Electronic Supplementary Material (ESI) for ChemComm.

Anion Ligand Promoted Selective C-F Bond Reductive Elimination Enables C(sp^2)-H Fluorination

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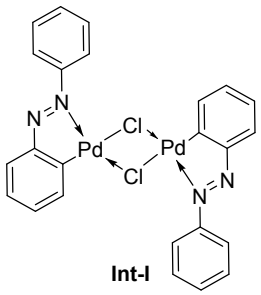
I. General

Unless otherwise stated, all experiments were carried out under air atmosphere. The reagents and solvents were purchased from commercial suppliers and used without further purification unless noted. ^{1}H NMR and ^{13}C NMR spectra were obtained on a Bruker AVANCE III 500 instrument in $CDCl_3$ using TMS as an internal standard, operating at 500 MHz and 125 MHz, respectively. Chemical shifts (δ) are expressed in ppm and coupling constants J are given in Hz. For $CDCl_3$ or DMSO-d_6 solutions the chemical shifts are reported as parts per million (ppm) to residual protium or carbon of the solvents; $CHCl_3$ δH (7.26 ppm) and $CDCl_3$ δC (77.03 ppm); DMSO δH (2.51 ppm) and DMSO-d_6 δC (39.52 ppm). ^{19}F NMR were recorded on a Bruker AVANCE III, Ascend400 or Anasazi Eft-90. Multiplicities are reported using the following abbreviations: s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, td = triplet of doublets, ddd = doublet of doublet of doublets, m = multiplet, br = broad resonance. GC experiments were carried out using Agilent 7890B GC. GC-MS experiments that used biphenyl as an internal standard were performed with a Thermo DSQ II, Trace GC Ultra. X-ray diffraction data were collected on a Bruker SMART APEX II. High resolution mass spectra (HRMS (ESI-TOF)) were obtained on an Agilent 6545 Q-TOF LCMS spectrometer equipped with an ESI source.

II. Preparation and characterization of starting materials

1. Preparation of Pd(II) complexes

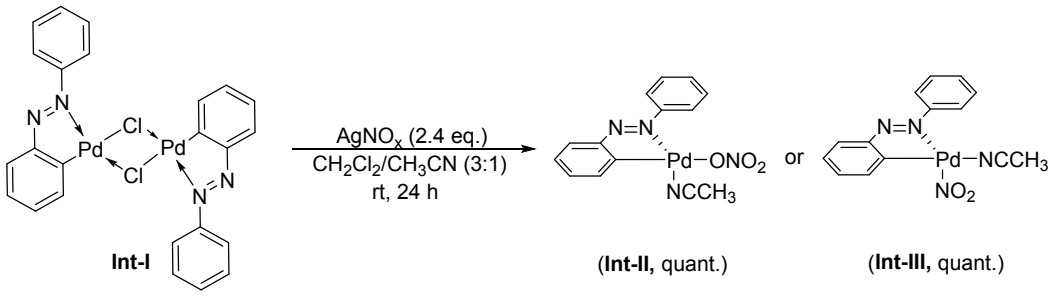
Int-I was prepared according to the literature procedure.[1]



Int-I

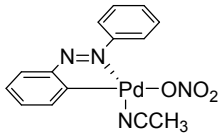
Dinuclear Pd(II)-Pd(II) complex **Int-I**: Red powder; ^{1}H NMR (500 MHz, DMSO-d_6): δ = 7.96 (dd, J_1 = 7.6 Hz, J_2 = 1.7 Hz, 1H), 7.78 (dd, J_1 = 7.8 Hz, J_2 = 1.8 Hz, 2H), 7.74 (d, J = 7.6 Hz , 1H), 7.57-7.52 (m, 3H), 7.29 (td, J_1 = 7.5 Hz, J_2 = 1.2 Hz, 1H), 7.23 (td, J_1 = 7.6 Hz, J_2 = 1.4 Hz, 1H) ppm; ^{13}C NMR (125 MHz, DMSO-d_6): δ = 163.5, 151.9, 131.5, 131.4, 130.9, 129.5, 128.4, 125.7, 123.8, 122.5 ppm.

The Pd(II) complexes **Int-II** and **Int-III** were prepared following the procedures.



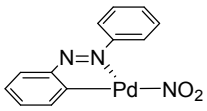
Int-I (**Int-II,** quant.) (**Int-III,** quant.)

A mixture of **Int-I** (343 mg, 0.5 mmol), $AgNO_x$ (1.2 mmol, 2.4 equiv) suspended in 24 mL of CH_2Cl_2/CH_3CN (3/1) were stirred at room temperature for 24 h. The reaction mixture was filtered and the filtrate was concentrated in vacuo to afford **Int-II** as a brown solid or **Int-III** as a yellow solid in quantitative yield.



Int-II

Mononuclear Pd(II) complex **Int-II**: Brown solid; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.90 (s, 1H), 7.78 (d, J = 7.3 Hz, 2H), 7.53-7.46 (m, 3H), 7.29-7.26 (m, 1H), 7.16-7.13 (m, 2H), 2.28 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 151.2, 133.5, 131.9, 130.0, 129.1, 126.9, 122.7, 119.0, 2.9 ppm. Crystals suitable for X-ray diffraction were grown by layering of a CH_2Cl_2 solution with hexane.

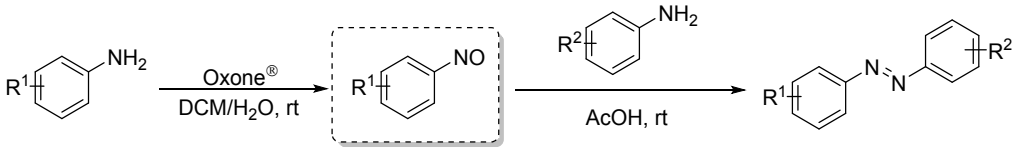


Int-III

Mononuclear Pd(II) complex **Int-III**: Yellow solid; ^{1}H NMR (500 MHz, DMSO-d_6): δ = 7.99 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.75 (dd, J_1 = 7.8 Hz, J_2 = 1.9 Hz, 2H), 7.60-7.55 (m, 3H), 7.34 (td, J_1 = 7.5 Hz, J_2 = 1.3 Hz, 1H), 7.27 (td, J_1 = 7.5 Hz, J_2 = 1.6 Hz, 1H), 7.07 (d, J = 7.7 Hz, 1H) ppm; ^{13}C NMR (125 MHz, DMSO-d_6): δ = 162.7, 150.8, 134.9, 132.8, 131.4, 130.1, 128.7 (2C), 126.4, 123.3 (2C) ppm. Crystals suitable for X-ray diffraction were grown by recrystallized from cold CH_3CN that placed in refrigerator. It seems that the CH_3CN ligand is easy to shed from the Pd(II) center.

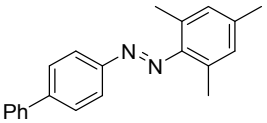
2. Preparation of substrates

Azobenzenes **1a** was purchased from Energy Chemical and other symmetrical azobenzenes **1b-d**, **1f-1k**, **1m**, and **1o-1t** were prepared according to the literature procedures.[2] The unsymmetrical substrates **3a-b**, **3e**, **3h-i**, **3l-p**, and **3u** were prepared following the procedure.



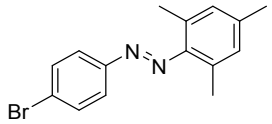
R^2 = donating electron groups

To a 250 mL three-necked, round-bottomed flask equipped with a magnetic stirring bar was added Oxone® (20 mmol) in water (120 mL) under nitrogen atmosphere. Aniline (10 mmol) in DCM (40 mL) was added at room temperature. The solution was stirred overnight. The layers were separated, the organic layer washed with water and concentrated under reduced pressure. Without any further purification the crude product was dissolved in 50 mL of acetic acid followed by adding alternative anilines containing electron-donating groups (10 mmol). The resulting mixture was stirred at room temperature for 12 h. Upon completion, H_2O (150 mL) was added, and the mixture was extracted with EtOAc (3 × 50 mL). The combined organic layers were successively washed with saturated solution of $NaHCO_3$ (75 mL), H_2O (75 mL), dried over $MgSO_4$, filtrated and then concentrated under reduced pressure. The crude product was purified by flash column chromatography on silica gel using petroleum ether as an eluent to give the desired unsymmetrical azobenzene as a red solid. *Unsymmetrical azobenzenes **3a**[3], **3b**[4], **3h**[4], **3p**[5], **3a' and 3m'**[6] are known compounds. All the new azo substrates were characterized as follows:*

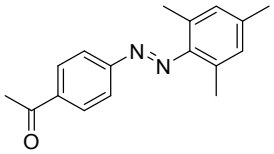


(*E*)-1-([1,1'-Biphenyl]-4-yl)-2-mesityldiazene (3e): Red solid; ^{1}H NMR (500 MHz, $CDCl_3$**): δ = 8.01-7.95 (m, 2H), 7.77 (d, J = 8.5 Hz, 2H), 7.71-7.68 (m, 2H), 7.51 (t, J = 7.7 Hz, 2H), 7.42 (t, J = 7.4 Hz, 1H), 6.99 (s, 2H), 2.44 (s, 6H), 2.37 (s, 3H) ppm; ^{13}C NMR (125 MHz,** $CDCl_3$**): δ = 152.1, 149.0, 143.5, 140.4, 138.5, 131.5 (2C), 130.0 (2C), 128.9 (2C), 127.83,**

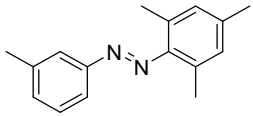
127.8 (2C), 127.2 (2C), 122.9 (2C), 21.1, 19.2 (2C) ppm.



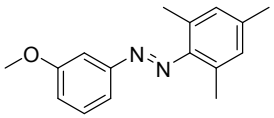
(*E*)-1-(4-Bromophenyl)-2-mesityldiazene (3i): Red solid; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.76-7.75 (m, 2H), 7.67-7.64 (m, 2H), 6.97 (s, 2H), 2.41 (s, 6H), 2.35 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 151.7, 148.5, 139.0, 132.3 (2C), 131.9 (2C), 130.1 (2C), 125.0, 123.9 (2C), 21.1, 19.4 (2C) ppm.



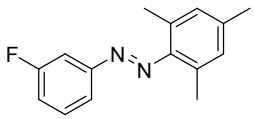
(*E*)-1-(4-(Mesityldiazenyl)phenyl)ethan-1-one (3l): Red solid; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.12 (d, J = 8.5 Hz, 2H), 7.93 (d, J = 8.5 Hz, 2H), 6.98 (s, 2H), 2.68 (s, 3H), 2.45 (s, 6H), 2.36 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 197.5, 155.5, 148.5, 139.7, 138.1, 132.5 (2C), 130.3 (2C), 129.4 (2C), 122.5 (2C), 26.9, 21.2, 19.7 (2C) ppm.



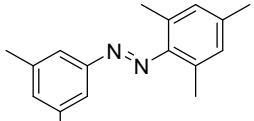
(*E*)-1-Mesityl-2-(m-tolyl)diazene (3m): Red solid; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.74-7.73 (m, 2H), 7.46-7.42 (m, 1H), 7.33 (d, J = 7.5 Hz, 1H), 6.98 (d, J = 1.2 Hz, 2H), 2.50 (s, 3H), 2.41 (s, 6H), 2.37 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 153.1, 149.0, 138.9, 138.2, 131.4, 131.2 (2C), 129.9 (2C), 128.9, 122.9, 119.7, 21.4, 21.1, 19.1 (2C) ppm.



(*E*)-1-Mesityl-2-(3-methoxyphenyl)diazene (3n): Red solid; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.55 (ddd, J_1 = 7.8, J_2 = 1.6, J_3 = 1.0 Hz, 1H), 7.47-7.44 (m, 2H), 7.07 (ddd, J_1 = 8.2, J_2 = 2.6, J_3 = 0.9 Hz, 1H), 6.97 (s, 2H), 3.92 (s, 3H), 2.40 (s, 6H), 2.36 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 160.3, 154.2, 148.8, 138.5, 131.4 (2C), 129.9 (2C), 129.7, 117.1, 116.5, 105.8, 55.5, 21.1, 19.1 (2C) ppm.

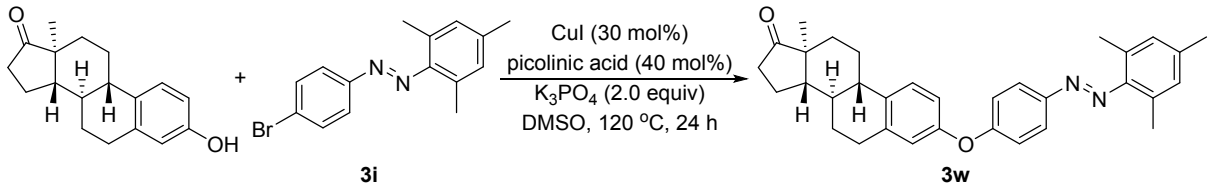


(*E*)-1-(3-Fluorophenyl)-2-mesityldiazene (3o): Red solid; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.74 (ddd, J_1 = 7.9, J_2 = 1.6, J_3 = 1.0 Hz, 1H), 7.57 (dt, J_1 = 9.8, J_2 = 2.2 Hz, 1H), 7.51 (td, J_1 = 8.1, J_2 = 5.9 Hz, 1H), 7.20 (tdd, J_1 = 8.2, J_2 = 2.6, J_3 = 0.9 Hz, 1H), 6.98 (s, 2H), 2.43 (s, 3H), 2.36 (s, 6H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 163.4 (d, J = 247.5 Hz), 154.6 (d, J = 6.5 Hz), 148.3, 139.2, 132.1 (2C), 130.2 (d, J = 8.3 Hz), 130.1 (2C), 120.1 (d, J = 2.9 Hz), 117.3 (d, J = 22.3 Hz), 107.5 (d, J = 22.7 Hz), 21.1, 19.4 (2C) ppm.



(*E*)-1-(3,5-Dimethylphenyl)-2-mesityldiazene (3u): Red solid; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.53 (s, 2H), 7.15 (s, 1H),

6.96 (s, 2H), 2.45 (s, 6H), 2.38 (s, 6H), 2.35 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 153.2, 149.2, 138.7 (2C), 138.1, 132.4, 131.0 (2C), 129.9 (2C), 120.2 (2C), 21.3 (2C), 21.1, 19.0 (2C) ppm.



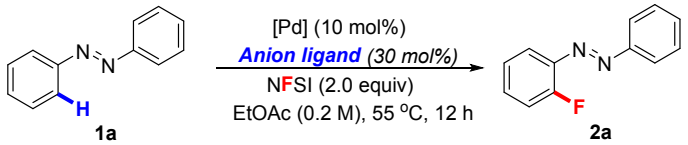
3i **3w**

To the diazo compound **3i** (302 mg, 1 mmol), CuI (57 mg, 30 mol%), picolinic acid (49 mg, 40 mol%), K_3PO_4 (425 mg, 2 mmol, 2.0 equiv) and Estrone (324 mg, 1.2 mmol, 1.2 equiv) in a Schlenk tube under N_2 was added DMSO (4 mL). The reaction mixture was heated at 120 °C for 24 h. The mixture was allowed to cool to r.t. and then diluted by EtOAc (25 mL) and H_2O (50 mL). The organic layer was separated and the aqueous layer was extracted with EtOAc (2 × 20 mL). The combined organic extracts were dried ($MgSO_4$) and concentrated reduced in vacuo. The product was purified by column chromatography on silica gel using petroleum ether as an eluent to give the desired azobenzene **3w** as a red solid (345 mg, 70% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.88-7.85 (m, 2H), 7.30 (d, J = 8.4 Hz, 1H), 7.11-7.08 (m, 2H), 6.93 (s, 2H), 6.89 (dd, J_1 = 8.5 Hz, J_2 = 2.6 Hz, 1H), 6.83 (d, J = 2.6 Hz, 1H), 2.93-2.90 (m, 2H), 2.52 (dd, J_1 = 19.1 Hz, J_2 = 8.6 Hz, 1H), 2.45-2.41 (m, 1H), 2.35 (s, 6H), 2.32 (s, 3H), 2.20-2.12 (m, 1H), 2.10-1.97 (m, 3H), 1.69-1.63 (m, 2H), 1.62-1.58 (m, 1H), 1.57-1.53 (m, 2H), 1.52-1.43 (m, 2H), 0.94 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 220.7, 160.1, 154.2, 148.9, 148.6, 138.5, 135.7, 131.1, 129.9 (2C), 129.1, 126.8, 124.1 (2C), 119.7, 118.3 (2C), 117.3, 117.1, 50.5, 48.0, 44.2, 38.2, 35.9, 31.6, 29.5, 26.4, 25.9, 21.6, 21.1, 19.1, 17.5, 13.9 ppm.

III. Catalytic and stoichiometric reactivity of the Pd complexes for the fluorination reaction

1. Preliminary optimization of the fluorinated reaction conditions

In a 10 mL test tube equipped with a stir bar, azobenzene (18.2 mg, 0.1 mmol), Pd complexes (0.01 mmol, 10 mol%), NFSI (63.1 mg, 0.2 mmol, 2.0 equiv), anion ligand (0.03 mmol, 30 mol%), biphenyl (7.7 mg, 0.05 mmol) and EtOAc (0.5 mL) were added successively. Then the tube was sealed and stirred at 55 °C oil bath for 12 h. Upon completion, the resulting mixture was cooled to room temperature, diluted with EtOAc and filtered, followed by GC experience (eq 1).



(1)

Conditions ([Pd] / Anion ligand)	*Yield of 2a*
$PdCl_2$ / $AgNO_3$	*76%*
$PdCl_2$ / $AgNO_2$	*73%*
$Pd(dba)_2$ / $AgNO_3$	*77%*
-- / $AgNO_3$	*0%*
$Pd(dba)_2$ / --	*16%*
$Pd(dba)_2$ / Ag_2SO_4 or Ag_2CO_3	*8%*

As shown in eq 1, **1a** was largely converted into desired product **2a** in 76% yield when a catalytic amount of $AgNO_3$ (30 mol%) was used as an additive in EtOAc (eq 1, line 1). It was noteworthy that $AgNO_2$ was also viable albeit with a slightly decreased yield, which implied that the nitrite ligand had the similar key feature with the nitrate (eq 1, line 2). Moreover, the combination of $Pd(dba)_2$ and $AgNO_3$ gave the similar result (eq 1, line 3). As anticipated, [Pd] catalyst and nitrate played an indispensable role in the reaction (eq 1, lines 4 & 5). Instead, the reaction efficiency dropped sharply when nitrate additive was replaced by other anion ligands such as SO_4^{2-} or CO_3^{2-} (eq 1, line 6).

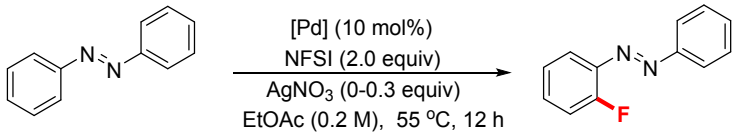
2. General procedure for the fluorination of Int-I, Int-II and Int-III around different anion ligands

In a 10 mL test tube equipped with a stir bar, Pd complexes (0.1 mmol, 100 mol% Pd), NFSI (63.1 mg, 0.2 mmol, 2.0 equiv),

anion ligand (0.03 mmol, 30 mol%) if necessary, biphenyl (7.7 mg, 0.05 mmol) and EtOAc (1.0 mL) were added successively. Then the tube was sealed and stirred at room temperature for 2 h. Upon completion, concentrated HCl (0.5 mL) was added to the resulting mixture and stirred vigorously for 30 min. The resulting acidic mixture was neutralized by NaOH aqueous, extracted with EtOAc and separated. The organic layer was filtered, followed by GC experience.

3. Full data of the catalytic evaluation of the [Pd] for the fluorination of azobenzene

Table S1. Full data of the catalytic evaluation of [Pd] for the fluorination of azobenzene



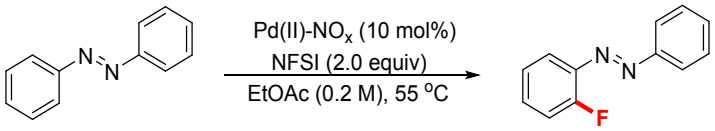
Entry	[Pd]	Eq. of $AgNO_3$	Conv. / % (GC)
1	$Pd(dba)_2$	0	18
2	$Pd(dba)_2$	0.1	76
3	$Pd(dba)_2$	0.3	95
4	$PdCl_2$	0	5
5	$PdCl_2$	0.1	66
6	$PdCl_2$	0.3	95
7	**Int-I**	0	30
8	**Int-I**	0.1	73
9	**Int-I**	0.3	98
10	**Int-II**	0	97
11	**Int-II**	0.1	99
12	**Int-II**	0.3	99
13	**Int-III**	0	60
14	**Int-III**	0.1	78
15	**Int-III**	0.3	93

4. Kinetic study for the fluorination of azobenzene by Pd(II)-NO_x complexes

In a 10 mL test tube equipped with a stir bar, azobenzene (18.2 mg, 0.1 mmol), Pd(II)-NO_x complexes (0.01 mmol, 10 mol%), NFSI (63.1 mg, 0.2 mmol, 2.0 equiv) and EtOAc (0.5 mL) were added successively. Then the tube was sealed and stirred at 55 °C oil bath for the indicated time. The resulting mixture was cooled to room temperature, diluted with EtOAc and filtered, followed by GC experience.

The data of kinetic curves from the catalytic Pd(II)-NO_x complexes runs are included below. Each data point is an average of three independent GC injections using biphenyl as an internal standard.

Table S2. Kinetic plots for the fluorination of azobenzene by Pd(II)-NO_x complexes



Pd(II)-NO_x complex	Time / min.	Conv. / % (GC)
Int-II	5	22.5
	10	31.3
	15	34.9
	30	47.0
	60	53.3
	90	65.2
	120	76.7
	180	84.9
	240	87.3
	300	90.5
Int-III	5	12.2
	10	17.0
	15	23.4
	30	37.0
	60	52.8
	90	56.6
	120	59.1
	180	59.7
	240	64.7
	300	61.1

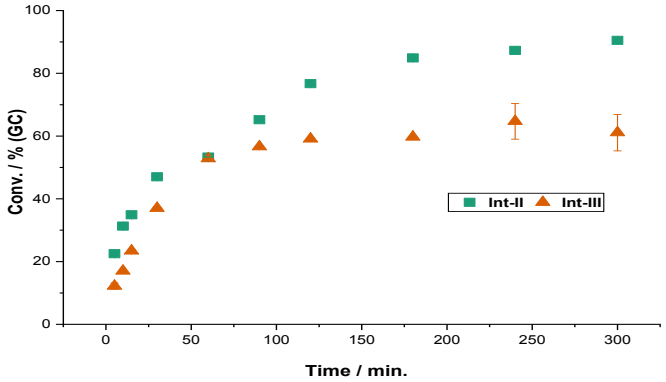


Figure S1. Kinetic plots for the fluorinated reaction of 1a

As shown in Figure S1, the time-conversion curves of fluorinated reaction displayed a lack of induction period, indicating that the cyclopalladatation complexes might be involved in the catalytic cycle.

5. HRMS (ESI-TOF) studies for the reaction of Int-II with NFSI

In a 10 mL test tube equipped with a stir bar, **Int-II** (39. 0 mg, 0.1 mmol, 1.0 equiv), NFSI (63.1 mg, 0.2 mmol, 2.0 equiv) and CH_3CN (0.5 mL) were added successively. Then the tube was sealed and stirred at room temperature for 30 min. The resulting

mixture was diluted with CH_3CN and filtered, followed by HRMS experience and the results are given on Figure S2 (bottom). The HRMS spectrum of **Int-II** was also obtained and exhibited on Figure S2 (top). It seems that the nitrate group has shed from the Pd center in HRMS (ESI-TOF).

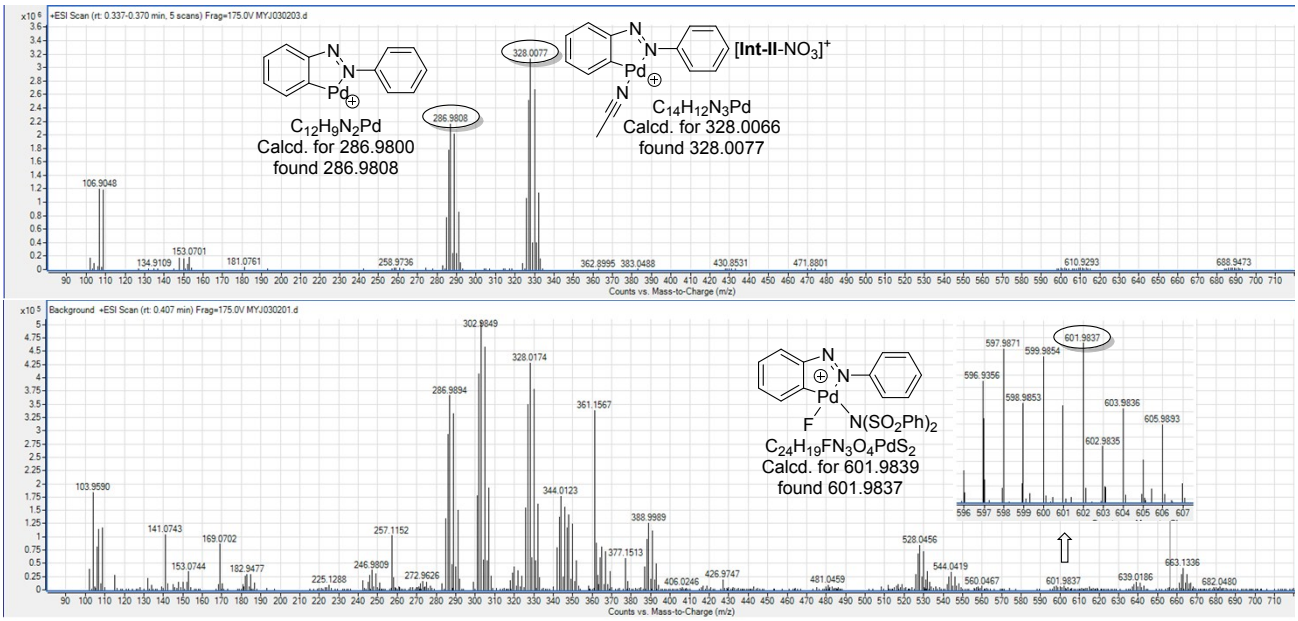


Figure S2. HRMS spectra of the Int-II and its diluted fluorination reaction mixture

6. ^{19}F NMR analysis for the reaction of Int-II with NFSI

To an NMR tube was successively added **Int-II** (39. 0 mg, 0.1 mmol, 1.0 equiv), NFSI (63.1 mg, 0.2 mmol, 2.0 equiv) and CD_3CN (0.5 mL). The tube was capped and shook for 2 min to fully mix the reactants, during which the suspension became a dark red solution very quickly. ^{19}F NMR spectra were recorded after 5 min, 30 min, and for another 25 min heating at 55 °C. The collected spectra are given on Figure S3 with comparison with *o*-fluoroazobenzene **2a**.

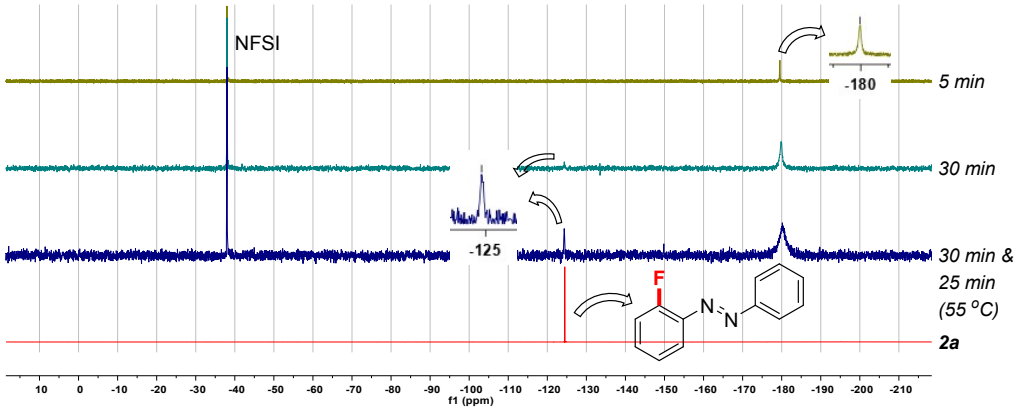


Figure S3. Fluorination of Int-II monitored by ^{19}F NMR spectroscopy (85 MHz)

IV. DFT calculations

Computational Details

All calculations were carried out with Gaussian 16 program.[7] The geometry optimizations were performed at the B3PW91[8]/BSI level. In the basis set BSI, the 6-31G(d) basis set was considered for all nonmetallic atoms, and the Stuttgart/Dresden effective core potential (ECP) together with associated basis set (MWB28) was used for Pd atom.[9] Each optimized structure was subsequently analyzed by harmonic vibration frequencies at the same level and characterized as a minimum without imaginary

frequency (N_{imag} = 0) or a transition state with only one imaginary frequency (N_{imag} = 1) and to obtain the thermodynamic corrections to Gibbs free energy. All of the structures were optimized without any symmetry restrictions. The subsequent single-point calculations were carried out at the level of M06[10]/BSII together with SMD model[11] for considering the ethylethanoate (ε = 5.9867) solvation effect. Gibbs free energies in the solution described in the text were obtained from such single-point calculations, including gas-phase free energy corrections. The three-dimensional images of the optimized structures were displayed using CYLview.[12]

As shown in Figure S4, the isomer A′ (the two coordinated N atoms at *cis*-position) has higher free energy than A (the two coordinated N atoms at *trans*-position) by 5.1 kcal/mol. The reductive elimination processes of F and Cl atoms in A′ were also considered. The results indicate that although the reductive elimination processes in A′ are significantly unfavorable than that in A (23.1 kcal/mol for TS′-A_F *vs* 14.6 kcal/mol for TS-A_F; 19.4 kcal/mol for TS′-A_{Cl} *vs* 12.6 kcal/mol for TS-A_{Cl}), the reductive elimination processes Cl atom is also favored than F atom in A′ (19.4 kcal/mol for TS′-A_{Cl} *vs* 23.1 kcal/mol for TS′-A_F;), similarly to the case of A. The corresponding 3D structures are shown in Figure S5.

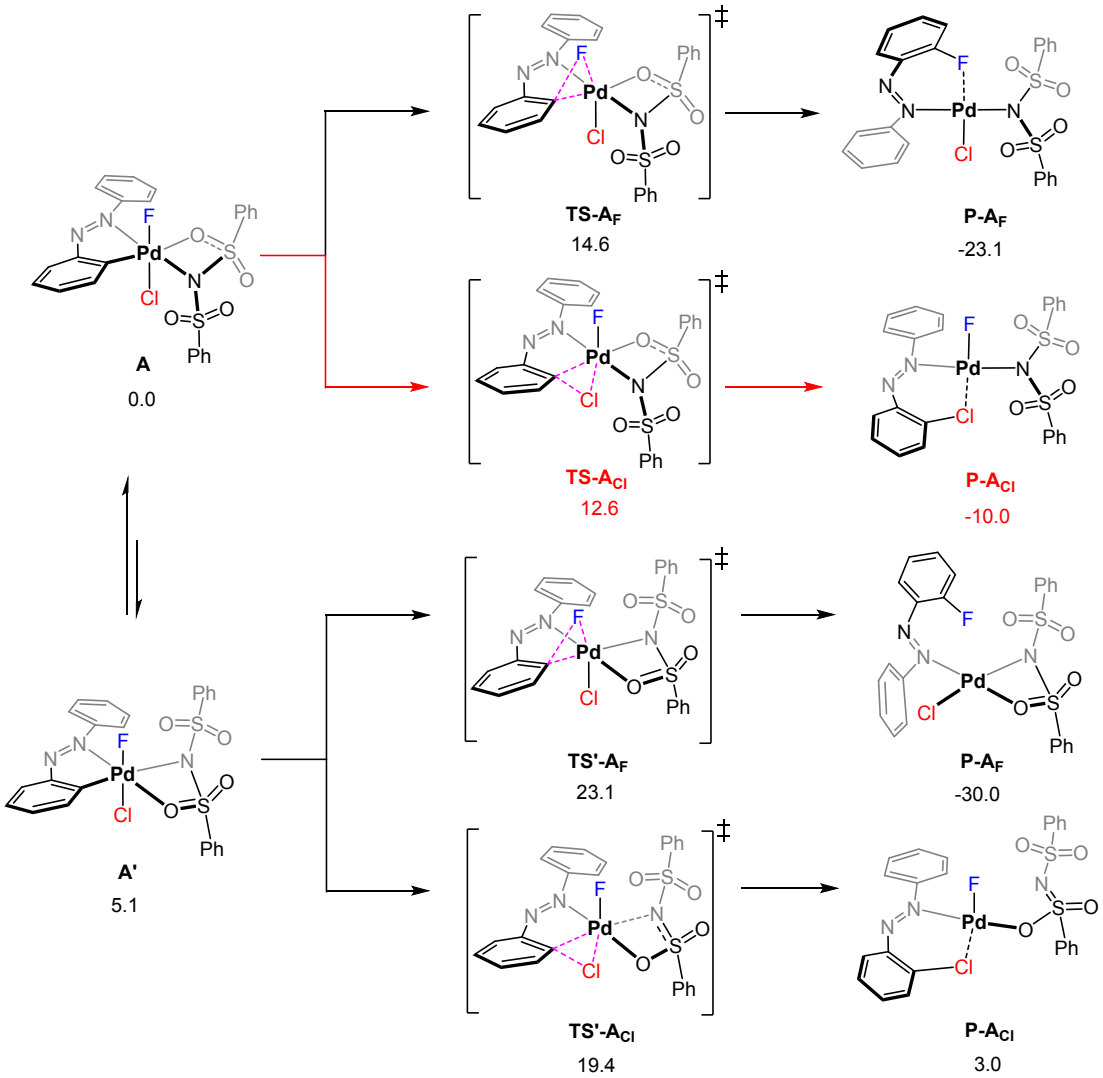


Figure S4. Computed reductive elimination processes of the species A and its isomer A′. Relative free energies are given in kcal/mol. The pathway with the red line is the most favorable one.

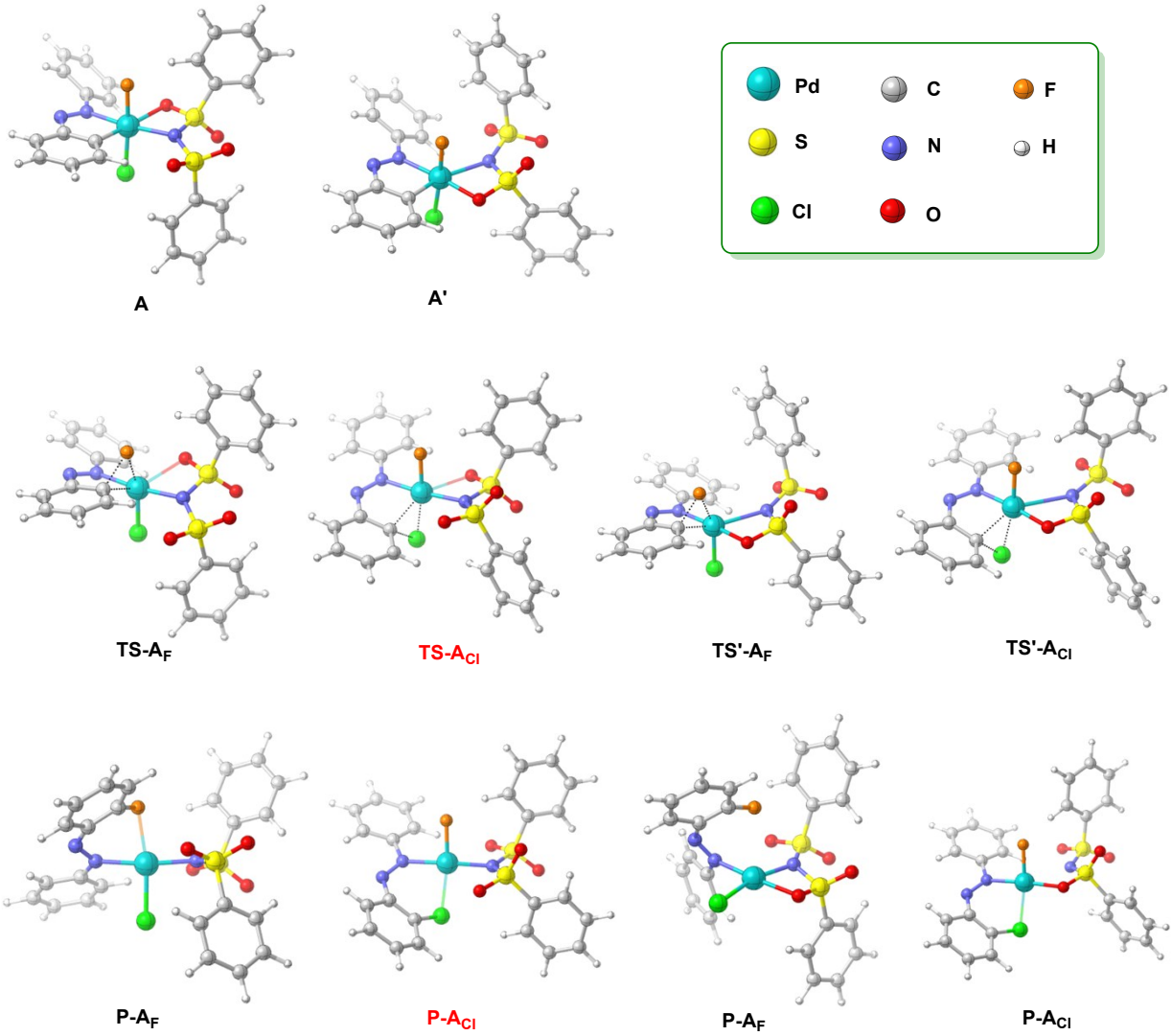


Figure S5. Optimized structures involved in reductive elimination processes of the species A and its isomer A′ shown in Figure S4.

Similar to complex A, complex B also has an isomer B′ with a higher free energy by 5.5 kcal/mol. Starting from B′, the reductive elimination processes F atom is more favored than NO_3 anion ligand (21.1 kcal/mol for TS′-B_F *vs* 31.6 kcal/mol for TS′-B_{NO3}) although the energy barriers are significantly higher than that of the corresponding processes based on B. The corresponding 3D structures are shown in Figure S7.

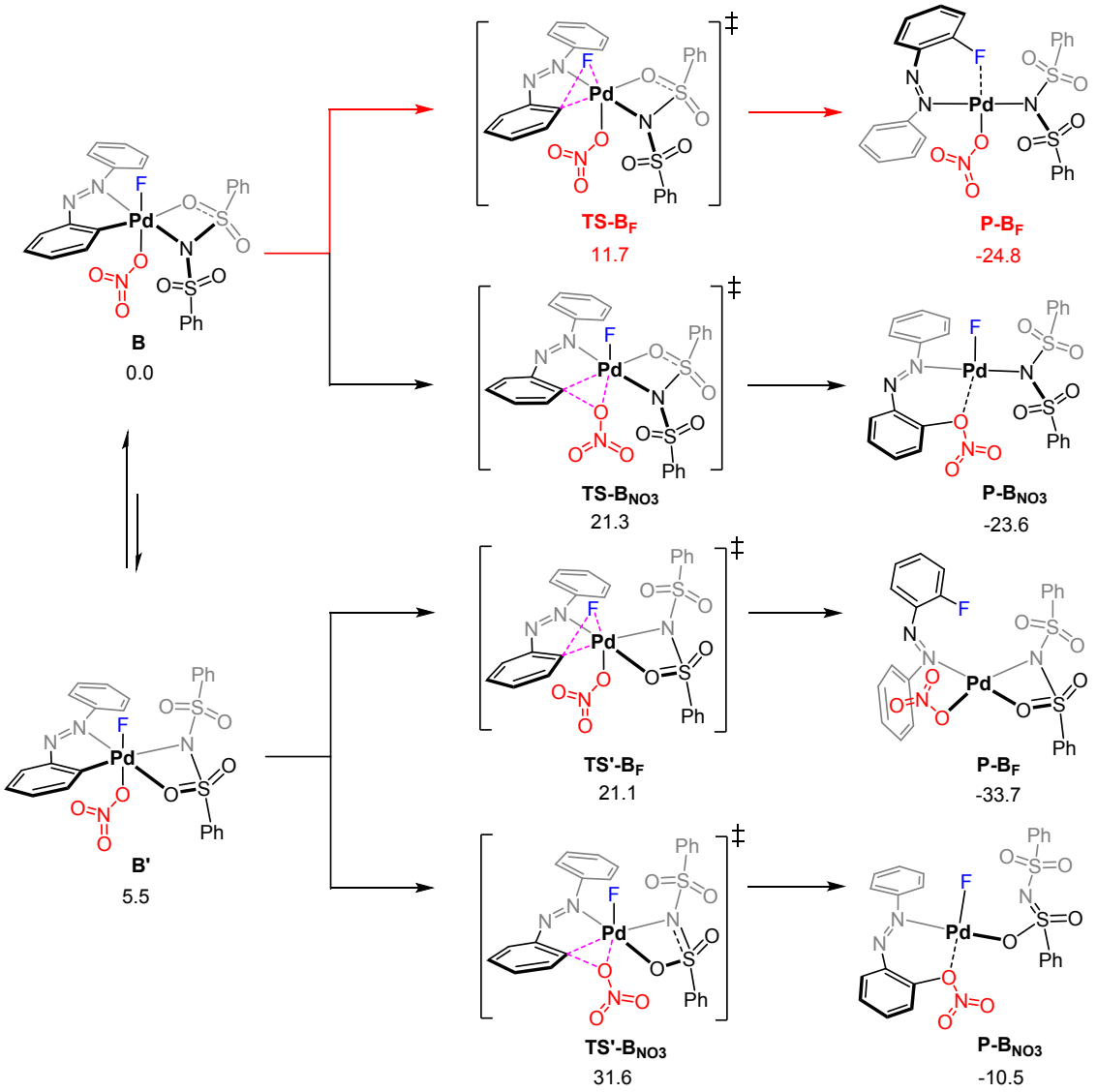


Figure S6. Computed reductive elimination processes of the species B and its isomer B′. Relative free energies are given in kcal/mol. The pathway with the red line is the most favorable one.

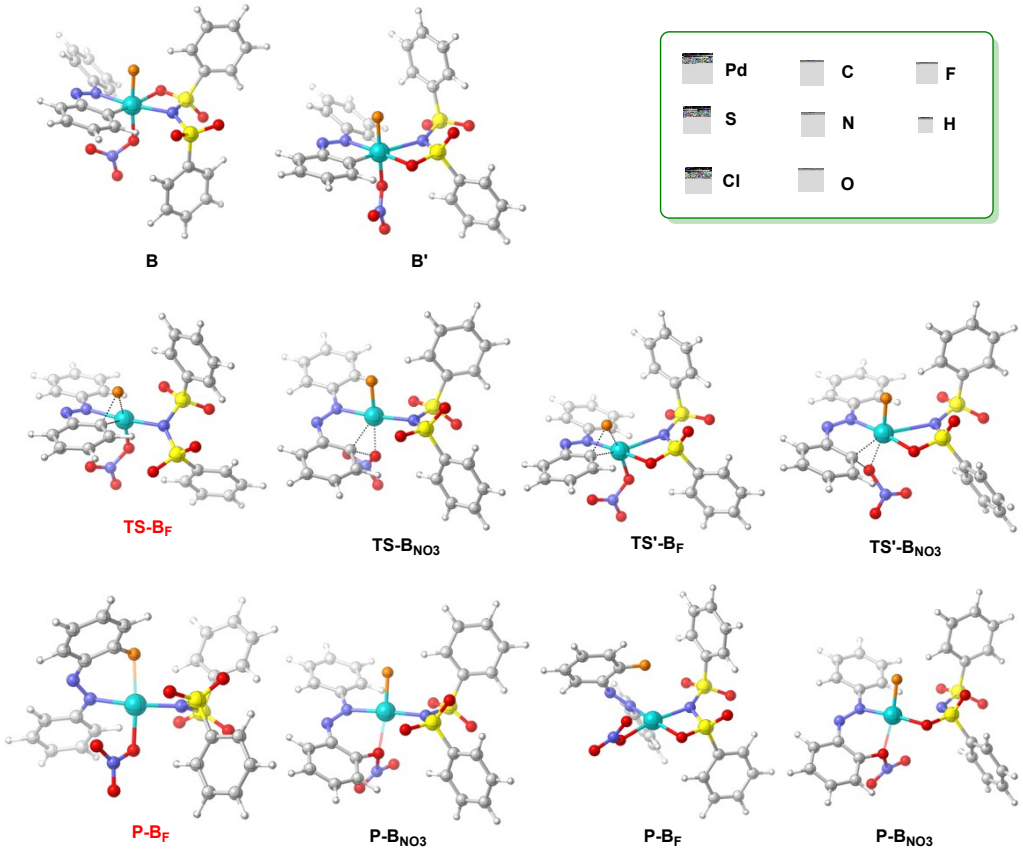


Figure S7. Optimized structures involved in reductive elimination processes of the species B and its isomer B′ shown in Figure S6.

As shown in Figure S8a, in the NO_2-containing case, several isomers may exist based on the orientation of $N(SO_2Ph)_2$ ligands and the coordination manner of the NO_2 moiety. The results show that the Pd-NO_2 coordination isomers (C and C′) are more stable than Pd-ONO coordination isomers (C″ and C‴) in the current system. Therefore, only C and C′ were selected to further investigate their reductive elimination transformations (Figure S8b). The result of the NO_2-containing case is similar to NO_3-containing case shown in Figure S6, in which the reductive elimination processes F atom is favored, leading to the fluorinated product. The corresponding 3D structures are shown in Figure S9.

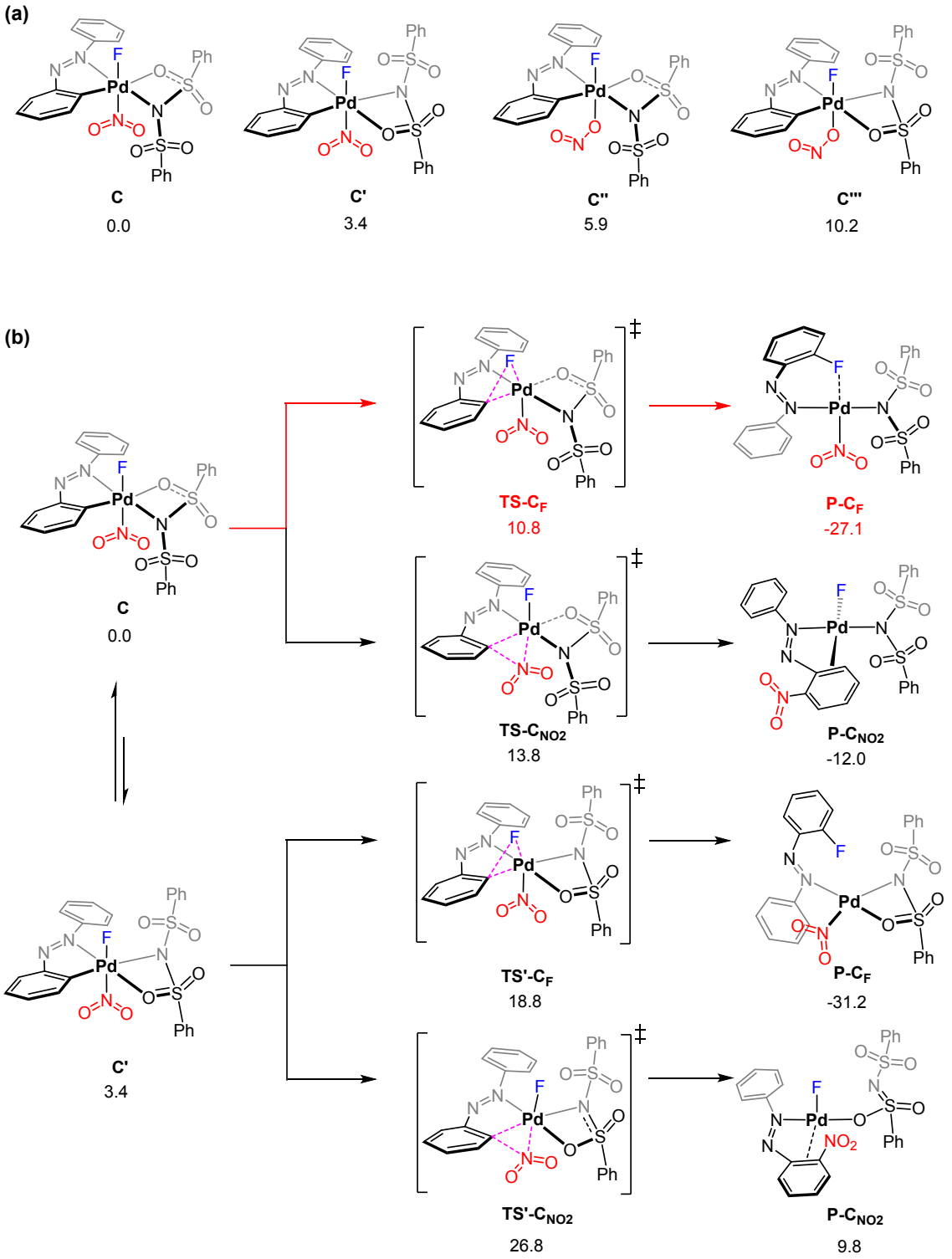


Figure S8. (a) Four NO_2-containing isomers C–C‴. (b) Computed reductive elimination processes of the species C and its isomer C′. Relative free energies are given in kcal/mol. The pathway with the red line is the most favorable one.

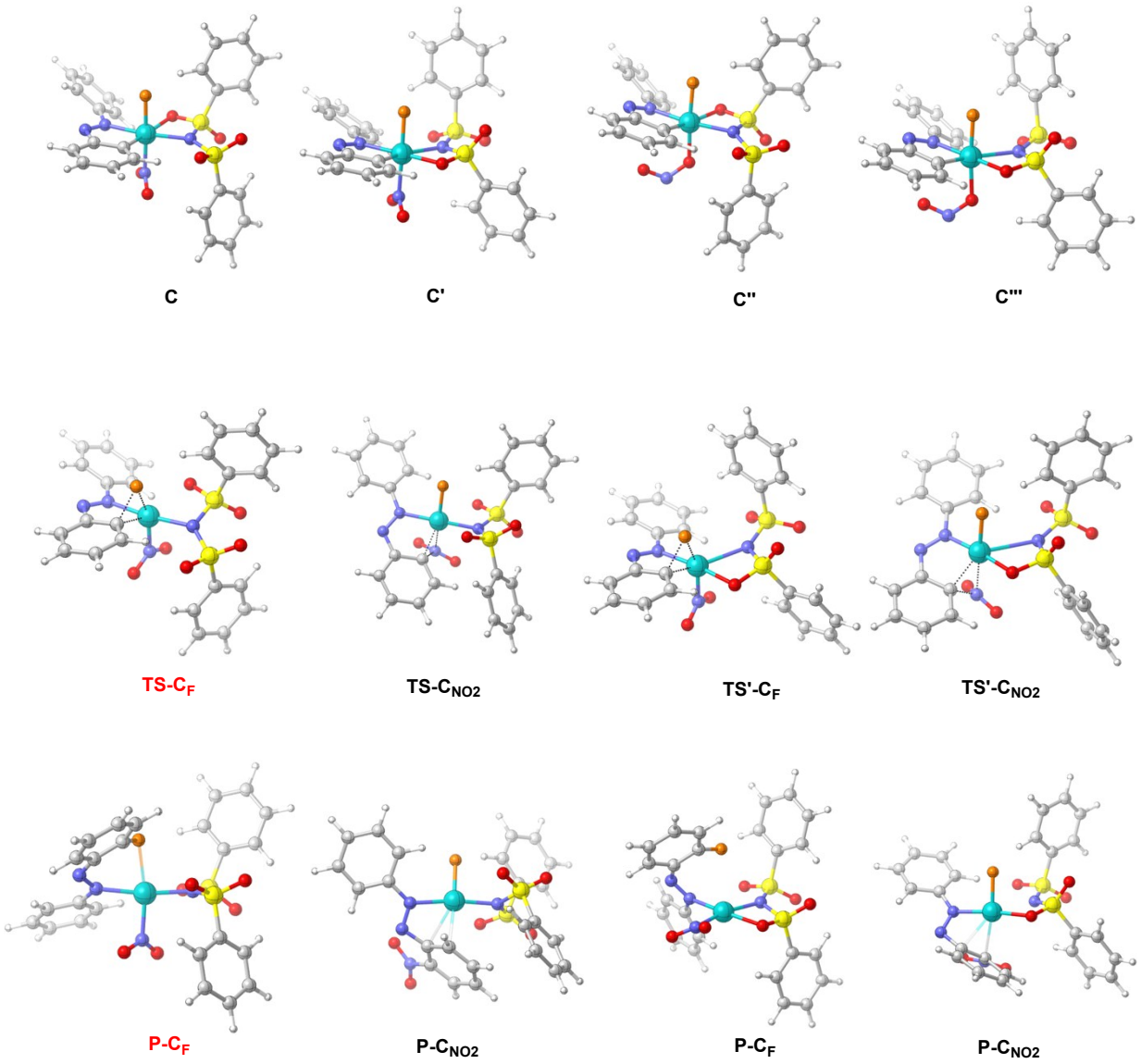


Figure S9. Optimized structures of C–C‴ and the structures involved in reductive elimination processes of the species C and its isomer C′ shown in Figure S8.

Optimized Cartesian coordinates and single-point calculation energies for all of the stationary as well as the imaginary frequencies of transition states.

A, $E_{(SCF\ Done)}$ = -2874.728182 a.u.

N	2.870538000	-0.389838000	0.182970000
N	3.511199000	-1.276424000	-0.430368000
C	3.578503000	0.557742000	0.957187000
C	4.881072000	0.922045000	0.585202000
C	2.964333000	1.109792000	2.085786000
C	5.570492000	1.841818000	1.361969000
H	5.321911000	0.490428000	-0.306744000
C	3.675463000	2.023742000	2.856970000
H	1.959251000	0.811638000	2.360461000
C	4.971290000	2.392795000	2.498493000
H	6.575653000	2.138419000	1.075915000
H	3.209086000	2.449712000	3.740249000
H	5.515386000	3.116023000	3.099845000
C	2.716709000	-2.078229000	-1.217189000
C	1.328694000	-1.831219000	-1.270838000
C	3.287240000	-3.114009000	-1.969476000
C	0.513294000	-2.568991000	-2.096269000
C	2.464253000	-3.882144000	-2.781927000
H	4.358124000	-3.282086000	-1.907461000
C	1.097030000	-3.604260000	-2.846159000
H	-0.546669000	-2.350905000	-2.178870000
H	2.884225000	-4.688942000	-3.374926000
H	0.457006000	-4.196723000	-3.495144000
Pd	0.854469000	-0.262707000	-0.148482000
Cl	0.489805000	-1.629119000	1.672170000
S	-2.630772000	-0.596456000	-0.752370000
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O	-3.637321000	0.454187000	-0.886081000
O	-2.194647000	1.575390000	1.664189000
O	0.227691000	1.628913000	0.913681000
N	-1.196336000	0.181929000	-0.341646000
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C	-3.923852000	-3.289298000	2.681301000
H	-4.241264000	-3.934289000	3.496607000
C	-4.322201000	-1.952725000	2.657625000
H	-4.949738000	-1.555335000	3.450540000

C	-3.921499000	-1.119768000	1.616102000
H	-4.223567000	-0.079556000	1.580572000
C	-1.596237000	2.945520000	-0.500187000
C	-0.761456000	3.203505000	-1.588227000
H	0.080188000	2.548020000	-1.799261000
C	-1.050536000	4.303243000	-2.391200000
H	-0.415894000	4.521896000	-3.245543000
C	-2.147482000	5.118065000	-2.105100000
H	-2.364818000	5.973749000	-2.739301000
C	-2.969342000	4.838831000	-1.013634000
H	-3.825320000	5.471561000	-0.796174000
C	-2.699233000	3.741777000	-0.199123000
H	-3.325749000	3.497990000	0.651745000
F	1.273824000	0.846070000	-1.700541000

TS-A_F, $E_{(SCF\ Done)}$ = -2874.701379 a.u., Imaginary frequency = *i*346.0684 cm^{-1}

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C	4.981697000	0.539750000	1.132755000
C	2.888378000	0.509526000	2.381680000
C	5.629721000	1.049611000	2.246951000
H	5.514637000	0.354928000	0.207025000
C	3.554085000	1.029358000	3.488003000
H	1.827303000	0.294158000	2.433809000
C	4.919856000	1.296847000	3.426997000
H	6.693161000	1.266031000	2.194969000
H	2.996799000	1.221878000	4.399820000
H	5.434299000	1.702276000	4.294010000
C	2.838425000	-0.993783000	-1.993735000
C	1.471303000	-0.635945000	-2.051665000
C	3.396115000	-1.731200000	-3.054640000
C	0.667989000	-0.962090000	-3.128493000
C	2.595427000	-2.106231000	-4.117746000
H	4.444689000	-2.006593000	-2.992721000
C	1.241481000	-1.733130000	-4.138997000
H	-0.372442000	-0.664628000	-3.157228000
H	3.010317000	-2.686741000	-4.935632000
H	0.613848000	-2.031137000	-4.974729000
Pd	0.866259000	-0.177960000	-0.111836000
Cl	0.674380000	-1.998420000	1.231952000
S	-2.477497000	-0.763500000	-0.715029000
S	-1.428282000	1.399763000	0.940292000
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O	-3.613300000	0.152584000	-0.816724000

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H	-4.825720000	-2.487866000	3.226870000
C	-3.780072000	-1.710839000	1.519669000
H	-4.158541000	-0.701427000	1.627512000
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H	0.107385000	3.261269000	-0.633749000
C	-1.316402000	4.706061000	-1.378748000
H	-0.566949000	5.287423000	-1.908737000
C	-2.656357000	5.094651000	-1.406741000
H	-2.950697000	5.980847000	-1.963084000
C	-3.619335000	4.352454000	-0.723439000
H	-4.662131000	4.656412000	-0.746610000
C	-3.250400000	3.215251000	-0.009030000
H	-3.982767000	2.620199000	0.524089000
F	1.238626000	1.118758000	-1.657116000

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N	-2.837744000	0.151868000	-0.007298000
N	-3.496516000	-0.051818000	1.045101000
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C	-4.992355000	0.263528000	-1.197707000
C	-2.946702000	1.078697000	-2.241824000
C	-5.705921000	0.627508000	-2.329515000
H	-5.482417000	-0.201757000	-0.350220000
C	-3.680666000	1.455064000	-3.363088000
H	-1.872732000	1.239854000	-2.209073000
C	-5.054204000	1.227384000	-3.412444000
H	-6.775106000	0.439661000	-2.373009000
H	-3.168748000	1.915328000	-4.202759000
H	-5.620401000	1.509087000	-4.296196000
C	-2.838262000	-0.303654000	2.251278000
C	-1.637255000	0.281069000	2.678972000
C	-3.512471000	-1.126502000	3.169709000
C	-1.088528000	0.048802000	3.922887000

C	-2.966588000	-1.398242000	4.416361000
H	-4.461827000	-1.553711000	2.861774000
C	-1.755792000	-0.812185000	4.792736000
H	-0.146653000	0.518673000	4.182573000
H	-3.489028000	-2.058924000	5.101195000
H	-1.327144000	-1.018589000	5.768700000
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Cl	-0.912687000	-1.523868000	-1.798374000
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S	1.926406000	1.108516000	-1.267805000
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O	3.040760000	0.443905000	-1.939180000
O	0.795583000	1.645900000	-2.032222000
N	1.200818000	0.095690000	-0.134266000
C	2.394579000	-2.464262000	-0.167182000
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H	0.618283000	-3.466548000	0.514634000
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H	4.726684000	-3.734887000	-2.265571000
C	3.557127000	-2.520406000	-0.935523000
H	4.228760000	-1.670736000	-0.966293000
C	2.598460000	2.472137000	-0.321251000
C	1.774088000	3.559771000	-0.032565000
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C	2.297119000	4.633071000	0.684593000
H	1.666291000	5.488794000	0.910448000
C	3.629295000	4.613869000	1.099279000
H	4.035053000	5.454279000	1.656728000
C	4.444147000	3.524071000	0.793516000
H	5.483052000	3.512919000	1.111658000
C	3.932888000	2.443276000	0.078323000
H	4.550159000	1.586456000	-0.164313000
F	-1.000501000	1.170017000	1.854413000

TS-A_{Cl}, $E_{(SCF\ Done)}$ = -2874.706251 a.u., Imaginary frequency = *i*238.1431 cm^{-1}

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C	5.275900000	0.555036000	0.282136000
C	3.280770000	1.839053000	0.849514000

C	6.064576000	1.628766000	0.663802000
H	5.716348000	-0.363598000	-0.087990000
C	4.089922000	2.902783000	1.239007000
H	2.200181000	1.918465000	0.925558000
C	5.476198000	2.804301000	1.144286000
H	7.145741000	1.551891000	0.589133000
H	3.627409000	3.811310000	1.612828000
H	6.102856000	3.640444000	1.442549000
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C	1.312648000	-2.408580000	-0.234165000
C	3.079344000	-3.574847000	-1.437130000
C	0.390607000	-3.369523000	-0.618100000
C	2.156603000	-4.524459000	-1.843055000
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C	0.818790000	-4.405158000	-1.448110000
H	-0.637680000	-3.316052000	-0.287648000
H	2.468026000	-5.354634000	-2.469045000
H	0.089935000	-5.144751000	-1.767556000
Pd	0.985740000	-0.252622000	-0.025701000
Cl	0.984189000	-1.802569000	1.742846000
S	-2.231025000	-0.505646000	-0.962118000
S	-1.297563000	1.518322000	0.939552000
O	-1.551638000	-1.548505000	-1.731870000
O	-2.962797000	0.550979000	-1.656666000
O	-2.406695000	1.337814000	1.873184000
O	0.060108000	1.760962000	1.475694000
N	-1.046600000	0.132848000	0.033615000
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C	-2.962620000	-1.954124000	1.298238000
H	-1.920374000	-1.904618000	1.596273000
C	-3.894434000	-2.632628000	2.079954000
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H	-6.708906000	-1.989541000	0.277903000
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C	-1.717363000	2.874723000	-0.143388000
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C	-1.235509000	4.270646000	-2.026068000
H	-0.632176000	4.500812000	-2.900032000
C	-2.322697000	5.079638000	-1.691478000
H	-2.561515000	5.945735000	-2.303625000

C	-3.108916000	4.777217000	-0.580669000
H	-3.959335000	5.403342000	-0.324425000
C	-2.811356000	3.664610000	0.203603000
H	-3.413322000	3.402294000	1.067112000
F	1.165314000	0.878192000	-1.578552000

P-A_{Cl}, $E_{(SCF\ Done)}$ = -2874.740812 a.u.

