SUPPORTING INFORMATION

The Quest for the Ideal Base: Rational Design of a Nickel Precatalyst Enables Mild, Homogeneous C–N Cross-Coupling

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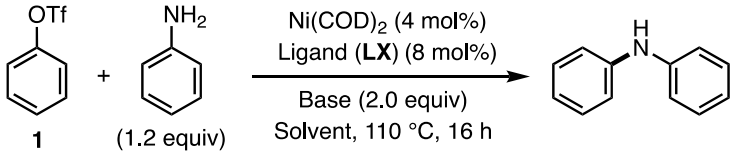
General Information

Unless noted, all chemicals were obtained from commercial sources, were stored at room temperature, and were used as received. All preparative C-N bond-forming reactions were carried out under an atmosphere of nitrogen using standard Schlenk techniques. Reaction screening, synthetic organometallic transformations, and mechanistic experiments were carried out with the aid of a nitrogen-filled glovebox. Anhydrous 2-methyl tetrahydrofuran (2-MeTHF) and triethylamine (TEA) were purchased from Sigma-Aldrich in Sure-Seal^{TM} bottles and were degassed prior to use by sparging the liquid with nitrogen gas for 10 min while submerged in a sonication bath. $CDCl_3$, DMSO-d_6, and acetone-d_6 were purchased from Cambridge Isotope Laboratories. Bis(3,5-di(trifluoromethyl)phenyl)chlorophosphine was purchased from Strem Chemicals. Other reagents were either prepared according to referenced literature procedures or were purchased from chemical suppliers (Sigma-Aldrich, Combi-Blocks, Alfa Aesar, or TCI-America) and were used as received unless otherwise noted. Isolated compounds were purified by flash chromatography using Silicycle SiliaFlashP60 (230-400 mesh) silica gel with the aid of a CombiFlash Automated Flash Chromatography System.

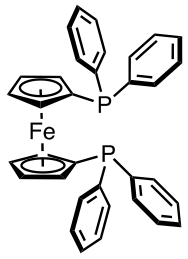
Instrumentation: ^{1}H, ^{13}C, ^{19}F, and ^{31}P spectra were recorded on a Bruker Avance-400 MHz spectrometer. ^{1}H and ^{13}C spectra were calibrated using residual solvent as an internal reference ($CHCl_3$: δ 7.26 ppm and δ 77.36 ppm, respectively; DMSO: 2.50 ppm and 39.52 ppm, respectively; acetone: δ 2.05 ppm and 29.92 ppm, respectively). ^{19}F NMR spectra were calibrated to an external standard of neat $CFCl_3$ (δ 0.0 ppm). ^{31}P NMR spectra were calibrated to an external standard of H_3PO_4 (δ 0.0 ppm). The following abbreviations were used to explain multiplicities: s = singlet, bs = broad singlet, d = doublet, t = triplet, q = quartet, m = multiplet. High-resolution mass spectra (HRMS) were recorded on an Agilent Technologies 6545 Q-TOF LC/MS system or JEOL AccuTOF 4G with an ionSense DART. Melting points were obtained using a Stanford Research Systems EZ-Melt melting point apparatus. Elemental Analyses were performed by Atlantic Microlabs Inc., Norcross, GA, USA.

General Procedure for Screening of Ni-Catalyzed C–N Coupling Reactions

All reactions were set up inside of a nitrogen-filled glovebox. An oven-dried vial (20 mL) equipped with a stir bar was sequentially charged with $Ni(COD)_2$ (8.3 mg, 30 μmol, 4 mol% Ni), a specific phosphine ligand (30 μmol, 4 mol%), and solvent (1.50 mL). The vial was capped and the solution was stirred for 2 min at RT. Then the cap was removed, phenyl triflate (122 μL, 0.75 mmol) and aniline (85 μL, 0.90 mmol, 1.2 equiv) were sequentially added via a micropipette, and the solution was stirred for 1 min. After this time, seven oven-dried reaction tubes (Fisher 16 x 125 mm tubes – Cat. No. 1495935A) containing stir bars were charged with an aliquot (228 μL each) of the stock solution. A specific base (0.20 mmol, 2.0 equiv) was then added to each reaction tube. The reaction tubes were each sealed with a screw cap (Kimble Chase, Open Top S/T, Part No. 73804-15425) containing a Teflon septum (Thermo Scientific, 10/90 Teflon/Sil, Cat. No. B7995-15), were removed from the glovebox and placed into a pre-heated oil bath set to 110 °C. The reaction mixtures were heated at this temperature for 16 h. After this time, the reaction mixtures were allowed to cool to RT and diluted with EtOAc. If an internal standard was used, hexamethylbenzene (1 equiv) was added at this time and the mixture stirred thoroughly. The reaction mixture was then analyzed by GC. Product yields are reported as a single run.

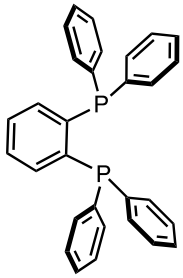


	Toluene	Cyclohexane	MeCN	MTBE	THF	1,4-dioxane
Et_3N	14%	Trace			6%	10%
DBU						
MTBD	Trace				Trace	
TBD						
TMG						
Quinuclidin-3-ol						
DABCO	Trace				Trace	Trace

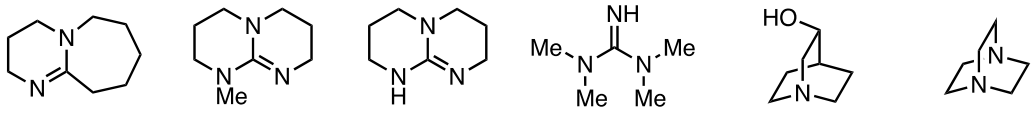


L1
DPPF

	Toluene	Cyclohexane	MeCN	MTBE	THF	1,4-dioxane
Et_3N	5%	Trace			Trace	
DBU						
MTBD						
TBD						
TMG						
Quinuclidin-3-ol						
DABCO	Trace					Trace



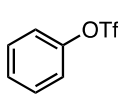
L4
DPPBz



DBU **MTBD** **TBD** **TMG** **quinuclidin-3-ol** **DABCO**

Figure S1: Results of reaction screening. Yields were determined relative to remaining phenyl triflate. Blank entries indicate 0% yield of the desired product.

Preparation of Aryl Triflates



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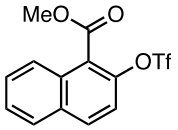
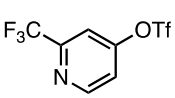


S1



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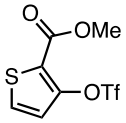

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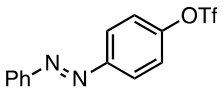

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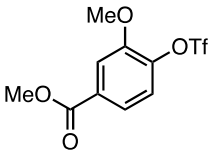

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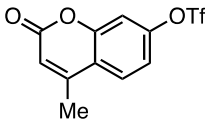

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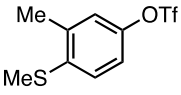

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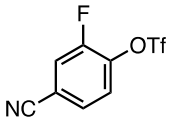

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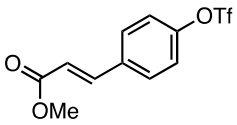

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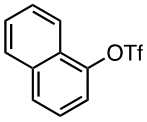

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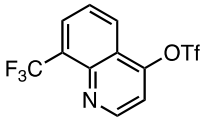

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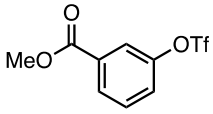

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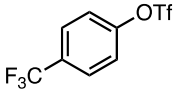

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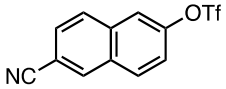

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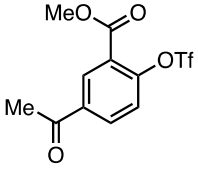

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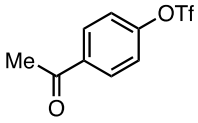
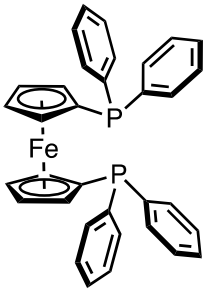


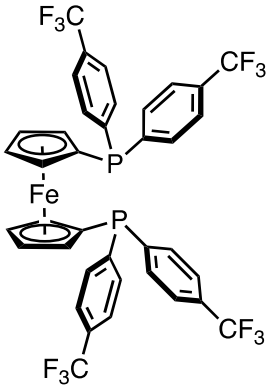
S16

Aryl triflates **1**, **S10**, **S13**, and **S16** were purchased from Sigma Aldrich. Aryl triflate **S1** was purchased from Alfa Aesar. The syntheses of aryl triflates **S2**,[1] **S3**,[2] **S4**,[3] **S5**,[4] **S6**,[5] **S7**[6] **S8**,[7] **S9**,[8] **S11**,[8] **S12**,[9] **S14**,[10] and **S15**,[11] have been previously reported.

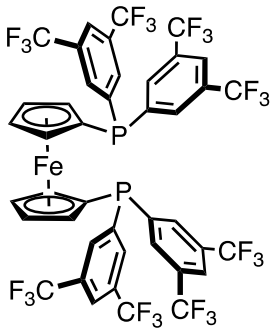
Preparation of Phosphine Ligands



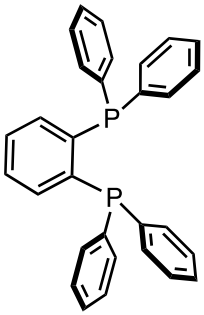
L1
DPPF



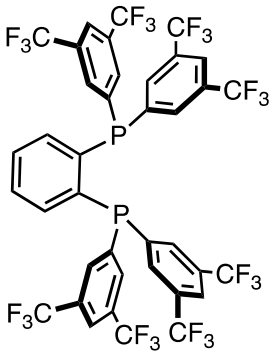
L2
$[CF_3]_4$-DPPF



L3
$[CF_3]_8$-DPPF



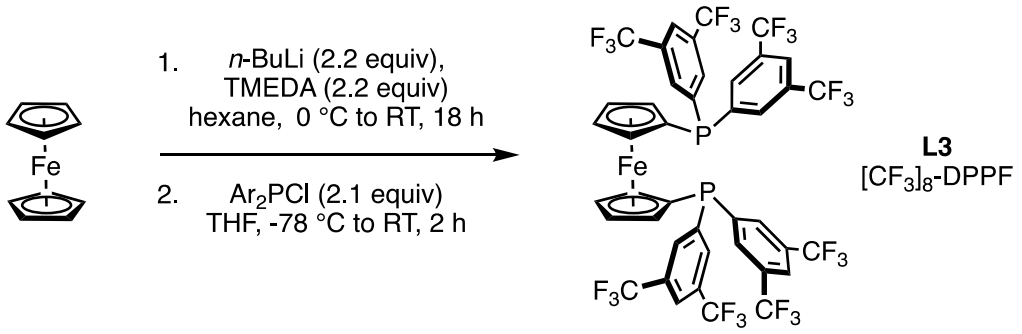
L4
DPPBz



L5
$[CF_3]_8$-DPPBz

Ligands **L1** and **L4** were purchased from Strem Chemicals. The syntheses of phosphines **L2**[12] and **L5**[13] have been previously reported. **L3** was prepared according to the following procedure:

Synthesis of [CF_3]$_8$-DPPF, L3



This procedure was adapted from previous syntheses of this ligand.[14]

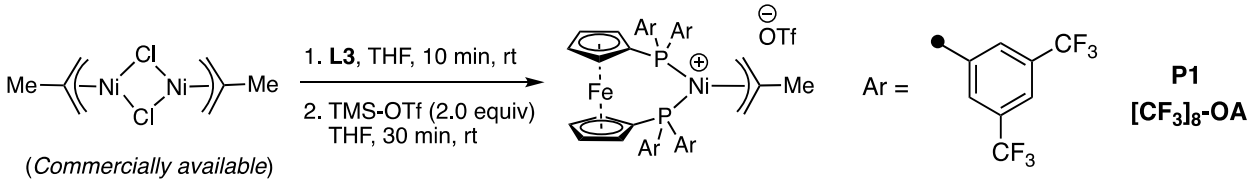
An oven-dried round bottom flask (500 mL) equipped with a stir bar was charged with ferrocene (1.41 g, 7.60 mmol) and was sealed with a rubber septum. The septum was pierced with a needle connected to a Schlenk line, and the flask was evacuated and backfilled with nitrogen (this process was repeated a total of three times). Following this sequence, hexane (anhydrous, 50 mL) and tetramethylethylenediamine (TMEDA, 2.50 mL, 16.7 mmol, 2.20 equiv) were sequentially added to the flask *via* syringe to afford a homogeneous, orange-colored solution. The reaction flask was submerged in an ice bath and the solution was allowed to cool for 10 min. Then *n*-butyl lithium (2.6 M in hexanes, 6.4 mL, 16.7 mmol, 2.20 equiv) was added dropwise to the solution *via* syringe. The reaction mixture was removed from the ice bath and the solution was allowed to stir for 18 h at RT. During this time, the lithiated ferrocene complex precipitated from solution as an orange/yellow-colored solid. (***Caution****: This solid is extremely pyrophoric!*). The reaction flask was submerged in a -78 °C bath (dry ice/acetone) and the mixture was allowed to cool for 10 min before THF (100 mL) was added to the solution. Under a positive pressure of nitrogen, a solution of bis(3,5-di(trifluoromethyl)phenyl)chlorophosphine (7.86 g, 16.0 mmol, 2.10 equiv, Strem Chemicals, CAS: 142421-57-6) in THF (20 mL) was added dropwise *via* syringe. Upon addition of the chlorophosphine, the solution turned from orange/yellow-colored to dark brown-colored. After stirring for 15 min, the reaction flask was removed from the -78 °C bath and the solution was allowed to warm to RT. After 1 h at RT, MeOH (25 mL) was *carefully* added to the flask via syringe to quench the reaction mixture. The septum was removed from the flask, the stir bar was

removed, and the reaction mixture was concentrated under reduced pressure with the aid of a rotary evaporator to afford a dark brown-colored semi-solid. The crude material was dissolved in hexane and CH_2Cl_2 (1:1 mixture, 25 mL) and was loaded onto a large plug of silica gel (230-400 mesh) held in a fritted filter (3-inch depth, 5-inch height) connected to a round bottom flask. Eluent (2% EtOAc in hexane) was passed through the silica gel and the desired product was collected as an orange solution (**Figure S2**). The solution was concentrated with the aid of a rotary evaporator to afford an orange-colored solid. The solid material was then recrystallized from hexane/CH_2Cl_2 (4:1 ratio, ~100 mL, refluxed to dissolve) and MeOH (anti-solvent, ~20 mL). The recrystallization solution was stored at -10 °C, which facilitated the formation of fine orange-colored crystals and a yellow-colored mother liquor. The mother liquor was decanted and the crystals were washed with cold hexane to afford the desired product: 4.65 g; 55% yield.

^{1}H NMR (400 MHz; $CDCl_3$): δ 7.89 (s, 4H), 7.71 (dd, *J* = 6.5, 1.8 Hz, 8H), 4.45 (t, *J* = 1.8 Hz, 4H), 4.03 (d, *J* = 1.9 Hz, 4H) ppm. **^{13}C NMR** (101 MHz; $CDCl_3$): δ 139.7 (d, *J* = 17.6 Hz), 132.3 (dd, *J* = 20.9, 3.9 Hz), 131.5 (qd, *J* = 33.5, 6.8 Hz), 122.8 (p, *J* = 3.7 Hz), 122.3 (q, *J* = 273.1 Hz) 73.2 (d, *J* = 7.1 Hz), 73.0 (d, *J* = 15.5 Hz), 72.6 (t, *J* = 2.2 Hz) ppm. **^{19}F NMR** (376 MHz, $CDCl_3$) -63.1 ppm. **^{31}P NMR** (162 MHz, $CDCl_3$) δ -15.6 ppm. **IR** (neat, cm^{-1}): 1616.2, 1351.8, 1274.9, 1105.9, 896.3, 703.4. **MP**: 154.1–156.9 °C. **Elemental Analysis:** Calculated for $C_{42}H_{20}F_{24}FeP_2$, 45.93; H, 1.84. Found: C, 45.65; H, 1.78.

Figure S2: Filtration of **L3** over silica gel (left), pure **P1** (middle), and a coupling reaction using P1 (right, see general procedure below).

Synthesis of P1

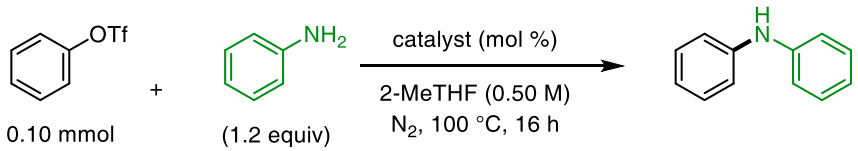


In a nitrogen-filled glovebox, an oven-dried round bottom flask (100 mL) equipped with a stir bar was sequentially charged with **L3** (3.00 g, 2.73 mmol, 1.0 equiv), methallyl nickel chloride dimer (408 mg, 2.73 mmol, 1.0 equiv, CAS: 12145-60-7), and THF (25 mL). The flask was sealed with a rubber septum and the dark burgundy/brown-colored mixture was stirred in the glovebox for 10 min at RT. Then trimethylsilyl triflate (0.987 mL, 5.47 mmol, 2.0 equiv) was added to the solution, at which time a color change from dark burgundy/brown to dark brown/orange was observed. The reaction mixture was left to stir in the glovebox for 30 min. (**Note**: the solution should not be stirred for >2 h. Otherwise, an insoluble gel will form, likely due to polymerization of THF). After this time, the solution was withdrawn into a syringe and was passed through a syringe filter (VWR®, 0.45 μm PFTE membrane, Part. No. 28145-497) to remove black particulates and afford a homogeneous, dark orange-colored solution. While still inside of the nitrogen-filled glovebox, the

solution was concentrated under reduced pressure with the aid of a high-vacuum pump equipped with an in-line, nitrogen-cooled trap to afford a dark brown/orange-colored semi-solid. To this solid, THF (3.0 mL) and pentane (30 mL) were added, which resulted in the formation of an orange/yellow solid. A stir bar was added to the flask, the flask was sealed with a rubber septum, and the mixture was agitated via stirring for 15 min at RT. The septum was removed from the flask and the orange-colored mother liquor was carefully decanted from the flask. To the remaining yellow/orange solid, additional THF (2.0 mL) and pentane (30 mL) were added to the solid. The flask was re-sealed with the rubber septum, the flask removed from the glovebox, and the mixture agitated at RT with aid of a sonication bath for 10 min to afford a fine, yellow/orange, free-flowing powder and a light yellow-colored mother liquor. The flask was returned to the nitrogen-filled glovebox, the septum and stir bar removed, and the solvent carefully decanted. The powder was dried under high-vacuum to afford the desired **P1**: 2.60 g, 70% yield.

^{1}H NMR (400 MHz, Acetone-d_6) δ 8.65 – 8.12 (m, 12H), 5.18 (bs, 2H), 4.92 (bs, 2H), 4.76 (bs, 2H), 4.53 – 4.40 (m, 4H), 3.39 (s, 2H), 2.17 (s, 3H) ppm. **^{13}C NMR** (101 MHz; Acetone-d_6): δ 209.2, 135.8, 135.3, 134.0 (d, J = 141.0 Hz), 133.8, 126.11 (d, J = 112.4 Hz), 132.2 (dd, J = 53.9, 31.7 Hz), 123.0 (q, J = 272.5 Hz), 76.3, 75.3, 75.1, 74.9, 71.9, 71.8 (d, J = 57.5 Hz) 68.4, 53.9, 22.0. Complex spectra; see attached (the observed complexity is due to C–P and C–F coupling). **^{19}F NMR** (376 MHz, THF-H_8): δ -63.3 (s, 24F), -79.0 (s, 3F) ppm. **^{31}P NMR** (162 MHz, Acetone-d_6) δ 30.5 ppm. **IR** (neat, cm^{-1}): 2863.8, 1619.6, 1354.0, 1276.2, 1118.6, 682.1. **MP**: 215.1–217.9 °C (decomposition). **HRMS** (ESI) Calcd. for $C_{46}H_{27}F_{24}FeNiP_2$ $[M\text{-}OTf]^+$: 1210.9902. Found: 1210.9925.

Stability of P1 and Robustness of Reactions Using P1



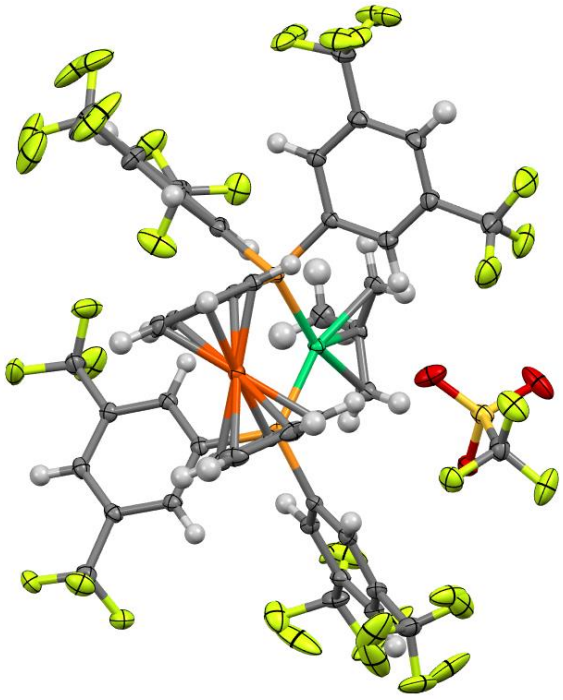
Precatalyst (mol%)	Yield (%)
P1 (4 mol%) freshly prepared[a]	98
P1 (4 mol%) aged 2 weeks in desiccator[b]	95
P1 (4 mol%) aged 6 weeks in desiccator[b]	95
P1 (4 mol%) + 1 equiv H_2O[c]	0
P1 (4 mol%) + 500 μL air[d]	18
P1 (4 mol%) heated to 60 °C in air for 10 min before reaction[e]	90
P1 (4 mol%) dissolved in 0.50 mL 2-MeTHF (MilliporeSigma, SureSeal) for 48 h before reaction[f]	91
P1 (4 mol%) dissolved in 0.50 mL EtOAc (MilliporeSigma, reagent grade) for 1 h before reaction[g]	0

Experimental details:

(a) The precatalyst was used within 1 h of its synthesis and isolation, and the reaction set-up was performed in a nitrogen-filled glovebox.
(b) The precatalyst was stored in a 20 mL scintillation vial under air for the indicated time. The vial was capped and placed in a benchtop desiccator during this time.
(c) After the reagents and solvent were added, distilled water (1 equiv) was added by syringe prior to heating.
(d) After the reagents and solvent were added, 500 μL of air was injected into the vial by syringe prior to heating.
(e) The solid precatalyst was weighed into an uncapped reaction tube, which was heated in an oil bath maintained at 60 °C for 10 min. Afterwards, the tube was removed and allowed to cool, and the remainder of the reagents were added. Then, the reaction was conducted as usual according to the general procedure.
(f) Under an atmosphere of N_2, the appropriate amount of precatalyst was dissolved in 2-MeTHF (0.50 mL, MilliporeSigma, SureSeal) and allowed to stir for 48 h. At this time, the solvent was removed with the aid of a rotary evaporator. Then, the reaction was conducted using the obtained solid according to the general procedure.
(g) Under an atmosphere of N_2, the appropriate amount of precatalyst was dissolved in EtOAc (0.50 mL, MilliporeSigma, reagent grade, stored open to air) and allowed to stir for 1 h. At this time, the solvent was removed with the aid of a rotary evaporator. Then, the reaction was conducted using the obtained solid according to the general procedure.

Crystallization Procedure and Structure Data

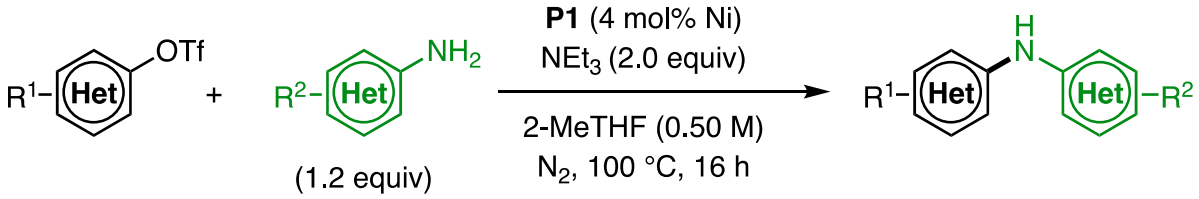
In a nitrogen-filled glovebox, an oven-dried vial (2.0 mL) was sequentially charged with **P1** (10.0 mg, 7.3 μmol) and pentane (1.5 mL). To this orange-colored suspension, a minimal amount of THF (~100 μL) was added to dissolve **P1**, resulting in a homogeneous, yellow/orange-colored solution. The uncapped vial was placed into a second glass vial (20 mL) containing pentane (2.0 mL). The larger vial was capped and was left undisturbed in a -30 °C glovebox freezer for crystallization via vapor diffusion (pentane into THF/pentane) to take place for 36 h. After decanting the solvent, this process afforded fine yellow crystals.



Crystal Data and Structure Refinement Information

Identification code	P19100	
Empirical formula	C47 H27 F27 Fe Ni O3 P2 S	
Formula weight	1361.24	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.5338(4) Å	a= 99.7349(17)°.
	b = 12.6851(5) Å	b= 104.7068(17)°.
	c = 19.8661(8) Å	g = 94.8618(17)°.
Volume	2507.81(17) $Å^3$	
Z	2	
Density (calculated)	1.803 Mg/m^3	
Absorption coefficient	0.914 mm^{-1}	
F(000)	1352	
Crystal size	0.150 x 0.085 x 0.050 mm^3	
Theta range for data collection	1.644 to 27.877°.	
Index ranges	-13<=h<=13, -16<=k<=16, -26<=l<=26	
Reflections collected	129313	
Independent reflections	11952 [R(int) = 0.0725]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6795	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11952 / 2960 / 873	
Goodness-of-fit on F^2	1.079	
Final R indices [I>2sigma(I)]	R1 = 0.0347, wR2 = 0.0833	
R indices (all data)	R1 = 0.0509, wR2 = 0.0885	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.734 and -0.413 $e.Å^{-3}$	

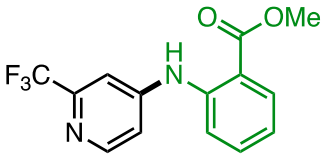
General Procedures for Amine Cross-Coupling Reactions



An oven-dried reaction tube (Fisher 16 x 125 mm tubes – Cat. No. 1495935A) equipped with a stir bar was sequentially charged with solid reagents, including precatalyst **P1** (54.5 mg, 0.04 mmol, 4.0 mol% Ni), aryl triflate (1.0 mmol, 1.0 equiv), and amine (1.2 mmol, 1.2 equiv). The reaction tube was sealed with a screw cap (Kimble Chase, Open Top S/T, Part No. 73804-15425) containing a Teflon septum (Thermo Scientific, 10/90 Teflon/Sil, Cat. No. B7995-15) and was pierced with a needle connected to a Schlenk line. The tube was evacuated and backfilled with nitrogen (this process was repeated a total of three times), then 2-MeTHF (2.0 mL) and triethylamine (280 μL, 2.0 mmol, 2.0 equiv) were added successively. If reagents were liquid, solvent was first added to the nitrogen-filled tube containing precatalyst, followed by the addition of aryl (pseudo)halide, amine, and base. The needle was removed from the septum and the top of the reaction tube was covered in parafilm. The reaction tube was placed into a pre-heated oil bath and the mixture was stirred at 100 °C for 16 h. The reaction tube was removed from the oil bath and allowed to cool to RT. Next, the tube was uncapped and the reaction solution was diluted with CH_2Cl_2 (2.0 mL), and the crude material was transferred to a round bottom flask. The solution containing the crude product was concentrated *in vacuo* with the aid of a rotary evaporator and then purified by automated silica gel column chromatography.

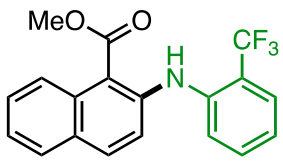
Characterization Data for Products 2a-2r

methyl 2-((2-(trifluoromethyl)pyridin-4-yl)amino)benzoate (2a)



The general procedure was followed on a 1.00 mmol scale using 2-(trifluoromethyl)pyridin-4-yl trifluoromethanesulfonate (294 mg, 1.00 mmol), methyl 2-aminobenzoate (181 mg, 1.20 mmol, 1.2 equiv), and **P1** (54.5 mg, 0.04 mmol, 4% Ni precatalyst). The product was purified via automated column chromatography (50 g silica gel, 0-10% EtOAc in hexane over 10 CV) to afford **2a** as a white solid. First run: 281 mg, 95% yield. Second run: 268 mg, 91% yield. **^{1}H NMR** (400 MHz; $CDCl_3$): δ 9.78 (s, 1H), 8.39 (d, *J* = 5.7 Hz, 1H), 7.99 (d, *J* = 8.0 Hz, 1H), 7.45 (m, 2H), 7.33 (d, *J* = 2.3 Hz, 1H), 7.13 (d, *J* = 3.2 Hz, 1H), 6.98 (dt, *J* = 7.5, 3.9 Hz, 1H), 3.86 (s, 3H). ppm. **^{13}C NMR** (101 MHz; $CDCl_3$): δ 168.4, 150.9, 149.8, 149.3 (q, *J* = 34.0 Hz), 142.8, 134.1, 132.0, 121.61 (q, *J* = 274.3 Hz), 121.59, 117.5, 116.4, 113.3, 108.7 (q, *J* = 3.0 Hz), 52.3 ppm. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -68.5 ppm. **IR** (neat, cm^{-1}): 3255.1, 2949.7, 1595.0, 1265.8, 1075.9, 752.8. **MP**: 77.4–79.0 °C. **Elemental Analysis:** Calcd. for $C_{14}H_{11}F_3N_2O_2$: C, 56.76; H, 3.74. Found: C, 56.47; H, 3.72.

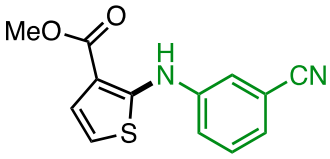
methyl 2-((2-(trifluoromethyl)phenyl)amino)-1-naphthoate (2b)



The general procedure was followed on a 1.00 mmol scale using methyl 2-(((trifluoromethyl)sulfonyl)oxy)-1-naphthoate (334 mg, 1.00 mmol), 2-(trifluoromethyl)aniline (193 mg, 1.20 mmol, 1.2 equiv), and **P1** (54.5 mg, 0.04 mmol, 4% Ni precatalyst). The product was purified via automated column chromatography (50 g silica gel, pure hexane for two CV followed by 0-10% EtOAc in hexane over 10 CV) to afford **2b** as a white solid. First run: 264 mg, 77% yield. Second run: 244 mg, 71% yield. **^{1}H NMR** (400 MHz; $CDCl_3$): δ 9.11 (s, 1H), 8.39 (d, *J* = 8.9 Hz, 1H), 7.85 – 7.63 (m, 3H), 7.61 – 7.31 (m, 5H), 7.13 (t, *J* = 7.6 Hz, 1H), 4.08 (s, 3H) ppm. **^{13}C NMR** (101 MHz; $CDCl_3$): δ 169.52, 143.87, 140.42, 133.69, 132.96, 132.69, 129.33, 128.76, 128.32, 127.40 (q, *J* = 5.4 Hz), 125.45, 124.64 (d, *J* = 272.7 Hz), 124.24, 122.70, 122.0, 121.82 (q, *J* = 29.5 Hz), 118.39, 112.10, 52.44 ppm. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.0 ppm **IR** (neat, cm^{-1}):

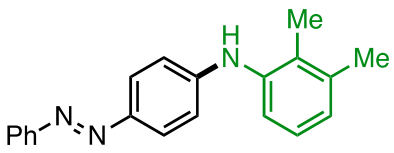
3051.3, 2951.9, 1676.6, 1504.4, 1204.6, 731.0. **MP**: 98.2–100.5 °C. **Elemental Analysis:** Calcd. for $C_{14}H_{11}F_3NO_2$: C, 66.09; H, 4.09. Found: C, 66.12; H, 4.14.

methyl 2-((3-cyanophenyl)amino)thiophene-3-carboxylate (2c)



The general procedure was followed on a 1.00 mmol scale using methyl 2-(((trifluoromethyl)sulfonyl)oxy)thiophene-3-carboxylate (290 mg, 1.00 mmol), 3-aminobenzonitrile (142 mg, 1.20 mmol, 1.2 equiv), and **P1** (54.5 mg, 0.04 mmol, 4% Ni precatalyst). The product was purified via automated column chromatography (100 g silica gel, 0-10% EtOAc in hexane over 15 CV) to afford **2c** as an opaque, slightly yellow-colored oil. Hexane (5 mL) was added to this oil and the mixture was agitated in a sonication bath, resulting in a white powder. Decanting the yellow mother liquor afforded the desired product as a powdery white solid. First run: 245 mg, 95% yield. Second run: 240 mg, 93% yield. **^{1}H NMR** (400 MHz; $CDCl_3$): δ 8.88 (s, 1H), 7.42 (d, *J* = 5.5 Hz, 1H), 7.39 – 7.32 (m, 2H), 7.30 (d, *J* = 8.7 Hz, 1H), 7.24 (d, *J* = 7.5 Hz, 1H), 7.07 (d, *J* = 5.5 Hz, 1H), 3.84 (s, 3H) ppm. **^{13}C NMR** (101 MHz; $CDCl_3$): δ ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.92, 149.22, 142.33, 132.23, 130.32, 125.74, 123.43, 121.62, 118.59, 117.67, 113.32, 105.53, 51.66 ppm. **IR** (neat, cm^{-1}): 3321.3, 2950.3, 2228.8, 1667.7, 1561.8, 1228.2, 678.5. **MP**: 72.1–73.4 °C. **Elemental Analysis:** Calcd. for $C_{13}H_{10}N_2O_2S$: C, 60.45; H, 3.90. Found: C, 60.15; H, 3.89.

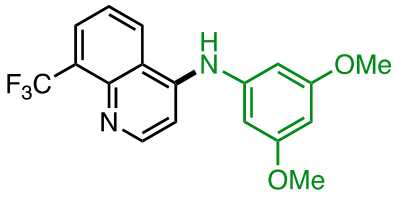
(*E*)-2,3-dimethyl-*N*-(4-(phenyldiazenyl)phenyl)aniline (2d)



The general procedure was followed on a 1.00 mmol scale using (*E*)-4-(phenyldiazenyl)phenyl trifluoromethanesulfonate (330 mg, 1.00 mmol), 2,3-dimethylaniline (145 mg, 1.20 mmol, 1.2 equiv), and **P1** (54.5 mg, 0.04 mmol, 4% Ni precatalyst). The product was purified via automated column chromatography (50 g silica gel, 0-10% EtOAc in hexane over 10 CV followed by 10% EtOAc (isocratic)) to afford **2d** as a bright orange-colored solid. First run: 262 mg, 87% yield. Second run: 266 mg, 88% yield. **^{1}H NMR** (400 MHz; $CDCl_3$): δ 7.93 (dd, *J* = 8.0, 4.4 Hz, 4H), 7.54 (t, *J* = 7.6 Hz, 2H), 7.45 (t, *J* = 7.3 Hz, 1H), 7.25 – 7.13 (m, 2H), 7.08 (d, *J* = 7.1 Hz, 1H), 6.87 (d, *J* =

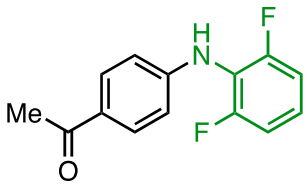
8.6 Hz, 2H), 5.78 (s, 1H), 2.39 (s, 3H), 2.22 (s, 3H) ppm. **^{13}C NMR** (101 MHz; $CDCl_3$): δ 153.3, 148.9, 146.1, 139.2, 138.6, 131.4, 130.1, 129.3, 126.9, 126.5, 125.3, 122.7, 122.0, 114.9, 20.9, 14.3 ppm. **IR** (neat, cm^{-1}): 3400.2, 2940.0, 1602.3, 1338.1, 1140.0, 833.9. **MP**: 131.0–132.7 °C. **Elemental Analysis:** Calcd. for $C_{20}H_{19}N_3$: C, 79.70; H, 6.35. Found: C, 79.54; H, 6.29.

***N*-(3,5-dimethoxyphenyl)-8-(trifluoromethyl)quinolin-4-amine (2e)**



The general procedure was followed on a 1.00 mmol scale using 8-(trifluoromethyl)quinolin-4-yl trifluoromethanesulfonate (345 mg, 1.00 mmol), 3,5-dimethoxyaniline (184 mg, 1.20 mmol, 1.2 equiv), and **P1** (54.5 mg, 0.04 mmol, 4% Ni precatalyst). The product was purified via automated column chromatography (100 g, 0-15% EtOAc in hexane over 10 CV followed by isocratic 15% EtOAc) to afford **2e** as a light yellow-colored solid foam. Hexane (5 mL) was added to this foam and the mixture was agitated in a sonication bath. Decanting the yellow mother liquor afforded the desired product as a powdery white solid. First run: 272 mg, 78% yield. Second run: 295 mg, 85% yield. **^{1}H NMR** (400 MHz; $CDCl_3$): δ 8.65 (d, *J* = 5.3 Hz, 1H), 8.14 (d, *J* = 8.5 Hz, 1H), 7.99 (d, *J* = 7.3 Hz, 1H), 7.43 (t, *J* = 7.9 Hz, 1H), 7.12 (d, *J* = 5.3 Hz, 1H), 6.97 (s, 1H), 6.42 (d, *J* = 2.2 Hz, 2H), 6.28 (s, 1H), 3.74 (s, 6H) ppm. **^{13}C NMR** (101 MHz; $CDCl_3$): δ 161.9, 151.8, 147.9, 146.0, 141.6, 128.2 (q, *J* = 5.7 Hz), 128.0 (q, *J* = 29.0 Hz), 125.0, 124.6 (q, *J* = 273.5 Hz), 123.9, 120.8, 104.2, 101.0, 97.0, 55.7 ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ 60.0 ppm. **IR** (neat, cm^{-1}): 2939.4, 2838.8, 1577.4, 1297.5, 1125.1, 1047.0, 817.9. **MP**: 102.6–104.8 °C. **Elemental Analysis:** Calcd. for $C_{14}H_{11}F_3N_2O_2$: C, 62.07; H, 4.34. Found: C, 61.78; H, 4.25.

1-(4-((2,6-difluorophenyl)amino)phenyl)ethan-1-one (2f)

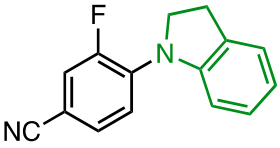


The general procedure was followed on a 1.00 mmol scale using 4-acetylphenyl trifluoromethanesulfonate (268 mg, 1.00 mmol), 2,6-difluoroaniline (155 mg, 1.20 mmol, 1.2 equiv), and **P1** (54.5 mg, 0.04 mmol, 4% Ni precatalyst). The product was purified via automated column chromatography (50 g silica gel, 0-15% EtOAc in hexane) to afford **2f** as a light yellow-colored oil. First run: 233 mg, 94% yield. Second run: 233 mg, 94% yield. **^{1}H NMR** (400 MHz; $CDCl_3$): δ 7.85 (d, *J* = 8.4 Hz, 1H), 7.11 (p, *J* = 6.5 Hz, 1H), 7.02 – 6.92 (m, 2H), 6.75 (d, *J* = 8.3 Hz, 1H), 6.13 (s, 1H), 2.51 (s, 3H) ppm. **^{13}C NMR** (101 MHz; $CDCl_3$): δ 197.1, 159.0 (d, *J* = 5.1 Hz), 156.5 (d, *J* = 5.2 Hz), 130.6, 129.5, 125.6 (t, *J* = 9.6 Hz), 117.7 (t, *J* = 15.6 Hz), 112.32 (d, *J* = 23.4 Hz), 112.32 (d, *J* = 12.3 Hz) ppm. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -118.8 ppm. **IR** (neat, cm^{-1}): 3303.0, 3050.7, 1679.5, 1514.0, 1391.0, 1149.3, 853.6. **Elemental Analysis**: Calcd for $C_{14}H_{11}F_2NO$: C, 68.01; H, 4.48. Found: C, 67.87; H, 4.40.

Additionally, the general procedure was followed on a 1.00 mmol scale (as outlined above) but a stir bar was not used. The product was obtained as a light yellow-colored oil: 230 mg, 93% yield.

Finally, the general procedure was followed on a 5.00 mmol scale, using a 25 mL round-bottom flask instead of the reaction vial, a rubber septum instead of a screw-top cap, and 2 mol% **P1** instead of 4 mol%. The product was obtained as a yellow-colored oil: 1.10 g, 88% yield.

