Supporting Information

Palladium-Catalyzed Oxidative Heck Reaction of Non-activated Alkenes Directed by Fluorinated Alcohol

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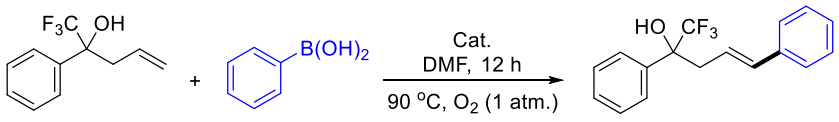
1. Materials and Methods

General Remarks

NMR spectra were recorded on a Bruker AV 400 spectrometer at 400 MHz (^{1}H NMR), 101 MHz (^{13}C NMR), 376 MHz (^{19}F NMR). Chemical shifts (δ) for ^{1}H and ^{13}C NMR spectra are given in ppm relative to TMS. The residual solvent signals were used as references for ^{1}H and ^{13}C NMR spectra, and the chemical shifts were converted to the TMS scale ($CDCl_3$: δ_H = 7.26 ppm, δ_C = 77.00 ppm; $(CD_3)_2SO$: δ_H = 2.50 ppm, δ_C = 40.00 ppm). ^{1}H, ^{13}C and ^{19}F multiplicities are reported as follows: singlet (s), doublet (d), triplet (t), quartet (q), double doublets (dd), double triplet (dt) and multiplet (m). Melting points were determined with a Buchi Melting Point B-545 instrument. IR spectra were obtained either as potassium bromide pellets or as liquid films between two potassium bromide pellets with a Bruker TENSOR 27 spectrometer. High-resolution mass spectra (APCI) were obtained with a LCMS-IT-TOF mass spectrometer. X-ray structural analysis was conducted on an X-ray analysis instrument. All the reaction temperatures reported are oil bath temperatures. Silica gel 60H (200-300 mesh) manufactured by Qingdao Haiyang Chemical Group Co. (China) was used for general silica gel flash column chromatography. Unless otherwise noted, all reagents and solvents were obtained from commercial suppliers and used without further purification.

Table S1. The Screening of the Catalyst[a]



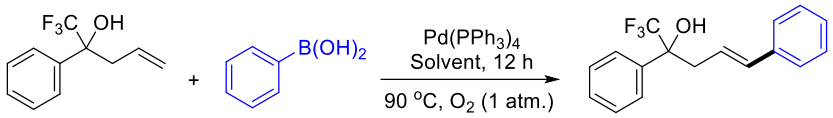
1a **2a** **3a**

Entry	Catalyst	Yield[b] (%)
1	$Pd(OAc)_2$	46
2	$PdCl_2$	0
3	$Pd(TFA)_2$	0
4	PdI_2	23
5	$Pd(dba)_2$	Trace
6	**$Pd(PPh_3)_4$**	**77(74[c])**

7	CuCl	0
8	-	0

[a]Reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), Catalyst (10 mol%), DMF (2.0 mL) in the tube at 90 °C for 12 h under O_2 atmosphere. [b]The yields were determined by ^{19}F NMR spectroscopy of the crude product with $PhCF_3$ as an internal standard. [c]The yields were isolated yields.

Table S2. Solvent Effects[a]

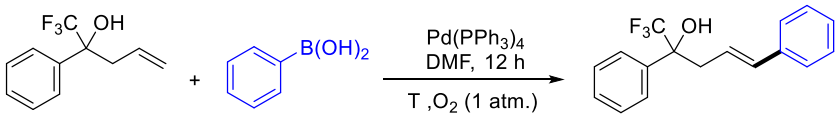


1a **2a** **3a**

Entry	Solvent	Yield[b] (%)
1	**DMSO**	**79**
2	Dioxane	0
3	Toluene	51
4	CH_3CN	0
5	THF	0
6	**DMF**	**79**
7	$MeNO_2$	50
8	Ethanol	0

[a]Reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), $Pd(PPh_3)_4$ (10 mol%), Solvent (2.0 mL) in the tube at 90 °C for 12 h under O_2 atmosphere. [b]The yields were determined by ^{19}F NMR spectroscopy of the crude product with $PhCF_3$ as an internal standard.

Table S3. Temperature Effects[a]



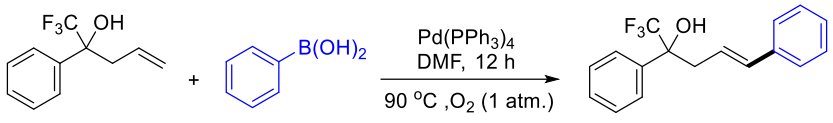
1a **2a** **3a**

Entry	T / °C	Yield[b] (%)
1	110	56
2	100	60
3	**90**	**79**
4	80	69

5	70	74
6	60	67
7	50	33
8	40	19

[a]Reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), $Pd(PPh_3)_4$ (10 mol%), DMF (2.0 mL) in the tube at 90 °C under O_2 atmosphere. [b]The yields were determined by ^{19}F NMR spectroscopy of the crude product with $PhCF_3$ as an internal standard.

Table S4. The Amount of Phenylboronic Acid Optimization[a]

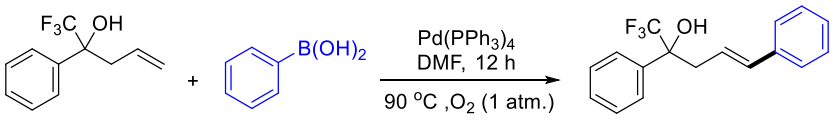


1a **2a** **3a**

Entry	**2a (mmol)**	Yield[b] (%)
1	0.3	15
2	0.4	74
3	0.5	73
4	**0.6**	**66**
5	0.7	64

[a]Reaction conditions: **1a** (0.2 mmol), **2a** (x mmol), $Pd(PPh_3)_4$ (10 mol%), DMF (2.0 mL) in the tube at 90 °C for 12 h under O_2 atmosphere. [b]The yields were determined by ^{19}F NMR spectroscopy of the crude product with $PhCF_3$ as an internal standard.

Table S5. The Amount of Catalyst Optimization[a]

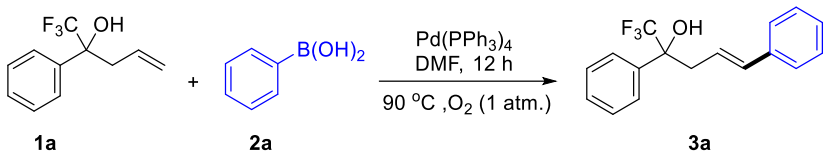


1a **2a** **3a**

Entry	$Pd(PPh_3)_4$ (mol %)	Yield[b] (%)
1	**5**	**89**
2	10	77
3	20	54
4	3	73
5	1	20

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), $Pd(PPh_3)_4$ (x mol%), DMF (2.0 mL) in the tube at 90 °C for 12 h under O_2 atmosphere. [b] The yields were determined by ^{19}F NMR spectroscopy of the crude product with $PhCF_3$ as an internal standard.

Table S6. The Effects of Reaction Time and Solvent Dosage[a]

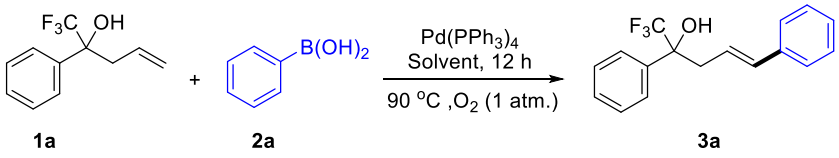


1a **2a** **3a**

Entry	**Solvent**	T / h	Yield[b] (%)
1	DMF(1 mL)	12	73
2	**DMF(2 mL)**	**12**	**89**
3	DMF(3 mL)	12	70
4	DMF(2 mL)	0.5	20
5	DMF(2 mL)	1	62
6	DMF(2 mL)	3	80
7	DMF(2 mL)	6	87
8	**DMF(2 mL)**	**9**	**89**

[a]Reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), $Pd(PPh_3)_4$ (5 mol%), DMF (2.0 mL) in the tube at 90 °C for 12 h under O_2 atmosphere. [b]The yields were determined by ^{19}F NMR spectroscopy of the crude product with $PhCF_3$ as an internal standard.

Table S7. The Effects of Mixed Solvents and Phenylboronic Acid Dosage[a]



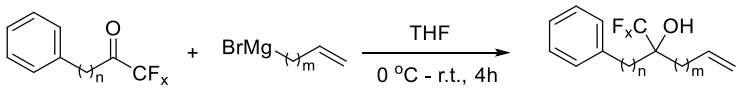
1a **2a** **3a**

Entry	2a	Solvent	Yield[b] (%)
1	0.4	DMF/DMSO (1 mL:1mL)	91
2	0.4	DMF/Toluene (1 mL:1mL)	complex
3	0.4	DMF/$MeNO_2$ (1 mL:1mL)	complex

4	0.4	DMSO/Toluene (1 mL:1mL)	82
5	0.4	DMSO/$MeNO_2$ (1 mL:1mL)	complex
6	**0.6**	**DMF/DMSO (1 mL:1mL)**	**95**
7[c]	0.6	DMF/DMSO (1 mL:1mL)	trace
8	0.8	DMF/DMSO (1 mL:1mL)	94

[a]Reaction conditions: **1a** (0.2 mmol), **2a** (x mmol), $Pd(PPh_3)_4$ (5 mol%), Solvent (2.0 mL) in the tube at 90 °C for 12 h under O_2 atmosphere. [b]The yields were Isolated. [c]air instead of O_2.

General procedure A for synthesis of alkene substrates



n = 0, 1, 2
x = 2, 3

m = 0,1

This compound was prepared following a literature procedure[1-2]. Add trifluoromethyl ketone (10 mmol) in a 50 mL oven-dried Schleck flask under nitrogen and add 10 mL of dry THF to the mixture *via* syringe. Add Grignard reagent (1.0 M in THF) dropwise to the reaction mixture at 0 °C using an ice bath. Stir the reaction mixture at room temperature for 4 hours. Quench the reaction mixture with saturated NH_4Cl (aq.). Extract the reaction mixture with ethyl acetate (3 x 30 mL). and wash the combined organic layers with brine. Dry the reaction mixture over Na_2SO_4, concentrate and purified by silica gel flash column chromatography to yield the corresponding product.

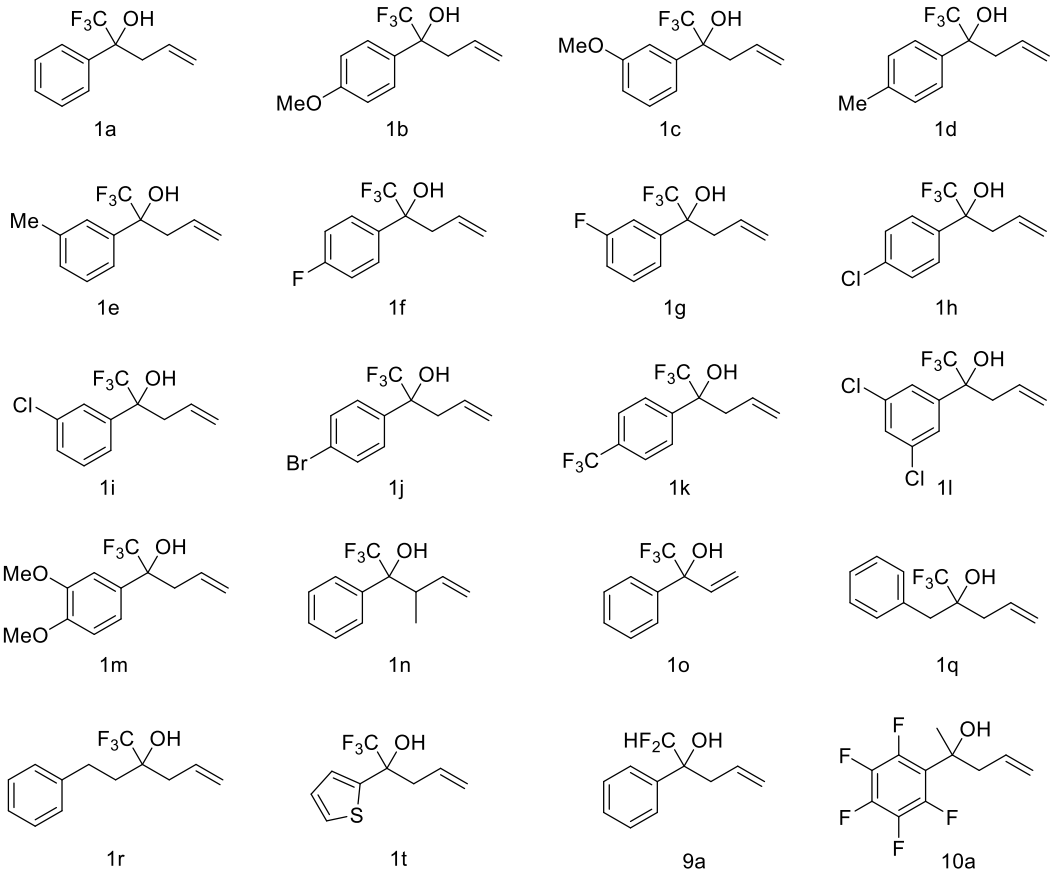
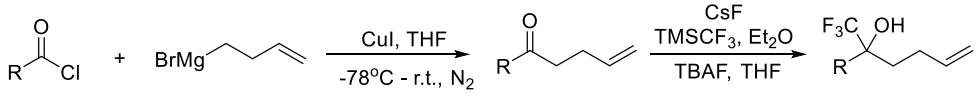


Figure S1. List of alkene substrates

General procedure B for synthesis of alkene substrates

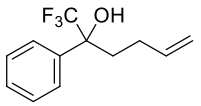


R = phenyl, cyclohexyl

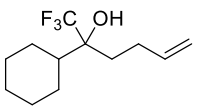
This compound was prepared following a literature procedure[3-4]. Add CuI (0.15 equiv) in a 250 mL oven-dried Schleck flask under nitrogen and evacuate the flask and refill with nitrogen (× 3). Then dry THF (40 mL) and acid chloride (20 mmol) was added. Stir the mixture at room temperature for 10 min and cool to -78 °C and add a freshly prepared solution of but-3-en-1-ylmagnesium bromide (1.1 equiv) by dropwise. Allow the mixture to warm to room temperature overnight. Quench the reaction mixture with saturated NH_4Cl (aq.). Extract the reaction mixture with ethyl acetate (3 × 30 mL) and wash the combined organic layers with brine. Dry the reaction mixture over Na_2SO_4, concentrate and purified by silica gel flash column chromatography to yield the enone.

This compound was prepared following a literature procedure[5-6]. Add CF_3TMS (12.0

mmol, 1.2 equiv) to a solution of enone (10 mmol) in Et_2O (30 mL). Add 1 mol% of dry CsF (0.1 mmol) to the mixture. Stir the reaction mixture at room temperature overnight. To cleave the alcohol formed by the reaction[9], the reaction mixture was cooled to 0 °C in an ice bath. H_2O (5 mL) and TBAF (30 mmol. 2 equiv) was then added and the reaction mixture was allowed to stir at room temperature for 6 h. After the reaction was completed, the mixture diluted with H_2O (20 mL), and extracted with ethyl acetate (10 mL × 3). The combined organic layer was dried over anhydrous Na_2SO_4 and concentrated in vacuum. The resulting materials were purified by flash column chromatography on silica gel with petroleum ether/ethyl acetate.



1p



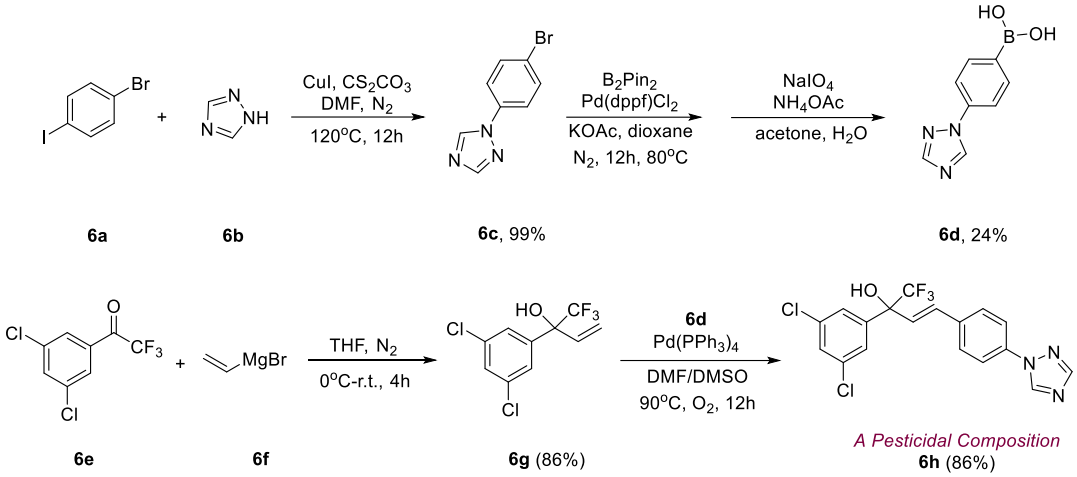
1s

General procedure for arylation of unactivated alkenes

To a 25 mL dried reaction tube was added the mixture of $Pd(PPh_3)_4$ (5 mol%), arylboronic acid (0.6 mmol, 3 equiv) andalkene substrate (0.2 mmol) in DMF/DMSO(1:1, 2 mL) successively. The mixture was stirred at 90 °C for 12 h under O_2 atmosphere. After the reaction was completed, the mixture was cooled to room temperature and diluted with H_2O (5 mL), and extracted with ethyl acetate (5 mL × 3). The combined organic layer was dried over anhydrous Na_2SO_4 and concentrated in vacuum. The resulting materials were purified by flash column chromatography on silica gel with petroleum ether/ethyl acetate.

2. Representative Derivatizations and Application of Strategy

The Synthesis of Pesticide Composition 6h



Scheme S1

This compound was prepared following a literature procedure[7]. To a stirred solution of 1-bromo-4-iodobenzene **6a** (26.6 mmol, 1.2 equiv), 1H-1,2,4-triazole **6b** (22.17 mmol) in DMF (50mL), Cs_2CO_3 (88.68 mmol, 4 equiv) was added anddegassed with nitrogen gas for 15 min. Then CuI (0.404 g, 2.12 mmol) was added and heated at 120 °C for 12h. After cooling, the reaction mixture was quenched with ice and extracted with ethyl acetate. The organic layer was washed with water and brine, dried over Na_2SO_4 and concentrated under reduced pressure. The product was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (5:1) to yield the white solid powder **6c** (4.895 g, 99%).

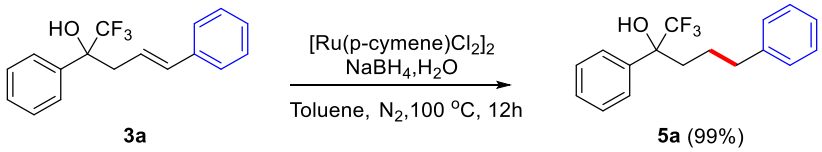
This compound was prepared following a literature procedure[8]. To a solution of bis(pinacolato)diboron (10 mmol, 2 equiv), $Pd(dppf)Cl_2$ (0.5 mmol, 0.05 equiv) and potassium acetate (15 mmol, 3 equiv) in 1,4-dioxane (60 ml) was added **6c** (5 mmol). The mixture was stirred under nitrogen at 80 °C for 12 h. Saturated sodium chloride solution (50 ml) was added and the resulting mixture was extracted with ethyl acetate (3 × 50 mL). The combined organic extracts were washed with waer, dried (Na_2SO_4) and concentrated in vacuo to give a dark brown oil. To the dark brown oil, n-hexane (10 mL) was added to precipitate crystals, and the crude product was obtained by filtration.

To a solution of sodium periodate (4 mmol, 2 equiv) and ammonium acetate (4 mmol, 2 equiv) and potassium acetate (15 mmol, 3 equiv) in acetone/H_2O (2:1, 21 mL) was added aryl borate (5 mmol). The mixture was stirred overnight at room temperature.

Saturated sodium chloride solution (20 ml) was added and the resulting mixture was extracted with ethyl acetate (3 × 10 mL). The combined organic were dried (Na_2SO_4) and concentrated in vacuo to give grey solid. Then the gray solid was washed with n-hexane (3 × 10 mL) and water (3 × 10 mL) to obtain pure arylboronic acid **6d** (171 mg ,45%).

This compound was prepared following a literature procedure[1-2]. Add trifluoromethyl ketone **6e** (5 mmol) in a 50 mL oven-dried Schleck flask under nitrogen and add 10 mL of dry THF to the mixture *via* syringe. Add alkenyl magnesium bromide **6f** (2.0 M in THF) dropwise to the reaction mixture at 0 °C using an ice bath. Stir the reaction mixture at room temperature for 4 hours. Quench the reaction mixture with saturated NH_4Cl (aq). Extract the reaction mixture with ethyl acetate (3 × 20 mL), and wash the combined organic layers with brine. Dry the reaction mixture over Na_2SO_4, concentrate and purified by silica gel flash column chromatography on eluting with ether/ethyl acetate (100:1-50:1 gradient) to yield the colorless oily product **6g** (1.163g, 86%).

To a 25 mL dried reaction tube was added the mixture of $Pd(PPh_3)_4$ (5 mol%), arylboronic acid **6d** (0.6 mmol, 3 equiv) andalkene substrate **6g** (0.2 mmol) in DMF/DMSO(1:1, 2 mL) successively. The mixture was stirred at 90 °C for 12 h under O_2 atmosphere. After the reaction was completed, the mixture was cooled to room temperature and diluted with H_2O (5 mL), and extracted with ethyl acetate (5 mL × 3). The combined organic layer was dried over anhydrous Na_2SO_4 and concentrated in vacuum. The resulting materials were purified by flash column chromatography on silica gel with petroleum ether/ethyl acetate (5:1) to yield white solid product **6h** (71 mg, 86%).

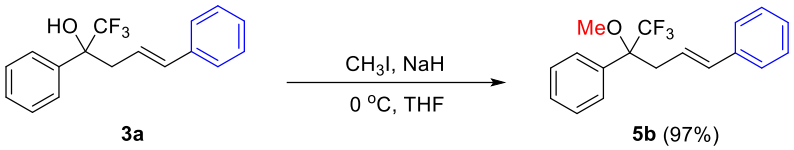


3a **5a** (99%)

Scheme S2

This compound was prepared following a literature procedure[10].Olefins **3a** (0.5 mmol), sodium borohydride (1 mmol, 2 equiv), water (1 mmol, 2 equiv) and [Ru(*p*-cymene)Cl_2]$_2$ (0.01 mmol, 2 mol%) in toluene (1 mL) were heated at 100 °C for12 h in

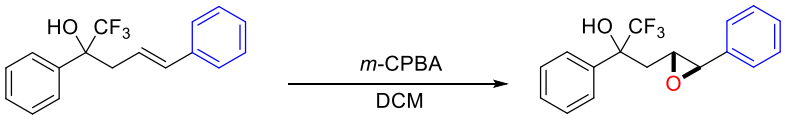
a pressure tube. After the reaction was completed, the mixture was cooled to room temperature and diluted with H_2O (5 mL), and extracted with ethyl acetate (5 mL × 3). The combined organic layer was dried over anhydrous Na_2SO_4 and concentrated in vacuum. The resulting materials were purified by flash column chromatography on silica gel with petroleum ether/ethyl acetate (100:1) to yield colorless oil product **5a** (145.5 mg, 99%).



3a **5b** (97%)

Scheme S3

This compound was prepared following a literature procedure[11]. To a stirring solution of sodium hydride (0.75 mmol, 1.5 equiv, 60% in mineral oil) in anhydrous THF (1 mL), alcohol **3a** (0.5 mmol) in anyhydrous THF (1 mL) was added at 0 °C under nitrogen. The resulting suspension was stirred at 0 °C for 1 h. Then iodomethane (0.75 mmol, 1.5 equiv) was added dropwise. The reaction mixture was stirred at room temperature overnight. The reaction was quenched with saturated ammonium chloride solution. The aqueous layer was extracted with ethyl acetate (3 × 5 mL). The combined organic extracts were washed with brine, dried over Na_2SO_4 and concentrated in vacuo. The residue was purified by flash column chromatography on silica gel with petroleum ether/ethyl acetate (100:1) to give the product **5b** as a yellow oil (148.4 mg, 97%).



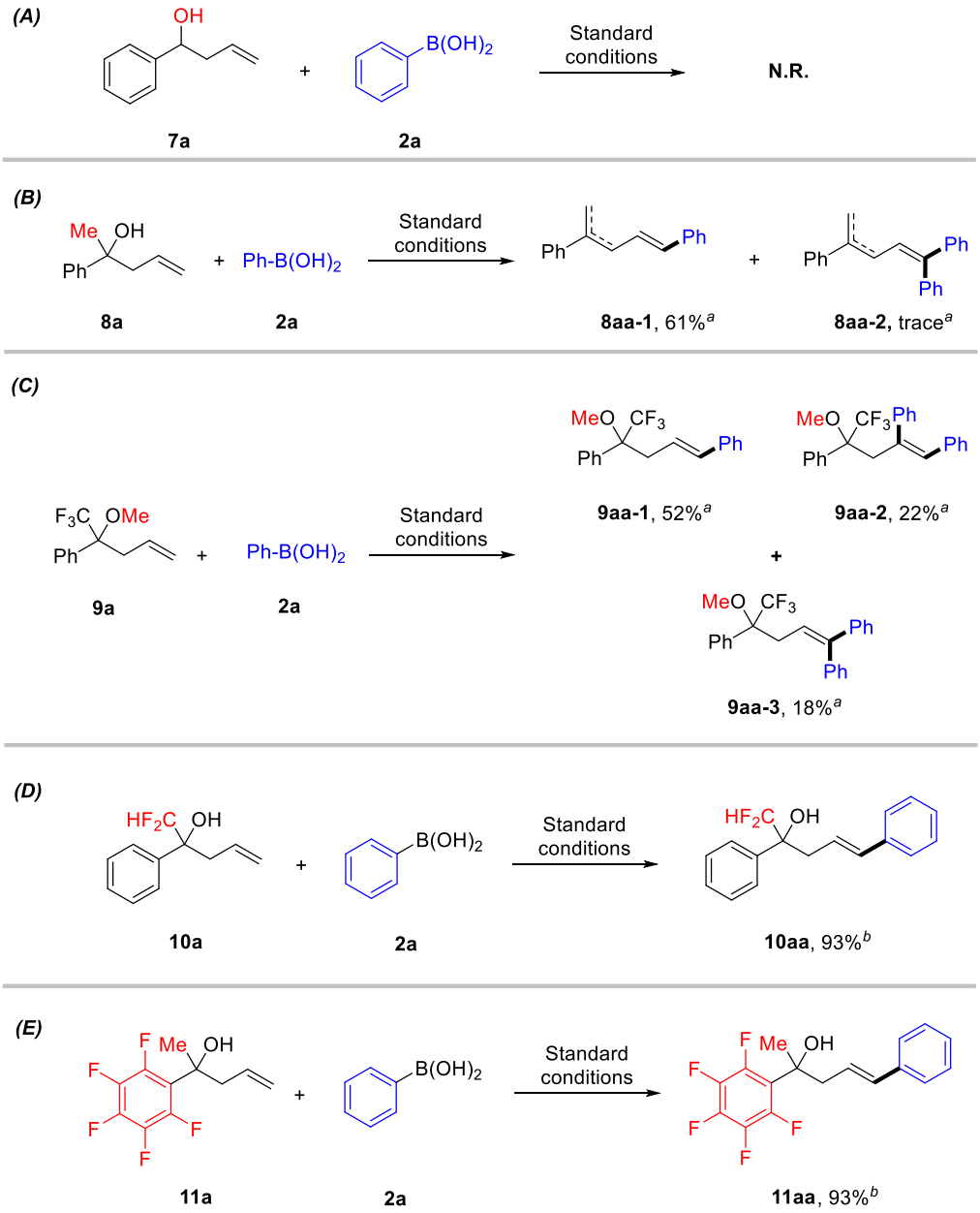
3a **5c** (99%)
d.r. = 1:2.57

Scheme S4

This compound was prepared following a literature procedure[12]. A flame dried test tube was charged with *m*-CPBA (0.3 mmol, 1.5 equiv) and DCM (2 mL) then cooled to 0 °C. Next added the compound **3a** (0.2 mmol) and increase the temperature gradually to room temperature and stirred overnight. After completion of reaction, mixture was quenched with saturated $NaHCO_3$ (5 mL). The organic layer was separated and the aqueous layer was extracted with additional DCM (3 × 5 mL). The organic

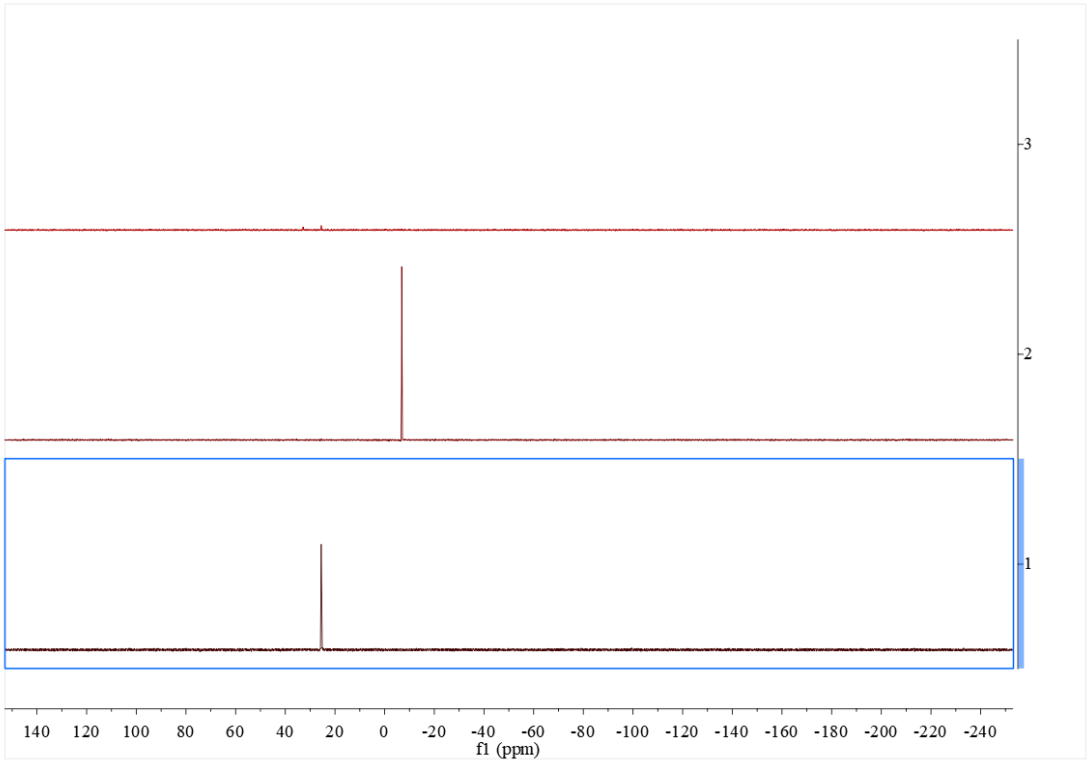
layers were combined and washed with brine (10 mL). The organic layer was separated, dried over Na_2SO_4, and concentrated over rotary evaporator. The d.r. was calculated from the crude reaction mixture by using the ^{19}F NMR. The crude product was purified by silica gel column chromatography (by using 20:1 petroleum ether/ethyl acetate as eluents) to obtain white solid **5c** (61 mg, 99%).

3. Control Experiment



[a]Determined by GC-MS. [b]Isolated yield.

Scheme S5



Scheme S6: ^{13}P NMR monitoring, 1) reaction solution, 2) triphenylphosphine, 3) tetrakis(triphenylphosphine)palladium

4. DFT Calculations

All DFT calculations were performed at PBE0/BS-I level using Gaussian 09 program, with Grimme's D3 empirical dispersion correction.[13-15] BSI denotes combination of the SDD basis set for Pd, and the 6-31G** basis sets for the other atoms. Additionally, single point calculations were performed to present better electronic energy with the PBE0 method and def2-TZVPP[16] basis set, using optimized geometries under PBE0/BS-I level. The mixed solvation effect (ε= 42.02) of DMF and DMSO was simulated by the SMD continuum solvent mode.[17] All transition states were further confirmed by vibrational analysis and characterized by the only one imaginary frequency. Intrinsic reaction coordinates (IRC)[18] calculations were performed in order to confirm intermediates along the reaction pathways. All energies discussed in the following parts are Gibbs free energies relative to **A1** and are calculated at 298.15 K unless otherwise stated. A correction factor of 1.89 kcal/mol was applied for the standard state change from 1 atm to 1 M. Total energies and Cartesian coordinates of all optimized structures are given in Supporting Information (SI).

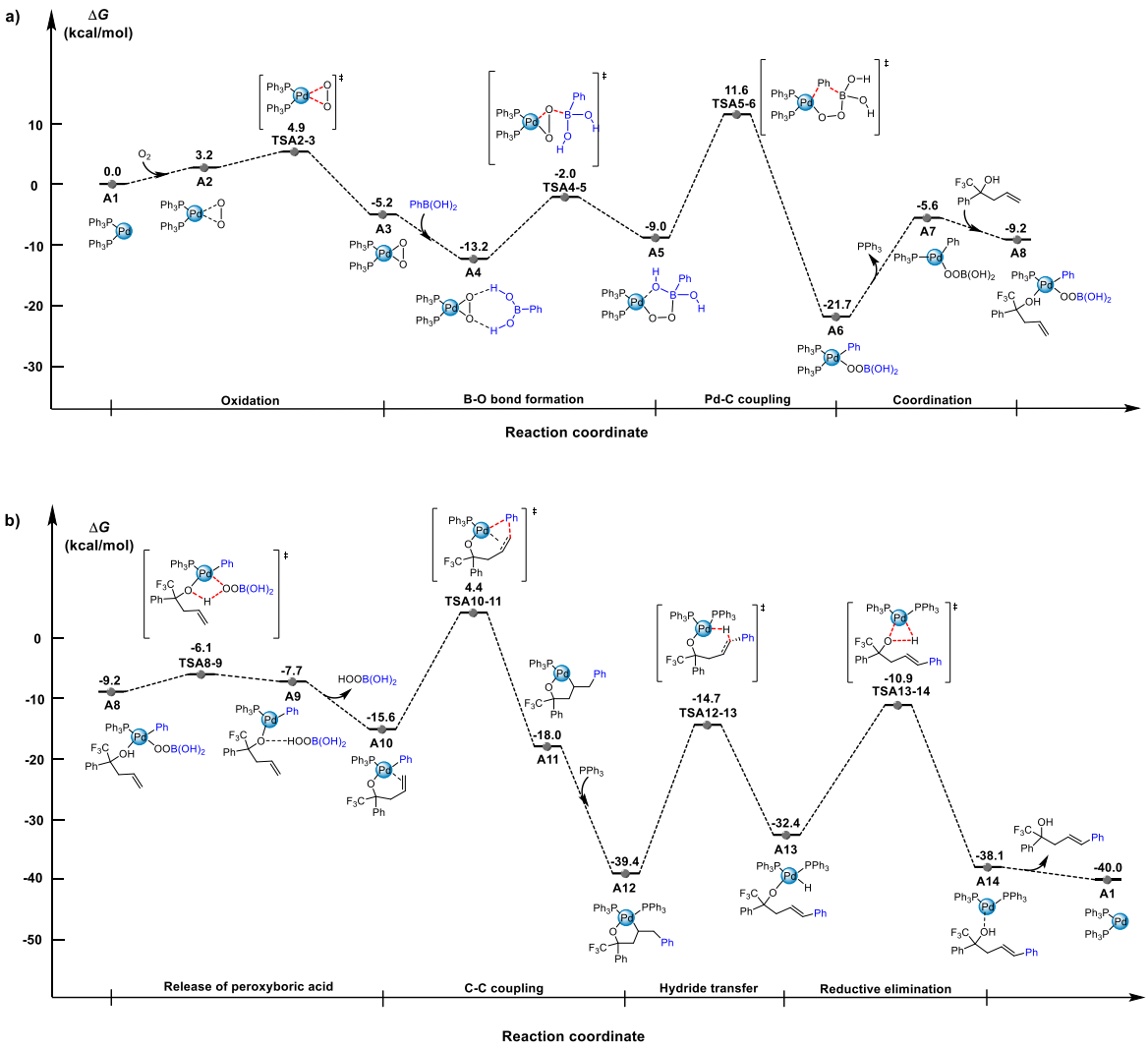


Figure S2. Gibbs free energy profiles for the oxidative Heck reaction of a) the catalyst oxidation and substrate coordination processes and b) product release and catalyst regeneration (unit: kcal/mol).

The electron-rich $Pd(PPh_3)_2$ could easily combine with oxygen to form **A2**, and then form the peroxo complex **A3** in the oxidation step via transition state **TSA2-3**, with an energy barrier of 1.7 kcal/mol. The oxygen atoms of **A3** could form hydrogen bond with the hydroxyl group of phenylboronic acid to provide a more stable compound **A4**, which is exergonic by 8.0 kcal/mol. Then electron-poor boron atom approachs the electron-rich oxygen atom via **TSA4-5**, with an energy barrier of 12.0 kcal/mol for the formation of B-O bond and the cleavage of Pd-O bond from **A4** to **A5**. Then the benzene moeity of **A5** is migrated to Pd center via **TSA5-6** to form **A6 in** the Pd-C coupling step, with a free energy barrier of 20.6 kcal/mol. One PPh_3 ligand is dissociated from **A6** to obtain intermediate **A7**, which is endergonic by 16.1 kcal/mol. The oxygen atom of **1a** substrate coordinates with Pd center of **A7** to form **A8**. Due to the electron-withdrawing trifluoromethyl group enhancing the acidity of the hydroxyl group, the proton of hydroxyl group of **A8** is easily transferred to obtain peroxyboric acid via **TSA8-9**, with an energy barrier of 3.1 kcal/mol. Then **A9** releases peroxyboric acid and

the olefin moiety coordinates with Pd to generate **A10**. In the C-C coupling step, the olefin moiety is inserted into the Pd-C bond via **TSA11-12** to form **A11** with a five-membered ring. The energy barrier for this step is 20.0 kcal/mol. Then one molecule PPh_3 coordinates with Pd center of **A11** to form **A12**, which is the most stable intermediate in the catalytic cycle . In the subsequent hydride transfer step (β-H elimination), the hydride is transferred to Pd center to form Pd-H intermediate **A13** via **TSA12-13**, with an energy barrier of 24.7 kcal/mol. Then **A13** undergo the reductive elimination via **TSA13-14** to obtain **A14**, and the energy barrier for this process is 21.5 kcal/mol. Finally, one molecule product **3a**, is released from **A14** and the active catalytic species **A1** is regenerated. The energetic span for this reaction is 28.5 kcal/mol (**A12→TSA13-14**). Meanwhile, the dissociative or associative effects of PPh_3 ligand in this reaction were also investigated.

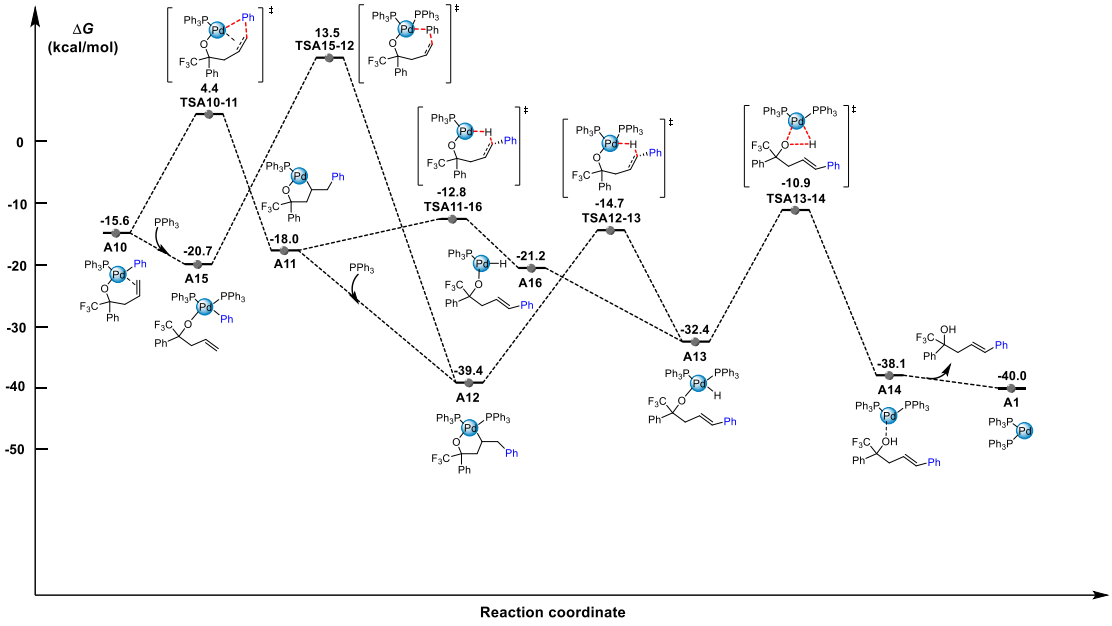


Figure S3. Effect of dissociation and association of PPh_3 ligand on the reaction (unit: kcal/mol)

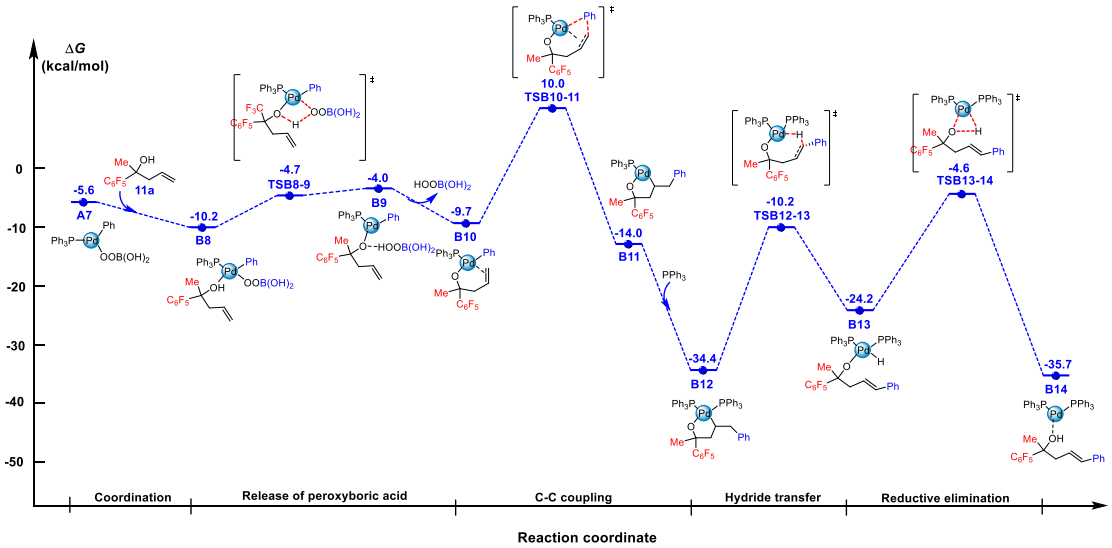


Figure S4. The Gibbs free energy profiles for the reactions of **11a** catalyzed by Pd complex (unit: kcal/mol).

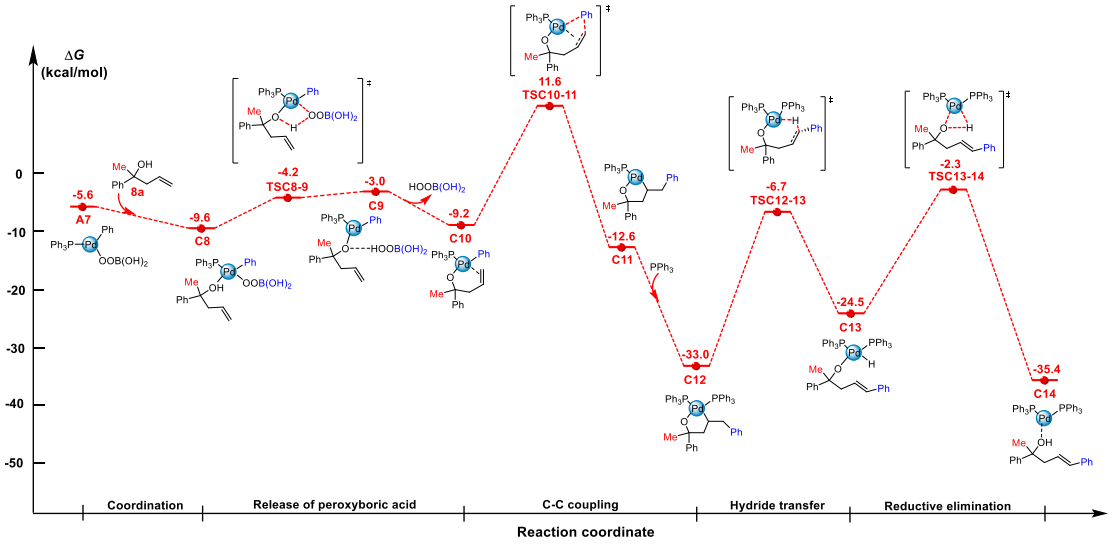


Figure S5. The Gibbs free energy profiles for the reactions of **8a** catalyzed by Pd complex (unit: kcal/mol).

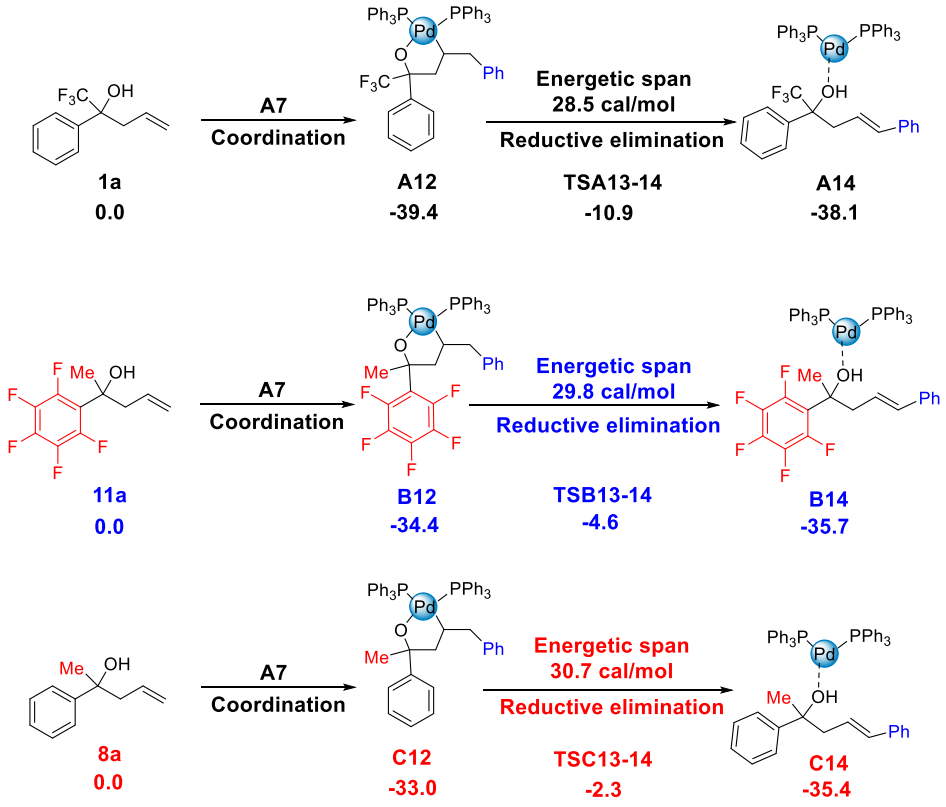


Figure S6. Effects of different substituents on reductive elimination process (unit: kcal/mol).

Table S8. The calculated absolute electronic energies (*E*, in a.u.), thermal free energies

(*G*, in a.u.), and relative Gibbs energies (Δ*G*, in kcal/mol) (Calculated at 298.15 K).

Complex	***E***	***G***	Δ*G*
A1	-2199.312321	-2198.835468	0.0
A2	-2349.572274	-2349.091006	3.2
TSA2-3	-2349.572119	-2349.088196	4.9
A3	-2349.593725	-2349.104344	-5.2
A4	-2757.610382	-2757.003434	-13.2
TSA4-5	-2757.592657	-2756.985696	-2.0
A5	-2757.604798	-2756.996953	-9.0
TSA5-6	-2757.571911	-2756.964113	11.6
A6	-2757.624554	-2757.017197	-21.7
A7	-1721.915420	-1721.570325	-5.6
A8	-2521.964582	-2521.430706	-9.2
TSA8-9	-2521.956881	-2521.425771	-6.1
A9	-2521.961443	-2521.428330	-7.7
A10	-2194.527497	-2194.040736	-15.6
TSA10-11	-2194.498214	-2194.008778	4.4
A11	-2194.535850	-2194.044531	-18.0
A12	-3230.250615	-3229.499753	-39.4
TSA12-13	-3230.204156	-3229.460328	-14.7
A13	-3230.231098	-3229.488605	-32.4
TSA13-14	-3230.192060	-3229.454383	-10.9
A14	-3230.239968	-3229.497616	-38.1
A1	-2199.312321	-2198.835468	-40.0
O_2	-150.247585	-150.263586	/
$PhB(OH)_2$	-407.982793	-407.889561	/
PPh_3	-1035.653051	-1035.424139	/
1a	-800.017250	-799.857649	/
$HOOB(OH)_2$	-327.427559	-327.403250	/

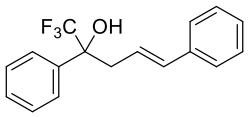
Pro-1a	-1030.901741	-1030.668254	/
A15	-3230.214870	-3229.469880	-20.7
TSA15-12	-3230.165026	-3229.415409	13.5
TSA11-16	-2194.519009	-2194.036225	-12.8
A16	-2194.533229	-2194.049666	-21.2
B8	-2720.289699	-2719.776857	-10.2
TSB8-9	-2720.280244	-2719.768094	-4.7
B9	-2720.281654	-2719.766953	-4.0
B10	-2392.842885	-2392.375721	-9.7
TSB10-11	-2392.814416	-2392.344416	10.0
B11	-2392.853063	-2392.382595	-14.0
B12	-3428.566060	-3427.836322	-34.4
TSB12-13	-3428.520540	-3427.797613	-10.2
B13	-3428.542904	-3427.819969	-24.2
TSB13-14	-3428.508127	-3427.788843	-4.6
B14	-3428.560186	-3427.838265	-35.7
11a	-998.341633	-998.202126	/
C8	-2224.371099	-2223.812130	-9.6
TSC8-9	-2224.360340	-2223.803549	-4.2
C9	-2224.361085	-2223.801636	-3.0
C10	-1896.924318	-1896.411395	-9.2
TSC10-11	-1896.892926	-1896.378137	11.6
C11	-1896.932180	-1896.416828	-12.6
C12	-2932.645820	-2931.870447	-33.0
TSC12-13	-2932.599057	-2931.828544	-6.7
C13	-2932.626030	-2931.856869	-24.5
TSC13-14	-2932.589189	-2931.821521	-2.3
C14	-2932.642718	-2931.874214	-35.4
8a	-502.424365	-502.238488	/

Table S9. Calculated imaginary frequencies of transition states at PBE0-D3/BS-I level.

TSA2-3	19.23*i*
TSA4-5	145.95*i*
TSA5-6	225.41*i*
TSA8-9	634.55*i*
TSC8-9	488.93*i*
TSB8-9	633.01*i*
TSA10-11	370.63*i*
TSC10-11	373.73*i*
TSB10-11	373.23*i*
TSA11-16	586.67*i*
TSA12-13	771.83*i*
TSC12-13	769.06*i*
TSB12-13	602.53*i*
TSA13-14	1031.46*i*
TSC13-14	1083.54*i*
TSB13-14	1056.97*i*
TSA15-12	389.49*i*

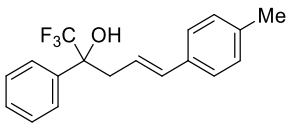
5. Supplementary Text

Characterization Data

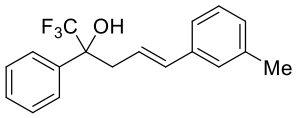


(*E*)-1,1,1-Trifluoro-2,5-diphenylpent-4-en-2-ol (3a): Yield: 55.5 mg (95%), yellow solid. M.p.: 84.0-85.1 °C. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.40. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 7.62(d, J = 8.0, 2H), 7.43-7.31 (m, 3H), 7.28-7.15 (m, 5H), 6.72 (s, 1H), 6.50 (d, J = 16.0 Hz, 1H), 5.96 (dt, J = 16.0, 8.0 Hz, 1H), 3.07 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ ppm 137.8, 137.3, 133.9, 129.0, 128.5, 128.4, 127.7, 127.4, 126.4 (q, $J_{C\text{-}F}$ = 262.6 Hz), 126.2, 123.5, 75.9 (q, $J_{C\text{-}F}$ = 26.3 Hz),

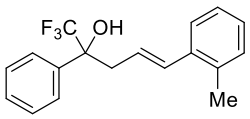
38.1. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -78.23. IR (KBr, cm^{-1}): υ_{max} = 3549, 3031, 2932, 1496, 1447, 1267, 1160, 1073, 1012, 969, 907, 741, 699, 636, 507. HRMS (APCI) calc. $C_{17}H_{14}F_3O^-$ [M-H]$^-$: 291.1002, found: 291.1006.



(*E*)-1,1,1-Trifluoro-2-phenyl-5-(*p*-tolyl)pent-4-en-2-ol (3b)：Yield: 57.5 mg (94%), yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.30. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 7.60 (d, J = 8.0 Hz, 2H), 7.41-7.30 (m, 3H), 7.10-7.04 (m, 4H), 6.68 (s, 1H), 6.43 (d, J = 16.0 Hz, 1H), 5.88 (dt, J = 16.0, 8.0 Hz, 1H), 3.04 (m, 2H), 2.22 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ ppm 137.3, 136.5, 134.1, 133.3, 129.1, 128.0, 127.9, 126.9, 125.9 (q, $J_{C\text{-}F}$ = 288.9 Hz) 125.7, 121.9, 76.0 (q, $J_{C\text{-}F}$ = 27.3 Hz), 37.7, 20.7. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -78.23. IR (KBr, cm^{-1}): υ_{max} = 3546, 3031, 2925, 2857, 1512, 1448, 1266, 1159, 1071, 1013, 969, 763, 701, 504. HRMS (APCI) calc. $C_{18}H_{16}F_3O^-$ [M-H]$^-$： 305.1159, found: 305.1162.

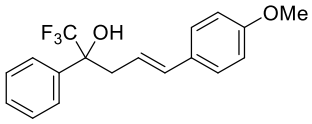


(*E*)-1,1,1-Trifluoro-2-phenyl-5-(*m*-tolyl)pent-4-en-2-ol (3c): Yield: 53.3 mg (87%), yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.40. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 7.60 (d, J = 8.0 Hz, 2H), 7.41-7.30 (m, 3H), 7.13 (t, J = 8.0 Hz, 1H), 7.01-6.97 (m, 3H), 6.70 (s, 1H), 6.44 (d, J = 16.0 Hz, 1H), 5.94 (dt, J = 16.0, 8.0 Hz, 1H), 3.05 (m, 2H), 2.22 (s, 3H).^{13}C NMR (101 MHz, DMSO-d_6) δ ppm 137.6, 137.3, 136.7, 133.5, 128.4, 128.0, 127.9, 127.9, 126.9, 126.3,125.9 (q, $J_{C\text{-}F}$=288.9 Hz), 123.0, 122.8, 75.9 (q, $J_{C\text{-}F}$ = 27.3 Hz), 37.7, 20.9. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -78.25. IR (KBr, cm^{-1}): υ_{max} = 3545, 3034, 2925, 2857, 1604, 1448, 1266, 1160, 1071, 1016, 970, 762, 771, 504. HRMS (APCI) calc. $C_{18}H_{16}F_3O^-$[M-H]$^-$: 305.1159, found: 305.1162.

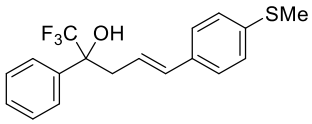


(*E*)-1,1,1-Trifluoro-2-phenyl-5-(*o*-tolyl)pent-4-en-2-ol (3d)：Yield：55.0 mg (90%),

yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.40. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 7.62 (d, J = 8.0 Hz, 2H), 7.42-7.31 (m, 3H), 7.14-7.04 (m, 4H), 6.71 (s, 1H), 6.65 (d, J = 16.0 Hz, 1H), 5.78 (dt, J = 16.0, 8.0 Hz, 1H), 3.08 (m, 2H), 2.13 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ ppm 137.3, 136.1, 134.5, 131.8, 123.0, 128.0, 127.9, 127.1, 127.0, 126.0 (q, $J_{C\text{-}F}$= 288.9 Hz), 126.0, 125.1, 124.3, 76.0 (q, $J_{C\text{-}F}$ = 27.3 Hz), 37.9, 19.2. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -78.27. IR (KBr, cm^{-1}): υ_{max} = 3547, 3288, 3029, 2926, 2858, 1489, 1450, 1267, 1160, 1072, 1018, 970, 751, 702, 509. HRMS (APCI) calc. $C_{18}H_{16}F_3O^-$ [M-H]$^-$: 305.1159, found: 305.1162.

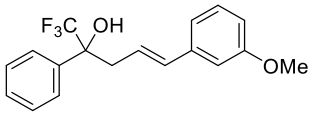


(*E*)-1,1,1-Trifluoro-5-(4-methoxyphenyl)-2-phenylpent-4-en-2-ol (3e): Yield: 61.2 mg (95%), yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.45. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 7.60 (d, J = 8.0 Hz, 2H), 7.42-7.30 (m, 3H), 7.13 (d, J = 8.0 Hz, 2H), 6.81 (d, J = 8.0 Hz, 2H), 6.66 (s, 1H), 6.41 (d, J = 16.0 Hz, 1H), 5.78 (dt, J = 16.0, 8.0 Hz, 1H), 3.70 (s, 3H), 3.03 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ ppm 159.1, 137.9, 133.4, 130.0, 128.5, 128.4, 127.4, 127.4, 126.4 (q, $J_{C\text{-}F}$ = 288.9 Hz), 121.0, 114.4, 76.4 (q, $J_{C\text{-}F}$ = 27.3 Hz), 55.5, 38.2. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -78.20. IR (KBr, cm^{-1}): υ_{max} = 3542, 3463, 3036, 2929, 2842, 1608, 1511, 1251, 1162, 1029, 970, 837, 762, 703, 520. HRMS (APCI) calc. $C_{18}H_{18}F_3O_2^+$ [M+H]$^+$: 323.1253, found: 323.1252.

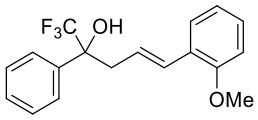


(*E*)-1,1,1-Trifluoro-5-(4-(methylthio)phenyl)-2-phenylpent-4-en-2-ol (3f): Yield: 43.9 mg (65%), yellow solid, M.p.: 98.2-99.7 °C. TLC (petroleum ether/ethyl acetate = 20/1, v/v): R_f = 0.30. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 7.59 (d, J = 7.6 Hz, 2H), 7.41-7.31 (m, 3H), 7.14 (s, 4H), 6.69 (s, 1H), 6.43 (d, J = 16.0 Hz, 1H), 5.90 (dt, J = 16.0, 8.0 Hz, 1H), 3.04 (m, 2H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ ppm 137.8, 137.5, 134.1, 133.3, 128.5, 128.4, 127.4, 126.8, 126.6, 126.4 (q, $J_{C\text{-}F}$ = 287.9 Hz),

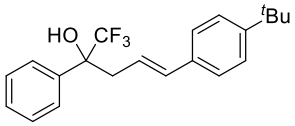
76.4 (q, $J_{C\text{-}F}$ = 26.3 Hz), 38.2, 15.2. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -78.21. IR (KBr, cm^{-1}): υ_{max} = 3543, 3033, 2924, 2854, 1596, 1494, 1267, 1160, 1012, 968, 763, 703, 213. HRMS (APCI) calc. $C_{18}H_{18}F_3O_1S_1^+$ $[M+H]^+$: 339.1025, found: 339.1026.



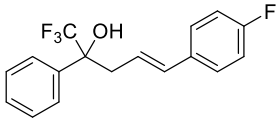
(*E*)-1,1,1-Trifluoro-5-(3-methoxyphenyl)-2-phenylpent-4-en-2-ol (3g): Yield: 59.9 mg (93%), yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.40. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 7.60 (d, J = 8.0 Hz, 2H), 7.41-7.31 (m, 3H), 7.16 (t, J = 8.0 Hz, 1H), 7.79-7.73 (m, 3H), 6.71 (s, 1H), 6.45 (d, J = 16.0 Hz), 5.96 (dt, J = 16.0, 8.0 Hz, 1H), 3.70 (s, 3H), 3.05 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ ppm 159.9, 138.8, 137.8, 133.8, 130.1, 128.5, 128.4, 127.4, 126.4(q, $J_{C\text{-}F}$ = 288.9 Hz), 123.9, 118.6, 113.2, 111.8, 76.4 (q, $J_{C\text{-}F}$ = 26.3 Hz), 55.4, 38.2. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -78.21. IR (KBr, cm^{-1}): υ_{max} = 3543, 3463, 3035, 2931, 2840, 1583, 1490, 1453, 1264, 1158, 1044, 970, 767, 701, 641. HRMS (APCI) calc. $C_{18}H_{18}F_3O_2^+$ $[M+H]^+$: 323.1253, found: 323.1252.



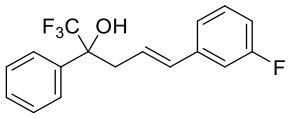
(*E*)-1,1,1-Trifluoro-5-(2-methoxyphenyl)-2-phenylpent-4-en-2-ol (3h): Yield: 59.9 mg (93%), yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.30. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 7.61 (d, J = 8.0 Hz, 2H), 7.41-7.31 (m, 3H), 7.18-7.13 (m, 2H), 6.92 (d, J = 8.0 Hz, 1H), 6.82 (t, J = 8.0 Hz, 1H), 6.70 (d, J = 16.0 Hz, 1H), 6.68 (s, 1H) 5.91 (dt, J = 16.0, 8.0 Hz, 1H), 3.72 (s, 3H), 3.06 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ ppm 155.9, 137.4, 128.4, 128.0, 127.9, 126.9, 126.0 (q, $J_{C\text{-}F}$ = 287.9 Hz), 125.9, 125.5, 123.4, 120.5, 111.3, 76.0 (q, $J_{C\text{-}F}$= 26.3 Hz), 55.3, 38.1. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -78.14. IR (KBr, cm^{-1}): υ_{max} = 3542, 3036, 2929, 2842, 1598, 1490, 1461, 1246, 1161, 1024, 976, 908, 755, 702, 635, 507. HRMS (APCI) calc. $C_{18}H_{16}F_3O_2^-$ $[M-H]^-$: 321.1108, found: 321.1108.



(*E*)-5-(4-(Tert-butyl)phenyl)-1,1,1-trifluoro-2-phenylpent-4-en-2-ol (3i): Yield: 65.4 mg (94%), yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.50. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 7.60 (d, J = 8.0 Hz, 2H), 7.40-7.24 (m, 6H), 7.12 (d, J = 8.4 Hz, 2H), 6.69 (s, 1H), 6.44 (d, J = 16.0 Hz, 1H), 5.90 (dt, J = 16.0, 8.0Hz, 1H), 3.05 (m, 2H), 1.22 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d_6) δ ppm 150.2, 137.8, 134.6, 133.7, 128.5, 128.4, 127.4, 126.3 (q, $J_{C\text{-}F}$ = 287.9 Hz), 126.0, 125.7, 122.6, 76.4 (q, $J_{C\text{-}F}$ = 27.3 Hz), 38.2, 34.6, 31.5. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -78.22. IR (KBr, cm^{-1}): υ_{max} = 3549, 3034, 2962, 2868, 1670, 1606, 1509, 1452, 1365, 1267, 1162, 1018, 971, 908, 826, 762, 702, 558. HRMS (APCI) calc. $C_{21}H_{22}F_3O^-$ [M-H]$^-$: 347.1628, found: 347.1630.

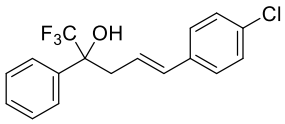


(*E*)-1,1,1-Trifluoro-5-(4-fluorophenyl)-2-phenylpent-4-en-2-ol (3j): Yield: 47.7 mg (77%), yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.55. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 7.60 (d, J = 8.0 Hz, 2H), 7.41-7.31 (m, 3H), 7.25-7.22 (m, 2H), 7.07 (t, J = 8.0 Hz, 2H), 6.70 (s, 1H), 6.48 (d, J = 16.0 Hz, 1H), 5.89 (dt, J = 16.0, 8.0 Hz, 1H), 3.05 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 161.9 (d, $J_{C\text{-}F}$ = 245.4 Hz), 137.8, 133.8 (d, $J_{C\text{-}F}$ = 3.0 Hz), 132.7, 128.5, 128.4, 128.1 (d, $J_{C\text{-}F}$ = 8.1 Hz), 127.4, 126.4 (q, $J_{C\text{-}F}$ = 287.9 Hz), 123.4 (d, $J_{C\text{-}F}$ = 2.0 Hz), 115.8 (d, $J_{C\text{-}F}$ = 21.2 Hz), 76.4 (q, $J_{C\text{-}F}$ = 26.3 Hz), 38.1. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -78.23, -115.03. IR (KBr, cm^{-1}): υ_{max} = 3557, 3040, 2928, 2855, 1601, 1508, 1448, 1628, 1229, 1160, 1072, 1013, 971, 843, 813, 764, 704, 512. HRMS (APCI) calc. $C_{17}H_{13}F_4O^-$ [M-H]$^-$: 309.0908, found: 309.0907.

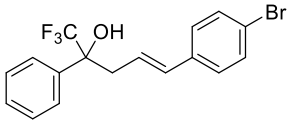


(*E*)-1,1,1-Trifluoro-5-(3-fluorophenyl)-2-phenylpent-4-en-2-ol (3k): Yield: 55.2 mg (89%), yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.50. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.62 (d, J = 8.0 Hz, 2H), 7.42-7.28 (m, 4H), 7.05-6.79 (m, 3H), 6.74 (s, 1H), 6.50 (d, J = 16.0 Hz, 1H), 6.04 (dt, J = 16.0, 8.0 Hz, 1H), 3.07 (m, 2H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 162.9 (d, $J_{C\text{-}F}$ = 244.4 Hz), 139.9 (d, $J_{C\text{-}F}$ = 8.1 Hz), 137.7, 132.8 (d, $J_{C\text{-}F}$ = 2.0 Hz), 130.9 (d, $J_{C\text{-}F}$ = 9.1 Hz), 128.6, 128.5, 127.4, 126.4 (q, $J_{C\text{-}F}$ = 288.9 Hz), 125.4, 122.4 (d, $J_{C\text{-}F}$ = 3.0 Hz), 114.36 (d, $J_{C\text{-}F}$ = 21.2 Hz), 112.6 (d, $J_{C\text{-}F}$ = 22.2 Hz), 76.4 (q, $J_{C\text{-}F}$ = 27.3 Hz), 38.2. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -78.23, -113.51. IR (KBr, cm^{-1}): υ_{max} = 6563, 3286, 3067, 3038, 2927, 2855, 1662, 1610, 1583, 1490, 1445, 1266, 1159, 1073, 1019, 967, 874, 766, 702, 639, 521. HRMS (APCI) calc. $C_{17}H_{13}F_4O^-$ [M-H]$^-$: 309.0908, found: 309.0909.

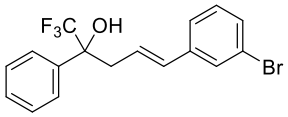


(*E*)-5-(4-Chlorophenyl)-1,1,1-trifluoro-2-phenylpent-4-en-2-ol (3l): Yield: 45.6 mg (70%), yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.60. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 7.60 (d, J = 8.0 Hz, 2H), 7.41-7.28 (m, 5H), 7.21 (d, J = 8.0 Hz, 2H), 6.72 (s, 1H), 6.48 (d, J = 16.0 Hz, 1H), 5.96 (dt, J = 16.0, 8.0 Hz, 1H), 3.06 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ ppm 137.7, 136.2, 132.7, 132.1, 129.0, 128.6, 128.5, 127.9, 127.4, 126.4 (q, $J_{C\text{-}F}$ = 287.9 Hz), 124.6, 76.5 (q, $J_{C\text{-}F}$ = 26.3 Hz), 38.1. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -78.25. IR (KBr, cm^{-1}): υ_{max} = 3560, 3277, 3035, 2925, 2854, 1492, 1448, 1267, 1160, 1095, 1013, 970, 826, 763, 705, 622, 502. HRMS (APCI) calc. $C_{17}H_{13}ClF_3O^-$ [M-H]$^-$: 325.0613, found: 325.0612.

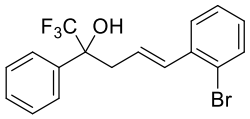


(*E*)-5-(4-Bromophenyl)-1,1,1-trifluoro-2-phenylpent-4-en-2-ol (3m): Yield: 63.6 mg (86%), yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.30. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.59 (d, J = 8.0 Hz, 2H), 7.45-7.30 (m, 5H), 7.18-7.13 (m, 2H), 6.72 (s, 1H), 6.46 (d, J = 16.0 Hz, 1H), 5.97 (dt, J = 16.0, 8.0 Hz, 1H), 3.05 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ ppm 136.4, 135.2, 131.5, 130.6, 127.3, 127.2, 127.0, 126.4 (q, $J_{C\text{-}F}$ = 295.9 Hz), 126.1, 123.4, 119.3, 75.1 (q, $J_{C\text{-}F}$ = 27.3 Hz), 36.9. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -78.27. IR (KBr, cm^{-1}): υ_{max} = 3251, 3034, 2926, 2854, 2253, 2126, 1898, 1725, 1588, 1488, 1449, 1401, 1265, 1160, 1008, 969,

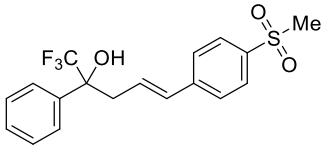
822, 762, 705, 508. HRMS (APCI) calc. $C_{17}H_{13}BrF_3O^-$ [M-H]$^-$: 369.0107, found: 369.0106.



(*E*)-5-(3-Bromophenyl)-1,1,1-trifluoro-2-phenylpent-4-en-2-ol (3n): Yield: 59.2 mg (80%), yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.35. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.60 (d, J = 8.0 Hz, 2H), 7.41-7.31 (m, 5H), 7.20 (d, J = 4.0 Hz, 2H), 6.72 (s, 1H), 6.47 (d, J = 16.0 Hz, 1H), 6.02 (dt, J = 16.0, 8.0 Hz, 1H), 3.06 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 139.8, 137.7, 132.5, 131.2, 130.4, 128.8, 128.6, 128.5, 127.4, 126.3(q, $J_{C\text{-}F}$ = 287.9 Hz), 125.6, 125.2, 122.5, 76.52, 76.4 (q, $J_{C\text{-}F}$ = 27.3 Hz), 38.17. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -78.24. IR (KBr, cm^{-1}): υ_{max} = 3556, 3278, 3064, 3035, 2926, 2854, 1591, 1562, 1474, 1448, 1266, 1160, 1072, 1017, 969, 905, 768, 701, 637, 504. HRMS (APCI) calc. $C_{17}H_{13}BrF_3O^-$ [M-H]$^-$: 369.0107, found: 369.0104.

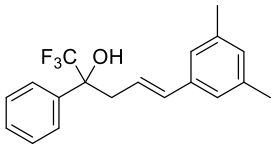


(*E*)-5-(2-Bromophenyl)-1,1,1-trifluoro-2-phenylpent-4-en-2-ol (3o): Yield: 55.5 mg (75%), yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.35. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.62 (d, J = 8.0 Hz, 2H), 7.53 (d, J = 8.0 Hz, 1H), 7.41-7.23 (m, 5H), 7.14-7.10 (m, 1H), 6.77 (s, 1H), 6.72 (d, J = 16.0 Hz, 1H), 5.95 (dt, J = 16.0, 8.0 Hz, 1H), 3.11 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 137.7, 136.9, 133.1, 132.4, 129.6, 128.6, 128.5, 128.4, 127.4, 127.4, 127.3, 126.3 (q, $J_{C\text{-}F}$ = 287.9 Hz), 122.7, 76.4 (q, $J_{C\text{-}F}$ = 27.3 Hz), 38.2. ^{19}F NMR (376 MHz, DMSO-d_6) δ -78.21. IR (KBr, cm^{-1}): υ_{max} = 3251, 3062, 2926, 2855, 1463, 1440, 1265, 1161, 1023, 967, 910, 820, 756, 704, 513. HRMS (APCI) calc. $C_{17}H_{13}BrF_3O^-$ [M-H]$^-$: 369.0107, found: 369.0106.

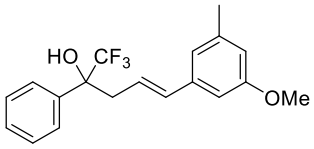


(*E*)-1,1,1-Trifluoro-5-(4-(methylsulfonyl)phenyl)-2-phenylpent-4-en-2-ol (3p): Yield: 44.4 mg (60%), white solid, M.p.: 126.0-127.5 °C. TLC (petroleum ether/ethyl

acetate = 2/1, v/v): R_f = 0.50. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.79 (d, J = 8.0 Hz, 2H), 7.61 (d, J = 8.0 Hz, 2H), 7.46-7.31 (m, 5H), 6.79 (s, 1H), 6.61 (d, J = 16.0 Hz, 1H), 6.17 (dt, J = 16.0, 8.0 Hz, 1H), 3.15 (s, 3H), 3.11 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 142.2, 139.6, 137.6, 132.6, 128.6, 128.5, 128.5, 127.9, 127.4, 126.9, 126.3 (q, $J_{C\text{-}F}$ = 26.3 Hz), 76.4 (q, $J_{C\text{-}F}$ = 26.3 Hz), 44.1, 38.3. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -78.24. IR (KBr, cm^{-1}): υ_{max} = 3462, 3035, 2927, 2854, 1594, 1449, 1303, 1264, 1152, 1074, 1018, 765, 703, 545. HRMS (APCI) calc. $C_{18}H_{18}F_3O_3S^+$ $[M+H]^+$: 371.0923, found: 371.0919.

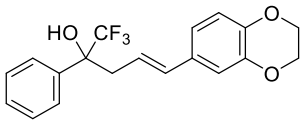


(*E*)-5-(3,5-Dimethylphenyl)-1,1,1-trifluoro-2-phenylpent-4-en-2-ol (3q): Yield: 58.2 mg (91%), yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.60. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 7.60 (d, J = 8.0 Hz, 2H), 7.41-7.30 (m, 3H), 6.80 (s, 3H), 6.69 (s, 1H), 6.40 (d, J = 16.0 Hz, 1H), 5.93 (dt, J = 16.0, 8.0 Hz, 1H), 3.05 (m, 2H), 2.18 (s, 6H). ^{13}C NMR (101 MHz, DMSO-d_6) δ ppm 137.9, 137.8, 137.2, 134.1, 129.2, 128.5, 128.4, 127.4, 126.4 (q, $J_{C\text{-}F}$ = 287.9 Hz), 124.1, 123.0, 76.4 (q, $J_{C\text{-}F}$ = 27.3 Hz), 38.2, 21.3. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -78.28. IR (KBr, cm^{-1}): υ_{max} = 3546, 3279, 3031, 2923, 2858, 1601, 1495, 1449, 1378, 1265, 1161, 1004, 970, 852, 819, 763, 703, 623, 511. HRMS (APCI) calc. $C_{19}H_{18}F_3O^-$ $[M-H]^-$: 319.1315, found: 319.1314.

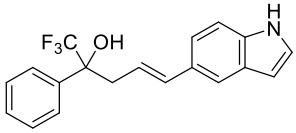


(*E*)-1,1,1-Trifluoro-5-(3-methoxy-5-methylphenyl)-2-phenylpent-4-en-2-ol (3r): Yield: 60.5 mg (90%), yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.55. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 7.61 (d, J = 8.0 Hz, 2H), 7.30-7.40 (m, 3H), 7.06 (d, J = 8.0 Hz, 1H), 6.62-6.68 (m, 3H), 6.56 (d, J = 16.0 Hz, 1H), 5.64 (dt, J = 16.0, 8.0 Hz, 1H), 3.67 (s, 3H), 3.04 (m, 2H), 2.12 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 158.8, 137.8, 136.5, 131.8, 129.2, 128.4, 128.4, 127.5, 126.7, 126.5 (q, $J_{C\text{-}}$

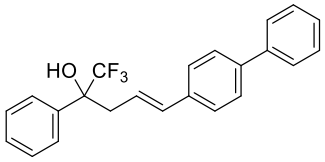
$_F$ = 287.9 Hz), 122.5, 115.6, 112.1, 76.5 (q, J_{C-F} = 26.3 Hz), 55.4, 38.3, 19.9. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -78.24. IR (KBr, cm^{-1}): υ_{max} = 3255, 2925, 2846, 2253, 1607, 1499, 1452, 1259, 1160, 1028, 819, 762, 706, 624, 454. HRMS (APCI) calc. $C_{19}H_{18}F_3O_2^-$ [M-H]$^-$: 335.1264, found: 335.1266.



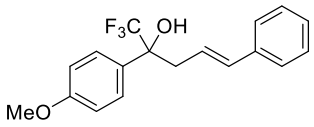
(*E*)-5-(2,3-Dihydrobenzo[*b*][1,4]dioxin-6-yl)-1,1,1-trifluoro-2-phenylpent-4-en-2-ol (3s): Yield: 67.2 mg (96%), yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.30. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.58 (d, J = 8.0 Hz, 2H), 7.4-7.30 (m, 3H), 6.73-6.65 (m, 4H), 6.34 (d, J = 16.0 Hz, 1H), 5.75 (dt, J = 16.0, 8.0 Hz, 1H), 4.17 (s, 4H), 3.00 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 143.8, 143.3, 137.8, 133.3, 130.9, 128.5, 128.4, 127.4, 126.4 (q, J_{C-F} = 288.9 Hz), 121.6, 119.3, 117.6, 114.6, 76.4 (q, J_{C-F} = 27.3 Hz), 64.5, 64.5, 38.1. ^{19}F NMR (376 MHz, DMSO-d_6) δ -78.23. IR (KBr, cm^{-1}): υ_{max} = 3261, 3038, 2980, 2931, 2878, 1582, 1503, 1453, 1295, 1161, 1066, 919, 884, 810, 764, 704, 607, 474. HRMS (APCI) calc. $C_{19}H_{16}F_3O_3^-$ [M-H]$^-$: 349.1057, found: 349.1058.



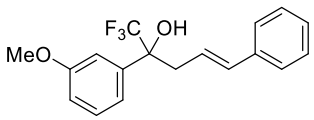
(*E*)-1,1,1-Trifluoro-5-(1*H*-indol-5-yl)-2-phenylpent-4-en-2-ol (3t): Yield: 63.6 mg (96%), yellow solid. M.p.: 105.5-106 °C. TLC (petroleum ether/ethyl acetate = 20/1, v/v): R_f = 0.50. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.1 (s, 1H), 7.64-7.63 (m, 2H), 7.42-7.27 (m, 6H), 7.01 (dd, J = 8.0, 1.7 Hz, 1H), 6.68 (s, 1H), 6.55 (d, J = 16.0 Hz, 1H), 6.37 (m, 1H), 5.83 (dt, J = 16.0, 8.0 Hz, 1H), 3.07 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 138.0, 135.9, 135.4, 128.6, 128.5, 128.4, 128.2, 127.5, 126.5 (q, J_{C-F} = 288.9 Hz), 126.2, 119.5, 118.5, 112.0, 101.8, 76.5 (q, J_{C-F} = 27.3 Hz), 38.3. ^{19}F NMR (376 MHz, DMSO-d_6) δ -78.19. IR (KBr, cm^{-1}): υ_{max} = 3399, 3243, 3034, 2924, 2844, 1610, 1454, 1263, 1163, 1016, 892, 765, 705. HRMS (APCI) calc. $C_{19}H_{15}F_3NO^-$ [M-H]$^-$: 330.1111, found: 330.1113.



(*E*)-5-([1,1'-Biphenyl]-4-yl)-1,1,1-trifluoro-2-phenylpent-4-en-2-ol (3u): Yield: 60.4 mg (82%), white solid. M.p: 152.6-153.6 °C. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.50. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 7.61 (d, J = 8.0 Hz, 4H), 7.56 (d, J = 8.0 Hz, 2H), 7.45-7.38 (m, 4H), 7.35-7.28 (m, 4H), 6.72 (s, 1H), 6.53 (d, J = 16.0 Hz, 1H), 6.00 (dt, J = 16.0, 8.0 Hz, 1H), 3.08 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ ppm 140.1, 139.4, 137.8, 136.5, 133.4, 129.4, 128.5, 128.5, 127.9, 127.4, 127.3, 126.9, 126.8, 126.6 (q, $J_{C\text{-}F}$ = 296.9 Hz), 123.8, 76.4 (q, $J_{C\text{-}F}$ = 26.3 Hz), 38.2. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -78.20. IR (KBr, cm^{-1}): υ_{max} = 3532, 3031, 2923, 1487, 1448, 1266, 1159, 1072, 967, 840, 761, 698, 510. HRMS (APCI) calc. $C_{23}H_{18}F_3^-$ [M-H]$^-$: 367.1315, found: 367.1319.

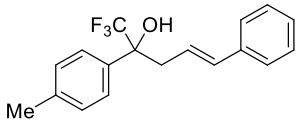


(*E*)-1,1,1-Trifluoro-2-(4-methoxyphenyl)-5-phenylpent-4-en-2-ol (4b): Yield: 61.2 mg (95%), yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.45. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 7.52 (d, J = 8.0 Hz, 2H), 7.27-7.15 (m, 5H), 6.94 (d, J = 8.0 Hz, 2H), 6.61 (s, 1H), 6.50 (d, J = 16.0 Hz, 1H), 5.98 (dt, J = 16.0, 8.0 Hz, 1H), 3.74 (s, 3H), 3.04 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ ppm 159.4, 137.4, 133.8, 129.6, 129.0, 128.8, 127.7, 126.5 (q, $J_{C\text{-}F}$ = 287.9 Hz), 126.2, 123.7, 113.8, 76.1 (q, $J_{C\text{-}F}$ = 27.3 Hz), 55.4, 38.1. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -78.62. IR (KBr, cm^{-1}): υ_{max} = 3548, 3029, 2933, 2842, 1611, 1514, 1449, 1255, 1160, 1104, 1028, 969, 830, 746, 696, 532. HRMS (APCI) calc. $C_{18}H_{16}F_3O_2^-$ [M-H]$^-$: 321.1108, found: 321.1108.

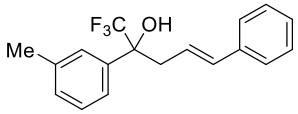


(*E*)-1,1,1-Trifluoro-2-(3-methoxyphenyl)-5-phenylpent-4-en-2-ol (4c): Yield: 58.0 mg (90%), yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.50. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 7.33-7.15 (m, 8H), 6.92-6.89 (m, 1H), 6.70 (s, 1H),

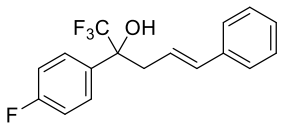
6.49 (d, J = 16.0 Hz, 1H), 5.96 (dt, J = 16.0, 8.0 Hz, 1H), 3.75 (s, 3H), 3.04 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 159.4, 139.5, 137.3, 133.9, 129.5, 129.0, 127.7, 126.4 (q, $J_{C\text{-}F}$ = 288.9 Hz), 126.3, 123.5, 119.6, 113.6, 113.6, 76.4 (q, $J_{C\text{-}F}$ = 27.3 Hz), 55.5, 38.3. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -78.12. IR (KBr, cm^{-1}): υ_{max} = 3550, 3270, 3031, 2931, 2842, 1666, 1601, 1492, 1438, 1257, 1176, 1023, 969, 878, 746, 699, 495. HRMS (APCI) calc. $C_{18}H_{16}F_3O_2^-$ [M-H]$^-$: 321.1108, found: 321.1107.



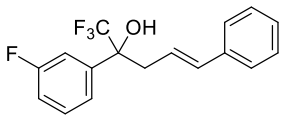
(*E*)-1,1,1-Trifluoro-5-phenyl-2-(*p*-tolyl)pent-4-en-2-ol (4d): Yield: 55.7 mg (91%), yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.50. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 7.47 (d, J = 8.0 Hz, 2H), 7.27-7.15 (m, 7H), 6.62 (s, 1H), 6.48 (d, J = 16.0 Hz, 1H), 5.95 (dt, J = 16.0. 8.0. Hz, 1H), 3.03 (m, 2H), 2.28 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ ppm 137.7, 137.3, 134.8, 133.8, 129.0, 127.7, 127.3, 126.4 (q, $J_{C\text{-}F}$ = 287.9 Hz), 126.2, 123.7, 76.3 (q, $J_{C\text{-}F}$ = 27.3 Hz), 38.1, 21.1. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -78.43. IR (KBr, cm^{-1}): υ_{max} = 3551, 3032, 2926, 2856, 1515, 1445, 1264, 1160, 1106, 1015, 969, 814, 746, 694, 513. HRMS (APCI) calc. $C_{18}H_{16}F_3O^-$ [M-H]$^-$: 305.1159, found: 305.1158.



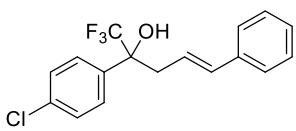
(*E*)-1,1,1-Trifluoro-5-phenyl-2-(*m*-tolyl)pent-4-en-2-ol (4e): Yield: 57.5 mg (94%), yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.55. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.44-7.38 (m, 2H), 7.29-7.13 (m 7H), 6.66 (s, 1H), 6.49 (d, J = 16.0 Hz, 1H), 5.95 (dt, J = 16.0, 8.0 Hz, 1H), 3.05 (m, 2H), 2.32 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 137.8, 137.5, 137.3, 133.9, 129.2, 129.0, 128.3, 127.9, 127.7, 126.4 (q, $J_{C\text{-}F}$ = 288.9 Hz), 126.3, 124.5, 123.6, 76.3 (q, $J_{C\text{-}F}$ = 27.3 Hz), 38.2, 21.7. ^{19}F NMR (376 MHz, DMSO-d_6) δ -78.17. IR (KBr, cm^{-1}): υ_{max} = 3550, 3274, 3031, 2926, 1598, 1487, 1434, 1263, 1165, 1023, 969, 747, 696, 493. HRMS (APCI) calc. $C_{18}H_{16}F_3O^-$ [M-H]$^-$: 305.1159, found: 305.1158.



(*E*)-1,1,1-Trifluoro-2-(4-fluorophenyl)-5-phenylpent-4-en-2-ol (4f): Yield: 53.9 mg (87%), yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.50. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.63 (dd, J = 8.0, 4.0 Hz, 2H), 7.27-7.15 (m, 7H), 6.79 (s, 1H), 6.48 (d, J = 16.0 Hz, 1H), 5.93 (dt, J = 16.0, 8.0 Hz, 1H), 3.05 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 162.3 (d, $J_{C\text{-}F}$ = 245.4 Hz), 137.2, 134.1, 133.9 (d, $J_{C\text{-}F}$ = 3.0 Hz), 129.7 (d, $J_{C\text{-}F}$ = 9.1 Hz), 129.1, 127.8, 126.3 (q, $J_{C\text{-}F}$ = 288.9 Hz), 126.3, 123.3, 115.3 (d, $J_{C\text{-}F}$ = 21.2 Hz), 76.2 (q, $J_{C\text{-}F}$ = 26.3 Hz), 38.0. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -78.52, -114.55. IR (KBr, cm^{-1}): υ_{max} = 3544, 2926, 1604, 1511, 1232, 1162, 1093, 1014, 969, 833, 745, 694, 524. HRMS (APCI) calc. $C_{17}H_{13}F_4O^-$ [M-H]$^-$: 309.0908, found: 309.0909.