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N	-3.799807000	-0.753820000	0.184370000
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C	-4.951185000	1.699105000	-0.057550000
C	-2.831581000	2.397282000	-1.042735000
C	-5.502968000	2.925935000	-0.392962000
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C	-3.406409000	3.617141000	-1.386345000
H	-1.793224000	2.190198000	-1.288822000
C	-4.734384000	3.885692000	-1.060729000
H	-6.534665000	3.140955000	-0.129074000
H	-2.805460000	4.359930000	-1.902145000
H	-5.173607000	4.845533000	-1.319238000
C	-3.319853000	-2.036090000	0.467060000
C	-2.216649000	-2.686260000	-0.118676000
C	-4.099877000	-2.770884000	1.375139000
C	-1.879775000	-3.990199000	0.212583000
C	-3.756313000	-4.066681000	1.733684000
H	-4.969496000	-2.279345000	1.800128000
C	-2.645296000	-4.677241000	1.152861000
H	-1.015725000	-4.454739000	-0.249553000
H	-4.359834000	-4.603369000	2.459148000
H	-2.370239000	-5.692282000	1.422916000
Pd	-0.975954000	0.108349000	-0.026523000
Cl	-1.256409000	-1.881077000	-1.351054000
S	1.842725000	-0.971406000	0.952228000
S	1.799186000	1.263070000	-0.999748000
O	0.798897000	-1.936968000	1.323517000
O	2.551341000	-0.227417000	1.991659000
O	2.908803000	0.700232000	-1.770658000
O	0.676078000	1.891550000	-1.709430000
N	1.056208000	0.040611000	-0.124655000
C	3.082081000	-1.842349000	-0.001548000
C	2.695719000	-2.688285000	-1.040125000
H	1.647858000	-2.781317000	-1.305216000
C	3.670771000	-3.398165000	-1.732937000
H	3.382874000	-4.054812000	-2.549716000
C	5.015677000	-3.264924000	-1.382246000

H	5.774323000	-3.820960000	-1.927061000
C	5.387720000	-2.420605000	-0.338000000
H	6.434554000	-2.317537000	-0.065187000
C	4.418940000	-1.701246000	0.360164000
H	4.682269000	-1.036175000	1.175905000
C	2.504227000	2.449049000	0.138456000
C	1.718206000	3.014034000	1.142041000
H	0.691438000	2.683683000	1.282350000
C	2.290712000	3.978416000	1.967653000
H	1.695774000	4.421527000	2.761900000
C	3.617890000	4.369599000	1.785246000
H	4.055188000	5.122898000	2.436035000
C	4.387516000	3.793210000	0.775593000
H	5.422217000	4.095045000	0.635390000
C	3.833038000	2.822934000	-0.056814000
H	4.411969000	2.354923000	-0.846061000
F	-0.986426000	1.597685000	1.201103000

A′, $E_{(\text{SCF Done})}$ = -2874.718262 a.u.

N	-2.634419000	0.107263000	0.470601000
N	-3.658128000	0.732843000	0.097105000
C	-2.796849000	-1.097978000	1.186954000
C	-3.999323000	-1.818097000	1.090141000
C	-1.750075000	-1.541272000	1.997972000
C	-4.144259000	-2.982274000	1.827891000
H	-4.787498000	-1.458806000	0.438125000
C	-1.914901000	-2.711490000	2.734542000
H	-0.823074000	-0.983802000	2.067614000
C	-3.105819000	-3.429951000	2.653422000
H	-5.066872000	-3.551192000	1.754306000
H	-1.095654000	-3.057240000	3.356104000
H	-3.226839000	-4.346579000	3.224429000
C	-3.384844000	1.880730000	-0.610987000
C	-2.041975000	2.225707000	-0.831578000
C	-4.408691000	2.704990000	-1.097432000
C	-1.679483000	3.348322000	-1.536282000
C	-4.059539000	3.851396000	-1.800797000
H	-5.444152000	2.430659000	-0.920356000
C	-2.714104000	4.166754000	-2.017215000
H	-0.635945000	3.587721000	-1.713060000
H	-4.835041000	4.505285000	-2.187788000
H	-2.455755000	5.065378000	-2.571412000
Pd	-0.825905000	0.855261000	-0.120545000
Cl	-0.703616000	2.004551000	1.888646000
S	1.820128000	-1.861652000	0.556761000

S	1.990066000	0.685157000	-0.684159000
O	1.150548000	-2.324119000	1.771417000
O	3.278676000	-1.740028000	0.511899000
O	2.571192000	0.205125000	-1.932415000
O	0.888276000	1.761141000	-0.826036000
N	1.152801000	-0.357251000	0.226890000
C	1.321019000	-2.943644000	-0.775717000
C	0.154591000	-3.694636000	-0.641491000
H	-0.433888000	-3.621699000	0.266757000
C	-0.224019000	-4.543000000	-1.679309000
H	-1.130392000	-5.135330000	-1.586527000
C	0.559469000	-4.635061000	-2.829406000
H	0.260088000	-5.298158000	-3.637035000
C	1.729035000	-3.883639000	-2.944814000
H	2.341447000	-3.960367000	-3.839049000
C	2.120103000	-3.031950000	-1.914818000
H	3.026392000	-2.441766000	-1.988510000
C	3.281368000	1.487109000	0.243322000
C	2.960408000	2.206518000	1.394737000
H	1.929108000	2.285383000	1.725104000
C	3.990929000	2.818518000	2.102084000
H	3.760371000	3.384890000	3.000057000
C	5.310947000	2.704890000	1.662288000
H	6.109821000	3.184508000	2.221920000
C	5.611005000	1.977566000	0.510995000
H	6.639481000	1.886784000	0.173068000
C	4.592746000	1.358415000	-0.209711000
H	4.799658000	0.783313000	-1.105275000
F	-1.057668000	-0.106547000	-1.783542000

TS′-A_F, $E_{(SCF\ Done)}$ = -2874.687463 a.u., Imaginary frequency = *i*351.7105 cm^{-1}

N	-2.673410000	0.038077000	-0.566649000
N	-3.733830000	-0.447198000	-0.080197000
C	-2.748860000	1.203358000	-1.359460000
C	-3.950829000	1.926419000	-1.455340000
C	-1.600634000	1.627324000	-2.036115000
C	-3.990318000	3.064431000	-2.245104000
H	-4.824932000	1.585901000	-0.912138000
C	-1.654667000	2.781794000	-2.812592000
H	-0.669715000	1.075435000	-1.962795000
C	-2.844760000	3.496910000	-2.924234000
H	-4.916614000	3.626596000	-2.325700000
H	-0.752949000	3.112629000	-3.317242000
H	-2.884301000	4.395706000	-3.533703000
C	-3.547771000	-1.501567000	0.767696000

C	-2.244150000	-1.789783000	1.234420000
C	-4.608815000	-2.349421000	1.137105000
C	-1.963762000	-2.896239000	2.022886000
C	-4.343960000	-3.466446000	1.907632000
H	-5.606629000	-2.119759000	0.775431000
C	-3.028280000	-3.740602000	2.326217000
H	-0.955355000	-3.081889000	2.375319000
H	-5.148601000	-4.139323000	2.185981000
H	-2.830979000	-4.628578000	2.921179000
Pd	-0.918960000	-0.824499000	0.000766000
Cl	-0.844962000	-1.876800000	-2.020272000
S	2.050664000	1.797624000	-0.448097000
S	1.954648000	-0.831168000	0.630483000
O	1.425943000	2.380562000	-1.636301000
O	3.499288000	1.586715000	-0.398585000
O	2.529709000	-0.502903000	1.933325000
O	0.772526000	-1.824883000	0.671027000
N	1.252393000	0.351215000	-0.203783000
C	1.600651000	2.830243000	0.943071000
C	0.477059000	3.649924000	0.844637000
H	-0.097174000	3.668582000	-0.075976000
C	0.125919000	4.448070000	1.931335000
H	-0.745566000	5.094157000	1.865757000
C	0.894994000	4.423846000	3.094959000
H	0.618330000	5.048844000	3.940212000
C	2.021963000	3.605515000	3.174979000
H	2.623892000	3.592533000	4.079574000
C	2.384117000	2.802468000	2.095929000
H	3.257342000	2.161304000	2.141481000
C	3.204649000	-1.669971000	-0.321651000
C	2.849360000	-2.327181000	-1.499881000
H	1.815311000	-2.343816000	-1.830082000
C	3.847827000	-2.962400000	-2.232398000
H	3.589235000	-3.482389000	-3.150616000
C	5.171744000	-2.932356000	-1.790814000
H	5.945707000	-3.429647000	-2.369719000
C	5.507011000	-2.266660000	-0.612378000
H	6.538525000	-2.241384000	-0.272347000
C	4.520640000	-1.625906000	0.133584000
H	4.756127000	-1.098883000	1.051371000
F	-1.485631000	-0.347551000	1.917443000

P′-A_F, $E_{(SCF\ Done)}$ = -2874.772185 a.u.

N	-1.425749000	-1.507370000	-0.680406000
N	-2.674951000	-1.491870000	-0.751610000

C	-0.770442000	-2.133492000	-1.787395000
C	-1.373276000	-2.150726000	-3.049937000
C	0.471782000	-2.735241000	-1.577183000
C	-0.723100000	-2.780700000	-4.102103000
H	-2.328089000	-1.657403000	-3.192603000
C	1.106633000	-3.374723000	-2.636811000
H	0.915630000	-2.719715000	-0.586136000
C	0.515117000	-3.394852000	-3.898991000
H	-1.177796000	-2.783233000	-5.088714000
H	2.067734000	-3.853587000	-2.474302000
H	1.021128000	-3.881923000	-4.728144000
C	-3.458782000	-0.882196000	0.233574000
C	-3.263386000	0.403553000	0.759506000
C	-4.608768000	-1.588172000	0.622189000
C	-4.138191000	0.947958000	1.686437000
C	-5.472390000	-1.067090000	1.574227000
H	-4.774994000	-2.567120000	0.183911000
C	-5.234738000	0.201284000	2.109337000
H	-3.946213000	1.949242000	2.058382000
H	-6.335169000	-1.643478000	1.893295000
H	-5.913798000	0.620219000	2.846283000
Pd	-0.281876000	-0.888698000	0.847386000
Cl	-1.125032000	-2.627136000	2.086207000
S	1.065827000	1.563521000	-1.309554000
S	1.849070000	0.791034000	1.406508000
O	0.448522000	0.764288000	-2.363140000
O	2.470490000	1.968859000	-1.390556000
O	2.159344000	2.137488000	1.867037000
O	1.032204000	-0.108783000	2.322233000
N	0.863879000	0.691850000	0.104395000
C	0.083043000	3.047281000	-1.122232000
C	-1.040057000	3.206843000	-1.931166000
H	-1.312438000	2.422590000	-2.629313000
C	-1.782098000	4.382660000	-1.831151000
H	-2.657747000	4.521150000	-2.459699000
C	-1.399808000	5.376497000	-0.931515000
H	-1.981032000	6.291959000	-0.856004000
C	-0.269644000	5.202712000	-0.130571000
H	0.029339000	5.979436000	0.567964000
C	0.485152000	4.036729000	-0.224291000
H	1.364115000	3.892031000	0.395194000
C	3.386379000	-0.073069000	1.138573000
C	3.482814000	-1.414753000	1.511334000
H	2.636280000	-1.916617000	1.969217000
C	4.692262000	-2.077322000	1.311817000

H	4.786699000	-3.118983000	1.605869000
C	5.776717000	-1.403501000	0.750552000
H	6.717694000	-1.925632000	0.598196000
C	5.662626000	-0.060011000	0.390907000
H	6.510009000	0.463840000	-0.042183000
C	4.463686000	0.619915000	0.585760000
H	4.357591000	1.661335000	0.305451000
F	-2.255710000	1.161540000	0.304482000

TS′-A_{Cl}, $E_{(SCF\ Done)}$ = -2874.694486 a.u., Imaginary frequency = *i*204.5458 cm^{-1}

N	-2.709922000	1.033793000	-0.279717000
N	-3.900109000	0.693759000	-0.030680000
C	-2.464600000	2.267882000	-0.914825000
C	-3.510355000	3.166004000	-1.191981000
C	-1.145947000	2.564001000	-1.274901000
C	-3.214309000	4.361201000	-1.826670000
H	-4.525065000	2.914753000	-0.905025000
C	-0.868640000	3.762419000	-1.925088000
H	-0.333335000	1.874011000	-1.067018000
C	-1.896585000	4.662154000	-2.196676000
H	-4.013499000	5.065907000	-2.039283000
H	0.158221000	3.972062000	-2.205940000
H	-1.678461000	5.602230000	-2.696355000
C	-4.033756000	-0.558171000	0.526908000
C	-3.000978000	-1.526745000	0.411050000
C	-5.158502000	-0.849931000	1.313485000
C	-3.052684000	-2.718039000	1.128792000
C	-5.214196000	-2.036697000	2.027924000
H	-5.938558000	-0.098273000	1.389204000
C	-4.150968000	-2.946860000	1.954753000
H	-2.252910000	-3.444244000	1.033289000
H	-6.072424000	-2.252852000	2.656051000
H	-4.187505000	-3.868426000	2.529206000
Pd	-1.223653000	-0.247347000	0.260118000
Cl	-2.129306000	-1.717410000	-1.362919000
S	2.578527000	1.009711000	-0.853894000
S	1.592116000	-1.248418000	0.570732000
O	1.923419000	1.964501000	-1.755884000
O	3.712297000	0.228774000	-1.356744000
O	2.439239000	-1.127505000	1.753558000
O	0.134483000	-1.666943000	0.877158000
N	1.337172000	0.031642000	-0.346205000
C	3.135428000	1.901628000	0.594025000
C	2.233979000	2.285965000	1.586516000
H	1.197286000	1.961969000	1.552669000

C	2.702318000	3.049672000	2.653831000
H	2.013569000	3.342754000	3.441673000
C	4.044067000	3.425665000	2.719141000
H	4.400316000	4.020603000	3.556489000
C	4.932882000	3.028924000	1.720268000
H	5.981115000	3.310615000	1.776793000
C	4.481900000	2.259885000	0.649898000
H	5.160590000	1.924764000	-0.128029000
C	2.226241000	-2.600433000	-0.409874000
C	1.914382000	-2.682639000	-1.766320000
H	1.332700000	-1.897687000	-2.238629000
C	2.391917000	-3.765317000	-2.499637000
H	2.167447000	-3.836682000	-3.560319000
C	3.168218000	-4.745210000	-1.879252000
H	3.541776000	-5.585755000	-2.458338000
C	3.478499000	-4.643498000	-0.523415000
H	4.094063000	-5.400438000	-0.045071000
C	3.009835000	-3.564061000	0.222433000
H	3.255009000	-3.453559000	1.273754000
F	-0.817638000	0.905524000	1.746539000

P′-A_{Cl}, $E_{(SCF\ Done)}$ = -2874.720587 a.u.

N	2.540893000	-1.269252000	-0.201995000
N	3.789200000	-1.127333000	-0.206403000
C	2.049095000	-2.518626000	-0.665143000
C	2.870242000	-3.657552000	-0.683968000
C	0.728862000	-2.569213000	-1.127689000
C	2.352643000	-4.848180000	-1.167999000
H	3.884604000	-3.595281000	-0.306363000
C	0.232243000	-3.767128000	-1.631210000
H	0.092954000	-1.687883000	-1.119213000
C	1.036969000	-4.904443000	-1.646301000
H	2.971457000	-5.741145000	-1.169344000
H	-0.787987000	-3.787519000	-2.000329000
H	0.641786000	-5.843550000	-2.024615000
C	4.386627000	0.076246000	0.177412000
C	3.922506000	1.381967000	-0.077512000
C	5.644672000	-0.055459000	0.788349000
C	4.661737000	2.501510000	0.278955000
C	6.376488000	1.057177000	1.179493000
H	6.016755000	-1.061649000	0.954371000
C	5.887270000	2.337529000	0.922685000
H	4.275371000	3.491396000	0.058757000
H	7.335045000	0.925512000	1.671794000
H	6.458341000	3.214578000	1.211878000

Pd	1.193506000	0.076566000	0.435375000
Cl	2.404235000	1.646190000	-0.923952000
S	-2.807159000	-0.564761000	-1.090820000
S	-1.588531000	1.326146000	0.662656000
O	-2.225885000	-1.502383000	-2.061928000
O	-3.828749000	0.379963000	-1.555417000
O	-2.475704000	1.119605000	1.805155000
O	-0.107190000	1.537154000	1.045990000
N	-1.487482000	0.203577000	-0.458446000
C	-3.527870000	-1.526551000	0.236581000
C	-2.718196000	-2.144413000	1.189724000
H	-1.646478000	-1.965836000	1.210078000
C	-3.318190000	-2.952979000	2.152843000
H	-2.699995000	-3.426333000	2.911097000
C	-4.700151000	-3.144112000	2.154685000
H	-5.159411000	-3.775711000	2.911271000
C	-5.495635000	-2.515778000	1.196991000
H	-6.573816000	-2.653742000	1.204916000
C	-4.911261000	-1.698902000	0.231392000
H	-5.512732000	-1.185472000	-0.512042000
C	-2.026615000	2.897675000	-0.074278000
C	-1.850902000	3.104413000	-1.441070000
H	-1.500650000	2.292351000	-2.069738000
C	-2.171677000	4.348566000	-1.979870000
H	-2.053701000	4.518269000	-3.046720000
C	-2.659086000	5.364666000	-1.157825000
H	-2.911727000	6.331992000	-1.584551000
C	-2.838884000	5.138985000	0.207259000
H	-3.232246000	5.926741000	0.844212000
C	-2.526669000	3.898516000	0.758211000
H	-2.680716000	3.695595000	1.813251000
F	0.490840000	-1.234322000	1.648783000

B, $E_{(\text{SCF Done})}$ = -2694.753468 a.u.

N	-2.806795000	0.144179000	0.016496000
N	-3.543421000	-0.462470000	0.828000000
C	-3.382220000	1.051694000	-0.900545000
C	-4.593093000	1.688179000	-0.590202000
C	-2.730807000	1.285899000	-2.115961000
C	-5.152153000	2.557598000	-1.515248000
H	-5.065628000	1.497837000	0.367086000
C	-3.311154000	2.154897000	-3.034418000
H	-1.793205000	0.790355000	-2.341402000
C	-4.515326000	2.791555000	-2.737783000
H	-6.084938000	3.062340000	-1.280197000

H	-2.814658000	2.334970000	-3.983111000
H	-4.957697000	3.476809000	-3.455610000
C	-2.850489000	-1.270089000	1.696468000
C	-1.440919000	-1.318475000	1.622343000
C	-3.537564000	-2.050903000	2.633825000
C	-0.711568000	-2.090629000	2.492241000
C	-2.809089000	-2.861990000	3.495087000
H	-4.621652000	-2.001656000	2.665570000
C	-1.415697000	-2.875756000	3.423775000
H	0.373772000	-2.081160000	2.482206000
H	-3.322621000	-3.476534000	4.228176000
H	-0.846324000	-3.499313000	4.108385000
Pd	-0.777918000	-0.016610000	0.267903000
S	2.634210000	-0.774779000	0.852128000
S	1.519081000	1.434028000	-0.656020000
O	2.229907000	-1.472338000	2.071072000
O	3.796335000	0.110067000	0.848828000
O	2.447794000	1.185950000	-1.751175000
O	0.067818000	1.643666000	-1.001921000
N	1.317557000	0.182063000	0.414263000
C	2.869729000	-2.007822000	-0.415918000
C	2.219585000	-3.236124000	-0.300340000
H	1.580979000	-3.437073000	0.553139000
C	2.418338000	-4.198238000	-1.286360000
H	1.913732000	-5.157264000	-1.211866000
C	3.262006000	-3.930374000	-2.364268000
H	3.412387000	-4.684005000	-3.132674000
C	3.914858000	-2.701822000	-2.458918000
H	4.576310000	-2.497748000	-3.296269000
C	3.723548000	-1.728039000	-1.481821000
H	4.221700000	-0.767314000	-1.539887000
C	2.077151000	2.864114000	0.239528000
C	1.295927000	3.366775000	1.281045000
H	0.370595000	2.869773000	1.560290000
C	1.745538000	4.500534000	1.951595000
H	1.154840000	4.908091000	2.767285000
C	2.946822000	5.108988000	1.582755000
H	3.289516000	5.993341000	2.113786000
C	3.712513000	4.587135000	0.540673000
H	4.649283000	5.059764000	0.259096000
C	3.281572000	3.451989000	-0.141778000
H	3.860552000	3.022092000	-0.951650000
F	-1.029173000	1.293659000	1.673520000
O	-0.393721000	-1.267588000	-1.252350000
N	-1.225317000	-2.253457000	-1.631594000

O	-0.839731000	-2.877797000	-2.597363000
O	-2.258654000	-2.440327000	-1.007104000

TS-B_F, $E_{(SCF\ Done)}$ = -2694.731345 a.u., Imaginary frequency = *i*335.2294 cm^{-1}

N	-2.899348000	0.085704000	-0.037481000
N	-3.536779000	0.443041000	0.989026000
C	-3.609404000	-0.171100000	-1.230544000
C	-5.013631000	-0.169908000	-1.255126000
C	-2.872314000	-0.430249000	-2.392729000
C	-5.667704000	-0.430807000	-2.449145000
H	-5.563063000	0.028802000	-0.342102000
C	-3.546032000	-0.678639000	-3.585199000
H	-1.785993000	-0.421787000	-2.376553000
C	-4.938864000	-0.684194000	-3.616496000
H	-6.753807000	-0.438604000	-2.473118000
H	-2.974702000	-0.872797000	-4.487870000
H	-5.460839000	-0.888406000	-4.547262000
C	-2.739651000	0.731206000	2.066519000
C	-1.345722000	0.880463000	1.912798000
C	-3.279194000	0.833819000	3.359096000
C	-0.491221000	1.165778000	2.952669000
C	-2.436538000	1.063465000	4.435095000
H	-4.349387000	0.697769000	3.481477000
C	-1.058799000	1.214757000	4.229713000
H	0.567095000	1.325676000	2.793968000
H	-2.842958000	1.127062000	5.439356000
H	-0.402065000	1.396493000	5.076005000
Pd	-0.837414000	0.031743000	0.068170000
S	2.280892000	-0.601742000	1.076233000
S	1.673869000	0.809466000	-1.450101000
O	1.410937000	-1.118761000	2.132380000
O	3.321335000	0.379274000	1.395769000
O	2.889841000	0.177427000	-1.950892000
O	0.421963000	0.766969000	-2.233469000
N	1.205057000	0.107586000	-0.008295000
C	3.078186000	-1.983198000	0.270986000
C	2.344017000	-3.130695000	-0.027013000
H	1.280074000	-3.178925000	0.172607000
C	3.003515000	-4.214662000	-0.600442000
H	2.441839000	-5.113070000	-0.840442000
C	4.372745000	-4.149157000	-0.860180000
H	4.880410000	-5.000528000	-1.306359000
C	5.092644000	-2.996564000	-0.548140000
H	6.159298000	-2.945958000	-0.749031000
C	4.446650000	-1.901847000	0.020773000

H	4.985974000	-0.995603000	0.272052000
C	2.045622000	2.529543000	-1.144613000
C	1.078298000	3.495025000	-1.418693000
H	0.109651000	3.195594000	-1.802462000
C	1.387198000	4.836214000	-1.201693000
H	0.643937000	5.599512000	-1.415215000
C	2.644316000	5.196061000	-0.717352000
H	2.880245000	6.243739000	-0.549331000
C	3.603122000	4.217159000	-0.452968000
H	4.583709000	4.499350000	-0.079758000
C	3.311698000	2.873150000	-0.669688000
H	4.046459000	2.102151000	-0.468649000
F	-0.981272000	1.993674000	0.490438000
O	-0.726285000	-1.928855000	-0.181295000
N	-1.412295000	-2.732920000	0.654831000
O	-1.218554000	-3.916085000	0.464606000
O	-2.139192000	-2.233085000	1.495710000

P-B_F, $E_{(SCF\ Done)}$ = -2694.789937 a.u.

N	-2.786255000	0.278762000	0.074540000
N	-3.390109000	0.633742000	1.116286000
C	-3.605616000	0.030098000	-1.063882000
C	-4.982107000	-0.203883000	-0.927756000
C	-2.997630000	0.031561000	-2.325397000
C	-5.744129000	-0.434361000	-2.062900000
H	-5.425769000	-0.217389000	0.061045000
C	-3.780323000	-0.187202000	-3.455744000
H	-1.929597000	0.205387000	-2.424329000
C	-5.147508000	-0.423111000	-3.328306000
H	-6.807513000	-0.633003000	-1.963654000
H	-3.311730000	-0.182464000	-4.435160000
H	-5.751261000	-0.608042000	-4.212616000
C	-2.677670000	0.940145000	2.278239000
C	-1.414210000	1.541139000	2.352813000
C	-3.346255000	0.714255000	3.492963000
C	-0.800247000	1.875731000	3.539674000
C	-2.741322000	1.015869000	4.705435000
H	-4.338532000	0.276649000	3.447681000
C	-1.471056000	1.595087000	4.730046000
H	0.186750000	2.324248000	3.521264000
H	-3.263141000	0.806974000	5.634015000
H	-0.996256000	1.835556000	5.676319000
Pd	-0.763620000	0.026759000	-0.068555000
S	2.158452000	-0.444209000	1.076031000
S	1.909022000	0.539907000	-1.698371000

O	1.147038000	-0.618620000	2.128447000
O	3.267148000	0.484990000	1.305879000
O	3.104812000	-0.239116000	-2.004569000
O	0.759802000	0.564565000	-2.609933000
N	1.251110000	0.033771000	-0.239229000
C	2.867301000	-2.034806000	0.678806000
C	2.159869000	-2.962618000	-0.083575000
H	1.203151000	-2.702175000	-0.524471000
C	2.721294000	-4.218436000	-0.300881000
H	2.181827000	-4.945814000	-0.900866000
C	3.967299000	-4.535716000	0.240161000
H	4.399540000	-5.517552000	0.064967000
C	4.665024000	-3.593895000	0.995732000
H	5.640771000	-3.836962000	1.407828000
C	4.118185000	-2.332316000	1.218368000
H	4.653099000	-1.580267000	1.789155000
C	2.416503000	2.239525000	-1.457662000
C	1.504633000	3.260659000	-1.725195000
H	0.511908000	3.015890000	-2.089676000
C	1.901348000	4.584451000	-1.549292000
H	1.202496000	5.389316000	-1.761441000
C	3.195760000	4.874263000	-1.116591000
H	3.503153000	5.908360000	-0.983189000
C	4.099978000	3.842405000	-0.864821000
H	5.110092000	4.070146000	-0.535562000
C	3.716209000	2.514170000	-1.035856000
H	4.405480000	1.700128000	-0.843607000
F	-0.763536000	1.867570000	1.183576000
O	-0.871451000	-1.723818000	-1.019662000
N	-1.576400000	-2.679881000	-0.392408000
O	-1.562633000	-3.758943000	-0.948204000
O	-2.156728000	-2.401811000	0.649356000

TS-B_{NO3}, $E_{(SCF\ Done)}$ = -2694.717477 a.u., Imaginary frequency = *i*391.277 cm^{-1}

N	-2.953535000	-0.142811000	0.232568000
N	-3.528901000	-1.189429000	0.622284000
C	-3.745089000	0.966365000	-0.140272000
C	-5.134960000	0.959635000	0.062260000
C	-3.109816000	2.067810000	-0.724675000
C	-5.878234000	2.064815000	-0.320913000
H	-5.604958000	0.095492000	0.517385000
C	-3.874414000	3.163336000	-1.115093000
H	-2.036424000	2.065742000	-0.888743000
C	-5.252537000	3.168471000	-0.911444000
H	-6.952678000	2.069073000	-0.160131000

H	-3.383754000	4.015387000	-1.575909000
H	-5.843417000	4.030222000	-1.209777000
C	-2.676824000	-2.226409000	0.919660000
C	-1.295800000	-2.192394000	0.607713000
C	-3.163865000	-3.304126000	1.681125000
C	-0.427191000	-3.182273000	1.030037000
C	-2.299752000	-4.285460000	2.136025000
H	-4.220590000	-3.305704000	1.930897000
C	-0.936436000	-4.206862000	1.827832000
H	0.619426000	-3.154582000	0.758688000
H	-2.676749000	-5.108637000	2.734495000
H	-0.252014000	-4.971998000	2.183064000
Pd	-0.897535000	-0.094067000	0.213158000
S	2.329792000	-0.426463000	1.108637000
S	1.435279000	1.438614000	-0.973223000
O	1.613548000	-1.337846000	2.003040000
O	3.151323000	0.644972000	1.665916000
O	2.509786000	1.102577000	-1.902980000
O	0.072504000	1.672357000	-1.506105000
N	1.144604000	0.189604000	0.099534000
C	3.390360000	-1.398397000	0.040972000
C	2.865353000	-2.141923000	-1.015387000
H	1.814333000	-2.065357000	-1.274272000
C	3.720355000	-2.950860000	-1.760258000
H	3.323793000	-3.522760000	-2.594735000
C	5.078681000	-3.013264000	-1.448178000
H	5.741128000	-3.643453000	-2.035905000
C	5.590812000	-2.258632000	-0.393383000
H	6.650775000	-2.297697000	-0.157090000
C	4.747670000	-1.442251000	0.357550000
H	5.130774000	-0.834174000	1.170644000
C	1.938694000	2.888291000	-0.062392000
C	1.188266000	3.324477000	1.029223000
H	0.339516000	2.743531000	1.380998000
C	1.574848000	4.497890000	1.670667000
H	1.009033000	4.847586000	2.529883000
C	2.684742000	5.215840000	1.222198000
H	2.979141000	6.130340000	1.730895000
C	3.422585000	4.761186000	0.130248000
H	4.290604000	5.316825000	-0.214100000
C	3.054039000	3.585996000	-0.521263000
H	3.617903000	3.205558000	-1.366330000
F	-1.042915000	1.205904000	1.612826000
O	-0.672212000	-1.720238000	-1.041644000
N	-1.498895000	-1.989580000	-2.158556000

O	-0.907082000	-2.585582000	-3.017689000
O	-2.646109000	-1.623482000	-2.116988000

P-B_{NO3}, $E_{(SCF\ Done)}$ = -2694.788214 a.u.

N	2.895045000	0.355087000	-0.221195000
N	3.644247000	-0.599391000	-0.564584000
C	3.552467000	1.566280000	0.125959000
C	4.866445000	1.823623000	-0.293449000
C	2.853262000	2.489787000	0.913884000
C	5.475897000	3.010929000	0.082303000
H	5.379986000	1.099329000	-0.915455000
C	3.486952000	3.667684000	1.297052000
H	1.834459000	2.283503000	1.229314000
C	4.790332000	3.932981000	0.880738000
H	6.487105000	3.225112000	-0.252087000
H	2.951013000	4.382398000	1.914230000
H	5.274076000	4.862105000	1.170074000
C	3.093312000	-1.842028000	-0.872971000
C	1.896633000	-2.378985000	-0.334414000
C	3.858738000	-2.648600000	-1.725913000
C	1.486579000	-3.670068000	-0.660111000
C	3.426480000	-3.922139000	-2.076286000
H	4.786668000	-2.241025000	-2.114700000
C	2.239652000	-4.433838000	-1.545489000
H	0.558764000	-4.038454000	-0.235832000
H	4.020377000	-4.521760000	-2.759560000
H	1.902494000	-5.429219000	-1.818122000
Pd	0.871447000	0.288586000	-0.181265000
S	-1.969870000	-0.793813000	-1.097616000
S	-1.916818000	1.258953000	1.020843000
O	-0.894052000	-1.560092000	-1.743823000
O	-2.911588000	-0.036647000	-1.920157000
O	-2.969595000	0.561442000	1.761968000
O	-0.799683000	1.869316000	1.751473000
N	-1.157669000	0.172579000	-0.009765000
C	-2.941099000	-1.940729000	-0.121649000
C	-2.382974000	-2.584343000	0.981527000
H	-1.387099000	-2.313689000	1.314482000
C	-3.134567000	-3.535975000	1.663858000
H	-2.715859000	-4.031545000	2.536026000
C	-4.429097000	-3.842000000	1.239879000
H	-5.013971000	-4.583779000	1.777691000
C	-4.976783000	-3.189509000	0.137022000
H	-5.987867000	-3.420344000	-0.187742000
C	-4.233866000	-2.230557000	-0.550458000

H	-4.644847000	-1.699977000	-1.403118000
C	-2.717663000	2.516002000	0.032537000
C	-1.981795000	3.247721000	-0.898615000
H	-0.936328000	3.007043000	-1.075395000
C	-2.626576000	4.259308000	-1.605751000
H	-2.070887000	4.833218000	-2.342713000
C	-3.976008000	4.532906000	-1.377339000
H	-4.470399000	5.324578000	-1.935086000
C	-4.694390000	3.790400000	-0.441233000
H	-5.746416000	4.000211000	-0.266457000
C	-4.066724000	2.770674000	0.271496000
H	-4.604772000	2.173562000	1.000091000
F	0.792922000	1.973130000	-1.100134000
O	1.129740000	-1.656374000	0.529317000
N	1.660069000	-1.821314000	2.134521000
O	1.098294000	-1.048792000	2.822934000
O	2.454957000	-2.687917000	2.263764000

B′, $E_{(\text{SCF Done})}$ = -2694.743135 a.u.

N	2.549922000	-0.201996000	0.491922000
N	3.552477000	-0.847125000	0.093365000
C	2.753588000	0.901882000	1.349223000
C	3.985293000	1.577563000	1.342153000
C	1.720606000	1.286041000	2.207219000
C	4.174000000	2.636545000	2.216059000
H	4.761387000	1.267926000	0.651200000
C	1.929887000	2.350303000	3.080495000
H	0.773041000	0.760921000	2.208236000
C	3.149782000	3.023028000	3.088718000
H	5.119398000	3.171779000	2.212662000
H	1.123301000	2.653696000	3.739458000
H	3.304556000	3.857537000	3.767281000
C	3.251568000	-1.879146000	-0.763466000
C	1.905484000	-2.114578000	-1.084719000
C	4.256958000	-2.687553000	-1.315719000
C	1.525621000	-3.092007000	-1.972133000
C	3.887287000	-3.695666000	-2.195235000
H	5.294011000	-2.500779000	-1.054208000
C	2.539850000	-3.890552000	-2.520914000
H	0.481786000	-3.248616000	-2.221388000
H	4.646276000	-4.333321000	-2.637921000
H	2.264301000	-4.681774000	-3.213262000
Pd	0.724156000	-0.756453000	-0.268646000
S	-1.643945000	2.145219000	0.519229000
S	-2.037608000	-0.300587000	-0.883795000

O	-1.011186000	2.427037000	1.806008000
O	-3.100334000	2.182456000	0.382727000
O	-2.581414000	0.276092000	-2.106759000
O	-1.022635000	-1.450965000	-1.104962000
N	-1.116864000	0.609201000	0.082613000
C	-0.942171000	3.261697000	-0.685150000
C	0.236395000	3.938569000	-0.377192000
H	0.710515000	3.785883000	0.586534000
C	0.772984000	4.816293000	-1.316880000
H	1.689894000	5.353400000	-1.089459000
C	0.133130000	5.007957000	-2.540960000
H	0.555647000	5.693287000	-3.271245000
C	-1.050404000	4.327927000	-2.830331000
H	-1.550021000	4.482242000	-3.782710000
C	-1.599864000	3.449236000	-1.900591000
H	-2.518999000	2.913404000	-2.110929000
C	-3.376216000	-1.027736000	0.034831000
C	-3.156708000	-1.468277000	1.340507000
H	-2.189227000	-1.335699000	1.814199000
C	-4.210547000	-2.065528000	2.025011000
H	-4.056288000	-2.414761000	3.041703000
C	-5.454995000	-2.211592000	1.409517000
H	-6.273604000	-2.677356000	1.951799000
C	-5.656285000	-1.758258000	0.106274000
H	-6.628265000	-1.865857000	-0.366863000
C	-4.612364000	-1.158927000	-0.594705000
H	-4.746074000	-0.788004000	-1.605226000
F	1.149151000	0.269632000	-1.839993000
O	0.303769000	-1.614366000	1.504846000
N	0.067440000	-2.932619000	1.639504000
O	-0.305273000	-3.248791000	2.752607000
O	0.234772000	-3.670640000	0.686399000

TS′-B_F, $E_{(SCF\ Done)}$ = -2694.716575 a.u., Imaginary frequency = *i*348.142 cm^{-1}

N	2.576024000	0.618903000	0.354925000
N	3.676672000	0.398150000	-0.225281000
C	2.494347000	1.671118000	1.292733000
C	3.575229000	2.549888000	1.484555000
C	1.310284000	1.820471000	2.022941000
C	3.457764000	3.566744000	2.418425000
H	4.480170000	2.420449000	0.902098000
C	1.205073000	2.856920000	2.946797000
H	0.468873000	1.151150000	1.879484000
C	2.274608000	3.725409000	3.150672000
H	4.289731000	4.248186000	2.573195000

H	0.275123000	2.974065000	3.493425000
H	2.190987000	4.531023000	3.875075000
C	3.638304000	-0.568556000	-1.188503000
C	2.391783000	-1.042038000	-1.654807000
C	4.811358000	-1.171278000	-1.675761000
C	2.267900000	-2.073127000	-2.567649000
C	4.712053000	-2.228945000	-2.563171000
H	5.768647000	-0.812997000	-1.309532000
C	3.450700000	-2.682829000	-2.985305000
H	1.292929000	-2.386329000	-2.924185000
H	5.609583000	-2.715681000	-2.930752000
H	3.385531000	-3.520125000	-3.675148000
Pd	0.954902000	-0.463130000	-0.269438000
S	-2.445259000	1.414253000	0.662030000
S	-1.905625000	-0.989564000	-0.763298000
O	-1.822435000	1.985852000	1.857109000
O	-3.810870000	0.889097000	0.714687000
O	-2.663353000	-0.672152000	-1.971579000
O	-0.547872000	-1.683206000	-1.022254000
N	-1.390001000	0.224359000	0.153803000
C	-2.388221000	2.668195000	-0.613283000
C	-1.449795000	3.694778000	-0.514966000
H	-0.783032000	3.735561000	0.340347000
C	-1.402766000	4.664479000	-1.514215000
H	-0.678664000	5.472184000	-1.447494000
C	-2.287524000	4.603039000	-2.591143000
H	-2.248447000	5.362264000	-3.368074000
C	-3.226835000	3.574732000	-2.670902000
H	-3.919665000	3.532035000	-3.506905000
C	-3.284490000	2.598537000	-1.678775000
H	-4.009089000	1.793027000	-1.724268000
C	-2.843775000	-2.171370000	0.184069000
C	-2.306420000	-2.693762000	1.361388000
H	-1.323763000	-2.386771000	1.705948000
C	-3.061318000	-3.613884000	2.082596000
H	-2.658868000	-4.031158000	3.001297000
C	-4.325609000	-3.996366000	1.630365000
H	-4.908790000	-4.714362000	2.201119000
C	-4.845613000	-3.460059000	0.453263000
H	-5.831813000	-3.755115000	0.105847000
C	-4.104547000	-2.537074000	-0.281475000
H	-4.488253000	-2.099982000	-1.196825000
F	1.340692000	0.305758000	-2.094979000
O	0.783796000	-1.413076000	1.459903000
N	1.768882000	-2.248170000	1.853009000

O	1.514505000	-2.853632000	2.871788000
O	2.785639000	-2.318270000	1.184391000

P′-B_F, $E_{(SCF\ Done)}$ = -2694.803476 a.u.

N	1.289901000	-1.200114000	1.164040000
N	2.526400000	-1.166483000	1.360494000
C	0.530122000	-1.738994000	2.249876000
C	1.038009000	-1.712897000	3.554405000
C	-0.719785000	-2.301664000	1.983511000
C	0.290626000	-2.264712000	4.585435000
H	2.000292000	-1.250751000	3.743146000
C	-1.454168000	-2.862600000	3.022774000
H	-1.103551000	-2.306762000	0.967276000
C	-0.953947000	-2.843057000	4.323609000
H	0.674968000	-2.234569000	5.601096000
H	-2.422786000	-3.307041000	2.814087000
H	-1.536489000	-3.268240000	5.136353000
C	3.411607000	-0.613166000	0.432977000
C	3.246554000	0.608305000	-0.239964000
C	4.634514000	-1.290834000	0.282006000
C	4.231620000	1.116085000	-1.071105000
C	5.609720000	-0.811487000	-0.578934000
H	4.772387000	-2.215392000	0.833907000
C	5.407116000	0.394250000	-1.255816000
H	4.055059000	2.064265000	-1.568004000
H	6.530907000	-1.368929000	-0.715977000
H	6.171386000	0.781217000	-1.923329000
Pd	0.329354000	-0.821498000	-0.583018000
S	-1.403099000	1.706237000	1.108706000
S	-1.911908000	0.509415000	-1.525974000
O	-0.835206000	1.106553000	2.311397000
O	-2.831135000	2.014094000	1.017048000
O	-2.301946000	1.759423000	-2.161407000
O	-0.942914000	-0.402152000	-2.256883000
N	-1.038599000	0.655063000	-0.145193000
C	-0.495755000	3.212942000	0.783472000
C	0.521870000	3.575886000	1.663362000
H	0.765824000	2.926906000	2.497518000
C	1.197055000	4.777247000	1.454078000
H	1.989943000	5.074099000	2.135343000
C	0.854035000	5.594019000	0.377812000
H	1.383402000	6.529711000	0.217299000
C	-0.170515000	5.217325000	-0.492462000
H	-0.438755000	5.856062000	-1.329450000
C	-0.859017000	4.024102000	-0.292324000

H	-1.656082000	3.722478000	-0.963956000
C	-3.383907000	-0.460933000	-1.256575000
C	-3.340570000	-1.836545000	-1.489013000
H	-2.426430000	-2.300865000	-1.844547000
C	-4.498429000	-2.585214000	-1.287594000
H	-4.483650000	-3.655394000	-1.474434000
C	-5.670857000	-1.961196000	-0.861980000
H	-6.571198000	-2.549977000	-0.707367000
C	-5.696466000	-0.583340000	-0.641989000
H	-6.612257000	-0.099059000	-0.315193000
C	-4.550833000	0.181869000	-0.841776000
H	-4.553145000	1.251681000	-0.668401000
F	2.148339000	1.343714000	-0.021056000
O	1.371953000	-2.387195000	-1.291361000
N	2.054296000	-2.122259000	-2.410395000
O	2.622253000	-3.070473000	-2.914071000
O	2.056917000	-0.967775000	-2.824237000

TS′-B_{NO3}, $E_{(SCF\ Done)}$ = -2694.700656 a.u., Imaginary frequency = i372.204 cm^{-1}

N	2.669302000	1.255885000	0.183613000
N	3.845120000	0.952759000	-0.164278000
C	2.447744000	2.420749000	0.943171000
C	3.508567000	3.276850000	1.289027000
C	1.139336000	2.694157000	1.354172000
C	3.236954000	4.408511000	2.040277000
H	4.515757000	3.042912000	0.963564000
C	0.886840000	3.828029000	2.120189000
H	0.312348000	2.038288000	1.098697000
C	1.929149000	4.687093000	2.459447000
H	4.048580000	5.079496000	2.307786000
H	-0.132860000	4.021000000	2.436748000
H	1.730386000	5.576564000	3.051231000
C	3.963783000	-0.253236000	-0.804658000
C	2.898462000	-1.188308000	-0.756336000
C	5.088985000	-0.546662000	-1.592401000
C	2.906681000	-2.356786000	-1.502195000
C	5.111276000	-1.708474000	-2.345912000
H	5.897670000	0.177281000	-1.625208000
C	4.015574000	-2.584805000	-2.316495000
H	2.077201000	-3.052931000	-1.465422000
H	5.967190000	-1.934095000	-2.973601000
H	4.027388000	-3.481370000	-2.930386000
Pd	1.187461000	-0.074807000	-0.291547000
S	-2.583418000	1.124033000	0.852835000
S	-1.594235000	-1.123278000	-0.610137000

O	-1.911330000	2.092290000	1.726198000
O	-3.701202000	0.343582000	1.390277000
O	-2.336541000	-0.937719000	-1.853367000
O	-0.125084000	-1.583929000	-0.815337000
N	-1.346709000	0.133435000	0.344114000
C	-3.184573000	1.992855000	-0.590795000
C	-2.303032000	2.429589000	-1.578996000
H	-1.252934000	2.154088000	-1.546223000
C	-2.807760000	3.177082000	-2.640725000
H	-2.134417000	3.510283000	-3.425902000
C	-4.166636000	3.486517000	-2.703862000
H	-4.551552000	4.069990000	-3.536530000
C	-5.035017000	3.038590000	-1.708876000
H	-6.095682000	3.269320000	-1.763411000
C	-4.547137000	2.284389000	-0.644004000
H	-5.207612000	1.911787000	0.132356000
C	-2.356994000	-2.475713000	0.268290000
C	-2.288244000	-2.544758000	1.658260000
H	-1.802742000	-1.755646000	2.219932000
C	-2.879063000	-3.628943000	2.302464000
H	-2.842584000	-3.691664000	3.386288000
C	-3.522488000	-4.620930000	1.562819000
H	-3.982393000	-5.463148000	2.073266000
C	-3.590022000	-4.531468000	0.171995000
H	-4.102882000	-5.298557000	-0.401692000
C	-3.010042000	-3.450878000	-0.486856000
H	-3.072481000	-3.348833000	-1.565405000
F	0.663586000	1.062354000	-1.732550000
O	2.304788000	-1.306866000	0.925390000
N	1.775045000	-2.541363000	1.428764000
O	2.407238000	-3.521210000	1.142531000
O	0.811534000	-2.406480000	2.128233000

P′-B_{NO3}, $E_{(SCF\ Done)}$ = -2694.767448 a.u.

N	-2.403250000	1.488445000	0.037374000
N	-3.657403000	1.362901000	0.055458000
C	-1.899771000	2.716091000	-0.463767000
C	-2.688811000	3.877670000	-0.457812000
C	-0.602163000	2.722697000	-0.991125000
C	-2.162771000	5.047372000	-0.982495000
H	-3.684277000	3.848358000	-0.029017000
C	-0.099795000	3.899456000	-1.536468000
H	0.007146000	1.823175000	-1.007413000
C	-0.871697000	5.059689000	-1.526326000
H	-2.755122000	5.957925000	-0.964632000

H	0.899909000	3.887378000	-1.958581000
H	-0.469432000	5.982361000	-1.936290000
C	-4.238204000	0.164963000	0.464684000
C	-3.656072000	-1.123811000	0.338095000
C	-5.548637000	0.257577000	0.952358000
C	-4.376191000	-2.264426000	0.694825000
C	-6.245706000	-0.880355000	1.341768000
H	-5.994962000	1.244346000	1.026105000
C	-5.661803000	-2.143134000	1.212189000
H	-3.900495000	-3.232607000	0.572965000
H	-7.252406000	-0.784071000	1.737158000
H	-6.210193000	-3.032805000	1.506593000
Pd	-1.095530000	0.110366000	0.663918000
S	2.826481000	0.453242000	-1.159411000
S	1.627976000	-1.287408000	0.771420000
O	2.218747000	1.414440000	-2.091366000
O	3.743948000	-0.557131000	-1.699273000
O	2.580660000	-1.058469000	1.856283000
O	0.161256000	-1.408776000	1.235639000
N	1.525050000	-0.227106000	-0.406803000
C	3.725599000	1.385349000	0.077035000
C	3.042217000	2.108398000	1.054655000
H	1.962588000	2.029275000	1.148905000
C	3.777003000	2.890075000	1.943306000
H	3.257877000	3.445115000	2.720286000
C	5.167710000	2.951221000	1.847766000
H	5.732992000	3.562995000	2.546705000
C	5.835641000	2.219161000	0.866726000
H	6.919895000	2.256761000	0.798856000
C	5.114975000	1.427683000	-0.025396000
H	5.614015000	0.836352000	-0.786476000
C	1.958684000	-2.922072000	0.118246000
C	1.809492000	-3.182556000	-1.241862000
H	1.541359000	-2.378889000	-1.918471000
C	2.052979000	-4.472529000	-1.710403000
H	1.956427000	-4.684753000	-2.771873000
C	2.436121000	-5.480436000	-0.826130000
H	2.627924000	-6.483732000	-1.198138000
C	2.590650000	-5.201458000	0.532588000
H	2.903373000	-5.983855000	1.219020000
C	2.357520000	-3.915581000	1.013065000
H	2.496273000	-3.674099000	2.062172000
F	-0.152180000	1.431781000	1.673196000
O	-2.397138000	-1.282048000	-0.149281000
N	-2.388626000	-1.489632000	-1.856916000

O	-3.464994000	-1.730853000	-2.281063000
O	-1.291532000	-1.380157000	-2.262931000

C, $E_{(\text{SCF Done})}$ = -2619.591362 a.u.

N	2.861865000	-0.655838000	0.228693000
N	3.421046000	-1.596426000	-0.389666000
C	3.674045000	0.286494000	0.901972000
C	4.975055000	0.534259000	0.436805000
C	3.163325000	0.958765000	2.017421000
C	5.767551000	1.453516000	1.107911000
H	5.333296000	0.016803000	-0.446202000
C	3.976493000	1.872441000	2.680758000
H	2.160408000	0.749246000	2.368823000
C	5.271868000	2.123002000	2.230828000
H	6.771712000	1.659253000	0.748020000
H	3.589762000	2.391091000	3.552920000
H	5.896131000	2.846149000	2.748663000
C	2.553369000	-2.352842000	-1.140395000
C	1.191501000	-1.983945000	-1.200163000
C	3.028648000	-3.453976000	-1.867396000
C	0.314682000	-2.667646000	-2.009119000
C	2.138787000	-4.167709000	-2.658150000
H	4.081524000	-3.711777000	-1.805302000
C	0.801396000	-3.770738000	-2.730400000
H	-0.721300000	-2.358037000	-2.098431000
H	2.484170000	-5.023700000	-3.229948000
H	0.109921000	-4.322249000	-3.362454000
Pd	0.845191000	-0.370377000	-0.087614000
S	-2.658298000	-0.275822000	-0.863298000
S	-1.065006000	1.675352000	0.568411000
O	-2.359127000	-1.202454000	-1.952319000
O	-3.461349000	0.921985000	-1.098226000
O	-2.045650000	1.827956000	1.637148000
O	0.384923000	1.557637000	0.964068000
N	-1.173128000	0.254090000	-0.272893000
C	-3.452581000	-1.213387000	0.433825000
C	-3.350143000	-2.603472000	0.428557000
H	-2.775043000	-3.102220000	-0.343054000
C	-4.003547000	-3.330411000	1.420782000
H	-3.930182000	-4.414296000	1.428552000
C	-4.746937000	-2.669549000	2.397798000
H	-5.254174000	-3.241200000	3.170649000
C	-4.846387000	-1.277905000	2.385051000
H	-5.430840000	-0.764706000	3.143604000
C	-4.201350000	-0.537736000	1.397967000

H	-4.272746000	0.543447000	1.372446000
C	-1.217387000	3.066902000	-0.528777000
C	-0.319607000	3.207538000	-1.587432000
H	0.443953000	2.452051000	-1.762439000
C	-0.446116000	4.324421000	-2.409236000
H	0.239616000	4.453413000	-3.242079000
C	-1.444168000	5.270164000	-2.169245000
H	-1.533546000	6.138074000	-2.817653000
C	-2.330447000	5.107142000	-1.104721000
H	-3.109104000	5.842458000	-0.922184000
C	-2.224493000	3.995692000	-0.272773000
H	-2.904105000	3.842218000	0.558051000
F	1.412096000	0.693119000	-1.655960000
N	0.321887000	-1.509678000	1.525689000
O	0.701133000	-1.094184000	2.606156000
O	-0.327091000	-2.518484000	1.340189000

TS-C_F, $E_{(SCF\ Done)}$ = -2619.570845 a.u., Imaginary frequency = *i*323.6746 cm^{-1}

N	2.909972000	-0.211244000	0.098601000
N	3.580419000	-0.697922000	-0.859385000
C	3.604189000	0.467531000	1.125135000
C	4.953334000	0.826403000	0.966145000
C	2.913908000	0.786786000	2.301008000
C	5.604708000	1.486819000	1.996588000
H	5.463200000	0.585022000	0.040411000
C	3.581791000	1.457263000	3.321654000
H	1.870631000	0.516444000	2.421324000
C	4.922971000	1.805162000	3.176000000
H	6.647759000	1.766797000	1.877623000
H	3.045520000	1.705877000	4.232528000
H	5.438970000	2.329696000	3.975545000
C	2.826638000	-1.139971000	-1.903526000
C	1.454215000	-0.785553000	-1.985846000
C	3.386160000	-1.966520000	-2.898662000
C	0.654015000	-1.215139000	-3.032883000
C	2.584357000	-2.438962000	-3.918403000
H	4.437392000	-2.226778000	-2.819399000
C	1.226875000	-2.072382000	-3.968436000
H	-0.387743000	-0.923857000	-3.087573000
H	2.997816000	-3.089664000	-4.682467000
H	0.598622000	-2.450085000	-4.771037000
Pd	0.845024000	-0.140838000	-0.119866000
S	-2.556191000	-0.718381000	-0.694210000
S	-1.435031000	1.484363000	0.847338000
O	-2.113707000	-1.407362000	-1.906326000

O	-3.695681000	0.196035000	-0.729000000
O	-2.439137000	1.279530000	1.886459000
O	-0.023108000	1.725419000	1.247783000
N	-1.230187000	0.165246000	-0.157164000
C	-2.894119000	-1.982500000	0.523503000
C	-2.429035000	-3.277373000	0.296212000
H	-1.862119000	-3.497893000	-0.601723000
C	-2.718789000	-4.269803000	1.230394000
H	-2.360609000	-5.282318000	1.066455000
C	-3.466007000	-3.963938000	2.367030000
H	-3.689252000	-4.741380000	3.093137000
C	-3.932648000	-2.665166000	2.574468000
H	-4.519122000	-2.430251000	3.458416000
C	-3.652517000	-1.662433000	1.650349000
H	-4.004954000	-0.648119000	1.798260000
C	-1.948106000	2.862872000	-0.157517000
C	-1.053205000	3.407480000	-1.079372000
H	-0.063122000	2.981429000	-1.204592000
C	-1.463509000	4.498173000	-1.840587000
H	-0.779975000	4.934113000	-2.563935000
C	-2.743777000	5.029294000	-1.674938000
H	-3.056496000	5.881724000	-2.272465000
C	-3.624022000	4.470681000	-0.749096000
H	-4.621340000	4.883156000	-0.624342000
C	-3.230714000	3.376524000	0.018175000
H	-3.898787000	2.919531000	0.739457000
F	1.256271000	1.020287000	-1.800509000
N	0.655478000	-1.690434000	1.133673000
O	0.371139000	-1.415790000	2.281531000
O	0.859943000	-2.795861000	0.676840000

P-C_F, $E_{(SCF\ Done)}$ = -2619.630375 a.u.

N	-2.807320000	0.386723000	-0.040889000
N	-3.451657000	0.682921000	0.997378000
C	-3.587863000	0.242074000	-1.224826000
C	-4.974112000	0.038080000	-1.170795000
C	-2.921773000	0.320699000	-2.453698000
C	-5.685002000	-0.092281000	-2.354618000
H	-5.466463000	-0.029743000	-0.207402000
C	-3.651744000	0.202974000	-3.633417000
H	-1.846534000	0.484803000	-2.485831000
C	-5.028334000	-0.007391000	-3.587037000
H	-6.756456000	-0.268738000	-2.320074000
H	-3.136369000	0.268856000	-4.586835000
H	-5.593052000	-0.112887000	-4.509385000

C	-2.767440000	0.913634000	2.193853000
C	-1.513202000	1.528573000	2.331591000
C	-3.459496000	0.595350000	3.374590000
C	-0.933777000	1.780685000	3.558003000
C	-2.885062000	0.815422000	4.618752000
H	-4.446169000	0.153292000	3.276577000
C	-1.622691000	1.405712000	4.710588000
H	0.046761000	2.242022000	3.594537000
H	-3.423983000	0.536214000	5.518755000
H	-1.170115000	1.583309000	5.681431000
Pd	-0.759379000	0.029433000	-0.125912000
S	2.096154000	-0.739438000	1.095766000
S	2.022992000	0.530425000	-1.569150000
O	1.193216000	-0.583259000	2.242887000
O	3.457579000	-0.206719000	1.147388000
O	3.079192000	-0.378966000	-2.010006000
O	0.899247000	0.862622000	-2.453245000
N	1.273253000	-0.028059000	-0.173203000
C	2.200762000	-2.490585000	0.750077000
C	1.291119000	-3.353796000	1.359652000
H	0.537865000	-2.955667000	2.031251000
C	1.380198000	-4.720072000	1.099783000
H	0.676178000	-5.403029000	1.567351000
C	2.368239000	-5.206152000	0.244651000
H	2.433248000	-6.272343000	0.043069000
C	3.275241000	-4.329565000	-0.352542000
H	4.045032000	-4.710473000	-1.018111000
C	3.199951000	-2.962201000	-0.102008000
H	3.890801000	-2.267755000	-0.566333000
C	2.798721000	2.082794000	-1.126239000
C	2.042511000	3.253320000	-1.189449000
H	1.006374000	3.209854000	-1.509672000
C	2.645997000	4.466778000	-0.868032000
H	2.068622000	5.386183000	-0.919509000
C	3.990143000	4.501784000	-0.495054000
H	4.458938000	5.450833000	-0.247485000
C	4.736351000	3.324450000	-0.447713000
H	5.784679000	3.353611000	-0.163328000
C	4.144251000	2.103859000	-0.765091000
H	4.706779000	1.178479000	-0.729489000
F	-0.851415000	1.954481000	1.213876000
N	-1.039776000	-1.768890000	-0.901253000
O	-0.441856000	-2.093300000	-1.900664000
O	-1.838345000	-2.452952000	-0.277442000

TS-C_{NO2}, $E_{(SCF\ Done)}$ = -2619.569273 a.u., Imaginary frequency = *i*303.6947 cm^{-1}

N	2.830714000	-0.898391000	-0.154383000
N	3.030761000	-2.141648000	-0.265591000
C	3.945754000	-0.040810000	-0.186894000
C	5.170675000	-0.462481000	-0.729369000
C	3.800349000	1.240442000	0.363186000
C	6.248302000	0.408536000	-0.716129000
H	5.251582000	-1.455395000	-1.157398000
C	4.897991000	2.093805000	0.384652000
H	2.848845000	1.547314000	0.783913000
C	6.115567000	1.685316000	-0.157758000
H	7.196613000	0.097529000	-1.145037000
H	4.796139000	3.083090000	0.820339000
H	6.965621000	2.362261000	-0.151709000
C	1.858004000	-2.876304000	-0.196688000
C	0.653855000	-2.292800000	0.292557000
C	1.847857000	-4.186472000	-0.677237000
C	-0.525706000	-3.029875000	0.299908000
C	0.650741000	-4.899032000	-0.705539000
H	2.772751000	-4.609920000	-1.056746000
C	-0.530293000	-4.318005000	-0.237287000
H	-1.419056000	-2.608206000	0.747795000
H	0.639596000	-5.915394000	-1.088008000
H	-1.460219000	-4.878014000	-0.255829000
Pd	0.895934000	-0.231830000	-0.071656000
S	-2.109158000	0.158670000	-1.183553000
S	-1.192415000	1.718620000	1.161338000
O	-1.329529000	-0.449737000	-2.262424000
O	-2.914892000	1.354958000	-1.415860000
O	-2.410149000	1.528434000	1.953819000
O	0.113196000	1.715542000	1.839544000
N	-1.023238000	0.447643000	0.062695000
C	-3.215957000	-1.122303000	-0.580746000
C	-3.495080000	-2.185452000	-1.440574000
H	-2.995945000	-2.239921000	-2.402623000
C	-4.409640000	-3.159250000	-1.040450000
H	-4.639938000	-3.987103000	-1.706343000
C	-5.028008000	-3.068122000	0.206451000
H	-5.738950000	-3.829650000	0.516987000
C	-4.738389000	-1.998254000	1.055248000
H	-5.220170000	-1.926805000	2.026710000
C	-3.835236000	-1.010887000	0.665044000
H	-3.600897000	-0.176730000	1.320580000
C	-1.376910000	3.266559000	0.285706000
C	-0.444822000	3.644247000	-0.679385000

H	0.347383000	2.959712000	-0.972331000
C	-0.582423000	4.893430000	-1.279130000
H	0.127413000	5.199068000	-2.043178000
C	-1.625186000	5.744352000	-0.910455000
H	-1.723831000	6.717691000	-1.384613000
C	-2.546157000	5.347384000	0.057980000
H	-3.362586000	6.006597000	0.340502000
C	-2.429381000	4.098067000	0.663136000
H	-3.140232000	3.762098000	1.410027000
F	1.360896000	1.256009000	-1.231866000
N	0.758876000	-1.439088000	1.961761000
O	-0.308407000	-1.329350000	2.496638000
O	1.862875000	-1.469461000	2.449107000

P-C_{NO2}, $E_{(SCF\ Done)}$ = -2619.610297 a.u.

