Supplemental Information

Expanding Chemical Space of Enol Silyl Ethers: Catalytic Dicarbofunctionalization Enabled by Iron Catalysis

Dinabandhu Sar, Shuai Yin,‡ Jacob Grygus,‡ Ángel Rentería-Gómez, Melanie Garcia, Osvaldo Gutierrez*

Department of Chemistry, Texas A&M University, College Station, Texas 77843, United States

og.labs@tamu.edu

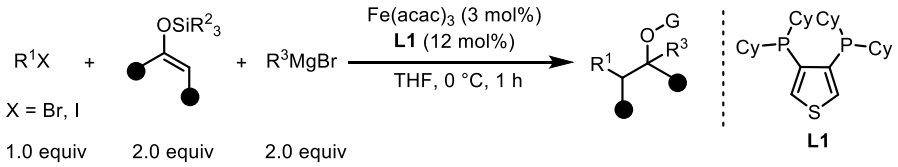
Table of Contents

1. General Consideration

Unless otherwise indicated, all reactions were carried out under a nitrogen atmosphere in oven- (110 °C) or flame-dried glassware. When necessary, solvents and reagents were dried prior to use. Tetrahydrofuran (THF) was dried by passage through activated alumina in Inert's PureSolv MB-SPS solvent purification system. All solvents were obtained from VWR, Sigma-Aldrich, or Fisher. Organometallic reagents were purchased from Sigma-Aldrich and Synthonix. Silicycle 250 μm silica-gel F-254 plates were used to perform analytical thin layer chromatography (TLC). Column chromatography was performed with Silica gel (230-400 mesh) and Biotage® Selekt Flash Systems silica gel chromatography was performed with prepacked silica-gel cartridges (Sfar; Biotage). NMR (^{1}H, ^{13}C and ^{19}F) spectra were recorded on Acsend^{TM} 400 (Bruker) NMR spectrometer. Chemical shifts (δ) are reported in parts per million (ppm) relative to the internal residual solvent resonance peak δ 7.26 ($CDCl_3$) and δ 0.00 (TMS) for all ^{1}H and δ 77.16 ($CDCl_3$) and δ 0.00 (TMS) for all ^{13}C. Other data are designated as follows: multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, qu = quintet, sept = septet, oct = octet, m = multiplet, dd= doublet of doublets, dt = doublet of triplets, td = triplet of doublets, dq = doublet of quartets, qd = quartet of doublets, tt = triplet of triplets, tdd = triplet of doublet of doublets, bs = broad singlet), coupling constants (*J*) are reported in Hertz (Hz), and number of protons. High Resolution Mass (HRMS) spectra using Electrospray ionization (ESI) mode and Atmospheric chemical ionization (APCI) mode were acquired on Thermo Scientific Q Exactive Focus mass spectrometer. Agilent 8890 GC system and 5977B MSD were used to measure GC-MS. Thermo Scientific Nicolet Summit FTIR spectrometer was employed for recording IR spectra and are reported in wavenumbers (cm^{-1}). Melting points were obtained and are uncorrected. A BRUKER Venture X-ray (kappa geometry) diffractometer was used for crystal screening, unit cell determination, and data collection.

2. General Procedure for Iron-Catalyzed 1,2-Dicarbofunctionalization of Enol Silyl Ether.

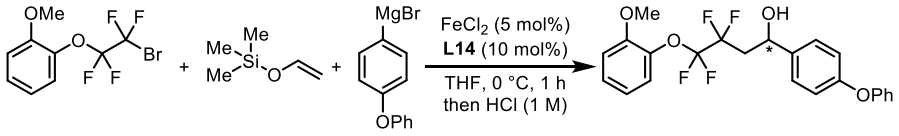
Procedure 1: Iron-Catalyzed cross-coupling for 1,2-Dicarbofunctionalization



G = H, when quench with HCl (aq)
G = $SiMe_3$, $SiEt_3$, $SiMe_2tBu$, when quench with sat. NH_4Cl (aq)

Standard-scale: In an argon-filled glovebox, $Fe(acac)_3$ (2.1 mg, 3 mol %), 3,4-bis(dicyclohexylphosphaneyl)thiophene **L1** (11.4 mg, 12 mol %), alkyl halide (0.2 mmol, 1.0 equiv.) and enol silyl ether (0.4 mmol, 2.0 equiv.) were weighted in a flame-dried 10 mL microwave vial equipped with a stir bar. The vial was sealed with a Teflon cap and brought out of the glovebox. The reaction mixture was then suspended in THF (0.2 mL). The resulting red solution was stirred at ambient temperature for 5 min and then cooled to 0 °C. A R^3MgBr solution (2.0 equiv.) was then added slowly for 1 h using a syringe pump. Over which time the heterogeneous solution turned from red to colorless or yellow, brown, grass green or orange color (depending on R^3MgBr and substrate). The resultant mixture was then stirred for an additional 10 min at 0 °C. After completion of the reaction, the mixture was quenched with a 1.0 M aqueous solution of hydrochloric acid (0.5 mL) and water (0.5 mL) or saturated aqueous solution of ammonium chloride (1.0 mL) (depending on products), then extracted with diethyl ether (3 x 4 mL). The organic solution was filtered over a short pad of silica and filtrate was concentrated under reduced pressure. The crude residue was then purified by Biotage® Selekt Flash Systems silica gel chromatography with prepacked silica-gel cartridges (Sfar; Biotage) and a gradient elution of hexane/EtOAc or hexane/DCM to obtain products.

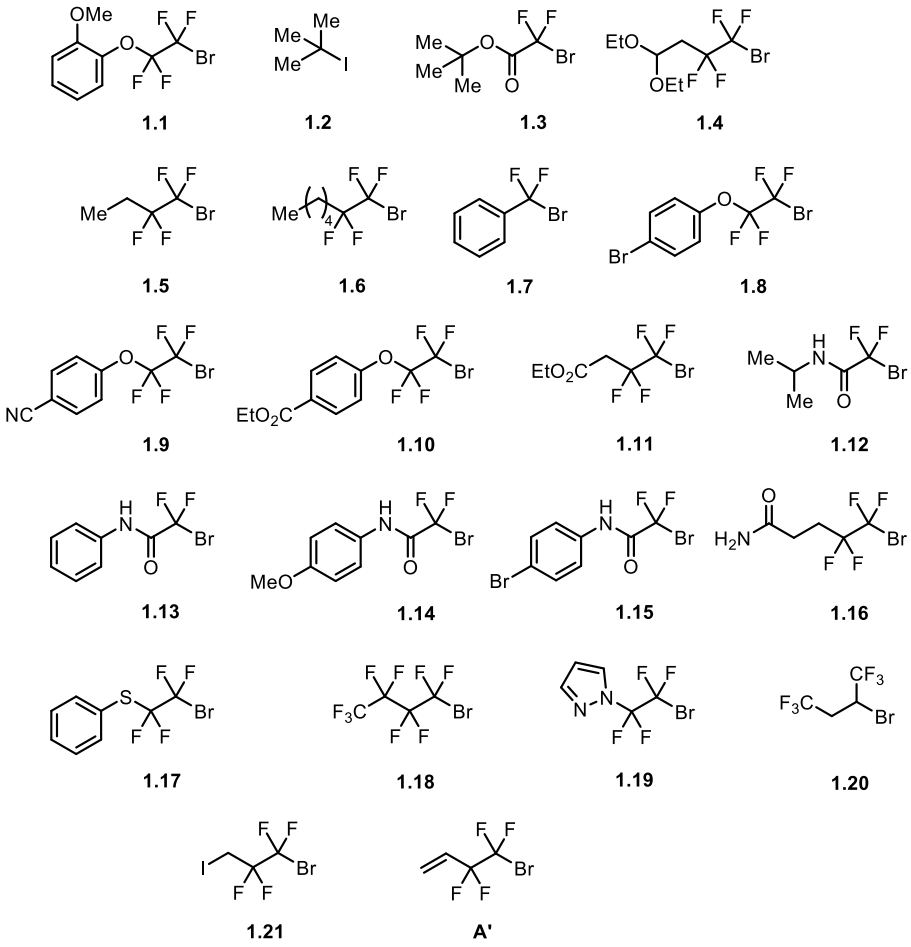
Procedure 2: Iron-catalyzed asymmetric 1,2-Dicarbofunctionalization of enol silyl ether



In an argon filled glovebox, a flame-dried microwave vial with a stir bar was transferred and the vial was charged with $FeCl_2$ (1.3 mg, 5 mol %), (*1R*,*1'R*,*2S*,*2'S*)-DuanPhos **L14** (7.6 mg, 10 mol %), alkyl halide (0.2 mmol, 1.0 equiv) and enol silyl ether (0.4 mmol, 2.0 equiv). The vial was brought out of the glovebox and THF (0.2 mL) was then added into the reaction mixture. The resulting solution was stirred at room temperature for 5 min and then cooled to 0 °C. Grignard solution (1.0 M solution in THF, 2.0 equiv.) was then added into the solution slowly for 1 h using a syringe pump. The resulting solution was stirred at 0 °C for an additional 10 min. After completion, the mixture was quenched with a 1.0 M aqueous solution of hydrochloric acid (0.5 mL) and water (0.5 mL) and then extracted with diethyl ether (3 x 4 mL). The organic solution was filtered through a short pad of silica and organic solvent was then evaporated by rotary evaporator. The crude residue was purified by Biotage® Selekt Flash Systems silica gel chromatography with prepacked silica-gel cartridges (Sfar; Biotage) and a gradient elution of hexane/EtOAc to obtain desired products.

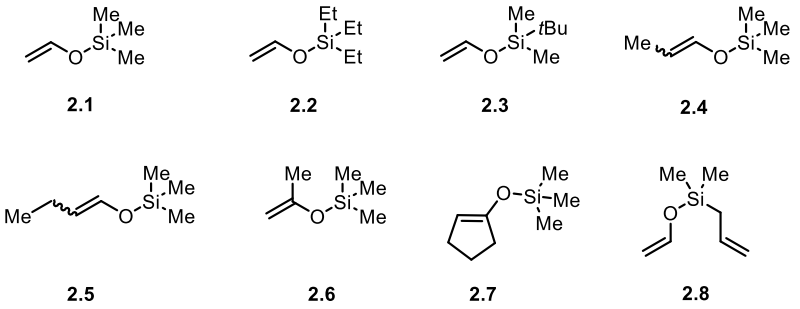
3. Structure of Starting Materials Used for Iron Catalyzed 1,2-Dicarbofunctionalization

Fig. S1. Structure of (Fluoro)alkyl halides



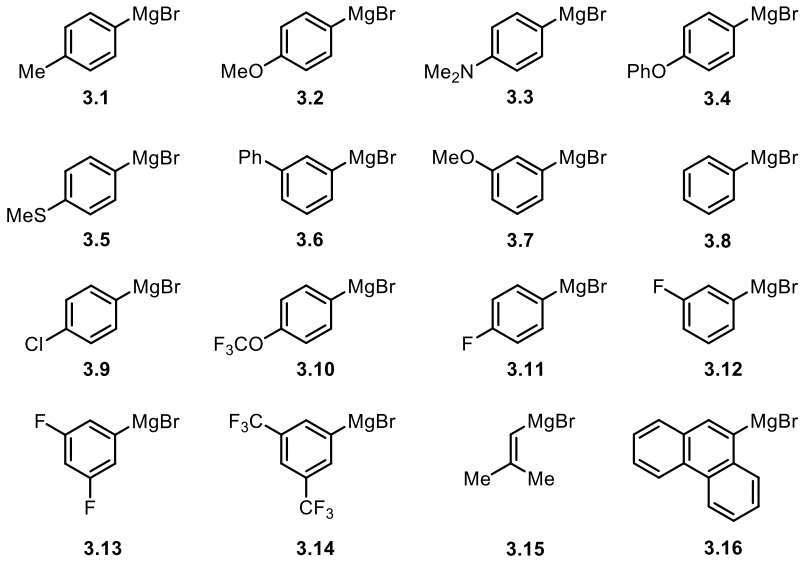
1.12 was synthesized according to the following procedure for synthesis of 2-bromo-2,2-difluoro-*N*-isopropylacetamide (**3.1.**).

Fig. S2. Structure of enol silyl ethers

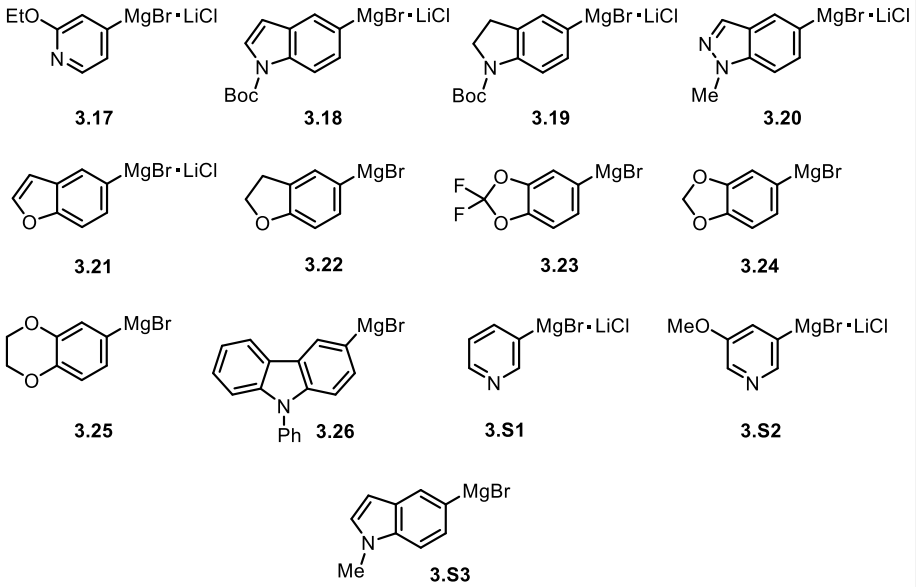


2.2-2.5 and **2.8** were prepared through the following General Procedure for Preparation of Silyl Enol Ether (**3.2.**). **2.1** and **2.7** were purchased from Sigma Aldrich and **2.6** was purchased from TCI America.

Fig. S3. Structure of Grignard reagents

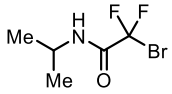


Continued…



3.17-26, 3.S1 and **3.S2** were prepared through the following General Procedure for Preparation of Grignard reagents (**3.3.**). **3.1-16** were purchased from Sigma Aldrich and **3.S3** was purchased from Synthonix.

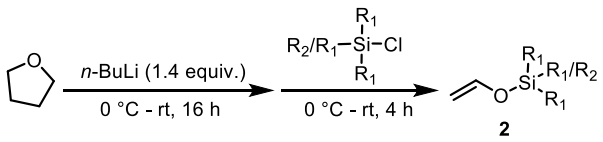
3.1. Procedure for Synthesis of 2-bromo-2,2-difluoro-*N*-isopropylacetamide[1]



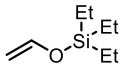
Ethyl bromodifluoroacetate (405.9 mg, 2 mmol) was added in an oven dried 10 mL microwave vial equipped with a stir bar. Isopropyl amine (0.17 mL, 2 mmol) was then added into the vial via syringe at room temperature. The mixture was stirred overnight at room temperature. After completion, the reaction mixture was quenched with 10% aqueous solution of hydrochloric acid and then extracted with ethyl acetate. The organic solution was successively washed with brine (10 mL) and dried over Na_2SO_4. The solvent was evaporated, and the residue was purified by flash chromatography on silica gel with hexane/EtOAc (9:1) to hexane/EtOAc (22:3). The product **1.12** was obtained as a colorless solid (349 mg, 81% yield). Spectral data matched those reported previously.[1]

3.2. General Procedure for Preparation of Enol Silyl Ether

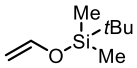
Procedure A: Preparation of monosubstituted enol silyl ethers[2]



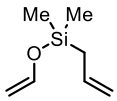
To an oven dried 50 mL round bottom flask, *n*-BuLi (2.8 mL, 2.5 M solution in *n*-hexane, 7.0 mmol, 1.4 equiv.) was slowly added to THF (8.3 mL) at 0 °C via syringe pump for 20 mins. The yellow solution was then stirred at room temperature for 16 h and resulted in the cloudy and grey-white solution. To the resulting solution was slowly added silane (5.0 mmol, 1.0 equiv.) at 0 °C. The reaction mixture was then stirred for another 4 h at room temperature. The solution was poured into *n*-pentane (20 mL), and then filtered through sand. The filtrate was concentrated under reduced pressure by rotary evaporator. The crude residue was then purified by silica gel column chromatography with *n*-pentane to obtain desired enolsilane as a colorless liquid.



Triethyl (vinyloxysilane) (2.2): Compound **2.2** was synthesized following the general procedure for preparation of Enolsilanes (procedure A), using chlorotriethylsilane (753.6 mg, 5 mmol). The product **2.2** was obtained as a colorless liquid (332 mg, 3.8 M solution in pentane, 42%). Spectral data matched those reported previously.[2]



***tert*-Butyldimethyl(vinyloxy)silane (2.3):** Compound **2.3** was synthesized following the general procedure for preparation of Enolsilanes (procedure A), using *tert*-Butylchlorodimethylsilane (753.6 mg, 5 mmol). The product **2.3** was obtained as a colorless liquid (300 mg, 4.0 M solution in pentane, 38%). Spectral data matched those reported previously.[2]



Allyldimethyl(vinyloxy)silane (2.8): Compound **2.8** was synthesized following the general procedure for preparation of Enolsilanes (procedure A), using allylchlorodimethylsilane (711.3 mg, 5 mmol). The product **2.8** was obtained as a colorless liquid (412 mg, 3.6 M solution in pentane, 58%). (*Note: Product was volatile under reduced pressure*.)

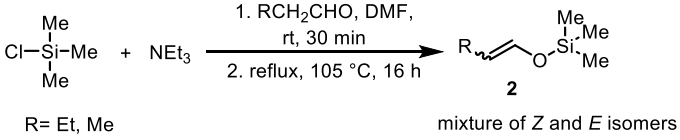
^{1}H NMR (400 MHz, $CDCl_3$) δ = 6.40 (dd, J = 13.6, 6.0 Hz, 1H), 5.79 (tdd, J = 12.6, 10.0, 8.0 Hz, 1H), 4.96-4.89 (m, 2H), 4.45 (dd, J = 13.6, 1.2 Hz, 1H), 4.15 (dd, J = 6.0, 1.2 Hz, 1H), 1.69 (dt, J = 8.0, 1.6 Hz, 2H), 0.20 (s, 6H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 145.9, 133.1, 114.5, 95.1, 24.1, -2.3;

IR (film) 2959, 2924, 2854, 1631, 1258, 1068, 804 cm^{-1};

HRMS (ESI) calcd for $C_7H_{14}OSi$ $[M+NH_4]^+$ m/z =160.1152; found: 160.1150.

Procedure B: Synthesis of disubstituted enol silyl ethers

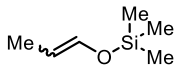


R= Et, Me

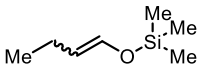
mixture of *Z* and *E* isomers

Following a modified procedure by Olmstead et al,[3] to a solution of chlorotrimethylsilane (2.61 g, 24.0 mmol, 1.2 equiv.) and triethylamine (4.86 g, 48.0 mmol, 2.5 equiv.) in anhydrous DMF (8 mL) was added aldehyde (20.0 mmol, 1.0 equiv.) via the syringe pump for 30 mins at room temperature. The resulting mixture, from which some white solid was formed, was refluxed for 16 h at 105 °C and then cooled to room temperature. The reaction mixture was then diluted with pentane (15 mL) and then washed with cold aqueous saturated sodium bicarbonate solution (25 mL) three times. The resulting organic layer was washed with cold hydrochloride acid solution (1.5 M, 15 mL) and cold aqueous saturated sodium bicarbonate solution (15 mL). The resulting organic solution was dried with anhydrous

sodium sulfate (Na_2SO_4) and the solvent was then removed via rotary evaporator. The crude residue was then purified by reduced-pressure distillation to obtain the desired product.



1-Trimethylsilyloxy-1-propene (2.4): Compound **2.4** was synthesized following the general procedure for synthesis of trimethyl silyl enol ethers (Procedure B) using propionaldehyde (1.16 g, 20 mmol). The product **2.4** was obtained as a colorless liquid (866.4 mg, 33%) after distillation at 40-50 °C under 200 mbar. The product is a mixture of *E/Z* isomers. *E/Z ratio*: 1:1.7. Spectral data matched those reported previously.[4]



1-Trimethylsilyloxy-1-butene (2.5): Compound **2.5** was synthesized following the general procedure for synthesis of trimethyl silyl enol ethers (Procedure B) using butyraldehyde (1.44 g, 20 mmol). The product **2.5** was obtained as a colorless liquid (1.19 g, 43%) after distillation at 58-65 °C under 50 mbar. The product is a mixture of *E/Z* isomers. *E/Z ratio*: 1:1.5. Spectral data matched those reported previously.[5]

3.3. General Procedure for Preparation of Grignard reagents[6]

Procedure A: Synthesis of heteroaryl Turbo Grignard reagents (**3.17**-**21**, **3.S1** and **3.S2**)

In an argon filled glovebox, a flame-dried two-necked 25 mL flask with a stir bar was transferred and the vial was charged with Mg powder (243 mg, 10 mmol, 2.0 equiv.) and LiCl (254.3 mg, 6.0 mmol, 1.2 equiv.). The flask was sealed with a Teflon cap and brought out of the glovebox. The flask was heated under vacuum for 2 min with stirring. Anhydrous THF (5 mL) and DIBALH (0.25 mL, 1.0 M solution in hexane, 0.25 mmol) were added to the cooled flask and the mixture was stirred vigorously. After 5 min at room temperature, heteroaryl halide (5.0 mmol, 1.0 equiv.) was added to the reaction mixture at specified

temperature. The resulting solution was stirred for specified time. The concentration of the resulting heteroaryl Grignard reagent was calculated via iodometric titration.

Using the above procedure, the solution was stirred at rt for 3 h to obtain heteroaryl Grignard reagents **3. 18** and **3.19**.

Using the above procedure, the solution was stirred at rt for 2 h to obtain heteroaryl Grignard reagent **3. 20**.

Using the above procedure, the solution was heated at 60 °C for 2 h to obtain heteroaryl Grignard reagents **3.17** and **3.21**.

Using the above procedure, the solution was stirred at 0 °C for 2 h to obtain heteroaryl Grignard reagents **3.S1** and **3.S2**.

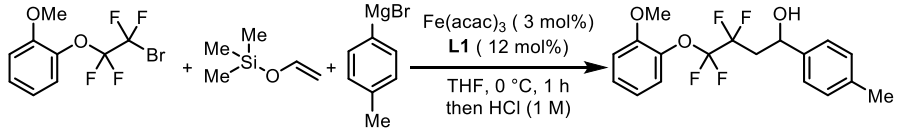
Procedure B: Synthesis of heteroaryl Grignard reagents **(3.22-26)**

In an argon filled glovebox, a flame-dried two-necked 25 mL flask with a stir bar was transferred and the vial was charged with Mg powder (175 mg, 7.2 mmol, 1.2 equiv.). The flask was sealed with a Teflon cap and brought out of the glovebox. The flask was heated under vacuum for 2 min with stirring. Anhydrous THF (5 mL) and I_2 (2 crystals) were added to the cooled flask and the mixture was stirred vigorously. Heteroaryl halide (6.0 mmol, 1.0 equiv.) was added dropwise to the reaction mixture at room temperature. The resulting solution was then heated at reflux for 2 h. The concentration of the heteroaryl Grignard reagent was calculated via iodometric titration.

Using the above procedure, the solution was heated at reflux for 3 h to obtain heteroaryl Grignard reagent **3.26**.

4. Screening of Reaction Conditions

Table S1. Screening of enol silyl ether and Grignard loading for iron catalyzed 1,2-dicarbofunctionalization.

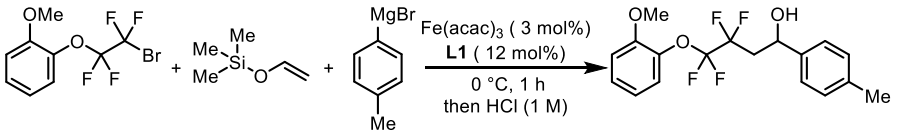


1.1 **2.1** **3.1** **4**

Entry	1.1 (equiv.)	2.1 (equiv.)	3.1 (equiv.)	Yield (%)*
1	1	1	1.5	78
2	1	2	1.5	85
3	**1**	**2**	**2**	**97**
4	1	2	3	87
5	1	3	2	95
6[†]	1	2	2	82

Reactions were conducted with a 0.10 mmol scale of 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (**1.1**), THF (0.1 mL) and Grignard addition for 1 h at 0 ºC. Reactions were then stirred an additional 10 min after Grignard addition. [*]Yields were determined by crude ^{1}H NMR with CH_2Br_2 as internal standard of the associated deprotected alcohol. [†]Neat (no additional THF solvent).

Table S2. Screening of solvents and rate of addition of Grignard reagent for iron-catalyzed 1,2-dicarbofunctionalization



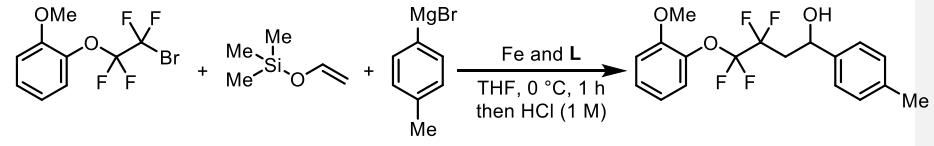
1.1 **2.1** **3.1** **4**

Entry	Solvents	Rate of addition (min)	Yield (%)*

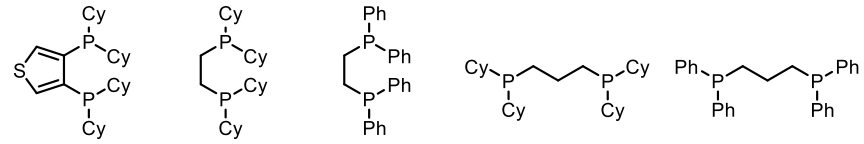
1	**THF**	**60**	**97**
2	Diethyl ether	60	57
3	1,4-Dioxane	60	34
4	THF	120	63
5	THF	30	18

Reactions were conducted with a 0.10 mmol scale of 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (**1.1**), THF (0.1 mL) at 0 ºC. Reactions were then stirred an additional 10 min after Grignard addition. *Yields were determined by crude ^{1}H NMR with CH_2Br_2 as internal standard of the associated deprotected alcohol.

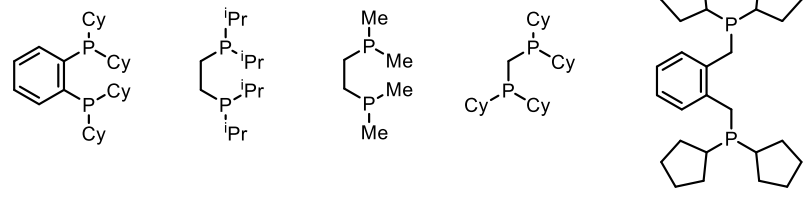
Table S3. Screening of ligands, iron salt and catalyst loading for 1,2-dicarbofunctionalization



1.1 **2.1** **3.1** **4**



L1 **L2** **L3** **L4** **L5**

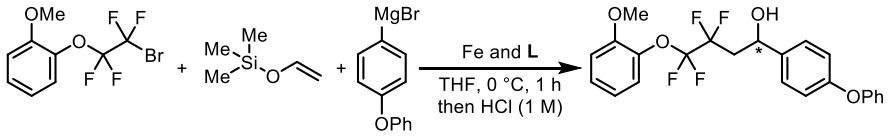


L6 **L7** **L8** **L9** **L10**

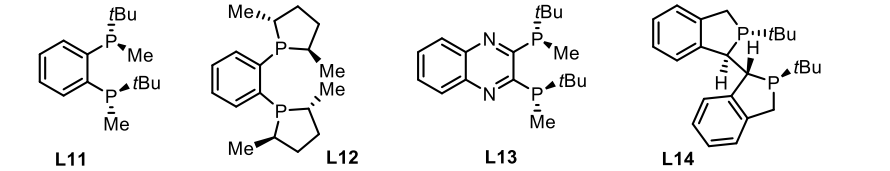
Entry	Fe	L	Fe/L (mol %)	Yield (%)*
1	**$Fe(acac)_3$**	**L1**	**3/12**	**97**
2	$Fe(acac)_3$	**L2**	3/12	93
3	$Fe(acac)_3$	**L3**	3/12	10
4	$Fe(acac)_3$	**L4**	3/12	46
5	$Fe(acac)_3$	**L5**	3/12	25
6	$Fe(acac)_3$	**L6**	3/12	89
7	$Fe(acac)_3$	**L7**	3/12	89
8	$Fe(acac)_3$	**L8**	3/12	0
9	$Fe(acac)_3$	**L9**	3/12	0
10	$Fe(acac)_3$	**L10**	3/12	0
11	$FeCl_3$	**L1**	3/12	83
12	$FeBr_2$	**L1**	3/12	82
13	FeF_3	**L1**	3/12	0
14	$Fe(OTf)_3$	**L1**	3/12	85
15	$Fe(OAc)_2$	**L1**	3/12	83
16	$Fe(acac)_3$	**L1**	3/6	89
17	$Fe(acac)_3$	**L1**	5/10	90
18	$Fe(acac)_3$	**L1**	5/20	72

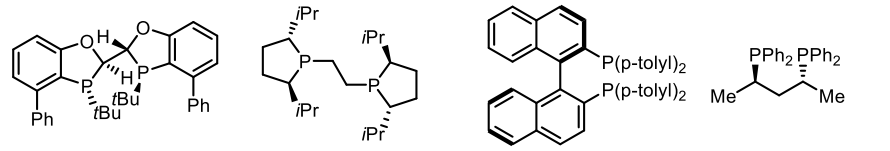
Reactions were carried out with a 0.10 mmol scale of 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (**1.1**), 2.0 equiv. of alkene (**2.1**), 2.0 equiv. of Grignard reagent (**3.1**), THF (0.1 mL) and Grignard addition for 1 h at 0 ºC. Reactions were then stirred an additional 10 min after Grignard addition. *Yields were determined by crude ^1H NMR with CH_2Br_2 as internal standard of the associated deprotected alcohol.

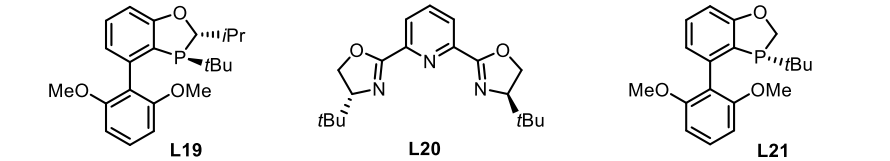
Table S4. Screening of chiral ligands, iron salt and catalyst loading for 1,2-dicarbofunctionalization



1.1 2.1 3.4 93







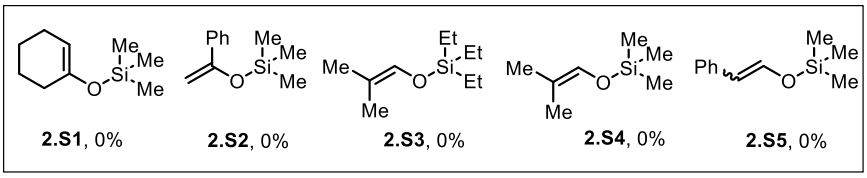
Entry	Fe	L	Fe/L (mol %)	Yield (%)*	Enantiomeric Ratio (er)
1	$FeBr_2$	**L11**	3/12	99	59:41
2	$FeBr_2$	**L12**	3/12	95	49:51
3	$FeCl_2$	**L13**	3/12	84	36:64
4	$FeCl_3$	**L13**	3/12	91	45:55
5	$FeCl_2$	**L13**	5/10	98	36:64
6	**$FeCl_2$**	**L14**	**5/10**	**69**	**70:30**

7	$Fe(acac)_3$	**L14**	5/10	50	68:32
8	$FeCl_2$	**L15**	5/10	20	50:50
9	$FeCl_2$	**L16**	5/10	15	50:50
10	$FeCl_2$	**L17**	5/10	19	50:50
11	$FeCl_2$	**L18**	5/10	19	53:47
12	$FeCl_2$	**L19**	5/10	23	50:50
13	$FeCl_2$	**L20**	5/10	8	51:49
14	$FeCl_2$	**L21**	5/10	13	50:50

Reactions were carried out with a 0.10 mmol scale of 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (**1.1**), 2.0 equiv. of alkene (**2.1**), 2.0 equiv. of Grignard reagent (**3.4**), THF (0.1 mL) and Grignard addition for 1 h at 0 ºC. Reactions were then stirred an additional 10 min after Grignard addition. *Yields were determined by crude ^1H NMR with CH_2Br_2 as internal standard. Enantiomeric ratio (er) values were determined by HPLC with the Daicel Chiralcel OJ-H column (Hexane/*i*-PrOH 90:10, 1.0 mL/min, 250 nm).

5. Current Limitation

Fig. S4: Current limitation of alkenes in iron catalyzed 1,2-Dicarbofunctionalization.



2.S1, 0% **2.S2**, 0% **2.S3**, 0% **2.S4**, 0% **2.S5**, 0%

Fig. S5: Current limitation or low yield of alkyl halides substrates in iron catalyzed 1,2-Dicarbofunctionalization.

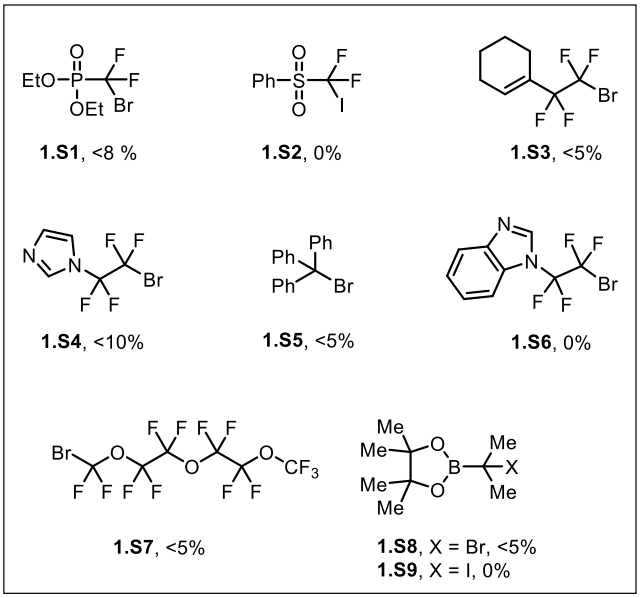
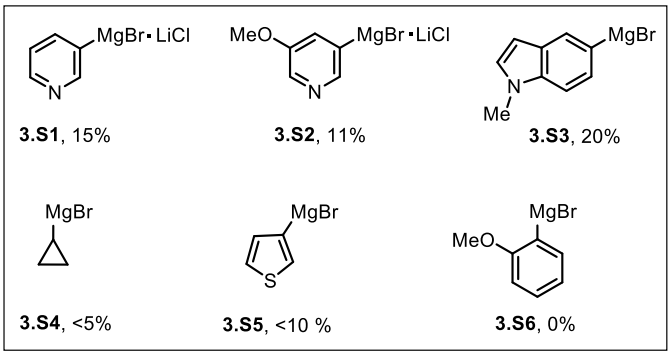
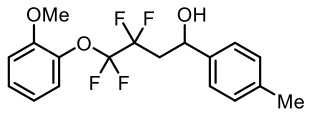


Fig. S6: Current limitation or low yield of Grignard nucleophiles in iron catalyzed 1,2-Dicarbofunctionalization.



6. Product Characterization Data



3,3,4,4-Tetrafluoro-4-(2-methoxyphenoxy)-1-(*p*-tolyl)butan-1-ol (4): Compound **4** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and *p*-tolylmagnesium bromide (0.4 mL, 1.0 M solution in THF, 0.4 mmol). The product **4** was obtained as a colorless liquid (62 mg, 86% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (4:1) to hexane/EtOAc (39:11).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.36 (d, J = 8.4 Hz, 2H), 7.28-7.21 (m, 4H), 7.01-6.94 (m, 2H), 5.30 (dt, J = 9.2, 3.2 Hz, 1H), 3.85 (s, 3H), 2.83-2.53 (m, 3H), 2.38 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.3, 140.4, 137.8, 137.7, 129.4, 127.6, 125.7, 123.8, 120.8, 119.3-116.8 (m), 112.8, 68.1 (t, J = 3.3 Hz), 56.0, 41.3 (t, J = 20.5 Hz), 21.2;

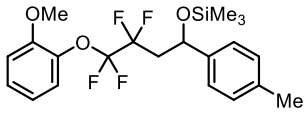
^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.07 to -88.89 (m, 2F), -113.69 to -114.49 (m, 1F), -114.93 to -115.73 (m, 1F);

IR (film) 3423, 2925, 1502, 1458, 1282, 1261, 1187, 1170, 1101, 1043, 1024, 819, 749 cm^{-1};

HRMS (ESI) calcd for $C_{18}H_{18}F_4O_3$ $[M+Na]^+$ m/z = 381.1084; found: 381.1074.

3,3,4,4-Tetrafluoro-4-(2-methoxyphenoxy)-1-(*p*-tolyl)butan-1-ol (4)-gram-scale: Compound **4** was synthesized following the general procedure, using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (1.6 g, 5.4 mmol), trimethyl(vinyloxy)silane (1.2 g, 10.8 mmol), *p*-tolylmagnesium bromide (10.8 mL, 1.0 M solution in THF, 10.8 mmol), $Fe(acac)_3$ (57.2 mg, 3 mol %), and 3,4-bis(dicyclohexylphosphaneyl)thiophene **L1** (308.9 mg, 12 mol %). The product **4** was obtained as a colorless liquid (1.6 g, 83% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (4:1) to hexane/EtOAc (39:11).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.36 (d, J = 8.0 Hz, 2H), 7.28-7.20 (m, 4H), 7.00-6.94 (m, 2H), 5.30 (dd, J = 9.2, 3.0 Hz, 1H), 3.85 (s, 3H), 2.82-2.53 (m, 3H), 2.38 (s, 3H); spectral data matched compound **4**.



Trimethyl(3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)-1-(*p*-tolyl)butoxy)silane (5): Compound **5** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.5 mg, 0.4 mmol) and *p*-tolylmagnesium bromide (0.4 mL, 1.0 M solution in THF, 0.4 mmol). The product **5** was obtained as a colorless liquid (55 mg, 64% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (9:1) to hexane/EtOAc (22:3).

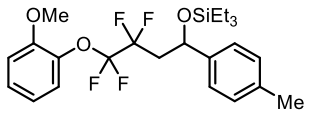
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.28-7.26 (m, 2H), 7.23-7.19 (m, 2H), 7.16-7.14 (m, 2H), 6.97-6.89 (m, 2H), 5.20 (dd, J = 8.8, 3.2 Hz, 1H), 3.80 (s, 3H), 2.71-2.56 (m, 1H), 2.54-2.40 (m, 1H), 2.34 (s, 3H), 0.05 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.5, 141.6, 137.9, 137.2, 129.1, 127.5, 125.8, 124.0, 120.6, 117.8-115.1 (m), 112.9, 68.7 (t, J = 2.5 Hz), 56.1, 41.7 (t, J = 20.3 Hz), 21.2, 0.1;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.86 to -88.89 (m, 2F), -114.47 to -115.27 (m, 1F), -117.56 to -118.36 (m, 1F);

IR (film) 2925, 1504, 1262, 1188, 1172, 1106, 921, 893, 748 cm^{-1};

HRMS (ESI) calcd for $C_{21}H_{26}F_4O_3Si$ $[M+H]^+$ m/z = 431.1660; found: 431.1656.



Triethyl(3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)-1-(*p*-tolyl)butoxy)silane (6): Compound **6** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol),

triethyl(vinyloxy)silane (0.1 mL, 3.8 M solution in pentane, 0.4 mmol) and *p*-tolylmagnesium bromide (0.4 mL, 1.0 M solution in THF, 0.4 mmol). The product **6** was obtained as a colorless liquid (49 mg, 52% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (19:1) to hexane/EtOAc (47:3).

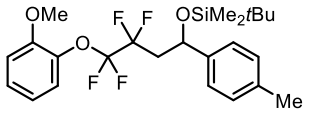
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.29 (d, J = 8.0 Hz, 2H), 7.23-7.19 (m, 2H), 7.15 (d, J = 8.0 Hz, 2H), 6.96-6.89 (m, 2H), 5.20 (dd, J = 8.4, 4.0 Hz, 1H), 3.80 (s, 3H), 2.74-2.59 (m, 1H), 2.53-2.39 (m, 1H), 2.35 (s, 3H), 0.87 (t, J = 8.0 Hz, 9H), 0.61-0.48 (m, 6H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.6, 141.8, 137.9, 137.3, 129.1, 127.5, 125.9, 124.0, 120.6, 119.0-113.9 (m), 112.9, 68.9 (t, J = 2.3 Hz), 56.0, 41.7 (t, J = 20.2 Hz), 21.3, 6.7, 4.8;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.99 to -89.01 (m, 2F), -114.72 to -115.52 (m, 1F), -117.44 to -118.42 (m, 1F);

IR (film) 2995, 1503, 1262, 1188, 1172, 1104, 1020, 912, 746 cm^{-1};

HRMS (ESI) calcd for $C_{24}H_{32}F_4O_3Si$ $[M+K]^+$ m/z = 511.1688; found: 511.1680.



***tert*-Butyldimethyl(3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)-1-(*p*-tolyl)butoxy)silane (7):** Compound **7** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), *tert*-butyldimethyl(vinyloxy)silane (0.1 mL, 4.0 M solution in pentane, 0.4 mmol) and *p*-tolylmagnesium bromide (0.4 mL, 1.0 M solution in THF, 0.4 mmol). The product **7** was obtained as a colorless liquid (46 mg, 49% yield) after purification by flash chromatography on silica gel with hexane.

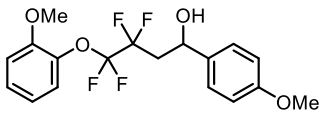
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.27-7.23 (m, 2H), 7.21 (d, J = 7.6 Hz, 2H), 7.15 (d, J = 8.0 Hz, 2H), 6.96-6.89 (m, 2H), 5.17 (dd, J = 8.8, 3.2 Hz, 1H), 3.80 (s, 3H), 2.17-2.56 (m, 1H), 2.51-2.37 (m, 1H), 2.34 (s, 3H), 0.87 (s, 9H), 0.07 (s, 3H), -0.17 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.5, 141.8, 137.9, 137.2, 129.1, 127.5, 125.9, 124.0, 120.6, 118.2-116.4 (m), 112.9, 69.1 (t, J = 2.1 Hz), 56.0, 41.0 (t, J = 20.4 Hz), 25.8, 21.2, 18.1, -4.4, -5.1;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.79 to -89.18 (m, 2F), -114.20 to -115.01 (m, 1F), -117.67 to -118.47 (m, 1F);

IR (film) 2954, 1503, 1260, 1187, 1102, 1044, 916, 836, 747 cm^{-1};

HRMS (ESI) calcd for $C_{24}H_{32}F_4O_3Si$ $[M+H]^+$ m/z = 473.2130; found: 473.2120.



3,3,4,4-Tetrafluoro-4-(2-methoxyphenoxy)-1-(4-methoxyphenyl)butan-1-ol (8): Compound **8** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-methoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **8** was obtained as a colorless liquid (59 mg, 79% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (77:23) to hexane/EtOAc (19:6).

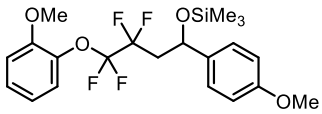
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.37 (d, J =8.8 Hz, 2H), 7.23-7.21 (m, 2H), 6.99-6.89 (m, 4H), 5.27 (dt, J = 9.2, 3.2 Hz, 1H), 3.83 (s, 3H), 3.81 (s, 3H), 2.80-2.51 (m, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 159.4, 152.3, 137.7, 135.6, 127.6, 127.0, 123.8, 120.7, 120.5-115.0 (m), 114.1, 112.8, 67.8 (t, J = 3.7 Hz), 56.0, 55.4, 41.2 (t, J = 20.5 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) $\boldsymbol{\delta}$ = -88.10 to -88.91 (m, 2F), -113.79 to -114.60 (m, 1F), -114.98 to -115.78 (m, 1F);

IR (film) 3440, 2946, 2840, 1611, 1501, 1458, 1302, 1248, 1169, 1097, 1025, 832, 790, 748, 703 cm^{-1};

HRMS (ESI) calcd for $C_{18}H_{18}F_4O_4$ $[M+Na]^+$ m/z = 397.1033; found: 397.1026.



Trimethyl(3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)-1-(4 methoxyphenyl)butoxy)silane (9): Compound **9** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene

(60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.5 mg, 0.4 mmol) and (4-methoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **9** was obtained as a colorless liquid (66.8 mg, 75% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (21:4) to hexane/EtOAc (41:9).

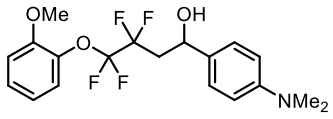
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.31 (d, J = 8.8 Hz, 2H), 7.23-7.19 (m, 2H), 6.97-6.89 (m, 2H), 6.89 (d, J = 8.8 Hz, 2H), 5.18 (dd, J = 8.8, 3.6 Hz, 1H), 3.81 (s, 3H), 3.80 (s, 3H), 2.72-2.57 (m, 1H), 2.53-2.39 (m, 1H), 0.04 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 159.1, 152.8, 137.9, 136.7, 127.5, 127.0, 124.0, 120.6, 119.0-115.1 (m), 113.8, 112.9, 68.5 (t, J = 2.6 Hz), 56.0, 55.3, 41.7 (t, J = 20.3 Hz), 0.1;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.88 to -88.89 (m, 2F), -114.56 to -115.37 (m, 1F), -117.53 to -118.33 (m, 1F);

IR (film) 2957, 1612, 1503, 1458, 1249, 1170, 1099, 1030, 918, 840, 771, 749 cm^{-1};

HRMS (ESI) calcd for $C_{21}H_{26}F_4O_4Si$ $[M+Na]^+$ m/z = 469.1429; found: 469.1423.



1-(4-(Dimethylamino)phenyl)-3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)butan-1-ol (10): Compound **10** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-(dimethylamino)phenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **10** was obtained as a yellowish liquid (52 mg, 67% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (37:13) to hexane/EtOAc (18:7).

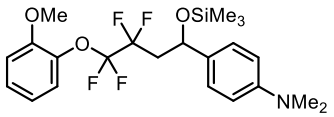
^{1}H NMR (400 MHz, $CDCl_3$) δ =7.31 (d, J = 8.8 Hz, 2H), 7.25-7.21 (m, 2H), 6.98-6.91 (m, 2H), 6.75 (d, J = 9.2 Hz, 2H), 5.22 (dt, J = 9.2, 3.0 Hz, 1H), 3.83 (s, 3H), 2.95 (s, 6H), 2.82-2.51 (m, 2H), 2.38-2.37 (m, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.3, 150.5, 137.8, 131.2, 127.5, 126.8, 123.9, 120.7, 120.5-114.3 (m), 112.8, 112.7, 68.0 (t, J = 3.5 Hz), 56.1, 40.8 (t, J = 20.3 Hz), 40.7;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.16 to -88.95 (m, 2F), -113.99 to -114.96 (m, 1F), -115.40 to -116.2 (m, 1F);

IR (film) 3410, 2893, 2842, 1607, 1524, 1503, 1458, 1261, 1187, 1170, 1106, 1024, 818, 749, 694 cm^{-1};

HRMS (ESI) calcd for $C_{19}H_{21}F_4NO_3$ $[M+H]^+$ m/z = 388.1530; found: 388.1522.



***N*,*N*-Dimethyl-4-(3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)-1-((trimethylsilyl)oxy)butyl)aniline (11):** Compound **11** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-(dimethylamino)phenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **11** was obtained as a colorless liquid (63 mg, 69% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (43:7) to hexane/EtOAc (21:4).

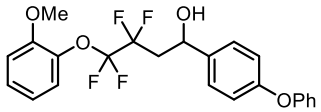
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.28-7.26 (m, 2H), 7.25-7.22 (m, 2H), 7.00-6.92 (m, 2H), 6.75 (d, *J* = 8.4 Hz, 2H), 5.18 (dd, *J* = 9.2, 3.2 Hz, 1H), 3.84 (s, 3H), 2.98 (s, 6H), 2.76-2.61 (m, 1H), 2.57-2.43 (m, 1H); 0.08 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.6, 150.1, 149.4, 137.9, 132.3, 129.9, 127.4, 127.1, 126.7, 124.0, 123.9-112.7 (m), 120.6, 113.2, 112.9, 112.4, 68.6 (t, *J* = 1.5 Hz), 56.1, 41.5 (t, *J* = 19.9), 40.9, 40.7, 0.1;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.87 to -88.89 (m, 2F), -114.56 to -115.36 (m, 1F), -117.70 to -118.50 (m, 1F);

IR (film) 2956, 2804, 1614, 1522, 1503, 1345, 1261, 1219, 1185, 1169, 1103, 1044, 918, 839, 773, 748, 693 cm^{-1};

HRMS (ESI) calcd for $C_{22}H_{29}F_4NO_3Si$ $[M+H]^+$ m/z = 460.1926; found: 460.1915.



3,3,4,4-Tetrafluoro-4-(2-methoxyphenoxy)-1-(4-phenoxyphenyl)butan-1-ol (12): Compound **12** was synthesized following the general procedure (standard-scale), using 1-(2-

bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **12** was obtained as a colorless liquid (78 mg, 89% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (37:13) to hexane/EtOAc (18:7).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.41 (d, J = 8.0 Hz, 2H), 7.34 (t, J = 7.6 Hz, 2H), 7.27-7.22 (m, 2H), 7.11 (t, J = 7.6 Hz, 1H), 7.03-6.92 (m, 6H), 5.31 (dt, J = 8.8, 3.2 Hz, 1H), 3.84 (s, 3H), 2.82-2.54 (m, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 157.2, 157.1, 152.2, 138.1, 137.7, 129.9, 127.7, 127.3, 123.8, 123.5, 120.8, 119.0, 118.0-115.0 (m), 112.8, 67.8 (t, J = 4.0 Hz), 56.1, 41.4 (t, J = 20.3 Hz);

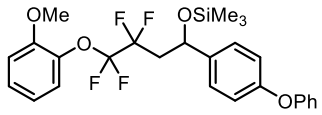
^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.03 to -88.84 (m, 2F), -113.62 to -114.41 (m, 1F), -114.70 to -115.49 (m, 1F);

IR (film) 3430, 2926, 1589, 1503, 1489, 1237, 1189, 1169, 1108, 870, 749, 692 cm^{-1};

HRMS (ESI) calcd for $C_{23}H_{20}F_4O_4$ $[M+Na]^+$ m/z = 459.1190; found: 459.1183.

Using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), triethyl(vinyloxy)silane (**2.2**) (63.3 mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **12** was obtained as a colorless liquid (51 mg, 58% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (37:13) to hexane/EtOAc (18:7).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.41 (d, J = 8.4 Hz, 2H), 7.34 (t, J = 7.6 Hz, 2H), 7.27-7.22 (m, 3H), 7.11 (t, J = 7.6 Hz, 1H), 7.03-6.92 (m, 5H), 5.31 (dt, J = 9.2, 3.0 Hz, 1H), 3.84 (s, 3H), 2.82-2.53 (m, 3H). Spectral data matched with compound **12**.



Trimethyl(3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)-1-(4-phenoxyphenyl)butoxy)silane (13): Compound **13** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene

(60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **13** was obtained as a colorless liquid (61 mg, 60% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (41:9) to hexane/EtOAc (4:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.36-7.32 (m, 4H), 7.24-7.20 (m, 2H), 7.11 (tt, J =7.2, 1.2 Hz, 1H), 7.03-6.90 (m, 6H), 5.23 (dd, J = 8.8, 3.6 Hz, 1H), 3.82 (s, 3H), 2.74-2.60 (m, 1H), 2.57-2.43 (m, 1H), 0.07 (s, 9H);

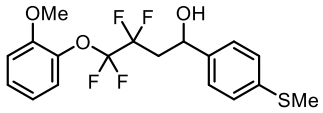
Commented [DS1]: Updated NMR

^{13}C NMR (100 MHz, $CDCl_3$) δ = 157.3, 156.7, 152.5, 139.4, 137.9, 129.8, 127.5, 127.3, 124.0, 123.4, 120.7, 119.0, 118.8, 118.2-113.5 (m), 112.9, 68.5 (J = 2.7 Hz), 56.0, 41.7 (t, J = 20.2 Hz), 0.1;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.84 (s, 2F), -114.49 to -115.28 (m, 1F), -117.39 to -118.18 (m, 1F)

IR (film) 2958, 1589, 1503, 1484, 1235, 1168, 1095, 918, 839, 747, 691 cm^{-1};

HRMS (ESI) calcd for $C_{26}H_{28}F_4O_4Si$ $[M+Na]^+$ m/z = 531.1585; found: 531.1581.



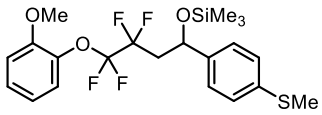
3,3,4,4-Tetrafluoro-4-(2-methoxyphenoxy)-1-(4-(methylthio)phenyl)butan-1-ol (14): Compound **14** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-(methylthio)phenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **14** was obtained as a colorless liquid (71 mg, 91% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (77:23) to hexane/EtOAc (19:6).

^{1}H NMR (400 MHz, $CDCl_3$) δ =7.34 (d, J = 8.4 Hz, 2H), 7.29-7.21 (m, 4H), 6.98-6.92 (m, 2H), 5.28 (dt, J = 9.2, 2.8 Hz, 1H), 3.83 (s, 3H), 2.79-2.54 (s, 3H), 2.49 (s, 3H);

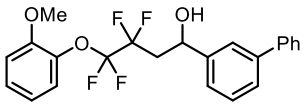
^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.2, 140.2, 138.3, 137.7, 127.6, 126.9, 126.3, 123.8, 120.8, 120.4-114.2 (m), 112.8, 67.8 (t, J = 4.0 Hz), 56.1, 41.3 (t, J = 20.5 Hz), 16.0;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.04 to -88.86 (m, 2F), -113.58 to -114.39 (m, 1F), -114.71 to -115.52 (m, 1F);

IR (film) 3432, 2923, 1601, 1501, 1457, 1260, 1186, 1168, 1098, 820, 748, 714 cm^{-1};
HRMS (ESI) calcd for $C_{18}H_{18}F_4O_3S$ $[M+K]^+$ m/z = 429.0544; found: 429.0538.



Trimethyl(3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)-1-(4-(methylthio)phenyl)butoxy)silane (15): Compound **15** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-(methylthio)phenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **15** was obtained as a colorless liquid (63 mg, 68% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (17:3) to hexane/EtOAc (83:17).
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.32 (d, *J* = 8.4 Hz, 2H), 7.25-7.20 (m, 4H), 6.97-6.89 (m, 2H), 5.20 (dd, *J* = 8.8, 3.2 Hz, 1H), 3.80 (s, 3H), 2.71-2.56 (m, 1H), 2.53-2.42 (m, 4H), 0.05 (s, 9H);
^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.5, 141.5, 137.8, 137.7, 127.5, 126.6, 126.4, 124.0, 120.6, 118.9-113.9 (m), 112.8, 68.5 (t, *J* = 3.0 Hz), 56.0, 41.6 (t, *J* = 20.1 Hz), 15.9, 0.1;
^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.87 to -88.89 (m, 2F), -114.46 to -115.27 (m, 1F); -117.44 to -118.24 (m, 1F);
IR (film) 2958, 1601, 1502, 1252, 1187, 1170, 1101, 919, 841, 718, 749 cm^{-1};
HRMS (ESI) calcd for $C_{21}H_{26}F_4O_3SSi$ $[M+K]^+$ m/z = 501.0940; found: 501.0936.



1-([1,1'-Biphenyl]-3-yl)-3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)butan-1-ol (16): Compound **16** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol),

trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and [1,1'-biphenyl]-3-ylmagnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **16** was obtained as a colorless liquid (69 mg, 82% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (77:23) to hexane/EtOAc (3:1).

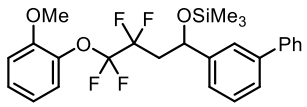
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.67 (t, J = 1.8 Hz, 1H), 7.62-7.60 (m, 2H), 7.55 (dt, J = 7.6, 1.6 Hz, 1H), 7.48-7.41 (m, 4H), 7.36 (tt, J = 7.2, 1.2 Hz, 1H), 7.27-7.21 (m, 2H), 6.98-6.92 (m, 2H), 5.39 (dt, J = 9.2, 2.8 Hz, 1H), 3.82 (s, 3H), 2.86-2.58 (m, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.2, 143.9, 141.8, 141.0, 137.7, 129.2, 128.9, 127.6, 127.5, 127.3, 126.9, 124.7, 124.6, 123.8, 120.8, 120.5-114.2 (m), 112.8, 68.3 (t, J = 4.5 Hz), 56.0, 41.5 (t, J =20.4 Hz),

^{19}F NMR (376 MHz, $CDCl_3$) $\boldsymbol{\delta}$ = -88.00 to -88.82 (m, 2F), -113.48 to -114.28 (m, 1F), -114.65 to -115.46 (m, 1F)

IR (film) 3436, 2946, 1602, 1502, 1261, 1188, 1170, 750, 702 cm^{-1};

HRMS (ESI) calcd for $C_{23}H_{20}F_4O_3$ $[M+Na]^+$ m/z = 443.1241; found: 443.1237.



(1-([1,1'-Biphenyl]-3-yl)-3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)butoxy)trimethylsilane (17): Compound **17** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and [1,1'-biphenyl]-3-ylmagnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **17** was obtained as a colorless liquid (80 mg, 81% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (17:3) to hexane/EtOAc (83:17).

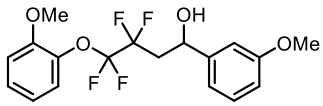
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.64-7.60 (m, 3H), 7.52 (dt, J = 7.2, 1.6 Hz, 1H), 7.47-7.40 (m, 3H), 7.39-7.33 (m, 2H), 7.23-7.20 (m, 2H), 6.97-6.91 (m, 2H), 5.31 (dd, J = 9.2, 3.2 Hz, 1H), 3.78 (s, 3H), 2.78-2.65 (m, 1H), 2.63-2.49 (m, 1H), 0.09 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.5, 145.1, 141.4, 141.1, 137.9, 129.0, 128.9, 127.6, 127.5, 127.2, 126.5, 124.8, 124.6, 124.0, 120.6, 119.3-113.9 (m), 112.8, 69.0 (t, J = 2.9 Hz), 56.0, 41.8 (t, J = 20.2 Hz), 0.1;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.81 to -88.84 (m, 2F), -114.33 to -115.13 (m, 1F), -117.47 to -118.27 (m, 1F);

IR (film) 2957, 1606, 1504, 1261, 1189, 1173, 1110, 1045, 917, 842, 771, 748 cm^{-1};

HRMS (ESI) calcd for $C_{26}H_{28}F_4O_3Si$ $[M+H]^+$ m/z = 493.1817; found: 493.1810.



3,3,4,4-Tetrafluoro-4-(2-methoxyphenoxy)-1-(3-methoxyphenyl)butan-1-ol (18): Compound **18** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (3-methoxyphenyl)magnesium bromide (0.4 mL, 1.0 M solution in THF, 0.4 mmol). The product **18** was obtained as a colorless liquid (51 mg, 68% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (19:6) to hexane/EtOAc (3:1).

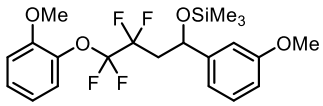
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.32-7.21 (m, 3H), 7.02-6.92 (m, 4H), 6.87-6.84 (m, 1H), 5.29 (dt, J = 9.2, 2.8 Hz, 1H), 3.84 (s, 3H), 3.83 (s, 3H), 2.79-2.53 (m, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 160.0, 152.2, 145.0, 137.7, 129.9, 127.6, 123.8, 120.8, 118.0, 119.3-113.9 (m), 113.6, 112.8, 111.3, 68.1 (t, J = 3.9 Hz), 56.1, 55.4, 41.4 (t, J = 20.4);

^{19}F NMR (376 MHz, $CDCl_3$) $\boldsymbol{\delta}$ = -88.02 to -88.85 (m, 2F), -113.52 to -114.33 (m, 1F), -114.82 to -115.63 (m, 1F);

IR (film) 3451, 2945, 2840, 1602, 1502, 1457, 1260, 1188, 1170, 1106, 1043, 858, 749, 699 cm^{-1};

HRMS (ESI) calcd for $C_{18}H_{18}F_4O_4$ $[M+Na]^+$ m/z = 397.1033; found: 397.1026.



Trimethyl(3,3,4,4-tetrafluoro-4-(2-methoxylphenoxy)-1-(3-methoxyphenyl)butoxy)silane (19): Compound **19** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene

(60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.5 mg, 0.4 mmol) and (3-methoxyphenyl)magnesium bromide (0.4 mL, 1.0 M solution in THF, 0.4 mmol). The product **19** was obtained as a colorless liquid (62 mg, 69% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (87:13) to hexane/EtOAc (43:7).

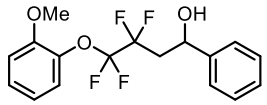
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.28-7.20 (m, 3H), 6.97- 6.89 (m, 4H), 6.83-6.80 (m, 1H), 5.22 (dd, J = 9.2, 3.2 Hz, 1H), 3.82 (s, 3H), 3.80 (s, 3H), 2.71- 2.42 (m, 2H), 0.07 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 159.8, 152.5, 146.3, 137.9, 129.5, 127.5, 124.0, 120.6, 119.0- 113.9 (m), 118.1, 113.1, 112.8, 111.2, 68.8 (t, J = 3.0 Hz), 56.0, 55.3, 41.7 (t, J = 20.0 Hz), 0.1;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.82 to -88.85 (m, 2F), -114.29 to -115.09 (m, 1F), -117.64 to -118.44 (m, 1F);

IR (film) 2958, 1602, 1504, 1262, 1189, 1172, 1109, 1044, 921, 843, 749, 698 cm^{-1};

HRMS (ESI) calcd for $C_{21}H_{26}F_4O_4Si$ $[M+H]^+$ m/z = 447.1609; found: 447.1607.



3,3,4,4-Tetrafluoro-4-(2-methoxyphenoxy)-1-phenylbutan-1-ol (20): Compound **20** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and phenylmagnesium bromide (0.4 mL, 1.0 M solution in THF, 0.4 mmol). The product **20** was obtained as a colorless liquid (61 mg, 89% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (39:11) to hexane/EtOAc (19:6).

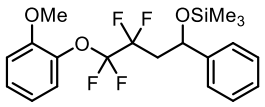
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.46-7.43 (m, 2H), 7.41-7.37 (m, 2H), 7.31 (tt, J =7.2, 1.6 Hz, 1H), 7.26-7.21 (m, 2H), 6.99-6.92 (m, 2H), 5.32 (dt, J = 8.8, 3.2 Hz, 1H), 3.83 (s, 3H), 2.81-2.53 (m, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.2, 143.3, 137.8, 137.7, 128.8, 128.1, 127.6, 125.8, 123.8, 120.8, 120.5-114.3 (m), 112.8, 68.2 (t, J = 3.7 Hz), 56.1, 41.4 (t, J = 20.5 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) $\boldsymbol{\delta}$ = -88.04 to -88.87 (m, 2F), -113.59 to -114.39 (m, 1F), -114.79 to -115.60 (m, 1F);

IR (film) 3426, 2947, 2842, 1604, 1501, 1457, 1260, 1187, 1169, 1103, 853, 748, 699 cm^{-1}

HRMS (ESI) calcd for $C_{17}H_{16}F_4O_3$ $[M+Na]^+$ m/z = 367.0928; found: 367.0926.



Trimethyl(3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)-1-phenylbutoxy)silane (21): Compound **21** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and phenylmagnesium bromide (0.4 mL, 1.0 M solution in THF, 0.4 mmol). The product **21** was obtained as a colorless liquid (53 mg, 64% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (97:3) to hexane/EtOAc (19:5).

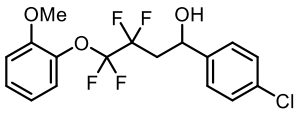
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.39-7.31 (m, 4H), 7.28-7.23 (m, 1H), 7.22-7.17 (m, 2H), 6.95-6.88 (m, 2H), 5.23 (dd, J = 8.8, 3.2 Hz, 1H), 3.78 (s, 3H), 2.72-2.42 (m, 2H), 0.04 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.5, 144.5, 137.9, 128.5, 127.6, 127.5, 125.8, 124.0, 120.6, 119.3-113.9 (m), 112.9, 68.9 (t, J = 3.2 Hz), 56.0, 41.7 (t, J = 20.3 Hz), 0.1;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.85 to -88.88 (m, 2F), -114.43 to -115.24 (m, 1F), -117.55 to -118.35 (m, 1F);

IR (film) 2958, 1503, 1456, 1261, 1251, 1187, 1170, 1105, 1027, 924, 840, 748, 699 cm^{-1};

HRMS (ESI) calcd for $C_{20}H_{24}F_4O_3Si$ $[M+Na]^+$ m/z = 439.1323; found: 439.1317.



1-(4-Chlorophenyl)-3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)butan-1-ol (22): Compound **22** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-chlorophenyl)magnesium bromide (0.4 mL, 1.0 M solution in diethyl ether, 0.4 mmol). The product **22** was obtained as a

colorless liquid (43 mg, 57% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (79:21) to hexane/EtOAc (77:23).

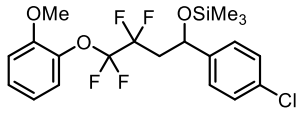
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.39-7.34 (m, 4H), 7.26-7.22 (m, 2H), 6.99-6.92 (m, 2H), 5.30 (dt, J = 8.8, 3.2 Hz, 1H), 3.83 (s, 3H), 2.74-2.52 (m, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.2, 141.8, 137.6, 133.7, 128.9, 127.7, 127.2, 123.8, 120.8, 120.4-114.1 (m), 112.8, 67.6 (t, J = 4.1 Hz), 56.0, 41.5 (t, J = 20.5 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.01 to -88.84 (m, 2F), -113.44 to -114.25 (m, 1F), -114.42 to -115.23 (m, 1F);

IR (film) 3435, 2946, 1603, 1502, 1458, 1261, 1189, 1170, 1108, 1014, 831, 748 cm^{-1};

HRMS (ESI) calcd for $C_{17}H_{15}ClF_4O_3$ $[M+Na]^+$ m/z = 401.0538; found: 401.0534.



(1-(4-Chlorophenyl)-3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)butoxy)trimethylsilane (23): Compound **23** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-chlorophenyl)magnesium bromide (0.4 mL, 1.0 M solution in diethyl ether, 0.4 mmol). The product **23** was obtained as a colorless liquid (69 mg, 76% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (24:1) to hexane/EtOAc (19:1).

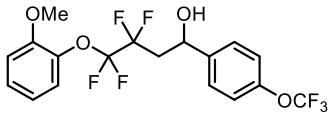
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.33-7.31 (m, 4H), 7.22 (d, J = 7.6 Hz, 2H), 6.97-6.89 (m, 2H), 5.20 (dd, J = 8.8, 3.2 Hz, 1H), 3.80 (s, 3H), 2.69-2.54 (m, 1H), 2.52-2.38 (m, 1H), 0.05 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.5, 143.1, 137.8, 133.3, 128.7, 127.6, 127.2, 124.0, 120.7, 117.7-116.2 (m), 112.9, 68.3 (t, J = 2.8 Hz), 56.0, 41.7 (t, J = 20.1 Hz), 0.0;

^{19}F NMR (376 MHz, $CDCl_3$) $\boldsymbol{\delta}$ = -88.51 to -89.37 (m, 2F), -114.48 to -115.28 (m, 1F), -117.29 to -118.10 (m, 1F);

IR (film) 2958, 1502, 1252, 1187, 1170, 1093, 918, 840, 747 cm^{-1};

HRMS (APCI) calcd for $C_{20}H_{23}ClF_4O_3Si$ $[M+H]^+$ m/z = 451.1114; found: 451.1100



3,3,4,4-Tetrafluoro-4-(2-methoxyphenoxy)-1-(4-(trifluoromethoxy)phenyl)butan-1-ol (24): Compound **24** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-(trifluoromethoxy)phenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **24** was obtained as a colorless liquid (59 mg, 69% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (77:23) to hexane/EtOAc (3:1).

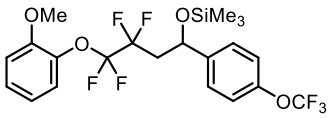
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.50 (d, J = 8.4 Hz, 2H), 7.27-7.23 (m, 4H), 7.01-6.94 (m, 2H), 5.35 (dt, J = 8.8, 2.8 Hz, 1H), 3.84 (s, 3H), 2.80-2.78 (m, 1H), 2.74-2.52 (m, 2H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.1, 148.9 (q, J = 1.9 Hz), 142.0, 137.6, 127.7, 127.3, 123.8, 121.3, 120.9, 120.6 (q, J = 255.4 Hz), 120.4-114.1 (m), 112.8, 67.5 (t, J = 4.0 Hz), 56.0, 41.6 (t, J = 20.7 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -57.89 (s, 3F), -87.95 to -88.82 (m, 2F), -113.41 to -114.22 (m, 1F), -114.33 to -115.14 (m, 1F);

IR (film) 3427, 2949, 2844, 1605, 1503, 1458, 1255, 1158, 1099, 855, 749, 675 cm^{-1};

HRMS (ESI) calcd for $C_{18}H_{15}F_7O_4$ $[M-H]^-$ m/z = 427.0775; found: 427.0785.



Trimethyl(3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)-1-(4-(trifluoromethoxy)phenyl)butoxy)silane (25): Compound **25** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-(trifluoromethoxy)phenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **25** was obtained as a colorless liquid (39 mg, 39% yield) after

purification by flash chromatography on silica gel with hexane/DCM (97:3) to hexane/DCM (19:1).

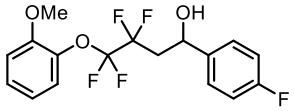
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.43 (d, J = 8.8 Hz, 2H), 7.24-7.19 (m, 4H), 6.98-6.90 (m, 2H), 5.25 (dd, J = 8.8, 3.6 Hz, 1H), 3.80 (s, 3H), 2.71-2.57 (m, 1H), 2.55-2.41 (m, 1H), 0.06 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.5, 148.6 (q, J = 2.1 Hz), 143.3, 137.8, 127.6, 127.2, 124.0, 121.0, 120.7, 120.6 (q, J = 255.3 Hz), 119.2-113.4 (m), 112.9, 68.2 (t, J = 3.2 Hz), 56.0, 41.7 (t, J = 20.3 Hz), 0.0;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -57.88 (s, 3F), -88.86 to -88.89 (m, 2F), -114.47 to -115.27 (m, 1F), -117.29 to -118.09 (m, 1F);

IR (film) 2925, 1504, 1459, 1260, 1219, 921, 844, 772 cm^{-1};

HRMS (ESI) calcd for $C_{21}H_{23}F_7O_4Si$ $[M+Na]^+$ m/z = 523.1146; found: 523.1141.



3,3,4,4-Tetrafluoro-1-(4-fluorophenyl)-4-(2-methoxyphenoxy)butan-1-ol (26): Compound **26** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-fluorophenyl)magnesium bromide (0.4 mL, 1.0 M solution in THF, 0.4 mmol). The product **26** was obtained as a colorless liquid (54 mg, 75% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (83:17) to hexane/EtOAc (81:19).

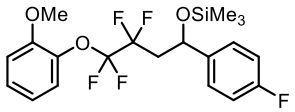
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.44-7.39 (m, 2H), 7.26-7.22 (m, 2 H), 7.07 (tt, J = 8.8, 2.8 Hz, 2H), 6.99-6.92 (m, 2 H), 5.31 (dt, J = 8.8, 3.2 Hz, 1H), 3.83 (s, 3H), 2.79-2.49 (m, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 163.7 (d, J = 244.4 Hz), 152.2, 139.1 (d, J = 3.2 Hz), 137.6, 127.7, 127.5 (d, J = 8.0 Hz), 123.8, 120.8, 120.4-113.8 (m), 115.7 (d, J = 21.3 Hz), 112.8, 67.6 (t, J = 3.9 Hz), 56.0, 41.5 (t, J = 20.5 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.04 to -88.86 (m, 2F), -113.58 to -114.46 (m, 2F), -114.56 to -115.37 (m, 1F);

IR (film) 3422, 2948, 2843, 1605, 1501, 1458, 1261, 1169, 1105, 836, 747 cm^{-1};

HRMS (ESI) calcd for $C_{17}H_{15}F_5O_3$ $[M+Na]^+$ m/z = 385.0834; found: 385.0825.



Trimethyl(3,3,4,4-tetrafluoro-1-(4-fluorophenyl)-4-(2-methoxyphenoxy)butoxy)silane (27): Compound **27** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-fluorophenyl)magnesium bromide (0.4 mL, 1.0 M solution in THF, 0.4 mmol). The product **27** was obtained as a colorless liquid (37 mg, 43% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (21:4) to hexane/EtOAc (83:17).

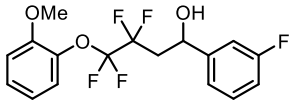
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.38-7.34 (m, 2H), 7.23-7.20 (m, 2H), 7.03 (t, J = 8.8 Hz, 2H), 6.97-6.90 (m, 2H), 5.22 (dd, J = 8.8, 3.2 Hz, 1H), 3.80 (s, 3H), 2.71-2.57 (m, 1H), 2.54-2.40 (m, 1H), 0.05 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 163.5 (d, J = 243.8 Hz), 152.5, 140.4 (d, J = 3.2 Hz), 137.8, 127.6, 127.5 (d, J = 8.1 Hz), 124.0, 120.7, 120.5-113.8 (m), 115.5 (d, J = 21.3 Hz), 112.9, 68.3 (t, J = 3.5 Hz), 56.0, 41.7 (t, J =20.3 Hz), 0.0;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.88 to -88.91 (m, 2F), -114.56 to -115.37 (m, 2F), -117.36 to -118.15 (m, 1F);

IR (film) 2959, 2849, 1735, 1605, 1504, 1219, 1110, 919, 843, 771cm^{-1};

HRMS (ESI) calcd for $C_{20}H_{23}F_5O_3Si$ $[M+H]^+$ m/z = 435.1409; found: 435.1400.



3,3,4,4-Tetrafluoro-1-(3-fluorophenyl)-4-(2-methoxyphenoxy)butan-1-ol (28): Compound **28** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (3-fluorophenyl)magnesium bromide

(0.4 mL, 1.0 M solution in THF, 0.4 mmol). The product **28** was obtained as a colorless liquid (62 mg, 85% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (77:23) to hexane/EtOAc (3:1).

