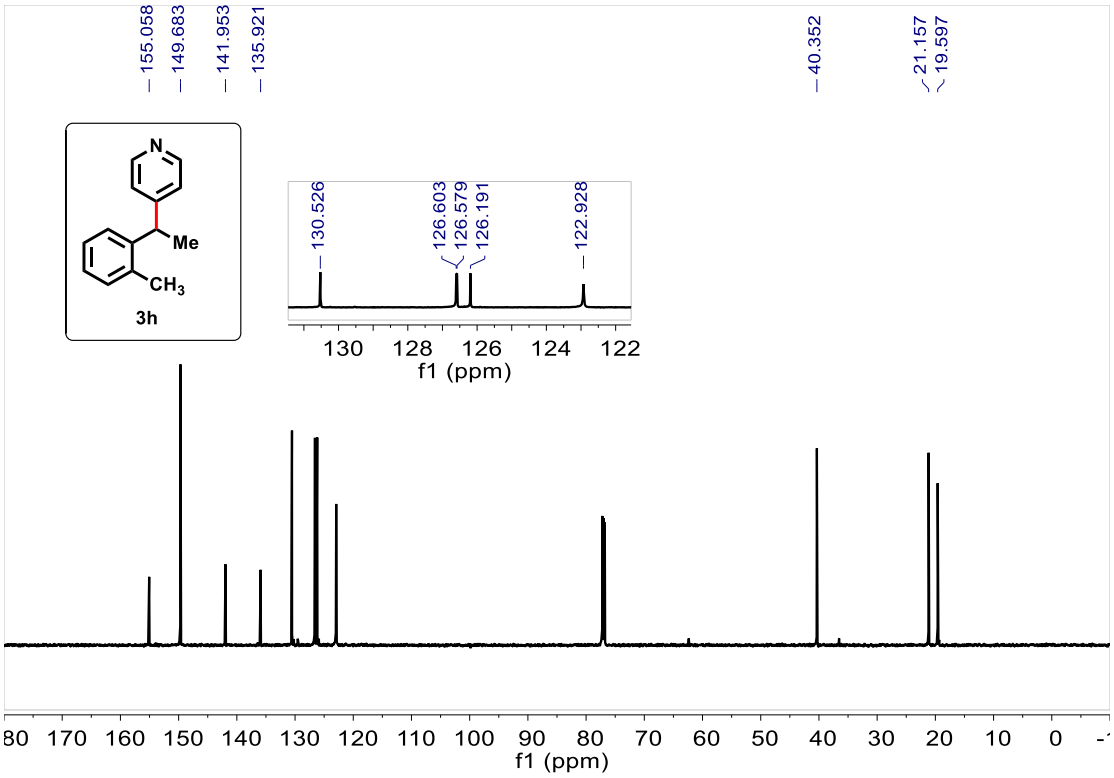

8.493
7.131
7.121
7.116
7.108
7.084
7.070
4.089
4.077
4.065
4.053
2.316
1.621
1.609
N
Me
H3C
3f
1.80
3.96
1.92
1.00
3.06
3.04
f1 (ppm)

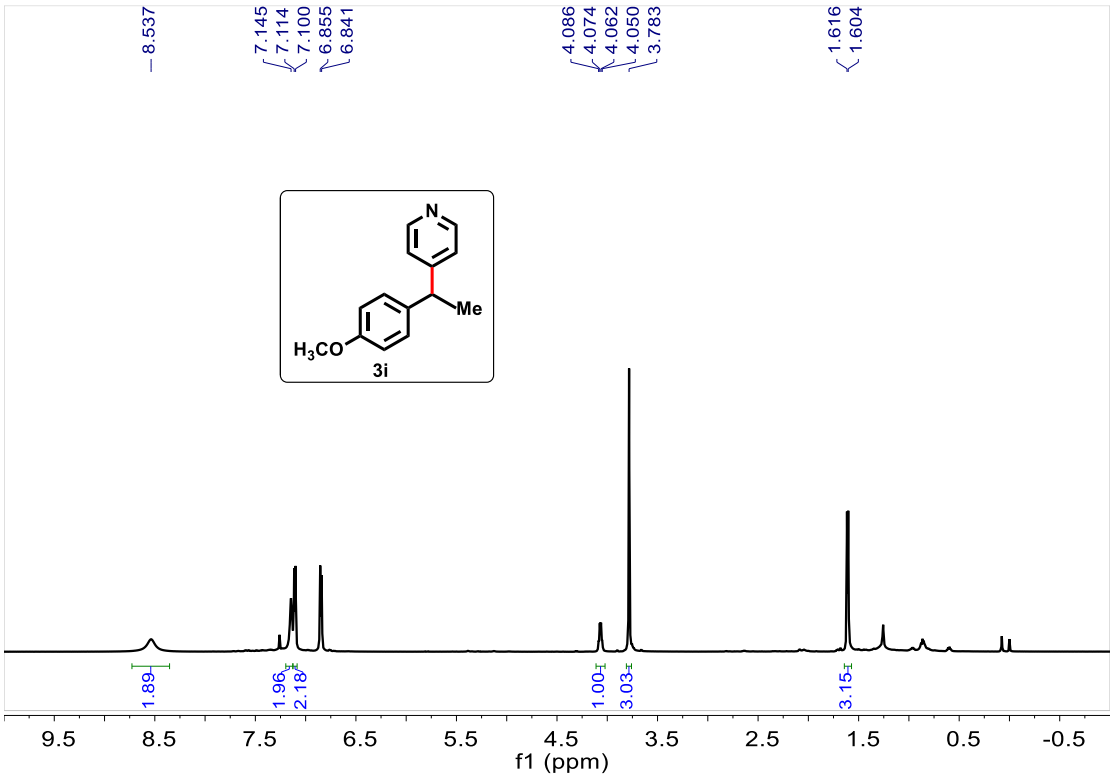

155.291
149.709
141.400
136.175
129.261
127.424
122.961
43.802
21.052
20.934
N
Me
H3C
3f
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

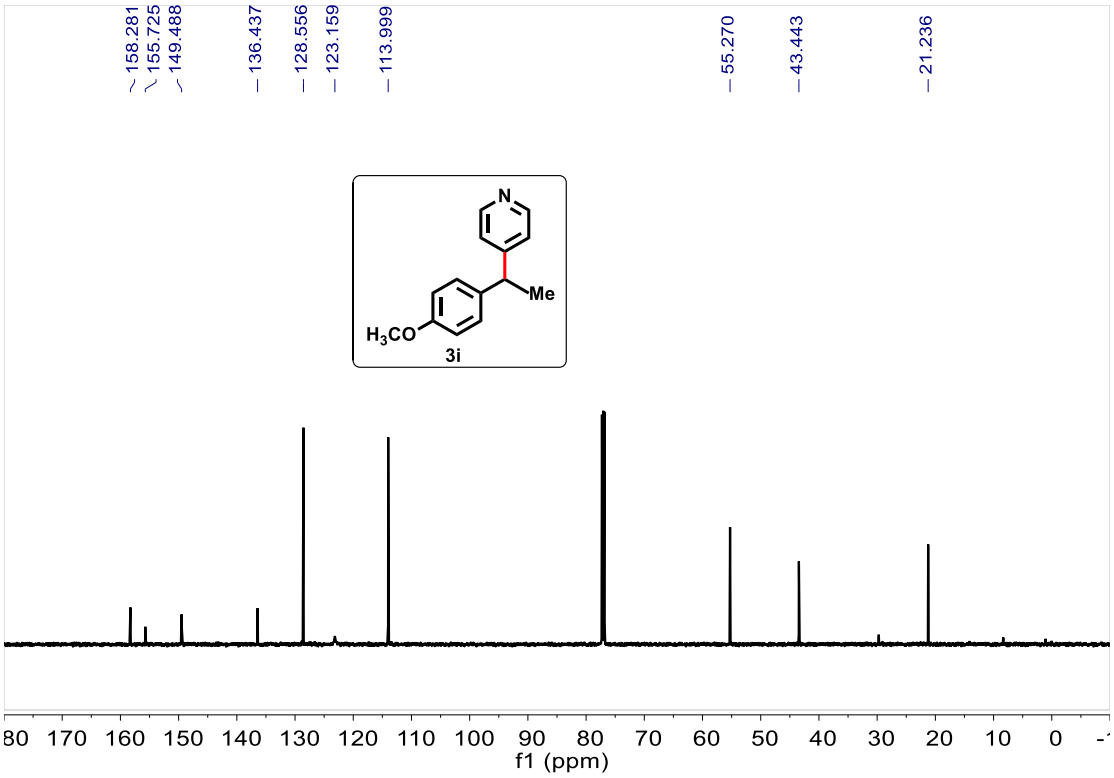

8.492
7.208
7.195
7.182
7.137
7.128
7.042
7.030
6.998
6.989
4.089
4.077
4.065
4.053
2.318
1.629
1.617
N
H3C
Me
3g
2.08
1.04
1.98
1.00
1.98
1.00
2.98
3.05
9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)

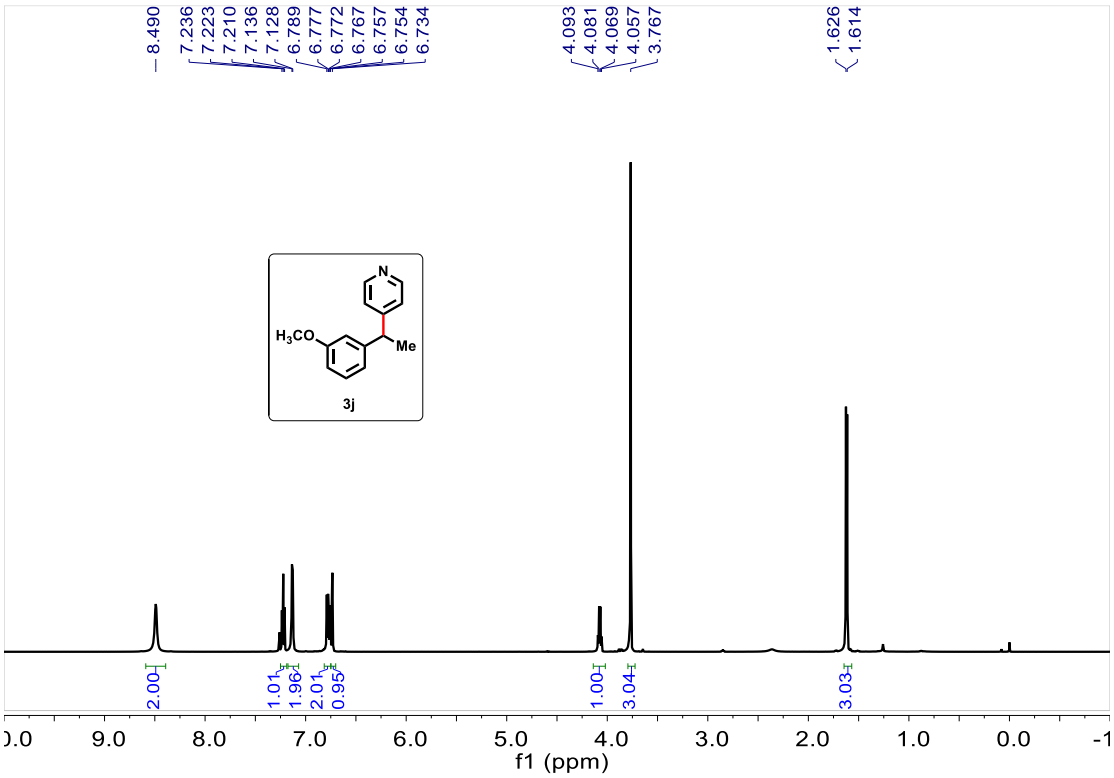

155.190
149.802
144.393
138.253
128.519
128.418
127.400
124.619
123.007
44.194
21.470
21.054
N
H3C
Me
3g
f1 (ppm)

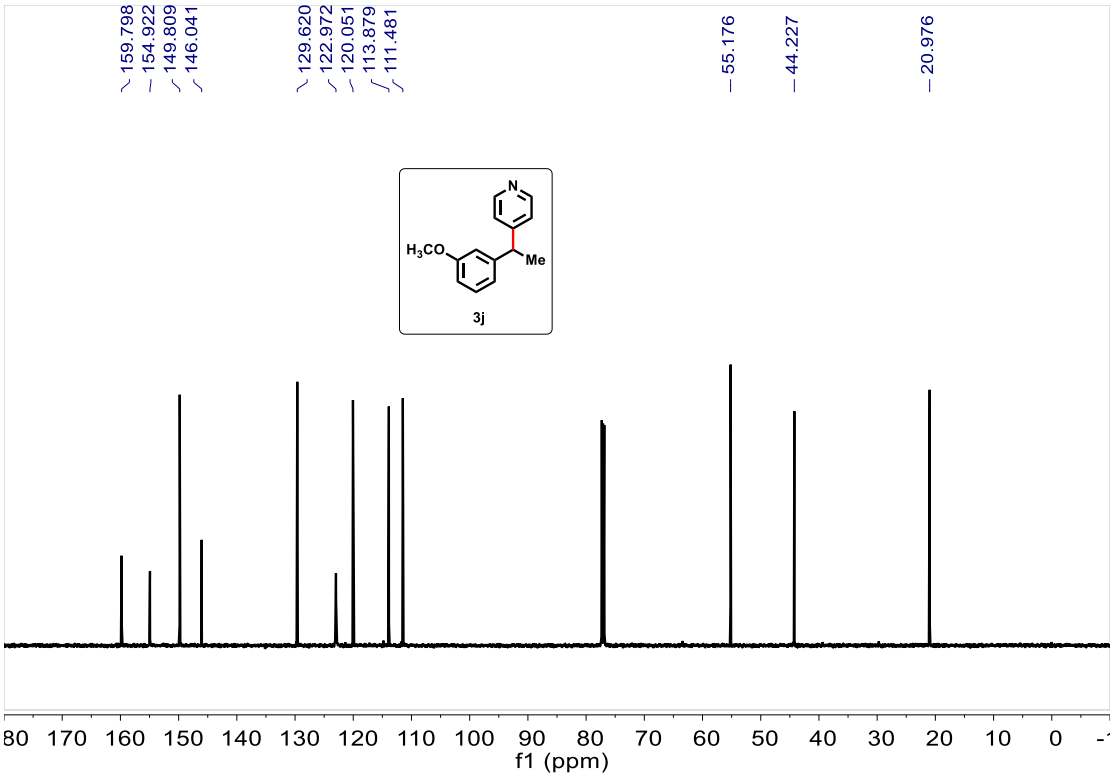

8.464
8.456
7.216
7.214
7.210
7.160
7.152
7.148
7.062
7.053
4.301
4.289
4.277
4.265
2.204
1.605
1.593
N
Me
CH3
3h
2.02
2.04
2.05
1.99
1.00
3.12
3.04
f1 (ppm)


155.058
149.683
141.953
135.921
40.352
21.157
19.597
130.526
126.603
126.579
126.191
122.928
N
Me
CH3
3h
130 128 126 124 122
f1 (ppm)
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.537
7.145
7.114
7.100
6.855
6.841
4.086
4.074
4.062
4.050
3.783
1.616
1.604
N
Me
H3CO
3i
1.89
1.96
2.18
1.00
3.03
3.15
9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.5
f1 (ppm)


158.281
155.725
149.488
136.437
128.556
123.159
113.999
55.270
43.443
21.236
N
Me
H3CO
3i
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.490
7.236
7.223
7.210
7.136
7.128
6.789
6.777
6.772
6.767
6.757
6.754
6.734
4.093
4.081
4.069
4.057
3.767
1.626
1.614
N
H3CO
Me
3j
2.00
1.01
1.96
2.01
0.95
1.00
3.04
3.03
9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)


159.798
154.922
149.809
146.041
129.620
122.972
120.051
113.879
111.481
55.176
44.227
20.976
N
H3CO
Me
3j
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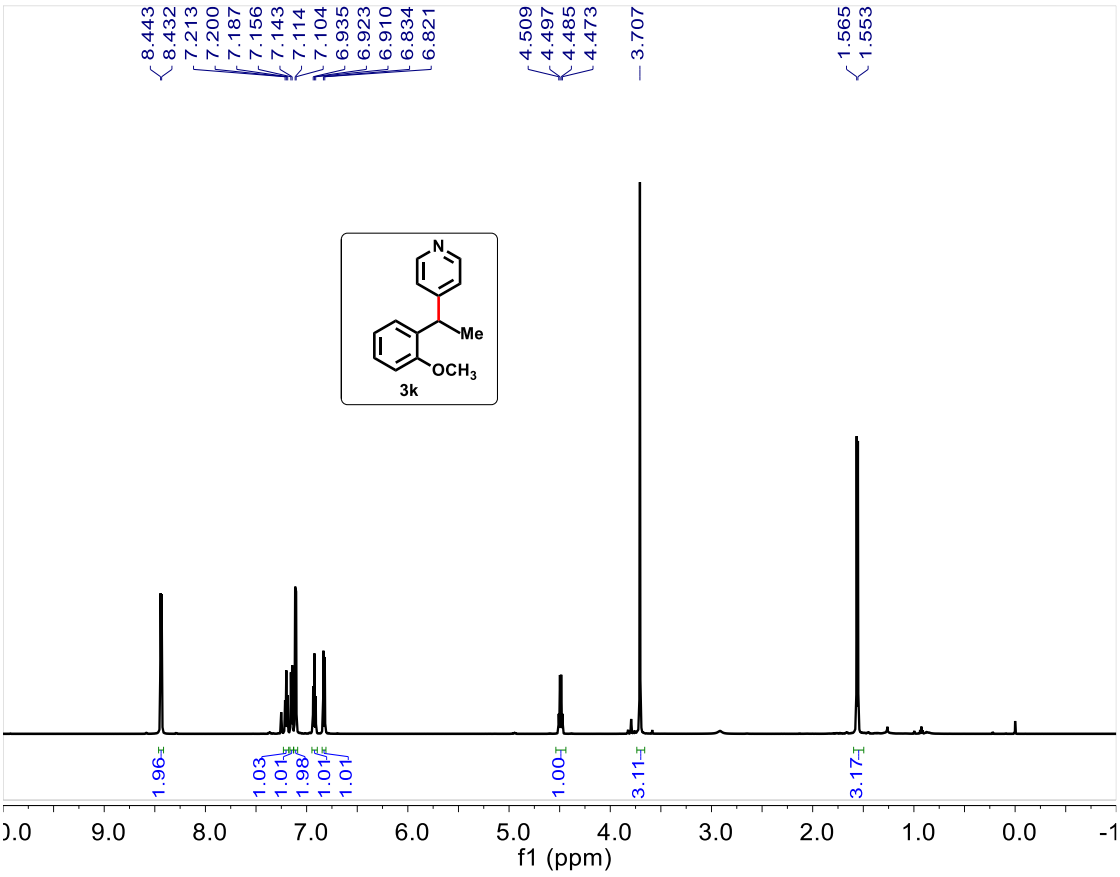
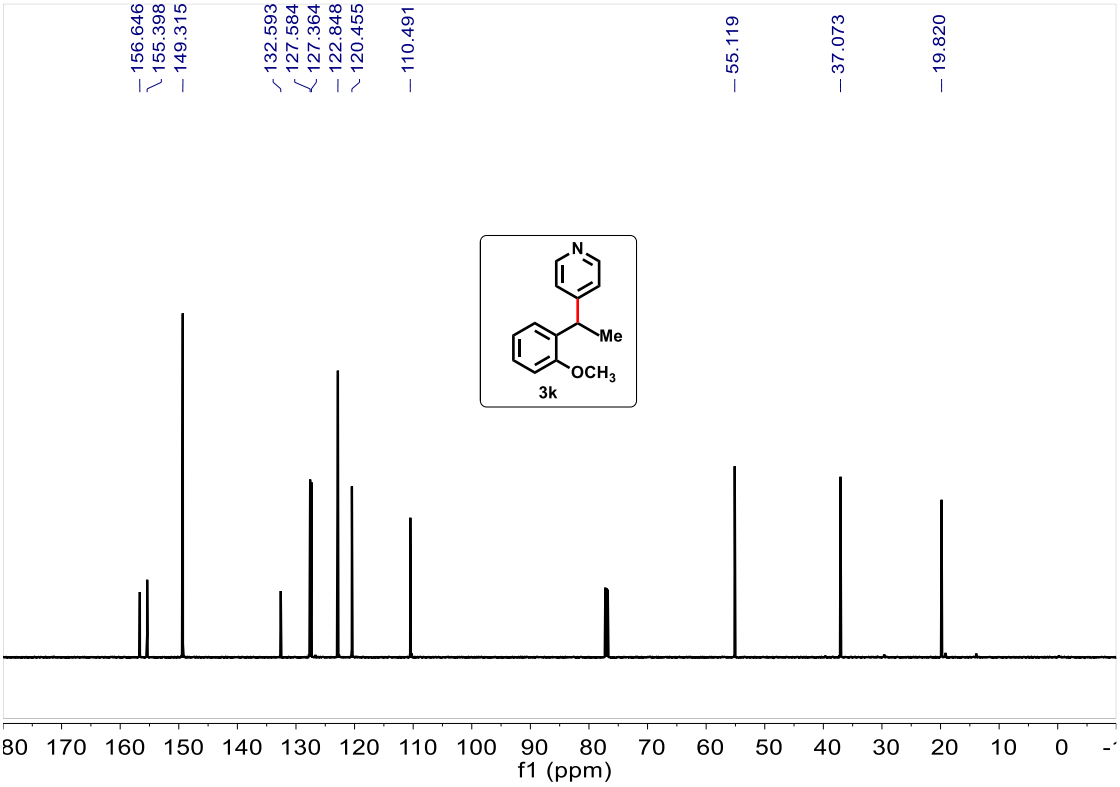
f1 (ppm)


8.443
8.432
7.213
7.200
7.187
7.156
7.143
7.114
7.104
6.935
6.923
6.910
6.834
6.821
4.509
4.497
4.485
4.473
3.707
1.565
1.553
N
Me
OCH3
3k
1.96
1.03
1.01
1.98
1.01
1.01
1.00
3.11
3.17
9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)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155.398
149.315
132.593
127.584
127.364
122.848
120.455
110.491
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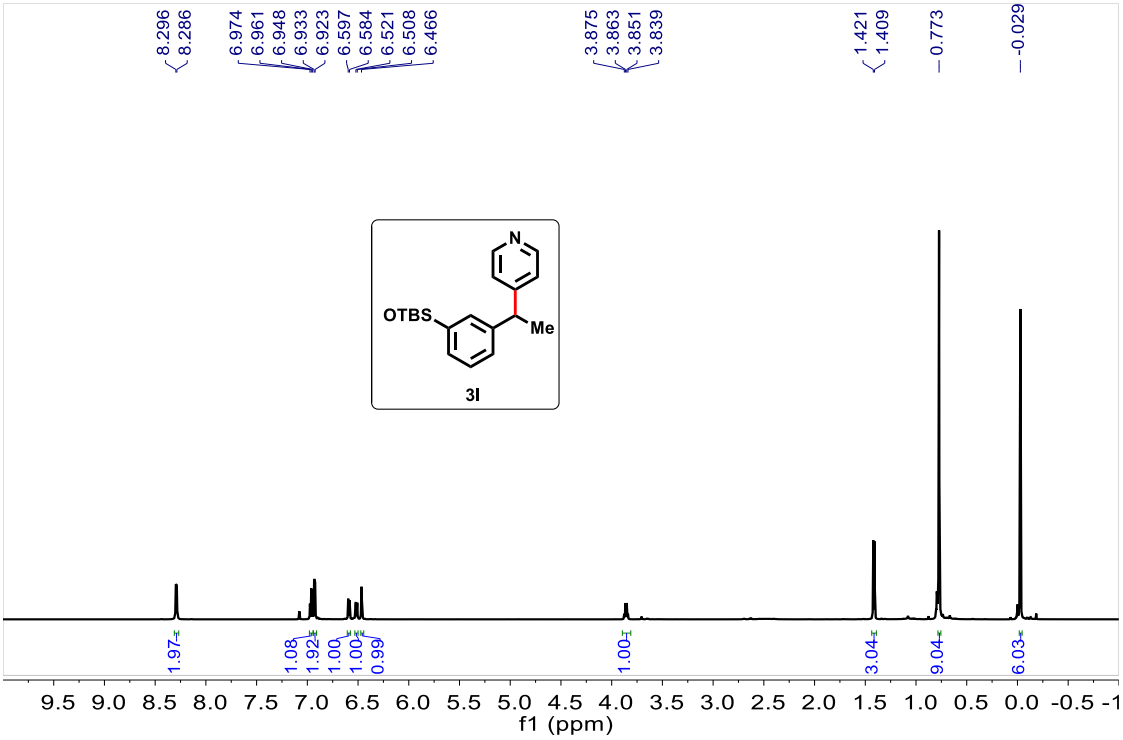
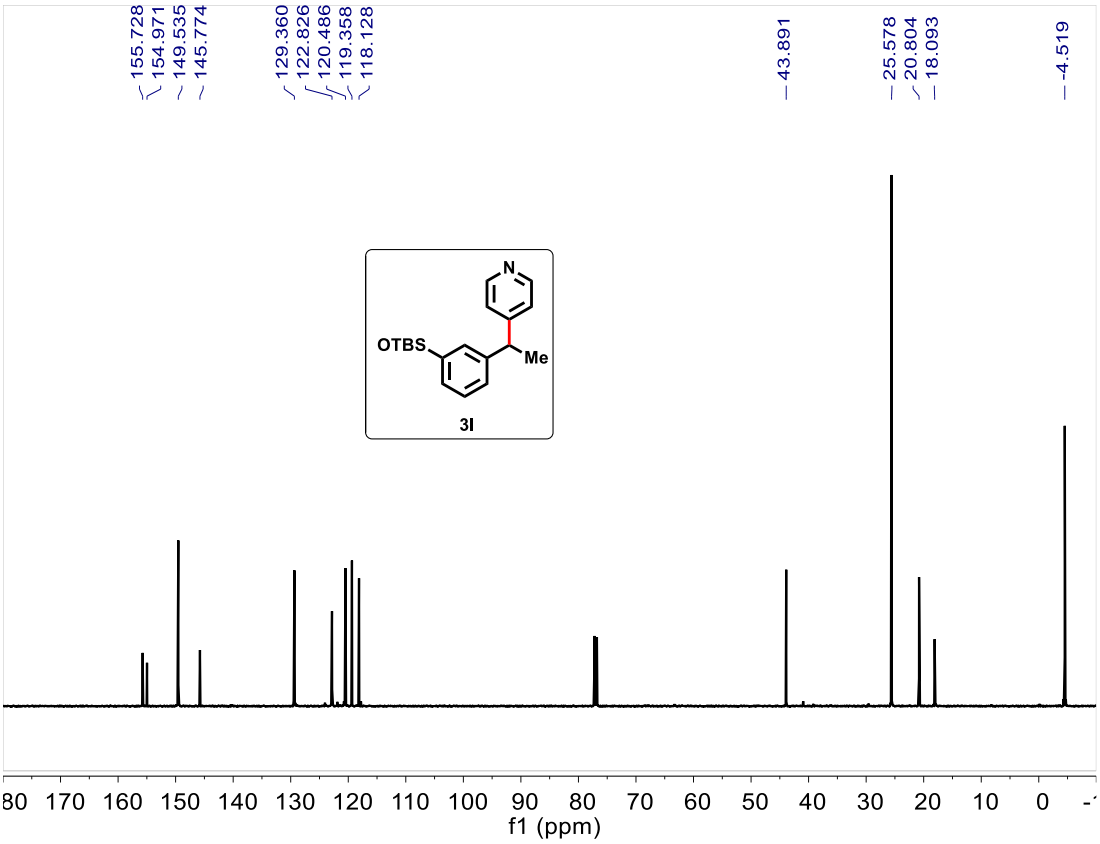
37.073
19.820
N
Me
OCH3
3k
f1 (ppm)


8.296
8.286
6.974
6.961
6.948
6.933
6.923
6.597
6.584
6.521
6.508
6.466
3.875
3.863
3.851
3.839
1.421
1.409
0.773
-0.029
N
OTBS
Me
3l
1.97
1.08
1.92
1.00
1.00
0.99
1.00
3.04
9.04
6.03
f1 (ppm)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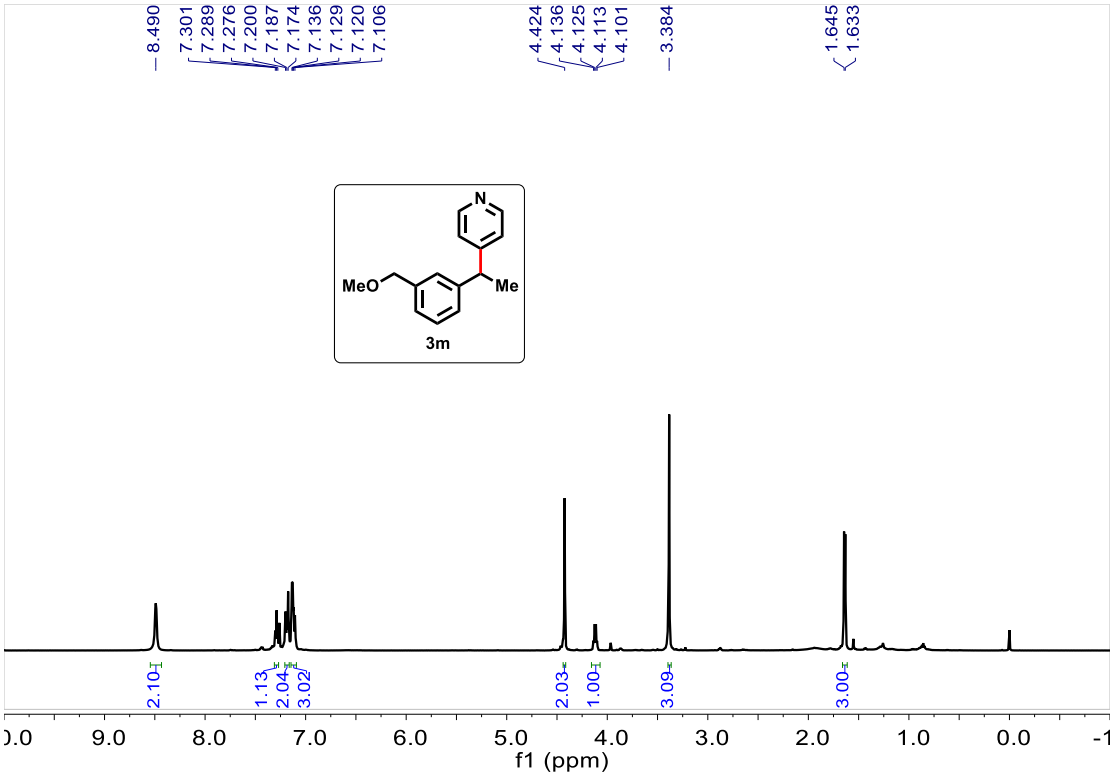
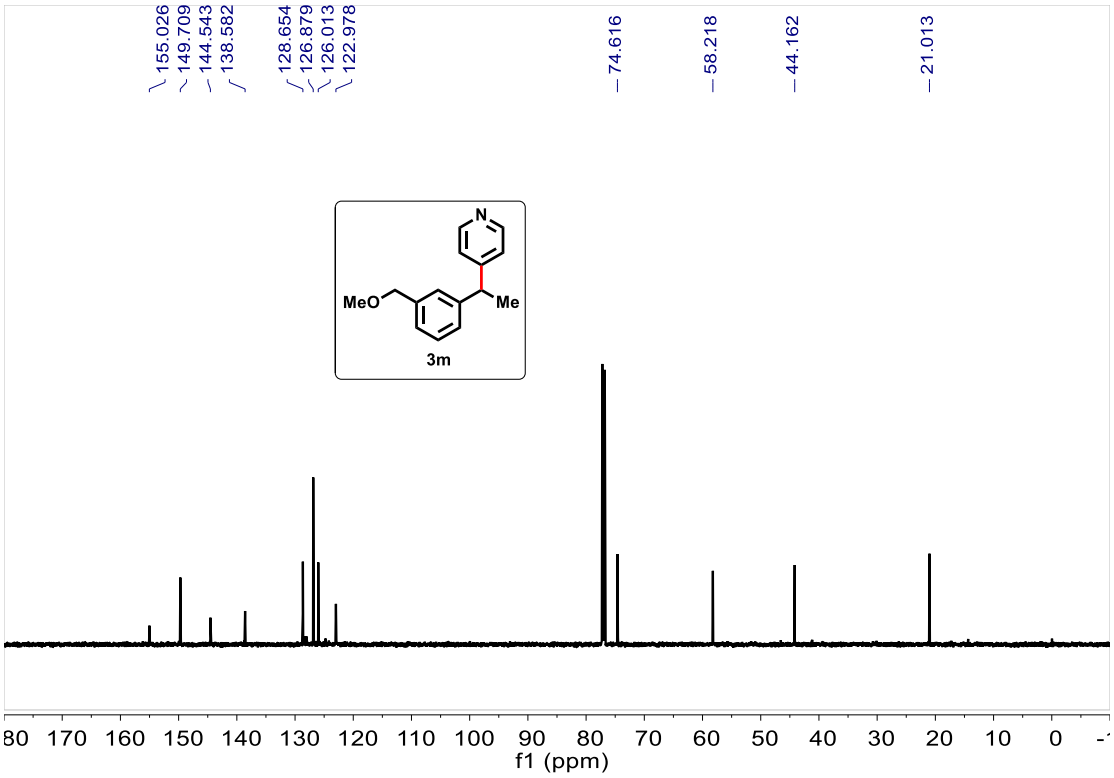
149.535
145.774
129.360
122.826
120.486
119.358
118.128
43.891
25.578
20.804
18.093
-4.519
OTBS
Me
N
3l
f1 (ppm)


8.490
7.301
7.289
7.276
7.200
7.187
7.174
7.136
7.129
7.120
7.106
4.424
4.136
4.125
4.113
4.101
3.384
1.645
1.633
MeO
Me
N
3m
2.10
1.13
2.04
3.02
2.03
1.00
3.09
3.00
f1 (ppm)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138.582
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126.013
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74.616
58.218
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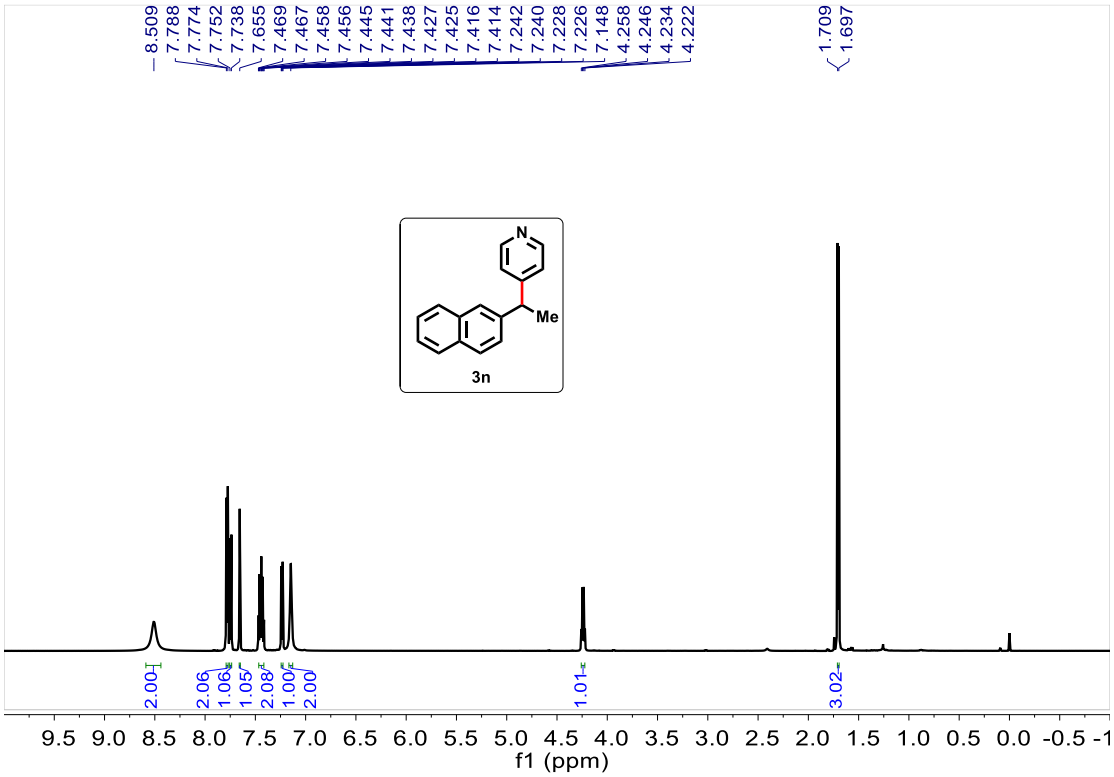
21.013
MeO
Me
3m
f1 (ppm)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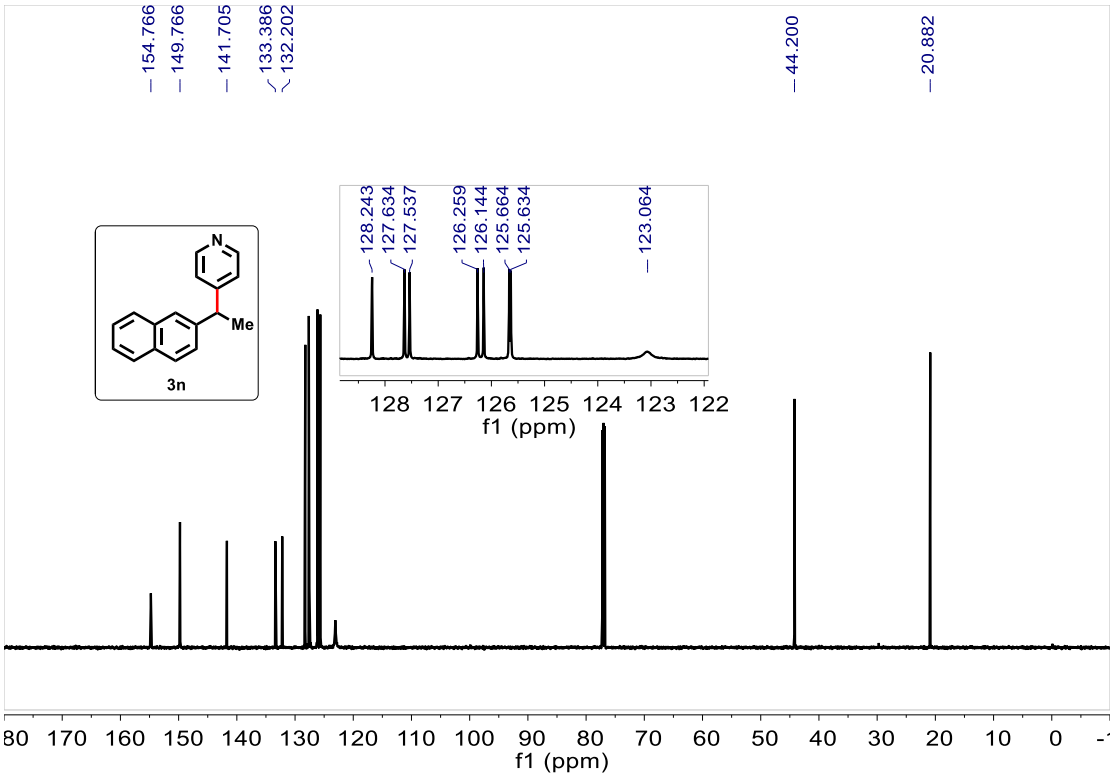
7.788
7.774
7.752
7.738
7.655
7.469
7.467
7.458
7.456
7.445
7.441
7.438
7.427
7.425
7.416
7.414
7.242
7.240
7.228
7.226
7.148
4.258
4.246
4.234
4.222
1.709
1.697
Me
3n
2.00
2.06
1.06
1.05
2.08
1.00
2.00
1.01
3.02
f1 (ppm)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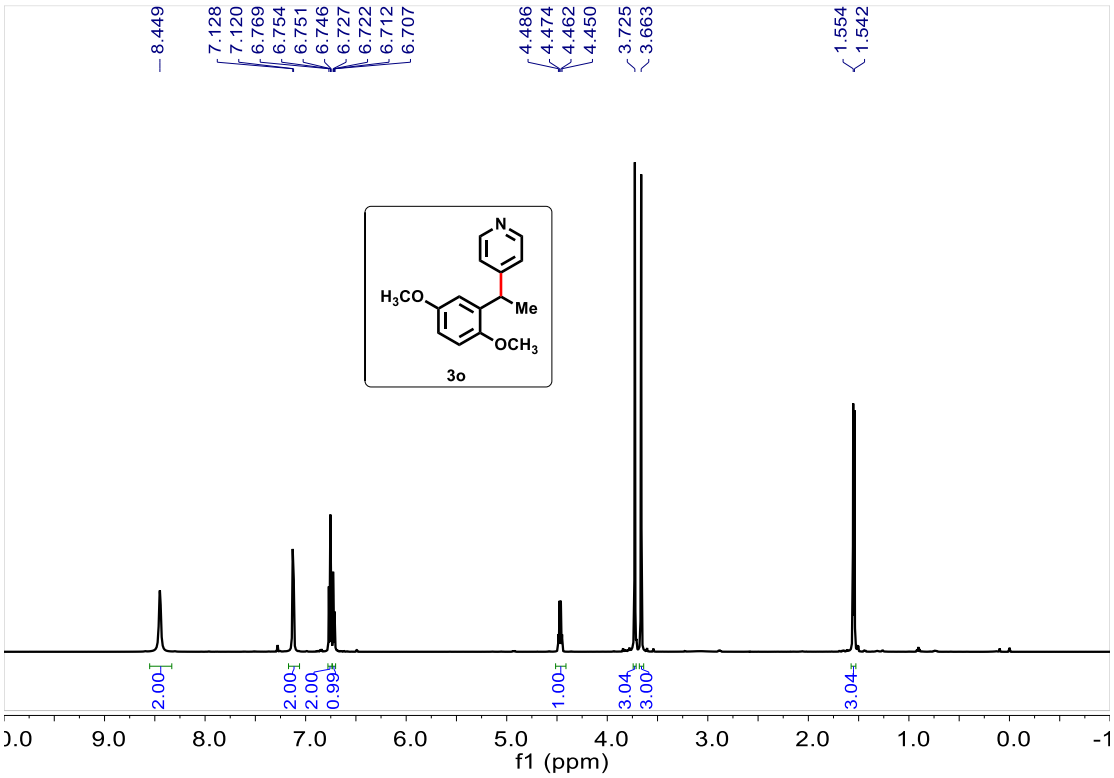
44.200
20.882
128.243
127.634
127.537
126.259
126.144
125.664
125.634
123.064
N
Me
3n
128 127 126 125 124 123 122
f1 (ppm)
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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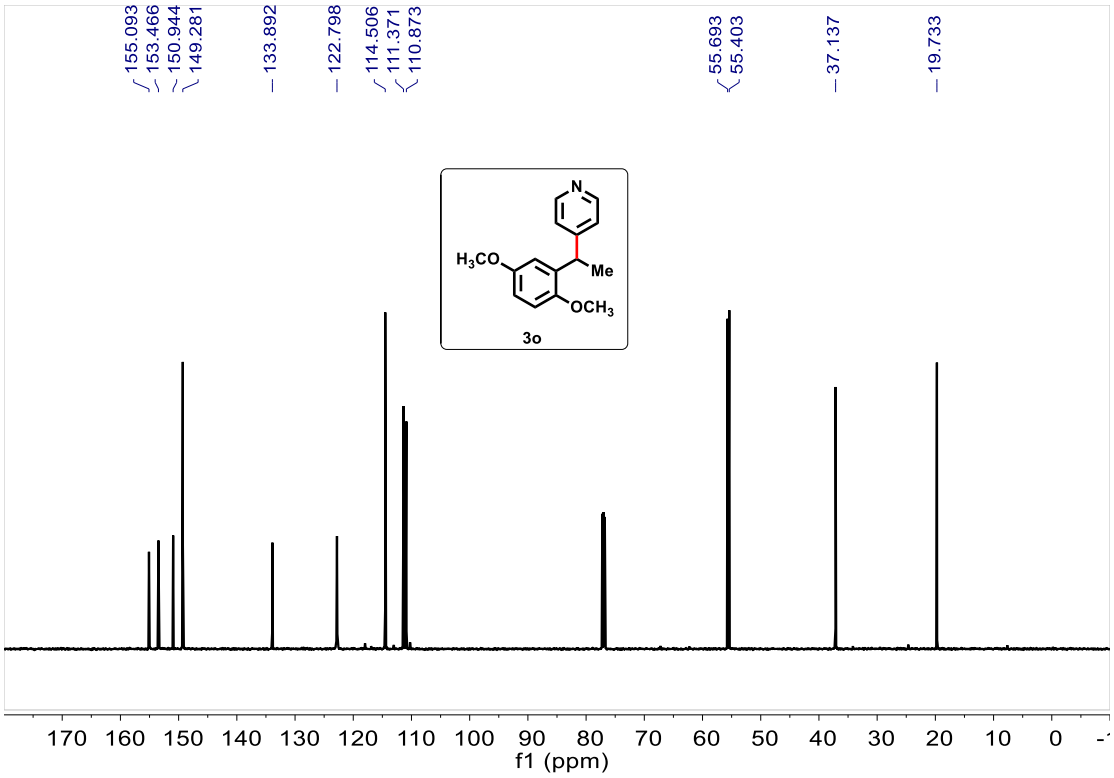
7.128
7.120
6.769
6.754
6.751
6.746
6.727
6.722
6.712
6.707
4.486
4.474
4.462
4.450
3.725
3.663
1.554
1.542
N
H3CO
Me
OCH3
3o
2.00
2.00
2.00
0.99
1.00
3.04
3.00
3.04
0.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1
f1 (ppm)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111.371
110.873
55.693
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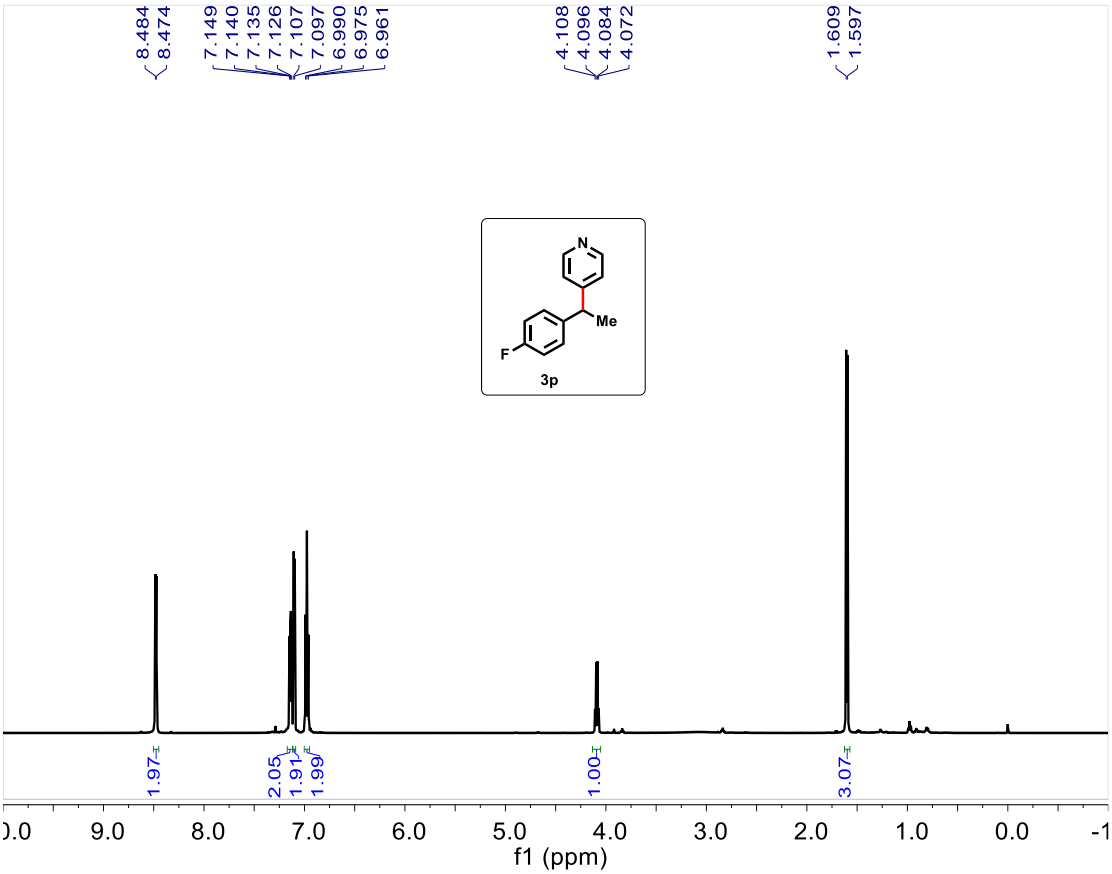
19.733
N
H3CO
Me
OCH3
3o
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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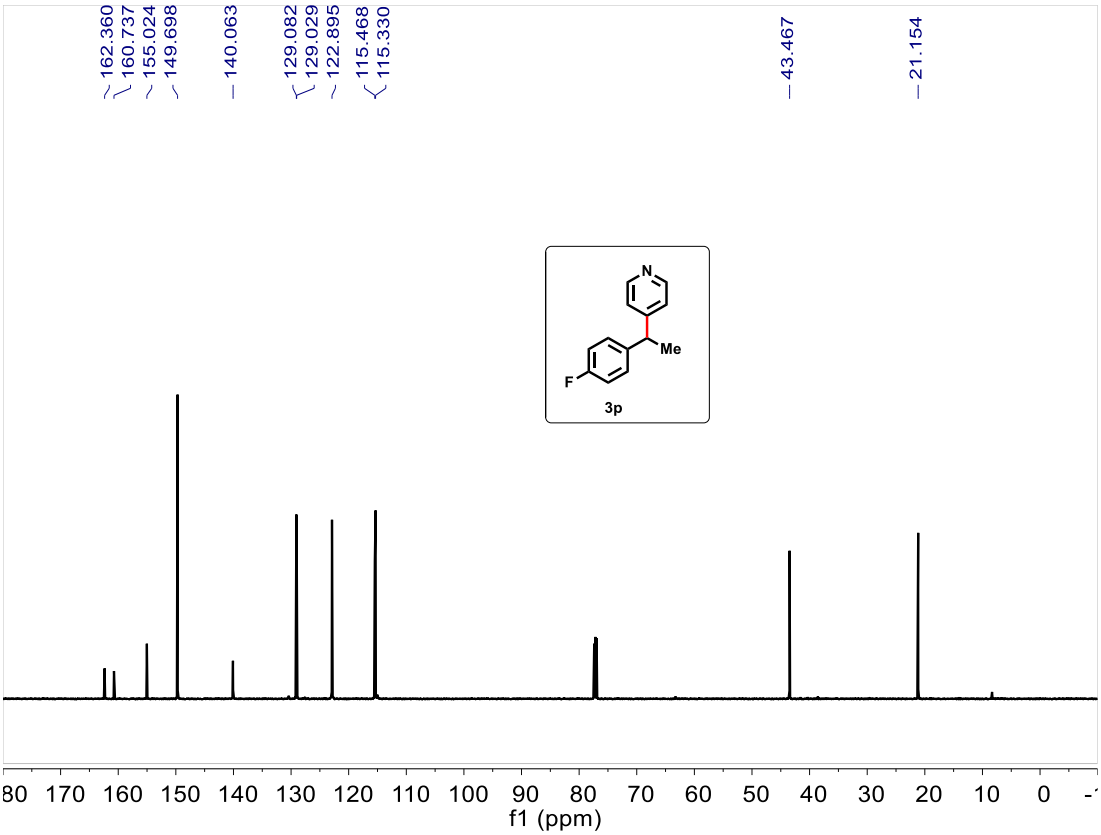
7.135
7.126
7.107
7.097
6.990
6.975
6.961
4.108
4.096
4.084
4.072
1.609
1.597
N
Me
F
3p
1.97
2.05
1.91
1.99
1.00
3.07
9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)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149.698
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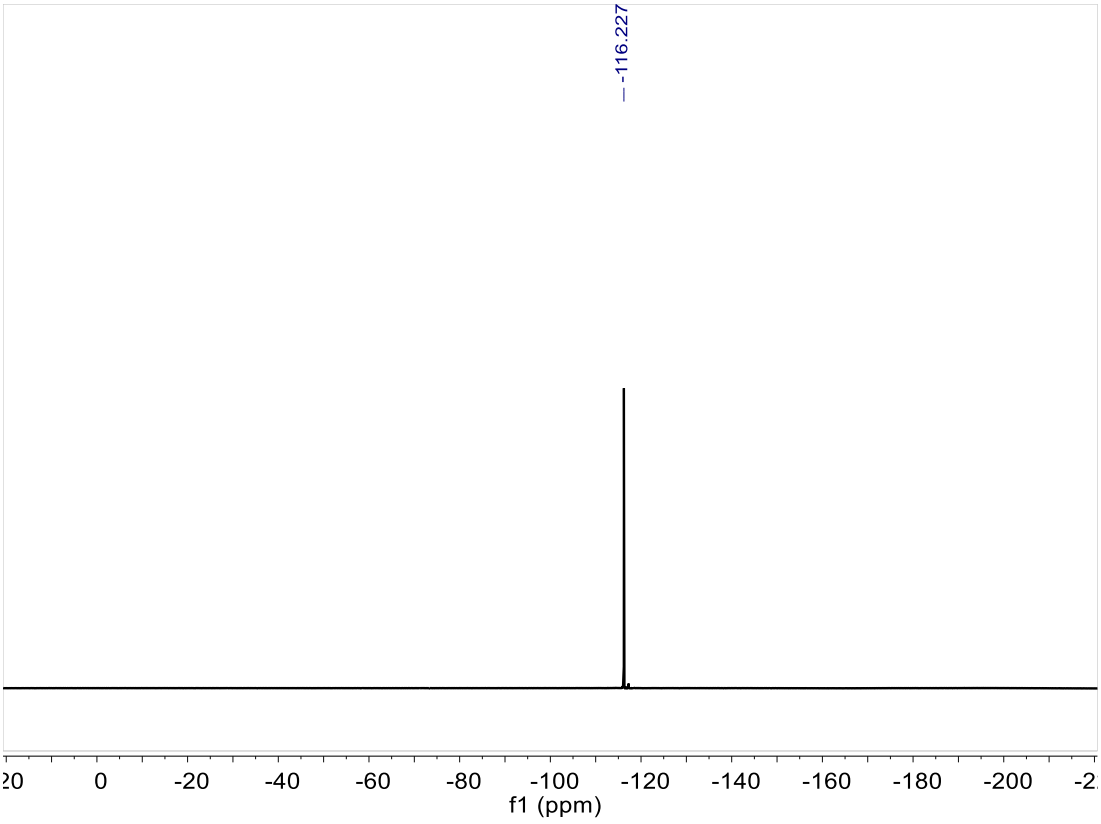
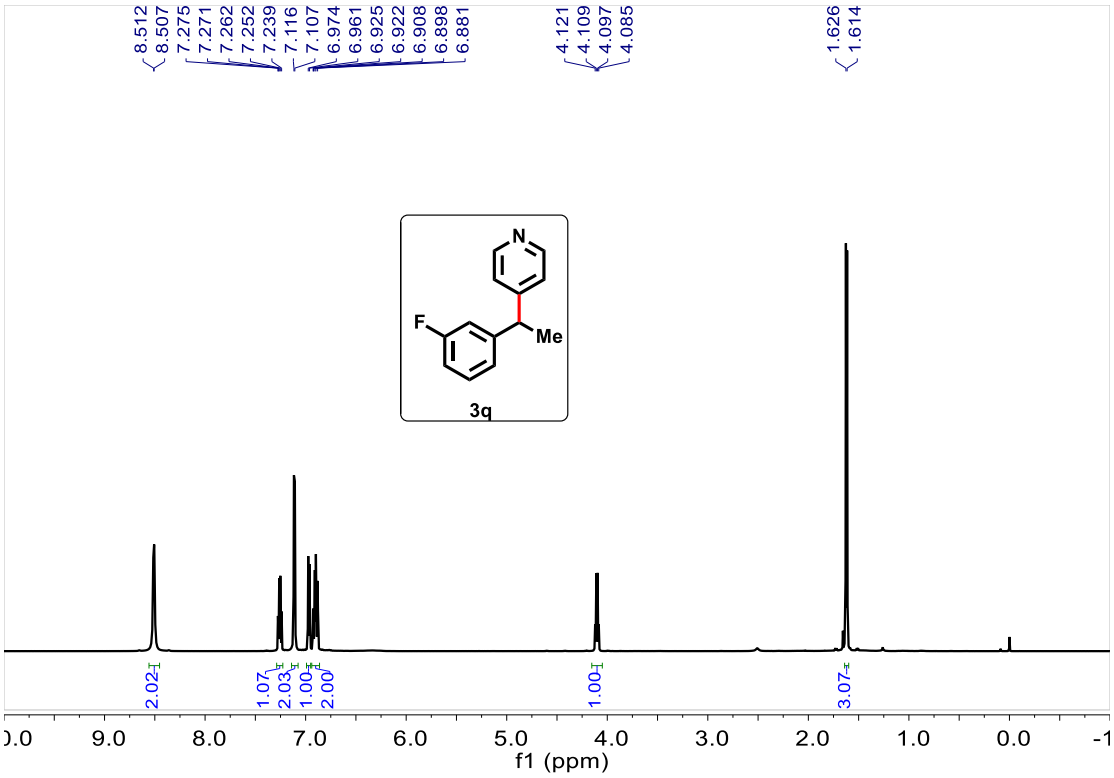
129.029
122.895
115.468
115.330
43.467
21.154
N
Me
F
3p
f1 (ppm)


