

Supporting Information

Silicon-fluorine non-covalent interaction guided distal functionalization of di- and tri- fluoro alkyl benzene

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1. General Consideration

Reagent information: Unless otherwise stated, all reactions were carried out under air atmosphere in screw cap reaction tubes. Palladium (II) acetate was purchased from Sigma-Aldrich. All the solvents were bought from Merck and α, α, α -Trifluorotoluene; [CAS: 98-08-8] ensure sealed bottle and were used as received. α, α -difluoromethylbenzene, *N*-Ac-Phe-OH, acrylates, silver acetate [CAS:2966-50-9] reagents were bought from Sigma Aldrich, Alfa-Aesar, TCI and Spectrochem. For column chromatography, silica gel (100–200 mesh) from SRL Co. A gradient elution using petroleum-ether and ethyl acetate was performed, based on Merck aluminium TLC sheets (silica gel 60F254).

Analytical Information: All isolated compounds were characterized by ^1H NMR, ^{13}C NMR Spectroscopy and high-resolution mass spectrometry (HRMS). Copies of the ^1H NMR, ^{13}C NMR can be found in the Supporting Information. Unless otherwise stated, all Nuclear Magnetic Resonance spectra were recorded on a Bruker 400 MHz and 500 MHz instrument. All ^1H NMR experiments were reported in units, parts per million (ppm), and were measured relative to the signals for residual chloroform (7.26 ppm) in the deuterated solvent, unless otherwise stated. All ^{13}C NMR spectra were reported in ppm relative to deuteron chloroform (77.00 ppm), unless otherwise stated, and all were obtained with ^1H decoupling. High-resolution mass spectra (HRMS) were recorded on a Q-TOF micromass (YA-105) mass spectrometer and a Bruker Maxis Impact (282001.00081) in ESI mode. Graphs were obtained using Origin Pro8 software. X-ray crystallography was recorded.

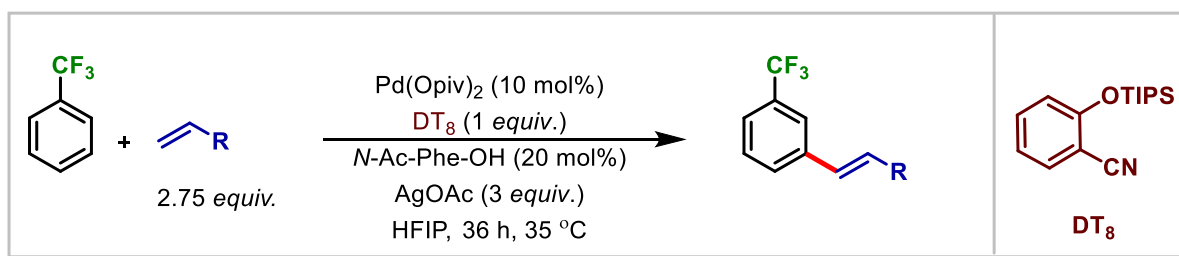


Description of Reaction Tube:

Pictorial description of reaction tube for olefination and lactamization: Fisher brand Disposable Borosilicate Glass Tubes (16*125mm) with Threaded End (Fisher Scientific, Order No. 1495935A) [left]; Kimble Black Phenolic Screw Thread Closures with Open Tops (Fisher Scientific Order No. 033407E) [left]; Thermo Scientific National PTFE/Silicone Septa for Sample Screw Thread Caps (Fisher Scientific Order No. 03394A)

[left].

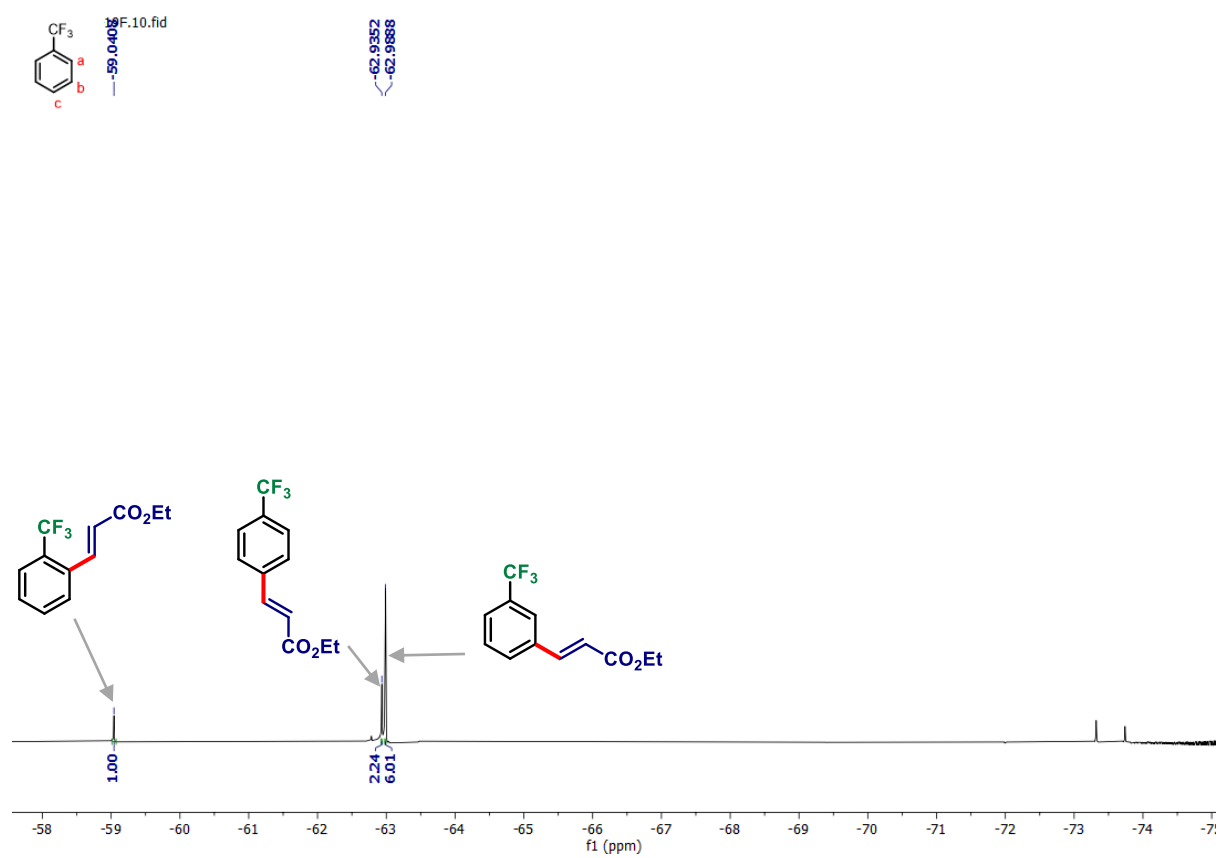
2. General procedure for Pd-catalysed olefination of tri/di-fluorotoluene (A):



A clean, oven-dried screw cap reaction tube with previously placed magnetic stir-bar was charged with tri/di-fluorotoluene (0.1 mmol), palladium (II) pivalate (10 mol %, 0.01 mmol, 3.1 mg) and *N*-acetyl phenyl alanine ligand (20 mol%, 0.02 mmol, 4.1 mg). Then AgOAc (3 equiv., 0.3 mmol, 51.6 mg) and directing ligand DT₈ (1 equiv., 0.1 mmol, 27.5 mg) were introduced in the reaction mixture. Then, olefin (2.75 equiv., 0.275 mmol) and HFIP (2 mL) was added to this mixture by syringe in the open atmosphere. The reaction mixture was vigorously stirred for 36 h in a preheated oil bath at 35 °C. After the stipulated time, the reaction mixture filtered through a celite bed using ethyl acetate as the eluent (3 mL). The crude reaction mixture was purified by column chromatography using silica gel (100-200 mesh size) and petroleum ether/ethyl acetate as the eluent to give the desired *meta*-olefinated product.

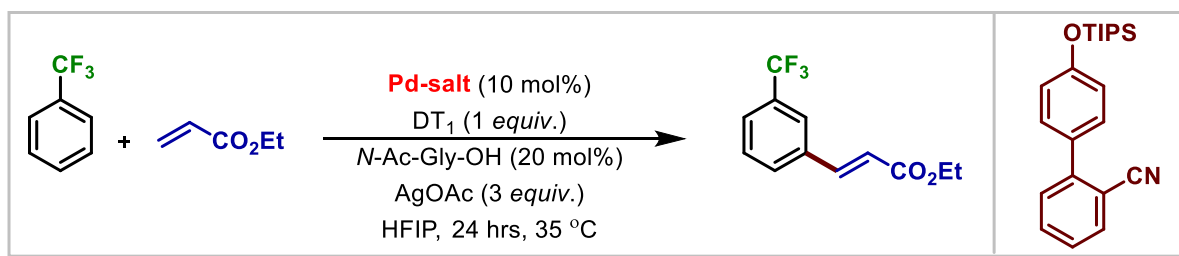
3. Crude NMR

The selectivity of the product is determined from ^{19}F NMR:



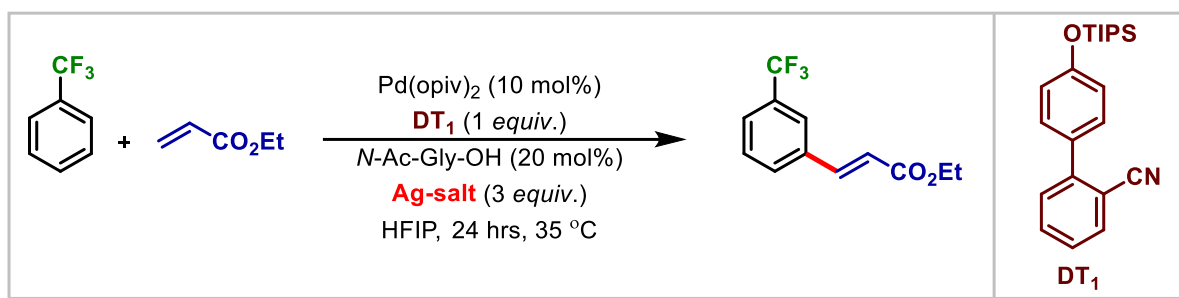
4. Optimization of Reaction

4.1: Table 1: Palladium salt optimization:



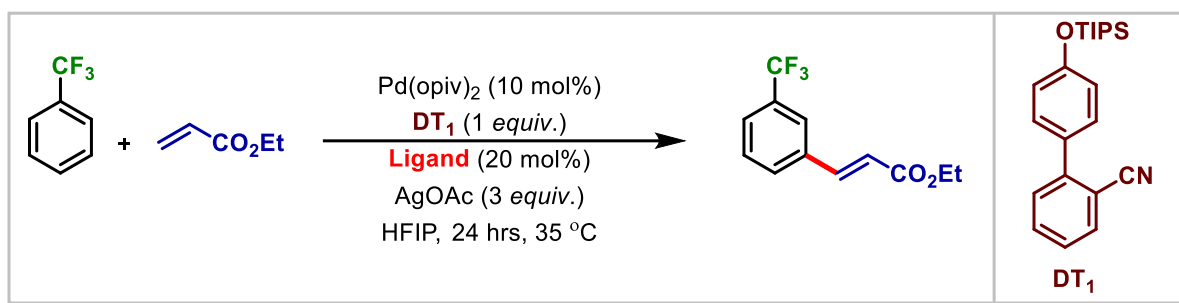
Entry	Pd Salt	Yield(%) and selectivity (o:m:p)
1.	Pd(PhCN) ₂ Cl ₂	27 (1:4.7:1.4)
2.	Pd(MeCN) ₂ Cl ₂	NR
3.	Pd(CF ₃ CO ₂) ₂	NR
4.	PdCl ₂	NR
5.	Pd(1,5-COD)Cl ₂	NR
6.	Pd (PPh ₃) ₂ Cl ₂	NR
7.	Pd(acac) ₂	NR
8.	[PdCl(p-cinnamyl)] ₂	Trace
9.	Pd(OAc) ₂	32 (1:5.2:1.3)
10.	Pd (OPiv)₂	37 (1:6:2.2)

4.2: Table 2: Silver salt optimization:



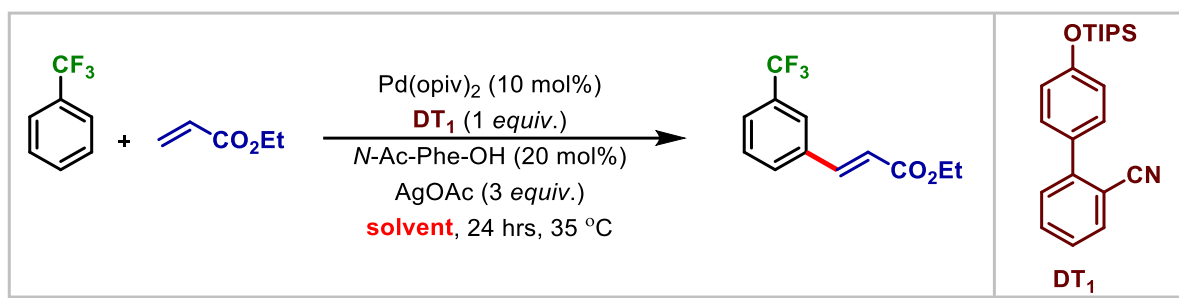
Entry	Oxidant	Yield(%) and selectivity (o:m:p)
1.	AgOAc	37 (1:6:2.2)
2.	Ag ₂ CO ₃	9 (1:6:2.2)
3.	AgTFA	trace
4.	Ag ₂ O	NR
5.	AgNO ₂	5 (1:5.4:2)
6.	AgCN	NR
7.	Ag ₃ PO ₄	NR
8.	AgPF ₆	NR
9.	AgOTf	7 (1:5.2:2.3)
10.	AgNO ₃	NR

4.3: Table 3: Ligand optimization:



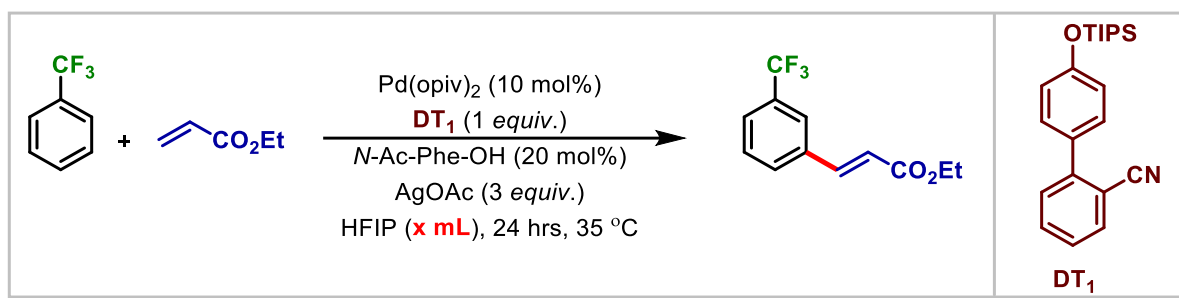
MPAA Ligand					
37% 1:6:2.2 (o:m:p)	39% 1:10.5:3.3 (o:m:p)	31% 3.7:1 (m:p)	28% 2:1 (m:p)		
35% 5.6:1 (m:p)	NR	NR	NR		
NR	NR	NR	NR		
Pyridone Ligand					
NR	NR	NR	NR	NR	NR

4.4: Table 4: Solvent optimization:



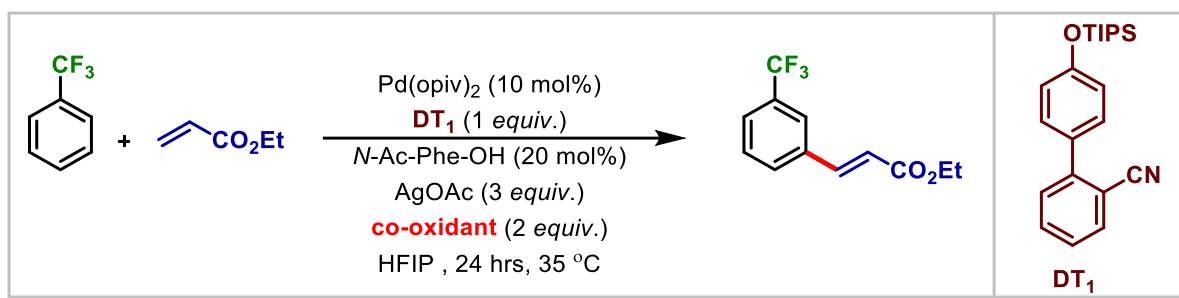
Entry	Solvent	Yield(%) and selectivity (o:m:p)
1.	HFIP	35 (5.6:1)
2.	DCE	NR
3.	1,2-Dibromoethane	NR
4.	THF	NR
5.	TFE	<5
6.	Hexafluorobenzene	NR
7.	Isopropanol	NR
8.	Methanol	NR
9.	DCB	NR
10.	MeCN	NR

4.5: Table 5: Solvent amount optimization:



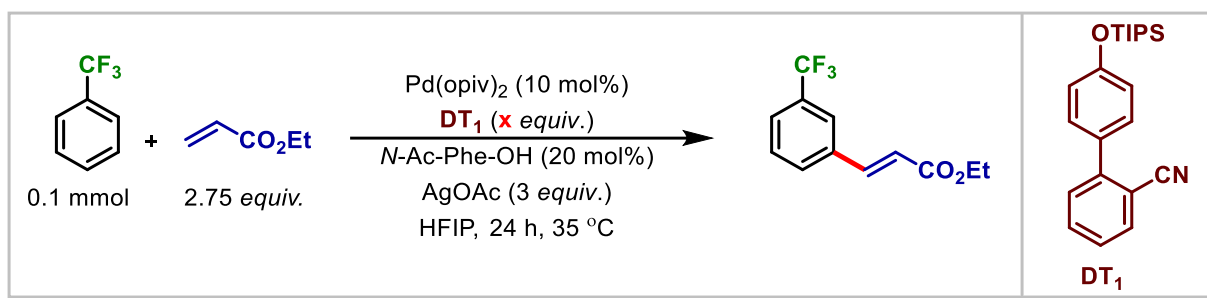
Entry	Solvent Amount	Yield(%) and selectivity (<i>m:p</i>)
1.	1.2	31 (4.8:1)
2.	1 mL	35 (5.6:1)
3.	0.8 mL	32 (5.2:1)
4.	0.6 mL	30 (4.9:1)
5.	0.4 mL	27 (4.8:1)
6.	0.2 mL	23 (4.8:1)

4.6: Table 6: Co-oxidant optimization:



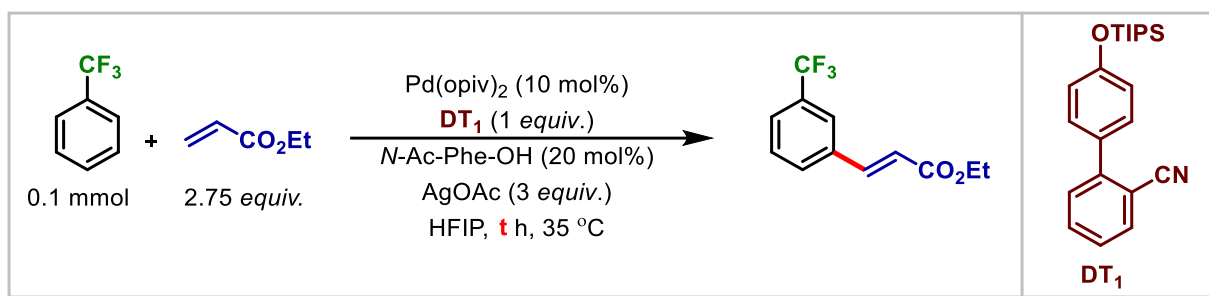
Entry	Co-Oxidant (Cu Salt)	Yield (%) and selectivity (<i>m:p</i>)
1.	CuCO_3	8 (3.3:1)
2.	$\text{Cu}_2\text{Cr}_2\text{O}_5$	11 (3.7:1)
3.	CuBr_2	6 (3.5:1)
4.	CuO	14 (3:1)
5.	$\text{Cu}(\text{OAc})_2$	19 (4.5:1)

4.7: Table 7: DT amount optimization:



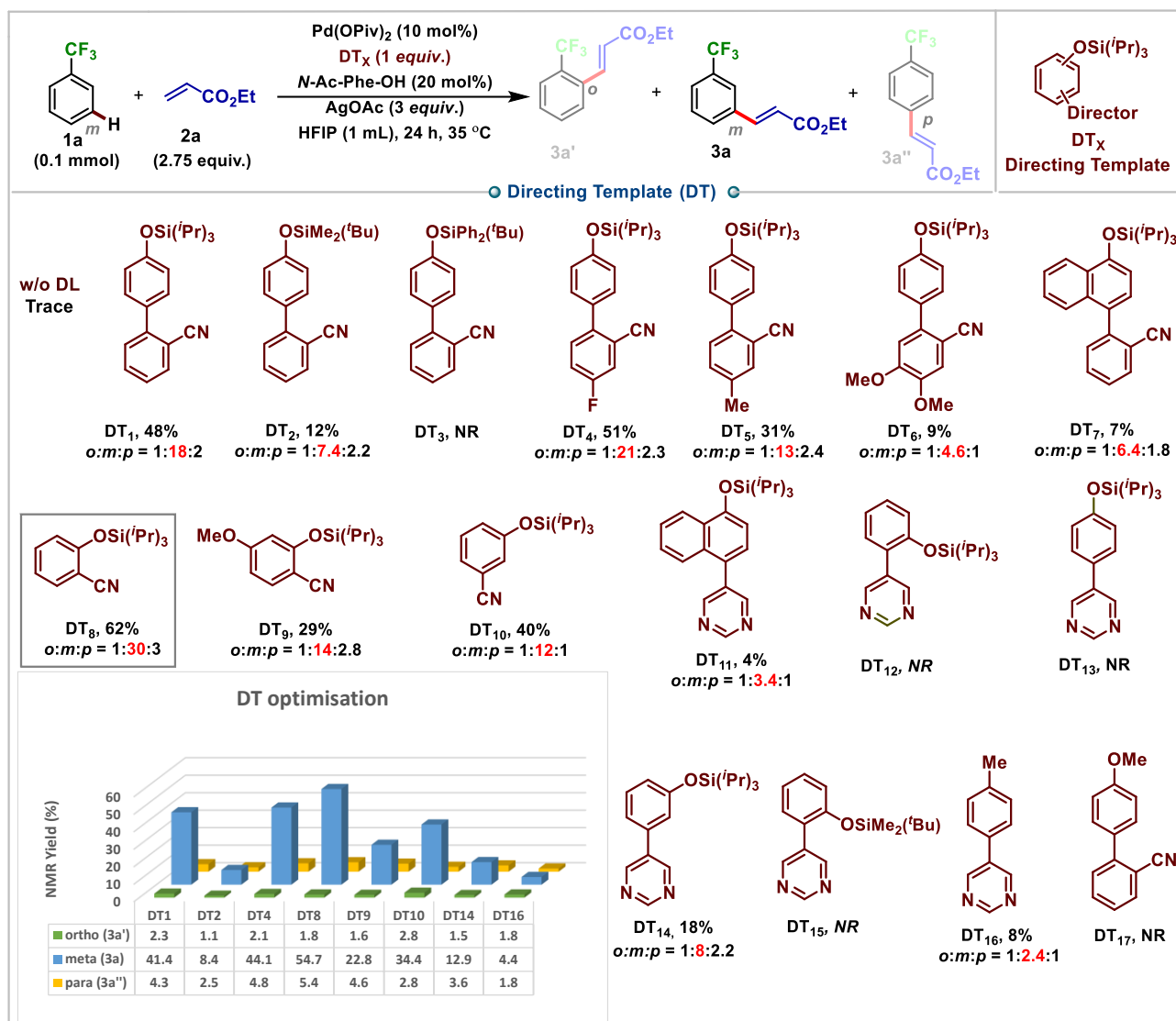
Entry	DT amount	Yield (%) and Selectivity (<i>m:p</i>)
1.	20 mol%	11 (4.9:1)
2.	40 mol%	19 (4.1:1)
3.	60 mol%	25 (4.5:1)
4.	80 mol%	28 (5.2:1)
5.	1 equiv.	35 (5.6:1)

4.8: Table 8: Time optimization:

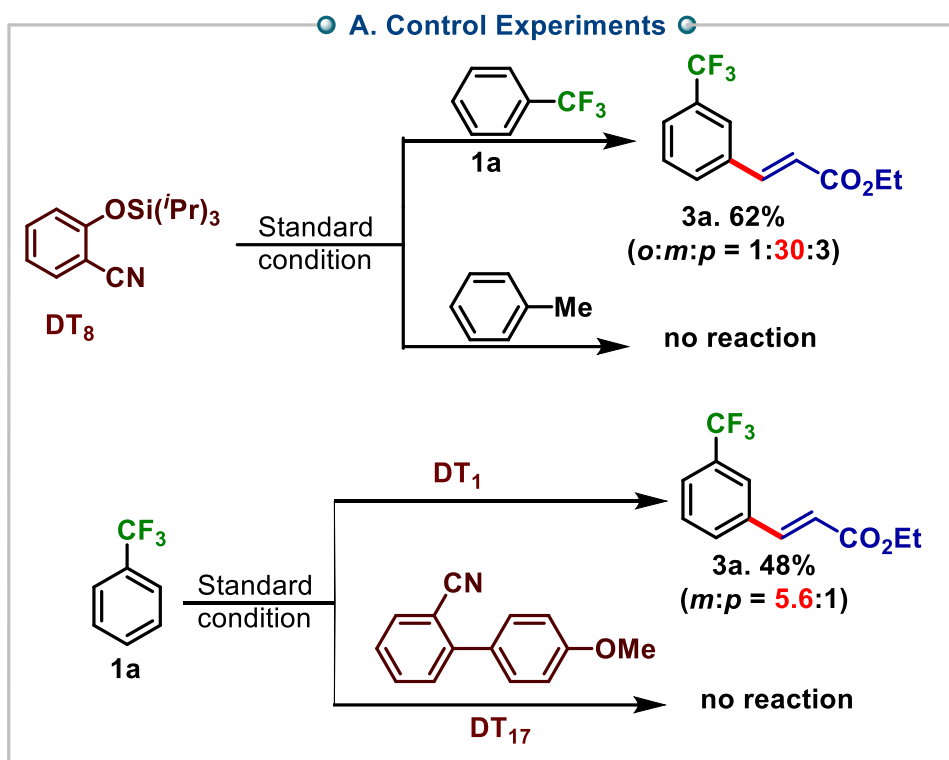


Entry	Time	Yield (%) and selectivity (<i>m:p</i>)
1.	12 h	19 (3.5:1)
2.	18 h	26 (3.9:1)
3.	24 h	35 (5.6:1)
4.	30 h	41 (5.4:1)
5.	36 h	48 (1:18:2)
6.	42 h	51 (5:1)

4.9: Table 9: Si-Directing Template (Si-DT):

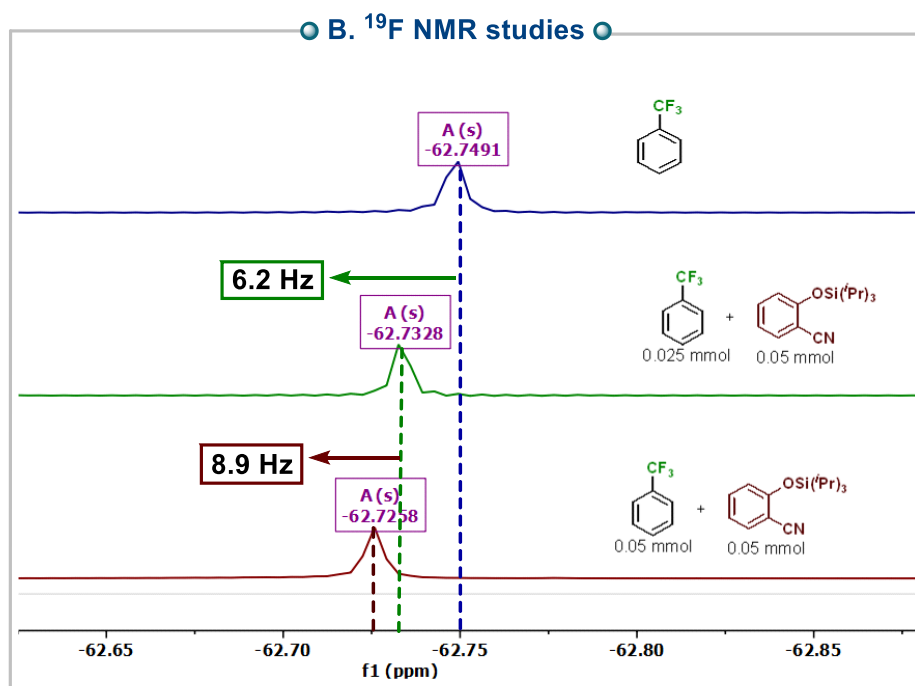


4. Control Experiment: A series of control experiments (Figure 6A) were used as a first step in understanding the mechanism of our protocol. When the trifluoromethyl substrate **1a** was replaced by toluene, no olefination product was observed. Similarly, no product formation was observed when the triisopropylsilyl (TIPS) protection of DT₁ was changed to the methyl protection of DT₁₇. These reactions justify the requirement of the fluorine-containing substrate as well as the presence of a silicon-containing directing group, which is consistent with our basic hypothesis of the Si–F interaction.

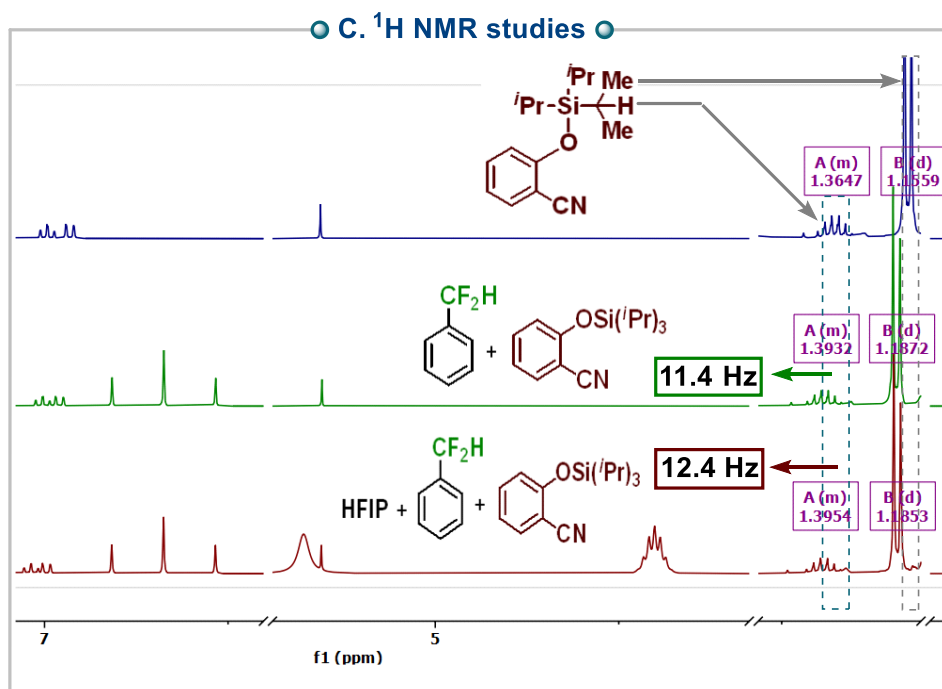


5. Mechanistic Studies:

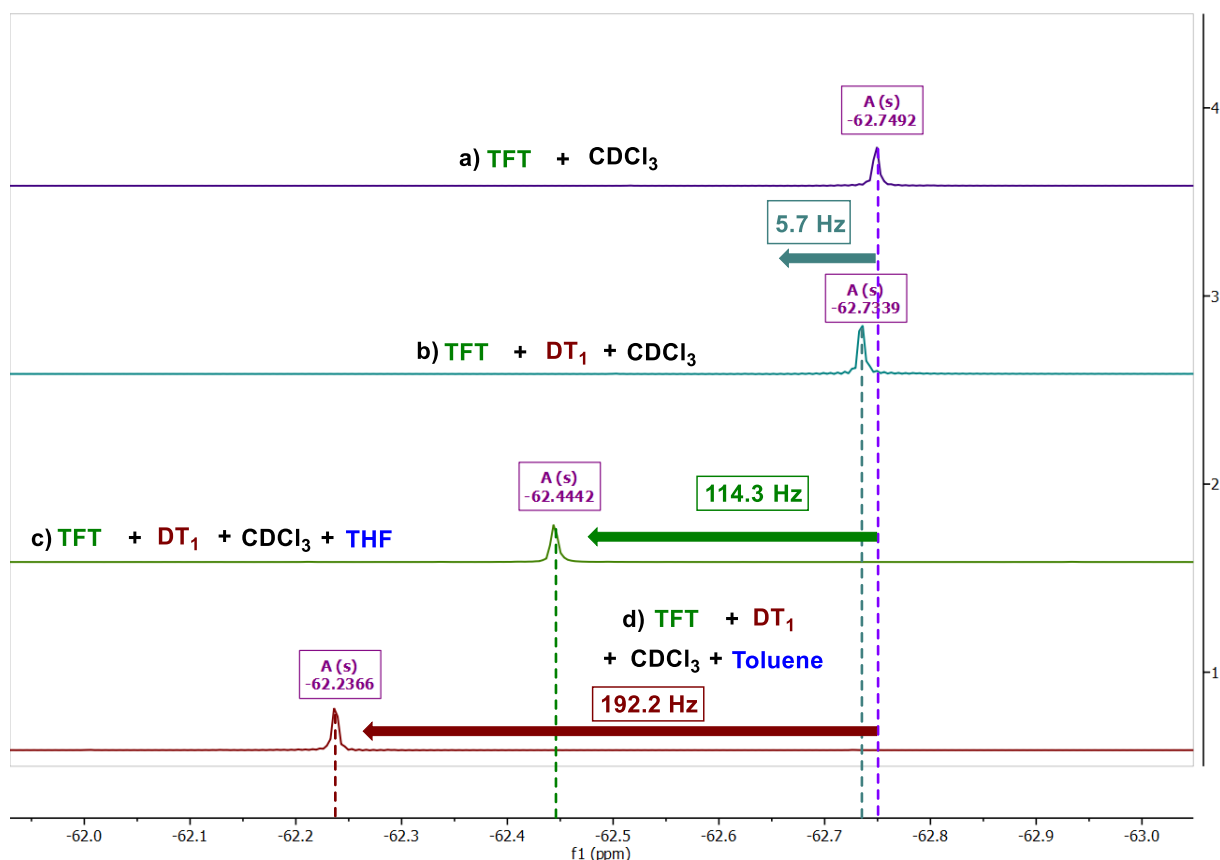
5.1: ^{19}F NMR studies for Si and F non-covalent interaction: This reaction confirms the necessity of a fluorine-containing substrate and a silicon-containing directing group, aligning with our basic hypothesis of Si/F interaction. To gather more evidence, we proceeded with NMR titration studies to explore the Si/F interaction. Starting with ^{19}F NMR studies, we used a mixture of trifluorotoluene and 0.5 equivalents of **DT**₈ in CDCl_3 , observing a significant shift of 6.2 Hz, which further increased to 8.9 Hz with equimolar quantities of **DT**₈.



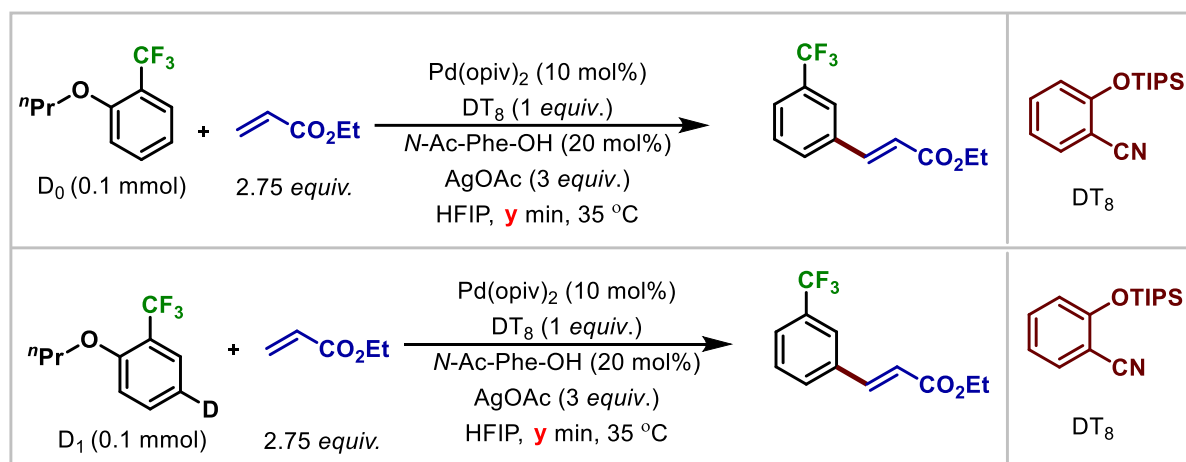
5.2: ^1H NMR studies for Si and F non-covalent interaction: A comparable shift was also observed in the ^1H NMR spectrum when the isopropyl protons of DT₈ were examined. Introduction of equimolar amounts of the substrate to DT₈ in CDCl_3 resulted in a significant shift of 11.7 Hz. The addition of HFIP to this mixture caused only a small shift (~ 0.9 Hz), ruling out the involvement of the fluorine atoms of HFIP in the Si/F interaction.



5.3: Solvent effect for Si and F non-covalent interaction: To verify the presence of non-covalent interactions with silicon and fluorine, ^{19}F NMR studies were carried out in different solvents in the presence of DT_1 and trifluoro toluene substrate. In the absence of DT_1 , the ^{19}F NMR peak came at -62.7492 ppm of trifluoro toluene (TFT) in CDCl_3 solvent. However, in the presence of an equimolecular amount of DT_1 , the ^{19}F NMR peaks shifted to 5.7 Hz. This indicates the presence of some interactions between silicon and fluorine. When we added 1 mL of THF and toluene along with TFT, DT_1 and CDCl_3 solvent, the ^{19}F NMR peaks shifted drastically to the down field up to 114.3 Hz and 192.2 Hz respectively. It is concluded that this noncovalent interaction between silicon and fluorine is dependent on the polarity of the solvent.



5.4: Parallel KIE determination:



The initial rates for the parallel experiments were determined according to general procedure C. Deuterium kinetic isotope effects (KIEs) were determined by dividing the initial rate of D-0 (k_H) by the initial rate of D-1 (k_D).

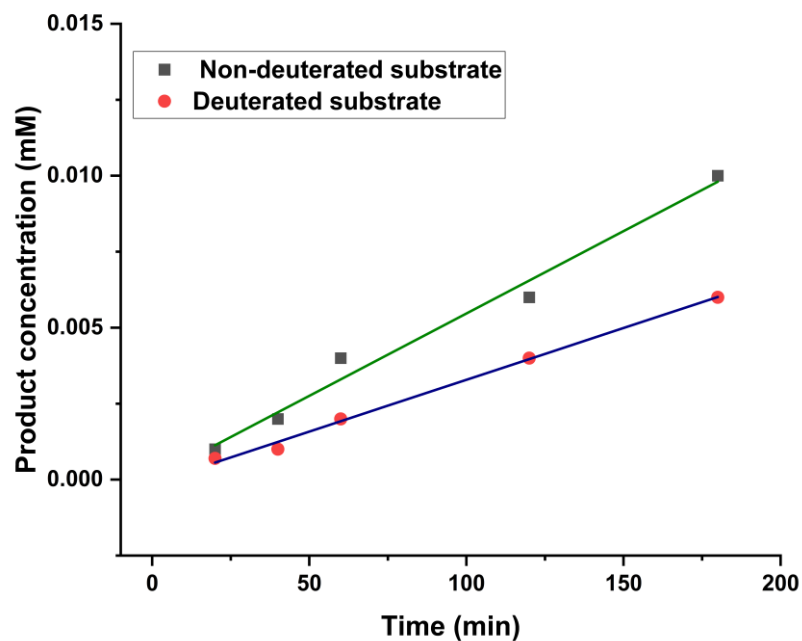
K_H/K_D experiments:

For D₀-deuterated Substrate

Entry	Time (min)	Concentration(mM)
1.	20	0.001
2.	40	0.002
3.	60	0.004
4.	120	0.006
5.	180	0.010

For D₁-deuterated Substrate

Entry	Time (min)	Concentration(mM)
1.	20	0.0005
2.	40	0.001
3.	60	0.002
4.	120	0.0035
5.	180	0.0055



$$\text{Parallel KIE} = 5.42 \times 10^{-5} / 3.40 \times 10^{-5} = 1.6$$

Plot of product (mM) vs. time (min) following general reaction conditions with linear fits for D-0 arene = 0.1 mmol (black), and D-1 arene = 0.1 mmol (red).

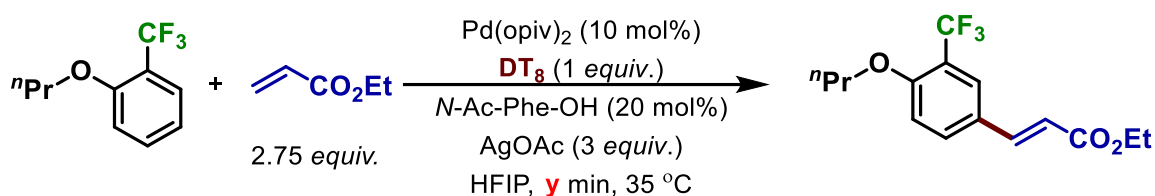
The substantial kinetic isotope effects observed indicate that the C–H activation step is not taking part in rate-limiting step.

5.5: Order determination studies:

Order determination studies were performed with respect to the substrate and aryl iodide. The general procedure was followed for all reactions; amount and components were varied necessarily. The yield of the olefination product in each reaction was measured by ^1H NMR of the crude reaction mixture using 1,4-bis(difluoromethyl)benzene as the internal standard. The product concentration (mM) was plotted against time (in minute). Here, we assume other than palladium acetate, the rate of the reaction is only dependent on concentration of the substrate, Olefin.

$$\text{So, rate} = k [\text{Subs}]^x [\text{Olefin}]^y \dots\dots\dots(1)$$

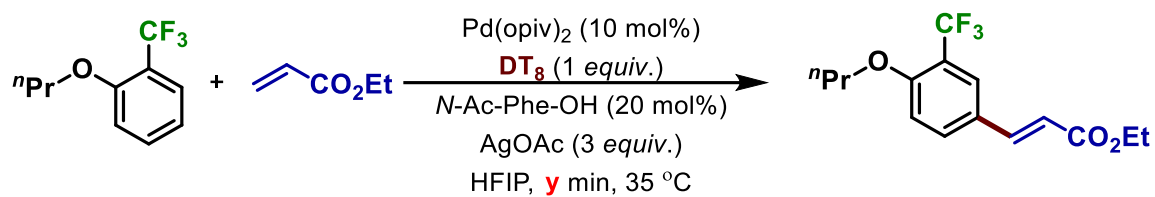
Run 1: Standard condition



Sr. No.	Substrate (mmol)	Olefin (mmol)	Pd(OPiv) ₂ (mmol)	DT ₈ (mmol)	N-Ac-Phe-OH (mmol)	AgOAc (mmol)
Run 1	0.1	0.275	0.01	0.1	0.02	0.3

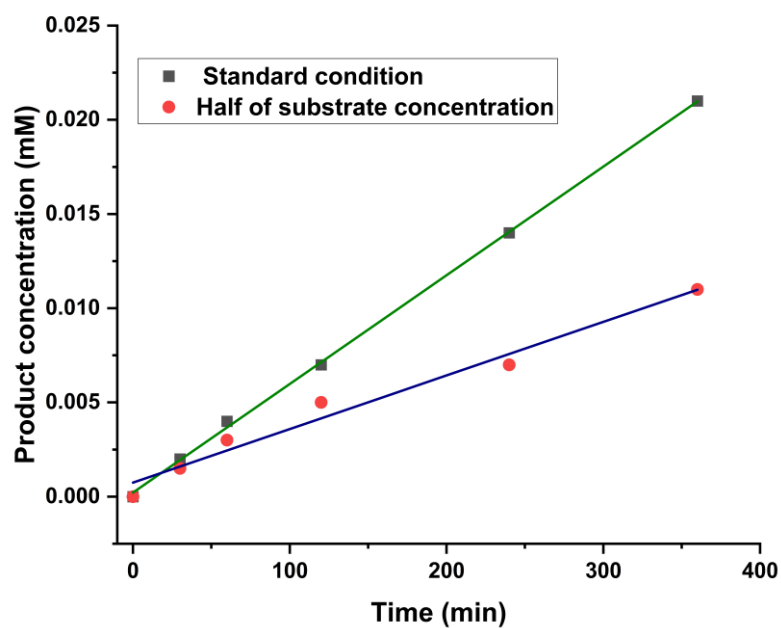
Entry	Time (min)	Product concentration (mM)
1	0	0
2	30	0.002
3	60	0.004
4	120	0.007
5	240	0.014
6	360	0.021

Run 2: Substrate concentration halved



Sr. No.	Substrate (mmol)	Olefin (mmol)	Pd(Opiv) ₂ (mmol)	DT ₈ (mmol)	N-Ac-Phe-OH (mmol)	AgOAc (mmol)
Run 2	0.05	0.275	0.01	0.1	0.02	0.3

Entry	Time (min)	Product concentration (mM)
1	0	0
2	30	0.0015
3	60	0.003
4	120	0.005
5	240	0.007
6	360	0.011



Run 1: Substrate (0.1 mmol)

$$\text{Rate} = [\text{substrate}]^x [\text{Olefin}]^y$$

For **Run 1**, initial rate, Rate 1 = $k \cdot [0.1]^x [0.275]^y$

$$5.76 \cdot 10^{-5} = k \cdot [0.1]^x [0.275]^y$$

Run 2: Substrate (0.05 mmol)

For **Run 2**, initial rate, Rate 2 = $k \cdot [0.05]^x [0.275]^y$

$$2.84 \cdot 10^{-5} = k \cdot [0.05]^x [0.275]^y$$

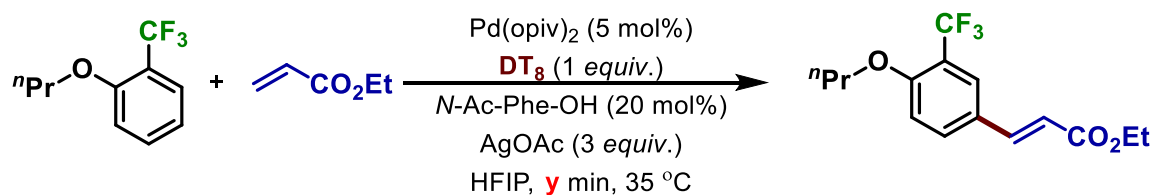
Hence, from Rate 2 / Rate 1 = $[0.5]^x$

$$\log (2.84 \cdot 10^{-5} / 5.76 \cdot 10^{-5}) = x \log (0.5)$$

$$x = 1.02 \sim 1$$

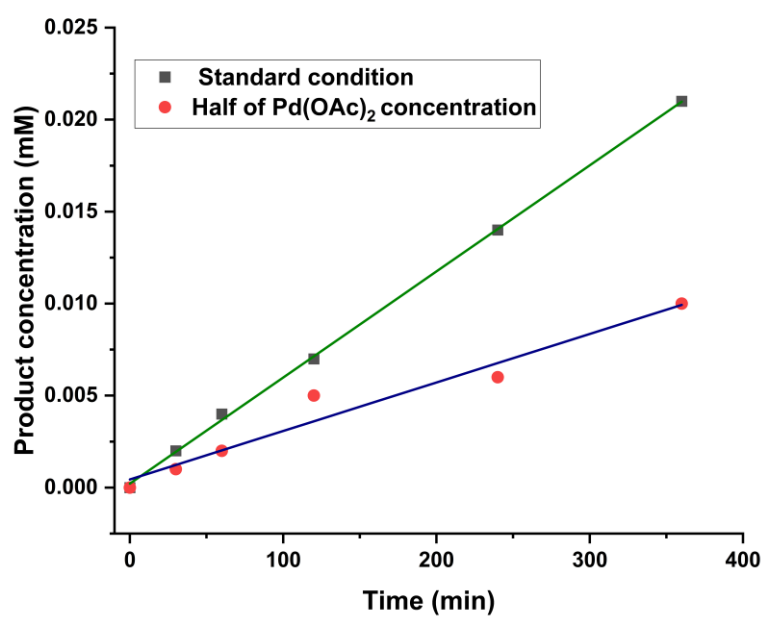
Order with respect to substrate is 1

Run 3: Pd(Opiv)₂ concentration halved:



Sr. No.	Substrate (mmol)	Olefin (mmol)	Pd(Opiv) ₂ (mmol)	DT ₈ (mmol)	N-Ac-Phe-OH (mmol)	AgOAc (mmol)
Run 3	0.1	0.275	0.005	0.1	0.02	0.3

Entry	Time (min)	Product concentration (mM)
1	0	0
2	30	0.001
3	60	0.002
4	120	0.005
5	240	0.006
6	360	0.010



Run 1: Pd (10 mol%)

$$\text{Rate} = [\text{substrate}]^x [\text{Olefin}]^y [\text{Pd}]^z$$

For **Run 1**, initial rate, Rate 1 = $k \cdot [0.1]^x [0.275]^y [\text{Pd}]^z$

$$5.76 \cdot 10^{-5} = k \cdot [0.1]^x [0.275]^y [\text{Pd}]^z$$

Run 3: Pd (5 mol%)

For **Run 3**, initial rate, Rate 3 = $k \cdot [0.1]^x [0.275]^y [0.5\text{Pd}]^z$

$$2.64 \cdot 10^{-5} = k \cdot [0.1]^x [0.275]^y [0.5\text{Pd}]^z$$

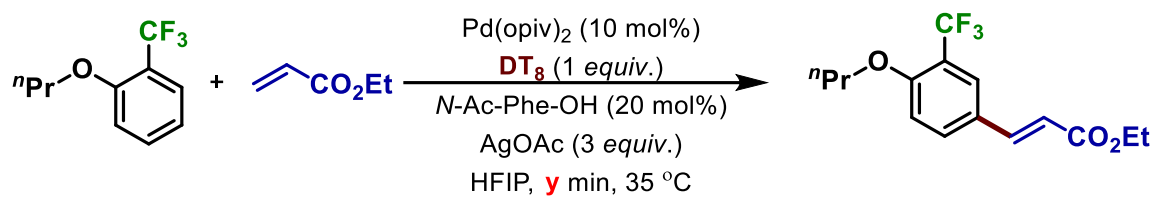
Hence, from Rate 3 / Rate 1 = $[0.5]^z$

$$\log (2.64 \cdot 10^{-5} / 5.76 \cdot 10^{-5}) = z \log (0.5)$$

$$z = 1.12 \sim 1$$

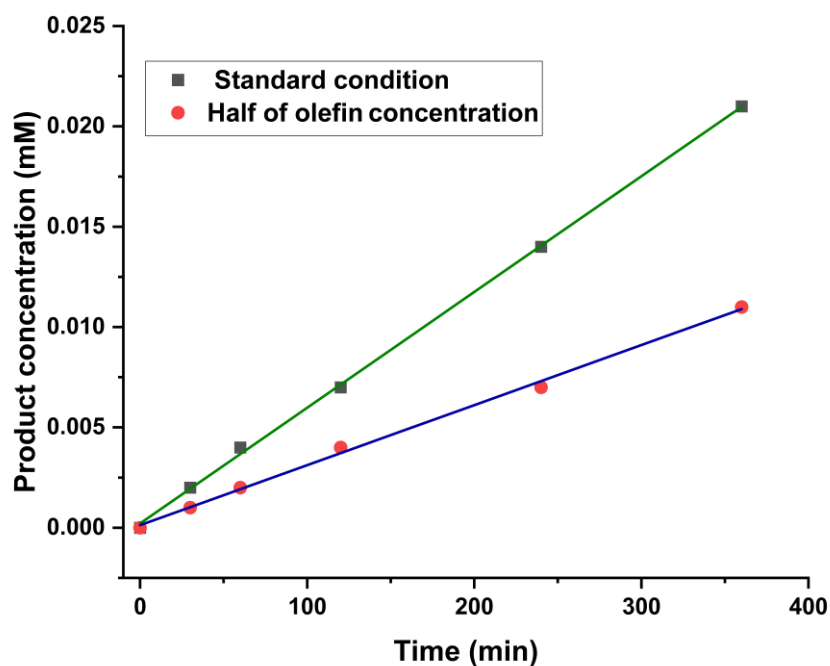
Order with respect to Pd(Opiv)₂ = 1.

Run 4: Olefin concentration halved.



Sr. No.	Substrate (mmol)	Olefin (mmol)	Pd(OPiv) ₂ (mmol)	DT ₈ (mmol)	N-Ac-Phe-OH (mmol)	AgOAc (mmol)
Run 4	0.1	0.0137	0.01	0.1	0.02	0.3

Entry	Time (min)	Product concentration (mM)
1	0	0
2	30	0.001
3	60	0.002
4	120	0.004
5	240	0.007
6	360	0.011



Run 1: Olefin (0.275 mmol)

$$\text{Rate} = [\text{substrate}]^x [\text{Olefin}]^y$$

For **Run 1**, initial rate, Rate 1 = $k \cdot [0.1]^x [0.275]^y$

$$5.76 \cdot 10^{-5} = k \cdot [0.1]^x [0.275]^y$$

Run 4: Olefin (0.137 mmol)

For **Run 4**, initial rate, Rate 4 = $k \cdot [0.1]^x [0.137]^y$

$$2.99 \cdot 10^{-5} = k \cdot [0.05]^x [0.137]^y$$

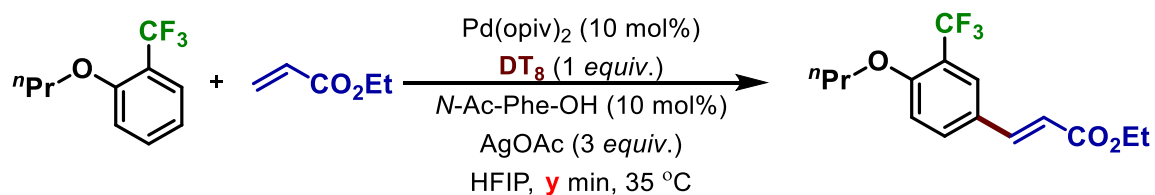
Hence, from Rate 4 / Rate 1 = $[0.5]^y$

$$\log (2.99 \cdot 10^{-5} / 5.76 \cdot 10^{-5}) = y \log (0.5)$$

$$y = 0.95 \sim 1$$

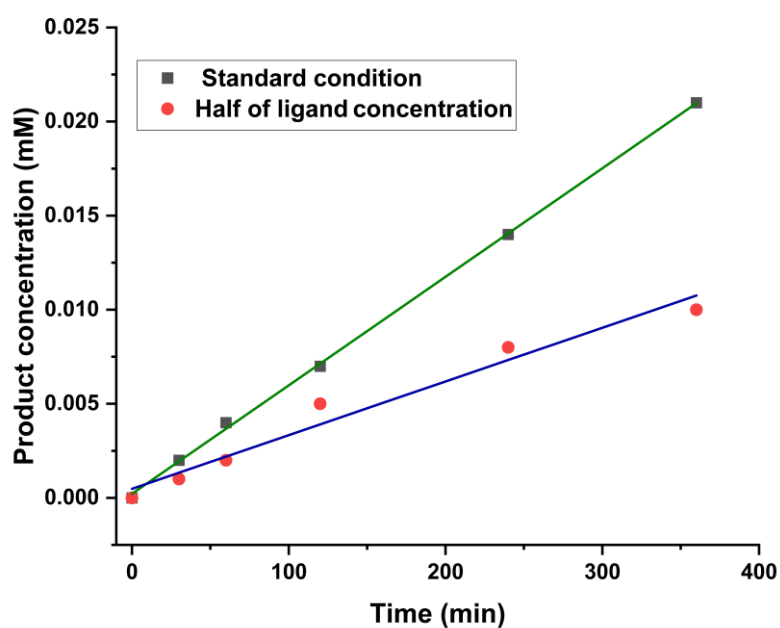
Order with respect to Olefin = 1.

Run 5: Ligand concentration 0.5 times:



Sr. No.	Substrate (mmol)	Olefin (mmol)	Pd(OPiv) ₂ (mmol)	DT ₈ (mmol)	<i>N</i> -Ac-Phe-OH (mmol)	AgOAc (mmol)
Run 5	0.1	0.275	0.01	0.1	0.01	0.3

Entry	Time (min)	Product concentration (mM)
1	0	0
2	30	0.001
3	60	0.002
4	120	0.005
5	240	0.008
6	360	0.010



Run 1: Ligand (20 mol%)

$$\text{Rate} = [\text{substrate}]^x [\text{Olefin}]^y [\text{ligand}]^z$$

For **Plot 2**, initial rate, Rate 1 = $k \cdot [0.1]^x [0.275]^y [0.02]^z$

$$5.76 \cdot 10^{-5} = k \cdot [0.1]^x [0.275]^y [0.02]^z$$

Run 5: Ligand (10 mol%)

For **Plot 4**, initial rate, Rate 5 = $k \cdot [0.1]^x [0.275]^y [0.01]^z$

$$2.85 \cdot 10^{-5} = k \cdot [0.1]^x [0.275]^y [0.01]^z$$

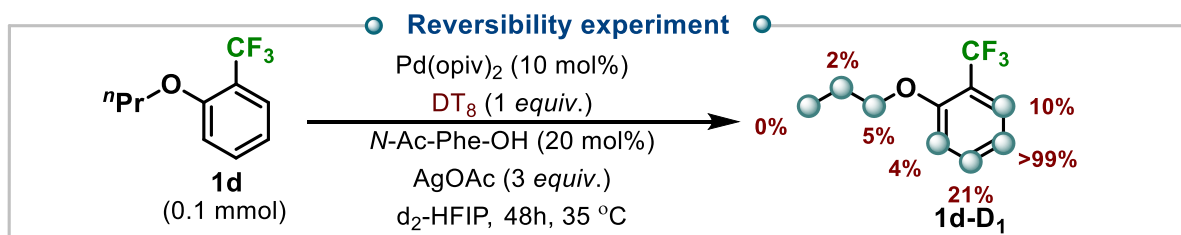
Hence, from Rate 5 / Rate 1 = $[0.5]^z$

$$\log (2.85 \cdot 10^{-5} / 5.76 \cdot 10^{-5}) = z \log (0.5)$$

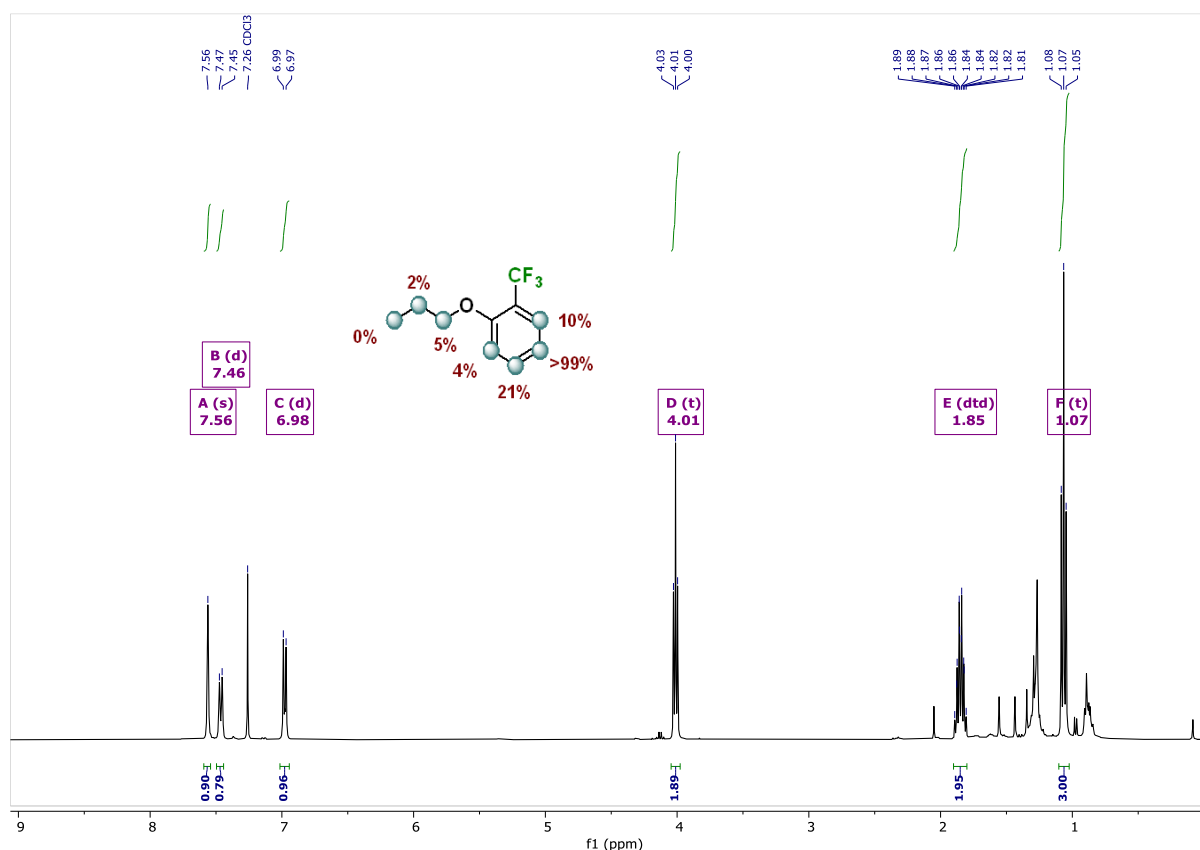
$$z = 1.02 \sim 1$$

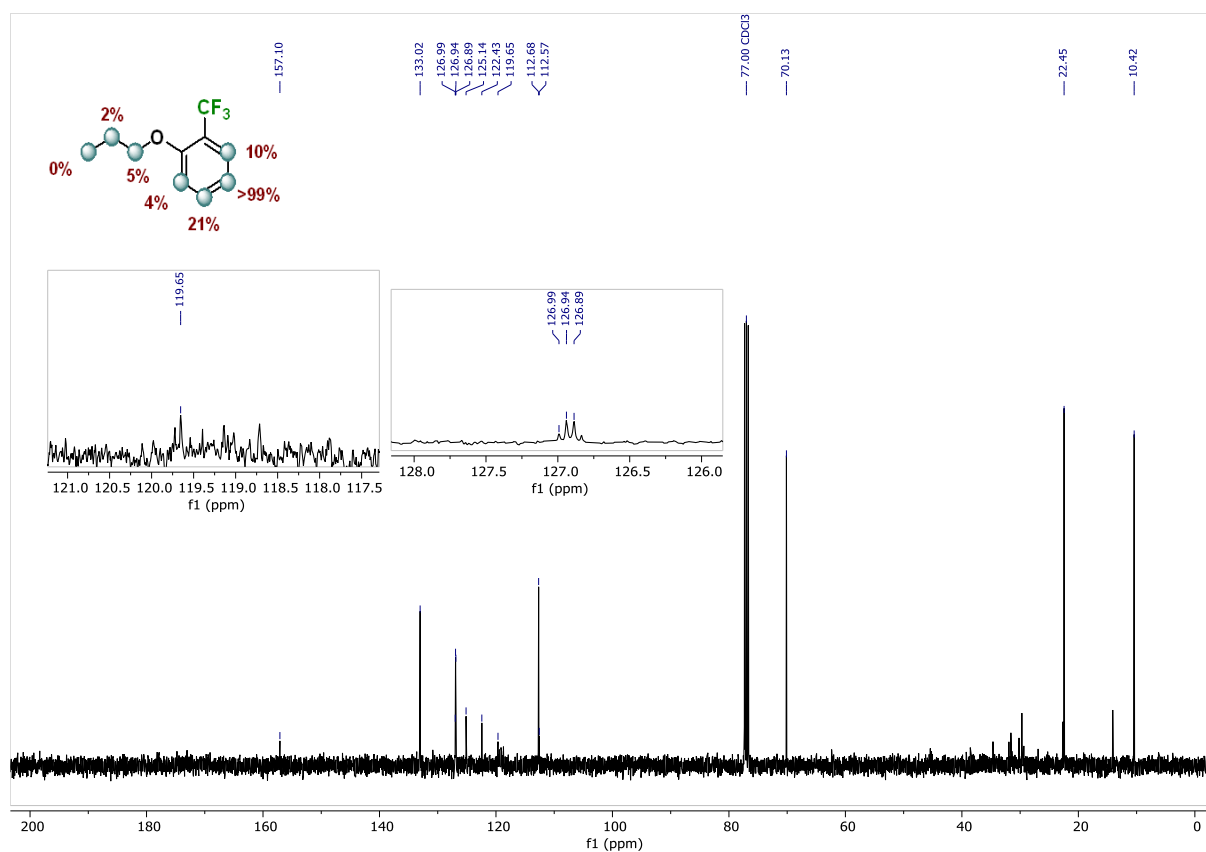
Order with respect to Ligand = 1.

5.6: Reversibility Experiments:

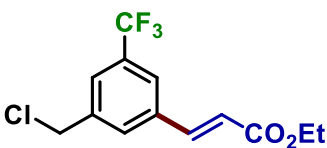
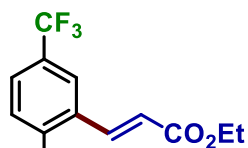
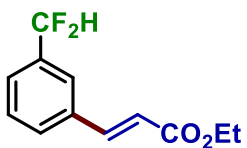


Reversibility of the *m*-C–H activation step was performed by using d₂-HFIP at room temperature. Deuterium scrambling was predominantly observed at the *meta*-position relative to the CF₃ group and the *para*-position relative to the alkoxy group, along with other positions in the recovered starting material. This suggest reversible nature of the C–H activation step and it is not likely to be the rate determining step of the reaction. Interestingly, kinetic isotope effect study of the corresponding **1d** substrate gave a value of 1.2, which is in agreement with our hypothesis that C–H activation is not the r.d.s. of the reaction. Also order determination study showed that reaction follows first order kinetics w.r.t. **1d** and olefine.





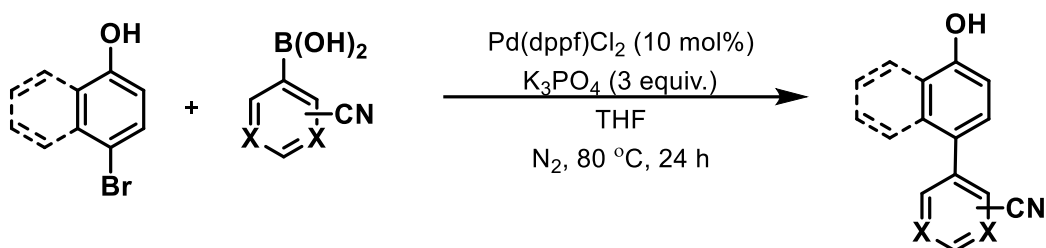
5.7: Competitive studies:

G. Competitive Studies			
			
	3f	3i	5a
Si-F interaction ^a :	52% (<i>m:others</i> > 20:1)	68% (<i>m:o</i> > 20:1)	59% (<i>o:m:p</i> = 1:13:3.5)
Non-directed ^b :	15% (<i>m:others</i> = 4:1)	24% (<i>m:o</i> = 5:1)	31% (<i>m:p</i> = 1.7:1)

Reaction was performed with 0.05 mmol of tri- and di- fluoro-methyl substrate according to the general procedure for Pd-catalysed alkenylation of fluoroalkyl arene in absence of **DT8**. The resulting solution was diluted with ethyl acetate, filtered on celite pad and ¹H NMR was recorded for the crude reaction mixture. The reaction mixture was mixed with 0.05 mmol of 4-fluoro-triifluoromethyl benzene to be considered as internal standard. Alkenylated product was formed with lower yield and with very low regioselectivity. Hence, the presence of **DT8** is playing a crucial role in this protocol.

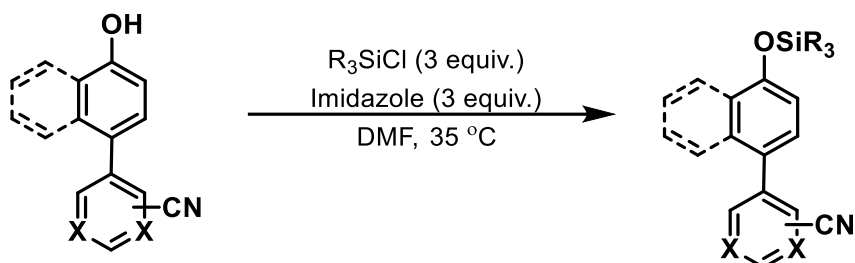
6. Directing Template (DT) synthesis:

Step 1:



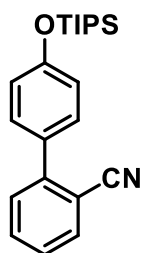
In an oven dried reaction tube, charged with stir-bar then Pd(dppf)Cl₂ (5 mol%), 2-cyano-bromo benzene or bromo-pyrimidine derivative or bromo-cyano derivative (2.0 mmol), hydroxyphenyl boronic acid (2.4 mmol) and K₃PO₄ (3.0 equiv.) were added. The reaction tubes were capped with Teflon cap and purged with N₂. THF was added to the reaction mixture (3 mL) and placed in a preheated 80 °C oil bath and allowed for vigorous stirring for 24 h. After 24 h, reaction mixture was allowed to cool and diluted with ethyl acetate and extracted with EtOAc for three times. The organic layer was dried over Na₂SO₄ and concentrated via evaporation. Concentrated organic part was purified by column chromatography. The solid coupling compound was isolated using ethyl acetate and petroleum ether as an eluent.

Step 2:



In an oven-dried Schlenk tube equipped with a PTFE-coated stirring bar, the mixture of phenol derivatives (2.0 mmol, 1.0 equiv.) and imidazole (6.0 mmol, 3.0 equiv.) in dimethylformamide (DMF, 6.0 mL) were added. Then, tri-alkyl silyl chloride (6.0 mmol, 3 equiv.) was added in dropwise fashion into the dimethylformamide solution. After stirring for 12 h at room temperature, NaHCO₃ (aq) was added to the reaction mixture. The organic phase was washed with NaCl (aq) three times, dried over Na₂SO₄, filtered, and concentrated under reduced pressure. The resulting residue was purified by flash column chromatography using ethyl acetate and petroleum ether as an eluent.

7. Characterization of spectral data of Directing Template (DT):



4'-((triisopropylsilyl)oxy)-[1,1'-biphenyl]-2-carbonitrile (Figure 2, DT₁):

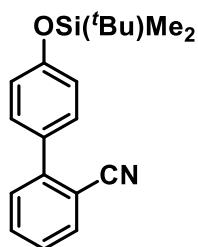
Yield: 81%

Eluent: 20% ethyl acetate in pet ether

Physical state: Yellow liquid

¹H NMR (400 MHz, CDCl₃) δ 7.73 (dd, J = 7.7, 1.3 Hz, 1H), 7.61 (td, J = 7.6, 1.4 Hz, 1H), 7.49 (dd, J = 8.0, 1.2 Hz, 1H), 7.44 (d, J = 8.6 Hz, 2H), 7.38 (td, J = 7.6, 1.3 Hz, 1H), 6.99 (d, J = 8.6 Hz, 2H), 1.38 – 1.25 (m, 3H), 1.13 (d, J = 7.3 Hz, 18H).

¹³C NMR (101 MHz, CDCl₃) δ 156.77, 145.28, 133.75, 132.68, 130.76, 129.91, 129.86, 126.93, 120.08, 118.93, 110.96, 17.90, 12.66.



4'-((tert-butyldimethylsilyl)oxy)-[1,1'-biphenyl]-2-carbonitrile (Figure 2, DT₂):

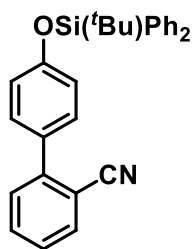
Yield: 81%

Eluent: 20% ethyl acetate in pet ether

Physical state: Yellow liquid

¹H NMR (400 MHz, CDCl₃) δ 7.73 (d, J = 7.7 Hz, 1H), 7.61 (t, J = 7.7 Hz, 1H), 7.49 (d, J = 7.9 Hz, 1H), 7.44 (d, J = 8.7 Hz, 2H), 7.39 (t, J = 7.6 Hz, 1H), 6.94 (d, J = 8.7 Hz, 2H), 1.01 (s, 9H), 0.25 (s, 6H).

¹³C NMR (101 MHz, CDCl₃) δ 156.37, 145.27, 133.77, 132.71, 131.06, 129.96, 129.90, 127.00, 120.23, 118.94, 110.99, 25.64, 18.20, -4.37.



4'-((tert-butyldiphenylsilyl)oxy)-[1,1'-biphenyl]-2-carbonitrile (Figure 2, DT₃):

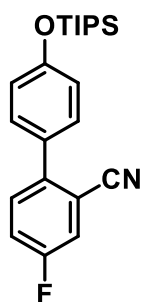
Yield: 81%

Eluent: 20% ethyl acetate in pet ether

Physical state: Yellow liquid

¹H NMR (400 MHz, CDCl₃) δ 7.78 – 7.66 (m, 6H), 7.57 (d, J = 7.7 Hz, 1H), 7.49 – 7.35 (m, 9H), 7.32 (d, J = 8.6 Hz, 1H), 6.88 (d, J = 8.7 Hz, 1H), 1.08 (s, 9H).

¹³C NMR (101 MHz, CDCl₃) δ 156.22, 135.49, 135.18, 134.78, 133.73, 132.65, 132.59, 130.83, 129.99, 129.84, 129.74, 129.61, 127.83, 127.69, 126.91, 119.93, 110.85, 30.90, 26.53.



4-fluoro-4'-((triisopropylsilyl)oxy)-[1,1'-biphenyl]-2-carbonitrile (Figure 2, DT₄):

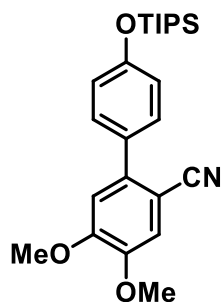
Yield: 81%

Eluent: 20% ethyl acetate in pet ether

Physical state: Yellow liquid

¹H NMR (400 MHz, CDCl₃) δ 7.49 – 7.41 (m, 2H), 7.39 (d, J = 8.6 Hz, 2H), 7.36 – 7.30 (m, 1H), 6.98 (d, J = 8.6 Hz, 2H), 1.33 – 1.29 (m, 3H), 1.13 (d, J = 7.3 Hz, 18H).

¹³C NMR (101 MHz, CDCl₃) δ 156.86, 131.82, 131.74, 129.90, 127.51, 124.45, 123.96, 120.52, 120.31, 120.23, 120.16, 119.99, 119.08, 117.62, 17.89, 12.66.



4,5-dimethoxy-4'-((triisopropylsilyl)oxy)-[1,1'-biphenyl]-2-carbonitrile (Figure 2, DT₆):

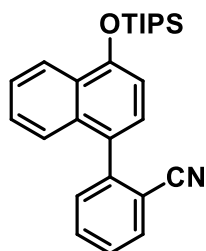
Yield: 81%

Eluent: 20% ethyl acetate in pet ether

Physical state: Yellow liquid

¹H NMR (400 MHz, CDCl₃) δ 7.41 (d, *J* = 8.6 Hz, 1H), 7.13 (s, 1H), 6.97 (d, *J* = 8.7 Hz, 1H), 6.91 (s, 1H), 3.96 (s, 2H), 3.93 (s, 2H), 1.37 – 1.23 (m, 2H), 1.12 (d, *J* = 7.4 Hz, 9H).

¹³C NMR (101 MHz, CDCl₃) δ 156.54, 152.47, 147.88, 140.12, 130.85, 129.77, 120.02, 119.33, 114.98, 112.30, 102.09, 56.25, 56.13, 17.91, 12.68.



2-((triisopropylsilyl)oxy)naphthalen-1-yl)benzonitrile (Figure 2, DT₇):

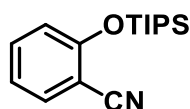
Yield: 81%

Eluent: 20% ethyl acetate in pet ether

Physical state: Yellow liquid

¹H NMR (500 MHz, CDCl₃) δ 8.29 (dd, *J* = 8.1, 3.0 Hz, 1H), 8.17 (dd, *J* = 8.5, 2.8 Hz, 1H), 7.59 (dd, *J* = 8.1, 2.6 Hz, 2H), 7.52 (ddd, *J* = 8.6, 5.2, 1.9 Hz, 1H), 6.76 (dd, *J* = 8.2, 2.5 Hz, 1H), 1.42 (dtd, *J* = 15.0, 7.5, 2.1 Hz, 3H), 1.16 (dd, *J* = 7.5, 2.5 Hz, 19H).

¹³C NMR (126 MHz, CDCl₃) δ 151.99, 132.91, 129.54, 128.93, 127.52, 126.97, 125.82, 123.15, 113.36, 112.38, 18.06, 13.01.



2-((triisopropylsilyl)oxy)benzonitrile (Figure 2, DT₈):

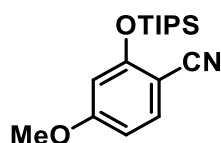
Yield: 81%

Eluent: 20% ethyl acetate in pet ether

Physical state: Yellow liquid

¹H NMR (400 MHz, CDCl₃) δ 7.51 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.41 (ddd, *J* = 8.4, 7.4, 1.8 Hz, 1H), 6.97 (td, *J* = 7.6, 1.0 Hz, 1H), 6.91 (dd, *J* = 8.4, 1.0 Hz, 1H), 1.42 – 1.27 (m, 3H), 1.13 (d, *J* = 7.4 Hz, 21H).

¹³C NMR (101 MHz, CDCl₃) δ 158.42, 133.97, 133.62, 121.00, 119.28, 116.97, 104.90, 17.65, 12.25.



4-methoxy-2-((triisopropylsilyl)oxy)benzonitrile (Figure 2, DT₉):

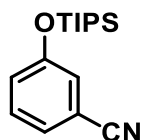
Yield: 81%

Eluent: 20% ethyl acetate in pet ether

Physical state: Yellow liquid

¹H NMR (400 MHz, CDCl₃) δ 7.42 (d, J = 8.7 Hz, 1H), 6.52 (dd, J = 8.7, 2.3 Hz, 1H), 6.41 (d, J = 2.3 Hz, 1H), 3.80 (s, 3H), 1.38 – 1.28 (m, 3H), 1.13 (d, J = 7.5 Hz, 18H).

¹³C NMR (101 MHz, CDCl₃) δ 164.09, 159.94, 134.52, 117.37, 107.09, 105.34, 97.14, 55.50, 17.66, 12.25.



3-((triisopropylsilyl)oxy)benzonitrile (Figure 2, DT₁₀):

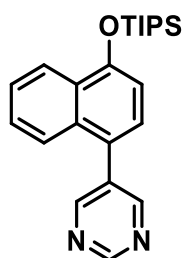
Yield: 81%

Eluent: 20% ethyl acetate in pet ether

Physical state: Yellow liquid

¹H NMR (500 MHz, CDCl₃) δ 7.31 (d, J = 7.9 Hz, 1H), 7.22 (d, J = 7.6 Hz, 1H), 7.13 (s, 1H), 7.10 (d, J = 5.9 Hz, 1H), 1.31 – 1.21 (m, 3H), 1.09 (d, J = 7.5 Hz, 18H).

¹³C NMR (126 MHz, CDCl₃) δ 156.40, 130.36, 124.87, 124.79, 123.14, 118.70, 113.11, 17.78, 17.67, 12.55, 12.25.

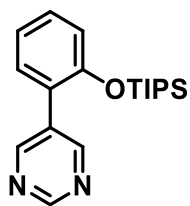


5-(4-((triisopropylsilyl)oxy)naphthalen-1-yl)pyrimidine (Figure 2, DT₁₁):

Yield: 81%

Eluent: 20% ethyl acetate in pet ether

Physical state: Yellow liquid



5-(2-((triisopropylsilyl)oxy)phenyl)pyrimidine (Figure 2, DT₁₂):

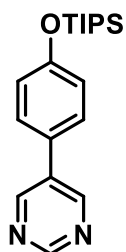
Yield: 81%

Eluent: 20% ethyl acetate in pet ether

Physical state: Yellow liquid

¹H NMR (400 MHz, CDCl₃) δ 9.11 (s, 1H), 8.85 (s, 2H), 7.25 (d, J = 7.3 Hz, 2H), 7.02 (td, J = 7.5, 1.1 Hz, 1H), 6.93 (d, J = 8.1 Hz, 1H), 1.21 – 1.08 (m, 3H), 0.94 (d, J = 7.5 Hz, 18H).

¹³C NMR (101 MHz, CDCl₃) δ 156.87, 156.78, 153.30, 132.86, 130.41, 130.20, 125.48, 121.55, 119.20, 17.75, 12.85.



5-(4-((triisopropylsilyl)oxy)phenyl)pyrimidine (Figure 2, DT₁₃):

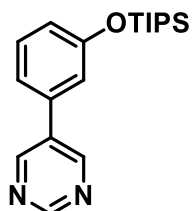
Yield: 81%

Eluent: 20% ethyl acetate in pet ether

Physical state: Yellow liquid

¹H NMR (400 MHz, CDCl₃) δ 9.14 (s, 1H), 8.91 (s, 2H), 7.45 (d, J = 8.6 Hz, 2H), 7.01 (d, J = 8.6 Hz, 2H), 1.41 – 1.21 (m, 3H), 1.12 (d, J = 7.3 Hz, 18H).

¹³C NMR (101 MHz, CDCl₃) δ 157.22, 156.77, 154.41, 134.01, 128.02, 126.70, 120.86, 17.88, 12.65.



5-(3-((triisopropylsilyl)oxy)phenyl)pyrimidine (Figure 2, DT₁₄):

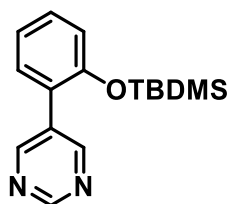
Yield: 81%

Eluent: 20% ethyl acetate in pet ether

Physical state: Yellow liquid

¹H NMR (400 MHz, CDCl₃) δ 9.20 (s, 1H), 8.92 (s, 2H), 7.36 (t, *J* = 7.9 Hz, 1H), 7.15 (ddd, *J* = 7.6, 1.7, 0.9 Hz, 1H), 7.08 (t, *J* = 2.1 Hz, 1H), 6.98 (ddd, *J* = 8.1, 2.4, 1.0 Hz, 1H), 1.32 – 1.26 (m, 3H), 1.13 (d, *J* = 7.3 Hz, 18H).

¹³C NMR (101 MHz, CDCl₃) δ 157.47, 156.97, 154.86, 135.51, 134.17, 130.46, 120.44, 119.59, 118.41, 17.91, 12.69.



5-(2-((tert-butyldimethylsilyl)oxy)phenyl)pyrimidine (Figure 2, DT₁₅):

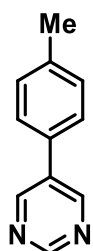
Yield: 81%

Eluent: 20% ethyl acetate in pet ether

Physical state: Yellow liquid

¹H NMR (400 MHz, CDCl₃) δ 9.15 (s, 1H), 8.88 (s, 2H), 7.37 – 7.28 (m, 2H), 7.08 (td, *J* = 7.5, 1.2 Hz, 1H), 6.99 – 6.85 (m, 1H), 0.83 (s, 9H), 0.05 (s, 6H).

¹³C NMR (101 MHz, CDCl₃) δ 156.94, 156.86, 152.91, 132.73, 130.38, 130.21, 126.00, 122.00, 120.06, 25.49, 18.03, -4.39.



5-(p-tolyl)pyrimidine (Figure 2, DT₁₆):

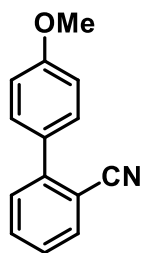
Yield: 81%

Eluent: 20% ethyl acetate in pet ether

Physical state: Yellow liquid

¹H NMR (400 MHz, CDCl₃) δ 9.17 (s, 1H), 8.93 (s, 2H), 7.47 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 7.9 Hz, 2H), 2.42 (s, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 157.15, 154.67, 139.10, 134.22, 131.26, 130.11, 126.76, 21.18.



4'-methoxy-[1,1'-biphenyl]-2-carbonitrile (Figure 2, DT₁₇):

Yield: 81%

Eluent: 20% ethyl acetate in pet ether

Physical state: Yellow liquid

¹H NMR (400 MHz, CDCl₃) δ 7.74 (d, J = 7.8 Hz, 1H), 7.62 (t, J = 7.7 Hz, 1H), 7.54 – 7.46 (m, 3H), 7.40 (t, J = 7.6 Hz, 1H), 7.02 (d, J = 8.8 Hz, 2H), 3.87 (s, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 160.04, 145.19, 133.73, 132.76, 130.50, 129.98, 129.86, 127.02, 118.97, 114.17, 111.01, 55.35.

8. Crystal data of 3a:

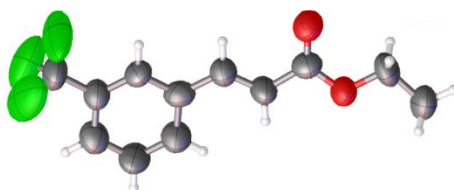
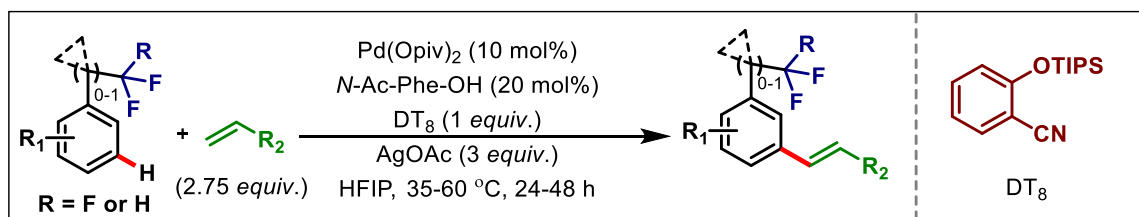


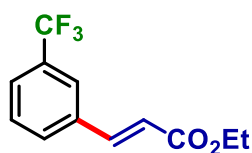
Table 1 Crystal data and structure refinement for 3a.	
Identification code	3a
Empirical formula	C ₂₄ H ₂₂ F ₆ O ₄
Formula weight	488.41
Temperature/K	298.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	9.129(2)
b/Å	11.280(3)
c/Å	11.308(3)
α /°	101.63(2)
β /°	92.39(2)
γ /°	94.33(2)
Volume/Å ³	1135.2(5)
Z	2
ρ_{calc} /cm ³	1.429
μ /mm ⁻¹	0.128
F(000)	504.0
Crystal size/mm ³	0.114 × 0.098 × 0.094
Radiation	Mo K α (λ = 0.71073)
2 θ range for data collection/°	3.684 to 49.998
Index ranges	-10 ≤ h ≤ 10, -13 ≤ k ≤ 13, -13 ≤ l ≤ 13
Reflections collected	14454
Independent reflections	3991 [R_{int} = 0.1457, R_{sigma} = 0.1622]
Data/restraints/parameters	3991/0/309
Goodness-of-fit on F ²	0.969
Final R indexes [$I \geq 2\sigma(I)$]	R_1 = 0.1169, wR_2 = 0.3132
Final R indexes [all data]	R_1 = 0.2961, wR_2 = 0.4383
Largest diff. peak/hole / e Å ⁻³	0.34/-0.29

9. General Procedure for palladium-catalyzed meta olefination of tri-fluorobenzene and di-fluorobenzene:



In an oven-dried screw capped reaction tube charged with magnetic stir-bar, substrate (fluoro alkyl arene) (1 equiv., 0.1 mmol), Pd(OAc)₂ (10 mol%, 2.24 mg), *N*-Ac-Phe-OH (20 mol%, 4.1 mg), Directing Template (DT₈) (1 equiv.), AgOAc (3 equiv.) in 1 mL of HFIP were added. After that, olefin (2.75 equiv.) was added to that reaction mixture. The reaction tube was well capped and placed in a RT (35 °C) or preheated oil bath at 60 °C with stirring (1000 rpm) for 36 h or 48 h. Upon completion of the reaction, the mixture was diluted with ethyl acetate and filtered through a celite pad. The filtrate was evaporated under reduced pressure and the crude mixture was purified by column chromatography using silica (100-200 mesh size) and petroleum ether/ethyl acetate as the eluent. The final meta-olefinated product was characterized by different spectroscopic techniques (¹H, ¹³C, ¹⁹F etc.).

10. Substrate scopes characterization data:



Ethyl (*E*)-3-(3-(trifluoromethyl)phenyl)acrylate (3a)¹:

Yield: 62% (15.2 mg)

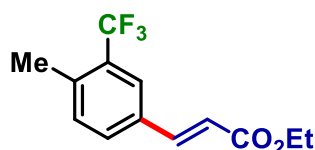
Eluent: 0.5% ethyl acetate in pet ether

Physical state: yellowish gammy liquid

¹H NMR (500 MHz, CDCl₃) δ 7.80 (s, 1H), 7.76 – 7.69 (m, 2H), 7.66 (d, *J* = 7.7 Hz, 1H), 7.55 (t, *J* = 7.7 Hz, 1H), 6.53 (d, *J* = 16.1 Hz, 1H), 4.31 (q, *J* = 7.1 Hz, 2H), 1.38 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (126 MHz, CDCl₃) δ 166.44, 142.74, 135.25, 131.44 (q, *J* = 32.6 Hz), 131.04, 129.43, 126.59 (q, *J* = 3.7 Hz), 124.56 (q, *J* = 3.8 Hz), 123.77 (q, *J* = 271.9 Hz), 120.26, 60.76, 14.27.

¹⁹F NMR (377 MHz, CDCl₃) δ -62.94.



Ethyl (*E*)-3-(4-methyl-3-(trifluoromethyl)phenyl)acrylate (3b):

Yield: 58% (15 mg)

Eluent: 1.5% ethyl acetate in pet ether

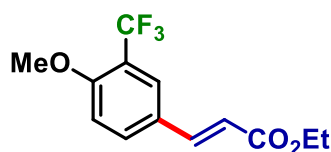
Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 7.71 (d, *J* = 26.7 Hz, 1H), 7.64 (s, 1H), 7.56 (d, *J* = 6.0 Hz, 1H), 7.31 (d, *J* = 7.9 Hz, 1H), 6.45 (d, *J* = 16.0 Hz, 1H), 4.27 (q, *J* = 7.1 Hz, 3H), 2.50 (s, 3H), 1.34 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 166.66, 142.89, 138.82, 132.55, 132.37, 130.73, 129.74, 125.28 (q, *J* = 5.6 Hz), 124.14 (q, *J* = 274.11 Hz), 122.77, 119.10, 114.09, 60.65, 19.32, 14.28.

¹⁹F NMR (377 MHz, CDCl₃) δ -62.03.

HRMS: [ESI, (+) ve]: calcd. [M+H] 259.0946 for (C₁₃H₁₄F₃O₂), found: 259.0940



Ethyl (*E*)-3-(4-methoxy-3-(trifluoromethyl)phenyl)acrylate (3c)²:

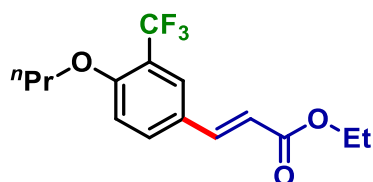
Yield: 72% (19.7 mg)

Eluent: 5% ethyl acetate in pet ether

Physical state: White solid

¹H NMR (400 MHz, CDCl₃) δ 7.74 (s, 1H), 7.68 – 7.56 (m, 2H), 7.01 (d, *J* = 8.6 Hz, 1H), 6.36 (d, *J* = 16.0 Hz, 1H), 4.26 (q, *J* = 7.1 Hz, 2H), 3.94 (s, 3H), 1.33 (t, *J* = 7.1 Hz, 3H).

¹⁹F NMR (377 MHz, CDCl₃) δ -62.84.



Ethyl (*E*)-3-(4-propoxy-3-(trifluoromethyl)phenyl)acrylate (3d):

Yield: 85% (25.6 mg)

Eluent: 5% ethyl acetate in pet ether

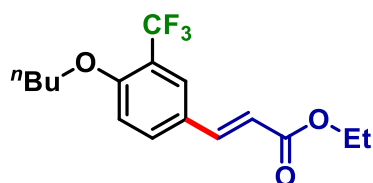
Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 7.73 (s, 1H), 7.66 – 7.59 (m, 2H), 6.98 (d, *J* = 8.6 Hz, 1H), 6.34 (d, *J* = 16.0 Hz, 1H), 4.26 (q, *J* = 7.1 Hz, 2H), 4.04 (t, *J* = 6.3 Hz, 2H), 1.85 (dtd, *J* = 13.6, 7.4, 6.2 Hz, 2H), 1.33 (t, *J* = 7.1 Hz, 3H), 1.05 (t, *J* = 7.4 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 166.89, 158.43, 142.89, 132.94, 126.76 (q, *J* = 5.2 Hz), 126.32, 123.26 (q, *J* = 272.6 Hz), 119.38 (q, *J* = 31.0 Hz), 117.22, 112.92, 70.43, 60.52, 22.33, 14.29, 10.36.

¹⁹F NMR (376 MHz, CDCl₃) δ -62.86.

HRMS: [ESI, (+) ve]: calcd. [M+H] 303.1208 for (C₁₅H₁₈F₃O₃), found: 303.1206



Ethyl (*E*)-3-(4-butoxy-3-(trifluoromethyl)phenyl)acrylate (3e):

Yield: 78% (24.7 mg)

Eluent: 5% ethyl acetate in pet ether

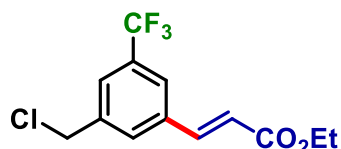
Physical state: yellowish liquid

¹H NMR (500 MHz, CDCl₃) δ 7.73 (s, 1H), 7.65 – 7.60 (m, 2H), 6.99 (d, *J* = 8.6 Hz, 1H), 6.35 (d, *J* = 16.0 Hz, 1H), 4.26 (q, *J* = 7.1 Hz, 2H), 4.08 (t, *J* = 6.3 Hz, 2H), 1.97 – 1.75 (m, 2H), 1.56 – 1.47 (m, 2H), 1.33 (t, *J* = 7.1 Hz, 3H), 0.97 (t, *J* = 7.4 Hz, 3H).

¹³C NMR (126 MHz, CDCl₃) δ 166.89, 158.44, 142.89, 132.95, 126.77 (q, *J* = 5.2 Hz), 126.34, 123.26 (q, *J* = 272.7 Hz), 119.41 (q, *J* = 30.9 Hz), 117.25, 112.94, 68.68, 60.52, 30.94, 19.00, 14.31, 13.69.

¹⁹F NMR (377 MHz, CDCl₃) δ -62.86.

HRMS: [ESI, (+) ve]: calcd. [M+H] 317.1365 for (C₁₆H₂₀F₃O₃), found: 317.1360



Ethyl (*E*)-3-(3-(chloromethyl)-5-(trifluoromethyl)phenyl)acrylate (3f):

Yield: 52% (15.2 mg)

Eluent: 1% ethyl acetate in pet ether

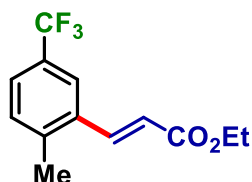
Physical state: yellowish liquid

¹H NMR (500 MHz, CDCl₃) δ 7.73 – 7.65 (m, 3H), 7.65 (s, 1H), 6.53 (d, *J* = 16.0 Hz, 1H), 4.63 (s, 2H), 4.28 (q, *J* = 7.1 Hz, 2H), 1.35 (t, *J* = 7.2 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 166.23, 142.05, 139.25, 135.98, 131.99 (q, *J* = 32.6 Hz), 130.96, 126.5 (q, *J* = 3.5 Hz), 124.43 (q, *J* = 3.6 Hz), 123.45 (q, *J* = 277.4 Hz), 120.99, 60.85, 44.75, 14.26.

¹⁹F NMR (377 MHz, CDCl₃) δ -62.92.

HRMS: [ESI, (+) ve]: calcd. [M+H] 293.0556 for (C₁₃H₁₃ClF₃O₃), found: 293.0555



Ethyl (*E*)-3-(2-methyl-5-(trifluoromethyl)phenyl)acrylate (3g)³:

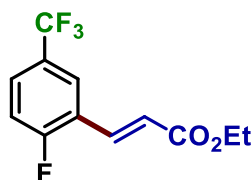
Yield: 59% (15.2 mg)

Eluent: 1.5% ethyl acetate in pet ether

Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 7.94 (d, *J* = 15.9 Hz, 1H), 7.77 (s, 1H), 7.51 (dd, *J* = 8.0, 1.9 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 1H), 6.42 (d, *J* = 15.9 Hz, 1H), 4.28 (q, *J* = 7.1 Hz, 2H), 2.48 (s, 1H), 1.35 (t, *J* = 7.1 Hz, 3H).

¹⁹F NMR (377 MHz, CDCl₃) δ -62.61.



Ethyl-(*E*)-3-(2-fluoro-5-(trifluoromethyl)phenyl)acrylate (3h)⁴:

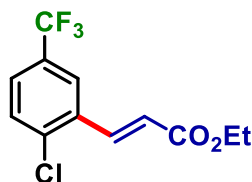
Yield: 66% (17.2 mg)

Eluent: 0.5% ethyl acetate in pet ether

Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 7.85 – 7.72 (m, 2H), 7.68 – 7.58 (m, 1H), 7.23 (t, *J* = 9.5 Hz, 1H), 6.60 (d, *J* = 16.3 Hz, 1H), 4.29 (q, *J* = 7.1 Hz, 2H), 1.35 (t, *J* = 7.1 Hz, 3H).

¹⁹F NMR (376 MHz, CDCl₃) δ -62.26, -109.15.



Ethyl (*E*)-3-(2-chloro-5-(trifluoromethyl)phenyl)acrylate (3i):

Yield: 68% (18.9 mg)

Eluent: 0.5% ethyl acetate in pet ether

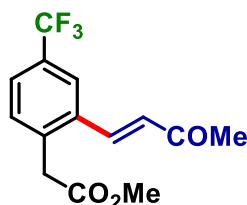
Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 8.06 (d, *J* = 16.0 Hz, 1H), 7.85 (s, 1H), 7.55 (d, *J* = 1.3 Hz, 2H), 6.50 (d, *J* = 16.0 Hz, 1H), 4.30 (q, *J* = 7.1 Hz, 2H), 1.35 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 165.97, 138.89, 138.26, 133.62, 130.79, 129.74 (q, *J* = 33.2 Hz), 127.25 (q, *J* = 3.9 Hz), 125.86 (q, *J* = 272.6 Hz), 124.55 (q, *J* = 3.7 Hz), 122.78, 60.96, 14.25.

¹⁹F NMR (377 MHz, CDCl₃) δ -62.83.

HRMS: [ESI, (+) ve]: calcd. [M+H] 279.0400 for (C₁₂H₁₁ClF₃O₂), found: 279.0402



Methyl (*E*)-2-(2-(3-oxobut-1-en-1-yl)-4-(trifluoromethyl)phenyl)acetate (3j):

Yield: 51% (14.5 mg)

Eluent: 10% ethyl acetate in pet ether

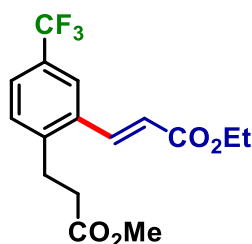
Physical state: yellowish liquid

¹H NMR (500 MHz, CDCl₃) δ 7.84 (s, 1H), 7.79 (d, J = 16.0 Hz, 1H), 7.60 (d, J = 7.8 Hz, 1H), 7.42 (d, J = 8.0 Hz, 1H), 6.71 (d, J = 15.9 Hz, 1H), 3.83 (s, 2H), 3.71 (s, 3H), 2.41 (s, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 197.61, 170.52, 138.52, 137.28, 134.98, 131.81, 130.40, 130.19 (q, J = 32.6 Hz), 126.57 (q, J = 3.6 Hz), 123.80 (q, J = 3.8 Hz), 123.69 (q, J = 273.6 Hz), 52.46, 38.76, 28.12.

¹⁹F NMR (377 MHz, CDCl₃) δ -62.85.

HRMS: [ESI, (+) ve]: calcd. [M+H] 287.0895 for (C₁₄H₁₄F₃O₃), found: 287.0890



Ethyl (*E*)-3-(2-(3-methoxy-3-oxopropyl)-5-(trifluoromethyl)phenyl)acrylate (3k):

Yield: 46% (15.1 mg)

Eluent: 1.5% ethyl acetate in pet ether

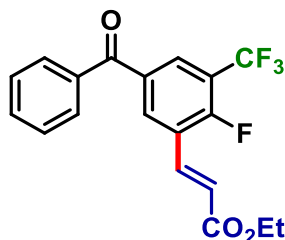
Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 7.96 (d, J = 15.8 Hz, 1H), 7.78 (s, 1H), 7.55 (d, J = 7.8 Hz, 1H), 7.37 (d, J = 8.1 Hz, 1H), 6.44 (d, J = 15.8 Hz, 1H), 4.29 (q, J = 7.1 Hz, 2H), 3.67 (s, 3H), 3.14 (t, J = 7.7 Hz, 2H), 2.61 (t, J = 7.7 Hz, 2H), 1.35 (t, J = 7.3 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 172.46, 166.34, 144.95, 143.49, 140.08, 133.96, 130.38, 126.41, 123.73, 122.09, 119.33, 60.83, 51.83, 34.78, 28.05, 14.27.

¹⁹F NMR (376 MHz, CDCl₃) δ -62.71.

HRMS: [ESI, (+) ve]: calcd. [M+H] 331.1157 for (C₁₆H₁₈F₃O₄), found: 331.1150



Ethyl (*E*)-3-(5-benzoyl-2-fluoro-3-(trifluoromethyl)phenyl)acrylate (3l):

Yield: 56% (20.5 mg)

Eluent: 2.5% ethyl acetate in pet ether

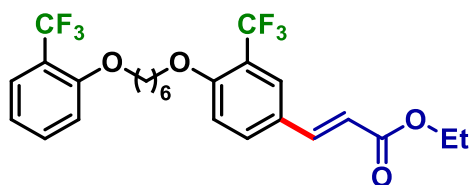
Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 8.12 (dd, J = 6.9, 2.2 Hz, 1H), 8.02 (ddd, J = 7.6, 4.8, 2.5 Hz, 1H), 7.90 (d, J = 1.8 Hz, 1H), 7.78 (d, J = 7.8 Hz, 1H), 7.76 – 7.69 (m, 2H), 7.55 (t, J = 7.7 Hz, 1H), 7.35 (t, J = 9.2 Hz, 1H), 6.50 (d, J = 16.0 Hz, 1H), 4.28 (q, J = 7.1 Hz, 2H), 1.34 (t, J = 7.1 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 193.26, 166.48, 162.27 (d, J = 266.6 Hz), 142.93, 141.17, 137.36, 135.84 (d, J = 9.8 Hz), 133.53 (d, J = 3.8 Hz), 132.04, 131.12, 129.24, 129.07, 128.10, 127.63, 122.03 (d, J = 273.8 Hz), 120.21, 117.27 (d, J = 21.1 Hz), 60.76, 14.28.

¹⁹F NMR (376 MHz, CDCl₃) δ -61.60 (d, J = 12.5 Hz), -106.95 (q, J = 12.5 Hz).