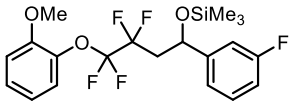
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.37-7.32 (m, 1H), 7.27-7.24 (m, 2H), 7.23-7.17 (m, 2H), 7.02-6.93 (m, 3H), 5.32 (dt, *J* = 8.8, 3.0 Hz, 1H), 3.84 (s, 3H), 2.77-2.76 (m, 1H), 2.73-2.52 (m, 2H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 164.3 (d, *J* = 244.7 Hz), 152.1, 146.0 (d, *J* = 6.9 Hz), 137.6, 130.3 (d, *J* = 8.1 Hz), 127.7, 123.8, 121.3 (d, *J* = 2.9 Hz), 120.8, 120.4-116.3 (m), 114.9 (d, *J* = 21.0 Hz), 112.9 (d, *J* = 22.1 Hz), 112.8, 67.6 (t, *J* = 4.8 Hz), 56.0, 41.5 (t, *J* = 20.5 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -87.97 to -88.82 (m, 2F), -112.41 to -112.47 (m, 1F), -113.30 to -114.11 (m, 1F), -114.40 to -115.22 (m, 1F);

IR (film) 3411, 2934, 2858, 1593, 1503, 1454, 1261, 1189, 1171, 1108, 875, 749, 699 cm^{-1};

HRMS (ESI) calcd for $C_{17}H_{15}F_5O_3$ $[M-H]^-$ m/z = 361.0858; found: 361.0870.



Trimethyl(3,3,4,4-tetrafluoro-1-(3-fluorophenyl)-4-(2-methoxyphenoxy)butoxy)silane (29): Compound **29** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (3-fluorophenyl)magnesium bromide (0.4 mL, 1.0 M solution in THF, 0.4 mmol). The product **29** was obtained as a colorless liquid (52 mg, 60% yield) after purification by flash chromatography on silica gel with hexane to hexane/EtOAc (99:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.33-7.28 (m, 1H), 7.24-7.20 (m, 2H), 7.16-7.11 (m, 2H), 6.99-6.90 (m, 3H), 5.23 (dd, *J* = 8.8, 3.2 Hz, 1H), 3.81 (s, 3H), 2.70-2.41 (m, 2H), 0.07 (s, 9H);

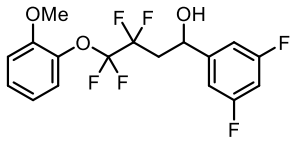
^{13}C NMR (100 MHz, $CDCl_3$) δ = 164.3 (d, *J* = 244.4 Hz), 152.5, 147.4 (d, *J* = 6.6 Hz), 137.8, 130.1 (d, *J* = 8.1 Hz), 127.6, 124.0, 121.4 (d, *J* = 2.9 Hz), 120.7, 120.5-116.3 (m),

114.6 (d, *J* = 21.1 Hz), 112.9 (d, *J* = 22.0 Hz), 112.8, 68.4 (t, *J* = 3.3 Hz), 56.0, 41.7 (t, *J* = 20.2 Hz), 0.0;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.46 to -89.24 (m, 2F), -112.80 to -112.86 (m, 1F), -114.28 to -115.08 (m, 1F), -117.38 to -118.18 (m, 1F);

IR (film) 2958, 1592, 1503, 1252, 1171, 1106, 1027, 918, 840, 747, 693 cm^{-1};

HRMS (APCI) calcd for $C_{20}H_{23}F_5O_3Si$ $[M+H]^+$ m/z = 435.1409; found: 435.1392.



1-(3,5-Difluorophenyl)-3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)butan-1-ol (30): Compound **30** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (3,5-difluorophenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **30** was obtained as a colorless liquid (49 mg, 64% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (77:23) to hexane/EtOAc (37:13).

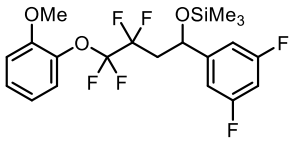
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.56-7.51 (m, 2H), 7.29-7.21(m, 4H), 7.05-6.99 (m, 1H), 5.58 (dt, *J* = 8.8, 3.0 Hz, 1H), 4.12 (s, 3H), 3.19 (s, 1H), 2.98-2.82 (m, 2H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 163.3 (dd, *J* = 247.6, 12.4 Hz), 152.1, 147.3 (t, *J* = 8.6 Hz), 137.5, 127.7, 123.8, 120.9, 120.4-114.0 (m), 112.8, 108.7 (dd, *J* = 18.7, 7.0 Hz), 103.3 (t, *J* = 25.1 Hz), 67.3 (t, *J* = 4.2 Hz), 56.0, 41.8 (t, *J* = 20.8 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -87.91 to -88.79 (m, 2F), -108.95 to -109.34 (m, 2F), -112.95 to -113.77 (m, 1F), -114.10 to -114.91 (m, 1F);

IR (film) 3442, 1625, 1599, 1503, 1262, 1172, 1118, 988, 860, 772 cm^{-1};

HRMS (ESI) calcd for $C_{17}H_{14}F_6O_3$ $[M+Na]^+$ m/z = 403.0739; found: 403.0734.



(1-(3,5-Difluorophenyl)-3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)butoxy)trimethylsilane (31): Compound **31** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (3,5-difluorophenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **31** was obtained as a colorless liquid (63 mg, 70% yield) after purification by flash chromatography on silica gel with hexane to hexane/EtOAc (49:1).

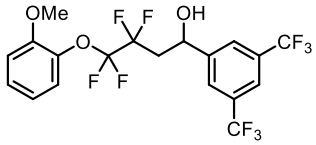
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.25-7.21 (m, 2H), 6.98-6.90 (m, 4H), 6.71 (tt, J =8.8, 2.4 Hz, 1H), 5.20 (dd, J = 8.8, 3.2 Hz, 1H), 3.82 (s, 3H), 2.67-2.40 (m, 2H), 0.08 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 163.2 (dd, J = 247.4, 12.4 Hz), 152.5, 148.9 (t, J =8.2 Hz), 137.8, 127.6, 123.9, 120.7, 120.5-113.0 (m), 112.8, 108.7 (dd, J = 18.5, 6.9 Hz), 103.0 (t, J = 25.1 Hz), 68.1 (t, J = 3.3 Hz), 55.9, 41.7 (t, J = 20.2 Hz), -0.0;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.43 to -89.24 (m, 2F), -109.27 to -109.31 (m, 2F), -114.03 to -114.83 (m, 1F), -117.24 to -118.04 (m, 1F);

IR (film) 2959, 1625, 1598, 1503, 1458, 1262, 1171, 1117, 989, 844, 749, 686 cm^{-1};

HRMS (APCI) calcd for $C_{20}H_{22}F_6O_3Si$ $[M+H]^+$ m/z = 453.1315; found: 453.1298.



1-(3,5-Bis(trifluoromethyl)phenyl)-3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)butan-1-ol (32): Compound **32** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (3,5-bis(trifluoromethyl)phenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **32** was obtained as a yellowish liquid (80 mg, 83% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (39:11) to hexane/EtOAc (19:6).

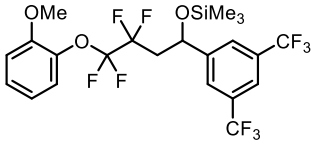
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.93-7.84 (m, 3H), 7.29-7.24 (m, 2H), 7.01-6.94 (m, 2H), 5.47 (dt, *J* = 9.2, 3.0 Hz, 1H), 3.85 (s, 3H), 3.14-3.12 (m, 1H), 2.80-2.54 (m, 2H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.0, 145.8, 137.5, 132.1 (q, *J* = 33.1 Hz), 127.8, 126.1 (q, *J* = 3.2 Hz), 123.7, 123.4 (q, *J* = 271.2 Hz), 121.9 (qu, *J* = 3.7 Hz), 121.0, 120.3-113.9 (m), 112.8, 67.2 (t, *J* = 4.2 Hz), 56.0, 42.0 (t, *J* = 20.4 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -62.84 (s, 6F), -87.83 to -88.72 (m, 2F), -112.61 to -113.42 (m, 1F), -113.55 to -114.36 (m, 1F);

IR (film) 3485, 2950, 1606, 1503, 1369, 1277, 1169, 1124, 900, 749, 682 cm^{-1};

HRMS (ESI) calcd for $C_{19}H_{14}F_{10}O_3$ $[M-H]^-$ m/z = 479.0700; found: 479.0710.



(1-(3,5-Bis(trifluoromethyl)phenyl)-3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)butoxy)trimethylsilane (33): Compound **33** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (3,5-bis(trifluoromethyl)phenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **33** was obtained as a colorless liquid (70 mg, 63% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (99:1) to hexane/EtOAc (49:1).

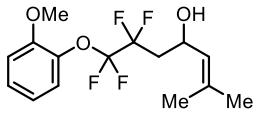
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.88 (s, 2H), 7.81 (s, 1H), 7.24-7.22 (m, 2H), 6.98-6.91 (m, 2H), 5.38 (dd, *J* = 8.8, 3.2 Hz, 1H), 3.80 (s, 3H), 2.73-2.45 (m, 2H), 0.09 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.4, 147.3, 137.7, 132.0 (q, *J* = 33.1 Hz), 127.7, 126.2 (q, *J* = 3.3 Hz), 123.9, 123.4 (q, *J* = 271.1 Hz), 121.7 (qu, *J* = 3.8 Hz), 120.7, 120.4-113.2 (m), 112.8, 68.1 (t, *J* = 3.4 Hz), 56.0, 41.82 (t, *J* = 20.5 Hz), -0.0;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -62.88 (s, 6H), -88.40 to -89.24 (m, 2H), -113.82 to -114.62 (m, 1H), -116.87 to -117.67 (m, 1H);

IR (film) 2960, 1504, 1278, 1172, 1131, 1044, 908, 843, 748, 682 cm^{-1};

HRMS (APCI) calcd for $C_{22}H_{22}F_{10}O_3Si$ $[M+H]^+$ m/z = 553.1251; found: 553.1238.



6,6,7,7-Tetrafluoro-7-(2-methoxyphenoxy)-2-methylhept-2-en-4-ol (34): Compound **34** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (2-methylprop-1-en-1-yl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **34** was obtained as a colorless liquid (23 mg, 35% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (79:21) to hexane/EtOAc (39:11).

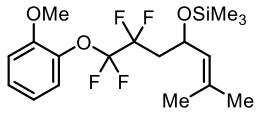
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.28-7.23 (m, 2H), 7.01-6.94 (m, 2H), 5.32 (dt, J = 8.8, 1.4 Hz, 1H), 4.98 (sept, J = 3.2 Hz, 1H), 3.87 (s, 3H), 2.64-2.49 (m, 1H), 2.44-2.30 (m, 1H), 2.13-2.12 (m, 1H), 1.76 (dd, J = 6.4, 1.2 Hz, 6H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.3, 137.8, 135.9, 127.6, 126.6, 123.9, 120.7, 120.5-114.0 (m), 112.8, 63.0 (t, J = 3.7 Hz), 56.1, 39.5 (t, J = 20.3 Hz), 25.8, 18.2;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.29 to -89.09 (m, 2F), -114.93 to -115.05 (m, 2F);

IR (film) 3385, 2935, 2843, 1604, 1503, 1458, 1261, 1172, 1181, 1108, 749 cm^{-1};

HRMS (ESI) calcd for $C_{15}H_{18}F_4O_3$ $[M+NH_4]^+$ m/z = 340.1530; found: 340.1523.



Trimethyl((6,6,7,7-tetrafluoro-7-(2-methoxyphenoxy)-2-methylhept-2-en-4-yl)oxy)silane (35): Compound **35** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (2-methylprop-1-en-1-yl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **35** was obtained as a colorless liquid (8 mg, 10% yield) after purification by flash chromatography on silica gel with hexane to hexane/EtOAc (24:1) to hexane/EtOAc (19:1).

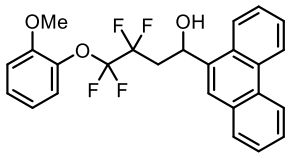
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.25-7.20 (m, 2H), 6.98-6.90 (m, 2H), 5.21 (dd, J = 8.8, 1.2 Hz, 1H), 4.91-4.86 (m, 1H), 3.84 (s, 3H), 2.56-2.41 (m, 1H), 2.35-2.21 (m, 1H), 1.71 (d, J = 8.0 Hz, 6H), 0.11(s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.6, 138.0, 132.8, 128.0, 127.5, 124.0, 120.6, 118.2-114.0 (m), 112.9, 63.7 (t, J = 3.3 Hz), 56.1, 39.4 (t, J = 20.1), 25.8, 18.2, 0.3;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -89.04 to -89.06 (m, 2F), -115.53 to -116.32 (m, 1F), -116.96 to -117.73 (m, 1F);

IR (film) 2960, 1503, 1261, 1186, 1171, 1102, 922, 839, 747 cm^{-1};

HRMS (ESI) calcd for $C_{18}H_{26}F_4O_3Si$ $[M+H]^+$ m/z = 395.1660; found: 395.1655.



3,3,4,4-Tetrafluoro-4-(2-methoxyphenoxy)-1-(phenanthren-9-yl)butan-1-ol (36): Compound **36** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and phenanthren-9-ylmagnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **36** was obtained as a white solid (54 mg, 61% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (83:17) to hexane/EtOAc (41:9).

mp: 89-90 °C

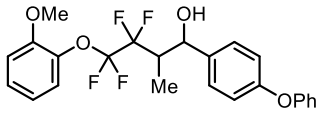
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.95-7.93 (m, 1H), 7.85 (d, J = 8.4 Hz, 1H), 7.32-7.30 (m, 1H), 7.09 (dd, J = 7.6, 1.6 Hz, 1H), 6.87-6.76 (m, 5H), 6.46-6.38 (m, 2H), 6.13-6.09 (m, 2H), 5.28 (dt, J = 9.2, 2.8 Hz, 1H), 2.92 (s, 3H), 2.20-2.19 (m, 1H), 2.12-1.90 (m, 2H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.2, 137.7, 136.9, 131.5, 131.0, 130.2, 129.0, 128.9, 127.6, 127.1, 127.0, 126.5, 124.1, 123.9, 123.6, 123.4, 122.6, 120.8, 120.6-114.6 (m), 112.8, 65.1 (t, J =3.6 Hz), 56.0, 40.9 (t, J = 20.3 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) $\boldsymbol{\delta}$ = -87.65 to -88.72 (s, 2F), -113.37 to -114.18 (m, 1F), -114.26 to -115.07 (m, 1F);

IR (film) 3464, 2930, 2841, 1604, 1501, 1456, 1261, 1188, 1170, 1107, 1025, 746 cm^{-1};

HRMS (ESI) calcd for $C_{25}H_{20}F_4O_3$ $[M-H]^-$ m/z = 443.1265; found: 443.1280.



3,3,4,4-Tetrafluoro-4-(2-methoxyphenoxy)-2-methyl-1-(4-phenoxyphenyl)butan-1-ol (37): Compound **37** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(prop-1-en-1-yloxy)silane (E/Z, 1/1.7) (52.1 mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **37** was obtained as a colorless liquid (14 mg, 15% yield, 3:1 dr,) after purification by flash chromatography on silica gel with hexane/EtOAc (22:3) to hexane/EtOAc (43:7).

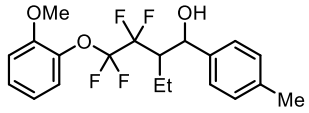
^{1}H NMR (400 MHz, $CDCl_3$, major) δ = 7.41 (d, J = 8.8 Hz, 2H), 7.36-7.29 (m, 3H), 7.27-7.23 (m, 1H), 7.10 (tt, J = 7.6, 0.8 Hz, 1H), 7.02-6.93 (m, 6H), 5.62 (d, J = 4.0 Hz, 1H), 3.84 (s, 3H), 2.74-2.57 (m, 2H), 1.14 (d, J = 7.2 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$, major) δ = 157.4, 156.4, 152.0, 137.6, 137.3, 129.8, 127.6, 127.1, 123.7, 123.3, 122.6-116.4 (m), 120.9, 118.9, 118.7, 112.7, 69.2 (t, J = 4.4 Hz), 56.0, 44.3 (t, J = 19.4 Hz), 5.0;

^{19}F NMR (376 MHz, $CDCl_3$, major) δ = -84.31 to -85.32 (m, 2F), -113.96 to -114.74 (m, 1F), -117.69 to -118.47 (m, 1F);

IR (film) 3524, 2951, 1589, 1504, 1489, 1238, 1170, 1108, 999, 750, 692 cm^{-1};

HRMS (ESI) calcd for $C_{24}H_{22}F_4O_4$ $[M+Na]^+$ m/z = 473.1346; found: 473.1341.



2-Ethyl-3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)-1-(*p*-tolyl)butan-1-ol (38): Compound **38** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), (but-1-en-1-yloxy)trimethylsilane (E/Z, 1/1.5) (57.7 mg, 0.4 mmol) and *p*-tolylmagnesium bromide (0.4

mL, 1.0 M solution in THF, 0.4 mmol). The product **38** was obtained as a colorless liquid (9 mg, 12% yield, 9:1 dr) after purification by flash chromatography on silica gel with hexane to hexane/EtOAc (9:1) to hexane/EtOAc (22:3).

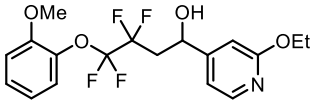
^{1}H NMR (400 MHz, $CDCl_3$, major) δ = 7.36 (d, J = 8.0 Hz, 2H), 7.27-7.23 (m, 2H), 7.18 (d, J = 7.6 Hz, 2H), 7.00-6.94 (m, 2H), 5.61 (d, J = 2.8 Hz, 1H), 3.84 (s, 3H), 2.70 (q, J = 2.0 Hz, 1H), 2.55-2.45 (m, 1H), 2.35 (s, 3H), 1.84-1.72 (m, 2H), 0.74 (t, J = 7.6 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$, major) δ = 151.9, 139.8, 137.7, 136.6, 129.0, 127.6, 125.5, 123.6, 120.9, 118.1-117.3 (m), 112.7, 69.3 (t, J = 3.4 Hz), 56.0, 51.3 (t, J = 18.1 Hz), 21.2, 14.8, 14.2;

^{19}F NMR (376 MHz, $CDCl_3$, major) δ =-84.12 to -84.56 (m, 1F), -85.54 to -85.95 (m, 1F), -109.56 to -110.36 (m, 1F), -116.54 to -117.34 (m, 1F);

IR (film) 3526, 2927, 1503, 1260, 1181, 1171, 1107, 1026, 748 cm^{-1};

HRMS (ESI) calcd for $C_{20}H_{22}F_4O_3$ $[M+Na]^+$ m/z = 409.1397; found: 409.1392.



1-(2-Ethoxypyridin-4-yl)-3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)butan-1-ol (39): Compound **39** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (2-ethoxypyridin-4-yl)magnesium bromide lithium chloride complex (0.54 mL, 0.74 M solution in THF, 0.4 mmol). The product **39** was obtained as a colorless liquid (69.2 mg, 89% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (41:9) to hexane/EtOAc (81:19).

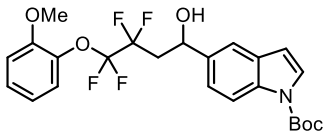
^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.14 (d, J = 5.2 Hz, 1H), 7.27-7.22 (m, 2H), 6.99-6.91 (m, 3H), 6.82 (t, J = 0.8 Hz, 1H), 5.25 (dt, J = 8.8, 3.2 Hz, 1H), 4.36 (q, J = 6.8 Hz, 2H), 3.84 (s, 3H), 2.95 (s, 1H), 2.73-2.51 (m, 2H), 1.39 (t, J = 7.2 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 164.5, 154.9, 152.1, 147.4, 137.6, 127.7, 123.8, 120.9, 120.4-114.1 (m), 113.8, 112.8, 107.8, 66.9 (t, J =4.0 Hz), 61.9, 56.0, 41.3 (t, J = 20.8 Hz), 14.7;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -87.90 to -88.79 (m, 2F), -113.05 to -113.86 (m, 1F), -114.17 to -114.98 (m, 1F);

IR (film) 3265, 2981, 1610, 1561, 1503, 1422, 1382, 1261, 1170, 1107, 1044, 750 cm^{-1};

HRMS (APCI) calcd for $C_{18}H_{19}F_4NO_4$ $[M+H]^+$ m/z = 390.1323; found: 390.1319.



***tert*-Butyl 5-(3,3,4,4-tetrafluoro-1-hydroxy-4-(2-methoxyphenoxy)butyl)-1*H*-indole-1-carboxylate (40)**: Compound **40** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (1-(*tert*-butoxycarbonyl)-1*H*-indol-5-yl)magnesium bromide lithium chloride complex (0.57 mL, 0.7 M solution in THF, 0.4 mmol). The product **40** was obtained as a brownish liquid (50.2 mg, 52% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (21:4) to hexane/EtOAc (83:17).

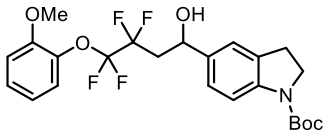
^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.15 (d, J = 8.4 Hz, 1H), 7.65 (d, J = 2.0 Hz, 1H), 7.61 (d, J = 3.6 Hz, 1H), 7.39-7.36 (m, 1H), 7.26-7.21 (m, 2H), 6.98-6.91 (m, 2H), 6.57 (d, J = 3.6 Hz, 1H), 5.41 (dt, J = 9.2, 2.8 Hz, 1H), 3.82 (s, 3H), 2.86-2.57 (m, 3H), 1.67 (s, 9H),

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.3, 149.8, 137.9, 137.7, 134.9, 130.9, 127.6, 126.7, 123.9, 122.1, 120.8, 120.2-114.3 (m), 118.2, 115.5, 112.8, 107.4, 83.9, 68.4 (t, J = 3.4 Hz), 56.1, 41.6 (t, J = 20.4 Hz), 28.3;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.07 to -88.89 (m, 2F), -113.66 to -114.47 (m, 1F), -114.92 to -115.73 (m, 1F);

IR (film) 3466, 2979, 1731, 1502, 1472, 1370, 1259, 1159, 1104, 1023, 852, 749 cm^{-1};

HRMS (ESI) calcd for $C_{24}H_{25}F_4NO_5$ $[M+Na]^+$ m/z = 506.1561; found: 506.1561.



***tert*-Butyl 5-(3,3,4,4-tetrafluoro-1-hydroxy-4-(2-methoxyphenoxy)butyl)indoline-1-carboxylate (41):** Compound **41** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (1-(*tert*-butoxycarbonyl)indolin-5-yl)magnesium bromide lithium chloride complex (0.52 mL, 0.76 M solution in THF, 0.4 mmol). The product **41** was obtained as a colorless liquid (23.3 mg, 24% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (21:4) to hexane/EtOAc (83:17).

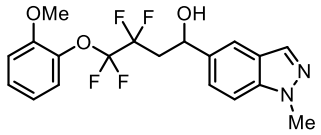
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.26-7.20 (m, 4H), 7.11 (d, J = 7.6 Hz, 1H), 6.99-6.92 (m, 2H), 5.30 (dt, J = 8.8, 2.8 Hz, 1H), 4.00 (t, J = 8.8 Hz, 2H), 3.82 (s, 3H), 3.13 (t, J = 8.6 Hz, 2H), 2.82-2.44 (m, 3H), 1.56 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.6, 152.2, 139.3, 137.7, 128.4, 127.7, 123.8, 120.8, 120.4-114.6 (m), 118.9, 114.3, 112.8, 88.4, 65.9 (t, J = 3.7 Hz), 56.1, 47.8, 40.1 (t, J = 20.4 Hz), 29.8, 28.5;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.03 to -88.88 (m, 2F), -114.87 to -114.92 (m, 2F);

IR (film) 3448, 2927, 1699, 1503, 1464, 1389, 1338, 1261, 1169, 1142, 1109, 854, 750 cm^{-1};

HRMS (ESI) calcd for $C_{24}H_{27}F_4NO_5$ $[M+Na]^+$ m/z = 508.1718; found: 508.1720.



3,3,4,4-Tetrafluoro-4-(2-methoxyphenoxy)-1-(1-methyl-1*H*-indazol-5-yl)butan-1-ol (42): Compound **42** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (1-methyl-1*H*-indazol-5-yl)magnesium bromide lithium chloride complex (0.4 mL, 1.0 M solution in THF, 0.4 mmol). The product

42 was obtained as a yellowish liquid (32.5 mg, 41% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (57:43) to hexane/EtOAc (14:11).

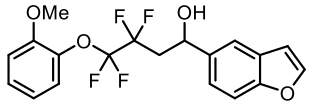
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.97 (s, 1H), 7.79 (d, J = 1.6 Hz, 1H), 7.48 (dd, J = 8.8, 1.6 Hz, 1H), 7.42 (d, J = 8.8 Hz, 1H), 7.26-7.21 (m, 2H), 6.99-6.92 (m, 2H), 5.43 (dd, J = 8.8, 2.8 Hz, 1H), 4.08 (s, 3H), 3.82 (s, 3H), 2.87-2.57 (m, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.2, 139.8, 137.7, 135.8, 133.0, 127.6, 124.6, 124.0, 123.8, 120.8, 120.5-115.0 (m), 118.2, 112.8, 109.5, 68.4 (t, J = 3.5 Hz), 56.1, 41.6 (t, J = 20.3 Hz), 35.7;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.05 to -88.87 (m, 2F), -113.71 to -114.51 (m, 1F), -114.73 to -115.53 (m, 1F);

IR (film) 3342, 2943, 1604, 1503, 1262, 1189, 1171, 1107, 751 cm^{-1};

HRMS (ESI) calcd for $C_{19}H_{18}F_4N_2O_3$ $[M+H]^+$ m/z = 399.1326; found: 399.1324.



1-(Benzofuran-5-yl)-3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)butan-1-ol (43): Compound **43** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and benzofuran-5-ylmagnesium bromide lithium chloride complex (0.48 mL, 0.82 M solution in THF, 0.4 mmol). The product **43** was obtained as a yellowish liquid (52.9 mg, 69% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (77:23) to hexane/EtOAc (19:6).

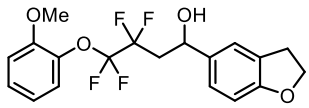
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.69 (d, J = 1.6 Hz, 1H), 7.65 (d, J = 2.4 Hz, 1H), 7.52 (d, J = 8.4 Hz, 1H), 7.37 (dd, J = 8.8, 2.0 Hz, 1H), 7.26-7.21 (m, 2H), 6.99-6.92 (m, 2H), 6.77 (dd, J = 2.4, 1.2 Hz, 1H), 5.42 (dd, J = 9.2, 2.8 Hz, 1H), 3.83 (s, 3H), 2.86-2.57 (m, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 154.7, 152.3, 145.8, 138.2, 137.7, 127.7, 127.6, 123.9, 122.2, 120.8, 120.5-116.8 (m), 118.5, 112.8, 111.7, 106.8, 68.4 (t, J = 3.6 Hz), 56.1, 41.8 (t, J = 20.3 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.05 to -88.86 (m, 2F), -113.68 to -114.49 (m, 1F), -114.81 to -115.61 (m, 1F);

IR (film) 3420, 2922, 1604, 1502, 1466, 1260, 1169, 1100, 1027, 742 cm^{-1};

HRMS (ESI) calcd for $C_{19}H_{16}F_4O_4$ $[M+Na]^+$ m/z = 407.0877; found: 407.0870.



1-(2,3-Dihydrobenzofuran-5-yl)-3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)butan-1-ol (44): Compound **44** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (2,3-dihydrobenzofuran-5-yl)magnesium bromide (0.49 mL, 0.81 M solution in THF, 0.4 mmol). The product **44** was obtained as a yellowish liquid (48.6 mg, 63% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (41:9) to hexane/EtOAc (81:19).

Commented [DS2]: Updated NMR

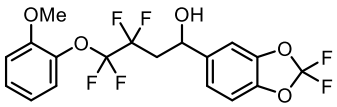
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.29-7.21 (m, 3H), 7.15 (dd, J = 8.0, 2.0 Hz, 1H), 6.99-6.92 (m, 2H), 6.78 (d, J = 8.0 Hz, 1H), 5.24 (dd, J = 9.2, 3.2 Hz, 1H), 4.58 (t, J = 8.6 Hz, 2H), 3.83 (s, 3H), 3.21 (t, J = 8.6 Hz, 2H), 2.80-2.49 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 160.0, 152.3, 137.7, 135.6, 127.6, 125.8, 123.9, 122.6, 120.8, 120.5-113.9 (m), 112.8, 109.3, 71.5, 68.1 (t, J = 3.5 Hz), 56.1, 41.3 (t, J = 20.3 Hz), 29.8;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.09 to -88.89 (m, 2F), -113.83 to -115.76 (m, 2F);

IR (film) 3447, 2963, 1604, 1503, 1261, 1189, 1171, 1107, 982, 751 cm^{-1};

HRMS (ESI) calcd for $C_{19}H_{18}F_4O_4$ $[M+Na]^+$ m/z = 409.1033; found: 409.1030.



1-(2,2-Difluorobenzo[*d*][1,3]dioxol-5-yl)-3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)butan-1-ol (45): Compound **45** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (2,2-

difluorobenzo[*d*][1,3]dioxol-5-yl)magnesium bromide (0.34 mL, 1.17 M solution in THF, 0.4 mmol). The product **45** was obtained as a colorless liquid (56.8 mg, 67% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (21:4) to hexane/EtOAc (83:17).

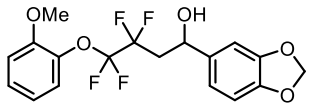
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.26-7.20 (m, 3H), 7.12 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.04 (d, *J* = 8.4 Hz, 1H), 6.99-6.92 (m, 2H), 5.30 (dt, *J* = 8.8, 2.8 Hz, 1H), 3.83 (s, 3H), 2.82 (bs, 1H), 2.76-2.47 (m, 2H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.1, 144.2, 143.3, 139.7, 137.6, 131.8 (t, *J* = 253.7 Hz), 127.7, 123.8, 121.0, 120.9, 120.4-114.0 (m), 112.8, 109.4, 107.3, 67.8 (t, *J* = 4.1 Hz), 56.1, 41.9 (t, *J* = 20.6 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -49.72 to -50.26 (m, 2F), -87.99 to -88.83 (m, 2F), -113.36 to -114.18 (m, 1F), -114.22 to -115.03 (m, 1F);

IR (film) 3434, 2844, 1605, 1501, 1449, 1239, 1169, 1107, 1033, 750, 704 cm^{-1};

HRMS (APCI) calcd for $C_{18}H_{14}F_6O_5$ $[M-H]^-$ m/z = 423.0662; found: 423.0676.



1-(Benzo[*d*][1,3]dioxol-5-yl)-3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)butan-1-ol (46): Compound **46** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and benzo[*d*][1,3]dioxol-5-ylmagnesium bromide (0.43 mL, 0.93 M solution in THF, 0.4 mmol). The product **46** was obtained as a colorless liquid (47.3 mg, 61% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (21:4) to hexane/EtOAc (83:17).

Commented [DS3]: Updated NMR

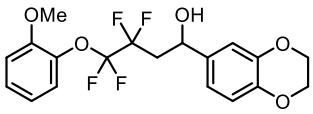
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.26-7.21 (m, 2H), 6.99-6.87 (m, 4H), 6.81 (d, *J* = 8.0 Hz, 1H), 5.96 (s, 2H), 5.22 (dt, *J* = 8.8, 2.4 Hz, 1H), 3.84 (s, 3H), 2.77-2.48 (m, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.2, 148.1, 147.4, 137.7, 137.4, 127.6, 123.8, 121.9-114.1 (m), 120.8, 119.2, 112.8, 108.4, 106.4, 101.2, 68.1 (t, *J* = 3.8 Hz), 56.1, 41.4 (t, *J* = 20.5 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.07 to -88.89 (m, 2F), -113.69 to -114.50 (m, 1F), -114.82 to -115.62 (m, 1F);

IR (film) 3429, 2902, 1605, 1502, 1443, 1248, 1169, 1102, 1038, 930, 750 cm^{-1};

HRMS (ESI) calcd for $C_{18}H_{16}F_4O_5$ $[M+Na]^+$ m/z = 411.0826; found: 411.0828.



1-(2,3-Dihydrobenzo[*b*][1,4]dioxin-6-yl)-3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)butan-1-ol (47): Compound **47** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)magnesium bromide (0.44 mL, 0.89 M solution in THF, 0.4 mmol). The product **47** was obtained as a colorless liquid (66.7 mg, 83% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (19:6) to hexane/EtOAc (3:1).

Commented [DS4]: Updated NMR

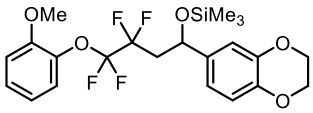
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.26-7.21 (m, 2 H), 6.99-6.85 (m, 5H), 5.20 (dd, J = 8.8, 2.8 Hz, 1H), 4.25 (s, 4H), 3.84 (s, 3H), 2.77-2.49 (m, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.3, 143.7, 143.3, 137.7, 136.8, 127.6, 123.8, 120.8, 120.5-114.2 (m), 118.8, 117.5, 114.8, 112.8, 67.8 (t, J = 3.8 Hz), 64.5, 56.1, 41.2 (t, J = 20.5 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.06 to -88.88 (m, 2F), -113.66 to -114.46 (m, 1F), -114.94 to -115.75 (m, 1F);

IR (film) 3465, 2880, 1592, 1504, 1285, 1260, 1189, 1171, 1106, 1067, 750 cm^{-1};

HRMS (ESI) calcd for $C_{19}H_{18}F_4O_5$ $[M+Na]^+$ m/z = 425.0983; found: 425.0978.



(1-(2,3-Dihydrobenzo[*b*][1,4]dioxin-6-yl)-3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)butoxy)trimethylsilane (48): Compound **48** was synthesized following

the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)magnesium bromide (0.44 mL, 0.89 M solution in THF, 0.4 mmol). The product **48** was obtained as a colorless liquid (73 mg, 77% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (22:3) to hexane/EtOAc (43:7).

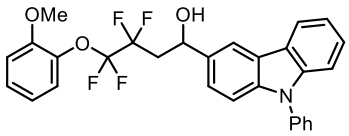
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.23-7.19 (m, 2H), 6.97-6.90 (m, 3H), 6.86-6.81 (m, 2H), 5.13 (dd, *J* = 8.8, 3.2 Hz, 1H), 4.25 (s, 4H), 3.81 (s, 3H), 2.68-2.39 (m, 2H), 0.06 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.5, 143.4, 142.9, 138.0, 137.9, 127.5, 124.0, 120.6, 118.9-113.5 (m), 118.8, 117.2, 114.7, 112.9, 68.4 (t, *J* = 3.1 Hz), 64.5, 64.4, 56.0, 41.7 (t, *J* = 20.1 Hz), 0.1;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.45 to -89.32 (m, 2F), -114.35 to -115.15 (m, 1F), -117.55 to -118.35 (m, 1F);

IR (film) 2957, 1592, 1504, 1285, 1260, 1187, 1172, 1108, 920, 843, 750 cm^{-1};

HRMS (ESI) calcd for $C_{22}H_{26}F_4O_5Si$ $[M+Na]^+$ m/z = 497.1378; found: 497.1369.



3,3,4,4-Tetrafluoro-4-(2-methoxyphenoxy)-1-(9-phenyl-9*H*-carbazol-3-yl)butan-1-ol (49): Compound **49** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (9-phenyl-9*H*-carbazol-3-yl)magnesium bromide (0.57 mL, 0.7 M solution in THF, 0.4 mmol). The product **49** was obtained as a greenish liquid (80.4 mg, 79% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (83:17) to hexane/EtOAc (41:9).

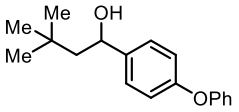
^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.09 (d, *J* = 1.6 Hz, 1H), 8.02 (dt, *J* = 8.0, 0.8 Hz, 1H), 7.49-7.45 (m, 2H), 7.43-7.40 (m, 2H), 7.35-7.32 (m, 2H), 7.28-7.27 (m, 2H), 7.18-7.07 (m, 4H), 6.85-6.78 (m, 2H), 5.39 (dt, *J* = 9.2, 2.4 Hz, 1H), 3.69 (s, 3H), 2.82-2.52 (m, 3H),

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.3, 141.4, 140.7, 137.8, 137.7, 135.2, 130.0, 127.7, 127.6, 127.2, 126.3, 123.93, 123.91, 123.6, 123.3, 120.8, 120.5, 120.2, 119.4-114.3 (m), 117.7, 112.8, 110.1, 110.0, 68.7 (t, J = 3.8 Hz), 56.1, 41.7 (t, J = 20.4 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.03 to -88.83 (m, 2F), -113.61 to -114.42 (m, 1F), -114.92 to -115.73 (m, 1F);

IR (film) 3408, 2840, 1599, 1502, 1457, 1261, 1233, 1189, 1108, 747, 700 cm^{-1};

HRMS (APCI) calcd for $C_{29}H_{23}F_4NO_3$ $[M-H]^-$ m/z = 508.1530; found: 508.1543.



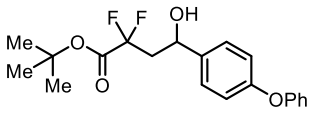
3,3-Dimethyl-1-(4-phenoxyphenyl)butan-1-ol (50): Compound **50** was synthesized following the general procedure (standard-scale), using *tert*-butyl iodide (36.8 mg, 0.2 mmol), trimethyl(vinyloxy)silane (325.8 mg, 2.8 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **50** was obtained as a colorless liquid (40 mg, 74% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (39:11) to hexane/EtOAc (77:23).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.35-7.30 (m, 4H), 7.09 (tt, J = 7.6, 1.0 Hz, 1H), 7.01-6.97 (m, 4H), 4.82 (dd, J = 8.4, 3.6 Hz, 1H), 1.77 (dd, J = 14.4, 8.4 Hz, 1H), 1.65-1.59 (m, 2H), 0.99 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 157.4, 156.5, 141.5, 129.8, 127.3, 123.3, 119.0, 118.9, 72.2, 53.0, 30.6, 30.3;

IR (film) 3395, 2951, 2866, 1589, 1505, 1489, 1237, 1165, 1070, 871, 752, 691 cm^{-1};

HRMS (ESI) calcd for $C_{18}H_{22}O_2$ $[M+Na]^+$ m/z = 293.1512; found: 293.1511.



***tert*-Butyl 2,2-difluoro-4-hydroxy-4-(4-phenoxyphenyl)butanoate (51):** Compound **51** was synthesized following the general procedure (standard-scale), using *tert*-butyl 2-bromo-2,2-difluoroacetate (46.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and

(4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **51** was obtained as a white solid (35 mg, 48% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (17:3) to hexane/EtOAc (83:17).

mp: 90-91 °C;

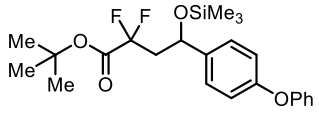
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.36-7.32 (m, 4H), 7.11 (tt, J = 7.2, 1.2 Hz, 1H), 7.01-6.97 (m, 4H), 5.04 (dt, J = 10, 3.2 Hz, 1H), 2.71-2.56 (m, 1H), 2.34 (qd, J = 14.4, 2.8 Hz, 1H), 2.22-2.20 (m, 1H), 1.54 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 163.2 (dd, J = 32.2, 30.6 Hz), 157.3, 157.1, 137.8, 129.9, 127.2, 123.6, , 119.1, 119.0, 115.2 (dd, J = 251.0, 248.3 Hz), 84.7, 68.5 (dd, J = 7.7, 3.7 Hz), 43.8 (t, J = 22.5 Hz), 27.8;

^{19}F NMR (376 MHz, $CDCl_3$) $\boldsymbol{\delta}$ = -101.69 to -102.46 (s, 1F), -106.60 to -107.39 (m, 1F);

IR (film) 3500, 2981, 1750, 1588, 1506, 1488, 1370, 1231, 1160, 1093, 870, 837, 748, 692 cm^{-1};

HRMS (ESI) calcd for $C_{20}H_{22}F_2O_4$ $[M+Na]^+$ m/z = 387.1378; found: 387.1373.

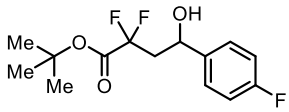


***tert*-Butyl 2,2-difluoro-4-(4-phenoxyphenyl)-4-((trimethylsilyl)oxy)butanoate (52):** Compound **52** was synthesized following the general procedure (standard-scale), using *tert*-butyl 2-bromo-2,2-difluoroacetate (46.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **52** was obtained as a colorless liquid (21 mg, 24% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (99:1) to hexane/EtOAc (49:1).

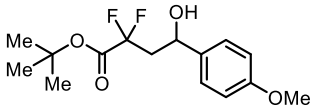
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.35-7.31 (m, 2H), 7.28-7.26 (m, 2H), 7.10 (tt, J = 7.6, 1.2 Hz, 1H), 7.01-6.95 (m, 4H), 4.96 (dd, J = 9.6, 3.6 Hz, 1H), 2.69-2.55 (m, 1H), 2.32-2.20 (m, 1H), 1.53 (s, 9H), -0.00 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 162.8 (dd, J = 33.0, 31.2 Hz), 157.2, 156.8, 138.9, 129.9, 127.4, 123.4, 119.0, 118.8, 114.9 (dd, J = 250.7, 246.8 Hz), 84.0, 69.3 (dd, J = 7.4, 4.1 Hz), 44.8 (t, J = 21.9 Hz), 28.0, 0.0;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -101.82 to -102.59 (m, 1F), -107.83 to -108.62 (m, 1F);
IR (film) 2979, 1768, 1590, 1505, 1489, 1370, 1237, 1119, 1093, 842, 751, 692 cm^{-1};
HRMS (ESI) calcd for $C_{23}H_{30}F_2O_4Si$ $[M+Na]^+$ m/z = 459.1774; found: 459.1770.



***tert*-Butyl 2,2-difluoro-4-(4-fluorophenyl)-4-hydroxybutanoate (53):** Compound **53** was synthesized following the general procedure (standard-scale), using *tert*-butyl 2-bromo-2,2-difluoroacetate (46.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-fluorophenyl)magnesium bromide (0.4 mL, 1.0 M solution in THF, 0.4 mmol). The product **53** was obtained as a colorless liquid (21.6 mg, 37% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (3:1) to hexane/EtOAc (73:27).
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.36-7.32 (m, 2H), 7.07-7.02 (m, 2H), 5.04 (dd, *J* = 10.0, 2.8 Hz, 1H), 2.67-2.52 (m, 1H), 2.37-2.26 (m, 2H), 1.54 (s, 9H);
^{13}C NMR (100 MHz, $CDCl_3$) δ = 163.8 (d, *J* = 244.9 Hz), 163.2 (dd, *J* = 32.3, 30.9 Hz), 138.8 (d, *J* = 3.0 Hz), 127.5 (d, *J* = 8.2 Hz), 115.8 (d, *J* = 21.5 Hz), 115.1 (dd, *J* = 250.6, 248.6 Hz), 84.8, 68.3 (dd, *J* = 7.6, 3.7 Hz), 43.9 (t, *J* = 22.5 Hz), 27.8;
^{19}F NMR (376 MHz, $CDCl_3$) δ = -101.75 to -102.51 (m, 1F), -106.52 to -107.32 (m, 1F), -114.13 to -114.20 (m, 1F);
IR (film) 3487, 2983, 1751, 1605, 1510, 1371, 1224, 1157, 1114, 1089, 836, 748, 652 cm^{-1};
HRMS (APCI) calcd for $C_{14}H_{17}F_3O_3$ $[M-H]^-$ m/z = 289.1046; found: 289.1057.



***tert*-Butyl 2,2-difluoro-4-hydroxy-4-(4-methoxyphenyl)butanoate (54):**
Compound **54** was synthesized following the general procedure (standard-scale), using *tert*-butyl 2-bromo-2,2-difluoroacetate (46.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-methoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **54** was obtained as a colorless liquid (15.9 mg, 23% yield) after

purification by flash chromatography on silica gel with hexane/EtOAc (73:27) to hexane/EtOAc (18:7).

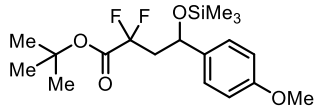
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.30 (d, J = 8.8 Hz, 2H), 6.90 (d, J = 8.4 Hz, 2H), 4.99 (dd, J =10.0, 2.8 Hz, 1H), 3.80 (s, 3H), 2.70-2.55 (m, 1H), 2.32 (qd, J = 14.4, 2.8 Hz, 1H), 2.10 (bs, 1H), 1.53 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 163.2 (dd, J = 32.3, 30.9 Hz), 159.5, 135.2, 127.0, 115.3 (dd, J = 250.6, 248.0 Hz), 114.2, 84.6, 68.5 (dd, J = 7.7, 3.7 Hz), 55.4, 43.8 (t, J = 22.4 Hz), 27.8;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -101.70 to -102.46 (m, 1F), -106.66 to -107.45 (m, 1F);

IR (film) 3502, 2981, 1752, 1612, 1513, 1370, 1248, 1161, 1099, 1034, 834, 749, 651 cm^{-1};

HRMS (APCI) calcd for $C_{15}H_{20}F_2O_4$ $[M-H]^-$ m/z = 301.1246; found: 301.1255.



***tert*-Butyl 2,2-difluoro-4-(4-methoxyphenyl)-4-((trimethylsilyl)oxy)butanoate (55):** Compound **55** was synthesized following the general procedure (standard-scale), using *tert*-butyl 2-bromo-2,2-difluoroacetate (46.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-methoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **55** was obtained as a colorless liquid (17.2 mg, 23% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (93:7) to hexane/EtOAc (23:2).

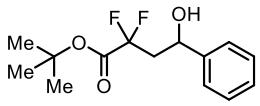
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.24 (d, J = 8.8 Hz, 2H), 6.86 (d, J = 8.8 Hz, 2H), 4.92 (dd, J = 9.6, 4.0 Hz, 1H), 3.80 (s, 3H), 2.68-2.54 (m, 1H), 2.29-2.17 (m, 1H), 1.52 (s, 9H), -0.02 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 162.8 (dd, J = 33.1, 30.9 Hz), 159.2, 136.2, 127.1, 115.0 (dd, J = 250.9, 246.7 Hz), 113.8, 83.9, 69.4 (dd, J = 7.5, 4.0 Hz), 55.3, 44.8 (t, J = 22.0 Hz), 28.0, 0.0;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -101.85 to -102.62 (m, 1F), -107.82 to -108.61 (m, 1F);

IR (film) 2957, 1768, 1613, 1513, 1370, 1250, 1121, 1095, 842, 772 cm^{-1};

HRMS (ESI) calcd for $C_{18}H_{28}F_2O_4Si$ $[M+Na]^+$ m/z = 397.1617; found: 397.1614.



***tert*-Butyl 2,2-difluoro-4-hydroxy-4-phenylbutanoate (56):**

Compound **56** was synthesized following the general procedure (standard-scale), using *tert*-butyl 2-bromo-2,2-difluoroacetate (46.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and phenylmagnesium bromide (0.4 mL, 1.0 M solution in THF, 0.4 mmol). The product **56** was obtained as a colorless liquid (28.3 mg, 52% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (87:13) to hexane/EtOAc (43:7).

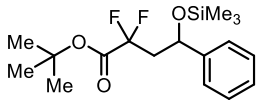
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.37-7.29 (m, 5H), 5.05 (dd, J = 10.4, 2.4 Hz, 1H), 2.70-2.56 (m, 1H), 2.40-2.29 (m, 1H), 2.17 (bs, 1H), 1.54 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 163.2 (dd, J = 32.4, 30.6 Hz), 143.0, 128.8, 128.2, 125.7, 115.2 (dd, J = 250.5, 248.3 Hz), 84.7, 68.9 (dd, J = 7.8, 3.7 Hz), 43.8 (t, J = 22.4 Hz), 27.8;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -101.71 to -102.47 (m, 1F), -106.63 to -107.42 (m, 1F);

IR (film) 3511, 2982, 1752, 1370, 1230, 1161, 1105, 1086, 837, 700 cm^{-1};

HRMS (ESI) calcd for $C_{14}H_{18}F_2O_3$ $[M+H]^+$ m/z = 273.1297; found: 273.1291.



***tert*-Butyl 2,2-difluoro-4-phenyl-4-((trimethylsilyl)oxy)butanoate (57):**

Compound **57** was synthesized following the general procedure (standard-scale), using *tert*-butyl 2-bromo-2,2-difluoroacetate (46.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and phenylmagnesium bromide (0.4 mL, 1.0 M solution in THF, 0.4 mmol). The product **57** was obtained as a colorless liquid (26.8 mg, 39% yield) after purification by flash chromatography on silica gel with hexane to hexane/EtOAc (99:1).

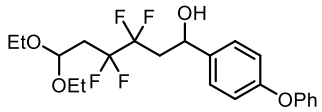
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.35-7.24 (m, 5H), 4.94 (dd, J = 9.6, 3.6 Hz, 1H), 2.69-2.55 (m, 1H), 2.32-2.20 (m, 1H), 1.52 (s, 9H), -0.01 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 162.8 (dd, J = 33.1, 31.5 Hz), 144.1, 128.5, 127.8, 125.9, 115.0 (dd, J = 250.9, 246.6 Hz), 84.0, 69.8 (dd, J = 7.4, 3.9 Hz), 44.7 (t, J = 22.1 Hz), 28.0, 0.0;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -101.86 to -102.64 (m, 1F), -107.85 to -108.64 (m, 1F),

IR (film) 2929, 2157, 1972, 1767, 1370, 1164, 1119, 842, 700 cm^{-1};

HRMS (ESI) calcd for $C_{17}H_{26}F_2O_3Si$ $[M+H]^+$ m/z = 345.1692; found: 345.1686.



6,6-Diethoxy-3,3,4,4-tetrafluoro-1-(4-phenoxyphenyl)hexan-1-ol (58): Compound **58** was synthesized following the general procedure (standard-scale), using 1-bromo-4,4-diethoxy-1,1,2,2-tetrafluorobutane (59.4 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **58** was obtained as a colorless liquid (62 mg, 72% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (21:4) to hexane/EtOAc (41:9).

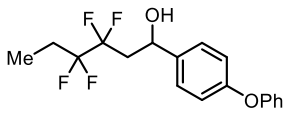
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.37-7.31 (m, 4H), 7.11 (tt, J = 7.2, 1.2 Hz, 1H), 7.02-6.98 (m, 4H), 5.18 (dt, J = 8.8, 3.2 Hz, 1H), 4.91 (t, J = 5.2 Hz, 1H), 3.67 (dq, J = 9.2, 7.2 Hz, 2H), 3.55 (dq, J = 9.6, 7.2 Hz, 2H), 2.62-2.31 (m, 4H), 2.25-2.23 (m, 1H); 1.21 (t, J = 7.2 Hz, 6H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 157.2, 157.1, 138.0, 129.9, 127.3, 123.5, 121.4-114.9 (m), 119.1, 119.0, 97.4 (t, J = 3.5 Hz), 68.0 (t, J = 3.4 Hz), 61.78, 61.76, 39.1 (t, J = 20.6 Hz), 34.7 (t, J =21.2 Hz), 15.2;

^{19}F NMR (376 MHz, $CDCl_3$) $\boldsymbol{\delta}$ = -112.80 to -113.64 (1F), -114.16 to -115.26 (3F);

IR (film) 3447, 2978, 2899, 1590, 1507, 1488, 1376, 1234, 1167, 1091, 870, 751, 692 cm^{-1};

HRMS (ESI) calcd for $C_{22}H_{26}F_4O_4$ $[M+Na]^+$ m/z = 453.1659; found: 453.1650.



3,3,4,4-Tetrafluoro-1-(4-phenoxyphenyl)hexan-1-ol (59): Compound **59** was synthesized following the general procedure (standard-scale), using 1-bromo-1,1,2,2-tetrafluorobutane (41.7 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **59** was obtained as a colorless liquid (47 mg, 69% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (9:1) to hexane/EtOAc (22:3).

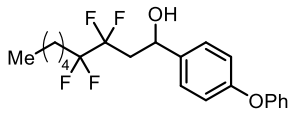
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.37-7.32 (m, 4H), 7.11 (tt, J = 7.6, 1.2 Hz, 1H), 7.02-6.99 (m, 4H), 5.20 (dd, J = 9.2, 3.2 Hz, 1H), 2.62-2.31 (m, 2H), 2.13-1.98 (m, 3H), 1.1 (t, J = 7.2 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 157.2, 157.1, 138.1, 129.9, 127.3, 123.5, 121.7-116.4 (m), 119.1, 119.0, 68.1 (t, J = 3.5 Hz), 39.5 (t, J = 20.6 Hz), 23.3 (t, J = 23.5 Hz), 4.9 (t, J = 4.7 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) $\boldsymbol{\delta}$ = -112.67 to -113.51 (s, 1F), -114.33 to -115.16 (m, 1F), -117.32 to -117.45 (m, 2F);

IR (film) 3405, 2951, 1590, 1507, 1489, 1237, 1170, 1092, 1003, 871, 692 cm^{-1};

HRMS (ESI) calcd for $C_{18}H_{18}F_4O_2$ $[M-H]^-$ m/z = 341.1159; found: 341.1166.



3,3,4,4-Tetrafluoro-1-(4-phenoxyphenyl)nonan-1-ol (60): Compound **60** was synthesized following the general procedure (standard-scale), using 1-bromo-1,1,2,2-tetrafluoroheptane (50.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **60** was obtained as a colorless liquid (51 mg, 67% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (9:1) to hexane/EtOAc (22:3).

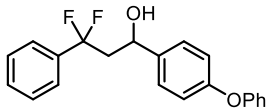
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.38-7.31 (m, 4H), 7.11 (tt, J = 7.2, 1.2 Hz, 1H), 7.02-6.99 (m, 4H), 5.20 (dt, J = 8.8, 3.2 Hz, 1H), 2.62-2.31 (m, 2H), 2.21 (t, J = 2.8 Hz, 1H), 2.06-1.93 (m, 2H), 1.61-1.54 (m, 2H), 1.37-1.32 (m, 4H), 0.93-0.89 (m, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 157.2, 157.1, 138.1, 129.9, 127.3, 123.5, 122.0-116.3 (m), 119.1, 119.0, 68.0 (t, J = 3.2 Hz), 39.4 (t, J = 20.8 Hz), 31.5, 29.8 (t, J = 22.7 Hz), 22.4, 20.2 (t, J = 3.6 Hz), 13.9;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -112.70 to -113.49 (m, 1F), -114.33 to -115.15 (m, 1F), -115.36 to -115.49 (m, 2F);

IR (film) 3395, 2957, 2873, 1590, 1507, 1488, 1234, 1167, 1091, 1034, 870, 750, 691 cm^{-1};

HRMS (ESI) calcd for $C_{21}H_{24}F_4O_2$ $[M-H]^-$ m/z = 383.1629; found: 383.1644.



3,3-Difluoro-1-(4-phenoxyphenyl)-3-phenylpropan-1-ol (61): Compound **61** was synthesized following the general procedure (standard-scale), using (bromodifluoromethyl)benzene (41.4 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and ((4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **61** was obtained as a colorless liquid (27 mg, 40% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (17:3) to hexane/EtOAc (83:17).

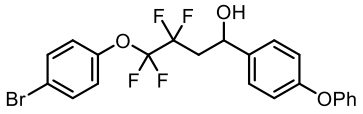
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.53-7.43 (m, 5H), 7.35-7.29 (m, 4H), 7.10 (tt, J = 7.6, 1.2 Hz, 1H), 7.00-6.95 (m, 4H), 4.99 (dt, J = 9.2, 2.6 Hz, 1H), 2.76-2.62 (m, 1H), 2.56-2.49 (m, 1H); 2.26-2.24 (m, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 157.2, 157.0, 138.2, 137.0 (t, J = 25.9 Hz), 130.1 (t, J = 1.9 Hz), 129.8, 128.7, 127.3, 125.0 (t, J = 6.2 Hz), 123.4, 120.2 (t, J = 246.1 Hz), 119.04, 119.02, 69.0 (t, J = 3.6 Hz), 48.4 (t, J = 25.6 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -92.79 to -93.54 (m, 1F), -94.93 to -95.67 (m, 1F);

IR (film) 3423, 2923, 2853, 1589, 1508, 1489, 1238, 1167, 1068, 871, 768, 696 cm^{-1};

HRMS (ESI) calcd for $C_{21}H_{18}F_2O_2$ $[M+NH_4]^+$ m/z = 363.1167; found: 363.1164.



4-(4-Bromophenoxy)-3,3,4,4-tetrafluoro-1-(4-phenoxyphenyl)butan-1-ol (62): Compound **62** was synthesized following the general procedure (standard-scale), using 1-bromo-4-(2-bromo-1,1,2,2-tetrafluoroethoxy)benzene (70.3 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **62** was obtained as a colorless liquid (64 mg, 66% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (43:7) to hexane/EtOAc (21:4).

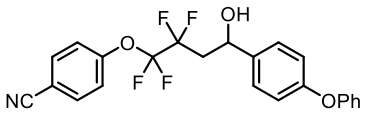
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.51-7.48 (m, 2H), 7.39-7.32 (m, 4H), 7.14-7.07 (m, 3H), 7.03-7.00 (m, 4H), 5.25 (dt, J = 8.8, 3.0 Hz, 1H), 2.76-2.42 (m, 2H), 2.25-2.24 (m, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 157.4, 157.0, 148.1, 137.8, 132.8, 129.9, 129.7, 127.3, 126.6-113.9 (m), 123.7, 123.6, 119.9, 119.1, 119.0, 67.9 (t, J = 3.3 Hz), 40.4 (t, J = 20.5 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) $\boldsymbol{\delta}$ = -88.08 to -88.92 (m, 2F), -115.37 to -116.17 (m, 1F), -116.69 to -117.49 (m, 1F);

IR (film) 3412, 3039, 1589, 1506, 1484, 1233, 1182, 1092, 1066, 1012, 850, 754, 691 cm^{-1};

HRMS (ESI) calcd for $C_{22}H_{17}BrF_4O_3$ $[M-H]^-$ m/z = 483.0213; found: 483.0225.



4-(1,1,2,2-Tetrafluoro-4-hydroxy-4-(4-phenoxyphenyl)butoxy)benzonitrile (63): Compound **63** was synthesized following the general procedure (standard-scale), using 4-(2-bromo-1,1,2,2-tetrafluoroethoxy)benzonitrile (59.6 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **63** was obtained as a colorless liquid (31 mg, 36% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (17:3) to hexane/EtOAc (83:17).

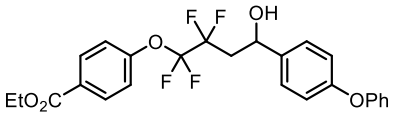
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.72-7.68 (m, 2H), 7.40-7.31 (m, 6H), 7.12 (tt, *J* = 7.2, 1.0 Hz, 1H), 7.04-6.99 (m, 4H), 5.25 (dt, *J* = 8.8, 3.2 Hz, 1H), 2.77-2.41 (m, 2H), 2.22-2.20 (m, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 157.5, 157.0, 152.4, 137.7, 134.1, 129.9, 127.3, 123.7, 122.2, 120.4-113.7 (m), 119.2, 119.0, 117.9, 110.6, 67.9 (t, *J* = 3.0 Hz), 40.2 (t, *J* = 20.6 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.04 to -88.88 (m, 2F), -115.50 to -116.30 (m, 1F), -116.69 to -117.49 (m, 1F);

IR (film) 3457, 3040, 2233, 1589, 1505, 1488, 1234, 1167, 1117, 1097, 867, 692 cm^{-1};

HRMS (ESI) calcd for $C_{23}H_{17}F_4NO_3$ $[M-H]^-$ m/z = 430.1061; found: 430.1073.



Ethyl 4-(1,1,2,2-tetrafluoro-4-hydroxy-4-(4-phenoxyphenyl)butoxy)benzoate (64): Compound **64** was synthesized following the general procedure (standard-scale), using ethyl 4-(2-bromo-1,1,2,2-tetrafluoroethoxy)benzoate (69 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **64** was obtained as a colorless liquid (34 mg, 36% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (81:19) to hexane/EtOAc (4:1).

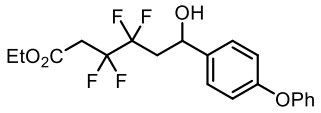
^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.08 (d, *J* = 8.8 Hz, 2H), 7.40-7.32 (m, 4H), 7.27-7.24 (m, 2H), 7.12 (tt, *J* = 7.6, 1.2 Hz, 1H), 7.03-7.00 (m, 4H), 5.26 (dt, *J* = 8.8, 3.2 Hz, 1H), 4.38 (q, *J* = 7.2 Hz, 2H), 2.78-2.63 (m, 1H), 2.58-2.44 (m, 1H), 2.26-2.24 (m, 1H), 1.39 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 165.7, 157.4, 157.0, 152.6, 137.8, 131.5, 129.9, 128.7, 127.3, 123.6, 121.1, 120.3-114.8 (m), 119.1, 119.0, 67.9 (t, *J* = 3.0 Hz), 61.3, 40.3 (t, *J* = 20.6 Hz), 14.4;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.02 to -88.85 (m, 2F), -115.42 to -116.22 (m, 1F), -116.77 to -117.57 (m, 1F);

IR (film) 3482, 2983, 1718, 1606, 1590, 1505, 1488, 1276, 1234, 1164, 1094, 1017, 869, 752, 691 cm^{-1};

HRMS (ESI) calcd for $C_{25}H_{22}F_4O_5$ $[M-H]^-$ m/z = 477.1320; found: 477.1327.



Ethyl 3,3,4,4-tetrafluoro-6-hydroxy-6-(4-phenoxyphenyl)hexanoate (65): Compound **65** was synthesized following the general procedure (standard-scale), using ethyl 4-bromo-3,3,4,4-tetrafluorobutanoate (53.4 mg, 0.2 mmol), trimethyl(vinyloxy)silane (92.9 mg, 0.8 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **65** was obtained as a yellowish liquid (22 mg, 27% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (21:4) to hexane/EtOAc (83:17).

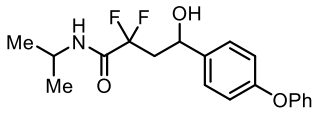
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.36-7.32 (m, 4H), 7.11 (tt, J = 7.2, 1.2 Hz, 1H), 7.02-6.99 (m, 4H), 5.19 (dt, J = 9.2, 3.2 Hz, 1H), 4.23 (q, J = 7.2 Hz, 2H), 3.13-3.03 (m, 2H), 2.65-2.50 (m, 1H), 2.48-2.34 (m, 1H), 2.17-2.16 (m, 1H), 1.29 (t, J = 7.2 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 165.3 (t, J = 2.3 Hz), 157.3, 157.0, 137.9, 129.9, 127.3, 123.6, 121.2-113.8 (m), 119.1, 119.0, 67.9 (t, J = 3.1 Hz), 61.7, 38.8 (t, J = 20.5 Hz), 36.0 (t, J = 22.5 Hz), 14.1;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -111.97 to -112.88 (m, 3F), -113.66 to -114.50 (m, 1F);

IR (film) 3481, 2985, 1744, 1580, 1570, 1489, 1236, 1092, 871, 693 cm^{-1};

HRMS (ESI) calcd for $C_{20}H_{20}F_4O_4$ $[M+Na]^+$ m/z = 423.1190; found: 423.1172.



2,2-Difluoro-4-hydroxy-*N*-isopropyl-4-(4-phenoxyphenyl)butanamide (66):

Compound **66** was synthesized following the general procedure (standard-scale), using 2-bromo-2,2-difluoro-*N*-isopropylacetamide (43.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **66** was obtained as a yellowish liquid (16.7 mg, 24% yield)

after purification by flash chromatography on silica gel with hexane/EtOAc (71:29) to hexane/EtOAc (7:3).

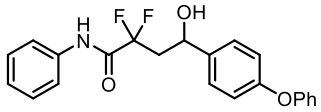
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.35-7.31 (m, 4H), 7.10 (tt, J = 7.2, 1.2 Hz, 1H), 7.01-6.97 (m, 4H), 6.29 (bs, 1H), 5.04 (dd, J =9.6, 2.4 Hz, 1H), 4.12 (oct, J = 6.4 Hz, 1H), 3.38 (bs, 1H), 2.68-2.53 (m, 1H), 2.49-2.37 (m, 1H), 1.24 (d, J = 6.8 Hz, 6H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 164.0 (t, J = 28.3 Hz), 157.2, 157.0, 138.0, 129.9, 127.3, 123.5, 119.0, 116.9 (t, J = 251.8 Hz), 68.3 (dd, J = 7.4, 4.5 Hz), 44.1 (t, J = 22.2 Hz), 42.2, 22.4, 22.3;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -99.25 to -100.02 (m, 1F), -104.38 to -105.17 (m, 1F);

IR (film) 3428, 3330, 2976, 1678, 1589, 1489, 1238, 1198, 1077, 870, 692 cm^{-1};

HRMS (ESI) calcd for $C_{19}H_{21}F_2NO_3$ $[M-H]^-$ m/z = 348.1406; found: 348.1419.



2,2-Difluoro-4-hydroxy-4-(4-phenoxyphenyl)-N-phenylbutanamide (67): Compound **67** was synthesized following the general procedure (standard-scale), using 2-bromo-2,2-difluoro-N-phenylacetamide (50.0 mg, 0.2 mmol), trimethyl(vinyloxy)silane (92.9 mg, 0.8 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **67** was obtained as an amorphous solid (16 mg, 21% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (83:17) to hexane/EtOAc (41:9).

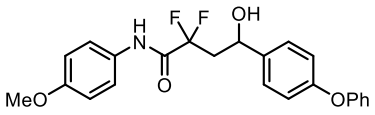
^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.10 (bs, 1H), 7.58-7.56 (m, 2H), 7.40-7.31 (m, 6H), 7.21 (tt, J = 7.6, 1.2 Hz, 1H), 7.11 (tt, J =7.2, 1.2 Hz, 1H), 7.00-6.96 (m, 4H), 5.08 (dt, J = 10, 3.2 Hz, 1H), 2.84-2.69 (m, 2H), 2.59-2.47 (m, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 162.4 (t, J = 28.4 Hz), 157.3, 157.0, 137.6, 136.0, 129.9, 129.3, 127.3, 125.9, 123.6, 120.5, 119.1, 118.9, 117.1 (t, J = 253.0 Hz), 68.5 (dd, J = 6.8, 4.8 Hz), 43.4 (t, J = 22.4 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) $\boldsymbol{\delta}$ = -99.28 to -100.06 (m, 1F), -104.20 to -105.00 (m, 1F);

IR (film) 3410, 3324, 3063, 1690, 1589, 1544, 1506, 1488, 1448, 1236, 1166, 1076, 870, 752, 691 cm^{-1};

HRMS (ESI) calcd for $C_{22}H_{19}F_2NO_3$ $[M+Na]^+$ m/z = 406.1225; found: 406.1218.



2,2-Difluoro-4-hydroxy-*N*-(4-methoxyphenyl)-4-(4-phenoxyphenyl)butanamide (68):
Compound **68** was synthesized following the general procedure (standard-scale), using 2-bromo-2,2-difluoro-*N*-(4-methoxyphenyl)acetamide (56.0 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **68** was obtained as a yellowish solid (21.2 mg, 26% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (71:29) to hexane/EtOAc (70:30).

mp: 128-129 °C

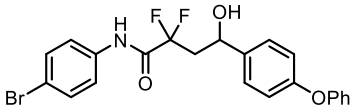
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.98 (bs, 1H), 7.49 (d, *J* = 9.2 Hz, 2H), 7.36-7.31 (m, 4H), 7.11 (tt, *J* = 7.6, 1.2 Hz, 1H), 7.00 (d, *J* = 8.8 Hz, 4H), 6.92 (d, *J* = 9.2 Hz, 2H), 5.09 (dd, *J* =10.0, 2.8 Hz, 1H), 3.81 (s, 3H), 2.82-2.68 (m, 1H), 2.59-2.47 (m, 1H), 1.56 (bs, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 162.3 (t, *J* = 28.1 Hz), 157.5, 157.2, 157.0, 137.7, 129.9, 128.9, 127.3, 123.5, 122.3, 119.1, 119.0, 117.2 (t, *J* = 252.9 Hz), 114.5, 68.5 (dd, *J* = 6.5, 5.4 Hz), 55.6, 43.6 (t, *J* = 22.2 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -99.15 to -99.93 (m, 1F), -103.97 to -104.76 (m, 1F);

IR (film) 3411, 3319, 2922, 1689, 1589, 1511, 1238, 1095, 829, 693 cm^{-1};

HRMS (APCI) calcd for $C_{23}H_{21}F_2NO_4$ $[M-H]^-$ m/z = 412.1355; found: 412.1363.



***N*-(4-Bromophenyl)-2,2-difluoro-4-hydroxy-4-(4-phenoxyphenyl)butanamide (69):**
Compound **69** was synthesized following the general procedure (standard-scale), using 2-bromo-*N*-(4-bromophenyl)-2,2-difluoroacetamide (65.7 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **69** was obtained as a yellowish

solid (17.5 mg, 19% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (83:17) to hexane/EtOAc (41:9).

mp: 111-112 °C

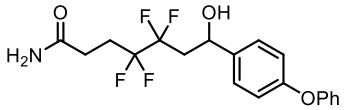
^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.04 (bs, 1H), 7.51-7.46 (m, 4H), 7.36-7.32 (m, 4H), 7.11 (tt, J = 7.2, 1.2 Hz, 1H), 7.00-6.96 (m, 4H), 5.07 (dd, J = 9.6, 2.8 Hz, 1H), 2.85-2.71 (m, 1H), 2.59-2.47 (m, 1H), 1.57 (bs, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 162.4 (t, J = 28.2 Hz), 157.4, 156.9, 137.3, 135.1, 132.4, 129.9, 127.3, 123.6, 122.0, 119.2, 118.9, 118.7, 117.1 (t, J = 252.8 Hz), 68.6 (dd, J = 6.8, 5.1 Hz), 43.2 (t, J = 22.3 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -99.35 to -100.13 (m, 1F), -104.65 to -105.44 (m, 1F);

IR (film) 3415, 3327, 2921, 1697, 1590, 1488, 1400, 1239, 1073, 824, 692 cm^{-1};

HRMS (APCI) calcd for $C_{22}H_{18}BrF_2NO_3$ $[M-H]^-$ m/z = 460.0354; found: 460.0367.



4,4,5,5-Tetrafluoro-7-hydroxy-7-(4-phenoxyphenyl)heptanamide (70):

Compound **70** was synthesized following the general procedure (standard-scale), using 5-bromo-4,4,5,5-tetrafluoropentanamide (50.4 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **70** was obtained as a white solid (52.4 mg, 68% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (1:4) to hexane/EtOAc (19:81).

mp: 75-76 °C

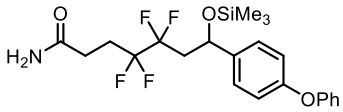
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.35-7.31 (m, 4H), 7.10 (tt, J = 7.2, 1.2 Hz, 1H), 7.01-6.98 (m, 4H), 5.69 (bs, 2H), 5.17 (dd, J = 9.2, 3.2 Hz, 1H), 2.62-2.29 (m, 7H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 173.0, 157.2, 157.1, 138.0, 129.9, 127.3, 123.5, 123.2-116.1 (m), 119.09, 119.05, 67.9 (dd, J = 2.2, 0.8 Hz), 39.3 (t, J = 20.9 Hz), 26.9 (t, J = 3.4 Hz), 25.7 (t, J = 22.4 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -112.72 to -115.04 (m, 2F), -115.50 to -115.62 (m, 2F);

IR (film) 3348, 3204, 2922, 1671, 1589, 1507, 1489, 1237, 1171, 1091, 871, 692 cm^{-1};

HRMS (APCI) calcd for $C_{19}H_{19}F_4NO_3$ $[M-H]^-$ m/z = 384.1217; found: 384.1229.



4,4,5,5-Tetrafluoro-7-(4-phenoxyphenyl)-7-((trimethylsilyl)oxy)heptanamide (71):

Compound **71** was synthesized following the general procedure (standard-scale), using 5-bromo-4,4,5,5-tetrafluoropentanamide (50.4 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **71** was obtained as a white solid (59.4 mg, 65% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (3:2) to hexane/EtOAc (57:43).

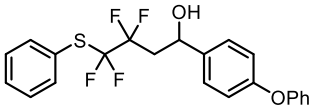
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.35-7.28 (m, 4H), 7.10 (tt, J = 7.6, 0.8 Hz, 1H), 7.02-6.95 (m, 4H), 5.43 (bs, 2H), 5.09 (dd, J = 8.8, 3.6 Hz, 1H), 2.51-2.27 (m, 6H), 0.03 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 173.1, 157.2, 156.7, 139.3, 129.9-112.2 (m), 129.8, 127.2, 123.4, 119.0, 118.8, 68.4 (dd, J = 4.0, 2.0 Hz), 40.4 (t, J = 10.6 Hz), 27.0 (t, J = 2.7 Hz), 25.7 (t, J = 22.7 Hz), 0.0;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -113.09 to -113.92 (m, 1F), -115.01 to -115.92 (m, 3F);

IR (film) 3342, 3199, 2957, 1671, 1589, 1505, 1489, 1367, 1237, 1173, 1092, 911, 842, 751, 692 cm^{-1};

HRMS (ESI) calcd for $C_{22}H_{27}F_4NO_3Si$ $[M+Na]^+$ m/z = 480.1589; found: 480.1582.



3,3,4,4-Tetrafluoro-1-(4-phenoxyphenyl)-4-(phenylthio)butan-1-ol (72):

Compound **72** was synthesized following the general procedure (standard-scale), using (2-bromo-1,1,2,2-tetrafluoroethyl)(phenyl)sulfane (57.8 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **72** was obtained as a yellowish

liquid (65.4 mg, 77% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (17:3) to hexane/EtOAc (21:4).

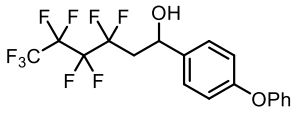
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.66 (d, J = 7.2 Hz, 2H), 7.48 (tt, J = 7.6, 1.2 Hz, 1H), 7.42-7.38 (m, 2H), 7.37-7.33 (m, 4H), 7.12 (tt, J = 7.2, 1.2 Hz, 1H), 7.03-7.00 (m, 4H), 5.21 (dd, J = 8.8, 3.2 Hz, 1H), 2.71-2.56 (m, 1H), 2.52-2.38 (m, 1H), 2.14 (bs, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 157.3, 157.0, 137.8, 137.2, 130.6, 129.9, 129.3, 127.3, 124.6-116.1 (m), 123.6, 119.1, 119.0, 68.0 (t, J = 2.8 Hz), 40.4 (t, J = 20.8 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.64 to -88.66 (m, 2F), -109.42 to -110.23 (m, 1F), -111.17 to -111.98 (m, 1F);

IR (film) 3402, 3062, 1589, 1507, 1488, 1237, 1093, 926, 871, 750, 690 cm^{-1};

HRMS (ESI) calcd for $C_{22}H_{18}F_4O_2S$ $[M-H]^-$ m/z = 421.0880; found: 421.0893.



3,3,4,4,5,5,6,6,6-Nonafluoro-1-(4-phenoxyphenyl)hexan-1-ol (73): Compound **73** was synthesized following the general procedure (standard-scale), using 1-bromo-1,1,2,2,3,3,4,4,4-nonafluorobutane (59.7 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **73** was obtained as a yellowish liquid (29 mg, 34% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (9:1) to hexane/EtOAc (89:11).

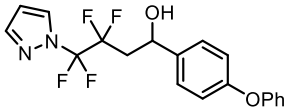
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.37-7.33 (m, 4H), 7.12 (tt, J = 7.2, 1.2 Hz, 1H), 7.03-6.99 (m, 4H), 5.21 (dt, J = 8.8, 3.2 Hz, 1H), 2.71-2.55 (m, 1H), 2.49-2.35 (m, 1H), 2.13-2.12 (m, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 157.6, 156.9, 137.4, 129.9, 127.3, 123.7, 120.3-116.0 (m), 119.2, 119.0, 67.6 (t, J = 3.2 Hz), 39.9 (t, J = 20.5 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -80.97 to -81.04 (m, 3F), -112.23 to -114.43 (m, 2F), -124.47 to -124.55 (m, 2F), -125.80 to -125.90 (m, 2F);

IR (film) 3420, 2924, 2157, 2016, 1591, 1490, 1235, 1134, 871, 754, 692 cm^{-1};

HRMS (ESI) calcd for $C_{18}H_{13}F_9O_2$ $[M-H]^-$ m/z = 431.0688; found: 431.0702.