-116.227
f1 (ppm)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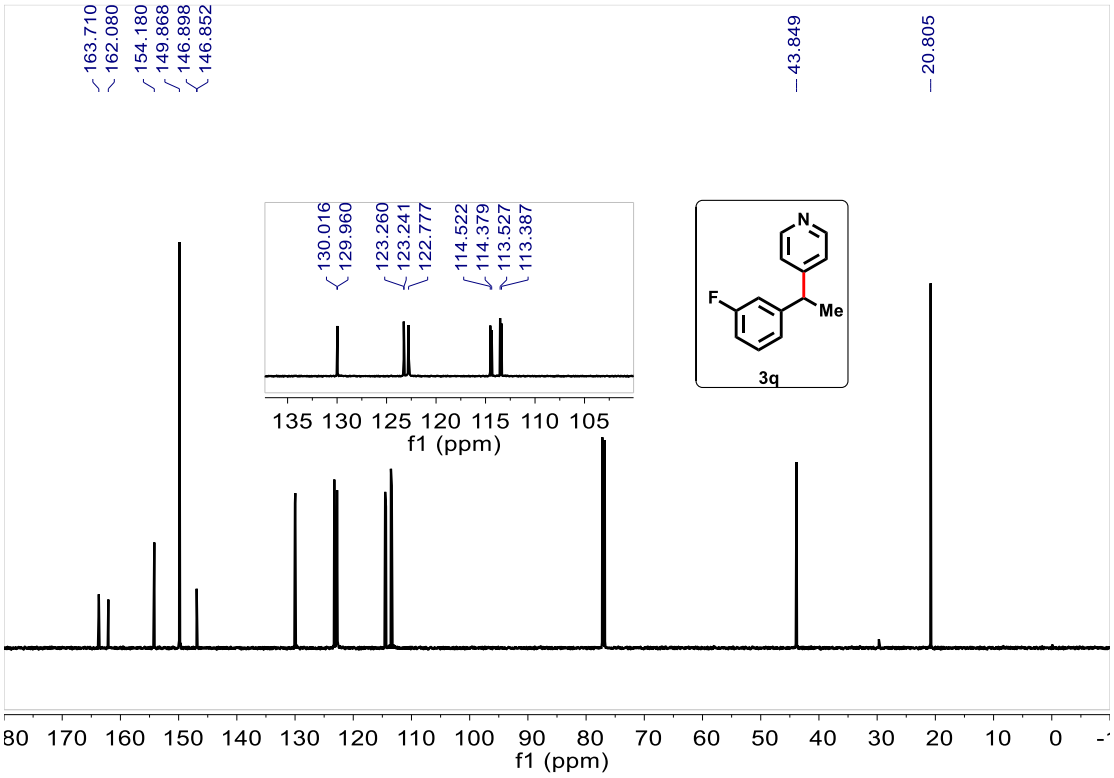
8.507
7.275
7.271
7.262
7.252
7.239
7.116
7.107
6.974
6.961
6.925
6.922
6.908
6.898
6.881
4.121
4.109
4.097
4.085
1.626
1.614
N
F
Me
3q
2.02
1.07
2.03
1.00
2.00
1.00
3.07
f1 (ppm)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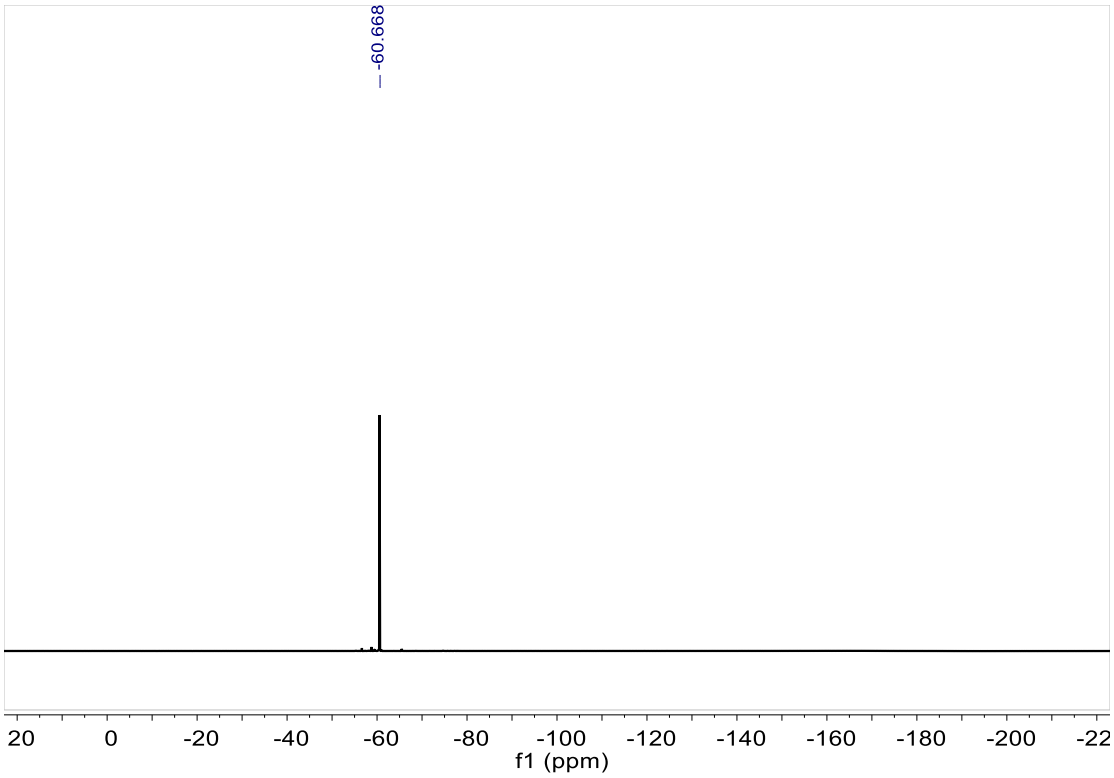
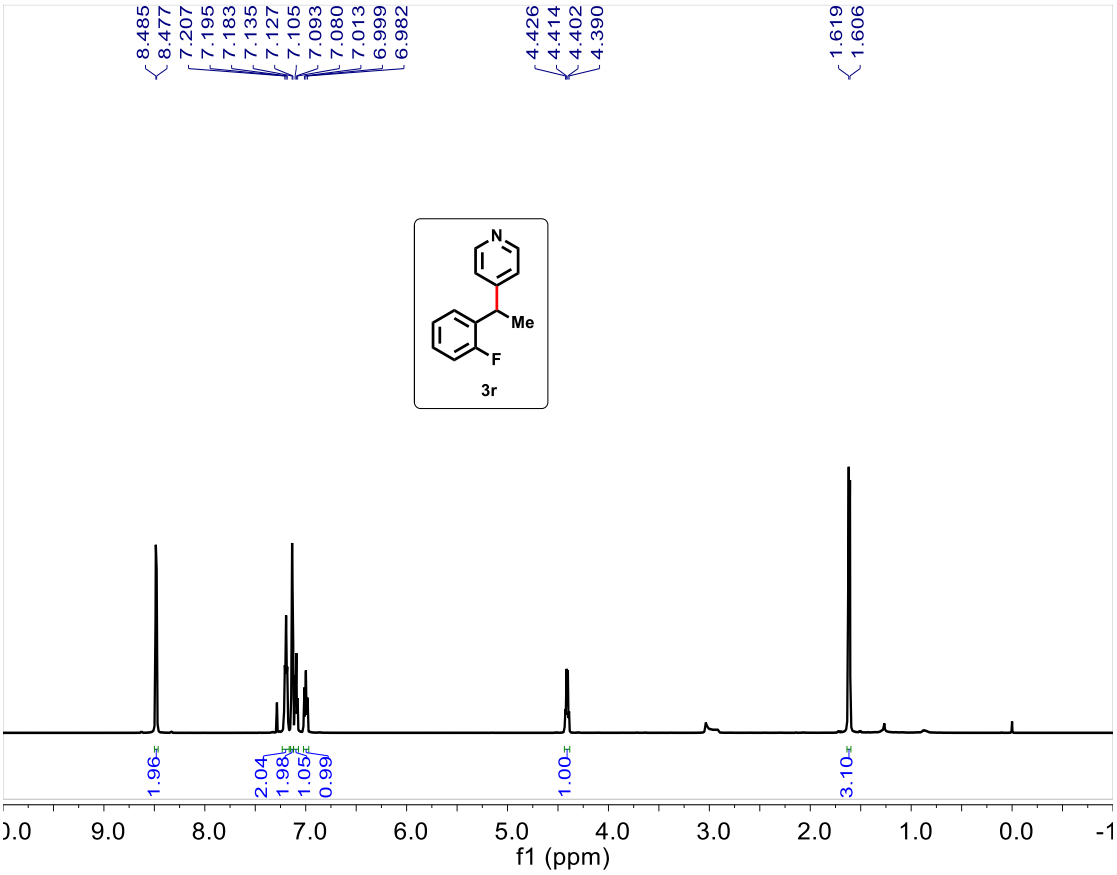
149.868
146.898
146.852
43.849
20.805
130.016
129.960
123.260
123.241
122.777
114.522
114.379
113.527
113.387
N
F
Me
3q
135 130 125 120 115 110 105
f1 (ppm)
f1 (ppm)


-60.668
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)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8.477
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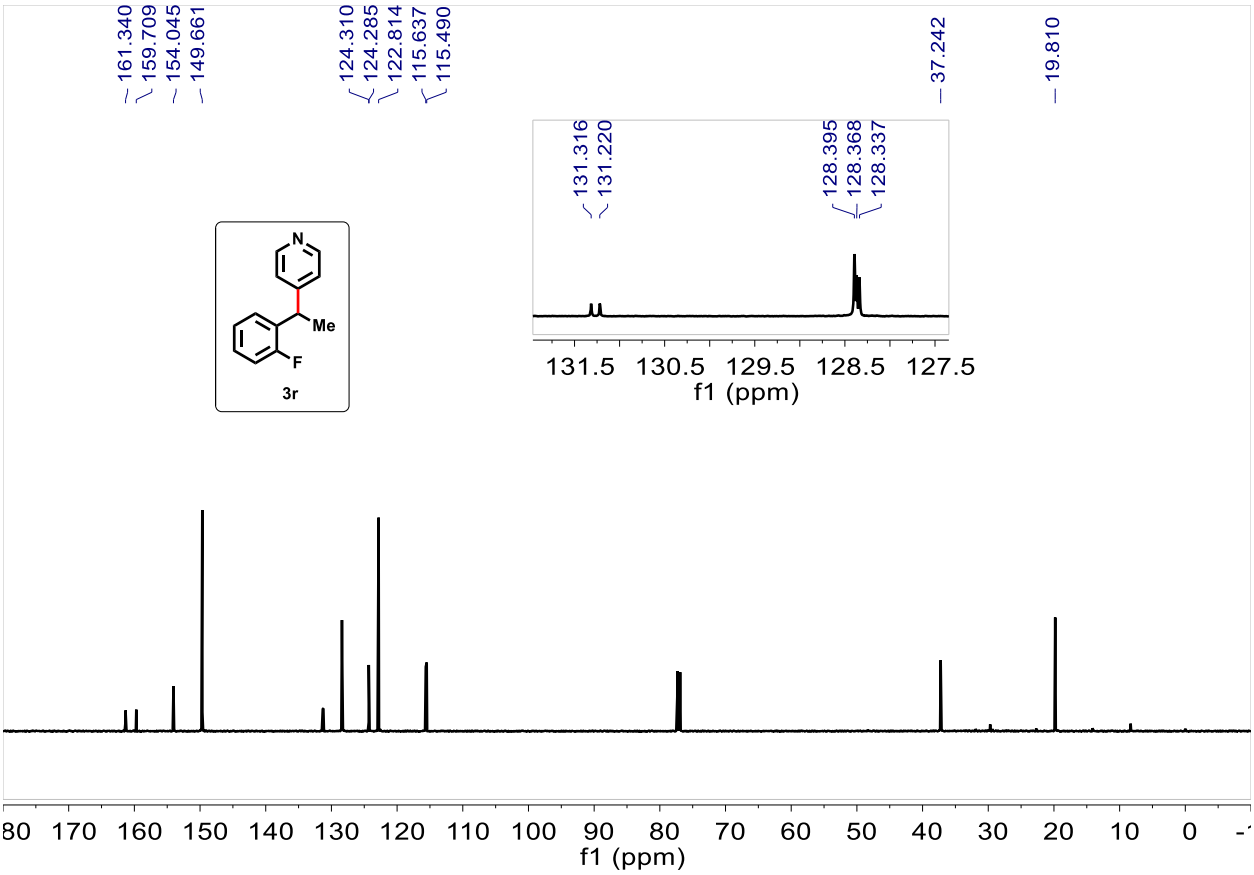
7.183
7.135
7.127
7.105
7.093
7.080
7.013
6.999
6.982
4.426
4.414
4.402
4.390
1.619
1.606
N
Me
F
3r
1.96
2.04
1.98
1.05
0.99
1.00
3.10
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


161.340
159.709
154.045
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124.310
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122.814
115.637
115.490
37.242
19.810
131.316
131.220
128.395
128.368
128.337
N
Me
F
3r
131.5 130.5 129.5 128.5 127.5
f1 (ppm)
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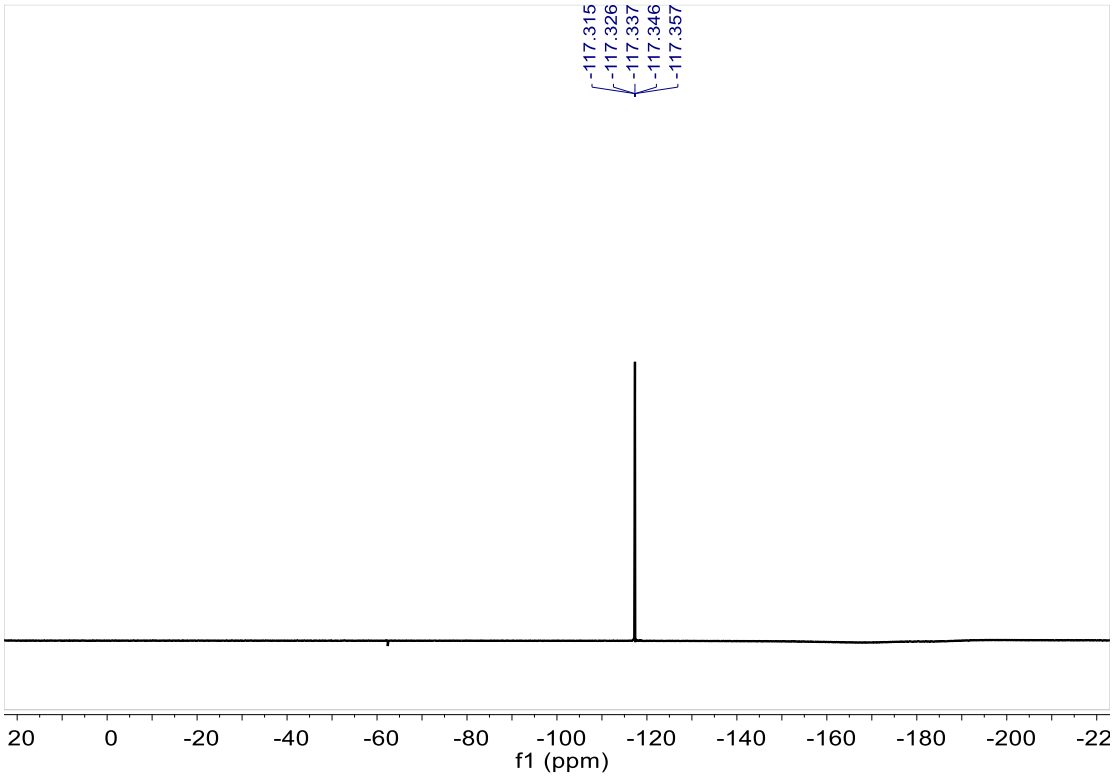
f1 (ppm)