N	2.855729000	-0.312381000	-0.262212000
N	3.078747000	-1.134678000	0.664065000
C	3.947096000	0.209754000	-0.987449000
C	5.270333000	-0.109668000	-0.640757000
C	3.654048000	1.045980000	-2.071291000
C	6.302582000	0.408379000	-1.406190000
H	5.465239000	-0.745575000	0.215707000
C	4.706032000	1.552639000	-2.829326000
H	2.619571000	1.310576000	-2.270867000
C	6.022817000	1.234516000	-2.502318000
H	7.331862000	0.173915000	-1.150214000
H	4.492638000	2.203436000	-3.672009000
H	6.840380000	1.635640000	-3.095484000
C	1.814179000	-1.557378000	1.175419000
C	1.496669000	-1.502299000	2.545757000
C	0.918683000	-2.212955000	0.291157000
C	0.318693000	-2.044571000	3.023057000
C	-0.277145000	-2.766051000	0.800719000
H	1.260146000	-2.489217000	-0.704441000
C	-0.575843000	-2.672410000	2.147265000
H	0.099946000	-1.947357000	4.080366000
H	-0.953248000	-3.271170000	0.118916000
H	-1.506545000	-3.075707000	2.531087000
Pd	0.840279000	0.044381000	-0.347313000
S	-2.056809000	-0.062797000	-1.678671000
S	-1.830703000	0.863730000	1.115656000
O	-1.066543000	-0.101648000	-2.754945000
O	-3.200165000	0.843937000	-1.716111000
O	-3.041875000	0.133497000	1.505016000
O	-0.686518000	0.874346000	2.038230000

N	-1.179098000	0.205235000	-0.277444000
C	-2.701175000	-1.734331000	-1.543030000
C	-2.153093000	-2.724611000	-2.358742000
H	-1.360759000	-2.463101000	-3.052961000
C	-2.652980000	-4.024868000	-2.279213000
H	-2.238283000	-4.801911000	-2.916208000
C	-3.690991000	-4.321327000	-1.395516000
H	-4.081022000	-5.334327000	-1.337004000
C	-4.240202000	-3.316011000	-0.596840000
H	-5.057658000	-3.545156000	0.081713000
C	-3.753279000	-2.012556000	-0.669228000
H	-4.166103000	-1.224964000	-0.048448000
C	-2.302680000	2.548641000	0.767024000
C	-1.423961000	3.391198000	0.087093000
H	-0.490066000	3.005418000	-0.315468000
C	-1.793890000	4.720956000	-0.098101000
H	-1.126834000	5.389876000	-0.635134000
C	-3.012363000	5.191690000	0.393131000
H	-3.291735000	6.231414000	0.242301000
C	-3.877440000	4.331653000	1.068332000
H	-4.830262000	4.696092000	1.442838000
C	-3.527026000	2.996801000	1.258625000
H	-4.189275000	2.305784000	1.769193000
F	0.949067000	1.792461000	-1.179080000
N	2.375384000	-0.801269000	3.480521000
O	2.209278000	-1.017601000	4.671947000
O	3.218080000	-0.049985000	3.005926000

C′, $E_{(\text{SCF Done})}$ = -2619.584169 a.u.

N	2.684522000	-0.047849000	0.448573000
N	3.704211000	-0.669935000	0.049956000
C	2.876108000	1.183237000	1.113133000
C	4.085755000	1.884096000	0.965153000
C	1.845773000	1.683855000	1.911911000
C	4.254536000	3.082815000	1.639327000
H	4.859904000	1.484541000	0.320104000
C	2.032531000	2.890575000	2.581296000
H	0.916499000	1.140968000	2.029518000
C	3.231043000	3.588288000	2.450188000
H	5.182758000	3.635554000	1.524141000
H	1.224502000	3.279068000	3.192350000
H	3.369704000	4.532896000	2.969282000
C	3.421279000	-1.802811000	-0.675952000
C	2.076521000	-2.120178000	-0.930181000
C	4.441185000	-2.626910000	-1.172543000

C	1.712912000	-3.212895000	-1.680308000
C	4.088563000	-3.746032000	-1.916787000
H	5.477296000	-2.370691000	-0.973488000
C	2.742989000	-4.033098000	-2.167641000
H	0.669420000	-3.433626000	-1.879575000
H	4.861531000	-4.398945000	-2.310544000
H	2.480995000	-4.910893000	-2.752597000
Pd	0.850735000	-0.779113000	-0.172193000
S	-1.843666000	1.856603000	0.644590000
S	-1.972881000	-0.632462000	-0.715780000
O	-1.075667000	2.327146000	1.795617000
O	-3.291830000	1.669451000	0.745562000
O	-2.607300000	-0.127820000	-1.926534000
O	-0.843869000	-1.663652000	-0.954768000
N	-1.147236000	0.380426000	0.233002000
C	-1.529072000	2.966258000	-0.717581000
C	-0.300453000	3.620276000	-0.797077000
H	0.454443000	3.456832000	-0.035486000
C	-0.069790000	4.488900000	-1.860125000
H	0.883878000	5.003968000	-1.936285000
C	-1.058854000	4.697581000	-2.821811000
H	-0.873163000	5.376710000	-3.649966000
C	-2.285353000	4.041467000	-2.723562000
H	-3.056044000	4.208519000	-3.470998000
C	-2.529666000	3.167806000	-1.666489000
H	-3.476748000	2.648673000	-1.571047000
C	-3.206661000	-1.501338000	0.230426000
C	-3.024824000	-1.705381000	1.597936000
H	-2.163863000	-1.286639000	2.108268000
C	-3.986972000	-2.427919000	2.297423000
H	-3.863717000	-2.588763000	3.364500000
C	-5.105541000	-2.933864000	1.634207000
H	-5.853373000	-3.495393000	2.187864000
C	-5.274554000	-2.713844000	0.267411000
H	-6.151872000	-3.099048000	-0.244665000
C	-4.323031000	-1.990184000	-0.446963000
H	-4.443256000	-1.791693000	-1.506852000
F	1.140677000	0.302372000	-1.779788000
N	0.591873000	-1.891536000	1.526482000
O	0.638263000	-1.265216000	2.573597000
O	0.386133000	-3.082709000	1.421409000

TS′-C_F, $E_{(SCF\ Done)}$ = -2619.557805 a.u., Imaginary frequency = *i*319.2294 cm^{-1}

N	2.707666000	0.022087000	0.540402000
N	3.743172000	-0.479220000	0.007096000

C	2.850088000	1.189368000	1.322678000
C	4.094452000	1.833024000	1.443199000
C	1.717960000	1.697340000	1.967869000
C	4.190479000	2.974297000	2.223649000
H	4.957477000	1.429838000	0.926091000
C	1.829190000	2.854538000	2.734614000
H	0.751917000	1.212741000	1.879352000
C	3.060680000	3.490620000	2.869794000
H	5.150412000	3.473696000	2.322838000
H	0.939172000	3.248660000	3.214341000
H	3.145656000	4.391140000	3.472027000
C	3.503942000	-1.497642000	-0.863702000
C	2.177929000	-1.725330000	-1.310214000
C	4.534487000	-2.350637000	-1.307350000
C	1.855610000	-2.781098000	-2.152877000
C	4.221544000	-3.417239000	-2.127044000
H	5.548103000	-2.160994000	-0.967140000
C	2.888307000	-3.633982000	-2.527679000
H	0.834724000	-2.924021000	-2.489087000
H	5.000805000	-4.094302000	-2.462043000
H	2.653941000	-4.484223000	-3.163081000
Pd	0.892360000	-0.776303000	-0.052984000
S	-2.011029000	1.849708000	0.478163000
S	-1.985422000	-0.766682000	-0.647556000
O	-1.304695000	2.422353000	1.624867000
O	-3.460958000	1.652265000	0.522178000
O	-2.568134000	-0.430277000	-1.944014000
O	-0.827460000	-1.785947000	-0.711721000
N	-1.247914000	0.387153000	0.195217000
C	-1.638782000	2.870212000	-0.941950000
C	-0.467809000	3.627378000	-0.946814000
H	0.193192000	3.607026000	-0.086321000
C	-0.179540000	4.415718000	-2.058369000
H	0.728556000	5.012451000	-2.074382000
C	-1.056811000	4.443999000	-3.142896000
H	-0.828167000	5.061191000	-4.007963000
C	-2.228970000	3.688380000	-3.118788000
H	-2.914179000	3.716627000	-3.961617000
C	-2.529263000	2.894673000	-2.014030000
H	-3.436544000	2.301925000	-1.976927000
C	-3.245049000	-1.559332000	0.332317000
C	-3.063268000	-1.710102000	1.706943000
H	-2.181510000	-1.305549000	2.193098000
C	-4.046318000	-2.367106000	2.440968000
H	-3.923046000	-2.486904000	3.513570000

C	-5.186648000	-2.860119000	1.804882000
H	-5.951382000	-3.369385000	2.385422000
C	-5.354274000	-2.694355000	0.430591000
H	-6.247232000	-3.070249000	-0.061063000
C	-4.380451000	-2.037787000	-0.318542000
H	-4.495011000	-1.883792000	-1.386307000
F	1.464808000	-0.197493000	-1.962857000
N	0.777554000	-1.804533000	1.667441000
O	0.322340000	-1.216158000	2.627370000
O	1.168438000	-2.950270000	1.629804000

P′-C_F, $E_{(SCF\ Done)}$ = -2619.636700 a.u.

N	-1.607721000	-1.256516000	-0.869025000
N	-2.850560000	-1.108959000	-0.913461000
C	-1.027805000	-1.861683000	-2.024441000
C	-1.721657000	-1.905186000	-3.240800000
C	0.245990000	-2.422307000	-1.911275000
C	-1.134296000	-2.523896000	-4.334709000
H	-2.701848000	-1.447819000	-3.312944000
C	0.820684000	-3.049058000	-3.011399000
H	0.774859000	-2.368291000	-0.963788000
C	0.134681000	-3.099488000	-4.223287000
H	-1.663365000	-2.551061000	-5.283168000
H	1.809715000	-3.488287000	-2.921945000
H	0.590494000	-3.577788000	-5.085983000
C	-3.519574000	-0.486462000	0.149005000
C	-3.178587000	0.765253000	0.683720000
C	-4.681792000	-1.116867000	0.618884000
C	-3.930689000	1.352076000	1.689376000
C	-5.421312000	-0.553979000	1.649992000
H	-4.957368000	-2.070805000	0.180634000
C	-5.044788000	0.679858000	2.185734000
H	-3.630273000	2.324469000	2.066118000
H	-6.295483000	-1.072503000	2.031204000
H	-5.626789000	1.129165000	2.985061000
Pd	-0.403451000	-0.849982000	0.744452000
S	1.363297000	1.523174000	-1.265539000
S	1.937845000	0.539998000	1.424036000
O	0.720578000	0.852032000	-2.391680000
O	2.803070000	1.792284000	-1.271392000
O	2.355703000	1.828335000	1.962661000
O	1.009854000	-0.316169000	2.269529000
N	1.012442000	0.591103000	0.077835000
C	0.521266000	3.085500000	-1.030496000
C	-0.546331000	3.396970000	-1.869894000

H	-0.864186000	2.679912000	-2.619228000
C	-1.174255000	4.633993000	-1.733068000
H	-2.005312000	4.890352000	-2.384751000
C	-0.734939000	5.538284000	-0.767411000
H	-1.226844000	6.502088000	-0.663567000
C	0.338845000	5.212848000	0.063249000
H	0.683106000	5.919936000	0.813072000
C	0.980218000	3.983981000	-0.066481000
H	1.814934000	3.721632000	0.574997000
C	3.400661000	-0.450500000	1.168567000
C	3.360524000	-1.812318000	1.470898000
H	2.455302000	-2.254205000	1.874144000
C	4.510033000	-2.575767000	1.278296000
H	4.496429000	-3.635220000	1.518886000
C	5.673397000	-1.979496000	0.792352000
H	6.567483000	-2.579453000	0.644348000
C	5.697377000	-0.614619000	0.503383000
H	6.605955000	-0.151062000	0.129626000
C	4.559186000	0.164311000	0.693083000
H	4.560654000	1.223899000	0.466283000
F	-2.147063000	1.447128000	0.164300000
N	-1.393002000	-2.215502000	1.801440000
O	-1.861534000	-3.208099000	1.256586000
O	-1.429242000	-1.994671000	3.001091000

TS′-C_{NO2}, $E_{(SCF\ Done)}$ = -2619.547183 a.u., Imaginary frequency = i318.2856 cm^{-1}

N	2.691176000	1.145226000	0.139703000
N	3.893024000	0.752752000	0.064250000
C	2.430152000	2.464796000	0.542891000
C	3.436368000	3.446666000	0.511319000
C	1.139286000	2.760438000	1.000897000
C	3.133287000	4.726456000	0.944382000
H	4.424075000	3.191770000	0.143966000
C	0.859481000	4.046071000	1.449236000
H	0.364215000	2.000564000	1.041403000
C	1.848076000	5.028072000	1.415754000
H	3.896887000	5.498503000	0.914217000
H	-0.137341000	4.262458000	1.819507000
H	1.622621000	6.035976000	1.753923000
C	4.002810000	-0.561140000	-0.352325000
C	2.873716000	-1.430355000	-0.309603000
C	5.196357000	-1.010565000	-0.920963000
C	2.935137000	-2.700795000	-0.882172000
C	5.246053000	-2.277376000	-1.496907000
H	6.047486000	-0.337244000	-0.950475000

C	4.115586000	-3.103761000	-1.502022000
H	2.072094000	-3.354969000	-0.811783000
H	6.168645000	-2.623148000	-1.953376000
H	4.164881000	-4.085867000	-1.963073000
Pd	1.238253000	-0.117733000	-0.445589000
S	-2.507697000	0.870392000	1.096729000
S	-1.565784000	-1.170368000	-0.677629000
O	-1.776795000	1.796697000	1.971100000
O	-3.550836000	0.022191000	1.680771000
O	-2.436981000	-0.895707000	-1.816998000
O	-0.106413000	-1.523654000	-1.073134000
N	-1.302731000	-0.031484000	0.401416000
C	-3.263916000	1.825373000	-0.214492000
C	-2.486548000	2.368970000	-1.237179000
H	-1.429242000	2.131049000	-1.316997000
C	-3.105713000	3.177478000	-2.187875000
H	-2.515007000	3.593950000	-2.999475000
C	-4.473441000	3.441441000	-2.108672000
H	-4.947888000	4.072892000	-2.855862000
C	-5.236396000	2.886855000	-1.081545000
H	-6.304116000	3.082425000	-1.025774000
C	-4.633481000	2.070714000	-0.126734000
H	-5.210432000	1.615119000	0.671696000
C	-2.163803000	-2.664512000	0.097302000
C	-1.953997000	-2.882586000	1.457674000
H	-1.460057000	-2.128817000	2.060101000
C	-2.417444000	-4.067386000	2.024544000
H	-2.271001000	-4.246011000	3.086084000
C	-3.076513000	-5.011952000	1.237843000
H	-3.438269000	-5.932911000	1.687879000
C	-3.286308000	-4.774180000	-0.121026000
H	-3.812190000	-5.504919000	-0.729533000
C	-2.833778000	-3.591988000	-0.701090000
H	-3.007949000	-3.375765000	-1.750227000
F	0.575686000	1.221210000	-1.696084000
N	2.035852000	-1.546961000	1.275521000
O	2.516089000	-0.862233000	2.152055000
O	1.339482000	-2.525764000	1.390256000

P′-C_{NO2}, $E_{(SCF\ Done)}$ = -2619.547183 a.u., Imaginary frequency = *i*318.2856 cm^{-1}

N	2.956364000	-0.003058000	-0.109577000
N	3.678179000	-1.035025000	-0.105848000
C	3.497805000	1.260531000	0.167931000
C	4.874752000	1.501903000	0.038056000
C	2.609840000	2.247877000	0.614844000

C	5.359115000	2.760228000	0.355226000
H	5.530230000	0.713405000	-0.316113000
C	3.121853000	3.497219000	0.948624000
H	1.553927000	2.027239000	0.743231000
C	4.484902000	3.755777000	0.811369000
H	6.418726000	2.973085000	0.247697000
H	2.447945000	4.264539000	1.316293000
H	4.875607000	4.738826000	1.060398000
C	2.796081000	-2.126428000	-0.391273000
C	1.644399000	-2.394461000	0.429110000
C	3.084692000	-2.966784000	-1.476233000
C	0.793914000	-3.467866000	0.076174000
C	2.220054000	-4.000019000	-1.798849000
H	3.971351000	-2.759945000	-2.066808000
C	1.059216000	-4.231222000	-1.042146000
H	-0.052470000	-3.673967000	0.721449000
H	2.442376000	-4.633542000	-2.652622000
H	0.385385000	-5.037626000	-1.312423000
Pd	1.118570000	-0.468686000	-0.715658000
S	-1.742045000	1.600112000	1.293853000
S	-1.868244000	-0.422796000	-0.772736000
O	-0.564322000	2.108504000	2.007348000
O	-2.907441000	1.161238000	2.068031000
O	-2.696847000	0.288662000	-1.742525000
O	-0.675801000	-1.184491000	-1.410782000
N	-1.124383000	0.370004000	0.376261000
C	-2.295635000	2.870627000	0.162091000
C	-1.495917000	3.245010000	-0.918186000
H	-0.582684000	2.700324000	-1.143711000
C	-1.921126000	4.293705000	-1.729877000
H	-1.316964000	4.586067000	-2.584704000
C	-3.118249000	4.957571000	-1.457594000
H	-3.442275000	5.774835000	-2.097358000
C	-3.905813000	4.568789000	-0.374800000
H	-4.842725000	5.079546000	-0.168034000
C	-3.497643000	3.516817000	0.443227000
H	-4.098838000	3.187192000	1.284444000
C	-2.874095000	-1.733893000	-0.086296000
C	-2.736779000	-2.093684000	1.253026000
H	-2.049938000	-1.551270000	1.893013000
C	-3.522010000	-3.132947000	1.751456000
H	-3.435486000	-3.413530000	2.797604000
C	-4.423822000	-3.794658000	0.918640000
H	-5.035729000	-4.601001000	1.314957000
C	-4.557099000	-3.413897000	-0.417974000

H	-5.271975000	-3.919610000	-1.061610000
C	-3.784893000	-2.374069000	-0.928628000
H	-3.893481000	-2.046880000	-1.957973000
F	0.925818000	1.188340000	-1.710778000
N	1.581508000	-1.969057000	1.859315000
O	2.584895000	-1.473462000	2.345329000
O	0.541032000	-2.200082000	2.449235000

C″, $E_{(\text{SCF Done})}$ = -2619.580586 a.u.

N	-2.826798000	-0.114772000	-0.093616000
N	-3.533379000	-0.798618000	0.686453000
C	-3.452886000	0.826378000	-0.942680000
C	-4.694265000	1.375321000	-0.589498000
C	-2.817309000	1.184981000	-2.135635000
C	-5.299589000	2.280563000	-1.449075000
H	-5.154243000	1.091199000	0.350411000
C	-3.442261000	2.089371000	-2.988360000
H	-1.854425000	0.758857000	-2.393479000
C	-4.677907000	2.638254000	-2.649075000
H	-6.256991000	2.717239000	-1.179053000
H	-2.955857000	2.366813000	-3.918705000
H	-5.156220000	3.351384000	-3.314863000
C	-2.797324000	-1.624534000	1.497289000
C	-1.386462000	-1.588966000	1.415295000
C	-3.438528000	-2.501979000	2.381597000
C	-0.615549000	-2.376285000	2.238671000
C	-2.664411000	-3.326989000	3.186418000
H	-4.523558000	-2.511597000	2.419058000
C	-1.271428000	-3.257672000	3.115239000
H	0.467233000	-2.302799000	2.235709000
H	-3.140407000	-4.015500000	3.878027000
H	-0.667075000	-3.891630000	3.759258000
Pd	-0.797899000	-0.142664000	0.184106000
S	2.659754000	-0.724224000	0.757734000
S	1.412201000	1.501628000	-0.610066000
O	2.296058000	-1.518358000	1.929567000
O	3.765284000	0.228778000	0.815017000
O	2.363777000	1.404878000	-1.710513000
O	-0.046748000	1.638686000	-0.962163000
N	1.287937000	0.159464000	0.353262000
C	2.985124000	-1.868784000	-0.575490000
C	2.477494000	-3.165078000	-0.498100000
H	1.891831000	-3.469061000	0.362743000
C	2.751798000	-4.059528000	-1.529628000
H	2.362144000	-5.072589000	-1.481023000

C	3.527128000	-3.656494000	-2.616676000
H	3.739032000	-4.357823000	-3.419517000
C	4.037166000	-2.359459000	-2.674232000
H	4.647198000	-2.049441000	-3.518144000
C	3.771286000	-1.454159000	-1.649959000
H	4.160232000	-0.442956000	-1.679114000
C	1.862202000	2.893920000	0.398905000
C	1.040171000	3.257951000	1.466517000
H	0.149943000	2.676585000	1.695606000
C	1.405422000	4.364942000	2.227385000
H	0.782241000	4.665868000	3.064958000
C	2.563453000	5.082168000	1.921132000
H	2.839715000	5.944297000	2.522827000
C	3.371109000	4.697168000	0.851465000
H	4.274544000	5.253888000	0.618771000
C	3.025206000	3.591348000	0.078585000
H	3.638543000	3.266153000	-0.754468000
F	-1.153994000	1.054592000	1.694741000
N	-1.044028000	-2.246910000	-1.897055000
O	-2.055347000	-2.554362000	-1.324602000
O	-0.329251000	-1.273986000	-1.441942000

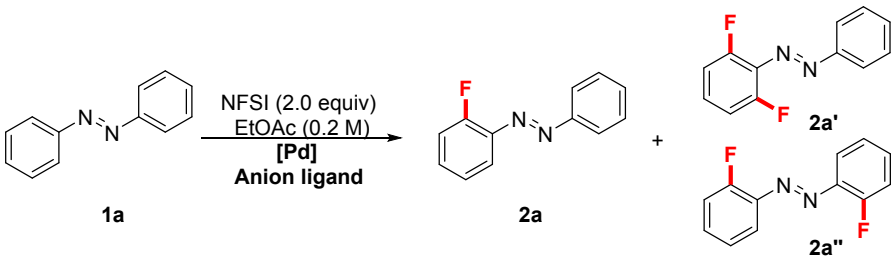
C‴, $E_{(\text{SCF Done})}$ = -2619.572447 a.u.

N	2.556514000	0.028653000	0.368467000
N	3.594518000	-0.468038000	-0.136316000
C	2.671125000	1.214252000	1.127275000
C	3.813207000	2.023675000	1.012490000
C	1.640564000	1.542038000	2.010159000
C	3.914153000	3.157566000	1.803121000
H	4.591528000	1.752550000	0.308436000
C	1.759434000	2.683286000	2.799292000
H	0.751888000	0.925401000	2.085397000
C	2.891857000	3.488491000	2.700483000
H	4.791055000	3.793167000	1.716893000
H	0.950317000	2.939921000	3.475014000
H	2.978730000	4.381307000	3.313814000
C	3.367442000	-1.629103000	-0.833279000
C	2.045729000	-2.099764000	-0.930191000
C	4.415310000	-2.362743000	-1.404111000
C	1.730297000	-3.257794000	-1.601033000
C	4.114681000	-3.548559000	-2.064055000
H	5.432711000	-1.993327000	-1.319614000
C	2.791147000	-3.989507000	-2.159369000
H	0.701147000	-3.587979000	-1.700849000
H	4.911293000	-4.134759000	-2.511912000

H	2.569997000	-4.916355000	-2.682376000
Pd	0.767579000	-0.797969000	-0.194617000
S	-1.924869000	1.810257000	0.555351000
S	-2.048227000	-0.717399000	-0.747433000
O	-1.290419000	2.226475000	1.805157000
O	-3.379044000	1.661378000	0.474076000
O	-2.666310000	-0.238489000	-1.977726000
O	-0.919038000	-1.755887000	-0.925036000
N	-1.223967000	0.335810000	0.165459000
C	-1.415724000	2.958371000	-0.716084000
C	-0.330783000	3.799502000	-0.476801000
H	0.189994000	3.751841000	0.473438000
C	0.053331000	4.701633000	-1.466747000
H	0.896286000	5.364891000	-1.292168000
C	-0.643539000	4.755498000	-2.673230000
H	-0.339807000	5.460062000	-3.443232000
C	-1.732692000	3.911861000	-2.894110000
H	-2.277461000	3.957851000	-3.833059000
C	-2.129539000	3.007002000	-1.913303000
H	-2.973252000	2.344602000	-2.071382000
C	-3.297955000	-1.560214000	0.200500000
C	-2.939265000	-2.237734000	1.366530000
H	-1.905655000	-2.252160000	1.697956000
C	-3.936405000	-2.887130000	2.088162000
H	-3.677255000	-3.420630000	2.998405000
C	-5.260666000	-2.852216000	1.647308000
H	-6.033281000	-3.360713000	2.218141000
C	-5.598519000	-2.166032000	0.481500000
H	-6.630471000	-2.135845000	0.143378000
C	-4.614057000	-1.509700000	-0.253492000
H	-4.850748000	-0.963415000	-1.159765000
F	1.014842000	0.183819000	-1.851291000
N	1.237610000	-2.289655000	2.342302000
O	2.404035000	-2.147941000	2.089186000
O	0.356125000	-1.800958000	1.532512000

V. Procedure for the optimization study

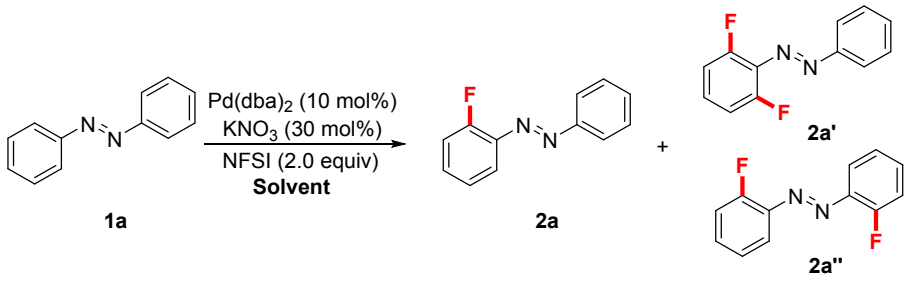
Table S3. Screening of catalysts [a]



Entry	[Pd]	Anion ligand	Conv. of 1a (%) [b]	Yield of 2a/(2a'+2a'') (%) [b]
1	$PdCl_2$	KNO_3	21	19/0
2	$PdCl_2$	$AgNO_3$	95	76/14
3	$PdCl_2$	$AgNO_2$	90	73/10
4	$Pd(dba)_2$	$AgNO_3$	95	77/16
5	/	$AgNO_3$	trace	0/0
6	$Pd(dba)_2$	/	20	16/0
7	$Pd(dba)_2$	Ag_2SO_4	11	8
8	$Pd(dba)_2$	Ag_2CO_3	14	8
9	**$Pd(dba)_2$**	KNO_3	**98**	**80/14**
10	$Pd(dba)_2$	KNO_2	23	19/0
11	$Pd(dba)_2$	$CsNO_3$	70	67/trace
12	$Pd(dba)_2$	$Cu(NO_3)_2 \cdot 2H_2O$	90	74/13
13	$Pd(dba)_2$	$Ca(NO_3)_2 \cdot 4H_2O$	68	66/trace
14	$Pd(dba)_2$	$Fe(NO_3)_3 \cdot 9H_2O$	29	26/0
15	$Pd(dba)_2$	$Bi(NO_3)_3 \cdot 5H_2O$	13	10/0
16	$Pd(NO_3)_2 \cdot 2H_2O$	/	98	73/23
17 [c]	$Pd(dba)_2$	KNO_3	67	60/3
18 [d]	$Pd(dba)_2$	KNO_3	77	65/8
19 [e]	$Pd_2(dba)_3$	KNO_3	72	64/5
20	$Pd(OAc)_2$	KNO_3	33	29/trace
21	$Pd(TFA)_2$	KNO_3	48	45/4
22	$Pd(PPh_3)_4$	KNO_3	75	67/6

[a] Reaction conditions: **1a** (0.1 mmol), [Pd] (10 mol%), NFSI = N-Fluorobenzenesulfoonimide (63 mg, 0.2 mmol), anion ligand (0.03 mmol), and EtOAc (0.5 mL), oil bath (55 °C), under air, 12 h. [b] GC-MS yields. [c] $Pd(dba)_2$ (5 mol%) was added. [d] KNO_3 (10 mol%). [e] $Pd_2(dba)_3$ (5 mol%) was added.

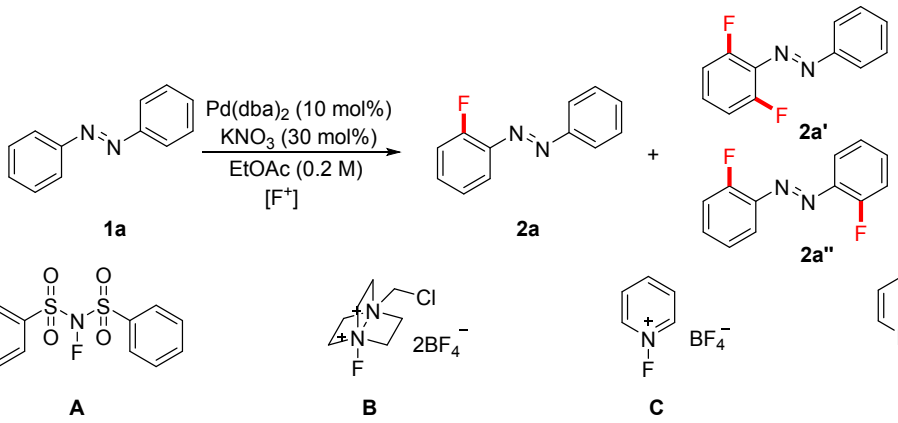
Table S4. Screening of solvents [a]



Entry	Solvent	T (°C)	Time (hr.)	Conv. of 1a (%) [b]	Yield of 2a/(2a'+2a'') (%) [b]
1	DCE	55	12	92	55/trace
2	CH_2Cl_2	55	12	99	58/trace
3	EtOAc	35	12	31	30/0
4	EtOAc	55	12	96	70/12
5 [c]	**EtOAc**	**55**	**12**	**98**	**80/14**
6	EtOAc	65	12	98	78/18
7	EtOAc	55	6	58	56/trace
8	Toulene	55	12	91	38/trace
9	$C_6H_5CF_3$	55	12	55	51/trace
10	1,4-dioxane	55	12	55	52/trace
11	THF	55	12	17	15/0
12	CH_3NO_2	55	12	17	14/0
13	DMF	55	12	trace	Trace/0
14	CH_3CN	55	12	16	14/0

[a] Reaction conditions: **1a** (0.1 mmol), $Pd(dba)_2$ (5.8 mg, 0.01 mmol), NFSI = N-Fluorobenzenesulfoonimide (63 mg, 0.2 mmol), KNO_3 (3.0 mg, 0.03 mmol), and solvents (1 mL), oil bath (55 °C), under air, [b] GC-MS yields. [c] EtOAc (0.5 mL).

Table S5. Screening of fluorination agents [a]



Entry	[F+]	Conv. of 1a (%) [b]	Yield of 2a/(2a'+2a'') (%) [b]
1 [c]	**A**	94	73/12
2	**A**	**98**	**80/14**
3	**B**	trace	trace/0
4	**C**	trace	trace/0
5	**D**	trace	trace/0

[a] Reaction conditions: **1a** (0.1 mmol), $Pd(dba)_2$ (5.8 mg, 0.01 mmol), [F+] (2.0 *equiv*), KNO_3 (3.0 mg, 0.03 mmol), and EtOAc (0.5 mL), oil bath (55 °C), under air, 12 h. [b] GC-MS yields. [c] A (1.5 *equiv*).

Considering of the inseparable mixture of mono- and difluorinated arenes, we proposed to eliminate the N=N framework by restoring azo double bond to corresponding anilines, which are widely found in various pharmaceuticals and medical intermediates (Figure S10). In addition, the reduction of major byproducts 1,2-bis(2-fluorophenyl)diazenes ***2a''*** *would give two equivalent of corresponding o-fluoroanilines* ***4a****, which unquestionably enhanced the synthetic utility of the protocol.*

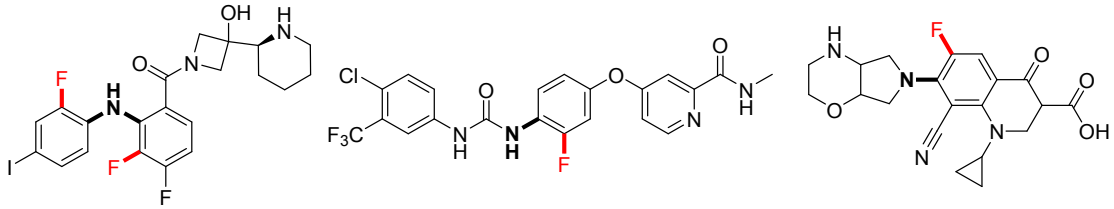
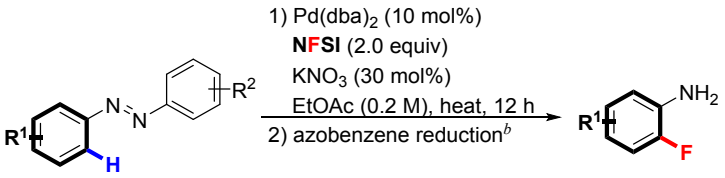


Figure S10. Pharmaceutical moleculars containing *o*-fluoroaniline segment

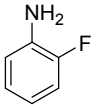
Cobimetinib and Regorafenib are used in the clinic for the treatment of cancer. Finafloxacin is an antibacterial drug indicated in the treatment of swimmer's ear caused by the bacteria. All of them can be synthesized from *o*-fluoroaniline derivatives.

VI. Procedure for the Pd-catalyzed fluorination of azobenzenes



In 10 ml test tube equipped with a stir bar, azobenzene (0.3 mmol), $Pd(dba)_2$ (17.3 mg, 0.03 mmol, 10 mol%), NFSI (189.0 mg, 0.6 mmol, 2.0 *equiv*), KNO_3 (9.1 mg, 0.09 mmol, 30 mol%) and EtOAc (1.5 mL) were added successively. Then the tube was sealed and stirred at the indicated oil bath temperature for 12 h. Upon completion, the resulting mixture was cooled to room temperature, diluted with EtOAc and filtered. The solvent was then removed *in vacuo* and the residue was purified through flash column chromatography on silica gel (eluent: petroleum ether) to give the crude *o*-mono or difluoroazobenzene products **2a-2w**.

A mixture of above obtained crude fluorinated azobenzene, $NaBH_4$ (79.4 mg, 2.1 mmol, 7.0 *equiv*), CuCl (178.2 mg, 1.8 mmol, 6.0 *equiv*) was stirred in EtOH (3 mL, 0.1 M) at room temperature or refluxed (for **2f, 2k, 2l, 2r**) for 5-30 min. After completed (monitored by TLC), the resulting mixture was diluted with H_2O (10 mL) and filtered, washed with CH_2Cl_2 (10 mL). The layers were separated and the aqueous layer was extracted with CH_2Cl_2 (3×15 mL). The combined organic layer was dried by $MgSO_4$, filtered and concentrated under reduced pressure. Then the residue was purified by silica gel chromatography to afford the desired *o*-fluoroanilines **4a-4w**.



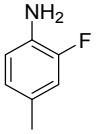
2-Fluoroaniline (4a):

From **1a** (54.6 mg, 0.3 mmol): **4a** was obtained as volatile oil (25.0 mg, 0.22 mmol, 75% yield based on **1a**);

From **3a** (67.2 mg, 0.3 mmol; Ar = Mes): **4a** was obtained as volatile oil (21.6 mg, 0.19 mmol, 65% yield);

From **3a'** (75.1 mg, 0.3 mmol; Ar = *m*-$CF_3C_6H_4$): **4a** was obtained as volatile oil (15.0 mg, 0.13 mmol, 45% yield);

^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.02-6.93 (m, 2H), 6.81-6.78(m, 1H), 6.73-6.69 (m, 1H), 3.62 (brs, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 151.7 (d, J = 236.9 Hz), 134.5 (d, J = 12.6 Hz), 124.4 (d, J = 3.5 Hz), 118.6 (d, J = 6.7 Hz), 116.9 (d, J = 3.5 Hz), 115.2 (d, J = 18.4 Hz) ppm; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -135.4 ppm.

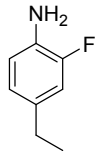


2-Fluoro-4-methylaniline (4b):

From **1b** (63.1 mg, 0.3 mmol): **4b** was obtained as volatile oil (27.0 mg, 0.22 mmol, 72% yield based on **1b**);

From **3b** (71.5 mg, 0.3 mmol; Ar = Mes): **4b** was obtained as volatile oil (25.1 mg, 0.20 mmol, 67% yield);

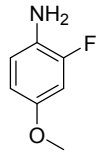
^{1}H NMR (500 MHz, $CDCl_3$): δ = 6.83 (dd, J_1 = 12.0 Hz, J_2 = 1.0 Hz, 1H), 6.77-6.75 (m, 1H), 6.73-6.69 (m, 1H), 3.45 (brs, 2H), 2.26 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 151.7 (d, J = 237.1 Hz), 131.4 (d, J = 12.9 Hz), 128.9 (d, J = 6.4 Hz), 124.8 (d, J = 3.3 Hz), 117.1 (d, J = 3.9 Hz), 115.8 (d, J = 18.3 Hz), 20.4 ppm; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -135.5 ppm.



4-Ethyl-2-fluoroaniline (4c):

From **1c** (54.6 mg, 0.3 mmol): **4c** was obtained as volatile oil (28.4 mg, 0.20 mmol, 68% yield based on **1c**);

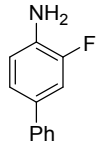
^{1}H NMR (500 MHz, $CDCl_3$): δ = 6.86 (dd, J_1 = 12.0 Hz, J_2 = 2.0 Hz, 1H), 6.80-6.78 (m, 1H), 6.74-6.71 (m, 1H), 3.51 (brs, 2H), 2.56 (q, J = 7.5 Hz, 2H), 1.21 (t, J = 7.5 Hz, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 151.7 (d, J = 237.0 Hz), 135.4 (d, J = 5.7 Hz), 131.8 (d, J = 13.1 Hz), 123.5 (d, J = 3.0 Hz), 117.0 (d, J = 3.6 Hz), 114.6 (d, J = 18.1 Hz), 27.9, 15.7 ppm; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -134.4 ppm.



2-Fluoro-4-methoxyaniline (4d):

From **1d** (72.7 mg, 0.3 mmol): **4d** was obtained as volatile oil (34.0 mg, 0.24 mmol, 81% yield based on **1d**);

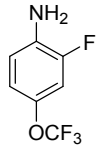
^{1}H NMR (500 MHz, $CDCl_3$): δ = 6.76-6.72 (m, 1H), 6.64 (dd, J_1 = 12.5 Hz, J_2 = 3.0 Hz, 1H), 6.57-6.54 (m, 1H), 3.75 (s, 3H), 3.13 (brs, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 152.1 (d, J = 237.7 Hz), 152.9 (d, J = 9.3 Hz), 127.7 (d, J = 13.3 Hz), 117.9 (d, J = 4.9 Hz), 109.8 (d, J = 3.3 Hz), 102.4 (d, J = 22.3 Hz), 55.9 ppm; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -131.7 ppm.



3-Fluoro-[1,1'-biphenyl]-4-amine (4e):

From **3e** (90.1 mg, 0.3 mmol; Ar = Mes): **4e** was obtained as white solid (40.4 mg, 0.22 mmol, 72% yield);

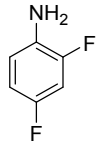
^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.55-7.53 (m, 2H), 7.44-7.41 (m, 2H), 7.34-7.27 (m, 2H), 7.24-7.22 (m, 1H), 6.88-6.85 (m, 1H), 3.77 (brs, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 151.9 (d, J = 237.3 Hz), 140.1 (d, J = 1.6 Hz), 133.7 (d, J = 12.9 Hz), 132.1 (d, J = 6.4 Hz), 128.8 (2C), 126.7, 126.4 (2C), 122.9 (d, J = 3.0 Hz), 117.1 (d, J = 3.9 Hz), 113.8 (d, J = 19.3 Hz) ppm; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -135.1 ppm.



2-Fluoro-4-(trifluoromethoxy)aniline (4f):

From **1f** (105.1 mg, 0.3 mmol): **4f** was obtained as volatile oil (34.5 mg, 0.18 mmol, 59% yield based on **1f**);

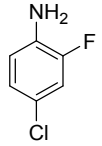
^{1}H NMR (500 MHz, $CDCl_3$): δ = 6.94 (d, J = 2.5 Hz, 1H), 6.87-6.85 (m, 1H), 6.77-6.74 (m, 1H), 3.74 (brs, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 150.6 (d, J = 240.4 Hz), 140.3 (d, J = 8.1 Hz), 133.6 (d, J = 12.7 Hz), 120.6 (d, J = 254.6 Hz), 117.6 (d, J = 3.4 Hz), 116.4 (d, J = 4.5 Hz), 109.7 (d, J = 22.1 Hz) ppm; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -58.7 (d, J = 15.8 Hz), -131.3 (d, J = 13.1 Hz) ppm.



2,4-Difluoroaniline (4g):

From **1g** (65.5 mg, 0.3 mmol): **4g** was obtained as volatile oil (27.1 mg, 0.21 mg, 70% yield based on **1g**);

^{1}H NMR (500 MHz, $CDCl_3$): δ = 6.81-6.77 (m, 1H), 6.75-6.68 (m, 2H), 3.46 (brs, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 155.3 (dd, J_1 = 237.1 Hz, J_2 = 10.7 Hz), 151.0 (dd, J_1 = 240.1 Hz, J_2 = 11.5 Hz), 130.7 (dd, J_1 = 12.7 Hz, J_2 = 3.0 Hz), 116.9 (dd, J_1 = 8.7 Hz, J_2 = 4.6 Hz), 110.9 (dd, J_1 = 21.9 Hz, J_2 = 3.7 Hz), 103.8 (dd, J_1 = 26.3 Hz, J_2 = 22.7 Hz) ppm; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -123.8-(-123.9) (m), -130.7-(-130.8)(m) ppm.

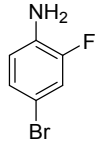


4-Chloro-2-fluoroaniline (4h):

From **1h** (75.3 mg, 0.3 mmol): **4h** was obtained as volatile oil (28.4 mg, 0.19 mmol, 65% yield based on **1h**);

From **3h** (77.6 mg, 0.3 mmol; Ar = Mes): **4h** was obtained as volatile oil (23.6 mg, 0.16 mmol, 54% yield);

^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.02 (dd, J_1 = 10.5 Hz, J_2 = 2.0 Hz, 1H), 6.94-6.92(m, 1H), 6.71 (t, J = 9.0 Hz, 1H), 3.58 (brs, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 151.2 (d, J = 240.9 Hz), 133.3 (d, J = 12.7 Hz), 124.5 (d, J = 3.5 Hz), 122.5 (d, J = 9.3 Hz), 117.3 (d, J = 4.4 Hz), 115.9 (d, J = 21.9 Hz) ppm; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -132.4 ppm.

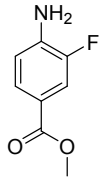


4-Bromo-2-fluoroaniline (4i):

From **1i** (102.0 mg, 0.3 mmol): **4i** was obtained as volatile oil (22.8 mg, 0.12 mmol, 40% yield based on **1i**);

From **3i** (91.0 mg, 0.3 mmol; Ar = Mes): **4i** was obtained as volatile oil (23.9 mg, 0.13 mmol, 42% yield);

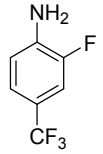
^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.15 (dd, J_1 = 10.5 Hz, J_2 = 2.5 Hz, 1H), 7.08-7.05 (m, 1H), 6.69-6.65 (m, 1H), 3.73 (brs, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 151.4 (d, J = 241.9 Hz), 133.8 (d, J = 12.6 Hz), 127.4 (d, J = 3.6 Hz), 118.7 (d, J = 21.6 Hz), 117.7 (d, J = 4.0 Hz), 108.9 (d, J = 8.5 Hz) ppm; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -132.3 ppm.



Methyl 4-amino-3-fluorobenzoate (4j):

From **1j** (89.5 mg, 0.3 mmol): **4j** was obtained as yellow solid (24.4 mg, 0.14 mmol, 48% yield based on **1j**);

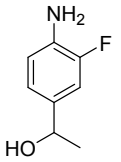
^{1}H NMR (500 MHz, $CDCl_3$): δ = 6.78-6.65 (m, 2H), 6.76-6.73 (m, 1H), 4.32 (q, J = 7.5 Hz, 2H), 4.08 (brs, 2H), 1.37 (t, J = 7.5 Hz, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 165.9 (d, J = 2.7 Hz), 150.3 (d, J = 237.6 Hz), 139.2 (d, J = 12.7 Hz), 126.8 (d, J = 2.9 Hz), 120.4 (d, J = 6.2 Hz), 116.5 (d, J = 19.7 Hz), 115.3 (d, J = 3.7 Hz), 60.7, 14.4 ppm; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -136.1 ppm.



2-Fluoro-4-(trifluoromethyl)aniline (4k):

From **1k** (95.5 mg, 0.3 mmol): **4k** was obtained as volatile oil (17.2 mg, 0.10 mmol, 32% yield based on **1k**);

^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.26-7.21 (m, 2H), 6.82 (t, J = 8.5 Hz, 1H), 4.04 (brs, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 150.4 (d, J = 238.9 Hz), 137.9 (d, J = 12.0 Hz), 124.0 (dd, J_1 = 269.0 Hz, J_2 = 2.6 Hz), 122.0-121.9 (m), 120.3 (dd, J_1 = 33.6 Hz, J_2 = 6.9 Hz), 116.0 (d, J = 4.0 Hz), 112.8 (dq, J_1 = 21.3 Hz, J_2 = 3.9 Hz) ppm; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -61.5, -134.3 ppm.

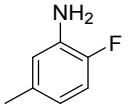


1-(4-Amino-3-fluorophenyl)ethan-1-ol (4l):

From **3l** (79.9 mg, 0.3 mmol; Ar = Mes): **4l** was obtained as white solid (14.9 mg, 0.12 mmol, 62% yield);

2,4,6-trimethylaniline (25.1 mg, 0.19 mmol) was recovered;

^{1}H NMR (500 MHz, DMSO-d_6): δ = 6.93 (dd, J_1 = 12.5 Hz, J_2 = 1.5 Hz, 1H), 6.83 (dd, J_1 = 8.5 Hz, J_2 = 2.0 Hz, 1H), 6.71-6.67 (m, 1H), 4.96-4.94 (m, 3H), 4.59-4.54 (m, 1H), 1.26 (d, J = 6.5 Hz, 3H) ppm; ^{13}C NMR (125 MHz, DMSO-d_6): δ = 150.4 (d, J = 234.6 Hz), 135.8 (d, J = 4.9 Hz), 134.6 (d, J = 13.0 Hz), 121.3 (d, J = 2.7 Hz), 115.7 (d, J = 4.6 Hz), 111.9 (d, J = 18.4 Hz), 67.3, 25.7 ppm; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -134.8 ppm.



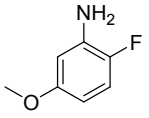
2-Fluoro-5-methylaniline (4m):

From **1m** (63.1 mg, 0.3 mmol): **4m** was obtained as volatile oil (23.3 mg, 0.19 mmol, 62% yield based on **1m**);

From **3m** (71.5 mg, 0.3 mmol; Ar = Mes): **4m** was obtained as volatile oil (26.7 mg, 0.21 mmol, 71% yield);

From **3m'** (69.2 mg, 0.3 mmol; Ar = p-ClC_6H_4): **4m** was obtained as volatile oil (18.4 mg, 0.15 mmol, 49% yield);

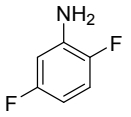
^{1}H NMR (500 MHz, $CDCl_3$): δ = 6.87 (dd, J_1 = 11.0 Hz, J_2 = 8.5 Hz, 1H), 6.61 (dd, J_1 = 8.5 Hz, J_2 = 2.0 Hz, 1H), 6.23-6.20 (m, 1H), 3.75 (brs, 5H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 150.0 (d, J = 234.4 Hz), 134.0 (d, J = 3.5 Hz), 133.8 (d, J = 13.0 Hz), 119.1 (d, J = 6.5 Hz), 117.6 (d, J = 3.1 Hz), 114.8 (d, J = 18.4 Hz), 20.8 ppm; ; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -132.4 ppm.



2-Fluoro-5-methoxyaniline (4n):

From **3n** (76.3 mg, 0.3 mmol; Ar = Mes): **4n** was obtained as volatile oil (28.3 mg, 0.21 mmol, 70% yield);

^{1}H NMR (500 MHz, $CDCl_3$): δ = 6.89 (dd, J_1 = 10.5 Hz, J_2 = 9.0 Hz, 1H), 6.34 (dd, J_1 = 7.5 Hz, J_2 = 3.0 Hz, 1H), 6.57-6.54 (m, 1H), 3.75 (s, 3H), 3.13 (brs, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 156.3 (d, J = 1.5 Hz), 146.6 (d, J = 229.9 Hz), 135.1 (d, J = 14.3 Hz), 115.3 (d, J = 20.0 Hz), 102.8 (d, J = 6.9Hz), 102.8 (d, J = 3.3 Hz), 55.6 ppm; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -145.4 ppm.

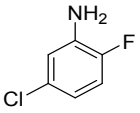


2,5-Difluoroaniline (4o):

From **1o** (65.5 mg, 0.3 mmol): **4o** was obtained as volatile oil (20.1 mg, 0.16 mmol, 52% yield based on **1o**);

From **3o** (72.7 mg, 0.3 mmol; Ar = Mes): **4o** was obtained as volatile oil (18.2 mg, 0.14 mmol, 47% yield);

^{1}H NMR (500 MHz, $CDCl_3$): δ = 6.94-6.89 (m, 1H), 6.51-6.47 (m, 1H), 6.39-6.34 (m, 1H), 3.82 (brs, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 159.3 (dd, J_1 = 238.2 Hz, J_2 = 1.9 Hz), 147.8 (dd, J_1 = 232.6 Hz, J_2 = 2.5 Hz), 135.7 (dd, J_1 = 15.3 Hz, J_2 = 11.4 Hz), 115.6 (dd, J_1 = 21.1 Hz, J_2 = 10.3 Hz), 104.2 (dd, J_1 = 24.1 Hz, J_2 = 7.1 Hz), 103.5 (dd, J_1 = 27.3 Hz, J_2 = 3.6 Hz) ppm; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -116.9 (d, J = 16.3 Hz), -128.3 (d, J = 16.3 Hz) ppm.

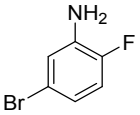


5-Chloro-2-fluoroaniline (4p):

From **1p** (75.3 mg, 0.3 mmol): **4p** was obtained as volatile oil (28.8 mg, 0.20 mmol, 66% yield based on **1p**);

From **3p** (77.6 mg, 0.3 mmol; Ar = Mes): **4p** was obtained as volatile oil (24.0 mg, 0.17 mmol, 55% yield);

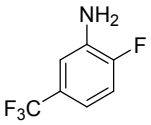
^{1}H NMR (500 MHz, $CDCl_3$): δ = 6.91 (dd, J_1 = 10.5 Hz, J_2 = 8.5 Hz, 1H), 6.77 (dd, J_1 = 7.5 Hz, J_2 = 2.5 Hz, 1H), 6.65 (ddd, J_1 = 8.5 Hz, J_2 = 4.0 Hz, J_3 = 2.5 Hz, 1H), 3.76 (brs, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 150.1 (d, J = 237.0 Hz), 135.6 (d, J = 14.0 Hz), 129.3 (d, J = 3.1 Hz), 118.1 (d, J = 6.9 Hz), 116.4 (d, J = 3.6 Hz), 116.1 (d, J = 20.3 Hz) ppm; ; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -138.0 ppm.



5-Bromo-2-fluoroaniline (4q):

From **1q** (102.0 mg, 0.3 mmol): **4q** was obtained as volatile oil (24.5 mg, 0.13 mmol, 43% yield based on **1q**);

^{1}H NMR (500 MHz, $CDCl_3$): δ = 6.92 (dd, J_1 = 8.0 Hz, J_2 = 2.5 Hz, 1H), 6.86 (dd, J_1 = 10.5 Hz, J_2 = 8.5 Hz, 1H), 6.79 (ddd, J_1 = 8.5 Hz, J_2 = 4.0 Hz, J_3 = 2.5 Hz, 1H), 3.78 (brs, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 150.7 (d, J = 237.6 Hz), 136.0 (d, J = 13.9 Hz), 121.0 (d, J = 6.9 Hz), 119.3 (d, J = 3.6 Hz), 116.7 (d, J = 3.3 Hz), 116.6 (d, J = 20.0 Hz) ppm; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -137.5 ppm.



2-Fluoro-5-(trifluoromethyl)aniline (4r):

From **1r** (95.5 mg, 0.3 mmol): **4r** was obtained as volatile oil (21.5 mg, 0.12 mmol, 40% yield based on **1r**);

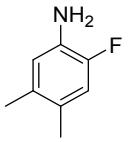
^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.09-7.02 (m, 2H), 6.98-6.96 (m, 1H), 4.04 (brs, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 150.4 (d, J = 238.9 Hz), 137.9 (d, J = 12.0 Hz), 124.0 (dd, J_1 = 269.0 Hz, J_2 = 2.6 Hz), 122.0-121.9 (m), 120.3 (dd, J_1 = 33.6 Hz, J_2 = 6.9 Hz), 116.0 (d, J = 4.0 Hz), 112.8 (dq, J_1 = 21.3 Hz, J_2 = 3.9 Hz) ppm; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -62.5 (dd, J_1 = 268.9 Hz, J_2 = 16.1 Hz), -135.4 (d, J = 15.8 Hz) ppm.

2,6-Difluoroaniline (4s):

From **1s** (65.5 mg, 0.3 mmol): **4s** was obtained as volatile oil (24.8 mg, 0.19 mmol, 64% yield based on **1s**);

From **3a** (67.3 mg, 0.3 mmol; Ar = Mes): **4s** was obtained as volatile oil (23.2 mg, 0.18 mmol, 60% yield);

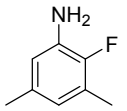
^{1}H NMR (500 MHz, $CDCl_3$): δ = 6.87-6.79 (m, 2H), 6.66-6.61 (m, 1H), 3.70 (brs, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 152.2 (dd, J_1 = 238.7 Hz, J_2 = 7.5 Hz, 2C), 124.0 (q, J = 16.1 Hz), 116.6 (q, J = 8.9 Hz), 111.0-110.7 (m, 2C) ppm; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -132.6 ppm.



2-Fluoro-4,5-dimethylaniline (4t):

From **1t** (71.5 mg, 0.3 mmol): **4t** was obtained as volatile oil (29.2 mg, 0.21 mmol, 70% yield based on **1t**);

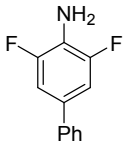
^{1}H NMR (500 MHz, $CDCl_3$): δ = 6.78 (d, J = 11.8 Hz, 1H), 6.60 (d, J = 9.2 Hz, 1H), 3.41 (brs, 2H), 2.16 (s, 6H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): = 149.9 (d, J = 234.4 Hz), 132.1 (d, J = 3.4 Hz), 131.4 (d, J = 12.7 Hz), 126.9 (d, J = 6.1 Hz), 118.5 (d, J = 3.5 Hz), 116.2 (d, J = 18.3 Hz), 19.1, 18.8 ppm; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -140.0 ppm.



2-Fluoro-3,5-dimethylaniline (4u):

From **3u** (75.7 mg, 0.3 mmol; Ar = Mes): **4u** was obtained as volatile oil (28.8 mg, 0.21 mmol, 69% yield);

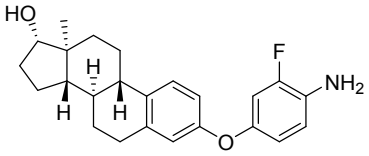
^{1}H NMR (500 MHz, $CDCl_3$): δ = 6.44 (d, J = 8.0 Hz, 1H), 6.38 (d, J = 6.5 Hz, 1H), 3.43 (brs, 2H), 2.21 (s, 6H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 148.7 (d, J = 233.1 Hz), 133.7 (d, J = 13.4 Hz), 133.1 (d, J = 4.1 Hz), 124.3 (d, J = 14.7 Hz), 121.1 (d, J = 3.5 Hz), 115.0 (d, J = 3.0 Hz), 20.7, 14.3 (d, J = 4.3 Hz) ppm; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -144.2 ppm.



3,5-Difluoro-[1,1'-biphenyl]-4-amine (4v):

From **3v** (90.1 mg, 0.3 mmol; Ar = Mes): **4v** was obtained as pale yellow solid (33.9 mg, 0.17 mmol, 55% yield);

^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.52-7.50 (m, 2H), 7.45-7.41 (m, 2H), 7.35-7.32 (m, 1H), 7.23-7.08 (m, 2H), 3.78 (brs, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 152.3 (dd, J_1 = 238.5 Hz, J_2 = 8.5 Hz, 2C), 139.2 (q, J = 2.5 Hz), 130.5 (q, J = 8.4 Hz), 128.9 (2C), 127.3, 126.4 (2C), 123.2-122.9 (m, 2C), 109.6-109.3 (m, 2C) ppm; ^{19}F NMR (376 MHz, $CDCl_3$): δ = -132.3 ppm.



(8R,9S,13S,14S,17S)-3-(4-Amino-3-fluorophenoxy)-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-ol (4w):

From **3w** (153.2 mg, 0.3 mmol; Ar = Mes): **4w** was obtained as white solid (62.9 mg, 0.17 mmol, 55% yield);

^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.21 (d, J = 8.5 Hz, 1H), 6.76-6.72 (m, 3H), 6.68-6.66 (m, 2H), 3.73 (t, J = 8.5 Hz, 1H), 3.58 (brs, 2H), 2.83-2.76 (m, 2H), 2.34-2.28 (m, 1H), 2.20 (td, J_1 = 11.4 Hz, J_2 = 4.2 Hz, 1H), 2.16-2.08 (m, 1H), 1.95 (dt, J_1 = 12.6

Hz, J_2 = 3.3 Hz, 1H), 1.90-1.85 (m, 1H), 1.74-1.67 (m, 1H), 1.55-1.41 (m, 3H), 1.40-1.25 (m, 3H), 1.20 (td, J_1 = 11.9 Hz, J_2 = 7.3 Hz, 1H), 0.79 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$): δ = 155.9, 151.7 (d, J = 240.8 Hz), 149.1 (d, J = 9.3 Hz), 138.4, 134.9, 130.3 (d, J = 13.3 Hz), 126.5, 117.8, 117.3 (d, J = 4.7 Hz), 115.6 (d, J = 3.4 Hz), 115.2, 107.8 (d, J = 21.4 Hz), 81.9, 50.1, 44.1, 43.3, 38.8, 36.7, 30.6, 29.7, 27.2, 26.3, 23.2, 11.1 ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -130.4 ppm.