3,3,4,4-Tetrafluoro-1-(4-phenoxyphenyl)-4-(1H-pyrazol-1-yl)butan-1-ol (74): Compound **74** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethyl)-1H-pyrazole (49.3 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **74** was obtained as a yellowish liquid (35 mg, 46% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (19:6) to hexane/EtOAc (37:13).

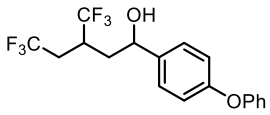
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.83 (d, J = 2.8 Hz, 1H), 7.75 (d, J = 1.6 Hz, 1H), 7.36-7.31 (m, 4H), 7.11 (tt, J = 7.2, 1.2 Hz, 1H), 7.02-6.97 (m, 4H), 6.46 (t, J = 2.0 Hz, 1H), 5.18 (dt, J = 8.8, 3.2 Hz, 1H), 2.76-2.48 (m, 2H), 2.46-2.44 (m, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 157.3, 157.1, 143.1, 137.8, 129.9, 129.3, 127.3, 123.6, 120.3-111.0 (m), 119.1, 119.0, 108.2, 67.8 (t, J = 3.5 Hz), 40.6 (t, J = 20.3 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -98.55 (s, 2F), -112.31 to -113.11 (m, 1F), -113.60 to -114.41 (m, 1F);

IR (film) 3396, 3040, 1589, 1506, 1488, 1391, 1233, 1165, 1096, 1070, 900, 755, 692 cm^{-1};

HRMS (ESI) calcd for $C_{19}H_{16}F_4N_2O_2$ $[M+Na]^+$ m/z = 403.1040; found: 403.1033.



5,5,5-Trifluoro-1-(4-phenoxyphenyl)-3-(trifluoromethyl)pentan-1-ol (75): Compound **75** was synthesized following the general procedure (standard-scale), using 1,1,1,4,4,4-hexafluoro-2-iodobutane (58.4 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **75** was obtained as a colorless liquid (11 mg, 15% yield, dr = 1:1.1,) after purification by flash chromatography on silica gel with hexane/EtOAc (23:2) to hexane/EtOAc (9:1). These two diastereomers are inseparable.

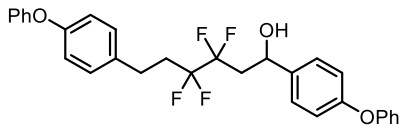
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.36-7.30 (m, 8H), 7.12 (tt, J = 7.2, 1.2 Hz, 2H), 7.02-6.99 (m, 8H), 4.86-4.78 (m, 2H), 2.94-2.85 (m, 1H), 2.79-2.69 (m, 1H), 2.60-2.29 (m, 4H), 2.24-1.82 (m, 6H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 157.5, 157.4, 157.1, 157.0, 138.5, 138.0, 129.9, 127.3, 127.2, 125.3 (q, J = 276.5 Hz), 125.2 (q, J = 276.1 Hz), 123.6, 119.19, 119.16, 119.1, 119.0, 71.6, 70.7, 38.2, 37.5, 35.4 (q, J = 2.6 Hz), 35.2 (q, J = 2.4 Hz), 33.6 (q, J = 3.0 Hz), 33.0 (q, J = 2.8 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -63.97 to -64.11 (m, 3F), -71.17 to -71.41 (m, 3F);

IR (film) 3429, 3040, 1589, 1507, 1489, 1239, 1144, 1109, 870, 749, 692 cm^{-1};

HRMS (ESI) calcd for $C_{18}H_{16}F_6O_2$ $[M-H]^-$ m/z = 377.0971; found: 377.0984.



3,3,4,4-Tetrafluoro-1,6-bis(4-phenoxyphenyl)hexan-1-ol (76): Compound **76** was synthesized following the general procedure (standard-scale), using 1-bromo-1,1,2,2-tetrafluoro-4-iodobutane (66.9 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **76** was obtained as a white solid (56 mg, 55% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (43:7) to hexane/EtOAc (21:4).

mp: 79-80 °C;

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.38-7.31 (m, 6H), 7.19 (d, J = 8.4 Hz, 2H), 7.14-7.07 (m, 2H), 7.02-6.95 (m, 8H), 5.21 (dt, J = 9.2, 2.8 Hz, 1H), 2.90-2.86 (m, 2H), 2.66-2.21 (m, 5H);

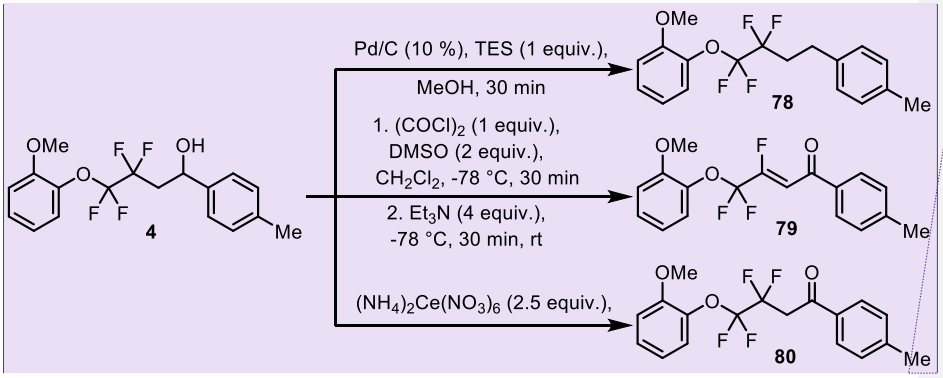
^{13}C NMR (100 MHz, $CDCl_3$) δ = 157.5, 157.2, 157.1, 155.8, 138.0, 135.0, 129.9, 129.8, 129.7, 127.3, 123.5, 123.2, 121.2-115.8 (m), 119.3, 119.1, 119.0, 118.8, 68.0 (t, J = 3.3 Hz), 39.4 (t, J = 20.8 Hz), 32.0 (t, J = 22.7 Hz), 26.2 (t, J = 4.6 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -112.59 to -113.42 (m, 1F), -114.18 to -115.00 (m, 1F), -115.52 to -115.66 (m, 2F);

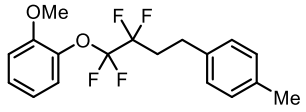
IR (film) 3419, 3039, 1589, 1506, 1487, 1231, 1166, 1071, 870, 751, 690 cm^{-1};

HRMS (ESI) calcd for $C_{30}H_{26}F_4O_3$ $[M+Na]^+$ m/z = 533.1710; found: 533.1708.

Derivatization



Commented [DS5]: (CoCl)2 has been changed to (COCl)2



1-Methoxy-2-(1,1,2,2-tetrafluoro-4-(*p*-tolyl)butoxy)benzene (78): Following a modified procedure by McMurray et al,[7] to an oven dried microwave vial, equipped with stir bar, 3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)-1-(*p*-tolyl)butan-1-ol (**4**) (100 mg, 0.27 mmol) and 10% Pd/C (10 mg, 10 wt% of **4**) was stirred in MeOH (1.1 mL) at rt under N_2. Triethylsilane (31.3 mg, 1.0 equiv.) was then added dropwise under N_2. The resultant mixture was stirred for 30 min under N_2. After completion, the reaction mixture was filtered over a short pad of celite, and filtrate was concentrated under reduced pressure. The product **78** was obtained as a colorless liquid (59 mg, 62% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (99:1) to hexane/EtOAc (97:3).

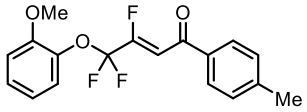
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.37-7.32 (m, 2H), 7.28-7.23 (m, 4H), 7.09-7.02 (m, 2H), 3.94 (s, 3H), 3.08-3.04 (m, 2H), 2.67-2.53 (m, 2H), 2.45 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.5, 137.9, 137.2, 136.0, 129.4, 128.3, 127.5, 124.0, 120.7, 119.5-114.5 (m), 112.9, 56.1, 33.6 (t, J = 22.0 Hz), 26.6 (t, J = 4.3 Hz), 21.1;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.08 to -88.11 (m, 2F), -117.30 to -117.41 (m, 2F),

IR (film) 2947, 1605, 1503, 1457, 1261, 1188, 1171, 1107, 1050, 748 cm^{-1};

HRMS (ESI) calcd for $C_{18}H_{18}F_4O_2$ $[M+K]^+$ m/z = 381.0875; found: 381.0867.



(*Z*)-3,4,4-Trifluoro-4-(2-methoxyphenoxy)-1-(*p*-tolyl)but-2-en-1-one (79):

Following a modified procedure by Swern et al,[8] to an oven dried microwave vial, equipped with stir bar, oxalyl chloride (25 µL, 0.28 mmol) was dissolved in CH_2Cl_2 (40 µL) and cooled to -78 °C. DMSO (40 µL, 0.56 mmol) was added dropwise and stirred for 5 minutes. Compound **4** (100 mg, 0.28 mmol) dissolved in CH_2Cl_2 (10 µL) was then added dropwise to the reaction mixture. The resultant mixture was stirred at -78 °C for 30 minutes. Triethylamine (156 µL, 1.12 mmol) was added dropwise and the resultant mixture is further stirred at -78 °C for 30 minutes. After completion of the reaction the mixture is warmed to room temperature and quenched with 1M HCl (1 mL). The organic phase is successfully extracted with three portions of CH_2Cl_2, washed with a saturated brine solution, dried over anhydrous Na_2SO_4, filtered, and concentrated in vacuo. The product **79** was obtained as a colorless liquid (56 mg, 59 % yield) after purification by flash chromatography on silica gel with hexane/EtOAc (17:3) to hexane/EtOAc (24:6).

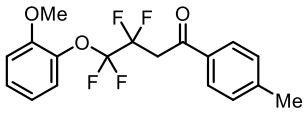
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.80 (d, J = 8.4 Hz, 2H), 7.28-7.21 (m, 4H), 6.99-6.91 (m, 2H), 6.81 (d, J = 32.0 Hz, 1H), 3.84 (s, 3H), 2.41 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 183.7, 154.1 (dt, J = 38.9, 283.4, Hz), 152.5, 145.1, 138.2, 134.4, 129.6, 129.0, 127.6, 123.9, 120.7, 116.6 (td, J = 37.1, 261.1 Hz), 112.9, 107.1 (q, J = 3.1 Hz), 56.1, 21.9;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -74.75 (d, J = 12.7 Hz, 2F), -113.65 to -113.81 (m, 1F);

IR (film) 2924, 1698, 1655, 1501, 1457, 1281, 1261, 1156, 1062, 815, 748, 695 cm^{-1};

HRMS (ESI) calcd for $C_{18}H_{15}F_3O_3$ $[M+H]^+$ m/z = 337.1046; found: 337.1043.



3,3,4,4-Tetrafluoro-4-(2-methoxyphenoxy)-1-(*p*-tolyl)butan-1-one (80): Following a modified procedure by Chakraborty et al,[9] 3,3,4,4-Tetrafluoro-4-(2-methoxyphenoxy)-1-(*p*-tolyl)butan-1-ol (**4**) (107.5 mg, 0.3 mmol) was dissolved in CH_3CN (10.5 mL) and H_2O (2.7

mL) in a flame-dried 50 mL round bottom flask, then cerium ammonium nitrate (411.2 mg, 0.75 mmol, 2.5 equiv.) was added into the flask, giving an orange-yellowish solution. The round bottom flask was then placed in an oil bath and the solution was stirred at 50 °C for 16 hours and resulted in the yellow-greenish solution. After quenching with H_2O (15 mL), the reaction mixture was extracted three times with EtOAc (15 mL). The organic layer was washed with brine and dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The product **80** was obtained as a colorless liquid (29 mg, 27% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (17:3) to hexane/EtOAc (21:4).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.92 (d, J = 8.0 Hz, 2H), 7.31 (d, J = 8.0 Hz, 2H), 7.26-7.22 (m, 2H), 7.00-6.92 (m, 2H), 3.89-3.80 (m, 5H), 2.43 (s, 3H);

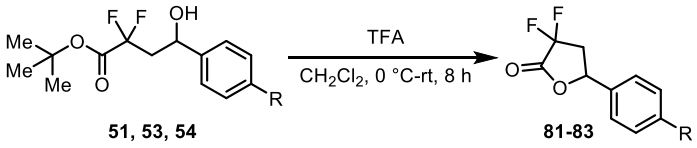
^{13}C NMR (100 MHz, $CDCl_3$) δ = 191.0, 152.4, 145.0, 137.8, 134.6, 129.6, 129.0, 127.7, 123.8, 120.7, 120.2-114.5 (m), 112.9, 56.1, 39.3 (t, J = 21.5), 21.8;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.84 (t, J = 4.1 Hz, 2F), -114.63 (tt, J = 17.6, 4.5 Hz, 2F);

IR (film) 2946, 1684, 1607, 1503, 1324, 1284, 1262, 1191, 1109, 1026, 750, 686 cm^{-1};

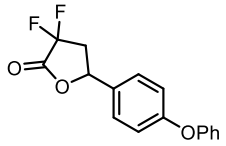
HRMS (ESI) calcd for $C_{18}H_{16}F_4O_3$ $[M+H]^+$ m/z = 357.1108; found: 357.1105.

General procedure for Synthesis of γ-lactones



51, 53, 54 **81-83**

Following a modified procedure by Petersen et al,[10] to an oven dried microwave vial, equipped with stir bar, alcohol (**51, 53 and 54**) was dissolved in CH_2Cl_2 (4.0 mL) and cooled at 0 °C. Trifluoroacetic acid (TFA) (15 µL) was then added dropwise to the solution at 0 °C. The reaction mixture was then stirred at rt for 8 h. After completion of the reaction the resultant mixture was diluted with Et_2O (15 mL) and washed with saturated sodium bicarbonate (2 x 5 mL). The organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product **81-83** was then purified by flash chromatography.



3,3-Difluoro-5-(4-phenoxyphenyl)dihydrofuran-2(3H)-one (81): Compound **81** was synthesized following the general procedure for synthesis of γ-lactones, using *tert*-butyl 2,2-difluoro-4-hydroxy-4-(4-phenoxyphenyl)butanoate (**51**) (50 mg, 0.13 mmol). The product **81** was obtained as a white solid (41 mg, 66% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (9:1) to hexane/EtOAc (89:11).

mp: 86-87 °C

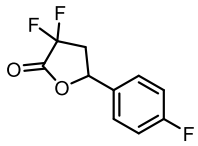
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.37 (t, J = 8.0 Hz, 2H), 7.32 (d, J = 8.8 Hz, 2H), 7.16 (t, J = 7.4 Hz, 1H), 7.05-7.02 (m, 4H), 5.58 (dd, J = 9.2, 6.0 Hz, 1H), 3.16-3.06 (m, 1H), 2.74-2.59 (m, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 164.9 (dd, J =33.7, 31.7 Hz), 158.9, 156.3, 130.4, 130.1, 127.7, 124.2, 119.6, 118.9, 115.8 (dd, J = 257.2, 248.4 Hz), 77.0 (dd, J = 7.3, 1.4 Hz), 40.0 (dd, J = 21.6, 21.1 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -106.15 to -107.00 (m, 1F), -108.75 to -109.54 (m, 1F);

IR (film) 2921, 1809, 1589, 1509, 1489, 1241, 1077, 750, 692 cm^{-1};

HRMS (APCI) calcd for $C_{16}H_{12}F_2O_3$ $[M+H]^+$ m/z = 291.0827; found: 291.0824.



3,3-Difluoro-5-(4-fluorophenyl)dihydrofuran-2(3H)-one (82): Compound **82** was synthesized following the general procedure for synthesis of γ-lactones, using *tert*-butyl 2,2-difluoro-4-(4-fluorophenyl)-4-hydroxybutanoate (**53**) (50.2 mg, 0.17 mmol). The product **82** was obtained as a yellowish liquid (21.7 mg, 58% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (21:4) to hexane/EtOAc (83:17).

Commented [DS6]: Updated NMR

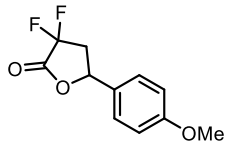
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.35-7.32 (m, 2H), 7.16-7.11 (m, 2H), 5.59 (dd, J = 9.2, 6.4 Hz, 1H), 3.18-3.08 (m, 1H), 2.70-2.55 (m, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 164.8 (dd, *J* = 33.6, 31.7 Hz), 164.6 (d, *J* = 247.8 Hz), 132.1 (d, *J* = 3.4 Hz), 127.9 (d, *J* = 8.6 Hz), 116.5 (d, *J* = 21.8 Hz), 115.6 (dd, *J* = 257.3, 248.7 Hz), 76.5 (dd, *J* = 6.9, 2.0 Hz), 40.1 (dd, *J* = 21.4, 20.7 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -106.17 to -107.02 (m, 1F), -108.70 to -109.49 (m, 1F), -111.05 to -111.12 (m, 1F);

IR (film) 2925, 1811, 1608, 1515, 1318, 1229, 1206, 1127, 1077, 1013, 953, 837, 746 cm^{-1};

HRMS (APCI) calcd for $C_{10}H_7F_3O_2$ $[M+H]^+$ m/z = 217.0471; found: 217.0469.



3,3-Difluoro-5-(4-methoxyphenyl)dihydrofuran-2(3H)-one (83):[11] Compound **83** was synthesized following the general procedure for synthesis of γ-lactones, using *tert*-butyl 2,2-difluoro-4-hydroxy-4-(4-methoxyphenyl)butanoate (**54**) (50.4 mg, 0.16 mmol). The product **83** was obtained as a yellowish liquid (17.5 mg, 46% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (83:17) to hexane/EtOAc (41:9).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.29 (d, *J* = 9.2 Hz, 2H), 6.96 (d, *J* = 8.8 Hz, 2H), 5.55 (dd, *J* = 8.4, 6.8 Hz, 1H), 3.83 (s, 3H), 3.13-3.03 (m, 1H), 2.73-2.58 (m, 1H);

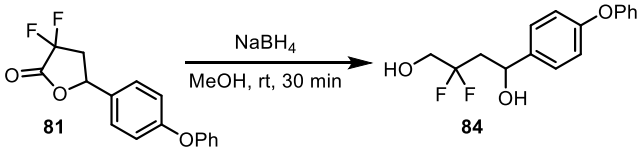
^{13}C NMR (100 MHz, $CDCl_3$) δ = 165.1 (dd, *J* = 33.6, 31.3 Hz), 160.8, 127.9, 127.7, 115.9 (dd, *J* = 257.4. 248.3 Hz), 114.6, 77.3 (dd, *J* = 7.2, 1.7 Hz), 55.5, 39.9 (dd, *J* = 22.2, 20.3 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -106.22 to -107.07 (m, 1F), -108.80 to -109.58 (m, 1F);

IR (film) 2938, 1807, 1613, 1518, 1321, 1250, 1207, 1179, 1114, 1078, 1031, 834, 747 cm^{-1};

HRMS (APCI) calcd for $C_{11}H_{10}F_2O_3$ $[M+H]^+$ m/z = 229.0671; found: 229.0669.

The Procedure for the synthesis of 3,3-Difluoro-1-(4-phenoxyphenyl)butane-1,4-diol (84):



Following a modified procedure by Singaram et al,[12] To an oven dried microwave vial, equipped with stir bar, 3,3-difluoro-5-(4-phenoxyphenyl)dihydrofuran-2(3H)-one (**81**) (58 mg, 0.2 mmol) was dissolved in MeOH (2 mL) and stirred at room temperature. Sodium borohydride (30.2 mg, 0.8 mmol) was then added into the solution. The resultant mixture was stirred for 30 min at ambient temperature. After completion, saturated NaCl solution (1 mL) was added to quench the reaction, then extracted with ethyl acetate (2 x 5 mL). The organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The product **84** was obtained as a white solid (31.7 mg, 54% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (71:29) to hexane/EtOAc (7:3).

mp: 82-83 °C

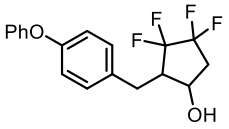
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.36-7.32 (m, 4H), 7.12 (tt, J = 7.6, 1.2 Hz, 1H), 7.02-6.99 (m, 4H), 5.01 (dt, J = 10.0, 2.0 Hz, 1H), 3.96-3.78 (m, 2H), 3.05 (bs, 1H), 2.80 (bs, 1H), 2.58-2.43 (m, 1H), 2.30-2.20 (m, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 157.4, 157.0, 137.9, 129.9, 127.2, 123.7, 122.6 (t, J = 241.9 Hz), 119.2, 119.0, 69.2 (dd, J =10.1, 2.4 Hz), 64.5 (t, J = 33.0 Hz), 43.5 (t, J = 24.3 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -98.89 to -99.71 (m, 1F), -106.85 to -107.69 (m, 1F),

IR (film) 3352, 2936, 1589, 1507, 1488, 1235, 1167, 1068, 870, 748, 692 cm^{-1};

HRMS (ESI) calcd for $C_{16}H_{16}F_2O_3$ $[M-H]^-$ m/z = 293.0984; found: 293.0996.



3,3,4,4-Tetrafluoro-2-(4-phenoxybenzyl)cyclopentan-1-ol (85): Compound **85** was synthesized following the general procedure (standard-scale), using 4-bromo-3,3,4,4-tetrafluorobut-1-ene (41.4 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The

product **85** was obtained as a colorless liquid (58.3 mg, 86% yield, 1.1:1 dr) after purification by flash chromatography on silica gel with hexane/EtOAc (83:17) to hexane/EtOAc (81:19).

^{1}H NMR (400 MHz, $CDCl_3$, major) δ = 7.35-7.31 (m, 2H), 7.25 (d, J = 8.4 Hz, 2H), 7.10 (tt, J = 7.2, 1.2 Hz, 1H), 7.01-6.95 (m, 4H), 4.23-4.17 (m, 1H), 3.05-2.95 (m, 2H), 2.68-2.52 (m, 2H), 2.42-2.29 (m, 1H), 1.70-1.68 (m, 1H);

^{13}C NMR (100 MHz, $CDCl_3$, major) δ = 157.2, 156.2, 132.6, 130.2, 129.9, 127.2-120.5 (m), 123.4, 119.3, 118.9, 64.9 (qu, J = 5.9 Hz), 49.2 (t, J = 20.0 Hz), 42.0 (t, J = 22.9 Hz), 26.4 (d, J = 4.2 Hz);

^{19}F NMR (376 MHz, $CDCl_3$, major) δ = -105.68 to -106.46 (m, 1F), -115.85 to -116.60 (m, 1F), -121.11 to -122.89 (m, 2F);

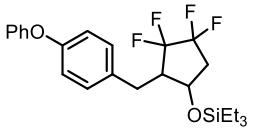
^{1}H NMR (400 MHz, $CDCl_3$, minor) δ = 7.36-7.32 (m, 2H), 7.24 (d, J = 8.8 Hz, 2H), 7.11 (tt, J = 7.6, 1.2 Hz, 1H), 7.01-6.97 (m, 4H), 4.15-4.11 (m, 1H), 3.10 (dd, J = 14.4, 6.0 Hz, 1H), 2.78 (dd, J = 14.0, 9.6 Hz, 1H), 2.73-2.49 (m, 2H), 2.26-2.13 (m, 1H), 1.40-1.39 (m, 1H);

^{13}C NMR (100 MHz, $CDCl_3$, minor) δ = 157.1, 156.5, 132.1, 130.2, 129.9, 127.3-117.9 (m), 123.6, 119.4, 119.1, 68.9 (qu, J = 5.8 Hz), 52.5 (t, J = 19.5 Hz), 39.7 (t, J = 22.1 Hz), 31.0 (d, J = 5.6 Hz);

^{19}F NMR (376 MHz, $CDCl_3$, minor) δ = -108.23 to -109.02 (m, 1F), -119.34 to -120.89 (m, 2F), -126.41 to -127.15 (m, 1F);

IR (film) 3456, 2929, 1589, 1507, 1488, 1350, 1236, 1131, 1093, 973, 870, 692 cm^{-1};

HRMS (ESI) calcd for $C_{18}H_{16}F_4O_2$ $[M+Cl]^-$ m/z = 375.0769; found: 375.0782.



Triethyl((3,3,4,4-tetrafluoro-2-(4-phenoxybenzyl)cyclopentyl)oxy)silane (86): Compound **86** was synthesized following the general procedure (standard-scale), using 4-bromo-3,3,4,4-tetrafluorobut-1-ene (41.4 mg, 0.2 mmol), triethyl(vinyloxy)silane (0.10 mL, 3.8 M solution in pentane, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **86** was obtained as a colorless liquid (50.7

mg, 56% yield, 2:1.2 dr) after purification by flash chromatography on silica gel with hexane/EtOAc (99:1) to hexane/EtOAc (49:1).

^{1}H NMR (400 MHz, $CDCl_3$, major) δ = 7.34-7.30 (m, 2H), 7.20 (d, J = 8.4 Hz, 2H), 7.10-7.07 (m, 1H), 6.99-6.94 (m, 4H), 4.28 (s, 1H), 2.96 (d, J = 7.6 Hz, 2H), 2.66-2.45 (m, 2H), 2.35-2.22 (m, 1H), 0.93 (t, J = 7.8 Hz, 9H), 0.56 (q, J = 7.8 Hz, 6H);

^{13}C NMR (100 MHz, $CDCl_3$, major) δ = 157.6, 155.7, 133.6, 130.2, 129.8, 128.3-119.1 (m), 123.1, 119.3, 118.6, 65.6 (qu, J = 5.1 Hz), 49.8 (t, J = 19.2 Hz), 42.6 (t, J = 21.0 Hz), 26.9 (d, J = 4.6 Hz), 6.8, 4.9;

^{19}F NMR (376 MHz, $CDCl_3$, major) δ = -106.13 to -106.88 (m, 1F), -114.62 to -115.35 (m, 1F), -119.04 to -119.74 (m, 1F), -121.19 to -121.93 (m, 1F);

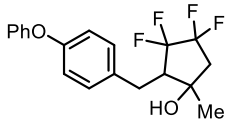
^{1}H NMR (400 MHz, $CDCl_3$, minor) δ = 7.34-7.30 (m, 2H), 7.21 (d, J = 8.4 Hz, 2H), 7.09 (tt, J = 7.6, 0.8 Hz, 1H), 7.00-6.93 (m, 4H), 3.99 (q, J = 8.2 Hz, 1H), 2.94 (dd, J = 14.4, 9.2 Hz, 1H), 2.84 (dd, J = 14.4, 6.0 Hz, 1H), 2.68-2.54 (m, 2H), 2.22-2.08 (m, 1H), 0.93 (t, J = 8.0 Hz, 9H), 0.56 (q, J = 8.2 Hz, 6H);

^{13}C NMR (100 MHz, $CDCl_3$, minor) δ = 157.5, 155.9, 133.0, 130.3, 129.8, 128.7-118.5 (m), 123.2, 119.1, 118.8, 69.0 (qu, J = 4.6 Hz), 53.1 (t, J = 18.6 Hz), 41.3 (t, J = 21.3 Hz), 31.1 (d, J = 4.9 Hz), 6.8, 4.7;

^{19}F NMR (376 MHz, $CDCl_3$, minor) δ = -107.32 to -108.08 (m, 1F), -116.85 to -118.33 (m, 2F), -125.66 to -126.38 (m, 1F);

IR (film) 2957, 2878, 1591, 1507, 1489, 1347, 1240, 1178, 1128, 1015, 871, 746, 692 cm^{-1};

HRMS (APCI) calcd for $C_{24}H_{30}F_4O_2Si$ $[M+H]^+$ m/z = 455.2024; found: 455.2026.



3,3,4,4-Tetrafluoro-1-methyl-2-(4-phenoxybenzyl)cyclopentan-1-ol (87):

Compound **87** was synthesized following the general procedure (standard-scale), using 4-bromo-3,3,4,4-tetrafluorobut-1-ene (41.4 mg, 0.2 mmol), trimethyl(prop-1-en-2-yloxy)silane (52.1mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **87** was obtained as a colorless liquid (12.3 mg,

18% yield, 5:1 dr) after purification by flash chromatography on silica gel with hexane/EtOAc (79:21) to hexane/EtOAc (39:11).

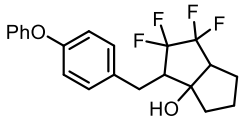
^{1}H NMR (400 MHz, $CDCl_3$, major) δ = 7.35-7.31 (m, 2H), 7.25-7.23 (m, 2H), 7.10 (tt, J = 7.2, 1.2 Hz, 1H), 7.01-6.94 (m, 4H), 3.01-2.96 (m, 1H), 2.89-2.73 (m, 2H), 2.52-2.33 (m, 2H), 1.54 (bs, 1H), 1.41 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$, major) δ = 157.2, 156.2, 132.5, 130.2, 129.9, 125.0-119.8 (m), 123.4, 119.2, 119.0, 72.9-72.7 (m), 54.8-54.6 (m), 47.8 (t, J = 21.9 Hz), 27.3 (d, J = 4.3 Hz), 25.6;

^{19}F NMR (376 MHz, $CDCl_3$, major) δ = -105.36 to -106.13 (m, 1F), -117.56 to -119.08 (m, 2F), -123.81 to -124.53 (m, 1F);

IR (film) 3540, 2957, 1590, 1507, 1488, 1346, 1237, 1181, 1136, 1101, 987, 871, 750, 692 cm^{-1};

HRMS (ESI) calcd for $C_{19}H_{18}F_4O_2$ $[M-H]^-$ m/z = 353.1159; found: 353.1174.



1,1,2,2-Tetrafluoro-3-(4-phenoxybenzyl)hexahydropentalen-3a(1H)-ol (88):

Compound **88** was synthesized following the general procedure (standard-scale), using 4-bromo-3,3,4,4-tetrafluorobut-1-ene (41.4 mg, 0.2 mmol), (cyclopent-1-en-1-yloxy)trimethylsilane (62.5 mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **88** was obtained as a colorless liquid (16.1 mg, 21% yield, 10:1 dr) after purification by flash chromatography on silica gel with hexane/EtOAc (21:4) to hexane/EtOAc (83:17).

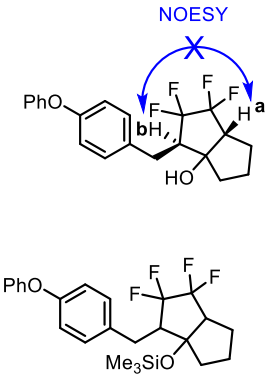
^{1}H NMR (400 MHz, $CDCl_3$, major) δ = 7.35-7.31 (m, 2H), 7.26-7.24 (m, 2H), 7.11 (tt, J = 7.6, 1.2 Hz, 1H), 7.00-6.95 (m, 4H), 3.09-3.03 (m, 1H), 2.88-2.81 (m, 2H), 2.61-2.48 (m, 1H), 2.10-2.03 (m, 1H), 1.88-1.81 (m, 2H), 1.76-1.60 (m, 4H);

^{13}C NMR (100 MHz, $CDCl_3$, major) δ = 157.1, 156.3, 132.6, 130.3, 129.9, 128.2-118.4 (m), 123.5, 119.3, 119.0, 85.7-85.5 (m), 55.7 (dd, J = 22.5, 19.8 Hz), 52.2 (dd, J = 19.0, 17.4 Hz), 37.7, 27.7 (d, J = 3.3 Hz), 26.7 (dd, J = 7.0, 4.4 Hz), 25.2;

^{19}F NMR (376 MHz, $CDCl_3$, major) δ = -102.21 to -102.93 (m, 1F), -120.65 to -121.34 (m, 1F), -124.42 to -125.15 (m, 1F), -130.01 to -130.71 (m, 1F);
IR (film) 3542, 2963, 1590, 1507, 1488, 1354, 1238, 1196, 1077, 1019, 870, 753, 692 cm^{-1};
HRMS (APCI) calcd for $C_{21}H_{20}F_4O_2$ $[M+H]^+$ m/z = 381.1472; found: 381.1473.

The stereochemistry of compound **88** was studied by 2D NOESY Spectrum (spectral data, compound **88**). The absence of ^{1}H-^{1}H interaction between CH proton "a" and CH proton "b" indicates that both protons are in the *trans* diastereomer.

Fig. S7: Confirmed the structure of **88** as *trans* based on NOESY NMR.



Trimethyl((1,1,2,2-tetrafluoro-3-(4-phenoxybenzyl)hexahydropentalen-3a(1H)-yl)oxy)silane (89):
Compound **89** was synthesized following the general procedure (standard-scale), using 4-bromo-3,3,4,4-tetrafluorobut-1-ene (41.4 mg, 0.2 mmol), (cyclopent-1-en-1-yloxy)trimethylsilane (62.5 mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **89** was obtained as a yellowish liquid (29.4 mg, 33% yield, 15:1 dr) after purification by flash chromatography on silica gel with hexane/EtOAc (97:3) to hexane/EtOAc (24:1).
^{1}H NMR (400 MHz, $CDCl_3$, major) δ = 7.32 (t, J = 8.0 Hz, 2H), 7.21 (d, J = 8.4 Hz, 2H), 7.08 (t, J = 7.6 Hz, 1H), 7.00 (d, J = 8.0 Hz, 2H), 6.95 (d, J = 8.8 Hz, 2H), 2.96 (dd, J = 14.4,

8.0 Hz, 1H), 2.88 (dd, J = 14.4, 6.4 Hz, 1H), 2.84-2.71 (m, 1H), 2.70-2.59 (m, 1H), 2.08-2.03 (m, 1H), 1.79-1.60 (m, 5H), 0.07 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$, major) δ = 157.5, 155.8, 133.6, 130.4, 129.8, 128.3-113.3 (m), 123.2, 119.0, 118.8, 88.0-87.8 (m), 55.1 (dd, J = 21.4, 17.4 Hz), 53.0 (dd, J = 18.7, 15.2 Hz), 37.7, 28.0 (d, J = 3.7 Hz), 26.5 (t, J = 5.5 Hz), 25.2, 2.1;

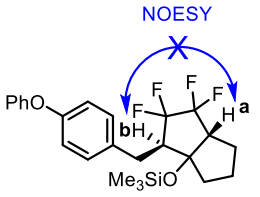
^{19}F NMR (376 MHz, $CDCl_3$, major) δ = -101.48 to -102.27 (m, 1F), -119.58 to -120.32 (m, 1F), -123.60 to -124.36 (m, 1F), -128.69 to -129.39 (m, 1F);

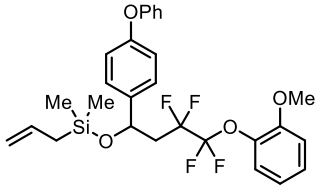
IR (film) 2960, 1590, 1507, 1489, 1353, 1240, 1197, 1088, 903, 840, 753, 691 cm^{-1};

HRMS (APCI) calcd for $C_{24}H_{28}F_4O_2Si$ $[M+H]^+$ m/z = 453.1867; found: 453.1841.

The stereochemistry of compound **89** was studied by 2D NOESY Spectrum (spectral data, compound **89**). The absence of ^{1}H-^{1}H interaction between CH proton "a" and CH proton "b" indicates that both protons are in the *trans* diastereomer.

Fig. S8: Confirmed the structure of **89** as *trans* based on NOESY NMR.





Allyldimethyl(3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)-1-(4-phenoxyphenyl)butoxy)silane (90): Compound **90** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), allyldimethyl(vinyloxy)silane (0.11 mL, 3.6 M solution in pentane, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4

mmol). The product **90** was obtained as a colorless liquid (28.8 mg, 27% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (24:1) to hexane/EtOAc (19:1).

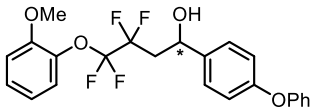
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.36-7.32 (m, 4H), 7.24-7.21 (m, 2H), 7.11 (t, J = 7.6 Hz, 1H), 7.02-6.90 (m, 6H), 5.75-5.64 (m, 1H), 5.23 (dd, J = 8.8, 3.2 Hz, 1H), 4.85-4.80 (m, 2H), 3.82 (s, 3H), 2.75-2.60 (m, 1H), 2.56-2.42 (m, 1H), 1.57-1.55 (m, 2H), 0.08 (s, 3H), 0.06 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 157.3, 156.8, 152.5, 139.2, 137.8, 134.0, 129.9, 127.6, 127.3, 124.0, 123.4, 120.7, 119.4-115.1 (m), 119.0, 118.8, 113.8, 112.9, 68.7 (t, J = 2.6 Hz), 56.1, 41.6 (t, J = 20.2 Hz), 24.9, -2.0;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.84 (s, 2F), -114.44 to -115.25 (m, 1F), -117.29 to -118.09 (m, 1F);

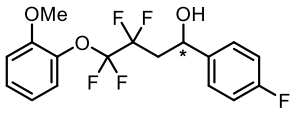
IR (film) 2921, 1590, 1503, 1489, 1236, 1187, 1169, 1096, 1044, 918, 836, 748, 692 cm^{-1};

HRMS (ESI) calcd for $C_{28}H_{30}F_4O_4Si$ $[M+H]^+$ m/z = 535.1922; found: 535.1924.



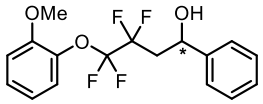
Trimethyl(3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)-1-(4-phenoxyphenyl)butoxy)silane (93): Compound **93** was synthesized following the general procedure 2, using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-phenoxyphenyl)magnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **93** was obtained as a colorless liquid (52.8 mg, 61% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (41:9) to hexane/EtOAc (4:1). HPLC (Daicel Chiralcel OJ-H column (Hexane/*i*-PrOH 90:10, 1.0 mL/min, 250 nm) t_{major} 28.7 min, t_{minor} 35.7 min, 70:30 er.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.42 (d, J = 8.4 Hz, 2H), 7.34 (t, J = 8.0 Hz, 2H), 7.27-7.22 (m, 2H), 7.11 (t, J = 7.4 Hz, 1H), 7.04-6.93 (m, 6H), 5.31 (dt, J = 8.8, 3.2 Hz, 1H), 3.84 (s, 3H), 2.82-2.53 (m, 3H); spectral data matched with compound 1**2**.



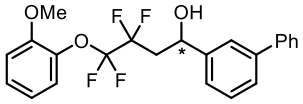
3,3,4,4-Tetrafluoro-1-(4-fluorophenyl)-4-(2-methoxyphenoxy)butan-1-ol (94): Compound **94** was synthesized following the general procedure 2, using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (4-fluorophenyl)magnesium bromide (0.4 mL, 1.0 M solution in THF, 0.4 mmol). The product **94** was obtained as a colorless liquid (45.4 mg, 63% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (83:17) to hexane/EtOAc (81:19). HPLC (Daicel Chiralcel OJ-H column (Hexane/*i*-PrOH 90:10, 1.0 mL/min, 250 nm) t_{major} 12.3 min, t_{minor} 13.6 min, 72:28 er.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.44-7.41 (m, 2H), 7.28-7.23 (m, 2H), 7.08 (tt, J = 8.8, 2.8 Hz, 2H), 7.01-6.94 (m, 2H), 5.32 (dt, J = 9.2, 2.8 Hz, 1H), 3.84 (S, 3H), 2.80-2.51 (m, 3H); spectral data matched with compound **26**.



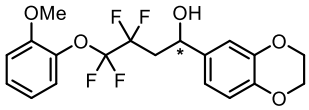
3,3,4,4-Tetrafluoro-4-(2-methoxyphenoxy)-1-phenylbutan-1-ol (95): Compound **95** was synthesized following the general procedure 2, using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and phenylmagnesium bromide (0.4 mL, 1.0 M solution in THF, 0.4 mmol). The product **95** was obtained as a colorless liquid (51.9 mg, 76% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (39:11) to hexane/EtOAc (19:6). HPLC (Daicel Chiralcel OJ-H column (Hexane/*i*-PrOH 90:10, 1.0 mL/min, 250 nm) t_{major} 12.1 min, t_{minor} 14.9 min, 59:41 er.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.46-7.43 (m, 2H), 7.41-7.37 (m, 2H), 7.32 (tt, J = 6.8, 2.0 Hz, 1H), 7.27-7.22 (m, 2H), 6.99-6.92 (m, 2H), 5.32 (dt, J = 9.2, 2.8 Hz, 1H), 3.83 (s, 3H), 2.82-2.54 (m, 3H); spectral data matched with compound **20**.



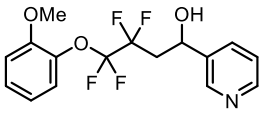
1-([1,1'-Biphenyl]-3-yl)-3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)butan-1-ol (96): Compound **96** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and [1,1'-biphenyl]-3-ylmagnesium bromide (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **96** was obtained as a colorless liquid (61 mg, 73% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (77:23) to hexane/EtOAc (3:1). HPLC (Daicel Chiralcel OJ-H column (Hexane/*i*-PrOH 90:10, 1.0 mL/min, 250 nm) t_{minor} 20.4 min, t_{major} 27.8 min, 37:63 er.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.67 (t, *J* = 2.0 Hz, 1H), 7.63-7.60 (m, 2H), 7.56 (dt, *J* = 7.2, 1.6 Hz, 1H), 7.48-7.42 (m, 4H), 7.36 (tt, *J* = 7.6, 1.2 Hz, 1H), 7.27-7.22 (m, 2H), 6.99-6.92 (m, 2H), 5.40 (dt, *J* = 9.2, 2.8 Hz, 1H), 3.82 (s, 3H), 2.86-2.59 (m, 3H); spectral data matched with compound **16**.



1-(2,3-Dihydrobenzo[*b*][1,4]dioxin-6-yl)-3,3,4,4-tetrafluoro-4-(2-methoxyphenoxy)butan-1-ol (97): Compound **97** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)magnesium bromide (0.23 mL, 1.7 M solution in THF, 0.4 mmol). The product **97** was obtained as a colorless liquid (34.9 mg, 44% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (19:6) to hexane/EtOAc (3:1). HPLC (Daicel Chiralcel OJ-H column (Hexane/*i*-PrOH 90:10, 1.0 mL/min, 250 nm) t_{major} 41.5 min, t_{minor} 51.2 min, 67:33 er.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.26-7.21 (m, 2H), 6.98-6.84 (m, 5H), 5.21 (dt, J = 9.2, 3.2 Hz, 1H), 4.26 (s, 4H), 3.84 (s, 3H), 2.77-2.49 (m, 3H); spectral data matched with compound **47**.



3,3,4,4-Tetrafluoro-4-(2-methoxyphenoxy)-1-(pyridin-3-yl)butan-1-ol (P1): Compound **P1** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and pyridin-3-ylmagnesium bromide lithium chloride complex (**3.S1**) (0.47 mL, 0.84 M solution in THF, 0.4 mmol). The product **P1** was obtained as a yellowish liquid (10.3 mg, 15% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (1:9) to hexane/EtOAc (2:23).

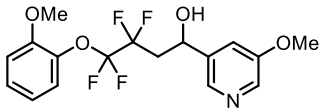
^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.68 (s, 1H), 8.57 (d, J = 4.8 Hz, 1H), 7.84 (d, J = 7.6 Hz, 1H), 7.34 (dd, J = 8.0, 4.8 Hz, 1H), 7.28-7.23 (m, 2H), 7.00-6.94 (m, 2H), 5.39 (dd, J =8.8, 2.8 Hz, 1H), 3.84 (s, 3H), 3.15-2.55 (m, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.1, 149.2, 147.6, 138.8, 137.6, 133.8, 127.7, 123.8, 120.9, 120.4-116.2 (m), 112.8, 66.1 (t, J = 3.9), 56.1, 41.5 (t, J = 20.6 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -87.99 to -88.83 (m, 2F), -113.19 to -114.00 (m, 1F), -114.23 to -115.04 (m, 1F);

IR (film) 3190, 2843, 1602, 1503, 1262, 1189, 1171, 1108, 1027, 751, 714 cm^{-1};

HRMS (ESI) calcd for $C_{16}H_{15}F_4NO_3$ $[M+H]^+$ m/z = 346.1061; found: 346.1054.



3,3,4,4-Tetrafluoro-4-(2-methoxyphenoxy)-1-(5-methoxypyridin-3-yl)butan-1-ol (P2): Compound **P2** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (5-methoxypyridin-3-yl)magnesium bromide lithium chloride complex (**3.S2**) (0.5 mL, 0.79 M solution in THF, 0.4 mmol). The product **P2** was obtained as a colorless liquid (8.3 mg, 11% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (12:13) to hexane/EtOAc (9:11).

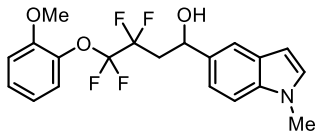
^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.27-8.26 (m, 2H), 7.35 (t, J = 2.0 Hz, 1H), 7.27-7.26 (m, 1H), 7.25-7.23 (m, 1H), 7.00-6.93 (m, 2H), 5.38 (dd, J = 8.8, 1.6 Hz, 1H), 3.89 (s, 3H), 3.84 (s, 3H), 2.92-2.53 (m, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 156.0, 152.1, 139.69, 139.61, 137.6, 137.2, 127.7, 123.8, 120.9, 117.9, 117.6-111.9 (m), 112.8, 65.9 (t, J = 3.9 Hz), 56.1, 55.7, 41.6 (t, J = 20.7 Hz);

^{19}F NMR (376 MHz, $CDCl_3$) δ = -87.96 to -88.81 (m, 2F), -113.03 to -115.06 (m, 2F);

IR (film) 3195, 2945, 1589, 1503, 1465, 1283, 1262, 1189, 1171, 1106, 1043, 750, 712 cm^{-1};

HRMS (APCI) calcd for $C_{17}H_{17}F_4NO_4$ $[M+H]^+$ m/z = 376.1161; found: 376.1151.



3,3,4,4-Tetrafluoro-4-(2-methoxyphenoxy)-1-(1-methyl-1H-indol-5-yl)butan-1-ol (P3): Compound **P3** was synthesized following the general procedure (standard-scale), using 1-(2-bromo-1,1,2,2-tetrafluoroethoxy)-2-methoxybenzene (60.2 mg, 0.2 mmol), trimethyl(vinyloxy)silane (46.4 mg, 0.4 mmol) and (1-methyl-1*H*-indol-5-yl)magnesium bromide (**3.S3**) (0.8 mL, 0.5 M solution in THF, 0.4 mmol). The product **P3** was obtained as a yellowish liquid (16 mg, 20% yield) after purification by flash chromatography on silica gel with hexane/EtOAc (39:11) to hexane/EtOAc (77:23).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.69 (t, J = 0.8 Hz, 1H), 7.35-7.29 (m, 2H), 7.25-7.20 (m, 2H), 7.08 (d, J = 3.2 Hz, 1H), 6.98-6.91 (m, 2H), 6.49 (dd, J = 3.2, 0.8 Hz, 1H), 5.42 (dt, J = 9.2, 2.8 Hz, 1H), 3.82 (s, 3H), 3.80 (s, 3H), 2.90-2.95 (m, 2H), 2.49-2.48 (m, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ = 152.4, 137.8, 136.6, 134.6, 129.6, 128.6, 127.5, 123.9, 121.0-116.9 (m), 120.7, 119.6, 118.2, 112.8, 109.6, 101.2, 68.9 (t, J = 3.5 Hz), 56.1, 41.4 (t, J = 20.4 Hz), 33.0;

^{19}F NMR (376 MHz, $CDCl_3$) δ = -88.12 to -88.92 (m, 2F), -113.88 to -114.68 (m, 1F), -115.32 to -116.13 (m, 1F);

IR (film) 3426, 2917, 2847, 1604, 1502, 1261, 1189, 1171, 1107, 750 cm^{-1};

HRMS (ESI) calcd for $C_{20}H_{19}F_4NO_3$ $[M+H]^+$ m/z = 398.1374; found: 398.1372.

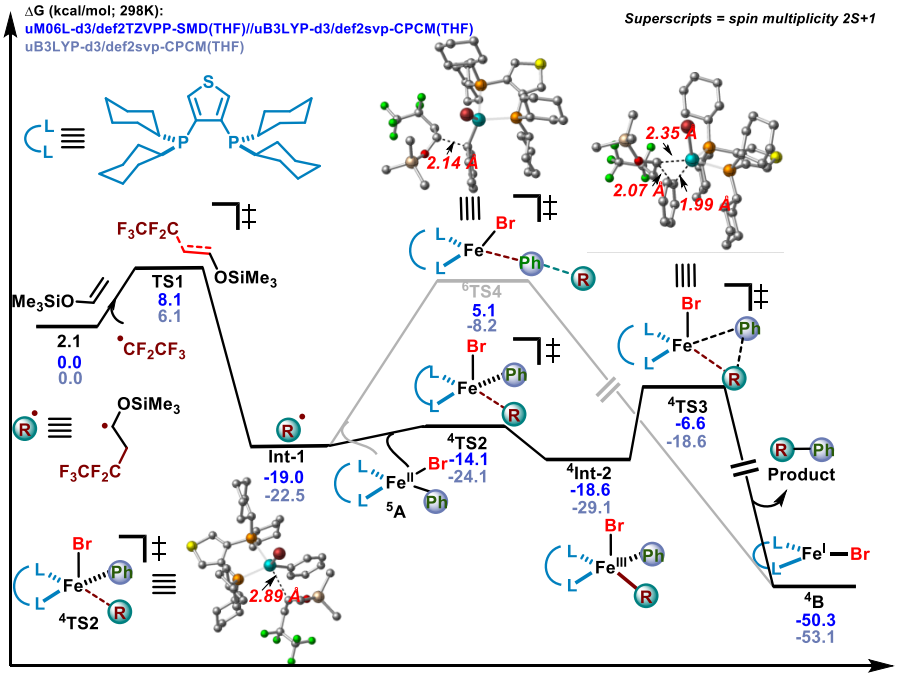
7. Computational Methods, Results, and Coordinates

7.1. Computational Methods

All geometry optimizations of intermediates and transition states were achieved using spin-unrestricted uB3LYP[13,14]-D3(*15-18*)/def2-SVP[19,20] method, in THF solvent using the CPCM solvent model[21-25] with "opt=noeigen" and "guess=mix" keywords as implemented in Gaussian16[26]. Frequency calculations were also conducted at the same level of theory to obtain vibrational frequencies to determine the identity of stationary points as intermediates (no imaginary frequencies) or transition states (only one imaginary frequency), as well as obtaining the thermochemistry: enthalpy (ΔH) and free energy (ΔG) at the temperature of 298 K. Also, extensive conformational and different spins search was performed for all the iron intermediates and transition states, and only the lowest-energy species were shown and discussed. For redox potential, lowest-energy species were reoptimized to the same level of theory but using acetonitrile as solvent. To compare energetics, we also carried out single-point energy calculations for the lowest energy structures using uM06L-d3/def2-TZVPP(19)-SMD(THF) [noted as uM06L-d3/def2-TZVPP-SMD(THF)//uB3LYP-d3/def2-SVP-CPCM(THF)] or using domain based local pair natural orbital coupled cluster method with single-, double-, and perturbative triple excitations and def2-SVP basis set along with def2-SVP/C[27] as auxiliary basis set [noted as DLPNO-CCSD(T)/def2-SVP-CPCM(THF)//uB3LYP-d3/def2-SVP-CPCM(THF)] with ORCA (version 4.1.1)[28]. All structural figures were generated with CYLview.[29] Distances in structural figures are shown in Å and energies are in kcal/mol.

7.2. Computational Results

Fig. S9. DFT calculation for dicarbofunctionalization of enol silyl ether. Calculated Gibbs free energies [uM06L-d3/def2tzvpp-SMD(THF)//uB3LYP-d3/def2-svp-CPCM(THF)] are given in kcal mol^{-1}.



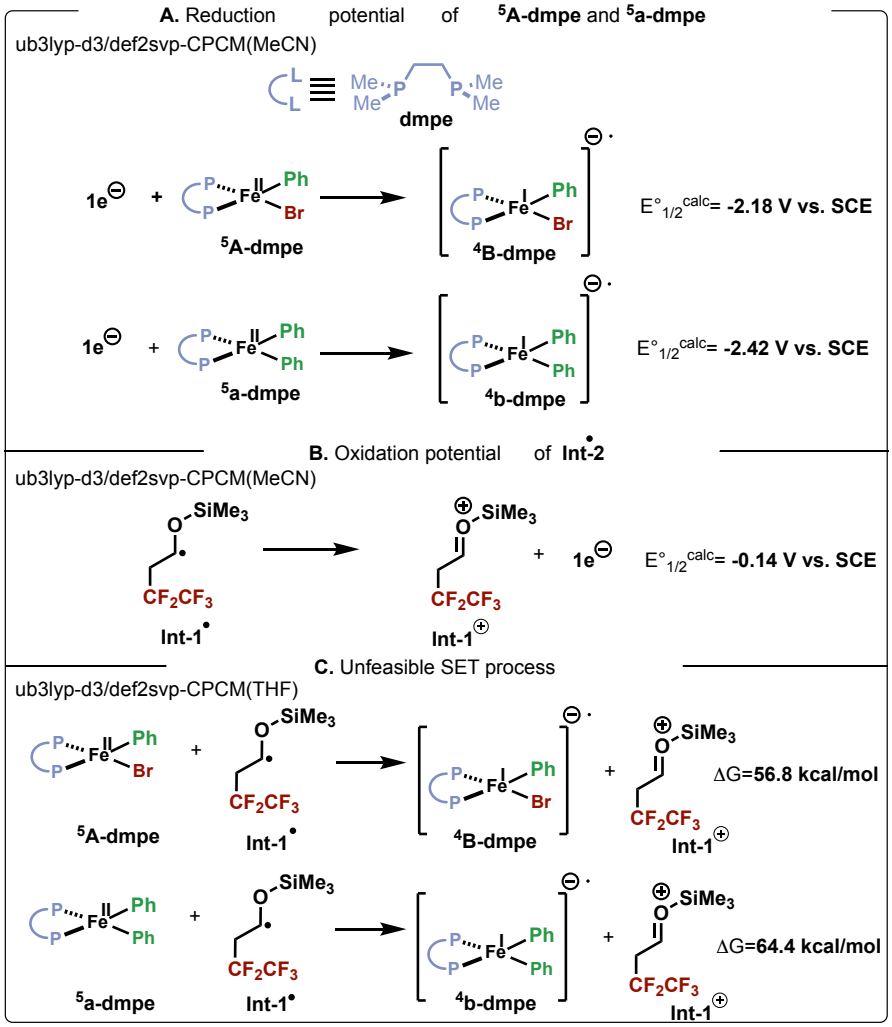
Redox potential

Redox potentials were computed from the relative Gibbs free energy differences (at the uB3LYP-d3/def2-SVP-CPCM(MeCN) level of theory) of the reduced and oxidized form of the compounds:[30]

$$E_{1/2}^{\mathrm{o,calc}} = -\frac{(G_{298}[\mathrm{reduced}] - G_{298}[\mathrm{oxidized}])}{n_e \mathcal{F}} - E_{1/2}^{\mathrm{o,SHE}} + E_{1/2}^{\mathrm{o,SCE}}$$

Where n_e is the number of electrons transferred (in all calculations here, n_e = 1 and is accordingly omitted from all subsequent expressions), $\mathcal{F}$ is the Faraday constant (value 23.061 kcal mol^{-1} V^{-1}), $E_{1/2}^{o,SHE}$ is the absolute value for the standard hydrogen electrode (SHE, value = 4.281 V) and $E_{1/2}^{o,SCE}$ is the potential of the saturated calomel electrode (SCE) relative to SHE in acetonitrile (value = - 0.141 V), and G_{298} [oxidized] and G_{298} [reduced] are the Gibbs free energies in acetonitrile as gathered from DFT calculations.

Fig. S10. Redox Potential calculated at the uB3LYP-d3/def2-SVP-CPCM(MeCN) level of theory.



The redox potential value is negative (E°cell = ~-2.4 V vs. SCE in MeCN) for bisphosphine-iron complex catalyzed oxidation of α-silyloxy radical to produce silyloxocarbonium via SET (Fig. S10).

Fig. S11. Energy profile of CF_3CF_2 radical addition on Silicon-tethered olefin (**2.8**). Calculated enthalpies and Gibbs free energies [DLPNO-CCSD(T)/def2TZVPP-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)] are given in kcal mol^{-1}.

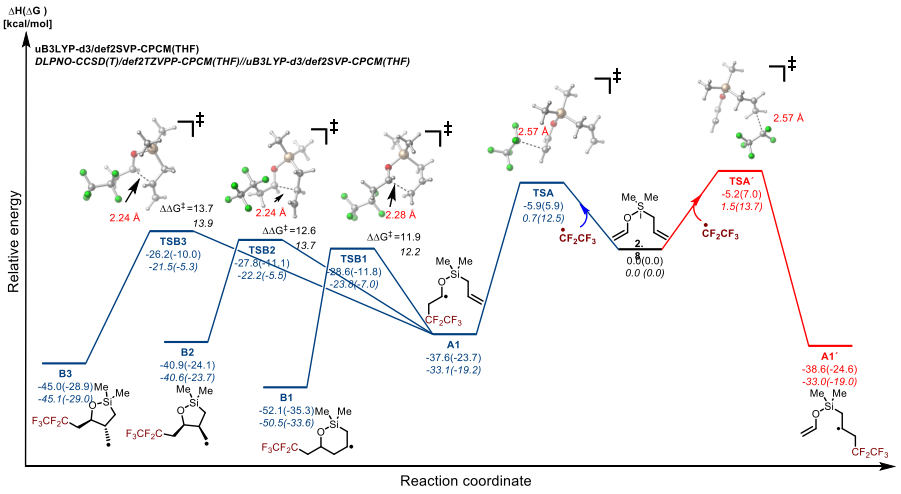


Fig. S12. Energy Profile for radical cascade annulation. Calculated enthalpies and Gibbs free energies [DLPNO-CCSD(T)/def2TZVPP-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)] are given in kcal mol^{-1}.

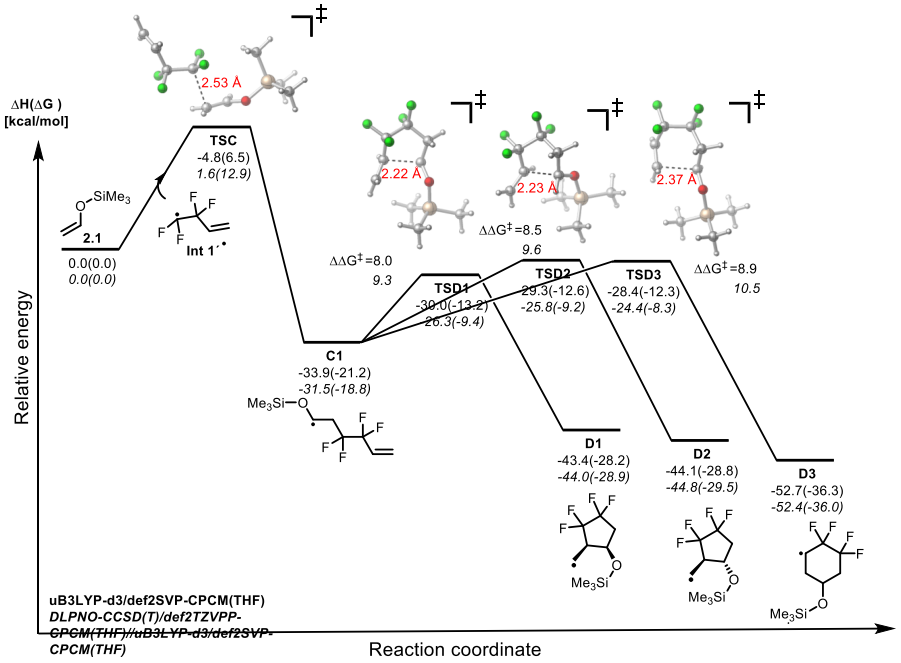
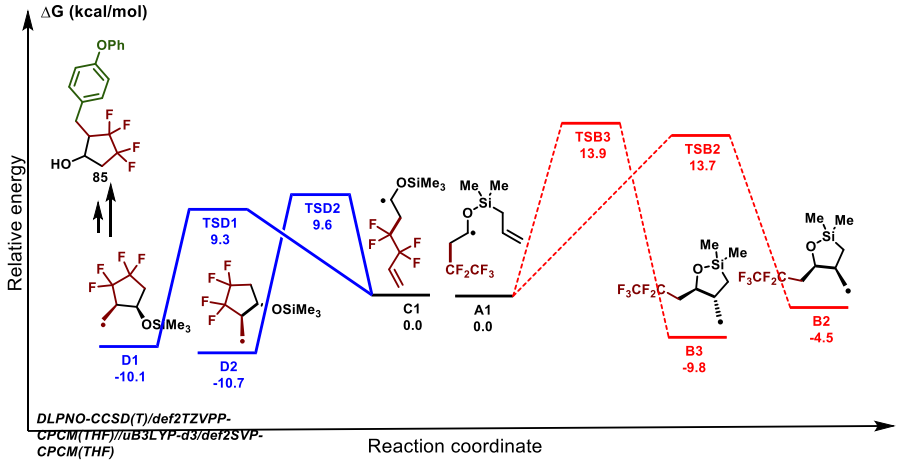
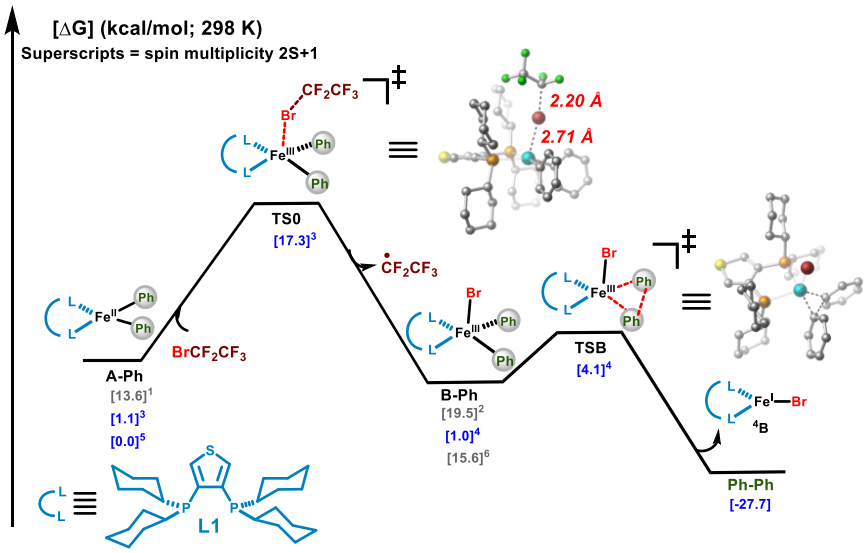


Fig. S13. Energy profile Comparison between 5-exo cyclization of A1 and C1 radical. Calculated Gibbs free energies [DLPNO-CCSD(T)/def2tzvpp-CPCM(THF)//uB3LYP-d3/def2-svp-CPCM(THF)] are given in kcal mol^{-1}.



We performed dispersion-corrected density functional theory (DFT) and domain-based local pair natural orbital coupled cluster method with single and double and perturbative triple excitation (DLPNO-CCSD(T)) calculations to gain insights into the radical cascade cyclization mechanism of silicon-tethered olefin (**2.8**) and enol silyl ether (**2.1**). First, the addition of electrophilic radical $^{\bullet}\mathbf{CF_2CF_3}$ for both olefin sites of silicon tethered diene (**2.8.**) was investigated (**Fig. S11**). Calculations shows that addition on the more electron-rich alkene site is kinetically favored ($\Delta G^{\ddagger}$ =12.5 vs. 13.7 kcal/mol) to form the stable radical **A1** ($\Delta G°$ = -19.2 kcal/mol). Notably, radical cyclization from the putative α-silyloxy radical (via **TSB2** and **TSB3**) is found to be ~5 kcal/mol higher compared to the annulation product (**TSD1** and **TSD2**) of the MAC reaction (Fig. S13). Therefore, **A1** prefers to undergo direct cross-coupling with organo-iron species, presumably kinetically more favored, which leads to the formation of the acyclic compound **90** (Fig. 5B).

Fig. S14. Energy profile for radical generation. Calculated Gibbs free energies [uB3LYP-d3/def2-svp-CPCM(THF)] are given in kcal mol^{-1}.



The active bis-phenyl bisphosphine-iron(II) species (**A-Ph**) abstract halogen of the corresponding fluoroalkyl halide through the selective triplet spin state **TS0** (barrier ~17 Kcal/mol) leading to the formation of **•CF_2CF_3** radical and distorted square pyramidal iron(III) species (**^{4}B-Ph).** Despite this process is reversible, **^{4}B-Ph** can undergo irreversible reductive elimination through the quartet spin state **TSB** to produces side product biphenyl (also confirmed by experimentally) and iron(I) species (**^{4}B)** which also might involve in the radical generation process.

7.3. Cartesian coordinates

Table S5. Cartesian coordinates (xyz format) of all the structures involved in each reaction mechanism studied calculated at the CPCM(THF) uB3LYP-d3/def2-SVP and single-point energies calculated at different levels of theory.

2.1
E(scf) = -601.557549899 a.u.
ν_{min} = 31.79 cm^{-1}

C	-1.217294	1.750125	0.211729	C	0.961362	-2.320598	-0.688153
C	-0.525967	0.818506	-0.459220	C	3.418422	-0.474590	-0.219644
C	-2.660954	2.072519	-0.042373	C	1.761518	-0.237222	-2.840078
O	0.781519	0.546025	-0.212684	H	-0.691205	2.310061	0.994224
Si	1.726855	-0.634110	-1.003956	H	-1.007989	0.229041	-1.254547

H	-2.797325	3.130170	-0.331310	H	3.831494	0.535092	-0.375963
H	-3.082432	1.449274	-0.847824	H	4.117808	-1.202801	-0.662515
H	-3.278425	1.915698	0.860311	H	3.369167	-0.663835	0.864949
H	-0.061453	-2.377923	-1.095555	H	0.749734	-0.273446	-3.276426
H	1.559101	-3.115028	-1.165457	H	2.174803	0.769669	-3.014591
H	0.912351	-2.530975	0.392788	H	2.388311	-0.964153	-3.383105

Zero-point correction= 0.184081 (Hartree/Particle)
Thermal correction to Energy= 0.196941
Thermal correction to Enthalpy= 0.197885
Thermal correction to Gibbs Free Energy= 0.144735
Sum of electronic and zero-point Energies= -601.373469
Sum of electronic and thermal Energies= -601.360609
Sum of electronic and thermal Enthalpies= -601.359665
Sum of electronic and thermal Free Energies= -601.412815

SMD(THF) uM06L-d3/def2-TZVPP
E(scf) = -562.606151921 a.u.

DLPNO-CCSD(T)/def2-SVP-CPCM(THF)
E= -561.636539905348 a.u.

$CF_2CF_3^{\bullet}$
E(scf) = -574.916403008 a.u.
ν_{min} = 51.75 cm^{-1}

C	1.452101	0.223043	4.039789
C	2.084227	1.549569	4.417129
F	0.183333	0.107438	4.379835
F	2.163709	-0.835119	4.375648
F	1.354135	2.553508	3.928895
F	3.320339	1.619095	3.920611
F	2.162527	1.702257	5.751346

Zero-point correction= 0.024518 (Hartree/Particle)
Thermal correction to Energy= 0.030706
Thermal correction to Enthalpy= 0.031650
Thermal correction to Gibbs Free Energy= -0.007299
Sum of electronic and zero-point Energies= -574.891885
Sum of electronic and thermal Energies= -574.885697
Sum of electronic and thermal Enthalpies= -574.884753
Sum of electronic and thermal Free Energies= -574.923702

SMD(THF) uM06L-d3/def2-TZVPP
E(scf) = -575.517332907 a.u.

DLPNO-CCSD(T)/def2-SVP-CPCM(THF)
E= -574.704172379334 a.u.

TS1
E(scf) = -1137.19270140 a.u.
ν_{min} = -55.10 cm^{-1}

C	1.566145	-1.574327	-1.095036	F	1.449787	-3.874121	-0.734417
C	-1.133615	-0.190179	-0.879236	H	-1.260402	0.457899	-1.758921
F	1.938849	-1.314852	0.155605	H	-1.168544	-1.986527	-1.999153
F	1.948456	-0.604786	-1.921596	H	-0.951074	-2.174612	-0.141272
C	-1.045224	-1.528950	-1.017049	H	-0.183082	1.514834	3.016569
O	-1.031516	0.421780	0.312087	H	-0.368566	3.267033	2.735006
Si	-0.451719	2.014081	0.597934	H	-1.798674	2.200771	2.680846
C	-0.728204	2.270894	2.428739	H	-1.317254	3.016785	-1.526959
C	-1.454033	3.206220	-0.449815	H	-1.137123	4.243657	-0.251079
C	1.364840	2.033805	0.133434	H	-2.528582	3.126616	-0.217922
C	1.957473	-2.955600	-1.563922	H	1.809734	3.024644	0.322243
F	3.292993	-3.137480	-1.607952	H	1.919953	1.282151	0.716424
F	1.477697	-3.168214	-2.794393	H	1.498257	1.791299	-0.932911

Zero-point correction= 0.181464 (Hartree/Particle)
Thermal correction to Energy= 0.200040
Thermal correction to Enthalpy= 0.200984
Thermal correction to Gibbs Free Energy= 0.130885
Sum of electronic and zero-point Energies= -1137.011237
Sum of electronic and thermal Energies= -1136.992662
Sum of electronic and thermal Enthalpies= -1136.991718
Sum of electronic and thermal Free Energies= -1137.061817
SMD(THF) uM06L-d3/def2-TZVPP
E(scf) = -1138.12977451 a.u.

Int-1•
E(scf) = -1137.24157831 a.u.
ν_{min} = 8.45 cm^{-1}

C	1.281642	-2.140142	-1.705124	C	-1.070407	2.359388	2.329117
C	0.324577	-0.045880	-0.755950	C	-1.349988	2.971985	-0.708429
F	2.528561	-1.868549	-1.237457	C	1.462358	2.922173	0.607357
F	1.203725	-1.628705	-2.966754	C	1.184307	-3.677134	-1.843101
C	0.217122	-1.534017	-0.814597	F	2.158324	-4.146858	-2.624961
O	-0.174498	0.534068	0.359324	F	0.007042	-4.021956	-2.378237
Si	-0.278908	2.223839	0.639783	F	1.287547	-4.255545	-0.640589

H	0.357104	0.535454	-1.685871	H	-0.902483	2.826665	-1.705150
H	-0.765555	-1.879957	-1.194782	H	-1.468344	4.056539	-0.547866
H	0.336207	-1.954040	0.195873	H	-2.352803	2.514567	-0.710816
H	-0.452660	1.861714	3.094079	H	1.451894	4.007992	0.798989
H	-1.182478	3.418034	2.615921	H	2.089499	2.443448	1.377013
H	-2.070112	1.895747	2.335440	H	1.934727	2.754070	-0.374213

Zero-point correction= 0.184122 (Hartree/Particle)
Thermal correction to Energy= 0.202180
Thermal correction to Enthalpy= 0.203125
Thermal correction to Gibbs Free Energy= 0.134234
Sum of electronic and zero-point Energies= -1137.057457
Sum of electronic and thermal Energies= -1137.039398
Sum of electronic and thermal Enthalpies= -1137.038454
Sum of electronic and thermal Free Energies= -1137.107344

SMD(THF) uM06L-d3/def2-TZVPP
E(scf) = -1138.17619464 a.u.

^{1}A
E(scf) = -6243.70036056 a.u.
ν_{min} = 17.49 cm^{-1}

Br	6.723396	2.788715	18.382574	H	9.148447	10.068758	17.784006
Fe	7.266099	5.047009	17.519770	C	10.645486	4.207175	18.660393
C	5.715492	5.011828	16.299616	H	11.440151	4.622410	19.306184
C	4.411767	4.993994	16.844705	C	11.053196	4.416359	17.189802
H	4.291469	4.928153	17.931533	H	10.216247	4.094041	16.543673
C	3.264708	5.060529	16.045656	H	11.210390	5.487727	16.988475
C	3.381982	5.121209	14.650533	C	12.312905	3.620449	16.828729
H	2.489992	5.174047	14.019932	H	13.169333	4.020871	17.401883
C	4.657827	5.100326	14.075958	H	12.552437	3.765619	15.761939
H	4.767340	5.130484	12.986967	C	12.143521	2.130813	17.147407
C	5.797835	5.047733	14.891264	H	13.069642	1.579017	16.914556
H	6.780176	5.041347	14.405401	H	11.352706	1.709886	16.499358
H	2.273574	5.060965	16.510969	C	11.751191	1.925123	18.615004
S	10.836082	9.212606	19.350843	H	11.597461	0.853832	18.827096
P	9.100045	5.194119	19.004001	H	12.582993	2.258294	19.263059
P	7.623155	7.273101	17.075989	C	10.482681	2.709710	18.978030
C	10.730840	7.515045	19.665544	H	10.247317	2.562346	20.043904
H	11.442807	7.047538	20.344003	H	9.622089	2.313074	18.413810
C	9.693633	6.929882	18.974126	C	8.636935	4.829894	20.770337
C	8.986561	7.878272	18.146524	H	8.337470	3.768729	20.705983
C	9.489055	9.155236	18.268871	C	9.744686	4.976256	21.823818

H	10.063621	6.031302	21.872801	H	10.053459	8.417327	11.943309
H	10.632571	4.384437	21.549770	C	8.780875	9.257622	13.499564
C	9.238129	4.552276	23.211022	H	7.854725	9.051536	12.932594
H	8.994636	3.474269	23.191992	H	9.054263	10.304728	13.287471
H	10.039218	4.681803	23.958017	C	8.499425	9.087226	15.000176
C	7.991254	5.347110	23.617338	H	7.699325	9.775564	15.315277
H	8.264929	6.412478	23.732204	H	9.405022	9.367084	15.563930
H	7.623278	5.009172	24.600590	C	6.226220	8.454775	17.447002
C	6.885915	5.224201	22.561793	H	6.687857	9.454068	17.540460
H	6.013398	5.838023	22.841819	C	5.154799	8.515387	16.341694
H	6.535212	4.176800	22.520574	H	4.760693	7.505331	16.155764
C	7.384599	5.631865	21.169425	H	5.594321	8.865343	15.395205
H	7.626216	6.710263	21.165823	C	4.000309	9.444944	16.742886
H	6.587452	5.479680	20.424564	H	4.374526	10.483097	16.815653
C	8.136138	7.628567	15.321368	H	3.234090	9.441092	15.949720
H	7.225373	7.362134	14.758170	C	3.384577	9.036777	18.085942
C	9.259254	6.678855	14.868586	H	2.933639	8.032648	17.985698
H	10.170855	6.893149	15.453373	H	2.568626	9.725962	18.360898
H	8.991458	5.631812	15.082158	C	4.450113	9.001493	19.187177
C	9.558162	6.851039	13.373628	H	4.010725	8.673998	20.144254
H	8.673377	6.530049	12.793884	H	4.839868	10.023095	19.351384
H	10.386568	6.185600	13.078773	C	5.610023	8.074009	18.807405
C	9.888883	8.307956	13.028217	H	5.240300	7.036128	18.744333
H	10.837838	8.589434	13.521136	H	6.383957	8.086371	19.591324

Zero-point correction= 0.785604 (Hartree/Particle)
Thermal correction to Energy= 0.826231
Thermal correction to Enthalpy= 0.827175
Thermal correction to Gibbs Free Energy= 0.711092
Sum of electronic and zero-point Energies= -6242.914757
Sum of electronic and thermal Energies= -6242.874129
Sum of electronic and thermal Enthalpies= -6242.873185
Sum of electronic and thermal Free Energies= -6242.989269

SMD(THF) uM06L-d3/def2-TZVPP
E(scf) = -6245.46274313 a.u.