-117.315
-117.326
-117.337
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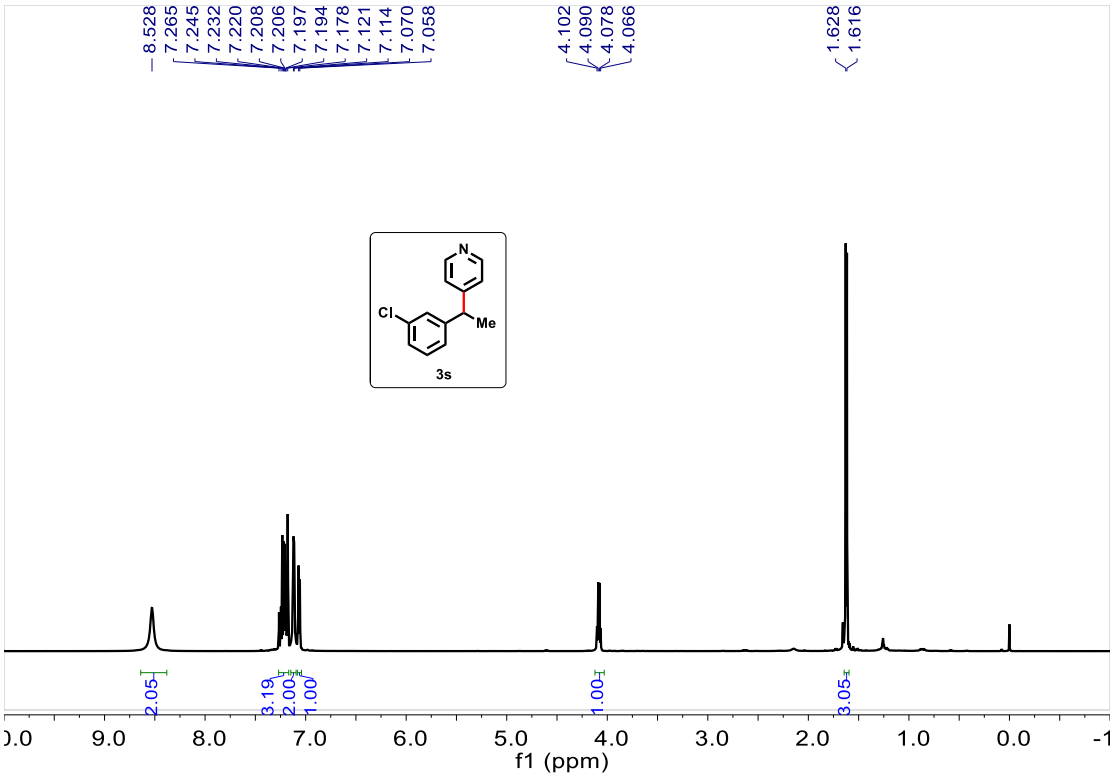
-117.357
20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -22
f1 (ppm)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7.245
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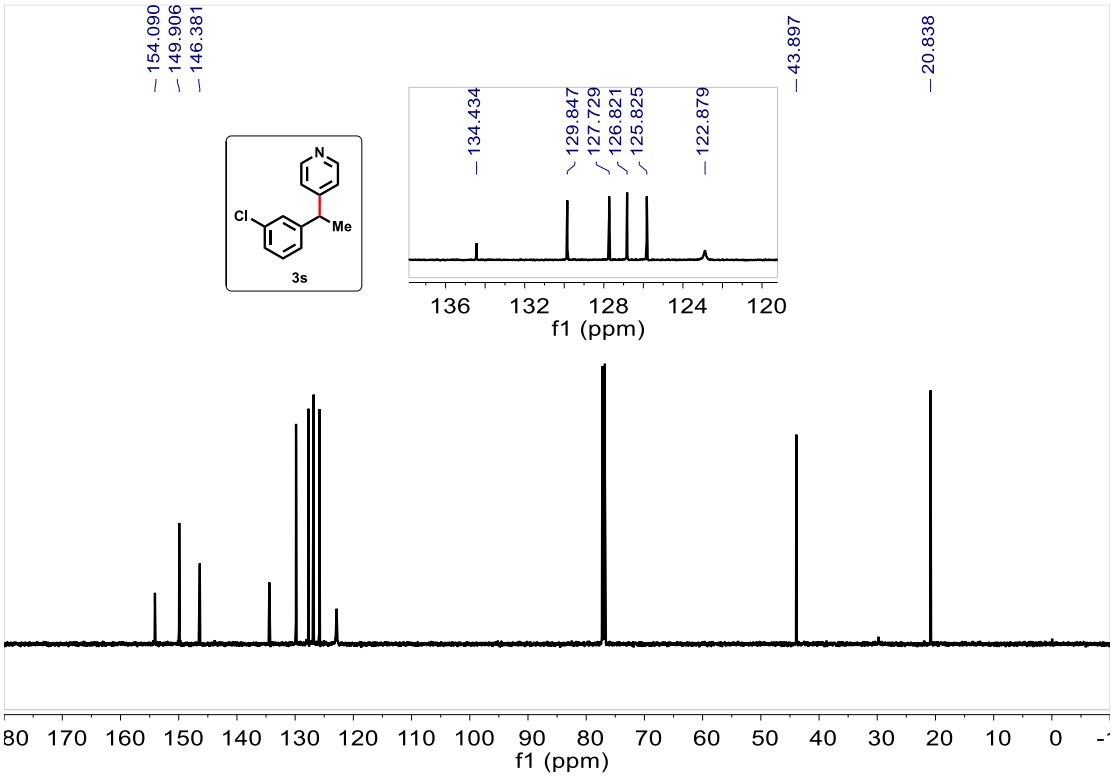
7.220
7.208
7.206
7.197
7.194
7.178
7.121
7.114
7.070
7.058
4.102
4.090
4.078
4.066
1.628
1.616
Cl
Me
N
3s
2.05
3.19
2.00
1.00
1.00
3.05
f1 (ppm)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149.906
146.381
134.434
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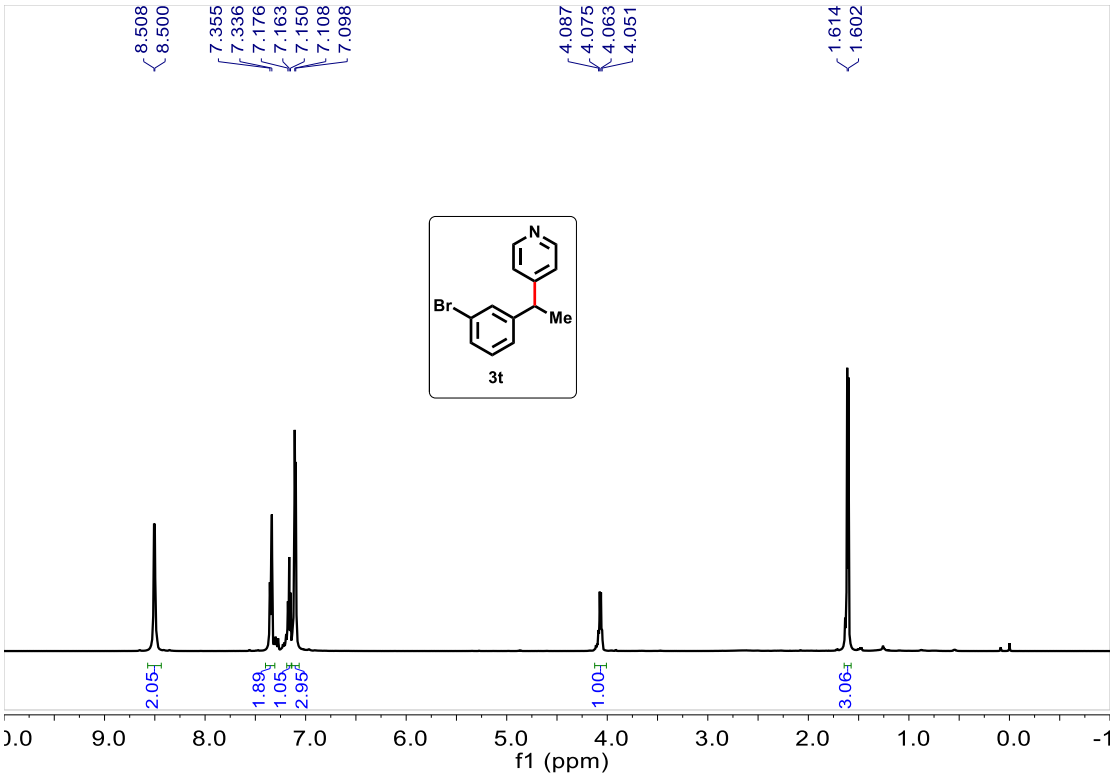
125.825
122.879
43.897
20.838
Cl
Me
N
3s
f1 (ppm)
f1 (ppm)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7.355
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7.176
7.163
7.150
7.108
7.098
4.087
4.075
4.063
4.051
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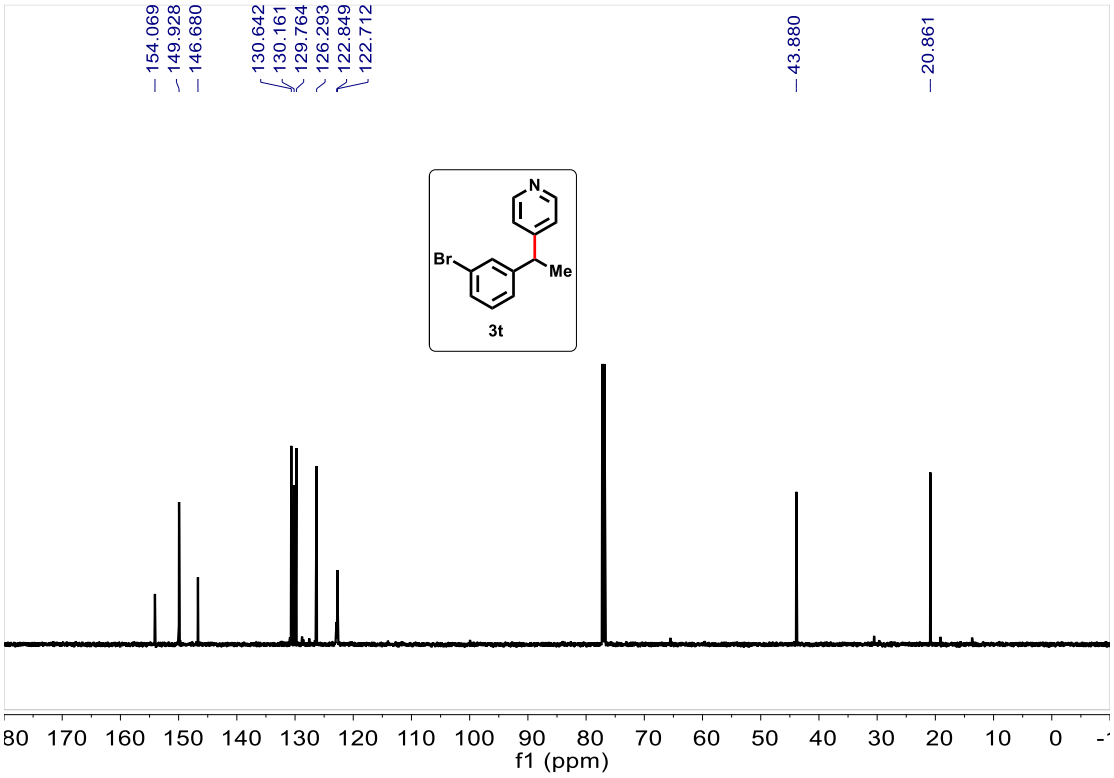
1.602
Br
Me
N
3t
2.05
1.89
1.05
2.95
1.00
3.06
f1 (ppm)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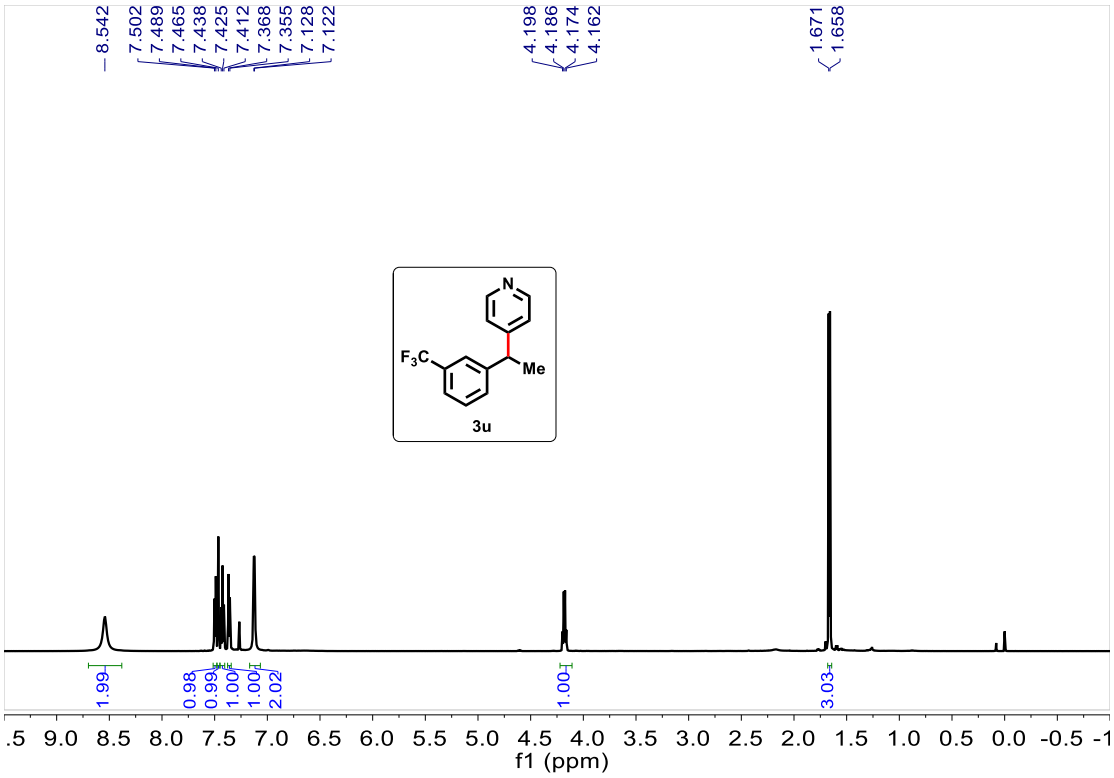
20.861
Br
Me
N
3t
f1 (ppm)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7.489
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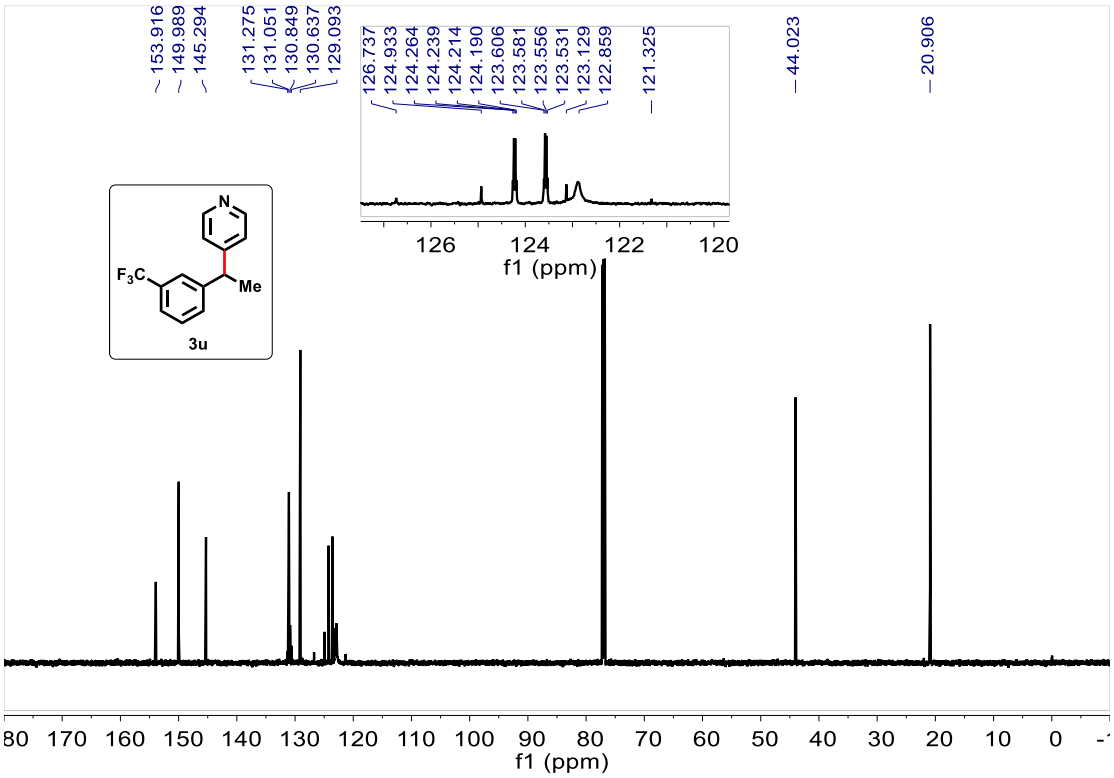
7.425
7.412
7.368
7.355
7.128
7.122
4.198
4.186
4.174
4.162
1.671
1.658
3u
1.99
0.98
0.99
1.00
1.00
2.02
1.00
3.03
f1 (ppm)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145.294
131.275
131.051
130.849
130.637
129.093
126.737
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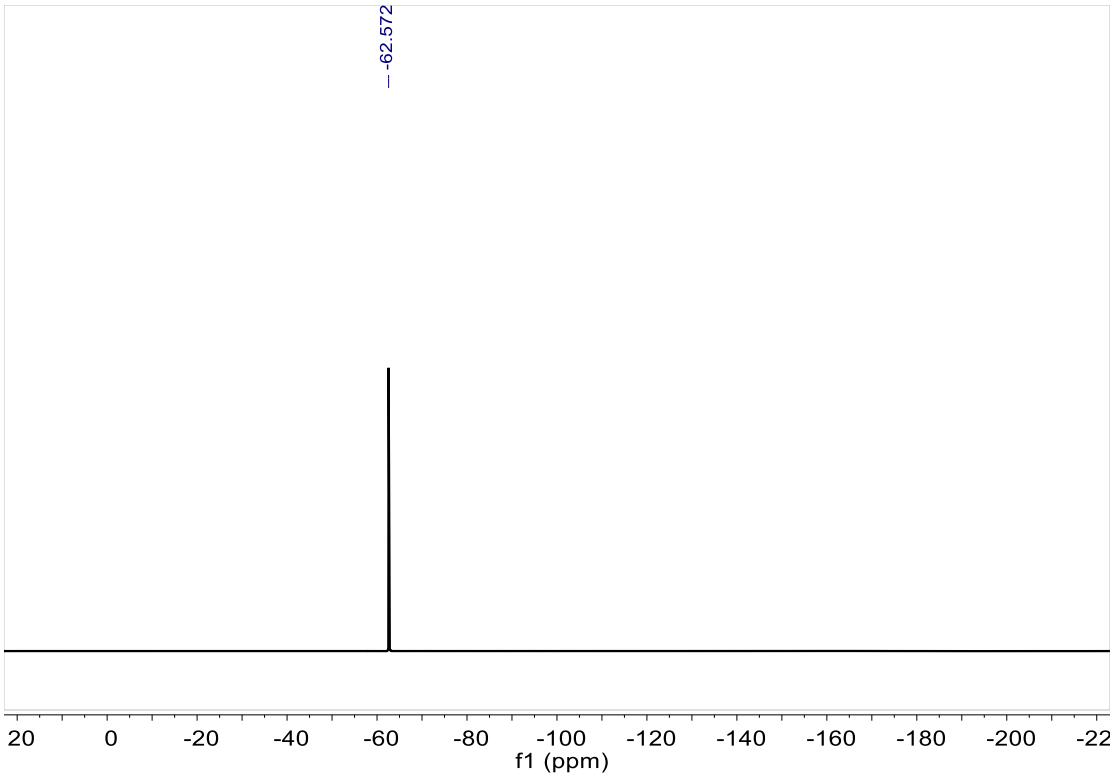
124.264
124.239
124.214
124.190
123.606
123.581
123.556
123.531
123.129
122.859
121.325
44.023
20.906
3u
f1 (ppm)
f1 (ppm)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-20
-40
-60
-80
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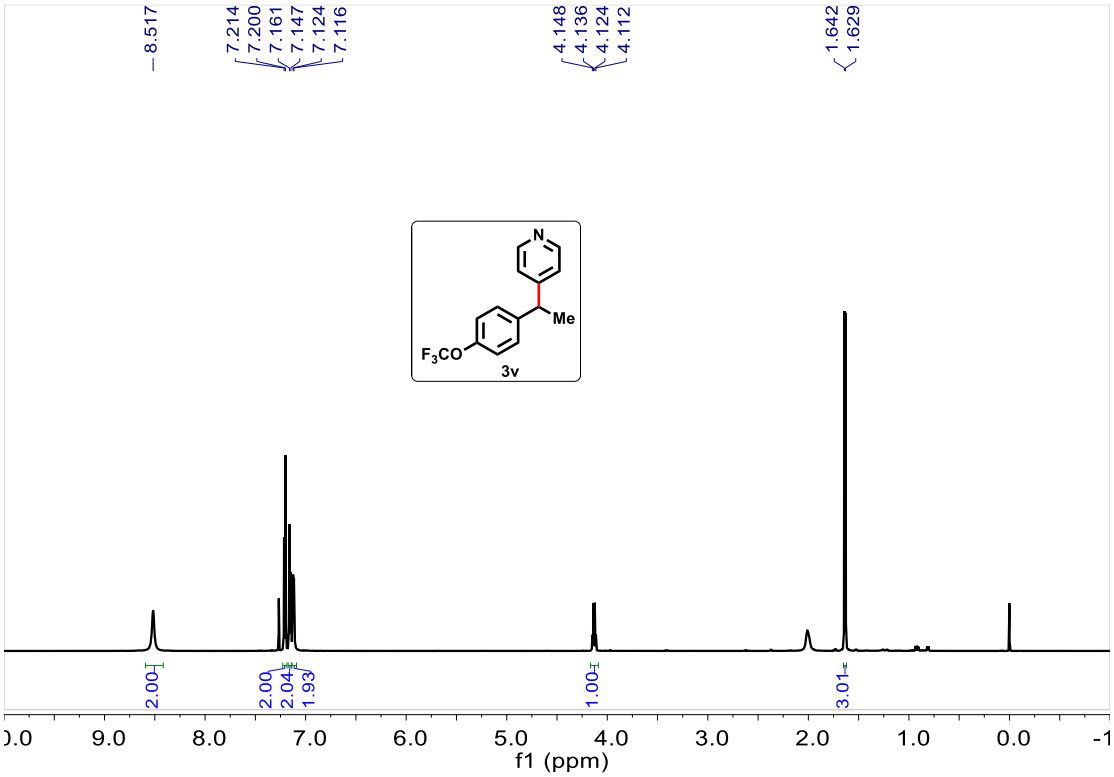
-120
-140
-160
-180
-200
-22
f1 (ppm)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7.214
7.200
7.161
7.147
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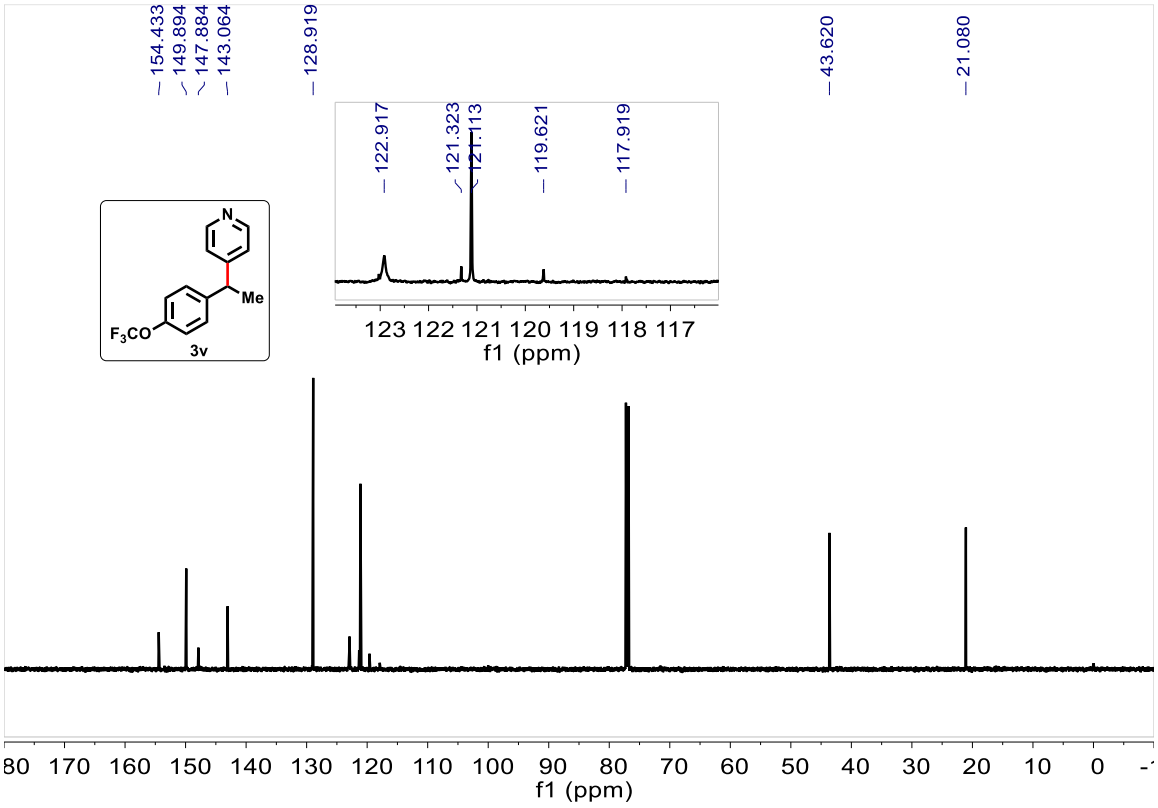
7.116
4.148
4.136
4.124
4.112
1.642
1.629
N
Me
F3CO
3v
2.00
2.00
2.04
1.93
1.00
3.01
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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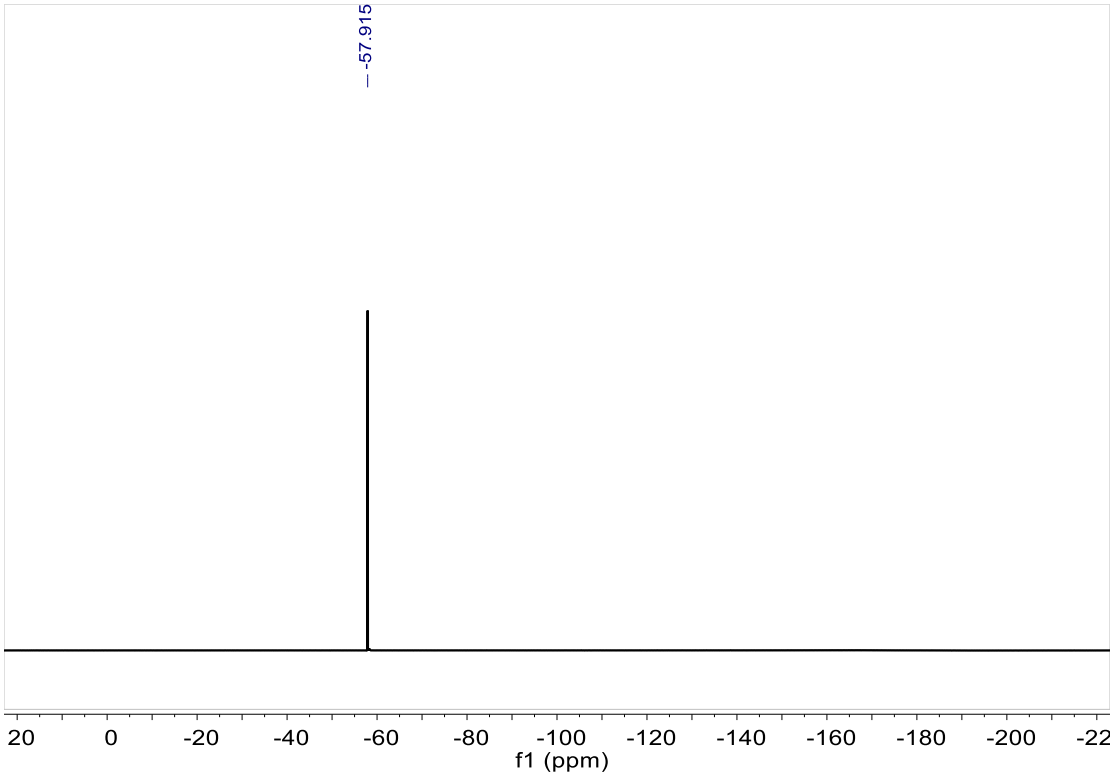
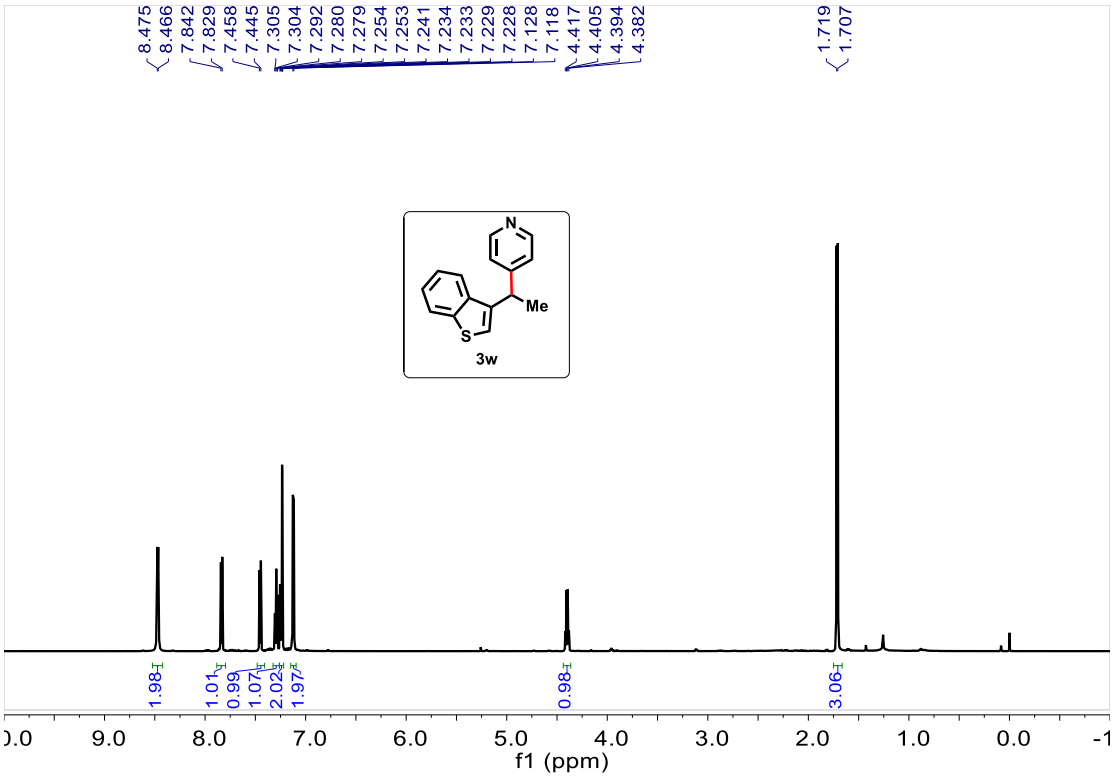
21.080
122.917
121.323
121.113
119.621
117.919
N
Me
F3CO
3v
123 122 121 120 119 118 117
f1 (ppm)
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-57.915
20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -22
f1 (ppm)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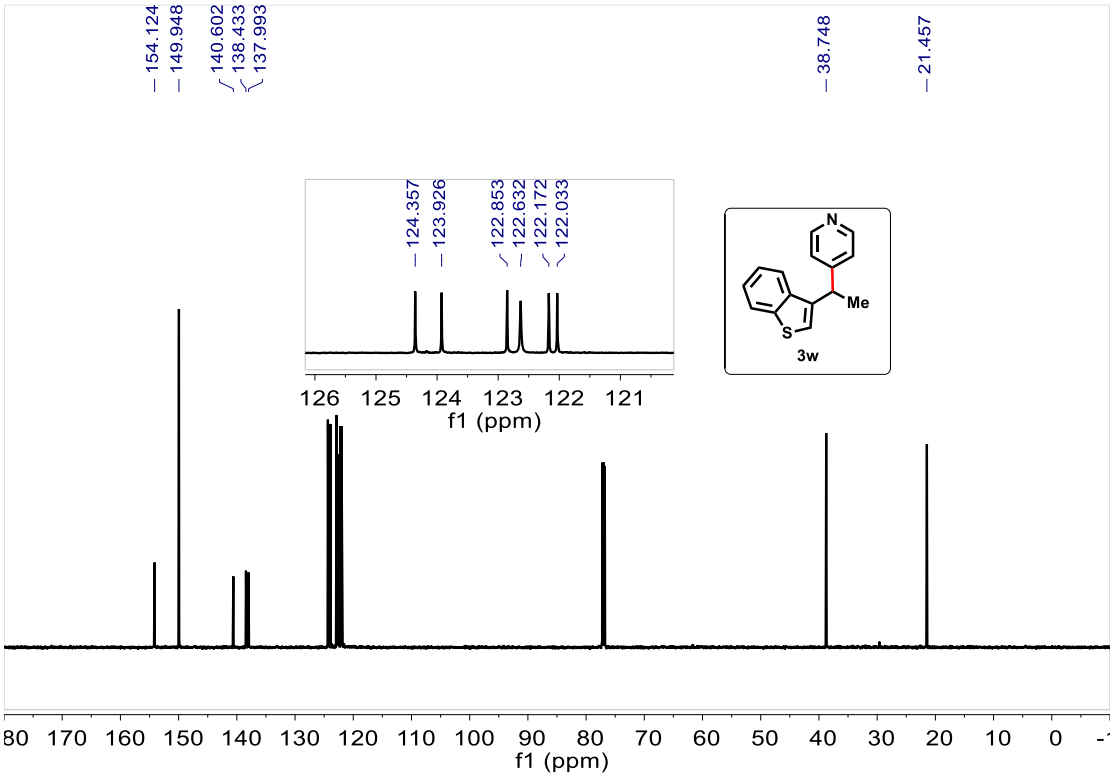
8.466
7.842
7.829
7.458
7.445
7.305
7.304
7.292
7.280
7.279
7.254
7.253
7.241
7.234
7.233
7.229
7.228
7.128
7.118
4.417
4.405
4.394
4.382
1.719
1.707
N
Me
S
3w
1.98
1.01
0.99
1.07
2.02
1.97
0.98
3.06
f1 (ppm)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138.433
137.993
38.748
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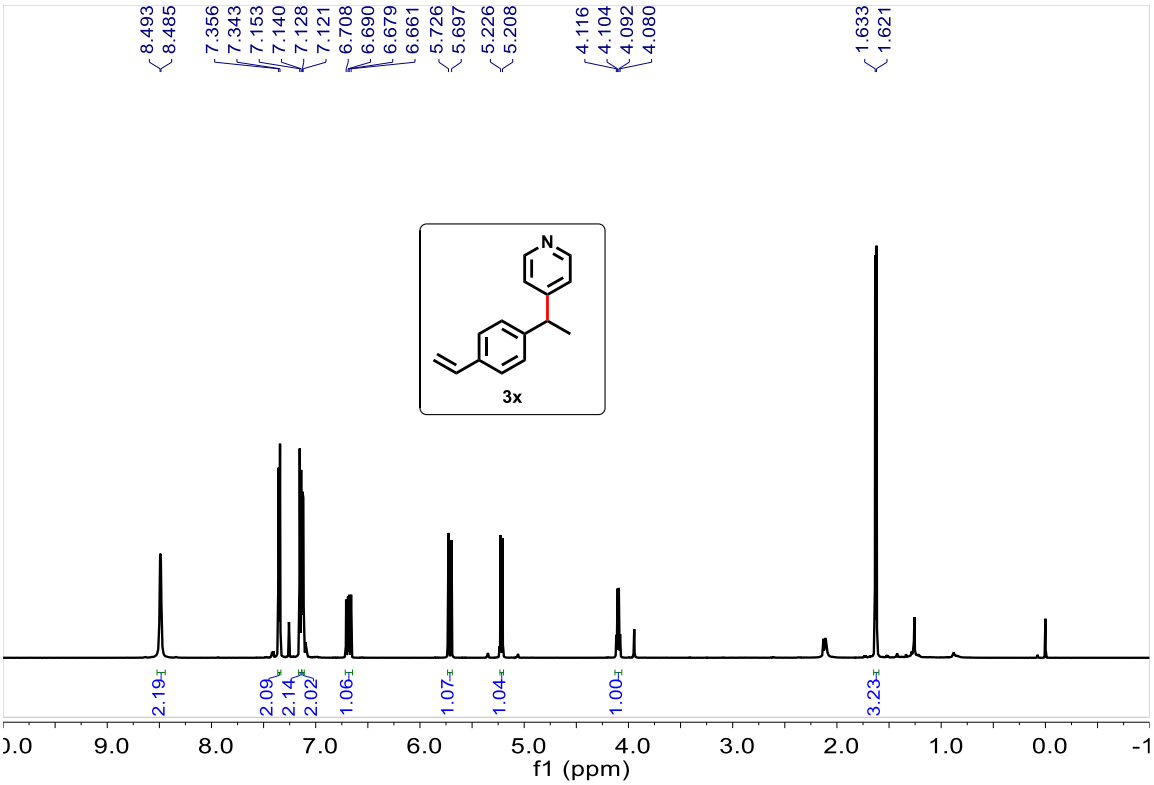
124.357
123.926
122.853
122.632
122.172
122.033
N
Me
S
3w
f1 (ppm)
f1 (ppm)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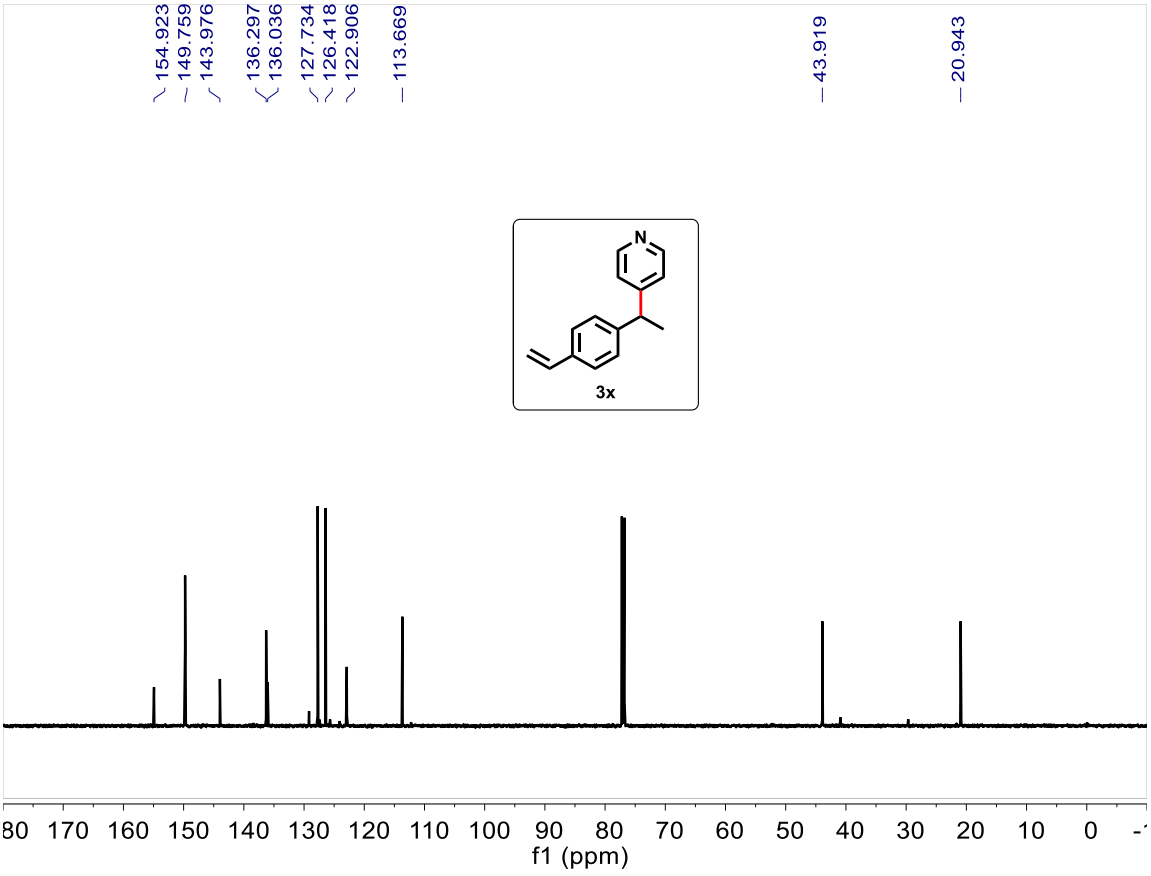
7.356
7.343
7.153
7.140
7.128
7.121
6.708
6.690
6.679
6.661
5.726
5.697
5.226
5.208
4.116
4.104
4.092
4.080
1.633
1.621
N
3x
2.19
2.09
2.14
2.02
1.06
1.07
1.04
1.00
3.23
f1 (ppm)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143.976
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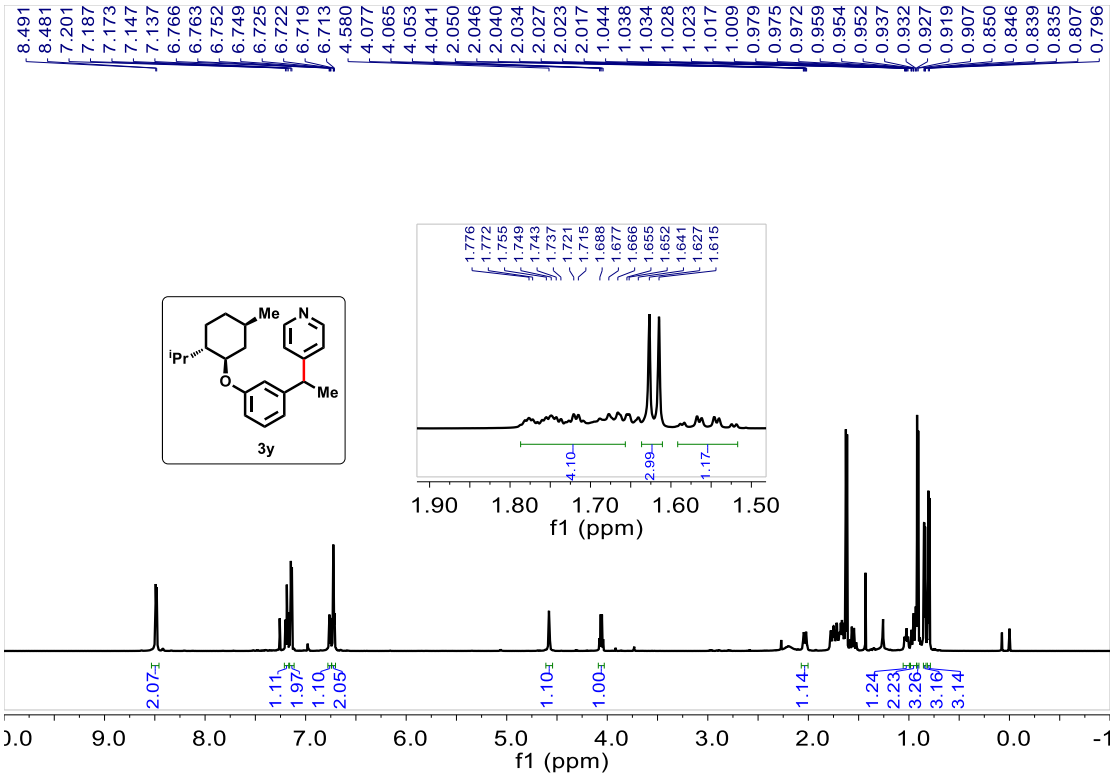
126.418
122.906
113.669
43.919
20.943
N
3x
f1 (ppm)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7.187
7.173
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7.137
6.766
6.763
6.752
6.749
6.725
6.722
6.719
6.713
4.580
4.077
4.065
4.053
4.041
2.050
2.046
2.040
2.034
2.027
2.023
2.017
1.044
1.038
1.034
1.028
1.023
1.017
1.009
0.979
0.975
0.972
0.959
0.954
0.952
0.937
0.932
0.927
0.919
0.907
0.850
0.846
0.839
0.835
0.807
0.796
Me
N
iPr
O
Me
3y
1.776
1.772
1.755
1.749
1.743
1.737
1.721
1.715
1.688
1.677
1.666
1.655
1.652
1.641
1.627
1.615
4.10
2.99
1.17
1.90
1.80
1.70
1.60
1.50
f1 (ppm)
2.07
1.11
1.97
1.10
2.05
1.10
1.00
1.14
1.24
2.23
3.26
3.16
3.14
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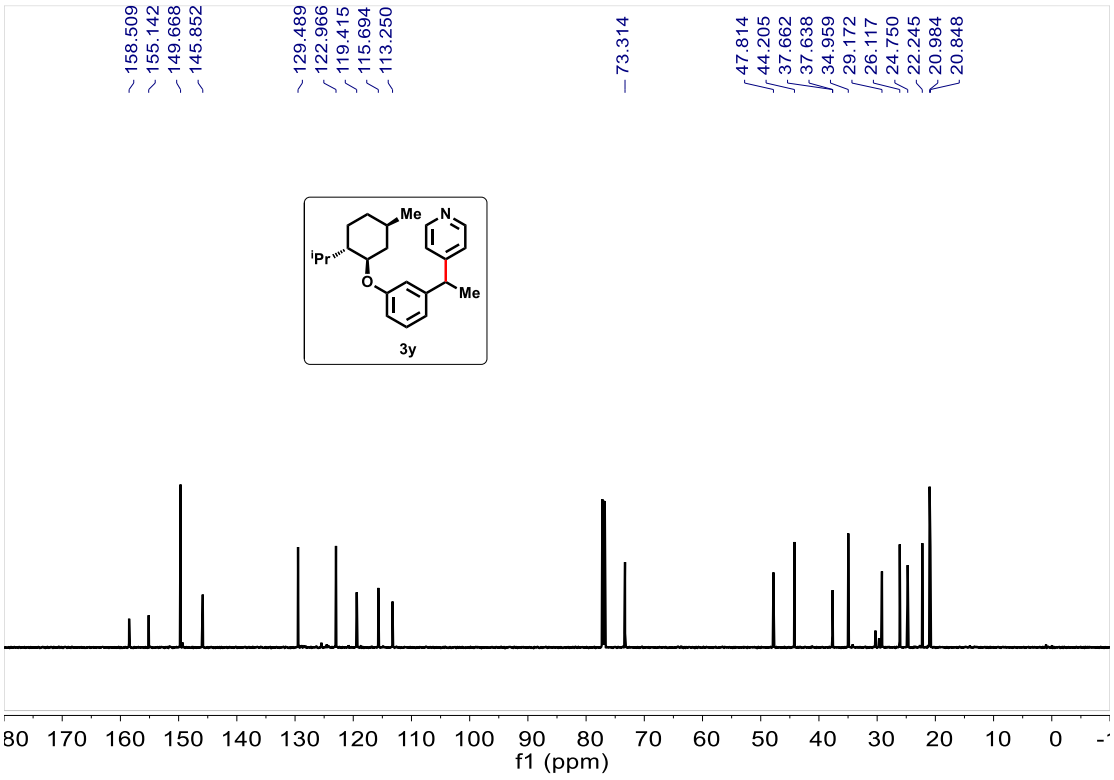
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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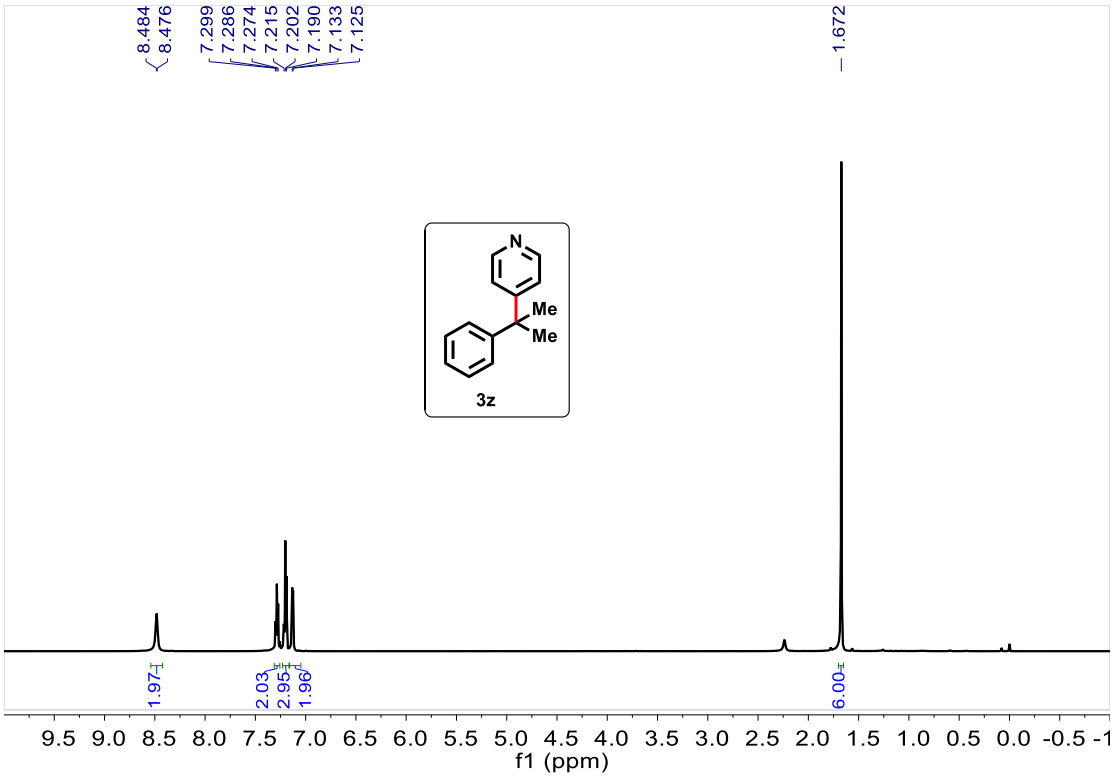
115.694
113.250
73.314
47.814
44.205
37.662
37.638
34.959
29.172
26.117
24.750
22.245
20.984
20.848
Me
N
iPr
O
Me
3y
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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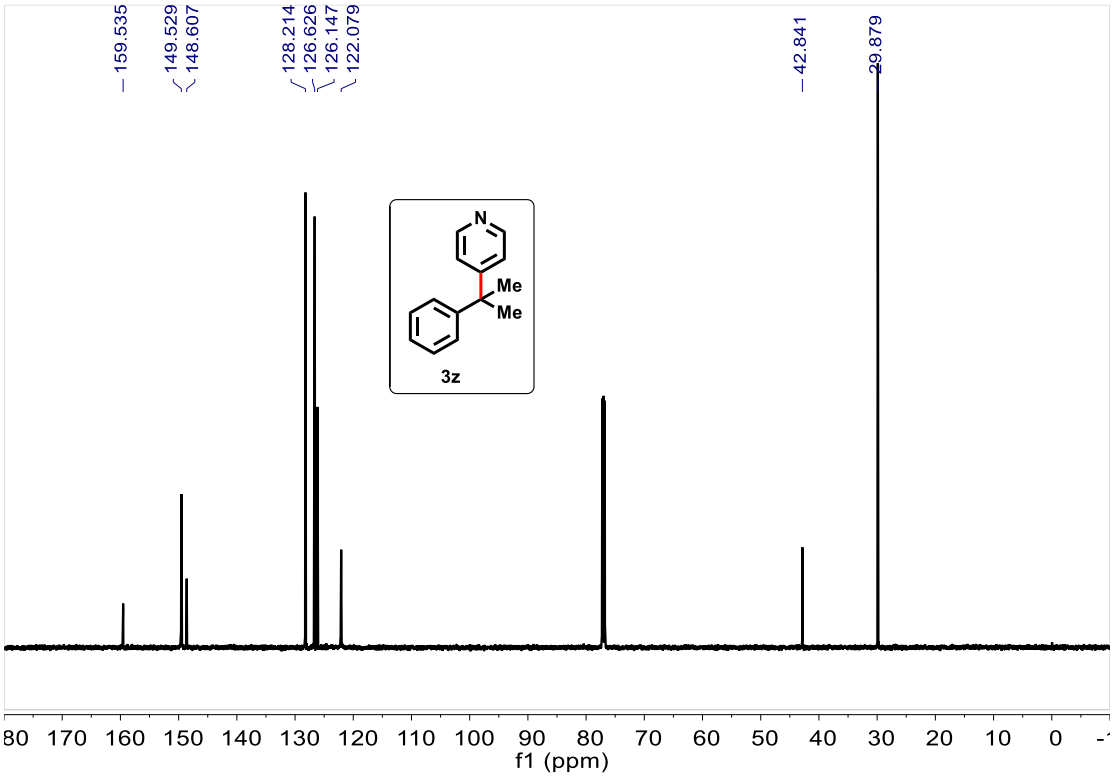
7.274
7.215
7.202
7.190
7.133
7.125
1.672
N
Me
Me
3z
1.97
2.03
2.95
1.96
6.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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126.147
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42.841
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N
Me
Me
3z
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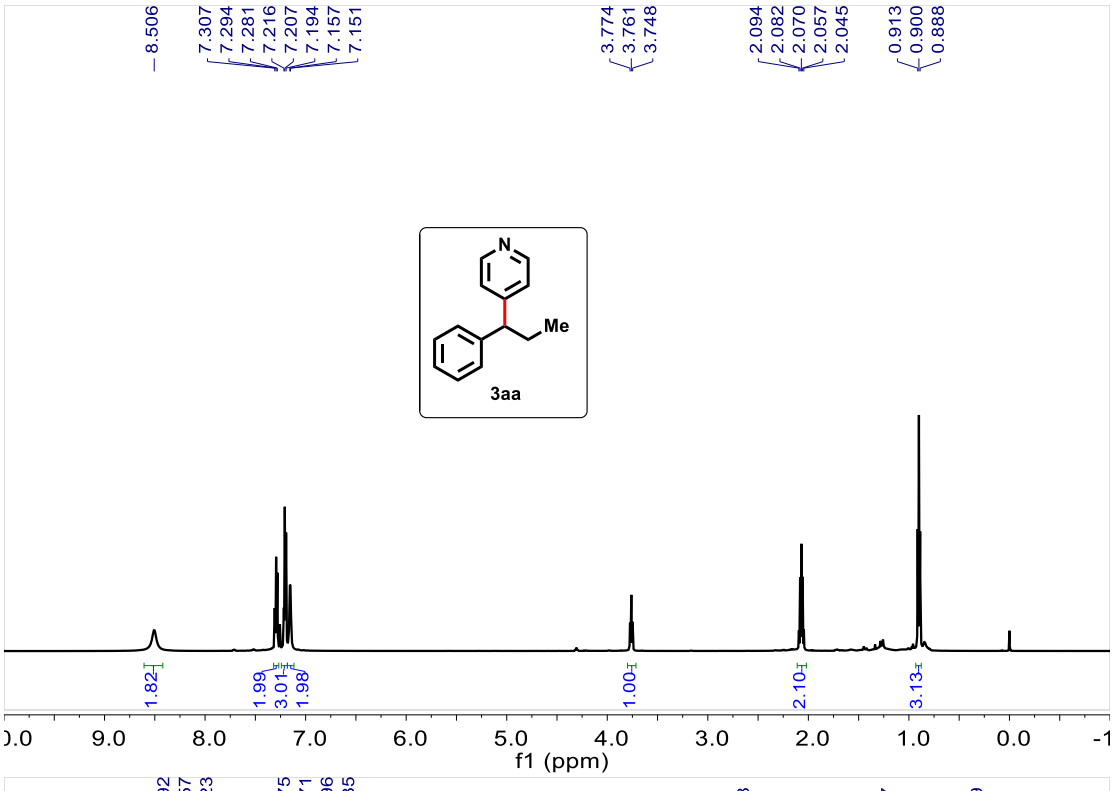
f1 (ppm)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7.194
7.157
7.151
3.774
3.761
3.748
2.094
2.082
2.070
2.057
2.045
0.913
0.900
0.888
N
Me
3aa
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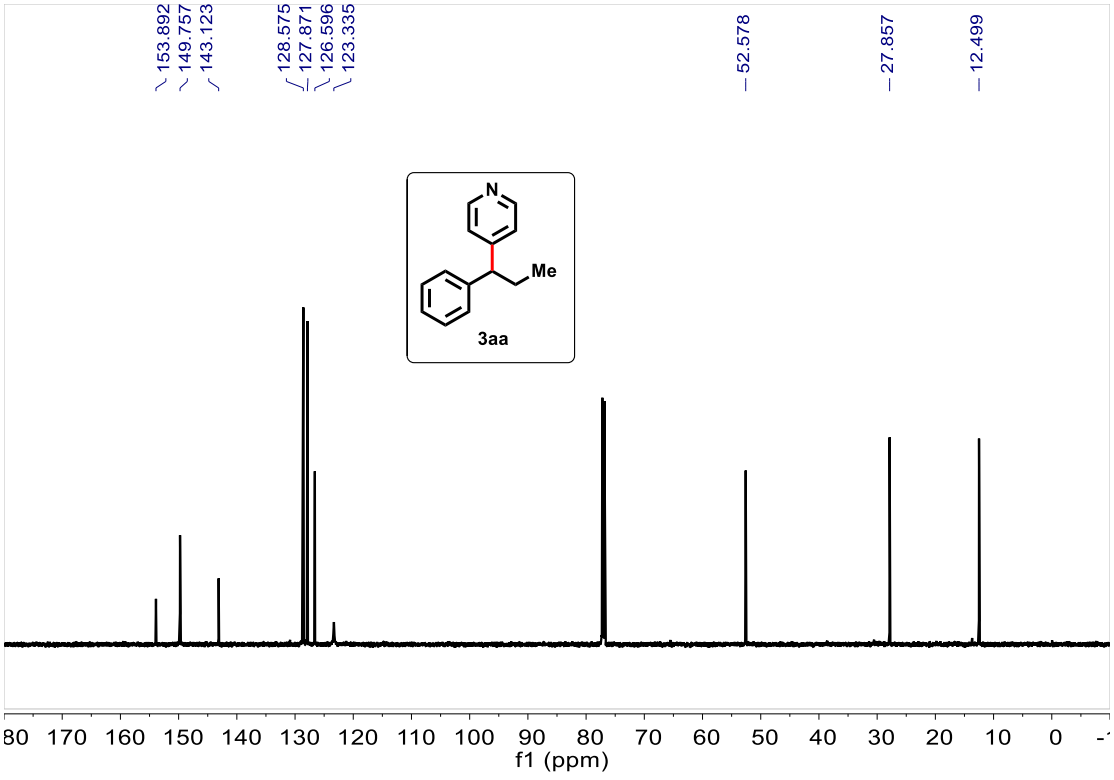
1.99
3.01
1.98
1.00
2.10
3.13
f1 (ppm)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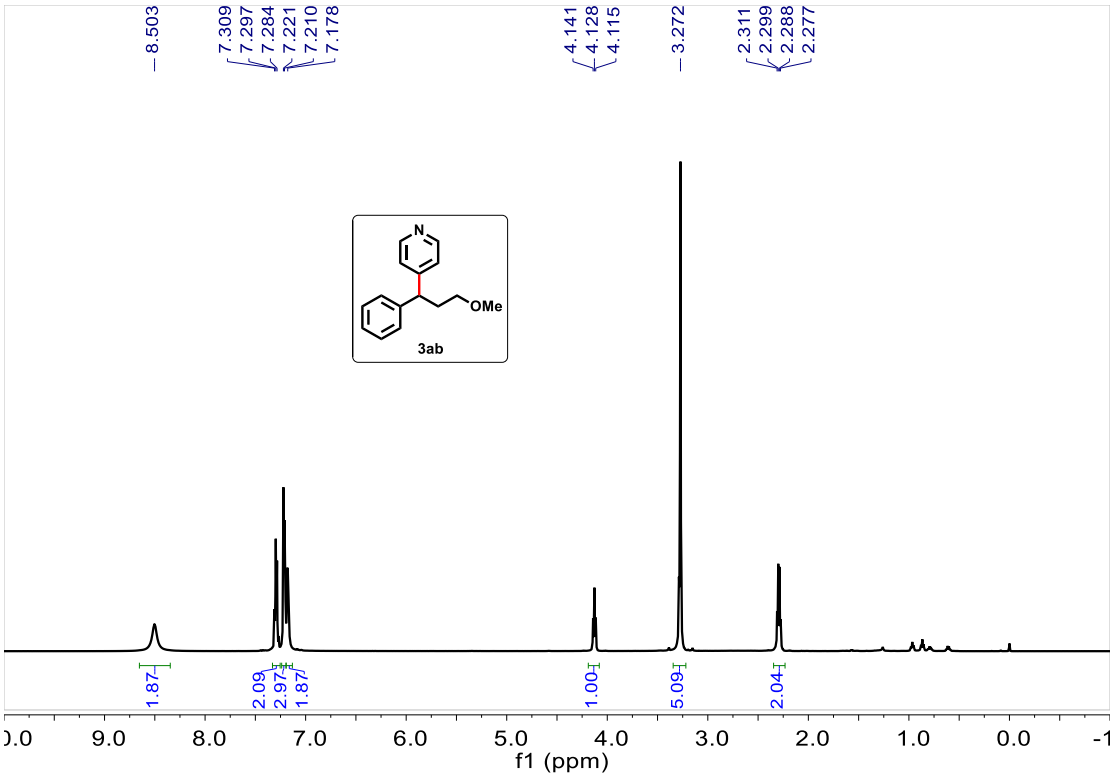
52.578
27.857
12.499
N
Me
3aa
f1 (ppm)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7.284
7.221
7.210
7.178
4.141
4.128
4.115
3.272
2.311
2.299
2.288
2.277
OMe
3ab
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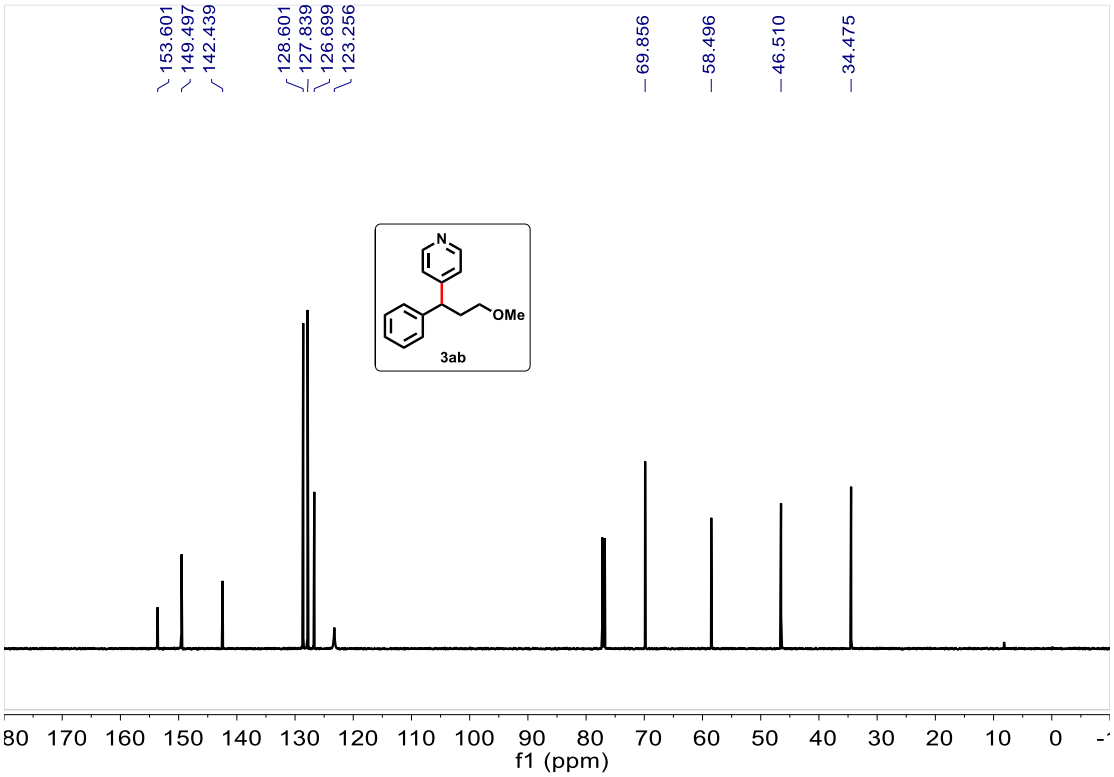
2.09
2.97
1.87
1.00
5.09
2.04
f1 (ppm)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46.510
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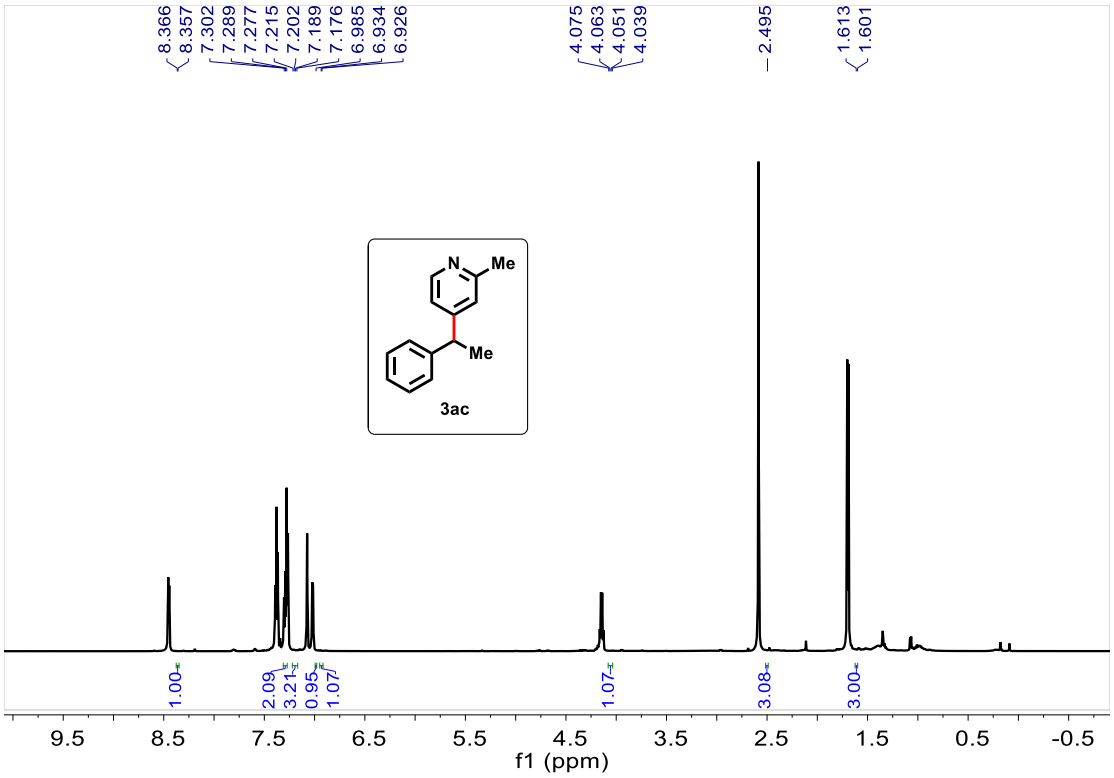
f1 (ppm)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6.934
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4.075
4.063
4.051
4.039
2.495
1.613
1.601
N
Me
Me
3ac
1.00
2.09
3.21
0.95
1.07
1.07
3.08
3.00
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
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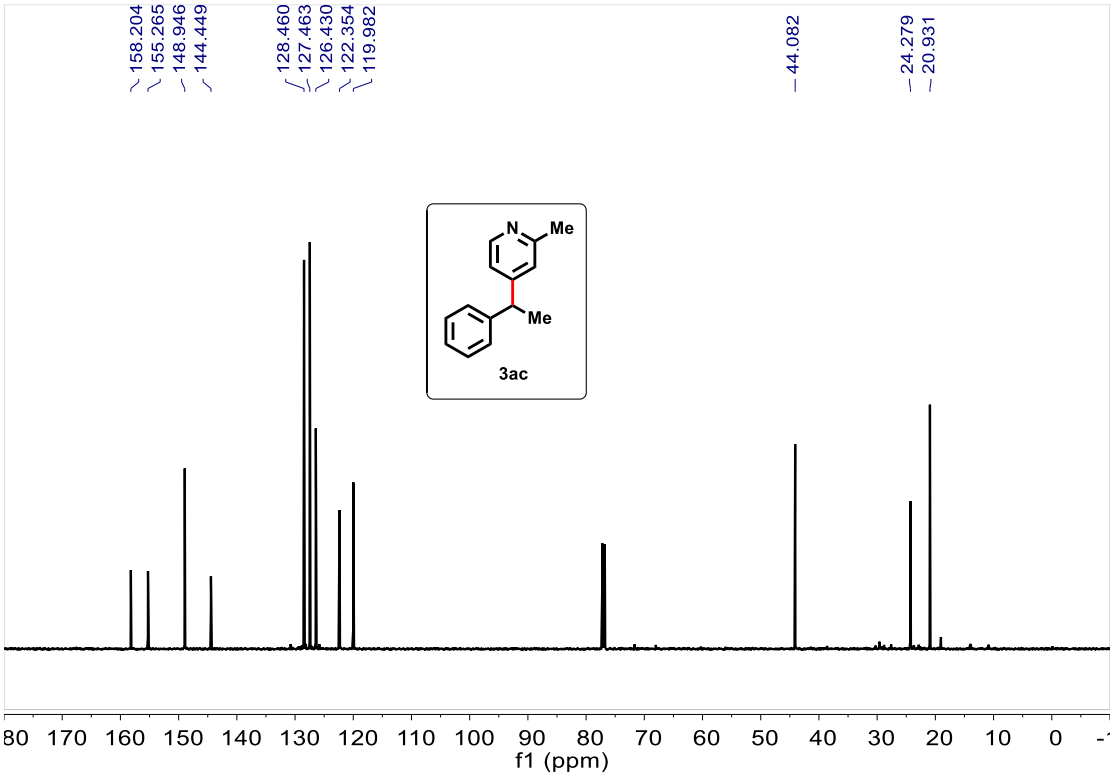
-0.5
f1 (ppm)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127.463
126.430
122.354
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24.279
20.931
N
Me
Me
3ac
80
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120
110
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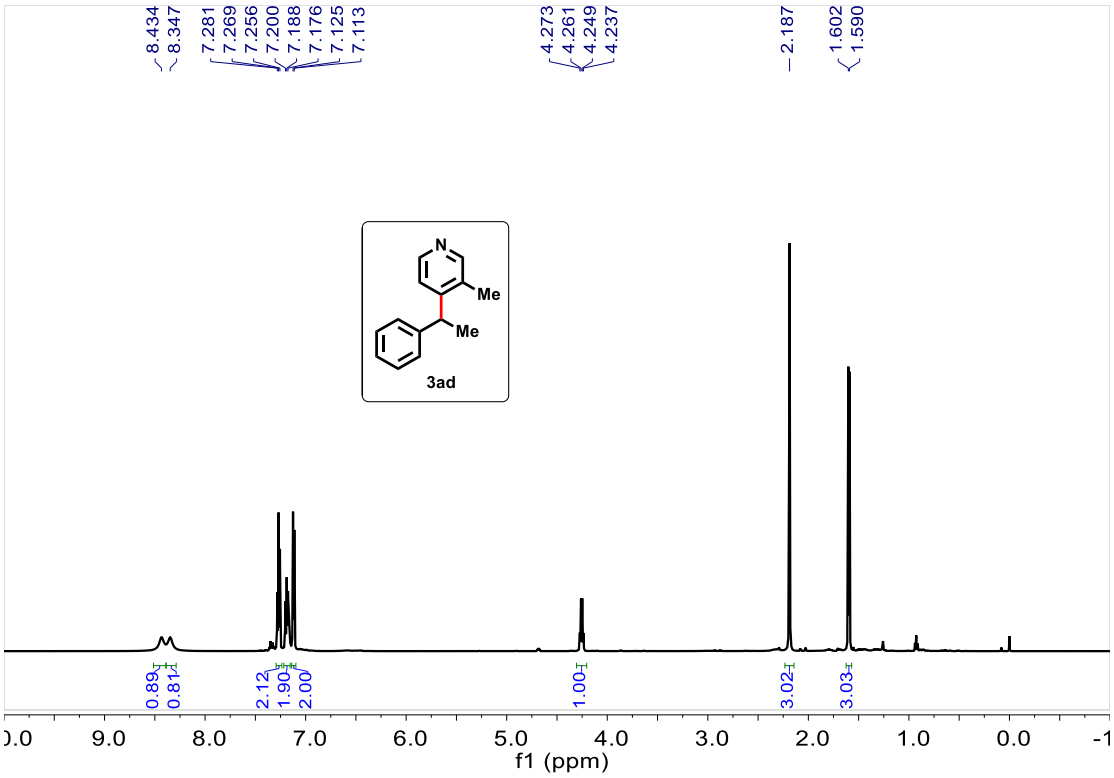
f1 (ppm)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7.176
7.125
7.113
4.273
4.261
4.249
4.237
2.187
1.602
1.590
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Me
Me
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1.00
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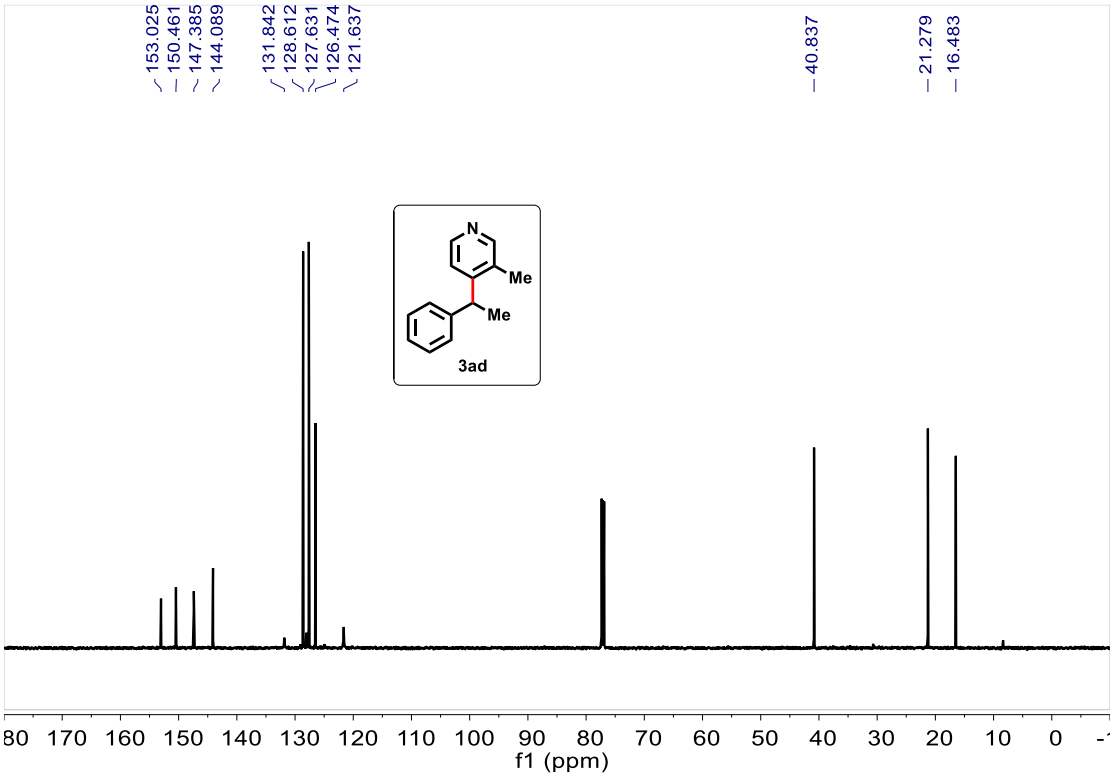
3.03
f1 (ppm)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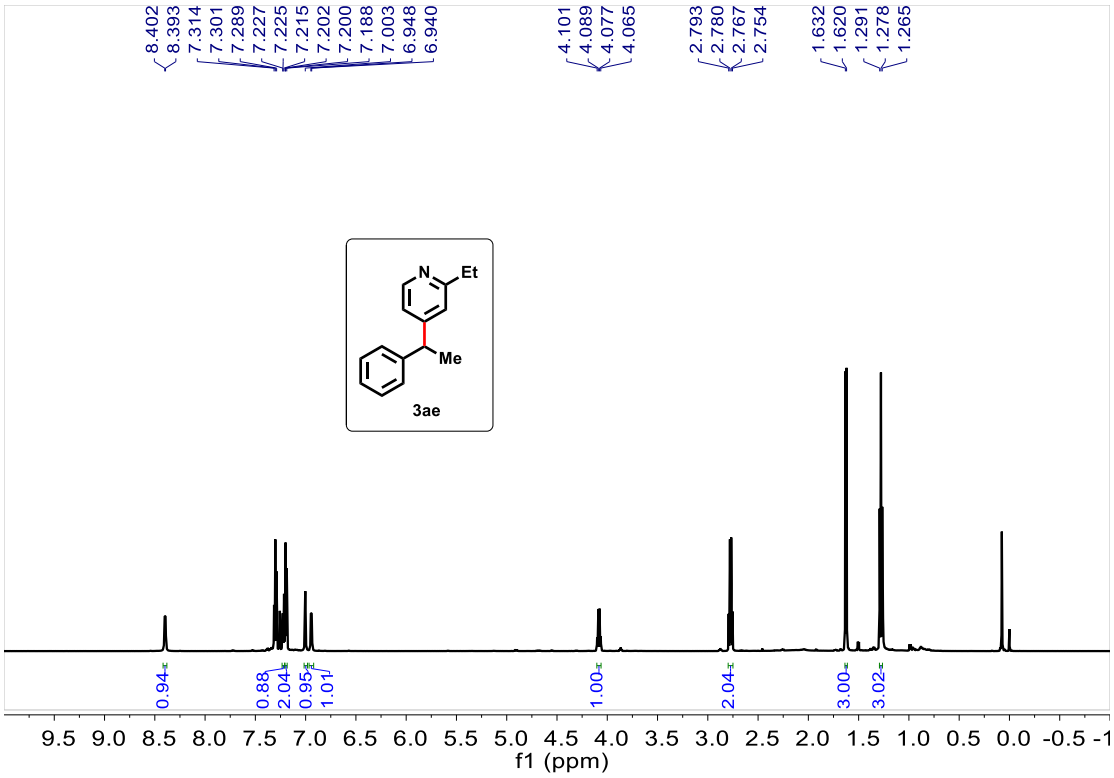
Me
Me
3ad
f1 (ppm)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7.200
7.188
7.003
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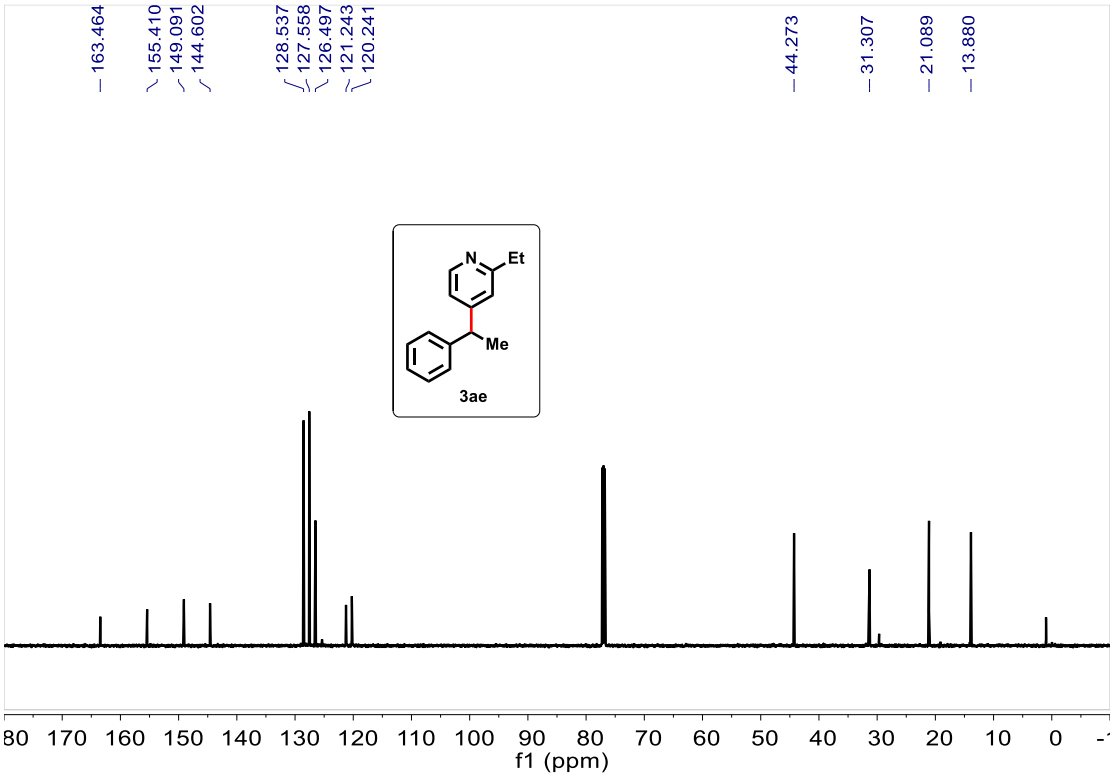
6.940
4.101
4.089
4.077
4.065
2.793
2.780
2.767
2.754
1.632
1.620
1.291
1.278
1.265
N
Et
Me
3ae
0.94
0.88
2.04
0.95
1.01
1.00
2.04
3.00
3.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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144.602
128.537
127.558
126.497
121.243
120.241
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31.307
21.089
13.880
N
Et
Me
3ae
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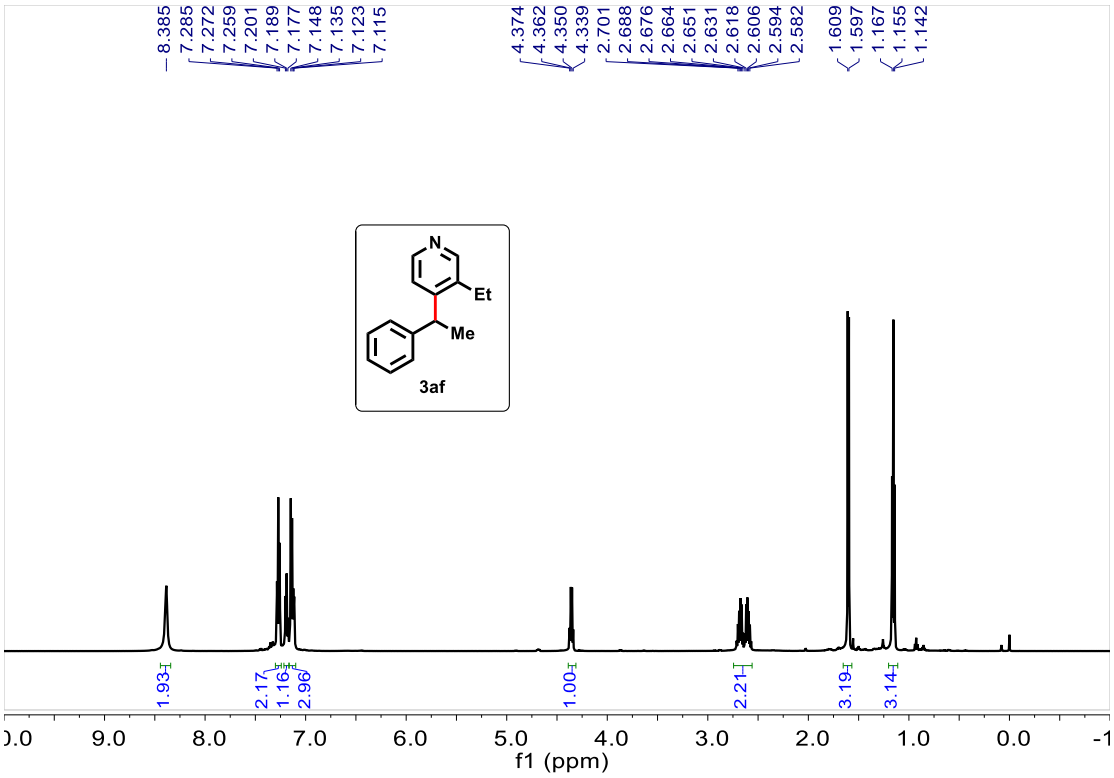
f1 (ppm)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4.350
4.339
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2.631
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2.582
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1.167
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Et
Me
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2.0
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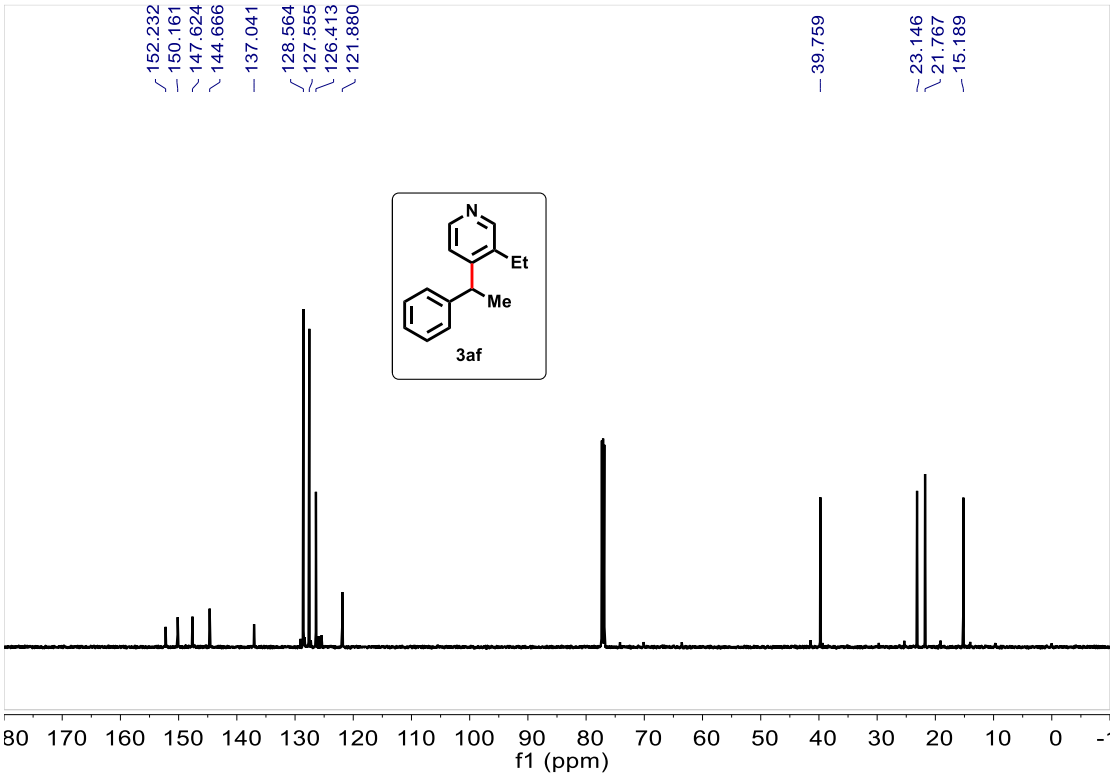
f1 (ppm)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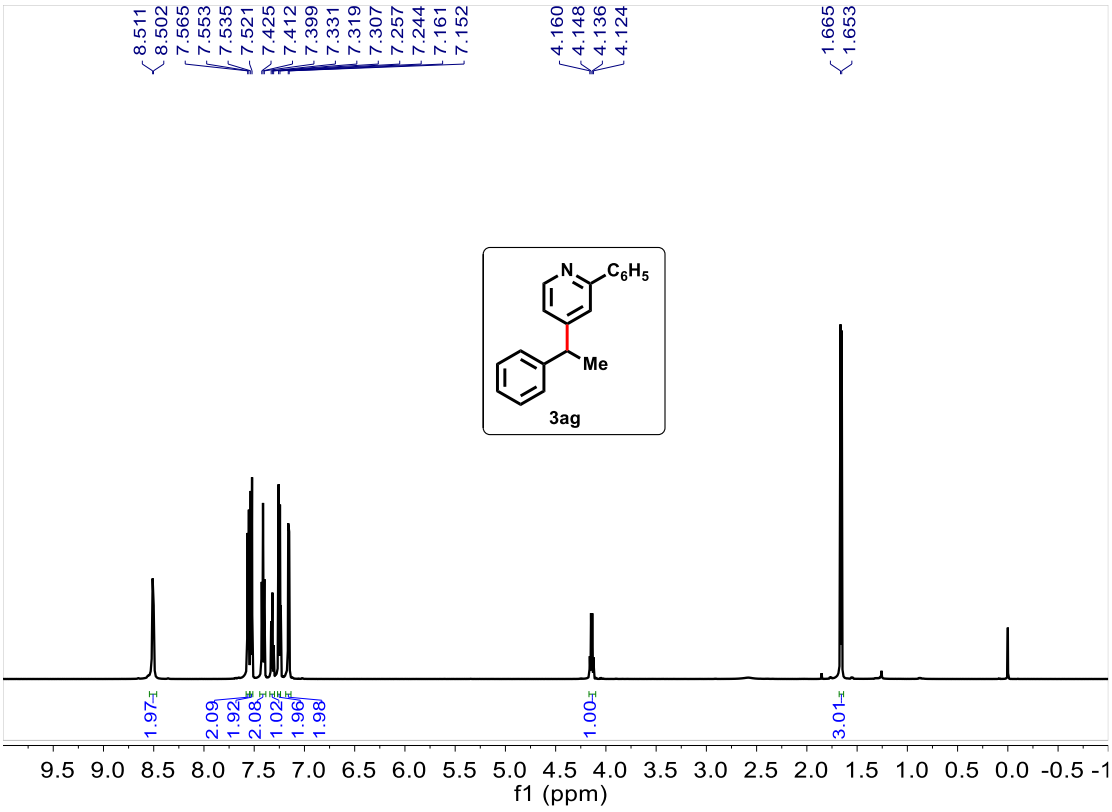
147.624
144.666
137.041
128.564
127.555
126.413
121.880
39.759
23.146
21.767
15.189
N
Et
Me
3af
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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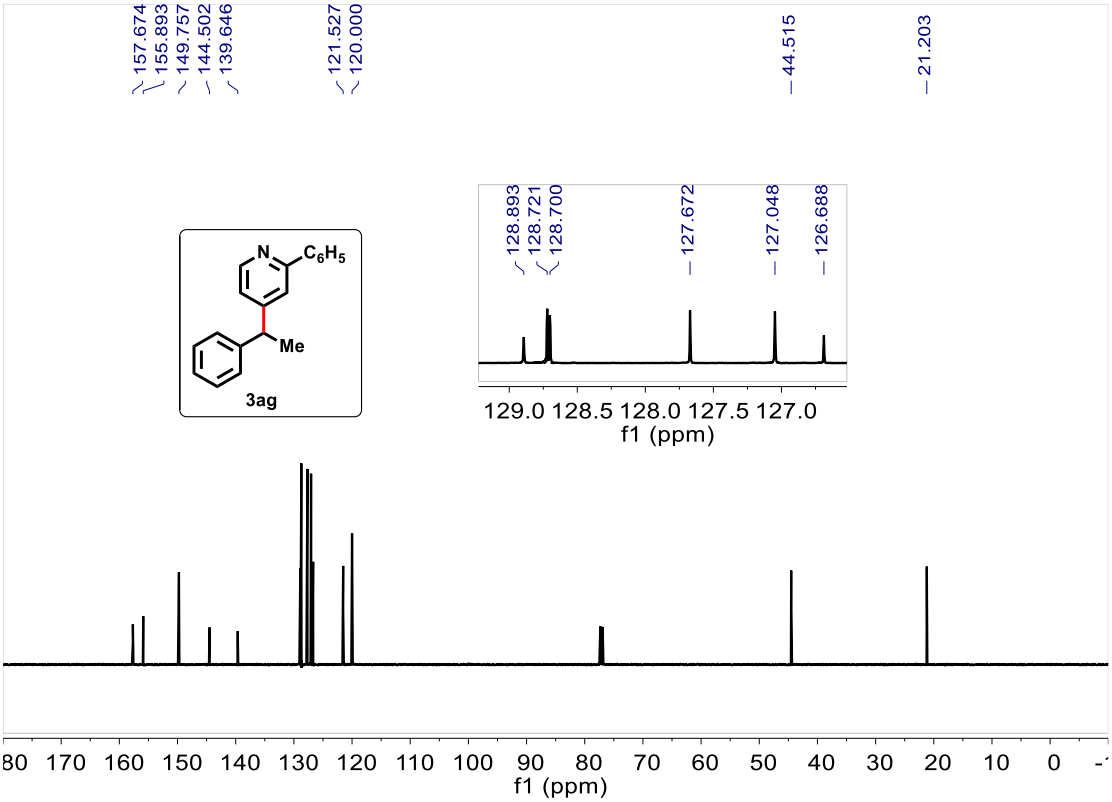
8.502
7.565
7.553
7.535
7.521
7.425
7.412
7.399
7.331
7.319
7.307
7.257
7.244
7.161
7.152
4.160
4.148
4.136
4.124
1.665
1.653
N
C6H5
Me
3ag
1.97
2.09
1.92
2.08
1.02
1.96
1.98
1.00
3.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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139.646
121.527
120.000
44.515
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128.721
128.700
127.672
127.048
126.688
N
C6H5
Me
3ag
129.0 128.5 128.0 127.5 127.0
f1 (ppm)
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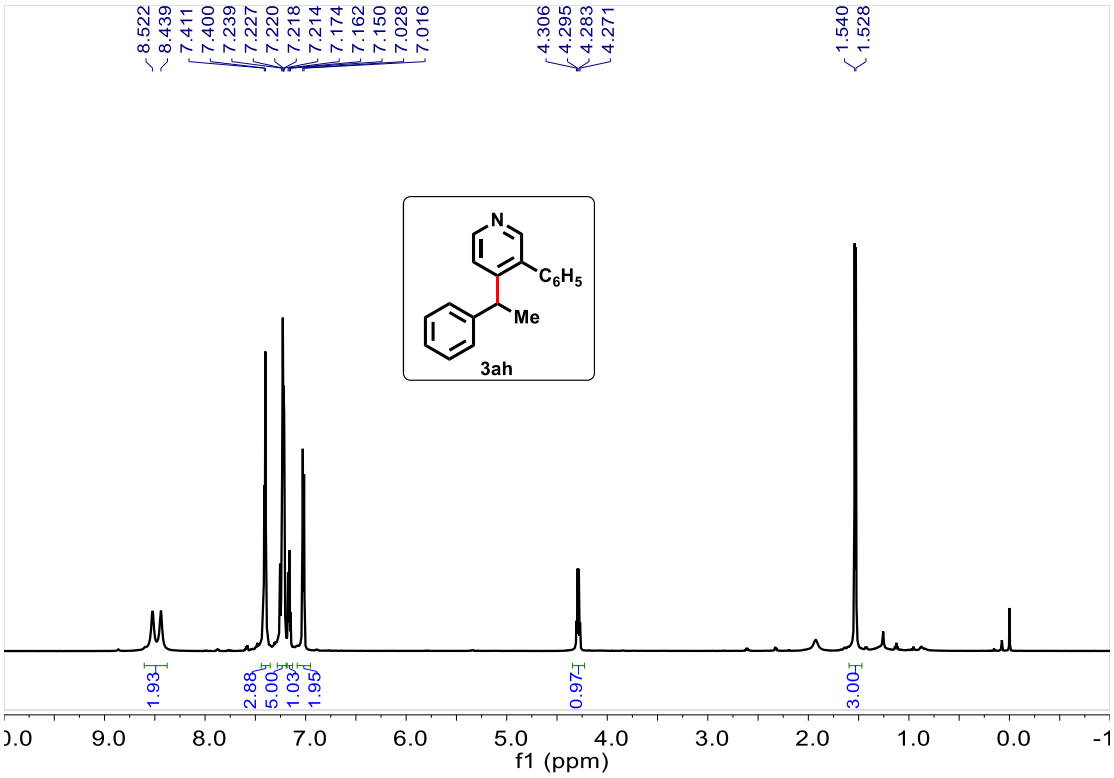
f1 (ppm)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8.439
7.411
7.400
7.239
7.227
7.220
7.218
7.214
7.174
7.162
7.150
7.028
7.016
4.306
4.295
4.283
4.271
1.540
1.528
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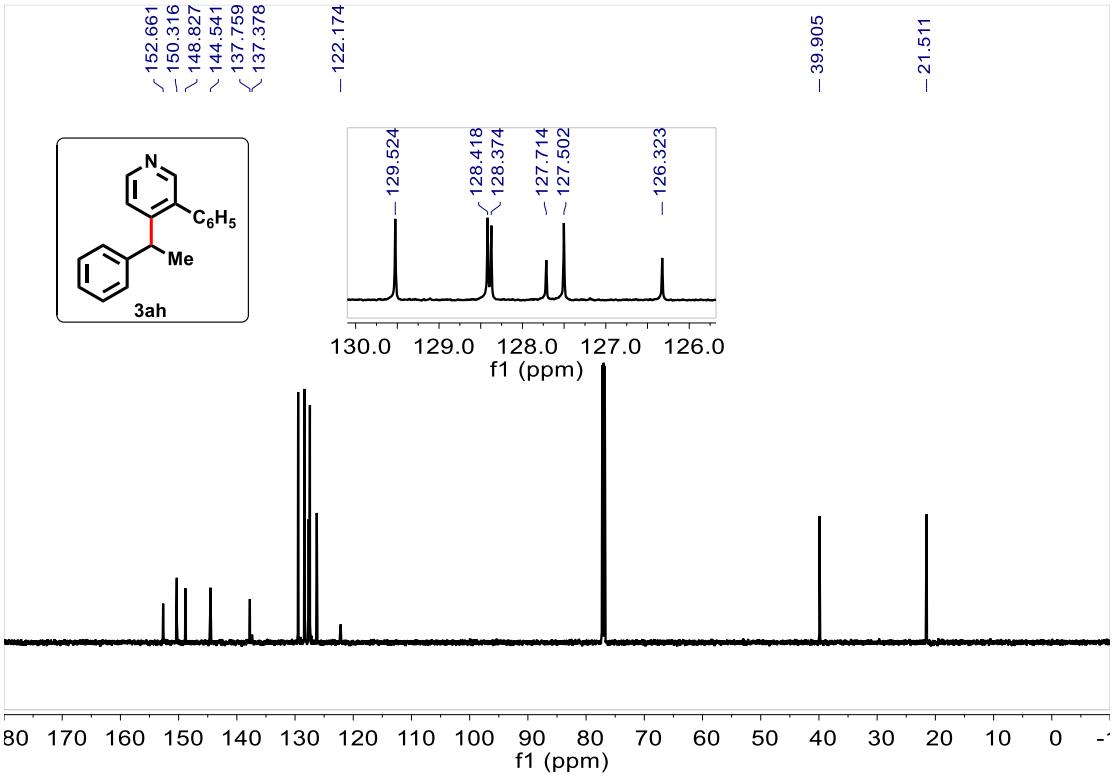
C6H5
Me
3ah
1.93
2.88
5.00
1.03
1.95
0.97
3.00
f1 (ppm)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150.316
148.827
144.541
137.759
137.378
122.174
39.905
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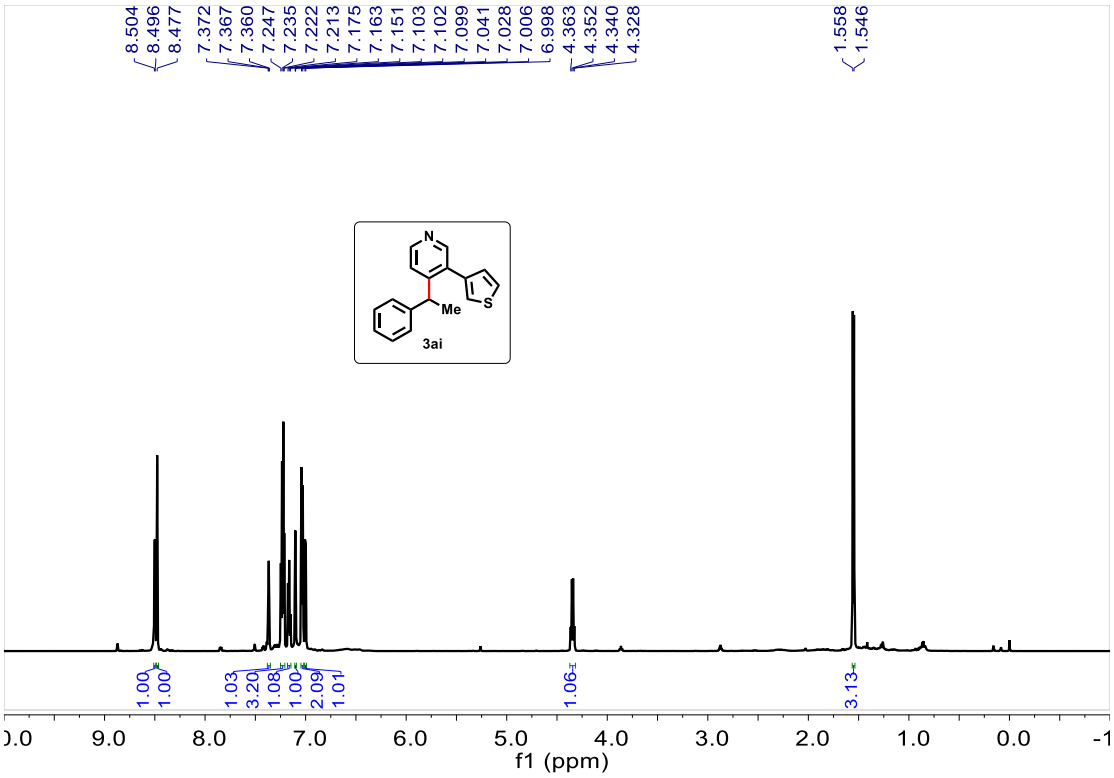
128.374
127.714
127.502
126.323
N
C6H5
Me
3ah
f1 (ppm)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8.477
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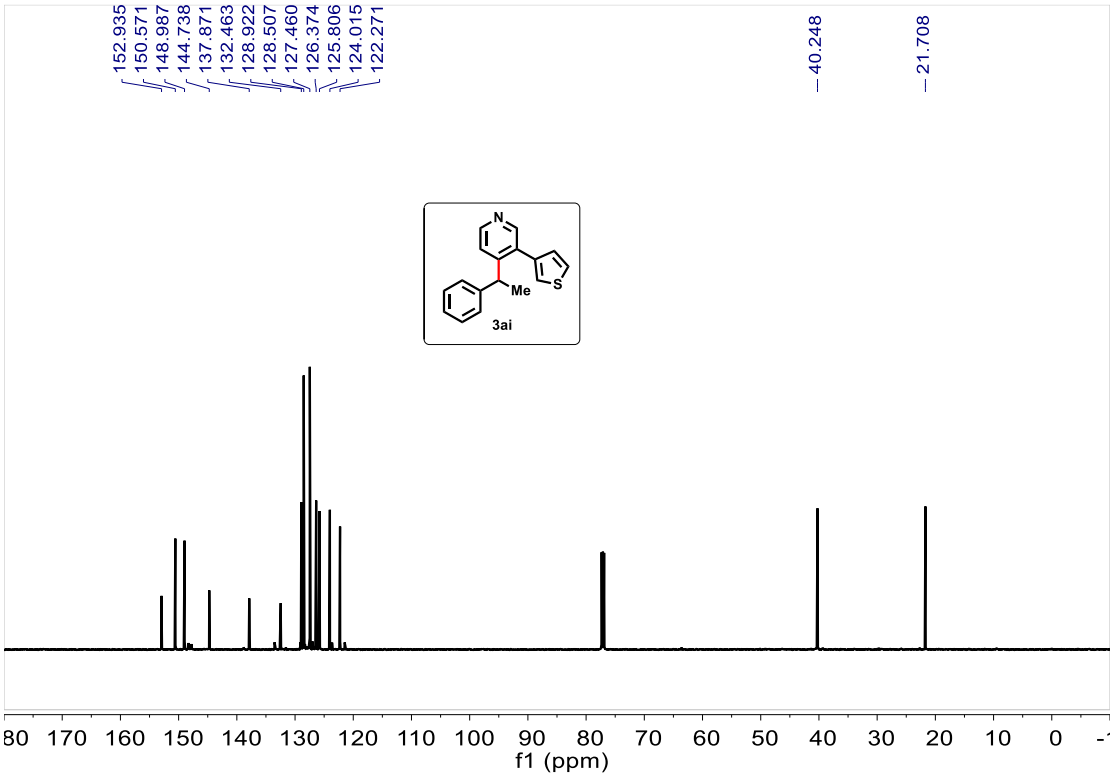
7.367
7.360
7.247
7.235
7.222
7.213
7.175
7.163
7.151
7.103
7.102
7.099
7.041
7.028
7.006
6.998
4.363
4.352
4.340
4.328
1.558
1.546
N
S
Me
3ai
1.00
1.00
1.03
3.20
1.08
1.00
2.09
1.01
1.06
3.13
f1 (ppm)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150.571
148.987
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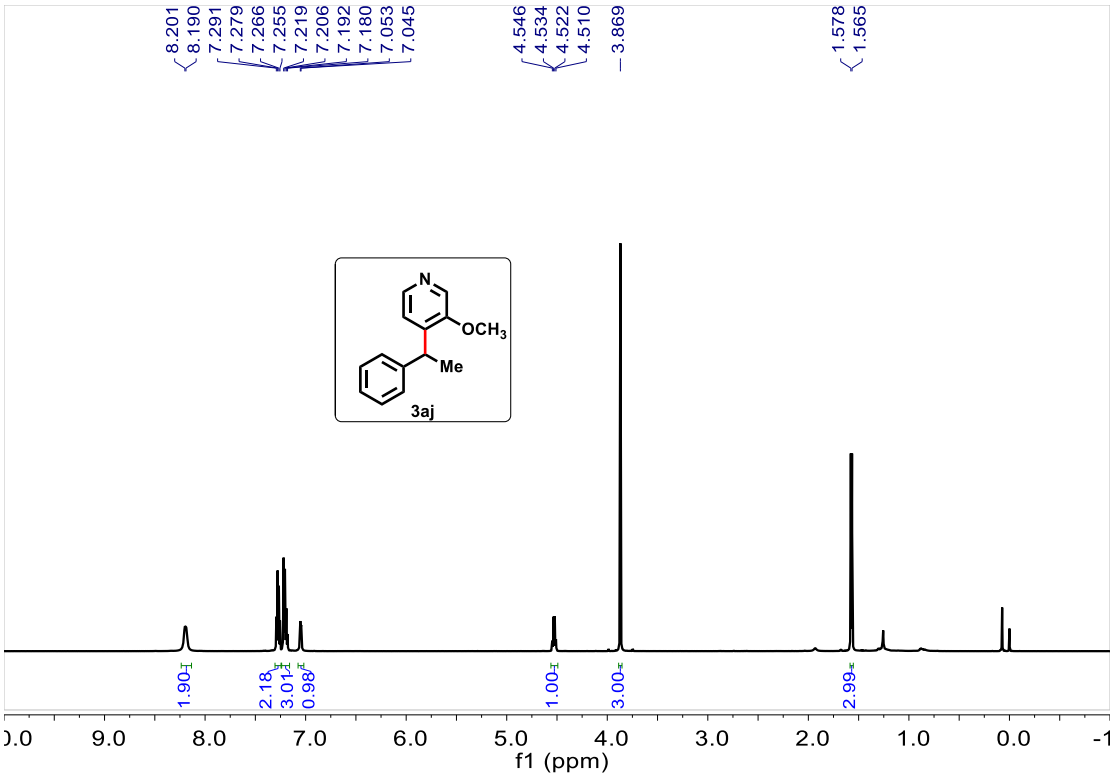
127.460
126.374
125.806
124.015
122.271
40.248
21.708
N
S
Me
3ai
f1 (ppm)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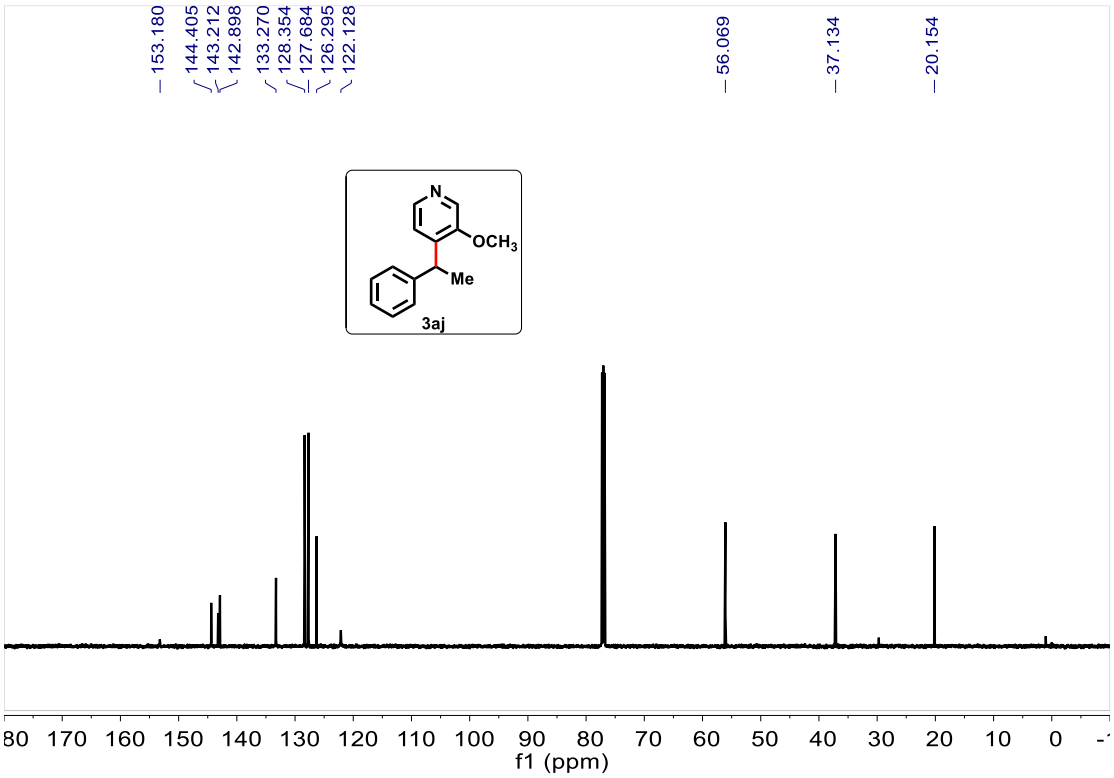
8.190
7.291
7.279
7.266
7.255
7.219
7.206
7.192
7.180
7.053
7.045
4.546
4.534
4.522
4.510
3.869
1.578
1.565
N
OCH3
Me
3aj
1.90
2.18
3.01
0.98
1.00
3.00
2.99
f1 (ppm)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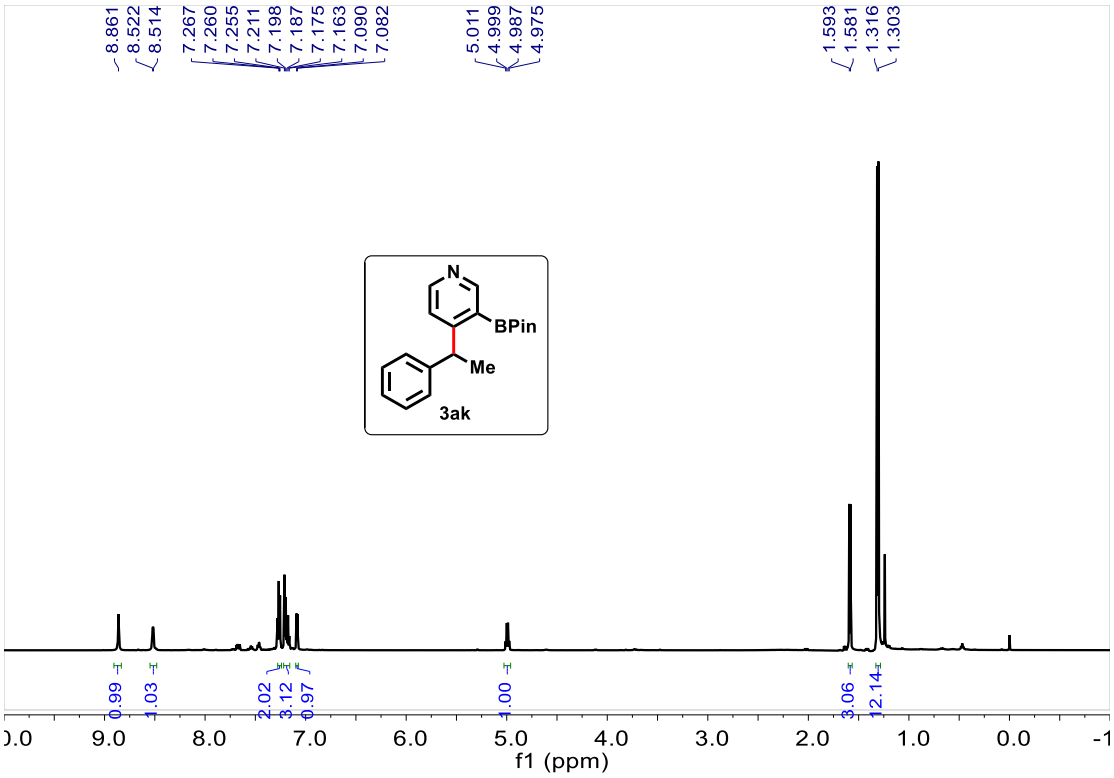
144.405
143.212
142.898
133.270
128.354
127.684
126.295
122.128
56.069
37.134
20.154
N
OCH3
Me
3aj
f1 (ppm)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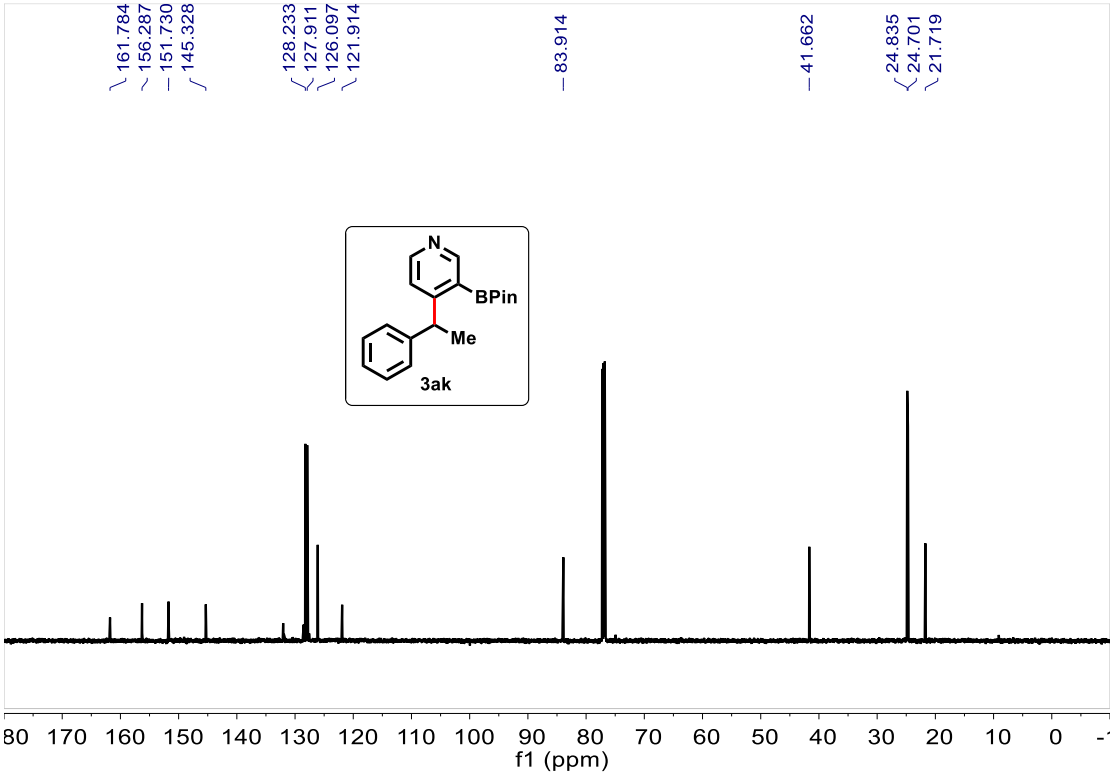
8.522
8.514
7.267
7.260
7.255
7.211
7.198
7.187
7.175
7.163
7.090
7.082
5.011
4.999
4.987
4.975
1.593
1.581
1.316
1.303
N
BPin
Me
3ak
0.99
1.03
2.02
3.12
0.97
1.00
3.06
12.14
f1 (ppm)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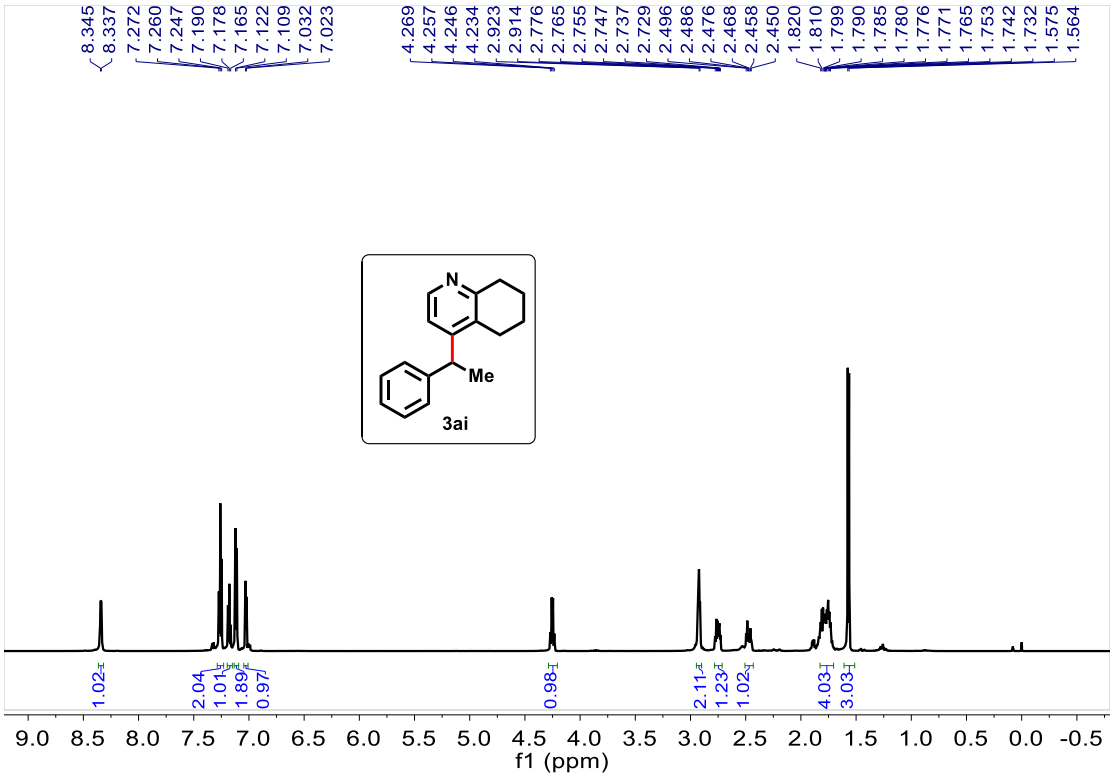
156.287
151.730
145.328
128.233
127.911
126.097
121.914
83.914
41.662
24.835
24.701
21.719
N
BPin
Me
3ak
f1 (ppm)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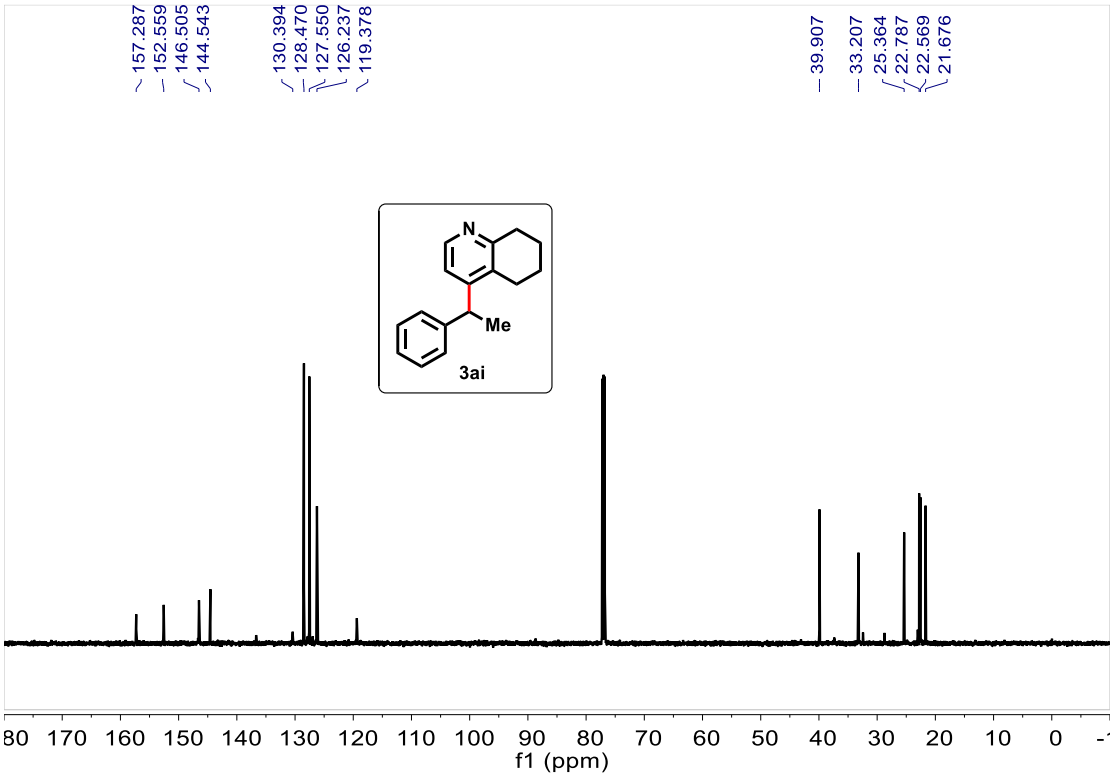
8.337
7.272
7.260
7.247
7.190
7.178
7.165
7.122
7.109
7.032
7.023
4.269
4.257
4.246
4.234
2.923
2.914
2.776
2.765
2.755
2.747
2.737
2.729
2.496
2.486
2.476
2.468
2.458
2.450
1.820
1.810
1.799
1.790
1.785
1.780
1.776
1.771
1.765
1.753
1.742
1.732
1.575
1.564
N
Me
3ai
1.02
2.04
1.01
1.89
0.97
0.98
2.11
1.23
1.02
4.03
3.03
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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146.505
144.543
130.394
128.470
127.550
126.237
119.378
39.907
33.207
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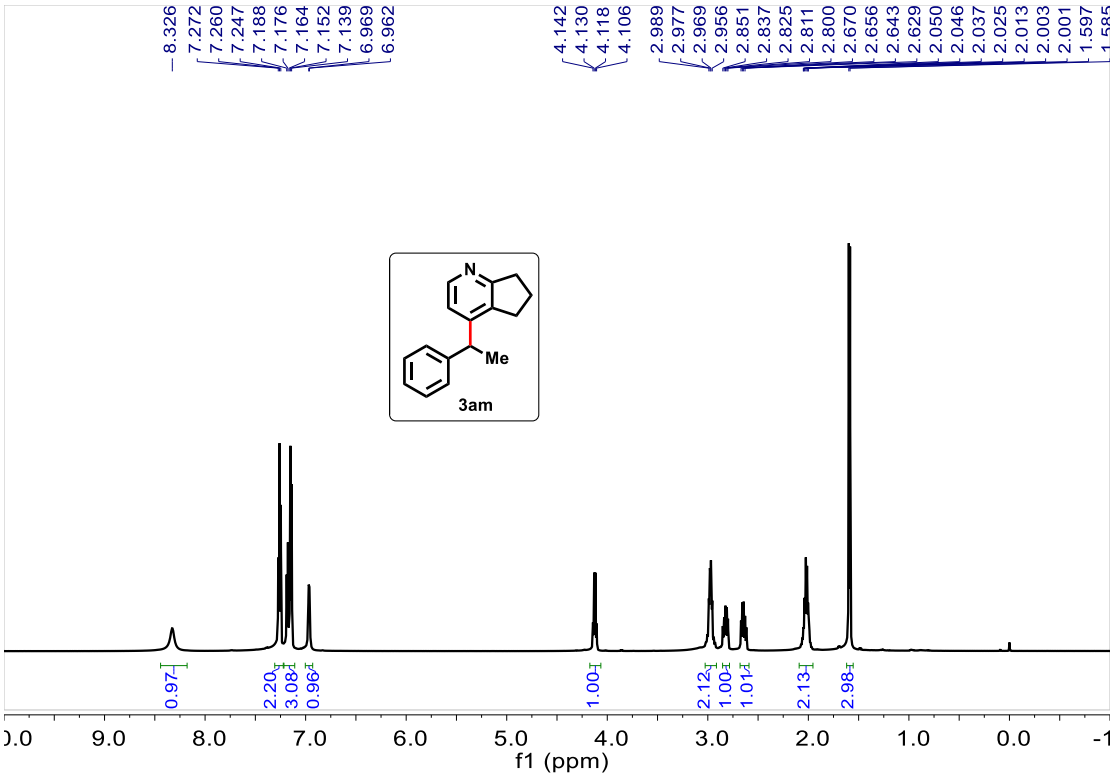
22.787
22.569
21.676
N
Me
3ai
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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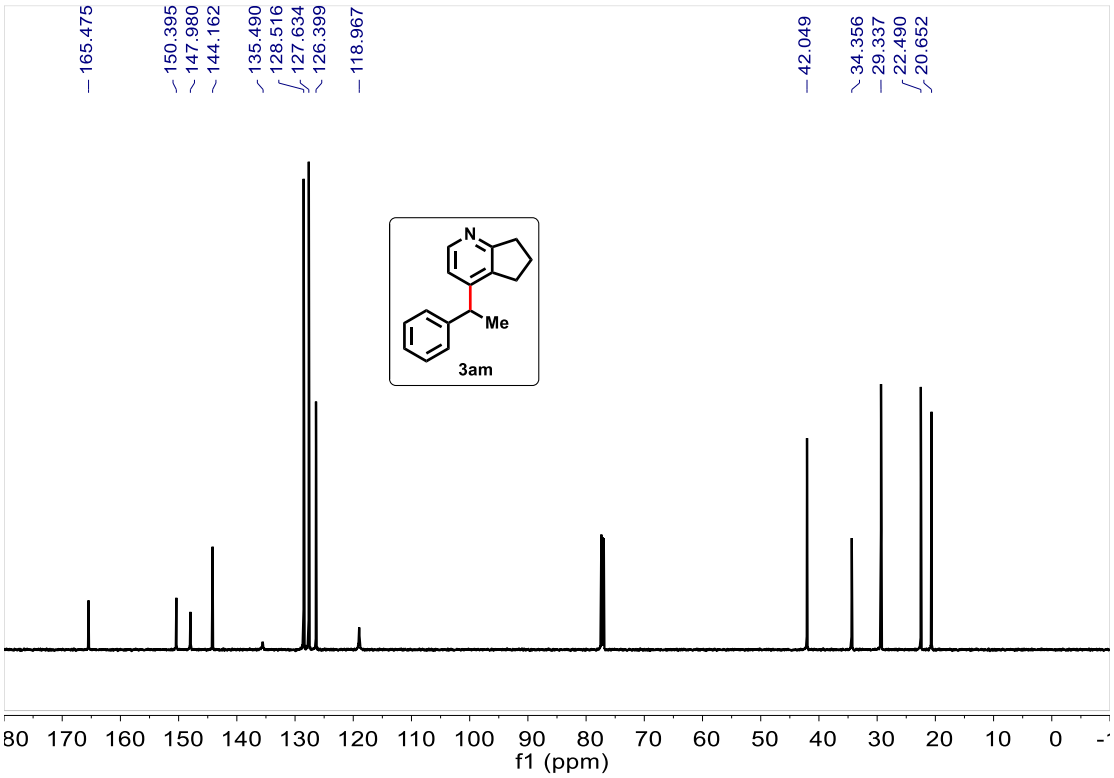
7.272
7.260
7.247
7.188
7.176
7.164
7.152
7.139
6.969
6.962
4.142
4.130
4.118
4.106
2.989
2.977
2.969
2.956
2.851
2.837
2.825
2.811
2.800
2.670
2.656
2.643
2.629
2.050
2.046
2.037
2.025
2.013
2.003
2.001
1.597
N
Me
3am
0.97
2.20
3.08
0.96
1.00
2.12
1.00
1.01
2.13
2.98
f1 (ppm)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135.490
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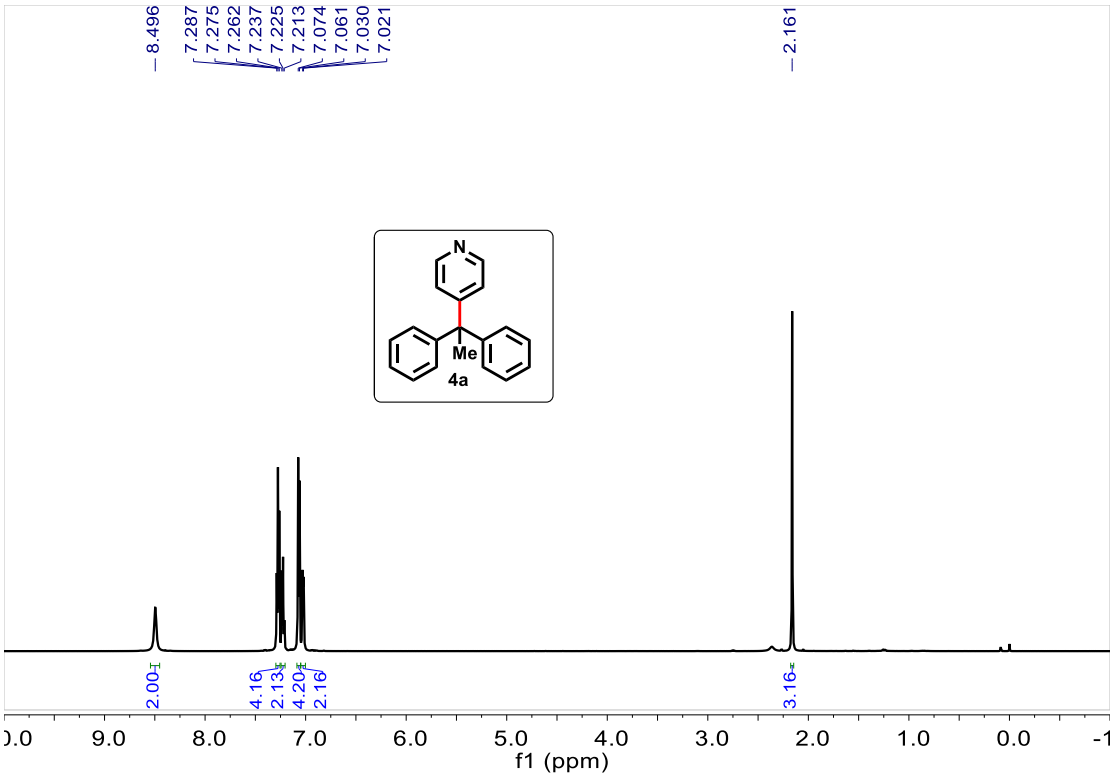
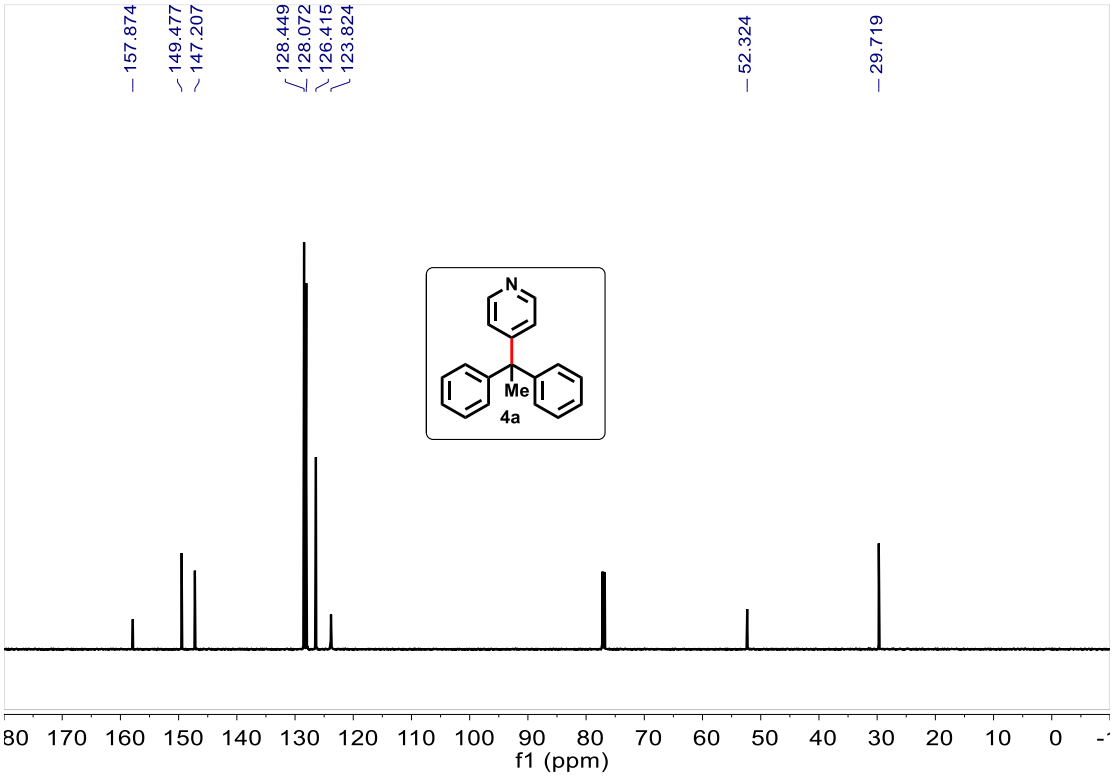
126.399
118.967
42.049
34.356
29.337
22.490
20.652
N
Me
3am
f1 (ppm)