HRMS: [ESI, (+) ve]: calcd. [M+H] 367.0957 for (C₁₉H₁₅F₄O₃), found: 367.0956



Ethyl (*E*)-3-(3-(trifluoromethyl)-4-((6-(2-(trifluoromethyl)phenoxy)hexyl)oxy)phenyl)acrylate (3m):

Yield: 73% (36.7 mg)

Eluent: 7% ethyl acetate in pet ether

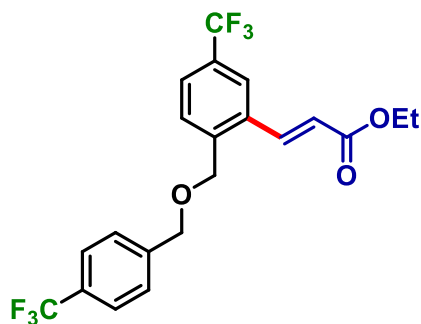
Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 7.72 (s, 1H), 7.67 – 7.58 (m, 2H), 7.55 (d, J = 8.7 Hz, 1H), 7.46 (t, J = 8.0 Hz, 1H), 6.98 (dd, J = 8.4, 6.0 Hz, 3H), 6.35 (d, J = 16.0 Hz, 1H), 4.26 (q, J = 7.1 Hz, 2H), 4.09 (t, J = 6.3 Hz, 2H), 4.05 (t, J = 6.2 Hz, 2H), 1.96 – 1.72 (m, 4H), 1.64 – 1.52 (m, 4H), 1.34 (t, J = 7.1 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 166.90, 158.36, 156.99, 142.89, 133.16, 132.97, 127.01 (q, J = 5.2 Hz), 126.76 (q, J = 5.2 Hz), 126.37, 125.76 (q, J = 273.7 Hz), 123.74 (q, J = 272.2 Hz), 119.72, 119.36 (q, J = 31.0 Hz), 118.78 (q, J = 29.8 Hz), 117.25, 112.95, 112.65, 68.67, 68.27, 60.53, 28.81, 28.70, 25.26, 25.22, 14.30.

¹⁹F NMR (377 MHz, CDCl₃) δ -62.41, -62.83.

HRMS: [ESI, (+) ve]: calcd. [M+H] 505.1814 for (C₂₅H₂₇F₆O₄), found: 505.1810



Ethyl-(*E*)-3-(5-(trifluoromethyl)-2-(((4-(trifluoromethyl)benzyl)oxy)methyl)phenyl)acrylate (3n):

Yield: 71% (30.6 mg)

Eluent: 8% ethyl acetate in pet ether

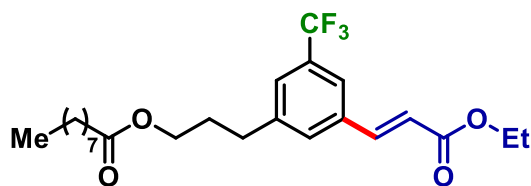
Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 7.97 (d, J = 15.9 Hz, 1H), 7.83 (d, J = 1.8 Hz, 1H), 7.65 – 7.55 (m, 4H), 7.49 (d, J = 8.0 Hz, 2H), 6.45 (d, J = 15.9 Hz, 1H), 4.71 (d, J = 15.9 Hz, 2H), 4.29 (q, J = 7.1 Hz, 2H), 1.34 (t, J = 7.1 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 166.32, 141.59, 140.26, 139.88, 134.20, 130.76 (q, J = 32.9 Hz), 130.07 (q, J = 32.5 Hz), 129.49, 127.71, 126.27 (q, J = 3.6 Hz), 125.47 (q, J = 3.7 Hz), 124.08 (q, J = 271.4 Hz), 123.73 (q, J = 273.4 Hz), 123.60 (q, J = 3.8 Hz), 122.03, 72.09, 69.83, 60.84, 14.26.

¹⁹F NMR (376 MHz, CDCl₃) δ -62.55, -62.81.

HRMS: [ESI, (+) ve]: calcd. [M+H] 433.1238 for (C₂₁H₁₉F₆O₃), found: 433.1233



(*E*)-3-(3-(3-ethoxy-3-oxoprop-1-en-1-yl)-5-(trifluoromethyl)phenyl)propylnonanoate (3o):

Yield: 67% (29.6 mg)

Eluent: 4% ethyl acetate in pet ether

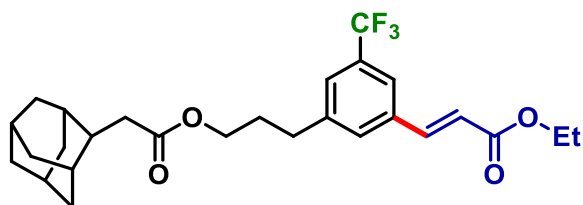
Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 7.67 (d, J = 16.0 Hz, 1H), 7.61 (s, 1H), 7.50 (s, 1H), 7.44 (s, 1H), 6.49 (d, J = 16.0 Hz, 1H), 4.28 (q, J = 7.1 Hz, 2H), 4.11 (t, J = 6.4 Hz, 2H), 2.77 (t, J = 7.8 Hz, 2H), 2.30 (t, J = 7.6 Hz, 2H), 2.05 – 1.93 (m, 2H), 1.69 – 1.59 (m, 2H), 1.36 – 1.20 (m, 13H), 0.87 (t, J = 6.7 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 173.84, 166.43, 143.09, 142.79, 135.44, 131.58 (q, *J* = 32.2 Hz), 131.11, 126.57 (q, *J* = 3.1 Hz), 124.39 (q, *J* = 272.1 Hz), 122.39 (q, *J* = 3.5 Hz), 120.21, 63.17, 60.73, 34.29, 32.04, 31.79, 29.96, 29.20, 29.16, 29.11, 24.97, 22.62, 14.27, 14.07.

¹⁹F NMR (376 MHz, CDCl₃) δ -62.79.

HRMS: [ESI, (+) ve]: calcd. [M+H] 443.2409 for (C₂₄H₃₄F₃O₄), found: 443.2408



(E)-3-(3-(3-ethoxy-3-oxoprop-1-en-1-yl)-5-(trifluoromethyl)phenyl)propyl nonanoate (3p):

Yield: 61% (29.2 mg)

Eluent: 3% ethyl acetate in pet ether

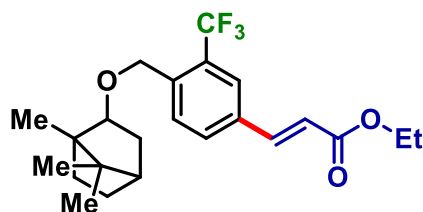
Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 7.67 (d, *J* = 16.1 Hz, 1H), 7.61 (s, 1H), 7.50 (s, 1H), 7.44 (s, 1H), 6.49 (d, *J* = 16.1 Hz, 1H), 4.27 (q, *J* = 7.1 Hz, 2H), 4.09 (t, *J* = 6.3 Hz, 2H), 2.78 (dd, *J* = 8.9, 6.7 Hz, 2H), 2.02 – 1.89 (m, 4H), 1.83 – 1.57 (m, 13H), 1.34 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 171.78, 166.43, 143.10, 142.80, 135.43, 131.58 (q, *J* = 32.3 Hz), 131.13, 126.58 (q, *J* = 3.5 Hz), 123.78 (q, *J* = 270.7 Hz), 122.38 (q, *J* = 3.9 Hz), 120.19, 62.82, 60.73, 48.93, 42.42, 36.69, 32.77, 32.12, 30.06, 28.57, 14.26.

¹⁹F NMR (376 MHz, CDCl₃) δ -62.78.

HRMS: [ESI, (+) ve]: calcd. [M+H] 479.2409 for (C₂₇H₃₄F₃O₄), found: 479.2401



Ethyl (E)-3-(3-(trifluoromethyl)-4-(((1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl)oxy)methyl)phenyl)acrylate (3q):

Yield: 47% (19.2 mg)

Eluent: 3% ethyl acetate in pet ether

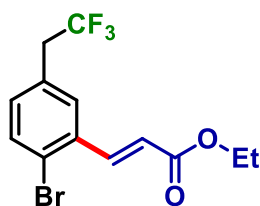
Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 7.86 – 7.72 (m, 2H), 7.72 – 7.64 (m, 2H), 6.47 (d, *J* = 16.1 Hz, 1H), 4.83 – 4.48 (m, 2H), 4.28 (qd, *J* = 7.1, 0.8 Hz, 2H), 3.37 (dd, *J* = 7.6, 3.5 Hz, 1H), 1.86 (dq, *J* = 12.7, 3.7 Hz, 1H), 1.79 – 1.63 (m, 3H), 1.58 – 1.48 (m, 1H), 1.40 – 1.30 (m, 4H), 1.05 (s, 3H), 0.97 (s, 3H), 0.84 (s, 3H).

¹³C NMR (101 MHz, CDCl₃) 166.60, 142.82, 133.20, 131.01, 128.88, 127.53 (q, *J* = 32.3 Hz), 124.90 (q, *J* = 5.6 Hz), 124.01 (q, *J* = 274.8 Hz), 120.61, 119.50, 87.36, 66.36, 60.69, 49.50, 46.53, 45.08, 38.29, 34.36, 27.25, 20.27, 20.23, 14.29, 11.96.

¹⁹F NMR (377 MHz, CDCl₃) δ -60.99.

HRMS: [ESI, (+) ve]: calcd. [M+H] 411.2147 for (C₂₃H₃₀F₃O₃), found: 411.2140



Ethyl (*E*)-3-(2-bromo-5-(2,2,2-trifluoroethyl)phenyl)acrylate (3r):

Yield: 46% (15.4 mg)

Eluent: 1% ethyl acetate in pet ether

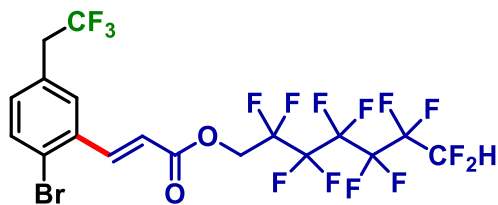
Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 8.01 (d, *J* = 15.9 Hz, 1H), 7.61 (d, *J* = 8.2 Hz, 1H), 7.51 (d, *J* = 2.0 Hz, 1H), 7.16 (d, *J* = 8.2 Hz, 1H), 6.40 (d, *J* = 16.1 Hz, 1H), 4.29 (q, *J* = 7.1 Hz, 2H), 3.35 (q, *J* = 10.6 Hz, 2H), 1.35 (t, *J* = 7.2 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 166.19, 142.33, 135.04, 133.75, 132.64, 129.94 (q, *J* = 2.8 Hz), 129.48 (q, *J* = 245.4 Hz), 129.44, 121.79, 118.88, 60.80, 39.69 (q, *J* = 30.2 Hz), 14.28.

¹⁹F NMR (376 MHz, CDCl₃) δ -65.88.

HRMS: [ESI, (+) ve]: calcd. [M+H] 337.0047 for (C₁₃H₁₃BrF₃O₂), found: 337.0041



2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoroheptyl (*E*)-3-(2-bromo-5-(2,2,2-trifluoroethyl)phenyl)acrylate (3s):

Yield: 46% (28.5 mg)

Eluent: 1% ethyl acetate in pet ether

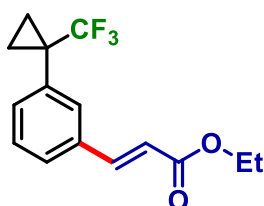
Physical state: yellowish liquid

¹H NMR (500 MHz, CDCl₃) δ 8.14 (d, *J* = 15.9 Hz, 1H), 7.63 (d, *J* = 8.2 Hz, 1H), 7.54 (s, 1H), 7.20 (dd, *J* = 8.3, 2.1 Hz, 1H), 6.45 (d, *J* = 16.0 Hz, 1H), 6.06 (tt, *J* = 51.9, 5.1 Hz, 1H), 4.74 (t, *J* = 13.5 Hz, 2H), 3.37 (q, *J* = 10.5 Hz, 2H).

¹³C NMR (126 MHz, CDCl₃) δ 164.42, 144.96, 134.36, 133.92, 133.73, 133.28, 130.81, 130.12 (q, *J* = 2.4 Hz), 129.54, 128.58, 125.40, 125.19 (q, *J* = 222.2 Hz), 119.20, 116.45, 109.58, 107.55, 59.83 (t, *J* = 22.2 Hz), 39.66 (q, *J* = 30.2 Hz).

¹⁹F NMR (376 MHz, CDCl₃) δ -65.87, -119.36, -122.14, -123.35, -123.43, -129.42, -136.99.

HRMS: [ESI, (+) ve]: calcd. [M+H] 622.9703 for (C₁₈H₁₁BrF₁₅O₂), found: 622.9695



Ethyl (*E*)-3-(3-(1-(trifluoromethyl)cyclopropyl)phenyl)acrylate (3t):

Yield: 75% (21.3 mg)

Eluent: 1% ethyl acetate in pet ether

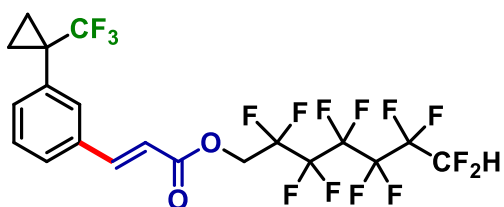
Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 7.67 (d, *J* = 16.1 Hz, 1H), 7.61 (d, *J* = 1.9 Hz, 1H), 7.48 (dt, *J* = 5.7, 2.5 Hz, 2H), 7.36 (t, *J* = 7.7 Hz, 1H), 6.46 (d, *J* = 16.0 Hz, 1H), 4.27 (q, *J* = 7.1 Hz, 2H), 1.94 – 1.26 (m, 5H), 1.22 – 0.83 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 166.79, 143.91, 136.90, 134.69, 133.01, 131.68, 128.93, 127.94, 127.86, 127.17 (q, *J* = 274.5 Hz), 118.90, 60.55, 28.25 (q, *J* = 33.7 Hz), 14.27, 9.69 (q, *J* = 2.4 Hz).

¹⁹F NMR (377 MHz, CDCl₃) δ -70.11.

HRMS: [ESI, (+) ve]: calcd. [M+H] 285.1102 for (C₁₅H₁₆F₃O₂), found: 285.1100



2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoroheptyl (*E*)-3-(3-(1-(trifluoromethyl)cyclopropyl)phenyl)acrylate (3u):

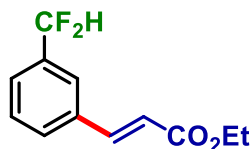
Yield: 73% (41.6 mg)

Eluent: 1% ethyl acetate in pet ether

Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 7.77 (d, *J* = 16.0 Hz, 1H), 7.64 (s, 1H), 7.55 – 7.48 (m, 2H), 7.39 (t, *J* = 7.7 Hz, 1H), 6.50 (d, *J* = 16.0 Hz, 1H), 6.06 (tt, *J* = 51.9, 5.1 Hz, 1H), 4.72 (t, *J* = 13.2 Hz, 2H), 1.43 – 1.36 (m, 2H), 1.07 – 1.01 (m, 2H).

HRMS: [ESI, (+) ve]: calcd. [M+H] 571.0754 for (C₂₀H₁₄F₁₅O₂), found: 571.0751



Ethyl (*E*)-3-(3-(difluoromethyl)phenyl)acrylate (5a):

Yield: 59% (13.3 mg)

Eluent: 1% ethyl acetate in pet ether

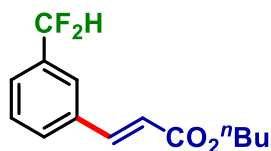
Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 7.70 (d, *J* = 16.0 Hz, 1H), 7.66 (s, 1H), 7.61 (t, *J* = 8.2 Hz, 1H), 7.56 – 7.45 (m, 2H), 6.66 (t, *J* = 56.3 Hz, 1H), 6.49 (d, *J* = 16.0 Hz, 1H), 4.28 (q, *J* = 7.1 Hz, 2H), 1.34 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (126 MHz, CDCl₃) δ 166.62, 143.28, 135.10 (d, *J* = 16.4 Hz), 130.12, 129.35, 128.21, 127.09 (t, *J* = 6.3 Hz), 124.94 (t, *J* = 6.3 Hz), 119.69, 114.22 (t, *J* = 239.4 Hz), 60.69, 14.29.

¹⁹F NMR (376 MHz, CDCl₃) δ -111.37.

HRMS: [ESI, (+) ve]: calcd. [M+H] 227.0884 for (C₁₂H₁₃F₂O₂), found: 227.0878



Ethyl (*E*)-3-(3-(difluoromethyl)phenyl)acrylate (5b):

Yield: 68% (17.2 mg)

Eluent: 1% ethyl acetate in pet ether

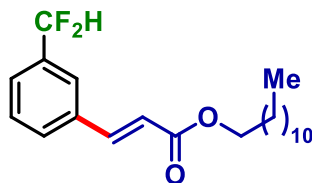
Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 7.69 (d, *J* = 16.1 Hz, 1H), 7.66 (s, 1H), 7.62 (t, *J* = 8.4 Hz, 1H), 7.56 – 7.44 (m, 2H), 6.66 (t, *J* = 56.3 Hz, 1H), 6.49 (d, *J* = 16.1 Hz, 1H), 4.22 (t, *J* = 6.7 Hz, 2H), 1.70 (dt, *J* = 14.2, 6.7 Hz, 2H), 1.44 (dq, *J* = 14.7, 7.4 Hz, 2H), 0.97 (t, *J* = 7.4 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 166.72, 143.25, 135.17 (t, *J* = 13.1 Hz), 130.14, 129.34, 128.22, 127.08 (t, *J* = 6.3 Hz), 124.94 (t, *J* = 6.1 Hz), 119.72, 114.23 (t, *J* = 239.4 Hz), 64.61, 30.73, 19.18, 13.72.

¹⁹F NMR (376 MHz, CDCl₃) δ -111.28.

HRMS: [ESI, (+) ve]: calcd. [M+H] 255.1917 for (C₁₄H₁₇F₂O₂), found: 255.1910



Dodecyl (*E*)-3-(3-(difluoromethyl)phenyl)acrylate (5c):

Yield: 61% (22.2 mg)

Eluent: 0.5% ethyl acetate in pet ether

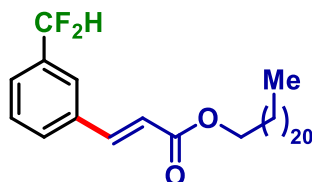
Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 7.73 – 7.58 (m, 3H), 7.54 – 7.45 (m, 2H), 6.66 (t, *J* = 56.3 Hz, 1H), 6.49 (d, *J* = 16.0 Hz, 1H), 4.21 (t, *J* = 6.7 Hz, 2H), 1.70 (p, *J* = 6.8 Hz, 2H), 1.40 – 1.13 (m, 18H), 0.88 (t, *J* = 6.7 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 166.73, 143.24, 135.11 (t, *J* = 22.8 Hz), 130.14, 129.34, 128.21, 127.08 (t, *J* = 5.5 Hz), 124.97 (t, *J* = 6.3 Hz), 119.71, 114.23 (t, *J* = 239.4 Hz), 64.92, 31.90, 29.69, 29.64, 29.62, 29.57, 29.52, 29.34, 29.27, 28.69, 25.96, 22.68, 14.11.

¹⁹F NMR (377 MHz, CDCl₃) δ -111.30.

HRMS: [ESI, (+) ve]: calcd. [M+H] 365.2292 for (C₂₂H₃₁F₂O₂), found: 365.2290



Docosyl (*E*)-3-(3-(difluoromethyl)phenyl)acrylate (5d):

Yield: 63% (31.9 mg)

Eluent: 0.5% ethyl acetate in pet ether

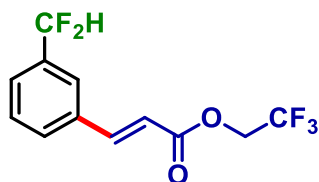
Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 7.69 (d, *J* = 16.2 Hz, 1H), 7.66 (s, 1H), 7.62 (t, *J* = 8.1 Hz, 1H), 7.55 – 7.45 (m, 2H), 6.66 (t, *J* = 56.4 Hz, 1H), 6.49 (d, *J* = 16.1 Hz, 1H), 4.21 (t, *J* = 6.7 Hz, 2H), 1.81 – 1.65 (m, 2H), 1.43 – 1.36 (m, 2H), 1.35 – 1.20 (m, 36H), 0.90 – 0.84 (m, 3H).

¹³C NMR (126 MHz, CDCl₃) δ 166.72, 143.24, 135.16 (t, *J* = 22.7 Hz), 130.14, 129.34, 128.22, 127.08 (t, *J* = 5.9 Hz), 124.94 (t, *J* = 6.3 Hz), 119.73, 114.23 (t, *J* = 239.9 Hz), 64.93, 31.92, 29.69, 29.65, 29.59, 29.53, 29.36, 29.28, 28.70, 25.97, 22.69, 14.11.

¹⁹F NMR (376 MHz, CDCl₃) δ -111.41.

HRMS: [ESI, (+) ve]: calcd. [M+H] 508.3857 for (C₃₂H₅₁F₂O₂), found: 508.3850



2,2,2-trifluoroethyl (*E*)-3-(3-(difluoromethyl)phenyl)acrylate (5e):

Yield: 66% (18.4 mg)

Eluent: 0.5% ethyl acetate in pet ether

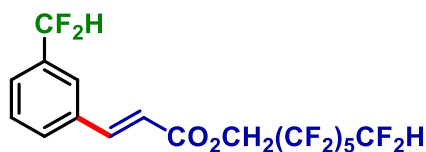
Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 7.80 (d, *J* = 16.1 Hz, 1H), 7.69 (s, 1H), 7.65 (t, *J* = 8.3 Hz, 1H), 7.53 (dt, *J* = 15.2, 7.2 Hz, 2H), 6.86 – 6.49 (m, 2H), 4.60 (q, *J* = 8.4 Hz, 2H).

¹³C NMR (126 MHz, CDCl₃) δ 164.81, 145.82, 134.47 (t, *J* = 22.7 Hz), 130.38, 129.49, 128.51, 127.79 (t, *J* = 5.9 Hz), 125.21 (t, *J* = 5.9 Hz), 124.11 (q, *J* = 272.6 Hz), 117.35, 114.09 (t, *J* = 239.2 Hz), 60.51 (q, *J* = 36.8 Hz).

¹⁹F NMR (376 MHz, CDCl₃) δ -73.69, -111.51.

HRMS: [ESI, (+) ve]: calcd. [M+H] 281.0601 for (C₁₂H₁₀F₅O₂), found: 281. 0598



2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoroheptyl (*E*)-3-(3-(difluoromethyl)phenyl)acrylate (5f):

Yield: 65% (33.3 mg)

Eluent: 1% ethyl acetate in pet ether

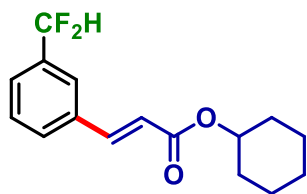
Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 7.79 (d, *J* = 16.0 Hz, 1H), 7.66 (dd, *J* = 16.2, 8.4 Hz, 2H), 7.53 (dt, *J* = 15.3, 7.7 Hz, 2H), 6.84 – 6.49 (m, 2H), 6.06 (tt, *J* = 51.9, 5.2 Hz, 1H), 4.73 (t, *J* = 13.4 Hz, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 164.83, 145.92, 135.33, 134.44, 130.42, 129.49, 128.54, 127.85, 127.79, 127.73, 126.30, 126.25, 126.20, 125.31, 125.25, 125.19, 117.26, 114.09, 107.56, 60.00, 59.73, 59.47, 17.68, 12.26.

¹⁹F NMR (376 MHz, CDCl₃) δ -111.50, -119.44, -122.17, -123.33, -123.37, -123.44, -129.43, -137.00.

HRMS: [ESI, (+) ve]: calcd. [M+H] 513.0535 for (C₁₇H₁₁F₁₄O₂), found: 513.0530



Cyclohexyl (*E*)-3-(3-(difluoromethyl)phenyl)acrylate (5g):

Yield: 57% (16 mg)

Eluent: 1% ethyl acetate in pet ether

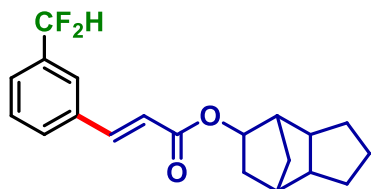
Physical state: yellowish liquid

¹H NMR (500 MHz, CDCl₃) δ 7.70 – 7.59 (m, 3H), 7.54 – 7.46 (m, 2H), 6.71 (t, J = 55.7 Hz, 1H), 6.48 (d, J = 16.0 Hz, 1H), 5.09 – 4.70 (m, 1H), 1.92 (dd, J = 12.3, 5.2 Hz, 2H), 1.77 (dt, J = 14.0, 4.5 Hz, 2H), 1.49 (dd, J = 12.4, 9.5 Hz, 2H), 1.41 (dt, J = 14.0, 10.7 Hz, 2H), 1.34 – 1.21 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 166.07, 142.95, 135.20 (t, J = 22.7 Hz), 130.11, 129.32, 128.18, 126.99 (t, J = 5.8 Hz), 124.91 (t, J = 6.1 Hz), 120.32, 114.25 (t, J = 240.4 Hz), 72.98, 31.70, 25.40, 23.78.

¹⁹F NMR (376 MHz, CDCl₃) δ -111.33.

HRMS: [ESI, (+) ve]: calcd. [M+Na] 303.1113 for (C₁₆H₁₈NaF₂O₂), found: 303.1116



Octahydro-1H-4,7-methanoinden-5-yl-(*E*)-3-(3-(difluoromethyl)phenyl)acrylate (5h):

Yield: 52% (17.2 mg)

Eluent: 1 % ethyl acetate in pet ether

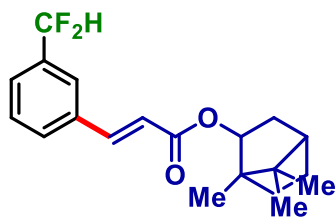
Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 7.68 – 7.58 (m, 3H), 7.54 – 7.43 (m, 2H), 6.65 (t, J = 56.3 Hz, 1H), 6.46 (d, J = 16.0 Hz, 1H), 4.78 – 4.61 (m, 1H), 2.14 (s, 1H), 2.06 (d, J = 4.7 Hz, 1H), 1.95 – 1.80 (m, 2H), 1.75 – 1.62 (m, 2H), 1.36 – 1.18 (m, 5H), 0.96 (ddt, J = 12.2, 7.9, 5.9 Hz, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 166.41, 142.89, 135.22 (t, J = 22.7 Hz), 130.11, 129.32, 128.18, 126.99 (t, J = 6.0 Hz), 124.91 (t, J = 6.2 Hz), 120.27, 114.25 (t, J = 239.5 Hz), 77.47, 47.30, 46.23, 43.03, 39.63, 39.15, 32.03, 31.69, 29.47, 27.73.

¹⁹F NMR (377 MHz, CDCl₃) δ -111.34.

HRMS: [ESI, (+) ve]: calcd. [M+H] 333.1666 for (C₂₀H₂₃F₂O₂), found: 333.1670



1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl (*E*)-3-(3-(difluoromethyl)phenyl)acrylate (5i):

Yield: 68% (22.7 mg)

Eluent: 1% ethyl acetate in pet ether

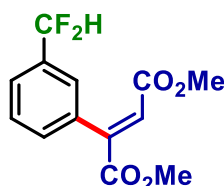
Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 7.72 – 7.56 (m, 2H), 7.54 – 7.44 (m, 2H), 7.17 – 7.08 (m, 1H), 6.66 (t, *J* = 56.3 Hz, 1H), 6.46 (d, *J* = 16.1 Hz, 1H), 4.81 (dd, *J* = 7.5, 4.1 Hz, 0H), 1.95 – 1.82 (m, 2H), 1.80 – 1.69 (m, 2H), 1.64 – 1.60 (m, 1H), 1.22 – 1.09 (m, 2H), 1.06 (s, 3H), 0.90 (s, 3H), 0.87 (s, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 166.16, 142.93, 135.16 (*t*, *J* = 22.6 Hz), 130.17, 129.32, 127.05 (*t*, *J* = 6.0 Hz), 125.76, 124.95 (*t*, *J* = 6.3 Hz), 120.27, 114.26 (*t*, *J* = 239.4 Hz), 81.35, 48.91, 47.00, 45.07, 38.84, 33.74, 27.05, 20.12, 20.01, 11.50.

¹⁹F NMR (376 MHz, CDCl₃) δ -111.28.

HRMS: [ESI, (+) ve]: calcd. [M+H] 335.1823 for (C₂₀H₂₅F₂O₂), found: 335.1820



Dimethyl 2-(3-(difluoromethyl)phenyl)fumarate (5j):

Yield: 49% (13.2 mg)

Eluent: 15% ethyl acetate in pet ether

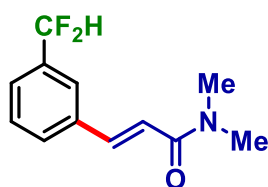
Physical state: colourless liquid

¹H NMR (400 MHz, CDCl₃) δ 7.60 (s, 1H), 7.59 – 7.55 (m, 2H), 7.53 – 7.49 (m, 1H), 6.66 (t, *J* = 56.2 Hz, 1H), 6.35 (s, 1H), 3.96 (s, 3H), 3.80 (s, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 167.86, 165.13, 147.79, 135.44 (*t*, *J* = 22.8 Hz), 129.55, 128.98, 127.54 (*t*, *J* = 5.9 Hz), 127.12, 123.90 (*t*, *J* = 6.2 Hz), 118.56, 114.00 (*t*, *J* = 239.7 Hz), 52.91, 52.20.

¹⁹F NMR (376 MHz, CDCl₃) δ -111.51.

HRMS: [ESI, (+) ve]: calcd. [M+H] 271.0782 for (C₁₃H₁₃F₂O₄), found: 271.0780



(E)-3-(3-(difluoromethyl)phenyl)-N,N-dimethylacrylamide (5k):

Yield: 67% (15 mg)

Eluent: 25% ethyl acetate in pet ether

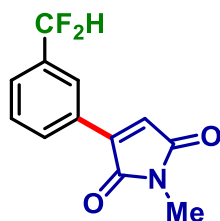
Physical state: yellowish liquid

¹H NMR (500 MHz, CDCl₃) δ 7.68 (d, J = 15.5 Hz, 2H), 7.61 (t, J = 6.7 Hz, 1H), 7.53 – 7.40 (m, 2H), 6.94 (d, J = 15.4 Hz, 1H), 6.67 (t, J = 56.4 Hz, 1H), 3.19 (s, 3H), 3.08 (s, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 166.29, 141.15, 136.00, 134.99 (t, J = 22.2 Hz), 130.24, 129.25, 126.44 (t, J = 6.1 Hz), 124.33 (t, J = 6.2 Hz), 118.77, 114.38 (d, J = 239.3 Hz), 37.46, 35.97.

¹⁹F NMR (376 MHz, CDCl₃) δ -111.07.

HRMS: [ESI, (+) ve]: calcd. [M+H] 226.1053 for (C₁₂H₁₄F₂ON), found: 226.1057



3-(3-(difluoromethyl)phenyl)-1-methyl-1H-pyrrole-2,5-dione (5l):

Yield: 52% (12.3 mg)

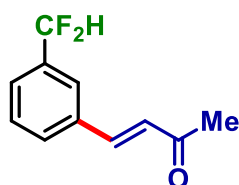
Eluent: 20% ethyl acetate in pet ether

Physical state: yellowish liquid

¹H NMR (500 MHz, CDCl₃) δ 8.06 (s, 1H), 8.05 – 7.99 (m, 1H), 7.70 – 7.48 (m, 2H), 6.83 – 6.54 (m, 2H), 3.10 (s, 3H).

¹⁹F NMR (376 MHz, CDCl₃) δ -111.40.

HRMS: [ESI, (+) ve]: calcd. [M+H] 238.0680 for (C₁₂H₁₀F₂O₂N), found: 238.0683



(E)-4-(3-(difluoromethyl)phenyl)but-3-en-2-one (5m):

Yield: 52% (10.2 mg)

Eluent: 9% ethyl acetate in pet ether

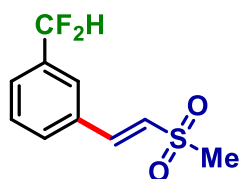
Physical state: yellowish liquid

^1H NMR (500 MHz, CDCl_3) δ 7.68 (s, 1H), 7.64 (dd, J = 12.9, 7.7 Hz, 1H), 7.57 – 7.46 (m, 3H), 6.85 – 6.52 (m, 2H), 2.40 (d, J = 1.4 Hz, 3H).

^{13}C NMR (126 MHz, CDCl_3) δ 198.08, 142.00, 135.25 (t, J = 20.9 Hz), 130.28, 129.43, 128.41, 128.11, 127.37 (t, J = 6.0 Hz), 125.15 (t, J = 6.1 Hz), 114.17 (t, J = 239.5 Hz), 27.74.

^{19}F NMR (376 MHz, CDCl_3) δ -112.02.

HRMS: [ESI, (+) ve]: calcd. $[\text{M}+\text{H}]$ 197.0778 for ($\text{C}_{11}\text{H}_{11}\text{F}_2\text{O}$), found: 197.0772



(E)-1-(difluoromethyl)-3-(2-(methylsulfonyl)vinyl)benzene (5n):

Yield: 69% (16 mg)

Eluent: 20% ethyl acetate in pet ether

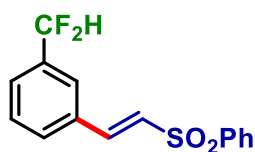
Physical state: yellowish liquid

^1H NMR (400 MHz, CDCl_3) δ 7.70 – 7.64 (m, 2H), 7.64 – 7.57 (m, 2H), 7.54 (t, J = 7.6 Hz, 1H), 6.98 (d, J = 15.5 Hz, 1H), 6.68 (t, J = 56.2 Hz, 1H), 3.05 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 142.80, 135.54, 132.75, 130.73, 129.70, 128.31 (t, J = 5.9 Hz), 127.64, 125.35 (t, J = 6.1 Hz), 115.10 (t, J = 239.9 Hz), 43.21.

^{19}F NMR (376 MHz, CDCl_3) δ -111.71.

HRMS: [ESI, (+) ve]: calcd. $[\text{M}+\text{H}]$ 233.0448 for ($\text{C}_{10}\text{H}_{11}\text{F}_2\text{O}_2\text{S}$), found: 233.0448



(E)-1-(difluoromethyl)-3-(2-(phenylsulfonyl)vinyl)benzene (5o):

Yield: 63% (18.5 mg)

Eluent: 7% ethyl acetate in pet ether

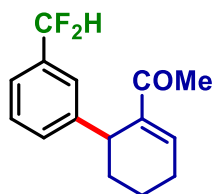
Physical state: yellowish solid

^1H NMR (400 MHz, CDCl_3) δ 8.02 – 7.92 (m, 2H), 7.71 (d, J = 15.4 Hz, 1H), 7.64 – 7.54 (m, 6H), 7.51 (d, J = 7.7 Hz, 1H), 6.93 (d, J = 15.4 Hz, 1H), 6.65 (t, J = 56.2 Hz, 1H).

¹³C NMR (101 MHz, CDCl₃) δ 141.09, 140.30, 135.41 (d, *J* = 22.4 Hz), 133.59, 133.01, 130.73, 129.59, 129.42, 128.81, 127.75, 126.33 (t, *J* = 6.1 Hz), 125.35 (t, *J* = 6.1 Hz), 113.92 (t, *J* = 239.9 Hz).

¹⁹F NMR (376 MHz, CDCl₃) δ -111.64.

HRMS: [ESI, (+) ve]: calcd. [M+H] 295.0604 for (C₁₅H₁₃F₂O₂S), found: 295.0601



1-(3'-(difluoromethyl)-1,4,5,6-tetrahydro-[1,1'-biphenyl]-2-yl)ethan-1-one (5p):

Yield: 45% (11.2 mg)

Eluent: 5% ethyl acetate in pet ether

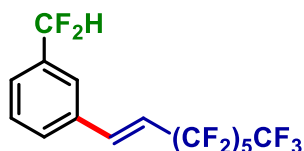
Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 7.43 – 7.27 (m, 2H), 7.25 – 7.16 (m, 3H), 6.60 (t, *J* = 56.7 Hz, 1H), 4.05 (d, *J* = 4.9 Hz, 1H), 2.50 – 2.32 (m, 2H), 2.25 (s, 3H), 1.93 – 1.71 (m, 2H), 1.54 – 1.43 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 198.35, 145.83, 142.80, 140.59, 134.20 (t, *J* = 22.2 Hz), 130.12, 128.53, 124.66 (t, *J* = 6.1 Hz), 123.17 (t, *J* = 6.1 Hz), 114.89 (t, *J* = 238.8 Hz), 38.24, 31.02, 26.11, 25.74, 16.74.

¹⁹F NMR (376 MHz, CDCl₃) δ -111.29.

HRMS: [ESI, (+) ve]: calcd. [M+H] 251.1247 for (C₁₅H₁₇F₂O), found: 251.1246



(E)-1-(difluoromethyl)-3-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooct-1-en-1-yl)benzene (5q):

Yield: 66% (31 mg)

Eluent: 0.5% ethyl acetate in pet ether

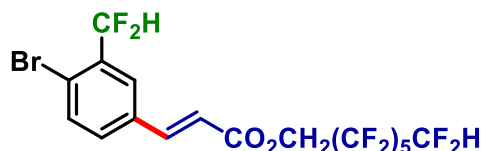
Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 7.62 (s, 1H), 7.59 (d, *J* = 7.3 Hz, 1H), 7.57 – 7.48 (m, 2H), 7.21 (dd, *J* = 16.2, 2.3 Hz, 1H), 6.67 (t, *J* = 56.3 Hz, 1H), 6.27 (dt, *J* = 16.1, 12.0 Hz, 1H).

¹³C NMR (101 MHz, CDCl₃) δ 138.75 (t, *J* = 9.5 Hz), 135.31 (t, *J* = 22.7 Hz), 134.13, 129.79, 129.47, 127.91, 127.20 (t, *J* = 6.0 Hz), 126.24 (t, *J* = 6.1 Hz), 124.64 (t, *J* = 6.1 Hz), 116.17, 116.04, 115.82, 115.58, 114.14 (t, *J* = 239.5 Hz).

¹⁹F NMR (376 MHz, CDCl₃) δ -81.54, -111.99, -112.11, -122.01, -123.31, -123.58, -126.70.

HRMS: [ESI, (+) ve]: calcd. [M+H] 473.0386 for (C₁₅H₈F₁₅), found: 473.0388



2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoroheptyl (*E*)-3-(4-bromo-3-(difluoromethyl)phenyl)acrylate (5r):

Yield: 68% (40 mg)

Eluent: 1% ethyl acetate in pet ether

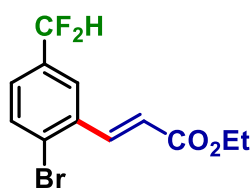
Physical state: yellowish solid

¹H NMR (400 MHz, CDCl₃) δ 8.21 (dd, *J* = 26.2, 15.9 Hz, 0.5H), 7.89 – 7.76 (m, 0.5H), 7.79 – 7.59 (m, 2H), 7.62 – 7.38 (m, 1H), 7.17 – 6.70 (m, 1H), 6.67 – 6.37 (m, 1H), 6.09 (tt, *J* = 51.9, 5.2 Hz, 1H), 4.84 – 4.68 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 164.30, 144.82, 133.98, 130.15, 128.87 (t, *J* = 6.2 Hz), 128.07, 126.74 (t, *J* = 6.1 Hz), 124.41, 113.59 (t, *J* = 239.4 Hz), 113.25, 110.87, 110.12, 107.89, 107.58, 101.93, 59.90 (t, *J* = 26.3 Hz).

¹⁹F NMR (376 MHz, CDCl₃) δ -115.09, -115.31, -119.36, -122.13, -123.40, -129.41, -137.02.

HRMS: [ESI, (+) ve]: calcd. [M+H] 590.9641 for (C₁₇H₁₀F₁₄O₂Br), found: 590.9640



Ethyl (*E*)-3-(2-bromo-5-(difluoromethyl)phenyl)acrylate (5s):

Yield: 76% (23.8 mg)

Eluent: 1% ethyl acetate in pet ether

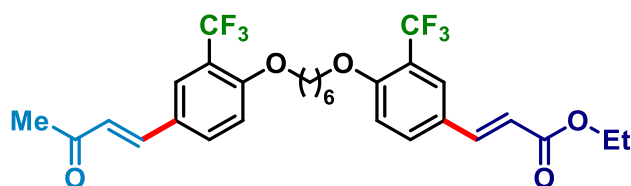
Physical state: yellowish solid

¹H NMR (400 MHz, CDCl₃) δ 8.03 (d, *J* = 15.9 Hz, 1H), 7.80 – 7.68 (m, 2H), 7.36 (dt, *J* = 8.3, 1.3 Hz, 1H), 6.63 (t, *J* = 56.2 Hz, 1H), 4.29 (q, *J* = 7.2 Hz, 2H), 1.35 (t, *J* = 7.2 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 166.05, 141.90, 135.25, 124.93 (t, *J* = 22.4 Hz), 133.94, 127.82, 124.93 (t, *J* = 5.9 Hz), 124.93 (t, *J* = 6.3 Hz), 122.40, 113.67 (t, *J* = 241.4 Hz), 60.88, 14.26.

¹⁹F NMR (377 MHz, CDCl₃) δ -111.72.

HRMS: [ESI, (+) ve]: calcd. [M+H] 304.9989 for (C₁₂H₁₂F₂O₂Br), found: 340.9986



Ethyl (*E*)-3-(4-(((6-(4-((*E*)-3-oxobut-1-en-1-yl)-2-(trifluoromethyl)phenoxy)hexyl)oxy)-3-(trifluoromethyl)phenyl)acrylate (7a):

Yield: 39% (22.3 mg)

Eluent: 15% ethyl acetate in pet ether

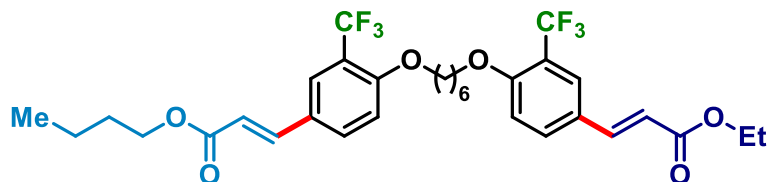
Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 7.72 (s, 1H), 7.66 – 7.59 (m, 2H), 7.54 (d, *J* = 8.3 Hz, 1H), 7.46 (t, *J* = 8.0 Hz, 1H), 7.01 – 6.86 (m, 4H), 6.35 (d, *J* = 16.0 Hz, 1H), 4.26 (q, *J* = 7.1 Hz, 2H), 4.09 (t, *J* = 6.3 Hz, 2H), 4.05 (t, *J* = 6.2 Hz, 2H), 2.15 (d, *J* = 5.0 Hz, 3H), 1.94 – 1.75 (m, 4H), 1.58 – 1.54 (m, 4H), 1.33 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 188.65, 166.90, 158.37, 156.98, 142.89, 133.16, 132.96, 130.39, 127.03, 126.98, 126.78, 126.73, 126.38, 124.76, 119.72, 117.26, 112.96, 112.66, 68.68, 68.28, 60.53, 28.81, 28.70, 25.63, 25.26, 25.22, 14.30.

¹⁹F NMR (377 MHz, CDCl₃) δ -62.41, -62.82.

HRMS: [ESI, (+) ve]: calcd. [M+H] 573.2076 for (C₂₉H₃₁F₆O₅Br), found: 573.2073



Butyl (*E*)-3-(4-(((6-(4-((*E*)-3-ethoxy-3-oxoprop-1-en-1-yl)-2-(trifluoromethyl)phenoxy)hexyl)oxy)-3-(trifluoromethyl)phenyl)acrylate (7b):

Yield: 57% (58.2 mg)

Eluent: 5% ethyl acetate in pet ether

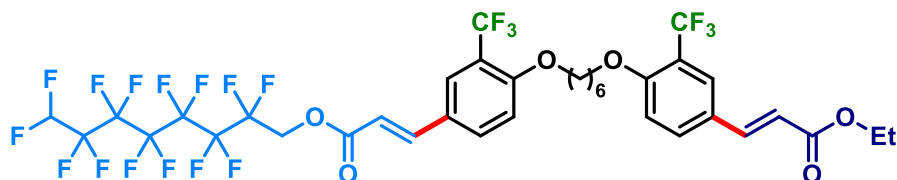
Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 7.72 (d, *J* = 2.2 Hz, 2H), 7.67 – 7.57 (m, 4H), 6.98 (d, *J* = 8.7 Hz, 2H), 6.35 (dd, *J* = 16.0, 1.4 Hz, 2H), 4.26 (q, *J* = 7.1 Hz, 2H), 4.20 (t, *J* = 6.7 Hz, 2H), 4.09 (t, *J* = 6.2 Hz, 4H), 2.34 (t, *J* = 7.5 Hz, 2H), 1.87 (dd, *J* = 7.8, 4.3 Hz, 4H), 1.76 – 1.65 (m, 2H), 1.57 (p, *J* = 3.5 Hz, 2H), 1.48 – 1.40 (m, 2H), 1.33 (t, *J* = 7.1 Hz, 3H), 0.96 (t, *J* = 7.4 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 167.01, 166.90, 158.33, 142.87, 142.83, 132.97, 126.76 (q, J = 5.2 Hz), 126.43, 124.61, 122.26 (q, J = 273.6 Hz), 117.32, 117.31, 112.94, 68.63, 64.48, 60.54, 33.74, 31.91, 28.68, 25.20, 22.68, 19.18, 14.30, 13.73.

¹⁹F NMR (377 MHz, CDCl₃) δ -62.80, -62.81.

HRMS: [ESI, (+) ve]: calcd. [M+H] 631.2494 for (C₃₂H₃₇F₆O₆), found: 631.2493



Ethyl (*E*)-3-(4-((6-(4-((*E*)-3-oxo-3-((2,2,3,3,4,4,5,5,6,6,7,7,8,8-tetradecafluorooctyl)oxy)prop-1-en-1-yl)-2-(trifluoromethyl)phenoxy)hexyl)oxy)-3-(trifluoromethyl)phenyl)acrylate (7c):

Yield: 33% (31 mg)

Eluent: 3% ethyl acetate in pet ether

Physical state: yellowish liquid

¹H NMR (400 MHz, CDCl₃) δ 7.75 (d, J = 2.3 Hz, 1H), 7.74 – 7.69 (m, 2H), 7.68 – 7.59 (m, 3H), 6.99 (t, J = 8.5 Hz, 2H), 6.39 (d, J = 16.0 Hz, 1H), 6.35 (d, J = 16.0 Hz, 1H), 6.06 (tt, J = 51.9, 5.2 Hz, 1H), 4.71 (t, J = 13.5 Hz, 2H), 4.26 (q, J = 7.1 Hz, 2H), 4.10 (q, J = 6.0 Hz, 4H), 1.99 – 1.80 (m, 4H), 1.66 – 1.49 (m, 4H), 1.33 (t, J = 7.1 Hz, 3H).

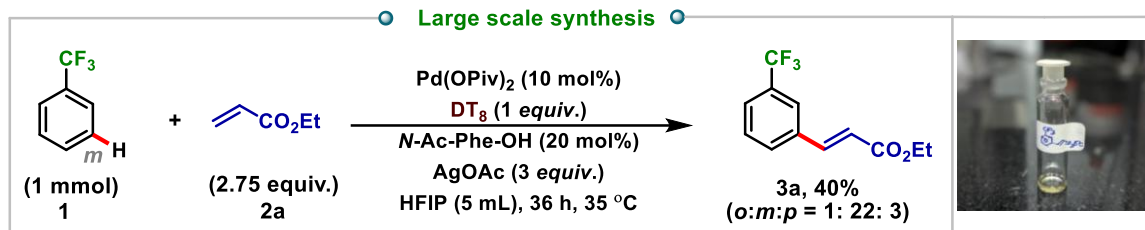
¹³C NMR (101 MHz, CDCl₃) δ 166.87, 165.07, 158.90, 158.34, 145.48, 142.83, 133.38, 132.96, 127.19 (q, J = 5.3 Hz), 126.77 (q, J = 5.3 Hz), 126.47, 125.80, 123.27 (q, J = 272.5 Hz); 123.16 (q, J = 272.9 Hz), 121.92, 121.81, 119.85, 119.71, 119.54, 119.40, 119.24, 119.09, 117.36, 114.79, 113.03, 112.96, 107.41 (q, J = 31.4 Hz), 105.18 (q, J = 30.3 Hz), 68.73, 68.63, 60.53, 59.62 (t, J = 26.9 Hz), 28.69, 28.66, 25.17, 14.29.

¹⁹F NMR (377 MHz, CDCl₃) δ -62.82, -62.89, -119.43, -122.13, -123.39, -129.42, -137.01.

HRMS: [ESI, (+) ve]: calcd. [M+] 938.1848 for (C₃₆H₃₀F₂₀O₆), found: 938.1847

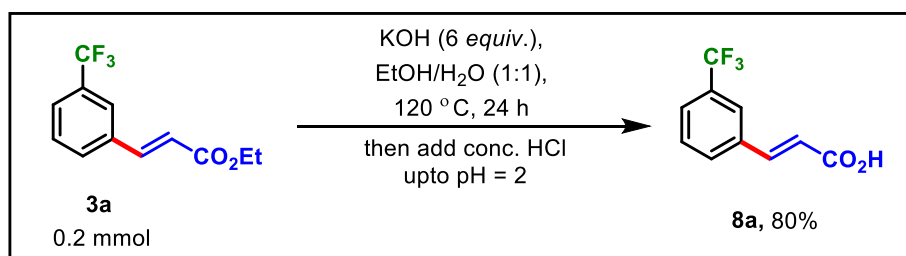
11. Applications:

11.1: Large scale synthesis:



In an oven-dried screw capped reaction tube charged with magnetic stir-bar, substrate **1a** (1 equiv., 1 mmol), Pd(OAc)_2 (10 mol%, 22.4 mg), $N\text{-Ac-Phe-OH}$ (20 mol%, 41 mg), Directing Template (DT_8) (1 equiv.), AgOAc (3 equiv.) in 5 mL of HFIP were added. After that, olefin **2a** (2.75 equiv.) was added to that reaction mixture. The reaction tube was well capped and placed in a RT (35 °C) with stirring (1000 rpm) for 36 h. Upon completion of the reaction, the mixture was diluted with ethyl acetate and filtered through a celite pad. The filtrate was evaporated under reduced pressure and the crude mixture was purified by column chromatography using silica (100-200 mesh size) and petroleum ether/ethyl acetate as the eluent.

11.2: Synthetic applications:



(E)-3-(3-(trifluoromethyl)phenyl)acrylic acid, (Figure 5, entry 8a)⁶: A mixture of **3a** (0.2 mmol) and KOH (6 equiv.) was dissolved in 2 mL of a 1:1 H_2O - EtOH solution in a Teflon screw-cap reaction tube equipped with a magnetic stir bar and stirred at 120 °C in an oil bath for 24 hours. After completion, as indicated by TLC, the reaction mixture was cooled to ambient temperature. The reaction mixture was then diluted with ethyl acetate, washed with water, and concentrated HCl was added to adjust the pH to 2. The organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography using ethyl acetate/hexane as the eluent, affording **8a** with an 80% yield.

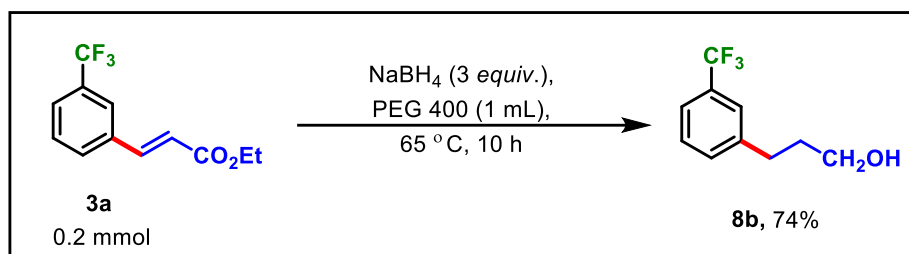
Yield: 80% (34.5 mg)

Eluent: 30% ethyl acetate in pet ether

Physical state: White solid

¹H NMR (500 MHz, CDCl₃) δ 7.86 – 7.71 (m, 3H), 7.61 (dd, J = 56.2, 7.8 Hz, 2H), 6.52 (d, J = 16.1 Hz, 1H).

¹³C NMR (126 MHz, CDCl₃) δ 171.61, 145.21, 134.78, 131.57 (q, J = 26.2 Hz), 131.27, 129.55, 127.12 (q, J = 2.7 Hz), 124.92 (q, J = 3.1 Hz), 123.69 (q, J = 218.2 Hz), 119.24.



3-(3-(trifluoromethyl)phenyl)propan-1-ol (Figure 5, entry 8b)⁷: A mixture of **3a** (0.2 mmol) and NaBH₄ (3 equiv.) was dissolved in 1 mL of PEG 400 solvent in a Teflon screw-cap reaction tube equipped with a magnetic stir bar and stirred at 65 °C in an oil bath for 10 hours. After completion, as indicated by TLC, the reaction mixture was cooled to ambient temperature. The reaction mixture was then diluted with ethyl acetate, washed with water. The organic layer was dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The crude product was purified by column chromatography using ethyl acetate/hexane as the eluent, affording **8b** with an 74% yield (30.2 mg).

Yield: 74% (30.2 mg)

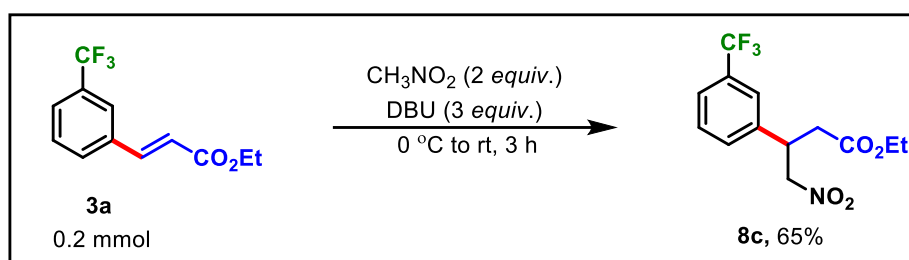
Eluent: 5% ethyl acetate in pet ether

Physical state: Yellow liquid

¹H NMR (400 MHz, CDCl₃) δ 7.49 – 7.41 (m, 2H), 7.40 (d, J = 2.5 Hz, 1H), 7.38 (d, J = 1.8 Hz, 1H), 3.68 (t, J = 6.4 Hz, 2H), 2.77 (d, J = 7.9 Hz, 2H), 2.02 – 1.83 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 142.70, 131.84, 130.65 (q, J = 32.1 Hz), 128.77, 125.08 (q, J = 3.9 Hz), 124.22 (q, J = 273.2 Hz), 122.75 (q, J = 3.9 Hz), 61.88, 33.91, 31.81.

¹⁹F NMR (377 MHz, CDCl₃) δ -62.57.



Ethyl (R)-4-nitro-3-(3-(trifluoromethyl)phenyl)butanoate (Figure 5, entry 8c)⁸: A mixture of **3a** (0.2 mmol) and DBU (6 equiv.) was added in a Teflon screw-cap reaction tube equipped

with a magnetic stir bar and stirred at 0 °C in 1 h. After completion, as indicated by TLC, the reaction mixture was cooled to ambient temperature. The crude product was purified by column chromatography using ethyl acetate/hexane as the eluent, affording **8c** with an 65% yield (34.5 mg).

Yield: 65%

Eluent: 10% ethyl acetate in pet ether

Physical state: Yellow liquid

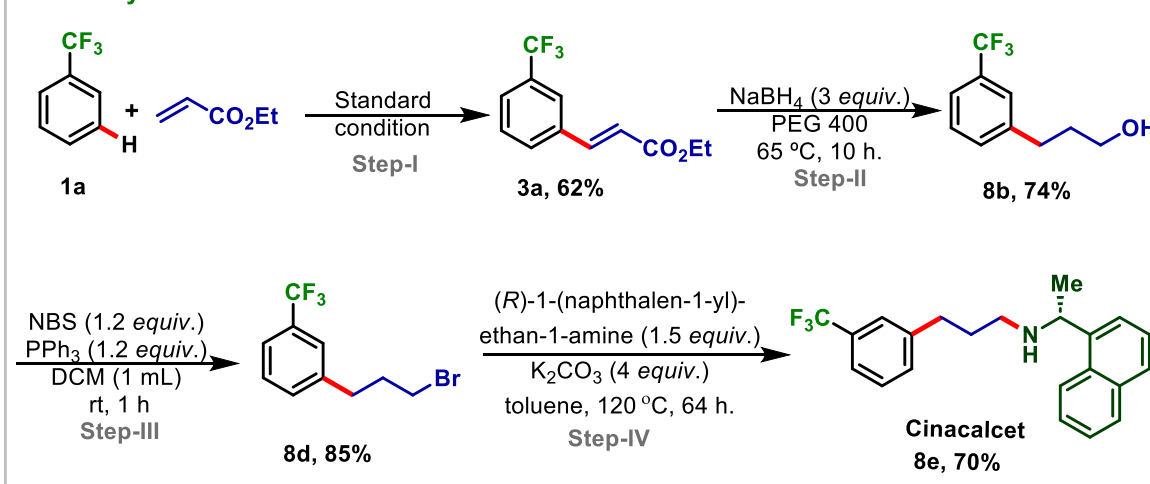
¹H NMR (400 MHz, CDCl₃) δ 7.56 (d, *J* = 7.6 Hz, 1H), 7.49 (s, 1H), 7.49 – 7.39 (m, 2H), 4.95 – 4.54 (m, 2H), 4.07 (dq, *J* = 12.9, 7.3 Hz, 3H), 3.07 – 2.54 (m, 2H), 1.17 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 170.15, 139.40, 131.42 (q, *J* = 32.2 Hz), 130.90, 129.60, 124.99 (q, *J* = 4.1 Hz), 124.21 (q, *J* = 3.8 Hz), 123.57 (q, *J* = 233.4 Hz), 78.89, 61.12, 39.94, 37.55, 13.98.

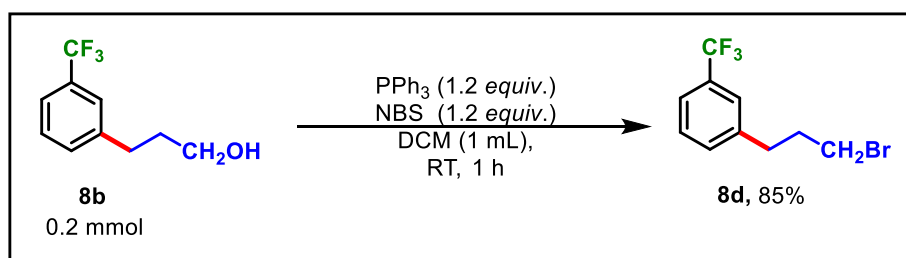
¹⁹F NMR (377 MHz, CDCl₃) δ -62.73.

11.3: Total synthesis of Cinacalcet:

D. Total synthesis of Cincalcet



For Step-III



1-(3-bromopropyl)-3-(trifluoromethyl)benzene (Figure 5, entry 8d)⁹: A mixture of **8b** (0.2 mmol), PPh₃ (1.2 *equiv.*) and NBS (1.2 *equiv.*) was dissolved in 1 mL of DCM solvent in a Teflon screw-cap reaction tube equipped with a magnetic stir bar at room temperature for 1 hour. After completion, as indicated by TLC. The reaction mixture was then diluted with ethyl acetate, washed with water. The organic layer was dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The crude product was purified by column chromatography using ethyl acetate/hexane as the eluent, affording **8d** with an 85% yield (45.4 mg).

Yield: 85% (45.4 mg)

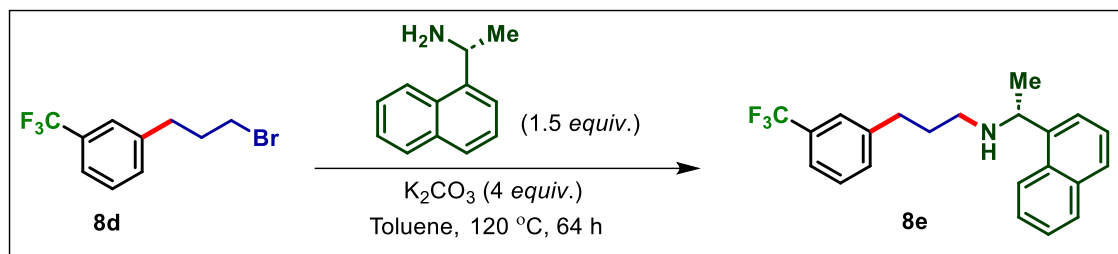
Eluent: 2% ethyl acetate in pet ether

Physical state: Yellow liquid

¹H NMR (400 MHz, CDCl₃) δ 7.50 – 7.45 (m, 2H), 7.44 – 7.38 (m, 2H), 3.40 (t, *J* = 6.5 Hz, 2H), 2.85 (t, *J* = 7.5 Hz, 2H), 2.29 – 1.95 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 141.44, 131.97, 130.83 (d, *J* = 31.7 Hz), 128.92, 125.18 (d, *J* = 3.8 Hz), 124.01 (d, *J* = 246.2 Hz), 123.11 (q, *J* = 3.8 Hz), 33.82, 33.76, 32.63.

For Step-IV



(R)-N-(1-(naphthalen-1-yl)ethyl)-3-(3-(trifluoromethyl)phenyl)propan-1-amine (Figure 5, entry 8e)¹⁰: Under an atmosphere of dry nitrogen, to an oven-dried 15 mL pressure vessel were added 1-(3-bromopropyl)-3-(trifluoromethyl)benzene (0.2 mmol), toluene (1.5 mL), 1-(naphthalen-1-yl)ethan-1-amine (1.5 *equiv.*), and K₂CO₃ (2.00 *equiv.*) in that order. The vial was capped with a PTFE lined septum cap and the reaction mixture stirred vigorously at 120 °C for 48 hours. Then, the mixture was cooled to room temperature and additional K₂CO₃ (2.00 *equiv.*) was added to the reaction mixture under a stream of dry nitrogen. The reaction mixture was then stirred vigorously heated at 120 °C for an additional 16 hours. Next, water (2 mL) was added to the cold reaction mixture and the organic products were partitioned between aqueous and organic phases. The aqueous phase was further extracted with toluene (3 x 1 mL) and the combined toluene fractions were combined and then extracted at 50 °C with 1 M

aqueous HCl (3 x 2 mL) and then dried over MgSO₄ and concentrated under vacuum. Addition of n-heptane and concentration led to the formation of a solid. The crude product was purified by column chromatography using ethyl acetate/hexane as the eluent, affording **8e** with an 70% yield (50 mg).

Yield: 70% (50 mg)

Eluent: 70% ethyl acetate in pet ether

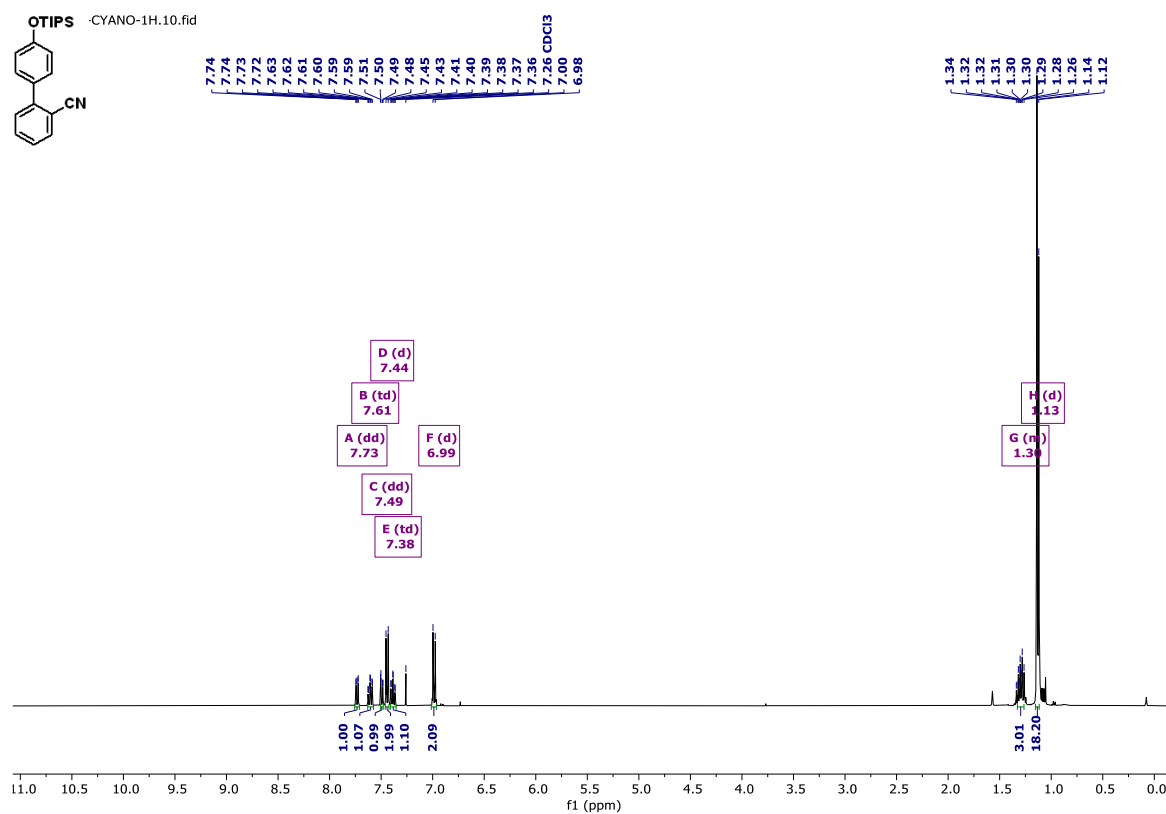
Physical state: White solid

¹H NMR (500 MHz, CDCl₃) δ 8.22 (d, *J* = 8.3 Hz, 1H), 7.90 (d, *J* = 7.9 Hz, 1H), 7.77 (d, *J* = 8.1 Hz, 1H), 7.67 (d, *J* = 7.1 Hz, 1H), 7.56 – 7.48 (m, 3H), 7.46 – 7.42 (m, 2H), 7.36 (t, *J* = 7.9 Hz, 1H), 7.32 (d, *J* = 7.7 Hz, 1H), 4.65 (q, *J* = 6.6 Hz, 1H), 2.81 – 2.57 (m, 4H), 1.86 (p, *J* = 7.4 Hz, 2H), 1.52 (d, *J* = 6.6 Hz, 3H).

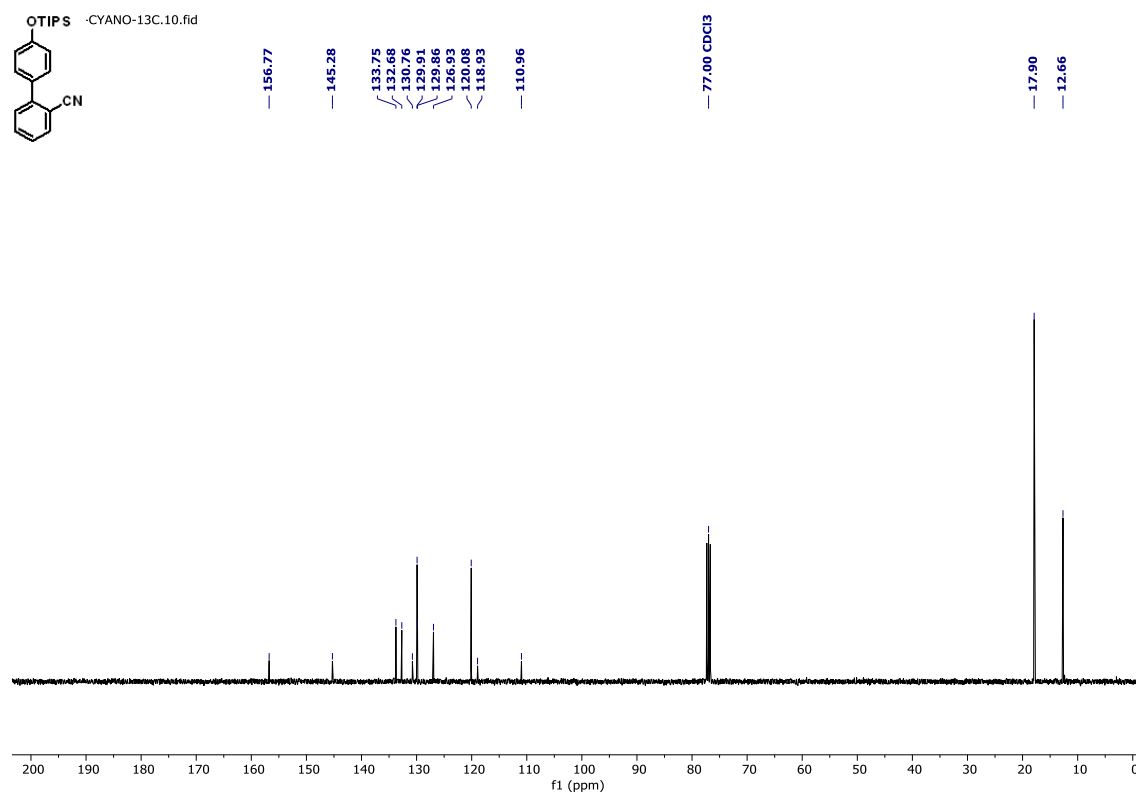
¹³C NMR (126 MHz, CDCl₃) δ 143.05, 141.16, 133.95, 131.74, 131.26, 130.65 (t, *J* = 31.9 Hz), 128.96, 128.63, 127.16, 125.73, 125.66, 125.29, 125.00 (q, *J* = 3.8 Hz), 124.24 (d, *J* = 272.1 Hz), 122.87, 122.59, 122.58 (d, *J* = 2.4 Hz), 53.70, 47.24, 33.38, 31.84, 23.58.

¹⁹F NMR (376 MHz, CDCl₃) δ -62.46.

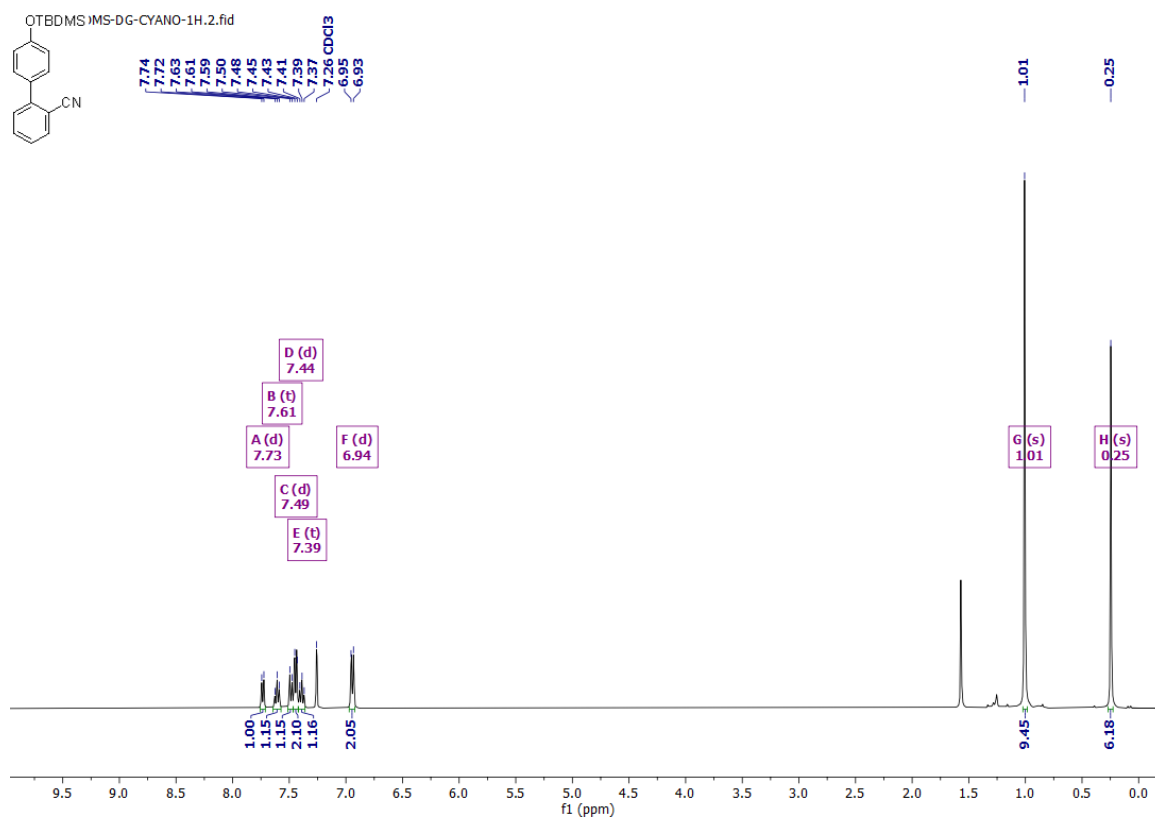
12. NMR spectra:



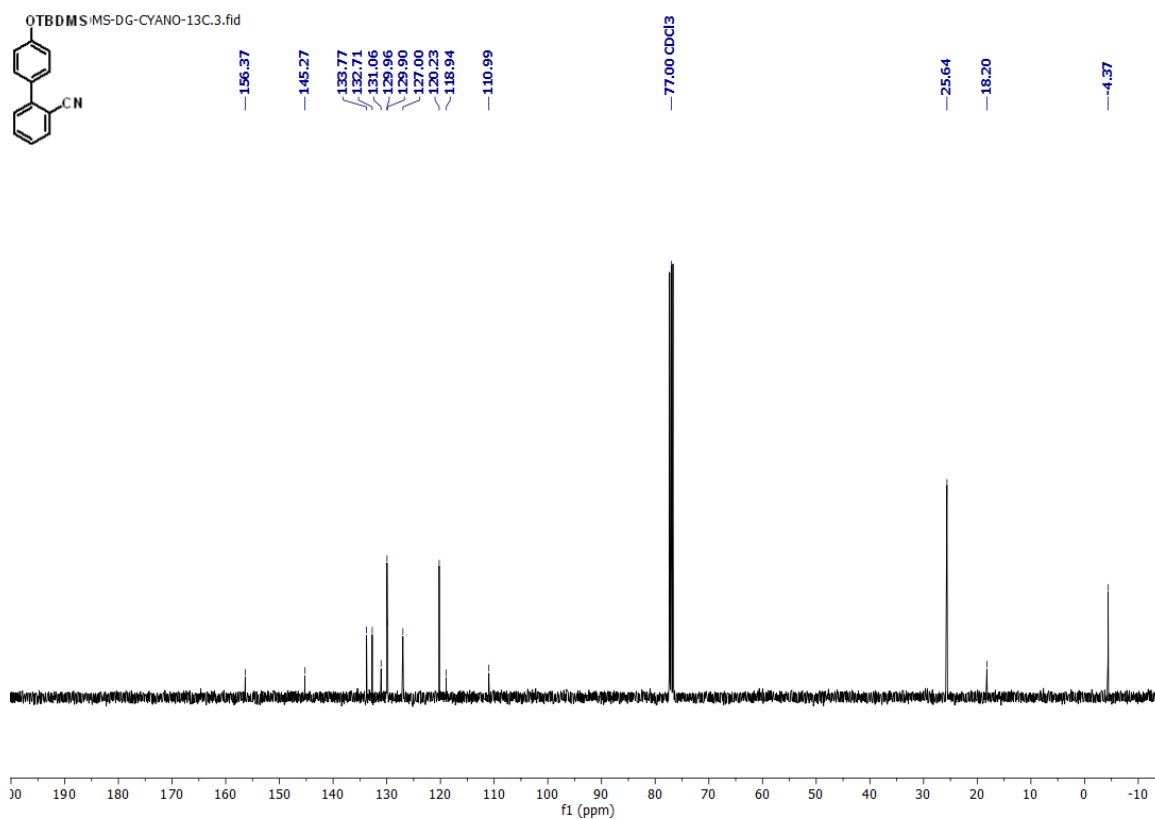
¹H NMR of DT₁



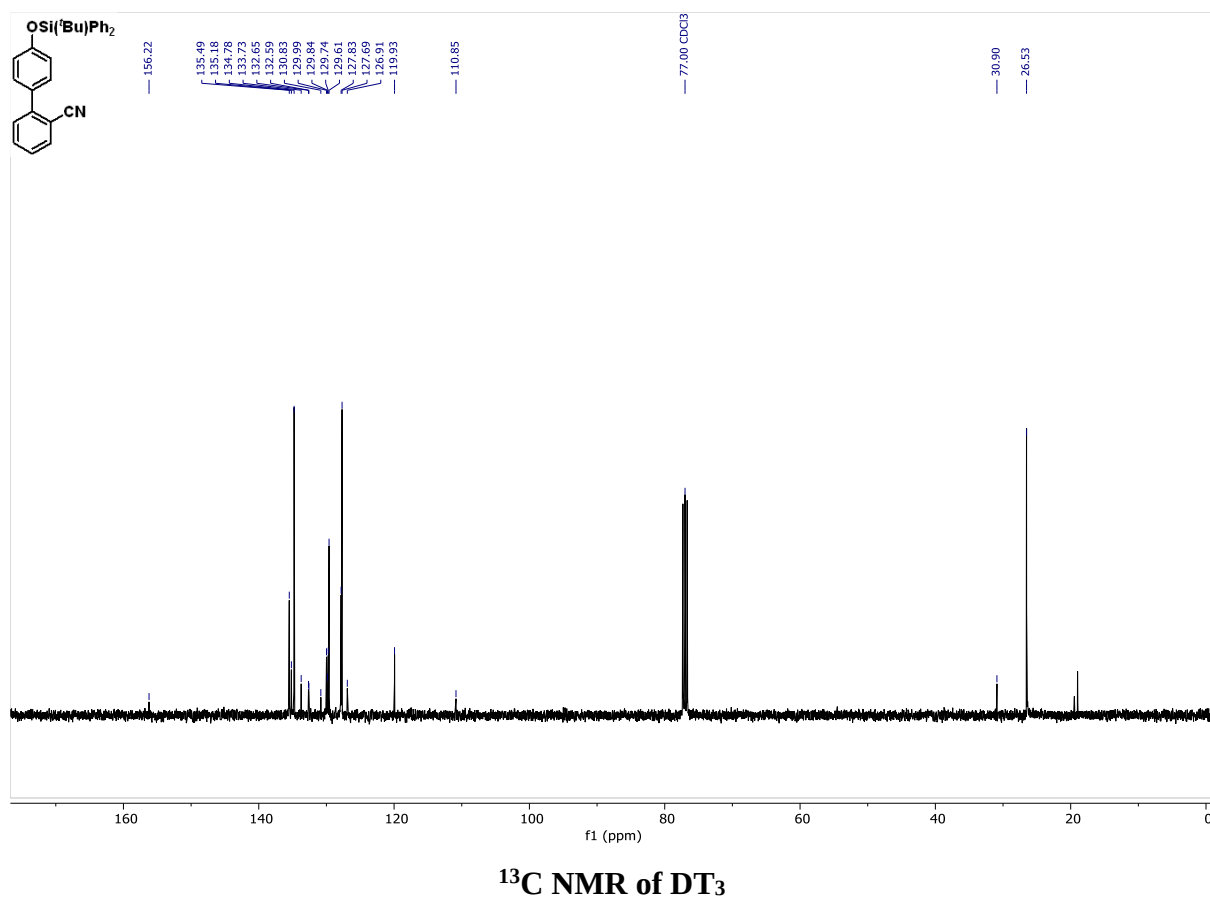
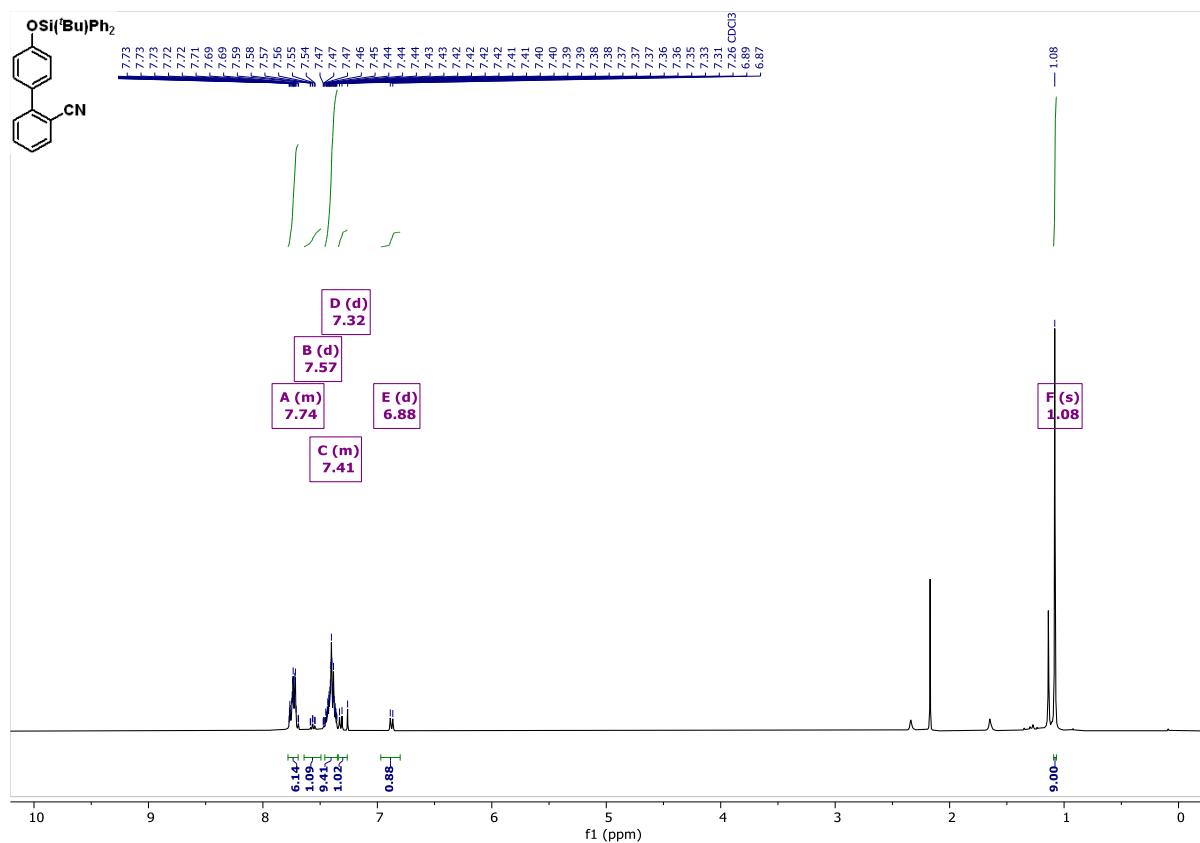
¹³C NMR of DT₁

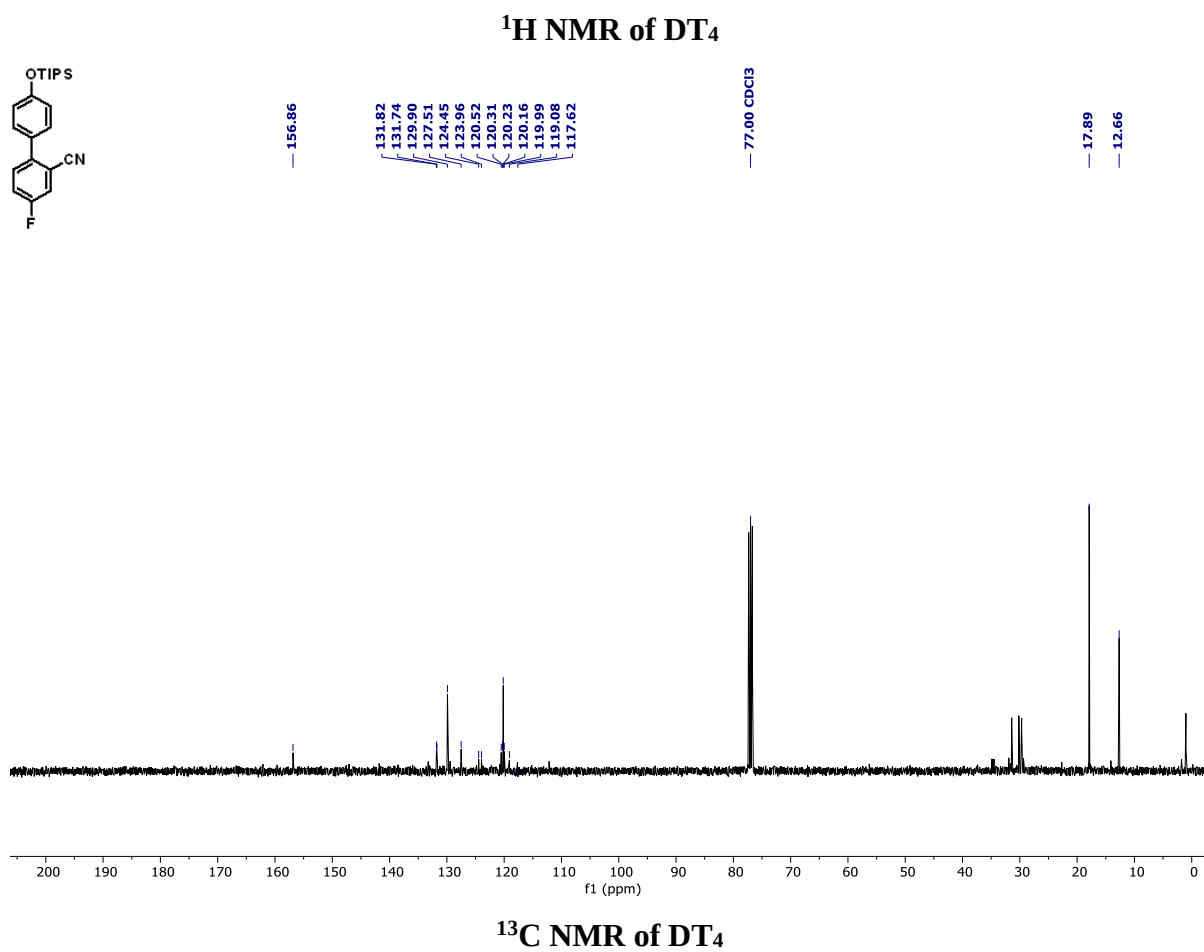
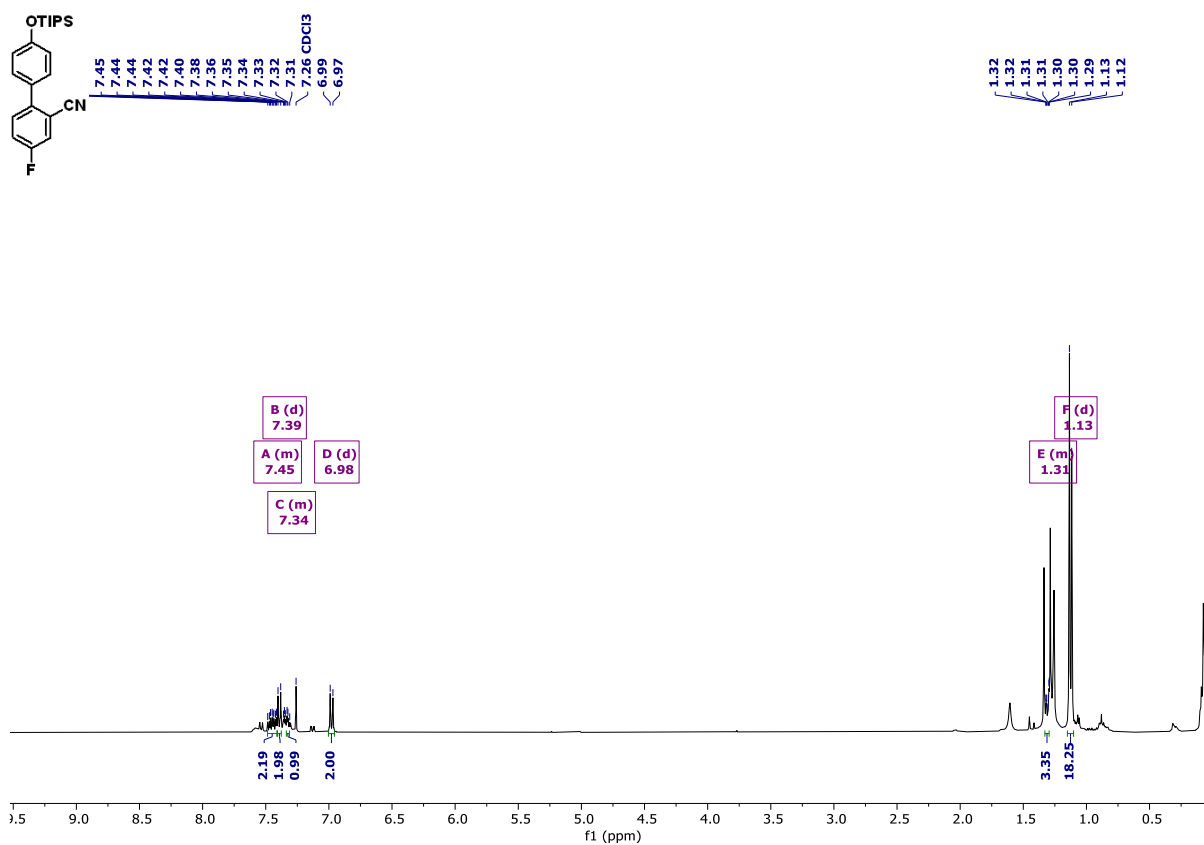


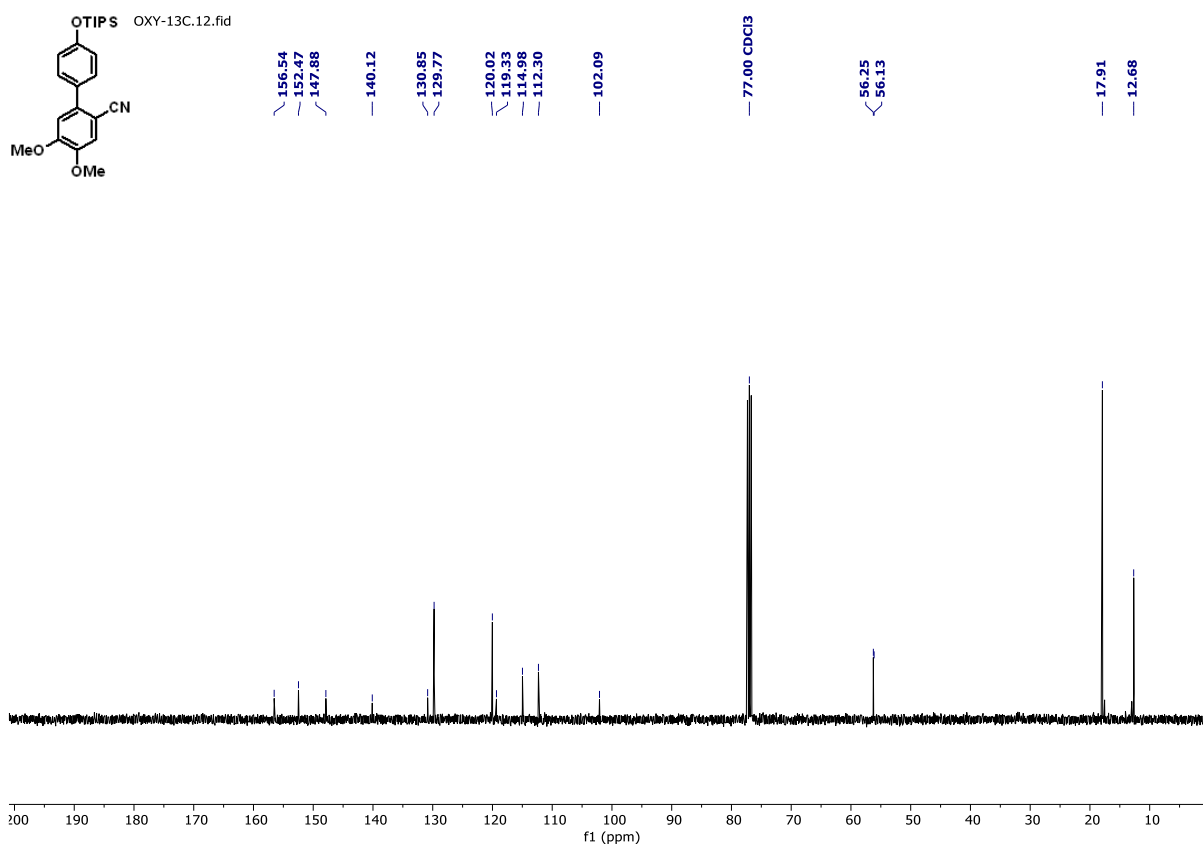
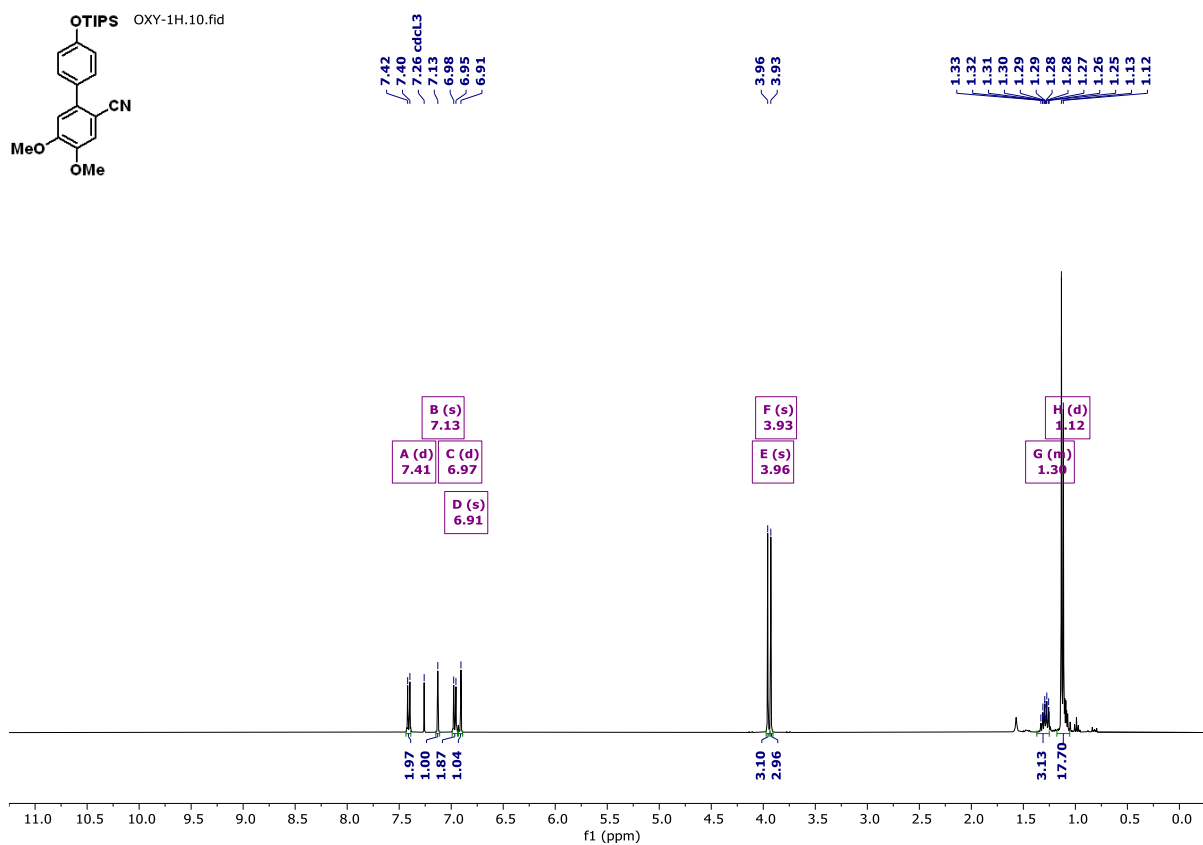
¹H NMR of DT₂

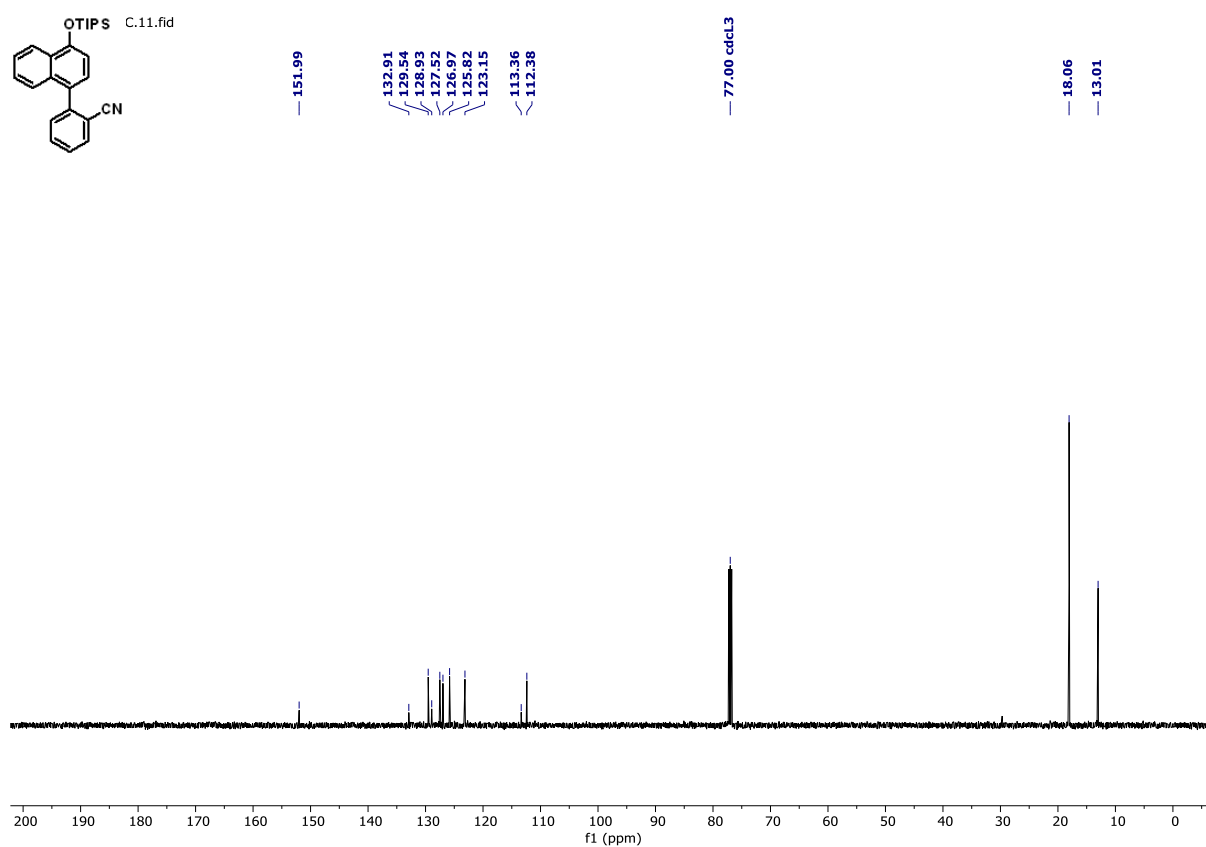
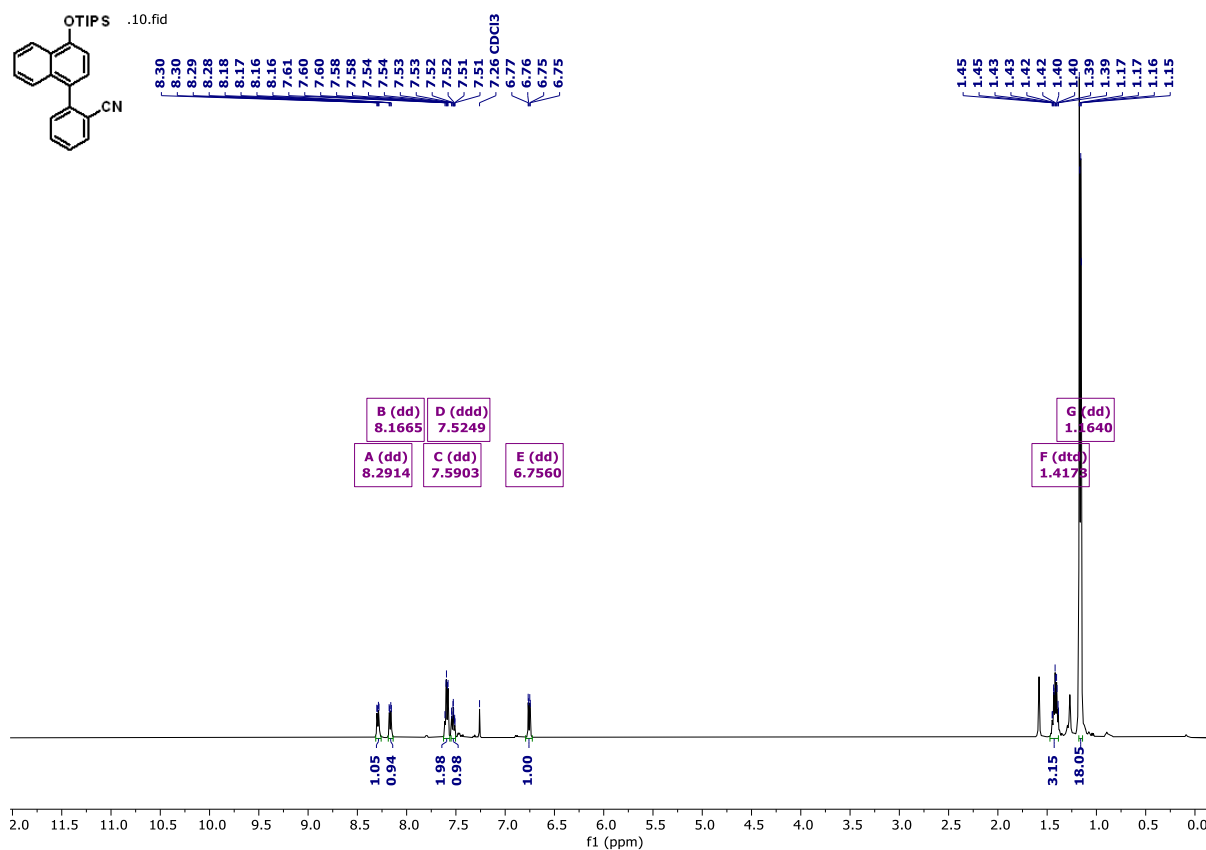