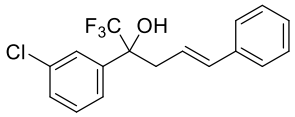


(*E*)-1,1,1-Trifluoro-2-(3-fluorophenyl)-5-phenylpent-4-en-2-ol (4g): Yield: 51.5 mg (83%), yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.50. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 7.46-7.41 (m, 3H), 7.28-7.16 (m, 6H), 6.91 (s, 1H), 6.50 (d, J = 16.0 Hz, 1H), 5.95 (dt, J = 16.0, 8.0 Hz, 1H), 3.08 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 162.5 (d, $J_{C\text{-}F}$ = 243.4 Hz), 140.8 (d, $J_{C\text{-}F}$ = 10.1 Hz), 137.2, 134.2, 130.5 (d, $J_{C\text{-}F}$ = 8.1 Hz), 129.0, 127.8, 126.3, 126.1 (q, $J_{C\text{-}F}$ = 287.9 Hz), 123.5, 123.1, 115.5 (d, $J_{C\text{-}F}$ = 21.2 Hz), 114.5(d, $J_{C\text{-}F}$ = 24.2 Hz), 76.3 (q, $J_{C\text{-}F}$ = 25.3 Hz), 38.0. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -78.28, -113.16. IR (KBr, cm^{-1}): υ_{max} = 3550, 3266, 3031, 2927, 2855, 1592, 1492, 1444, 1259, 1175, 1024, 969, 867, 788, 748, 698, 492. HRMS (APCI) calc. $C_{17}H_{13}F_4O^-$ [M-H]$^-$: 309.0908, found: 309.0909.

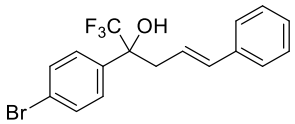


(*E*)-2-(4-Chlorophenyl)-1,1,1-trifluoro-5-phenylpent-4-en-2-ol (4h): Yield: 55.4 mg (85%), yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.45. ^{1}H NMR

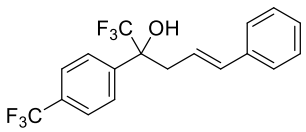
(400 MHz, DMSO-d_6) δ ppm 7.63 (d, J = 8.0 Hz, 2H), 7.45 (d, J = 8.0 Hz, 2H), 7.27-7.17 (m, 5H), 6.87 (s, 1H), 6.49 (d, J = 16.0 Hz, 1H), 5.95 (dt, J = 16.0, 8.0Hz, 1H), 3.07 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 137.2, 136.8, 134.2, 133.5, 129.4, 129.0, 128.5, 127.8, 126.3, 126.2 (q, $J_{C\text{-}F}$ = 288.9 Hz), 123.1, 76.3 (q, $J_{C\text{-}F}$ = 27.3 Hz), 38.0. ^{19}F NMR (376 MHz, DMSO-d_6) δ -78.44. IR (KBr, cm^{-1}): υ_{max} = 3550. 3266, 3030, 2927, 1597, 1494, 1262, 1162, 1098, 1016, 970, 825, 752, 697, 512. HRMS (APCI) calc. $C_{17}H_{13}ClF_3O^-$ [M-H]$^-$: 325.0613, found, 325.0613.



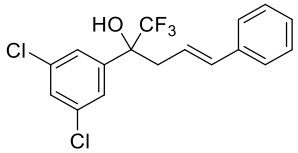
(*E*)-2-(3-Chlorophenyl)-1,1,1-trifluoro-5-phenylpent-4-en-2-ol (4i): Yield: 59.3 mg (91%), yellow oil. TLC (petroleum ether/ethyl acetate = 20/1, v/v): R_f = 0.30. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.64-7.55 (m, 2H), 7.46-7.40 (m, 2H), 7.29-7.16 (m, 5H), 6.93 (s, 1H), 6.50 (d, J = 16.0 Hz, 1H), 5.94 (dt, J = 12.0, 8.0 Hz, 1H), 3.07 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 140.3, 137.2, 134.3, 133.4, 130.4, 129.1, 128.7, 127.8, 127.4, 126.3, 126.2, 126.1 (q, $J_{C\text{-}F}$ = 287.9 Hz), 123.0, 76.3 (q, $J_{C\text{-}F}$ = 26.3 Hz), 37.9. ^{19}F NMR (376 MHz, DMSO-d_6) δ -78.29. IR (KBr, cm^{-1}): υ_{max} = 3256, 3031, 2926, 2857, 1599, 1489, 1436, 1262, 1161, 1025, 969, 786, 749, 699, 890, 749, 699, 494, 449. HRMS (APCI) calc. $C_{17}H_{13}ClF_3O^-$ [M-H]$^-$: 325.0613, found, 325.0612.



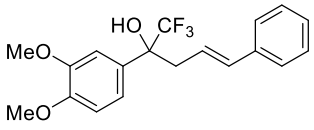
(*E*)-2-(4-Bromophenyl)-1,1,1-trifluoro-5-phenylpent-4-en-2-ol (4j): 65.1 mg Yield: (88%): yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.45. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.61-7.54 (m, 4H), 7.27-7.15 (m, 5H), 6.86 (s, 1H), 6.49 (d, J = 16.0 Hz, 1H), 5.95 (dt, J = 16.0, 8.0 Hz, 1H), 3.06 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 137.24, 137.20, 134.23, 131.43, 129.78, 129.04, 127.78, 126.28, 123.10, 122.18, 76.3 (q, $J_{C\text{-}F}$ = 27.3 Hz), 37.9. ^{19}F NMR (376 MHz, DMSO-d_6) δ -78.41. IR (KBr, cm^{-1}): υ_{max} = 3548, 3271, 3030, 2926, 2854, 1593, 1491, 1444, 1401, 1263, 1163, 1008, 970, 821, 750, 695, 510. HRMS (APCI) calc. $C_{17}H_{13}BrF_3O^-$ [M-H]$^-$: 369.0107, found, 369.0109.



(*E*)-1,1,1-Trifluoro-5-phenyl-2-(4-(trifluoromethyl)phenyl)pent-4-en-2-ol (4k): Yield: 67.0 mg (93%), colourless oil. TLC (petroleum ether/ethyl acetate = 20/1, v/v): R_f = 0.40. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.85 (d, J = 8.0 Hz, 2H), 7.76 (d, J = 8.4 Hz, 2H), 7.30-7.14 (m, 5H), 7.02 (s, 1H), 6.50 (d, J = 16.0 Hz, 1H), 5.94 (dt, J = 16.0, 8.0 Hz, 1H), 3.12 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 142.5, 137.2, 134.4, 129.3 (q, $J_{C\text{-}F}$ = 32.3 Hz), 129.1, 128.4, 127.8, 126.3, 126.1 (q, $J_{C\text{-}F}$ = 287.9 Hz), 125.4 (q, $J_{C\text{-}F}$ = 4.0 Hz), 124.6 (q, $J_{C\text{-}F}$ = 273.1 Hz), 122.9, 76.5 (q, $J_{C\text{-}F}$ = 27.3 Hz), 38.0. ^{19}F NMR (376 MHz, DMSO-d_6) δ -61.21, -78.21. IR (KBr, cm^{-1}): υ_{max} = 3263, 3031, 2929, 1621, 1496, 1417, 1328, 1266, 1168, 1072, 1019, 838, 748, 694, 645, 492. HRMS (APCI) calc. $C_{18}H_{13}F_6O^-$ [M-H]$^-$: 359.0876, found: 359.0877.

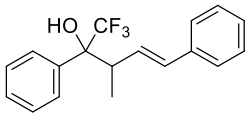


(*E*)-2-(3,5-Dichlorophenyl)-1,1,1-trifluoro-5-phenylpent-4-en-2-ol (4l): Yield: 67.7 mg (94%), colourless oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.50. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 7.63 (m, 3H), 7.32-7.17 (m, 5H), 7.12 (s, 1H), 6.53 (d, J = 16.0 Hz, 1H), 5.94 (dt, J = 16.0, 8.0 Hz,1H), 3.10 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ ppm 142.1, 137.1, 134.6, 134.5, 129.1, 128.6, 127.9, 126.4, 126.3, 126.2 (q, $J_{C\text{-}F}$ = 288.9 Hz), 122.7, 76.2 (q, $J_{C\text{-}F}$ = 26.3Hz), 37.6. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -78.28. IR (KBr, cm^{-1}): υ_{max} = 3544, 2927, 1569, 1423, 1271, 1170, 1024, 969, 862, 801, 747, 691, 494. HRMS (APCI) calc. $C_{17}H_{12}Cl_2F_3O^-$ [M-H]$^-$: 359.0223, found: 359.0225.

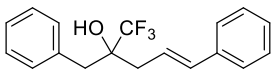


(*E*)-2-(3,4-Dimethoxyphenyl)-1,1,1-trifluoro-5-phenylpent-4-en-2-ol (4m): Yield: 66.2 mg (94%), yellow oil. TLC (petroleum ether/ethyl acetate = 5/1, v/v): R_f = 0.50. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.30-7.21 (m, 4H), 7.21-7.10 (m, 3H), 6.96 (d, J =

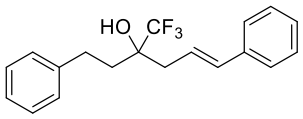
8.5 Hz, 1H), 6.63 (s, 1H), 6.52 (d, J = 16.0 Hz, 1H), 5.99 (dt, J = 16.0, 7.0 Hz, 1H), 3.75 (s, 3H), 3.75 (s, 3H), 3.05 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ ppm 149.0, 148.5, 137.4, 133.8, 130.0, 129.0, 127.7, 126.5 (q, $J_{C\text{-}F}$ = 287.9 Hz), 126.3, 123.8, 120.0, 111.5, 111.5, 76.2 (q, $J_{C\text{-}F}$ = 26.3 Hz), 56.0, 55.8, 38.2. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -78.43. IR (KBr, cm^{-1}): υ_{max} = 3252, 2931, 2841, 1667, 1599, 1516, 1459, 1261, 1142, 1025, 965, 810, 749, 696, 492. HRMS (APCI) calc. $C_{19}H_{18}F_3O_3^-$ [M-H]$^-$: 351.1214, found: 351.1215.



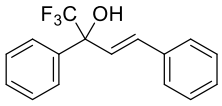
(*E*)-1,1,1-Trifluoro-3-methyl-2,5-diphenylpent-4-en-2-ol (4n): Yield: 56.9 mg (93%), yellow oil. TLC (petroleum ether/ethyl acetate = 20/1, v/v): R_f = 0.40. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.63 (d, J = 8.0 Hz, 2H), 7.45-7.32 (m, 7H), 7.25-7.21 (m, 1H), 6.57 (m, 3H), 3.23 (dt, J = 16.0, 8.0 Hz, 1H), 0.77 (d, J = 8.0 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 139.0, 137.8, 131.2, 130.1, 129.1, 128.6, 128.4, 127.6, 126.5, 126.5, 43.5, 16.1. ^{19}F NMR (376 MHz, DMSO-d_6) δ -72.60. IR (KBr, cm^{-1}): υ_{max} = 3278, 2975, 2932, 1724, 1494, 1451, 1267, 1161, 1021, 977, 914, 756, 699, 512. HRMS (APCI) calc. $C_{18}H_{16}F_3O^-$ [M-H]$^-$: 305.1159, found, 305.1158.



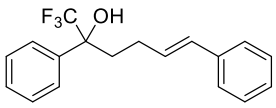
(*E*)-2-Benzyl-1,1,1-trifluoro-5-phenylpent-4-en-2-ol (4o): Yield: 55.1 mg (90%), yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.70. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 7.39-7.36 (m, 4H), 7.33-7.29 (m, 4H), 7.27-7.20 (m, 2H), 6.41 (d, J = 16.0 Hz, 1H), 6.28 (dt, J = 16.0, 8.0 Hz, 1H), 6.15 (s, 1H), 2.98 (dd, J = 24.0, 16.0 Hz, 2H), 2.43 (d, J = 8.0 Hz, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 137.5, 135.7, 133.1, 131.4, 129.0, 128.3, 127.7, 127.3 (q, $J_{C\text{-}F}$ = 294.9 Hz), 127.1, 126.5, 124.2, 75.4 (q, $J_{C\text{-}F}$ = 25.3 Hz), 37.6. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -77.88. IR (KBr, cm^{-1}): υ_{max} = 3549, 3309, 3032, 2929, 2855, 1601, 1495, 1450, 1278, 1166, 1109, 1028, 972, 821, 741, 670, 496. HRMS (APCI) calc. $C_{18}H_{16}F_3O^-$ [M-H]$^-$: 305.1159, found: 305.1160.



(*E*)-1,6-Diphenyl-3-(trifluoromethyl)hex-5-en-3-ol (4p): Yield: 57.6 mg (82%), yellow oil. TLC (petroleum ether/ethyl acetate = 20/1, v/v): R_f = 0.60. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 7.41 (d, J = 8.0 Hz, 2H), 7.34-7.14 (m, 8H), 6.58 (d, J = 16.0 Hz, 1H), 6.29 (dt, J = 16.0, 8.0 Hz, 1H), 6.11 (s, 1H), 2.76-2.63 (m, 2H), 2.64 (d, J = 8.0 Hz, 2H), 1.92-1.87 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 142.2, 137.4, 133.6, 129.1, 128.9, 128.7, 127.8, 127.3 (q, $J_{C\text{-}F}$ = 259.6 Hz), 126.5, 126.4, 124.1, 74.6 (q, $J_{C\text{-}F}$ = 25.3 Hz), 37.5, 36.0, 28.9. ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -77.88. IR (KBr, cm^{-1}): υ_{max} = 3550, 3352, 3029, 2930, 2858, 1601, 1496, 1452, 1261, 1164, 1115, 1029, 972, 746, 698, 499. HRMS (APCI) calc. $C_{19}H_{18}F_3O^-$ [M-H]$^-$: 319.1315, found: 319.1317.

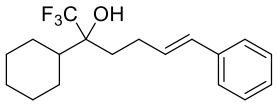


(*E*)-1,1,1-Trifluoro-2,4-diphenylbut-3-en-2-ol (4q): Yield: 55.3 mg (94%), yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.50. ^{1}H NMR (400 MHz, DMSO-d_6) δ ppm 7.72 (d, J = 4.0 Hz, 2H), 7.56 (d, J = 8.0 Hz, 2H), 7.45-7.28 (m, 6H), 7.04 (s, 1H), 6.92 (dd, J = 24.0, 8.0 Hz, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 139.2, 136.1, 132.6, 129.2, 128.8, 128.7, 128.6, 127.4, 127.4, 127.4, 125.8 (q, $J_{C\text{-}F}$ = 287.9 Hz), 76.7(q, $J_{C\text{-}F}$ = 28.3 Hz). ^{19}F NMR (376 MHz, DMSO-d_6) δ ppm -77.13. IR (KBr, cm^{-1}): υ_{max} = 3550, 3062, 2926, 2854, 1653, 1600, 1495, 1451, 1251, 1159, 977, 940, 748, 701,573, 500. HRMS (APCI) calc. $C_{16}H_{12}F_3O^-$ [M-H]$^-$: 277.0846, found: 277.0847.

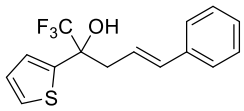


(*E*)-1,1,1-Trifluoro-2,6-diphenylhex-5-en-2-ol (4r): Yield: 42.8 mg (70%), yellow oil. TLC (petroleum ether/ethyl acetate = 20/1, v/v): R_f = 0.35. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, J = 8.0 Hz, 2H), 7.50-7.41 (m, 3H), 7.34 (d, J = 4.0 Hz, 4H), 7.28-7.23 (m, 1H), 6.38 (d, J = 16.0 Hz, 1H), 6.19 (dt, J = 16.0, 6.0 Hz, 1H), 2.47-2.41 (m, 1H), 2.36-2.21 (m, 2H), 2.14-2.01 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.3, 136.3, 130.9, 129.1, 128.6, 128.6, 128.5, 127.2, 126.3, 126.0, 125.6 (q, $J_{C\text{-}F}$ = 286.8 Hz), 77.5 (q, $J_{C\text{-}}$

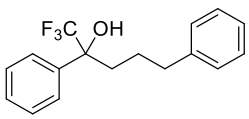
$_F$ = 28.3 Hz), 34.9, 26.1. ^{19}F NMR (376 MHz, $CDCl_3$) δ -79.99. IR (KBr, cm^{-1}): υ_{max} = 3544, 3028, 2958, 2832, 1608, 1495, 1450, 1366, 1249, 1160, 1070, 963, 900, 742, 699. HRMS (APCI) calc. $C_{18}H_{16}F_3O^-$ [M-H]$^-$: 305.1159, found: 305.1156.



(*E*)-2-Cyclohexyl-1,1,1-trifluoro-6-phenylhex-5-en-2-ol (4s): Yield: 43.1 mg (69%), colourless oil. TLC (petroleum ether/ethyl acetate = 50/1, v/v): R_f = 0.30. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.30 (m, 4H), 7.26-7.21 (m, 1H), 6.48 (d, J = 16.0 Hz, 1H), 6.23 (dt, J = 16.0, 8.0 Hz, 1H), 2.40-2.34 (m, 2H), 1.91-1.85 (m, 6H), 1.80-1.71 (m, 2H), 1.34-1.17 (m, 5H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.4, 130.8, 129.5, 128.6, 127.2, 126.8 (q, $J_{C\text{-}F}$ = 289.9 Hz), 126.0, 77.4 (q, $J_{C\text{-}F}$ = 31.3 Hz), 43.1, 31.6, 27.0, 26.8, 26.4, 26.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ -74.25. IR (KBr, cm^{-1}): υ_{max} = 3554, 3027, 2939, 2857, 1599, 1494, 1450, 1276, 1233, 1161, 965, 893, 744, 696. 505. HRMS (APCI) calc. $C_{18}H_{24}F_3O^+$ [M+H]$^+$: 313.1774, found: 313.1765.

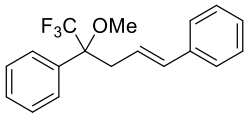


(*E*)-1,1,1-Trifluoro-5-phenyl-2-(thiophen-2-yl)pent-4-en-2-ol (4t): Yield: 57.2 mg (96%), yellow oil. TLC (petroleum ether/ethyl acetate = 20/1, v/v): R_f = 0.30. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (dd, J = 4.0, 1.0 Hz, 1H), 7.34-7.26 (m, 5H), 7.21 (d, J = 4.0 Hz, 1H), 7.10 (dd, J = 4.0, 4.0 Hz, 1H), 6.63 (d, J = 16.0 Hz, 1H), 6.04 (dt, J = 16.0, 8.0 Hz, 1H), 3.08 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.2, 137.0, 136.3, 128.7, 128.1, 127.3, 126.5, 126.3, 125.9, 124.8 (q, $J_{C\text{-}F}$ = 286.9 Hz), 120.8, 75.9 (t, $J_{C\text{-}F}$ = 30.3 Hz), 40.7. ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.09. IR (KBr, cm^{-1}): υ_{max} = 3540, 3032, 2925, 2857, 1658, 1495, 1439, 1274, 1175, 970, 837, 705, 503. HRMS (APCI) calc. $C_{15}H_{12}F_3OS^-$ [M-H]$^-$: 297.0566, found: 297.0565.

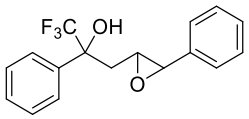


1,1,1-Trifluoro-2,5-diphenylpentan-2-ol (5a): Yield: 58.2 mg (99%), colourless oil. TLC (petroleum ether/ethyl acetate = 20/1, v/v): R_f = 0.35. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, J = 8.0 Hz, 2H), 7.47-7.41 (m, 3H), 7.35-7.31 (m, 2H), 7.28-7.23 (m, 1H),

7.16 (d, J = 8.0 Hz, 2H), 2.73-2.59 (m, 2H), 2.30 (td, J = 12.0, 8.0 Hz, 1H), 2.12-2.05 (m, 1H), 1.82-1.70 (m, 1H), 1.51-1.35 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.5, 136.3, 128.5, 128.4, 128.4, 126.3, 126.1, 125.7 (q, $J_{C\text{-}F}$ = 286.8 Hz), 77.4 (q. $J_{C\text{-}F}$ = 28.3 Hz), 35.6, 34.6, 24.0. ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.02. IR (KBr, cm^{-1}): υ_{max} = 3554, 3069, 3031, 2953, 2868, 1657, 1606, 1497, 1455, 1387, 1276, 1163, 1075, 973, 905, 806, 750, 700. HRMS (APCI) calc. $C_{17}H_{16}F_3O^-$ [M-H]$^-$: 293.1159, found: 293.1157.

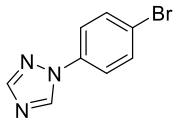


(*E*)-(5,5,5-Trifluoro-4-methoxypent-1-ene-1,4-diyl)dibenzene (5b): Yield: 59.4 mg (97%), yellow oil. TLC (petroleum ether/ethyl acetate = 50/1, v/v): R_f = 0.65. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, J = 8.0 Hz, 2H), 7.52-7.43 (m, 3H), 7.40-7.34 (m, 4H), 7.30-7.27 (t, J = 6.6 Hz, 1H), 6.56 (d, J = 16.0 Hz, 1H), 6.23 (dt, J = 16.0, 8.0 Hz, 1H), 3.50 (s, 3H), 3.20 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.3, 135.7, 133.8, 128.7, 128.6, 128.4, 127.7, 127.5, 126.3, 125.6(q, $J_{C\text{-}F}$ = 289.9 Hz), 123.0, 81.8 (q, $J_{C\text{-}F}$ = 26.3 Hz), 52.5, 36.8. ^{19}F NMR (376 MHz, $CDCl_3$) δ -73.32. IR (KBr, cm^{-1}): υ_{max} = 3033, 2950, 2843, 1654, 1608, 1493, 1448, 1262, 1167, 1115, 964, 743, 697, 501. HRMS (APCI) calc. $C_{18}H_{18}F_3O^+$ [M+H]$^+$: 307.1304, found: 307.1299.

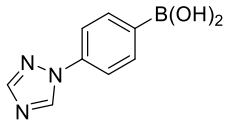


1,1,1-Trifluoro-2-phenyl-3-(3-phenyloxiran-2-yl)propan-2-ol (5c): Yield: 61.0 mg (99%), colorless liquid. TLC (petroleum ether/ethyl acetate = 5/1, v/v): R_f = 0.50. ^{1}H NMR (400 MHz, $CDCl_3$, major) δ 7.61 (d, J = 4.0 Hz, 2H), 7.44-7.34 (m, 8H), 4.68 (d, J = 8.0 Hz, 1H), 4.34 (q, J = 8.0 Hz, 1H), 2.83 (m, 2H). ^{1}H NMR (400 MHz, $CDCl_3$, minor) δ 8.11-7.95 (m, 3H), 7.68 (d, J = 8.0 Hz, 2H), 7.49 (m, 5H), 4.95 (d, J = 8.0 Hz, 1H), 4.02 (q, J = 8.0 Hz, 1H), 2.85 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.2 (minor), 138.4 (major), 138.4 (minor), 138.3 (major), 138.0 (minor), 134.7 (minor), 133.9 (major), 131.1 (minor), 129.9 (major), 128.9 (major), 128.8 (minor), 128.6 (major), 128.6 (minor), 128.4 (major), 128.3 (minor), 126.2 (major), 123.5 (q, $J_{C\text{-}F}$ = 284.8 Hz, major), 125.5 (q, $J_{C\text{-}F}$ = 285.8 Hz, minor), 87.4 (minor), 86.4 (major), 83.9

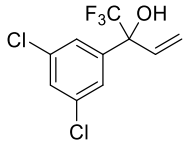
(q, $J_{C\text{-}F}$ = 29.3 Hz, major), 83.3 (q, $J_{C\text{-}F}$ = 30.3 Hz, minor), 77.8 (major), 76.8 (minor), 42.3 (major), δ41.6 (minor). ^{19}F NMR (376 MHz, $CDCl_3$) δ -79.04 (minor), -79.25 (major). IR (KBr, cm^{-1}): υ_{max} = 2832, 1608, 1453, 1366, 1310, 1169, 1091, 1039, 757, 703. HRMS (APCI) calc. $C_{17}H_{14}F_3O_2^-$ [M-H]$^-$: 307.0951, found: 307.0950.



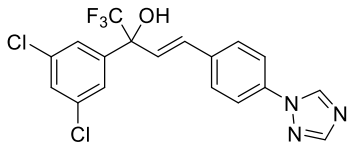
1-(4-Bromophenyl)-1*H*-1,2,4-triazole (6c): Yield： 4.895g (99%), white solid. M.p.: 148.5-150.0 °C. TLC (petroleum ether/ethyl acetate = 2/1, v/v): R_f = 0.50. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (s, 1H), 8.06 (s, 1H), 7.55 (q, J = 12.0 Hz, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.8, 140.8, 138.8, 136.0, 132.9, 121.40. IR (KBr, cm^{-1}): υ_{max} = 2831, 1606, 1507, 1362, 1273, 1069, 817, 775, 672, 501. HRMS (APCI) calc. $C_8H_7BrN_3^+$ [M+H]$^+$: 223.9818, found: 223.9814.



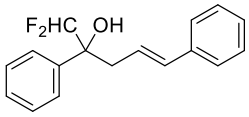
(4-(1*H*-1,2,4-Triazol-1-yl)phenyl)boronic acid (6d): Yield: 171 mg (45%), grey solid. M.p.: 275.0-276.0 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.33 (s, 1H), 8.25 (s, 1H), 8.19 (s, 2H), 7.90(dd, J = 48.0, 8.0 Hz, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 152.9, 142.8, 138.5, 136.0, 118.6. IR (KBr, cm^{-1}): υ_{max} = 3770, 2831, 1612, 1374, 772, 645. HRMS (APCI) calc. $C_8H_9BN_3O_2^+$ [M+H]$^+$: 190.0782, found: 190.0779.



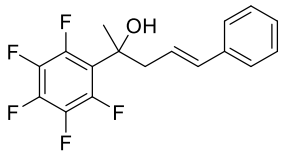
2-(3,5-Dichlorophenyl)-1,1,1-trifluorobut-3-en-2-ol (6g): Yield: 1.163g (86%), colourless oil. TLC (petroleum ether/ethyl acetate = 20/1, v/v): R_f = 0.40. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (s, 2H), 7.40 (s, 1H), 6.38 (dd, J = 16.0, 8.0 Hz, 1H), 5.66-5.57 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.2, 135.0, 134.6, 129.0, 125.6, 124.4 (q, $J_{C\text{-}F}$ = 287.9 Hz), 119.6, 76.6 (q, $J_{C\text{-}F}$ = 29.3 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -78.77. IR (KBr, cm^{-1}): υ_{max} = 2965, 1658, 1602, 1420, 1267, 1176, 1101, 1020, 866, 805, 733, 689. HRMS (APCI) calc. $C_{10}H_6Cl_2F_3O^-$ [M-H]$^-$: 268.9753, found: 268.9752.



(*E*)-4-(4-(1*H*-1,2,4-Triazol-1-yl)phenyl)-2-(3,5-dichlorophenyl)-1,1,1-trifluorobut-3-en-2-ol (6h): Yield: 71.0 mg (86%), white solid. M.p.: 175.0-176.0 °C. TLC (petroleum ether/ethyl acetate = 2/1, v/v): R_f = 0.50. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.35 (s, 1H), 8.25 (s, 1H), 7.89-7.77 (m, 4H), 7.77 (m, 2H), 7.68-7.67 (m, 1H), 7.50 (s, 1H), 7.07 (dd, J = 76.0, 16.0 Hz, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 152.9, 143.1, 142.8, 136.9, 135.3, 134.6, 132.4, 129.0, 128.8, 126.8, 126.3, 125.2 (q, $J_{C\text{-}F}$ = 287.9 Hz), 119.9. 76.4 (q, $J_{C\text{-}F}$ = 28.3 Hz). ^{19}F NMR (376 MHz, DMSO-d_6) δ -77.43. IR (KBr, cm^{-1}): υ_{max} = 3500, 2920, 2830, 1651, 1609, 1373, 1168, 767. HRMS (APCI) calc. $C_{18}H_{13}Cl_2F_3N_3O^+$ $[M+H]^+$: 414.0382, found: 414.0375.



(*E*)-1,1-Difluoro-2,5-diphenylpent-4-en-2-ol (10aa): Yield: 51.0 mg (93%), yellow oil. TLC (petroleum ether/ethyl acetate = 10/1, v/v): R_f = 0.55. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.55 (d, J = 7.4 Hz, 2H), 7.37 (t, J = 8.0 Hz, 2H), 7.29-7.14 (m, 6H), 6.42 (d, J = 16.0 Hz, 1H), 6.22-5.94 (m, 3H), 2.87 (ddd, J = 36.0, 12.0, 8.0 Hz, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 140.2, 137.5, 133.4, 129.0, 128.3, 127.8, 127.6, 127.1, 126.3, 124.6, 117.7 (t, $J_{C\text{-}F}$ = 249.5 Hz), 75.9 (t, $J_{C\text{-}F}$ = 20.2 Hz), 39.2. ^{19}F NMR (376 MHz, DMSO-d_6) δ -128.52 (d, J = 274.5 Hz), -128.67 (d, J = 274.5 Hz), -130.49 (d, J = 274.5 Hz), -130.63 (d, J = 270.7 Hz). IR (KBr, cm^{-1}): υ_{max} = 3556, 3031, 2925, 2853, 1599, 1495, 1447, 1350, 1152, 1067, 970, 901, 818, 749, 699, 557, 501. HRMS (APCI) calc. $C_{17}H_{15}F_2O^-$ $[M-H]^-$: 273.1096, found: 273.1098.



(*E*)-2-(Perfluorophenyl)-5-phenylpent-4-en-2-ol (11aa): Yield: 61.0 mg (93%), colourless oil. TLC (petroleum ether/ethyl acetate = 20/1, v/v): R_f = 0.30. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.24 (m, 5H), 6.54 (d, J = 16.0 Hz, 1H), 6.13 (dt, J = 16.0, 8.0 Hz,

1H), 2.88 (m, 2H), 1.80 (t, J = 2.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.8, 135.4, 128.6, 127.7, 126.3, 123.3, 75.8, 46.6, 28.9. ^{19}F NMR (376 MHz, $CDCl_3$) δ -140.45 (d, J = 16.5 Hz), -155.75 (tt, J = 21.3, 2.4 Hz), -161.79 (td, J = 22.4, 7.1 Hz). IR (KBr, cm^{-1}): υ_{max} = 3501, 2928, 1724, 1652, 1604, 1525, 1484, 1387, 1301, 1133, 982, 803, 745, 695. HRMS (APCI) calc. $C_{17}H_{12}F_5^+$ $[M\text{-}H_2O+H]^+$: 311.0854, found: 311.0847.

6. Studies on X-ray Crystallographic Analysis

X-ray Crystallographic Analysis for Product 3u

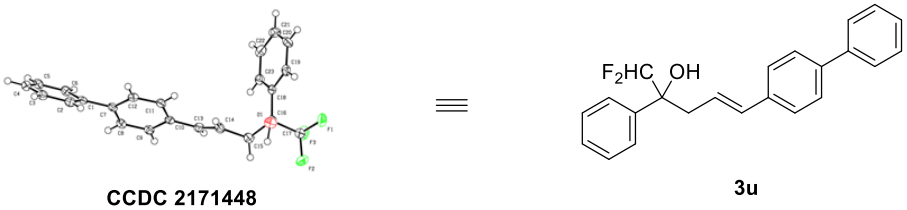


Fig. S7. Crystal data and structure refinement for 3u

Table S4. Crystal data and structure refinement for 3u

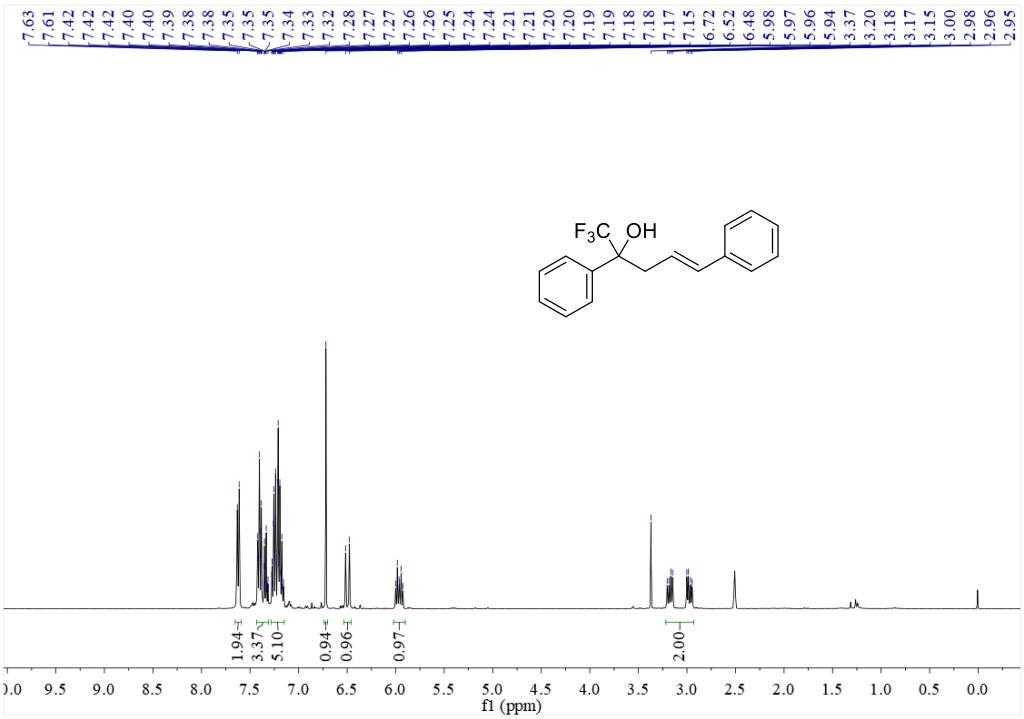
Empirical formula	$C_{23}H_{19}F_3O$
Formula weight	368.38
Temperature	150.0(2) K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 18.1043(13) Å, α = 90°
	b = 5.8211(4) Å, β = 98.663(7)°
	c = 16.8027(12) Å, γ = 90°
Volume/Å^3	1750.6(2)
Z	4
Density(calcd g cm^{-3})	1.398
Absorption coeff. (mm^{-1})	0.106
F(000)	768.0
Crystal size	0.13 × 0.11 × 0.1 mm^3
Theta range for data collection	4.552 to 49.988
Index ranges	$-13 \le h \le 21$, $-5 \le k \le 6$, $-19 \le l \le 19$
Reflections collected	6954
Independent reflections	3066 [R_{int} = 0.0522, R_{sigma} = 0.0665]
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	3066/0/248
Goodness-of-fit on F^2	1.007
Final R indices [$I > 2sigma(I)$]	R_1 = 0.0555, wR_2 = 0.1320
Final R indexes [all data]	R_1 = 0.0718, wR_2 = 0.1449

For detailed crystal data and structure refinement, please refer to the attached cif-Z-3o and checkcif-Z-3o files

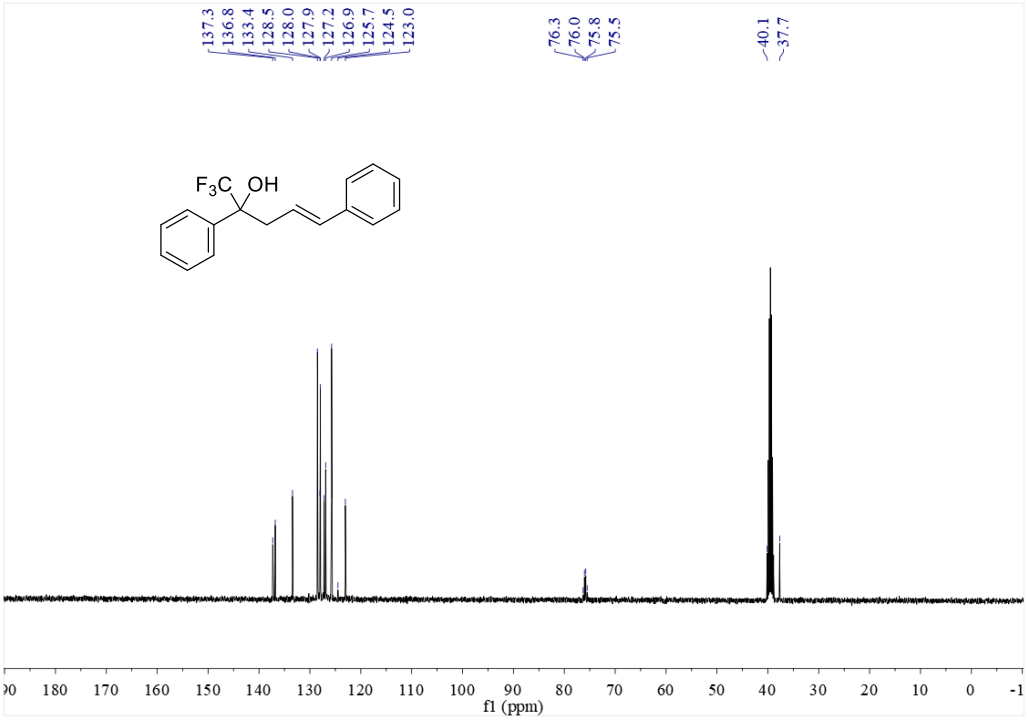
7. ^{1}H, ^{13}C, ^{19}F NMR Spectra for All the Compounds

(*E*)-1,1,1-Trifluoro-2,5-diphenylpent-4-en-2-ol (3a)

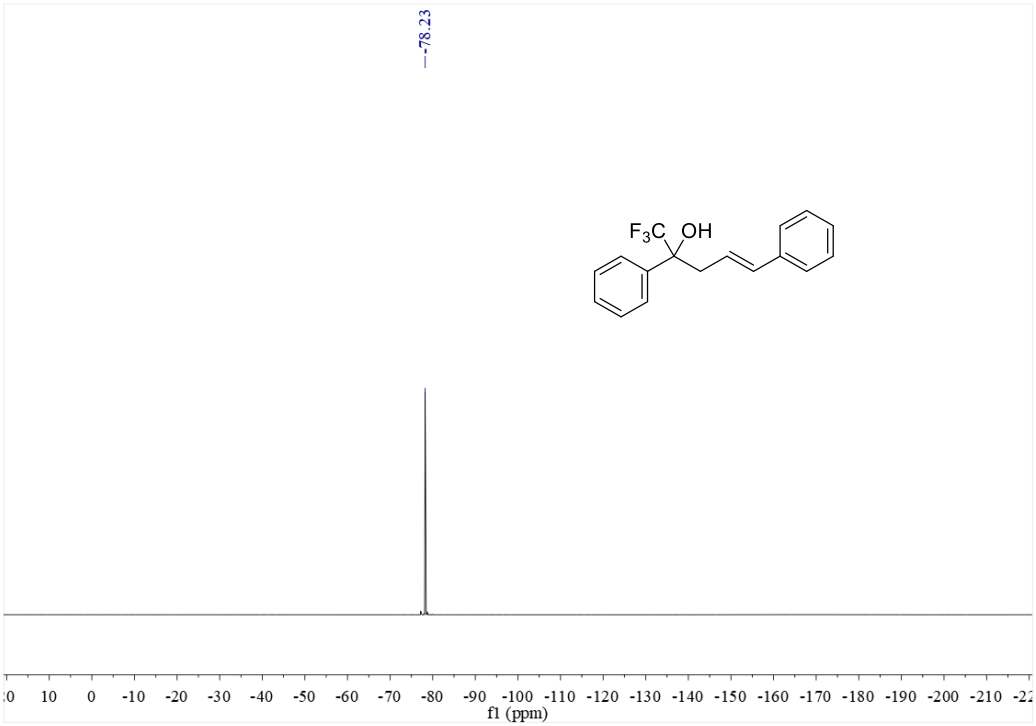
^{1}H NMR of 3a



^{13}C NMR of 3a

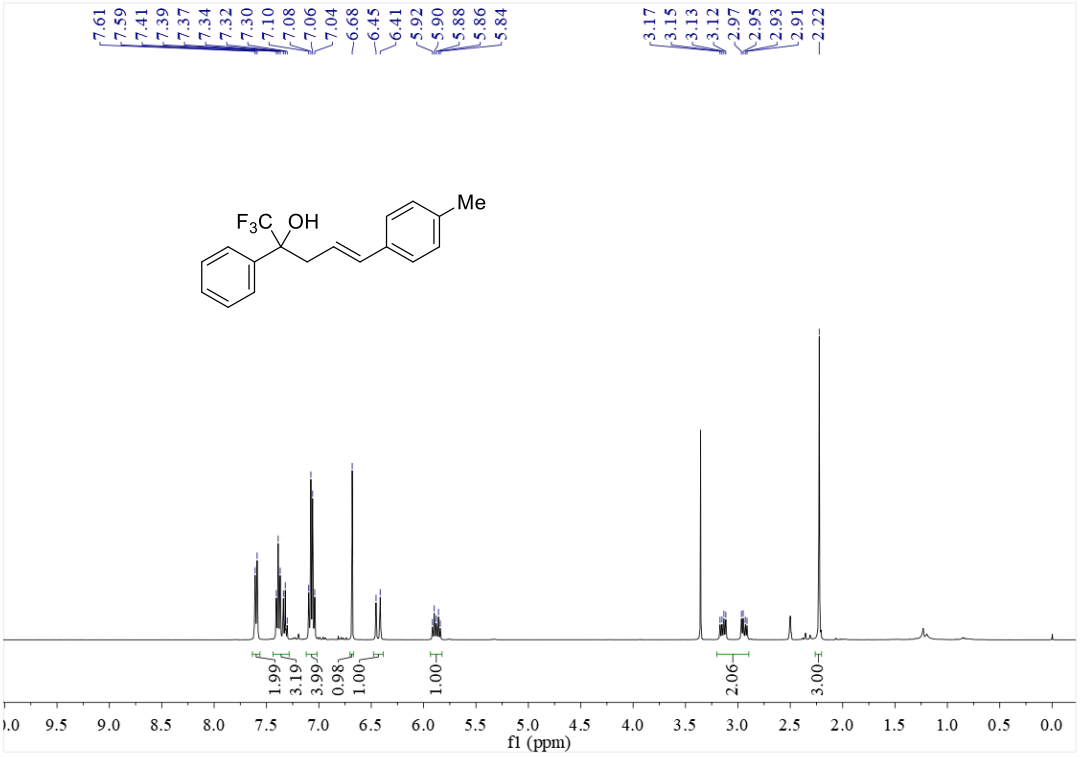


^{19}F NMR of 3a

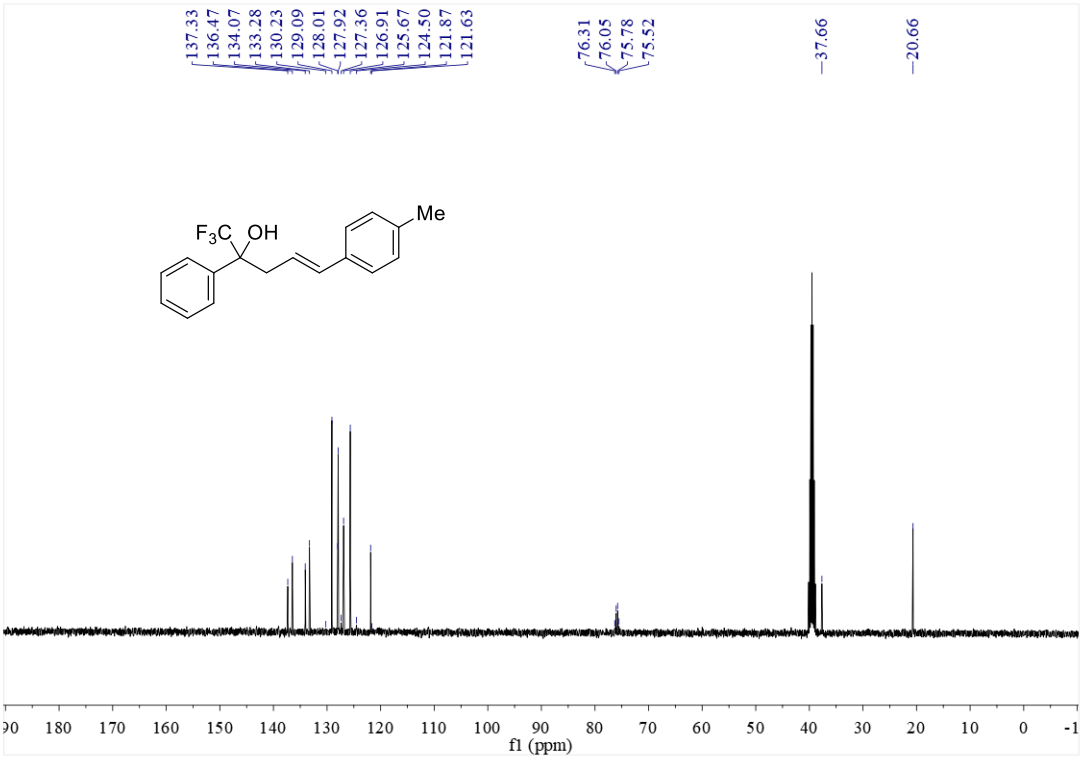


(*E*)-1,1,1-Trifluoro-2-phenyl-5-(*p*-tolyl)pent-4-en-2-ol (3b)

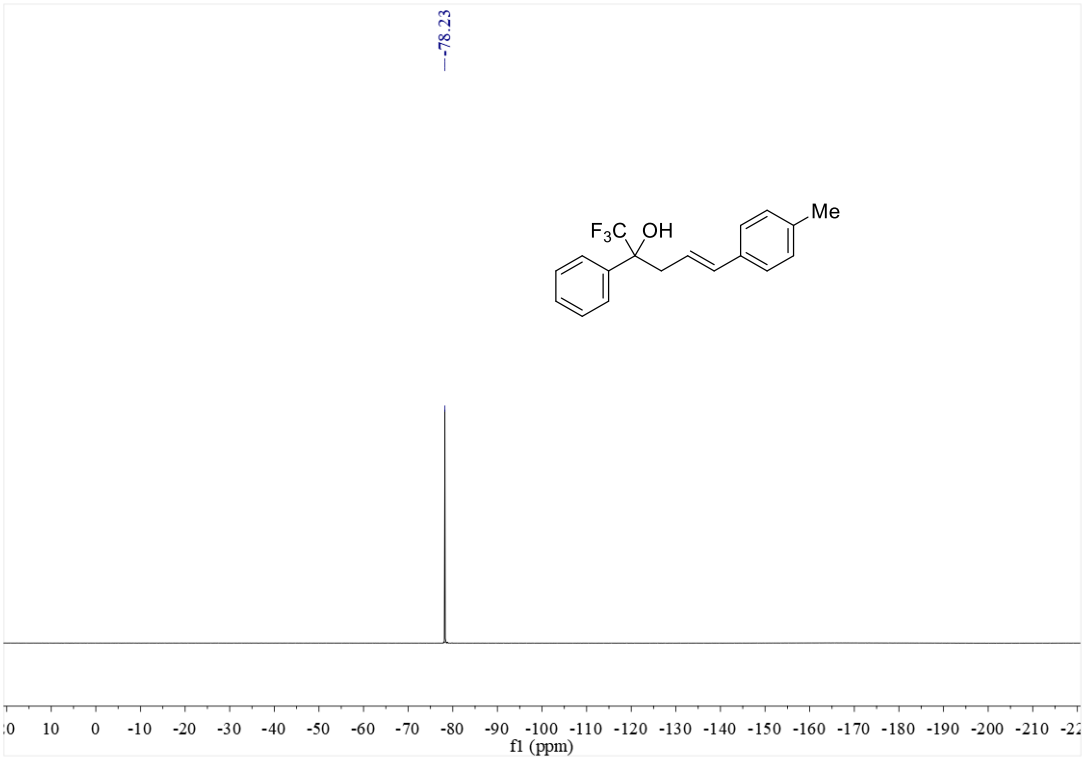
^{1}H NMR of 3b



^{13}C NMR of 3b

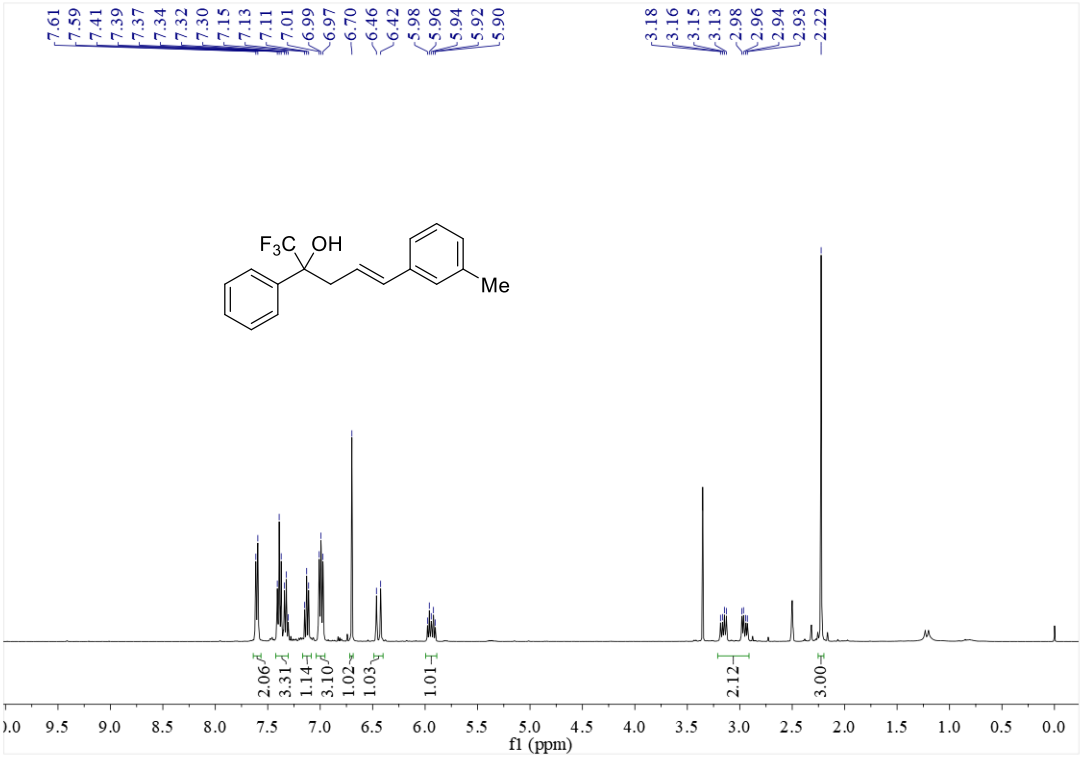


^{19}F NMR of 3b

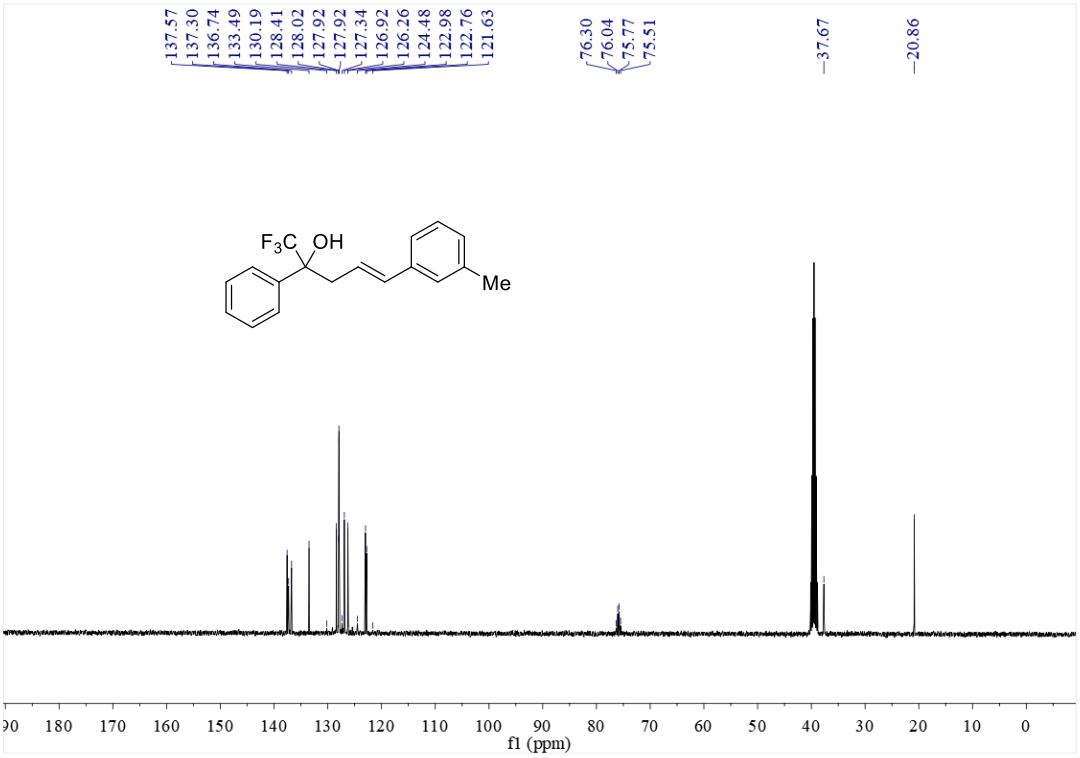


(*E*)-1,1,1-Trifluoro-2-phenyl-5-(*m*-tolyl)pent-4-en-2-ol (3c)

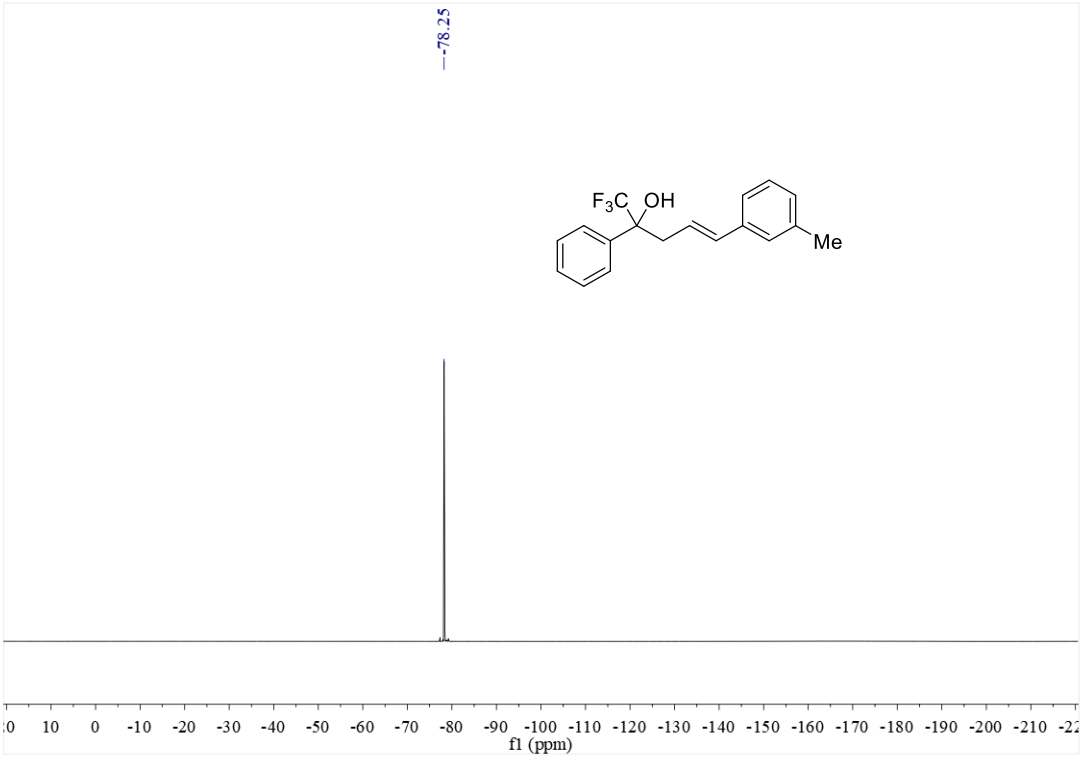
^{1}H NMR of 3c



^{13}C NMR of 3c

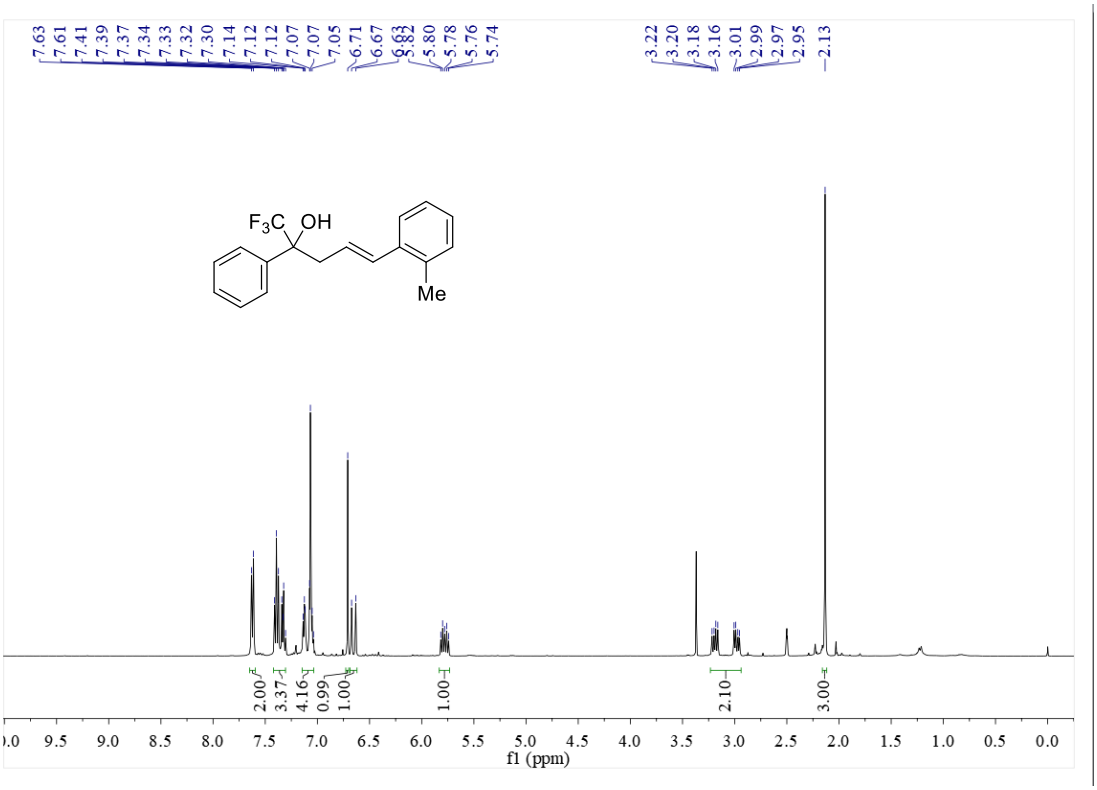


^{19}F NMR of 3c

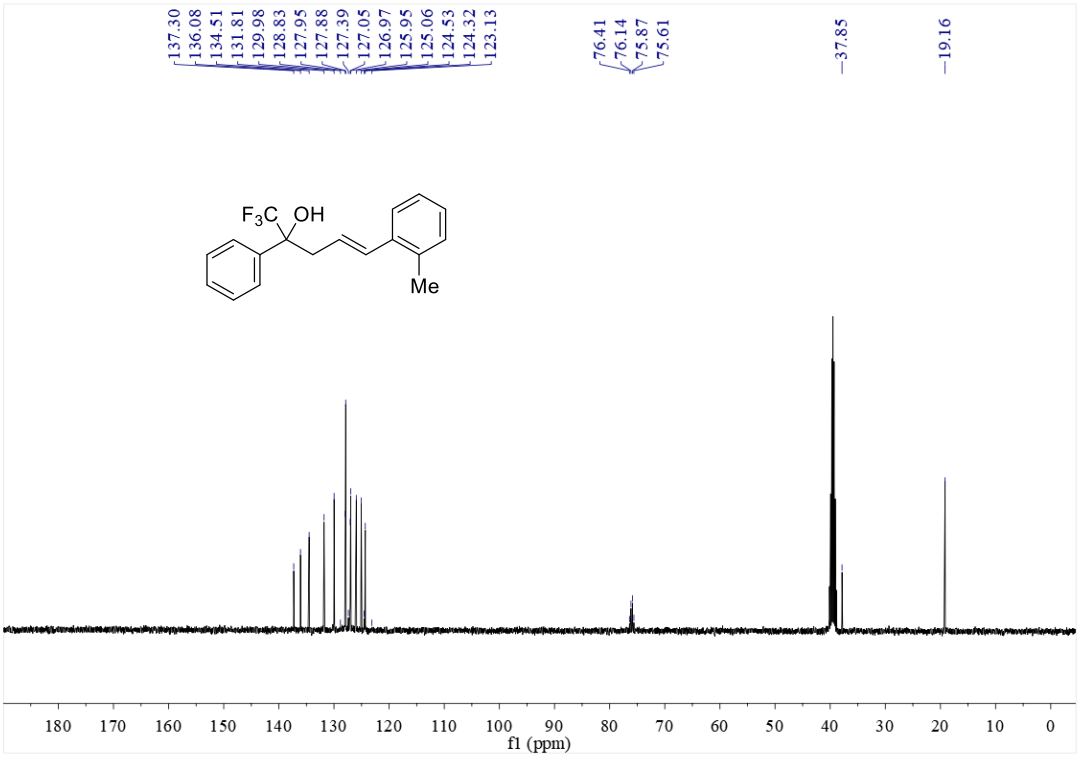


(*E*)-1,1,1-Trifluoro-2-phenyl-5-(*o*-tolyl)pent-4-en-2-ol (3d)

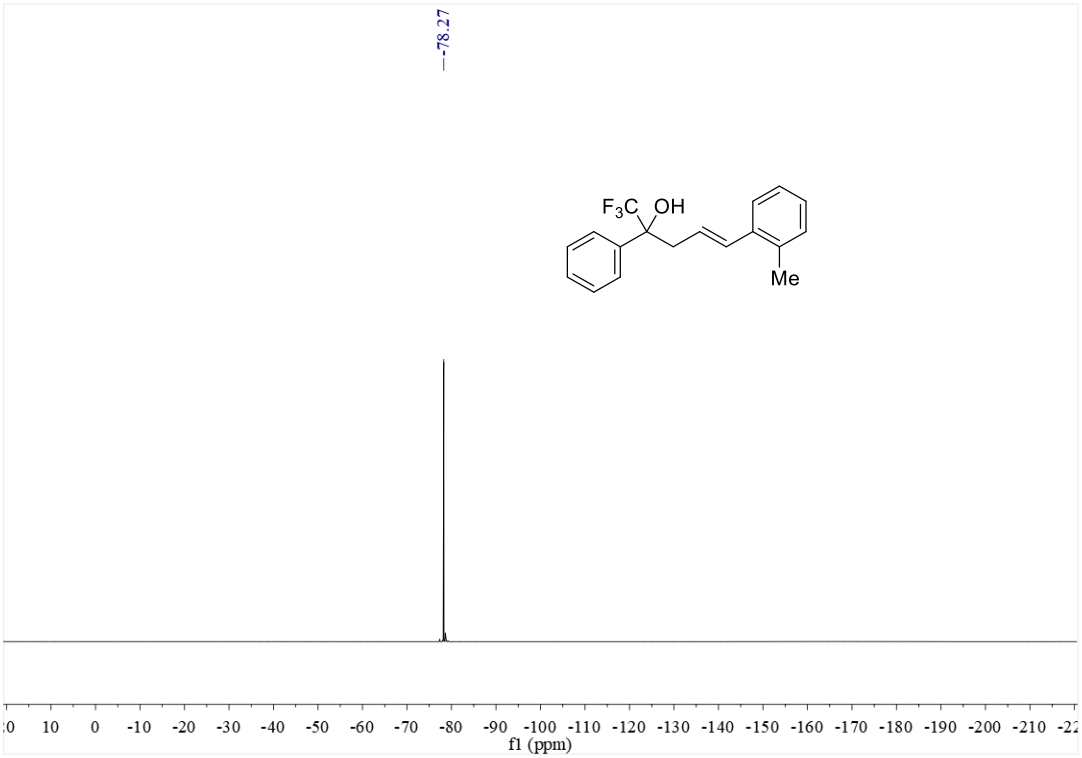
^{1}H NMR of 3d



^{13}C NMR of 3d

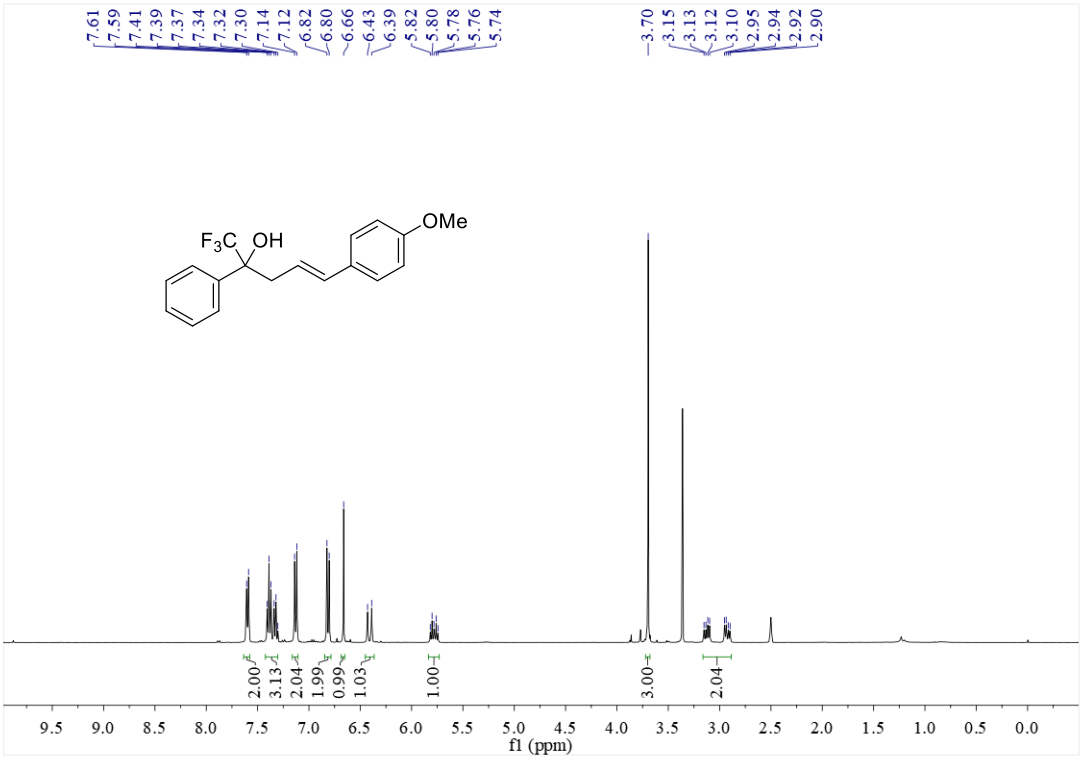


^{13}F NMR of 3d

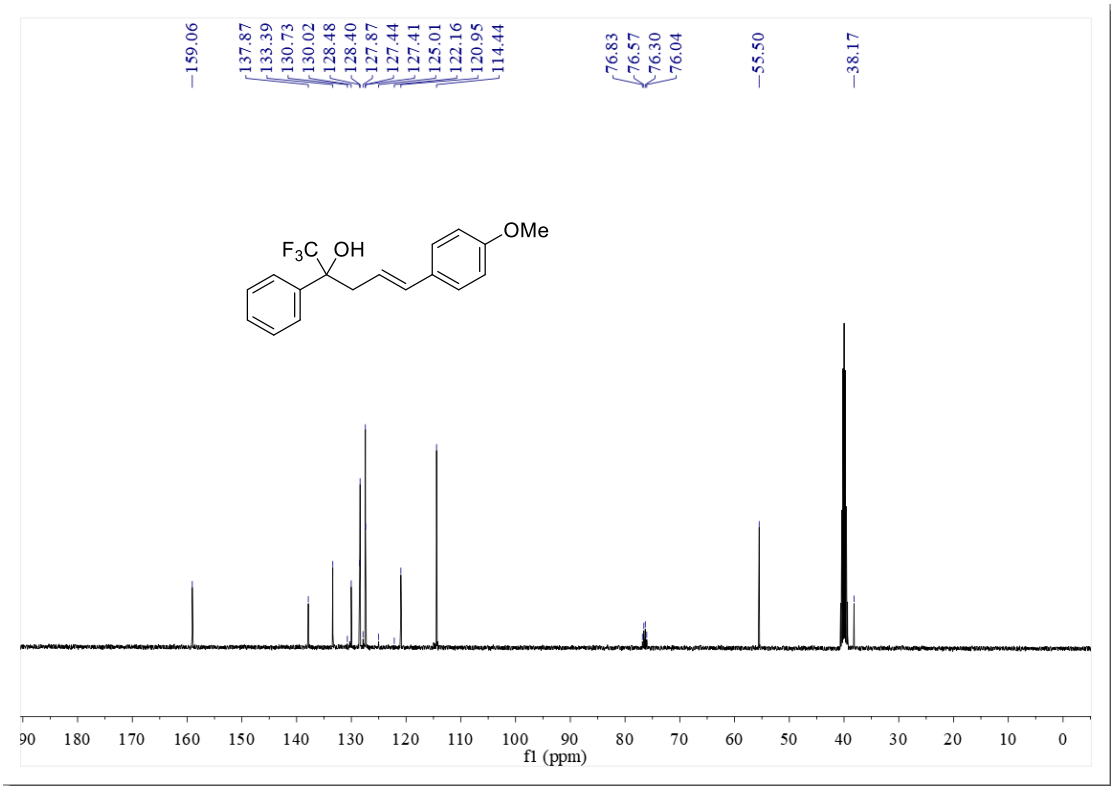


(*E*)-1,1,1-Trifluoro-5-(4-methoxyphenyl)-2-phenylpent-4-en-2-ol (3e)

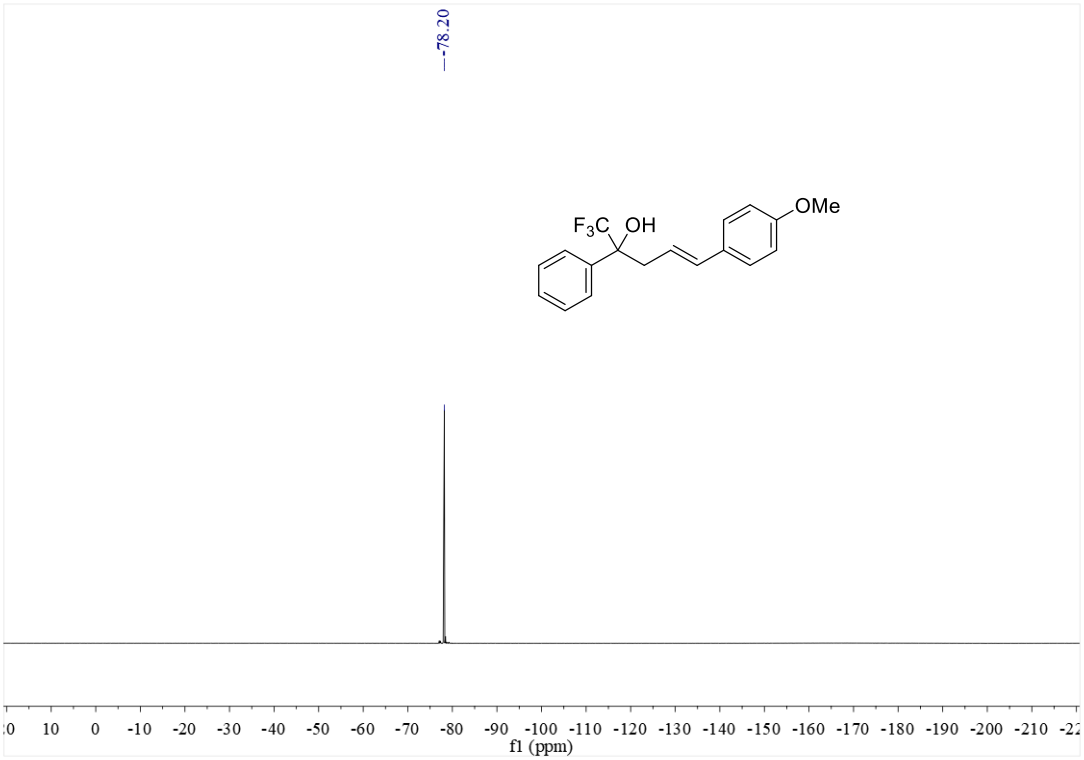
^{1}H NMR of 3e



^{13}C NMR of 3e

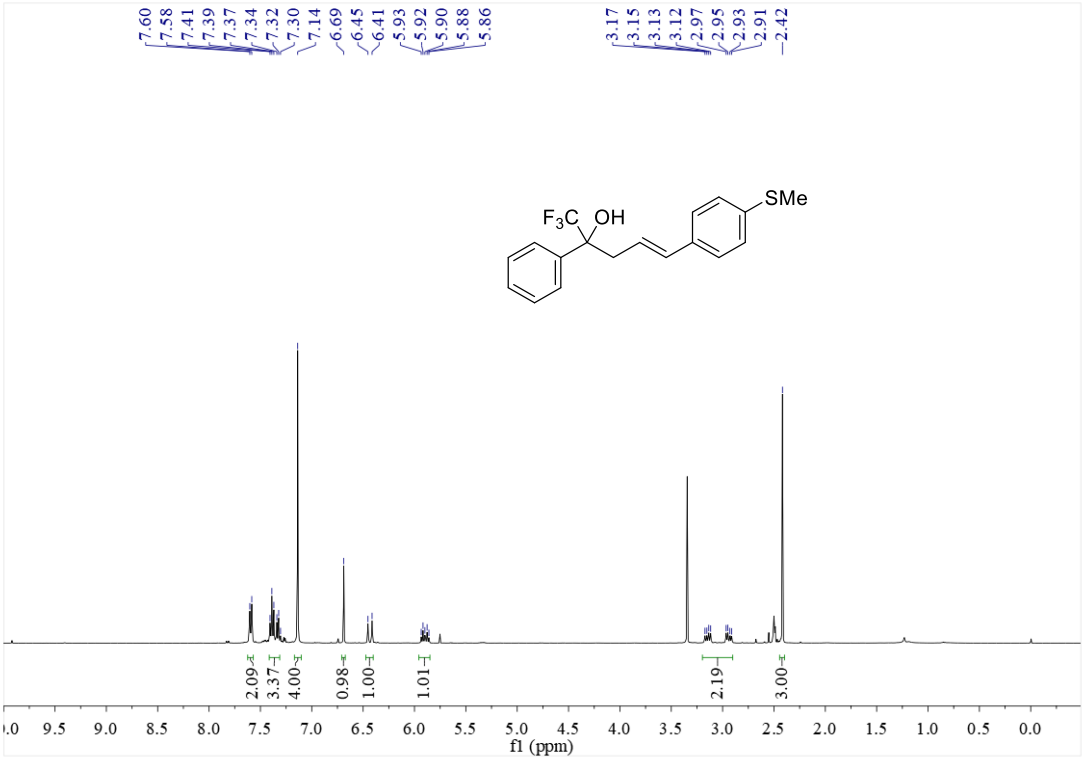


^{19}F NMR of 3e

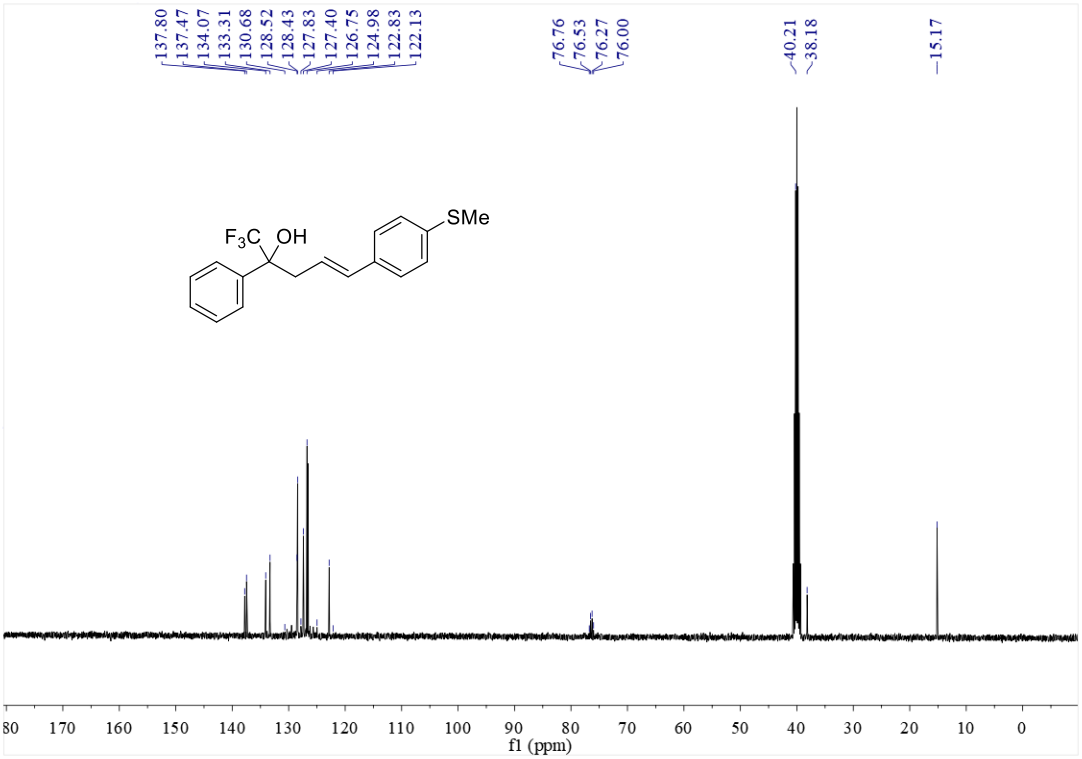


(*E*)-1,1,1-Trifluoro-5-(4-(methylthio)phenyl)-2-phenylpent-4-en-2-ol (3f)

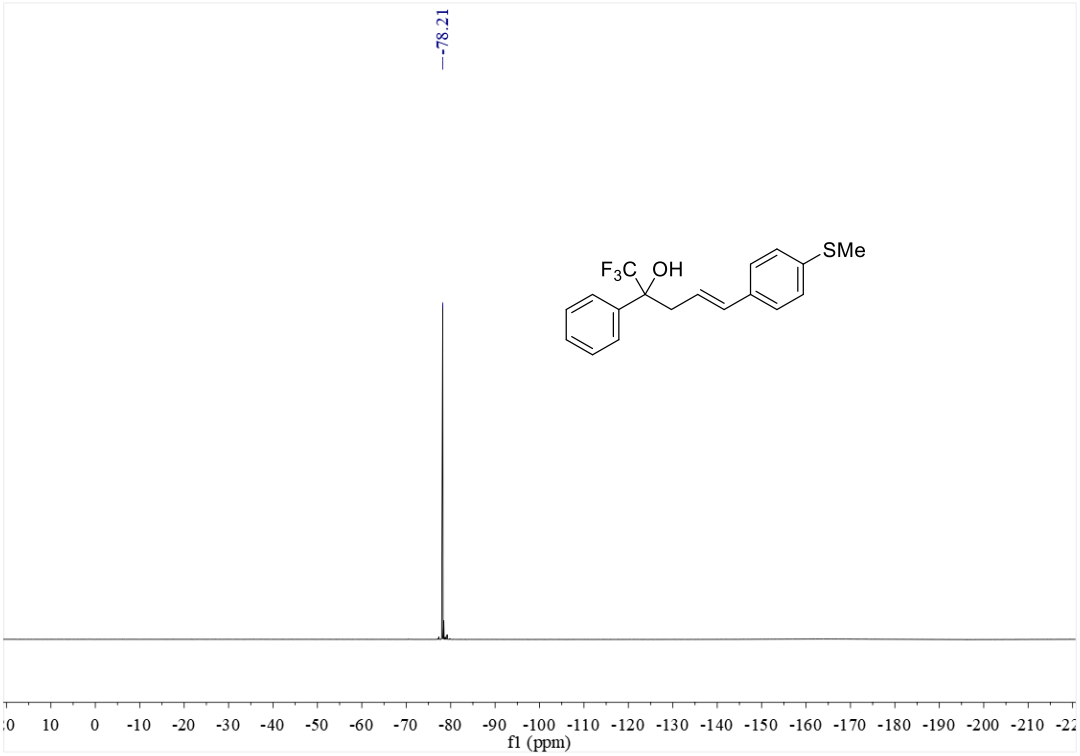
^{1}H NMR of 3f



^{13}C NMR of 3f

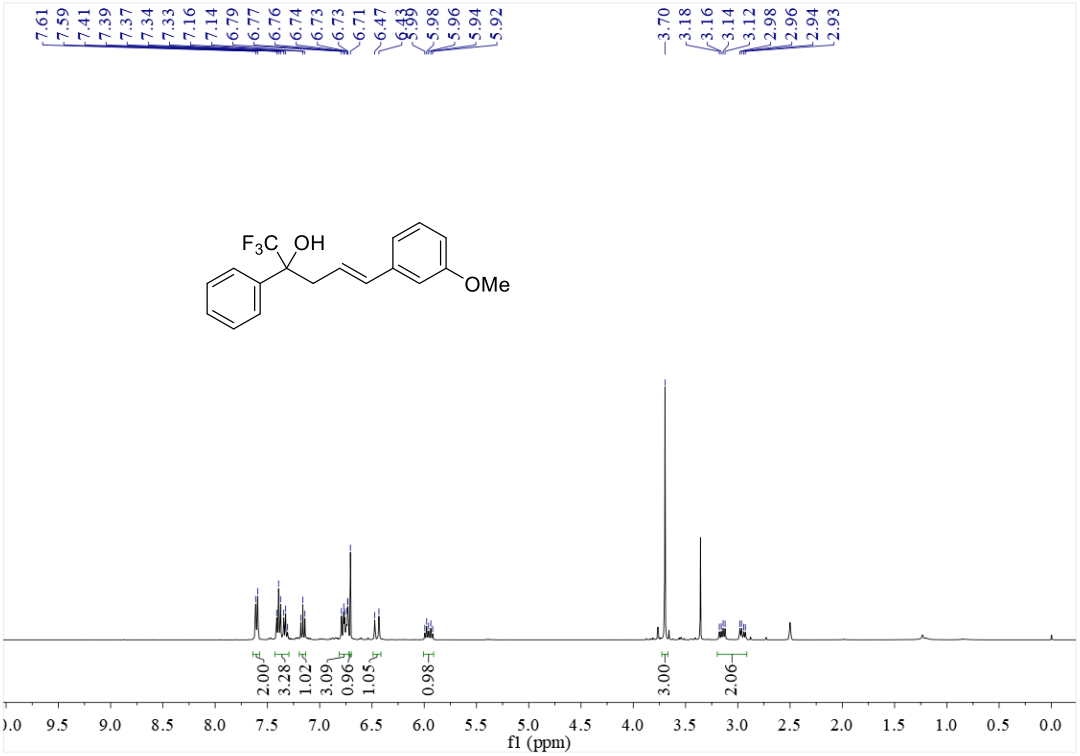


^{19}F NMR of 3f

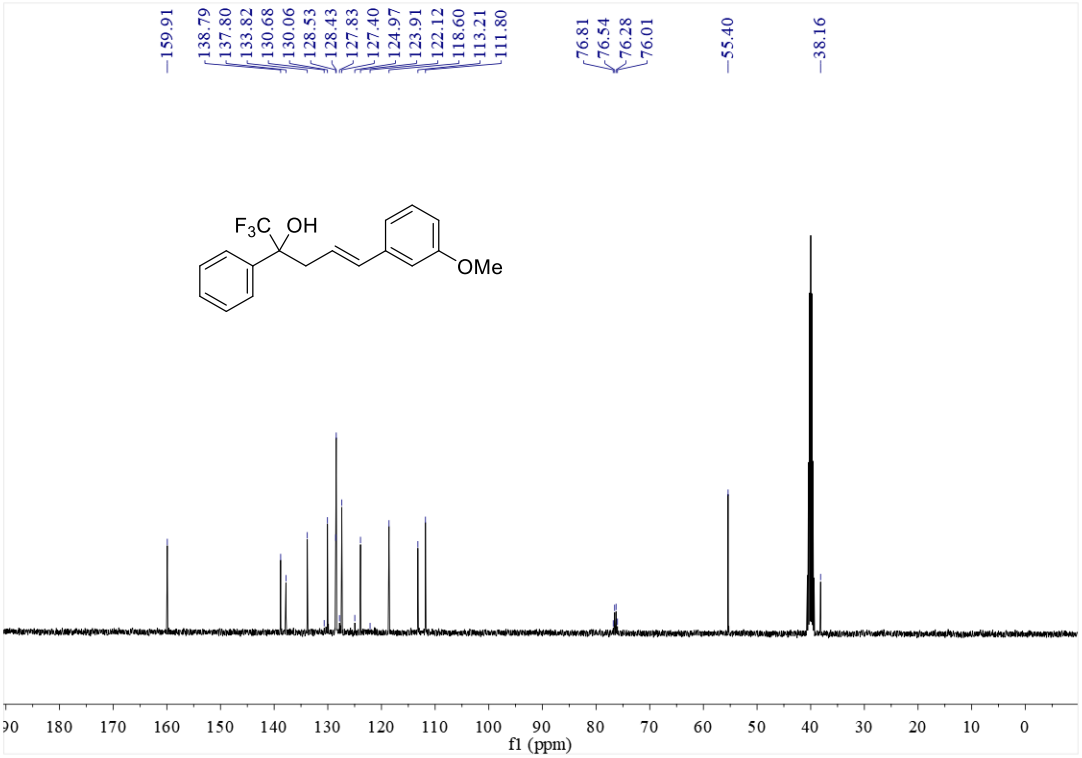


(*E*)-1,1,1-Trifluoro-5-(3-methoxyphenyl)-2-phenylpent-4-en-2-ol (3g)