8.496
7.287
7.275
7.262
7.237
7.225
7.213
7.074
7.061
7.030
7.021
2.161
N
Me
4a
2.00
4.16
2.13
4.20
2.16
3.16
f1 (ppm)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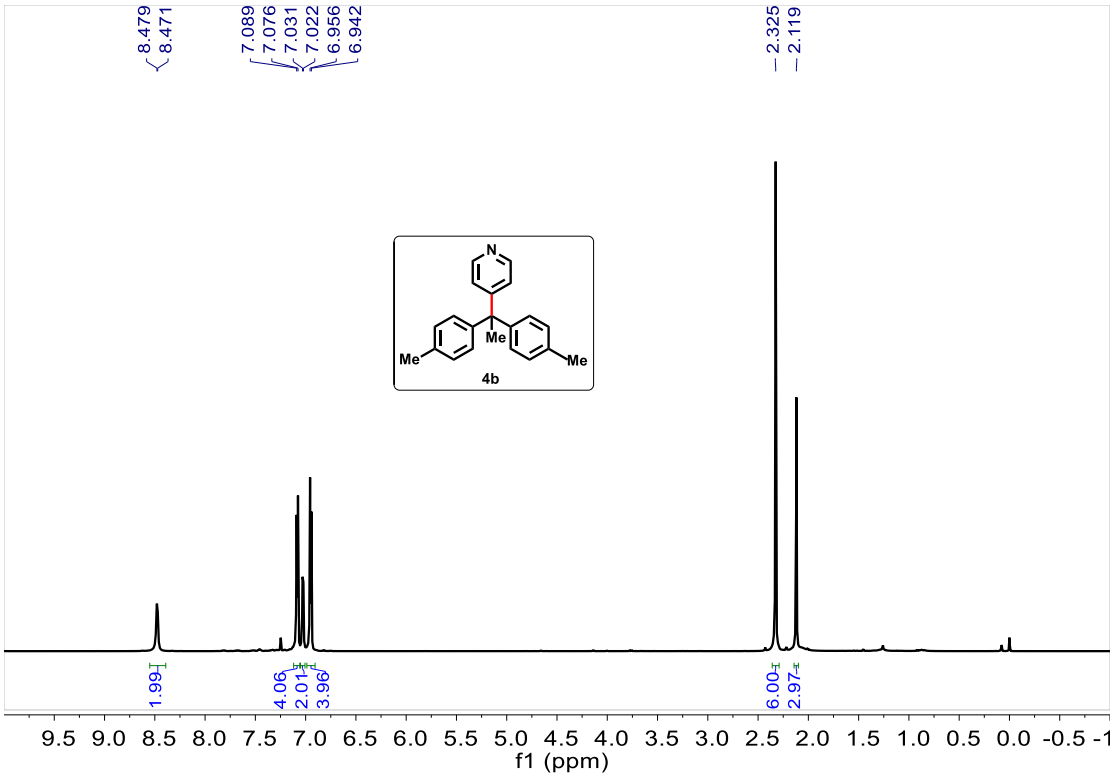
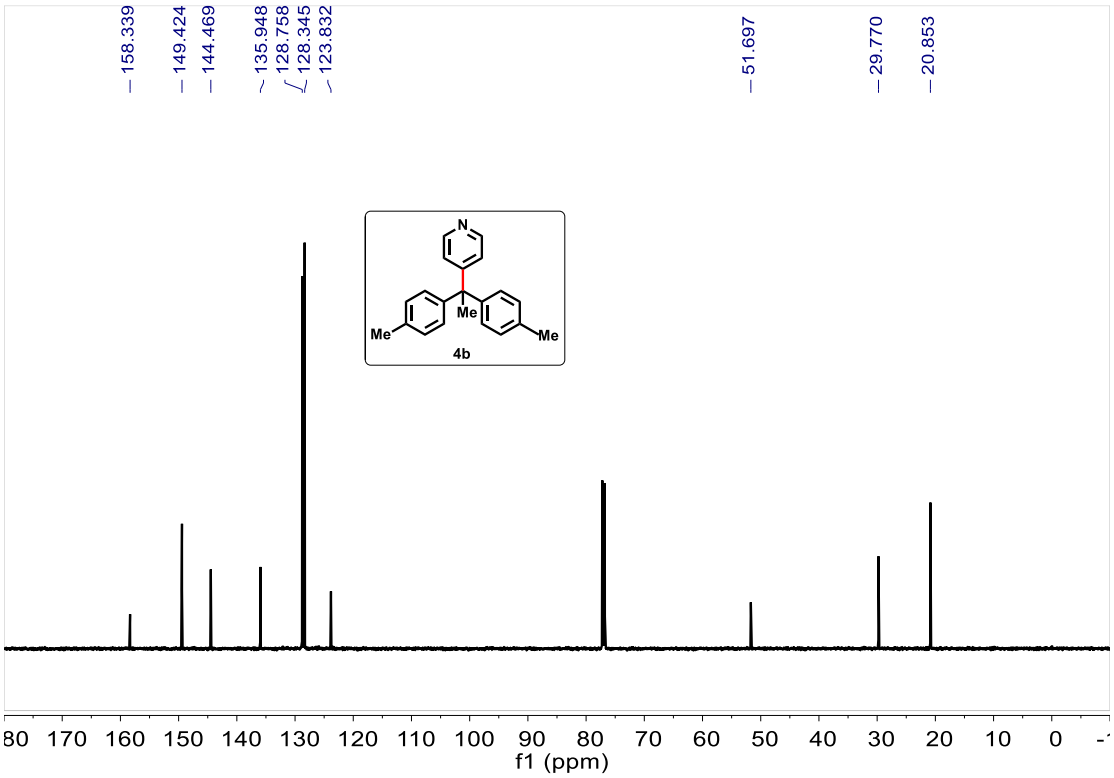
128.072
126.415
123.824
52.324
29.719
N
Me
4a
f1 (ppm)