VII. X-ray data for Int-II, Int-III and 4w

X-ray data for **Int-II**

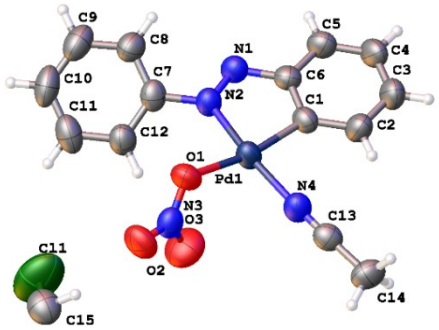


Figure S11. X-ray structure of **Int-II**

Table S6. Crystal data and structure refinement for 170301_myj20170227_1 (**Int-II**)

Identification code	170301_myj20170227_1 **(Int-II)**
Empirical formula	$C_{29}H_{25}Cl_2N_8O_6Pd_2$
Formula weight	866.28
Temperature/K	293.15
Crystal system	Orthorhombic
Space group	Pbcn
a/Å	23.9255 (13)
b/Å	7.4483 (7)
c/Å	18.7126 (11)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3334.7 (4)
Z	4
ρ_{calc}g/cm^3	1.725
μ/mm^{-1}	1.293
F(000)	1720.0
Crystal size/mm^3	0.48 × 0.38 × 0.32
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.728 to 50.698
Index ranges	-28 ≤ h ≤ 24, -8 ≤ k ≤ 8, -21 ≤ l ≤ 22
Reflections collected	19430
Independent reflections	3047 [R_{int} = 0.0559, R_{sigma} = 0.0324]

Data/restraints/parameters	3047 / 0 / 214
Goodness-of-fit on F^2	1.057
Final R indexes [I>=2σ (I)]	R_1 = 0.0598, wR_2 = 0.1480
Final R indexes [all data]	R_1 = 0.0823, wR_2 = 0.1668
Largest diff. peak/hole / e $Å^{-3}$	2.50 / -1.62

X-ray data for **Int-III**

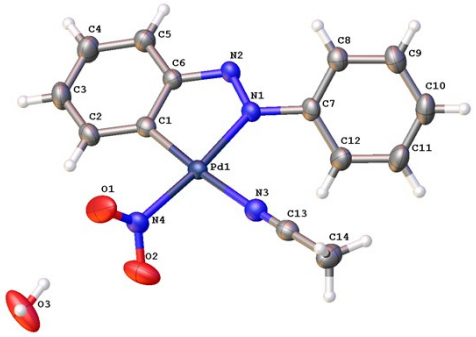


Figure S12. X-ray structure of **Int-III**

Table S7. Crystal data and structure refinement for mjr17026_0m (**Int-III**)

Identification code	mjr17026_0m (**Int-III**)	
Empirical formula	C_{14} H_{14} N_4 O_3 Pd	
Formula weight	392.69	
Temperature	302.25 K	
Wavelength	1.34139 Å	
Crystal system	Monoclinic	
Space group	C 1 2/c 1	
Unit cell dimensions	a = 33.8026 (6) Å	α = 90°.
	b = 4.69190 (10) Å	β = 101.1400 (10)°.
	c = 20.2989 (4) Å	γ = 90°.
Volume	3158.71(11) $Å^3$	
Z	8	
Density (calculated)	1.652 mg/m^3	
Absorption coefficient	6.429 mm^{-1}	
F(000)	1568	
Crystal size	? x ? x ? mm^3	
Theta range for data collection	4.876 to 60.617°.	
Index ranges	-43<=h<=43, -5<=k<=6, -26<=l<=26	
Reflections collected	19305	
Independent reflections	3586 [R(int) = 0.0485]	
Completeness to theta = 53.594°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7519 and 0.4874	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3586 / 0 / 203	
Goodness-of-fit on F^2	1.062	
Final R indices [I>2sigma(I)]	R_1 = 0.0301, wR_2 = 0.0730	

R indices (all data)	$R_1 = 0.0426$, $wR_2 = 0.0819$
Extinction coefficient	n/a
Largest diff. peak and hole	0.538 and -1.074 e.Å^{-3}

X-ray data for **6**

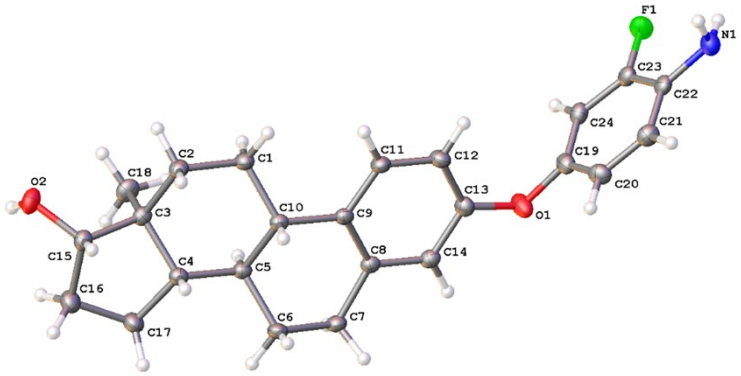


Figure S13. X-ray structure of **4w**

Table S8. Crystal data and structure refinement for 1905055737_0m (**4w**).

Identification code	1905055737_0m (**4w**)	
Empirical formula	C_{24} H_{28} F N O_2	
Formula weight	381.47	
Temperature	169.97 K	
Wavelength	1.34139 Å	
Crystal system	Triclinic	
Space group	P1	
Unit cell dimensions	a = 7.3870 (2) Å	α = 73.1920 (10)°.
	b = 9.3722 (2) Å	β = 85.0490 (10)°.
	c = 15.5339 (4) Å	γ = 75.3100 (10)°.
Volume	995.76(4) Å^3	
Z	2	
Density (calculated)	1.272 mg/m^3	
Absorption coefficient	0.446 mm^{-1}	
F(000)	408	
Crystal size	0.12 × 0.08 × 0.05 mm^3	
Theta range for data collection	5.176 to 54.900°.	
Index ranges	-9<=h<=8, -11<=k<=11, -18<=l<=18	
Reflections collected	18763	
Independent reflections	7233 [R(int) = 0.0302]	
Completeness to theta = 53.594°	98.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7508 and 0.6502	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7233 / 3 / 521	
Goodness-of-fit on F^2	1.042	
Final R indices [I>2sigma(I)]	$R_1 = 0.0360$, $wR_2 = 0.0994$	
R indices (all data)	$R_1 = 0.0365$, $wR_2 = 0.1003$	

Absolute structure parameter	0.02 (4)
Extinction coefficient	n/a
Largest diff. peak and hole	0.539 and -0.282 e.Å^{-3}

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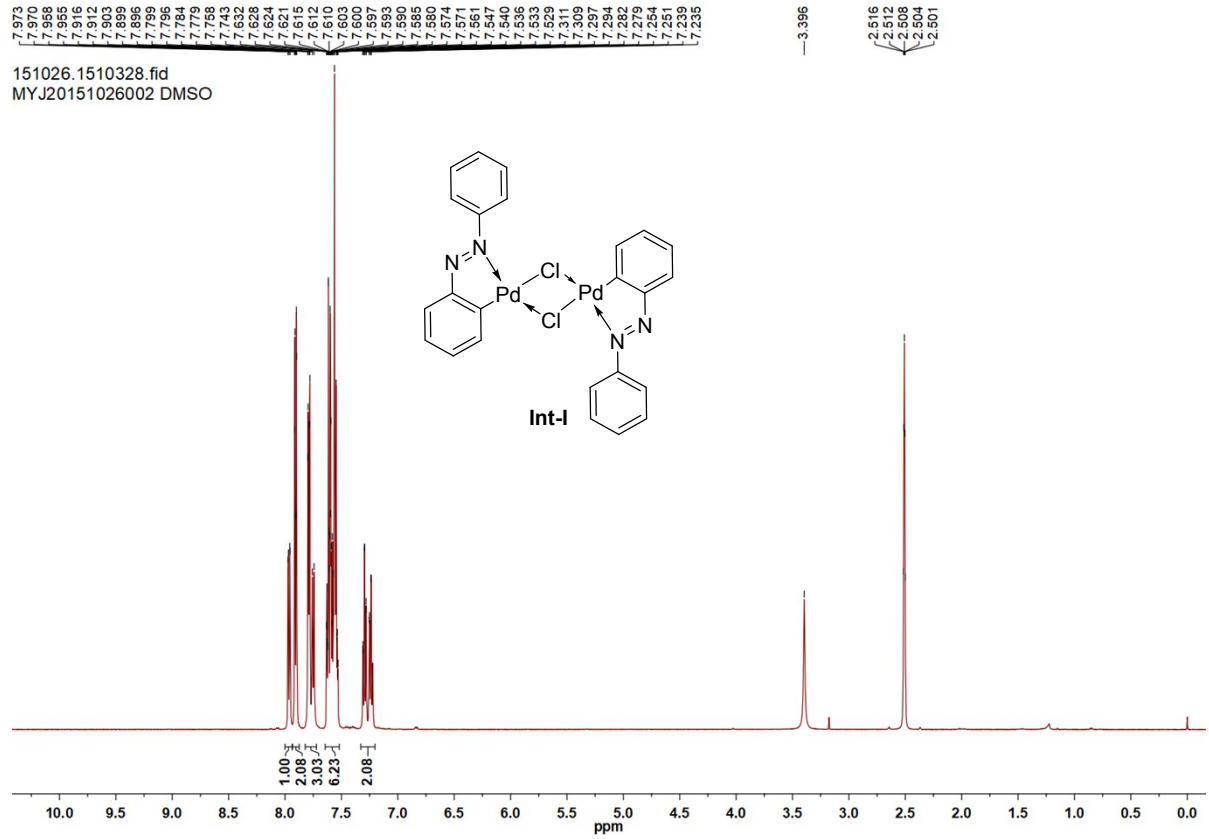
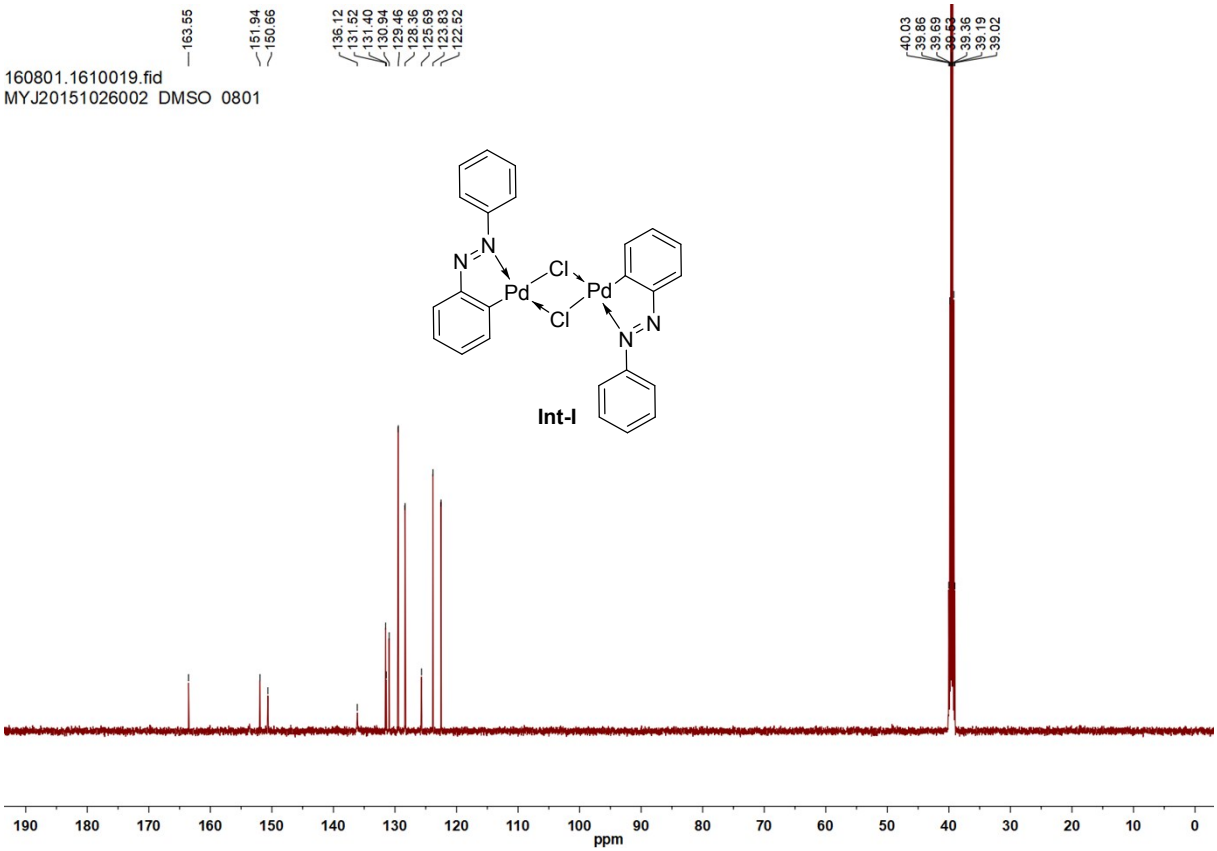
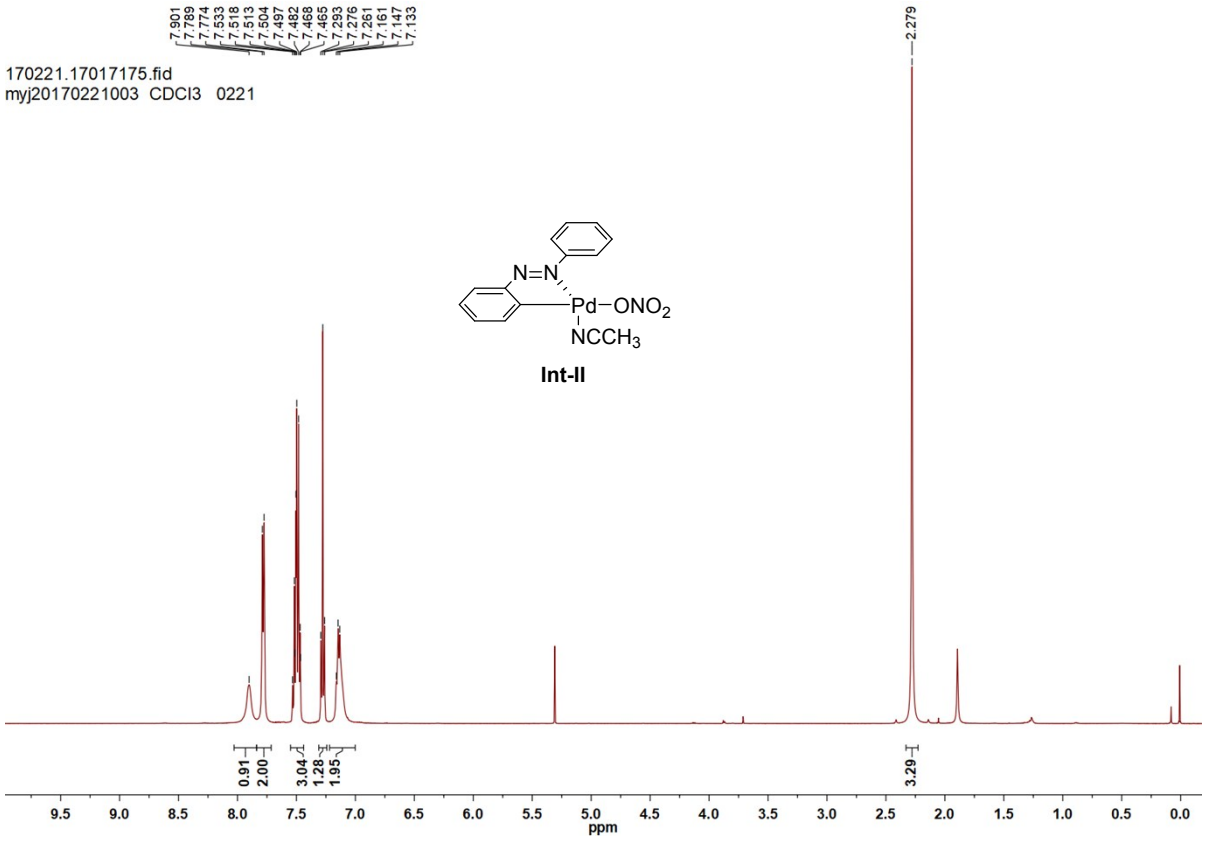
IX. NMR spectra



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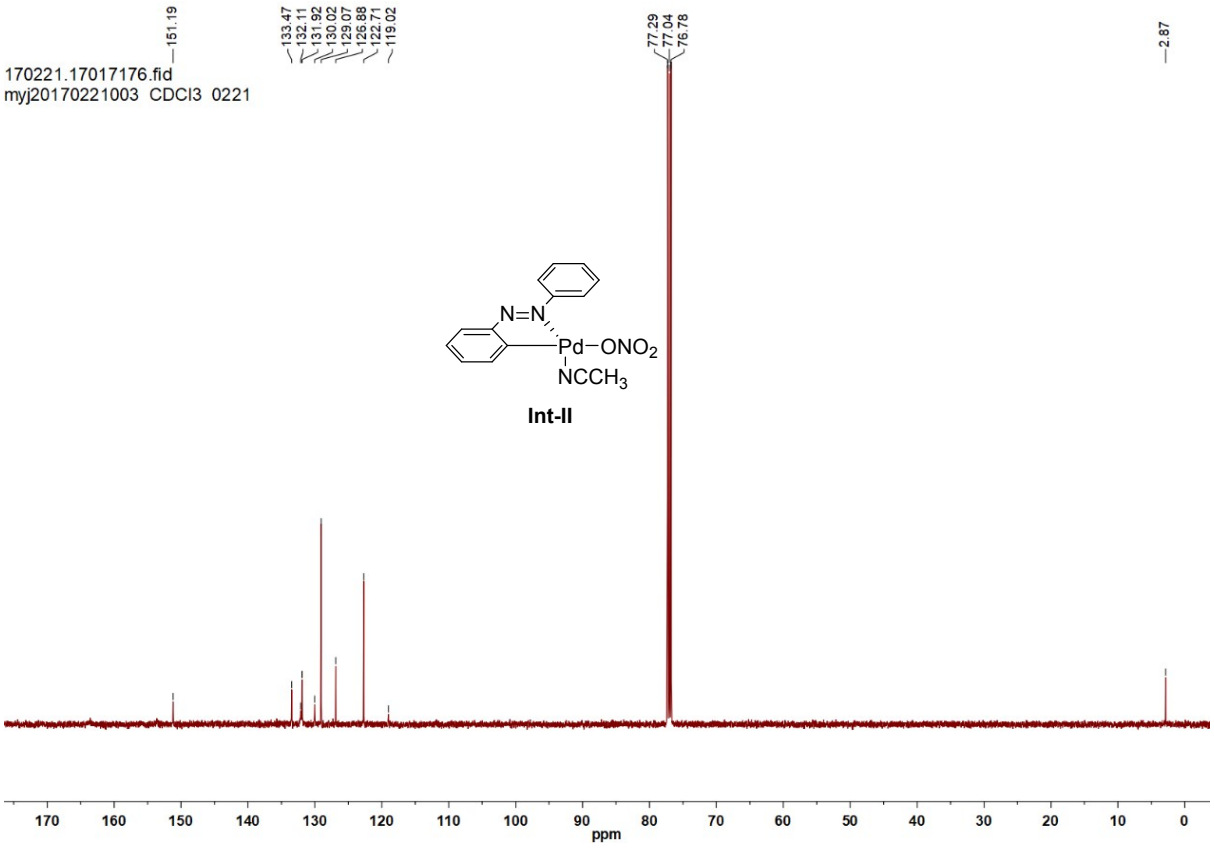
Int-II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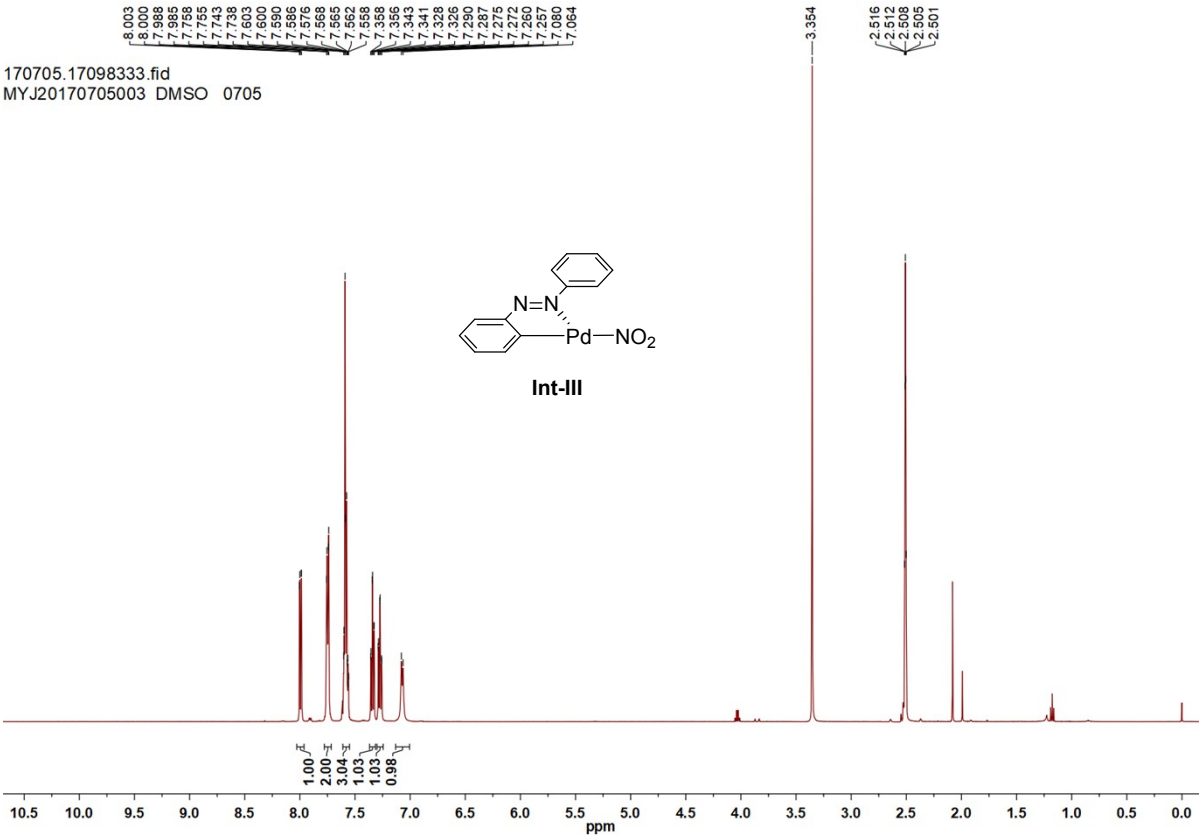
Int-II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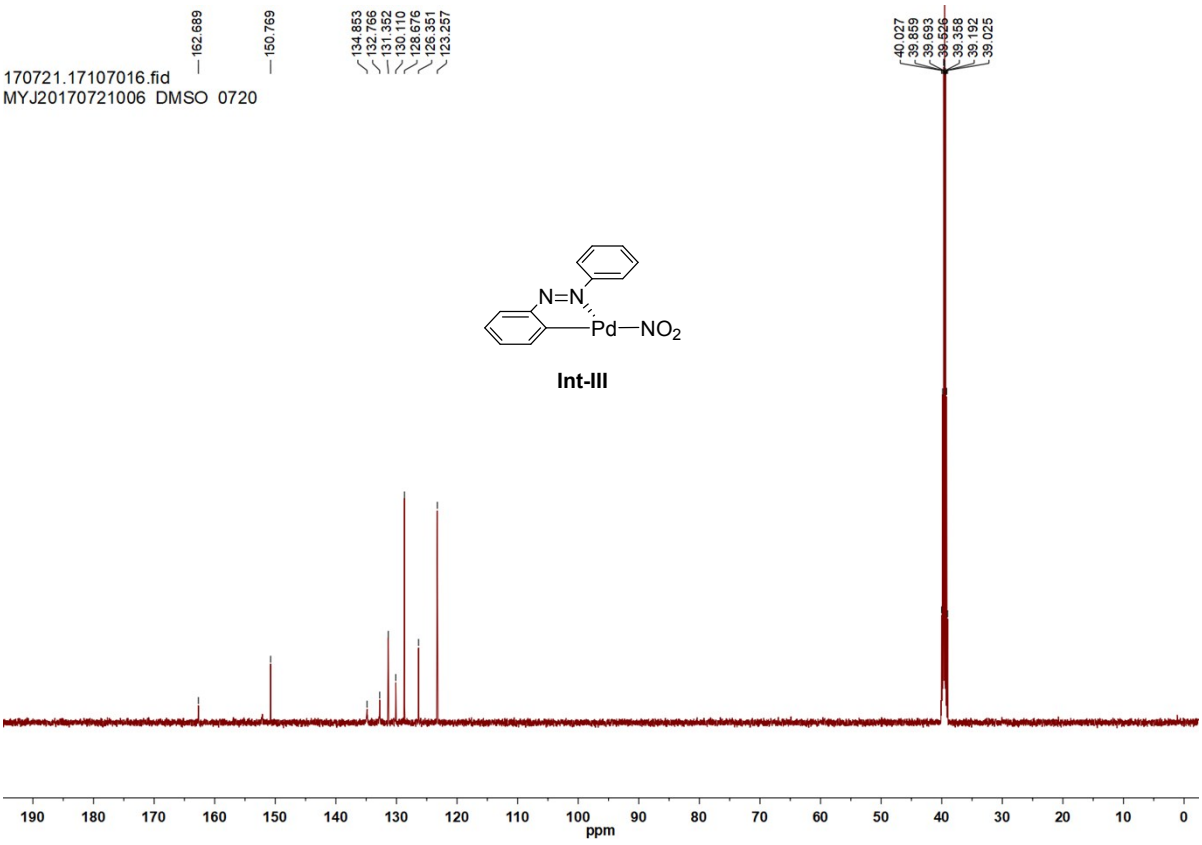
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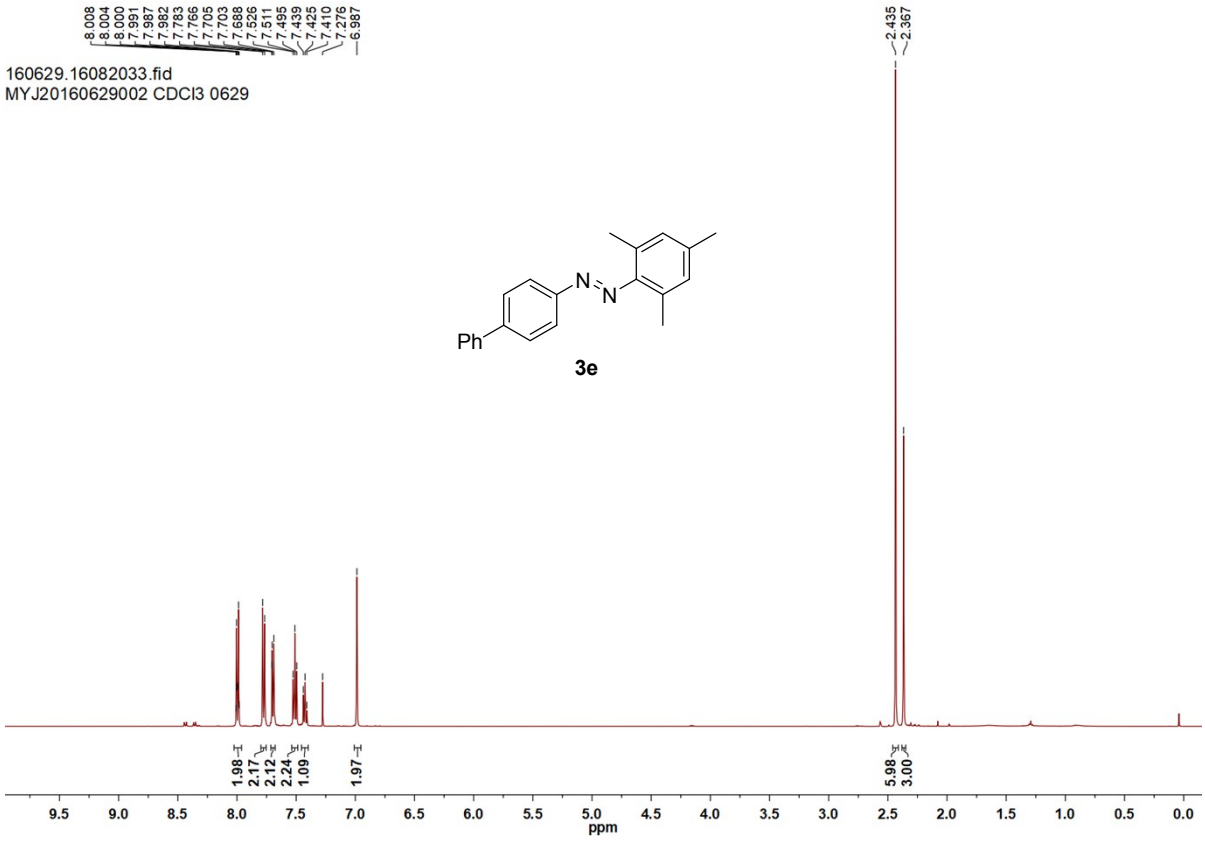
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7.511
7.495
7.439
7.425
7.410
7.276
6.987
2.435
2.367
160629.16082033.fid
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N
N
Ph
3e
1.98
2.17
2.12
2.24
1.09
1.97
5.98
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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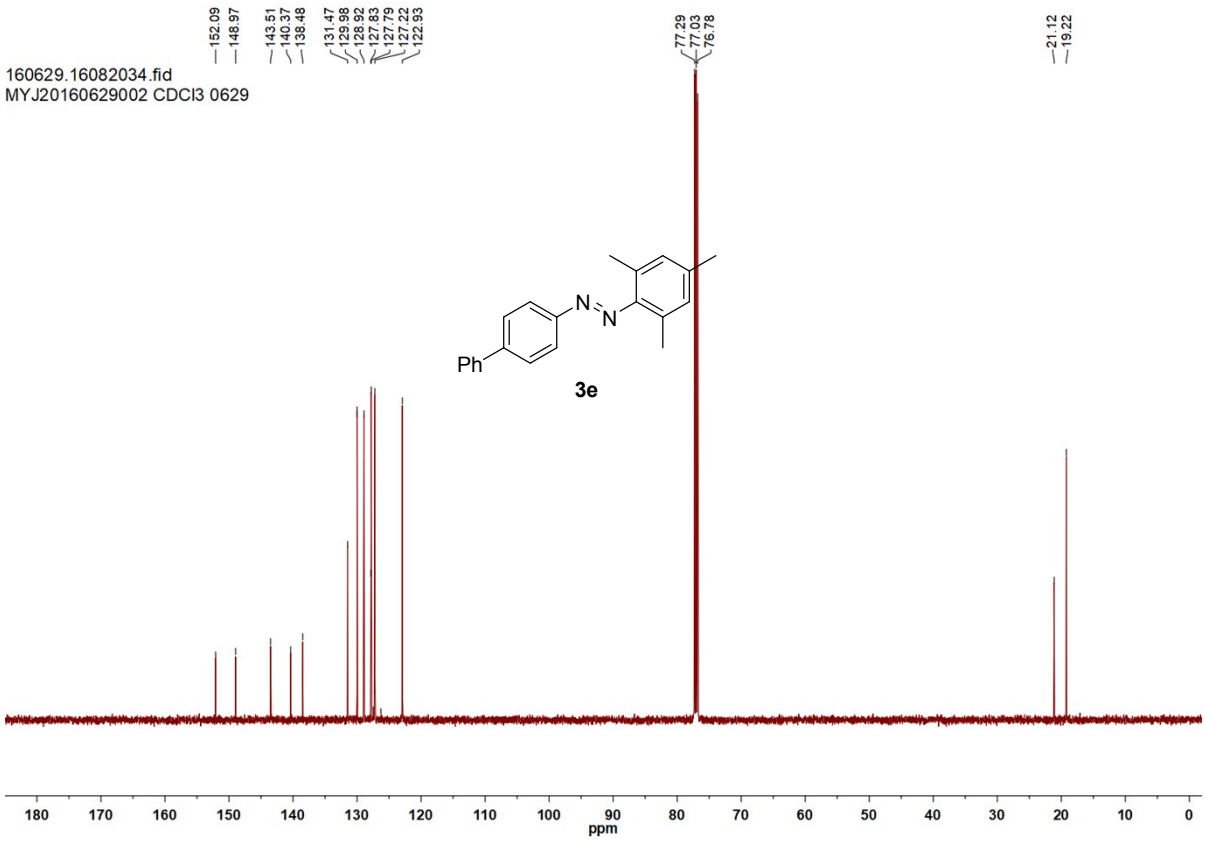
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127.79
127.22
122.93
77.29
77.03
76.78
21.12
19.22
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N
Ph
3e
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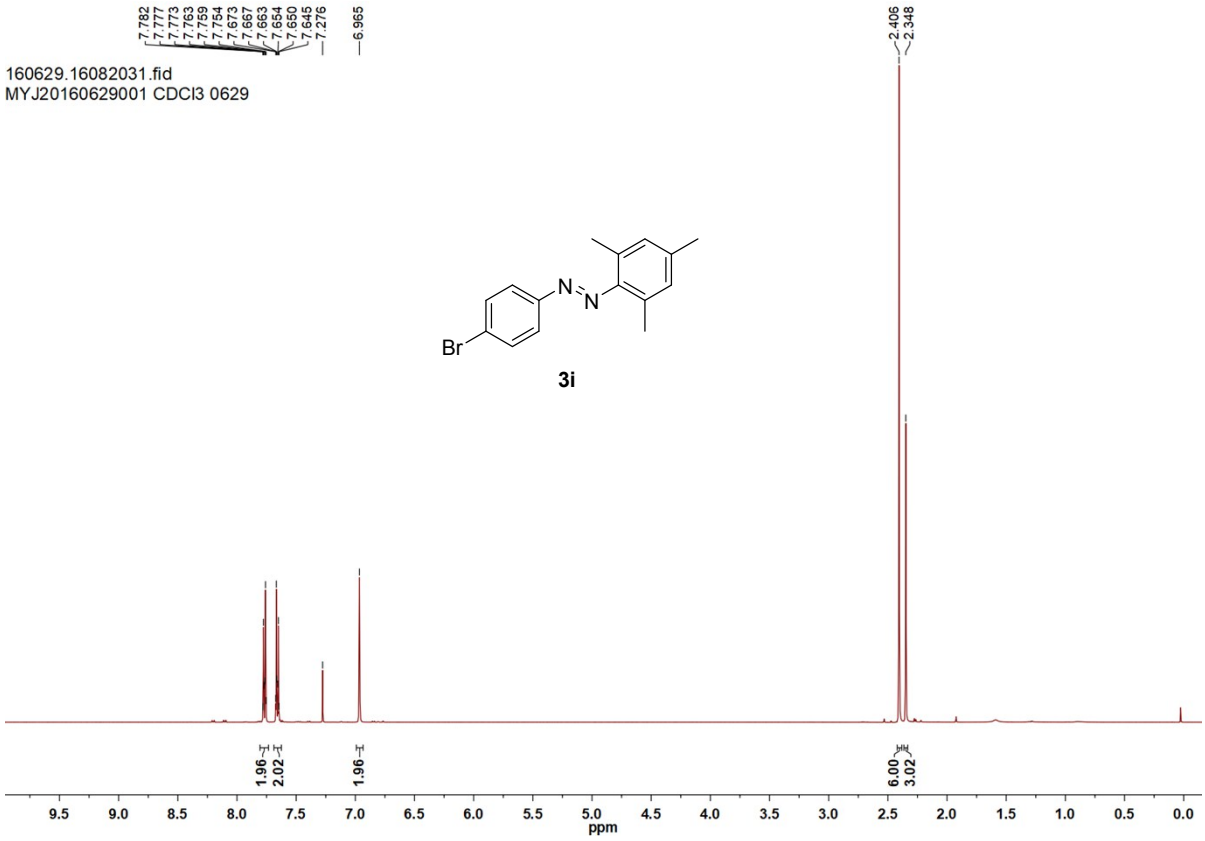
ppm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7.645
7.276
6.965
2.406
2.348
160629.16082031.fid
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Br
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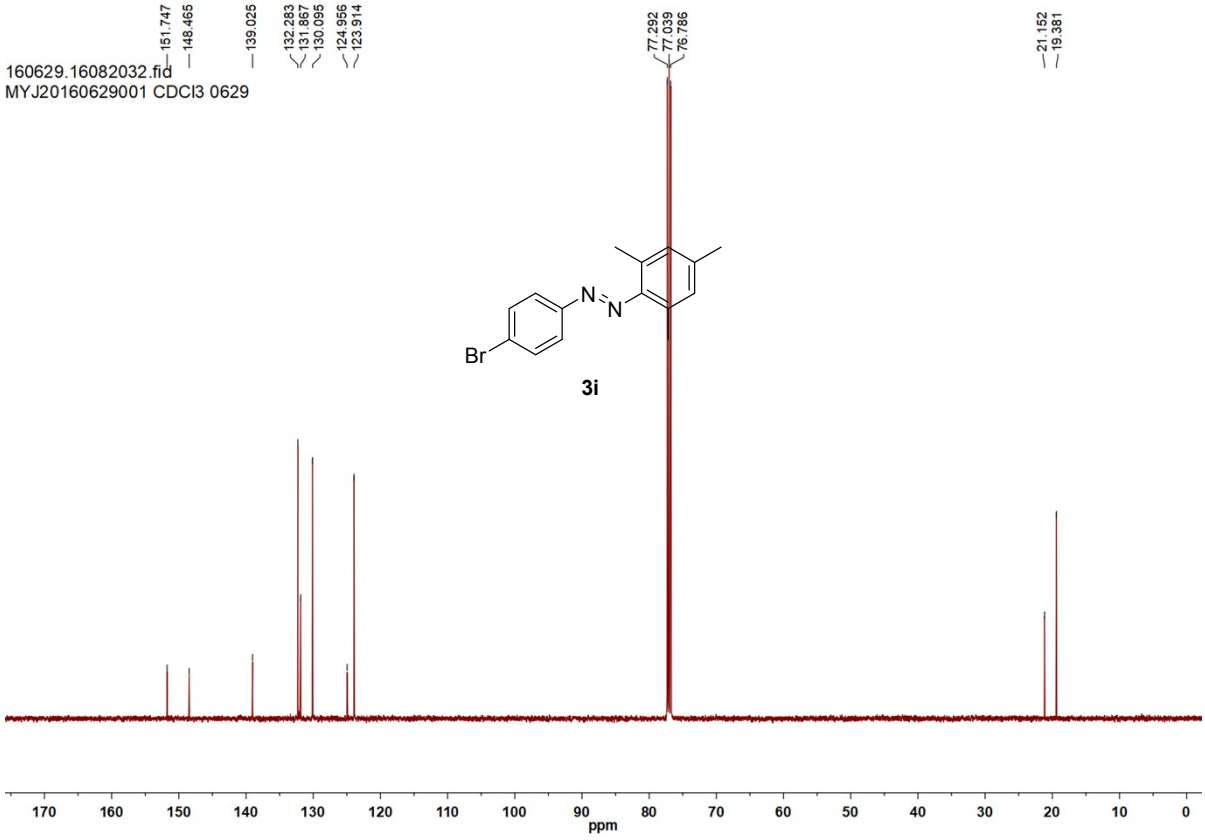
N
3i
1.96
2.02
1.96
6.00
3.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm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Br
N
N
3i
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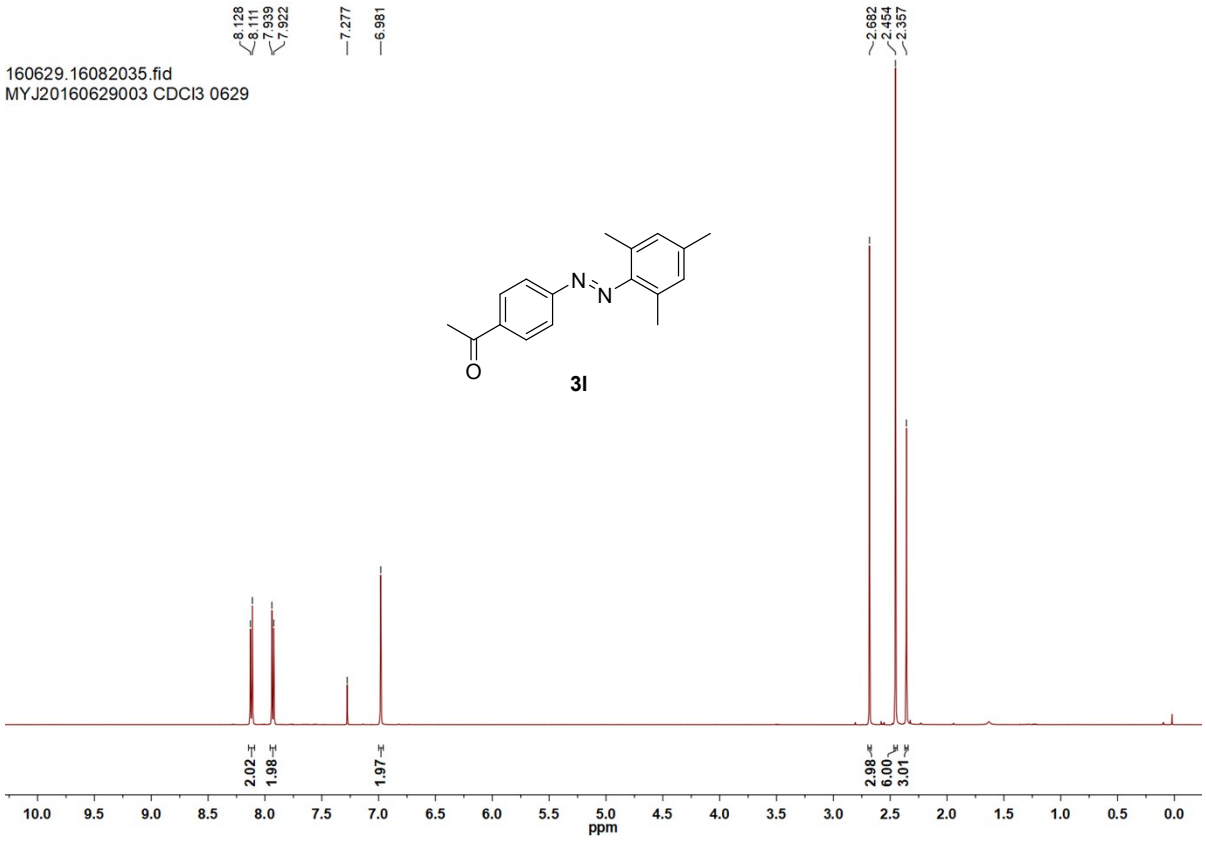
ppm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1.97
2.98
6.00
3.01
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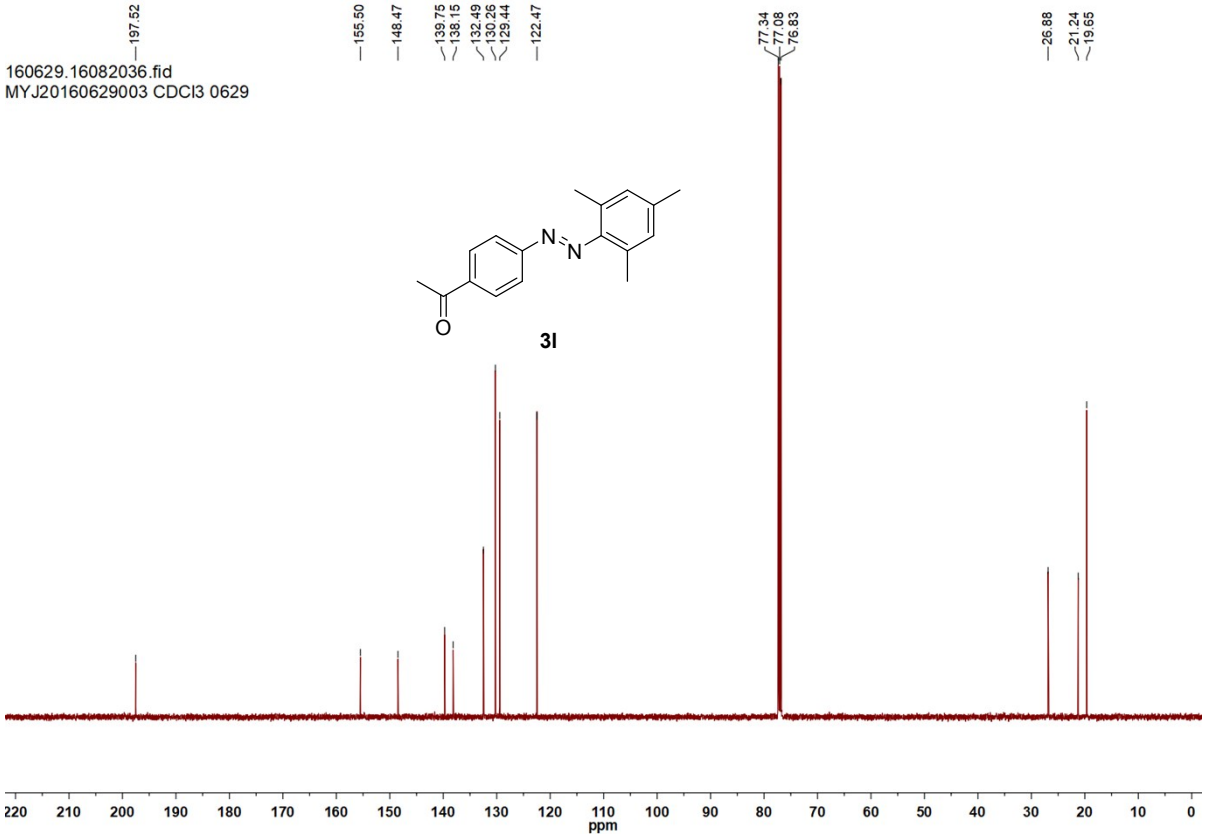
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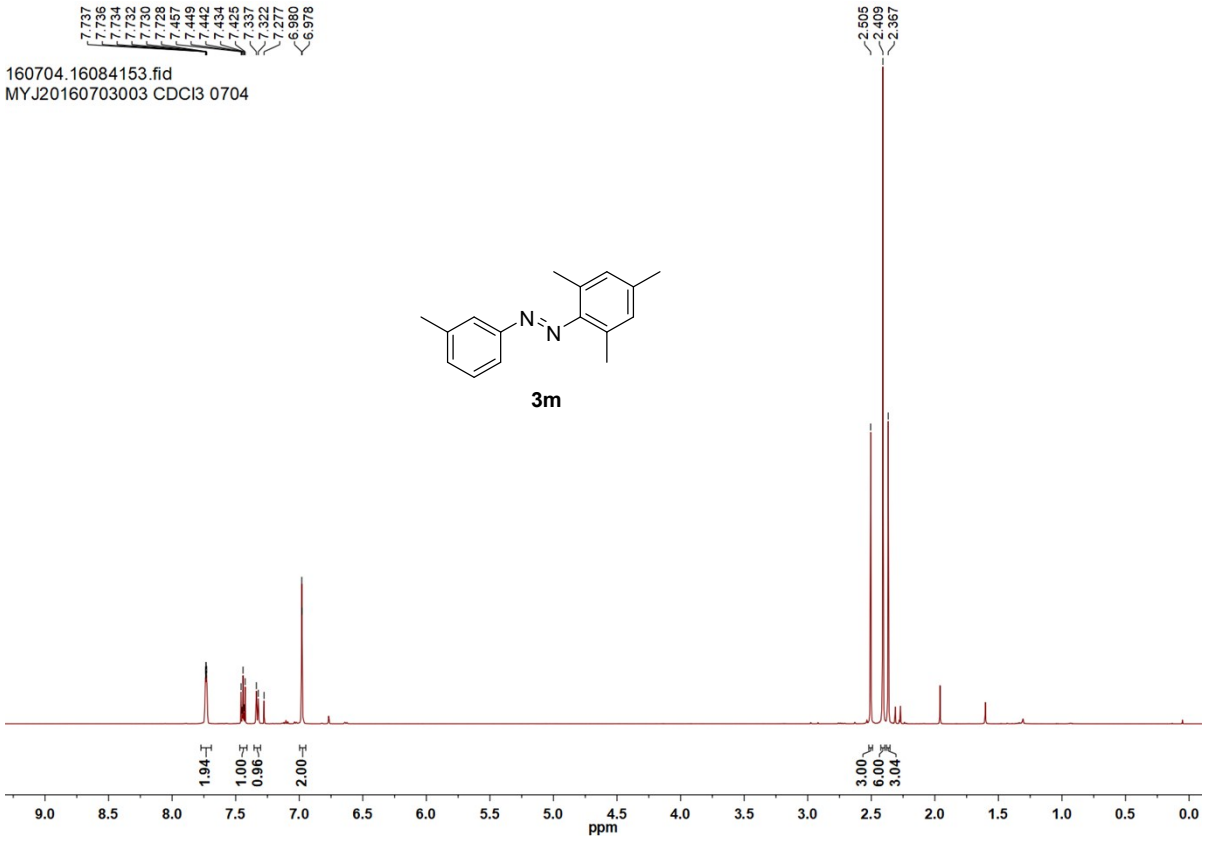
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7.425
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2.505
2.409
2.367
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N
3m
1.94
1.00
0.96
2.00
3.00
6.00
3.04
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.0
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3.0
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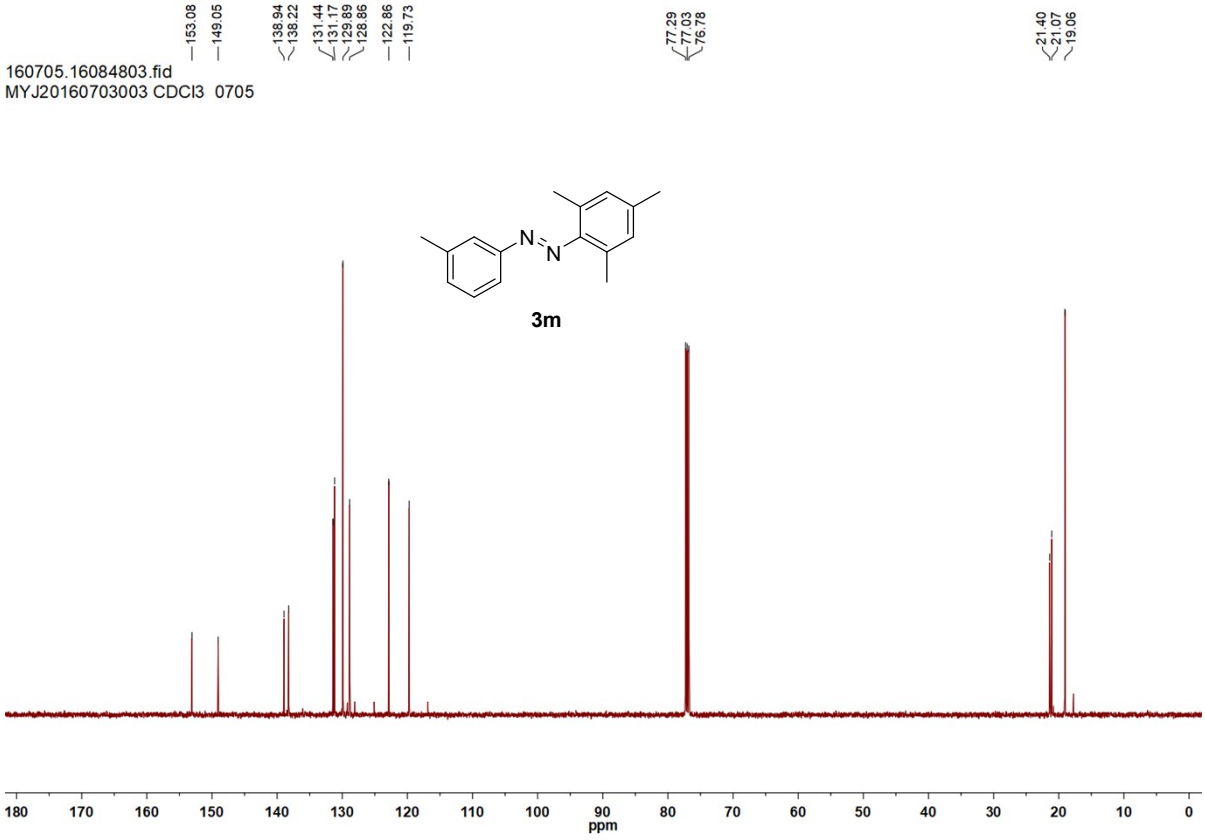
1.5
1.0
0.5
0.0
ppm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128.86
122.86
119.73
77.29
77.03
76.78
21.40
21.07
19.06
160705.16084803.fid
MYJ20160703003 CDCl3 0705
N
N
3m
180
170
160
150
140
130
120
110
100
90
80
70
60
50
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30
20
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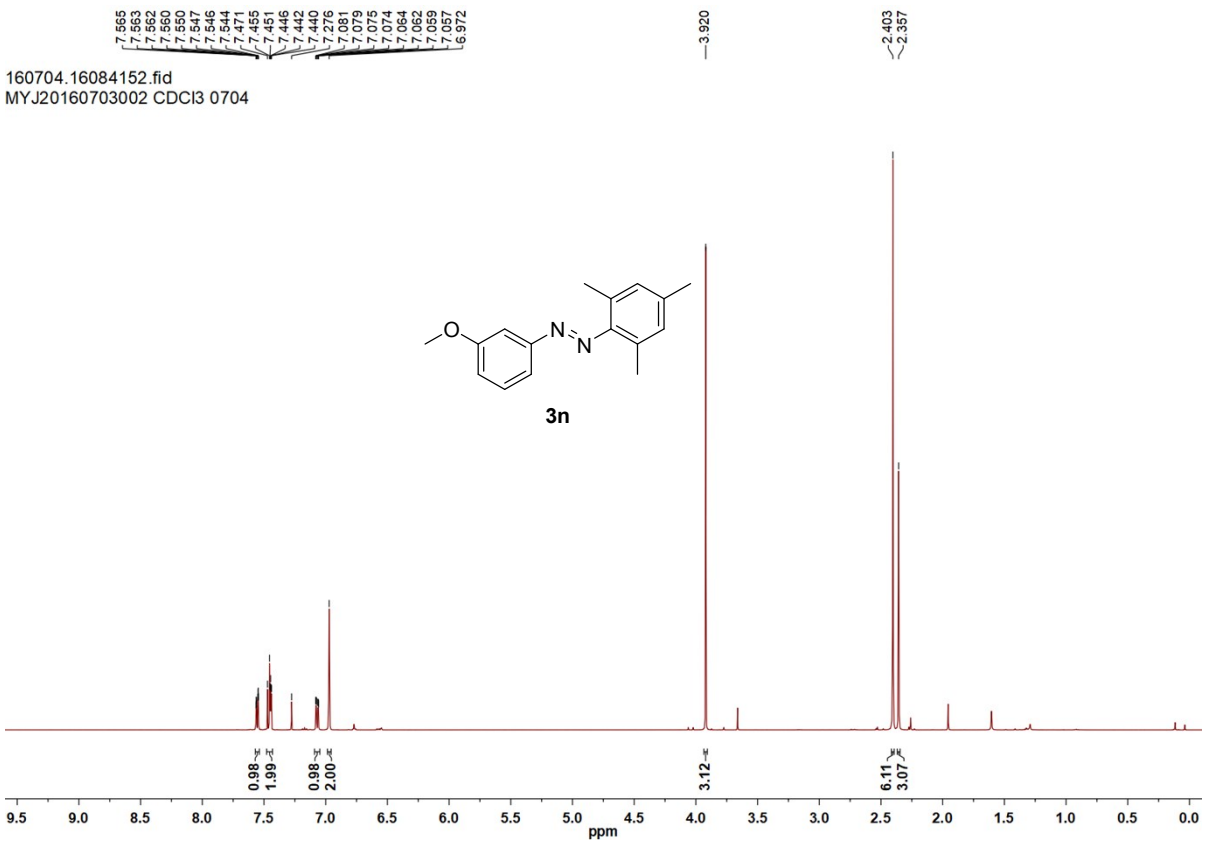
0
ppm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7.547
7.546
7.544
7.471
7.455
7.451
7.446
7.442
7.440
7.276
7.081
7.079
7.075
7.074
7.064
7.062
7.059
7.057
6.972
3.920
2.403
2.357
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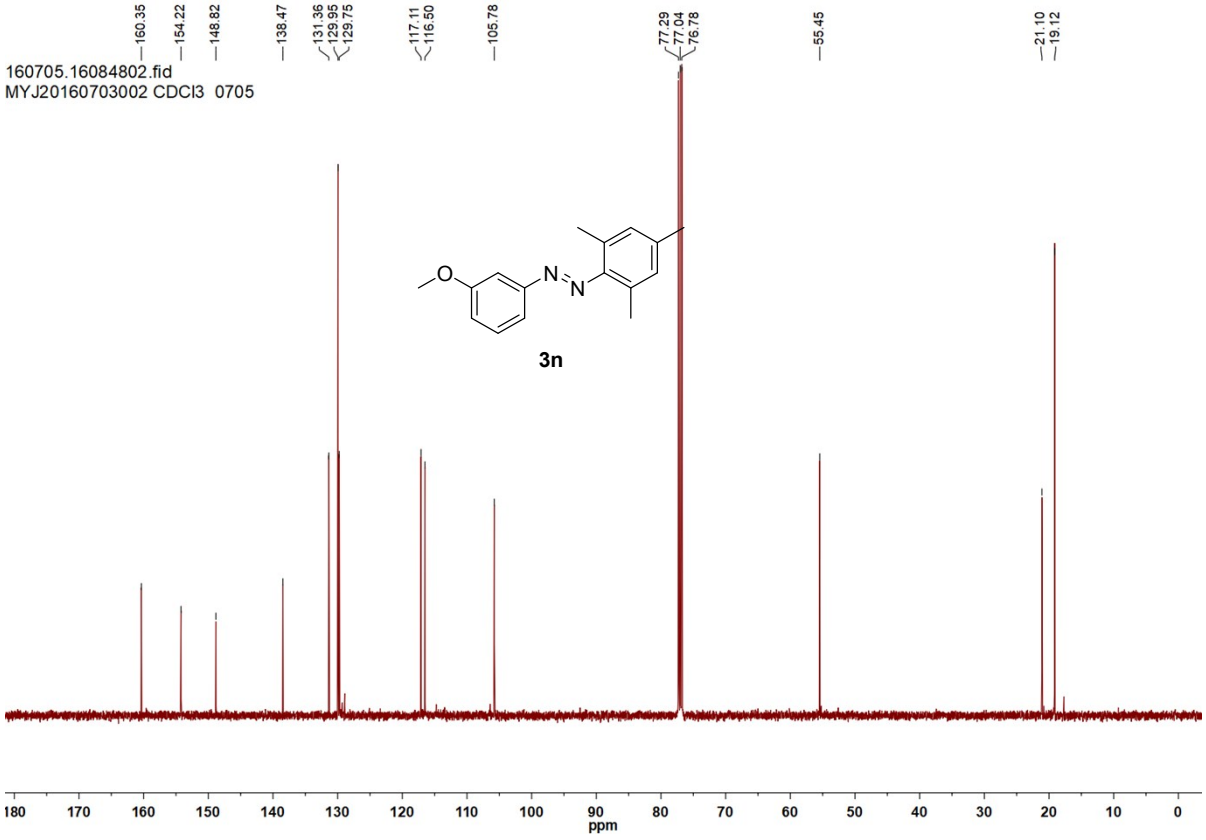
N
3n
0.98
1.99
0.98
2.00
3.12
6.11
3.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm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117.11
116.50
105.78
77.29
77.04
76.78
55.45
21.10
19.12
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N
3n
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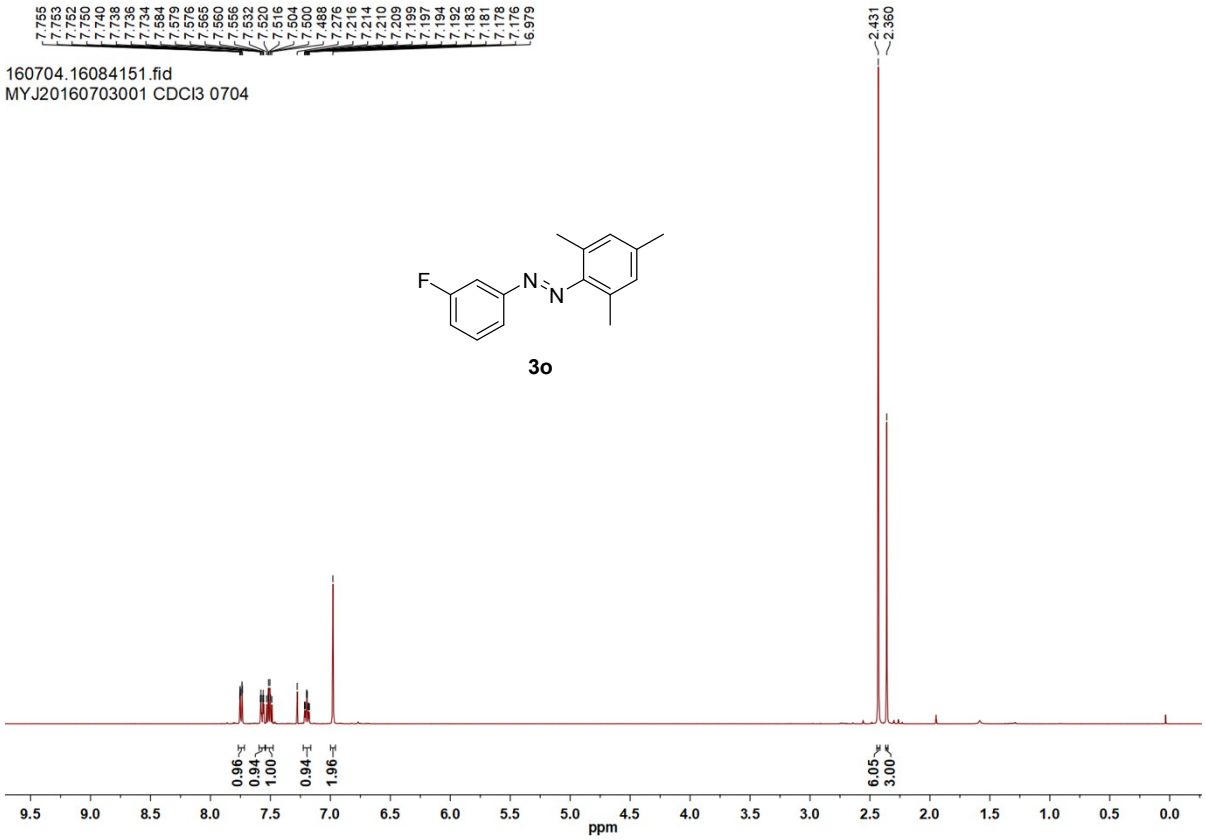
ppm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7.738
7.736
7.734
7.584
7.579
7.576
7.565
7.560
7.556
7.532
7.520
7.516
7.504
7.500
7.488
7.276
7.216
7.214
7.210
7.209
7.199
7.197
7.194
7.192
7.183
7.181
7.178
7.176
6.979
2.431
2.360
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N
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0.94
1.00
0.94
1.96
6.05
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.5
3.0
2.5
2.0
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1.0
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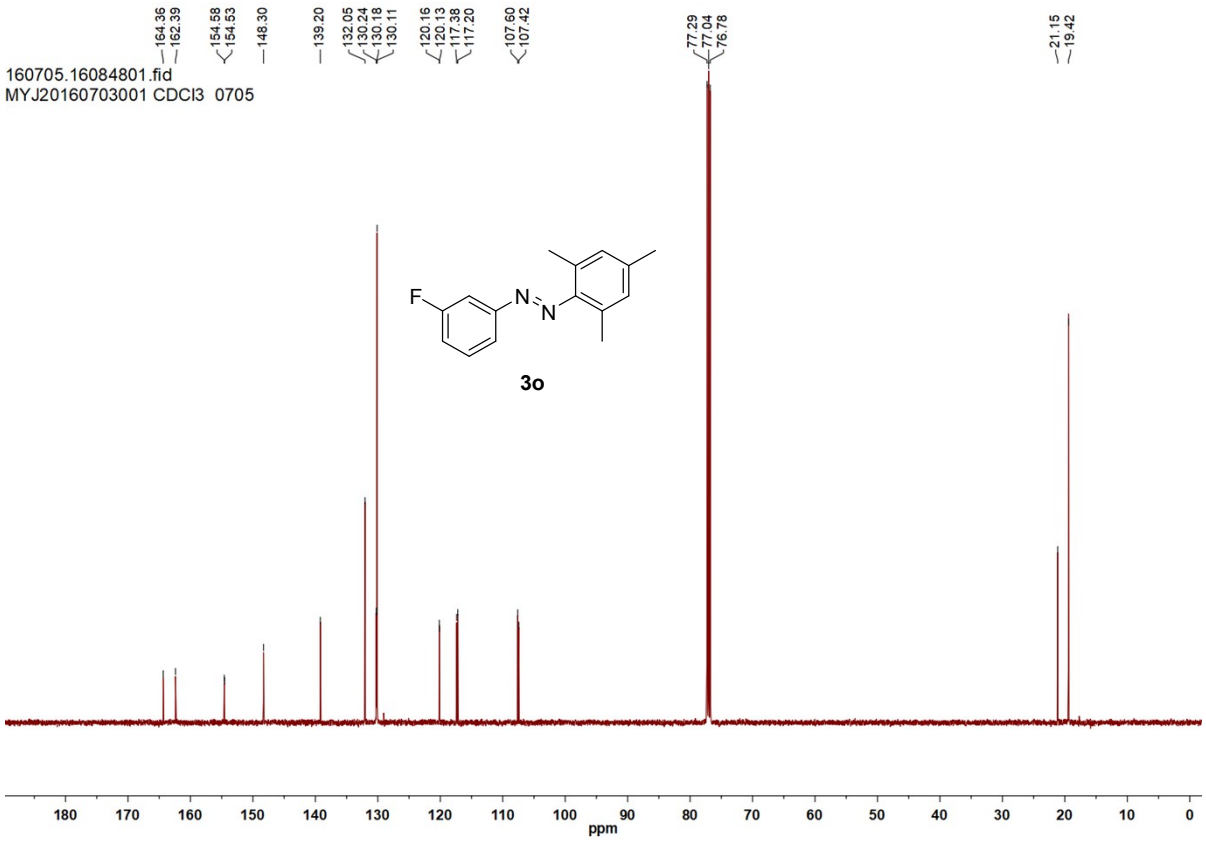
0.0
ppm