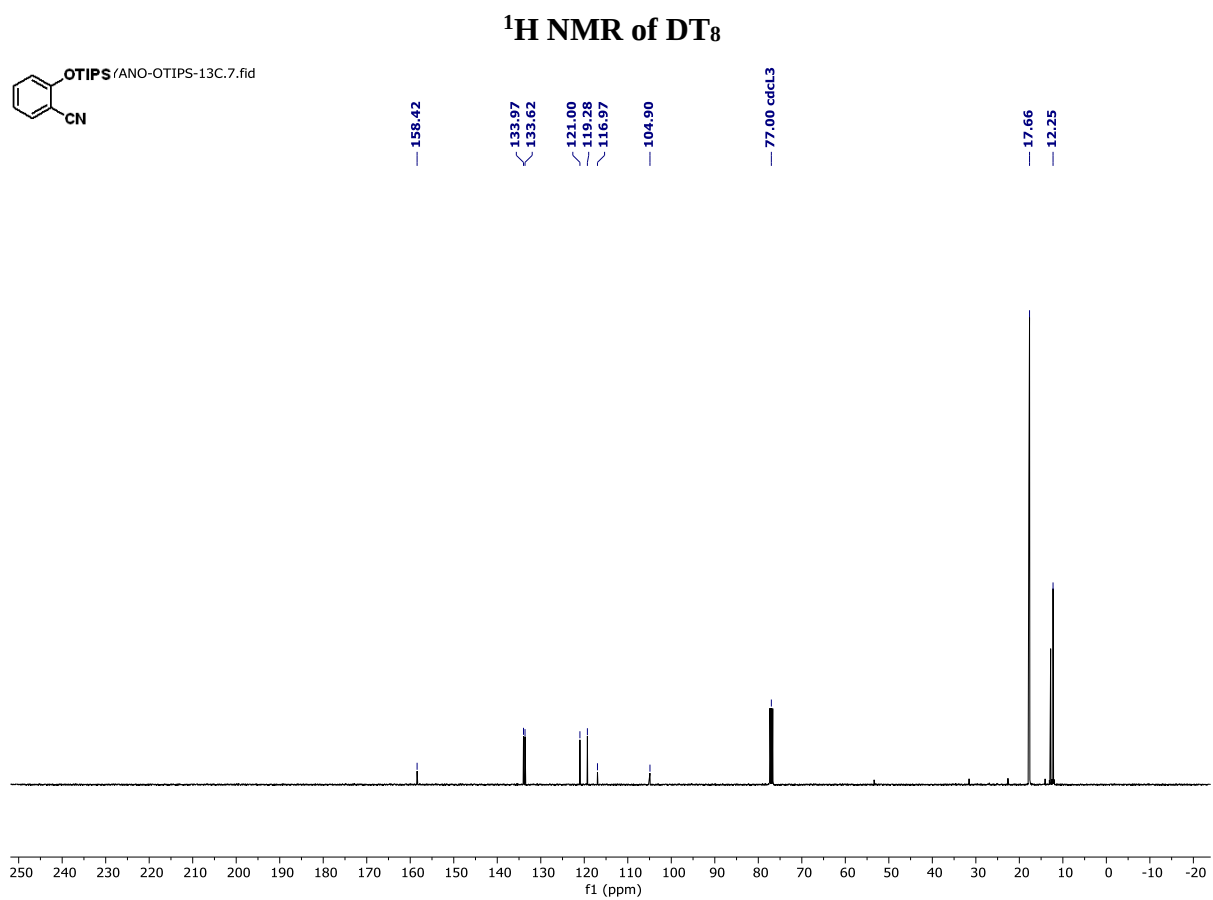
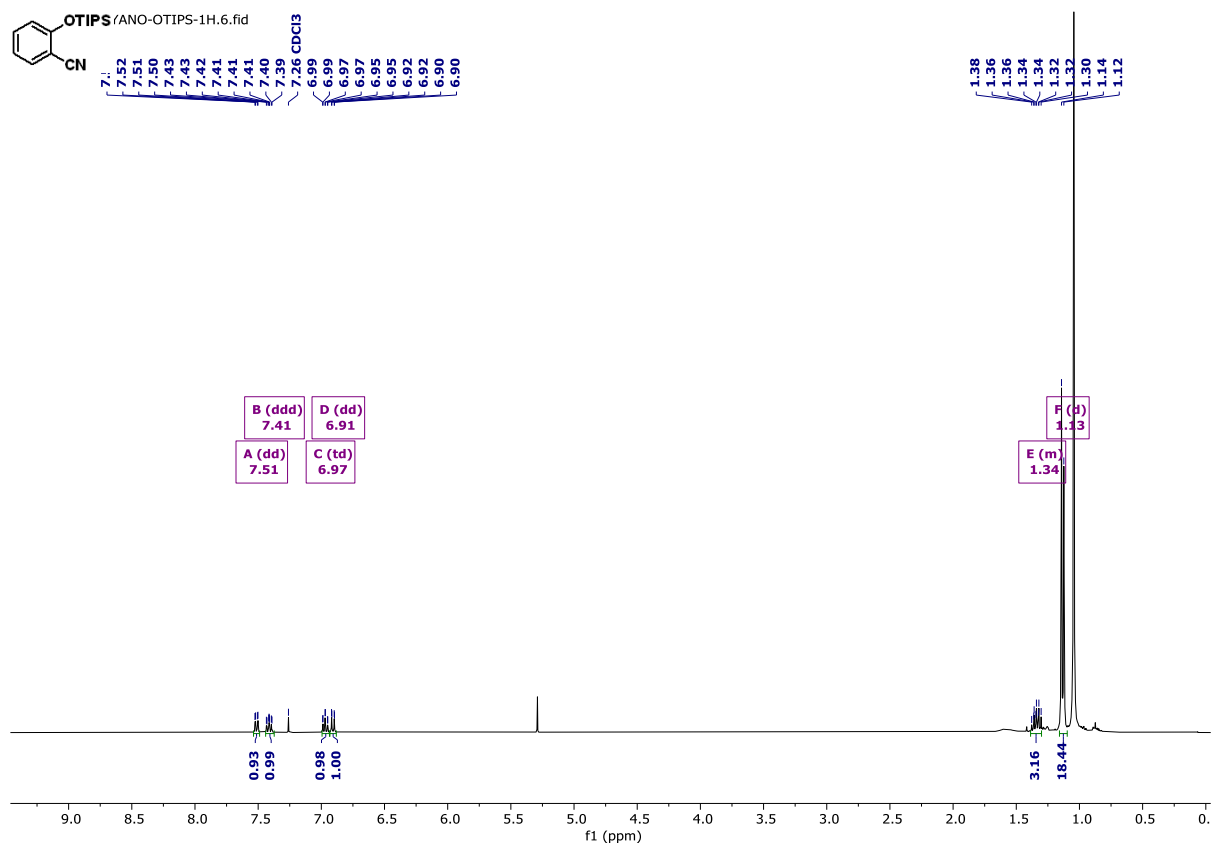
¹³C NMR of DT₂



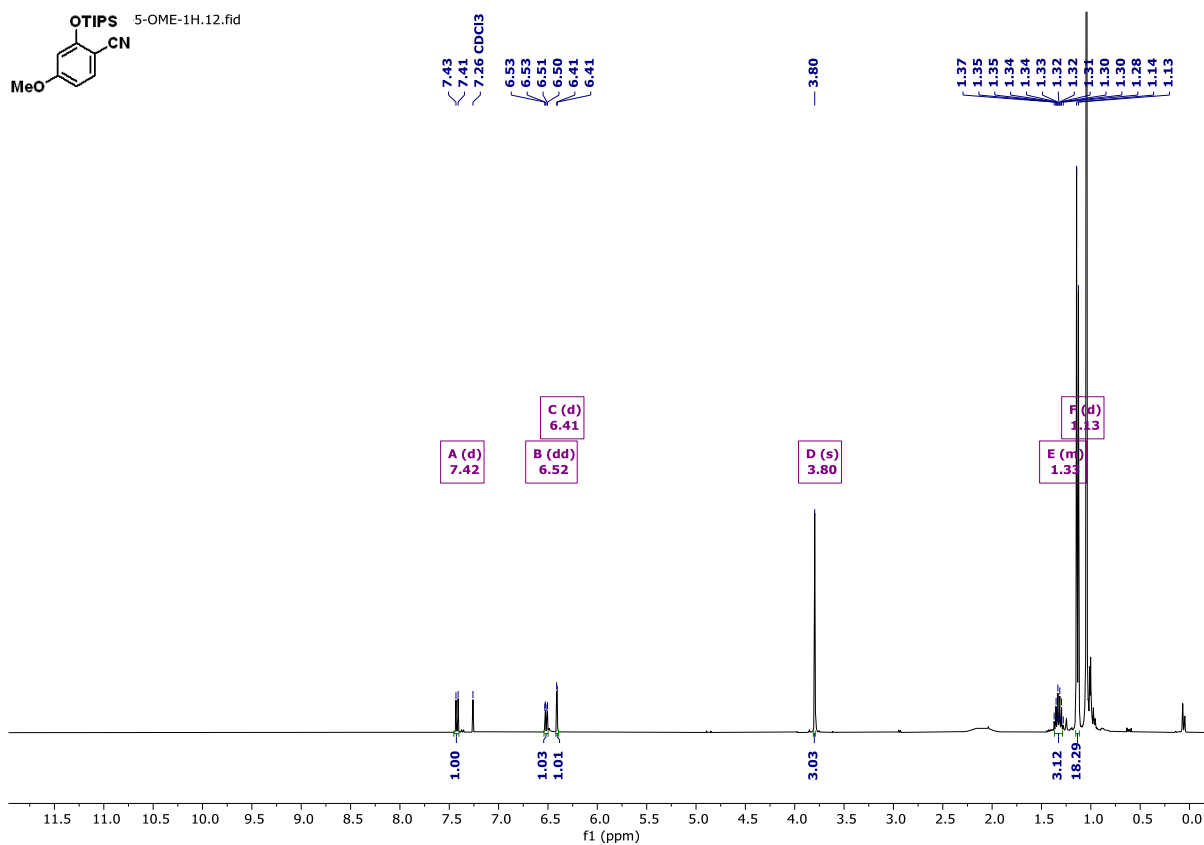




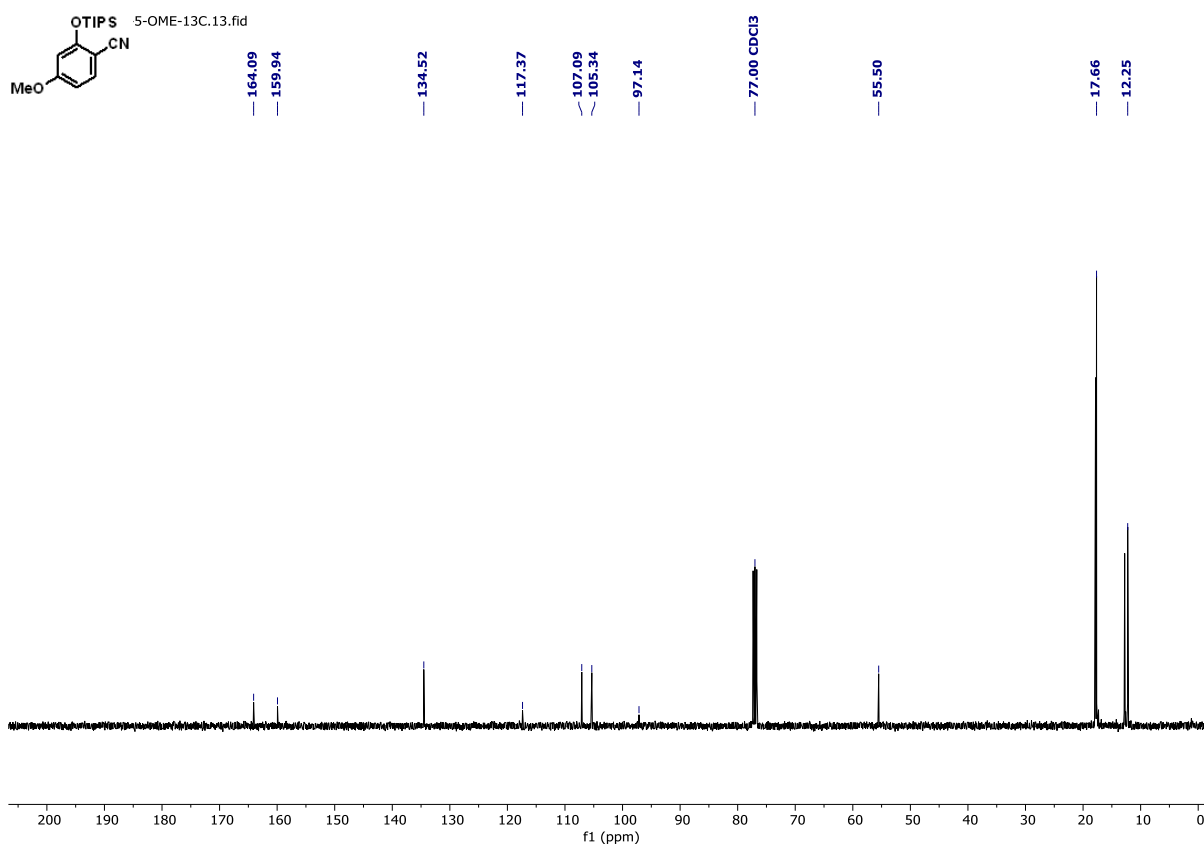




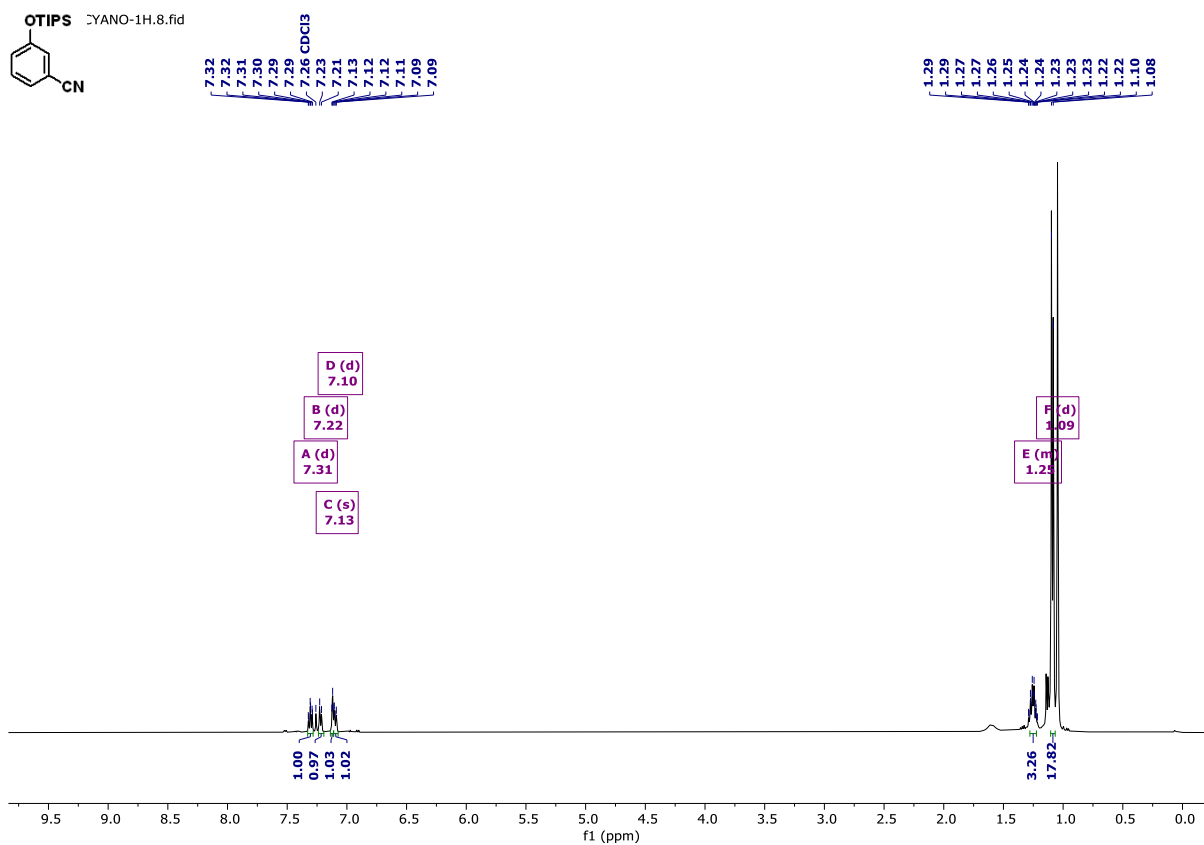
¹³C NMR of DT₈



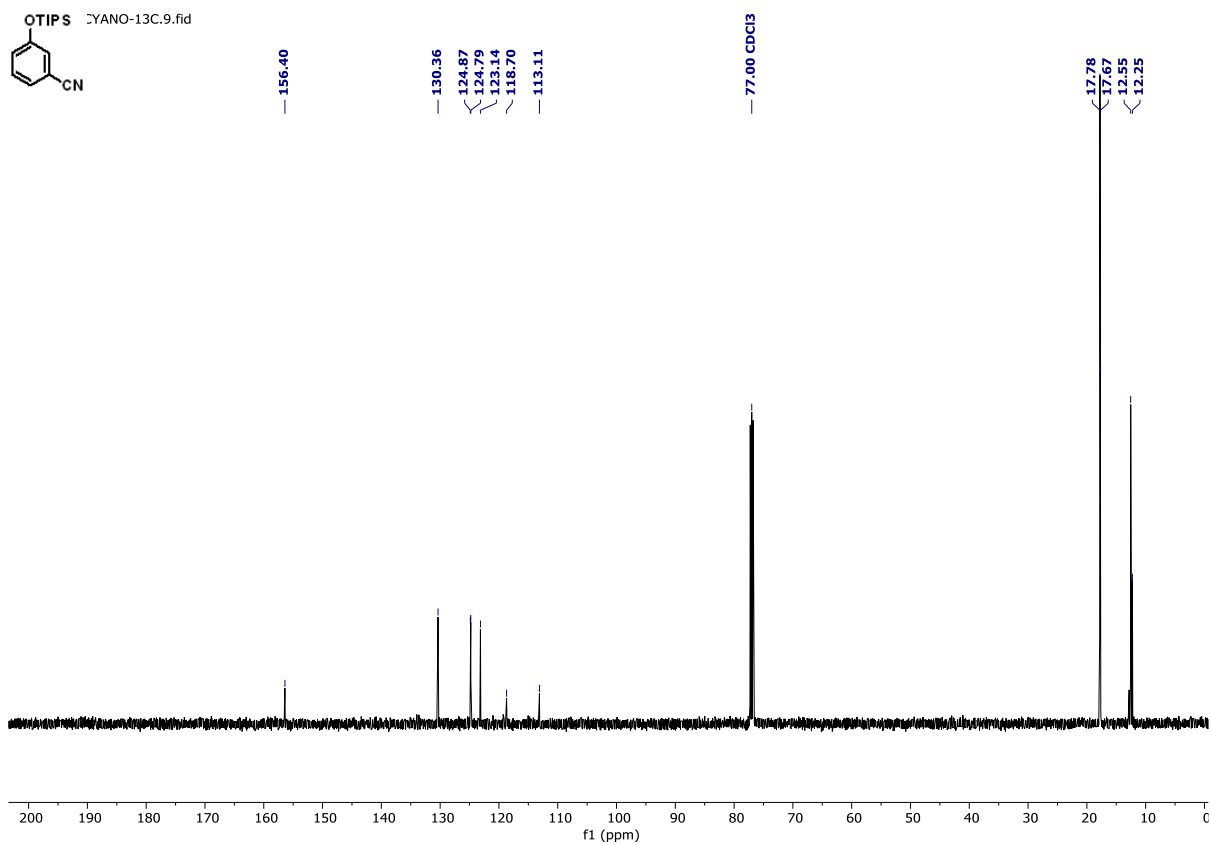
¹H NMR of DT₉



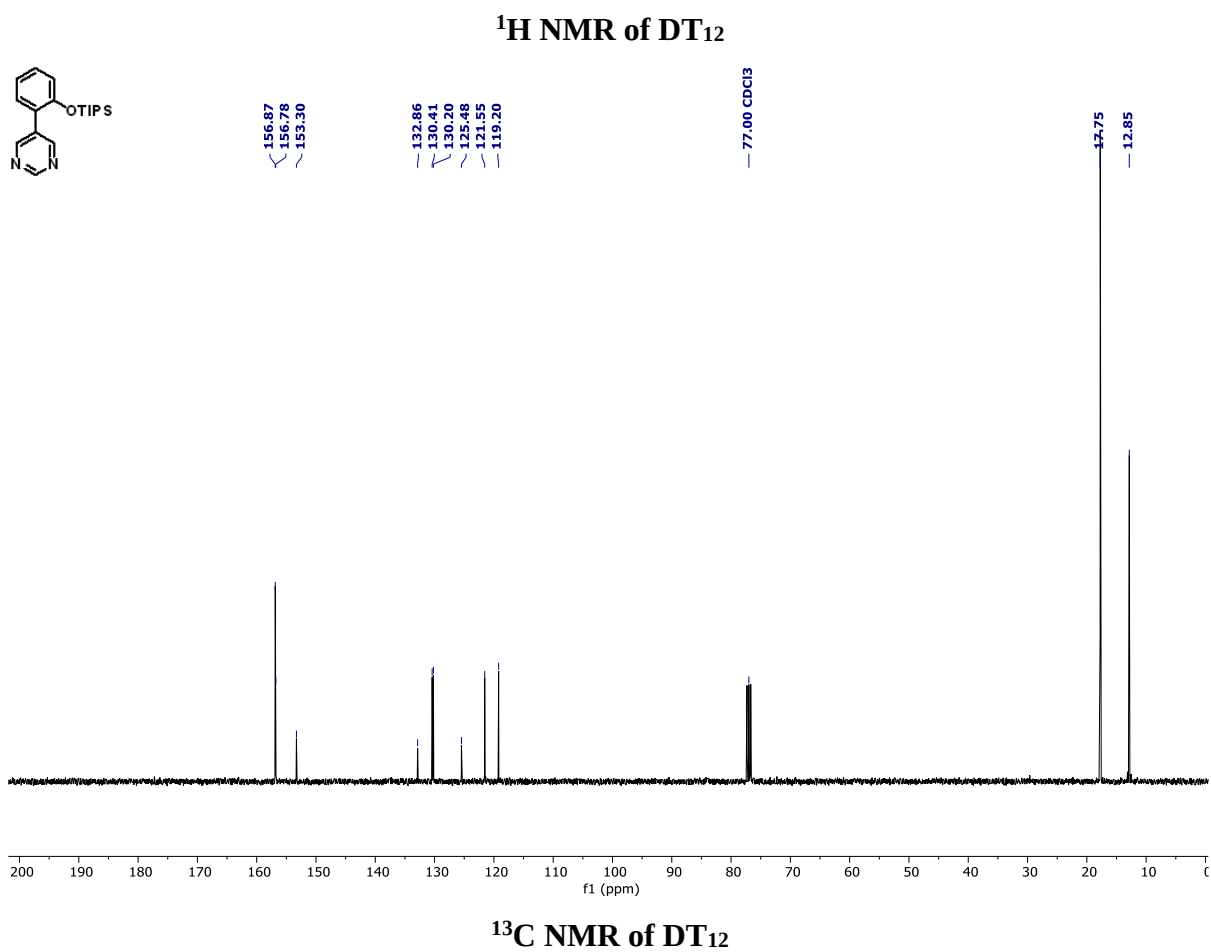
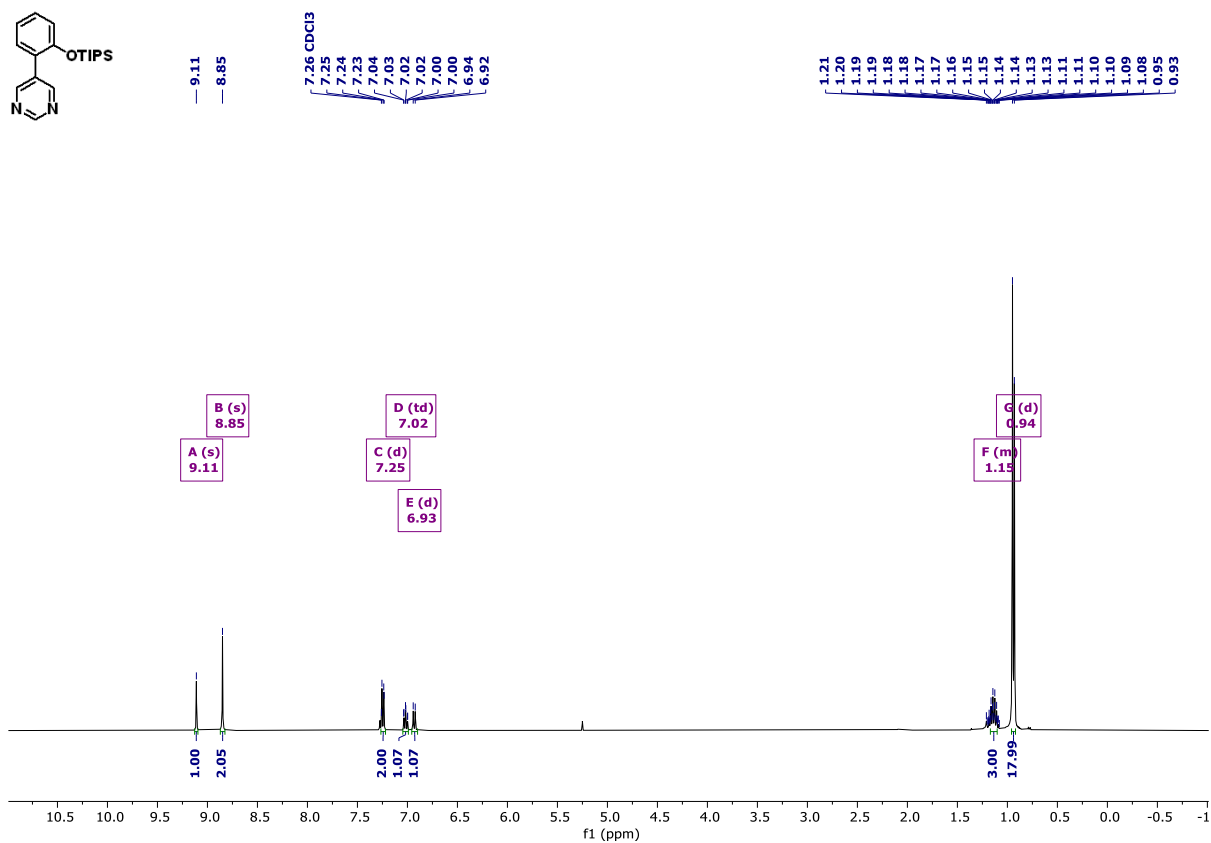
¹³C NMR of DT₉

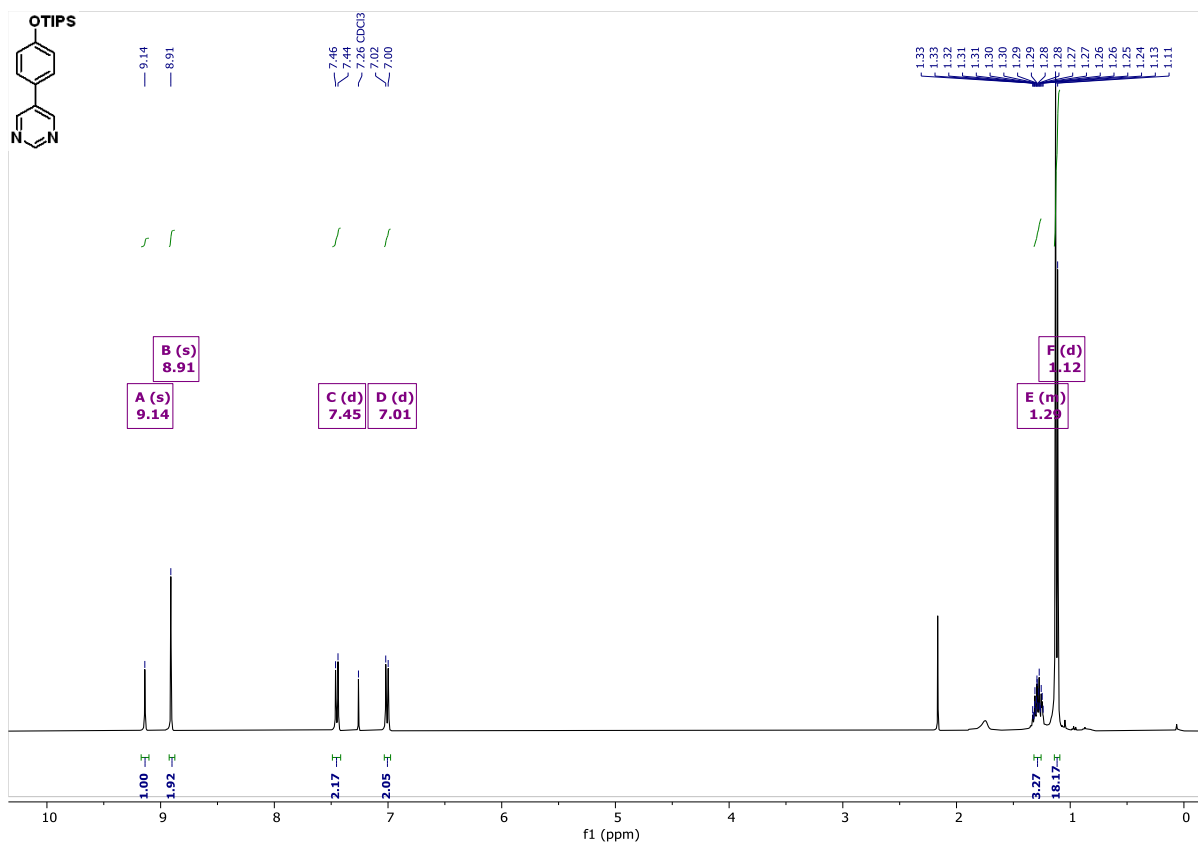


^1H NMR of DT₁₀

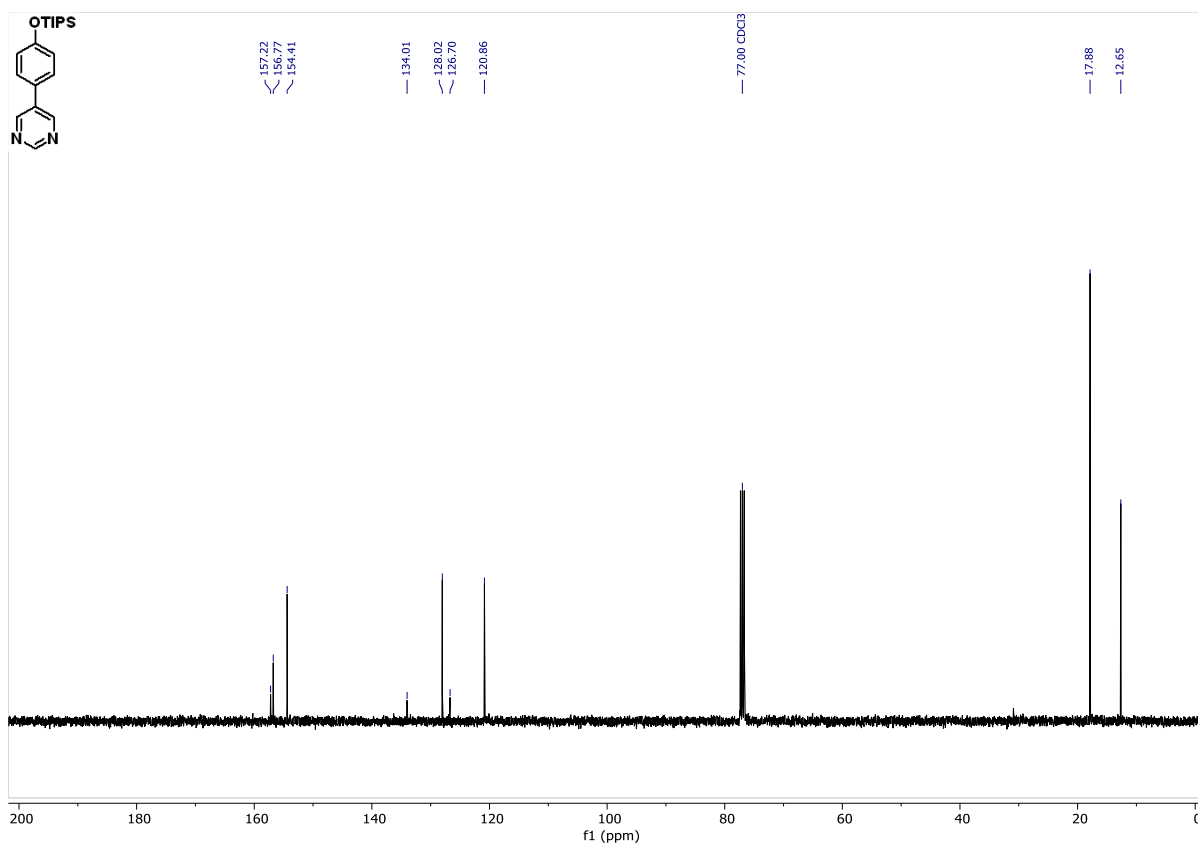


^{13}C NMR of DT₁₀

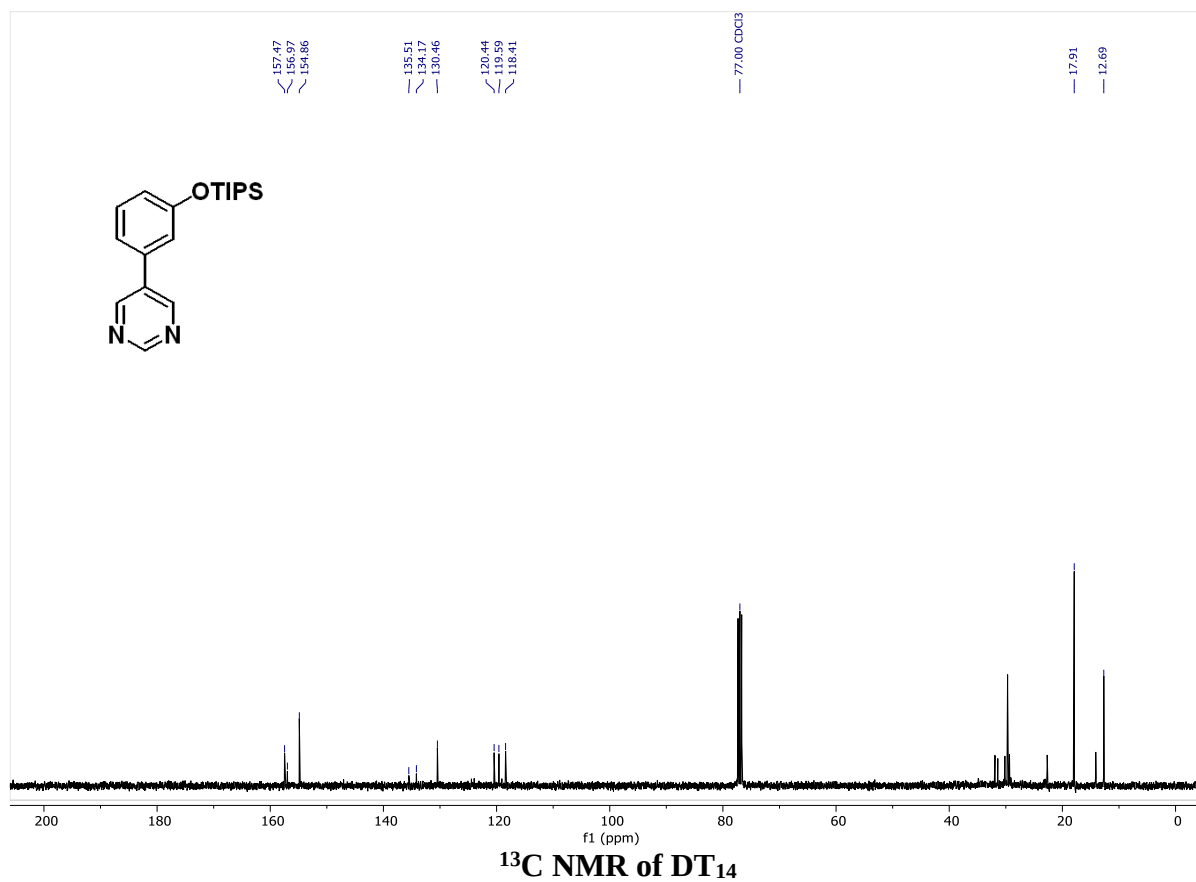
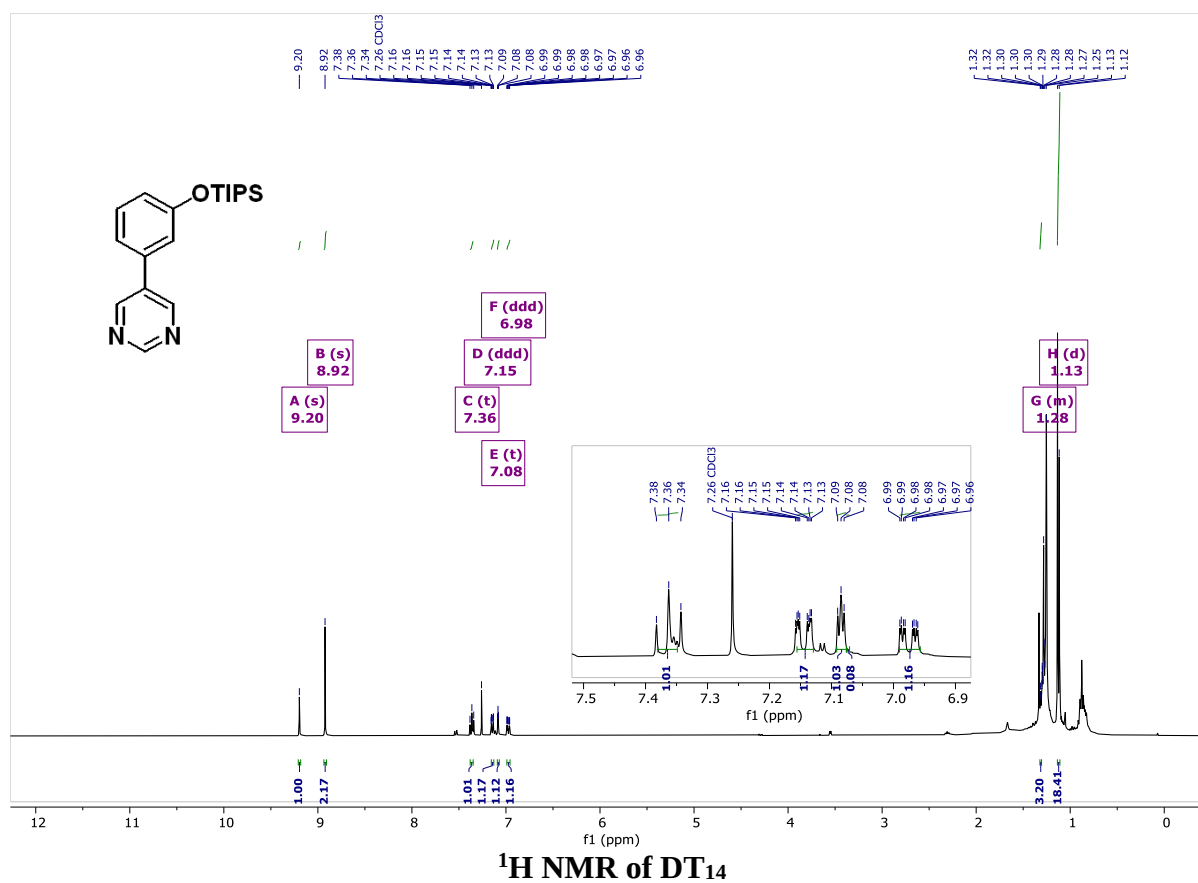


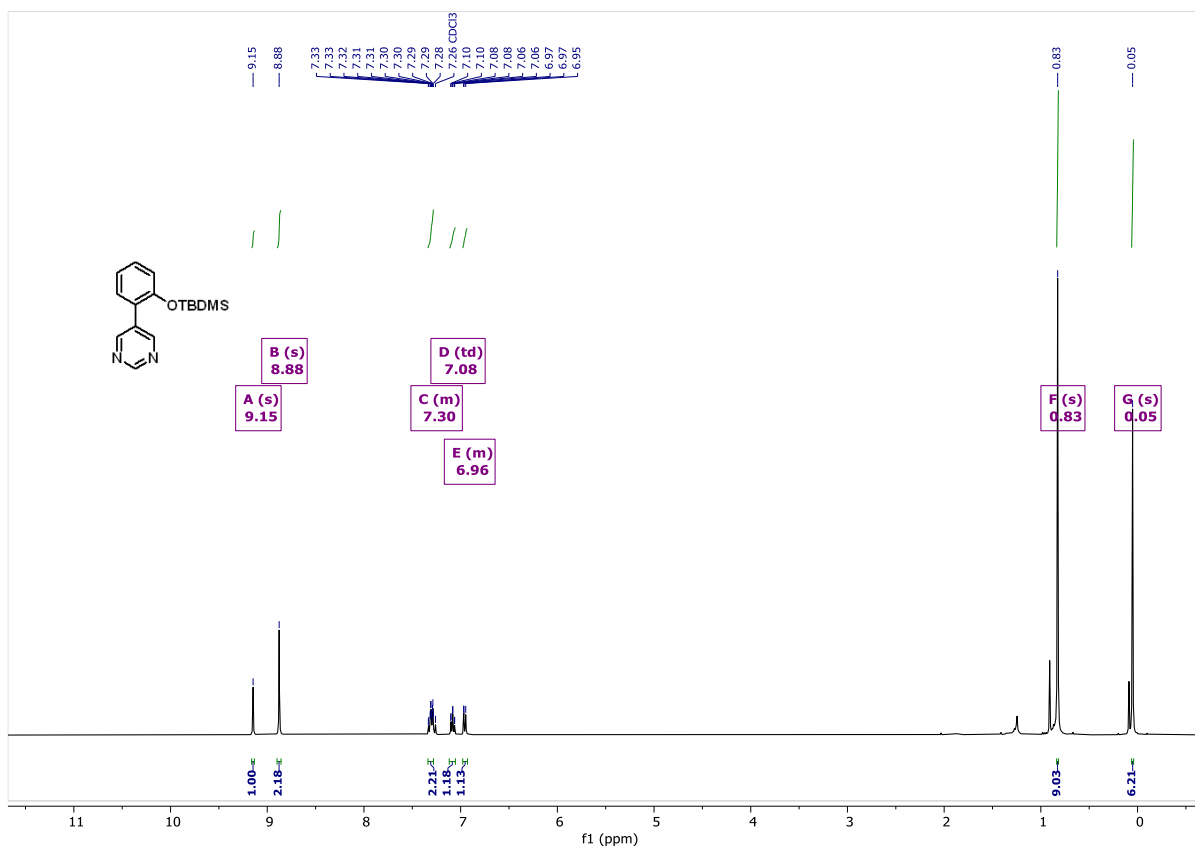


¹H NMR of DT₁₃

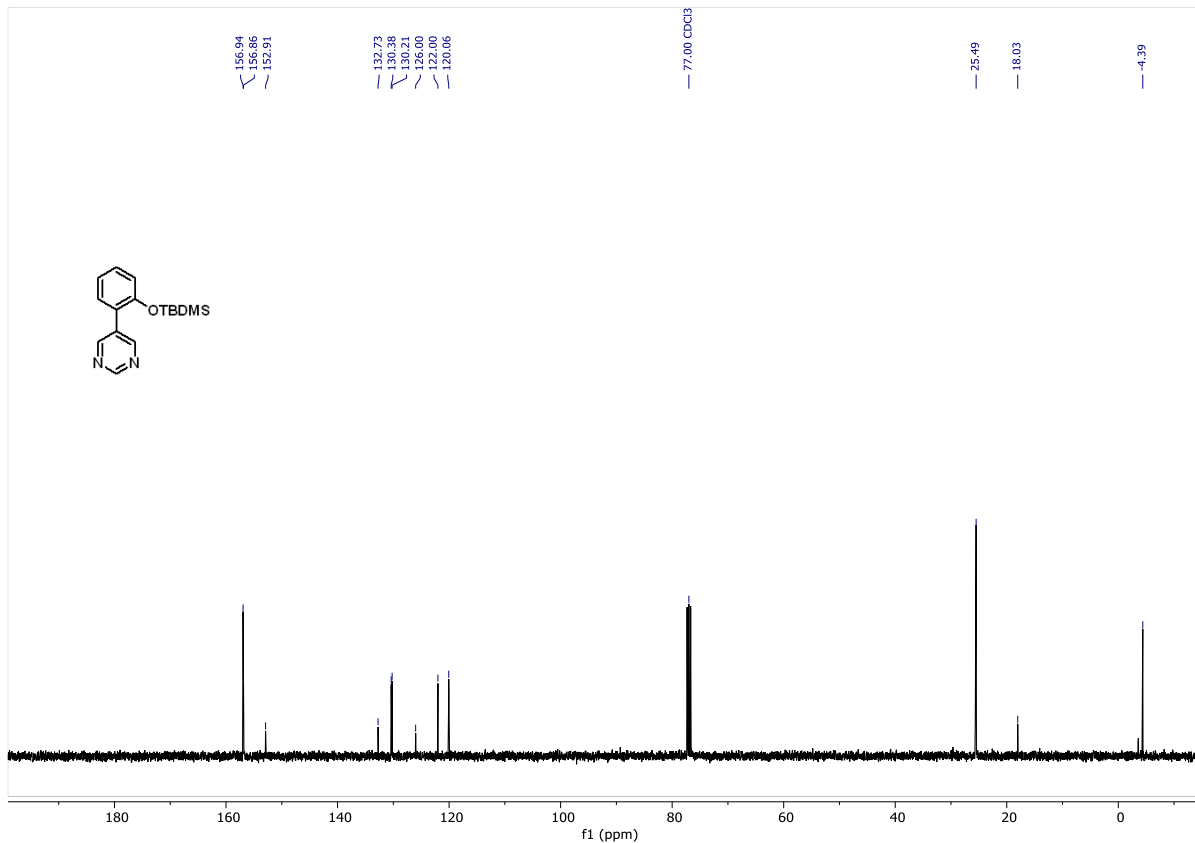


¹³C NMR of DT₁₃

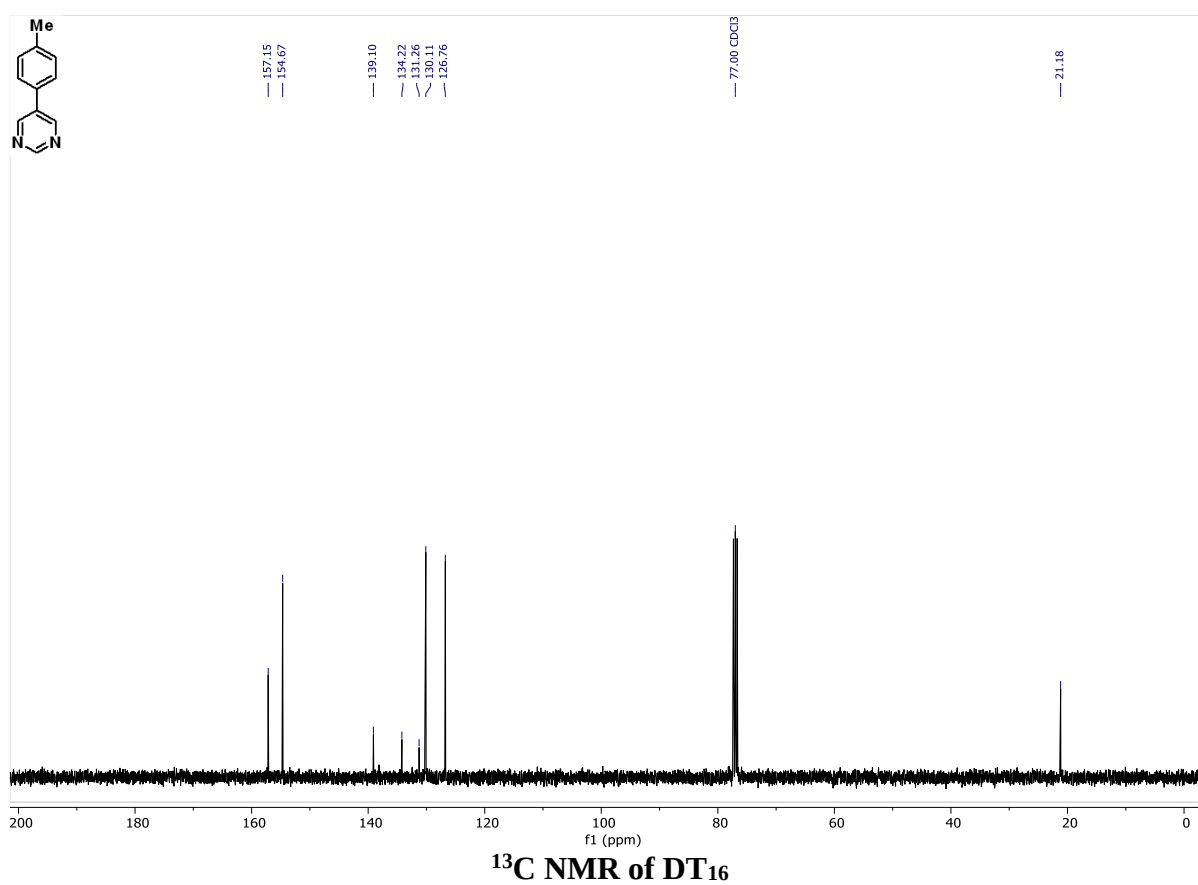
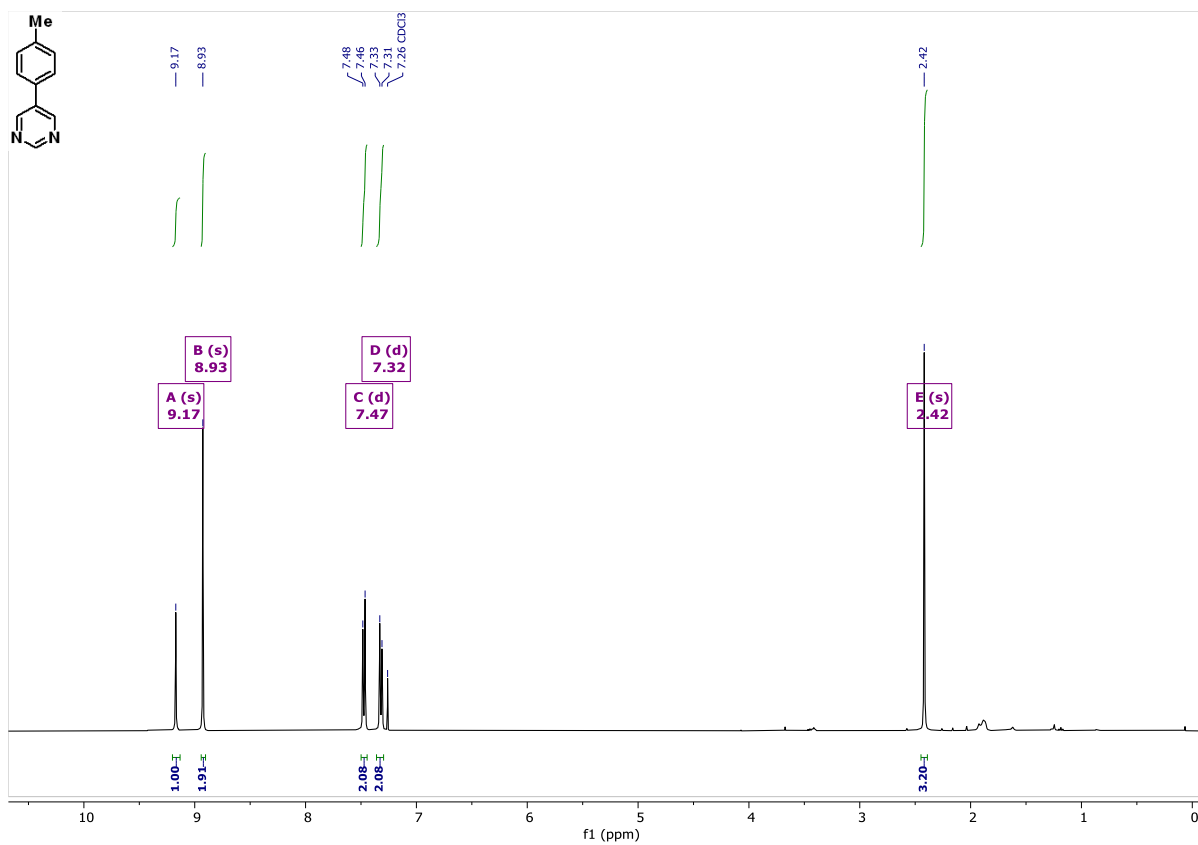


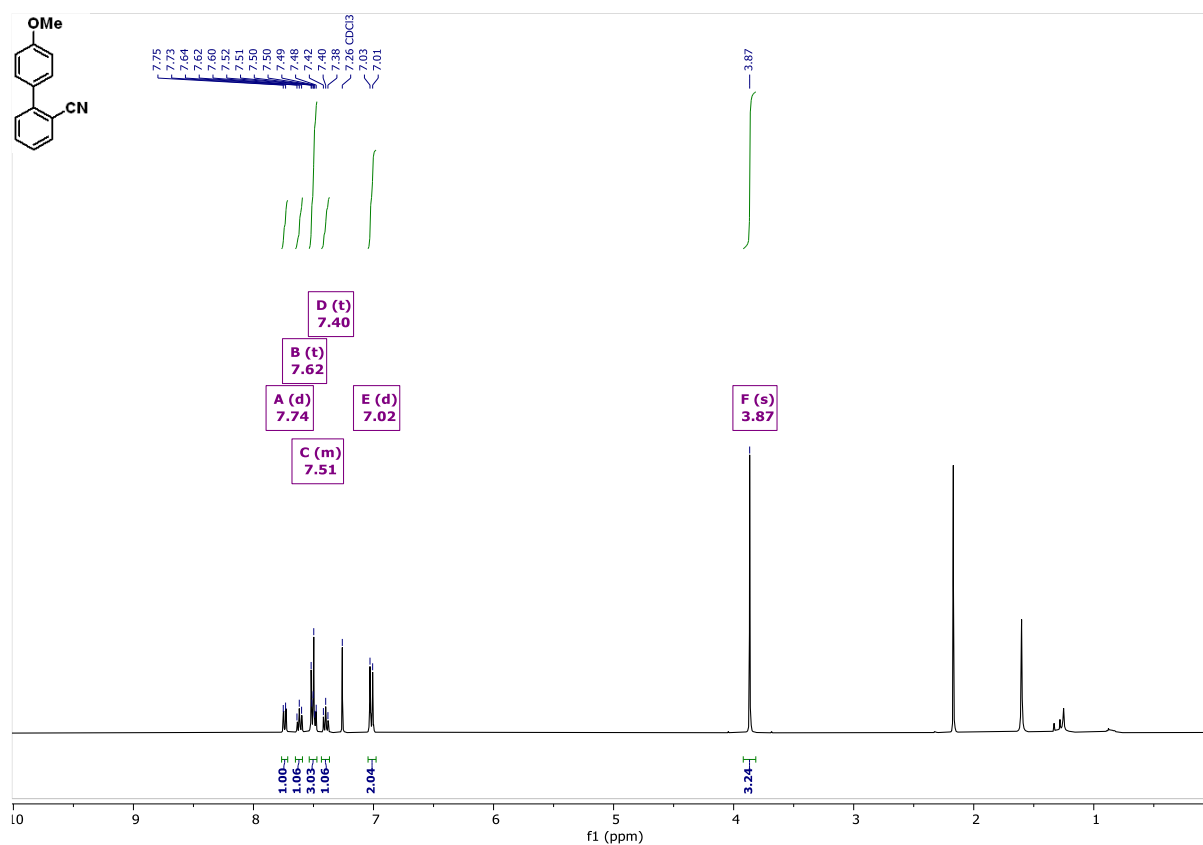


¹H NMR of DT₁₅

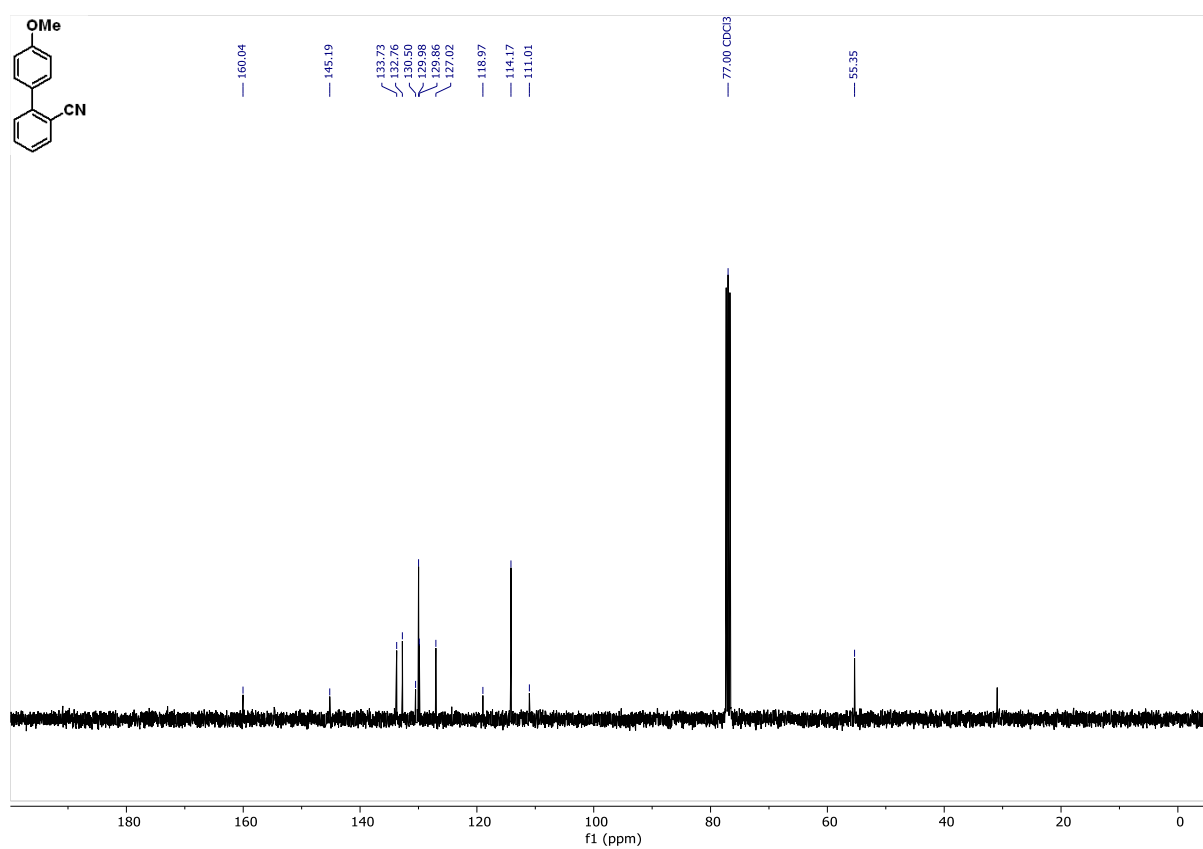


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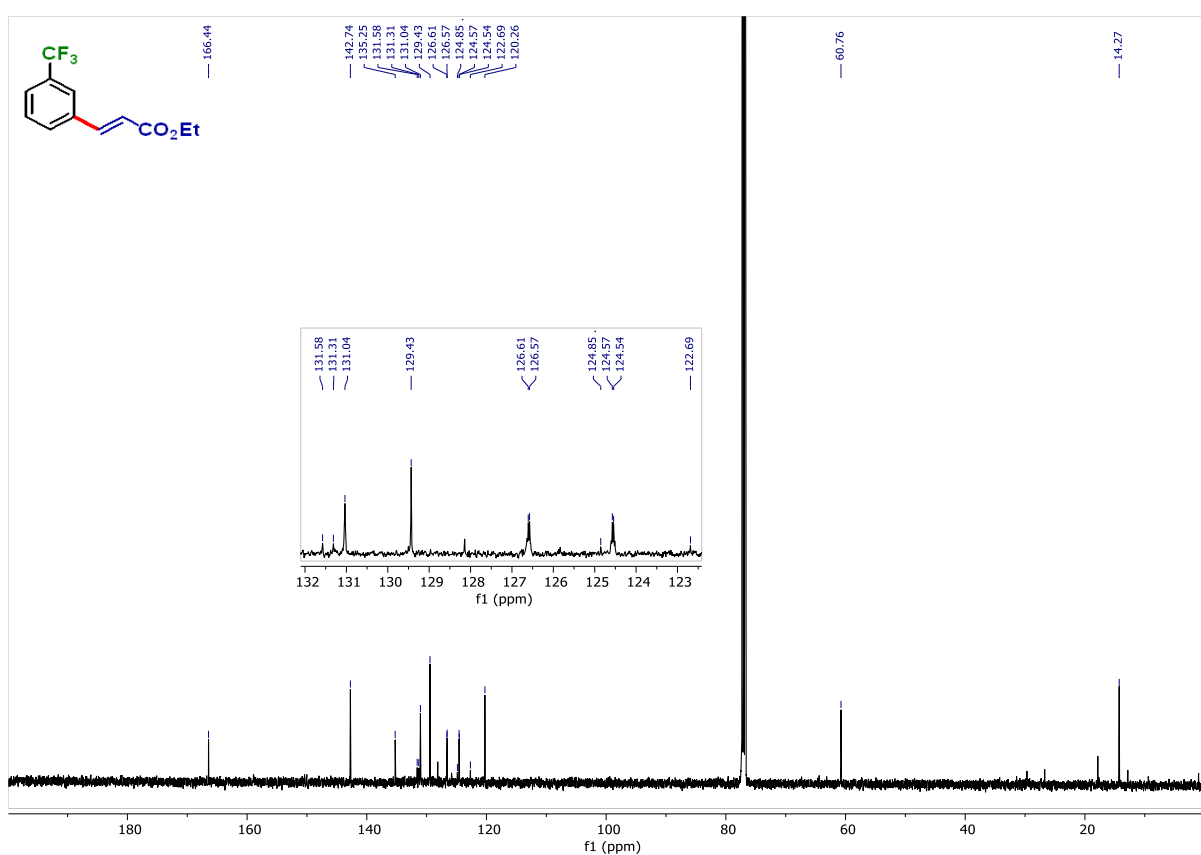
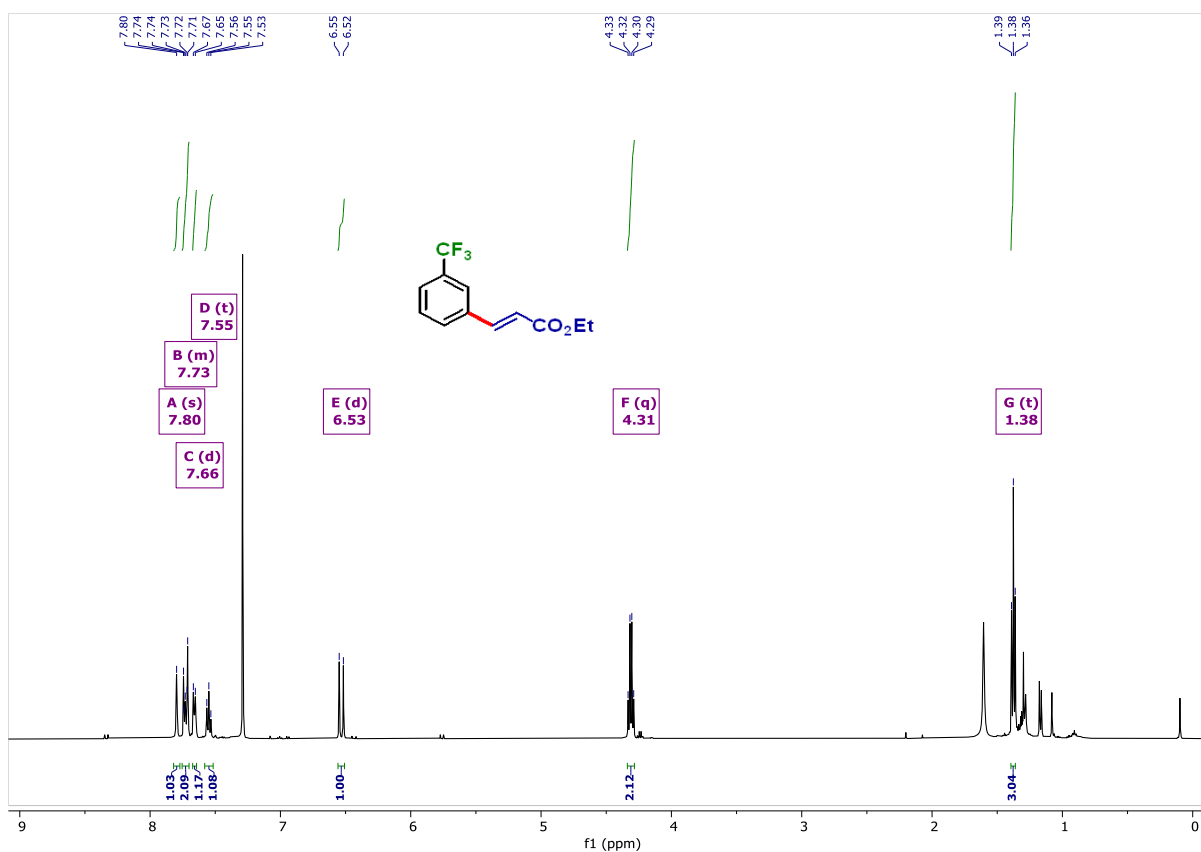


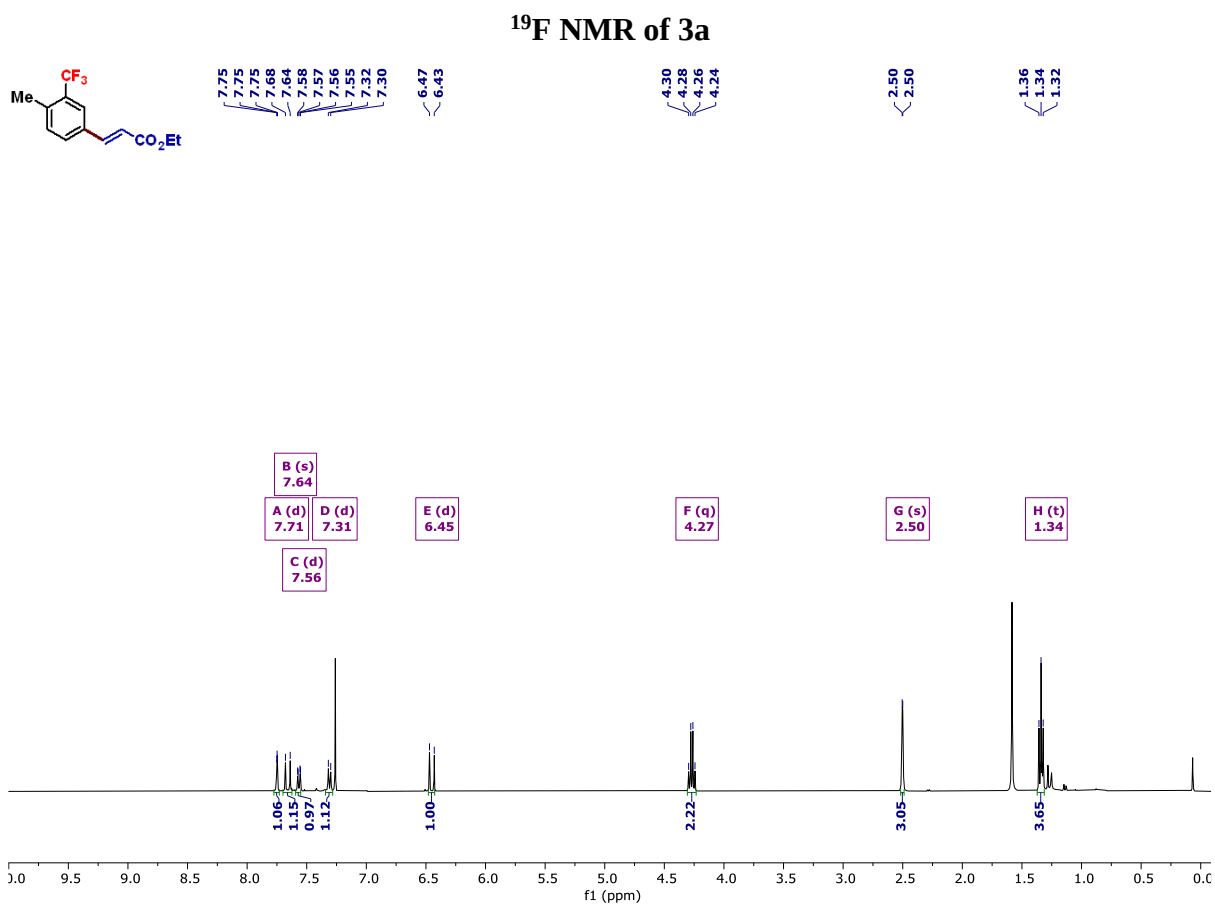
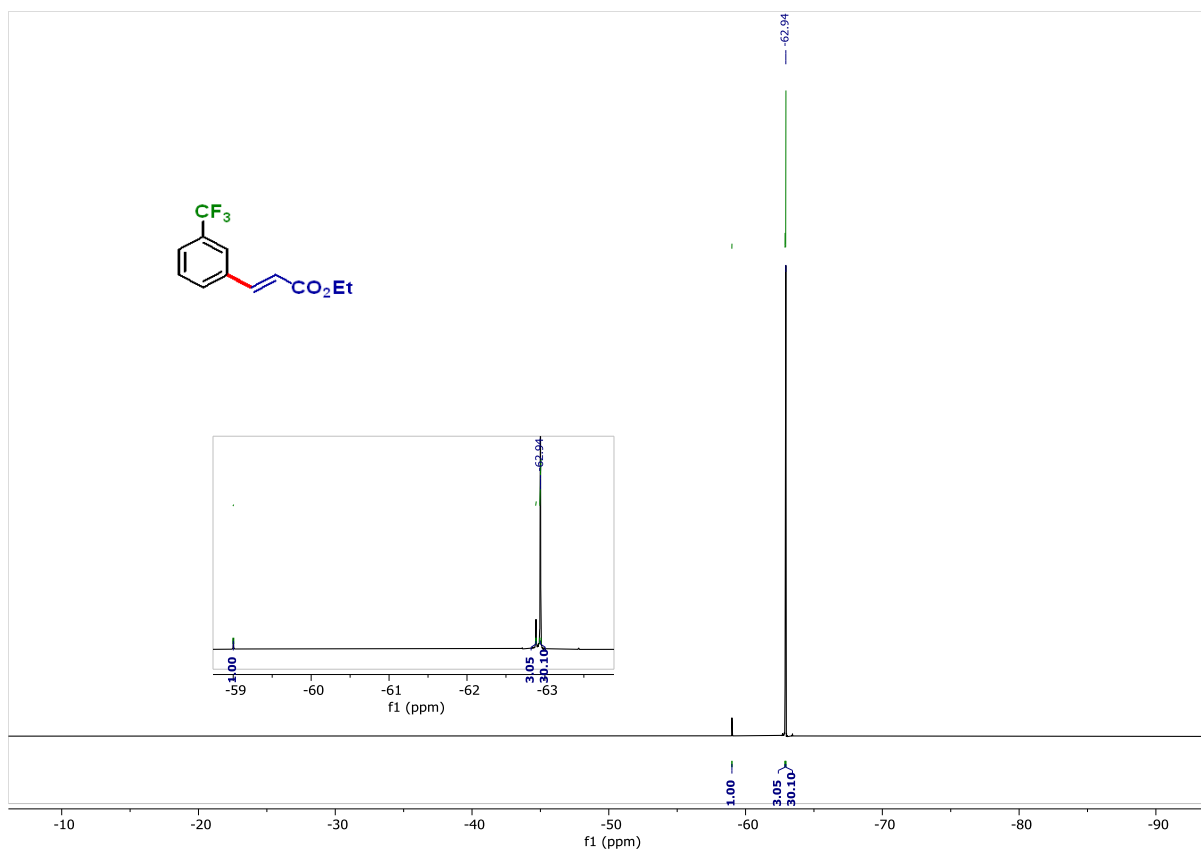


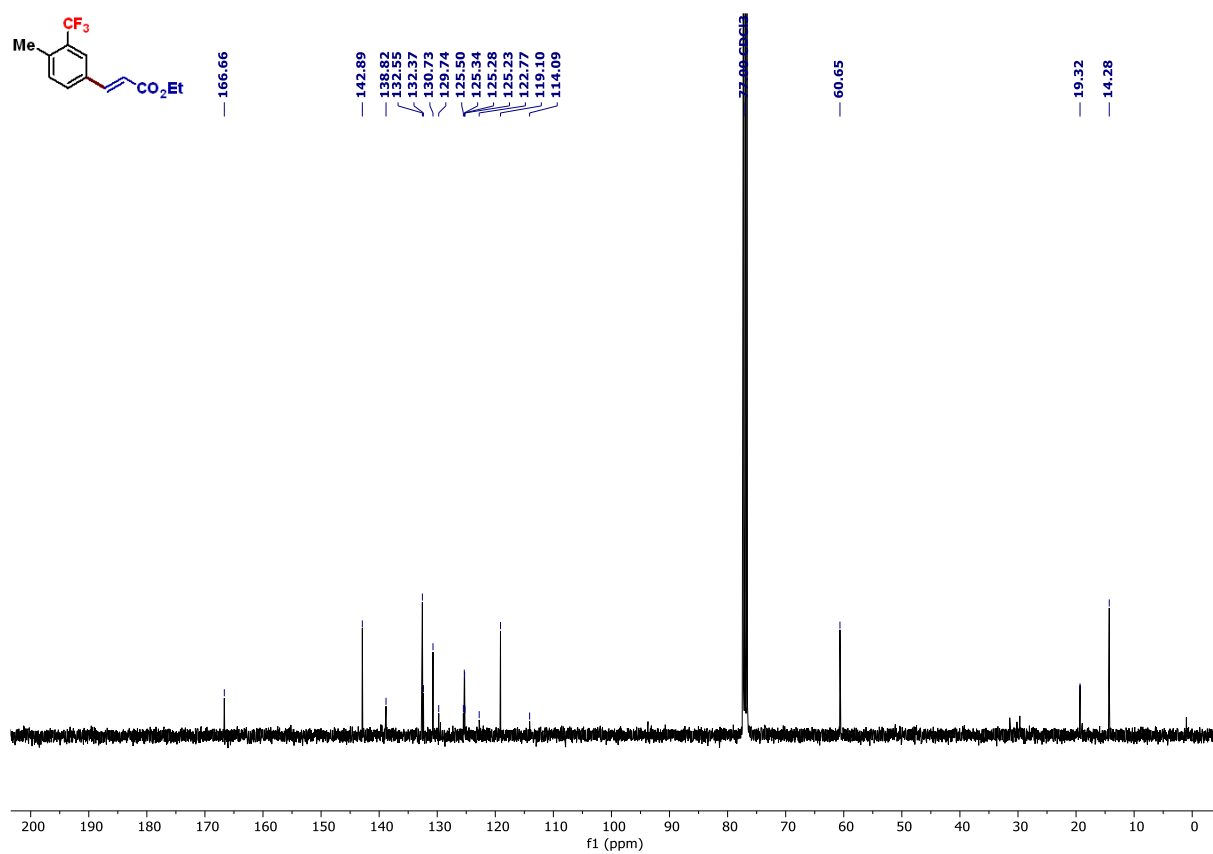
¹H NMR of DT₁₇



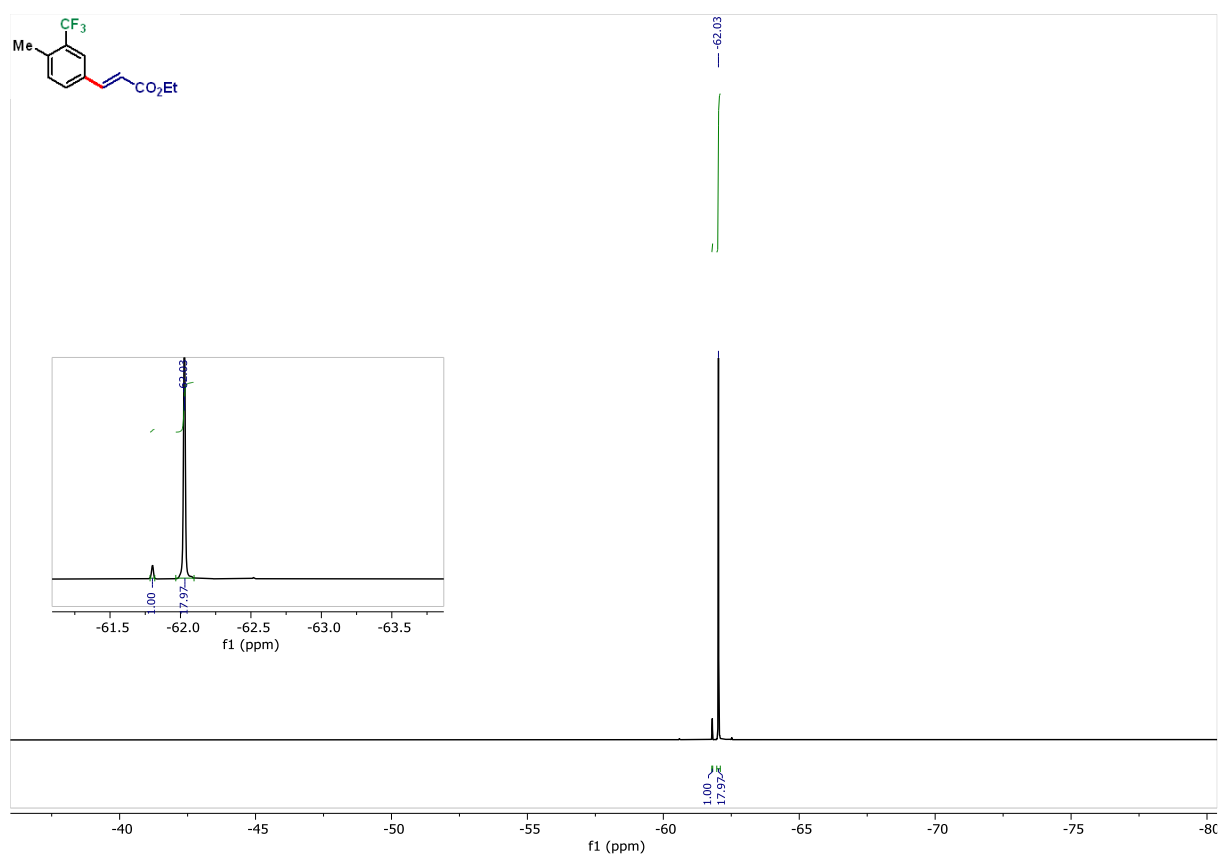
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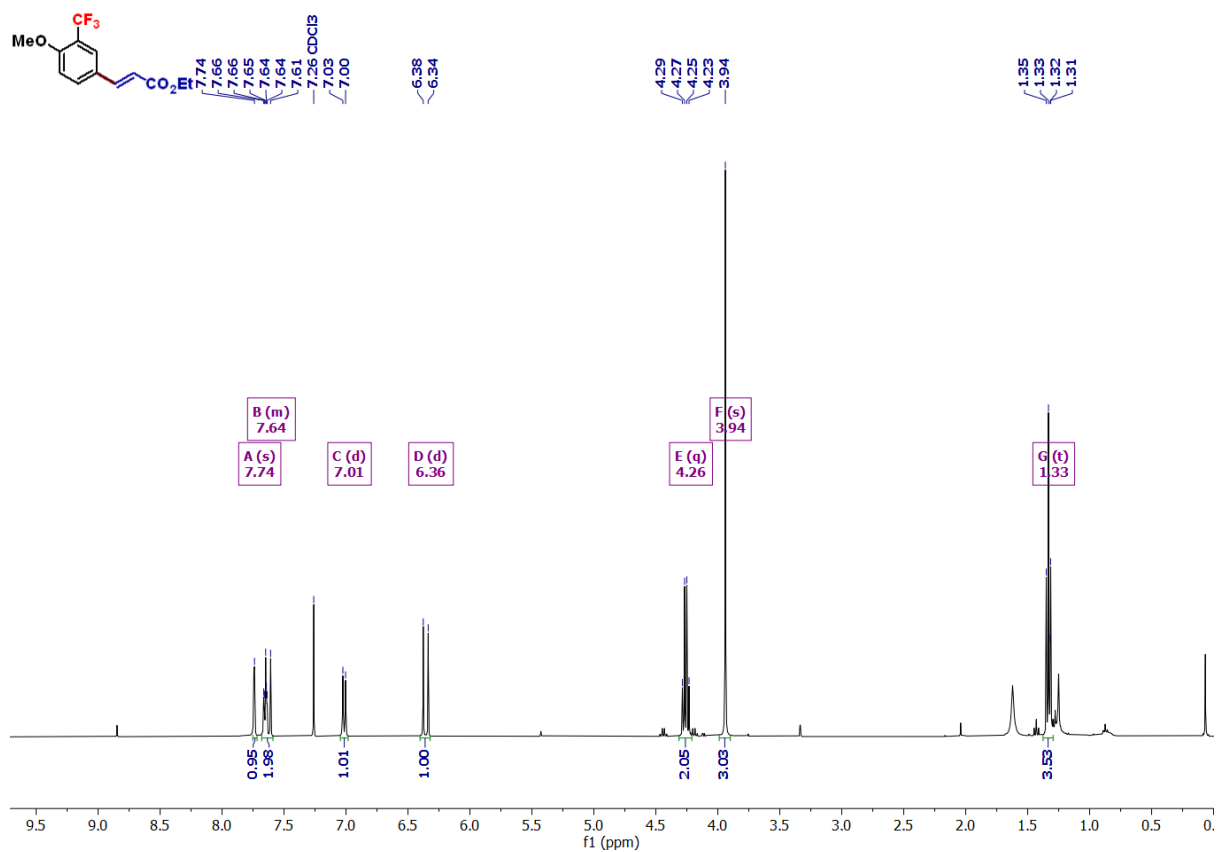




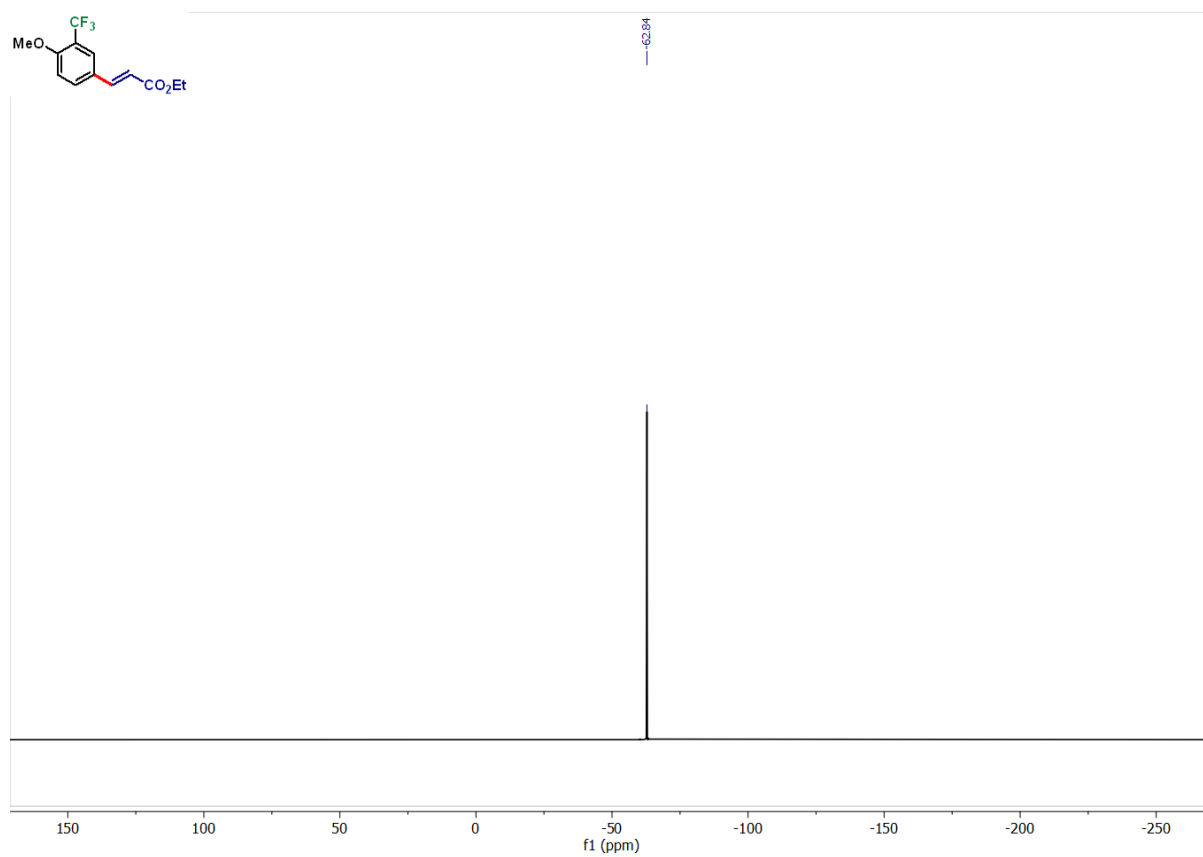
^{13}C NMR of 3b



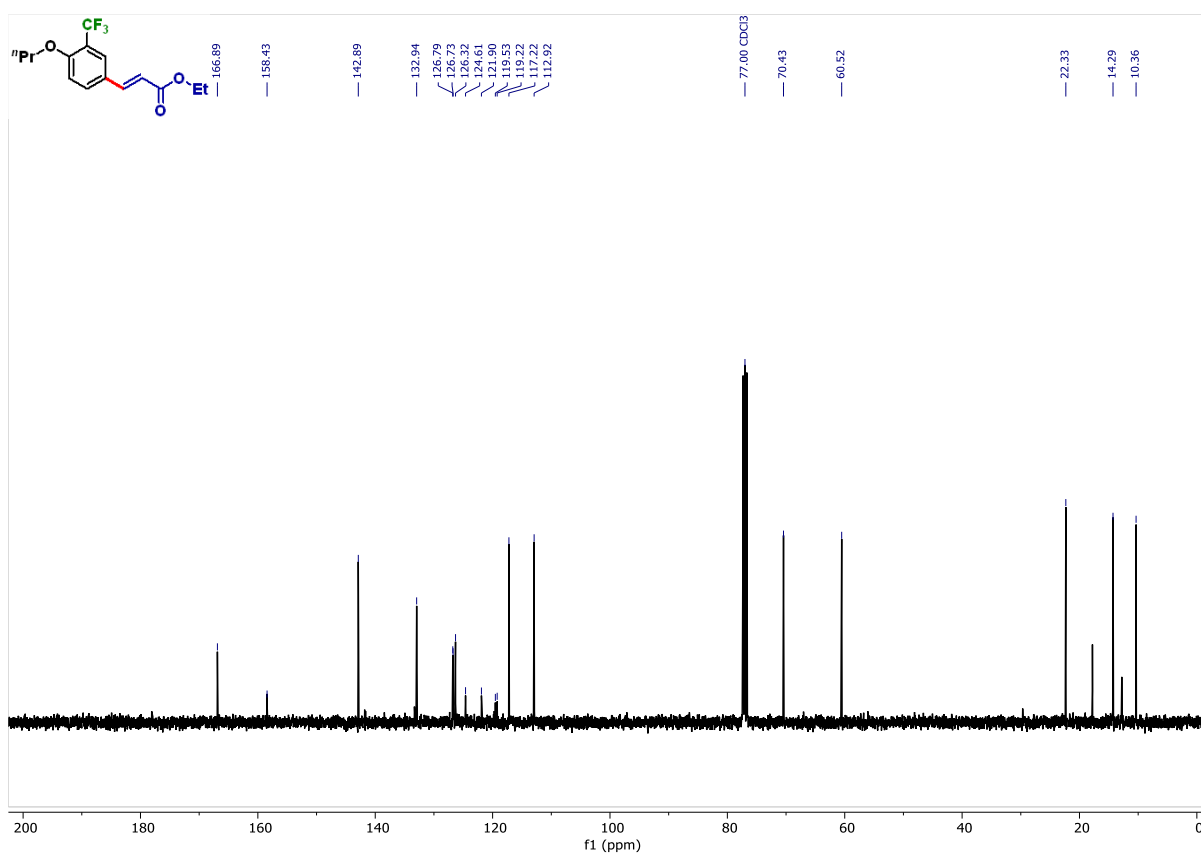
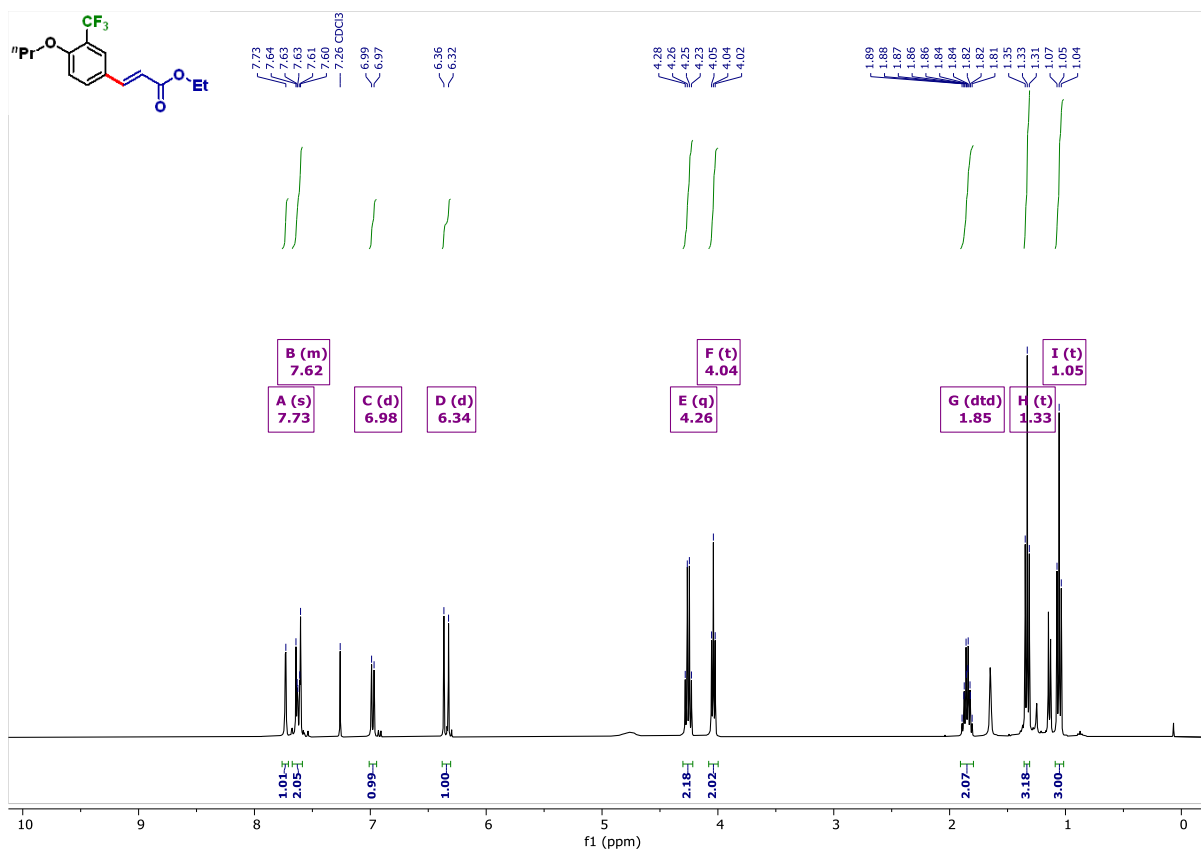
^{19}F NMR of 3b

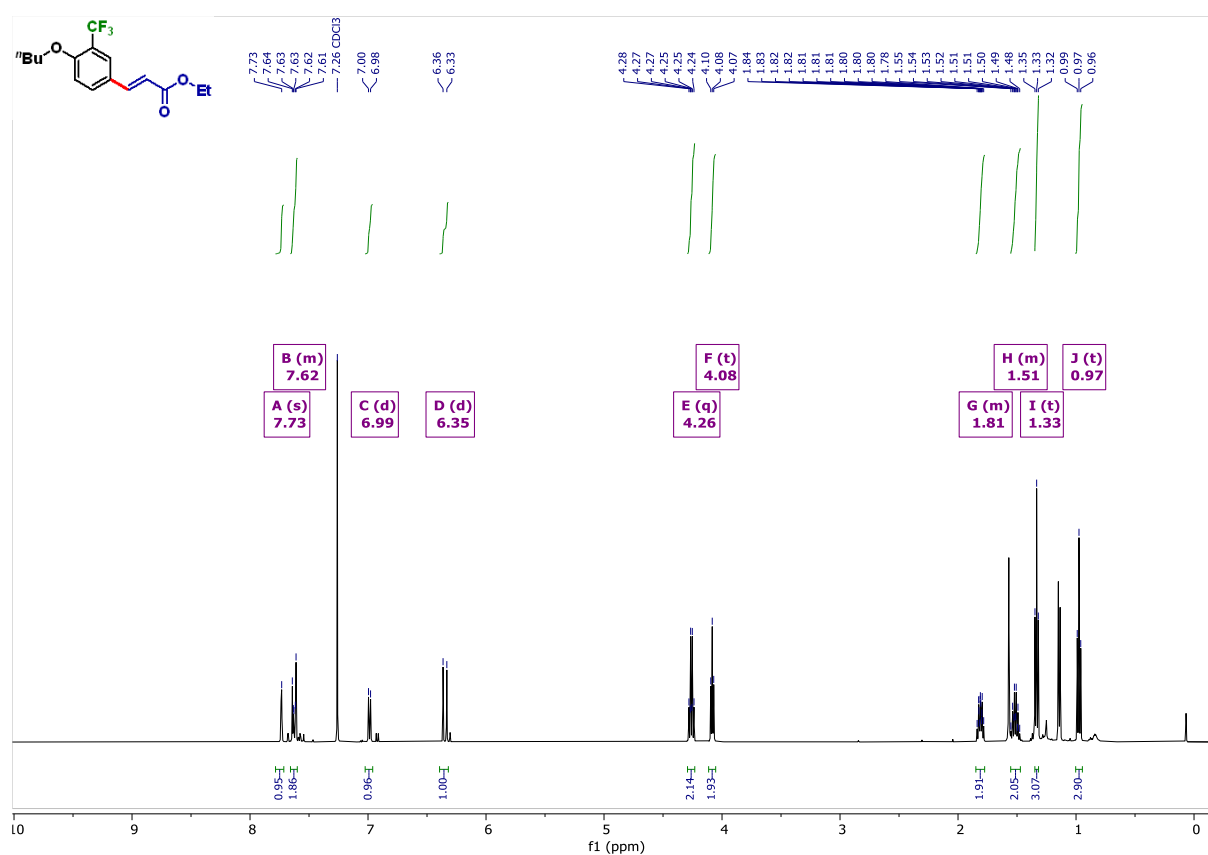
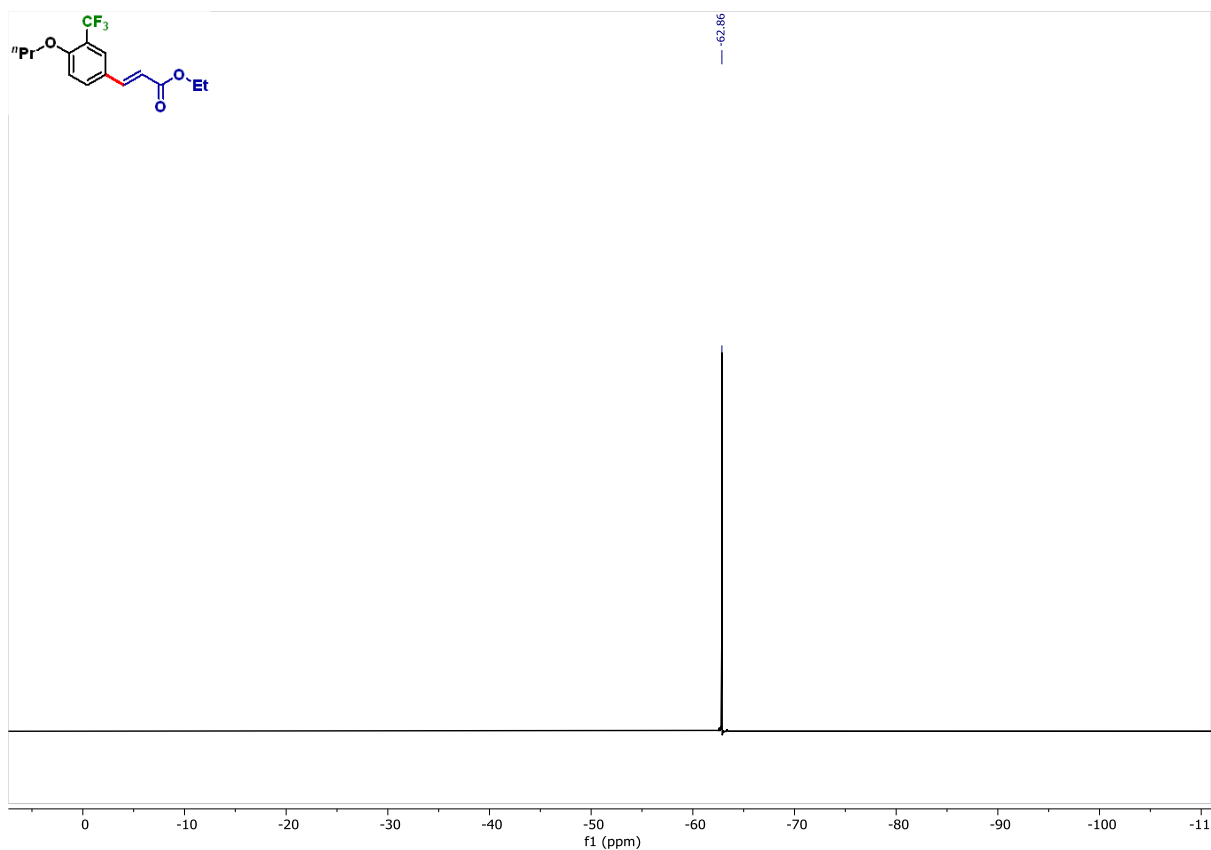


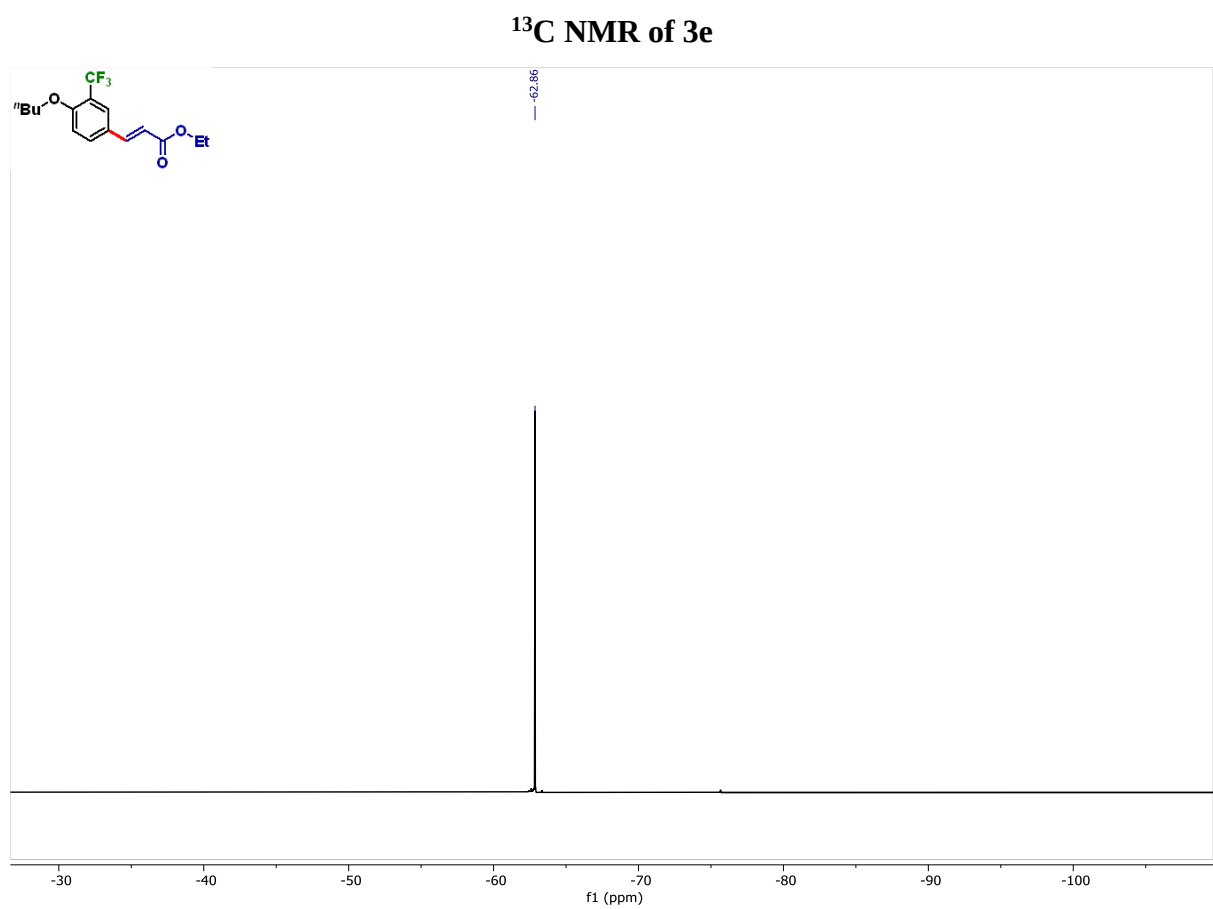
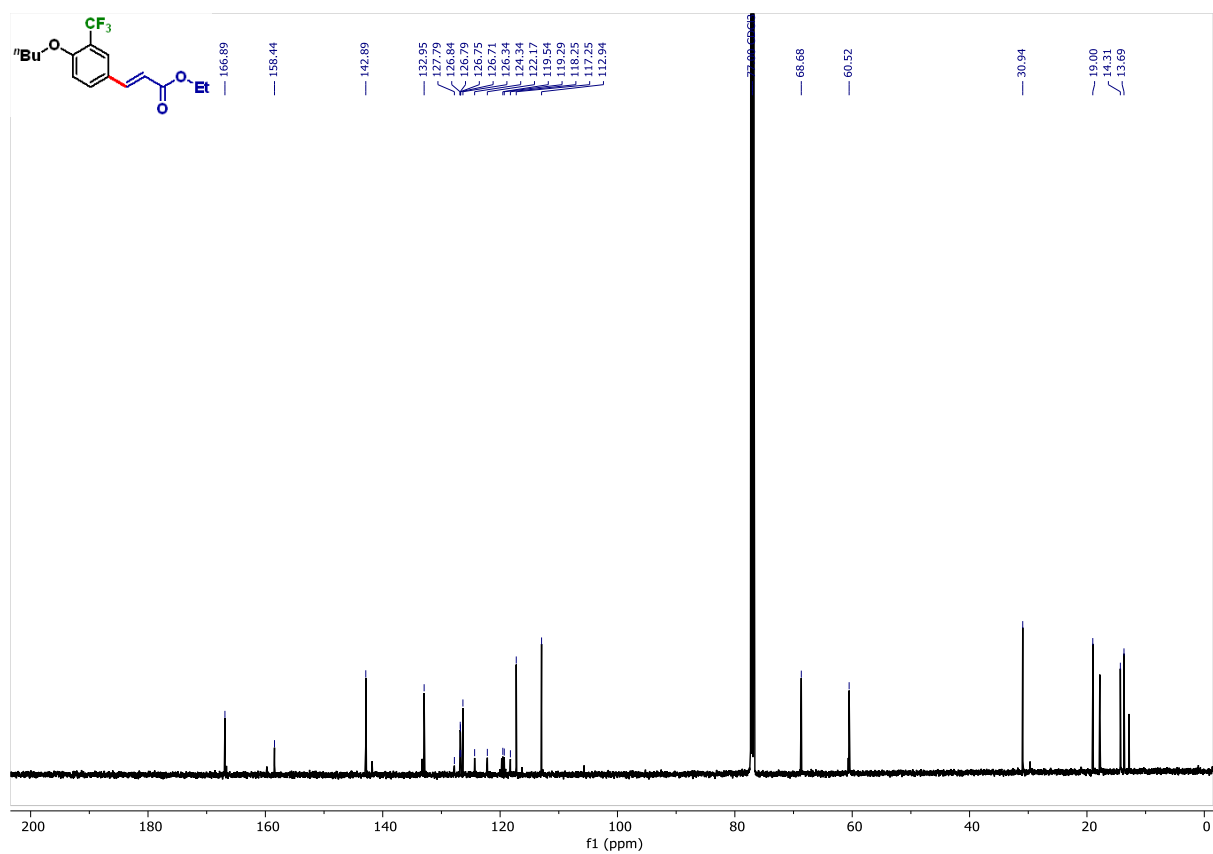
¹H NMR of 3c