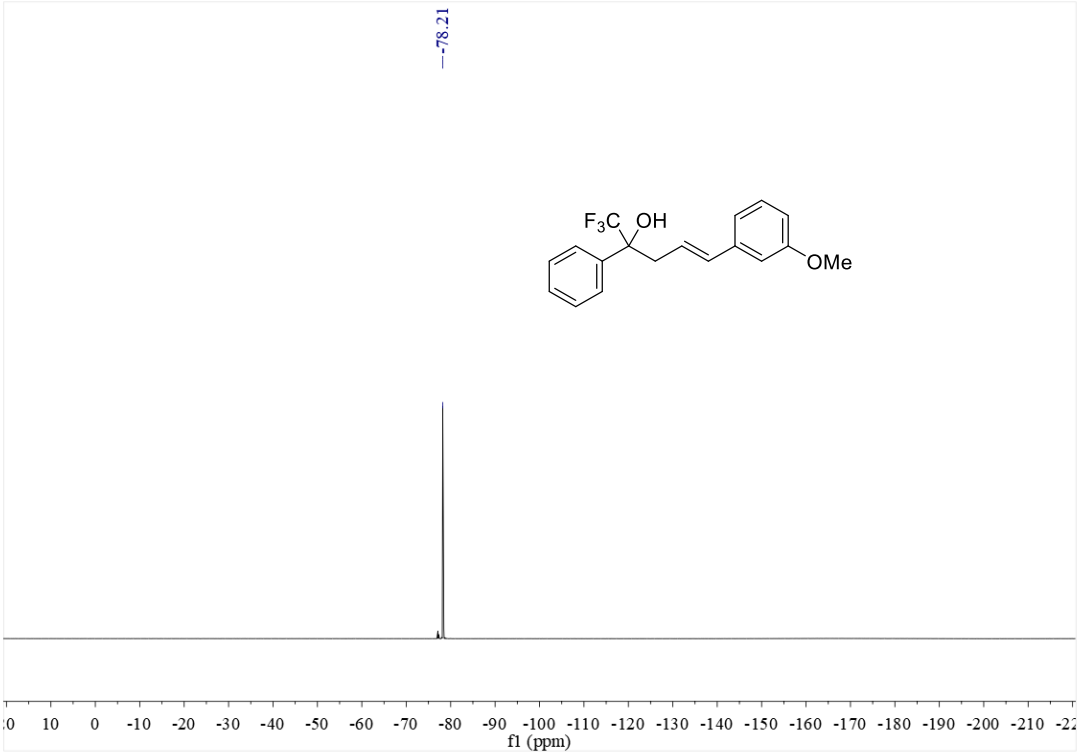
^{1}H NMR of 3g



^{13}C NMR of 3g

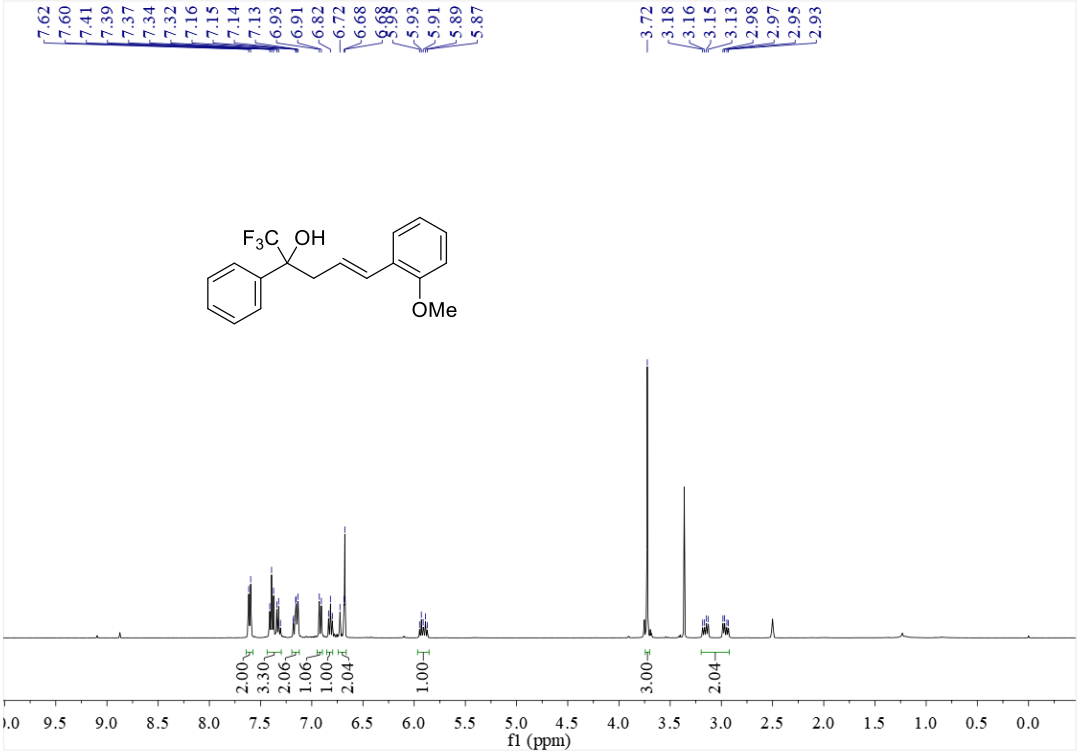


^{19}F NMR of 3g

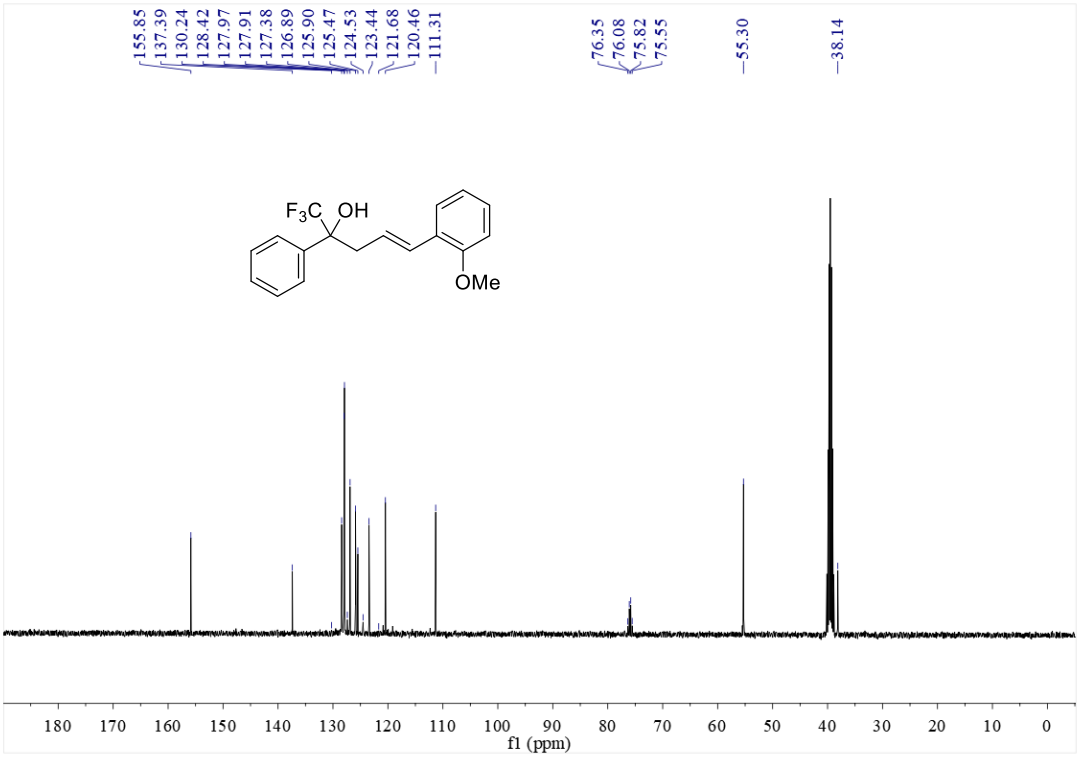


(*E*)-1,1,1-Trifluoro-5-(2-methoxyphenyl)-2-phenylpent-4-en-2-ol (3h)

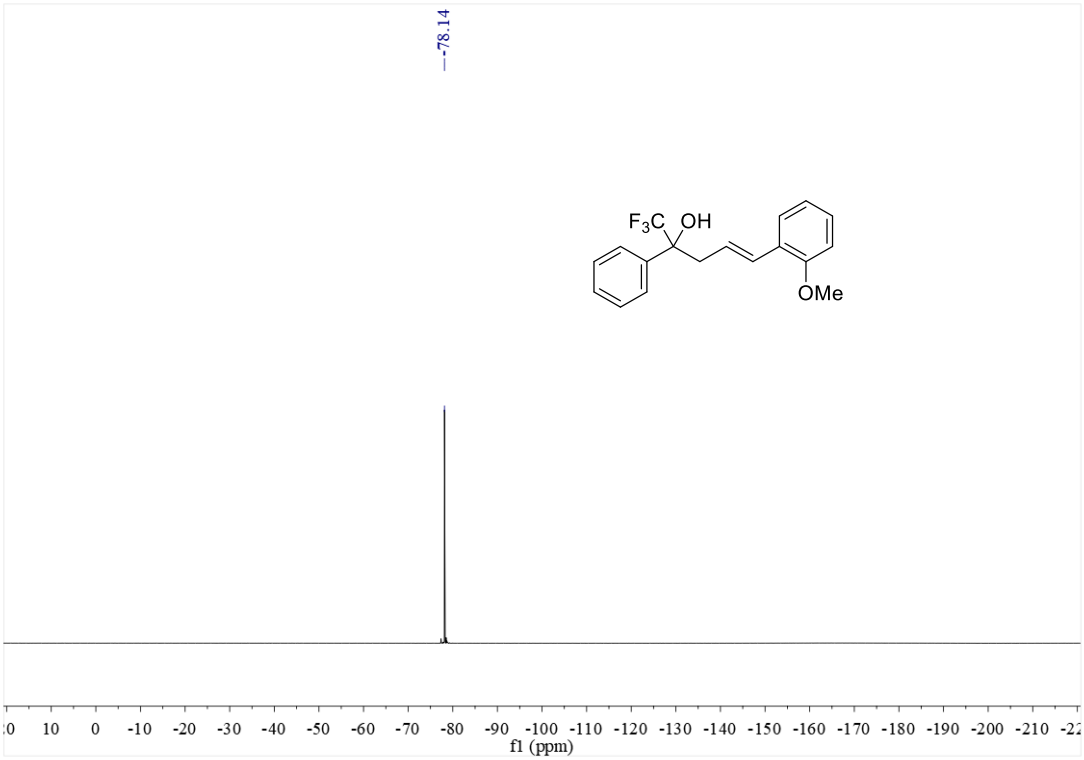
^{1}H NMR of 3h



^{13}C NMR of 3h

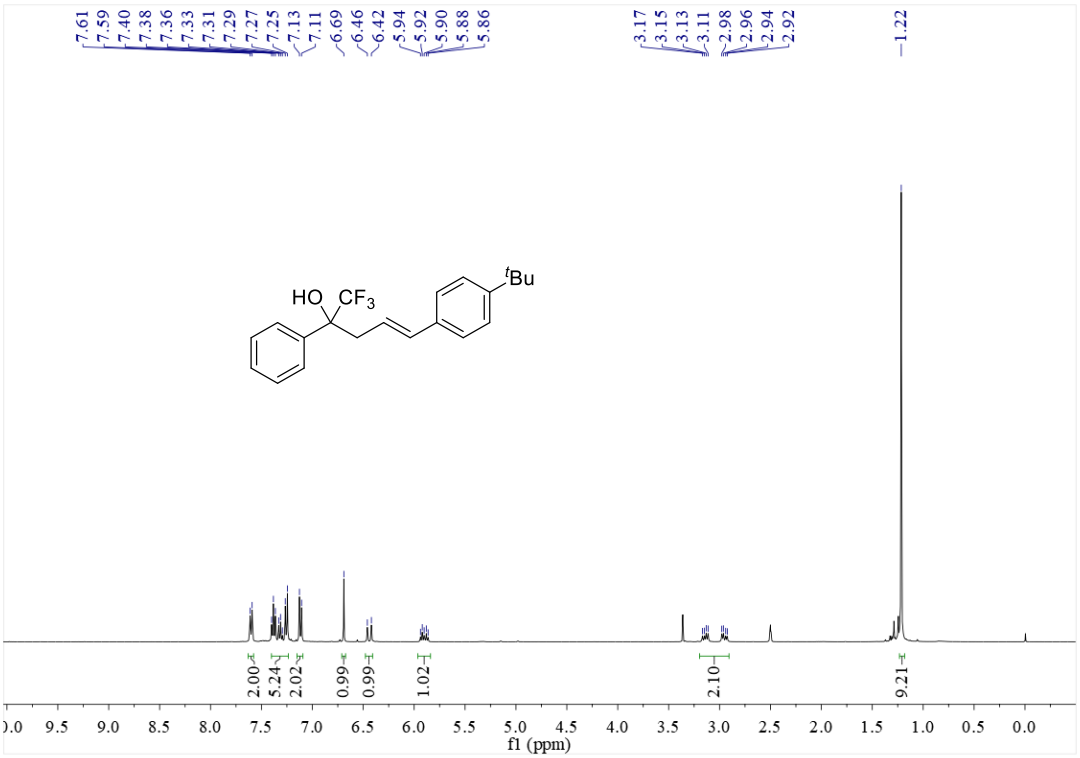


^{19}F NMR of 3h

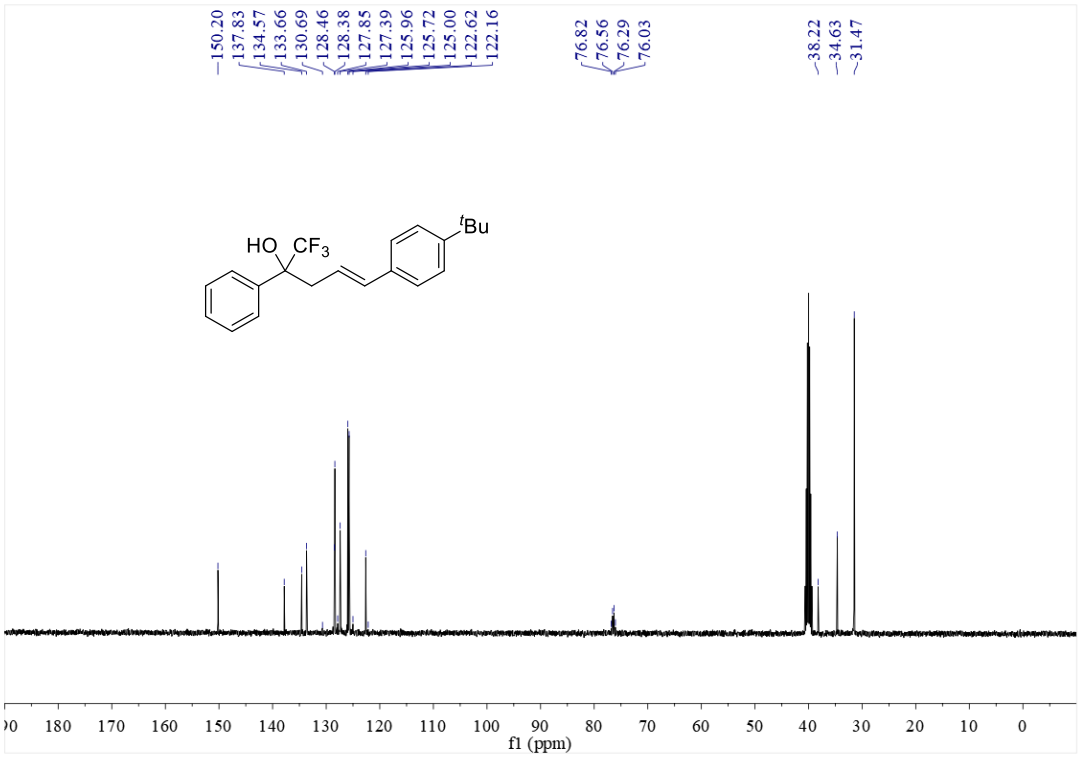


(*E*)-5-(4-(Tert-butyl)phenyl)-1,1,1-trifluoro-2-phenylpent-4-en-2-ol (3i)

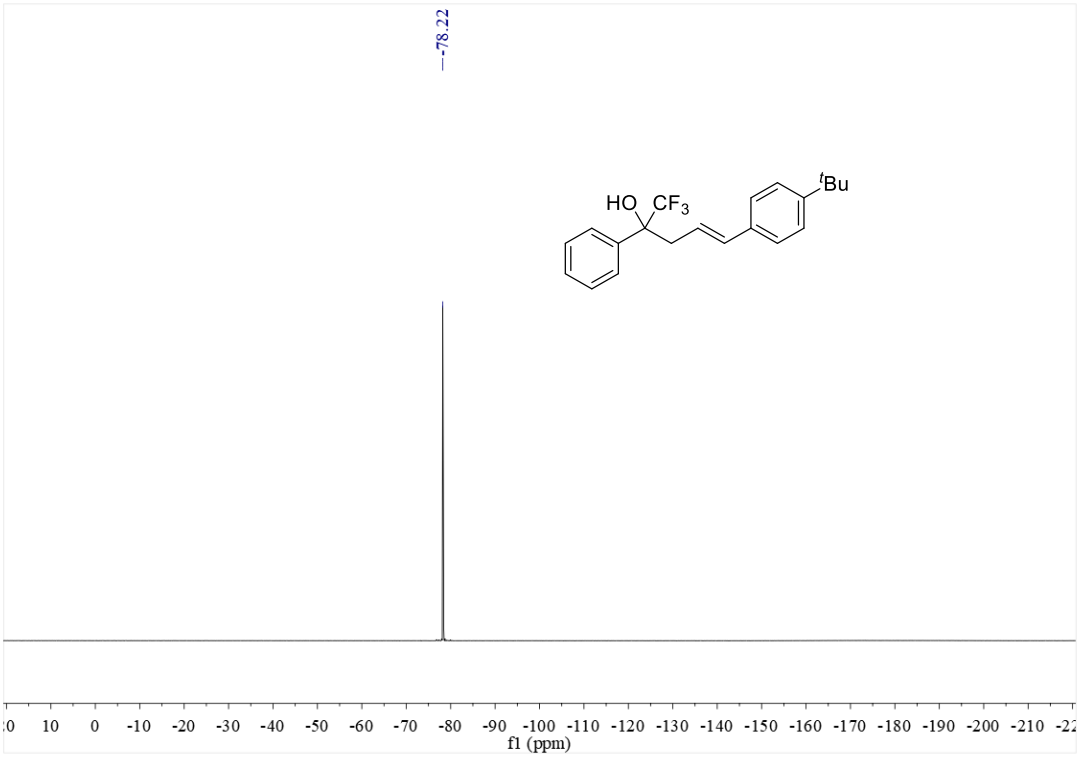
^{1}H NMR of 3i



^{13}C NMR of 3i

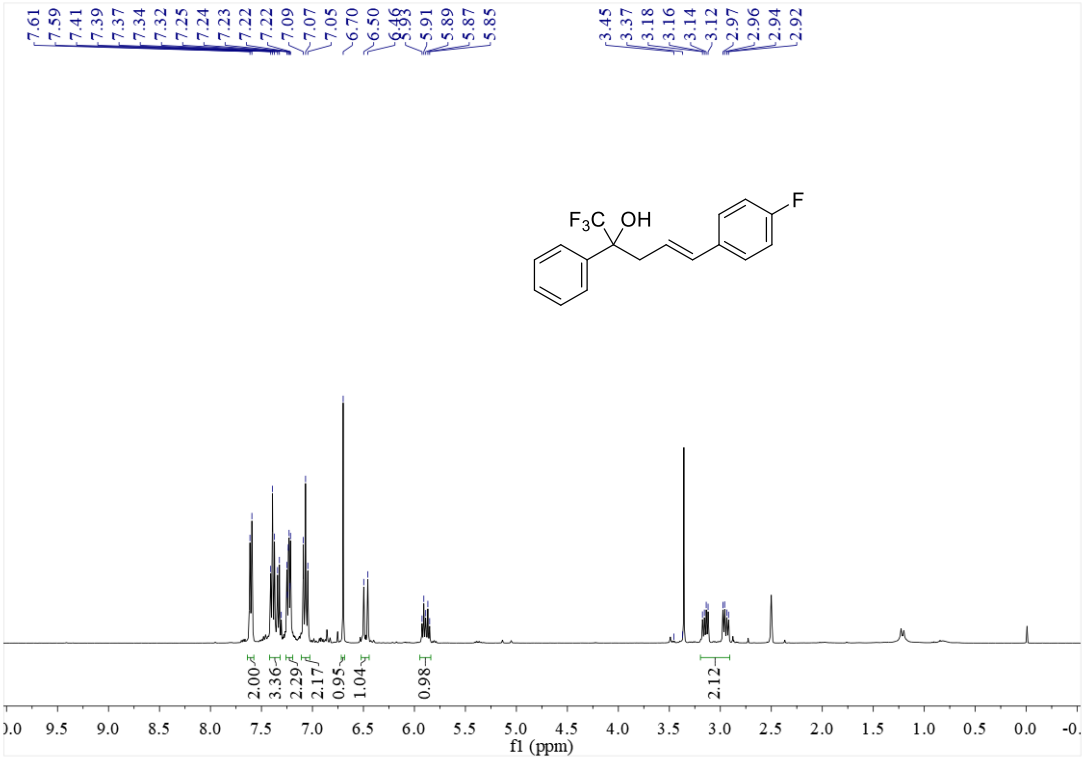


^{19}F NMR of 3i

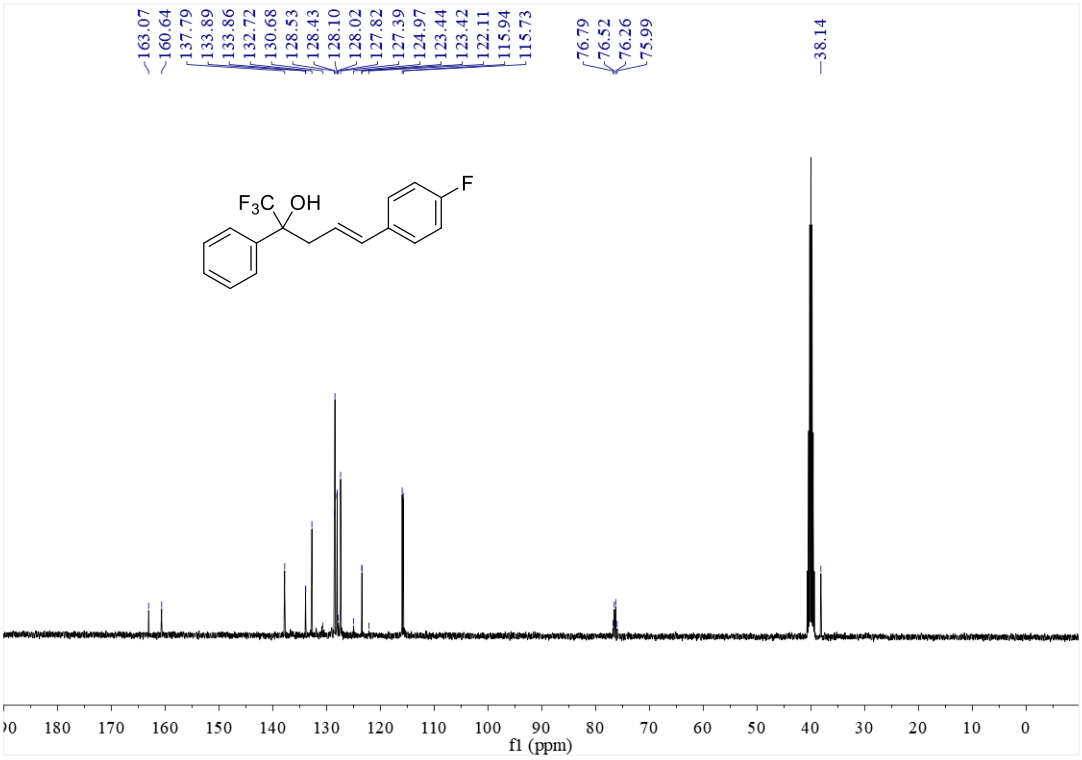


(*E*)-1,1,1-Trifluoro-5-(4-fluorophenyl)-2-phenylpent-4-en-2-ol (3j)

^{1}H NMR of 3j



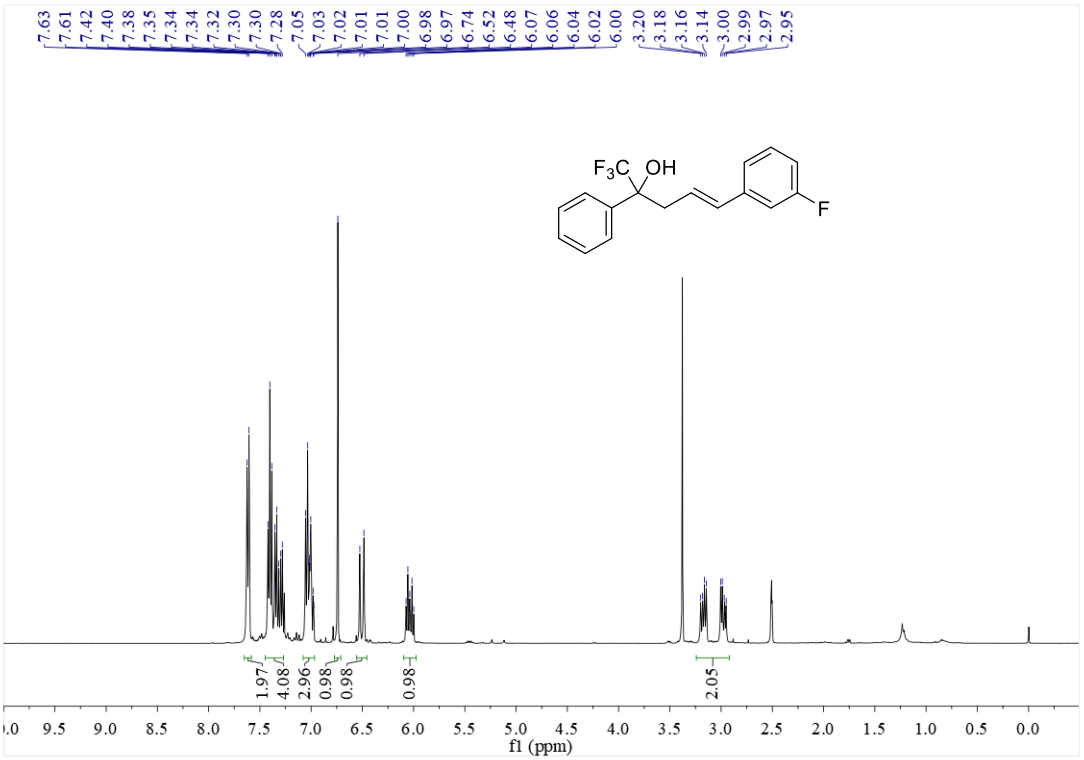
^{13}C NMR of 3j



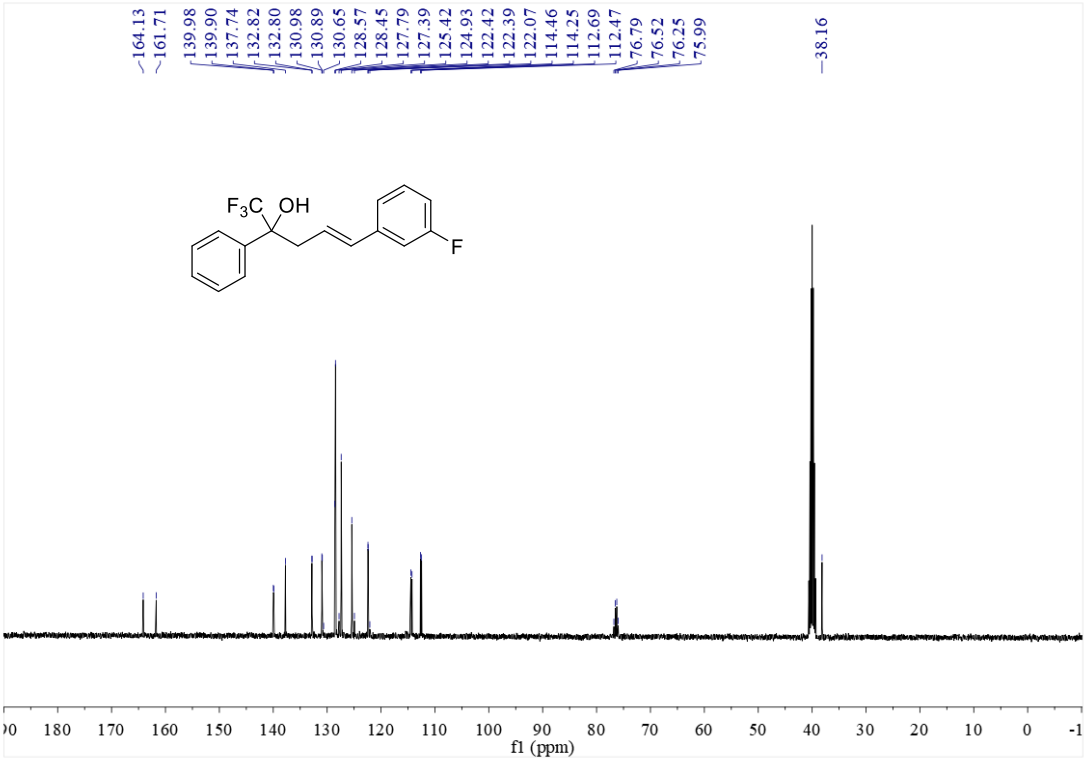
^{19}F NMR of 3j

(*E*)-1,1,1-Trifluoro-5-(3-fluorophenyl)-2-phenylpent-4-en-2-ol (3k)

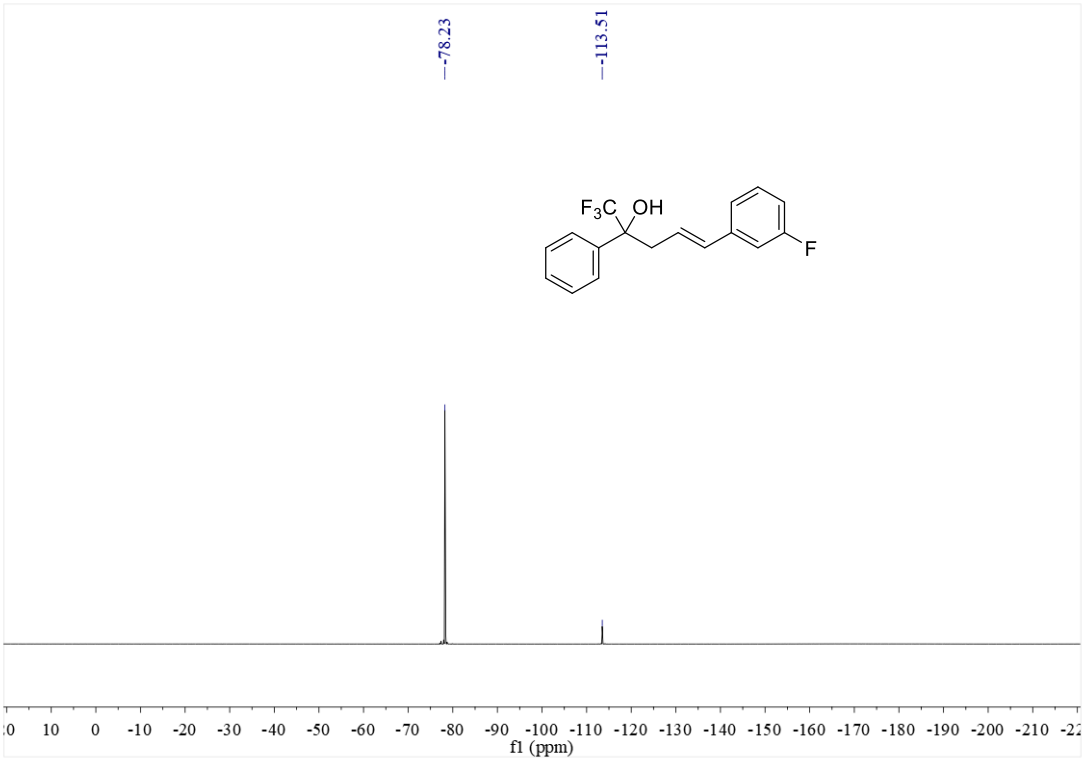
^{1}H NMR of 3k



^{13}C NMR of 3k

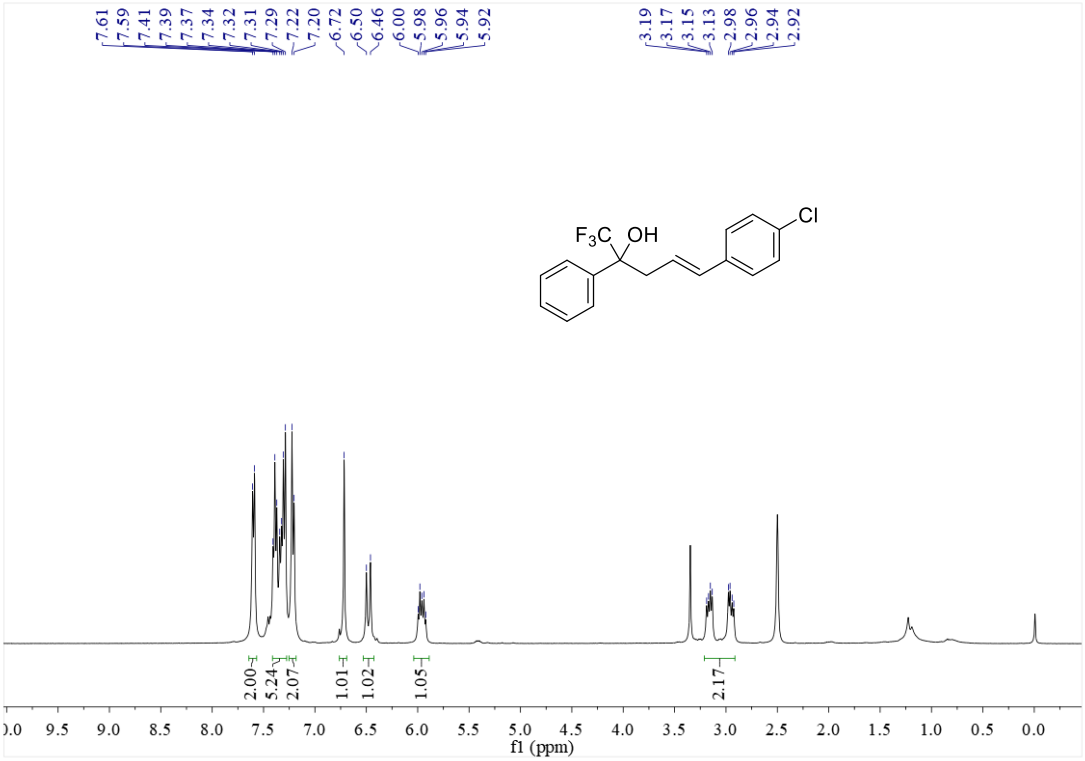


^{19}F NMR of 3k

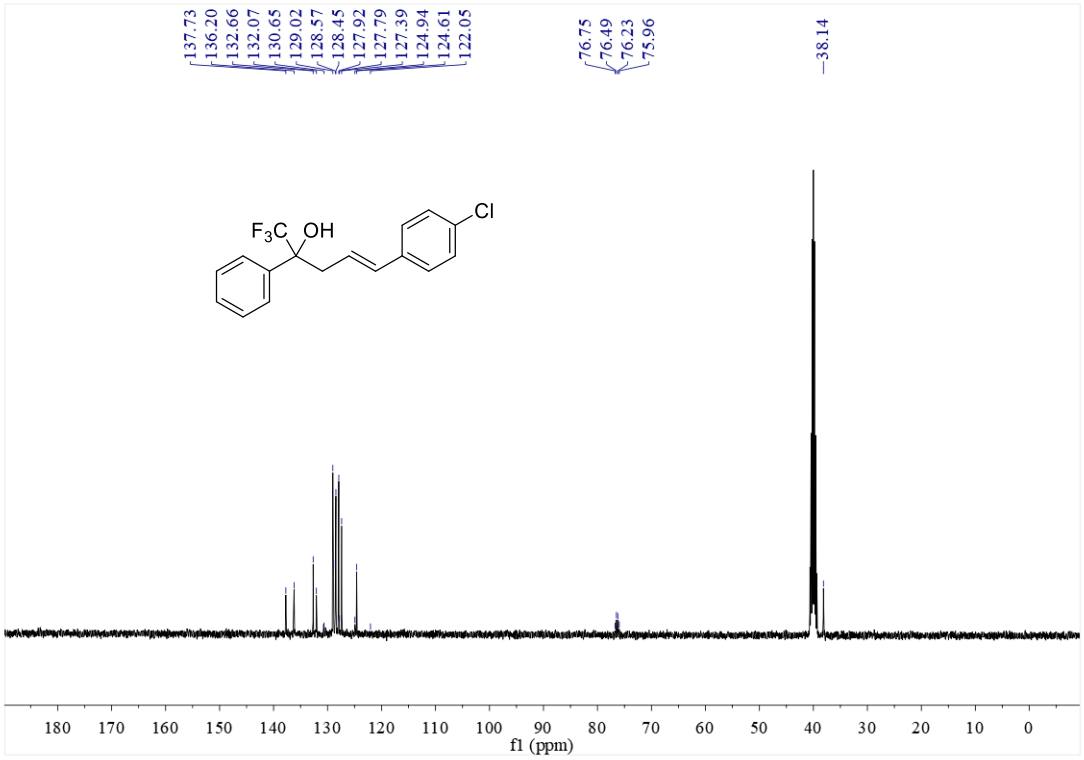


(*E*)-5-(4-Chlorophenyl)-1,1,1-trifluoro-2-phenylpent-4-en-2-ol (3l)

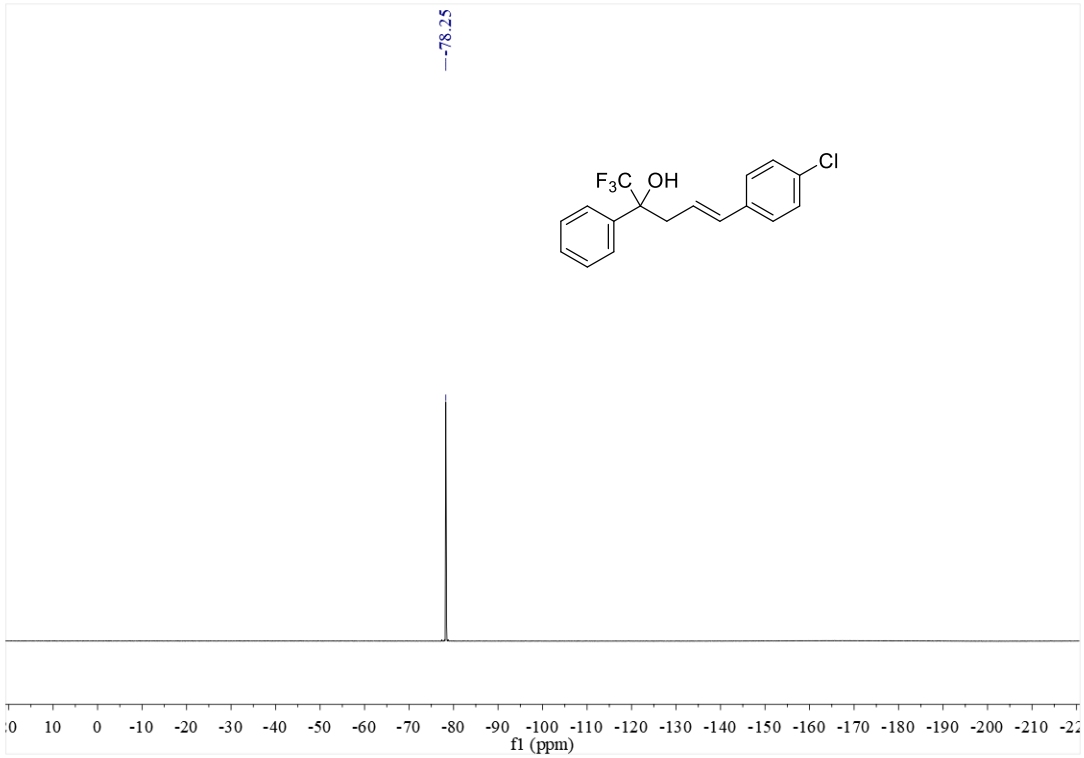
^{1}H NMR of 3l



^{13}C NMR of 3l

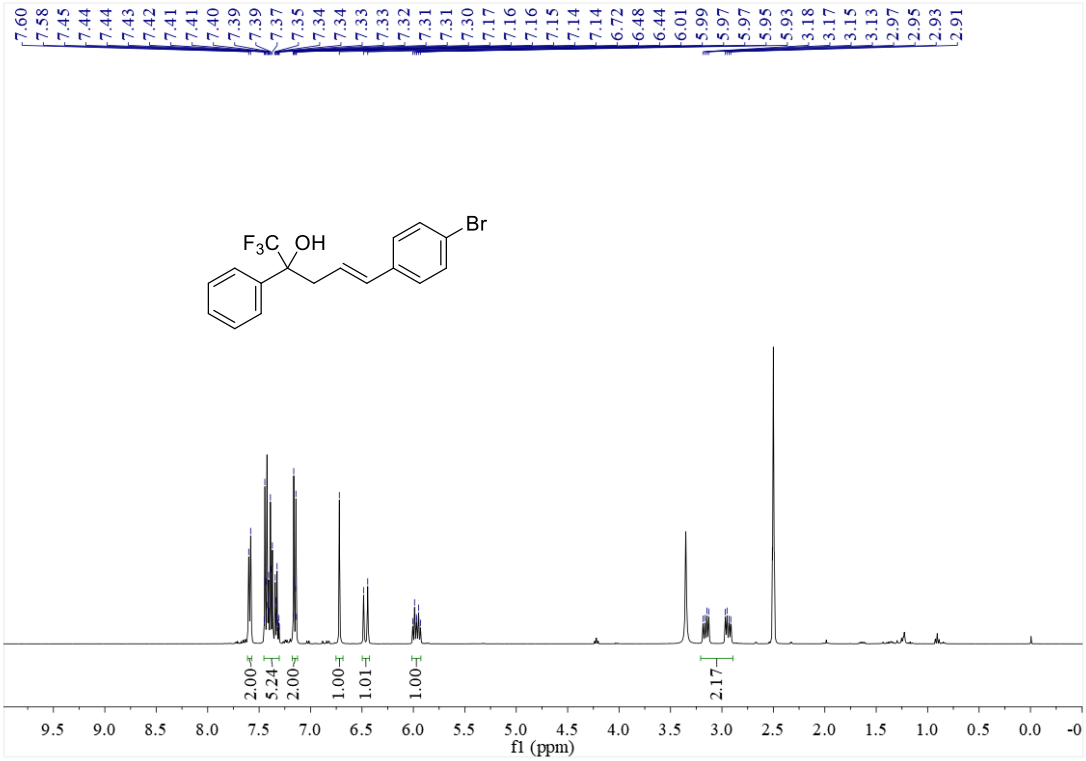


^{19}F NMR of 3l

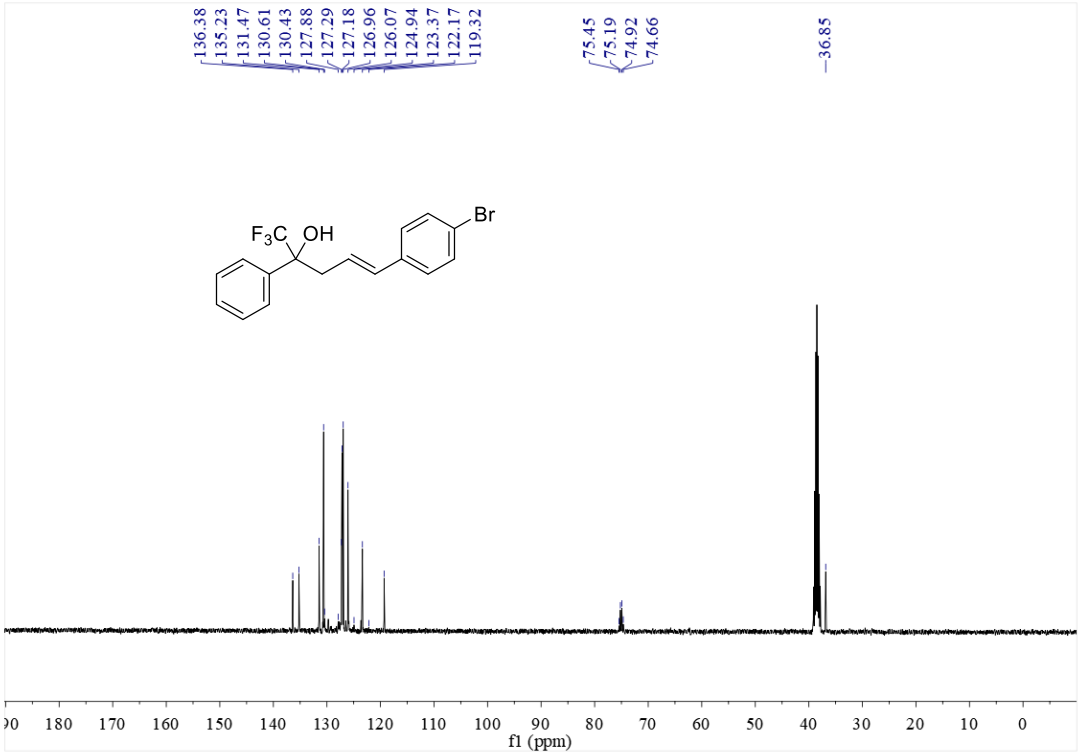


(*E*)-5-(4-Bromophenyl)-1,1,1-trifluoro-2-phenylpent-4-en-2-ol (3m)

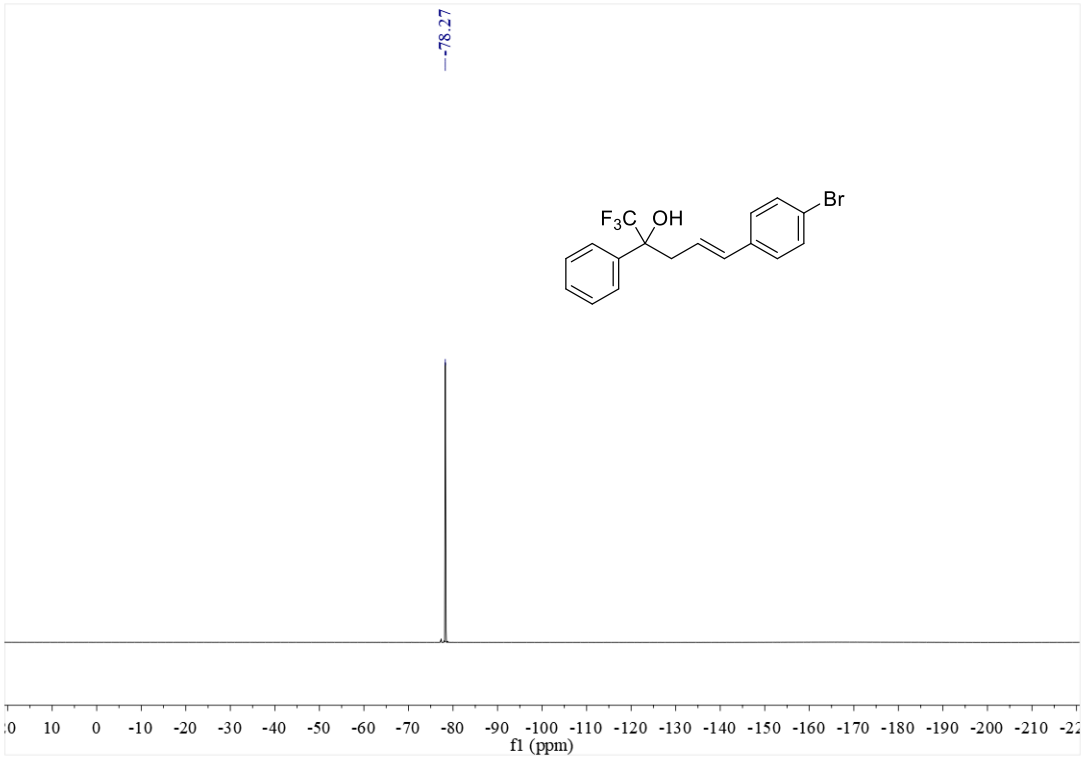
^{1}H NMR of 3m



^{13}C NMR of 3m

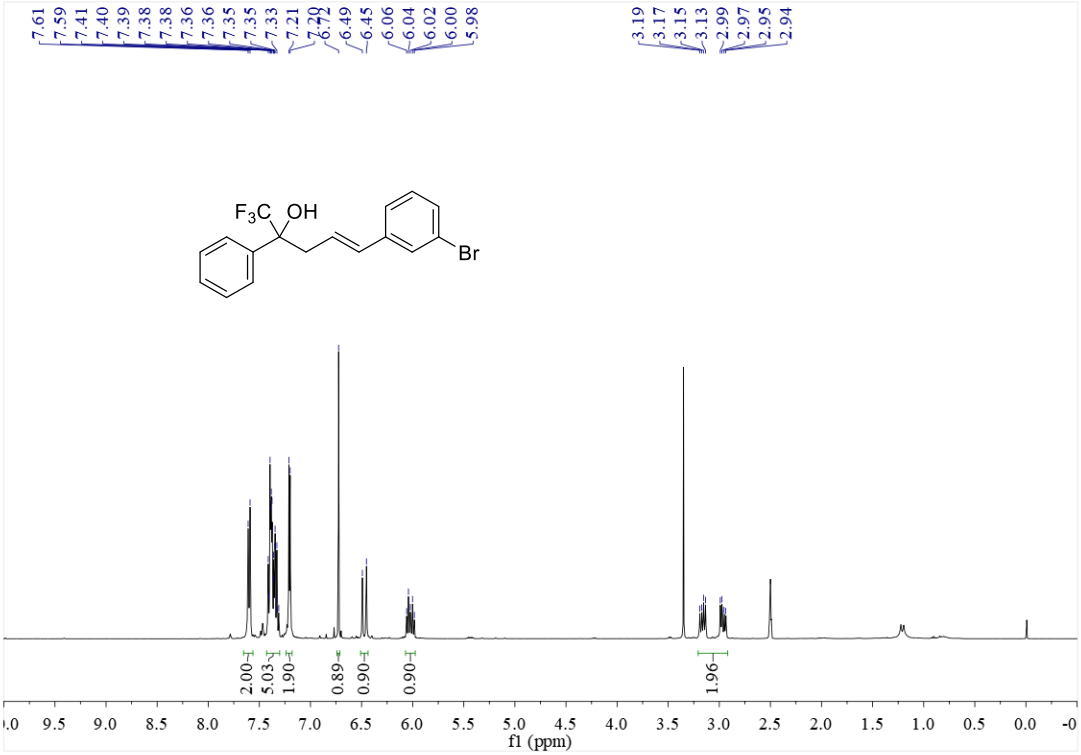


^{19}F NMR of 3m

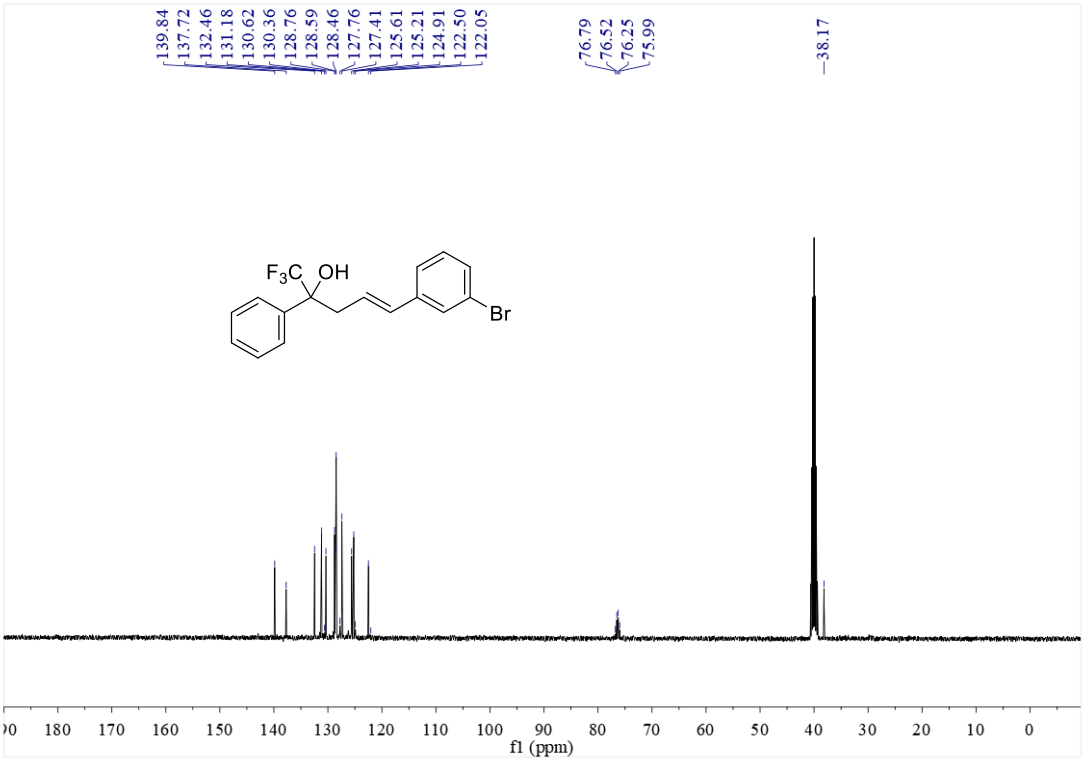


(*E*)-5-(3-Bromophenyl)-1,1,1-trifluoro-2-phenylpent-4-en-2-ol (3n)

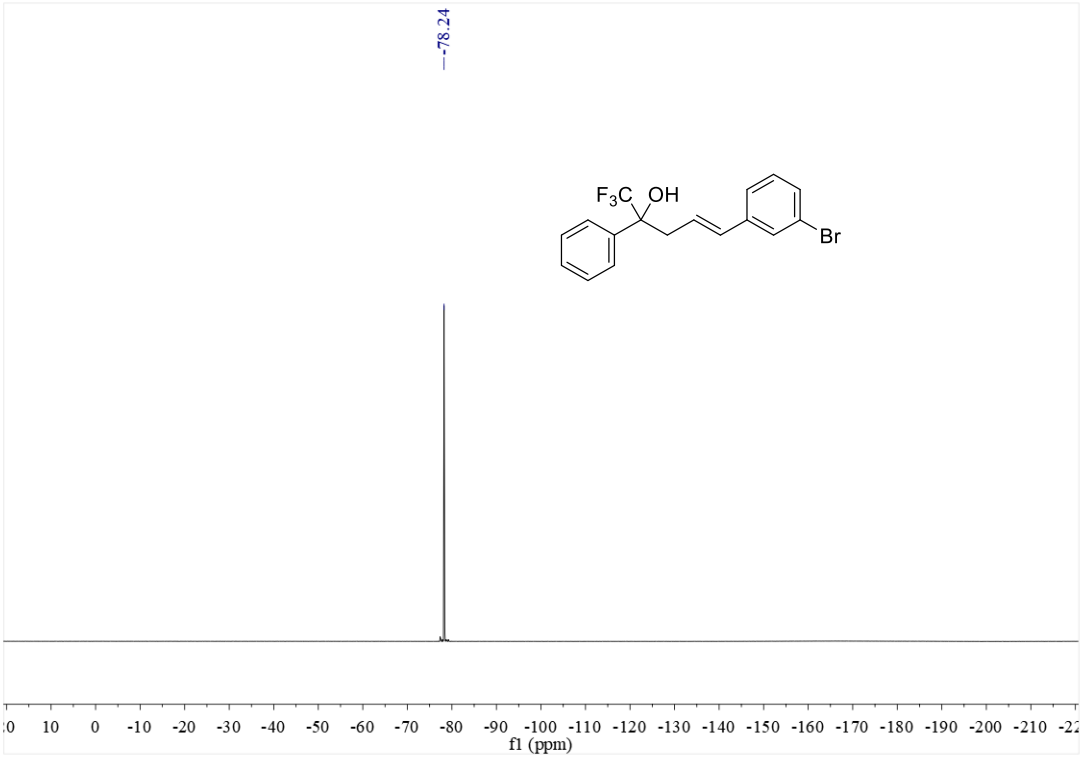
^{1}H NMR of 3n



^{13}C NMR of 3n

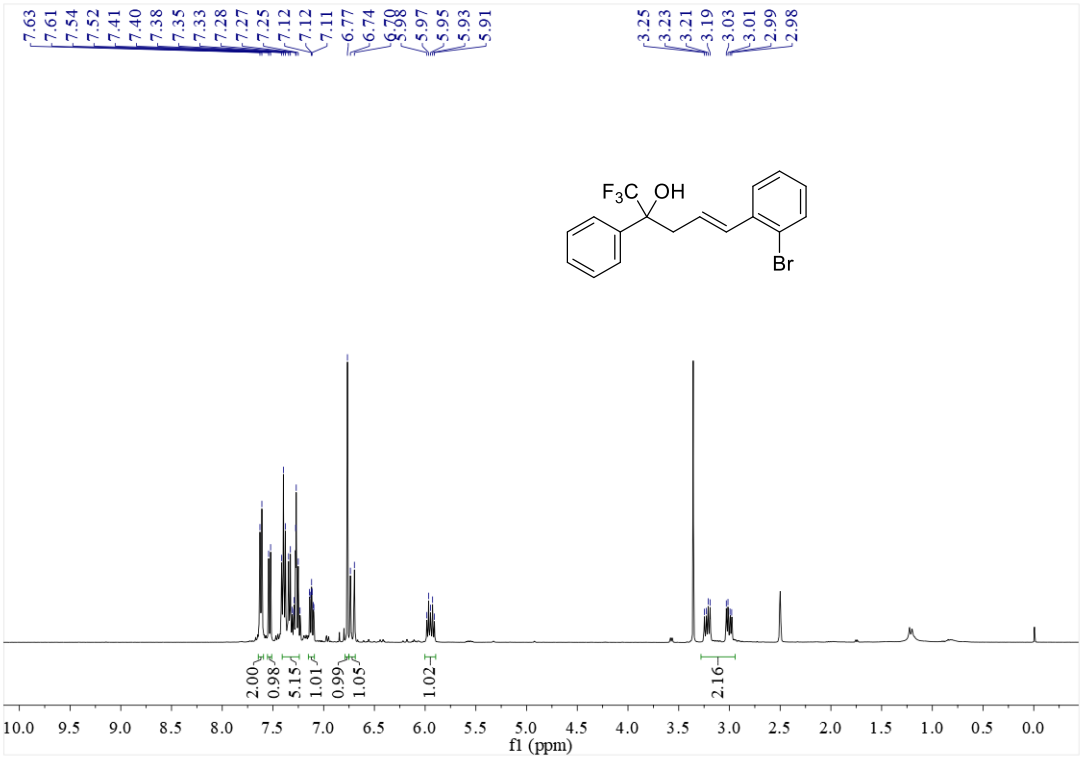


^{19}F NMR of 3n

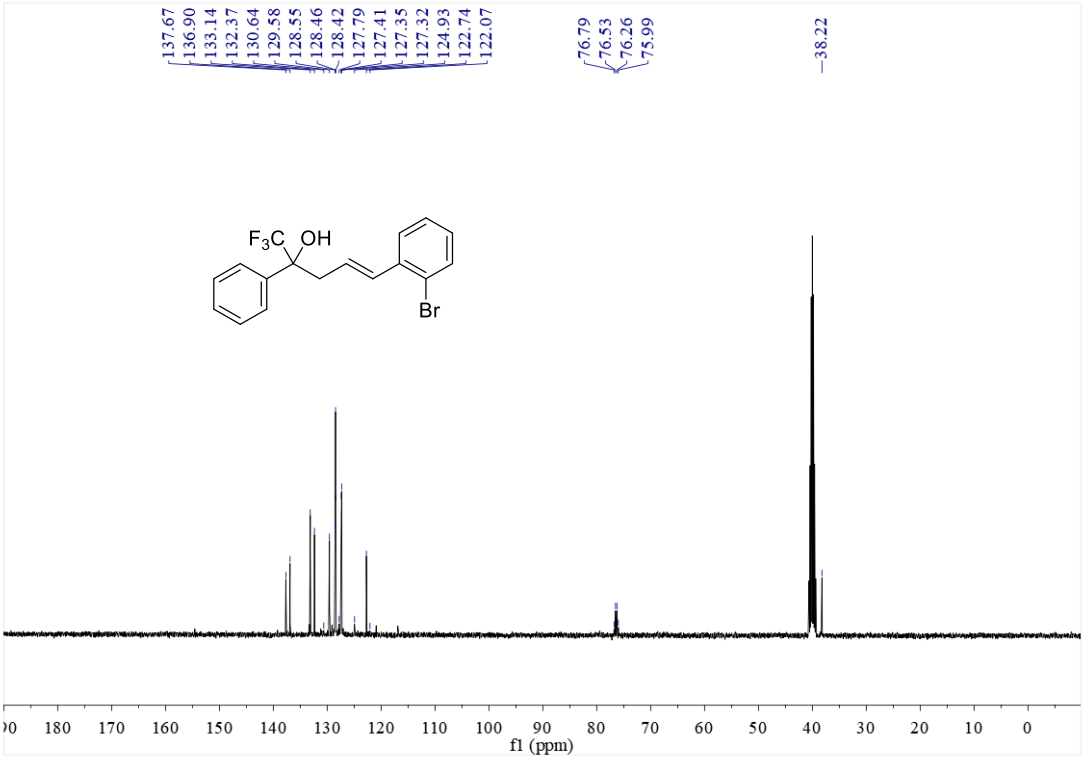


(*E*)-5-(2-Bromophenyl)-1,1,1-trifluoro-2-phenylpent-4-en-2-ol (3o)

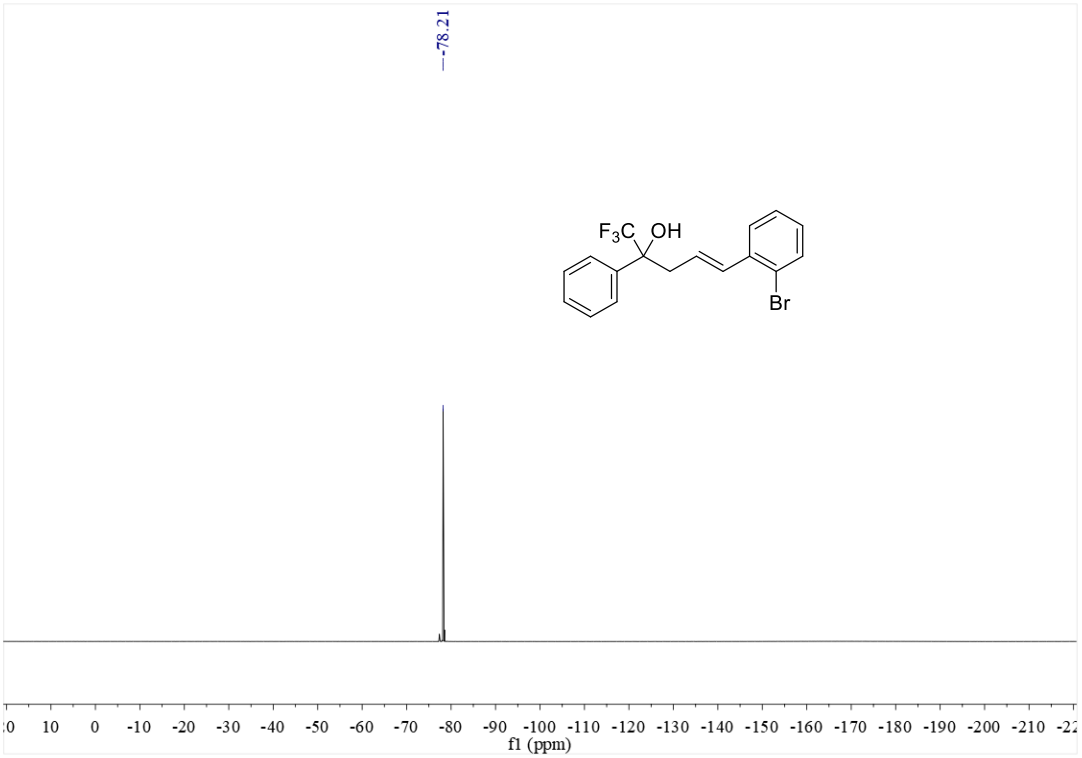
^{1}H NMR of 3o



^{13}C NMR of 3o

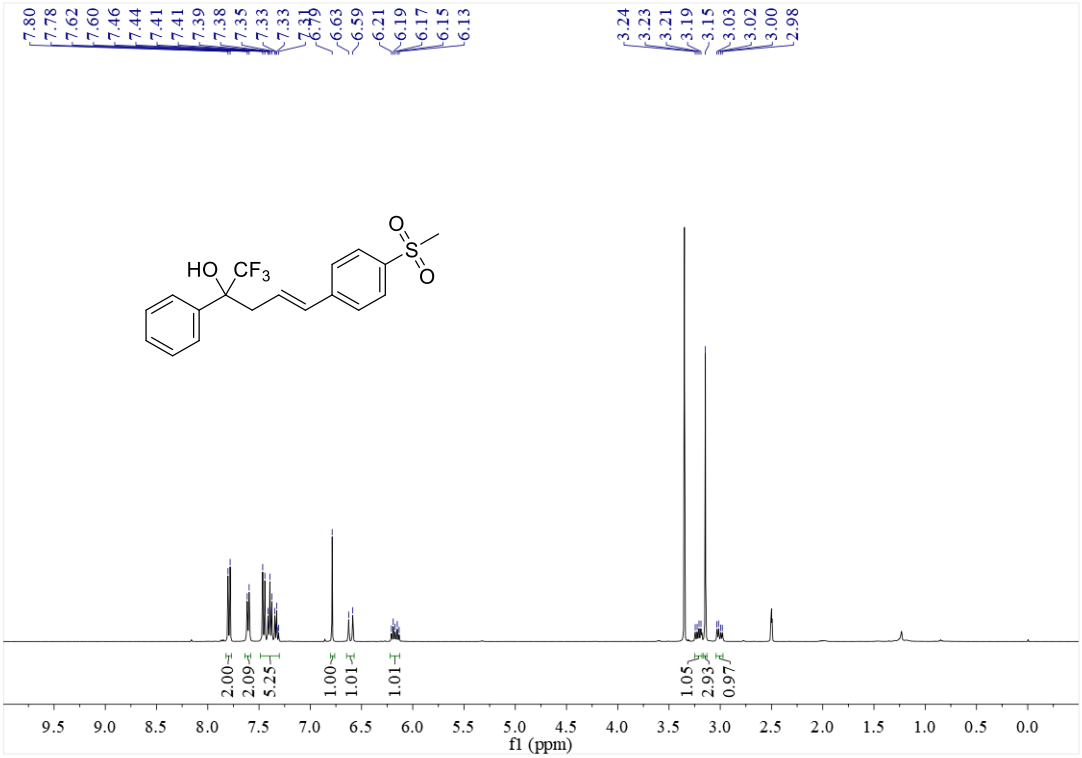


^{19}F NMR of 3o

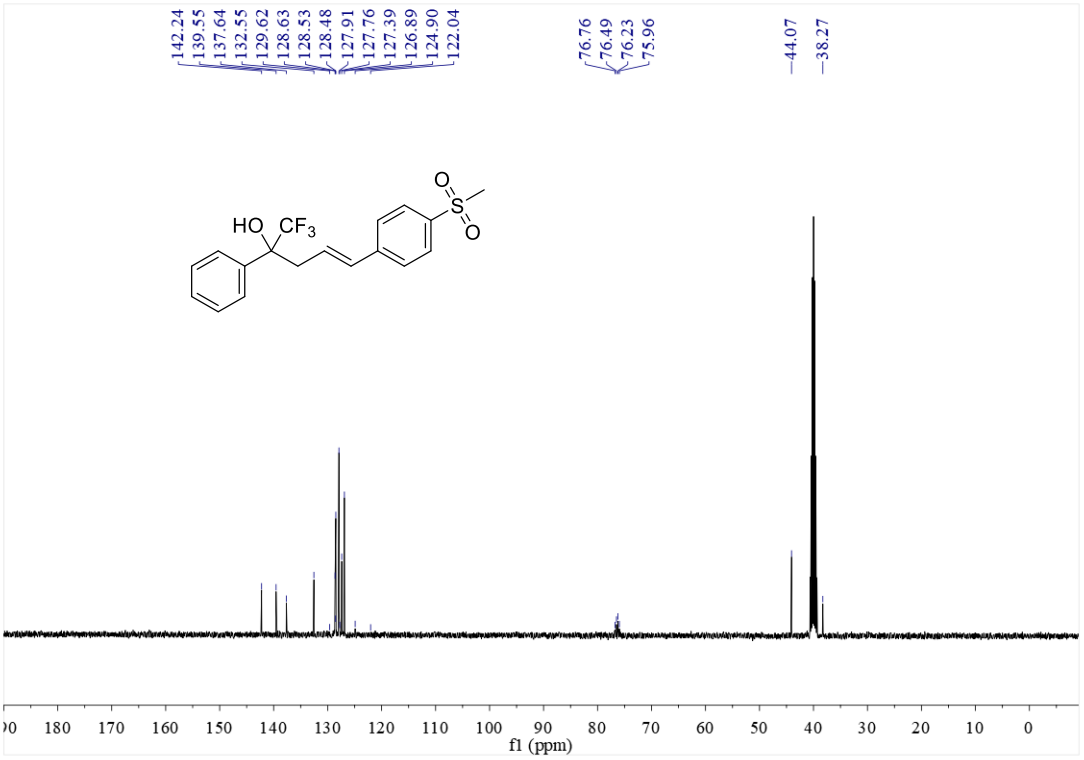


(*E*)-1,1,1-Trifluoro-5-(4-(methylsulfonyl)phenyl)-2-phenylpent-4-en-2-ol (3p)

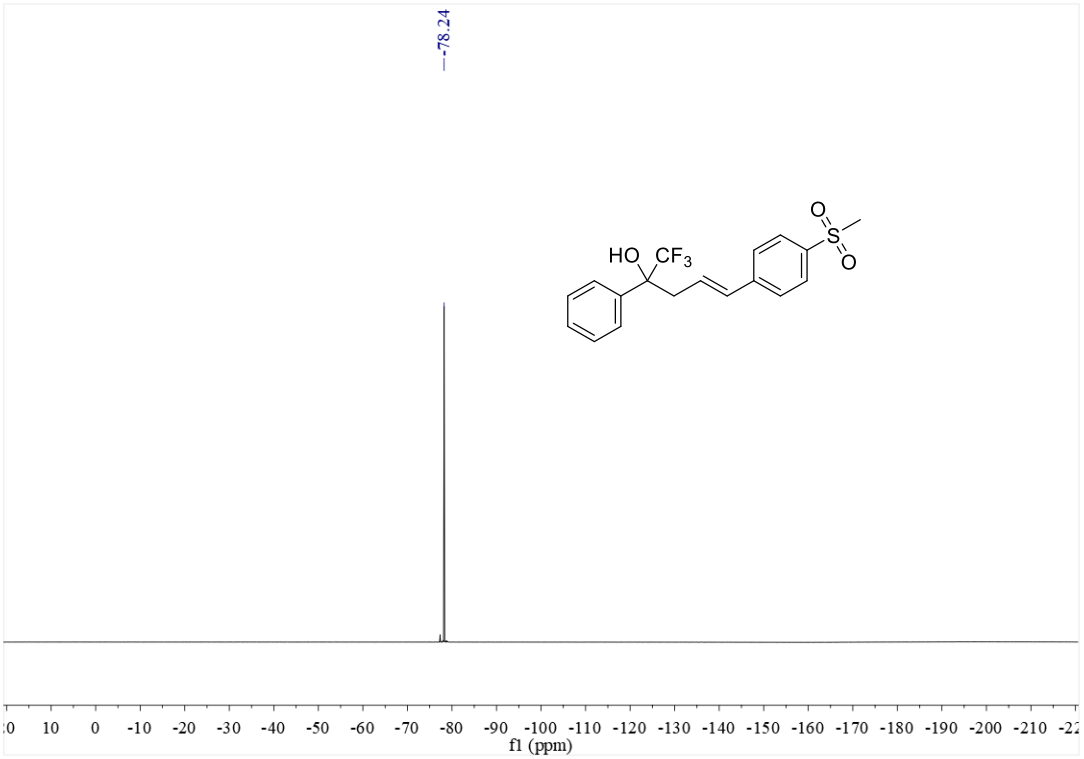
^{1}H NMR of 3p



^{13}C NMR of 3p

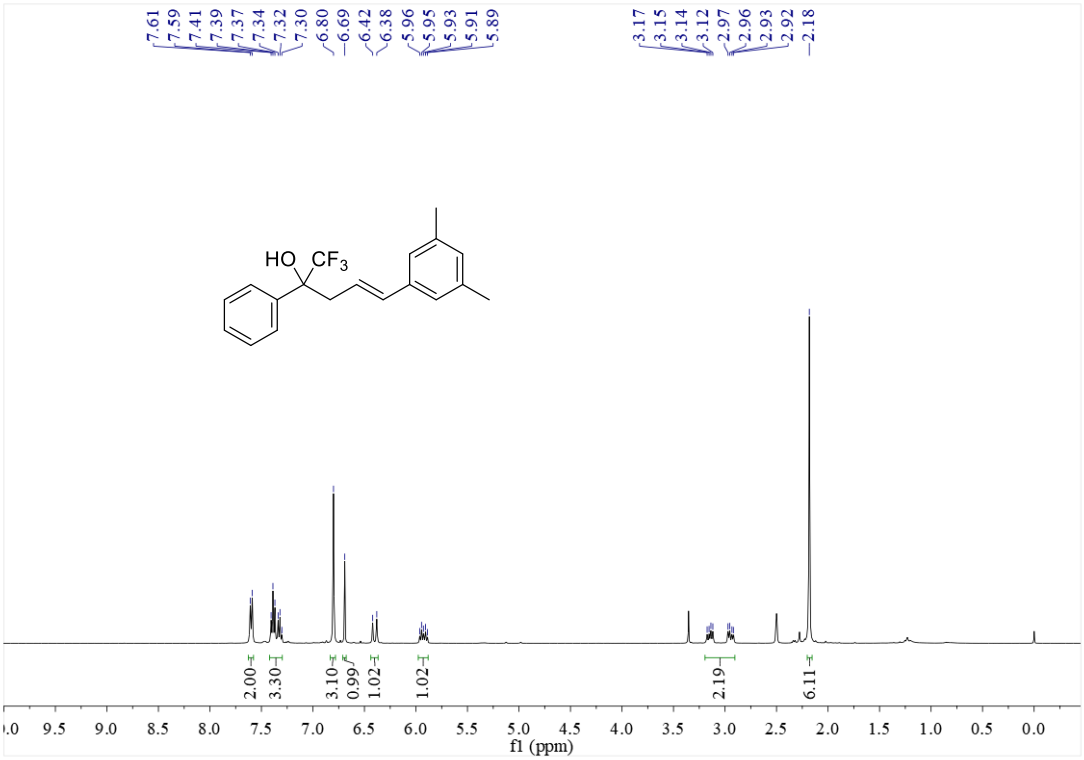


^{19}F NMR of 3p

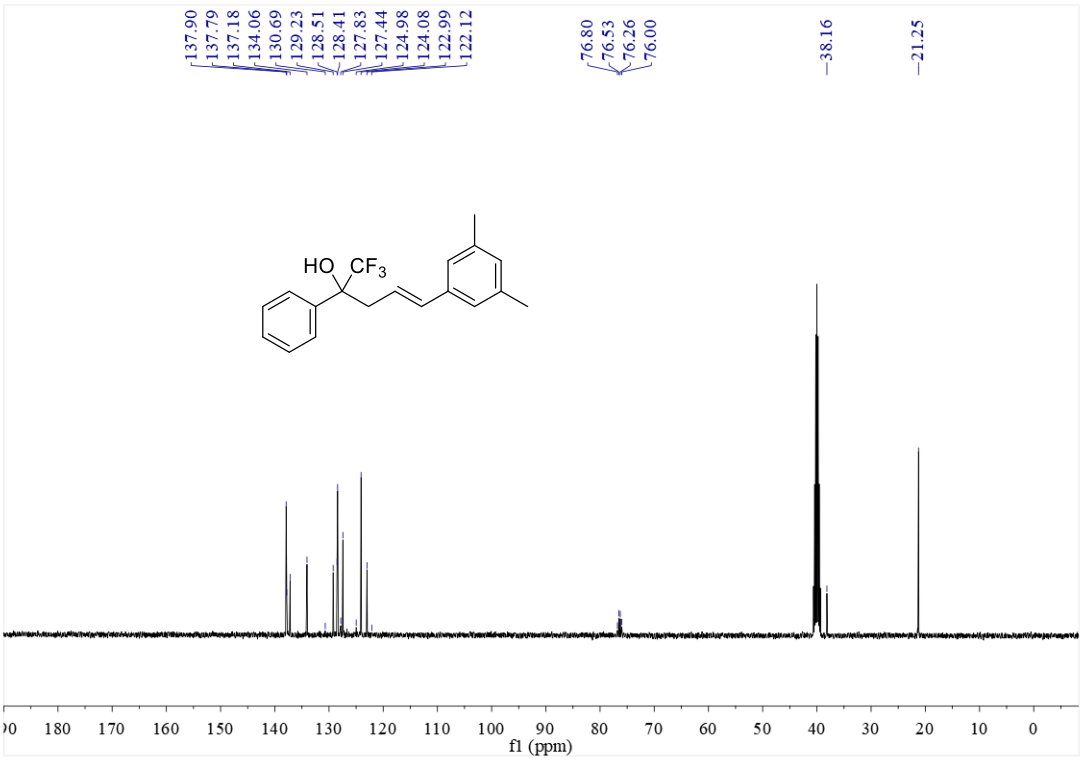


(*E*)-5-(3,5-Dimethylphenyl)-1,1,1-trifluoro-2-phenylpent-4-en-2-ol (3q)

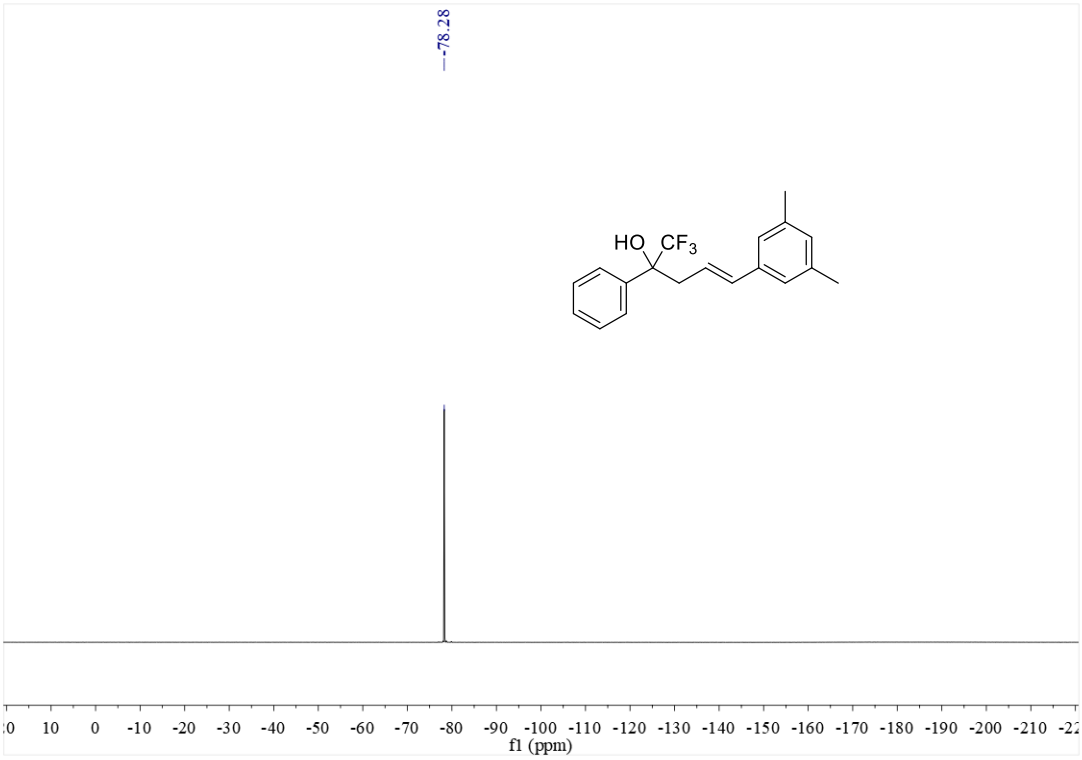
^{1}H NMR of 3q



^{13}C NMR of 3q

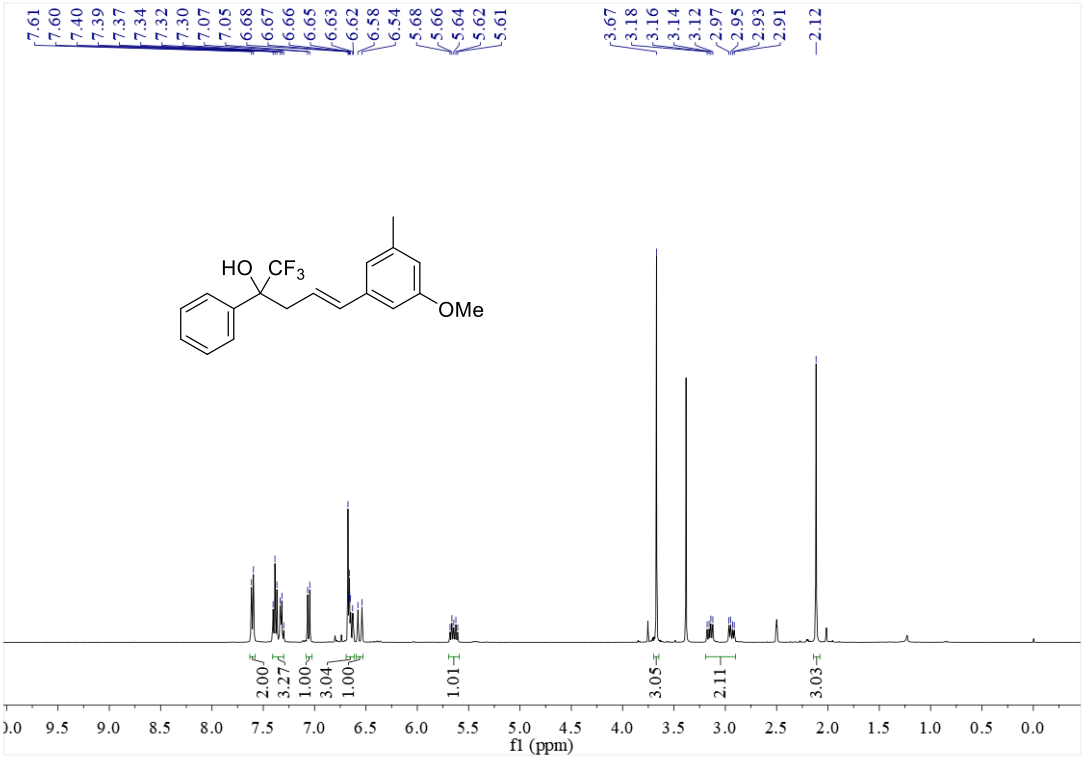


^{19}F NMR of 3q

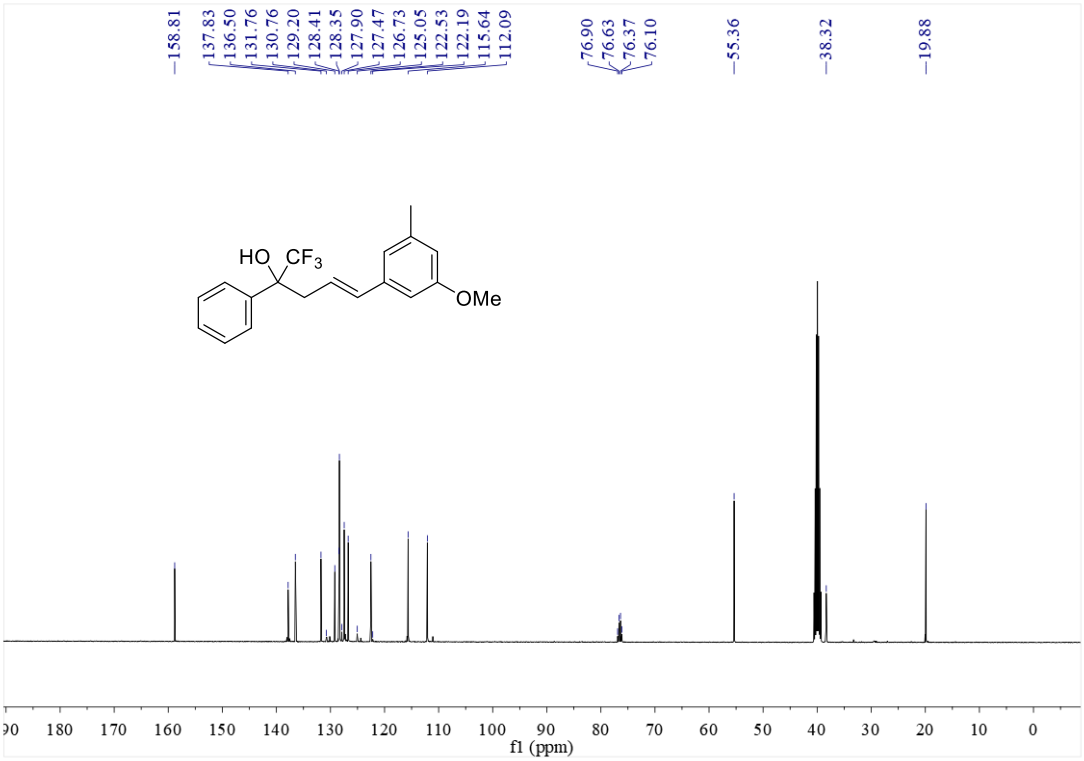


(*E*)-1,1,1-Trifluoro-5-(3-methoxy-5-methylphenyl)-2-phenylpent-4-en-2-ol (3r)