3o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139.20
132.05
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130.11
120.16
120.13
117.38
117.20
107.60
107.42
77.29
77.04
76.78
21.15
19.42
160705.16084801.fid
MYJ20160703001 CDCl3 0705
F
N
N
180
170
160
150
140
130
120
110
100
90
80
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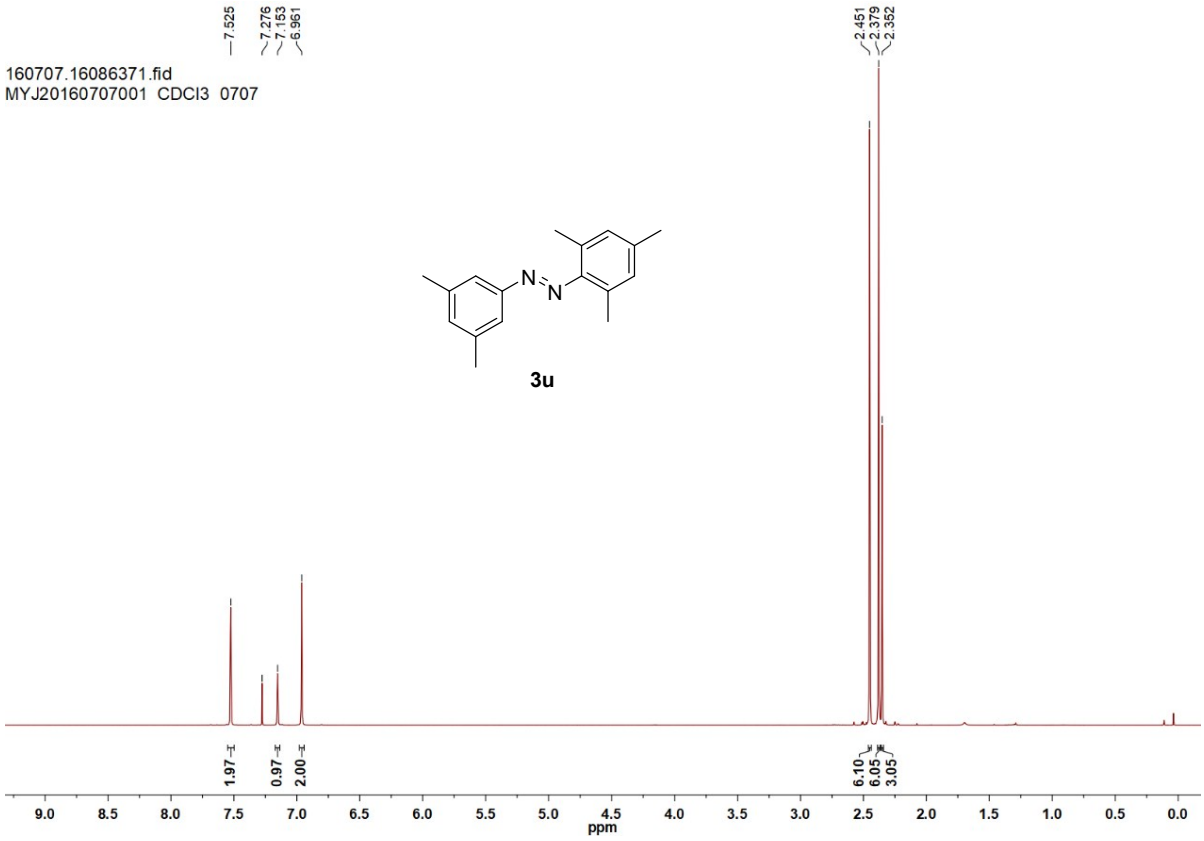
50
40
30
20
10
0
ppm

3o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2.352
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3u
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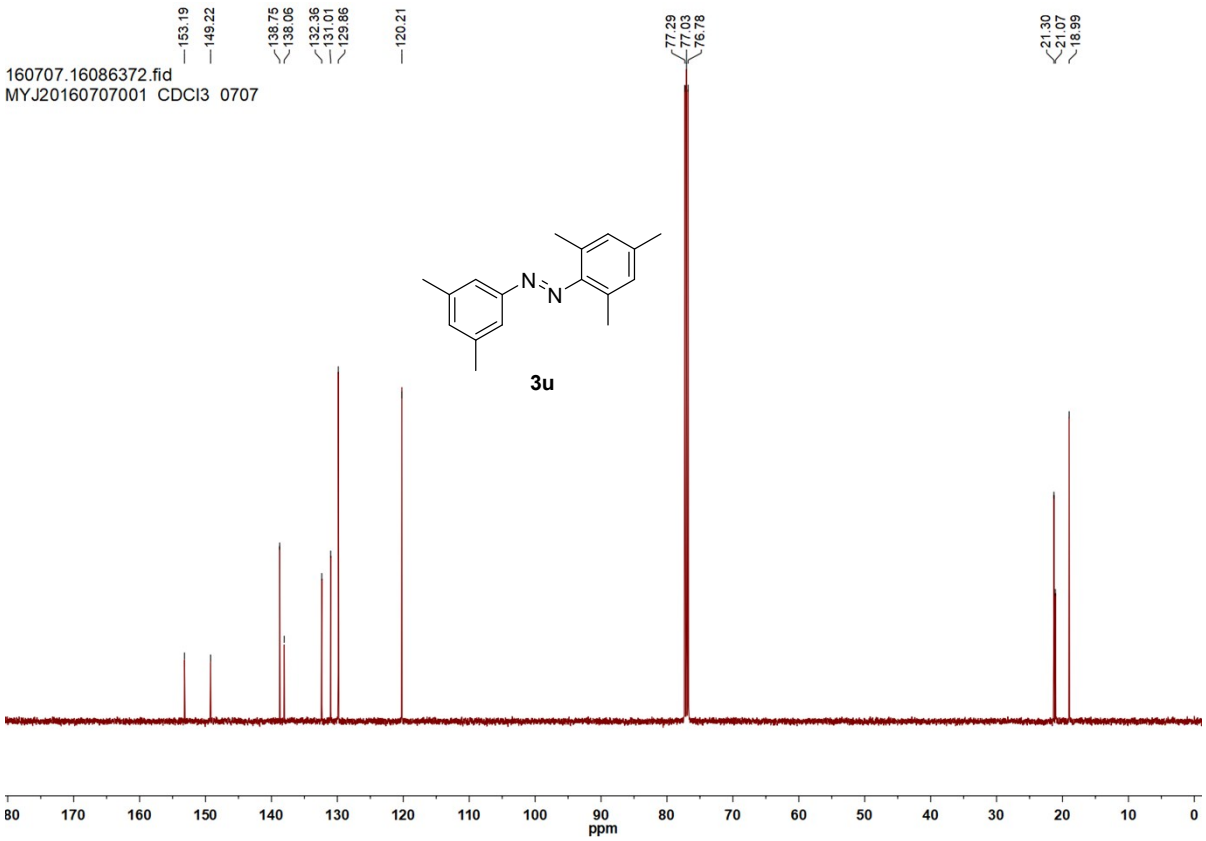
2.00
6.10
6.05
3.05
ppm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120.21
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21.07
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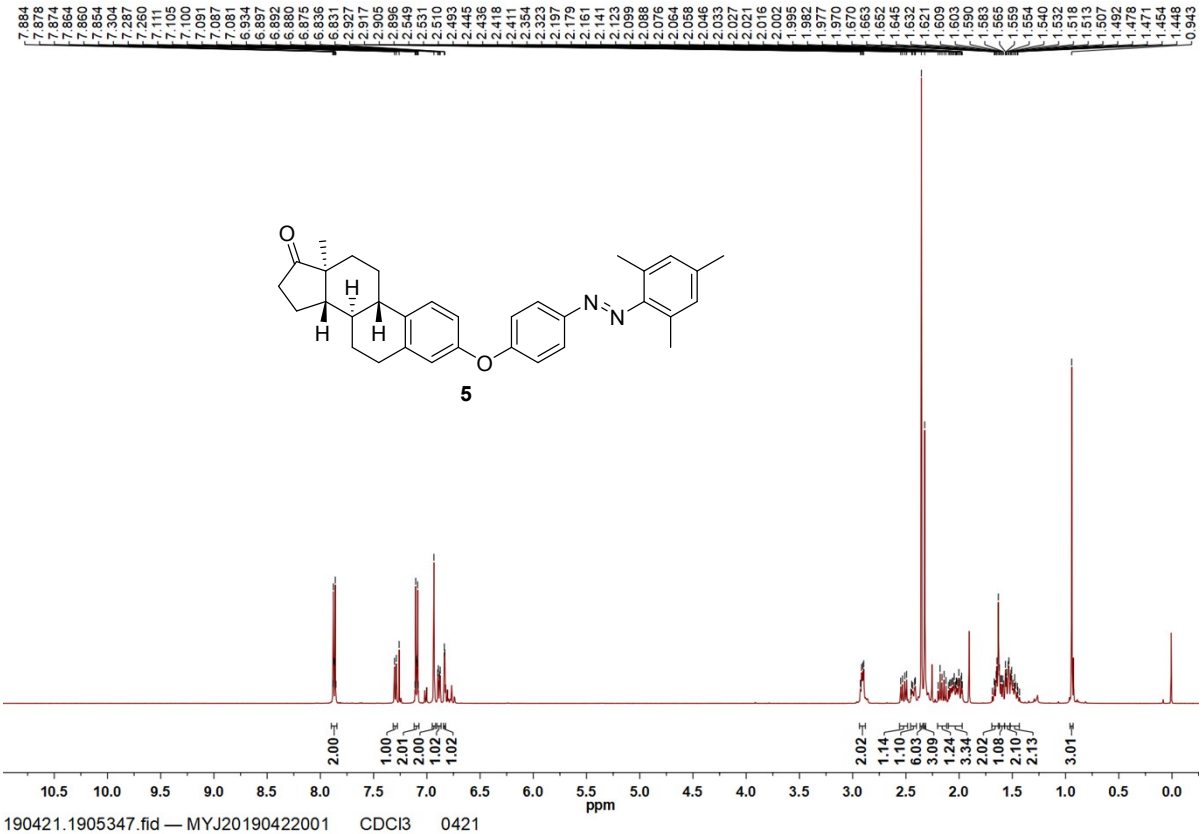
3u
ppm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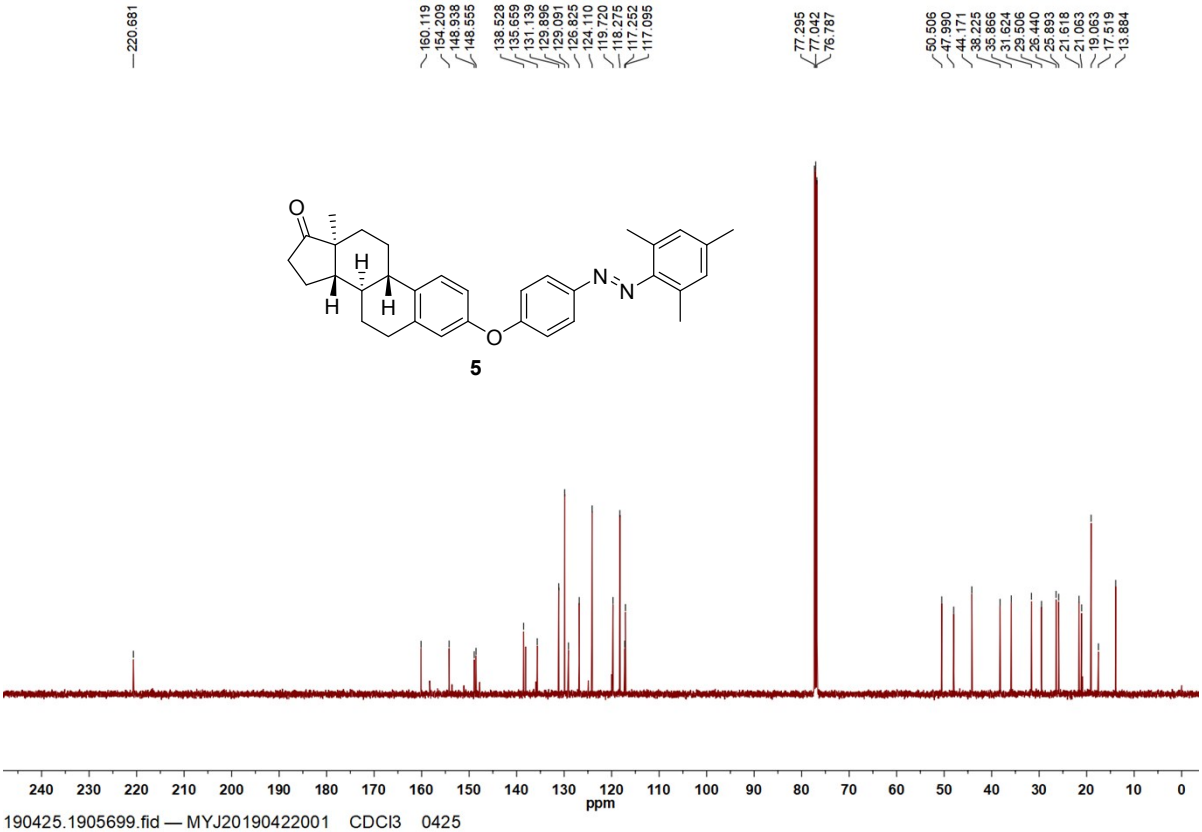
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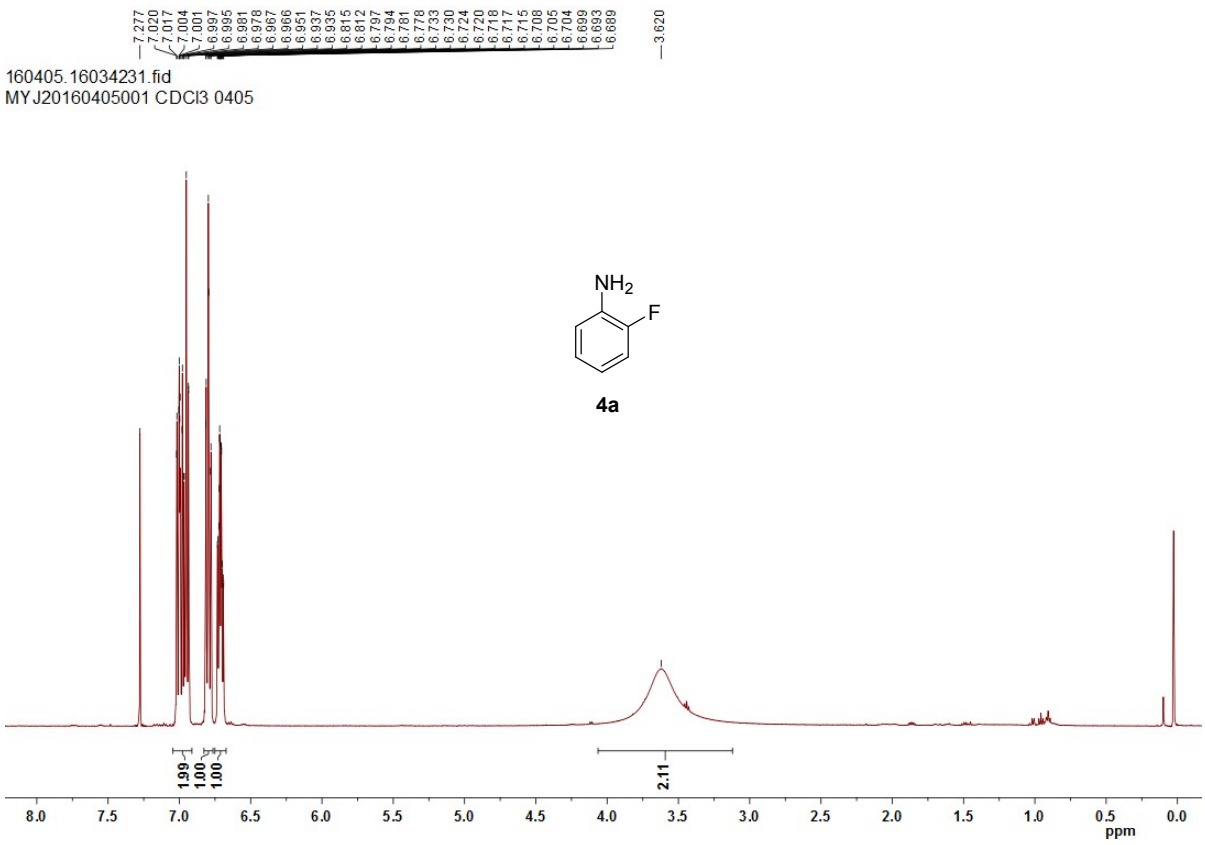
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6.937
6.935
6.815
6.812
6.797
6.794
6.781
6.778
6.733
6.730
6.724
6.720
6.718
6.717
6.715
6.708
6.705
6.704
6.699
6.693
6.689
3.620
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NH2
F
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1.00
1.00
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8.0
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7.0
6.5
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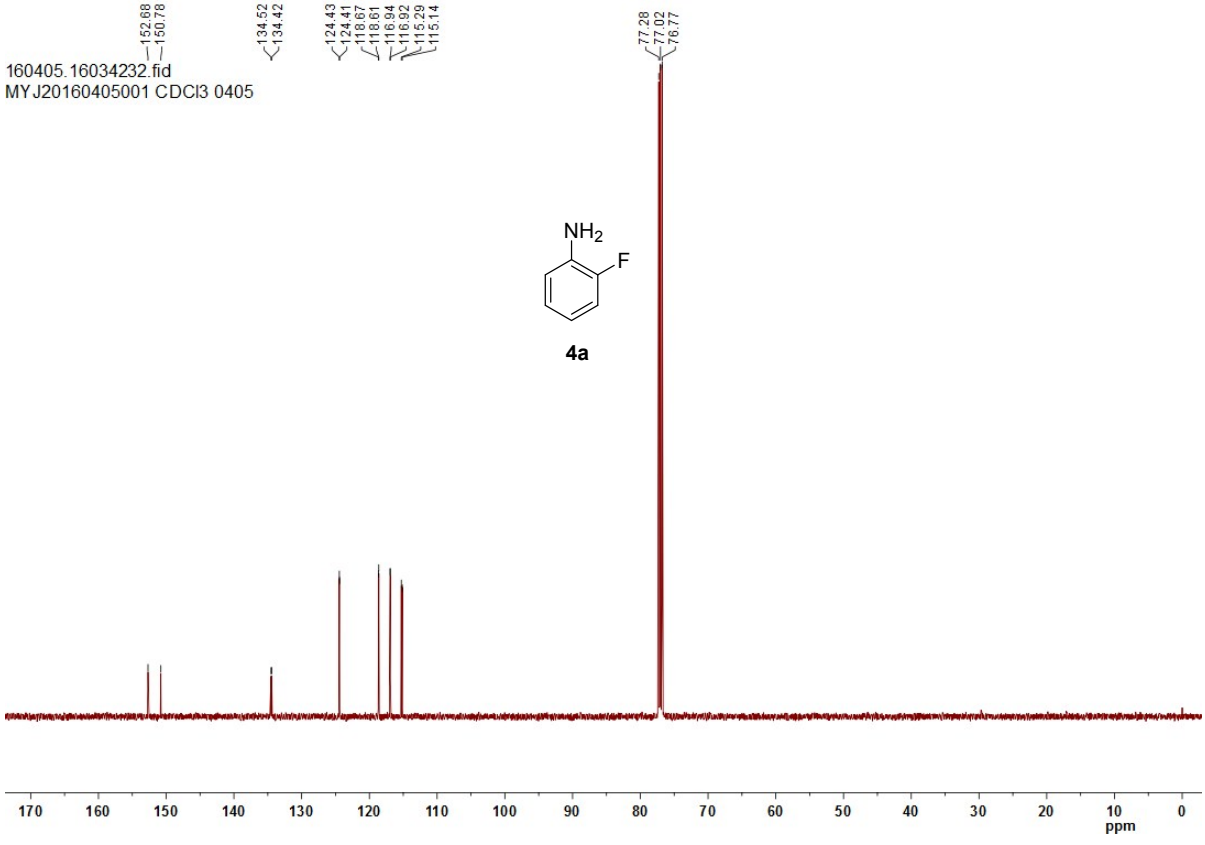
ppm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124.41
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115.14
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77.02
76.77
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NH2
F
4a
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160
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140
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110
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80
70
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myj-1.10.fid

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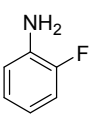

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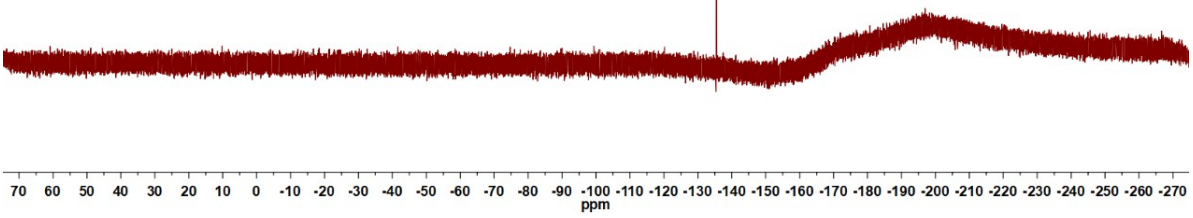

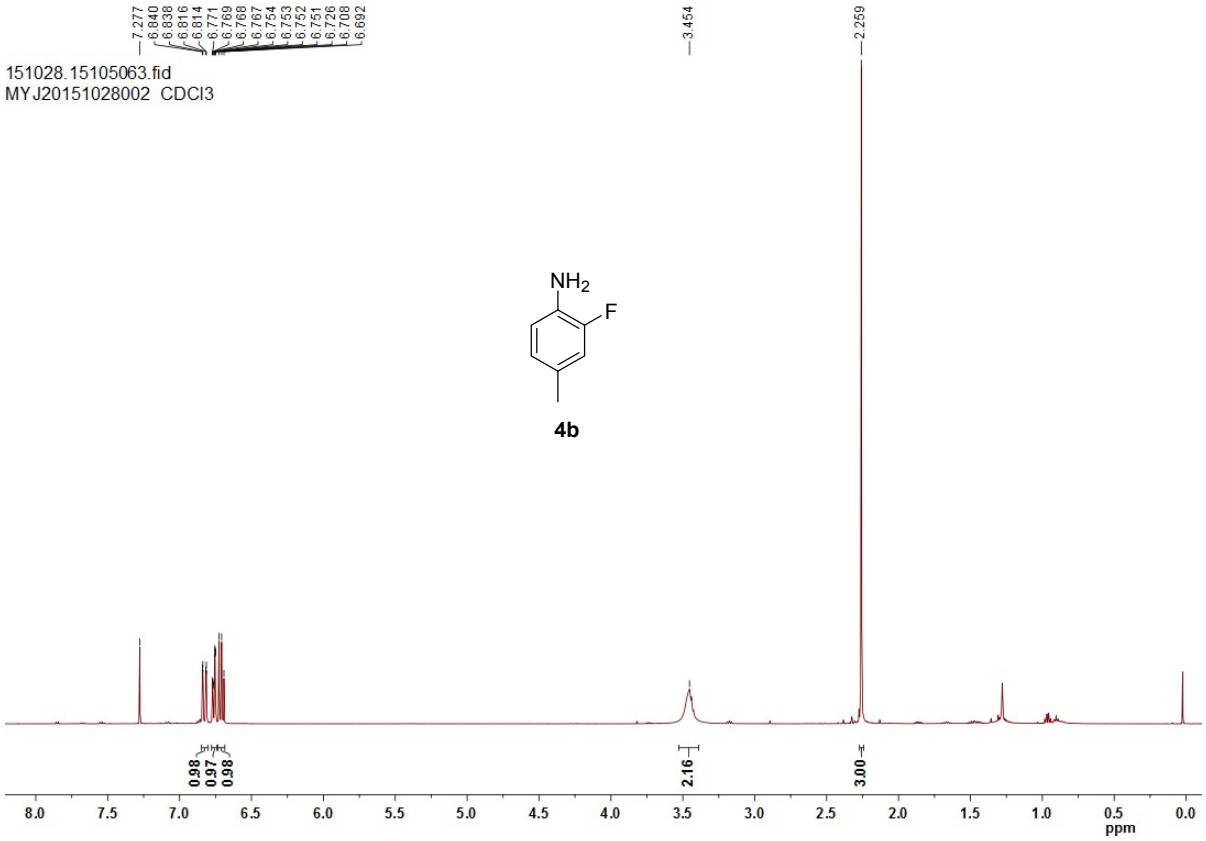
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6.753
6.752
6.751
6.726
6.708
6.692
3.454
2.259
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NH2
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4b
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3.00
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7.5
7.0
6.5
6.0
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4.0
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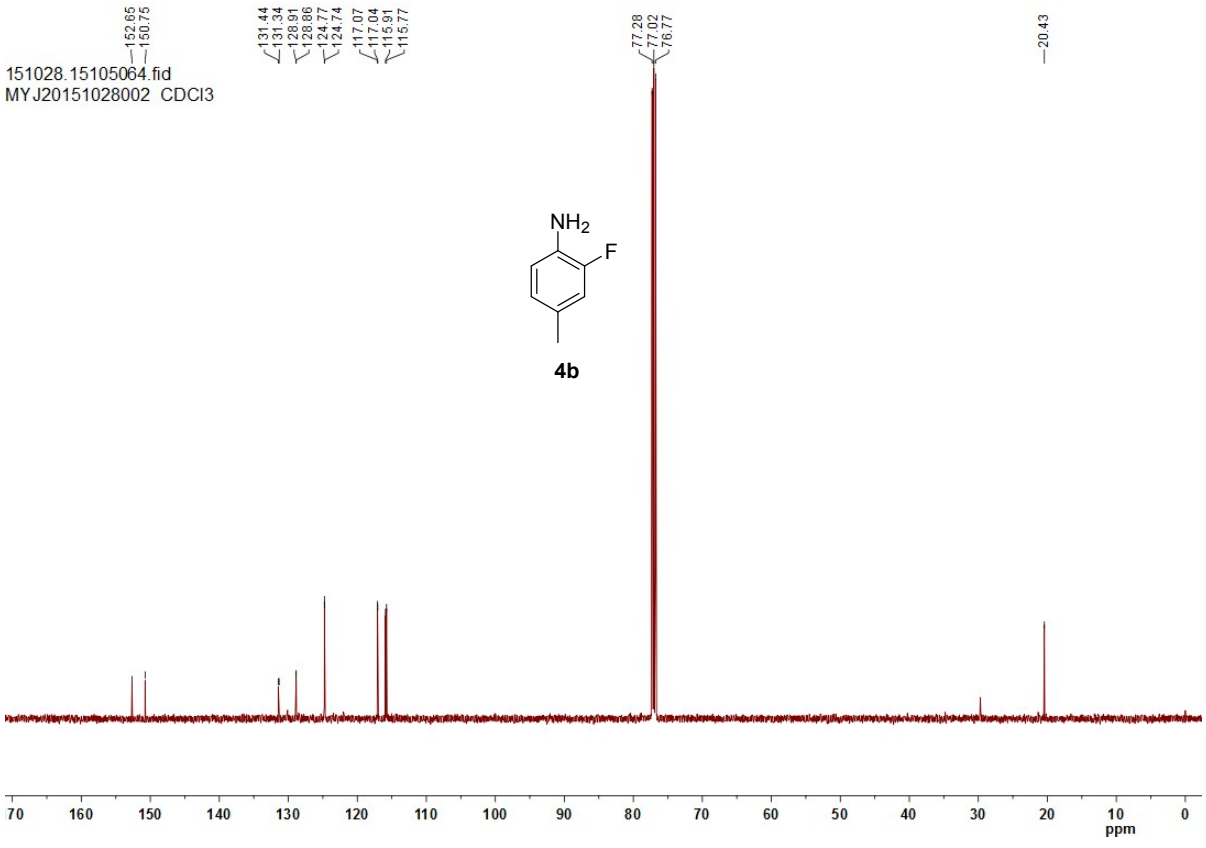
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117.04
115.91
115.77
77.28
77.02
76.77
20.43
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NH2
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80
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60
50
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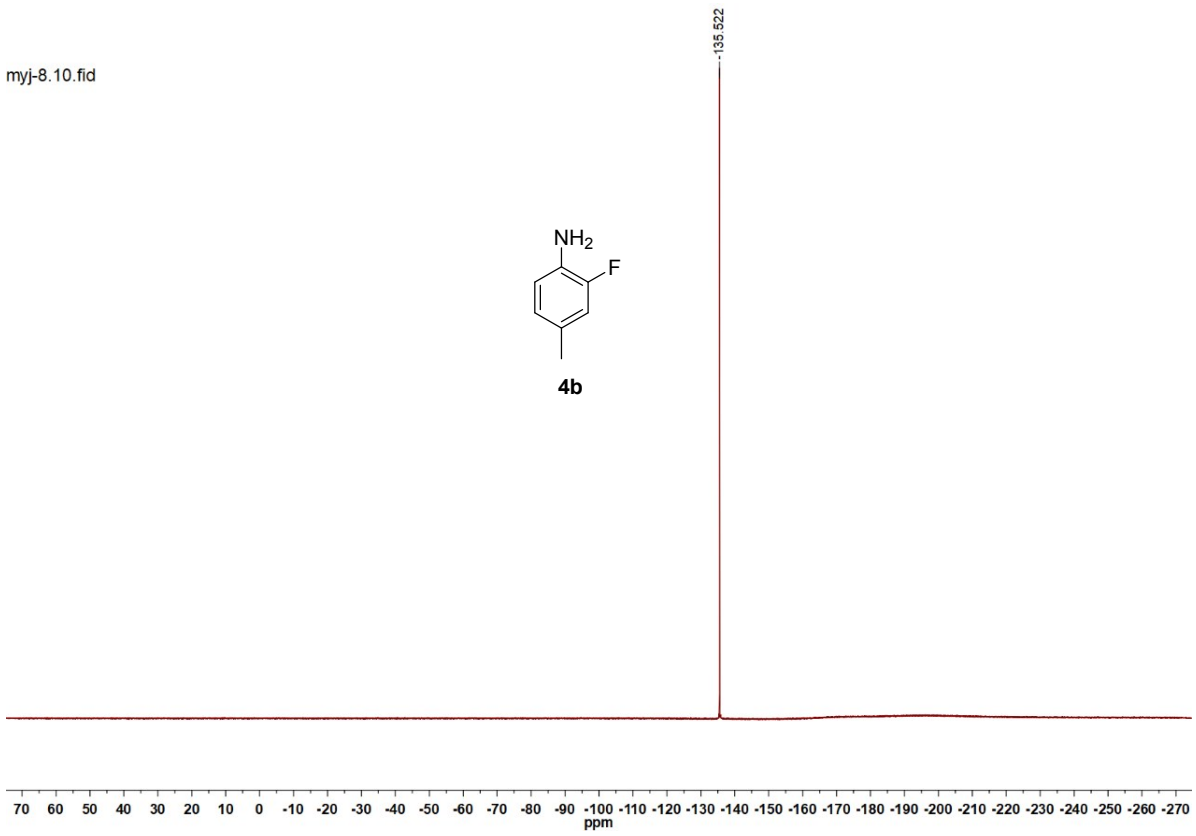
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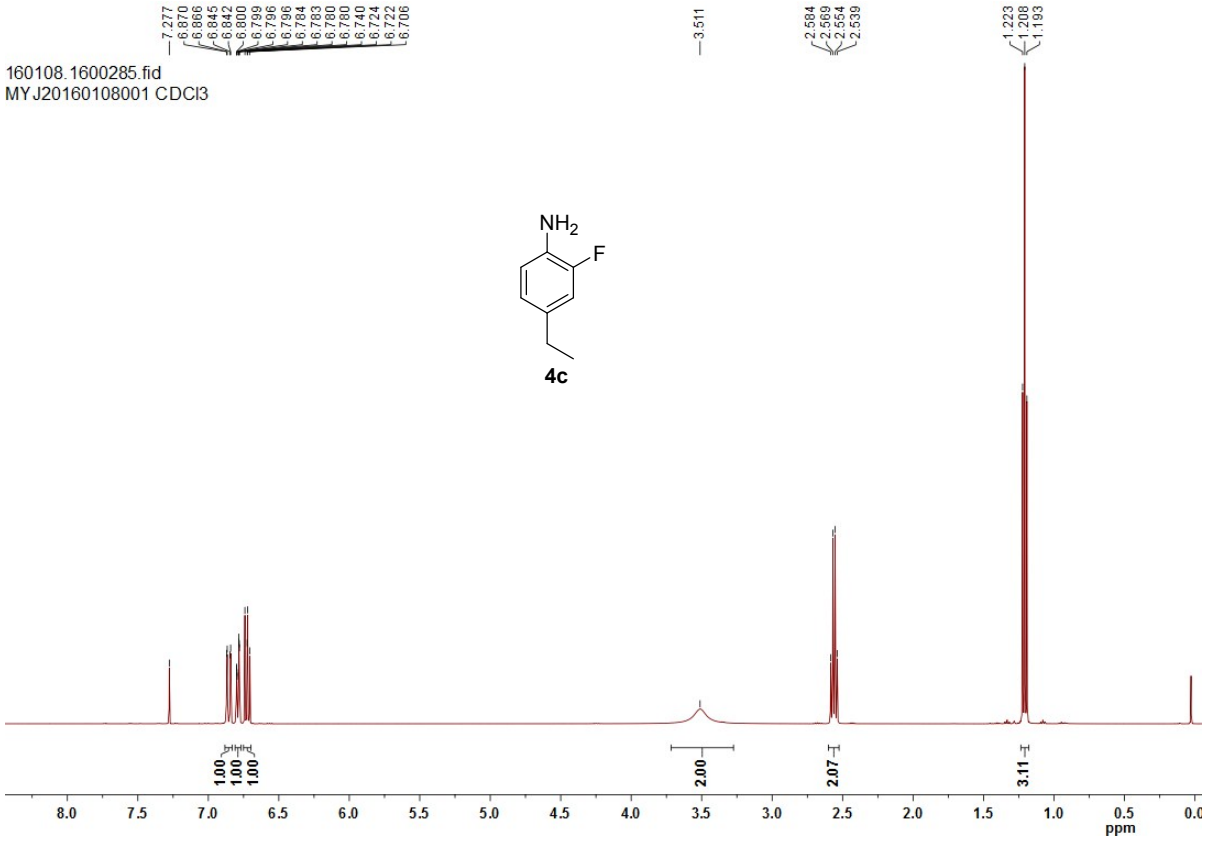
ppm