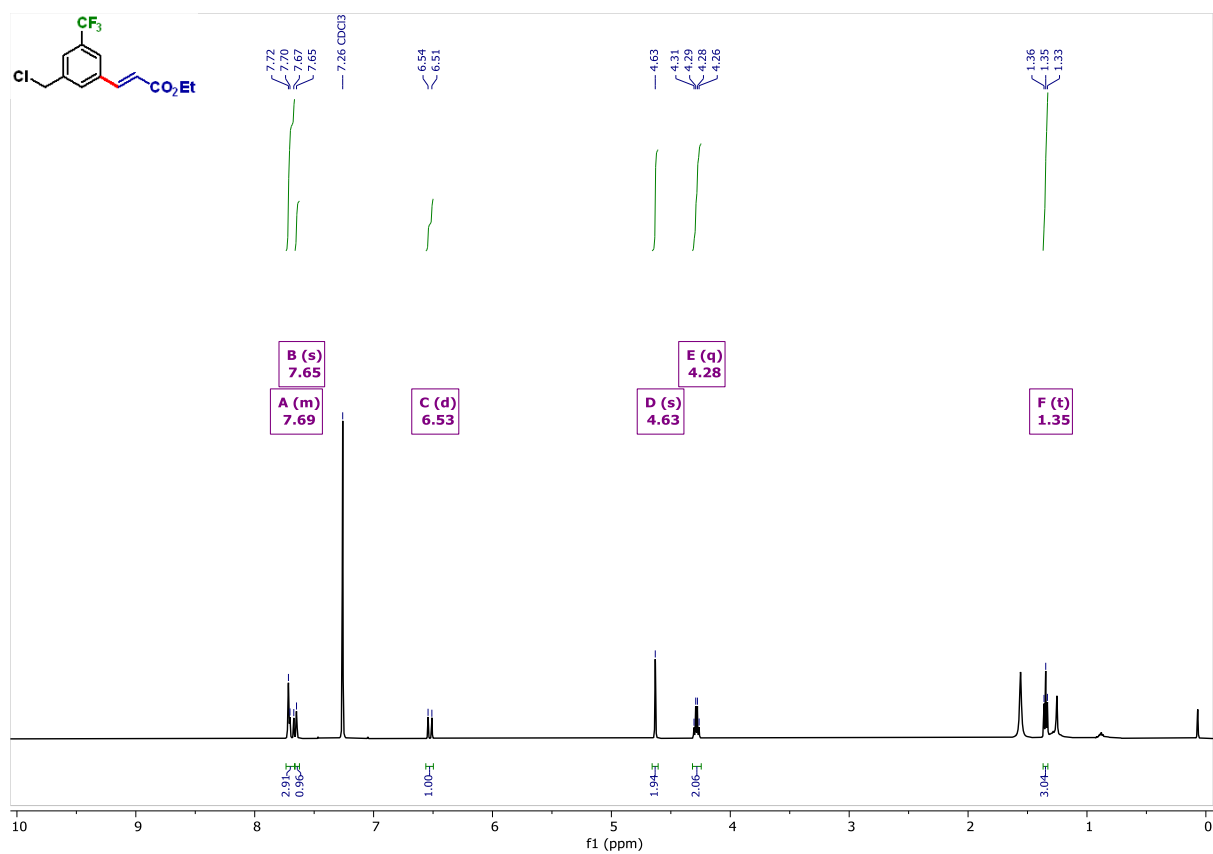


¹⁹F NMR of 3c

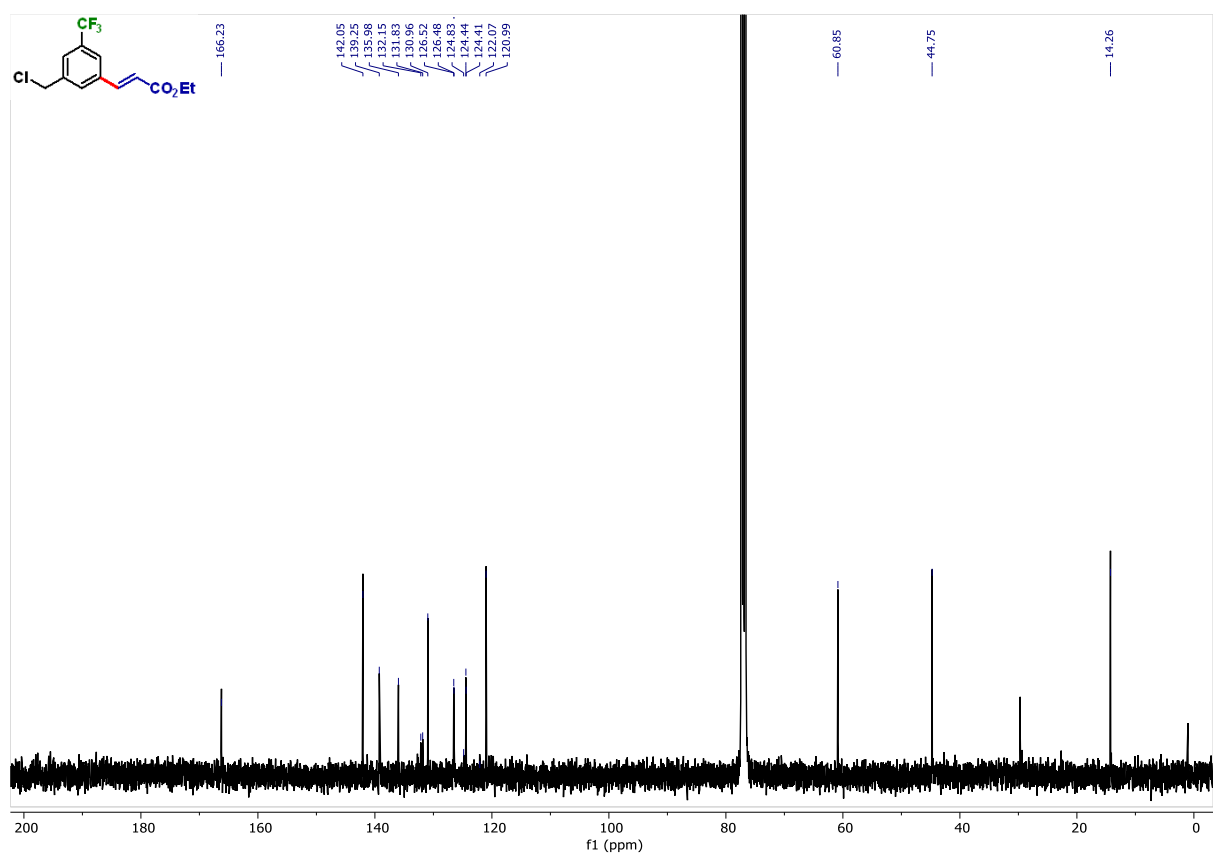




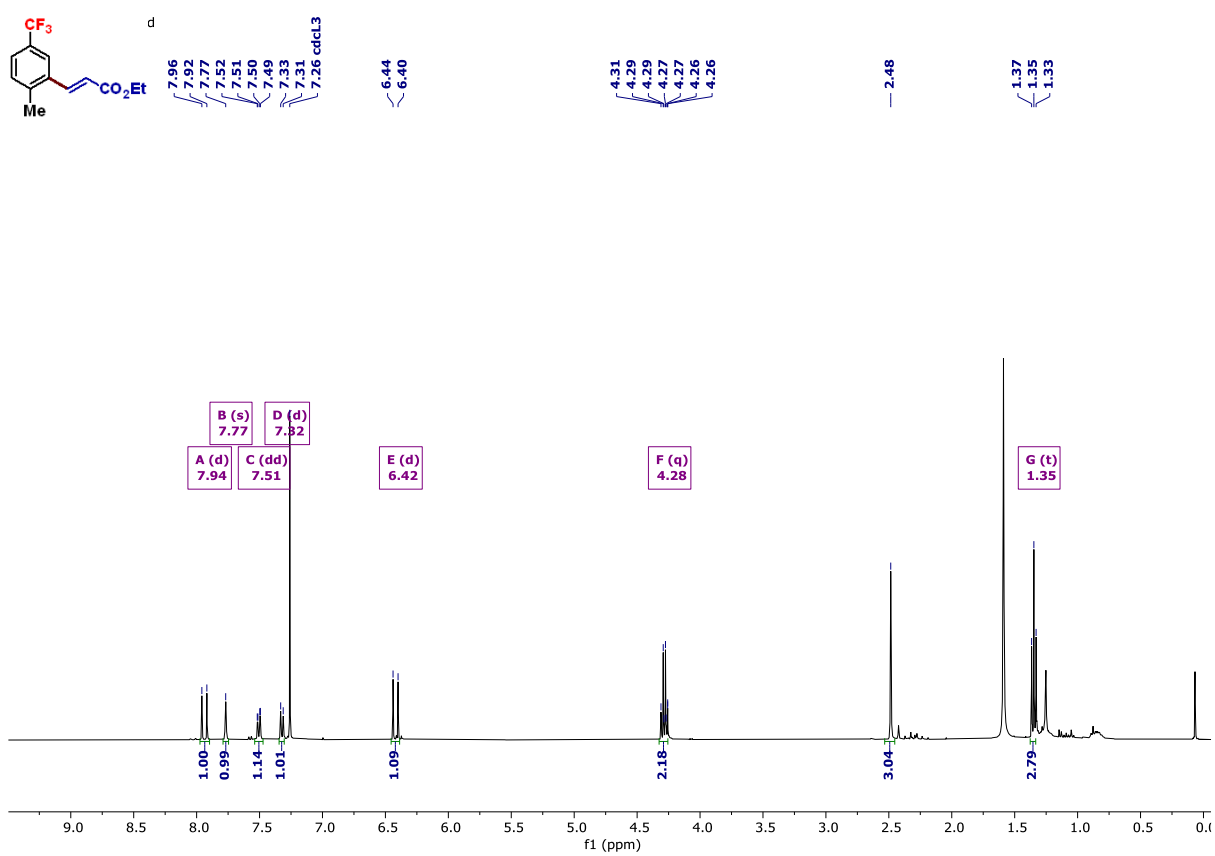
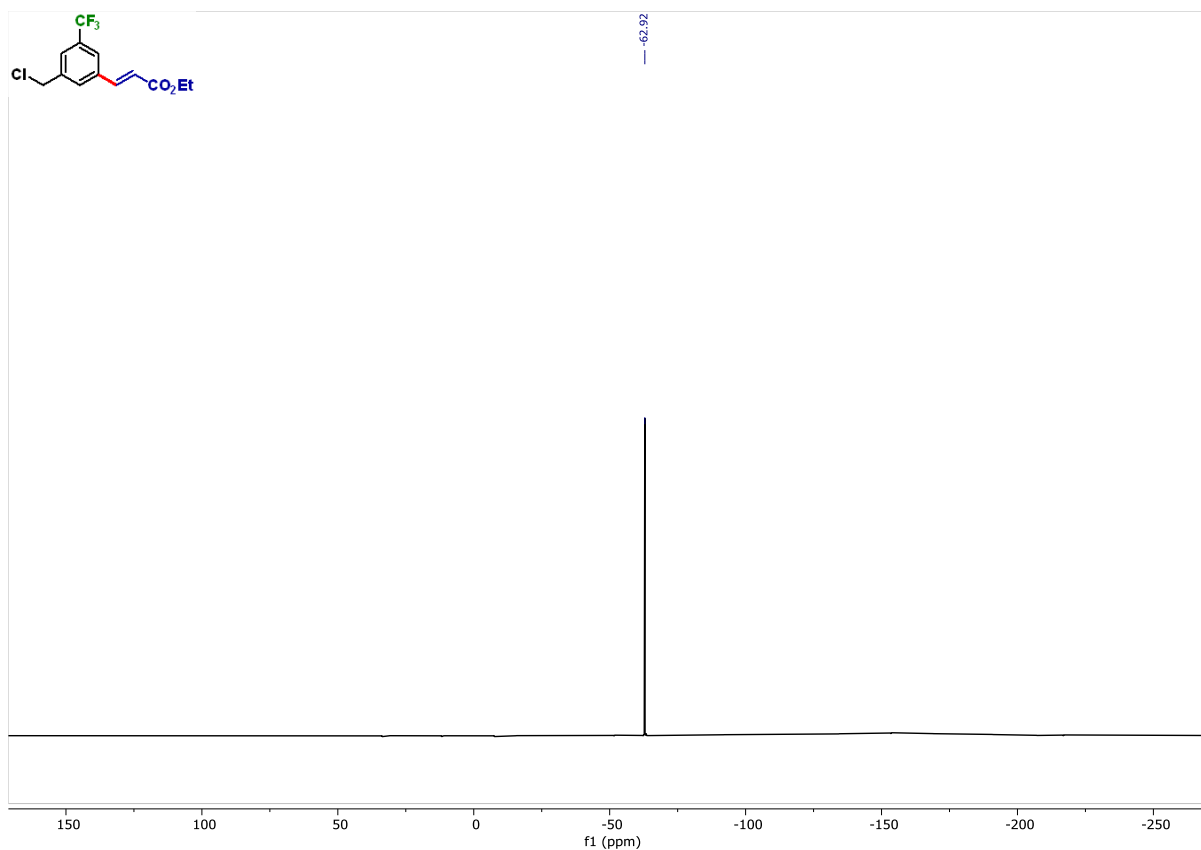


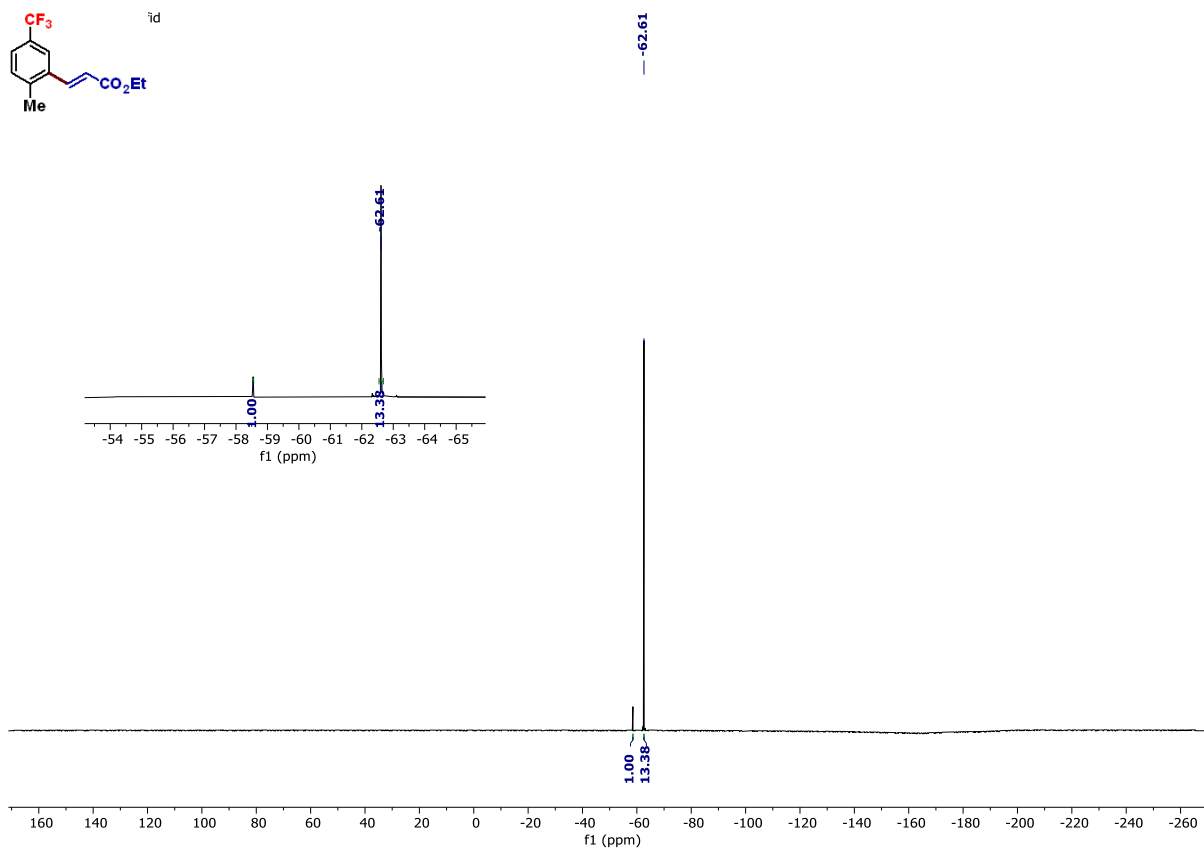


¹H NMR of 3f

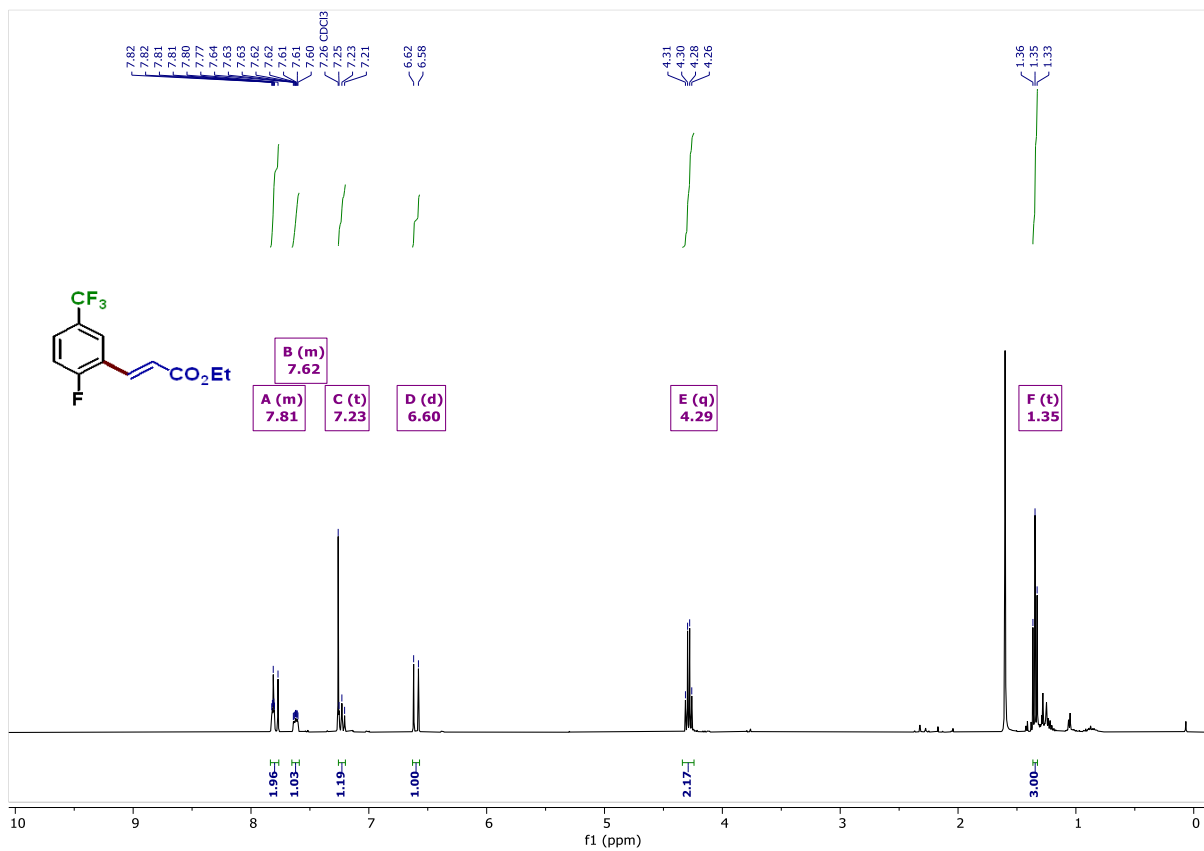


¹³C NMR of 3f

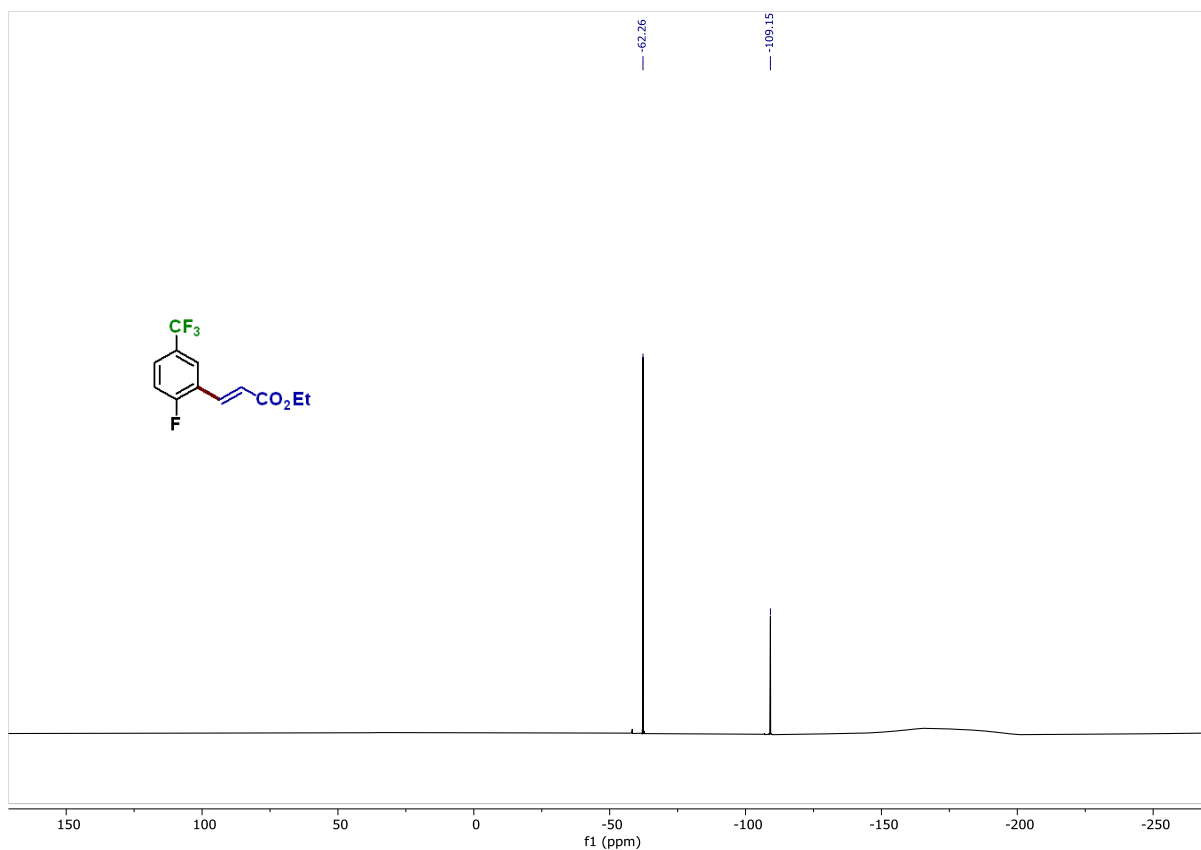




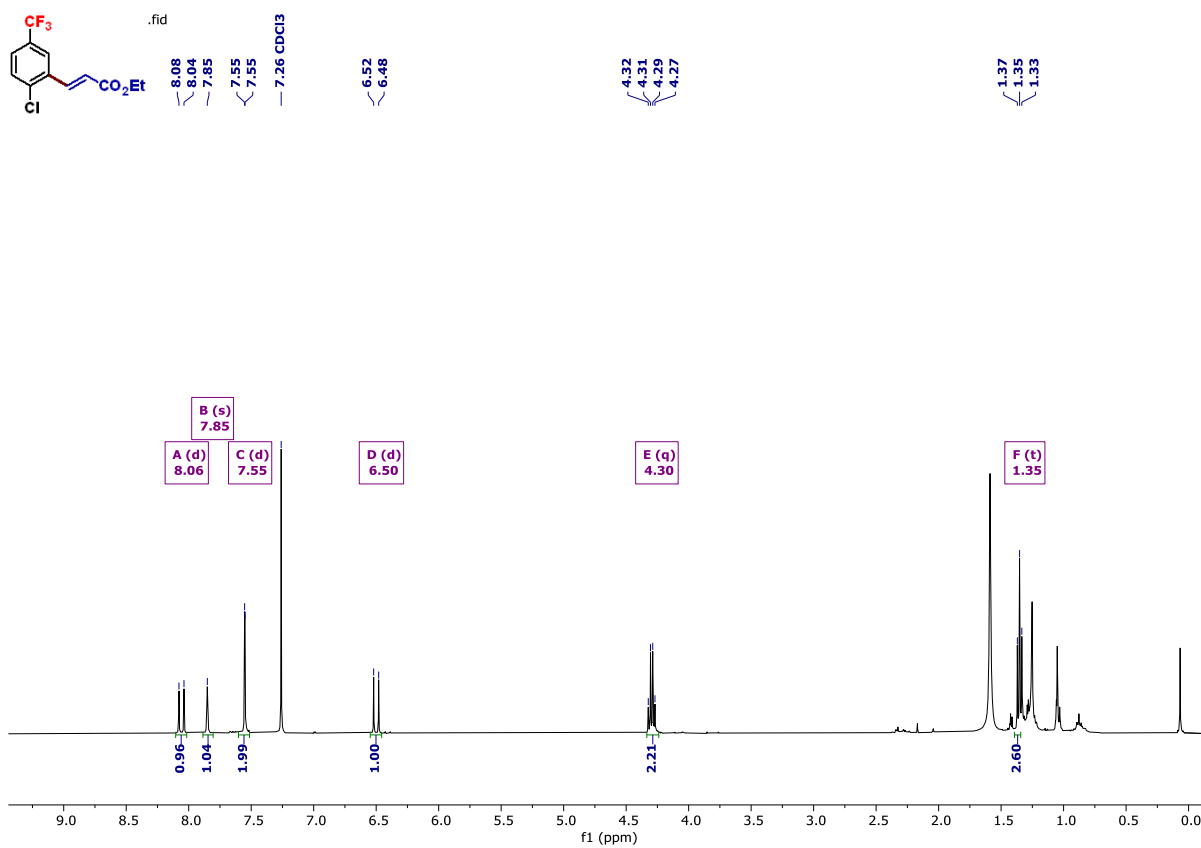
¹⁹F NMR of 3g



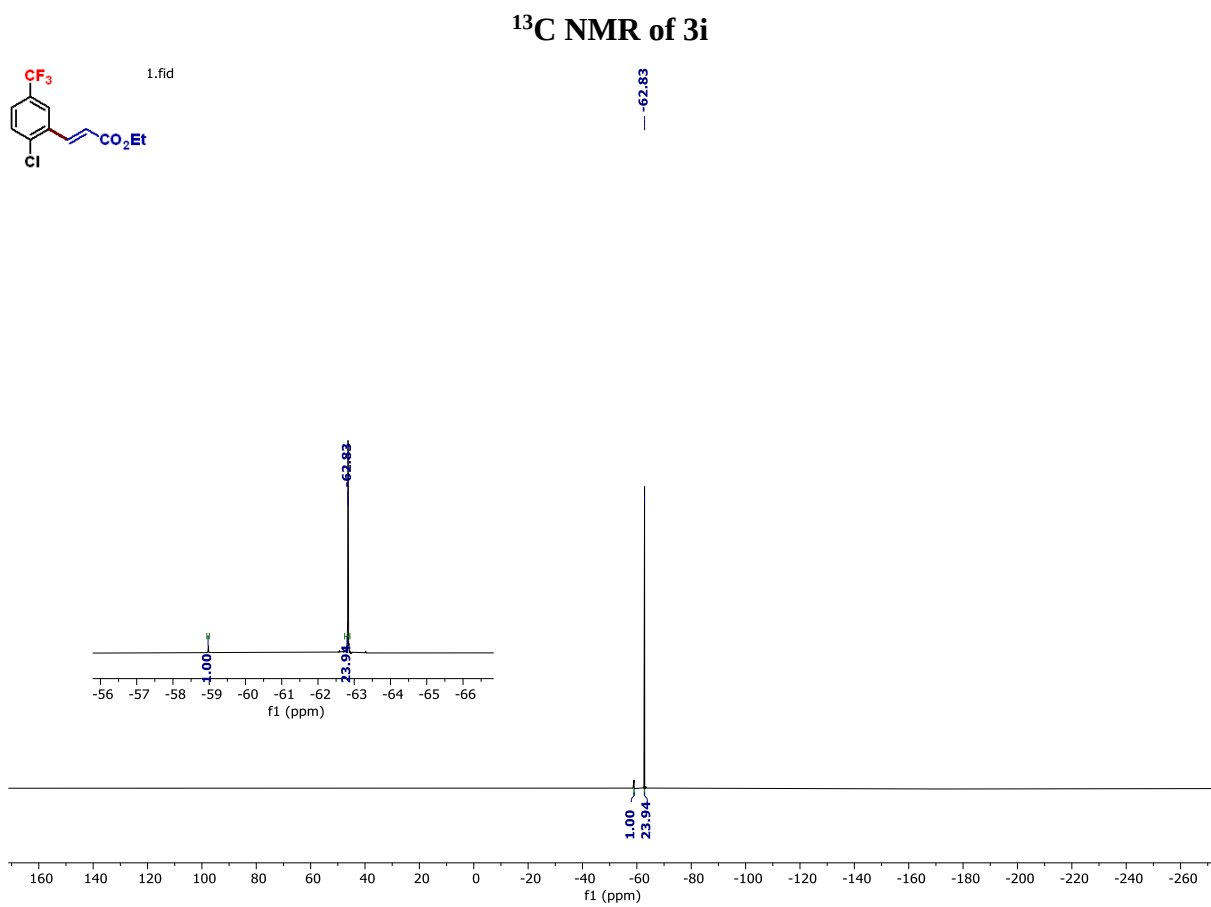
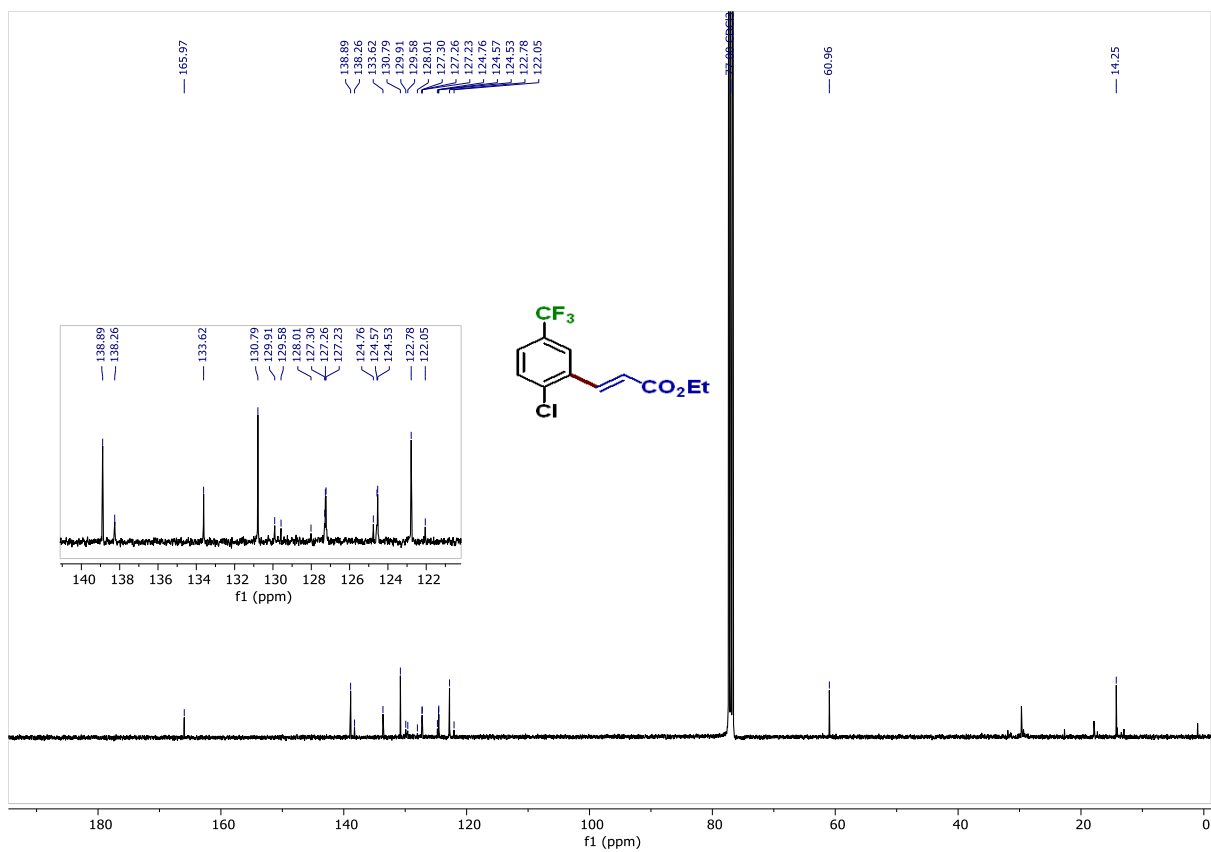
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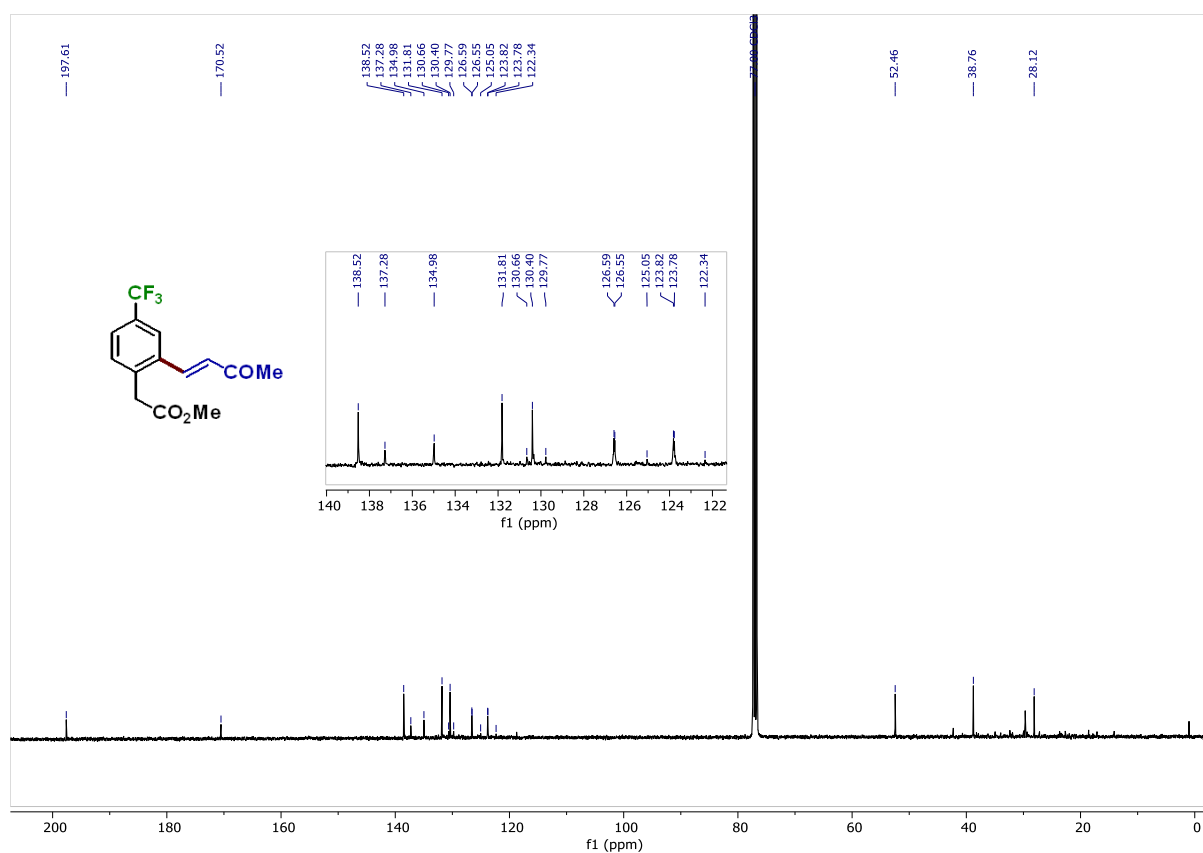
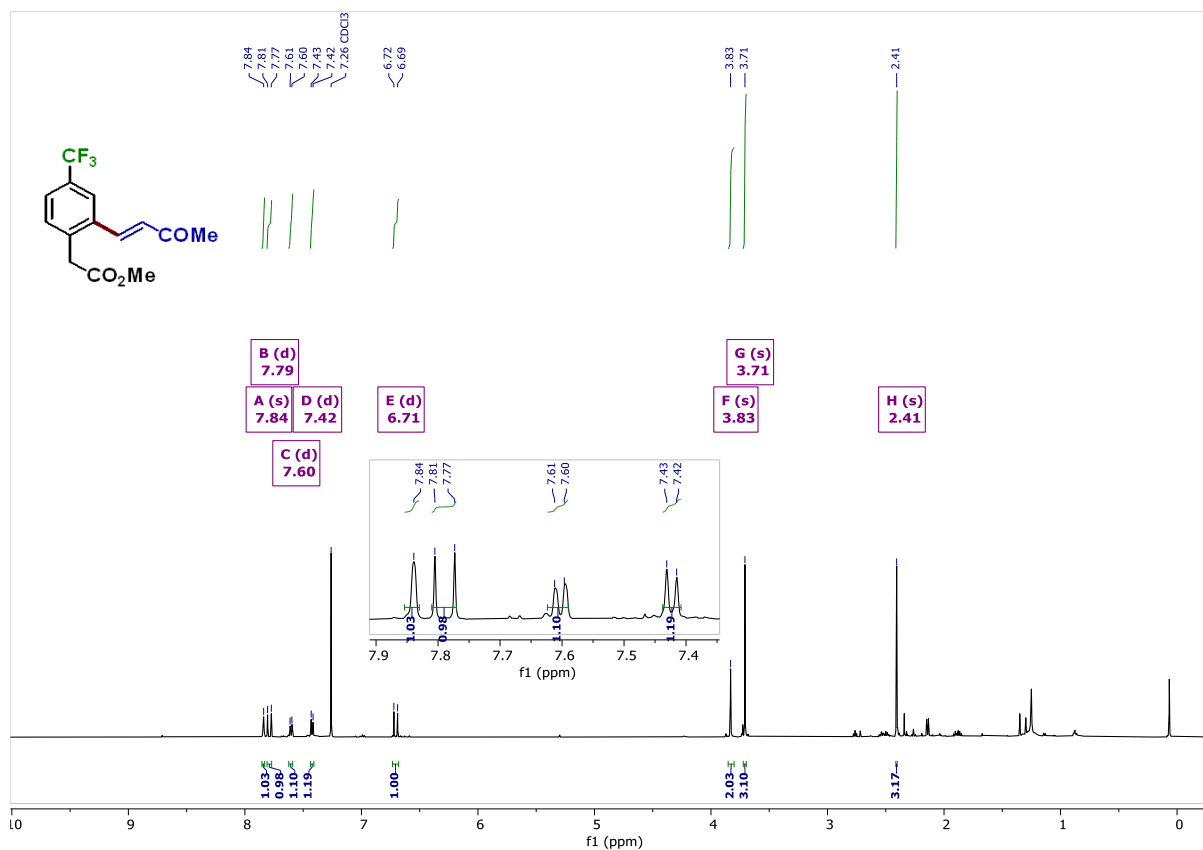


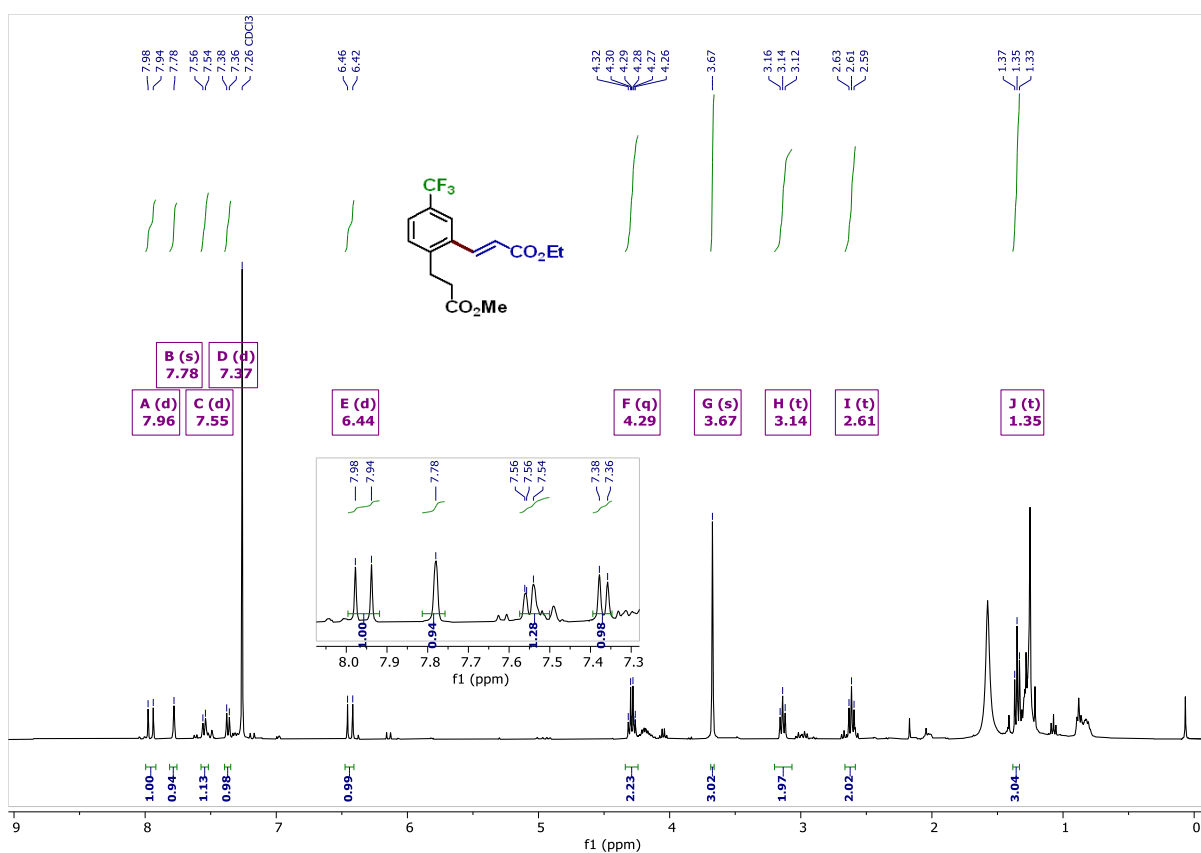
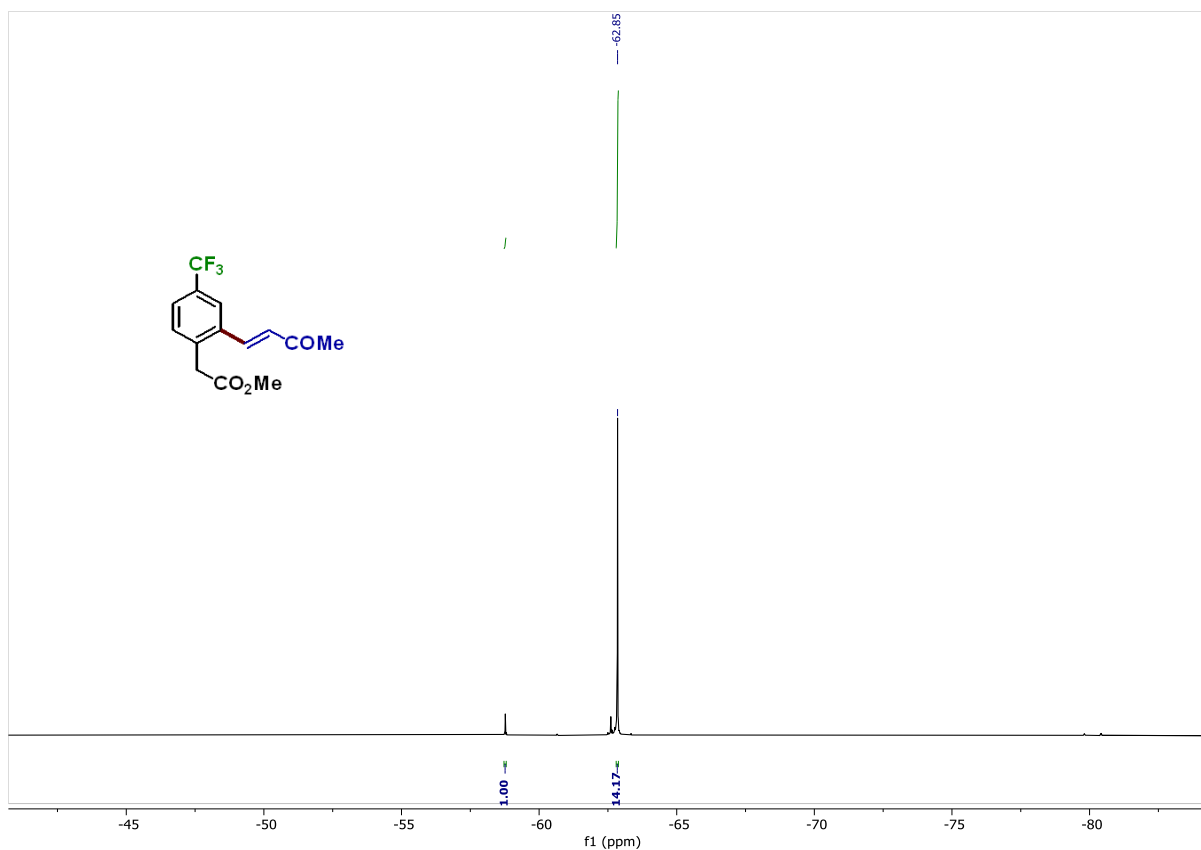
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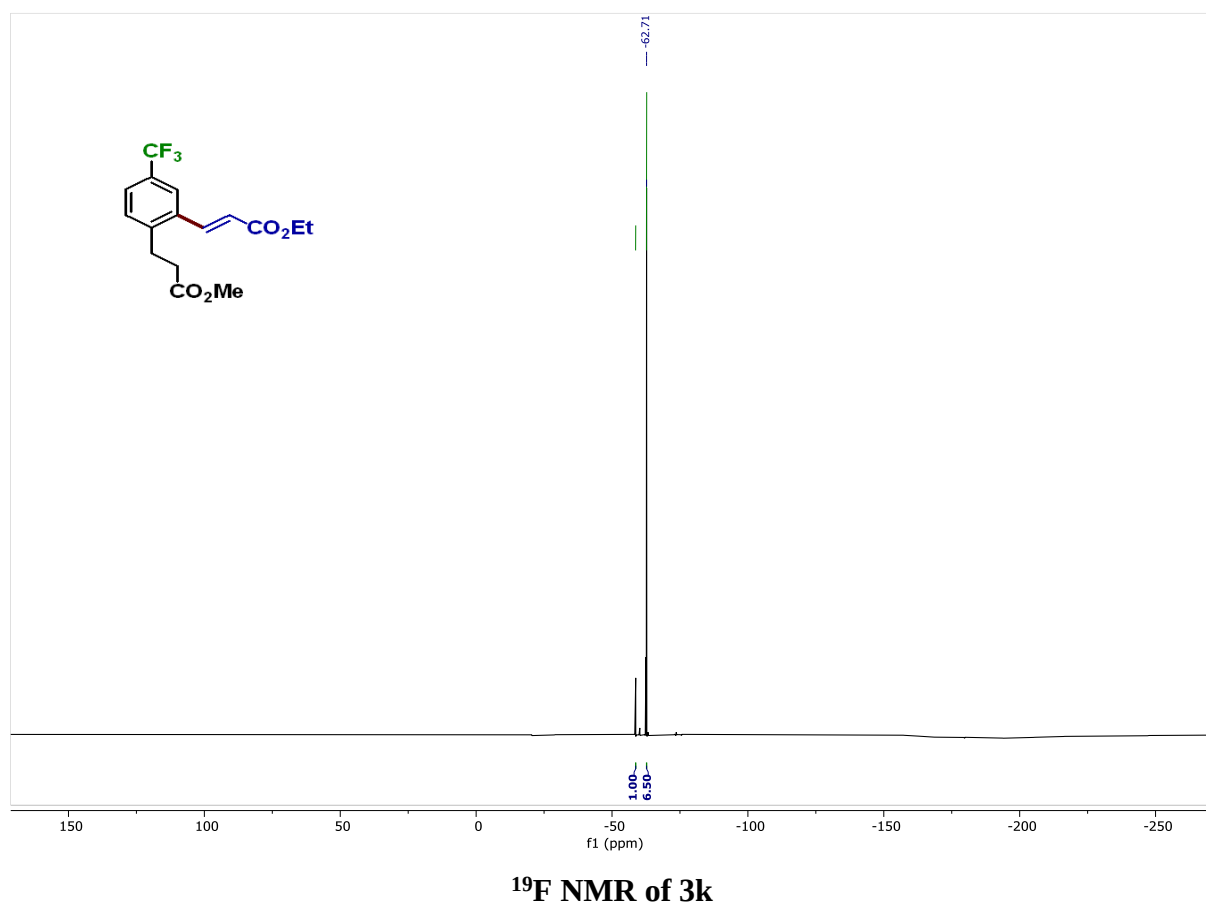
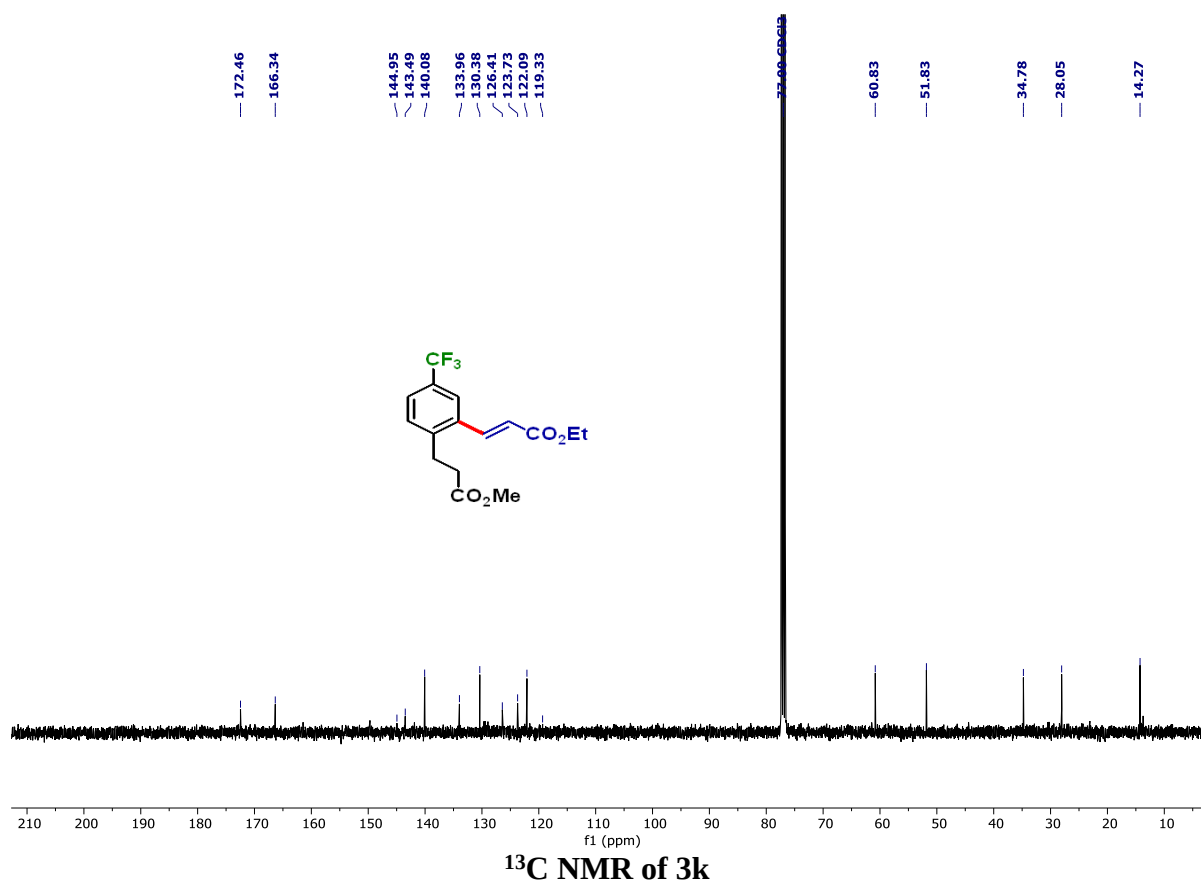


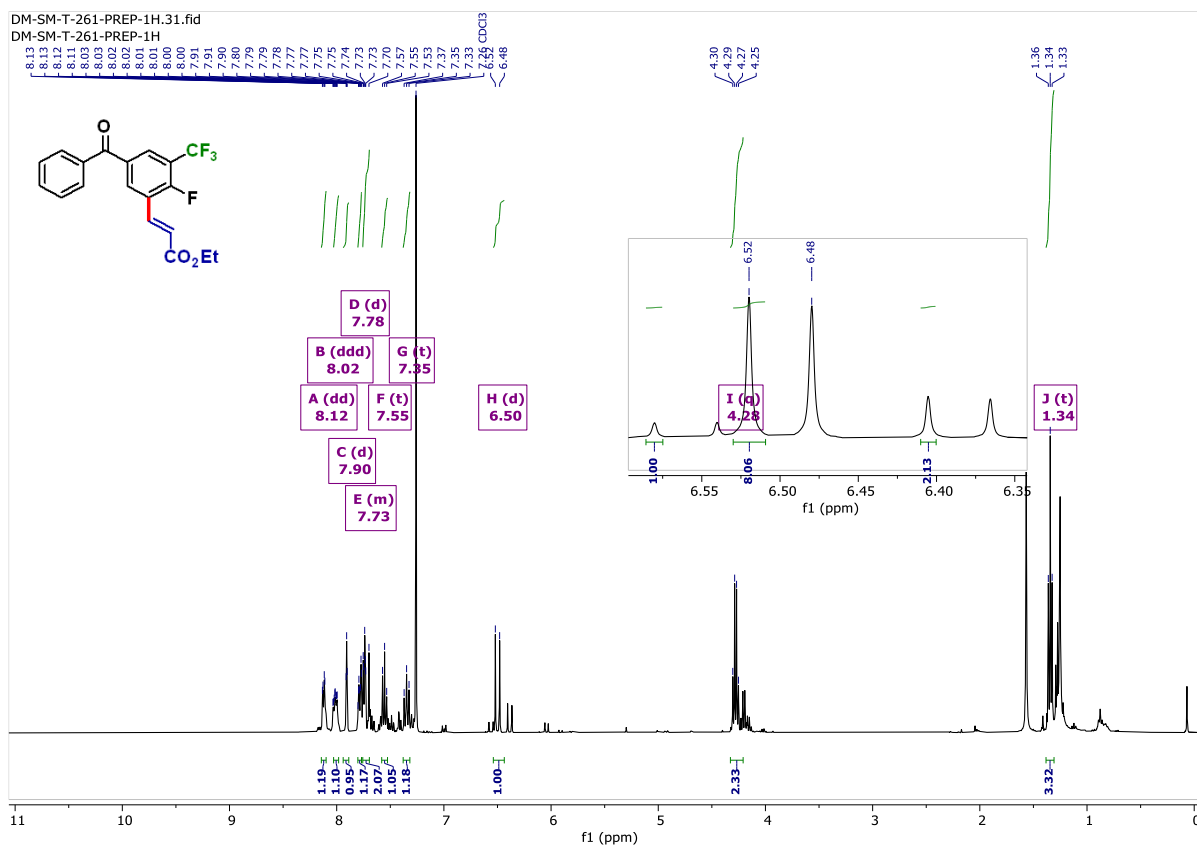
¹H NMR of 3i



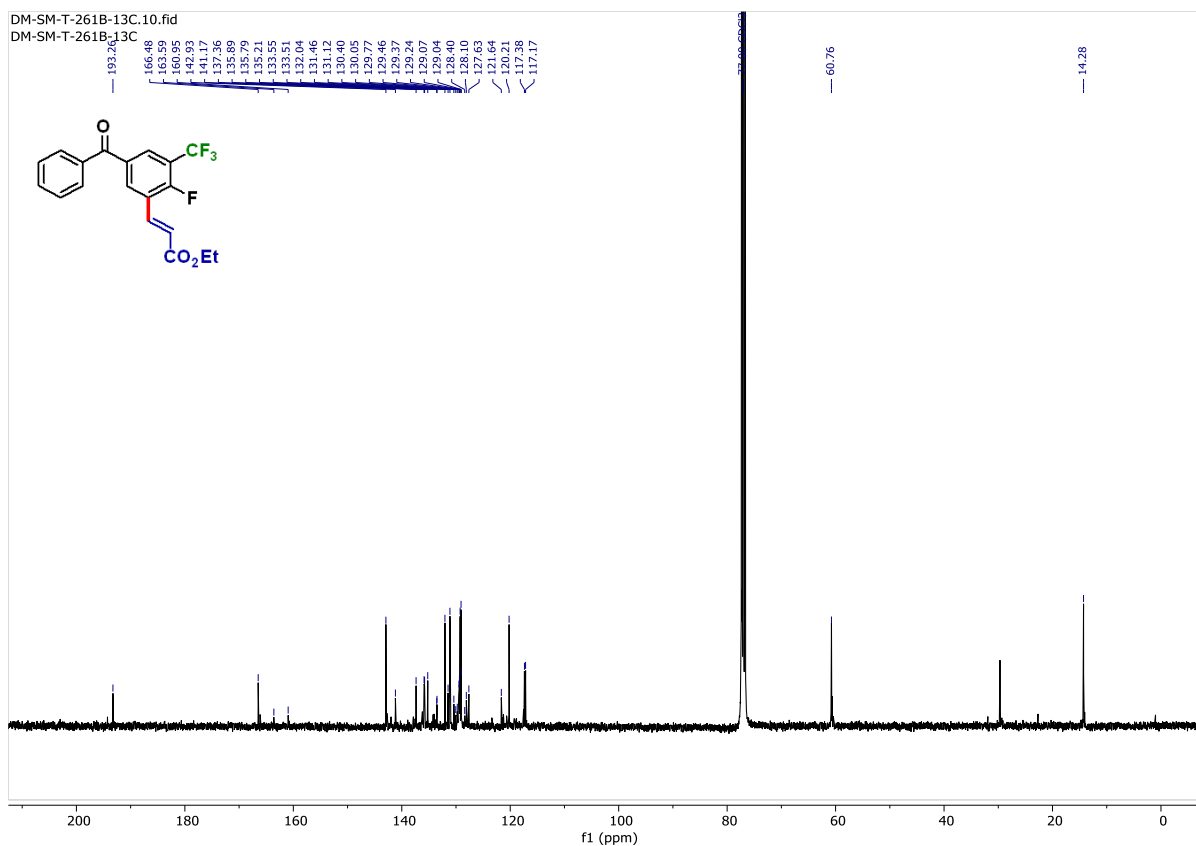




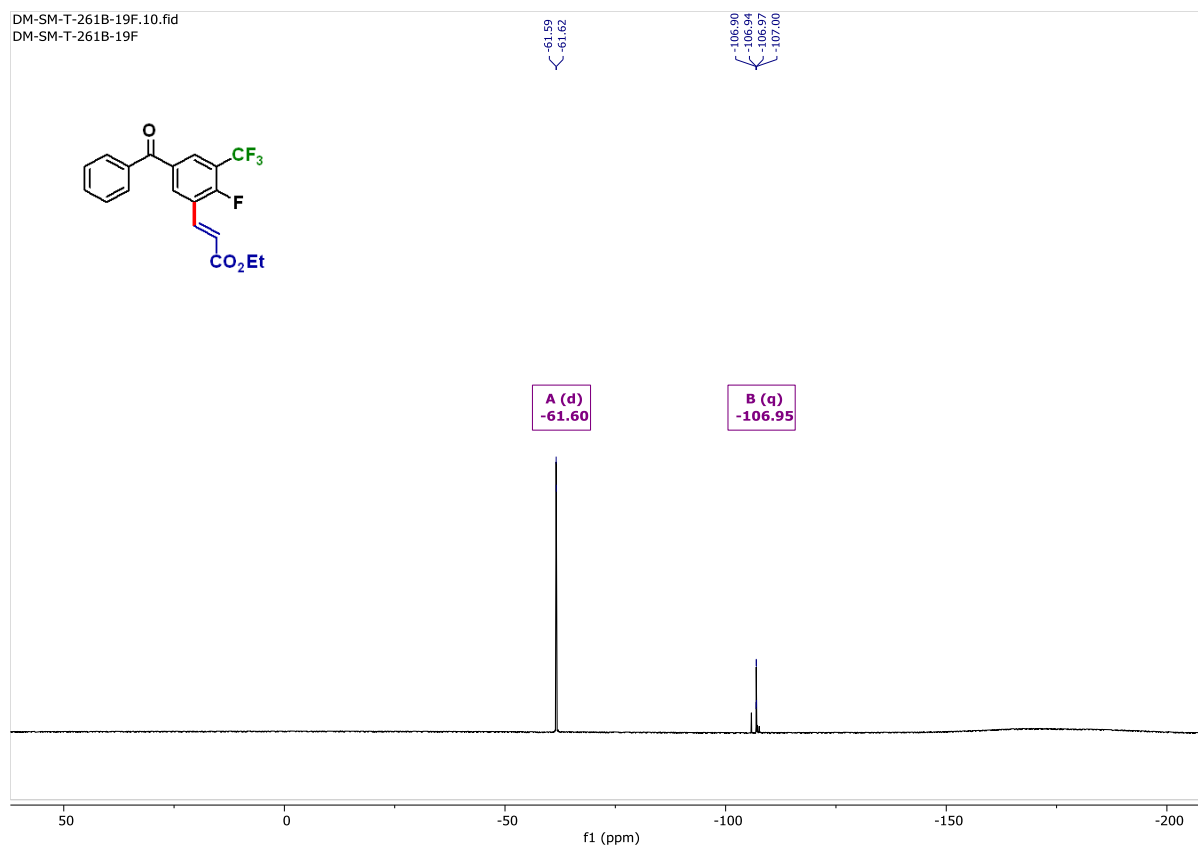




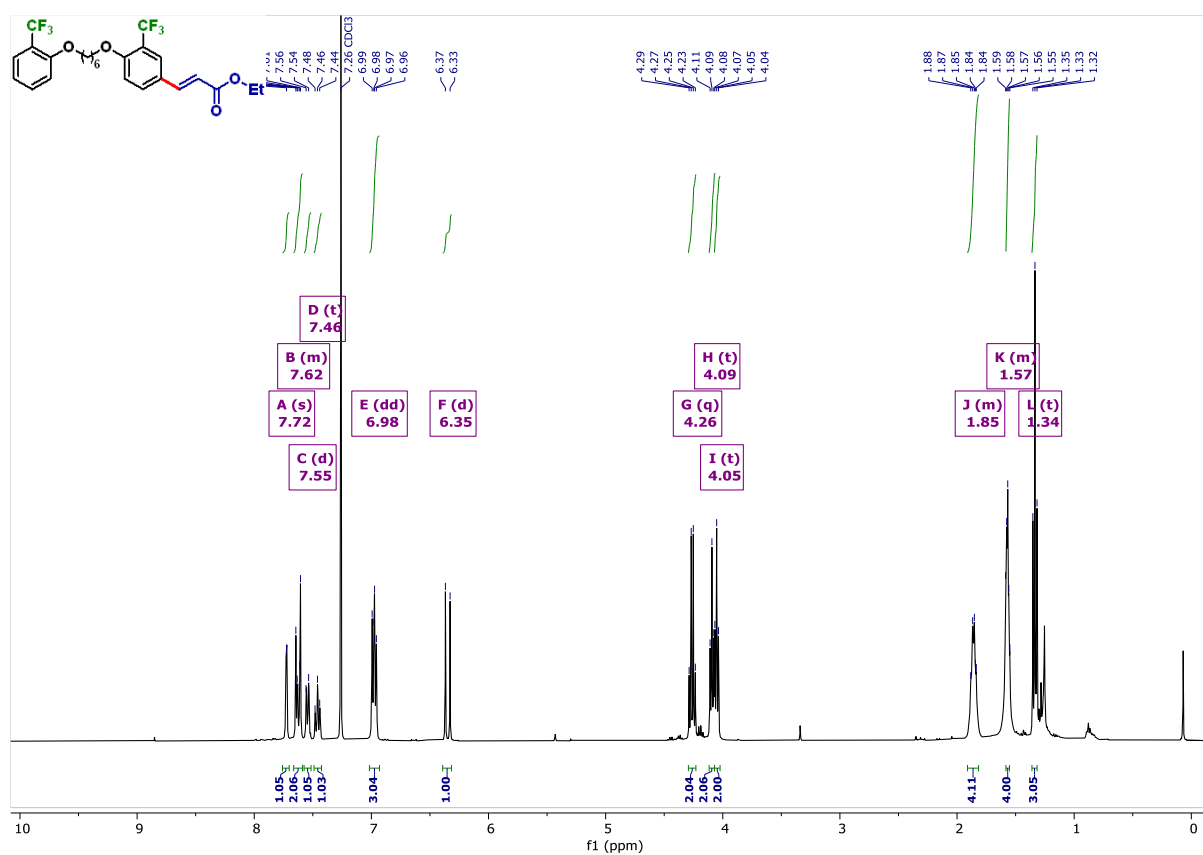
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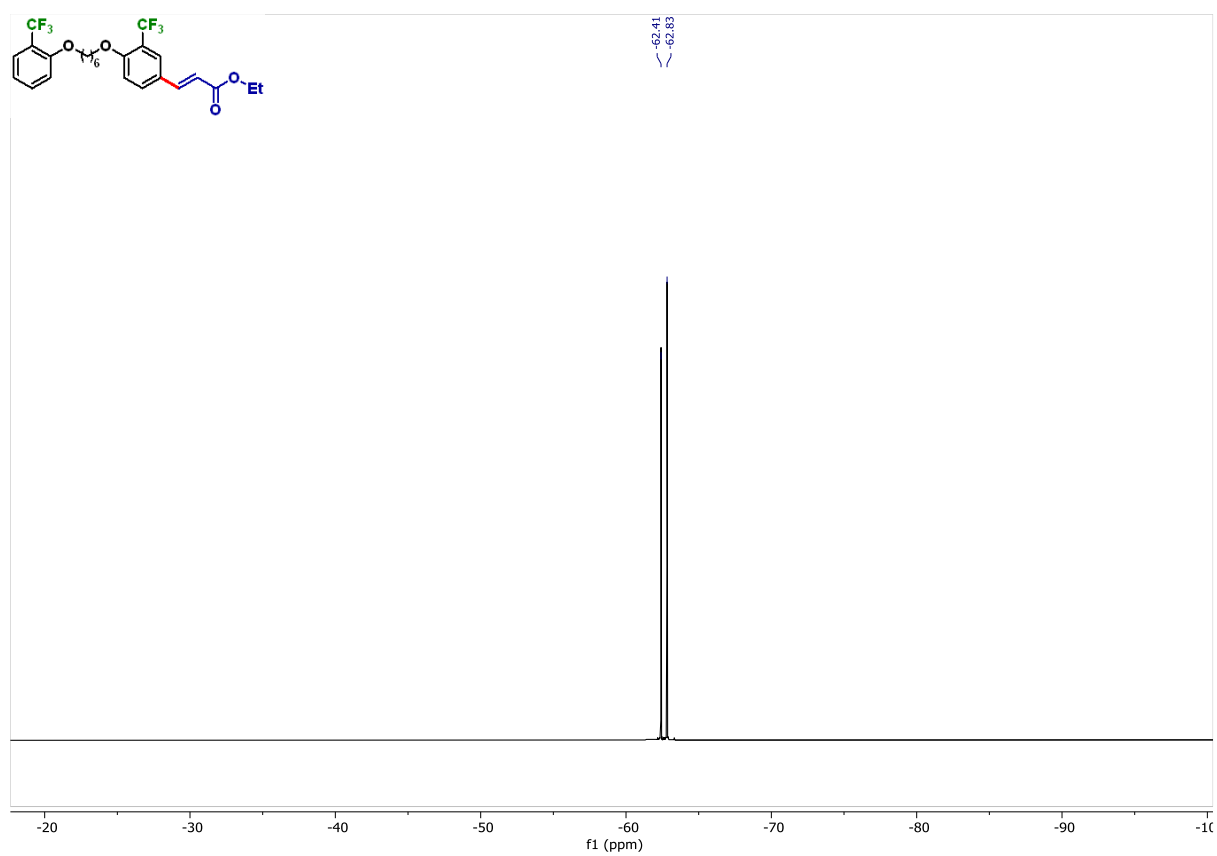
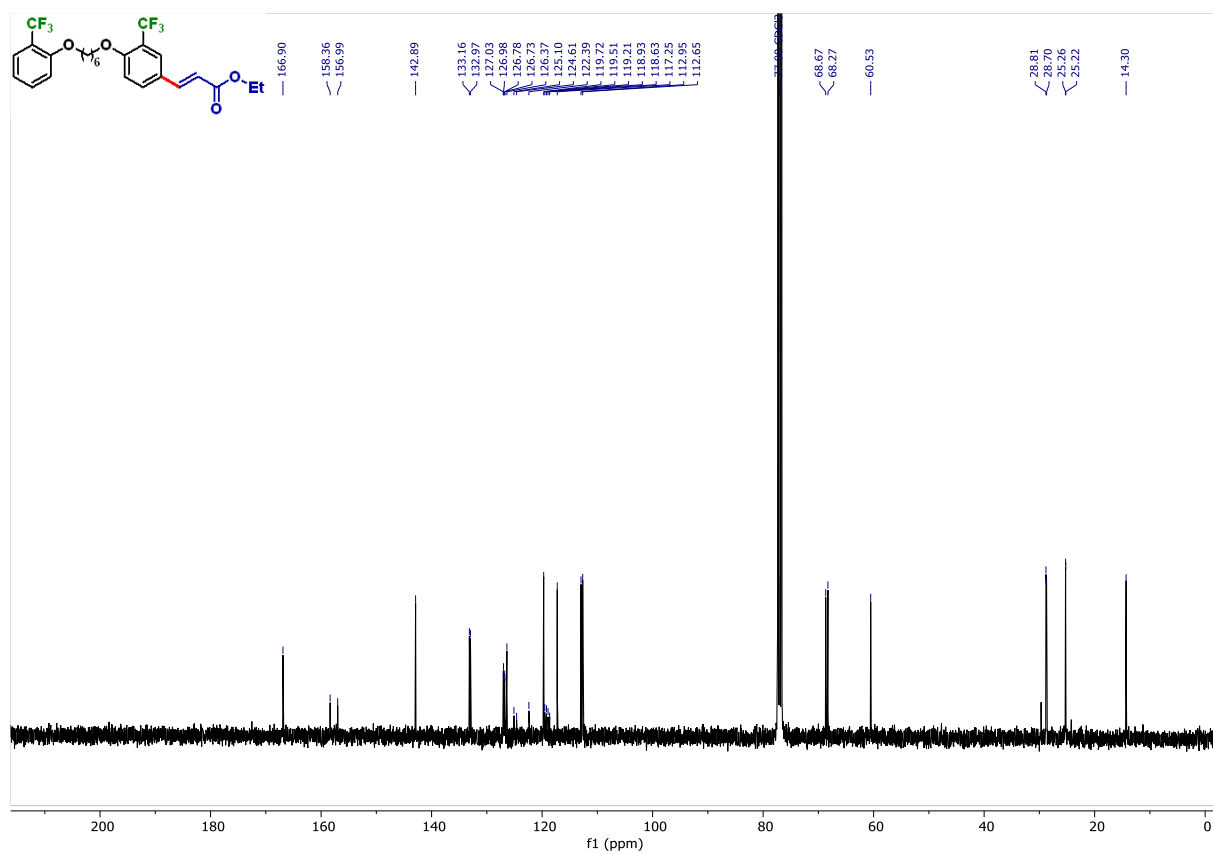
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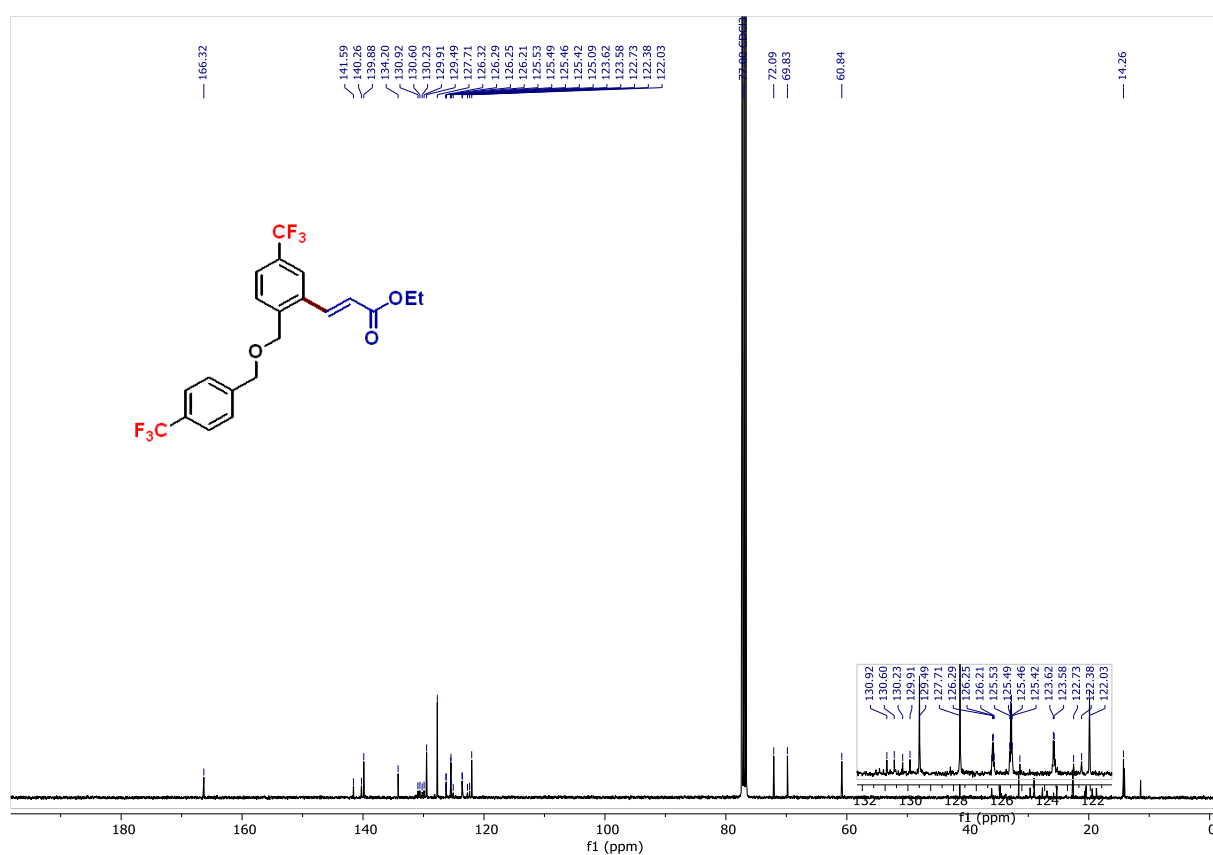
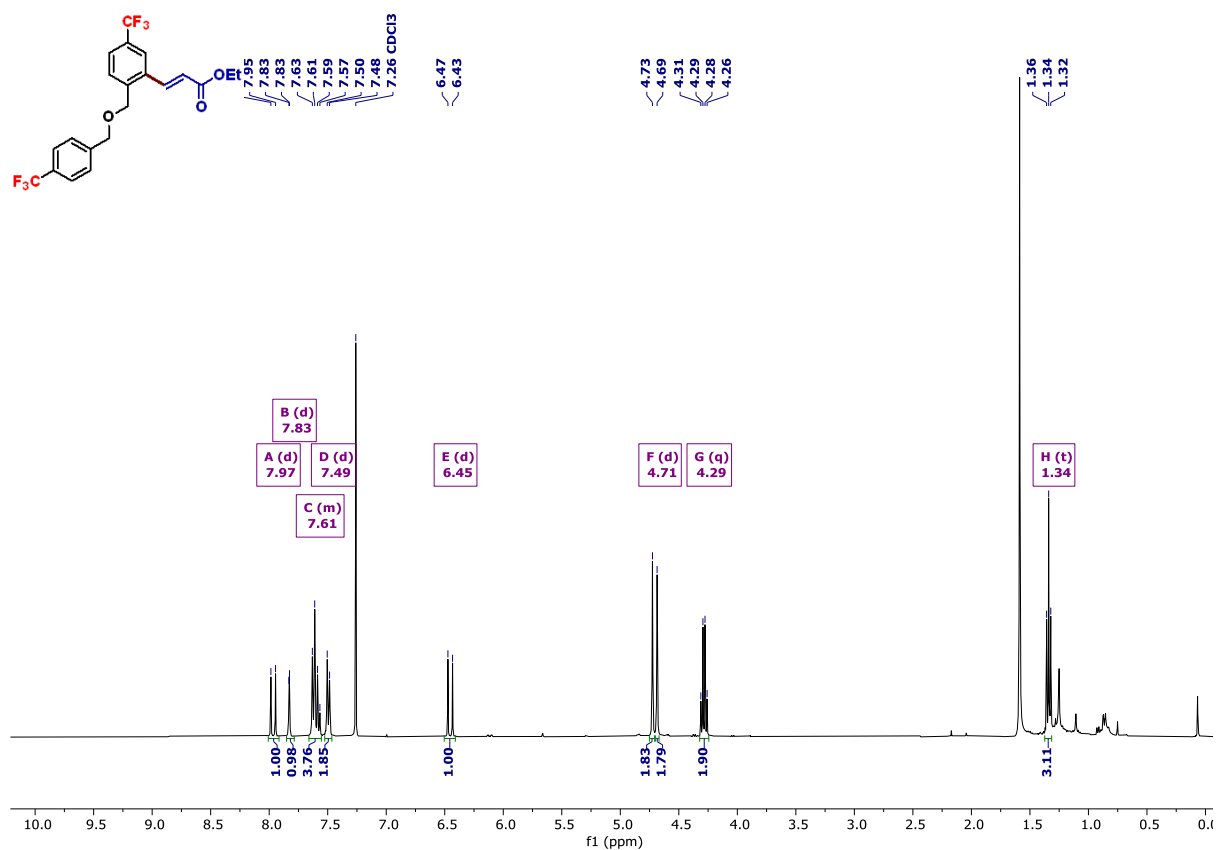


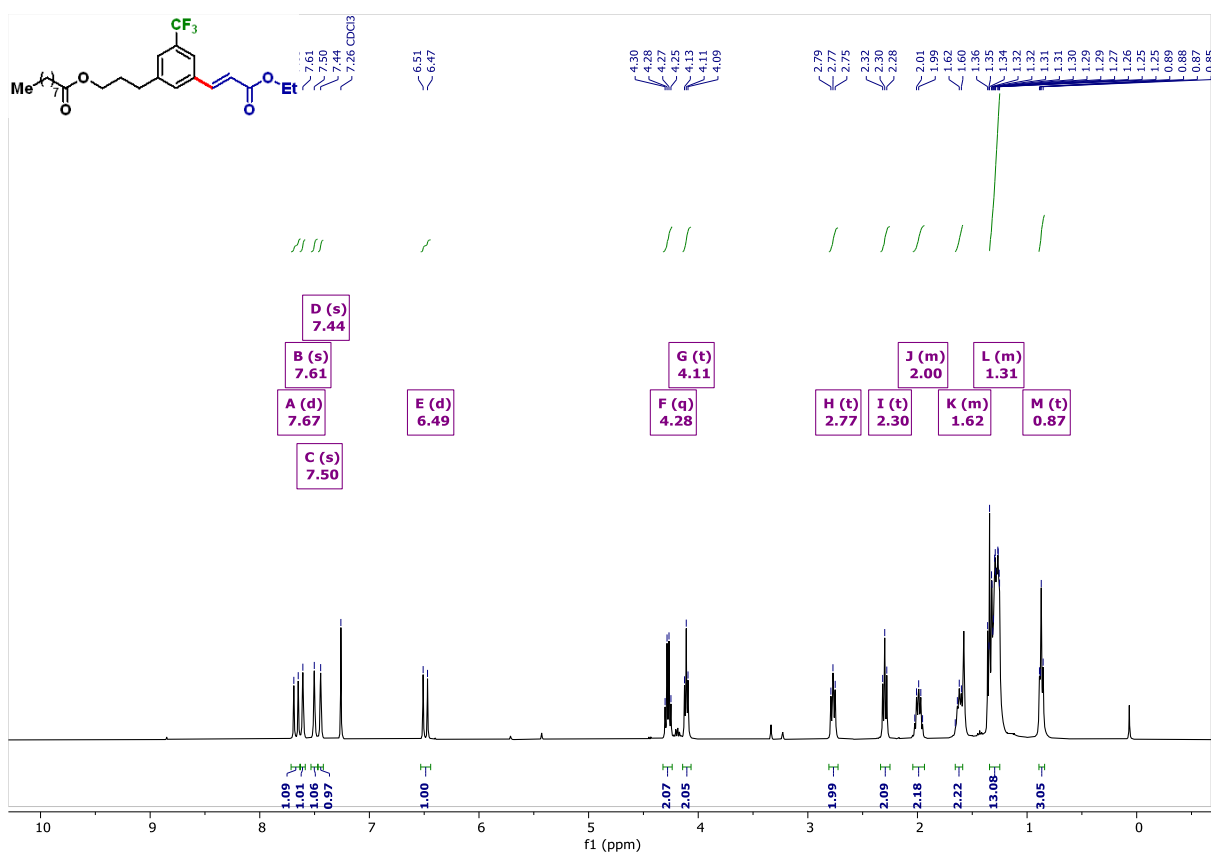
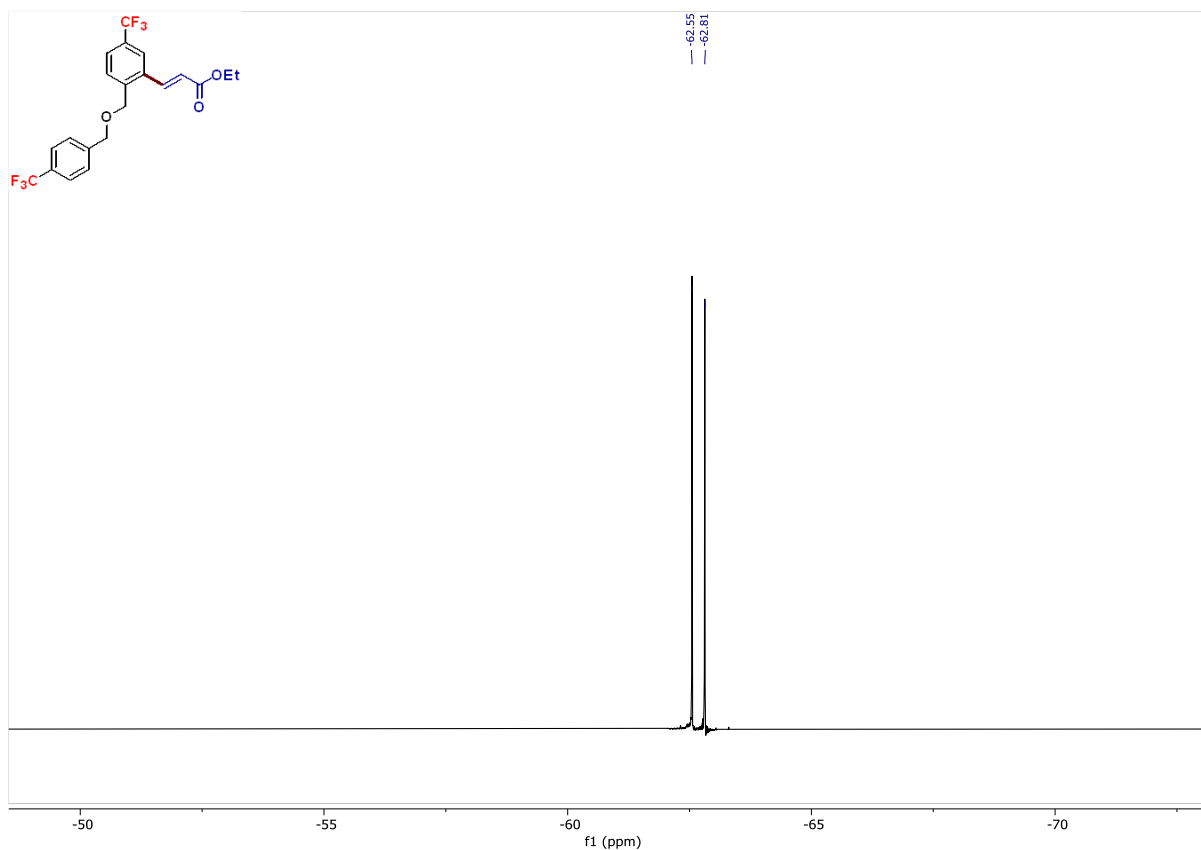
¹⁹F NMR of 3l

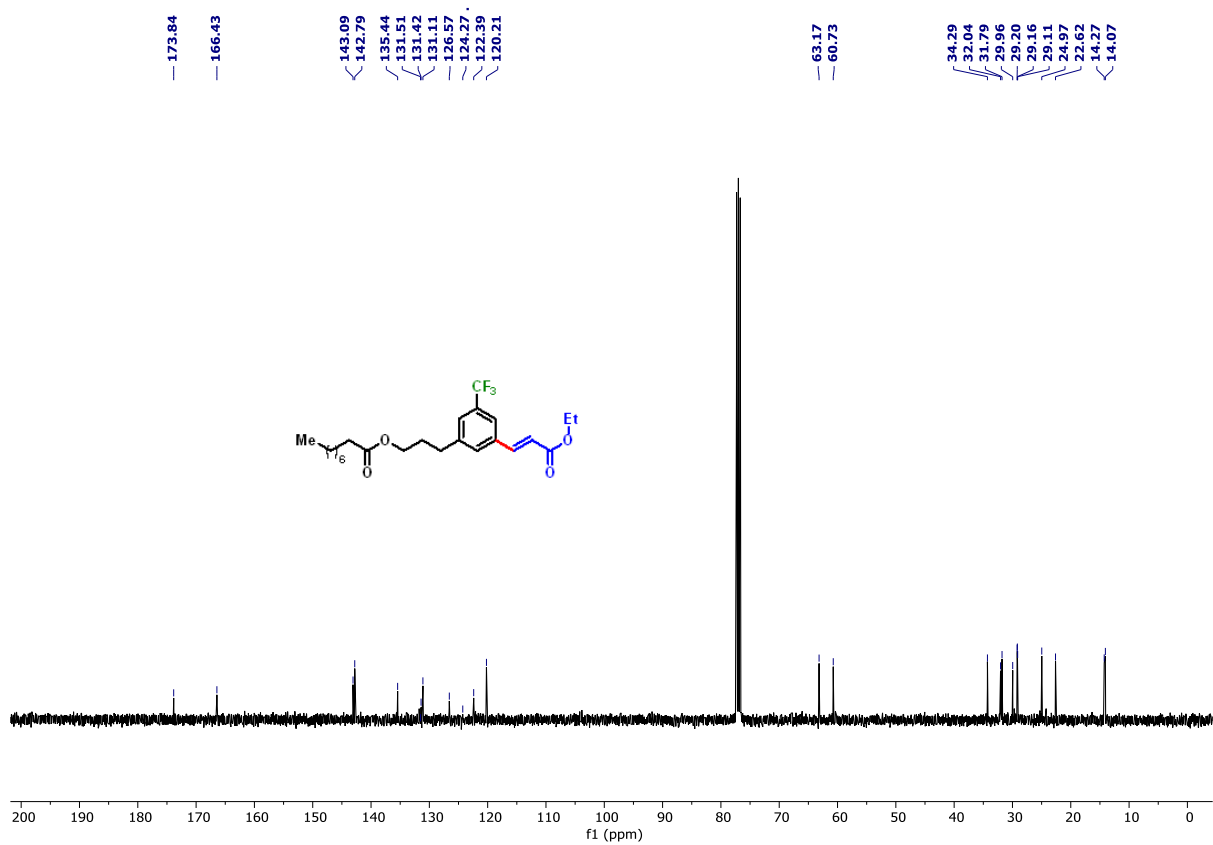


¹H NMR of 3m

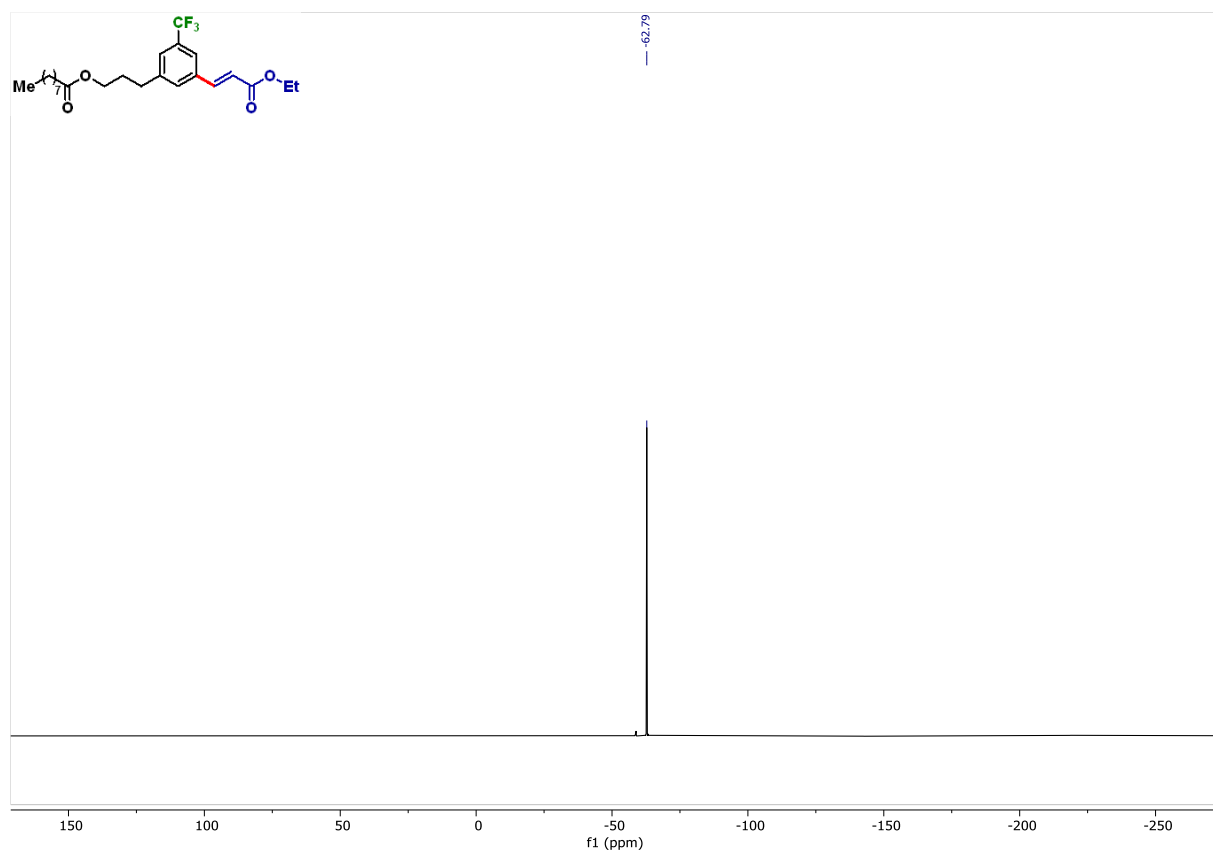




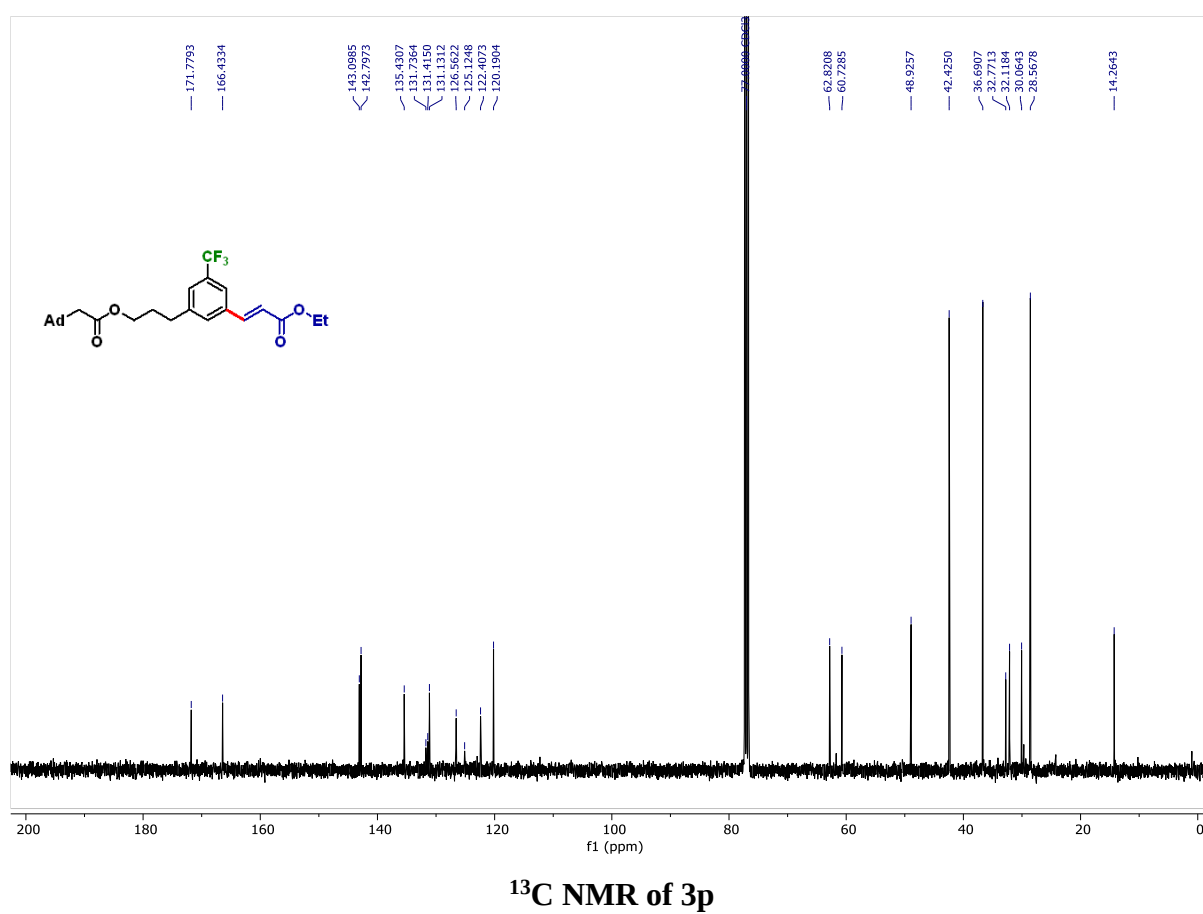
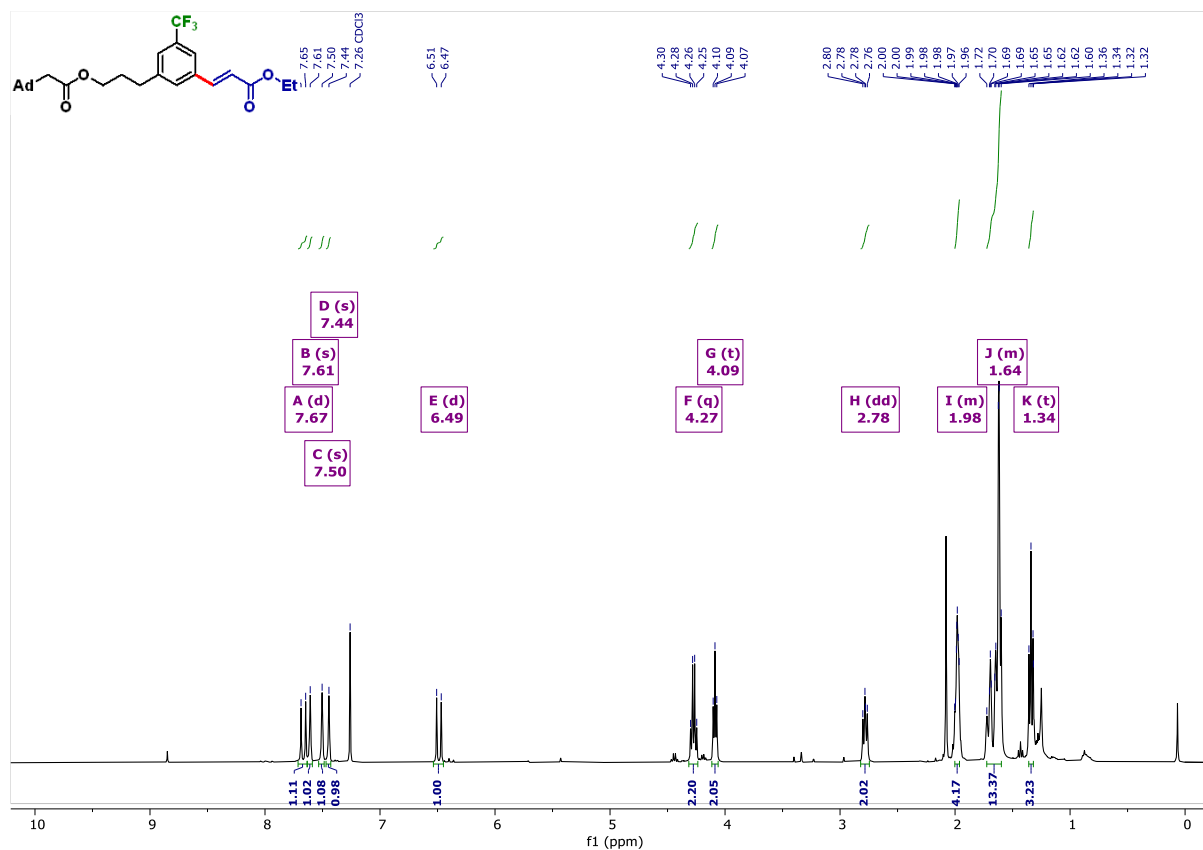


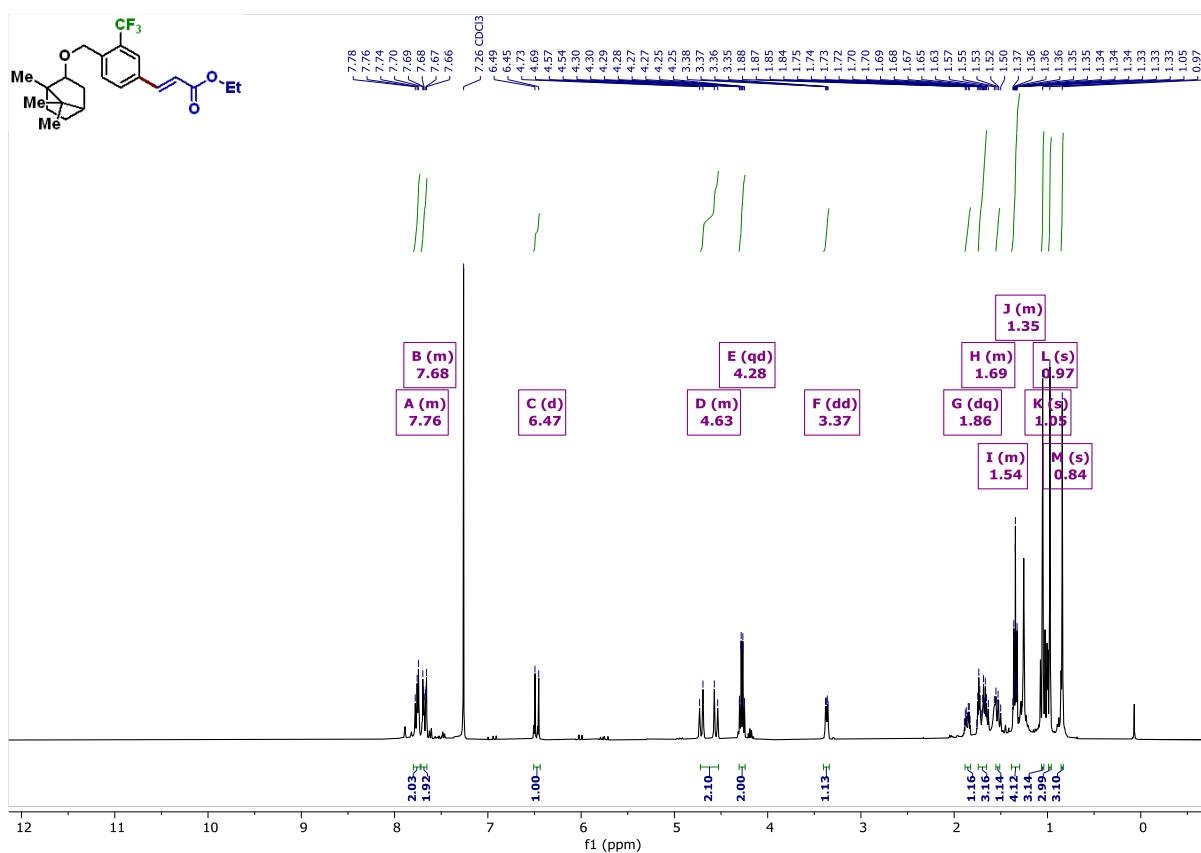
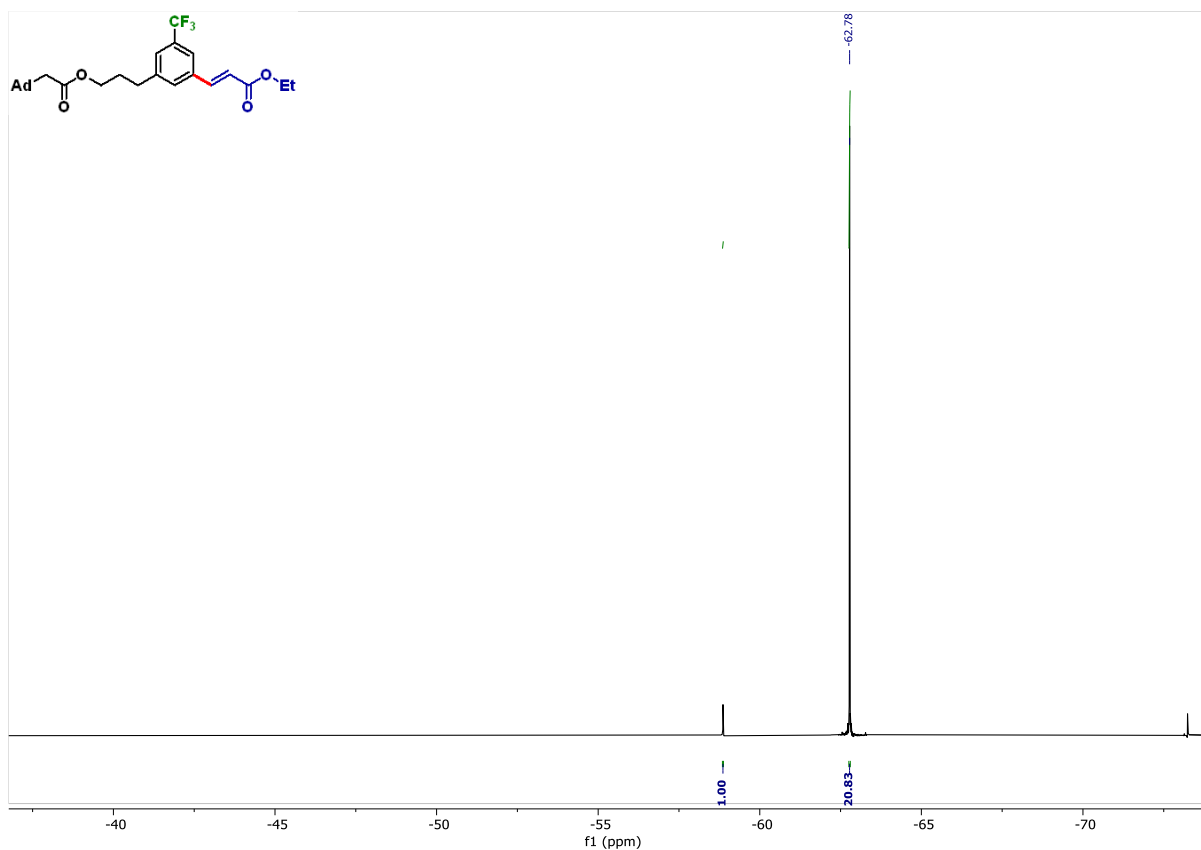