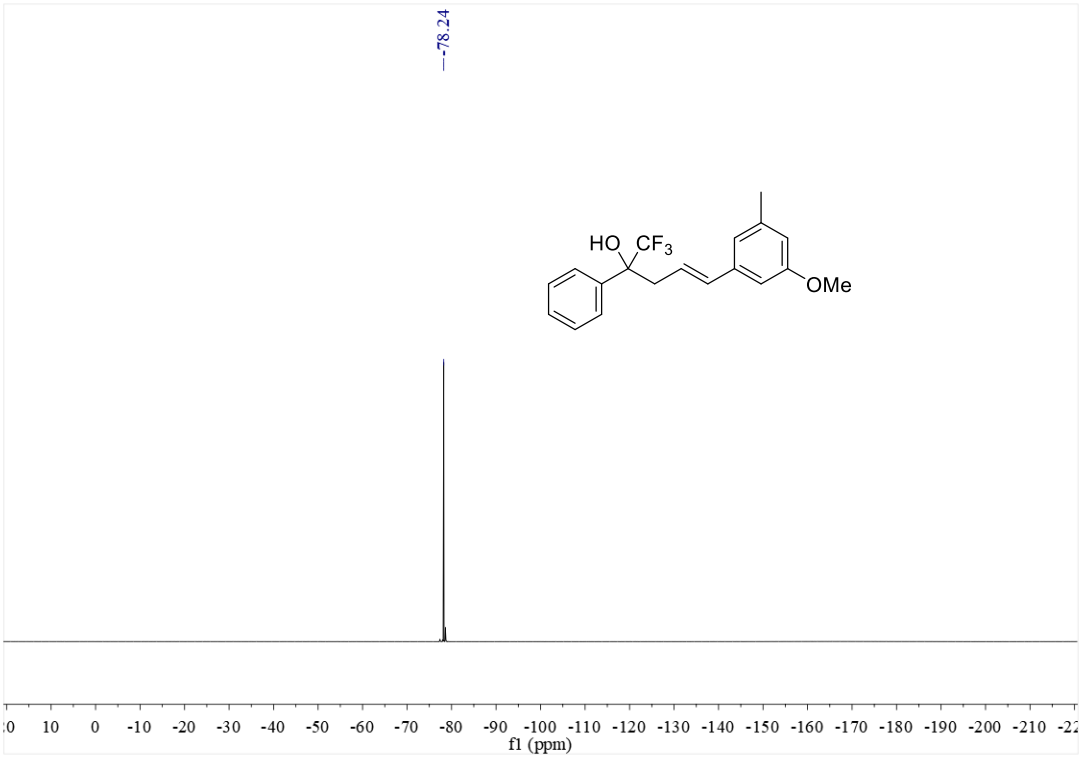
^{1}H NMR of 3r



^{13}C NMR of 3r

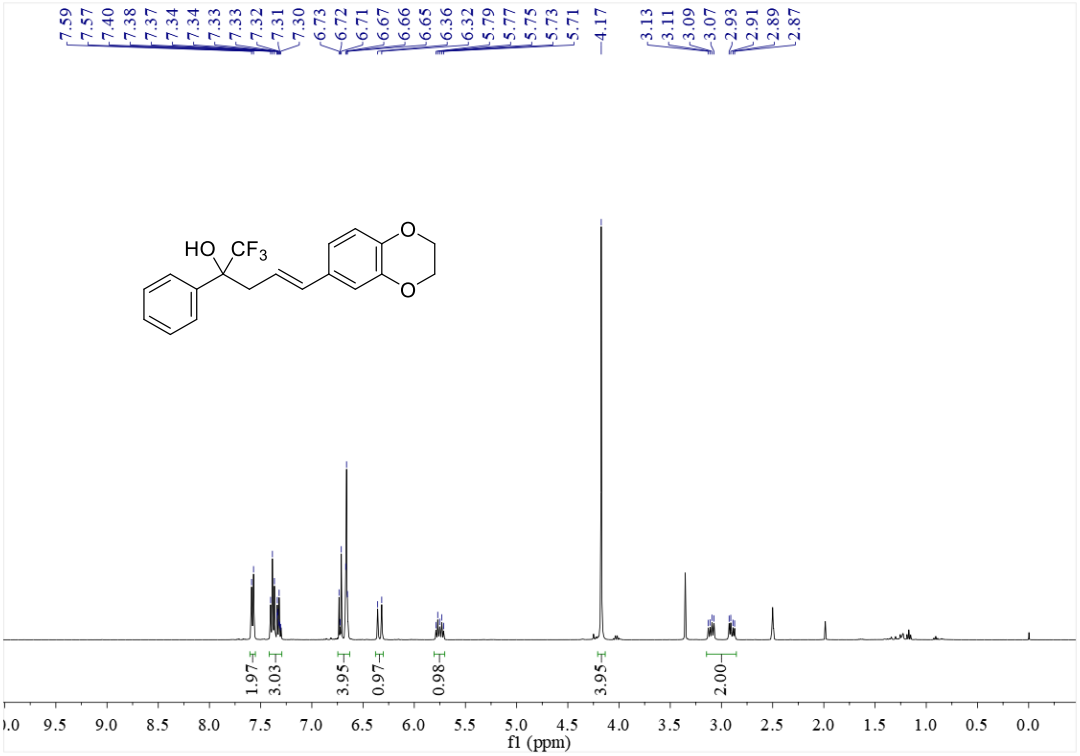


^{19}F NMR of 3r

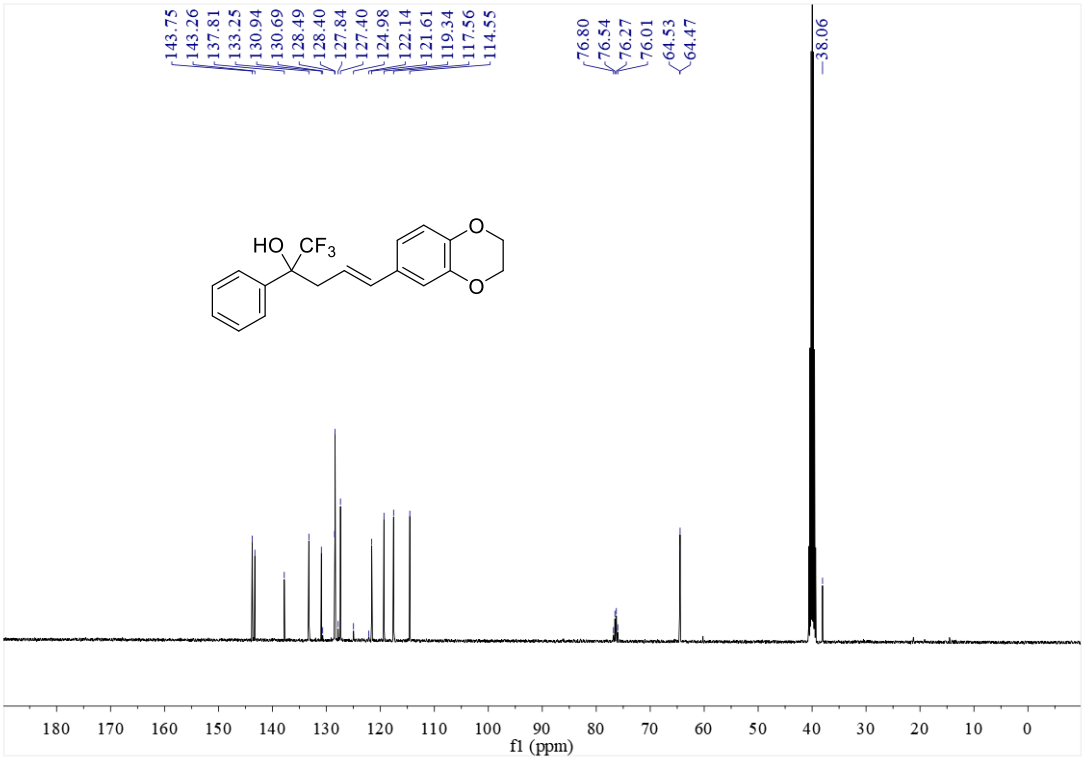


(*E*)-5-(2,3-Dihydrobenzo[*b*][1,4]dioxin-6-yl)-1,1,1-trifluoro-2-phenylpent-4-en-2-ol (3s)

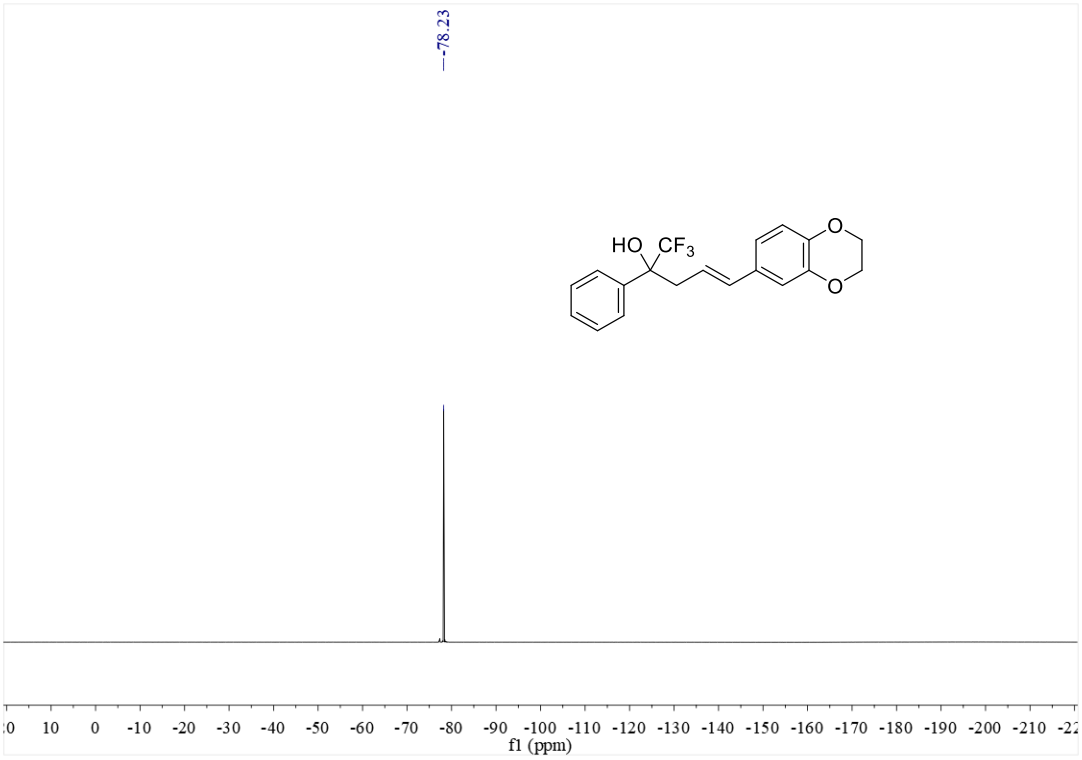
^{1}H NMR of 3s



^{13}C NMR of 3s

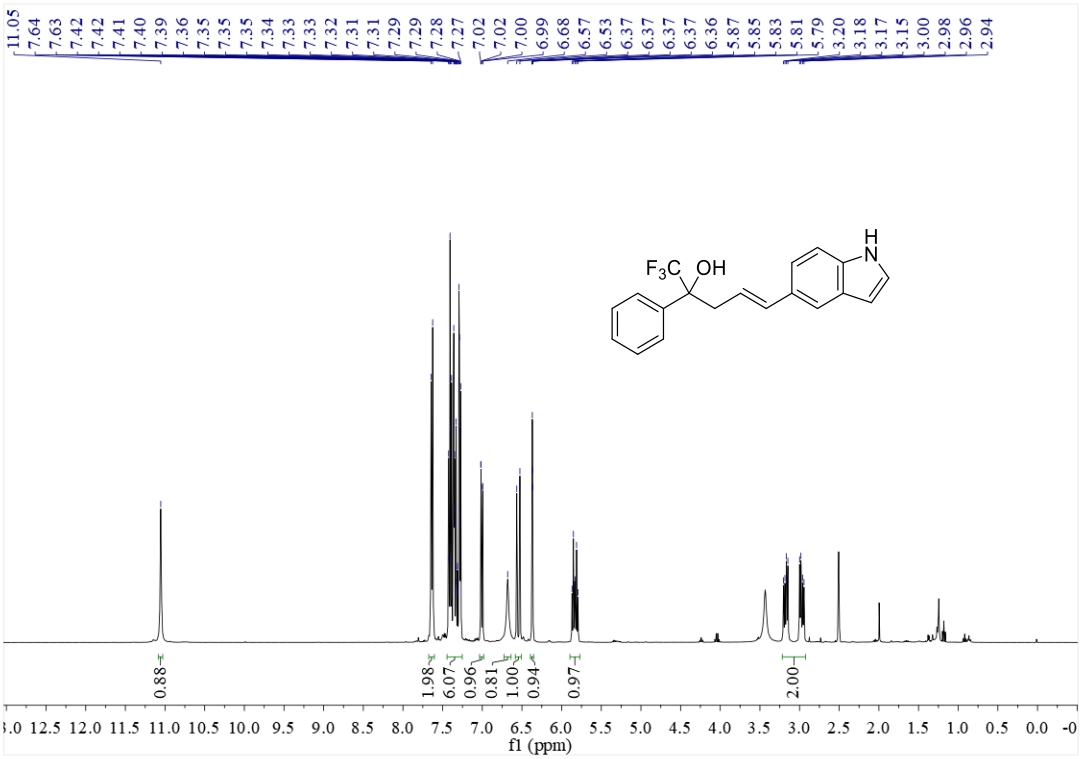


^{19}F NMR of 3s

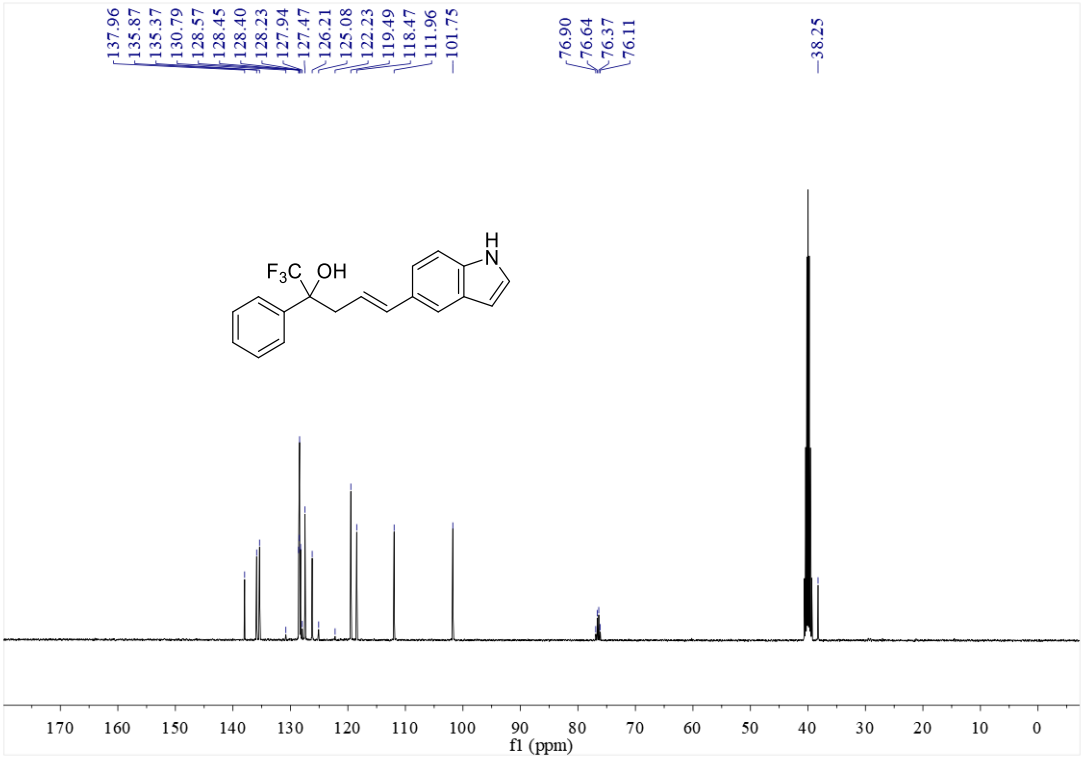


(*E*)-1,1,1-Trifluoro-5-(1*H*-indol-5-yl)-2-phenylpent-4-en-2-ol (3t)

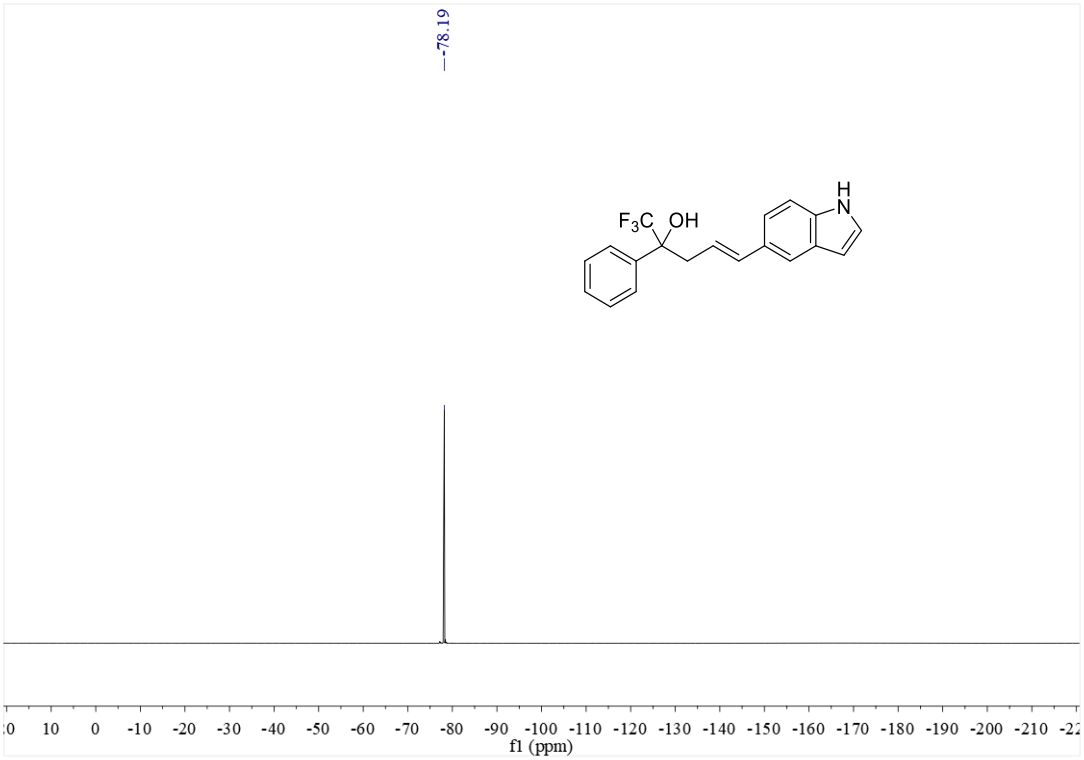
^{1}H NMR of 3t



^{13}C NMR of 3t

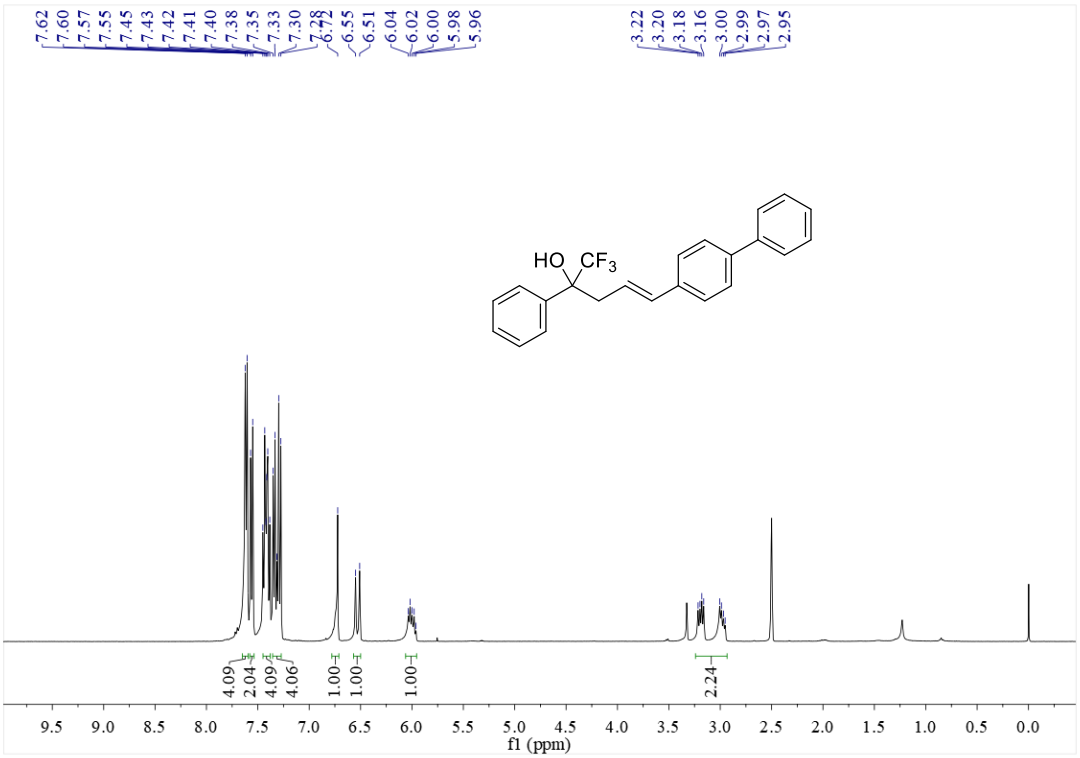


^{19}F NMR of 3t

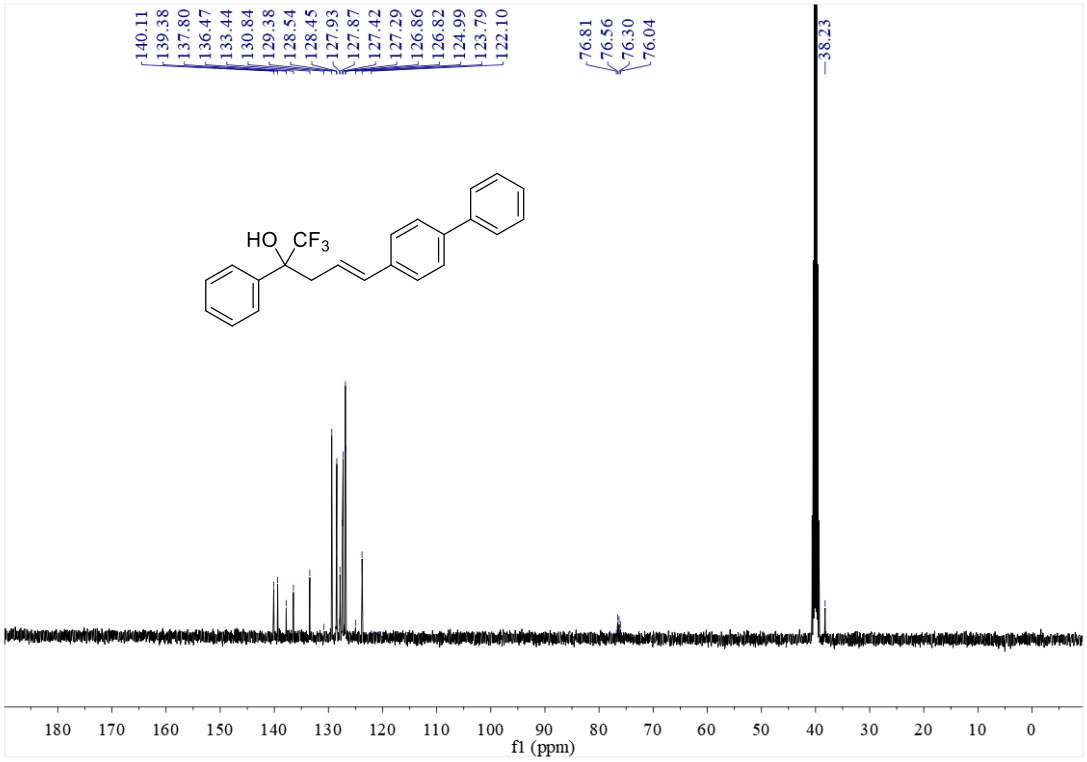


(*E*)-5-([1,1'-Biphenyl]-4-yl)-1,1,1-trifluoro-2-phenylpent-4-en-2-ol (3u)

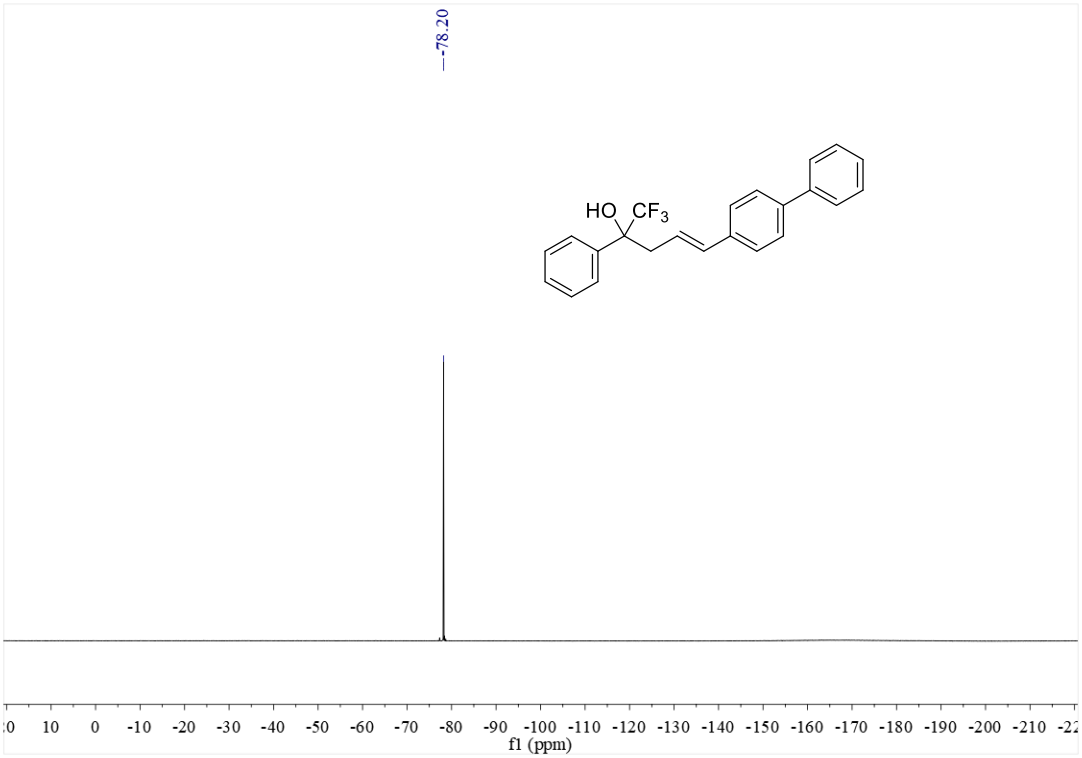
^{1}H NMR of 3u



^{13}C NMR of 3u

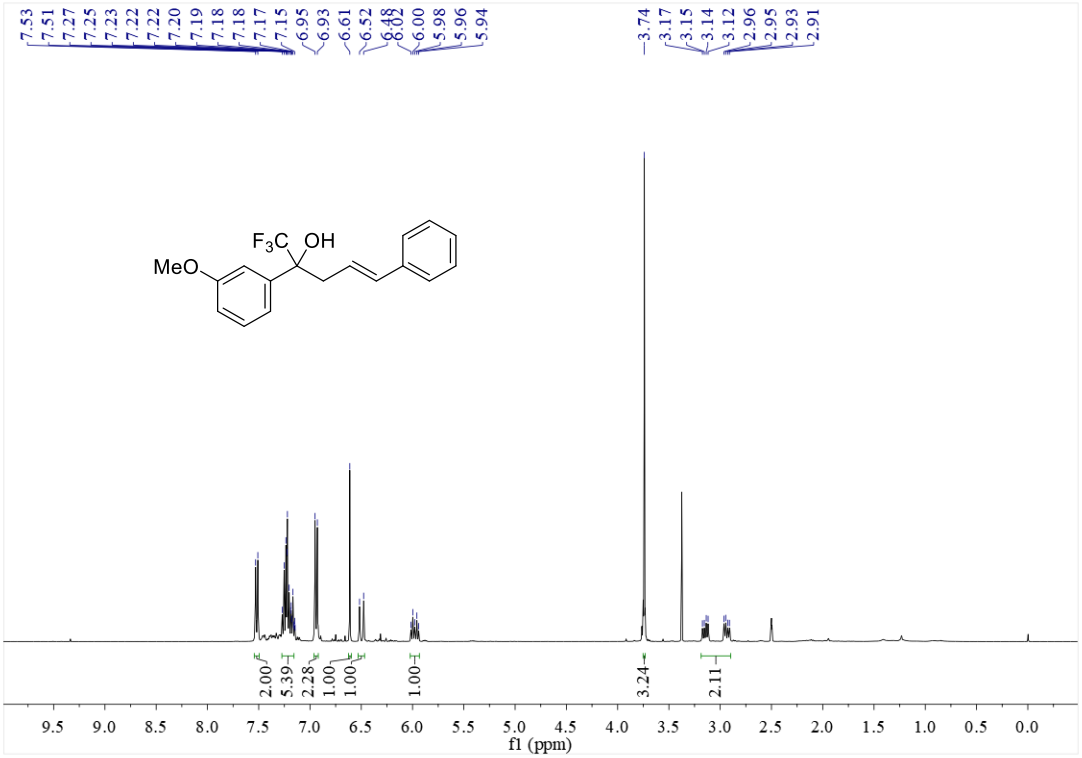


^{19}F NMR of 3u

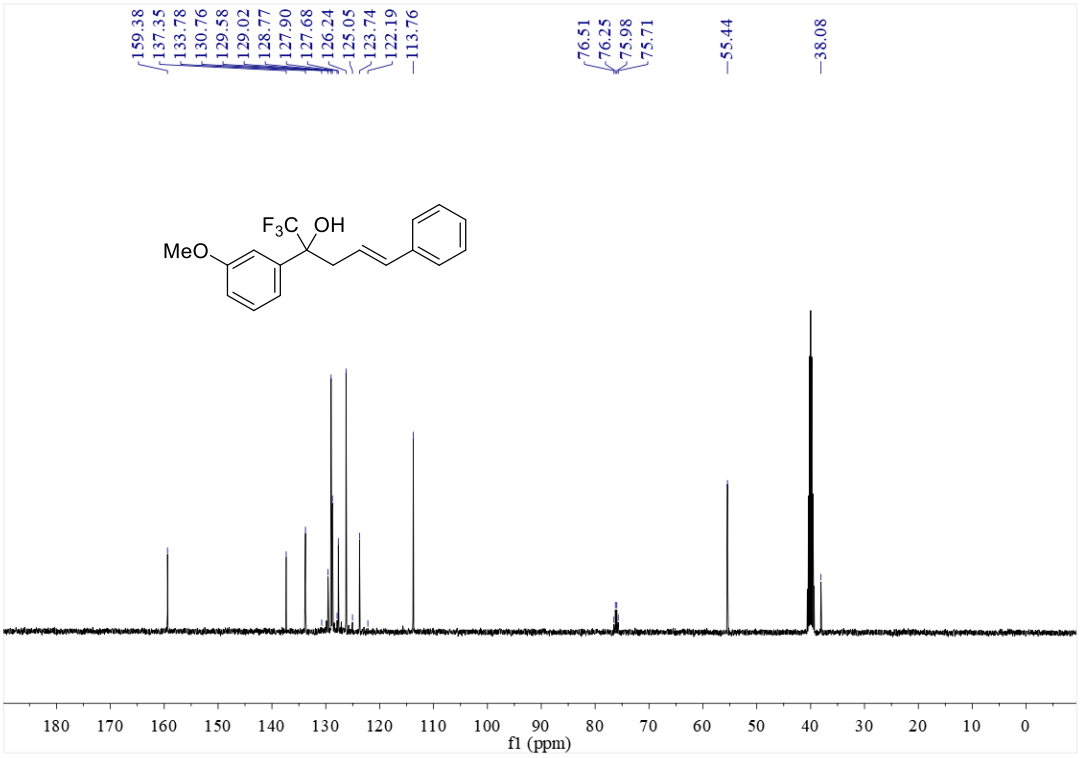


(*E*)-1,1,1-Trifluoro-2-(4-methoxyphenyl)-5-phenylpent-4-en-2-ol (4b)

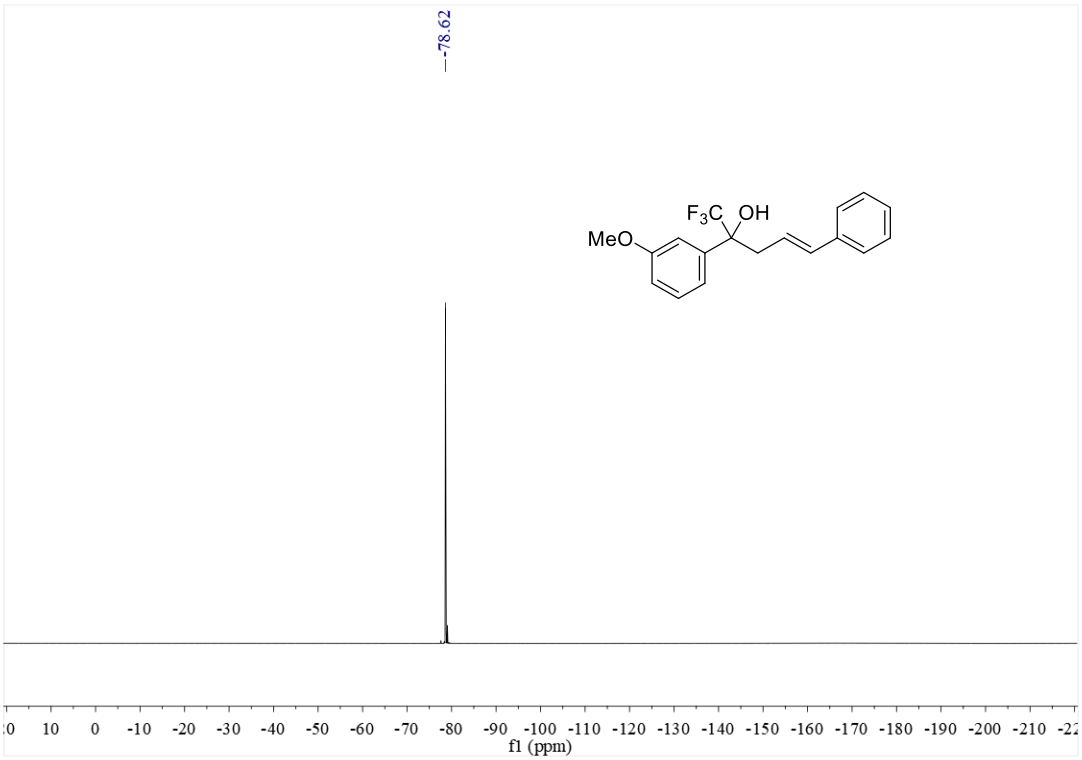
^{1}H NMR of 4b



^{13}C NMR of 4b

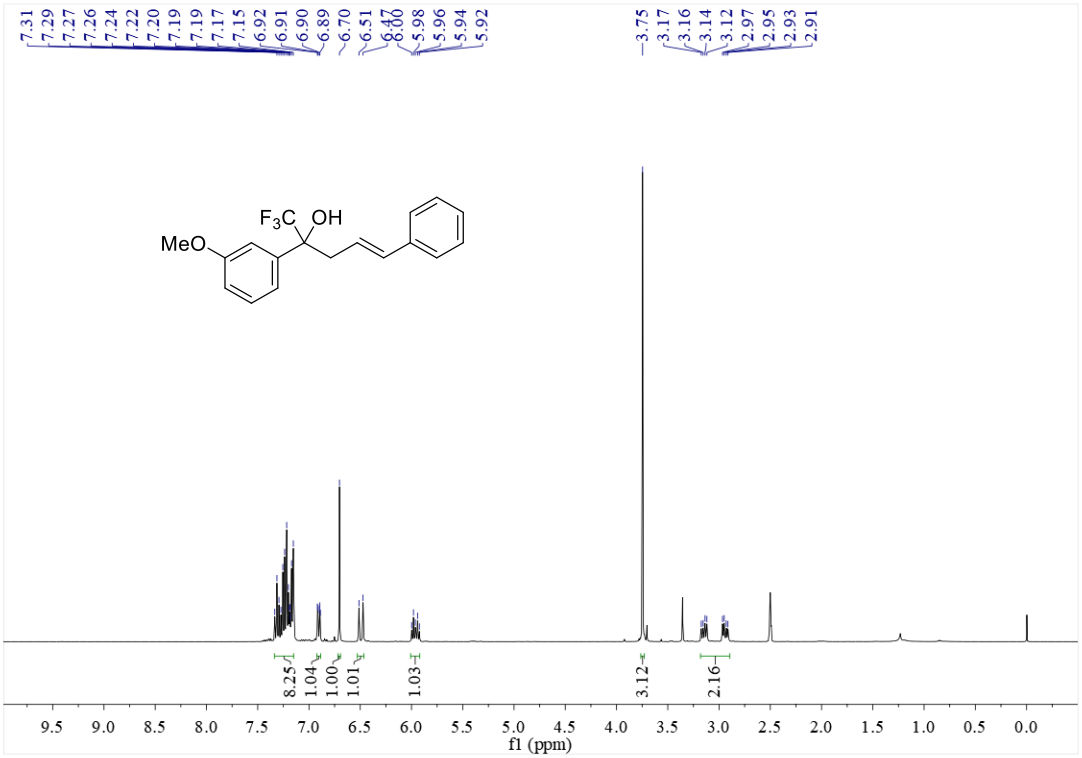


^{19}F NMR of 4b

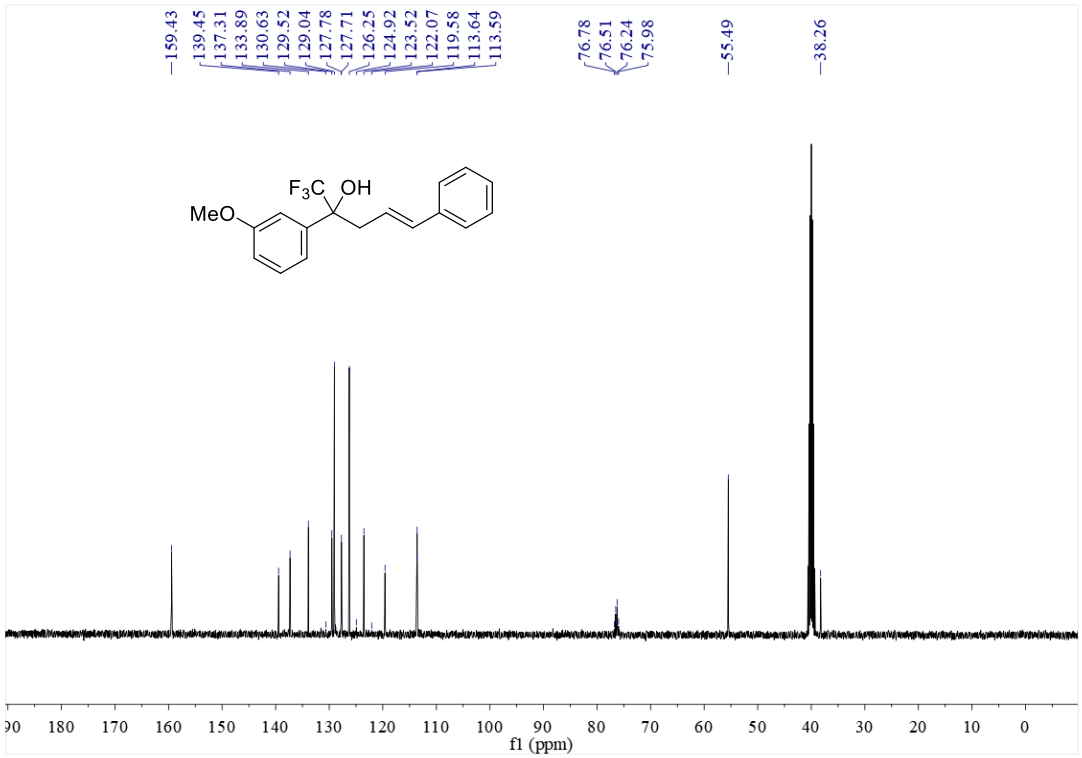


(*E*)-1,1,1-Trifluoro-2-(3-methoxyphenyl)-5-phenylpent-4-en-2-ol (4c)

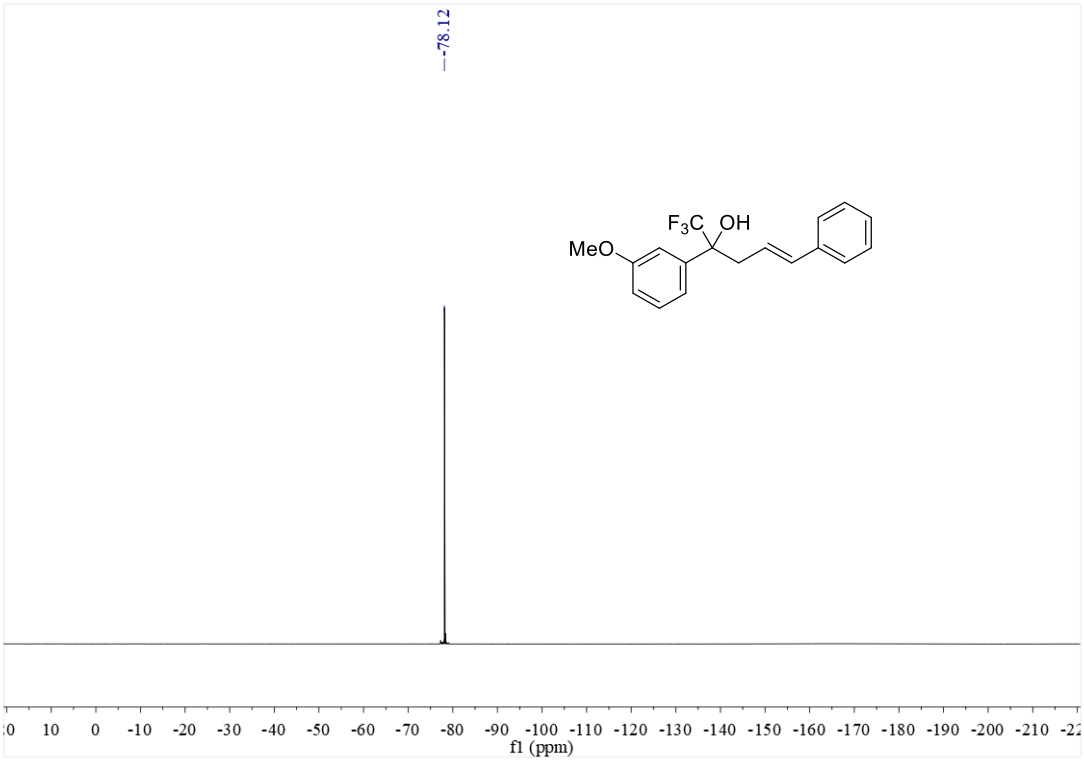
^{1}H NMR of 4c



^{13}C NMR of 4c

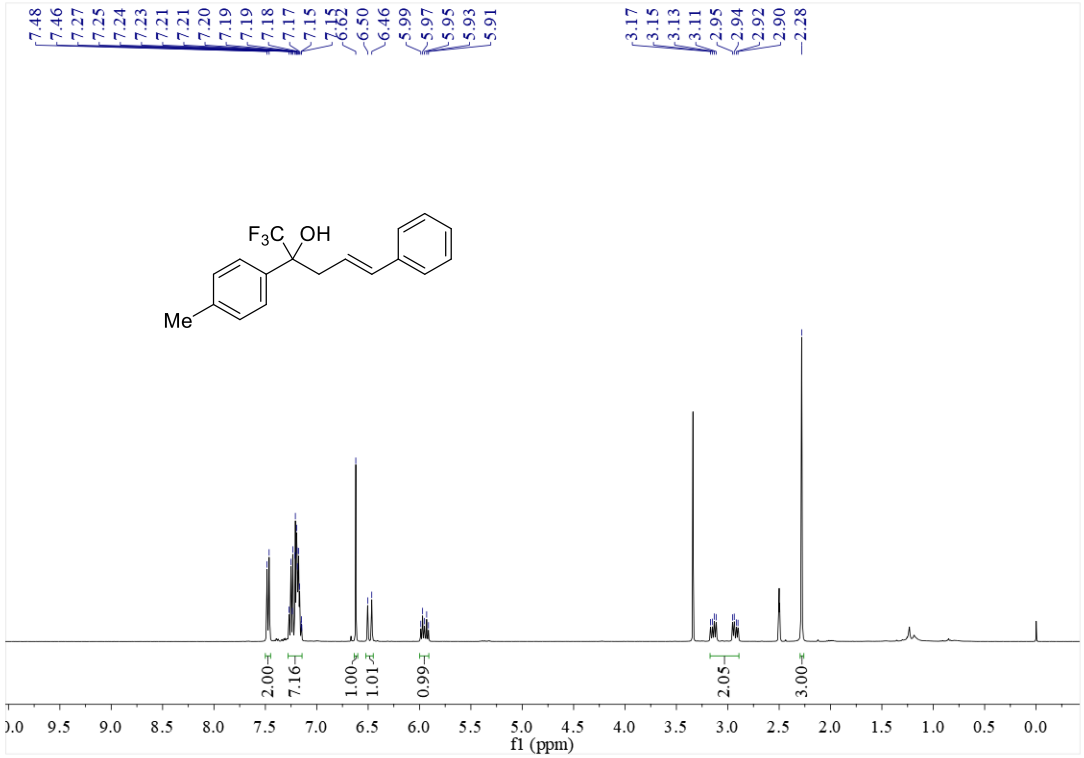


^{19}F NMR of 4c

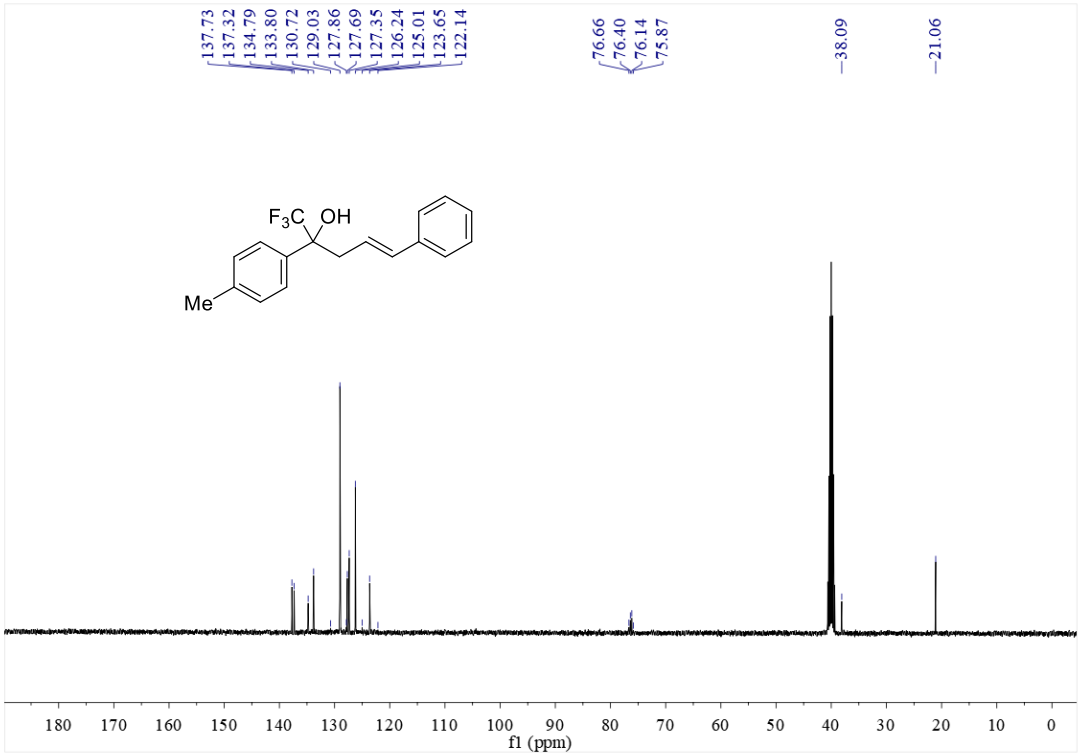


(*E*)-1,1,1-Trifluoro-5-phenyl-2-(p-tolyl)pent-4-en-2-ol (4d)

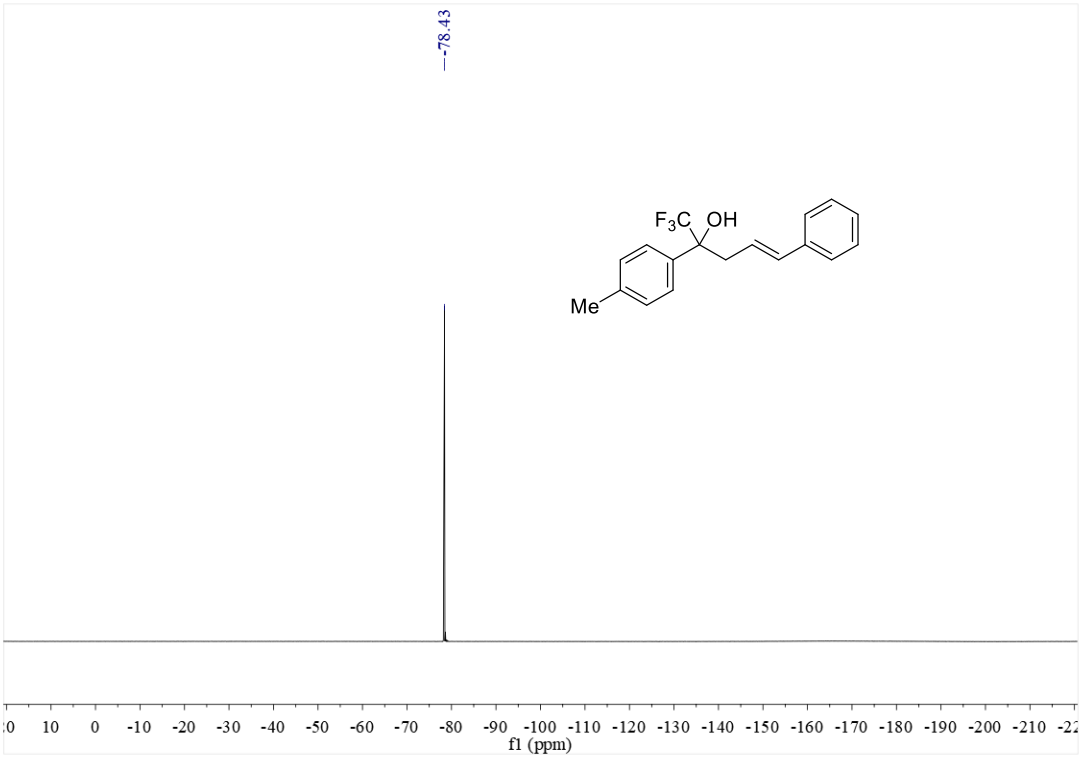
^{1}H NMR of 4d



^{13}C NMR of 4d

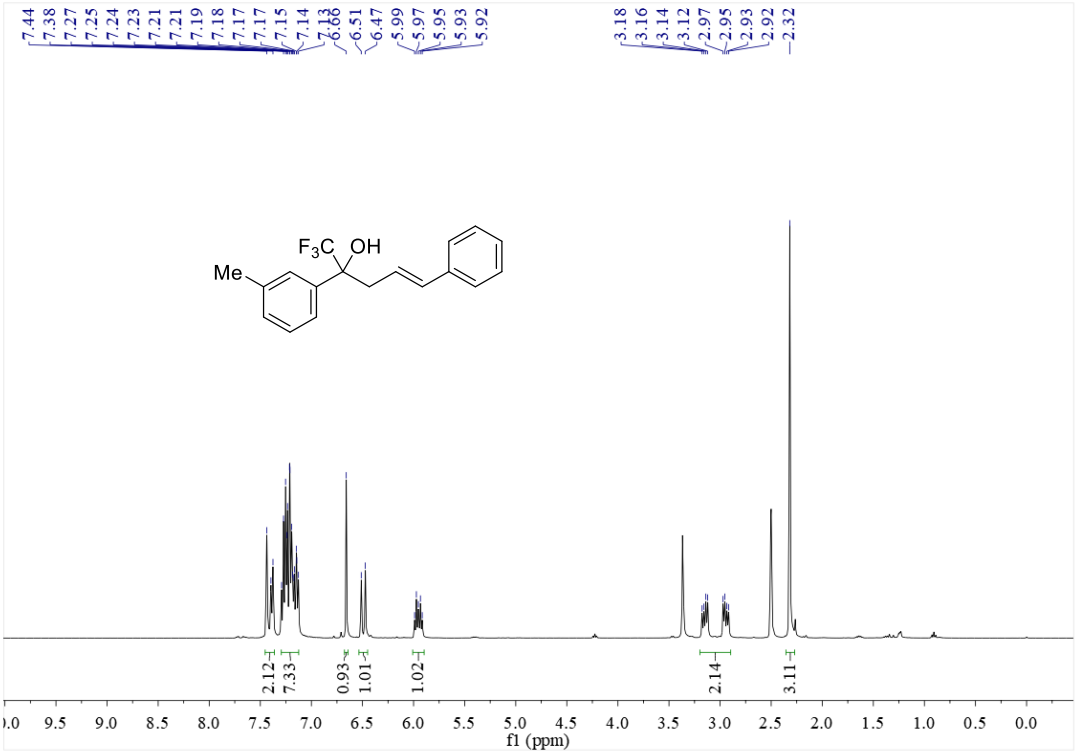


^{19}F NMR of 4d

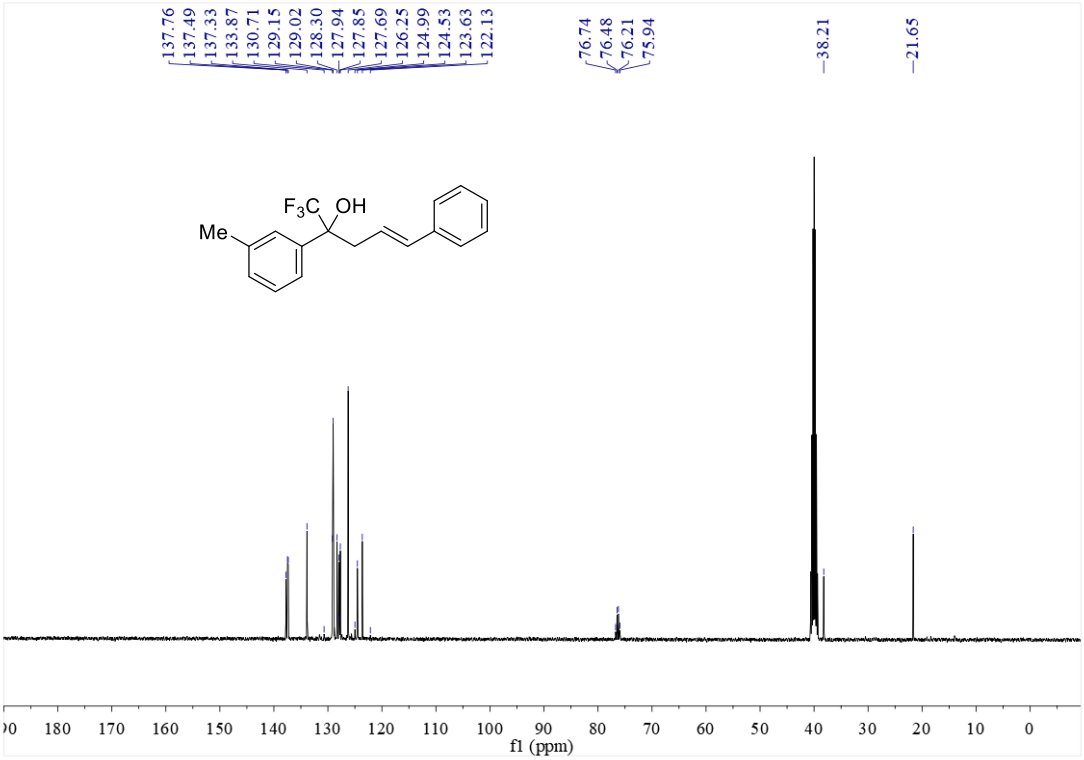


(*E*)-1,1,1-Trifluoro-5-phenyl-2-(m-tolyl)pent-4-en-2-ol (4e)

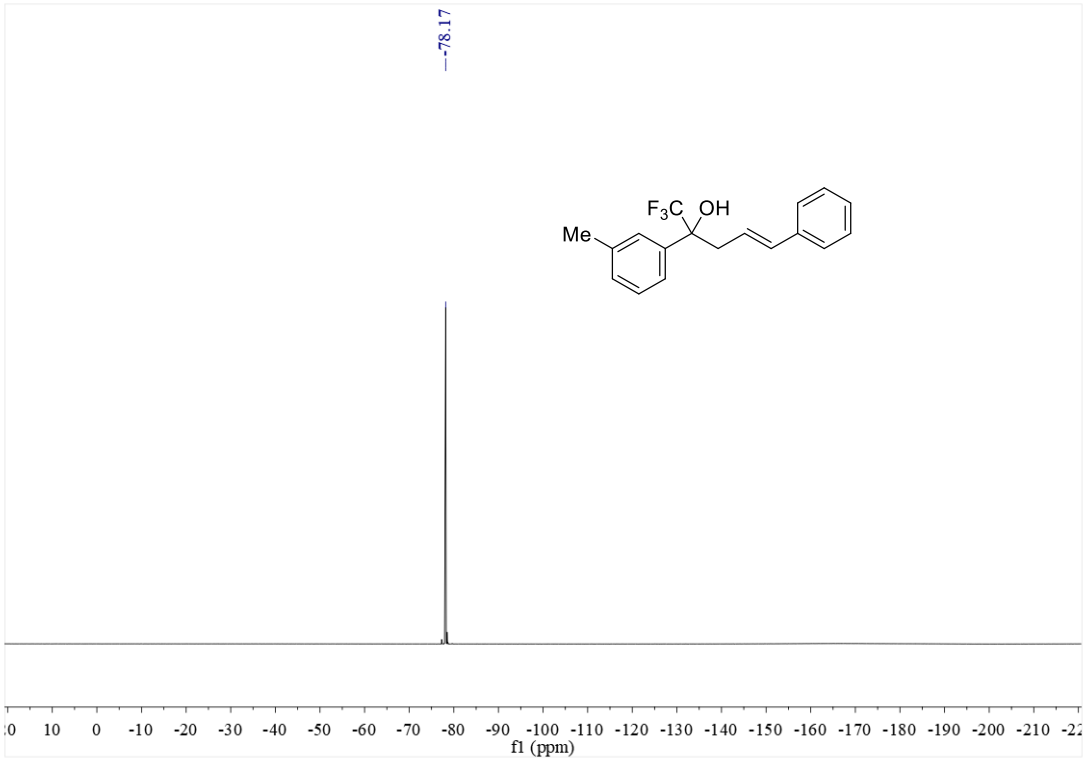
^{1}H NMR of 4e



^{13}C NMR of 4e

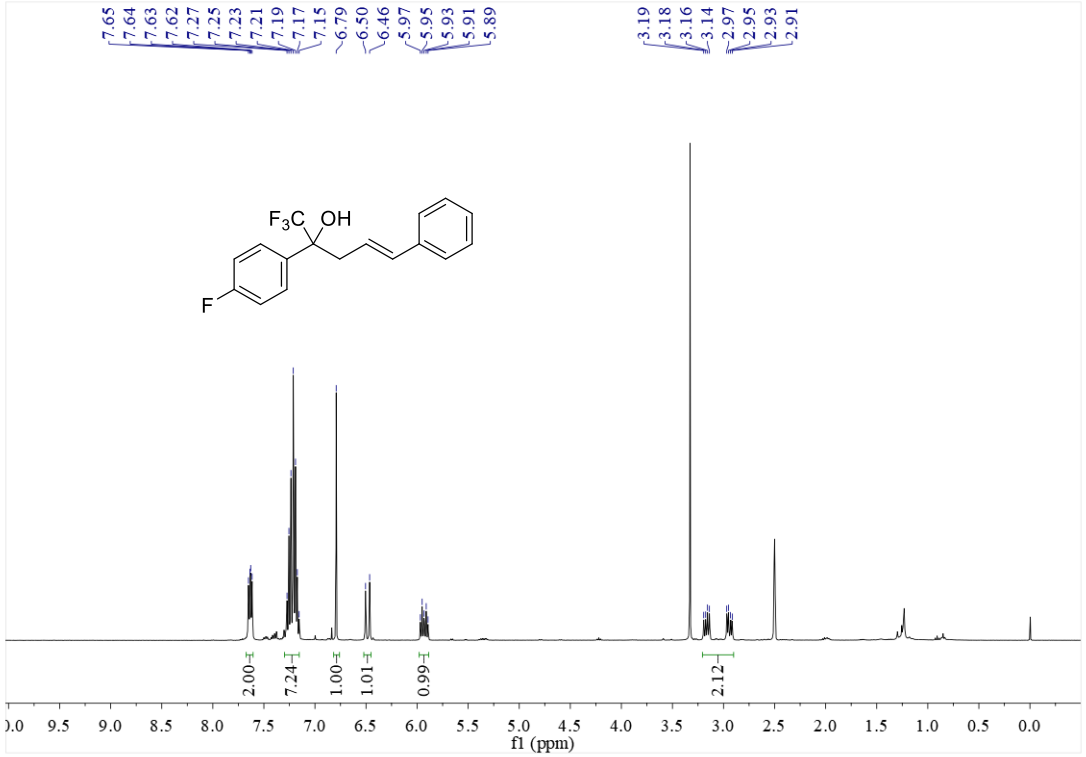


^{19}F NMR of 4e

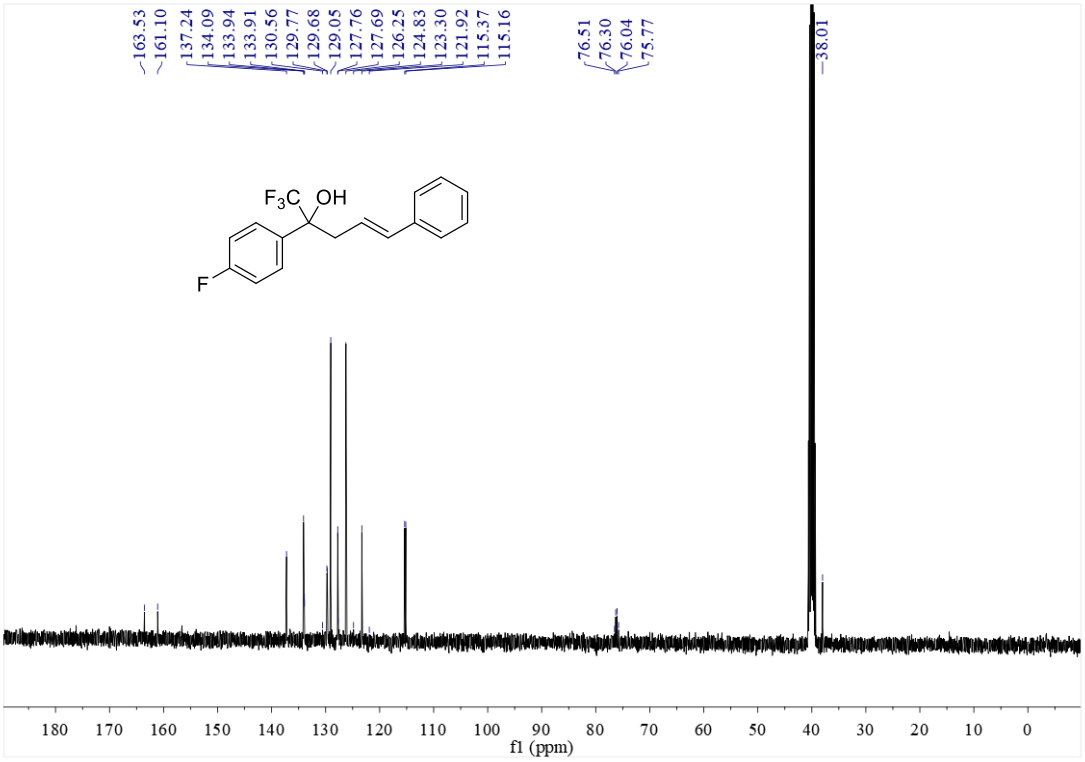


(*E*)-1,1,1-Trifluoro-2-(4-fluorophenyl)-5-phenylpent-4-en-2-ol (4f)

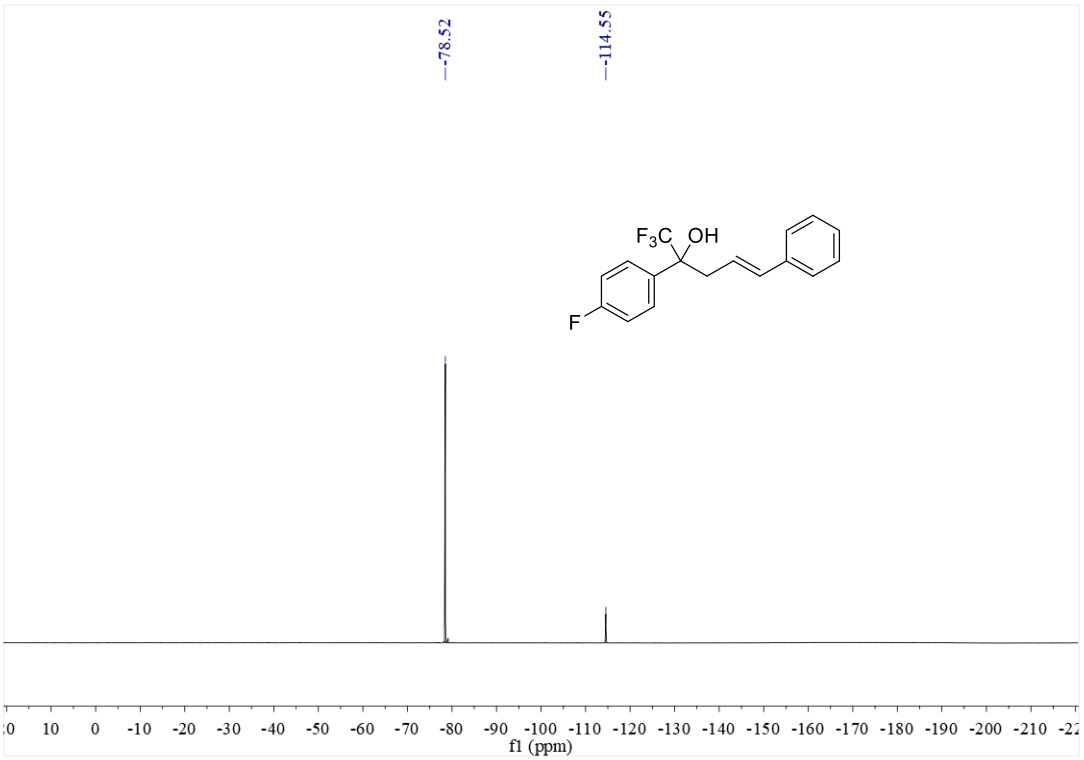
^{1}H NMR of 4f



^{13}C NMR of 4f

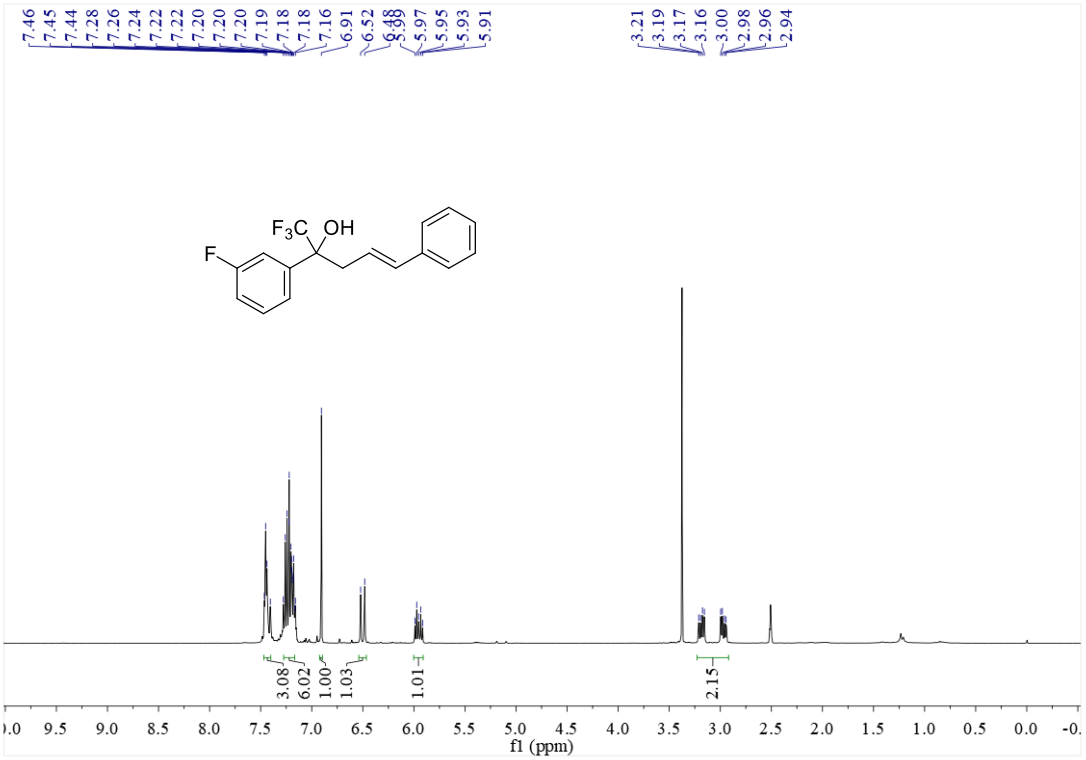


^{19}F NMR of 4f

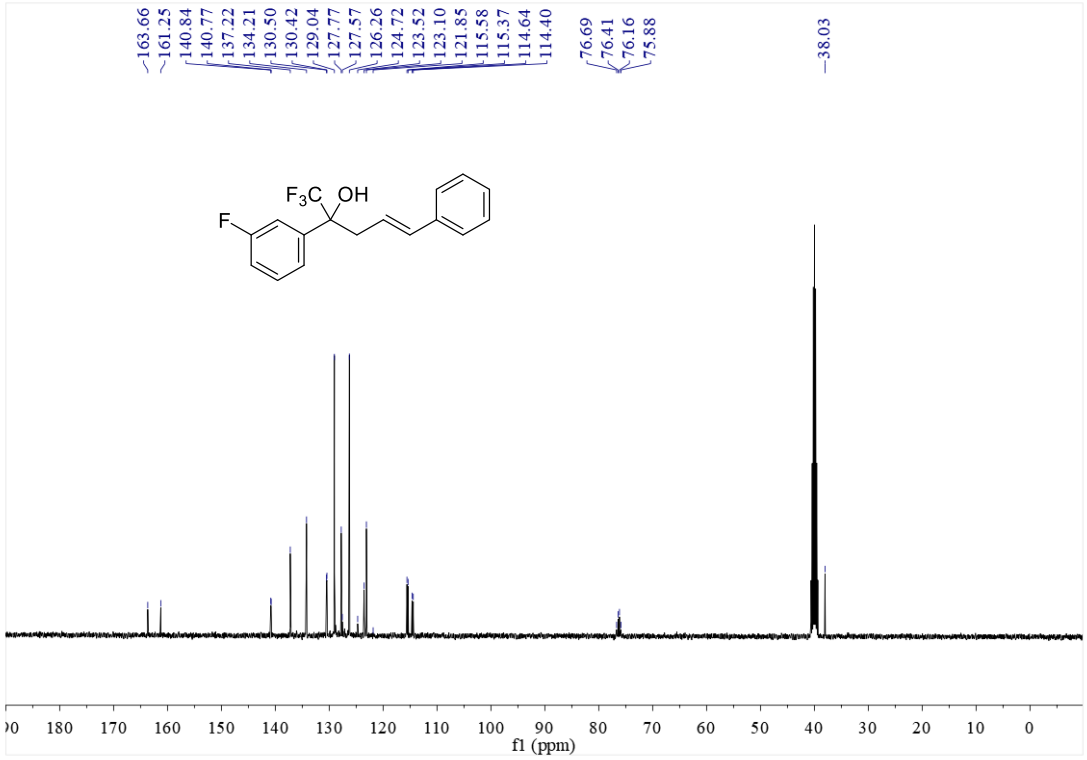


(*E*)-1,1,1-Trifluoro-2-(3-fluorophenyl)-5-phenylpent-4-en-2-ol (4g)

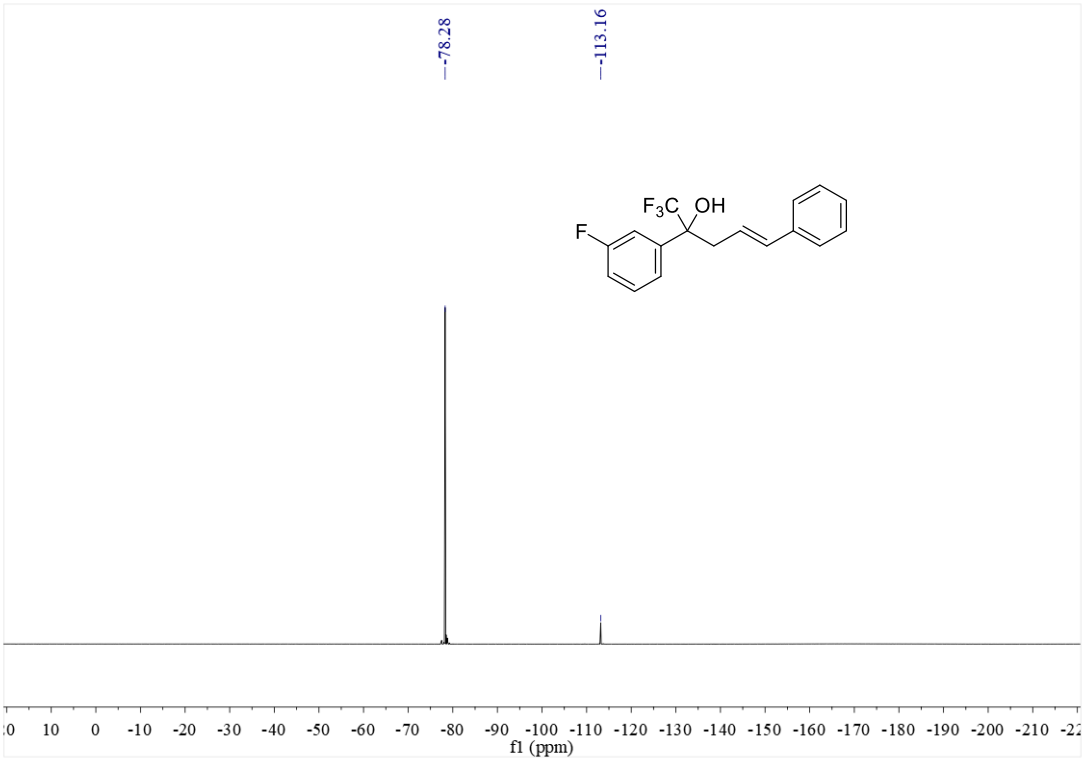
^{1}H NMR of 4g



^{13}C NMR of 4g

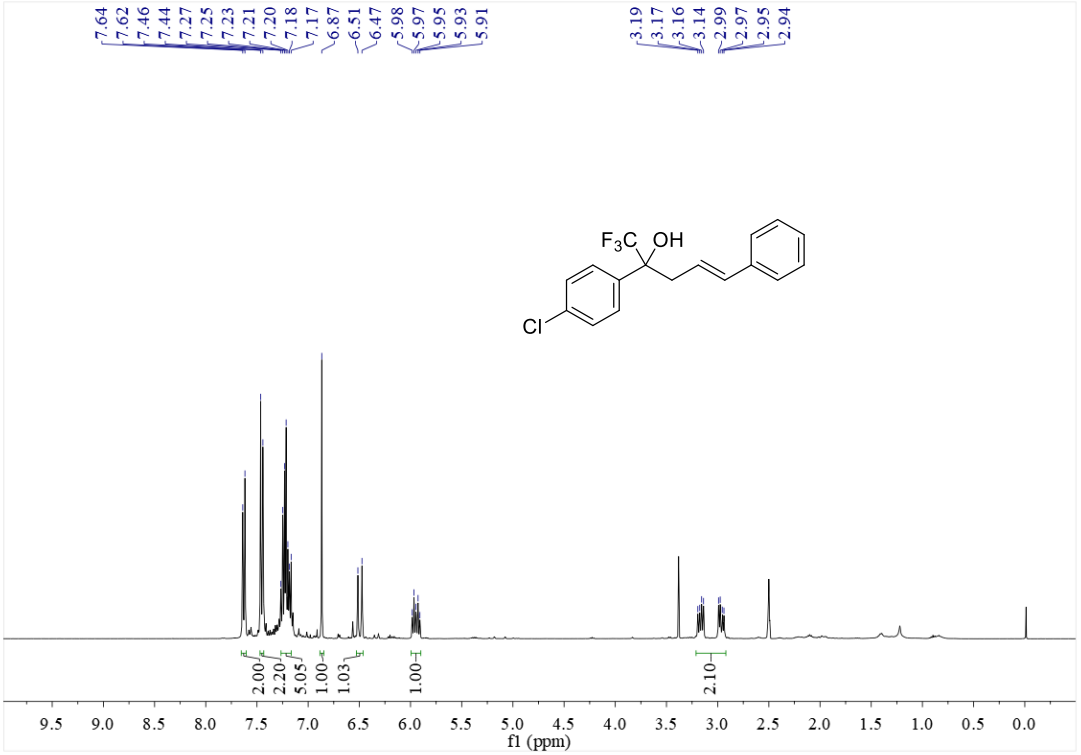


^{19}F NMR of 4g

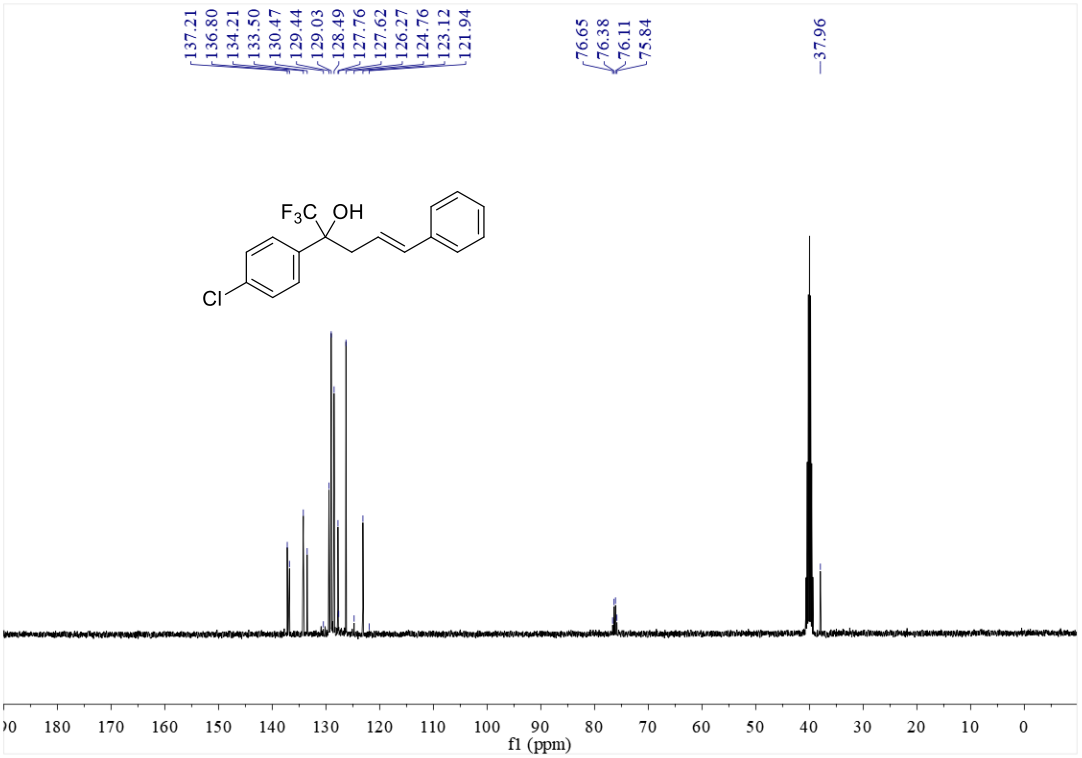


(*E*)-2-(4-Chlorophenyl)-1,1,1-trifluoro-5-phenylpent-4-en-2-ol (4h)

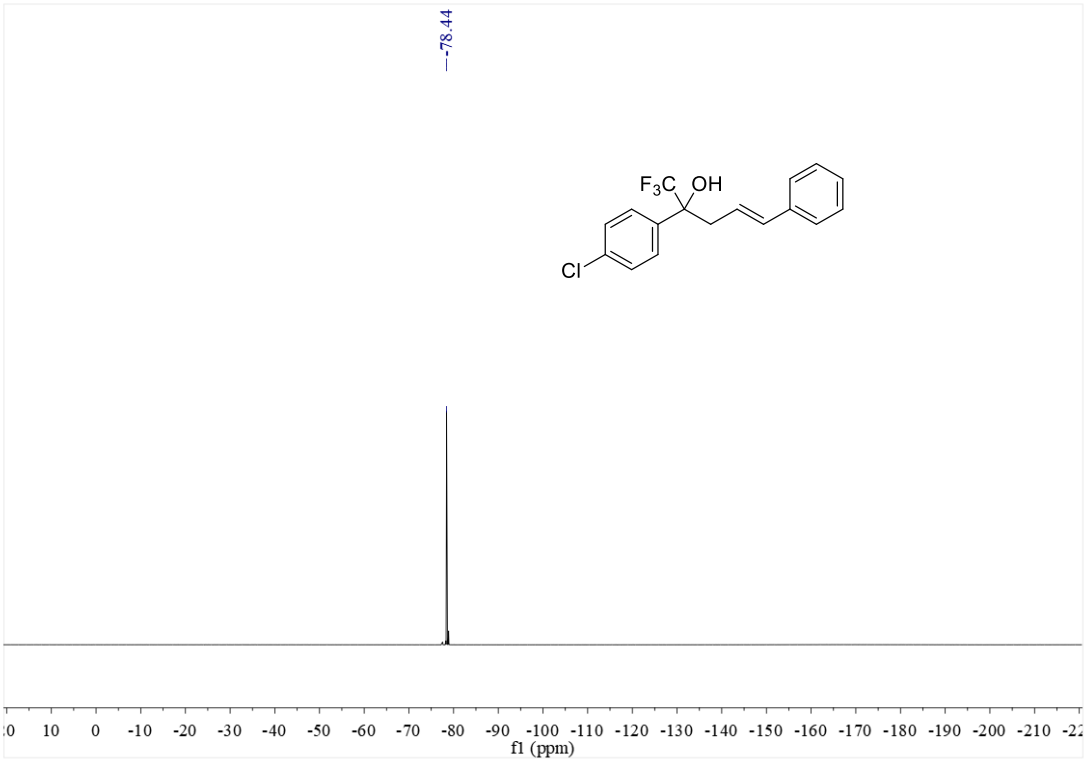
^{1}H NMR of 4h



^{13}C NMR of 4h

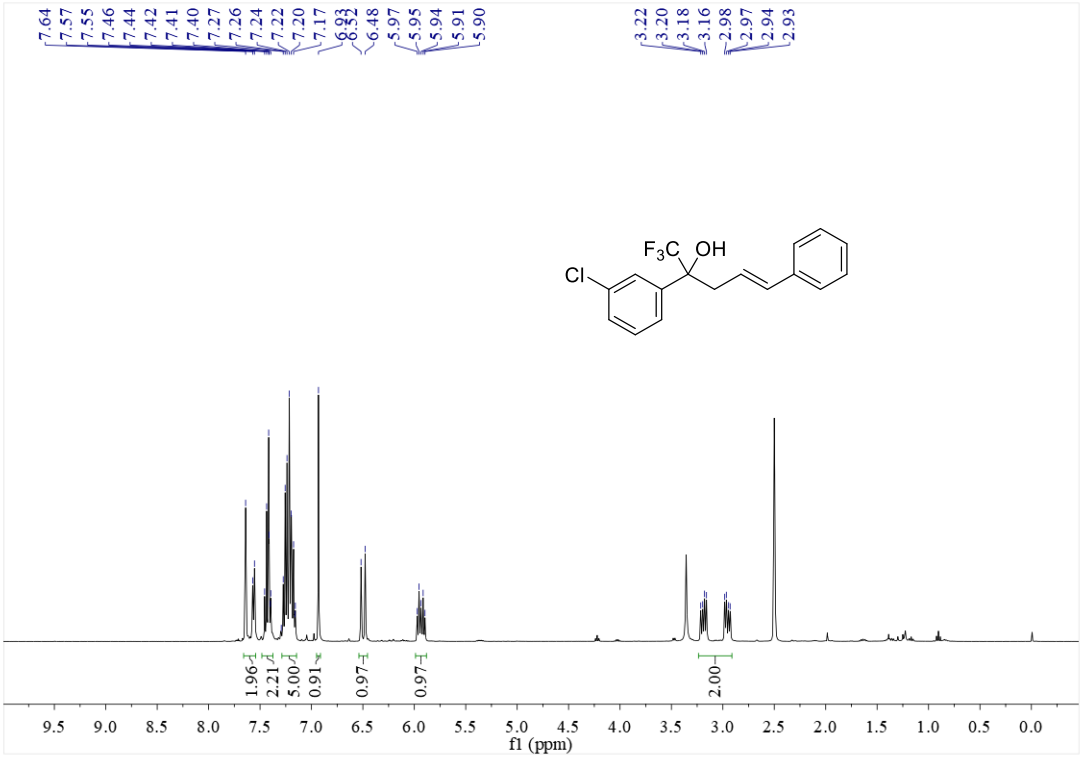


^{19}F NMR of 4h

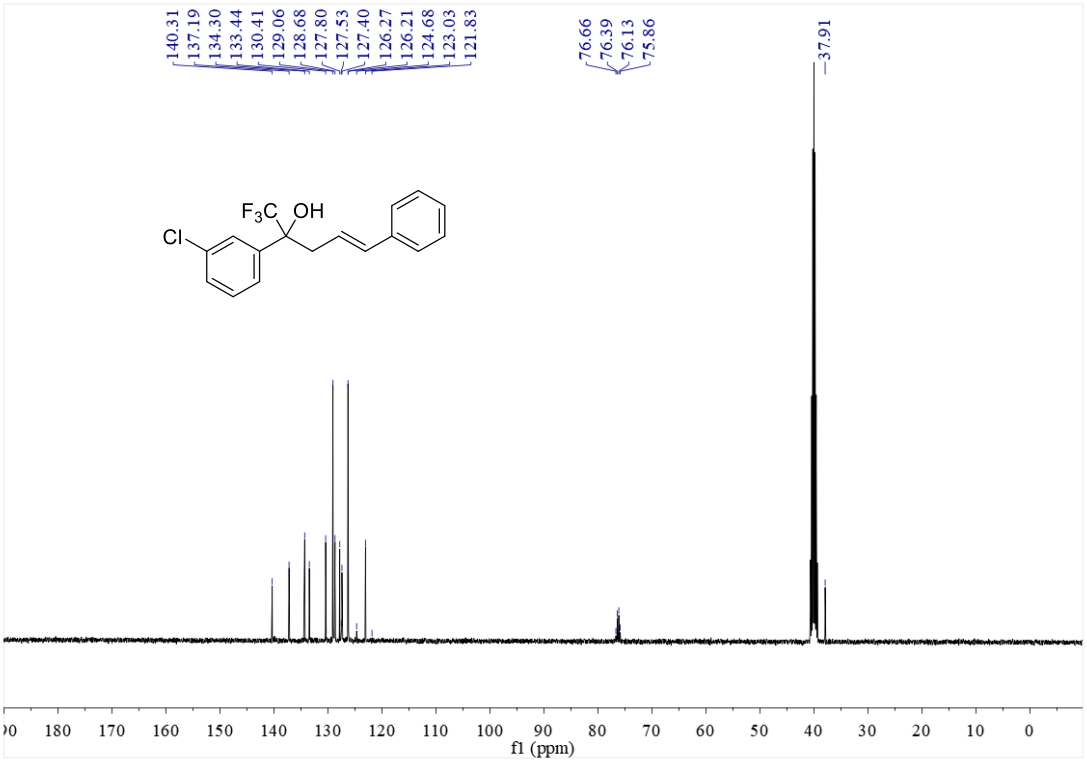


(*E*)-2-(3-Chlorophenyl)-1,1,1-trifluoro-5-phenylpent-4-en-2-ol (4i)