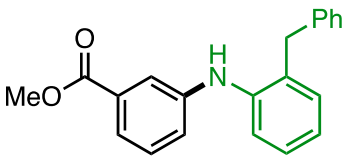
3-fluoro-4-(indolin-1-yl)benzonitrile (2g)



The general procedure was followed on a 1.00 mmol scale using 4-cyano-2-fluorophenyl trifluoromethanesulfonate (269 mg, 1.00 mmol), indoline (143 mg, 1.20 mmol, 1.2 equiv), and **P1** (54.5 mg, 0.04 mmol, 4% Ni precatalyst). The product was purified via automated column chromatography (0-20% EtOAc in hexane over 12 CV followed by isocratic 20% EtOAc) to afford **2g** as a light yellow-colored powder. Hexane (5 mL) was added to this powder and the mixture was agitated in a sonication bath. Decanting the yellow mother liquor afforded the desired product as a powdery white solid. First run: 201 mg, 84% yield. Second run: 215 mg, 90% yield. **^{1}H NMR** (400 MHz; $CDCl_3$): δ 7.50 (t, *J* = 8.1 Hz, 1H), 7.30 – 7.27 (m, 2H), 7.19 (t, *J* = 7.8 Hz, 1H), 7.02 (dd, *J* = 8.7, 2.3 Hz,

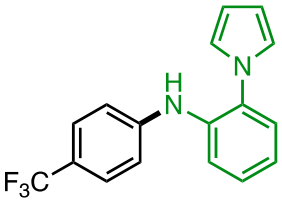
1H), 7.00 – 6.91 (m, 2H), 4.00 (t, *J* = 8.3 Hz, 2H), 3.21 (t, *J* = 8.3 Hz, 2H) ppm. **^{13}C NMR** (101 MHz; $CDCl_3$): δ 164.6 (d, *J* = 255.2 Hz), 149.3 (d, *J* = 11.2 Hz), 144.1, 134.1 (d, *J* = 2.6 Hz), 132.6, 127.5, 125.8, 122.0, 115.4, 111.9 (d, *J* = 2.3 Hz), 110.7, 102.6 (d, *J* = 23.7 Hz), 90.3 (d, *J* = 16.0 Hz), 52.1, 28.1 ppm. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -105.5 ppm. **IR** (neat, cm^{-1}): 2219.7, 1620.11, 1509.7, 1383.9, 905.4, 646.0. **MP**: 95.0–96.7 °C. **Elemental Analysis**: Calcd. For $C_{15}H_{11}FN_3$: C, 75.62; H, 4.65. Found: C, 75.81; H, 4.76.

methyl 3-((2-benzylphenyl)amino)benzoate (2h)



The general procedure was followed on a 1.00 mmol scale using methyl 3-(((trifluoromethyl)sulfonyl)oxy)benzoate (284 mg, 1.00 mmol), 2-benzylaniline (213 mg, 1.20 mmol, 1.2 equiv), and **P1** (54.5 mg, 0.04 mmol, 4% Ni precatalyst). The product was purified via automated column chromatography (50 g silica gel, 0-10% EtOAc in hexane over 12 CV) to afford **2h** as a light yellow-colored oil. First run: 295 mg, 93% yield. Second run: 280 mg, 88% yield. **^{1}H NMR** (400 MHz; $CDCl_3$): δ 7.65 – 7.59 (m, 2H), 7.44 – 7.24 (m, 9H), 7.15 (td, *J* = 7.4, 1.4 Hz, 1H), 7.06 (dd, *J* = 8.1, 1.6 Hz, 2H), 5.58 (s, 1H), 4.08 (s, 2H), 3.95 (s, 3H). ppm. **^{13}C NMR** (101 MHz; $CDCl_3$): δ 167.3, 144.8, 140.8, 139.7, 132.5, 131.6, 131.4, 129.4, 129.0, 128.7, 127.8, 126.7, 123.4, 121.2, 121.0, 120.9, 117.5, 52.2, 38.4 ppm. **IR** (neat, cm^{-1}): 3367.9, 2935.1, 1734.0, 1577.7, 1149.3, 719.2. **HRMS** (DART) Calcd. for $C_{21}H_{20}NO_2$ $[M+H]^+$: 318.1489. Found: 318.1499.

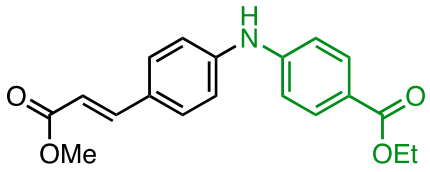
2-(1*H*-pyrrol-1-yl)-*N*-(4-(trifluoromethyl)phenyl)aniline (2i)



The general procedure was followed on a 1.00 mmol scale using 4-(trifluoromethyl)phenyl trifluoromethanesulfonate (294 mg, 1.00 mmol), 2-(1*H*-pyrrol-1-yl)aniline (190 mg, 1.20 mmol, 1.2 equiv), and **P1** (54.5 mg, 0.04 mmol, 4% Ni precatalyst). The product was purified via automated column chromatography (50 g silica gel, 0-5% EtOAc in hexane over 10 CV) to afford **2i** as a light yellow-colored oil. First run: 295 mg, 93% yield. Second run: 280 mg, 97% yield. **^{1}H NMR** (400 MHz; $CDCl_3$): δ 7.54 (dd, *J* = 13.4, 8.4 Hz, 3H), 7.40 – 7.36 (m, 2H) 7.15 (t, *J* = 7.6

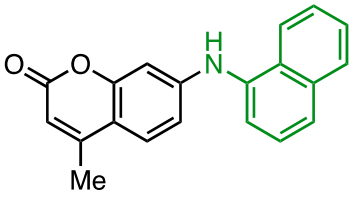
Hz, 1H), 7.10 (d, *J* = 8.3 Hz, 2H), 6.90 (s, 2H), 6.44 (s, 2H), 5.78 (s, 2H) ppm. **^{13}C NMR** (101 MHz; $CDCl_3$): δ 146.29, 137.01, 132.19, 128.53, 127.78, 127.07 (q, *J* = 3.8 Hz), 124.83 (q, *J* = 270.9 Hz), 123.0, 122.99 (q, *J* = 32.8 Hz), 122.09, 119.80, 116.76, 110.47 ppm**. ^{19}F NMR** (376 MHz, $CDCl_3$) δ 61.5 ppm. **IR** (neat, cm^{-1}): 3396.3, 1598.1, 1313.5, 1107.9, 1063.9, 725.2. **Elemental Analysis:** Calcd. for $C_{17}H_{13}F_3N_2$: C, 67.54; H, 4.33. Found: C, 67.27; H, 4.43.

ethyl (*E*)-4-((4-(3-methoxy-3-oxoprop-1-en-1-yl)phenyl)amino)benzoate (2j)



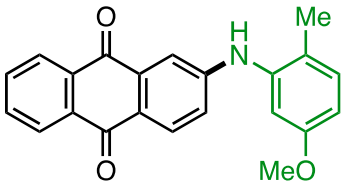
The general procedure was followed on a 1.00 mmol scale using methyl (*E*)-3-(4-(((trifluoromethyl)-sulfonyl)oxy)phenyl)acrylate (310 mg, 1.00 mmol), ethyl 4-aminobenzoate(198 mg, 1.20 mmol, 1.2 equiv), and **P1** (54.5 mg, 0.04 mmol, 4% Ni precatalyst). The product was purified via automated column chromatography (50 g, 0-20% EtOAc in hexanes over 15 CV followed by isocratic 20% EtOAc) to afford **2j** as a light yellow-colored powder. Hexane (5 mL) was added to this powder and the mixture was agitated in a sonication bath. Decanting the yellow mother liquor afforded the desired product as a white solid powder. First run: 265 mg, 82% yield. **2j** may also be purified via precipitation of the desired product from the crude reaction mixture. The general procedure was followed on a 1.00 mmol scale, as outlined above. After concentrating the reaction mixture, hexane and CH_2Cl_2 (3:1 mixture, 15 mL) were added to the flask, resulting in a light yellow-colored precipitate and yellow-colored mother liquor. The mixture was filtered and the filter cake was washed with additional hexane and CH_2Cl_2 (3:1 mixture, 20 mL) to afford the desired product as a white powdery solid. Second run: 258 mg, 79% yield. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 9.12 (s, 1H), 7.85 (d, *J* = 8.8 Hz, 2H), 7.73 – 7.49 (m, 3H), 7.29 – 7.09 (m, 4H), 6.46 (d, *J* = 15.9 Hz, 1H), 4.26 (q, *J* = 7.1 Hz, 2H), 3.70 (s, 3H), 1.29 (t, *J* = 7.1 Hz, 3H) ppm. **^{13}C NMR** (101 MHz, DMSO-d_6) δ 167.0, 165.42, 146.9, 144.4, 144.0, 131.0, 129.9, 126.6, 120.8, 117.6, 115.6, 114.4, 60.1, 51.3, 14.3 ppm. **IR** (neat, cm^{-1}): 3311.4, 3193.6, 1676.8, 1588.6, 1162.2, 825.4, 767.2. **MP**: 165.3–167.4 °C. **HRMS** (DART) Calcd. for $C_{19}H_{20}NO_4$ $[M+H]^+$: 326.1387. Found: 326.1399.

4-methyl-7-(naphthalen-1-ylamino)-2*H*-chromen-2-one (2k)



The general procedure was followed on a 1.00 mmol scale using methyl-2-oxo-2*H*-chromen-7-yl trifluoromethanesulfonate (308 mg, 1.00 mmol), 1-naphthylamine (172 mg, 1.20 mmol, 1.2 equiv), and **P1** (54.5 mg, 0.04 mmol, 4% Ni precatalyst). The product was purified via automated column chromatography (0-40% EtOAc in hexane over 12 CV followed by isocratic 40% EtOAc) to afford **2k** as a light yellow-colored powder. First run: 264 mg, 88% yield. Second run: 272 mg, 90% yield. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.97 (s, 1H), 8.06 (d, *J* = 7.9 Hz, 1H), 7.95 (d, *J* = 7.1 Hz, 1H), 7.74 (d, *J* = 6.9 Hz, 1H), 7.60 – 7.41 (m, 5H), 6.92 (dd, *J* = 8.8, 2.2 Hz, 1H), 6.68 (d, *J* = 2.2 Hz, 1H), 6.02 (s, 1H), 2.32 (s, 3H) ppm. **^{13}C NMR** (101 MHz, DMSO-d_6) δ 160.4, 155.0, 153.4, 150.1, 136.7, 134.4, 128.4, 128.3, 126.4, 126.3, 126.1, 125.9, 124.5, 122.81, 119.4, 111.8, 109.1, 99.9, 18.0 ppm. **IR** (neat, cm^{-1}): 3302.8, 1658.7, 1623.3, 1274.8, 1177.7, 726.7. **MP**: 168.0–169.9 °C. **HRMS** (DART) Calcd. $C_{20}H_{16}NO_2$ $[M+H]^+$: 302.1176. Found: 302.1182.

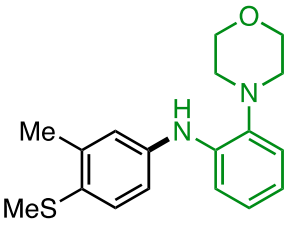
2-((5-methoxy-2-methylphenyl)amino)anthracene-9,10-dione (2l)



The general procedure was followed on a 1.00 mmol scale using 9,10-dioxo-9,10-dihydroanthracen-2-yl trifluoromethanesulfonate (356 mg, 1.00 mmol, 1.00 equiv), 5-methoxy-2-methylaniline (165 mg, 1.20 mmol, 1.20 equiv), and **P1** (54.5 mg, 0.04 mmol, 4% Ni precatalyst). The product was purified via automated column chromatography (100 g silica gel, 0–20% acetone in hexane over 12 CV) to afford **2l** as a red solid. First run: 303 mg, 88% yield. Second run: 285 mg, 83% yield. **^{1}H NMR** (400 MHz; $(CD_3)_2SO$): δ 8.83 (s, 1H), 8.21–8.08 (m, 2H), 8.03 (d, *J* = 8.6 Hz, 1H), 7.86 (dtd, *J* = 16.7, 7.4, 1.6 Hz, 2H), 7.44 (d, *J* = 2.5 Hz, 1H), 7.24 (d, *J* = 8.4 Hz, 1H), 7.15 (dd, *J* = 8.6, 2.5 Hz, 1H), 6.83 (d, *J* = 2.6 Hz, 1H), 6.77 (dd, *J* = 8.4, 2.7 Hz, 1H), 3.73 (s, 3H), 2.13 (s, 3H) ppm. **^{13}C NMR** (101 MHz; $(CD_3)_2SO$): δ 183.1, 180.4, 158.2, 151.4, 138.9, 134.8, 134.5, 133.63, 133.60, 133.0, 131.9, 129.6, 126.6, 126.5, 124.5, 123.0, 118.3, 111.0, 110.0, 109.9, 55.2, 17.0 ppm. **IR** (neat, cm^{-1}): 3365.3, 1673.7, 1587.9, 1415.0, 1327.6,

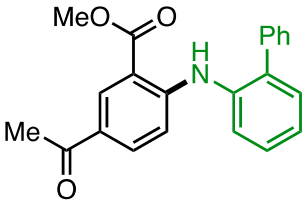
1106.8, 1038.3, 995.2, 931.2. **MP**: 190.7–192.1 °C. **HRMS** (DART) Calcd. for $C_{22}H_{17}NO_3$ $[M+H]^+$: 344.1281. Found: 344.1294.

3-methyl-4-(methylthio)-*N*-(2-morpholinophenyl)aniline (2m)



The general procedure was followed on a 1.00 mmol scale using 3-methyl-4-(methylthio)phenyl trifluoromethanesulfonate (286 mg, 1.00 mmol), 2-morpholinoaniline (267 mg, 1.50 mmol, 1.5 equiv), and **P1** (54.5 mg, 0.04 mmol, 4% Ni precatalyst). The product was purified via automated column chromatography (50 g silica gel, 0-15% EtOAc in hexane over 12 CV) to afford **2m** as a light yellow-colored oil. First run: 258 mg, 82% yield. Second run: 269 mg, 86% yield. **^{1}H NMR** (400 MHz; $CDCl_3$): δ 7.30 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.23 (d, *J* = 8.1 Hz, 1H), 7.12 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.08 – 6.99 (m, 3H), 6.90 (td, *J* = 7.6, 1.5 Hz, 1H), 6.53 (s, 1H), 3.93 – 3.80 (m, 3H), 2.97 – 2.91 (m, 3H), 2.45 (s, 3H), 2.40 (s, 3H) ppm. **^{13}C NMR** (101 MHz, $CDCl_3$) δ 141.0, 140.9, 139.0, 138.5, 129.3, 129.1, 125.1, 120.7, 120.4, 120.4, 117.1, 114.9, 67.9, 52.2, 20.7, 17.3 ppm. **IR** (neat, cm^{-1}): 3346.0, 2958.7, 2849.1, 1586.3, 1506.4, 906.8, 726.7. **Elemental Analysis:** calcd. for $C_{18}H_{22}N_2OS$: C, 68.75; H, 7.05. Found: C, 68.79; H, 7.22.

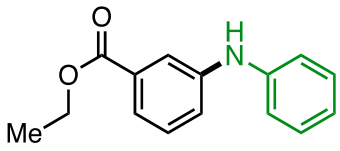
methyl 2-([1,1'-biphenyl]-2-ylamino)-5-acetylbenzoate (2n)



The general procedure was followed on a 1.00 mmol scale using methyl methyl 5-acetyl-2-(((trifluoromethyl)sulfonyl)oxy)benzoate (326 mg, 1.00 mmol), 2-amino biphenyl (203 mg, 1.20 mmol, 1.2 equiv), and **P1** (54.5 mg, 0.04 mmol, 4% Ni precatalyst). The product was purified via automated column chromatography (50 g silica gel, 0-10% EtOAc in hexane over 12 CV) to afford **2n** as a light yellow-colored powder. First run: 293 mg, 85% yield. Second run: 301 mg, 87% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.73 (s, 1H), 8.56 (d, *J* = 2.3 Hz, 1H), 7.88 (dd, *J* = 9.0, 2.3 Hz, 1H), 7.52 – 7.26 (m, 9H), 7.03 (d, *J* = 8.9 Hz, 1H), 3.86 (s, 3H), 2.54 (s, 3H) ppm. **^{13}C NMR** (101 MHz, $CDCl_3$) δ 195.7, 168.2, 152.0, 138.7, 137.9, 136.4, 133.8, 133.6, 131.4, 129.0, 128.4, 128.4, 127.5, 126.14, 126.09, 125.6, 113.3, 110.4, 52.0, 26.0 ppm. **IR** (neat, cm^{-1}): 3301.8, 2952.1,

1667.4, 1580.2, 1215.6, 956.0. **MP**: 86.8–88.3 °C. **HRMS** (DART) Calcd. for $C_{22}H_{20}NO_3$ $[M+H]^+$: 346.1438. Found: 346.1443.

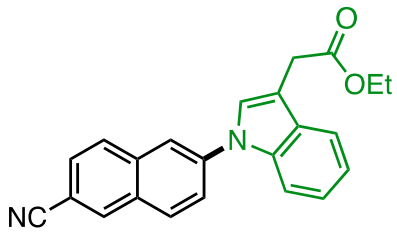
ethyl 3-(phenylamino)benzoate (2o)



The general procedure was followed on a 1.00 mmol scale using ethyl 3-(((trifluoromethyl)sulfonyl)oxy)benzoate (298 mg, 1.00 mmol, 1.00 equiv), aniline (112 mg, 1.20 mmol, 1.20 equiv), and **P1** (54.5 mg, 0.04 mmol, 4% Ni precatalyst). The product was purified via automated column chromatography (50 g silica gel, 0–10% EtOAc in hexane over 14 CV) to afford **2o** as a yellow oil. First run: 192 mg, 80% yield. Second run: 205 mg, 85% yield. **^{1}H NMR** (400 MHz; $CDCl_3$): δ 7.72 (t, *J* = 2.0 Hz, 1H), 7.59 (dt, *J* = 7.5, 1.4 Hz, 1H), 7.41–7.19 (m, 4H), 7.09 (dd, *J* = 8.6, 1.2 Hz, 2H), 6.98 (tt, *J* = 7.2, 1.2 Hz, 1H), 5.81 (s, 1H), 4.37 (q, *J* = 7.1 Hz, 2H), 1.38 (t, *J* = 7.1 Hz, 3H) ppm. **^{13}C NMR** (101 MHz; $CDCl_3$): δ 166.7, 143.6, 142.6, 131.9, 129.6, 129.4, 121.9, 121.8, 121.5, 118.5, 118.4, 61.1, 14.5 ppm.

Characterization data is consistent with that previously reported.[15]

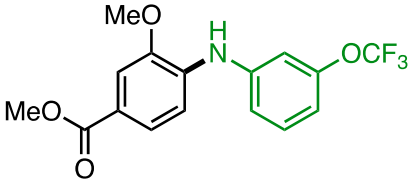
ethyl 2-(1-(6-cyanonaphthalen-2-yl)-1*H*-indol-3-yl)acetate (2p)



The general procedure was followed on a 1.00 mmol scale using 6-cyanonaphthalen-2-yl trifluoromethanesulfonate (301 mg, 1.00 mmol), ethyl 2-(1*H*-indol-3-yl)acetate (244 mg, 1.20 mmol, 1.2 equiv), and **P1** (54.5 mg, 0.04 mmol, 4% Ni precatalyst). The product was purified via automated column chromatography (100 g silica gel basified with triethyl amine, 0-10% of a 1:1 EtOAc:Acetone mixture in hexane over 12 CV followed by isocratic 10% 1:1 EtOAc:Acetone) to afford **2q** as a yellow-colored oil. First run: 265 mg, 82% yield. Second run: 258 mg, 79% yield. **^{1}H NMR** (400 MHz; $CDCl_3$): δ

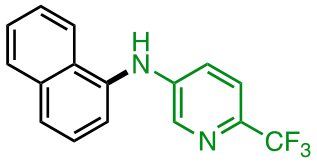
8.27 (s, 1H), 8.02 (d, *J* = 8.8 Hz, 1H), 7.97 – 7.87 (m, 2H), 7.80 (dd, *J* = 8.8, 2.2 Hz, 1H), 7.75 (d, *J* = 7.6 Hz, 1H), 7.70 – 7.64 (m, 2H), 7.50 (s, 1H), 7.30 (p, *J* = 6.9 Hz, 2H), 4.26 (q, *J* = 7.1 Hz, 2H), 3.89 (s, 2H), 1.34 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (101 MHz; $CDCl_3$): δ 171.9, 140.1, 136.0, 135.6, 134.2, 130.5, 129.5, 129.1, 127.7, 126.7, 124.7, 123.5, 121.3, 121.1, 119.9, 119.4, 111.4, 110.8, 109.5, 61.2, 31.5, 14.6. **IR** (neat, cm^{-1}): 2980.5, 1729.5, 1483.5, 1455.2, 1151.4, 904.9, 725.9. **HRMS** (DART) Calcd. for $C_{23}H_{19}N_2O_2$ $[M+H]^+$: 355.1441. Found: 355.1454.

methyl 3-methoxy-4-((3-(trifluoromethoxy)phenyl)amino)benzoate (2q)



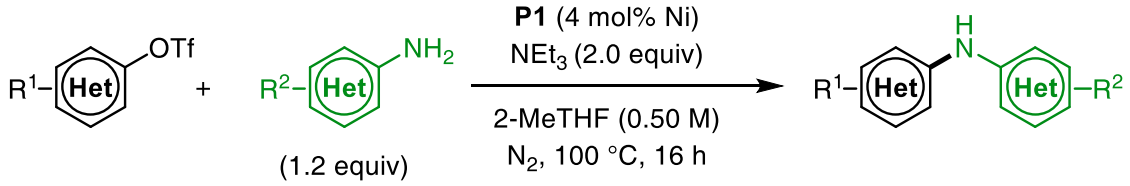
The general procedure was followed on a 1.00 mmol scale using methyl 3-methoxy-4-(((trifluoromethyl)sulfonyl)oxy)benzoate (314 mg, 1.00 mmol), 3-(trifluoromethoxy)aniline (213 mg, 1.20 mmol, 1.2 equiv), and **P1** (54.5 mg, 0.04 mmol, 4% Ni precatalyst). The product was purified via automated column chromatography (100 g silica gel, 0-10% EtOAc in hexane over 12 CV followed by isocratic 10% EtOAc) to afford **2q** as a light yellow-colored solid foam. Residual aniline starting material was removed from the product by heating the solid foam to 100 °C under vacuum (~100 millitorr). This process resulted in a slightly yellow-colored solid. First run: 240 mg, 71% yield. Second run: 230 mg, 68% yield. **^{1}H NMR** (400 MHz; $CDCl_3$): δ 7.64 (d, *J* = 8.4 Hz, 1H), 7.56 (s, 1H), 7.31 (t, *J* = 8.2 Hz, 1H), 7.25 (d, *J* = 8.4 Hz, 1H), 7.15 – 7.05 (m, 2H), 6.88 (d, *J* = 8.2 Hz, 1H), 6.67 (s, 1H), 3.92 (s, 3H), 3.90 (s, 3H) ppm. **^{13}C NMR** (101 MHz; $CDCl_3$): δ 167.2, 150.4, 150.4, 150.3, 150.3, 147.3, 142.8, 137.0, 130.7, 123.9, 121.5, 120.7 (q, *J* = 257.1 Hz), 118.0, 114.6, 112.3, 112.1, 111.4, 55.9, 52.0 ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ 57.4 ppm. **IR** (neat, cm^{-1}): 3333.4, 2954.4, 1688.8, 1593.4, 1205.0, 987.0, 761.8. **MP**: 89.2–91.6 °C. **Elemental Analysis:** Calcd. for $C_{16}H_{13}F_3NO_4$: C, 56.31; H, 4.13. Found: C, 56.07; H, 4.11.

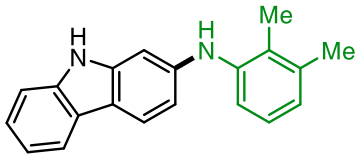
***N*-(naphthalen-1-yl)-6-(trifluoromethyl)pyridin-3-amine (2r)**



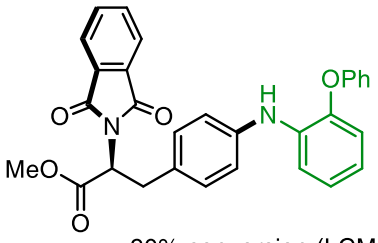
The general procedure was followed on a 1.00 mmol scale using 2-(trifluoromethyl)pyridin-4-yl trifluoromethanesulfonate (294 mg, 1.00 mmol), methyl 2-aminobenzoate (181 mg, 1.20 mmol, 1.2 equiv), and **P1** (54.5 mg, 0.04 mmol, 4% Ni precatalyst). The product was purified via automated column chromatography (50 g silica gel, 0-10% EtOAc in hexane over 10 CV followed by isocratic 10% EtOAc) to afford **2r** as a slightly-yellow solid. Hexane (5 mL) was added to this solid and the mixture was agitated in a sonication bath. Decanting the yellow mother liquor afforded the desired product as a white powder. First run: 236 mg, 82% yield. Second run: 248 mg, 86% yield. **^{1}H NMR** (400 MHz; $CDCl_3$): δ 8.25 (s, 1H), 7.91 (d, *J* = 8.3 Hz, 2H), 7.76 (d, *J* = 8.2 Hz, 1H), 7.55 – 7.36 (m, 5H),7.02 (d, *J* = 8.5 Hz, 1H), 6.45 (d, *J* = 11.0 Hz, 1H) ppm. **^{13}C NMR** (101 MHz; $CDCl_3$): δ 145.1, 138.1 (q, *J* = 37.1 Hz), 137.7, 135.7, 135.0, 129.4, 128.9, 126.8, 126.8, 126.5, 126.1, 122.5 (d, *J* = 272.2 Hz), 122.4, 122.4, 121.5 (q, *J* = 2.9 Hz), 120.9, 120.5 ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.3 ppm. **IR** (neat, cm^{-1}): 3237.9, 3062.3, 1590.7, 1345.2, 1085.2, 774.1. **MP**: 77.1–79.0 °C. **Elemental Analysis:** Calcd. for $C_{16}H_{11}F_3N_2$: C, 66.66; H, 3.85. Found: C, 66.96; H, 6.72.

Additional Substrate Scope Data

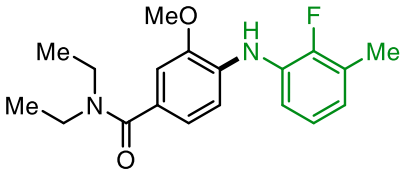




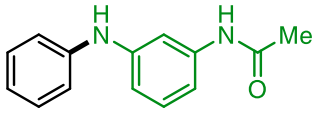
27% isolated yield



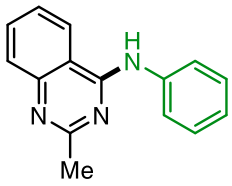
>90% conversion (LCMS)
(Difficult purification)



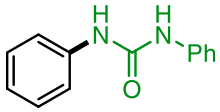
>90% conversion (LCMS)
(Difficult purification)



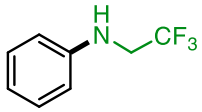
~25% product (LC/MS)



Trace product



No conversion



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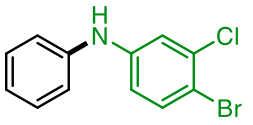

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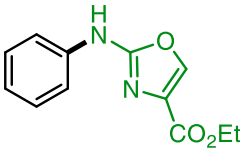

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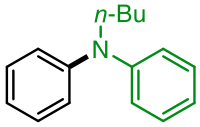

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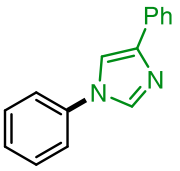

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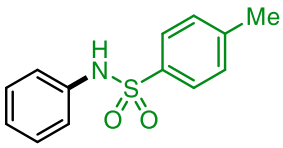

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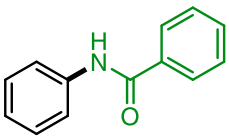
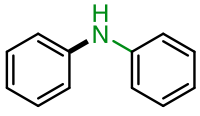
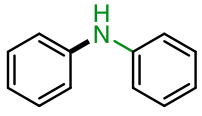


No conversion

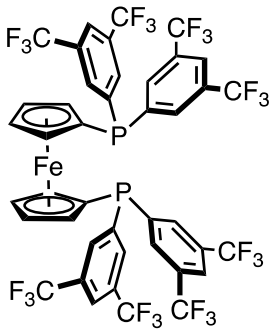


From Ph**OTs**
or Ph**OMs**
No conversion

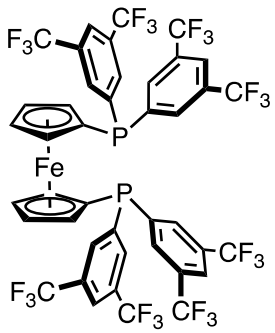


From Ph**Br**

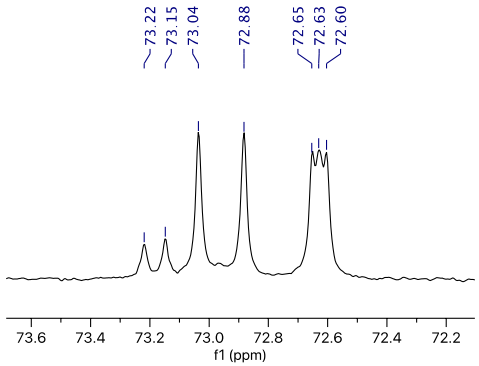
Trace product

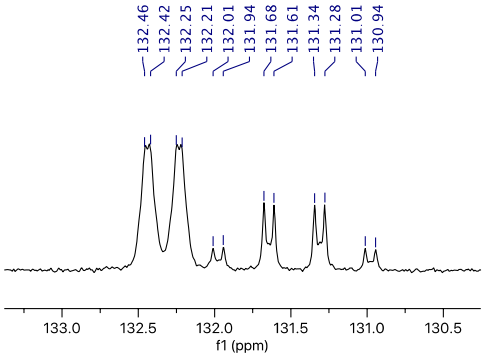


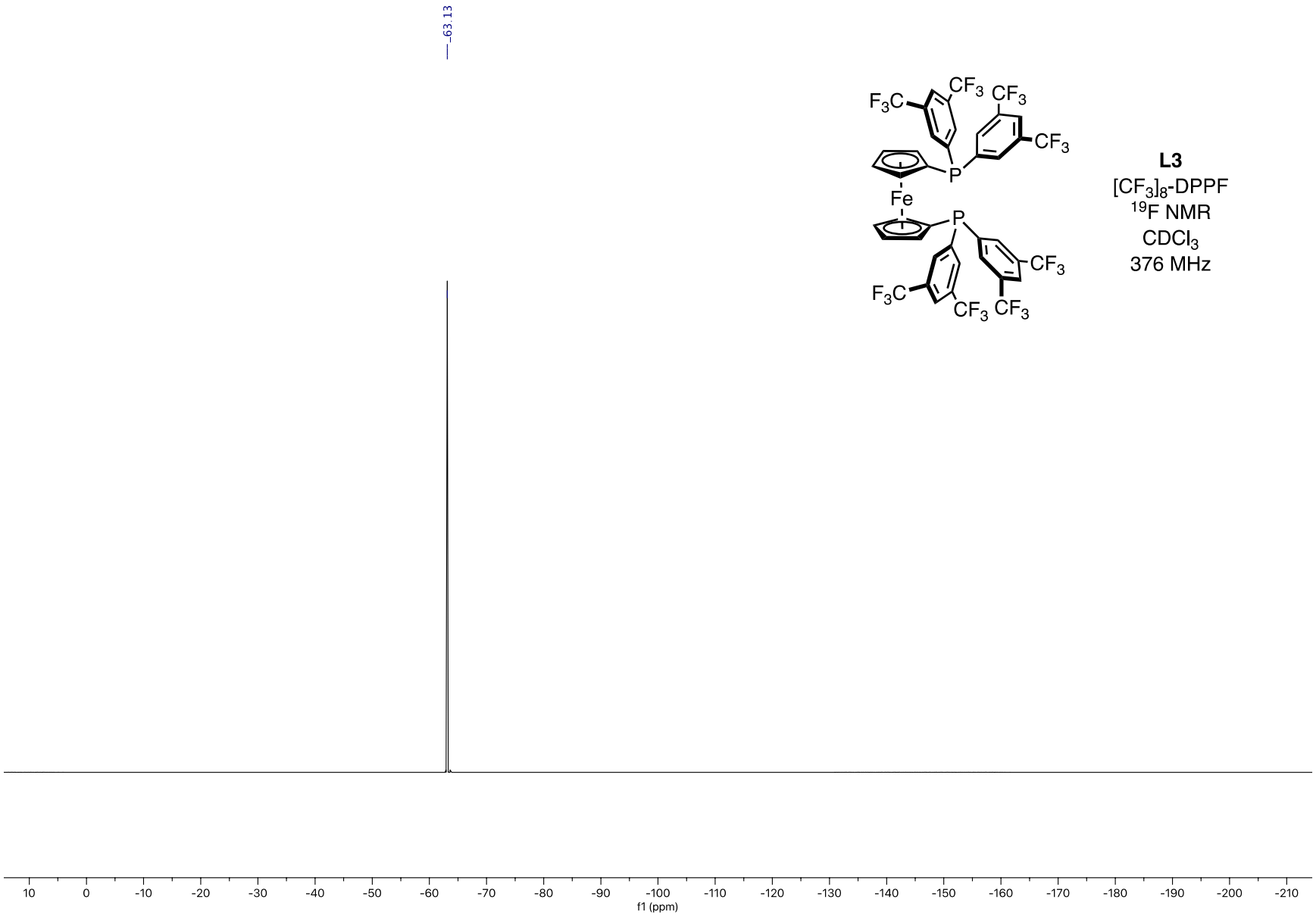
L3
$[CF_3]_8$-DPPF
^{1}H NMR
$CDCl_3$
400 MHz

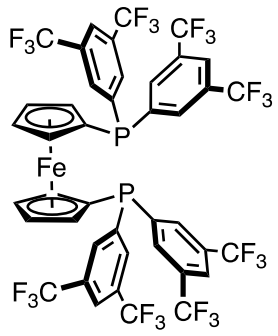


L3
$[CF_3]_8$-DPPF
^{13}C NMR
$CDCl_3$
101 MHz

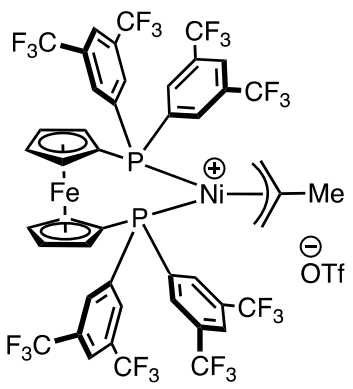




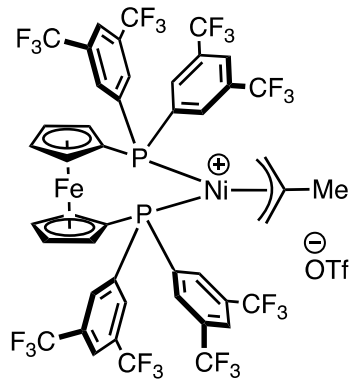

-63.13
F3C
CF3
CF3
CF3
P
Fe
P
CF3
F3C
CF3
CF3
L3
[CF3]8-DPPF
19F NMR
CDCl3
376 MHz
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)



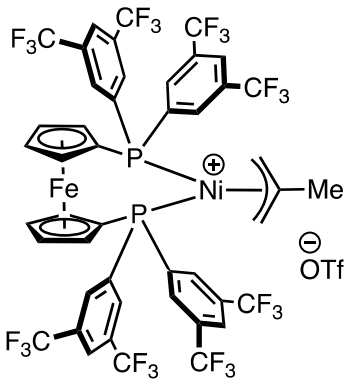
L3
$[CF_3]_8$-DPPF
^{31}P NMR
$CDCl_3$
162 MHz