8.479
8.471
7.089
7.076
7.031
7.022
6.956
6.942
2.325
2.119
N
Me
Me
Me
4b
1.99
4.06
2.01
3.96
6.00
2.97
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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135.948
128.758
128.345
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51.697
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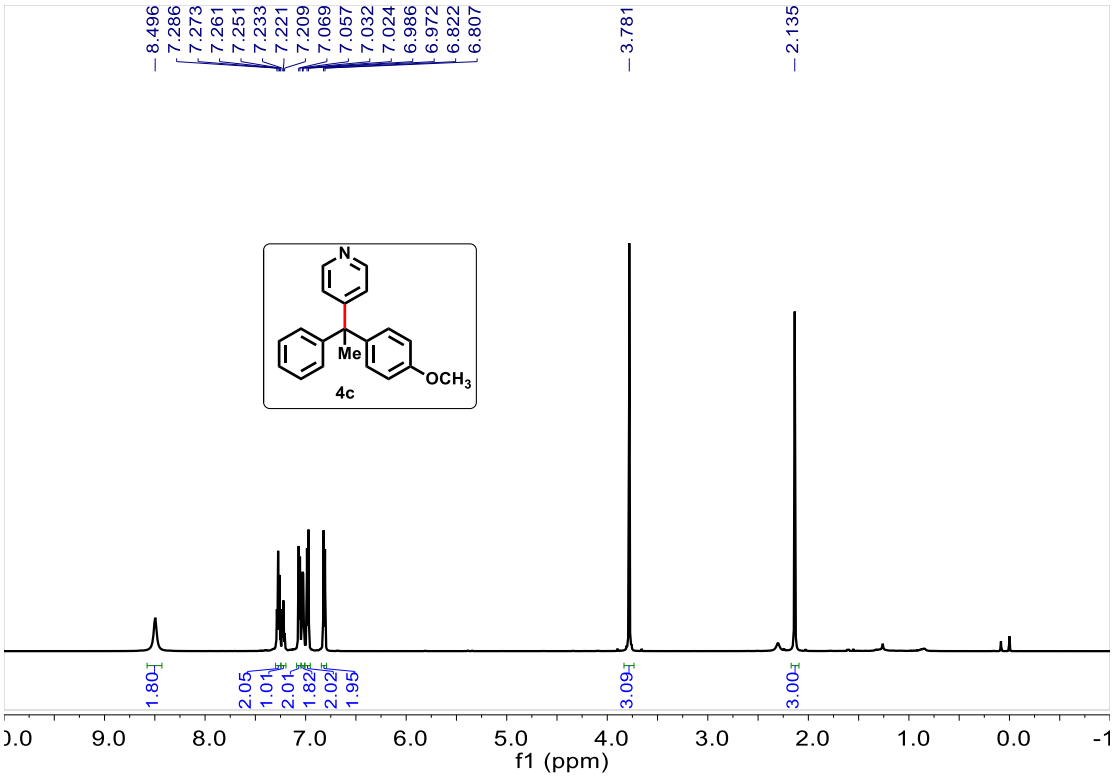
20.853
N
Me
Me
Me
4b
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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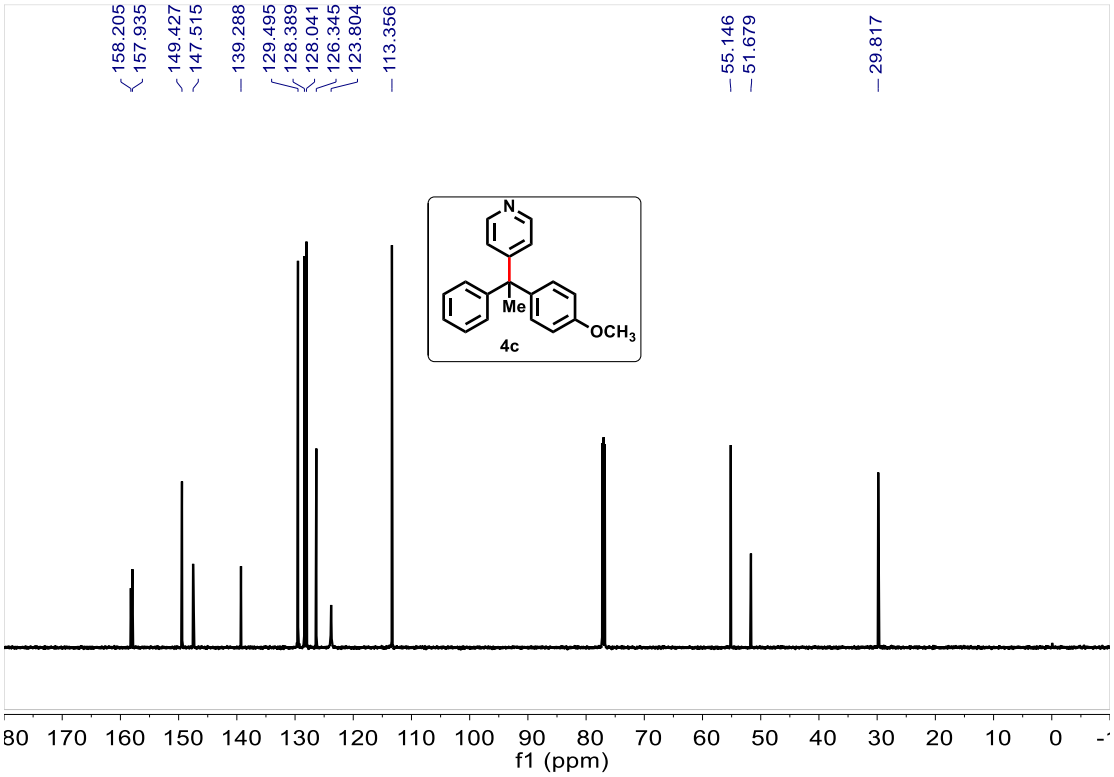
7.273
7.261
7.251
7.233
7.221
7.209
7.069
7.057
7.032
7.024
6.986
6.972
6.822
6.807
3.781
2.135
N
Me
OCH3
4c
1.80
2.05
1.01
2.01
1.82
2.02
1.95
3.09
3.00
f1 (ppm)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128.041
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55.146
51.679
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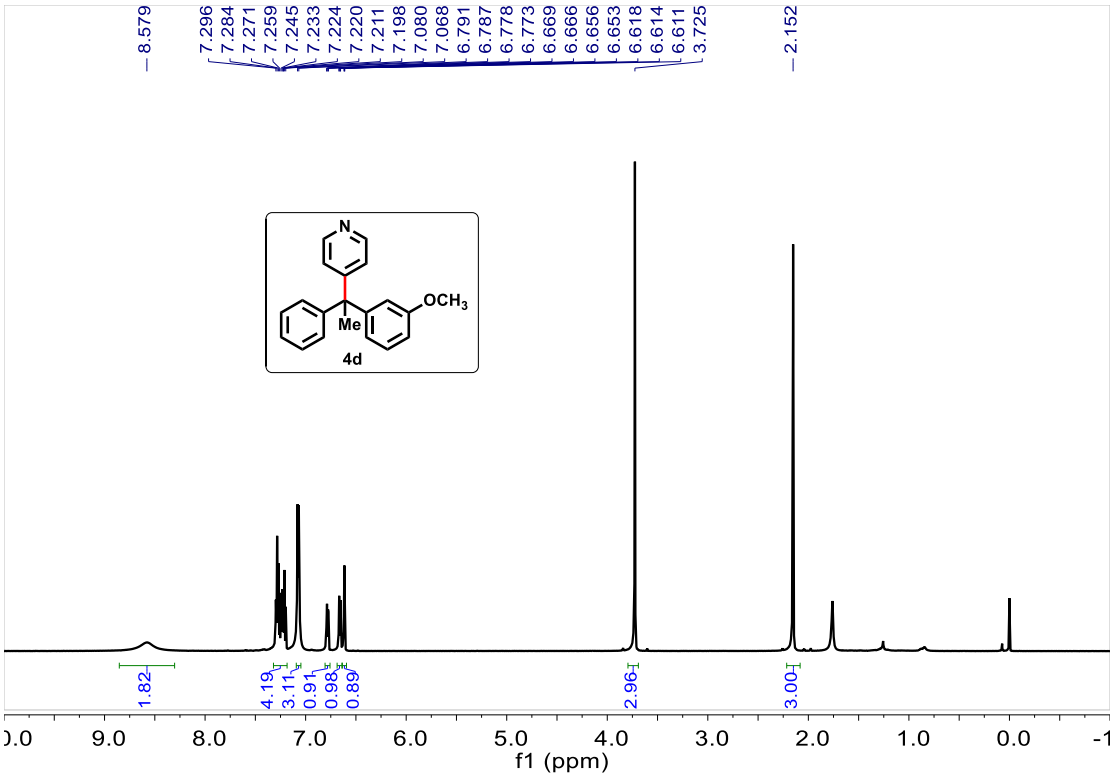
Me
OCH3
4c
f1 (ppm)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7.245
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7.224
7.220
7.211
7.198
7.080
7.068
6.791
6.787
6.778
6.773
6.669
6.666
6.656
6.653
6.618
6.614
6.611
3.725
2.152
N
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Me
4d
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3.11
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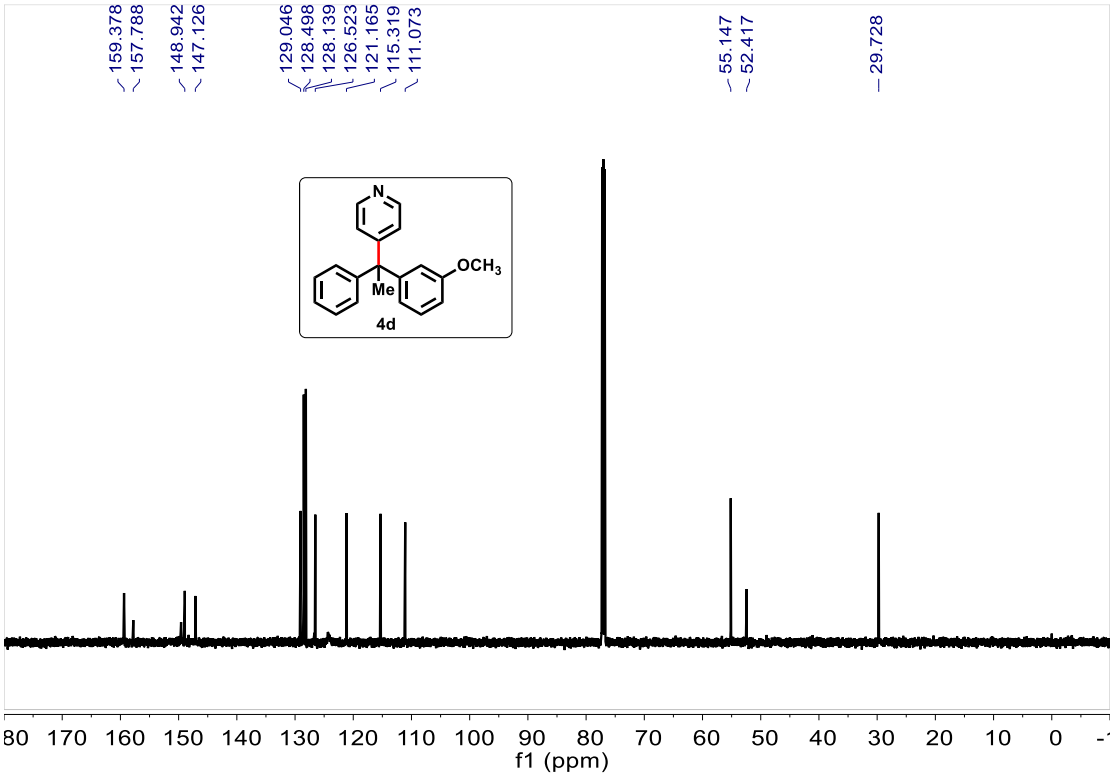
2.96
3.00
f1 (ppm)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55.147
52.417
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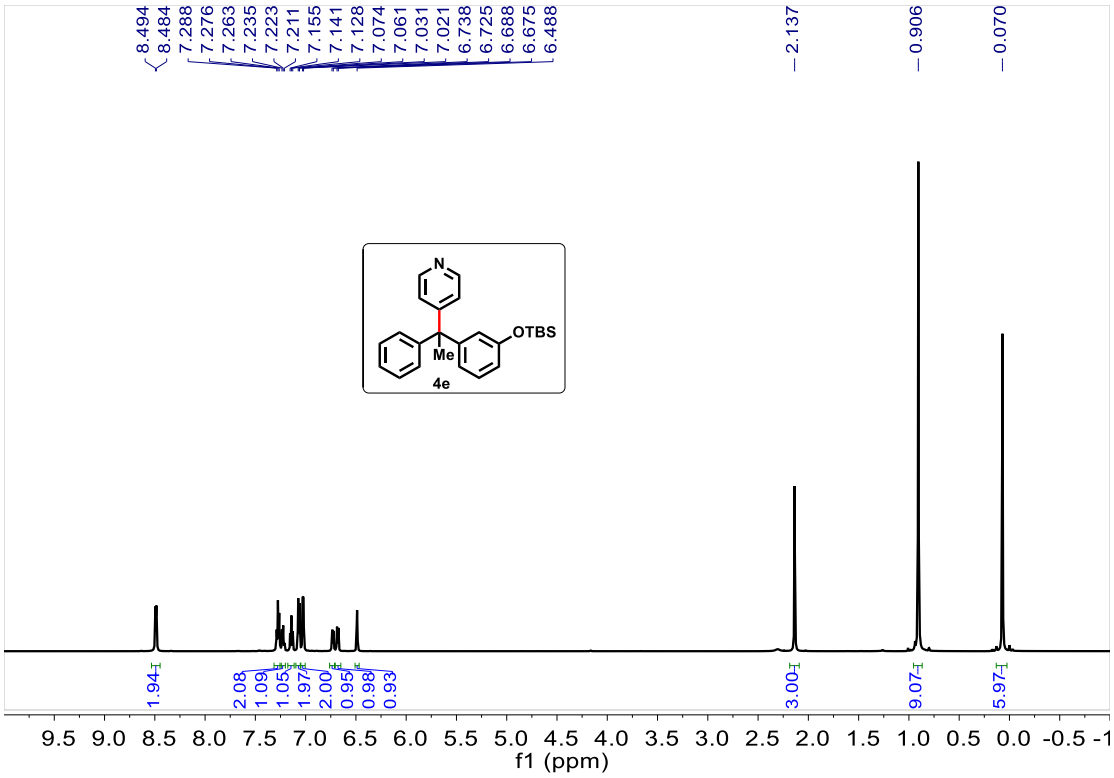
N
OCH3
Me
4d
f1 (ppm)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7.263
7.235
7.223
7.211
7.155
7.141
7.128
7.074
7.061
7.031
7.021
6.738
6.725
6.688
6.675
6.488
2.137
0.906
0.070
N
OTBS
Me
4e
1.94
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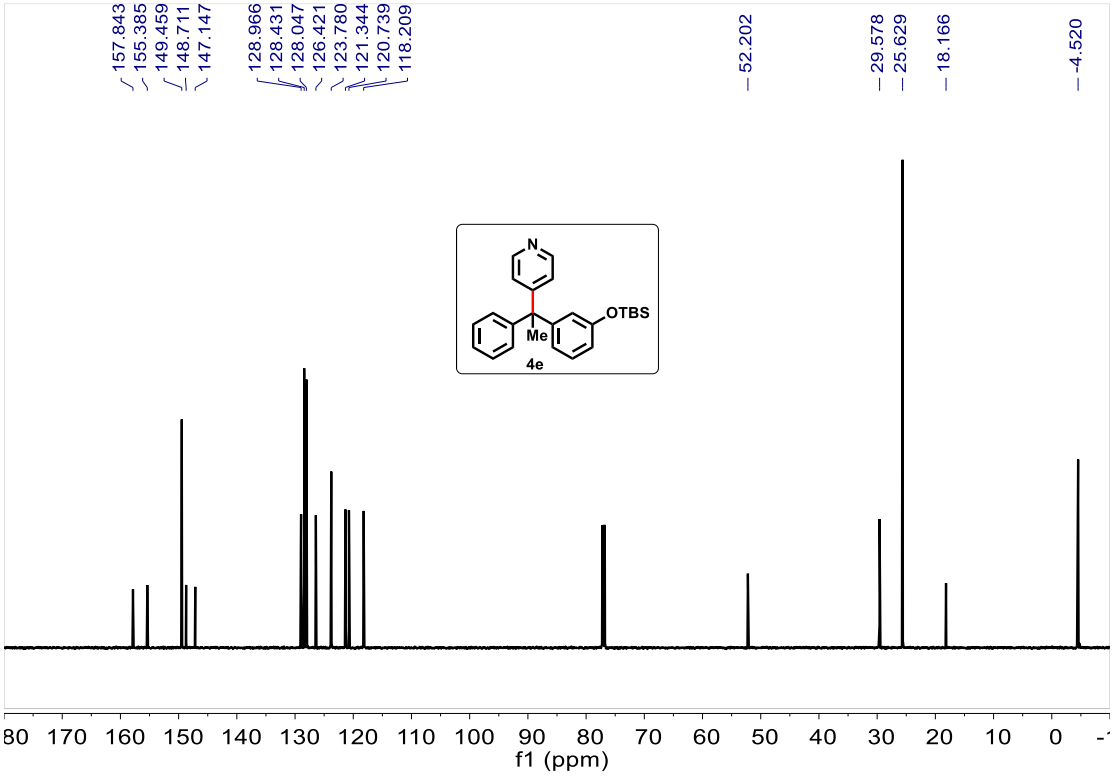
1.09
1.05
1.97
2.00
0.95
0.98
0.93
3.00
9.07
5.97
f1 (ppm)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128.966
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-4.520
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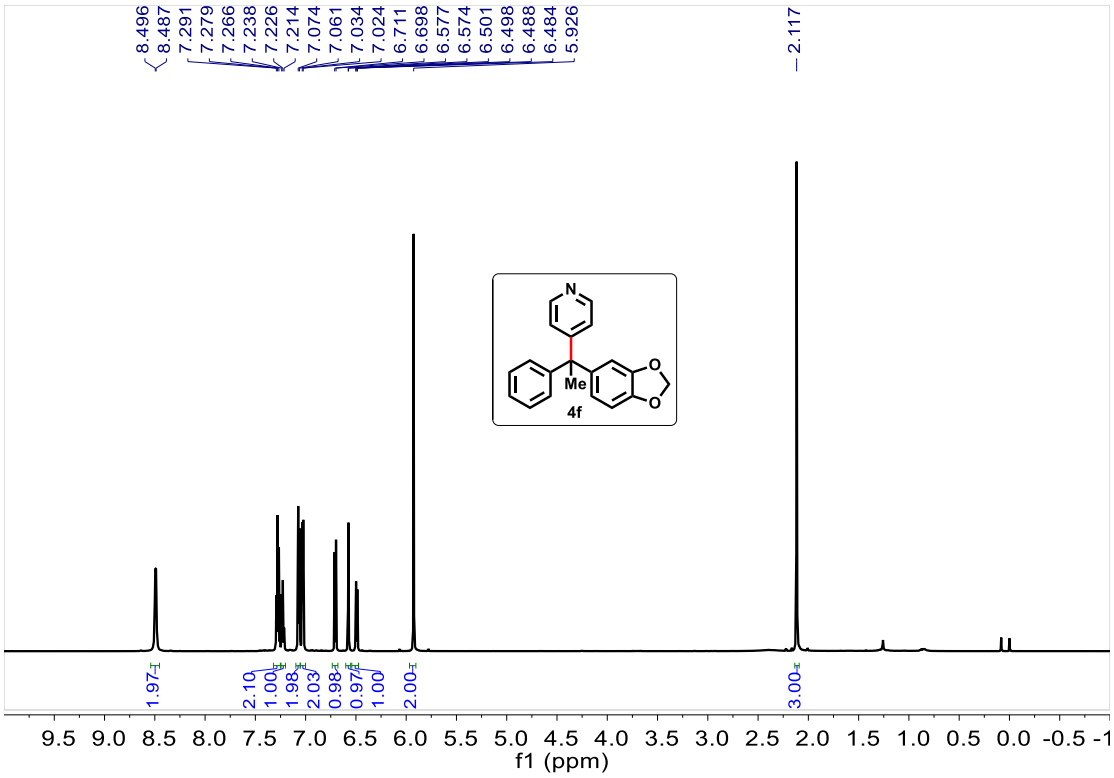
OTBS
Me
4e
f1 (ppm)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7.214
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7.061
7.034
7.024
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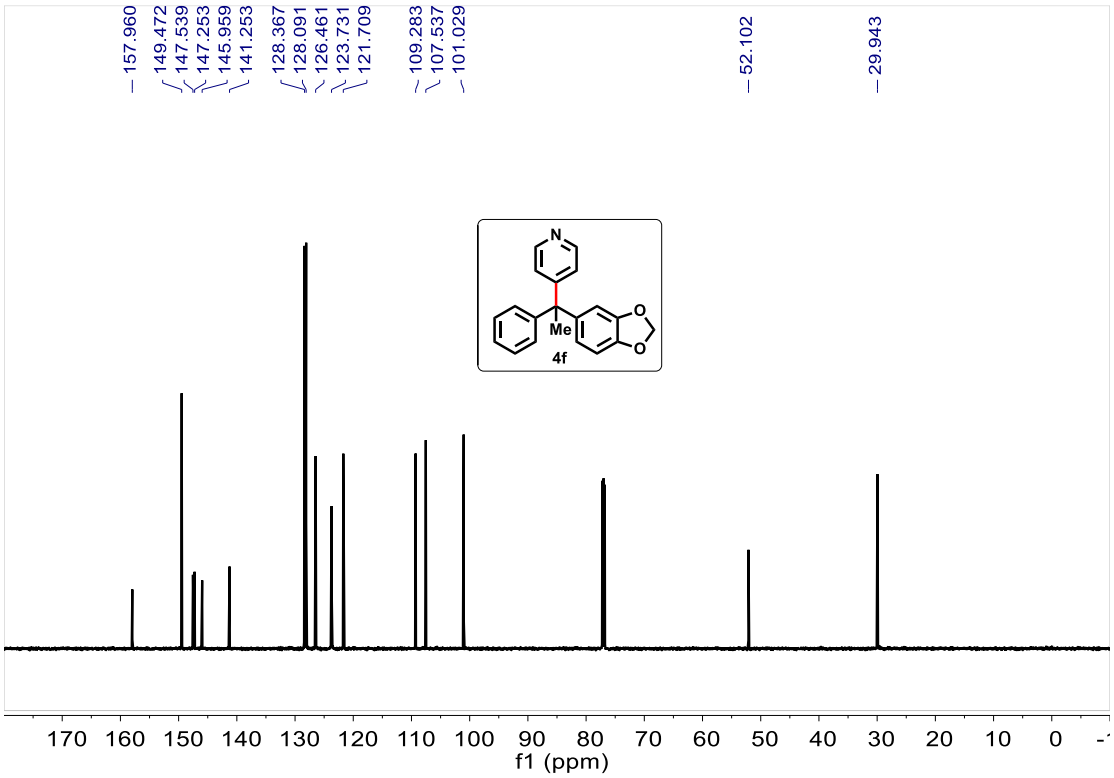
6.577
6.574
6.501
6.498
6.488
6.484
5.926
2.117
1.97
2.10
1.00
1.98
2.03
0.98
0.97
1.00
2.00
3.00
N
Me
O
O
4f
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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128.091
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123.731
121.709
109.283
107.537
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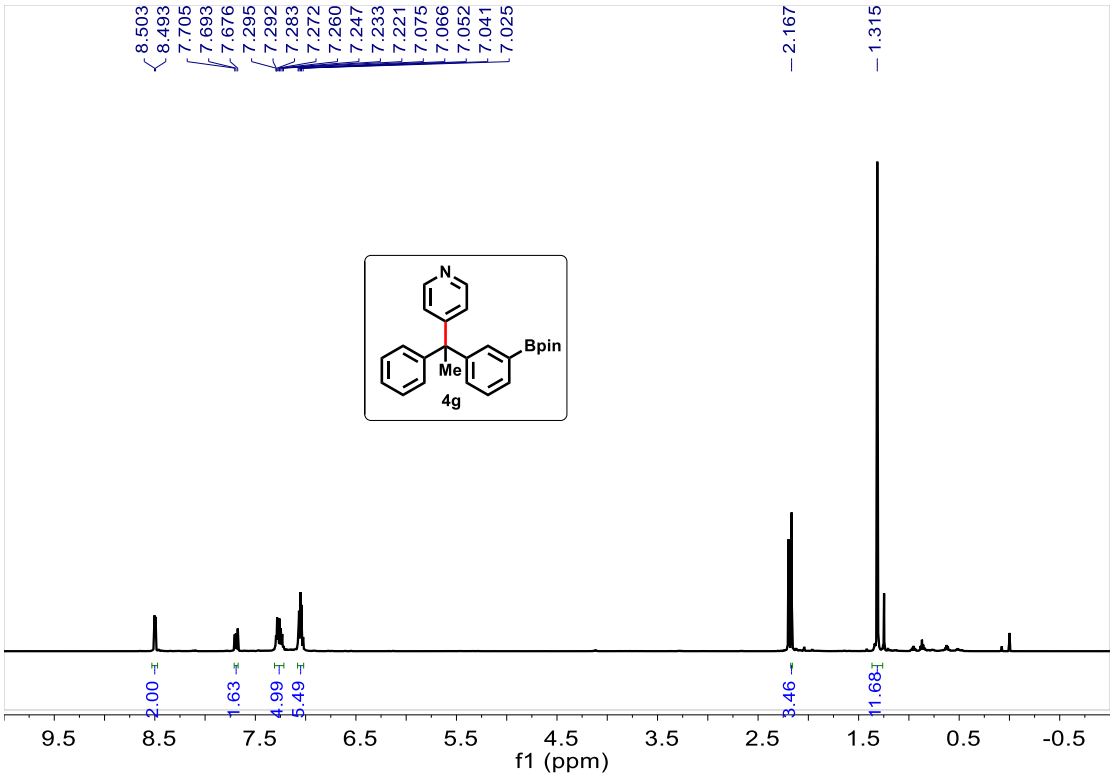
29.943
N
Me
O
O
4f
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.283
7.272
7.260
7.247
7.233
7.221
7.075
7.066
7.052
7.041
7.025
2.167
1.315
N
Bpin
Me
4g
2.00
1.63
4.99
5.49
3.46
11.68
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
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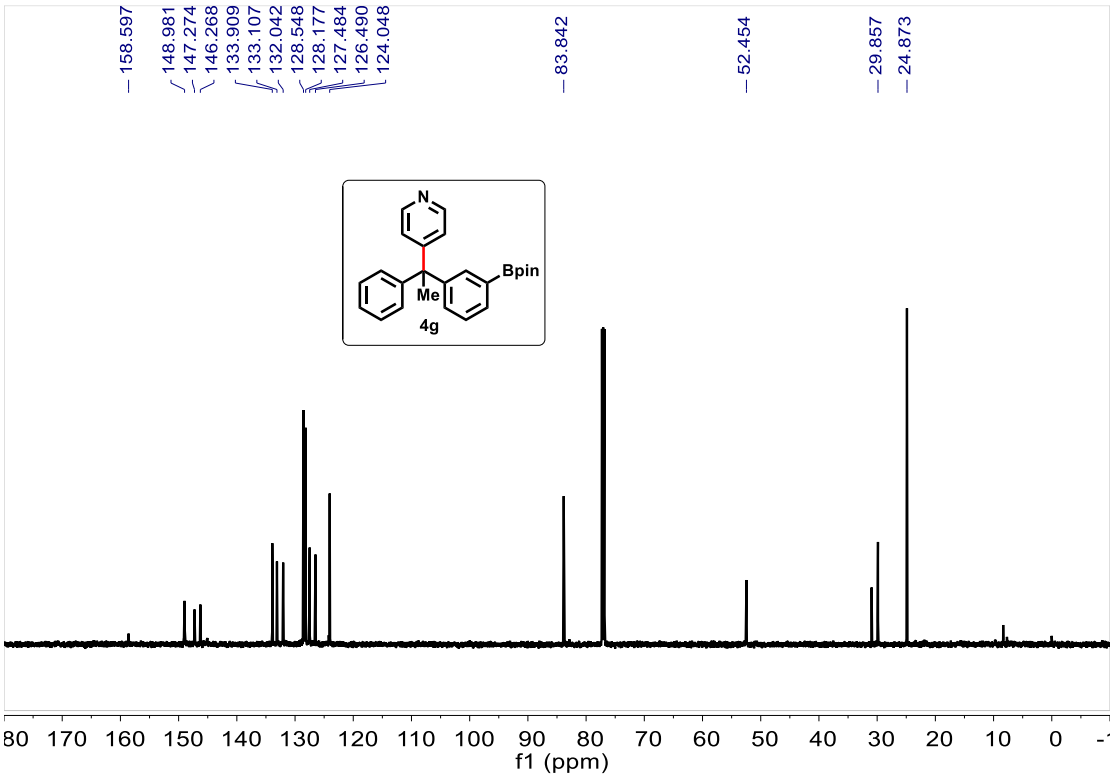
-0.5
f1 (ppm)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133.909
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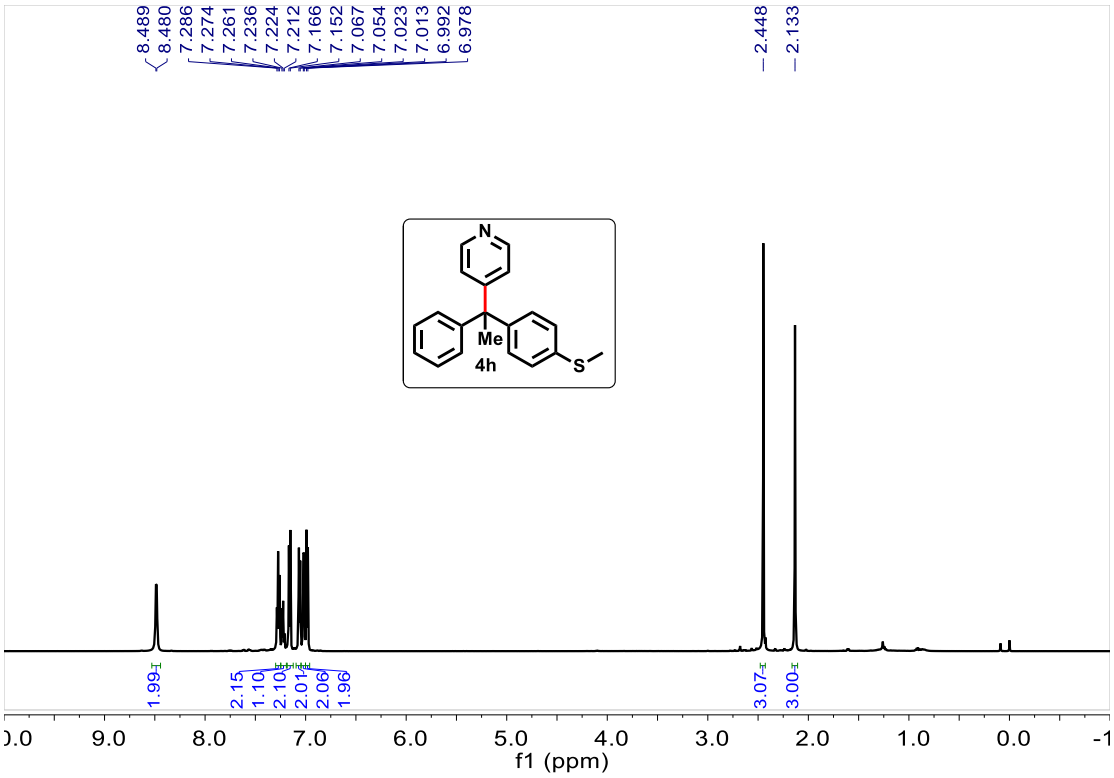
132.042
128.548
128.177
127.484
126.490
124.048
83.842
52.454
29.857
24.873
N
Bpin
Me
4g
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.274
7.261
7.236
7.224
7.212
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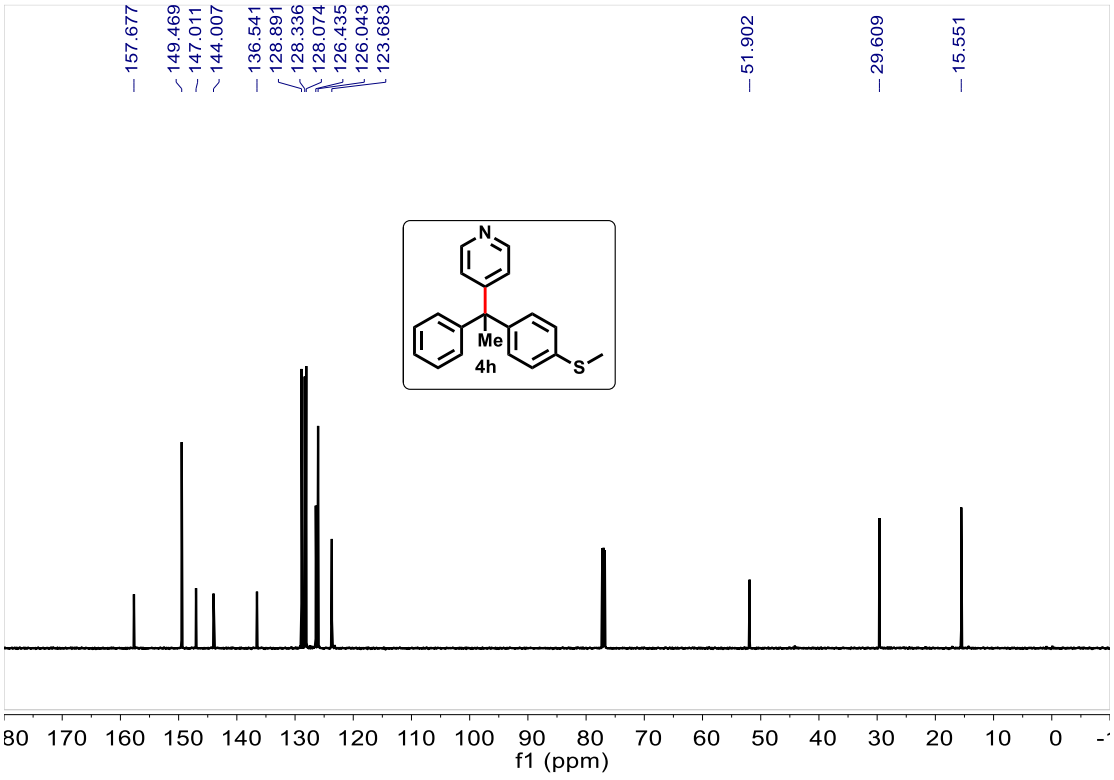
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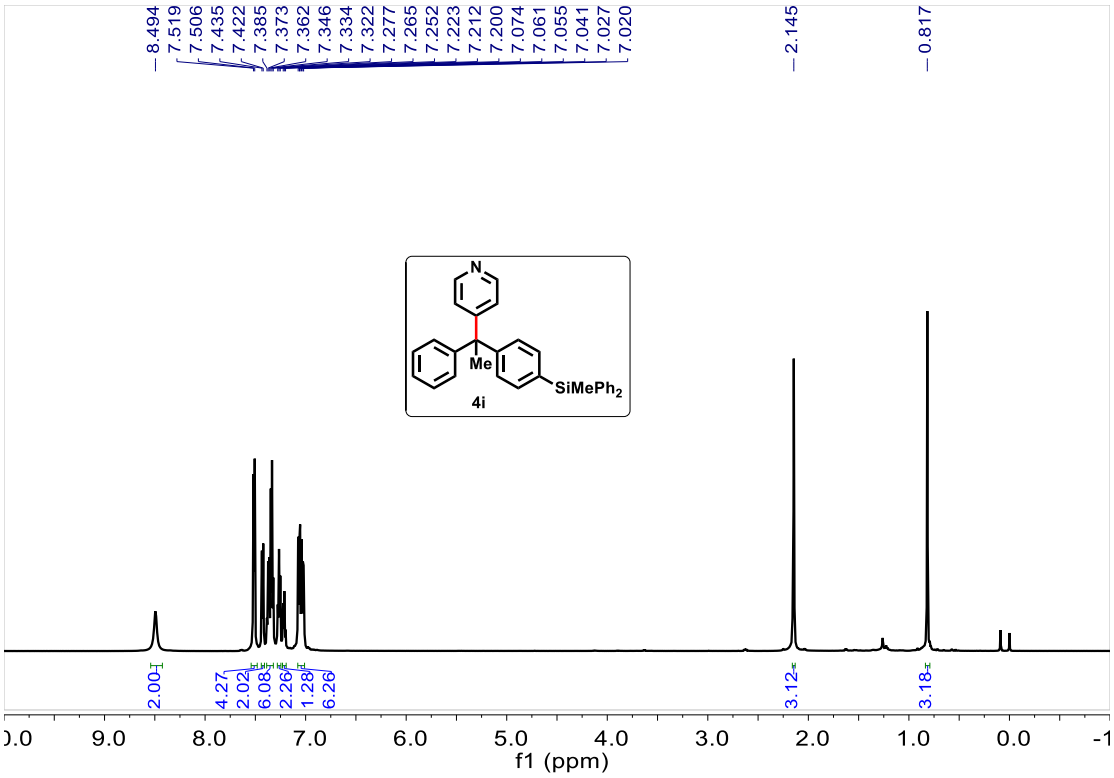
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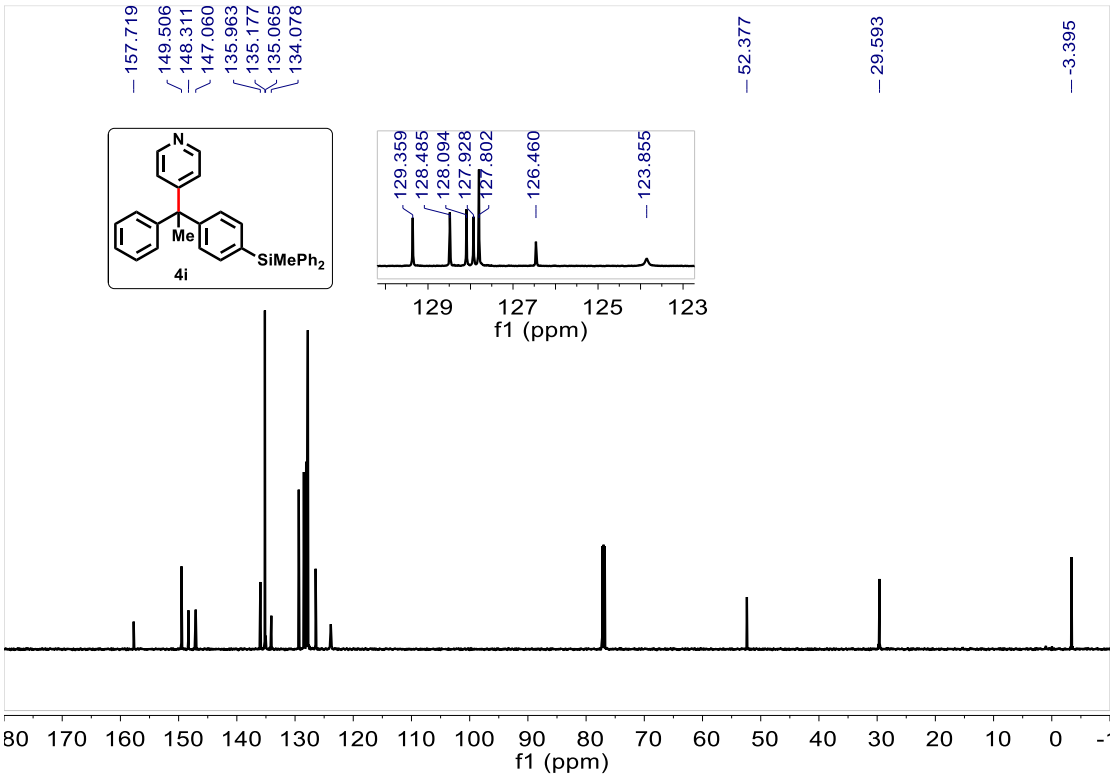
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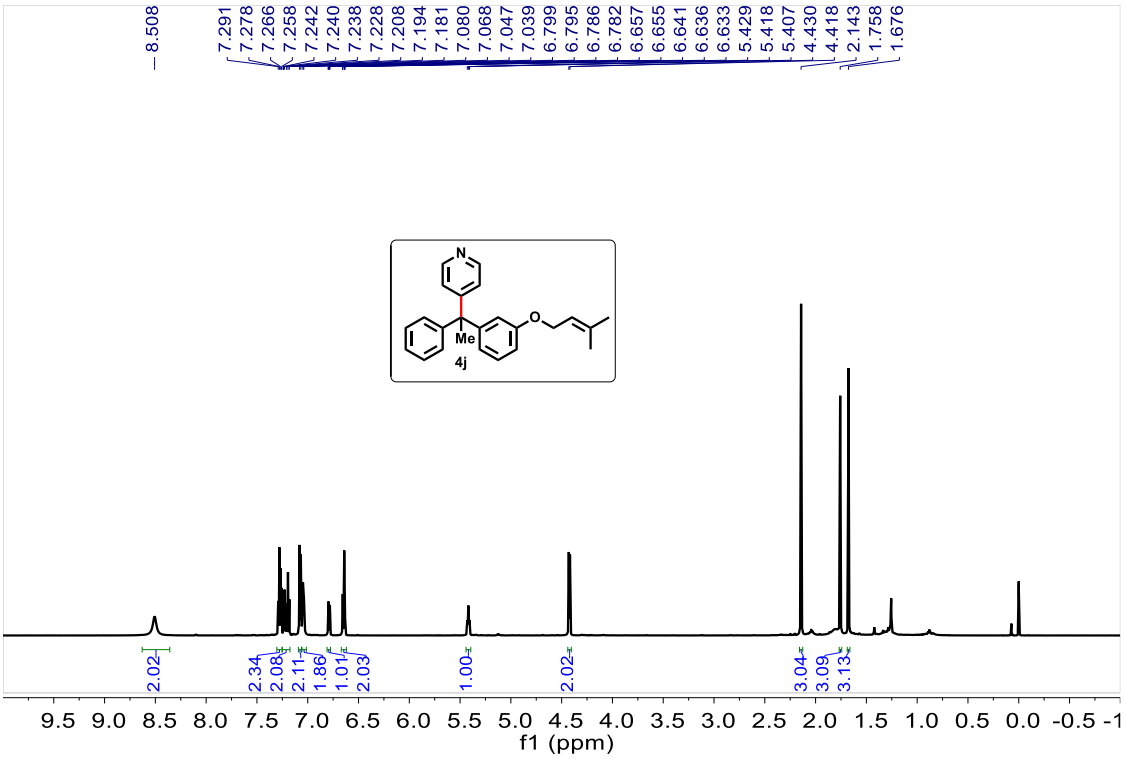
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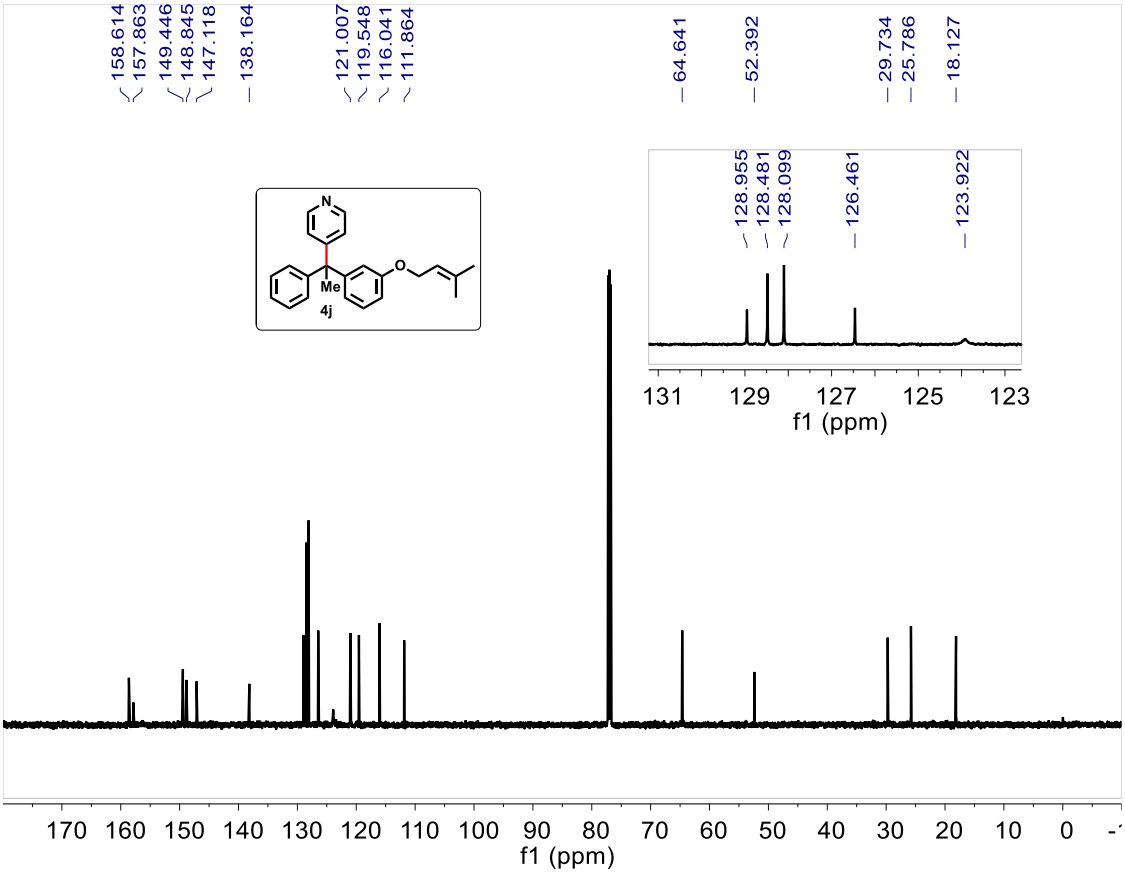
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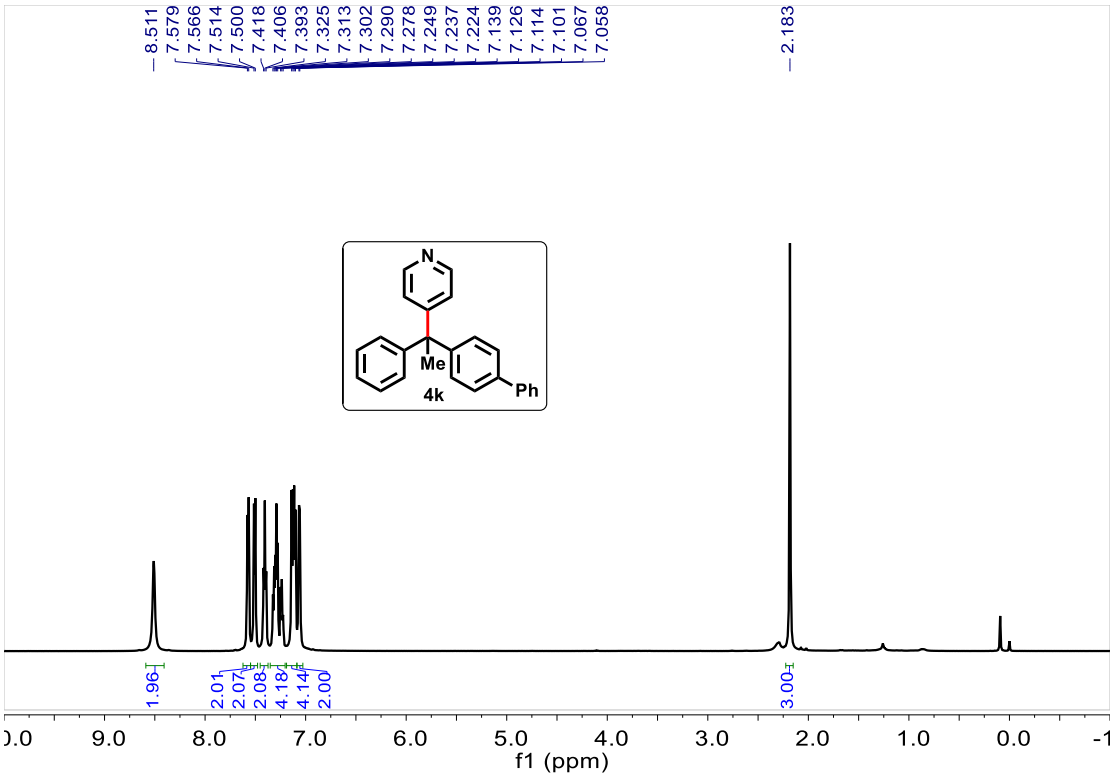
f1 (ppm)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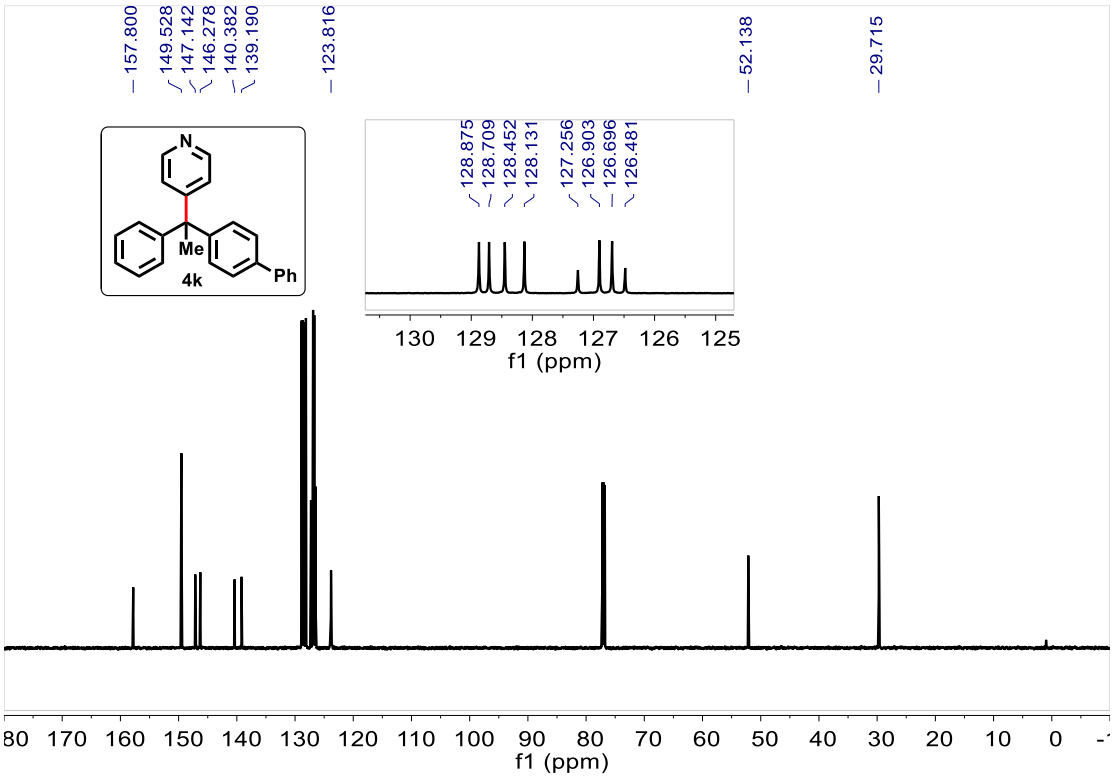
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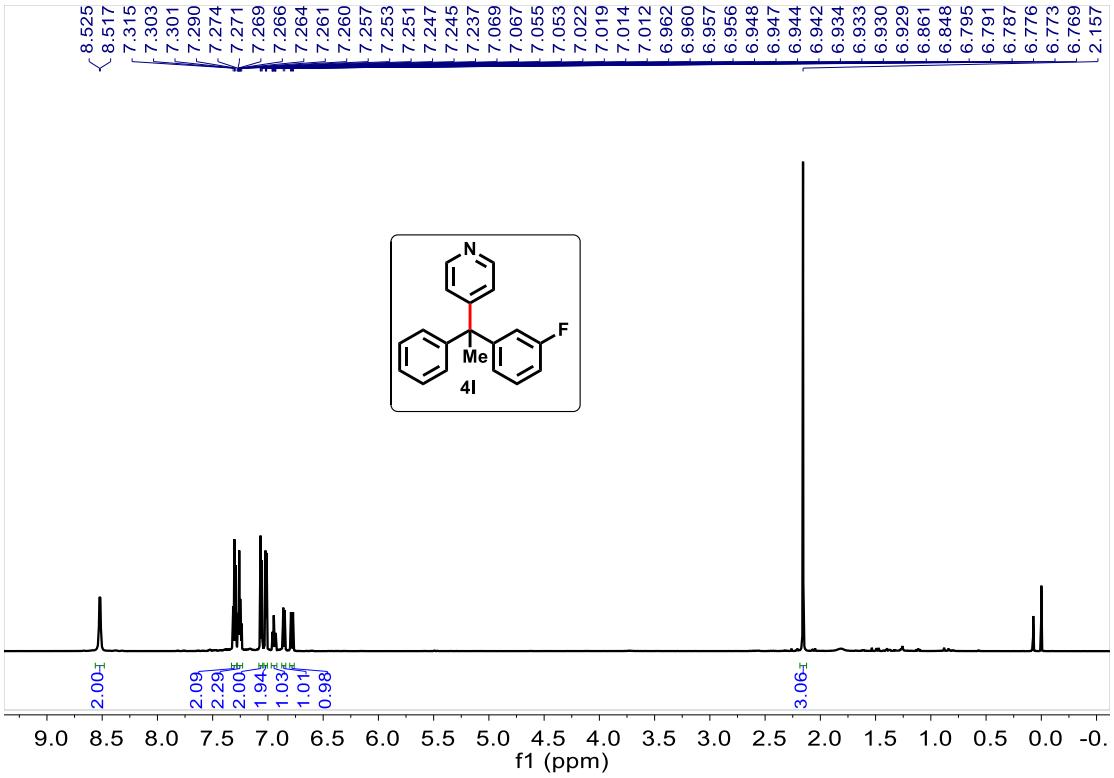
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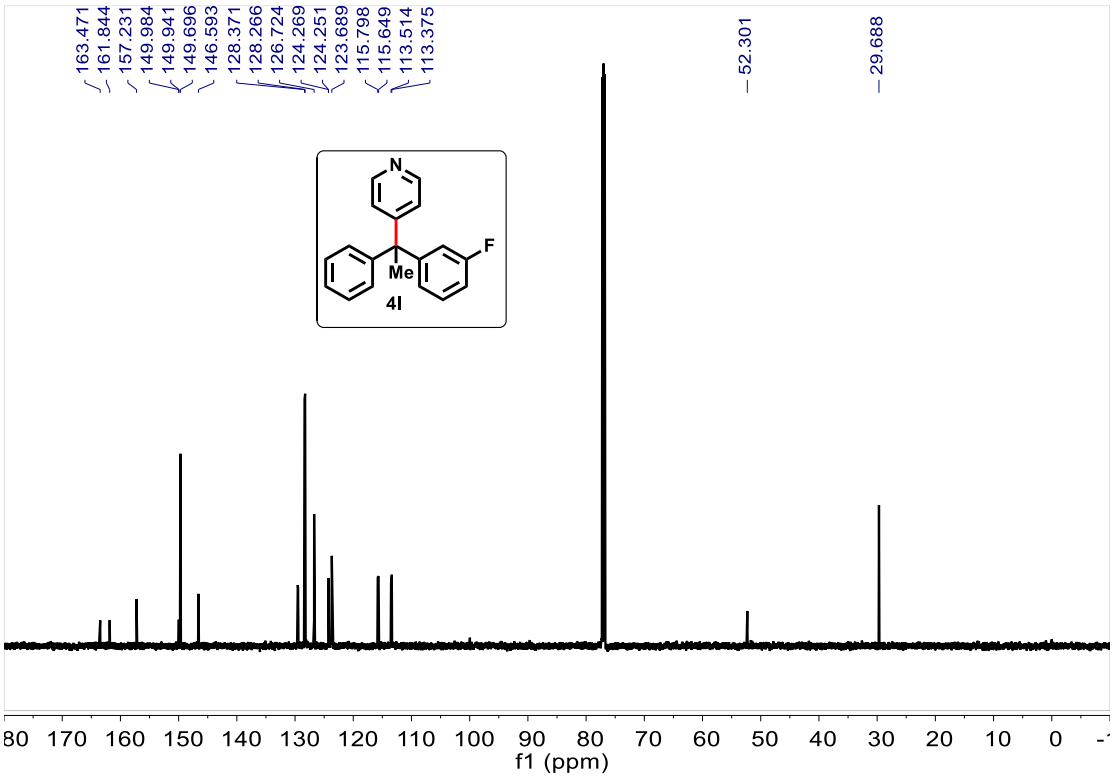
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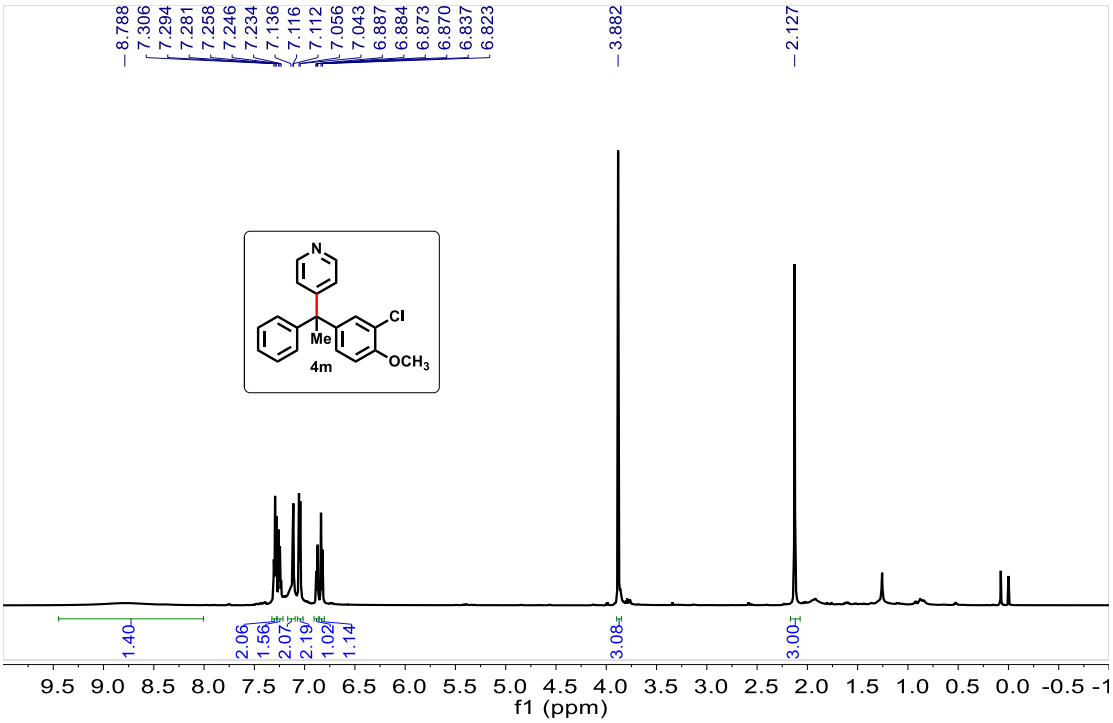
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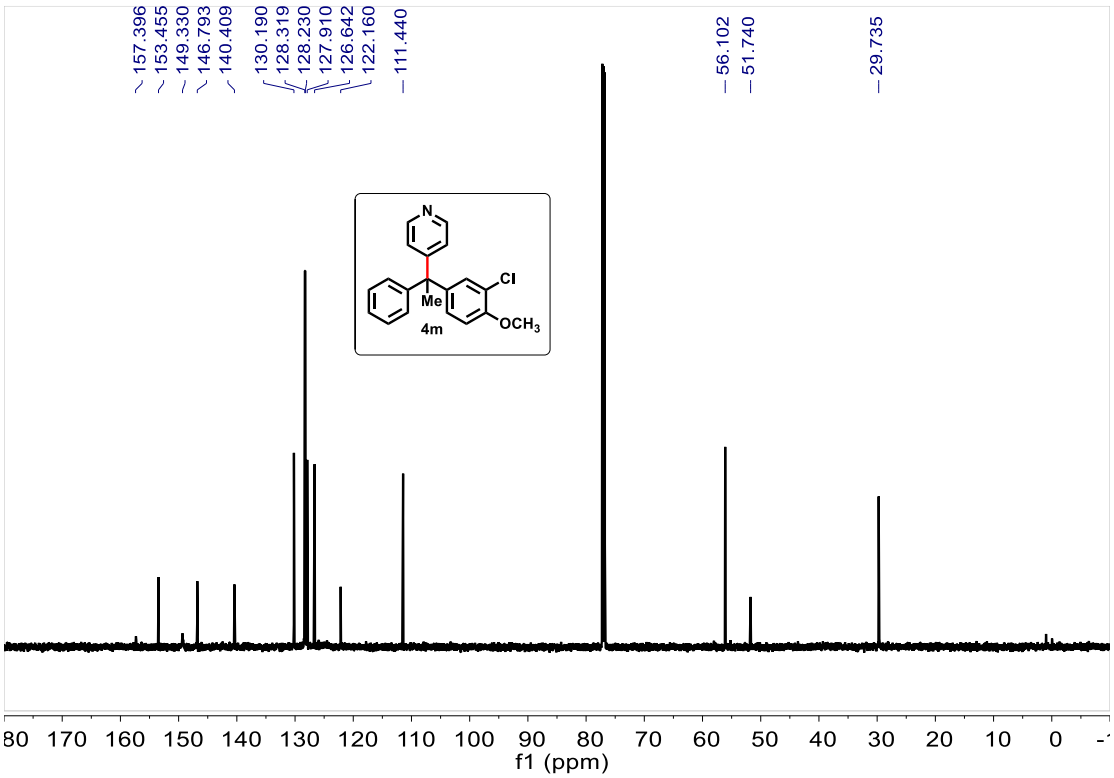
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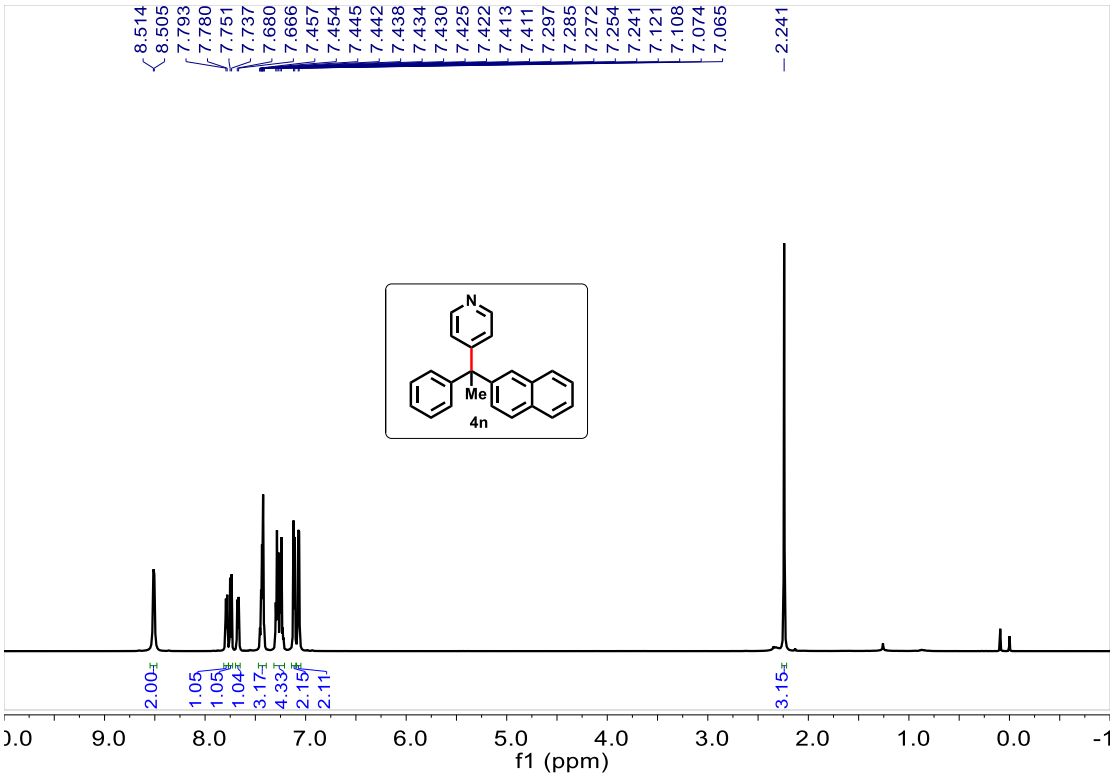
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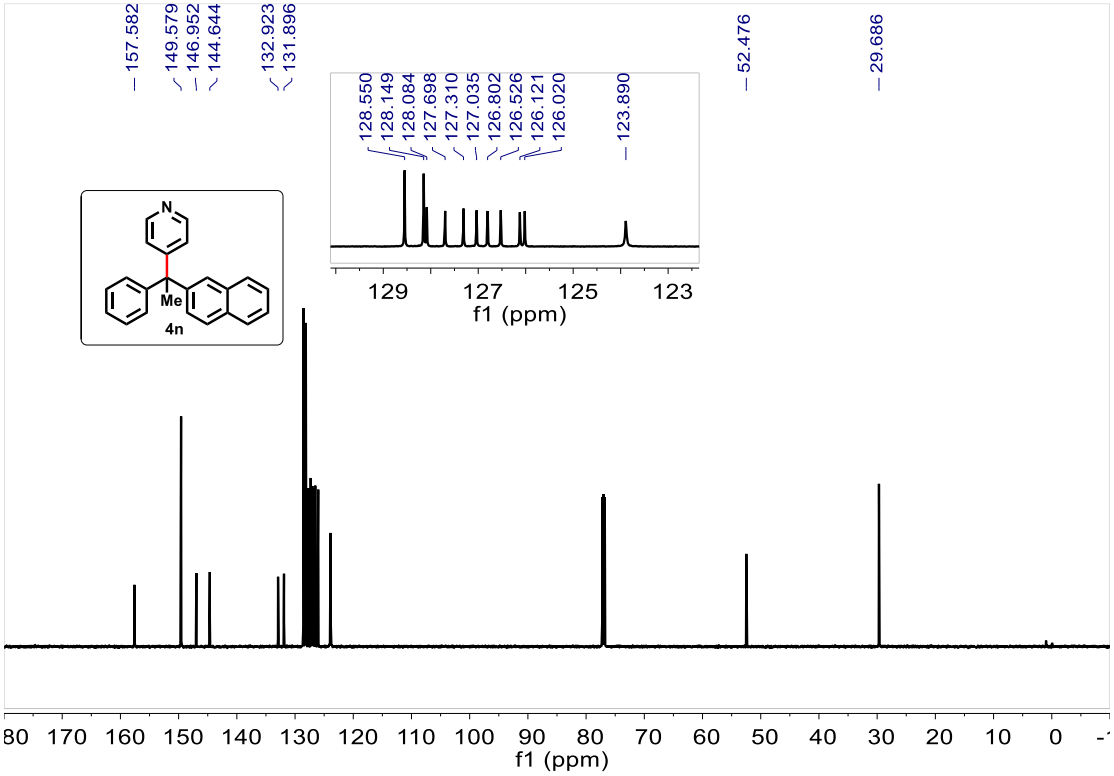
f1 (ppm)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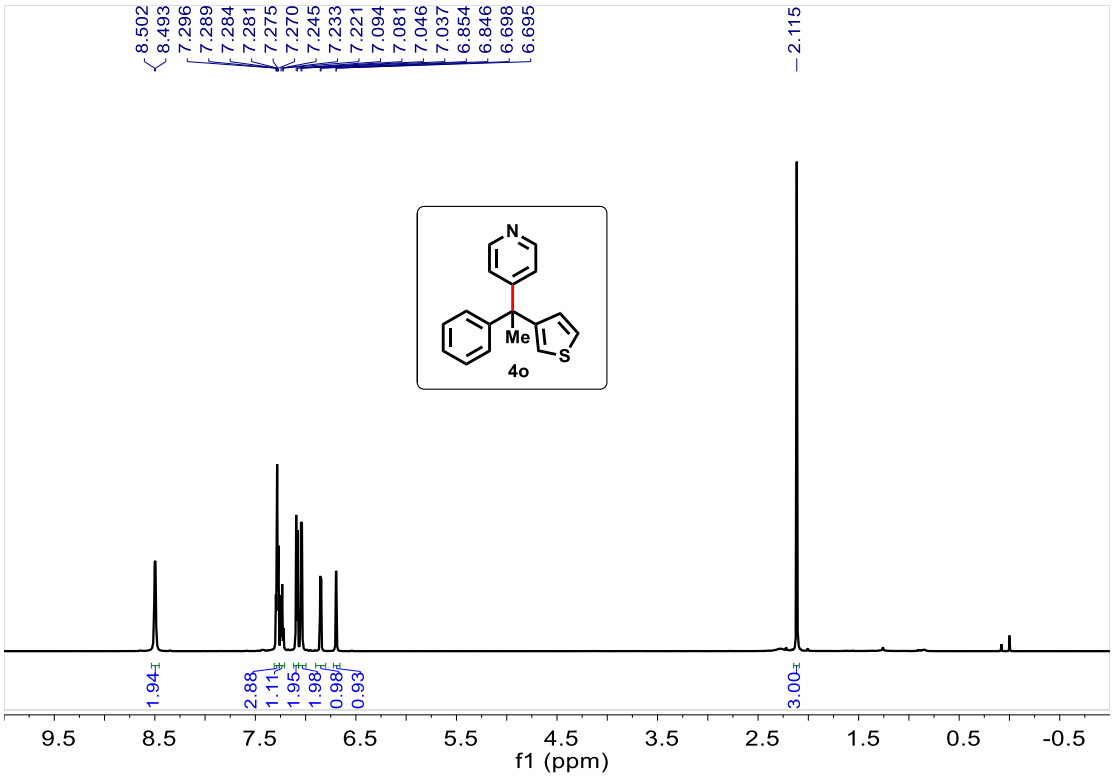
f1 (ppm)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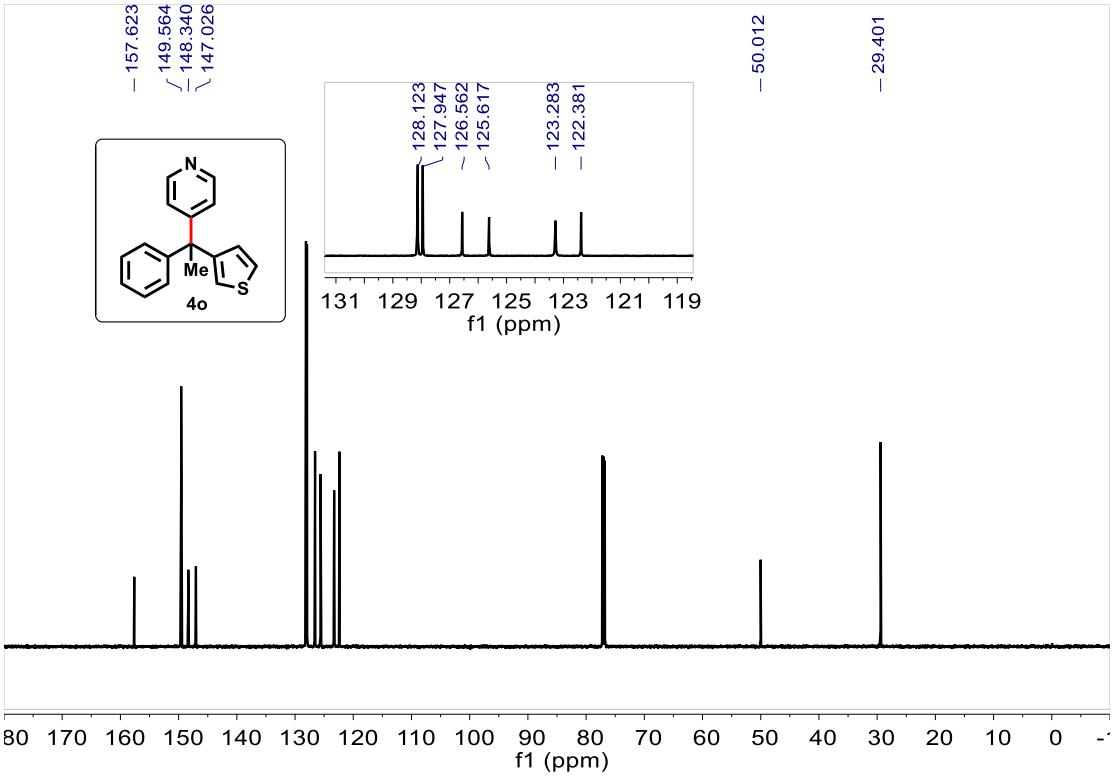
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S
4o
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f1 (ppm)
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f1 (ppm)