^{3}A
E(scf) = -6243.72015914 a.u.
ν_{min} = 12.10 cm^{-1}

Br	6.745345	2.777327	18.406765	C	5.693278	4.994760	16.321168
Fe	7.269347	5.028947	17.521423	C	4.401830	4.980332	16.892938

H	4.302346	4.904741	17.980897	C	8.004284	5.381950	23.611866
C	3.240594	5.061173	16.115613	H	8.270349	6.450104	23.718478
C	3.332459	5.132496	14.719272	H	7.638199	5.049154	24.597578
H	2.429118	5.196057	14.106115	C	6.900461	5.243020	22.556696
C	4.596870	5.107525	14.119806	H	6.023470	5.852836	22.831466
H	4.685596	5.145063	13.029231	H	6.557137	4.192886	22.523283
C	5.751820	5.040823	14.912386	C	7.397282	5.643574	21.161721
H	6.724892	5.031109	14.408740	H	7.631657	6.723493	21.150217
H	2.258356	5.063936	16.599255	H	6.602845	5.480367	20.416363
S	10.828521	9.232439	19.314749	C	8.121576	7.601594	15.306832
P	9.116846	5.202098	19.001007	H	7.207291	7.334627	14.749718
P	7.616390	7.261601	17.066844	C	9.238953	6.643845	14.856699
C	10.734234	7.536540	19.641715	H	10.153594	6.858417	15.436523
H	11.451230	7.077738	20.320839	H	8.967209	5.599823	15.080100
C	9.698042	6.940797	18.957923	C	9.532950	6.803759	13.359462
C	8.982279	7.879067	18.126718	H	8.644909	6.481850	12.785205
C	9.477768	9.159753	18.238252	H	10.357802	6.133068	13.066554
H	9.130165	10.067914	17.748301	C	9.867812	8.256857	13.002075
C	10.667496	4.221870	18.663407	H	10.819440	8.538536	13.489717
H	11.458244	4.643313	19.310059	H	10.029127	8.357534	11.915837
C	11.079198	4.427469	17.193369	C	8.764835	9.214098	13.469941
H	10.246800	4.098275	16.545028	H	7.835930	9.006832	12.907918
H	11.231646	5.498923	16.988548	H	9.041117	10.258544	13.248684
C	12.344668	3.636767	16.840954	C	8.488278	9.056496	14.972859
H	13.196503	4.043899	17.416238	H	7.691252	9.749625	15.285463
H	12.588078	3.778980	15.774654	H	9.396697	9.337931	15.531260
C	12.181702	2.147479	17.164719	C	6.219918	8.445545	17.433950
H	13.111695	1.599689	16.937928	H	6.682216	9.445579	17.515822
H	11.395883	1.719877	16.514965	C	5.143273	8.497392	16.333384
C	11.784370	1.945228	18.631453	H	4.746912	7.486547	16.157868
H	11.635005	0.873998	18.846912	H	5.578685	8.838762	15.381822
H	12.611857	2.284879	19.281659	C	3.991387	9.431213	16.732032
C	10.510683	2.724972	18.986655	H	4.366461	10.469758	16.794142
H	10.272265	2.580931	20.052322	H	3.221408	9.420888	15.942560
H	9.653938	2.321873	18.421126	C	3.382017	9.034663	18.081436
C	8.655366	4.847140	20.769677	H	2.930754	8.029673	17.991899
H	8.363133	3.783520	20.713349	H	2.567340	9.726206	18.354281
C	9.761772	5.008943	21.822310	C	4.452865	9.009034	19.177794
H	10.074198	6.066326	21.862899	H	4.017961	8.690325	20.139887
H	10.653370	4.420299	21.553448	H	4.843363	10.032095	19.330889
C	9.257015	4.592733	23.212581	C	5.610890	8.077863	18.801163
H	9.021097	3.512923	23.202067	H	5.242189	7.039047	18.750956
H	10.056674	4.733852	23.959007	H	6.389109	8.098590	19.580679

Zero-point correction= 0.785456 (Hartree/Particle)
Thermal correction to Energy= 0.826164
Thermal correction to Enthalpy= 0.827109
Thermal correction to Gibbs Free Energy= 0.709426
Sum of electronic and zero-point Energies= -6242.934703
Sum of electronic and thermal Energies= -6242.893995
Sum of electronic and thermal Enthalpies= -6242.893051
Sum of electronic and thermal Free Energies= -6243.010733

SMD(THF) uM06L-d3/def2-TZVPP
E(scf) = -6245.48033817 a.u.

^{5}A
E(scf) = -6243.73201780 a.u.
ν_{min} = 18.59 cm^{-1}

Br	-0.397740	-4.217114	3.439686	H	-3.676518	0.681161	3.431559
Fe	1.290840	-2.838938	2.301963	H	-3.612478	-0.525455	4.726192
C	2.067664	-3.632045	0.575236	C	-4.144555	-1.328256	2.770202
C	3.375744	-4.128988	0.388770	H	-5.230720	-1.203828	2.915598
H	4.075605	-4.140772	1.229986	H	-3.899809	-2.364272	3.068076
C	3.825419	-4.612047	-0.847901	C	-3.777259	-1.130653	1.294998
C	2.964549	-4.619031	-1.951497	H	-4.312133	-1.857833	0.661518
H	3.310904	-4.989428	-2.920600	H	-4.105789	-0.126477	0.969249
C	1.652822	-4.152564	-1.800032	C	-2.265061	-1.262800	1.068586
H	0.967256	-4.162008	-2.653320	H	-2.027499	-1.080722	0.007466
C	1.221033	-3.673169	-0.556356	H	-1.947663	-2.296657	1.295925
H	0.187039	-3.319038	-0.469730	C	0.754393	-0.105614	-0.009899
H	4.850032	-4.983360	-0.951023	H	0.334567	-0.941230	-0.597734
S	2.042137	2.791723	3.935180	C	0.140998	1.203883	-0.527619
P	0.347695	-0.603183	1.742964	H	0.528520	2.049489	0.066108
P	2.640327	-1.550908	3.955767	H	-0.954115	1.201183	-0.408876
C	0.971621	1.992042	2.839254	C	0.502941	1.425626	-2.004899
H	0.241775	2.573123	2.277437	H	0.032815	0.630437	-2.612022
C	1.182967	0.631065	2.810853	H	0.077317	2.381275	-2.354206
C	2.228046	0.223738	3.727458	C	2.020339	1.399966	-2.226449
C	2.786167	1.298264	4.385001	H	2.475781	2.260443	-1.701912
H	3.597479	1.299027	5.111380	H	2.253041	1.525324	-3.297233
C	-1.471380	-0.301311	1.975132	C	2.638700	0.102979	-1.690920
H	-1.693498	0.740733	1.683815	H	3.734989	0.118224	-1.810802
C	-1.854754	-0.494415	3.455078	H	2.268947	-0.754172	-2.282642
H	-1.537054	-1.501762	3.772725	C	2.280491	-0.122678	-0.217193
H	-1.311393	0.227470	4.085473	H	2.737520	0.672265	0.398973
C	-3.367586	-0.354808	3.664394	H	2.693934	-1.079803	0.132765

C	2.264912	-1.921721	5.747531	C	4.489149	-1.626461	3.769626
H	2.379215	-3.020676	5.792210	H	4.937491	-0.927813	4.497799
C	0.789561	-1.595005	6.050740	C	4.990206	-3.052211	4.069030
H	0.634898	-0.505861	5.950837	H	4.446274	-3.763578	3.421580
H	0.138597	-2.083671	5.311279	H	4.755541	-3.336572	5.107425
C	0.404297	-2.034627	7.468684	C	6.499471	-3.182343	3.822139
H	0.456100	-3.137156	7.529007	H	7.038276	-2.554279	4.555092
H	-0.643934	-1.758253	7.671774	H	6.817173	-4.222252	4.005216
C	1.335739	-1.422748	8.521557	C	6.882656	-2.742973	2.404258
H	1.197808	-0.325561	8.532206	H	6.424018	-3.433129	1.672691
H	1.069368	-1.783204	9.529266	H	7.973875	-2.814994	2.262757
C	2.804031	-1.739065	8.213114	C	6.398431	-1.316243	2.119875
H	2.969280	-2.828363	8.302707	H	6.643733	-1.023272	1.085391
H	3.467113	-1.258374	8.951795	H	6.932437	-0.611068	2.783138
C	3.194349	-1.290371	6.796180	C	4.888311	-1.180513	2.349732
H	4.247035	-1.548512	6.601589	H	4.350386	-1.804019	1.615868
H	3.115952	-0.191361	6.737270	H	4.565924	-0.141937	2.174742

Zero-point correction= 0.784098 (Hartree/Particle)
Thermal correction to Energy= 0.825551
Thermal correction to Enthalpy= 0.826496
Thermal correction to Gibbs Free Energy= 0.705118
Sum of electronic and zero-point Energies= -6242.947920
Sum of electronic and thermal Energies= -6242.906466
Sum of electronic and thermal Enthalpies= -6242.905522
Sum of electronic and thermal Free Energies= -6243.026900

SMD(THF) uM06L-d3/def2-TZVPP
E(scf) = -6245.49334891 a.u.

^{2}TS2
E(scf) = -7380.97466965 a.u.
ν_{min} = -279.25 cm^{-1}

Fe	8.867503	6.408598	12.611770	H	10.625254	1.622064	12.620703
Br	7.648228	5.662921	14.635917	H	11.359511	3.759433	8.941255
C	9.685592	4.815297	11.757367	H	11.620797	1.689203	10.325920
C	9.832550	3.631196	12.507693	C	7.039561	5.607779	11.119062
C	10.248551	4.819382	10.466014	S	11.199535	11.664215	13.734663
C	10.523214	2.521258	12.004525	P	10.971845	7.306569	13.373058
H	9.400401	3.577915	13.509944	P	8.177828	8.771386	12.440557
C	10.933232	3.712554	9.948265	C	11.815618	10.049112	13.705586
H	10.166618	5.711615	9.838810	H	12.856034	9.862953	13.969113
C	11.081188	2.554482	10.720533	C	10.845562	9.137331	13.354161

C	9.577750	9.768590	13.077256
C	9.624744	11.133307	13.259488
H	8.822825	11.859989	13.136290
C	12.619629	6.974642	12.566536
H	13.357194	7.562040	13.142283
C	12.637322	7.487751	11.113879
H	11.855833	6.965626	10.540574
H	12.393012	8.561324	11.084755
C	14.000200	7.236898	10.454797
H	14.767130	7.848227	10.965586
H	13.973578	7.577951	9.406168
C	14.399856	5.758370	10.530789
H	15.393561	5.605627	10.077186
H	13.683235	5.158761	9.940950
C	14.388750	5.258702	11.980246
H	14.640748	4.185752	12.019543
H	15.169165	5.789280	12.557036
C	13.020848	5.488075	12.636390
H	13.037313	5.134966	13.679134
H	12.266596	4.883584	12.116389
C	11.197120	6.929256	15.202115
H	10.896784	5.868059	15.268361
C	12.616401	7.085068	15.776000
H	12.923399	8.143836	15.706919
H	13.353045	6.501795	15.206077
C	12.653484	6.642097	17.248268
H	12.437153	5.559145	17.296510
H	13.671719	6.776850	17.650324
C	11.633084	7.399527	18.105831
H	11.925526	8.464737	18.156797
H	11.646765	7.019594	19.141273
C	10.223867	7.298329	17.510857
H	9.512364	7.902919	18.098264
H	9.868961	6.253204	17.564927
C	10.207163	7.755250	16.048317
H	10.496049	8.818983	15.998769
H	9.193659	7.675531	15.636887
C	8.019106	9.361564	10.672195
H	7.257782	8.687209	10.256326
C	9.343072	9.122810	9.919229
H	10.117900	9.788954	10.336472
H	9.709777	8.096823	10.085185
C	9.187135	9.396903	8.417993
H	8.486197	8.661168	7.985183
H	10.154507	9.248224	7.910105
C	8.657676	10.813643	8.166581
H	9.416681	11.546972	8.496311
H	8.505537	10.980909	7.087298
C	7.353663	11.062553	8.933791
H	6.566313	10.394672	8.539288
H	7.002522	12.095668	8.774619
C	7.518390	10.795277	10.439056
H	6.556545	10.963240	10.947726
H	8.240420	11.515625	10.860490
C	6.666037	9.413082	13.319555
H	6.531371	10.463232	13.007145
C	5.433655	8.598503	12.879234
H	5.606938	7.542765	13.148199
H	5.304886	8.634908	11.785235
C	4.158819	9.087987	13.577611
H	3.933040	10.117685	13.244528
H	3.304980	8.461576	13.269709
C	4.318203	9.069958	15.102265
H	4.443040	8.024290	15.438494
H	3.405736	9.452967	15.589143
C	5.542041	9.884704	15.538772
H	5.666988	9.836148	16.633533
H	5.379907	10.949232	15.286759
C	6.821236	9.387744	14.851757
H	7.026793	8.354707	15.173745
H	7.682951	10.000719	15.158627
O	6.739811	4.286441	11.218869
Si	5.629238	3.383752	12.150477
C	4.785501	2.249440	10.909268
H	4.162481	1.507050	11.435780
H	4.146994	2.808612	10.210610
H	5.540487	1.701998	10.321006
C	6.573453	2.319824	13.370493
H	7.359585	1.753643	12.845741
H	7.048371	2.931637	14.149499
H	5.885970	1.599698	13.845906
C	4.409044	4.558802	12.960758
H	4.918242	5.196741	13.698758
H	3.929414	5.202125	12.206059
H	3.618671	3.989593	13.477880
H	6.332109	6.276030	11.627191

C	7.367650	5.991145	9.693957	F	5.622151	4.208835	8.215842
H	8.070574	6.829604	9.654539	F	4.356136	5.199643	9.680052
H	7.851096	5.141759	9.195456	F	4.272940	5.789906	7.599995
C	6.198230	6.429228	8.830384	F	6.662827	6.813473	7.607858
C	5.090166	5.380505	8.573451	F	5.563964	7.517696	9.369789

Zero-point correction= 0.973567 (Hartree/Particle)
Thermal correction to Energy= 1.032236
Thermal correction to Enthalpy= 1.033180
Thermal correction to Gibbs Free Energy= 0.878785
Sum of electronic and zero-point Energies= -7380.001102
Sum of electronic and thermal Energies= -7379.942434
Sum of electronic and thermal Enthalpies= -7379.941489
Sum of electronic and thermal Free Energies= -7380.095885

SMD(THF) uM06L-d3/def2-TZVPP
E(scf) = -7383.662116 a.u.

^{4}TS2
E(scf) = -7381.01104480 a.u.
ν_{min} = -30.80 cm^{-1}

Fe	9.095192	6.396917	12.653751	H	9.013448	11.919520	12.921217
Br	7.903180	5.529044	14.666093	C	12.797791	7.052677	12.927476
C	9.853928	4.960731	11.404433	H	13.572911	7.618350	13.474269
C	9.915702	3.667207	11.969675	C	12.791382	7.530835	11.463540
C	10.403200	5.102317	10.114872	H	11.950420	7.051025	10.939793
C	10.507175	2.588180	11.301828	H	12.618325	8.617910	11.419654
H	9.487449	3.497586	12.963123	C	14.100596	7.171626	10.748906
C	10.996000	4.032219	9.430041	H	14.932607	7.737729	11.207530
H	10.375312	6.074614	9.612045	H	14.046671	7.491258	9.694437
C	11.054916	2.767028	10.024839	C	14.398937	5.670173	10.840989
H	10.539060	1.602296	11.776818	H	15.356218	5.437521	10.344759
H	11.415271	4.188037	8.431046	H	13.613239	5.111548	10.301445
H	11.518917	1.928412	9.497997	C	14.426270	5.205098	12.301447
C	6.898137	5.489886	11.006077	H	14.606659	4.118468	12.357293
S	11.301908	11.793488	13.804495	H	15.268917	5.693167	12.825650
P	11.157010	7.413078	13.732962	C	13.114455	5.546842	13.020295
P	8.397289	8.804045	12.461734	H	13.167193	5.225762	14.073565
C	11.909948	10.186039	13.989251	H	12.288557	4.981273	12.559016
H	12.915867	10.031699	14.377283	C	11.393015	7.094192	15.565713
C	10.989103	9.236929	13.603997	H	11.197781	6.008777	15.643768
C	9.763439	9.835280	13.120612	C	12.784509	7.385491	16.152165
C	9.795352	11.211489	13.191354	H	13.004064	8.462960	16.053911

H	13.571411	6.847980	15.602129	H	4.123821	10.038948	13.345750
C	12.843980	6.996331	17.637995	H	3.537485	8.367330	13.331539
H	12.721347	5.901058	17.724167	C	4.562611	8.947410	15.166518
H	13.841120	7.233731	18.045474	H	4.716234	7.895475	15.469677
C	11.749339	7.692345	18.455088	H	3.649227	9.294806	15.677752
H	11.938705	8.781911	18.457663	C	5.774273	9.776948	15.608808
H	11.788831	7.363649	19.507256	H	5.918803	9.697337	16.699333
C	10.361951	7.427913	17.859229	H	5.583624	10.844652	15.392989
H	9.588480	7.977724	18.421625	C	7.052719	9.332949	14.885725
H	10.117155	6.354228	17.955051	H	7.288169	8.294558	15.170304
C	10.304484	7.822344	16.378596	H	7.905398	9.955118	15.199455
H	10.457350	8.911976	16.286880	O	6.603328	4.183485	11.110485
H	9.312174	7.598539	15.964702	Si	5.519662	3.340367	12.141548
C	8.187728	9.353669	10.689975	C	4.476180	2.305360	10.972989
H	7.415075	8.661457	10.323247	H	3.806986	1.637491	11.540759
C	9.482954	9.083350	9.900769	H	3.862052	2.942662	10.319433
H	10.274790	9.759980	10.267467	H	5.121386	1.679147	10.335072
H	9.846719	8.061626	10.092343	C	6.547660	2.232431	13.245765
C	9.273030	9.301744	8.396609	H	7.223926	1.611056	12.636405
H	8.560739	8.547868	8.016677	H	7.153970	2.833651	13.939110
H	10.221963	9.137450	7.859514	H	5.895571	1.561876	13.830298
C	8.725377	10.704864	8.108691	C	4.490028	4.597968	13.077987
H	9.490884	11.455025	8.380516	H	5.125019	5.186916	13.757599
H	8.533266	10.827348	7.029738	H	3.982385	5.283557	12.380349
C	7.447956	10.978620	8.912209	H	3.718908	4.087219	13.678138
H	6.651654	10.289835	8.576245	H	6.346988	6.185284	11.645825
H	7.084173	12.002152	8.722499	C	7.262306	5.936430	9.622523
C	7.673174	10.775545	10.419690	H	8.011516	6.737292	9.647015
H	6.734113	10.964413	10.963003	H	7.706929	5.097587	9.071430
H	8.411428	11.513215	10.777201	C	6.113748	6.493700	8.799000
C	6.875184	9.399953	13.357421	C	4.927527	5.531977	8.546368
H	6.717359	10.454940	13.072105	F	5.368116	4.348754	8.110477
C	5.655651	8.568927	12.914979	F	4.235132	5.338047	9.678597
H	5.859156	7.511810	13.156739	F	4.095144	6.038897	7.634623
H	5.507147	8.627801	11.824769	F	6.571250	6.887362	7.578179
C	4.379834	9.006162	13.645597	F	5.580616	7.605016	9.397434

Zero-point correction= 0.972379 (Hartree/Particle)
Thermal correction to Energy= 1.031716
Thermal correction to Enthalpy= 1.032661
Thermal correction to Gibbs Free Energy= 0.874204
Sum of electronic and zero-point Energies= -7380.038666
Sum of electronic and thermal Energies= -7379.979328

Sum of electronic and thermal Enthalpies= -7379.978384
Sum of electronic and thermal Free Energies= -7380.136841

SMD(THF) uM06L-d3/def2-TZVPP
E(scf) = -7383.69660786 a.u.

^{6}TS2
E(scf) = -7380.99141016 a.u.
ν_{min} = -126.13 cm^{-1}

Fe	8.660989	6.073536	12.518803	C	14.473223	5.364311	11.983466
Br	7.745186	5.400657	14.691125	H	14.760857	4.300834	12.036978
C	9.809239	4.586785	11.648574	H	15.257176	5.932066	12.518558
C	10.104209	3.434620	12.407713	C	13.124633	5.568570	12.686724
C	10.352248	4.644736	10.349540	H	13.193158	5.240325	13.736207
C	10.911886	2.404530	11.907450	H	12.368609	4.928877	12.209144
H	9.703093	3.345247	13.423019	C	11.294529	6.961709	15.261238
C	11.160814	3.622888	9.834575	H	11.098661	5.876684	15.342900
H	10.159449	5.516769	9.716279	C	12.696971	7.252885	15.822502
C	11.447570	2.497879	10.617130	H	12.906869	8.333209	15.732785
H	11.128406	1.527663	12.525883	H	13.477113	6.728422	15.251849
H	11.573754	3.706388	8.824497	C	12.788685	6.844125	17.301871
H	12.082984	1.699571	10.223465	H	12.672007	5.747216	17.374825
C	6.825278	5.682984	11.034933	H	13.793440	7.079403	17.691792
S	11.053144	11.665059	13.737012	C	11.709862	7.523851	18.153060
P	11.013448	7.295427	13.429553	H	11.900280	8.613039	18.173487
P	8.128156	8.684787	12.448307	H	11.769134	7.174570	19.197711
C	11.731180	10.074365	13.732286	C	10.310867	7.273787	17.578124
H	12.777594	9.934071	14.000019	H	9.550209	7.818071	18.163094
C	10.802369	9.116753	13.389477	H	10.062136	6.199955	17.660137
C	9.511834	9.696168	13.094026	C	10.232458	7.694775	16.106039
C	9.504856	11.064818	13.260844	H	10.406592	8.782279	16.032805
H	8.676876	11.758811	13.123946	H	9.226784	7.502861	15.709185
C	12.669452	7.038652	12.601312	C	7.973200	9.265336	10.679335
H	13.403854	7.666728	13.136912	H	7.204477	8.595622	10.269486
C	12.615902	7.509845	11.135463	C	9.296410	8.996111	9.934948
H	11.832524	6.941931	10.607442	H	10.079871	9.654227	10.348822
H	12.329543	8.572376	11.086014	H	9.644389	7.965522	10.118512
C	13.960438	7.291061	10.428861	C	9.154562	9.258660	8.430074
H	14.723945	7.941875	10.894034	H	8.449884	8.528262	7.994725
H	13.881506	7.604023	9.373930	H	10.124179	9.095388	7.930942
C	14.415553	5.829802	10.523793	C	8.642740	10.679289	8.162130
H	15.397556	5.700656	10.038198	H	9.408724	11.406782	8.488642
H	13.700238	5.191839	9.974365	H	8.499160	10.837059	7.080234

C	7.336990	10.952946	8.918695	Si	5.350029	3.516941	12.134783
H	6.544280	10.289914	8.527636	C	4.300408	2.543302	10.913370
H	7.000129	11.988411	8.744490	H	3.679467	1.811022	11.456716
C	7.492609	10.702480	10.427995	H	3.637802	3.193853	10.325329
H	6.532836	10.889540	10.934858	H	4.945460	1.988726	10.212343
H	8.224269	11.417642	10.840817	C	6.270319	2.293092	13.216706
C	6.624990	9.337129	13.335906	H	6.918273	1.656921	12.591129
H	6.550973	10.413243	13.099232	H	6.898446	2.805241	13.958829
C	5.353221	8.631085	12.829909	H	5.556209	1.638415	13.744008
H	5.455363	7.550289	13.021845	C	4.313152	4.756352	13.091413
H	5.238710	8.753769	11.740361	H	4.932421	5.298696	13.821775
C	4.102079	9.144619	13.553743	H	3.849748	5.486252	12.407549
H	3.944577	10.208481	13.298088	H	3.504010	4.240345	13.634450
H	3.215255	8.597703	13.192447	H	6.053134	6.375453	11.398150
C	4.241446	9.000577	15.073699	C	7.274178	5.940766	9.611064
H	4.295903	7.926336	15.329333	H	8.037185	6.726946	9.555284
H	3.348533	9.401811	15.581554	H	7.732188	5.026927	9.211401
C	5.507769	9.701011	15.581368	C	6.194325	6.385094	8.641784
H	5.618414	9.557166	16.669202	C	5.012627	5.408520	8.436777
H	5.413190	10.790151	15.415338	F	5.457467	4.169826	8.208687
C	6.761955	9.185790	14.862795	F	4.232511	5.392096	9.527167
H	6.909386	8.120077	15.103886	F	4.262268	5.786945	7.399044
H	7.654885	9.721793	15.220796	F	6.742286	6.606486	7.413693
O	6.523302	4.351522	11.223927	F	5.631925	7.570236	9.040032

Zero-point correction= 0.972335 (Hartree/Particle)
Thermal correction to Energy= 1.031586
Thermal correction to Enthalpy= 1.032530
Thermal correction to Gibbs Free Energy= 0.874116
Sum of electronic and zero-point Energies= -7380.019075
Sum of electronic and thermal Energies= -7379.959824
Sum of electronic and thermal Enthalpies= -7379.958880
Sum of electronic and thermal Free Energies= -7380.117294

SMD(THF) uM06L-d3/def2-TZVPP
E(scf) = -7383.6838248 a.u.

^{2}Int2
E(scf) = -7381.00000364 a.u.
ν_{min} = 23.64 cm^{-1}

Fe	8.613656	6.156199	12.532570	C	9.944605	3.865425	11.170144
Br	7.541230	5.637439	14.712224	C	10.751464	2.489988	13.438626
C	9.586410	4.407954	12.422225	H	9.761852	4.040005	14.548581
C	10.014295	3.676296	13.550743	C	10.667814	2.673421	11.040154

H	9.675900	4.399144	10.263198
C	11.081442	1.975934	12.179758
H	11.069450	1.963297	14.344015
H	10.919616	2.299041	10.042926
H	11.653770	1.048619	12.088841
C	7.022248	5.710437	11.481224
S	10.947942	11.562429	13.320247
P	10.800093	7.186916	13.111269
P	7.891968	8.538212	12.512402
C	11.609437	9.967350	13.228206
H	12.685016	9.825372	13.321922
C	10.628366	9.014830	13.060558
C	9.313448	9.598447	12.971149
C	9.337648	10.967695	13.117075
H	8.502145	11.666027	13.099445
C	12.273190	6.865403	12.007875
H	13.032825	7.623097	12.270638
C	11.836450	7.095784	10.548770
H	10.981991	6.433698	10.333438
H	11.474705	8.128162	10.425563
C	12.965456	6.816127	9.550553
H	13.761200	7.572430	9.681365
H	12.584117	6.934038	8.522266
C	13.560829	5.418526	9.750877
H	14.389797	5.248171	9.043579
H	12.789110	4.659307	9.527697
C	14.038258	5.232962	11.195779
H	14.446868	4.218698	11.339770
H	14.864101	5.939508	11.401157
C	12.896538	5.468347	12.193569
H	13.263956	5.338320	13.222156
H	12.129652	4.700650	12.038724
C	11.371062	6.891614	14.871739
H	11.283549	5.795889	14.977082
C	12.816107	7.305020	15.207339
H	12.911004	8.400075	15.112768
H	13.541790	6.861039	14.511699
C	13.171133	6.898804	16.647044
H	13.148981	5.796145	16.722433
H	14.204678	7.208623	16.876302
C	12.193602	7.497226	17.665338
H	12.309128	8.596984	17.670263
H	12.439517	7.150409	18.683199
C	10.742645	7.151062	17.312089
H	10.046835	7.644899	18.011280
H	10.582857	6.063146	17.426164
C	10.404101	7.555185	15.872281
H	10.487230	8.651862	15.773484
H	9.367086	7.286323	15.636558
C	7.480279	9.158640	10.777651
H	6.846536	8.357730	10.361943
C	8.776755	9.216497	9.946041
H	9.475313	9.928360	10.415550
H	9.265373	8.233148	9.971871
C	8.537974	9.666091	8.499121
H	7.963711	8.897536	7.957063
H	9.506783	9.750518	7.978742
C	7.774641	10.992736	8.442600
H	8.399524	11.793428	8.879635
H	7.578206	11.280208	7.396298
C	6.462907	10.894855	9.227896
H	5.804126	10.148453	8.747158
H	5.920757	11.854772	9.199910
C	6.705736	10.483843	10.688116
H	5.739669	10.408674	11.209508
H	7.280102	11.282970	11.187814
C	6.492651	9.160229	13.582109
H	6.312847	10.199206	13.256945
C	5.211249	8.343304	13.324374
H	5.402063	7.290333	13.586606
H	4.946682	8.364280	12.253590
C	4.037426	8.872550	14.158739
H	3.777451	9.892052	13.818103
H	3.146948	8.245355	13.985269
C	4.386816	8.912822	15.650899
H	4.555908	7.881118	16.009711
H	3.541602	9.317169	16.233003
C	5.653210	9.742062	15.896580
H	5.911327	9.743825	16.969036
H	5.457242	10.794589	15.618215
C	6.840449	9.210363	15.081986
H	7.097540	8.199579	15.429735
H	7.726066	9.844078	15.244448
O	7.870729	5.919241	10.376927
Si	7.703689	5.577883	8.698942
C	9.336205	6.084237	7.924727

H	9.253030	5.987607	6.829446	H	6.201840	6.443020	11.501224
H	9.619579	7.119824	8.153687	C	6.492373	4.294630	11.687844
H	10.152736	5.424430	8.256468	H	7.094310	3.563483	11.136828
C	7.443574	3.739948	8.394673	H	6.566295	4.033463	12.752342
H	8.235961	3.134488	8.860579	C	5.032772	4.144512	11.329895
H	6.470274	3.385804	8.759804	C	4.495302	2.704472	11.484166
H	7.479747	3.563750	7.305909	F	5.160917	1.879394	10.662984
C	6.240139	6.546228	8.032119	F	4.664642	2.277193	12.739683
H	5.315838	6.235501	8.539864	F	3.196332	2.639610	11.184886
H	6.356505	7.631300	8.160668	F	4.773023	4.510199	10.036094
H	6.123799	6.341867	6.954632				
F	4.261677	4.945755	12.118723				

Zero-point correction= 0.976544 (Hartree/Particle)
Thermal correction to Energy= 1.034941
Thermal correction to Enthalpy= 1.035885
Thermal correction to Gibbs Free Energy= 0.883134
Sum of electronic and zero-point Energies= -7380.023460
Sum of electronic and thermal Energies= -7379.965062
Sum of electronic and thermal Enthalpies= -7379.964118
Sum of electronic and thermal Free Energies= -7380.116870

SMD(THF) uM06L-d3/def2-TZVPP
E(scf) = -7383.68241462 a.u.

^{4}Int2
E(scf) = -7381.02420747 a.u.
ν_{min} = 19.67 cm^{-1}

Fe	8.631666	6.272759	12.357911	P	10.829510	7.210563	13.364247
Br	7.636627	5.654611	14.576502	P	8.067568	8.749113	12.273411
C	9.628913	4.816789	11.404105	C	11.684506	9.942391	13.685942
C	9.765316	3.624480	12.138115	H	12.702695	9.737497	14.014242
C	10.234161	4.883742	10.140492	C	10.712540	9.043579	13.305208
C	10.508392	2.549158	11.639209	C	9.482962	9.701152	12.934311
H	9.288562	3.536595	13.117646	C	9.559332	11.070223	13.077533
C	10.980117	3.810331	9.632452	H	8.786073	11.813489	12.889184
H	10.138052	5.785711	9.529858	C	12.499241	6.899450	12.579677
C	11.124824	2.639691	10.383839	H	13.229050	7.462422	13.188275
H	10.608660	1.635622	12.233227	C	12.555276	7.457853	11.144743
H	11.451120	3.893070	8.648507	H	11.786559	6.958799	10.535222
H	11.708772	1.802018	9.993220	H	12.316981	8.532836	11.142333
C	7.052365	5.554110	11.188949	C	13.934818	7.223961	10.513664
S	11.116538	11.573521	13.629166	H	14.688149	7.819114	11.062515

H	13.935978	7.596907	9.475480
C	14.334121	5.743929	10.553872
H	15.341297	5.606333	10.125659
H	13.636430	5.163704	9.923724
C	14.279372	5.196835	11.985059
H	14.528081	4.122377	11.996212
H	15.042995	5.705685	12.602466
C	12.892695	5.410075	12.606194
H	12.872791	5.016317	13.634578
H	12.153994	4.829582	12.038988
C	11.052731	6.870030	15.205191
H	10.696738	5.828481	15.298891
C	12.481814	6.958149	15.770441
H	12.847884	7.996670	15.683209
H	13.182169	6.326196	15.206816
C	12.504753	6.537301	17.249452
H	12.230713	5.468467	17.316556
H	13.531377	6.623241	17.643766
C	11.532072	7.361692	18.100414
H	11.881084	8.410554	18.132066
H	11.532265	6.998548	19.142011
C	10.115871	7.325974	17.514641
H	9.441185	7.976225	18.096876
H	9.707143	6.301844	17.587422
C	10.114401	7.761391	16.045085
H	10.461022	8.806633	15.979558
H	9.094979	7.734505	15.641213
C	7.903909	9.358109	10.513545
H	7.128868	8.695432	10.102452
C	9.216093	9.099509	9.746571
H	10.002134	9.763491	10.146332
H	9.577803	8.072554	9.917670
C	9.035339	9.358654	8.245504
H	8.315112	8.626516	7.837942
H	9.989611	9.191206	7.719055
C	8.519750	10.779783	7.988381
H	9.295946	11.505607	8.293684
H	8.348066	10.936833	6.910492
C	7.235031	11.058243	8.778262
H	6.427856	10.402748	8.403284
H	6.900273	12.096474	8.617155
C	7.422474	10.798777	10.282375
H	6.473424	10.986272	10.808104
H	8.164417	11.509738	10.684137
C	6.575022	9.404488	13.179471
H	6.452790	10.456863	12.868739
C	5.319334	8.613491	12.764090
H	5.469601	7.555759	13.040854
H	5.175601	8.640633	11.672652
C	4.067437	9.139810	13.477526
H	3.864682	10.173457	13.141789
H	3.192834	8.535244	13.184710
C	4.247443	9.125121	14.999881
H	4.347725	8.078025	15.339978
H	3.352927	9.535741	15.497469
C	5.499324	9.907546	15.415155
H	5.640672	9.857192	16.507831
H	5.361445	10.975685	15.164011
C	6.754500	9.377393	14.708808
H	6.940220	8.339559	15.027888
H	7.635356	9.968952	15.002209
O	6.731238	4.206394	11.276404
Si	5.662721	3.297181	12.225866
C	4.824151	2.115197	11.022368
H	4.234921	1.363342	11.573945
H	4.154435	2.642171	10.327946
H	5.582080	1.579835	10.426497
C	6.629784	2.254229	13.453496
H	7.398072	1.667154	12.924365
H	7.126404	2.878167	14.209439
H	5.950430	1.549181	13.962428
C	4.410562	4.429727	13.054323
H	4.908245	5.100397	13.770581
H	3.882025	5.041089	12.306445
H	3.660905	3.832149	13.599780
H	6.275863	6.182944	11.660990
C	7.244525	5.923649	9.719918
H	7.931126	6.769629	9.600104
H	7.704065	5.073453	9.201151
C	6.015835	6.331432	8.932391
C	4.921299	5.258686	8.722540
F	5.461042	4.101475	8.331137
F	4.242258	5.055927	9.858759
F	4.050150	5.655159	7.790040
F	6.402959	6.734863	7.687358
F	5.383606	7.401084	9.510773

Zero-point correction= 0.975019 (Hartree/Particle)
Thermal correction to Energy= 1.033961
Thermal correction to Enthalpy= 1.034905
Thermal correction to Gibbs Free Energy= 0.879429
Sum of electronic and zero-point Energies= -7380.049189
Sum of electronic and thermal Energies= -7379.990247
Sum of electronic and thermal Enthalpies= -7379.989303
Sum of electronic and thermal Free Energies= -7380.144779

SMD(THF) uM06L-d3/def2-TZVPP
E(scf) = -7383.70899037 a.u.

^{6}Int2
E(scf) = -7380.99167081 a.u.
ν_{min} = 18.84 cm^{-1}

Fe	8.576850	6.053484	12.472626	C	13.988627	7.312417	10.428122
Br	7.764335	5.401019	14.678713	H	14.743904	7.966024	10.902716
C	9.816009	4.591681	11.683736	H	13.916494	7.629771	9.374014
C	10.127513	3.455895	12.458629	C	14.452777	5.853840	10.520195
C	10.360758	4.649712	10.386375	H	15.439407	5.733292	10.041817
C	10.955956	2.436468	11.970591	H	13.746208	5.213617	9.962022
H	9.723957	3.371009	13.472835	C	14.501731	5.382126	11.978171
C	11.189942	3.637539	9.885400	H	14.795948	4.320301	12.029248
H	10.152898	5.511625	9.744499	H	15.277587	5.952576	12.522126
C	11.493759	2.526270	10.680916	C	13.146051	5.574296	12.671030
H	11.186728	1.570426	12.598863	H	13.207591	5.240815	13.719162
H	11.604955	3.718269	8.876076	H	12.399222	4.931648	12.184074
H	12.144891	1.735633	10.297835	C	11.290222	6.949773	15.240511
C	6.860289	5.692857	11.070139	H	11.085146	5.866519	15.322080
S	11.061658	11.654488	13.747235	C	12.692928	7.229426	15.807464
P	11.016497	7.286127	13.405949	H	12.910869	8.308504	15.721263
P	8.128721	8.688236	12.452870	H	13.471641	6.701017	15.238748
C	11.739699	10.063741	13.722349	C	12.776358	6.815571	17.286046
H	12.788056	9.921245	13.981168	H	12.651222	5.719323	17.355012
C	10.808181	9.108893	13.379358	H	13.781543	7.041937	17.680179
C	9.515643	9.691273	13.100760	C	11.699958	7.500486	18.136149
C	9.509333	11.058514	13.279358	H	11.899404	8.587929	18.162151
H	8.680365	11.753579	13.154178	H	11.752319	7.146125	19.179474
C	12.681601	7.041545	12.588996	C	10.301116	7.265023	17.554700
H	13.408731	7.671245	13.132593	H	9.543078	7.814279	18.138472
C	12.636911	7.518967	11.124724	H	10.042146	6.193259	17.631769
H	11.861443	6.948755	10.587267	C	10.233444	7.692252	16.083922
H	12.344032	8.579846	11.077626	H	10.421248	8.777745	16.015894

H	9.226846	7.515622	15.682774	H	5.606066	9.550304	16.669369
C	7.977222	9.272026	10.685319	H	5.416956	10.791543	15.421163
H	7.206839	8.605743	10.273165	C	6.754970	9.179202	14.866343
C	9.300351	8.999398	9.942431	H	6.892520	8.111082	15.102397
H	10.085967	9.653952	10.357783	H	7.650696	9.705784	15.231274
H	9.643362	7.967225	10.125636	O	6.532905	4.345374	11.236414
C	9.160376	9.264397	8.437901	Si	5.354770	3.524802	12.140413
H	8.452344	8.537800	8.001432	C	4.299041	2.542621	10.929067
H	10.129405	9.097506	7.938849	H	3.679346	1.814233	11.479100
C	8.655255	10.687915	8.172350	H	3.634928	3.188733	10.337884
H	9.424483	11.411131	8.500721	H	4.941523	1.982660	10.229823
H	8.513059	10.848475	7.090701	C	6.251855	2.295452	13.239214
C	7.350288	10.966417	8.928575	H	6.897947	1.648277	12.622776
H	6.554565	10.308229	8.535405	H	6.880228	2.802522	13.984621
H	7.018770	12.003923	8.756366	H	5.526491	1.651056	13.763956
C	7.502947	10.711841	10.437519	C	4.316772	4.769154	13.092561
H	6.543240	10.901576	10.943497	H	4.935358	5.313412	13.822209
H	8.237120	11.422711	10.853406	H	3.856145	5.498255	12.406030
C	6.625543	9.339965	13.339865	H	3.505748	4.257079	13.636565
H	6.559213	10.417947	13.109320	H	6.049762	6.367294	11.387768
C	5.351335	8.645461	12.824096	C	7.284773	5.942119	9.630324
H	5.443830	7.562989	13.010521	H	8.045953	6.728751	9.555466
H	5.243110	8.773639	11.734665	H	7.739251	5.026311	9.230886
C	4.101093	9.165828	13.544591	C	6.195476	6.378938	8.670240
H	3.953440	10.232118	13.293221	C	5.010491	5.404248	8.478337
H	3.211567	8.627882	13.176602	F	5.449860	4.163881	8.249896
C	4.232009	9.013500	15.064519	F	4.237238	5.394303	9.573340
H	4.276092	7.937632	15.315273	F	4.253274	5.781414	7.444268
H	3.340102	9.419868	15.570025	F	6.732320	6.594244	7.435302
C	5.501634	9.700811	15.581845	F	5.636282	7.567156	9.065991

Zero-point correction= 0.973038 (Hartree/Particle)
Thermal correction to Energy= 1.032786
Thermal correction to Enthalpy= 1.033731
Thermal correction to Gibbs Free Energy= 0.874350
Sum of electronic and zero-point Energies= -7380.018633
Sum of electronic and thermal Energies= -7379.958884
Sum of electronic and thermal Enthalpies= -7379.957940
Sum of electronic and thermal Free Energies= -7380.117321

SMD(THF) uM06L-d3/def2-TZVPP
E(scf) = -7383.68675697 a.u.

^{2}TS3

E(scf) = -7380.97072283 a.u.

ν_{min} = -365.66 cm^{-1}

Fe	8.743088	6.333588	12.553783	H	12.089163	4.848012	12.137035
Br	7.815312	5.421156	14.700206	C	11.097043	6.934930	15.279593
C	9.355266	4.912842	11.278746	H	10.780322	5.881398	15.378452
C	9.562544	3.681433	11.946245	C	12.518820	7.078830	15.849510
C	10.102934	5.140520	10.103226	H	12.853273	8.126496	15.747513
C	10.500947	2.756497	11.490076	H	13.240711	6.459255	15.298233
H	8.975669	3.456348	12.835208	C	12.550443	6.683458	17.335207
C	11.030949	4.203473	9.635757	H	12.312484	5.607219	17.419868
H	9.970227	6.062095	9.535641	H	13.571769	6.811225	17.732021
C	11.240314	3.004750	10.324262	C	11.545919	7.488303	18.167538
H	10.648019	1.825306	12.044883	H	11.854567	8.550244	18.177087
H	11.594774	4.420087	8.724250	H	11.557942	7.147799	19.216729
H	11.963954	2.272933	9.957358	C	10.133752	7.384521	17.580861
C	7.362204	5.298527	11.116401	H	9.431411	8.016300	18.150703
S	11.135097	11.617173	13.539512	H	9.767888	6.345676	17.671192
P	10.861421	7.246185	13.436692	C	10.114725	7.790841	16.103146
P	8.161119	8.694652	12.191189	H	10.402652	8.852622	16.015562
C	11.700395	9.992950	13.713489	H	9.099913	7.695881	15.699108
H	12.698992	9.807818	14.107165	C	7.940762	9.301907	10.436268
C	10.753195	9.074413	13.318787	H	7.181113	8.610601	10.041501
C	9.547327	9.705373	12.840958	C	9.245884	9.083944	9.647712
C	9.613628	11.079906	12.920667	H	10.012032	9.783285	10.025594
H	8.852460	11.811579	12.655007	H	9.646799	8.074847	9.834205
C	12.527576	6.896039	12.671138	C	9.028328	9.317058	8.147717
H	13.266928	7.434689	13.289704	H	8.328287	8.553645	7.763796
C	12.637466	7.442298	11.236190	H	9.977720	9.180913	7.603559
H	11.869303	6.965683	10.608552	C	8.452344	10.714422	7.885464
H	12.436857	8.524963	11.222172	H	9.206061	11.473189	8.166147
C	14.027278	7.155410	10.650558	H	8.252957	10.851832	6.809599
H	14.783576	7.722885	11.224215	C	7.173794	10.954606	8.698560
H	14.078276	7.525717	9.612625	H	6.385026	10.264160	8.347703
C	14.368950	5.660938	10.702924	H	6.796927	11.977316	8.530881
H	15.386970	5.486771	10.315423	C	7.402043	10.721304	10.201500
H	13.677723	5.110259	10.042029	H	6.460196	10.882450	10.748547
C	14.237521	5.107193	12.126877	H	8.127343	11.463126	10.575822
H	14.428312	4.020816	12.135081	C	6.686481	9.356676	13.131841
H	15.007770	5.568910	12.772370	H	6.632551	10.438405	12.915761
C	12.849106	5.392223	12.714546	C	5.383973	8.691779	12.653536
H	12.790312	5.007724	13.745692	H	5.471168	7.598125	12.782563

H	5.226334	8.870315	11.580236	C	6.685724	2.117471	13.453275
C	4.169845	9.190909	13.448311	H	7.412704	1.459745	12.949679
H	4.014272	10.264261	13.233452	H	7.211338	2.724756	14.202830
H	3.262491	8.666342	13.104945	H	5.952801	1.475861	13.972139
C	4.366202	9.000989	14.956141	C	4.609295	4.408025	12.994247
H	4.428738	7.919850	15.179122	H	5.152318	5.030978	13.721084
H	3.495174	9.389403	15.510110	H	4.145643	5.063353	12.241862
C	5.654469	9.684276	15.428747	H	3.805872	3.873751	13.528571
H	5.808936	9.515138	16.507683	H	6.802719	5.976442	11.797112
H	5.559150	10.777437	15.290947	C	7.299383	5.819379	9.687824
C	6.873133	9.175422	14.648794	H	7.938674	6.702285	9.599031
H	7.016673	8.103645	14.861098	H	7.698907	5.059476	9.005367
H	7.784058	9.694750	14.984392	C	5.964626	6.278178	9.128744
O	6.879014	4.012661	11.192799	C	4.920423	5.190859	8.759441
Si	5.778665	3.174523	12.193680	F	5.514205	4.128276	8.209908
C	4.909712	1.981001	11.027489	F	4.254323	4.794663	9.849520
H	5.660508	1.400460	10.465648	F	4.029833	5.674593	7.890536
H	4.303175	1.267841	11.610591	F	6.210522	6.970247	7.977705
H	4.254694	2.485679	10.305019	F	5.335711	7.139951	9.979764

Zero-point correction= 0.974434 (Hartree/Particle)
Thermal correction to Energy= 1.032859
Thermal correction to Enthalpy= 1.033803
Thermal correction to Gibbs Free Energy= 0.879934
Sum of electronic and zero-point Energies= -7379.996288
Sum of electronic and thermal Energies= -7379.937864
Sum of electronic and thermal Enthalpies= -7379.936920
Sum of electronic and thermal Free Energies= -7380.090789

SMD(THF) uM06L-d3/def2-TZVPP
E(scf) = -7383.65303886 a.u.

^{4}TS3
E(scf) = -7381.00787777 a.u.
ν_{min} = -316.56 cm^{-1}

Fe	8.792765	6.316048	12.514614	H	9.983623	5.935537	9.495211
Br	7.680819	5.531451	14.644691	C	11.218898	2.898197	10.413612
C	9.329034	4.847400	11.267870	H	10.605538	1.789300	12.173007
C	9.524881	3.642912	11.988670	H	11.598977	4.246291	8.761716
C	10.095875	5.029639	10.093402	H	11.944388	2.150277	10.084694
C	10.465909	2.698196	11.580304	C	7.304210	5.245401	11.044465
H	8.930359	3.457569	12.882846	S	11.131716	11.658893	13.566377
C	11.022096	4.069749	9.673836	P	10.928489	7.284845	13.445337

P	8.143613	8.727691	12.276921	C	9.252884	9.055381	9.734195
C	11.726314	10.041148	13.699158	H	10.025555	9.745083	10.116360
H	12.742227	9.866529	14.051322	H	9.637148	8.040963	9.928834
C	10.778943	9.111061	13.332707	C	9.059644	9.281085	8.229548
C	9.543590	9.730990	12.909390	H	8.356901	8.523724	7.839301
C	9.594977	11.105249	13.002635	H	10.015927	9.130154	7.701611
H	8.812958	11.827621	12.773611	C	8.503371	10.682485	7.948549
C	12.580852	6.937102	12.658173	H	9.259384	11.435838	8.237570
H	13.342834	7.477276	13.247297	H	8.323849	10.814707	6.868558
C	12.642531	7.460257	11.211537	C	7.213496	10.938510	8.738170
H	11.847625	6.977105	10.621051	H	6.426555	10.249349	8.380749
H	12.446304	8.543702	11.187235	H	6.845633	11.961894	8.555401
C	14.007052	7.154607	10.578499	C	7.416434	10.717538	10.246363
H	14.788373	7.723343	11.116119	H	6.466457	10.888487	10.776433
H	14.022289	7.510675	9.534489	H	8.139966	11.458324	10.626997
C	14.337661	5.657959	10.638250	C	6.658669	9.388464	13.192376
H	15.339690	5.469680	10.217206	H	6.552029	10.454178	12.923269
H	13.618725	5.105644	10.009234	C	5.393658	8.632129	12.745089
C	14.252114	5.122613	12.072702	H	5.543554	7.554002	12.933235
H	14.432062	4.034497	12.087161	H	5.232909	8.745993	11.662777
H	15.049660	5.583703	12.684502	C	4.151201	9.105330	13.510878
C	12.889155	5.429127	12.707440	H	3.937627	10.155953	13.240590
H	12.865499	5.058077	13.745032	H	3.275110	8.514407	13.195127
H	12.101198	4.885699	12.163983	C	4.352817	9.004400	15.026820
C	11.165680	6.973448	15.285304	H	4.471253	7.941098	15.305408
H	10.882187	5.909545	15.381147	H	3.460838	9.374854	15.559389
C	12.580899	7.159713	15.857735	C	5.601990	9.777686	15.465618
H	12.883159	8.216780	15.751995	H	5.758330	9.674365	16.552594
H	13.320685	6.560311	15.306875	H	5.451234	10.855647	15.269500
C	12.621745	6.770323	17.344634	C	6.849820	9.291493	14.717399
H	12.417270	5.687477	17.432741	H	7.042965	8.240155	14.984494
H	13.637360	6.931362	17.743950	H	7.732728	9.871447	15.028305
C	11.590007	7.546515	18.171347	O	6.831504	3.955517	11.092965
H	11.864747	8.617734	18.177037	Si	5.717800	3.139648	12.098009
H	11.610601	7.210974	19.221975	C	4.870432	1.923637	10.940707
C	10.182381	7.396025	17.583173	H	5.626960	1.300343	10.435241
H	9.459576	8.006613	18.150417	H	4.212301	1.251499	11.516435
H	9.850120	6.346162	17.677668	H	4.268512	2.425815	10.170858
C	10.152366	7.797495	16.104119	C	6.608025	2.135260	13.410857
H	10.405394	8.868061	16.014732	H	7.359784	1.473478	12.951380
H	9.141742	7.668133	15.696226	H	7.103228	2.782306	14.148827
C	7.941818	9.298093	10.506742	H	5.873646	1.501509	13.937250
H	7.180754	8.602913	10.119916	C	4.532332	4.385803	12.854594

H	5.058872	5.009771	13.592823	C	5.978776	6.280047	9.048004
H	4.092143	5.039838	12.087292	C	4.936024	5.209232	8.632788
H	3.712678	3.857824	13.370315	F	5.533030	4.174048	8.035891
H	6.735641	5.908577	11.719189	F	4.271285	4.760827	9.703252
C	7.295406	5.793943	9.627746	F	4.044260	5.729616	7.786333
H	7.943921	6.675067	9.579904	F	6.252922	6.994771	7.917148
H	7.707993	5.048348	8.936848	F	5.338880	7.129326	9.904871

SMD(THF) uM06L-d3/def2-TZVPP
E(scf) = -7383.69029314 a.u.

^{6}TS4
E(scf) = -7380.98594151 a.u.
ν_{min} = -365.16 cm^{-1}

Fe	8.841815	6.546858	12.742940	C	13.783925	6.891238	10.613789
Br	7.379513	5.817816	14.606857	H	14.646368	7.449560	11.023105
C	9.150046	4.952665	11.422911	H	13.723021	7.148421	9.542776
C	9.356434	3.747190	12.189485	C	14.020545	5.386225	10.790199
C	9.902407	4.996881	10.192010	H	14.964798	5.086876	10.304840
C	10.145623	2.693370	11.745335	H	13.210045	4.833318	10.285609
H	8.858258	3.656030	13.160429	C	14.035582	4.994490	12.272451
C	10.668733	3.932537	9.733500	H	14.151134	3.902939	12.379771
H	9.863044	5.896754	9.570608	H	14.911229	5.455655	12.765978
C	10.805410	2.761773	10.503868	C	12.756466	5.449411	12.988910
H	10.259677	1.802313	12.370710	H	12.810286	5.180813	14.056881
H	11.199189	4.019368	8.779539	H	11.888150	4.912416	12.569509
H	11.425833	1.932897	10.153739	C	11.235739	7.226230	15.493930
C	7.101043	4.827870	10.802760	H	11.071102	6.138318	15.604878
S	11.414213	11.840119	13.399531	C	12.630181	7.565469	16.044883
P	10.964190	7.488601	13.662543	H	12.826284	8.642147	15.902655
P	8.264594	8.972102	12.378859	H	13.415895	7.020783	15.499076
C	11.903684	10.214080	13.719475	C	12.721665	7.237348	17.543462
H	12.904102	10.018502	14.102747	H	12.620997	6.144664	17.677239
C	10.908937	9.307109	13.426189	H	13.720429	7.509955	17.923683
C	9.722326	9.952658	12.904542	C	11.626800	7.947971	18.347729
C	9.859021	11.322920	12.852861	H	11.791984	9.040209	18.295839
H	9.128017	12.062413	12.529263	H	11.691961	7.670005	19.413044
C	12.536304	6.964843	12.818476	C	10.235129	7.624845	17.792034
H	13.368313	7.507913	13.301025	H	9.458765	8.179944	18.344852
C	12.505123	7.348433	11.327929	H	10.020433	6.550822	17.941394
H	11.633441	6.864227	10.858367	C	10.136964	7.949653	16.296416
H	12.371564	8.435945	11.214157	H	10.245701	9.039238	16.151682

H	9.145661	7.670630	15.911681	H	6.027544	10.195750	16.650119
C	8.006338	9.366137	10.573851	H	5.746194	11.343775	15.331413
H	7.198650	8.665673	10.304547	C	7.056297	9.697178	14.806660
C	9.261249	8.983131	9.766318	H	7.210320	8.649454	15.110721
H	10.087091	9.661091	10.045130	H	7.972013	10.248443	15.073180
H	9.599040	7.969042	10.032138	O	6.799671	3.537762	10.471887
C	8.999895	9.081543	8.257894	Si	5.925995	2.353674	11.337909
H	8.243285	8.328910	7.975039	C	4.824479	1.546051	10.048545
H	9.919580	8.834293	7.702055	H	5.434619	1.143955	9.222712
C	8.492586	10.476275	7.870882	H	4.257232	0.709515	10.489460
H	9.293799	11.216591	8.051757	H	4.110989	2.269541	9.627194
H	8.264630	10.515751	6.792657	C	7.101374	1.068797	12.038477
C	7.256254	10.864729	8.691327	H	7.817752	0.732844	11.272319
H	6.424818	10.181279	8.440764	H	7.676382	1.464649	12.888019
H	6.922211	11.882360	8.428995	H	6.525471	0.193129	12.383637
C	7.529200	10.777929	10.201770	C	4.949219	3.193180	12.703987
H	6.618625	11.045555	10.759988	H	5.618843	3.697706	13.419640
H	8.305016	11.514688	10.472078	H	4.258721	3.945826	12.292927
C	6.832177	9.743387	13.283329	H	4.356265	2.444998	13.256087
H	6.778573	10.801837	12.971504	H	6.619082	5.198999	11.716769
C	5.522088	9.035292	12.888342	C	7.054325	5.768766	9.629703
H	5.627551	7.957180	13.101545	H	7.710028	6.627578	9.823401
H	5.340608	9.125090	11.806522	H	7.427429	5.261543	8.729162
C	4.324637	9.597415	13.665964	C	5.716351	6.397621	9.300584
H	4.156923	10.647819	13.363925	C	4.576377	5.443007	8.872948
H	3.412202	9.041944	13.391674	F	5.007317	4.580408	7.948211
C	4.557009	9.539340	15.179958	F	4.125948	4.749033	9.926842
H	4.631956	8.482117	15.493873	F	3.550577	6.131568	8.365447
H	3.696368	9.970627	15.718255	F	5.875959	7.289276	8.275105
C	5.850516	10.267617	15.563815	F	5.244874	7.109451	10.367163

Zero-point correction= 0.972142 (Hartree/Particle)
Thermal correction to Energy= 1.031145
Thermal correction to Enthalpy= 1.032089
Thermal correction to Gibbs Free Energy= 0.874515
Sum of electronic and zero-point Energies= -7380.013800
Sum of electronic and thermal Energies= -7379.954797
Sum of electronic and thermal Enthalpies= -7379.953852
Sum of electronic and thermal Free Energies= -7380.111427

SMD(THF) uM06L-d3/def2-TZVPP
E(scf) = -7383.66642104 a.u.

^{2}B

E(scf) = -6012.19440287 a.u.
ν_{min} = 22.77 cm^{-1}

Fe	-3.057741	4.845546	-2.845686	H	-7.976129	6.961503	-4.047140
Br	-1.947612	6.630442	-3.970117	H	-6.939317	6.856854	-5.478429
S	-6.750047	0.736719	-1.335843	C	-6.468009	5.400322	-3.951896
P	-4.444165	3.464307	-3.914509	H	-6.979142	4.888186	-3.117137
P	-3.689999	3.881944	-0.928592	H	-5.696058	6.044682	-3.501149
C	-6.227981	1.388851	-2.854146	C	-2.347664	2.981815	0.016406
H	-6.637939	0.990275	-3.781048	H	-1.646519	3.800020	0.265609
C	-5.297326	2.388481	-2.686508	C	-1.607872	2.018316	-0.928073
C	-4.977038	2.612895	-1.295885	H	-2.306613	1.228327	-1.257187
C	-5.703612	1.801118	-0.455288	H	-1.297949	2.558025	-1.837627
H	-5.692930	1.765989	0.633085	C	-0.397273	1.373456	-0.242163
C	-3.729181	2.255306	-5.146331	H	0.351379	2.156755	-0.022635
H	-4.528323	1.558226	-5.455763	H	0.087050	0.658322	-0.928291
C	-2.608326	1.454654	-4.459356	C	-0.796976	0.678401	1.065207
H	-1.875048	2.172786	-4.049760	H	-1.463749	-0.172825	0.832981
H	-3.011932	0.898217	-3.598369	H	0.091374	0.255073	1.563356
C	-1.901977	0.501289	-5.429510	C	-1.528289	1.644287	2.005576
H	-2.617661	-0.271776	-5.765226	H	-0.833103	2.444965	2.318429
H	-1.088093	-0.028946	-4.906738	H	-1.842657	1.123311	2.925655
C	-1.359345	1.252971	-6.650110	C	-2.749162	2.278161	1.320789
H	-0.880093	0.552624	-7.354640	H	-3.244671	2.980579	2.010216
H	-0.573550	1.957515	-6.320109	H	-3.478151	1.482541	1.092142
C	-2.474326	2.037257	-7.350768	C	-4.512105	4.975689	0.344169
H	-2.069926	2.605054	-8.205518	H	-4.903017	4.339923	1.158264
H	-3.211423	1.325452	-7.766174	C	-3.499461	5.978938	0.926106
C	-3.192016	2.992527	-6.387134	H	-3.024386	6.521355	0.086744
H	-4.010274	3.503994	-6.918626	H	-2.691517	5.451662	1.458448
H	-2.492796	3.781239	-6.052485	C	-4.170252	6.983943	1.872644
C	-5.797127	4.350946	-4.855595	H	-4.547909	6.444032	2.760501
H	-5.220226	4.903131	-5.620375	H	-3.422615	7.707256	2.239294
C	-6.842472	3.480291	-5.567365	C	-5.335468	7.712058	1.193382
H	-7.396697	2.894833	-4.814247	H	-4.942367	8.330009	0.364873
H	-6.357522	2.757455	-6.243153	H	-5.821333	8.404798	1.900855
C	-7.842453	4.343423	-6.351796	C	-6.354205	6.713188	0.632913
H	-7.307829	4.866466	-7.165913	H	-7.168685	7.242383	0.110076
H	-8.597228	3.699220	-6.833590	H	-6.822134	6.161432	1.469055
C	-8.519456	5.377940	-5.444662	C	-5.688366	5.713983	-0.319790
H	-9.131126	4.850191	-4.689341	H	-5.301886	6.251164	-1.204755
H	-9.213374	6.006199	-6.028049	H	-6.428394	4.989262	-0.695259
C	-7.480829	6.250241	-4.729441				

Zero-point correction= 0.693868 (Hartree/Particle)
Thermal correction to Energy= 0.729489
Thermal correction to Enthalpy= 0.730433
Thermal correction to Gibbs Free Energy= 0.622940
Sum of electronic and zero-point Energies= -6011.500534
Sum of electronic and thermal Energies= -6011.464914
Sum of electronic and thermal Enthalpies= -6011.463970
Sum of electronic and thermal Free Energies= -6011.571462

SMD(THF) uM06L-d3/def2-TZVPP
E(scf) = -6013.760585 a.u.

^{4}B
E(scf) = -6012.22445837 a.u.
ν_{min} = 18.56 cm^{-1}

Fe	-2.982453	5.004705	-2.840938	H	-2.387811	3.677099	-6.156161
Br	-2.768159	7.366800	-3.301078	C	-5.719427	4.365348	-4.915506
S	-6.716722	0.822610	-1.407882	H	-5.154256	4.957114	-5.659609
P	-4.344619	3.487678	-3.988879	C	-6.739926	3.492679	-5.660182
P	-3.678729	3.961700	-0.874589	H	-7.286699	2.873152	-4.929287
C	-6.127447	1.446117	-2.912845	H	-6.236870	2.801299	-6.355146
H	-6.495054	1.027338	-3.848530	C	-7.752700	4.357919	-6.426441
C	-5.208945	2.454844	-2.728316	H	-7.222562	4.917397	-7.219075
C	-4.953281	2.709774	-1.326951	H	-8.488321	3.712278	-6.935332
C	-5.716559	1.911315	-0.505394	C	-8.461076	5.348956	-5.495073
H	-5.752403	1.898012	0.583031	H	-9.070035	4.784493	-4.764475
C	-3.679147	2.229030	-5.195564	H	-9.161591	5.980804	-6.066748
H	-4.501528	1.551132	-5.485545	C	-7.449106	6.218035	-4.739089
C	-2.579055	1.397907	-4.509766	H	-7.967029	6.893711	-4.037578
H	-1.802526	2.086661	-4.129395	H	-6.913476	6.863335	-5.459543
H	-2.990392	0.876662	-3.630657	C	-6.425407	5.364674	-3.980258
C	-1.938462	0.392924	-5.474544	H	-6.936094	4.805717	-3.175251
H	-2.696396	-0.353710	-5.775239	H	-5.675967	6.007854	-3.492887
H	-1.136848	-0.162530	-4.959150	C	-2.361311	3.009314	0.051172
C	-1.392082	1.090781	-6.725454	H	-1.647927	3.804344	0.337061
H	-0.964665	0.352272	-7.424296	C	-1.632150	2.066371	-0.923798
H	-0.564757	1.763226	-6.431720	H	-2.343668	1.302278	-1.284776
C	-2.484632	1.912710	-7.418931	H	-1.303578	2.628063	-1.814129
H	-2.073214	2.442965	-8.294146	C	-0.439762	1.372912	-0.253175
H	-3.263972	1.229016	-7.802978	H	0.322295	2.132389	0.001077
C	-3.134536	2.919520	-6.459495	H	0.035883	0.674075	-0.961774
H	-3.937392	3.463676	-6.982077	C	-0.864386	0.637904	1.024181

H	-1.545783	-0.190498	0.754935	C	-4.198310	6.972080	2.008019
H	0.011341	0.178554	1.512621	H	-4.606167	6.415694	2.872103
C	-1.584367	1.582311	1.994710	H	-3.449576	7.674352	2.411601
H	-0.876137	2.356583	2.342818	C	-5.335483	7.734792	1.319246
H	-1.916360	1.033472	2.892087	H	-4.913456	8.364768	0.514480
C	-2.786928	2.265077	1.324883	H	-5.827305	8.418221	2.031725
H	-3.274432	2.952081	2.035357	C	-6.355032	6.764590	0.711746
H	-3.530072	1.493629	1.061388	H	-7.152120	7.318458	0.187601
C	-4.529095	5.012627	0.413617	H	-6.846520	6.196135	1.522991
H	-4.947193	4.355236	1.196694	C	-5.680191	5.786717	-0.256843
C	-3.517821	5.982893	1.051751	H	-5.266728	6.347865	-1.113864
H	-3.012102	6.539652	0.240945	H	-6.419860	5.082811	-0.671200
H	-2.733988	5.426692	1.591201				

Zero-point correction= 0.693561 (Hartree/Particle)
Thermal correction to Energy= 0.729334
Thermal correction to Enthalpy= 0.730279
Thermal correction to Gibbs Free Energy= 0.621586
Sum of electronic and zero-point Energies= -6011.530898
Sum of electronic and thermal Energies= -6011.495124
Sum of electronic and thermal Enthalpies= -6011.494180
Sum of electronic and thermal Free Energies= -6011.602872

SMD(THF) uM06L-d3/def2-TZVPP
E(scf) = -6013.78432785 a.u.

^{6}B
E(scf) = -6012.17612951 a.u.
ν_{min} = 18.70 cm^{-1}

Fe	-3.060679	5.356359	-2.938720	H	-1.886459	2.091368	-4.109598
Br	-0.704577	4.678177	-3.387310	H	-3.122672	0.888214	-3.706830
S	-6.555469	0.807077	-1.360229	C	-2.004997	0.461688	-5.527299
P	-4.432656	3.552220	-4.048389	H	-2.764967	-0.249462	-5.901153
P	-3.636573	4.040269	-0.875017	H	-1.242464	-0.138906	-5.003347
C	-6.071240	1.477892	-2.881382	C	-1.380744	1.206014	-6.713648
H	-6.450737	1.044132	-3.805180	H	-0.932470	0.492700	-7.425563
C	-5.203359	2.537281	-2.727628	H	-0.558458	1.845950	-6.344323
C	-4.904510	2.796777	-1.334760	C	-2.420145	2.083714	-7.420664
C	-5.584520	1.946694	-0.490666	H	-1.954510	2.645433	-8.247749
H	-5.567596	1.920135	0.597871	H	-3.193483	1.436939	-7.874871
C	-3.711406	2.318381	-5.244614	C	-3.093143	3.060006	-6.445947
H	-4.530494	1.669858	-5.603166	H	-3.860002	3.647416	-6.977189
C	-2.661162	1.437565	-4.542700	H	-2.345506	3.778200	-6.064195

C	-5.864484	4.349335	-4.958852	H	-1.646452	-0.048618	1.094809
H	-5.345026	5.018952	-5.670396	H	0.020782	0.276275	1.595120
C	-6.790189	3.418198	-5.756621	C	-1.385402	1.877744	2.043977
H	-7.283551	2.714579	-5.064366	H	-0.579277	2.621064	2.184551
H	-6.216250	2.813487	-6.476142	H	-1.639811	1.496293	3.047226
C	-7.871328	4.218476	-6.499631	C	-2.607428	2.578752	1.429265
H	-7.386989	4.856826	-7.261253	H	-2.931900	3.400545	2.086214
H	-8.537339	3.528787	-7.044860	H	-3.442822	1.859467	1.378455
C	-8.678879	5.100153	-5.540127	C	-4.464936	5.095007	0.420036
H	-9.240332	4.452862	-4.841038	H	-4.786060	4.437977	1.247529
H	-9.428613	5.687612	-6.096306	C	-3.465950	6.138007	0.954103
C	-7.759269	6.027461	-4.736803	H	-3.077927	6.714406	0.092081
H	-8.344215	6.624473	-4.017007	H	-2.596398	5.645619	1.419190
H	-7.277150	6.746463	-5.424501	C	-4.125926	7.091459	1.958913
C	-6.672188	5.239304	-3.995777	H	-4.421689	6.519385	2.857641
H	-7.140152	4.604002	-3.222275	H	-3.393969	7.845675	2.293294
H	-5.988423	5.927007	-3.467558	C	-5.364177	7.770672	1.362601
C	-2.291648	3.090173	0.014588	H	-5.050571	8.424428	0.527862
H	-1.481768	3.840089	0.084645	H	-5.843134	8.423130	2.111804
C	-1.786495	1.946722	-0.885500	C	-6.363171	6.732898	0.837169
H	-2.599979	1.212442	-1.023934	H	-7.230083	7.231738	0.372044
H	-1.535174	2.341344	-1.879962	H	-6.756896	6.143342	1.685860
C	-0.571597	1.245351	-0.266014	C	-5.706327	5.785669	-0.173881
H	0.274052	1.956397	-0.229350	H	-5.391160	6.358014	-1.067176
H	-0.252435	0.411179	-0.913349	H	-6.430826	5.033122	-0.524501
C	-0.874691	0.741610	1.149948				

Zero-point correction= 0.693601 (Hartree/Particle)
Thermal correction to Energy= 0.729403
Thermal correction to Enthalpy= 0.730347
Thermal correction to Gibbs Free Energy= 0.621923
Sum of electronic and zero-point Energies= -6011.482529
Sum of electronic and thermal Energies= -6011.446727
Sum of electronic and thermal Enthalpies= -6011.445782
Sum of electronic and thermal Free Energies= -6011.554207

SMD(THF) uM06L-d3/def2-TZVPP
E(scf) = -6013.73842942 a.u.

Product
E(scf) = -1368.80720023 a.u.
ν_{min} = 17.69 cm^{-1}

C	8.767305	4.412472	10.955391	C	9.529136	5.114304	11.899120

C	9.346894	3.330231	10.277652	H	7.838746	1.959875	12.695188
C	10.852967	4.744006	12.160520	H	6.507424	0.791501	12.928544
H	9.081909	5.954132	12.439238	C	5.154887	3.838499	12.977422
C	10.668493	2.957951	10.537512	H	5.999543	4.278347	13.532852
H	8.745306	2.771878	9.557272	H	4.528266	4.659022	12.593540
C	11.425889	3.664653	11.479562	H	4.555493	3.250888	13.692443
H	11.435489	5.295710	12.902889	H	6.960402	5.420172	11.504464
H	11.109182	2.110318	10.006160	C	7.295379	5.736775	9.410404
H	12.458380	3.371250	11.685815	H	8.098924	6.485933	9.467685
C	7.335635	4.830066	10.647879	H	7.456720	5.131652	8.506924
O	6.501945	3.720985	10.397814	C	6.030795	6.552356	9.229362
Si	5.753904	2.742843	11.570042	C	4.700071	5.791081	8.973989
C	4.337836	1.931370	10.648772	F	4.879634	4.800061	8.097768
H	4.715212	1.360018	9.784814	F	4.204430	5.283944	10.109176
H	3.785297	1.237167	11.302934	F	3.784128	6.630158	8.475830
H	3.637969	2.695307	10.275892	F	6.201844	7.376232	8.157686
C	6.984731	1.469583	12.201131	F	5.814910	7.343891	10.318532
H	7.378098	0.861453	11.370385				

Zero-point correction= 0.279844 (Hartree/Particle)
Thermal correction to Energy= 0.301746
Thermal correction to Enthalpy= 0.302691
Thermal correction to Gibbs Free Energy= 0.227071
Sum of electronic and zero-point Energies= -1368.527357
Sum of electronic and thermal Energies= -1368.505454
Sum of electronic and thermal Enthalpies= -1368.504510
Sum of electronic and thermal Free Energies= -1368.580129

SMD(THF) uM06L-d3/def2-TZVPP
E(scf) = -1369.94450734 a.u.