4b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6.780
6.780
6.740
6.724
6.722
6.706
3.511
2.584
2.569
2.554
2.539
1.223
1.208
1.193
160108.1600285.fid
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NH2
F
4c
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1.00
1.00
2.00
2.07
3.11
8.0
7.5
7.0
6.5
6.0
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1.5
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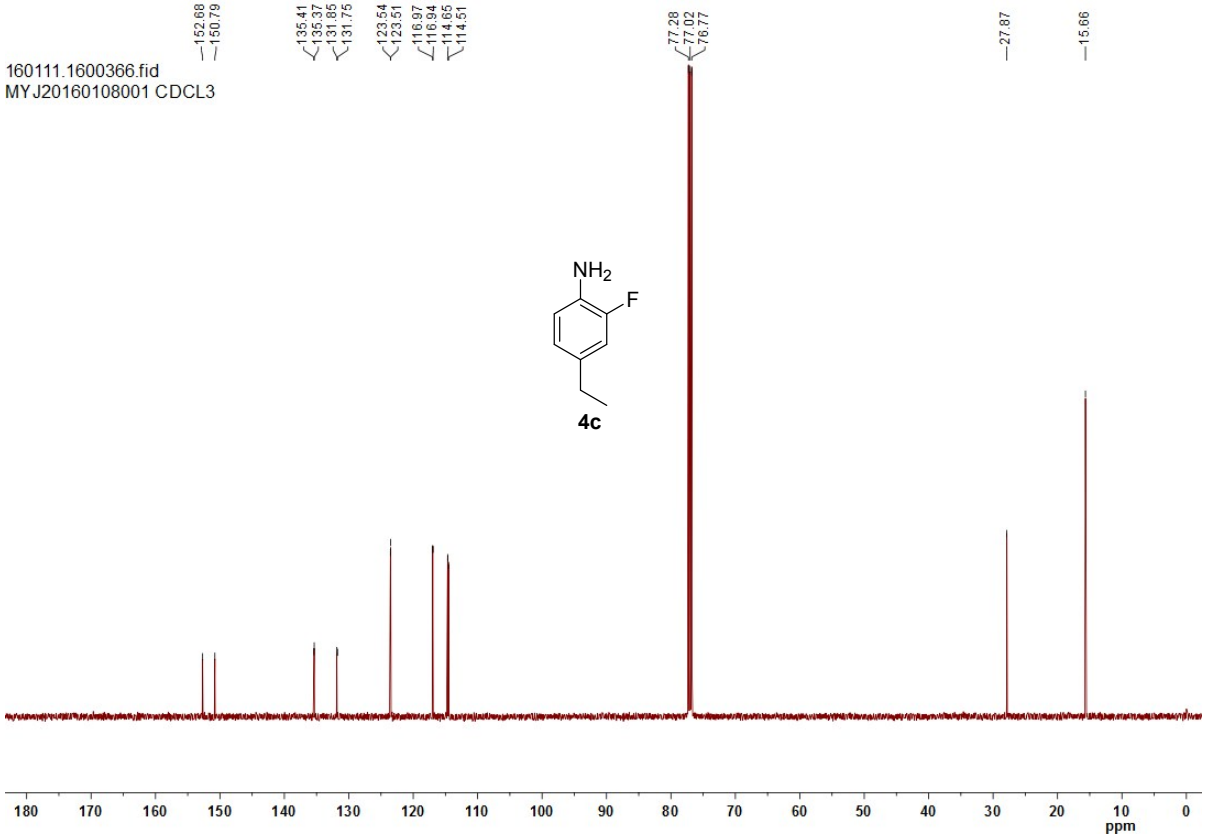
ppm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123.51
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116.94
114.65
114.51
77.28
77.02
76.77
27.87
15.66
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NH2
F
4c
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140
130
120
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100
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80
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60
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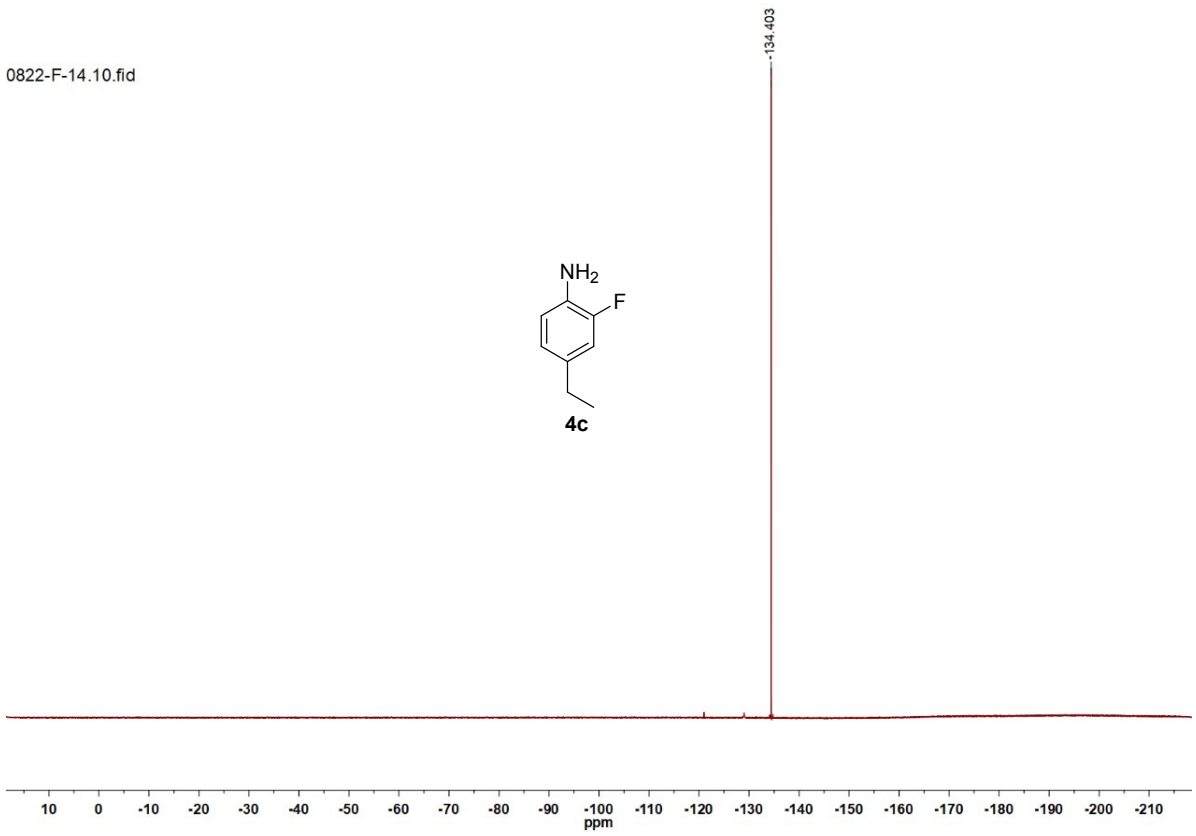
20
10
0
ppm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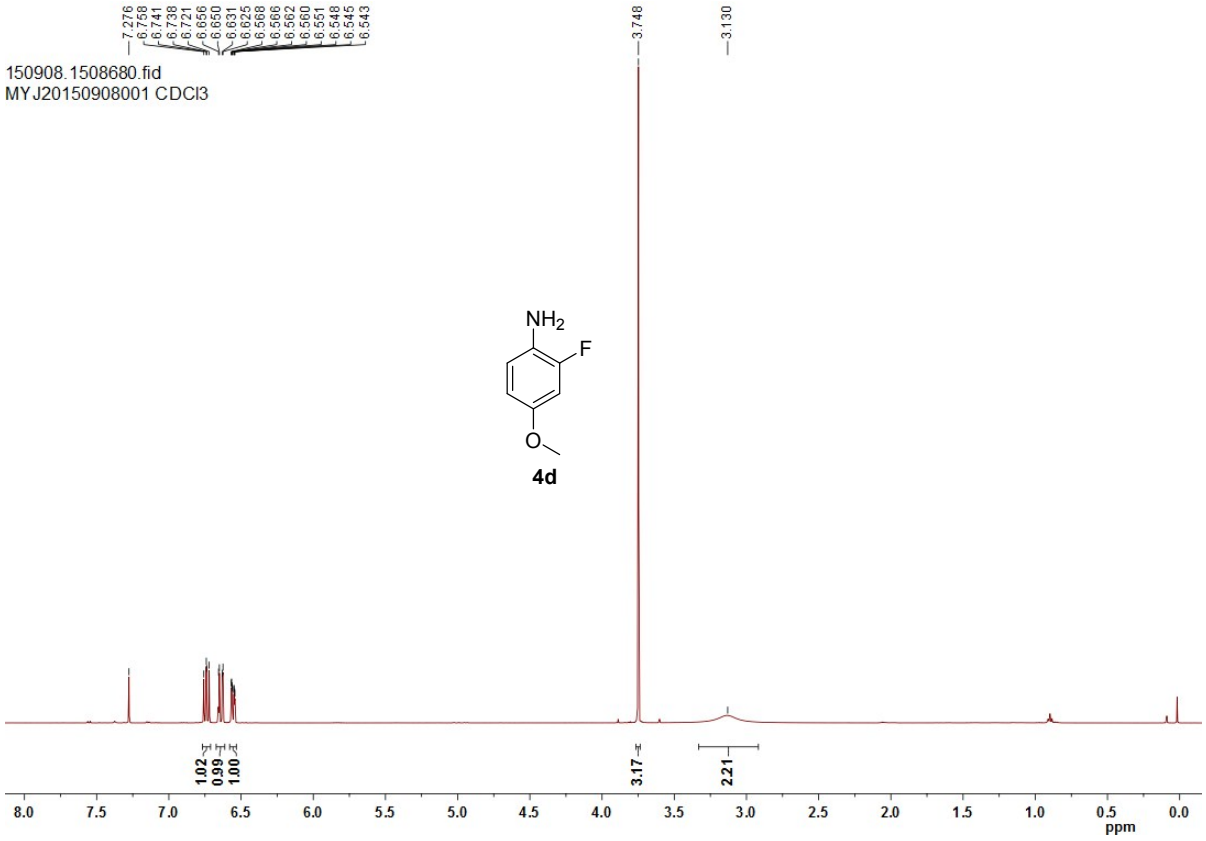
ppm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6.568
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6.562
6.560
6.551
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6.545
6.543
3.748
3.130
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O
4d
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1.00
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2.21
8.0
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7.0
6.5
6.0
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4.0
3.5
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1.5
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0.5
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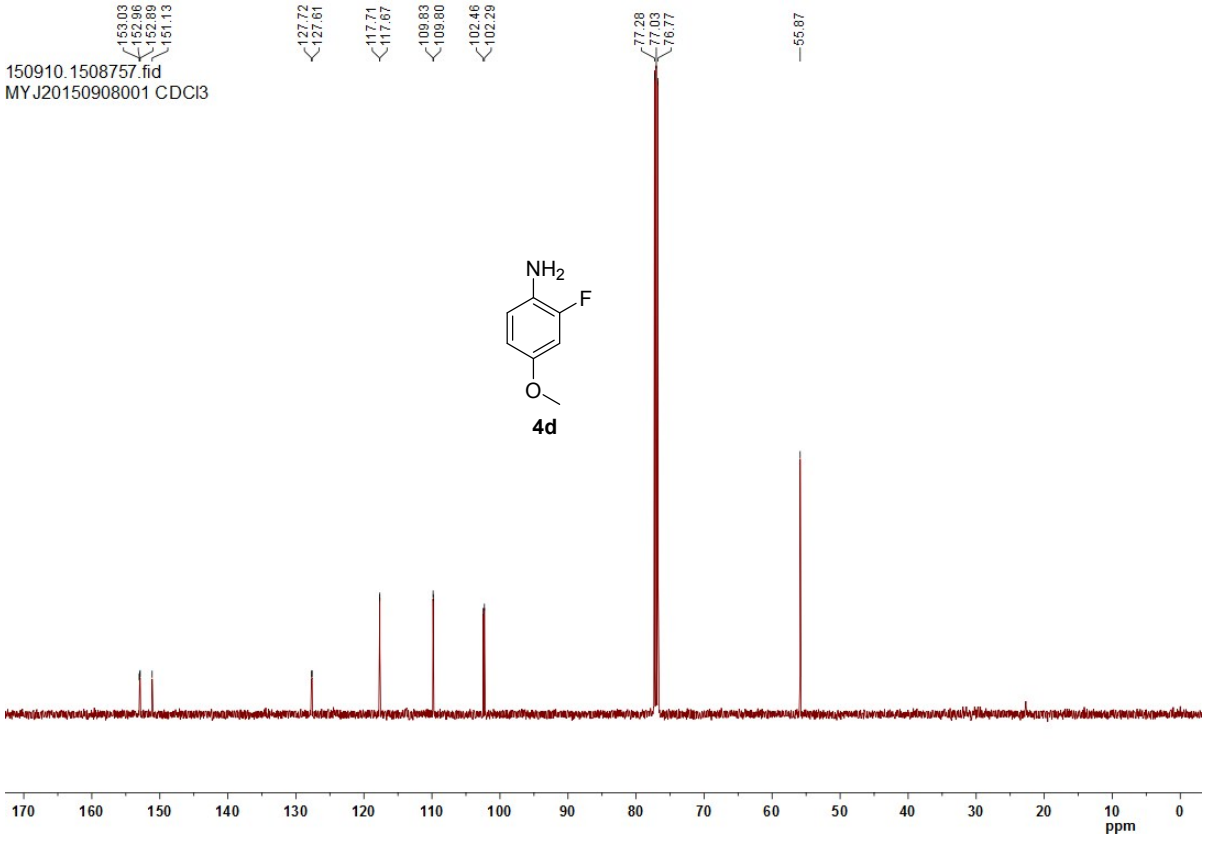
ppm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NH2
F
O
4d
170
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110
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80
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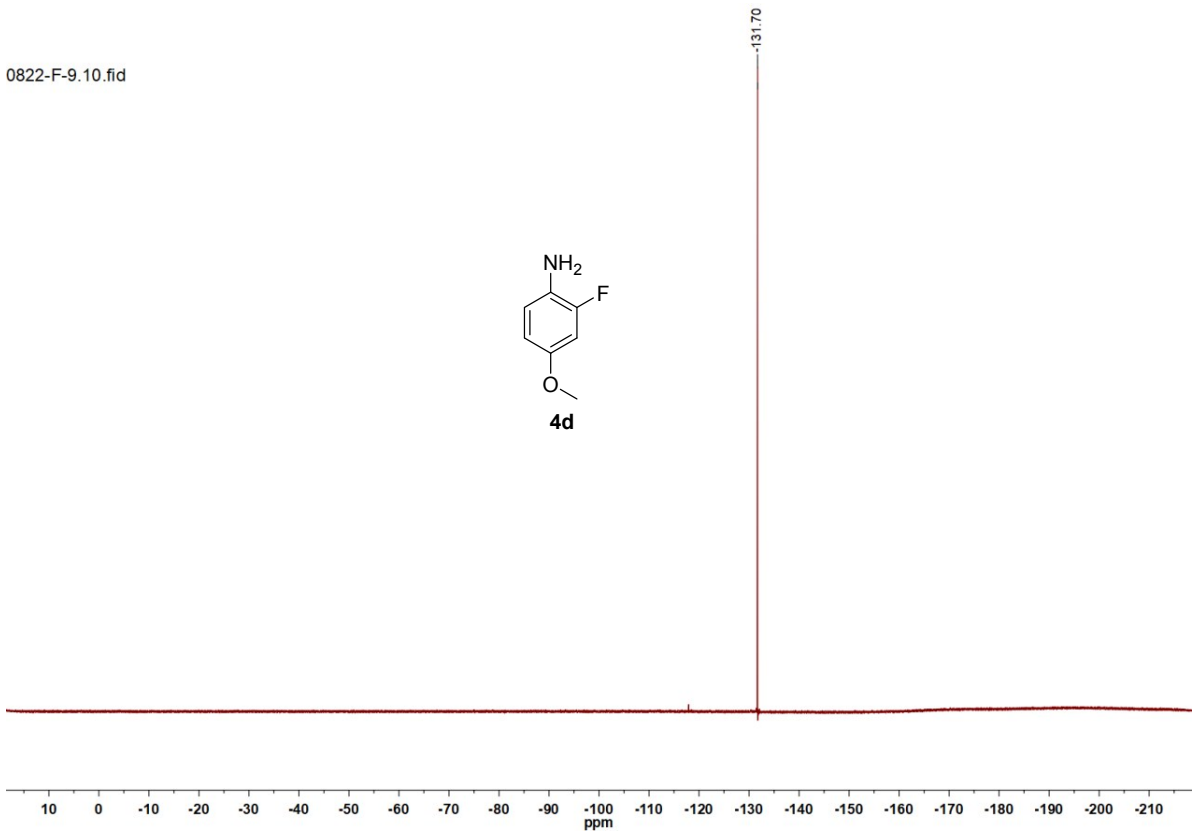
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O
4d
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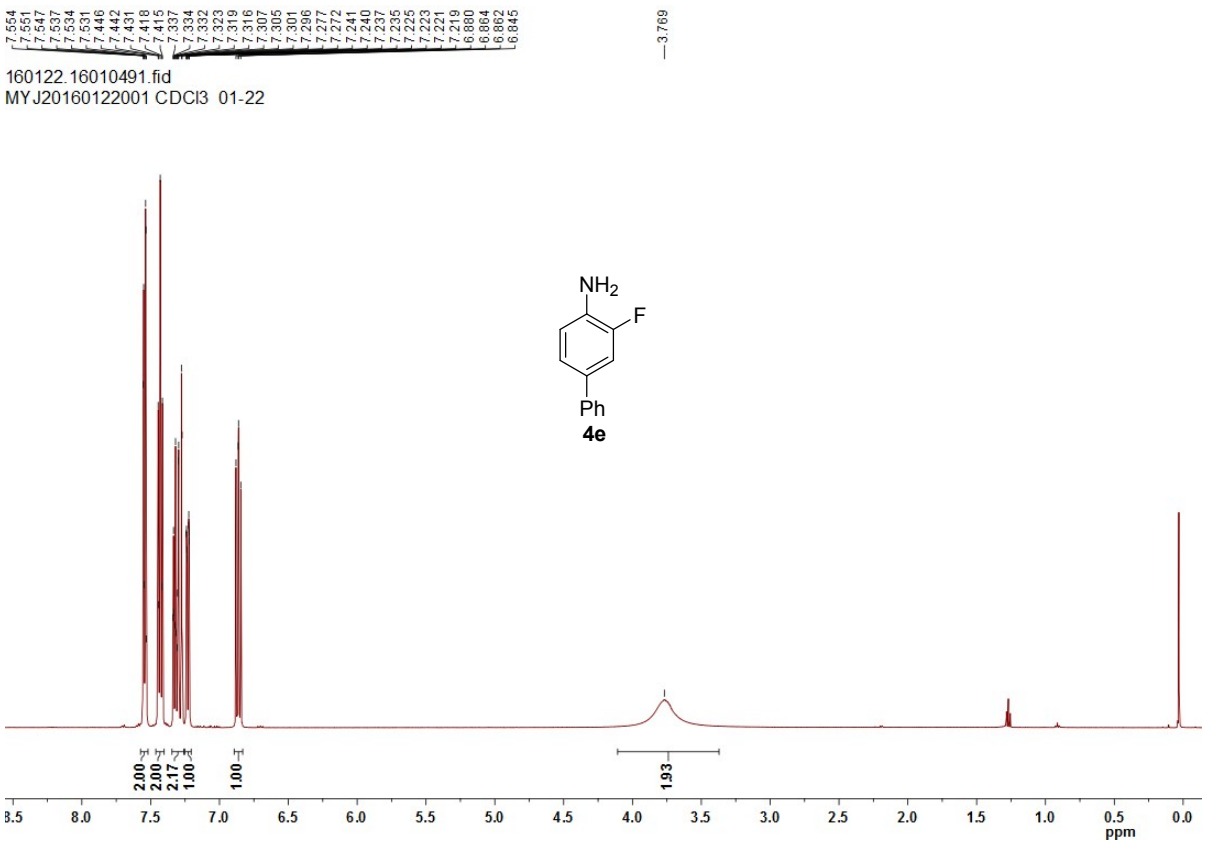
ppm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7.547
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7.531
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7.442
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7.337
7.334
7.332
7.323
7.319
7.316
7.307
7.305
7.301
7.296
7.277
7.272
7.241
7.240
7.237
7.235
7.225
7.223
7.221
7.219
6.880
6.864
6.862
6.845
3.769
160122.16010491.fid
MYJ20160122001 CDCl3 01-22
NH2
F
Ph
4e
2.00
2.00
2.17
1.00
1.00
1.93
8.5
8.0
7.5
7.0
6.5
6.0
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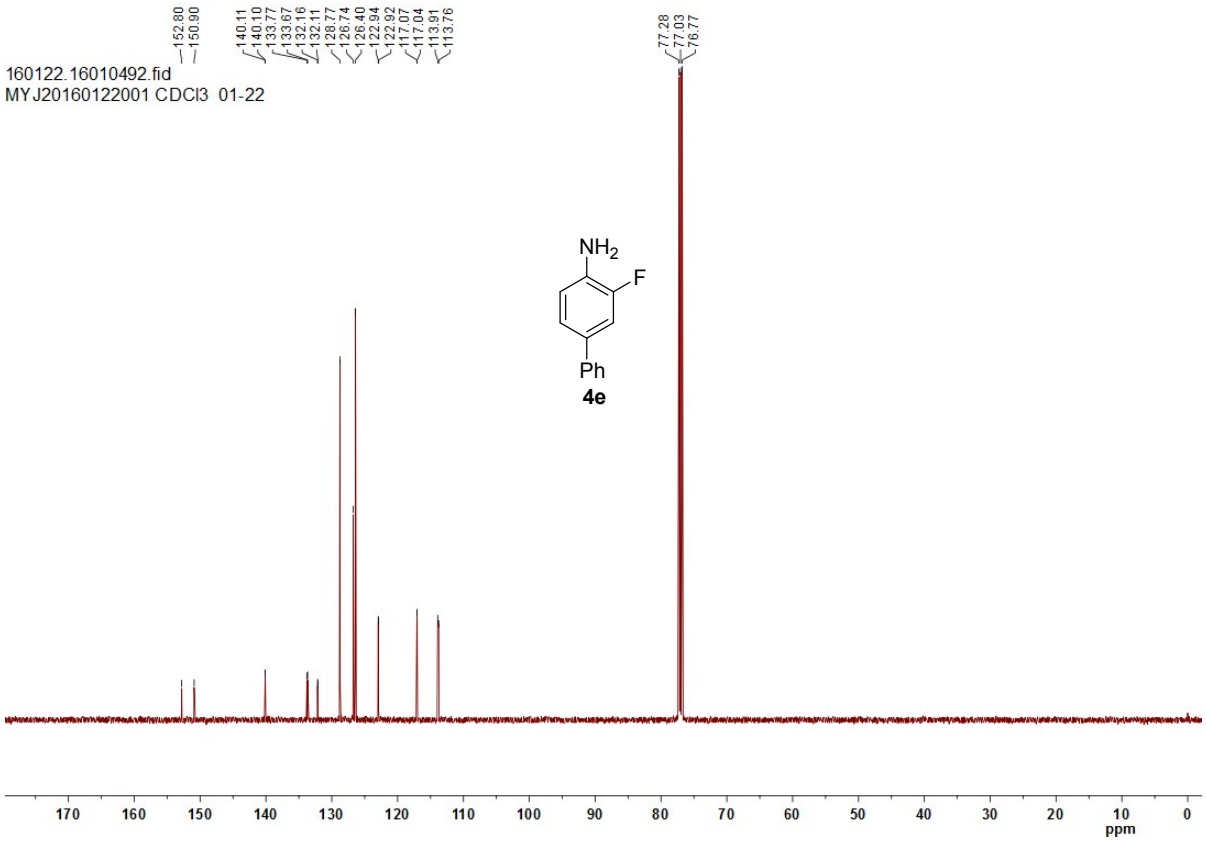
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132.11
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128.74
126.40
122.94
122.92
117.07
117.04
113.91
113.76
77.28
77.03
76.77
160122.16010492.fid
MYJ20160122001 CDCl3 01-22
NH2
F
Ph
4e
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160
150
140
130
120
110
100
90
80
70
60
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20
10
0
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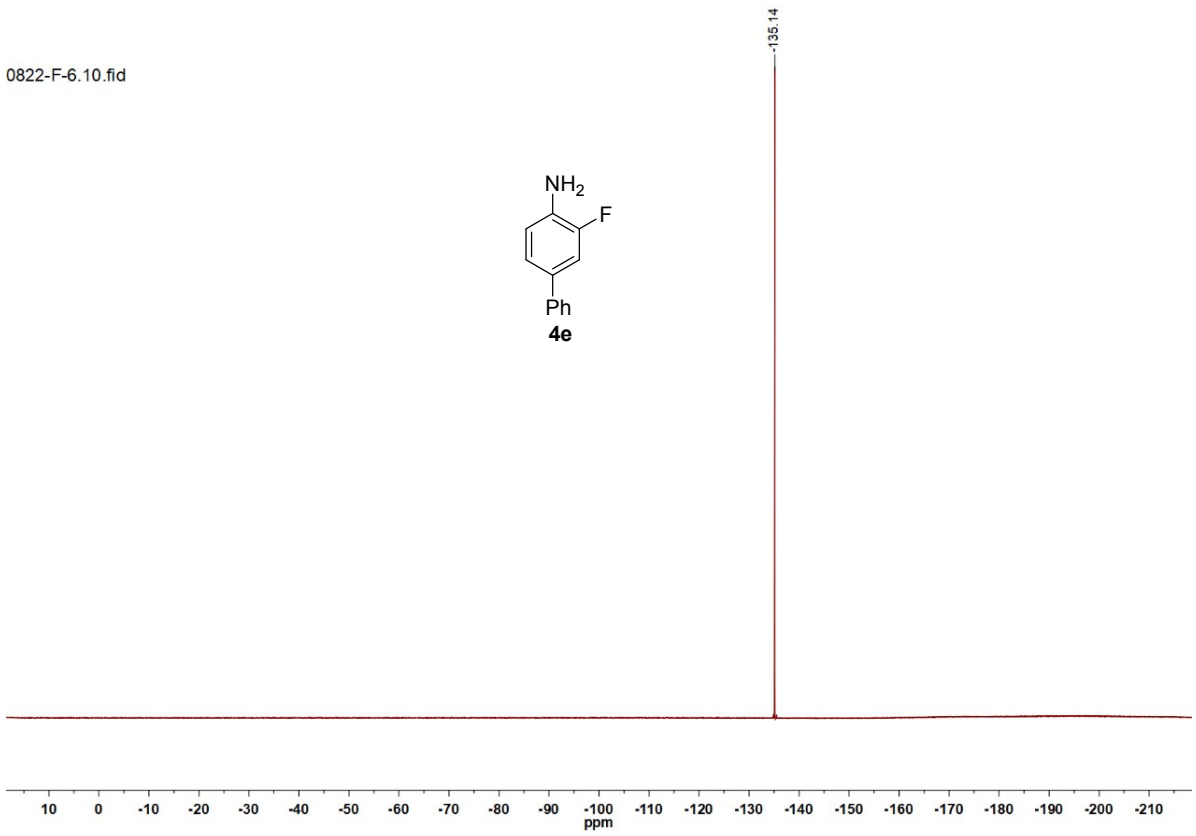
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F
Ph
4e
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-20
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-40
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-60
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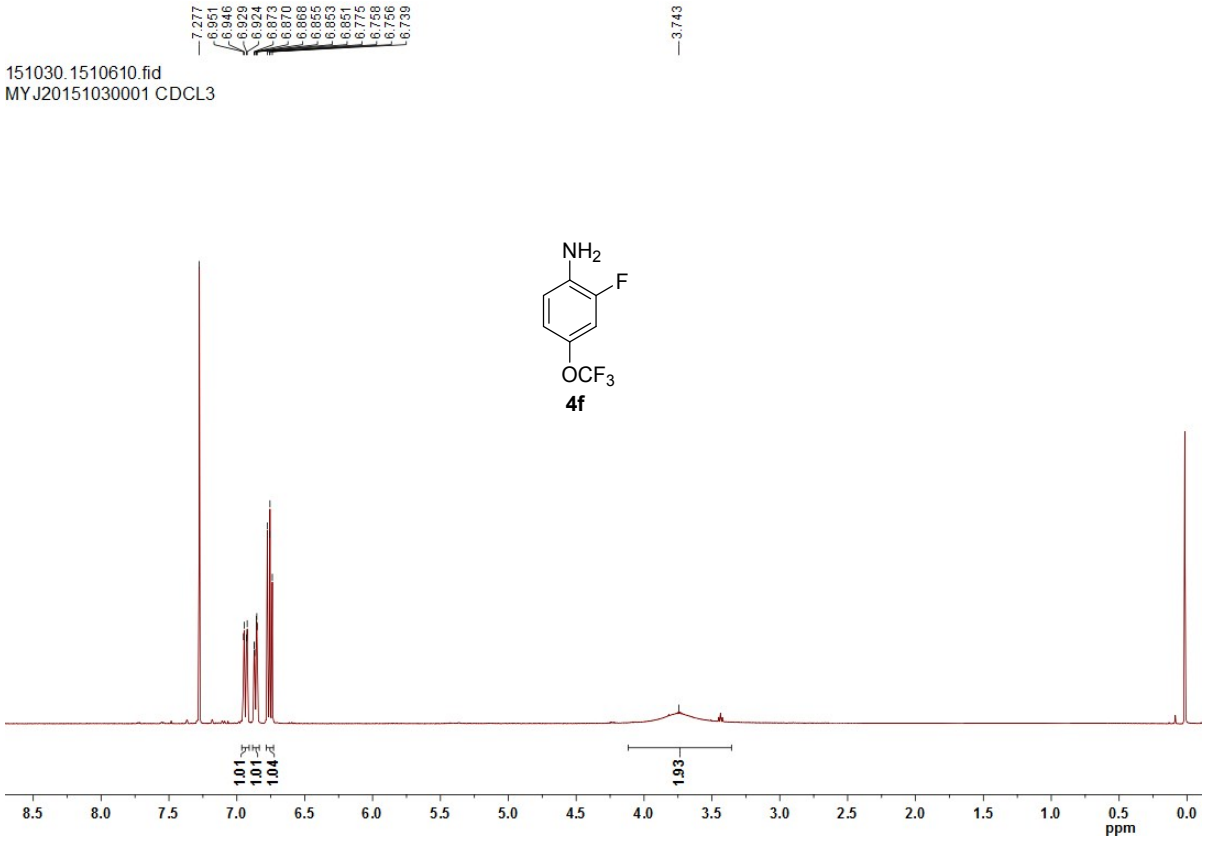
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
ppm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6.946
6.929
6.924
6.873
6.870
6.868
6.855
6.853
6.851
6.775
6.758
6.756
6.739
3.743
151030.1510610.fid
MYJ20151030001 CDCL3
NH2
F
OCF3
4f
1.01
1.01
1.04
1.93
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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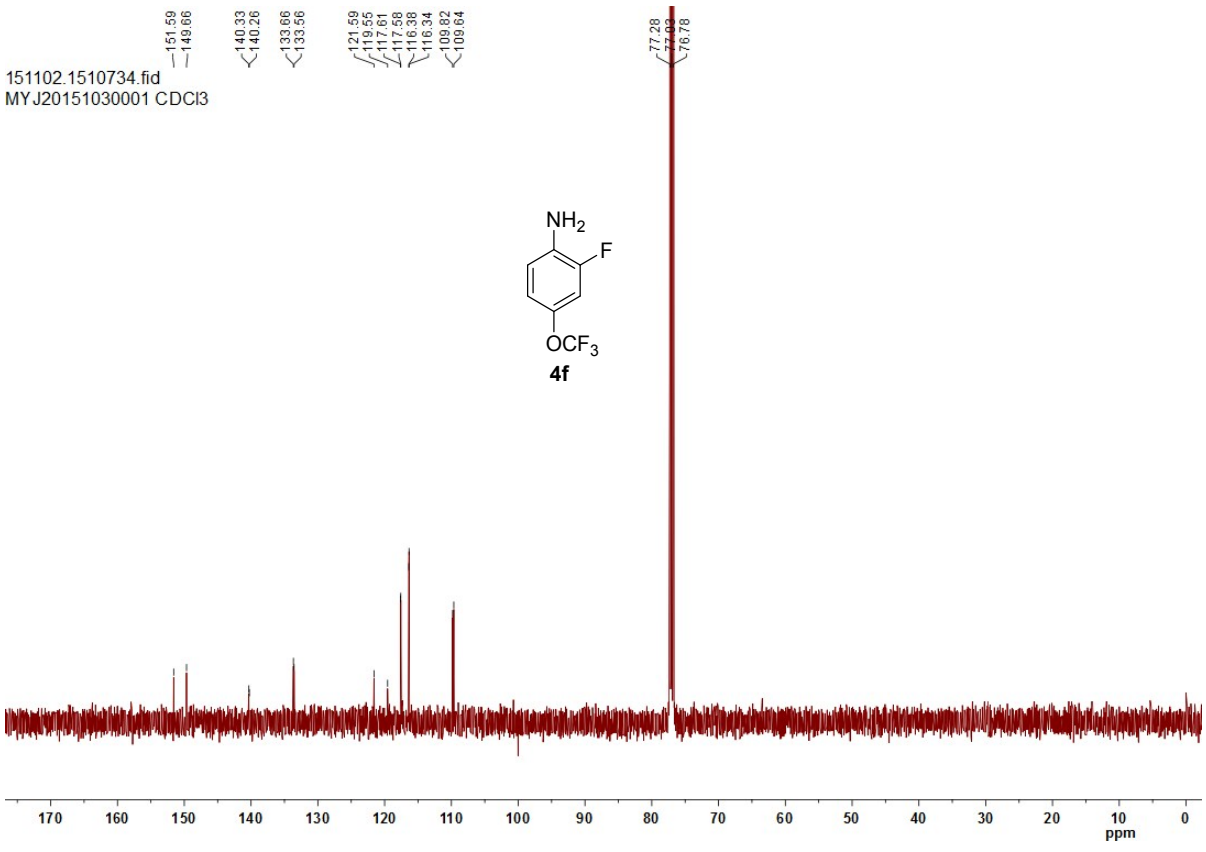
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm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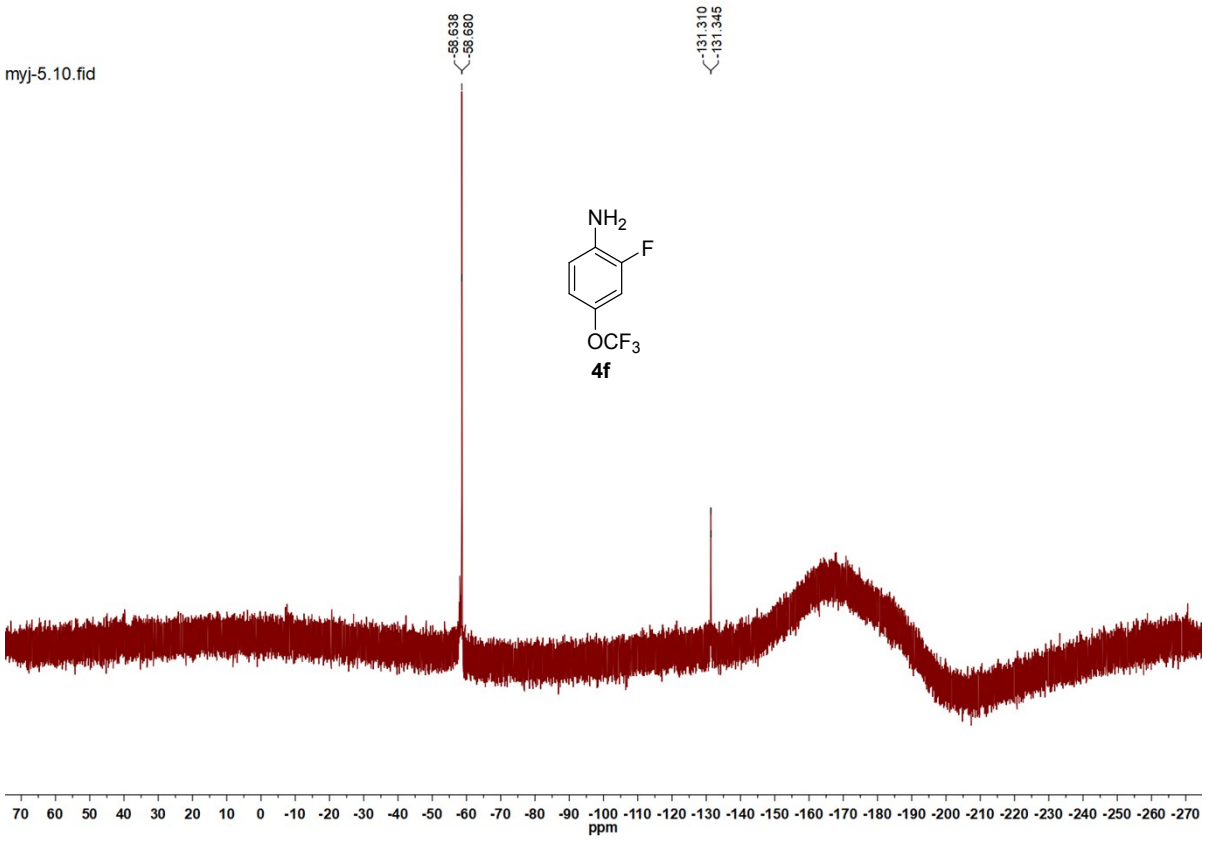
140.26
133.66
133.56
121.59
119.55
117.61
117.58
116.38
116.34
109.82
109.64
77.28
77.03
76.78
151102.1510734.fid
MYJ20151030001 CDCl3
NH2
F
OCF3
4f
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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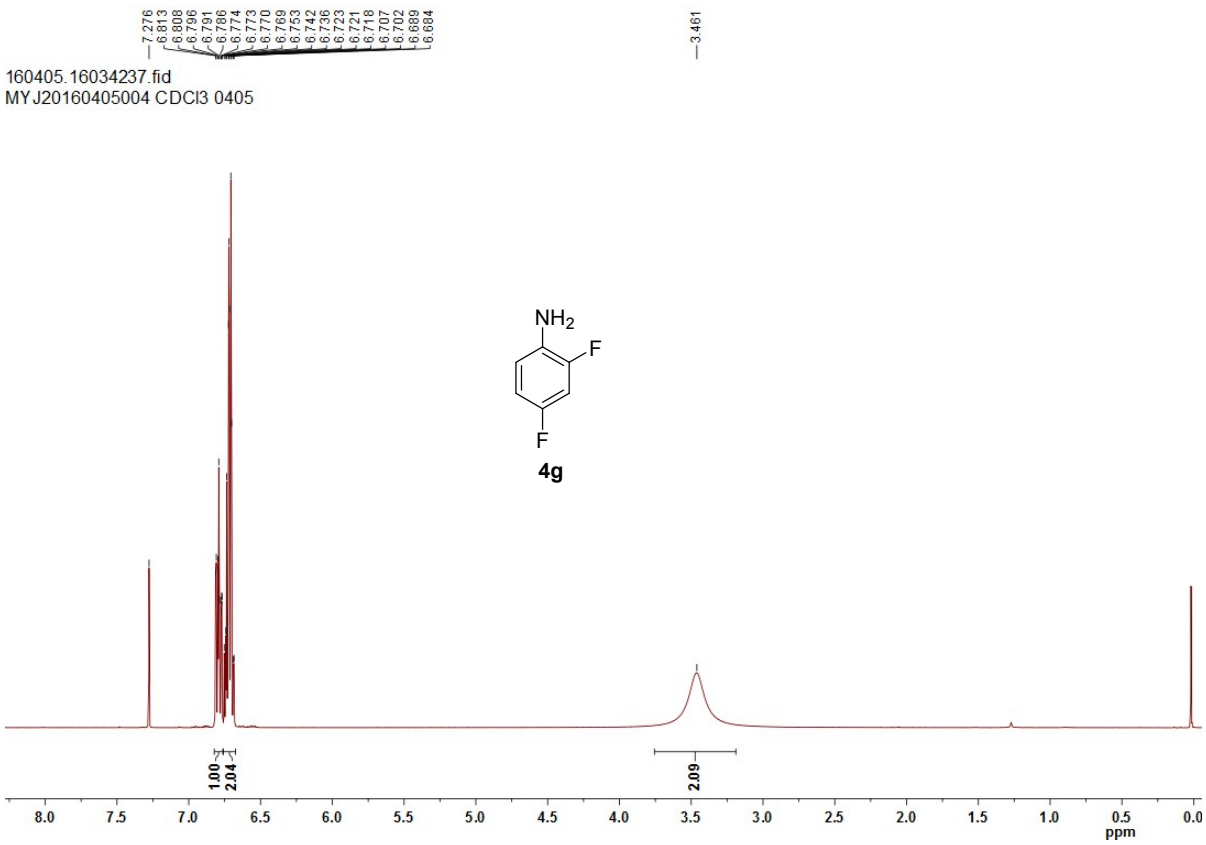
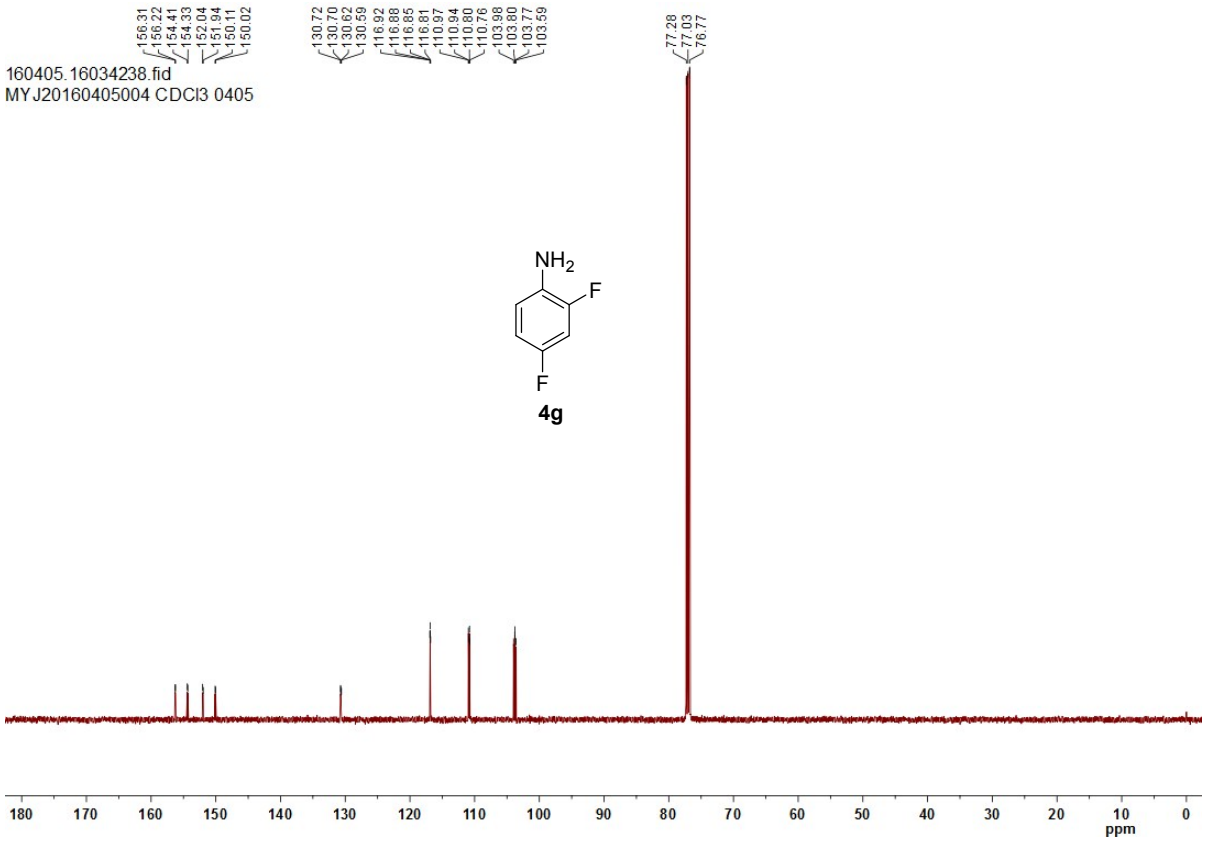
-58.680
-131.310
-131.345
NH2
F
OCF3
4f
70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -250 -260 -270
ppm


7.276
6.813
6.808
6.796
6.791
6.786
6.774
6.773
6.770
6.769
6.753
6.742
6.736
6.723
6.721
6.718
6.707
6.702
6.689
6.684
3.461
160405.16034237.fid
MYJ20160405004 CDCl3 0405
NH2
F
F
4g
1.00
2.04
2.09
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
ppm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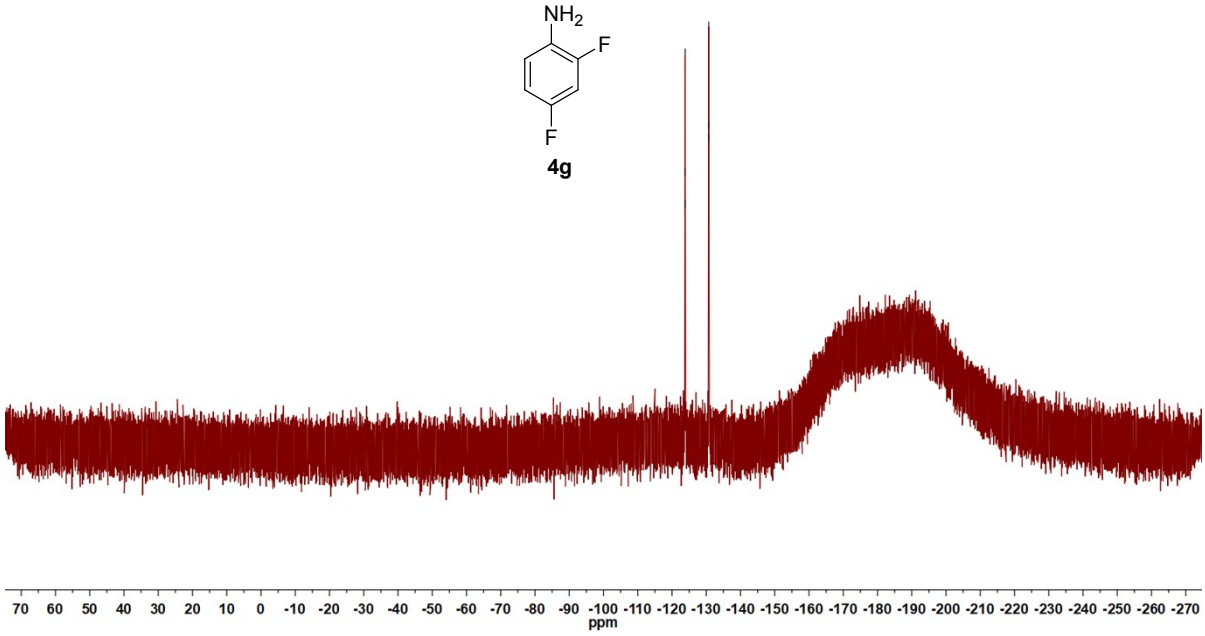
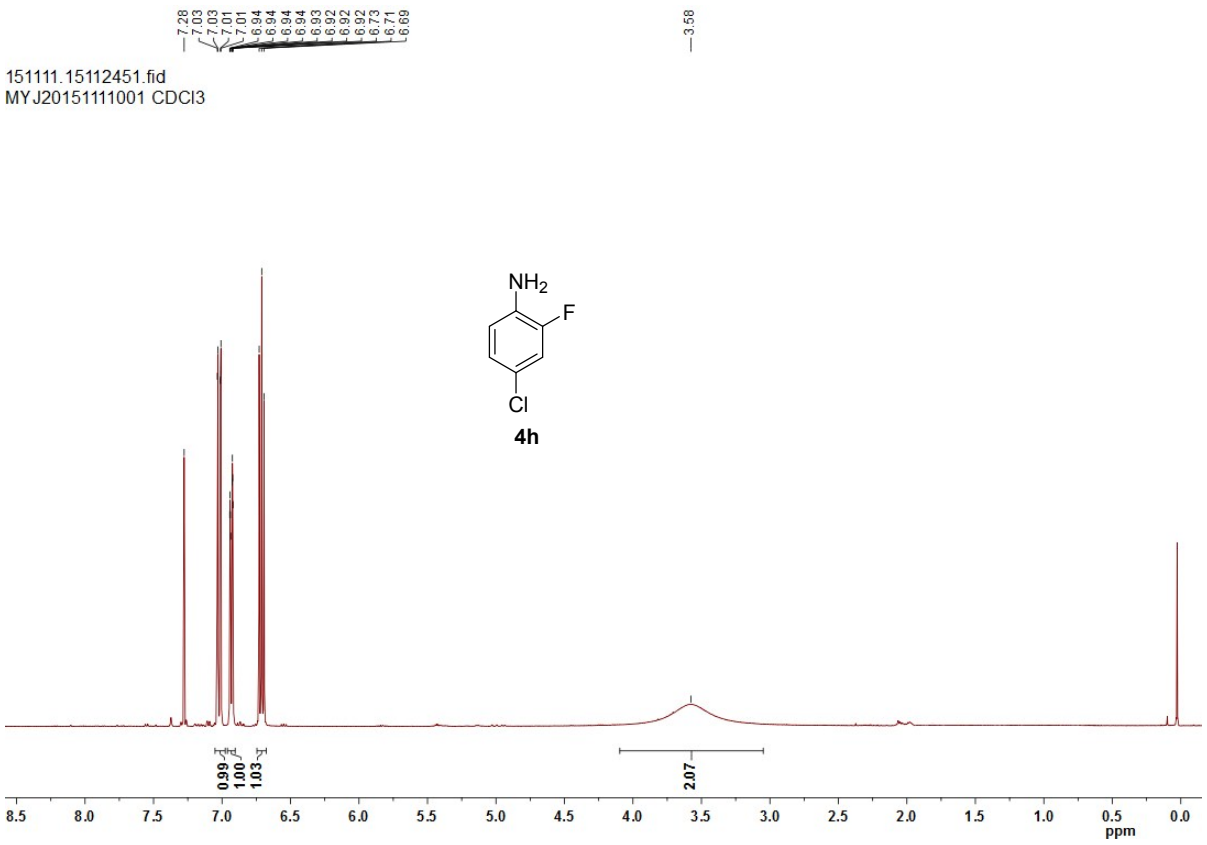
156.22
154.41
154.33
152.04
151.94
150.11
150.02
130.72
130.70
130.62
130.59
116.92
116.88
116.85
116.81
110.97
110.94
110.90
110.76
103.98
103.80
103.77
103.59
77.28
77.03
76.77
160405.16034238.fid
MYJ20160405004 CDCl3 0405
NH2
F
F
4g
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

myj-3.10.fid

123.847
123.869
123.878
130.715
130.722
130.748



4g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7.03
7.03
7.01
7.01
6.94
6.94
6.94
6.94
6.93
6.92
6.92
6.92
6.73
6.71
6.69
3.58
151111.15112451.fid
MYJ20151111001 CDCl3
NH2
F
Cl
4h
0.99
1.00
1.03
2.07
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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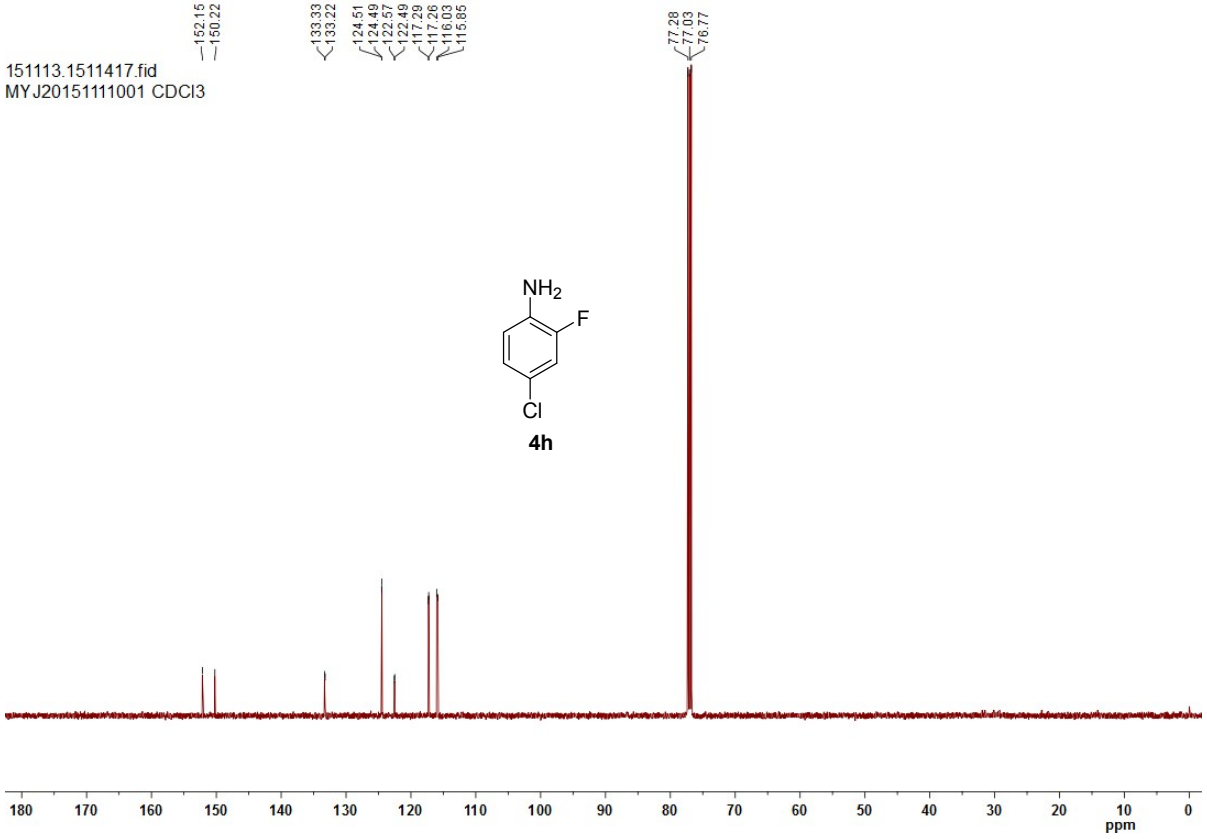
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm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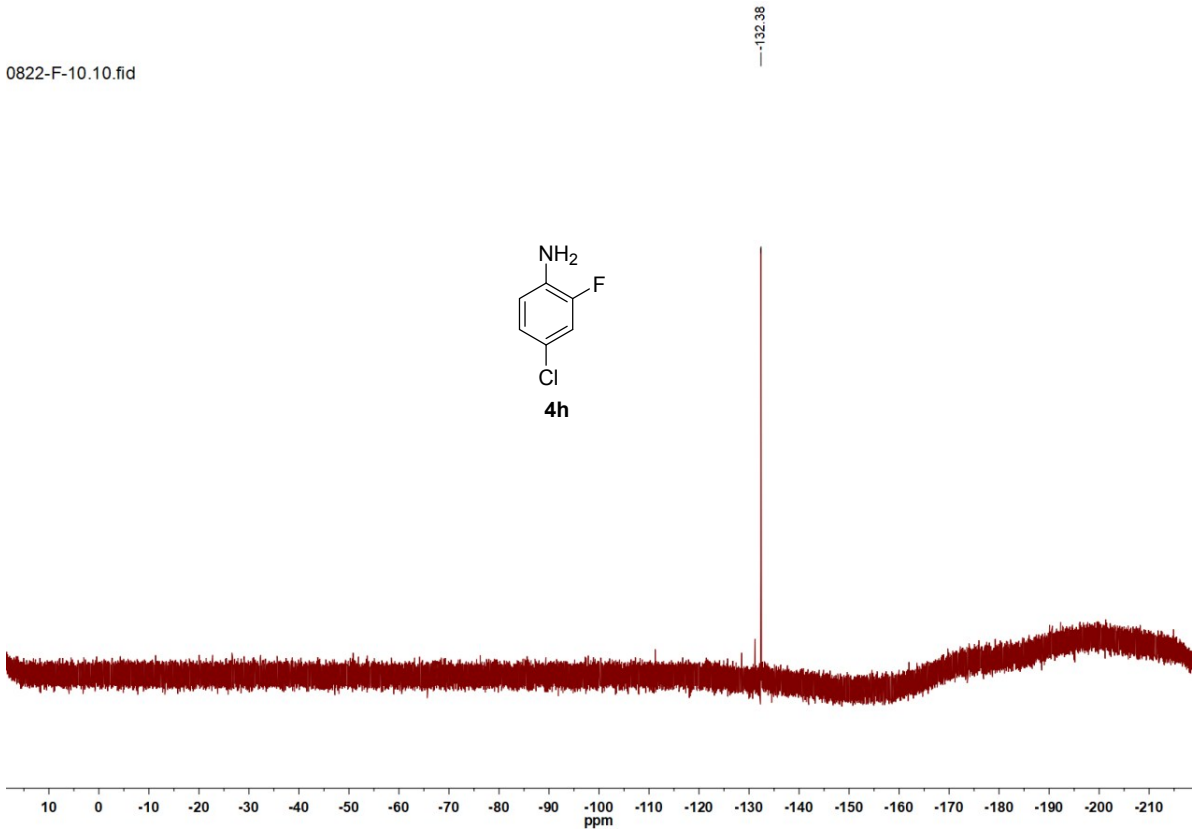
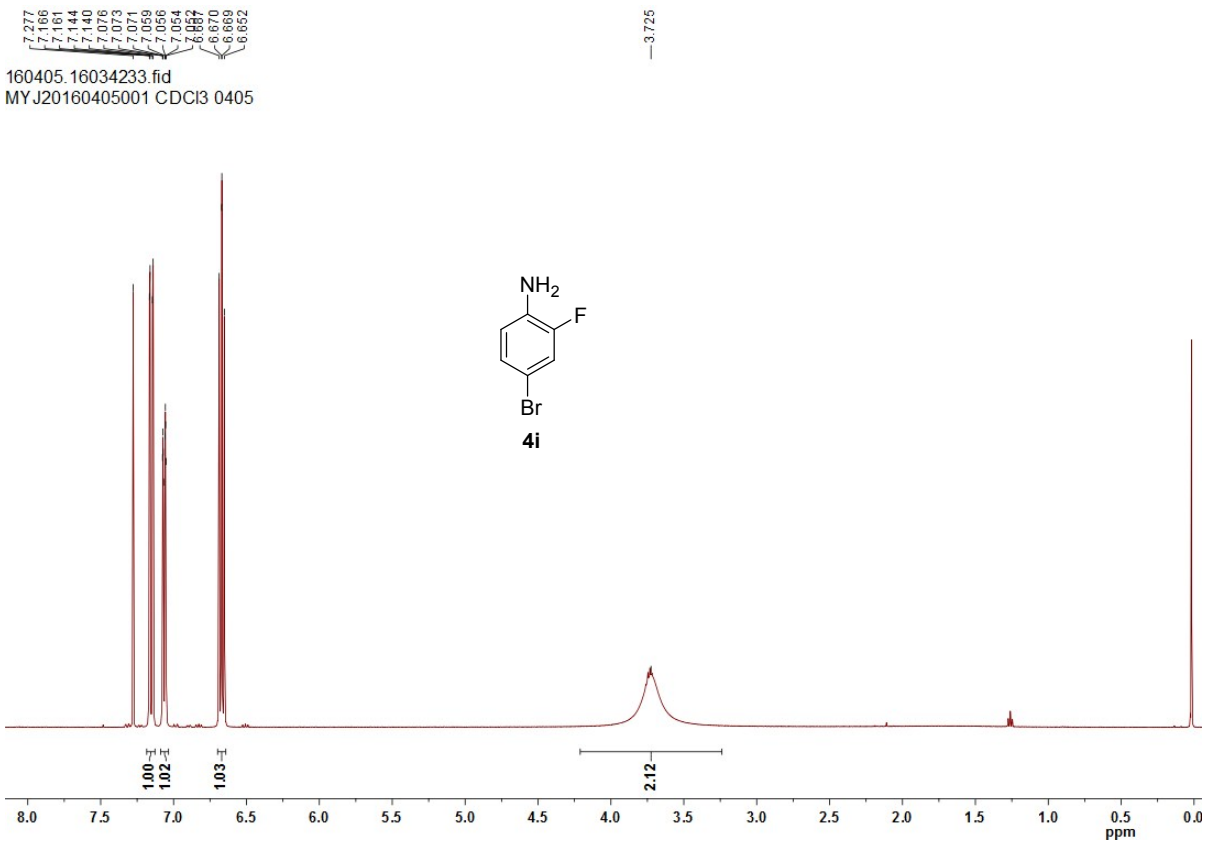
133.33
133.22
124.51
124.49
122.57
122.49
117.29
117.26
116.03
115.85
77.28
77.03
76.77
151113.1511417.fid
MYJ20151111001 CDCl3
NH2
F
Cl
4h
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

0822-F-10.10.fid



4h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7.161
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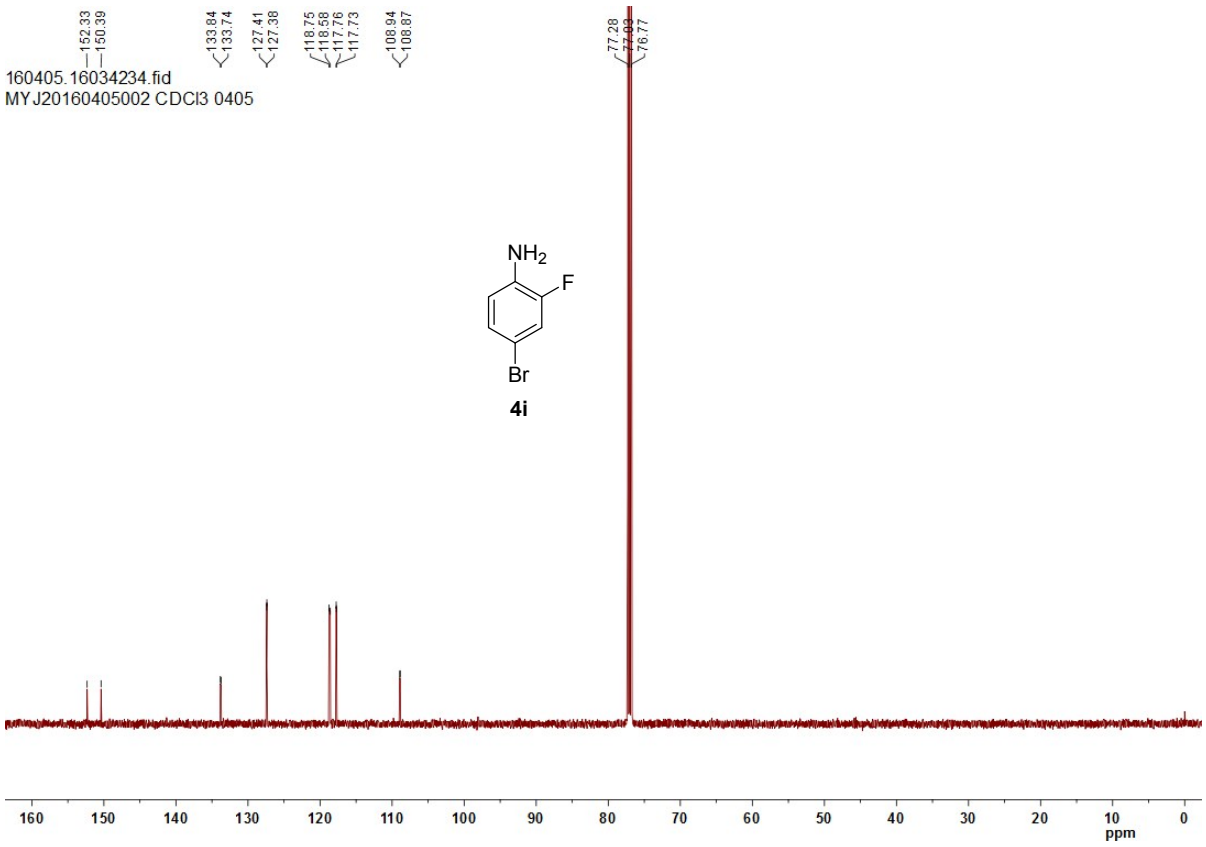
7.076
7.073
7.071
7.059
7.056
7.054
6.670
6.669
6.652
3.725
160405.16034233.fid
MYJ20160405001 CDCl3 0405
NH2
F
Br
4i
1.00
1.02
1.03
2.12
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm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127.41
127.38
118.75
118.58
117.76
117.73
108.94
108.87
77.28
77.03
76.77
160405.16034234.fid
MYJ20160405002 CDCl3 0405
NH2
F
Br
4i
160
150
140
130
120
110
100
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80
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60
50
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20
10
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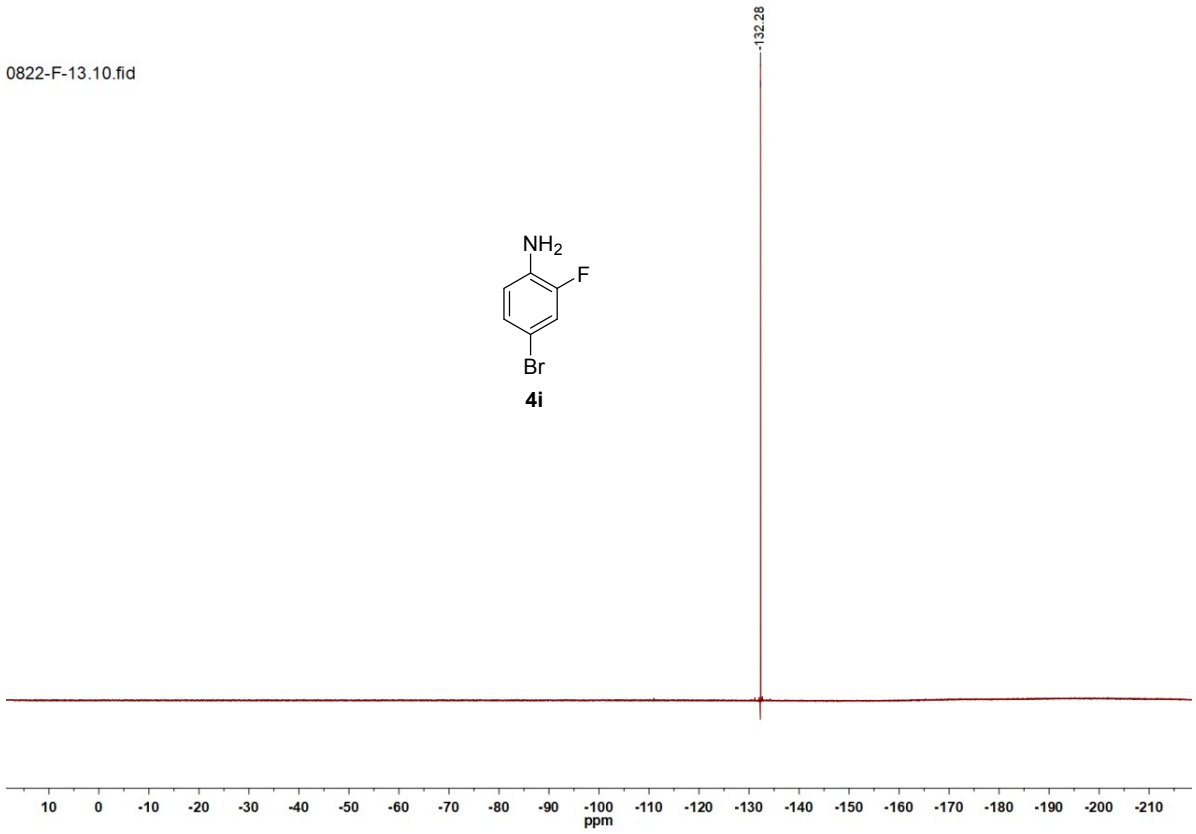
ppm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Br
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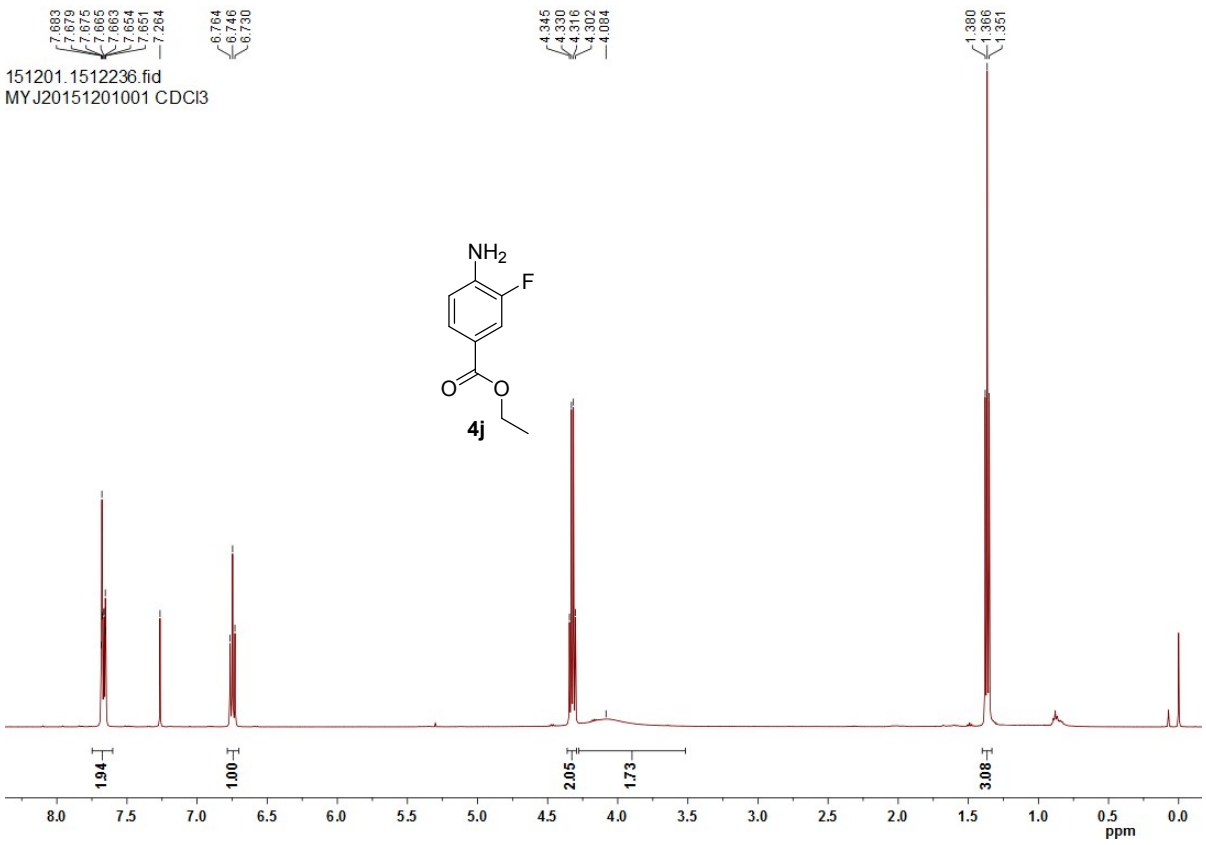
ppm