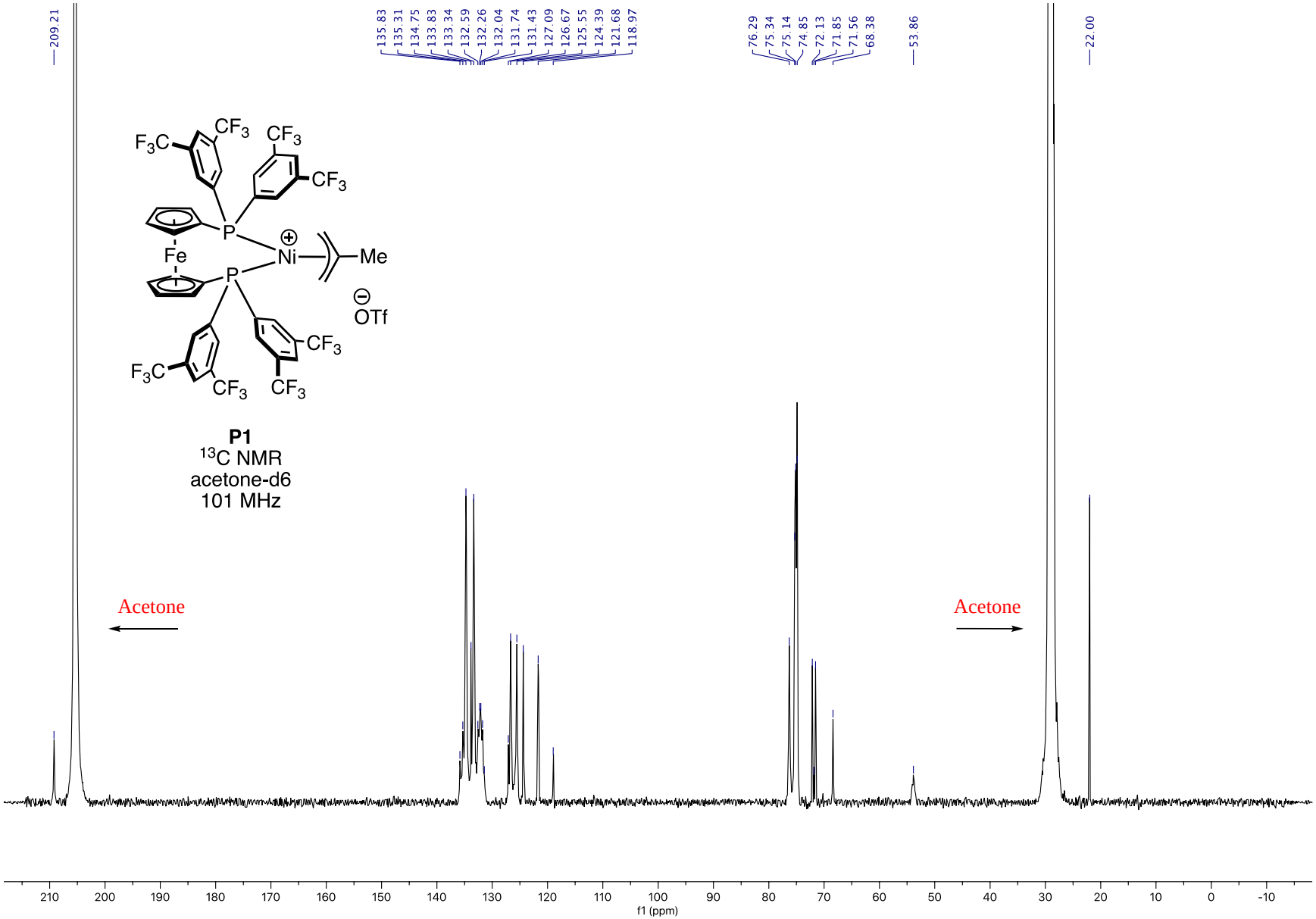
P1
^{1}H NMR
acetone-d6
400 MHz

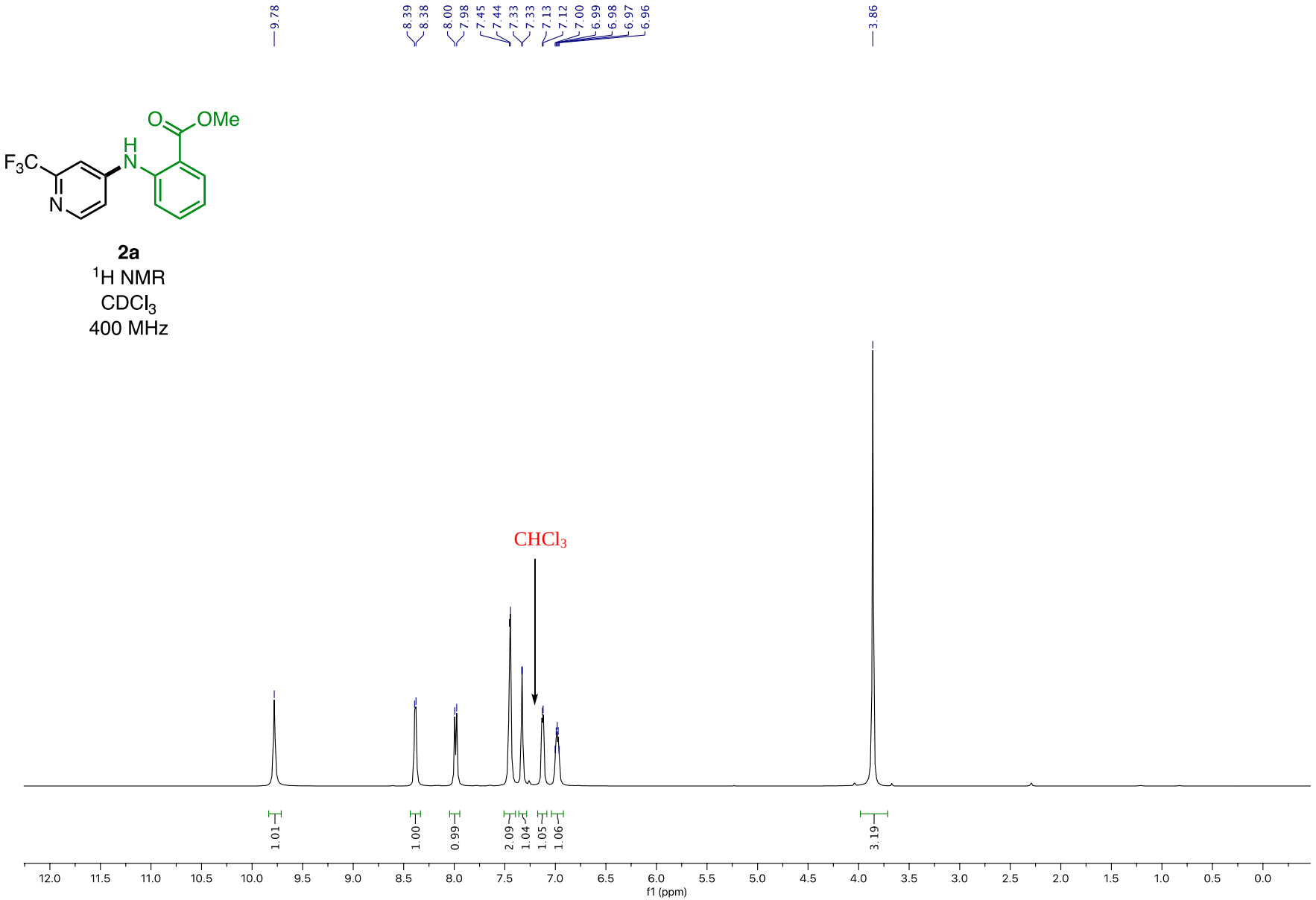


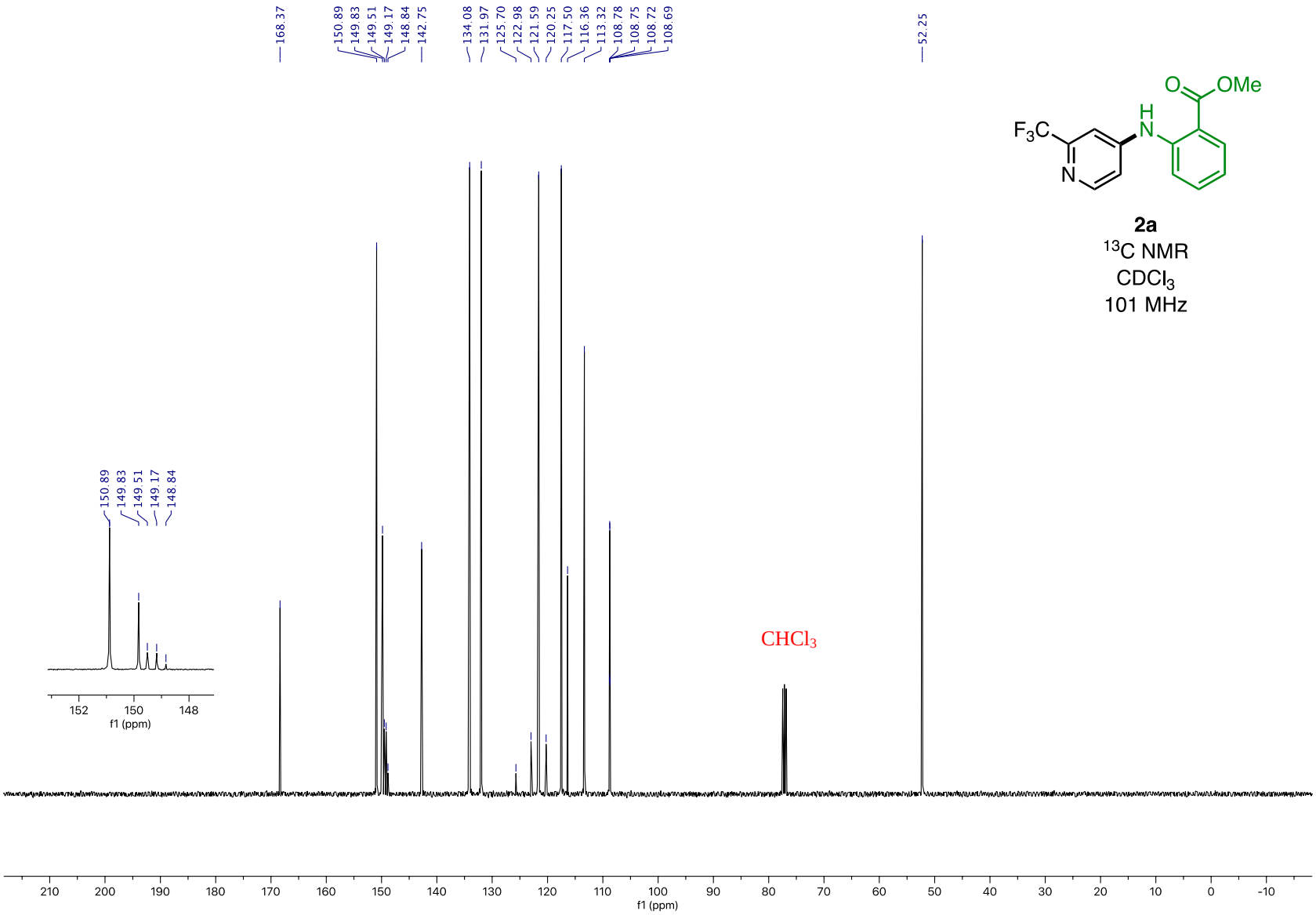
P1
^{19}F NMR
THF-H_8
376 MHz

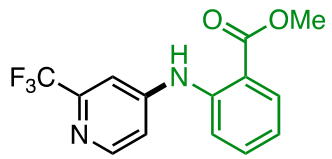


P1
^{31}P NMR
acetone-d6
162 MHz

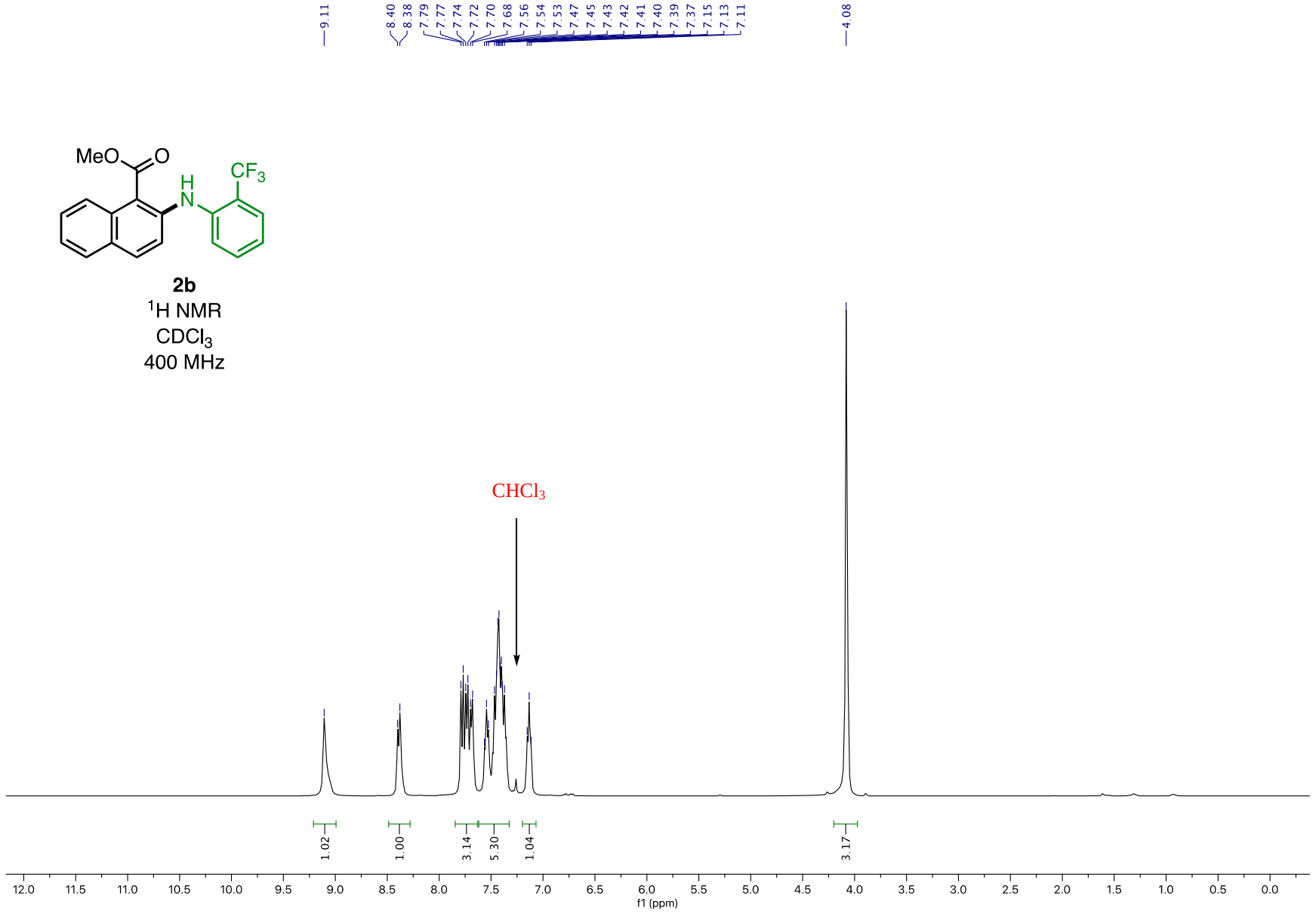

209.21
135.83
135.31
134.75
133.83
133.34
132.59
132.26
132.04
131.74
131.43
127.09
126.67
125.55
124.39
121.68
118.97
76.29
75.34
75.14
74.85
72.13
71.85
71.56
68.38
53.86
22.00
F3C
CF3
CF3
CF3
P
Fe
P
Ni
Me
OTf
CF3
F3C
CF3
CF3
P1
13C NMR
acetone-d6
101 MHz
Acetone
Acetone
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

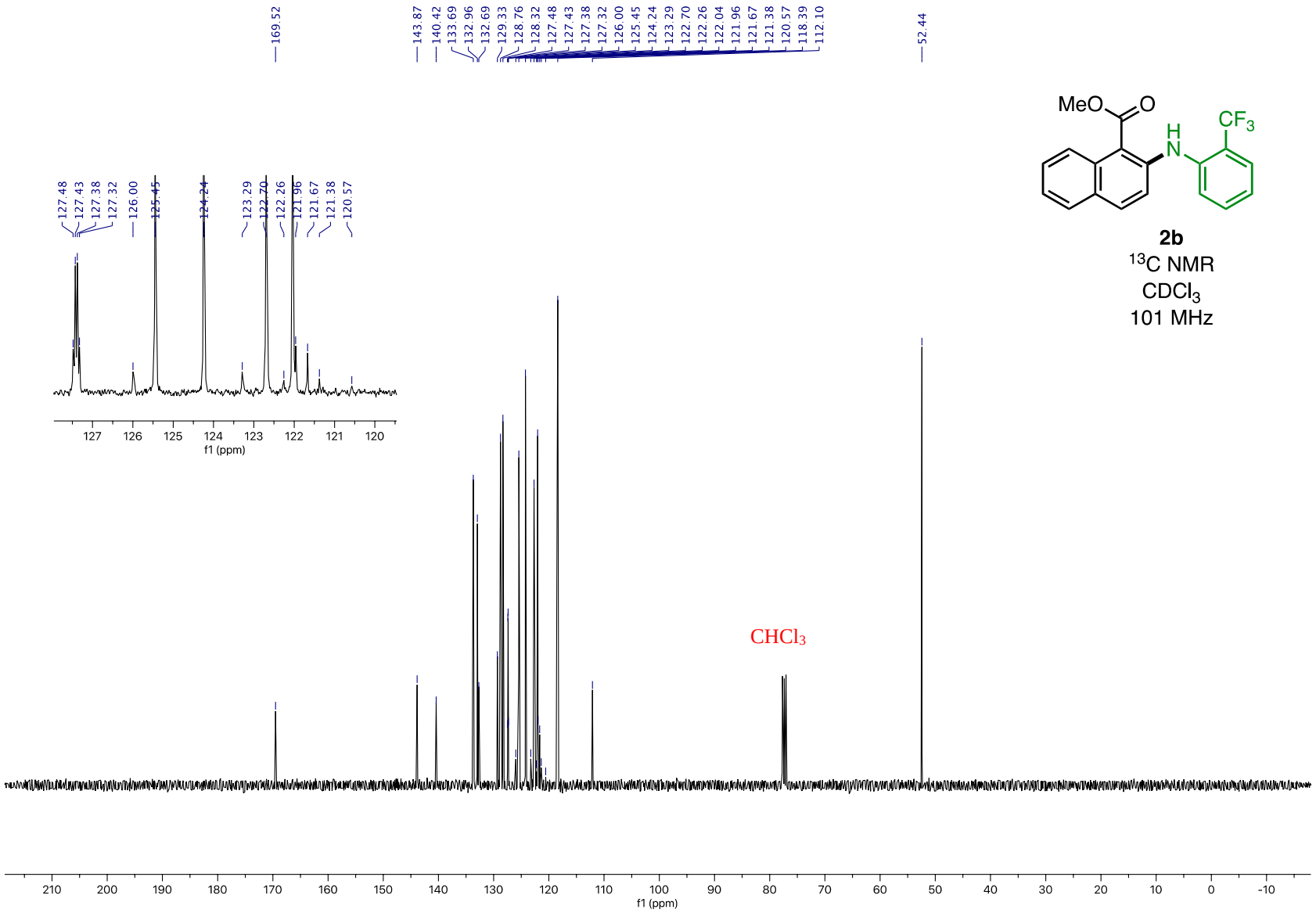

9.78
8.39
8.38
8.00
7.98
7.45
7.44
7.33
7.33
7.13
7.12
7.00
6.99
6.98
6.97
6.96
3.86
O
OMe
H
N
F3C
N
2a
1H NMR
CDCl3
400 MHz
CHCl3
1.01
1.00
0.99
2.09
1.04
1.05
1.06
3.19
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

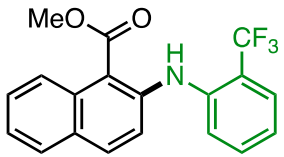

168.37
150.89
149.83
149.51
149.17
148.84
142.75
134.08
131.97
125.70
122.98
121.59
120.25
117.50
116.36
113.32
108.78
108.75
108.72
108.69
52.25
CHCl3
f1 (ppm)
2a
13C NMR
CDCl3
101 MHz



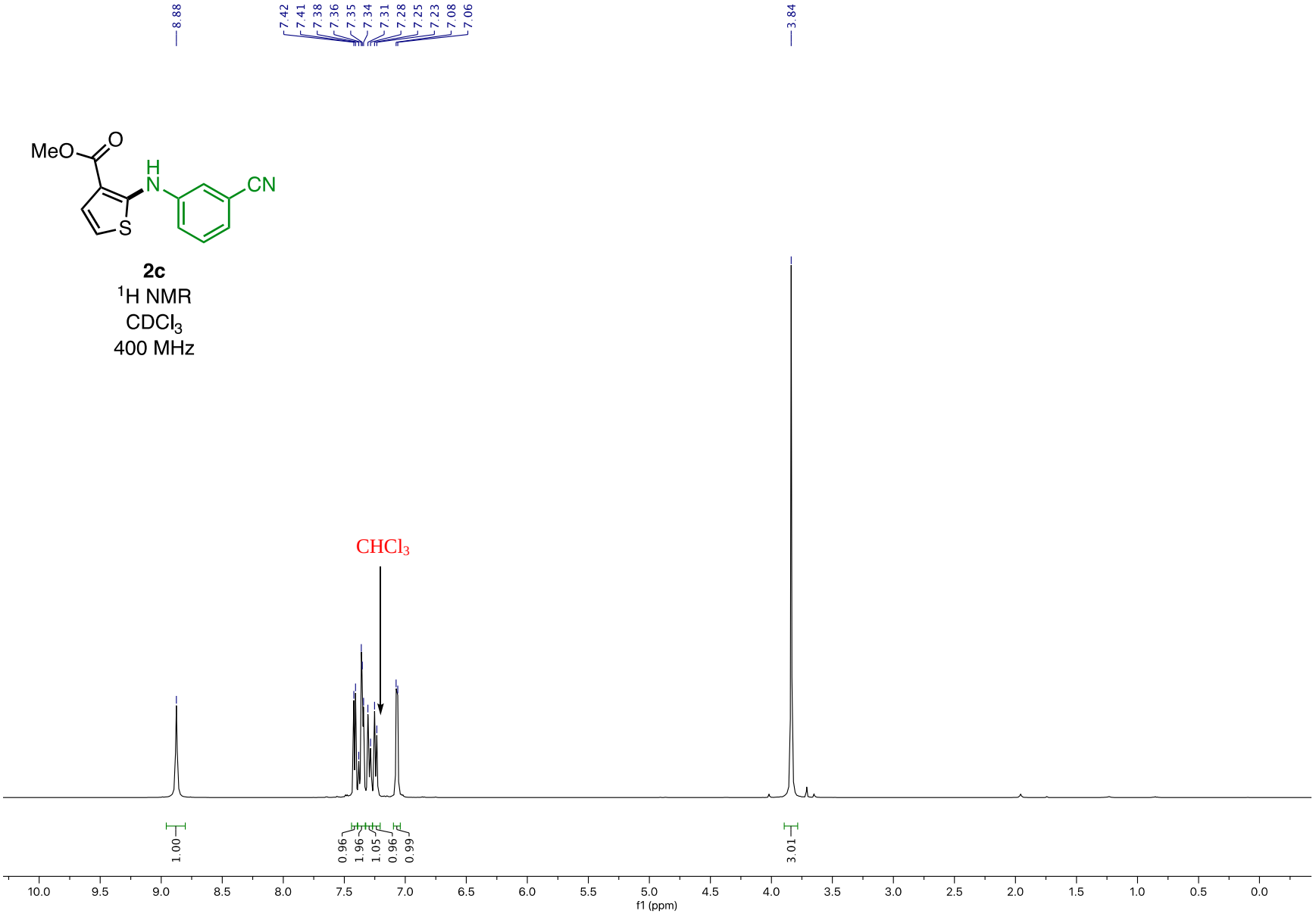
2a
^{19}F NMR
$CDCl_3$
376 MHz

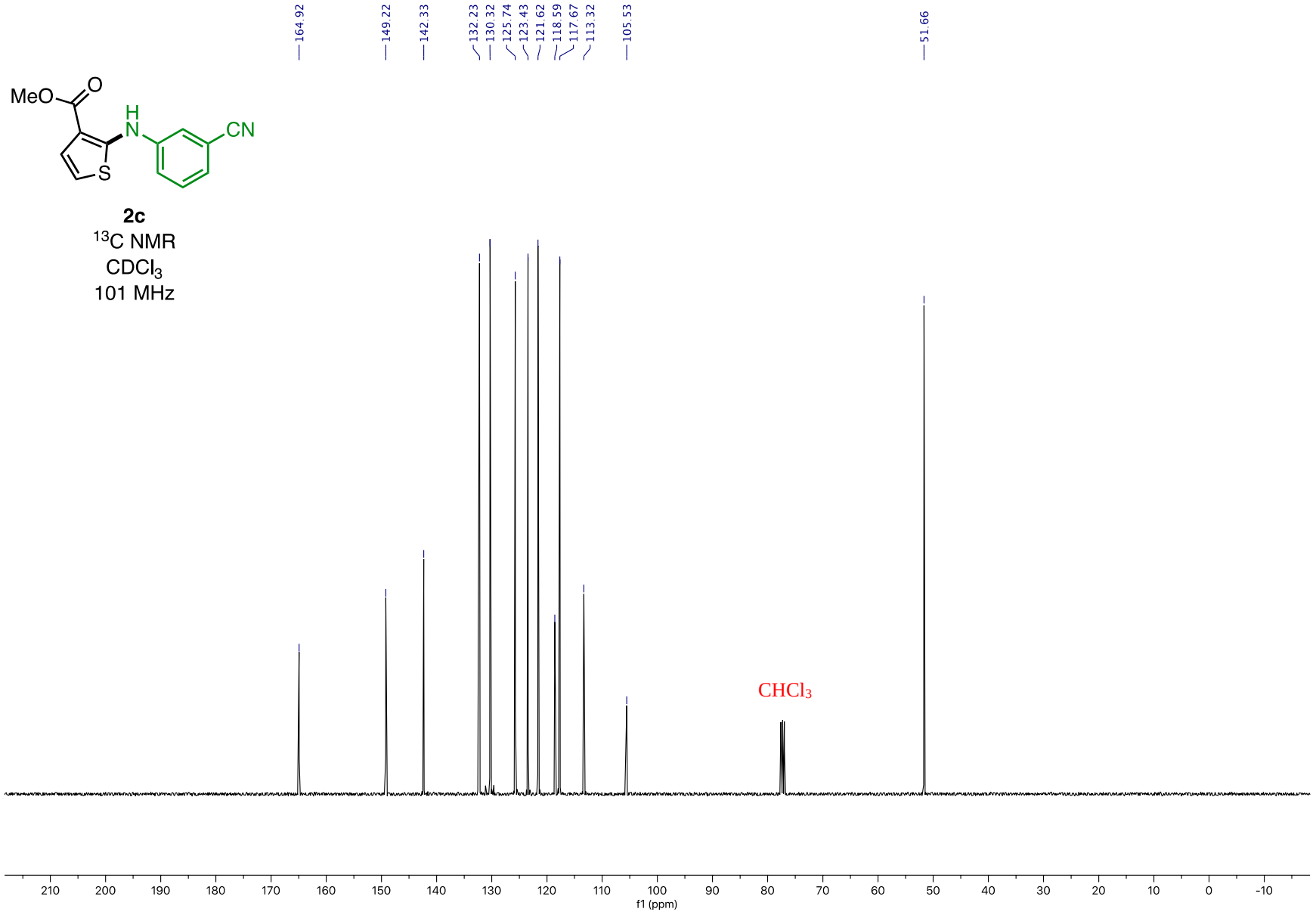

9.11
8.40
8.38
7.79
7.77
7.74
7.72
7.70
7.68
7.56
7.54
7.53
7.47
7.45
7.43
7.42
7.41
7.40
7.39
7.37
7.15
7.13
7.11
4.08
MeO
O
H
N
CF3
2b
1H NMR
CDCl3
400 MHz
CHCl3
1.02
1.00
3.14
5.30
1.04
3.17
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

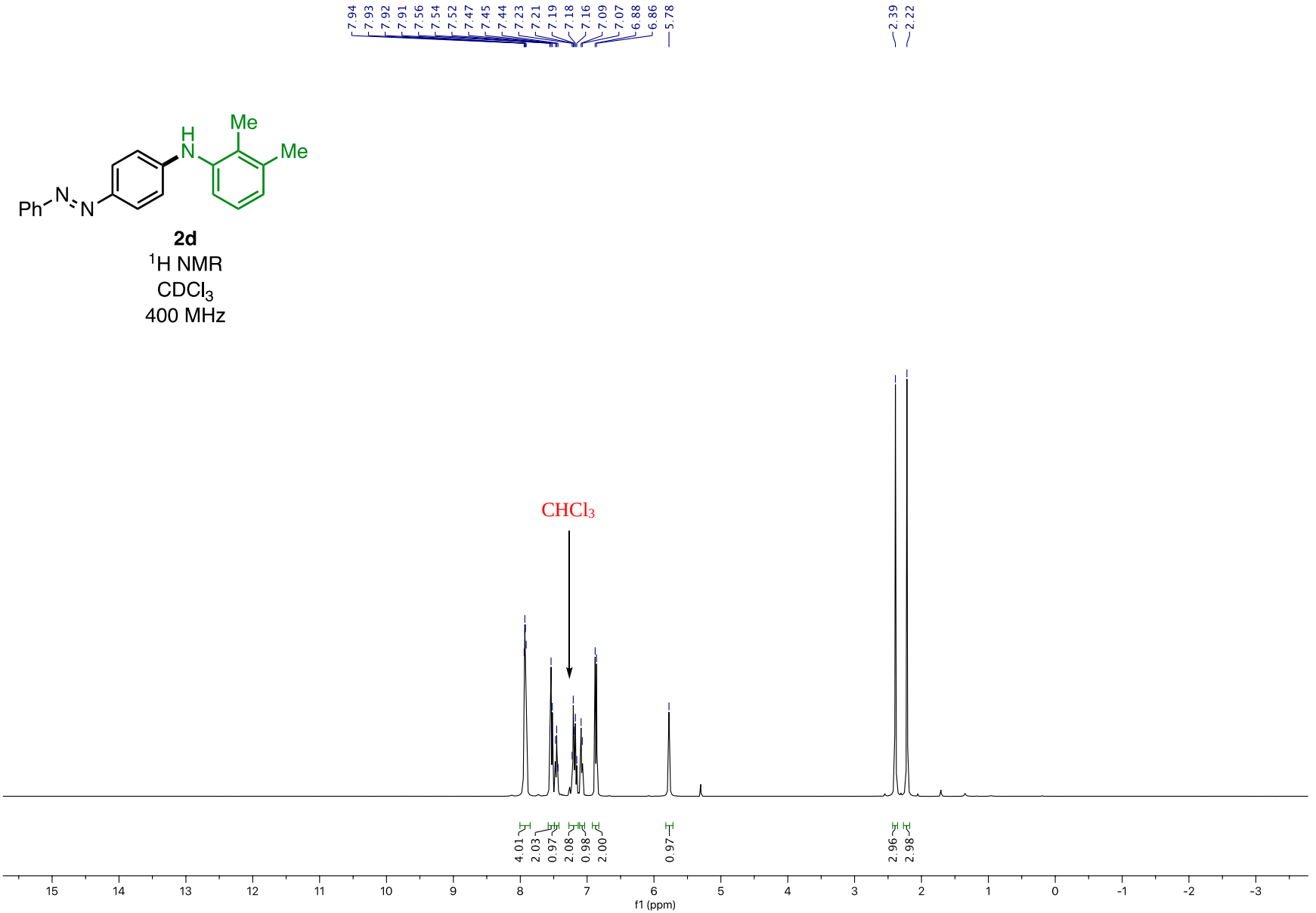

169.52
143.87
140.42
133.69
132.96
132.69
129.33
128.76
128.32
127.48
127.43
127.38
127.32
126.00
125.45
124.24
123.29
122.70
122.26
122.04
121.96
121.67
121.38
120.57
118.39
112.10
52.44
MeO
O
H
N
CF3
2b
13C NMR
CDCl3
101 MHz
CHCl3
f1 (ppm)

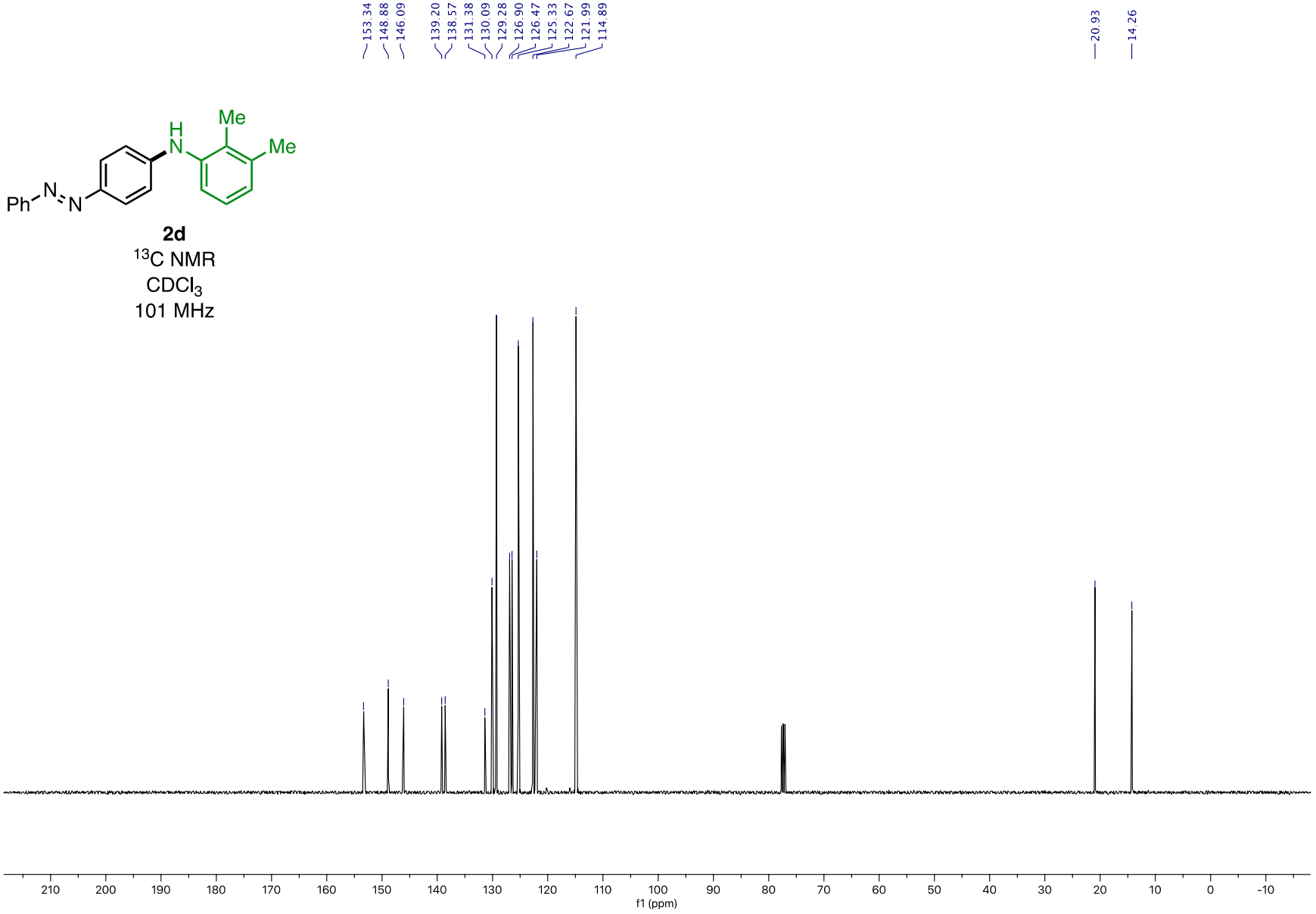


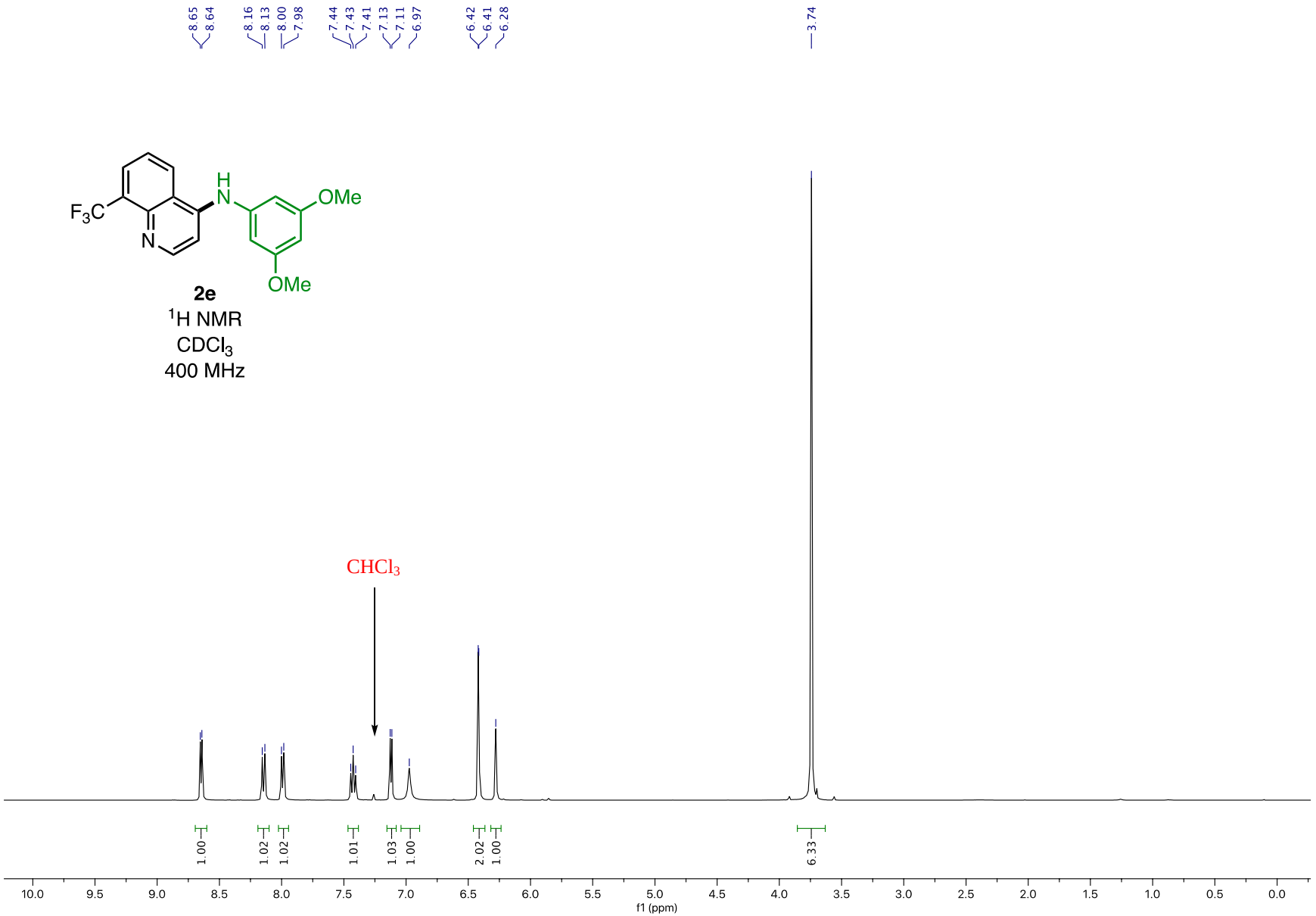
2b
^{19}F NMR
$CDCl_3$
376 MHz

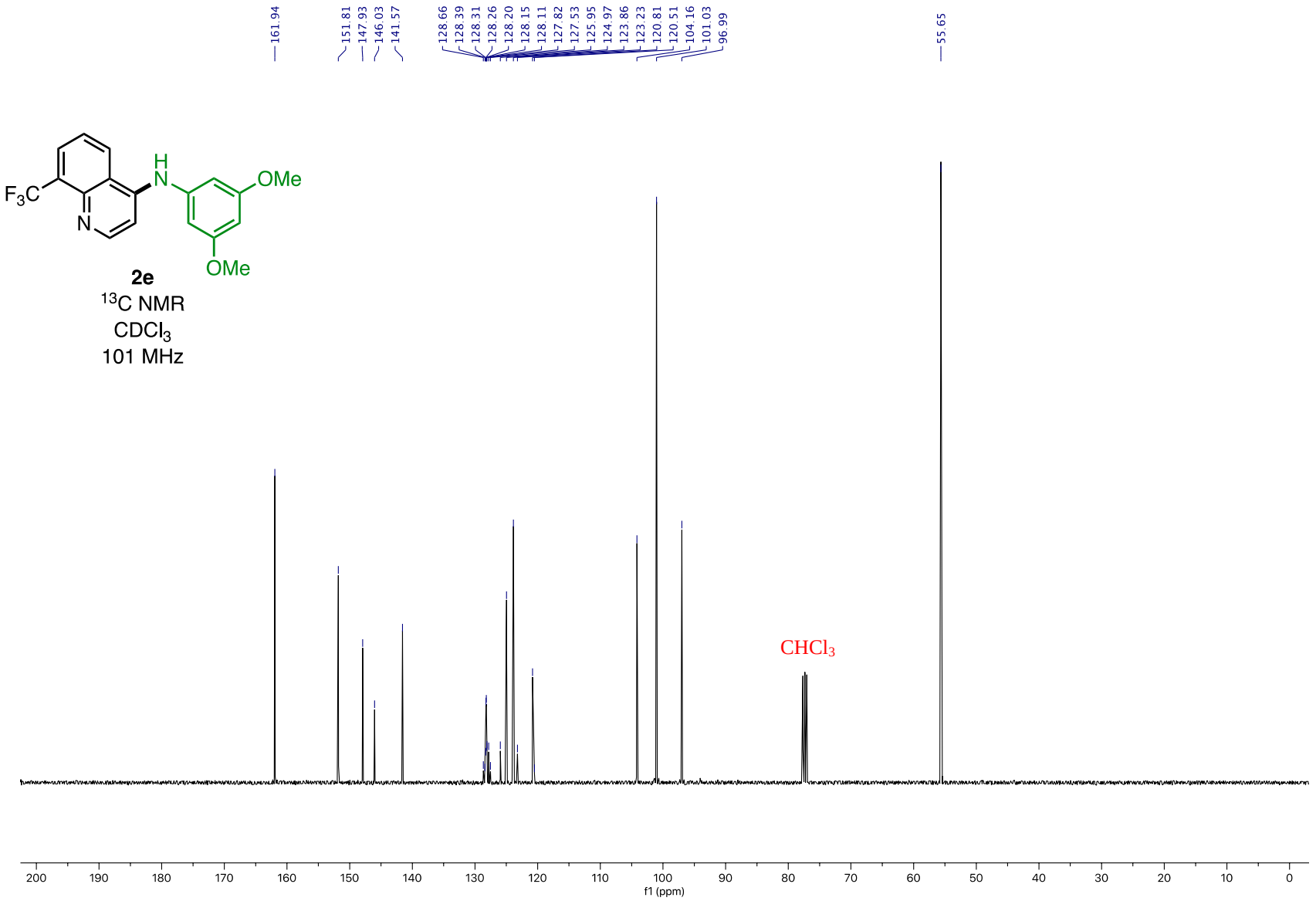

8.88
7.42
7.41
7.38
7.36
7.35
7.34
7.31
7.28
7.25
7.23
7.08
7.06
3.84
MeO
O
H
N
CN
S
2c
1H NMR
CDCl3
400 MHz
CHCl3
1.00
0.96
1.96
1.05
0.96
0.99
3.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

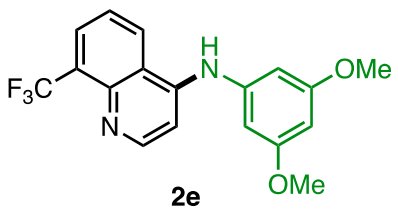

164.92
149.22
142.33
132.23
130.32
125.74
123.43
121.62
118.59
117.67
113.32
105.53
51.66
MeO
O
H
N
CN
S
2c
13C NMR
CDCl3
101 MHz
CHCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.94
7.93
7.92
7.91
7.56
7.54
7.52
7.47
7.45
7.44
7.23
7.21
7.19
7.18
7.16
7.09
7.07
6.88
6.86
5.78
2.39
2.22
Me
H
N
Me
Ph
N
N
2d
1H NMR
CDCl3
400 MHz
CHCl3
4.01
2.03
0.97
2.08
0.98
2.00
0.97
2.96
2.98
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

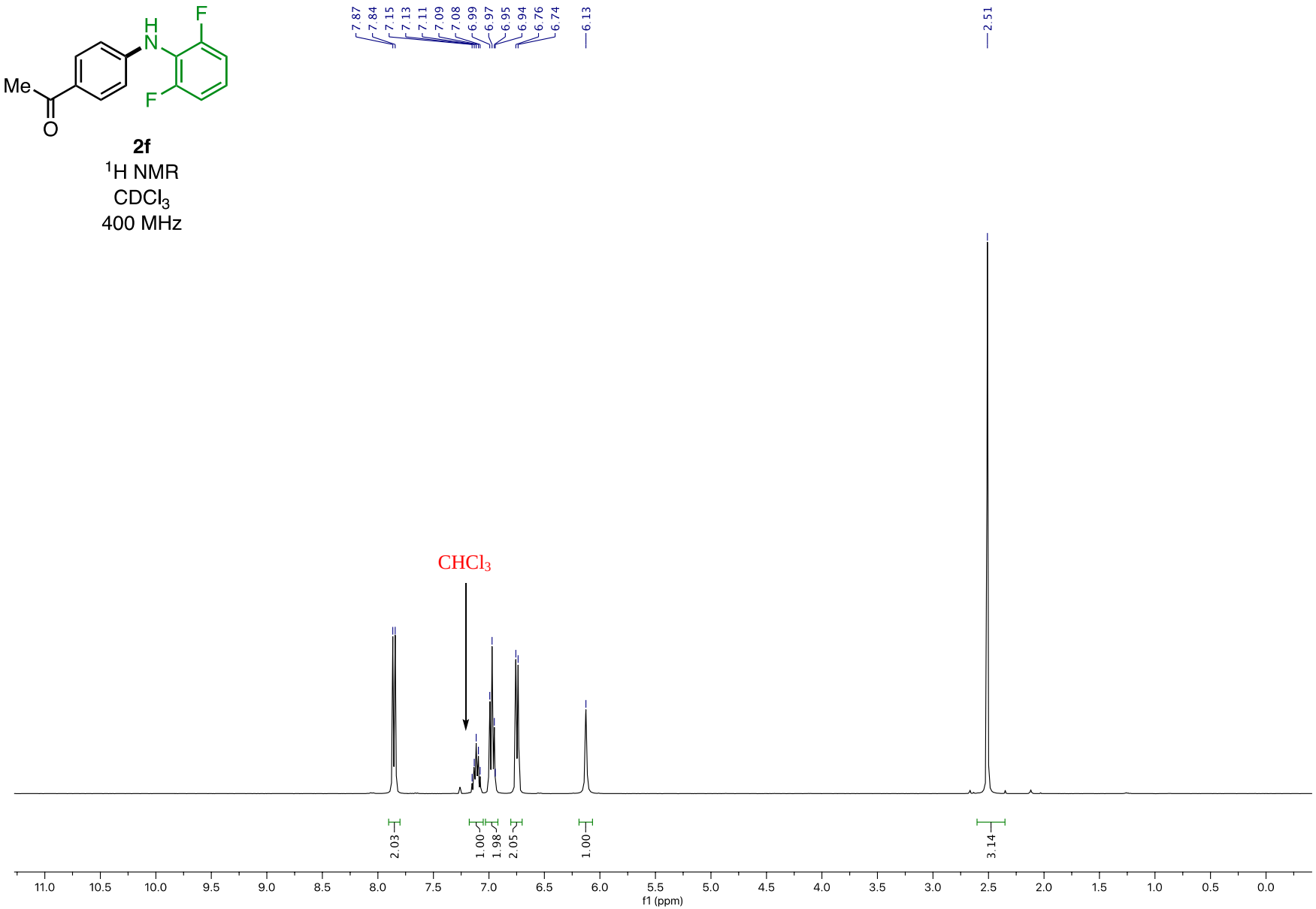

153.34
148.88
146.09
139.20
138.57
131.38
130.09
129.28
126.90
126.47
125.33
122.67
121.99
114.89
20.93
14.26
Me
H
N
Me
Ph
N
N
2d
13C NMR
CDCl3
101 MHz
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