Int-1^{+}
E(scf) = -1137.08064798 a.u.
ν_{min} = 25.39 cm^{-1}

C	6.023894	4.892748	10.600373	H	3.421357	2.964064	10.887095
H	5.093574	4.793845	10.011910	H	2.473860	3.096309	12.384823
O	6.072370	4.478106	11.763940	C	4.752476	4.842399	14.265658
Si	4.801278	3.645900	12.848627	H	5.748514	4.958043	14.719876
C	5.647693	2.026756	13.171353	H	4.384835	5.828434	13.942169
H	6.637563	2.181822	13.627222	H	4.065278	4.453716	15.035518
H	5.033416	1.439006	13.873664	C	7.219093	5.493450	9.962854
H	5.762412	1.444666	12.244039	H	7.917956	5.874551	10.719702
C	3.273273	3.573110	11.792599	H	7.721878	4.672639	9.414935
H	2.919433	4.576367	11.507441	C	6.836120	6.573659	8.959663

C	8.056073	7.173002	8.217427	F	7.659684	8.095518	7.348246
F	5.991502	6.064057	8.030659	F	8.702363	6.202941	7.565089
F	6.193536	7.582274	9.593465	F	8.889842	7.728817	9.099233

Zero-point correction= 0.186863 (Hartree/Particle)
Thermal correction to Energy= 0.204551
Thermal correction to Enthalpy= 0.205496
Thermal correction to Gibbs Free Energy= 0.139879
Sum of electronic and zero-point Energies= -1136.893785
Sum of electronic and thermal Energies= -1136.876097
Sum of electronic and thermal Enthalpies= -1136.875152
Sum of electronic and thermal Free Energies= -1136.940769

^{1}A-dmpe
E(scf) = -4989.69603309 a.u.
ν_{min} = 17.20 cm^{-1}

Br	10.465588	4.360277	13.855241	H	4.706516	3.521209	10.703949
Fe	9.388696	6.382257	12.930912	C	6.650950	4.395537	10.297352
P	8.440561	8.350668	12.367957	H	6.630091	4.144302	9.231708
P	11.164283	7.699410	13.685719	C	7.757018	5.067150	10.836943
C	9.395904	9.769834	13.111136	H	8.585511	5.329144	10.166697
H	9.170439	10.709206	12.580888	H	4.788741	4.095873	13.136582
H	9.024799	9.881027	14.143918	H	13.611509	7.994640	13.638956
C	10.899445	9.452852	13.109608	H	13.093219	6.269779	13.546024
H	11.468423	10.167685	13.725627	H	12.967324	7.3142	12.103152
H	11.304950	9.508649	12.085368	H	12.077797	8.472868	15.843987
C	6.701753	8.666725	12.851597	H	10.297677	8.220855	15.899349
C	8.462831	8.672765	10.559519	H	11.386311	6.807586	15.915863
C	12.885355	7.293199	13.200108	H	9.500144	8.630417	10.196117
C	11.250306	7.824045	15.517781	H	7.885595	7.881515	10.059425
C	7.836721	5.410042	12.204582	H	8.029537	9.65751	10.327096
C	6.735914	5.036856	13.006156	H	6.38389	9.676635	12.550415
H	6.748654	5.271513	14.077493	H	6.064491	7.911382	12.370183
C	5.622284	4.368769	12.480867	H	6.605167	8.558407	13.941883
C	5.573126	4.043840	11.118814				

Zero-point correction= 0.299132 (Hartree/Particle)
Thermal correction to Energy= 0.321156
Thermal correction to Enthalpy= 0.322100
Thermal correction to Gibbs Free Energy= 0.245792
Sum of electronic and zero-point Energies= -4989.396901
Sum of electronic and thermal Energies= -4989.374877
Sum of electronic and thermal Enthalpies= -4989.373933
Sum of electronic and thermal Free Energies= -4989.450241

^{3}A-dmpe
E(scf) = -4989.71600265 a.u.
ν_{min} = 12.73 cm^{-1}

Br	10.508247	4.355366	13.839613	H	4.674723	3.564863	10.709146
Fe	9.402124	6.367223	12.932171	C	6.626142	4.418617	10.293307
P	8.446627	8.338489	12.358575	H	6.591497	4.180118	9.225158
P	11.167149	7.706361	13.700593	C	7.746469	5.069142	10.829187
C	9.385660	9.762327	13.112788	H	8.571653	5.327652	10.154175
H	9.157801	10.700536	12.581398	H	4.788888	4.107061	13.147701
H	9.003214	9.868859	14.141845	H	13.612042	8.013428	13.635262
C	10.891279	9.457790	13.125197	H	13.102244	6.285587	13.545601
H	11.448574	10.176523	13.747338	H	12.959277	7.329825	12.104392
H	11.305867	9.518012	12.104907	H	12.090985	8.475439	15.855188
C	6.703043	8.640639	12.834985	H	10.311789	8.218715	15.920784
C	8.473498	8.666425	10.551238	H	11.404581	6.808354	15.926638
C	12.886400	7.308046	13.201945	H	9.512543	8.634818	10.191926
C	11.263051	7.825537	15.532299	H	7.905038	7.872179	10.045918
C	7.842408	5.394023	12.199839	H	8.031798	9.647968	10.321012
C	6.746593	5.024538	13.009465	H	6.381814	9.650994	12.538795
H	6.773854	5.244284	14.083396	H	6.072355	7.885476	12.344859
C	5.618993	4.377938	12.486903	H	6.601212	8.524262	13.923896
C	5.552090	4.071211	11.121538				

Zero-point correction= 0.299067 (Hartree/Particle)
Thermal correction to Energy= 0.321155
Thermal correction to Enthalpy= 0.322099
Thermal correction to Gibbs Free Energy= 0.244213
Sum of electronic and zero-point Energies= -4989.416935
Sum of electronic and thermal Energies= -4989.394848
Sum of electronic and thermal Enthalpies= -4989.393904
Sum of electronic and thermal Free Energies= -4989.471789

^{5}A-dmpe
E(scf) = -4989.72792644 a.u.
ν_{min} = 16.99 cm^{-1}

Br	10.629980	5.676614	10.074860	H	8.723421	9.483642	13.810011
Fe	9.387243	6.129936	12.150752	C	10.724972	9.241197	12.970928
P	8.362130	8.362727	11.696068	H	11.208577	9.915474	13.697264
P	11.009905	7.466341	13.467063	H	11.242015	9.379821	12.006493
C	9.227732	9.562364	12.832040	C	6.583895	8.736077	11.970932
H	9.075395	10.594343	12.474858	C	8.704868	9.036219	10.019534

C	12.830032	7.276092	13.323021	H	13.368706	8.080535	13.847863
C	10.696479	7.483941	15.280268	H	13.122319	6.303475	13.746479
C	8.207189	5.062709	13.440756	H	13.096089	7.282580	12.255533
C	8.762098	4.294779	14.489367	H	9.777425	8.922442	9.805555
H	9.852180	4.237444	14.595586	H	8.152320	8.438588	9.279338
C	7.966621	3.598462	15.409040	H	8.411516	10.094479	9.937620
C	6.570966	3.651717	15.306168	H	6.375997	9.812805	11.868380
H	5.943987	3.111363	16.021354	H	5.983607	8.178350	11.236603
C	5.985445	4.403962	14.280560	H	6.299252	8.399110	12.978693
H	4.895229	4.451343	14.192768	H	11.315417	8.238878	15.789951
C	6.796376	5.093861	13.368998	H	9.632031	7.696313	15.458604
H	6.310639	5.677006	12.577822	H	10.913873	6.487210	15.691425
H	8.432997	3.013168	16.208086				

^{1}a-dmpe

E(scf) = -2647.24001070 a.u.

ν_{min} = 16.08 cm^{-1}

Fe	9.381518	6.411653	12.941585	H	13.561627	8.030138	13.722216
P	8.445232	8.416932	12.298567	H	13.076558	6.296010	13.662969
P	11.116084	7.712433	13.713884	H	12.965334	7.297451	12.192429
C	9.410311	9.828163	13.052953	H	11.971114	8.523893	15.884245
H	9.235801	10.767525	12.503326	H	10.192799	8.259015	15.900455
H	9.004837	9.966090	14.069724	H	11.292153	6.857188	15.974209
C	10.903663	9.470219	13.115569	H	9.560511	8.682333	10.149268
H	11.468638	10.175699	13.746472	H	7.943492	7.949226	9.975007
H	11.350077	9.505602	12.107257	H	8.097629	9.724813	10.233875
C	6.698712	8.796210	12.721941	H	6.406748	9.803134	12.385624
C	8.514945	8.737930	10.487192	H	6.056446	8.042125	12.243619
C	12.855613	7.305935	13.287249	H	6.566594	8.719353	13.811547
C	11.157081	7.862933	15.548413	C	10.230747	4.751452	13.577744
C	7.837802	5.385496	12.275724	C	11.224708	4.056205	12.850910
C	6.765752	5.010663	13.117511	C	9.910940	4.217664	14.847564
H	6.820284	5.243153	14.188536	C	11.857369	2.909748	13.350043
C	5.631034	4.343342	12.637669	H	11.517244	4.421435	11.858143
C	5.526877	4.014278	11.279622	C	10.540817	3.077495	15.364546
H	4.644841	3.490513	10.899986	H	9.136881	4.705719	15.453567
C	6.574047	4.364120	10.417406	C	11.520962	2.412866	14.616171
H	6.512061	4.110844	9.353488	H	12.618398	2.400056	12.749218
C	7.699854	5.036833	10.911812	H	10.262137	2.700119	16.354413
H	8.500738	5.297183	10.207571	H	12.012977	1.519692	15.011912
H	4.823676	4.072767	13.326832				

Zero-point correction= 0.386959 (Hartree/Particle)

Thermal correction to Energy= 0.412615
Thermal correction to Enthalpy= 0.413559
Thermal correction to Gibbs Free Energy= 0.329196
Sum of electronic and zero-point Energies= -2646.853052
Sum of electronic and thermal Energies= -2646.827396
Sum of electronic and thermal Enthalpies= -2646.826452
Sum of electronic and thermal Free Energies= -2646.910815

^{3}a-dmpe
E(scf) = -2647.25954564 a.u.
ν_{min} = 15.56 cm^{-1}

Fe	9.383664	6.392320	12.930090	H	13.566765	8.023001	13.675172
P	8.440500	8.409612	12.297715	H	13.081714	6.288733	13.621696
P	11.122061	7.704846	13.707347	H	12.945533	7.292157	12.154324
C	9.404565	9.816459	13.059768	H	12.015029	8.499480	15.867716
H	9.226286	10.759063	12.516884	H	10.235480	8.245346	15.910575
H	9.000619	9.946079	14.078144	H	11.327153	6.836473	15.959908
C	10.899050	9.463113	13.116479	H	9.531816	8.706503	10.140298
H	11.463376	10.168445	13.748158	H	7.920474	7.958676	9.974965
H	11.342160	9.503483	12.106983	H	8.059176	9.733070	10.249659
C	6.696006	8.772251	12.743594	H	6.394839	9.781313	12.422108
C	8.489196	8.748161	10.488979	H	6.053429	8.019914	12.262974
C	12.854189	7.298978	13.250774	H	6.575966	8.681607	13.833468
C	11.191662	7.845282	15.541561	C	10.234943	4.732897	13.588415
C	7.834521	5.369073	12.249433	C	11.242276	4.037390	12.880743
C	6.760767	4.995021	13.088957	C	9.912588	4.220520	14.866215
H	6.824384	5.202931	14.164227	C	11.888518	2.911372	13.408134
C	5.612699	4.357558	12.600005	H	11.534797	4.384922	11.881981
C	5.498375	4.057515	11.236234	C	10.556304	3.100915	15.410636
H	4.606353	3.556119	10.849815	H	9.126448	4.708050	15.456383
C	6.548644	4.405359	10.376876	C	11.551229	2.436189	14.682357
H	6.478997	4.172766	9.308767	H	12.660019	2.399884	12.822472
C	7.687797	5.048679	10.879574	H	10.275960	2.739179	16.405809
H	8.490481	5.307950	10.177480	H	12.053325	1.558428	15.099321
H	4.803529	4.086566	13.286805				

Zero-point correction= 0.386949 (Hartree/Particle)
Thermal correction to Energy= 0.412662
Thermal correction to Enthalpy= 0.413606
Thermal correction to Gibbs Free Energy= 0.327963
Sum of electronic and zero-point Energies= -2646.872597
Sum of electronic and thermal Energies= -2646.846884
Sum of electronic and thermal Enthalpies= -2646.845940

Sum of electronic and thermal Free Energies= -2646.931582

^{5}a-dmpe

E(scf) = -2647.25839195 a.u.

ν_{min} = 11.99 cm^{-1}

Fe	9.425616	6.161628	12.140219	H	13.279921	8.207711	14.104204
P	8.369445	8.385575	11.727483	H	13.135321	6.435638	13.850970
P	10.978425	7.515546	13.542202	H	13.146249	7.531306	12.443048
C	9.144576	9.575651	12.938813	H	9.899575	9.046293	9.954087
H	8.967127	10.613544	12.610777	H	8.328953	8.539885	9.298926
H	8.607149	9.443310	13.893134	H	8.498983	10.175414	10.031780
C	10.645814	9.303795	13.124603	H	6.371339	9.833590	11.785001
H	11.073794	9.957694	13.902839	H	6.023250	8.204268	11.114562
H	11.195046	9.511887	12.190711	H	6.226884	8.410039	12.874902
C	6.574961	8.756138	11.890364	H	11.171528	8.195230	15.908148
C	8.811778	9.121404	10.097859	H	9.523030	7.603668	15.490411
C	12.814799	7.423211	13.486474	H	10.840736	6.435640	15.718185
C	10.600774	7.441361	15.343316	C	10.395954	5.680009	10.382580
C	8.245640	5.108978	13.466049	C	9.730531	5.685699	9.134133
C	8.804203	4.310783	14.491912	C	11.770395	5.348245	10.342816
H	9.895276	4.228908	14.573390	C	10.381194	5.384504	7.930041
C	8.017906	3.616973	15.421549	H	8.663429	5.937755	9.096566
C	6.621251	3.700180	15.356266	C	12.439441	5.044236	9.148814
H	6.000692	3.163712	16.080090	H	12.344339	5.328367	11.277043
C	6.028711	4.479435	14.355170	C	11.744233	5.062186	7.933551
H	4.937729	4.552235	14.294829	H	9.827267	5.401748	6.985558
C	6.832681	5.165684	13.434184	H	13.505319	4.793505	9.163701
H	6.337524	5.770647	12.665096	H	12.259754	4.828167	6.997454
H	8.492298	3.011097	16.200679				

Zero-point correction= 0.386450 (Hartree/Particle)
Thermal correction to Energy= 0.412826
Thermal correction to Enthalpy= 0.413770
Thermal correction to Gibbs Free Energy= 0.324665
Sum of electronic and zero-point Energies= -2646.871941
Sum of electronic and thermal Energies= -2646.845566
Sum of electronic and thermal Enthalpies= -2646.844622
Sum of electronic and thermal Free Energies= -2646.933727

^{2}B-dmpe

E(scf) = -4989.77374464 a.u.

ν_{min} = 16.34 cm^{-1}

Br	10.540930	5.423496	10.121354	H	5.744932	3.163051	15.681694
Fe	9.456876	6.234125	12.213926	C	6.000394	4.355681	13.879770
P	8.409425	8.141496	11.821569	H	4.978406	4.181414	13.523051
P	10.993068	7.357876	13.427777	C	6.875071	5.155599	13.133688
C	9.169272	9.444372	12.947929	H	6.500575	5.592996	12.199948
H	8.955409	10.461903	12.576483	H	8.091855	3.579354	16.453772
H	8.666515	9.338184	13.925005	H	13.370136	8.132294	13.600582
C	10.671787	9.186499	13.089786	H	13.228939	6.348176	13.457446
H	11.131556	9.814363	13.872748	H	12.984582	7.366908	12.016664
H	11.188224	9.418633	12.142077	H	9.731148	8.937548	9.926611
C	6.606514	8.510471	12.080257	H	8.148697	8.336183	9.394239
C	8.655536	8.945063	10.159255	H	8.273137	9.978757	10.119276
C	12.825775	7.310677	13.104645	H	6.391822	9.590774	12.023616
C	11.021120	7.368457	15.290172	H	6.013603	7.987626	11.313659
C	8.217281	5.428861	13.522435	H	6.303918	8.125139	13.065397
C	8.598511	4.817619	14.748430	H	11.647310	8.185096	15.686136
H	9.618388	4.968476	15.118294	H	9.992494	7.478449	15.664397
C	7.737300	4.020479	15.514659	H	11.414278	6.407835	15.657128
C	6.424137	3.781437	15.086761				

Zero-point correction= 0.296745 (Hartree/Particle)
Thermal correction to Energy= 0.318911
Thermal correction to Enthalpy= 0.319855
Thermal correction to Gibbs Free Energy= 0.242438
Sum of electronic and zero-point Energies= -4989.476999
Sum of electronic and thermal Energies= -4989.454833
Sum of electronic and thermal Enthalpies= -4989.453889
Sum of electronic and thermal Free Energies= -4989.531306

^{4}B-dmpe
E(scf) = -4989.80188038 a.u.
ν_{min} = 18.48 cm^{-1}

Br	10.539758	5.288136	10.129823	C	8.772628	9.044147	10.086521
Fe	9.429401	6.201806	12.209835	C	12.793396	7.383892	13.097860
P	8.460763	8.258066	11.743233	C	10.949873	7.394736	15.267585
P	10.965337	7.470858	13.410112	C	8.177208	5.192148	13.524343
C	9.165270	9.558798	12.902752	C	8.647789	4.470265	14.654545
H	8.967343	10.575219	12.520055	H	9.719974	4.492617	14.888922
H	8.614421	9.453346	13.853326	C	7.814850	3.728129	15.503692
C	10.659932	9.304988	13.119478	C	6.436002	3.665154	15.260863
H	11.069843	9.911239	13.945837	H	5.777126	3.091383	15.920129
H	11.226612	9.569323	12.209852	C	5.920001	4.354989	14.155388
C	6.646077	8.602994	11.928546	H	4.844309	4.320265	13.945718

C	6.773919	5.090365	13.321384	H	8.372663	10.069381	10.015014
H	6.322651	5.619311	12.472206	H	6.411381	9.677475	11.845005
H	8.240981	3.196197	16.362612	H	6.093217	8.052993	11.151055
H	13.353480	8.176031	13.622472	H	6.315656	8.228523	12.909324
H	13.165966	6.400860	13.425827	H	11.628328	8.134917	15.723366
H	12.963554	7.466878	12.013419	H	9.921753	7.572297	15.617470
H	9.858522	9.056830	9.907093	H	11.243454	6.384190	15.590381
H	8.315486	8.416620	9.305596				

Zero-point correction= 0.296159 (Hartree/Particle)
Thermal correction to Energy= 0.318774
Thermal correction to Enthalpy= 0.319718
Thermal correction to Gibbs Free Energy= 0.240098
Sum of electronic and zero-point Energies= -4989.505721
Sum of electronic and thermal Energies= -4989.483107
Sum of electronic and thermal Enthalpies= -4989.482163
Sum of electronic and thermal Free Energies= -4989.561782

^{6}B-dmpe
E(scf) = -4989.74991478 a.u.
ν_{min} = 19.38 cm^{-1}

Br	12.482878	8.454100	9.575594	H	5.830003	3.510476	16.272789
Fe	9.375218	5.875556	11.989139	C	5.905701	4.626418	14.410858
P	8.336923	8.144791	11.645804	H	4.816580	4.697221	14.316695
P	10.987504	7.237827	13.367635	C	6.733314	5.198845	13.436038
C	9.188054	9.332631	12.809824	H	6.258751	5.700610	12.584774
H	9.021874	10.371002	12.474947	H	8.320765	3.353624	16.455036
H	8.680747	9.221899	13.783765	H	13.314716	7.853940	13.892981
C	10.686418	9.026209	12.938696	H	13.134586	6.099656	13.543462
H	11.160608	9.672347	13.697159	H	13.096852	7.290617	12.195717
H	11.206722	9.190155	11.978916	H	9.675892	8.890153	9.758488
C	6.557126	8.498751	11.977216	H	8.051600	8.349768	9.240386
C	8.600310	8.928268	9.999837	H	8.247570	9.972872	9.991638
C	12.818753	7.111460	13.246541	H	6.344507	9.576582	11.893350
C	10.698136	7.211947	15.193517	H	5.934850	7.951118	11.253496
C	8.145669	5.143845	13.504236	H	6.303210	8.149109	12.988502
C	8.674488	4.454901	14.621402	H	11.258370	8.016535	15.696335
H	9.762548	4.360812	14.723480	H	9.621713	7.325358	15.386629
C	7.865033	3.875289	15.606375	H	11.011508	6.240382	15.601921
C	6.469426	3.960296	15.507463				

Zero-point correction= 0.298006 (Hartree/Particle)
Thermal correction to Energy= 0.320416

Thermal correction to Enthalpy= 0.321360
Thermal correction to Gibbs Free Energy= 0.242206
Sum of electronic and zero-point Energies= -4989.451908
Sum of electronic and thermal Energies= -4989.429499
Sum of electronic and thermal Enthalpies= -4989.428555
Sum of electronic and thermal Free Energies= -4989.507709

^{2}b-dmpe
E(scf) = -2647.30755265 a.u.
ν_{min} = 20.02 cm^{-1}

Fe	9.463045	6.287447	12.251338	H	13.502099	7.609850	13.668630
P	8.527606	8.236068	11.939180	H	13.127205	5.858476	13.578059
P	11.048156	7.158694	13.454634	H	13.057484	6.851006	12.097034
C	9.520123	9.461931	12.977550	H	9.536967	9.075019	9.868378
H	9.426463	10.486089	12.576098	H	7.858970	8.554751	9.601733
H	9.060041	9.463138	13.981067	H	8.179977	10.153712	10.355011
C	10.979682	9.005210	13.067217	H	6.602979	9.753098	12.455108
H	11.551223	9.585646	13.812961	H	6.077009	8.144665	11.857016
H	11.482994	9.135333	12.094404	H	6.674173	8.306322	13.526155
C	6.805130	8.669327	12.495741	H	11.884341	7.885276	15.702127
C	8.520858	9.106650	10.288690	H	10.105410	7.651315	15.672444
C	12.865601	6.852256	13.180367	H	11.181009	6.233971	15.739208
C	11.067985	7.247415	15.323200	C	10.487055	6.071184	10.593832
C	8.115379	5.522650	13.482213	C	10.233341	4.768733	10.069010
C	8.018607	5.287313	14.880351	C	11.380294	6.847138	9.806050
H	8.763273	5.736155	15.546248	C	10.803088	4.286763	8.884327
C	7.013787	4.501192	15.462873	H	9.551197	4.095373	10.613008
C	6.038168	3.887137	14.665964	C	11.960410	6.383633	8.617846
H	5.253150	3.271551	15.115909	H	11.635823	7.861545	10.137050
C	6.086564	4.086649	13.278063	C	11.677669	5.094967	8.142315
H	5.330206	3.622923	12.633793	H	10.565926	3.275429	8.533382
C	7.086968	4.891174	12.719605	H	12.642248	7.031781	8.054358
H	7.061310	5.046527	11.629616	H	12.128129	4.728347	7.214965
H	6.991717	4.361653	16.550359				

Zero-point correction= 0.385424 (Hartree/Particle)
Thermal correction to Energy= 0.410432
Thermal correction to Enthalpy= 0.411377
Thermal correction to Gibbs Free Energy= 0.329713
Sum of electronic and zero-point Energies= -2646.922129
Sum of electronic and thermal Energies= -2646.897120
Sum of electronic and thermal Enthalpies= -2646.896176
Sum of electronic and thermal Free Energies= -2646.977840

^{4}b-dmpe
E(scf) = -2647.32480952 a.u.
ν_{min} = 15.69 cm^{-1}

Fe	9.452544	6.278051	12.176185	H	13.301021	8.292175	13.766857
P	8.423327	8.344909	11.820713	H	13.161249	6.516093	13.554486
P	10.936927	7.545539	13.456233	H	12.996649	7.584538	12.139285
C	9.137058	9.636109	12.988506	H	9.695183	9.277761	9.950324
H	8.929893	10.657354	12.623270	H	8.141279	8.619164	9.396228
H	8.600776	9.516151	13.945862	H	8.187255	10.231066	10.189462
C	10.633843	9.382902	13.181687	H	6.344035	9.708079	12.066420
H	11.055621	9.980745	14.008626	H	6.033920	8.105332	11.321999
H	11.189085	9.653723	12.266893	H	6.328177	8.216393	13.074635
C	6.607714	8.637384	12.097017	H	11.547634	8.201877	15.794118
C	8.621676	9.217200	10.185861	H	9.844639	7.638871	15.645668
C	12.780312	7.491875	13.214371	H	11.167424	6.452612	15.644240
C	10.880532	7.464011	15.317541	C	10.468613	5.766535	10.430308
C	8.205752	5.237292	13.480142	C	9.860124	5.809470	9.146038
C	8.688491	4.499678	14.595634	C	11.787267	5.235108	10.423180
H	9.758936	4.542373	14.834899	C	10.492726	5.377842	7.972005
C	7.870230	3.717925	15.422868	H	8.840240	6.206025	9.057191
C	6.493952	3.627921	15.172625	C	12.441564	4.797224	9.263194
H	5.846335	3.023165	15.815129	H	12.334490	5.166164	11.371826
C	5.966345	4.331563	14.081211	C	11.797118	4.866871	8.020490
H	4.892541	4.276536	13.865968	H	9.968631	5.441546	7.010925
C	6.805675	5.106563	13.268746	H	13.462150	4.401046	9.325328
H	6.345418	5.644834	12.430443	H	12.300954	4.530765	7.108811
H	8.305519	3.176122	16.271043				

Zero-point correction= 0.383870 (Hartree/Particle)
Thermal correction to Energy= 0.410051
Thermal correction to Enthalpy= 0.410995
Thermal correction to Gibbs Free Energy= 0.323412
Sum of electronic and zero-point Energies= -2646.940940
Sum of electronic and thermal Energies= -2646.914758
Sum of electronic and thermal Enthalpies= -2646.913814
Sum of electronic and thermal Free Energies= -2647.001397

^{6}b-dmpe
E(scf) = -2647.27210183 a.u.
ν_{min} = 24.18 cm^{-1}

Fe	10.520468	5.062773	12.713015	P	8.220740	8.224183	11.977538

P	11.255765	7.176247	13.685648	H	13.408888	6.492152	14.601737
C	9.526441	9.320725	12.766112	H	13.608288	7.332172	13.044140
H	9.509821	10.296437	12.246640	H	9.587895	7.827171	9.981630
H	9.186552	9.515773	13.798017	H	7.873918	8.026628	9.561541
C	10.964829	8.790783	12.774013	H	8.864310	9.478262	9.925497
H	11.627674	9.554324	13.218345	H	7.098365	10.436391	11.627613
H	11.319426	8.619671	11.743945	H	5.957768	9.059435	11.490264
C	6.818839	9.455801	12.051399	H	6.506008	9.597356	13.098312
C	8.687358	8.421317	10.190284	H	10.836485	8.549943	15.699545
C	13.073596	7.355164	14.007015	H	9.455694	7.458906	15.306902
C	10.550779	7.543436	15.353956	H	10.919562	6.794976	16.070196
C	8.702247	4.581922	13.606913	C	10.673734	5.412865	10.668944
C	8.523309	4.558343	15.013011	C	9.759768	4.872249	9.727193
H	9.376752	4.801913	15.659409	C	11.700615	6.214591	10.103934
C	7.308193	4.227812	15.626000	C	9.844604	5.118940	8.351488
C	6.197375	3.879949	14.842506	H	8.946272	4.229173	10.084732
H	5.247059	3.607258	15.311644	C	11.801385	6.479704	8.734158
C	6.328204	3.890620	13.446317	H	12.459147	6.653472	10.766401
H	5.468980	3.630466	12.817274	C	10.867904	5.930369	7.840160
C	7.548594	4.240755	12.855128	H	9.107164	4.679710	7.669788
H	7.601916	4.260495	11.760047	H	12.609100	7.116613	8.355808
H	7.224515	4.232968	16.718899	H	10.939839	6.128500	6.766543
H	13.314695	8.293766	14.534885				

Zero-point correction= 0.384669 (Hartree/Particle)
Thermal correction to Energy= 0.410945
Thermal correction to Enthalpy= 0.411889
Thermal correction to Gibbs Free Energy= 0.324707
Sum of electronic and zero-point Energies= -2646.887433
Sum of electronic and thermal Energies= -2646.861157
Sum of electronic and thermal Enthalpies= -2646.860213
Sum of electronic and thermal Free Energies= -2646.947395

2.8

E(scf) = -639.607152592 a.u.

ν_{min} = 35.68 cm^{-1}

C	-1.939668	1.153153	-1.751043	C	0.585966	0.609036	1.722856
C	-1.612427	-0.125066	-1.509412	C	-0.636971	0.627747	2.268445
O	-0.390899	-0.638025	-1.254459	H	-2.983746	1.407157	-1.942947
Si	1.127482	0.104244	-1.016628	H	-1.207755	1.963582	-1.768643
C	0.988088	1.297767	0.452633	H	-2.385391	-0.904466	-1.507151
C	2.264374	-1.328360	-0.624279	H	0.270430	2.091282	0.186519
C	1.653418	1.005548	-2.575990	H	1.978492	1.776796	0.560292

H	3.284853	-0.964579	-0.420161	H	2.682454	1.385197	-2.461508
H	2.314134	-2.032752	-1.470189	H	1.367227	0.011762	2.211757
H	1.910983	-1.878043	0.262517	H	-0.862681	0.070133	3.181986
H	1.637338	0.319837	-3.438904	H	-1.455615	1.198299	1.816168
H	0.998741	1.860490	-2.804532				

Zero-point correction= 0.190524 (Hartree/Particle)
Thermal correction to Energy= 0.203766
Thermal correction to Enthalpy= 0.204710
Thermal correction to Gibbs Free Energy= 0.150571
Sum of electronic and zero-point Energies= -639.416628
Sum of electronic and thermal Energies= -639.403387
Sum of electronic and thermal Enthalpies= -639.402442
Sum of electronic and thermal Free Energies= -639.456581

DLPNO-CCSD(T)/def2-SVP-CPCM(THF)
E= -638.883752714910 a.u.

TSA´
E(scf) = -1214.53268573 a.u.
ν_{min} = -77.93 cm^{-1}

C	-1.620522	1.491003	-0.678905	H	1.904075	-2.020022	-2.618824
C	-1.500255	0.243293	-1.155360	H	1.865497	-2.484060	-0.893930
O	-0.372598	-0.477643	-1.329106	H	1.463552	1.008587	-3.401628
Si	1.281330	-0.089949	-1.179440	H	1.133129	2.215988	-2.129225
C	1.637113	0.435649	0.611442	H	2.773812	1.540046	-2.312085
C	2.155076	-1.688168	-1.598612	H	1.978754	-1.204088	2.069657
C	1.698739	1.301202	-2.365352	H	-0.903036	-0.193004	1.585244
C	1.198994	-0.569075	1.632314	H	-0.334323	-1.506975	2.779102
C	-0.075176	-0.735563	2.049811	C	-0.280962	1.058011	3.877060
H	-2.615248	1.930782	-0.588264	C	-1.000019	2.222381	3.228685
H	-0.770779	2.094267	-0.354955	F	-0.977664	0.498217	4.859086
H	-2.391040	-0.325900	-1.450582	F	0.954674	1.352528	4.259395
H	1.132758	1.400949	0.775625	F	-2.168189	1.814639	2.722132
H	2.721277	0.626185	0.679825	F	-0.252099	2.727635	2.237328
H	3.247707	-1.555290	-1.538199	F	-1.254323	3.220610	4.095536

Zero-point correction= 0.215863 (Hartree/Particle)
Thermal correction to Energy= 0.236283
Thermal correction to Enthalpy= 0.237227
Thermal correction to Gibbs Free Energy= 0.163603
Sum of electronic and zero-point Energies= -1214.316823
Sum of electronic and thermal Energies= -1214.296403
Sum of electronic and thermal Enthalpies= -1214.295459

Sum of electronic and thermal Free Energies= -1214.369083

DLPNO-CCSD(T)/def2-SVP-CPCM(THF)
E= -1213.586375908980 a.u.

A1´
E(scf) = -1214.58757143 a.u.
ν_{min} = 15.10 cm^{-1}

C	-1.623067	-0.434536	0.091671	H	3.434455	-1.838719	-0.778602
C	-0.631354	-0.192363	-0.774966	H	3.338492	-0.972228	0.783719
O	0.643994	-0.589030	-0.560672	H	2.102069	-0.472793	-3.343806
Si	2.078715	0.237508	-0.957803	H	1.304114	1.115156	-3.165920
C	2.021499	1.924029	-0.060508	H	3.081043	1.000678	-3.102597
C	3.452191	-0.844686	-0.303653	H	3.047853	1.913527	1.919535
C	2.144728	0.493975	-2.815964	H	0.646478	2.276685	2.972512
C	2.082333	1.816290	1.418129	H	-0.010342	1.342498	1.615287
C	0.883199	1.477313	2.245012	C	0.974846	0.196849	3.066538
H	-2.642827	-0.124583	-0.142843	C	2.024647	0.201016	4.204037
H	-1.426143	-0.945325	1.037630	F	-0.228500	-0.042436	3.660813
H	-0.820775	0.333895	-1.723004	F	1.258572	-0.882602	2.288544
H	1.085520	2.408882	-0.400744	F	1.855696	1.272178	4.988610
H	2.861403	2.522595	-0.454181	F	3.266917	0.236868	3.703393
H	4.434068	-0.384691	-0.501978	F	1.910338	-0.896334	4.955517

Zero-point correction= 0.218287 (Hartree/Particle)
Thermal correction to Energy= 0.237982
Thermal correction to Enthalpy= 0.238926
Thermal correction to Gibbs Free Energy= 0.168061
Sum of electronic and zero-point Energies= -1214.369285
Sum of electronic and thermal Energies= -1214.349589
Sum of electronic and thermal Enthalpies= -1214.348645
Sum of electronic and thermal Free Energies= -1214.419510

DLPNO-CCSD(T)/def2-SVP-CPCM(THF)
E= -1213.643050022326 a.u.

TSA
E(scf) = -1214.53382052 a.u.
ν_{min} = -62.94 cm^{-1}

C	-1.979027	1.376734	-1.184862	Si	1.062499	0.120914	-0.732659
C	-1.718908	0.060047	-1.015292	C	1.093826	1.217968	0.814386
O	-0.520282	-0.521676	-0.887479	C	2.124859	-1.402373	-0.523673

C	1.518329	1.090125	-2.270927	H	0.926334	2.010153	-2.385389
C	0.678458	0.484946	2.055460	H	2.583344	1.372365	-2.225609
C	-0.515931	0.580047	2.653475	H	1.418085	-0.212473	2.470741
H	-3.015575	1.710493	-1.238425	H	-0.759433	-0.013503	3.539318
H	-1.205109	2.143962	-1.134349	H	-1.293065	1.252154	2.273130
H	-2.537811	-0.669930	-1.021736	C	-1.697100	1.510268	-3.741962
H	0.445670	2.091382	0.633425	C	-3.124629	1.547762	-4.237287
H	2.128386	1.596275	0.906018	F	-0.995170	2.591113	-4.077131
H	3.180038	-1.117887	-0.379465	F	-1.058166	0.394992	-4.089760
H	2.062056	-2.046982	-1.415083	F	-3.777418	0.457054	-3.823321
H	1.803084	-1.989453	0.351021	F	-3.207616	1.590760	-5.582335
H	1.360108	0.475594	-3.170590	F	-3.744360	2.632612	-3.757866

Zero-point correction= 0.215899 (Hartree/Particle)
Thermal correction to Energy= 0.236287
Thermal correction to Enthalpy= 0.237231
Thermal correction to Gibbs Free Energy= 0.162986
Sum of electronic and zero-point Energies= -1214.317921
Sum of electronic and thermal Energies= -1214.297533
Sum of electronic and thermal Enthalpies= -1214.296589
Sum of electronic and thermal Free Energies= -1214.370835

DLPNO-CCSD(T)/def2-SVP-CPCM(THF)
E= -1213.587718214199 a.u.

A1
E(scf) = -1214.58657672 a.u.
ν_{min} = 19.17 cm^{-1}

O	-0.428331	-0.449571	1.032390	F	3.264659	1.733428	2.841378
C	0.751646	-0.879414	0.530113	H	0.792064	-1.204397	-0.515427
C	-0.960177	0.487514	-2.472079	H	-1.743084	-0.006772	-3.062611
C	-1.421279	1.137330	-1.200732	H	-2.326718	1.743606	-1.386437
Si	-1.867861	-0.081153	0.187493	H	-0.650606	1.811503	-0.789881
C	-2.596510	-1.669351	-0.491413	H	-2.828671	-2.373469	0.323738
C	-2.955147	0.722331	1.478145	H	-3.528290	-1.462112	-1.043831
C	2.362449	1.040306	0.766325	H	-1.894735	-2.159987	-1.184894
F	2.707765	1.048477	-0.552885	H	-3.944076	0.963555	1.055284
F	1.325189	1.910066	0.913707	H	-3.104331	0.048042	2.336971
C	0.302006	0.434588	-2.918089	H	-2.500451	1.656050	1.846561
C	1.973910	-0.367076	1.213717	H	0.553234	-0.084066	-3.847953
C	3.558513	1.640502	1.539118	H	1.124708	0.894598	-2.362637
F	3.862569	2.858648	1.085765	H	1.807110	-0.329305	2.302146
F	4.634009	0.855379	1.402637	H	2.842179	-1.013901	1.016998

Zero-point correction= 0.218850 (Hartree/Particle)
Thermal correction to Energy= 0.238534
Thermal correction to Enthalpy= 0.239479
Thermal correction to Gibbs Free Energy= 0.168544
Sum of electronic and zero-point Energies= -1214.367727
Sum of electronic and thermal Energies= -1214.348042
Sum of electronic and thermal Enthalpies= -1214.347098
Sum of electronic and thermal Free Energies= -1214.418033

DLPNO-CCSD(T)/def2-SVP-CPCM(THF)
E= -1213.643817347945 a.u.

TSB1
E(scf) = -1214.57114692 a.u.
ν_{min} = -425.66 cm^{-1}

O	-0.644800	0.588222	0.311750	F	0.385311	-4.314326	-0.951383
C	0.394758	-0.241471	0.631494	H	0.804778	-0.119732	1.643618
C	2.117027	0.788503	-0.454380	H	1.643932	0.483824	-1.390313
C	1.983845	2.083843	-0.019439	H	2.947787	0.164483	-0.114569
C	0.820702	2.934918	-0.432719	H	2.580870	2.424597	0.834830
Si	-0.686822	2.279843	0.528254	H	0.974481	4.006646	-0.224204
C	-2.327894	2.816692	-0.189293	H	0.592980	2.822695	-1.507885
C	-0.535866	2.661450	2.359989	H	-2.404024	2.526588	-1.249467
C	0.342714	-1.965019	-1.257569	H	-3.166084	2.355468	0.357982
F	1.661008	-1.951283	-1.603972	H	-2.436574	3.911678	-0.122710
F	-0.286922	-1.050445	-2.042629	H	-0.603871	3.748084	2.534887
C	0.161811	-1.671297	0.222521	H	-1.342659	2.171896	2.929450
C	-0.199773	-3.352601	-1.676022	H	0.429827	2.314264	2.760607
F	0.041560	-3.588300	-2.967162	H	-0.871907	-1.961142	0.488128
F	-1.520993	-3.415766	-1.473422	H	0.845674	-2.341459	0.761914

Zero-point correction= 0.219286 (Hartree/Particle)
Thermal correction to Energy= 0.237449
Thermal correction to Enthalpy= 0.238393
Thermal correction to Gibbs Free Energy= 0.172059
Sum of electronic and zero-point Energies= -1214.351861
Sum of electronic and thermal Energies= -1214.333698
Sum of electronic and thermal Enthalpies= -1214.332754
Sum of electronic and thermal Free Energies= -1214.399088

DLPNO-CCSD(T)/def2-SVP-CPCM(THF)
E= -1213.627892177234 a.u.

TSB2

E(scf) = -1214.56929572 a.u.
ν_{min} = -433.51 cm^{-1}

O	-0.478030	-0.900708	0.733837	F	3.840017	1.060077	2.102189
C	0.639402	-1.016321	-0.036167	H	0.819509	-2.023407	-0.439982
C	0.005947	-0.077100	-1.971004	H	-0.200388	-1.082220	-2.359742
C	-1.209301	0.663604	-1.449478	H	-2.007221	0.649197	-2.213533
Si	-1.876609	-0.111209	0.146683	H	-0.961616	1.719633	-1.259675
C	-3.198028	-1.405075	-0.163894	H	-3.437559	-1.951551	0.763099
C	-2.412077	1.129967	1.440989	H	-4.125572	-0.933712	-0.529774
C	1.675006	0.998738	1.136778	H	-2.863234	-2.135342	-0.918512
F	0.874207	1.816349	0.393434	H	-3.283316	1.709004	1.092578
F	1.086303	0.872479	2.356003	H	-2.694548	0.622403	2.377824
C	1.115155	0.566054	-2.484657	H	-1.588358	1.827398	1.657390
C	1.889614	-0.351893	0.482071	H	1.891902	0.011462	-3.019138
C	2.991342	1.781543	1.360570	H	1.314475	1.617063	-2.256112
F	2.756151	2.935749	1.987081	H	2.393869	-0.977475	1.239995
F	3.576636	2.047693	0.186247	H	2.591615	-0.224810	-0.356657

Zero-point correction= 0.218696 (Hartree/Particle)
Thermal correction to Energy= 0.236920
Thermal correction to Enthalpy= 0.237864
Thermal correction to Gibbs Free Energy= 0.171366
Sum of electronic and zero-point Energies= -1214.350600
Sum of electronic and thermal Energies= -1214.332376
Sum of electronic and thermal Enthalpies= -1214.331432
Sum of electronic and thermal Free Energies= -1214.397930

DLPNO-CCSD(T)/def2-SVP-CPCM(THF)
E= -1213.624776696574 a.u.

TSB3
E(scf) = -1214.56676485 a.u.
ν_{min} = -440.32 cm^{-1}

O	-0.625130	-0.683171	1.224227	F	0.989722	1.607112	1.849966
C	0.416576	-0.757315	0.342514	C	0.551365	0.485084	-2.335297
C	-0.198981	0.736986	-1.206101	C	1.766046	-0.471605	0.948932
C	-1.676089	0.414464	-1.095481	C	3.249693	1.173529	2.236278
Si	-2.123924	-0.056229	0.685023	F	3.500662	2.468733	2.435479
C	-3.430696	-1.391776	0.805549	F	4.346030	0.600321	1.725616
C	-2.525757	1.415942	1.771583	F	2.986686	0.605560	3.418753
C	2.053678	0.985934	1.272205	H	0.403653	-1.634507	-0.320834
F	2.362489	1.690227	0.145290	H	0.139617	1.557809	-0.566507

H	-2.275310	1.290983	-1.402829	H	-2.631785	1.103825	2.823656
H	-1.943982	-0.408809	-1.780527	H	-1.717667	2.162303	1.716022
H	-4.399192	-1.018660	0.432329	H	1.568211	0.876382	-2.426741
H	-3.148185	-2.273295	0.207848	H	0.201017	-0.207691	-3.107431
H	-3.571804	-1.711099	1.851130	H	1.858574	-1.042568	1.890426
H	-3.469565	1.893553	1.460740	H	2.567284	-0.809117	0.276883

Zero-point correction= 0.218535 (Hartree/Particle)
Thermal correction to Energy= 0.236905
Thermal correction to Enthalpy= 0.237849
Thermal correction to Gibbs Free Energy= 0.170612
Sum of electronic and zero-point Energies= -1214.348230
Sum of electronic and thermal Energies= -1214.329860
Sum of electronic and thermal Enthalpies= -1214.328916
Sum of electronic and thermal Free Energies= -1214.396153

DLPNO-CCSD(T)/def2-SVP-CPCM(THF)
E= -1213.623664444264 a.u.

B1
E(scf) = -1214.61156207 a.u.
ν_{min} = 24.22 cm^{-1}

O	-0.491262	0.618535	0.269615	F	0.628637	-4.184512	-1.127298
C	0.731286	-0.077085	0.445617	H	0.996795	-0.087786	1.521367
C	1.891640	0.631219	-0.308681	H	1.670452	0.578279	-1.388545
C	2.021256	2.062081	0.112698	H	2.820650	0.066505	-0.130356
C	0.929364	3.003754	-0.260347	H	2.673617	2.304932	0.958413
Si	-0.660508	2.285717	0.520272	H	1.115572	4.038377	0.068574
C	-2.241684	2.778077	-0.351374	H	0.757042	3.011414	-1.354773
C	-0.722107	2.649160	2.362410	H	-2.192577	2.522498	-1.421975
C	0.374276	-1.845090	-1.417551	H	-3.108844	2.258798	0.088924
F	1.583148	-1.764536	-2.048302	H	-2.412804	3.863425	-0.261193
F	-0.463398	-0.984727	-2.052267	H	-0.872313	3.726540	2.544142
C	0.509572	-1.546391	0.062477	H	-1.551886	2.102967	2.840443
C	-0.162908	-3.269481	-1.700433	H	0.216868	2.349670	2.855304
F	-0.206766	-3.508707	-3.012346	H	-0.410430	-1.883914	0.561552
F	-1.397284	-3.407397	-1.202493	H	1.338994	-2.166022	0.433027

Zero-point correction= 0.222347 (Hartree/Particle)
Thermal correction to Energy= 0.240367
Thermal correction to Enthalpy= 0.241311
Thermal correction to Gibbs Free Energy= 0.175087
Sum of electronic and zero-point Energies= -1214.389215
Sum of electronic and thermal Energies= -1214.371196

Sum of electronic and thermal Enthalpies= -1214.370251
Sum of electronic and thermal Free Energies= -1214.436475

DLPNO-CCSD(T)/def2-SVP-CPCM(THF)
E= -1213.673273377819 a.u.

B2
E(scf) = -1214.59256101 a.u.
ν_{min} = 30.52 cm^{-1}

O	-0.477867	-0.575025	0.566995	F	4.204059	0.379858	1.768131
C	0.538886	-0.722277	-0.411612	H	0.595307	-1.787876	-0.706963
C	0.143396	0.057807	-1.730847	H	0.679530	-0.471049	-2.543301
C	-1.390248	-0.131720	-1.869439	H	-1.617190	-1.134419	-2.270498
Si	-1.980112	-0.078040	-0.068406	H	-1.835435	0.604585	-2.554703
C	-3.302939	-1.333137	0.363470	H	-3.443692	-1.392401	1.455427
C	-2.407390	1.616700	0.612158	H	-4.269819	-1.048125	-0.084373
C	1.920502	0.736863	1.227612	H	-3.033036	-2.335232	-0.006387
F	1.112737	1.788671	0.920628	H	-3.297573	2.034814	0.113554
F	1.521073	0.267334	2.439008	H	-2.622411	1.552945	1.691914
C	0.542469	1.493998	-1.784499	H	-1.564243	2.310221	0.472606
C	1.911511	-0.369715	0.183570	H	1.597114	1.777015	-1.826959
C	3.331751	1.339079	1.435251	H	-0.186860	2.291643	-1.623796
F	3.322152	2.257277	2.402858	H	2.334063	-1.244009	0.698857
F	3.756574	1.920206	0.304392	H	2.608191	-0.110794	-0.626545

Zero-point correction= 0.220934 (Hartree/Particle)
Thermal correction to Energy= 0.239187
Thermal correction to Enthalpy= 0.240131
Thermal correction to Gibbs Free Energy= 0.173952
Sum of electronic and zero-point Energies= -1214.371627
Sum of electronic and thermal Energies= -1214.353374
Sum of electronic and thermal Enthalpies= -1214.352430
Sum of electronic and thermal Free Energies= -1214.418610

DLPNO-CCSD(T)/def2-SVP-CPCM(THF)
E= -1213.656396401948 a.u.

B3
E(scf) = -1214.59915873 a.u.
ν_{min} = 29.95 cm^{-1}

O	-0.636633	-0.587698	1.157653	C	-1.661459	0.278868	-1.115977
C	0.333767	-0.531405	0.120851	Si	-2.178385	-0.035586	0.678722
C	-0.131568	0.501338	-0.962735	C	-3.451343	-1.386622	0.932188

C	-2.605739	1.510381	1.649645	H	-2.144468	1.129791	-1.619186
C	1.993689	1.129124	1.209352	H	-1.855508	-0.623077	-1.724005
F	2.238465	1.969845	0.159765	H	-4.442911	-1.058424	0.577880
F	0.951185	1.658032	1.904255	H	-3.171908	-2.298817	0.381142
C	0.643151	0.399115	-2.229420	H	-3.543773	-1.641486	2.000943
C	1.719013	-0.281478	0.726085	H	-3.566382	1.938738	1.318708
C	3.231730	1.225592	2.133395	H	-2.689061	1.281285	2.725135
F	3.469111	2.492125	2.479313	H	-1.818598	2.270372	1.523688
F	4.312682	0.745106	1.507072	H	1.464610	1.084628	-2.450017
F	3.035313	0.510809	3.247180	H	0.465691	-0.440063	-2.909278
H	0.391524	-1.522769	-0.371865	H	1.837930	-0.965180	1.578915
H	0.018299	1.505320	-0.535165	H	2.503176	-0.519463	-0.006938

Zero-point correction= 0.220680 (Hartree/Particle)
Thermal correction to Energy= 0.239270
Thermal correction to Enthalpy= 0.240214
Thermal correction to Gibbs Free Energy= 0.172813
Sum of electronic and zero-point Energies= -1214.378479
Sum of electronic and thermal Energies= -1214.359889
Sum of electronic and thermal Enthalpies= -1214.358944
Sum of electronic and thermal Free Energies= -1214.426345

DLPNO-CCSD(T)/def2-SVP-CPCM(THF)
E= -1213.663605182422 a.u.

Int-1´ •
E(scf) = -553.092711190 a.u.
ν_{min} = 64.48 cm^{-1}

C	3.570734	2.455392	-0.552485
C	4.479420	2.896325	0.318564
C	1.476287	1.162764	-0.005374
C	2.931466	1.099641	-0.457785
F	3.588878	0.296122	0.419497
F	2.941747	0.495517	-1.681291
F	0.678327	1.813749	-0.839358
F	1.309827	1.572137	1.241955
H	3.196213	3.070620	-1.375663
H	4.906357	3.898102	0.227428
H	4.825946	2.267930	1.143113

Zero-point correction= 0.064709 (Hartree/Particle)
Thermal correction to Energy= 0.072529
Thermal correction to Enthalpy= 0.073473
Thermal correction to Gibbs Free Energy= 0.030871

Sum of electronic and zero-point Energies= -553.028002
Sum of electronic and thermal Energies= -553.020182
Sum of electronic and thermal Enthalpies= -553.019238
Sum of electronic and thermal Free Energies= -553.061840

DLPNO-CCSD(T)/def2-SVP-CPCM(THF)
E= -552.810290058477 a.u.

TSC
E(scf) = -1115.36802653 a.u.
ν_{min} = -115.17 cm^{-1}

C	3.077370	2.152977	-1.169390	H	3.100069	1.788027	-2.200290
C	3.281450	3.434081	-0.858431	H	3.502639	4.173663	-1.631976
C	-0.346548	-1.264537	1.507621	H	3.237070	3.778925	0.177896
C	1.002405	-1.221155	1.464101	H	-0.906432	-0.667467	2.242170
C	1.284072	0.631326	-0.232384	H	1.558290	-1.848013	0.764062
C	2.727532	1.102484	-0.156493	H	1.555892	-0.663151	2.219662
F	2.934903	1.546850	1.115470	H	-1.661744	-0.170967	-1.798871
F	3.512119	-0.002972	-0.347289	H	-3.358532	0.294310	-1.466966
F	0.972966	0.085266	-1.412323	H	-2.043362	0.818541	-0.374907
F	0.400123	1.579528	0.083964	H	-3.845122	-2.198634	2.097587
O	-1.074835	-1.987171	0.635775	H	-4.802710	-1.074719	1.095169
Si	-2.620674	-1.569241	0.017718	H	-3.467057	-0.452204	2.092430
C	-2.406108	-0.010635	-1.002998	H	-4.092682	-2.880057	-1.486747
C	-3.787677	-1.298859	1.463619	H	-2.373674	-3.221591	-1.821613
C	-3.108389	-3.046987	-1.019038	H	-3.172142	-3.958558	-0.403061

Zero-point correction= 0.221699 (Hartree/Particle)
Thermal correction to Energy= 0.241857
Thermal correction to Enthalpy= 0.242801
Thermal correction to Gibbs Free Energy= 0.168820
Sum of electronic and zero-point Energies= -1115.146328
Sum of electronic and thermal Energies= -1115.126170
Sum of electronic and thermal Enthalpies= -1115.125225
Sum of electronic and thermal Free Energies= -1115.199207

DLPNO-CCSD(T)/def2-SVP-CPCM(THF)
E= -1114.445118537647 a.u.

C1
E(scf) = -1115.41661581 a.u.
ν_{min} = 16.66 cm^{-1}

C	3.714115	2.318654	-0.534438	C	4.434562	3.054448	0.311205

C	-0.587864	-0.239341	0.127067	H	4.871586	4.005892	-0.001633
C	0.902711	-0.320907	0.124417	H	4.608758	2.727985	1.339671
C	1.545962	1.015325	-0.186393	H	-1.090027	0.550282	0.700221
C	3.095050	1.004928	-0.159296	H	1.236394	-1.044502	-0.634559
F	3.479011	0.603103	1.084694	H	1.315133	-0.662174	1.095246
F	3.501657	0.035114	-1.037802	H	-3.252111	-0.881042	-2.416411
F	1.171884	1.456146	-1.423847	H	-4.758631	-0.674324	-1.480249
F	1.133771	1.961690	0.709262	H	-3.424303	0.495180	-1.292479
O	-1.239187	-1.409514	-0.074904	H	-3.103907	-1.645377	2.430523
Si	-2.941202	-1.612765	-0.056305	H	-4.669173	-1.215676	1.687836
C	-3.661531	-0.570936	-1.441148	H	-3.376355	0.003842	1.801619
C	-3.578724	-1.064777	1.622822	H	-4.264287	-3.688587	-0.358390
C	-3.189127	-3.445108	-0.341094	H	-2.752927	-3.756193	-1.304142
H	3.515571	2.629870	-1.563016	H	-2.717410	-4.036837	0.460020

Zero-point correction= 0.224423 (Hartree/Particle)
Thermal correction to Energy= 0.244084
Thermal correction to Enthalpy= 0.245028
Thermal correction to Gibbs Free Energy= 0.173241
Sum of electronic and zero-point Energies= -1115.192193
Sum of electronic and thermal Energies= -1115.172532
Sum of electronic and thermal Enthalpies= -1115.171588
Sum of electronic and thermal Free Energies= -1115.243375

DLPNO-CCSD(T)/def2-SVP-CPCM(THF)
E= -1114.500113206080 a.u.

TSD1
E(scf) = -1115.40930235 a.u.
ν_{min} = -379.91 cm^{-1}

C	-2.468971	-0.771006	-1.576031	C	3.046824	0.548466	1.558605
C	-2.007806	0.485117	-0.887614	C	0.411624	2.175118	1.731429
C	-0.419715	-0.602076	0.232174	H	-2.583694	0.705536	0.015421
C	-0.706714	-1.972950	-0.318642	H	-0.808695	-0.385231	1.235783
C	-2.164531	-2.011709	-0.712357	H	-0.501139	-2.786171	0.398899
C	-1.438383	1.516617	-1.602845	H	-0.101631	-2.134838	-1.221502
F	-3.807688	-0.737837	-1.846737	H	-1.007300	1.346612	-2.591251
F	-1.828065	-0.948557	-2.769814	H	-1.318594	2.505584	-1.157098
F	-2.503590	-3.150319	-1.366213	H	1.317708	2.688903	-1.413567
F	-2.957074	-1.937028	0.402054	H	2.788912	3.133846	-0.500410
O	0.780086	-0.091875	-0.082270	H	2.785155	1.679506	-1.534207
Si	1.597043	1.256199	0.603253	H	2.698188	-0.099675	2.379167
C	2.173220	2.287862	-0.848449	H	3.655888	1.357156	1.995904

H	3.696288	-0.049324	0.898596	H	-0.482589	2.516113	1.186950
H	0.912927	3.061768	2.153776	H	0.084944	1.542841	2.572960

Zero-point correction= 0.224894 (Hartree/Particle)
Thermal correction to Energy= 0.242909
Thermal correction to Enthalpy= 0.243853
Thermal correction to Gibbs Free Energy= 0.178626
Sum of electronic and zero-point Energies= -1115.184409
Sum of electronic and thermal Energies= -1115.166393
Sum of electronic and thermal Enthalpies= -1115.165449
Sum of electronic and thermal Free Energies= -1115.230676

DLPNO-CCSD(T)/def2-SVP-CPCM(THF)
E= -1114.490600412316 a.u.

TSD2
E(scf) = -1115.40809621 a.u.
ν_{min} = -379.87 cm^{-1}

C	-1.567895	-1.143430	-2.483199	H	-0.667128	0.686562	-1.740588
C	-0.383412	-0.323448	-2.045769	H	0.351896	-1.514336	0.197854
C	-0.596542	-0.976033	0.077909	H	-1.588097	-2.851672	-0.291617
C	-1.845318	-1.799634	-0.108002	H	-2.511729	-1.735284	0.767589
C	-2.582117	-1.293264	-1.331065	H	1.681314	0.155212	-2.410636
C	0.872077	-0.563845	-2.556499	H	1.113850	-1.518931	-3.027955
F	-2.197211	-0.583613	-3.558053	H	2.423230	-0.111998	0.648616
F	-1.189522	-2.401521	-2.859549	H	2.821637	0.996970	1.983467
F	-3.604591	-2.107379	-1.697818	H	1.916533	-0.503476	2.318073
F	-3.117451	-0.058561	-1.096649	H	-1.225234	2.450127	2.720855
O	-0.759223	0.138310	0.821244	H	0.434130	2.760477	3.297551
Si	0.445564	1.254594	1.325695	H	-0.366381	1.210138	3.677995
C	2.047823	0.315707	1.592485	H	1.070972	2.138673	-0.929783
C	-0.243120	1.984681	2.904030	H	-0.353866	2.992531	-0.270283
C	0.625339	2.556865	-0.013634	H	1.279769	3.372308	0.337298

Zero-point correction= 0.224935 (Hartree/Particle)
Thermal correction to Energy= 0.242931
Thermal correction to Enthalpy= 0.243875
Thermal correction to Gibbs Free Energy= 0.178329
Sum of electronic and zero-point Energies= -1115.183161
Sum of electronic and thermal Energies= -1115.165165
Sum of electronic and thermal Enthalpies= -1115.164221
Sum of electronic and thermal Free Energies= -1115.229767

DLPNO-CCSD(T)/def2-SVP-CPCM(THF)

E= -1114.489890247163 a.u.

TSD3
E(scf) = -1115.40675025 a.u.
ν_{min} = -303.39 cm^{-1}

C	0.604758	2.802598	-0.818152	H	1.111691	3.352003	-0.022031
C	0.998675	1.562746	-1.218881	H	1.952005	1.145186	-0.889142
C	-0.570517	0.234056	-0.037309	H	0.528813	1.074166	-2.075350
C	-1.822309	0.952210	-0.459704	H	-0.185954	0.445171	0.970001
C	-1.811539	2.456766	-0.243816	H	-2.021378	0.757608	-1.524901
C	-0.788946	3.235423	-1.116224	H	-2.698336	0.573182	0.102605
F	-0.966930	4.566623	-0.889408	H	2.484480	-0.798213	0.641832
F	-1.136405	2.991396	-2.421578	H	3.000843	-2.474115	0.329176
F	-3.057518	2.951084	-0.492127	H	2.564045	-1.410657	-1.035690
F	-1.525677	2.743135	1.064348	H	-0.870982	-4.023714	-0.935754
O	-0.493030	-1.035603	-0.486908	H	0.796539	-4.601458	-0.671124
Si	0.533758	-2.269778	0.127698	H	0.441275	-3.500690	-2.029968
C	2.310414	-1.678757	0.002597	H	0.166493	-1.681645	2.526516
C	0.191244	-3.734276	-0.982455	H	-1.017166	-2.898945	1.972639
C	0.037597	-2.585767	1.909323	H	0.659691	-3.383830	2.347474

Zero-point correction= 0.224983 (Hartree/Particle)
Thermal correction to Energy= 0.243028
Thermal correction to Enthalpy= 0.243972
Thermal correction to Gibbs Free Energy= 0.177588
Sum of electronic and zero-point Energies= -1115.181767
Sum of electronic and thermal Energies= -1115.163722
Sum of electronic and thermal Enthalpies= -1115.162778
Sum of electronic and thermal Free Energies= -1115.229163

DLPNO-CCSD(T)/def2-SVP-CPCM(THF)
E= -1114.487716600590 a.u.

D1
E(scf) = -1115.43256478 a.u.
ν_{min} = 17.94 cm^{-1}

C	-2.194866	-0.953837	-1.638131	F	-1.339351	-0.627711	-2.642410
C	-2.249888	0.137369	-0.558531	F	-1.069222	-3.079554	-1.732653
C	-0.905720	-0.082606	0.196904	F	-2.678271	-2.808319	-0.273228
C	-0.653872	-1.617354	0.144138	O	0.122904	0.615312	-0.461386
C	-1.628317	-2.181824	-0.884129	Si	1.431487	1.387921	0.292910
C	-2.497036	1.511804	-1.055717	C	2.380179	2.181018	-1.113289
F	-3.398696	-1.211287	-2.203129	C	2.464488	0.096939	1.190345

C	0.765258	2.667850	1.499436	H	3.275080	2.701001	-0.733460
H	-3.068213	-0.189393	0.106194	H	2.708547	1.421361	-1.841129
H	-1.019092	0.260533	1.238813	H	1.874167	-0.414233	1.969002
H	-0.828187	-2.110148	1.109998	H	3.336236	0.561447	1.680780
H	0.375941	-1.814581	-0.176614	H	2.835273	-0.665953	0.486026
H	-1.657662	2.114460	-1.404667	H	1.591918	3.231335	1.963482
H	-3.516812	1.878095	-1.185758	H	0.108828	3.385429	0.980460
H	1.754726	2.917956	-1.642831	H	0.185173	2.198171	2.310773

Zero-point correction= 0.226349 (Hartree/Particle)
Thermal correction to Energy= 0.244879
Thermal correction to Enthalpy= 0.245823
Thermal correction to Gibbs Free Energy= 0.177970
Sum of electronic and zero-point Energies= -1115.206215
Sum of electronic and thermal Energies= -1115.187686
Sum of electronic and thermal Enthalpies= -1115.186742
Sum of electronic and thermal Free Energies= -1115.254595

DLPNO-CCSD(T)/def2-SVP-CPCM(THF)
E= -1114.520882507916 a.u.

D2
E(scf) = -1115.43337272 a.u.
ν_{min} = 21.00 cm^{-1}

C	-1.644858	-1.411623	-2.521856	H	-2.353761	0.392866	-1.693212
C	-1.361131	-0.025403	-1.966669	H	0.381917	-0.642368	-0.867851
C	-0.659908	-0.359939	-0.628188	H	-0.729647	-2.350764	0.359755
C	-1.404592	-1.612393	-0.091315	H	-2.145738	-1.300087	0.656248
C	-2.137175	-2.215563	-1.288657	H	-0.089471	1.743409	-2.442193
C	-0.631305	0.897574	-2.869796	H	-0.758544	0.835315	-3.952479
F	-2.532069	-1.429069	-3.542764	H	1.518883	-1.061874	1.595306
F	-0.495321	-1.992584	-2.976106	H	2.031322	0.052278	2.886293
F	-1.923371	-3.544867	-1.447967	H	0.370399	-0.603220	2.882299
F	-3.486452	-2.035341	-1.187539	H	-0.466603	3.433655	1.636888
O	-0.707566	0.728044	0.251267	H	0.704317	3.027334	2.920237
Si	0.605865	1.231245	1.208600	H	-0.903402	2.252506	2.903665
C	1.184713	-0.231169	2.239081	H	2.299762	1.041217	-0.622427
C	-0.081013	2.614697	2.265668	H	1.636945	2.694993	-0.526169
C	1.977235	1.833982	0.072382	H	2.858871	2.149248	0.654999

Zero-point correction= 0.225974 (Hartree/Particle)
Thermal correction to Energy= 0.244598
Thermal correction to Enthalpy= 0.245543
Thermal correction to Gibbs Free Energy= 0.177792

Sum of electronic and zero-point Energies= -1115.207399
Sum of electronic and thermal Energies= -1115.188774
Sum of electronic and thermal Enthalpies= -1115.187830
Sum of electronic and thermal Free Energies= -1115.255581

DLPNO-CCSD(T)/def2-SVP-CPCM(THF)
E= -1114.521750742088 a.u.

D3
E(scf) = -1115.44820547 a.u.
ν_{min} = 19.02 cm^{-1}

C	0.362860	2.894223	-1.224446	H	1.085136	3.689478	-1.417179
C	0.626982	1.461912	-1.532408	H	1.706069	1.257315	-1.589304
C	-0.031855	0.506512	-0.516501	H	0.203208	1.204828	-2.526349
C	-1.507072	0.871887	-0.291563	H	0.491941	0.630717	0.450392
C	-1.653216	2.310443	0.149757	H	-2.070368	0.733851	-1.226559
C	-1.018990	3.292754	-0.861532	H	-1.951970	0.228280	0.481282
F	-1.067638	4.555174	-0.363409	H	2.551135	-0.823583	0.958563
F	-1.838048	3.278034	-1.978753	H	2.885977	-2.572210	0.975762
F	-2.958791	2.637656	0.339597	H	3.068558	-1.644583	-0.539086
F	-1.018030	2.500131	1.348857	H	-0.550508	-3.779464	-1.452123
O	0.066196	-0.815576	-0.989769	H	0.873979	-4.509088	-0.662987
Si	0.664848	-2.108282	-0.064467	H	1.085207	-3.474720	-2.101443
C	2.459053	-1.753324	0.372994	H	-0.328843	-1.356600	2.104346
C	0.502197	-3.606429	-1.175447	H	-1.435748	-2.456683	1.237588
C	-0.379054	-2.272375	1.492014	H	-0.025916	-3.110779	2.115372

Zero-point correction= 0.227842 (Hartree/Particle)
Thermal correction to Energy= 0.245789
Thermal correction to Enthalpy= 0.246733
Thermal correction to Gibbs Free Energy= 0.180752
Sum of electronic and zero-point Energies= -1115.220363
Sum of electronic and thermal Energies= -1115.202417
Sum of electronic and thermal Enthalpies= -1115.201473
Sum of electronic and thermal Free Energies= -1115.267454

DLPNO-CCSD(T)/def2-SVP-CPCM(THF)
E= -1114.535043032628 a.u.

Table S6. Cartesian coordinates (xyz format) and energies of all the structures involved in redox potential calculated at the CPCM(MeCN) uB3LYP-d3/def2-svp level of theory.
Int-1•
E(scf) = -1137.24209058 a.u.

ν_{min} = 15.82 cm^{-1}

C	5.883043	5.165971	10.688409	H	5.477514	5.287878	14.402249
H	4.859317	5.449224	10.413680	H	4.141604	5.848592	13.358025
O	6.066603	4.139284	11.549496	H	3.824746	4.658300	14.648617
Si	4.908877	3.575653	12.685848	C	7.003211	5.416470	9.733014
C	5.749608	2.122650	13.510685	H	7.964812	5.202845	10.224448
H	6.683485	2.436357	14.004614	H	6.951505	4.773490	8.831011
H	5.088962	1.683258	14.276159	C	7.026096	6.854284	9.258643
H	5.991878	1.337369	12.776463	C	8.138400	7.159468	8.228837
C	3.368442	3.064397	11.743056	F	5.843590	7.186367	8.665971
H	2.916094	3.919899	11.215586	F	7.209860	7.713332	10.296395
H	3.604860	2.285759	10.999623	F	8.110334	8.443828	7.866306
H	2.612709	2.658753	12.436097	F	7.978217	6.406491	7.134301
C	4.555691	4.974027	13.885855	F	9.339818	6.892253	8.754192

Zero-point correction= 0.184161 (Hartree/Particle)
Thermal correction to Energy= 0.202147
Thermal correction to Enthalpy= 0.203092
Thermal correction to Gibbs Free Energy= 0.135246
Sum of electronic and zero-point Energies= -1137.057929
Sum of electronic and thermal Energies= -1137.039943
Sum of electronic and thermal Enthalpies= -1137.038999
Sum of electronic and thermal Free Energies= -1137.106844

Int-1^{+}
E(scf) = -1137.08957084 a.u.
ν_{min} = 26.71 cm^{-1}

C	6.016589	4.898333	10.600965	H	5.749975	4.955242	14.718327
H	5.086019	4.801789	10.013106	H	4.384403	5.825252	13.942998
O	6.066658	4.480248	11.763094	H	4.066940	4.448849	15.036188
Si	4.800763	3.645456	12.846807	C	7.213648	5.498306	9.965766
C	5.650760	2.027391	13.166996	H	7.908852	5.881780	10.724657
H	6.641827	2.185147	13.619213	H	7.719022	4.674389	9.425063
H	5.039283	1.438599	13.870702	C	6.838207	6.574660	8.957119
H	5.763518	1.447775	12.237951	C	8.062313	7.168418	8.217372
C	3.268209	3.569404	11.798001	F	5.996642	6.066481	8.024307
H	2.912085	4.572366	11.515076	F	6.196734	7.590219	9.581741
H	3.415375	2.961631	10.891644	F	7.669772	8.087197	7.340369
H	2.473473	3.090243	12.394457	F	8.712118	6.196576	7.571512
C	4.752931	4.839564	14.266432	F	8.893158	7.730885	9.097717

Zero-point correction= 0.186878 (Hartree/Particle)

Thermal correction to Energy= 0.204546
Thermal correction to Enthalpy= 0.205490
Thermal correction to Gibbs Free Energy= 0.139994
Sum of electronic and zero-point Energies= -1136.902693
Sum of electronic and thermal Energies= -1136.885025
Sum of electronic and thermal Enthalpies= -1136.884081
Sum of electronic and thermal Free Energies= -1136.949576

^{5}A-dmpe
E(scf) = -4989.73067971 a.u.
ν_{min} = 18.38 cm^{-1}

Br	10.608936	5.636534	10.068242	H	5.951085	3.100921	16.028005
Fe	9.381443	6.133298	12.153011	C	5.985549	4.402968	14.293879
P	8.363527	8.368644	11.692322	H	4.894940	4.453548	14.212799
P	11.010303	7.469581	13.463219	C	6.792908	5.096536	13.381625
C	9.227377	9.565903	12.830920	H	6.304123	5.686122	12.597147
H	9.075634	10.598013	12.474227	H	8.441084	2.997706	16.201132
H	8.721121	9.486301	13.807700	H	13.365054	8.082014	13.861229
C	10.724399	9.245154	12.972108	H	13.122272	6.305595	13.743355
H	11.205170	9.916575	13.702792	H	13.104590	7.298934	12.260631
H	11.244308	9.388661	12.010000	H	9.786463	8.933128	9.807743
C	6.584747	8.741903	11.960969	H	8.164179	8.441965	9.273941
C	8.712212	9.040927	10.016416	H	8.415597	10.098119	9.933585
C	12.831181	7.281239	13.326129	H	6.378274	9.818390	11.853943
C	10.690144	7.479218	15.275025	H	5.986382	8.181774	11.226958
C	8.204104	5.062313	13.445603	H	6.297888	8.409554	12.969594
C	8.763322	4.287662	14.487114	H	11.306358	8.233887	15.788172
H	9.853835	4.229266	14.588017	H	9.624928	7.690098	15.450247
C	7.971466	3.587536	15.407305	H	10.908803	6.481652	15.683386
C	6.575217	3.643727	15.312150				

Zero-point correction= 0.298191 (Hartree/Particle)
Thermal correction to Energy= 0.320957
Thermal correction to Enthalpy= 0.321902
Thermal correction to Gibbs Free Energy= 0.241345
Sum of electronic and zero-point Energies= -4989.432489
Sum of electronic and thermal Energies= -4989.409722
Sum of electronic and thermal Enthalpies= -4989.408778
Sum of electronic and thermal Free Energies= -4989.489335

^{4}B-dmpe
E(scf) = -4989.81134608 a.u.
ν_{min} = 17.20 cm^{-1}

Br	10.487327	5.225023	10.148555	H	5.772323	3.051580	15.898135
Fe	9.422436	6.210155	12.226995	C	5.916077	4.332730	14.146279
P	8.460484	8.268867	11.746912	H	4.841953	4.292462	13.930318
P	10.972098	7.481654	13.411466	C	6.769602	5.082537	13.324563
C	9.172705	9.569396	12.899587	H	6.319023	5.617822	12.478894
H	8.976215	10.584700	12.513922	H	8.232017	3.171962	16.358037
H	8.624737	9.469145	13.852311	H	13.359205	8.182606	13.621406
C	10.667560	9.313101	13.111898	H	13.171860	6.407629	13.428863
H	11.081303	9.921914	13.934114	H	12.972003	7.472600	12.013718
H	11.231848	9.572567	12.199461	H	9.859497	9.052339	9.904353
C	6.647329	8.617023	11.932332	H	8.311075	8.415965	9.308056
C	8.773801	9.043602	10.085701	H	8.378427	10.070140	10.010879
C	12.799491	7.389762	13.097941	H	6.415586	9.691468	11.843140
C	10.957085	7.410849	15.268355	H	6.092219	8.064438	11.158301
C	8.171124	5.192788	13.536965	H	6.316842	8.249634	12.915786
C	8.640177	4.464308	14.663861	H	11.641089	8.148350	15.719615
H	9.710309	4.494155	14.906909	H	9.930953	7.598299	15.618983
C	7.807563	3.707792	15.500876	H	11.244783	6.399759	15.594851
C	6.430798	3.636243	15.248303				

Zero-point correction= 0.296165 (Hartree/Particle)
Thermal correction to Energy= 0.318826
Thermal correction to Enthalpy= 0.319770
Thermal correction to Gibbs Free Energy= 0.239787
Sum of electronic and zero-point Energies= -4989.515181
Sum of electronic and thermal Energies= -4989.492520
Sum of electronic and thermal Enthalpies= -4989.491576
Sum of electronic and thermal Free Energies= -4989.571559

^{5}a-dmpe
E(scf) = -2647.26061858 a.u.
ν_{min} = 13.03 cm^{-1}

Fe	9.440885	6.184113	12.156444	C	8.821395	9.133772	10.105978
P	8.380101	8.403431	11.738184	C	12.826479	7.449331	13.495206
P	10.990557	7.541630	13.553628	C	10.613985	7.465655	15.354729
C	9.152414	9.597322	12.946687	C	8.252477	5.112704	13.461323
H	8.974041	10.633809	12.615112	C	8.803859	4.312570	14.489837
H	8.614184	9.467316	13.900797	H	9.894349	4.245852	14.590576
C	10.653936	9.328260	13.134426	C	8.010887	3.599348	15.399244
H	11.079420	9.982953	13.913194	C	6.614431	3.664205	15.310147
H	11.204251	9.537222	12.201449	H	5.988671	3.112842	16.018169
C	6.584277	8.766683	11.898638	C	6.028882	4.445472	14.306207

H	4.938198	4.505080	14.228124	H	9.536040	7.626029	15.502643
C	6.839452	5.151314	13.405786	H	10.858592	6.460997	15.729570
H	6.349785	5.758614	12.634997	C	10.391731	5.677257	10.393870
H	8.479858	2.993228	16.181511	C	9.710306	5.661799	9.153950
H	13.291360	8.233632	14.113221	C	11.765928	5.345492	10.341964
H	13.147630	6.461585	13.858602	C	10.345504	5.339753	7.946775
H	13.156647	7.559526	12.451590	H	8.643203	5.915221	9.125791
H	9.910288	9.067085	9.966071	C	12.419688	5.020946	9.144667
H	8.344145	8.545053	9.308915	H	12.352291	5.344090	11.268714
H	8.501160	10.185112	10.034602	C	11.708692	5.017330	7.938228
H	6.377353	9.843221	11.791174	H	9.779667	5.341629	7.009182
H	6.035691	8.211531	11.122980	H	13.486056	4.771794	9.149929
H	6.236767	8.421520	12.883690	H	12.212256	4.767563	6.999662
H	11.183069	8.221591	15.918302				

Zero-point correction= 0.386387 (Hartree/Particle)
Thermal correction to Energy= 0.412789
Thermal correction to Enthalpy= 0.413733
Thermal correction to Gibbs Free Energy= 0.324588
Sum of electronic and zero-point Energies= -2646.874231
Sum of electronic and thermal Energies= -2646.847830
Sum of electronic and thermal Enthalpies= -2646.846885
Sum of electronic and thermal Free Energies= -2646.936030

^{4}b-dmpe

E(scf) = -2647.33314688 a.u.

ν_{min} = 16.06 cm^{-1}

Fe	9.457123	6.311442	12.183705	C	6.513324	3.570865	15.111321
P	8.424419	8.379025	11.830828	H	5.870086	2.941512	15.734102
P	10.943886	7.578369	13.464801	C	5.983179	4.292921	14.033055
C	9.141054	9.667122	12.998693	H	4.911858	4.227899	13.808973
H	8.933711	10.688494	12.634588	C	6.817023	5.099415	13.245752
H	8.606149	9.547121	13.956778	H	6.354491	5.652143	12.418043
C	10.638318	9.414143	13.189537	H	8.322635	3.121161	16.214270
H	11.060615	10.012052	14.015874	H	13.308284	8.320343	13.771800
H	11.192345	9.685759	12.274295	H	13.166383	6.544891	13.557911
C	6.609181	8.666798	12.110343	H	13.001334	7.615921	12.144070
C	8.619490	9.250316	10.195637	H	9.692794	9.315153	9.959844
C	12.786010	7.521387	13.219235	H	8.139646	8.650937	9.406547
C	10.888325	7.494585	15.325438	H	8.182237	10.262756	10.199518
C	8.214002	5.244579	13.470181	H	6.343725	9.736830	12.078926
C	8.699040	4.488755	14.572843	H	6.034727	8.133004	11.337026
H	9.766678	4.542672	14.822752	H	6.332057	8.247593	13.089450
C	7.886153	3.675663	15.375108	H	11.561117	8.227251	15.801582

H	9.854335	7.678266	15.655092
H	11.168560	6.480903	15.651082
C	10.463038	5.772508	10.440147
C	9.847977	5.794803	9.158106
C	11.773682	5.220687	10.438597
C	10.466016	5.322573	7.991709
H	8.834850	6.207510	9.064407
C	12.413236	4.742123	9.286317
H	12.326316	5.168392	11.385286
C	11.761759	4.790298	8.046089
H	9.937797	5.371528	7.032151
H	13.427752	4.331519	9.352147
H	12.254128	4.422496	7.140536

Zero-point correction= 0.383954 (Hartree/Particle)
Thermal correction to Energy= 0.410110
Thermal correction to Enthalpy= 0.411054
Thermal correction to Gibbs Free Energy= 0.323603
Sum of electronic and zero-point Energies= -2646.949193
Sum of electronic and thermal Energies= -2646.923037
Sum of electronic and thermal Enthalpies= -2646.922093
Sum of electronic and thermal Free Energies= -2647.009544

$BrCF_2CF_3$
E(scf) = -3148.85017715 a.u.
ν_{min} = 57.97 cm^{-1}

C	6.140795	6.344525	8.918287
C	5.000318	5.353062	8.548110
F	5.482602	4.329288	7.848738
F	4.405889	4.895623	9.646822
F	4.097463	5.996067	7.805166
F	6.687081	6.800563	7.788332
F	5.607680	7.372077	9.583906
Br	7.511598	5.486461	10.015666

Zero-point correction= 0.026754 (Hartree/Particle)
Thermal correction to Energy= 0.034169
Thermal correction to Enthalpy= 0.035113
Thermal correction to Gibbs Free Energy= -0.006909
Sum of electronic and zero-point Energies= -3148.823423
Sum of electronic and thermal Energies= -3148.816008
Sum of electronic and thermal Enthalpies= -3148.815064
Sum of electronic and thermal Free Energies= -3148.857086

SMD(THF) uM06L-d3/def2-TZVPP
E(scf) = -3149.64706062 a.u.