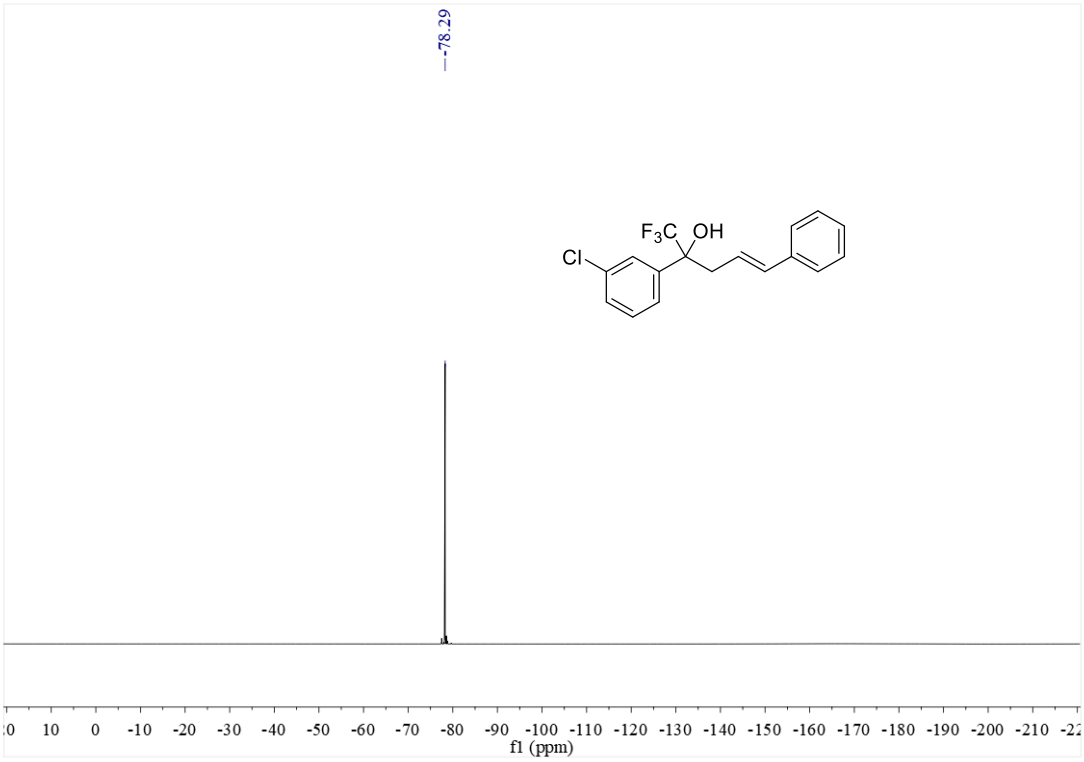
^{1}H NMR of 4i



^{13}C NMR of 4i

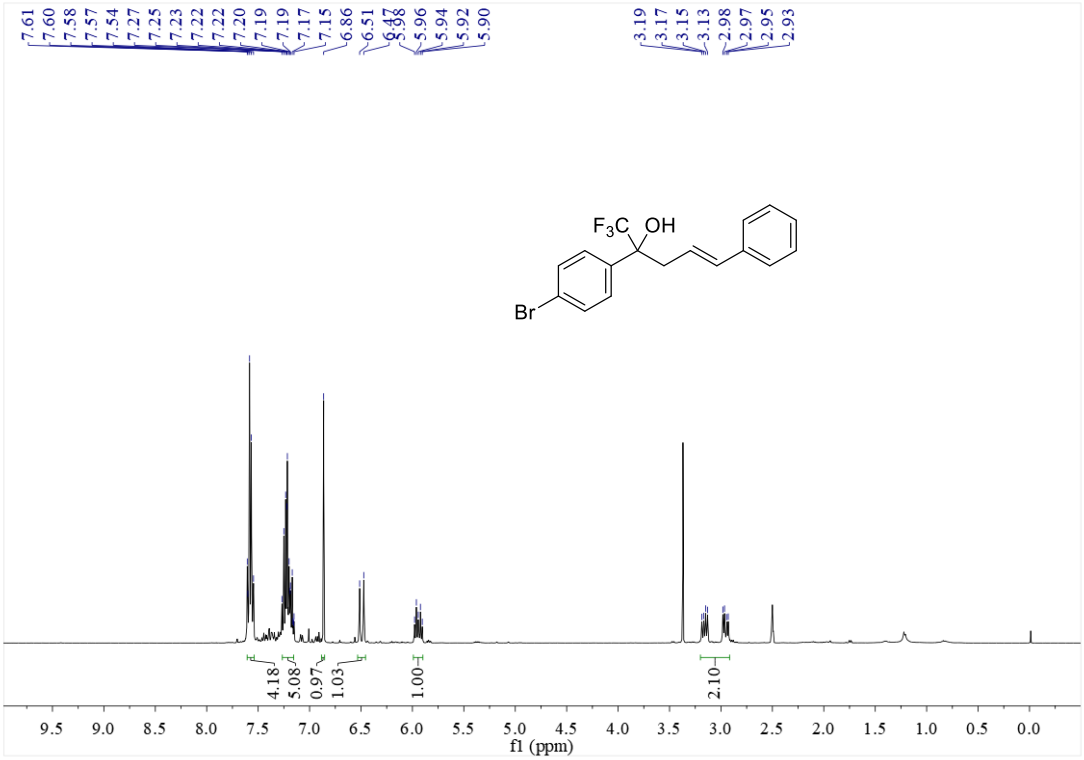


^{19}F NMR of 4i

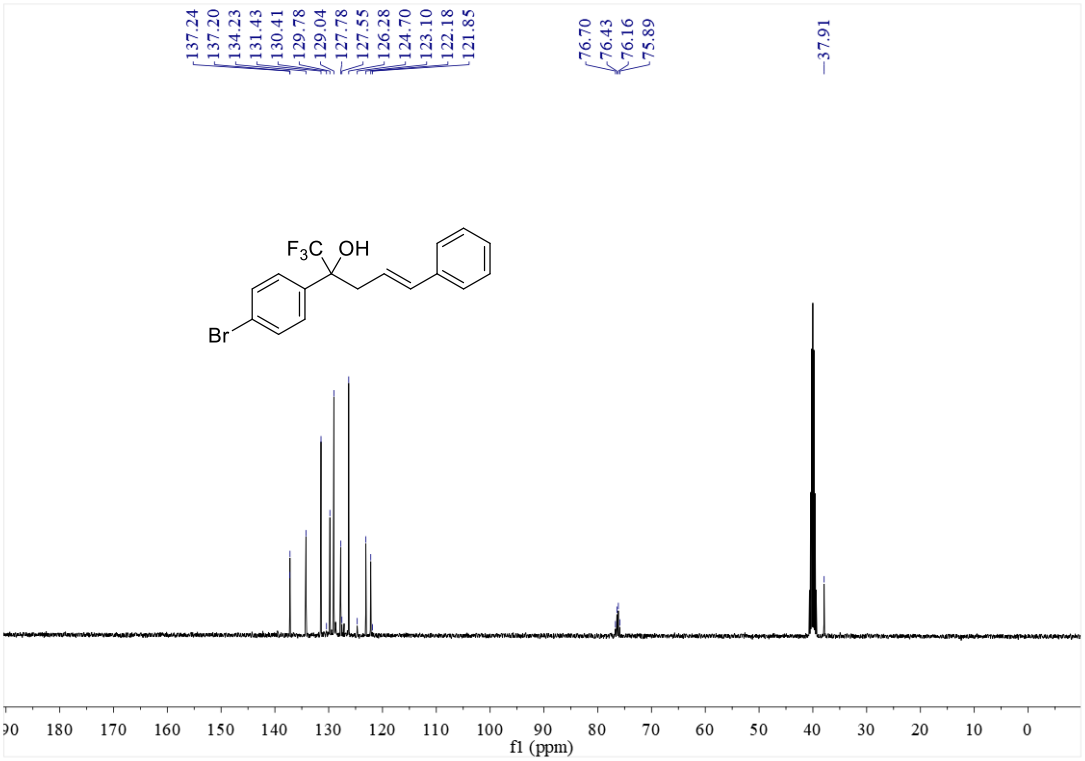


(*E*)-2-(4-Bromophenyl)-1,1,1-trifluoro-5-phenylpent-4-en-2-ol (4j)

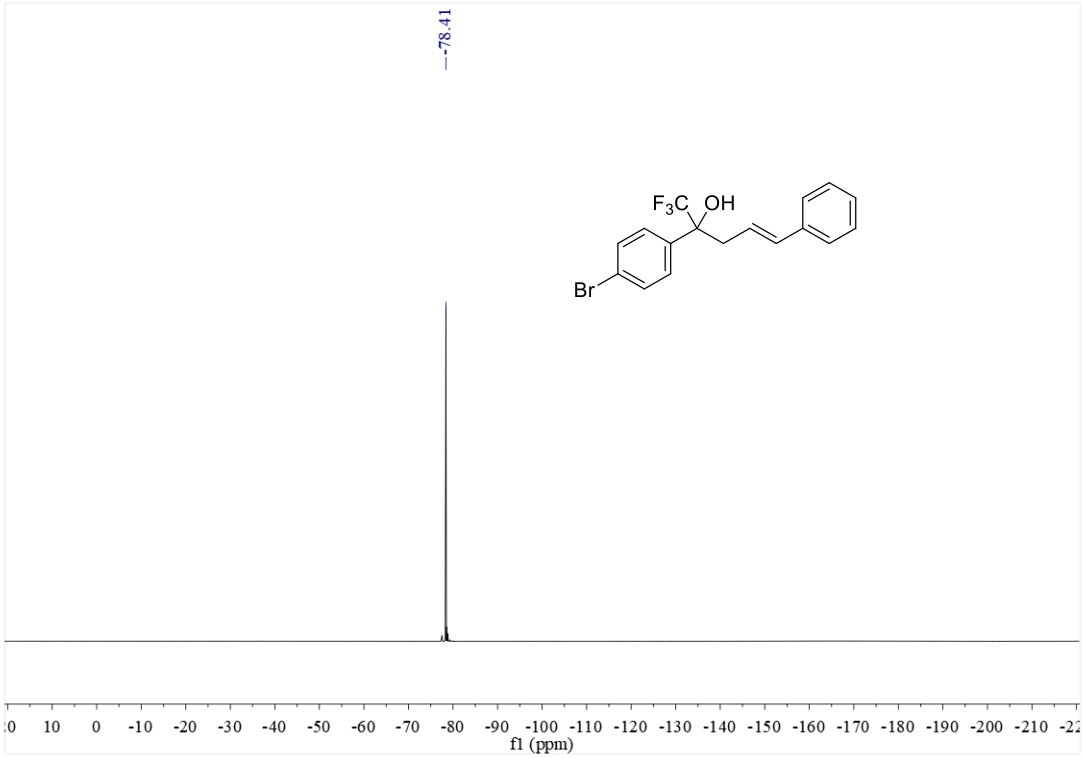
^{1}H NMR of 4j



^{13}C NMR of 4j

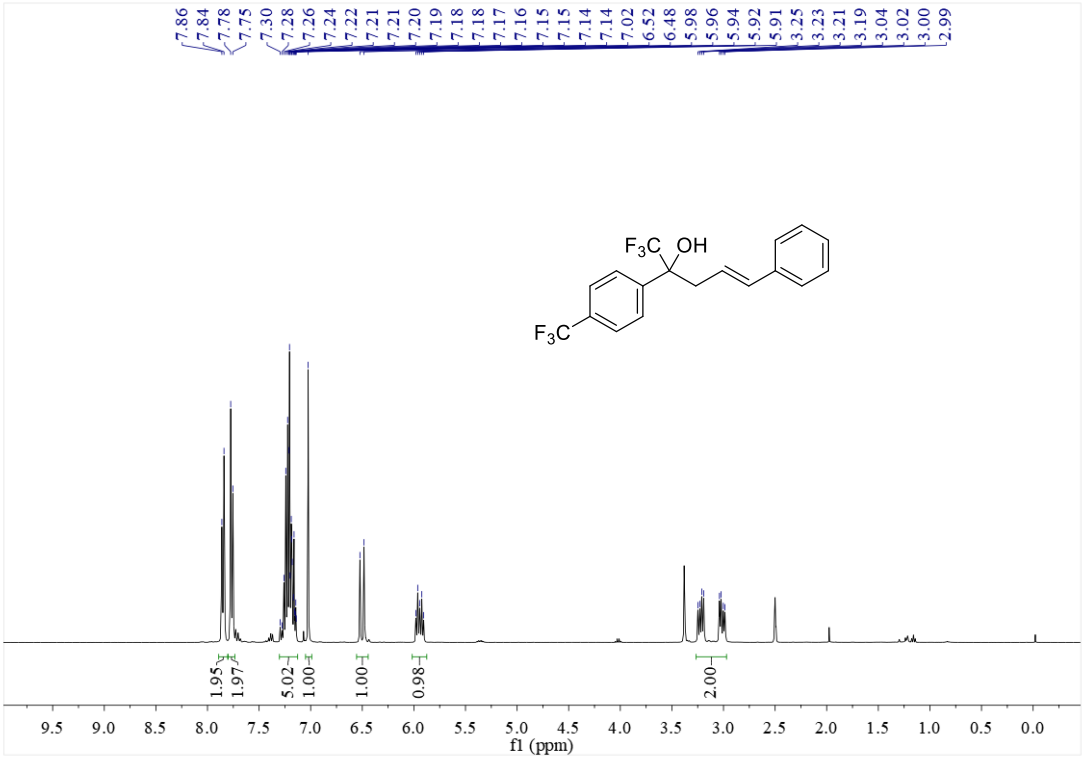


^{19}F NMR of 4j

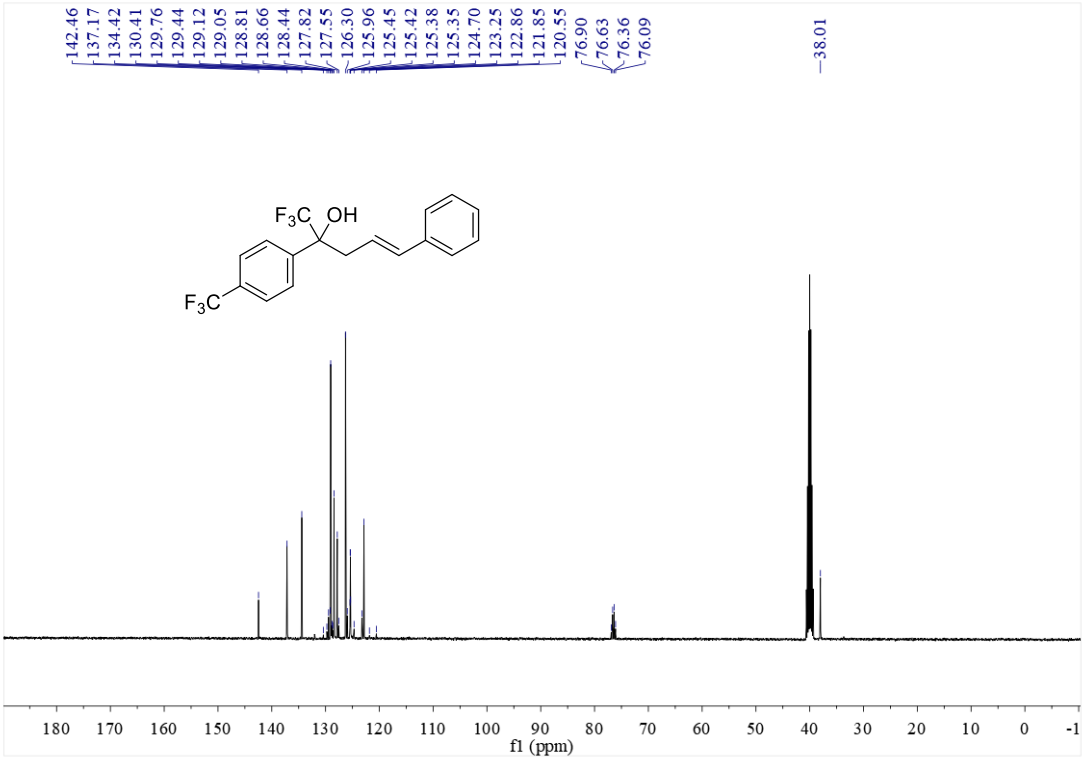


(*E*)-1,1,1-Trifluoro-5-phenyl-2-(4-(trifluoromethyl)phenyl)pent-4-en-2-ol (4k)

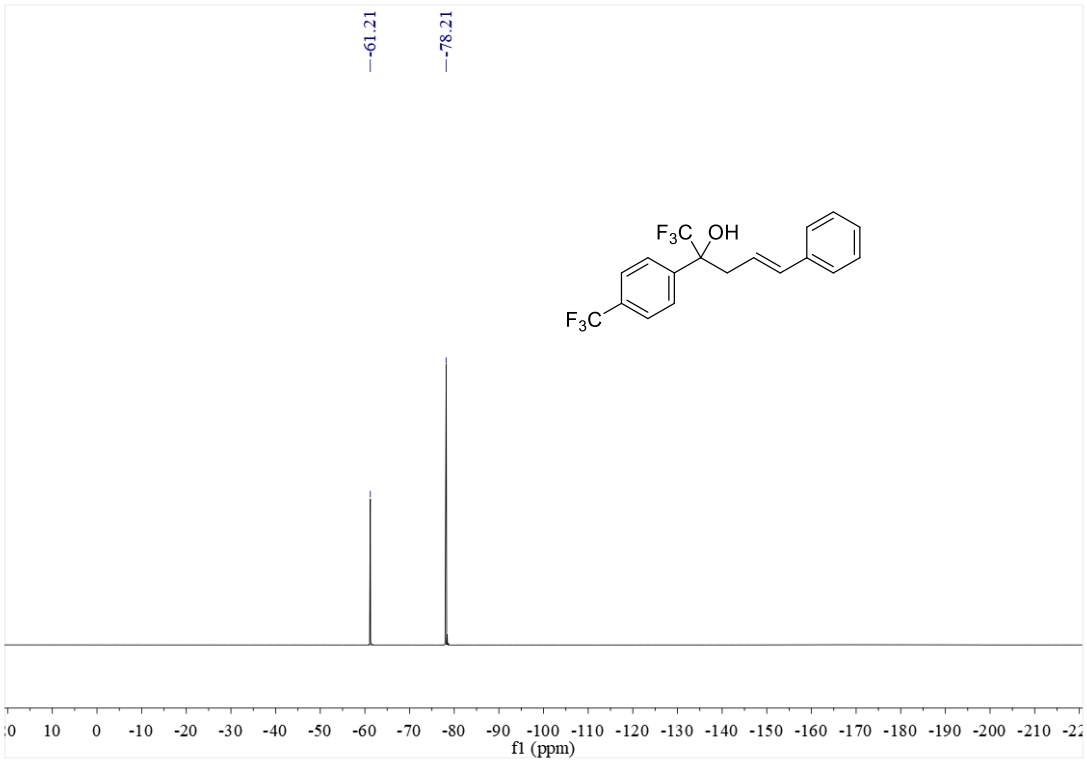
^{1}H NMR of 4k



^{13}C NMR of 4k

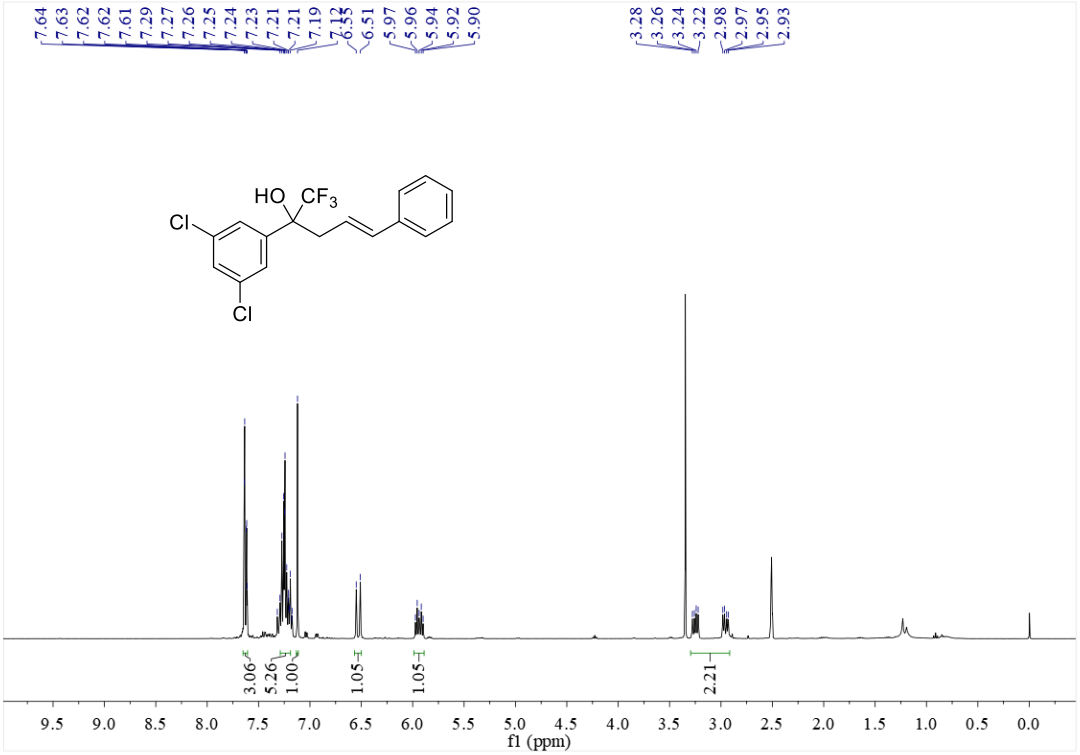


^{19}F NMR of 4k

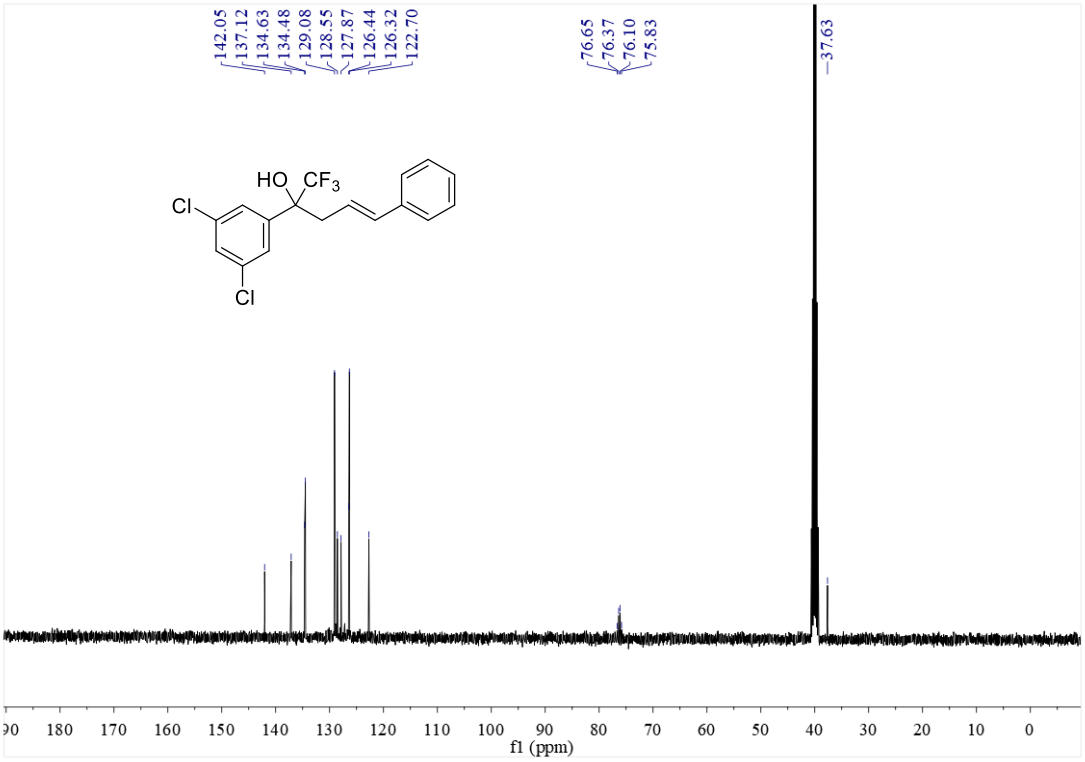


(*E*)-2-(3,5-Dichlorophenyl)-1,1,1-trifluoro-5-phenylpent-4-en-2-ol (4l)

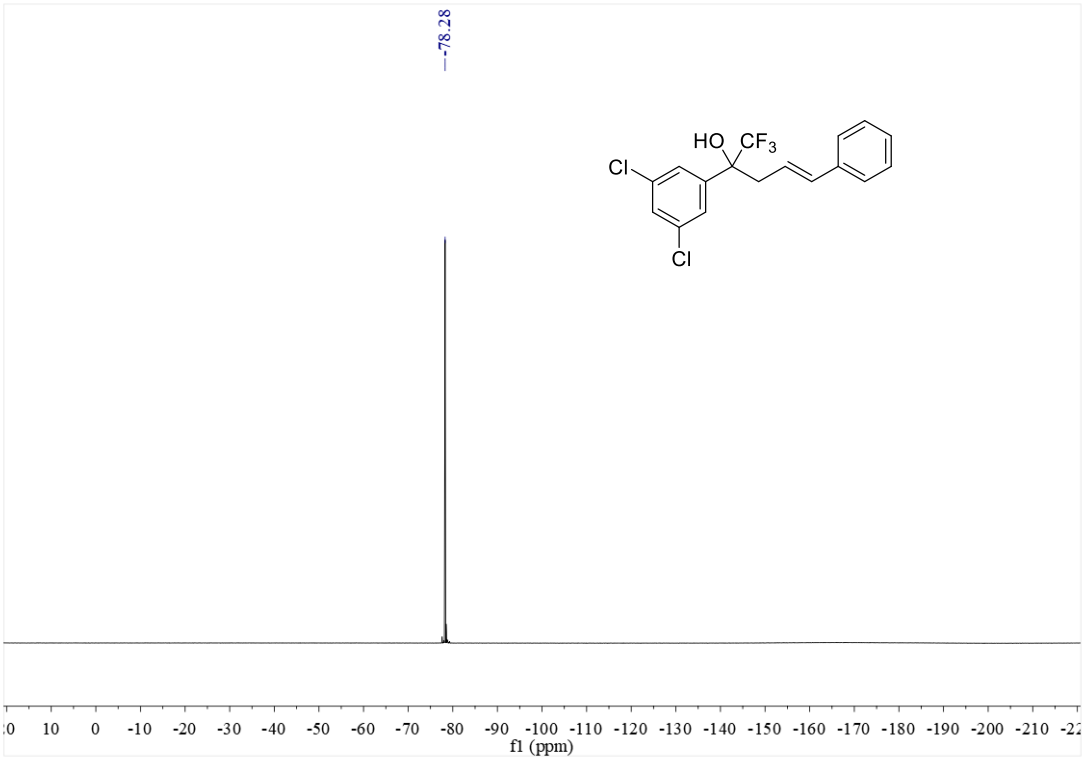
^{1}H NMR of 4l



^{13}C NMR of 4l

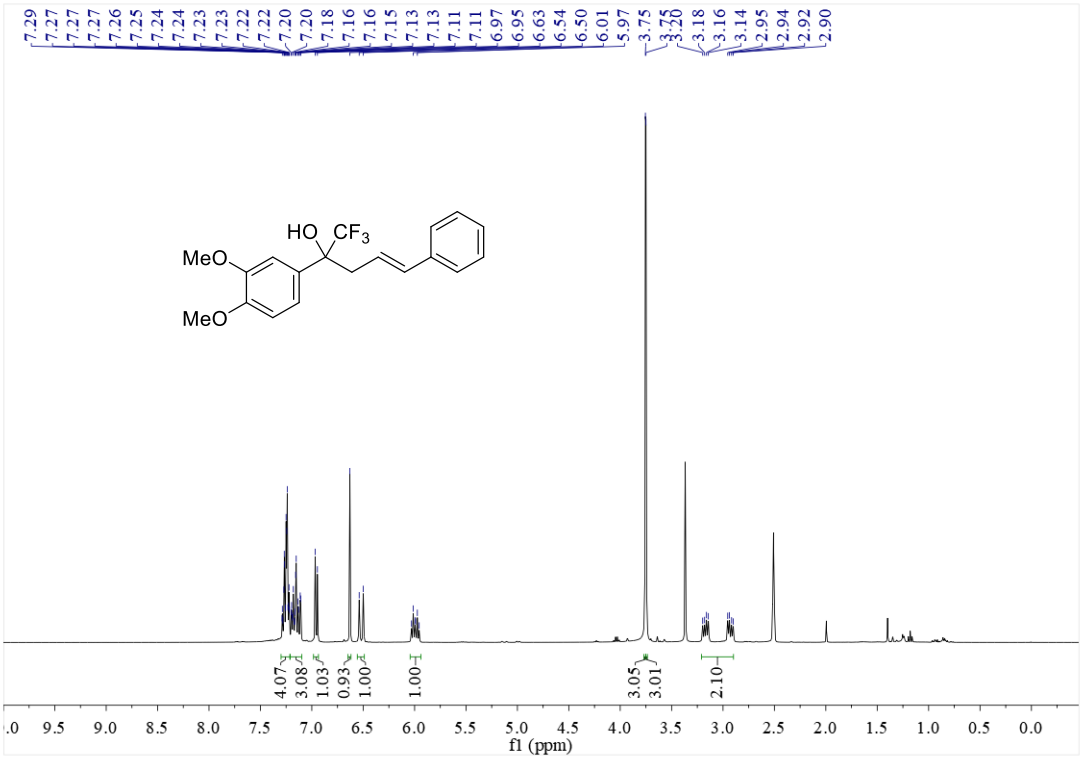


^{19}F NMR of 4l

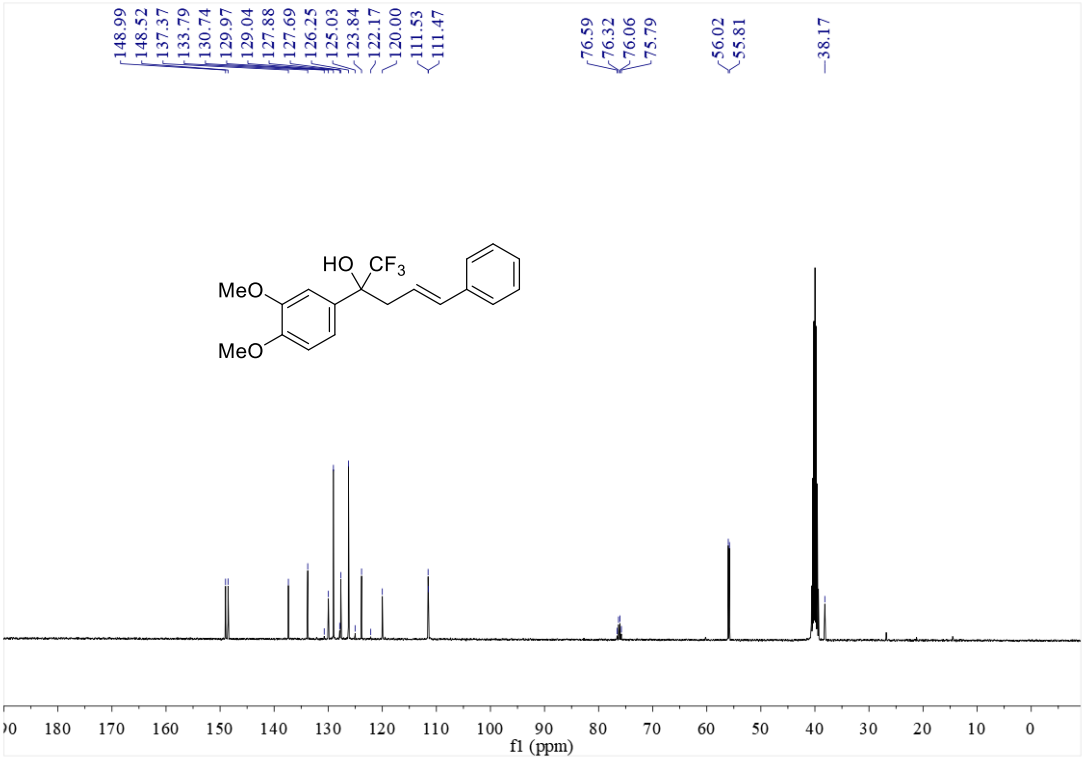


(*E*)-2-(3,4-Dimethoxyphenyl)-1,1,1-trifluoro-5-phenylpent-4-en-2-ol (4m)

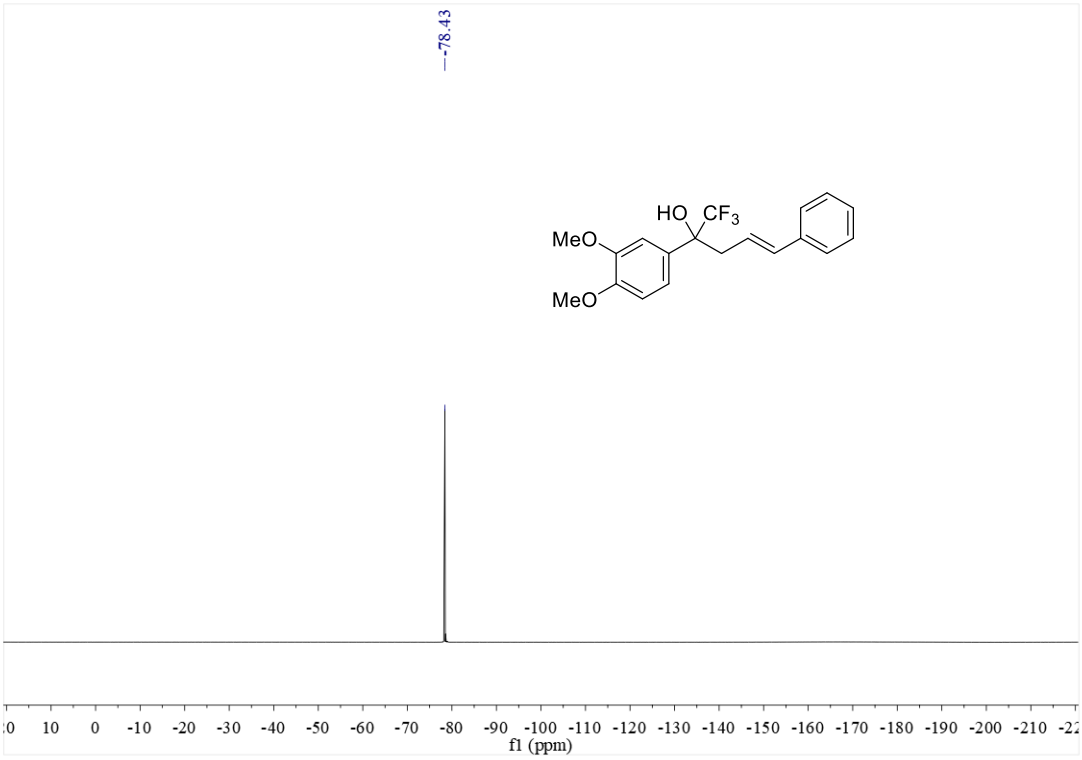
^{1}H NMR of 4m



^{13}C NMR of 4m

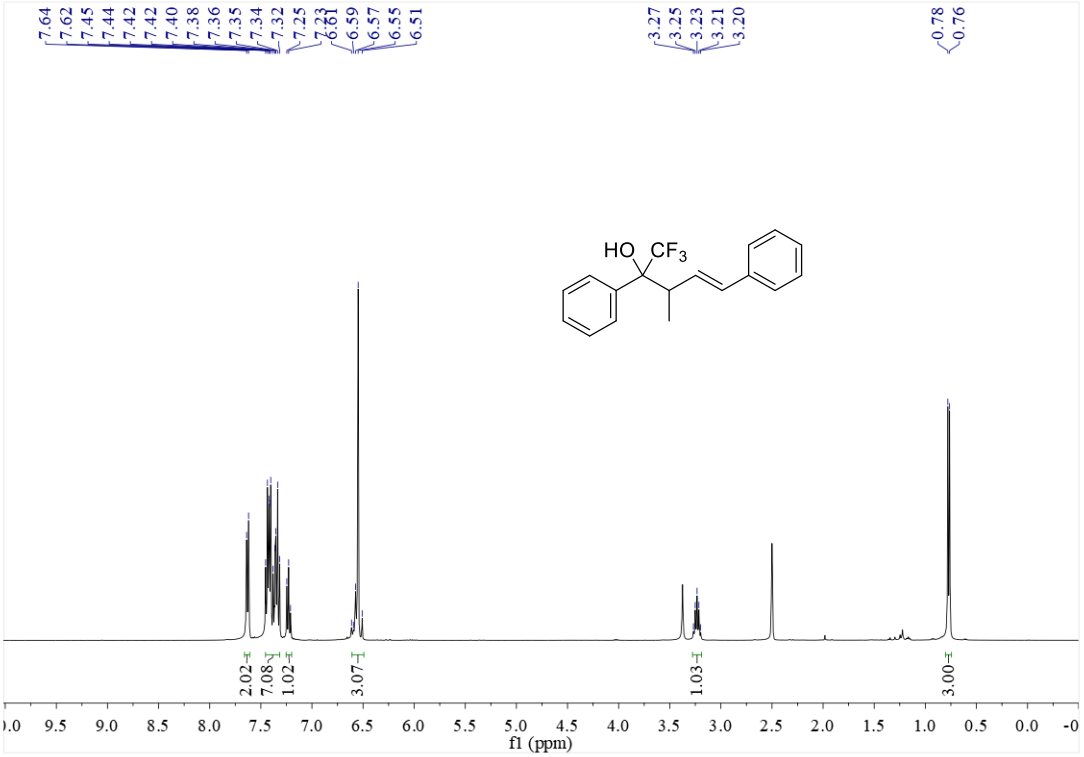


^{19}F NMR of 4m

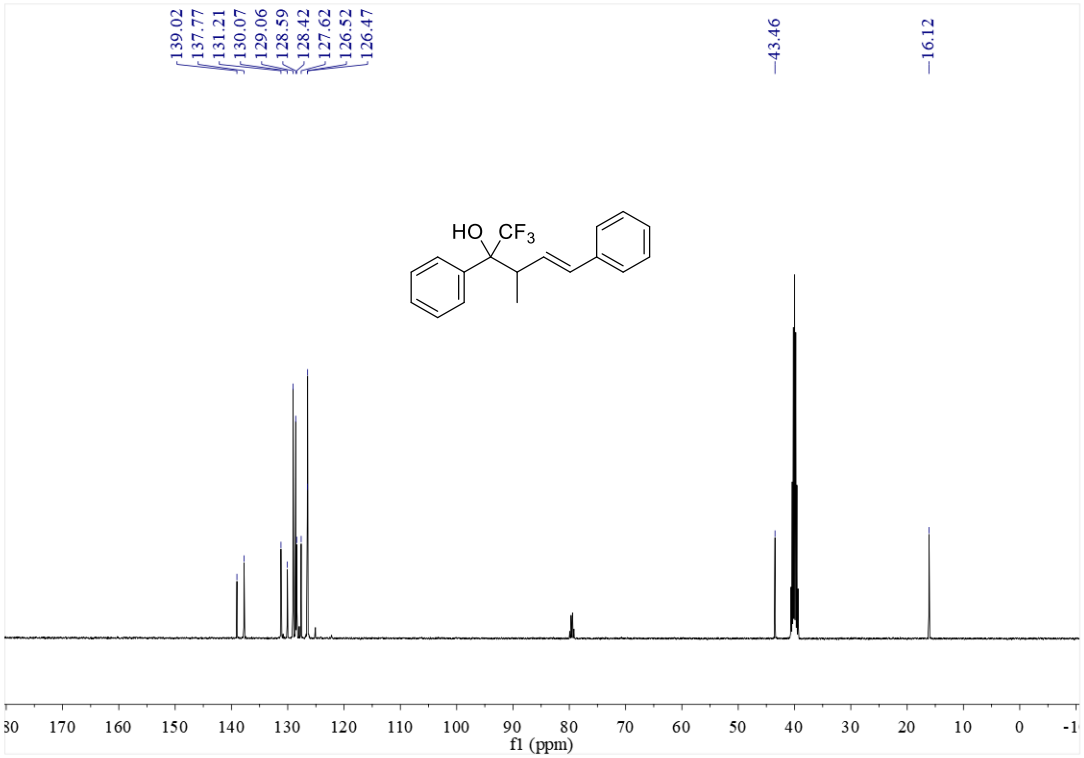


(*E*)-1,1,1-Trifluoro-3-methyl-2,5-diphenylpent-4-en-2-ol (4n)

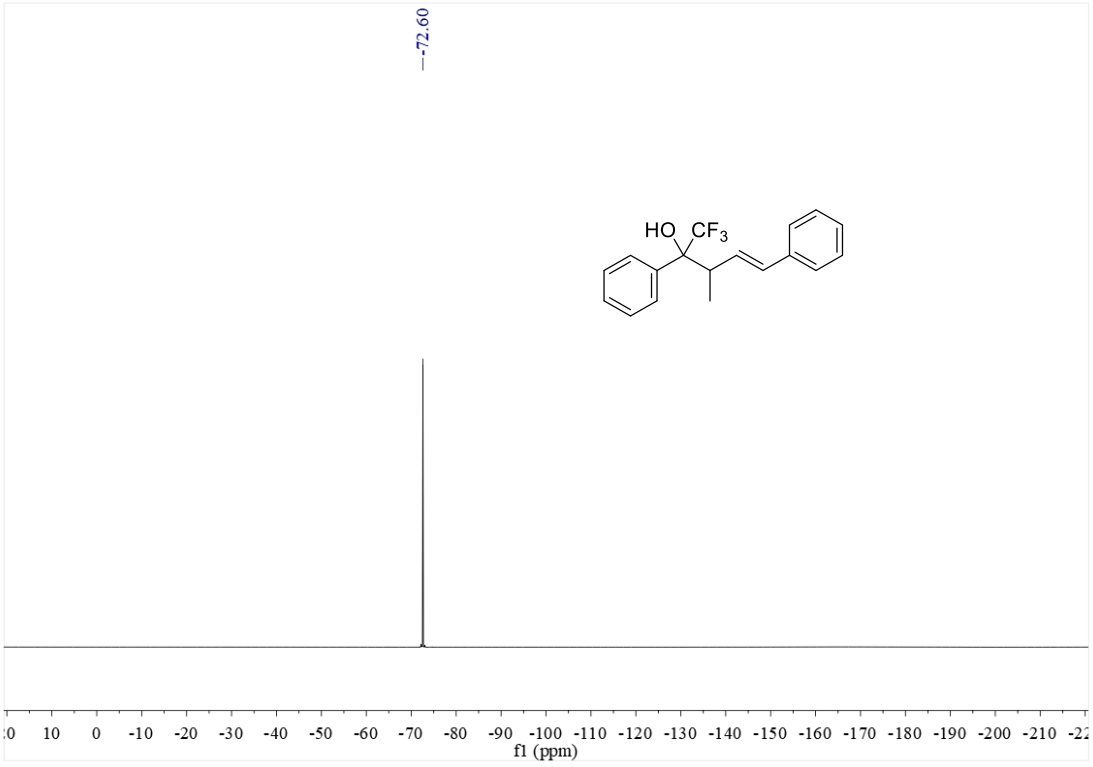
^{1}H NMR of 4n



^{13}C NMR of 4n

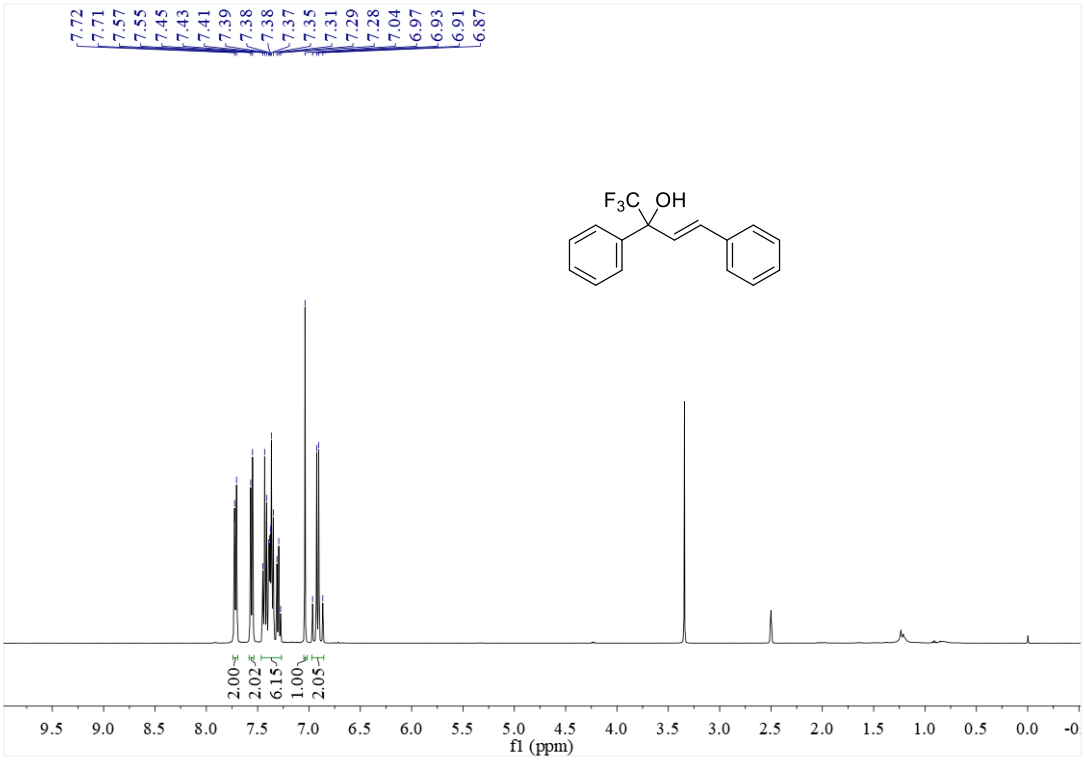


^{19}F NMR of 4n

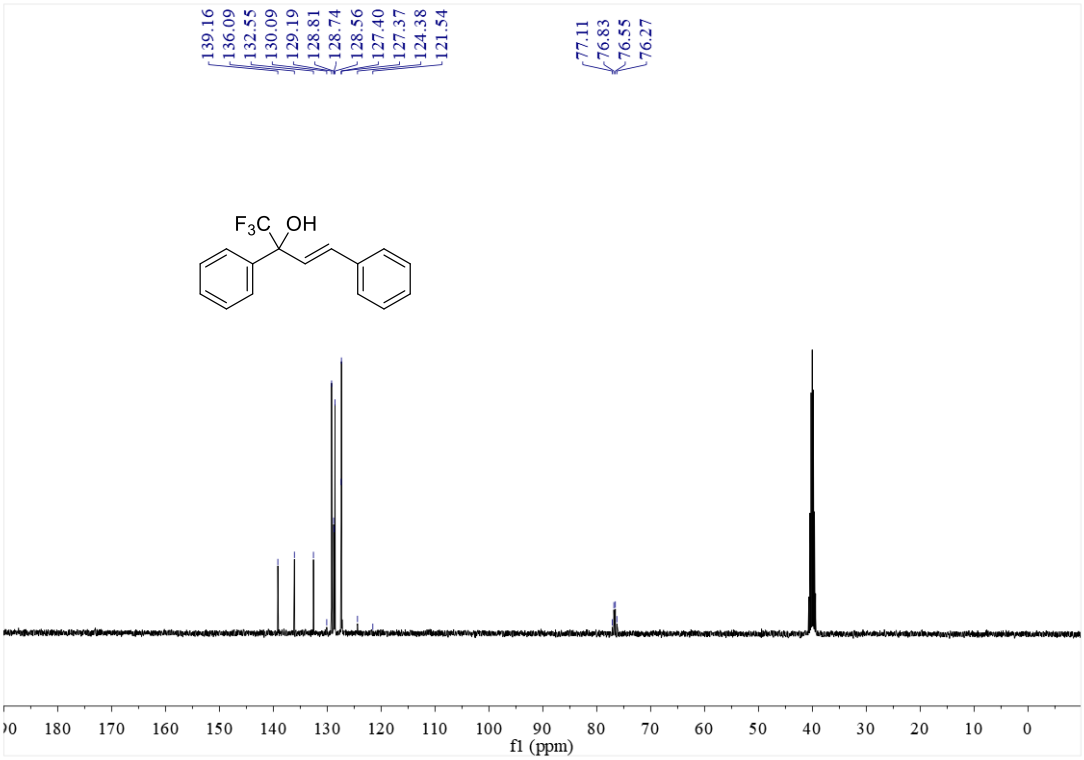


(*E*)-1,1,1-Trifluoro-2,4-diphenylbut-3-en-2-ol (4o)

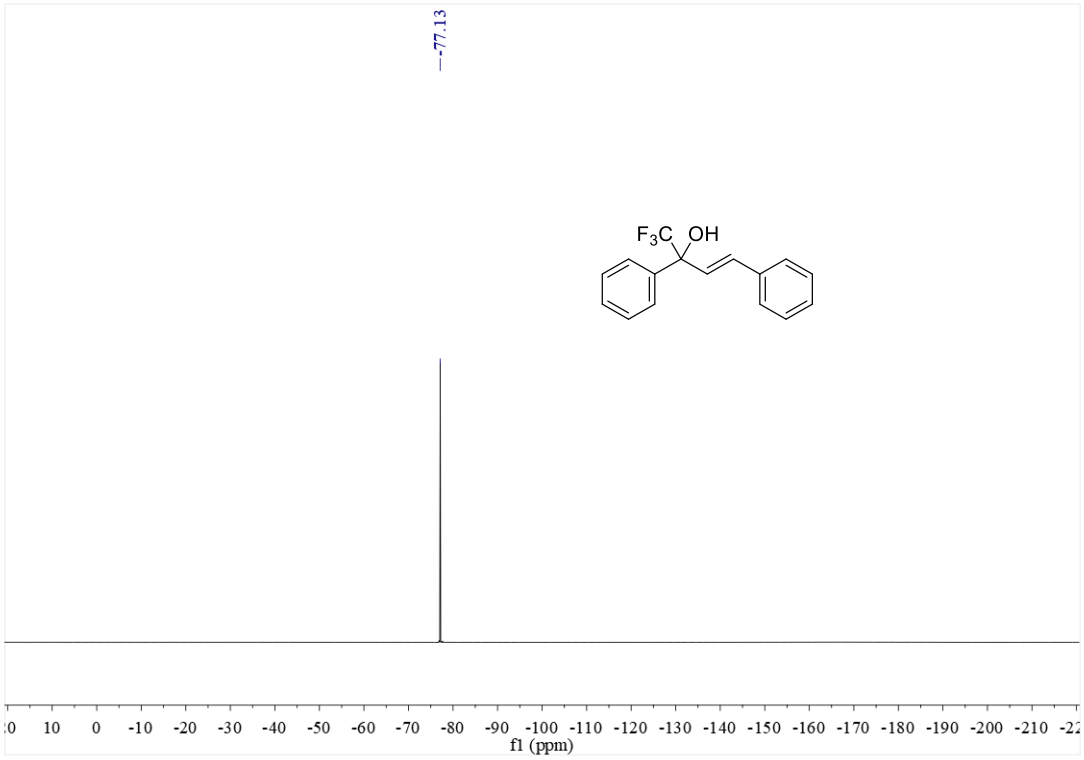
^{1}H NMR of 4o



^{13}C NMR of 4o

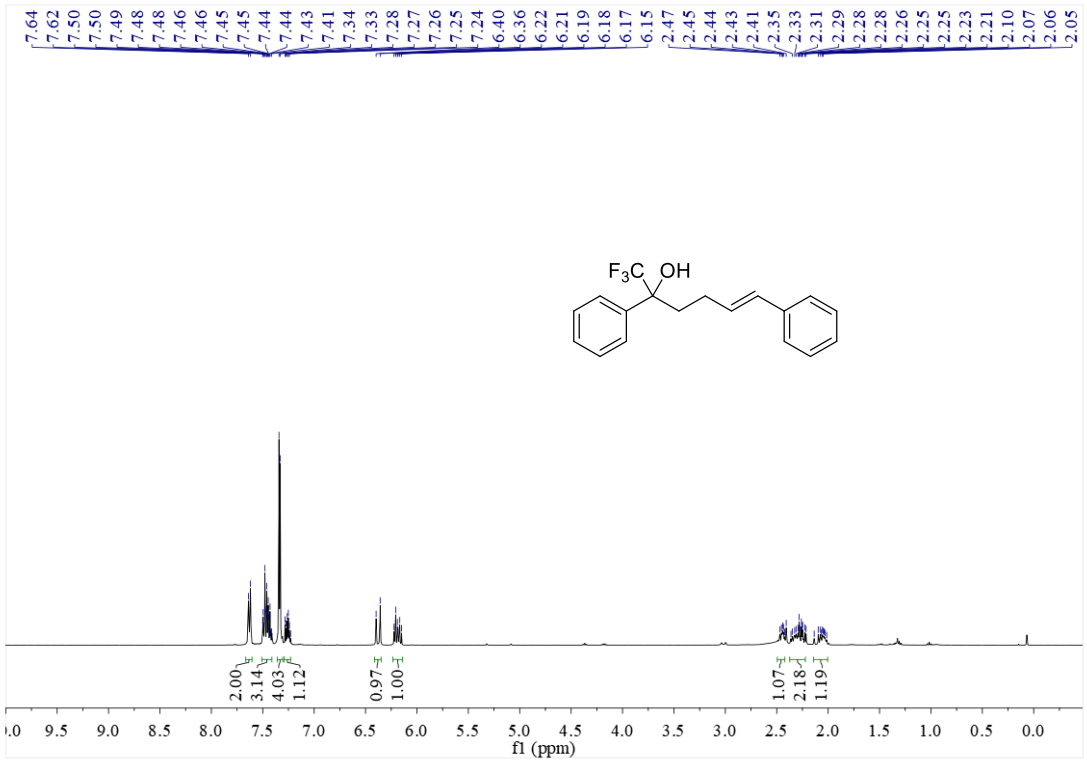


^{19}F NMR of 4o

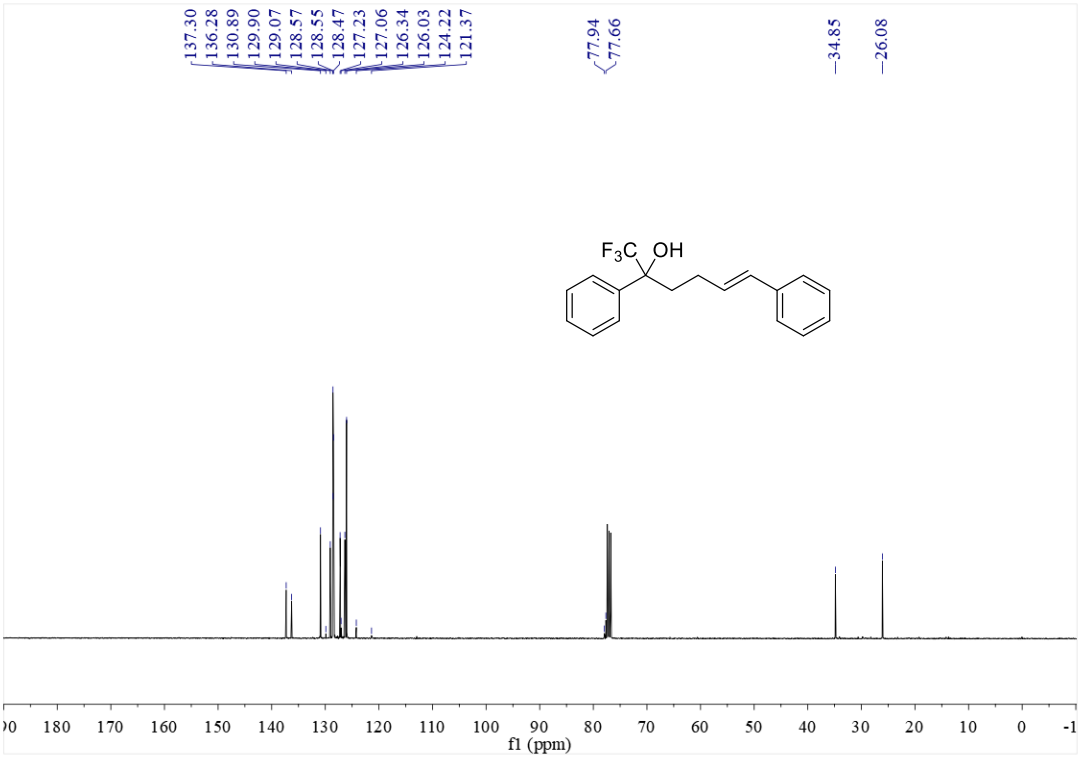


(*E*)-1,1,1-Trifluoro-2,6-diphenylhex-5-en-2-ol (4p)

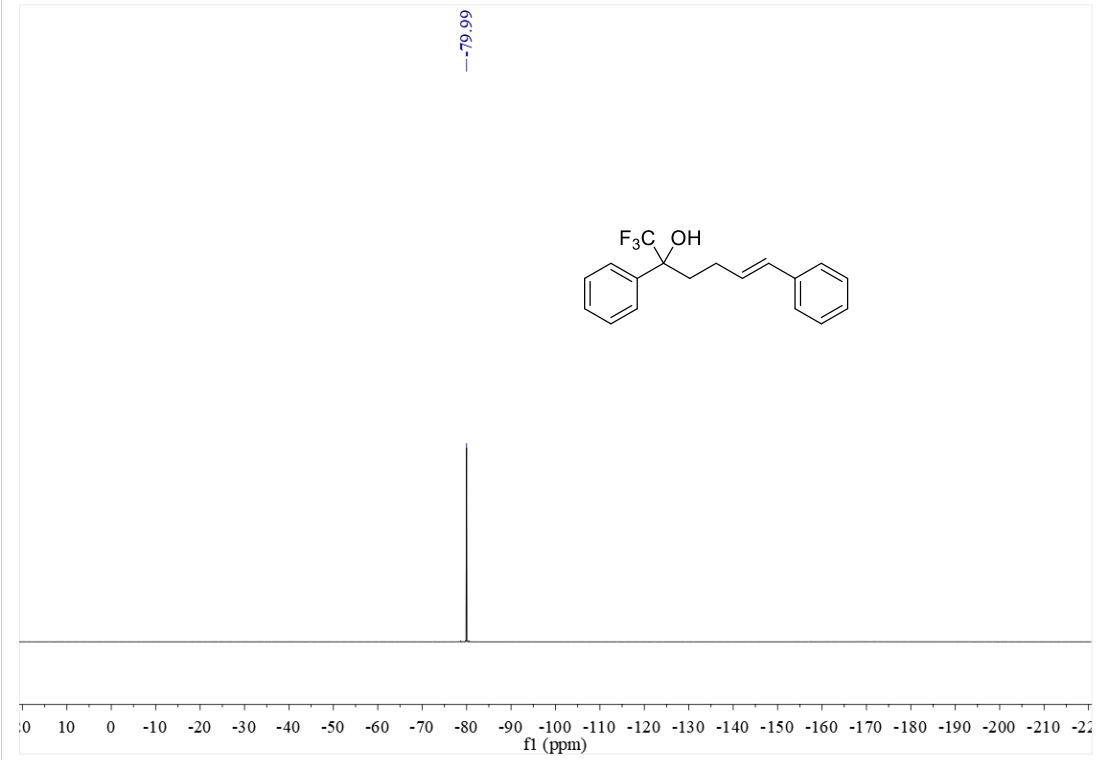
^{1}H NMR of 4p



^{13}C NMR of 4p

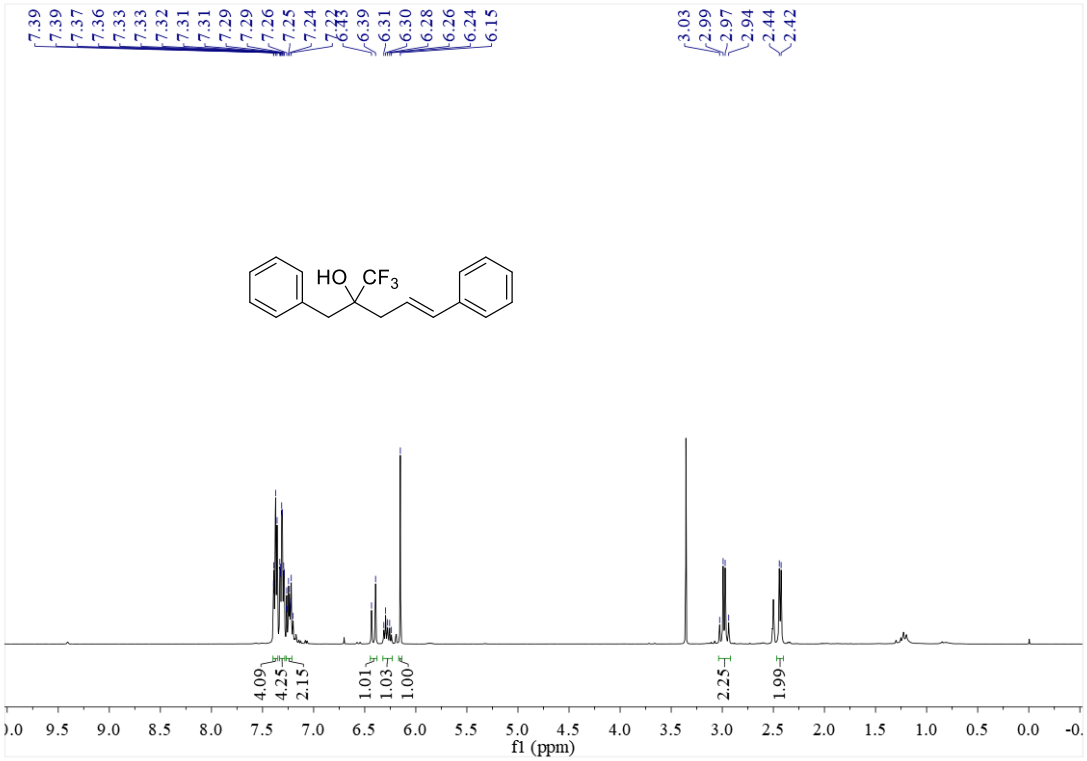


^{19}F NMR of 4p

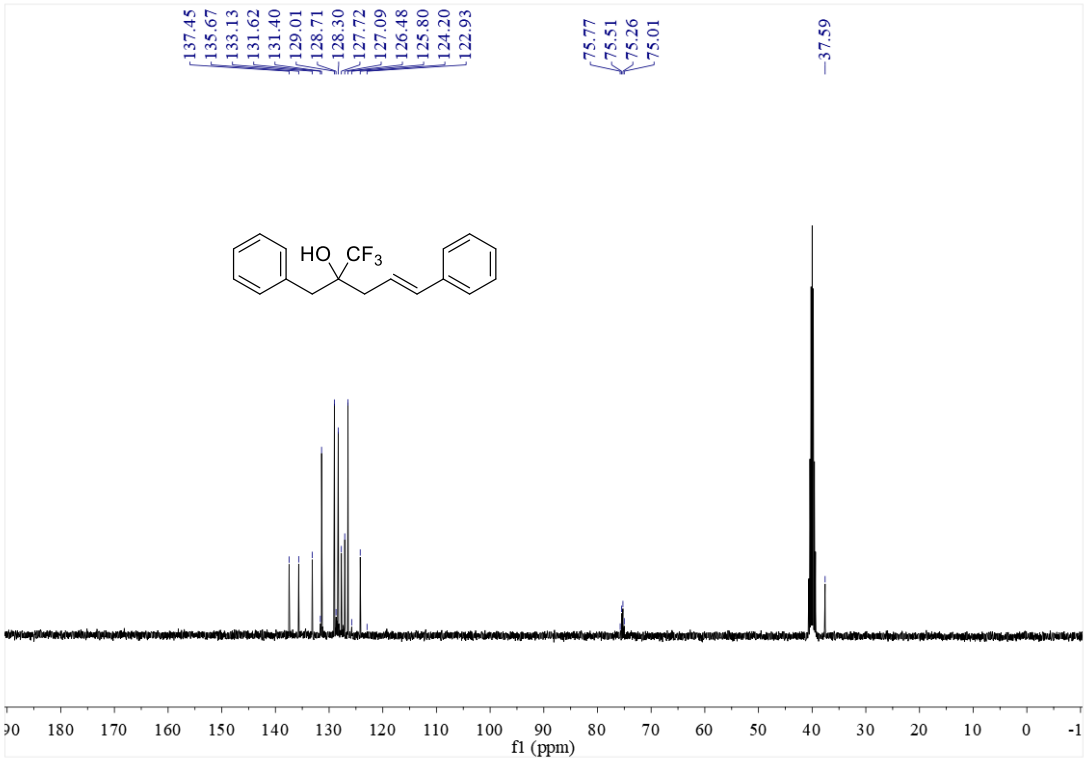


(*E*)-2-Benzyl-1,1,1-trifluoro-5-phenylpent-4-en-2-ol (4q)

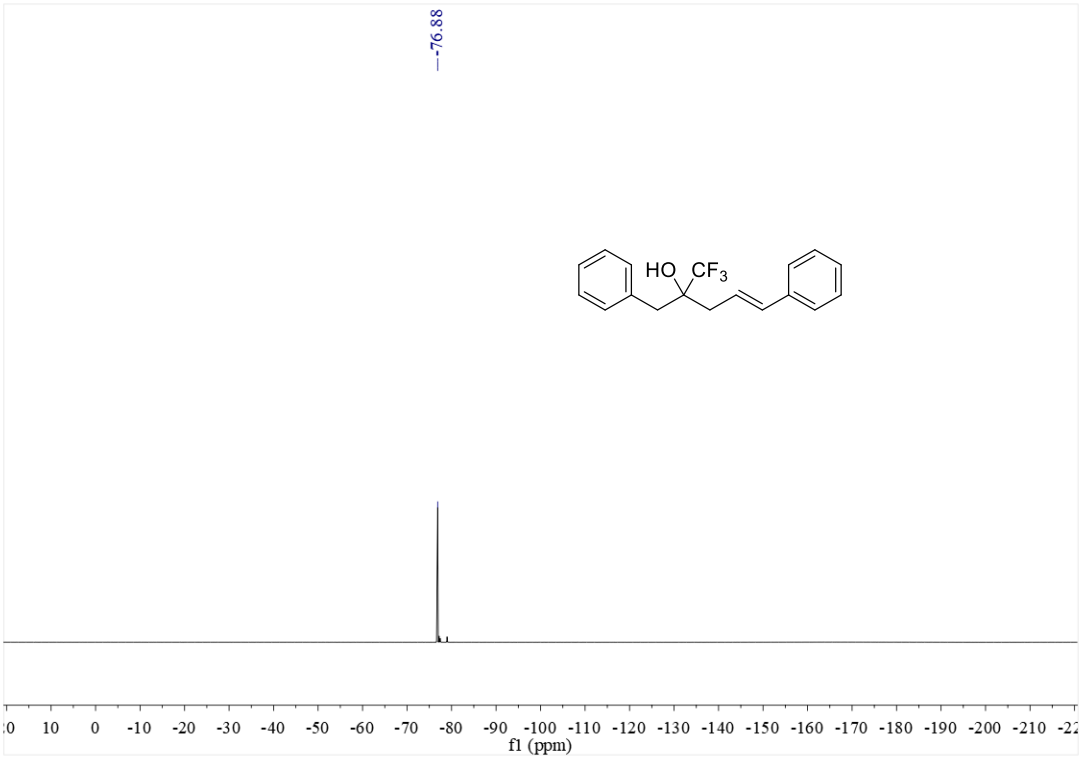
^{1}H NMR of 4q



^{13}C NMR of 4q

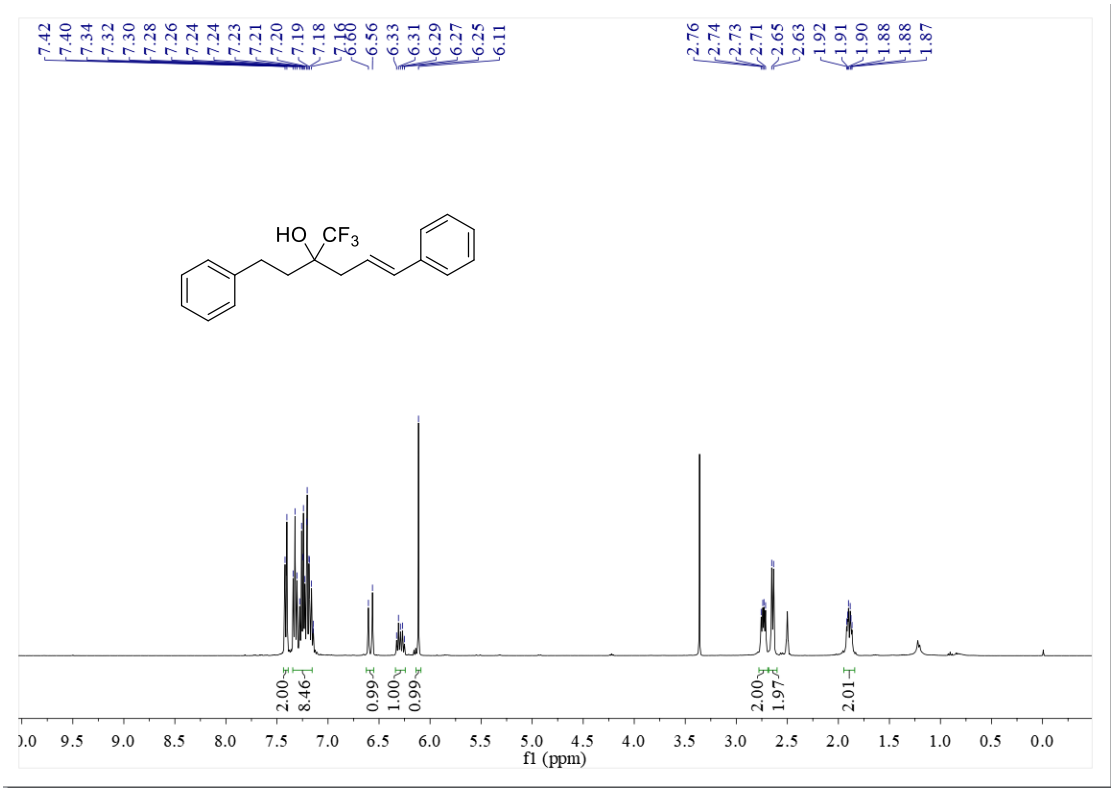


^{19}F NMR of 4q

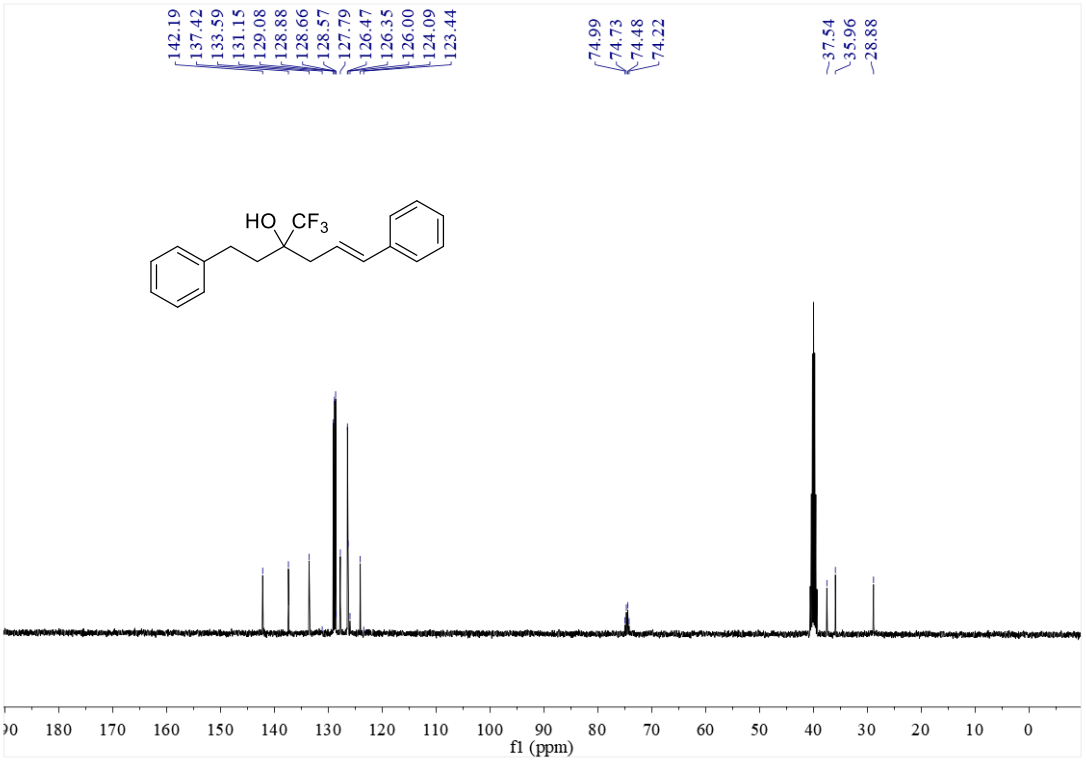


(*E*)-1,6-Diphenyl-3-(trifluoromethyl)hex-5-en-3-ol (4r)

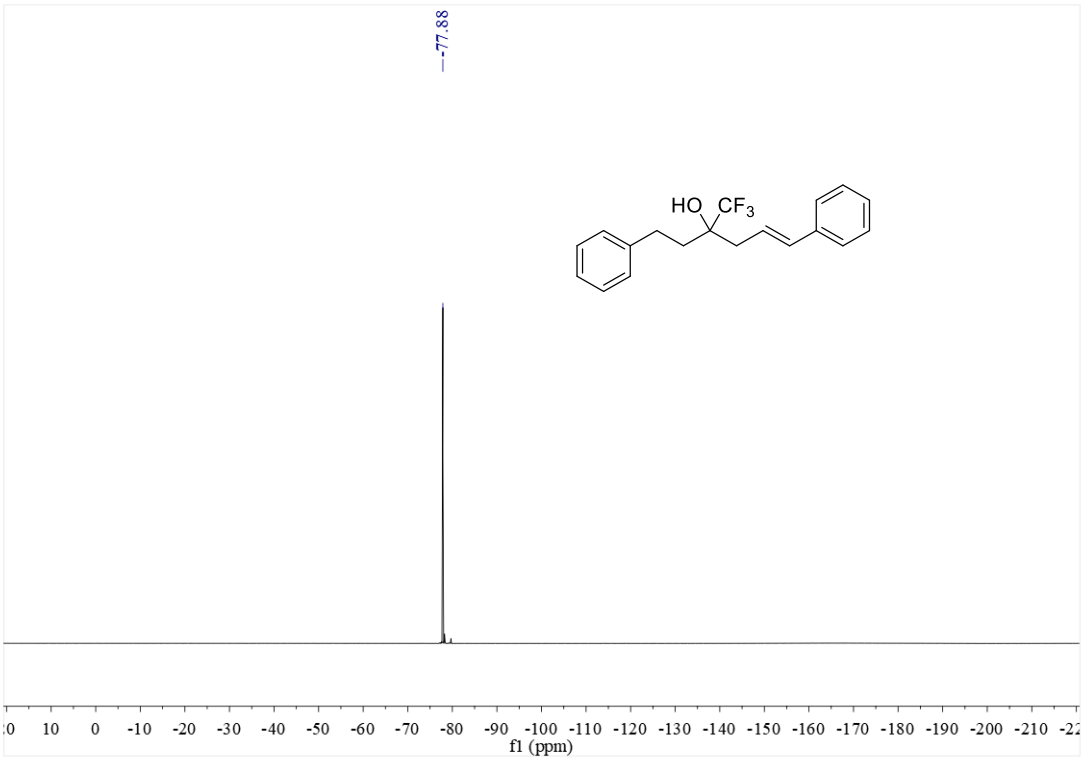
^{1}H NMR of 4r



^{13}C NMR of 4r

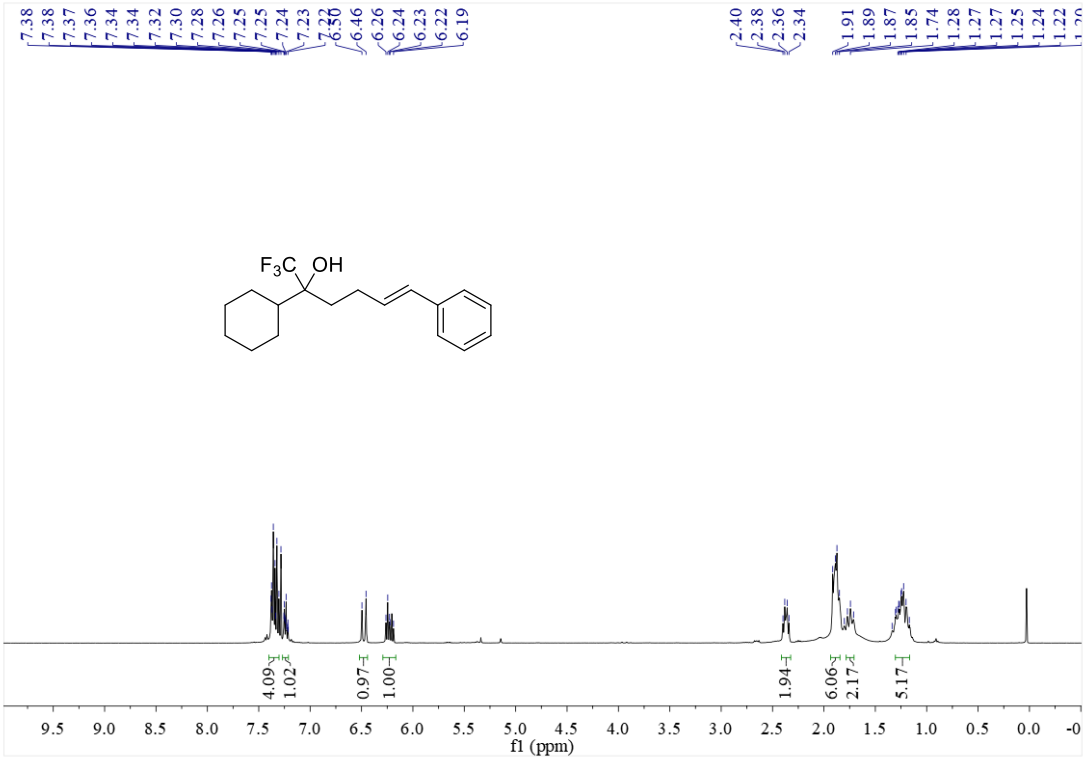


^{19}F NMR of 4r

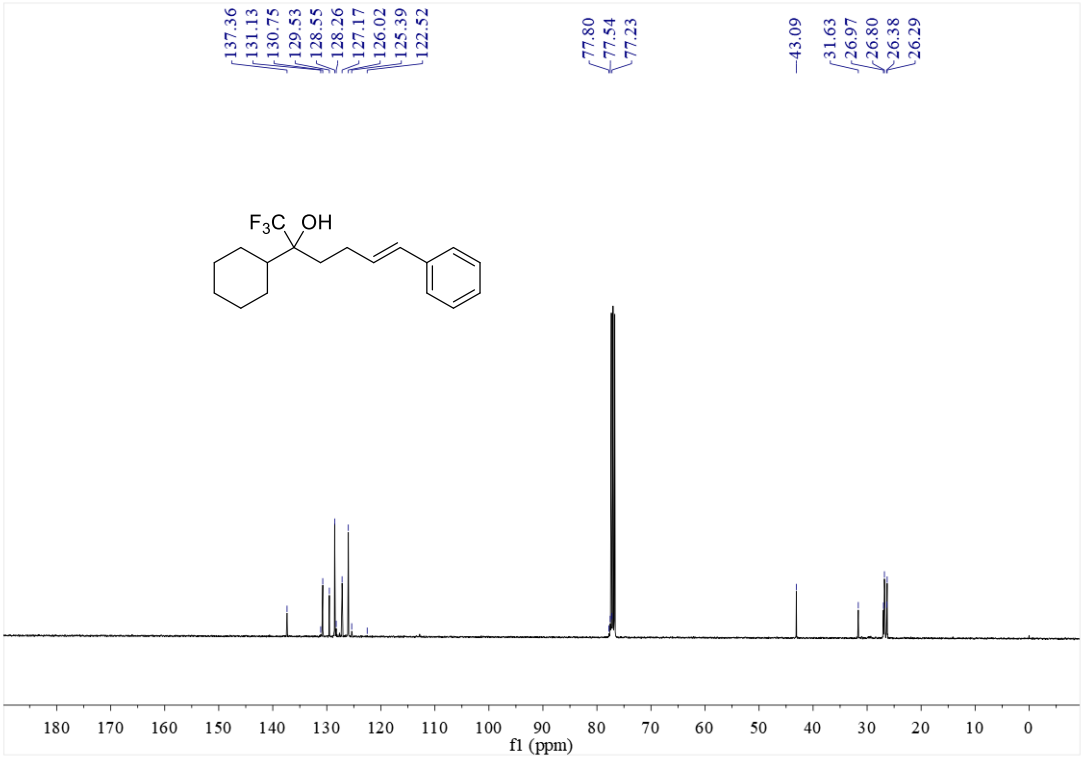


(*E*)-2-Cyclohexyl-1,1,1-trifluoro-6-phenylhex-5-en-2-ol (4s)

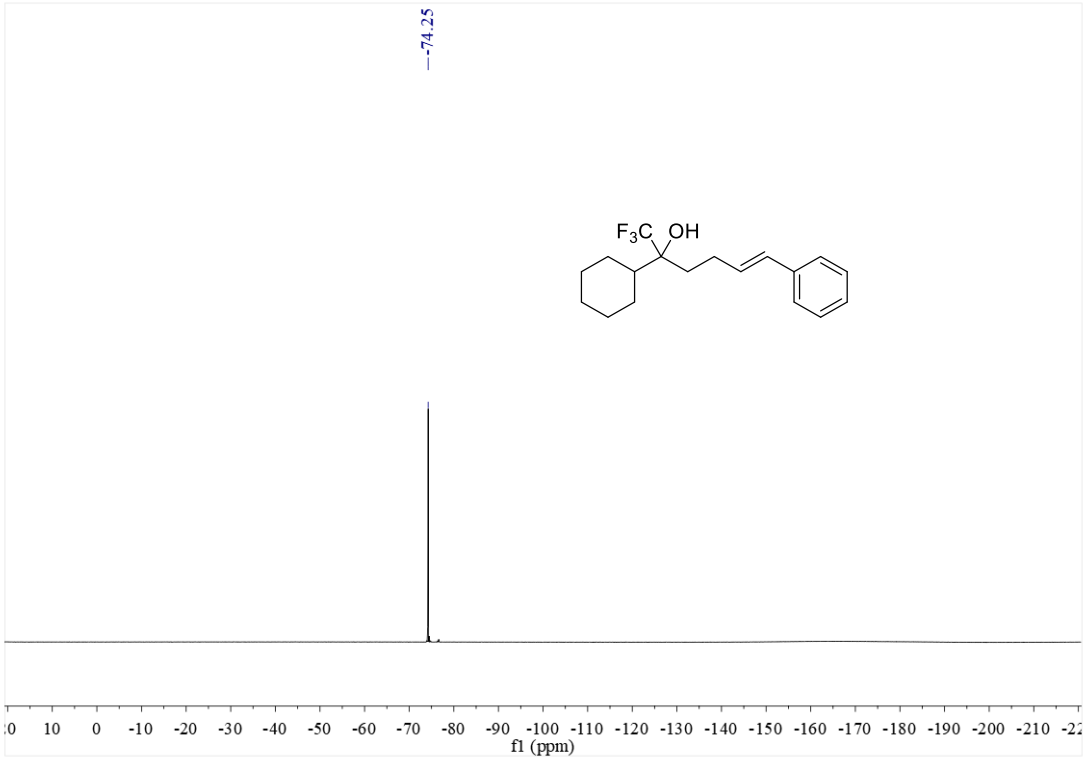
^{1}H NMR of 4s



^{13}C NMR of 4s

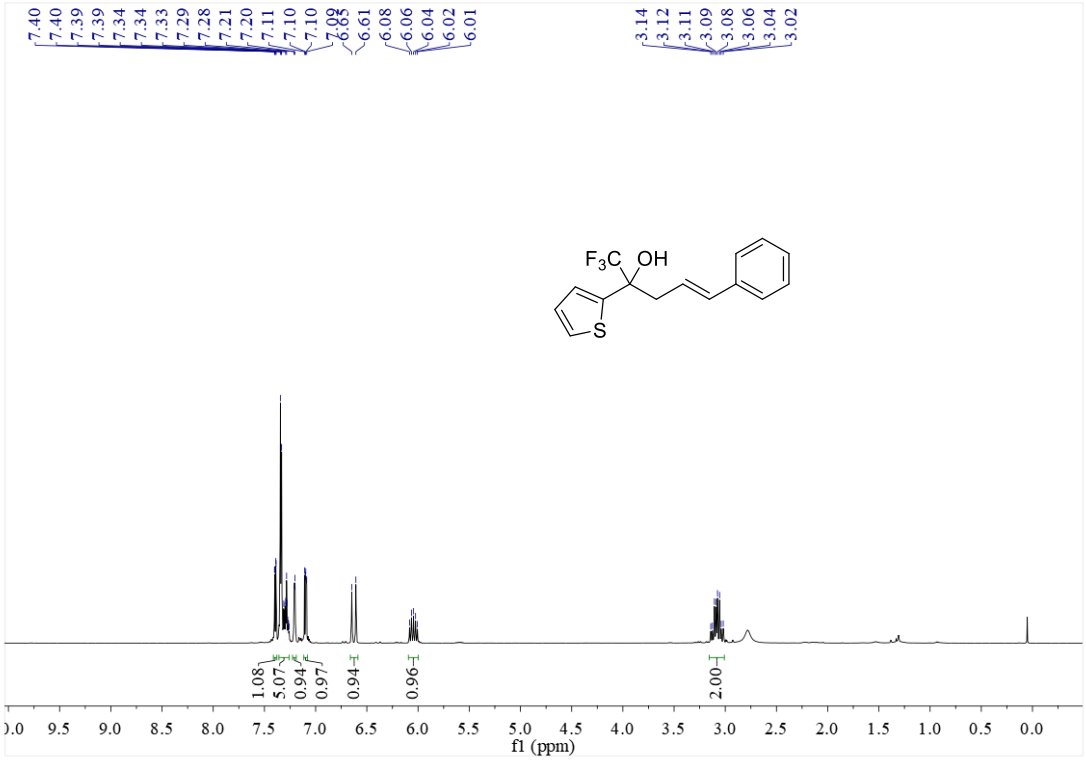


^{19}F NMR of 4s

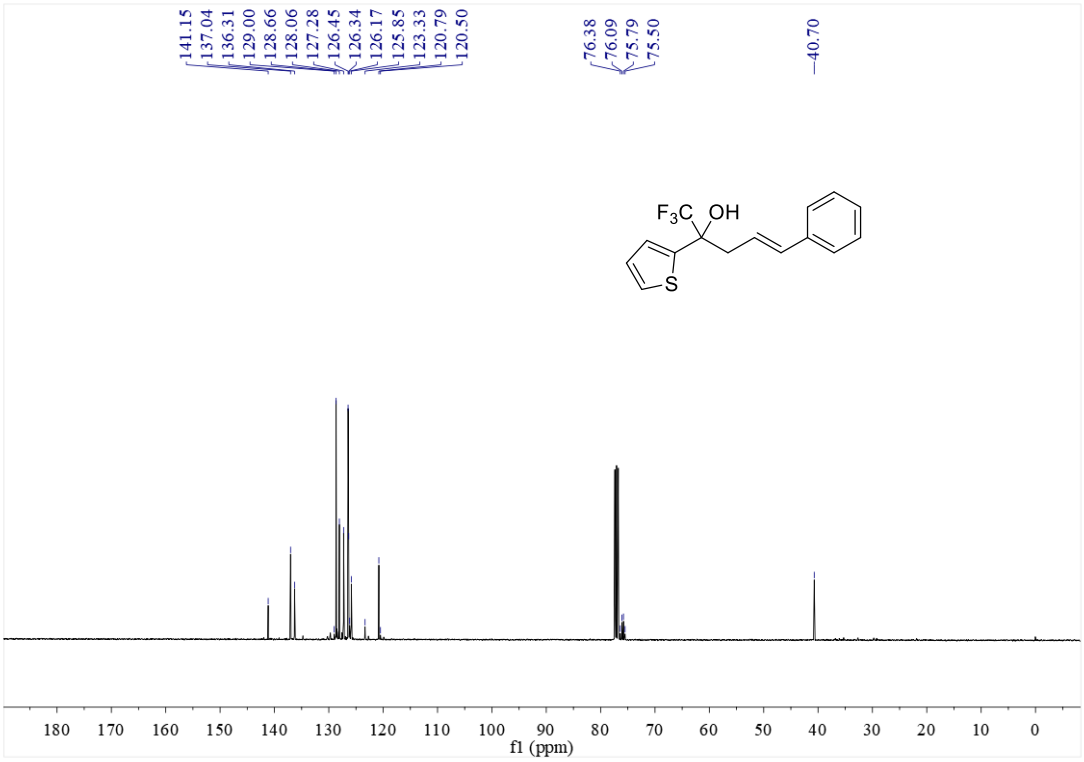


(*E*)-1,1,1-Trifluoro-5-phenyl-2-(thiophen-2-yl)pent-4-en-2-ol (4t)