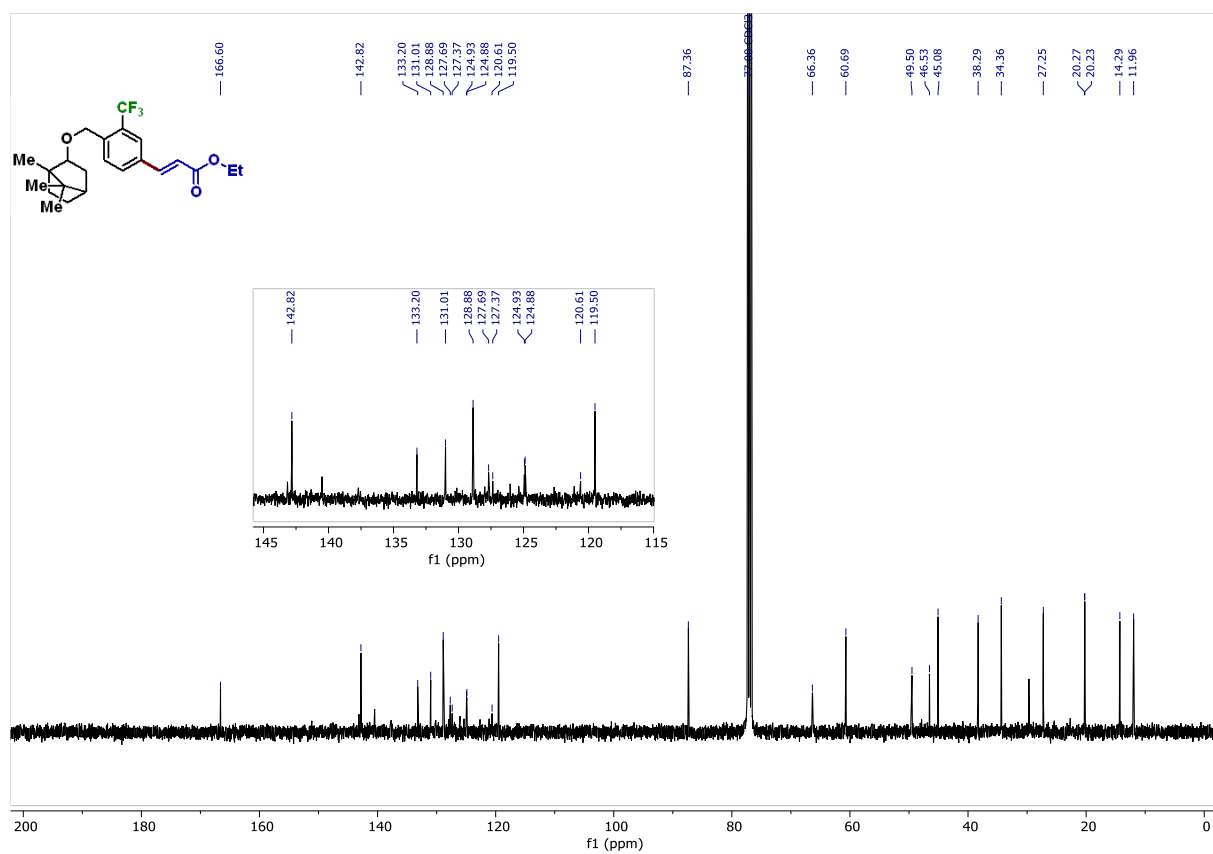
¹³C NMR of 3o



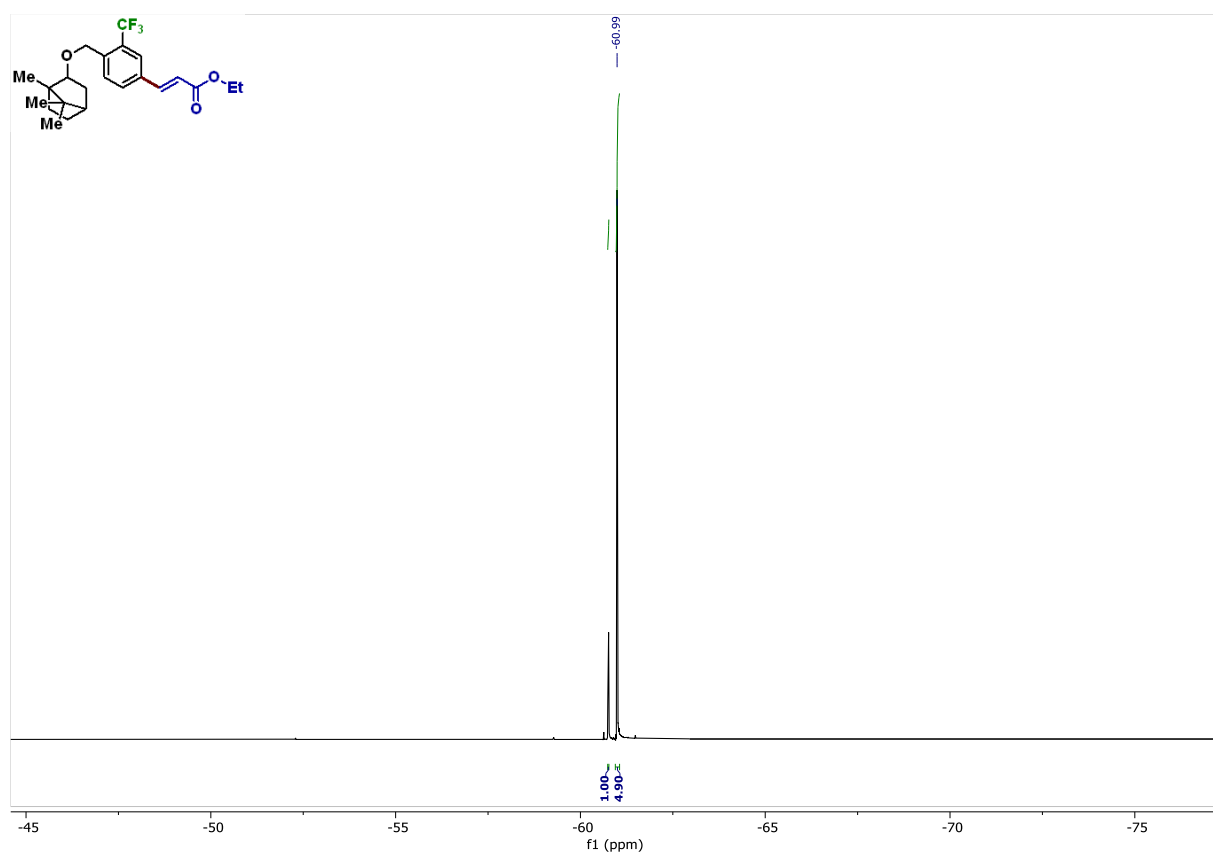
¹⁹F NMR of 3o



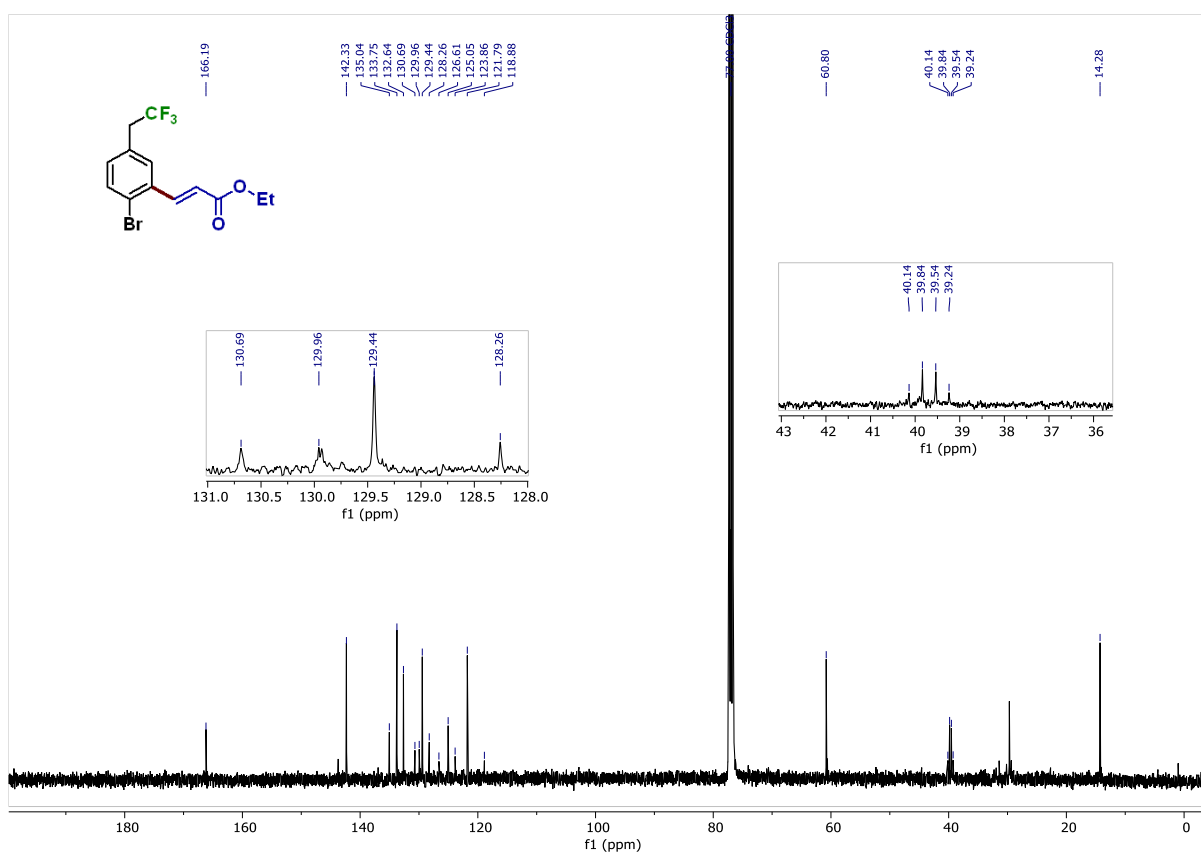
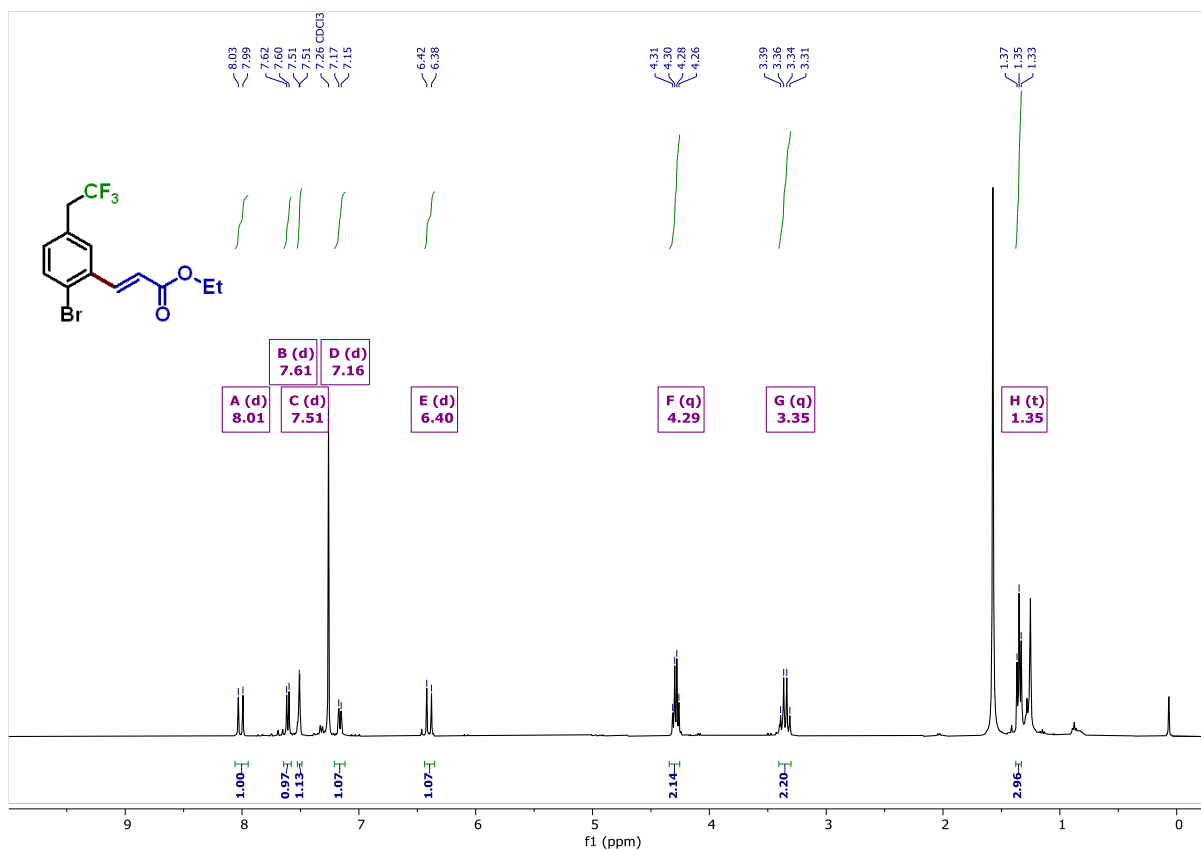


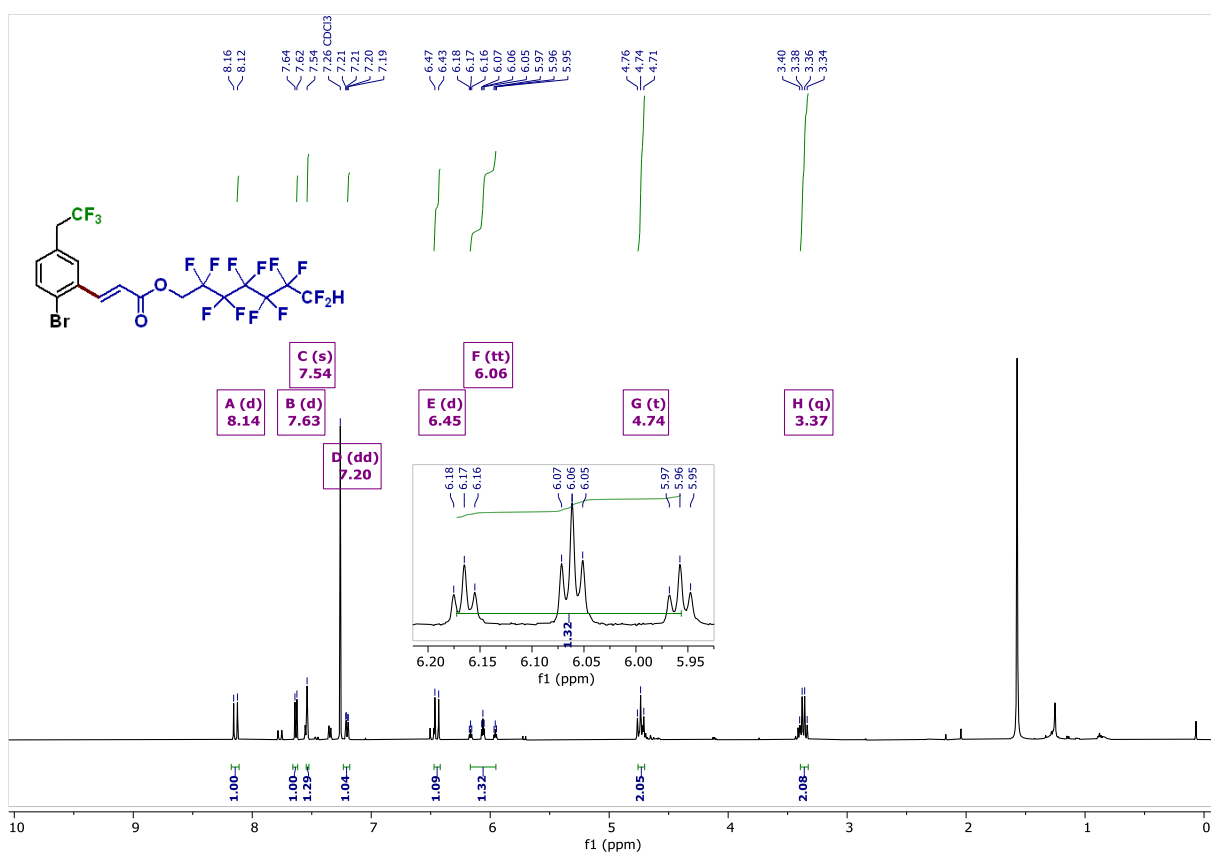
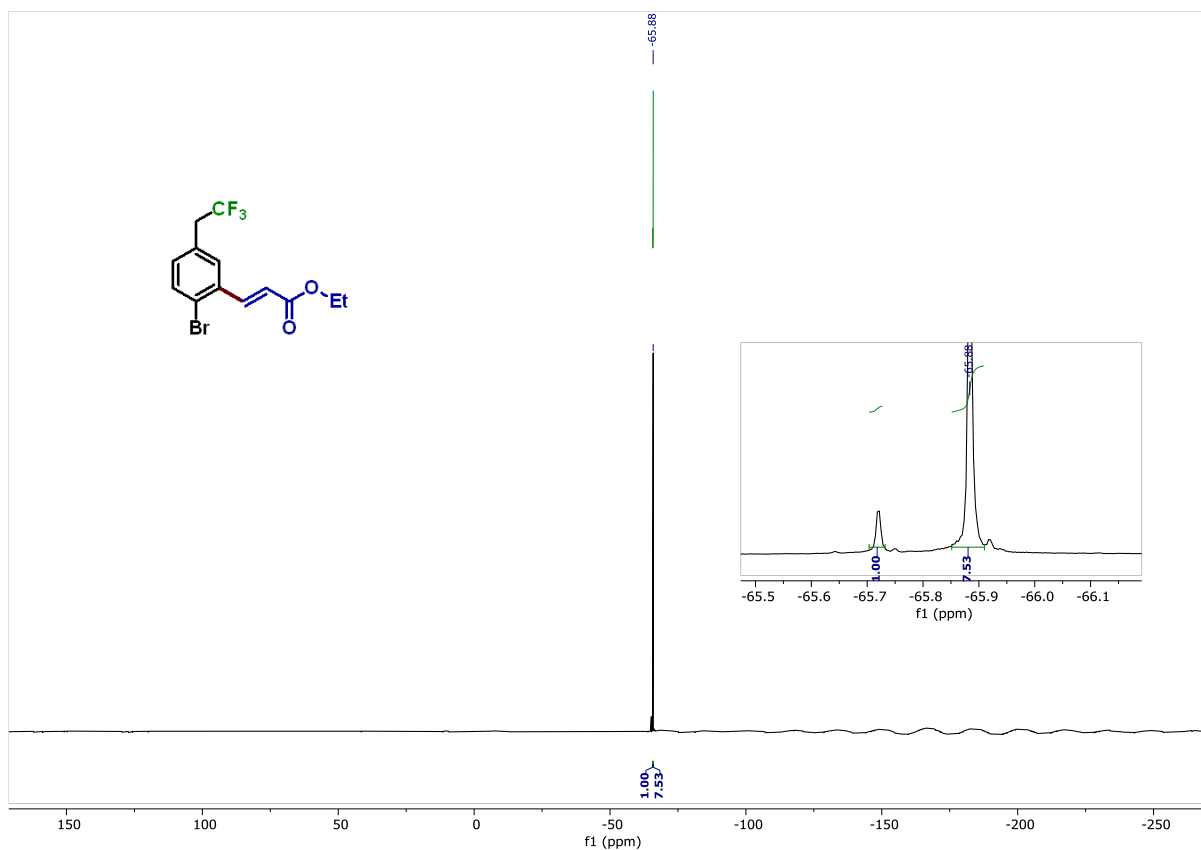


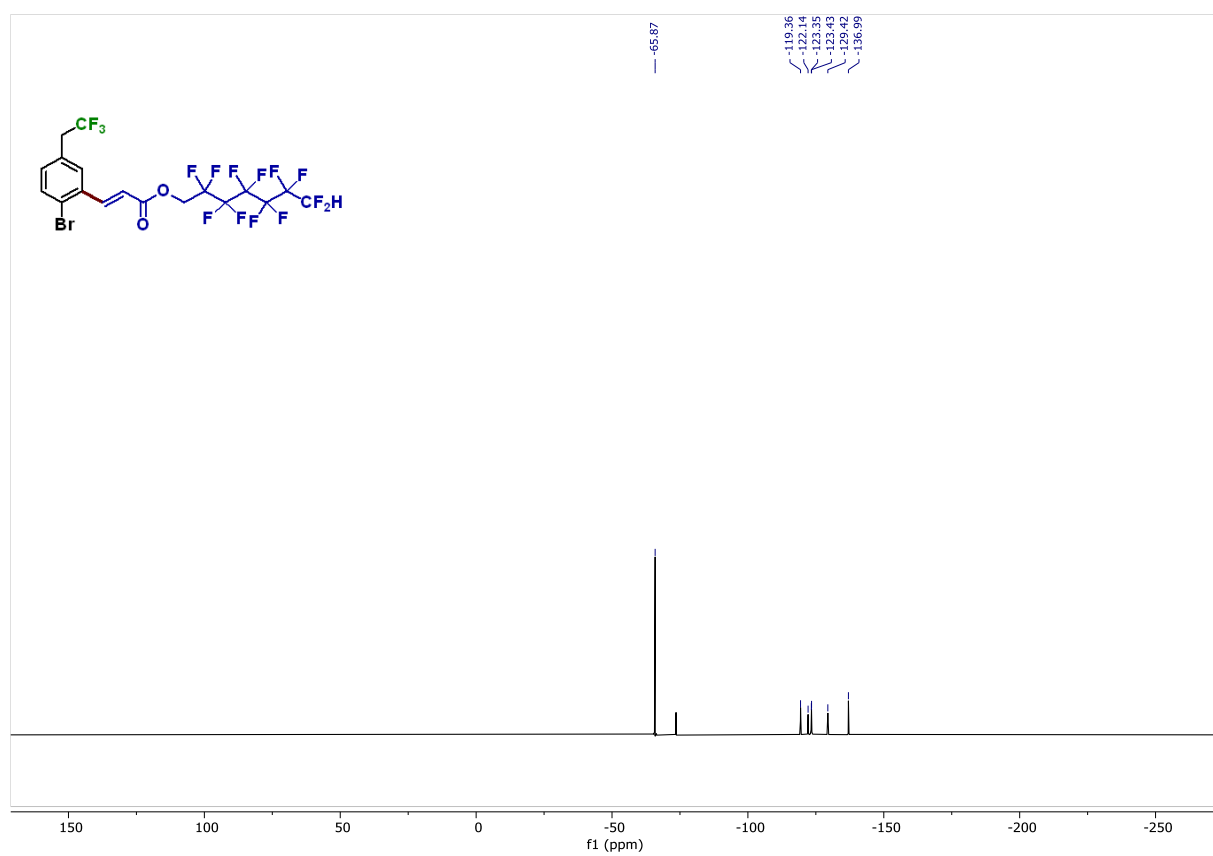
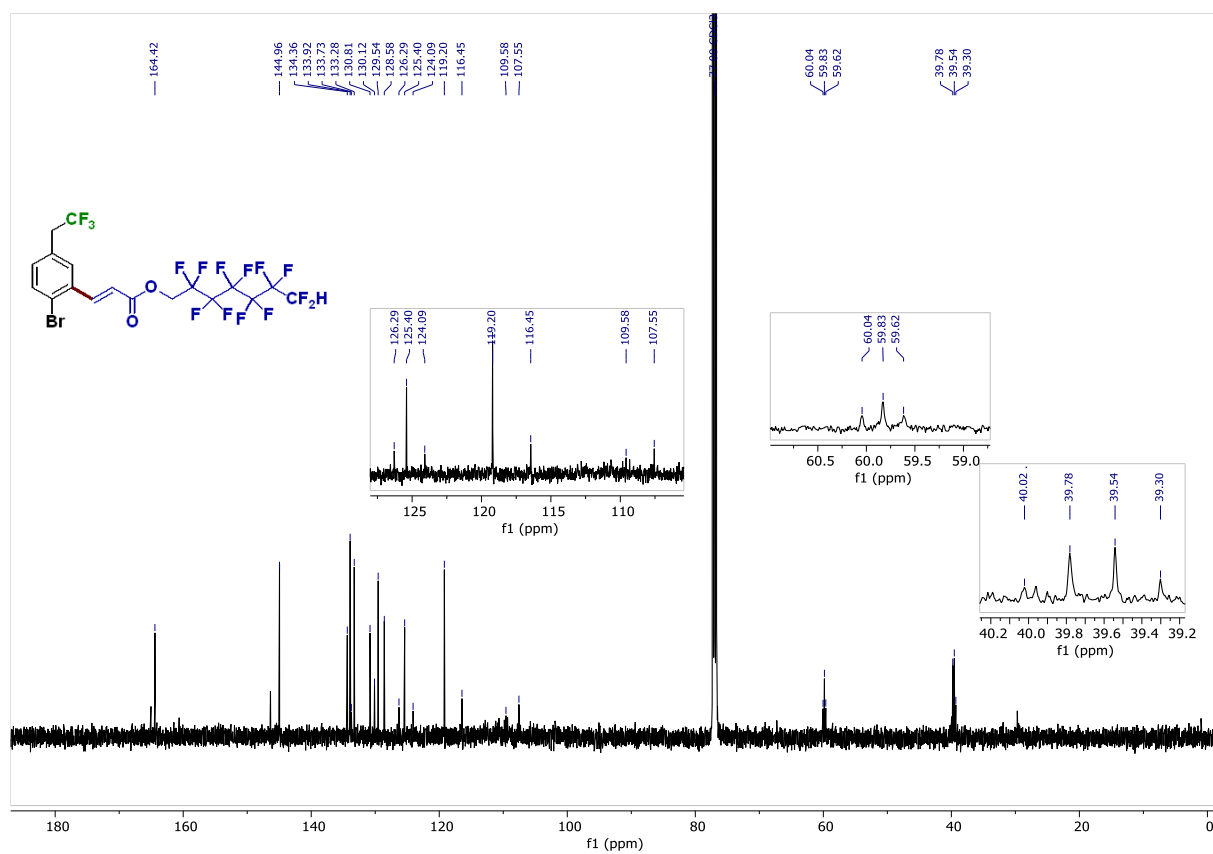
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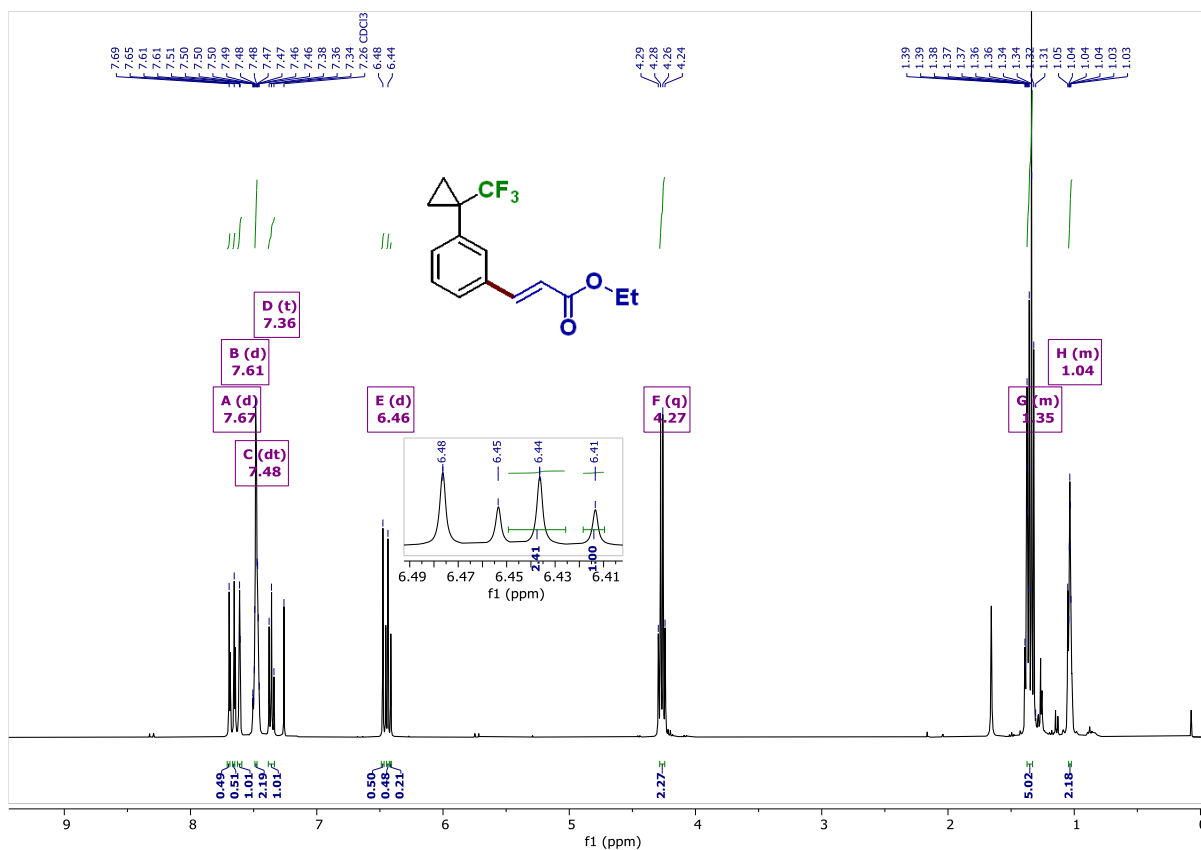


¹⁹F NMR of 3q

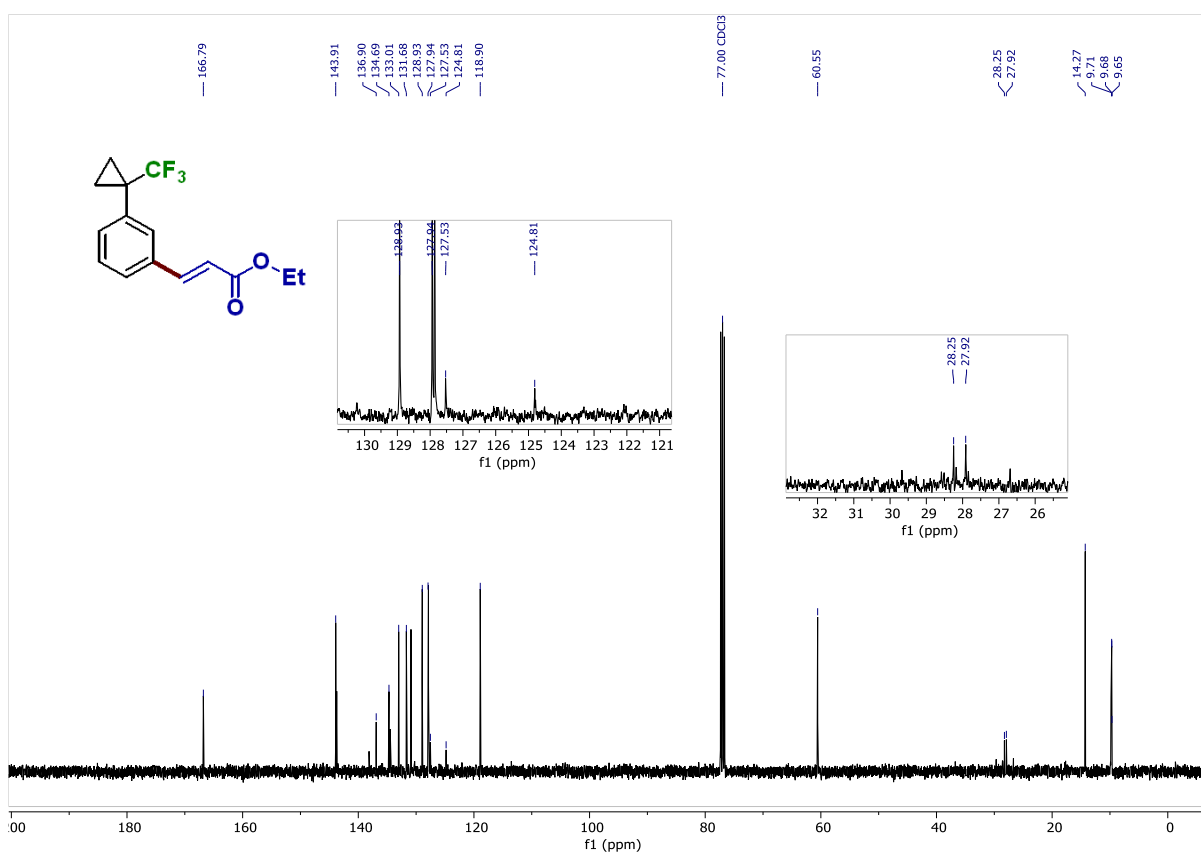




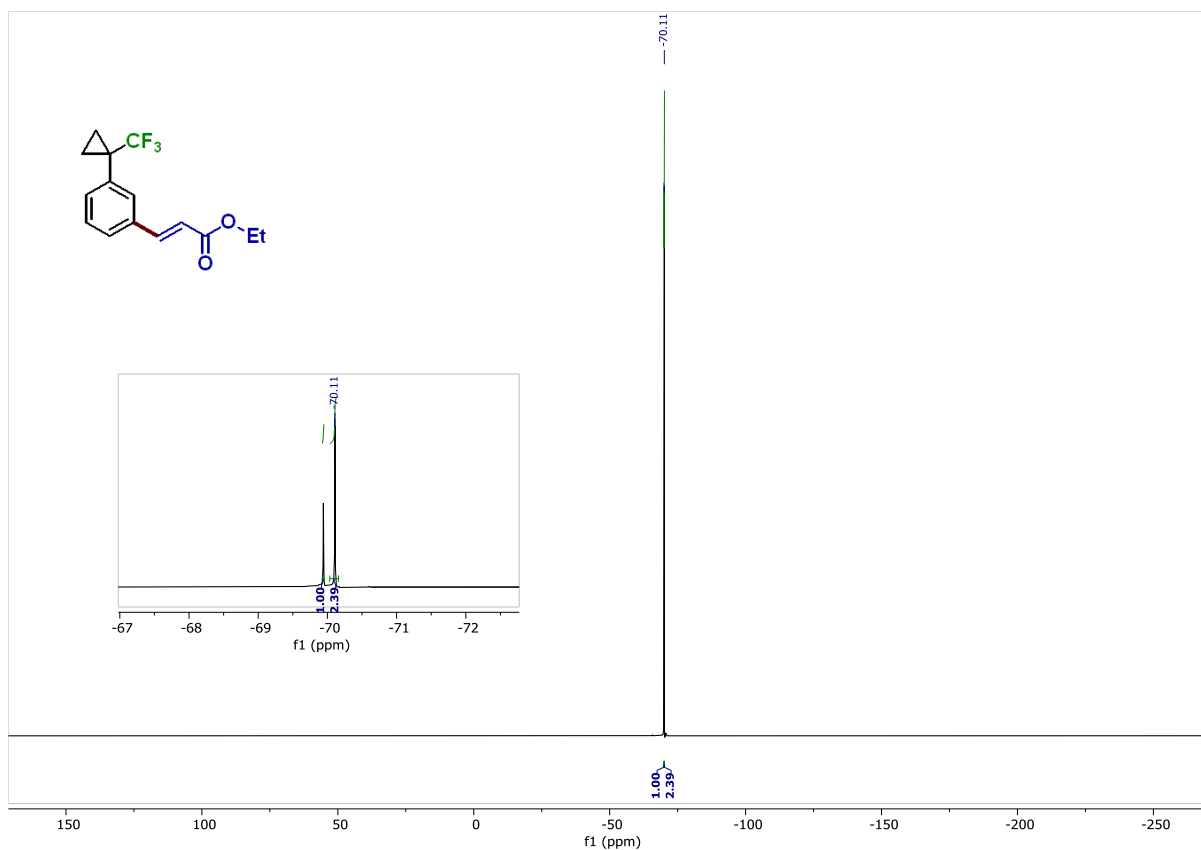




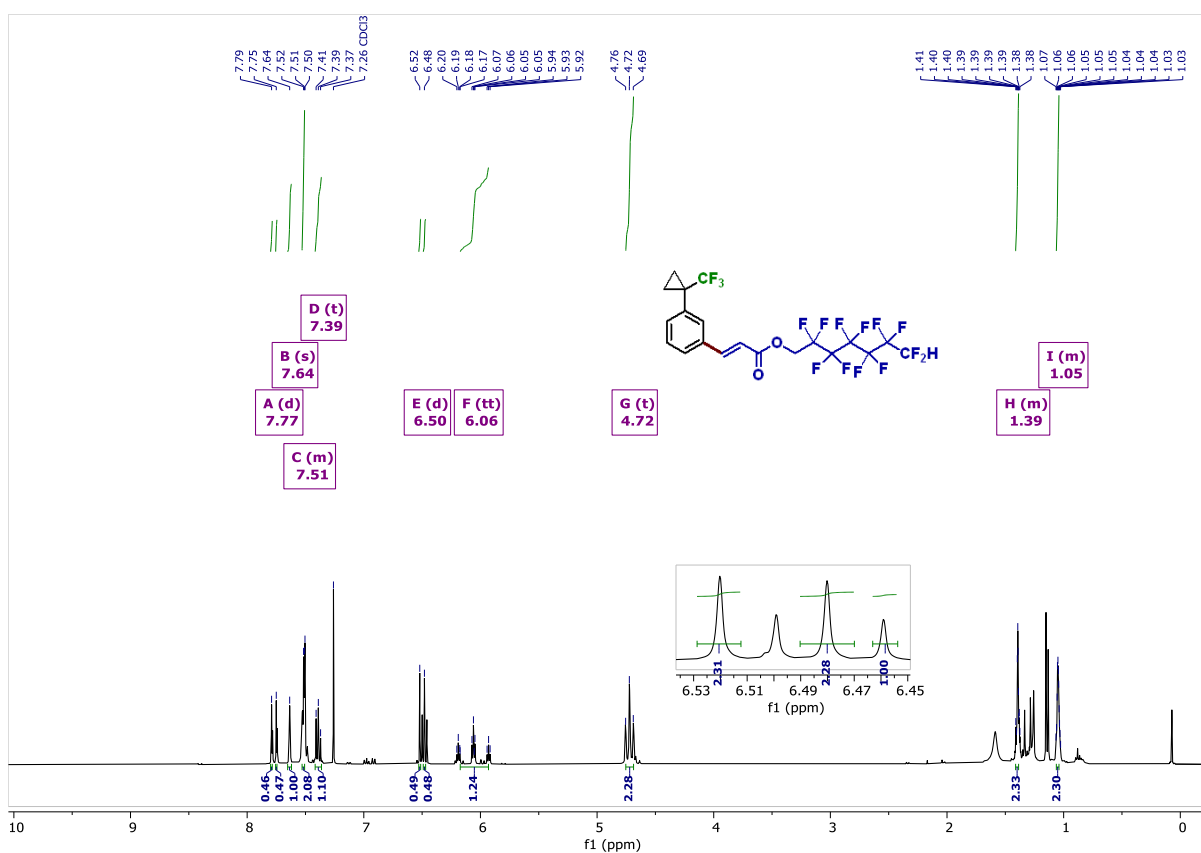
¹H NMR of 3u

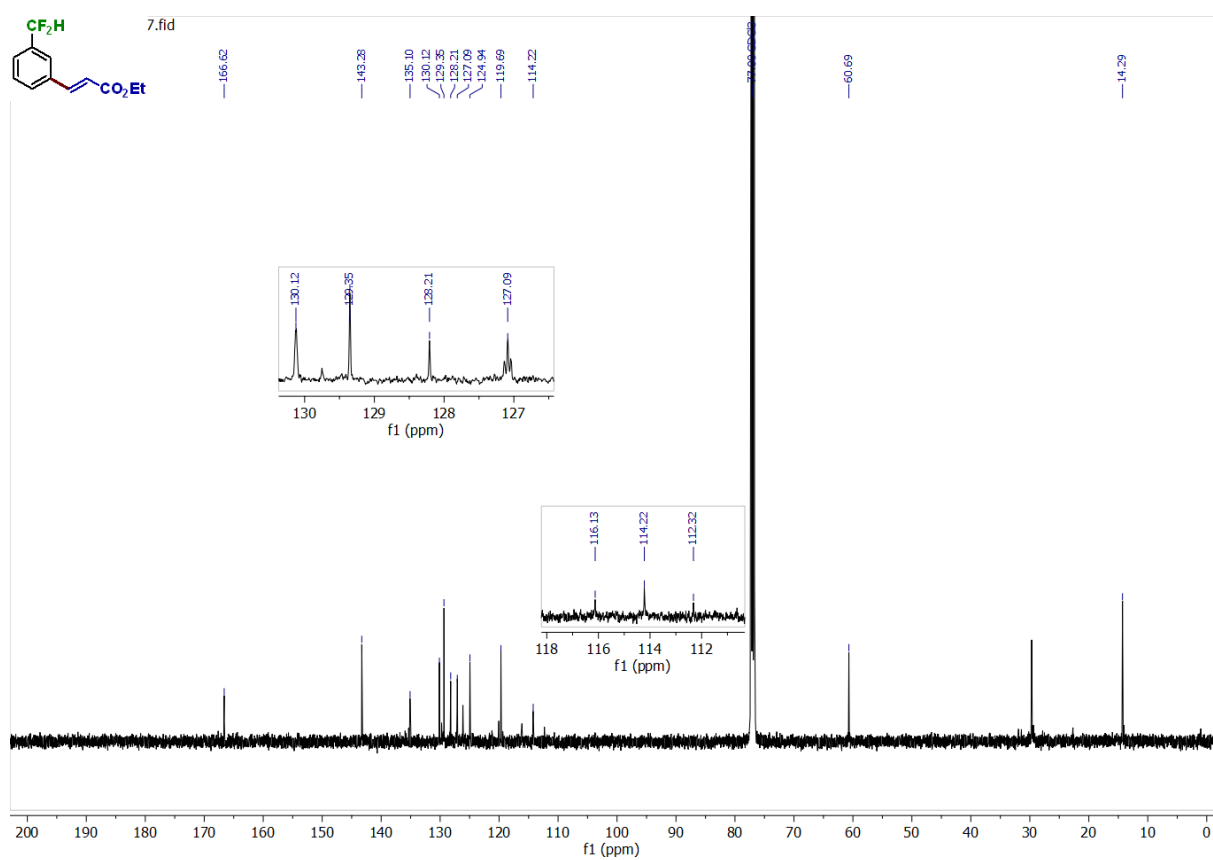
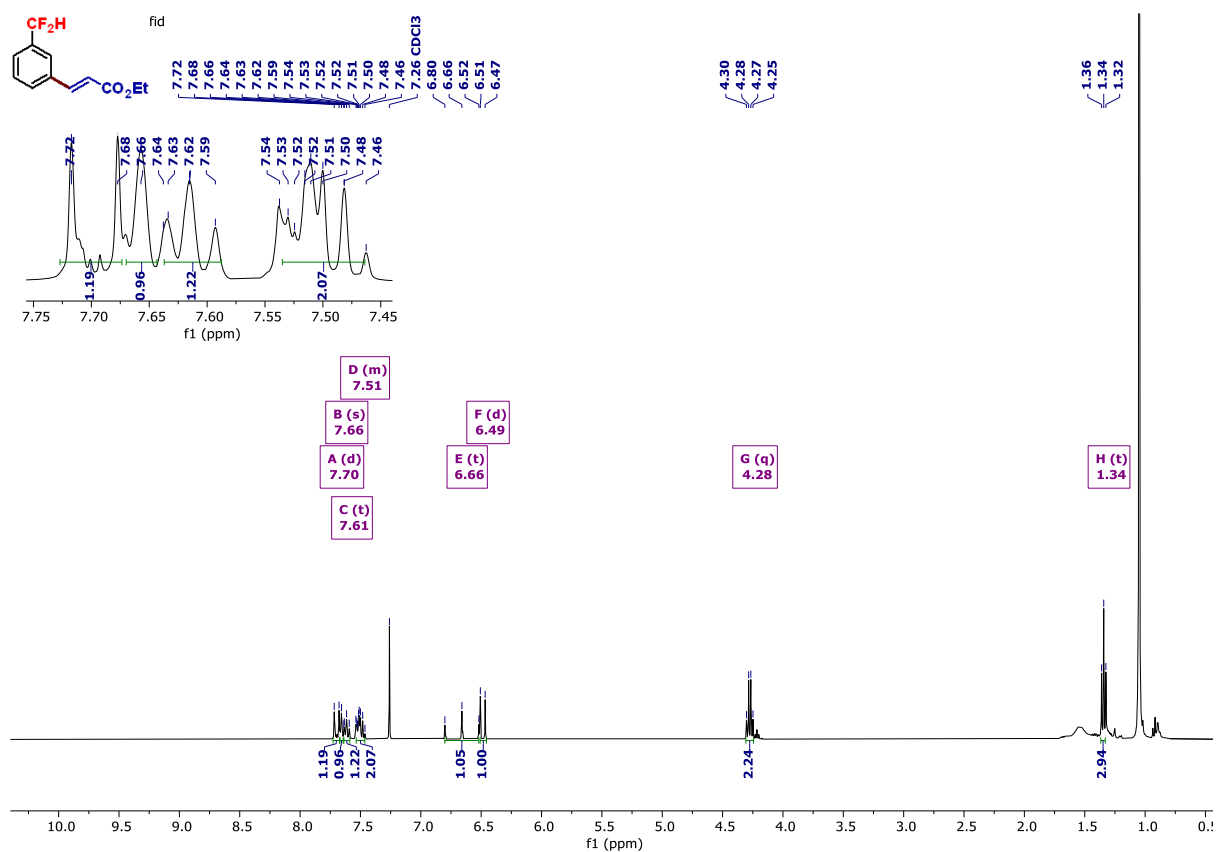


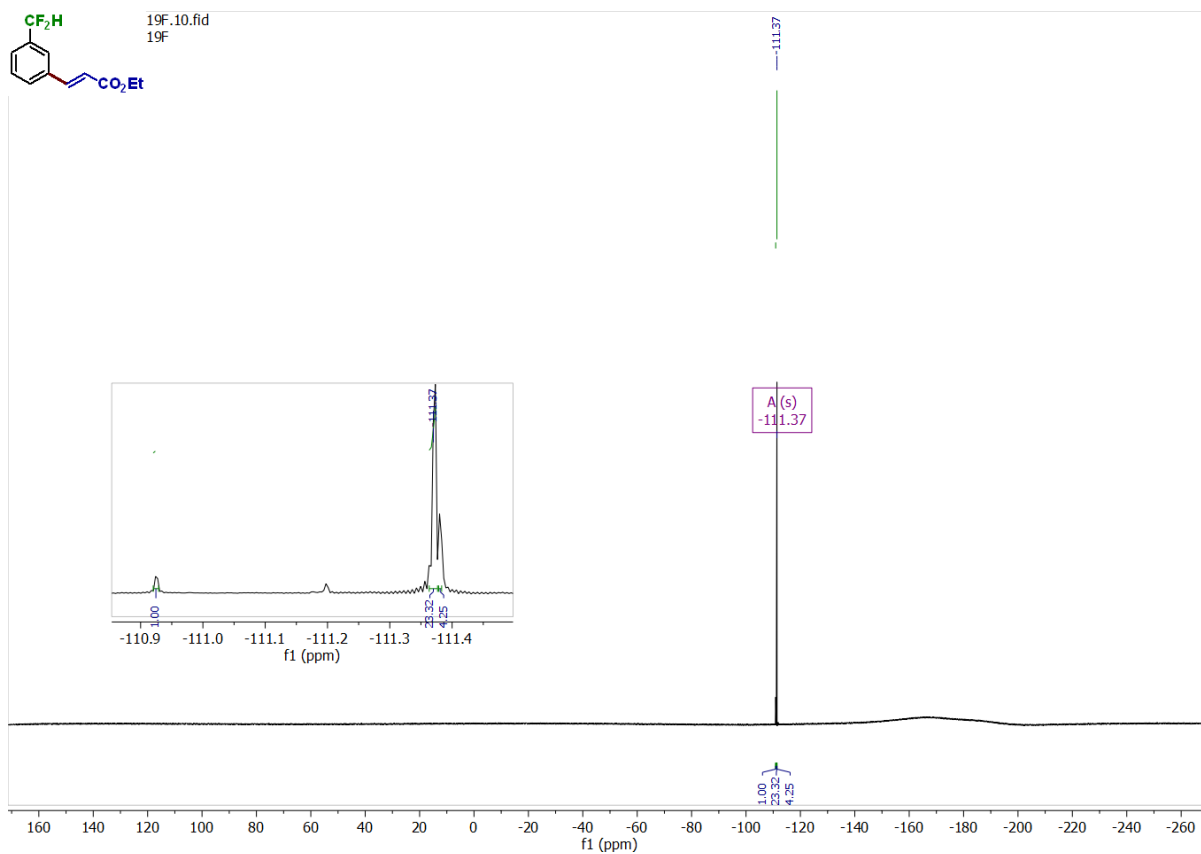
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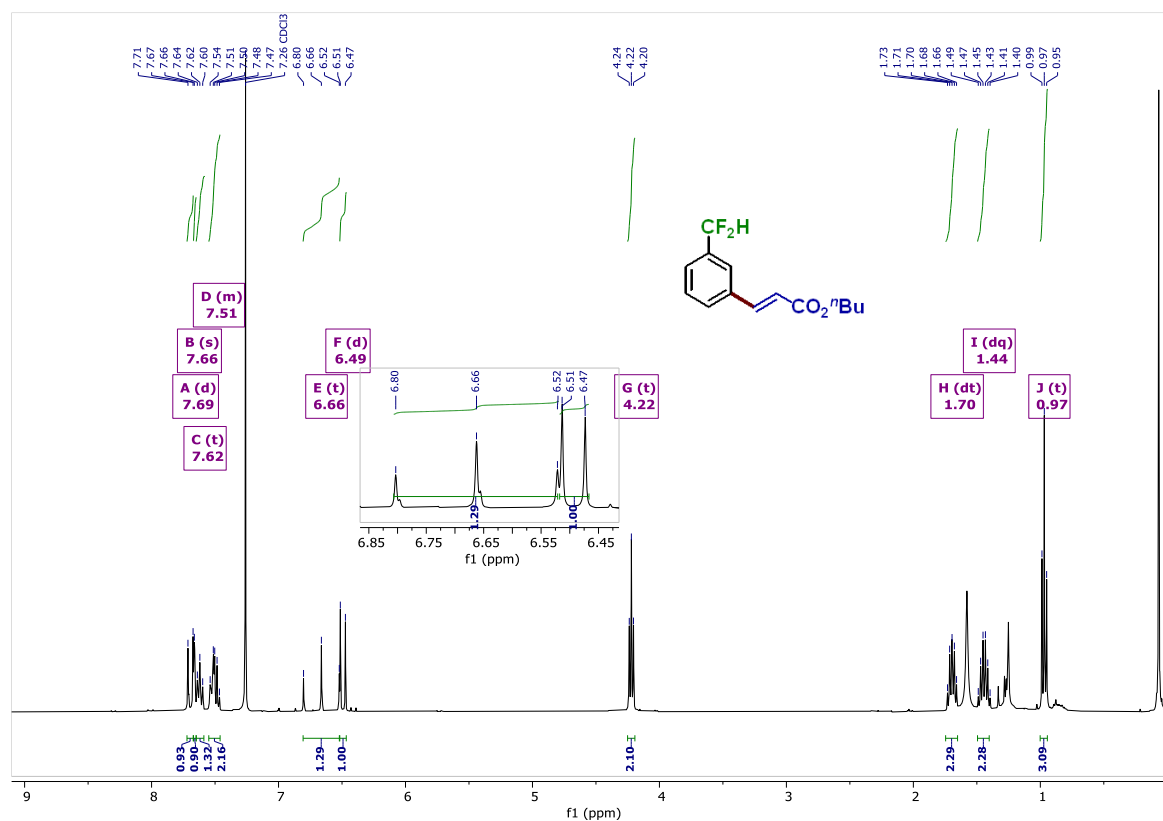
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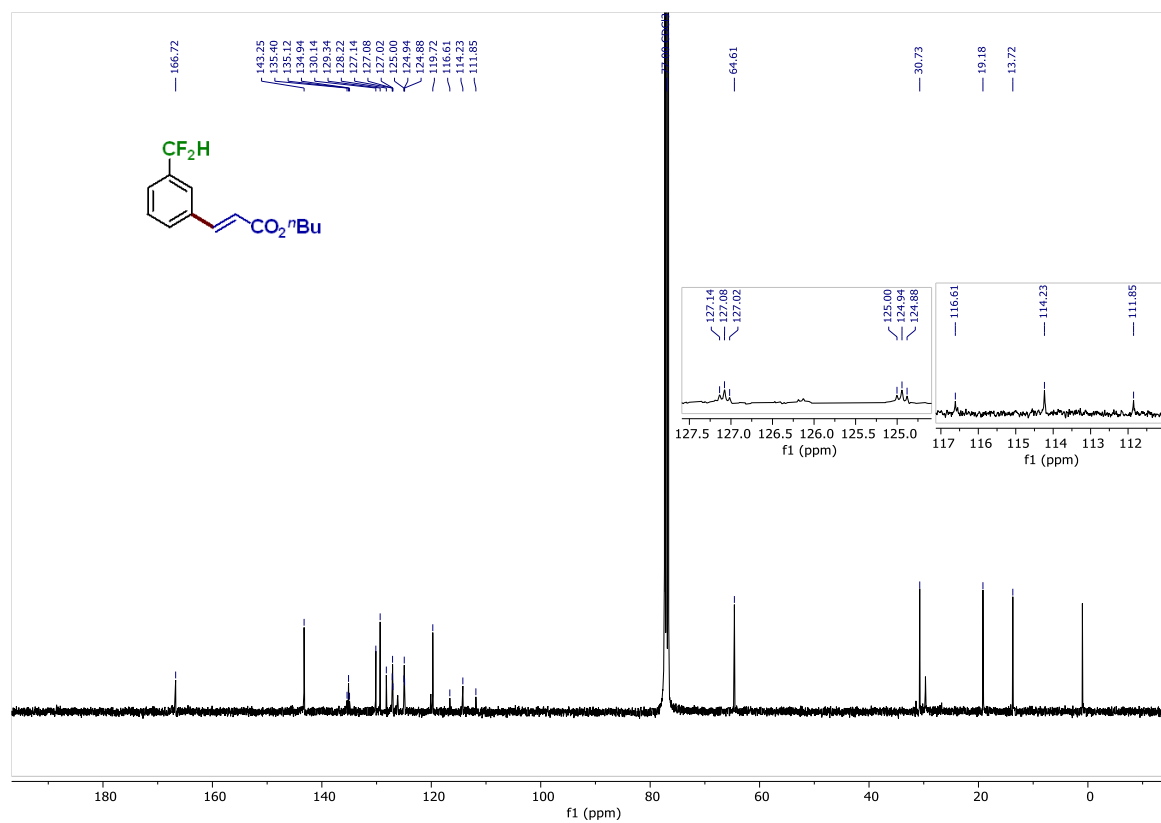




¹⁹F NMR of 5a

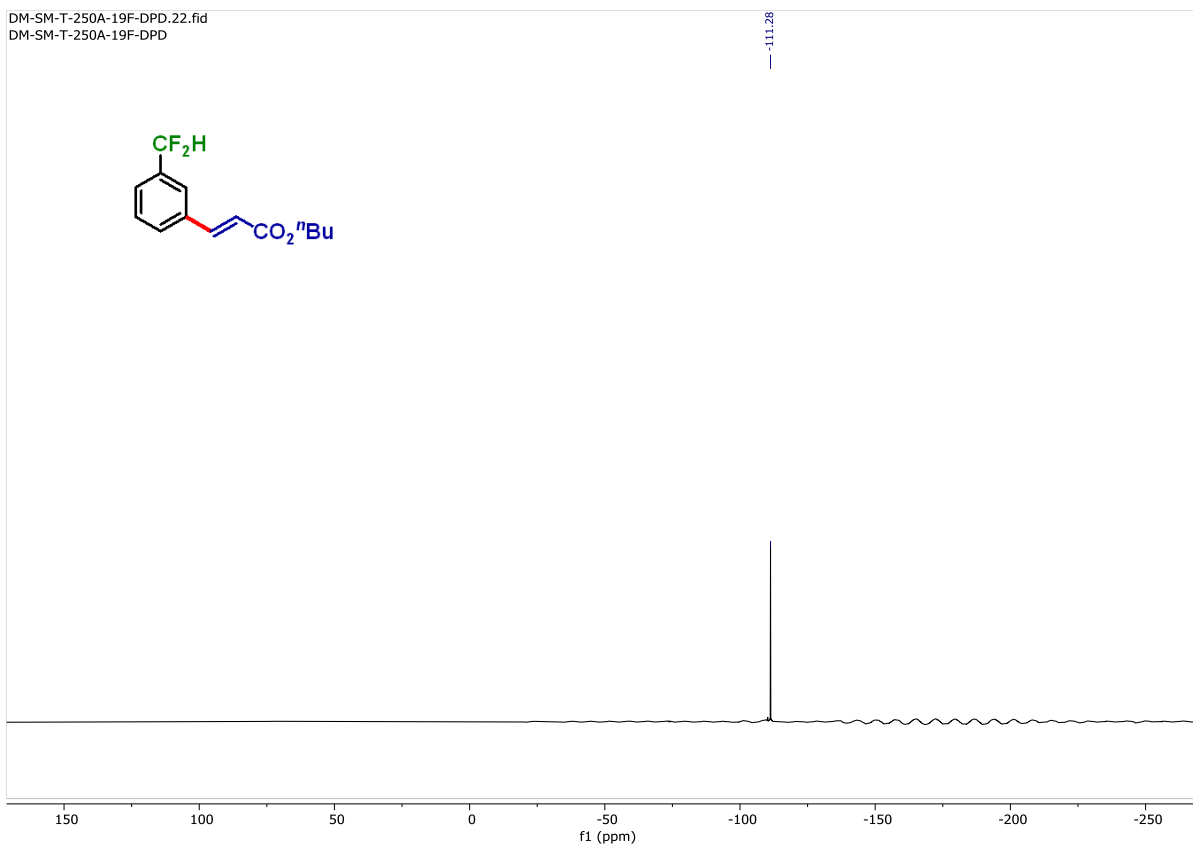


^1H NMR of 5b

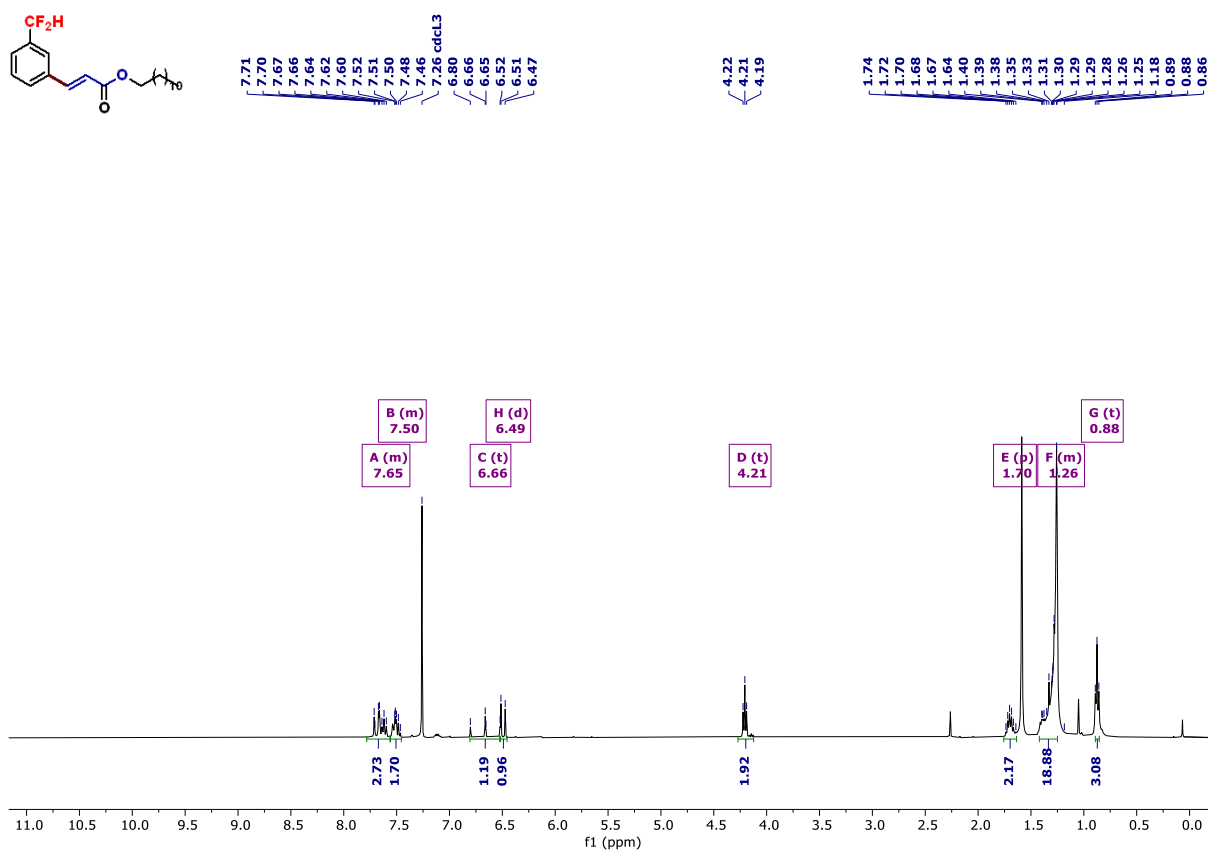


^{13}C NMR of 5b

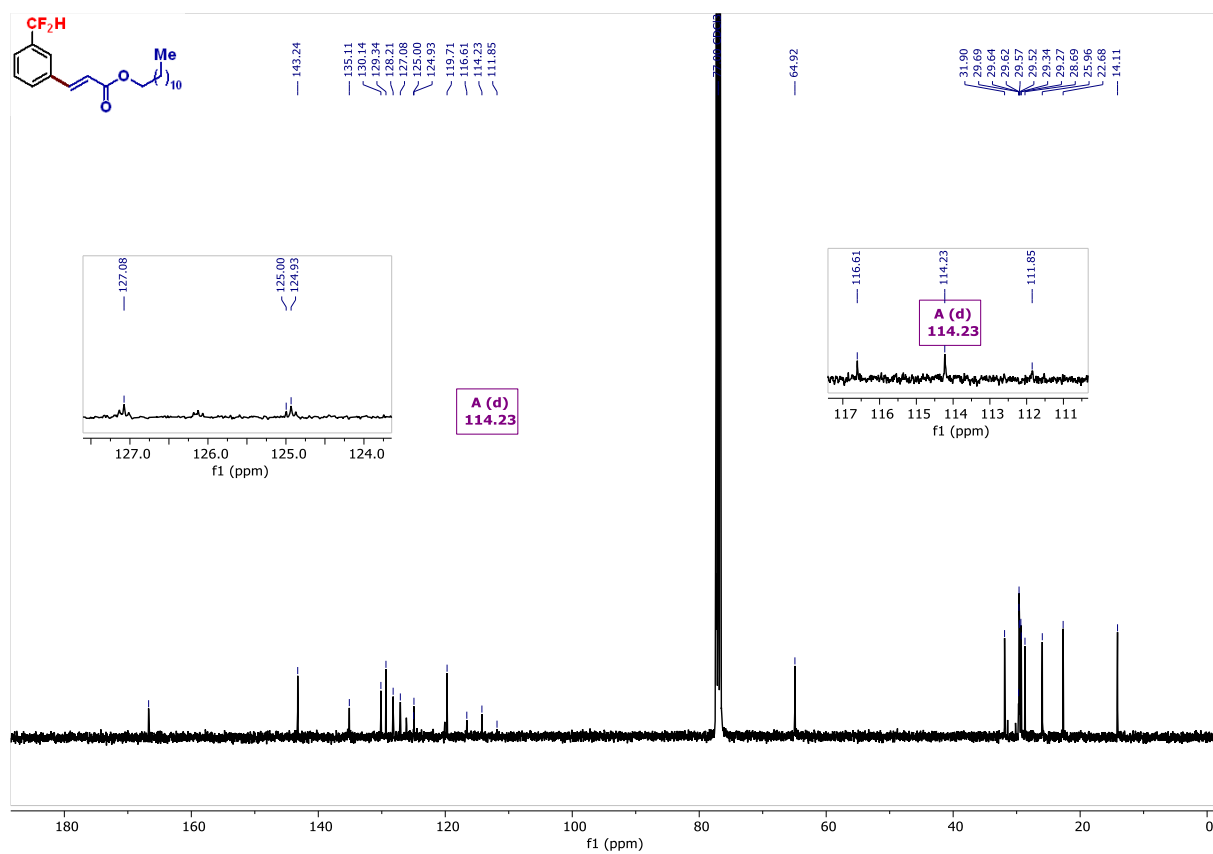
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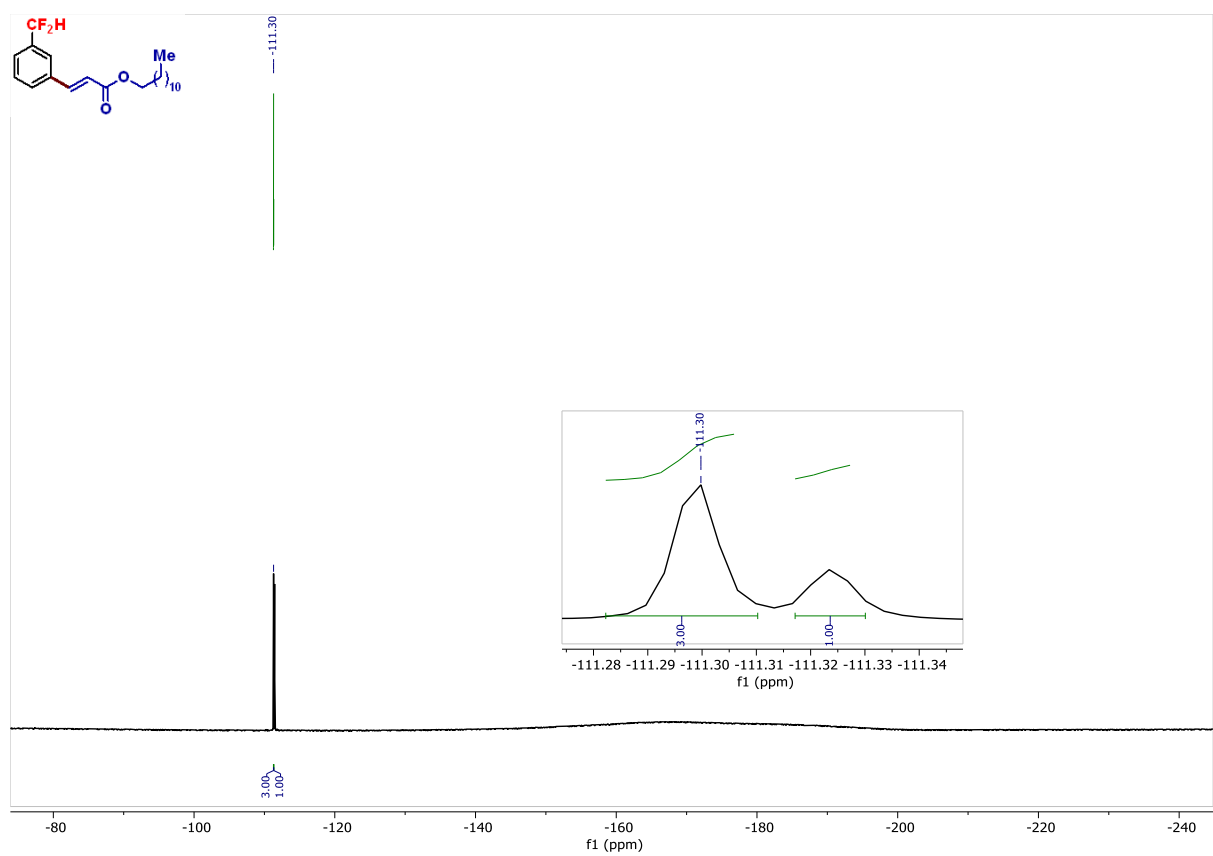
¹⁹F NMR of 5b



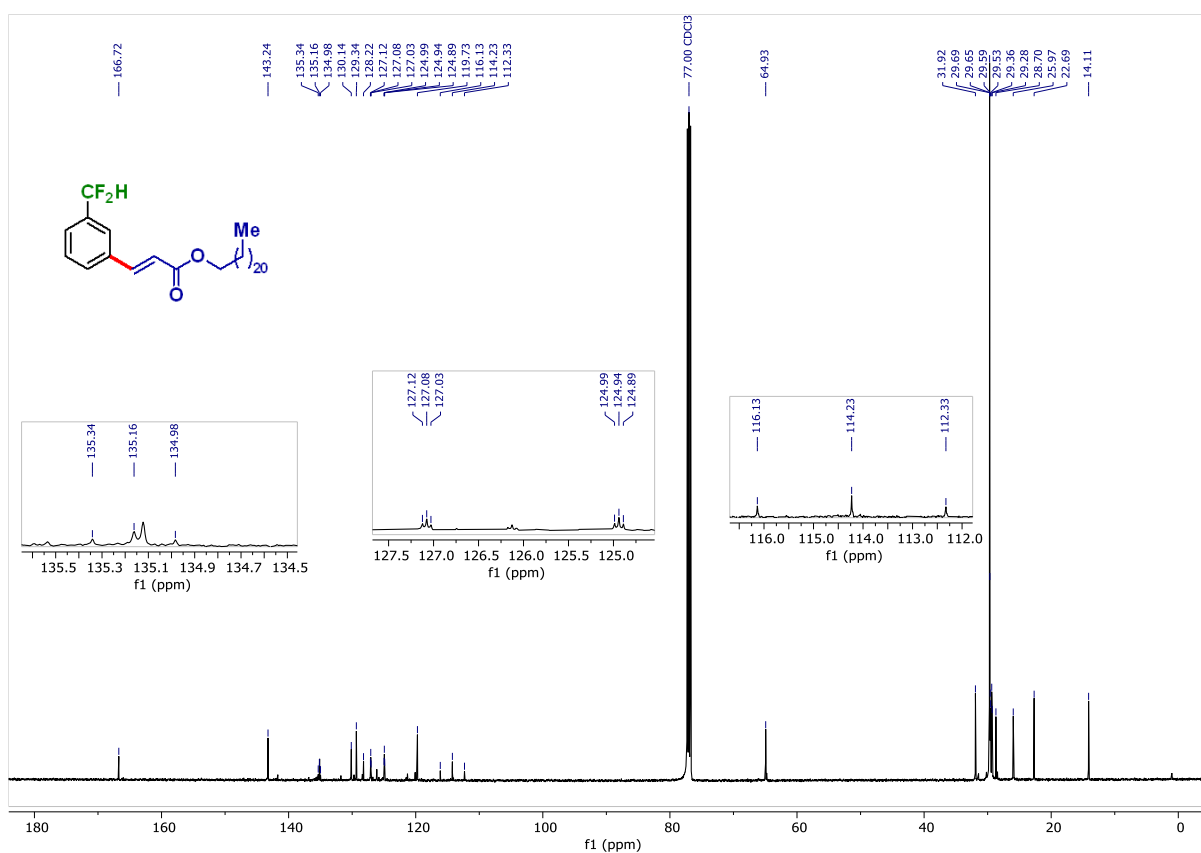
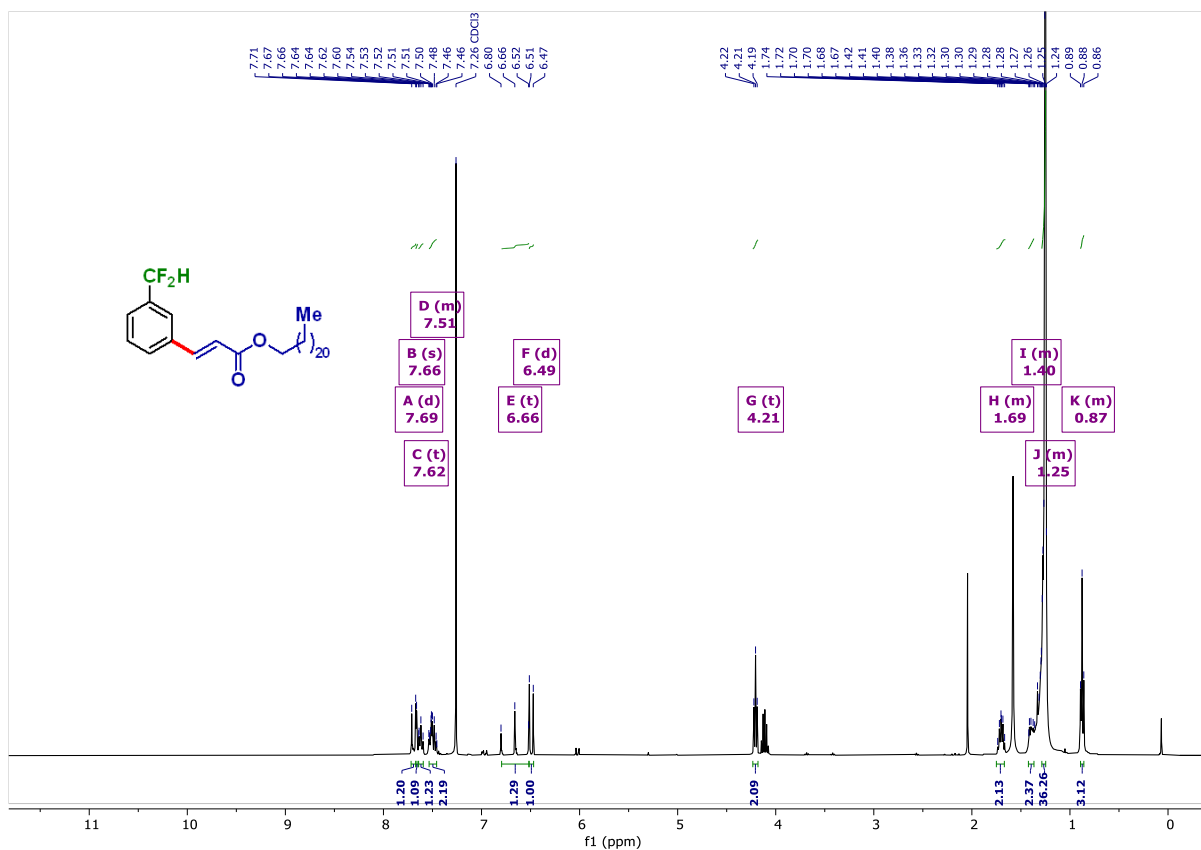
¹H NMR of 5c

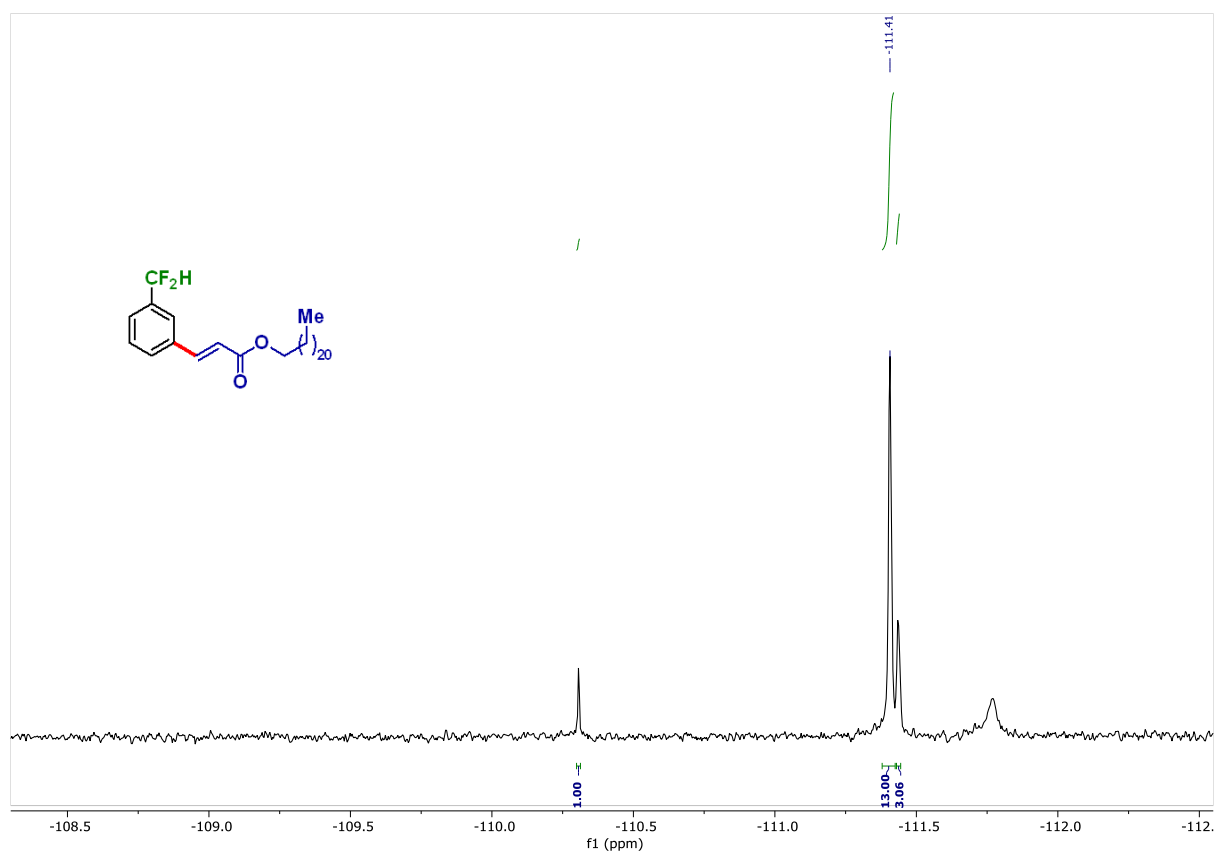


¹³C NMR of 5c

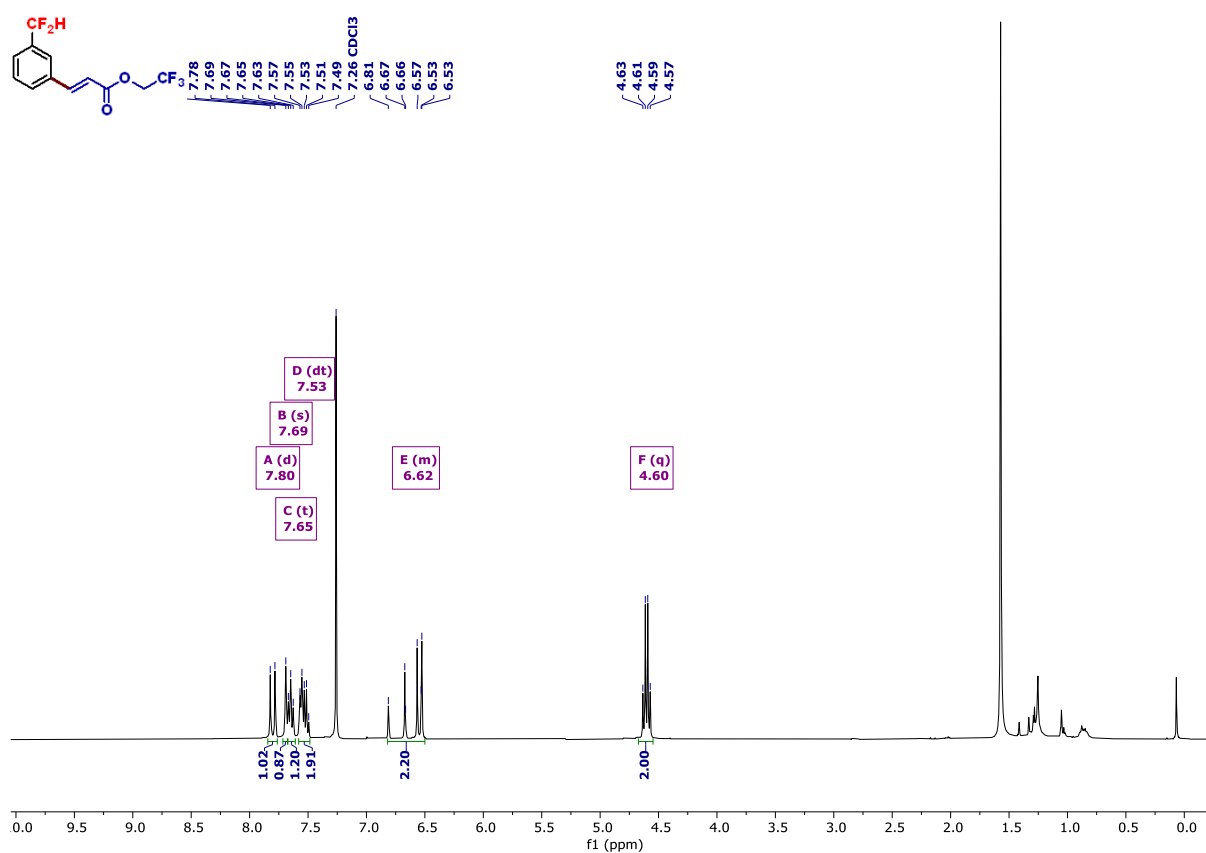


¹⁹F NMR of 5c

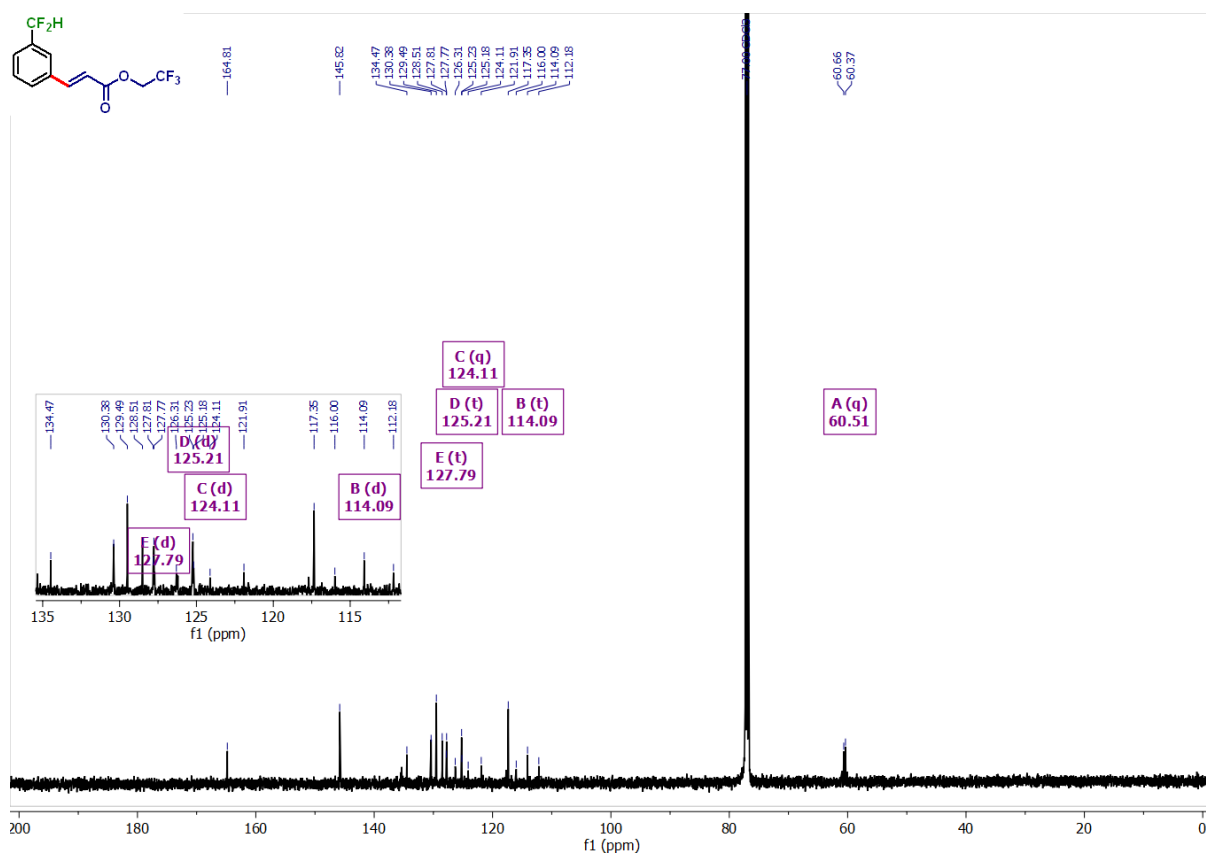




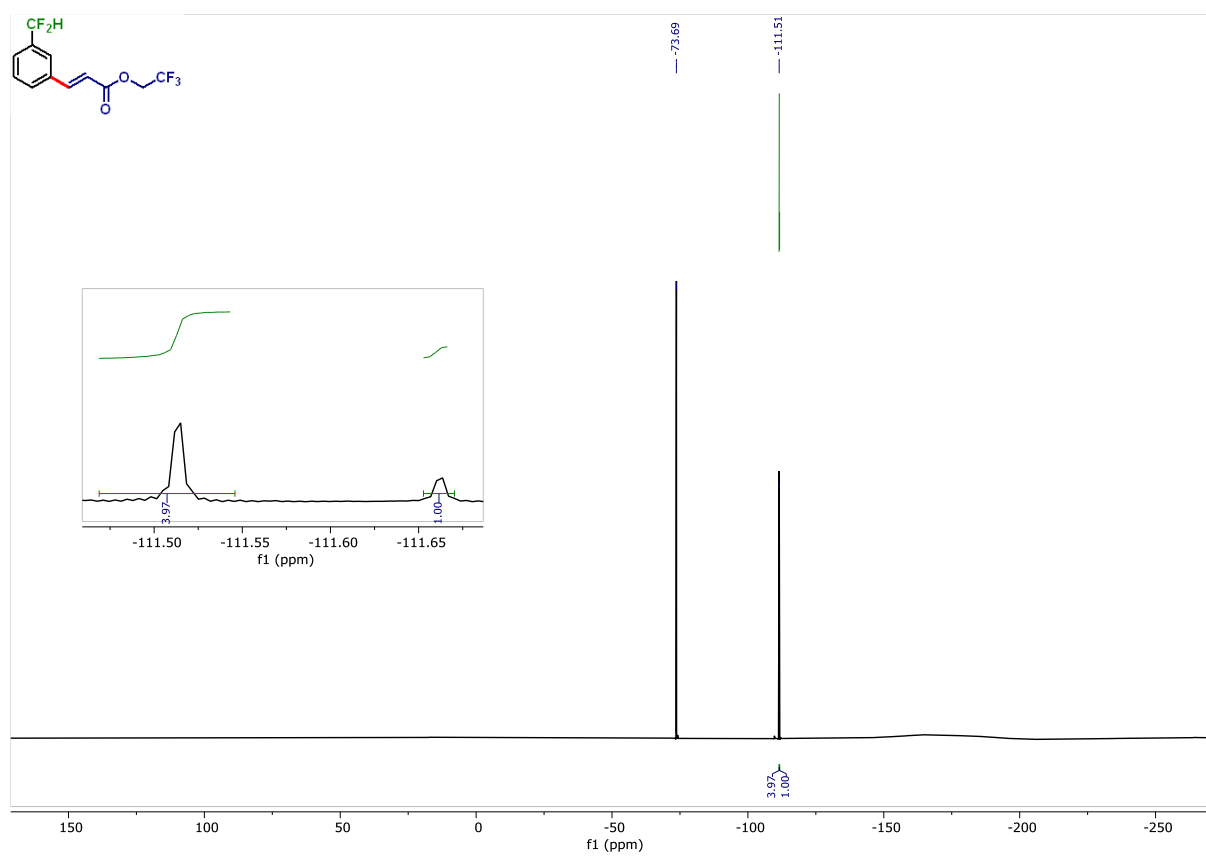
¹⁹F NMR of 5d



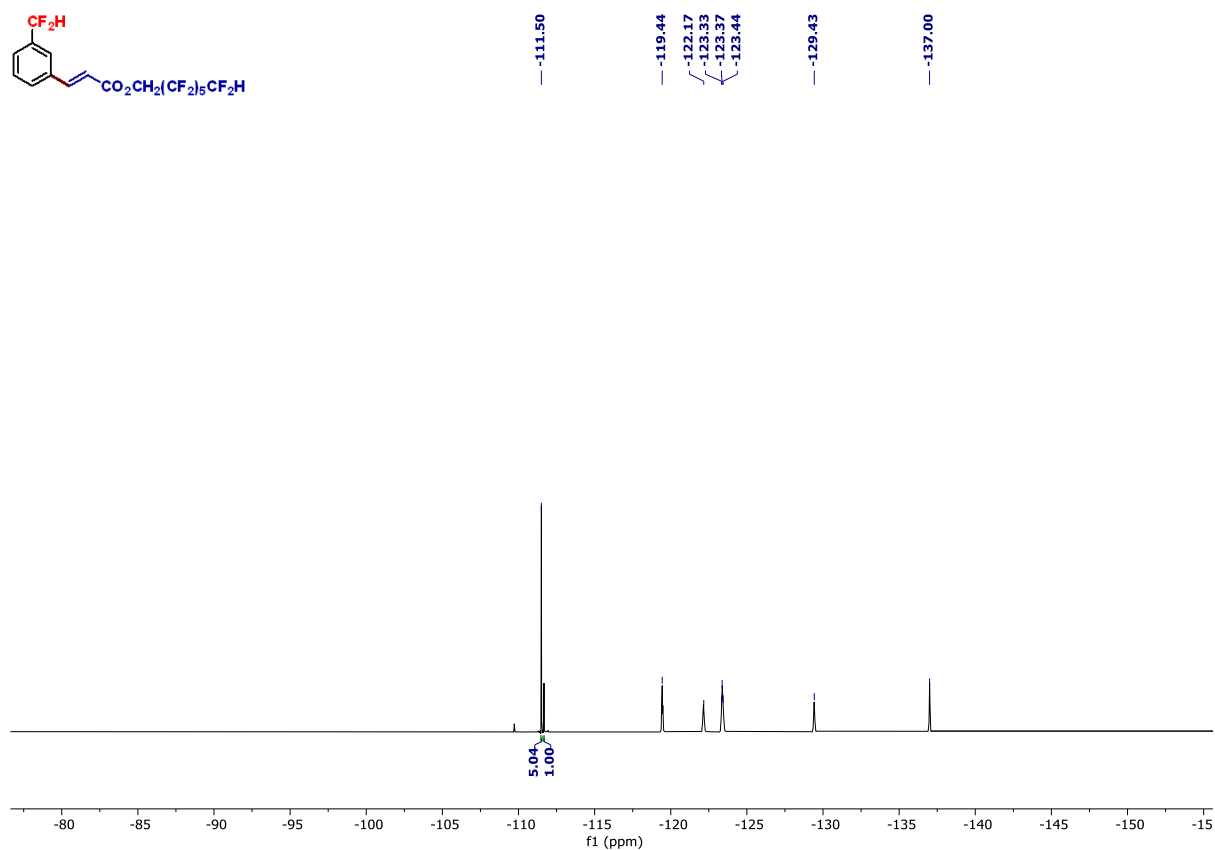
¹H NMR of 5e



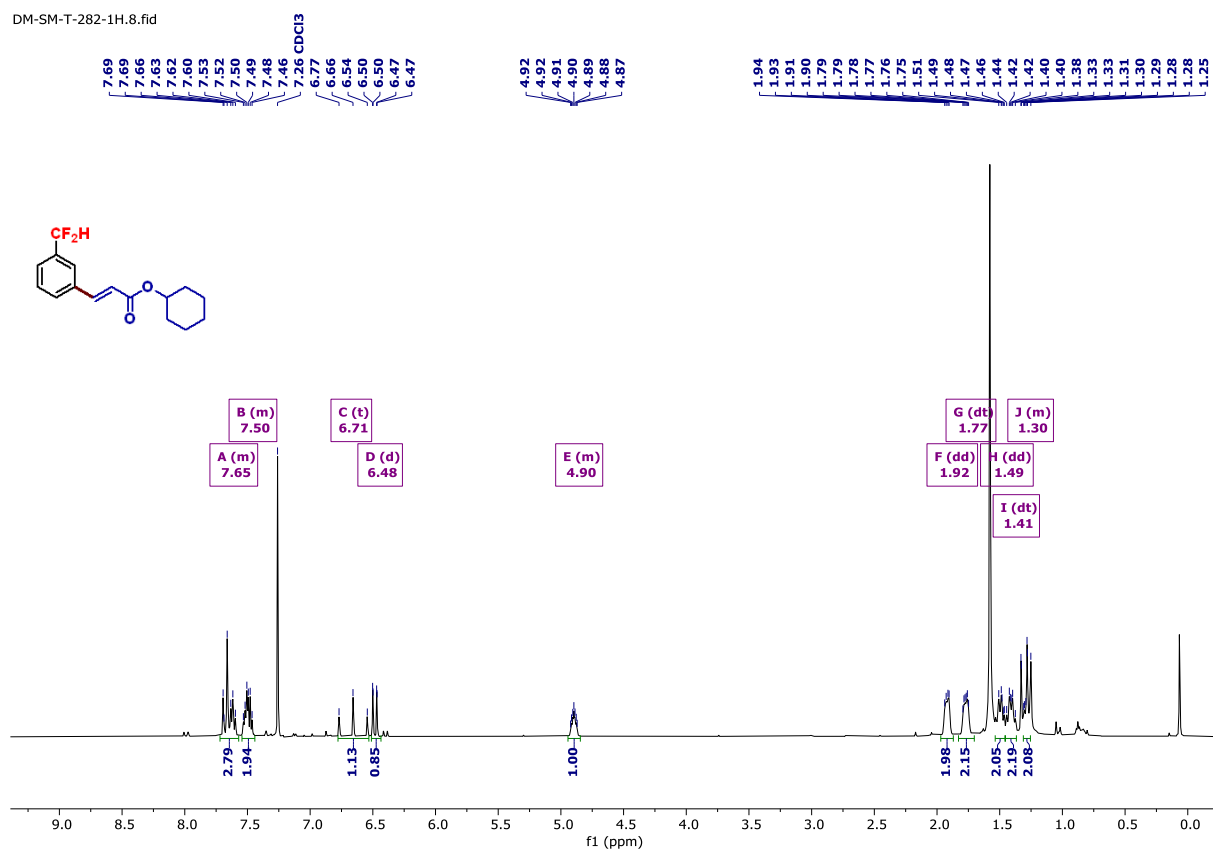
¹³C NMR of 5e



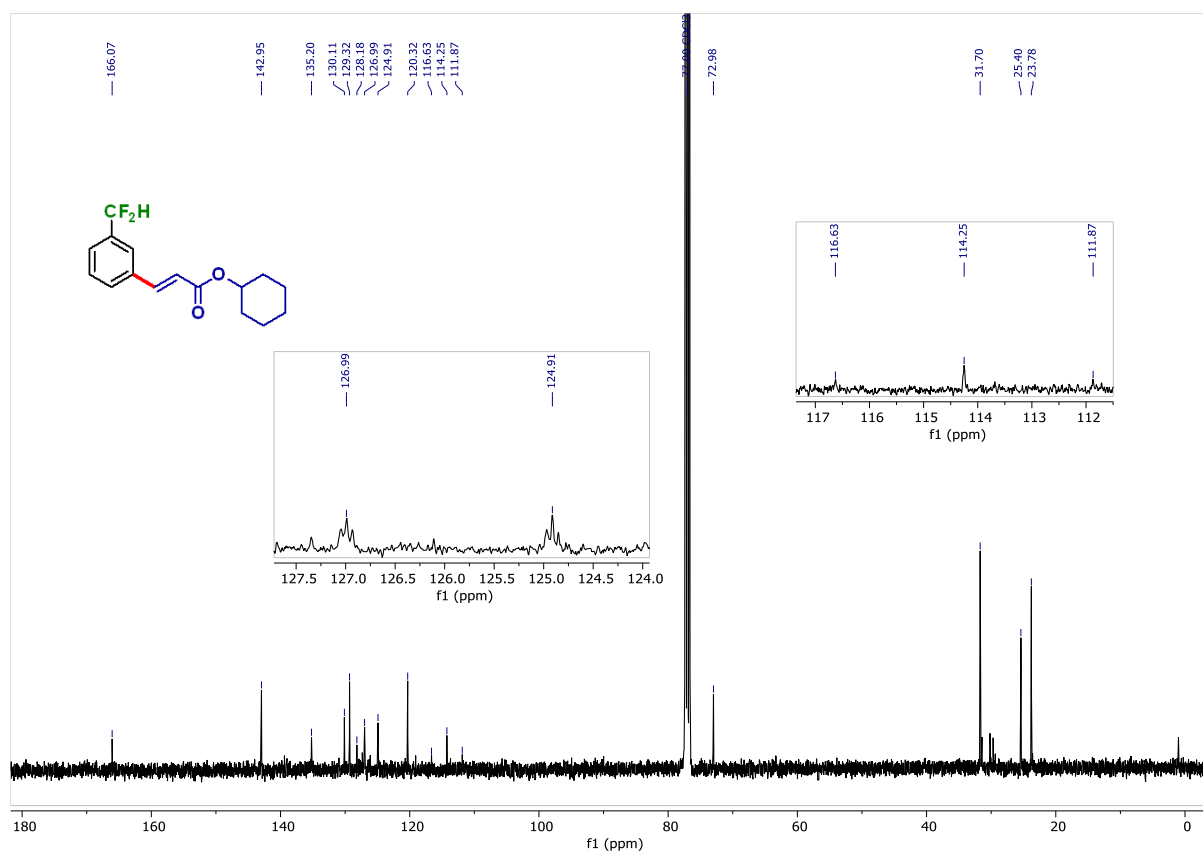
¹⁹F NMR of 5e



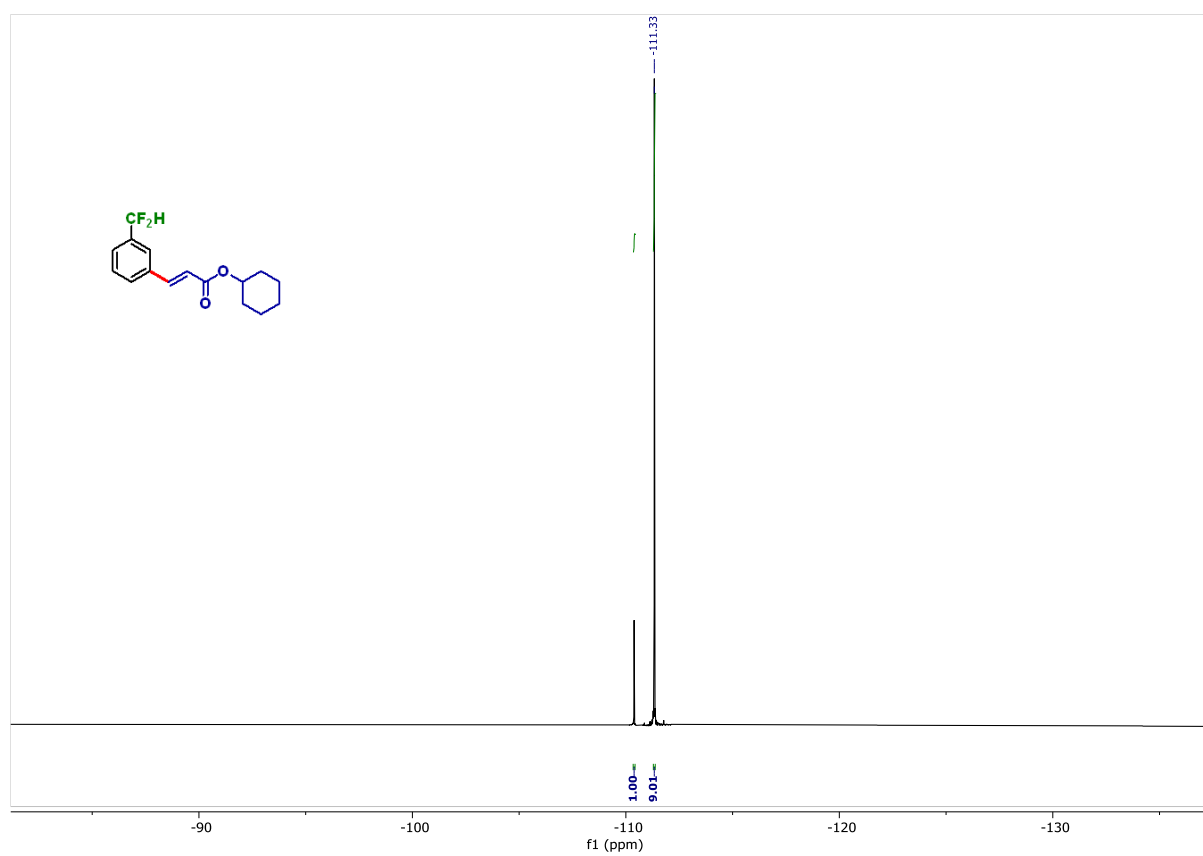
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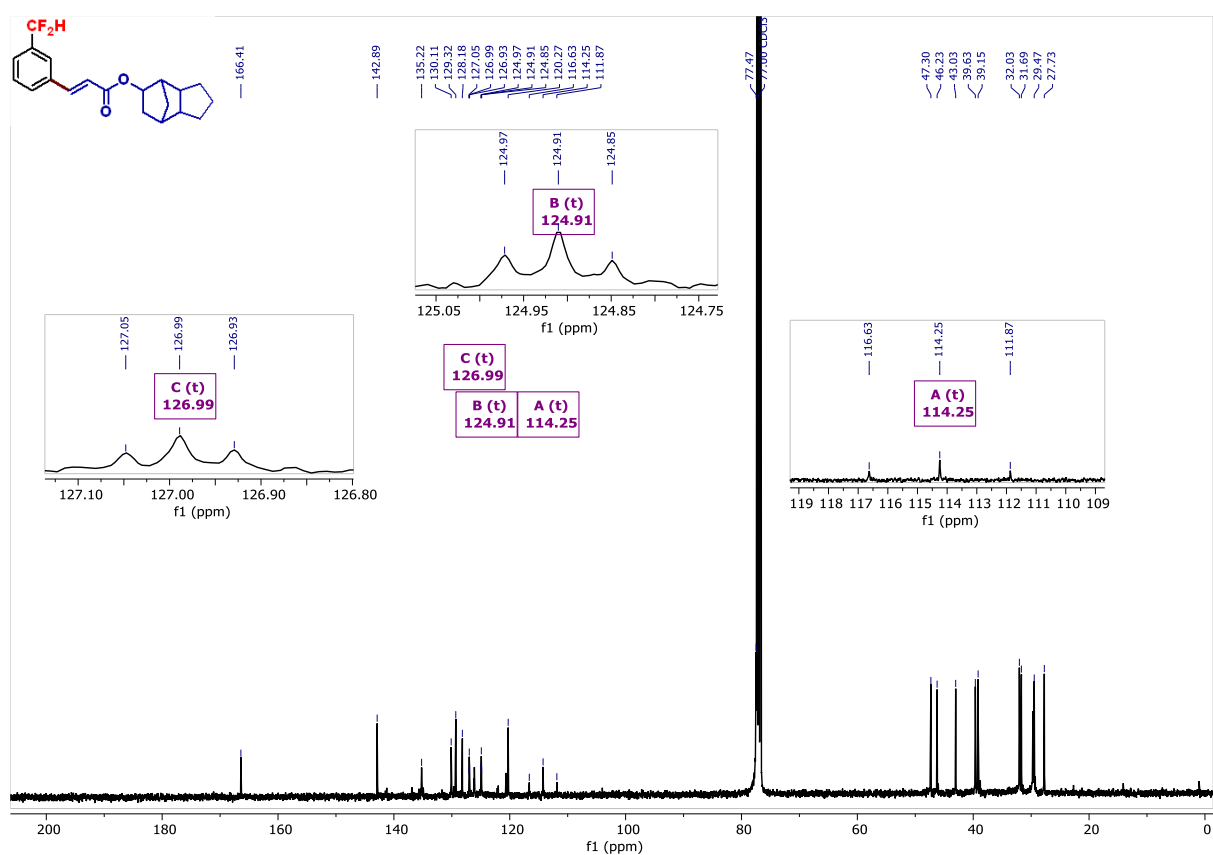
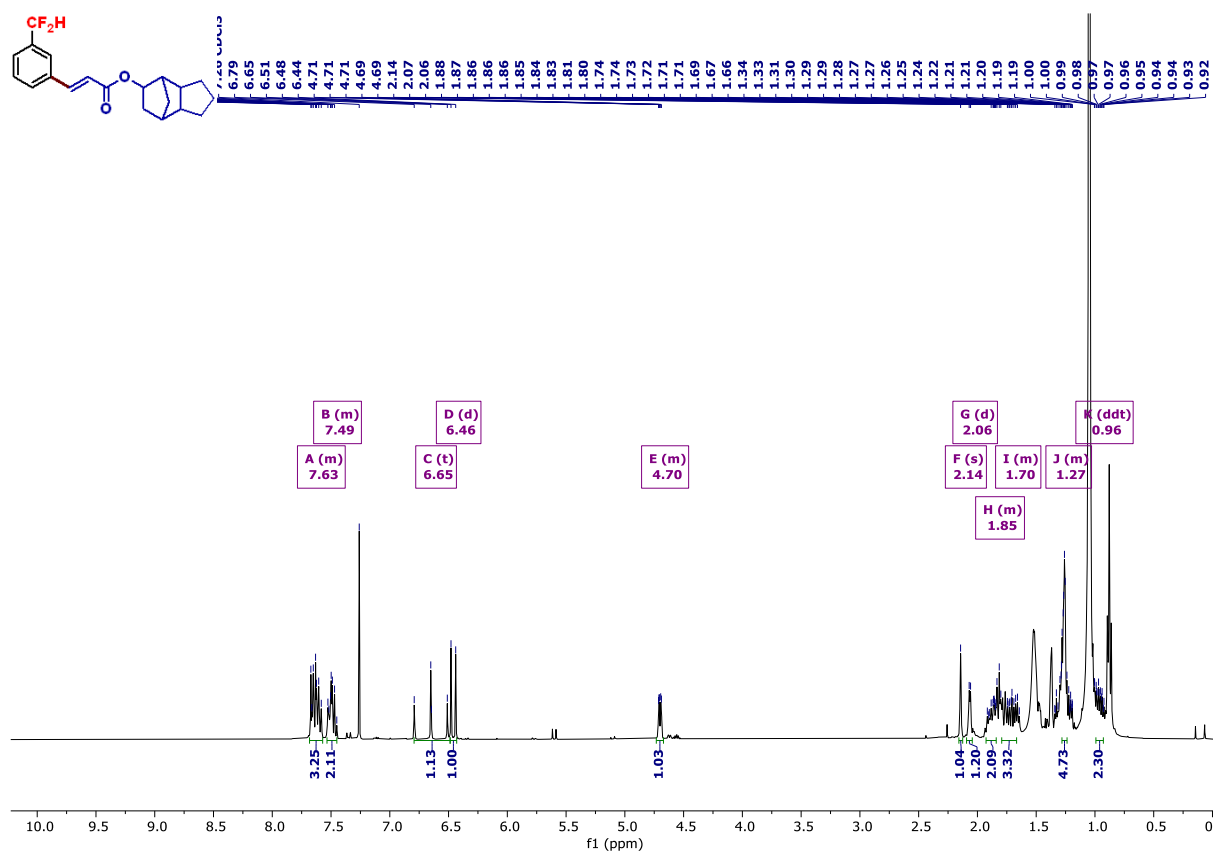
Page | 120