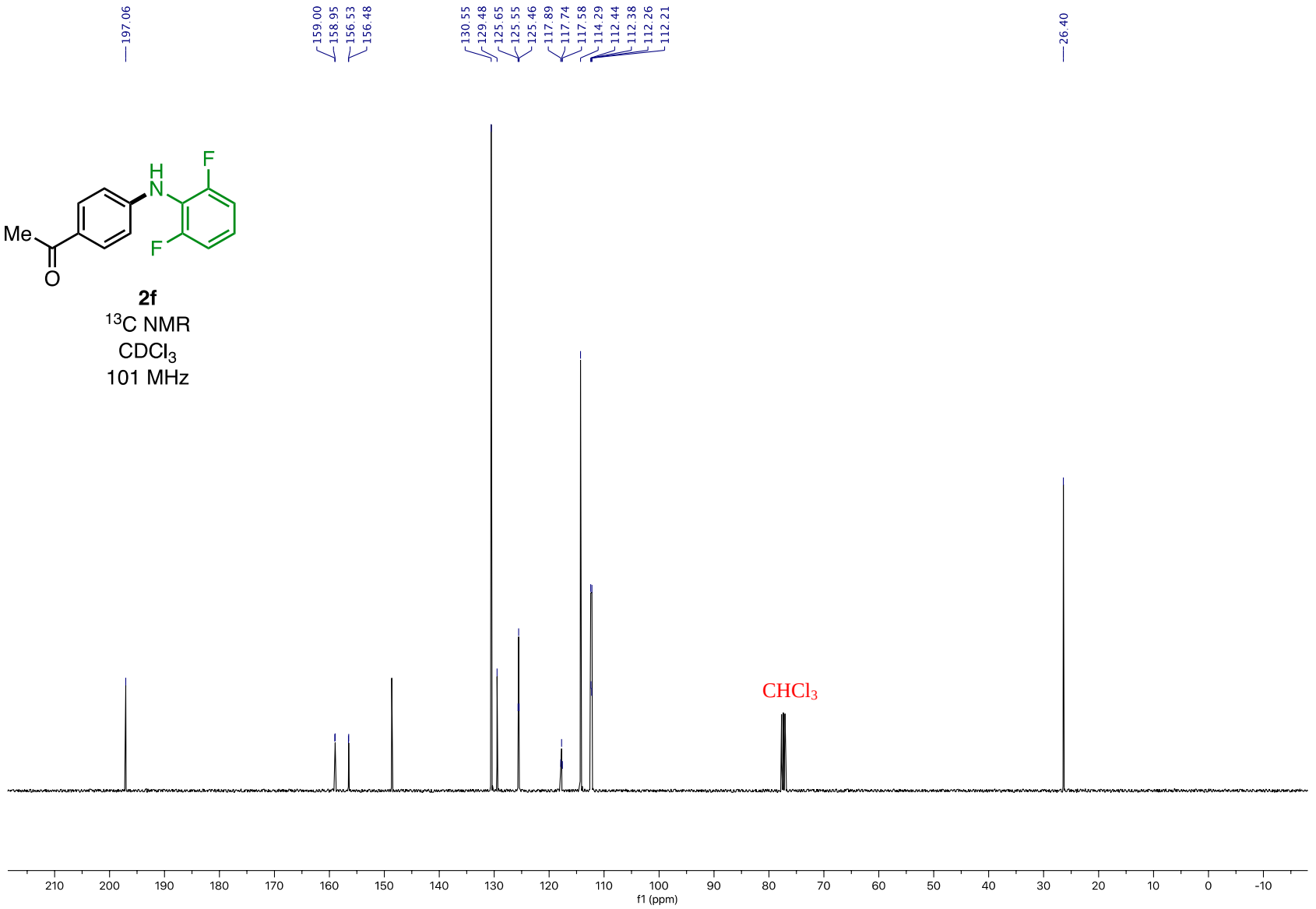

8.65
8.64
8.16
8.13
8.00
7.98
7.44
7.43
7.41
7.13
7.11
6.97
6.42
6.41
6.28
3.74
F3C
N
H
N
OMe
OMe
2e
1H NMR
CDCl3
400 MHz
CHCl3
1.00
1.02
1.02
1.01
1.03
1.00
2.02
1.00
6.33
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

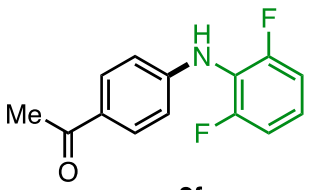

161.94
151.81
147.93
146.03
141.57
128.66
128.39
128.31
128.26
128.20
128.15
128.11
127.82
127.53
125.95
124.97
123.86
123.23
120.81
120.51
104.16
101.03
96.99
55.65
F3C
N
H
N
OMe
OMe
2e
13C NMR
CDCl3
101 MHz
CHCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



2e
^{19}F NMR
$CDCl_3$
376 MHz


Me
O
H
N
F
F
2f
^{1}H NMR
$CDCl_3$
400 MHz
7.87
7.84
7.15
7.13
7.11
7.09
7.08
6.99
6.97
6.95
6.94
6.76
6.74
6.13
2.51
$CHCl_3$
2.03
1.00
1.98
2.05
1.00
3.14
11.0
10.5
10.0
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
f1 (ppm)


197.06
159.00
158.95
156.53
156.48
130.55
129.48
125.65
125.55
125.46
117.89
117.74
117.58
114.29
112.44
112.38
112.26
112.21
26.40
Me
O
H
N
F
F
2f
13C NMR
CDCl3
101 MHz
CHCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

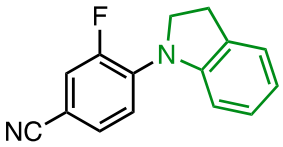


2f

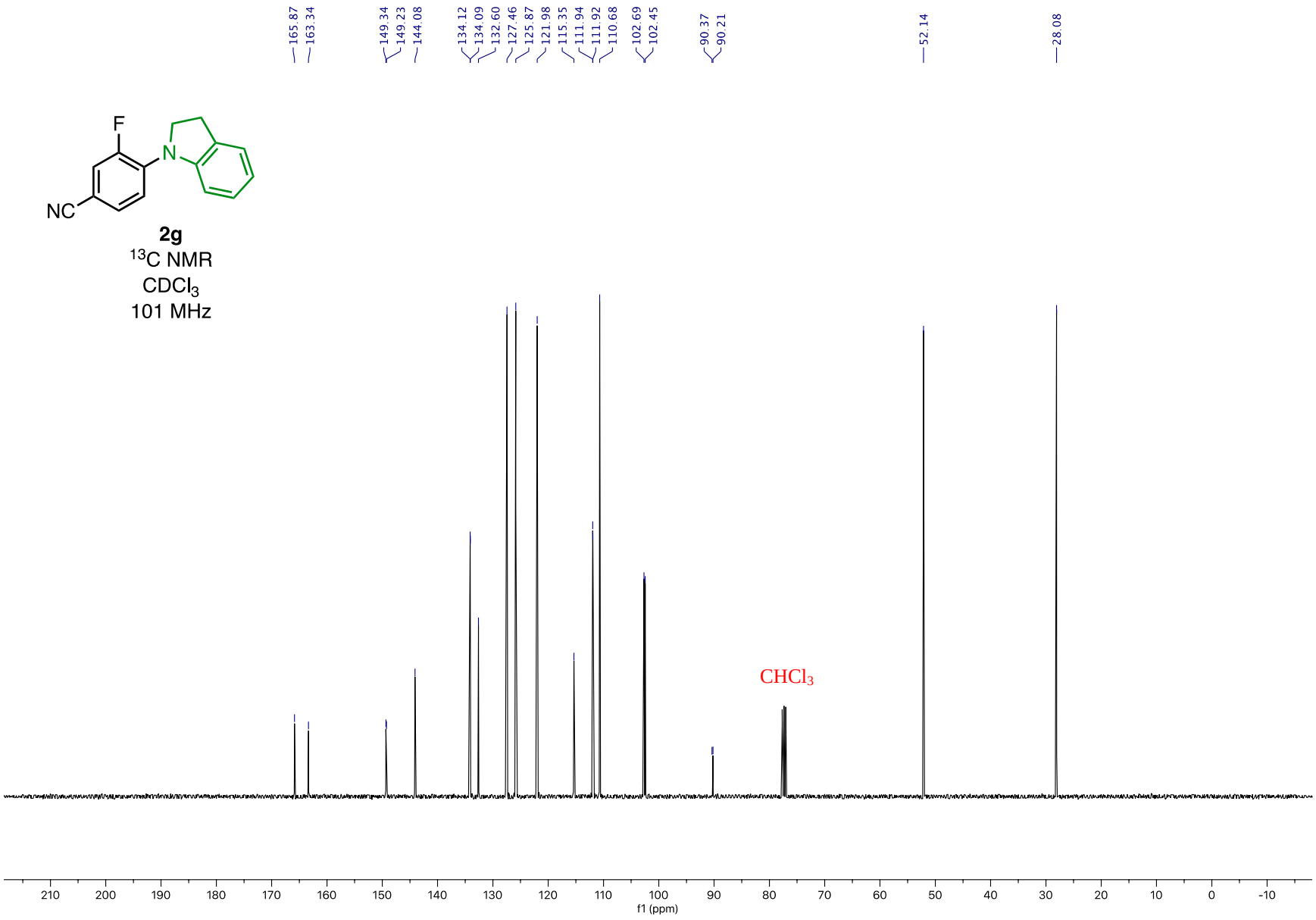
^{19}F NMR

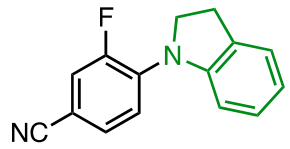
$CDCl_3$

376 MHz



2g
^{1}H NMR
$CDCl_3$
400 MHz


165.87
163.34
149.34
149.23
144.08
134.12
134.09
132.60
127.46
125.87
121.98
115.35
111.94
111.92
110.68
102.69
102.45
90.37
90.21
52.14
28.08
F
N
NC
2g
13C NMR
CDCl3
101 MHz
CHCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

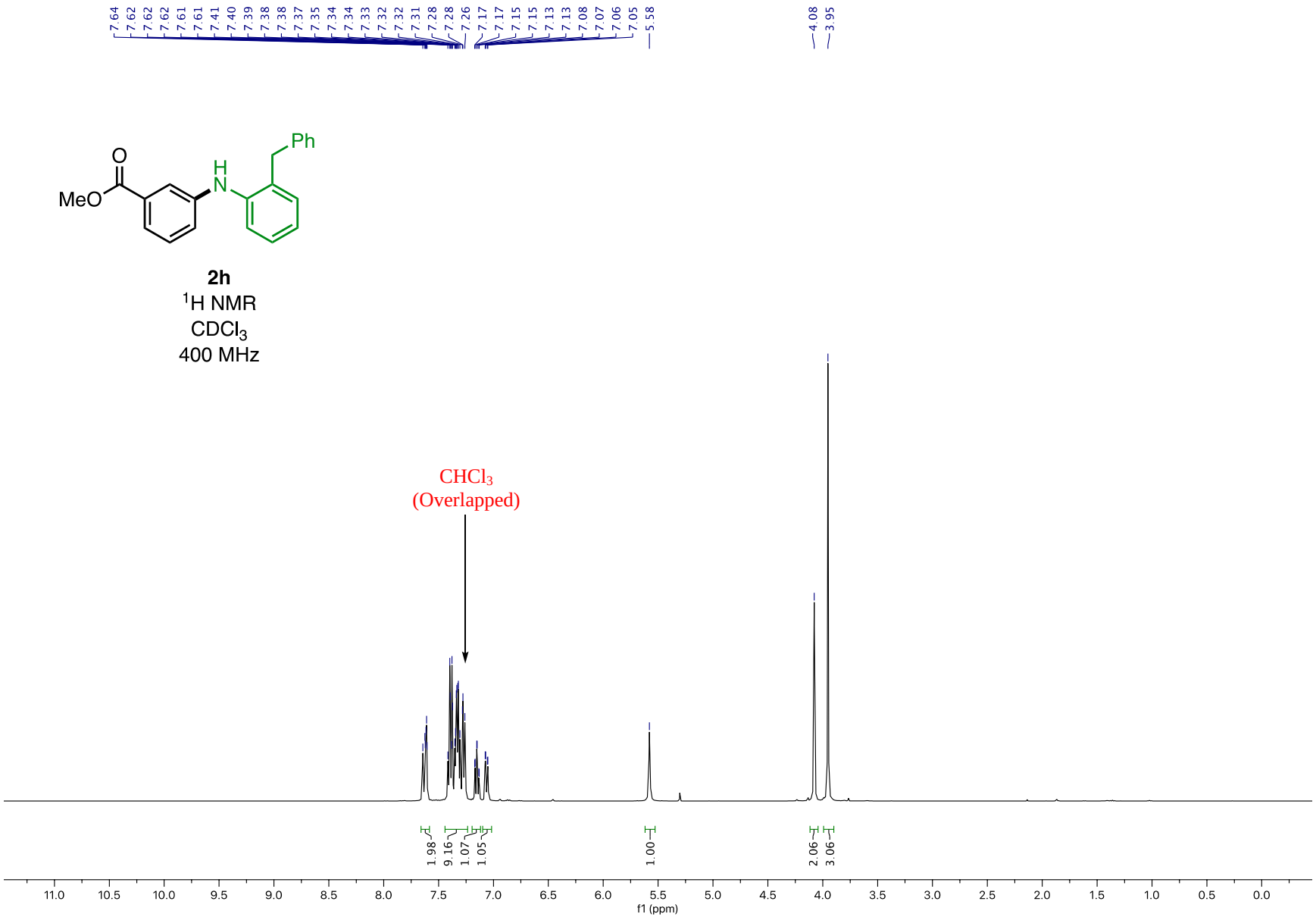


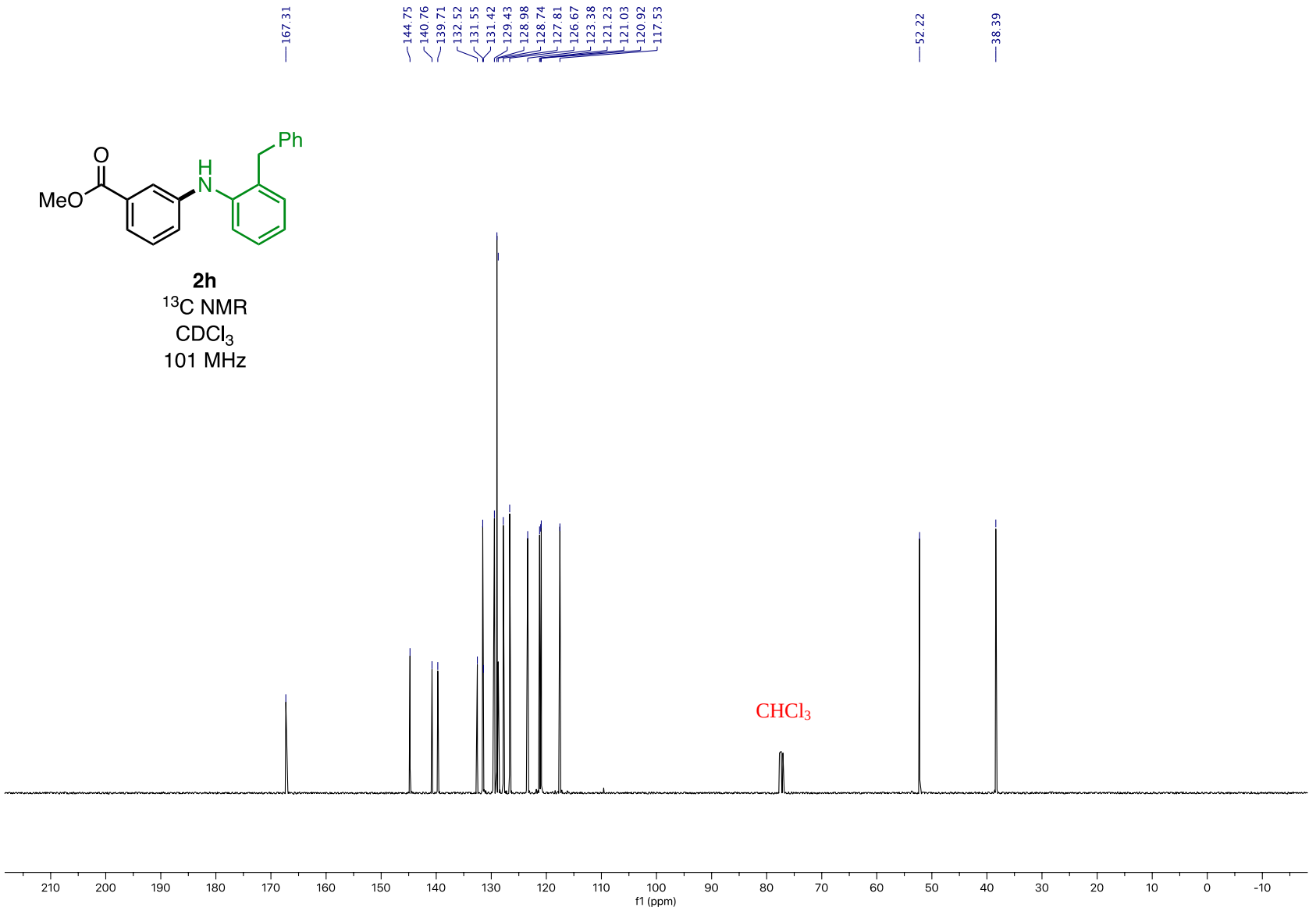
2g

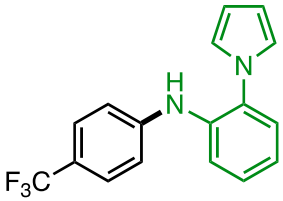
^{19}F NMR

$CDCl_3$

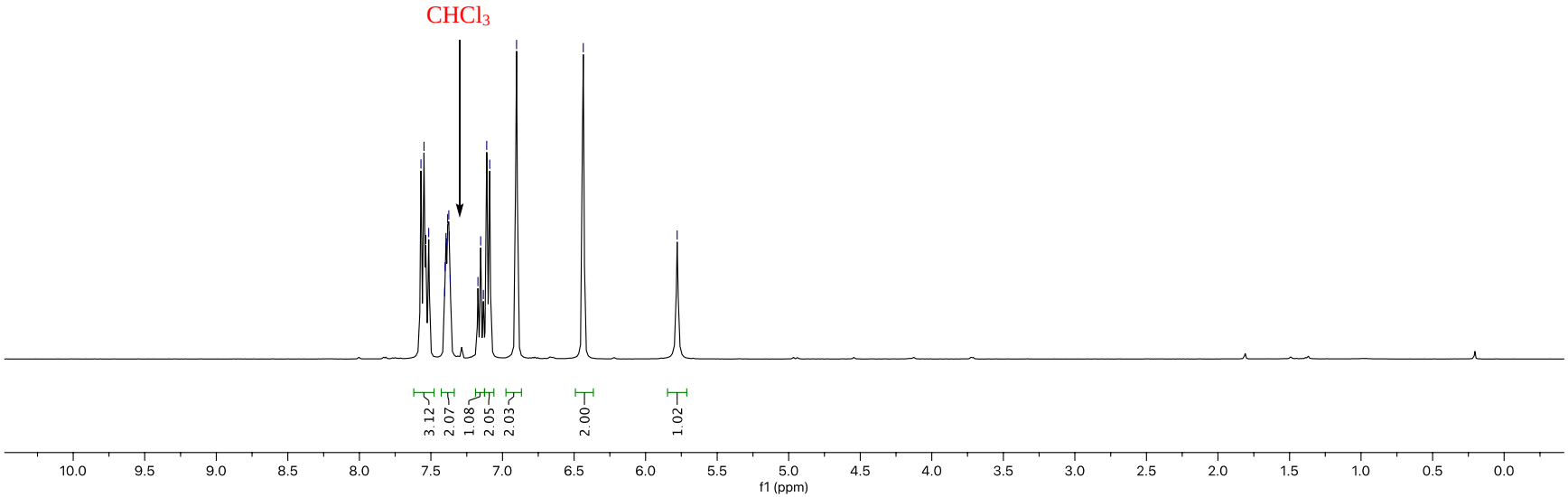
376 MHz

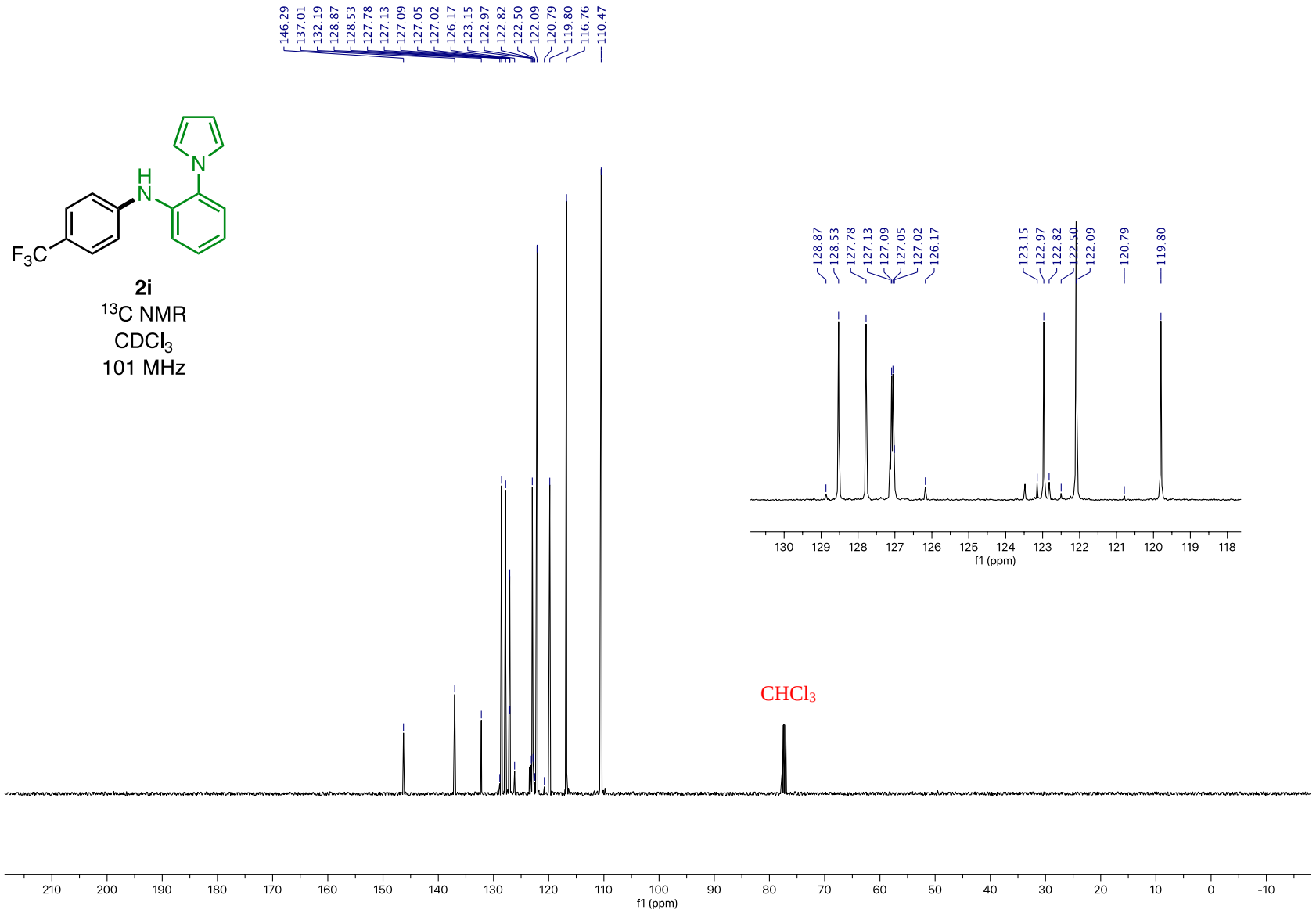

7.64
7.62
7.62
7.62
7.61
7.61
7.41
7.40
7.39
7.38
7.38
7.37
7.35
7.34
7.34
7.33
7.32
7.32
7.31
7.28
7.28
7.26
7.17
7.17
7.15
7.15
7.13
7.13
7.08
7.07
7.06
7.05
5.58
4.08
3.95
O
MeO
H
N
Ph
2h
1H NMR
CDCl3
400 MHz
CHCl3
(Overlapped)
1.98
9.16
1.07
1.05
1.00
2.06
3.06
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
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
f1 (ppm)

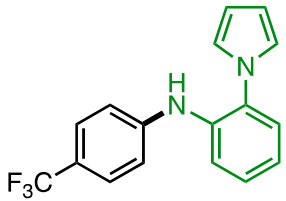

167.31
144.75
140.76
139.71
132.52
131.55
131.42
129.43
128.98
128.74
127.81
126.67
123.38
121.23
121.03
120.92
117.53
52.22
38.39
Ph
H
N
O
MeO
2h
13C NMR
CDCl3
101 MHz
CHCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



2i
^{1}H NMR
$CDCl_3$
400 MHz




146.29
137.01
132.19
128.87
128.53
127.78
127.13
127.09
127.05
127.02
126.17
123.15
122.97
122.82
122.50
122.09
120.79
119.80
116.76
110.47
F3C
H
N
N
2i
13C NMR
CDCl3
101 MHz
CHCl3
f1 (ppm)