9. **Calculation datas**

9.1 The DFT calculations were performed with M06[11] method as implemented in Gaussian 09[12] program. Solvation effects were included with the universal solvation model (SMD).[13] The 6-31++G(d,p) and 6-31G(d) basis sets were used for H atom and the other atoms (B, C, N, O, Na), respectively. Frequency calculations were carried out at the same theoretical level to verify the stationary points to be equilibriums or transition states. The thermodynamic energy corrections to the Gibbs energy were evaluated at 298.15 K and 1 atm. Intrinsic reaction coordinate (IRC)[14,15] analysis was performed to ensure the correct transition states connecting reactants and products. In order to consider the change in standard states from gas phase to aqueous solution, the translational entropy was corrected with the method developed by Whitesides et al (see the following section).[16] Images of the 3D structures were prepared with *CYLview* visualization program.[17]

9.2 We evaluated the electronic energy (E_{sol}) with zero-point energy correction in solution. For each species, the E_{sol} is defined through equation (S1):

$$E_{sol} = E_{sol}^{pot} + E_{gas}^{v_0} \qquad \text{(S1)}$$

where E_{sol}^{pot} is the potential energy including non-electrostatic energy in solution and $E_{gas}^{v_0}$ represents the zero-point vibrational energy in the gas phase. In a bimolecular process, such as the coordination of the BEt_3 with the substrate or the intermediate, the entropy change must be taken into consideration because the entropy considerably decreases. In this case, Gibbs energy (G_{sol}^{o}) must be evaluated as follows:

$$\begin{aligned} G_{sol}^{o} &= H_0 - T(S_r^o + S_v^o + S_t^o) \\ &= E^T + P\Delta V - T(S_r^o + S_v^o + S_t^o) \\ &= E_{sol} + E_{therm} - T(S_r^o + S_v^o + S_t^o) \end{aligned} \qquad \text{(S2)}$$

where ΔV is 0 in solution, E_{therm} is the thermal correction by translational, vibrational, and rotational movement, and S_r^o, S_v^o, and S_t^o are rotational, vibrational, and translational entropies, respectively. In general, the Sackur-Tetrode equation is used to evaluate translational entropyS_t^o. In solution, however, the usual Sackur-Tetrode equation cannot be directly applied to the evaluation of S_t^o, because the translation movement is suppressed very much in solution. In this context, the translational entropy was corrected with the method developed by Whitesides et al., where the rotational entropy was evaluated in a normal manner. Thermal correction and entropy contributions of vibration movements to the Gibbs energy were evaluated with the frequencies calculated at 298.15 K and 1 atm.

9.3 Result and discussion

The lone pair of N atom in pyridine interacts with the empty orbital of B atom of BEt_3 to produce a stable complex **Sub2** with Gibbs free energy change ($\Delta G°$) of –4.1 kcal/mol, as shown in

Fig.S11a. Thus, the **Sub2** directly participates in the reaction. At the beginning of the reaction, catalyst $NaHBEt_3$ is combined with styrene substrate (**Sub1a**) through the electrostatic interaction to form an intermediate **1'** with a $\Delta G°$ value of −5.1 kcal/mol (Fig. S11b). Subsequently, the extra BEt_3 is involved in the hydride ion insertion process (**1'** → **2'** transformation) through the transition state **TS1** to generate an intermediate **2'** and release the BEt_3 of the $NaHBEt_3$ with a small Gibbs activation energy ($\Delta G°^{‡}$) of 5.3 kcal/mol and a $\Delta G°$ value of −2.5 kcal/mol. Then, **2'** is isomerized to a stable intermediate **3'** with a $\Delta G°$ value of −4.3 kcal/mol. The following electrophilic nuclear attack between **3** and **Sub2** occurs through the transition state **TS2** to afford an intermediate **4'** with the $\Delta G°^{‡}$ and $\Delta G°$ values of 20.0 and 1.6 kcal/mol. Finally, the extra BEt_3 as Lewis acid is again involved in the hydride ion transfer through the transition state **TS3** to obtain the target product **5** and regenerate the catalyst $NaHBEt_3$. Such hydride ion transfer is the rate-determining step of the whole reaction, which requires a moderate $\Delta G°^{‡}$ value of 25.0 kcal/mol relative to **3**. The present calculations are consistent with the experimental results. This reaction can be achieved at a temperature of 373 K and the H atom on pyridine was detected on $NaHBEt_3$ by a series of isotope labeling experiments.

By contrast, we also investigated the hydride ion insertion process without the extra BEt_3 (the top red line in Fig. S12). Obviously, these results clearly show that the participation of the extra BEt_3 dramatically accelerates the hydride ion insertion and following reaction steps.

According to the experimental observations, the reaction could unexpectedly occur at low temperature when 1,1-diarylalkenes was employed as a substrate. To better understand the substituent effect on the mechanism, we calculated the reaction of 1, 1-diarylalkenes as a substrate. According to the above calculations, the C–B bond generated during the H^- insertion can stabilize the activity of the species, which may be an important factor for the reaction barriers. Here, we compared two modes of interaction between styrene (or 1,1-diarylalkenes.) and BEt_3, as illustrated in Fig. S13. For styrene, the presence of the C–B bond stabilizes the energy by −15.3 kcal/mol. For 1, 1-diarylalkenes, however, the C–B bond destabilizes the energy increased by 3.0 kcal/mol. In other words, 1,1-diarylalkenes cannot get enough stabilization energy due to the formation of C–B bond, which means that the reaction mechanism involving 1, 1-diarylalkenes may be different from styrene (Fig. S11). Similar to the above styrene case, catalyst $NaBEt_3H$ is combined with 1, 1-diarylalkenes substrate (**Sub1a**) through the electrostatic interaction to form an intermediate **9** with a $\Delta G°$ value of −8.2 kcal/mol (Fig. S14). Subsequently, **9** is transformed to an intermediate **10'** through the transition state **TS7**. The H^- insertion requires the $\Delta G°^{‡}$ and $\Delta G°$ values of 20.7 and 6.5 kcal/mol, respectively. Then, the following electrophilic nuclear attack and H^- transfer occur through the transition states **TS8** and **TS9** to provide the product **12'** and regenerate the catalyst $NaBEt_3H$ with the $\Delta G°^{‡}$ values of 14.5 and 20.7 kcal/mol relative to **9'**. It can be found by comparing the corresponding rate-determining steps that the reaction involving 1, 1-diarylalkenes is easier to occur than that involving styrene (20.7 versus 25.0 kcal/mol). This means

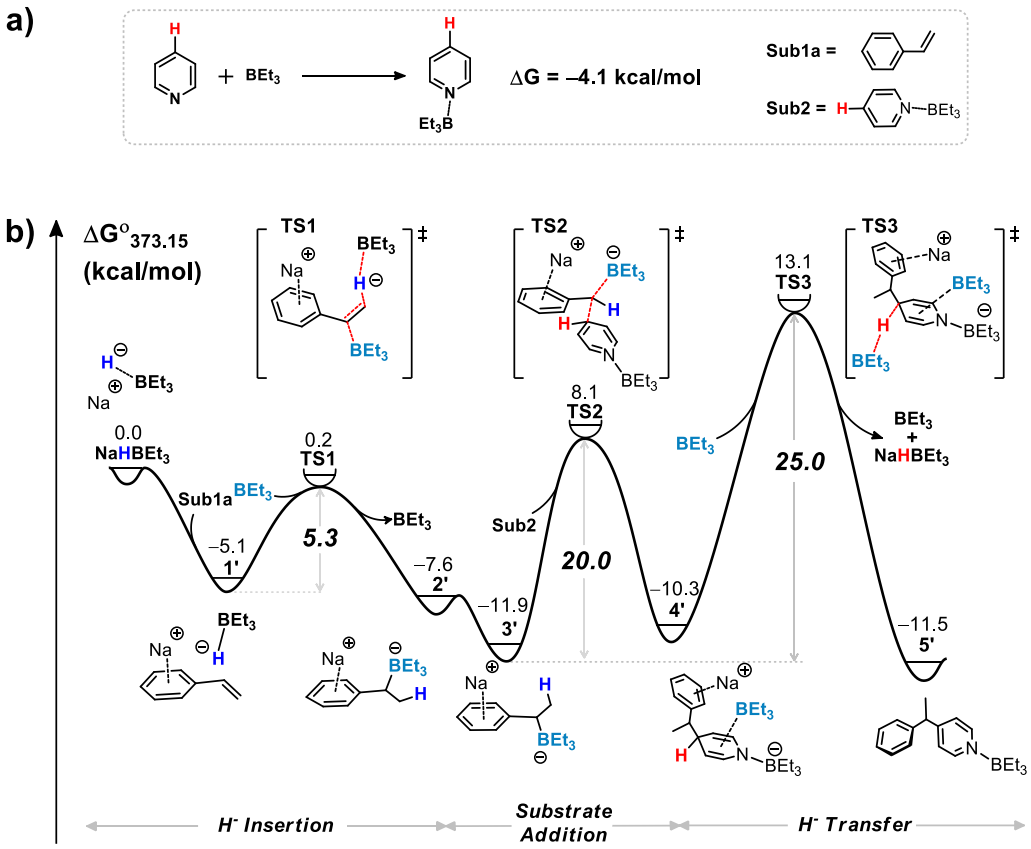

Figure. S11. Gibbs energy profiles ($\Delta G°_{298.15}$) of reaction of styrene as substrate with BEt_3 in the H^- insertion process.

that the yield of the former is higher than that of the latter under the same reaction conditions, which is consistent with the experimental results.

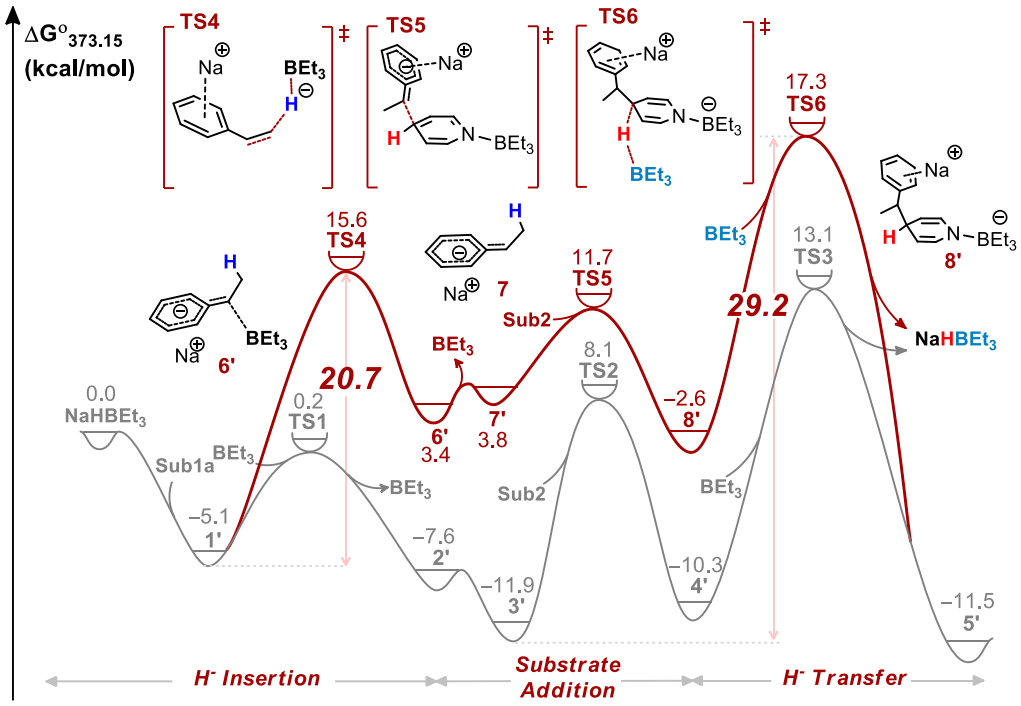

Figure.S12. Gibbs energy profiles ($\Delta G°_{298.15}$) of styrene as substrate without BEt_3 in the H^- insertion process.

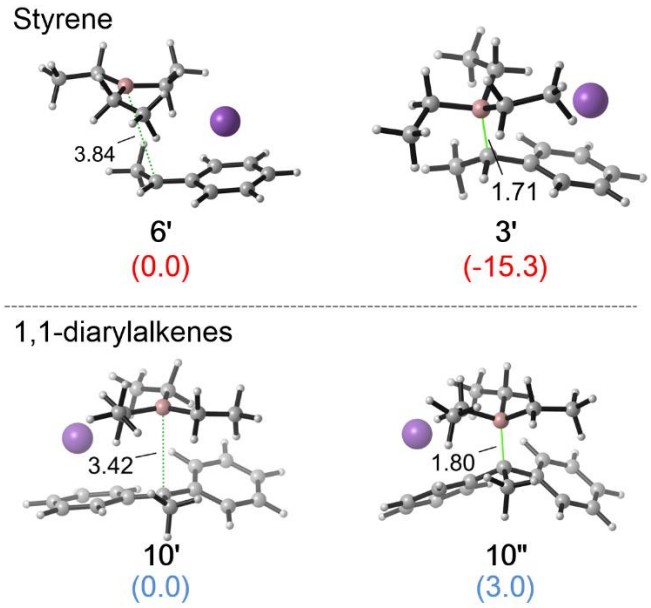

Figure. S13. The relative Gibbs energies and structures of different C–B interactions between **Sub1a** and **Sub2** and between **Sub1b** and **Sub2**. Gibbs energies are given in kcal/mol, the lengths are given in Å. White, pink, gray spheres represent H, B, C, Na atoms, respectively.

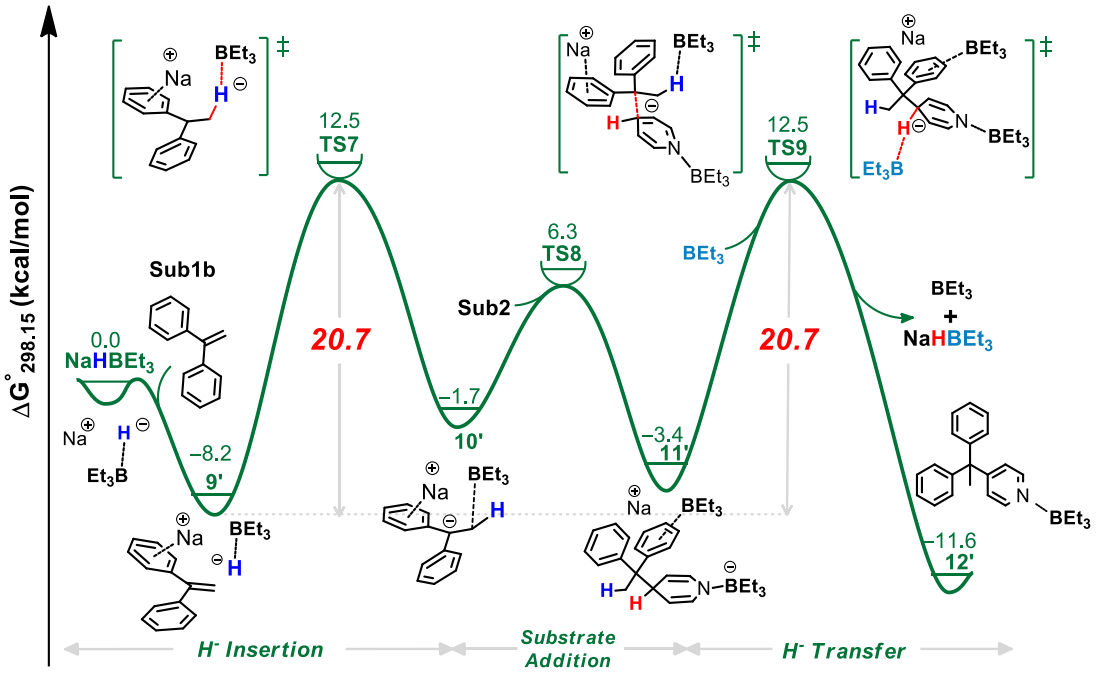

Figure. S14. Gibbs energy profiles ($\Delta G°_{298.15}$) of 1,1-diarylalkenes as substrate.