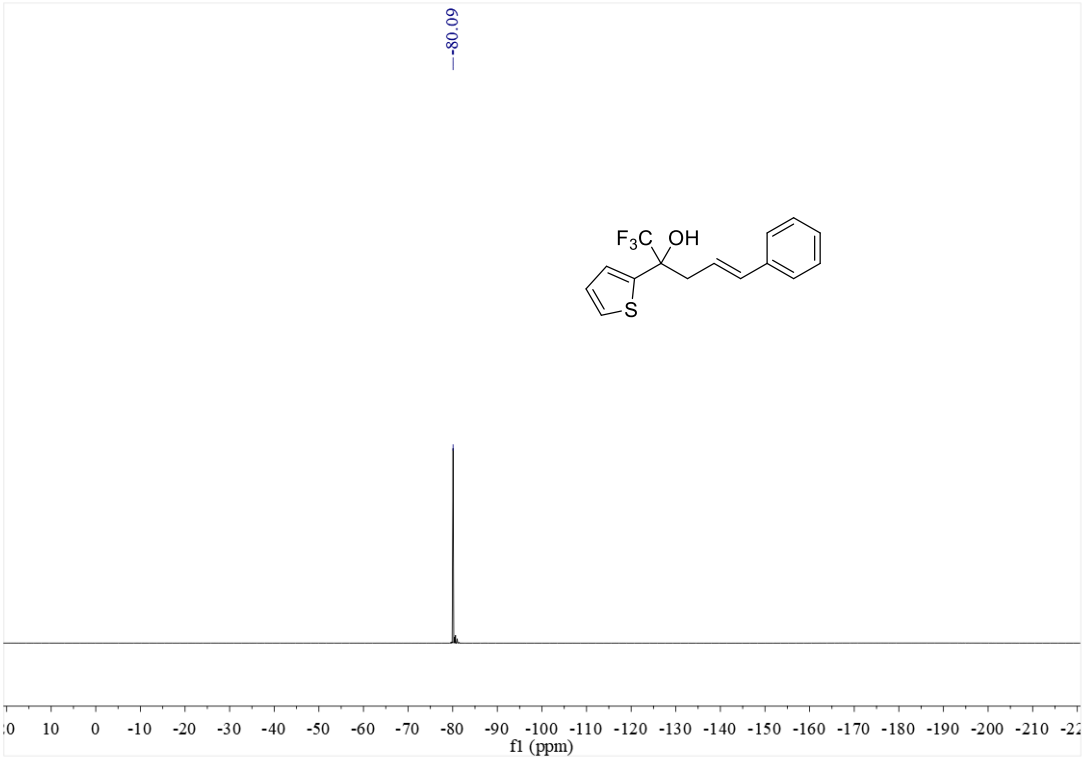
^{1}H NMR of 4t



^{13}C NMR of 4t

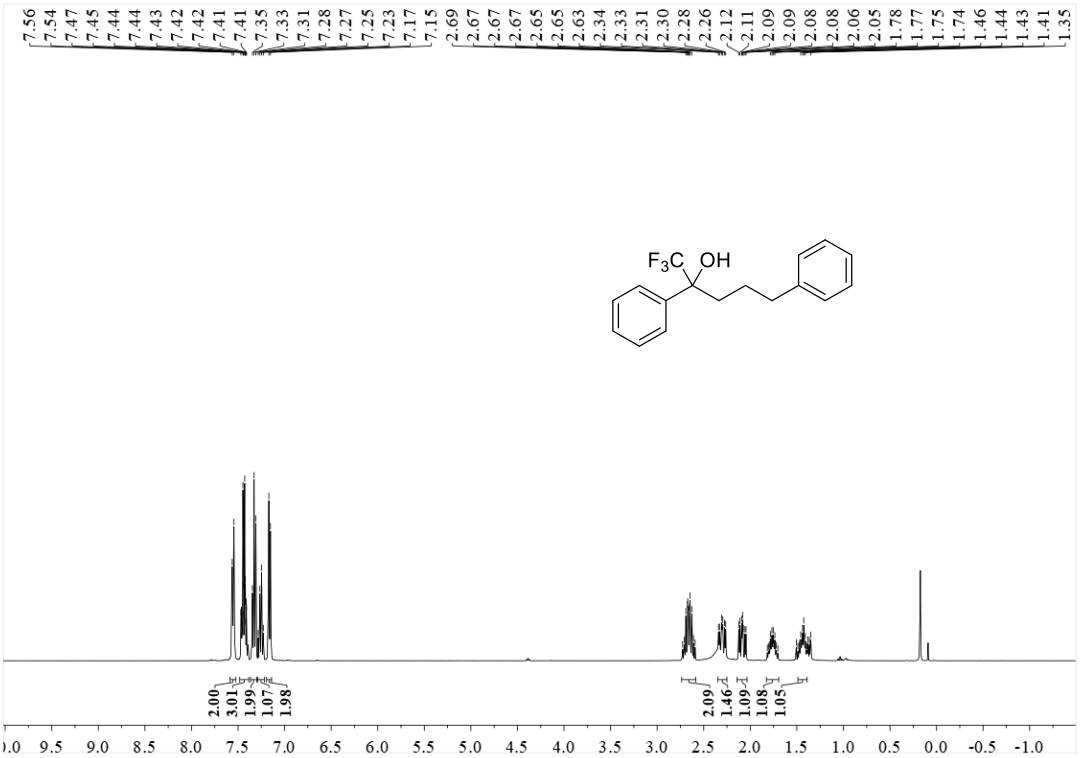


^{19}F NMR of 4t

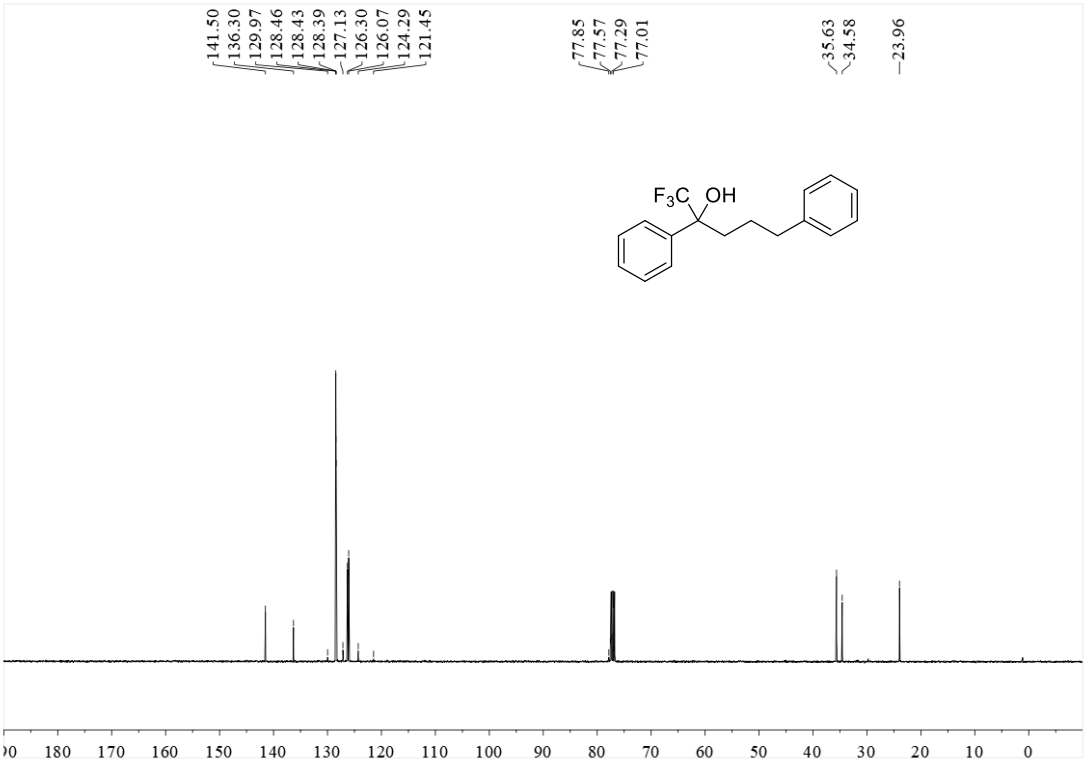


1,1,1-Trifluoro-2,5-diphenylpentan-2-ol (5a)

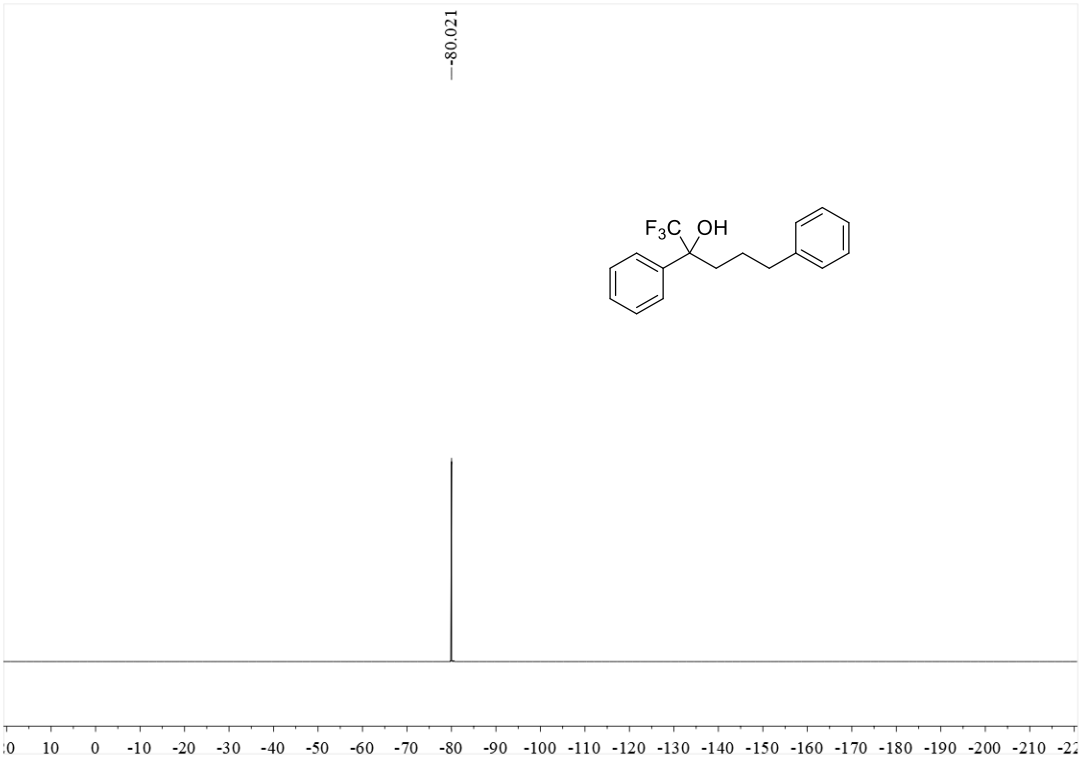
^{1}H NMR of 5a



^{13}C NMR of 5a

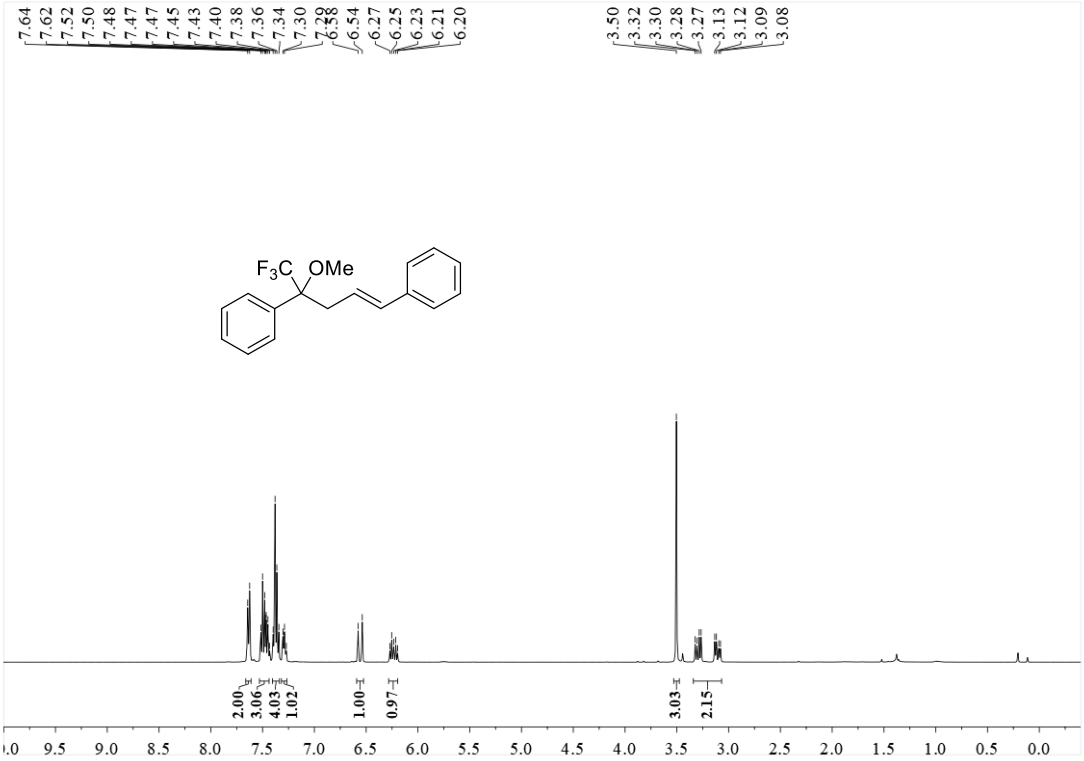


^{19}F NMR of 5a

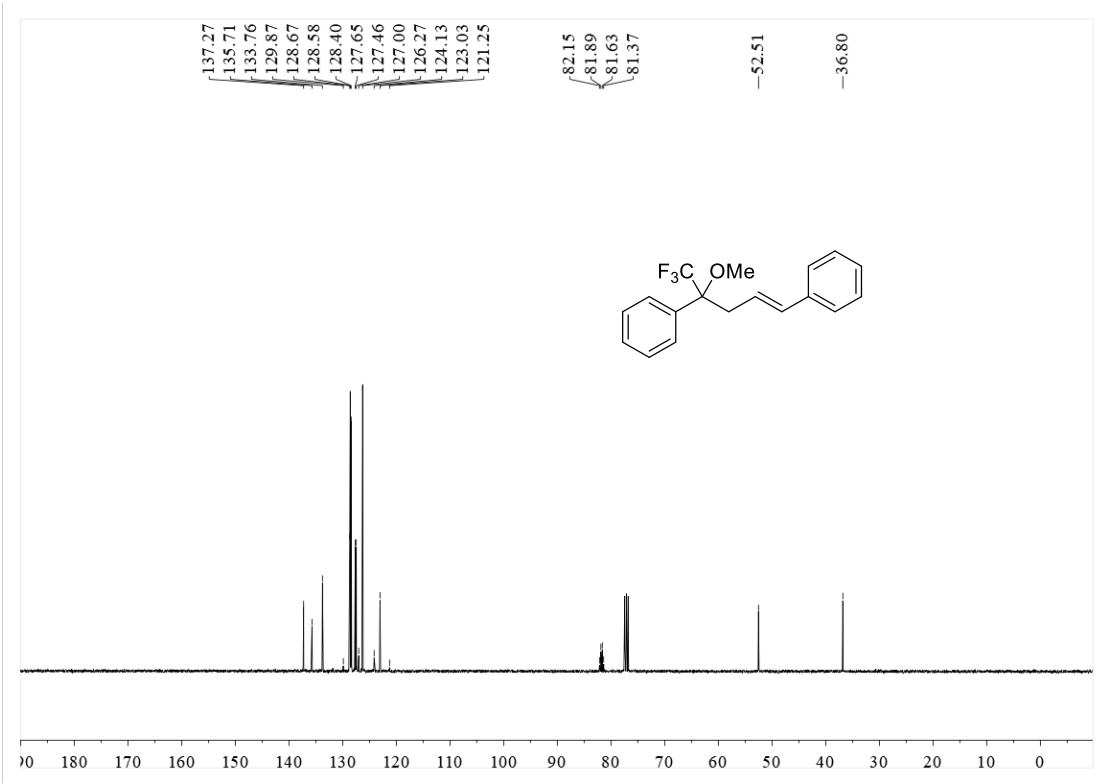


(*E*)-(5,5,5-Trifluoro-4-methoxypent-1-ene-1,4-diyl)dibenzene (5b)

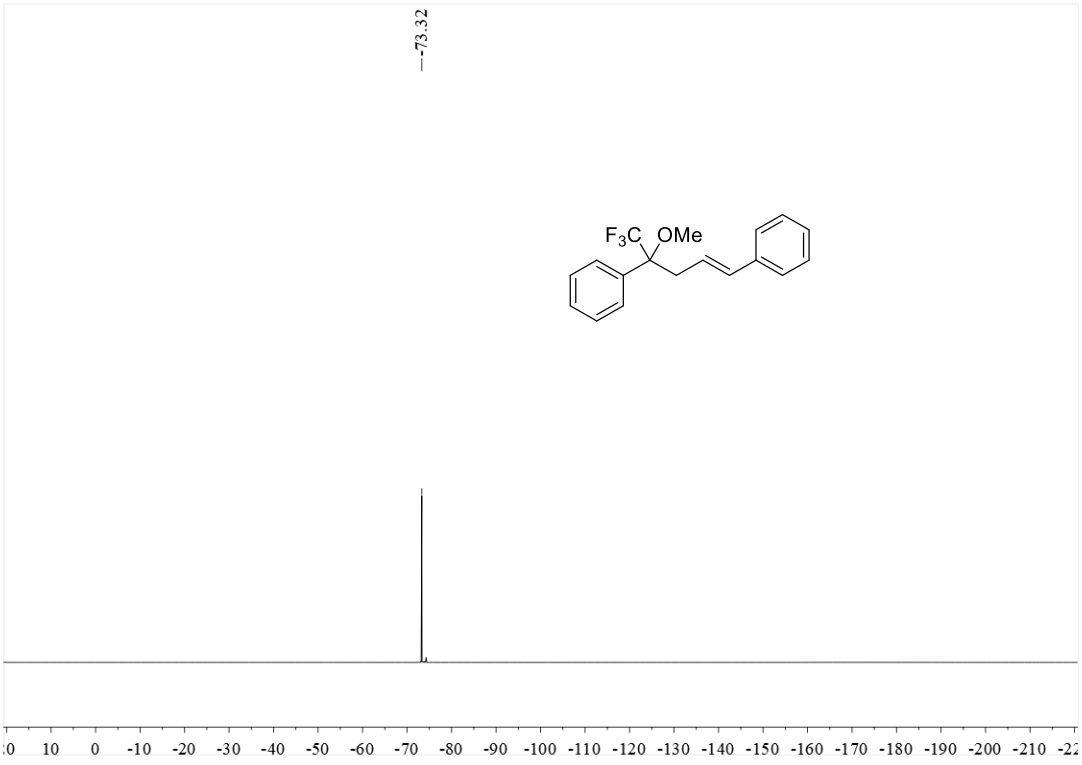
^{1}H NMR of 5b



^{13}C NMR of 5b

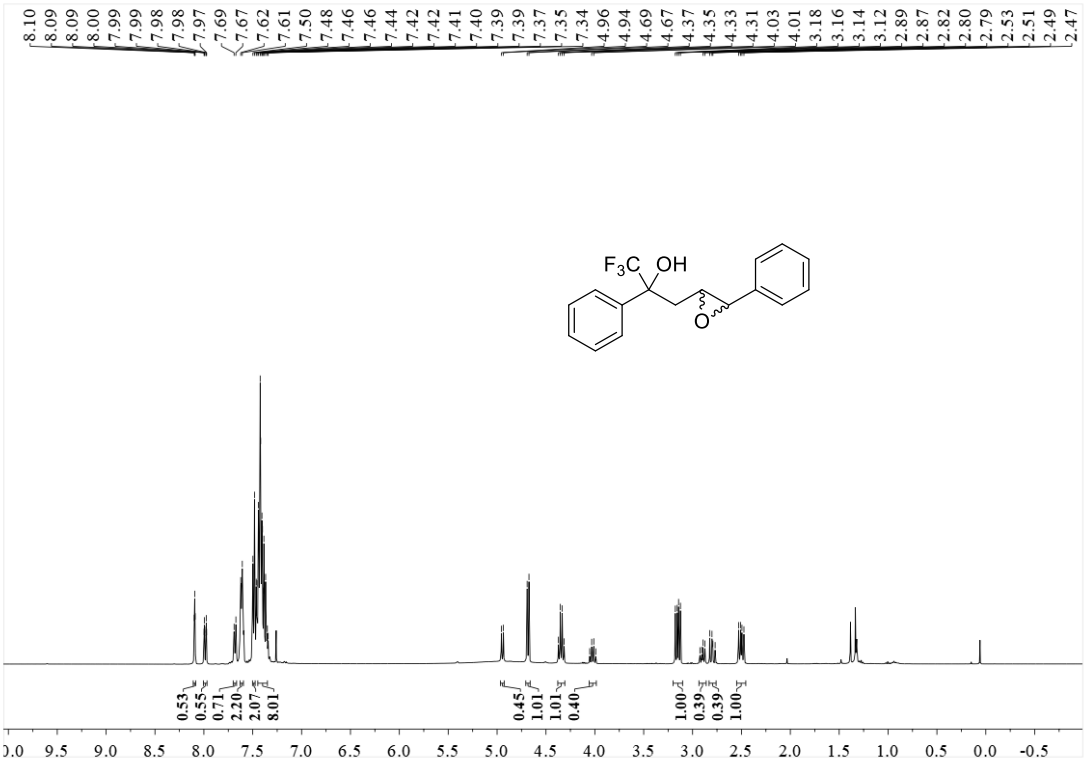


^{19}F NMR of 5b

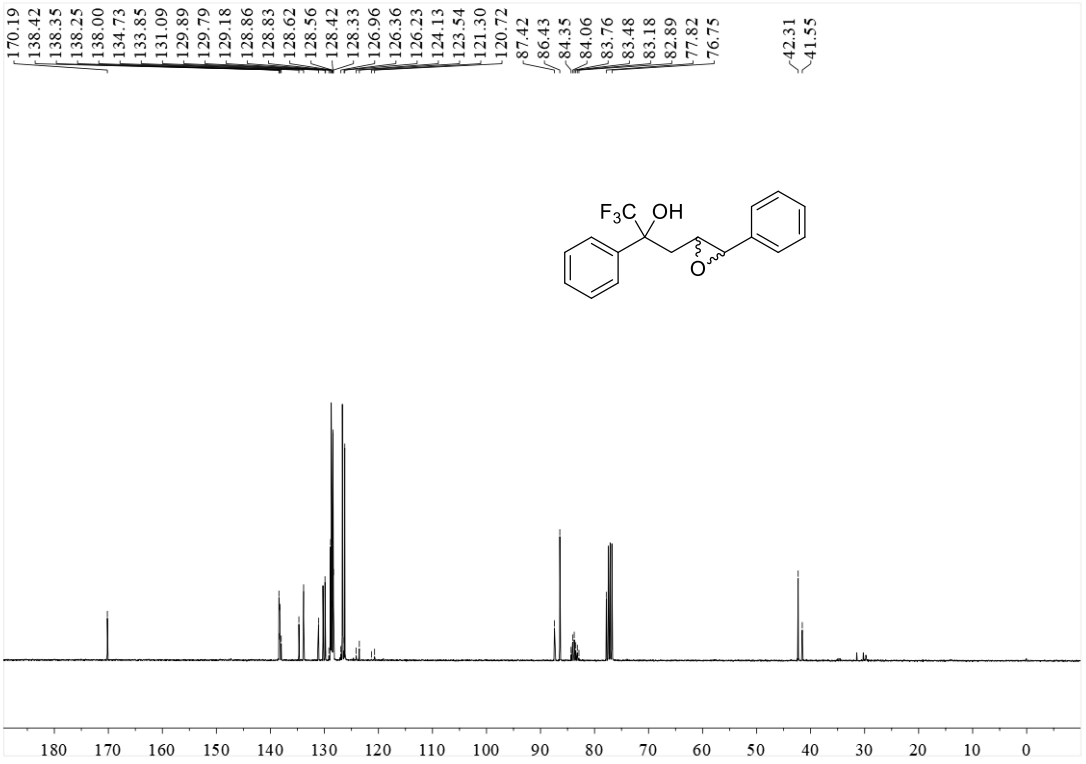


1,1,1-Trifluoro-2-phenyl-3-(3-phenyloxiran-2-yl)propan-2-ol (5c)

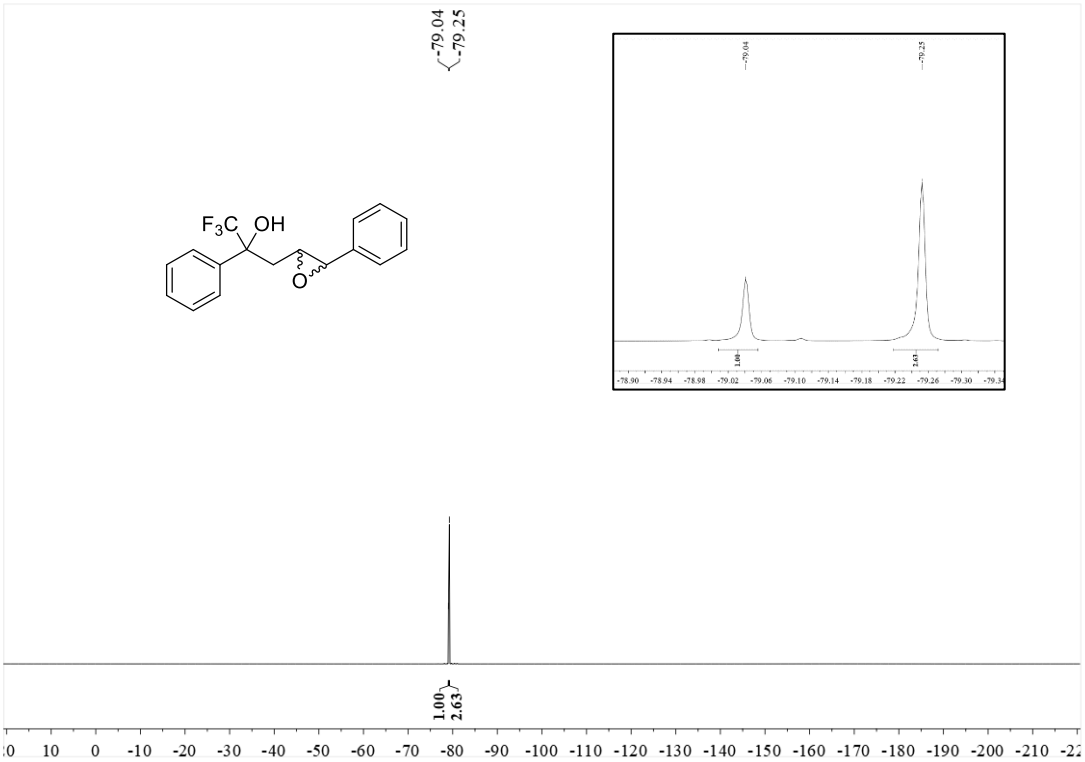
^{1}H NMR of 5c



^{13}C NMR of 5c

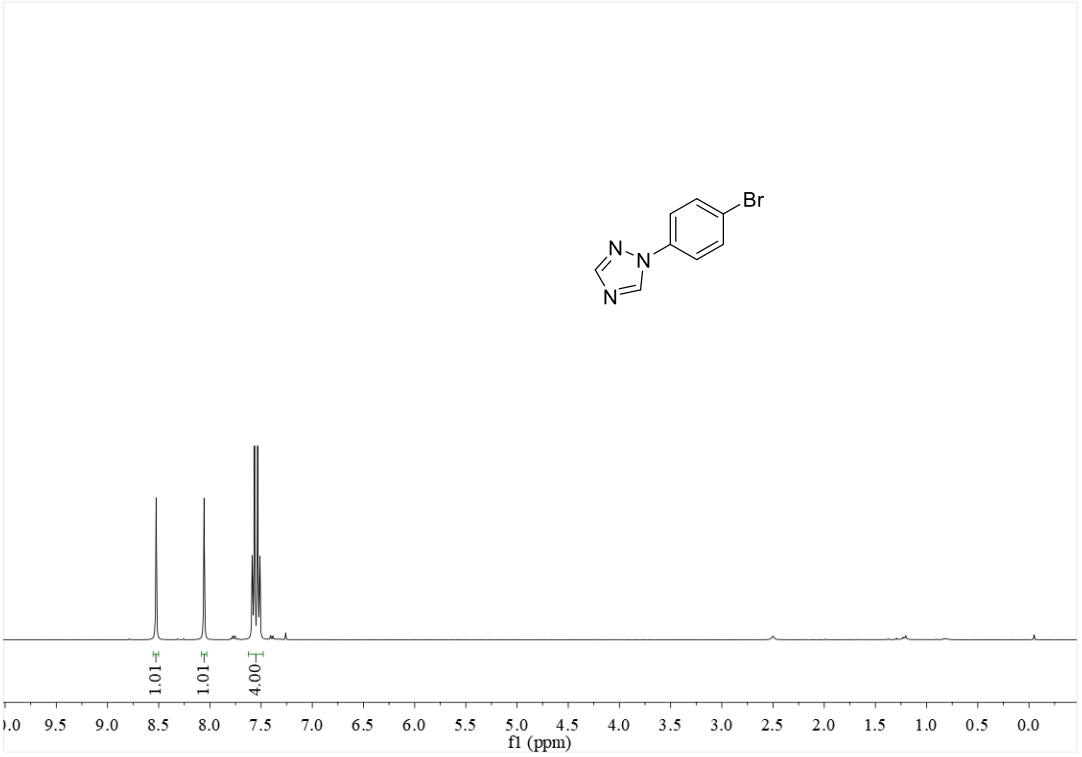


^{19}F NMR of 5c

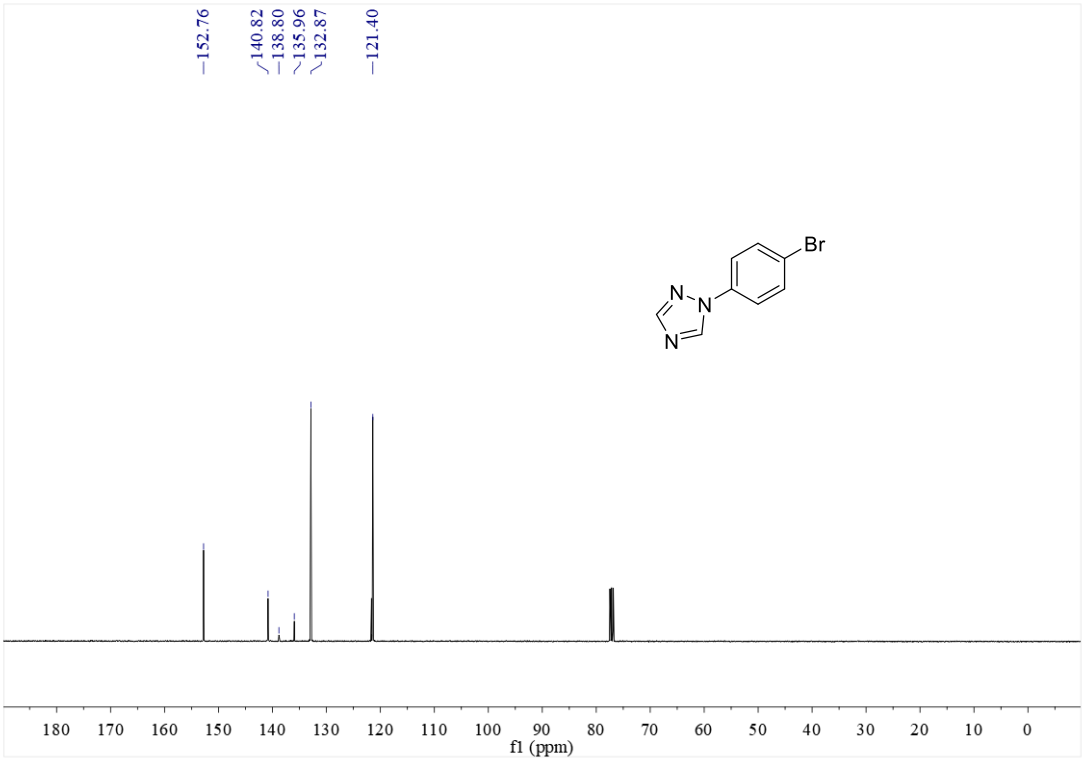


1-(4-Bromophenyl)-1*H*-1,2,4-triazole (6c)

^{1}H NMR of 6c

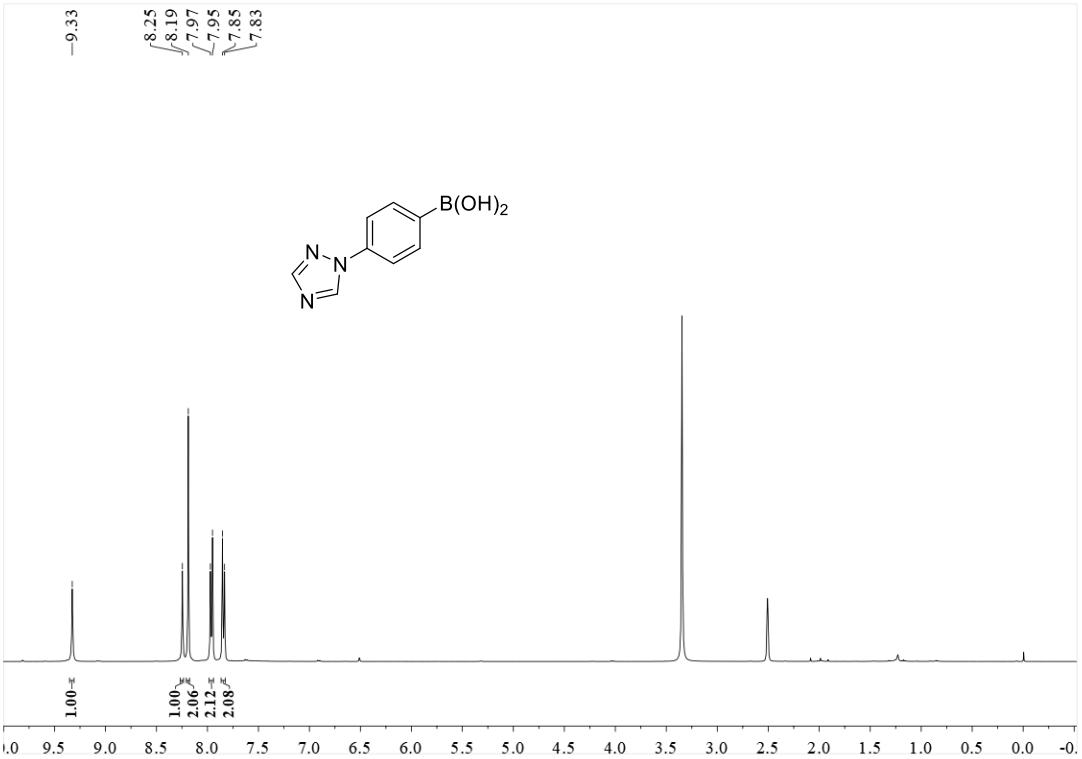


^{13}C NMR of 6c

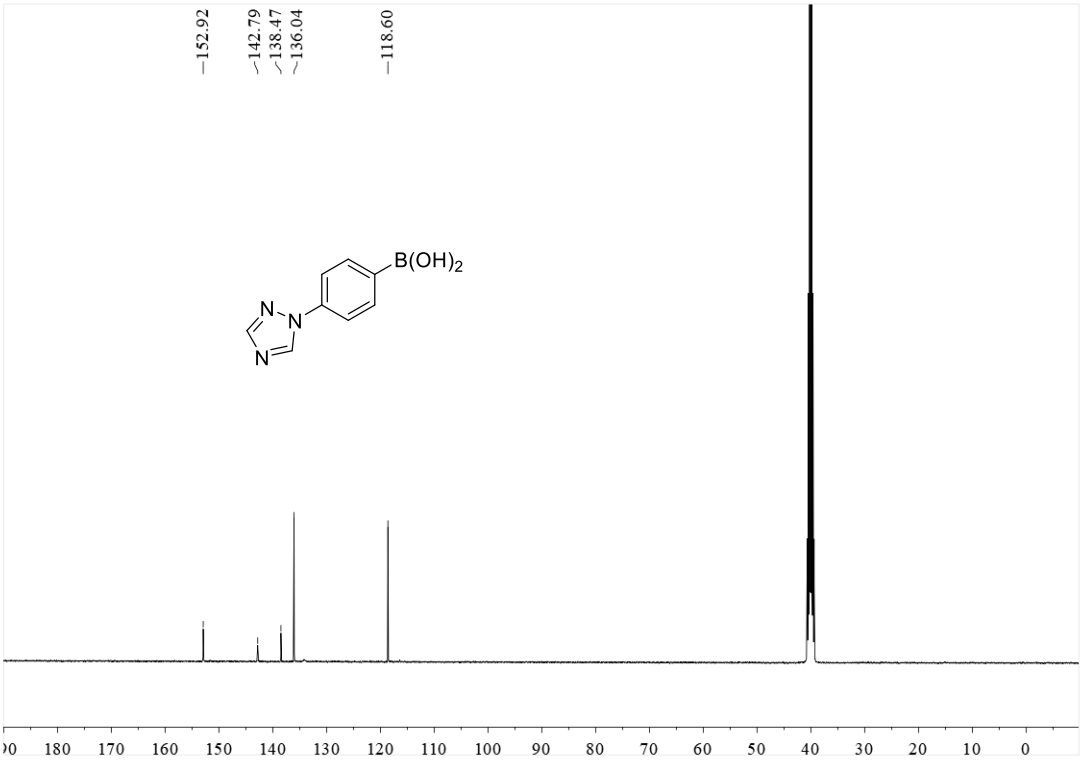


(4-(1*H*-1,2,4-Triazol-1-yl)phenyl)boronic acid (6d)

^{1}H NMR of 6d

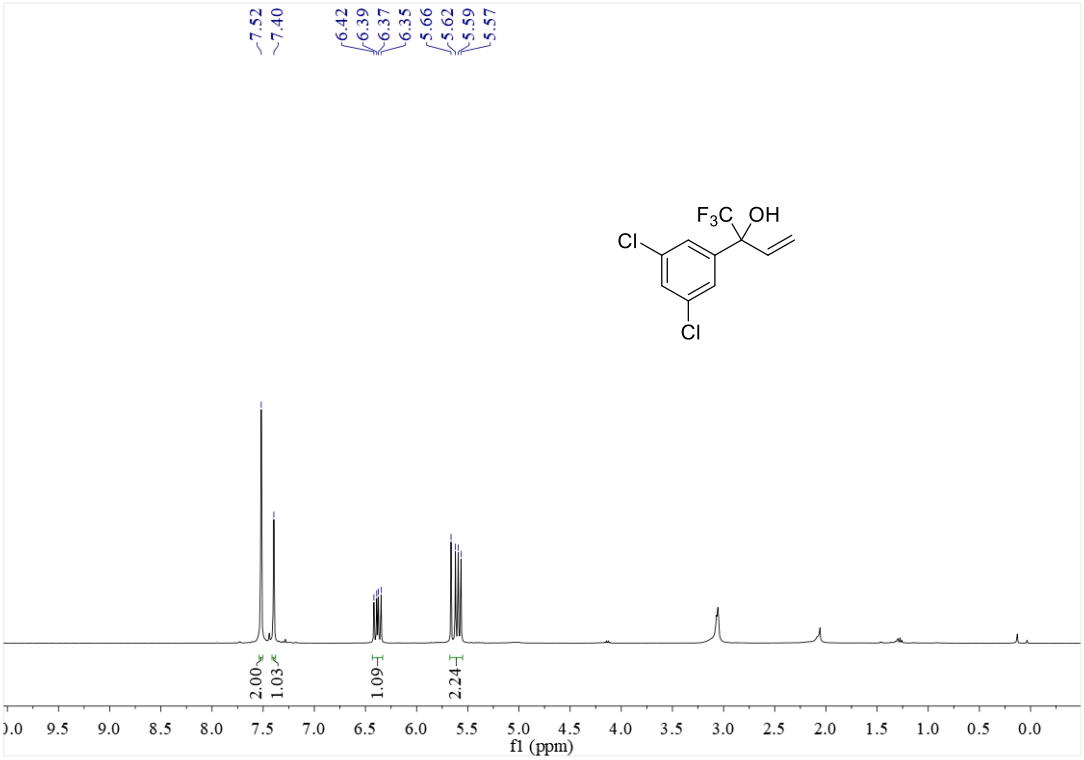


^{13}C NMR of 6d

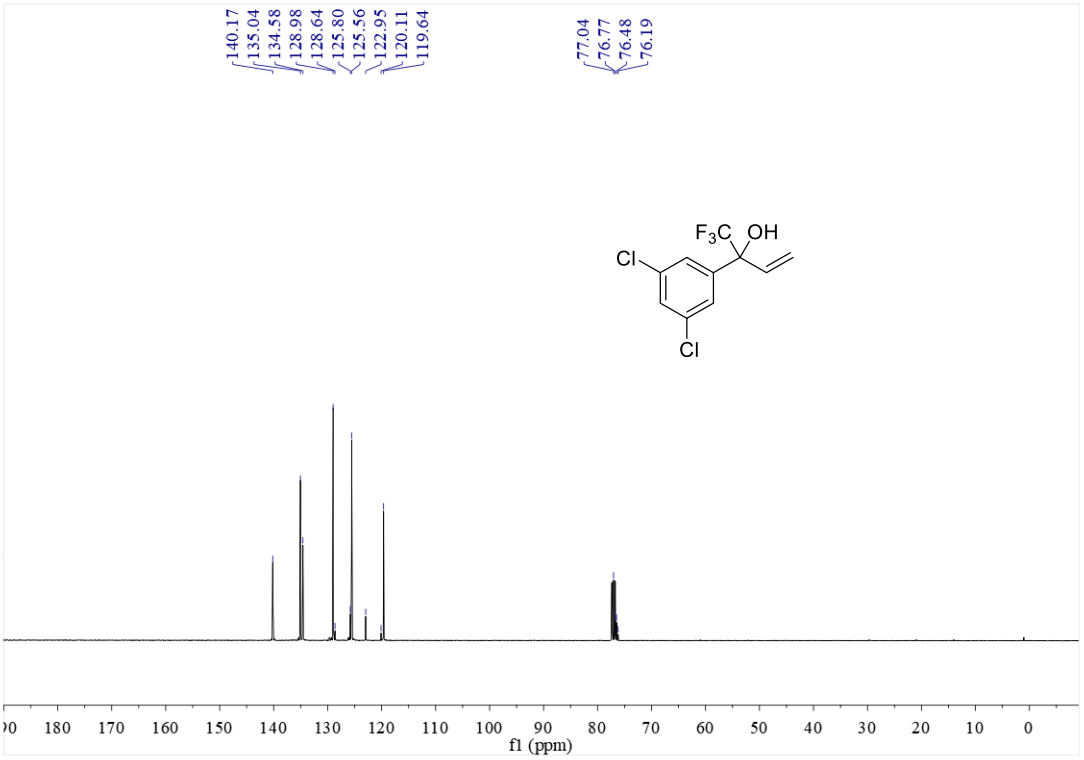


2-(3,5-Dichlorophenyl)-1,1,1-trifluorobut-3-en-2-ol (6g)

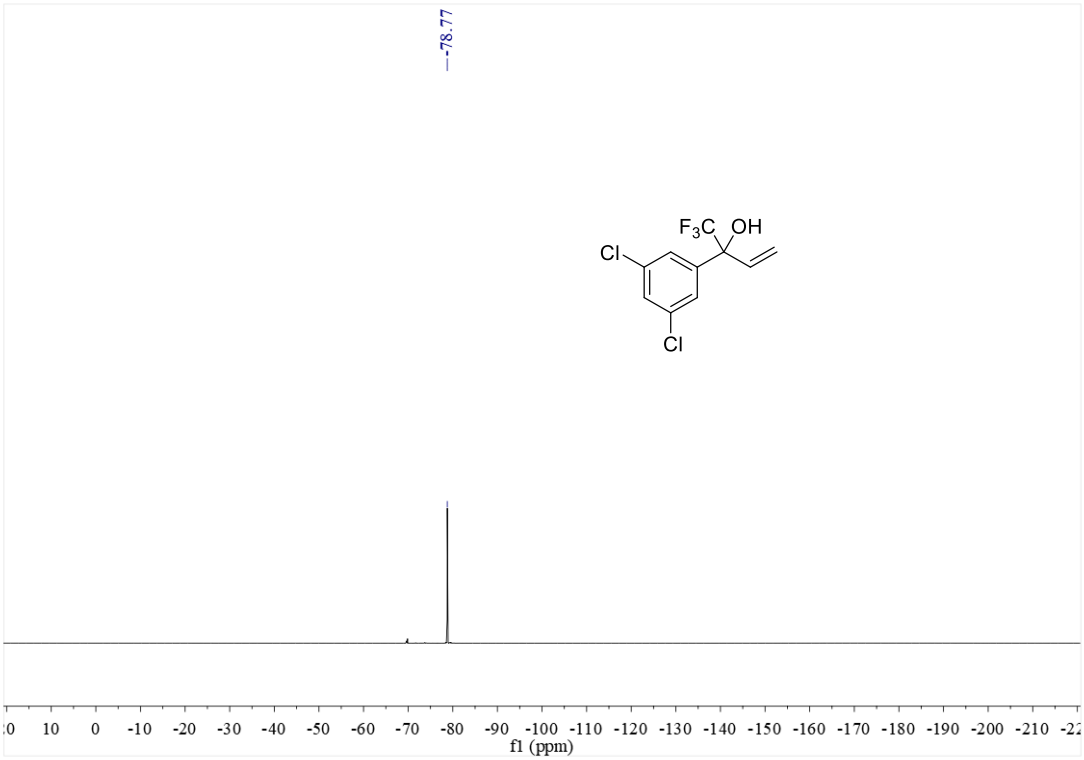
^{1}H NMR of 6g



^{13}C NMR of 6g

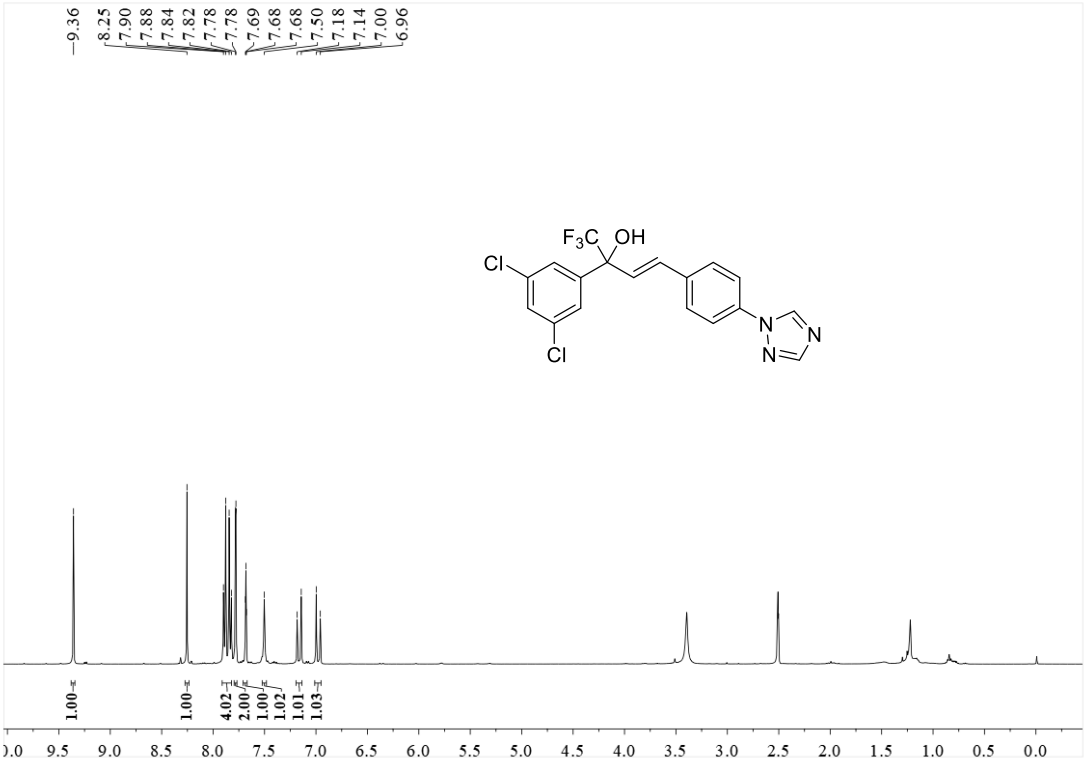


^{19}F NMR of 6g

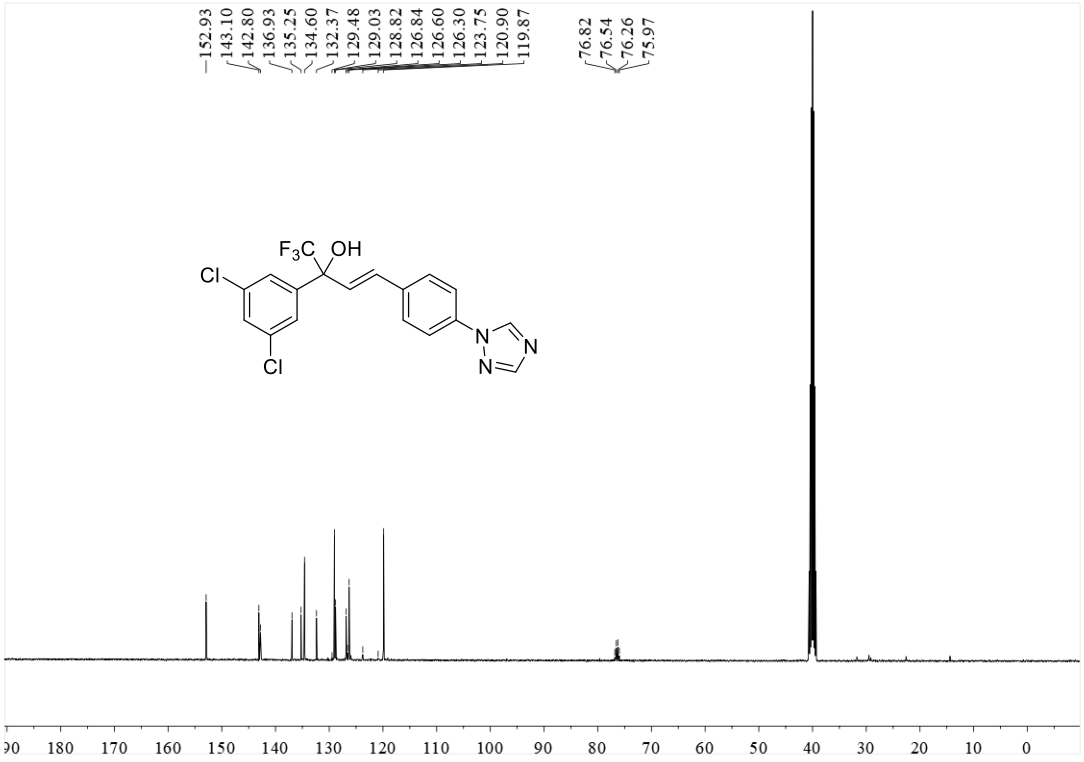


(*E*)-4-(4-(1*H*-1,2,4-Triazol-1-yl)phenyl)-2-(3,5-dichlorophenyl)-1,1,1-trifluorobut-3-en-2-ol (6h)

^{1}H NMR of 6h



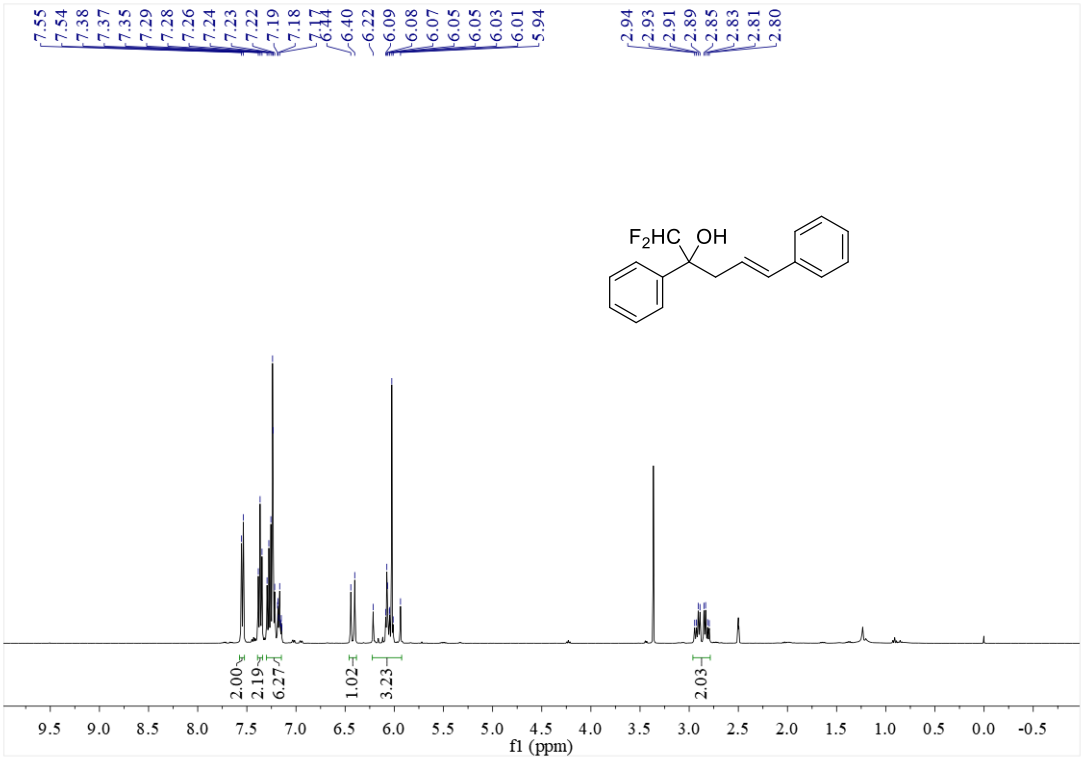
^{13}C NMR of 6h



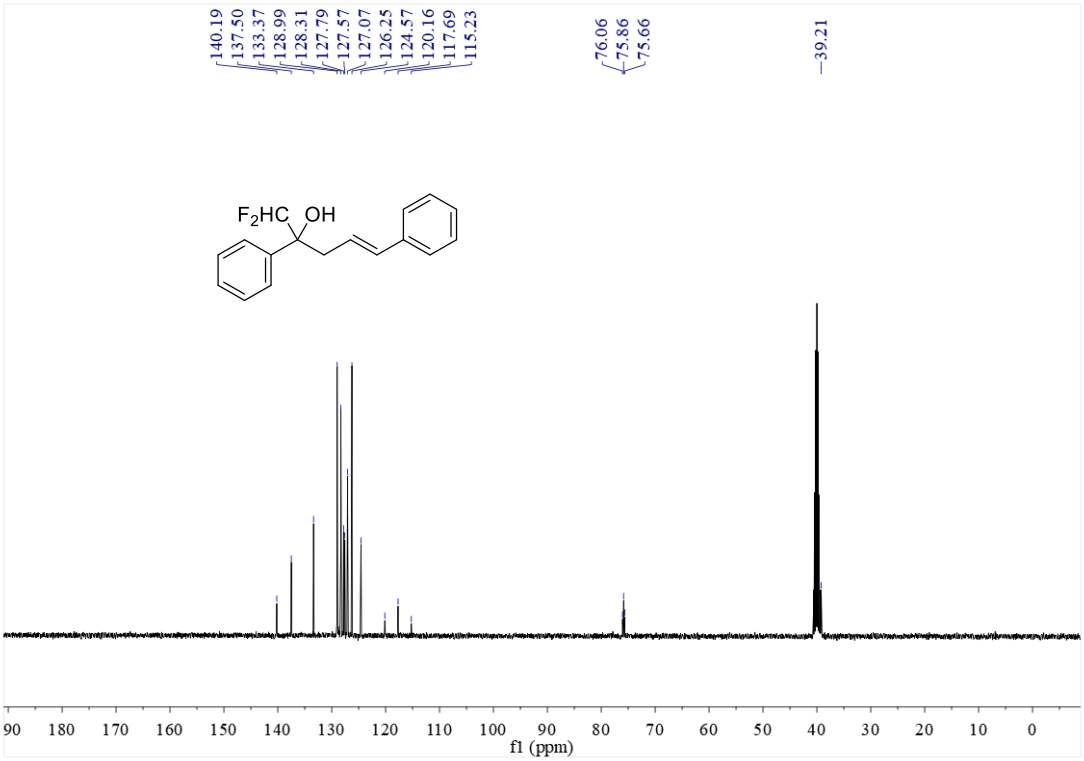
^{19}F NMR of 6h

(*E*)-1,1-Difluoro-2,5-diphenylpent-4-en-2-ol (10aa)

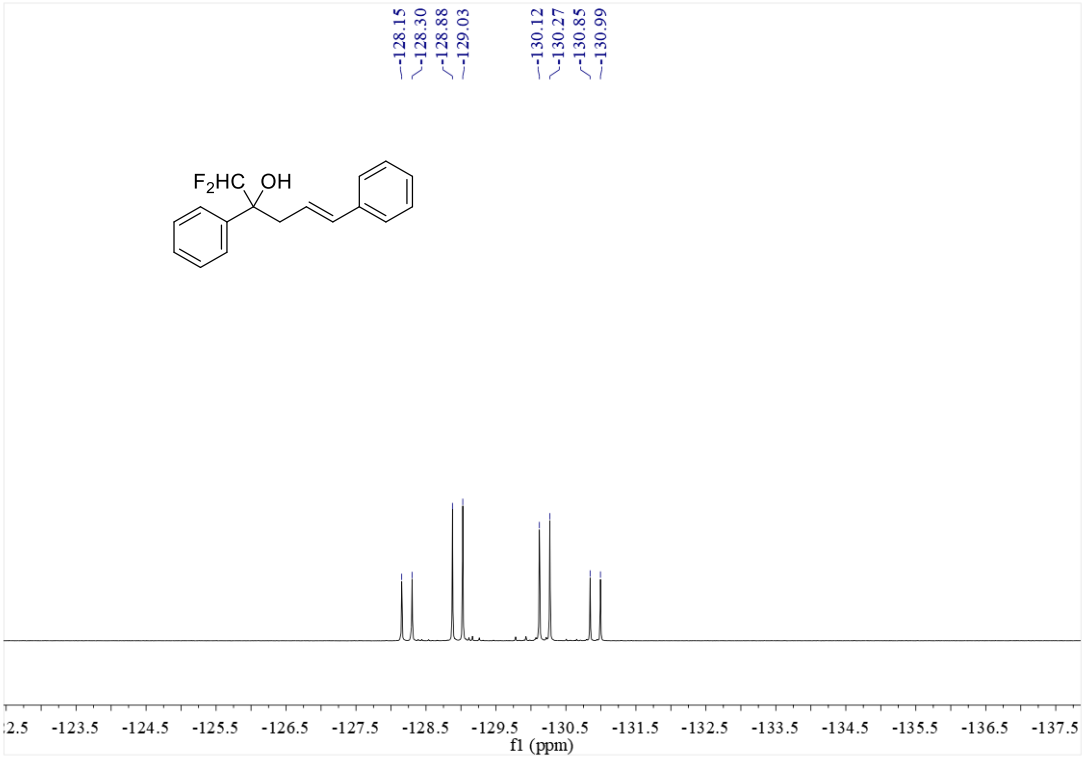
^{1}H NMR of 10aa



^{13}C NMR of 10aa

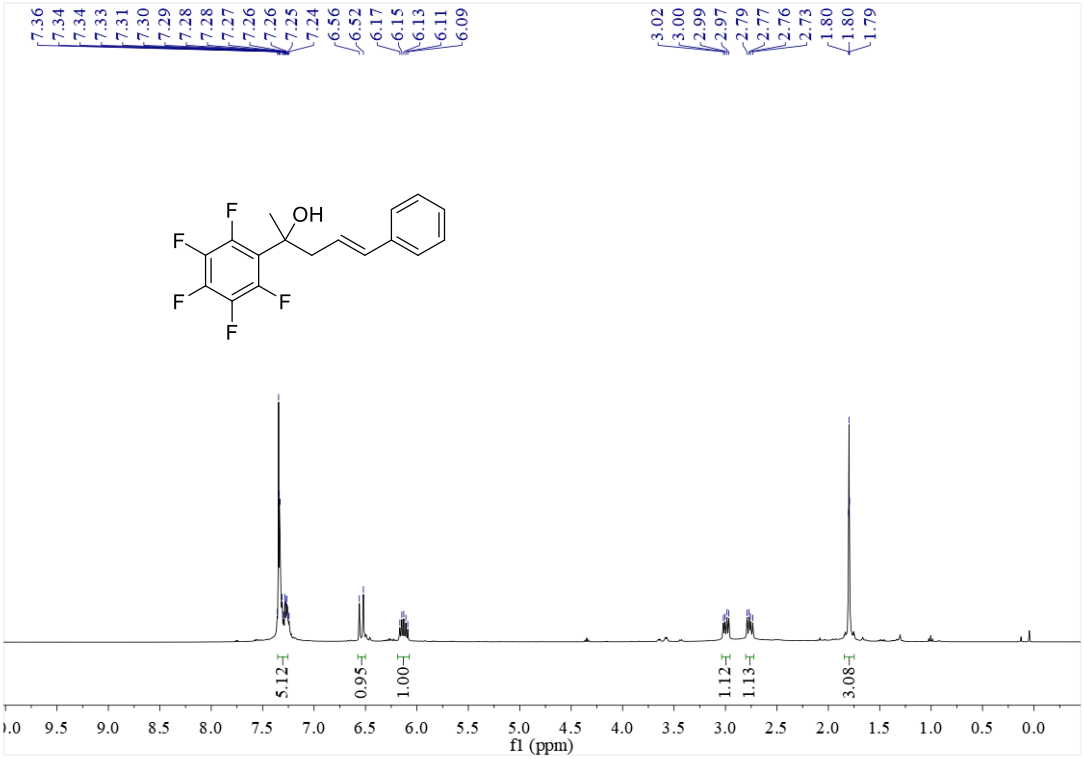


^{19}F NMR of 10aa

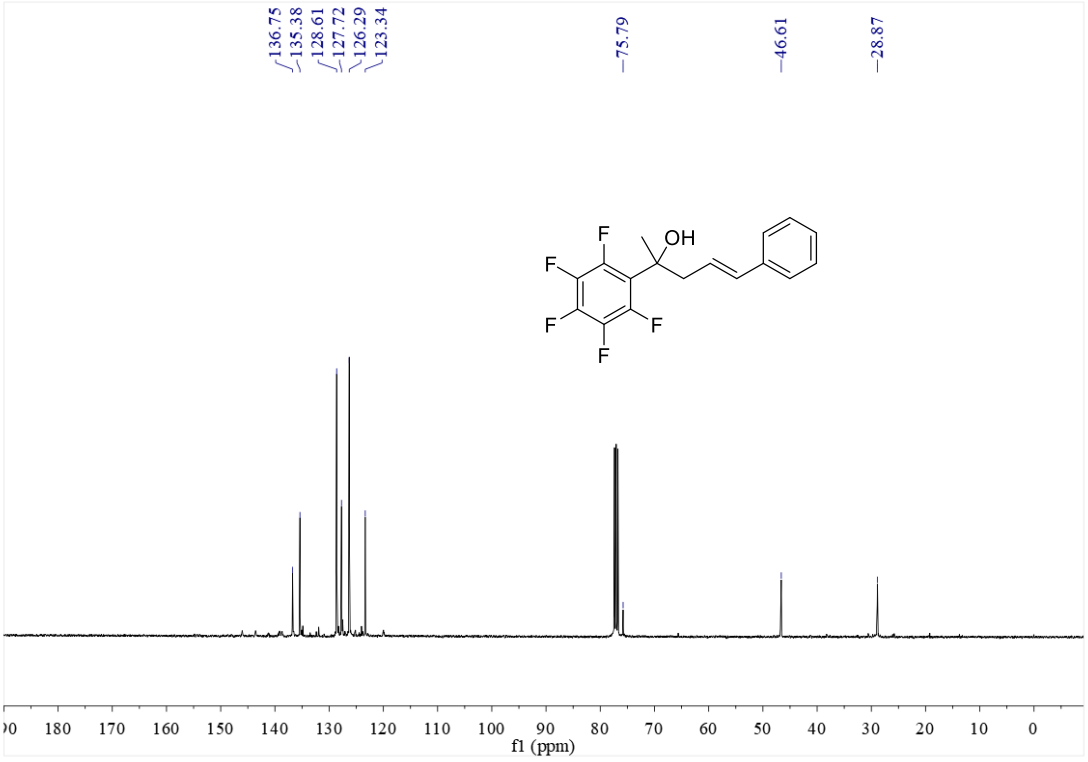


(E)-2-(Perfluorophenyl)-5-phenylpent-4-en-2-ol (11aa)

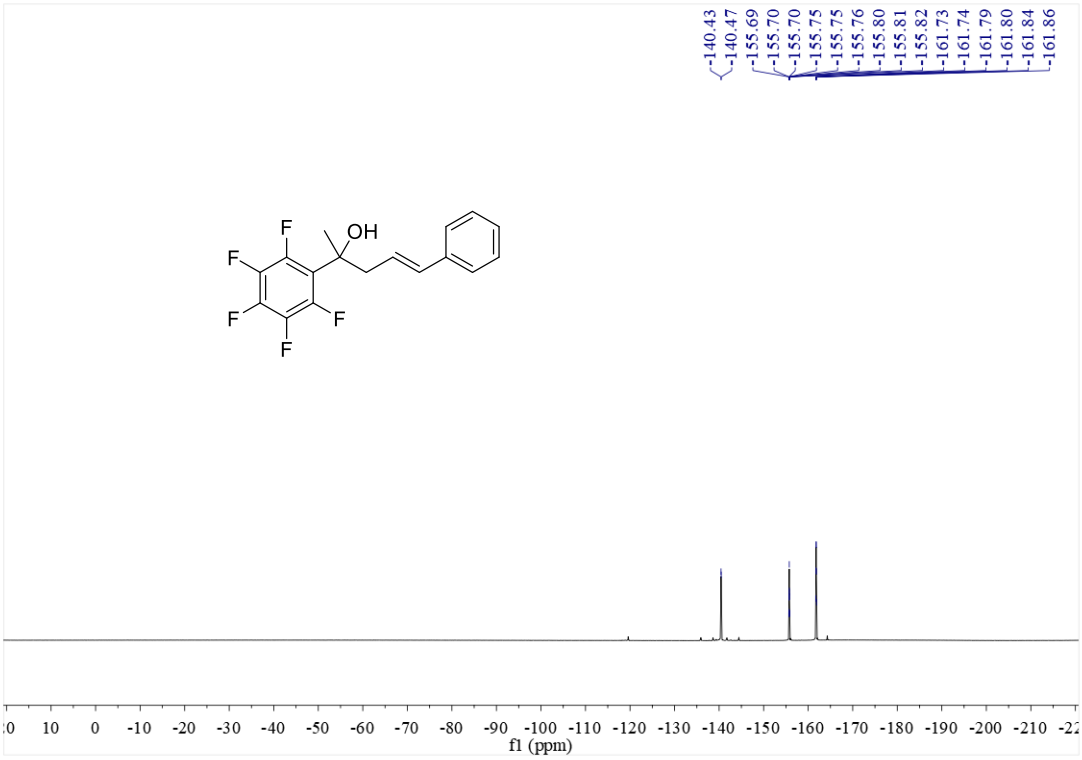
^{1}H NMR of 11aa



^{13}C NMR of 11aa



^{19}F NMR of 11aa



8. Supplementary References

1. Qiao, C.; Villar-Yanez, A.; Sprachmann, J.; Limburg, B.; Bo, C.; Kleij, A. W. Organocatalytic Trapping of Elusive Carbon Dioxide Based Heterocycles by a Kinetically Controlled Cascade Process. *Angew. Chem. Int. Ed.* **59**, 18446-18451(2020).
2. Chen, Y.; Ni, N.; Cheng, D.; Xu, X. The Coupling of Alkylboronic Acids with *α*-(trifluoromethyl)styrenes by Lewis Base/Photoredox Dual Catalysis. *Tetrahedron Lett.* **61**, 152425 (2020).
3. Davies, J.; Sheikh, N. S.; Leonori, D. Photoredox Imino Functionalizations of Olefins. *Angew. Chem. Int. Ed.* **56**, 13361-13365 (2017).
4. Guven, S.; Kundu, G.; Weßels, A.; Ward, J. S.; Rissanen, K.; Schoenebeck, F. Selective Synthesis of *Z*-Silyl Enol Ethers *via* Ni-Catalyzed Remote Functionalization of Ketones. *J. Am. Chem. Soc.* **143**, 8375-8380 (2021).
5. Iakovenko, R. O.; Kazakova, A. N.; Vasilyev, A. V. et al. Reactions of CF_3-Enones with Arenes under Superelectrophilic Activation: A Pathway to Trans-1,3-diaryl-1-CF_3-indanes, New Cannabinoid Receptor Ligands. *Org. Biomol. Chem.* **13**, 8827-8842 (2015).

6. Mercadante, M. A.; Kelly, C. B.; Tilley, L. J. et al. 1,3-γ-Silyl-Elimination in Electron-Deficient Cationic Systems. *Chem. Sci.* **5**, 3983-3994 (2014).

7. Jagannath, M. R. R.; Madhavan, G. R.; Shanmugam, P. Preparation of Oxoindolylidene Derivatives for Use as AMPK Activators. World Intellectual Property Organization, WO2014202528, A1, 2014-12-24.

8. Skaff, O.; Jolliffe, K. A.; Hutton, C. A. Synthesis of the Side Chain Cross-Linked Tyrosine Oligomers Dityrosine, Trityrosine, and Pulcherosine. *J. Org. Chem.* **70**, 7353-7363 (2005).

9. Wen, K.; Chow, S.; Sanghvi, Y. S.; Theodorakis, E. A. Synthesis of 2'-*O*-Methoxyethylguanosine Using a Novel Silicon-Based Protecting Group. *J. Org. Chem.* **67**, 7887-7889 (2002).

10. Adair, G. R. A.; Kapoor, K. K.; Scolan, A. L. B.; Williams, J. M. J. Ruthenium Catalysed Reduction of Alkenes using Sodium Borohydride. *Tetrahedron Lett.* **47**, 8943-8944 (2006).

11. Zhou, Y.; Klinger, G. E., Hegg, E. L.; Saffron, C. M.; Jackson, J. E. Multiple Mechanisms Mapped in Aryl Alkyl Ether Cleavage *via* Aqueous Electrocatalytic Hydrogenation over Skeletal Nickel. *J. Am. Chem. Soc*. **142**, 4037-4050 (2020).

12. Punna, N., Haradaa, K.; Shibata, N. Stille Cross-Coupling of Secondary and Tertiary α-(Trifluoromethyl)-Benzyl Chlorides with Allylstannanes. *Chem. Commun.* **54**, 7171-7174 (2018).

13. Gaussian 09 v. *Gaussian 09*, *Revision D. 01* (Gaussian, Inc,Wallingford., CT 2010).

14. Adamo, C.; Barone, V. Toward Reliable Density Functional Methods Without Adjustable Parameters: The PBE0 Model. *J. Chem. Phys.* **110**, 6158-6170 (1999).

15. Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. A Consistent and Accurate *ab initio* Parametrization of Density Functional Dispersion Correction (DFT-D) for the 94 Elements H-Pu. *J. Chem. Phys.* **132**, 154104 (2010).

16. Weigend, F.; Ahlrichs, R. Balanced Basis Sets of Split Valence, Triple Zeta Valence and Quadruple Zeta Valence Quality for H to Rn: Design and Assessment of Accuracy. *Phys. Chem. Chem. Phys.* **7**, 3297-3305 (2005).

17. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B* **113**, 6378-6396 (2009).

18. Hratchian, H. P.; Schlegel, H. B. Accurate Reaction Paths Using a Hessian Based Predictor-corrector Integrator. *J. Chem. Phys.* **120**, 9918 (2004).

9. Atomic cartesian coordinates of intermediates and transition states (presented in Å).

11a

	Coordinates (Angstroms)		
	X	Y	Z
C	2.654333	-0.368725	-0.149435
C	2.214362	0.942741	-0.153730
C	0.861688	1.232100	-0.005365
C	-0.104819	0.236302	0.148745
C	0.385162	-1.072389	0.162446
C	1.727361	-1.385414	0.014334
C	-1.611389	0.508522	0.310456
C	-2.373870	-0.177301	-0.842653
H	-1.987937	0.257649	-1.773785
H	-2.147837	-1.245255	-0.854124
C	-3.853099	0.032613	-0.762511
H	-4.192081	1.067271	-0.778497
C	-4.745505	-0.953094	-0.673713
H	-4.439474	-1.997844	-0.650510
H	-5.813171	-0.751657	-0.629002
O	-1.914666	1.879142	0.165107
H	-1.544211	2.351853	0.920460
C	-2.071644	0.019865	1.682707
H	-1.916997	-1.054160	1.805972
H	-3.136645	0.234961	1.803424
H	-1.517540	0.538219	2.472764
F	-0.443974	-2.113127	0.326222
F	0.560236	2.535082	0.003472

F	3.092036	1.935099	-0.293661
F	3.945610	-0.648320	-0.291242
F	2.125841	-2.656012	0.030182

1a

	Coordinates (Angstroms)		
	X	Y	Z

C	-3.826488	-0.281773	-0.473435
C	-3.343586	-0.816127	0.716772
C	-1.979888	-0.781618	0.998651
C	-1.081823	-0.209221	0.096067
C	-1.571651	0.313103	-1.105774
C	-2.934299	0.280244	-1.383978
H	-4.889895	-0.305853	-0.693630
H	-4.027360	-1.264648	1.431902
H	-1.610176	-1.214743	1.922214
H	-0.894639	0.751255	-1.830549
H	-3.298784	0.695995	-2.319070
C	0.411010	-0.235368	0.420313
C	1.097517	-1.330380	-0.411999
H	0.568747	-2.256426	-0.152839
H	0.911008	-1.137537	-1.472389
C	2.562486	-1.500646	-0.156384
H	2.852423	-1.680602	0.877422
C	3.490884	-1.469737	-1.110048
H	3.232002	-1.288352	-2.151767
H	4.542416	-1.627731	-0.884100

O	0.647751	-0.539656	1.774235
H	0.168566	0.105353	2.314244
C	1.054275	1.139242	0.157096
F	2.283310	1.218900	0.680018
F	1.165517	1.425246	-1.151704
F	0.328181	2.121877	0.725131

8a

Coordinates (Angstroms)

	X	Y	Z
C	3.469186	-0.470902	-0.316340
C	2.981668	0.814573	-0.533728
C	1.633392	1.100073	-0.322121
C	0.753376	0.109067	0.116392
C	1.251791	-1.182350	0.326654
C	2.596340	-1.470360	0.112348
H	4.519605	-0.694650	-0.480975
H	3.651008	1.601460	-0.871745
H	1.252155	2.100330	-0.501295
H	0.585238	-1.974443	0.657758
H	2.964175	-2.478970	0.281538
C	-0.725153	0.422144	0.334005
C	-1.542367	-0.239294	-0.793175
H	-1.179472	0.186711	-1.738327
H	-1.318796	-1.311157	-0.809953
C	-3.016413	-0.019182	-0.671822
H	-3.343922	1.019871	-0.662785

C	-3.919562	-0.994072	-0.571087
H	-3.626937	-2.043021	-0.571707
H	-4.982844	-0.780262	-0.491599
O	-0.972121	1.816770	0.209095
H	-0.605114	2.242776	0.994554
C	-1.186084	-0.052879	1.709627
H	-1.109213	-1.138738	1.813088
H	-2.230496	0.229711	1.868362
H	-0.575467	0.405318	2.495796

A1

	Coordinates (Angstroms)		
	X	Y	Z

H	5.743676	-3.602415	-0.250412
C	4.803274	-3.221447	-0.639350
C	3.052644	-1.551957	-0.606928
C	4.263895	-2.048549	-0.114510
H	4.787753	-1.521957	0.678613
C	-3.057208	-1.207211	-1.134536
C	-2.421379	-2.444848	-1.296373
C	-2.973751	-3.416641	-2.124893
H	-1.487372	-2.637931	-0.771490
H	-2.473374	-4.373837	-2.242665
P	-2.275518	0.000263	-0.001080
P	2.277471	-0.007730	0.000825
C	-3.034873	1.596073	-0.481299
C	-4.230729	2.073911	0.064355

C	-2.370538	2.356564	-1.452183
C	-4.755551	3.292282	-0.362101
H	-4.753818	1.497753	0.822833
C	-2.902138	3.567881	-1.883233
H	-1.430005	1.993589	-1.862498
C	-4.095179	4.038287	-1.336441
H	-5.683297	3.658027	0.068846
H	-2.379761	4.149531	-2.637985
H	-4.506249	4.988491	-1.665397
C	-3.046411	-0.375971	1.616479
C	-2.395331	0.088364	2.766586
C	-4.242178	-1.089887	1.745143
C	-2.941373	-0.142898	4.025272
H	-1.454715	0.627630	2.667499
C	-4.781349	-1.328395	3.007641
H	-4.754263	-1.460134	0.861269
C	-4.134667	-0.854185	4.146945
H	-2.429852	0.222873	4.911389
H	-5.710286	-1.884926	3.099491
H	-4.557473	-1.043190	5.129671
C	3.042930	0.242516	1.645613
C	4.219844	0.972388	1.840079
C	2.403658	-0.337764	2.748897
C	4.751960	1.112716	3.120332
H	4.721988	1.433482	0.994096
C	2.943103	-0.204512	4.024385
H	1.476849	-0.889332	2.599894
C	4.117514	0.523665	4.211840
H	5.665559	1.683399	3.263487
H	2.441320	-0.659901	4.873723

H	4.534377	0.636251	5.208776
C	3.046079	1.294706	-1.031527
C	2.398106	2.535287	-1.094084
C	4.234864	1.104826	-1.742657
C	2.939234	3.573821	-1.845262
H	1.464016	2.677721	-0.553570
C	4.768826	2.143568	-2.502589
H	4.744814	0.146314	-1.705640
C	4.124286	3.377805	-2.553171
H	2.429583	4.532564	-1.886594
H	5.690834	1.986447	-3.055491
H	4.541837	4.185052	-3.148249
Pd	0.000516	-0.009350	-0.003836
C	-4.158338	-3.155000	-2.812202
H	-4.585054	-3.909116	-3.467710
C	-4.790449	-1.922313	-2.663416
H	-5.711451	-1.713816	-3.200898
C	4.141509	-3.903049	-1.658943
H	4.564455	-4.817829	-2.064847
C	2.932384	-3.414692	-2.152144
H	2.408945	-3.947072	-2.941768
C	2.386421	-2.248995	-1.623317
H	1.433153	-1.873138	-1.991198
C	-4.245502	-0.951106	-1.825877
H	-4.746769	0.006125	-1.712085

A10

Coordinates (Angstroms)

	X	Y	Z
C	-0.114572	2.219590	-0.540425
C	0.343488	2.123764	-1.860570
C	1.170295	3.108959	-2.388843
H	0.067627	1.264298	-2.466049
H	1.520065	3.026829	-3.413969
P	-1.167384	0.871245	0.091019
C	-1.275925	1.087326	1.891509
C	-2.005495	2.142475	2.455911
C	-0.604952	0.186041	2.722590
C	-2.049014	2.294483	3.837703
H	-2.539512	2.840963	1.817728
C	-0.654187	0.341392	4.105759
H	-0.048776	-0.635043	2.282280
C	-1.373840	1.395173	4.662924
H	-2.613404	3.114760	4.271687
H	-0.132396	-0.364101	4.746102
H	-1.413527	1.515618	5.741838
C	-2.854145	1.235446	-0.500552
C	-3.950817	0.737420	0.215063
C	-3.067907	1.902424	-1.709705
C	-5.240022	0.900915	-0.279132
H	-3.799271	0.209810	1.151771
C	-4.361948	2.063381	-2.200091
H	-2.229081	2.300209	-2.272883
C	-5.448741	1.561052	-1.489384
H	-6.083034	0.506947	0.281285
H	-4.517586	2.586325	-3.139473
H	-6.456570	1.685033	-1.875349

Pd	-0.220023	-1.120078	-0.533293
C	1.567786	4.184934	-1.595619
H	2.225888	4.947263	-2.003109
C	1.127579	4.275362	-0.277510
H	1.440427	5.107646	0.346616
C	0.285025	3.298815	0.250744
H	-0.046306	3.377552	1.281394
C	-2.573973	-2.488991	0.565227
C	-3.865349	-3.023090	0.591179
C	-4.672380	-2.963815	-0.542752
C	-4.175288	-2.375578	-1.706026
C	-2.887034	-1.842616	-1.728692
C	-2.067273	-1.884320	-0.592420
H	-1.965681	-2.534706	1.467266
H	-4.240773	-3.480772	1.503772
H	-5.679299	-3.372001	-0.521605
H	-4.795048	-2.325627	-2.598487
H	-2.524362	-1.377489	-2.643271
O	1.617916	-0.216863	-0.287506
C	2.687538	-1.044482	-0.082909
C	3.991293	-0.299490	-0.399892
C	2.558443	-2.317232	-0.954898
C	2.739010	-1.446536	1.403787
C	3.919846	1.074280	-0.638358
C	5.232520	-0.938171	-0.481990
H	2.800637	-2.014185	-1.977927
H	3.278919	-3.086779	-0.656544
C	1.170933	-2.900398	-0.932099
F	1.626555	-2.114313	1.793004
F	3.775894	-2.255015	1.704677

F	2.833047	-0.371532	2.202799
C	5.065138	1.799526	-0.955982
H	2.946236	1.549490	-0.581447
C	6.378254	-0.212893	-0.802717
H	5.314758	-2.005013	-0.297814
H	0.916357	-3.574572	-0.115517
C	0.307928	-2.789869	-1.988434
C	6.299364	1.158130	-1.040526
H	4.990806	2.868222	-1.142003
H	7.335489	-0.723261	-0.869383
H	0.604864	-2.259352	-2.891906
H	-0.592039	-3.391991	-2.047801
H	7.194145	1.721028	-1.292514

A11

Coordinates (Angstroms)

	X	Y	Z
C	1.335668	1.941139	-1.394419
C	0.206094	1.919200	-2.222261
C	0.046935	2.887211	-3.210844
H	-0.557848	1.162368	-2.055982
H	-0.833093	2.864410	-3.848132
P	1.479809	0.663739	-0.092073
C	3.277637	0.592119	0.222690
C	3.816138	0.691269	1.507821
C	4.131605	0.333682	-0.858515
C	5.187153	0.536214	1.708755

H	3.169403	0.890651	2.357147
C	5.499605	0.191921	-0.656653
H	3.725612	0.246177	-1.863212
C	6.031477	0.289095	0.629791
H	5.593833	0.616117	2.713058
H	6.151701	-0.000773	-1.503987
H	7.099896	0.173161	0.788255
C	0.778228	1.457981	1.398957
C	0.453097	0.633173	2.484204
C	0.497008	2.824677	1.470452
C	-0.133964	1.169816	3.625512
H	0.648949	-0.435150	2.424846
C	-0.103938	3.357466	2.609904
H	0.734353	3.475507	0.634024
C	-0.418977	2.533396	3.687923
H	-0.381874	0.521098	4.461066
H	-0.326886	4.419970	2.652660
H	-0.890461	2.951133	4.573030
Pd	0.084110	-1.281146	-0.438257
C	1.009931	3.878957	-3.383885
H	0.886306	4.630018	-4.159260
C	2.132084	3.908742	-2.557601
H	2.882541	4.684204	-2.683767
C	2.295703	2.946111	-1.565259
H	3.171923	2.978205	-0.924446
C	1.500460	-3.093404	-0.816883
C	2.873841	-2.779629	-0.716146
C	3.479709	-2.681308	0.520116
C	2.725628	-2.883565	1.687939
C	1.381901	-3.199816	1.611392

C	0.744513	-3.348849	0.356800
H	1.084104	-3.340046	-1.791448
H	3.448737	-2.624173	-1.624176
H	4.534425	-2.434865	0.592858
H	3.204209	-2.795357	2.659366
H	0.804715	-3.376374	2.515346
C	-5.262076	1.590008	2.333740
C	-3.945389	1.984015	2.107358
C	-3.149480	1.284174	1.203126
C	-3.657728	0.182384	0.512755
C	-4.979908	-0.212088	0.746614
C	-5.775415	0.488962	1.649943
H	-5.884246	2.133093	3.040038
H	-3.531453	2.837646	2.638399
H	-2.118285	1.568643	1.021975
H	-5.395751	-1.068325	0.224844
H	-6.800163	0.170294	1.822257
C	-2.718686	-0.592136	-0.418874
C	-2.583045	-2.046197	0.060979
H	-2.452253	-1.993816	1.148136
H	-3.496506	-2.633150	-0.117687
C	-1.355543	-2.698802	-0.550989
H	-1.477587	-2.937924	-1.610822
C	-0.693659	-3.822867	0.233836
H	-1.126985	-3.920962	1.234403
H	-0.747566	-4.803494	-0.254680
O	-1.475013	0.020157	-0.455472
C	-3.281437	-0.528882	-1.848226
F	-2.445787	-1.079086	-2.753702
F	-4.461894	-1.169213	-1.992556

F	-3.476413	0.742972	-2.242604

A12

	Coordinates (Angstroms)		
	X	Y	Z

H	3.519436	3.666395	-2.447069
C	3.800351	2.863685	-1.771395
C	3.265954	0.780097	-0.664975
C	2.917847	1.813725	-1.540822
H	1.950492	1.795682	-2.038459
C	-1.517368	2.906111	-0.314687
C	-2.545231	3.544712	0.381123
C	-3.530568	4.243462	-0.314666
H	-2.584283	3.492376	1.465442
H	-4.333641	4.729287	0.232682
P	-0.192561	1.974260	0.529817
P	2.141205	-0.661074	-0.558182
C	1.103502	3.254734	0.740467
C	1.030844	4.488054	0.085129
C	2.203542	2.994347	1.568747
C	2.035383	5.438888	0.255415
H	0.188661	4.715285	-0.559992
C	3.198058	3.948558	1.747188
H	2.282772	2.045692	2.088114
C	3.118390	5.174954	1.088025
H	1.963046	6.391528	-0.261854
H	4.041155	3.729820	2.396142

H	3.899026	5.918275	1.222863
C	-0.819887	1.740473	2.240493
C	-0.488324	2.596082	3.296921
C	-1.682434	0.661106	2.481422
C	-0.992305	2.362184	4.574935
H	0.162683	3.448117	3.129587
C	-2.188205	0.436324	3.758453
H	-1.973683	0.025528	1.648455
C	-1.837318	1.280488	4.810793
H	-0.723579	3.031824	5.387223
H	-2.857577	-0.402606	3.929150
H	-2.225971	1.100304	5.809264
C	2.731512	-1.532013	-2.058153
C	4.020698	-2.076171	-2.131637
C	1.939548	-1.498068	-3.210331
C	4.479733	-2.631177	-3.321527
H	4.676915	-2.053192	-1.266753
C	2.407180	-2.043837	-4.403701
H	0.963013	-1.025812	-3.178302
C	3.671340	-2.623848	-4.457694
H	5.477252	-3.059134	-3.364165
H	1.781503	-2.010713	-5.291182
H	4.034668	-3.054842	-5.386300
C	2.730875	-1.576672	0.906133
C	3.221437	-2.884012	0.882818
C	2.562045	-0.934691	2.141215
C	3.539610	-3.533870	2.074284
H	3.342776	-3.413156	-0.056182
C	2.902179	-1.575374	3.325468
H	2.135070	0.063126	2.176686