4i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7.651
7.264
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6.746
6.730
4.345
4.330
4.316
4.302
4.084
1.380
1.366
1.351
151201.1512236.fid
MYJ20151201001 CDCl3
NH2
F
O
O
4j
1.94
1.00
2.05
1.73
3.08
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
3.5
3.0
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2.0
1.5
1.0
0.5
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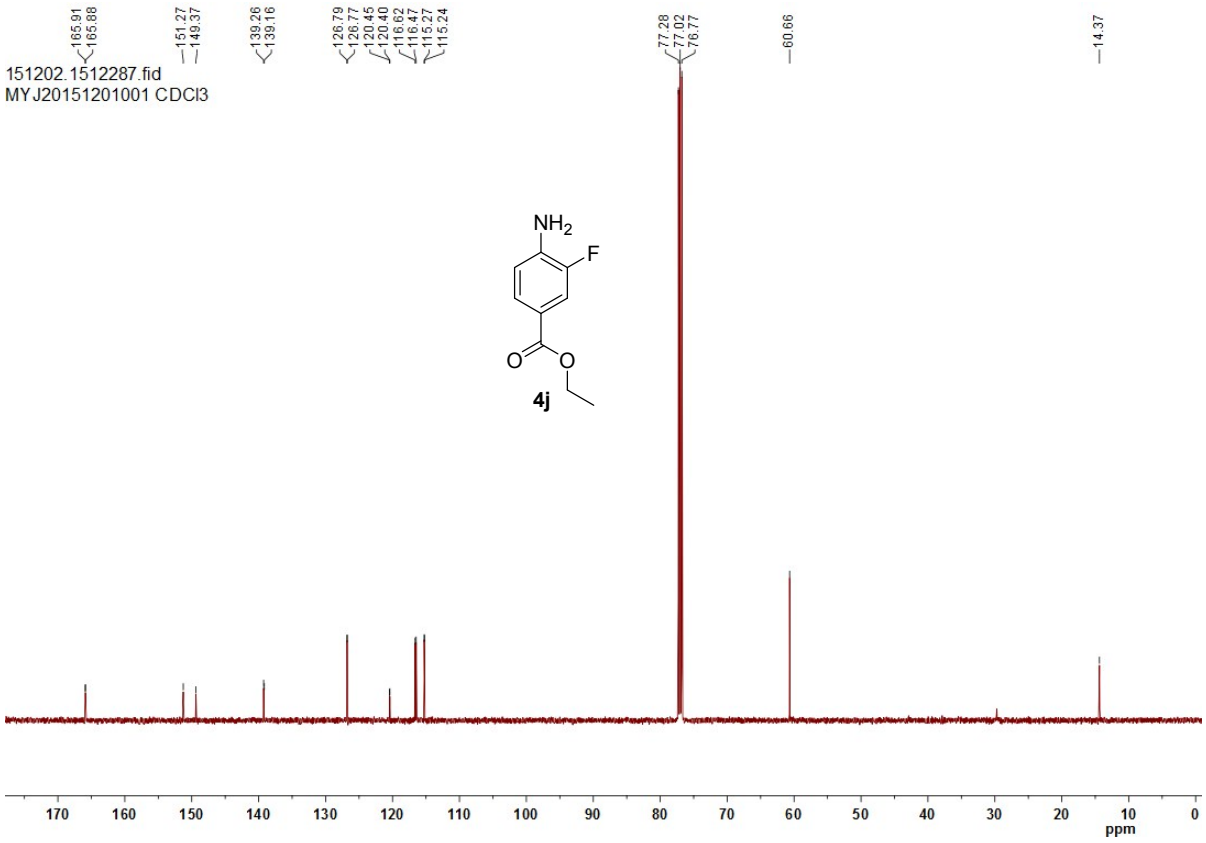
ppm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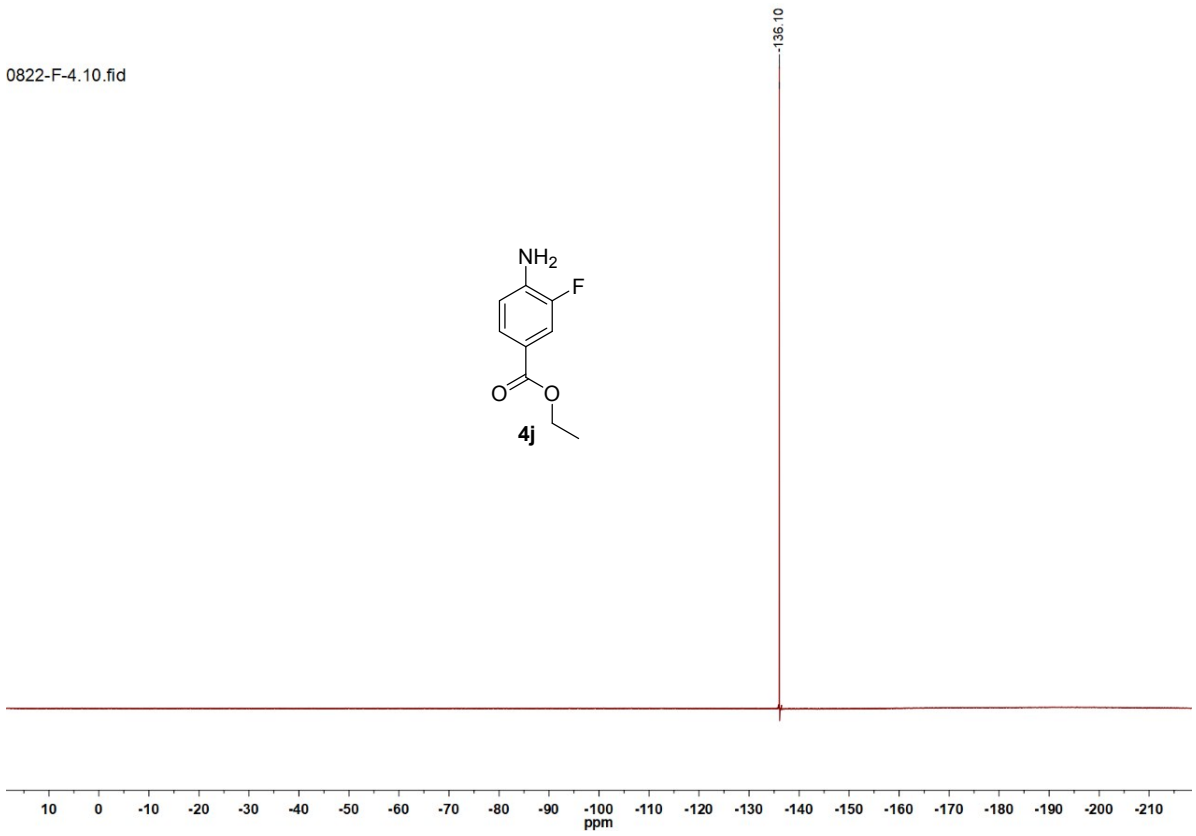
139.26
139.16
126.79
126.77
120.45
120.40
116.62
116.47
115.27
115.24
77.28
77.02
76.77
60.66
14.37
151202.1512287.fid
MYJ20151201001 CDCl3
NH2
F
O
O
4j
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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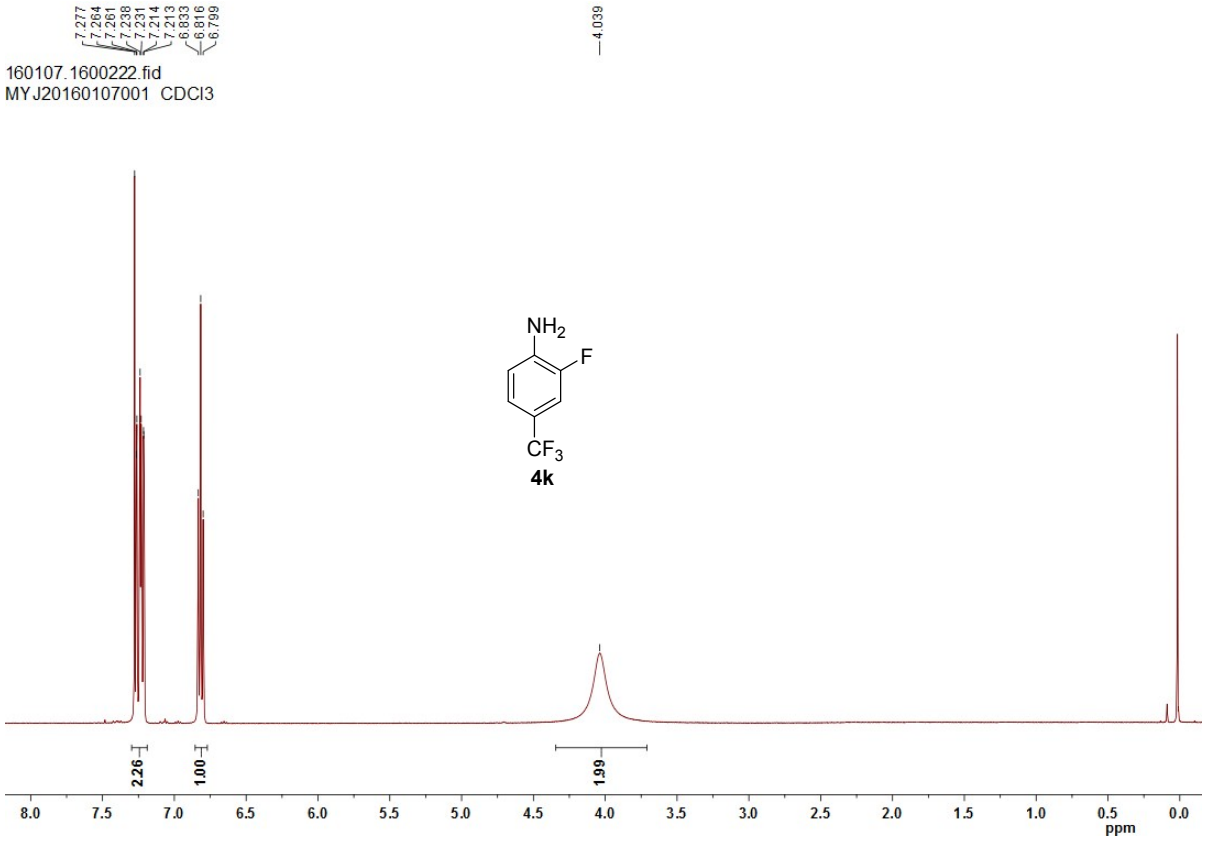
F
O
O
4j
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
ppm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7.231
7.214
7.213
6.833
6.816
6.799
4.039
160107.1600222.fid
MYJ20160107001 CDCl3
NH2
F
CF3
4k
2.26
1.00
1.99
8.0
7.5
7.0
6.5
6.0
5.5
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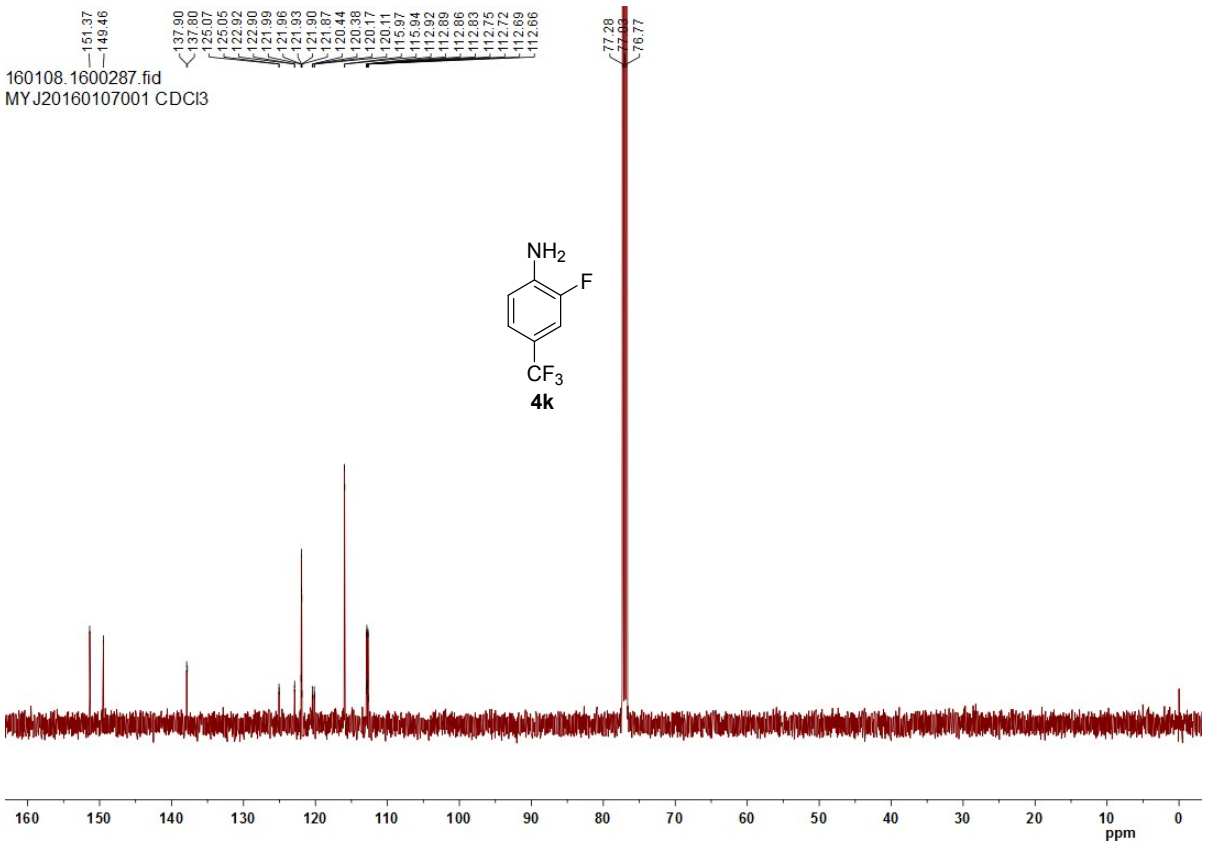
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm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121.96
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120.11
115.97
115.94
112.92
112.89
112.86
112.83
112.75
112.72
112.69
112.66
77.28
77.03
76.77
160108.1600287.fid
MYJ20160107001 CDCl3
NH2
F
CF3
4k
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140
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120
110
100
90
80
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60
50
40
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20
10
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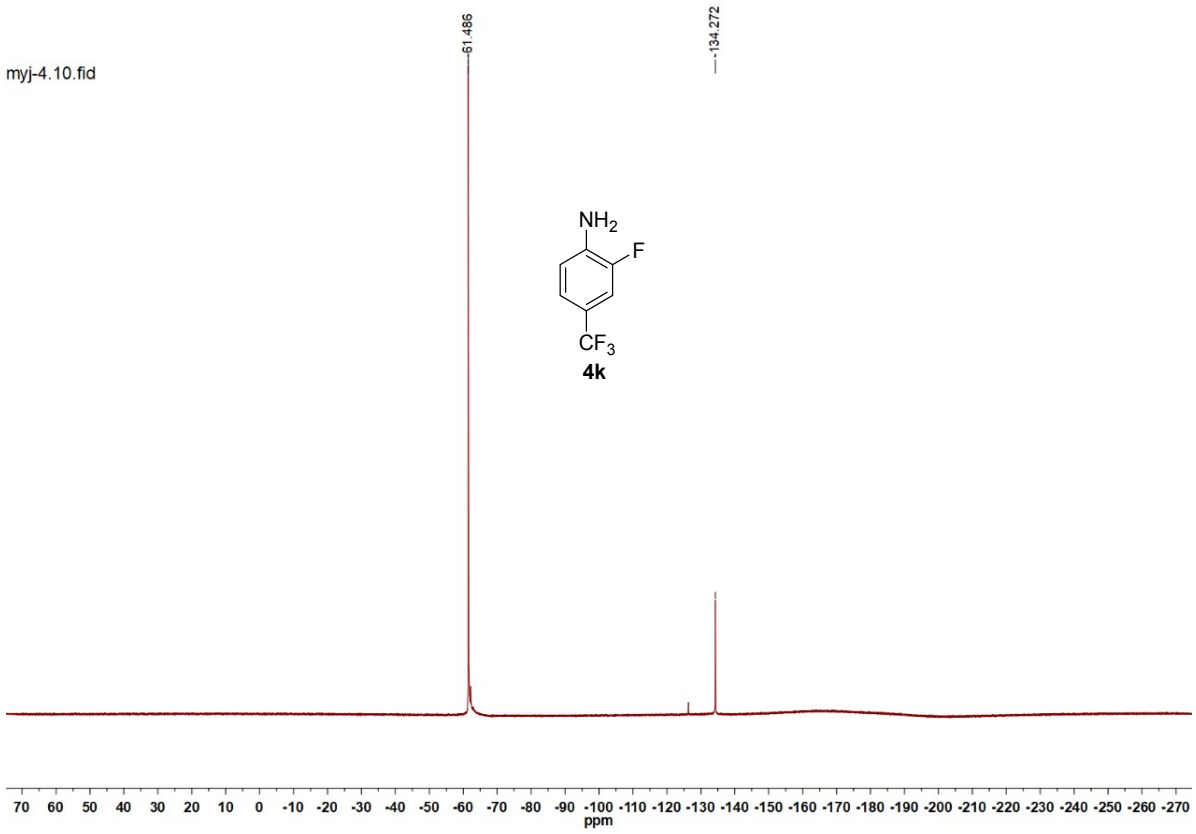
ppm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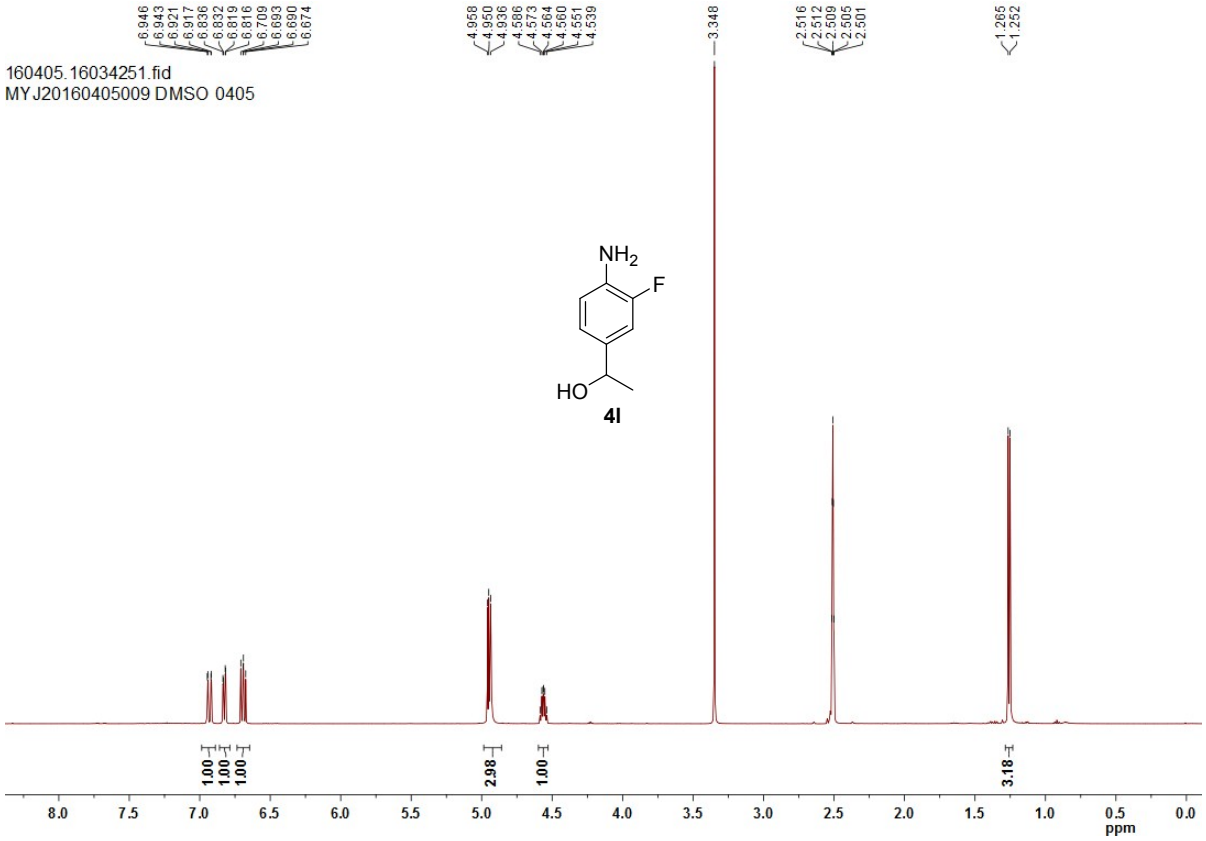
F
CF3
4k
70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -250 -260 -270
ppm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4.573
4.564
4.560
4.551
4.539
3.348
2.516
2.512
2.509
2.505
2.501
1.265
1.252
NH2
F
HO
4l
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1.00
1.00
2.98
1.00
3.18
8.0
7.5
7.0
6.5
6.0
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4.0
3.5
3.0
2.5
2.0
1.5
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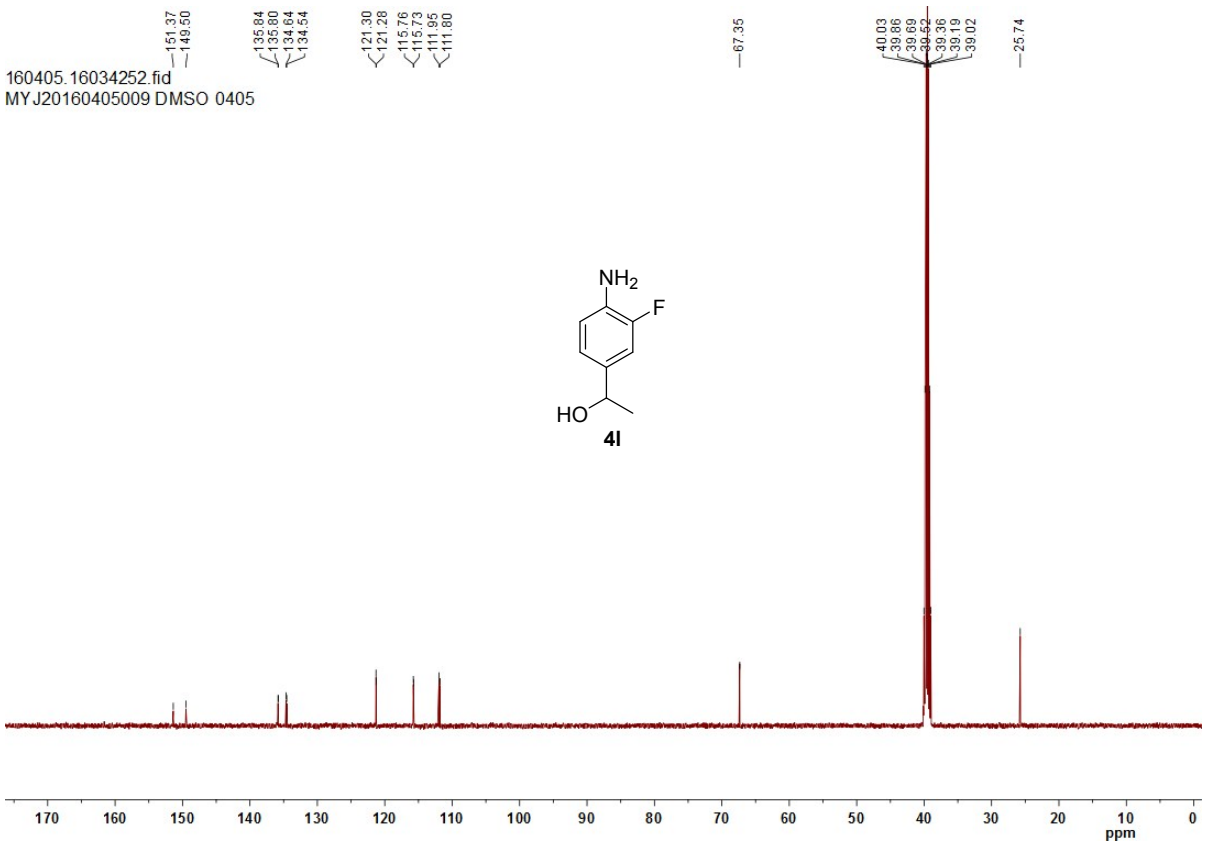
ppm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111.95
111.80
67.35
40.03
39.86
39.69
39.52
39.36
39.19
39.02
25.74
NH2
F
HO
4l
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120
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100
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80
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60
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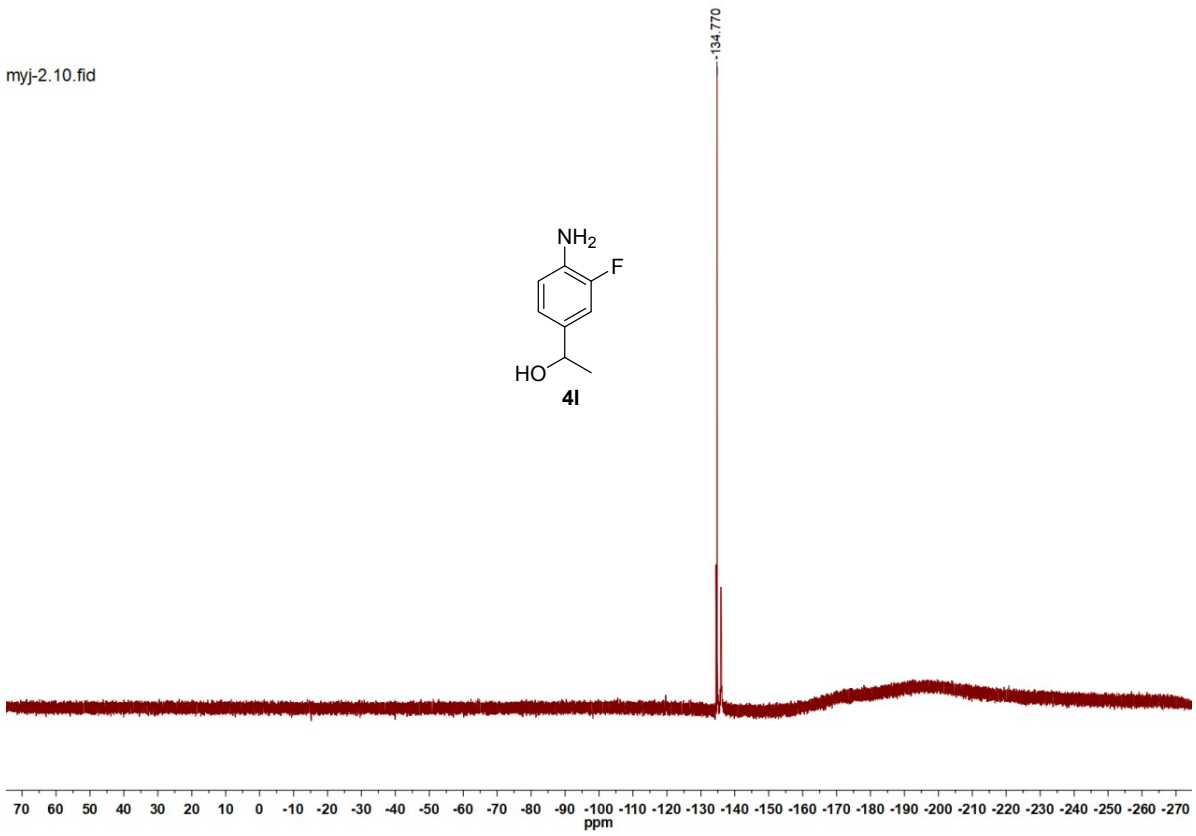
20
10
0
ppm


myj-2.10.fid
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NH2
F
HO
4l
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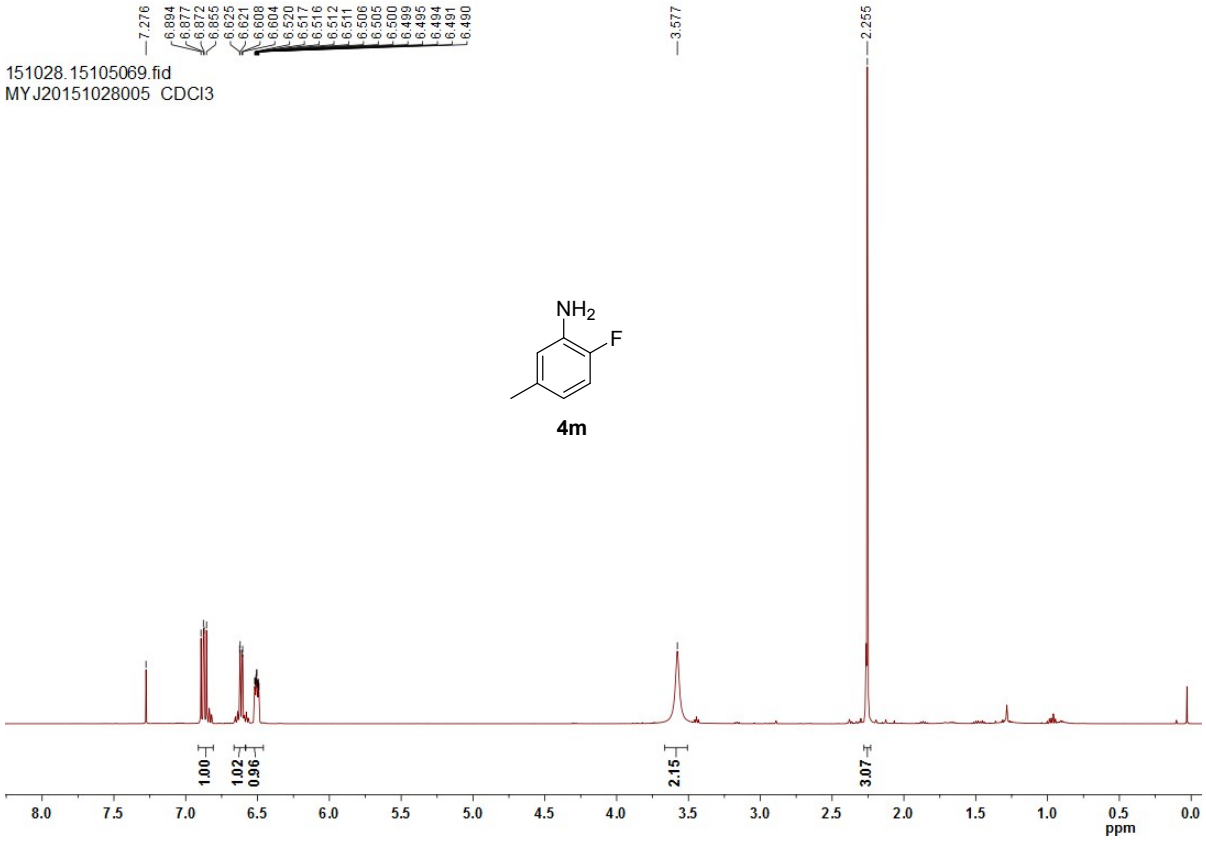
ppm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6.512
6.511
6.506
6.505
6.500
6.499
6.495
6.494
6.491
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3.577
2.255
151028.15105069.fid
MYJ20151028005 CDCl3
NH2
F
4m
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1.02
0.96
2.15
3.07
8.0
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
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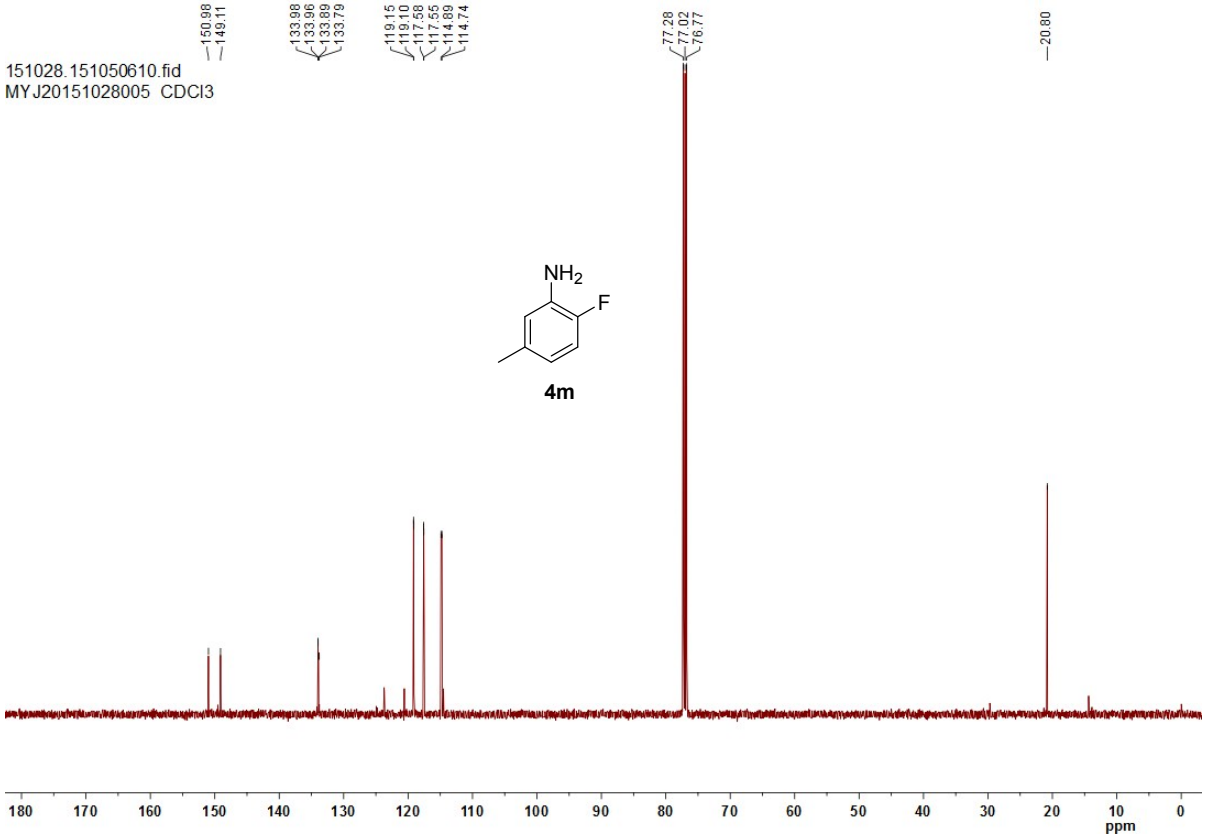
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114.89
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77.28
77.02
76.77
20.80
151028.151050610.fid
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NH2
F
4m
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80
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60
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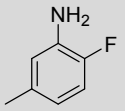

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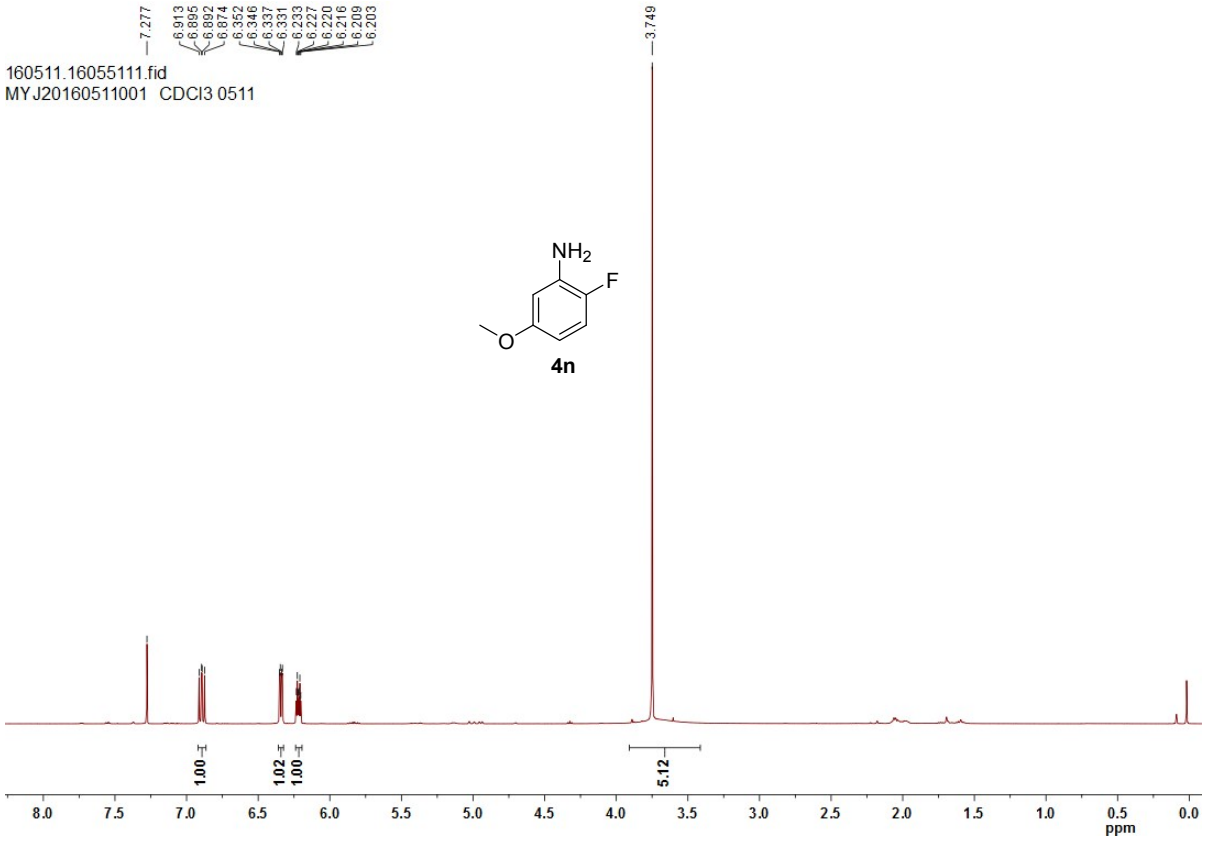
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6.337
6.331
6.233
6.227
6.220
6.216
6.209
6.203
3.749
160511.16055111.fid
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NH2
F
O
4n
1.00
1.02
1.00
5.12
8.0
7.5
7.0
6.5
6.0
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4.0
3.5
3.0
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1.5
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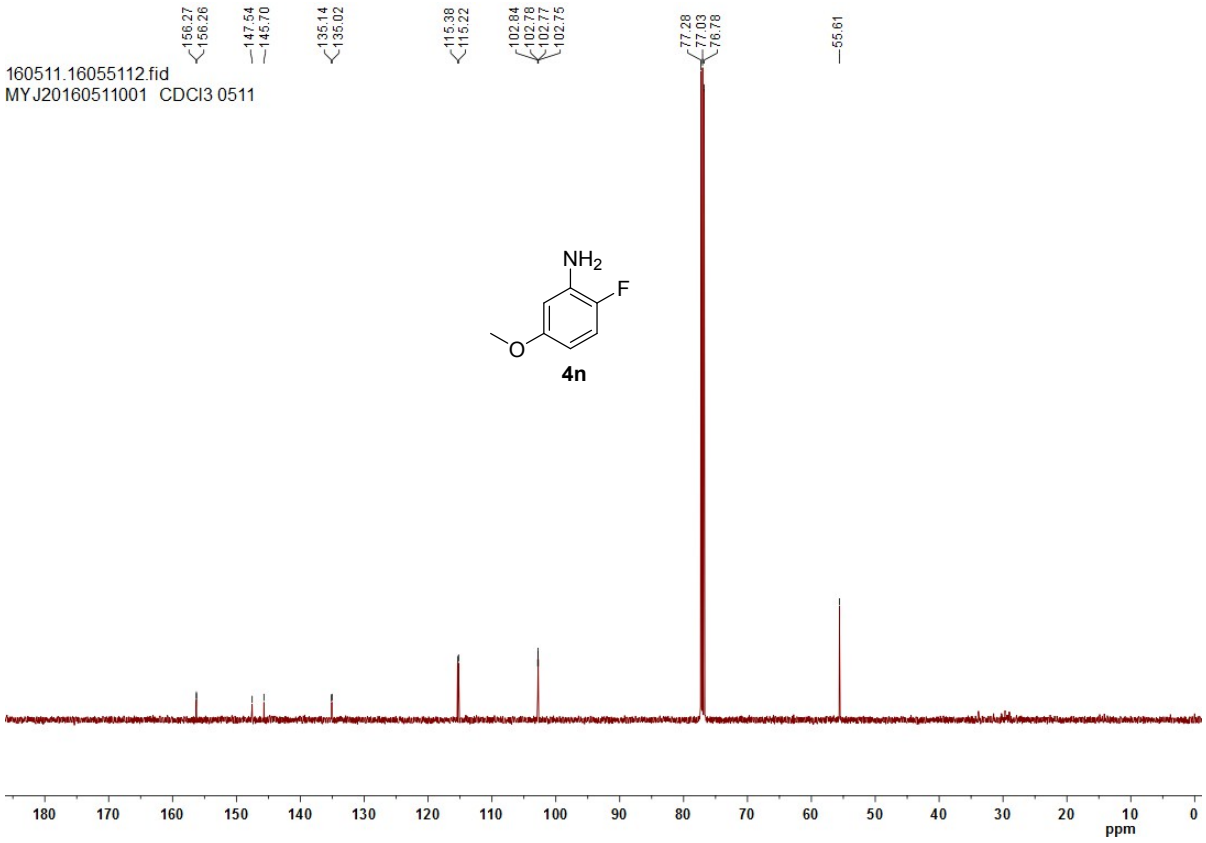
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115.22
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102.78
102.77
102.75
77.28
77.03
76.78
55.61
160511.16055112.fid
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NH2
F
O
4n
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170
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20
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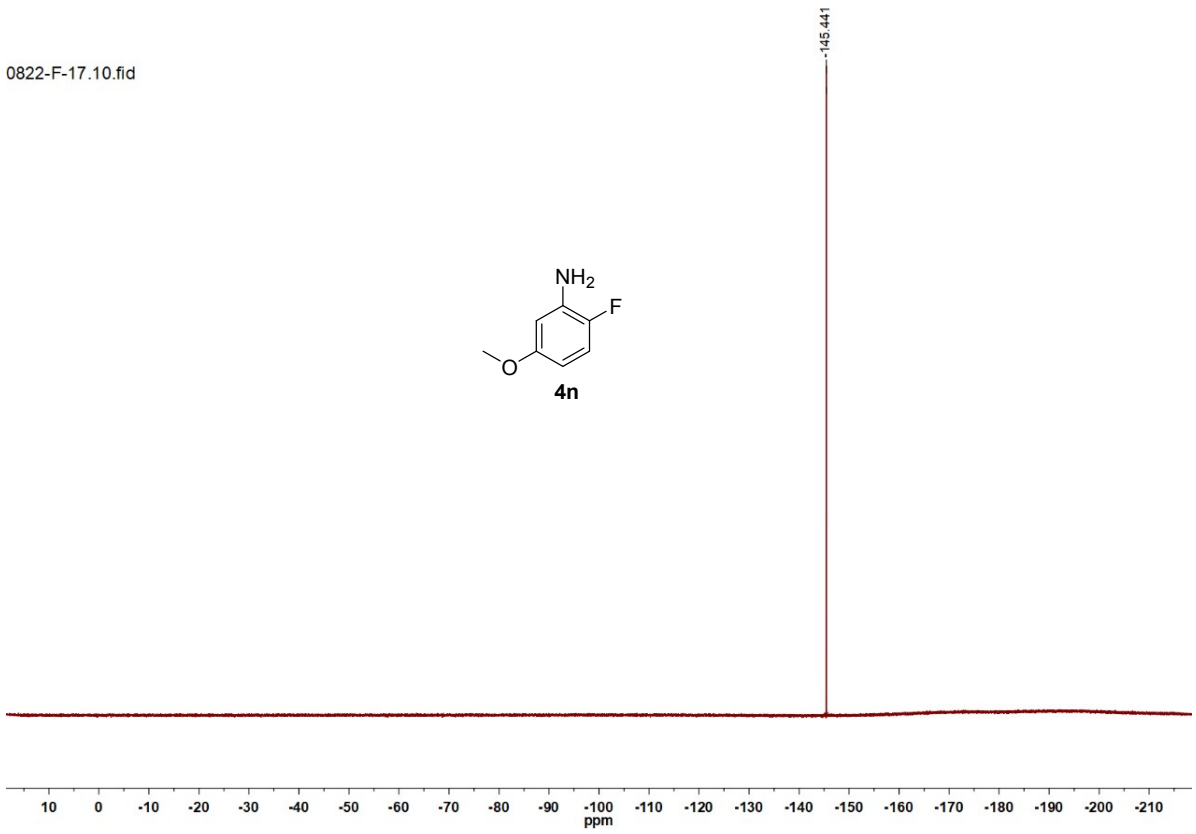
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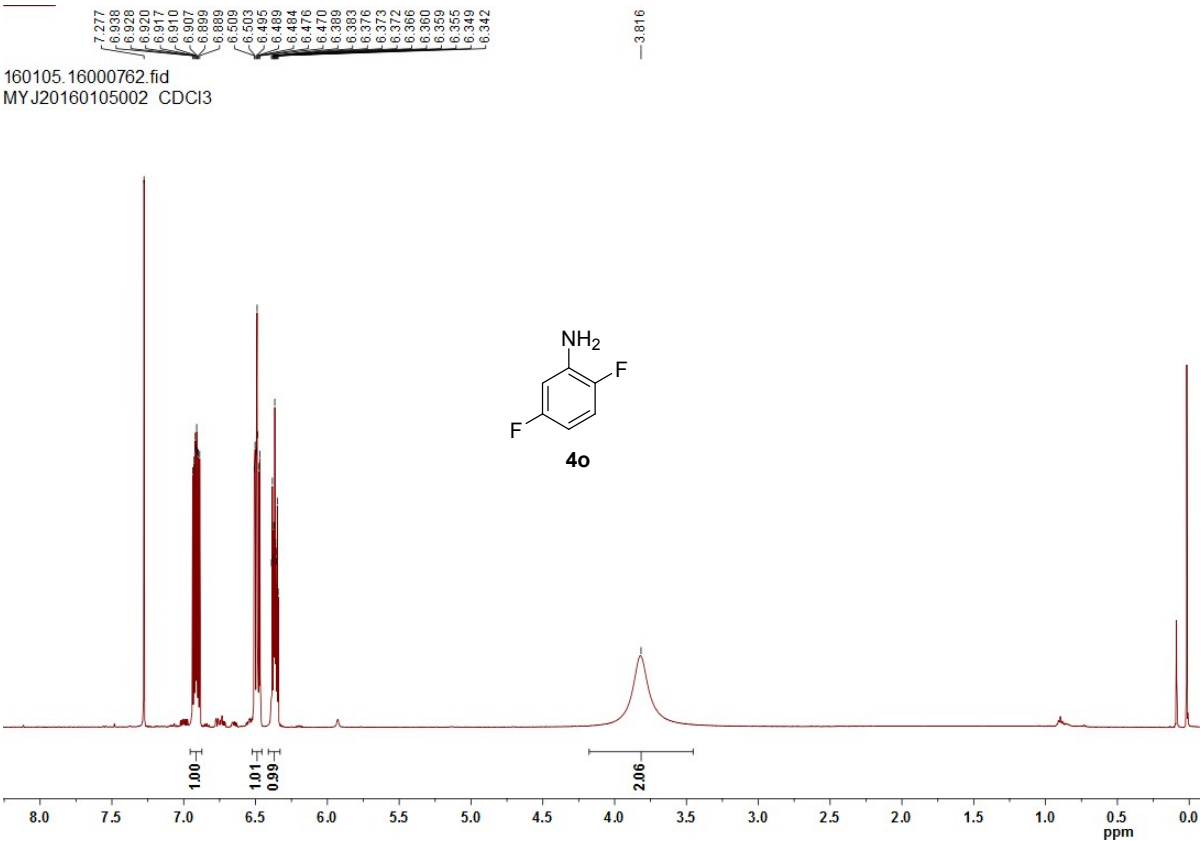
ppm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6.484
6.476
6.470
6.389
6.383
6.376
6.373
6.372
6.366
6.360
6.359
6.355
6.349
6.342
3.816
160105.16000762.fid
MYJ20160105002 CDCl3
NH2
F
F
4o
1.00
1.01
0.99
2.06
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
3.5
3.0
2.5
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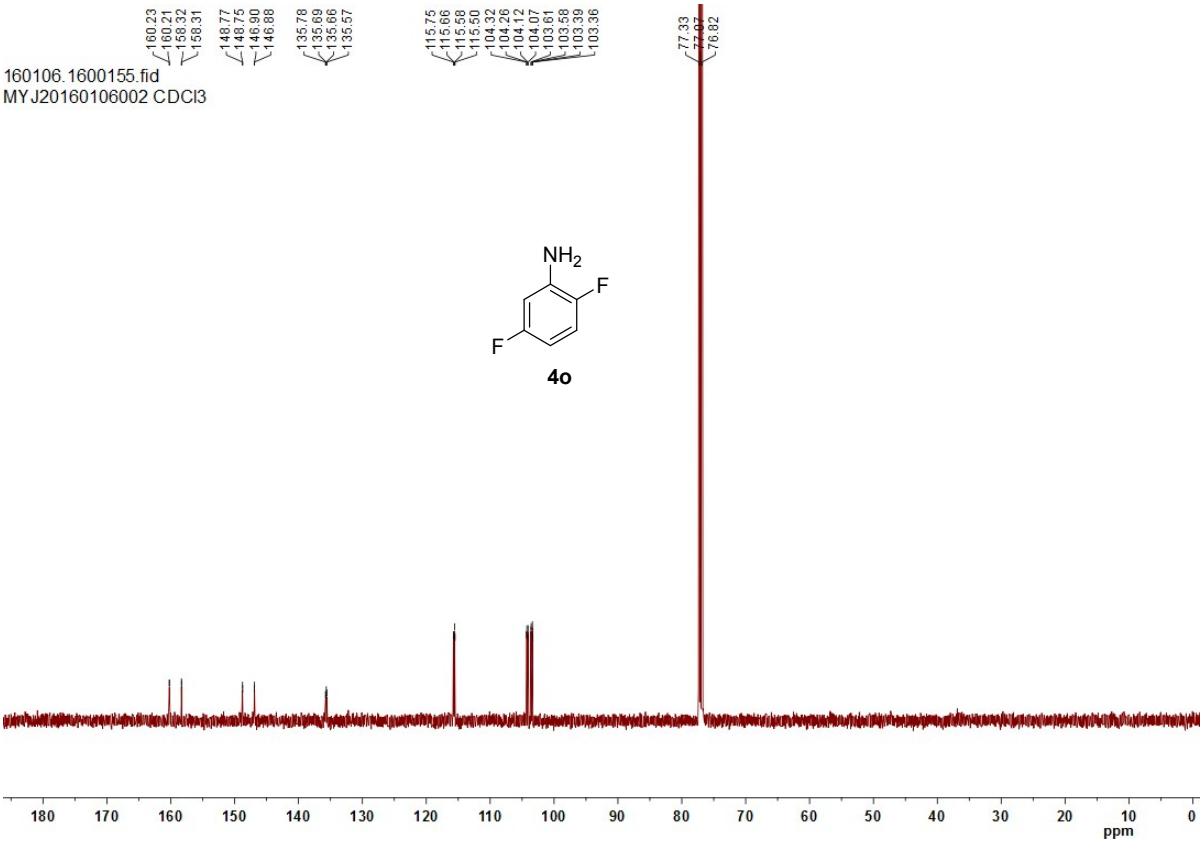
1.5
1.0
0.5
0.0
ppm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146.88
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135.69
135.66
135.57
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115.58
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104.26
104.12
104.07
103.61
103.58
103.39
103.36
77.33
77.07
76.82
160106.1600155.fid
MYJ20160106002 CDCl3
NH2
F
F
4o
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170
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150
140
130
120
110
100
90
80
70
60
50
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30
20
10
0
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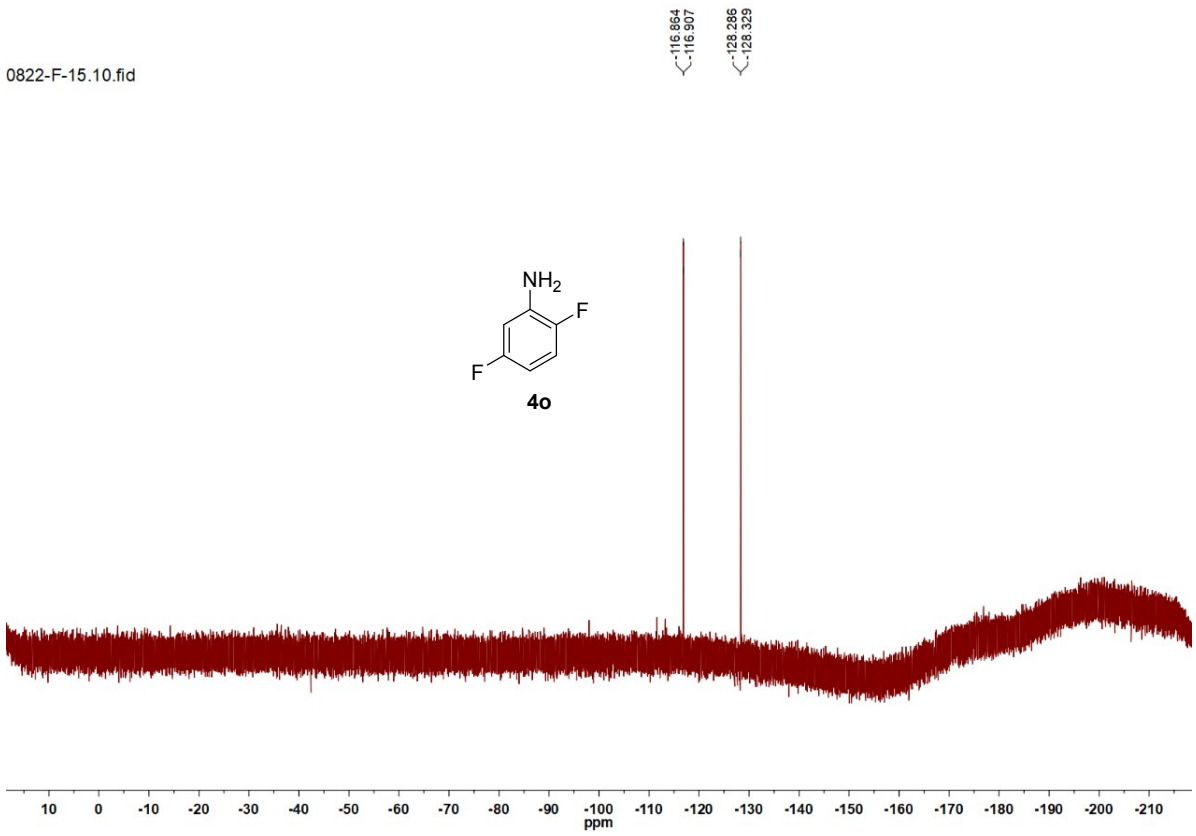
0822-F-15.10.fid
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-116.907
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-128.329
NH2
F
F
4o
10
0
-10
-20
-30
-40
-50
-60
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-140
-150
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-170
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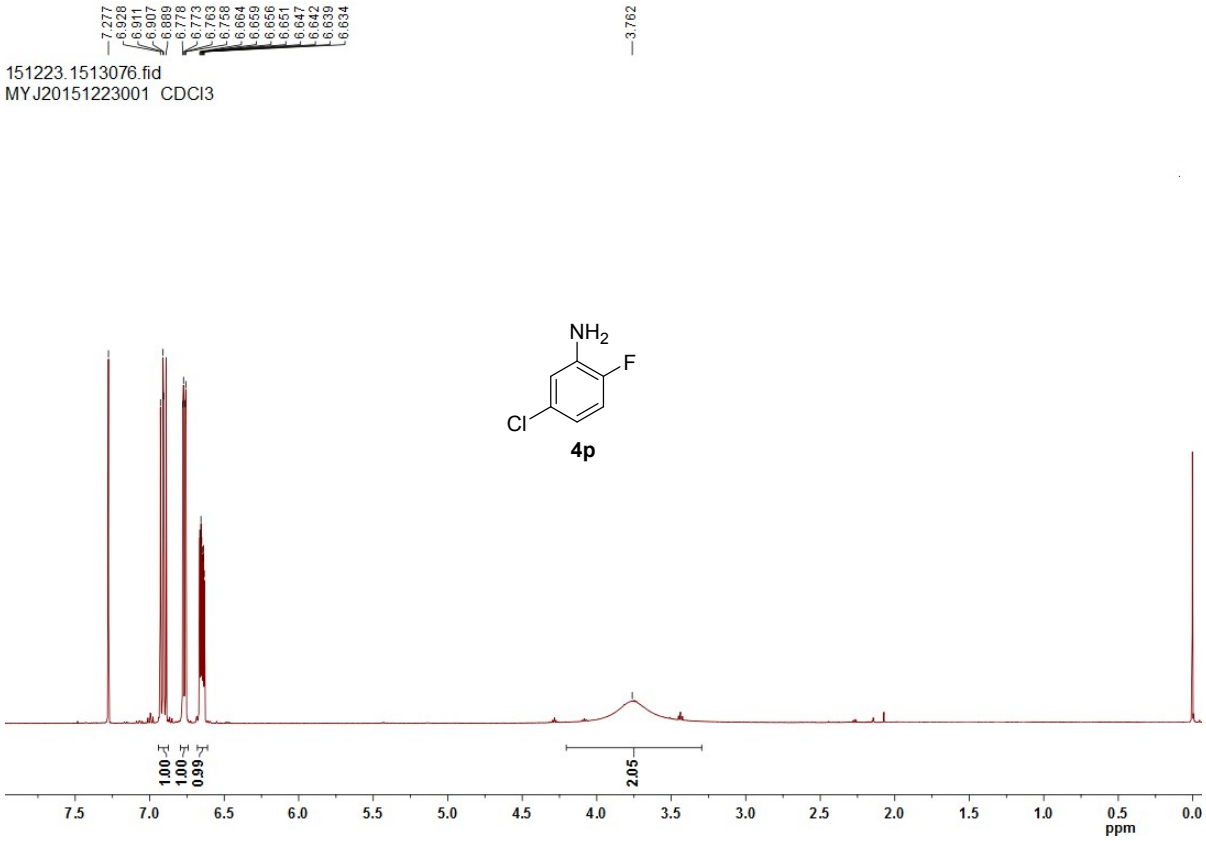
-200
-210
ppm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6.907
6.889
6.778
6.773
6.763
6.758
6.664
6.659
6.656
6.651
6.647
6.642
6.639
6.634
3.762
151223.1513076.fid
MYJ20151223001 CDCl3
NH2
F
Cl
4p
1.00
1.00
0.99
2.05
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
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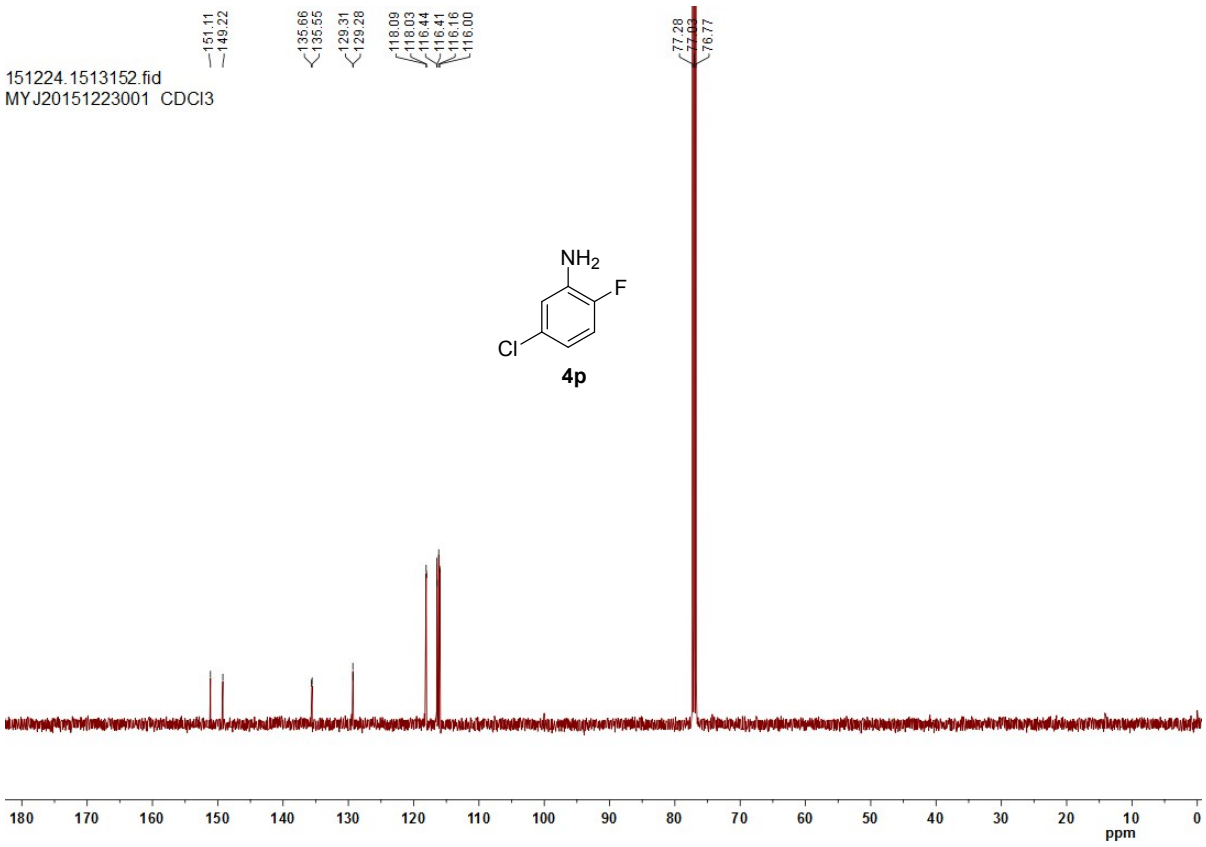
ppm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129.28
118.09
118.03
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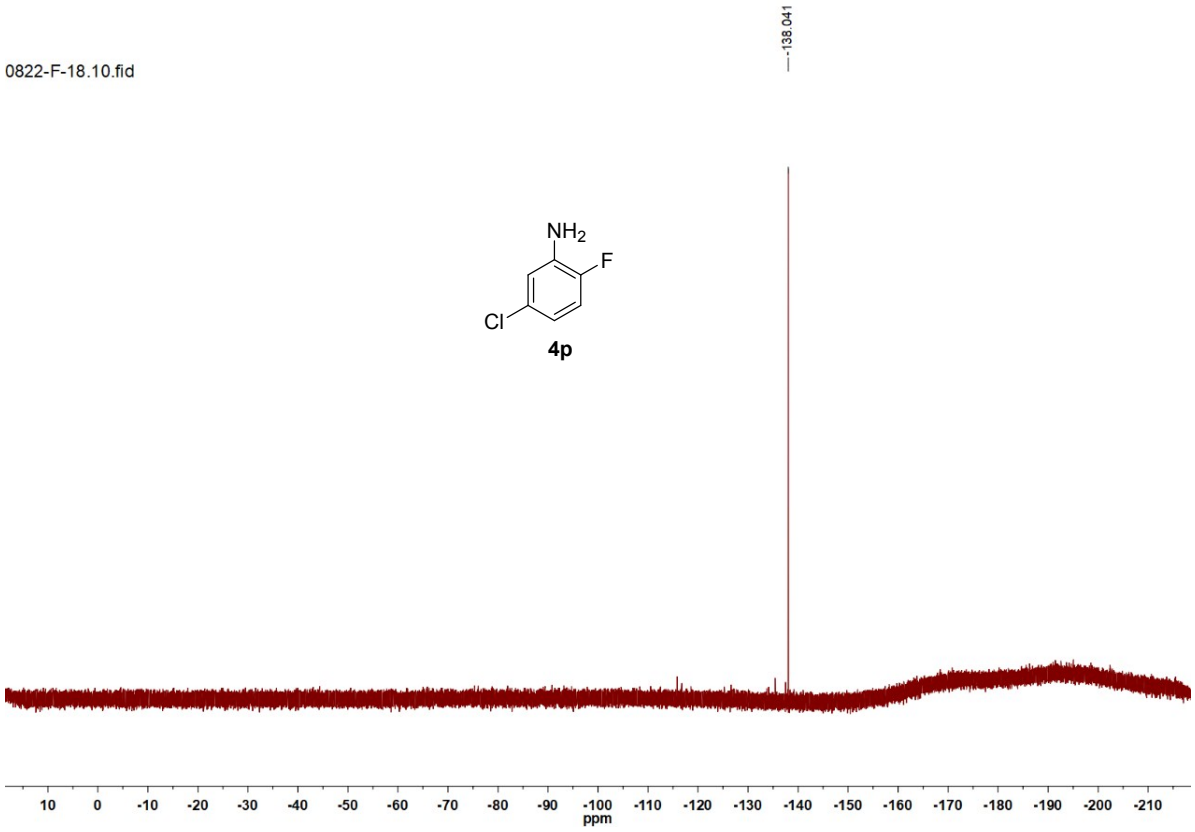
116.41
116.16
116.00
77.28
77.03
76.77
151224.1513152.fid
MYJ20151223001 CDCl3
NH2
F
Cl
4p
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