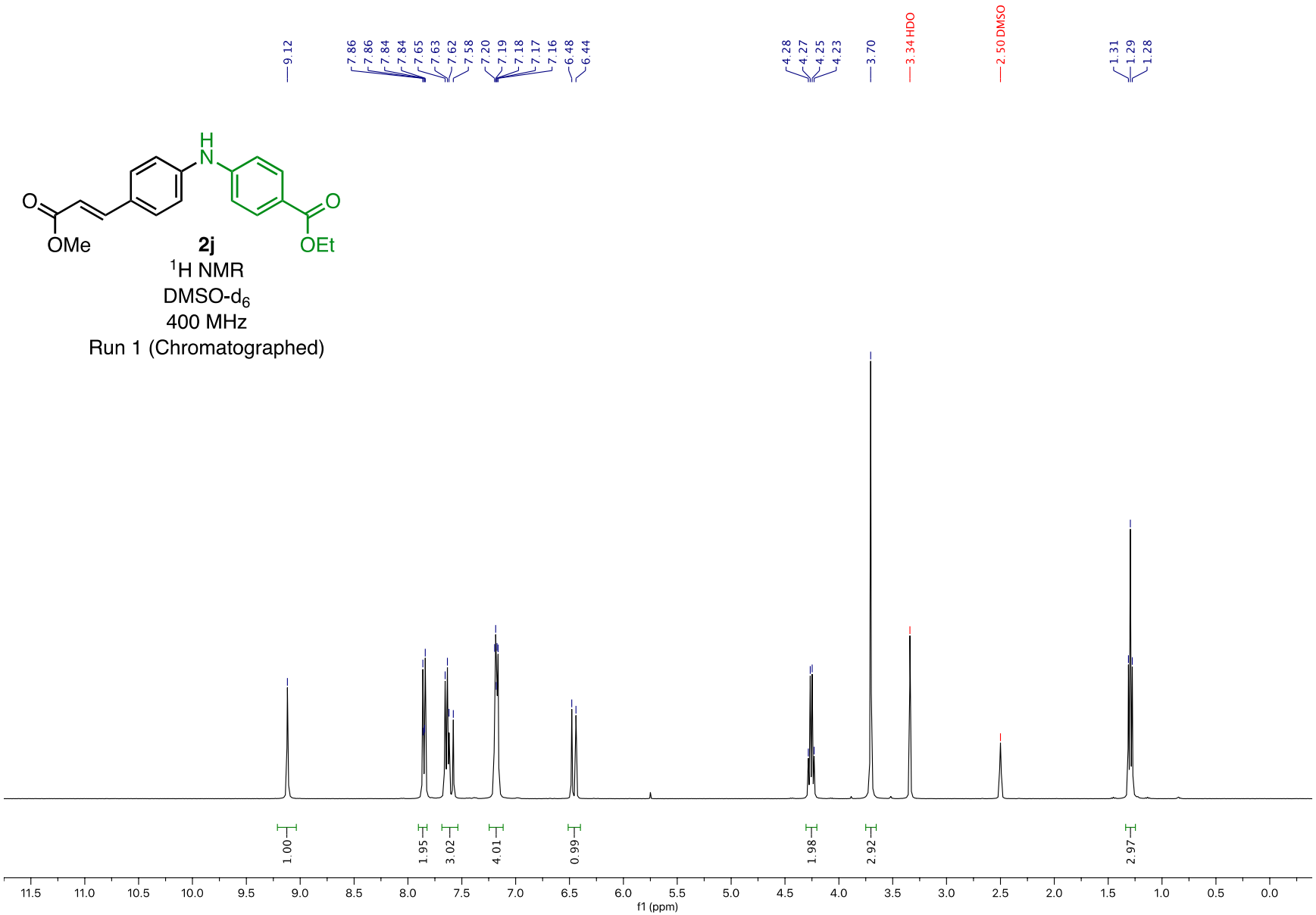


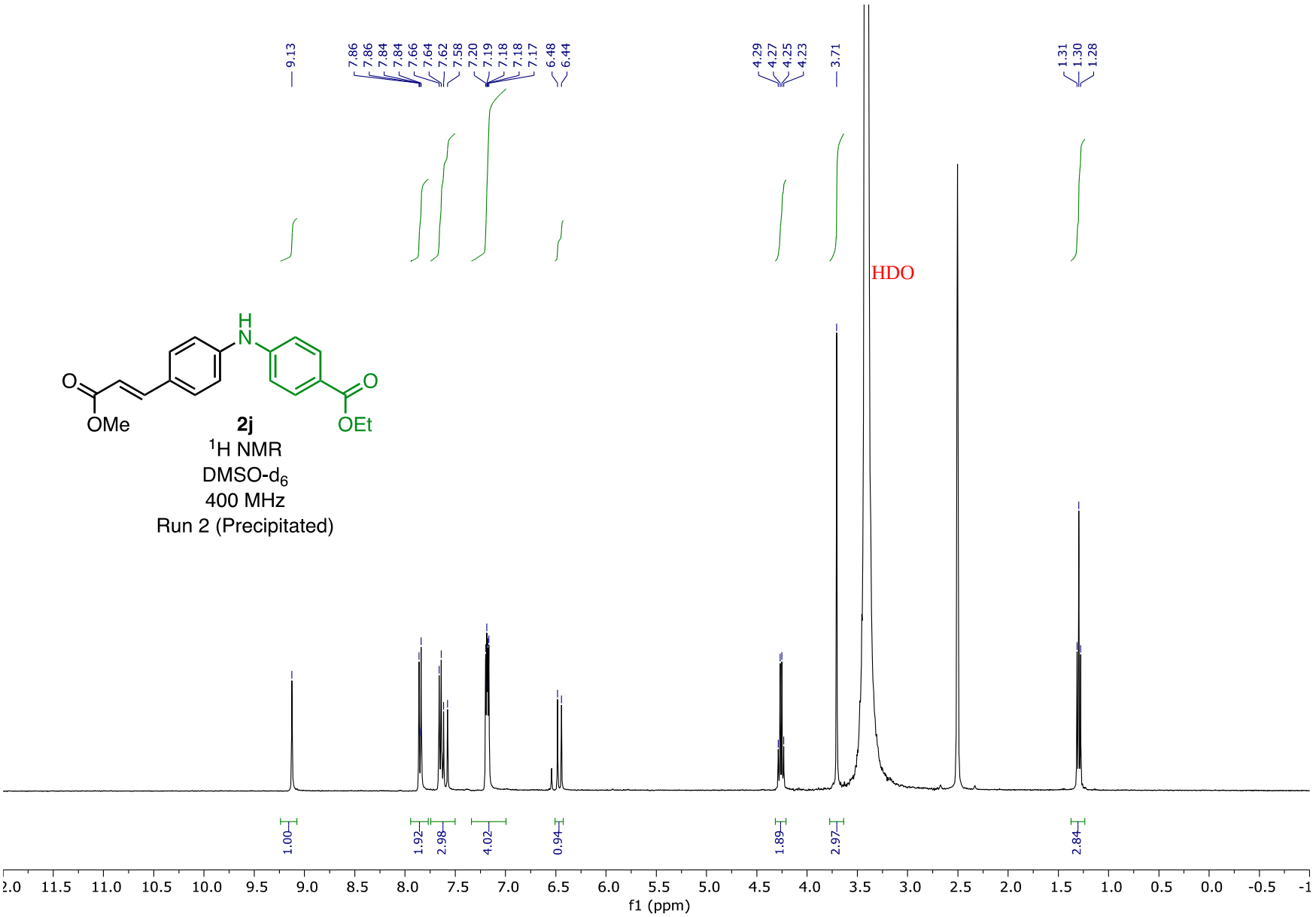
2i

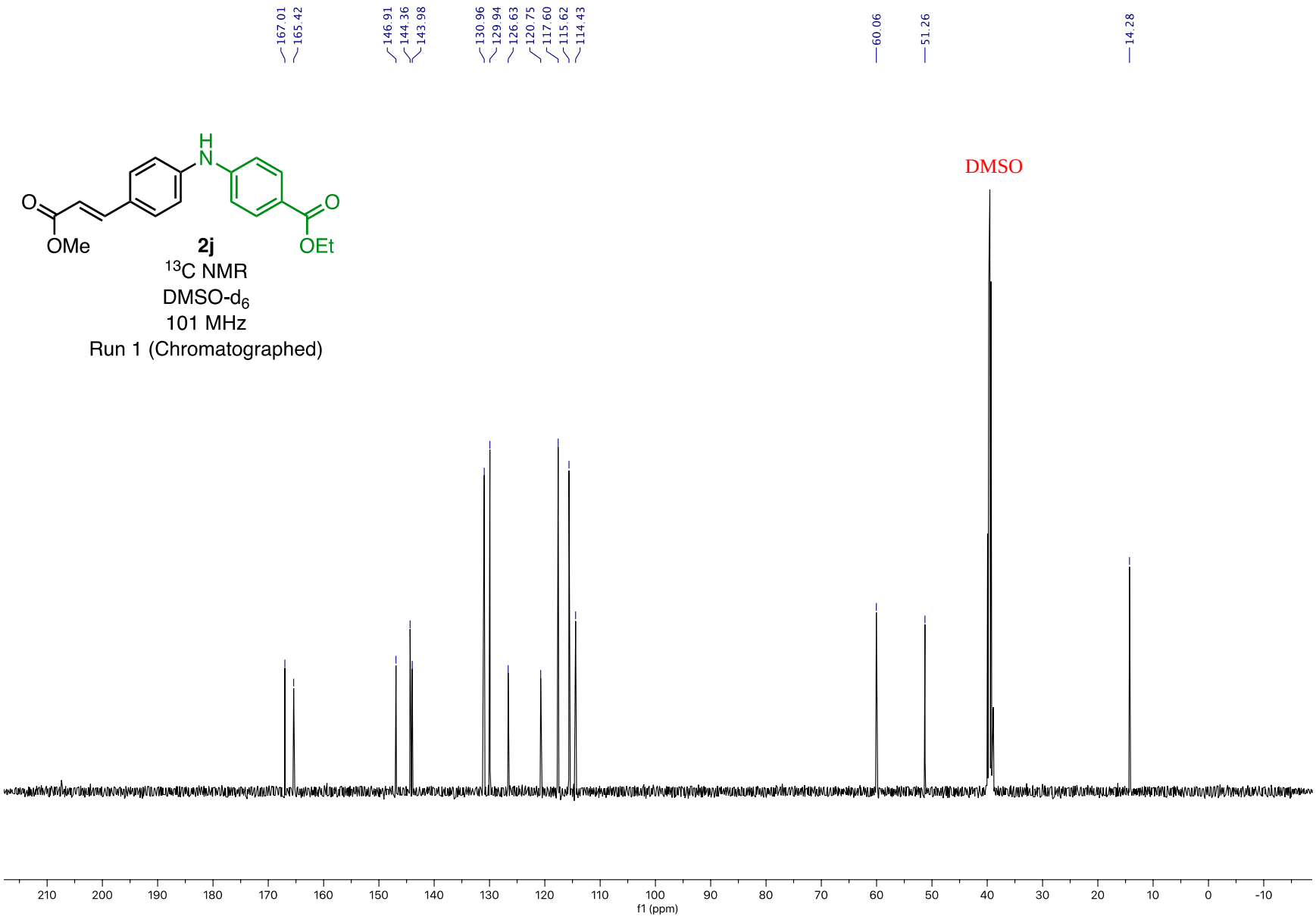
^{19}F NMR

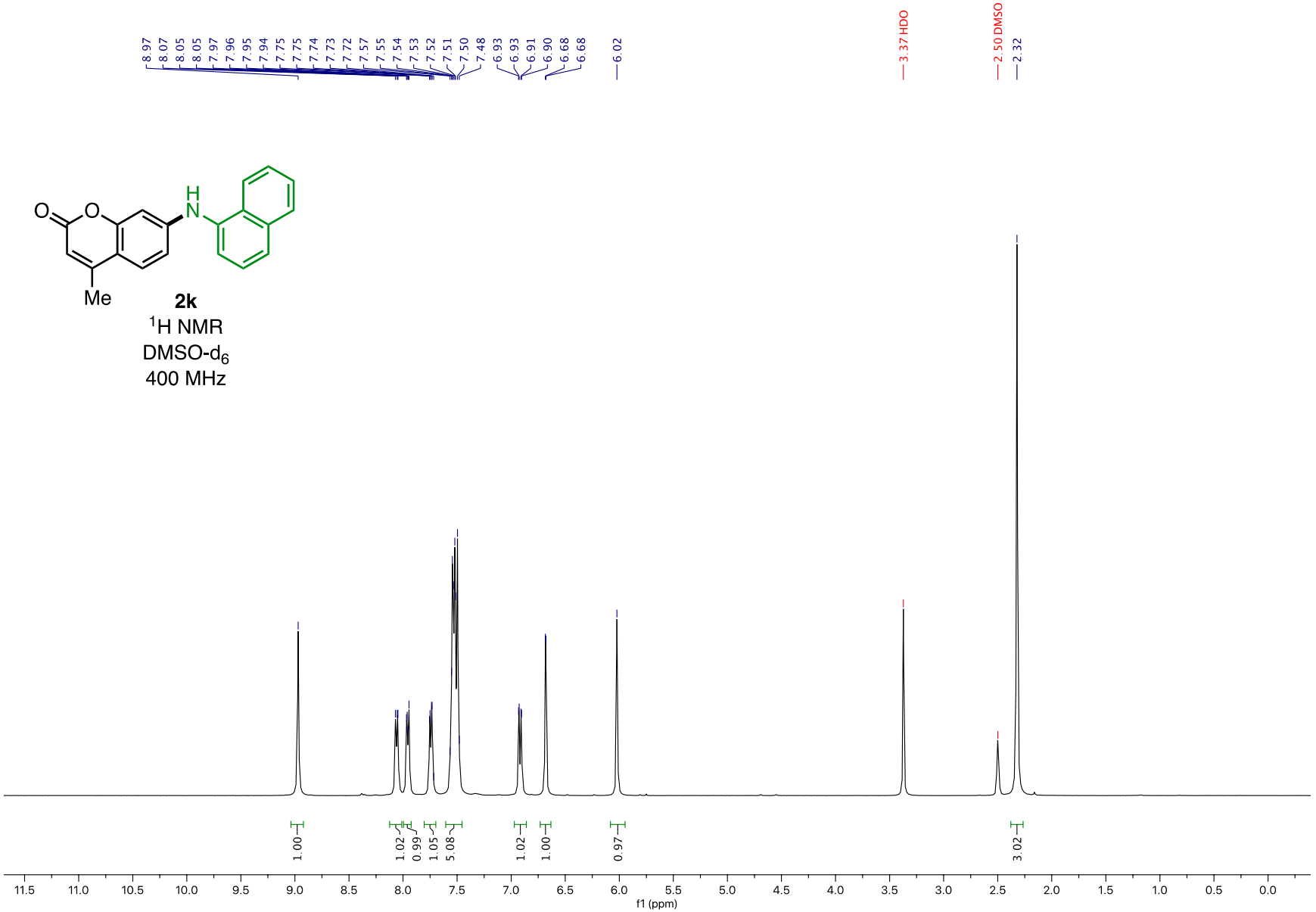
$CDCl_3$

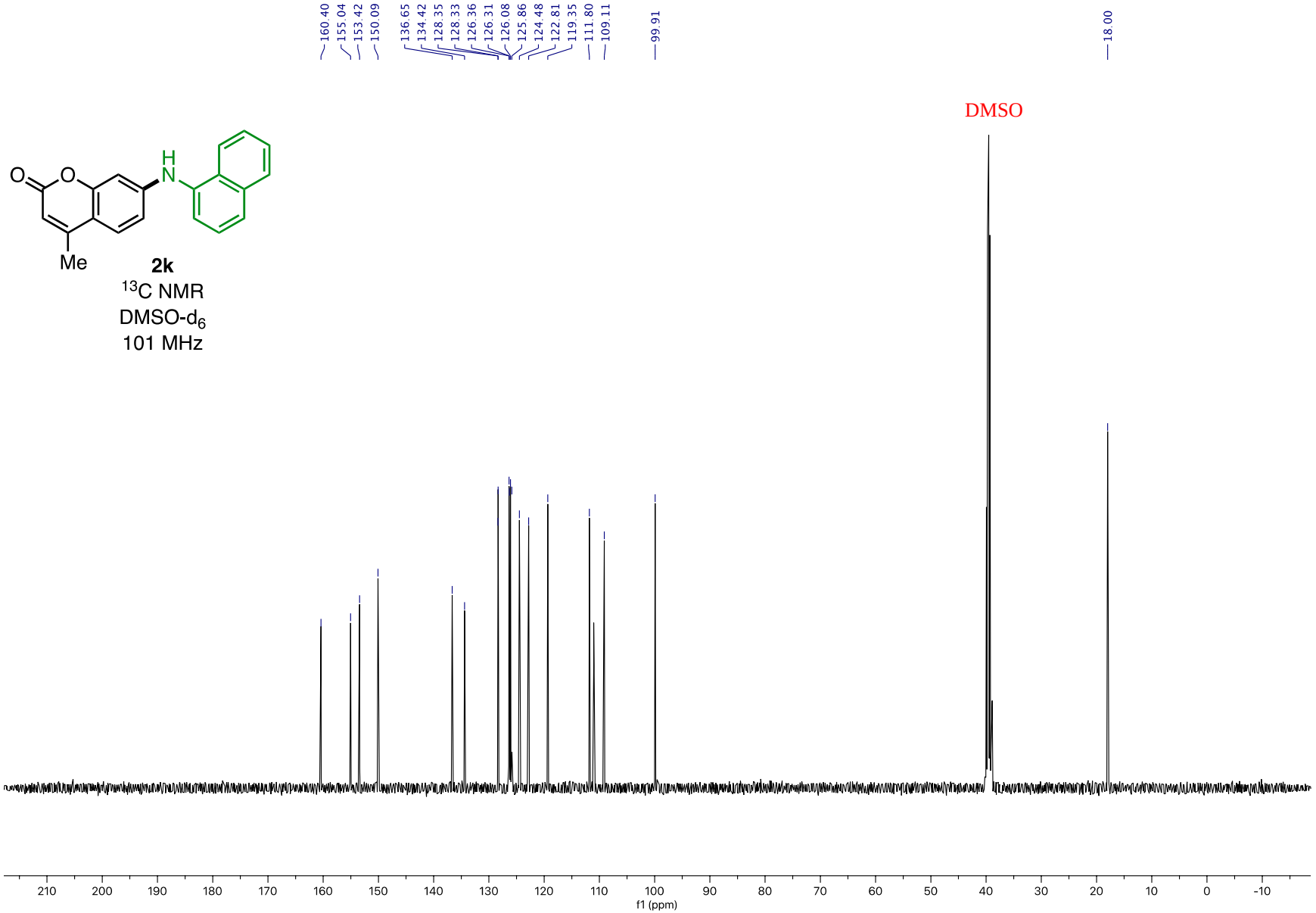
376 MHz

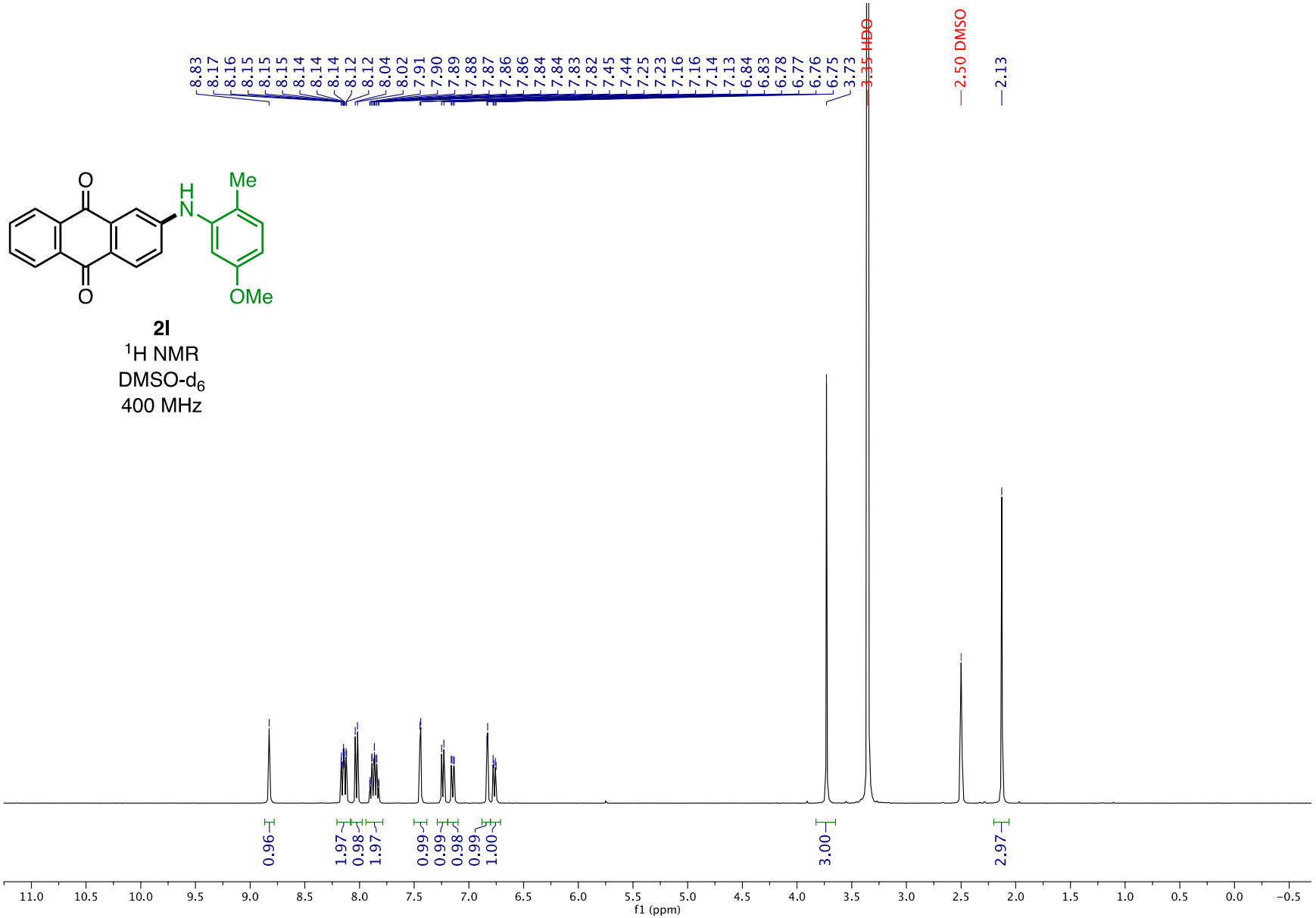

9.12
7.86
7.86
7.84
7.84
7.65
7.63
7.62
7.58
7.20
7.19
7.18
7.17
7.16
6.48
6.44
4.28
4.27
4.25
4.23
3.70
3.34 HDO
2.50 DMSO
1.31
1.29
1.28
H
N
O
OMe
O
OEt
2j
1H NMR
DMSO-d6
400 MHz
Run 1 (Chromatographed)
1.00
1.95
3.02
4.01
0.99
1.98
2.92
2.97
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

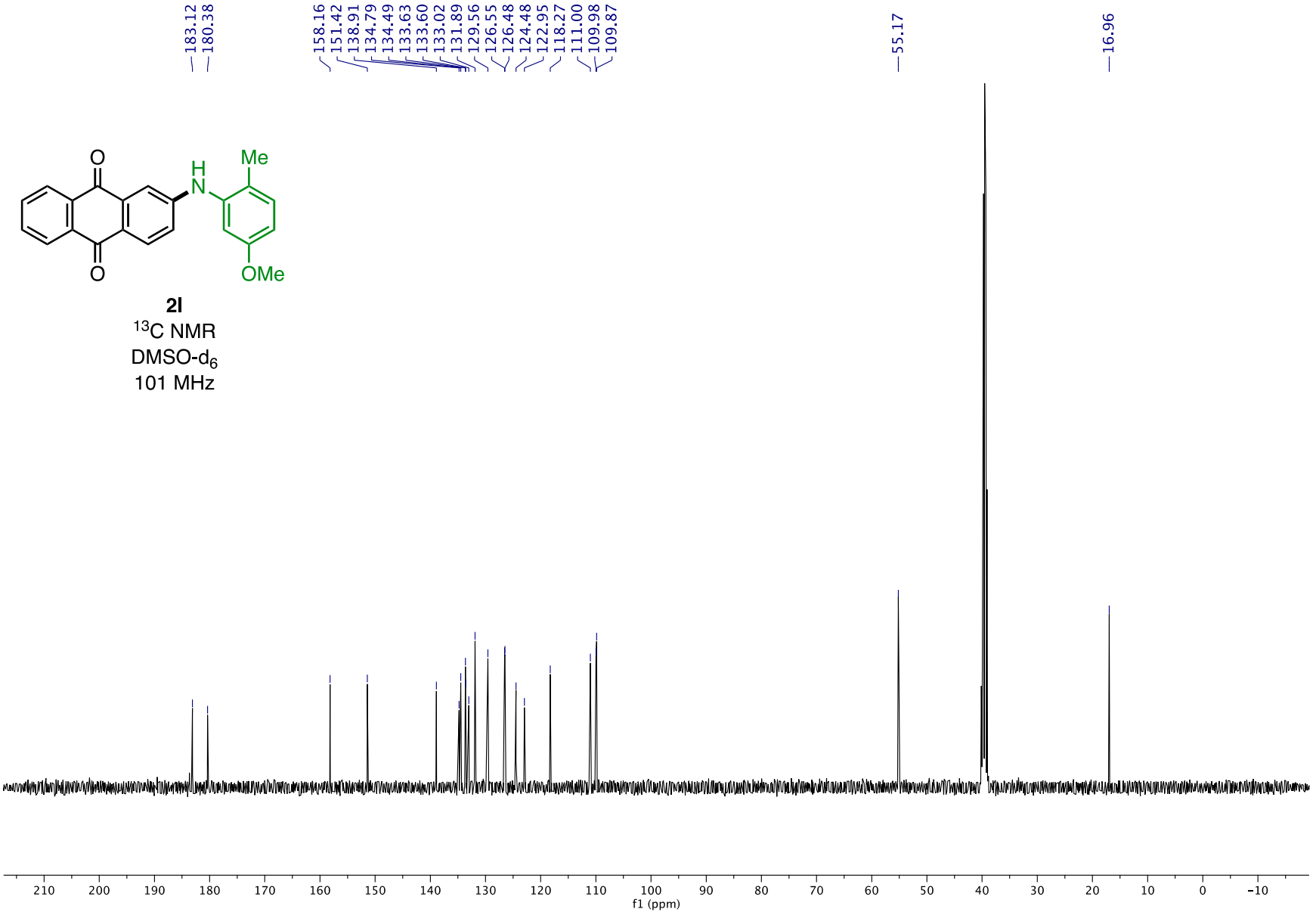

9.13
7.86
7.86
7.84
7.84
7.66
7.64
7.62
7.58
7.20
7.19
7.18
7.18
7.17
6.48
6.44
4.29
4.27
4.25
4.23
3.71
1.31
1.30
1.28
HDO
O
OMe
H
N
O
OEt
2j
1H NMR
DMSO-d6
400 MHz
Run 2 (Precipitated)
1.00
1.92
2.98
4.02
0.94
1.89
2.97
2.84
f1 (ppm)

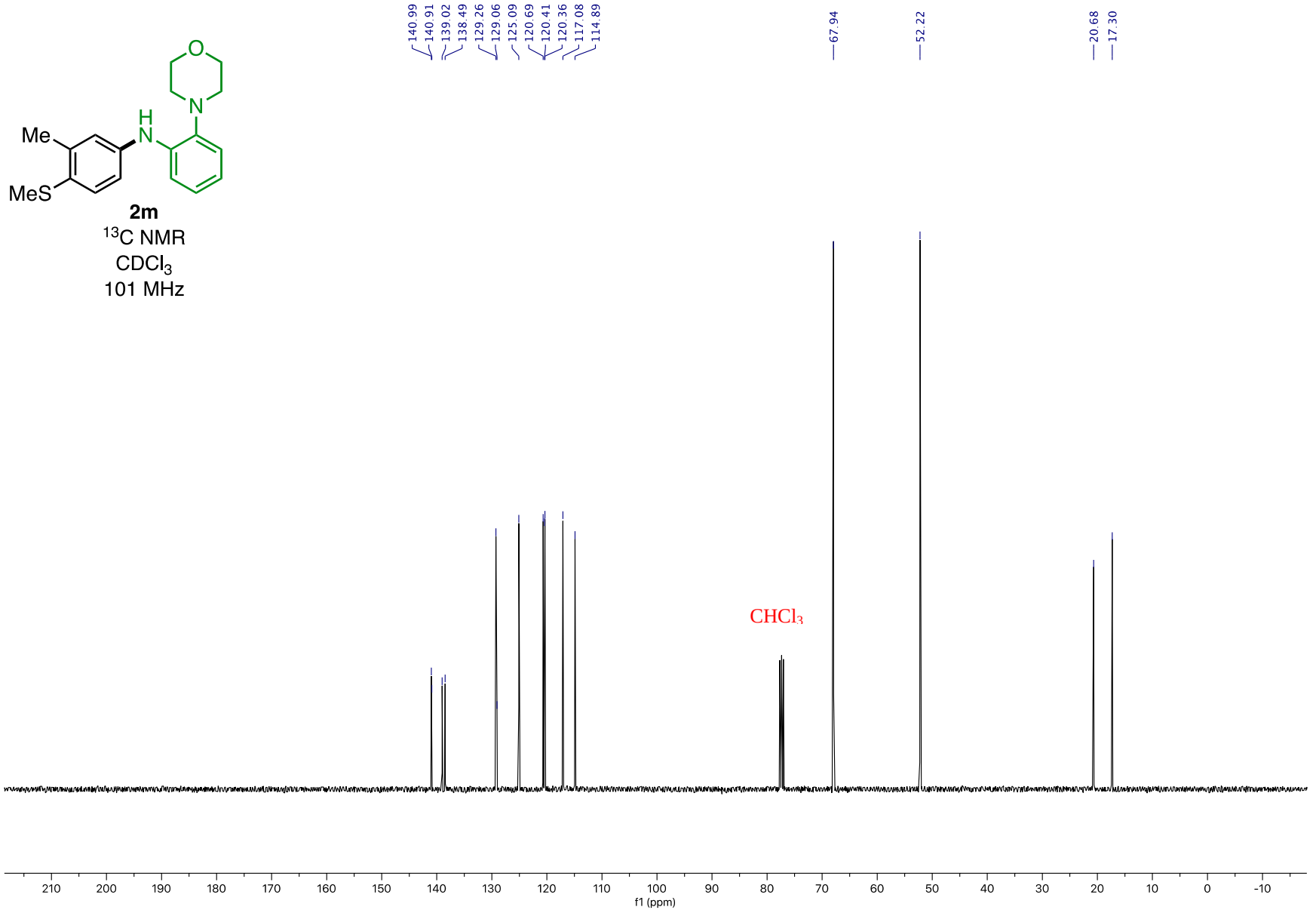

167.01
165.42
146.91
144.36
143.98
130.96
129.94
126.63
120.75
117.60
115.62
114.43
60.06
51.26
14.28
DMSO
H
N
O
OMe
O
OEt
2j
13C NMR
DMSO-d6
101 MHz
Run 1 (Chromatographed)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

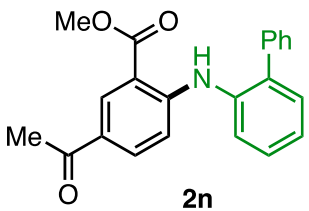

8.97
8.07
8.05
8.05
7.97
7.96
7.95
7.94
7.75
7.75
7.74
7.73
7.72
7.57
7.55
7.54
7.53
7.52
7.51
7.50
7.48
6.93
6.93
6.91
6.90
6.68
6.68
6.02
3.37 HDO
2.50 DMSO
2.32
O
O
H
N
Me
2k
1H NMR
DMSO-d6
400 MHz
1.00
1.02
0.99
1.05
5.08
1.02
1.00
0.97
3.02
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


160.40
155.04
153.42
150.09
136.65
134.42
128.35
128.33
126.36
126.31
126.08
125.86
124.48
122.81
119.35
111.80
109.11
99.91
18.00
DMSO
O
O
H
N
Me
2k
^{13}C NMR
DMSO-d$_6$
101 MHz
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.83
8.17
8.16
8.15
8.15
8.15
8.14
8.14
8.14
8.12
8.12
8.04
8.02
7.91
7.90
7.89
7.88
7.87
7.86
7.86
7.84
7.84
7.83
7.82
7.45
7.44
7.25
7.23
7.16
7.16
7.14
7.13
6.84
6.83
6.78
6.77
6.76
6.75
3.73
3.35 HDO
2.50 DMSO
2.13
O
H
N
Me
O
OMe
2l
1H NMR
DMSO-d6
400 MHz
0.96
1.97
0.98
1.97
0.99
0.99
0.98
0.99
1.00
3.00
2.97
11.0
10.5
10.0
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)


183.12
180.38
158.16
151.42
138.91
134.79
134.49
133.63
133.60
133.02
131.89
129.56
126.55
126.48
124.48
122.95
118.27
111.00
109.98
109.87
55.17
16.96
O
H
N
Me
O
OMe
2l
13C NMR
DMSO-d6
101 MHz
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


Me
MeS
H
N
O
N
2m
13C NMR
CDCl3
101 MHz
140.99
140.91
139.02
138.49
129.26
129.06
125.09
120.69
120.41
120.36
117.08
114.89
67.94
52.22
20.68
17.30
CHCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

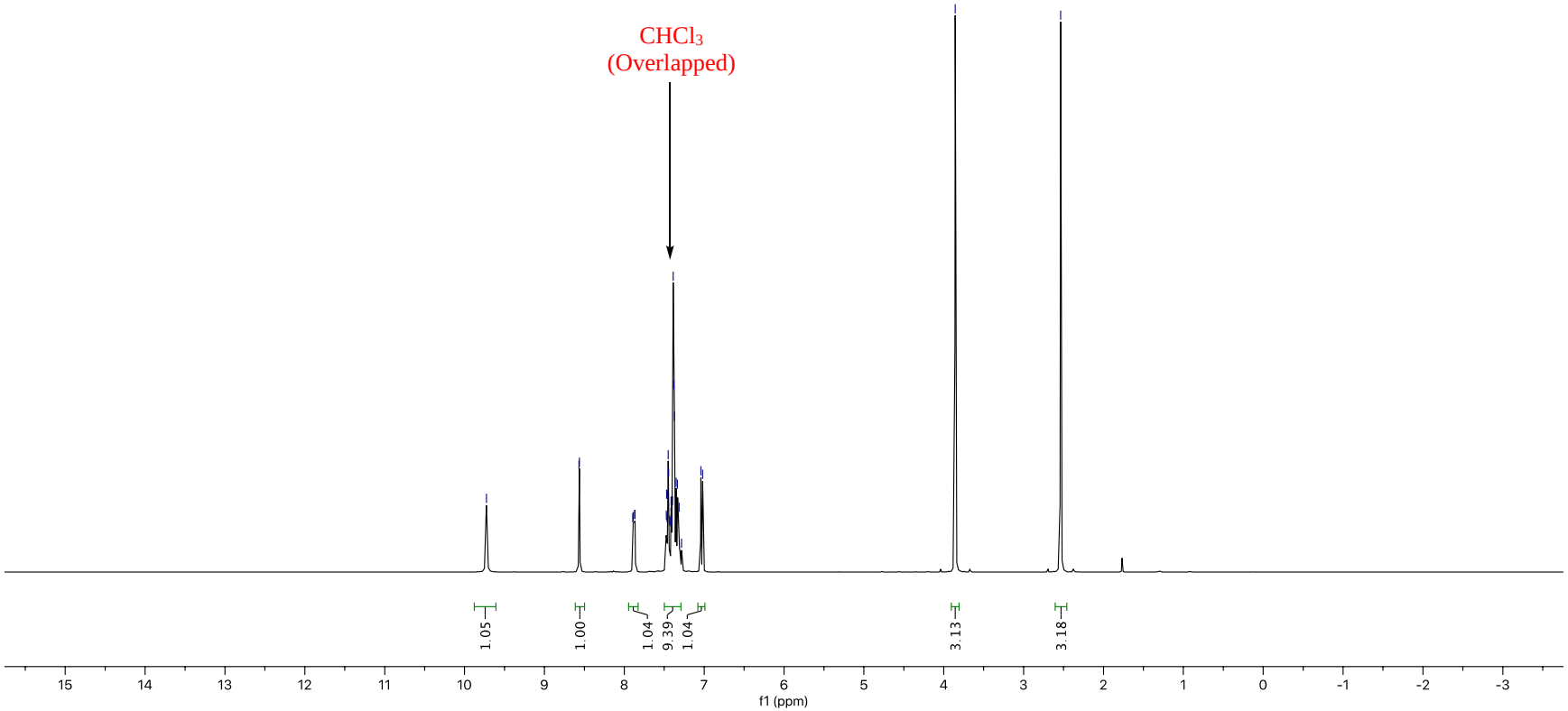


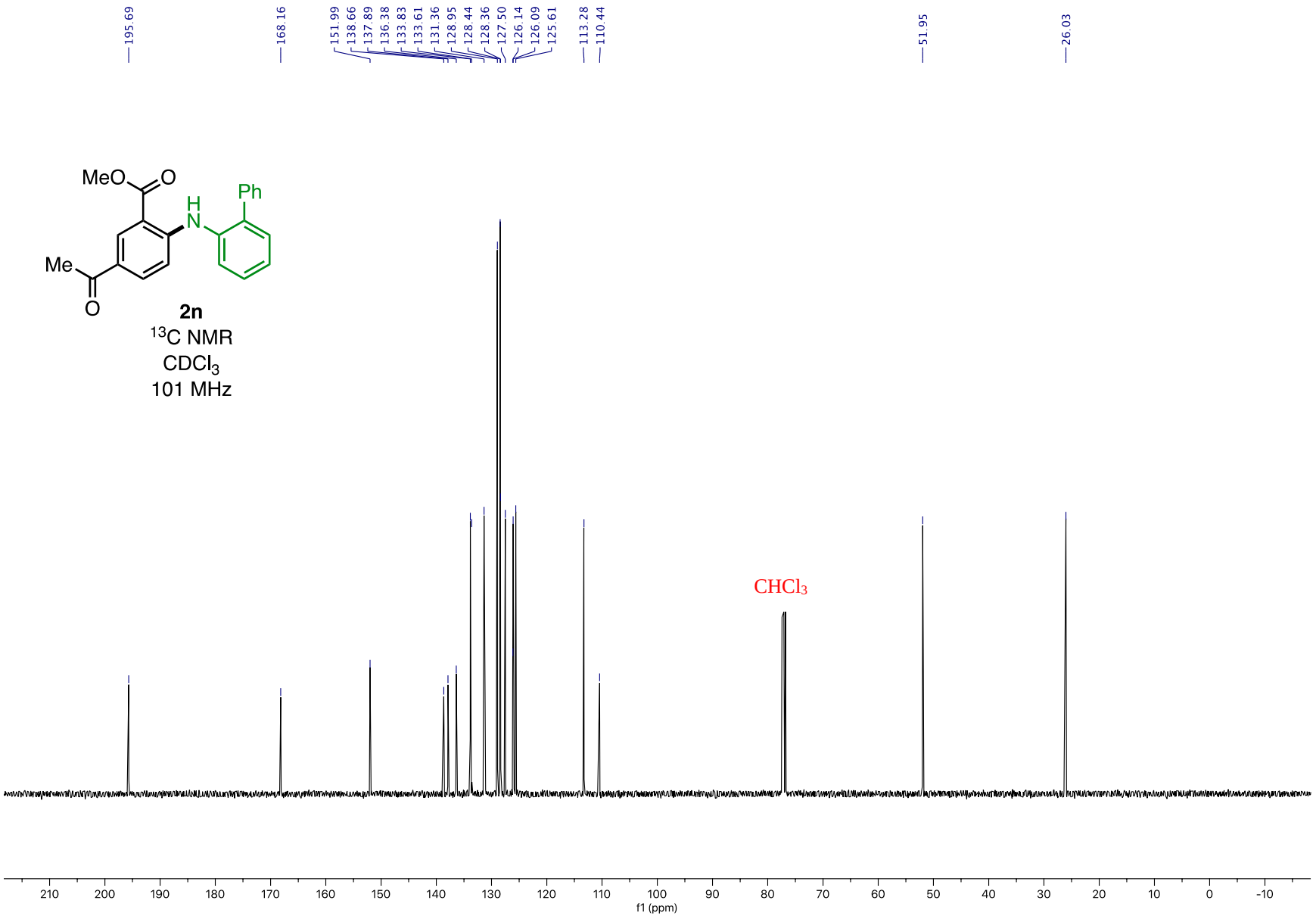
2n

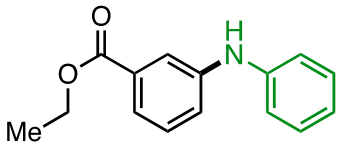
^{1}H NMR

$CDCl_3$

400 MHz




195.69
168.16
151.99
138.66
137.89
136.38
133.83
133.61
131.36
128.95
128.44
128.36
127.50
126.14
126.09
125.61
113.28
110.44
51.95
26.03
MeO
O
H
N
Ph
Me
O
2n
13C NMR
CDCl3
101 MHz
CHCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