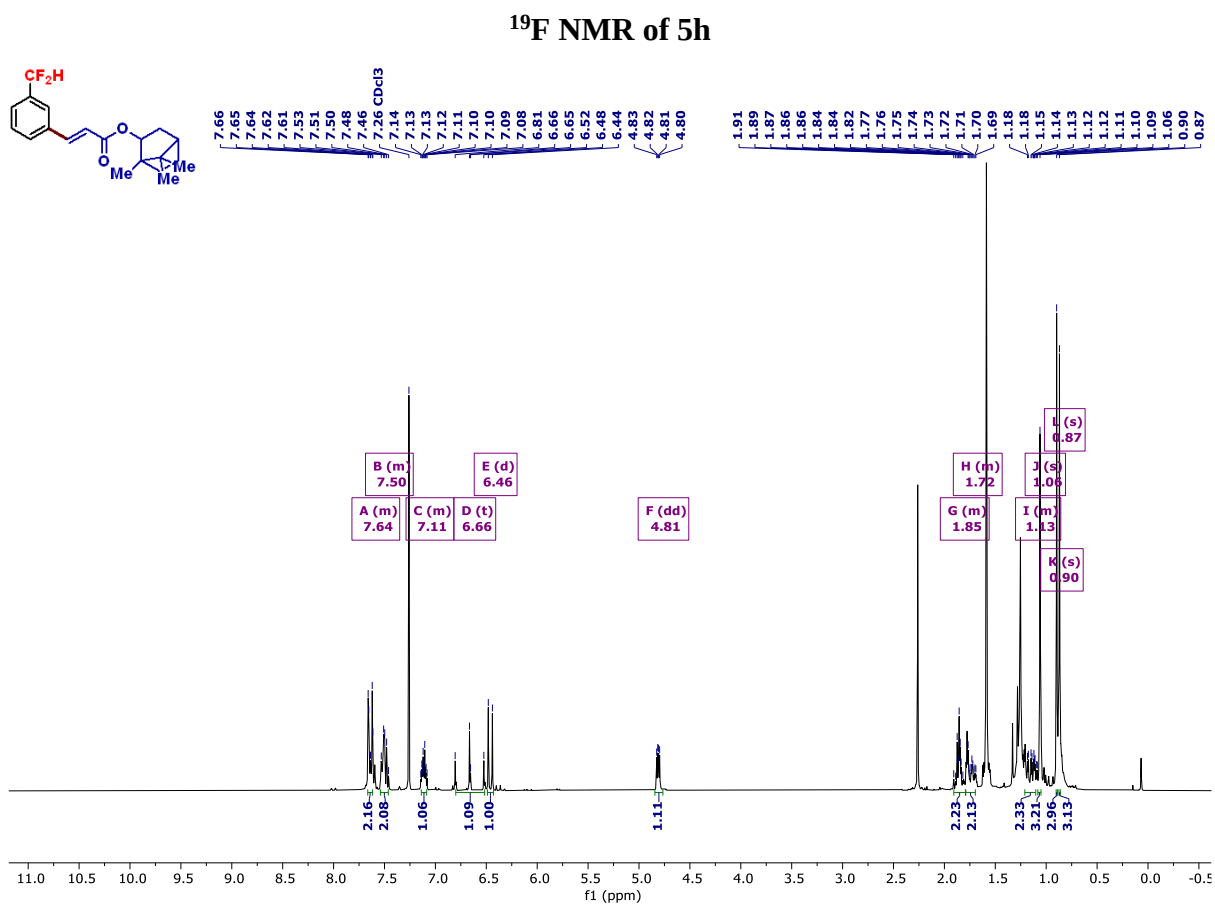
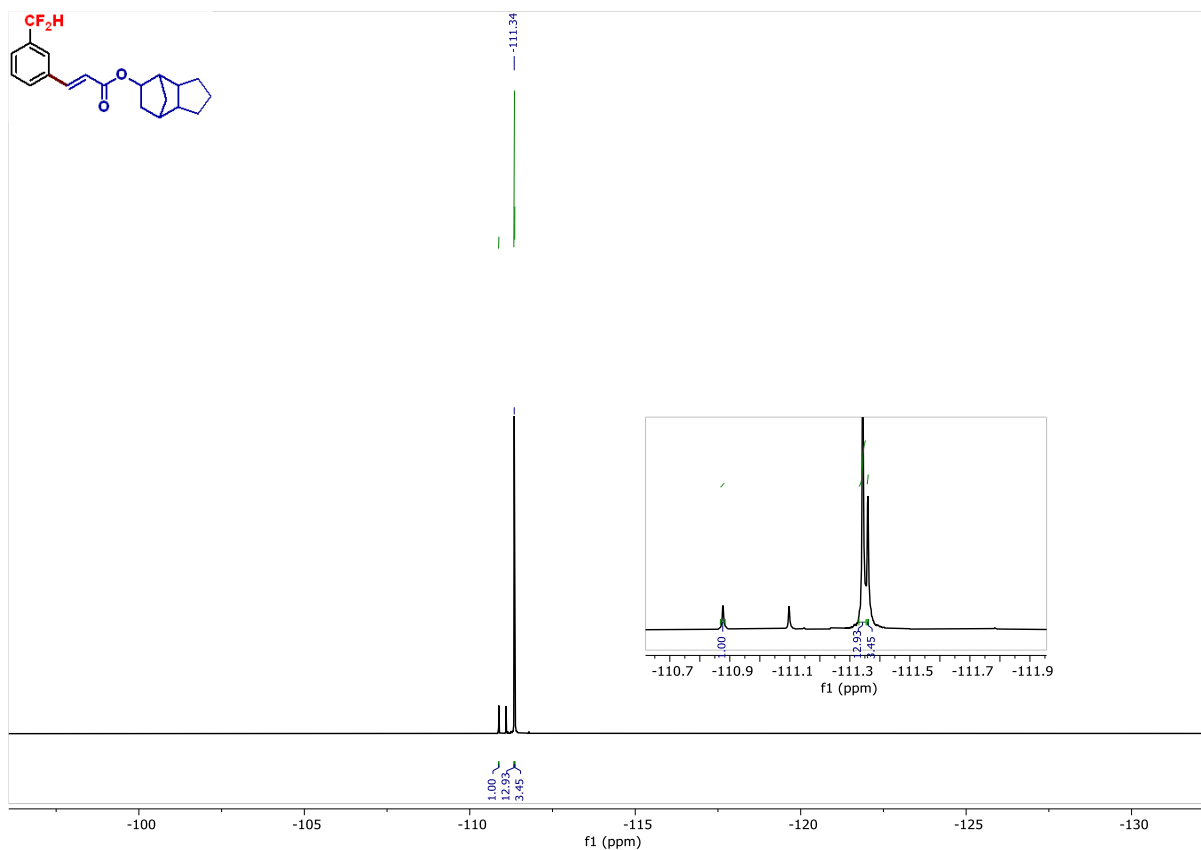


¹³C NMR of 5g

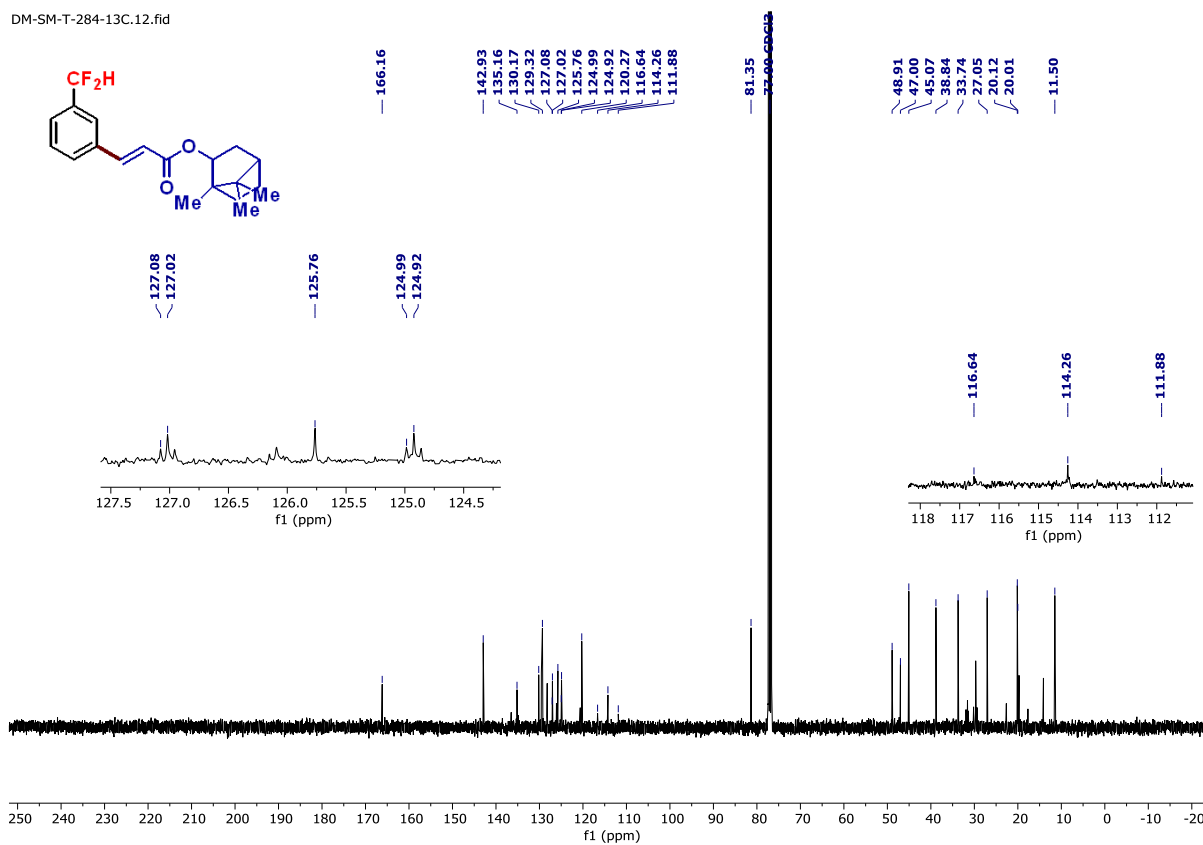


¹⁹F NMR of 5g

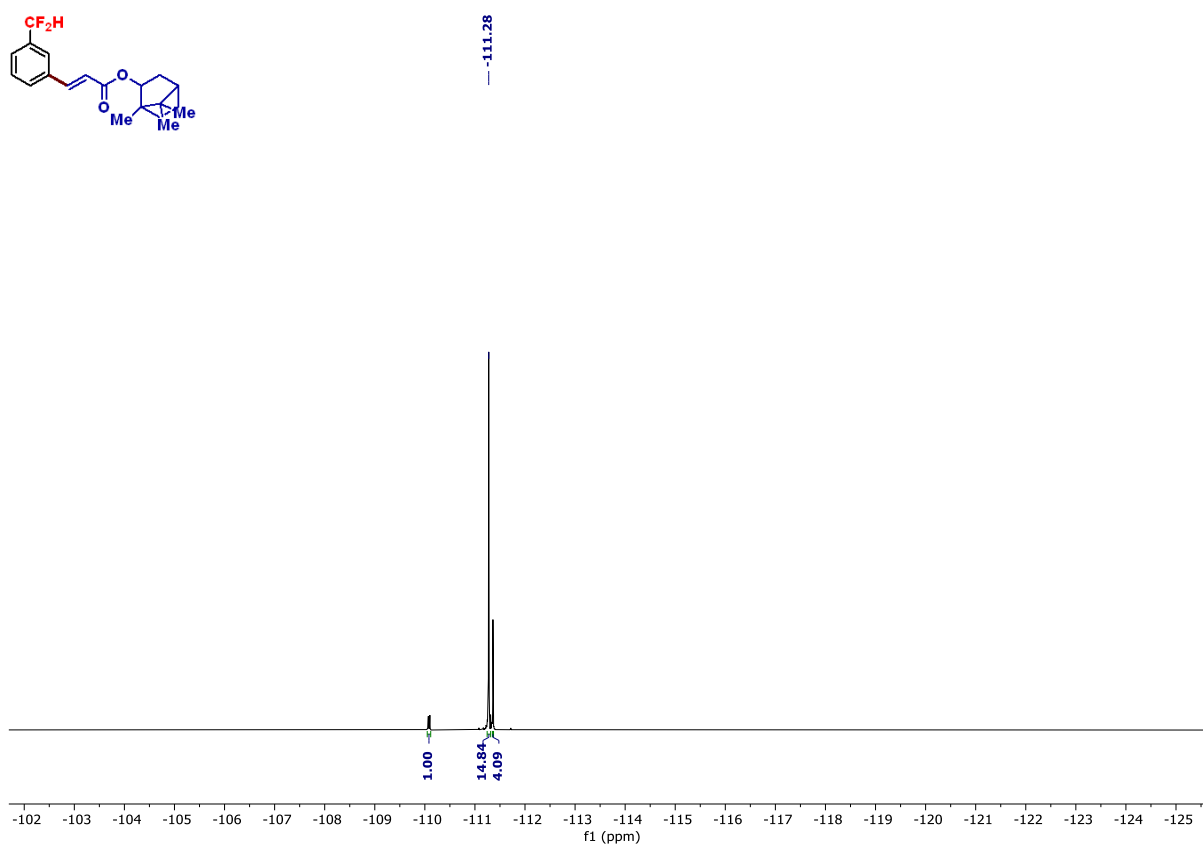




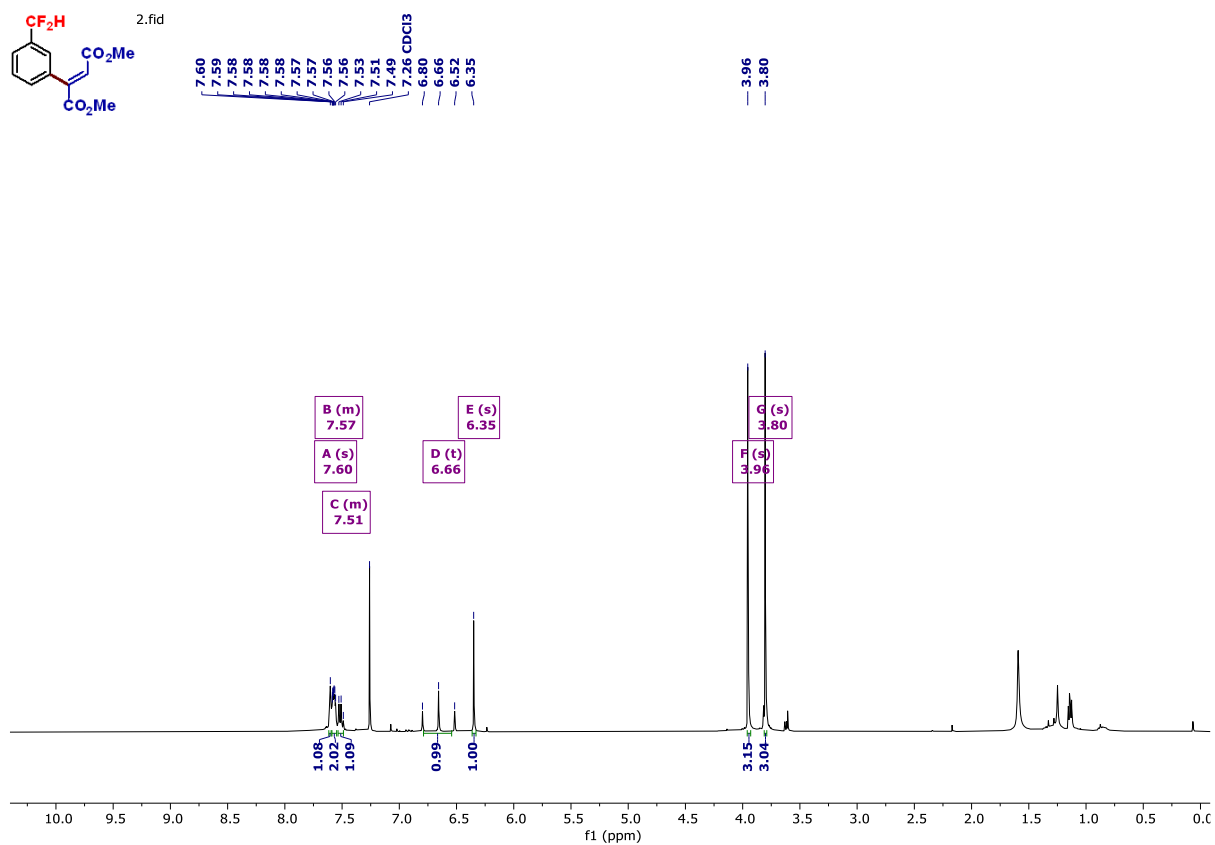
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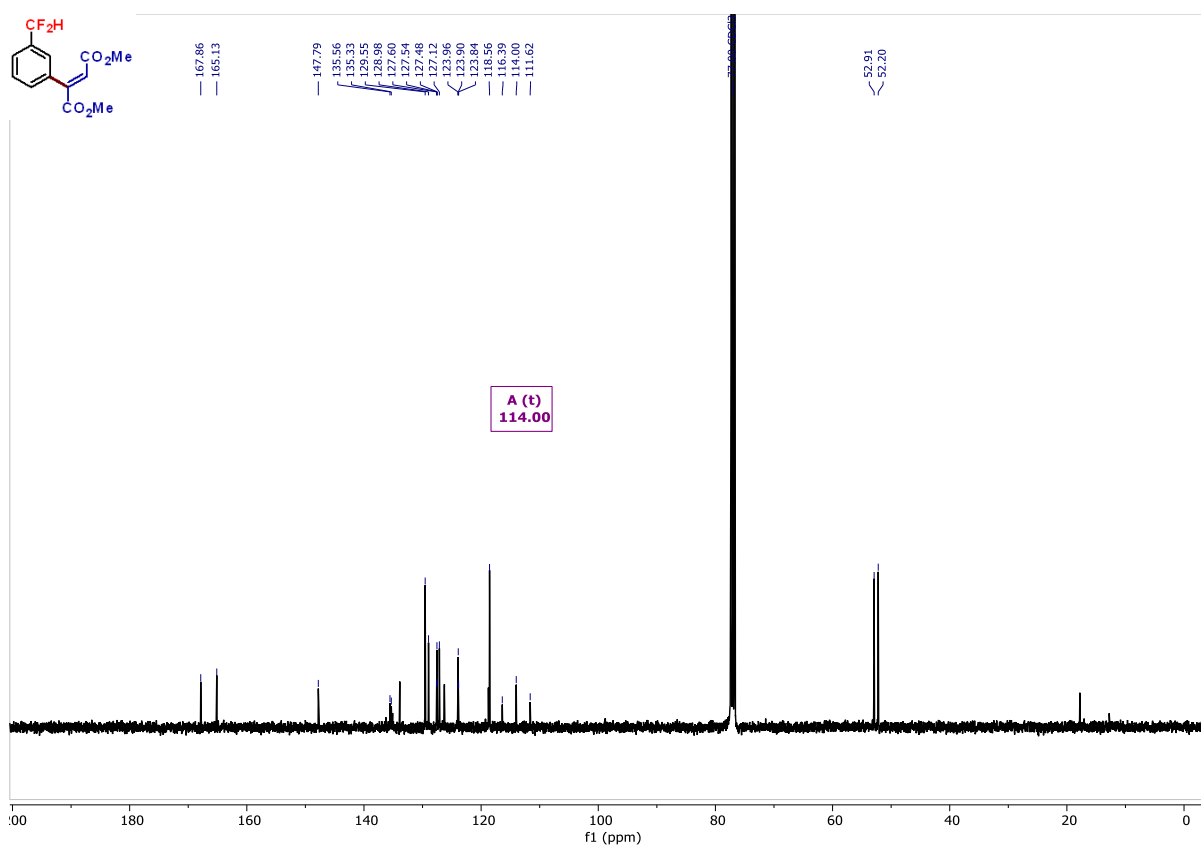
¹³C NMR of 5i



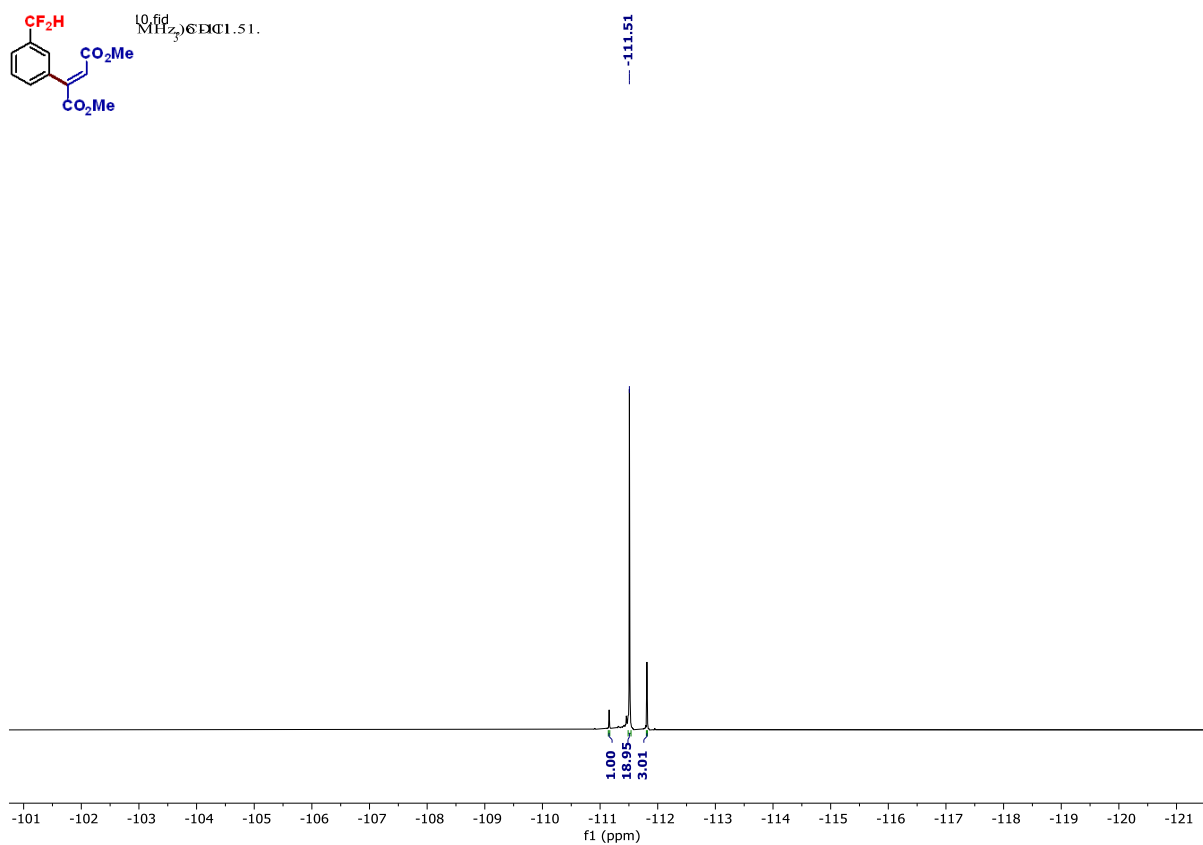
¹⁹F NMR of 5i



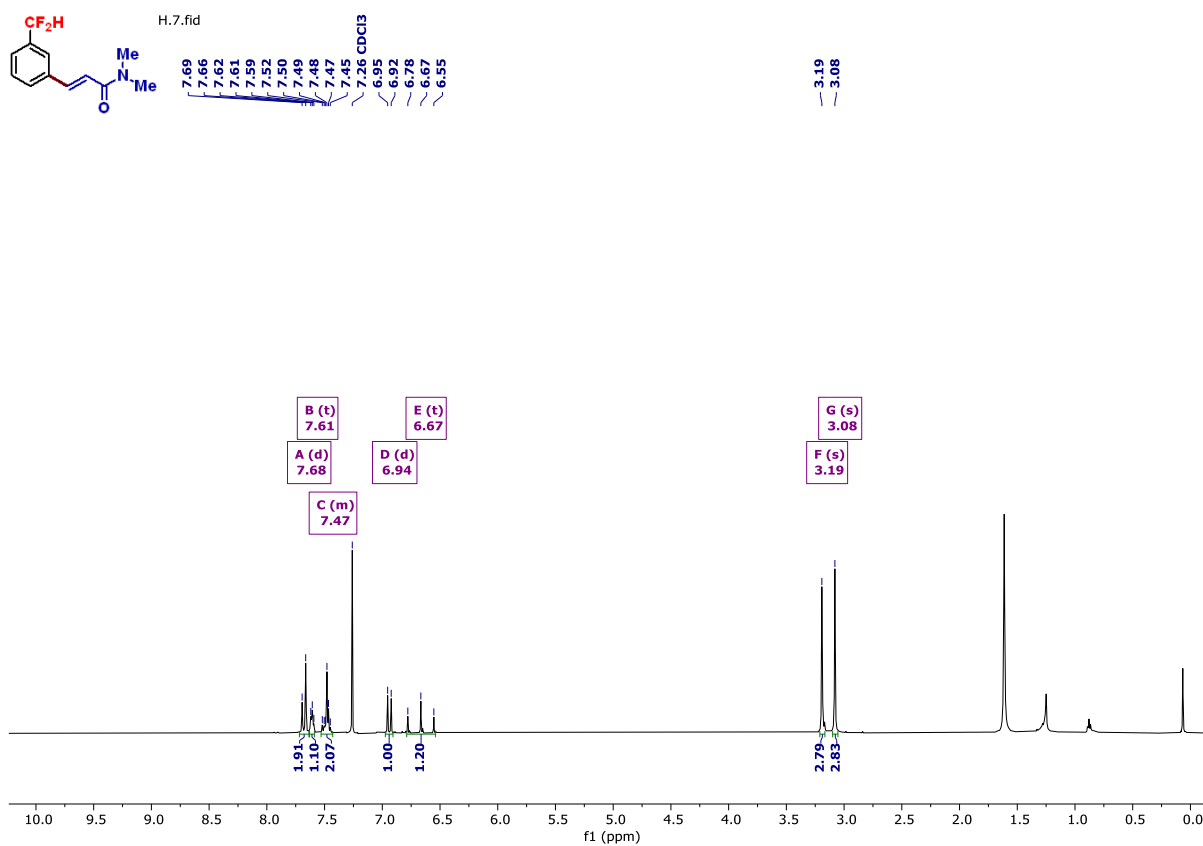
¹H NMR of 5j



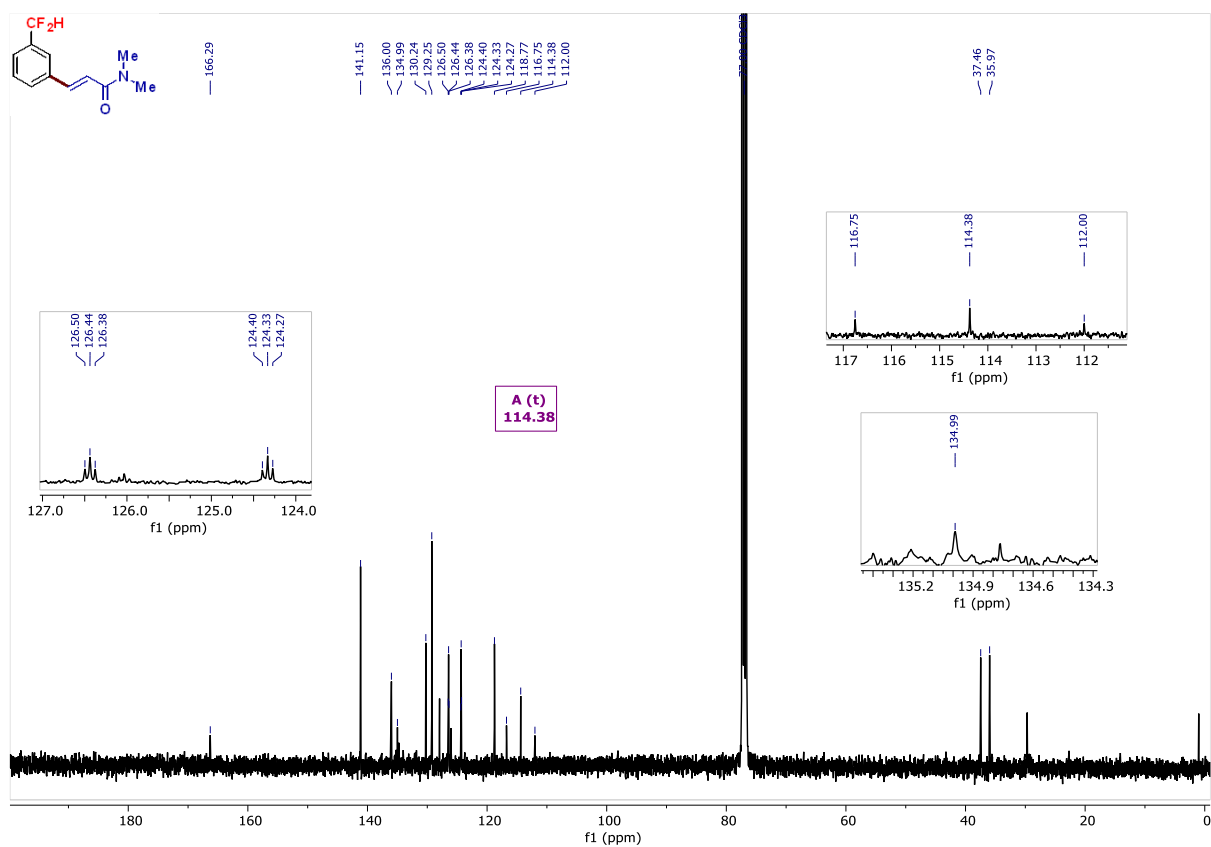
¹³C NMR of 5j



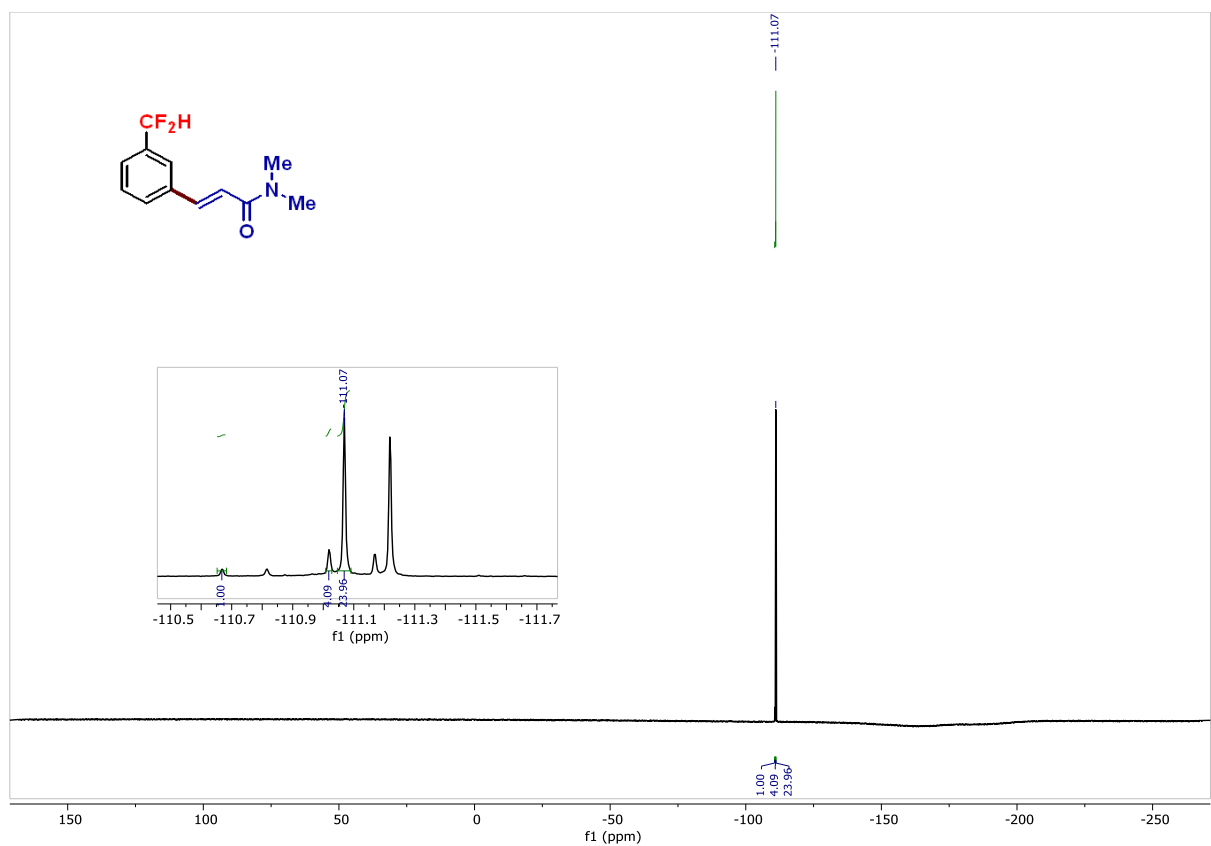
^{19}F NMR of 5j



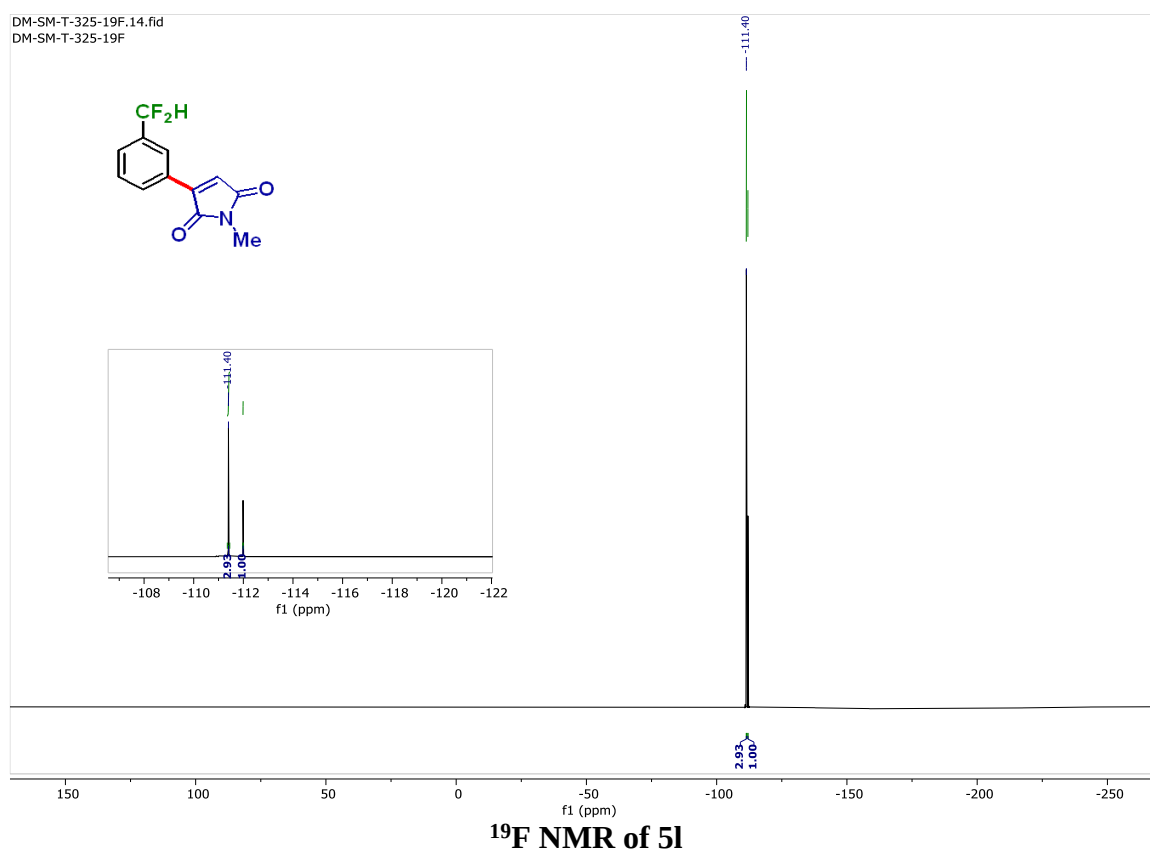
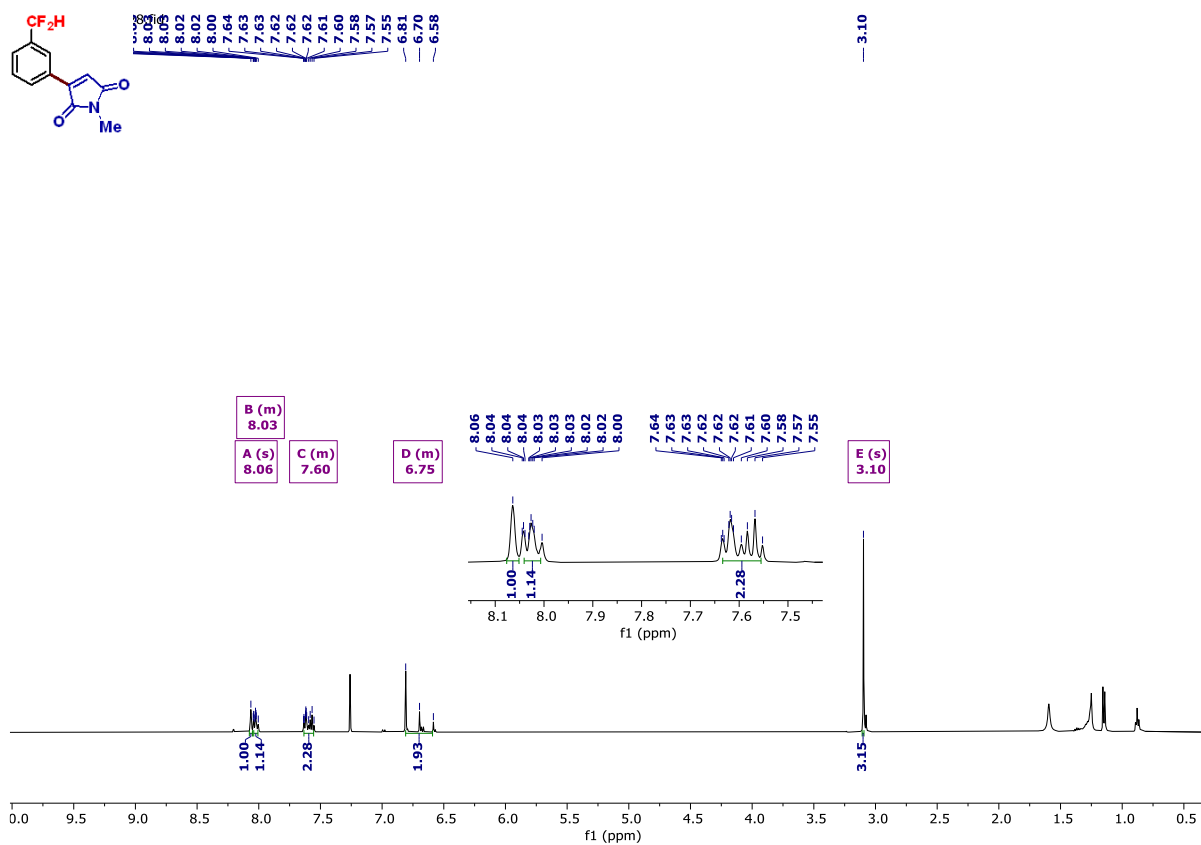
^1H NMR of 5k

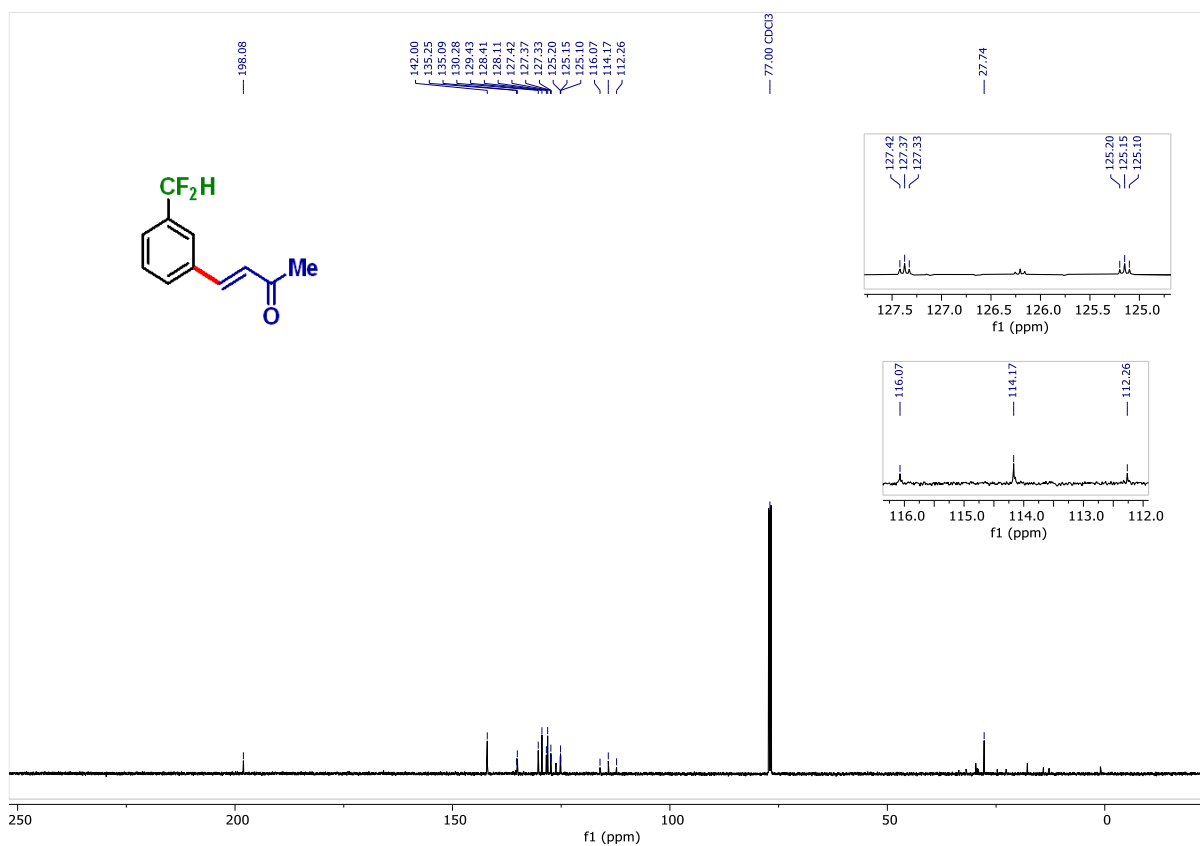
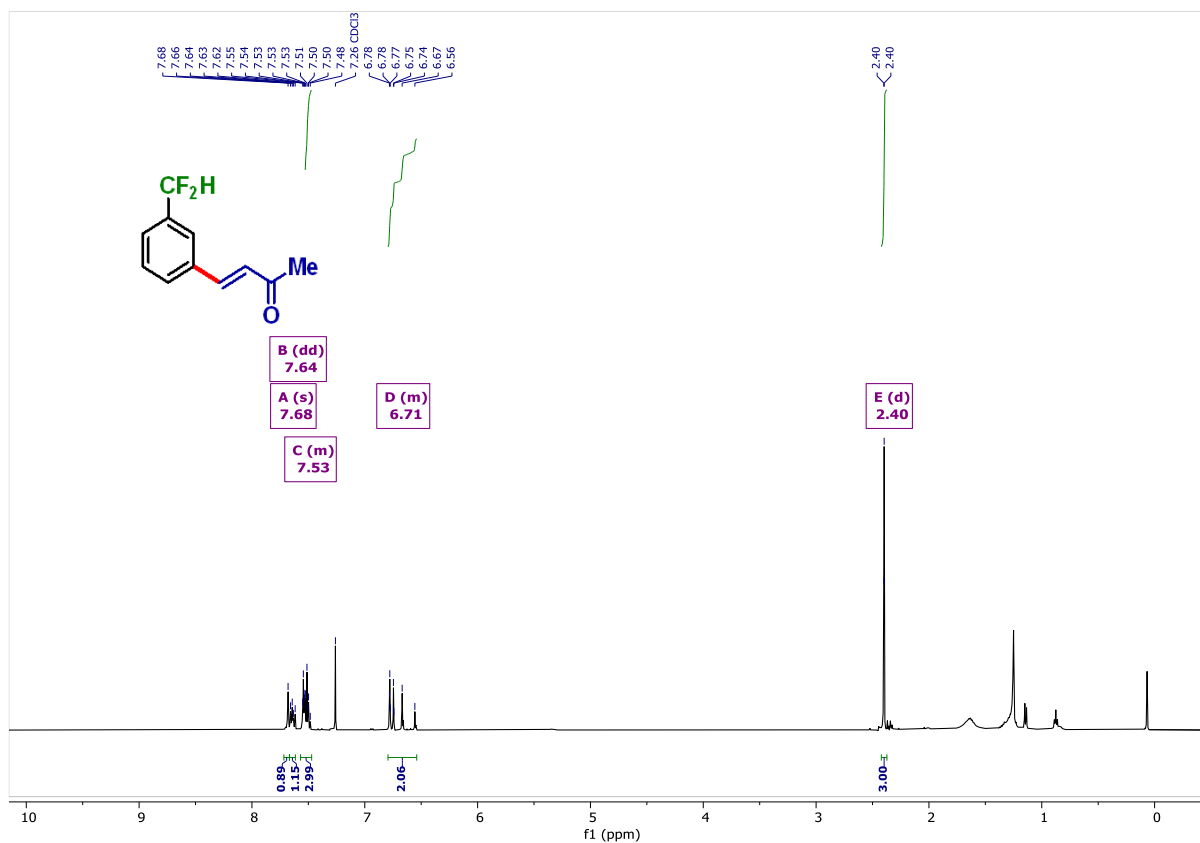


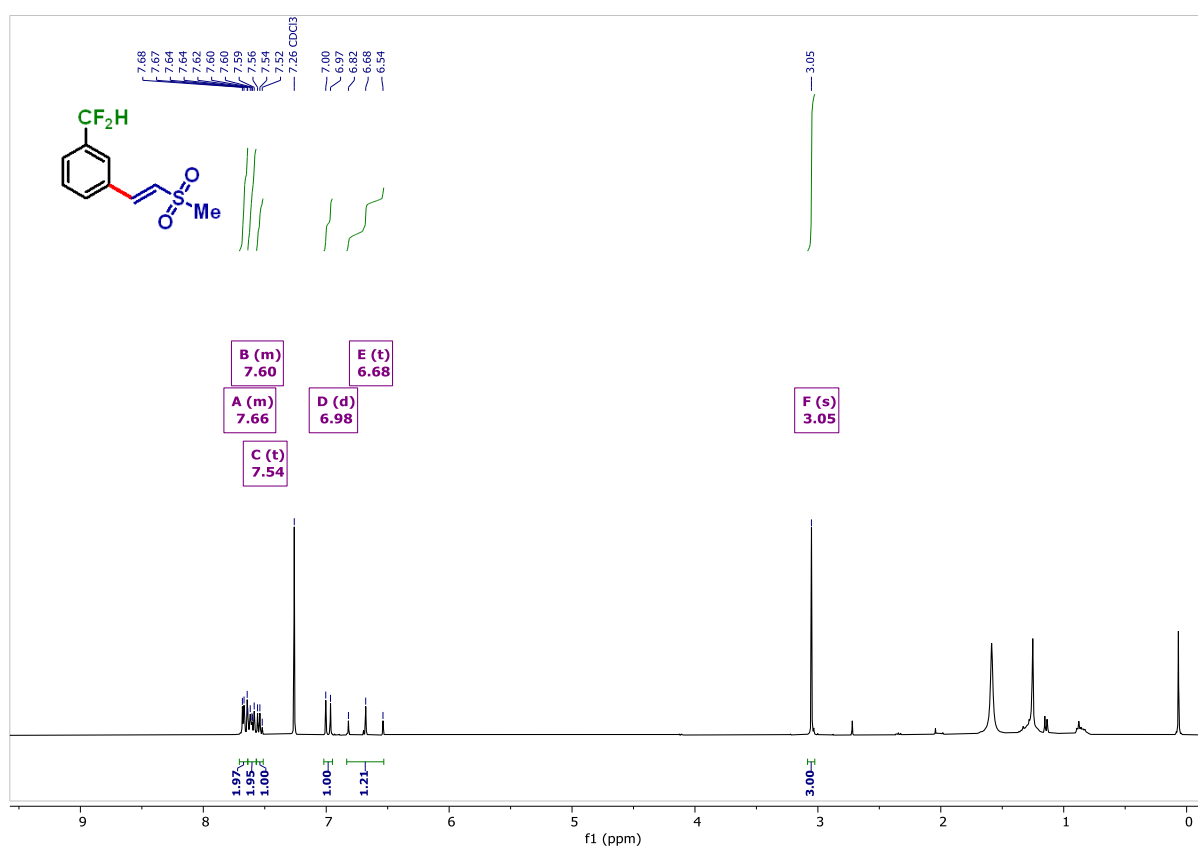
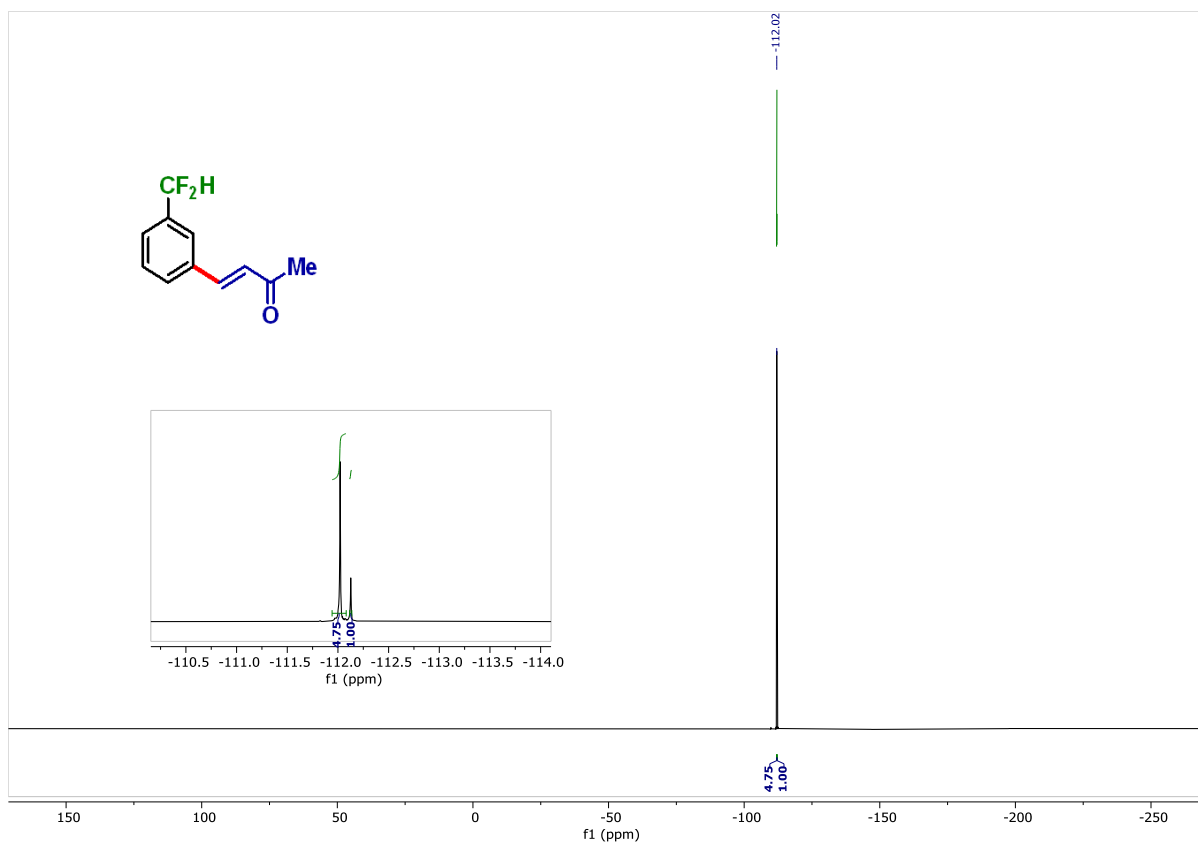
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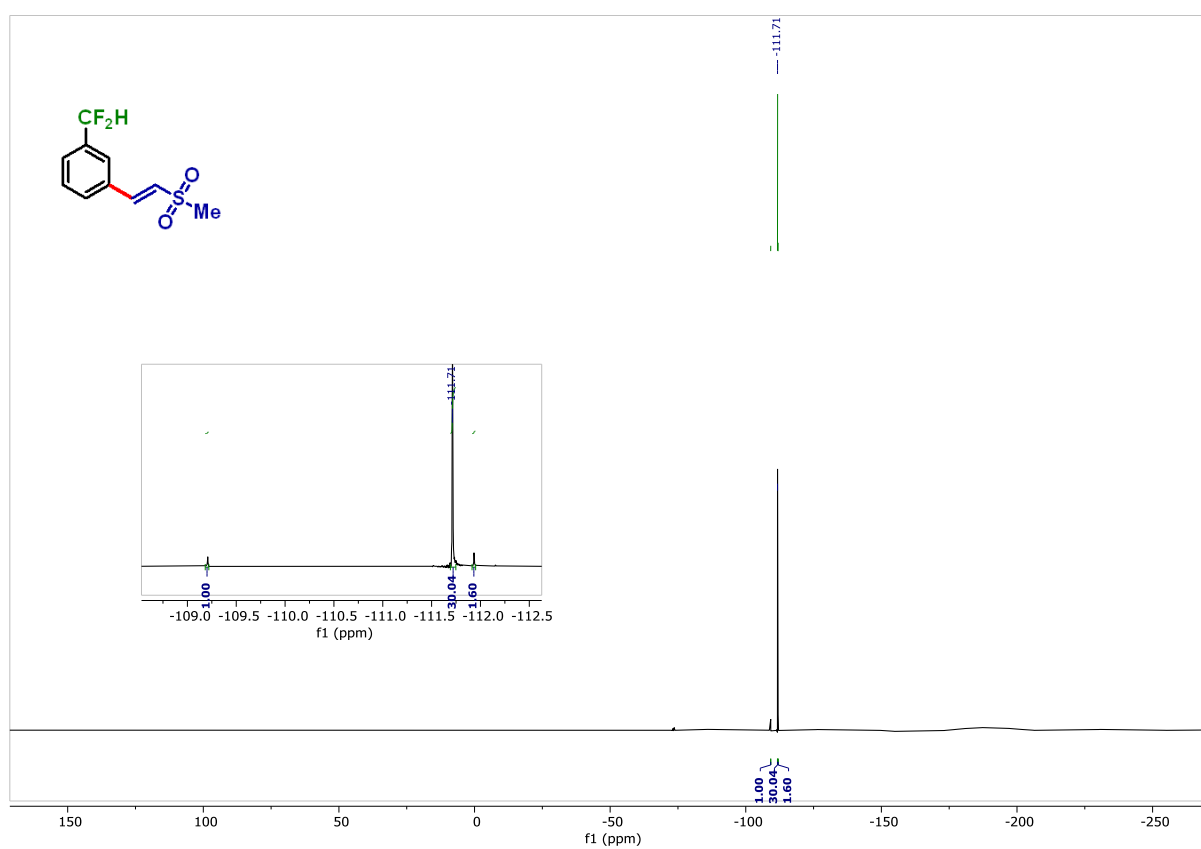
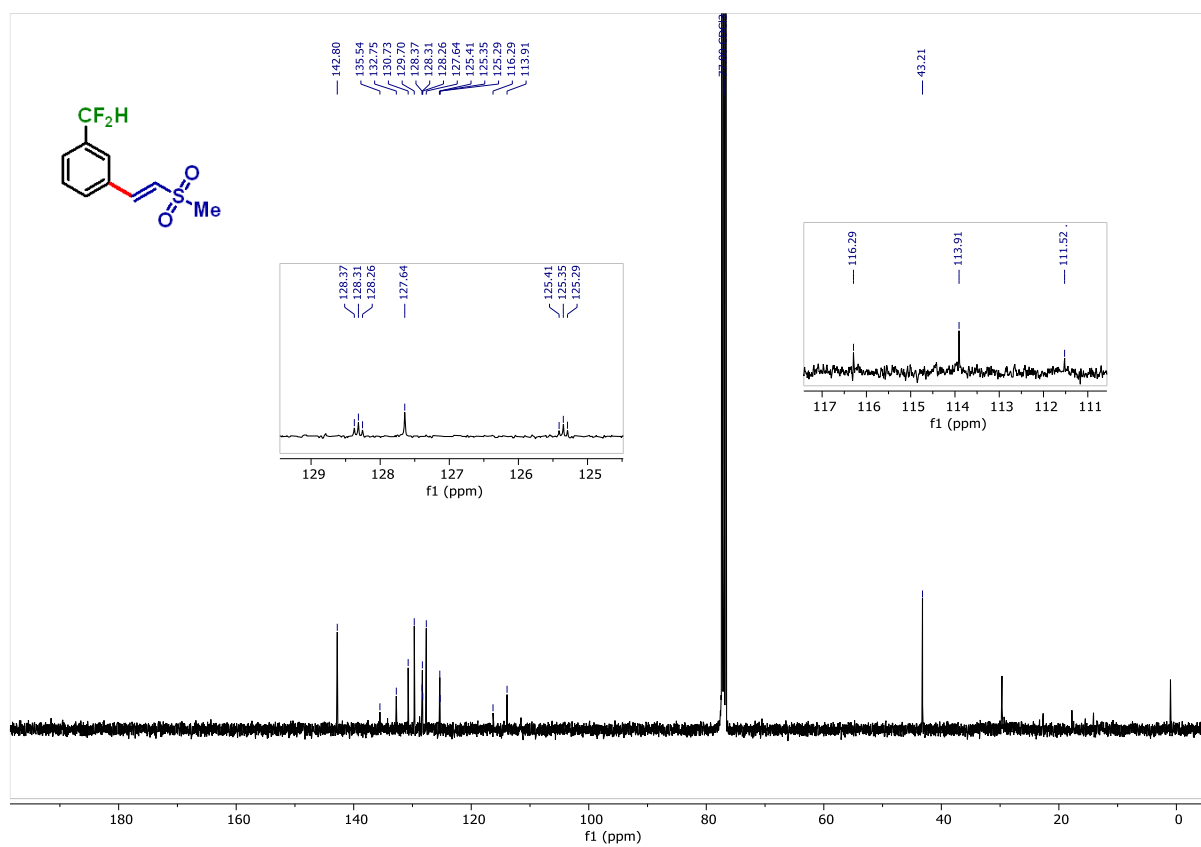


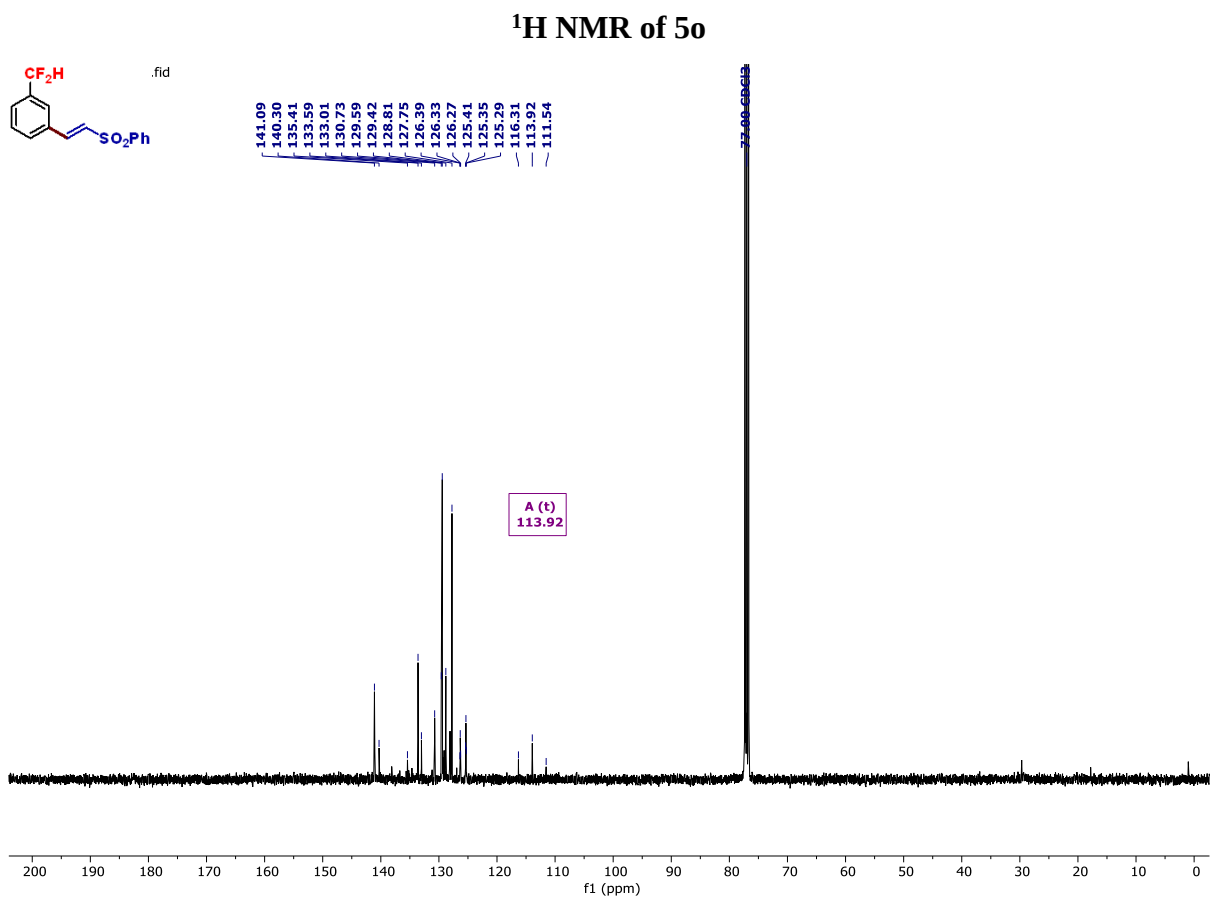
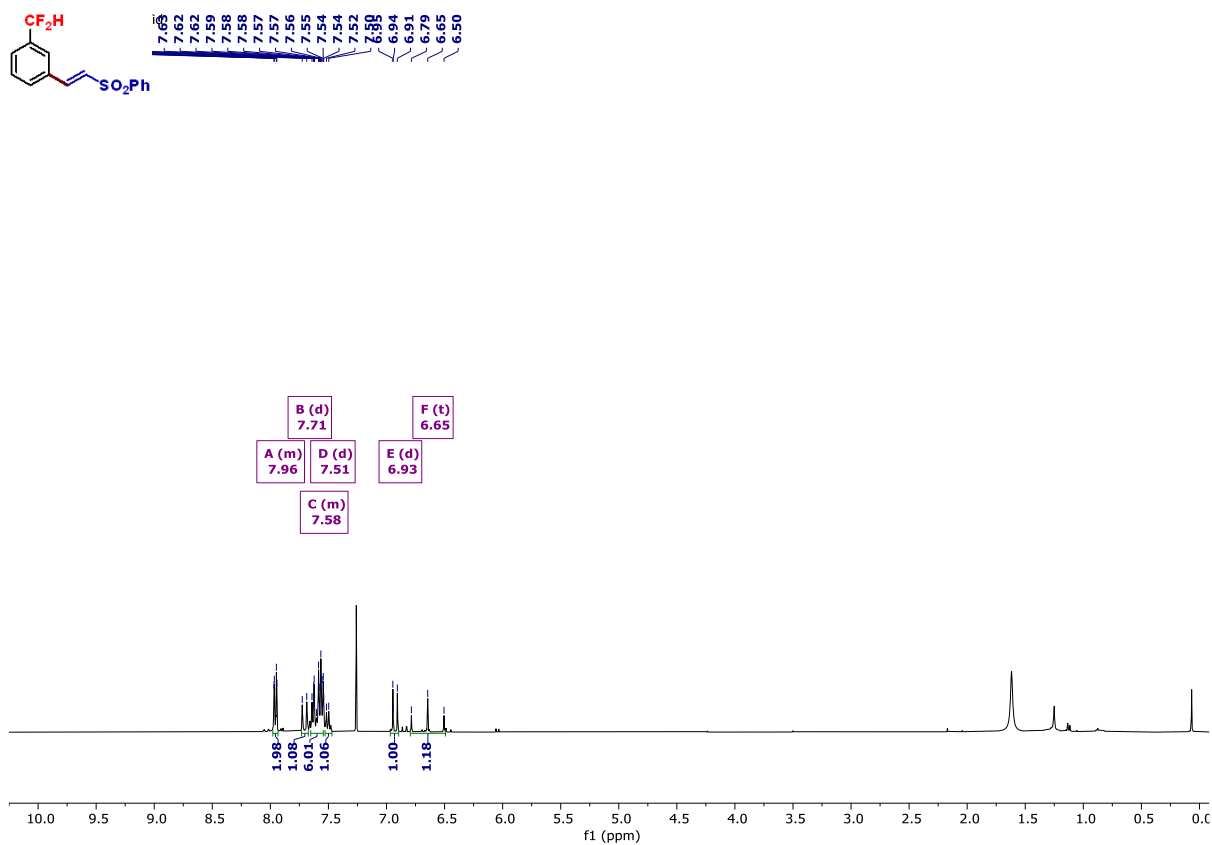
¹⁹F NMR of 5k

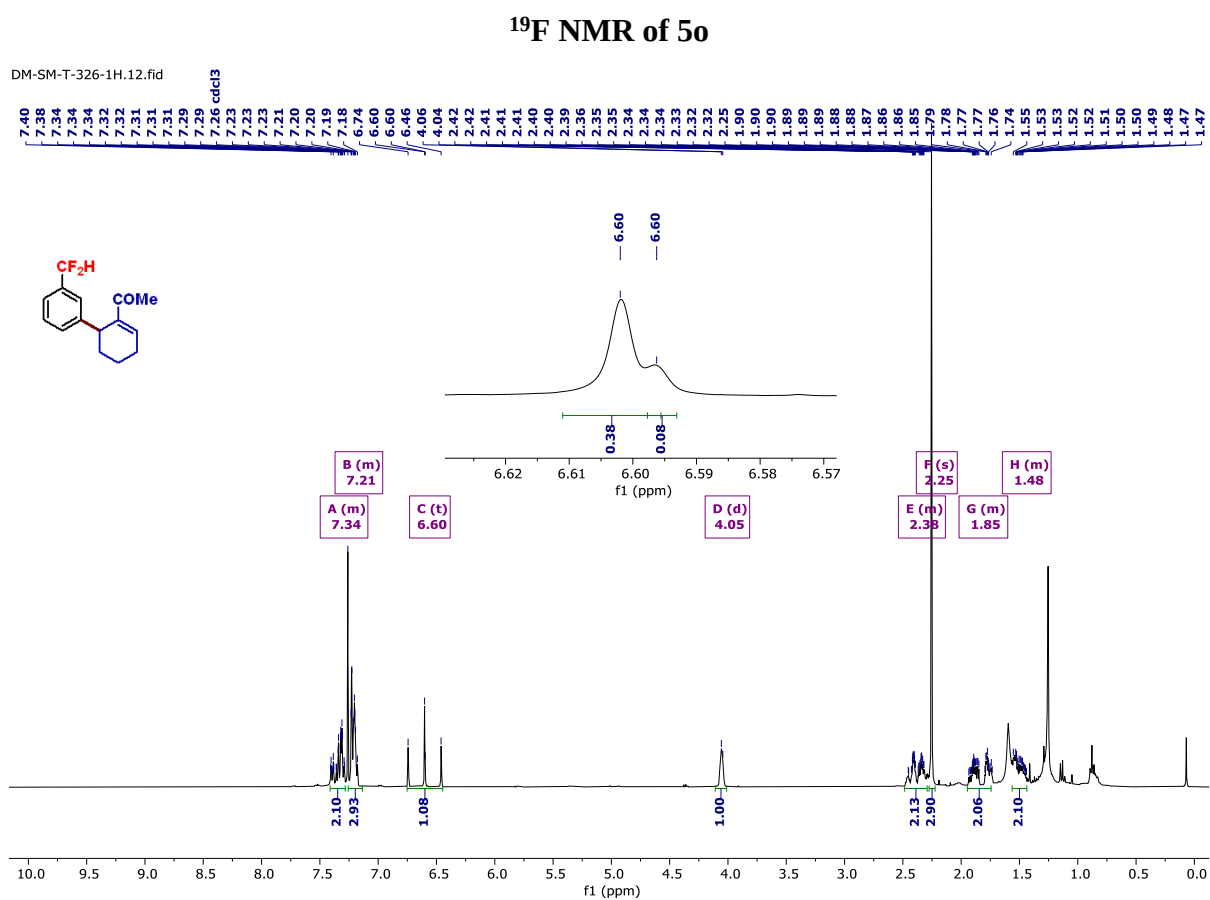
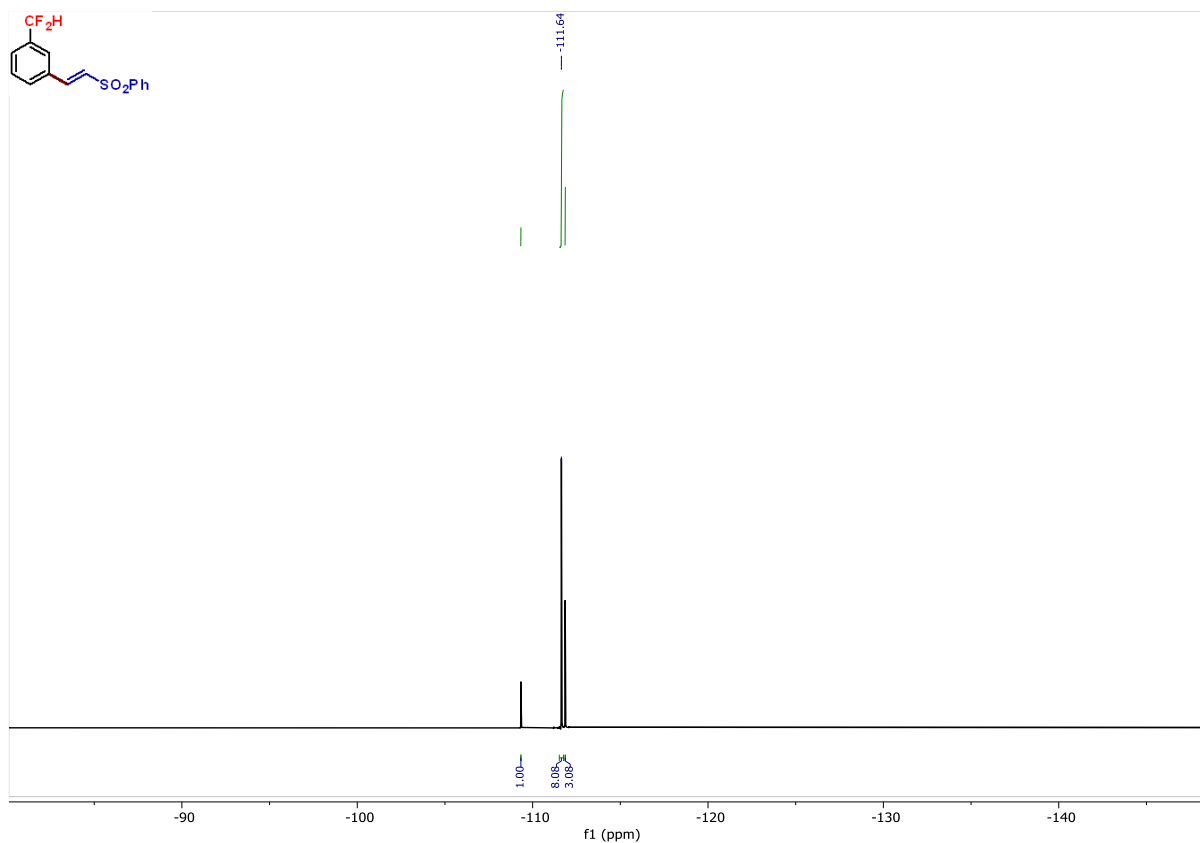


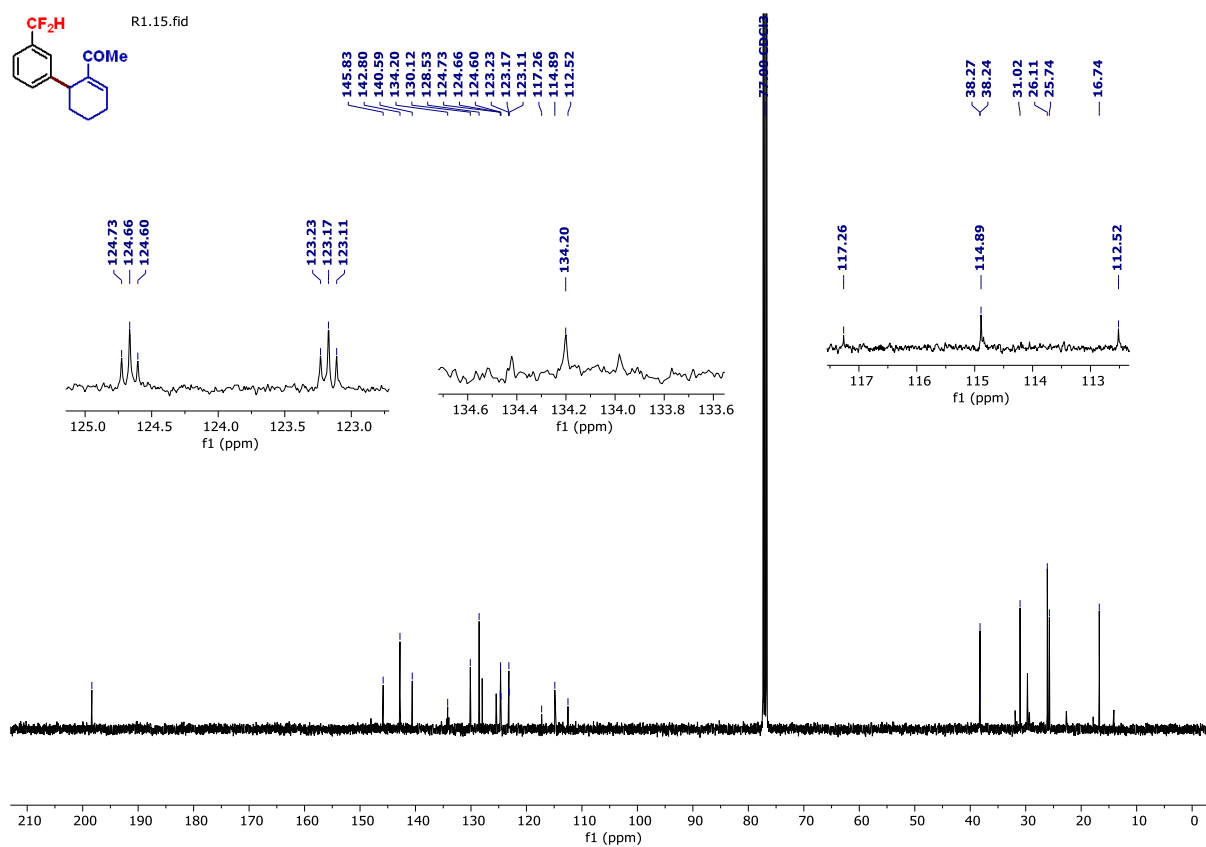




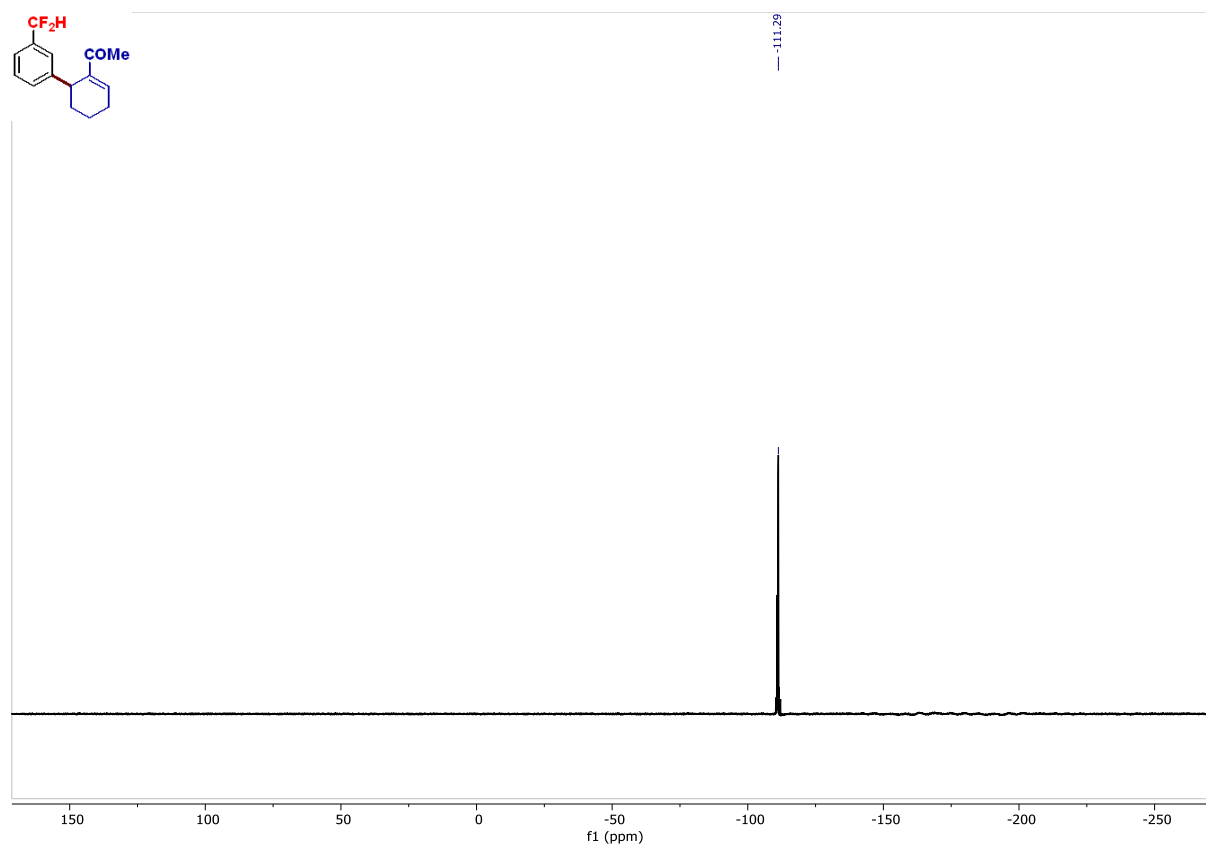




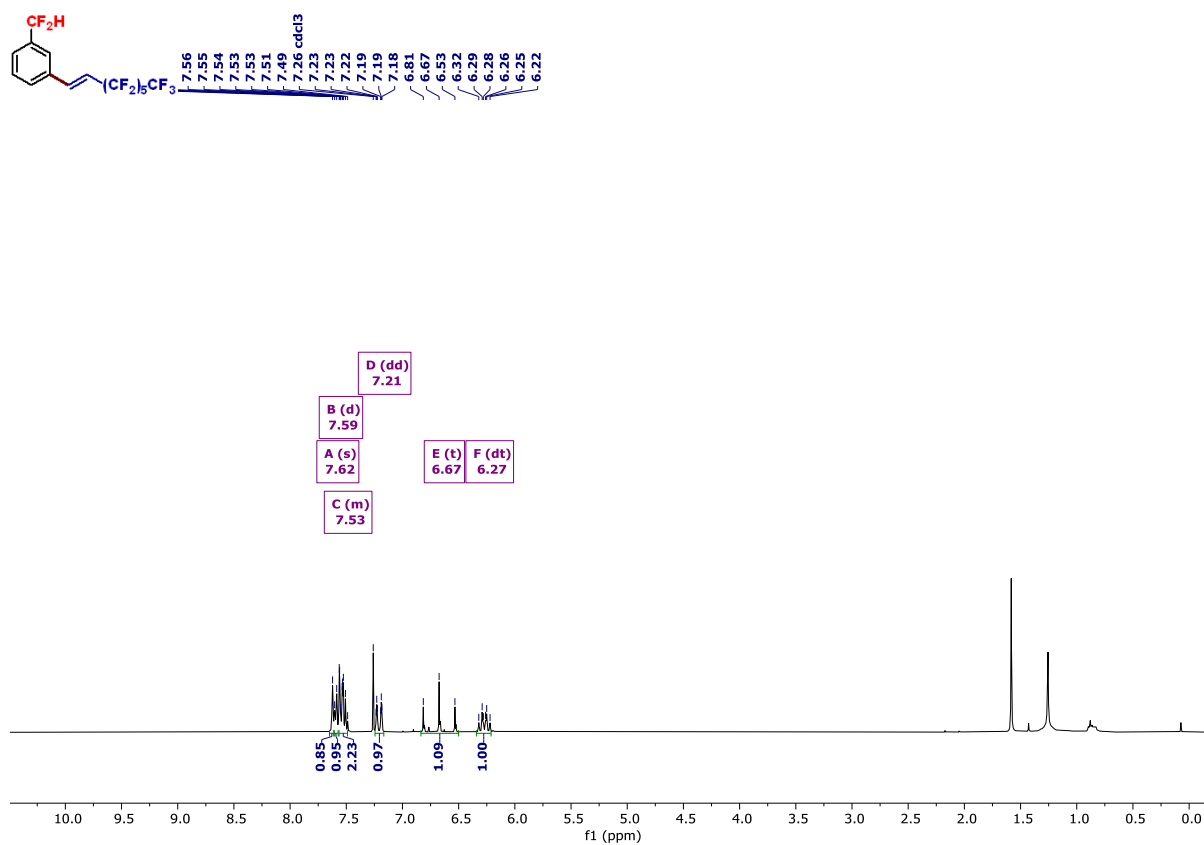




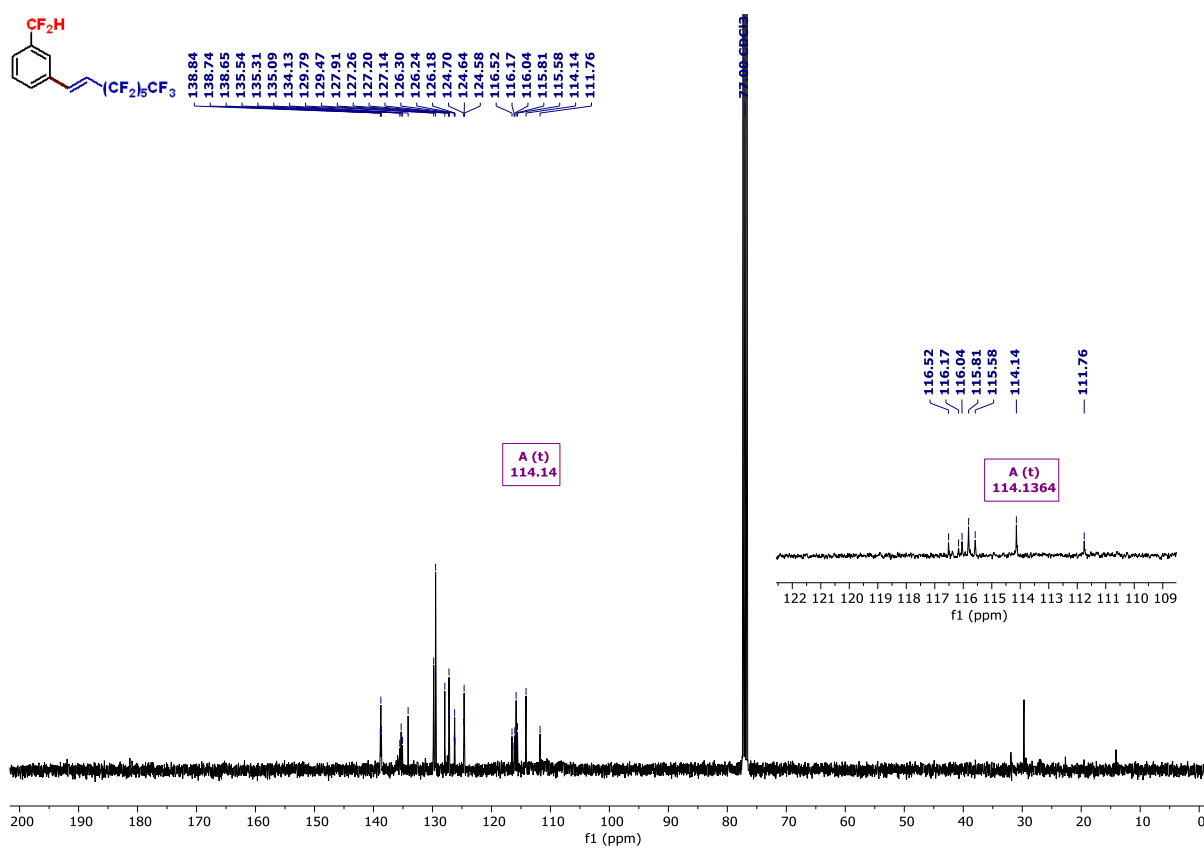
¹³C NMR of 5p



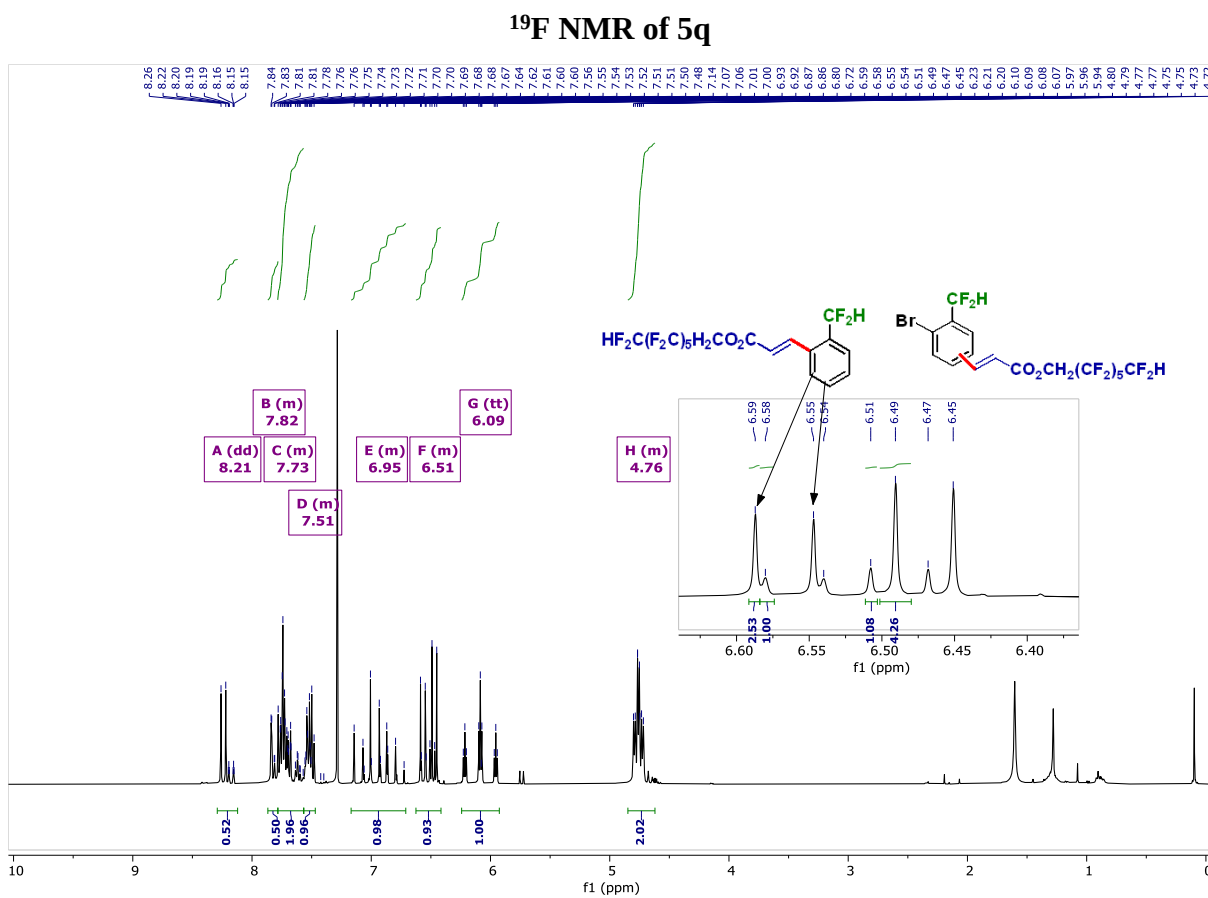
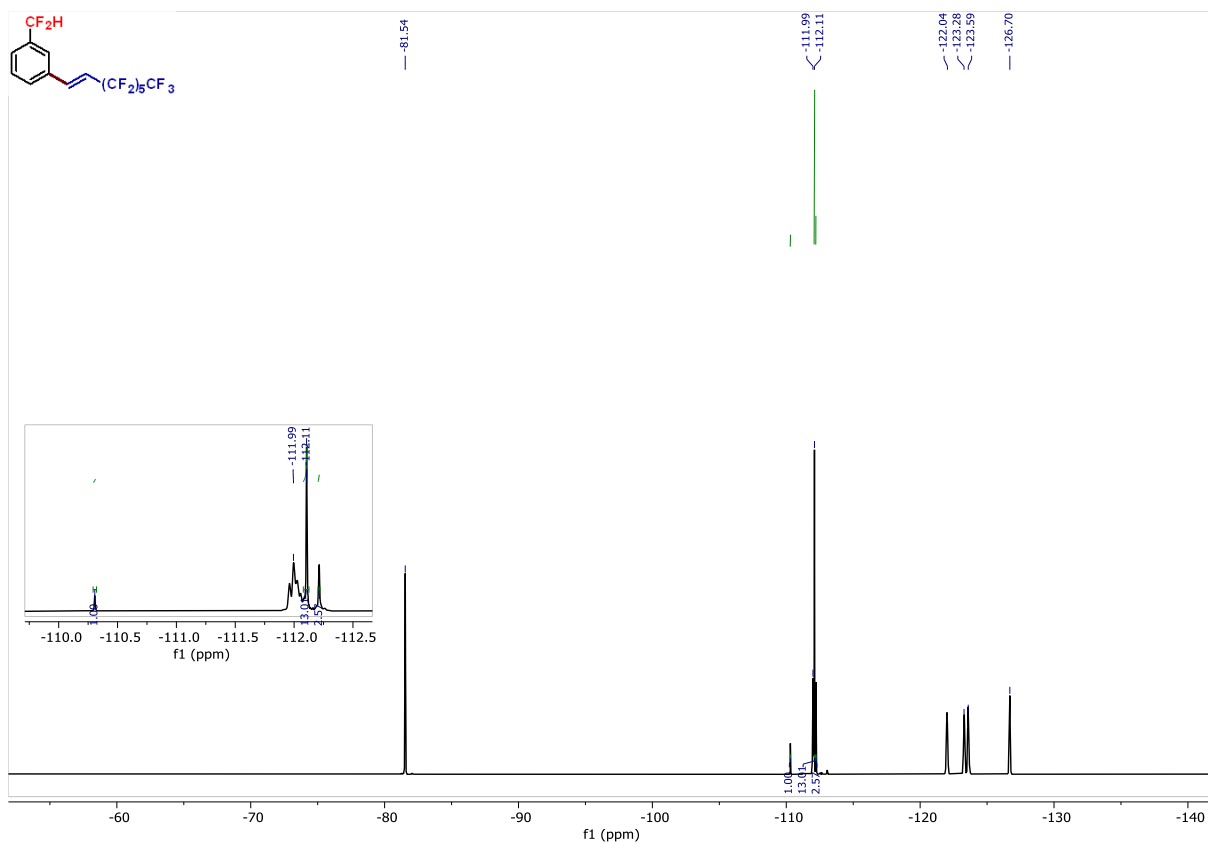
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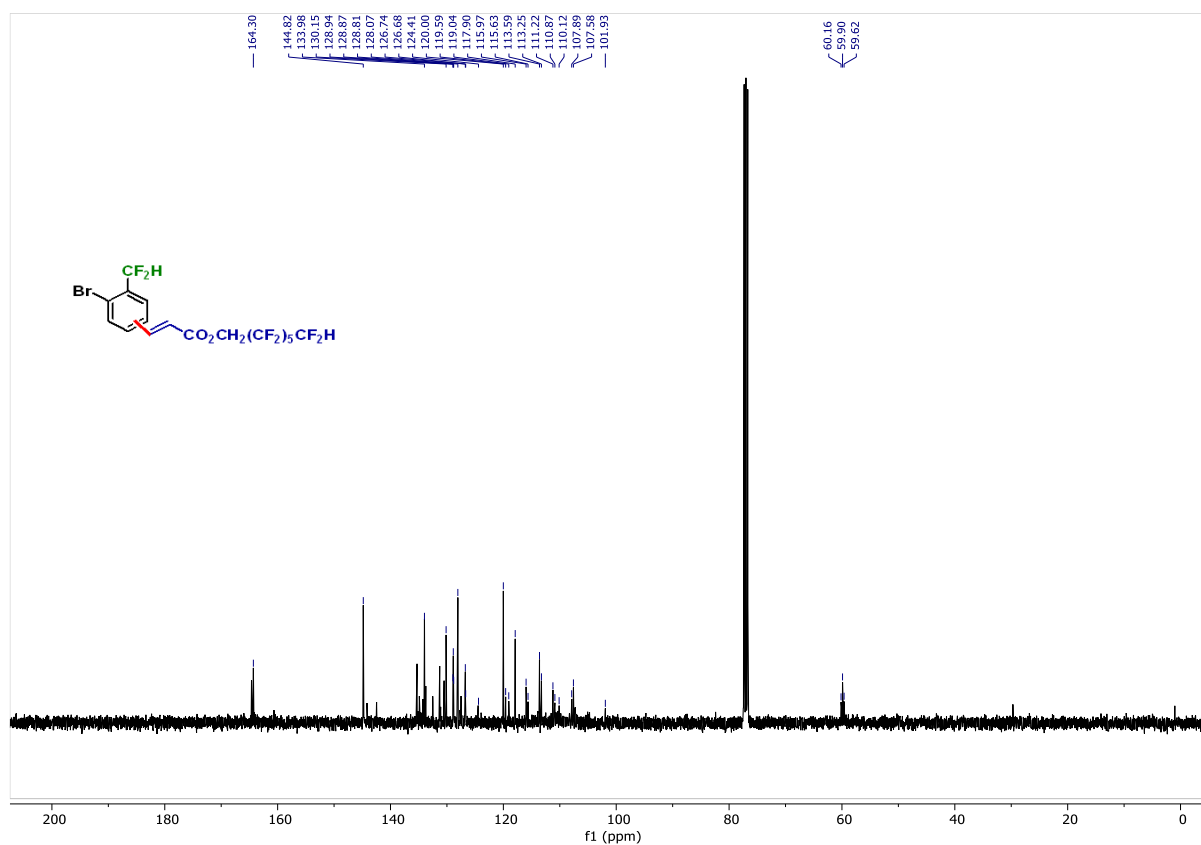


¹H NMR of 5q

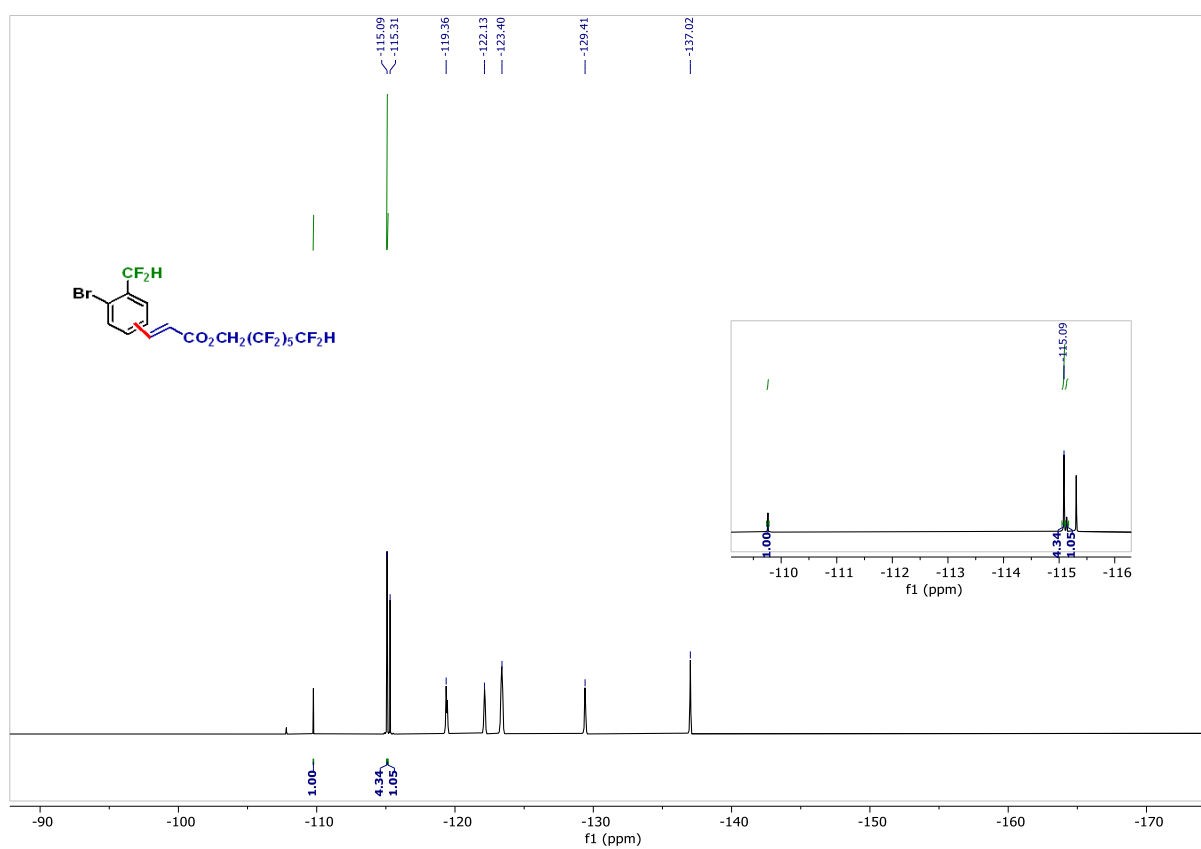


¹³C NMR of 5q

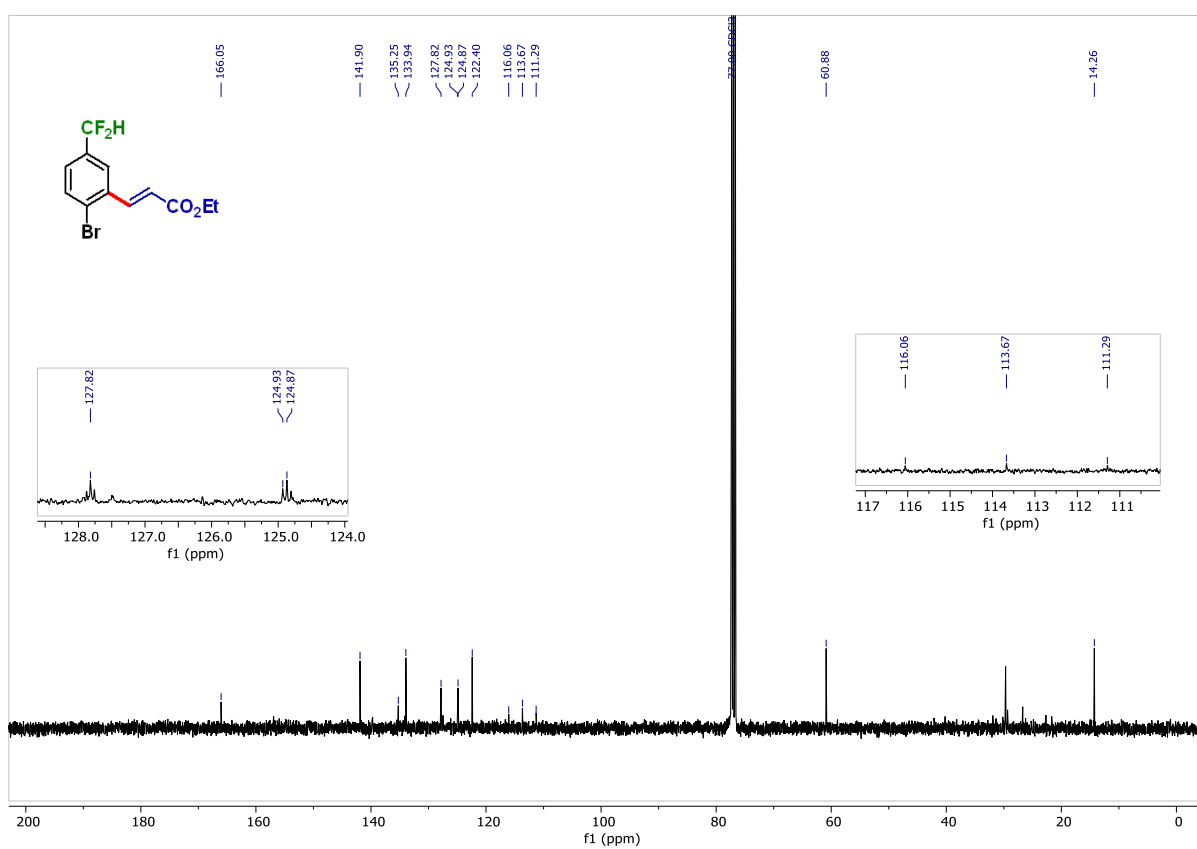
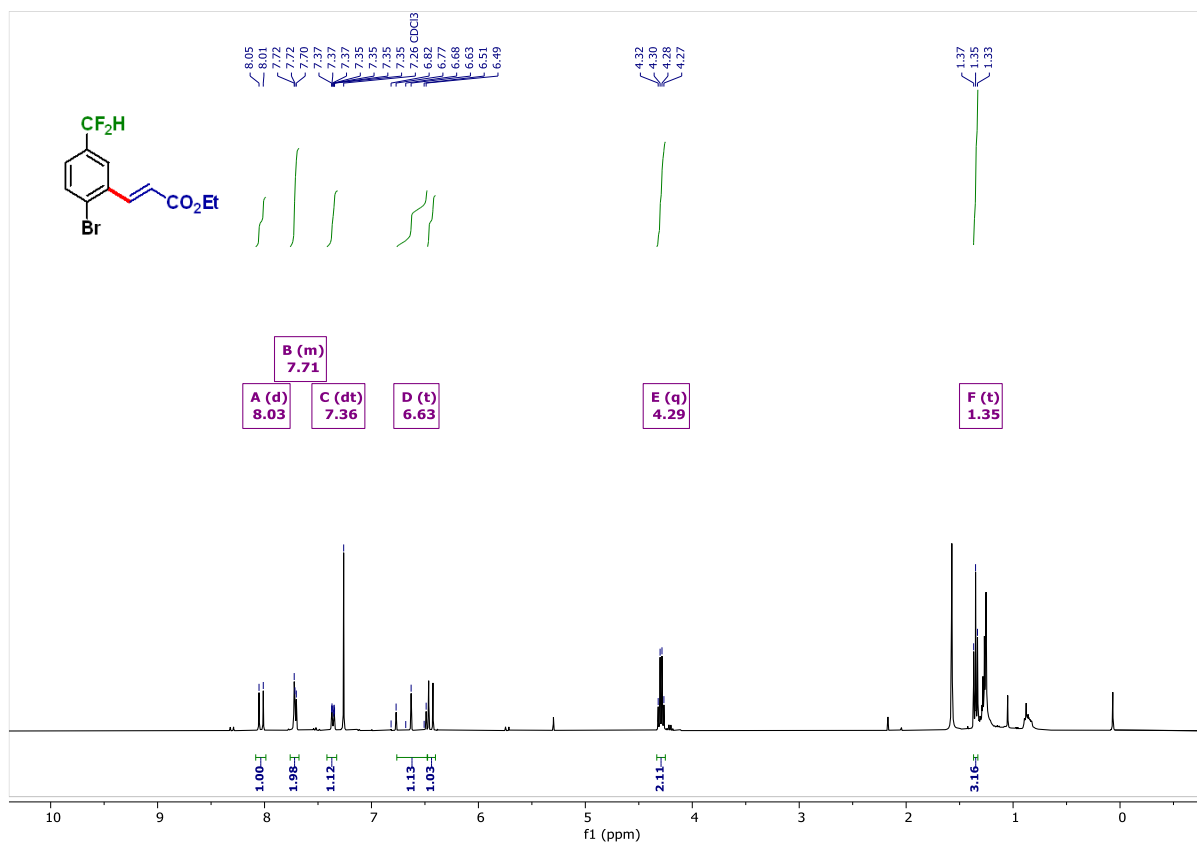