TS5
E(scf) = -4286.09861832 a.u.
ν_{min} = -182.46 cm^{-1}

C	6.878272	5.353483	10.463511	H	7.813901	1.304767	10.714613
O	6.567347	4.071766	10.416010	H	8.647599	2.307755	11.939096
Si	6.263598	2.958985	11.726570	H	7.564195	0.982118	12.452547
C	4.650186	2.151695	11.240755	C	6.169384	3.955352	13.308185
H	4.731834	1.710100	10.234458	H	7.136426	4.437957	13.521129
H	4.388407	1.349597	11.949910	H	5.387154	4.730005	13.259416
H	3.833194	2.889228	11.225600	H	5.927968	3.286262	14.150690
C	7.711803	1.778462	11.704126	H	6.474085	5.942227	11.298620

C	6.901347	6.037186	9.121769	F	5.029811	7.437099	9.498884
H	7.511352	6.950122	9.160934	Br	9.094962	5.493431	11.255631
H	7.322748	5.358633	8.367953	C	11.201945	5.392262	12.364034
C	5.530041	6.503707	8.645264	C	11.072390	4.330501	13.457859
C	4.438018	5.411663	8.496919	F	11.456460	6.588693	12.885199
F	4.917733	4.355951	7.834032	F	12.139527	5.060903	11.481502
F	4.014232	5.007873	9.701766	F	10.083985	4.641811	14.298487
F	3.388831	5.893732	7.828590	F	10.823090	3.134537	12.916026
F	5.667611	7.088481	7.428614	F	12.208447	4.234331	14.168384

Zero-point correction= 0.213021 (Hartree/Particle)
Thermal correction to Energy= 0.239516
Thermal correction to Enthalpy= 0.240460
Thermal correction to Gibbs Free Energy= 0.150447
Sum of electronic and zero-point Energies= -4285.885597
Sum of electronic and thermal Energies= -4285.859102
Sum of electronic and thermal Enthalpies= -4285.858158
Sum of electronic and thermal Free Energies= -4285.948172

SMD(THF) uM06L-d3/def2-TZVPP
E(scf) = -4287.82266224 a.u.

C
E(scf) = -3711.18313596 a.u.
ν_{min} = 16.92 cm^{-1}

C	7.003937	5.222698	11.059790	H	3.787508	3.751619	13.635322
O	6.544924	3.960852	10.950465	H	6.362885	5.892701	11.652632
Si	5.595931	3.065092	12.084143	C	7.326971	5.812483	9.695555
C	4.648094	1.874162	10.999262	H	7.949820	6.710978	9.797950
H	5.343072	1.257435	10.406630	H	7.871601	5.070981	9.095946
H	4.028031	1.199512	11.611846	C	6.106825	6.279394	8.916089
H	3.992587	2.420967	10.304589	C	5.042462	5.214260	8.533340
C	6.773924	2.187788	13.245541	F	5.626009	4.106412	8.071607
H	7.475670	1.552591	12.681307	F	4.286193	4.895267	9.593173
H	7.360673	2.912848	13.830330	F	4.233585	5.694572	7.586008
H	6.213743	1.544788	13.944822	F	6.533996	6.829630	7.749981
C	4.492654	4.289094	12.980103	F	5.447542	7.246749	9.611654
H	5.078969	4.975507	13.612496	Br	8.749013	5.280309	12.172624
H	3.906978	4.886256	12.263036				

Zero-point correction= 0.188904 (Hartree/Particle)
Thermal correction to Energy= 0.207710
Thermal correction to Enthalpy= 0.208654
Thermal correction to Gibbs Free Energy= 0.139969

Sum of electronic and zero-point Energies= -3710.994232
Sum of electronic and thermal Energies= -3710.975426
Sum of electronic and thermal Enthalpies= -3710.974482
Sum of electronic and thermal Free Energies= -3711.043167

SMD(THF) uM06L-d3/def2-TZVPP
E(scf) = -3712.30670802 a.u.

^{1}A-Ph
E(scf) = -3901.24760535 a.u.
ν_{min} = 18.97 cm^{-1}

F			
e	1.247247	-2.523049	2.340971
C	0.107046	-3.455355	1.041188
C	0.368728	-3.572842	-0.342037
H	1.321376	-3.204347	-0.742027
C	-0.556657	-4.131761	-1.234156
C	-1.791635	-4.600912	-0.768591
H	-2.520985	-5.028857	-1.462188
C	-2.071684	-4.525130	0.602616
H	-3.026663	-4.900085	0.985925
C	-1.132111	-3.974368	1.482580
H	-1.376110	-3.936678	2.551644
H	-0.316725	-4.195723	-2.300885
S	2.090818	2.981582	3.938747
P	0.620969	-0.415954	1.566568
P	2.357679	-1.404506	4.055142
C	1.181788	2.220452	2.678319
H	0.606384	2.831775	1.984609
C	1.310316	0.849769	2.709871
C	2.144641	0.404448	3.802830
C	2.646712	1.455892	4.536776
H	3.310884	1.424636	5.399388
C	-1.182959	0.049044	1.438615
H	-1.232377	1.148585	1.341292
C	-1.885957	-0.356738	2.748732
H	-1.738974	-1.439807	2.903456
H	-1.412481	0.151044	3.604206
C	-3.387098	-0.047472	2.713035
H	-3.531593	1.047799	2.665819
H	-3.859754	-0.387271	3.650001
C	-4.061045	-0.698585	1.500090
H	-5.134630	-0.446863	1.473915
H	-3.993341	-1.797810	1.594402
C	-3.376798	-0.266116	0.198442
H	-3.847415	-0.760985	-0.667694
H	-3.519652	0.821519	0.057247
C	-1.875186	-0.584362	0.216022
H	-1.413532	-0.227575	-0.717675
H	-1.735241	-1.675687	0.241929
C	1.349772	-0.037467	-0.109130
H	0.838517	-0.775255	-0.753178
C	1.091758	1.368463	-0.671993
H	1.581534	2.112517	-0.021212
H	0.015613	1.603320	-0.673291
C	1.661429	1.504884	-2.092118
H	1.118598	0.817592	-2.766608
H	1.482747	2.525075	-2.471315
C	3.158359	1.173909	-2.127359
H	3.708034	1.927762	-1.533689
H	3.544050	1.243142	-3.158281
C	3.433075	-0.218372	-1.546734
H	4.516432	-0.424488	-1.531101
H	2.975627	-0.982816	-2.201281
C	2.853910	-0.365695	-0.133611
H	3.383588	0.317023	0.554642
H	3.032245	-1.385879	0.242572
C	1.614455	-1.776738	5.725534
H	1.857714	-2.846861	5.851148

C	0.080405	-1.654174	5.677353	H	6.340369	-4.101447	5.446594
H	-0.191544	-0.601159	5.484830	C	6.739973	-3.003090	3.607224
H	-0.328159	-2.239322	4.837397	H	6.367796	-3.825082	2.968715
C	-0.557042	-2.113936	6.994860	H	7.834619	-3.121708	3.672624
H	-0.373855	-3.196768	7.121237	C	6.383724	-1.661223	2.957785
H	-1.651085	-1.982870	6.947394	H	6.815049	-1.592228	1.944893
C	0.023941	-1.359371	8.196597	H	6.831353	-0.840364	3.548121
H	-0.255320	-0.291942	8.122213	C	4.865294	-1.462947	2.888669
H	-0.416170	-1.734958	9.135510	H	4.427560	-2.219231	2.213795
C	1.552568	-1.473964	8.238077	H	4.627153	-0.478707	2.454250
H	1.835932	-2.527637	8.415321	C	1.931666	-4.277185	2.908340
H	1.960469	-0.891663	9.081326	C	3.021447	-4.853863	2.216119
C	2.184644	-0.998572	6.921182	C	1.468188	-4.992731	4.034942
H	3.280663	-1.097142	6.970859	C	3.641584	-6.035072	2.641680
H	1.965244	0.074637	6.790230	H	3.407559	-4.355623	1.318049
C	4.200908	-1.603883	4.272451	C	2.073549	-6.179600	4.469812
H	4.550033	-0.776359	4.915943	H	0.612052	-4.606885	4.601682
C	4.580591	-2.940090	4.940059	C	3.174805	-6.704100	3.781169
H	4.135910	-3.771589	4.372106	H	4.492798	-6.438182	2.082711
H	4.166402	-2.993842	5.958805	H	1.687431	-6.696867	5.354660
C	6.103792	-3.122532	4.996795	H	3.655582	-7.625758	4.121138
H	6.540445	-2.354971	5.662713				

Zero-point correction= 0.873635 (Hartree/Particle)
Thermal correction to Energy= 0.917782
Thermal correction to Enthalpy= 0.918726
Thermal correction to Gibbs Free Energy= 0.795104
Sum of electronic and zero-point Energies= -3900.373971
Sum of electronic and thermal Energies= -3900.329823
Sum of electronic and thermal Enthalpies= -3900.328879
Sum of electronic and thermal Free Energies= -3900.452501

^{3}A-Ph
E(scf) = -3901.26692595 a.u.
ν_{min} = 19.66 cm^{-1}

Fe	1.258050	-2.534126	2.329554	C	-1.815038	-4.574126	-0.777795
C	0.105949	-3.470771	1.032219	H	-2.553110	-4.986339	-1.471664
C	0.358606	-3.573532	-0.353859	C	-2.085126	-4.513403	0.595946
H	1.312396	-3.210345	-0.755598	H	-3.040981	-4.884221	0.980959
C	-0.578566	-4.111515	-1.246289	C	-1.134320	-3.983261	1.476835

H	-1.370008	-3.957736	2.547774	H	4.509136	-0.433229	-1.507886
H	-0.346429	-4.164964	-2.315262	H	2.969950	-0.986415	-2.186125
S	2.056562	2.981365	3.948721	C	2.839985	-0.370558	-0.118534
P	0.603028	-0.417253	1.571543	H	3.367985	0.310506	0.572600
P	2.365398	-1.400762	4.051361	H	3.011608	-1.390901	0.260837
C	1.146890	2.216354	2.691074	C	1.616616	-1.786317	5.716491
H	0.562673	2.824570	2.001973	H	1.869935	-2.854218	5.841138
C	1.287721	0.846826	2.717435	C	0.081707	-1.678989	5.659281
C	2.132869	0.405300	3.803495	H	-0.199382	-0.628148	5.467949
C	2.629602	1.458652	4.538264	H	-0.314713	-2.265058	4.814224
H	3.298367	1.430163	5.397437	C	-0.558729	-2.148023	6.971934
C	-1.202173	0.039724	1.439321	H	-0.365293	-3.229187	7.097381
H	-1.255985	1.139388	1.345473	H	-1.653749	-2.027987	6.918236
C	-1.908560	-0.374175	2.745088	C	0.007448	-1.389736	8.178431
H	-1.757514	-1.457153	2.896123	H	-0.282279	-0.325091	8.104170
H	-1.440606	0.132456	3.604301	H	-0.434291	-1.771391	9.114129
C	-3.410828	-0.071056	2.704108	C	1.536926	-1.488748	8.228942
H	-3.559933	1.023723	2.659787	H	1.829932	-2.539774	8.406203
H	-3.885908	-0.415950	3.637973	H	1.933749	-0.903746	9.075600
C	-4.076800	-0.721279	1.486261	C	2.172343	-1.004816	6.916751
H	-5.151453	-0.474574	1.456547	H	3.268955	-1.093108	6.972803
H	-4.004099	-1.820482	1.576997	H	1.943695	0.066529	6.786066
C	-3.389414	-0.281085	0.188894	C	4.209159	-1.584990	4.275721
H	-3.853954	-0.775401	-0.680828	H	4.549049	-0.755764	4.921965
H	-3.536971	0.806303	0.050706	C	4.595445	-2.919180	4.943767
C	-1.886371	-0.592109	0.211368	H	4.159167	-3.753362	4.373269
H	-1.422772	-0.229133	-0.718952	H	4.177421	-2.976743	5.960693
H	-1.741529	-1.682843	0.233181	C	6.119568	-3.091172	5.006987
C	1.336779	-0.037914	-0.101472	H	6.547872	-2.321681	5.676078
H	0.826667	-0.773857	-0.748531	H	6.360708	-4.069160	5.456367
C	1.084449	1.369165	-0.663451	C	6.761164	-2.965185	3.620522
H	1.571821	2.111385	-0.008687	H	6.397649	-3.788812	2.979148
H	0.008631	1.605793	-0.670279	H	7.856301	-3.076217	3.690772
C	1.662339	1.505703	-2.080329	C	6.398452	-1.624811	2.971581
H	1.120855	0.821092	-2.758610	H	6.834214	-1.551002	1.960940
H	1.488996	2.526958	-2.459125	H	6.837279	-0.801766	3.565476
C	3.158462	1.169937	-2.108468	C	4.878964	-1.437416	2.895166
H	3.707528	1.921240	-1.511018	H	4.449993	-2.195675	2.216893
H	3.549358	1.239580	-3.137397	H	4.635965	-0.454167	2.461187
C	3.426458	-0.224056	-1.528496	C	1.964006	-4.288291	2.893355

C	3.069595	-4.849032	2.213989	H	0.635352	-4.627979	4.578130
C	1.504044	-5.001685	4.022754	C	3.245696	-6.681383	3.797849
C	3.708395	-6.014531	2.655671	H	4.571131	-6.406790	2.106828
H	3.453209	-4.351849	1.314692	H	1.746156	-6.688687	5.359948
C	2.129287	-6.171947	4.473557	H	3.740981	-7.590750	4.149818

Zero-point correction= 0.873773 (Hartree/Particle)
Thermal correction to Energy= 0.917908
Thermal correction to Enthalpy= 0.918853
Thermal correction to Gibbs Free Energy= 0.794420
Sum of electronic and zero-point Energies= -3900.393153
Sum of electronic and thermal Energies= -3900.349018
Sum of electronic and thermal Enthalpies= -3900.348073
Sum of electronic and thermal Free Energies= -3900.472506

^{5}A-Ph
E(scf) = -3901.26311466 a.u.
ν_{min} = 16.15 cm^{-1}

Fe	1.184823	-2.845945	2.269599	H	-1.662762	0.886007	1.657262
C	2.004830	-3.581994	0.521787	C	-1.933052	-0.427839	3.354424
C	3.311433	-4.095586	0.358869	H	-1.669968	-1.461910	3.634281
H	3.992641	-4.119962	1.215716	H	-1.366509	0.233216	4.029346
C	3.786115	-4.578384	-0.868849	C	-3.440420	-0.221190	3.546001
C	2.953441	-4.570789	-1.994088	H	-3.688945	0.841605	3.369372
H	3.319134	-4.940065	-2.956610	H	-3.715320	-0.439577	4.591512
C	1.644024	-4.089477	-1.870295	C	-4.250673	-1.096332	2.582563
H	0.978803	-4.085843	-2.739954	H	-5.330971	-0.919371	2.715913
C	1.189040	-3.610596	-0.634453	H	-4.072713	-2.160362	2.824381
H	0.157759	-3.241868	-0.573361	C	-3.843353	-0.834795	1.127924
H	4.809224	-4.960293	-0.948689	H	-4.405306	-1.491862	0.443419
S	2.057692	2.805505	3.870336	H	-4.109521	0.203602	0.857658
P	0.301599	-0.572571	1.694515	C	-2.336485	-1.035066	0.916280
P	2.609239	-1.544699	3.862239	H	-2.070233	-0.798437	-0.126551
C	0.950268	2.015118	2.803402	H	-2.081599	-2.099593	1.068104
H	0.209741	2.603334	2.263328	C	0.757861	-0.068133	-0.047513
C	1.155417	0.653493	2.762175	H	0.330549	-0.885551	-0.654926
C	2.224449	0.237702	3.644748	C	0.194351	1.264095	-0.564199
C	2.808198	1.305526	4.290294	H	0.595842	2.091474	0.045606
H	3.639242	1.297385	4.994216	H	-0.902396	1.296066	-0.467737
C	-1.506568	-0.181277	1.894064	C	0.592256	1.489034	-2.031826

H	0.112526	0.712848	-2.655904	C	4.464206	-1.637595	3.756339
H	0.200769	2.459444	-2.380723	H	4.894396	-0.941816	4.498159
C	2.112516	1.422880	-2.223291	C	4.933109	-3.068182	4.084618
H	2.580383	2.266902	-1.683112	H	4.402387	-3.777537	3.423850
H	2.370254	1.549598	-3.288259	H	4.656532	-3.339370	5.116306
C	2.684237	0.105924	-1.684610	C	6.447572	-3.225605	3.892840
H	3.782999	0.093015	-1.780673	H	6.971370	-2.600594	4.639232
H	2.305207	-0.737081	-2.290601	H	6.741327	-4.269201	4.094551
C	2.287659	-0.120374	-0.220961	C	6.886739	-2.803793	2.485987
H	2.748719	0.660827	0.409744	H	6.437521	-3.489316	1.743947
H	2.670370	-1.088732	0.132551	H	7.980375	-2.898988	2.380942
C	2.165690	-1.900636	5.643509	C	6.440906	-1.369475	2.177849
H	2.293494	-2.995600	5.709562	H	6.730461	-1.086104	1.152084
C	0.673468	-1.598952	5.878388	H	6.963594	-0.671717	2.857861
H	0.505562	-0.511615	5.777963	C	4.925954	-1.205551	2.350810
H	0.066663	-2.092211	5.105286	H	4.405282	-1.821659	1.598351
C	0.231953	-2.056179	7.273599	H	4.629099	-0.161860	2.160615
H	0.307128	-3.157508	7.327814	C	0.041485	-4.109981	3.438381
H	-0.830715	-1.805566	7.430425	C	0.704848	-4.954553	4.360321
C	1.100408	-1.427971	8.370236	C	-1.364765	-4.244504	3.391984
H	0.934364	-0.334632	8.379797	C	0.021671	-5.849332	5.194753
H	0.798609	-1.800531	9.363583	H	1.798347	-4.913226	4.435918
C	2.589333	-1.704762	8.127660	C	-2.067190	-5.132722	4.218588
H	2.778515	-2.789583	8.224905	H	-1.942456	-3.634210	2.690271
H	3.204819	-1.208158	8.896581	C	-1.374715	-5.936858	5.131425
C	3.032597	-1.245623	6.729180	H	0.577161	-6.478644	5.897774
H	4.098727	-1.480157	6.582049	H	-3.158236	-5.196820	4.151581
H	2.931939	-0.148620	6.664189	H	-1.916588	-6.627710	5.783837

Zero-point correction= 0.872328 (Hartree/Particle)
Thermal correction to Energy= 0.917383
Thermal correction to Enthalpy= 0.918327
Thermal correction to Gibbs Free Energy= 0.788915
Sum of electronic and zero-point Energies= -3900.390786
Sum of electronic and thermal Energies= -3900.345732
Sum of electronic and thermal Enthalpies= -3900.344788
Sum of electronic and thermal Free Energies= -3900.474199

^{3}TS0
E(scf) = -7050.11520070 a.u.
ν_{min} = -407.64 cm^{-1}

Fe	7.003999	4.751983	17.446797	C	9.615225	4.839946	21.712449
C	5.114756	4.838128	16.814504	H	10.099735	5.830801	21.688705
C	4.127142	5.083384	17.792651	H	10.395844	4.093202	21.500392
H	4.402419	5.110858	18.850410	C	9.041181	4.600477	23.118240
C	2.788284	5.314241	17.459270	H	8.637245	3.572968	23.170161
C	2.384335	5.283337	16.118687	H	9.850193	4.659127	23.865358
H	1.339815	5.463655	15.850206	C	7.927628	5.599786	23.453615
C	3.335964	5.014690	15.129775	H	8.358421	6.616890	23.504157
H	3.036398	4.985095	14.077477	H	7.507376	5.385931	24.450457
C	4.677462	4.798716	15.475375	C	6.822615	5.577151	22.390993
H	5.396075	4.616723	14.673953	H	6.054873	6.336864	22.613185
H	2.058191	5.520110	18.247940	H	6.313445	4.596365	22.411765
S	10.809325	8.946358	19.109084	C	7.395493	5.811764	20.988426
P	9.011028	4.962197	18.870051	H	7.818168	6.830151	20.930068
P	7.526848	7.112712	16.861468	H	6.592088	5.769590	20.236804
C	10.698252	7.246949	19.399454	C	8.220349	7.484914	15.152691
H	11.432441	6.760219	20.039687	H	7.590772	6.865829	14.488746
C	9.619502	6.685938	18.750680	C	9.676117	6.986930	15.028772
C	8.884112	7.655257	17.975480	H	10.315783	7.585169	15.699752
C	9.408886	8.923023	18.096780	H	9.761959	5.943270	15.355092
H	9.064762	9.846761	17.633805	C	10.188686	7.129383	13.590189
C	10.538719	3.917311	18.682688	H	9.599305	6.469527	12.932078
H	11.260514	4.296789	19.428030	H	11.230102	6.772853	13.534211
C	11.154264	4.083855	17.282750	C	10.082754	8.577016	13.100855
H	10.412087	3.776633	16.531573	H	10.766049	9.211888	13.694972
H	11.383706	5.143355	17.087522	H	10.411688	8.656480	12.051029
C	12.417255	3.228357	17.122973	C	8.652030	9.103919	13.252696
H	13.203809	3.607716	17.801126	H	7.983287	8.543462	12.574038
H	12.802340	3.336510	16.096008	H	8.593538	10.162566	12.948714
C	12.141111	1.753459	17.439244	C	8.135934	8.952068	14.692270
H	13.069363	1.163176	17.358633	H	7.108059	9.335637	14.750072
H	11.442954	1.351729	16.684762	H	8.749932	9.580293	15.360608
C	11.522780	1.589694	18.832421	C	6.201331	8.387445	17.191246
H	11.288293	0.530162	19.028921	H	6.687859	9.369079	17.050207
H	12.257525	1.897921	19.599121	C	5.006667	8.290448	16.224220
C	10.251548	2.435298	18.984548	H	4.541637	7.301568	16.321179
H	9.837007	2.312441	19.997932	H	5.337461	8.377240	15.177669
H	9.479442	2.071052	18.287938	C	3.959035	9.366686	16.538866
C	8.498376	4.788826	20.658256	H	4.393279	10.368713	16.363989
H	8.045091	3.783441	20.681372	H	3.107497	9.265305	15.845459

C	3.480915	9.264541	17.991985	C	5.702200	1.660103	20.119550
H	2.965209	8.297244	18.130233	H	5.664723	3.794091	19.989053
H	2.743768	10.054642	18.213117	C	6.062454	0.453159	19.509227
C	4.661439	9.348132	18.966669	H	6.971823	-0.444087	17.762613
H	4.314733	9.228084	20.006888	H	5.212091	1.657373	21.098104
H	5.117940	10.353124	18.900893	H	5.858827	-0.501436	20.002245
C	5.730060	8.292143	18.654796	Br	7.973519	3.826431	15.084170
H	5.313664	7.286476	18.825553	C	9.055452	3.242242	13.255754
H	6.584105	8.405324	19.340487	C	10.544441	3.013526	13.538599
C	6.609155	2.946996	18.223676	F	8.513813	2.111261	12.788485
C	6.950888	1.714578	17.630358	F	8.915163	4.207839	12.335119
C	5.967852	2.876120	19.479192	F	10.698796	2.032177	14.432715
C	6.684470	0.489179	18.257101	F	11.112128	4.125594	14.020924
H	7.447959	1.699925	16.658548	F	11.202175	2.666415	12.421469

Zero-point correction= 0.901994 (Hartree/Particle)
Thermal correction to Energy= 0.955056
Thermal correction to Enthalpy= 0.956001
Thermal correction to Gibbs Free Energy= 0.811435
Sum of electronic and zero-point Energies= -7049.213206
Sum of electronic and thermal Energies= -7049.160144
Sum of electronic and thermal Enthalpies= -7049.159200
Sum of electronic and thermal Free Energies= -7049.303765

^{2}B-Ph

E(scf) = -6475.17428937 a.u.

ν_{min} = 21.82 cm^{-1}

Fe	7.246253	4.675965	17.118752	P	7.448039	7.142748	17.045578
C	5.609654	4.775698	16.000262	C	10.688716	7.292426	19.453828
C	4.288019	4.700470	16.479520	H	11.498723	6.804307	19.993935
H	4.099070	4.454429	17.524586	C	9.649647	6.712948	18.760752
C	3.185133	4.941355	15.647818	C	8.771927	7.695263	18.176636
C	3.372187	5.263846	14.300520	C	9.151108	8.984936	18.480793
H	2.514266	5.459239	13.651526	H	8.679817	9.919882	18.181120
C	4.675199	5.319681	13.792323	C	10.834442	4.086339	18.433436
H	4.843118	5.556180	12.737173	H	11.467881	4.412197	19.277482
C	5.769443	5.070138	14.628399	C	11.528269	4.535915	17.133869
H	6.772485	5.099399	14.195852	H	10.884268	4.288533	16.276327
H	2.173842	4.878435	16.061078	H	11.661978	5.629304	17.134405
S	10.588062	9.018591	19.439305	C	12.886448	3.839475	16.972569
P	9.194556	4.935419	18.695857	H	13.566641	4.174170	17.777960

H	13.350942	4.147717	16.020754	H	10.274371	8.864269	12.289004
C	12.748083	2.313342	17.033202	C	8.727851	9.448483	13.707234
H	13.736628	1.833246	16.938371	H	7.911023	9.167476	13.017655
H	12.144503	1.971445	16.172670	H	8.888967	10.532014	13.579765
C	12.061155	1.872797	18.331530	C	8.287468	9.158401	15.150975
H	11.935695	0.777193	18.350097	H	7.374715	9.727947	15.384026
H	12.706523	2.131244	19.191752	H	9.072766	9.512612	15.839586
C	10.695875	2.553194	18.497349	C	6.002249	8.259225	17.409542
H	10.226901	2.241205	19.444511	H	6.426307	9.272349	17.527202
H	10.024676	2.226652	17.688762	C	4.964990	8.296201	16.270608
C	8.755443	4.600252	20.496759	H	4.595409	7.279026	16.077974
H	8.197946	3.651067	20.445705	H	5.424426	8.647186	15.334543
C	9.919080	4.417828	21.485539	C	3.781365	9.203088	16.635108
H	10.506012	5.350775	21.547695	H	4.132917	10.248015	16.720462
H	10.607280	3.626692	21.154073	H	3.041544	9.184671	15.817637
C	9.384423	4.065726	22.883880	C	3.131253	8.779222	17.956934
H	8.881562	3.082653	22.833271	H	2.698965	7.768778	17.837983
H	10.227502	3.952482	23.585981	H	2.296423	9.453926	18.209720
C	8.391858	5.113319	23.400955	C	4.161713	8.754247	19.091455
H	8.924953	6.069560	23.556753	H	3.698238	8.411124	20.031363
H	7.993684	4.811080	24.384147	H	4.528593	9.780620	19.275921
C	7.250028	5.332768	22.402111	C	5.349705	7.849909	18.742649
H	6.575367	6.131223	22.754510	H	4.994493	6.809817	18.650783
H	6.642316	4.414334	22.324217	H	6.094792	7.865599	19.553929
C	7.794562	5.688483	21.014584	C	6.529933	3.421157	18.463974
H	8.336436	6.647668	21.075906	C	6.952121	2.083115	18.571622
H	6.969982	5.840983	20.306470	C	5.572593	3.877229	19.384364
C	8.076772	7.649162	15.358267	C	6.447773	1.244316	19.574015
H	7.273791	7.309950	14.682368	H	7.691385	1.693410	17.871694
C	9.359663	6.871992	15.010032	C	5.067407	3.045393	20.392027
H	10.159522	7.164302	15.713357	H	5.215336	4.908019	19.338246
H	9.203230	5.791617	15.142785	C	5.506525	1.721547	20.493301
C	9.811143	7.166149	13.574375	H	6.798610	0.209831	19.637187
H	9.051239	6.775346	12.873063	H	4.331098	3.438071	21.099045
H	10.745793	6.621511	13.360254	H	5.117780	1.068061	21.278727
C	9.995886	8.669428	13.338161	Br	8.429946	3.136647	15.578251
H	10.835026	9.032078	13.960288				

Zero-point correction= 0.877365 (Hartree/Particle)
Thermal correction to Energy= 0.923162

Thermal correction to Enthalpy= 0.924106
Thermal correction to Gibbs Free Energy= 0.797904
Sum of electronic and zero-point Energies= -6474.296924
Sum of electronic and thermal Energies= -6474.251128
Sum of electronic and thermal Enthalpies= -6474.250183
Sum of electronic and thermal Free Energies= -6474.376386

^{4}B-Ph
E(scf) = -6475.20116556 a.u.
ν_{min} = 16.08 cm^{-1}

Fe	7.313142	4.723760	17.174232	H	13.399833	1.498437	17.204768
C	5.346936	4.752214	16.783581	H	11.874970	1.854246	16.375281
C	4.359782	5.048428	17.736869	C	11.680489	1.715655	18.525155
H	4.627621	5.145695	18.791487	H	11.412336	0.646175	18.504099
C	3.022120	5.235014	17.367561	H	12.314361	1.865071	19.418709
C	2.639151	5.106340	16.027867	C	10.409037	2.562573	18.660654
H	1.596374	5.252324	15.734090	H	9.870241	2.291643	19.583593
C	3.606529	4.778740	15.070554	H	9.724842	2.340676	17.824974
H	3.319992	4.665247	14.020618	C	8.563822	4.782356	20.546436
C	4.944716	4.599277	15.444338	H	8.127047	3.770762	20.506042
H	5.686993	4.352867	14.681713	C	9.628065	4.795444	21.654948
H	2.278620	5.482732	18.130772	H	10.112760	5.786126	21.692789
S	10.686686	9.113060	19.296262	H	10.417403	4.055853	21.449836
P	9.162283	5.044917	18.794722	C	8.990440	4.497449	23.021523
P	7.605092	7.219935	16.831892	H	8.593670	3.465835	23.013978
C	10.679068	7.395928	19.487003	H	9.763235	4.531887	23.807456
H	11.423514	6.919054	20.123003	C	7.853101	5.473648	23.343350
C	9.659490	6.805586	18.772185	H	8.270053	6.492062	23.450960
C	8.883260	7.769558	18.030232	H	7.390592	5.218548	24.311336
C	9.321082	9.058693	18.238398	C	6.798010	5.480208	22.231199
H	8.932802	9.982415	17.811133	H	6.011039	6.221931	22.446672
C	10.735742	4.068427	18.640402	H	6.300934	4.493738	22.191873
H	11.351514	4.314396	19.523436	C	7.431583	5.778136	20.867005
C	11.534696	4.447502	17.379833	H	7.843043	6.802534	20.871944
H	10.902265	4.284442	16.492783	H	6.661493	5.764580	20.079336
H	11.792455	5.518191	17.399999	C	8.370566	7.689566	15.176838
C	12.804802	3.594799	17.260758	H	7.849641	7.018054	14.471933
H	13.482232	3.824985	18.104041	C	9.871537	7.331870	15.145382
H	13.346844	3.864808	16.339004	H	10.413362	8.001888	15.834190
C	12.475805	2.096917	17.270965	H	10.031583	6.306169	15.500292

C	10.442107	7.500350	13.732775	H	2.953679	8.175124	17.963886
H	9.943270	6.783872	13.055433	H	2.631967	9.918306	17.978756
H	11.514345	7.241203	13.731153	C	4.561623	9.347450	18.812850
C	10.235394	8.929912	13.219631	H	4.188388	9.245264	19.845750
H	10.837195	9.623254	13.836030	H	4.965595	10.372945	18.723882
H	10.603161	9.029096	12.184455	C	5.693935	8.340291	18.571259
C	8.760753	9.340201	13.301601	H	5.321490	7.322376	18.764370
H	8.173201	8.729580	12.591861	H	6.518163	8.519204	19.279163
H	8.634074	10.391093	12.991388	C	6.761996	2.948299	17.958410
C	8.182178	9.145195	14.712985	C	7.061115	1.761226	17.265098
H	7.122961	9.437680	14.710040	C	6.193753	2.822275	19.238122
H	8.699551	9.823710	15.414233	C	6.846025	0.505537	17.849190
C	6.206694	8.421259	17.120832	H	7.481678	1.815854	16.259874
H	6.637163	9.427324	16.970628	C	5.980078	1.571179	19.829462
C	5.054775	8.228885	16.115190	H	5.899613	3.711944	19.797159
H	4.648417	7.214278	16.217939	C	6.313303	0.401183	19.138491
H	5.418947	8.314140	15.079457	H	7.098578	-0.398545	17.286620
C	3.933970	9.246764	16.365026	H	5.547847	1.515296	20.833093
H	4.312699	10.267016	16.168175	H	6.148683	-0.578799	19.594339
H	3.111276	9.071555	15.651807	Br	8.512578	4.057846	15.061105
C	3.418799	9.164752	17.806881				

Zero-point correction= 0.876548 (Hartree/Particle)
Thermal correction to Energy= 0.922617
Thermal correction to Enthalpy= 0.923561
Thermal correction to Gibbs Free Energy= 0.795241
Sum of electronic and zero-point Energies= -6474.324617
Sum of electronic and thermal Energies= -6474.278549
Sum of electronic and thermal Enthalpies= -6474.277604
Sum of electronic and thermal Free Energies= -6474.405925

^{6}B-Ph

E(scf) = -6475.17472596 a.u.

ν_{min} = 21.74 cm^{-1}

Fe	7.127974	4.495619	17.070444	C	4.576733	5.579216	13.631816
C	5.484689	4.921256	15.815034	H	4.745733	5.832807	12.580648
C	4.165878	4.916549	16.308700	C	5.658913	5.239754	14.453234
H	3.976826	4.655177	17.352869	H	6.664220	5.218164	14.020943
C	3.072969	5.247661	15.495301	H	2.060742	5.241721	15.911240
C	3.277205	5.592388	14.154647	S	10.600688	9.054297	19.465973
H	2.429319	5.860641	13.518303	P	9.300298	4.938634	18.756921

P	7.493666	7.159459	17.035274	H	6.927129	5.607802	20.255265
C	10.706383	7.329915	19.524996	C	8.104489	7.684455	15.350448
H	11.504026	6.857455	20.096537	H	7.256419	7.419874	14.695842
C	9.693662	6.726028	18.813024	C	9.315992	6.832390	14.927959
C	8.825678	7.690872	18.176246	H	10.162564	7.049318	15.604045
C	9.194450	8.988029	18.465179	H	9.094281	5.760642	15.038290
H	8.728809	9.914290	18.132026	C	9.725803	7.137105	13.481366
C	10.952395	4.117611	18.489903	H	8.912263	6.815577	12.805276
H	11.616264	4.446811	19.309374	H	10.612570	6.539584	13.211460
C	11.580276	4.561979	17.154774	C	9.998217	8.631206	13.271718
H	10.884383	4.322361	16.334065	H	10.886553	8.922285	13.862407
H	11.721202	5.654783	17.148229	H	10.242278	8.834044	12.215459
C	12.920175	3.855043	16.910594	C	8.802793	9.482443	13.717078
H	13.648962	4.180222	17.676166	H	7.938894	9.274661	13.059533
H	13.330768	4.163665	15.934445	H	9.031195	10.555877	13.607568
C	12.770982	2.330101	16.972895	C	8.411477	9.180575	15.172142
H	13.747600	1.840932	16.819538	H	7.553834	9.803974	15.470111
H	12.115667	1.997599	16.147153	H	9.252497	9.457405	15.829520
C	12.155813	1.890933	18.307048	C	6.060393	8.280494	17.454346
H	12.020218	0.796604	18.328969	H	6.487739	9.273364	17.680452
H	12.852192	2.139310	19.129379	C	5.051602	8.441905	16.301086
C	10.809973	2.584459	18.556127	H	4.692929	7.453485	15.982725
H	10.397046	2.271971	19.529138	H	5.534810	8.900729	15.425450
H	10.087593	2.264551	17.787348	C	3.851092	9.296078	16.731745
C	8.819928	4.564723	20.531864	H	4.190249	10.327472	16.941886
H	8.349267	3.569761	20.453300	H	3.132850	9.363784	15.897644
C	9.952810	4.486387	21.567735	C	3.170549	8.724360	17.980639
H	10.453070	5.467465	21.643499	H	2.757567	7.727558	17.740838
H	10.719930	3.757550	21.265248	H	2.319274	9.358281	18.280190
C	9.396958	4.099886	22.948083	C	4.170442	8.590591	19.134507
H	8.980660	3.077447	22.890623	H	3.686576	8.146728	20.020596
H	10.217735	4.064996	23.684183	H	4.518353	9.596090	19.434920
C	8.300006	5.065557	23.411813	C	5.379387	7.740477	18.727397
H	8.744118	6.065766	23.571231	H	5.048794	6.706066	18.530966
H	7.892532	4.743708	24.384954	H	6.106896	7.690601	19.553245
C	7.180654	5.173120	22.369736	C	6.384557	3.249766	18.556254
H	6.425671	5.912208	22.687237	C	6.923306	1.959696	18.734930
H	6.658246	4.204256	22.283514	C	5.370559	3.654414	19.444219
C	7.738057	5.558986	20.995093	C	6.480925	1.118255	19.763991
H	8.178103	6.569956	21.052828	H	7.712508	1.608827	18.064454

C	4.918843	2.820392	20.475662	H	4.134376	3.167581	21.154545
H	4.926152	4.649945	19.352046	H	5.131597	0.894683	21.446398
C	5.477067	1.547852	20.640358	Br	8.392565	3.041305	15.534692
H	6.922399	0.124112	19.883573				

Zero-point correction= 0.875127 (Hartree/Particle)
Thermal correction to Energy= 0.921735
Thermal correction to Enthalpy= 0.922679
Thermal correction to Gibbs Free Energy= 0.792108
Sum of electronic and zero-point Energies= -6474.299599
Sum of electronic and thermal Energies= -6474.252991
Sum of electronic and thermal Enthalpies= -6474.252047
Sum of electronic and thermal Free Energies= -6474.382618

Ph-Ph
E(scf) = -462.996149266 a.u.
ν_{min} = 68.09 cm^{-1}

C	4.718110	3.728793	17.157581	C	5.531553	2.678498	17.827440
C	3.692461	4.402699	17.849192	C	5.949858	1.529397	17.128129
H	3.474003	4.134477	18.885535	C	5.905964	2.803867	19.179666
C	2.929359	5.390084	17.220693	C	6.714143	0.543052	17.756809
C	3.174127	5.727288	15.885003	H	5.654074	1.395135	16.085021
H	2.577452	6.499644	15.393196	C	6.670262	1.817910	19.808963
C	4.189424	5.066968	15.184426	H	5.613517	3.695107	19.739864
H	4.395241	5.327240	14.142877	C	7.078358	0.682486	19.100519
C	4.952185	4.079691	15.813518	H	7.020148	-0.343490	17.195265
H	5.756504	3.589365	15.260137	H	6.954973	1.941580	20.857086
H	2.133544	5.893384	17.775931	H	7.676246	-0.088849	19.592457

Zero-point correction= 0.181784 (Hartree/Particle)
Thermal correction to Energy= 0.190597
Thermal correction to Enthalpy= 0.191541
Thermal correction to Gibbs Free Energy= 0.147252
Sum of electronic and zero-point Energies= -462.814365
Sum of electronic and thermal Energies= -462.805552
Sum of electronic and thermal Enthalpies= -462.804608
Sum of electronic and thermal Free Energies= -462.848898

^{4}TSB
E(scf) = -6475.19568538 a.u.
ν_{min} = -254.60 cm^{-1}

Fe	7.349593	4.767789	17.105671	C	4.425227	4.970003	17.930098
C	5.354235	4.448268	17.005901	H	4.719677	5.131562	18.968459

C	3.120451	5.283962	17.544299
C	2.704110	5.083688	16.222302
H	1.683909	5.331753	15.919782
C	3.610267	4.549100	15.297426
H	3.299493	4.379650	14.262486
C	4.911857	4.218662	15.684158
H	5.602923	3.796516	14.952287
H	2.425263	5.691291	18.283336
S	10.728453	9.101265	19.320432
P	9.144145	5.053558	18.805403
P	7.634338	7.273303	16.824374
C	10.697102	7.381712	19.495245
H	11.435425	6.889617	20.126769
C	9.668658	6.809670	18.778541
C	8.904776	7.792972	18.043456
C	9.360371	9.073598	18.263471
H	8.984300	10.004974	17.841728
C	10.700101	4.045823	18.675393
H	11.347999	4.296128	19.533861
C	11.463606	4.369781	17.377617
H	10.787839	4.222899	16.519004
H	11.763729	5.429903	17.370457
C	12.691855	3.465362	17.214767
H	13.416044	3.677917	18.023173
H	13.201939	3.699978	16.265399
C	12.302009	1.983031	17.262902
H	13.195361	1.344521	17.159315
H	11.646329	1.755317	16.402315
C	11.556861	1.653363	18.561510
H	11.247742	0.594750	18.573980
H	12.240736	1.793143	19.419015
C	10.326832	2.550764	18.746300
H	9.833049	2.318476	19.704198
H	9.588348	2.331179	17.955283
C	8.537935	4.822379	20.559365
H	8.107675	3.807313	20.536389
C	9.588189	4.860472	21.679986
H	10.064086	5.855552	21.707824
H	10.386457	4.124856	21.495245
C	8.935501	4.579965	23.043298
H	8.545474	3.545616	23.047948
H	9.697105	4.632464	23.839227
C	7.787549	5.553761	23.334773
H	8.197085	6.576307	23.431391
H	7.314281	5.311484	24.300918
C	6.746219	5.537703	22.209292
H	5.953001	6.278744	22.403574
H	6.253888	4.548208	22.180340
C	7.397435	5.816280	20.849599
H	7.803958	6.842746	20.843504
H	6.643645	5.786943	20.047367
C	8.416882	7.770678	15.184509
H	7.897901	7.111255	14.466748
C	9.912957	7.394623	15.157821
H	10.458881	8.042390	15.864695
H	10.053191	6.358453	15.492763
C	10.498252	7.582650	13.753738
H	9.999583	6.881907	13.060076
H	11.568482	7.314830	13.756534
C	10.307875	9.022341	13.262588
H	10.907115	9.700969	13.897751
H	10.689000	9.136345	12.233685
C	8.835197	9.442245	13.333601
H	8.252108	8.844774	12.609016
H	8.719423	10.497945	13.035252
C	8.240071	9.231208	14.735682
H	7.180459	9.525442	14.724197
H	8.749937	9.900803	15.451167
C	6.223384	8.458955	17.092523
H	6.611183	9.476431	16.909303
C	5.089202	8.171193	16.089088
H	4.739007	7.136891	16.230148
H	5.457831	8.236747	15.052695
C	3.915697	9.139648	16.289349
H	4.244645	10.165138	16.038464
H	3.103160	8.887919	15.587325
C	3.401267	9.110797	17.733809
H	2.967720	8.116582	17.938517
H	2.588895	9.844982	17.866512
C	4.531469	9.378926	18.735298
H	4.155033	9.306986	19.769653
H	4.897886	10.414046	18.604861
C	5.702094	8.405978	18.540016
H	5.365439	7.381402	18.765030

H	6.513461	8.637699	19.247688	H	5.945403	3.619678	19.831135
C	6.522186	3.026190	17.823655	C	6.660075	0.415506	18.934065
C	6.809408	1.904791	17.017316	H	7.139788	-0.223266	16.921606
C	6.235844	2.791672	19.184678	H	6.111930	1.372703	20.801364
C	6.892755	0.622619	17.569722	H	6.724939	-0.587346	19.363376
H	6.997490	2.041534	15.952385	Br	8.484582	4.133616	14.904865
C	6.318187	1.511834	19.736263				

Zero-point correction= 0.875410 (Hartree/Particle)
Thermal correction to Energy= 0.920984
Thermal correction to Enthalpy= 0.921929
Thermal correction to Gibbs Free Energy= 0.794667
Sum of electronic and zero-point Energies= -6474.320276
Sum of electronic and thermal Energies= -6474.274701
Sum of electronic and thermal Enthalpies= -6474.273757
Sum of electronic and thermal Free Energies= -6474.401018

8. References

1. A. Tarui, S. Shinohara, K. Sato, M. Omote and A. Ando, *Org. Lett.*, 2016, **18**, 1128-1131.

2. L. Schreyer, P. S. J. Kaib, V. N. Wakchaure, C. Obradors, R. Properzi, S. Lee and B. List, *Science*, 2011, **362**, 216-219.

3. H. O. House, L. J. Czuba, M. Gall and H. D. Olmstead, *J. Org. Chem.*, 1969, **34**, 2324-2336.

4. S. E. Denmark and S. K. Ghosh, *Angew. Chem. Int. Ed*., 2001, **40**, 4759-4762.

5. P. Duhamel, L. Hennequin, J. M. Poirier, G. Tavel and C. Vottero, *Tetrahedron.*, 1986, **42**, 4777-4786.

6. J. Nugent, B. R. Shire, D. F. J. Caputo, H. D. Pickford, F. Nightingale, I.T.T. Houlsby, J. J. Mousseau and E. A. Anderson, *Angew. Chem. Int. Ed*., 2020, **59**, 11866-11870.

7. P. K. Mandal and J. S. McMurray, *J. Org. Chem*., 2007, **72**, 6599-6601.

8. A. J. Mancuso, S. -L. Huang and D. Swern, *J. Org. Chem*., 1978, **43**, 2480-2482.

9. R. R. Gowda and D. Chakraborty, *Chin. J. Chem*., 2011, **29**, 2379-2384.

10. G. Qabaja, J. E. Wilent, A. R. Benavides, G. E. Bullard and K. S. Petersen, *Org. Lett*., 2013, **15**, 1266-1269.

11. R. Giri, I. Mosiagin, I. Franzoni, N. Y. Notel, S. Patra and D. Katayev, *Angew. Chem. Int. Ed.*, 2022, **61**, e202209143.

12. P. C. P., E. Joseph, A. A, N. D. S., I. Ibnusaud, J. Raskatov and B. Singaram, *J. Org. Chem*., 2018, **83**, 1431-1440.
13. C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B.*, 1988, **37**, 785-789.

14. A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648-5652.

15. S. Grimme, *J. Comput. Chem*., 2004, **25**, 1463-147.

16. S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys*., 2010, **132**, 154104.

17. S. Grimme, *WIREs Comput Mol Sci*., 2011, **1**, 211-228.

18. S. Ehrlich, J. Moellmann and S. Grimme, *Acc. Chem. Res.*, 2012, **46**, 916-926.

19. F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys*., 2005, **7**, 3297-3305.

20. F. Weigend, *Phys. Chem. Chem. Phys*., 2006, **8**, 1057-1065.

21. A. Klamt and G. Schüürmann, *J. Chem. Soc. Perkin Trans*., 1993, **2**, 799-805.

22. J. Tomasi and M. Persico, *Chem. Rev.*, 1994, **94**, 2027-2094.

23. J. Andzelm, C. Kölmel and A. Klamt, *J. Chem. Phys.*, 1995, **103**, 9312-9320.

24. V. Barone and M. Cossi, *J. Phys. Chem. A*., 1998, **102**, 1995-2001.

25. M. Cossi, N. Rega, G. Scalmani and V. Barone, *J. Comput. Chem*., 2003, **24**, 669-681.

26. M. J. Frisch, G. Trucks, H. Schlegel, G. Scuseria, M. Robb, J. Cheeseman, G. Scalmani, V. Barone, G. Petersson and H. Nakatsuji, Gaussian 16 (Gaussian, Inc. Wallingford, CT), 2016.

27. A. Hellweg, C. Hättig, S. Höfener and W. Klopper, *Theor. Chem. Acc.*, 2007, **117**, 587-597.

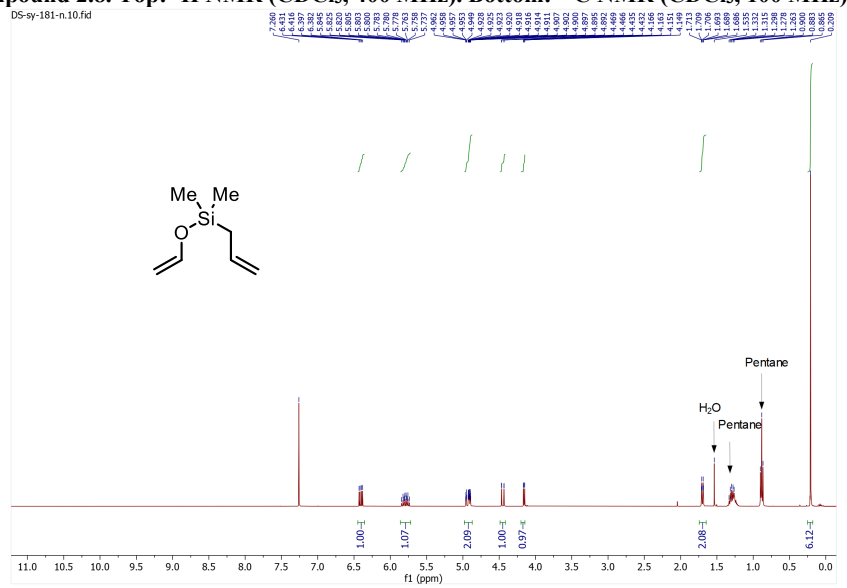
28. F. Neese, *WIREs Comput Mol Sci*., 2012, **2**, 73-78.

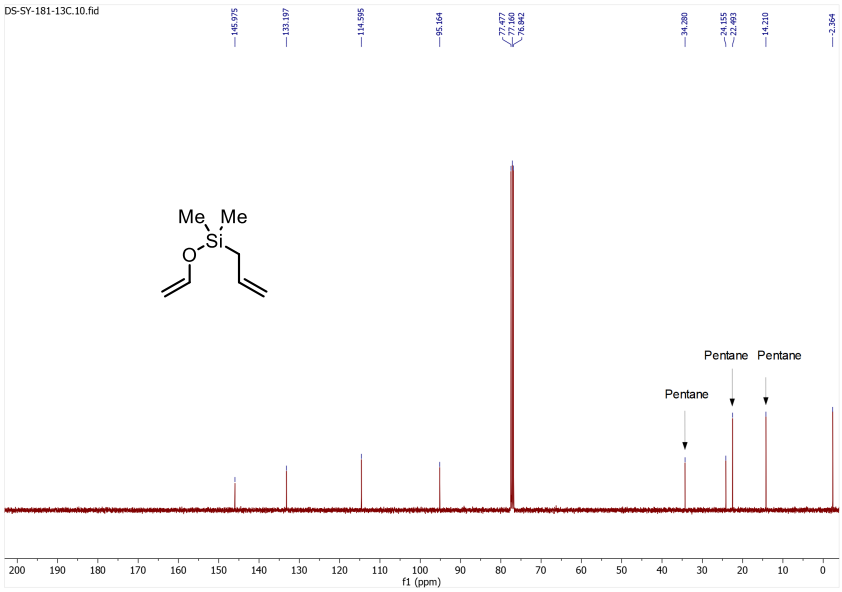
29. C. Legault, (2009). CYLview, 1.0 b. Université de Sherbrooke 436, 437.

30. H. G. Roth, N. A. Romero and D. A. Nicewicz, *Synlett*., 2016, **27**, 714-723.

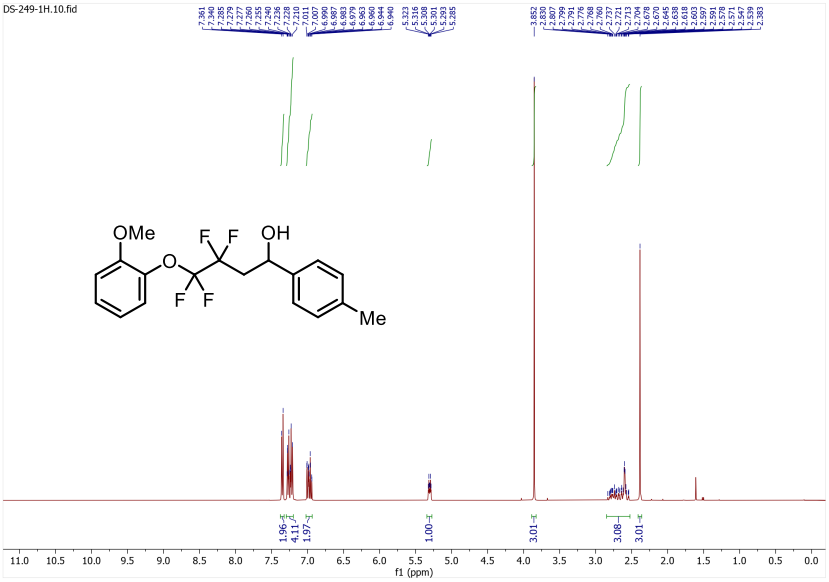
9. Spectral data

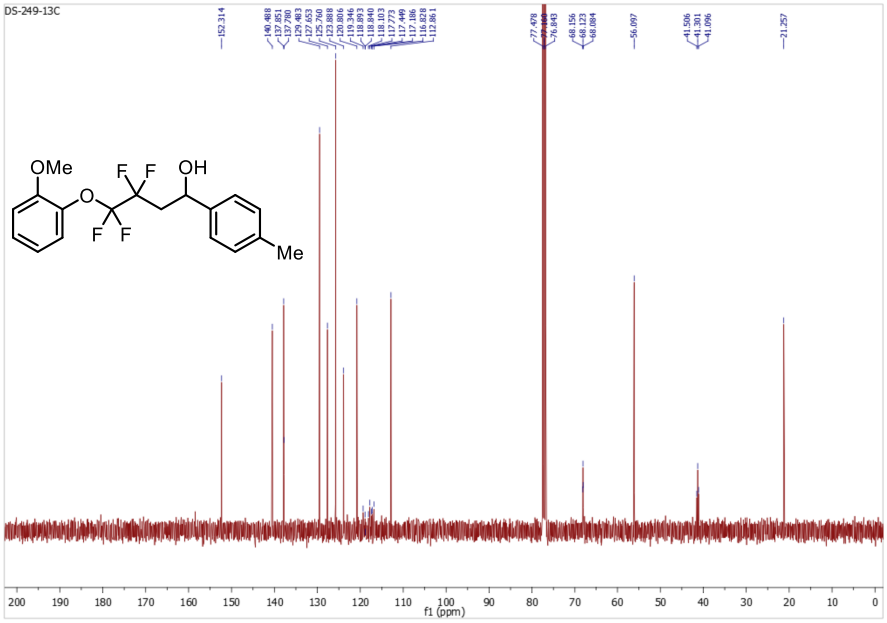
Compound 2.8. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)



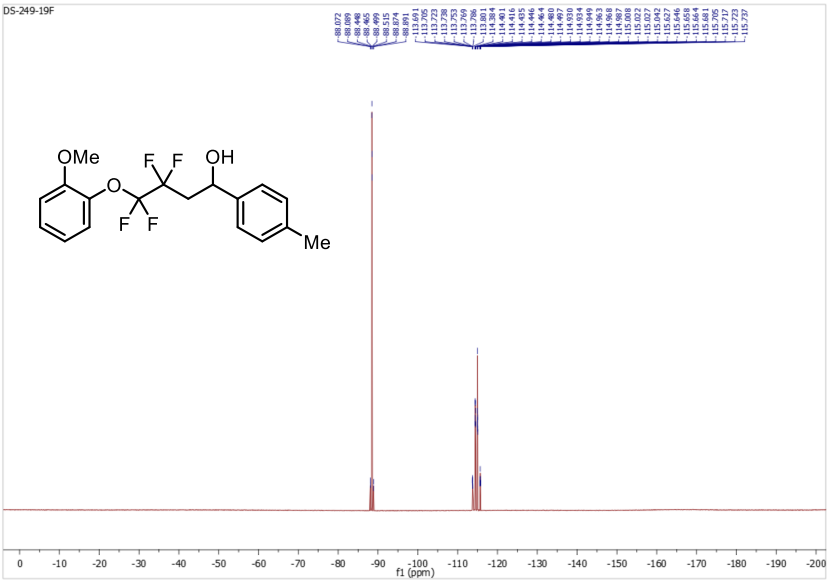


Compound 4. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

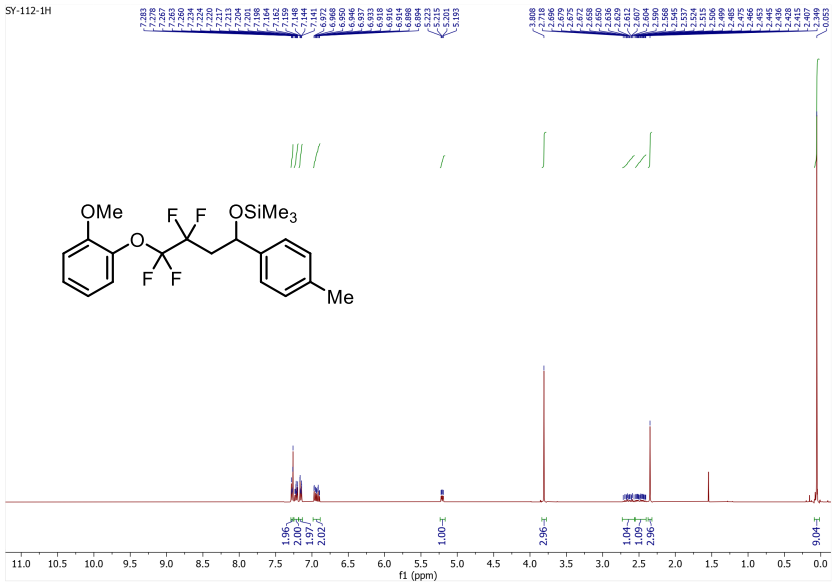


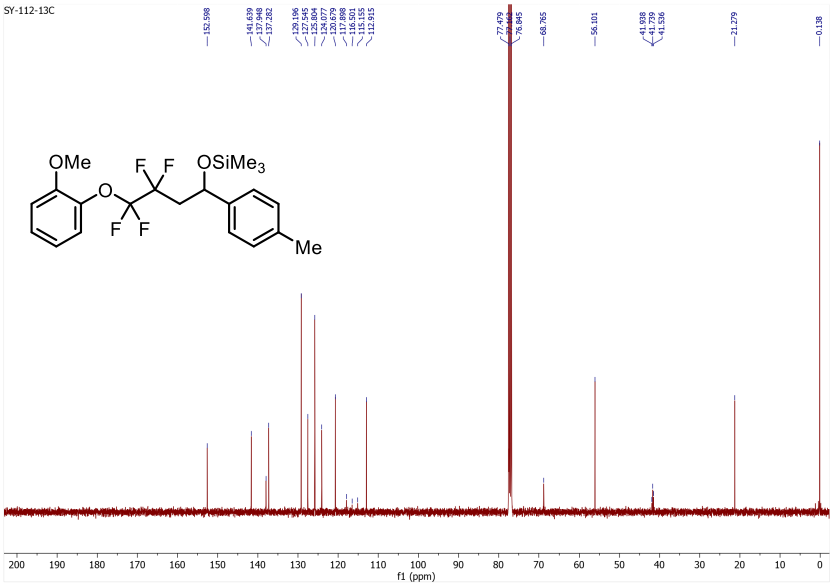


Compound 4. ^{19}F NMR ($CDCl_3$, 376 MHz)

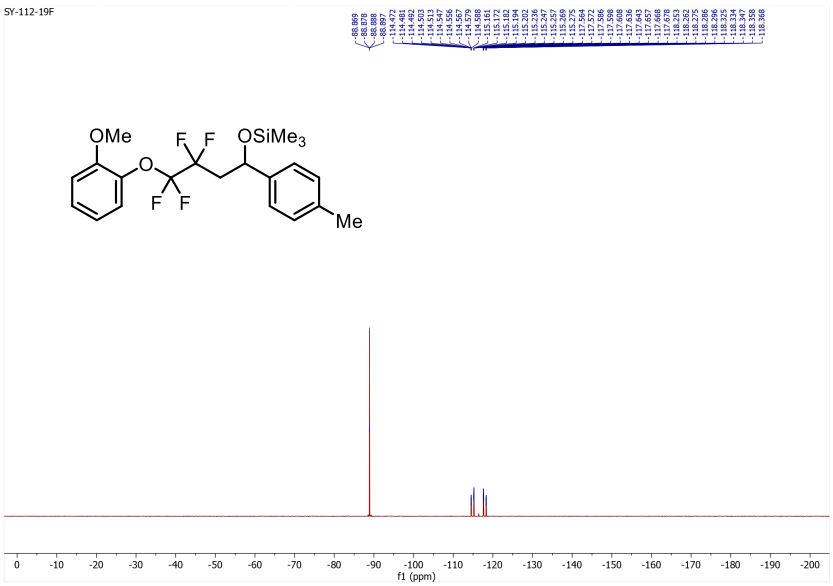


Compound 5. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

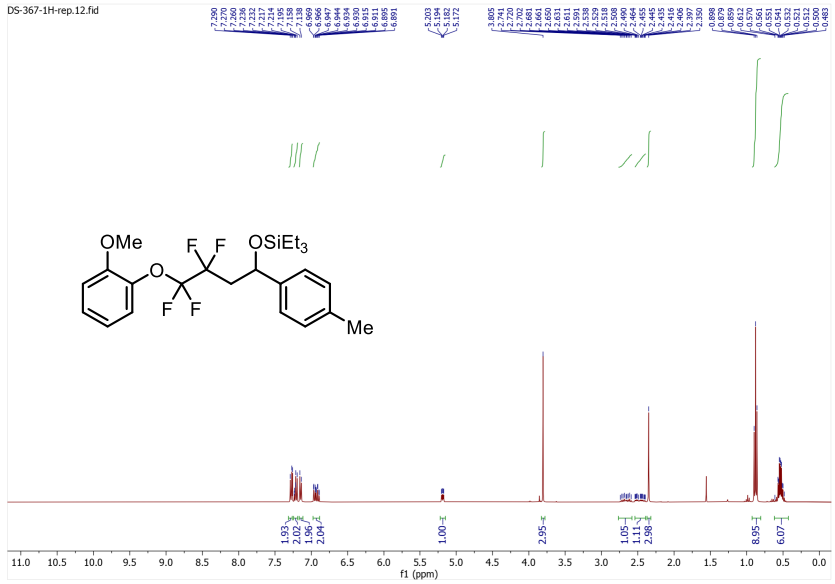


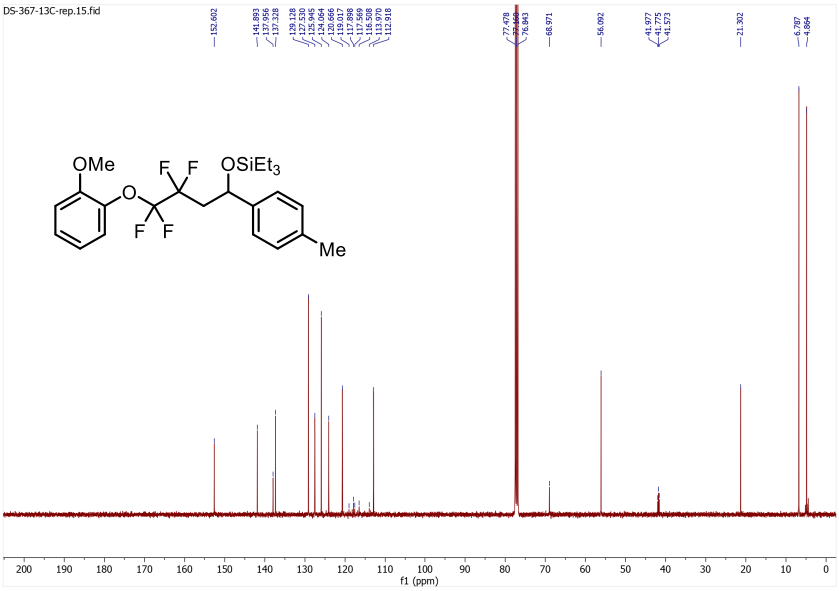


Compound 5. ^{19}F NMR ($CDCl_3$, 376 MHz)

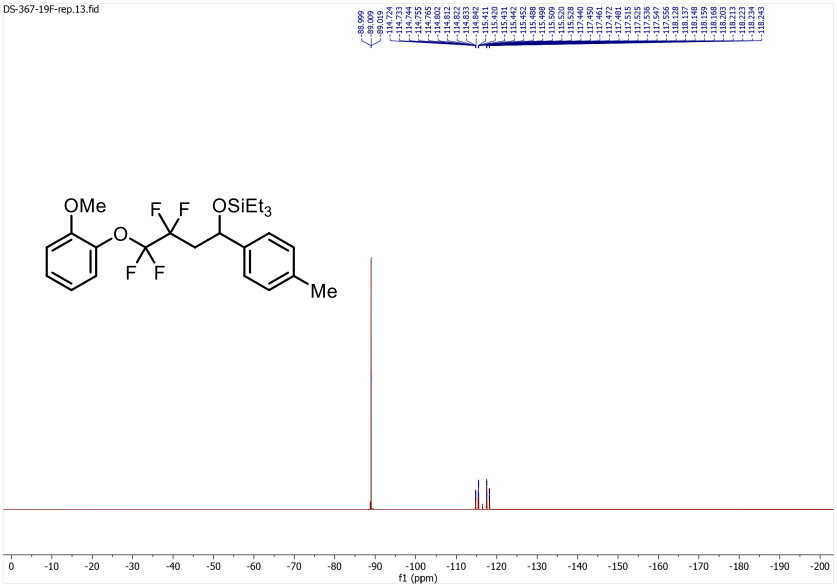


Compound 6. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

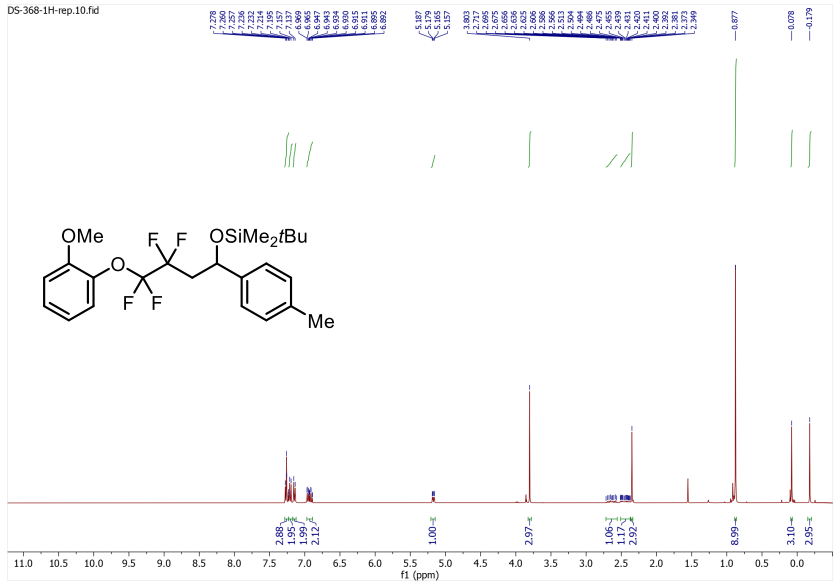


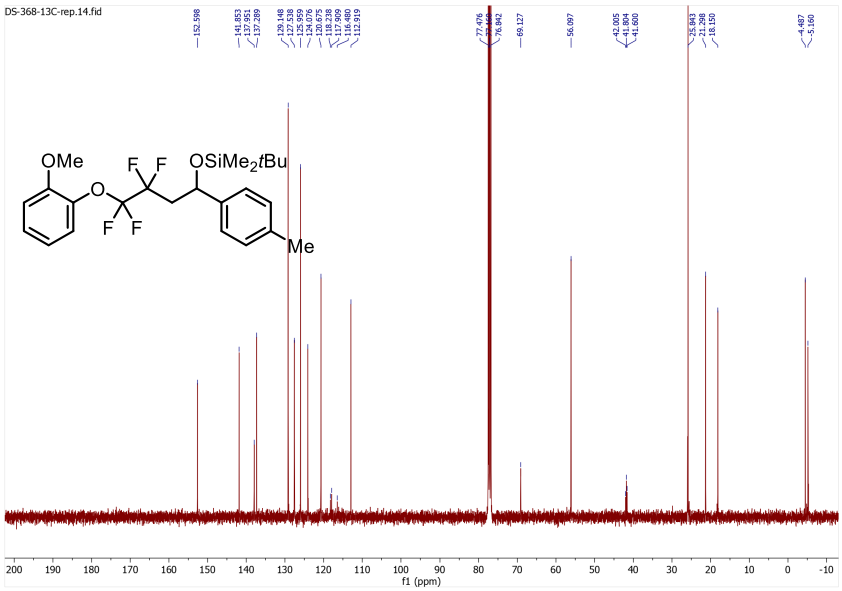


Compound 6. ^{19}F NMR ($CDCl_3$, 376 MHz)

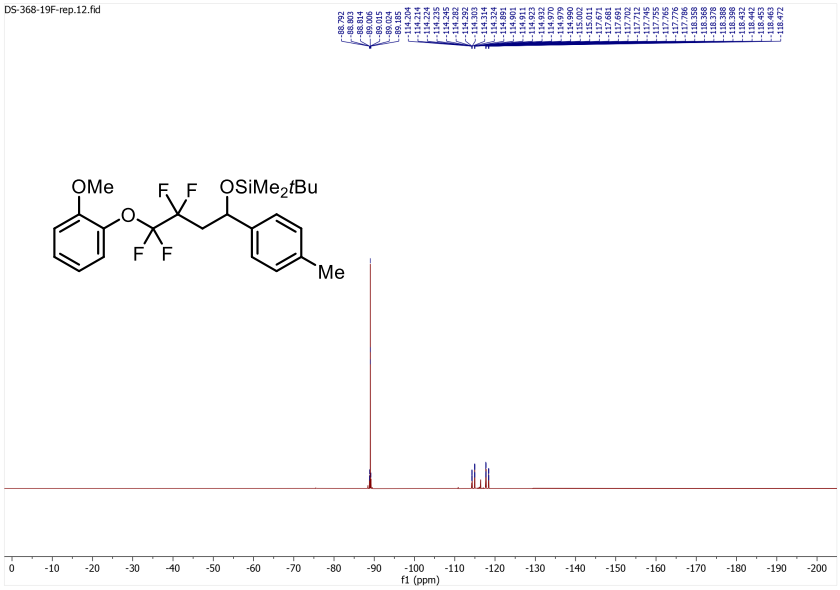


Compound 7. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

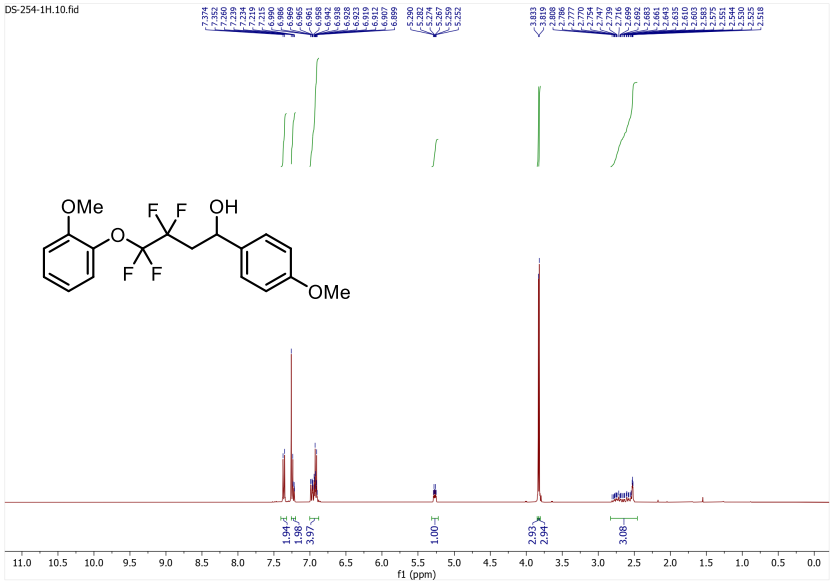


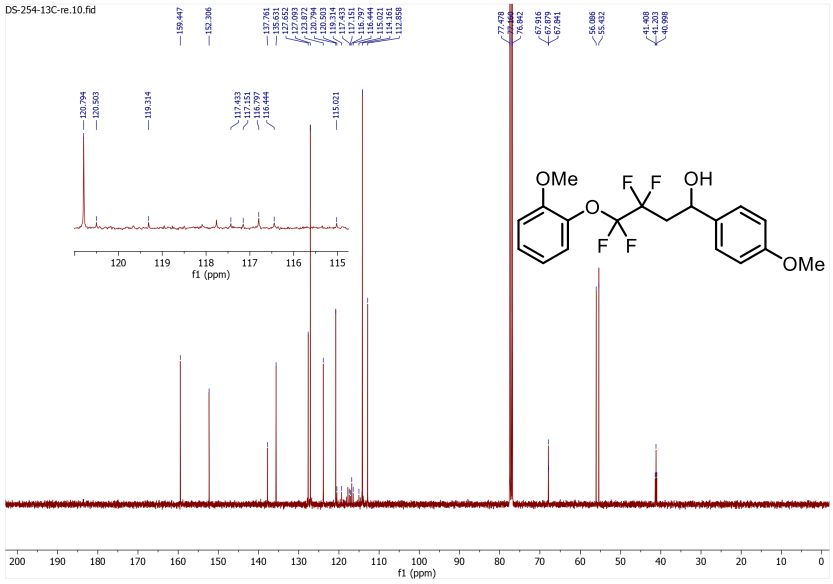


Compound 7. ^{19}F NMR ($CDCl_3$, 376 MHz)