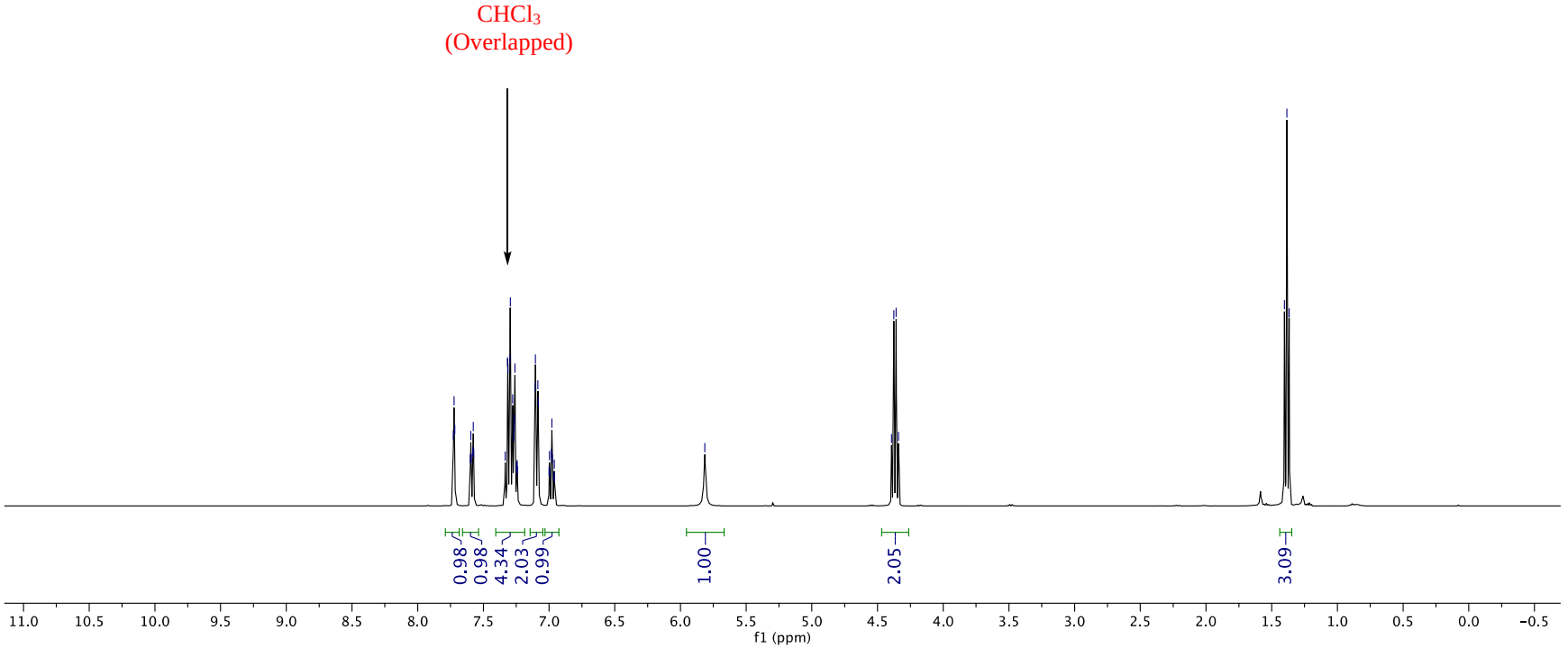


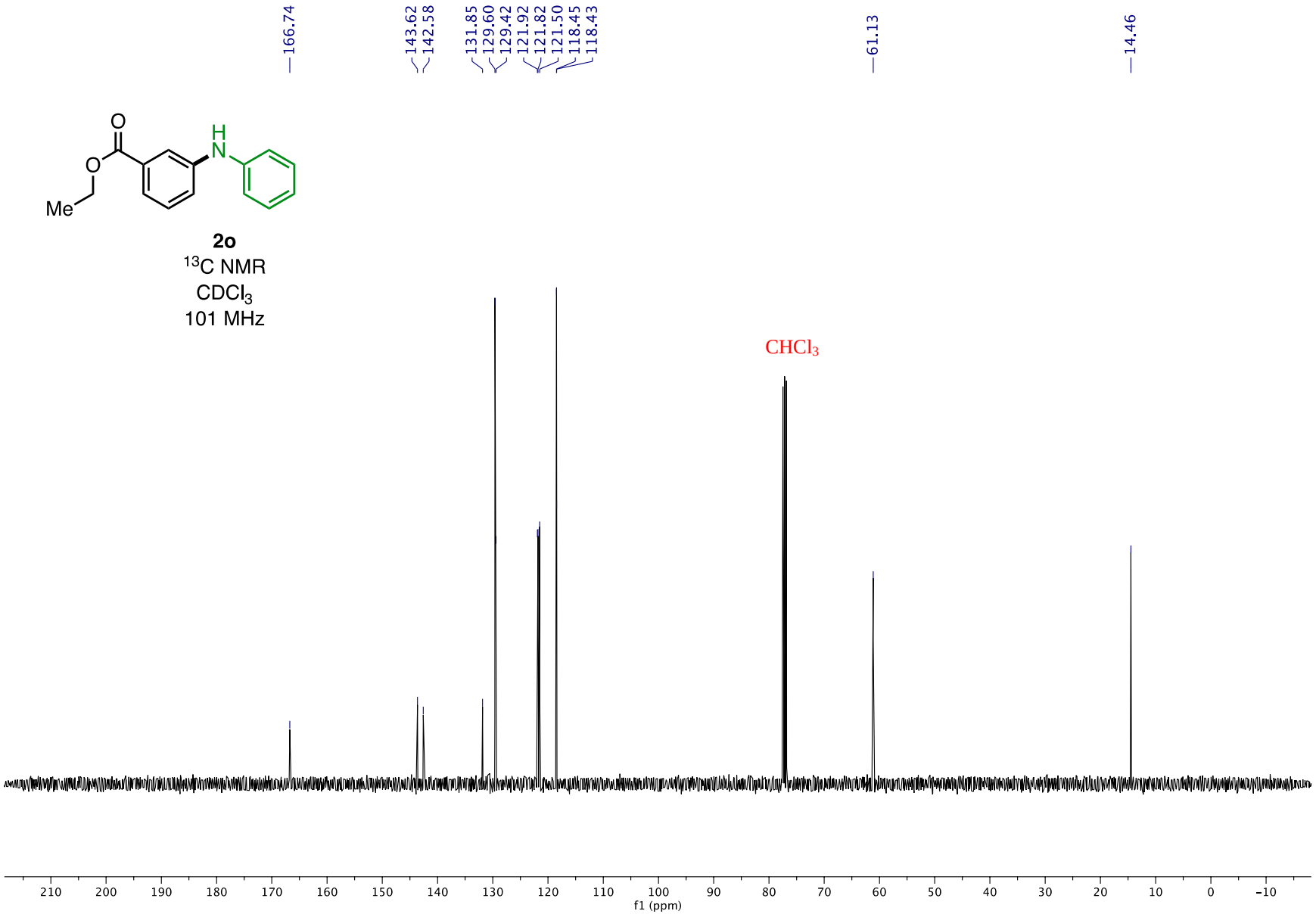
2o

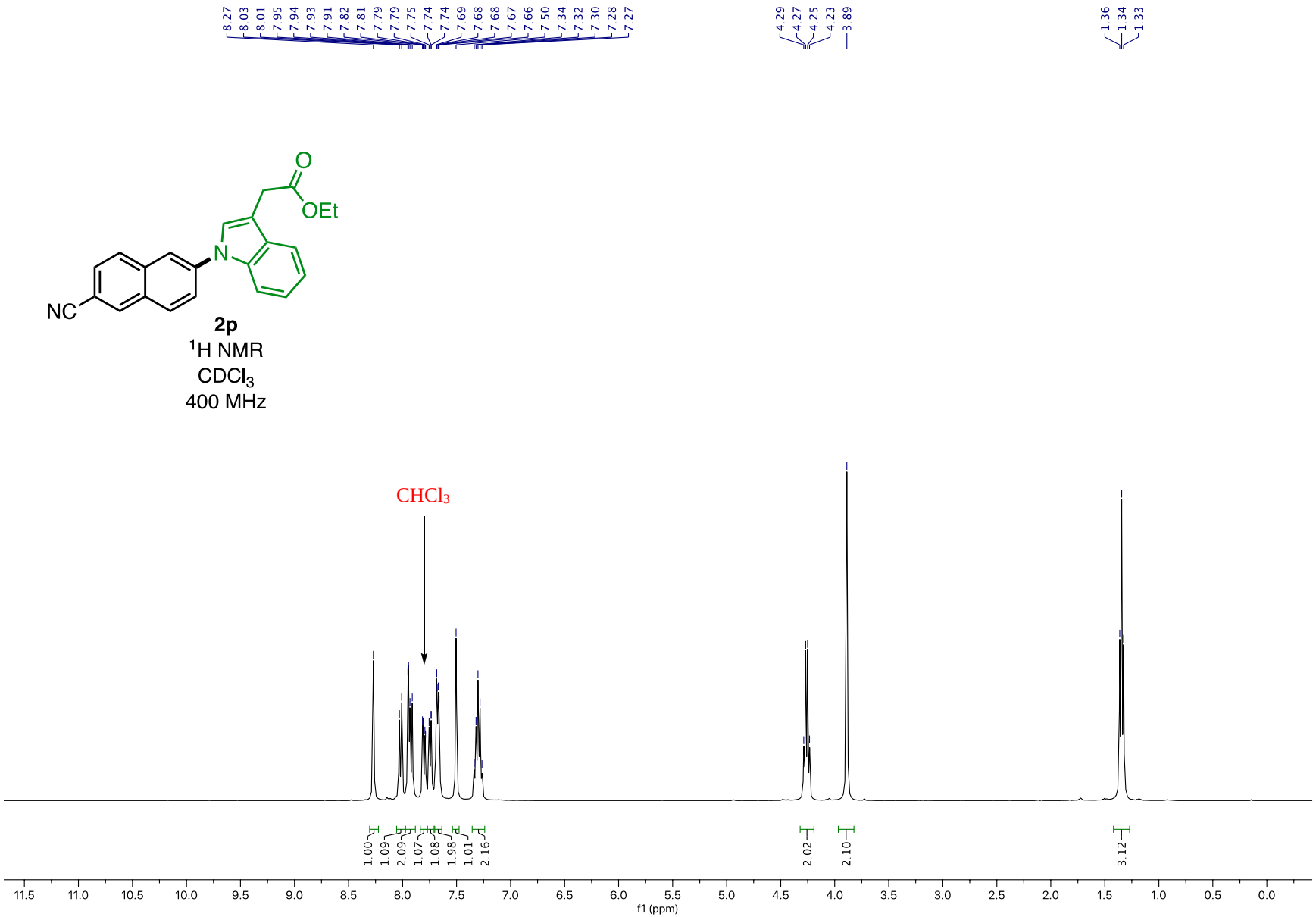
^{1}H NMR

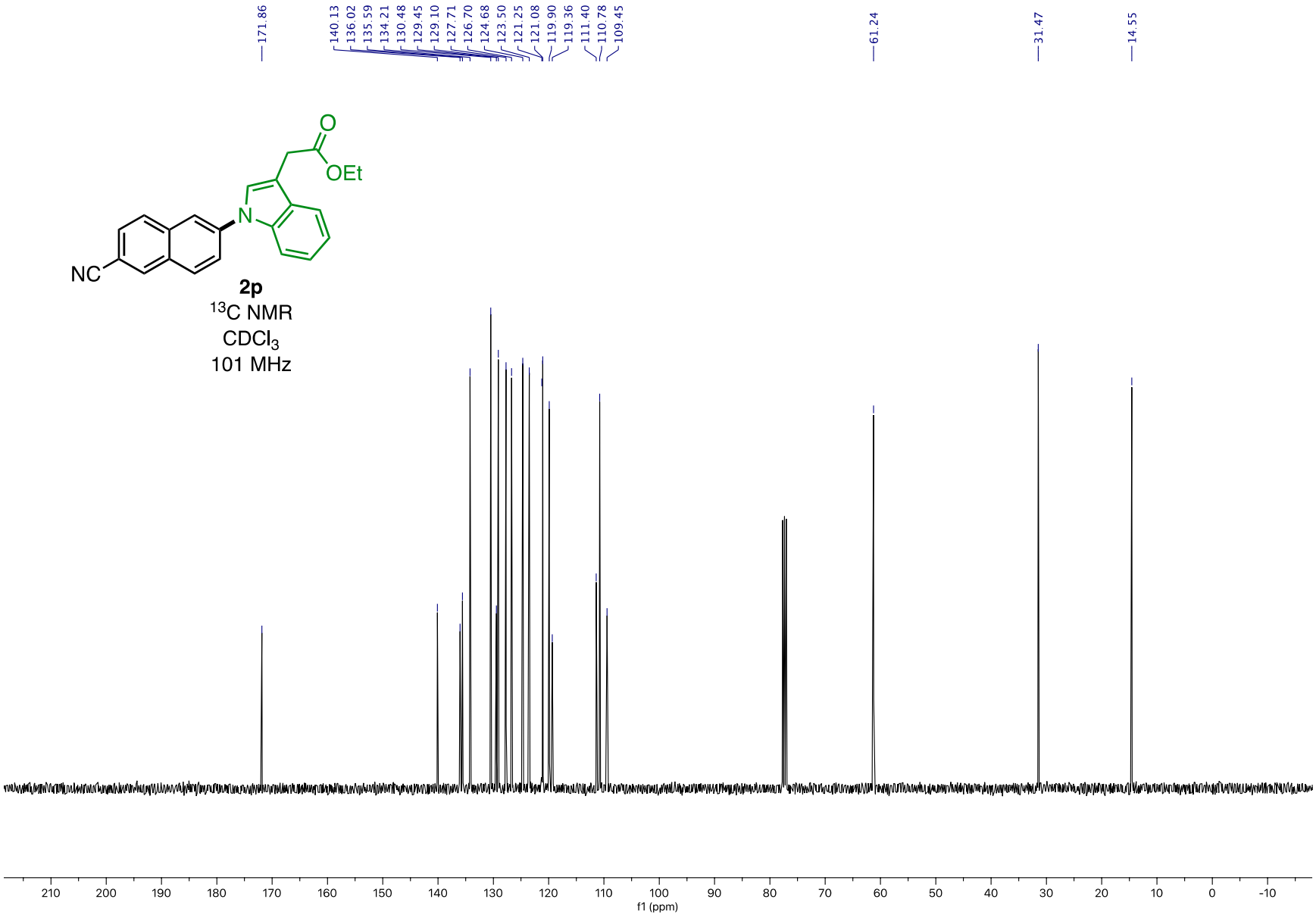
$CDCl_3$

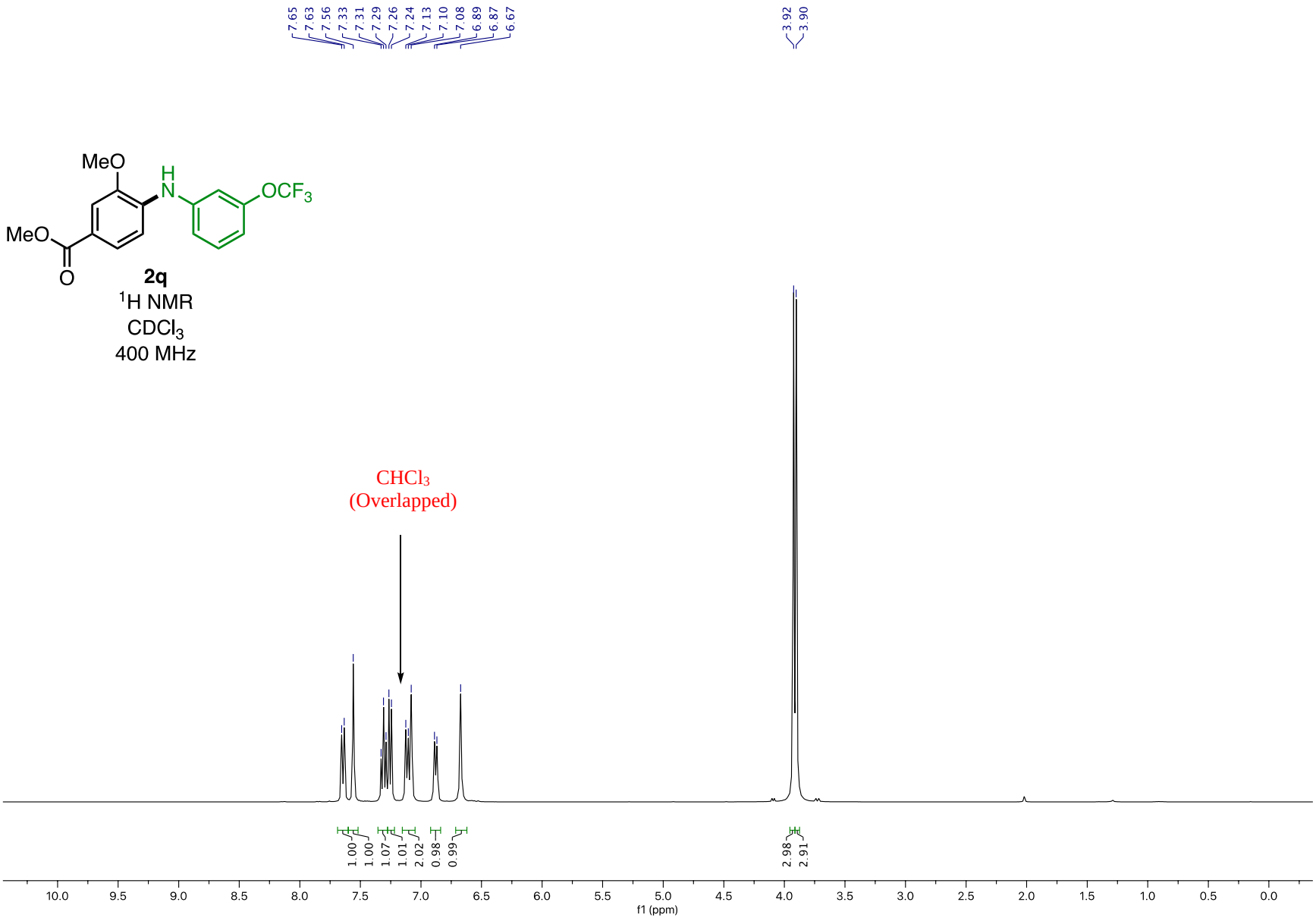
400 MHz

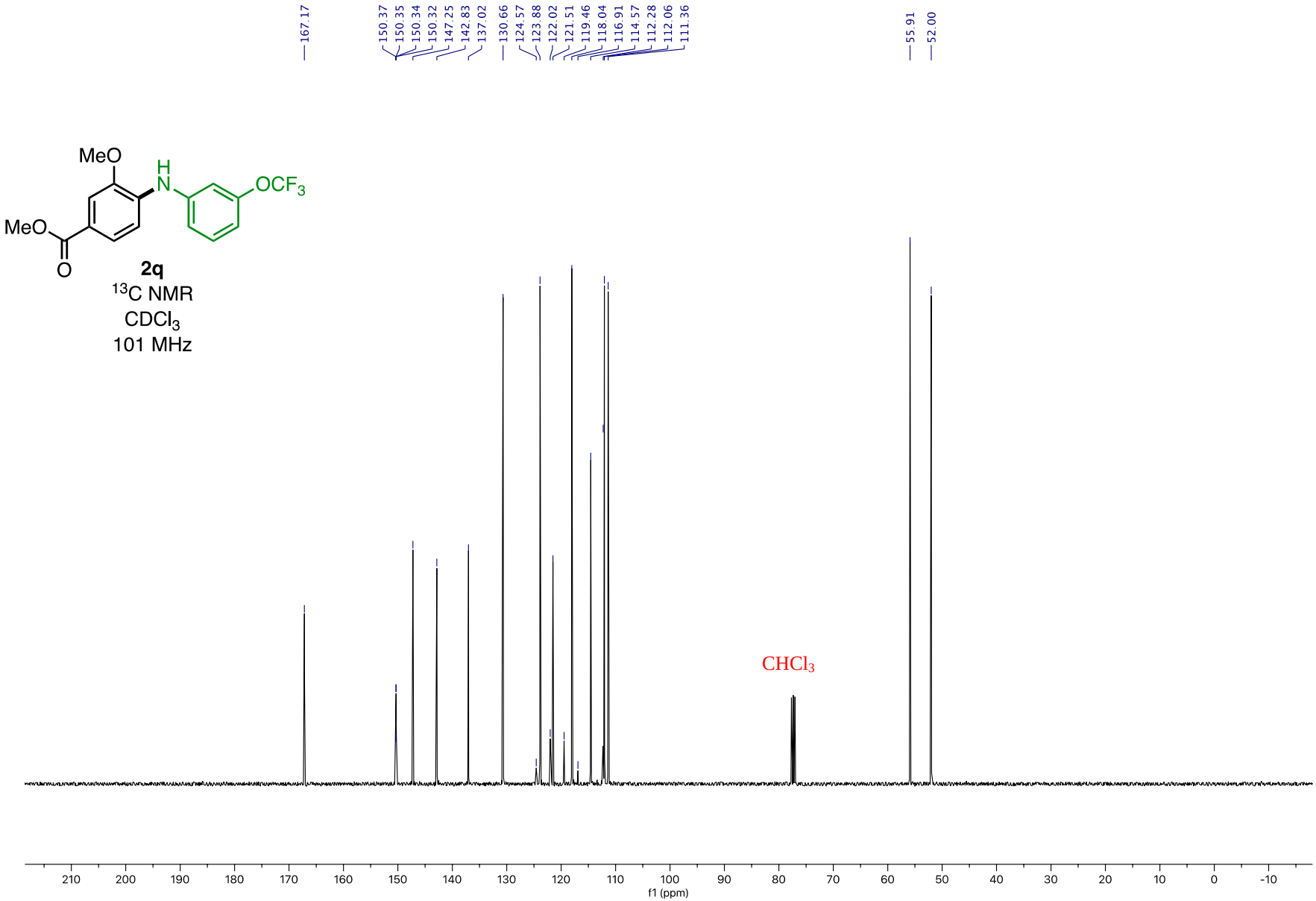


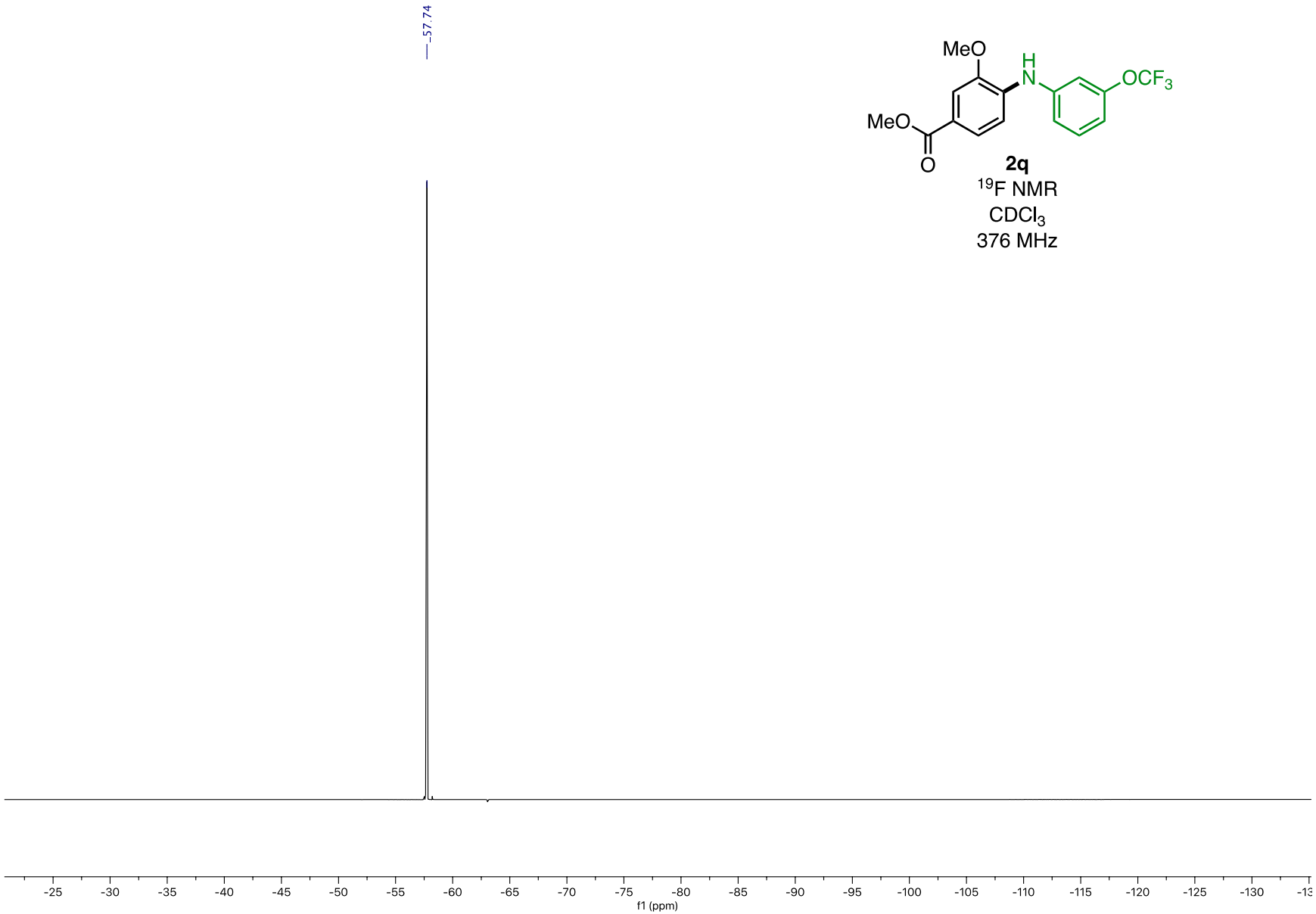

166.74
143.62
142.58
131.85
129.60
129.42
121.92
121.82
121.50
118.45
118.43
61.13
14.46
O
O
H
N
Me
2o
13C NMR
CDCl3
101 MHz
CHCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

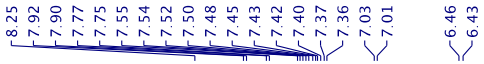

8.27
8.03
8.01
7.95
7.94
7.93
7.91
7.82
7.81
7.79
7.79
7.75
7.74
7.74
7.69
7.68
7.68
7.67
7.66
7.50
7.34
7.32
7.30
7.28
7.27
4.29
4.27
4.25
4.23
3.89
1.36
1.34
1.33
O
OEt
N
NC
2p
1H NMR
CDCl3
400 MHz
CHCl3
1.00
1.09
2.09
1.07
1.08
1.98
1.01
2.16
2.02
2.10
3.12
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
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
f1 (ppm)

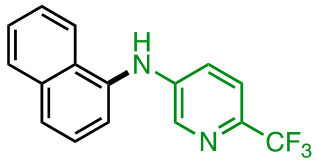

171.86
140.13
136.02
135.59
134.21
130.48
129.45
129.10
127.71
126.70
124.68
123.50
121.25
121.08
119.90
119.36
111.40
110.78
109.45
61.24
31.47
14.55
O
OEt
N
NC
2p
13C NMR
CDCl3
101 MHz
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.65
7.63
7.56
7.33
7.31
7.29
7.26
7.24
7.13
7.10
7.08
6.89
6.87
6.67
3.92
3.90
MeO
H
N
OCF3
MeO
O
2q
1H NMR
CDCl3
400 MHz
CHCl3
(Overlapped)
1.00
1.00
1.07
1.01
2.02
0.98
0.99
2.98
2.91
10.0
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
f1 (ppm)

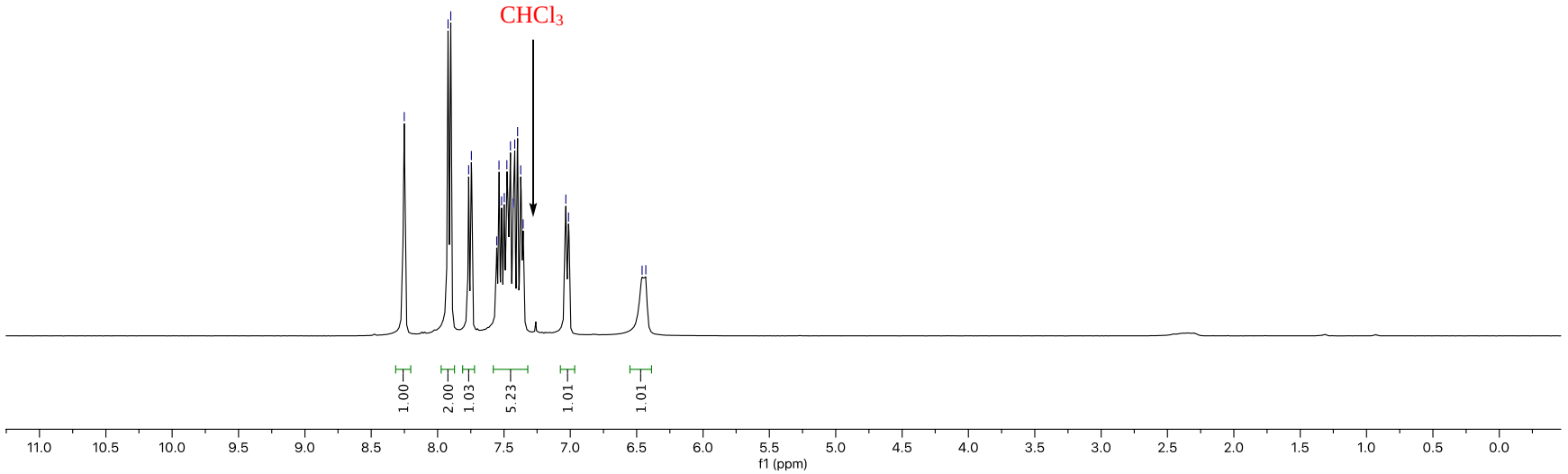

167.17
150.37
150.35
150.34
150.32
147.25
142.83
137.02
130.66
124.57
123.88
122.02
121.51
119.46
118.04
116.91
114.57
112.28
112.06
111.36
55.91
52.00
MeO
MeO
O
H
N
OCF3
2q
13C NMR
CDCl3
101 MHz
CHCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

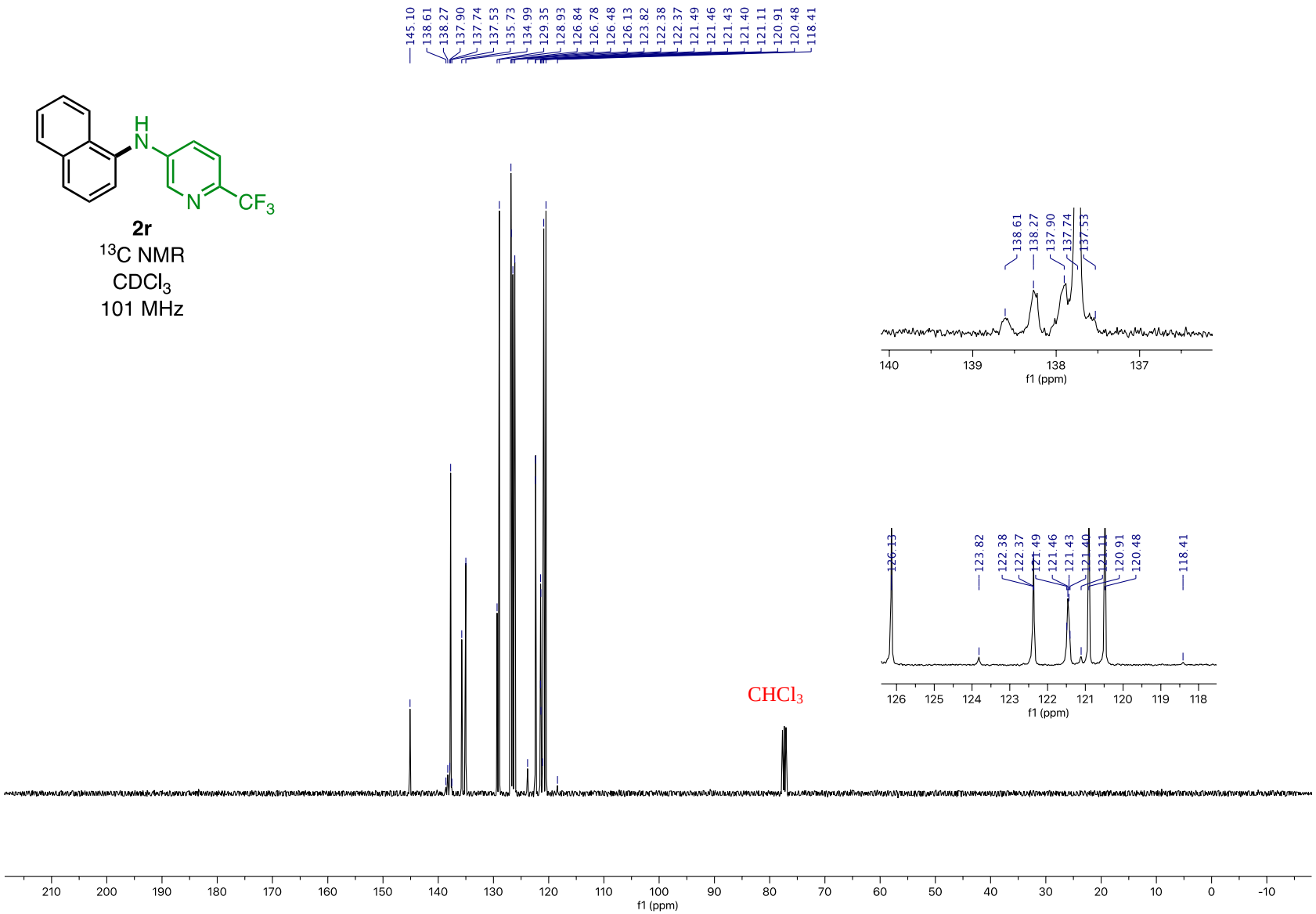

-57.74
MeO
H
N
OCF3
MeO
O
2q
19F NMR
CDCl3
376 MHz
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
f1 (ppm)

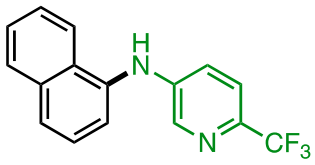




2r
^{1}H NMR
$CDCl_3$
400 MHz




145.10
138.61
138.27
137.90
137.74
137.53
135.73
134.99
129.35
128.93
126.84
126.78
126.48
126.13
123.82
122.38
122.37
121.49
121.46
121.43
121.40
121.11
120.91
120.48
118.41
H
N
N
CF3
2r
13C NMR
CDCl3
101 MHz
CHCl3
f1 (ppm)



2r

^{19}F NMR

$CDCl_3$

376 MHz

Computational Details

All reported calculations were performed using the ORCA software[16] or GAUSSIAN 03[17]. Images of the 3D structures were rendered using CYLView.[18] The geometry of all reactants and transition states were optimized using the B3LYP functional in the gas phase. In these geometry optimizations, a mixed basis set of SDD for Ni and Fe and 6-31G(d) for all other atoms was used. Ground and transition state geometries were validated by vibrational analysis at the same level, showing zero and one imaginary frequencies respectively. Single point energies were calculated using the M06[19,20] functional on a mixed basis set of SDD for Ni and Fe and 6-311+G(d,p) for all other atoms. In these energy calculations, the SMD solvation model[21] with THF as solvent was applied. The reported Gibbs free energies and enthalpies include zero-point and thermal corrections calculated at 298 K using B3LYP/SDD(Ni,Fe)–6-31G(d).

Cartesian Coordinates and Calculated Thermodynamic Parameters for Optimized Structures

```
L3-Ni0 (I)
Charge: 0
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -4986.318881
Gibbs Free Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -4985.879513
Electronic Energy (M06/6-311+G(d,p)-SDD(Ni,Fe)/SMD(THF)): -4985.677839
Total Gibbs Free Energy: -4985.23847
Geometry:
P           1.92103        -0.10137         0.11281
P          -1.91722         0.11321         0.10206
C           1.73253         0.37528        -1.65236
C           2.06103        -0.37918        -2.82906
C           1.14003         1.60989        -2.09712
C           1.68573         0.38318        -3.97294
H           2.49386        -1.37003        -2.84389
C           1.12490         1.61392        -3.52084
H           0.77050         2.40372        -1.46207
H           1.77914         0.06510        -5.00353
H           0.71887         2.39790        -4.14707
Fe          0.01239         0.00544        -2.78487
C          -1.65389        -0.37415        -3.98196
C          -2.03626         0.38941        -2.84116
C          -1.09536        -1.60418        -3.52503
H          -1.74139        -0.05751        -5.01351
C          -1.71452        -0.36352        -1.66175
H          -2.46961         1.37998        -2.85937
C          -1.11878        -1.59835        -2.10141
H          -0.68537        -2.38877        -4.14792
H          -0.75282        -2.39106        -1.46283
Ni         -0.00047         0.00950         0.98244
C           2.64300        -1.80822        -0.04044
C           1.77488        -2.88590         0.15803
C           3.97908        -2.07289        -0.37337
C           2.21725        -4.20120        -0.00424
H           0.74458        -2.69124         0.44387
```

C	4.42354	-3.38880	-0.51356
H	4.68079	-1.25839	-0.51773
C	3.54362	-4.46094	-0.33830
H	3.89222	-5.48071	-0.45105
C	3.39740	0.89430	0.64380
C	3.65380	0.98228	2.02006
C	4.23168	1.58329	-0.24417
C	4.73162	1.72852	2.49491
H	2.99884	0.47699	2.72427
C	5.30285	2.34251	0.23774
H	4.05140	1.53450	-1.31289
C	5.56012	2.41652	1.60537
H	6.38946	3.00795	1.97531
C	-3.39085	-0.89226	0.62214
C	-3.65064	-0.99218	1.99686
C	-4.22010	-1.57744	-0.27366
C	-4.72668	-1.74683	2.46275
H	-2.99972	-0.48980	2.70685
C	-5.28944	-2.34475	0.19909
H	-4.03724	-1.51935	-1.34145
C	-5.54994	-2.43093	1.56550
H	-6.37781	-3.02873	1.92848
C	-2.64747	1.81583	-0.05701
C	-1.78187	2.89771	0.12948
C	-3.98515	2.07368	-0.38871
C	-2.22670	4.20979	-0.05043
H	-0.75014	2.70871	0.41380
C	-4.43323	3.38708	-0.54192
H	-4.68174	1.25561	-0.53712
C	-3.55439	4.46289	-0.38491
H	-3.90107	5.47975	-0.52594
C	1.21521	-5.31170	0.17120
C	5.84748	-3.66146	-0.92915
C	5.03415	1.75886	3.97195
C	6.14361	3.13343	-0.73261
C	-5.03279	-1.79057	3.93874
C	-6.12449	-3.13172	-0.77941
C	-5.88798	3.65595	-0.83583
C	-1.22328	5.32328	0.09515
F	-5.55062	-4.32024	-1.06997
F	-7.35599	-3.39146	-0.29359
F	-6.27428	-2.46986	-1.94742
F	-5.89797	-0.81325	4.28961
F	-3.92051	-1.62305	4.68464
F	-5.59501	-2.96460	4.29536
F	-6.58987	3.85693	0.30051
F	-6.46612	2.62258	-1.48404
F	-6.04473	4.75888	-1.59902
F	-1.77457	6.53929	-0.07862
F	-0.63698	5.30482	1.31106
F	-0.22710	5.19207	-0.81666
F	1.76201	-6.53020	0.00041
F	0.20363	-5.18812	-0.72427
F	0.65050	-5.28026	1.39708
F	6.31006	-4.81107	-0.39496
F	6.67865	-2.66788	-0.55322
F	5.95012	-3.77974	-2.27287

F 3.91990 1.58629 4.71373
F 5.89721 0.77725 4.31630
F 5.59717 2.92886 4.34030
F 7.37183 3.39243 -0.23826
F 6.30124 2.47548 -1.90188
F 5.57064 4.32239 -1.02306

PhOTf
Charge: 0
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy (B3LYP/6-31G(d)): -1193.031425
Gibbs Free Energy (B3LYP/6-31G(d)): -1192.953538
Electronic Energy (M06/6-311+G(d,p)): -1192.887124
Total Gibbs Free Energy: -1192.809237
Geometry:
O 0.52691 -0.57959 1.62774
S 1.04162 -0.79374 0.28560
O 1.70081 -2.01947 -0.12540
O -0.10628 -0.43909 -0.84181
C 2.20420 0.61238 -0.11667
F 2.57554 0.54328 -1.39028
F 3.27006 0.50703 0.67375
F 1.59572 1.77955 0.11123
C -1.42006 -0.12582 -0.42573
C -2.36939 -1.14288 -0.42966
C -1.74303 1.18954 -0.10807
C -3.68873 -0.82647 -0.10191
H -2.07416 -2.15351 -0.69209
C -3.06581 1.49080 0.21890
H -0.97259 1.95223 -0.11807
C -4.03717 0.48673 0.22270
H -4.44251 -1.60834 -0.10134
H -3.33518 2.51250 0.47016
H -5.06501 0.72776 0.47779

L3-Ni0-PhOTf precomplex (II)
Charge: 0
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -6179.373130
Gibbs Free Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -6178.823114
Electronic Energy (M06/6-311+G(d,p)-SDD(Ni,Fe)/SMD(THF)): -6178.613805
Total Gibbs Free Energy: -6178.063789
Geometry:
P 1.66636 0.40642 0.51708
P -1.90181 -0.08908 0.40454
C 1.51667 -0.01144 2.29334
C 1.79308 0.78371 3.45938
C 0.99972 -1.27388 2.75800
C 1.44908 0.02202 4.61270
H 2.15221 1.80328 3.46483
C 0.96414 -1.24693 4.18042
H 0.69480 -2.09868 2.12911
H 1.50819 0.36638 5.63746
H 0.59588 -2.03961 4.81872
Fe -0.21365 0.28705 3.37083

C	-1.96673	0.64242	4.45737
C	-2.24080	-0.17694	3.32600
C	-1.42196	1.87317	3.99157
H	-2.11381	0.36042	5.49202
C	-1.86152	0.53895	2.13756
H	-2.63361	-1.18278	3.36013
C	-1.34470	1.81346	2.57031
H	-1.08444	2.69690	4.60721
H	-0.95620	2.59822	1.93667
Ni	-0.02145	-0.17375	-0.81558
C	0.79522	-0.58533	-2.58640
C	-0.64630	-0.60093	-2.70039
C	1.55562	0.45374	-3.22379
C	-1.25321	0.49951	-3.40373
H	-1.18342	-1.54548	-2.66953
C	0.91338	1.51211	-3.81255
H	2.63689	0.36697	-3.24526
C	-0.50974	1.54043	-3.90142
H	-2.32202	0.46612	-3.59020
H	1.49692	2.31051	-4.26287
H	-0.99709	2.35476	-4.42961
C	1.83815	2.25249	0.53702
C	0.79738	2.99599	-0.02829
C	2.91616	2.93790	1.11538
C	0.79926	4.39163	0.03076
H	-0.01963	2.47469	-0.51967
C	2.92787	4.33395	1.15140
H	3.75592	2.39014	1.53018
C	1.86381	5.06872	0.62155
H	1.87312	6.15184	0.65900
C	3.40105	-0.13085	0.13957
C	4.13451	0.51745	-0.86227
C	3.95460	-1.26619	0.74654
C	5.38435	0.03533	-1.25623
H	3.73134	1.39780	-1.35099
C	5.20681	-1.74019	0.35263
H	3.41191	-1.78848	1.52587
C	5.92953	-1.09633	-0.65230
H	6.89831	-1.47143	-0.95917
C	-3.27734	0.89572	-0.36289
C	-4.01916	0.33507	-1.41208
C	-3.50108	2.23974	-0.03394
C	-4.96741	1.09270	-2.10096
H	-3.86927	-0.70188	-1.69528
C	-4.44495	2.99616	-0.73203
H	-2.95318	2.70934	0.77311
C	-5.18609	2.42867	-1.76805
H	-5.92650	3.01373	-2.30046
C	-2.70881	-1.73459	0.69947
C	-1.89614	-2.87171	0.72288
C	-4.07314	-1.87107	1.00072
C	-2.42801	-4.11816	1.07120
H	-0.84285	-2.79245	0.47770
C	-4.60500	-3.12206	1.31283
H	-4.72373	-1.00351	1.00659
C	-3.78269	-4.25162	1.36012
H	-4.19351	-5.21674	1.63059

C	-0.41810	5.13294	-0.45778
C	4.06066	5.05043	1.84315
C	6.14179	0.77797	-2.32548
C	5.73979	-3.00862	0.96859
C	-5.69208	0.46902	-3.26530
C	-4.62074	4.45939	-0.40939
C	-6.08447	-3.26459	1.56854
C	-1.49367	-5.29908	1.16016
F	-3.82499	5.23003	-1.18356
F	-5.89130	4.86477	-0.62347
F	-4.31462	4.73159	0.87582
F	-6.01137	-0.81910	-3.02266
F	-4.91494	0.47764	-4.37707
F	-6.82792	1.12739	-3.56837
F	-6.75977	-3.51143	0.42543
F	-6.60807	-2.14092	2.10443
F	-6.34733	-4.28341	2.41435
F	-2.12274	-6.40995	1.59671
F	-0.93287	-5.58789	-0.02919
F	-0.48102	-5.04050	2.02287
F	-0.17545	6.43982	-0.66440
F	-1.41446	5.04734	0.46390
F	-0.90029	4.60967	-1.60209
F	4.25378	6.28568	1.33889
F	5.22094	4.37169	1.73360
F	3.80810	5.19361	3.16519
F	6.70348	1.90882	-1.84435
F	7.12929	0.03317	-2.85943
F	5.31827	1.15197	-3.33540
F	7.08444	-3.08531	0.87797
F	5.41005	-3.10501	2.27433
F	5.23630	-4.10190	0.35228
O	1.30829	-2.91958	-0.33571
S	1.16134	-3.13915	-1.77755
O	-0.04989	-3.76637	-2.29109
O	1.56690	-1.84026	-2.62794
C	2.63413	-4.14893	-2.33674
F	2.58504	-4.32912	-3.65211
F	2.56069	-5.32356	-1.71528
F	3.76451	-3.53180	-2.00394

L3-Ni-PhOTf oxidative addition TS (II-TS)
Charge: 0
Multiplicity: 1
Imaginary Frequencies: 1
Electronic Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -6179.358144
Gibbs Free Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -6178.809343
Electronic Energy (M06/6-311+G(d,p)-SDD(Ni,Fe)/SMD(THF)): -6178.598268
Total Gibbs Free Energy: -6178.049467
Geometry:

P	-1.67422	0.40195	-0.47659
P	1.92054	-0.09953	-0.43896
C	-1.53864	-0.06061	-2.23907
C	-1.82978	0.72034	-3.41223
C	-1.04582	-1.33707	-2.69076
C	-1.51829	-0.06507	-4.55821
H	-2.17841	1.74337	-3.42783

C	-1.03804	-1.33152	-4.11302
H	-0.75256	-2.15692	-2.05051
H	-1.59484	0.26243	-5.58727
H	-0.69129	-2.13892	-4.74483
Fe	0.17202	0.20679	-3.35802
C	1.90386	0.51147	-4.49704
C	2.19730	-0.27377	-3.34733
C	1.37876	1.76129	-4.05982
H	2.02633	0.19548	-5.52498
C	1.84974	0.48516	-2.17602
H	2.58200	-1.28321	-3.35512
C	1.33240	1.75017	-2.63650
H	1.03406	2.56701	-4.69487
H	0.96892	2.55990	-2.02012
Ni	0.03376	-0.15678	0.85608
C	-0.67652	-0.30986	2.54912
C	0.68768	-0.63685	2.79260
C	-1.38702	0.58841	3.37343
C	1.37203	0.10881	3.80141
H	1.09164	-1.60510	2.50481
C	-0.67102	1.31090	4.30933
H	-2.45413	0.73271	3.24788
C	0.71274	1.08411	4.51882
H	2.39494	-0.15666	4.05178
H	-1.18348	2.06924	4.89633
H	1.23359	1.64040	5.29265
C	-1.80224	2.24973	-0.53778
C	-0.73144	2.99180	-0.03063
C	-2.89079	2.93700	-1.09562
C	-0.71792	4.38592	-0.12104
H	0.09872	2.47500	0.44248
C	-2.88538	4.33131	-1.16399
H	-3.75263	2.39242	-1.46640
C	-1.79439	5.06374	-0.68776
H	-1.79219	6.14598	-0.74751
C	-3.40032	-0.08850	-0.04080
C	-4.08687	0.60891	0.95707
C	-4.00645	-1.20840	-0.62678
C	-5.35055	0.18770	1.37776
H	-3.64100	1.48128	1.42228
C	-5.27342	-1.61366	-0.21355
H	-3.48912	-1.77710	-1.38865
C	-5.95179	-0.92351	0.79408
H	-6.92900	-1.25601	1.12577
C	3.27178	0.90914	0.33277
C	3.96125	0.38764	1.43716
C	3.53505	2.22676	-0.06230
C	4.89918	1.16220	2.11963
H	3.77117	-0.62636	1.77217
C	4.46452	3.00277	0.63469
H	3.02825	2.66109	-0.91472
C	5.15413	2.47597	1.72538
H	5.87762	3.07938	2.26119
C	2.70997	-1.75651	-0.66982
C	1.89778	-2.89587	-0.66508
C	4.07711	-1.88915	-0.96135
C	2.44205	-4.14573	-0.98429

H	0.84165	-2.82544	-0.42093
C	4.61647	-3.14326	-1.24205
H	4.72241	-1.01788	-0.98435
C	3.79820	-4.27671	-1.26642
H	4.21414	-5.24553	-1.51508
C	0.52532	5.12094	0.30851
C	-4.03173	5.05131	-1.83079
C	-6.06066	0.98016	2.44348
C	-5.94564	-2.80791	-0.84300
C	5.67763	0.55496	3.25962
C	4.68013	4.44570	0.24905
C	6.09733	-3.28571	-1.49000
C	1.51720	-5.33786	-1.05710
F	3.89726	5.26931	0.97994
F	5.95823	4.82747	0.45898
F	4.39360	4.66601	-1.05029
F	6.78475	-0.07859	2.81936
F	4.94061	-0.36213	3.93122
F	6.07483	1.48897	4.14649
F	6.76682	-3.52898	-0.34300
F	6.62267	-2.16302	-2.02673
F	6.36387	-4.30661	-2.33150
F	2.16358	-6.44661	-1.47933
F	0.95845	-5.61595	0.13039
F	0.51021	-5.09983	-1.93143
F	0.30732	6.43376	0.49734
F	1.48629	5.00256	-0.64707
F	1.04154	4.61208	1.44464
F	-4.21705	6.28102	-1.31090
F	-5.18808	4.36952	-1.70867
F	-3.79874	5.20800	-3.15446
F	-6.61817	2.10323	1.93691
F	-7.04378	0.27345	3.03219
F	-5.20053	1.37749	3.41260
F	-7.06384	-2.43668	-1.51002
F	-5.14485	-3.44288	-1.72027
F	-6.32905	-3.70318	0.09081
O	-1.28198	-2.78913	0.21987
S	-1.31464	-3.08209	1.67681
O	-0.10159	-3.69822	2.22982
O	-1.85831	-1.92016	2.49833
C	-2.67950	-4.33762	1.88616
F	-2.81817	-4.65194	3.17467
F	-2.36873	-5.43669	1.19436
F	-3.83929	-3.84881	1.42872

L3-Ni(Ph)OTf oxidative addition complex (III)
Charge: 0
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -6179.406265
Gibbs Free Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -6178.862384
Electronic Energy (M06/6-311+G(d,p)-SDD(Ni,Fe)/SMD(THF)): -6178.64988
Total Gibbs Free Energy: -6178.105999
Geometry:

P	-1.91058	-0.04845	-0.54810
P	1.67910	-0.06280	-0.67441

C	-1.74099	-0.34995	-2.33985
C	-2.19557	0.45267	-3.44547
C	-1.17076	-1.55127	-2.89809
C	-1.89969	-0.24190	-4.65181
H	-2.64533	1.43336	-3.37804
C	-1.27075	-1.47650	-4.31599
H	-0.73287	-2.36468	-2.33411
H	-2.07996	0.12865	-5.65262
H	-0.89515	-2.21235	-5.01503
Fe	-0.15866	0.12264	-3.54381
C	1.50400	0.57939	-4.72839
C	1.88992	-0.20264	-3.60249
C	0.90081	1.77962	-4.25073
H	1.62330	0.29469	-5.76575
C	1.51427	0.50518	-2.41093
H	2.35575	-1.17772	-3.63652
C	0.89971	1.73952	-2.82737
H	0.48129	2.56914	-4.86082
H	0.51045	2.50620	-2.17075
Ni	-0.21039	-0.81256	0.66016
C	-1.49744	-1.35053	1.95314
C	-1.81305	-0.47882	3.00284
C	-2.05603	-2.63424	1.94007
C	-2.68908	-0.88275	4.01857
H	-1.36134	0.50891	3.05886
C	-2.93052	-3.03575	2.95447
H	-1.80756	-3.33660	1.14660
C	-3.25697	-2.15748	3.99106
H	-2.91871	-0.19943	4.83266
H	-3.35337	-4.03761	2.93530
H	-3.94258	-2.46728	4.77477
C	-2.16021	1.77682	-0.40843
C	-1.17186	2.55734	0.19747
C	-3.30446	2.40855	-0.91909
C	-1.30491	3.94797	0.26167
H	-0.29497	2.08488	0.62758
C	-3.43317	3.79544	-0.85091
H	-4.10453	1.82304	-1.35908
C	-2.43161	4.57367	-0.26482
H	-2.53683	5.65042	-0.20847
C	-3.61795	-0.69815	-0.23850
C	-4.36320	-0.23975	0.85997
C	-4.16876	-1.67522	-1.07022
C	-5.62672	-0.76181	1.11678
H	-3.95677	0.50827	1.52842
C	-5.44188	-2.19376	-0.80648
H	-3.62328	-2.03811	-1.93375
C	-6.17523	-1.74308	0.28482
H	-7.16472	-2.13892	0.48260
C	2.63615	1.33837	0.06176
C	2.45833	1.67572	1.41142
C	3.50908	2.10674	-0.72248
C	3.13991	2.76562	1.95788
H	1.80340	1.09716	2.05484
C	4.18863	3.19123	-0.16652
H	3.66037	1.87050	-1.77026
C	4.00419	3.52808	1.17409

H	4.52377	4.37781	1.60075
C	2.87614	-1.45409	-0.86089
C	2.34761	-2.72635	-1.09477
C	4.26473	-1.29524	-0.80134
C	3.19097	-3.81845	-1.30372
H	1.27382	-2.88039	-1.09235
C	5.10391	-2.39377	-0.99250
H	4.70373	-0.32519	-0.60040
C	4.57367	-3.65875	-1.25268
H	5.23009	-4.50644	-1.40911
C	-0.18086	4.74963	0.86980
C	-4.63291	4.45803	-1.48282
C	-6.41218	-0.31086	2.32322
C	-5.98222	-3.27131	-1.71165
C	2.96806	3.09779	3.42233
C	5.06849	4.03486	-1.05382
C	6.59843	-2.22572	-0.86992
C	2.56523	-5.15270	-1.61326
F	4.33499	4.90602	-1.78424
F	5.95758	4.75642	-0.34392
F	5.75868	3.27348	-1.93058
F	3.84586	2.41874	4.18412
F	1.73038	2.79897	3.85817
F	3.17711	4.41560	3.64939
F	7.02417	-2.46769	0.38443
F	6.98429	-0.97170	-1.19143
F	7.25747	-3.07783	-1.68674
F	3.46676	-6.15139	-1.63183
F	1.60935	-5.47131	-0.71540
F	1.96023	-5.12999	-2.82877
F	-0.49927	6.04922	1.00801
F	0.92587	4.67996	0.09017
F	0.16185	4.27150	2.08237
F	-4.88434	5.66320	-0.93792
F	-5.74196	3.70186	-1.35402
F	-4.43335	4.64760	-2.80764
F	-5.91341	0.82081	2.85947
F	-7.70470	-0.07804	2.00181
F	-6.41246	-1.25376	3.28852
F	-7.30094	-3.47558	-1.52628
F	-5.79343	-2.95649	-3.01325
F	-5.35493	-4.44902	-1.50008
O	1.12290	-1.85141	1.59122
S	1.93739	-1.58913	2.86705
O	3.37633	-1.63419	2.58899
O	1.41420	-0.46591	3.65811
C	1.56561	-3.13471	3.83773
F	2.30889	-3.14601	4.94851
F	1.85998	-4.21463	3.10385
F	0.27547	-3.17975	4.17757