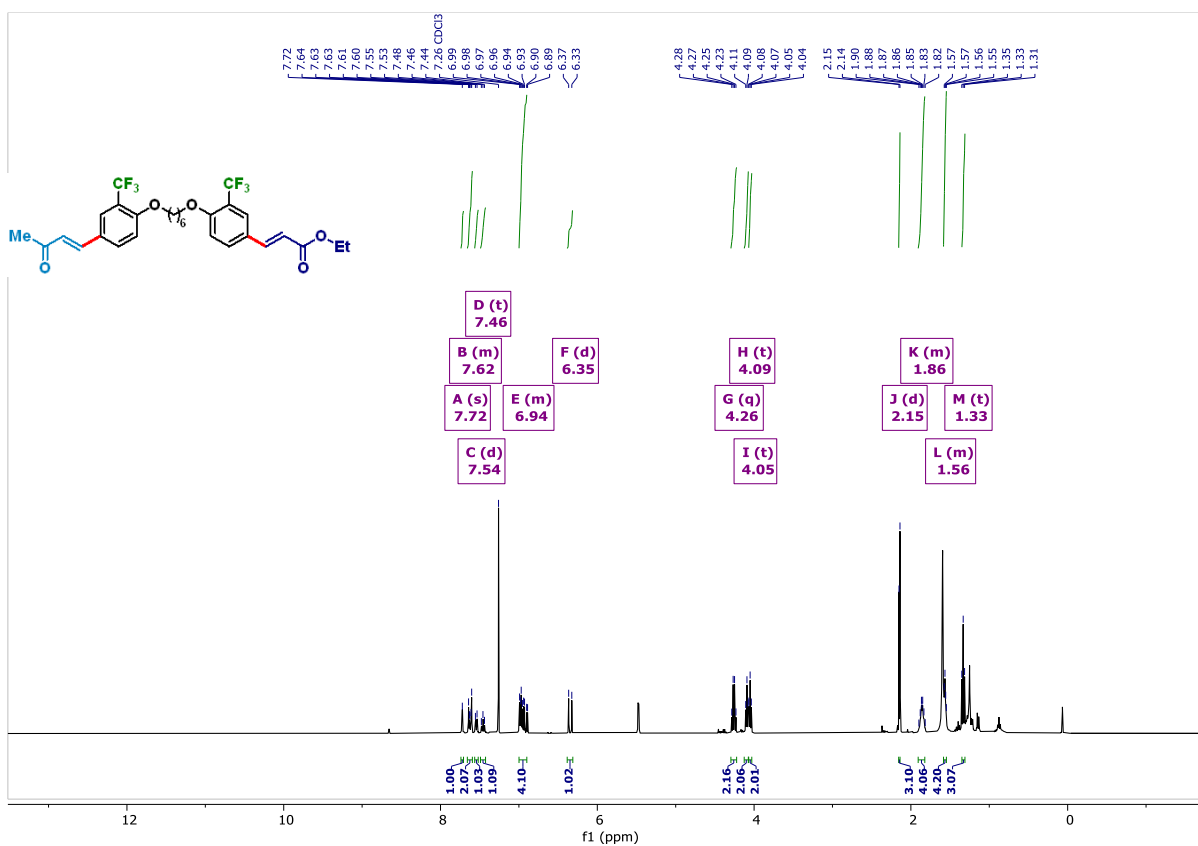
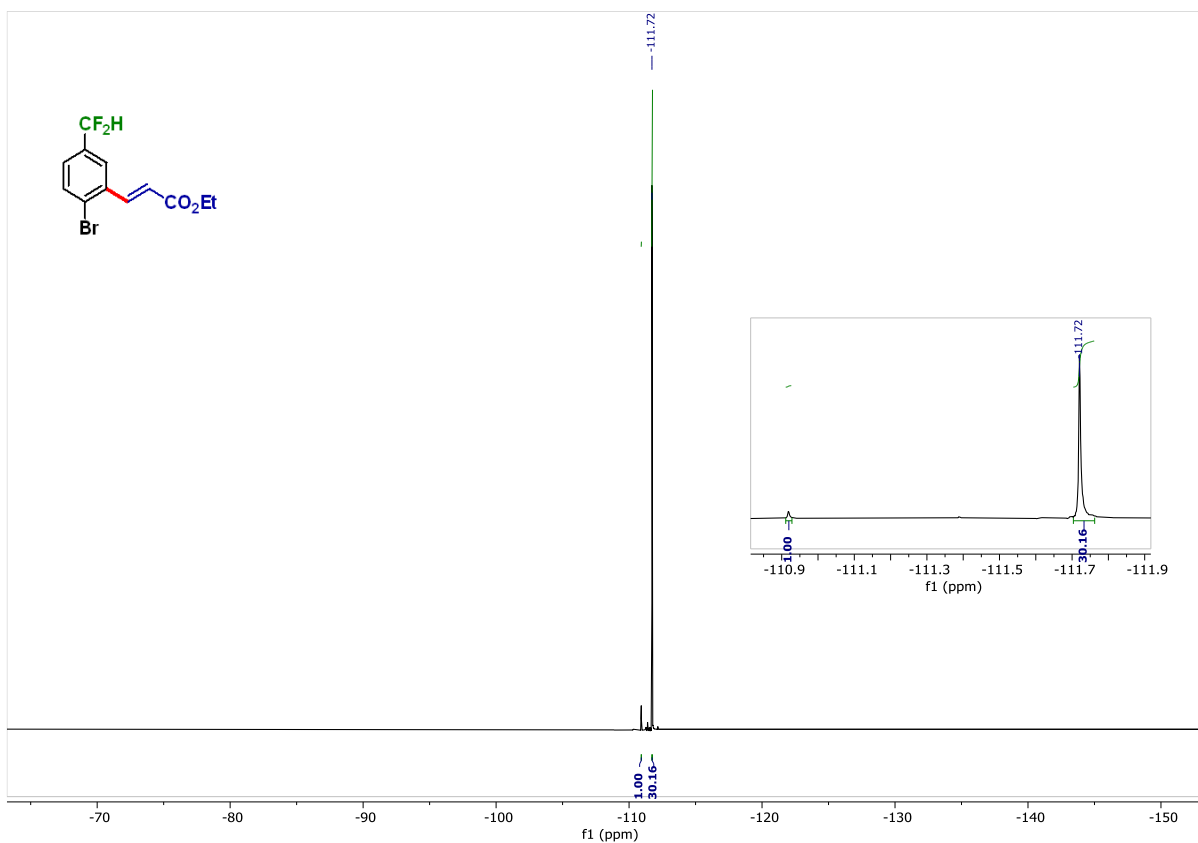


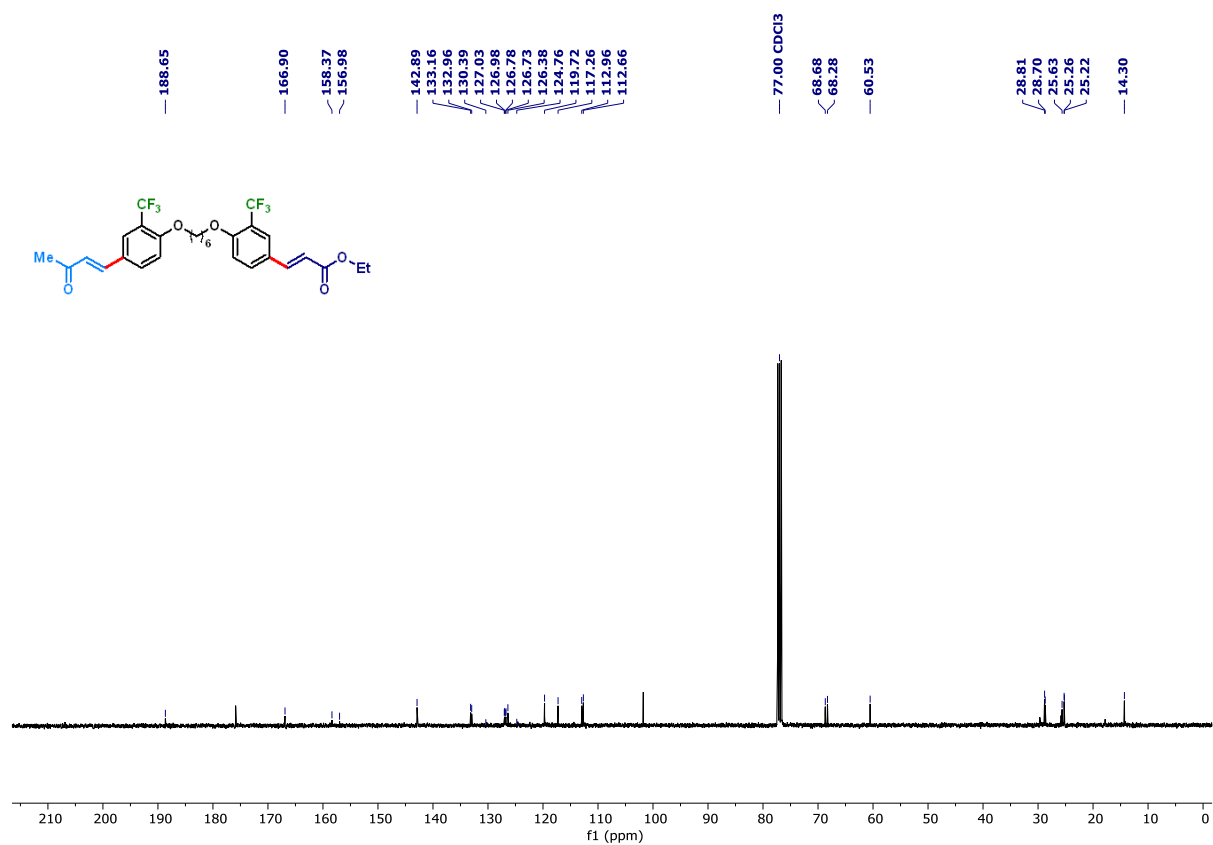
¹³C NMR of 5r



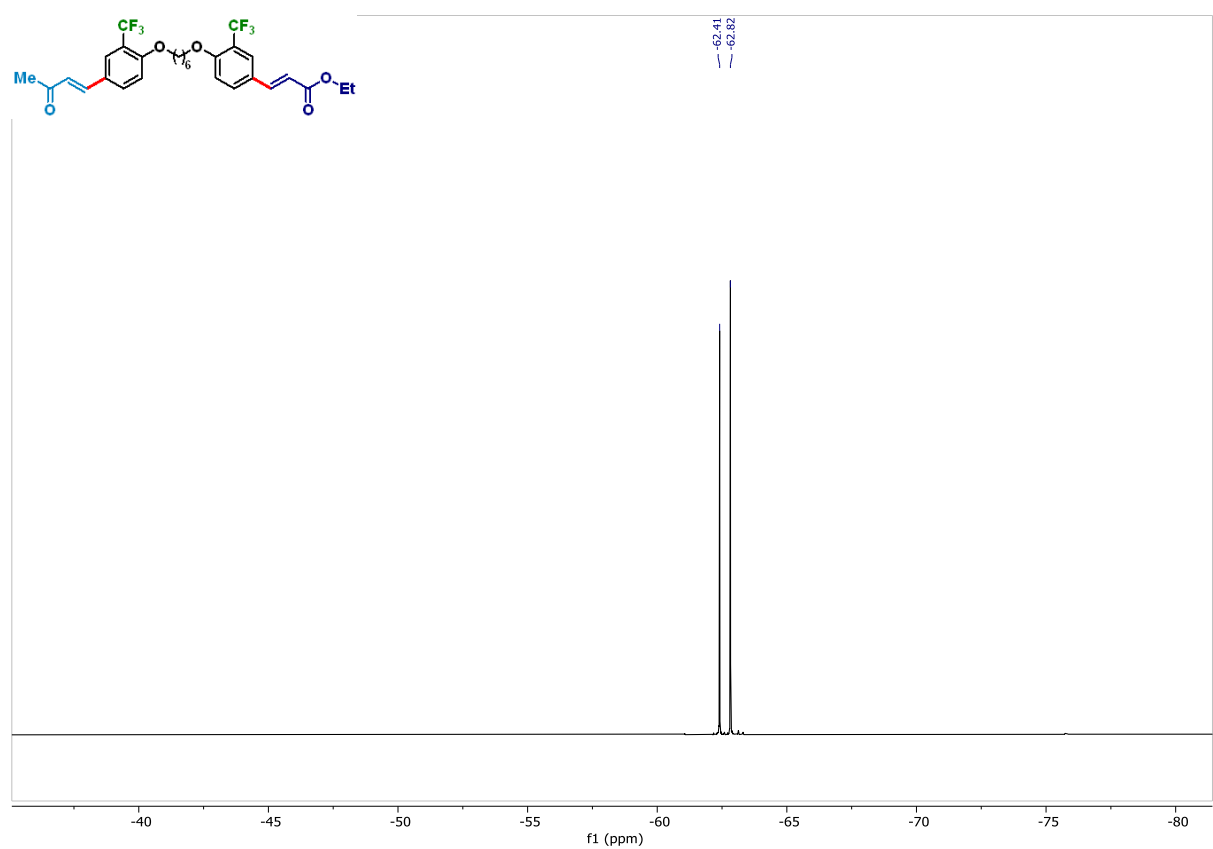
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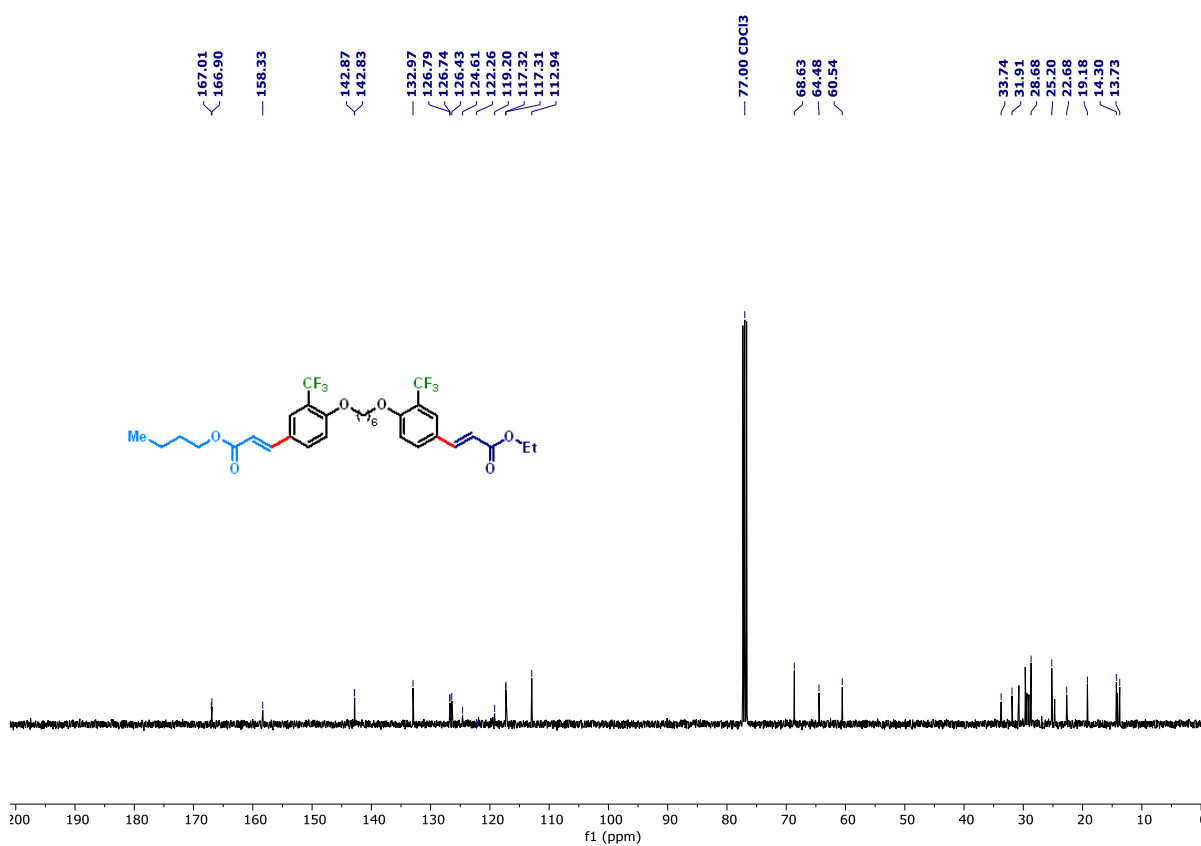
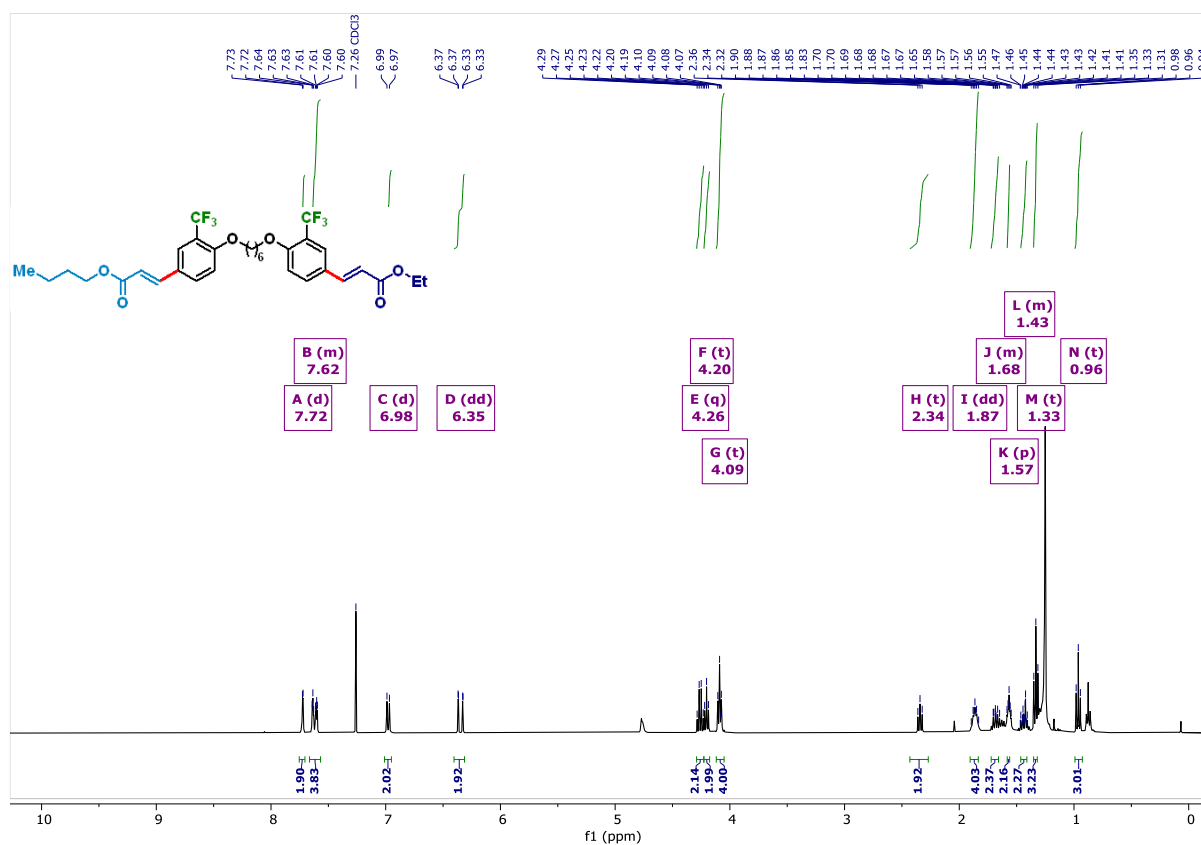


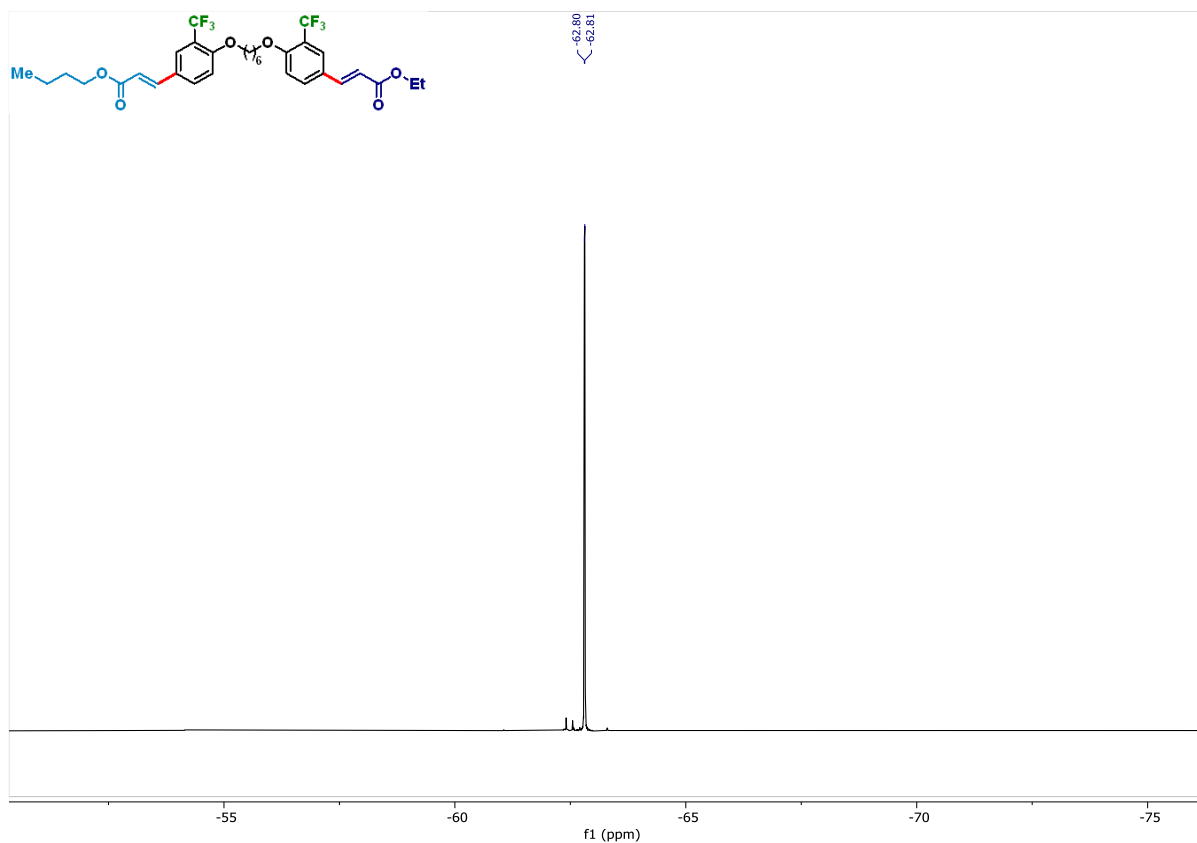


¹³C NMR of 7a

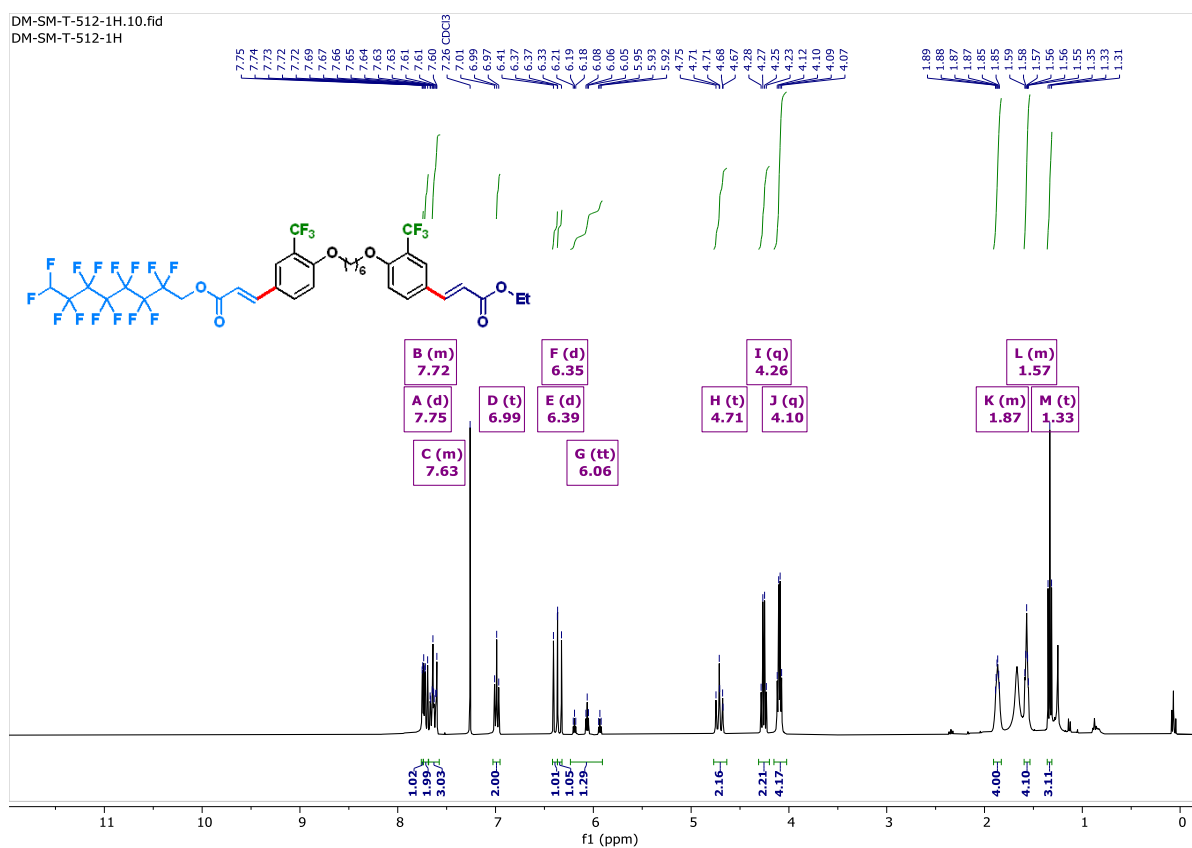


¹⁹F NMR of 7a

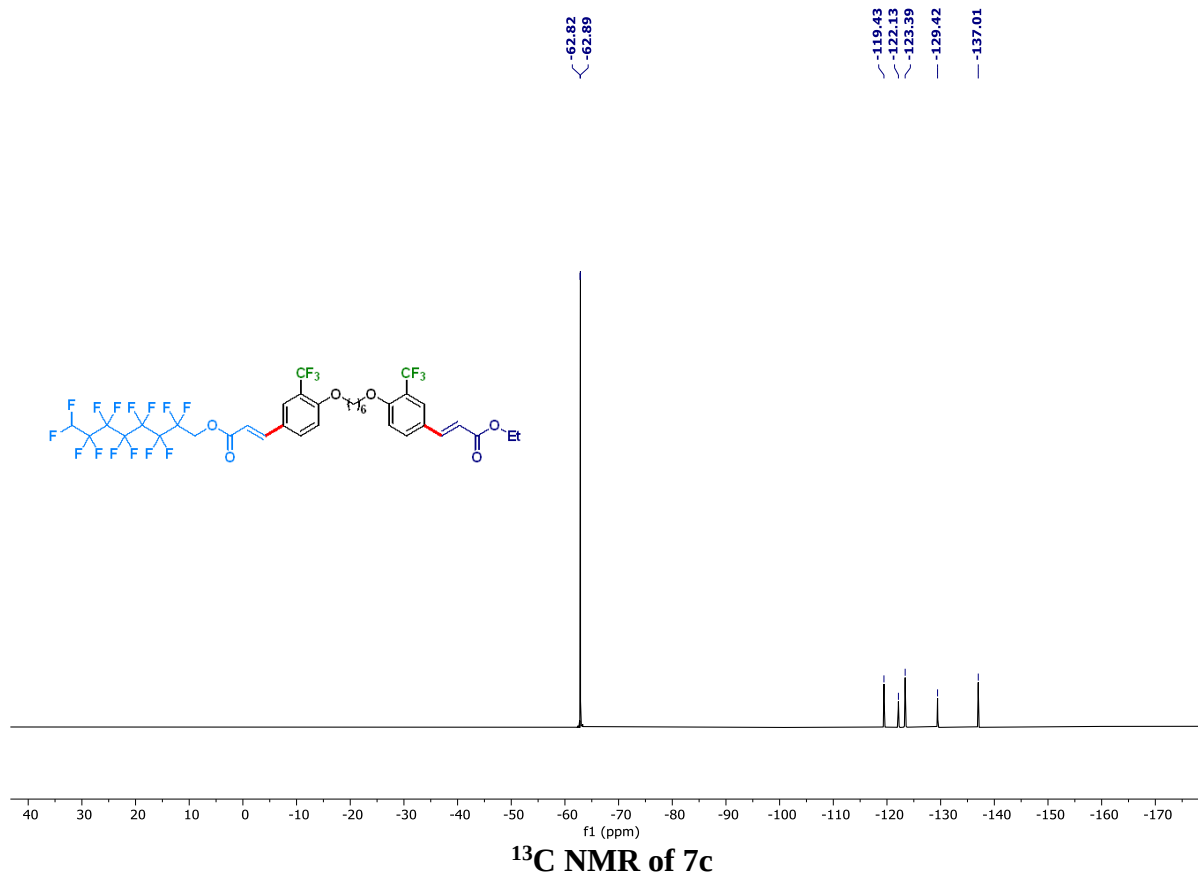
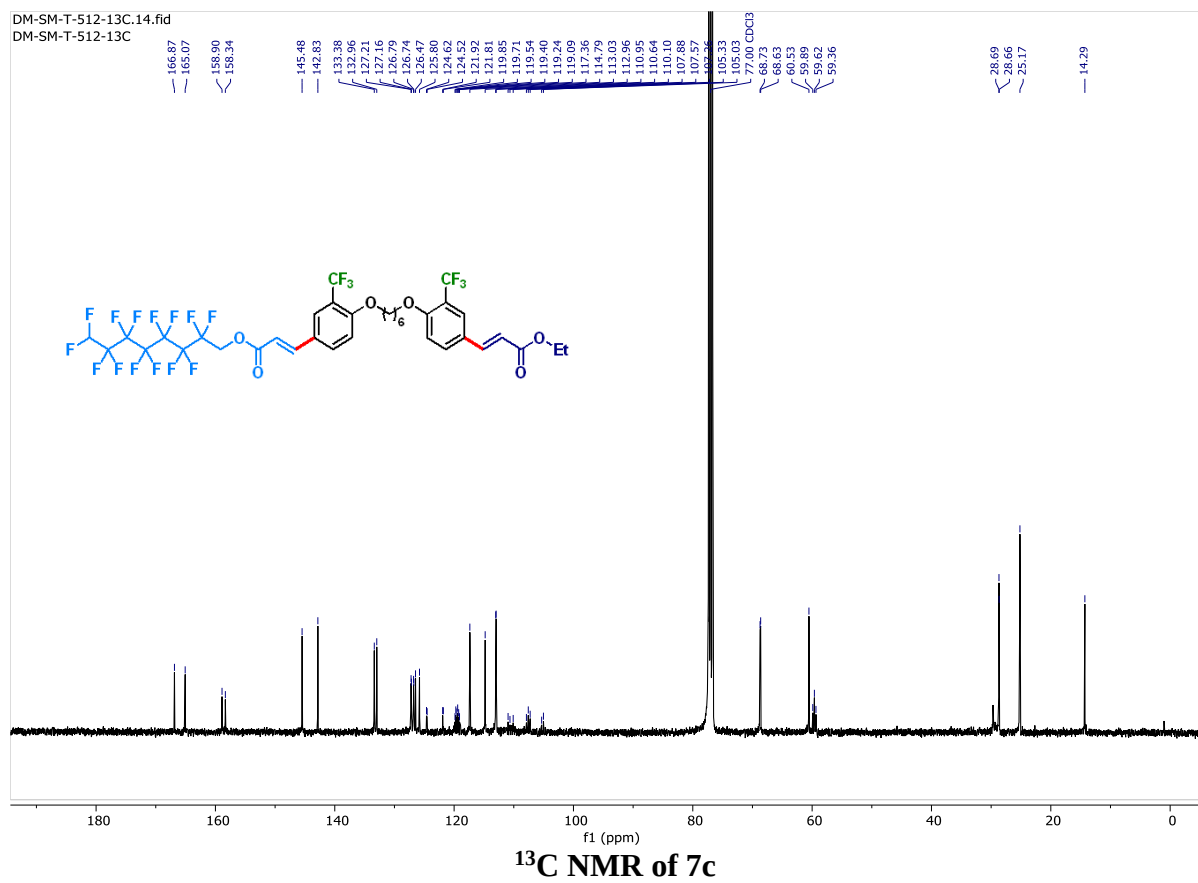


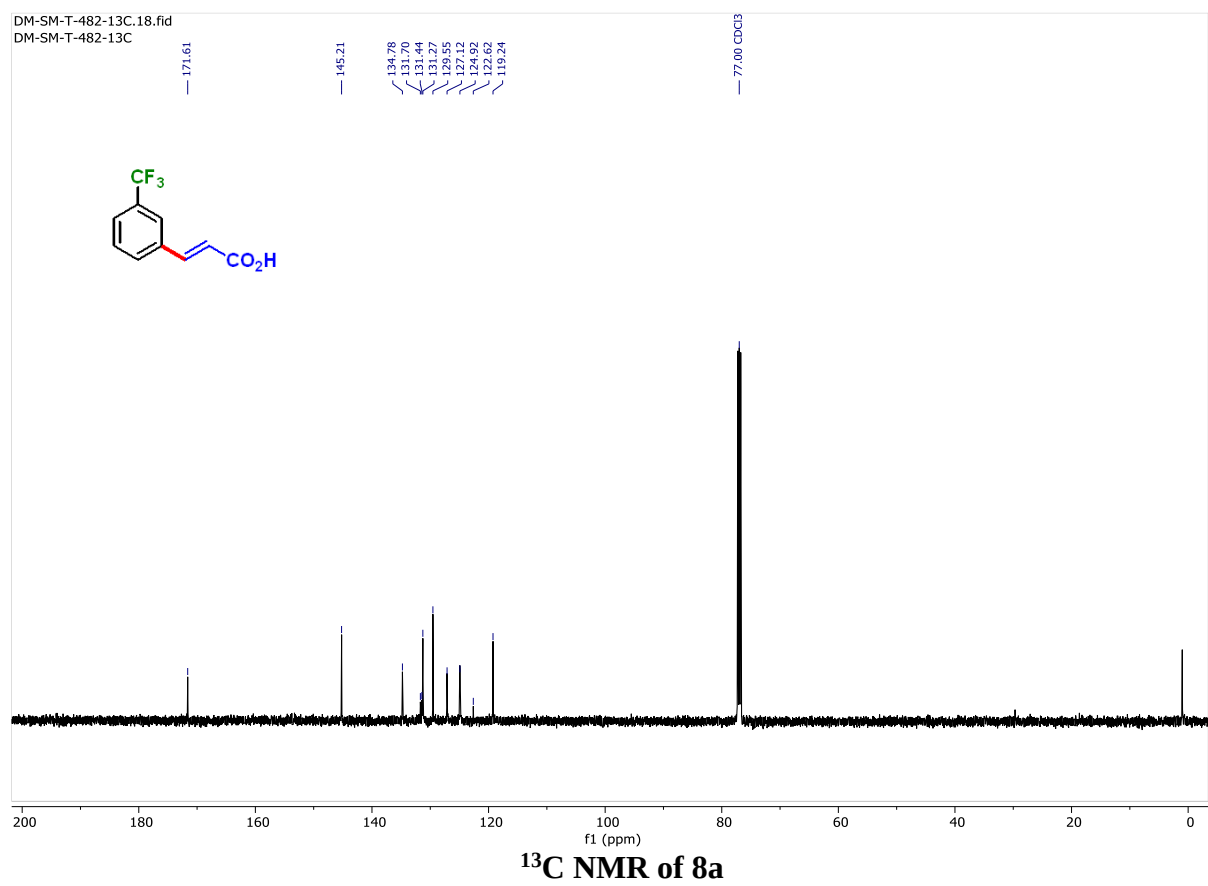
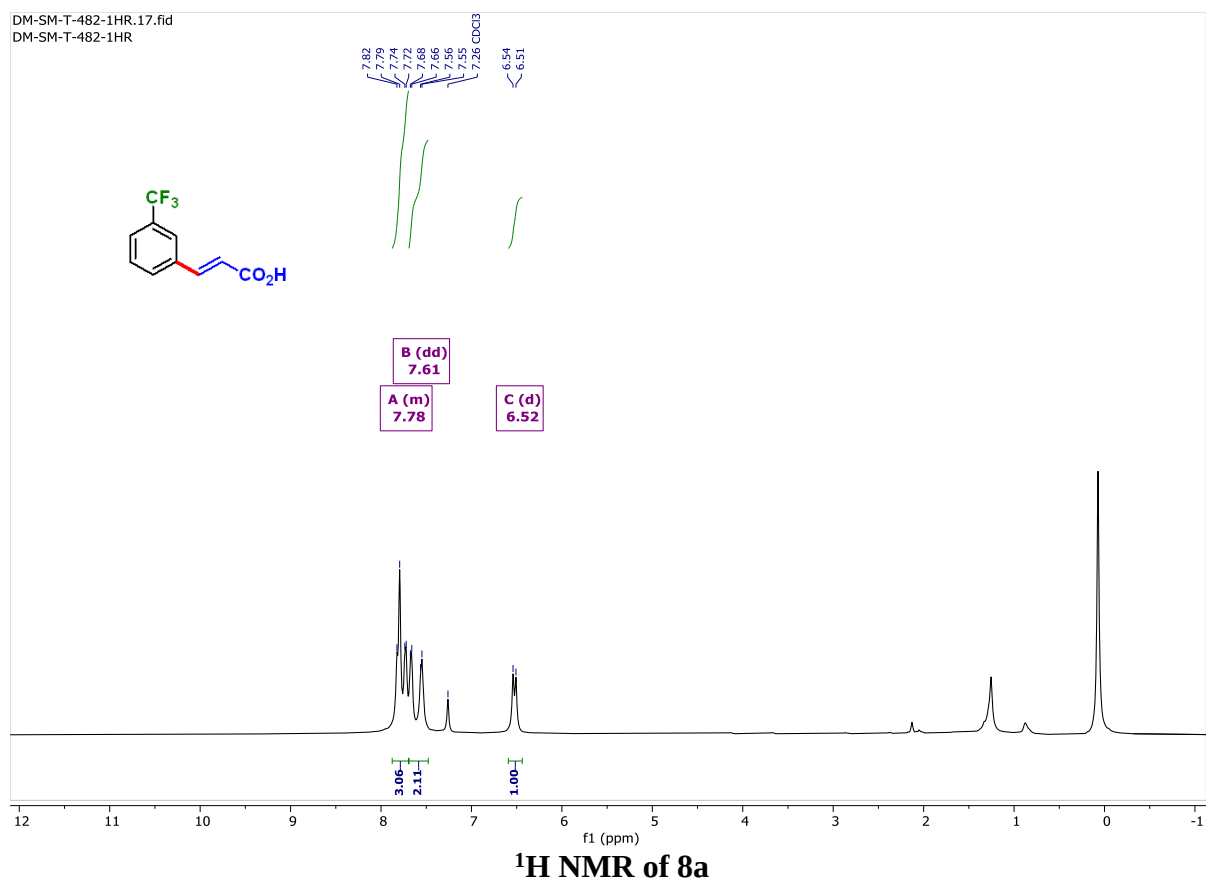


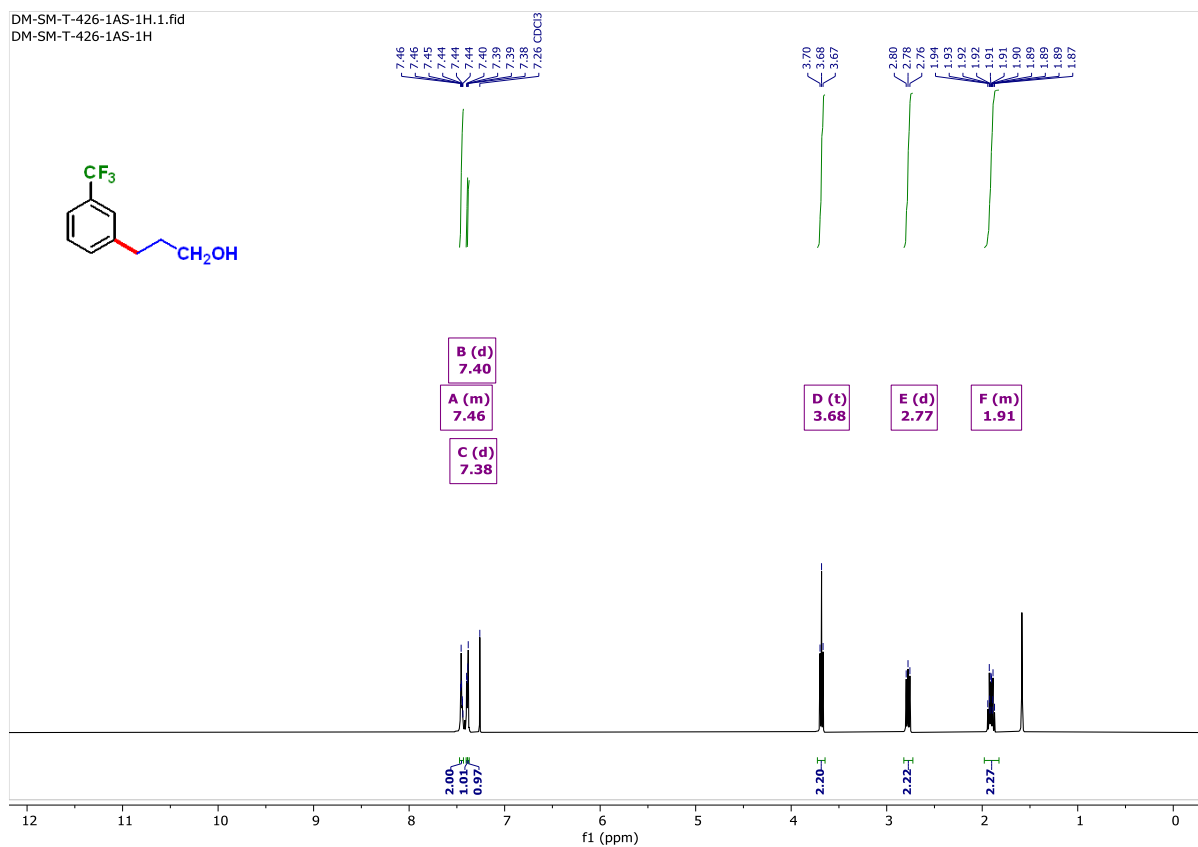
^{19}F NMR of 7b



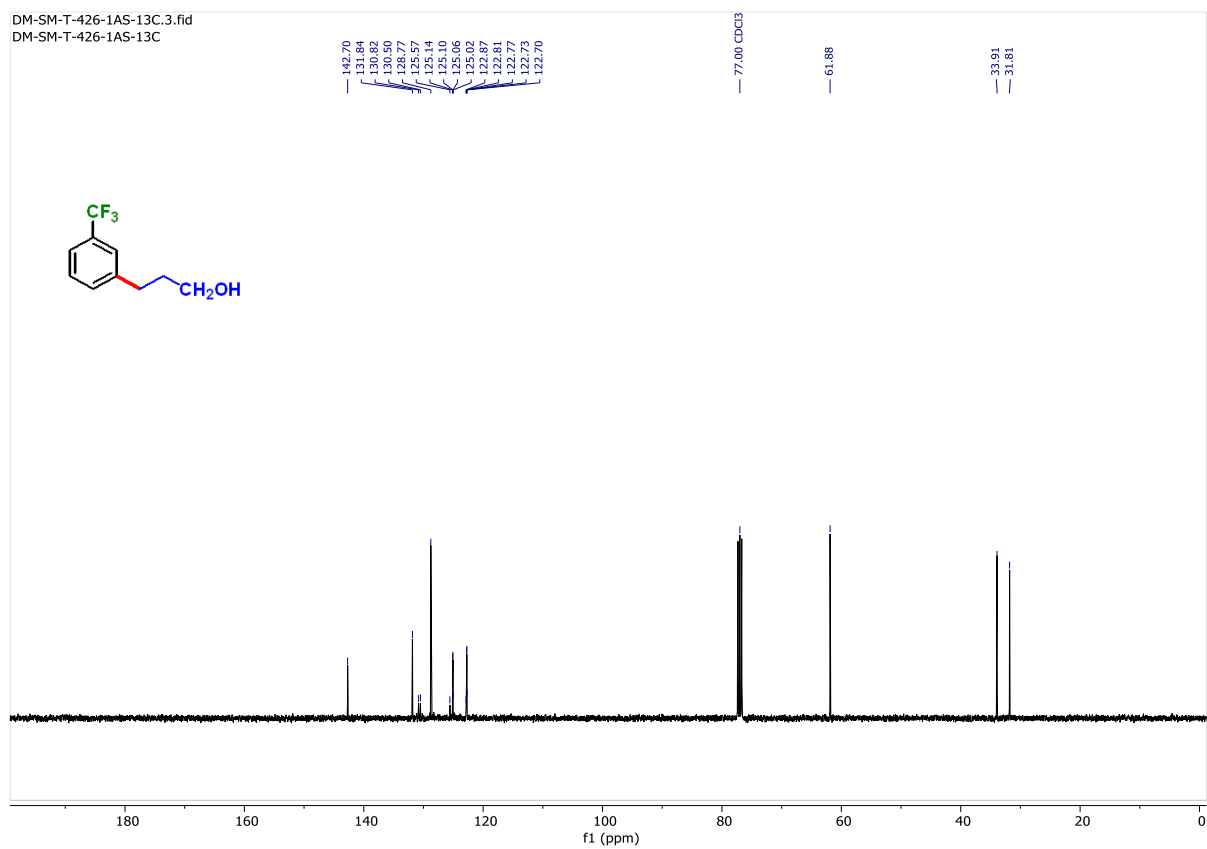
^1H NMR of 7c





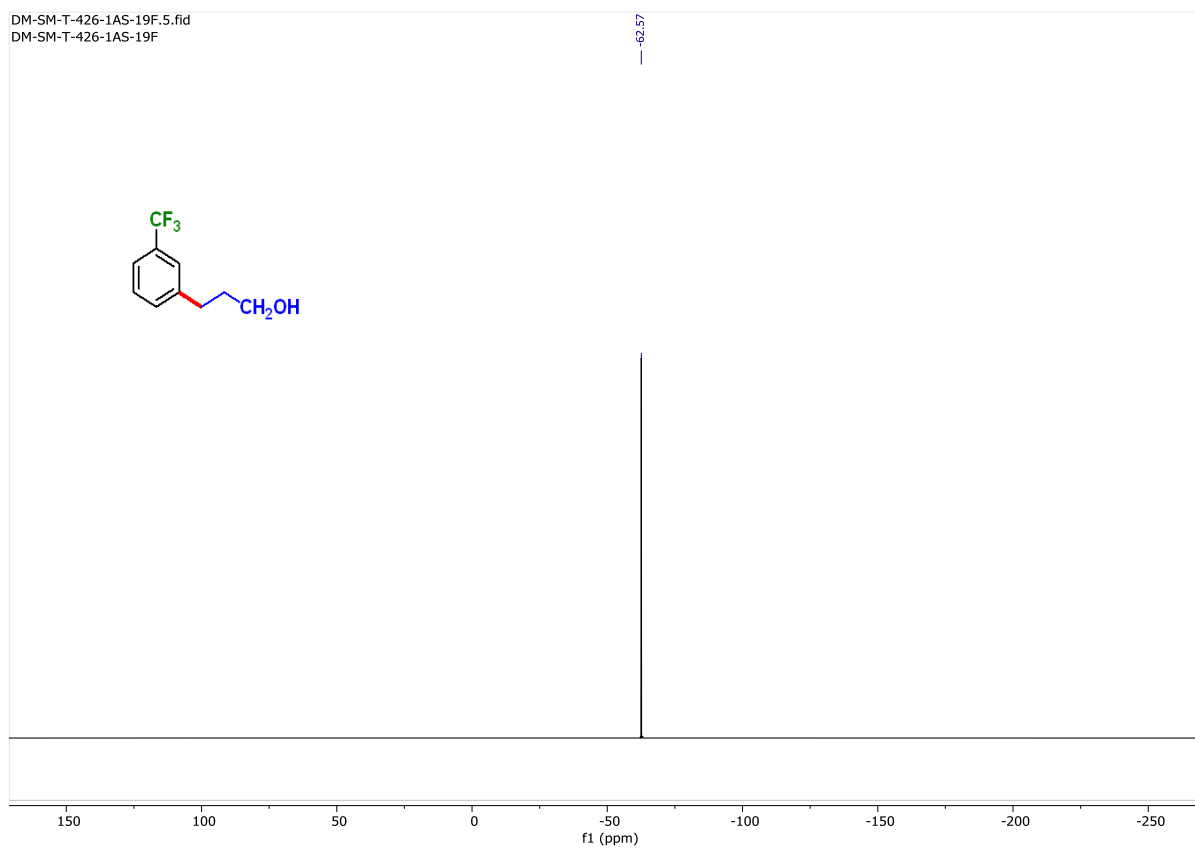


¹H NMR of 8b



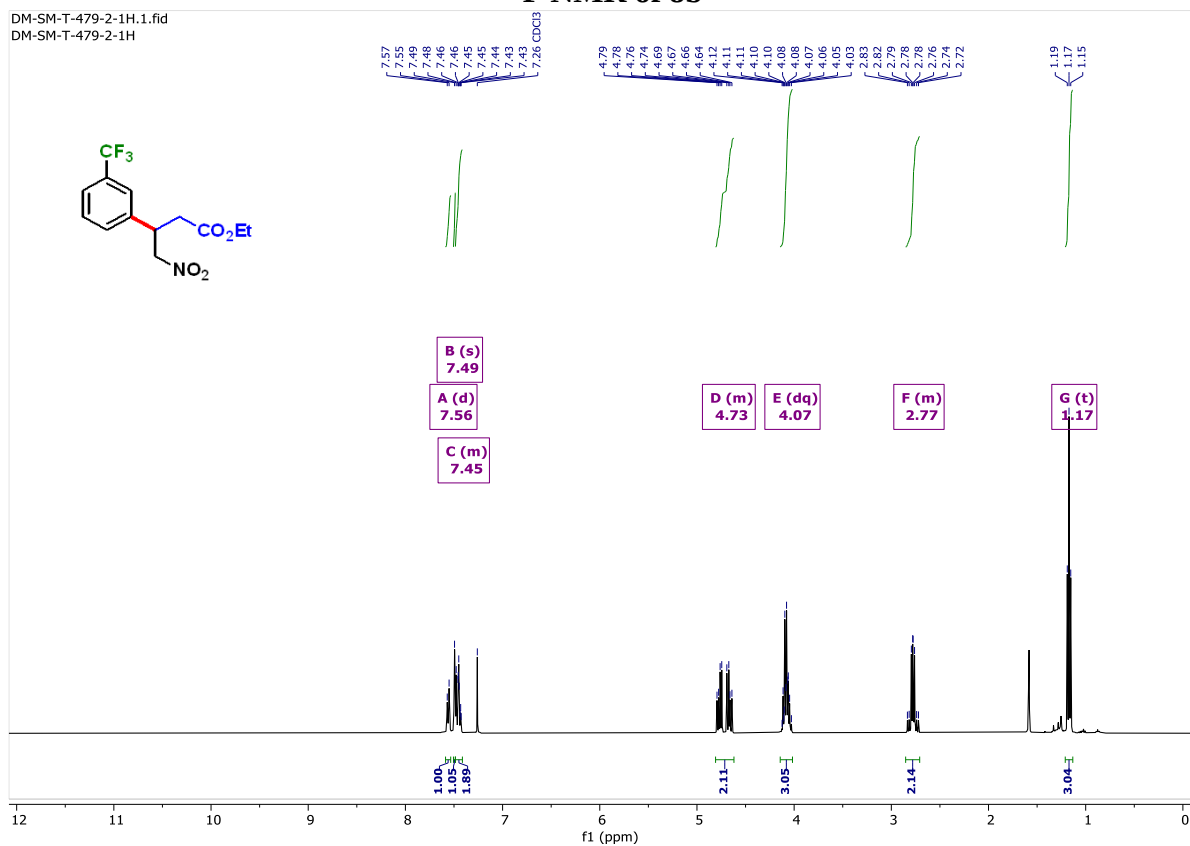
¹³C NMR of 8b

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DM-SM-T-426-1AS-19F

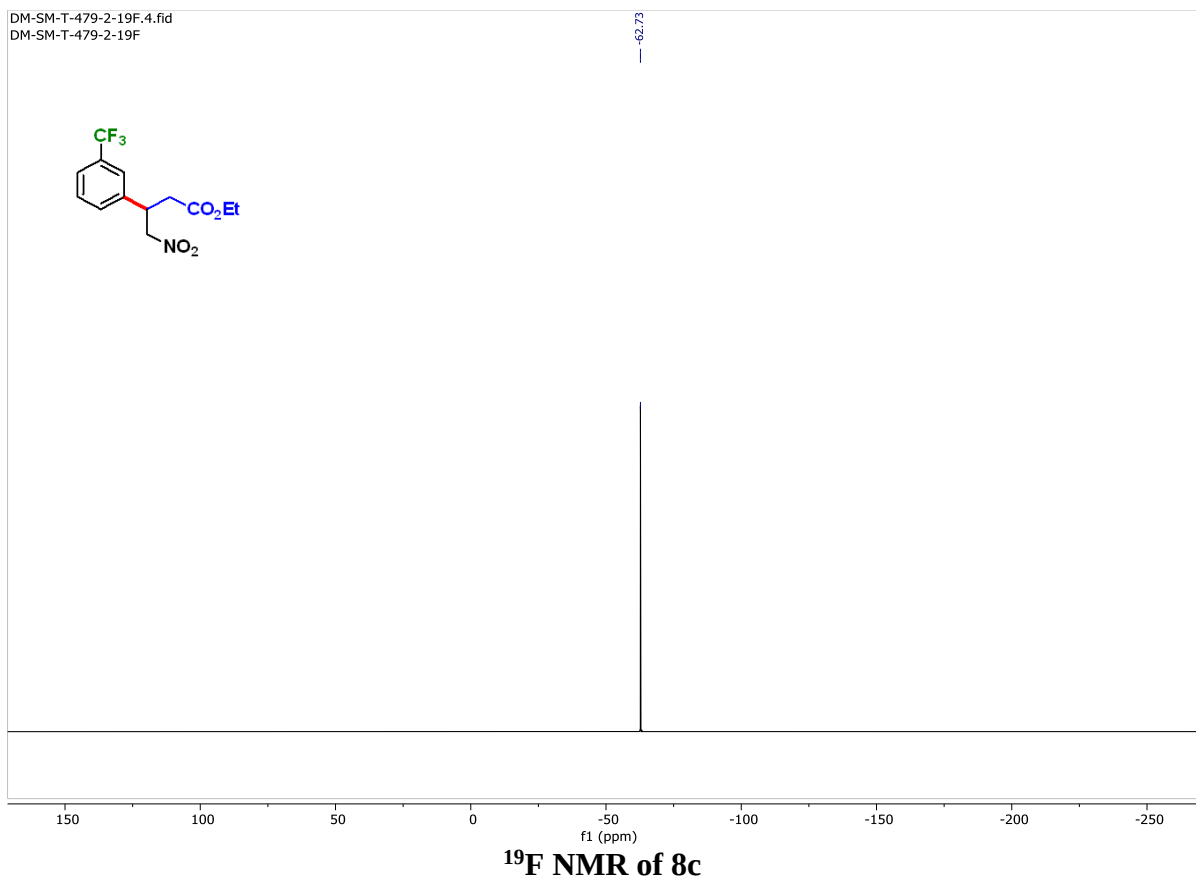
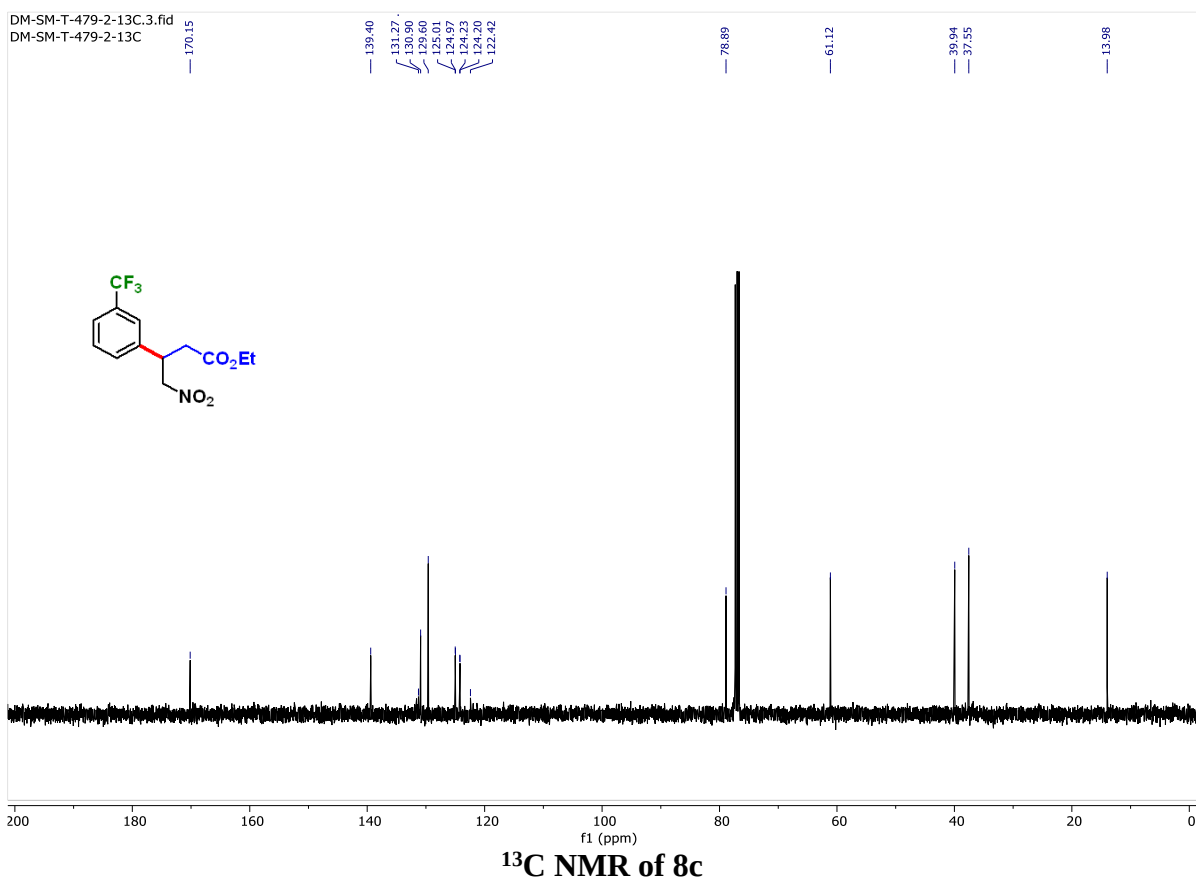


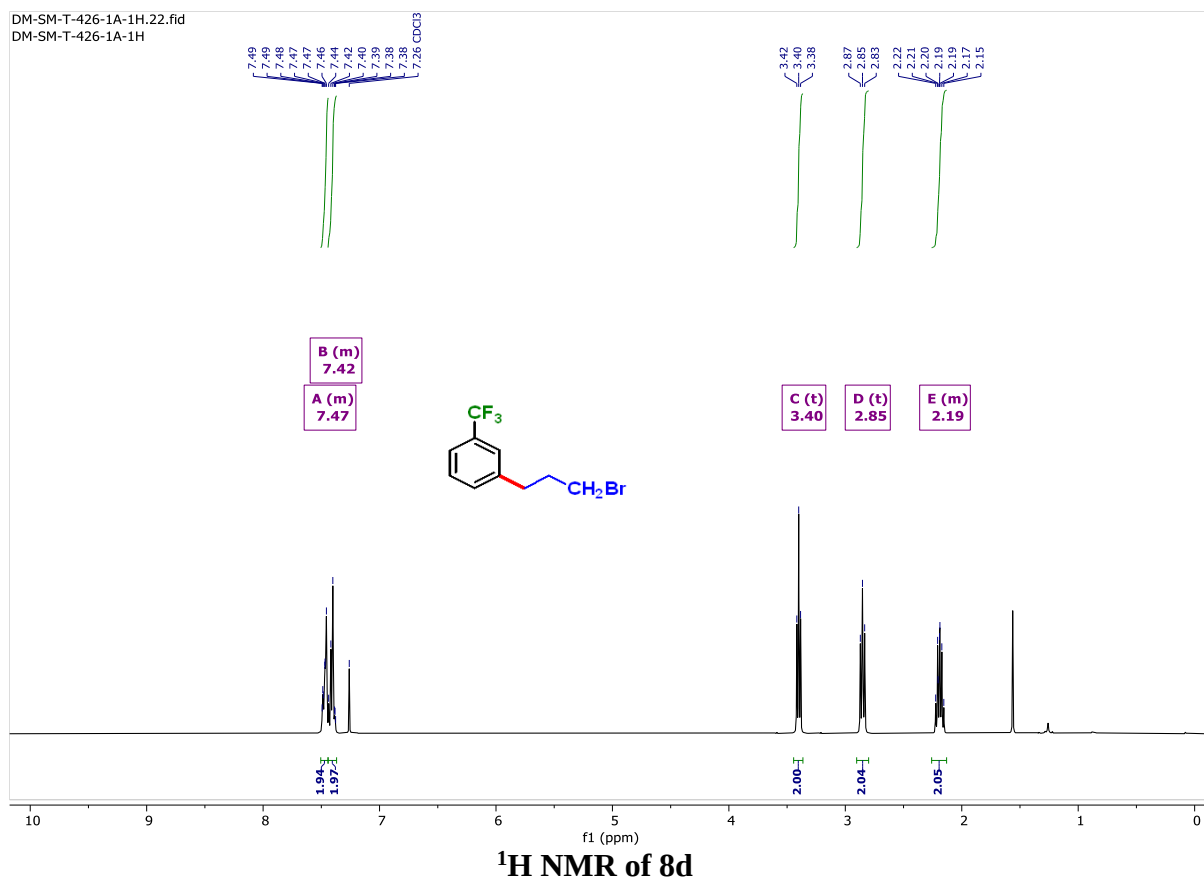
¹⁹F NMR of 8b

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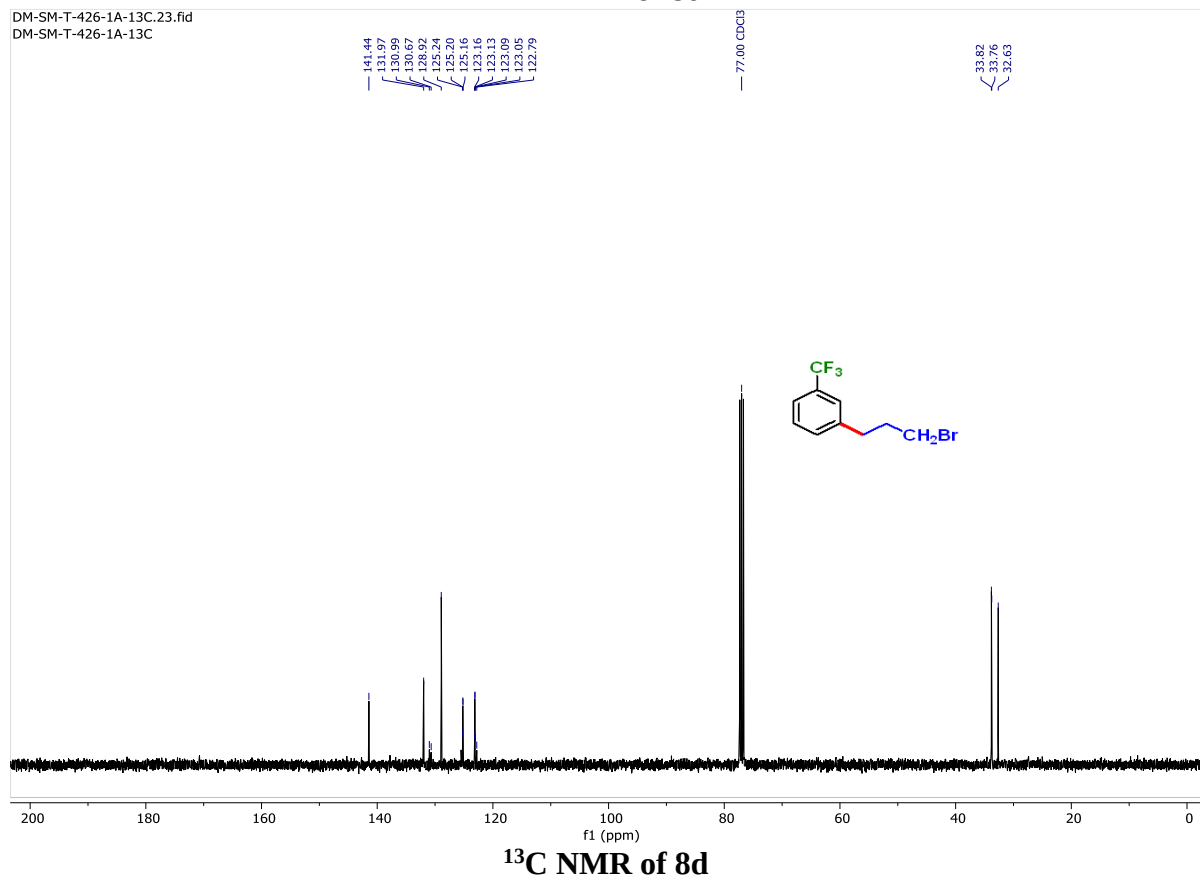


¹H NMR of 8c

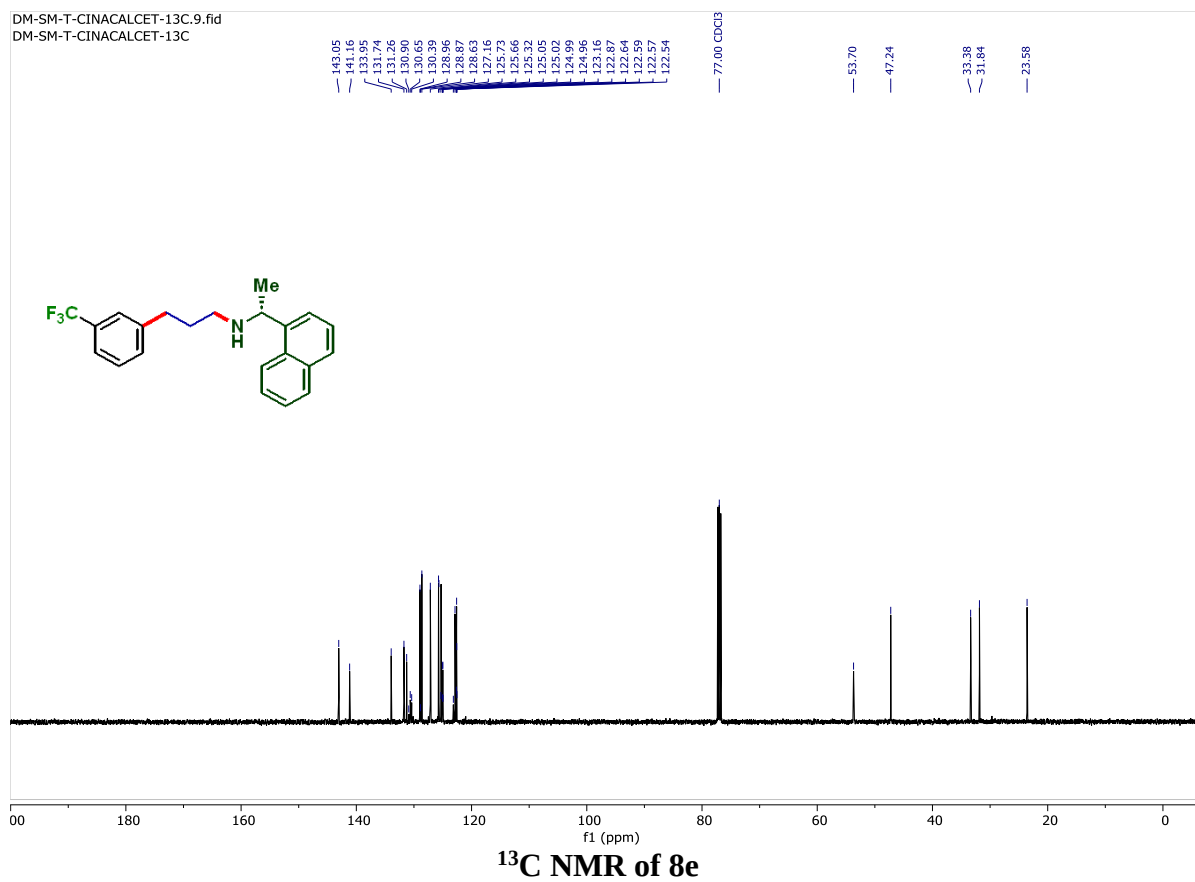
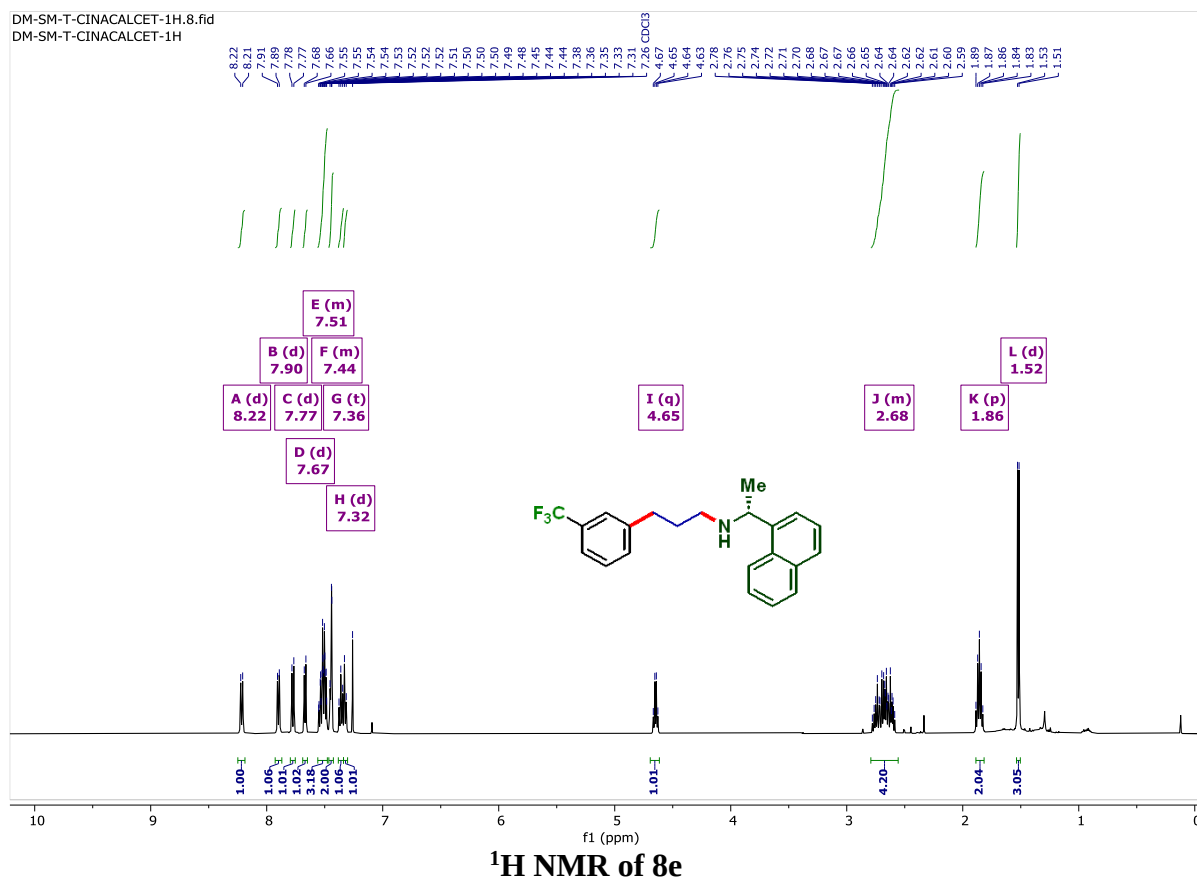




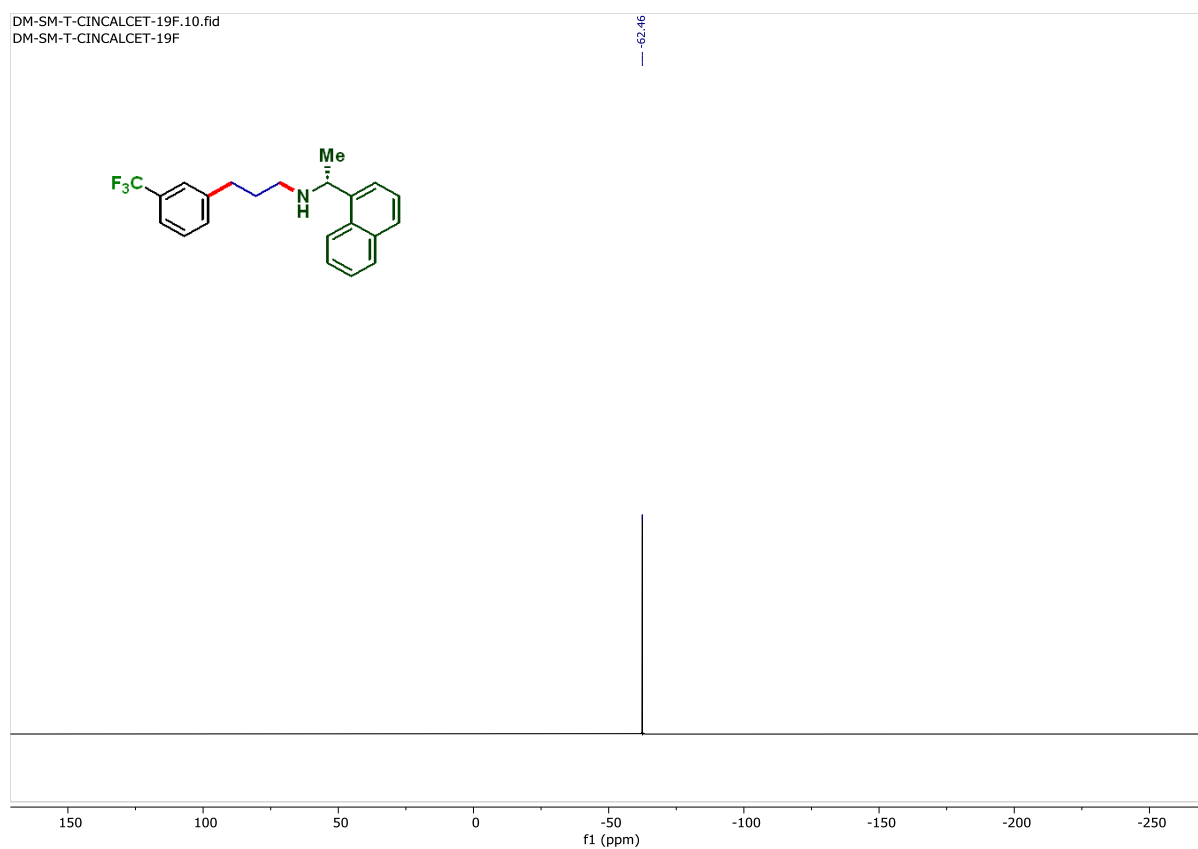
¹H NMR of 8d



¹³C NMR of 8d



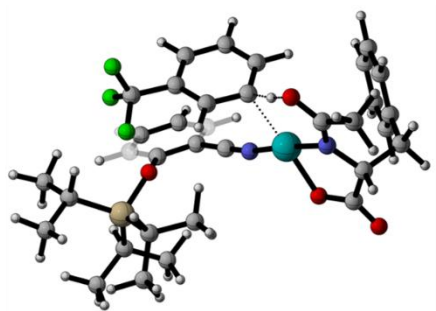
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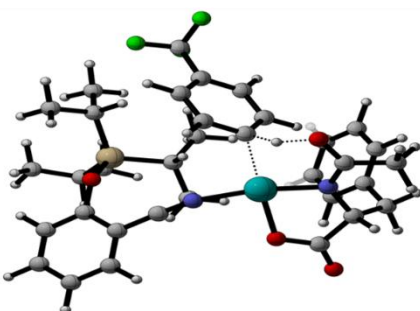
^{19}F NMR of 8e

13. Computational part:

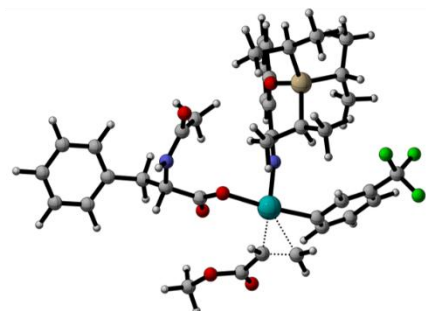
DFT Optimized Structures of Transition States:



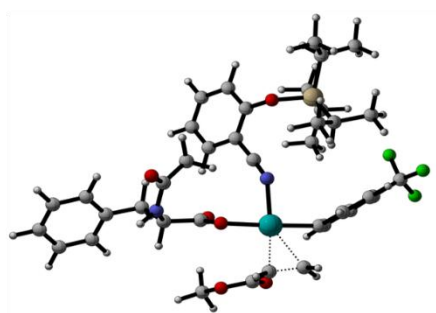
TS-1_m



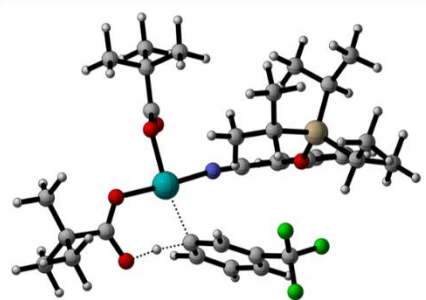
TS-1_p



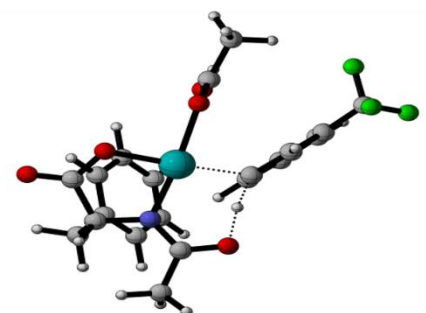
TS-2_m



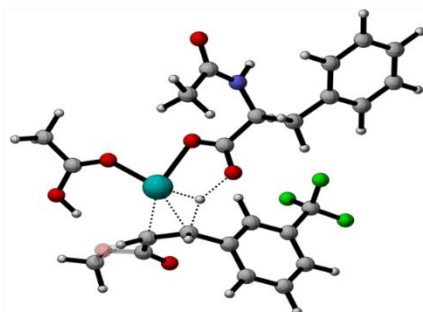
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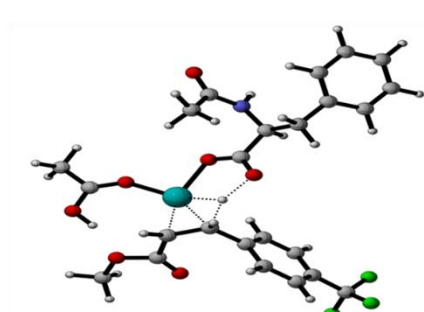
TS-I_m



TS-1_{m''}

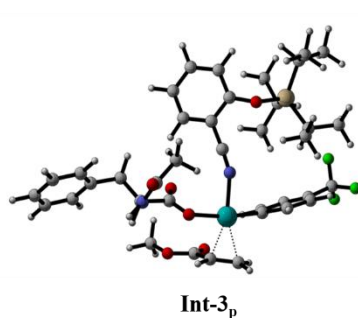
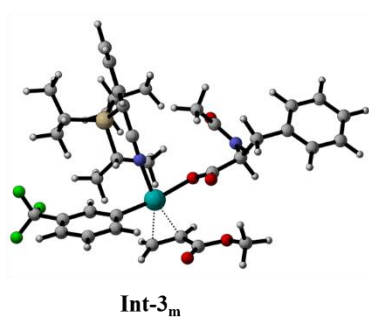
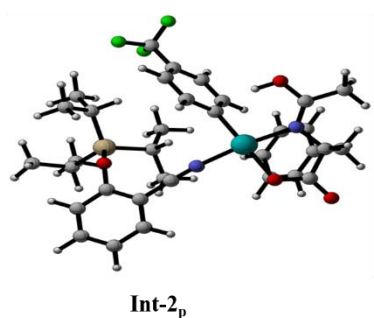
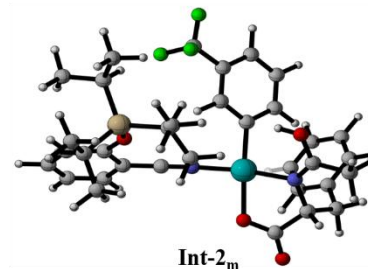
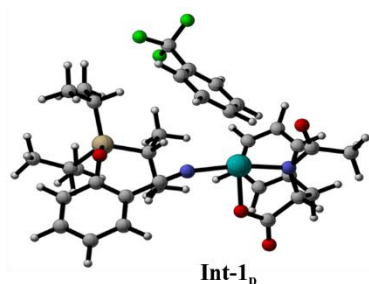
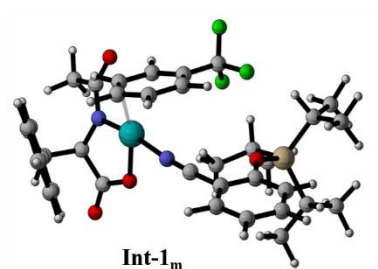


TS-III_m



TS-III_p

DFT Optimized Structures of Intermediates:



Subs

Number of Imaginary Frequency: 0

Electronic Energy: HF= -569.3601356

Zero-point correction=	0.105562
(Hartree/Particle)	
Thermal correction to Energy=	0.113199
Thermal correction to Enthalpy=	0.114143
Thermal correction to Gibbs Free Energy=	0.072373
Sum of electronic and zero-point Energies=	-
569.254573	
Sum of electronic and thermal Energies=	-
569.246937	
Sum of electronic and thermal Enthalpies=	-
569.245993	
Sum of electronic and thermal Free Energies=	-
569.287763	

6	-0.460200000	-0.086805000	0.018561000
6	0.932499000	-0.083889000	-0.002597000

6	1.628993000	1.123945000	-0.015151000
6	0.931992000	2.331650000	-0.004884000
6	-0.460562000	2.334009000	0.016382000
6	-1.155244000	1.123415000	0.026439000
1	-1.009444000	-1.029616000	0.034867000
1	1.476379000	-1.030554000	-0.006243000
1	2.720972000	1.124168000	-0.030223000
1	1.475558000	3.278486000	-0.010346000
1	-1.010198000	3.276676000	0.031065000
6	-2.662816000	1.124308000	-0.004647000
9	-3.172042000	2.195814000	0.611787000
9	-3.126255000	1.139447000	-1.260785000
9	-3.173565000	0.039633000	0.586769000

DG_ipr

Number of Imaginary Frequency: 0

Electronic Energy: HF= -1044.3580541

<i>Zero-point correction=</i>	<i>0.377397</i>
<i>(Hartree/Particle)</i>	
<i>Thermal correction to Energy=</i>	<i>0.398364</i>
<i>Thermal correction to Enthalpy=</i>	<i>0.399309</i>
<i>Thermal correction to Gibbs Free Energy=</i>	<i>0.330370</i>
<i>Sum of electronic and zero-point Energies=</i>	<i>-</i>
<i>1043.980657</i>	
<i>Sum of electronic and thermal Energies=</i>	<i>-</i>
<i>1043.959690</i>	
<i>Sum of electronic and thermal Enthalpies=</i>	<i>-</i>
<i>1043.958746</i>	
<i>Sum of electronic and thermal Free Energies=</i>	<i>-</i>
<i>1044.027684</i>	

6	-0.436903000	-0.446158000	0.348885000
6	0.607431000	-0.128383000	-0.510805000

6	1.116559000	1.176679000	-0.550103000
6	0.581567000	2.177241000	0.289183000
6	-0.475345000	1.843735000	1.146125000
6	-0.975010000	0.545576000	1.171637000
1	-0.832589000	-1.462362000	0.377343000
1	1.038608000	-0.885614000	-1.167822000
1	-0.892812000	2.614058000	1.797439000
1	-1.797415000	0.303612000	1.848427000
6	2.169780000	1.536368000	-1.457275000
7	3.001384000	1.833916000	-2.205765000
8	1.116116000	3.396138000	0.241120000
14	0.406501000	4.940552000	0.019040000
6	1.826388000	5.899041000	-0.764118000
6	-0.167064000	5.555738000	1.718691000
6	-1.056398000	4.659868000	-1.145548000
6	3.024911000	6.041219000	0.182622000
1	3.324100000	5.071490000	0.607690000
1	3.896627000	6.453800000	-0.350798000
1	2.801428000	6.725323000	1.017718000
6	1.424410000	7.244948000	-1.379853000
1	2.286232000	7.711669000	-1.884365000
1	0.627466000	7.137761000	-2.131385000
1	1.069624000	7.957767000	-0.619161000
6	-0.332687000	7.081385000	1.770726000
1	-0.787208000	7.394148000	2.724944000
1	0.642923000	7.587548000	1.695825000
1	-0.968640000	7.469206000	0.960323000
6	0.721019000	5.062095000	2.869044000
1	0.304236000	5.369047000	3.842480000
1	0.825554000	3.967285000	2.876213000
1	1.736243000	5.482370000	2.800315000
6	-2.056035000	5.821708000	-1.202660000
1	-1.596353000	6.742697000	-1.595604000
1	-2.901824000	5.574897000	-1.865234000

1	-2.475360000	6.055977000	-0.212024000
6	-0.587224000	4.237111000	-2.543965000
1	-1.441749000	3.937143000	-3.172012000
1	-0.073909000	5.062467000	-3.063084000
1	0.113507000	3.388582000	-2.509981000
1	-1.171045000	5.106875000	1.851163000
1	2.137319000	5.229364000	-1.587499000
1	-1.586071000	3.797118000	-0.697597000

Alkene

Number of Imaginary Frequency: 0

Electronic Energy: HF= -306.4938186

<i>Zero-point correction=</i>	<i>0.095818</i>
<i>(Hartree/Particle)</i>	
<i>Thermal correction to Energy=</i>	<i>0.101925</i>
<i>Thermal correction to Enthalpy=</i>	<i>0.102869</i>
<i>Thermal correction to Gibbs Free Energy=</i>	<i>0.066311</i>
<i>Sum of electronic and zero-point Energies=</i>	<i>-</i>
<i>306.398000</i>	
<i>Sum of electronic and thermal Energies=</i>	<i>-</i>
<i>306.391894</i>	
<i>Sum of electronic and thermal Enthalpies=</i>	<i>-</i>
<i>306.390950</i>	
<i>Sum of electronic and thermal Free Energies=</i>	<i>-</i>
<i>306.427507</i>	

6	1.969190000	-1.393110000	-0.734732000
6	0.902681000	-2.191711000	-0.764013000
6	2.647065000	-1.085375000	0.553209000
8	2.318262000	-1.503064000	1.634097000
8	3.691451000	-0.269266000	0.364610000
6	4.417958000	0.095288000	1.525325000

1	5.224370000	0.756481000	1.189273000
1	3.771308000	0.619796000	2.243883000
1	2.386241000	-0.937135000	-1.635591000
1	4.836715000	-0.792890000	2.020691000
1	0.519590000	-2.626323000	0.163617000
1	0.391715000	-2.429430000	-1.699343000

Int-1m (CH_act_reac)

Number of Imaginary Frequency: 0

Electronic Energy: HF= -2448.0274725

<i>Zero-point correction=</i>	<i>0.692296</i>
<i>(Hartree/Particle)</i>	
<i>Thermal correction to Energy=</i>	<i>0.738024</i>
<i>Thermal correction to Enthalpy=</i>	<i>0.738968</i>
<i>Thermal correction to Gibbs Free Energy=</i>	<i>0.613881</i>
<i>Sum of electronic and zero-point Energies=</i>	<i>-</i>
<i>2447.335176</i>	
<i>Sum of electronic and thermal Energies=</i>	<i>-</i>
<i>2447.289449</i>	
<i>Sum of electronic and thermal Enthalpies=</i>	<i>-</i>
<i>2447.288504</i>	
<i>Sum of electronic and thermal Free Energies=</i>	<i>-</i>
<i>2447.413591</i>	

6	-4.341829000	1.220289000	2.246381000
6	-4.320822000	1.747194000	3.531823000
6	-3.143581000	0.946106000	1.567537000
6	-1.921061000	1.732321000	3.553798000
1	-0.964354000	1.917837000	4.045076000
6	-0.242278000	-2.506795000	1.004861000
6	1.019877000	-2.439381000	0.370849000
6	-0.360120000	-2.272329000	2.360515000
6	2.151574000	-2.113808000	1.132099000

6	0.776702000	-1.931961000	3.117935000
6	2.015331000	-1.846376000	2.515922000
1	3.140013000	-2.229051000	0.683360000
1	2.901588000	-1.588287000	3.096412000
46	1.758477000	-0.133316000	-0.129757000
8	3.278357000	3.084001000	-1.867533000
8	1.859020000	1.686613000	-0.896330000
8	2.926536000	-2.699930000	-1.746463000
7	3.221726000	-0.468431000	-1.424848000
6	3.894322000	0.769417000	-1.784000000
6	2.967666000	1.964952000	-1.530336000
6	3.476896000	-1.641024000	-2.044121000
6	4.492931000	-1.645107000	-3.181092000
1	4.113262000	-1.076073000	-4.043377000
1	5.459824000	-1.210395000	-2.893171000
1	4.639946000	-2.687820000	-3.483254000
1	4.120662000	0.802326000	-2.860998000
1	0.671092000	-1.740529000	4.187519000
1	-1.337151000	-2.339118000	2.841787000
1	1.177728000	-2.756983000	-0.664121000
6	-1.441178000	-2.881858000	0.175427000
9	-2.589409000	-2.721526000	0.845299000
9	-1.388806000	-4.155052000	-0.222849000
9	-1.521148000	-2.132209000	-0.932631000
6	-1.931631000	1.204099000	2.253572000
6	-0.716462000	0.865711000	1.592423000
7	0.241596000	0.524043000	1.053285000
6	-3.117810000	2.011970000	4.194102000
1	-5.292500000	1.006650000	1.759407000
1	-5.269455000	1.952609000	4.032646000
1	-3.119575000	2.426772000	5.202602000
8	-3.071807000	0.442576000	0.347900000
14	-3.973704000	0.530953000	-1.126446000
6	-5.038723000	-1.029382000	-1.157317000

1	-4.314855000	-1.820390000	-0.892312000
6	-4.959455000	2.146533000	-1.020863000
1	-5.509426000	2.083727000	-0.065527000
6	-2.679802000	0.471495000	-2.502409000
1	-2.524359000	-0.609534000	-2.669594000
6	5.223087000	0.996049000	-1.025603000
1	5.579390000	2.000947000	-1.298605000
1	5.969690000	0.272297000	-1.384318000
6	5.082092000	0.868235000	0.469314000
6	5.460079000	-0.309981000	1.122601000
6	4.529537000	1.906220000	1.231131000
6	5.308215000	-0.446386000	2.501647000
1	5.889817000	-1.129841000	0.540397000
6	4.358682000	1.766040000	2.607030000
1	4.229972000	2.832727000	0.734655000
6	4.752951000	0.592106000	3.248873000
1	5.628468000	-1.367962000	2.994504000
1	3.926192000	2.586959000	3.183476000
1	4.635476000	0.490408000	4.330508000
6	-6.142723000	-1.041682000	-0.094882000
1	-6.725944000	-1.975630000	-0.145188000
1	-5.727819000	-0.978336000	0.922268000
1	-6.853742000	-0.208601000	-0.227347000
6	-5.587716000	-1.363137000	-2.551338000
1	-4.785551000	-1.458977000	-3.298279000
1	-6.130127000	-2.322423000	-2.532432000
1	-6.293512000	-0.599809000	-2.915676000
6	-6.019206000	2.309885000	-2.119199000
1	-6.588542000	3.241643000	-1.967688000
1	-5.572344000	2.363096000	-3.122787000
1	-6.743946000	1.481578000	-2.120583000
6	-4.035917000	3.369629000	-0.933825000
1	-3.298924000	3.280583000	-0.120258000
1	-3.474080000	3.518651000	-1.868924000

1	-4.617537000	4.288023000	-0.752042000
6	-3.189300000	1.072683000	-3.821298000
1	-3.301275000	2.165988000	-3.748388000
1	-2.468184000	0.878116000	-4.631160000
1	-4.158792000	0.658862000	-4.139502000
6	-1.323751000	1.068818000	-2.112024000
1	-0.886985000	0.546973000	-1.253724000
1	-0.606570000	0.984420000	-2.943518000
1	-1.390911000	2.136381000	-1.851044000

TS-1m (CH_{act}_TS)

One Imaginary Frequency: -1217.8 cm⁻¹

Electronic Energy: HF= -2448.0075434

Zero-point correction=	0.687784
(Hartree/Particle)	
Thermal correction to Energy=	0.732686
Thermal correction to Enthalpy=	0.733631
Thermal correction to Gibbs Free Energy=	0.611366
Sum of electronic and zero-point Energies=	-
2447.319759	
Sum of electronic and thermal Energies=	-
2447.274857	
Sum of electronic and thermal Enthalpies=	-
2447.273913	
Sum of electronic and thermal Free Energies=	-
2447.396177	

6	-3.787884000	2.536797000	3.268149000
6	-3.693652000	3.064501000	4.550102000
6	-2.650313000	2.426570000	2.455341000
6	-1.331263000	3.396613000	4.288166000
1	-0.360672000	3.724571000	4.664025000

6	-0.410692000	-0.796018000	1.847313000
6	0.560594000	-0.414647000	0.926802000
6	-0.140171000	-0.722783000	3.217857000
6	1.810351000	0.069536000	1.350974000
6	1.111605000	-0.300028000	3.657127000
6	2.081273000	0.080418000	2.730000000
1	2.770367000	-0.186963000	0.490365000
1	3.056268000	0.431438000	3.078037000
46	2.333245000	2.012862000	0.496415000
8	4.301632000	5.081611000	-1.127488000
8	2.691486000	3.839943000	-0.230137000
8	3.682489000	-0.656590000	-0.327829000
7	3.966015000	1.570197000	-0.528000000
6	4.743028000	2.750780000	-0.881064000
6	3.861536000	4.012258000	-0.767401000
6	4.333456000	0.329406000	-0.774875000
6	5.562684000	0.007152000	-1.586870000
1	5.881280000	0.822695000	-2.246001000
1	6.387719000	-0.231560000	-0.899062000
1	5.354908000	-0.892473000	-2.178668000
1	5.075548000	2.709136000	-1.930926000
1	1.325077000	-0.258409000	4.727147000
1	-0.909746000	-1.005406000	3.939359000
1	0.343066000	-0.468280000	-0.142174000
6	-1.736534000	-1.338660000	1.388531000
9	-2.749687000	-0.901162000	2.149650000
9	-1.769923000	-2.675273000	1.441140000
9	-2.011249000	-0.994802000	0.121840000
6	-1.418556000	2.869828000	2.990067000
6	-0.248336000	2.756599000	2.184412000
7	0.701160000	2.635301000	1.543960000
6	-2.470544000	3.497153000	5.070917000
1	-4.748059000	2.194701000	2.884960000
1	-4.597224000	3.136492000	5.159380000

1	-2.410968000	3.907679000	6.079490000
8	-2.663900000	1.919996000	1.229717000
14	-3.685594000	2.123309000	-0.150015000
6	-4.935877000	0.702447000	-0.175838000
1	-4.298995000	-0.188233000	-0.040626000
6	-4.451477000	3.838358000	0.096425000
1	-4.892524000	3.799481000	1.109557000
6	-2.523024000	1.951570000	-1.634713000
1	-2.547011000	0.870079000	-1.863238000
6	5.985790000	2.932523000	0.019504000
1	6.427320000	3.904501000	-0.245661000
1	6.727524000	2.155371000	-0.218740000
6	5.639626000	2.876485000	1.486824000
6	5.802966000	1.692700000	2.214456000
6	5.074180000	3.984169000	2.131312000
6	5.414163000	1.611548000	3.550950000
1	6.242598000	0.817964000	1.726928000
6	4.670808000	3.902115000	3.462327000
1	4.937910000	4.914912000	1.575035000
6	4.838998000	2.716415000	4.177501000
1	5.561414000	0.680442000	4.103664000
1	4.226378000	4.775108000	3.945474000
1	4.530825000	2.656403000	5.223916000
6	-5.955940000	0.714360000	0.967069000
1	-6.689405000	-0.098965000	0.842959000
1	-5.470037000	0.554765000	1.940230000
1	-6.525155000	1.658242000	1.013380000
6	-5.625279000	0.557357000	-1.541672000
1	-4.901438000	0.430015000	-2.360232000
1	-6.278947000	-0.329991000	-1.547583000
1	-6.257090000	1.425517000	-1.786973000
6	-5.594812000	4.173952000	-0.869847000
1	-6.013044000	5.167940000	-0.641151000
1	-5.258336000	4.197522000	-1.917277000

1	-6.420191000	3.449389000	-0.800886000
6	-3.378726000	4.937082000	0.111975000
1	-2.578175000	4.731470000	0.839431000
1	-2.902015000	5.052747000	-0.873696000
1	-3.820091000	5.911367000	0.377505000
6	-3.030370000	2.697315000	-2.878481000
1	-2.978591000	3.788824000	-2.741946000
1	-2.405274000	2.453635000	-3.752494000
1	-4.069655000	2.444455000	-3.138608000
6	-1.066791000	2.317347000	-1.329322000
1	-0.661618000	1.698797000	-0.519673000
1	-0.432490000	2.166175000	-2.217857000
1	-0.952303000	3.369822000	-1.025906000

Int-2m (CH_act_pdt)

Number of Imaginary Frequency: 0

Electronic Energy: HF= -2448.0360366

<i>Zero-point correction=</i>	<i>0.693062</i>
<i>(Hartree/Particle)</i>	
<i>Thermal correction to Energy=</i>	<i>0.737698</i>
<i>Thermal correction to Enthalpy=</i>	<i>0.738642</i>
<i>Thermal correction to Gibbs Free Energy=</i>	<i>0.617268</i>
<i>Sum of electronic and zero-point Energies=</i>	<i>-</i>
<i>2447.342974</i>	
<i>Sum of electronic and thermal Energies=</i>	<i>-</i>
<i>2447.298339</i>	
<i>Sum of electronic and thermal Enthalpies=</i>	<i>-</i>
<i>2447.297395</i>	
<i>Sum of electronic and thermal Free Energies=</i>	<i>-</i>
<i>2447.418769</i>	

6	-4.510430000	2.397663000	1.901916000
6	-4.586487000	3.236507000	3.007852000

6	-3.273041000	1.896229000	1.471539000
6	-2.209156000	3.126267000	3.316522000
1	-1.297145000	3.401705000	3.848531000
6	-0.467923000	-2.874096000	0.897022000
6	-0.155413000	-1.561174000	0.527673000
6	0.525544000	-3.743038000	1.340894000
6	1.161880000	-1.089745000	0.583414000
6	1.840472000	-3.284751000	1.409851000
6	2.152997000	-1.980967000	1.033156000
1	1.648399000	-1.336729000	-1.374235000
1	3.191402000	-1.647682000	1.088247000
46	1.676177000	0.804982000	0.188592000
8	4.341536000	3.738689000	-0.365629000
8	2.362987000	2.734746000	-0.098687000
8	2.251742000	-1.417127000	-2.141070000
7	3.157976000	0.432408000	-1.170596000
6	4.159827000	1.506779000	-1.145101000
6	3.589131000	2.789793000	-0.471617000
6	3.175869000	-0.481182000	-2.076865000
6	4.216026000	-0.641657000	-3.142400000
1	4.689104000	0.306906000	-3.417199000
1	4.996682000	-1.323591000	-2.772720000
1	3.755908000	-1.100612000	-4.025405000
1	4.379247000	1.834131000	-2.174168000
1	2.631301000	-3.951356000	1.761365000
1	0.274247000	-4.763845000	1.631143000
1	-0.962677000	-0.896702000	0.210554000
6	-1.903814000	-3.311500000	0.825567000
9	-2.688029000	-2.558768000	1.616027000
9	-2.080989000	-4.581431000	1.191097000
9	-2.401325000	-3.188803000	-0.419735000
6	-2.121115000	2.279715000	2.201497000
6	-0.859361000	1.797902000	1.744688000
7	0.139388000	1.406667000	1.323808000