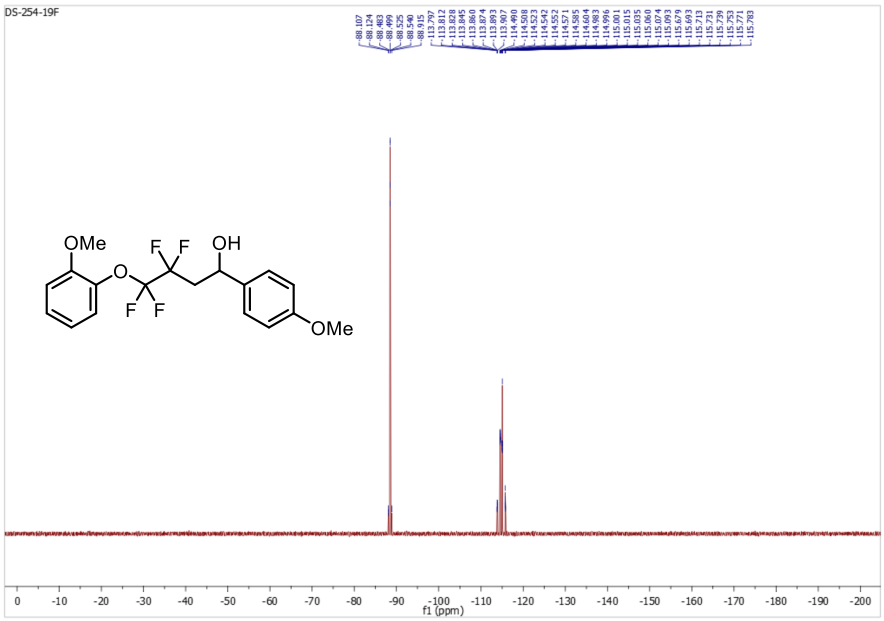


Compound 8. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

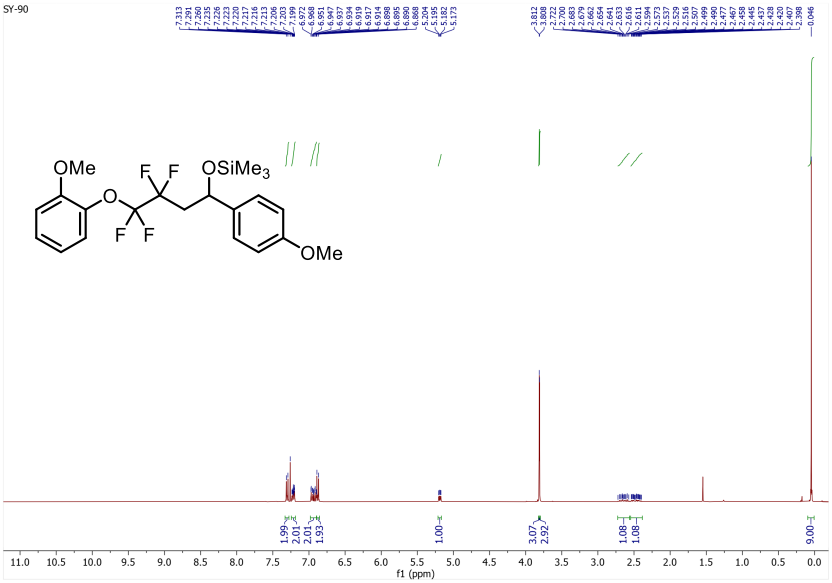


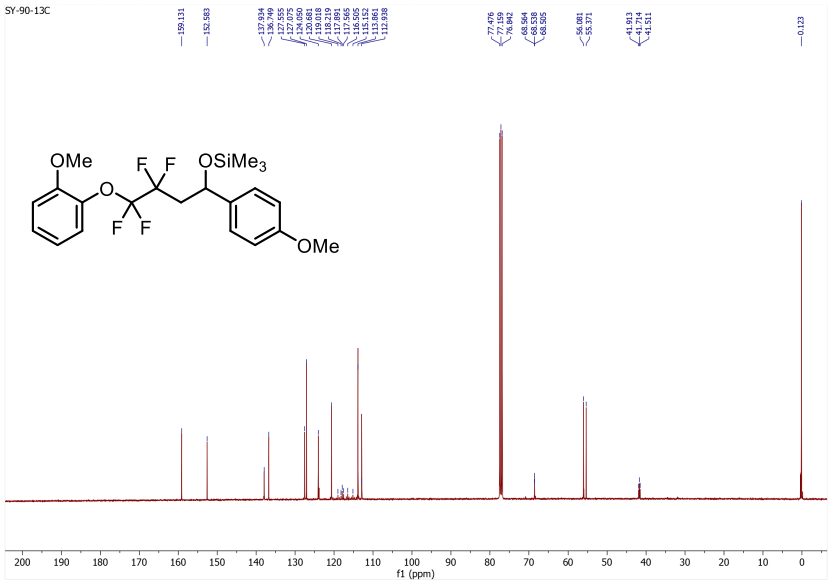


Compound 8. ^{19}F NMR ($CDCl_3$, 376 MHz)

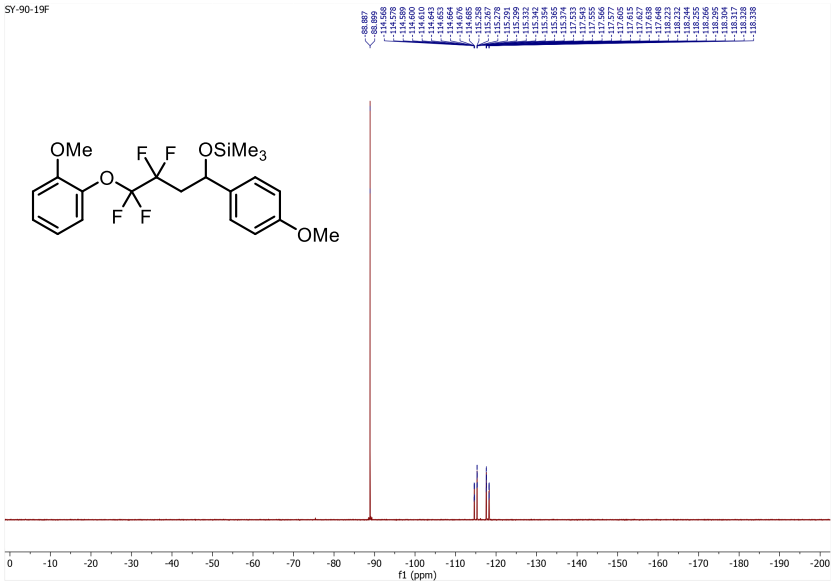


Compound 9. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

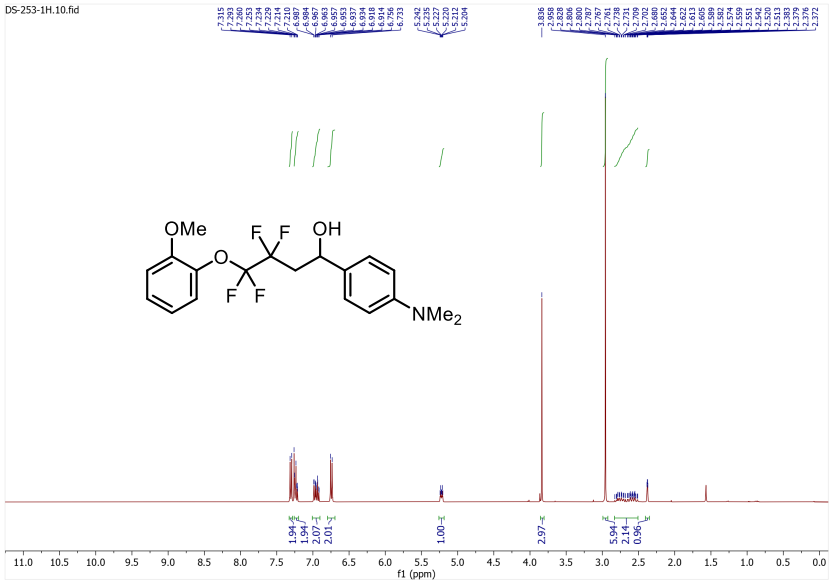


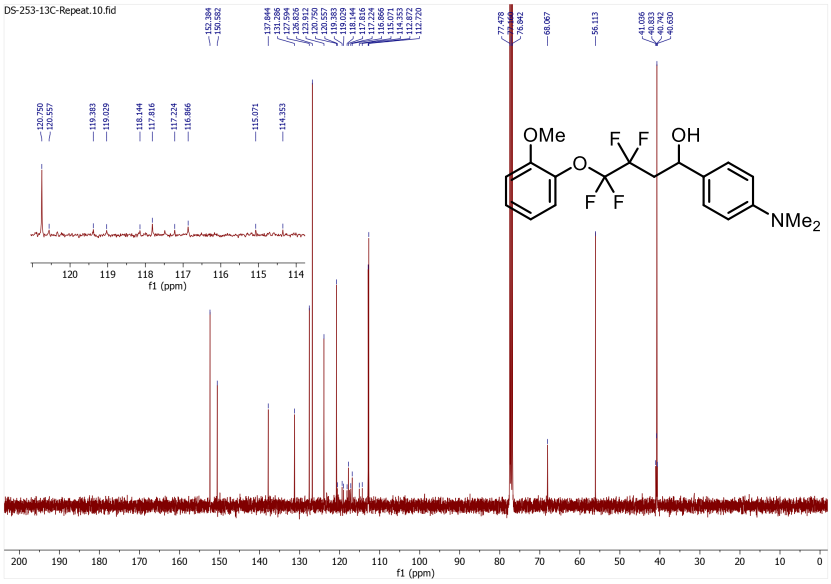


Compound 9. ^{19}F NMR ($CDCl_3$, 376 MHz)

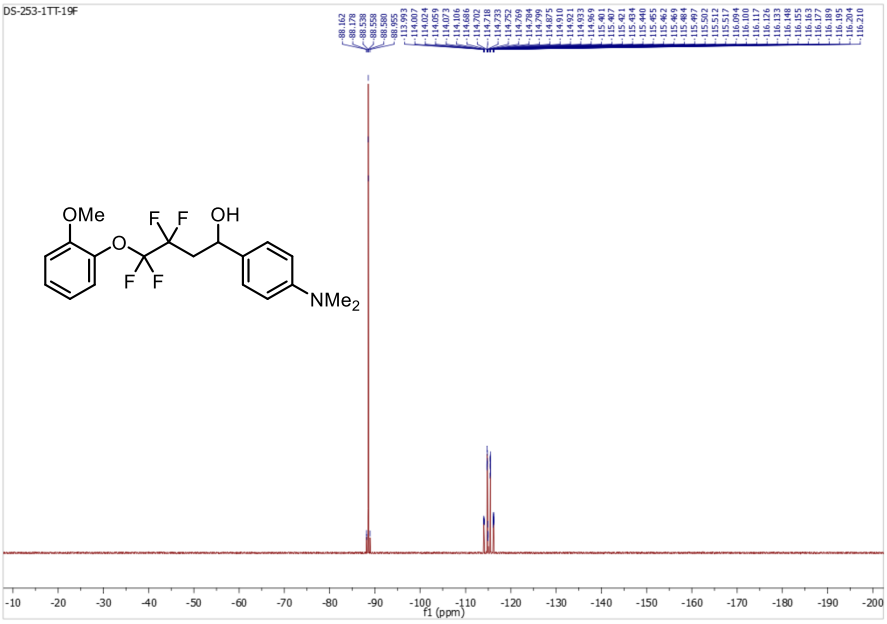


Compound 10. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

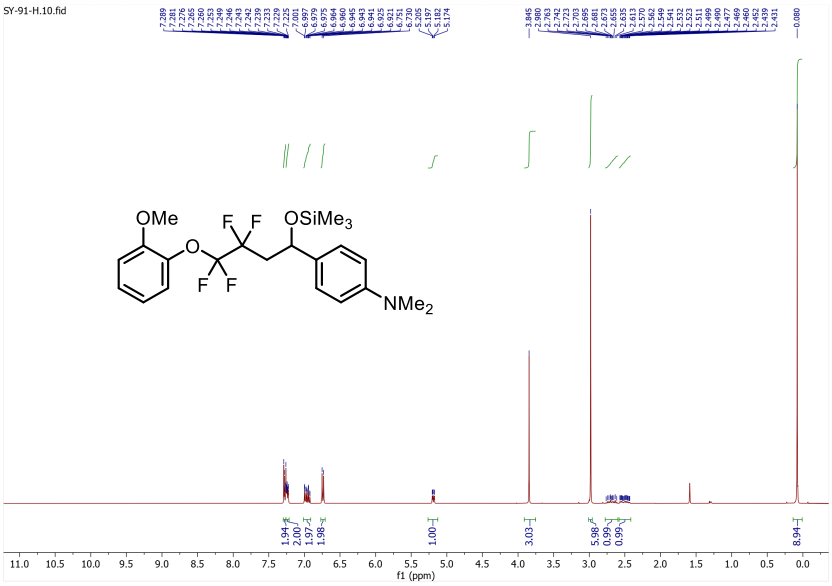


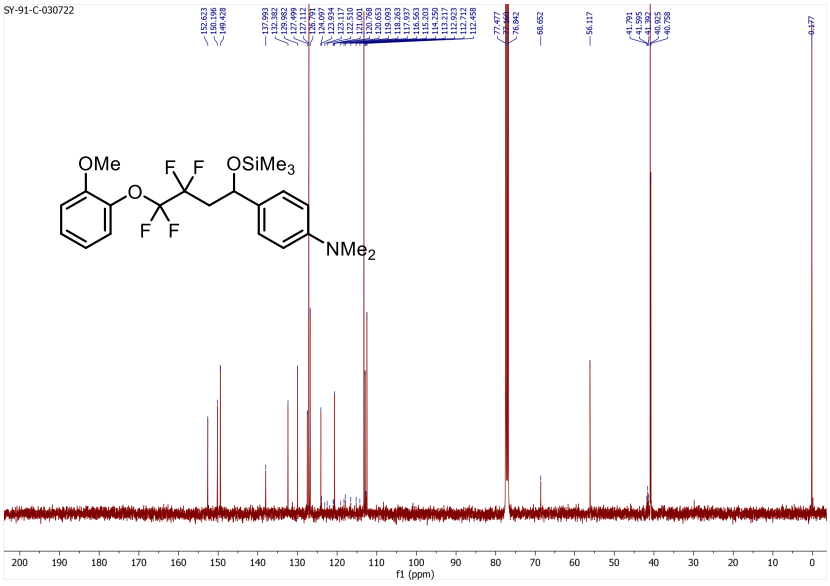


Compound 10. ^{19}F NMR ($CDCl_3$, 376 MHz)

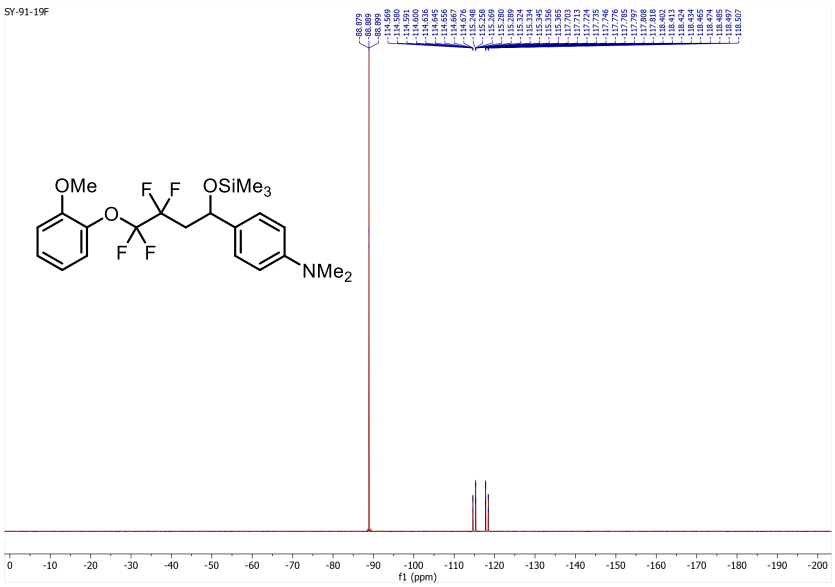


Compound 11. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

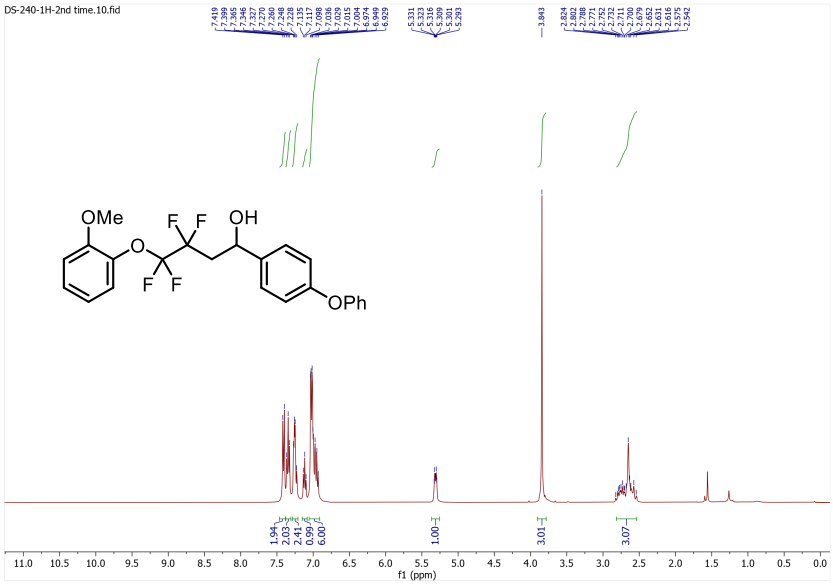


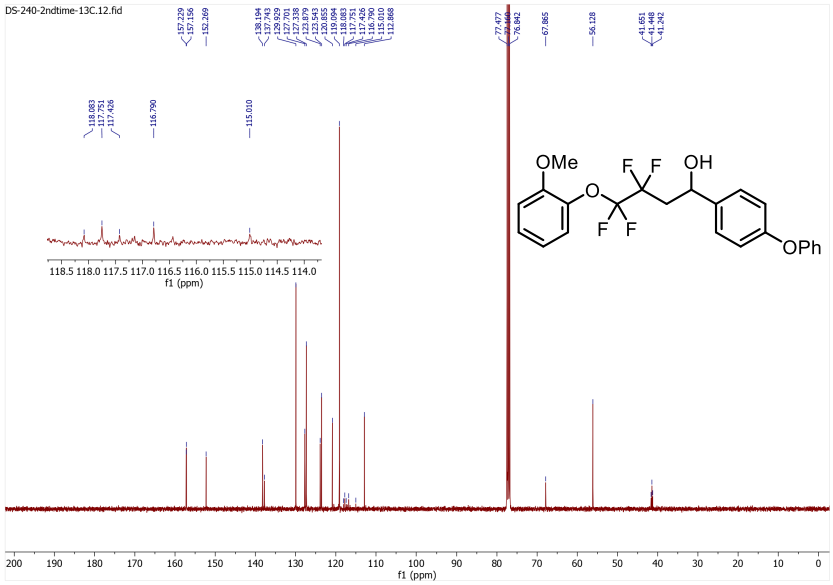


Compound 11. ^{19}F NMR ($CDCl_3$, 376 MHz)

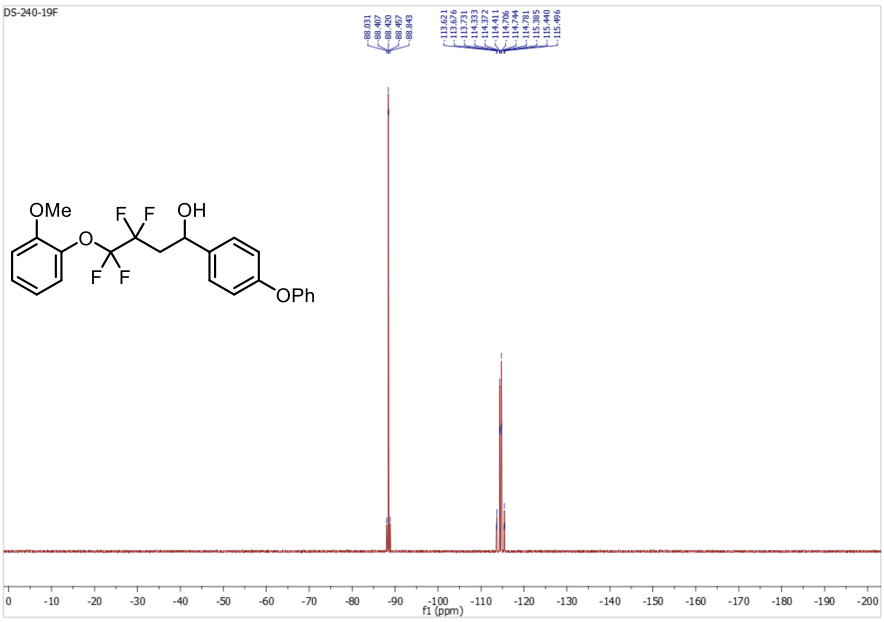


Compound 12. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

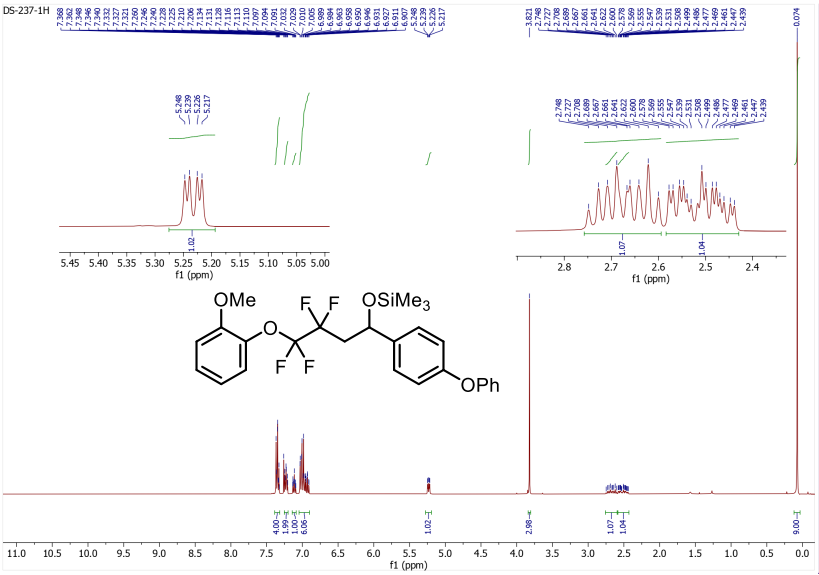


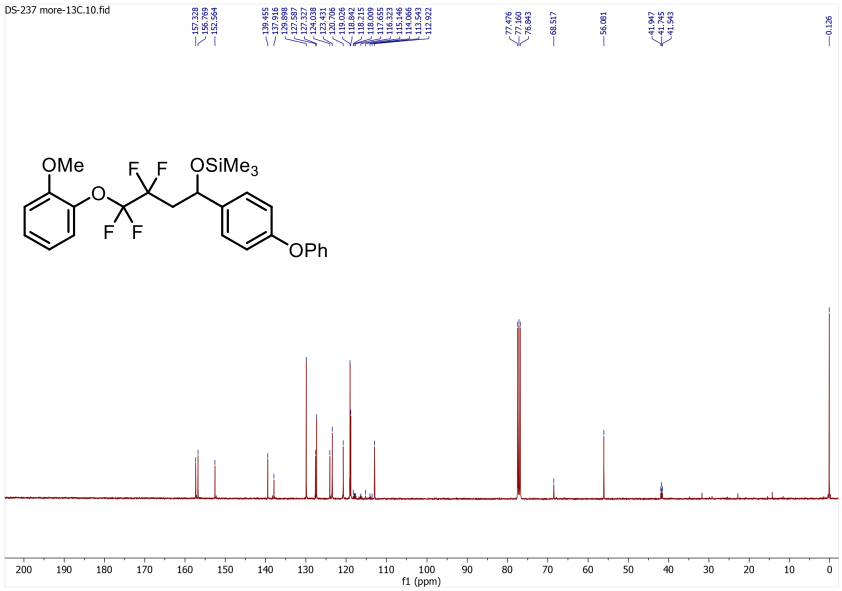


Compound 12. ^{19}F NMR ($CDCl_3$, 376 MHz)



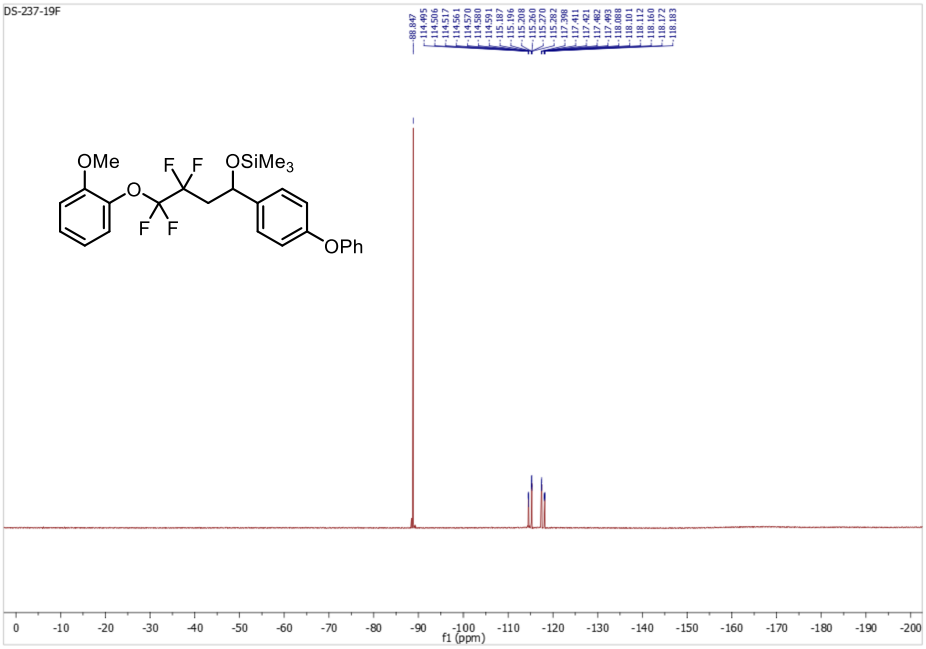
Compound 13. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)



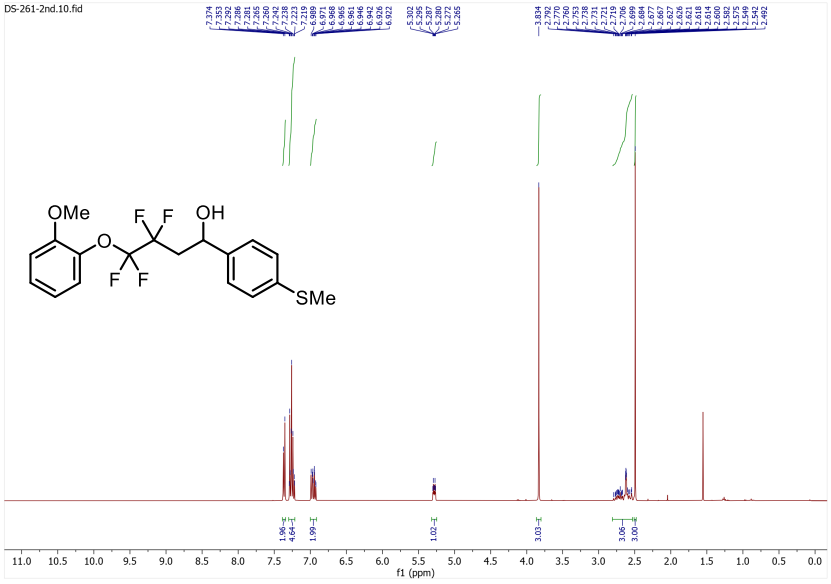


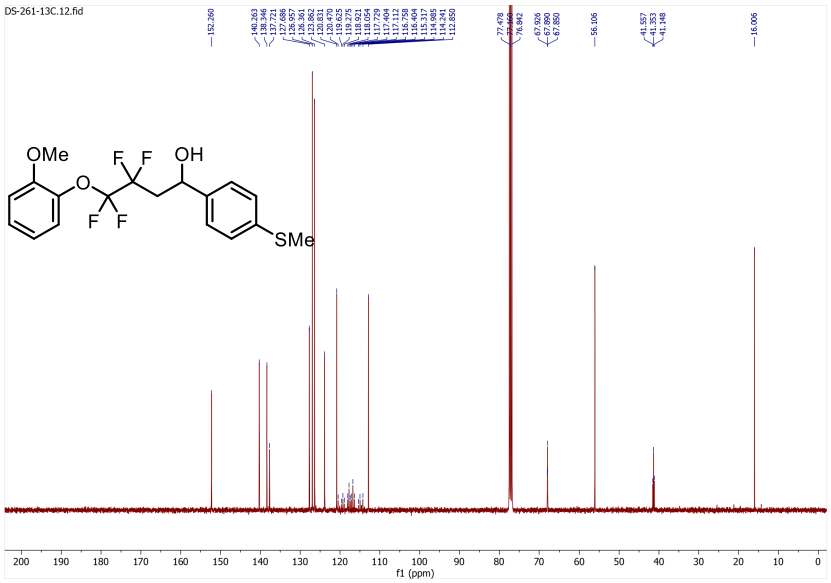
Commented [DS7]: Changed the spectra

Compound 13. ^{19}F NMR ($CDCl_3$, 376 MHz)

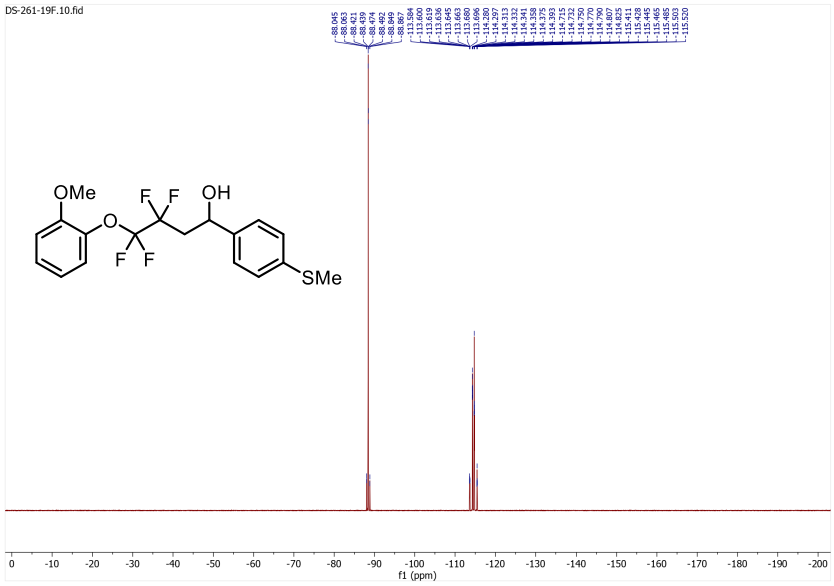


Compound 14. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

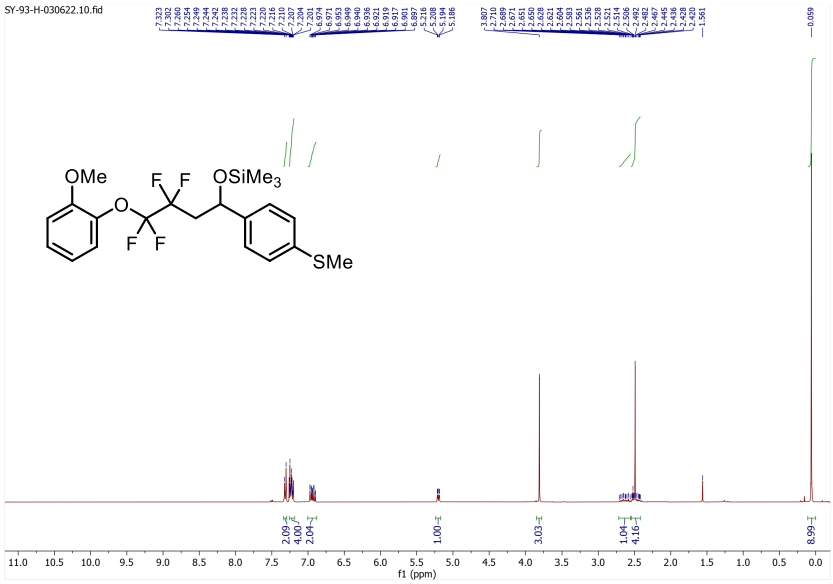


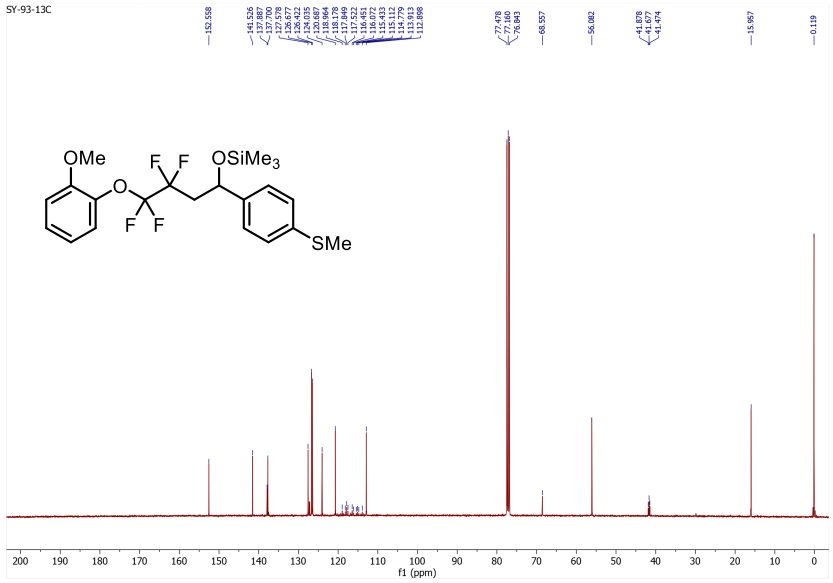


Compound 14. ^{19}F NMR ($CDCl_3$, 376 MHz)

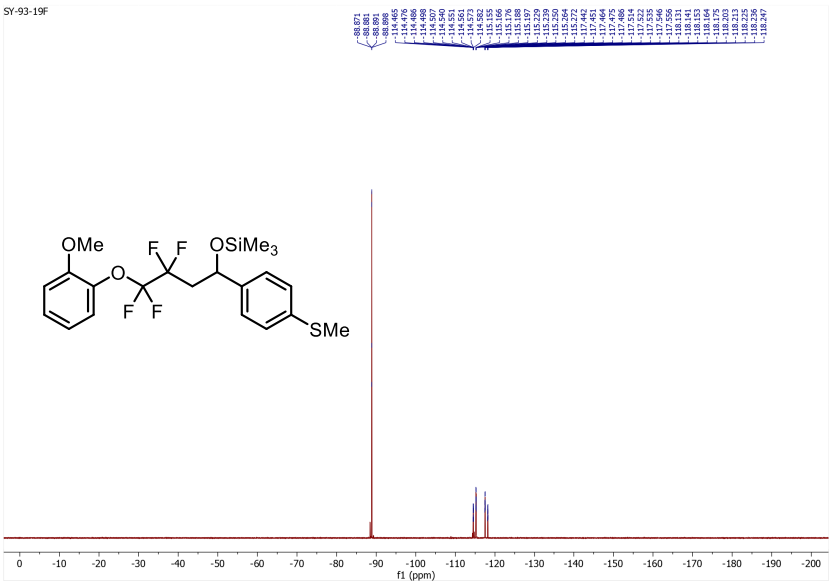


Compound 15. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

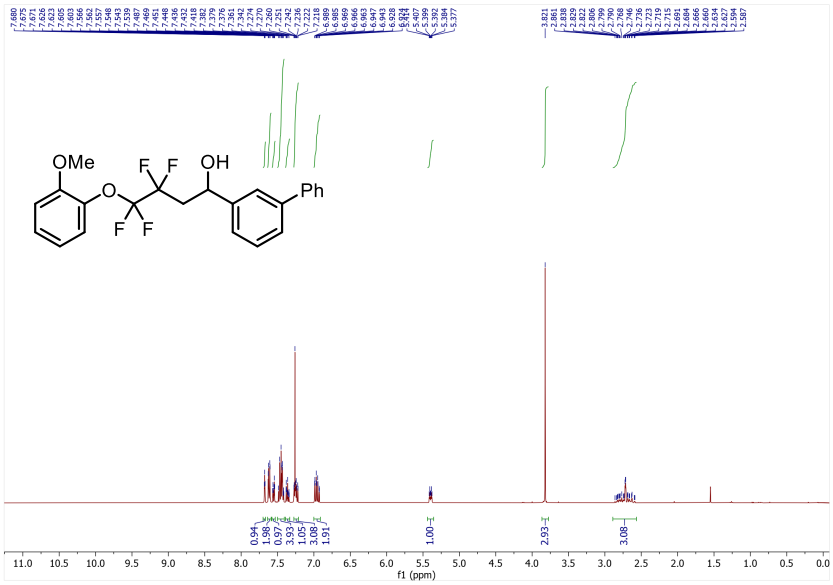


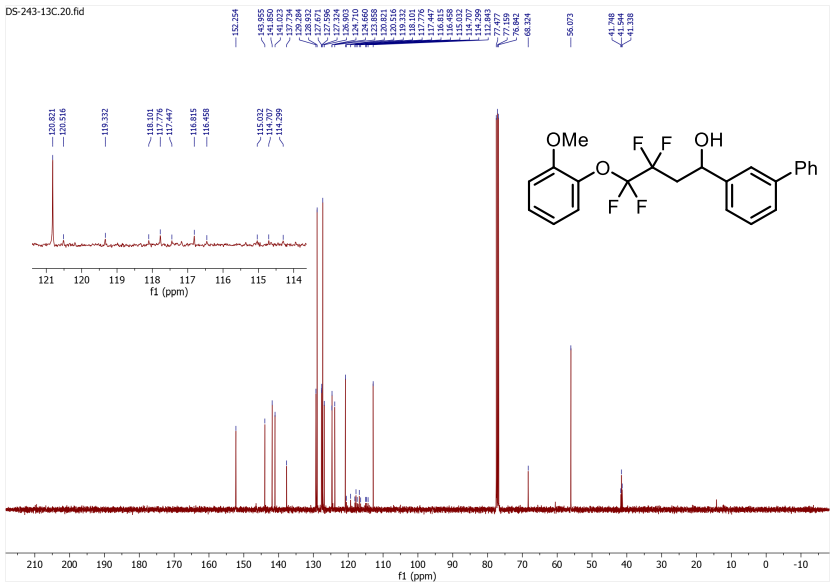


Compound 15. ^{19}F NMR ($CDCl_3$, 376 MHz)

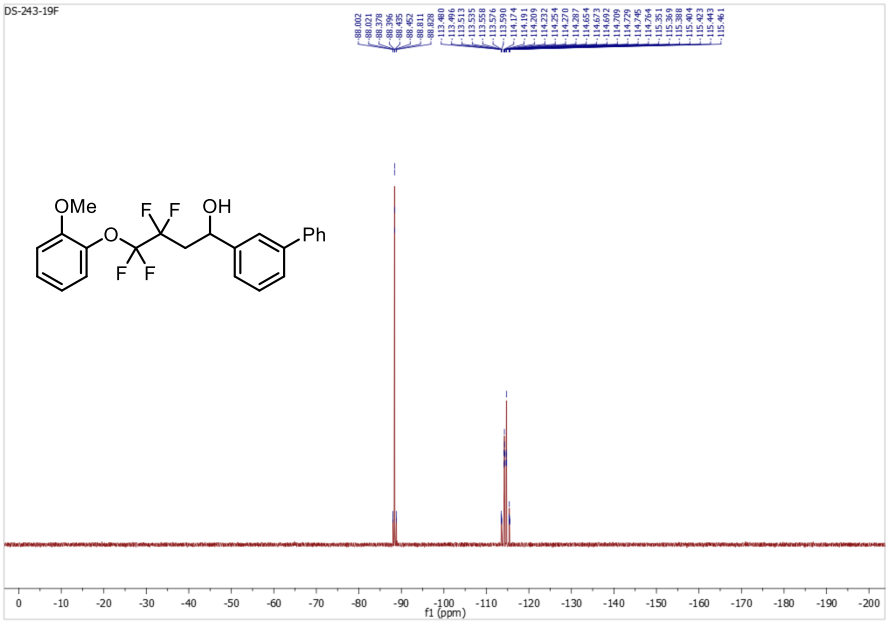


Compound 16. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

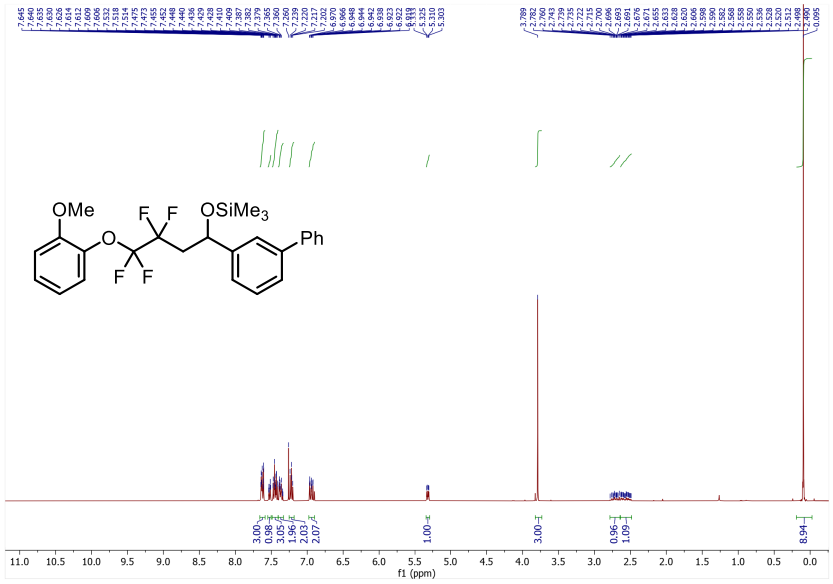


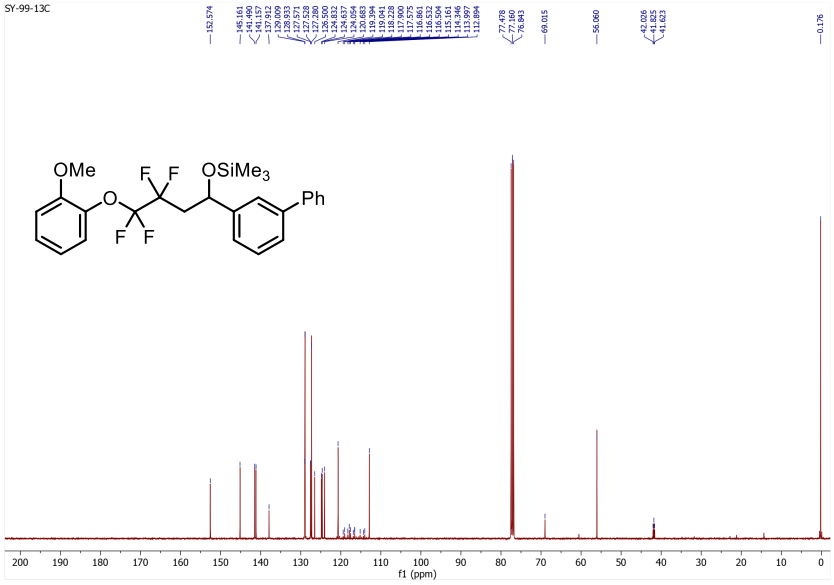


Compound 16. ^{19}F NMR ($CDCl_3$, 376 MHz)

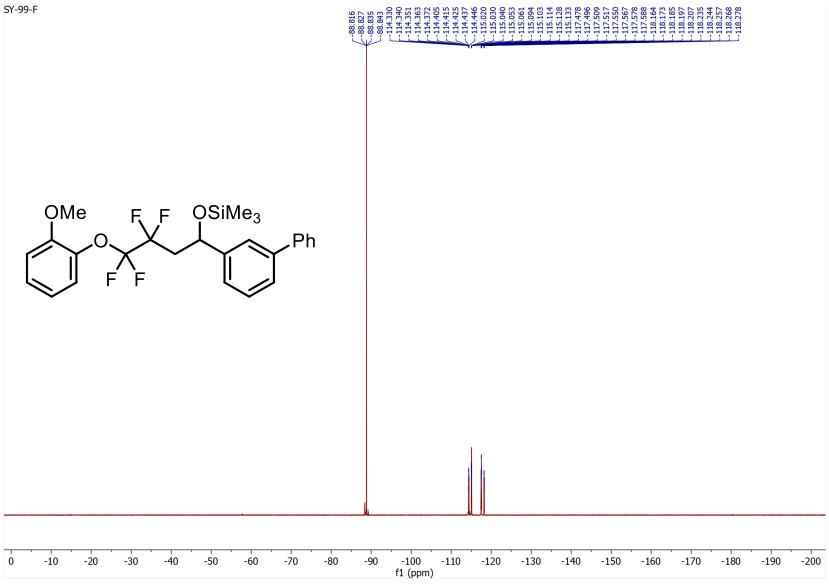


Compound 17. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

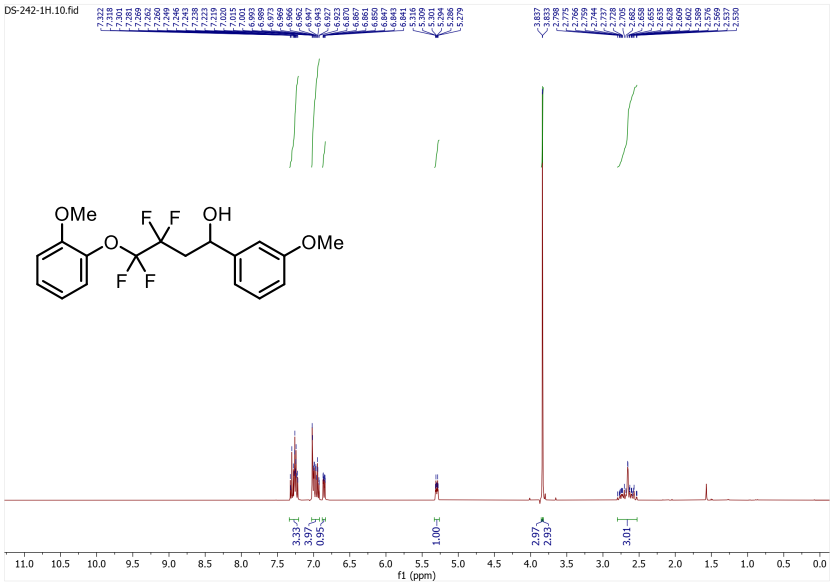


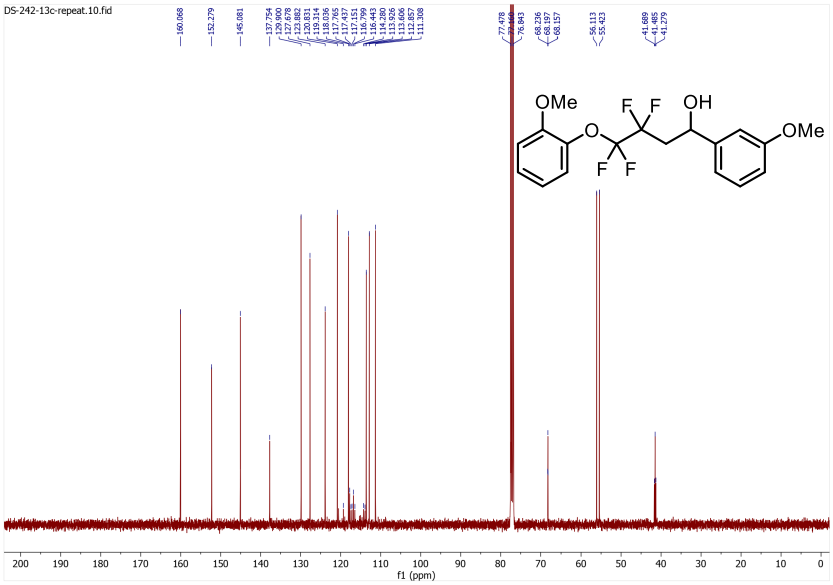


Compound 17. ^{19}F NMR ($CDCl_3$, 376 MHz)

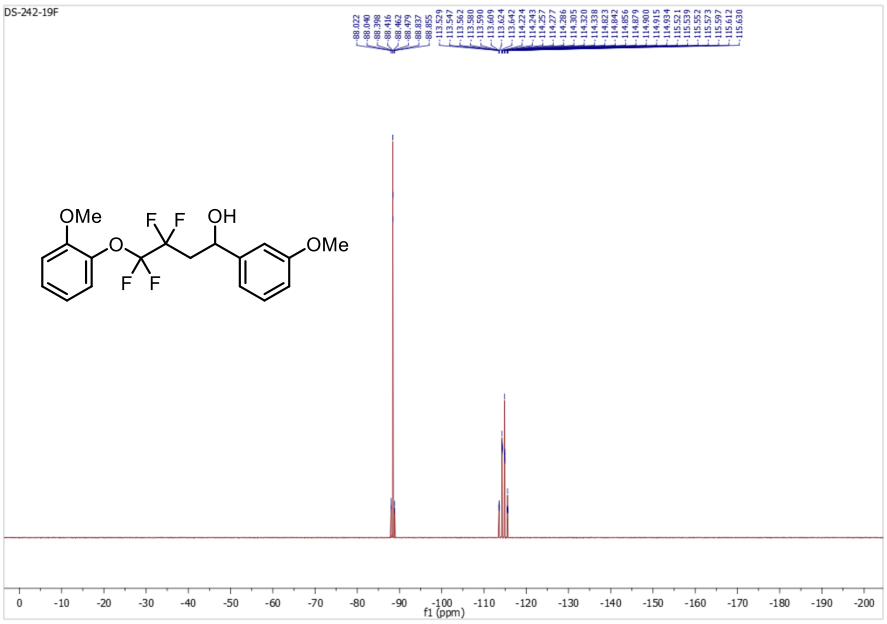


Compound 18. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

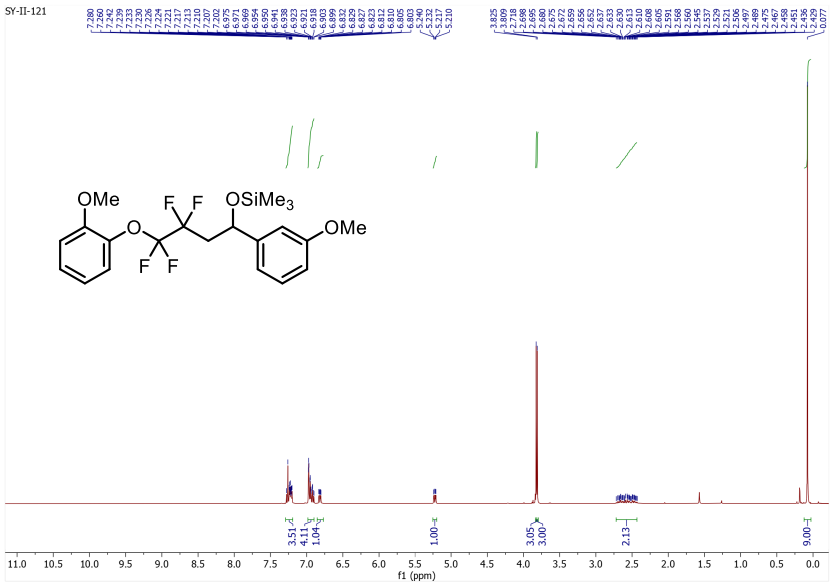


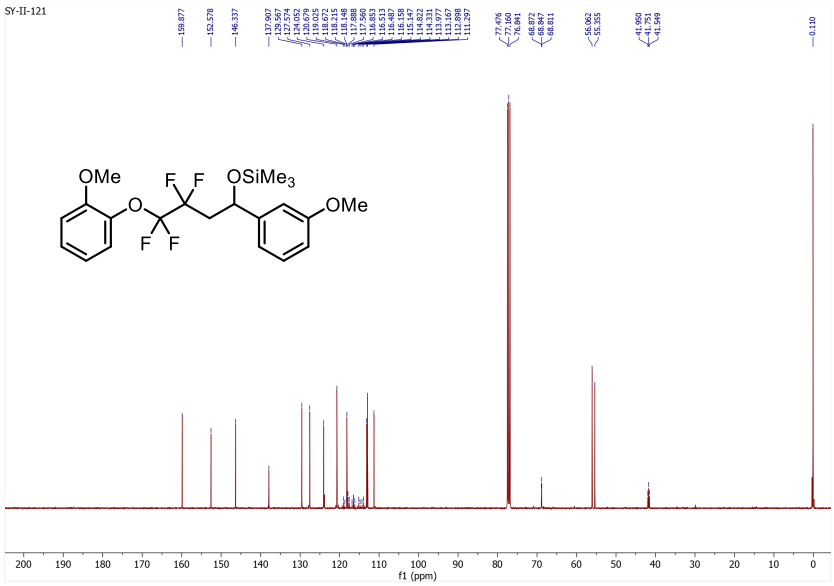


Compound 18. ^{19}F NMR ($CDCl_3$, 376 MHz)

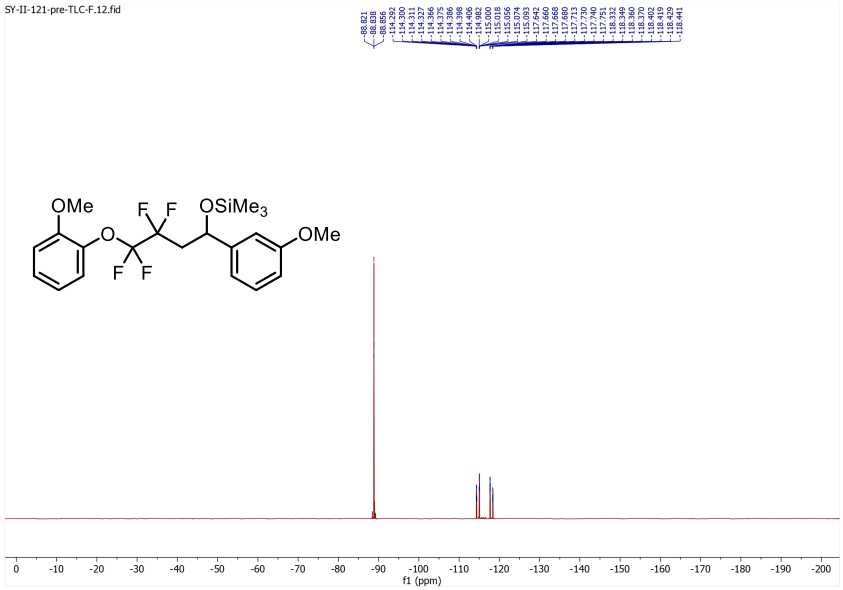


Compound 19. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

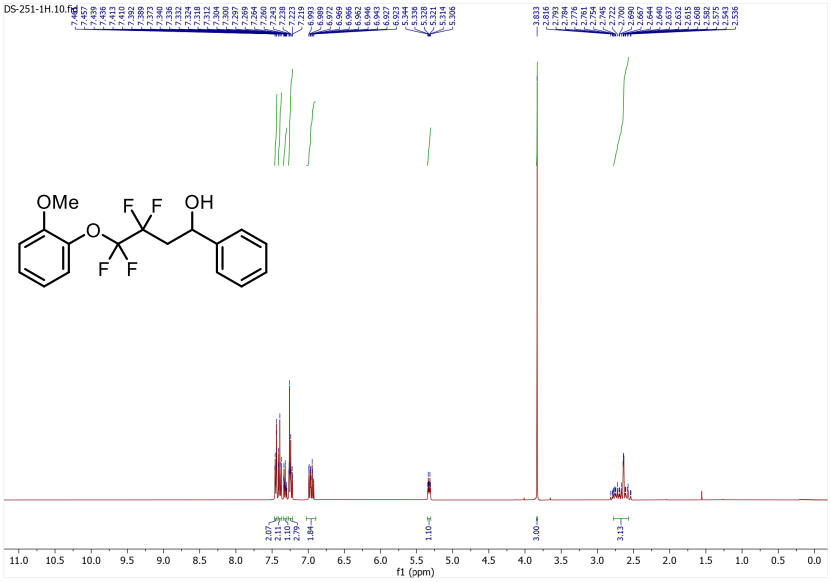


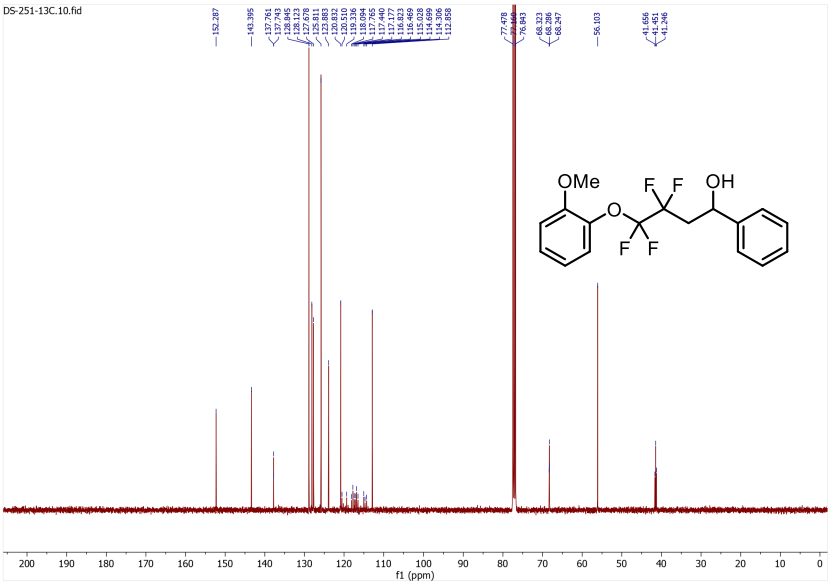


Compound 19. ^{19}F NMR ($CDCl_3$, 376 MHz)

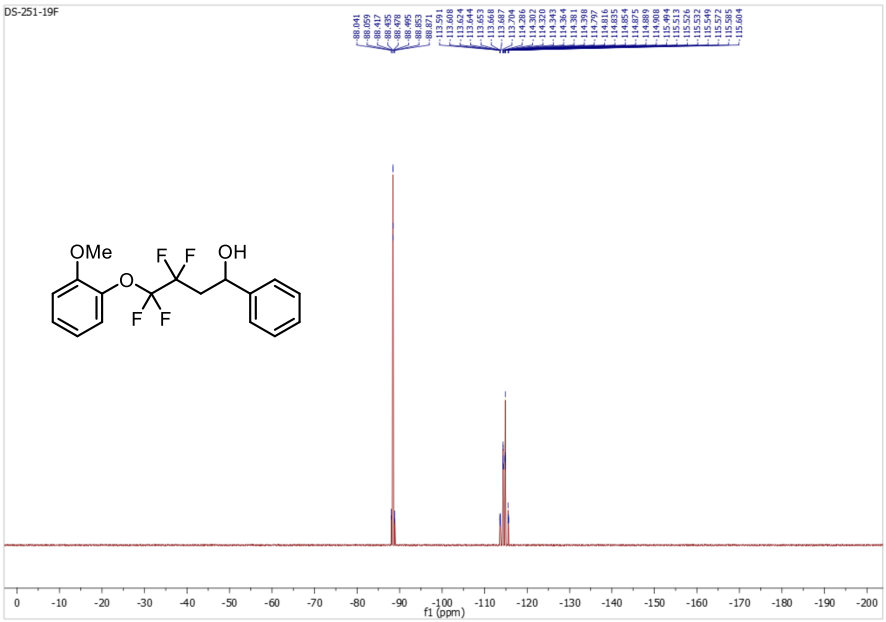


Compound 20. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

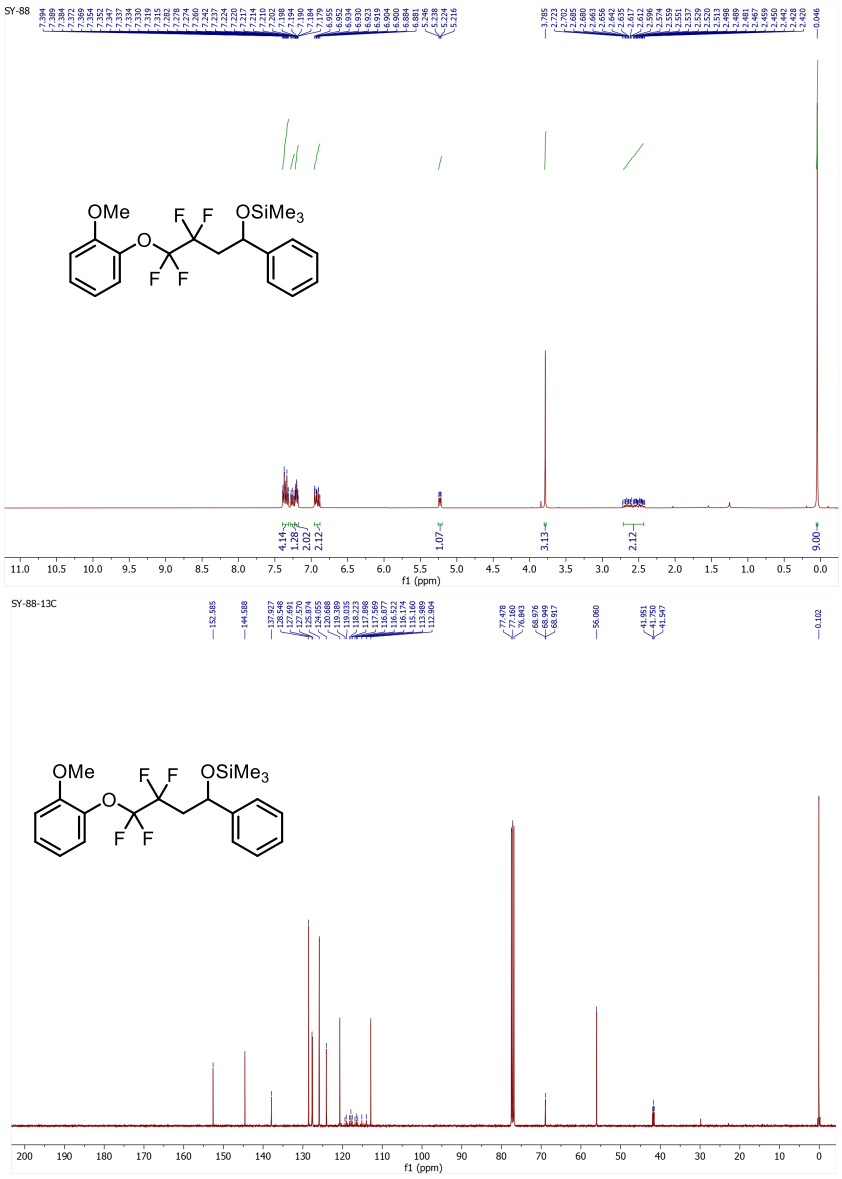




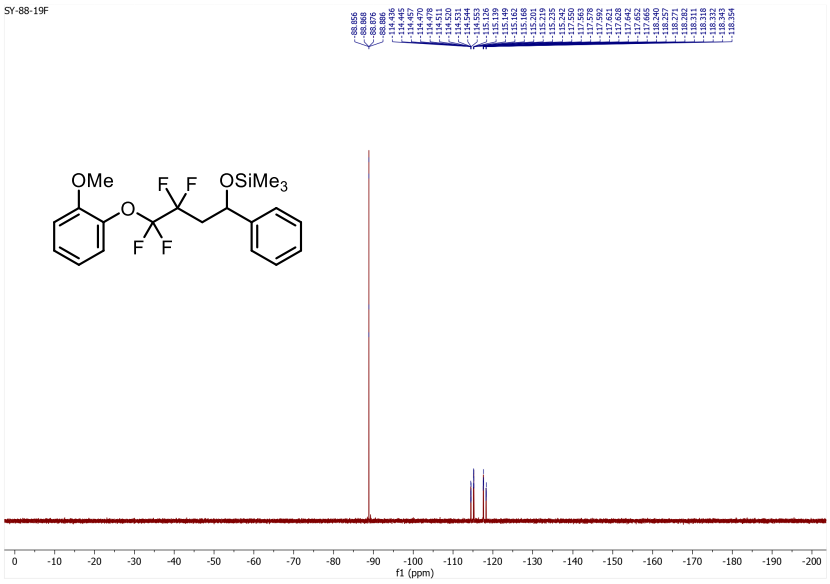
Compound 20. ^{19}F NMR ($CDCl_3$, 376 MHz)



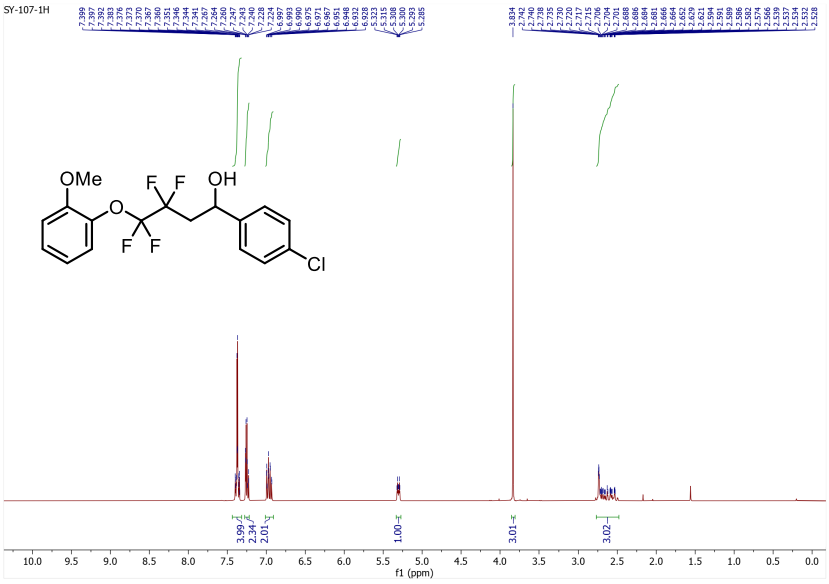
Compound 21. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

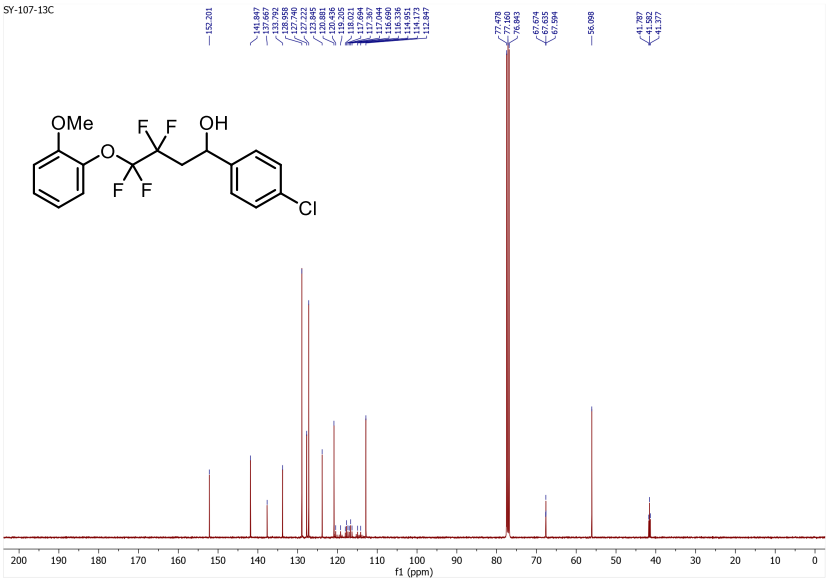


Compound 21. ^{19}F NMR ($CDCl_3$, 376 MHz)

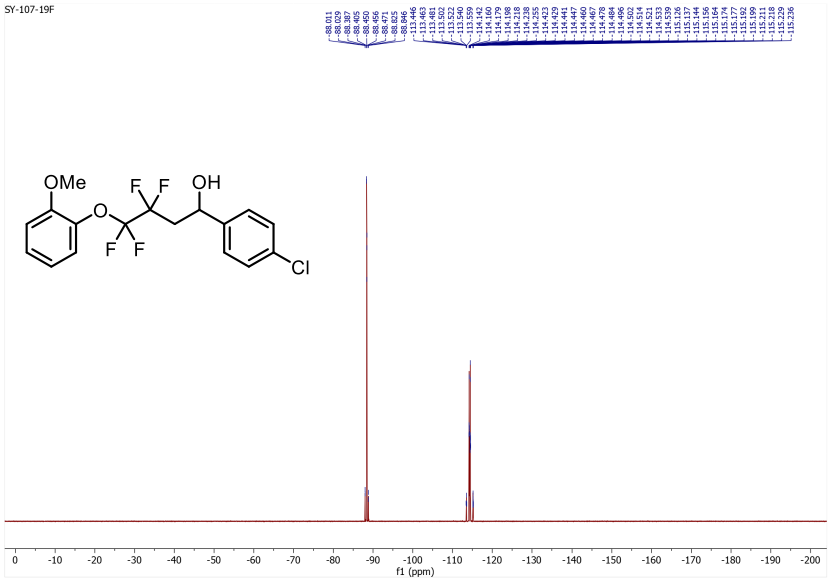


Compound 22. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

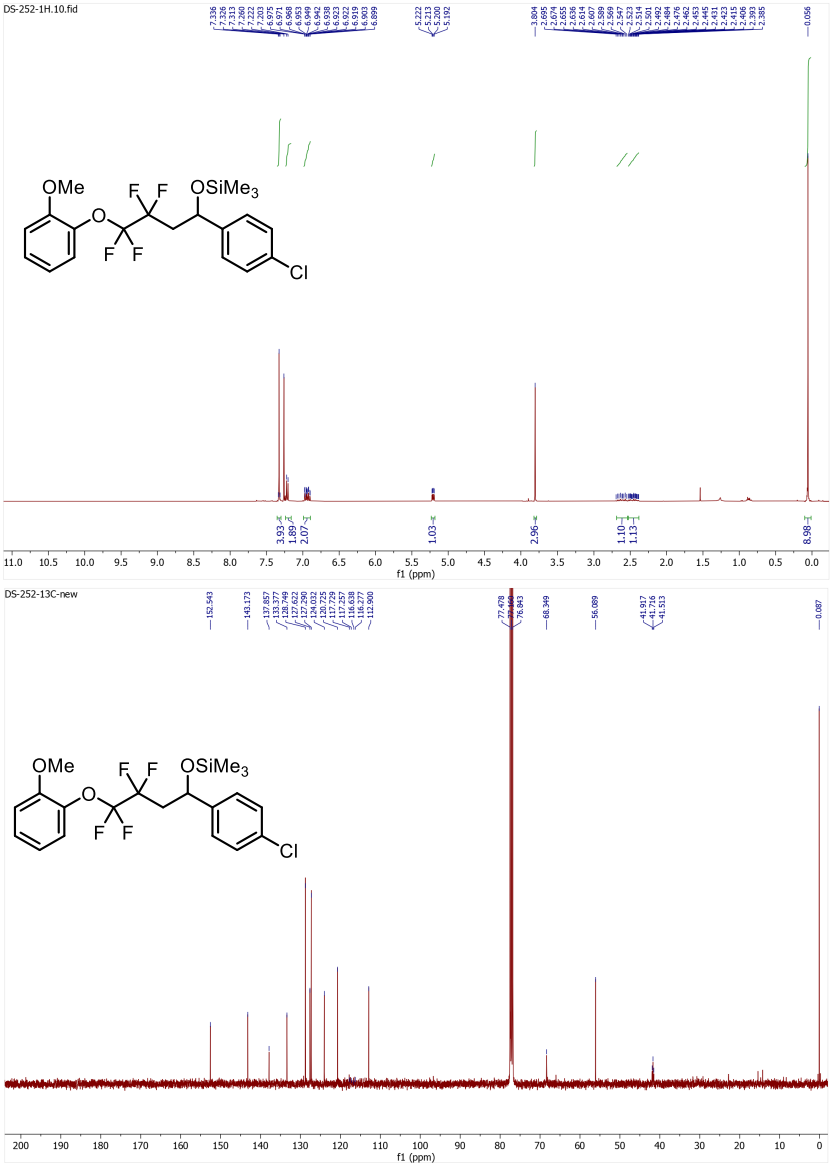




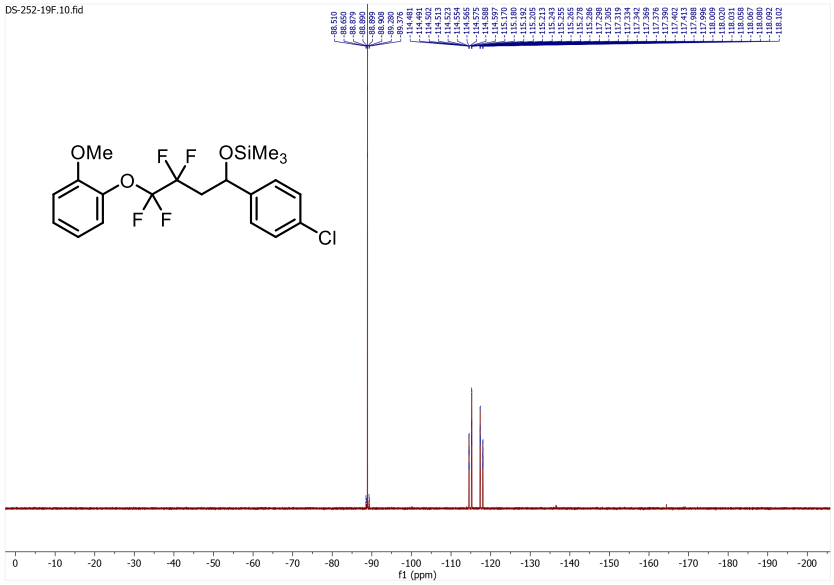
Compound 22. ^{19}F NMR ($CDCl_3$, 376 MHz)



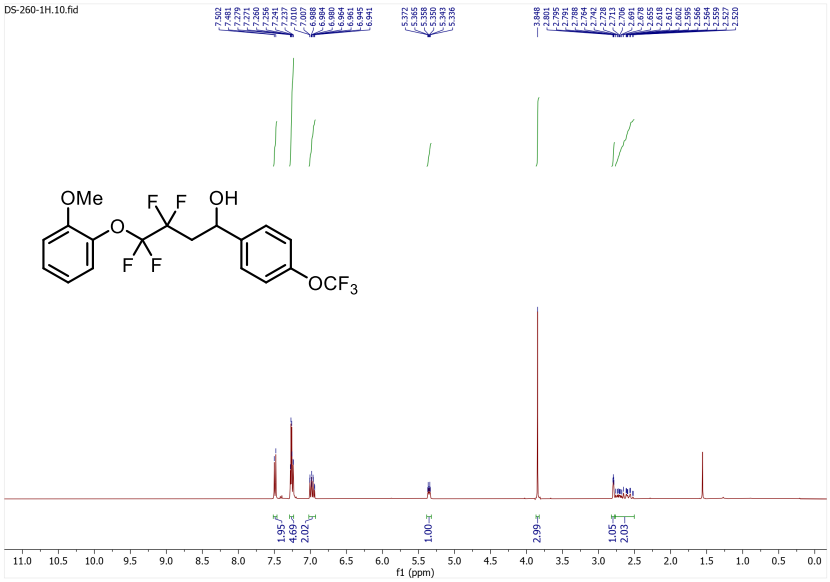
Compound 23. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

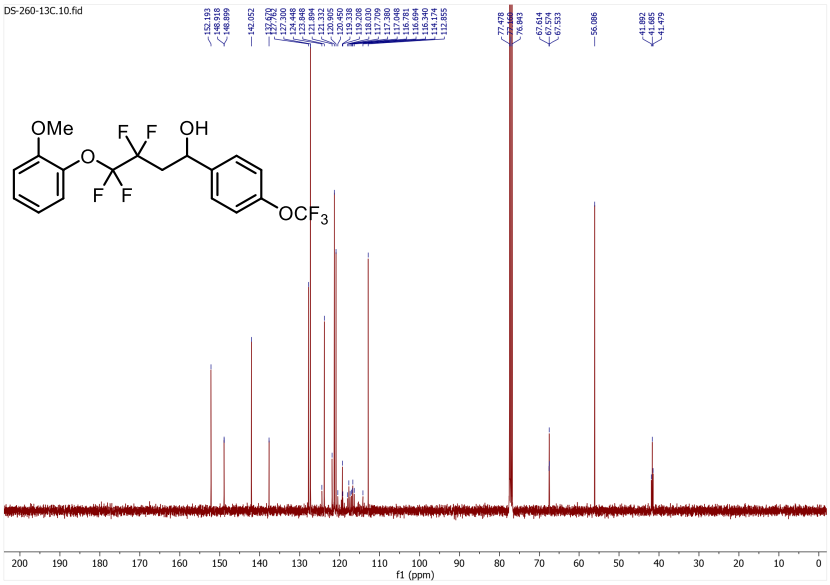


Compound 23. ^{19}F NMR ($CDCl_3$, 376 MHz)