0822-F-18.10.fid



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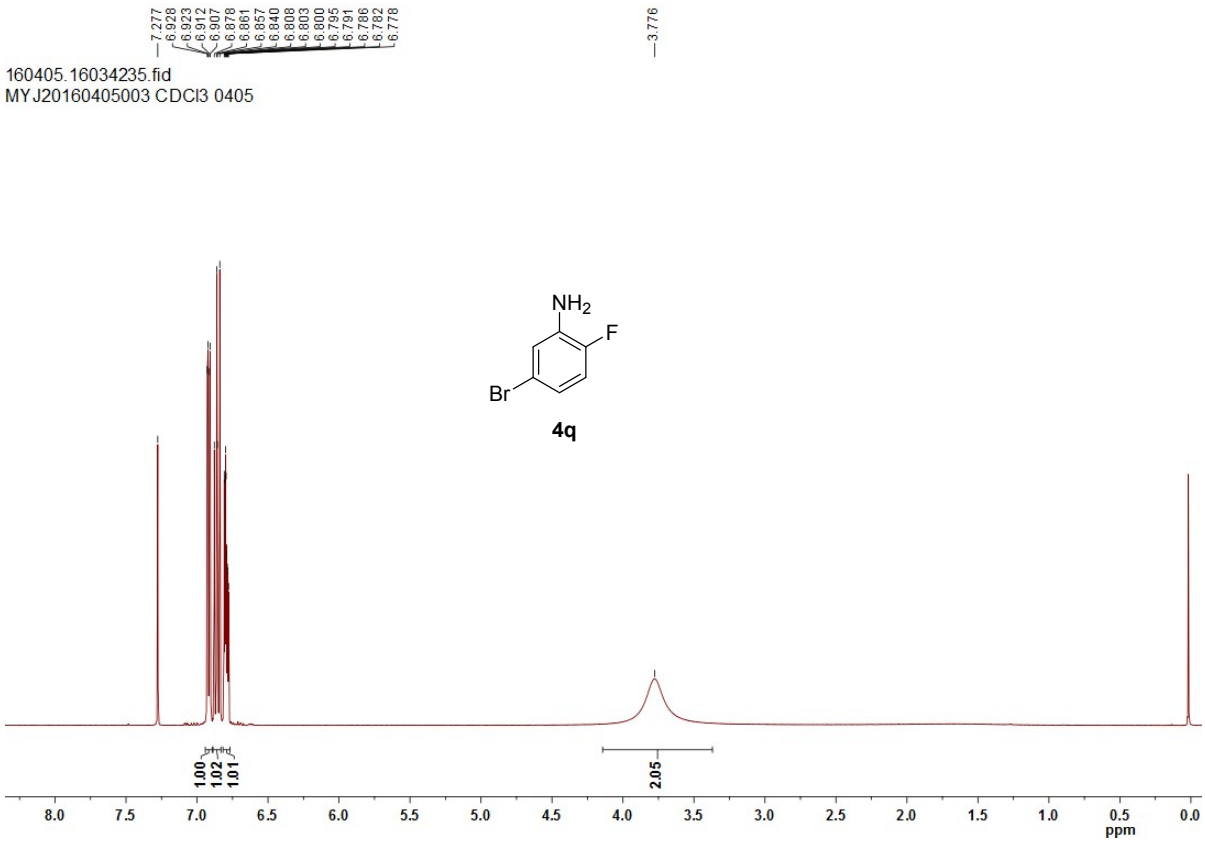
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6.857
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6.808
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6.800
6.795
6.791
6.786
6.782
6.778
3.776
160405.16034235.fid
MYJ20160405003 CDCl3 0405
NH2
F
Br
4q
1.00
1.02
1.01
2.05
8.0
7.5
7.0
6.5
6.0
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4.0
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3.0
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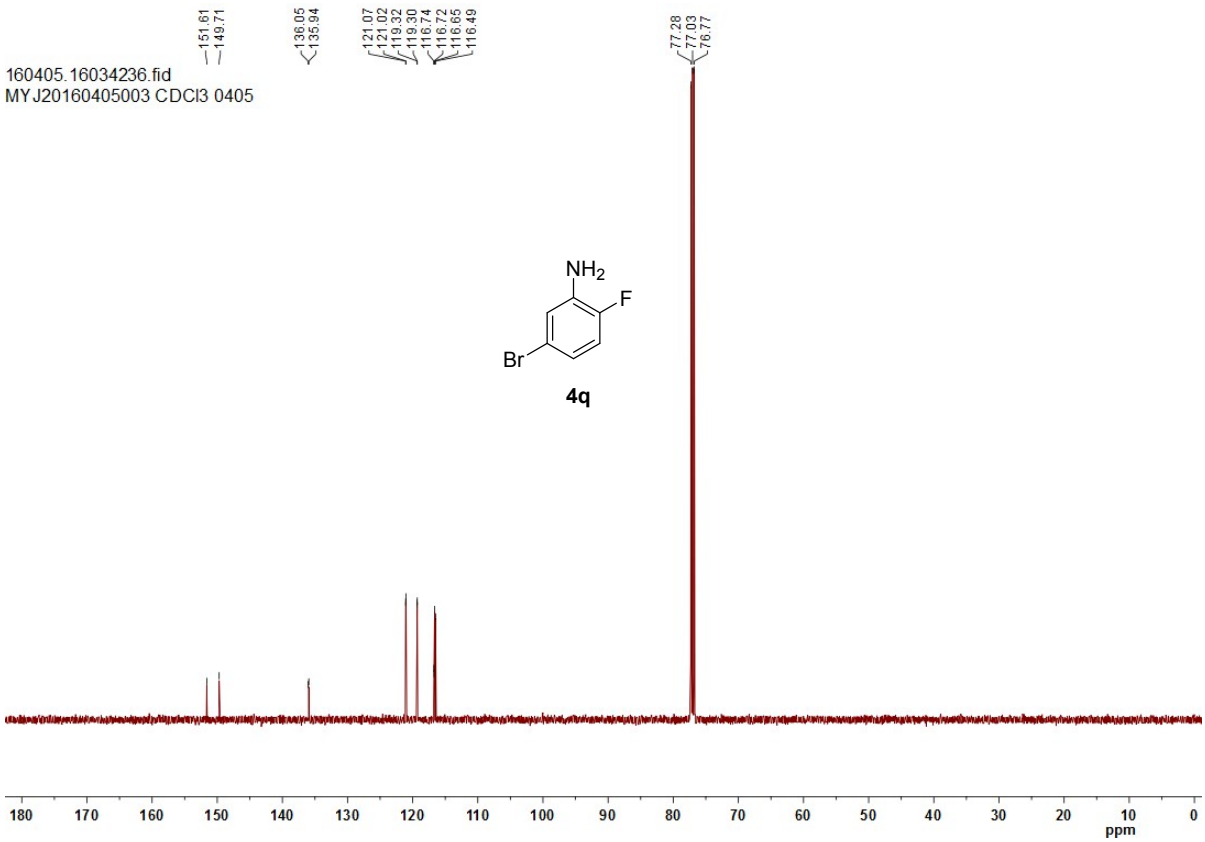
2.0
1.5
1.0
0.5
0.0
ppm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121.02
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119.30
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116.72
116.65
116.49
77.28
77.03
76.77
160405.16034236.fid
MYJ20160405003 CDCl3 0405
NH2
F
Br
4q
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170
160
150
140
130
120
110
100
90
80
70
60
50
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30
20
10
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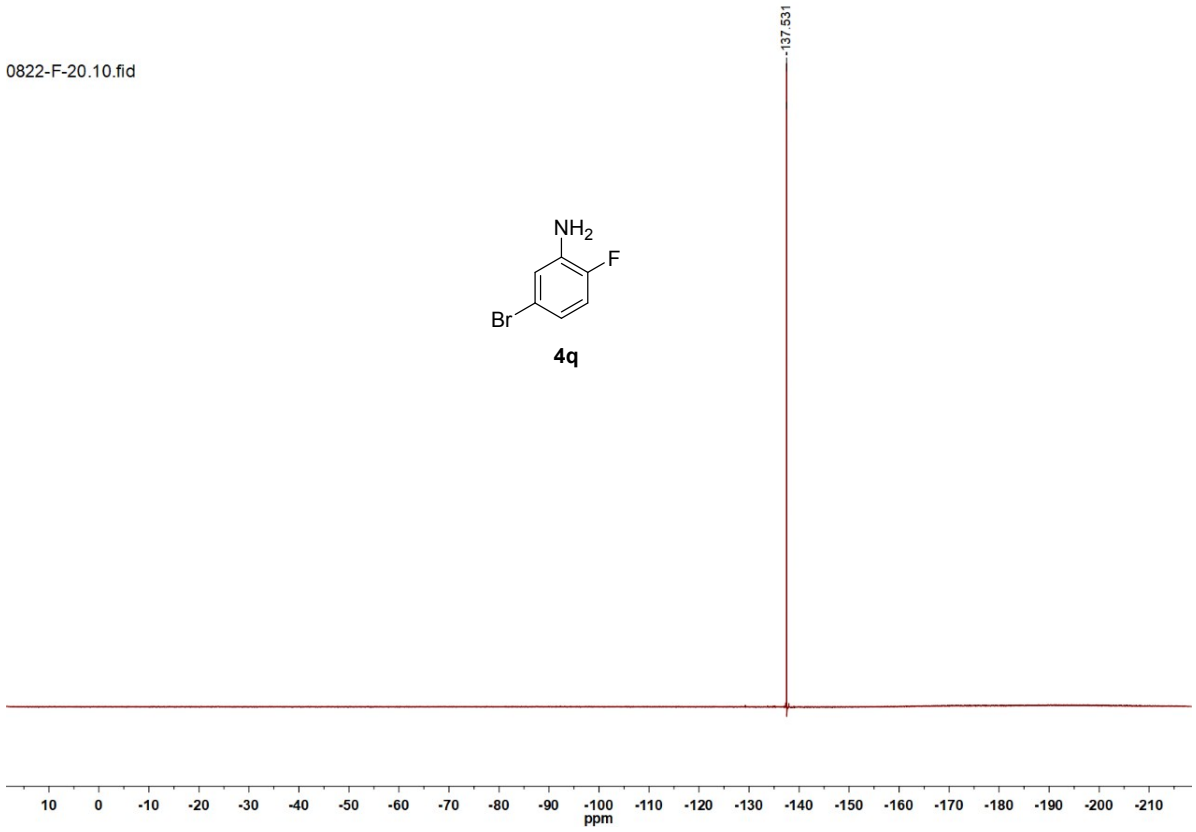
ppm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F
Br
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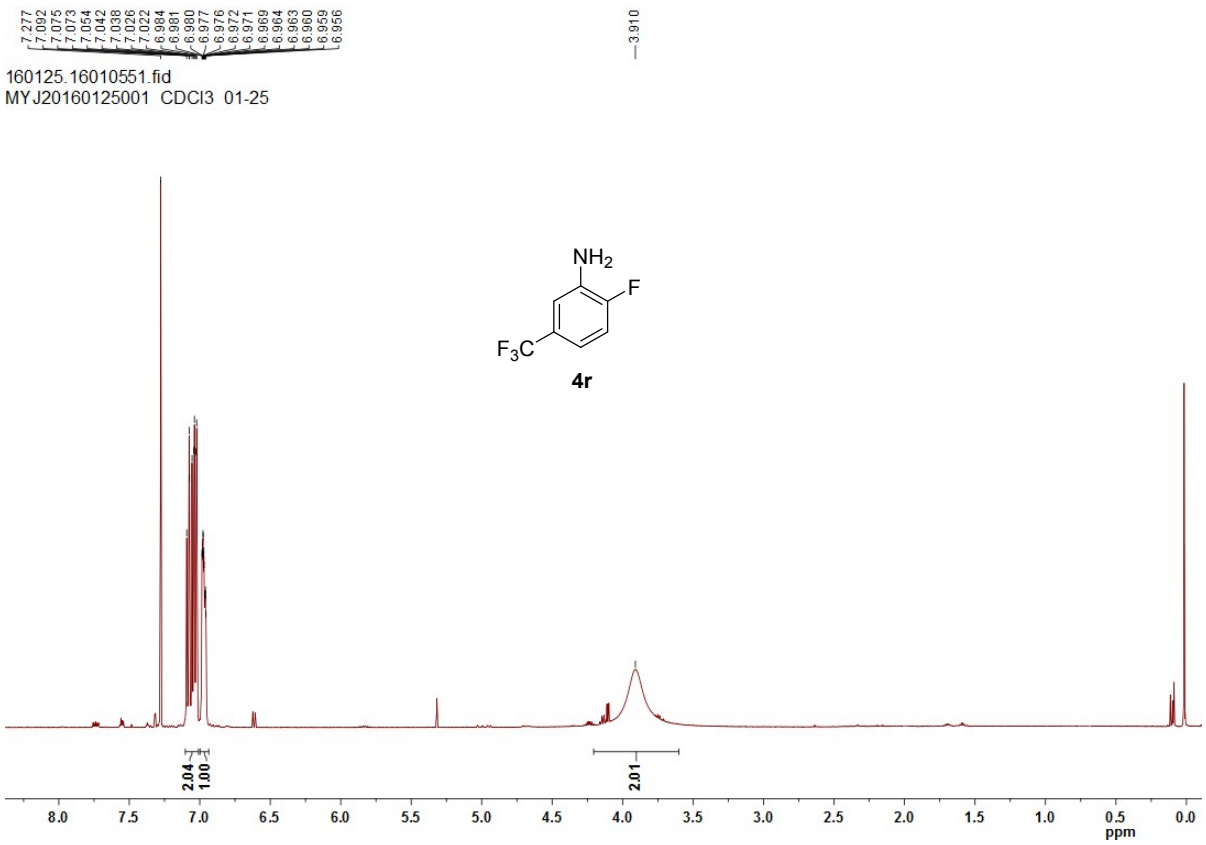
ppm

4q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7.054
7.042
7.038
7.026
7.022
6.984
6.981
6.980
6.977
6.976
6.972
6.971
6.969
6.964
6.963
6.960
6.959
6.956
3.910
160125.16010551.fid
MYJ20160125001 CDCl3 01-25
NH2
F
F3C
4r
2.04
1.00
2.01
8.0
7.5
7.0
6.5
6.0
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5.0
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4.0
3.5
3.0
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1.5
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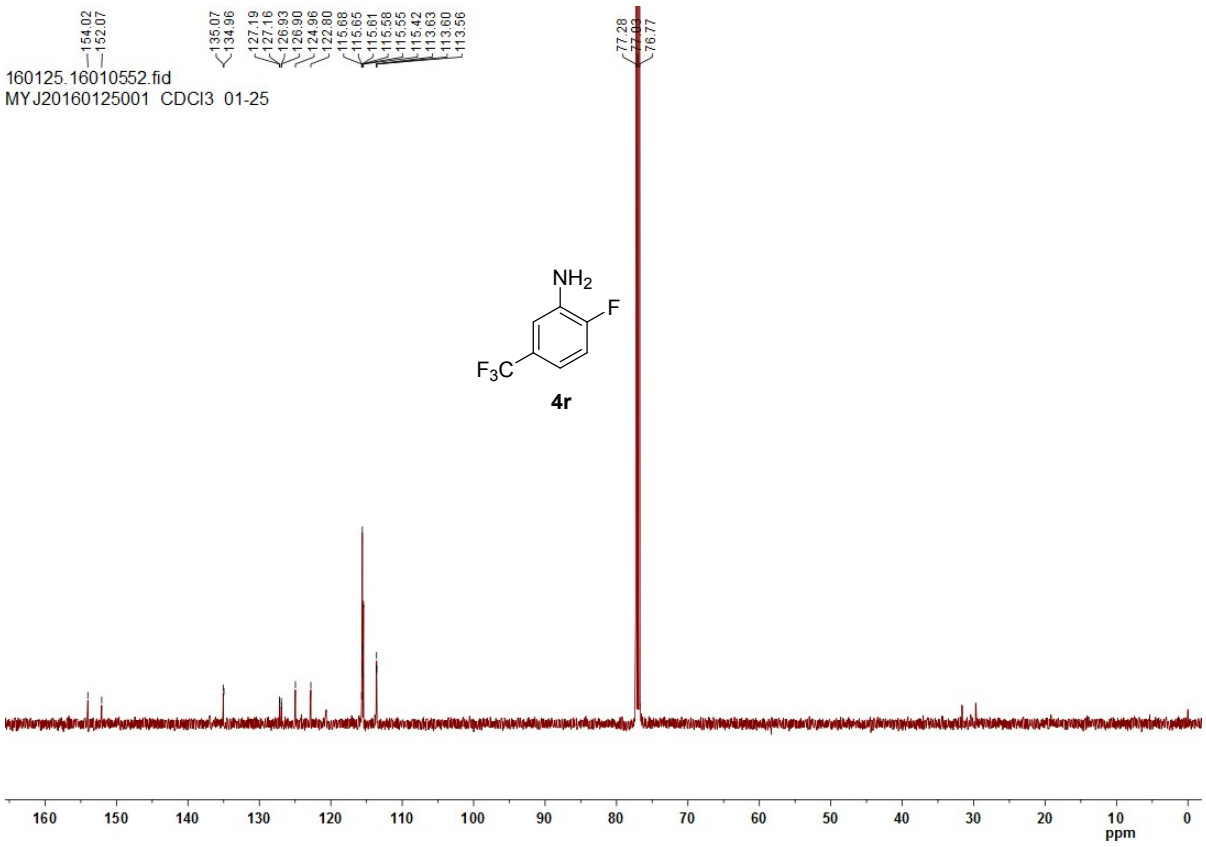
0.5
0.0
ppm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124.96
122.80
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115.61
115.58
115.55
115.42
113.63
113.60
113.56
77.28
77.03
76.77
160125.16010552.fid
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NH2
F
F3C
4r
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140
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110
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60
50
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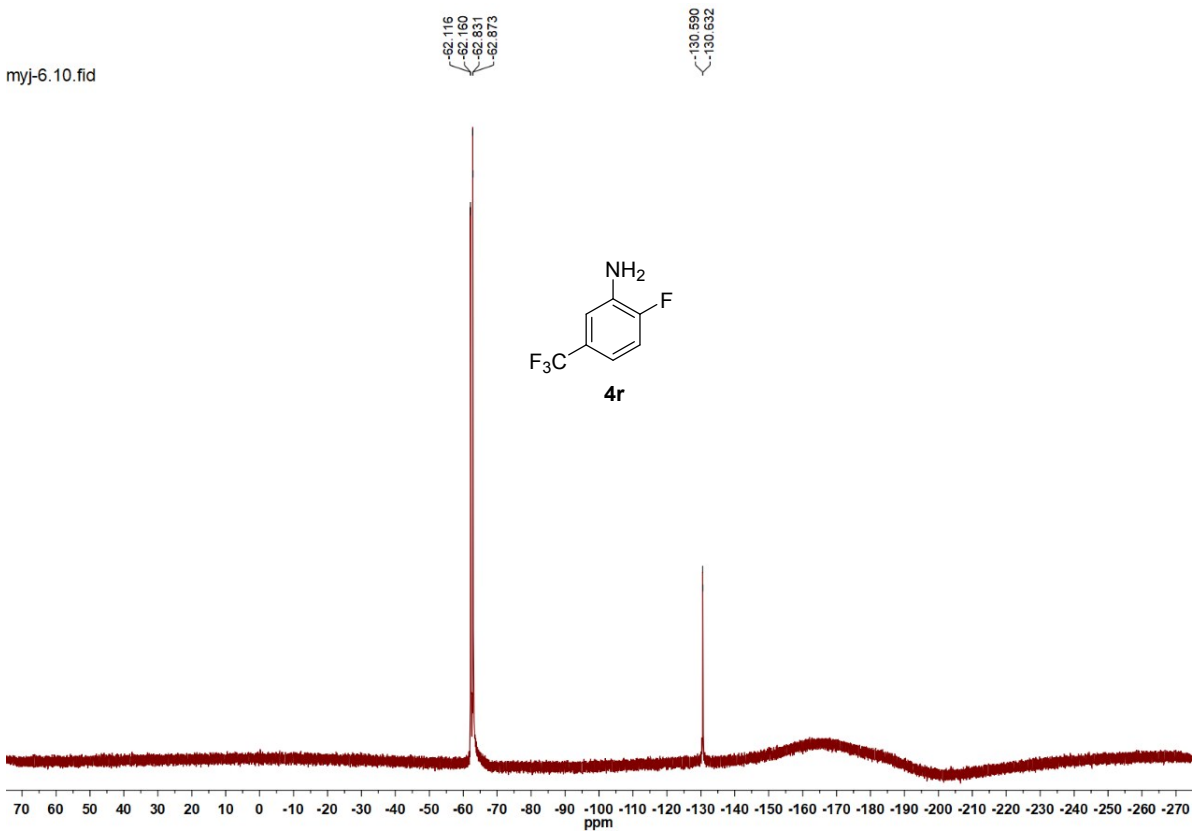
30
20
10
0
ppm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-62.873
-130.590
-130.632
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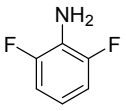
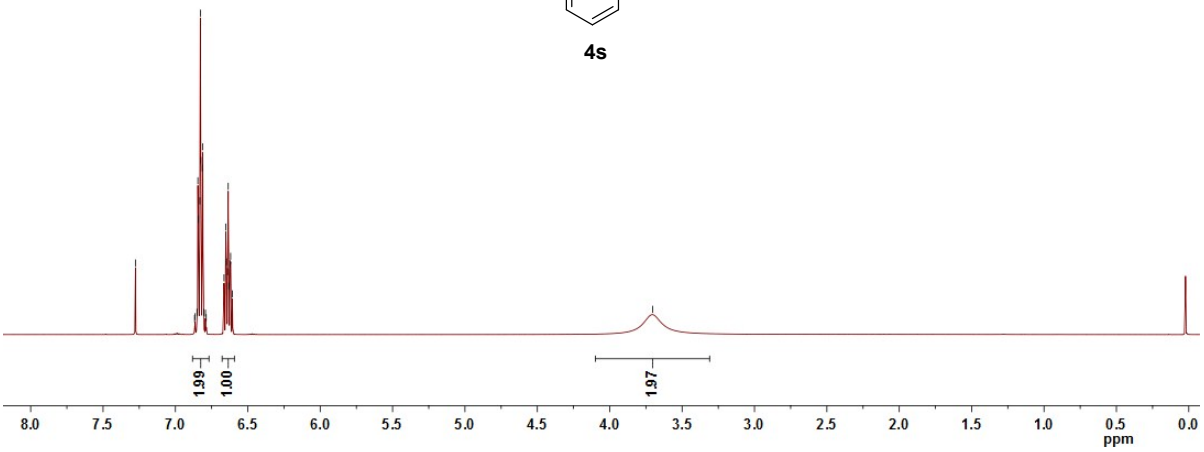
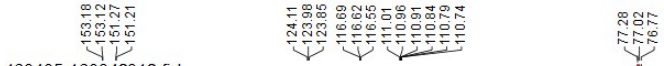
F
F3C
4r
70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -250 -260 -270
ppm

160405.160342311.fid
MYJ20160405006 CDCl3 0405



4s





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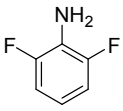
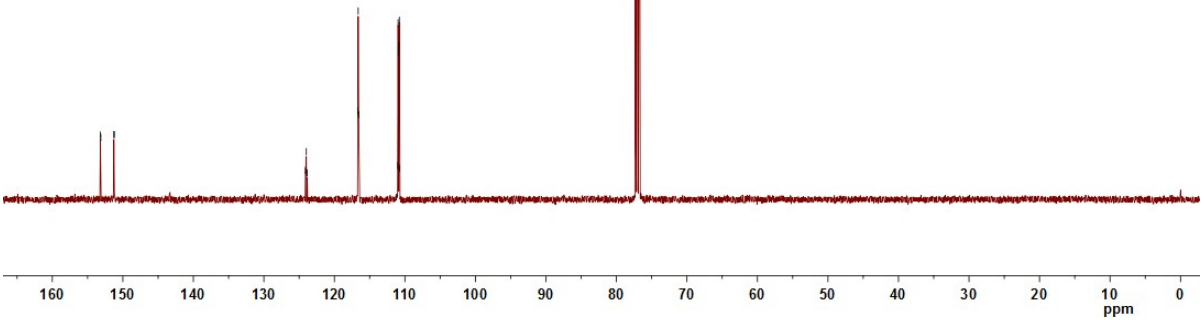
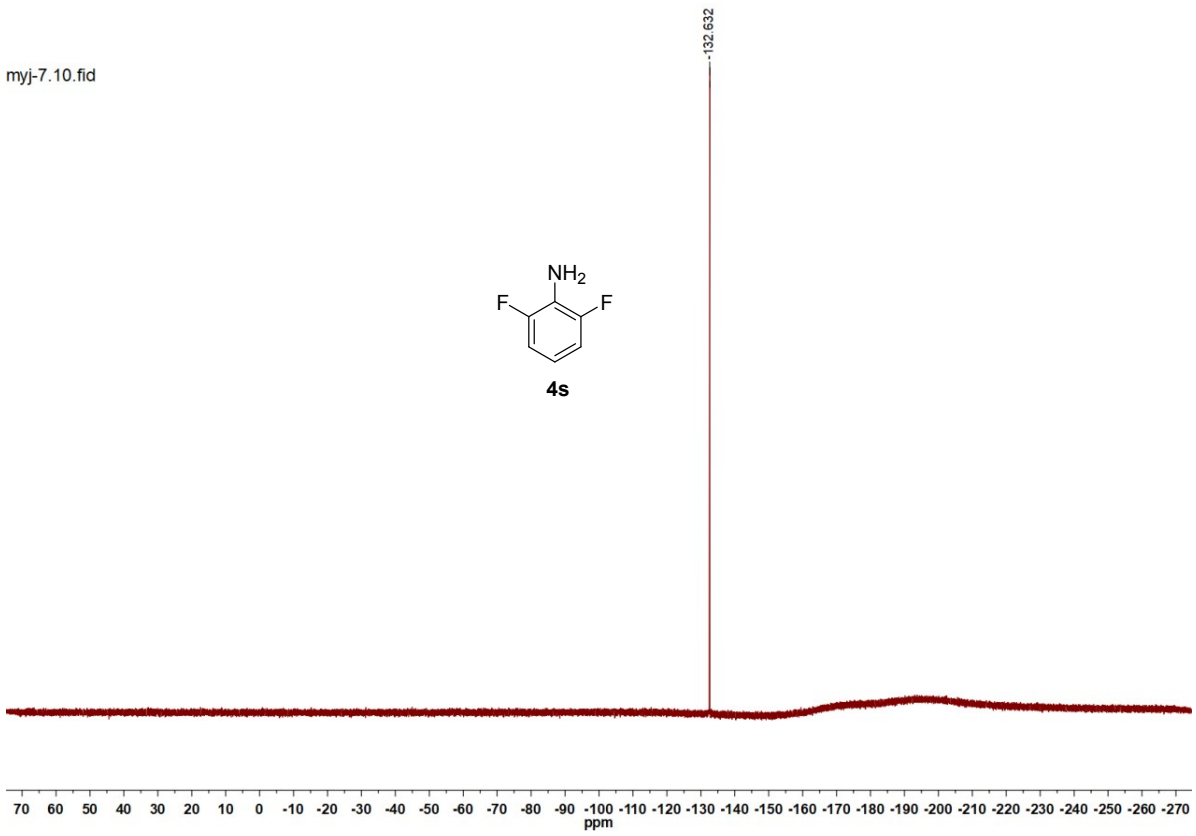


4s

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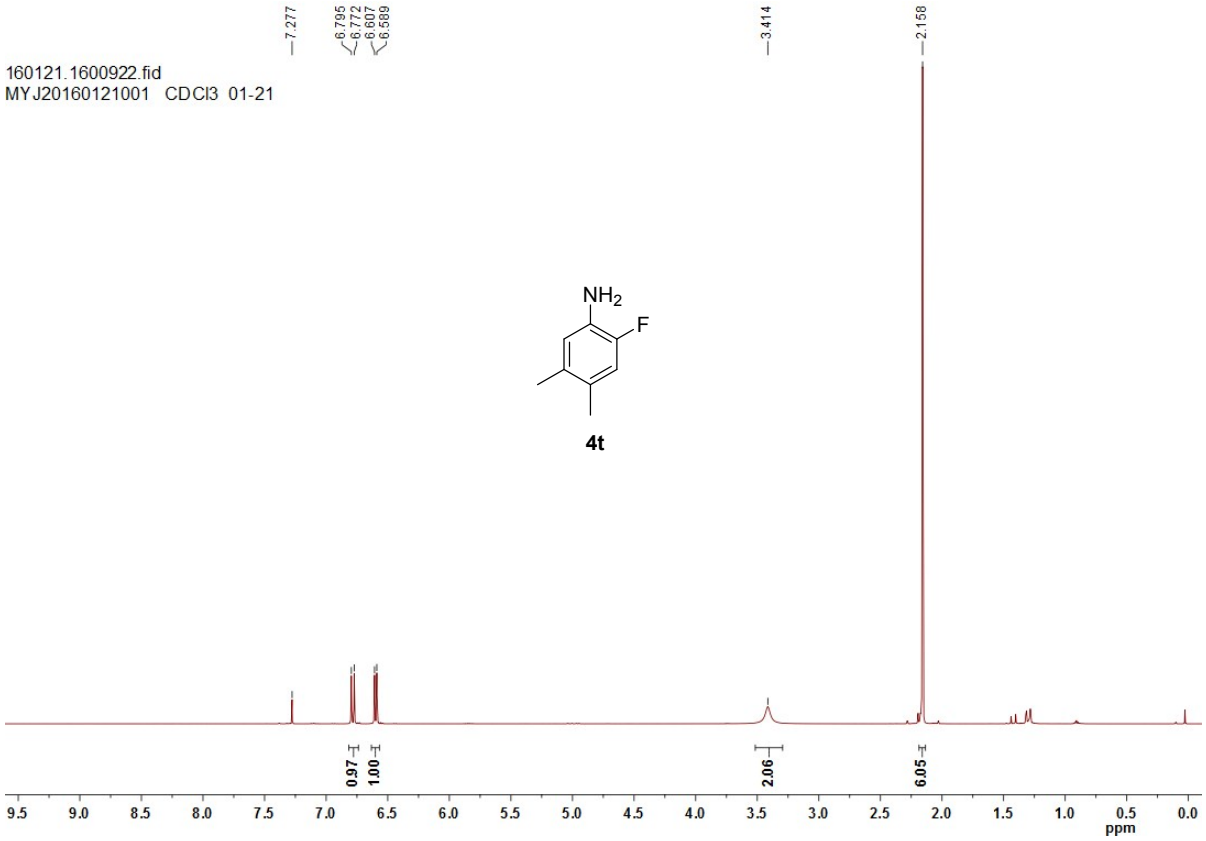
F
F
4s
70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -250 -260 -270
ppm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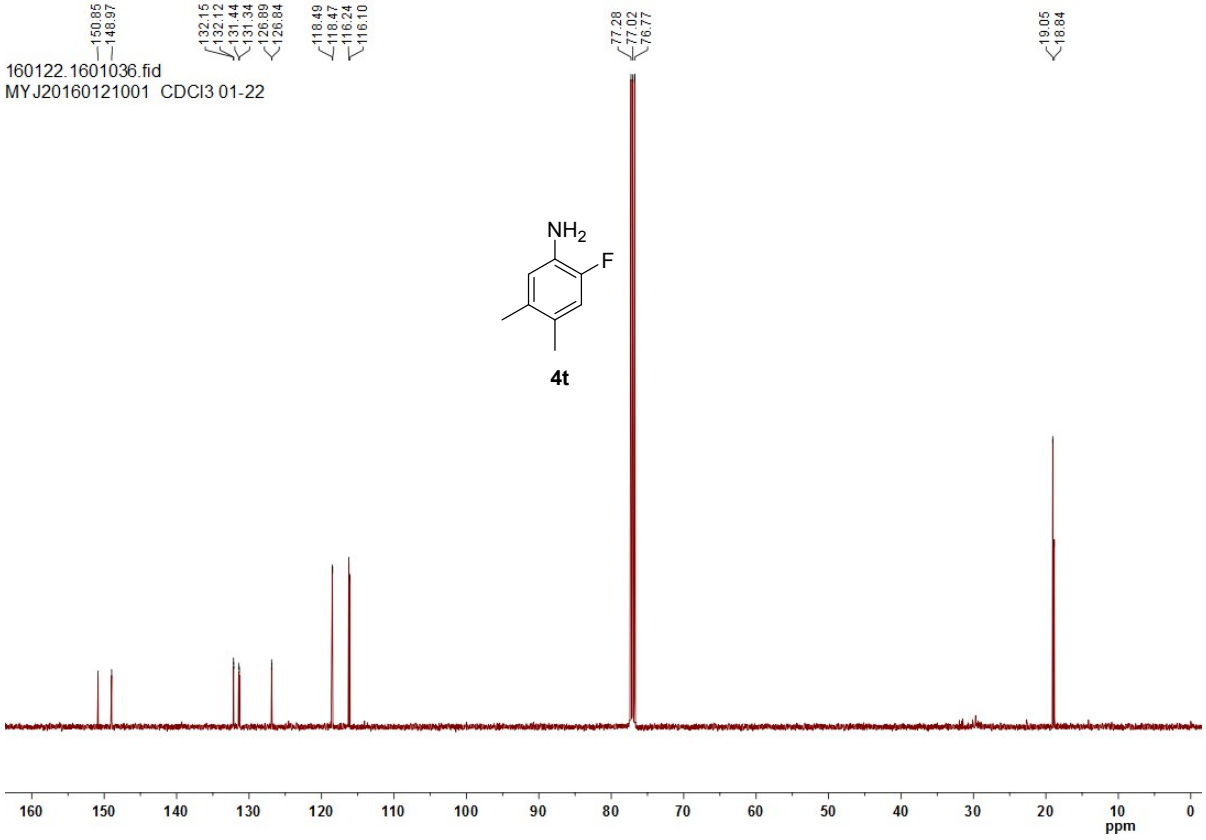
6.05
ppm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19.05
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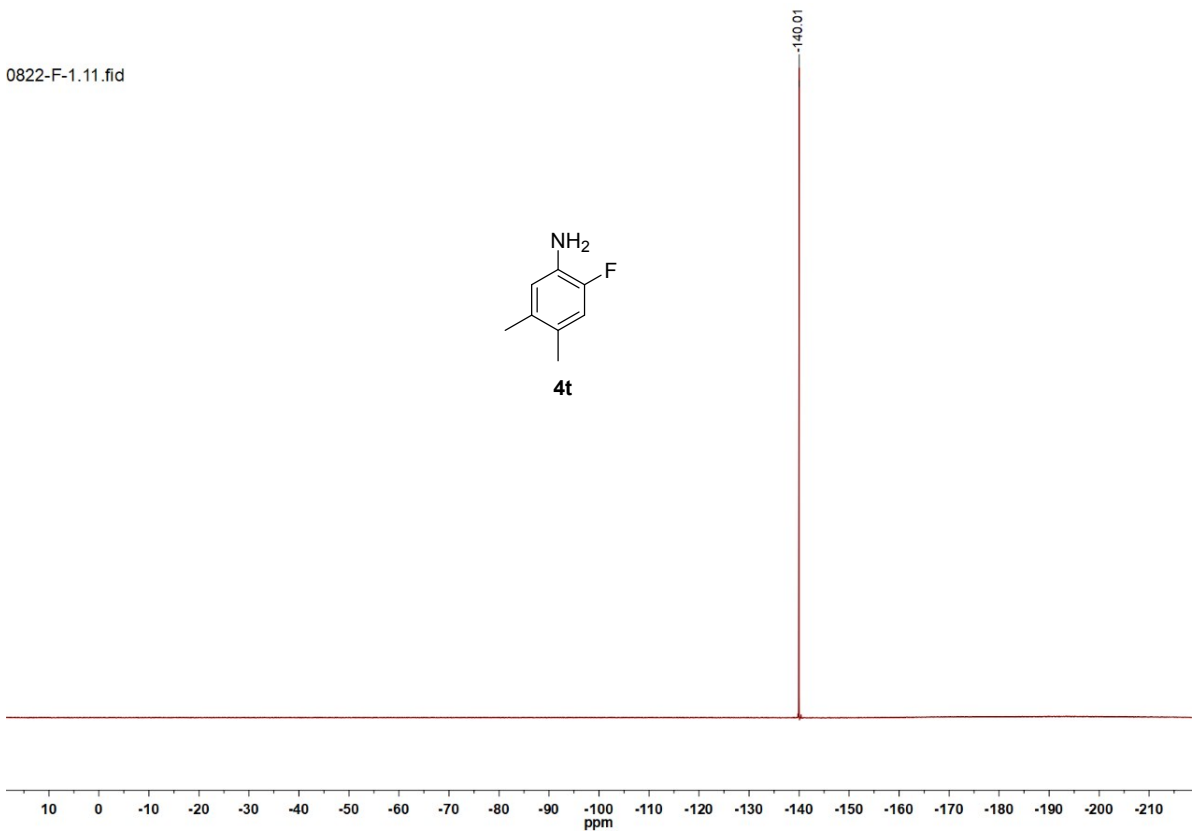
NH2
F
4t
ppm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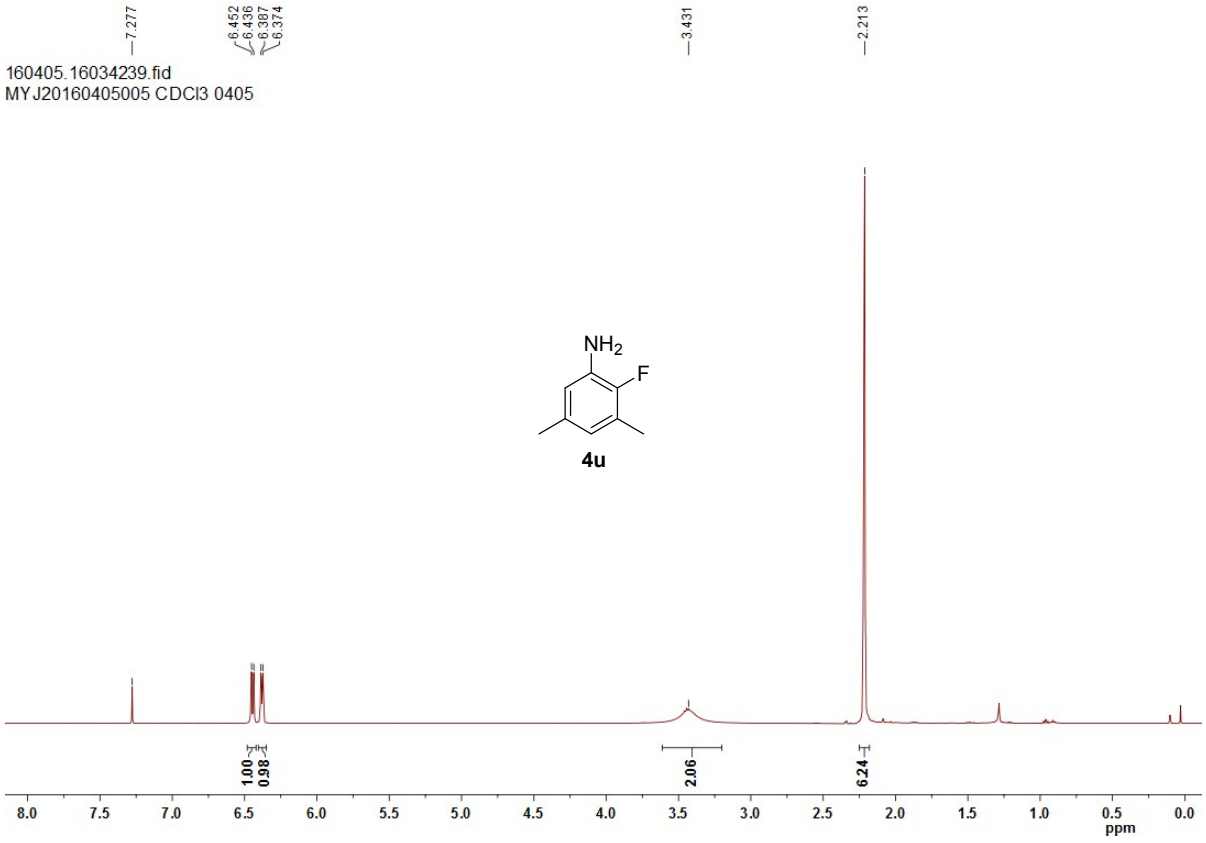
ppm

4t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F
4u
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2.06
6.24
8.0
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7.0
6.5
6.0
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4.0
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3.0
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1.5
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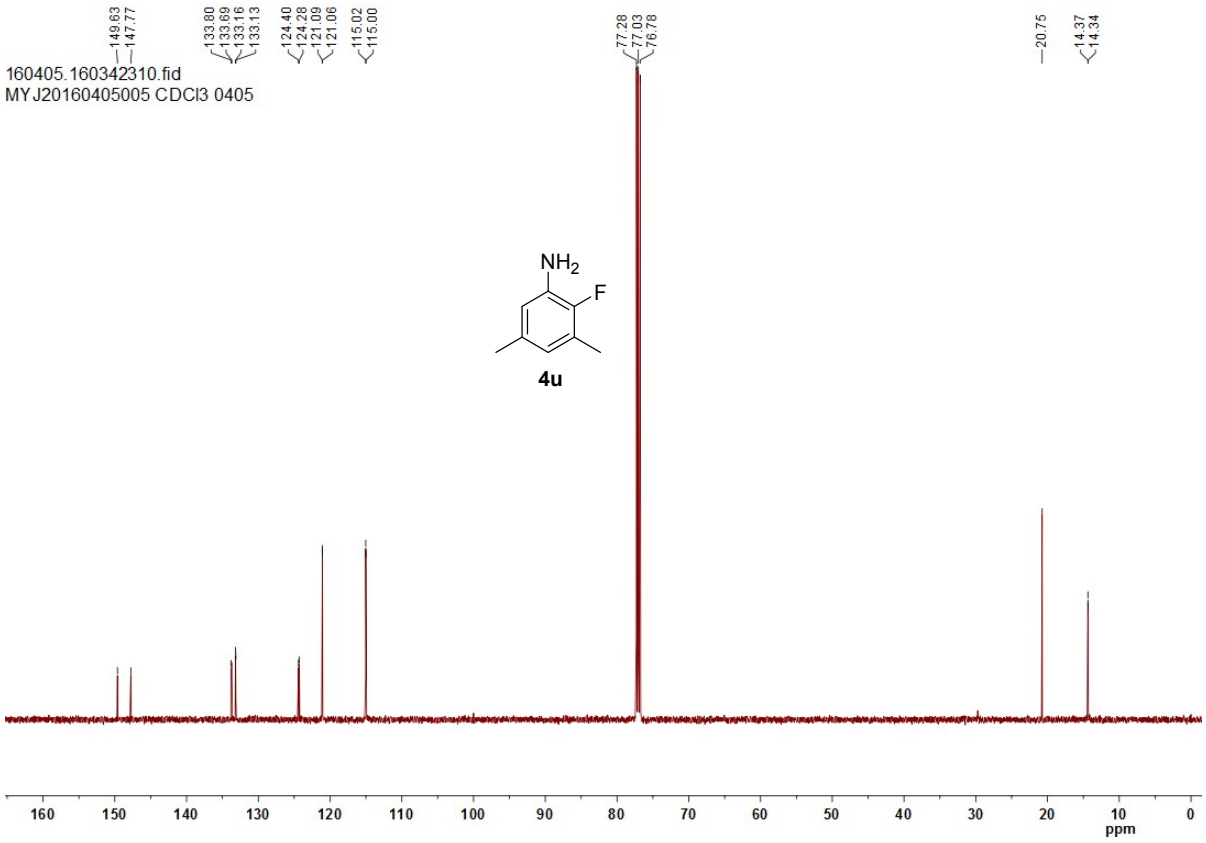
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124.28
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121.06
115.02
115.00
77.28
77.03
76.78
20.75
14.37
14.34
160405.160342310.fid
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NH2
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60
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40
30
20
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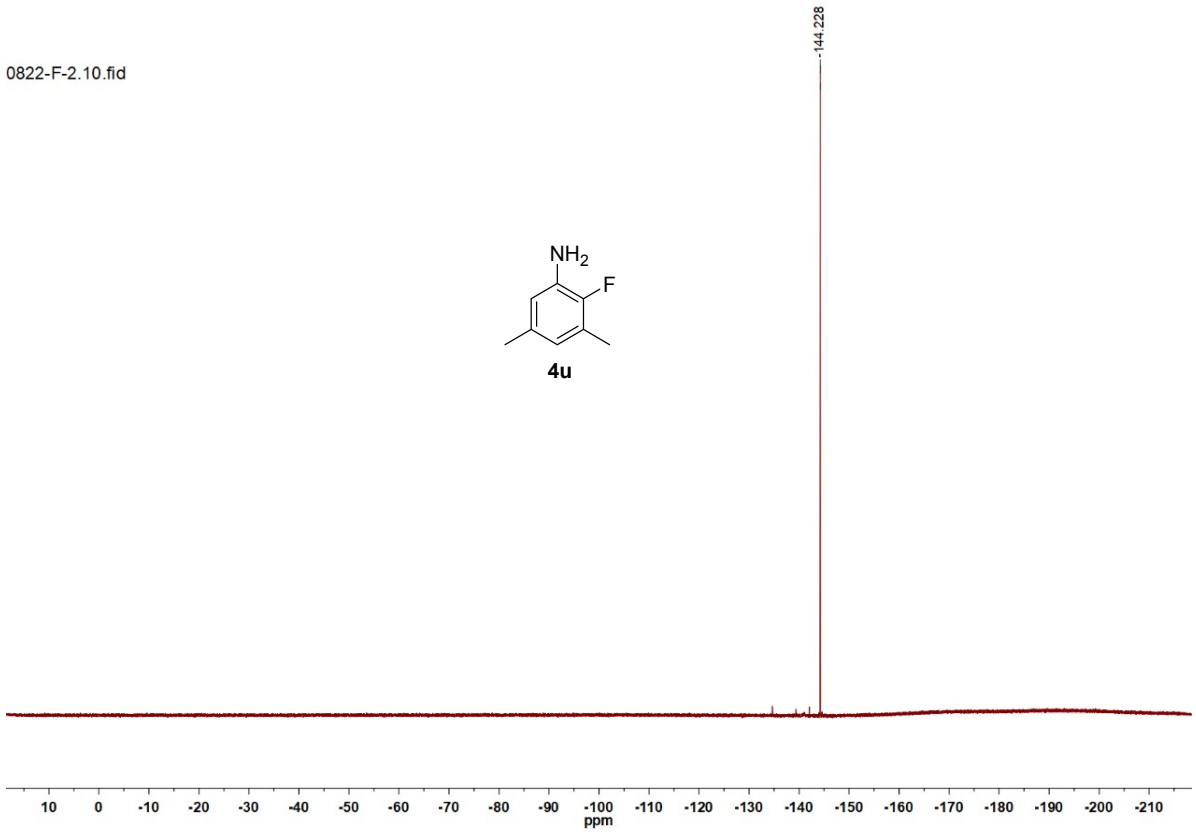
0
ppm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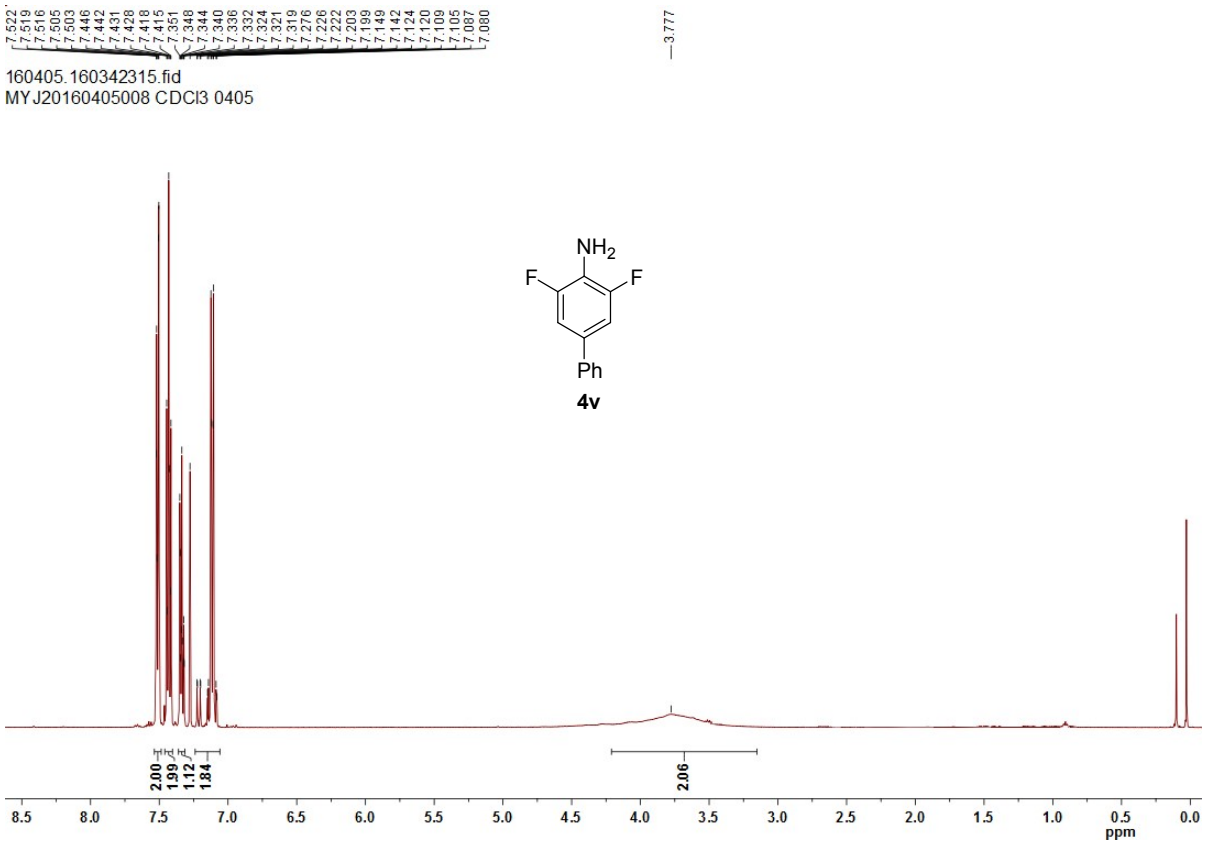
ppm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7.344
7.340
7.336
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7.226
7.222
7.203
7.199
7.149
7.142
7.124
7.120
7.109
7.105
7.087
7.080
3.777
160405.160342315.fid
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NH2
F
F
Ph
4v
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1.12
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2.06
8.5
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6.0
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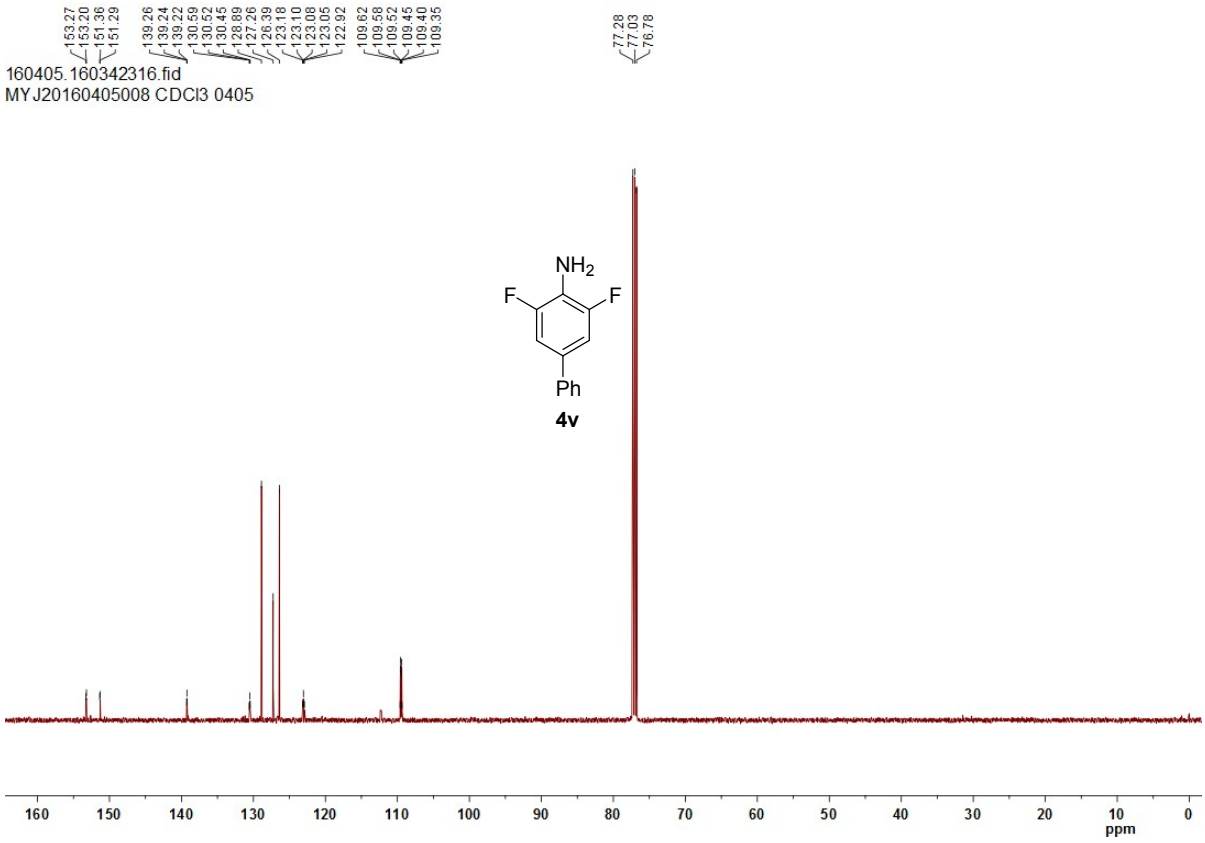
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109.58
109.52
109.45
109.40
109.35
77.28
77.03
76.78
160405.160342316.fid
MYJ20160405008 CDCl3 0405
NH2
F
F
Ph
4v
160
150
140
130
120
110
100
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80
70
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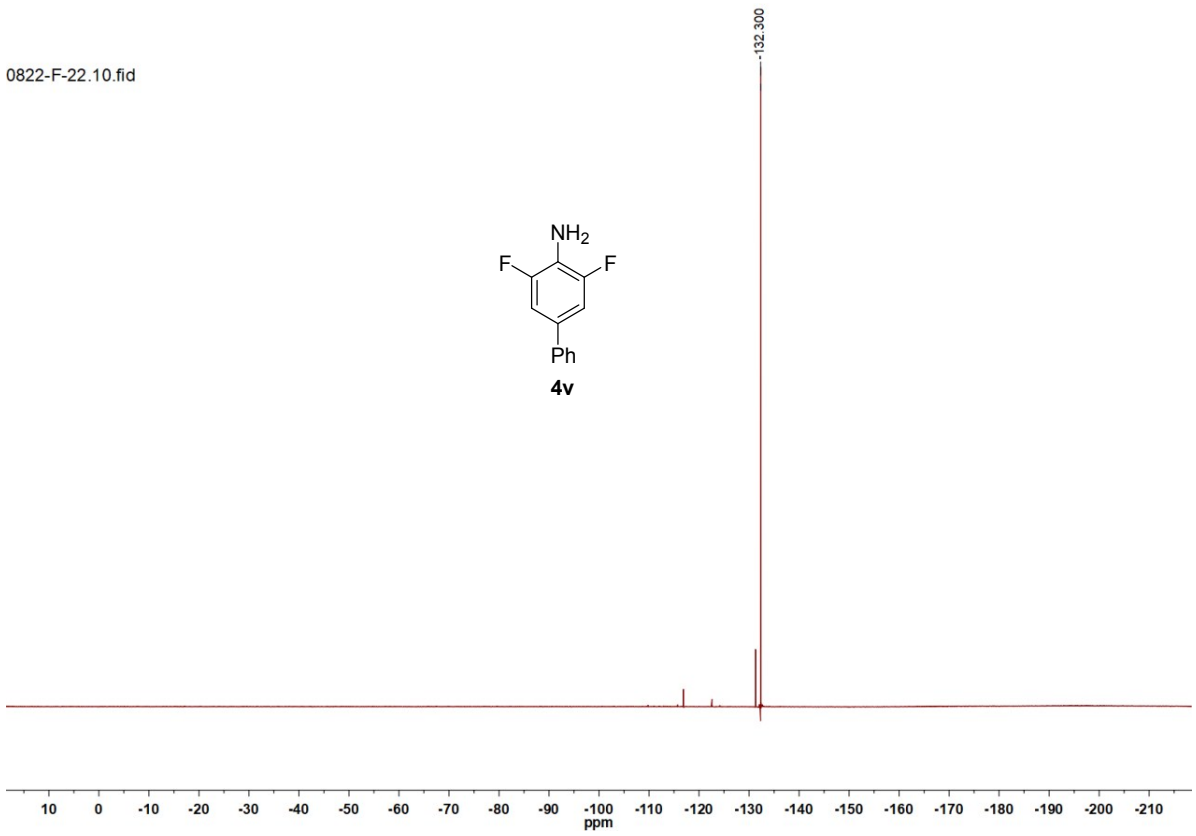
20
10
0
ppm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-132.300
NH2
F
F
Ph
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4v

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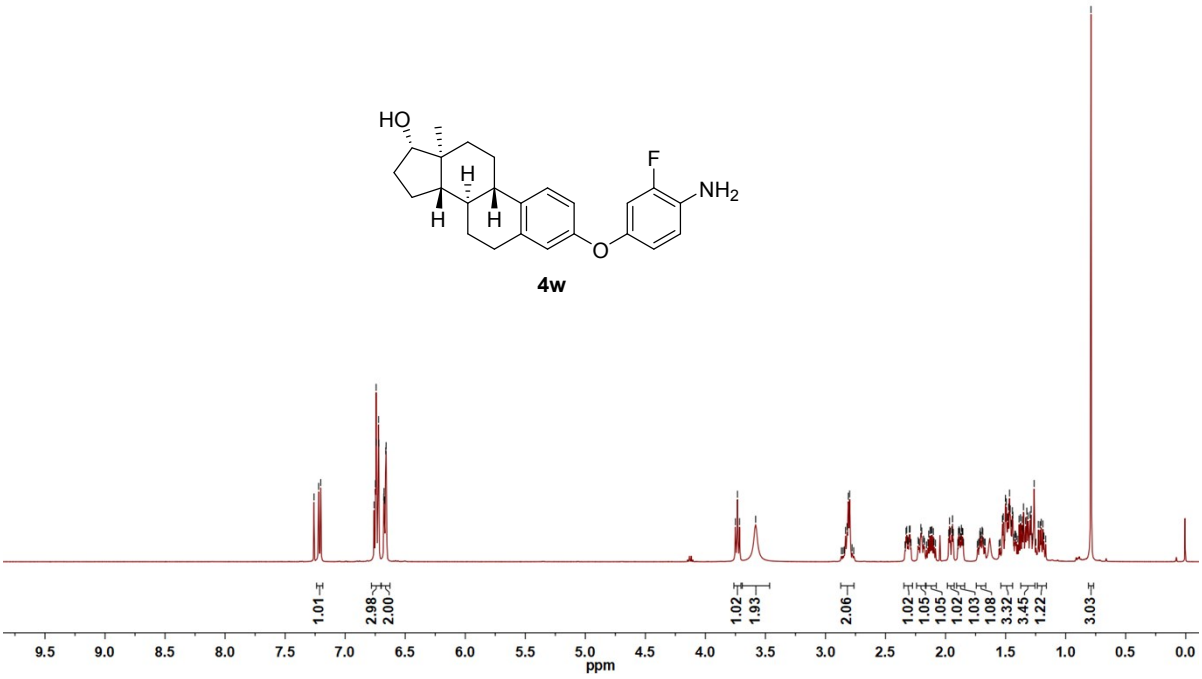

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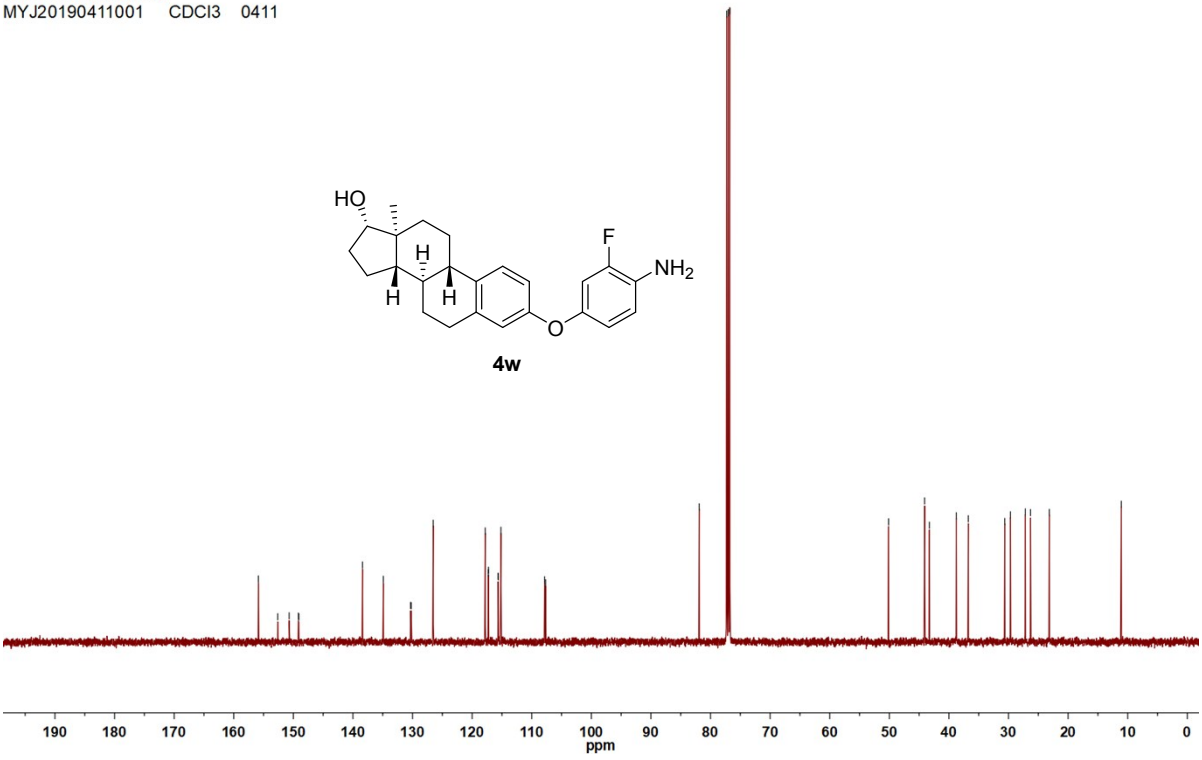

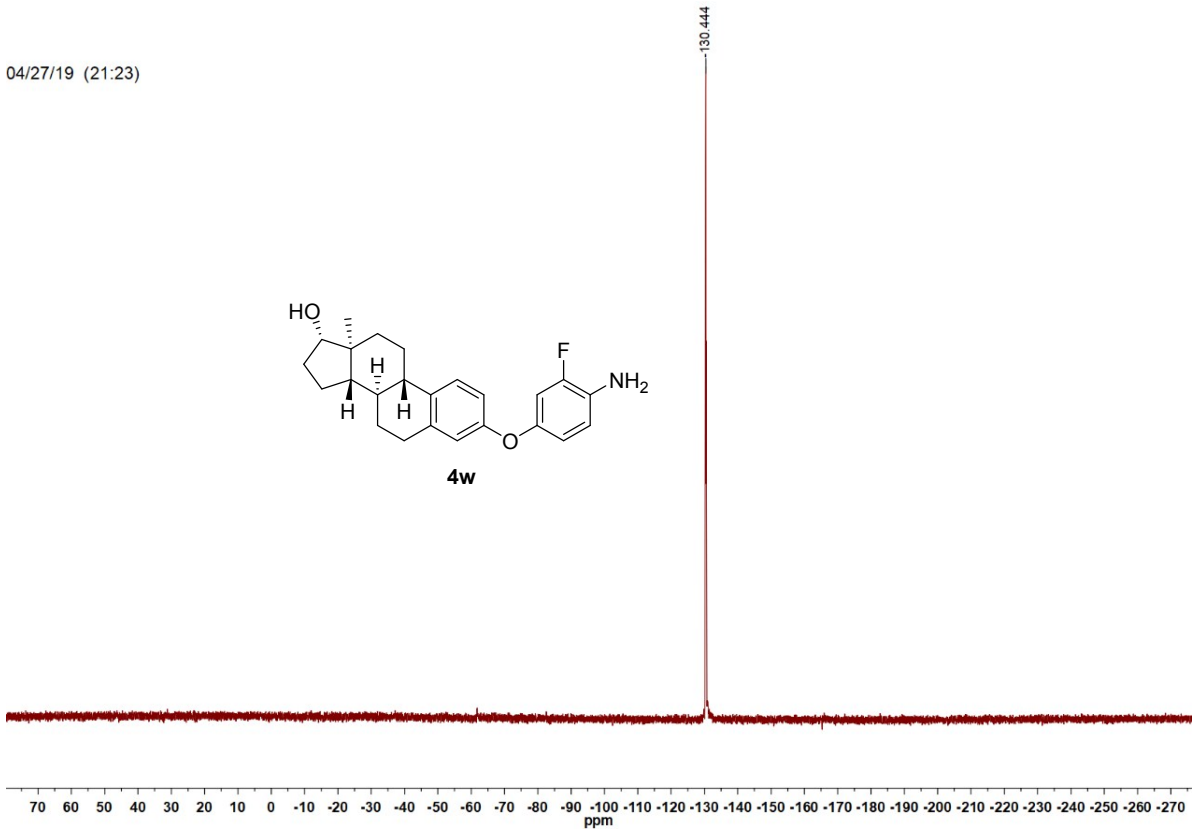
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HO
H
H
H
F
NH2
O
4w
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ppm