L3-Ni(Ph) cation
Charge: 1
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -5217.757964
Gibbs Free Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -5217.240372

Electronic Energy (M06/6-311+G(d,p)-SDD(Ni,Fe)/SMD(THF)): -5217.040839
Total Gibbs Free Energy: -5216.523247
Geometry:

P	1.75397	-0.02521	-0.34849
P	-1.97988	0.14732	-0.29768
C	1.42627	0.60146	-2.02385
C	1.79384	-0.03543	-3.26409
C	0.80374	1.85982	-2.36091
C	1.41096	0.82093	-4.33153
H	2.25947	-1.00583	-3.36502
C	0.80568	1.98598	-3.77786
H	0.41743	2.59435	-1.66649
H	1.52426	0.60233	-5.38541
H	0.38243	2.81039	-4.33666
Fe	-0.25545	0.28062	-3.17381
C	-1.94898	-0.02865	-4.37747
C	-2.30187	0.62586	-3.16510
C	-1.35313	-1.28205	-4.05357
H	-2.08247	0.37398	-5.37314
C	-1.91380	-0.22265	-2.07124
H	-2.74959	1.60628	-3.08012
C	-1.31988	-1.40929	-2.63807
H	-0.95888	-2.00043	-4.76055
H	-0.93065	-2.25935	-2.09398
Ni	-0.01304	-0.07344	0.91860
C	0.99191	-0.31118	2.42710
C	1.09155	-1.59739	2.98353
C	1.13922	0.83200	3.23199
C	1.25186	-1.73091	4.36743
H	1.03107	-2.48851	2.36400
C	1.29377	0.68185	4.61376
H	1.13481	1.82942	2.79773
C	1.35171	-0.59622	5.17697
H	1.30816	-2.72242	4.80808
H	1.38614	1.56186	5.24422
H	1.49161	-0.70829	6.24806
C	2.33814	-1.74583	-0.61569
C	1.42477	-2.78669	-0.43897
C	3.64574	-2.04535	-1.02701
C	1.79766	-4.10978	-0.68091
H	0.41492	-2.57286	-0.10181
C	4.01442	-3.37011	-1.26177
H	4.38084	-1.25865	-1.15672
C	3.09342	-4.40939	-1.09171
H	3.38933	-5.43744	-1.26691
C	3.23916	0.90850	0.21250
C	3.95502	0.46156	1.33429
C	3.66716	2.06034	-0.45852
C	5.08096	1.15723	1.76907
H	3.63775	-0.42096	1.87797
C	4.79072	2.75789	-0.00676
H	3.14711	2.41782	-1.33895
C	5.50216	2.31152	1.10464
H	6.37444	2.85385	1.45106
C	-3.31469	-0.91623	0.38709
C	-3.40982	-1.03686	1.78076
C	-4.21135	-1.61932	-0.42706

C	-4.39578	-1.84170	2.35142
H	-2.71791	-0.50877	2.43213
C	-5.19207	-2.42720	0.15215
H	-4.15205	-1.54461	-1.50765
C	-5.29011	-2.54043	1.53955
H	-6.05203	-3.17092	1.98304
C	-2.63130	1.86239	-0.19121
C	-1.74758	2.87116	0.19999
C	-3.95689	2.19954	-0.50397
C	-2.16184	4.20397	0.24292
H	-0.72535	2.62350	0.47141
C	-4.37111	3.53001	-0.44111
H	-4.66768	1.43489	-0.80037
C	-3.47430	4.54036	-0.07652
H	-3.79829	5.57419	-0.04694
C	0.74881	-5.17568	-0.48505
C	5.40752	-3.68466	-1.76254
C	5.87102	0.62613	2.94385
C	5.19415	4.03737	-0.70373
C	-4.50697	-1.91328	3.85716
C	-6.10975	-3.23448	-0.73843
C	-5.81609	3.87324	-0.73110
C	-1.13216	5.24617	0.60209
F	-5.54817	-4.41921	-1.05432
F	-7.28509	-3.48663	-0.13636
F	-6.35944	-2.58634	-1.89508
F	-5.19187	-0.85843	4.34117
F	-3.28330	-1.89286	4.43156
F	-5.13606	-3.03159	4.25602
F	-6.56632	3.77338	0.38250
F	-6.33767	3.03264	-1.64841
F	-5.93715	5.12925	-1.19729
F	-1.64709	6.48114	0.65369
F	-0.56330	4.97209	1.79644
F	-0.13043	5.24571	-0.31307
F	1.22262	-6.40958	-0.69680
F	-0.29093	-4.97171	-1.33133
F	0.24346	-5.12253	0.76828
F	5.84402	-4.86173	-1.28156
F	6.28514	-2.72868	-1.40186
F	5.42030	-3.76291	-3.10901
F	5.06353	0.00980	3.83301
F	6.78743	-0.27628	2.54054
F	6.52208	1.61293	3.58486
F	6.50665	4.28665	-0.55722
F	4.92186	3.97863	-2.02454
F	4.51744	5.09044	-0.20132

TfO anion
Charge: -1
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy (B3LYP/6-31G(d)): -961.487293
Gibbs Free Energy (B3LYP/6-31G(d)): -961.492511
Electronic Energy (M06/6-311+G(d,p)/SMD(THF)): -961.550566
Total Gibbs Free Energy: -961.555784
Geometry:

```
O          -1.24082         1.44268        -0.10432
S          -0.92486        -0.00006        -0.00018
O          -1.24205        -0.63087         1.30113
O          -1.24207        -0.81138        -1.19715
C           0.93919        -0.00011        -0.00001
F           1.44345        -1.25147         0.08872
F           1.44213         0.70228         1.03976
F           1.44355         0.54899        -1.12785
```

aniline
Charge: 0
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy (B3LYP/6-31G(d)): -287.595892
Gibbs Free Energy (B3LYP/6-31G(d)): -287.507607
Electronic Energy (M06/6-311+G(d,p)/SMD(THF)): -287.468212
Total Gibbs Free Energy: -287.379927
Geometry:

```
C          -0.93907        -0.00001        -0.01030
C          -0.22132         1.20844        -0.00519
C          -0.22130        -1.20844        -0.00512
C           1.17206         1.20289         0.00342
H          -0.76329         2.15199        -0.01329
C           1.17209        -1.20288         0.00334
H          -0.76324        -2.15201        -0.01313
C           1.88215         0.00001         0.00833
H           1.70585         2.15006         0.00889
H           1.70589        -2.15003         0.00882
H           2.96810         0.00003         0.01655
N          -2.33786        -0.00000        -0.07876
H          -2.77792        -0.83518         0.28826
H          -2.77793         0.83513         0.28834
```

L3-Ni(Ph)-aniline complex (V)
Charge: 1
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -5505.391082
Gibbs Free Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -5504.748870
Electronic Energy (M06/6-311+G(d,p)-SDD(Ni,Fe)/SMD(THF)): -5504.559369
Total Gibbs Free Energy: -5503.917157
Geometry:

```
P           1.75496         0.15051        -0.43929
P          -1.83742         0.34858        -0.63979
C           1.58700         0.93675        -2.07971
C           2.08086         0.45786        -3.34528
C           0.98658         2.22630        -2.32361
C           1.78177         1.43145        -4.33777
H           2.56254        -0.49347        -3.52243
C           1.11223         2.52077        -3.71033
H           0.51417         2.86105        -1.58586
H           1.99316         1.33830        -5.39510
H           0.72805         3.40294        -4.20564
Fe          0.03152         0.75180        -3.39214
C          -1.58594         0.52883        -4.72054
C          -2.00915         1.07149        -3.47640
C          -0.98410        -0.73817        -4.47653
```

H	-1.67549	1.01646	-5.68257
C	-1.66055	0.13675	-2.43692
H	-2.47175	2.03822	-3.33919
C	-1.02167	-0.98866	-3.07742
H	-0.53860	-1.38573	-5.22028
H	-0.62815	-1.86982	-2.59047
Ni	-0.04022	0.07214	0.94625
C	1.25714	0.10856	2.35388
C	1.83812	-1.05454	2.87736
C	1.53855	1.34022	2.96729
C	2.69585	-0.98705	3.98252
H	1.62351	-2.02623	2.43818
C	2.38739	1.40461	4.07888
H	1.10788	2.26723	2.58985
C	2.97554	0.24201	4.58226
H	3.14241	-1.89806	4.37276
H	2.59334	2.36606	4.54256
H	3.64714	0.29391	5.43385
C	2.13967	-1.60747	-0.83818
C	1.13848	-2.55802	-0.62042
C	3.34800	-2.02175	-1.41796
C	1.31267	-3.88630	-1.01278
H	0.20908	-2.26409	-0.14057
C	3.52696	-3.35581	-1.78898
H	4.15627	-1.31545	-1.57617
C	2.50824	-4.29384	-1.59932
H	2.65105	-5.32554	-1.89852
C	3.35831	0.86894	0.13859
C	4.24128	0.12727	0.93703
C	3.68713	2.18847	-0.19023
C	5.42415	0.70171	1.39666
H	4.01165	-0.89246	1.21582
C	4.87645	2.75713	0.27358
H	3.03024	2.78846	-0.80877
C	5.75035	2.01922	1.06718
H	6.67385	2.46155	1.42333
C	-3.32745	-0.66968	-0.21794
C	-4.34961	-0.20463	0.62073
C	-3.34980	-2.01239	-0.62459
C	-5.37088	-1.06512	1.03833
H	-4.37145	0.82894	0.95126
C	-4.35898	-2.86894	-0.18648
H	-2.57439	-2.41133	-1.26983
C	-5.37832	-2.40152	0.64456
H	-6.15892	-3.07078	0.98566
C	-2.39445	2.08977	-0.42370
C	-1.56614	2.94179	0.31353
C	-3.57863	2.60856	-0.97165
C	-1.89518	4.28702	0.49057
H	-0.64828	2.55771	0.75135
C	-3.90610	3.95310	-0.78948
H	-4.24703	1.97451	-1.54545
C	-3.06617	4.80090	-0.06053
H	-3.32357	5.84540	0.07085
C	0.14895	-4.82868	-0.83625
C	4.81115	-3.76166	-2.47728
C	6.33814	-0.08076	2.31006

C	5.22781	4.16271	-0.15250
C	-6.47889	-0.50729	1.90273
C	-4.25903	-4.33519	-0.53873
C	-5.20810	4.47283	-1.35955
C	-0.92205	5.15405	1.25110
F	-3.29684	-4.92709	0.21285
F	-5.41034	-4.98798	-0.31546
F	-3.91510	-4.50861	-1.82834
F	-7.15602	-1.47885	2.53579
F	-7.35620	0.19928	1.16469
F	-5.97582	0.33150	2.83731
F	-6.24092	4.16557	-0.55148
F	-5.45776	3.91630	-2.56352
F	-5.18381	5.80783	-1.51138
F	-1.41739	6.36974	1.51492
F	-0.58204	4.57073	2.42639
F	0.22358	5.30731	0.54901
F	0.44761	-6.08903	-1.17022
F	-0.89387	-4.42732	-1.61662
F	-0.30171	-4.82060	0.43709
F	5.04397	-5.07941	-2.35388
F	5.86648	-3.09568	-1.97062
F	4.74999	-3.47633	-3.79618
F	6.13207	-1.40959	2.19990
F	7.63296	0.16418	2.03405
F	6.13378	0.25375	3.60219
F	6.11209	4.73137	0.68591
F	5.76926	4.17302	-1.38836
F	4.12762	4.94659	-0.19466
C	-1.37816	-1.46034	3.20556
C	-1.08623	-1.44699	4.56984
C	-1.68069	-2.65938	2.55930
C	-1.09835	-2.64350	5.28876
H	-0.84325	-0.51295	5.07009
C	-1.70016	-3.85055	3.28578
H	-1.91016	-2.67373	1.50010
C	-1.40808	-3.84630	4.65108
H	-0.86937	-2.63006	6.35006
H	-1.94512	-4.77632	2.77463
H	-1.42271	-4.77393	5.21501
H	-2.34755	-0.05131	2.11898
H	-1.18085	0.55835	3.09339
N	-1.39195	-0.20548	2.44842

L3-Ni(Ph)-NHPh (VI)
Charge: 0
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -5504.965112
Gibbs Free Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -5504.337720
Electronic Energy (M06/6-311+G(d,p)-SDD(Ni,Fe)/SMD(THF)): -5504.095151
Total Gibbs Free Energy: -5503.467759
Geometry:

P	1.72079	-0.06353	-0.48548
P	-1.86319	0.17801	-0.45975
C	1.52848	0.56635	-2.20662
C	1.89652	-0.09349	-3.43191

C	0.95284	1.83540	-2.57829
C	1.55746	0.75473	-4.52328
H	2.32549	-1.08151	-3.51627
C	0.98137	1.94638	-3.99762
H	0.55490	2.58006	-1.90329
H	1.68120	0.51390	-5.57129
H	0.59123	2.77578	-4.57312
Fe	-0.14113	0.29119	-3.39129
C	-1.84831	0.01130	-4.57328
C	-2.17087	0.69886	-3.36894
C	-1.28405	-1.25213	-4.22954
H	-1.97481	0.39989	-5.57577
C	-1.79821	-0.13435	-2.25838
H	-2.58503	1.69545	-3.30382
C	-1.24714	-1.34800	-2.81016
H	-0.91092	-1.99341	-4.92432
H	-0.85922	-2.18384	-2.24257
Ni	-0.02836	-0.27793	0.97995
C	1.25277	-0.41783	2.39601
C	1.77824	-1.64237	2.84266
C	1.63616	0.74735	3.08636
C	2.67619	-1.69776	3.91528
H	1.47224	-2.57378	2.37195
C	2.52341	0.69390	4.16650
H	1.25259	1.71999	2.77926
C	3.05544	-0.52956	4.57957
H	3.06980	-2.65948	4.23726
H	2.80448	1.61123	4.67920
H	3.75456	-0.57147	5.41016
C	2.39935	-1.75305	-0.80051
C	1.59140	-2.85206	-0.49834
C	3.65763	-1.97686	-1.37725
C	2.01681	-4.15109	-0.78642
H	0.62845	-2.69908	-0.02237
C	4.08232	-3.27685	-1.65703
H	4.31337	-1.14322	-1.60591
C	3.26299	-4.37122	-1.36749
H	3.59639	-5.37840	-1.58718
C	3.19592	0.89367	0.10676
C	4.14096	0.30162	0.95905
C	3.32097	2.25353	-0.19619
C	5.19937	1.05299	1.46635
H	4.04983	-0.73900	1.24493
C	4.37338	3.00592	0.33280
H	2.61048	2.74743	-0.84653
C	5.32232	2.40922	1.15829
H	6.14992	2.98882	1.55153
C	-3.53415	-0.44891	0.00413
C	-4.10565	-0.04047	1.21772
C	-4.21539	-1.37692	-0.79072
C	-5.33006	-0.56853	1.62922
H	-3.58872	0.66987	1.84947
C	-5.44538	-1.89285	-0.37590
H	-3.79291	-1.71129	-1.73165
C	-6.00575	-1.49694	0.83791
H	-6.95593	-1.90452	1.16132
C	-2.10276	2.01137	-0.34695

C	-1.07075	2.77399	0.20699
C	-3.24852	2.67165	-0.81336
C	-1.14967	4.16783	0.24777
H	-0.19599	2.27349	0.61248
C	-3.33280	4.06455	-0.75677
H	-4.07724	2.10551	-1.22590
C	-2.27985	4.82200	-0.23656
H	-2.34224	5.90341	-0.21197
C	1.10623	-5.29701	-0.42395
C	5.40746	-3.48522	-2.34692
C	6.19920	0.42680	2.40635
C	4.43635	4.48634	0.05416
C	-5.88616	-0.15890	2.96889
C	-6.19392	-2.83418	-1.28249
C	-4.59104	4.74852	-1.23233
C	0.05197	4.93449	0.73545
F	-5.35300	-3.63135	-1.97815
F	-7.04057	-3.62897	-0.59678
F	-6.93374	-2.15803	-2.19297
F	-7.21088	-0.40491	3.06039
F	-5.69995	1.16179	3.19426
F	-5.28451	-0.81861	3.98026
F	-5.53569	4.76710	-0.26997
F	-5.12192	4.11070	-2.29924
F	-4.35761	6.02731	-1.59279
F	-0.22444	6.22753	0.97474
F	0.55967	4.39822	1.86501
F	1.04228	4.89615	-0.19566
F	1.50998	-6.45911	-0.97329
F	-0.15816	-5.05756	-0.85354
F	1.04167	-5.47321	0.90989
F	5.89941	-4.72060	-2.12898
F	6.32799	-2.59139	-1.93119
F	5.28477	-3.33266	-3.68619
F	6.18136	-0.91918	2.34242
F	7.45702	0.83472	2.12143
F	5.95751	0.77658	3.68826
F	5.69951	4.95587	0.13065
F	3.96134	4.78404	-1.17479
F	3.69738	5.18482	0.94426
N	-1.32680	-0.61765	2.31853
H	-1.11044	-0.11110	3.17497
C	-1.67653	-1.92411	2.63945
C	-2.07024	-2.27811	3.95273
C	-1.71045	-2.94944	1.66483
C	-2.47722	-3.57182	4.26142
H	-2.05715	-1.51466	4.72822
C	-2.11193	-4.24570	1.98341
H	-1.41939	-2.71692	0.64355
C	-2.50128	-4.57231	3.28346
H	-2.77319	-3.80354	5.28208
H	-2.10299	-5.00625	1.20665
H	-2.80855	-5.58377	3.53268

Et3NH-OTf
Charge: 0
Multiplicity: 1

Imaginary Frequencies: 0
Electronic Energy (B3LYP/6-31G(d)): -1254.446321
Gibbs Free Energy (B3LYP/6-31G(d)): -1254.242079
Electronic Energy (M06/6-311+G(d,p)/SMD(THF)): -1254.298611
Total Gibbs Free Energy: -1254.094369
Geometry:

O	0.70610	0.96656	1.19038
S	1.23992	0.82089	-0.18643
O	1.91171	1.97714	-0.78140
O	0.23405	0.13689	-1.08590
C	2.55700	-0.47947	-0.02362
F	3.10051	-0.75823	-1.21357
F	2.03272	-1.62039	0.47461
F	3.52081	-0.06823	0.80661
C	-2.88361	1.12757	-0.02297
H	-2.71625	1.48146	-1.04113
H	-3.95013	0.90074	0.09119
C	-2.05420	-0.69056	1.49630
H	-1.53314	0.09065	2.04721
H	-3.08079	-0.77885	1.87073
C	-2.71369	-1.21355	-0.87155
H	-2.09381	-2.10332	-0.76004
H	-3.72485	-1.45197	-0.52212
C	-1.27900	-1.99573	1.64729
H	-1.12567	-2.17287	2.71676
H	-1.80947	-2.86385	1.24544
H	-0.29207	-1.92307	1.18291
C	-2.69914	-0.77177	-2.33342
H	-2.95081	-1.63595	-2.95672
H	-3.43116	0.01169	-2.54830
H	-1.70250	-0.42272	-2.61966
C	-2.42791	2.19181	0.97234
H	-2.86195	3.14928	0.66629
H	-2.77061	1.98547	1.99029
H	-1.33884	2.29068	0.98371
H	-1.14795	-0.01195	-0.27294
N	-2.14382	-0.18751	0.07563

L3-Ni(Ph)-NHPh reductive elimination TS (VI-TS)
Charge: 0
Multiplicity: 1
Imaginary Frequencies: 1
Electronic Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -5504.935035
Gibbs Free Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -5504.308833
Electronic Energy (M06/6-311+G(d,p)-SDD(Ni,Fe)/SMD(THF)): -5504.067837
Total Gibbs Free Energy: -5503.441635
Geometry:

P	1.79684	-0.00941	-0.39401
P	-1.79713	0.27437	-0.59722
C	1.68981	0.66610	-2.10027
C	2.11570	0.05995	-3.33213
C	1.17256	1.96934	-2.43375
C	1.86632	0.97327	-4.39531
H	2.52528	-0.93490	-3.43812
C	1.29104	2.15379	-3.84125
H	0.76819	2.68906	-1.73450
H	2.04693	0.78522	-5.44597

H	0.96147	3.02356	-4.39490
Fe	0.08668	0.50547	-3.39946
C	-1.54722	0.37684	-4.70156
C	-1.92801	0.98108	-3.46992
C	-1.04893	-0.92910	-4.42225
H	-1.59293	0.84540	-5.67642
C	-1.66044	0.05079	-2.40669
H	-2.30939	1.98582	-3.35209
C	-1.10986	-1.13497	-3.01523
H	-0.65590	-1.62990	-5.14748
H	-0.79266	-2.02927	-2.49520
Ni	-0.00002	-0.07263	0.91952
C	0.78643	-0.28269	2.71121
C	1.37734	-1.51799	3.10204
C	1.27066	0.89930	3.34743
C	2.36929	-1.55444	4.08161
H	1.03452	-2.44917	2.66386
C	2.26414	0.83589	4.31877
H	0.85416	1.86865	3.07524
C	2.82096	-0.38906	4.70812
H	2.79552	-2.51689	4.35760
H	2.61269	1.75943	4.77609
H	3.59942	-0.42889	5.46238
C	2.32405	-1.75370	-0.73857
C	1.34805	-2.74754	-0.63275
C	3.61876	-2.12304	-1.12788
C	1.64326	-4.07985	-0.92823
H	0.34784	-2.47546	-0.30937
C	3.91455	-3.45766	-1.41436
H	4.40259	-1.37675	-1.20193
C	2.92885	-4.44396	-1.32032
H	3.16477	-5.47827	-1.54028
C	3.38158	0.76792	0.18859
C	4.04134	0.24403	1.31429
C	3.92210	1.89175	-0.44690
C	5.23332	0.81831	1.75823
H	3.63402	-0.61164	1.84184
C	5.10296	2.47531	0.02030
H	3.43419	2.32282	-1.31251
C	5.76945	1.93700	1.11677
H	6.69577	2.37821	1.46574
C	-3.44703	-0.46294	-0.21044
C	-4.08798	-0.10271	0.98762
C	-4.03220	-1.44436	-1.01711
C	-5.28104	-0.71317	1.36255
H	-3.65620	0.65296	1.63217
C	-5.23101	-2.05401	-0.63375
H	-3.56852	-1.73411	-1.95381
C	-5.86018	-1.69585	0.55553
H	-6.79022	-2.16953	0.84844
C	-2.17161	2.08418	-0.43501
C	-1.22140	2.88699	0.20213
C	-3.34987	2.68353	-0.90407
C	-1.42616	4.26081	0.35304
H	-0.31501	2.42923	0.59262
C	-3.54967	4.05774	-0.75756
H	-4.12026	2.08107	-1.37462

C	-2.58883	4.85550	-0.12883
H	-2.75272	5.91971	-0.00924
C	0.53012	-5.08837	-0.82540
C	5.29491	-3.82078	-1.90270
C	5.95726	0.26535	2.96151
C	5.69016	3.64322	-0.72900
C	-5.98993	-0.30904	2.62996
C	-5.80866	-3.14234	-1.50177
C	-4.78685	4.68997	-1.34502
C	-0.34935	5.06062	1.03778
F	-7.12660	-3.32244	-1.27602
F	-5.65249	-2.86211	-2.81509
F	-5.19894	-4.32773	-1.27916
F	-7.15714	0.31879	2.35602
F	-5.25120	0.53232	3.38415
F	-6.29443	-1.38214	3.38922
F	-5.86257	3.88560	-1.22194
F	-4.62432	4.93368	-2.66618
F	-5.07892	5.86614	-0.75490
F	-0.66670	6.36311	1.14956
F	-0.10489	4.58643	2.28115
F	0.81759	4.97735	0.35499
F	0.94053	-6.33984	-1.09597
F	-0.47033	-4.78777	-1.69132
F	-0.01978	-5.09157	0.41097
F	5.39565	-3.64761	-3.24103
F	5.59574	-5.10953	-1.64448
F	6.24369	-3.05096	-1.33219
F	5.65233	-1.02609	3.19034
F	7.29883	0.34398	2.79714
F	5.66442	0.96005	4.08317
F	6.52168	4.37141	0.04420
F	6.40197	3.23227	-1.80377
F	4.72750	4.47120	-1.19150
N	-0.96960	-0.26391	2.55290
H	-1.19634	0.57036	3.08279
C	-1.70616	-1.37200	2.99441
C	-2.55017	-1.26053	4.11774
C	-1.61533	-2.61938	2.35077
C	-3.29299	-2.35209	4.55806
H	-2.63223	-0.30551	4.63258
C	-2.34942	-3.71261	2.80968
H	-0.97040	-2.73063	1.48553
C	-3.19717	-3.58894	3.91124
H	-3.94886	-2.23570	5.41671
H	-2.25388	-4.66439	2.29337
H	-3.77337	-4.43974	4.26255

Ph2NH
Charge: 0
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy (B3LYP/6-31G(d)): -518.641219
Gibbs Free Energy (B3LYP/6-31G(d)): -518.479604
Electronic Energy (M06/6-311+G(d,p)/SMD(THF)): -518.389429
Total Gibbs Free Energy: -518.227814
Geometry:

C	-1.26722	-0.43881	0.01907
C	-2.36537	-1.19561	-0.43077
C	-1.50119	0.85542	0.51737
C	-3.65470	-0.67264	-0.38899
H	-2.19599	-2.19728	-0.82069
C	-2.79558	1.37378	0.53832
H	-0.67775	1.44117	0.90974
C	-3.88133	0.62101	0.08731
H	-4.48564	-1.27864	-0.74096
H	-2.95416	2.37604	0.92844
H	-4.88604	1.03254	0.11031
N	0.00001	-1.03206	0.00012
H	0.00001	-2.04208	0.00007
C	1.26724	-0.43884	-0.01896
C	1.50113	0.85545	-0.51724
C	2.36544	-1.19560	0.43072
C	2.79548	1.37380	-0.53834
H	0.67761	1.44119	-0.90948
C	3.65478	-0.67258	0.38885
H	2.19618	-2.19730	0.82061
C	3.88134	0.62104	-0.08744
H	2.95404	2.37607	-0.92846
H	4.48570	-1.27864	0.74075
H	4.88600	1.03265	-0.11058

PhNH anion
Charge: -1
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy (B3LYP/6-31G(d)): -286.98001
Gibbs Free Energy (B3LYP/6-31G(d)): -286.906462
Electronic Energy (M06/6-311+G(d,p)/SMD(THF)): -286.944222
Total Gibbs Free Energy: -286.870668
Geometry:

N	-2.39359	-0.13326	0.00016
H	-2.77591	0.82326	0.00063
C	-1.06718	-0.03067	0.00007
C	-0.29376	1.19741	-0.00018
C	-0.24296	-1.22477	-0.00024
C	1.09430	1.21479	-0.00005
H	-0.84290	2.14254	-0.00053
C	1.14006	-1.18349	0.00007
H	-0.76946	-2.17889	-0.00057
C	1.85301	0.03284	0.00015
H	1.60742	2.18075	-0.00011
H	1.69396	-2.12632	-0.00007
H	2.94123	0.05489	0.00064

L1-Ni(Ph)-aniline complex
Charge: 1
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -2809.145002
Gibbs Free Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -2808.494308
Electronic Energy (M06/6-311+G(d,p)-SDD(Ni,Fe)/SMD(THF)): -2808.297250
Total Gibbs Free Energy: -2807.646556
Geometry:

P	1.87844	-0.15412	0.36660
P	-1.61238	-0.67604	-0.20104
C	2.11376	-1.60889	-0.70526
C	2.67526	-2.89508	-0.38511
C	1.76289	-1.64190	-2.10330
C	2.65692	-3.69596	-1.56094
H	3.00697	-3.22037	0.58986
C	2.09477	-2.92557	-2.61982
H	1.31597	-0.82795	-2.65825
H	2.97527	-4.72849	-1.62518
H	1.91859	-3.26725	-3.63152
Fe	0.72584	-3.06962	-1.03439
C	-0.75027	-4.52230	-1.35254
C	-1.26190	-3.22143	-1.61999
C	-0.31125	-4.55804	0.00311
H	-0.68158	-5.33262	-2.06660
C	-1.13246	-2.43164	-0.42526
H	-1.66011	-2.88022	-2.56498
C	-0.53744	-3.27603	0.57929
H	0.15324	-5.39993	0.50021
H	-0.29635	-2.98332	1.59214
Ni	0.09756	1.05407	-0.36133
C	1.36441	2.36421	-0.96086
C	1.92439	3.37014	-0.15942
C	1.61482	2.40724	-2.34361
C	2.70438	4.38736	-0.71946
H	1.77466	3.36078	0.91836
C	2.40406	3.41893	-2.90652
H	1.19973	1.64631	-3.00508
C	2.94847	4.41401	-2.09433
H	3.12675	5.15627	-0.07728
H	2.58926	3.42528	-3.97801
H	3.55803	5.20206	-2.52718
C	1.71009	-0.77931	2.09208
C	0.56320	-0.47821	2.83805
C	2.73841	-1.52278	2.70086
C	0.42017	-0.94257	4.14850
H	-0.22290	0.12441	2.39913
C	2.59319	-1.99014	4.00618
H	3.66390	-1.71479	2.16757
C	1.43071	-1.70736	4.73060
H	-0.47926	-0.70162	4.70765
H	3.39324	-2.56574	4.46283
H	1.32333	-2.06972	5.74890
C	3.55954	0.60470	0.40306
C	3.99788	1.30039	1.54101
C	4.40655	0.51533	-0.71115
C	5.26226	1.88884	1.56413
H	3.36134	1.37527	2.41753
C	5.67033	1.10662	-0.68420
H	4.08739	-0.01819	-1.60053
C	6.10105	1.79374	0.45191
H	5.59229	2.41798	2.45366
H	6.31926	1.02427	-1.55137
H	7.08704	2.24897	0.47228
C	-2.73931	-0.75729	1.25748
C	-2.87101	0.35785	2.10015

C	-3.48000	-1.91766	1.54489
C	-3.72392	0.31510	3.20517
H	-2.31337	1.26660	1.89788
C	-4.33196	-1.95644	2.64898
H	-3.38979	-2.79329	0.90983
C	-4.45432	-0.84149	3.48209
H	-3.81569	1.18792	3.84504
H	-4.89776	-2.85954	2.85928
H	-5.11548	-0.87591	4.34327
C	-2.73784	-0.42718	-1.65395
C	-2.16252	-0.18031	-2.91524
C	-4.13602	-0.46938	-1.54888
C	-2.96497	0.00747	-4.04290
H	-1.08045	-0.14450	-3.02107
C	-4.93705	-0.27412	-2.67762
H	-4.60428	-0.65593	-0.58830
C	-4.35640	-0.03660	-3.92463
H	-2.50357	0.18851	-5.00959
H	-6.01824	-0.31153	-2.57920
H	-4.98265	0.11362	-4.79899
C	-2.16003	3.10832	-0.05819
C	-3.54996	3.00012	-0.14562
C	-1.57565	3.89619	0.93904
C	-4.35649	3.67090	0.77653
H	-4.00288	2.39708	-0.92795
C	-2.38982	4.56692	1.85224
H	-0.49624	3.99459	0.98522
C	-3.78084	4.45308	1.77838
H	-5.43662	3.58530	0.70264
H	-1.93362	5.18560	2.61965
H	-4.40998	4.97959	2.48968
H	-0.72835	3.08143	-1.51042
H	-1.89501	1.94969	-1.71238
N	-1.31039	2.40702	-1.01005

L1-Ni(Ph)-NHPh
Charge: 0
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -2808.695922
Gibbs Free Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -2808.062833
Electronic Energy (M06/6-311+G(d,p)-SDD(Ni,Fe)/SMD(THF)): -2807.819009
Total Gibbs Free Energy: -2807.185920
Geometry:

P	1.64723	-0.71653	0.31468
P	-1.86145	-0.24761	-0.15922
C	1.38637	-2.30522	-0.55403
C	1.53299	-3.64891	-0.06381
C	1.00884	-2.40487	-1.94025
C	1.24646	-4.55062	-1.12849
H	1.77563	-3.92584	0.95249
C	0.92528	-3.78319	-2.28757
H	0.80475	-1.57042	-2.59739
H	1.23155	-5.63082	-1.05627
H	0.62872	-4.17722	-3.25118
Fe	-0.39534	-3.32240	-0.73351
C	-2.23772	-4.27181	-0.96589

C	-2.33986	-2.90174	-1.34575
C	-1.82525	-4.32218	0.39889
H	-2.41423	-5.12328	-1.61090
C	-1.98312	-2.08697	-0.21935
H	-2.61202	-2.53137	-2.32451
C	-1.65655	-2.98368	0.85867
H	-1.62940	-5.21853	0.97371
H	-1.32662	-2.68942	1.84599
Ni	0.26005	0.97079	-0.29893
C	1.68340	1.93517	-1.13262
C	2.38121	3.02102	-0.58264
C	2.01534	1.55424	-2.44549
C	3.36920	3.69381	-1.30890
H	2.14021	3.36967	0.41795
C	2.99611	2.22957	-3.18135
H	1.51044	0.71116	-2.91808
C	3.68137	3.30378	-2.61275
H	3.89085	4.53324	-0.85306
H	3.22415	1.91087	-4.19702
H	4.44679	3.83014	-3.17792
C	1.47871	-1.13812	2.11150
C	0.41720	-0.60216	2.85595
C	2.41151	-1.96265	2.76407
C	0.27246	-0.90554	4.21265
H	-0.29754	0.06112	2.37890
C	2.26475	-2.26824	4.11720
H	3.26528	-2.35223	2.21754
C	1.19217	-1.74377	4.84381
H	-0.55564	-0.47879	4.77181
H	2.99419	-2.90811	4.60679
H	1.08286	-1.97789	5.89935
C	3.47584	-0.48890	0.17567
C	4.08784	0.51543	0.94299
C	4.26905	-1.27307	-0.67199
C	5.46440	0.71871	0.87391
H	3.48614	1.14268	1.59402
C	5.64886	-1.06294	-0.74446
H	3.81602	-2.04958	-1.27950
C	6.24936	-0.07046	0.02913
H	5.92297	1.50035	1.47343
H	6.25099	-1.67929	-1.40689
H	7.32242	0.09193	-0.02738
C	-3.07613	0.15108	1.18378
C	-3.02734	1.41656	1.79332
C	-4.03719	-0.77462	1.62667
C	-3.91239	1.74066	2.82304
H	-2.30817	2.14963	1.45009
C	-4.92182	-0.44435	2.65539
H	-4.09779	-1.75835	1.17292
C	-4.86029	0.81299	3.25871
H	-3.85643	2.72450	3.28115
H	-5.65857	-1.17321	2.98354
H	-5.54766	1.06777	4.06125
C	-2.74699	0.19992	-1.72360
C	-1.98966	0.42712	-2.88372
C	-4.14439	0.28622	-1.80256
C	-2.61406	0.72438	-4.09675

H	-0.90460	0.39190	-2.83365
C	-4.76821	0.58865	-3.01445
H	-4.74884	0.12673	-0.91527
C	-4.00623	0.80571	-4.16440
H	-2.01128	0.90265	-4.98330
H	-5.85200	0.65815	-3.05759
H	-4.49409	1.04386	-5.10578
N	-0.86642	2.49324	-0.46913
H	-1.14018	2.66329	-1.43488
C	-0.69320	3.68834	0.19715
C	-1.04844	4.93278	-0.38258
C	-0.22431	3.71940	1.53579
C	-0.95294	6.12038	0.33454
H	-1.40332	4.94799	-1.41177
C	-0.12330	4.91626	2.24201
H	0.06506	2.78192	2.00743
C	-0.48921	6.13043	1.65501
H	-1.23686	7.05384	-0.14722
H	0.24455	4.89777	3.26619
H	-0.41305	7.06135	2.20964

L2-Ni(Ph)-aniline complex
Charge: 1
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -4157.263469
Gibbs Free Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -4156.618537
Electronic Energy (M06/6-311+G(d,p)-SDD(Ni,Fe)/SMD(THF)): -4156.428095
Total Gibbs Free Energy: -4155.783164
Geometry:

P	-1.92467	-0.21625	-0.45640
P	1.64698	-0.19398	-0.54667
C	-1.81939	-0.77887	-2.18608
C	-2.26856	-0.12740	-3.38936
C	-1.23503	-2.03620	-2.58480
C	-1.95565	-0.96632	-4.49460
H	-2.72148	0.85087	-3.45593
C	-1.31873	-2.14136	-4.00107
H	-0.80585	-2.77053	-1.91626
H	-2.13284	-0.72845	-5.53553
H	-0.93403	-2.95642	-4.60003
Fe	-0.22944	-0.44061	-3.42152
C	1.43329	-0.06725	-4.64530
C	1.83250	-0.69966	-3.43457
C	0.78207	1.15660	-4.31564
H	1.57717	-0.46474	-5.64158
C	1.41764	0.12998	-2.33538
H	2.34067	-1.65027	-3.35614
C	0.76203	1.28375	-2.89821
H	0.34047	1.85233	-5.01739
H	0.32295	2.09973	-2.34127
Ni	-0.21369	-1.08810	0.75336
C	-1.53068	-2.19754	1.60037
C	-2.28879	-1.81665	2.71736
C	-1.61301	-3.53174	1.16719
C	-3.10092	-2.74018	3.38447
H	-2.27091	-0.78747	3.07084

C	-2.43219	-4.45646	1.82856
H	-1.04236	-3.87113	0.30280
C	-3.17666	-4.06216	2.94074
H	-3.67862	-2.42235	4.24878
H	-2.48450	-5.48199	1.47140
H	-3.81080	-4.77708	3.45682
C	-1.96271	1.62961	-0.49119
C	-0.99592	2.36432	0.20663
C	-2.97993	2.32453	-1.17100
H	-0.22172	1.85032	0.76393
H	-3.77557	1.78278	-1.67139
C	-2.00811	4.43629	-0.50676
C	-3.67227	-0.60108	-0.00050
C	-4.34132	0.18002	0.95526
C	-4.34167	-1.68423	-0.58581
H	-3.84521	1.02574	1.42133
H	-3.84498	-2.30399	-1.32482
C	-6.31500	-1.19129	0.71883
C	2.55544	1.31634	0.00457
C	2.41943	1.77324	1.32422
C	3.38747	2.02680	-0.87864
H	1.79093	1.23982	2.02970
H	3.50632	1.69445	-1.90481
C	3.91930	3.61116	0.86690
C	2.93492	-1.52730	-0.58696
C	2.51938	-2.84543	-0.85557
C	4.29608	-1.28628	-0.35460
H	1.47004	-3.05658	-1.04559
H	4.64717	-0.28170	-0.14616
C	4.79287	-3.63582	-0.65851
C	1.72772	-1.20581	3.12114
C	3.12034	-1.14444	3.20670
C	0.93320	-0.52682	4.05089
C	3.71963	-0.38803	4.21676
H	3.73669	-1.68615	2.49443
C	1.54082	0.22180	5.05975
H	-0.14765	-0.60188	3.99471
C	2.93397	0.29894	5.14299
H	4.80281	-0.34667	4.28194
H	0.92193	0.73962	5.78671
H	3.40215	0.87989	5.93167
C	4.06643	3.16511	-0.44966
H	4.71277	3.70371	-1.13472
C	3.09763	2.91413	1.75394
H	2.99350	3.25333	2.77887
C	-5.65509	-0.11164	1.31156
H	-6.16563	0.49542	2.05193
C	-5.65732	-1.97728	-0.22845
H	-6.16978	-2.81727	-0.68484
C	-2.99641	3.71644	-1.18698
H	-3.77723	4.24494	-1.72409
C	-1.01261	3.76053	0.19815
H	-0.25124	4.31763	0.73355
C	5.21875	-2.33423	-0.38998
H	6.27104	-2.13565	-0.21624
C	3.43936	-3.89177	-0.89748
H	3.10932	-4.90141	-1.12001

C	4.60728	4.88078	1.31094
C	5.77588	-4.78314	-0.63519
C	-7.75902	-1.46398	1.06265
C	-2.06677	5.94599	-0.48211
F	3.84164	5.95996	1.04656
F	4.85002	4.87271	2.63693
F	5.78161	5.05278	0.67350
F	5.45601	-5.71897	-1.55055
F	5.77620	-5.38581	0.57286
F	7.03120	-4.36629	-0.88239
F	-8.58688	-0.71881	0.29964
F	-8.08298	-2.75725	0.86422
F	-8.02342	-1.16300	2.35096
F	-2.88477	6.37912	0.49870
F	-0.85072	6.48429	-0.26436
F	-2.53717	6.43587	-1.64628
H	0.49608	-2.70245	2.48759
H	1.80637	-2.48203	1.53428
N	1.09019	-1.98510	2.06741

L2-Ni(Ph)-NHPh
Charge: 0
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -4156.830546
Gibbs Free Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -4156.203973
Electronic Energy (M06/6-311+G(d,p)-SDD(Ni,Fe)/SMD(THF)): -4155.956223
Total Gibbs Free Energy: -4155.329650
Geometry:

P	-1.79936	-0.12726	-0.57190
P	1.77032	-0.15666	-0.52473
C	-1.61782	-0.59351	-2.33039
C	-1.98273	0.13412	-3.51643
C	-1.07026	-1.85368	-2.76492
C	-1.66081	-0.66435	-4.65066
H	-2.39104	1.13453	-3.54458
C	-1.09964	-1.89137	-4.18779
H	-0.68694	-2.62925	-2.11579
H	-1.77963	-0.36907	-5.68539
H	-0.72233	-2.69379	-4.80838
Fe	0.04286	-0.27812	-3.50373
C	1.77219	-0.00893	-4.64275
C	2.08657	-0.65762	-3.41351
C	1.18053	1.25265	-4.33896
H	1.92772	-0.41878	-5.63259
C	1.68436	0.19519	-2.33113
H	2.52771	-1.63925	-3.30939
C	1.11307	1.37889	-2.92115
H	0.80618	1.97121	-5.05699
H	0.69651	2.21802	-2.38050
Ni	-0.15753	-0.84220	0.82115
C	-1.34175	-2.05527	1.70168
C	-1.96895	-1.84537	2.93877
C	-1.55750	-3.29259	1.06898
C	-2.78058	-2.82723	3.51684
H	-1.81036	-0.91553	3.47863
C	-2.36008	-4.28309	1.64743