In addition, we also employed *para*-OMe substituted styrene as substrate to study the Gibbs energy profile of this reaction. As shown in Fig.S11 and S15, The two mechanisms involving styrene and *para*-OMe substituted styrene are the same, only the energy barriers are different. Comparing the rate-determining steps of these two reactions, the energy barrier of latter case is higher than that of former case by 2.2 kcal/mol. Thus, this means that the yield of the reaction involving *para*-OMe substituted styrene is lower than that of styrene under the same reaction conditions, which is consistent with the experimental results. In view of the large difference in the energy barrier of hydride ion insertion (Fig.S11 and S15), we investigated the electronic process of this process using the fragment molecular orbital analyses.[18-20] As shown in Fig. S16, **TS1** is divided into two fragments as $NaHBEt_3$ and **Sub1** moieties. The electron population of the LUMO of the **Sub1** moiety considerably increases to 0.508e. the population of the HOMO of the $NaHBEt_3$ moiety greatly decreases to 1.567e. These results clearly show that charge transfer (CT) occurs from the HOMO of the $NaHBEt_3$ to the LUMO of the **Sub1** in this step with a 4.48 eV gap. Similarly, **TS10** is divided into two fragments as $NaHBEt_3$ and **Sub1-OMe** moieties. The CT occurs from the HOMO of the $NaHBEt_3$ to the LUMO of the **Sub1-OMe** in this step with a 5.49 eV gap. In addition, the back donation from the *para*-OMe group to the Na cation exists in **TS10**. Thus, from the perspective of CT, the hydride ion insertion involving **Sub1-OMe** requires more energy barrier than that involving **Sub1**.

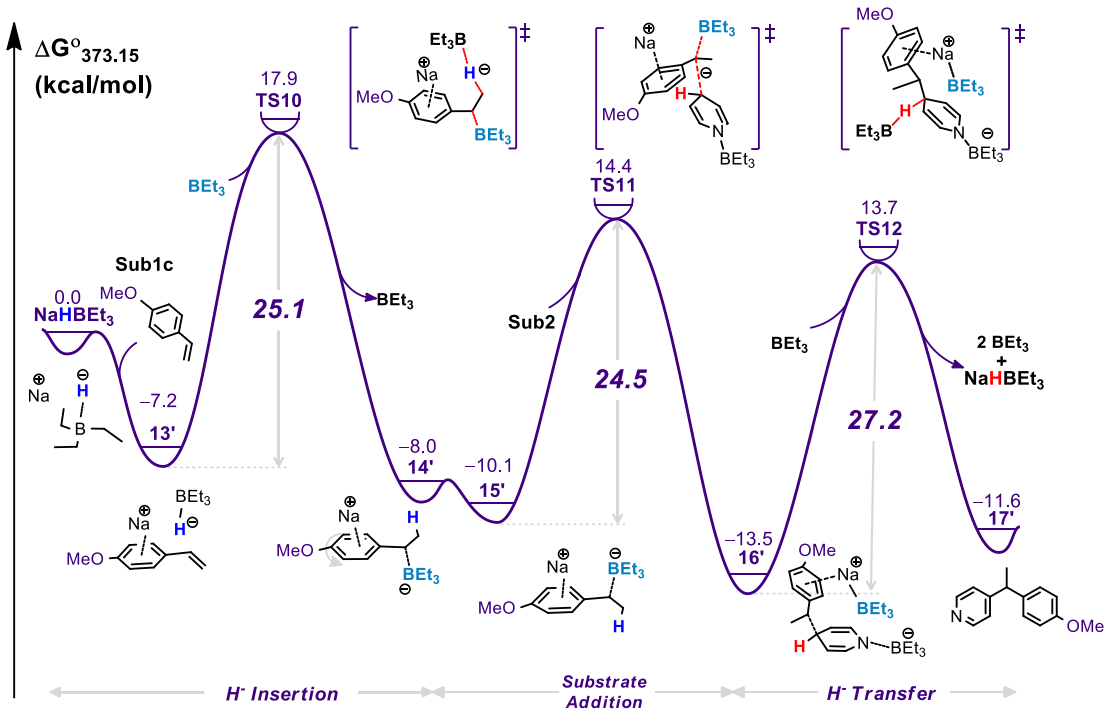

Figure. S15. Gibbs energy profiles ($\Delta G°_{298.15}$) of *para*-OMe substituted styrene as substrate.

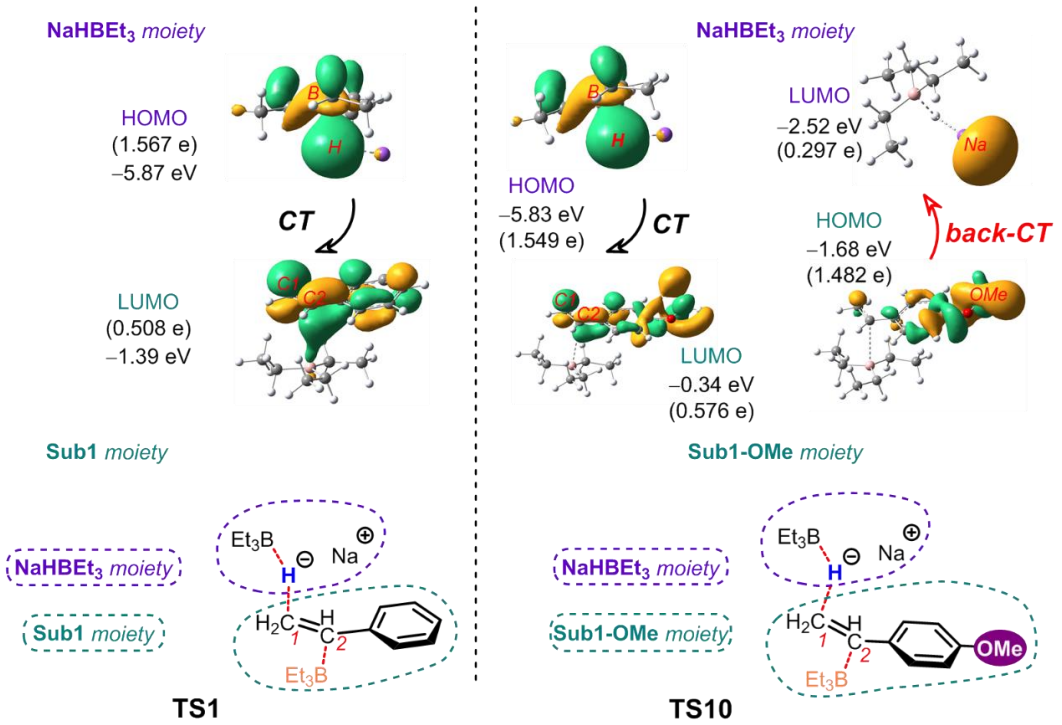

Figure. S16. Important Kohn−Sham orbitals and their electron populations of $NaHBEt_3$ and **Sub1** (and **Sub1-OMe**) moieties in **TS1** (and **TS10**).

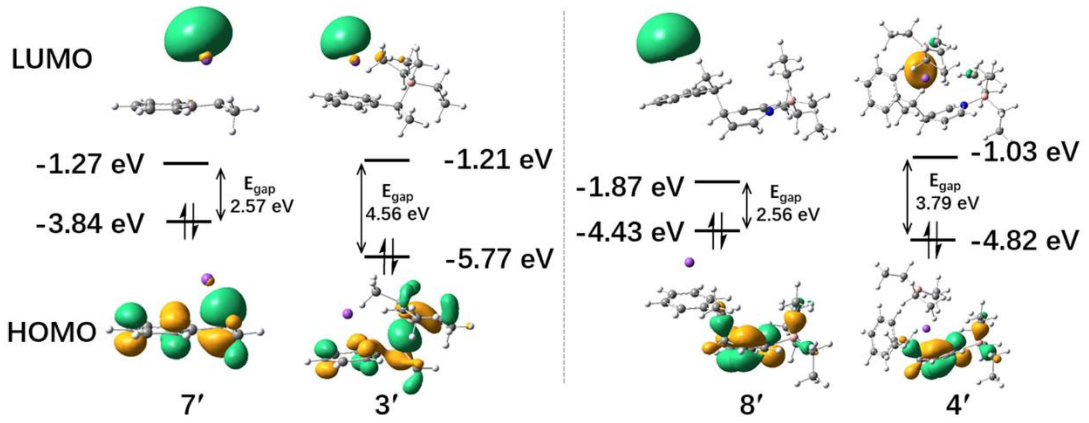

Figure S17. Frontier molecular orbital energy levels, distributions and energy gaps (E_{gap}) of intermediates **7′**, **3′**, **8′** and **4′**.

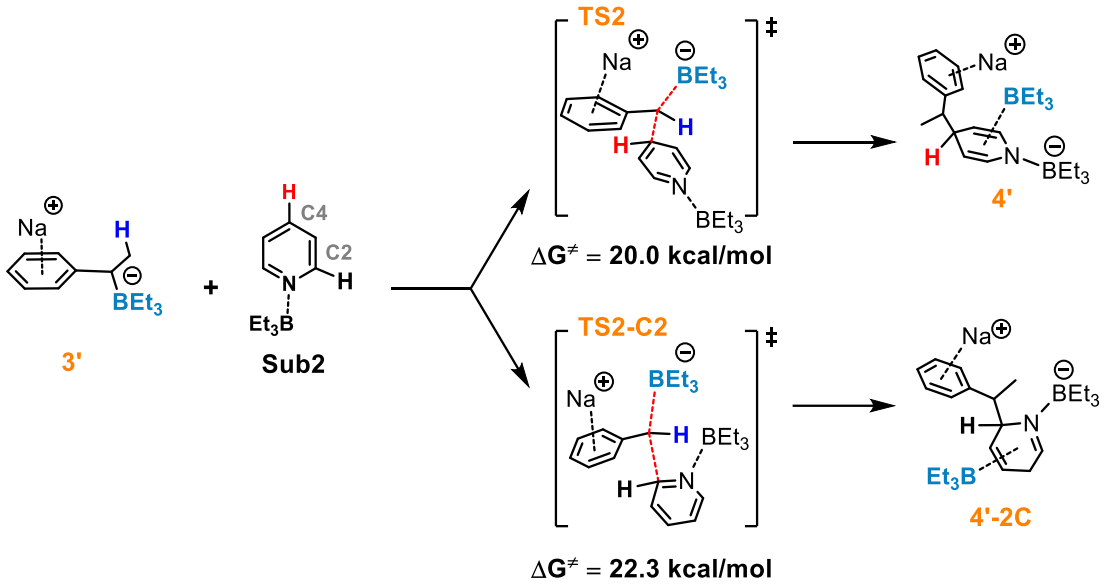

Figure S18. Nucleophilic addition processes for C4-position and C2-position of **Sub2**, respectively.

Cartesian Coordinates of Optimized Structures

1

C	2.74463800	-1.25722200	-1.23609400
C	2.08418400	-0.06214500	-1.51849100
C	1.99033900	0.96089100	-0.56086300
C	2.59130400	0.75178300	0.69244000
C	3.24815800	-0.44245000	0.97741500
C	3.32608200	-1.45499400	0.01674100
H	2.79994900	-2.03531200	-1.99426100
H	1.61360400	0.08256100	-2.49034400
H	2.54626600	1.52999300	1.45217300

H	3.70568400	-0.58377100	1.95407900
H	3.84292300	-2.38478000	0.24176700
C	1.23038600	2.17134700	-0.89478700
C	0.89723200	3.15791400	-0.05755100
H	0.88919100	2.22216300	-1.93057100
H	1.18166000	3.16514600	0.99394600
H	-1.06630800	0.08476200	-0.46372000
H	0.30731600	4.00283900	-0.40434400
C	-3.21559300	0.93978200	-0.17222700
C	-3.29568000	1.37286300	-1.63234800
H	-3.00368200	1.83437200	0.44248300
H	-4.21643200	0.59768800	0.15880600
H	-4.07638300	2.12266300	-1.83240300
H	-2.34006900	1.80829400	-1.96331200
H	-3.49595100	0.51975600	-2.29802600
C	-2.66064600	-1.68355300	-0.45754300
C	-1.65967200	-2.83730000	-0.51324300
H	-3.06353000	-1.54408600	-1.47646800
H	-3.52690100	-2.00882400	0.15037400
H	-2.08333300	-3.77559200	-0.89858200
H	-0.81228500	-2.60778100	-1.18453700
H	-1.26004700	-3.09675400	0.48313900
C	-1.87212400	-0.34678800	1.77074000
C	-1.08857300	0.80613100	2.40028300
H	-1.42736400	-1.30808100	2.11047800
H	-2.87569800	-0.37445900	2.23248200
H	-1.04552900	0.76536900	3.49839600
H	-0.04226000	0.85846700	2.05022200
H	-1.53111200	1.77440500	2.12805200
B	-2.13478200	-0.24534100	0.13775500
Na	0.33945400	-1.17089800	0.49677900

TS1

C	2.05576900	3.35782400	0.72105700
C	1.66243900	2.07620700	1.07912000
C	0.85427100	1.28287100	0.22802100
C	0.42510700	1.88226200	-0.98168200
C	0.82373600	3.16895400	-1.33185500
C	1.64508900	3.91765100	-0.49141500
H	2.68766300	3.93101200	1.39757600
H	1.99086200	1.65388200	2.03025400
H	-0.21310000	1.32103400	-1.66510700
H	0.48188100	3.59042600	-2.27595300
H	1.95219300	4.92304600	-0.76926100
C	0.43990900	-0.03927500	0.63587200
C	-0.49112100	-0.81321400	-0.06766900
H	0.69552800	-0.33648100	1.65659900

H	-0.53742000	-0.74293600	-1.15852100
H	-1.90027800	-0.37804800	0.04069700
H	-0.68127200	-1.82339300	0.30013600
C	-3.52374600	-1.07359300	-1.52509700
C	-3.23315700	-2.56185100	-1.68599100
H	-2.91678100	-0.50817400	-2.25568500
H	-4.57003300	-0.88297300	-1.83366000
H	-3.35364100	-2.90912800	-2.72194900
H	-2.20602700	-2.81295000	-1.38326700
H	-3.90195200	-3.17255700	-1.06396400
C	-3.67075100	-1.39398700	1.21236400
C	-3.22279500	-0.87204400	2.57523300
H	-3.24175000	-2.39923900	1.06885500
H	-4.76606200	-1.55346800	1.23187900
H	-3.49466000	-1.53663700	3.40652500
H	-2.12430400	-0.77524600	2.62519100
H	-3.66386300	0.10785000	2.81401600
C	-3.92255400	1.06732400	0.05996300
C	-3.51065600	2.07445300	-1.01276100
H	-3.84478800	1.53628200	1.06161000
H	-5.01349700	0.90928900	-0.02293400
H	-3.97494700	3.06035100	-0.87809400
H	-2.41951700	2.23799900	-1.05683300
H	-3.79156900	1.71903500	-2.01198100
B	-3.32391700	-0.44715200	-0.05015900
Na	-1.57446300	1.44981300	1.29518000
C	2.24026300	-3.02954900	0.08371200
C	1.46932900	-3.67391500	-1.06086300
H	1.62122500	-3.00073800	0.99547000
H	3.08527000	-3.68527800	0.36922300
H	1.07330100	-4.66232100	-0.79295700
H	0.61462000	-3.05763500	-1.37295600
H	2.10113900	-3.81033400	-1.94852700
C	2.98869200	-1.01975800	-1.61850700
C	3.71779800	0.30322000	-1.81742200
H	1.96976100	-0.95857500	-2.03791000
H	3.46923100	-1.80319600	-2.23359300
H	3.71343600	0.62674600	-2.86683400
H	3.26086600	1.11064600	-1.22905400
H	4.76902000	0.23764300	-1.50577400
C	3.72214000	-0.93535800	1.01158600
C	3.50643900	-1.42042500	2.43856700
H	3.61686600	0.16012700	0.95630000
H	4.77787500	-1.10713400	0.72360800
H	4.15593600	-0.90310900	3.15727400
H	2.46993200	-1.25950700	2.76804600

H	3.70725600	-2.49524600	2.54003400
B	2.89661400	-1.61000600	-0.15361000

2

C	2.76099500	1.36718300	-0.17748700
C	1.53775500	0.94692500	-0.69676300
C	0.89543900	-0.22799900	-0.24381000
C	1.59126400	-0.98839700	0.72264200
C	2.81576000	-0.56927600	1.24752100
C	3.41279800	0.61363400	0.80510600
H	3.21409100	2.28476100	-0.54872700
H	1.05086400	1.54474300	-1.46676200
H	1.15020800	-1.91166000	1.09394000
H	3.30857100	-1.17600400	2.00535000
H	4.36607500	0.94109900	1.21297200
C	-0.44172000	-0.61528700	-0.75029800
C	-0.62933500	-2.12856200	-0.78917700
H	-0.52512000	-0.23819200	-1.78438700
H	-0.76866700	-2.56624800	0.20977300
H	0.22862800	-2.65352600	-1.24808700
H	-1.51670600	-2.39309300	-1.37566800
Na	3.28726400	-1.09143800	-1.45839700
C	-3.15993800	-0.38872200	-0.43930300
C	-3.75141300	-1.61884700	0.25098100
H	-3.13485500	-0.57665500	-1.53097900
H	-3.90075200	0.42755700	-0.32014000
H	-4.74440000	-1.89166800	-0.13998300
H	-3.11800100	-2.51052100	0.14833000
H	-3.87754800	-1.44968300	1.33010500
C	-1.58773000	0.05893000	1.71849700
C	-0.65469200	1.00563700	2.47618200
H	-1.33452600	-0.98355300	1.99619900
H	-2.60259100	0.20822800	2.13727200
H	-0.62532700	0.80221800	3.55853600
H	0.38344600	0.95593400	2.11672600
H	-0.97187300	2.05232500	2.36418500
C	-1.65761000	1.81525900	-0.32321500
C	-1.96178400	2.17280300	-1.77644000
H	-0.69016200	2.27393300	-0.04732500
H	-2.40091200	2.33412500	0.31468900
H	-1.90815000	3.25347100	-1.98197800
H	-1.26546100	1.68568600	-2.47775700
H	-2.96989300	1.84678300	-2.07082900
B	-1.70511600	0.21721600	0.08005900

3

C	-3.02385400	0.56862200	-1.20277100
C	-1.65514400	0.42428500	-1.42551200

C	-0.88861000	-0.55735500	-0.76614600
C	-1.58343700	-1.40183100	0.12500100
C	-2.95487800	-1.26793800	0.34813100
C	-3.68783100	-0.27467900	-0.30664300
H	-3.57698600	1.33960200	-1.73641100
H	-1.15544400	1.08507700	-2.13481500
H	-1.03747900	-2.18405900	0.65099100
H	-3.45384600	-1.94440700	1.03994600
H	-4.75716800	-0.17277300	-0.13738200
C	0.58141800	-0.66605000	-0.97810900
C	1.01426200	-2.13053800	-1.10126900
H	0.78890900	-0.18229300	-1.94921200
H	0.35652800	-2.70699100	-1.77197600
H	1.02934800	-2.65523100	-0.13687700
H	2.03066200	-2.20197500	-1.50623800
C	3.09959800	-0.15361600	-0.10072300
C	3.69169700	0.20641000	-1.46109700
H	3.28207000	-1.22702900	0.08196700
H	3.69032300	0.36596100	0.68054200
H	4.74990700	-0.07936000	-1.56458800
H	3.15189800	-0.28543400	-2.28509800
H	3.63741900	1.28724600	-1.65573200
C	1.39577700	1.87081900	-0.15537000
C	0.24182600	2.71406700	0.39223500
H	1.46316900	2.06980400	-1.24098200
H	2.31974500	2.31378200	0.26378200
H	0.41363000	3.79525800	0.29047900
H	-0.70111000	2.53137400	-0.14808500
H	0.09715800	2.55253800	1.47509100
C	1.15690700	-0.04771400	1.73121100
C	1.55236100	-1.38715100	2.35386800
H	0.08498700	0.09475200	1.98619400
H	1.66760100	0.74955800	2.30684400
H	1.37500900	-1.42272600	3.43979600
H	0.99551300	-2.22780000	1.91544500
H	2.61833800	-1.60153100	2.19829500
B	1.51267300	0.23569100	0.13804800
Na	-1.84310000	1.10401900	1.32099500

TS2

C	2.83273200	-1.87040400	1.82332500
C	2.07114100	-1.12786200	0.93354700
C	2.33191800	-1.12727800	-0.47759300
C	3.43356500	-1.94118800	-0.90278900
C	4.18195000	-2.68711800	0.00265500
C	3.91237100	-2.65494500	1.37946200
H	2.59312300	-1.83102600	2.88597700

H	1.24543400	-0.51877200	1.30393000
H	3.68234500	-1.98639100	-1.96254400
H	5.00686500	-3.29485000	-0.36848400
H	4.50699700	-3.23579500	2.07971600
C	1.49996600	-0.42759700	-1.36879200
C	1.87164800	-0.20863500	-2.80109000
H	0.80538000	0.28655100	-0.91946800
H	1.97231700	-1.15702400	-3.35798900
H	2.82943300	0.32659500	-2.93973600
H	1.10445000	0.38098500	-3.31993500
C	0.95282400	3.05957900	-1.23385100
C	-0.51457300	2.91699300	-1.62000100
H	1.59271700	2.57632700	-1.98952400
H	1.24987000	4.12543200	-1.28571100
H	-0.70924800	3.26373900	-2.64353600
H	-0.84418000	1.86837800	-1.56560200
H	-1.17271600	3.49067100	-0.95361700
C	0.29510900	2.33186300	1.31677000
C	0.75318200	2.05420700	2.74354800
H	-0.33785200	1.50004700	0.95100600
H	-0.40262400	3.18797500	1.30713000
H	-0.09281900	1.92389100	3.43119500
H	1.35990800	1.13895400	2.80850900
H	1.36714600	2.87441200	3.14040400
C	2.91801000	2.53792700	0.59684500
C	3.94614200	2.44881100	-0.52656100
H	3.05357100	1.74960800	1.36043300
H	3.09168400	3.46380700	1.17600200
H	4.98726200	2.45713400	-0.16645000
H	3.79087800	1.55970900	-1.15979300
H	3.86655900	3.30373600	-1.20812400
B	1.38493800	2.59601000	0.20906700
Na	4.62508400	-0.05000100	0.68577200
C	-5.08565600	-0.83301100	-0.16385100
C	-5.22649800	-2.33518600	0.06006100
H	-5.14221200	-0.63442500	-1.24963900
H	-5.96699900	-0.31836200	0.26335900
H	-6.13014600	-2.76124500	-0.40062800
H	-4.36820300	-2.88220600	-0.36024500
H	-5.26646900	-2.58536000	1.12999000
C	-3.64124700	-0.43203500	2.07916800
C	-2.50597700	0.26561400	2.82639500
H	-3.61611100	-1.51040400	2.31652000
H	-4.60094800	-0.08642100	2.50592500
H	-2.49224500	0.03957600	3.90339100
H	-1.51703000	-0.01635200	2.42988800

H	-2.57552300	1.35839900	2.73000700
C	-3.69082000	1.47835400	0.21621700
C	-4.30388800	2.09131700	-1.04351300
H	-2.64936600	1.83798900	0.31324200
H	-4.21923900	1.93168700	1.07573900
H	-4.29035100	3.19177200	-1.01842500
H	-3.78126600	1.80339100	-1.96710100
H	-5.35400000	1.79161200	-1.17030400
B	-3.74693400	-0.14703900	0.47214400
C	-1.18810000	-1.15815800	-2.29860300
C	-2.23413500	-0.61722900	-1.59924800
C	-1.65104400	-1.76780300	0.31501300
C	-0.58014100	-2.35638800	-0.31288400
C	-0.21246100	-1.93609800	-1.61757800
H	-1.08093000	-0.92580300	-3.35546200
H	-2.95872000	0.02645900	-2.08927800
H	-1.90830400	-2.03511300	1.33611900
H	0.01211100	-3.08988300	0.22796700
H	0.51023800	-2.51832200	-2.18738400
N	-2.45897700	-0.85547300	-0.27813400

4

C	-3.51083100	-3.43307900	-0.61680200
C	-2.61546200	-2.97236100	0.34385300
C	-2.30755100	-1.60988000	0.44151800
C	-2.94472000	-0.72982200	-0.44211600
C	-3.84026700	-1.18562200	-1.41143900
C	-4.12176600	-2.54562700	-1.50316900
H	-3.73144400	-4.49685200	-0.67855500
H	-2.14183500	-3.68086800	1.02292700
H	-2.74605700	0.34162200	-0.35650300
H	-4.32004100	-0.47415800	-2.08232700
C	-1.33151000	-1.07210700	1.46070800
C	-2.00308700	-0.95880900	2.82698800
H	-1.05563400	-0.05056000	1.13881200
H	-2.26723600	-1.95529200	3.20884400
H	-2.92792600	-0.36946900	2.77139600
H	-1.34063000	-0.47891800	3.55837500
C	-1.85637100	2.75557100	1.54484900
C	-0.51418900	2.68047100	2.26026100
H	-2.53075400	1.96217600	1.92223500
H	-2.38724600	3.68145100	1.82549300
H	-0.62502800	2.72899700	3.35139200
H	0.02103900	1.74626400	2.03449000
H	0.14664000	3.50654800	1.96478000
C	-0.57136100	2.28014300	-0.81923600
C	-0.67841500	2.02089600	-2.31980900

H	-0.04565200	1.46119600	-0.28905400
H	0.11966000	3.12557800	-0.64876700
H	0.26947600	1.68086700	-2.76539600
H	-1.47489300	1.30074500	-2.57701500
H	-0.95644100	2.93242600	-2.86214700
C	-3.23945900	2.89710800	-0.79644900
C	-4.54181400	2.87481300	-0.00513200
H	-3.32268100	2.24409300	-1.68068500
H	-3.08927500	3.90281800	-1.23683000
H	-5.41008800	3.11464900	-0.63191200
H	-4.72641800	1.88464400	0.43606400
H	-4.53133900	3.59616400	0.82175600
B	-1.89149600	2.62907300	-0.02306100
Na	-0.46990500	-0.73319200	-1.69506100
C	4.92785700	-0.04316700	0.52841500
C	5.37966800	-1.49325600	0.67597800
H	4.78664000	0.38243400	1.53780300
H	5.75401200	0.55052100	0.09249300
H	6.23267300	-1.62281800	1.35906100
H	4.56277100	-2.12455900	1.06049800
H	5.68000000	-1.92386300	-0.29024300
C	3.89616300	-0.44221500	-1.90814700
C	2.96074600	-0.05324700	-3.05174700
H	3.99617100	-1.54233500	-1.88748200
H	4.90671300	-0.08676800	-2.18197000
H	3.22231700	-0.53208100	-4.00700800
H	1.90925100	-0.32556500	-2.85290100
H	2.96358000	1.03119700	-3.22614100
C	3.21829000	1.76251100	-0.55889500
C	3.10299000	2.60374700	0.70935100
H	2.27388900	1.86084100	-1.12873800
H	3.98724000	2.22584600	-1.20766500
H	2.86379400	3.65960400	0.50588400
H	2.31845400	2.22798000	1.38240100
H	4.04107300	2.59782400	1.28376100
B	3.60250300	0.17315200	-0.41142400
C	1.05426600	-1.08487700	2.27844400
C	2.06562800	-0.47016500	1.62702800
C	1.66982100	-1.63616400	-0.31406400
C	0.58853000	-2.27422800	0.21757400
C	-0.00163300	-1.88099200	1.55394000
H	0.97766400	-0.95142000	3.35676300
H	2.76285200	0.15777600	2.17904000
H	2.06363800	-1.96672900	-1.27677200
H	0.20498500	-3.15212000	-0.30428000
H	-0.24744000	-2.79325700	2.12887200

N	2.36155800	-0.62102400	0.28151800
H	-4.81660000	-2.91332900	-2.25471000

TS3

C	-3.83893400	-0.43264200	-2.41590200
C	-2.78465300	-0.40948700	-1.49742500
C	-2.67401700	0.61344800	-0.54816000
C	-3.66215300	1.61353100	-0.55319600
C	-4.72113300	1.58802800	-1.45722100
C	-4.81602100	0.55894700	-2.39629200
H	-3.89266600	-1.24090400	-3.14284800
H	-2.05193700	-1.21204500	-1.51979200
H	-3.59512100	2.42999100	0.16612100
H	-5.46863400	2.37782800	-1.43317600
H	-5.63649800	0.53832300	-3.10945900
C	-1.58741100	0.68895700	0.51118900
C	-2.19763300	0.52498900	1.90336500
H	-1.19928500	1.72409600	0.45709300
H	-2.50899100	-0.51462800	2.07653500
H	-3.06755500	1.18017600	2.03123100
H	-1.48590800	0.78461600	2.69496400
C	0.43262600	3.85577200	2.04154000
C	1.74306000	3.36610000	2.64142200
H	-0.40871600	3.25537900	2.43730300
H	0.20206400	4.87365500	2.40325400
H	1.73986100	3.41100800	3.73847300
H	1.94481700	2.32314600	2.35996500
H	2.59847000	3.96153700	2.29452600
C	1.42846200	3.34082200	-0.45381900
C	1.20028500	3.33279500	-1.95949100
H	1.67712700	2.32123300	-0.10222900
H	2.33993200	3.91514700	-0.20761600
H	2.05538500	2.91544700	-2.50864100
H	0.32093500	2.73147100	-2.23160500
H	1.02848900	4.34478600	-2.35083500
C	-1.07016700	4.40704300	-0.16270400
C	-2.20040100	4.82309700	0.76966100
H	-1.43014700	3.65658000	-0.89008000
H	-0.78488800	5.25732900	-0.80887700
H	-3.09555300	5.14715500	0.22184000
H	-2.50544000	4.00130900	1.43463900
H	-1.90367200	5.65565900	1.42110800
B	0.27013900	3.86690900	0.47360100
Na	-4.80181000	-1.04687000	0.26182400
C	4.76106900	-1.55304200	0.65732400
C	4.23076000	-2.97590600	0.81330300
H	4.70165700	-1.04922000	1.63844000

H	5.84494600	-1.59545500	0.44047100
H	4.75120300	-3.54982500	1.59466400
H	3.16169200	-2.97927700	1.07483200
H	4.32216900	-3.55072200	-0.12001000
C	4.28449400	-1.45317700	-1.97923000
C	4.40083000	-0.63936200	-3.26993700
H	3.49345300	-2.21554800	-2.10606000
H	5.21694200	-2.04057300	-1.89135000
H	4.53497800	-1.27595000	-4.15727600
H	3.52276500	-0.00669000	-3.46928400
H	5.26265200	0.04161400	-3.23780900
C	4.73132500	0.84313300	-0.60123600
C	4.72550300	1.63474000	0.70166000
H	4.20876000	1.43639000	-1.37529700
H	5.77481100	0.76186500	-0.96027400
H	5.10330700	2.66275600	0.58865600
H	3.70940100	1.71817200	1.11471100
H	5.34285700	1.15117300	1.47254800
B	4.09887600	-0.66504700	-0.54492500
C	0.66162600	-0.19561300	1.30968700
C	1.98321900	-0.39865000	1.02323100
C	1.58871500	-0.32310800	-1.23094800
C	0.24947900	-0.12940300	-1.03883500
C	-0.35046200	-0.18592600	0.27712000
H	0.37953500	-0.11731400	2.35722100
H	2.70884000	-0.46580500	1.83105100
H	1.99722000	-0.30549300	-2.23793700
H	-0.35471900	0.06996200	-1.91911400
H	-1.05664300	-1.52430400	0.44377500
N	2.48843000	-0.50521000	-0.23360200
C	-0.69785300	-3.63700100	-0.63945600
C	0.81788100	-3.78838200	-0.73991700
H	-1.07069200	-3.12783200	-1.54817300
H	-1.14690400	-4.64745400	-0.69877600
H	1.13954300	-4.18890900	-1.71290600
H	1.34229200	-2.83454400	-0.59579900
H	1.20289300	-4.47391200	0.02785000
C	-0.38536400	-3.19968900	2.02533100
C	-0.93888300	-2.73857400	3.37004900
H	0.62978100	-2.78805100	1.89718700
H	-0.23291400	-4.29609900	2.07095500
H	-0.28213800	-3.00428500	4.21114000
H	-1.07140600	-1.64730800	3.40572700
H	-1.92168100	-3.18325400	3.58406900
C	-2.87155100	-3.20338300	0.96085800
C	-3.76518800	-3.53178500	-0.23862300

H	-3.31313600	-2.40979500	1.59669700
H	-2.91622100	-4.08199800	1.63035300
H	-4.82736700	-3.67130500	0.02559900
H	-3.70031200	-2.79925600	-1.05709200
H	-3.45694000	-4.47828200	-0.69786000
B	-1.27638300	-2.94133400	0.70377200

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C	-3.40108900	-0.58320300	-0.76093000
C	-2.25027400	0.10222200	-1.14461900
C	-1.23316600	0.35876200	-0.22453700
C	-1.38829800	-0.08726800	1.09153800
C	-2.53600000	-0.77092800	1.47725100
C	-3.54693400	-1.02092100	0.55128000
H	-4.18476700	-0.77498000	-1.49147500
H	-2.13678100	0.44557600	-2.17329200
H	-0.59596900	0.09742900	1.81784500
H	-2.64125400	-1.11197500	2.50553600
H	-4.44385700	-1.55827600	0.85277000
C	-0.00226500	1.14476900	-0.63600000
C	-0.04156700	2.54728700	-0.03830100
H	-0.03964900	1.24333700	-1.73223900
H	-0.06776000	2.51923000	1.05849400
H	-0.94620500	3.06740400	-0.37344100
H	0.82679600	3.14267800	-0.34632800
C	2.17024300	0.74565700	0.66573800
C	3.29493100	-0.04468000	0.88754600
C	2.69533500	-1.51364700	-0.74181300
C	1.54494200	-0.79699800	-1.03395700
C	1.26048300	0.37125900	-0.32106400
H	2.02131900	1.64218500	1.26288000
H	4.01162700	0.24018000	1.65852200
H	2.92781000	-2.42231700	-1.29764400
H	0.86684600	-1.14290600	-1.81378200
N	3.57197200	-1.15734600	0.20562300

TS4

C	-4.28509600	-0.53415800	-0.22573100
C	-3.18941800	-1.25235800	0.22884900
C	-2.03738300	-0.60673700	0.74602800
C	-2.05440600	0.81188500	0.74411400
C	-3.16086200	1.52318100	0.28697400
C	-4.28567200	0.86357400	-0.20292300
H	-5.15231800	-1.07072100	-0.60848300
H	-3.20698500	-2.34273600	0.20498200
H	-1.19144400	1.36065900	1.12325800
H	-3.13527300	2.61204300	0.31029100
H	-5.14503600	1.42398300	-0.56367200

C	-0.88350600	-1.37289200	1.14271200
C	0.33886100	-0.79977100	1.52760200
H	-0.91727600	-2.44713900	0.94588900
H	0.33725500	0.15736800	2.05771300
H	1.14604000	-0.25439900	0.45441600
H	1.10801400	-1.47968400	1.89909000
C	2.90358100	1.28418100	0.84599000
C	3.61584000	0.68527200	2.05441900
H	2.10055600	1.95685500	1.19900100
H	3.60791800	1.95586200	0.31742900
H	3.95808600	1.44944400	2.76679500
H	2.96491500	-0.00308400	2.61261400
H	4.50164400	0.10823200	1.75505700
C	3.11961600	-1.12376400	-0.49581700
C	2.36463800	-2.19792900	-1.27535200
H	3.45264000	-1.56075800	0.45988500
H	4.05309200	-0.87573000	-1.03658900
H	2.95989800	-3.10298800	-1.45750200
H	1.47288700	-2.53746400	-0.72142400
H	2.04045200	-1.84523600	-2.26704300
C	1.80507100	0.99825900	-1.59642100
C	0.88378700	2.20762200	-1.44170400
H	1.41828000	0.32963800	-2.39161900
H	2.75093200	1.34894900	-2.04899700
H	0.59831500	2.65718900	-2.40208300
H	-0.05211700	1.97198900	-0.90539500
H	1.36849800	2.99329500	-0.84873100
B	2.30810900	0.24858300	-0.23903100
Na	-0.30816600	-0.63333300	-1.24474200

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C	3.62742600	0.96721100	-0.14827000
C	2.52561400	1.28237500	0.62261500
C	1.63124200	0.27169400	1.16443400
C	2.00800300	-1.09025100	0.81828600
C	3.11767900	-1.37608700	0.03796600
C	3.94432200	-0.36770500	-0.49427200
H	4.25956700	1.77838800	-0.51271300
H	2.31746800	2.32740300	0.86042500
H	1.40302200	-1.91351400	1.19882300
H	3.34288500	-2.42122200	-0.18108900
H	4.82378800	-0.60644400	-1.08639600
C	0.49681400	0.58807200	1.88454300
C	-0.43068600	-0.43566800	2.46446200
H	0.28884200	1.64193600	2.08195200
H	0.01808600	-1.04879000	3.26864200
H	-0.80401400	-1.16380600	1.71926900

H	-1.31951100	0.04034000	2.90086400
C	-3.67084500	-0.72190600	0.00157700
C	-4.76527100	0.11243200	0.65350300
H	-3.32224800	-1.50326000	0.69867200
H	-4.08592600	-1.30422300	-0.84202800
H	-5.61251300	-0.50111100	0.98587200
H	-4.38924400	0.64686700	1.53618200
H	-5.16506300	0.87011100	-0.03350400
C	-2.33660000	1.59237900	-0.60239800
C	-1.04360900	2.24862600	-1.07119700
H	-2.58725200	1.95323900	0.41049800
H	-3.18905200	1.93748700	-1.21464500
H	-1.10380500	3.34411300	-1.06584400
H	-0.21566600	1.97279900	-0.39948000
H	-0.78211500	1.95487800	-2.09958900
C	-1.17240800	-0.80885600	-1.10173700
C	-1.23981600	-2.32841100	-1.15846100
H	-0.37853300	-0.49047500	-0.39626700
H	-0.91112800	-0.39673500	-2.09483500
H	-0.29986800	-2.77438600	-1.51195800
H	-1.44277900	-2.75767200	-0.16876800
H	-2.03648000	-2.67382200	-1.83012500
B	-2.40550500	0.01858500	-0.56622100
Na	1.55162500	0.12650300	-1.61992400

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C	1.98601200	-0.81255900	-0.59761700
C	0.62550000	-0.84397400	-0.86081000
C	-0.27666700	0.16248300	-0.37860000
C	0.34653700	1.21990100	0.35628200
C	1.71033400	1.23444700	0.61035200
C	2.55766000	0.22118700	0.15266700
H	2.61854500	-1.60753900	-0.99530200
H	0.21597000	-1.65388800	-1.47331900
H	-0.26956200	2.03906000	0.72721300
H	2.12786600	2.06685500	1.17908500
H	3.62573600	0.24380100	0.35750100
C	-1.68531600	0.04374300	-0.54084900
C	-2.58358500	1.21736300	-0.25292200
H	-1.99263700	-0.58616300	-1.38555500
H	-2.36404700	2.12346200	-0.85562500
H	-2.53796200	1.54869000	0.79768900
H	-3.63530300	0.96623200	-0.44552700
Na	-1.26104100	-1.79964100	1.01480200

TS5

C	2.09769000	-1.97125800	-0.01707900

C	1.79327200	-0.71238900	0.48237700
C	2.57781600	0.44442500	0.16556400
C	3.71720300	0.20703500	-0.66921800
C	4.00550400	-1.05906500	-1.16942600
C	3.21362600	-2.17239100	-0.84683900
H	1.45848700	-2.81403800	0.24648200
H	0.91324300	-0.58159400	1.11495200
H	4.36184300	1.04257200	-0.93938800
H	4.87678700	-1.18767200	-1.81111900
H	3.44590500	-3.15744500	-1.24308500
C	2.13671900	1.72969600	0.53707900
C	2.97861200	2.95296700	0.35290300
H	1.39933500	1.76115900	1.34097400
H	3.32526500	3.06047200	-0.68796000
H	3.88504700	2.98515000	0.98278000
H	2.40185400	3.85865100	0.58676400
Na	4.27337300	-1.29775200	1.57024200
C	-0.57269100	2.57836700	-0.23477900
C	-1.63460100	1.77925500	0.09232500
C	-0.86478500	0.07649200	-1.26364400
C	0.23162600	0.80968900	-1.63793000
C	0.50305300	2.05616600	-1.01167500
H	-0.52507300	3.58681400	0.17126700
H	-2.42677900	2.14250200	0.74187900
H	-1.03969500	-0.90678600	-1.69084900
H	0.92496000	0.38296100	-2.36009700
H	1.21675800	2.73744400	-1.47125400
N	-1.79348500	0.50793400	-0.37527500
C	-3.31195800	-1.63878300	-0.91253700
C	-2.52128000	-2.94830100	-0.93883900
H	-3.30104600	-1.19279800	-1.92396000
H	-4.37058600	-1.91071800	-0.74821700
H	-2.84812300	-3.62222700	-1.74488900
H	-1.43928900	-2.79902900	-1.07364300
H	-2.63734300	-3.50368800	0.00226900
C	-2.29767900	-1.19063100	1.56093200
C	-1.97091600	-0.26370200	2.72704200
H	-1.37906600	-1.74253900	1.28172200
H	-3.00100500	-1.96751200	1.91589200
H	-1.52586700	-0.78890000	3.58568500
H	-1.25862600	0.52294600	2.43358600
H	-2.86857500	0.25066500	3.10008200
C	-4.27685900	0.37463400	0.56679100
C	-4.94834400	1.04733000	-0.62738500
H	-4.09467400	1.13496000	1.34650100
H	-4.99598800	-0.32417900	1.03336700

H	-5.83489500	1.63894900	-0.35441900
H	-4.25735500	1.72860300	-1.14676100
H	-5.27606700	0.30936200	-1.37327000
B	-2.94363700	-0.50431200	0.22100100

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C	3.41476500	-2.01012100	-0.20538400
C	2.38831200	-1.11888500	0.11405000
C	2.53226900	0.26340900	-0.09191600
C	3.74241900	0.72202200	-0.63745100
C	4.77245900	-0.16473200	-0.95691700
C	4.61528300	-1.53570200	-0.73865500
H	3.27574700	-3.07575700	-0.03604500
H	1.45359200	-1.49364800	0.52928700
H	3.88030000	1.78610000	-0.82313200
H	5.70018500	0.21655600	-1.37825600
H	5.41698800	-2.22655100	-0.98802100
C	1.39519900	1.19718100	0.21109800
C	1.83745900	2.48179800	0.89834500
H	0.69643500	0.66164300	0.87414000
H	2.41733000	3.12677000	0.22326000
H	2.45277500	2.28638300	1.78787500
H	0.96223500	3.05571900	1.22378000
Na	4.44509300	-0.40699900	1.87662000
C	-0.65730900	2.31071800	-0.75633700
C	-1.79102400	1.66132700	-0.39885700
C	-1.07481000	-0.30547800	-1.37802200
C	0.09460600	0.25467800	-1.76504700
C	0.57166900	1.51075500	-1.09093200
H	-0.61437400	3.39720300	-0.69864800
H	-2.65000800	2.21146400	-0.01317100
H	-1.38268600	-1.27339600	-1.77048300
H	0.72418900	-0.25686000	-2.49215000
H	1.25229500	2.08102000	-1.74814900
N	-1.98903200	0.30714100	-0.55014400
C	-3.38600700	-1.96664000	-0.40327600
C	-2.42999400	-3.11712600	-0.08301500
H	-3.47255400	-1.86881900	-1.50129100
H	-4.39534400	-2.28179100	-0.07750000
H	-2.67471900	-4.04152600	-0.62865900
H	-1.38283800	-2.87626600	-0.32161600
H	-2.45069800	-3.36891600	0.98677000
C	-2.54324900	-0.70154500	1.82098400
C	-2.38068500	0.55133100	2.67712700
H	-1.56564500	-1.22085700	1.77579500
H	-3.21548100	-1.40335900	2.35294300
H	-1.98218400	0.34478600	3.68285100

H	-1.69764900	1.27569900	2.20682600
H	-3.33923700	1.07240400	2.81784800
C	-4.50583900	0.36401500	0.28459100
C	-5.14507900	0.55360600	-1.08773600
H	-4.38623700	1.35642800	0.75500900
H	-5.22013500	-0.16529900	0.94403800
H	-6.05775900	1.16894500	-1.06934400
H	-4.44578100	1.03618500	-1.78778600
H	-5.42200500	-0.40952300	-1.54022600
B	-3.11043900	-0.49828100	0.28926900

TS6

C	3.58018500	-2.93896900	-1.02867200
C	2.66085200	-2.43227200	-0.10986500
C	2.73219100	-1.10231100	0.33740300
C	3.77539100	-0.30331300	-0.14738000
C	4.70124800	-0.80561300	-1.06690900
C	4.60672600	-2.12386200	-1.51393800
H	3.49631300	-3.97025200	-1.36379300
H	1.86506500	-3.07443900	0.26652100
H	3.86660300	0.72823200	0.18630200
H	5.49382900	-0.15816800	-1.43688000
H	5.32408300	-2.51322900	-2.23230500
C	1.71839000	-0.59643100	1.33983800
C	2.31571000	0.39345000	2.32856700
H	1.40987000	-1.48544900	1.91655300
H	2.56453300	1.34603500	1.84743200
H	3.22980400	-0.01577700	2.77903700
H	1.62113500	0.60415400	3.14847400
Na	5.18148100	-2.33470700	1.24549100
C	-0.65579300	0.23224100	1.63490000
C	-1.97650600	0.04772400	1.32950600
C	-1.45635100	-0.94647200	-0.67208900
C	-0.11378900	-0.81301200	-0.44632300
C	0.38656000	-0.13035000	0.71399500
H	-0.41110000	0.69619200	2.58753500
H	-2.74644500	0.34842800	2.03596500
H	-1.81049500	-1.43250800	-1.57755900
H	0.57465000	-1.18960600	-1.19995300
H	0.93933800	1.25764300	0.14634100
N	-2.42059300	-0.52573000	0.18394900
C	-4.31658800	-0.74633600	-1.69811900
C	-4.23300300	-2.00186400	-2.56796600
H	-3.68764000	0.04199500	-2.15078100
H	-5.34786900	-0.36125800	-1.79739700
H	-4.47501200	-1.79748700	-3.62166500
H	-3.23742100	-2.47013000	-2.56238800

H	-4.93579900	-2.77478200	-2.22664900
C	-4.25855900	-2.38208600	0.47653100
C	-4.01355000	-2.60924900	1.96461200
H	-3.63444300	-3.09664800	-0.09147300
H	-5.30174500	-2.66506700	0.24100600
H	-4.19753000	-3.64726800	2.28011600
H	-2.97387100	-2.37514100	2.24039200
H	-4.65686100	-1.97014300	2.58664100
C	-4.91919000	0.22759200	0.72514900
C	-4.76466500	1.68789400	0.30687000
H	-4.79371500	0.16135800	1.82067000
H	-5.96791700	-0.07985900	0.55596500
H	-5.46935000	2.36044300	0.81845400
H	-3.75398800	2.06767000	0.51947900
H	-4.92339400	1.82037500	-0.77334000
B	-4.01087700	-0.86465000	-0.08353400
C	2.43357400	2.96224400	-0.69664600
C	3.04856600	2.37819600	-1.96672400
H	3.08887200	2.74220400	0.16631200
H	2.45773500	4.06745600	-0.77904200
H	4.13037800	2.56606000	-2.05463800
H	2.90208100	1.28927800	-2.02669600
H	2.57992300	2.79966500	-2.86630700
C	0.01373700	2.37944500	-1.76100700
C	-1.50725100	2.41229500	-1.64349400
H	0.31008700	1.46480900	-2.30845200
H	0.31908800	3.20666500	-2.43171900
H	-2.01216200	2.27053200	-2.61192700
H	-1.88896400	1.63483400	-0.96965400
H	-1.86034800	3.37360200	-1.24276000
C	0.15102500	3.44095900	0.72859800
C	0.92522200	3.79932100	1.99248800
H	-0.81203800	2.98298700	1.01898900
H	-0.13703800	4.38351500	0.22127000
H	0.37707400	4.49373100	2.64692500
H	1.15107500	2.90902300	2.59668800
H	1.88905600	4.27637100	1.76081200
B	0.88840100	2.53875000	-0.39777100

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C	0.08166900	2.98180400	-1.58209000
C	-0.84367000	2.17143100	-0.92474300
C	-0.73520500	1.92085500	0.45229900
C	0.35356900	2.47767700	1.14276100
C	1.27582400	3.29266300	0.48984400
C	1.14295800	3.55320600	-0.87682300
H	-0.03120200	3.17267000	-2.64701200

H	-1.66952400	1.73669600	-1.48499800
H	0.48946000	2.24884800	2.19800500
H	2.11006200	3.71363100	1.04706100
H	1.86234100	4.18984700	-1.38693700
C	-2.47188700	0.04921500	0.41141900
C	-1.76180100	-0.94291700	-0.27591600
C	-3.87013100	0.00823000	0.39668500
C	-2.43522500	-1.95340200	-0.95386100
H	-0.67105500	-0.94345900	-0.24665900
C	-4.54349400	-1.00117900	-0.28565200
H	-4.42849700	0.78632600	0.91571200
C	-3.82855600	-1.98360100	-0.96431600
H	-1.86473300	-2.72434400	-1.47082400
H	-5.63168100	-1.01478200	-0.29166900
H	-4.35410200	-2.77198900	-1.49922600
C	-1.76156800	1.11736700	1.15947800
C	-2.08566600	1.37991500	2.43492900
H	-1.63039900	2.19678700	2.99117900
H	-2.82794400	0.77997000	2.95734900
H	1.36050900	-0.67736700	0.52387900
C	1.54864100	-2.25759300	-1.27397700
C	1.26144700	-1.33322000	-2.45873800
H	0.62932300	-2.83706800	-1.07332200
H	2.28853200	-3.01061100	-1.60770200
H	0.93964200	-1.86954500	-3.36289000
H	0.44204600	-0.62317300	-2.24562300
H	2.15067800	-0.75828800	-2.77154900
C	3.65941800	-1.02920200	-0.08026900
C	4.17915800	-0.12489500	1.03706800
H	3.83911500	-0.52811300	-1.05673300
H	4.31810500	-1.91426300	-0.14341600
H	5.22795900	0.18071600	0.91140200
H	3.59320900	0.80575800	1.14450300
H	4.10204000	-0.62605700	2.01166600
C	2.10671200	-2.73269800	1.31650200
C	0.71987300	-3.11014900	1.82951800
H	2.71346900	-2.39478700	2.17673900
H	2.61560300	-3.64612200	0.94951400
H	0.73381400	-3.88340400	2.61274900
H	0.20385000	-2.23322900	2.25127000
H	0.07557100	-3.48952600	1.02219500
B	2.12345800	-1.61270500	0.12710900
Na	1.89492000	0.84521400	-0.82044600