C	3.387080	-2.882564	3.294424
H	3.905434	-4.556113	2.043371
H	2.766517	-1.062649	4.273450
H	3.635711	-3.394338	4.219741
Pd	-0.075515	-0.235256	-0.457754
C	-3.486013	4.319407	-1.704494
H	-4.256089	4.862765	-2.244940
C	-2.451803	3.694967	-2.401926
H	-2.413373	3.750300	-3.486359
C	5.034939	2.891522	-1.123560
H	5.721427	3.715096	-1.298227
C	5.382952	1.866534	-0.246703
H	6.342081	1.887293	0.263097
C	4.503808	0.810453	-0.017975
H	4.785410	0.012649	0.662828
C	-1.475569	2.985272	-1.710922
H	-0.681983	2.480582	-2.256904
C	-0.270203	-2.725517	1.892571
C	-0.367278	-3.045687	3.244805
C	-0.220436	-4.365147	3.666113
C	0.019495	-5.360262	2.719405
C	0.108090	-5.033622	1.368918
C	-0.028960	-3.710756	0.931111
H	-0.371690	-1.690928	1.570554
H	-0.553021	-2.256291	3.969269
H	-0.294251	-4.616861	4.720655
H	0.132948	-6.394849	3.033102
H	0.290500	-5.817818	0.636547
C	-6.840065	-1.016783	0.471774
C	-5.971146	0.032079	0.765946

C	-4.681689	0.042769	0.239304
C	-4.242453	-0.994088	-0.586212
C	-5.121941	-2.039695	-0.885590
C	-6.410903	-2.051722	-0.357083
H	-7.845118	-1.028557	0.884768
H	-6.297528	0.845631	1.409005
H	-3.989782	0.848356	0.462648
H	-4.804497	-2.850778	-1.533914
H	-7.080851	-2.874426	-0.592941
C	-2.805676	-0.958427	-1.117037
C	-2.090859	-2.282025	-0.869521
H	-2.291220	-2.532265	0.178196
H	-2.499937	-3.108135	-1.469864
C	-0.580472	-2.165241	-1.089812
H	-0.377365	-2.138513	-2.163262
C	0.120223	-3.400964	-0.540293
H	-0.257760	-4.275957	-1.094159
H	1.190062	-3.367001	-0.783378
O	-2.097104	0.051933	-0.501872
C	-2.890836	-0.642394	-2.624097
F	-1.686694	-0.391730	-3.181731
F	-3.430549	-1.653653	-3.340060
F	-3.643485	0.447539	-2.864096

A13

Coordinates (Angstroms)		
X	Y	Z

H	2.842202	2.676518	4.592510
C	2.678070	2.836978	3.530628
C	1.310115	2.508256	1.561743
C	1.536282	2.313200	2.926612
H	0.822821	1.755234	3.525234
C	2.849943	-0.451549	0.836725
C	2.151442	-1.177396	1.810993
C	2.649596	-1.273147	3.105485
H	1.223134	-1.678886	1.550126
H	2.100498	-1.840690	3.851334
P	2.144019	-0.455091	-0.847320
P	-0.160548	1.831230	0.705886
C	3.152624	0.677858	-1.855734
C	4.500074	0.417261	-2.133419
C	2.547860	1.826327	-2.376657
C	5.238207	1.315492	-2.897630
H	4.970419	-0.486662	-1.755523
C	3.289500	2.721542	-3.143491
H	1.493514	2.009482	-2.178686
C	4.635281	2.469116	-3.398797
H	6.284649	1.112641	-3.106651
H	2.813962	3.612575	-3.543418
H	5.214503	3.166595	-3.997316
C	2.640577	-2.118687	-1.453032
C	2.082090	-2.616612	-2.636107
C	3.584051	-2.890729	-0.768222
C	2.448502	-3.869047	-3.116492
H	1.345510	-2.027339	-3.176229
C	3.943696	-4.149552	-1.247377
H	4.035820	-2.521043	0.146509

C	3.374293	-4.643439	-2.417216
H	2.002116	-4.245052	-4.032734
H	4.668827	-4.744081	-0.698875
H	3.649341	-5.627978	-2.784786
C	-1.328960	1.472173	2.062708
C	-2.319551	2.372507	2.464477
C	-1.228187	0.230956	2.704037
C	-3.191061	2.038763	3.499336
H	-2.420457	3.332468	1.967359
C	-2.088788	-0.091572	3.748490
H	-0.477306	-0.485292	2.383320
C	-3.073854	0.811023	4.146729
H	-3.962478	2.742418	3.799295
H	-1.995586	-1.051920	4.247300
H	-3.752152	0.554917	4.955696
C	-0.838864	3.313982	-0.124521
C	-1.540221	3.135713	-1.322379
C	-0.686433	4.604027	0.399491
C	-2.084672	4.232935	-1.985425
H	-1.674754	2.129274	-1.708160
C	-1.230121	5.697563	-0.268473
H	-0.141553	4.756081	1.326715
C	-1.928290	5.514117	-1.461622
H	-2.631001	4.083302	-2.912805
H	-1.108196	6.695225	0.144069
H	-2.349239	6.370634	-1.980979
Pd	-0.041178	0.002949	-0.855563
C	3.846646	-0.640889	3.439292
H	4.235586	-0.711335	4.451170
C	4.537944	0.089520	2.476174

H	5.464079	0.594316	2.735653
C	3.601091	3.561164	2.781580
H	4.488308	3.970404	3.256383
C	3.382955	3.756192	1.418411
H	4.097884	4.318577	0.824195
C	2.247209	3.232001	0.811107
H	2.083507	3.399371	-0.248947
C	4.044524	0.185565	1.175851
H	4.590315	0.760845	0.435042
C	-6.383320	-1.449352	1.153642
C	-5.365679	-0.567662	1.510685
C	-4.292110	-0.349663	0.650263
C	-4.212917	-1.012057	-0.576055
C	-5.243797	-1.888357	-0.932543
C	-6.318544	-2.106684	-0.073315
H	-7.220298	-1.623950	1.824408
H	-5.404917	-0.046163	2.463486
H	-3.483985	0.323405	0.914504
H	-5.220264	-2.408569	-1.885003
H	-7.107022	-2.795504	-0.365215
C	-2.993536	-0.745042	-1.482857
C	-2.424220	-2.074391	-2.026253
H	-3.221109	-2.657382	-2.504218
H	-1.723436	-1.830355	-2.836699
C	-1.678416	-2.940803	-1.065378
H	-1.145827	-3.764563	-1.542963
C	-1.541081	-2.768842	0.256208
H	0.035352	-1.169183	-1.856626
O	-2.102473	0.070862	-0.837193
C	-3.495933	0.048594	-2.708631

F	-2.475262	0.401776	-3.520736
F	-4.369800	-0.633333	-3.480705
F	-4.107032	1.191105	-2.349625
H	-2.074543	-1.957224	0.744195
C	-0.648335	-3.547778	1.120538
C	-0.826060	-3.496273	2.511720
C	0.441439	-4.280116	0.619591
C	0.044684	-4.156914	3.373715
H	-1.661189	-2.928226	2.913480
C	1.311167	-4.939528	1.480453
H	0.631719	-4.303993	-0.449820
C	1.120028	-4.880671	2.861368
H	-0.114519	-4.101919	4.447398
H	2.155928	-5.486827	1.070770
H	1.808926	-5.387153	3.531497

A14

Coordinates (Angstroms)

	X	Y	Z
H	1.785710	1.328735	4.991632
C	2.079213	0.653634	4.192322
C	2.662809	0.305341	1.866822
C	2.288936	1.158293	2.909534
H	2.152436	2.220025	2.725421
C	-1.128166	-2.152614	1.034496
C	-2.067700	-3.149779	1.316499
C	-2.687096	-3.198386	2.563435

H	-2.323186	-3.891111	0.566191
H	-3.419074	-3.974119	2.769110
P	-0.176412	-2.053810	-0.530321
P	2.718078	0.881470	0.121746
C	1.231886	-3.192816	-0.205260
C	1.307238	-4.027351	0.912792
C	2.322423	-3.131511	-1.084613
C	2.459645	-4.775804	1.154114
H	0.476372	-4.083480	1.609606
C	3.469989	-3.878638	-0.843765
H	2.278605	-2.466274	-1.944183
C	3.543666	-4.698028	0.283748
H	2.510408	-5.414666	2.031734
H	4.313560	-3.805716	-1.524844
H	4.445152	-5.270773	0.482813
C	-1.170638	-2.995426	-1.748167
C	-1.801681	-2.282051	-2.772296
C	-1.308626	-4.388719	-1.701136
C	-2.594825	-2.941107	-3.709272
H	-1.662012	-1.206880	-2.836155
C	-2.099629	-5.046790	-2.638500
H	-0.793641	-4.960000	-0.933149
C	-2.750387	-4.323545	-3.637862
H	-3.083507	-2.375491	-4.497736
H	-2.205570	-6.127058	-2.591611
H	-3.366583	-4.840284	-4.368313
C	3.188371	2.648087	0.278155
C	4.510974	3.094936	0.186359
C	2.164975	3.580627	0.491570
C	4.803443	4.450623	0.313131

H	5.316394	2.387457	0.013354
C	2.462623	4.933741	0.629930
H	1.132116	3.247368	0.546926
C	3.782200	5.371456	0.539323
H	5.833706	4.787352	0.236419
H	1.659618	5.646369	0.795532
H	4.013922	6.428420	0.637246
C	4.216408	0.082674	-0.559827
C	4.226059	-0.212398	-1.928446
C	5.327213	-0.258332	0.220628
C	5.326781	-0.837031	-2.508701
H	3.355098	0.035429	-2.532058
C	6.422798	-0.892738	-0.358996
H	5.333817	-0.036521	1.284046
C	6.424241	-1.183257	-1.722455
H	5.321928	-1.064416	-3.571045
H	7.277726	-1.159923	0.255913
H	7.279122	-1.681593	-2.170949
Pd	0.883817	-0.057392	-0.842843
C	-2.381110	-2.249746	3.537026
H	-2.871384	-2.287208	4.505789
C	-1.454083	-1.246282	3.260303
H	-1.212963	-0.499214	4.011429
C	2.247333	-0.704331	4.450514
H	2.081209	-1.095421	5.450298
C	2.632936	-1.558778	3.417680
H	2.769175	-2.620184	3.606392
C	2.833937	-1.061120	2.135148
H	3.116039	-1.741411	1.336554
C	-0.833438	-1.196687	2.015496

H	-0.108794	-0.415773	1.793378
C	-5.044942	5.014184	0.717778
C	-3.982864	4.637753	1.535857
C	-2.927075	3.892851	1.016519
C	-2.926581	3.506603	-0.325017
C	-3.988919	3.896420	-1.145141
C	-5.041998	4.643461	-0.625094
H	-5.870422	5.592445	1.123299
H	-3.973566	4.923338	2.584157
H	-2.103945	3.594636	1.655825
H	-4.007128	3.615923	-2.193333
H	-5.865199	4.931795	-1.272813
C	-1.760634	2.695800	-0.878604
C	-2.196068	1.577685	-1.832343
H	-2.599926	2.018110	-2.750000
H	-1.283632	1.040086	-2.147013
C	-3.168562	0.573951	-1.302128
H	-3.607115	-0.058175	-2.072768
C	-3.516961	0.374385	-0.024622
H	-0.443131	1.456039	-0.100374
O	-1.009893	2.207218	0.205316
C	-0.845944	3.660369	-1.660274
F	0.258807	3.031964	-2.113204
F	-1.456881	4.190033	-2.732695
F	-0.432444	4.677165	-0.892160
H	-3.105563	1.018801	0.748301
C	-4.446606	-0.656941	0.446761
C	-5.021471	-0.517477	1.717999
C	-4.764530	-1.799913	-0.305083
C	-5.900848	-1.474016	2.216863

H	-4.770469	0.354687	2.317271
C	-5.641901	-2.755256	0.193484
H	-4.299701	-1.957311	-1.274511
C	-6.216470	-2.597325	1.455511
H	-6.335641	-1.344627	3.204386
H	-5.867714	-3.637005	-0.400495
H	-6.897046	-3.349554	1.844561

A15

Coordinates (Angstroms)

	X	Y	Z

H	-5.336047	-2.227902	1.045493
C	-4.579590	-2.448592	0.297505
C	-2.243127	-2.489383	-0.354419
C	-3.239522	-2.221434	0.594048
H	-2.970742	-1.842255	1.572648
C	-2.400553	0.675446	1.748987
C	-1.480012	0.142989	2.659800
C	-1.912973	-0.397198	3.867967
H	-0.422882	0.131538	2.407244
H	-1.188829	-0.824252	4.556107
P	-1.735966	1.321592	0.170917
P	-0.504388	-2.026852	-0.005080
C	-3.013706	1.141002	-1.112299
C	-4.229701	1.837255	-1.064135
C	-2.747002	0.298466	-2.195830
C	-5.174511	1.659813	-2.068826

H	-4.432450	2.531941	-0.254372
C	-3.694151	0.126573	-3.202189
H	-1.792000	-0.217893	-2.246916
C	-4.910055	0.800919	-3.135497
H	-6.116066	2.199271	-2.023084
H	-3.479112	-0.534704	-4.036536
H	-5.649730	0.666767	-3.919751
C	-1.669512	3.120988	0.485543
C	-1.890364	4.036615	-0.548551
C	-1.276378	3.585772	1.744454
C	-1.709602	5.398111	-0.326073
H	-2.187956	3.687726	-1.532428
C	-1.095829	4.948832	1.962090
H	-1.097872	2.885156	2.555344
C	-1.308391	5.856941	0.927465
H	-1.878392	6.101373	-1.136638
H	-0.786610	5.299725	2.942666
H	-1.163398	6.920042	1.097580
C	-0.107395	-2.848993	1.576769
C	-0.949238	-3.749585	2.234932
C	1.134370	-2.528718	2.138567
C	-0.563541	-4.294164	3.458723
H	-1.905027	-4.028600	1.803554
C	1.518250	-3.080666	3.355542
H	1.793618	-1.860214	1.592391
C	0.663592	-3.956329	4.024865
H	-1.226596	-4.987650	3.968478
H	2.484901	-2.825003	3.781236
H	0.956788	-4.381241	4.980828
C	0.421630	-2.983801	-1.254045

C	0.926839	-4.259912	-0.996078
C	0.596220	-2.416306	-2.521072
C	1.602075	-4.958598	-1.994857
H	0.797622	-4.709987	-0.015879
C	1.253689	-3.123754	-3.522277
H	0.226714	-1.412524	-2.715928
C	1.763031	-4.394504	-3.258506
H	1.998996	-5.947836	-1.784347
H	1.382618	-2.676021	-4.503684
H	2.287261	-4.942532	-4.036483
Pd	0.219380	0.282838	-0.276546
C	-3.271188	-0.404315	4.176716
H	-3.615143	-0.837818	5.111493
C	-4.190580	0.144800	3.282918
H	-5.250327	0.141860	3.521616
C	-4.946175	-2.954186	-0.947822
H	-5.993037	-3.126243	-1.181416
C	-3.961048	-3.247022	-1.887411
H	-4.235111	-3.652146	-2.857512
C	-2.619128	-3.016842	-1.595131
H	-1.867706	-3.240425	-2.345540
C	-3.760314	0.686212	2.075104
H	-4.492577	1.085185	1.381446
C	0.555879	2.270406	-2.382666
C	0.930674	3.455266	-3.022041
C	1.542829	4.476596	-2.299112
C	1.767112	4.304642	-0.933295
C	1.384480	3.123203	-0.298213
C	0.788174	2.079300	-1.014236
H	0.079277	1.487171	-2.969004

H	0.741012	3.576362	-4.086365
H	1.834624	5.400142	-2.792339
H	2.236379	5.096668	-0.353872
H	1.554521	3.026238	0.769205
C	3.502461	2.904967	2.973279
C	2.576271	1.862941	2.999418
C	2.549626	0.928298	1.968632
C	3.432829	1.016877	0.889555
C	4.380456	2.043111	0.891354
C	4.408909	2.985329	1.918762
H	3.520255	3.644638	3.769083
H	1.866614	1.781624	3.819143
H	1.813145	0.133244	1.977052
H	5.091912	2.135139	0.076954
H	5.141780	3.787454	1.890426
C	3.318181	-0.013886	-0.248715
C	3.763207	0.616256	-1.596504
H	3.273031	1.589272	-1.687336
H	4.844619	0.804036	-1.570028
C	3.452821	-0.214369	-2.802522
H	3.679477	-1.276035	-2.742517
C	2.961534	0.274165	-3.941922
H	2.716827	1.328668	-4.051829
H	2.798061	-0.362792	-4.808133
O	2.094357	-0.625323	-0.317049
C	4.312404	-1.139993	0.118915
F	4.248684	-2.189556	-0.720964
F	5.596018	-0.721005	0.114804
F	4.082271	-1.635383	1.352369

A16

	Coordinates (Angstroms)		
	X	Y	Z
H	4.824152	-4.280266	-1.656981
C	4.586880	-3.320361	-1.207414
C	2.942483	-1.738056	-0.407909
C	3.257750	-2.977046	-0.978736
H	2.467074	-3.672821	-1.244400
P	1.209634	-1.319132	-0.036843
C	0.219251	-2.257226	-1.243880
C	-0.385986	-3.476929	-0.932620
C	0.047590	-1.701200	-2.517272
C	-1.164252	-4.129717	-1.887241
H	-0.259311	-3.915680	0.052520
C	-0.722590	-2.360155	-3.468624
H	0.506002	-0.743870	-2.754172
C	-1.334921	-3.572978	-3.152217
H	-1.638264	-5.074840	-1.638199
H	-0.856164	-1.921418	-4.453361
H	-1.946709	-4.081754	-3.891796
C	0.869169	-2.092112	1.577820
C	-0.428049	-1.965060	2.093664
C	1.849109	-2.771367	2.305375
C	-0.738191	-2.524118	3.327831
H	-1.172542	-1.421944	1.515276
C	1.529872	-3.323100	3.545103
H	2.856200	-2.873709	1.912366

C	0.240126	-3.201879	4.056138
H	-1.744549	-2.422372	3.724783
H	2.293514	-3.850068	4.110112
H	-0.003235	-3.633492	5.023002
Pd	0.503516	0.826664	-0.075725
C	5.607579	-2.436730	-0.861848
H	6.644100	-2.706007	-1.044001
C	5.297942	-1.206199	-0.286449
H	6.090296	-0.513822	-0.017126
C	3.969894	-0.854795	-0.063167
H	3.729091	0.109505	0.376518
C	-6.125716	-0.203412	-1.675038
C	-4.989110	-1.007899	-1.721667
C	-3.814115	-0.596873	-1.097086
C	-3.758550	0.621148	-0.417625
C	-4.902146	1.425251	-0.373040
C	-6.077236	1.014377	-0.998796
H	-7.042871	-0.520721	-2.163913
H	-5.014494	-1.958601	-2.248454
H	-2.914035	-1.202780	-1.128785
H	-4.885401	2.375372	0.152319
H	-6.957661	1.650367	-0.958635
C	-2.425398	1.032504	0.220709
C	-2.000600	2.425716	-0.291770
H	-2.059961	2.378951	-1.383799
H	-2.689436	3.209950	0.044240
C	-0.601098	2.795948	0.115387
H	-0.455401	3.102228	1.149489
C	0.400750	3.027580	-0.798253
H	1.996526	1.176693	-0.054135

O	-1.452986	0.112214	-0.067232
C	-2.629319	1.063024	1.749127
F	-1.474854	1.268528	2.419185
F	-3.477958	2.028096	2.159955
F	-3.121319	-0.107003	2.200474
H	0.167557	2.865395	-1.851758
C	1.652554	3.773114	-0.557167
C	2.434504	4.129133	-1.661992
C	2.077754	4.162591	0.721233
C	3.614889	4.850198	-1.498832
H	2.110865	3.834118	-2.657483
C	3.254893	4.881197	0.883153
H	1.491260	3.894372	1.595558
C	4.030441	5.227852	-0.225245
H	4.208433	5.115998	-2.369187
H	3.571775	5.173833	1.880473
H	4.951105	5.788999	-0.093092

A2

Coordinates (Angstroms)

	X	Y	Z
H	-2.295456	2.042621	4.275861
C	-1.938035	2.156201	3.256143
C	-1.711461	1.277828	1.014024
C	-2.182046	1.150006	2.324577
H	-2.717340	0.256204	2.629490
C	1.708605	-0.833228	1.431869

C	2.219131	-2.120239	1.634910
C	1.965932	-2.797451	2.825672
H	2.809442	-2.601559	0.860517
H	2.367478	-3.796813	2.969461
P	1.856990	-0.014487	-0.197122
P	-1.886597	-0.027356	-0.256825
C	2.339159	1.706013	0.190082
C	2.920299	2.094419	1.402112
C	2.106039	2.672222	-0.796525
C	3.247792	3.429780	1.625763
H	3.110283	1.358876	2.177934
C	2.444578	4.003605	-0.575632
H	1.641535	2.376644	-1.734851
C	3.009794	4.385591	0.640290
H	3.690962	3.722653	2.573430
H	2.255671	4.744207	-1.347636
H	3.262482	5.426775	0.820069
C	3.392698	-0.753969	-0.871932
C	3.268885	-1.800659	-1.791994
C	4.667959	-0.336838	-0.474583
C	4.402769	-2.431220	-2.299143
H	2.277865	-2.116379	-2.109233
C	5.799666	-0.960272	-0.991776
H	4.778968	0.475928	0.237800
C	5.669213	-2.009155	-1.901504
H	4.295788	-3.245312	-3.010572
H	6.786605	-0.627938	-0.681854
H	6.555039	-2.493661	-2.302585
C	-2.265845	-1.549508	0.682351
C	-3.518988	-1.776344	1.266027

C	-1.258360	-2.508745	0.828185
C	-3.747003	-2.934323	2.003497
H	-4.316424	-1.048234	1.143791
C	-1.488163	-3.665654	1.568538
H	-0.292912	-2.340521	0.359068
C	-2.731465	-3.877507	2.159544
H	-4.720285	-3.101767	2.456420
H	-0.696151	-4.401027	1.678564
H	-2.913590	-4.780515	2.735589
C	-3.502910	0.356095	-1.031902
C	-4.035057	-0.572331	-1.938441
C	-4.195594	1.545556	-0.788844
C	-5.242063	-0.318311	-2.579122
H	-3.502520	-1.499941	-2.138174
C	-5.401497	1.800924	-1.440611
H	-3.799625	2.272272	-0.085605
C	-5.928005	0.871934	-2.333584
H	-5.647241	-1.048287	-3.274506
H	-5.932368	2.728109	-1.242330
H	-6.868799	1.072497	-2.838453
Pd	0.002608	-0.174784	-1.595407
C	1.202827	-2.199469	3.826360
H	1.003160	-2.731768	4.752042
C	0.699378	-0.914064	3.634017
H	0.106502	-0.435370	4.408620
C	-1.230277	3.299209	2.887045
H	-1.031537	4.076146	3.619920
C	-0.775251	3.442121	1.577387
H	-0.218818	4.327572	1.282875
C	-1.013484	2.434706	0.647076

H	-0.635408	2.531604	-0.367428
C	0.948279	-0.235227	2.445591
H	0.550293	0.764472	2.308357
O	-0.558913	-0.358585	-3.806707
O	0.725860	-0.320161	-3.729724

A3

Coordinates (Angstroms)

	X	Y	Z
H	-2.150895	2.211564	4.246543
C	-1.843413	2.299100	3.208329
C	-1.639082	1.329419	1.004643
C	-2.044296	1.229917	2.338559
H	-2.491953	0.313763	2.709778
C	1.639696	-0.749756	1.482594
C	2.077601	-2.062320	1.698300
C	1.844827	-2.687619	2.919593
H	2.593472	-2.601859	0.909158
H	2.187449	-3.706724	3.074927
P	1.779260	-0.019843	-0.183796
P	-1.779186	-0.033245	-0.198702
C	2.220863	1.734162	0.069153
C	2.834449	2.212715	1.231400
C	1.948324	2.620782	-0.979595
C	3.152171	3.563581	1.347047
H	3.056540	1.537431	2.051938
C	2.277619	3.967668	-0.865471

H	1.462530	2.252741	-1.880550
C	2.873660	4.442062	0.301980
H	3.619333	3.929248	2.257016
H	2.058341	4.647990	-1.683391
H	3.119984	5.495801	0.397306
C	3.330122	-0.765313	-0.811099
C	3.310572	-1.532712	-1.978208
C	4.533876	-0.590583	-0.115251
C	4.485551	-2.123620	-2.443302
H	2.377845	-1.654716	-2.525546
C	5.701689	-1.180497	-0.584112
H	4.558916	0.001372	0.795828
C	5.678571	-1.949212	-1.748867
H	4.464924	-2.719262	-3.351770
H	6.631906	-1.041925	-0.040305
H	6.592926	-2.409543	-2.112802
C	-2.192231	-1.523918	0.767631
C	-3.437479	-1.673076	1.392013
C	-1.238882	-2.540147	0.877734
C	-3.706831	-2.812627	2.143068
H	-4.195312	-0.900677	1.289352
C	-1.511606	-3.678821	1.631711
H	-0.284086	-2.434070	0.371414
C	-2.743015	-3.813302	2.267881
H	-4.672320	-2.922404	2.628680
H	-0.761877	-4.460254	1.717138
H	-2.957489	-4.701979	2.854831
C	-3.342237	0.326388	-1.078642
C	-3.649238	-0.439703	-2.210097
C	-4.241935	1.302450	-0.640460

C	-4.847975	-0.237962	-2.885895
H	-2.939165	-1.182029	-2.565319
C	-5.437812	1.506291	-1.326593
H	-4.014769	1.901308	0.236624
C	-5.743456	0.736537	-2.446019
H	-5.079561	-0.836385	-3.762647
H	-6.132324	2.266994	-0.981208
H	-6.676363	0.897423	-2.979017
Pd	0.001791	-0.308921	-1.626069
C	1.171359	-2.012266	3.935931
H	0.985467	-2.504004	4.886544
C	0.742484	-0.703273	3.730085
H	0.223432	-0.165964	4.518898
C	-1.238809	3.469988	2.754600
H	-1.071235	4.295803	3.440188
C	-0.849253	3.580680	1.420569
H	-0.376262	4.489581	1.059923
C	-1.050934	2.515215	0.549288
H	-0.734947	2.595075	-0.487070
C	0.975381	-0.072660	2.510980
H	0.642387	0.948914	2.366184
O	-0.715094	-0.664021	-3.466674
O	0.669793	-0.668719	-3.498685

A4

Coordinates (Angstroms)		
X	Y	Z

H	-6.293467	-0.728234	1.538519
C	-5.591982	-0.574785	0.723665
C	-3.356893	-0.776803	-0.171954
C	-4.268391	-0.982361	0.868721
H	-3.949515	-1.455852	1.792078
C	-1.345629	2.450787	0.874786
C	-1.247823	2.862138	2.207497
C	-2.387460	3.277007	2.890942
H	-0.293413	2.835731	2.723323
H	-2.307756	3.583833	3.929925
P	0.072455	1.815067	-0.072276
P	-1.614865	-1.296101	-0.083685
C	0.667874	3.258727	-1.023491
C	-0.091664	4.422665	-1.167200
C	1.922705	3.168238	-1.642232
C	0.399556	5.486064	-1.922895
H	-1.061364	4.509023	-0.686521
C	2.407723	4.235006	-2.390327
H	2.519139	2.265053	-1.539686
C	1.646953	5.395366	-2.533870
H	-0.195020	6.389321	-2.026635
H	3.382701	4.159519	-2.863746
H	2.027820	6.226939	-3.120000
C	1.412566	1.515421	1.122951
C	1.794036	0.201271	1.404444
C	2.072839	2.578996	1.753398
C	2.800695	-0.053037	2.332307
H	1.308777	-0.619525	0.886600
C	3.083377	2.320443	2.673546
H	1.800482	3.605288	1.522050

C	3.444483	1.005155	2.967170
H	3.095483	-1.077714	2.538408
H	3.592944	3.147487	3.159554
H	4.237951	0.807349	3.682317
C	-1.189353	-1.397067	1.688922
C	-0.332208	-2.402778	2.150420
C	-1.607179	-0.394015	2.571132
C	0.113366	-2.391501	3.468838
H	0.000354	-3.190540	1.481341
C	-1.157521	-0.386937	3.887983
H	-2.282390	0.384152	2.233866
C	-0.290924	-1.380098	4.338092
H	0.781604	-3.174809	3.814935
H	-1.486320	0.400528	4.560257
H	0.064009	-1.369848	5.364602
C	-1.640736	-3.043128	-0.623202
C	-0.446031	-3.637324	-1.046097
C	-2.815270	-3.802683	-0.587577
C	-0.427029	-4.979196	-1.417647
H	0.471422	-3.056553	-1.087266
C	-2.790971	-5.141102	-0.969470
H	-3.749972	-3.354675	-0.264548
C	-1.598550	-5.732057	-1.382831
H	0.505734	-5.432058	-1.742259
H	-3.708135	-5.722698	-0.943174
H	-1.583992	-6.776644	-1.680754
Pd	-0.284860	0.010958	-1.439438
C	-3.626048	3.287486	2.251643
H	-4.514285	3.599620	2.793581
C	-3.724743	2.897306	0.917231

H	-4.685959	2.903348	0.411656
C	-6.015666	0.024434	-0.460852
H	-7.048308	0.344186	-0.567828
C	-5.115636	0.211711	-1.508836
H	-5.442747	0.676308	-2.434521
C	-3.790075	-0.184299	-1.364249
H	-3.078554	-0.020995	-2.171039
C	-2.588252	2.480511	0.231327
H	-2.667054	2.163913	-0.804296
O	0.140039	-0.923773	-3.210666
O	0.662649	0.375200	-3.194272
C	6.062373	-2.106813	1.452172
C	6.121227	-0.885617	0.780532
C	5.205752	-0.605936	-0.230559
C	4.218541	-1.532369	-0.595918
C	4.182565	-2.756620	0.086902
C	5.091574	-3.045335	1.102545
H	6.770629	-2.326125	2.247048
H	6.876034	-0.152282	1.052697
H	5.241544	0.354153	-0.739712
H	3.420235	-3.485803	-0.177128
H	5.042951	-3.997359	1.625062
B	3.122662	-1.169614	-1.662019
O	3.083237	0.102484	-2.151440
H	2.240455	0.258021	-2.655538
O	2.226997	-2.135583	-2.026788
H	1.477983	-1.780408	-2.571947

A5

	Coordinates (Angstroms)		
	X	Y	Z
H	-2.814644	-0.202311	4.613024
C	-2.921434	0.140352	3.587985
C	-2.409841	-0.119460	1.238886
C	-2.280508	-0.550364	2.563512
H	-1.683478	-1.425961	2.798173
C	0.372964	1.639165	1.893215
C	1.033013	0.551657	2.482057
C	1.043767	0.402569	3.864633
H	1.541249	-0.176023	1.853436
H	1.563242	-0.441063	4.310430
P	0.503002	1.762509	0.081952
P	-1.554454	-1.006645	-0.108077
C	-0.692025	2.978550	-0.550054
C	-0.668625	4.316364	-0.133814
C	-1.593286	2.580246	-1.541921
C	-1.572665	5.226687	-0.670801
H	0.062997	4.650187	0.596553
C	-2.490075	3.497266	-2.084613
H	-1.589360	1.550145	-1.889028
C	-2.486771	4.817361	-1.641807
H	-1.556779	6.260536	-0.338374
H	-3.188094	3.177500	-2.852967
H	-3.187589	5.533321	-2.061767
C	2.100557	2.602739	-0.200932
C	2.327796	3.183463	-1.455417
C	3.112237	2.624192	0.761688

C	3.552583	3.775878	-1.740026
H	1.545286	3.174832	-2.210597
C	4.339525	3.217347	0.469900
H	2.949728	2.184406	1.740986
C	4.562979	3.791425	-0.778163
H	3.719064	4.226543	-2.714420
H	5.119673	3.232491	1.225841
H	5.519990	4.254320	-1.001607
C	-1.318147	-2.681587	0.568325
C	-2.352814	-3.621657	0.572915
C	-0.087221	-2.997783	1.154313
C	-2.158810	-4.864696	1.168778
H	-3.308402	-3.390052	0.111231
C	0.096184	-4.237227	1.760562
H	0.726905	-2.279805	1.119485
C	-0.937988	-5.171019	1.767523
H	-2.963895	-5.594002	1.165988
H	1.053050	-4.475473	2.215587
H	-0.790906	-6.140672	2.235000
C	-2.806477	-1.125590	-1.427385
C	-2.379887	-1.150301	-2.760442
C	-4.174699	-1.195951	-1.135856
C	-3.313876	-1.236925	-3.788929
H	-1.314791	-1.118743	-2.974713
C	-5.102622	-1.286021	-2.169132
H	-4.518468	-1.171028	-0.106277
C	-4.674385	-1.302180	-3.495141
H	-2.977079	-1.251372	-4.821631
H	-6.162271	-1.338348	-1.936289
H	-5.401997	-1.364403	-4.299517

Pd	0.436639	-0.290645	-0.927383
C	0.381059	1.328318	4.668586
H	0.381100	1.210045	5.748386
C	-0.293828	2.398207	4.085121
H	-0.826278	3.111359	4.707845
C	-3.693590	1.263860	3.301797
H	-4.193218	1.799480	4.103955
C	-3.821898	1.699409	1.984587
H	-4.423217	2.573658	1.751968
C	-3.184840	1.012405	0.956283
H	-3.304976	1.353021	-0.066368
C	-0.298057	2.559233	2.701206
H	-0.838672	3.389875	2.260311
O	0.542038	-2.117853	-1.761826
O	1.599482	-2.117413	-2.728135
C	3.575575	-1.292689	0.387163
C	3.939034	-1.854335	1.613088
C	3.984891	-3.239812	1.757291
C	3.669819	-4.050688	0.665151
C	3.299316	-3.473824	-0.548324
C	3.235677	-2.082983	-0.721820
H	3.537822	-0.209465	0.289417
H	4.183085	-1.210697	2.455965
H	4.265979	-3.684982	2.708538
H	3.702541	-5.133261	0.767732
H	3.028679	-4.117973	-1.382864
B	2.765398	-1.455712	-2.142059
O	3.766685	-1.396586	-3.173520
H	4.631899	-1.428295	-2.759013
O	2.301200	-0.008021	-1.804423

H	2.220309	0.471834	-2.639341

A6

Coordinates (Angstroms)

	X	Y	Z
H	-3.723364	-4.571747	0.739862
C	-3.162405	-3.731631	1.139421
C	-2.268715	-1.501861	0.855225
C	-2.995148	-2.588615	0.360390
H	-3.421840	-2.557697	-0.636320
C	0.606628	-2.563817	-0.412110
C	0.015681	-2.586247	-1.681676
C	-0.602999	-3.739158	-2.154340
H	0.033571	-1.693706	-2.299005
H	-1.058326	-3.738392	-3.140626
P	1.438554	-1.011667	0.084363
P	-1.991773	0.037782	-0.092654
C	1.842721	-1.137506	1.854743
C	2.679429	-2.143314	2.356443
C	1.330577	-0.172001	2.727361
C	2.963690	-2.199164	3.717083
H	3.117930	-2.875431	1.684168
C	1.620777	-0.227374	4.088095
H	0.705477	0.624835	2.329417
C	2.431241	-1.245317	4.584163
H	3.607647	-2.985491	4.100070
H	1.215847	0.526406	4.757215

H	2.658284	-1.290921	5.645518
C	3.078697	-1.158982	-0.726666
C	4.216632	-0.649464	-0.089629
C	3.194463	-1.670131	-2.022667
C	5.443226	-0.639184	-0.745108
H	4.143754	-0.241386	0.912835
C	4.424863	-1.658355	-2.675395
H	2.328259	-2.077702	-2.533880
C	5.550529	-1.139130	-2.041744
H	6.316344	-0.234397	-0.241155
H	4.500036	-2.058211	-3.682759
H	6.508175	-1.126126	-2.554347
C	-2.805240	-0.198370	-1.706505
C	-4.179694	-0.453936	-1.807546
C	-2.043422	-0.070370	-2.871841
C	-4.770223	-0.611919	-3.056556
H	-4.787825	-0.522732	-0.909651
C	-2.638122	-0.225799	-4.121990
H	-0.985140	0.168076	-2.795579
C	-3.999378	-0.502739	-4.214263
H	-5.834939	-0.815155	-3.127281
H	-2.038129	-0.123592	-5.021693
H	-4.464821	-0.624033	-5.188401
C	-3.097431	1.257777	0.723136
C	-3.596120	2.321915	-0.042405
C	-3.397896	1.205705	2.088177
C	-4.383788	3.304841	0.547817
H	-3.366010	2.382473	-1.100046
C	-4.183652	2.195276	2.675457
H	-3.034486	0.388705	2.702223

C	-4.677979	3.246727	1.908759
H	-4.767233	4.120011	-0.059577
H	-4.412959	2.136118	3.735765
H	-5.292715	4.015703	2.368109
Pd	0.243638	0.878304	-0.357739
C	-0.647158	-4.880273	-1.356686
H	-1.136800	-5.779914	-1.718435
C	-0.076801	-4.858484	-0.085795
H	-0.125225	-5.739198	0.548174
C	-2.611235	-3.803603	2.416266
H	-2.745522	-4.697811	3.018218
C	-1.873633	-2.730012	2.910637
H	-1.423140	-2.778804	3.898035
C	-1.696423	-1.591659	2.131422
H	-1.101908	-0.770739	2.518145
C	0.550093	-3.708099	0.387595
H	0.974863	-3.705967	1.385410
O	-0.751911	2.628853	-0.795265
O	0.033701	3.837263	-0.773887
C	2.713477	2.344532	0.490610
C	3.930180	3.006669	0.306328
C	4.502591	3.084025	-0.961160
C	3.847612	2.496772	-2.044486
C	2.635822	1.833173	-1.855081
C	2.047955	1.750021	-0.586953
H	2.291580	2.291760	1.491527
H	4.432037	3.458836	1.159171
H	5.452285	3.592888	-1.104521
H	4.286132	2.548319	-3.038697
H	2.152565	1.365909	-2.711141

B	0.080796	4.329139	0.514324
O	0.823419	5.453280	0.763913
H	1.308458	5.717811	-0.025124
O	-0.612681	3.737751	1.526932
H	-1.082669	3.009225	1.078424

A7

Coordinates (Angstroms)

	X	Y	Z

C	2.491689	-1.151924	-0.440822
C	2.378129	-1.888896	-1.626853
C	3.422300	-2.711680	-2.040545
H	1.472575	-1.810155	-2.226573
H	3.329769	-3.279828	-2.961587
P	1.098359	-0.076563	0.028565
C	1.175658	0.072355	1.838643
C	1.982600	1.017874	2.480541
C	0.420388	-0.827516	2.599641
C	2.032818	1.056442	3.871475
H	2.566776	1.724326	1.898127
C	0.476935	-0.787115	3.989135
H	-0.216879	-1.551490	2.095575
C	1.282091	0.156133	4.625219
H	2.659353	1.792744	4.366538
H	-0.114130	-1.485641	4.574396
H	1.321277	0.192665	5.710229
C	1.525158	1.572572	-0.616689

C	0.841101	2.699127	-0.139816
C	2.476275	1.719971	-1.630576
C	1.110833	3.954639	-0.672969
H	0.098872	2.595824	0.646517
C	2.737916	2.980262	-2.163580
H	3.015611	0.854899	-2.005077
C	2.057121	4.097508	-1.687094
H	0.576925	4.822455	-0.296449
H	3.479958	3.086432	-2.949748
H	2.263747	5.079322	-2.103580
Pd	-0.793347	-1.065014	-0.723847
C	4.579285	-2.805689	-1.270333
H	5.393128	-3.450029	-1.590514
C	4.693588	-2.076645	-0.087196
H	5.595770	-2.151508	0.513070
C	3.654229	-1.251177	0.330400
H	3.748409	-0.686648	1.253484
O	-2.417436	-2.114912	-1.381852
O	-3.704009	-1.475694	-1.284932
C	-2.187918	0.940374	0.898155
C	-2.891953	2.130579	1.100314
C	-3.135059	2.996330	0.036698
C	-2.675242	2.666717	-1.237832
C	-1.971605	1.481229	-1.449308
C	-1.731626	0.615255	-0.379825
H	-1.992107	0.285526	1.741384
H	-3.243532	2.378948	2.098800
H	-3.677245	3.923740	0.199373
H	-2.857143	3.337031	-2.074401
H	-1.610877	1.241654	-2.445746

B	-4.210604	-1.607939	-0.007193
O	-5.410206	-1.016721	0.285324
H	-5.735066	-0.516091	-0.471020
O	-3.557312	-2.331294	0.943657
H	-2.760147	-2.636805	0.473385

A8

Coordinates (Angstroms)

	X	Y	Z
C	0.244194	-1.801301	1.486171
C	0.483517	-0.888863	2.523078
C	1.322061	-1.231129	3.579872
H	0.013519	0.092406	2.496966
H	1.498158	-0.518174	4.380172
P	-0.932701	-1.278846	0.194657
C	-0.790486	-2.415793	-1.215436
C	-1.081751	-3.780825	-1.089848
C	-0.401614	-1.902834	-2.457087
C	-0.939510	-4.624655	-2.186240
H	-1.426256	-4.181093	-0.140342
C	-0.267433	-2.750323	-3.554027
H	-0.208247	-0.837405	-2.559227
C	-0.526677	-4.111848	-3.415947
H	-1.158289	-5.683442	-2.082828
H	0.037639	-2.345693	-4.514661
H	-0.419029	-4.774465	-4.269956
C	-2.572659	-1.665496	0.902741

C	-3.646341	-1.903953	0.035792
C	-2.799551	-1.617872	2.280563
C	-4.929909	-2.072969	0.542954
H	-3.483050	-1.946062	-1.036331
C	-4.086507	-1.794144	2.783703
H	-1.978410	-1.441156	2.968151
C	-5.153991	-2.014954	1.917852
H	-5.756891	-2.249331	-0.138893
H	-4.251895	-1.757589	3.856707
H	-6.157943	-2.144882	2.311806
Pd	-0.521163	0.871894	-0.387266
C	1.944445	-2.477558	3.598162
H	2.607969	-2.742329	4.416346
C	1.723713	-3.379206	2.559704
H	2.219443	-4.345479	2.562098
C	0.873138	-3.048578	1.507789
H	0.715997	-3.758509	0.703108
O	-0.094276	2.848927	-0.918019
O	-0.458548	3.713878	0.181304
C	-3.142388	0.946408	-1.675107
C	-4.514449	1.195408	-1.750622
C	-5.213071	1.627148	-0.625131
C	-4.532626	1.817270	0.577085
C	-3.161252	1.573553	0.656672
C	-2.460438	1.135017	-0.470146
H	-2.613725	0.592973	-2.557297
H	-5.036840	1.043727	-2.692284
H	-6.282415	1.811459	-0.682316
H	-5.070893	2.152127	1.460645
H	-2.647581	1.709859	1.604894

B	-1.566527	4.469077	-0.174315
O	-2.081414	5.332495	0.752219
H	-1.590878	5.287212	1.580086
O	-2.112077	4.383508	-1.413038
H	-1.595434	3.678605	-1.841507
O	1.716880	1.141199	-0.694723
C	2.970359	0.919299	-0.074055
C	3.291541	-0.562680	-0.185611
C	2.993263	1.423733	1.378609
C	3.989662	1.698536	-0.925001
C	2.750390	-1.301172	-1.241594
C	4.154714	-1.195000	0.711855
H	2.377667	0.718990	1.948290
H	4.012092	1.351916	1.767425
C	2.475637	2.812934	1.585600
F	3.639027	2.992536	-1.041937
F	5.213483	1.656587	-0.382289
F	4.080686	1.212291	-2.170761
C	3.045191	-2.653164	-1.385059
H	2.089994	-0.813400	-1.947802
C	4.458755	-2.545938	0.559758
H	4.595443	-0.646730	1.537442
H	1.458604	3.021068	1.253100
C	3.168440	3.777426	2.188811
C	3.904455	-3.279963	-0.485487
H	2.598562	-3.214606	-2.201314
H	5.127635	-3.025261	1.268794
H	4.185279	3.615109	2.542492
H	2.741056	4.764082	2.350061
H	4.137249	-4.335402	-0.595213

H	1.457900	2.099779	-0.731940

A9

	Coordinates (Angstroms)		
	X	Y	Z

C	0.240600	-2.055288	-1.176079
C	0.312705	-1.742066	-2.542547
C	-0.427822	-2.470132	-3.466396
H	0.939370	-0.921044	-2.882489
H	-0.362498	-2.224246	-4.522208
P	1.211254	-1.021987	-0.035766
C	0.989359	-1.632753	1.660591
C	1.257185	-2.972092	1.973986
C	0.619092	-0.742106	2.672207
C	1.113313	-3.418844	3.282682
H	1.578448	-3.662336	1.198451
C	0.489851	-1.192858	3.983884
H	0.427997	0.301724	2.434554
C	0.727744	-2.530906	4.287509
H	1.310533	-4.460046	3.520447
H	0.200215	-0.496907	4.765818
H	0.621782	-2.883249	5.309600
C	2.964756	-1.414512	-0.366956
C	3.908530	-0.993079	0.580026
C	3.394971	-2.058699	-1.528228
C	5.264324	-1.185804	0.348433
H	3.583081	-0.502520	1.492396

C	4.756886	-2.255448	-1.751881
H	2.679362	-2.412911	-2.262300
C	5.692304	-1.811937	-0.822776
H	5.988366	-0.845052	1.082871
H	5.082403	-2.758504	-2.657925
H	6.753079	-1.959018	-1.004779
Pd	0.474153	1.082200	-0.252624
C	-1.266430	-3.496911	-3.033117
H	-1.854771	-4.058001	-3.753419
C	-1.358477	-3.793384	-1.676037
H	-2.022822	-4.580673	-1.332534
C	-0.607123	-3.078360	-0.745556
H	-0.702411	-3.309100	0.309886
O	-0.417164	3.120905	-0.494162
O	-0.290267	4.049591	0.586114
C	2.953220	2.254223	0.703394
C	4.253434	2.753479	0.602199
C	4.956432	2.644837	-0.596112
C	4.349675	2.048200	-1.700714
C	3.051808	1.545830	-1.603622
C	2.347784	1.645004	-0.400014
H	2.420547	2.335130	1.648687
H	4.718614	3.219849	1.467338
H	5.972538	3.022801	-0.669063
H	4.890678	1.962305	-2.639954
H	2.599054	1.057026	-2.463109
B	-0.505796	3.530263	1.876632
O	-0.105785	4.365608	2.878772
H	0.356379	5.140364	2.539201
O	-1.079655	2.353060	2.183652

H	-1.456529	1.820747	1.428881
O	-1.690167	1.094119	0.027818
C	-2.801897	0.442688	-0.480710
C	-3.123172	-0.835117	0.296728
C	-2.660826	0.127997	-1.991039
C	-3.969390	1.420739	-0.267469
C	-2.532706	-1.041456	1.542754
C	-3.987137	-1.811700	-0.209356
H	-2.103128	-0.811327	-2.056185
H	-3.648392	-0.055177	-2.424570
C	-1.940882	1.167245	-2.788852
F	-3.737285	2.611650	-0.851113
F	-5.131595	0.960673	-0.762122
F	-4.165769	1.667309	1.040234
C	-2.762518	-2.214897	2.256876
H	-1.870958	-0.284108	1.942863
C	-4.224268	-2.982921	0.505419
H	-4.471728	-1.674266	-1.170834
H	-0.891904	1.327257	-2.532818
C	-2.472107	1.855370	-3.798214
C	-3.606031	-3.193460	1.737027
H	-2.274435	-2.363750	3.216515
H	-4.890306	-3.736569	0.094119
H	-3.511130	1.720898	-4.094669
H	-1.886987	2.577174	-4.362954
H	-3.784001	-4.112874	2.287973
H	-1.284267	2.615463	-0.364543

B10

	Coordinates (Angstroms)		
	X	Y	Z
C	-0.689838	2.046723	-0.807368
C	-0.352718	1.730169	-2.129294
C	0.354563	2.640045	-2.907761
H	-0.633147	0.763063	-2.539657
H	0.611561	2.388543	-3.932872
P	-1.627050	0.802700	0.136700
C	-1.542033	1.266841	1.892361
C	-2.222327	2.388474	2.385664
C	-0.791140	0.474493	2.764239
C	-2.132312	2.716522	3.734473
H	-2.825725	2.999341	1.720075
C	-0.706857	0.804770	4.114374
H	-0.275976	-0.397656	2.375408
C	-1.374731	1.926477	4.599069
H	-2.658781	3.588195	4.112438
H	-0.122345	0.182377	4.786084
H	-1.311948	2.183769	5.652667
C	-3.372938	1.105633	-0.297985
C	-4.374388	0.642200	0.565087
C	-3.730812	1.690217	-1.515220
C	-5.712543	0.752178	0.206042
H	-4.108816	0.183784	1.512851
C	-5.074007	1.798744	-1.870136
H	-2.966612	2.059667	-2.192373
C	-6.065565	1.326943	-1.014959
H	-6.481140	0.383916	0.879565

H	-5.342449	2.255741	-2.818432
H	-7.111774	1.408190	-1.295861
Pd	-0.728511	-1.262758	-0.304357
C	0.747272	3.863241	-2.365877
H	1.310906	4.569238	-2.969275
C	0.424033	4.175919	-1.047776
H	0.735279	5.124830	-0.620209
C	-0.296772	3.273400	-0.268512
H	-0.536645	3.524447	0.759964
C	-3.155553	-2.609662	0.679127
C	-4.464560	-3.099350	0.650230
C	-5.240474	-2.961429	-0.498412
C	-4.694042	-2.339300	-1.621479
C	-3.388564	-1.850498	-1.588148
C	-2.600383	-1.968623	-0.435240
H	-2.570822	-2.718781	1.591366
H	-4.877753	-3.584844	1.531659
H	-6.260571	-3.335482	-0.520112
H	-5.288796	-2.227451	-2.525318
H	-2.986895	-1.354717	-2.469771
O	1.132894	-0.402417	-0.037325
C	2.129688	-1.274663	0.340498
C	3.520378	-0.636502	0.108312
C	2.001191	-2.545842	-0.538505
C	3.722999	0.694978	-0.267085
C	4.689999	-1.378642	0.298334
H	2.215744	-2.261374	-1.574379
H	2.710369	-3.324742	-0.243191
C	0.612869	-3.104470	-0.453708
C	4.996004	1.229198	-0.455298

C	5.965982	-0.868750	0.115924
H	0.348722	-3.659863	0.446645
C	-0.253516	-3.129022	-1.513559
C	6.124347	0.452809	-0.266941
H	0.046619	-2.731976	-2.482253
H	-1.153659	-3.732967	-1.490244
C	2.040110	-1.638804	1.833379
H	1.074285	-2.114449	2.034747
H	2.833023	-2.322027	2.151170
H	2.102487	-0.727503	2.435646
F	4.633467	-2.663471	0.686198
F	2.732028	1.563531	-0.465406
F	5.128577	2.506957	-0.816801
F	7.338992	0.965553	-0.447636
F	7.035691	-1.641691	0.309098

B11

Coordinates (Angstroms)

	X	Y	Z

C	-1.571584	2.106745	1.277807
C	-0.809792	1.969657	2.446007
C	-0.797442	2.991859	3.392033
H	-0.205055	1.074353	2.582780
H	-0.204544	2.880134	4.296104
P	-1.536052	0.737303	0.063469
C	-3.067668	0.995407	-0.900798
C	-3.062785	1.089723	-2.294724

C	-4.293599	0.996129	-0.221025
C	-4.263340	1.184564	-2.997577
H	-2.122783	1.088187	-2.838761
C	-5.488633	1.101911	-0.923282
H	-4.313157	0.914651	0.862990
C	-5.476986	1.192940	-2.315823
H	-4.245810	1.257107	-4.081551
H	-6.431540	1.108058	-0.383535
H	-6.411308	1.270604	-2.864599
C	-0.205065	1.208474	-1.102437
C	0.370371	0.198873	-1.885089
C	0.265336	2.519156	-1.222572
C	1.396016	0.497926	-2.777115
H	0.018609	-0.825421	-1.781177
C	1.296621	2.815075	-2.111333
H	-0.167228	3.310895	-0.617580
C	1.863917	1.806624	-2.887788
H	1.840766	-0.293387	-3.374152
H	1.663134	3.834503	-2.189937
H	2.679958	2.037138	-3.567088
Pd	-0.842691	-1.407959	0.933669
C	-1.542524	4.151161	3.185455
H	-1.535467	4.943623	3.928915
C	-2.295146	4.294011	2.021193
H	-2.872637	5.198654	1.851786
C	-2.309604	3.278165	1.068760
H	-2.897616	3.399025	0.163664
C	-2.662116	-2.873066	0.725775
C	-3.760951	-2.286063	0.064222
C	-3.789174	-2.211557	-1.315481

C	-2.713304	-2.712976	-2.063417
C	-1.630168	-3.300597	-1.432772
C	-1.595016	-3.425295	-0.026034
H	-2.727735	-3.075106	1.793471
H	-4.588386	-1.899396	0.651648
H	-4.634143	-1.753250	-1.820079
H	-2.733543	-2.646985	-3.147824
H	-0.808092	-3.708158	-2.015573
C	4.635663	0.963033	-1.089128
C	3.812182	1.611805	-0.184808
C	3.009535	0.879931	0.679686
C	2.961469	-0.518419	0.665718
C	3.848307	-1.129464	-0.219693
C	4.659716	-0.419956	-1.097017
C	1.973983	-1.277096	1.583495
C	1.605023	-2.662398	1.010859
H	1.585644	-2.604706	-0.083517
H	2.342517	-3.436500	1.270828
C	0.213672	-3.042819	1.481331
H	0.131767	-3.156752	2.566414
C	-0.474486	-4.150910	0.695987
H	0.197407	-4.618614	-0.031924
H	-0.883196	-4.942032	1.334007
O	0.810421	-0.507780	1.681821
C	2.618387	-1.407757	2.968567
H	3.588420	-1.914938	2.921842
H	2.764225	-0.413890	3.402616
H	1.956215	-1.977724	3.629274
F	2.287775	1.606544	1.536169
F	3.969133	-2.464347	-0.276851

F	5.461302	-1.069307	-1.944118
F	5.385233	1.660526	-1.940422
F	3.786542	2.945465	-0.153483

B12

	Coordinates (Angstroms)		
	X	Y	Z

H	4.467438	2.862598	-2.852584
C	4.606836	2.105425	-2.086322
C	3.731445	0.269192	-0.778719
C	3.563360	1.242306	-1.769291
H	2.611799	1.324151	-2.290149
C	-0.743200	3.107711	-0.553844
C	-1.528814	4.028043	0.142294
C	-2.429934	4.838781	-0.545415
H	-1.444521	4.108967	1.222562
H	-3.045481	5.546035	0.003660
P	0.479575	2.041301	0.287431
P	2.396249	-0.964119	-0.557509
C	1.946138	3.145122	0.339095
C	2.020883	4.288462	-0.464051
C	3.029902	2.839346	1.173937
C	3.147660	5.107331	-0.428604
H	1.197758	4.549739	-1.120692
C	4.146678	3.665997	1.219145
H	3.003485	1.957148	1.803661
C	4.210724	4.803740	0.415995

H	3.186369	5.990649	-1.060025
H	4.972991	3.413321	1.877243
H	5.086467	5.445730	0.447321
C	-0.088654	1.994388	2.033263
C	0.443801	2.801034	3.044208
C	-1.117849	1.093575	2.345226
C	-0.024356	2.687181	4.352232
H	1.224065	3.520838	2.820239
C	-1.586977	0.991828	3.651499
H	-1.561499	0.507787	1.541889
C	-1.033868	1.779161	4.660826
H	0.401677	3.315336	5.129684
H	-2.386941	0.292784	3.881037
H	-1.394352	1.691364	5.682052
C	2.891739	-2.077163	-1.926029
C	4.064611	-2.841633	-1.876037
C	2.165738	-2.019792	-3.120221
C	4.464894	-3.582296	-2.983487
H	4.678552	-2.848786	-0.980593
C	2.576108	-2.752586	-4.231338
H	1.286754	-1.385269	-3.182578
C	3.717712	-3.546100	-4.160128
H	5.370520	-4.179850	-2.930277
H	2.002997	-2.699276	-5.152671
H	4.035258	-4.123333	-5.023894
C	2.792348	-1.775145	1.029331
C	3.075035	-3.133670	1.187417
C	2.670494	-0.969703	2.171042
C	3.242186	-3.671048	2.462997
H	3.146381	-3.788802	0.326058

C	2.856131	-1.502653	3.439622
H	2.396512	0.075343	2.066385
C	3.140015	-2.860005	3.588866
H	3.447819	-4.732035	2.571634
H	2.756939	-0.862666	4.311735
H	3.268487	-3.284936	4.580231
Pd	0.254864	-0.230299	-0.544579
C	-2.538885	4.745617	-1.930870
H	-3.241932	5.378687	-2.465081
C	-1.745828	3.836747	-2.631343
H	-1.829170	3.758749	-3.711899
C	5.823354	2.006492	-1.411787
H	6.636192	2.684629	-1.655672
C	5.992178	1.043014	-0.420079
H	6.937228	0.965457	0.110199
C	4.951341	0.172678	-0.104750
H	5.092670	-0.581494	0.663853
C	-0.857669	3.015140	-1.944639
H	-0.258414	2.287771	-2.486068
C	-0.373916	-2.535669	1.914794
C	-0.531997	-2.767712	3.279218
C	-0.530608	-4.069499	3.775333
C	-0.374507	-5.135631	2.890543
C	-0.220700	-4.896016	1.527427
C	-0.210105	-3.592989	1.015367
H	-0.366471	-1.516304	1.534321
H	-0.650713	-1.924203	3.955146
H	-0.652937	-4.252457	4.839487
H	-0.375350	-6.157221	3.261978
H	-0.100869	-5.734579	0.843927

C	-6.745679	-0.248275	-0.245101
C	-5.827966	0.632627	0.296373
C	-4.476990	0.544449	-0.032581
C	-3.981981	-0.429797	-0.903411
C	-4.947635	-1.289344	-1.435888
C	-6.296471	-1.219770	-1.124404
C	-2.496905	-0.591866	-1.290351
C	-2.022187	-2.001866	-0.935027
H	-2.296377	-2.174725	0.112437
H	-2.511044	-2.787111	-1.527715
C	-0.505324	-2.098860	-1.096941
H	-0.268412	-2.157342	-2.164450
C	0.018832	-3.381374	-0.462877
H	-0.442839	-4.233440	-0.988343
H	1.093256	-3.485394	-0.663988
O	-1.714237	0.285698	-0.553623
C	-2.366587	-0.293619	-2.792807
H	-2.954276	-0.975662	-3.414388
H	-2.691972	0.731984	-2.991462
H	-1.312949	-0.374810	-3.079524
F	-3.711425	1.470211	0.548373
F	-4.602664	-2.253815	-2.304017
F	-7.160003	-2.079918	-1.666737
F	-8.036463	-0.163108	0.068791
F	-6.241626	1.581434	1.138906

B13

Coordinates (Angstroms)

	X	Y	Z
H	3.970411	3.357175	3.591307
C	3.741717	3.192046	2.542096
C	2.160147	2.539654	0.832534
C	2.467977	2.757475	2.177040
H	1.716366	2.595076	2.943581
C	3.045349	-0.726413	0.930774
C	2.222689	-1.093181	2.004322
C	2.672450	-0.958888	3.312524
H	1.234270	-1.502341	1.811851
H	2.024215	-1.247534	4.135210
P	2.349924	-0.974126	-0.739346
P	0.502665	2.003490	0.266532
C	3.627029	-0.457501	-1.931988
C	4.887540	-1.066067	-1.974300
C	3.320191	0.560402	-2.840073
C	5.836246	-0.636109	-2.896493
H	5.127269	-1.874891	-1.289214
C	4.271388	0.986064	-3.764153
H	2.330368	1.012037	-2.817048
C	5.530804	0.392120	-3.788246
H	6.814545	-1.107380	-2.922342
H	4.026609	1.779252	-4.464767
H	6.274232	0.723745	-4.507627
C	2.370618	-2.811381	-0.868642
C	1.644415	-3.453403	-1.877676
C	3.138498	-3.586076	0.009093
C	1.670291	-4.839340	-1.997144
H	1.042369	-2.866817	-2.566358

C	3.158720	-4.974124	-0.108210
H	3.718577	-3.111935	0.794038
C	2.420547	-5.604932	-1.105937
H	1.093687	-5.321328	-2.781585
H	3.752084	-5.561155	0.587110
H	2.429465	-6.687940	-1.190142
C	-0.516599	2.149203	1.777296
C	-1.162138	3.337314	2.133633
C	-0.628684	1.032110	2.611410
C	-1.905426	3.405079	3.309439
H	-1.088386	4.211655	1.493744
C	-1.357020	1.108011	3.795038
H	-0.150456	0.099181	2.331244
C	-1.999985	2.293753	4.144359
H	-2.409435	4.330544	3.573871
H	-1.429013	0.236577	4.439719
H	-2.577297	2.350235	5.062958
C	-0.016016	3.443668	-0.746843
C	-1.035387	3.261134	-1.689611
C	0.551510	4.713480	-0.580510
C	-1.474731	4.338003	-2.456533
H	-1.475742	2.267691	-1.796361
C	0.107943	5.784021	-1.352628
H	1.338124	4.870575	0.151297
C	-0.903474	5.598259	-2.293571
H	-2.264884	4.189314	-3.188234
H	0.554391	6.765376	-1.217442
H	-1.244643	6.435100	-2.896955
Pd	0.335259	-0.039099	-1.025812
C	3.950196	-0.457884	3.560146

H	4.303989	-0.349420	4.581531
C	4.771306	-0.094437	2.495975
H	5.764669	0.302326	2.684736
C	4.713716	3.417429	1.571441
H	5.703697	3.759143	1.860225
C	4.413013	3.196913	0.227447
H	5.165781	3.364717	-0.537977
C	3.145838	2.758626	-0.139181
H	2.917305	2.601406	-1.189112
C	4.323312	-0.226131	1.182142
H	4.969228	0.069279	0.361986
C	-6.486510	-0.203915	0.130584
C	-5.373609	0.414753	0.668167
C	-4.138762	0.336299	0.028892
C	-3.950519	-0.358688	-1.169793
C	-5.104692	-0.970949	-1.670569
C	-6.344663	-0.908050	-1.053078
C	-2.593692	-0.454874	-1.929224
C	-2.203878	-1.948791	-2.022314
H	-3.025859	-2.518429	-2.471884
H	-1.383775	-2.011275	-2.754364
C	-1.738592	-2.652501	-0.790687
H	-1.397987	-3.673377	-0.972223
C	-1.649866	-2.162765	0.454637
H	0.309281	-1.161254	-2.088082
O	-1.667194	0.348659	-1.304035
H	-1.993379	-1.151328	0.655897
C	-1.067455	-2.869411	1.601345
C	-1.357704	-2.419598	2.898524
C	-0.166754	-3.937976	1.458751

C	-0.771075	-3.009856	4.014196
H	-2.052111	-1.593012	3.023744
C	0.418002	-4.529193	2.572786
H	0.107698	-4.284958	0.466710
C	0.123604	-4.067010	3.856022
H	-1.011723	-2.642812	5.008551
H	1.123959	-5.344177	2.436404
H	0.592126	-4.523658	4.723326
C	-2.805843	0.071702	-3.361932
H	-3.168470	1.103809	-3.324274
H	-1.829929	0.070094	-3.859350
H	-3.502535	-0.523708	-3.956882
F	-3.154936	0.961075	0.679928
F	-5.481580	1.091048	1.813655
F	-7.668077	-0.129128	0.738406
F	-7.398253	-1.520650	-1.595194
F	-5.073172	-1.681815	-2.810422

B14

Coordinates (Angstroms)

	X	Y	Z
H	-1.576871	-2.011644	4.863604
C	-2.121356	-1.515253	4.064877
C	-2.752572	-1.405205	1.728021
C	-2.061628	-2.030165	2.770323
H	-1.468639	-2.919386	2.578551
C	-0.228144	2.395908	1.081277

C	0.311002	3.649501	1.386948
C	0.865633	3.888008	2.642878
H	0.307462	4.443754	0.647943
H	1.288831	4.863460	2.865093
P	-1.065518	1.989683	-0.498954
P	-2.524194	-1.901829	-0.029103
C	-2.806315	2.474497	-0.153533
C	-3.201490	3.149409	1.003863
C	-3.783792	2.053376	-1.066122
C	-4.554005	3.386196	1.250797
H	-2.458286	3.477392	1.724560
C	-5.131132	2.292805	-0.820372
H	-3.483423	1.508761	-1.958460
C	-5.520037	2.954092	0.345876
H	-4.850853	3.904931	2.158360
H	-5.878572	1.945222	-1.528453
H	-6.573110	3.128775	0.547877
C	-0.527377	3.293431	-1.668274
C	0.294219	2.921699	-2.736961
C	-0.914970	4.633609	-1.538149
C	0.757587	3.877707	-3.638872
H	0.564075	1.877102	-2.862638
C	-0.451083	5.587866	-2.438594
H	-1.582192	4.931071	-0.733245
C	0.392151	5.212905	-3.484577
H	1.398509	3.577647	-4.463267
H	-0.751157	6.626070	-2.326588
H	0.752409	5.960242	-4.186007
C	-2.188334	-3.702945	0.072281
C	-3.164211	-4.678002	-0.160607

C	-0.880255	-4.105880	0.375761
C	-2.838357	-6.030122	-0.081692
H	-4.181062	-4.387025	-0.406369
C	-0.563137	-5.458014	0.471202
H	-0.104514	-3.359042	0.528837
C	-1.540993	-6.423485	0.239332
H	-3.603974	-6.778046	-0.269173
H	0.452874	-5.756210	0.715497
H	-1.291406	-7.479004	0.302101
C	-4.214372	-1.794761	-0.720524
C	-4.351464	-1.378996	-2.049768
C	-5.361927	-2.081045	0.028850
C	-5.614185	-1.250947	-2.623206
H	-3.459690	-1.138841	-2.625569
C	-6.623619	-1.945418	-0.543194
H	-5.270022	-2.401414	1.063039
C	-6.751465	-1.529038	-1.868007
H	-5.709028	-0.922489	-3.654416
H	-7.509152	-2.164006	0.047037
H	-7.737994	-1.419000	-2.309622
Pd	-1.228441	-0.256641	-0.904299
C	0.892350	2.878734	3.602762
H	1.331693	3.067055	4.578463
C	0.365008	1.623607	3.303050
H	0.385181	0.828134	4.043040
C	-2.875350	-0.376273	4.335202
H	-2.918186	0.024404	5.343993
C	-3.576732	0.245409	3.302366
H	-4.169932	1.134029	3.500055
C	-3.513518	-0.260161	2.008717

H	-4.052185	0.245394	1.212031
C	-0.188445	1.383067	2.049265
H	-0.597197	0.403473	1.809986
C	6.405376	-2.401657	0.041897
C	5.484593	-2.158707	1.044262
C	4.142294	-1.951670	0.739368
C	3.662132	-1.969144	-0.572879
C	4.628267	-2.211384	-1.553996
C	5.968394	-2.425085	-1.272181
C	2.204991	-1.735341	-0.987288
C	2.100386	-0.493689	-1.891092
H	2.555871	-0.715184	-2.860322
H	1.019029	-0.357806	-2.098257
C	2.651395	0.796803	-1.372826
H	2.845089	1.543453	-2.142144
C	2.902007	1.107868	-0.093732
H	0.582866	-1.148077	-0.080868
O	1.438862	-1.553795	0.190471
H	2.727937	0.363327	0.678254
C	3.413622	2.394927	0.385161
C	4.005064	2.453591	1.655236
C	3.301092	3.584375	-0.352699
C	4.482884	3.655480	2.168845
H	4.082136	1.540652	2.241761
C	3.774861	4.785315	0.161951
H	2.811939	3.574878	-1.322931
C	4.369140	4.827863	1.424085
H	4.937569	3.678071	3.155593
H	3.667449	5.697384	-0.419292
H	4.732772	5.769556	1.825777

C	1.669405	-2.960461	-1.735052
H	1.737468	-3.846930	-1.099392
H	0.614745	-2.785606	-1.975896
H	2.209146	-3.151572	-2.664226
F	3.367061	-1.707720	1.798077
F	4.296763	-2.236062	-2.852734
F	6.832922	-2.650770	-2.259807
F	7.686617	-2.604007	0.331496
F	5.883740	-2.119898	2.315077

B8

Coordinates (Angstroms)

	X	Y	Z
C	1.004265	-1.041849	1.489351
C	0.893925	0.014365	2.402895
C	1.847588	0.179272	3.403125
H	0.053821	0.701831	2.330381
H	1.754288	1.001931	4.106047
P	-0.365261	-1.260798	0.305034
C	0.234275	-2.298970	-1.061527
C	0.591320	-3.641200	-0.870603
C	0.314832	-1.738182	-2.339976
C	1.052455	-4.396549	-1.943243
H	0.496979	-4.098226	0.110534
C	0.773219	-2.500172	-3.411748
H	0.014460	-0.704669	-2.490096
C	1.147122	-3.826131	-3.212765

H	1.331821	-5.434768	-1.789104
H	0.836404	-2.056139	-4.400903
H	1.504796	-4.421186	-4.048287
C	-1.525055	-2.346824	1.210813
C	-2.366443	-3.208813	0.497495
C	-1.661904	-2.245325	2.597924
C	-3.339004	-3.946333	1.163942
H	-2.272205	-3.295348	-0.580137
C	-2.635623	-2.988292	3.261123
H	-1.013816	-1.585647	3.167175
C	-3.478714	-3.835144	2.546525
H	-3.990926	-4.607236	0.599812
H	-2.733076	-2.902732	4.339701
H	-4.241347	-4.409582	3.064649
Pd	-1.181076	0.725070	-0.434490
C	2.921953	-0.703208	3.492153
H	3.671583	-0.570984	4.266839
C	3.041946	-1.747294	2.577532
H	3.888224	-2.425735	2.632368
C	2.089601	-1.917969	1.576531
H	2.201075	-2.730182	0.865968
O	-1.934930	2.528400	-1.163267
O	-2.635232	3.191283	-0.084872
C	-3.461902	-0.758893	-1.520597
C	-4.754262	-1.288460	-1.506380
C	-5.550017	-1.170096	-0.368731
C	-5.051562	-0.509708	0.753857
C	-3.762785	0.024043	0.741916
C	-2.958329	-0.100922	-0.394894
H	-2.848572	-0.873835	-2.411467

H	-5.134489	-1.800856	-2.387065
H	-6.551766	-1.590887	-0.355491
H	-5.665215	-0.412416	1.646361
H	-3.382777	0.522686	1.630084
B	-3.992542	3.219212	-0.367088
O	-4.829160	3.799945	0.546002
H	-4.337261	4.120962	1.309608
O	-4.481648	2.714774	-1.527568
H	-3.693808	2.326910	-1.949712
O	0.538833	2.097539	-0.886412
C	1.780499	2.664722	-0.449541
C	2.760537	1.494649	-0.421682
C	1.567359	3.343376	0.918421
C	2.804210	0.612304	-1.508085
C	3.681828	1.238621	0.594468
H	1.365695	2.564254	1.660717
H	2.486347	3.856438	1.209589
C	0.428251	4.316586	0.902503
C	3.642215	-0.492035	-1.548790
C	4.552550	0.156254	0.557829
H	-0.574670	3.907507	0.775785
C	0.571139	5.633111	1.054197
C	4.521800	-0.727495	-0.504910
H	1.550297	6.089341	1.191570
H	-0.287010	6.301061	1.050963
H	-0.143050	2.786973	-1.055946
C	2.244479	3.684757	-1.487003
H	1.528663	4.510728	-1.546934
H	3.216134	4.096477	-1.199581
H	2.334276	3.222415	-2.471992

F	2.042267	0.804984	-2.587984
F	3.621300	-1.312384	-2.597213
F	5.323944	-1.786356	-0.523653
F	5.399905	-0.046530	1.564541
F	3.791778	2.020831	1.672220

B9

Coordinates (Angstroms)

	X	Y	Z
C	-0.718366	-1.696195	-1.124090
C	-0.956334	-1.056219	-2.346759
C	-1.991976	-1.484994	-3.171544
H	-0.324583	-0.222531	-2.646430
H	-2.171907	-0.981180	-4.116709
P	0.751352	-1.168405	-0.186402
C	0.567026	-1.669472	1.550377
C	0.521505	-3.023148	1.914278
C	0.519490	-0.684127	2.541686
C	0.392343	-3.378154	3.252232
H	0.605850	-3.798254	1.157868
C	0.398966	-1.047333	3.880871
H	0.582094	0.365438	2.268831
C	0.328737	-2.391188	4.235962
H	0.352812	-4.427766	3.528506
H	0.361629	-0.275994	4.644815
H	0.234516	-2.673243	5.280817
C	2.068553	-2.264968	-0.820907

C	3.163195	-2.575763	-0.004587
C	2.048349	-2.709313	-2.145476
C	4.228746	-3.307636	-0.515874
H	3.192897	-2.233063	1.024760
C	3.117831	-3.444797	-2.651539
H	1.203633	-2.481636	-2.788573
C	4.210681	-3.740176	-1.841424
H	5.076789	-3.537571	0.122798
H	3.093253	-3.786740	-3.682261
H	5.045999	-4.309216	-2.239429
Pd	1.053172	1.047480	-0.373722
C	-2.799030	-2.549960	-2.777142
H	-3.612986	-2.880829	-3.415522
C	-2.571502	-3.181425	-1.556241
H	-3.211631	-3.998693	-1.237315
C	-1.535949	-2.758143	-0.727706
H	-1.377633	-3.252361	0.224991
O	1.309993	3.251388	-0.575852
O	1.947801	3.952276	0.494028
C	3.683655	0.681306	0.804746
C	5.070388	0.515464	0.806329
C	5.753096	0.300459	-0.389023
C	5.046310	0.263452	-1.590869
C	3.660800	0.426224	-1.597651
C	2.973265	0.636422	-0.398667
H	3.160464	0.831061	1.746689
H	5.614081	0.546131	1.747519
H	6.830485	0.159542	-0.385010
H	5.572496	0.097163	-2.527764
H	3.119111	0.368733	-2.538767

B	1.531478	3.602332	1.789214
O	2.327627	4.105217	2.779107
H	3.105411	4.548086	2.421608
O	0.445286	2.880783	2.115846
H	-0.162645	2.603112	1.375275
O	-0.780791	2.198628	-0.076971
C	-2.132533	2.245348	-0.443925
C	-2.830130	0.968605	0.063328
C	-2.246552	2.402459	-1.980564
C	-2.571468	0.523222	1.364052
C	-3.749099	0.196132	-0.648136
H	-1.974732	1.451197	-2.448210
H	-3.283976	2.619591	-2.246679
C	-1.353926	3.477197	-2.514866
C	-3.101978	-0.645225	1.890431
C	-4.320703	-0.960753	-0.131550
H	-0.292455	3.241932	-2.580017
C	-1.772056	4.672321	-2.932033
C	-3.983290	-1.400138	1.134709
H	-2.824723	4.949222	-2.901644
H	-1.078881	5.413111	-3.323611
H	0.292207	3.218207	-0.397271
C	-2.787041	3.448120	0.243494
H	-2.308117	4.369863	-0.101124
H	-3.854850	3.503404	0.009247
H	-2.670961	3.378987	1.327925
F	-5.176861	-1.665521	-0.870977
F	-4.150982	0.516881	-1.884164
F	-1.800084	1.233325	2.193400
F	-2.785322	-1.032462	3.125879

F	-4.492595	-2.530817	1.615314

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Coordinates (Angstroms)

	X	Y	Z
B	0.524626	0.060921	0.000514
O	0.369022	1.405325	0.009012
H	-0.577123	1.603478	-0.007764
O	1.770451	-0.482354	0.014401
H	1.751867	-1.446061	0.001417
O	-0.553295	-0.830025	-0.026370
O	-1.786313	-0.103658	-0.089940
H	-2.196792	-0.376319	0.746953

C10

Coordinates (Angstroms)

	X	Y	Z
C	0.247700	1.923304	-0.888605
C	0.697829	1.479584	-2.138070
C	1.564365	2.265108	-2.890487
H	0.382668	0.508010	-2.508978
H	1.908103	1.913089	-3.859009
P	-0.878150	0.833986	0.044071
C	-0.886993	1.435974	1.759558

C	-1.554975	2.613412	2.120591
C	-0.193008	0.707291	2.730026
C	-1.516134	3.056550	3.438961
H	-2.107017	3.179750	1.375793
C	-0.158304	1.154588	4.048056
H	0.321934	-0.203473	2.439714
C	-0.818342	2.328835	4.402506
H	-2.034529	3.970306	3.714938
H	0.381915	0.583115	4.797568
H	-0.793903	2.676585	5.431395
C	-2.551236	1.212660	-0.573487
C	-3.657992	0.934256	0.239174
C	-2.753414	1.651525	-1.884619
C	-4.946641	1.084080	-0.260536
H	-3.514073	0.587247	1.257830
C	-4.046972	1.799545	-2.380475
H	-1.904938	1.876332	-2.523976
C	-5.144034	1.512437	-1.573015
H	-5.798500	0.860073	0.375180
H	-4.194331	2.141624	-3.400971
H	-6.151715	1.623858	-1.963184
Pd	-0.119954	-1.317895	-0.129908
C	2.007185	3.489527	-2.391221
H	2.694506	4.097723	-2.972558
C	1.573351	3.927342	-1.142320
H	1.921281	4.877068	-0.745962
C	0.692396	3.150410	-0.392197
H	0.366447	3.500145	0.582625
C	-2.670717	-2.341556	0.942558
C	-4.008978	-2.744368	0.930827

C	-4.730589	-2.747374	-0.260822
C	-4.100205	-2.353703	-1.441779
C	-2.765059	-1.951156	-1.425168
C	-2.028179	-1.929425	-0.232424
H	-2.129032	-2.336932	1.887397
H	-4.487952	-3.051174	1.858183
H	-5.773141	-3.054038	-0.270635
H	-4.652389	-2.353537	-2.379002
H	-2.298606	-1.633594	-2.355929
O	1.740822	-0.475164	0.085098
C	2.761079	-1.315688	0.502842
C	4.106044	-0.706589	0.100440
C	2.578489	-2.676018	-0.209776
C	4.133177	0.533989	-0.540709
C	5.320354	-1.356733	0.350044
H	2.757838	-2.529074	-1.280802
H	3.299701	-3.418522	0.155314
C	1.188350	-3.203171	-0.007703
C	5.341332	1.114975	-0.922070
H	3.183246	1.023161	-0.731632
C	6.529113	-0.781116	-0.034897
H	5.325415	-2.323511	0.848433
H	0.941068	-3.602587	0.976365
C	0.287940	-3.376112	-1.023767
C	6.545121	0.459623	-0.672130
H	5.339736	2.082371	-1.419223
H	7.462103	-1.302780	0.163632
H	0.560414	-3.144121	-2.052373
H	-0.622586	-3.946533	-0.876723
H	7.488447	0.908850	-0.971331

C	2.742300	-1.509764	2.027590
H	1.792191	-1.957027	2.340044
H	3.556064	-2.153838	2.378978
H	2.837070	-0.537333	2.521482

C11

Coordinates (Angstroms)

	X	Y	Z

C	1.163264	2.026153	-1.325265
C	0.130642	2.011318	-2.271615
C	0.045799	3.021782	-3.226485
H	-0.618205	1.221358	-2.218571
H	-0.757758	3.005214	-3.958185
P	1.202108	0.681350	-0.084294
C	2.948807	0.660006	0.455585
C	3.307549	0.668962	1.805912
C	3.950986	0.529783	-0.515779
C	4.645878	0.553229	2.178585
H	2.544759	0.765904	2.572917
C	5.286118	0.428200	-0.141694
H	3.686648	0.512567	-1.570075
C	5.637556	0.436474	1.208481
H	4.911481	0.561855	3.232114
H	6.053671	0.337454	-0.905316
H	6.680417	0.352824	1.501034
C	0.298084	1.370446	1.350630
C	-0.151024	0.475751	2.331050

C	-0.005217	2.728661	1.474210
C	-0.881741	0.934933	3.422278
H	0.062956	-0.585528	2.226914
C	-0.749405	3.184377	2.561173
H	0.328681	3.433228	0.718028
C	-1.187747	2.290663	3.535882
H	-1.225720	0.232002	4.175919
H	-0.987658	4.241197	2.643969
H	-1.771001	2.648163	4.379854
Pd	-0.060029	-1.290373	-0.702711
C	0.987587	4.048446	-3.248240
H	0.923812	4.832011	-3.998391
C	2.011350	4.071623	-2.302508
H	2.744053	4.873943	-2.310151
C	2.099755	3.067258	-1.342204
H	2.900096	3.094466	-0.608652
C	1.478645	-3.023536	-1.035872
C	2.820016	-2.662276	-0.784602
C	3.301633	-2.617251	0.508804
C	2.449038	-2.916581	1.583853
C	1.133305	-3.277303	1.358224
C	0.624907	-3.374224	0.041357
H	1.168554	-3.225772	-2.059004
H	3.471460	-2.430896	-1.622284
H	4.333087	-2.336705	0.698406
H	2.828022	-2.869130	2.600997
H	0.480515	-3.528225	2.190421
C	-5.796901	1.298117	1.497592
C	-4.464094	1.703122	1.485875
C	-3.538062	1.051782	0.672346

C	-3.926845	-0.012585	-0.145309
C	-5.269007	-0.412217	-0.126960
C	-6.195423	0.235218	0.687008
H	-6.520148	1.803801	2.131926
H	-4.139912	2.529143	2.114725
H	-2.494857	1.350680	0.655019
H	-5.595959	-1.241124	-0.750228
H	-7.232396	-0.091421	0.689025
C	-2.886849	-0.737963	-0.998589
C	-2.706669	-2.168383	-0.461210
H	-2.624273	-2.107185	0.631973
H	-3.578670	-2.806929	-0.678125
C	-1.422976	-2.754363	-1.016986
H	-1.467705	-2.939559	-2.095396
C	-0.771464	-3.897404	-0.249946
H	-1.288595	-4.090447	0.695824
H	-0.727845	-4.841810	-0.806380
O	-1.657772	-0.064591	-0.894448
C	-3.333065	-0.746751	-2.466926
H	-4.293383	-1.252151	-2.616003
H	-3.429024	0.282476	-2.828308
H	-2.579801	-1.250556	-3.081229

C12

Coordinates (Angstroms)

	X	Y	Z
H	3.301574	3.888764	-2.371506

C	3.584880	3.107017	-1.672563
C	3.107871	0.996443	-0.591612
C	2.756575	2.003379	-1.496782
H	1.829396	1.921974	-2.060044
C	-1.926203	2.737207	-0.394944
C	-2.939454	3.347893	0.346221
C	-4.001445	3.974786	-0.304426
H	-2.907287	3.329929	1.432114
H	-4.791731	4.439238	0.278912
P	-0.505131	1.906552	0.399363
P	2.076182	-0.515823	-0.557728
C	0.655780	3.305365	0.648878
C	0.478431	4.522291	-0.018528
C	1.764575	3.158258	1.494098
C	1.383122	5.567171	0.160656
H	-0.369927	4.663448	-0.680147
C	2.655844	4.207777	1.685456
H	1.934987	2.222916	2.015209
C	2.469883	5.416691	1.016339
H	1.228652	6.503988	-0.367552
H	3.503882	4.075482	2.350991
H	3.170995	6.233929	1.160079
C	-1.111365	1.528513	2.092159
C	-0.773092	2.272784	3.226394
C	-1.961760	0.420643	2.227702
C	-1.253039	1.897363	4.480429
H	-0.136435	3.147160	3.142011
C	-2.447303	0.058896	3.480450
H	-2.246530	-0.131188	1.332346
C	-2.084505	0.788474	4.612342

H	-0.977499	2.480039	5.355170
H	-3.107144	-0.799765	3.572204
H	-2.454478	0.497813	5.591690
C	2.887930	-1.374932	-1.958835
C	4.201726	-1.853558	-1.870041
C	2.237185	-1.395458	-3.196430
C	4.826117	-2.397737	-2.987577
H	4.747733	-1.788926	-0.933732
C	2.869146	-1.930899	-4.316414
H	1.240004	-0.975083	-3.284576
C	4.158351	-2.445741	-4.210663
H	5.841290	-2.775509	-2.904824
H	2.351879	-1.942004	-5.271646
H	4.649357	-2.869353	-5.082203
C	2.560448	-1.362515	0.987231
C	3.107580	-2.646040	1.050637
C	2.222718	-0.710312	2.181925
C	3.323678	-3.257519	2.284829
H	3.351572	-3.188792	0.143905
C	2.456484	-1.313025	3.410994
H	1.744967	0.263787	2.150533
C	3.006668	-2.593416	3.465499
H	3.736743	-4.261562	2.317100
H	2.188131	-0.790601	4.324914
H	3.174593	-3.075300	4.424418
Pd	-0.169157	-0.254271	-0.653855
C	-4.047837	4.007100	-1.695806
H	-4.876426	4.494906	-2.201654
C	-3.029534	3.410413	-2.439714
H	-3.063714	3.429920	-3.525611

C	4.765666	3.215997	-0.938948
H	5.408723	4.081566	-1.070614
C	5.115820	2.217870	-0.032012
H	6.033803	2.301467	0.543047
C	4.292635	1.107561	0.140555
H	4.576044	0.328618	0.842644
C	-1.978429	2.769895	-1.792241
H	-1.203667	2.272524	-2.369603
C	-0.416012	-2.854856	1.585110
C	-0.589284	-3.241701	2.911934
C	-0.336686	-4.555775	3.299670
C	0.084805	-5.479061	2.344053
C	0.251542	-5.086200	1.018548
C	0.012007	-3.766790	0.615725
H	-0.605582	-1.824530	1.291974
H	-0.918572	-2.508508	3.644190
H	-0.470067	-4.858779	4.334708
H	0.281846	-6.509037	2.630475
H	0.580135	-5.814096	0.278974
C	-6.977813	-1.431366	-0.698505
C	-6.205987	-0.412214	-0.145145
C	-4.846298	-0.321356	-0.439041
C	-4.234050	-1.243043	-1.292367
C	-5.020205	-2.259260	-1.849360
C	-6.377653	-2.356151	-1.552882
H	-8.037332	-1.505738	-0.468247
H	-6.663618	0.316452	0.519950
H	-4.232249	0.466018	-0.013069
H	-4.567978	-2.984319	-2.521975
H	-6.969369	-3.156028	-1.991134

C	-2.747784	-1.114451	-1.615769
C	-2.002232	-2.412648	-1.319228
H	-2.280290	-2.724295	-0.305187
H	-2.293746	-3.235009	-1.992755
C	-0.491177	-2.186031	-1.393687
H	-0.196743	-2.100650	-2.445033
C	0.267614	-3.377250	-0.821606
H	0.035941	-4.258862	-1.441774
H	1.348362	-3.230246	-0.949491
O	-2.187979	-0.133757	-0.793352
C	-2.613331	-0.715822	-3.095074
H	-3.040189	-1.468257	-3.768461
H	-3.129151	0.233905	-3.269709
H	-1.557188	-0.579805	-3.353158

C13

Coordinates (Angstroms)

	X	Y	Z
H	2.003971	2.969704	4.654876
C	1.998826	3.039586	3.570691
C	0.922176	2.558638	1.457951
C	0.945466	2.475680	2.852033
H	0.139792	1.979162	3.384059
C	2.539032	-0.424667	1.051410
C	1.707666	-1.114706	1.944187
C	2.006216	-1.143468	3.301743
H	0.833433	-1.643278	1.573111

H	1.355353	-1.684692	3.982518
P	2.075960	-0.497656	-0.713505
P	-0.430761	1.850145	0.446146
C	3.276734	0.528939	-1.620717
C	4.638705	0.208599	-1.672317
C	2.805649	1.659794	-2.295123
C	5.519335	1.029057	-2.370335
H	5.009961	-0.681323	-1.170869
C	3.689866	2.477908	-2.993921
H	1.741374	1.886687	-2.270237
C	5.046699	2.164910	-3.027748
H	6.575942	0.779458	-2.404831
H	3.317407	3.355558	-3.514566
H	5.737379	2.801195	-3.573917
C	2.560392	-2.219201	-1.143442
C	2.105205	-2.795642	-2.334536
C	3.398795	-2.964805	-0.306707
C	2.467142	-4.094850	-2.675594
H	1.450229	-2.229923	-2.991547
C	3.754439	-4.268531	-0.646601
H	3.770064	-2.536892	0.618833
C	3.285425	-4.838999	-1.826673
H	2.098908	-4.530008	-3.600374
H	4.397002	-4.838486	0.018602
H	3.555652	-5.858998	-2.084955
C	-1.770531	1.558392	1.653278
C	-2.809094	2.470882	1.857703
C	-1.755718	0.360229	2.378424
C	-3.818073	2.189377	2.776464
H	-2.837607	3.399218	1.295500