H	-1.10231	-3.50415	0.10080
C	-2.97924	-4.05193	2.87627
H	-3.25206	-2.63393	4.47828
H	-2.50142	-5.23191	1.13330
H	-3.60693	-4.81537	3.32881
C	-1.93753	1.72301	-0.59831
C	-0.93729	2.50200	0.00104
C	-3.03865	2.37354	-1.18149
H	-0.09147	2.02169	0.48270
H	-3.84603	1.79318	-1.61701
C	-2.10370	4.52735	-0.60870
C	-3.55443	-0.59286	-0.21965
C	-4.14108	-0.15287	0.97805
C	-4.31271	-1.37713	-1.09759
H	-3.56529	0.44008	1.68162
H	-3.87875	-1.73641	-2.02448
C	-6.20943	-1.25398	0.39445
C	2.87970	1.21458	0.05611
C	2.95148	1.50059	1.42987
C	3.63777	1.99304	-0.83557
H	2.39483	0.89482	2.13347
H	3.60871	1.79078	-1.90061
C	4.48990	3.31684	0.99807
C	2.87377	-1.64697	-0.52269
C	2.28904	-2.92114	-0.46182
C	4.26986	-1.55039	-0.61621
H	1.21211	-3.01912	-0.35844
H	4.74794	-0.57688	-0.65000
C	4.46403	-3.96038	-0.60352
N	1.14755	-1.14622	2.16701
H	1.51622	-2.09510	2.13218
C	1.01283	-0.74011	3.48277
C	1.52479	-1.50300	4.56103
C	0.42485	0.50893	3.80409
C	1.46408	-1.03709	5.87019
H	1.97445	-2.47192	4.35094
C	0.35907	0.96233	5.12028
H	0.01510	1.11553	2.99838
C	0.88075	0.19950	6.16797
H	1.87029	-1.65163	6.67057
H	-0.10258	1.92558	5.32761
H	0.83264	0.55753	7.19222
C	4.43730	3.03551	-0.36891
H	5.02405	3.62395	-1.06690
C	3.74808	2.54555	1.89584
H	3.79449	2.75242	2.96006
C	-5.45963	-0.47516	1.28153
H	-5.90161	-0.13700	2.21296
C	-5.63415	-1.70716	-0.79264
H	-6.21236	-2.31988	-1.47623
C	-3.11895	3.76375	-1.19390
H	-3.96839	4.25612	-1.65647
C	-1.01583	3.89601	-0.00458
H	-0.23262	4.48658	0.45886
C	5.06050	-2.69756	-0.65488
H	6.14066	-2.61084	-0.71554
C	3.07569	-4.07184	-0.50500

H	2.61252	-5.05115	-0.44577
C	5.30049	4.48534	1.49322
C	5.31801	-5.19633	-0.70965
C	-7.65304	-1.55206	0.69962
C	-2.22708	6.02908	-0.57567
F	4.56806	5.62375	1.50560
F	5.74849	4.29136	2.75136
F	6.37521	4.71931	0.70755
F	5.56194	-5.51463	-2.00299
F	4.72591	-6.26958	-0.14425
F	6.51842	-5.02865	-0.11481
F	-8.46401	-0.55420	0.27334
F	-8.07452	-2.68457	0.09659
F	-7.86763	-1.69029	2.02554
F	-2.98584	6.43790	0.46532
F	-1.02511	6.62991	-0.45400
F	-2.81046	6.50332	-1.69868

L4-Ni(Ph)-aniline complex
Charge: 1
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy (B3LYP/6-31G(d)-SDD(Ni)): -5226.635560
Gibbs Free Energy (B3LYP/6-31G(d)-SDD(Ni)): -5226.059354
Electronic Energy (M06/6-311+G(d,p)-SDD(Ni)/SMD(THF)): -5225.864123
Total Gibbs Free Energy: -5225.287917
Geometry:

P	-1.53437	-0.12991	-0.45527
P	1.56018	-0.51330	-0.51119
Ni	-0.05406	-0.43111	1.13803
C	-1.55848	-0.48376	2.33668
C	-2.16615	0.65824	2.87974
C	-1.99846	-1.74547	2.77512
C	-3.18299	0.54233	3.83714
H	-1.84931	1.65258	2.57581
C	-3.01018	-1.86244	3.73498
H	-1.56906	-2.65727	2.35936
C	-3.60861	-0.71666	4.26473
H	-3.63996	1.43993	4.24624
H	-3.33553	-2.84747	4.05929
H	-4.40229	-0.80549	5.00054
C	-2.12505	1.60810	-0.55527
C	-1.30990	2.60249	-0.00098
C	-3.29651	1.97910	-1.22867
C	-1.65347	3.94902	-0.12500
H	-0.40253	2.33321	0.53139
C	-3.63626	3.32732	-1.34605
H	-3.95700	1.23050	-1.65173
C	-2.81804	4.31721	-0.79730
H	-3.08897	5.36288	-0.89038
C	-3.01991	-1.20789	-0.48231
C	-4.14349	-0.88567	0.29439
C	-2.99930	-2.41748	-1.18693
C	-5.23203	-1.75401	0.34192
H	-4.17400	0.03120	0.87140
C	-4.09356	-3.28438	-1.12785
H	-2.14587	-2.69100	-1.79750

C	-5.21460	-2.95616	-0.36892
H	-6.06832	-3.62332	-0.33712
C	2.66515	0.94878	-0.68432
C	3.90320	1.02100	-0.03689
C	2.17799	2.08903	-1.34477
C	4.62898	2.21632	-0.03175
H	4.31818	0.15465	0.46858
C	2.90905	3.27386	-1.34019
H	1.22448	2.06328	-1.85949
C	4.13719	3.34732	-0.67720
H	4.69779	4.27478	-0.66036
C	2.64378	-1.99766	-0.46757
C	2.15927	-3.11072	0.23250
C	3.88111	-2.09303	-1.12301
C	2.89489	-4.29631	0.28093
H	1.19858	-3.06158	0.73777
C	4.61276	-3.27967	-1.06856
H	4.28490	-1.25121	-1.67486
C	4.12507	-4.38563	-0.36744
H	4.69894	-5.30441	-0.32779
C	-0.78993	4.99400	0.54176
C	-4.86945	3.72355	-2.12742
C	-6.40877	-1.42510	1.23187
C	-4.01673	-4.60502	-1.85759
C	5.92497	2.25983	0.74222
C	2.39266	4.48447	-2.08495
C	5.97284	-3.34741	-1.72912
C	2.31180	-5.48343	1.01253
F	1.05787	4.40925	-2.28540
F	2.65015	5.61737	-1.41016
F	2.97535	4.58816	-3.29539
F	6.59071	3.40794	0.55480
F	6.73093	1.23749	0.39556
F	5.68298	2.13354	2.07276
F	6.93861	-2.95863	-0.87433
F	6.03018	-2.53362	-2.80365
F	6.25926	-4.59704	-2.13219
F	3.25162	-6.38676	1.32923
F	1.70736	-5.08557	2.15771
F	1.37557	-6.09809	0.26437
F	-0.90189	6.18967	-0.05637
F	0.51571	4.63408	0.52183
F	-1.13548	5.14500	1.83722
F	-5.43090	4.83713	-1.62529
F	-5.79366	2.74168	-2.11290
F	-4.55916	3.96780	-3.41687
F	-6.56411	-0.09330	1.37098
F	-7.55384	-1.93186	0.73976
F	-6.23335	-1.94229	2.46662
F	-5.23420	-5.13225	-2.06803
F	-3.40787	-4.46223	-3.05500
F	-3.29549	-5.50080	-1.15082
C	1.47932	0.37754	3.60192
C	0.67526	0.71037	4.69459
C	2.62600	1.12012	3.31745
C	1.01916	1.80567	5.48900
H	-0.20716	0.12293	4.92628

C	2.96251	2.21274	4.11726
H	3.27250	0.84434	2.49162
C	2.15702	2.56228	5.20212
H	0.39538	2.05990	6.34070
H	3.86150	2.77665	3.88957
H	2.42028	3.41018	5.82679
C	0.66871	-0.58939	-2.11858
C	-0.72740	-0.41117	-2.09519
C	1.32778	-0.77861	-3.34274
C	-1.44364	-0.41029	-3.30240
C	0.60515	-0.78833	-4.53360
H	2.40389	-0.92046	-3.36947
C	-0.78074	-0.60033	-4.51317
H	-2.52030	-0.27086	-3.30022
H	1.12042	-0.93956	-5.47723
H	-1.34415	-0.60368	-5.44131
H	1.98566	-1.25212	2.48598
H	0.58089	-1.42654	3.30819
N	1.13038	-0.76442	2.75735

L4-Ni(Ph)-NHPh
Charge: 0
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy (B3LYP/6-31G(d)-SDD(Ni)): -5226.203451
Gibbs Free Energy (B3LYP/6-31G(d)-SDD(Ni)): -5225.644753
Electronic Energy (M06/6-311+G(d,p)-SDD(Ni)/SMD(THF)): -5225.394255
Total Gibbs Free Energy: -5224.835557
Geometry:

P	1.43846	-0.19714	-0.54299
P	-1.59115	0.37706	-0.45584
Ni	-0.03557	-0.18901	1.09730
C	1.34013	-0.27617	2.43302
C	1.90384	-1.46822	2.91911
C	1.80452	0.93368	2.98447
C	2.90435	-1.45208	3.89813
H	1.55299	-2.43000	2.55227
C	2.79823	0.95383	3.96986
H	1.39146	1.88617	2.65192
C	3.35975	-0.24117	4.42385
H	3.32243	-2.39142	4.25385
H	3.13767	1.90457	4.37444
H	4.13790	-0.22893	5.18254
C	2.24654	-1.83367	-0.80274
C	1.59126	-2.95905	-0.29102
C	3.45512	-2.00288	-1.49225
C	2.13051	-4.23454	-0.47183
H	0.66673	-2.84480	0.26767
C	3.98594	-3.28051	-1.67369
H	4.00157	-1.14520	-1.86990
C	3.32719	-4.40231	-1.16383
H	3.74970	-5.39141	-1.29450
C	2.82453	1.01058	-0.47979
C	3.87874	0.78656	0.42211
C	2.78021	2.21653	-1.18905
C	4.88040	1.74323	0.57818
H	3.91997	-0.12664	1.00476

C	3.78210	3.17537	-1.01543
H	1.97718	2.41598	-1.88946
C	4.83814	2.94161	-0.13747
H	5.62389	3.67856	-0.01730
C	-3.14998	-0.57210	-0.61993
C	-4.04128	-0.53428	0.46889
C	-3.42490	-1.42036	-1.69702
C	-5.19777	-1.30958	0.45065
H	-3.81015	0.07591	1.33478
C	-4.58891	-2.19626	-1.70261
H	-2.74536	-1.48341	-2.54012
C	-5.48167	-2.14104	-0.63649
H	-6.38859	-2.73330	-0.65078
C	-2.13272	2.12156	-0.19599
C	-1.23385	2.96706	0.46240
C	-3.35188	2.64423	-0.64765
C	-1.53250	4.31832	0.64667
H	-0.29840	2.56784	0.84333
C	-3.65114	3.99279	-0.45071
H	-4.07355	2.00728	-1.14701
C	-2.74156	4.83808	0.19114
H	-2.97581	5.88643	0.33541
C	1.41575	-5.41010	0.14848
C	5.25149	-3.45920	-2.47476
C	5.98666	1.52016	1.58057
C	3.67749	4.49227	-1.74243
C	-6.12824	-1.29686	1.63966
C	-4.84768	-3.08648	-2.89080
C	-4.98576	4.54350	-0.88925
C	-0.50039	5.20130	1.30230
F	-3.89041	-4.03216	-3.01274
F	-6.03562	-3.71508	-2.81011
F	-4.83807	-2.37502	-4.04275
F	-7.40842	-1.51222	1.26092
F	-6.08698	-0.11529	2.28891
F	-5.80827	-2.25759	2.52713
F	-5.86300	4.58155	0.13534
F	-5.53970	3.79126	-1.86423
F	-4.86783	5.80351	-1.35886
F	-1.01957	6.37967	1.69697
F	0.03872	4.60128	2.38699
F	0.51788	5.46722	0.45445
F	1.93455	-6.58669	-0.25658
F	0.10271	-5.40685	-0.17477
F	1.49213	-5.36947	1.49416
F	5.95556	-4.53162	-2.06149
F	6.05405	-2.37733	-2.38736
F	4.97639	-3.64359	-3.78594
F	6.19928	0.21026	1.81045
F	7.15060	2.05808	1.15239
F	5.69714	2.09871	2.76521
F	4.88657	5.06084	-1.92595
F	3.10512	4.34237	-2.95827
F	2.91923	5.37287	-1.05518
N	-1.36878	-0.39200	2.45574
H	-1.16310	0.22673	3.23980
C	-1.52819	-1.68848	2.94036

C	-1.64493	-1.96756	4.32170
C	-1.61875	-2.78955	2.05446
C	-1.84535	-3.26593	4.78259
H	-1.57353	-1.14534	5.03137
C	-1.79971	-4.08896	2.52395
H	-1.56514	-2.60571	0.98344
C	-1.91834	-4.34222	3.89285
H	-1.93236	-3.44022	5.85279
H	-1.84275	-4.90889	1.81111
H	-2.06158	-5.35482	4.25859
C	-0.79524	0.42093	-2.12379
C	0.58929	0.14508	-2.15978
C	-1.46819	0.73300	-3.31512
C	1.26219	0.15595	-3.39097
C	-0.78720	0.74409	-4.53115
H	-2.52889	0.96655	-3.29492
C	0.57852	0.44896	-4.56967
H	2.32547	-0.06101	-3.43210
H	-1.31981	0.98247	-5.44726
H	1.11089	0.45274	-5.51638

L1-Ni(Ph)-NHPh reductive elimination TS
Charge: 0
Multiplicity: 1
Imaginary Frequencies: 1
Electronic Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -2808.665340
Gibbs Free Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -2808.031665
Electronic Energy (M06/6-311+G(d,p)-SDD(Ni,Fe)/SMD(THF)): -2807.792199
Total Gibbs Free Energy: -2807.158524
Geometry:

P	1.67193	-0.62539	0.30675
P	-1.89003	-0.32459	-0.13404
C	1.47719	-2.25306	-0.52252
C	1.68160	-3.58316	-0.02017
C	1.04801	-2.38473	-1.88964
C	1.38326	-4.51040	-1.06065
H	1.96688	-3.83746	0.99109
C	0.99436	-3.77033	-2.21701
H	0.80706	-1.55830	-2.54593
H	1.40547	-5.58950	-0.97304
H	0.67833	-4.18838	-3.16439
Fe	-0.28544	-3.33994	-0.62023
C	-2.07681	-4.40699	-0.70246
C	-2.28302	-3.07481	-1.16654
C	-1.60450	-4.33919	0.64149
H	-2.22917	-5.30918	-1.28136
C	-1.93235	-2.16533	-0.11385
H	-2.62854	-2.79551	-2.15188
C	-1.50282	-2.96475	1.00352
H	-1.32673	-5.18009	1.26428
H	-1.14663	-2.58478	1.95171
Ni	0.13379	0.85447	-0.28092
C	1.08070	2.13544	-1.37849
C	2.25229	2.87801	-1.08471
C	0.84669	1.78909	-2.73824
C	3.16368	3.18579	-2.08772

H	2.44501	3.20264	-0.06766
C	1.78617	2.08929	-3.72722
H	-0.08266	1.29778	-3.01803
C	2.95411	2.78709	-3.41595
H	4.06419	3.73787	-1.82604
H	1.58589	1.79135	-4.75513
H	3.67818	3.03144	-4.18789
C	1.69636	-1.06961	2.10875
C	0.65258	-0.62982	2.93675
C	2.74028	-1.81552	2.68238
C	0.63681	-0.94615	4.29801
H	-0.14957	-0.03124	2.51487
C	2.72503	-2.13256	4.04132
H	3.57679	-2.13554	2.06786
C	1.67110	-1.70194	4.85193
H	-0.18041	-0.59454	4.92222
H	3.54068	-2.71004	4.46886
H	1.66302	-1.94590	5.91098
C	3.46242	-0.25817	0.01414
C	4.08069	0.73454	0.79270
C	4.20954	-0.88567	-0.99203
C	5.41639	1.07411	0.58483
H	3.51655	1.23882	1.57312
C	5.54510	-0.53627	-1.20765
H	3.75332	-1.65206	-1.61022
C	6.15329	0.43989	-0.41868
H	5.88006	1.83905	1.20240
H	6.10963	-1.03433	-1.99174
H	7.19351	0.70745	-0.58462
C	-3.00288	0.08919	1.28591
C	-2.79079	1.29887	1.96716
C	-4.04246	-0.75547	1.71035
C	-3.60091	1.65543	3.04824
H	-1.99492	1.96535	1.64951
C	-4.84691	-0.39916	2.79326
H	-4.22130	-1.69441	1.19490
C	-4.62740	0.80668	3.46498
H	-3.42328	2.59598	3.56274
H	-5.64573	-1.06369	3.11248
H	-5.25437	1.08140	4.30929
C	-2.93159	0.07667	-1.61543
C	-2.42220	-0.20494	-2.89682
C	-4.17285	0.72305	-1.51947
C	-3.14464	0.12343	-4.04380
H	-1.45185	-0.68318	-2.99776
C	-4.88862	1.06611	-2.67013
H	-4.58778	0.95890	-0.54530
C	-4.38211	0.76350	-3.93394
H	-2.73564	-0.11126	-5.02309
H	-5.84764	1.56840	-2.57298
H	-4.94168	1.02877	-4.82678
N	-0.47221	2.64750	-0.57450
H	-1.07815	2.83460	-1.36764
C	-0.39420	3.73727	0.28897
C	-0.97734	4.97576	-0.05684
C	0.26435	3.64012	1.53358
C	-0.91435	6.06094	0.81188

H	-1.48355	5.07468	-1.01524
C	0.33950	4.74044	2.38628
H	0.70329	2.68712	1.81812
C	-0.25286	5.95741	2.04032
H	-1.37890	7.00053	0.52192
H	0.85592	4.63906	3.33828
H	-0.20250	6.80815	2.71380

L2-Ni(Ph)-NHPh reductive elimination TS
Charge: 0
Multiplicity: 1
Imaginary Frequencies: 1
Electronic Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -4156.801349
Gibbs Free Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -4156.173959
Electronic Energy (M06/6-311+G(d,p)-SDD(Ni,Fe)/SMD(THF)): -4155.930494
Total Gibbs Free Energy: -4155.303103
Geometry:

P	-1.81887800	-0.18935400	-0.64608300
P	1.81138200	-0.14626500	-0.60737300
C	-1.60610500	-0.63908400	-2.40472500
C	-1.97831800	0.08145700	-3.59205800
C	-1.02597600	-1.88428400	-2.83540300
C	-1.63290300	-0.70851000	-4.72541500
H	-2.41002100	1.07206000	-3.62118400
C	-1.04789000	-1.92337400	-4.25880800
H	-0.63447500	-2.65302300	-2.18170700
H	-1.75485900	-0.41552600	-5.76054500
H	-0.65263600	-2.71791600	-4.87864500
Fe	0.05904800	-0.28569400	-3.57719900
C	1.77687700	0.03058100	-4.72017500
C	2.11760800	-0.61498000	-3.49660300
C	1.15535600	1.27524300	-4.40626100
H	1.93673800	-0.37066900	-5.71269400
C	1.70610900	0.22336900	-2.40748700
H	2.58383500	-1.58575400	-3.39977000
C	1.09283400	1.39234200	-2.98672400
H	0.75902000	1.98738500	-5.11882000
H	0.65657800	2.21728900	-2.43946800
Ni	-0.25807200	-0.92531500	0.73505100
C	-1.00210900	-2.12553600	1.98477900
C	-2.00666900	-1.89951700	2.97839500
C	-0.99195400	-3.44172500	1.40379400
C	-2.86349900	-2.90791400	3.38901600
H	-2.08465100	-0.90622900	3.42848600
C	-1.87797000	-4.43281300	1.82022100
H	-0.31104200	-3.66687500	0.58076100
C	-2.81039900	-4.19681400	2.83550400
H	-3.59303600	-2.67781200	4.16374000
H	-1.82589800	-5.40581800	1.33413700
H	-3.47999900	-4.97883800	3.17860800
C	-2.03364400	1.65371100	-0.67117200
C	-1.07003900	2.46413700	-0.05411100
C	-3.15315200	2.26693400	-1.25856400
H	-0.21344400	2.00555000	0.43086000
H	-3.93157800	1.65849800	-1.70895100
C	-2.31235300	4.44874200	-0.64741000
C	-3.55157000	-0.73880100	-0.30933000

C	-4.11788500	-0.41316500	0.93401700
C	-4.29325400	-1.51842100	-1.20649200
H	-3.54671600	0.16260400	1.65550600
H	-3.87046800	-1.79888500	-2.16560200
C	-6.14053600	-1.59531500	0.34986400
C	2.71879700	1.33875200	0.03975900
C	2.73982300	1.51684400	1.43303500
C	3.36650400	2.28739200	-0.76910000
H	2.25606400	0.79247600	2.08149000
H	3.37215900	2.17339300	-1.84757900
C	4.02200800	3.54915400	1.18829700
C	3.14244100	-1.45081800	-0.60088400
C	2.74838900	-2.79209600	-0.71465300
C	4.51488100	-1.16195200	-0.51769200
H	1.69102900	-3.04122500	-0.77506300
H	4.85636200	-0.13812400	-0.41898700
C	5.05038800	-3.51643700	-0.67266700
N	0.56223800	-1.54417300	2.30856700
H	1.09751400	-2.40403500	2.23232900
C	0.73717700	-0.98404100	3.59259200
C	1.36044300	-1.74182600	4.59959100
C	0.23669200	0.28729300	3.91582800
C	1.52065200	-1.21789800	5.88080700
H	1.72257300	-2.74275100	4.37433300
C	0.38851700	0.79896700	5.20534700
H	-0.27451100	0.86383100	3.14964700
C	1.04332700	0.05815000	6.19135800
H	2.01661300	-1.81597000	6.64090000
H	-0.00123200	1.78715200	5.43723400
H	1.16992300	0.46524200	7.19034000
C	4.01061900	3.38505900	-0.19959700
H	4.51397500	4.10795500	-0.83353900
C	3.39045900	2.60868600	2.00555200
H	3.40622300	2.72447200	3.08430000
C	-5.40519900	-0.82806600	1.25879900
H	-5.83237400	-0.57350000	2.22314600
C	-5.58060600	-1.94597900	-0.87897600
H	-6.14637100	-2.55257200	-1.57838600
C	-3.29135900	3.65286400	-1.25118200
H	-4.15702500	4.11700800	-1.71299500
C	-1.20310900	3.85370600	-0.04404300
H	-0.44799800	4.47018100	0.43231100
C	5.45987400	-2.18470600	-0.55147900
H	6.51658400	-1.94882000	-0.47712900
C	3.69089000	-3.82001100	-0.75591000
H	3.36684600	-4.85208600	-0.83985400
C	4.66421600	4.76789400	1.79635800
C	6.08153000	-4.60938800	-0.77012500
C	-7.55412800	-1.99212700	0.67903500
C	-2.49748700	5.94274600	-0.59281000
F	3.78308900	5.78978000	1.90103900
F	5.13221000	4.52265700	3.03879800
F	5.69788400	5.21515300	1.04998400
F	6.50440400	-4.77487400	-2.04551400
F	5.59633300	-5.79951300	-0.35764700
F	7.17514800	-4.33293700	-0.02723900
F	-8.43383100	-1.02117200	0.33258700

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F                 -7.93216800   -3.11286000    0.02644200
F                 -7.72024300   -2.21371600    2.00097600
F                 -3.27903200    6.30592100    0.44904200
F                 -1.32197900    6.59150900   -0.45307600
F                 -3.09247700    6.41128900   -1.71229600

L4-Ni(Ph)-NHPh reductive elimination TS
Charge: 0
Multiplicity: 1
Imaginary Frequencies: 1
Electronic Energy (B3LYP/6-31G(d)-SDD(Ni)): -5226.175481
Gibbs Free Energy (B3LYP/6-31G(d)-SDD(Ni)): -5225.615330
Electronic Energy (M06/6-311+G(d,p)-SDD(Ni)/SMD(THF)): -5225.361618
Total Gibbs Free Energy: -5224.801467
Geometry:
P           1.60635        -0.05049        -0.45323
P          -1.53239        -0.01316        -0.44833
Ni          0.11819         0.12775         1.11299
C           1.11770        -0.08874         2.76759
C           1.00837        -1.41658         3.24155
C           2.25579         0.66572         3.14296
C           2.05258        -1.99171         3.97229
H           0.11231        -1.99789         3.04437
C           3.27588         0.08471         3.88974
H           2.35232         1.70163         2.82373
C           3.19143        -1.25358         4.29983
H           1.96442        -3.02719         4.29248
H           4.15129         0.68076         4.13670
H           3.99187        -1.70288         4.88003
C           2.74082        -1.50655        -0.55130
C           2.34624        -2.66672         0.12400
C           3.94953        -1.51402        -1.26312
C           3.13757        -3.81753         0.08067
H           1.42973        -2.66604         0.70372
C           4.73355        -2.66667        -1.30746
H           4.29783        -0.61958        -1.76796
C           4.33141        -3.82453        -0.63587
H           4.94733        -4.71592        -0.66581
C           2.73974         1.39820        -0.51212
C           3.85709         1.43369         0.33838
C           2.38960         2.56404        -1.21063
C           4.59650         2.60892         0.48489
H           4.14551         0.55349         0.90145
C           3.13908         3.73148        -1.06385
H           1.52319         2.57135        -1.86364
C           4.24608         3.76408        -0.21303
H           4.81910         4.67522        -0.09188
C          -2.70126        -1.43759        -0.60294
C          -3.80963        -1.51595         0.25882
C          -2.42521        -2.52967        -1.43783
C          -4.62272        -2.64822         0.26632
H          -4.03619        -0.69804         0.93503
C          -3.24387        -3.66182        -1.42241
H          -1.57217        -2.50706        -2.10673
C          -4.34698        -3.72962        -0.57405
H          -4.97984        -4.60905        -0.56383
C          -2.62056         1.47662        -0.58022
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C	-2.10281	2.66935	-0.05948
C	-3.88475	1.49662	-1.18522
C	-2.82092	3.86213	-0.16437
H	-1.14362	2.65802	0.44928
C	-4.60554	2.68873	-1.27291
H	-4.32428	0.58464	-1.57429
C	-4.07540	3.87940	-0.77031
H	-4.64029	4.80168	-0.83545
C	2.71122	-5.02654	0.87505
C	5.99724	-2.69010	-2.12998
C	5.72394	2.63316	1.48474
C	2.76021	4.95106	-1.86541
C	-5.76881	-2.73935	1.24237
C	-2.96208	-4.78672	-2.38641
C	-5.94037	2.70106	-1.97473
C	-2.19283	5.13006	0.35671
F	-1.63634	-4.95036	-2.58465
F	-3.46178	-5.96013	-1.94953
F	-3.51395	-4.54270	-3.59689
F	-6.77500	-3.49756	0.76063
F	-6.27120	-1.52580	1.54274
F	-5.37282	-3.30666	2.40869
F	-6.75241	3.66169	-1.48898
F	-6.57871	1.51795	-1.85066
F	-5.79538	2.93473	-3.29921
F	-3.08600	6.13398	0.45994
F	-1.64206	4.94089	1.57655
F	-1.20059	5.55096	-0.45909
F	3.31467	-6.15196	0.44067
F	1.37646	-5.21818	0.79697
F	3.01387	-4.88714	2.18447
F	6.94750	-3.45785	-1.55835
F	6.51040	-1.45262	-2.29642
F	5.76888	-3.19500	-3.36354
F	6.43121	1.48451	1.46656
F	6.58057	3.64951	1.26116
F	5.24839	2.78143	2.74654
F	3.24129	6.08357	-1.31402
F	3.24503	4.88228	-3.12649
F	1.41914	5.07864	-1.96653
N	-0.44905	0.91464	2.74140
H	-0.02351	1.78972	3.02483
C	-1.52802	0.58237	3.56276
C	-1.88732	1.41637	4.64240
C	-2.28979	-0.58024	3.33794
C	-2.98710	1.11256	5.43839
H	-1.30195	2.31217	4.84117
C	-3.38714	-0.88083	4.14555
H	-2.01566	-1.24055	2.52079
C	-3.74744	-0.03693	5.19744
H	-3.25026	1.77768	6.25703
H	-3.96751	-1.77616	3.94073
H	-4.60289	-0.27228	5.82363
C	-0.66065	-0.00111	-2.09227
C	0.75012	-0.02368	-2.09813
C	-1.35197	0.04625	-3.31293
C	1.43494	-0.01413	-3.32308

C	-0.66077	0.05534	-4.52278
H	-2.43773	0.07461	-3.32038
C	0.73645	0.02258	-4.52810
H	2.52057	-0.03184	-3.33849
H	-1.20998	0.08933	-5.45939
H	1.27965	0.02972	-5.46876

L3-Ni(Ph)-DBU complex
Charge: 1
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -5679.904089
Gibbs Free Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -5679.133786
Electronic Energy (M06/6-311+G(d,p)-SDD(Ni,Fe)/SMD(THF)): -5678.992460
Total Gibbs Free Energy: -5678.222156
Geometry:

P	1.88909	-0.05094	0.55918
P	-1.68886	0.37512	0.69341
C	1.65238	-0.35305	2.34725
C	2.22181	0.36651	3.45701
C	0.87766	-1.43498	2.90464
C	1.80213	-0.26293	4.66150
H	2.83464	1.25463	3.39210
C	0.97631	-1.37327	4.32419
H	0.31430	-2.16769	2.34109
H	2.03705	0.07384	5.66294
H	0.47793	-2.03247	5.02299
Fe	0.14963	0.38131	3.53421
C	-1.39431	1.16545	4.72197
C	-1.92178	0.39273	3.64901
C	-0.62195	2.22699	4.17162
H	-1.53956	0.96061	5.77469
C	-1.46401	0.96874	2.41286
H	-2.54619	-0.48168	3.76044
C	-0.65689	2.11404	2.75454
H	-0.07434	2.97410	4.73118
H	-0.17473	2.78647	2.05915
Ni	0.08544	-0.54736	-0.70891
C	1.27383	-0.64042	-2.20994
C	1.46419	0.56274	-2.90961
C	1.84736	-1.80762	-2.73242
C	2.20143	0.59360	-4.10262
H	1.04897	1.49944	-2.54486
C	2.58599	-1.77800	-3.91890
H	1.73675	-2.75275	-2.20958
C	2.76598	-0.57614	-4.60902
H	2.33308	1.53765	-4.62535
H	3.02333	-2.69644	-4.30330
H	3.34324	-0.55304	-5.52869
C	2.54522	1.66752	0.49828
C	1.70032	2.69369	0.07049
C	3.83726	1.99354	0.93875
C	2.12049	4.02568	0.10675
H	0.70279	2.46274	-0.28678
C	4.25670	3.32378	0.96235
H	4.52466	1.21768	1.25832
C	3.39975	4.34851	0.55105

H	3.72947	5.38059	0.57315
C	3.35148	-1.11601	0.18388
C	4.27331	-0.76394	-0.81346
C	3.48294	-2.35262	0.82202
C	5.31114	-1.63228	-1.14705
H	4.17650	0.17220	-1.35104
C	4.50610	-3.23208	0.45816
H	2.79769	-2.64630	1.60901
C	5.42875	-2.87630	-0.52137
H	6.22419	-3.55782	-0.79965
C	-2.33700	1.90264	-0.11982
C	-1.89158	2.24194	-1.40025
C	-3.23692	2.76013	0.53472
C	-2.33507	3.41184	-2.02385
H	-1.18689	1.60271	-1.91990
C	-3.67437	3.92660	-0.08989
H	-3.59593	2.52454	1.53105
C	-3.22725	4.25859	-1.37295
H	-3.57129	5.16692	-1.85394
C	-3.16080	-0.73602	0.80432
C	-3.07395	-1.89457	1.58707
C	-4.32357	-0.52048	0.05417
C	-4.13609	-2.79773	1.64509
H	-2.17945	-2.10075	2.16523
C	-5.37112	-1.44398	0.09181
H	-4.42731	0.36669	-0.55988
C	-5.29166	-2.58180	0.89485
H	-6.11627	-3.28375	0.93855
C	1.14305	5.08749	-0.33061
C	5.62384	3.65862	1.51438
C	6.33813	-1.21919	-2.17543
C	4.53951	-4.59424	1.10409
C	-1.86599	3.69916	-3.42965
C	-4.59169	4.87122	0.65411
C	-6.56258	-1.24535	-0.81453
C	-3.97162	-4.04540	2.47505
F	-3.88119	5.75806	1.37950
F	-5.37092	5.56803	-0.19295
F	-5.39336	4.20169	1.50746
F	-2.10947	4.96548	-3.79781
F	-2.48382	2.88288	-4.31329
F	-0.53767	3.47266	-3.55485
F	-6.32210	-1.79577	-2.03274
F	-6.82281	0.05953	-1.01572
F	-7.66880	-1.82802	-0.32448
F	-5.13815	-4.65678	2.71864
F	-3.16818	-4.94189	1.83331
F	-3.37584	-3.77610	3.65520
F	1.62912	6.32728	-0.17881
F	-0.00348	4.99692	0.39344
F	0.79353	4.92733	-1.62471
F	6.10191	4.80188	0.99345
F	6.50848	2.67513	1.25850
F	5.56820	3.81176	2.85539
F	5.84080	-0.30806	-3.03605
F	7.41894	-0.66938	-1.58487
F	6.76501	-2.27801	-2.89172

F	5.70472	-5.22795	0.89827
F	4.33221	-4.51230	2.43483
F	3.55219	-5.38265	0.60476
N	-1.22081	-1.58431	-1.77741
C	-1.47185	-2.85450	-1.53024
C	-1.89367	-0.93242	-2.91233
C	-0.67086	-3.55431	-0.44887
N	-2.38447	-3.59663	-2.20686
H	-1.21018	-0.18344	-3.31903
H	-2.79035	-0.40696	-2.55447
C	-2.27338	-1.93070	-4.00085
C	0.15043	-4.77626	-0.93393
H	0.01129	-2.80213	-0.03635
H	-1.33407	-3.86680	0.36706
C	-2.81493	-4.93655	-1.75791
C	-3.08651	-3.05611	-3.38186
H	-1.36247	-2.33380	-4.45864
H	-2.85203	-1.43600	-4.78708
C	-0.64529	-6.08531	-1.01593
H	0.59481	-4.55158	-1.91115
H	0.98745	-4.91534	-0.23969
C	-1.80236	-6.05933	-2.02161
H	-3.74420	-5.14215	-2.29566
H	-3.07559	-4.90382	-0.69433
H	-3.22169	-3.87462	-4.09646
H	-4.08465	-2.70597	-3.08458
H	-1.04489	-6.32210	-0.01936
H	0.03979	-6.90125	-1.27436
H	-2.33798	-7.01557	-1.97382
H	-1.42149	-5.96349	-3.04723

L3-Ni(Ph)-NEt3 complex
Charge: 1
Multiplicity: 1
Imaginary Frequencies: 0
Electronic Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -5510.168580
Gibbs Free Energy (B3LYP/6-31G(d)-SDD(Ni,Fe)): -5509.437492
Electronic Energy (M06/6-311+G(d,p)-SDD(Ni,Fe)/SMD(THF)): -5509.330140
Total Gibbs Free Energy: -5508.599052
Geometry:

P	-1.80056	-0.32468	-0.44574
P	1.79595	-0.19562	-0.51126
C	-1.50119	-0.94608	-2.13335
C	-2.01571	-0.43460	-3.37997
C	-0.76433	-2.14627	-2.44424
C	-1.58999	-1.30083	-4.42426
H	-2.59100	0.47050	-3.51236
C	-0.81951	-2.35345	-3.85128
H	-0.24370	-2.76995	-1.72947
H	-1.78281	-1.15627	-5.47942
H	-0.32825	-3.15127	-4.39283
Fe	0.04561	-0.50269	-3.36898
C	1.66626	0.01550	-4.59995
C	2.10910	-0.58445	-3.38897
C	0.91829	1.18245	-4.27231
H	1.84617	-0.36761	-5.59590
C	1.62210	0.20865	-2.28856

H	2.68425	-1.49591	-3.31049
C	0.88475	1.31006	-2.85589
H	0.42902	1.84404	-4.97528
H	0.39996	2.10519	-2.30775
Ni	-0.12714	-0.70833	1.03441
C	-1.52796	-0.44517	2.29790
C	-1.59364	0.82157	2.90124
C	-2.37997	-1.45491	2.77024
C	-2.45858	1.05542	3.97905
H	-0.95987	1.63997	2.56842
C	-3.23597	-1.22478	3.85112
H	-2.38899	-2.43585	2.30044
C	-3.27848	0.03311	4.45822
H	-2.48613	2.04006	4.43844
H	-3.87758	-2.02573	4.20959
H	-3.95272	0.21675	5.28947
C	-2.15469	1.47077	-0.67284
C	-1.23475	2.41632	-0.21313
C	-3.30300	1.91728	-1.34373
C	-1.43947	3.77941	-0.43870
H	-0.35060	2.09727	0.32685
C	-3.50045	3.27972	-1.57234
H	-4.05562	1.21316	-1.68183
C	-2.57002	4.21925	-1.12378
H	-2.73114	5.27646	-1.29768
C	-3.47496	-1.04740	-0.12613
C	-4.41103	-0.38073	0.67971
C	-3.81570	-2.28434	-0.68083
C	-5.66495	-0.94110	0.90901
H	-4.16282	0.56491	1.14733
C	-5.07033	-2.84974	-0.42962
H	-3.12027	-2.81713	-1.31990
C	-6.00122	-2.18217	0.35999
H	-6.97322	-2.62162	0.55102
C	2.51520	1.35373	0.18750
C	2.21652	1.66922	1.51699
C	3.29175	2.25141	-0.56124
C	2.70203	2.83945	2.10167
H	1.59584	1.00355	2.10813
C	3.76454	3.42625	0.02438
H	3.52120	2.04757	-1.60177
C	3.47836	3.72509	1.35912
H	3.85331	4.63712	1.80858
C	3.19700	-1.40385	-0.62274
C	2.87256	-2.76184	-0.69537
C	4.54591	-1.02718	-0.66053
C	3.87376	-3.73056	-0.78332
H	1.83487	-3.07838	-0.66940
C	5.54325	-1.99937	-0.75925
H	4.83167	0.01791	-0.61337
C	5.21513	-3.35591	-0.81651
H	5.99357	-4.10642	-0.88679
C	-0.38213	4.74466	0.03565
C	-4.70451	3.71413	-2.37687
C	-6.68317	-0.18642	1.73200
C	-5.36961	-4.21020	-1.01177
C	2.32806	3.11721	3.53634

C	4.52346	4.41926	-0.82657
C	6.99481	-1.57500	-0.73187
C	3.46103	-5.18034	-0.74907
F	3.66880	5.22874	-1.48468
F	5.33142	5.19411	-0.08176
F	5.27769	3.79123	-1.75166
F	2.60570	2.04364	4.31772
F	0.99879	3.34332	3.65443
F	2.97504	4.17690	4.03879
F	7.42414	-1.43067	0.53921
F	7.16777	-0.39098	-1.35220
F	7.78531	-2.48312	-1.33032
F	4.47182	-6.00945	-1.04101
F	3.00068	-5.50363	0.48724
F	2.45039	-5.42074	-1.61297
F	-0.75885	6.02372	-0.09473
F	0.76373	4.57452	-0.67167
F	-0.07152	4.52511	1.33337
F	-4.96759	5.02132	-2.21691
F	-5.80161	3.01469	-2.02744
F	-4.49185	3.49328	-3.69357
F	-6.08703	0.64060	2.61653
F	-7.47737	0.56884	0.94660
F	-7.47695	-1.02858	2.42087
F	-6.65718	-4.55740	-0.85177
F	-5.08624	-4.24347	-2.33159
F	-4.60792	-5.15922	-0.42249
C	2.60584	-1.53240	2.71300
H	2.84354	-1.31322	1.67644
H	2.81166	-0.62021	3.28038
C	0.61718	-1.34937	4.15321
H	-0.40258	-1.71884	4.24065
H	0.54891	-0.25861	4.13377
C	0.71201	-3.14625	2.38550
H	1.35239	-3.42821	1.54581
H	-0.30877	-3.06881	1.99705
C	3.56746	-2.64450	3.15722
H	4.59019	-2.27767	3.01032
H	3.46361	-2.91805	4.20817
H	3.45883	-3.54815	2.54976
C	0.71467	-4.28127	3.41930
H	0.02206	-4.08473	4.24264
H	0.37148	-5.19274	2.91613
H	1.70280	-4.48640	3.83511
C	1.40722	-1.74586	5.40903
H	1.50867	-2.82493	5.54189
H	2.40306	-1.29522	5.44328
H	0.85367	-1.35884	6.27229
N	1.12661	-1.76323	2.79902

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