TS7

C	-3.47585200	2.66758500	0.16263600
C	-2.90922100	1.44799200	0.50072900

C	-1.51074100	1.29204500	0.63419800
C	-0.72406500	2.44472600	0.41174100
C	-1.29848900	3.66842600	0.07159700
C	-2.67681700	3.79068400	-0.06367700
H	-4.55886800	2.74594000	0.08050900
H	-3.55796800	0.59535300	0.69373300
H	0.35950400	2.38875100	0.51681300
H	-0.65224600	4.52954300	-0.09357400
H	-3.12559200	4.74411400	-0.33334900
C	-0.89334400	0.01117800	0.98511900
C	0.43390200	0.00618500	1.45614800
H	0.79849200	0.87746300	2.00450900
H	1.46097800	0.13505200	0.40556100
H	0.84444500	-0.93142600	1.83064900
C	3.67205100	0.83336200	0.85296100
C	3.98456900	0.14068500	2.17584300
H	3.21417300	1.81674800	1.06351700
H	4.62835500	1.08042400	0.35171400
H	4.57581900	0.77220700	2.85422700
H	3.07024900	-0.14155200	2.71744600
H	4.55709800	-0.78422600	2.02103500
C	2.96141700	-1.58933900	-0.24580300
C	1.96552800	-2.39425800	-1.07905600
H	2.97245700	-2.00484300	0.77519900
H	3.97988800	-1.77596300	-0.63829900
H	2.21523300	-3.46239700	-1.13418600
H	0.95007000	-2.35792000	-0.64602900
H	1.91002900	-2.04390800	-2.12198700
C	2.74653000	0.71713200	-1.67813900
C	2.41875600	2.20544200	-1.78246600
H	2.19338000	0.16450300	-2.46391300
H	3.79297600	0.57872200	-2.00890800
H	2.56132300	2.59966200	-2.79759400
H	1.38032700	2.44187600	-1.49682200
H	3.05511000	2.79806500	-1.11239300
B	2.76368600	0.01513800	-0.20340900
Na	0.14350800	0.00133900	-1.38865300
C	-1.48052300	-1.26768400	0.54443100
C	-1.18332000	-2.47368700	1.21501600
C	-2.26452800	-1.38029100	-0.62591100
C	-1.61561900	-3.70301100	0.73692400
H	-0.60976900	-2.43873600	2.13976300
C	-2.69532900	-2.61548300	-1.10654800
H	-2.55935300	-0.48167800	-1.17000100
C	-2.36994900	-3.78893100	-0.43424100
H	-1.36586600	-4.60678400	1.29020300

H	-3.29035300	-2.65247700	-2.01760900
H	-2.70664700	-4.75348600	-0.80699900
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C	-2.64178200	2.48514500	0.73310200
C	-1.36280100	2.08706000	0.38146500
C	-1.09240300	1.17425000	-0.70577600
C	-2.28902400	0.76412100	-1.41049800
C	-3.56470900	1.17271500	-1.04141000
C	-3.78499300	2.01282500	0.06018600
H	-2.75562400	3.18928900	1.55756600
H	-0.53202200	2.53028400	0.92156400
H	-2.19920100	0.13494300	-2.29210200
H	-4.41252800	0.81967200	-1.62922500
H	-4.78377500	2.33936100	0.33740500
C	0.18697300	0.73390700	-1.11360800
C	0.27530300	-0.03073900	-2.41191000
H	0.08984200	0.58333300	-3.31347500
H	-0.44961700	-0.85833500	-2.45909700
H	1.26211200	-0.49129700	-2.54092700
C	1.42079200	-2.80875800	-0.47408000
C	2.84273200	-2.35342100	-0.17013600
H	1.16496700	-2.58273300	-1.52225100
H	1.36200900	-3.91334000	-0.42808800
H	3.57162800	-2.77942500	-0.87204700
H	2.93248100	-1.25909600	-0.23281800
H	3.15926800	-2.64542000	0.84012800
C	0.62463700	-1.71059600	1.87896600
C	-0.44066200	-1.04410900	2.74012400
H	1.48971100	-1.03701100	1.78045300
H	1.03522900	-2.58569600	2.41882400
H	-0.08907400	-0.84476300	3.75994000
H	-0.71368200	-0.05565900	2.33451700
H	-1.34365300	-1.66431800	2.84906200
C	-1.24307200	-2.53019300	0.01459400
C	-1.52334000	-3.64350700	-0.99188600
H	-1.53167900	-1.57093000	-0.46246800
H	-1.89773400	-2.66922100	0.89398900
H	-2.58209000	-3.68220700	-1.27811800
H	-0.94290400	-3.50902300	-1.91308800
H	-1.25948300	-4.62789400	-0.58449000
B	0.26063300	-2.29668800	0.46156200
Na	-2.80472700	-0.24053800	1.12484800
C	1.44501000	1.17069500	-0.52185700
C	1.64393800	1.40594400	0.86285800
C	2.60425000	1.32720000	-1.32651700
C	2.88347600	1.74701500	1.39085600

H	0.82100400	1.25593000	1.55673000
C	3.84287600	1.66783300	-0.79706300
H	2.52415900	1.19002100	-2.40320300
C	4.00390200	1.88119400	0.57164400
H	2.97519000	1.89075200	2.46751800
H	4.69394200	1.77484400	-1.46935900
H	4.97373700	2.14581800	0.98759700

TS8

C	3.39777700	0.48912800	3.18239300
C	2.69813100	1.07144200	2.12699300
C	1.56477200	0.45564100	1.53215200
C	1.17862300	-0.77894500	2.12025600
C	1.86306600	-1.34048800	3.19017100
C	2.99056800	-0.72283400	3.73145200
H	4.27060500	1.00463100	3.58050900
H	3.05566900	2.03386100	1.76781900
H	0.32920800	-1.32501100	1.72069900
H	1.51564200	-2.29087200	3.59370400
H	3.53368500	-1.17498900	4.55784600
C	0.83184300	0.98705200	0.37251200
C	0.15067200	-0.05573200	-0.48249900
H	-0.51733100	-0.69423600	0.10671900
H	0.84921900	-0.73599700	-1.00725800
H	-0.47527900	0.41106100	-1.25251500
Na	3.59214900	0.60187200	-0.45175700
C	-1.54482500	0.90507900	2.09058700
C	-2.65121800	0.24633900	1.62237100
C	-2.80495300	1.64081300	-0.20616100
C	-1.70506500	2.35300200	0.18782500
C	-0.90279700	1.89822100	1.28403100
H	-1.13773700	0.62608400	3.05915400
H	-3.10618400	-0.55090500	2.20536500
H	-3.37856900	1.95060500	-1.07460300
H	-1.41147400	3.22998000	-0.38637100
H	-0.24692000	2.61523600	1.77739300
N	-3.27626700	0.54790300	0.45427900
C	-5.22676300	0.31325000	-1.37187600
C	-4.61216300	0.31365100	-2.77271900
H	-5.47021200	1.35226500	-1.08357600
H	-6.21233200	-0.18164100	-1.44869700
H	-5.19737600	0.90536400	-3.49260800
H	-3.58675700	0.71340100	-2.79125400
H	-4.54805900	-0.70467100	-3.18024500
C	-3.64841700	-1.77879300	-0.74485100
C	-2.96374200	-2.71165900	0.25039600
H	-2.90361900	-1.47232900	-1.50383500

H	-4.39970900	-2.36660400	-1.30637300
H	-2.53321800	-3.60545900	-0.22681700
H	-2.13778200	-2.21190700	0.78126800
H	-3.66268700	-3.06910700	1.02094400
C	-5.46510000	-0.83131100	1.03805400
C	-6.24427300	0.34667000	1.61631800
H	-4.97392600	-1.36828300	1.86866900
H	-6.17956600	-1.56775200	0.62482900
H	-6.92187600	0.06419600	2.43590100
H	-5.56506200	1.11627600	2.01440900
H	-6.86014100	0.83928400	0.85053900
B	-4.42340100	-0.45382400	-0.16460700
C	1.37413000	2.13870300	-0.37398800
C	1.45566800	2.13132300	-1.78803000
C	1.77625400	3.34308600	0.25564600
C	1.93632900	3.22333500	-2.50995200
H	1.13111300	1.25287900	-2.34355900
C	2.24618000	4.43246800	-0.46688700
H	1.67944100	3.44493500	1.33397700
C	2.34278700	4.38255900	-1.85767000
H	1.98425500	3.16017900	-3.59594200
H	2.52972500	5.33822900	0.06667600
H	2.71446600	5.23633000	-2.41947600
C	1.19769100	-3.68392300	-0.95479200
C	0.04132000	-3.80067400	-1.93869600
H	0.81943400	-3.41298300	0.04748400
H	1.65411500	-4.67813500	-0.79402400
H	-0.70076100	-4.54186000	-1.61527900
H	-0.48817400	-2.84359800	-2.05413100
H	0.38430200	-4.10288900	-2.93721800
C	2.53254600	-2.14731200	-2.77317000
C	3.47983300	-0.99151900	-3.07371200
H	1.54334500	-1.94182600	-3.20930200
H	2.87603800	-3.04569200	-3.32490500
H	3.66100100	-0.87309600	-4.14879900
H	3.04821400	-0.02713100	-2.75939600
H	4.46836500	-1.11689900	-2.60891600
C	3.45818400	-2.41128600	-0.18003100
C	3.78135800	-3.55160100	0.78634300
H	2.97997800	-1.61569700	0.42873000
H	4.40075800	-2.00348900	-0.58282300
H	4.49414900	-3.24011300	1.56001700
H	2.88052500	-3.91124900	1.29862500
H	4.22173100	-4.40795900	0.25988200
B	2.39130100	-2.71866500	-1.31112300

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C	-3.48666600	1.44507200	-1.82382500
C	-2.74890300	0.52685800	-1.08021400
C	-3.09272700	-0.83509500	-1.02580500
C	-4.19623500	-1.24207000	-1.78221200
C	-4.94050300	-0.32740900	-2.52751400
C	-4.60039100	1.02057100	-2.54623800
H	-3.17417100	2.48884900	-1.85063600
H	-1.84573600	0.86574900	-0.57007800
H	-4.49288600	-2.28772700	-1.79599400
H	-5.79849900	-0.67894400	-3.09729100
H	-5.18510300	1.73058800	-3.12650600
C	-2.24967000	-1.81092100	-0.20671300
C	-2.98008100	-3.14875200	-0.01758000
H	-2.99057300	-3.72370200	-0.95179100
H	-4.02093600	-3.02876700	0.30135500
H	-2.47275900	-3.75634700	0.73930700
Na	-3.30247700	1.42355200	1.45172600
C	-0.00139500	-3.07795200	-0.28206900
C	1.29424800	-2.78185200	-0.02518200
C	1.21409200	-0.85835700	-1.28571800
C	-0.09798300	-1.02691900	-1.58031300
C	-0.92560400	-2.16315100	-1.03845400
H	-0.38375100	-4.02915200	0.08497900
H	1.88985600	-3.47608000	0.56443400
H	1.75603300	-0.02228500	-1.72736800
H	-0.54763500	-0.33906400	-2.29621700
H	-1.38007500	-2.70006200	-1.89627400
N	1.96666300	-1.67067400	-0.47314900
C	4.33515700	-0.99582200	-1.55096400
C	4.38342200	0.43229100	-2.09608800
H	3.98482400	-1.67118200	-2.35412900
H	5.38576600	-1.29605300	-1.37663000
H	5.02833500	0.52377900	-2.98386000
H	3.39693000	0.81724400	-2.39346200
H	4.77933200	1.13409500	-1.34649800
C	3.52619300	-0.03019400	0.85729700
C	2.98162300	-0.28837600	2.25772600
H	2.94494500	0.79427300	0.39926500
H	4.55760000	0.36352900	0.94401400
H	2.86668600	0.62699700	2.86252200
H	1.99450100	-0.77643800	2.21564600
H	3.63726300	-0.96132900	2.82887100
C	4.22757600	-2.61666900	0.57044000
C	4.49111200	-3.83618200	-0.31249300
H	3.67782000	-2.94167400	1.47227500
H	5.19899600	-2.25687100	0.96037800

H	4.92987800	-4.68418800	0.23524000
H	3.57055800	-4.20530500	-0.78902900
H	5.18390600	-3.59513400	-1.13073500
B	3.51881000	-1.32398700	-0.14962100
C	-2.01784800	-1.18382000	1.17365200
C	-3.05632300	-1.22385900	2.12334500
C	-0.85239600	-0.49194500	1.53367800
C	-2.94447900	-0.59782200	3.36584800
H	-3.98204600	-1.74725100	1.89293400
C	-0.73820700	0.14007400	2.77451600
H	-0.02103200	-0.42568900	0.83612300
C	-1.78144700	0.09923000	3.69684700
H	-3.76893800	-0.65813100	4.07366200
H	0.18257200	0.66978200	3.01613900
H	-1.68630100	0.59157900	4.66173000
C	1.66025400	3.29843600	1.41135300
C	3.12204000	3.56483600	1.74619300
H	1.39892500	2.25514000	1.69185900
H	1.00177200	3.91181800	2.04811400
H	3.33571400	3.42314400	2.81374000
H	3.79220300	2.89516700	1.19072500
H	3.41003500	4.59416600	1.49310400
C	2.27837400	3.45744400	-1.24272900
C	1.81012700	3.29289100	-2.68267700
H	3.06927900	2.72285200	-1.01525600
H	2.79541600	4.42762100	-1.12010800
H	2.64376400	3.32943800	-3.39610400
H	1.30068800	2.32967700	-2.83387700
H	1.10005900	4.07819700	-2.97506000
C	-0.32533800	3.34022000	-0.46313900
C	-1.34338900	3.47757500	0.66073500
H	-0.45085900	2.37111800	-0.98522000
H	-0.53324500	4.08073200	-1.25213000
H	-2.37641800	3.40991000	0.28032600
H	-1.17026100	2.72254300	1.44494600
H	-1.27134500	4.45134300	1.16081900
B	1.20753600	3.39153000	-0.09345900

TS9

C	-2.8000002	-2.7838434	1.9746308
C	-2.2455602	-2.0718394	0.9135418
C	-3.0017712	-1.1668544	0.1485398
C	-4.3458342	-1.0117244	0.4937168
C	-4.9123062	-1.7312924	1.5468058
C	-4.1484172	-2.6200204	2.2933018
H	-2.1714132	-3.4595914	2.5545778
H	-1.1892982	-2.2172684	0.6816418

H	-4.9747672	-0.3136934	-0.0517892
H	-5.9629042	-1.5804534	1.7867998
H	-4.5918822	-3.1738974	3.1172918
C	-2.3714242	-0.4585914	-1.0609802
C	-3.4390902	0.2621786	-1.8914662
H	-3.8190522	1.1285496	-1.3432402
H	-4.2875852	-0.3840334	-2.1309432
H	-3.0263922	0.6093926	-2.8435912
Na	-2.1677422	-4.3018744	-0.6694362
C	-0.6448302	1.2646426	-1.7621312
C	0.6502478	1.7019766	-1.7016362
C	0.9373578	0.8050476	0.3894808
C	-0.3410352	0.3172966	0.4100328
C	-1.2597502	0.5679806	-0.6673332
H	-1.2043602	1.4753566	-2.6692022
H	1.0851928	2.2262686	-2.5480722
H	1.5987408	0.6350986	1.2372918
H	-0.6690862	-0.1989674	1.3086498
H	-2.2615602	1.6397706	0.0065848
N	1.4745828	1.4956286	-0.6474022
C	3.5397978	2.4456796	0.7882768
C	4.0864858	1.4862416	1.8447918
H	2.7223618	3.0380906	1.2376858
H	4.3369708	3.1850766	0.5898758
H	4.4404968	2.0121606	2.7441608
H	3.3401558	0.7558536	2.1897958
H	4.9376988	0.9041826	1.4620778
C	3.8245288	0.4535196	-1.0523352
C	3.4656068	-0.1582674	-2.4020902
H	3.6102048	-0.2921134	-0.2626792
H	4.9188498	0.6095296	-1.0077002
H	3.9734198	-1.1158594	-2.5970912
H	2.3826108	-0.3505154	-2.4808172
H	3.7249818	0.5119066	-3.2343062
C	3.3295068	3.0081466	-1.8158572
C	2.6853408	4.3681096	-1.5513202
H	3.0550718	2.6750456	-2.8326332
H	4.4260408	3.1419976	-1.8642522
H	2.9342498	5.1201736	-2.3146222
H	1.5865588	4.3036916	-1.5156442
H	2.9998058	4.7797586	-0.5818322
B	3.0793548	1.8608456	-0.6803982
C	-1.7655272	-1.5910194	-1.9289742
C	-2.6405702	-2.4264534	-2.6469762
C	-0.3999342	-1.9006704	-1.9819492
C	-2.1751552	-3.5156544	-3.3842672

H	-3.7117122	-2.2372764	-2.6277502
C	0.0699758	-2.9915594	-2.7171992
H	0.3224708	-1.2986914	-1.4348392
C	-0.8106602	-3.8095754	-3.4195872
H	-2.8842912	-4.1314044	-3.9340722
H	1.1390828	-3.1998614	-2.7306242
H	-0.4421692	-4.6561484	-3.9937372
C	-4.1433082	2.5070146	1.2145888
C	-4.1394832	1.6761836	2.4959748
H	-4.8080342	2.0285776	0.4728068
H	-4.6276312	3.4807666	1.4314758
H	-5.1471702	1.3787556	2.8258868
H	-3.5560212	0.7495106	2.3762248
H	-3.6822892	2.2278426	3.3286648
C	-1.5648292	3.1375116	1.7368498
C	-0.2941882	3.8797736	1.3299328
H	-1.2792232	2.2086986	2.2658588
H	-2.0763762	3.7422186	2.5118318
H	0.4060598	4.0118606	2.1696128
H	0.2564948	3.3573386	0.5366448
H	-0.5170552	4.8849866	0.9442418
C	-2.6613962	3.9298506	-0.6041112
C	-3.7678952	3.9003796	-1.6540552
H	-1.6809792	3.9327216	-1.1165032
H	-2.7011202	4.9127276	-0.0938622
H	-3.7516912	4.7795166	-2.3157792
H	-3.6915652	3.0191196	-2.3064452
H	-4.7664082	3.8679096	-1.1935722
B	-2.6748662	2.8263256	0.5867928
C	3.1446898	-3.3913554	-0.0683722
C	4.6323778	-3.1750594	-0.3186172
H	2.5554108	-2.7132054	-0.7236662
H	2.8426908	-4.3995104	-0.3956812
H	4.9158088	-3.3975964	-1.3555932
H	4.9319148	-2.1376904	-0.1159352
H	5.2440228	-3.8190574	0.3275748
C	3.4240628	-2.2202254	2.3774178
C	2.7369878	-1.6793544	3.6248188
H	3.9099048	-1.3996864	1.8227888
H	4.2763998	-2.8649364	2.6646418
H	3.4192378	-1.0903804	4.2515728
H	1.8913768	-1.0235604	3.3697388
H	2.3355488	-2.4849024	4.2540498
C	1.1326738	-3.5607354	1.7768288
C	0.4285058	-4.5647264	0.8740828
H	0.5346288	-2.6317724	1.8618338

H	1.1591198	-3.9386174	2.8115008
H	-0.5715592	-4.8214524	1.2614078
H	0.3535908	-4.1780944	-0.1551652
H	0.9814468	-5.5097944	0.8057488
B	2.5784708	-3.0780584	1.3671878

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C	1.51797500	-2.84768600	-1.30973300
C	0.62856100	-1.88218900	-0.84259000
C	0.93416500	-1.10190300	0.27569500
C	2.16725400	-1.31164800	0.90481600
C	3.05586400	-2.27658700	0.44286400
C	2.73429600	-3.05199800	-0.66802300
H	1.25250400	-3.44254000	-2.18164500
H	-0.31727500	-1.73858900	-1.36186500
H	2.44958500	-0.70422400	1.76258300
H	4.00573600	-2.42032500	0.95458700
H	3.42761700	-3.80835200	-1.03020800
C	-0.00194000	0.00977700	0.76852000
C	0.01039600	0.05212600	2.31202000
H	0.94256800	0.48524600	2.68998200
H	-0.08497400	-0.95251900	2.73717300
H	-0.81683400	0.65888600	2.69506900
C	-0.07482900	2.55040100	0.76419300
C	0.36479600	3.77632600	0.28651400
C	1.82417700	2.79135300	-1.14680200
C	1.45305000	1.51493000	-0.73155700
C	0.48092000	1.37036200	0.25724500
H	-0.85815100	2.52360500	1.51864200
H	-0.06336600	4.69720000	0.68295200
H	2.58526200	2.90527500	-1.91930500
H	1.92759800	0.64878700	-1.18679100
N	1.30435300	3.91739600	-0.65608400
C	-1.43130100	-0.25481300	0.27801500
C	-2.20978800	-1.23380800	0.90646100
C	-1.97025300	0.39680400	-0.83426100
C	-3.48889500	-1.53562000	0.45285200
H	-1.80889000	-1.78237800	1.75657700
C	-3.25093600	0.09442200	-1.29341800
H	-1.38564200	1.14923600	-1.36047300
C	-4.01812200	-0.86976100	-0.64984500
H	-4.07319300	-2.29860900	0.96383300
H	-3.64578000	0.61880700	-2.16154900
H	-5.01957700	-1.10421200	-1.00478900

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C	2.34207900	-0.13744400	-1.54839800
C	1.30105100	0.77328300	-1.66579100

C	0.96147800	1.64781300	-0.61670700
C	1.72284600	1.56844300	0.55761700
C	2.77134600	0.66009700	0.69425200
C	3.09744100	-0.19532000	-0.36777000
H	2.59772100	-0.80738000	-2.36631300
H	0.71919400	0.80210300	-2.58653900
H	1.50005200	2.22927800	1.39342000
H	3.33689000	0.63790700	1.62123700
C	-0.18471900	2.54898500	-0.77964400
C	-0.73396200	3.32823700	0.15743000
H	-0.63295300	2.53382600	-1.77558100
H	-0.36010600	3.38280900	1.17940800
H	-1.69833800	-0.04005000	-0.43532800
H	-1.60191000	3.94143600	-0.07274700
C	-3.94382500	0.16121900	0.15231400
C	-4.28450200	0.74403900	-1.21549800
H	-3.90425000	0.99232500	0.88084300
H	-4.78265400	-0.47801300	0.49305900
H	-5.25158900	1.26866400	-1.24946800
H	-3.51560800	1.46571400	-1.53204800
H	-4.31719300	-0.03577500	-1.99138800
C	-2.75290600	-2.15999800	-0.56034700
C	-1.47926900	-2.93227900	-0.90080000
H	-3.31944800	-2.02102700	-1.49849100
H	-3.39363000	-2.80744200	0.06919200
H	-1.65962300	-3.89268100	-1.40468000
H	-0.83220500	-2.35880400	-1.58875500
H	-0.89308600	-3.19120900	-0.00110500
C	-2.09658200	-0.94186000	1.77232600
C	-1.59618600	0.29618400	2.51872500
H	-1.36865700	-1.76971800	1.92449300
H	-2.99227300	-1.31915900	2.29827500
H	-1.38652700	0.11525400	3.58307200
H	-0.67184200	0.72060300	2.08711100
H	-2.33408300	1.10829600	2.46667600
B	-2.56537700	-0.71547600	0.19872200
Na	0.09943500	-0.89786800	0.26399800
C	4.91911900	-1.14913000	0.81135500
H	5.67311400	-1.91388800	0.61600500
H	5.42089700	-0.18966700	0.99288700
H	4.34296600	-1.43618800	1.70127700
O	4.09972200	-1.09461200	-0.34456300

TS10

C	-3.14500200	-1.18187600	1.26895800
C	-2.07046100	-0.32950300	1.44811000
C	-1.01732400	-0.23748500	0.50256300

C	-1.10263600	-1.10728300	-0.60586300
C	-2.18390000	-1.97186500	-0.79310300
C	-3.21988100	-2.00994800	0.13985600
H	-3.94912700	-1.22763800	2.00141600
H	-2.03804100	0.30619400	2.33457100
H	-0.31645900	-1.09647300	-1.36214000
H	-2.19851300	-2.61011200	-1.67298300
C	0.09630800	0.66260500	0.71879200
C	1.23976400	0.68135900	-0.09659900
H	0.14651300	1.14984400	1.69663200
H	1.12724800	0.50595400	-1.17207000
H	2.13148700	-0.44805900	0.02925200
H	1.99432300	1.43877200	0.12749400
C	3.66906300	-0.99542600	-1.68468600
C	4.25266900	0.36145700	-2.06553600
H	2.76333400	-1.17940200	-2.29106100
H	4.37524800	-1.78641400	-2.00386800
H	4.41503100	0.46488800	-3.14782700
H	3.59625800	1.18976600	-1.76062100
H	5.22286400	0.53354400	-1.57946200
C	4.29713200	-0.53063500	0.96724500
C	3.76920800	-0.51862200	2.40015100
H	4.52313900	0.50776100	0.67435400
H	5.27381900	-1.05127300	0.94916000
H	4.47042100	-0.07379900	3.11921900
H	2.84649400	0.08133800	2.47929100
H	3.55497400	-1.53138800	2.77584200
C	2.97816000	-2.79176800	0.20258700
C	1.94081900	-3.48601200	-0.67819000
H	2.77331300	-3.01801800	1.26835600
H	3.94719300	-3.30293500	0.05238000
H	1.79305500	-4.54232600	-0.41662300
H	0.94875800	-3.00407900	-0.63607000
H	2.23860200	-3.45259700	-1.73385800
B	3.33750000	-1.23544500	-0.12384600
Na	0.99739300	-1.58610200	1.59050200
C	0.30028600	4.03926500	-0.18680300
C	1.25456500	4.03504700	-1.37448300
H	0.84000000	3.77807200	0.73843600
H	-0.04060800	5.07643800	-0.00104600
H	2.13018100	4.67655800	-1.20723700
H	1.63090000	3.02569100	-1.59144400
H	0.76474100	4.39260000	-2.29014800
C	-1.50443400	2.62592100	-1.68417700
C	-2.86476100	1.94372400	-1.76916400
H	-0.71872900	1.95717100	-2.07637400

H	-1.48095000	3.48334100	-2.38245600
H	-3.08964300	1.59146500	-2.78504900
H	-2.92465200	1.07095900	-1.10439200
H	-3.67680000	2.62407900	-1.47840000
C	-2.05760700	3.23855300	0.92248600
C	-1.54825300	3.66834500	2.29226700
H	-2.59407900	2.27874500	0.99455400
H	-2.83959600	3.94788600	0.58725300
H	-2.34314300	3.67482700	3.05039000
H	-0.75839500	2.99717300	2.65961000
H	-1.11843700	4.67880800	2.26915600
B	-1.03662500	3.19566500	-0.28303200
C	-4.41657700	-3.65036000	-1.07476800
H	-3.58809800	-4.37207400	-1.12363400
H	-5.35527100	-4.19988100	-0.97199700
H	-4.44449900	-3.07369300	-2.01073300
O	-4.31392300	-2.81108100	0.05414100
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C	2.33908500	-0.61410400	0.77308700
C	1.01216400	-0.27956900	1.06279300
C	0.23585600	0.55587600	0.23799900
C	0.90166800	1.09495600	-0.88595600
C	2.22264500	0.77546800	-1.19066900
C	2.95220300	-0.10133900	-0.37663900
H	2.87639900	-1.27926700	1.44418000
H	0.55842800	-0.69704700	1.96175600
H	0.36646700	1.76375500	-1.55801500
H	2.70510700	1.18784900	-2.07490200
C	-1.20019600	0.82395200	0.53124900
C	-1.61988200	2.22367800	0.09160200
H	-1.32072500	0.77313600	1.62826100
H	-1.72651200	2.31186600	-0.99936200
H	-0.90453600	3.00843600	0.40271800
H	-2.59043400	2.49089500	0.52562700
Na	2.11500300	2.26067700	1.26662300
C	-3.80582800	0.03125200	0.18449200
C	-4.51353700	0.88083100	-0.87224700
H	-3.92209200	0.52677500	1.16900200
H	-4.39023600	-0.90623200	0.28041600
H	-5.57307400	1.06611700	-0.63387100
H	-4.04676800	1.86572100	-1.00984100
H	-4.49707200	0.39027800	-1.85628200
C	-1.97371500	-0.73373400	-1.65633200
C	-0.82948500	-1.67566700	-2.03608600
H	-1.86233700	0.20814800	-2.22989300
H	-2.90339100	-1.18350000	-2.05735700

H	-0.72528200	-1.80938300	-3.12472400
H	0.14604000	-1.32890900	-1.66530200
H	-0.98241100	-2.67857200	-1.61203000
C	-1.96571600	-1.79249600	0.82161500
C	-2.35836400	-1.75356100	2.29704700
H	-0.91217600	-2.12100500	0.75087500
H	-2.54272900	-2.60707900	0.33963500
H	-2.14262800	-2.69063500	2.83424500
H	-1.83608900	-0.95172700	2.84348000
H	-3.43327600	-1.55907100	2.42401300
B	-2.22594900	-0.41842700	-0.05496100
C	4.96919900	-1.27740600	0.02152300
H	5.12477900	-0.89890000	1.04195200
H	4.48658000	-2.26288200	0.07264900
H	5.94032400	-1.38387000	-0.46668200
O	4.22197200	-0.36987900	-0.76368200

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C	-2.34010600	0.93737100	-1.21589200
C	-0.97837000	0.72815500	-1.40155300
C	-0.29263500	-0.36091000	-0.82514000
C	-1.07492500	-1.23251900	-0.04980700
C	-2.44986000	-1.04554400	0.14796200
C	-3.09844300	0.04132000	-0.44778000
H	-2.84576400	1.78022000	-1.68325300
H	-0.41891100	1.43032100	-2.02076100
H	-0.60468500	-2.09608600	0.41969400
H	-3.00056600	-1.76567600	0.74762300
C	1.17941000	-0.55191400	-1.01960300
C	1.49669400	-2.02331000	-1.31053000
H	1.43576100	0.01481900	-1.93309000
H	0.81588200	-2.45858700	-2.06024100
H	1.43663000	-2.65733400	-0.41582600
H	2.51678100	-2.13327600	-1.69769400
C	3.72378700	-0.33463600	-0.09466600
C	4.35144500	0.11135000	-1.41313000
H	3.82508600	-1.43126600	-0.01875300
H	4.34625200	0.06060300	0.73341500
H	5.38537000	-0.24355800	-1.54496700
H	3.78134900	-0.25338000	-2.28162900
H	4.38152100	1.20718000	-1.49904800
C	2.18044300	1.80629600	0.06765400
C	1.08147100	2.67553800	0.68195800
H	2.28593300	2.10993800	-0.99037400
H	3.12589700	2.13087200	0.54356100
H	1.32500000	3.74770400	0.67494300
H	0.13372900	2.60610700	0.12316200

H	0.91376500	2.43226300	1.74623400
C	1.79247000	-0.28352100	1.74135900
C	2.03785700	-1.72460000	2.19080200
H	0.75165600	-0.05013800	2.05304600
H	2.40173300	0.37642400	2.39046500
H	1.87368500	-1.87129300	3.26944900
H	1.37883900	-2.43604300	1.67241400
H	3.06804000	-2.04156500	1.97977400
B	2.16561900	0.14345600	0.18237600
Na	-1.06868400	1.09378100	1.38933700
C	-5.21880400	-0.60227400	0.38902900
H	-4.91450000	-0.64388300	1.44477100
H	-6.24495000	-0.23288400	0.33216600
H	-5.17994900	-1.61439400	-0.03669600
O	-4.42359400	0.30490300	-0.34837000

TS11

C	2.80644100	-1.59105800	0.94660000
C	1.87877600	-0.75471700	0.34267500
C	2.00944100	-0.32331600	-1.01973800
C	3.16803800	-0.80817300	-1.71143700
C	4.08800300	-1.65560900	-1.09775900
C	3.92287400	-2.05459600	0.23337900
H	2.67419600	-1.90256300	1.98311200
H	1.01478500	-0.41018200	0.91263400
H	3.32454100	-0.52546000	-2.75172000
H	4.95454300	-2.01964800	-1.64987800
C	1.01211100	0.45535500	-1.63355200
C	1.21210100	1.10359200	-2.96581600
H	0.26461400	0.89529600	-0.96891100
H	1.37801400	0.36624500	-3.77178800
H	2.07626600	1.79361400	-3.00804100
H	0.32947300	1.68998100	-3.25419200
C	-0.08165800	3.60841500	-0.47663600
C	-1.53881600	3.30237200	-0.80108200
H	0.54050300	3.48540700	-1.37723000
H	0.02809400	4.68263000	-0.22895300
H	-1.90345400	3.88480000	-1.65754000
H	-1.67710400	2.23940300	-1.04996300
H	-2.20528400	3.51876700	0.04488200
C	-0.32038100	2.11741400	1.80140100
C	0.33913500	1.55461900	3.05463700
H	-0.86108100	1.31481900	1.26321300
H	-1.13299900	2.81023800	2.08356400
H	-0.39216800	1.10762000	3.74097800
H	1.07139100	0.76972700	2.81410700
H	0.87410900	2.33306200	3.61604600

C	2.14017200	2.97087800	0.98156300
C	3.02435800	3.32100800	-0.21170300
H	2.48227900	2.06332000	1.51248600
H	2.24254400	3.75487100	1.75465600
H	4.09102800	3.41869000	0.04666800
H	2.91380300	2.59122100	-1.03168300
H	2.74165000	4.28697200	-0.64581100
B	0.58020200	2.85466100	0.73870500
Na	4.19004000	0.79493900	0.24676100
C	-5.24609400	-1.50755200	-0.11203900
C	-5.11097600	-3.00728100	-0.35407500
H	-5.48202200	-1.01810100	-1.07456800
H	-6.13266500	-1.32367400	0.52359300
H	-5.98677400	-3.44708900	-0.85402600
H	-4.23867700	-3.23231000	-0.98732000
H	-4.97073700	-3.56063700	0.58572800
C	-3.59682700	-1.48514900	2.02506500
C	-2.48643800	-0.82595800	2.84172300
H	-3.37721800	-2.56282100	1.92472600
H	-4.52981300	-1.45569200	2.61779000
H	-2.28613500	-1.33625900	3.79598700
H	-1.53181200	-0.79541500	2.29155200
H	-2.73457000	0.21727400	3.08376700
C	-4.19918400	0.82814400	0.83167500
C	-5.11802800	1.62262900	-0.09727500
H	-3.22348900	1.34601800	0.89302200
H	-4.62439200	0.92400700	1.84810200
H	-5.24491100	2.66386800	0.23662600
H	-4.75343400	1.67762000	-1.13326600
H	-6.12398900	1.18190800	-0.14406800
B	-3.96318900	-0.78468800	0.59385500
C	-1.65511400	-0.44438500	-2.53702500
C	-2.67103700	-0.33056500	-1.62510100
C	-1.68828500	-1.87798900	-0.22119200
C	-0.63097700	-2.05166800	-1.08193300
C	-0.50278600	-1.20864400	-2.21440000
H	-1.71496700	0.11248200	-3.46917200
H	-3.53435600	0.29690900	-1.82680600
H	-1.76936300	-2.47660000	0.68176900
H	0.12776900	-2.79289700	-0.84507800
H	0.22573400	-1.44826400	-2.98709300
N	-2.68983800	-0.99112700	-0.43511800
C	5.86160200	-2.24627700	1.51057100
H	6.46230300	-1.62211100	0.82736000
H	5.46747700	-1.61320400	2.32297100
H	6.51613500	-3.00560100	1.94909500

O	4.82310300	-2.91293400	0.82252100

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C	3.79846100	-2.31679700	-0.51239400
C	2.71512600	-1.91000200	-1.28894300
C	2.10654600	-0.66444700	-1.11228500
C	2.65236800	0.17832600	-0.13328900
C	3.72560900	-0.20906100	0.66150800
C	4.30714300	-1.46822500	0.47652700
H	4.23429600	-3.29720200	-0.68269000
H	2.32968500	-2.59432400	-2.04469200
H	2.22391900	1.17325100	0.01094700
H	4.13752200	0.45755600	1.41757300
C	0.90825800	-0.21634900	-1.91531800
C	1.33431700	0.29334300	-3.28934900
H	0.45672200	0.63247800	-1.37052100
H	1.77750500	-0.52059600	-3.88116000
H	2.08499600	1.09029100	-3.20738200
H	0.47959700	0.69351400	-3.84964900
C	0.60004500	3.59129200	-1.08671500
C	-0.73709500	3.31276800	-1.76076000
H	1.42003600	3.11911400	-1.66195500
H	0.84181200	4.66607800	-1.15321900
H	-0.73944200	3.62459600	-2.81346900
H	-0.99540200	2.24372200	-1.74271800
H	-1.55756800	3.84714900	-1.26294000
C	-0.29214700	2.27202000	1.13316200
C	-0.00850000	1.76353000	2.54384600
H	-0.59546400	1.45282700	0.45058300
H	-1.20952500	2.88768000	1.14989600
H	-0.79527600	1.09187800	2.92069100
H	0.96724100	1.25500100	2.63335800
H	0.05224100	2.59144300	3.26061100
C	2.11232900	3.57799000	1.18028600
C	3.29538800	4.10728000	0.37943000
H	2.44648200	2.78332300	1.86762600
H	1.74492700	4.36590600	1.86745000
H	4.11574700	4.44047800	1.02781200
H	3.70631200	3.33596600	-0.28772000
H	3.01566300	4.95967700	-0.25265100
B	0.81227600	3.13669500	0.40536700
Na	0.53599900	-0.79051400	1.33186800
C	-5.23080700	-0.98748400	-0.18424100
C	-5.37311000	-2.45329700	-0.58374300
H	-5.32580500	-0.36819800	-1.09384100
H	-6.09834500	-0.69649900	0.43847400

H	-6.25843400	-2.65635400	-1.20506400
H	-4.49522300	-2.79410600	-1.15556100
H	-5.44685000	-3.10767800	0.29680300
C	-3.79122600	-1.57603200	1.99367100
C	-2.80118800	-1.19518800	3.09321100
H	-3.64565300	-2.63989200	1.73352100
H	-4.80176900	-1.54518800	2.44101700
H	-2.78610800	-1.90888000	3.93038200
H	-1.76243600	-1.13247100	2.72373300
H	-3.02875200	-0.20793500	3.51788300
C	-3.83660900	0.94695700	1.10935200
C	-4.05944600	2.01680000	0.04426800
H	-2.88067600	1.16554900	1.62295700
H	-4.61120300	1.07362300	1.89114000
H	-4.05450900	3.04007400	0.45244000
H	-3.28332200	1.98619200	-0.73429900
H	-5.02489500	1.88565800	-0.46660700
B	-3.86648000	-0.62944900	0.65124400
C	-1.51005600	-0.66889600	-2.47391800
C	-2.53141400	-0.46449400	-1.61322000
C	-1.60652200	-1.83621200	-0.01819800
C	-0.49512900	-2.06726700	-0.77362900
C	-0.20832000	-1.29797800	-2.04437700
H	-1.61976900	-0.31556500	-3.49845800
H	-3.42389000	0.06192800	-1.94681600
H	-1.77247800	-2.43225800	0.88077200
H	0.14544700	-2.90506700	-0.49357000
H	0.14692300	-1.99903400	-2.82313000
N	-2.59209700	-0.93980800	-0.31299500
O	5.34163400	-1.77160400	1.29030400
C	5.96593800	-3.03154900	1.12846100
H	6.40383300	-3.14044700	0.12687100
H	6.76482900	-3.07729200	1.87146800
H	5.26395800	-3.85722300	1.30897600

TS12

C	3.80033000	-0.59123300	1.65751600
C	2.61886400	-0.51457200	0.90757200
C	2.38242000	0.51802700	-0.00140600
C	3.39364700	1.49098100	-0.13244200
C	4.57208500	1.43063900	0.59357900
C	4.78520900	0.38867200	1.51021500
H	3.92500400	-1.41529500	2.35497400
H	1.88136700	-1.30282000	1.04134000
H	3.24639900	2.32247700	-0.82251400
H	5.33728200	2.19578900	0.48411000
C	1.14947800	0.64870300	-0.87991900

C	1.52786800	0.49301300	-2.35314900
H	0.80879300	1.69409000	-0.75172400
H	1.76149900	-0.55513400	-2.58894800
H	2.39348800	1.11641000	-2.60881100
H	0.71478900	0.79694200	-3.02174100
C	-0.93817100	3.92327400	-2.07839200
C	-2.36469900	3.48171000	-2.37452300
H	-0.22493400	3.29579300	-2.64661400
H	-0.75692400	4.93370000	-2.48588100
H	-2.59603800	3.51581900	-3.44729200
H	-2.54139300	2.45112600	-2.03610600
H	-3.10169100	4.11616100	-1.86370500
C	-1.37789300	3.41244100	0.57359500
C	-0.82352200	3.38093800	1.99189200
H	-1.72846800	2.40386900	0.28220600
H	-2.30344900	4.01523000	0.53748700
H	-1.54922500	2.98373600	2.71436600
H	0.07469400	2.74986900	2.06092700
H	-0.53608400	4.38257800	2.33959900
C	1.01927500	4.42952300	-0.25176700
C	1.94961600	4.77450200	-1.40736200
H	1.50208400	3.70275300	0.42560400
H	0.88172400	5.31626200	0.39460400
H	2.93957700	5.10224600	-1.06244300
H	2.10697500	3.91495300	-2.07590500
H	1.54233800	5.58217200	-2.02950500
B	-0.43700300	3.91813600	-0.58364600
Na	4.17570700	-1.19643000	-1.23702000
C	-5.25897500	-1.25204000	-0.11689600
C	-4.87221900	-2.67898000	-0.49672000
H	-5.32363100	-0.64804600	-1.03940600
H	-6.29325200	-1.25449700	0.27544300
H	-5.55501400	-3.13281700	-1.23062600
H	-3.86247900	-2.72091400	-0.93310600
H	-4.85688500	-3.34284100	0.37994600
C	-4.33762500	-1.48357300	2.38898900
C	-4.21423700	-0.82385100	3.76411800
H	-3.57019000	-2.27487700	2.30237800
H	-5.29567300	-2.03529000	2.38967100
H	-4.23941000	-1.55809800	4.58330300
H	-3.28597500	-0.24685300	3.89111200
H	-5.03750800	-0.11899100	3.94643100
C	-4.85500300	0.97876700	1.36080100
C	-5.00690900	1.90997700	0.16334100
H	-4.17130400	1.45064300	2.09138300
H	-5.82724000	0.91102400	1.88408500

H	-5.27412200	2.94080900	0.44314300
H	-4.07203500	1.97288600	-0.41360100
H	-5.78404700	1.55650300	-0.52959600
B	-4.34568200	-0.54124300	1.03701300
C	-1.23180500	-0.11507000	-1.33183100
C	-2.49964400	-0.27666100	-0.84630900
C	-1.75206000	-0.30723800	1.31737200
C	-0.45256000	-0.15695200	0.92222000
C	-0.06928700	-0.18851500	-0.47401900
H	-1.11707700	0.00186600	-2.40708800
H	-3.34646400	-0.27319700	-1.52938300
H	-1.99762500	-0.31050200	2.37647600
H	0.29041500	-0.01311000	1.70133400
H	0.54079900	-1.54331400	-0.78559900
N	-2.80423100	-0.41892000	0.46953100
C	0.25093700	-3.67471800	0.28879900
C	-1.23538600	-3.76840600	0.62524100
H	0.78748000	-3.20781400	1.13638400
H	0.65838700	-4.70379400	0.25072200
H	-1.41669200	-4.18404100	1.62766800
H	-1.73327100	-2.79050300	0.58655000
H	-1.76606200	-4.41525300	-0.08726800
C	-0.46145900	-3.14149500	-2.27918700
C	-0.10662200	-2.67143100	-3.68675800
H	-1.42059700	-2.68661000	-1.97986000
H	-0.67567000	-4.22769700	-2.32082500
H	-0.90552500	-2.87690600	-4.41388600
H	0.08237400	-1.58853200	-3.72287000
H	0.80043000	-3.16330700	-4.06708500
C	2.15625000	-3.29773700	-1.62962200
C	3.22144800	-3.66480300	-0.59228600
H	2.51995900	-2.52975500	-2.34170000
H	2.04554100	-4.17998600	-2.28641500
H	4.22106100	-3.83814300	-1.02545900
H	3.31649500	-2.93700500	0.22794400
H	2.95805100	-4.60269000	-0.08976100
B	0.64055700	-2.96517700	-1.11338200
O	5.94969800	0.41898900	2.18517500
C	6.17634600	-0.58116900	3.16409900
H	6.20876100	-1.58380300	2.71677600
H	7.14801800	-0.36020300	3.60974500
H	5.40791600	-0.55673600	3.94763300

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C	2.58249600	0.75025200	1.16332200
C	1.28482600	1.23911900	1.17599500
C	0.35744800	0.86002600	0.20096000

C	0.77433300	-0.03077700	-0.78727000
C	2.07339400	-0.53249500	-0.81793400
C	2.98676100	-0.13911200	0.16374400
H	3.30382600	1.04425200	1.92316800
H	0.98131100	1.93268500	1.96058800
H	0.06835100	-0.35182100	-1.55440100
H	2.36054800	-1.22497900	-1.60432800
C	-1.04240000	1.44273100	0.19357800
C	-1.17857600	2.49504400	-0.90174300
H	-1.18078800	1.94738400	1.16301800
H	-1.00826200	2.06340100	-1.89674900
H	-0.43076500	3.28271000	-0.75470100
H	-2.17031300	2.96411000	-0.89553400
C	-2.97411100	0.18488500	-0.92906600
C	-3.89557300	-0.85884700	-0.89025700
C	-3.14213000	-1.56742100	1.13526700
C	-2.18691700	-0.56450300	1.18729500
C	-2.08794700	0.34953800	0.13355400
H	-2.96202500	0.85522600	-1.78534200
H	-4.59215600	-0.99598400	-1.71805300
H	-3.22966800	-2.28075500	1.95512000
H	-1.51591200	-0.49096400	2.04273600
N	-3.99560700	-1.72906000	0.11557400
C	4.71720900	-1.46367500	-0.76434200
H	4.65112900	-1.02550300	-1.77022000
H	5.76456000	-1.67955000	-0.54135700
H	4.14910400	-2.40453900	-0.74566700
O	4.27092800	-0.56510500	0.22926000

TS2-C2

C	2.6702926	-2.8255391	1.8530183
C	1.9234606	-1.7707411	1.3489393
C	1.5511486	-1.6929911	-0.0306827
C	2.0756676	-2.7263461	-0.8699737
C	2.8219356	-3.7827941	-0.3514967
C	3.1327766	-3.8553271	1.0125413
H	2.9086886	-2.8476671	2.9157283
H	1.5766086	-0.9877301	2.0255533
H	1.8569326	-2.7074311	-1.9362487
H	3.1788646	-4.5596991	-1.0270827
H	3.7103916	-4.6848751	1.4122713
C	0.6028716	-0.7434991	-0.4890647
C	0.3649796	-0.5463751	-1.9549947
H	0.4612646	0.1350529	0.1469573
H	0.0604286	-1.4841511	-2.4446177
H	1.2512286	-0.1822951	-2.5076997
H	-0.4381364	0.1824649	-2.1251317

C	2.1813056	2.6303909	-1.7110787
C	0.8218256	3.2635549	-1.9729297
H	2.3369956	1.7748459	-2.3892667
H	2.9879336	3.3336639	-1.9973207
H	0.7051726	3.5817759	-3.0170947
H	0.0103226	2.5559919	-1.7561587
H	0.6498876	4.1464419	-1.3427167
C	1.6942626	2.7697129	0.9736813
C	2.0732876	2.3325159	2.3827653
H	0.6276526	2.5583019	0.7801843
H	1.7478506	3.8714669	0.8936033
H	1.4411636	2.8009849	3.1482863
H	1.9723806	1.2443679	2.5079693
H	3.1143176	2.5880889	2.6235053
C	3.8385956	1.3623239	0.0523973
C	4.6015636	0.8119369	-1.1490797
H	3.5408646	0.5765499	0.7737293
H	4.5052546	2.0076439	0.6504863
H	5.5560616	0.3266939	-0.8852337
H	3.9946946	0.1152999	-1.7500957
H	4.8824686	1.6167879	-1.8382317
B	2.5359406	2.2146599	-0.2353047
Na	4.4282676	-1.6216161	0.1006763
C	-4.5342614	0.2653519	0.5219723
C	-5.1995704	-0.9430721	1.1757483
H	-4.9215784	0.3639189	-0.5065577
H	-4.8846214	1.1827999	1.0312343
H	-6.2956104	-0.9412471	1.0793143
H	-4.8421304	-1.8871111	0.7354263
H	-4.9756264	-0.9958891	2.2503513
C	-2.4574214	0.1742839	2.1753793
C	-1.1042774	0.7235749	2.6209983
H	-2.5594034	-0.8671181	2.5318773
H	-3.2295894	0.7302599	2.7386073
H	-0.9427884	0.6335039	3.7064113
H	-0.2597474	0.2175389	2.1325733
H	-1.0047574	1.7904569	2.3741893
C	-2.2900144	1.6586099	-0.0822537
C	-2.7895174	2.0334679	-1.4746357
H	-1.1862314	1.6057499	-0.1049057
H	-2.5166604	2.4973889	0.6038463
H	-2.3559034	2.9735699	-1.8495517
H	-2.5477544	1.2585599	-2.2187057
H	-3.8817114	2.1609609	-1.4926487
B	-2.8961244	0.2986869	0.5958213
C	-2.7444204	-2.5960591	-2.0155507

C	-2.9802824	-1.4060961	-1.3723807
C	-1.2538274	-1.7548301	0.1733973
C	-1.0980494	-3.0823871	-0.3379067
C	-1.8009934	-3.4812031	-1.4405857
H	-3.3168314	-2.8601081	-2.8996077
H	-3.7640934	-0.7385491	-1.7201347
H	-0.9407284	-1.5619141	1.1962603
H	-0.3816524	-3.7427271	0.1461923
H	-1.6645034	-4.4812181	-1.8489617
N	-2.3367924	-1.0115981	-0.2460057

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