C	-2.754597	0.091394	3.309182
H	-0.963530	-0.363881	2.210848
C	-3.790342	1.003577	3.506744
H	-4.625976	2.900868	2.922359
H	-2.728263	-0.835199	3.875416
H	-4.576233	0.787406	4.224896
C	-0.979407	3.320065	-0.503496
C	-1.566202	3.130750	-1.760245
C	-0.836017	4.619041	0.001335
C	-1.995687	4.228481	-2.503063
H	-1.712178	2.113105	-2.118746
C	-1.268451	5.711453	-0.745225
H	-0.386043	4.779537	0.976672
C	-1.844335	5.518678	-2.000296
H	-2.450231	4.072938	-3.478054
H	-1.153976	6.715269	-0.345621
H	-2.175628	6.374069	-2.582743
Pd	-0.069891	0.022611	-1.078516
C	3.134752	-0.479313	3.781052
H	3.367710	-0.497008	4.841982
C	3.958328	0.214033	2.898140
H	4.832522	0.742031	3.268109
C	3.034139	3.691965	2.907366
H	3.850536	4.134383	3.471151
C	3.020212	3.771561	1.515272
H	3.825214	4.275088	0.987128
C	1.973943	3.206749	0.795016
H	1.967676	3.285295	-0.288055
C	3.664712	0.242864	1.535367
H	4.311931	0.790962	0.858540

C	-6.607063	-1.354135	-0.013841
C	-5.627870	-0.502754	0.492136
C	-4.435848	-0.308691	-0.204524
C	-4.194377	-0.962500	-1.415324
C	-5.191403	-1.806749	-1.920226
C	-6.383502	-2.003780	-1.227316
H	-7.536277	-1.508898	0.528225
H	-5.789060	0.013891	1.435231
H	-3.660178	0.345696	0.178332
H	-5.042263	-2.321310	-2.866545
H	-7.140503	-2.668222	-1.636741
C	-2.874957	-0.721750	-2.173968
C	-2.215012	-2.079254	-2.505458
H	-2.929634	-2.704461	-3.059506
H	-1.406537	-1.876843	-3.224120
C	-1.619601	-2.890376	-1.401968
H	-1.025977	-3.738748	-1.747721
C	-1.702040	-2.664003	-0.082923
H	0.152157	-0.947383	-2.265818
O	-2.085992	0.144306	-1.432117
H	-2.304479	-1.832210	0.272890
C	-1.004776	-3.427825	0.957529
C	-1.424562	-3.298779	2.290723
C	0.116936	-4.232098	0.693956
C	-0.754725	-3.947829	3.323889
H	-2.289711	-2.678599	2.510007
C	0.786085	-4.880439	1.725585
H	0.490106	-4.324456	-0.322152
C	0.357498	-4.740646	3.046236
H	-1.100115	-3.830917	4.347798

H	1.659917	-5.485416	1.498406
H	0.890055	-5.239812	3.850867
C	-3.220937	-0.055261	-3.518850
H	-3.735944	0.894529	-3.341330
H	-2.293249	0.150921	-4.065645
H	-3.861237	-0.681180	-4.151094

C14

Coordinates (Angstroms)

	X	Y	Z

H	1.840261	1.709440	4.815626
C	2.117311	0.992368	4.047628
C	2.669675	0.523302	1.735780
C	2.317069	1.430522	2.738912
H	2.190211	2.483439	2.505628
C	-1.213411	-1.841308	1.068790
C	-2.229400	-2.744065	1.398649
C	-2.859085	-2.668770	2.639274
H	-2.537577	-3.505624	0.689622
H	-3.652686	-3.369704	2.881821
P	-0.256415	-1.902094	-0.494451
P	2.718429	0.999685	-0.041090
C	1.096207	-3.078712	-0.082491
C	1.139883	-3.816772	1.102962
C	2.176134	-3.154799	-0.973166
C	2.252123	-4.605379	1.398663
H	0.314920	-3.766553	1.807481

C	3.283203	-3.942529	-0.678376
H	2.156325	-2.569621	-1.889860
C	3.326794	-4.664621	0.515209
H	2.278499	-5.168524	2.327643
H	4.119768	-3.977476	-1.371010
H	4.197388	-5.268666	0.754958
C	-1.298190	-2.888281	-1.635196
C	-1.925104	-2.227680	-2.696616
C	-1.481435	-4.269011	-1.485509
C	-2.754275	-2.925485	-3.572539
H	-1.755596	-1.164325	-2.838170
C	-2.308304	-4.965593	-2.362031
H	-0.975135	-4.799852	-0.683467
C	-2.951772	-4.293735	-3.401132
H	-3.239264	-2.401065	-4.391168
H	-2.449242	-6.035477	-2.235711
H	-3.596324	-4.840195	-4.083956
C	3.195740	2.770563	0.006972
C	4.506669	3.215953	-0.192621
C	2.183415	3.711341	0.243397
C	4.800420	4.576937	-0.146404
H	5.302784	2.503401	-0.385847
C	2.484340	5.069266	0.305348
H	1.155096	3.380702	0.373391
C	3.793195	5.505300	0.107909
H	5.821872	4.911122	-0.306657
H	1.691815	5.787462	0.497638
H	4.026413	6.565756	0.145671
C	4.208801	0.141851	-0.664590
C	4.180724	-0.340113	-1.978189

C	5.345940	-0.079335	0.121867
C	5.271418	-1.030671	-2.500806
H	3.286232	-0.187729	-2.579190
C	6.432153	-0.776868	-0.399035
H	5.378121	0.284136	1.145309
C	6.395938	-1.253893	-1.708997
H	5.237264	-1.404926	-3.520108
H	7.308224	-0.950471	0.219583
H	7.243498	-1.802541	-2.110183
Pd	0.862213	0.044088	-0.932248
C	-2.485162	-1.690556	3.558271
H	-2.984193	-1.630632	4.521478
C	-1.478757	-0.781973	3.233930
H	-1.184211	-0.012999	3.942769
C	2.274017	-0.352773	4.371075
H	2.114877	-0.692222	5.390672
C	2.638647	-1.261546	3.377519
H	2.764792	-2.313934	3.616979
C	2.830147	-0.829938	2.069947
H	3.093005	-1.551398	1.301467
C	-0.849383	-0.854778	1.995015
H	-0.066391	-0.146040	1.733281
C	-4.834978	5.558352	-0.116458
C	-4.014515	5.033509	0.878159
C	-2.973982	4.166129	0.548493
C	-2.739475	3.807173	-0.780401
C	-3.563552	4.346173	-1.774476
C	-4.602815	5.211729	-1.446815
H	-5.647795	6.232024	0.140459
H	-4.183844	5.296845	1.919079

H	-2.338806	3.755369	1.325527
H	-3.395568	4.087791	-2.816841
H	-5.234348	5.615647	-2.233645
C	-1.597411	2.874586	-1.157668
C	-2.094502	1.684467	-1.994729
H	-2.440572	2.059360	-2.965357
H	-1.205085	1.066842	-2.229607
C	-3.145445	0.789557	-1.418984
H	-3.635919	0.149574	-2.152357
C	-3.509760	0.691071	-0.133174
H	-0.408532	1.671763	-0.173447
O	-0.998819	2.425286	0.051902
H	-3.039707	1.343295	0.597826
C	-4.517713	-0.233320	0.394922
C	-5.086533	0.027422	1.650031
C	-4.913303	-1.397512	-0.284179
C	-6.031945	-0.831918	2.202400
H	-4.776463	0.916921	2.193771
C	-5.856706	-2.256011	0.267551
H	-4.455941	-1.649348	-1.237131
C	-6.422652	-1.977921	1.512607
H	-6.459986	-0.608818	3.176060
H	-6.142132	-3.156345	-0.270328
H	-7.154872	-2.654549	1.944375
C	-0.559603	3.644382	-1.980458
H	-0.187267	4.502321	-1.414402
H	0.285871	2.986460	-2.215629
H	-0.986028	4.008631	-2.920172

C8

	Coordinates (Angstroms)		
	X	Y	Z
C	1.315158	-1.153500	1.447077
C	1.138041	-0.218259	2.476023
C	2.087080	-0.099078	3.486705
H	0.255624	0.418421	2.480632
H	1.939753	0.626638	4.281321
P	-0.024755	-1.278732	0.216190
C	0.564632	-2.294508	-1.172570
C	0.942890	-3.632112	-0.994562
C	0.613183	-1.728364	-2.450402
C	1.404063	-4.374081	-2.076902
H	0.872121	-4.094780	-0.013901
C	1.068307	-2.476888	-3.532980
H	0.290210	-0.699586	-2.592563
C	1.472671	-3.796180	-3.344615
H	1.704134	-5.407767	-1.931772
H	1.104515	-2.028649	-4.521626
H	1.830638	-4.380227	-4.187706
C	-1.266086	-2.352391	1.024654
C	-2.161051	-3.068684	0.219733
C	-1.408451	-2.394485	2.413707
C	-3.194485	-3.796685	0.798402
H	-2.059464	-3.048284	-0.860872
C	-2.442291	-3.130467	2.989035
H	-0.718387	-1.854934	3.054527
C	-3.340672	-3.825646	2.184739

H	-3.887891	-4.340987	0.163614
H	-2.542704	-3.157468	4.070372
H	-4.150088	-4.392842	2.635484
Pd	-0.693185	0.778571	-0.475381
C	3.228617	-0.897666	3.466521
H	3.975495	-0.798976	4.249076
C	3.416485	-1.815192	2.435715
H	4.312612	-2.428147	2.407897
C	2.464093	-1.947632	1.428424
H	2.628454	-2.659656	0.627063
O	-1.281027	2.641900	-1.193336
O	-1.927812	3.379322	-0.130985
C	-3.175151	-0.386841	-1.495607
C	-4.511987	-0.785667	-1.435776
C	-5.227200	-0.669780	-0.245724
C	-4.600580	-0.146658	0.884821
C	-3.264989	0.253732	0.828168
C	-2.543028	0.134185	-0.362917
H	-2.626930	-0.494855	-2.428791
H	-4.991556	-1.192661	-2.322992
H	-6.265167	-0.987840	-0.197729
H	-5.150141	-0.054321	1.818723
H	-2.784831	0.642390	1.722878
B	-3.274578	3.523332	-0.423898
O	-4.063994	4.183324	0.477634
H	-3.551899	4.466337	1.242998
O	-3.797654	3.051905	-1.583133
H	-3.042765	2.594050	-1.995271
O	1.169159	1.943611	-0.999816
C	2.417073	2.383431	-0.437301

C	3.369735	1.201373	-0.506658
C	2.199508	2.874517	1.005605
C	3.209880	0.240333	-1.509556
C	4.456618	1.082202	0.364533
H	1.941364	2.003508	1.617763
H	3.142701	3.278284	1.385720
C	1.131068	3.914203	1.131479
C	4.101115	-0.822562	-1.630701
H	2.374813	0.325384	-2.194661
C	5.357330	0.027000	0.235034
H	4.614266	1.811361	1.153167
H	0.111206	3.608208	0.896455
C	1.350340	5.171656	1.516976
C	5.182866	-0.931863	-0.760050
H	3.944844	-1.566513	-2.407899
H	6.193899	-0.048866	0.924234
H	2.349246	5.526993	1.765695
H	0.537486	5.889405	1.600566
H	5.881532	-1.758650	-0.853004
H	0.555863	2.699962	-1.133554
C	2.946647	3.509543	-1.322563
H	2.263078	4.365714	-1.309501
H	3.923002	3.848021	-0.963245
H	3.057738	3.158978	-2.352643

C9

Coordinates (Angstroms)

X Y Z

C	-0.504923	-1.947650	-1.105990
C	-0.370370	-1.744168	-2.488101
C	-1.276017	-2.321066	-3.371185
H	0.433140	-1.120480	-2.872345
H	-1.161059	-2.162245	-4.439390
P	0.684984	-1.105019	-0.017374
C	0.336171	-1.579138	1.702490
C	0.311853	-2.931012	2.069773
C	0.159791	-0.590839	2.674569
C	0.073171	-3.285216	3.392898
H	0.479323	-3.703422	1.323910
C	-0.067762	-0.951601	4.000915
H	0.193038	0.459206	2.393645
C	-0.119205	-2.296528	4.358435
H	0.044185	-4.334254	3.672599
H	-0.206374	-0.179222	4.751961
H	-0.301078	-2.577094	5.392010
C	2.299029	-1.910571	-0.312229
C	3.318288	-1.661046	0.617509
C	2.563994	-2.710674	-1.424632
C	4.590880	-2.179002	0.415805
H	3.118639	-1.050232	1.492895
C	3.841627	-3.234841	-1.617790
H	1.783828	-2.934467	-2.144111
C	4.857469	-2.962908	-0.707349
H	5.376407	-1.970024	1.136237
H	4.037842	-3.857328	-2.486115
H	5.853864	-3.365481	-0.865849
Pd	0.468634	1.105787	-0.322371

C	-2.340435	-3.077831	-2.882416
H	-3.057404	-3.514976	-3.571407
C	-2.490051	-3.262347	-1.510586
H	-3.325488	-3.838748	-1.124384
C	-1.573601	-2.705562	-0.620836
H	-1.709628	-2.849198	0.445332
O	0.072719	3.293758	-0.550760
O	0.442187	4.131313	0.549436
C	3.143768	1.704583	0.630939
C	4.524710	1.888168	0.537812
C	5.196026	1.579316	-0.643732
C	4.479453	1.097633	-1.738609
C	3.100037	0.908251	-1.648250
C	2.424223	1.209886	-0.461555
H	2.634765	1.940712	1.563085
H	5.075826	2.266065	1.395662
H	6.272284	1.712743	-0.711138
H	4.995986	0.856840	-2.664677
H	2.559042	0.503930	-2.500876
B	0.050495	3.705553	1.829764
O	0.631608	4.411240	2.846000
H	1.286158	5.038384	2.519081
O	-0.833382	2.734573	2.122798
H	-1.283695	2.295954	1.342512
O	-1.625602	1.681815	-0.067952
C	-2.878378	1.329110	-0.598544
C	-3.503155	0.196096	0.212895
C	-2.724462	0.867927	-2.070070
C	-2.955537	-0.184537	1.437777
C	-4.633823	-0.489447	-0.248028

H	-2.289814	-0.135957	-2.058210
H	-3.716809	0.791502	-2.525902
C	-1.860704	1.765603	-2.895044
C	-3.497054	-1.236683	2.174762
H	-2.083900	0.338057	1.808790
C	-5.180339	-1.539640	0.484596
H	-5.092949	-0.209246	-1.192074
H	-0.787277	1.709716	-2.703183
C	-2.304442	2.603069	-3.833086
C	-4.609556	-1.924430	1.697991
H	-3.037487	-1.521893	3.118069
H	-6.053765	-2.062640	0.103844
H	-3.365432	2.684883	-4.064875
H	-1.626276	3.232749	-4.404363
H	-5.032073	-2.749140	2.265364
H	-0.891639	2.924959	-0.396157
C	-3.780758	2.563152	-0.522854
H	-3.369168	3.366788	-1.143304
H	-4.793511	2.339656	-0.872843
H	-3.843632	2.917303	0.511206

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o2

Coordinates (Angstroms)			
	X	Y	Z

O	0.000000	0.000000	0.601149
O	0.000000	0.000000	-0.601149

PhBOH2

	Coordinates (Angstroms)		
	X	Y	Z
C	2.640000	-0.000001	0.000040
C	1.941661	-1.206516	-0.000047
C	0.549638	-1.201982	-0.000094
C	-0.172603	0.000002	-0.000056
C	0.549640	1.201983	0.000037
C	1.941664	1.206515	0.000076
H	3.726859	-0.000003	0.000077
H	2.483934	-2.148325	-0.000040
H	0.009769	-2.145437	-0.000173
H	0.009774	2.145440	0.000069
H	2.483937	2.148324	0.000100
B	-1.739091	0.000000	-0.000140
O	-2.377410	-1.209163	0.000178
H	-3.340118	-1.147731	0.000137
O	-2.377413	1.209162	-0.000099
H	-3.340121	1.147728	0.000156

PPh3

	Coordinates (Angstroms)		
	X	Y	Z
C	-1.132125	-1.198666	-0.436404

C	-1.213566	-2.480604	-0.996177
C	-2.040904	-3.447657	-0.433777
H	-0.624047	-2.722519	-1.877829
H	-2.090796	-4.439034	-0.875405
P	0.000810	-0.001231	-1.247004
C	-0.467378	1.578857	-0.435659
C	0.150872	2.079388	0.715355
C	-1.509838	2.310528	-1.019429
C	-0.270393	3.284662	1.272560
H	0.961915	1.526203	1.180399
C	-1.937503	3.508250	-0.454730
H	-1.990439	1.938458	-1.921571
C	-1.316013	3.999061	0.692032
H	0.218442	3.663968	2.165783
H	-2.750249	4.063064	-0.915089
H	-1.642947	4.938129	1.129613
C	1.603768	-0.384504	-0.436503
C	2.757573	0.162558	-1.012882
C	1.728618	-1.177284	0.709248
C	4.007944	-0.063037	-0.445526
H	2.675138	0.770295	-1.911272
C	2.982374	-1.411940	1.269334
H	0.844336	-1.610202	1.168049
C	4.122792	-0.853635	0.696423
H	4.893834	0.371541	-0.900160
H	3.066933	-2.029747	2.159160
H	5.099094	-1.037008	1.136247
C	-2.812089	-3.140203	0.685813
H	-3.465526	-3.891447	1.120375
C	-2.746001	-1.865068	1.242279

H	-3.345672	-1.619960	2.114655
C	-1.908648	-0.899506	0.687763
H	-1.859060	0.089517	1.133791

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pro-1a

	Coordinates (Angstroms)		
	X	Y	Z

C	-5.390141	-0.401179	-1.154666
C	-4.946421	-1.381993	-0.273604
C	-3.652673	-1.329881	0.240020
C	-2.787381	-0.294511	-0.116953
C	-3.234561	0.681884	-1.013730
C	-4.527863	0.629162	-1.523620
H	-6.399043	-0.439814	-1.555255
H	-5.605432	-2.195644	0.015921
H	-3.310052	-2.108384	0.913597
H	-2.578836	1.490146	-1.318008
H	-4.861130	1.397984	-2.214943
C	-1.359050	-0.300307	0.425227
C	-0.389192	-0.716501	-0.694016
H	-0.744195	-1.701974	-1.022262
H	-0.511616	-0.032880	-1.538868
C	1.045699	-0.806521	-0.288998
H	1.267983	-1.471453	0.543009
C	2.025265	-0.130941	-0.902745
H	1.756395	0.548812	-1.712314
O	-1.197449	-1.224877	1.474046

H	-1.833939	-1.003864	2.169339
C	-0.982532	1.081043	0.992117
F	0.159265	1.038585	1.688532
F	-0.825609	2.014049	0.037576
F	-1.934340	1.522507	1.837587
C	3.456248	-0.187973	-0.587786
C	4.012864	-1.142121	0.279613
C	4.316001	0.749887	-1.178198
C	5.374455	-1.143256	0.554608
H	3.377706	-1.896207	0.735676
C	5.679813	0.749017	-0.902338
H	3.901416	1.490378	-1.858251
C	6.215546	-0.197226	-0.032457
H	5.785044	-1.891032	1.227731
H	6.324854	1.488252	-1.369345
H	7.280121	-0.203058	0.183508

TSA10-11

Coordinates (Angstroms)

	X	Y	Z
C	-1.031271	1.860774	1.695245
C	0.138475	1.737188	2.457774
C	0.335168	2.560585	3.563622
H	0.889680	1.001944	2.167943
H	1.244284	2.462764	4.151054
P	-1.209260	0.788597	0.226907
C	-2.995069	0.836545	-0.134849

C	-3.502943	1.312700	-1.346510
C	-3.873761	0.307936	0.820543
C	-4.872090	1.259607	-1.600065
H	-2.831112	1.724415	-2.093763
C	-5.240007	0.263969	0.566303
H	-3.487599	-0.069840	1.764220
C	-5.741267	0.734855	-0.647077
H	-5.258243	1.630828	-2.545278
H	-5.914042	-0.147342	1.312386
H	-6.808136	0.693040	-0.847578
C	-0.439976	1.752771	-1.123239
C	0.049461	1.054842	-2.234609
C	-0.309613	3.143867	-1.074494
C	0.654140	1.738626	-3.284806
H	-0.031551	-0.029597	-2.262714
C	0.303285	3.824986	-2.123607
H	-0.678682	3.696254	-0.214841
C	0.785196	3.124901	-3.228382
H	1.036093	1.187693	-4.139679
H	0.407479	4.905311	-2.075676
H	1.268955	3.658948	-4.041339
Pd	-0.097595	-1.279665	0.277072
C	-0.629282	3.500961	3.921490
H	-0.474494	4.137390	4.788394
C	-1.794201	3.622925	3.166504
H	-2.548674	4.354817	3.441256
C	-1.996341	2.808595	2.054823
H	-2.906031	2.911555	1.470460
C	-2.394445	-3.074125	0.575366
C	-3.763043	-3.288878	0.444624

C	-4.415293	-2.941125	-0.739224
C	-3.693755	-2.367125	-1.785958
C	-2.328028	-2.135891	-1.650810
C	-1.661196	-2.474670	-0.463776
H	-1.880624	-3.389975	1.480677
H	-4.319353	-3.742224	1.260913
H	-5.481058	-3.121498	-0.847427
H	-4.198314	-2.091522	-2.708221
H	-1.772032	-1.688433	-2.471252
C	4.690455	2.038174	-2.075006
C	3.728441	2.375732	-1.125551
C	3.128271	1.382690	-0.354576
C	3.478326	0.042124	-0.521428
C	4.452665	-0.289512	-1.468739
C	5.051397	0.702054	-2.242562
H	5.155083	2.809756	-2.682994
H	3.435989	3.413730	-0.990470
H	2.359923	1.623659	0.372331
H	4.744384	-1.325887	-1.612888
H	5.800827	0.428963	-2.980821
C	2.752201	-1.016868	0.316842
C	2.331525	-2.212244	-0.573315
H	2.076674	-1.818218	-1.563290
H	3.156881	-2.922258	-0.724028
C	1.117100	-2.912213	0.002208
H	1.255105	-3.425800	0.953078
C	0.037668	-3.361667	-0.820318
H	0.114759	-3.172058	-1.889751
H	-0.406193	-4.323314	-0.581562
O	1.666297	-0.472026	0.982792

C	3.718224	-1.503948	1.406368
F	3.157843	-2.448907	2.189031
F	4.849528	-2.049537	0.909360
F	4.095449	-0.503344	2.219695

TSA11-16

	Coordinates (Angstroms)		
	X	Y	Z

H	4.286821	-4.554934	-1.991602
C	4.118117	-3.608116	-1.486367
C	2.602280	-2.027081	-0.462238
C	2.827420	-3.247837	-1.107692
H	1.994917	-3.913781	-1.317697
P	0.940653	-1.507397	0.081354
C	-0.209263	-2.334447	-1.073598
C	-0.816733	-3.561798	-0.793644
C	-0.511996	-1.671903	-2.270544
C	-1.712173	-4.120035	-1.704391
H	-0.597516	-4.080625	0.135310
C	-1.401132	-2.235368	-3.179400
H	-0.056907	-0.705819	-2.479049
C	-2.004760	-3.459819	-2.895798
H	-2.183707	-5.072466	-1.479011
H	-1.634144	-1.711912	-4.102367
H	-2.708740	-3.894999	-3.599433
C	0.669643	-2.362785	1.670048
C	-0.396851	-1.913298	2.462129

C	1.454563	-3.435369	2.102398
C	-0.679099	-2.549848	3.667218
H	-0.992978	-1.063211	2.128180
C	1.170310	-4.060481	3.314782
H	2.285816	-3.785009	1.497052
C	0.102841	-3.622237	4.095169
H	-1.507828	-2.202074	4.278144
H	1.784262	-4.892494	3.648163
H	-0.116987	-4.112980	5.039283
Pd	0.442014	0.739649	0.102467
C	5.188916	-2.756532	-1.220094
H	6.194458	-3.039553	-1.518475
C	4.969335	-1.538832	-0.578601
H	5.801191	-0.870039	-0.376440
C	3.679523	-1.171496	-0.206076
H	3.503223	-0.213761	0.279359
C	-5.161028	-0.767048	-1.844297
C	-4.298748	-1.368095	-0.930500
C	-3.385680	-0.594328	-0.216932
C	-3.321233	0.786292	-0.405792
C	-4.194634	1.385572	-1.320053
C	-5.106311	0.613158	-2.035577
H	-5.870081	-1.368612	-2.406658
H	-4.329341	-2.443553	-0.777109
H	-2.690810	-1.044029	0.484393
H	-4.163679	2.459031	-1.482962
H	-5.774512	1.090996	-2.747260
C	-2.263058	1.581347	0.368808
C	-1.503931	2.535971	-0.605328
H	-1.504592	2.083691	-1.602100

H	-2.008541	3.507155	-0.701083
C	-0.076897	2.709814	-0.139813
H	0.070187	3.225681	0.808204
C	1.061941	2.614625	-1.004435
H	1.602855	1.262424	-0.900940
O	-1.405991	0.741481	1.063369
C	-2.972863	2.425397	1.437246
F	-2.098336	3.181767	2.131588
F	-3.885397	3.281317	0.926343
F	-3.620400	1.658942	2.329521
H	0.853543	2.544088	-2.073823
C	2.312598	3.356697	-0.662215
C	2.853560	4.255711	-1.583604
C	2.937681	3.185571	0.577202
C	3.994134	4.988500	-1.261812
H	2.376073	4.385048	-2.551670
C	4.074828	3.919263	0.897973
H	2.529608	2.460522	1.279755
C	4.605542	4.824188	-0.021177
H	4.406611	5.686707	-1.984865
H	4.554665	3.777107	1.862387
H	5.497762	5.392291	0.226518

TSA12-13

Coordinates (Angstroms)		
X	Y	Z

H	-0.205309	4.851074	3.658716

C	0.200847	3.901246	3.322294
C	0.838988	2.431414	1.514304
C	0.325896	3.652367	1.956019
H	0.010237	4.406961	1.242831
C	-2.534541	1.232943	1.365314
C	-2.838087	2.095743	0.301788
C	-3.303158	3.384586	0.540387
H	-2.703645	1.751065	-0.719920
H	-3.529382	4.038403	-0.297522
P	-1.838066	-0.404120	0.934358
P	0.977088	1.946349	-0.238789
C	-1.537365	-1.212562	2.549289
C	-2.574116	-1.477149	3.456076
C	-0.232256	-1.606162	2.859057
C	-2.300249	-2.098661	4.669505
H	-3.595377	-1.196124	3.210969
C	0.035572	-2.236286	4.074845
H	0.558085	-1.450095	2.124603
C	-0.992553	-2.475043	4.982240
H	-3.106718	-2.294590	5.370918
H	1.050448	-2.549471	4.305724
H	-0.782122	-2.965141	5.929149
C	-3.294854	-1.365214	0.359720
C	-3.164568	-2.762455	0.320113
C	-4.486801	-0.786189	-0.086070
C	-4.209195	-3.558187	-0.137528
H	-2.243670	-3.229679	0.660404
C	-5.529360	-1.586790	-0.549500
H	-4.614890	0.291647	-0.060808
C	-5.397470	-2.972826	-0.573547

H	-4.093973	-4.638599	-0.154126
H	-6.451345	-1.121204	-0.887158
H	-6.213511	-3.593801	-0.932081
C	0.457760	3.416081	-1.194312
C	1.146723	4.631789	-1.083375
C	-0.628120	3.324849	-2.067699
C	0.734658	5.739351	-1.816857
H	2.006572	4.712187	-0.423360
C	-1.038604	4.433967	-2.804447
H	-1.148514	2.378063	-2.173485
C	-0.360955	5.643134	-2.675250
H	1.271510	6.678927	-1.721496
H	-1.885119	4.349245	-3.480159
H	-0.679217	6.509704	-3.248002
C	2.782693	1.914577	-0.546041
C	3.220385	1.327338	-1.739684
C	3.720902	2.459008	0.334119
C	4.574417	1.293524	-2.053116
H	2.492513	0.882998	-2.415000
C	5.079576	2.414803	0.022504
H	3.395720	2.915894	1.264238
C	5.507661	1.835227	-1.169129
H	4.904076	0.829043	-2.978313
H	5.803405	2.835610	0.715030
H	6.567166	1.797316	-1.406142
Pd	0.093362	-0.161769	-0.660803
C	-3.458094	3.837500	1.850097
H	-3.808967	4.847842	2.040604
C	-3.148877	2.991778	2.912290
H	-3.254632	3.341665	3.935525

C	0.580795	2.935957	4.250685
H	0.475158	3.132418	5.313983
C	1.089470	1.712669	3.812768
H	1.377093	0.950343	4.531641
C	1.216888	1.458867	2.451906
H	1.603840	0.504144	2.101029
C	-2.689341	1.697321	2.674960
H	-2.437547	1.059129	3.515559
C	6.424792	-2.184334	-0.550417
C	5.727486	-1.393217	0.360571
C	4.337200	-1.448447	0.414375
C	3.623482	-2.296085	-0.433913
C	4.329515	-3.096970	-1.337373
C	5.720204	-3.035428	-1.399901
H	7.509293	-2.136652	-0.600969
H	6.266966	-0.722133	1.023999
H	3.771633	-0.819557	1.093705
H	3.798667	-3.771216	-2.003110
H	6.254124	-3.655509	-2.115339
C	2.089663	-2.291571	-0.339763
C	1.464701	-2.347029	-1.752525
H	2.025742	-1.647793	-2.381820
H	1.573108	-3.340676	-2.209548
C	0.003014	-1.945481	-1.759421
H	-0.704125	-2.639460	-1.312295
C	-0.490705	-1.027684	-2.728882
H	-0.688505	0.285980	-1.970817
O	1.646321	-1.200742	0.376867
C	1.690368	-3.560212	0.438366
F	0.351768	-3.688481	0.566641

F	2.116702	-4.700692	-0.149027
F	2.193868	-3.556032	1.685596
H	0.236589	-0.641676	-3.445025
C	-1.893404	-1.076726	-3.243547
C	-2.466287	0.066372	-3.816483
C	-2.643819	-2.255143	-3.202474
C	-3.761784	0.037560	-4.319022
H	-1.888144	0.986880	-3.859655
C	-3.941262	-2.285069	-3.710142
H	-2.211397	-3.158009	-2.782773
C	-4.507126	-1.140075	-4.263644
H	-4.191298	0.935876	-4.753917
H	-4.509727	-3.209639	-3.669612
H	-5.520652	-1.164535	-4.653751

TSA13-14

Coordinates (Angstroms)

	X	Y	Z
H	3.391681	-0.433114	4.896752
C	3.586718	-0.614703	3.843442
C	3.290131	0.027382	1.524173
C	3.050824	0.243765	2.887467
H	2.440376	1.084757	3.205391
C	-0.127816	-2.667368	1.314620
C	-1.405377	-3.109253	1.676901
C	-1.662454	-3.509801	2.986261
H	-2.204872	-3.139987	0.943007

H	-2.658396	-3.851885	3.252557
P	0.205932	-1.965848	-0.339484
P	2.411720	1.055210	0.290754
C	1.808434	-2.684354	-0.861667
C	2.347248	-3.861458	-0.335565
C	2.499254	-2.002090	-1.869137
C	3.577939	-4.327805	-0.792776
H	1.819445	-4.407475	0.440853
C	3.722735	-2.475080	-2.333443
H	2.083243	-1.082418	-2.271315
C	4.269003	-3.635424	-1.786369
H	3.999306	-5.235251	-0.369103
H	4.254987	-1.926516	-3.105869
H	5.231746	-4.000451	-2.132988
C	-0.941999	-2.824744	-1.476697
C	-1.475995	-2.100951	-2.545039
C	-1.222847	-4.192128	-1.362660
C	-2.292277	-2.728551	-3.484311
H	-1.249483	-1.041485	-2.632780
C	-2.052892	-4.813099	-2.290332
H	-0.798195	-4.771269	-0.547195
C	-2.588673	-4.082875	-3.352109
H	-2.703519	-2.156184	-4.311078
H	-2.277629	-5.871134	-2.188775
H	-3.234151	-4.572076	-4.076163
C	2.392056	2.701660	1.095142
C	3.562202	3.374543	1.468834
C	1.146993	3.282811	1.353946
C	3.483375	4.614868	2.092068
H	4.534431	2.929062	1.275706

C	1.072969	4.527243	1.980177
H	0.233875	2.769940	1.052333
C	2.238178	5.192185	2.349547
H	4.393518	5.134191	2.379363
H	0.101444	4.974797	2.172866
H	2.181128	6.161837	2.836552
C	3.589325	1.248690	-1.094444
C	3.037871	1.452252	-2.365192
C	4.980912	1.208920	-0.951586
C	3.861448	1.612911	-3.475969
H	1.956180	1.473965	-2.479070
C	5.802932	1.361806	-2.064997
H	5.425969	1.045178	0.025543
C	5.246171	1.561993	-3.327206
H	3.421515	1.767099	-4.457279
H	6.882066	1.323039	-1.945602
H	5.891318	1.676253	-4.193748
Pd	0.189961	0.268065	-0.219623
C	-0.653441	-3.470636	3.945620
H	-0.857866	-3.784544	4.965371
C	0.618751	-3.023297	3.592023
H	1.412819	-2.984875	4.332702
C	4.368389	-1.700729	3.452828
H	4.785309	-2.370401	4.199687
C	4.611708	-1.921848	2.098666
H	5.217146	-2.766452	1.781647
C	4.074018	-1.067648	1.138784
H	4.263722	-1.262215	0.088188
C	0.880580	-2.618310	2.287231
H	1.873296	-2.264451	2.025812

C	-5.316707	4.665273	1.253737
C	-4.233084	4.125357	1.942848
C	-3.265978	3.390428	1.262045
C	-3.368863	3.178348	-0.114570
C	-4.453070	3.732505	-0.801765
C	-5.421316	4.467170	-0.121111
H	-6.074593	5.236056	1.783297
H	-4.139433	4.275744	3.015186
H	-2.423266	2.956189	1.789080
H	-4.554293	3.597660	-1.874036
H	-6.261224	4.884752	-0.669783
C	-2.270282	2.372164	-0.824852
C	-2.855821	1.406944	-1.873494
H	-3.495325	1.951957	-2.576840
H	-2.022100	1.030800	-2.484785
C	-3.588074	0.213942	-1.352017
H	-3.912486	-0.470628	-2.134850
C	-3.808820	-0.112625	-0.070174
H	-1.371185	0.304507	-0.247087
O	-1.475243	1.752501	0.121491
C	-1.383760	3.379291	-1.586209
F	-0.324505	2.772354	-2.165859
F	-2.041526	4.016234	-2.575296
F	-0.887445	4.323576	-0.772784
H	-3.495374	0.574795	0.711504
C	-4.390942	-1.371944	0.402862
C	-4.747153	-1.485467	1.754779
C	-4.539879	-2.501684	-0.419009
C	-5.247476	-2.678232	2.268590
H	-4.622118	-0.624136	2.406963

C	-5.032686	-3.694799	0.095472
H	-4.238735	-2.458269	-1.461352
C	-5.390406	-3.790571	1.441435
H	-5.517359	-2.741499	3.319328
H	-5.125318	-4.560151	-0.555473
H	-5.769824	-4.726500	1.841815

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	Coordinates (Angstroms)		
	X	Y	Z

H	-5.051306	0.346382	2.514772
C	-4.822989	-0.050288	1.529197
C	-3.231148	-1.079193	0.013836
C	-3.558450	-0.571942	1.278218
H	-2.824485	-0.593064	2.076064
C	-0.935703	1.288288	2.286295
C	0.023506	0.414367	2.814131
C	-0.068711	-0.006954	4.138480
H	0.828397	0.043191	2.180217
H	0.677921	-0.689140	4.535867
P	-0.713048	1.795700	0.534972
P	-1.498219	-1.633780	-0.256010
C	-2.246528	2.656151	0.060956
C	-2.725641	3.799888	0.717965
C	-2.986955	2.122272	-0.998871
C	-3.919221	4.391808	0.316024
H	-2.171809	4.229741	1.546981

C	-4.182071	2.714512	-1.397343
H	-2.626236	1.230086	-1.501391
C	-4.648068	3.851199	-0.742117
H	-4.280329	5.276418	0.832623
H	-4.749157	2.283746	-2.217364
H	-5.579822	4.315463	-1.052822
C	0.584575	3.081340	0.712059
C	0.402583	4.436157	0.429360
C	1.850384	2.627505	1.114247
C	1.460456	5.331816	0.588078
H	-0.551597	4.804085	0.068652
C	2.897619	3.526158	1.279897
H	2.027658	1.559628	1.235459
C	2.703468	4.883813	1.024964
H	1.306962	6.383991	0.364412
H	3.874323	3.159560	1.585325
H	3.522980	5.586216	1.149687
C	-1.254117	-2.697429	1.209071
C	-2.274166	-3.537767	1.679690
C	-0.018874	-2.673787	1.857572
C	-2.053684	-4.345355	2.789208
H	-3.238475	-3.558343	1.179062
C	0.197879	-3.491913	2.966691
H	0.760042	-2.008824	1.481680
C	-0.815419	-4.322365	3.434688
H	-2.846533	-4.993787	3.151727
H	1.162958	-3.474470	3.465510
H	-0.645780	-4.953894	4.302715
C	-1.641517	-2.820259	-1.643795
C	-1.409858	-4.190595	-1.489874

C	-1.901095	-2.315612	-2.927099
C	-1.457426	-5.039815	-2.594142
H	-1.188937	-4.600002	-0.509244
C	-1.963678	-3.167952	-4.024474
H	-2.050932	-1.247690	-3.067442
C	-1.739746	-4.534171	-3.860264
H	-1.273539	-6.102160	-2.459890
H	-2.176278	-2.762193	-5.009546
H	-1.777899	-5.199988	-4.717686
Pd	0.105498	0.076348	-0.849232
C	-1.121776	0.422696	4.942380
H	-1.196948	0.083680	5.971860
C	-2.084988	1.281246	4.416257
H	-2.916392	1.613224	5.032046
C	-5.789563	-0.043691	0.525378
H	-6.777817	0.363502	0.719188
C	-5.482711	-0.575274	-0.724788
H	-6.234158	-0.592827	-1.509445
C	-4.212427	-1.086851	-0.982257
H	-4.000096	-1.496242	-1.963862
C	-1.992759	1.715757	3.096631
H	-2.764300	2.366464	2.700765
C	-0.182637	2.370799	-2.889087
C	0.098093	3.674668	-3.296533
C	1.356463	4.226918	-3.067268
C	2.327371	3.470595	-2.409343
C	2.040068	2.178836	-1.979437
C	0.778668	1.608723	-2.212388
H	-1.154306	1.941782	-3.114355
H	-0.668352	4.252229	-3.807603

H	1.580018	5.237776	-3.396795
H	3.309714	3.893333	-2.214929
H	2.801273	1.612549	-1.452466
C	6.765766	0.487505	0.867420
C	5.673472	0.552851	1.731513
C	4.460363	-0.026084	1.367498
C	4.315734	-0.679881	0.141998
C	5.421887	-0.758070	-0.709506
C	6.635434	-0.171020	-0.353652
H	7.711555	0.946266	1.143057
H	5.766503	1.058722	2.689465
H	3.591548	0.028924	2.015589
H	5.342566	-1.273863	-1.662251
H	7.481453	-0.229565	-1.033721
C	2.932434	-1.270949	-0.197112
C	2.687357	-1.225833	-1.728627
H	3.153621	-0.315091	-2.112366
H	3.186391	-2.057679	-2.245135
C	1.226982	-1.216126	-2.118408
H	0.683051	-2.154217	-2.081975
C	0.831468	-0.239872	-3.067834
H	1.603778	0.217383	-3.677541
H	-0.117738	-0.354002	-3.585250
O	1.944631	-0.652583	0.506968
C	3.001301	-2.763926	0.193131
F	1.902154	-3.444483	-0.203893
F	4.051226	-3.413777	-0.361501
F	3.106749	-2.938944	1.523525

TSA2-3

	Coordinates (Angstroms)		
	X	Y	Z
H	2.278298	-1.189203	4.586887
C	1.924105	-1.492437	3.605503
C	1.710410	-1.051841	1.236870
C	2.177446	-0.681666	2.501627
H	2.715319	0.251586	2.636064
C	-1.694384	1.064774	1.274369
C	-2.170823	2.380560	1.261651
C	-1.909381	3.233943	2.331142
H	-2.740600	2.746656	0.412513
H	-2.283457	4.253721	2.306862
P	-1.850722	-0.008607	-0.199831
P	1.887888	-0.007253	-0.254563
C	-2.379697	-1.624651	0.471000
C	-3.022331	-1.774891	1.704913
C	-2.115921	-2.759532	-0.305584
C	-3.384048	-3.041889	2.156075
H	-3.233710	-0.905057	2.319605
C	-2.487305	-4.023660	0.142268
H	-1.600406	-2.645719	-1.256901
C	-3.116968	-4.166576	1.377789
H	-3.876969	-3.149671	3.118194
H	-2.273803	-4.897363	-0.467040
H	-3.397349	-5.153657	1.734555
C	-3.352109	0.653085	-1.014909
C	-3.177791	1.583692	-2.046353

C	-4.647213	0.286943	-0.633164
C	-4.281831	2.149958	-2.678586
H	-2.170877	1.861330	-2.351004
C	-5.748993	0.844647	-1.275924
H	-4.797549	-0.436346	0.163355
C	-5.568821	1.777760	-2.295976
H	-4.135997	2.874110	-3.475227
H	-6.751675	0.550863	-0.977793
H	-6.431211	2.211203	-2.794666
C	2.245326	1.667326	0.384116
C	3.485762	2.009970	0.938297
C	1.231729	2.628793	0.326396
C	3.694081	3.287983	1.447941
H	4.288271	1.277914	0.970270
C	1.440572	3.905545	0.842136
H	0.279074	2.366871	-0.124928
C	2.670844	4.235033	1.405881
H	4.657640	3.545647	1.878661
H	0.642915	4.641811	0.798691
H	2.836851	5.231316	1.806211
C	3.512831	-0.516993	-0.933460
C	4.073536	0.259434	-1.958325
C	4.178620	-1.672590	-0.513318
C	5.281212	-0.107953	-2.540235
H	3.563814	1.158611	-2.297862
C	5.385145	-2.042631	-1.106096
H	3.761729	-2.284332	0.281598
C	5.940184	-1.262840	-2.116897
H	5.708366	0.506213	-3.328197
H	5.894101	-2.941475	-0.768849

H	6.881720	-1.552152	-2.575018
Pd	0.003955	-0.179943	-1.597657
C	-1.172707	2.784822	3.424955
H	-0.965475	3.453562	4.255542
C	-0.707263	1.471311	3.450103
H	-0.137571	1.107885	4.300998
C	1.208106	-2.679468	3.457289
H	0.999846	-3.300697	4.323891
C	0.757571	-3.065581	2.196021
H	0.195149	-3.986716	2.070969
C	1.008098	-2.254640	1.092986
H	0.634206	-2.540334	0.113193
C	-0.964724	0.616141	2.383500
H	-0.598069	-0.404383	2.415418
O	0.591990	-0.595700	-3.754084
O	-0.694692	-0.637823	-3.712397

TSA4-5

Coordinates (Angstroms)

	X	Y	Z
H	6.227724	-1.765282	-1.527127
C	5.298063	-1.285050	-1.818311
C	3.253502	-0.150688	-1.204881
C	4.457973	-0.762167	-0.839054
H	4.740398	-0.837406	0.206530
C	0.176733	-2.646087	-0.456825
C	0.274360	-3.715990	0.436384

C	1.171656	-4.751339	0.184137
H	-0.331032	-3.735967	1.337146
H	1.249279	-5.577019	0.885689
P	-0.935837	-1.226963	-0.193337
P	2.107792	0.562612	0.015593
C	-2.393611	-1.668736	-1.206016
C	-2.646337	-2.990214	-1.593760
C	-3.286428	-0.658105	-1.576290
C	-3.784843	-3.292355	-2.336343
H	-1.958440	-3.783466	-1.316698
C	-4.423656	-0.966403	-2.316719
H	-3.090128	0.369426	-1.287489
C	-4.674540	-2.282716	-2.698181
H	-3.975142	-4.319965	-2.632900
H	-5.110675	-0.173266	-2.597509
H	-5.560029	-2.521718	-3.280512
C	-1.505064	-1.372694	1.530052
C	-0.940327	-0.531508	2.492843
C	-2.477334	-2.305033	1.909510
C	-1.324875	-0.634783	3.826328
H	-0.207220	0.210373	2.193904
C	-2.863863	-2.401835	3.243104
H	-2.935813	-2.950923	1.166017
C	-2.286584	-1.570578	4.202508
H	-0.877937	0.021168	4.567962
H	-3.619897	-3.125877	3.532833
H	-2.591862	-1.648581	5.242142
C	2.407812	-0.337655	1.574998
C	2.384741	0.345153	2.797498
C	2.563519	-1.728716	1.570055

C	2.495659	-0.356778	3.993881
H	2.272562	1.424659	2.821854
C	2.675713	-2.424918	2.769908
H	2.604980	-2.271649	0.632299
C	2.634489	-1.743209	3.983544
H	2.473707	0.183878	4.935714
H	2.793697	-3.504580	2.750809
H	2.717361	-2.289521	4.918734
C	2.750232	2.237454	0.360283
C	1.880619	3.179840	0.922752
C	4.079177	2.588495	0.104679
C	2.339975	4.455478	1.236619
H	0.841998	2.918819	1.108855
C	4.530678	3.869444	0.411967
H	4.762160	1.868191	-0.335729
C	3.664837	4.802332	0.978861
H	1.658367	5.180111	1.672838
H	5.562991	4.137853	0.206195
H	4.021221	5.800881	1.215485
Pd	-0.034399	0.801317	-0.791412
C	1.977656	-4.720941	-0.952274
H	2.687480	-5.522435	-1.136053
C	1.871780	-3.662399	-1.854293
H	2.496930	-3.631802	-2.742209
C	4.948654	-1.193935	-3.164073
H	5.604767	-1.608032	-3.924378
C	3.757352	-0.572150	-3.534266
H	3.480552	-0.499287	-4.582010
C	2.911242	-0.054889	-2.558871
H	1.971160	0.410571	-2.844595

C	0.968976	-2.632901	-1.610270
H	0.888488	-1.804115	-2.307668
O	-0.011761	2.561339	-1.767134
O	-1.314309	2.069796	-1.808510
C	-5.409417	0.811165	1.143717
C	-5.716137	1.541188	-0.005023
C	-4.759931	2.383123	-0.570388
C	-3.480142	2.516426	-0.011887
C	-3.203745	1.787209	1.152475
C	-4.150057	0.941059	1.727480
H	-6.149944	0.147993	1.583775
H	-6.699426	1.448398	-0.460158
H	-5.003625	2.946000	-1.468470
H	-2.220342	1.883073	1.605861
H	-3.904423	0.379107	2.625253
B	-2.365788	3.429007	-0.672392
O	-2.814803	4.247191	-1.710071
H	-2.114524	4.860532	-1.955954
O	-1.269475	3.801940	0.110335
H	-0.481642	3.635815	-0.449491

TSA5-6

Coordinates (Angstroms)			
	X	Y	Z

H	3.532987	4.512960	-0.697493
C	3.067225	3.794602	-0.029036
C	2.235050	1.561587	0.375004

C	2.837287	2.494510	-0.473094
H	3.126531	2.214809	-1.480691
C	-0.633060	2.315279	-0.804429
C	-0.233368	2.007206	-2.111653
C	0.244582	2.999400	-2.960651
H	-0.288008	0.979858	-2.459267
H	0.555334	2.739875	-3.968820
P	-1.352324	0.923302	0.152247
P	1.933635	-0.163136	-0.138248
C	-1.409742	1.321992	1.925222
C	-1.917944	2.518849	2.448056
C	-0.930118	0.337721	2.799897
C	-1.892234	2.747182	3.820488
H	-2.354221	3.267109	1.794656
C	-0.918276	0.568157	4.173357
H	-0.571196	-0.611382	2.400596
C	-1.383625	1.777696	4.683511
H	-2.277949	3.682354	4.215806
H	-0.540337	-0.198622	4.843823
H	-1.364355	1.961411	5.754051
C	-3.095966	1.024171	-0.418555
C	-4.156036	1.286050	0.453739
C	-3.361200	0.850647	-1.782438
C	-5.456481	1.391356	-0.033862
H	-3.977887	1.398116	1.517673
C	-4.662188	0.953127	-2.264518
H	-2.554816	0.627061	-2.474629
C	-5.713572	1.228453	-1.392108
H	-6.270478	1.597012	0.655596
H	-4.853475	0.811911	-3.324514

H	-6.728835	1.309662	-1.769807
C	2.826906	-0.351926	-1.714128
C	4.222365	-0.243232	-1.757469
C	2.113686	-0.596927	-2.890305
C	4.890936	-0.359442	-2.971514
H	4.784726	-0.063576	-0.844805
C	2.787391	-0.713037	-4.103743
H	1.035360	-0.717213	-2.847499
C	4.173932	-0.590550	-4.145469
H	5.973125	-0.270633	-3.001271
H	2.227873	-0.906015	-5.014675
H	4.699310	-0.682246	-5.091947
C	2.950814	-1.122421	1.056466
C	2.865202	-2.522221	1.032734
C	3.839294	-0.507570	1.945683
C	3.636725	-3.285938	1.903908
H	2.197224	-2.993770	0.316286
C	4.608975	-1.280020	2.813659
H	3.943590	0.571460	1.966981
C	4.505106	-2.667872	2.801839
H	3.555837	-4.369285	1.879622
H	5.293587	-0.789029	3.499562
H	5.102877	-3.265644	3.484185
Pd	-0.206572	-1.023638	-0.275580
C	0.333730	4.314898	-2.510967
H	0.711428	5.092665	-3.168579
C	-0.048277	4.625428	-1.208337
H	0.036775	5.645139	-0.843670
C	2.698127	4.174524	1.258878
H	2.878755	5.189949	1.600013

C	2.092336	3.249107	2.107172
H	1.798422	3.534654	3.113229
C	1.862004	1.949943	1.668950
H	1.405301	1.233484	2.343587
C	-0.530582	3.633943	-0.356532
H	-0.797258	3.899258	0.658998
O	0.681408	-2.663950	-1.036162
O	0.191713	-3.826160	-0.341838
C	-3.057689	-1.971403	0.653247
C	-4.388679	-2.041341	0.260457
C	-4.704243	-2.411212	-1.047483
C	-3.686587	-2.714448	-1.954912
C	-2.359615	-2.661759	-1.541652
C	-2.002922	-2.315592	-0.219073
H	-2.817145	-1.690393	1.676735
H	-5.182639	-1.795942	0.960876
H	-5.743582	-2.454403	-1.363096
H	-3.935577	-2.991029	-2.976626
H	-1.564494	-2.929859	-2.233750
B	-0.818261	-3.467586	0.627104
O	-1.580508	-4.621742	0.969342
H	-1.876131	-5.038419	0.153947
O	-0.341836	-2.785345	1.815345
H	0.611487	-2.914404	1.860574

TSA8-9

Coordinates (Angstroms)

X	Y	Z

C	0.276464	-2.023631	-1.197958
C	0.335321	-1.655854	-2.551525
C	-0.424382	-2.338005	-3.494861
H	0.968788	-0.829682	-2.865750
H	-0.368993	-2.050130	-4.540590
P	1.257231	-1.033536	-0.027028
C	1.018703	-1.701382	1.645379
C	1.299432	-3.045765	1.923097
C	0.606740	-0.849784	2.674582
C	1.129823	-3.536613	3.212829
H	1.649188	-3.705620	1.133469
C	0.449169	-1.344702	3.967221
H	0.408367	0.198831	2.464550
C	0.702201	-2.687789	4.234410
H	1.338297	-4.581561	3.422987
H	0.127290	-0.679053	4.762849
H	0.575332	-3.074321	5.241650
C	3.008621	-1.410475	-0.373273
C	3.958950	-0.961982	0.554343
C	3.430001	-2.063756	-1.532562
C	5.313776	-1.142232	0.306821
H	3.639786	-0.459010	1.462489
C	4.791073	-2.246511	-1.772586
H	2.706971	-2.433397	-2.252109
C	5.733073	-1.779658	-0.861529
H	6.043992	-0.781586	1.025491
H	5.110996	-2.756516	-2.676748
H	6.793040	-1.916046	-1.056173
Pd	0.500663	1.077612	-0.204057

C	-1.269324	-3.372500	-3.093262
H	-1.873166	-3.896733	-3.828360
C	-1.346666	-3.724635	-1.748495
H	-2.013853	-4.519781	-1.429468
C	-0.575218	-3.056603	-0.799551
H	-0.655347	-3.332646	0.246221
O	-0.493814	2.973730	-0.405762
O	-0.272768	3.932533	0.636903
C	2.968024	2.318381	0.701188
C	4.267592	2.814321	0.576039
C	4.956072	2.688176	-0.628844
C	4.335575	2.075161	-1.716468
C	3.039828	1.572334	-1.595649
C	2.352470	1.688986	-0.384177
H	2.446803	2.419083	1.650465
H	4.742495	3.294549	1.428206
H	5.970716	3.065999	-0.720213
H	4.864007	1.975883	-2.661531
H	2.577330	1.070713	-2.442220
B	-0.451647	3.501828	1.945716
O	-0.006821	4.367695	2.906688
H	0.445764	5.122022	2.513227
O	-1.028597	2.345191	2.359262
H	-1.437961	1.811204	1.652764
O	-1.746425	1.085125	0.093412
C	-2.871518	0.469833	-0.478005
C	-3.173082	-0.832409	0.255516
C	-2.687479	0.212843	-1.990131
C	-4.035205	1.441745	-0.232860
C	-2.576491	-1.090599	1.489274

C	-4.035468	-1.787651	-0.291826
H	-2.112318	-0.715182	-2.070425
H	-3.664049	0.025810	-2.445859
C	-1.971236	1.288280	-2.743339
F	-3.802904	2.643951	-0.786578
F	-5.191014	0.986094	-0.737863
F	-4.222584	1.649088	1.081287
C	-2.802667	-2.295165	2.150586
H	-1.914159	-0.356277	1.928300
C	-4.270052	-2.987756	0.373366
H	-4.522236	-1.608980	-1.245137
H	-0.933424	1.470025	-2.457737
C	-2.496272	1.982357	-3.751285
C	-3.647874	-3.250361	1.592618
H	-2.310030	-2.484515	3.100495
H	-4.937134	-3.722719	-0.068307
H	-3.523574	1.826444	-4.076275
H	-1.916632	2.730846	-4.285888
H	-3.823518	-4.192455	2.104354
H	-1.437391	2.162587	-0.201439

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Coordinates (Angstroms)			
	X	Y	Z

C	-1.239183	2.133641	1.366518
C	-0.471411	1.913881	2.517461
C	-0.416244	2.890759	3.509004

H	0.097086	0.988695	2.607681
H	0.180226	2.718772	4.401168
P	-1.262618	0.822404	0.096086
C	-2.828050	1.123630	-0.791736
C	-2.880990	1.368484	-2.166787
C	-4.021765	1.030633	-0.063222
C	-4.111298	1.517680	-2.804181
H	-1.962979	1.442262	-2.742238
C	-5.246762	1.187877	-0.701627
H	-3.991359	0.835807	1.006011
C	-5.294072	1.426752	-2.075013
H	-4.142609	1.707439	-3.873502
H	-6.166740	1.115131	-0.128401
H	-6.251979	1.542616	-2.574236
C	0.035362	1.299814	-1.100979
C	0.623115	0.285555	-1.868241
C	0.458217	2.621217	-1.270828
C	1.610191	0.590565	-2.800475
H	0.310707	-0.745524	-1.716849
C	1.454264	2.922289	-2.196837
H	0.017242	3.415828	-0.675624
C	2.029272	1.910146	-2.963092
H	2.064088	-0.203247	-3.387021
H	1.785979	3.949852	-2.315173
H	2.813805	2.147099	-3.676236
Pd	-0.751280	-1.343048	0.828583
C	-1.124652	4.082081	3.363693
H	-1.083492	4.839142	4.142134
C	-1.888145	4.302628	2.218478
H	-2.440255	5.230895	2.100273

C	-1.946649	3.333043	1.220927
H	-2.545558	3.509109	0.331941
C	-3.452432	-2.531427	0.685206
C	-4.734457	-2.492134	0.145283
C	-4.910365	-2.324179	-1.228964
C	-3.796528	-2.187773	-2.057562
C	-2.514272	-2.218374	-1.517420
C	-2.322318	-2.374267	-0.136352
H	-3.320257	-2.704049	1.751236
H	-5.597999	-2.605094	0.795659
H	-5.910612	-2.303593	-1.652148
H	-3.927345	-2.052955	-3.128008
H	-1.651229	-2.116541	-2.171447
C	4.656143	0.654646	-1.098727
C	3.848129	1.310436	-0.187368
C	3.033413	0.589262	0.677670
C	2.963688	-0.807173	0.657706
C	3.842552	-1.425444	-0.232368
C	4.659088	-0.729549	-1.113119
C	2.000402	-1.600815	1.579361
C	1.499294	-2.885044	0.849603
H	1.531135	-2.739044	-0.235592
H	2.139082	-3.750345	1.067335
C	0.065195	-3.176718	1.235635
H	-0.125316	-3.424592	2.280332
C	-0.894834	-3.630771	0.276815
H	-0.537164	-3.788690	-0.739130
H	-1.614023	-4.375098	0.605058
O	0.910033	-0.808597	1.923324
C	2.776288	-1.964352	2.851354

H	3.694494	-2.519071	2.628402
H	3.042199	-1.051409	3.393310
H	2.143296	-2.579372	3.500568
F	2.330222	1.334401	1.532704
F	3.850712	2.644172	-0.144026
F	5.415091	1.344347	-1.947809
F	5.449299	-1.387767	-1.964040
F	3.944267	-2.763273	-0.278727

TSB12-13

Coordinates (Angstroms)

	X	Y	Z

H	-1.208375	5.586783	2.092967
C	-0.703948	4.624748	2.076515
C	0.194911	2.764470	0.824357
C	-0.444504	4.005294	0.854579
H	-0.751580	4.487343	-0.068291
C	-3.072879	1.277748	0.963120
C	-3.378914	1.784020	-0.309402
C	-3.963976	3.037342	-0.455656
H	-3.146764	1.190254	-1.190273
H	-4.191445	3.411996	-1.450007
P	-2.226601	-0.345490	1.022253
P	0.494683	1.807557	-0.699696
C	-1.876025	-0.631557	2.795872
C	-2.892732	-0.707925	3.759287
C	-0.543591	-0.811866	3.183146

C	-2.575888	-0.925808	5.095785
H	-3.932690	-0.597715	3.462190
C	-0.233020	-1.035634	4.525302
H	0.240165	-0.807018	2.421417
C	-1.243395	-1.084060	5.481547
H	-3.367843	-0.975652	5.838189
H	0.803815	-1.177114	4.820373
H	-0.998872	-1.255965	6.526403
C	-3.583249	-1.555548	0.755044
C	-3.365398	-2.876916	1.175590
C	-4.777313	-1.246733	0.095429
C	-4.328323	-3.857125	0.959778
H	-2.442944	-3.135908	1.690173
C	-5.739600	-2.231558	-0.118580
H	-4.969940	-0.232433	-0.241027
C	-5.521803	-3.537314	0.314199
H	-4.146105	-4.873252	1.299206
H	-6.665143	-1.972882	-0.625792
H	-6.275118	-4.301871	0.146713
C	0.005528	2.923127	-2.061225
C	0.682370	4.129345	-2.286858
C	-1.055358	2.566015	-2.896277
C	0.289273	4.967663	-3.324703
H	1.517289	4.410157	-1.649719
C	-1.449133	3.407381	-3.934868
H	-1.565725	1.620780	-2.733457
C	-0.778961	4.609091	-4.147678
H	0.818105	5.901543	-3.493490
H	-2.275688	3.120395	-4.578968
H	-1.082530	5.265344	-4.958554

C	2.322247	1.775119	-0.846951
C	2.869585	0.984850	-1.865933
C	3.177744	2.474181	0.007590
C	4.247509	0.896450	-2.026928
H	2.209676	0.422708	-2.523229
C	4.560439	2.372289	-0.145980
H	2.771621	3.093788	0.801188
C	5.097497	1.585226	-1.160713
H	4.660349	0.273532	-2.815656
H	5.216882	2.908686	0.533587
H	6.174835	1.494277	-1.268575
Pd	-0.286705	-0.373322	-0.563902
C	-4.237358	3.814071	0.669654
H	-4.682841	4.798659	0.558471
C	-3.922575	3.326592	1.935409
H	-4.118832	3.931737	2.816267
C	-0.332149	4.010673	3.269490
H	-0.542652	4.494638	4.219160
C	0.305204	2.769697	3.243032
H	0.590013	2.279987	4.170370
C	0.566644	2.147134	2.027878
H	1.063490	1.179865	1.997763
C	-3.343900	2.067168	2.084612
H	-3.091312	1.712254	3.078396
C	6.151914	-1.301880	0.215822
C	5.336754	-0.788058	1.210999
C	3.994542	-1.134595	1.261487
C	3.388399	-1.964307	0.310625
C	4.254756	-2.493972	-0.643710
C	5.605228	-2.169558	-0.710913

C	1.851941	-2.161686	0.354442
C	1.298086	-2.619558	-1.014281
H	1.772389	-2.032312	-1.807767
H	1.520290	-3.676219	-1.213954
C	-0.198791	-2.394801	-1.092837
H	-0.831126	-3.004438	-0.448493
C	-0.795876	-1.842780	-2.263715
H	-1.110773	-0.381274	-1.933872
O	1.303429	-0.927615	0.691329
H	-0.120252	-1.625857	-3.093418
C	-2.188257	-2.193935	-2.683419
C	-2.969237	-1.278741	-3.400355
C	-2.714768	-3.460569	-2.414559
C	-4.243431	-1.620946	-3.838663
H	-2.572854	-0.286611	-3.607632
C	-3.991094	-3.804452	-2.855550
H	-2.118820	-4.186889	-1.869575
C	-4.759507	-2.887774	-3.567842
H	-4.836411	-0.895995	-4.389544
H	-4.384995	-4.792868	-2.636644
H	-5.756003	-3.156271	-3.906955
C	1.537582	-3.215081	1.428367
H	2.006164	-4.180585	1.205222
H	1.895509	-2.872690	2.403695
H	0.453981	-3.361608	1.496322
F	3.828630	-3.355101	-1.581387
F	3.312809	-0.624008	2.291136
F	5.846307	0.051932	2.114796
F	7.434534	-0.949444	0.143996
F	6.370348	-2.684305	-1.676411

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	Coordinates (Angstroms)		
	X	Y	Z
H	-3.490517	-1.435976	4.855422
C	-3.767252	-1.281110	3.816253
C	-3.268133	-1.552144	1.459075
C	-2.929269	-1.742615	2.805154
H	-2.004673	-2.251210	3.065507
C	-1.406935	2.390600	1.425150
C	-0.401669	3.288192	1.804986
C	-0.273167	3.671945	3.137620
H	0.287163	3.685587	1.065462
H	0.509919	4.370833	3.417703
P	-1.471563	1.712167	-0.269102
P	-2.051830	-1.992660	0.165025
C	-3.243408	1.674748	-0.734240
C	-4.238025	2.430747	-0.108081
C	-3.586202	0.844719	-1.807873
C	-5.562189	2.323888	-0.528435
H	-3.988724	3.091115	0.717110
C	-4.907035	0.747219	-2.234003
H	-2.814271	0.258572	-2.298906
C	-5.900497	1.478766	-1.584279
H	-6.332962	2.902317	-0.026588
H	-5.159638	0.087038	-3.059360
H	-6.935915	1.393743	-1.901903

C	-0.874806	3.056285	-1.360252
C	-0.172055	2.705871	-2.515927
C	-1.184513	4.401456	-1.124826
C	0.225665	3.685994	-3.423304
H	0.063737	1.660699	-2.698584
C	-0.768781	5.380840	-2.021128
H	-1.746197	4.686051	-0.239257
C	-0.064450	5.024923	-3.171900
H	0.772022	3.403155	-4.318779
H	-1.000600	6.423915	-1.824885
H	0.255880	5.791806	-3.871514
C	-1.299023	-3.524388	0.834213
C	-2.046394	-4.678114	1.101031
C	0.075048	-3.512405	1.096700
C	-1.423330	-5.807024	1.621703
H	-3.114792	-4.694912	0.903211
C	0.694222	-4.646913	1.622655
H	0.663284	-2.621069	0.872819
C	-0.052238	-5.792123	1.884350
H	-2.006788	-6.700651	1.825832
H	1.762357	-4.633011	1.823534
H	0.430562	-6.676055	2.292120
C	-3.042365	-2.572561	-1.257233
C	-2.469735	-2.409631	-2.524863
C	-4.307616	-3.160372	-1.148732
C	-3.148690	-2.826957	-3.666158
H	-1.491947	-1.938215	-2.610175
C	-4.989198	-3.568850	-2.292240
H	-4.770015	-3.287713	-0.174208
C	-4.412943	-3.402289	-3.550614

H	-2.695996	-2.692713	-4.644632
H	-5.974261	-4.017618	-2.199407
H	-4.950217	-3.718373	-4.440384
Pd	-0.428903	-0.270941	-0.257633
C	-1.138437	3.162370	4.103523
H	-1.035571	3.464753	5.141879
C	-2.133413	2.259257	3.732564
H	-2.810236	1.851014	4.478107
C	-4.956308	-0.626651	3.498174
H	-5.610795	-0.268190	4.287629
C	-5.300712	-0.435164	2.161571
H	-6.223633	0.076180	1.902189
C	-4.461115	-0.887994	1.146674
H	-4.736694	-0.715481	0.111315
C	-2.264826	1.869620	2.403422
H	-3.036703	1.156925	2.128670
C	6.623705	-1.893054	0.379829
C	5.628160	-1.531186	1.268441
C	4.328984	-1.299894	0.823777
C	3.964328	-1.408296	-0.521664
C	5.004822	-1.773874	-1.381902
C	6.304363	-2.012010	-0.962334
C	2.536596	-1.171094	-1.072690
C	2.576969	-0.012216	-2.093976
H	3.309161	-0.227028	-2.879746
H	1.600294	-0.018714	-2.605349
C	2.788769	1.374091	-1.573938
H	2.725412	2.144307	-2.342952
C	2.956855	1.747375	-0.295609
H	0.977735	0.402617	-0.291389

O	1.682513	-0.906499	-0.009790
H	3.017530	0.982881	0.473442
C	2.981720	3.123471	0.208526
C	3.328356	3.339080	1.550887
C	2.592782	4.231998	-0.561502
C	3.299074	4.615406	2.105231
H	3.615016	2.486762	2.163070
C	2.556995	5.505566	-0.006653
H	2.285703	4.093210	-1.593509
C	2.909471	5.705395	1.329182
H	3.571714	4.757725	3.147540
H	2.238425	6.346400	-0.617143
H	2.873743	6.701423	1.761456
C	2.063943	-2.445617	-1.788777
H	2.115045	-3.298905	-1.106352
H	1.015413	-2.296177	-2.071888
H	2.640187	-2.679623	-2.686915
F	3.478837	-0.938355	1.789506
F	4.793258	-1.909242	-2.700677
F	7.242308	-2.356914	-1.844456
F	7.864324	-2.116912	0.804008
F	5.915119	-1.402620	2.564404

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	Coordinates (Angstroms)		
	X	Y	Z

C	-0.654608	-1.716615	-1.138974

C	-0.922151	-1.050693	-2.341787
C	-1.957372	-1.482106	-3.165907
H	-0.314285	-0.194480	-2.627094
H	-2.160061	-0.958327	-4.095477
P	0.806382	-1.170446	-0.197384
C	0.632210	-1.703432	1.530766
C	0.629274	-3.062078	1.878170
C	0.543915	-0.732105	2.533040
C	0.500979	-3.436891	3.210887
H	0.744507	-3.824505	1.112869
C	0.423030	-1.114651	3.866744
H	0.578345	0.321966	2.272718
C	0.394782	-2.464369	4.205248
H	0.494344	-4.490383	3.474918
H	0.353519	-0.354201	4.639294
H	0.300647	-2.761986	5.245784
C	2.155794	-2.212635	-0.850839
C	3.262929	-2.496196	-0.041726
C	2.148794	-2.633793	-2.183215
C	4.352664	-3.181477	-0.566813
H	3.282019	-2.169827	0.993335
C	3.242486	-3.322474	-2.702915
H	1.295248	-2.424131	-2.821038
C	4.346664	-3.592672	-1.899164
H	5.209943	-3.391662	0.066297
H	3.228303	-3.647591	-3.739260
H	5.200644	-4.125172	-2.307981
Pd	1.033872	1.060872	-0.362607
C	-2.734784	-2.575469	-2.790660
H	-3.548065	-2.908867	-3.428562

C	-2.479503	-3.232032	-1.588414
H	-3.097340	-4.071633	-1.283769
C	-1.444646	-2.805966	-0.760629
H	-1.265073	-3.319231	0.178258
O	1.109206	3.229142	-0.547370
O	1.781740	3.954465	0.487191
C	3.679575	0.797691	0.806753
C	5.070266	0.669400	0.803820
C	5.756274	0.483163	-0.394510
C	5.047740	0.435750	-1.594734
C	3.658090	0.560089	-1.597551
C	2.968256	0.741410	-0.395502
H	3.155538	0.928415	1.750911
H	5.614778	0.708397	1.744224
H	6.837215	0.372847	-0.393888
H	5.575677	0.291495	-2.534282
H	3.116613	0.495946	-2.538152
B	1.466842	3.605793	1.799875
O	2.290352	4.148899	2.747530
H	3.024765	4.623947	2.343167
O	0.438863	2.831381	2.213254
H	-0.192213	2.541875	1.517456
O	-0.870370	2.169793	-0.030478
C	-2.232941	2.223825	-0.401258
C	-2.881602	0.919258	0.086628
C	-2.344456	2.408269	-1.931043
C	-2.600481	0.460580	1.378643
C	-3.768366	0.122975	-0.639657
H	-2.001818	1.486754	-2.413353
H	-3.393211	2.555702	-2.198220

C	-1.535734	3.559933	-2.439761
C	-3.084147	-0.736333	1.884673
C	-4.294799	-1.062935	-0.140800
H	-0.452782	3.443444	-2.436799
C	-2.059582	4.692980	-2.906959
C	-3.937885	-1.510815	1.117086
H	-3.136533	4.851705	-2.934950
H	-1.432777	5.499240	-3.280336
H	-0.018926	3.028758	-0.312264
C	-2.894425	3.400804	0.318203
H	-2.426294	4.336907	-0.001127
H	-3.961482	3.450468	0.080728
H	-2.781779	3.303155	1.400451
F	-5.125621	-1.786008	-0.890253
F	-4.178085	0.445006	-1.871764
F	-1.849612	1.180976	2.218703
F	-2.747907	-1.132776	3.111245
F	-4.402471	-2.667554	1.578663

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Coordinates (Angstroms)

	X	Y	Z

C	0.660565	2.095990	-1.424949
C	-0.409616	1.963162	-2.320425
C	-0.611821	2.928091	-3.304382
H	-1.079540	1.106496	-2.225126
H	-1.442452	2.822894	-3.997437

P	0.848351	0.823120	-0.126149
C	2.579111	1.014736	0.416481
C	2.925639	1.348924	1.728601
C	3.591268	0.748467	-0.515655
C	4.266317	1.414634	2.103125
H	2.150667	1.557344	2.460351
C	4.927815	0.824728	-0.140285
H	3.331101	0.481572	-1.537227
C	5.267956	1.152543	1.171980
H	4.526127	1.673816	3.125740
H	5.705350	0.618530	-0.870419
H	6.312426	1.204051	1.466228
C	-0.142735	1.469990	1.268842
C	-0.603215	0.562701	2.231754
C	-0.473555	2.822942	1.388200
C	-1.379198	1.003743	3.299334
H	-0.364187	-0.493728	2.131567
C	-1.258856	3.260073	2.452474
H	-0.126082	3.536021	0.646089
C	-1.712901	2.352682	3.407806
H	-1.736088	0.291381	4.037873
H	-1.518310	4.312009	2.532941
H	-2.330729	2.695524	4.233009
Pd	0.019810	-1.316045	-0.622225
C	0.247728	4.020374	-3.407358
H	0.089520	4.767379	-4.180393
C	1.312008	4.153275	-2.517526
H	1.983284	5.004227	-2.592903
C	1.519072	3.196604	-1.526855
H	2.348581	3.308967	-0.834910

C	2.575447	-2.755690	-0.919195
C	3.937706	-2.827110	-0.643820
C	4.400874	-2.620457	0.656392
C	3.493615	-2.333362	1.676452
C	2.132047	-2.251564	1.400016
C	1.652985	-2.444925	0.095438
H	2.216082	-2.959298	-1.925675
H	4.638726	-3.056447	-1.442257
H	5.463174	-2.685995	0.874091
H	3.848402	-2.168912	2.690583
H	1.431694	-2.034583	2.203152
C	-5.548814	0.819118	1.519485
C	-4.426757	1.432291	0.967151
C	-3.567457	0.709667	0.140189
C	-3.811480	-0.634166	-0.149201
C	-4.947100	-1.239303	0.404477
C	-5.806488	-0.521775	1.232727
H	-6.218339	1.378712	2.167376
H	-4.213801	2.476119	1.184462
H	-2.682226	1.168066	-0.288503
H	-5.160352	-2.284702	0.192029
H	-6.679890	-1.010641	1.657294
C	-2.835989	-1.414962	-1.032249
C	-2.333290	-2.650843	-0.242699
H	-2.215192	-2.380304	0.814089
H	-3.061808	-3.474832	-0.276312
C	-0.992200	-3.097146	-0.781577
H	-0.972390	-3.434289	-1.819050
C	0.060548	-3.566253	0.065384
H	-0.144375	-3.598165	1.134300

H	0.649122	-4.407722	-0.287833
O	-1.749178	-0.605901	-1.392687
C	-3.556849	-1.854627	-2.314041
H	-4.465431	-2.432006	-2.110312
H	-3.834617	-0.970651	-2.897329
H	-2.885804	-2.467644	-2.925960

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	Coordinates (Angstroms)		
	X	Y	Z

H	0.218757	5.023070	3.229121
C	0.554374	4.016722	2.994724
C	1.100859	2.331915	1.352082
C	0.679390	3.626380	1.661929
H	0.436552	4.329026	0.870952
C	-2.369148	1.324980	1.292505
C	-2.664679	2.104687	0.164147
C	-3.052114	3.433665	0.298271
H	-2.585800	1.664345	-0.826613
H	-3.275976	4.021088	-0.588078
P	-1.762873	-0.376156	0.994609
P	1.216231	1.669998	-0.344323
C	-1.481945	-1.056639	2.670575
C	-2.515277	-1.179793	3.611009
C	-0.192307	-1.483876	3.001356
C	-2.251946	-1.693409	4.876179
H	-3.525587	-0.871841	3.352864

C	0.064817	-2.002298	4.271551
H	0.592227	-1.442806	2.241893
C	-0.958404	-2.099289	5.210166
H	-3.055034	-1.779478	5.603136
H	1.068183	-2.336295	4.523871
H	-0.755428	-2.500788	6.199448
C	-3.269770	-1.310282	0.513471
C	-3.191620	-2.711239	0.563375
C	-4.450356	-0.717026	0.055840
C	-4.273898	-3.495718	0.180326
H	-2.280912	-3.189842	0.917276
C	-5.531442	-1.506638	-0.332543
H	-4.537700	0.364381	0.012293
C	-5.449965	-2.895326	-0.268501
H	-4.198834	-4.578545	0.232681
H	-6.443842	-1.029891	-0.680492
H	-6.296163	-3.507112	-0.568185
C	0.826667	3.089076	-1.429445
C	1.660558	4.214858	-1.466607
C	-0.309439	3.054338	-2.240698
C	1.349884	5.289810	-2.292868
H	2.555007	4.248664	-0.849741
C	-0.620013	4.131510	-3.068296
H	-0.947140	2.176085	-2.229162
C	0.207466	5.250795	-3.092752
H	2.001353	6.158889	-2.314862
H	-1.506677	4.091448	-3.694969
H	-0.032033	6.090995	-3.738516
C	3.017559	1.469806	-0.618891
C	3.417883	0.844047	-1.806829

C	3.988715	1.898328	0.288505
C	4.766613	0.653539	-2.082853
H	2.665428	0.493289	-2.509825
C	5.341733	1.694860	0.014741
H	3.695394	2.388255	1.212118
C	5.732888	1.074269	-1.168228
H	5.065198	0.163250	-3.005292
H	6.089400	2.027097	0.729714
H	6.786791	0.913854	-1.377282
Pd	0.162335	-0.382596	-0.597568
C	-3.135011	4.010985	1.564895
H	-3.425592	5.052241	1.672293
C	-2.831442	3.248898	2.689798
H	-2.880971	3.694763	3.679398
C	0.846055	3.121118	4.020236
H	0.741217	3.428216	5.057068
C	1.265481	1.826039	3.714025
H	1.484188	1.119140	4.509777
C	1.389334	1.430589	2.386970
H	1.706946	0.420492	2.136810
C	-2.450352	1.914462	2.558002
H	-2.202286	1.341654	3.445615
C	6.116662	-3.576370	-0.195329
C	5.646803	-2.358066	0.289850
C	4.277399	-2.098944	0.329235
C	3.353674	-3.049133	-0.110826
C	3.836227	-4.272220	-0.594430
C	5.203645	-4.533374	-0.639000
H	7.183631	-3.780683	-0.229352
H	6.348538	-1.602492	0.635304

H	3.885627	-1.154392	0.693377
H	3.139278	-5.030214	-0.944645
H	5.558623	-5.487405	-1.021184
C	1.858525	-2.717026	-0.074959
C	1.318535	-2.751575	-1.523360
H	1.962882	-2.119121	-2.146604
H	1.355232	-3.767273	-1.945521
C	-0.098109	-2.224546	-1.585593
H	-0.866932	-2.819859	-1.095789
C	-0.517189	-1.327078	-2.607553
H	-0.615739	0.036789	-1.922626
O	1.668704	-1.444571	0.465674
H	0.237067	-1.047463	-3.345238
C	-1.920977	-1.288646	-3.121352
C	-2.400131	-0.134709	-3.755898
C	-2.766801	-2.396338	-3.016016
C	-3.697042	-0.081312	-4.252715
H	-1.746686	0.729893	-3.851011
C	-4.066862	-2.343475	-3.515276
H	-2.408050	-3.308679	-2.549853
C	-4.539150	-1.186390	-4.128120
H	-4.052651	0.824617	-4.735889
H	-4.711293	-3.212743	-3.421379
H	-5.554693	-1.146280	-4.511659
C	1.130879	-3.773447	0.775265
H	1.245076	-4.788047	0.376835
H	1.520715	-3.761399	1.798119
H	0.061888	-3.539529	0.821722

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	Coordinates (Angstroms)		
	X	Y	Z
H	3.251237	-0.236312	4.844519
C	3.444559	-0.483059	3.804239
C	3.200592	0.049310	1.451041
C	2.962220	0.349865	2.798753
H	2.394168	1.237429	3.064779
C	-0.376967	-2.416275	1.417958
C	-1.693487	-2.690188	1.808272
C	-1.983086	-2.980946	3.139138
H	-2.497225	-2.674316	1.078039
H	-3.008295	-3.196635	3.426458
P	0.003972	-1.851595	-0.276936
P	2.381003	1.054599	0.160323
C	1.550927	-2.710682	-0.752214
C	2.011746	-3.888098	-0.156201
C	2.279770	-2.141852	-1.802292
C	3.205774	-4.463764	-0.585461
H	1.451826	-4.349068	0.652297
C	3.465300	-2.724643	-2.239176
H	1.922860	-1.225196	-2.263459
C	3.936178	-3.882424	-1.621387
H	3.567156	-5.369918	-0.107109
H	4.027416	-2.263593	-3.046864
H	4.869655	-4.332921	-1.946852
C	-1.204479	-2.706092	-1.355081
C	-1.670844	-2.030958	-2.485490

C	-1.604046	-4.029263	-1.130508
C	-2.535223	-2.662439	-3.377917
H	-1.355421	-1.005183	-2.658529
C	-2.482670	-4.651820	-2.011388
H	-1.235063	-4.571602	-0.264283
C	-2.949368	-3.970002	-3.136005
H	-2.892905	-2.127938	-4.253524
H	-2.799453	-5.673923	-1.823689
H	-3.633404	-4.460327	-3.822955
C	2.485175	2.750096	0.850698
C	3.698698	3.339857	1.226367
C	1.290958	3.461458	1.006083
C	3.714153	4.628087	1.749606
H	4.630636	2.792390	1.113550
C	1.312573	4.753668	1.532483
H	0.345178	3.006708	0.704745
C	2.520698	5.336683	1.903460
H	4.657628	5.082281	2.039876
H	0.380826	5.301313	1.649664
H	2.537674	6.343260	2.312375
C	3.553388	1.086888	-1.242350
C	3.000618	1.226619	-2.521325
C	4.942970	0.993807	-1.104885
C	3.820930	1.272126	-3.645223
H	1.919005	1.285792	-2.630979
C	5.761208	1.030344	-2.230754
H	5.388435	0.878557	-0.121008
C	5.203099	1.168282	-3.500847
H	3.380254	1.377919	-4.632594
H	6.838503	0.950037	-2.115241

H	5.845264	1.192338	-4.376813
Pd	0.106915	0.387714	-0.290276
C	-0.968292	-2.993546	4.093713
H	-1.197819	-3.221666	5.130790
C	0.341806	-2.707455	3.712975
H	1.139984	-2.707976	4.450220
C	4.170378	-1.628099	3.479142
H	4.546004	-2.278182	4.264239
C	4.411812	-1.933413	2.141072
H	4.974656	-2.824053	1.875640
C	3.928133	-1.104159	1.131782
H	4.115562	-1.363225	0.094839
C	0.637292	-2.414927	2.385125
H	1.660318	-2.184651	2.102398
C	-4.786041	5.555486	0.536973
C	-3.950692	4.811332	1.366129
C	-3.060868	3.886811	0.821170
C	-2.990084	3.684970	-0.559416
C	-3.828435	4.444711	-1.384216
C	-4.719173	5.368147	-0.843037
H	-5.481666	6.275480	0.959567
H	-3.990372	4.949246	2.443881
H	-2.408274	3.299793	1.458923
H	-3.788549	4.320765	-2.463663
H	-5.362945	5.944501	-1.502639
C	-1.975891	2.694403	-1.146772
C	-2.670731	1.716322	-2.118610
H	-3.231905	2.281841	-2.873964
H	-1.876209	1.207325	-2.688485
C	-3.539077	0.642352	-1.546400

H	-3.884559	-0.083222	-2.283143
C	-3.842418	0.444993	-0.253696
H	-1.444074	0.547434	-0.347586
O	-1.346918	2.037471	-0.084425
H	-3.503581	1.172525	0.479192
C	-4.525837	-0.727040	0.301753
C	-4.898647	-0.711744	1.654414
C	-4.750162	-1.904331	-0.432126
C	-5.483270	-1.823895	2.253184
H	-4.717408	0.186510	2.240430
C	-5.329239	-3.016680	0.166572
H	-4.441482	-1.963560	-1.471330
C	-5.699060	-2.984209	1.512334
H	-5.762534	-1.787221	3.302801
H	-5.479748	-3.920759	-0.417619
H	-6.144879	-3.858078	1.979101
C	-0.936496	3.489477	-1.951214
H	-0.464134	4.245508	-1.316729
H	-0.158898	2.802345	-2.307305
H	-1.379023	3.994026	-2.817341

TSC8-9

	Coordinates (Angstroms)		
	X	Y	Z

C	-0.467377	-1.918849	-1.146870
C	-0.324053	-1.679000	-2.522347
C	-1.240419	-2.209092	-3.423514

H	0.494347	-1.063209	-2.887163
H	-1.118378	-2.022981	-4.486530
P	0.721241	-1.117859	-0.026194
C	0.356365	-1.649765	1.672884
C	0.327368	-3.012301	1.997784
C	0.160890	-0.691742	2.671275
C	0.066477	-3.406834	3.305232
H	0.506626	-3.761426	1.231137
C	-0.090251	-1.092868	3.981695
H	0.200070	0.366198	2.422193
C	-0.145409	-2.448236	4.296815
H	0.034151	-4.463933	3.552415
H	-0.243717	-0.344244	4.753587
H	-0.345431	-2.760509	5.317857
C	2.340304	-1.902126	-0.341453
C	3.362526	-1.653654	0.585319
C	2.606022	-2.684848	-1.465965
C	4.638784	-2.156813	0.369585
H	3.162044	-1.055643	1.469474
C	3.887528	-3.193815	-1.673329
H	1.823389	-2.906311	-2.183530
C	4.905941	-2.923750	-0.765060
H	5.426772	-1.949325	1.087750
H	4.084879	-3.802971	-2.550810
H	5.905216	-3.314511	-0.934586
Pd	0.475124	1.099695	-0.278780
C	-2.324432	-2.953605	-2.959294
H	-3.049532	-3.353285	-3.662395
C	-2.482831	-3.173397	-1.593631
H	-3.333176	-3.740059	-1.225797

C	-1.555227	-2.664861	-0.686616
H	-1.697395	-2.835713	0.374656
O	-0.020976	3.223258	-0.508028
O	0.387309	4.088771	0.558461
C	3.143040	1.725728	0.676902
C	4.522135	1.922841	0.583318
C	5.192669	1.644667	-0.606182
C	4.477001	1.178702	-1.708313
C	3.099586	0.974662	-1.618069
C	2.425488	1.246441	-0.423466
H	2.635260	1.938818	1.615044
H	5.072263	2.288118	1.447245
H	6.267376	1.789726	-0.674083
H	4.992548	0.961529	-2.640747
H	2.559746	0.583385	-2.477365
B	0.080797	3.689860	1.860607
O	0.693286	4.430537	2.834175
H	1.312615	5.063581	2.454090
O	-0.755763	2.696424	2.236203
H	-1.245617	2.257751	1.498582
O	-1.657863	1.658386	0.012475
C	-2.912990	1.341240	-0.555268
C	-3.553830	0.200367	0.227776
C	-2.730933	0.892768	-2.025855
C	-2.986414	-0.259179	1.415789
C	-4.715424	-0.426812	-0.239171
H	-2.275885	-0.102051	-2.010292
H	-3.717614	0.796129	-2.489424
C	-1.879033	1.809828	-2.841889
C	-3.542409	-1.331119	2.112401

H	-2.087792	0.214893	1.787506
C	-5.274887	-1.497084	0.452880
H	-5.188779	-0.084681	-1.155547
H	-0.808546	1.792338	-2.628104
C	-2.331535	2.621522	-3.797969
C	-4.686681	-1.960051	1.630139
H	-3.068351	-1.677654	3.027511
H	-6.172766	-1.974288	0.069060
H	-3.389795	2.664968	-4.051398
H	-1.663069	3.266750	-4.363162
H	-5.120258	-2.800159	2.165618
H	-1.031036	2.721374	-0.298058
C	-3.791509	2.589228	-0.475941
H	-3.355654	3.395381	-1.075847
H	-4.799722	2.388637	-0.850996
H	-3.869900	2.927827	0.562058