6	-3.444502000	3.606279000	3.723410000
1	-5.417361000	2.120362000	1.366542000
1	-5.564447000	3.609773000	3.319489000
1	-3.520962000	4.265497000	4.588649000
8	-3.105929000	1.088162000	0.435854000
14	-3.977523000	0.537160000	-0.949588000
6	-5.026288000	-0.924583000	-0.365346000
1	-4.343324000	-1.462138000	0.313752000
6	-5.003678000	1.997497000	-1.581378000
1	-5.619335000	2.311272000	-0.719705000
6	-2.589902000	-0.028665000	-2.104955000
1	-2.316740000	-1.021345000	-1.701658000
6	5.488483000	1.078397000	-0.502098000
1	6.060711000	2.009612000	-0.369917000
1	6.053728000	0.445958000	-1.203980000
6	5.344578000	0.347197000	0.810640000
6	5.771690000	-0.978610000	0.935265000
6	4.770101000	0.969726000	1.928047000
6	5.631601000	-1.671883000	2.138623000
1	6.228672000	-1.477882000	0.075850000
6	4.610593000	0.274223000	3.123987000
1	4.452071000	2.013042000	1.861134000
6	5.041042000	-1.048816000	3.235278000
1	5.978373000	-2.705104000	2.214221000
1	4.151605000	0.773470000	3.979995000
1	4.917967000	-1.589741000	4.175917000
6	-6.258025000	-0.514381000	0.451435000
1	-6.820222000	-1.404825000	0.776787000
1	-5.984295000	0.038274000	1.362086000
1	-6.954165000	0.112394000	-0.130505000
6	-5.400884000	-1.904686000	-1.485909000
1	-4.512158000	-2.318323000	-1.983220000
1	-5.963833000	-2.757285000	-1.072575000
1	-6.037151000	-1.439231000	-2.256098000

6	-5.981489000	1.611937000	-2.700635000
1	-6.597526000	2.478948000	-2.990188000
1	-5.458127000	1.269949000	-3.605896000
1	-6.669528000	0.809921000	-2.393006000
6	-4.127053000	3.191692000	-1.979304000
1	-3.426737000	3.480522000	-1.180115000
1	-3.528660000	2.966047000	-2.876120000
1	-4.745399000	4.073308000	-2.213807000
6	-3.050375000	-0.230125000	-3.556758000
1	-3.259622000	0.736145000	-4.042981000
1	-2.257545000	-0.719978000	-4.144665000
1	-3.954390000	-0.850145000	-3.645019000
6	-1.333813000	0.851341000	-2.067173000
1	-0.985530000	1.046895000	-1.045727000
1	-0.506125000	0.365827000	-2.610352000
1	-1.507716000	1.828801000	-2.542797000

Int-1p (CH_act_para_reac)

Number of Imaginary Frequency: 0

Electronic Energy: HF= -2448.0169743

<i>Zero-point correction=</i>	<i>0.691791</i>
<i>(Hartree/Particle)</i>	
<i>Thermal correction to Energy=</i>	<i>0.737297</i>
<i>Thermal correction to Enthalpy=</i>	<i>0.738242</i>
<i>Thermal correction to Gibbs Free Energy=</i>	<i>0.613692</i>
<i>Sum of electronic and zero-point Energies=</i>	<i>-</i>
<i>2447.325183</i>	
<i>Sum of electronic and thermal Energies=</i>	<i>-</i>
<i>2447.279677</i>	
<i>Sum of electronic and thermal Enthalpies=</i>	<i>-</i>
<i>2447.278733</i>	

Sum of electronic and thermal Free Energies= -
2447.403282

6	-3.411179000	4.332164000	-0.970551000
6	-3.071439000	5.643744000	-0.661784000
6	-2.430428000	3.331299000	-0.996831000
6	-0.762911000	5.032882000	-0.393788000
1	0.274421000	5.280037000	-0.162290000
6	-0.188244000	-1.403844000	-2.958515000
6	0.899645000	-0.616612000	-2.594965000
6	-0.505231000	-2.534004000	-2.201148000
6	1.671571000	-0.961775000	-1.481546000
6	0.242018000	-2.864257000	-1.068451000
6	1.337814000	-2.084426000	-0.715496000
1	2.721139000	-0.536857000	-1.383486000
1	1.943892000	-2.348962000	0.152943000
46	2.239841000	0.692766000	0.090432000
8	3.008451000	1.789160000	3.791673000
8	2.369576000	1.860145000	1.671795000
7	3.806430000	-0.175262000	0.910997000
6	4.042674000	0.232855000	2.285298000
6	3.075991000	1.370733000	2.660288000
1	5.039741000	0.698641000	2.386416000
1	-0.019026000	-3.739249000	-0.470282000
1	1.165894000	0.257443000	-3.191409000
6	-1.098731000	3.704562000	-0.705781000
6	-0.095875000	2.693122000	-0.678325000
7	0.716501000	1.880019000	-0.591911000
6	-1.751153000	6.003864000	-0.371933000
1	-4.440885000	4.062037000	-1.203081000
1	-3.854486000	6.404987000	-0.647787000
1	-1.499487000	7.036631000	-0.128430000
8	-2.708164000	2.075247000	-1.325236000
14	-3.383143000	0.713188000	-0.504950000

6	-1.987836000	-0.011552000	0.538066000
1	-1.140279000	-0.018216000	-0.174227000
6	-4.847122000	1.371290000	0.497082000
1	-4.454041000	2.282504000	0.988270000
6	-3.817908000	-0.456450000	-1.918090000
1	-2.856520000	-0.961171000	-2.115480000
6	3.966176000	-0.903275000	3.320872000
1	3.996598000	-0.419534000	4.308961000
1	4.862748000	-1.533462000	3.236884000
6	2.735220000	-1.761981000	3.192084000
6	2.805000000	-3.025325000	2.595680000
6	1.491881000	-1.309728000	3.654313000
6	1.668845000	-3.825003000	2.468025000
1	3.768350000	-3.393817000	2.232439000
6	0.355662000	-2.105258000	3.527660000
1	1.424287000	-0.327620000	4.129609000
6	0.438730000	-3.366024000	2.934662000
1	1.748242000	-4.812801000	2.007579000
1	-0.603591000	-1.739448000	3.900941000
1	-0.453122000	-3.990349000	2.843477000
6	-1.585006000	0.853248000	1.740416000
1	-0.613136000	0.530322000	2.146476000
1	-1.488073000	1.921938000	1.495142000
1	-2.326060000	0.776222000	2.552214000
6	-2.219033000	-1.468306000	0.957644000
1	-2.424974000	-2.122015000	0.099845000
1	-1.319102000	-1.861694000	1.452321000
1	-3.056991000	-1.566379000	1.666788000
6	-5.301340000	0.411683000	1.606121000
1	-6.136935000	0.847070000	2.178235000
1	-5.654519000	-0.547295000	1.194761000
1	-4.495580000	0.190578000	2.320738000
6	-6.034310000	1.783232000	-0.384654000
1	-5.736596000	2.410748000	-1.238214000

1	-6.542508000	0.900121000	-0.801920000
1	-6.783563000	2.343933000	0.197661000
6	-4.831682000	-1.538337000	-1.519087000
1	-5.837365000	-1.112402000	-1.376649000
1	-4.907616000	-2.302162000	-2.308637000
1	-4.557476000	-2.060035000	-0.590464000
6	-4.236939000	0.243526000	-3.215329000
1	-3.497448000	0.992013000	-3.533477000
1	-4.350203000	-0.493106000	-4.027367000
1	-5.204576000	0.758346000	-3.102834000
1	-0.781391000	-1.153353000	-3.838852000
6	-1.604827000	-3.469012000	-2.643224000
9	-2.408418000	-3.810161000	-1.624984000
9	-1.103102000	-4.605009000	-3.133811000
9	-2.377746000	-2.933396000	-3.593927000
6	4.758016000	-0.696046000	0.103331000
6	6.057177000	-1.179353000	0.724416000
1	6.485386000	-0.465312000	1.441212000
1	5.887415000	-2.126862000	1.256871000
1	6.770652000	-1.357229000	-0.087675000
8	4.591086000	-0.828839000	-1.109764000

TS-1p (CH_act_para_TS)

One Imaginary Frequency: -991.9 cm⁻¹

Electronic Energy: HF= -2448.0090037

<i>Zero-point correction=</i>	<i>0.687844</i>
<i>(Hartree/Particle)</i>	
<i>Thermal correction to Energy=</i>	<i>0.732620</i>
<i>Thermal correction to Enthalpy=</i>	<i>0.733564</i>
<i>Thermal correction to Gibbs Free Energy=</i>	<i>0.612257</i>
<i>Sum of electronic and zero-point Energies=</i>	<i>-</i>
2447.321159	

Sum of electronic and thermal Energies= -
2447.276384

Sum of electronic and thermal Enthalpies= -
2447.275440

Sum of electronic and thermal Free Energies= -
2447.396747

6	-3.050194000	6.241519000	-0.280983000
6	-2.725806000	7.542022000	0.086335000
6	-2.067580000	5.242410000	-0.300257000
6	-0.429557000	6.922152000	0.429721000
1	0.597148000	7.160971000	0.712070000
6	0.323211000	0.583203000	-2.342328000
6	1.363221000	1.363185000	-1.845004000
6	-0.096656000	-0.541392000	-1.628804000
6	1.992932000	1.039509000	-0.632960000
6	0.507907000	-0.875618000	-0.415120000
6	1.546461000	-0.092198000	0.071937000
1	3.266829000	1.174730000	-0.592839000
1	2.034310000	-0.369677000	1.009024000
46	2.622346000	2.604736000	0.743859000
8	3.889342000	3.845364000	4.289288000
8	2.988226000	3.859583000	2.258193000
7	4.256864000	1.735115000	1.427500000
6	4.645018000	2.170843000	2.758473000
6	3.784158000	3.387743000	3.173689000
1	5.678050000	2.561542000	2.749958000
1	0.173580000	-1.751405000	0.144264000
1	1.703013000	2.230151000	-2.415746000
6	-0.749884000	5.605489000	0.058480000
6	0.255691000	4.596080000	0.088976000
7	1.072323000	3.787972000	0.176419000
6	-1.419538000	7.891879000	0.443523000
1	-4.068907000	5.979411000	-0.565442000

1	-3.509950000	8.302246000	0.093320000
1	-1.179597000	8.915762000	0.732292000
8	-2.329989000	3.997299000	-0.680851000
14	-3.037764000	2.613493000	0.070996000
6	-1.696713000	1.881108000	1.178667000
1	-0.812583000	1.881526000	0.512452000
6	-4.558719000	3.243850000	1.005104000
1	-4.197451000	4.146023000	1.535780000
6	-3.385761000	1.468974000	-1.384753000
1	-2.411035000	0.974706000	-1.538555000
6	4.573259000	1.065015000	3.826284000
1	4.698419000	1.569439000	4.796459000
1	5.423867000	0.379007000	3.700755000
6	3.288411000	0.275888000	3.797395000
6	3.270510000	-1.038815000	3.320260000
6	2.082193000	0.844542000	4.230021000
6	2.086216000	-1.775637000	3.278883000
1	4.203237000	-1.499215000	2.982500000
6	0.897126000	0.114009000	4.183656000
1	2.080653000	1.865609000	4.620322000
6	0.893508000	-1.198892000	3.709478000
1	2.098226000	-2.803826000	2.909814000
1	-0.032578000	0.570415000	4.530946000
1	-0.036175000	-1.771941000	3.684061000
6	-1.362547000	2.745290000	2.402528000
1	-0.399826000	2.440794000	2.842645000
1	-1.281447000	3.817912000	2.168852000
1	-2.133428000	2.645040000	3.183621000
6	-1.942204000	0.421547000	1.581743000
1	-2.087284000	-0.230683000	0.709503000
1	-1.072007000	0.033375000	2.133074000
1	-2.823432000	0.314857000	2.234655000
6	-5.069761000	2.261248000	2.068060000
1	-5.939606000	2.681231000	2.599269000

1	-5.392294000	1.307968000	1.619868000
1	-4.304596000	2.031733000	2.823576000
6	-5.696259000	3.671140000	0.066993000
1	-5.353262000	4.318302000	-0.754385000
1	-6.176319000	2.795953000	-0.397642000
1	-6.479666000	4.216560000	0.618132000
6	-4.412198000	0.374705000	-1.059365000
1	-5.426232000	0.792816000	-0.959125000
1	-4.443468000	-0.373391000	-1.866679000
1	-4.181463000	-0.164473000	-0.128730000
6	-3.738117000	2.190199000	-2.690085000
1	-2.986948000	2.948240000	-2.953376000
1	-3.800539000	1.467621000	-3.519831000
1	-4.713993000	2.697168000	-2.622156000
1	-0.155556000	0.838375000	-3.288839000
6	-1.150841000	-1.460176000	-2.193254000
9	-2.022619000	-1.851004000	-1.250677000
9	-0.608971000	-2.571175000	-2.699572000
9	-1.859181000	-0.884809000	-3.171274000
6	5.014111000	1.036383000	0.594681000
6	6.354480000	0.494297000	1.025716000
1	6.868037000	1.140752000	1.748399000
1	6.206692000	-0.491409000	1.491871000
1	6.978213000	0.360003000	0.134791000
8	4.625949000	0.775704000	-0.570940000

Int-2p (CH_act_para_pdt)

Number of Imaginary Frequency: 0

Electronic Energy: HF = -2448.0439033

Zero-point correction= 0.693350

(Hartree/Particle)

Thermal correction to Energy= 0.737747

Thermal correction to Enthalpy= 0.738691

Thermal correction to Gibbs Free Energy= 0.618558
 Sum of electronic and zero-point Energies= -
 2447.350553
 Sum of electronic and thermal Energies= -
 2447.306156
 Sum of electronic and thermal Enthalpies= -
 2447.305212
 Sum of electronic and thermal Free Energies= -
 2447.425345

6	-3.521699000	4.198886000	-0.375754000
6	-3.279195000	5.442257000	0.196094000
6	-2.496902000	3.247094000	-0.470721000
6	-0.983637000	4.859622000	0.600629000
1	0.014124000	5.092806000	0.976558000
6	-0.020006000	-1.373878000	-2.913736000
6	0.777953000	-0.457643000	-2.229030000
6	-0.419778000	-2.551991000	-2.284539000
6	1.204494000	-0.700808000	-0.912808000
6	-0.000530000	-2.818237000	-0.979632000
6	0.802144000	-1.903178000	-0.306514000
1	3.004766000	-1.382646000	-1.481941000
1	1.114933000	-2.122526000	0.716325000
46	2.251980000	0.639156000	0.137208000
8	4.758934000	1.980255000	2.985086000
8	3.290517000	1.989251000	1.302672000
7	3.958874000	-0.454571000	0.445497000
6	4.657486000	0.029808000	1.645420000
6	4.211409000	1.469002000	2.026559000
1	5.734316000	0.127947000	1.437271000
1	-0.316123000	-3.737311000	-0.481116000
1	1.064371000	0.468935000	-2.733017000
6	-1.221466000	3.599706000	0.026082000
6	-0.167183000	2.641714000	-0.033254000

7	0.698166000	1.881464000	-0.035272000
6	-2.014753000	5.781726000	0.687509000
1	-4.508033000	3.948519000	-0.765403000
1	-4.095247000	6.165581000	0.257443000
1	-1.838007000	6.761167000	1.133392000
8	-2.678486000	2.059311000	-1.039173000
14	-3.452356000	0.600165000	-0.532440000
6	-2.323544000	-0.146875000	0.781742000
1	-1.324511000	-0.070916000	0.312448000
6	-5.153502000	1.115476000	0.119862000
1	-4.937605000	1.967439000	0.793031000
6	-3.466324000	-0.465222000	-2.086061000
1	-2.474165000	-0.947400000	-2.059059000
6	4.495414000	-0.914230000	2.848625000
1	4.998104000	-0.409970000	3.687276000
1	5.035655000	-1.854397000	2.657294000
6	3.061237000	-1.223227000	3.203560000
6	2.518403000	-2.487823000	2.955696000
6	2.239459000	-0.243925000	3.779731000
6	1.189294000	-2.775007000	3.269630000
1	3.148562000	-3.265449000	2.514100000
6	0.909806000	-0.524320000	4.082331000
1	2.654432000	0.742729000	3.999005000
6	0.378680000	-1.790003000	3.829256000
1	0.786782000	-3.771845000	3.074466000
1	0.285975000	0.250963000	4.533114000
1	-0.662072000	-2.009554000	4.078438000
6	-2.292726000	0.658893000	2.086398000
1	-1.496838000	0.286661000	2.749681000
1	-2.100893000	1.730585000	1.921678000
1	-3.245976000	0.579493000	2.634092000
6	-2.570653000	-1.637137000	1.049212000
1	-2.523375000	-2.236309000	0.128289000
1	-1.798495000	-2.031417000	1.730057000

1	-3.550404000	-1.817310000	1.520129000
6	-5.843775000	0.034641000	0.963210000
1	-6.814219000	0.396972000	1.340554000
1	-6.042948000	-0.875725000	0.376492000
1	-5.242325000	-0.257992000	1.836205000
6	-6.081335000	1.617387000	-0.995561000
1	-5.591739000	2.343007000	-1.663345000
1	-6.425326000	0.785363000	-1.629269000
1	-6.980224000	2.099275000	-0.577111000
6	-4.519452000	-1.581717000	-2.037390000
1	-5.541462000	-1.177607000	-2.110919000
1	-4.380132000	-2.275986000	-2.880181000
1	-4.463401000	-2.179165000	-1.114921000
6	-3.550824000	0.325994000	-3.395570000
1	-2.768108000	1.095415000	-3.457578000
1	-3.434712000	-0.351621000	-4.257017000
1	-4.524179000	0.831285000	-3.503398000
1	-0.352064000	-1.158863000	-3.930934000
6	-1.296797000	-3.546370000	-2.993845000
9	-2.237728000	-4.040889000	-2.173422000
9	-0.604132000	-4.592842000	-3.456776000
9	-1.933690000	-3.003371000	-4.039301000
6	4.483781000	-1.357862000	-0.307856000
6	5.788365000	-2.056807000	-0.073622000
1	6.473022000	-1.485772000	0.560827000
1	5.587350000	-3.024340000	0.410680000
1	6.258717000	-2.260846000	-1.043214000
8	3.888866000	-1.791869000	-1.397964000

Int-Im (CH_act_wl_reac)

Number of Imaginary Frequency: 0

Electronic Energy: HF = -2434.6503983

Zero-point correction= 0.759319
 (Hartree/Particle)
 Thermal correction to Energy= 0.808426
 Thermal correction to Enthalpy= 0.809370
 Thermal correction to Gibbs Free Energy= 0.676746
 Sum of electronic and zero-point Energies= -
 2433.891080
 Sum of electronic and thermal Energies= -
 2433.841972
 Sum of electronic and thermal Enthalpies= -
 2433.841028
 Sum of electronic and thermal Free Energies= -
 2433.973652

6	-3.699357000	1.356080000	3.059189000
6	-3.385940000	1.713680000	4.365563000
6	-2.714743000	0.833381000	2.207938000
6	-1.105686000	1.026136000	4.059379000
1	-0.083992000	0.893496000	4.419297000
6	-0.608855000	-3.073593000	-0.345626000
6	0.783387000	-3.064014000	-0.602781000
6	-1.079569000	-3.238906000	0.942650000
6	1.684465000	-3.226285000	0.465098000
6	-0.176871000	-3.409882000	2.008392000
6	1.183594000	-3.400607000	1.777359000
1	2.759266000	-3.319936000	0.282855000
1	1.889276000	-3.532147000	2.599084000
46	1.740945000	-0.937114000	-0.128149000
8	2.210422000	0.976199000	-0.450123000
8	4.554400000	-2.129560000	-0.225921000
6	2.508320000	1.735169000	0.564444000
6	4.197352000	-1.725735000	-1.321086000
6	5.162745000	-1.593734000	-2.511375000

1	-0.562042000	-3.543344000	3.020989000
1	-2.153969000	-3.230710000	1.133462000
1	1.151764000	-3.052430000	-1.630304000
6	-1.577912000	-2.967200000	-1.495692000
9	-2.728918000	-2.390487000	-1.119365000
9	-1.889029000	-4.171430000	-1.985838000
9	-1.080016000	-2.248586000	-2.503318000
6	-1.416220000	0.658208000	2.740739000
6	-0.414599000	0.095707000	1.900679000
7	0.388234000	-0.368379000	1.220531000
6	-2.092381000	1.560310000	4.873408000
1	-4.716178000	1.476577000	2.686198000
1	-4.172108000	2.122829000	5.003896000
1	-1.860643000	1.853675000	5.897828000
8	-2.939887000	0.478353000	0.947726000
14	-3.711683000	1.244322000	-0.400597000
6	-5.344321000	0.318946000	-0.626579000
1	-5.029261000	-0.740648000	-0.588557000
6	-3.893829000	3.063005000	0.098388000
1	-4.385597000	3.038834000	1.086971000
6	-2.589802000	0.942504000	-1.892379000
1	-2.908853000	-0.042901000	-2.276826000
6	-6.346963000	0.547744000	0.509273000
1	-7.274443000	-0.022284000	0.336767000
1	-5.945347000	0.219270000	1.479554000
1	-6.631951000	1.609382000	0.600029000
6	-5.986554000	0.549572000	-2.001864000
1	-5.305771000	0.285111000	-2.824644000
1	-6.890270000	-0.071091000	-2.115113000
1	-6.293955000	1.597481000	-2.146660000
6	-4.809035000	3.880483000	-0.823516000
1	-4.912311000	4.911067000	-0.446243000
1	-4.413038000	3.948760000	-1.847379000
1	-5.821404000	3.453190000	-0.885825000

6	-2.527427000	3.738402000	0.288019000
1	-1.879949000	3.186376000	0.987556000
1	-1.980640000	3.824077000	-0.663773000
1	-2.646715000	4.757884000	0.689129000
6	-2.805741000	1.967236000	-3.016345000
1	-2.435496000	2.963790000	-2.729007000
1	-2.247558000	1.665357000	-3.916869000
1	-3.862254000	2.075087000	-3.306487000
6	-1.107228000	0.826709000	-1.529966000
1	-0.934208000	-0.023646000	-0.861962000
1	-0.490365000	0.669628000	-2.428593000
1	-0.719083000	1.723941000	-1.024047000
8	2.984344000	-1.349120000	-1.608086000
8	2.568907000	1.374618000	1.725601000
6	2.771401000	3.195787000	0.137879000
6	6.509705000	-2.219936000	-2.148978000
1	7.216257000	-2.108127000	-2.986671000
1	6.940169000	-1.741540000	-1.258531000
1	6.402348000	-3.291852000	-1.926549000
6	4.561985000	-2.289658000	-3.740964000
1	4.405369000	-3.363816000	-3.552598000
1	3.595483000	-1.843272000	-4.012297000
1	5.244772000	-2.195226000	-4.600297000
6	5.328905000	-0.090592000	-2.792228000
1	5.739691000	0.430849000	-1.914005000
1	6.020152000	0.063969000	-3.636074000
1	4.361422000	0.369544000	-3.037510000
6	3.941356000	3.215703000	-0.856691000
1	4.855713000	2.809764000	-0.396701000
1	3.711190000	2.611885000	-1.745128000
1	4.152152000	4.248866000	-1.176531000
6	3.108671000	4.030410000	1.373716000
1	3.302903000	5.075455000	1.083820000
1	2.282027000	4.015983000	2.098633000

1	3.998554000	3.636694000	1.884592000
6	1.501831000	3.736691000	-0.538170000
1	1.259377000	3.154574000	-1.438324000
1	0.639050000	3.688433000	0.146163000
1	1.642284000	4.790296000	-0.828388000

TS-Im (CH_act_wl_TS)

One Imaginary Frequency: -1305.2 cm⁻¹

Electronic Energy: HF = -2198.7131143

<i>Zero-point correction=</i>	<i>0.584976</i>
<i>(Hartree/Particle)</i>	
<i>Thermal correction to Energy=</i>	<i>0.625400</i>
<i>Thermal correction to Enthalpy=</i>	<i>0.626345</i>
<i>Thermal correction to Gibbs Free Energy=</i>	<i>0.513355</i>
<i>Sum of electronic and zero-point Energies=</i>	<i>-</i>
2198.128138	
<i>Sum of electronic and thermal Energies=</i>	<i>-</i>
2198.087714	
<i>Sum of electronic and thermal Enthalpies=</i>	<i>-</i>
2198.086770	
<i>Sum of electronic and thermal Free Energies=</i>	<i>-</i>
2198.199759	

6	-3.739107000	2.610894000	3.241588000
6	-3.642254000	3.224922000	4.484986000
6	-2.604978000	2.456161000	2.432049000
6	-1.282696000	3.554736000	4.189516000
1	-0.311774000	3.915100000	4.533768000
6	-0.366540000	-0.836606000	1.828658000
6	0.659436000	-0.455678000	0.967527000
6	-0.195614000	-0.725780000	3.211650000

6	1.860959000	0.079991000	1.463395000
6	1.011533000	-0.259765000	3.726923000
6	2.028030000	0.133399000	2.859138000
1	2.962047000	-0.208084000	0.746521000
1	2.963074000	0.524218000	3.269656000
46	2.367705000	1.989943000	0.534312000
8	2.602302000	3.818786000	-0.251764000
8	3.984395000	-0.658250000	0.139327000
6	2.810543000	4.782912000	0.596715000
6	4.489855000	0.299103000	-0.501577000
6	5.749161000	0.052748000	-1.286246000
1	5.857145000	0.797733000	-2.082403000
1	6.603653000	0.145270000	-0.599206000
1	5.747659000	-0.965920000	-1.692366000
1	1.148939000	-0.188779000	4.807693000
1	-1.007830000	-1.009426000	3.883951000
1	0.513913000	-0.540589000	-0.111907000
6	-1.646996000	-1.412322000	1.287742000
9	-2.708343000	-1.056192000	2.023654000
9	-1.622312000	-2.749865000	1.270901000
9	-1.884609000	-1.015746000	0.028228000
6	-1.373220000	2.937083000	2.932523000
6	-0.202566000	2.765794000	2.139060000
7	0.749769000	2.597197000	1.516548000
6	-2.420420000	3.702124000	4.967849000
1	-4.698837000	2.238101000	2.886244000
1	-4.543398000	3.331781000	5.092804000
1	-2.359673000	4.183189000	5.944692000
8	-2.625789000	1.876386000	1.237055000
14	-3.623448000	2.065333000	-0.162188000
6	-4.882842000	0.653610000	-0.167389000
1	-4.251043000	-0.237743000	-0.012593000
6	-4.376803000	3.792748000	0.036414000
1	-4.825557000	3.783744000	1.046645000

6	-2.452988000	1.854626000	-1.636166000
1	-2.488527000	0.769909000	-1.845391000
6	-5.901622000	0.696998000	0.975603000
1	-6.632992000	-0.121810000	0.878020000
1	-5.413522000	0.570123000	1.952672000
1	-6.472978000	1.640570000	0.993200000
6	-5.571693000	0.484379000	-1.530265000
1	-4.847307000	0.338888000	-2.345421000
1	-6.228639000	-0.400527000	-1.520048000
1	-6.199973000	1.350031000	-1.792816000
6	-5.510705000	4.112689000	-0.946214000
1	-5.922272000	5.115550000	-0.745765000
1	-5.167642000	4.106483000	-1.991726000
1	-6.342400000	3.396852000	-0.863892000
6	-3.295881000	4.883676000	0.032144000
1	-2.506413000	4.694689000	0.775960000
1	-2.806287000	4.966108000	-0.950589000
1	-3.733197000	5.868573000	0.263158000
6	-2.942392000	2.582681000	-2.897212000
1	-2.881836000	3.676070000	-2.780999000
1	-2.312700000	2.316471000	-3.761368000
1	-3.981913000	2.334481000	-3.161121000
6	-0.994769000	2.205565000	-1.325052000
1	-0.606019000	1.590090000	-0.505144000
1	-0.354976000	2.036060000	-2.206350000
1	-0.866745000	3.259436000	-1.031628000
8	4.021839000	1.469099000	-0.508709000
8	2.858047000	4.661265000	1.808542000
6	3.004003000	6.124683000	-0.089410000
1	3.099278000	6.918196000	0.661218000
1	3.910861000	6.089645000	-0.710296000
1	2.157772000	6.332879000	-0.759161000

Int-Im (CH_act_wl_pdt)

Number of Imaginary Frequency: 0

Electronic Energy: HF = -2434.6676151

Zero-point correction= 0.756264
(Hartree/Particle)
Thermal correction to Energy= 0.803470
Thermal correction to Enthalpy= 0.804415
Thermal correction to Gibbs Free Energy= 0.678246
Sum of electronic and zero-point Energies= -
2433.911352
Sum of electronic and thermal Energies= -
2433.864145
Sum of electronic and thermal Enthalpies= -
2433.863200
Sum of electronic and thermal Free Energies= -
2433.989369

6	-3.678440000	4.037154000	1.681710000
6	-3.380284000	4.745032000	2.839844000
6	-2.714256000	3.204785000	1.097665000
6	-1.146285000	3.849912000	2.872403000
1	-0.150573000	3.772386000	3.312582000
6	-0.374073000	-1.697139000	-3.120012000
6	0.374623000	-0.658921000	-2.564746000
6	-0.934935000	-2.683996000	-2.306874000
6	0.562277000	-0.581427000	-1.181313000
6	-0.749455000	-2.611519000	-0.929629000
6	-0.017585000	-1.561738000	-0.368596000
1	4.224669000	-0.420815000	0.651297000
1	0.115502000	-1.524584000	0.715862000
46	1.795706000	0.758259000	-0.436097000
8	3.146318000	2.150521000	0.432283000
8	4.334855000	-1.292715000	0.003838000
6	3.959445000	1.786715000	1.321894000

6	3.910947000	-1.158165000	-1.191365000
6	4.234651000	-2.284714000	-2.166317000
1	-1.177541000	-3.381301000	-0.283746000
1	-1.512409000	-3.497122000	-2.748867000
1	0.825608000	0.087289000	-3.222273000
6	-0.503929000	-1.792272000	-4.616264000
9	-1.604209000	-2.462102000	-4.985344000
9	0.540922000	-2.431166000	-5.161363000
9	-0.563042000	-0.586414000	-5.195475000
6	-1.441514000	3.127173000	1.705225000
6	-0.458615000	2.310139000	1.072646000
7	0.330700000	1.661357000	0.539802000
6	-2.120694000	4.653984000	3.443598000
1	-4.657791000	4.117103000	1.207551000
1	-4.145197000	5.386739000	3.282583000
1	-1.901783000	5.218069000	4.350956000
8	-2.941946000	2.516735000	-0.013908000
14	-3.810046000	1.053518000	-0.306635000
6	-3.446427000	-0.087550000	1.159110000
1	-2.349615000	-0.001989000	1.286120000
6	-5.623432000	1.582357000	-0.390835000
1	-5.787883000	2.105713000	0.570856000
6	-3.042013000	0.398712000	-1.895458000
1	-2.179592000	-0.187786000	-1.531725000
6	-4.117809000	0.350789000	2.467011000
1	-3.817181000	-0.306079000	3.299689000
1	-3.857949000	1.381004000	2.753794000
1	-5.216159000	0.296301000	2.391643000
6	-3.746748000	-1.560610000	0.849012000
1	-3.217203000	-1.906670000	-0.049838000
1	-3.430045000	-2.204712000	1.686008000
1	-4.823264000	-1.736591000	0.695113000
6	-6.623917000	0.421132000	-0.448695000
1	-7.659350000	0.799653000	-0.450888000

1	-6.497292000	-0.183266000	-1.359789000
1	-6.525713000	-0.254445000	0.414396000
6	-5.858773000	2.592634000	-1.521191000
1	-5.147739000	3.432067000	-1.476954000
1	-5.745285000	2.118324000	-2.509184000
1	-6.878222000	3.009674000	-1.475448000
6	-3.957330000	-0.561064000	-2.667688000
1	-4.812640000	-0.030215000	-3.116423000
1	-3.402042000	-1.039447000	-3.489628000
1	-4.360525000	-1.367997000	-2.036131000
6	-2.484085000	1.492796000	-2.813627000
1	-1.759280000	2.131187000	-2.289228000
1	-1.971364000	1.035302000	-3.674029000
1	-3.281506000	2.143252000	-3.208090000
8	3.207869000	-0.206046000	-1.584303000
8	4.330496000	0.605663000	1.527462000
6	4.505021000	2.898565000	2.234089000
6	3.185437000	-3.381152000	-1.881878000
1	3.344337000	-4.226323000	-2.568894000
1	3.267785000	-3.751931000	-0.849685000
1	2.163790000	-3.001519000	-2.037651000
6	4.087193000	-1.798877000	-3.610850000
1	3.059848000	-1.472545000	-3.818741000
1	4.763749000	-0.958014000	-3.823716000
1	4.331539000	-2.620700000	-4.300703000
6	5.647165000	-2.822063000	-1.912221000
1	5.761592000	-3.165345000	-0.875423000
1	5.850183000	-3.667806000	-2.586547000
1	6.406553000	-2.047722000	-2.100670000
6	5.190993000	3.951625000	1.350467000
1	6.051300000	3.519061000	0.816517000
1	4.490334000	4.350701000	0.604054000
1	5.560750000	4.784371000	1.969507000
6	5.493876000	2.332289000	3.253512000

1	5.875494000	3.139381000	3.898906000
1	5.019028000	1.571211000	3.888652000
1	6.347650000	1.854324000	2.752735000
6	3.302407000	3.533520000	2.953004000
1	2.587950000	3.940780000	2.222910000
1	2.779711000	2.790863000	3.577657000
1	3.638953000	4.351270000	3.609787000

Int-3m (Olefin_reac)

Number of Imaginary Frequency: 0

Electronic Energy: HF = -2754.5462343

<i>Zero-point correction=</i>	<i>0.790384</i>
<i>(Hartree/Particle)</i>	
<i>Thermal correction to Energy=</i>	<i>0.842797</i>
<i>Thermal correction to Enthalpy=</i>	<i>0.843741</i>
<i>Thermal correction to Gibbs Free Energy=</i>	<i>0.704440</i>
<i>Sum of electronic and zero-point Energies=</i>	<i>-</i>
<i>2753.755850</i>	
<i>Sum of electronic and thermal Energies=</i>	<i>-</i>
<i>2753.703437</i>	
<i>Sum of electronic and thermal Enthalpies=</i>	<i>-</i>
<i>2753.702493</i>	
<i>Sum of electronic and thermal Free Energies=</i>	<i>-</i>
<i>2753.841795</i>	

6	-2.784188000	-4.009411000	0.720454000
6	-1.764160000	-3.183491000	0.246515000
6	-2.719387000	-4.545899000	2.007821000
6	-0.673740000	-2.877485000	1.063411000
6	-1.624340000	-4.250326000	2.814025000
1	-3.516475000	-5.196525000	2.372478000

6	-0.602010000	-3.420547000	2.347183000
1	0.262520000	-3.209438000	2.981813000
7	-0.736898000	-0.139405000	1.034280000
46	0.682332000	-1.513679000	0.509752000
6	2.519548000	-2.580836000	0.020584000
6	1.500158000	-3.444792000	-0.298132000
6	3.234255000	-2.676259000	1.336204000
8	2.875407000	-3.357849000	2.262093000
8	4.310552000	-1.899066000	1.334630000
6	4.951901000	-1.698770000	2.587810000
1	5.888934000	-1.174457000	2.370100000
1	4.304193000	-1.075164000	3.220499000
1	-1.560533000	-4.672777000	3.819169000
1	2.970755000	-1.927729000	-0.728586000
1	-1.829263000	-2.785761000	-0.767603000
6	-3.717488000	3.436653000	0.050204000
6	-4.249799000	3.871979000	1.257795000
6	-2.804560000	2.374911000	0.027644000
6	-2.973093000	2.231889000	2.472975000
1	-2.667359000	1.753940000	3.404954000
6	-2.433664000	1.784273000	1.257772000
6	-1.494889000	0.714742000	1.183882000
6	-3.886255000	3.275288000	2.470910000
1	-3.989245000	3.911175000	-0.894076000
1	-4.961970000	4.700046000	1.256991000
1	-4.312616000	3.631082000	3.409484000
8	-2.239409000	1.943624000	-1.086957000
14	-2.640366000	1.012147000	-2.479384000
6	-4.375649000	0.296181000	-2.249767000
6	-2.514248000	2.226170000	-3.914423000
1	-3.465309000	2.790881000	-3.895637000
6	-1.380414000	-0.395037000	-2.475753000
1	-1.397010000	-0.726581000	-1.422372000
6	-5.524234000	1.301556000	-2.390758000

1	-6.498273000	0.790160000	-2.322147000
1	-5.500807000	2.056719000	-1.589428000
1	-5.499461000	1.832498000	-3.354484000
6	-2.441426000	1.494190000	-5.261776000
1	-2.486978000	2.208857000	-6.099287000
1	-1.497001000	0.936731000	-5.364062000
1	-3.268088000	0.777330000	-5.397010000
6	-1.375167000	3.241660000	-3.739488000
1	-1.521332000	3.856661000	-2.839438000
1	-0.383843000	2.775784000	-3.635430000
1	-1.332572000	3.923034000	-4.605003000
6	-1.794201000	-1.595605000	-3.336773000
1	-1.860544000	-1.334669000	-4.404982000
1	-1.046304000	-2.402227000	-3.250913000
1	-2.762503000	-2.021138000	-3.033429000
6	0.051803000	0.053455000	-2.781357000
1	0.384391000	0.876561000	-2.136704000
1	0.757937000	-0.778511000	-2.621650000
1	0.163520000	0.382718000	-3.826100000
6	-3.989391000	-4.302368000	-0.133867000
9	-3.806148000	-3.951874000	-1.413553000
9	-4.305775000	-5.601328000	-0.120011000
9	-5.071621000	-3.638245000	0.299735000
6	-4.489964000	-0.502011000	-0.942359000
1	-3.661240000	-1.212140000	-0.805652000
1	-4.497867000	0.166751000	-0.066417000
1	-5.422118000	-1.086629000	-0.912115000
1	-4.463798000	-0.422411000	-3.087025000
1	5.153735000	-2.658016000	3.083088000
7	3.175421000	2.415997000	-0.649500000
6	1.975675000	2.855075000	-1.127503000
8	1.834553000	3.116753000	-2.309877000
6	0.840815000	3.076429000	-0.149659000
1	-0.087214000	2.756442000	-0.639264000

1	0.943200000	2.560959000	0.812056000
1	0.763444000	4.158230000	0.039823000
6	3.464813000	1.818057000	0.636575000
1	4.438413000	1.313534000	0.516385000
6	2.515777000	0.656927000	1.013096000
6	3.632219000	2.835165000	1.778852000
1	3.774825000	2.262488000	2.704521000
1	2.699565000	3.406390000	1.900469000
8	1.928336000	0.110028000	0.017858000
8	2.426208000	0.306484000	2.185705000
6	4.787893000	3.772000000	1.542194000
6	4.631302000	4.931639000	0.774017000
6	6.061369000	3.472038000	2.039917000
6	5.714728000	5.768036000	0.511587000
1	3.644925000	5.179569000	0.374191000
6	7.148482000	4.305194000	1.780355000
1	6.200146000	2.571574000	2.645630000
6	6.978047000	5.456983000	1.013445000
1	5.571146000	6.668928000	-0.089351000
1	8.133206000	4.055608000	2.182383000
1	7.827482000	6.112687000	0.809636000
1	1.244556000	-4.257957000	0.382570000
1	1.116060000	-3.503854000	-1.319191000
1	3.857883000	2.292890000	-1.387382000

Ts-2m (Olefin_TS)

One Imaginary Frequency: -283.4 cm⁻¹

Electronic Energy: HF = -2754.5369555

Zero-point correction= 0.790552

(Hartree/Particle)

Thermal correction to Energy= 0.842936

Thermal correction to Enthalpy= *0.843880*
Thermal correction to Gibbs Free Energy= *0.703851*
Sum of electronic and zero-point Energies= *-*
2753.746403
Sum of electronic and thermal Energies= *-*
2753.694020
Sum of electronic and thermal Enthalpies= *-*
2753.693076
Sum of electronic and thermal Free Energies= *-*
2753.833104

6	-3.310616000	-2.167419000	-0.894946000
6	-2.026390000	-1.724808000	-1.212482000
6	-3.676814000	-2.373029000	0.435531000
6	-1.101558000	-1.469762000	-0.196263000
6	-2.743298000	-2.149880000	1.446545000
1	-4.684618000	-2.713372000	0.678133000
6	-1.457316000	-1.714575000	1.136026000
1	-0.721887000	-1.550589000	1.928285000
7	-1.347956000	1.443316000	-0.141721000
46	0.225746000	0.088045000	-0.477485000
6	1.829069000	-1.171564000	-0.698960000
6	0.779591000	-2.124799000	-0.711200000
6	2.622637000	-1.030937000	0.561875000
8	2.306283000	-1.528600000	1.615118000
8	3.709668000	-0.290542000	0.374257000
6	4.427163000	0.081702000	1.544036000
1	5.339140000	0.579191000	1.195075000
1	3.813328000	0.776752000	2.134657000
1	-3.021523000	-2.318538000	2.488787000
1	2.316982000	-0.863294000	-1.627760000
1	-1.755302000	-1.561957000	-2.258339000
6	-4.177279000	5.176422000	-1.059639000
6	-4.674394000	5.612748000	0.162680000

6	-3.317234000	4.073101000	-1.115285000
6	-3.462994000	3.888637000	1.326702000
1	-3.167448000	3.378797000	2.244996000
6	-2.960790000	3.439765000	0.096385000
6	-2.072714000	2.328034000	0.000928000
6	-4.325097000	4.974568000	1.358242000
1	-4.437424000	5.681137000	-1.991290000
1	-5.346056000	6.473638000	0.187230000
1	-4.720842000	5.331611000	2.309732000
8	-2.790374000	3.643764000	-2.252712000
14	-3.288725000	2.622978000	-3.549070000
6	-4.978920000	1.886831000	-3.115615000
6	-3.369977000	3.779398000	-5.034602000
1	-4.003084000	4.612165000	-4.671435000
6	-2.000287000	1.250442000	-3.641480000
1	-2.220630000	0.637962000	-2.747899000
6	-6.145616000	2.879169000	-3.207242000
1	-7.108306000	2.365275000	-3.051161000
1	-6.066843000	3.658160000	-2.432379000
1	-6.196528000	3.384685000	-4.183104000
6	-4.062153000	3.167401000	-6.260180000
1	-4.170755000	3.917778000	-7.060327000
1	-3.476954000	2.333956000	-6.678265000
1	-5.067760000	2.780718000	-6.033019000
6	-1.995120000	4.358548000	-5.400854000
1	-1.422909000	4.714754000	-4.530375000
1	-1.374367000	3.599051000	-5.902018000
1	-2.101999000	5.200888000	-6.103479000
6	-2.198468000	0.359508000	-4.875094000
1	-1.909277000	0.889822000	-5.796451000
1	-1.561130000	-0.538356000	-4.811577000
1	-3.235784000	0.011700000	-4.995822000
6	-0.549057000	1.724215000	-3.522430000
1	-0.373203000	2.311952000	-2.613976000

1	0.135123000	0.859413000	-3.477947000
1	-0.237799000	2.346404000	-4.373445000
6	-4.285516000	-2.481703000	-2.000688000
9	-4.076603000	-1.720113000	-3.083653000
9	-4.182395000	-3.754815000	-2.398643000
9	-5.552752000	-2.291874000	-1.619249000
6	-4.995398000	1.155259000	-1.764532000
1	-4.119495000	0.506339000	-1.618060000
1	-5.022264000	1.870411000	-0.927255000
1	-5.888614000	0.517598000	-1.674723000
1	-5.122530000	1.122859000	-3.903923000
1	4.679622000	-0.801342000	2.146928000
7	2.545725000	4.044840000	-1.680930000
6	1.333512000	4.501932000	-2.108105000
8	1.140040000	4.763626000	-3.282848000
6	0.251289000	4.741937000	-1.076537000
1	-0.710117000	4.567991000	-1.572900000
1	0.323120000	4.117517000	-0.177827000
1	0.289827000	5.798294000	-0.767968000
6	2.896951000	3.494208000	-0.388252000
1	3.876188000	3.007624000	-0.532766000
6	1.986478000	2.326590000	0.063791000
6	3.084636000	4.550727000	0.714009000
1	3.276216000	4.011171000	1.650591000
1	2.143727000	5.102389000	0.857820000
8	1.429885000	1.706220000	-0.905745000
8	1.895731000	2.048913000	1.253544000
6	4.207854000	5.505505000	0.404314000
6	3.996924000	6.634222000	-0.396367000
6	5.504698000	5.252593000	0.866636000
6	5.050021000	7.486026000	-0.724553000
1	2.991922000	6.845975000	-0.769754000
6	6.561713000	6.101270000	0.541334000
1	5.686082000	4.376864000	1.496828000

6	6.337053000	7.221798000	-0.257255000
1	4.863906000	8.361984000	-1.350181000
1	7.565448000	5.888354000	0.916573000
1	7.162800000	7.889579000	-0.512777000
1	0.727931000	-2.808355000	0.138110000
1	0.475290000	-2.546895000	-1.670447000
1	3.192953000	3.897814000	-2.445447000

Int-4m (Olefin_pdt)

Number of Imaginary Frequency: 0

Electronic Energy: HF = -2754.5774087

Zero-point correction= 0.792419
(Hartree/Particle)
Thermal correction to Energy= 0.844957
Thermal correction to Enthalpy= 0.845902
Thermal correction to Gibbs Free Energy= 0.704622
Sum of electronic and zero-point Energies= -
2753.784989
Sum of electronic and thermal Energies= -
2753.732451
Sum of electronic and thermal Enthalpies= -
2753.731507
Sum of electronic and thermal Free Energies= -
2753.872787

6	-2.354065000	-3.711354000	0.182068000
6	-1.048459000	-3.879778000	-0.244322000
6	-2.633267000	-3.374992000	1.519362000
6	0.027270000	-3.762417000	0.666910000
6	-1.595994000	-3.230614000	2.418913000
1	-3.667393000	-3.243679000	1.838839000
6	-0.259560000	-3.424205000	2.009878000

1	0.544767000	-3.460771000	2.751470000
7	-0.989763000	-0.252324000	1.254207000
46	0.660828000	-1.562406000	0.884840000
6	2.222339000	-2.767271000	0.458151000
6	1.464356000	-4.072995000	0.264080000
6	3.109002000	-2.709887000	1.656291000
8	2.940236000	-3.358547000	2.665706000
8	4.108640000	-1.840024000	1.501880000
6	4.864663000	-1.529702000	2.662885000
1	5.715590000	-0.928859000	2.320854000
1	4.243240000	-0.943167000	3.354940000
1	-1.803649000	-2.982239000	3.460754000
1	2.702174000	-2.352936000	-0.435683000
1	-0.839118000	-4.148749000	-1.282429000
6	-3.612076000	3.509294000	-0.051889000
6	-4.156993000	4.048635000	1.107679000
6	-2.789659000	2.378935000	0.020367000
6	-3.069480000	2.376856000	2.456831000
1	-2.841466000	1.927415000	3.424632000
6	-2.521264000	1.822484000	1.291574000
6	-1.677747000	0.671714000	1.312962000
6	-3.892574000	3.489699000	2.363064000
1	-3.804065000	3.954788000	-1.029232000
1	-4.797929000	4.929933000	1.034271000
1	-4.323870000	3.928729000	3.263448000
8	-2.211938000	1.841855000	-1.042964000
14	-2.714663000	0.896488000	-2.393053000
6	-4.430487000	0.196511000	-2.000529000
6	-2.734543000	2.097595000	-3.845407000
1	-3.384418000	2.919253000	-3.485435000
6	-1.453272000	-0.499947000	-2.490959000
1	-1.722619000	-1.161081000	-1.645712000
6	-5.591828000	1.180826000	-2.190765000
1	-6.559795000	0.678174000	-2.030141000

1	-5.534892000	2.008855000	-1.466346000
1	-5.613506000	1.621973000	-3.198007000
6	-3.372991000	1.525201000	-5.118709000
1	-3.464544000	2.305572000	-5.891805000
1	-2.758530000	0.718810000	-5.547031000
1	-4.379389000	1.113476000	-4.945789000
6	-1.345427000	2.685588000	-4.135771000
1	-0.807879000	3.017753000	-3.234363000
1	-0.703101000	1.939046000	-4.629101000
1	-1.422119000	3.545771000	-4.820542000
6	-1.599930000	-1.316759000	-3.781780000
1	-1.244666000	-0.744116000	-4.653335000
1	-0.989765000	-2.233359000	-3.730416000
1	-2.636711000	-1.628657000	-3.982495000
6	-0.005053000	-0.050595000	-2.277919000
1	0.130799000	0.483876000	-1.330601000
1	0.667892000	-0.924358000	-2.248599000
1	0.351490000	0.615367000	-3.077080000
6	-3.472510000	-3.974185000	-0.798013000
9	-3.361213000	-3.216377000	-1.897888000
9	-3.462444000	-5.246208000	-1.207938000
9	-4.674644000	-3.735314000	-0.269563000
6	-4.496422000	-0.448804000	-0.607608000
1	-3.605668000	-1.050785000	-0.372977000
1	-4.591049000	0.318792000	0.176464000
1	-5.371364000	-1.111143000	-0.521413000
1	-4.545382000	-0.613947000	-2.745449000
1	5.218170000	-2.443606000	3.159553000
7	3.024607000	2.296430000	-0.497923000
6	1.828707000	2.791712000	-0.925131000
8	1.644906000	3.060690000	-2.100286000
6	0.743343000	3.052479000	0.097093000
1	-0.197526000	2.710348000	-0.348775000
1	0.883767000	2.572859000	1.072635000

1	0.668622000	4.140318000	0.246308000
6	3.366132000	1.758682000	0.802114000
1	4.307151000	1.202883000	0.653614000
6	2.398481000	0.661557000	1.301409000
6	3.641261000	2.830844000	1.870068000
1	3.808532000	2.308527000	2.821078000
1	2.742683000	3.451828000	2.004724000
8	1.801570000	0.042564000	0.350746000
8	2.302819000	0.424510000	2.497531000
6	4.823523000	3.694242000	1.514996000
6	4.678367000	4.812473000	0.685541000
6	6.107621000	3.360879000	1.961776000
6	5.783477000	5.576168000	0.314095000
1	3.683857000	5.085794000	0.324158000
6	7.216240000	4.121406000	1.593268000
1	6.237852000	2.492211000	2.614020000
6	7.057060000	5.232523000	0.766238000
1	5.648666000	6.445575000	-0.333451000
1	8.209245000	3.846853000	1.956811000
1	7.923510000	5.831349000	0.476861000
1	1.863463000	-4.880968000	0.895471000
1	1.495161000	-4.399236000	-0.783838000
1	3.673689000	2.138219000	-1.258715000

Int-3p (Olefin_para_reac)

Number of Imaginary Frequency: 0

Electronic Energy: HF = -2754.5419123

<i>Zero-point correction=</i>	<i>0.789610</i>
<i>(Hartree/Particle)</i>	
<i>Thermal correction to Energy=</i>	<i>0.842377</i>
<i>Thermal correction to Enthalpy=</i>	<i>0.843321</i>
<i>Thermal correction to Gibbs Free Energy=</i>	<i>0.700427</i>

Sum of electronic and zero-point Energies= -
2753.752302
Sum of electronic and thermal Energies= -
2753.699535
Sum of electronic and thermal Enthalpies= -
2753.698591
Sum of electronic and thermal Free Energies= -
2753.841485

6	-1.676613000	-3.962431000	-1.183670000
6	-0.580098000	-3.139363000	-1.436726000
6	-1.954092000	-4.372321000	0.119422000
6	0.244913000	-2.725875000	-0.388733000
6	-1.105523000	-3.995717000	1.162958000
6	-0.006800000	-3.178559000	0.910221000
1	0.657765000	-2.891730000	1.729101000
7	-0.007515000	-0.010762000	-0.665012000
46	1.598872000	-1.288141000	-0.680750000
6	3.568288000	-2.125934000	-0.308987000
6	2.830283000	-3.165450000	-0.822299000
6	3.720488000	-1.927540000	1.170499000
8	3.138913000	-2.562554000	2.013447000
8	4.567251000	-0.935385000	1.418848000
6	4.628082000	-0.467313000	2.760190000
1	5.476030000	0.225064000	2.802344000
1	3.694299000	0.063054000	2.996318000
1	-1.311962000	-4.329456000	2.182012000
1	4.206768000	-1.509414000	-0.944395000
1	-0.394630000	-2.800165000	-2.458556000
6	-3.380900000	3.165918000	0.690311000
6	-2.684799000	4.072141000	1.484153000
6	-2.710270000	2.078799000	0.118259000
6	-0.627197000	2.860652000	1.166945000
1	0.438083000	2.688981000	1.346324000

6	-1.326111000	1.952482000	0.354922000
6	-0.631943000	0.853971000	-0.227331000
6	-1.315447000	3.924563000	1.732025000
1	-4.448707000	3.287129000	0.501341000
1	-3.224150000	4.914067000	1.923875000
1	-0.789934000	4.639511000	2.366286000
8	-3.305124000	1.174940000	-0.653010000
14	-4.521628000	-0.009788000	-0.364244000
6	-4.427854000	-0.579266000	1.434746000
6	-6.170158000	0.827607000	-0.749763000
1	-6.185433000	1.706669000	-0.076897000
6	-4.014756000	-1.417000000	-1.509273000
1	-3.223148000	-1.924527000	-0.931019000
6	-5.042709000	0.390654000	2.452183000
1	-5.043779000	-0.053313000	3.461026000
1	-4.464573000	1.326516000	2.511377000
1	-6.082772000	0.656450000	2.209899000
6	-7.393773000	-0.032645000	-0.405557000
1	-8.324244000	0.544936000	-0.530610000
1	-7.467496000	-0.911626000	-1.063207000
1	-7.371959000	-0.400422000	0.631960000
6	-6.228295000	1.342564000	-2.193105000
1	-5.354568000	1.963625000	-2.443007000
1	-6.257960000	0.506963000	-2.911027000
1	-7.133188000	1.948757000	-2.362402000
6	-5.137383000	-2.437713000	-1.731839000
1	-5.929175000	-2.028879000	-2.380248000
1	-4.749450000	-3.342670000	-2.227107000
1	-5.604938000	-2.766531000	-0.791189000
6	-3.382125000	-0.970853000	-2.831133000
1	-2.533711000	-0.291766000	-2.666628000
1	-3.011701000	-1.845227000	-3.392445000
1	-4.106363000	-0.451510000	-3.478725000
6	-3.005029000	-0.980039000	1.848712000

1	-2.515606000	-1.637689000	1.116386000
1	-2.363336000	-0.094569000	1.982334000
1	-3.014880000	-1.518396000	2.809989000
1	-5.039906000	-1.502250000	1.430197000
1	4.775815000	-1.300119000	3.460667000
7	3.954735000	2.861068000	-1.579991000
6	2.985648000	3.263958000	-2.458051000
8	3.285401000	3.753324000	-3.529983000
6	1.538497000	3.040580000	-2.070460000
1	1.269576000	2.002954000	-2.314339000
1	1.337540000	3.191751000	-1.001456000
1	0.919239000	3.723064000	-2.663623000
6	3.819848000	2.434277000	-0.206276000
1	4.793960000	1.992202000	0.065625000
6	2.848844000	1.252057000	-0.001241000
6	3.558693000	3.591120000	0.776793000
1	3.406413000	3.155917000	1.773070000
1	2.618373000	4.095087000	0.501106000
8	2.811523000	0.419536000	-0.966181000
8	2.236240000	1.154397000	1.063546000
6	4.692216000	4.584074000	0.797967000
6	4.781309000	5.603534000	-0.158068000
6	5.717327000	4.468929000	1.744450000
6	5.863852000	6.481744000	-0.166672000
1	3.994629000	5.708987000	-0.909552000
6	6.800995000	5.345594000	1.740276000
1	5.661007000	3.680338000	2.500715000
6	6.877764000	6.355569000	0.782249000
1	5.914743000	7.269987000	-0.921121000
1	7.588011000	5.241227000	2.490753000
1	7.725063000	7.044756000	0.776488000
1	2.406130000	-3.915981000	-0.153909000
1	2.876734000	-3.408064000	-1.886233000
1	4.889405000	3.054223000	-1.919337000

6	-3.211395000	-5.133878000	0.430842000
9	-3.746941000	-5.702326000	-0.653378000
9	-3.009306000	-6.097267000	1.334136000
9	-4.153292000	-4.319063000	0.946126000
1	-2.331501000	-4.265001000	-2.002679000

TS-2p (Olefin_para_TS)

One Imaginary Frequency: -300.7 cm⁻¹

Electronic Energy: HF = -2754.5316087

Zero-point correction= 0.789431
(Hartree/Particle)
Thermal correction to Energy= 0.841299
Thermal correction to Enthalpy= 0.842244
Thermal correction to Gibbs Free Energy= 0.702479
Sum of electronic and zero-point Energies= -
2753.742177
Sum of electronic and thermal Energies= -
2753.690309
Sum of electronic and thermal Enthalpies= -
2753.689365
Sum of electronic and thermal Free Energies= -
2753.829130

6	-2.781588000	-3.180400000	-1.430033000
6	-1.555561000	-2.581098000	-1.711406000
6	-3.195010000	-3.328891000	-0.107952000
6	-0.742173000	-2.121958000	-0.671941000
6	-2.368616000	-2.903494000	0.937389000
6	-1.142899000	-2.313945000	0.658887000
1	-0.483692000	-1.998225000	1.471749000
7	-1.368307000	0.789602000	-0.840896000
46	0.371826000	-0.412514000	-0.982413000

6	2.132138000	-1.441473000	-0.840100000
6	1.235905000	-2.534774000	-0.979391000
6	2.628900000	-1.123659000	0.534967000
8	2.202464000	-1.638670000	1.541025000
8	3.567528000	-0.183401000	0.514329000
6	3.937516000	0.366249000	1.772350000
1	4.793470000	1.022162000	1.577647000
1	3.094323000	0.947415000	2.174074000
1	-2.686365000	-3.034161000	1.973749000
1	2.737276000	-1.094715000	-1.682319000
1	-1.244441000	-2.457078000	-2.751313000
6	-4.342344000	4.322163000	0.584849000
6	-3.577103000	5.061141000	1.480902000
6	-3.801584000	3.187473000	-0.030655000
6	-1.701111000	3.578673000	1.185136000
1	-0.675726000	3.255114000	1.388572000
6	-2.471925000	2.834789000	0.275727000
6	-1.896090000	1.694543000	-0.356279000
6	-2.261607000	4.695505000	1.787876000
1	-5.366711000	4.609039000	0.341912000
1	-4.015684000	5.943864000	1.951610000
1	-1.675855000	5.285155000	2.494314000
8	-4.491026000	2.468508000	-0.911918000
14	-5.549423000	1.117267000	-0.818948000
6	-5.680193000	0.510422000	0.966228000
6	-7.206329000	1.800689000	-1.415738000
1	-7.356424000	2.686614000	-0.769035000
6	-4.767590000	-0.202346000	-1.920679000
1	-3.982073000	-0.651952000	-1.285958000
6	-6.422392000	1.480771000	1.895313000
1	-6.563798000	1.033300000	2.892666000
1	-5.851699000	2.412568000	2.036757000
1	-7.417855000	1.754316000	1.514257000
6	-8.395046000	0.857067000	-1.190070000

1	-9.342977000	1.356485000	-1.449414000
1	-8.323083000	-0.044764000	-1.816613000
1	-8.475574000	0.523620000	-0.143999000
6	-7.145444000	2.296083000	-2.865923000
1	-6.294367000	2.973750000	-3.032346000
1	-7.046232000	1.454890000	-3.570768000
1	-8.065785000	2.838914000	-3.136781000
6	-5.767578000	-1.310001000	-2.276116000
1	-6.547394000	-0.939221000	-2.960467000
1	-5.263204000	-2.142924000	-2.791635000
1	-6.267792000	-1.732641000	-1.391704000
6	-4.072877000	0.345573000	-3.172272000
1	-3.343816000	1.130298000	-2.928458000
1	-3.532453000	-0.461706000	-3.694348000
1	-4.795188000	0.770951000	-3.886352000
6	-4.343290000	0.078343000	1.583144000
1	-3.754832000	-0.566569000	0.915438000
1	-3.721311000	0.949866000	1.840736000
1	-4.510946000	-0.484985000	2.515279000
1	-6.300042000	-0.401087000	0.861789000
1	4.215047000	-0.425184000	2.481767000
7	2.473241000	3.805592000	-1.955610000
6	1.425830000	4.191704000	-2.747178000
8	1.626353000	4.702119000	-3.832500000
6	0.021660000	3.924786000	-2.248436000
1	-0.234598000	2.880752000	-2.477913000
1	-0.097944000	4.065441000	-1.165961000
1	-0.662419000	4.592350000	-2.784721000
6	2.469305000	3.344257000	-0.586722000
1	3.482423000	2.944511000	-0.407841000
6	1.575103000	2.114001000	-0.325390000
6	2.239936000	4.465371000	0.445779000
1	2.217139000	4.002716000	1.441109000
1	1.247530000	4.914154000	0.279973000

8	1.434658000	1.333147000	-1.322916000
8	1.115638000	1.933842000	0.803433000
6	3.306835000	5.527275000	0.376506000
6	3.226068000	6.573903000	-0.550242000
6	4.435990000	5.455049000	1.200939000
6	4.244207000	7.520629000	-0.649391000
1	2.355978000	6.646350000	-1.207712000
6	5.456159000	6.400333000	1.106066000
1	4.513087000	4.645577000	1.932977000
6	5.363248000	7.436880000	0.178307000
1	4.162053000	8.328763000	-1.379633000
1	6.326774000	6.328614000	1.762140000
1	6.160516000	8.179502000	0.101881000
1	1.155000000	-3.213811000	-0.129358000
1	1.143975000	-3.006131000	-1.959920000
1	3.370984000	4.024815000	-2.370173000
6	-4.540854000	-3.916661000	0.221271000
9	-5.138855000	-4.449918000	-0.845871000
9	-4.452620000	-4.868958000	1.153991000
9	-5.373803000	-2.979594000	0.710481000
1	-3.419329000	-3.527204000	-2.243817000

Int-4p (Olefin_para_pdt)

Number of Imaginary Frequency: 0

Electronic Energy: HF = -2754.5419123

<i>Zero-point correction=</i>	<i>0.792872</i>
<i>(Hartree/Particle)</i>	
<i>Thermal correction to Energy=</i>	<i>0.844367</i>
<i>Thermal correction to Enthalpy=</i>	<i>0.845311</i>
<i>Thermal correction to Gibbs Free Energy=</i>	<i>0.709067</i>
<i>Sum of electronic and zero-point Energies=</i>	<i>-</i>
<i>2753.782500</i>	

Sum of electronic and thermal Energies= -
2753.731005

Sum of electronic and thermal Enthalpies= -
2753.730061

Sum of electronic and thermal Free Energies= -
2753.866304

6	-1.476680000	-4.405123000	-0.566666000
6	-0.270948000	-4.344306000	-1.230522000
6	-1.517165000	-4.309282000	0.839497000
6	0.945596000	-4.193637000	-0.515173000
6	-0.352199000	-4.157638000	1.561906000
6	0.890055000	-4.083851000	0.892880000
1	1.821511000	-4.090697000	1.466881000
7	-0.407736000	-1.009103000	1.022200000
46	1.218178000	-1.970238000	-0.065879000
6	2.825575000	-2.769869000	-0.984620000
6	2.301467000	-4.181405000	-1.209848000
6	3.898321000	-2.630060000	0.043692000
8	4.082190000	-3.410688000	0.952360000
8	4.613913000	-1.518458000	-0.127952000
6	5.469191000	-1.136936000	0.938662000
1	6.110149000	-0.338868000	0.546489000
1	4.860267000	-0.753533000	1.770844000
1	-0.380812000	-4.085625000	2.649377000
1	3.014880000	-2.168326000	-1.880642000
1	-0.239911000	-4.424141000	-2.319220000
6	-2.003119000	3.489993000	1.410170000
6	-1.347735000	4.026144000	2.512516000
6	-1.816519000	2.145882000	1.063461000
6	-0.278553000	1.919544000	2.964814000
1	0.420565000	1.296978000	3.524507000
6	-0.940220000	1.370180000	1.854817000
6	-0.668646000	0.038738000	1.433978000

6	-0.489473000	3.247853000	3.297648000
1	-2.663063000	4.097964000	0.789603000
1	-1.501588000	5.078047000	2.762630000
1	0.028457000	3.688111000	4.150285000
8	-2.385926000	1.632787000	-0.018094000
14	-3.722453000	0.637964000	-0.434570000
6	-4.768012000	0.332663000	1.111691000
6	-4.669959000	1.712116000	-1.666836000
1	-4.749009000	2.679459000	-1.135098000
6	-3.021264000	-0.971506000	-1.134707000
1	-2.684478000	-1.536677000	-0.247882000
6	-5.371645000	1.627024000	1.675255000
1	-6.043316000	1.408762000	2.521459000
1	-4.586387000	2.302512000	2.051913000
1	-5.956160000	2.182334000	0.926206000
6	-6.095755000	1.227190000	-1.959705000
1	-6.626111000	1.946916000	-2.604592000
1	-6.097716000	0.260439000	-2.486177000
1	-6.694901000	1.104690000	-1.044198000
6	-3.883827000	1.964104000	-2.959329000
1	-2.851819000	2.288596000	-2.757891000
1	-3.832841000	1.054566000	-3.578842000
1	-4.367195000	2.744587000	-3.569021000
6	-4.116510000	-1.801039000	-1.818034000
1	-4.469689000	-1.317344000	-2.742762000
1	-3.730358000	-2.792530000	-2.104995000
1	-4.990232000	-1.969228000	-1.169088000
6	-1.802670000	-0.793887000	-2.048052000
1	-1.002917000	-0.212793000	-1.570389000
1	-1.377130000	-1.776570000	-2.311093000
1	-2.063908000	-0.287569000	-2.989626000
6	-4.056990000	-0.463098000	2.214147000
1	-3.598545000	-1.388657000	1.841631000
1	-3.268184000	0.137120000	2.694220000

1	-4.767499000	-0.748328000	3.006742000
1	-5.600972000	-0.293387000	0.736490000
1	6.079197000	-1.984233000	1.279826000
7	2.704344000	2.347932000	-1.533960000
6	1.598071000	2.455613000	-2.332843000
8	1.718658000	2.618398000	-3.532127000
6	0.235119000	2.415120000	-1.678852000
1	0.175852000	1.661345000	-0.887415000
1	-0.014461000	3.396883000	-1.248192000
1	-0.500592000	2.184809000	-2.457300000
6	2.828506000	2.023405000	-0.131929000
1	3.911830000	1.988471000	0.064537000
6	2.344162000	0.616208000	0.286661000
6	2.256576000	3.085254000	0.832322000
1	2.420649000	2.701265000	1.847627000
1	1.168110000	3.165753000	0.697143000
8	1.837138000	-0.099935000	-0.645098000
8	2.475955000	0.286023000	1.461825000
6	2.903162000	4.435261000	0.671560000
6	2.420738000	5.365321000	-0.255939000
6	4.036719000	4.771482000	1.421036000
6	3.050240000	6.596582000	-0.429127000
1	1.539395000	5.121428000	-0.853724000
6	4.670343000	6.001408000	1.251994000
1	4.425753000	4.056156000	2.151715000
6	4.178212000	6.918811000	0.324442000
1	2.658162000	7.307573000	-1.159821000
1	5.551578000	6.245904000	1.849667000
1	4.672270000	7.883574000	0.189699000
1	2.962605000	-4.941325000	-0.767847000
1	2.179029000	-4.397311000	-2.279137000
1	3.559252000	2.366252000	-2.076191000
6	-2.848227000	-4.412699000	1.536920000
9	-3.276517000	-5.677355000	1.593942000

9	-2.800610000	-3.949252000	2.787120000
9	-3.794699000	-3.715485000	0.888083000
1	-2.404750000	-4.525316000	-1.128220000

Int-5m (Beta_reac)

Number of Imaginary Frequency: 0

Electronic Energy: HF = -2754.5743159

<i>Zero-point correction=</i>	<i>0.793209</i>
<i>(Hartree/Particle)</i>	
<i>Thermal correction to Energy=</i>	<i>0.845499</i>
<i>Thermal correction to Enthalpy=</i>	<i>0.846444</i>
<i>Thermal correction to Gibbs Free Energy=</i>	<i>0.706315</i>
<i>Sum of electronic and zero-point Energies=</i>	<i>-</i>
<i>2753.781107</i>	
<i>Sum of electronic and thermal Energies=</i>	<i>-</i>
<i>2753.728817</i>	
<i>Sum of electronic and thermal Enthalpies=</i>	<i>-</i>
<i>2753.727872</i>	
<i>Sum of electronic and thermal Free Energies=</i>	<i>-</i>
<i>2753.868001</i>	

6	-1.289458000	2.469254000	2.141003000
6	-1.575945000	2.808614000	3.470862000
6	-2.650067000	3.639849000	3.745435000
6	-3.437054000	4.112098000	2.689584000
6	-3.151833000	3.789981000	1.367741000
6	-2.053454000	2.972751000	1.061616000
1	-0.960827000	2.392148000	4.269612000
1	-2.886904000	3.910274000	4.775104000
1	-3.774323000	4.174813000	0.559971000
6	-0.303212000	1.499366000	1.817443000
6	-2.090092000	-0.838276000	3.976106000
6	-0.983160000	-1.475439000	3.415386000

6	-1.971307000	-0.145757000	5.181747000
6	0.269026000	-1.412608000	4.035019000
6	-0.731227000	-0.085668000	5.809517000
6	0.377112000	-0.707181000	5.237714000
1	1.350993000	-0.635402000	5.723142000
7	0.404645000	0.646453000	1.499545000
46	1.202910000	-0.962906000	0.681731000
6	1.193389000	-2.110402000	-1.521302000
8	1.854852000	-2.540636000	-0.526830000
8	0.405898000	-1.147315000	-1.389421000
6	1.369288000	-2.767762000	-2.887543000
1	0.519307000	-3.467367000	-2.960771000
6	2.264838000	-1.381149000	2.349878000
6	1.467165000	-2.115708000	3.431102000
6	2.972958000	-0.146517000	2.815408000
8	2.790229000	0.434444000	3.858359000
8	3.870326000	0.274433000	1.909843000
6	4.554401000	1.475523000	2.214291000
1	3.848968000	2.314564000	2.307431000
1	5.112687000	1.384277000	3.157384000
1	-0.625348000	0.448991000	6.755861000
1	3.014091000	-2.064358000	1.919170000
1	1.132097000	-3.071152000	2.999009000
1	2.164177000	-2.375614000	4.246285000
1	-2.844457000	0.337179000	5.623726000
1	-4.295688000	4.752790000	2.902421000
1	-1.096189000	-2.024679000	2.477070000
8	-1.678446000	2.654693000	-0.168196000
14	-2.546206000	2.115875000	-1.567168000
6	-3.648203000	0.731684000	-0.904980000
1	-4.084424000	1.149206000	0.022500000
6	-3.549717000	3.599095000	-2.201524000
1	-4.440726000	3.636876000	-1.544472000
6	-1.190161000	1.511768000	-2.718635000

1	-0.591002000	0.828891000	-2.090272000
6	-0.262890000	2.627475000	-3.218976000
1	0.156060000	3.218057000	-2.389161000
1	0.569781000	2.195529000	-3.796886000
1	-0.791037000	3.321892000	-3.892945000
6	-1.731969000	0.671289000	-3.887220000
1	-0.901053000	0.364368000	-4.541283000
1	-2.239602000	-0.239668000	-3.535351000
1	-2.445309000	1.231122000	-4.512384000
6	-4.815682000	0.347952000	-1.822311000
1	-4.466729000	-0.033896000	-2.794996000
1	-5.424033000	-0.447025000	-1.360625000
1	-5.485775000	1.199290000	-2.018592000
6	-2.810594000	-0.490960000	-0.505635000
1	-2.315156000	-0.953269000	-1.372720000
1	-2.014818000	-0.228703000	0.207503000
1	-3.441658000	-1.254286000	-0.025700000
6	-2.806929000	4.937196000	-2.073432000
1	-3.465318000	5.776326000	-2.352973000
1	-2.438807000	5.124680000	-1.054105000
1	-1.933171000	4.971307000	-2.741385000
6	-4.052221000	3.404372000	-3.639950000
1	-4.737182000	4.219207000	-3.926438000
1	-3.215290000	3.417718000	-4.355514000
1	-4.591069000	2.455550000	-3.779988000
6	-3.416485000	-0.851403000	3.265452000
9	-3.570370000	0.238850000	2.491473000
9	-3.555234000	-1.915587000	2.469254000
9	-4.443735000	-0.854820000	4.120979000
6	2.656547000	-3.605645000	-2.996449000
1	3.530676000	-2.939916000	-2.938609000
1	2.705561000	-4.265940000	-2.119957000
6	2.693565000	-4.408061000	-4.272164000
6	3.172855000	-3.846088000	-5.461253000

6	2.194955000	-5.715475000	-4.305774000
6	3.154566000	-4.570771000	-6.651585000
1	3.564768000	-2.825839000	-5.454470000
6	2.175392000	-6.444103000	-5.494018000
1	1.821186000	-6.171517000	-3.384320000
6	2.654718000	-5.872326000	-6.671739000
1	3.534054000	-4.115356000	-7.568952000
1	1.787020000	-7.465070000	-5.498997000
1	2.641947000	-6.441596000	-7.603722000
7	1.186976000	-1.810427000	-3.954593000
6	1.744850000	-0.571546000	-4.107697000
8	1.441915000	0.123758000	-5.061425000
6	2.713107000	-0.066962000	-3.060097000
1	3.457091000	0.559420000	-3.566784000
1	2.150695000	0.563856000	-2.355919000
1	3.220730000	-0.847324000	-2.479417000
1	0.544641000	-2.049416000	-4.700146000
1	5.244256000	1.656010000	1.382350000

TS-3m (Beta_TS)

One Imaginary Frequency: -840.7 cm⁻¹

Electronic Energy: HF = -2754.539682

<i>Zero-point correction=</i>	<i>0.787306</i>
<i>(Hartree/Particle)</i>	
<i>Thermal correction to Energy=</i>	<i>0.839429</i>
<i>Thermal correction to Enthalpy=</i>	<i>0.840374</i>
<i>Thermal correction to Gibbs Free Energy=</i>	<i>0.700085</i>
<i>Sum of electronic and zero-point Energies=</i>	<i>-</i>
<i>2753.752376</i>	
<i>Sum of electronic and thermal Energies=</i>	<i>-</i>
<i>2753.700253</i>	
<i>Sum of electronic and thermal Enthalpies=</i>	<i>-</i>
<i>2753.699308</i>	

Sum of electronic and thermal Free Energies= -
2753.839597

6	0.257503000	2.861149000	-1.462763000
6	-0.009539000	3.165962000	-0.117792000
6	-1.295505000	3.510122000	0.264990000
6	-2.310854000	3.538110000	-0.695756000
6	-2.060738000	3.222075000	-2.025423000
6	-0.766971000	2.869044000	-2.437601000
1	0.792840000	3.076736000	0.614872000
1	-1.514782000	3.737683000	1.308575000
1	-2.870090000	3.238641000	-2.755490000
6	1.547911000	2.411984000	-1.857751000
6	-0.530879000	-1.839321000	0.257000000
6	0.697480000	-1.349864000	-0.164048000
6	-0.615378000	-3.065034000	0.924776000
6	1.874735000	-2.066459000	0.084697000
6	0.545413000	-3.789949000	1.161933000
6	1.781014000	-3.293841000	0.742219000
1	2.686800000	-3.875681000	0.930110000
7	2.577891000	1.962814000	-2.145590000
46	3.145606000	-0.077452000	-1.936891000
6	2.553590000	-1.991432000	-3.924748000
8	2.912733000	-2.730933000	-2.980370000
8	2.473005000	-0.736234000	-3.868636000
6	2.127949000	-2.681268000	-5.226719000
1	1.085578000	-2.977684000	-5.018300000
6	3.763530000	-0.255430000	-0.010891000
6	3.219466000	-1.566230000	-0.367731000
6	3.144304000	0.739841000	0.903403000
8	1.969373000	0.913832000	1.128872000
8	4.099580000	1.507418000	1.446145000
6	3.665121000	2.575330000	2.267217000
1	3.121592000	3.326349000	1.673688000

1	3.006546000	2.215110000	3.070188000
1	0.492528000	-4.751351000	1.676128000
1	4.857380000	-0.208988000	0.036365000
1	3.165650000	-1.808469000	-1.778335000
1	3.979611000	-2.359176000	-0.328768000
1	-1.583941000	-3.447108000	1.253249000
1	-3.328124000	3.802567000	-0.398740000
1	0.744260000	-0.393070000	-0.681677000
8	-0.446952000	2.537468000	-3.679286000
14	-1.319329000	1.647211000	-4.880121000
6	-1.998722000	0.143128000	-3.955517000
1	-2.374805000	0.550027000	-2.999045000
6	-2.698999000	2.790486000	-5.511857000
1	-3.520650000	2.675475000	-4.778333000
6	0.018029000	1.199706000	-6.119106000
1	0.759542000	0.649393000	-5.508881000
6	0.733621000	2.414999000	-6.721957000
1	1.094743000	3.103640000	-5.943135000
1	1.600157000	2.079984000	-7.313151000
1	0.069487000	2.982072000	-7.395597000
6	-0.472252000	0.244660000	-7.218353000
1	0.375229000	-0.028829000	-7.867002000
1	-0.908593000	-0.679664000	-6.804180000
1	-1.238863000	0.704868000	-7.859195000
6	-3.177579000	-0.557610000	-4.640673000
1	-2.892640000	-0.987456000	-5.614651000
1	-3.548308000	-1.385381000	-4.014447000
1	-4.023250000	0.126041000	-4.814015000
6	-0.869204000	-0.838742000	-3.619892000
1	-0.466093000	-1.304758000	-4.533281000
1	-0.021283000	-0.346435000	-3.120634000
1	-1.229517000	-1.645252000	-2.962554000
6	-2.285498000	4.268786000	-5.532250000
1	-3.128529000	4.904610000	-5.849541000

1	-1.948552000	4.626122000	-4.548073000
1	-1.459841000	4.441452000	-6.239778000
6	-3.253618000	2.366411000	-6.879163000
1	-4.148879000	2.956189000	-7.135483000
1	-2.513028000	2.539175000	-7.675556000
1	-3.536777000	1.303423000	-6.914148000
6	-1.792589000	-1.056477000	0.001998000
9	-1.552961000	0.132196000	-0.560941000
9	-2.627393000	-1.717257000	-0.817000000
9	-2.469615000	-0.832083000	1.133361000
6	2.903740000	-3.987210000	-5.495539000
1	3.952287000	-3.749255000	-5.730639000
1	2.907464000	-4.568737000	-4.564667000
6	2.284926000	-4.778480000	-6.619147000
6	2.629698000	-4.530299000	-7.952874000
6	1.301354000	-5.738260000	-6.352638000
6	2.009976000	-5.222661000	-8.991805000
1	3.392565000	-3.781583000	-8.181342000
6	0.679268000	-6.433402000	-7.388389000
1	1.022345000	-5.945909000	-5.315428000
6	1.031865000	-6.176324000	-8.712650000
1	2.293182000	-5.014562000	-10.025973000
1	-0.082763000	-7.182000000	-7.159734000
1	0.546692000	-6.720227000	-9.526105000
7	2.060759000	-1.793995000	-6.362056000
6	3.006561000	-0.955461000	-6.882096000
8	2.764024000	-0.301511000	-7.882364000
6	4.343661000	-0.835645000	-6.186112000
1	5.100103000	-0.619928000	-6.950228000
1	4.289299000	0.013394000	-5.490592000
1	4.638923000	-1.721160000	-5.609419000
1	1.209459000	-1.810493000	-6.909409000
1	4.569866000	3.025804000	2.689947000

Int-6m (Beta_pdt)

Number of Imaginary Frequency: 0

Electronic Energy: HF = -2754.5642421

Zero-point correction= 0.792797
(Hartree/Particle)
Thermal correction to Energy= 0.845412
Thermal correction to Enthalpy= 0.846357
Thermal correction to Gibbs Free Energy= 0.705513
Sum of electronic and zero-point Energies= -
2753.771445
Sum of electronic and thermal Energies= -
2753.718830
Sum of electronic and thermal Enthalpies= -
2753.717885
Sum of electronic and thermal Free Energies= -
2753.858729

6	-0.539852000	3.231921000	1.466838000
6	-0.769186000	3.580826000	2.806888000
6	-2.029582000	4.001215000	3.204261000
6	-3.059373000	4.062511000	2.263628000
6	-2.845690000	3.706463000	0.936654000
6	-1.579717000	3.280586000	0.512626000
1	0.037495000	3.460975000	3.530643000
1	-2.215589000	4.260294000	4.247097000
1	-3.664602000	3.751141000	0.218515000
6	0.733923000	2.728234000	1.064915000
6	-1.577757000	-1.359461000	3.094594000
6	-0.296847000	-0.824332000	3.044774000
6	-1.779011000	-2.737648000	3.216124000
6	0.831332000	-1.660035000	3.110260000
6	-0.671708000	-3.573733000	3.289102000
6	0.615065000	-3.039736000	3.233421000

1	1.475412000	-3.712978000	3.277533000
7	1.756536000	2.254199000	0.791101000
46	2.334799000	0.172876000	1.328225000
6	1.742007000	-1.750374000	-0.906740000
8	2.149207000	-2.596860000	0.009585000
8	1.682845000	-0.549543000	-0.719835000
6	1.296581000	-2.411561000	-2.201526000
1	0.272252000	-2.748032000	-1.960625000
6	2.837514000	0.064141000	3.328178000
6	2.230822000	-1.174716000	2.944181000
6	2.266524000	1.207462000	4.073929000
8	1.102665000	1.471939000	4.285724000
8	3.258257000	2.009164000	4.496490000
6	2.874290000	3.206795000	5.141085000
1	2.359830000	3.881338000	4.439119000
1	2.205717000	3.005627000	5.990457000
1	-0.808213000	-4.652931000	3.383453000
1	3.926100000	0.028240000	3.440079000
1	2.353940000	-2.057613000	0.818717000
1	2.946132000	-2.008691000	2.929278000
1	-2.790012000	-3.147818000	3.245402000
1	-4.056708000	4.384668000	2.571040000
1	-0.163329000	0.251932000	2.957305000
8	-1.304422000	2.917861000	-0.738020000
14	-2.214609000	1.965168000	-1.847287000
6	-2.823708000	0.491616000	-0.829555000
1	-3.197816000	0.942668000	0.107381000
6	-3.644807000	3.043690000	-2.480157000
1	-4.425317000	2.959892000	-1.699066000
6	-0.929610000	1.484538000	-3.132952000
1	-0.139620000	0.995248000	-2.532381000
6	-0.289774000	2.687778000	-3.836763000
1	0.076548000	3.433557000	-3.115279000
1	0.562938000	2.354320000	-4.448515000

1	-1.006433000	3.188824000	-4.508584000
6	-1.440095000	0.453453000	-4.150429000
1	-0.623175000	0.180897000	-4.837812000
1	-1.810721000	-0.464303000	-3.663614000
1	-2.263926000	0.845914000	-4.764596000
6	-3.989517000	-0.288008000	-1.447941000
1	-3.709042000	-0.769315000	-2.398938000
1	-4.323468000	-1.084130000	-0.763058000
1	-4.859227000	0.357190000	-1.646859000
6	-1.655591000	-0.428729000	-0.453184000
1	-1.215904000	-0.900856000	-1.347689000
1	-0.843336000	0.114199000	0.054236000
1	-1.989486000	-1.233418000	0.221304000
6	-3.261648000	4.524752000	-2.610902000
1	-4.135538000	5.128625000	-2.906401000
1	-2.865617000	4.942774000	-1.673998000
1	-2.488161000	4.668633000	-3.380935000
6	-4.259501000	2.530137000	-3.789948000
1	-5.177142000	3.089786000	-4.034477000
1	-3.563542000	2.667651000	-4.632325000
1	-4.524887000	1.462776000	-3.748816000
6	-2.774912000	-0.447434000	3.033711000
9	-2.471956000	0.759793000	2.545408000
9	-3.741709000	-0.955383000	2.249717000
9	-3.322331000	-0.258845000	4.239249000
6	2.096667000	-3.683383000	-2.564553000
1	3.133109000	-3.407878000	-2.810175000
1	2.136752000	-4.332516000	-1.679926000
6	1.461055000	-4.412122000	-3.721739000
6	1.773447000	-4.076593000	-5.043864000
6	0.496432000	-5.399551000	-3.491022000
6	1.138263000	-4.712480000	-6.109039000
1	2.521468000	-3.305267000	-5.244542000
6	-0.140421000	-6.038070000	-4.553719000

1	0.243851000	-5.676060000	-2.463098000
6	0.178854000	-5.694649000	-5.866698000
1	1.394783000	-4.437464000	-7.134265000
1	-0.887293000	-6.809853000	-4.355088000
1	-0.318160000	-6.194130000	-6.701029000
7	1.160683000	-1.466469000	-3.276577000
6	2.093733000	-0.627835000	-3.835014000
8	1.818995000	0.002889000	-4.837773000
6	3.437852000	-0.474539000	-3.160345000
1	4.166126000	-0.185746000	-3.926922000
1	3.362209000	0.336019000	-2.421113000
1	3.790796000	-1.372719000	-2.636921000
1	0.298647000	-1.499151000	-3.806892000
1	3.799467000	3.679095000	5.490230000

Int-5p (Beta_para_reac)

Number of Imaginary Frequency: 0

Electronic Energy: HF = -2754.5766971

<i>Zero-point correction=</i>	<i>0.793492</i>
<i>(Hartree/Particle)</i>	
<i>Thermal correction to Energy=</i>	<i>0.844754</i>
<i>Thermal correction to Enthalpy=</i>	<i>0.845698</i>
<i>Thermal correction to Gibbs Free Energy=</i>	<i>0.709114</i>
<i>Sum of electronic and zero-point Energies=</i>	<i>-</i>
<i>2753.783205</i>	
<i>Sum of electronic and thermal Energies=</i>	<i>-</i>
<i>2753.731943</i>	
<i>Sum of electronic and thermal Enthalpies=</i>	<i>-</i>
<i>2753.730999</i>	
<i>Sum of electronic and thermal Free Energies=</i>	<i>-</i>
<i>2753.867583</i>	

6	-1.072463000	2.963478000	1.735428000
6	-1.384034000	3.526892000	2.981006000
6	-2.397592000	4.467466000	3.068793000
6	-3.094713000	4.832705000	1.911774000
6	-2.777180000	4.295235000	0.670182000
6	-1.741932000	3.356173000	0.553624000
1	-0.829025000	3.203418000	3.862884000
1	-2.655370000	4.910459000	4.031387000
1	-3.324610000	4.601839000	-0.221696000
6	-0.135366000	1.902029000	1.609772000
6	-1.934878000	0.416537000	4.296237000
6	-0.643437000	-0.063866000	4.486116000
6	-2.780791000	-0.192567000	3.367802000
6	-0.174192000	-1.160032000	3.753731000
6	-2.347450000	-1.323409000	2.677601000
6	-1.056422000	-1.800706000	2.876850000
1	-0.717223000	-2.675497000	2.315711000
7	0.557816000	0.993168000	1.460647000
46	1.405036000	-0.732750000	1.007685000
6	1.521636000	-2.249667000	-0.951969000
8	2.097260000	-2.512313000	0.148851000
8	0.785666000	-1.242785000	-1.057979000
6	1.724336000	-3.175685000	-2.148688000
1	0.877829000	-3.880610000	-2.085243000
6	2.217178000	-0.889933000	2.863626000
6	1.268773000	-1.609736000	3.832770000
6	2.673200000	0.454597000	3.337291000
8	2.188855000	1.097078000	4.240411000
8	3.713779000	0.903885000	2.620660000
6	4.175065000	2.205413000	2.929711000
1	3.385298000	2.951383000	2.754963000
1	4.492131000	2.273909000	3.980489000
1	-3.013029000	-1.824663000	1.974598000

1	3.106063000	-1.504980000	2.654025000
1	1.315105000	-2.685963000	3.611044000
1	1.642318000	-1.475144000	4.861296000
1	-3.904960000	5.561901000	1.979520000
1	0.034662000	0.440543000	5.175238000
8	-1.337623000	2.825691000	-0.590184000
14	-2.173473000	2.210398000	-1.973715000
6	-3.542691000	1.142512000	-1.232139000
1	-3.993974000	1.783892000	-0.451589000
6	-2.876330000	3.703086000	-2.913155000
1	-3.815217000	3.952030000	-2.380617000
6	-0.841821000	1.237156000	-2.874478000
1	-0.389353000	0.603319000	-2.090258000
6	0.269794000	2.126111000	-3.449729000
1	0.723851000	2.766753000	-2.677571000
1	1.059232000	1.502366000	-3.897854000
1	-0.107847000	2.781675000	-4.251527000
6	-1.405632000	0.288291000	-3.944752000
1	-0.580629000	-0.244487000	-4.443134000
1	-2.081731000	-0.464596000	-3.511199000
1	-1.963771000	0.825194000	-4.728085000
6	-4.661602000	0.763111000	-2.209398000
1	-4.287952000	0.155866000	-3.049067000
1	-5.437297000	0.169839000	-1.697890000
1	-5.157027000	1.649952000	-2.633951000
6	-2.957660000	-0.085066000	-0.523392000
1	-2.468415000	-0.774594000	-1.229468000
1	-2.203519000	0.191854000	0.229066000
1	-3.753806000	-0.642709000	-0.004725000
6	-1.964680000	4.937551000	-2.865508000
1	-2.453463000	5.800990000	-3.346383000
1	-1.702507000	5.230153000	-1.838061000
1	-1.020175000	4.756546000	-3.400500000
6	-3.251468000	3.363743000	-4.363486000

1	-3.771365000	4.210975000	-4.839929000
1	-2.354130000	3.152981000	-4.965981000
1	-3.912067000	2.486964000	-4.438744000
6	3.011539000	-4.016322000	-2.055031000
1	3.887323000	-3.355413000	-2.136043000
1	3.047492000	-4.466137000	-1.053600000
6	3.060884000	-5.081743000	-3.120338000
6	3.546305000	-4.795798000	-4.401721000
6	2.568270000	-6.366640000	-2.864833000
6	3.539881000	-5.767608000	-5.400718000
1	3.933451000	-3.797226000	-4.619431000
6	2.560408000	-7.341781000	-3.860975000
1	2.190179000	-6.608243000	-1.867116000
6	3.045805000	-7.043853000	-5.133485000
1	3.924189000	-5.525910000	-6.394134000
1	2.176656000	-8.340514000	-3.640760000
1	3.042375000	-7.806469000	-5.915299000
7	1.557261000	-2.467959000	-3.396904000
6	2.098252000	-1.275107000	-3.790494000
8	1.763745000	-0.769451000	-4.847385000
6	3.095891000	-0.585938000	-2.885659000
1	2.553676000	0.169556000	-2.298533000
1	3.619480000	-1.245857000	-2.182739000
1	3.826095000	-0.072453000	-3.522845000
1	0.888258000	-2.834719000	-4.062782000
1	5.024589000	2.397011000	2.264739000
6	-4.122848000	0.418144000	3.074382000
1	-2.287821000	1.279319000	4.864355000
9	-4.012637000	1.452608000	2.218955000
9	-4.709902000	0.899659000	4.174826000
9	-4.968473000	-0.452760000	2.514492000

TS-3p (Beta_para_TS)

One Imaginary Frequency: -491.3 cm⁻¹

Electronic Energy: HF = -2754.5341753

Zero-point correction= 0.787347
(Hartree/Particle)
Thermal correction to Energy= 0.838733
Thermal correction to Enthalpy= 0.839677
Thermal correction to Gibbs Free Energy= 0.701972
Sum of electronic and zero-point Energies= -
2753.746828
Sum of electronic and thermal Energies= -
2753.695442
Sum of electronic and thermal Enthalpies= -
2753.694498
Sum of electronic and thermal Free Energies= -
2753.832203

6	0.772928000	3.412978000	-1.290356000
6	0.557676000	4.136302000	-0.106377000
6	-0.725631000	4.526889000	0.238906000
6	-1.794074000	4.172485000	-0.591672000
6	-1.596242000	3.451631000	-1.762809000
6	-0.301105000	3.066890000	-2.147927000
1	1.401829000	4.346642000	0.549200000
1	-0.901229000	5.084562000	1.159146000
1	-2.446139000	3.184840000	-2.391282000
6	2.045437000	2.850864000	-1.592093000
6	-1.386897000	0.058058000	0.075741000
6	-0.008483000	0.137002000	0.233035000
6	-2.012899000	-1.183778000	0.000195000
6	0.768895000	-1.023077000	0.335306000
6	-1.254777000	-2.349296000	0.117620000
6	0.122610000	-2.265501000	0.282035000
1	0.712249000	-3.183422000	0.330082000
7	3.032548000	2.274036000	-1.800334000

46	2.984528000	0.151406000	-1.331632000
6	2.428657000	-1.903641000	-3.206326000
8	2.451175000	-2.569258000	-2.151481000
8	2.550339000	-0.648182000	-3.281716000
6	2.185294000	-2.690429000	-4.502700000
1	1.124725000	-2.980186000	-4.420535000
6	3.185986000	0.064802000	0.701743000
6	2.273739000	-1.021929000	0.345488000
6	2.942236000	1.340855000	1.421959000
8	1.910386000	1.956176000	1.558533000
8	4.106528000	1.794085000	1.905598000
6	4.081332000	3.059973000	2.538817000
1	3.825841000	3.850509000	1.817099000
1	3.348422000	3.078094000	3.357771000
1	-1.736667000	-3.326471000	0.050923000
1	4.199268000	-0.290337000	0.922734000
1	2.585885000	-1.458455000	-0.939733000
1	2.668700000	-2.005318000	0.641570000
1	-2.810850000	4.461823000	-0.316642000
1	0.463715000	1.115074000	0.283423000
8	-0.013544000	2.397016000	-3.245503000
14	-0.953034000	1.644209000	-4.490687000
6	-1.873382000	0.235258000	-3.625983000
1	-2.225632000	0.673728000	-2.673372000
6	-2.139699000	2.960682000	-5.178154000
1	-3.013324000	2.957254000	-4.498577000
6	0.381480000	1.053521000	-5.668426000
1	1.037235000	0.444335000	-5.018013000
6	1.240898000	2.191469000	-6.235265000
1	1.624900000	2.847637000	-5.439436000
1	2.101793000	1.770205000	-6.777078000
1	0.672068000	2.814319000	-6.945826000
6	-0.139107000	0.142661000	-6.790270000
1	0.710421000	-0.203683000	-7.400770000

1	-0.673196000	-0.740050000	-6.400858000
1	-0.831034000	0.666571000	-7.466488000
6	-3.113198000	-0.269257000	-4.374739000
1	-2.849891000	-0.720222000	-5.345462000
1	-3.629808000	-1.041661000	-3.783242000
1	-3.839847000	0.535260000	-4.567101000
6	-0.918616000	-0.912505000	-3.275817000
1	-0.515461000	-1.382661000	-4.186830000
1	-0.061667000	-0.568423000	-2.677286000
1	-1.438982000	-1.694120000	-2.701831000
6	-1.546787000	4.376809000	-5.180148000
1	-2.278166000	5.101156000	-5.575114000
1	-1.257525000	4.716645000	-4.175084000
1	-0.651283000	4.434744000	-5.817444000
6	-2.658251000	2.596167000	-6.577620000
1	-3.455861000	3.290663000	-6.888036000
1	-1.854857000	2.669033000	-7.327042000
1	-3.069648000	1.576738000	-6.629729000
6	2.984012000	-4.011911000	-4.538736000
1	4.058263000	-3.792525000	-4.631989000
1	2.838495000	-4.507801000	-3.570345000
6	2.536330000	-4.902681000	-5.668540000
6	3.089622000	-4.779383000	-6.948169000
6	1.508434000	-5.832748000	-5.473768000
6	2.630076000	-5.564518000	-8.004124000
1	3.890542000	-4.055833000	-7.120672000
6	1.045871000	-6.620430000	-6.526560000
1	1.066988000	-5.942759000	-4.478866000
6	1.605798000	-6.487470000	-7.796607000
1	3.074909000	-5.453216000	-8.995455000
1	0.246048000	-7.344109000	-6.353453000
1	1.245980000	-7.104089000	-8.623182000
7	2.279490000	-1.910066000	-5.711846000
6	3.291026000	-1.131719000	-6.199450000

8	3.152999000	-0.547669000	-7.261616000
6	4.568630000	-0.990865000	-5.404544000
1	4.514714000	-0.046621000	-4.845705000
1	4.751422000	-1.795315000	-4.682661000
1	5.400422000	-0.930892000	-6.117471000
1	1.484656000	-1.942559000	-6.337813000
1	5.091417000	3.227772000	2.928031000
6	-3.498013000	-1.285269000	-0.222612000
1	-1.968024000	0.976845000	-0.016646000
9	-4.023215000	-0.129578000	-0.647315000
9	-4.150993000	-1.629972000	0.891935000
9	-3.790860000	-2.214199000	-1.145238000

Int-6p (Beta_para_Pdt)

Number of Imaginary Frequency: 0

Electronic Energy: HF = -2754.5625453

<i>Zero-point correction=</i>	<i>0.791681</i>
<i>(Hartree/Particle)</i>	
<i>Thermal correction to Energy=</i>	<i>0.843072</i>
<i>Thermal correction to Enthalpy=</i>	<i>0.844016</i>
<i>Thermal correction to Gibbs Free Energy=</i>	<i>0.706269</i>
<i>Sum of electronic and zero-point Energies=</i>	<i>-</i>
<i>2753.770864</i>	
<i>Sum of electronic and thermal Energies=</i>	<i>-</i>
<i>2753.719473</i>	
<i>Sum of electronic and thermal Enthalpies=</i>	<i>-</i>
<i>2753.718529</i>	
<i>Sum of electronic and thermal Free Energies=</i>	<i>-</i>
<i>2753.856277</i>	

6	-0.093575000	3.390518000	1.313842000
6	-0.343322000	4.027694000	2.538045000

6	-1.633515000	4.420705000	2.864508000
6	-2.673826000	4.165152000	1.968002000
6	-2.438862000	3.533412000	0.751781000
6	-1.139557000	3.141510000	0.395365000
1	0.476247000	4.156787000	3.244342000
1	-1.831738000	4.907493000	3.819977000
1	-3.267383000	3.339067000	0.070468000
6	1.200792000	2.860772000	1.018179000
6	-2.144869000	0.347707000	2.819642000
6	-0.785295000	0.374458000	3.104091000
6	-2.788488000	-0.861874000	2.559609000
6	-0.027522000	-0.808435000	3.124365000
6	-2.061623000	-2.052035000	2.613624000
6	-0.700805000	-2.020681000	2.889321000
1	-0.138976000	-2.958231000	2.902292000
7	2.224199000	2.348067000	0.822850000
46	2.211993000	0.156134000	1.593653000
6	1.770497000	-1.866336000	-0.572082000
8	2.033276000	-2.641065000	0.455580000
8	1.734157000	-0.652552000	-0.489466000
6	1.462474000	-2.632114000	-1.849195000
1	0.411847000	-2.937990000	-1.698657000
6	2.414568000	0.114386000	3.664400000
6	1.450966000	-0.861454000	3.269702000
6	2.271654000	1.480285000	4.214667000
8	1.274013000	2.157159000	4.342229000
8	3.480735000	1.943656000	4.569300000
6	3.536551000	3.282166000	5.020822000
1	3.248271000	3.977142000	4.217386000
1	2.868754000	3.440256000	5.879954000
1	-2.556368000	-3.005161000	2.417107000
1	3.393139000	-0.300758000	3.927288000
1	2.170979000	-2.030255000	1.230744000
1	1.806445000	-1.892004000	3.402111000

1	-3.694772000	4.458635000	2.222268000
1	-0.298093000	1.323207000	3.317602000
8	-0.827405000	2.550903000	-0.748606000
14	-1.759411000	1.770818000	-1.968998000
6	-2.648682000	0.351821000	-1.089368000
1	-3.029180000	0.798787000	-0.152496000
6	-2.972513000	3.047079000	-2.683690000
1	-3.850033000	3.027735000	-2.009389000
6	-0.421194000	1.179317000	-3.147604000
1	0.248446000	0.600485000	-2.484399000
6	0.410365000	2.320919000	-3.746583000
1	0.786619000	3.001097000	-2.967616000
1	1.275626000	1.909705000	-4.289567000
1	-0.178360000	2.917140000	-4.463354000
6	-0.929255000	0.227318000	-4.240125000
1	-0.078387000	-0.131366000	-4.841524000
1	-1.454875000	-0.647583000	-3.822438000
1	-1.628579000	0.722244000	-4.930251000
6	-3.860992000	-0.205222000	-1.845503000
1	-3.571929000	-0.673300000	-2.800678000
1	-4.368875000	-0.973329000	-1.241495000
1	-4.603626000	0.576011000	-2.069776000
6	-1.663472000	-0.755368000	-0.694146000
1	-1.184341000	-1.198629000	-1.582911000
1	-0.863604000	-0.375580000	-0.039364000
1	-2.182582000	-1.562575000	-0.155592000
6	-2.410365000	4.475683000	-2.687381000
1	-3.157133000	5.184622000	-3.081522000
1	-2.125605000	4.819258000	-1.682261000
1	-1.516726000	4.552300000	-3.325615000
6	-3.473284000	2.661404000	-4.083474000
1	-4.280005000	3.339196000	-4.407087000
1	-2.665821000	2.740679000	-4.828101000
1	-3.867299000	1.634682000	-4.128482000

6	2.276365000	-3.937492000	-2.006303000
1	3.338880000	-3.692555000	-2.153095000
1	2.203504000	-4.507203000	-1.070605000
6	1.764506000	-4.759565000	-3.162347000
6	2.235765000	-4.546978000	-4.462652000
6	0.758853000	-5.711941000	-2.961410000
6	1.715394000	-5.268590000	-5.535471000
1	3.018268000	-3.804879000	-4.640863000
6	0.236494000	-6.435932000	-4.031682000
1	0.382562000	-5.893021000	-1.950207000
6	0.713642000	-6.214653000	-5.322882000
1	2.095245000	-5.089028000	-6.543430000
1	-0.544626000	-7.178717000	-3.855613000
1	0.306533000	-6.781190000	-6.163049000
7	1.466216000	-1.786904000	-3.012251000
6	2.476720000	-1.021396000	-3.541305000
8	2.331620000	-0.495089000	-4.627897000
6	3.735838000	-0.809083000	-2.732902000
1	3.585934000	0.066531000	-2.084683000
1	4.015049000	-1.655808000	-2.092403000
1	4.550886000	-0.594103000	-3.433446000
1	0.672386000	-1.867112000	-3.636325000
1	4.577182000	3.465035000	5.311333000
6	-4.257711000	-0.896493000	2.245582000
1	-2.700238000	1.286737000	2.784225000
9	-4.696814000	0.272295000	1.757589000
9	-5.001242000	-1.170555000	3.323577000
9	-4.546648000	-1.837343000	1.331323000

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