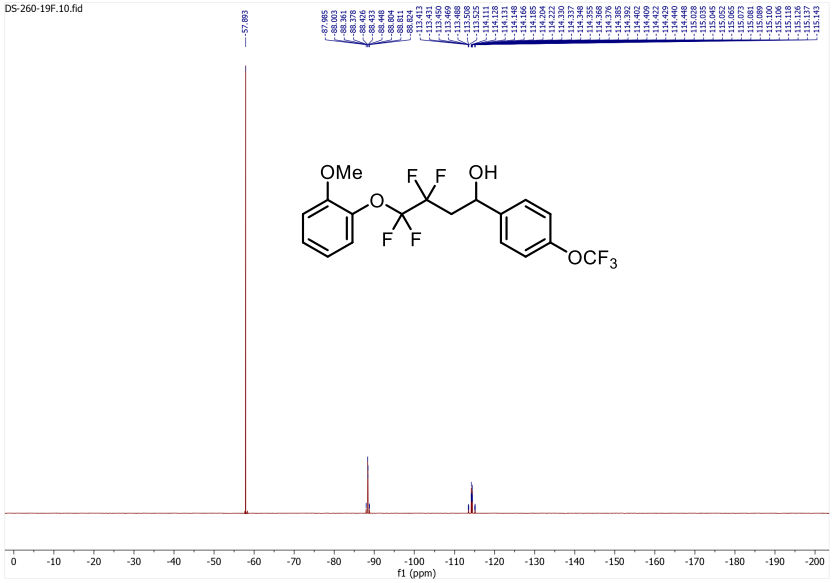


Compound 24. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

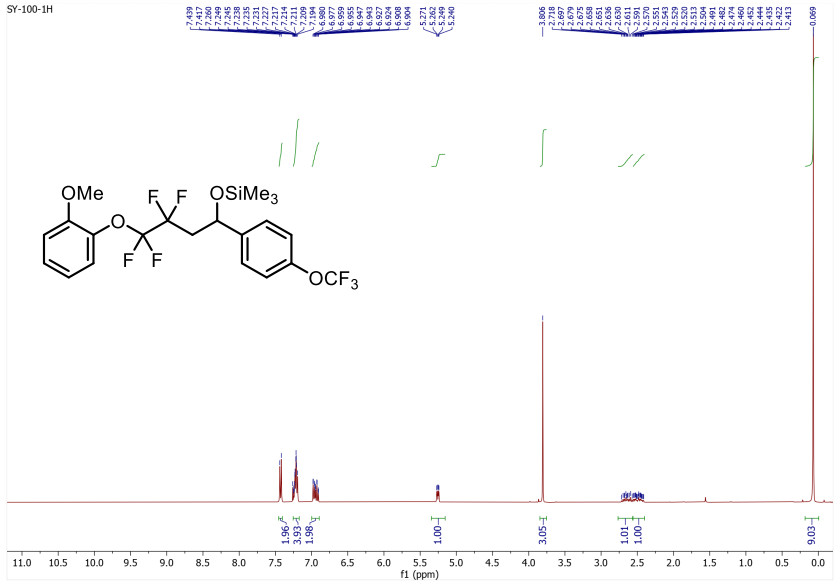


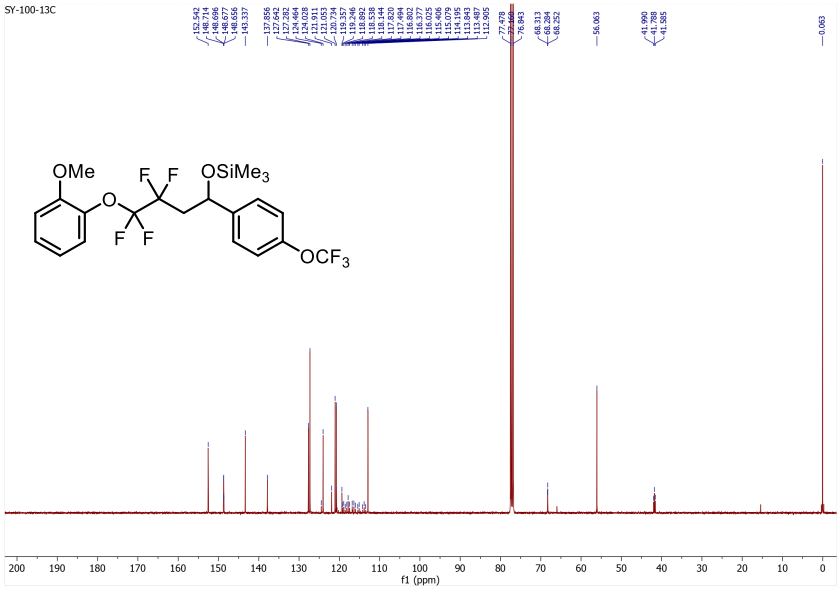


Compound 24. ^{19}F NMR ($CDCl_3$, 376 MHz)

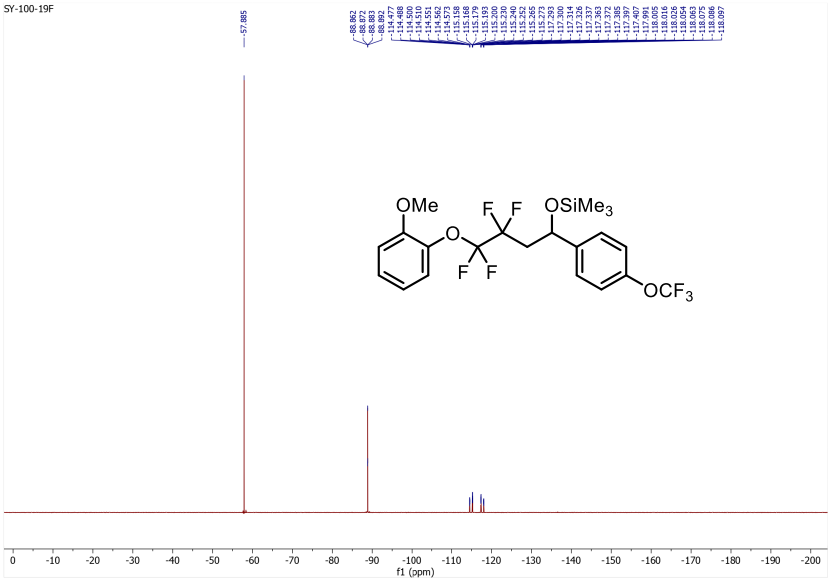


Compound 25. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

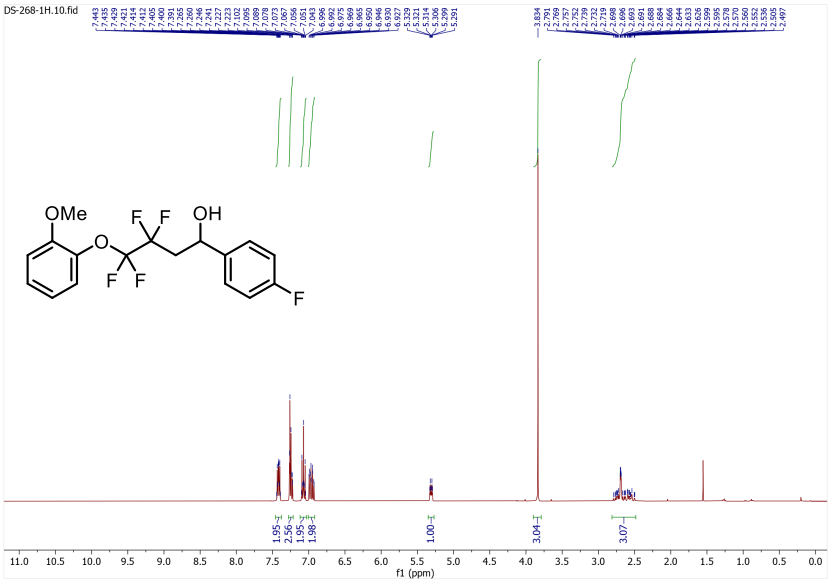


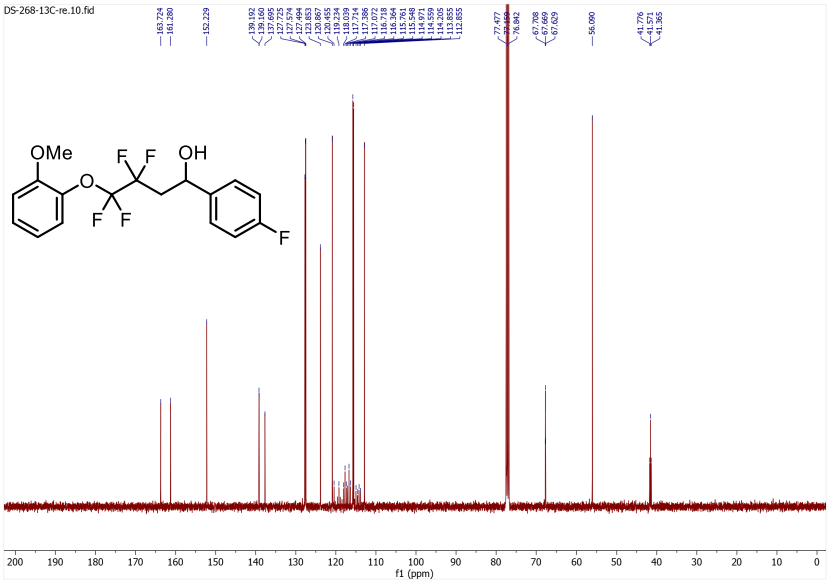


Compound 25. ^{19}F NMR ($CDCl_3$, 376 MHz)

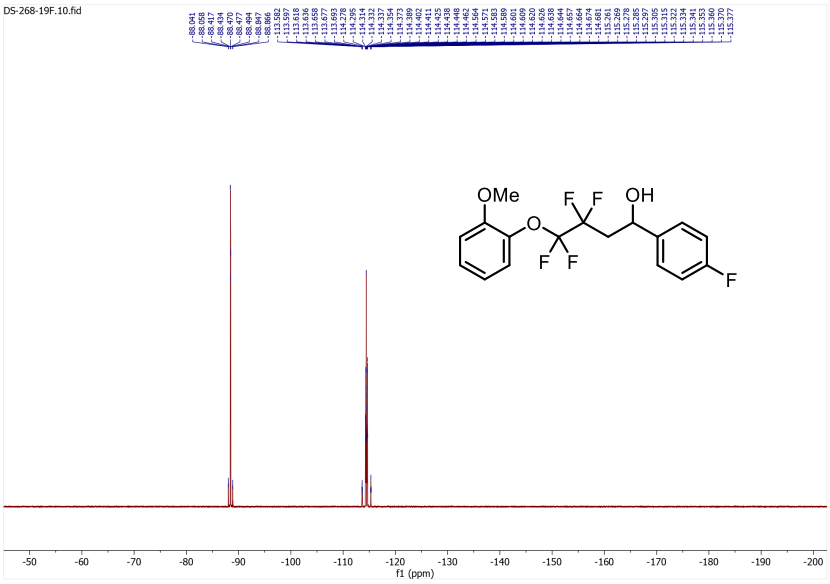


Compound 26. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

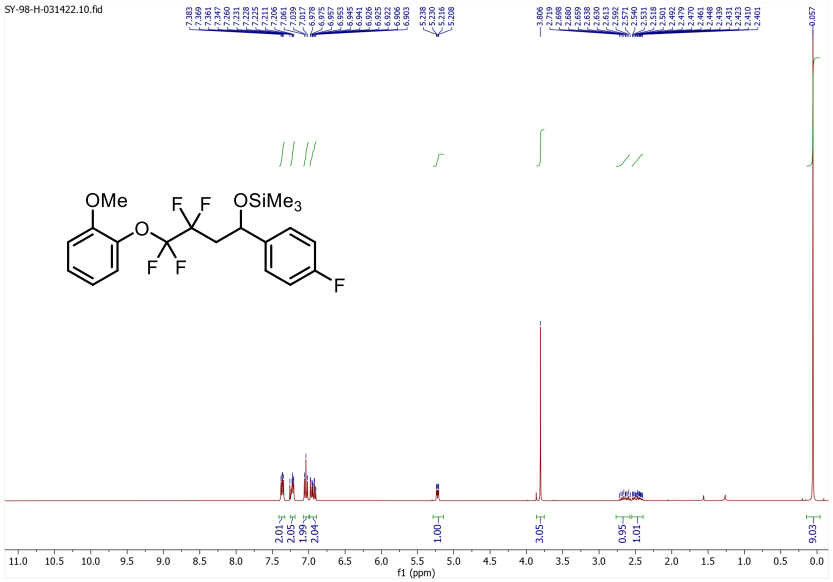


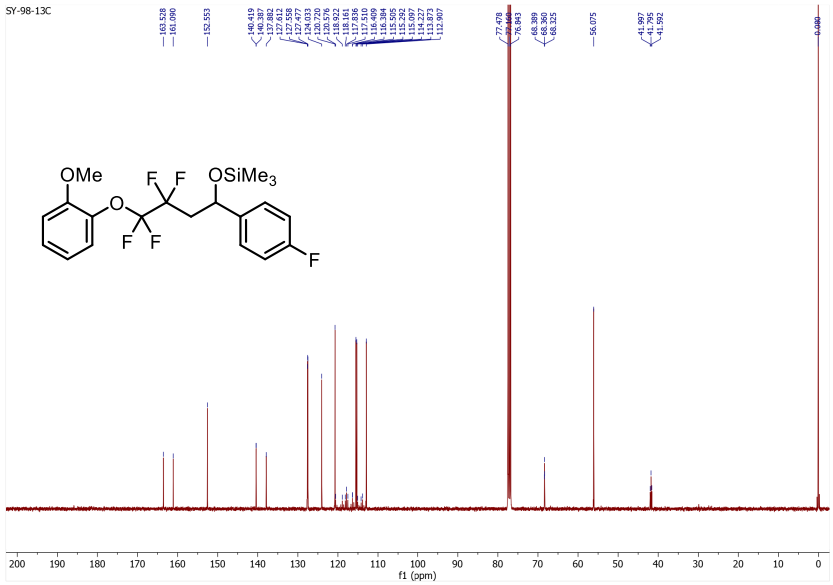


Compound 26. ^{19}F NMR ($CDCl_3$, 376 MHz)

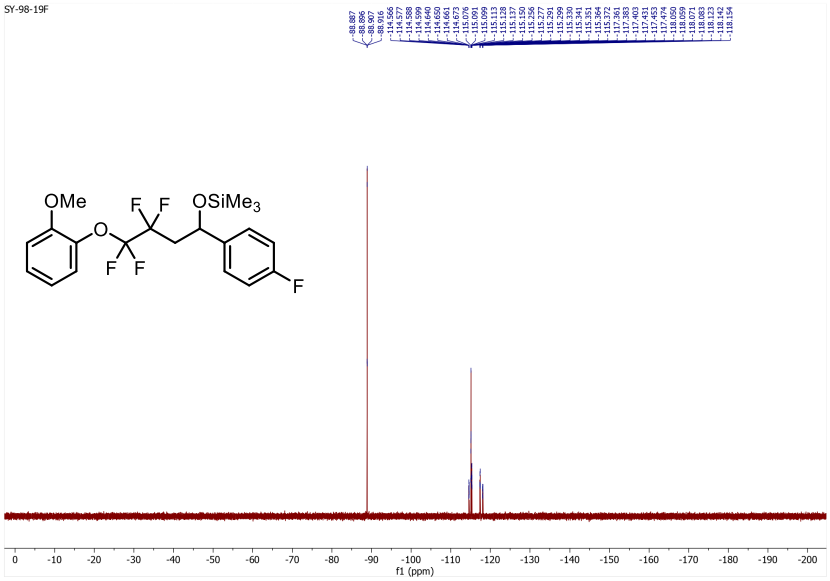


Compound 27. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

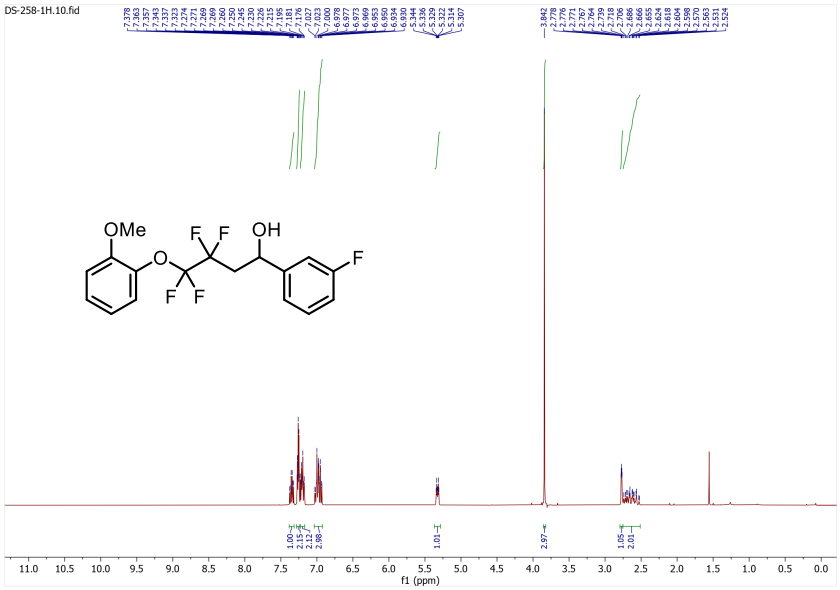


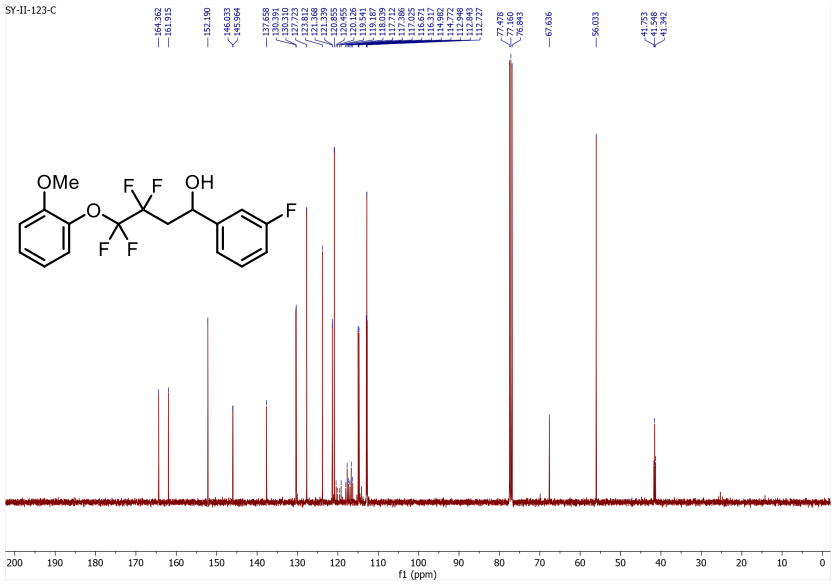


Compound 27. ^{19}F NMR ($CDCl_3$, 376 MHz)

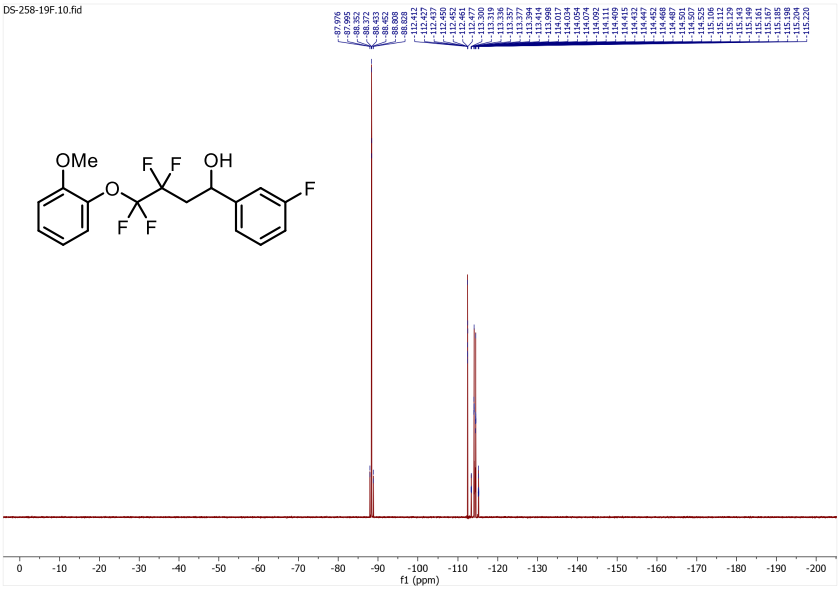


Compound 28. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

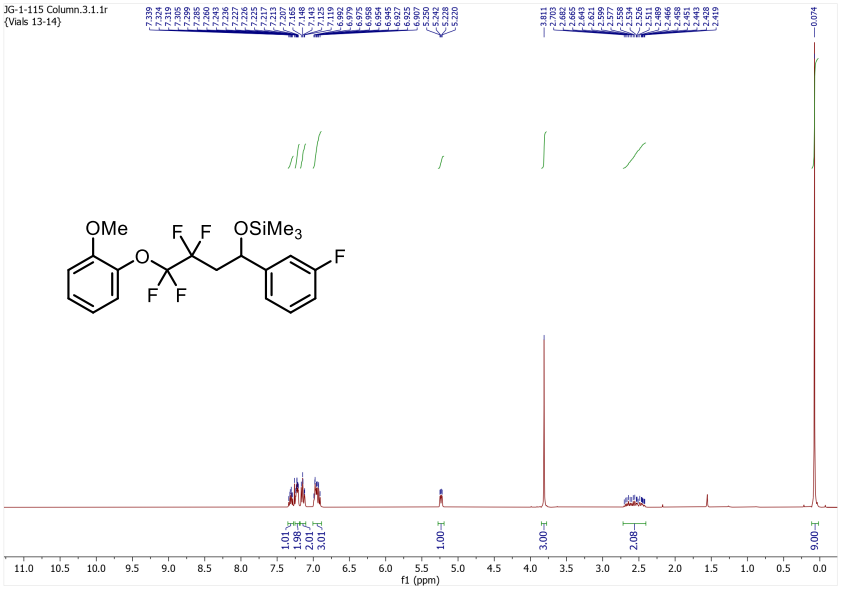


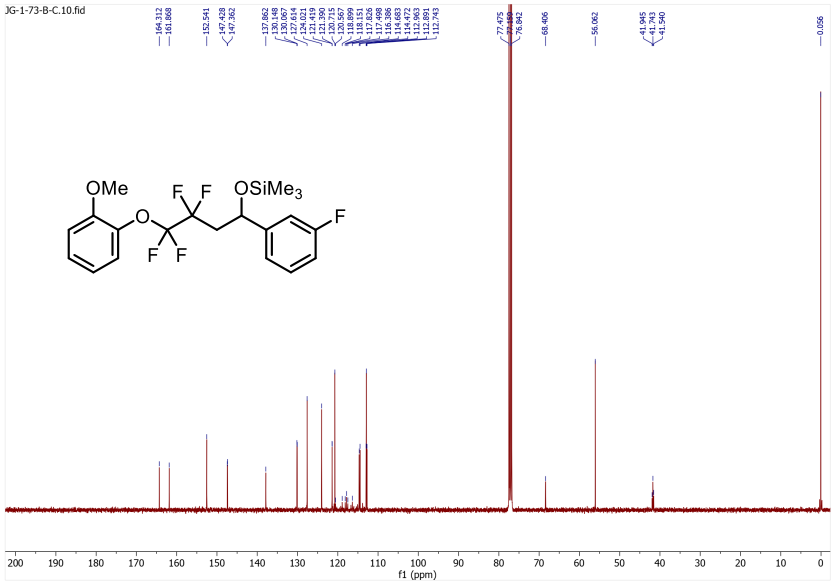


Compound 28. ^{19}F NMR ($CDCl_3$, 376 MHz)

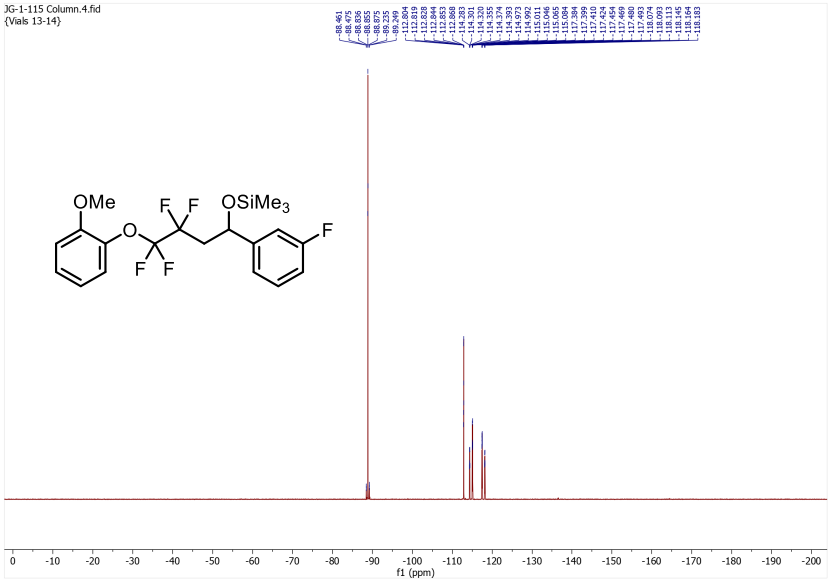


Compound 29. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

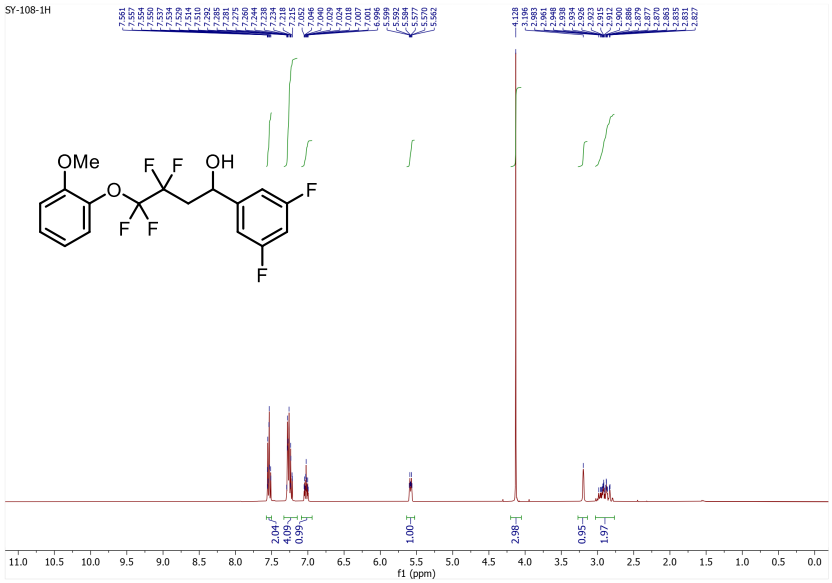


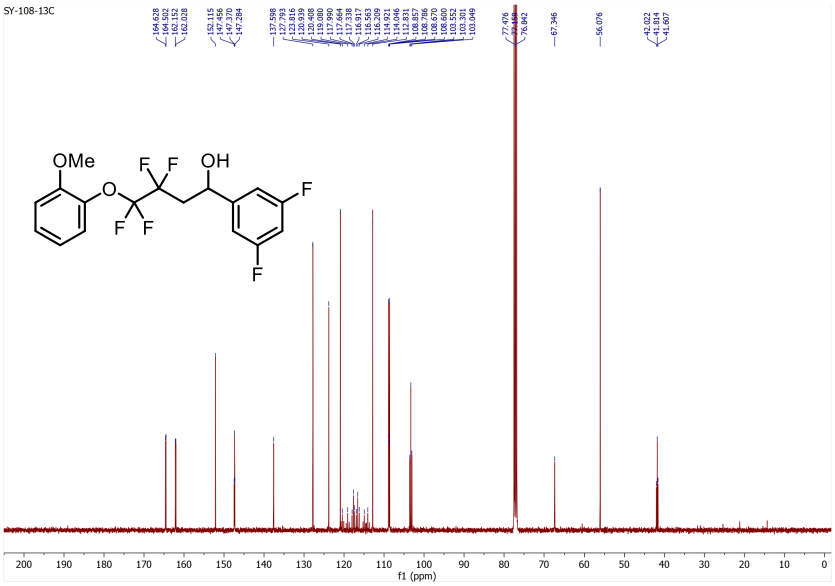


Compound 29. ^{19}F NMR ($CDCl_3$, 376 MHz)

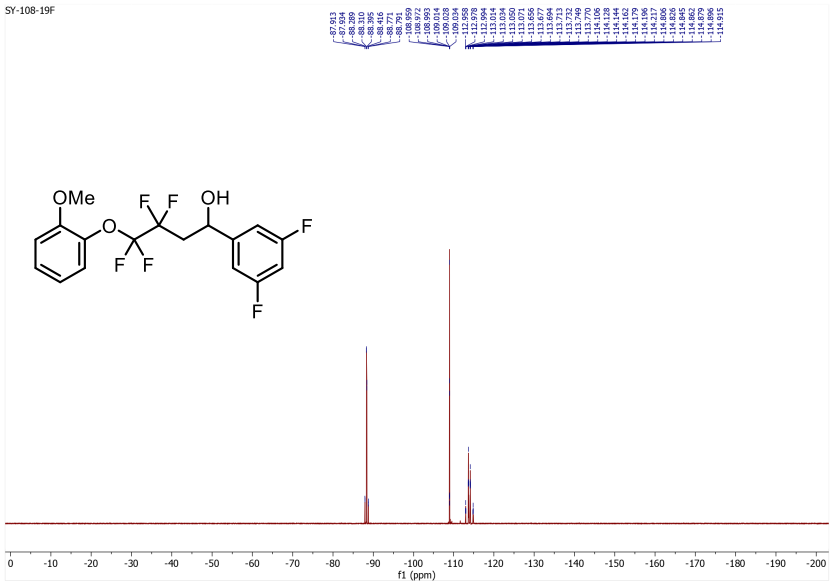


Compound 30. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

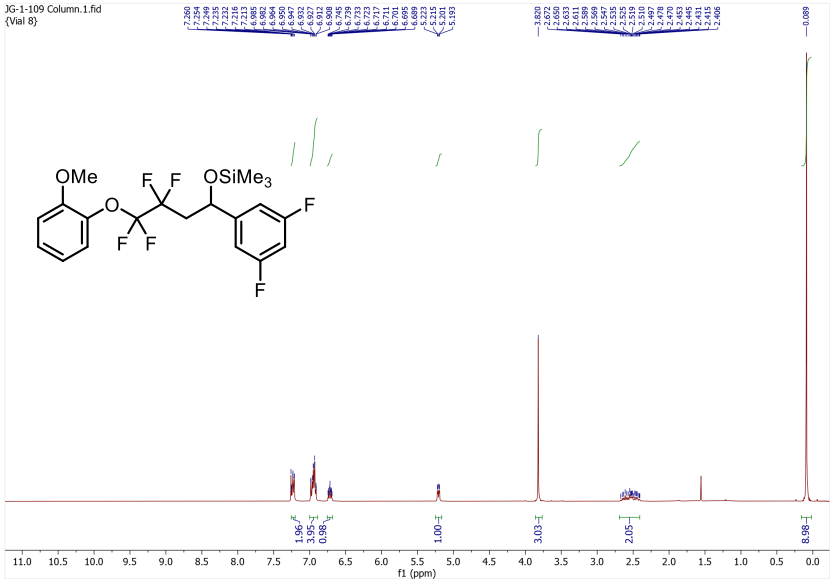


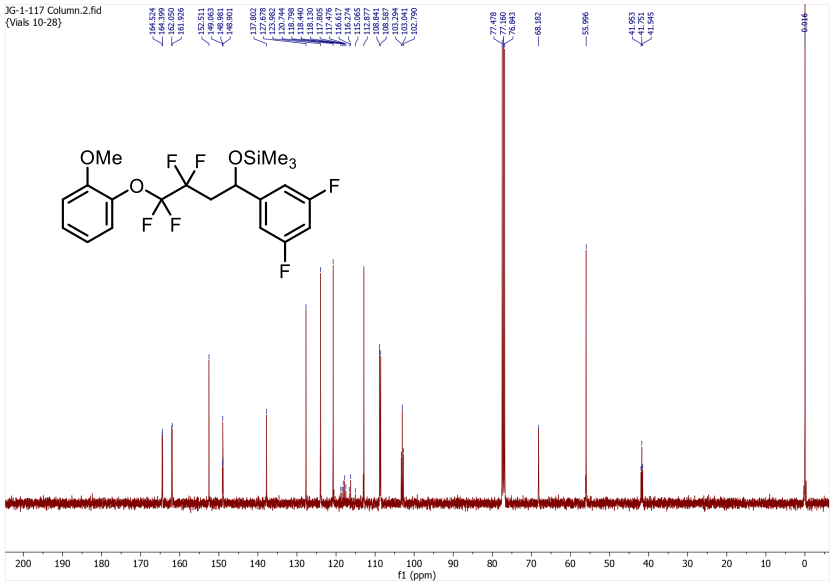


Compound 30. ^{19}F NMR ($CDCl_3$, 376 MHz)

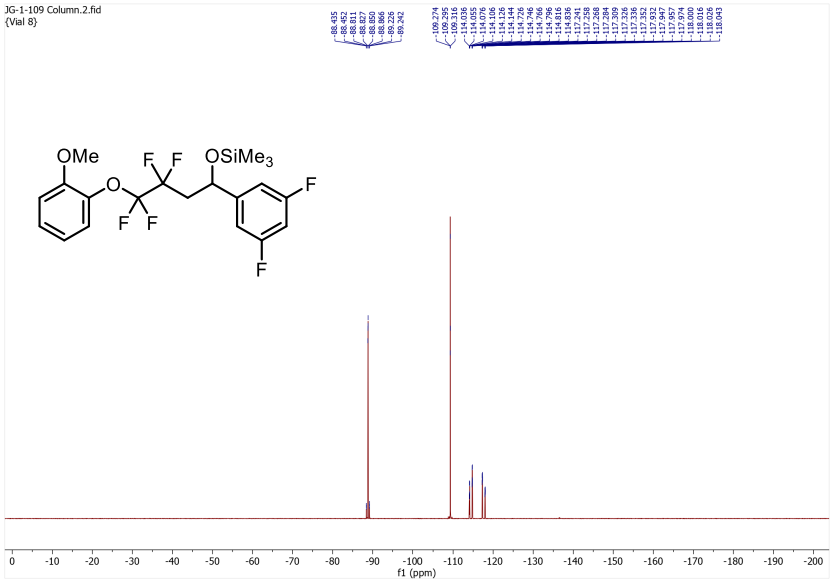


Compound 31. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

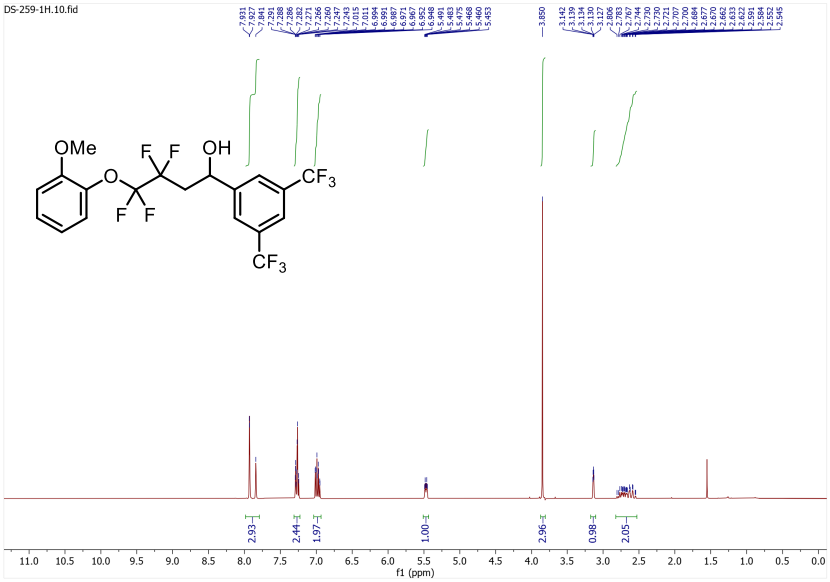


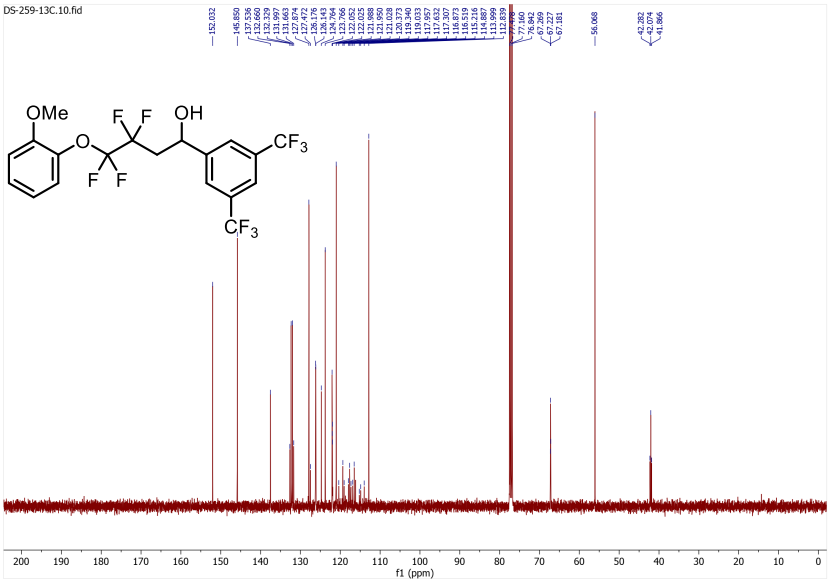


Compound 31. ^{19}F NMR ($CDCl_3$, 376 MHz)

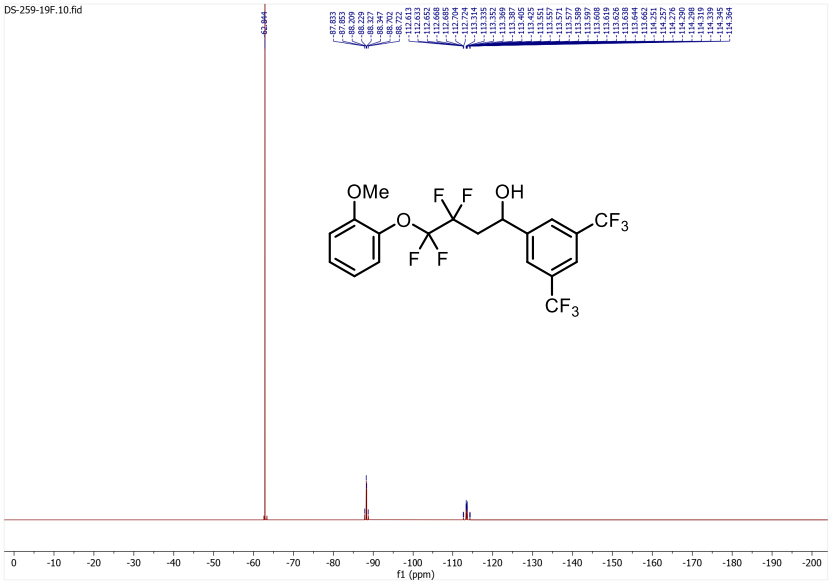


Compound 32. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

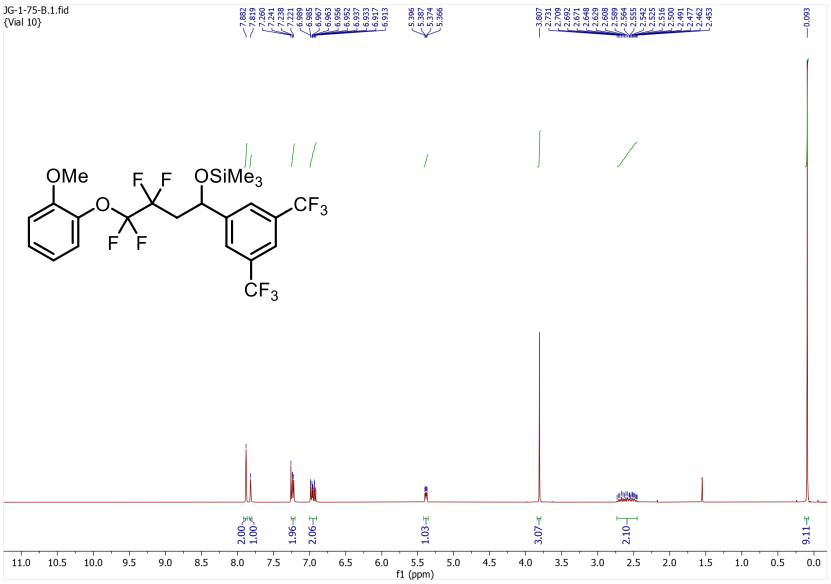


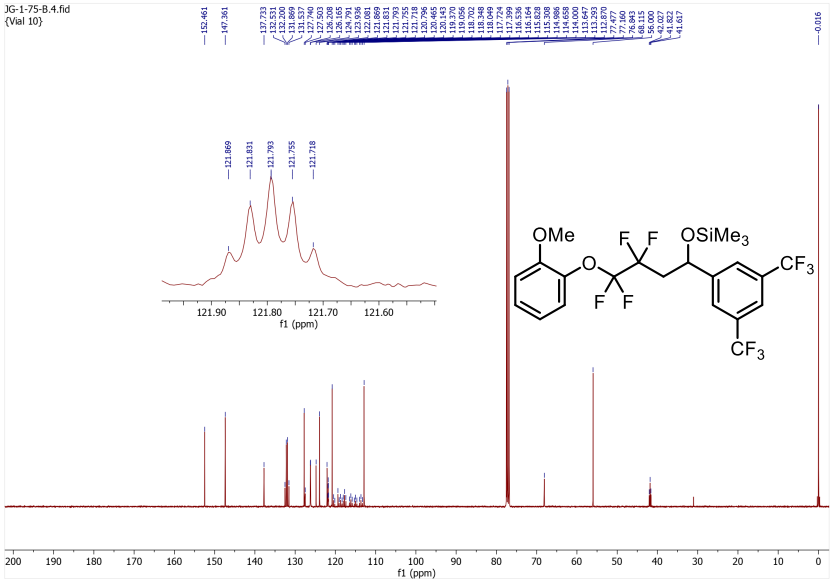


Compound 32. ^{19}F NMR ($CDCl_3$, 376 MHz)

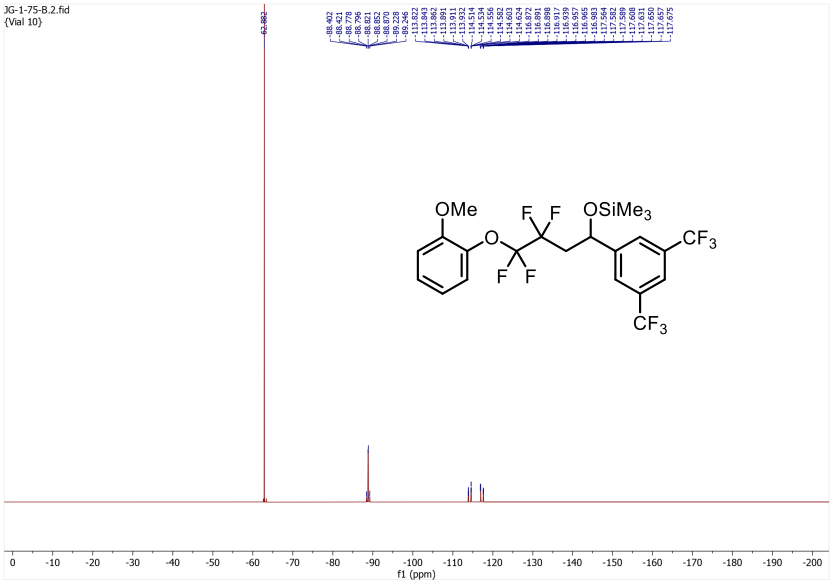


Compound 33. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

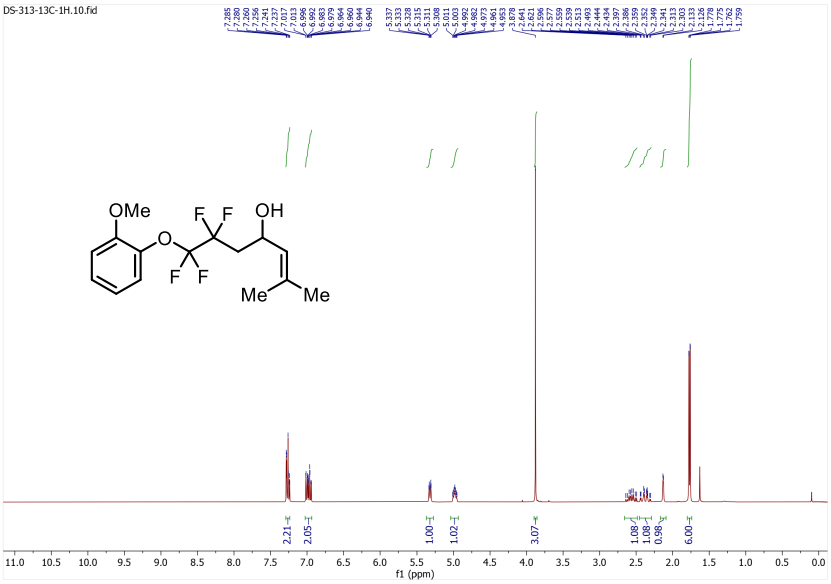


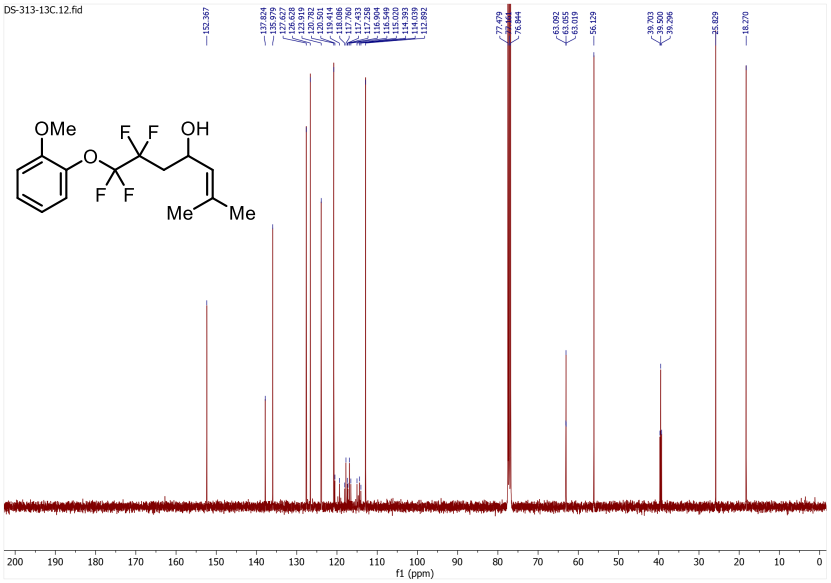


Compound 33. ^{19}F NMR ($CDCl_3$, 376 MHz)

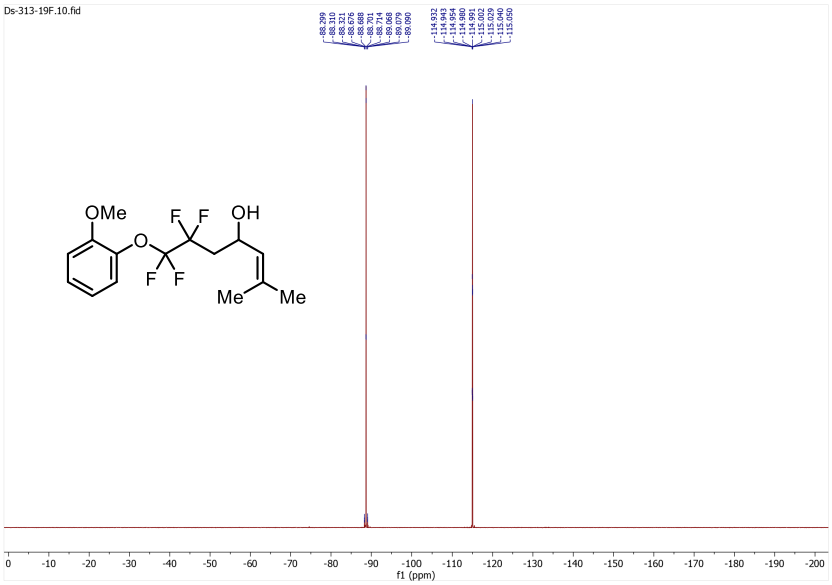


Compound 34. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

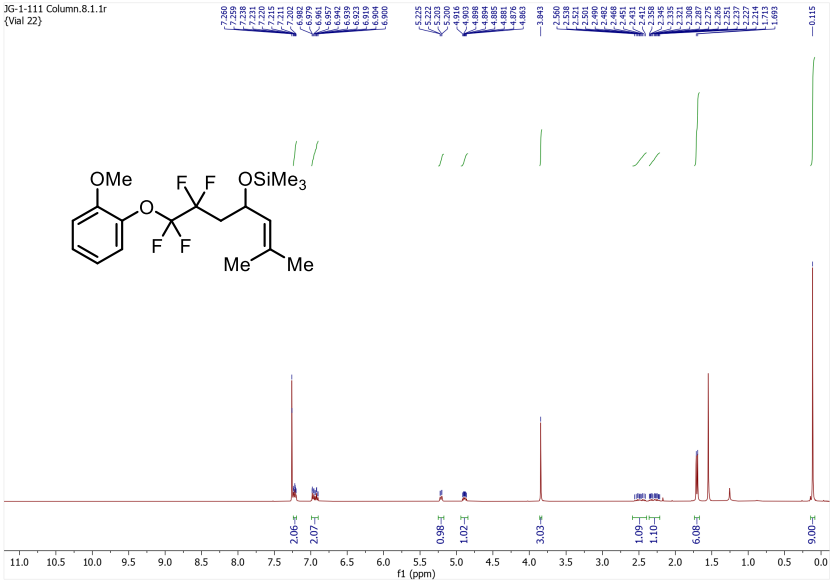


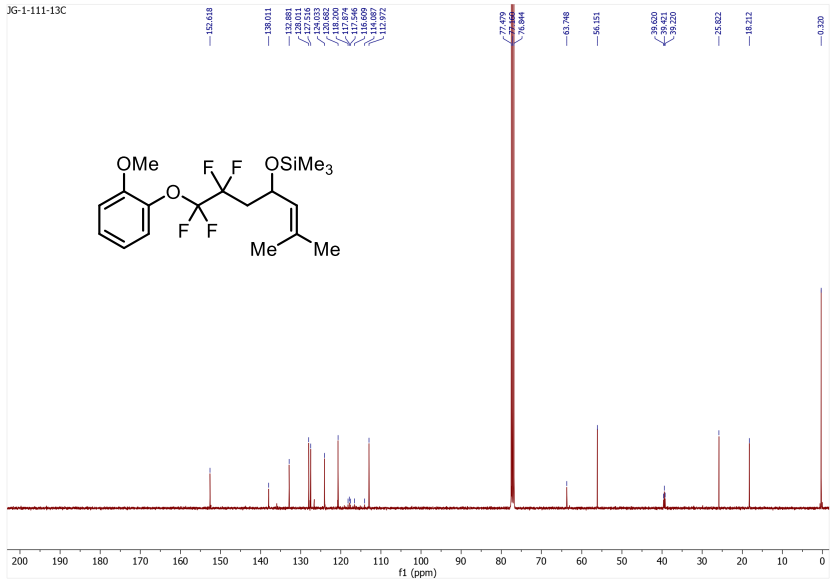


Compound 34. ^{19}F NMR ($CDCl_3$, 376 MHz)

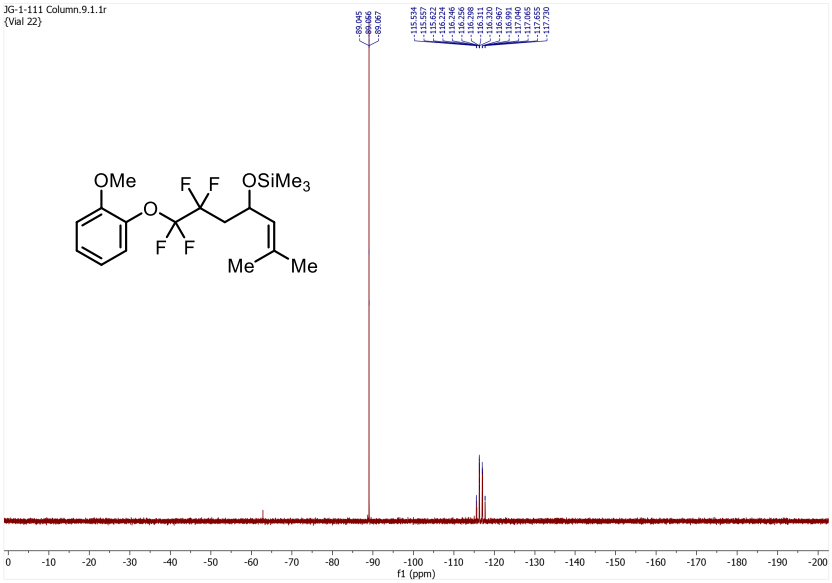


Compound 35. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

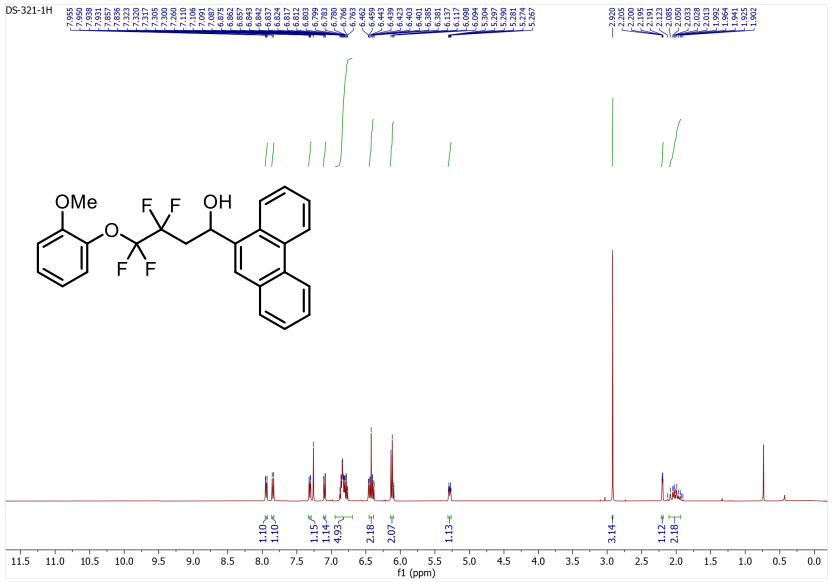


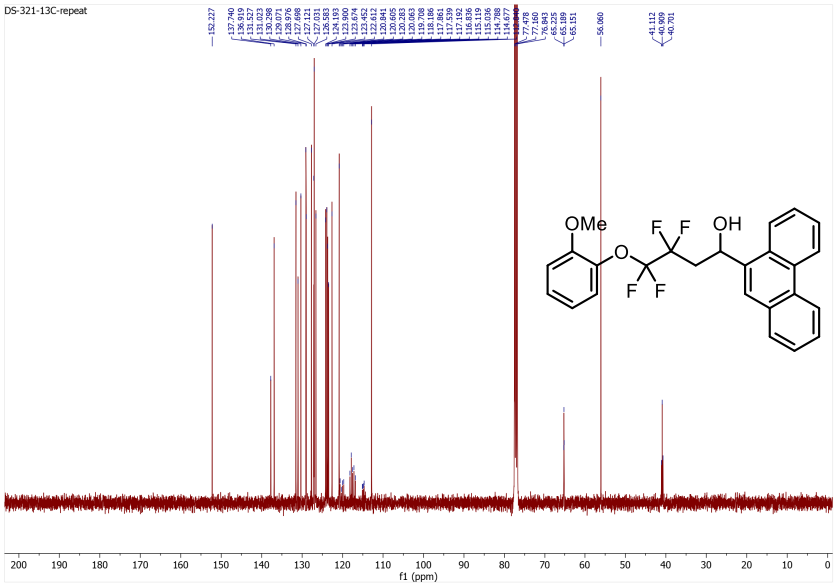


Compound 35. ^{19}F NMR ($CDCl_3$, 376 MHz)

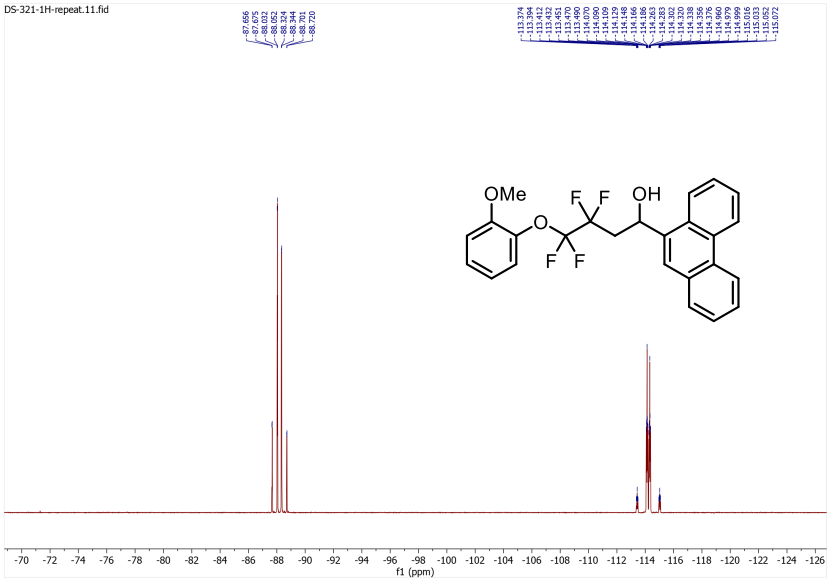


Compound 36. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

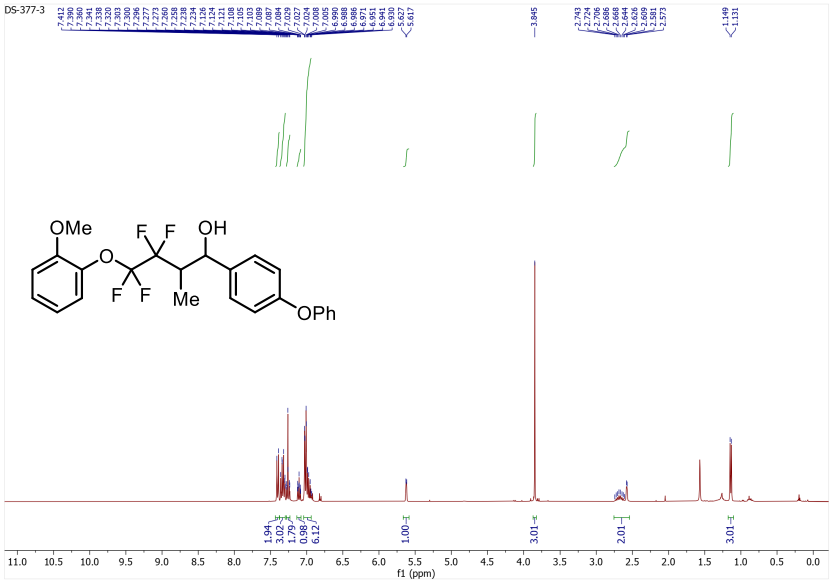


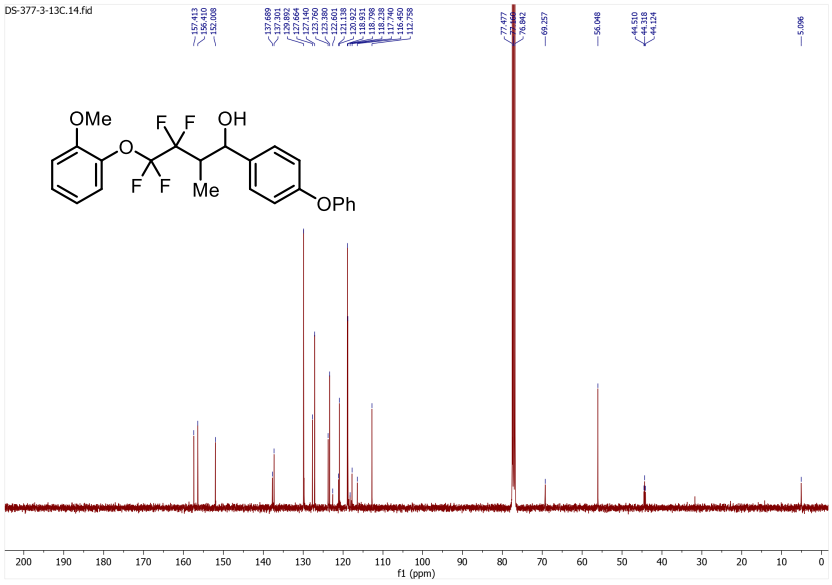


Compound 36. ^{19}F NMR ($CDCl_3$, 376 MHz)

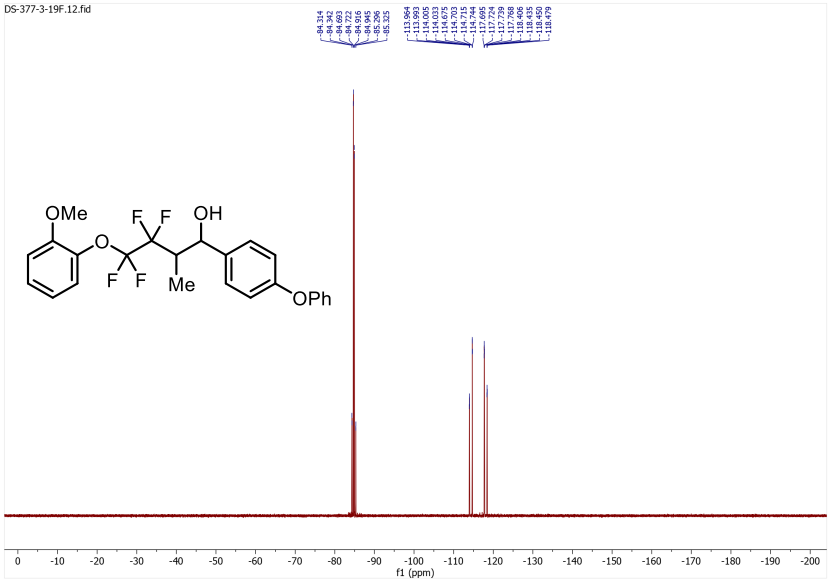


Compound 37. Top: (major) ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

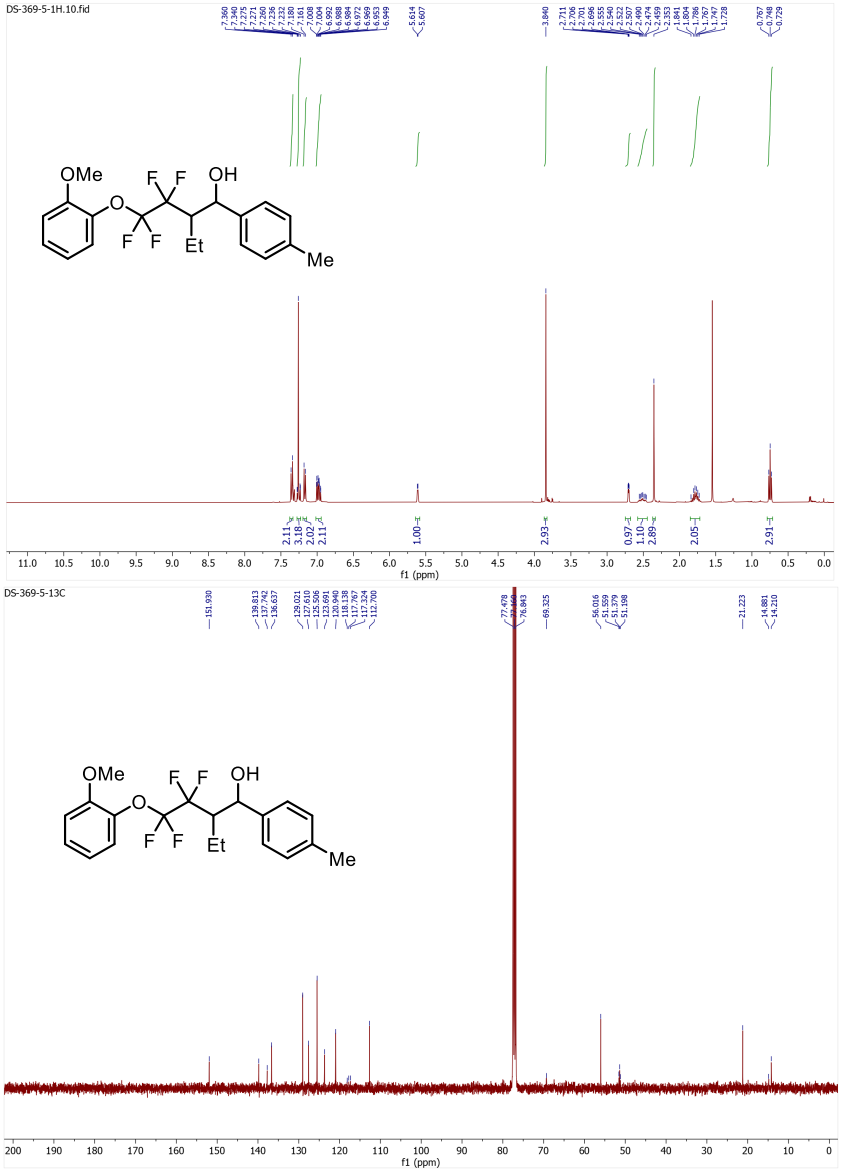




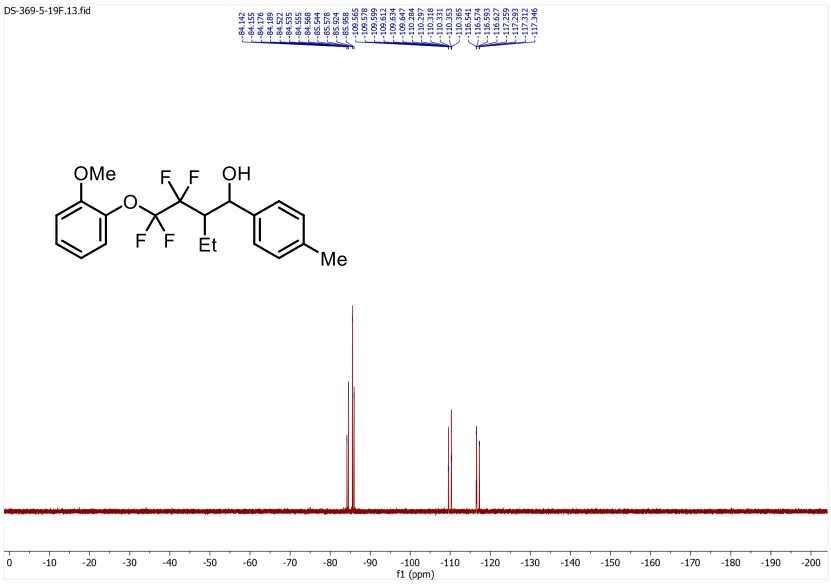
Compound 37. (major) ^{19}F NMR ($CDCl_3$, 376 MHz)



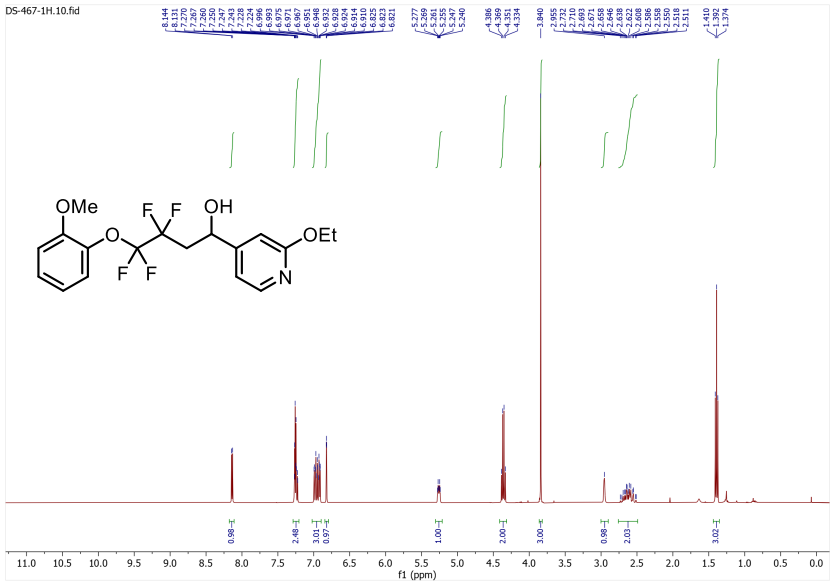
Compound 38. Top: (major) ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

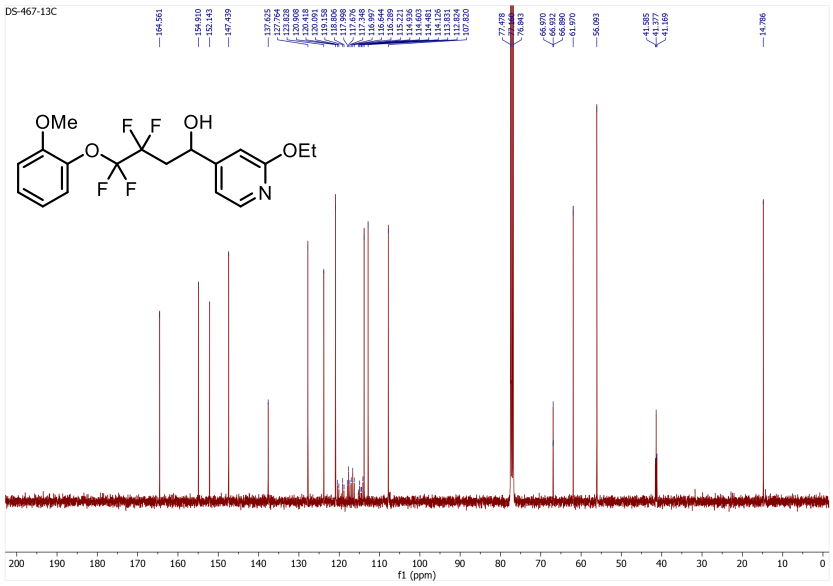


Compound 38. (major) ^{19}F NMR ($CDCl_3$, 376 MHz)

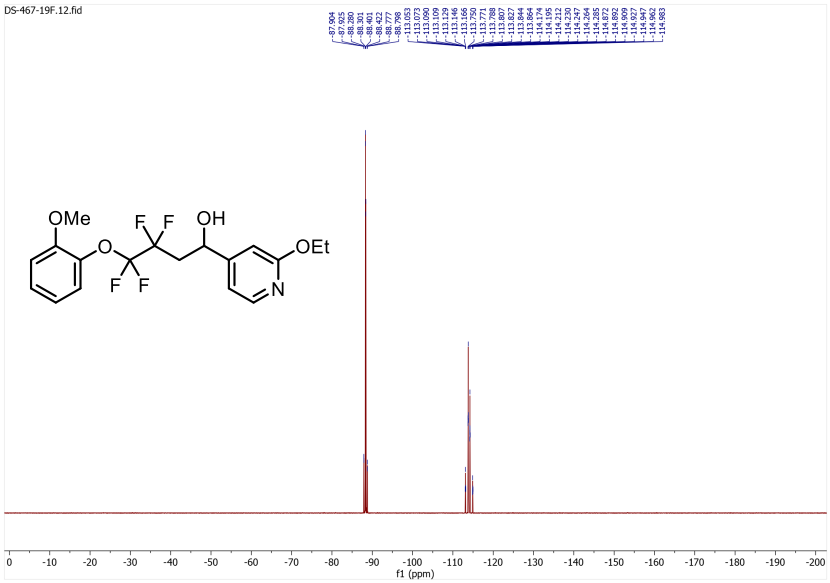


Compound 39. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

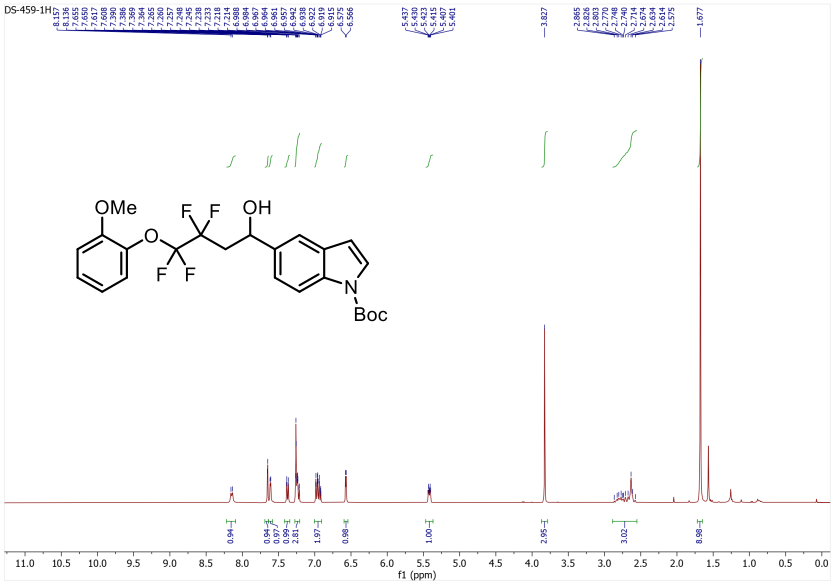


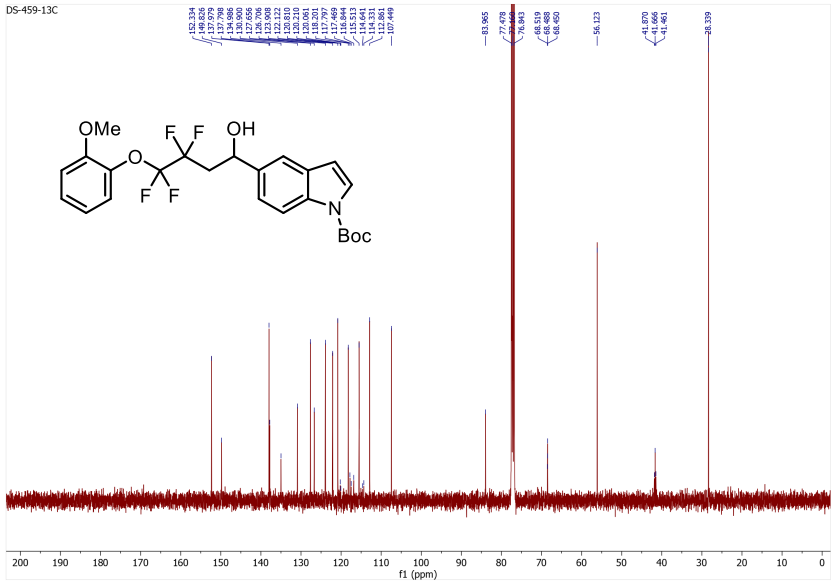


Compound 39. ^{19}F NMR ($CDCl_3$, 376 MHz)

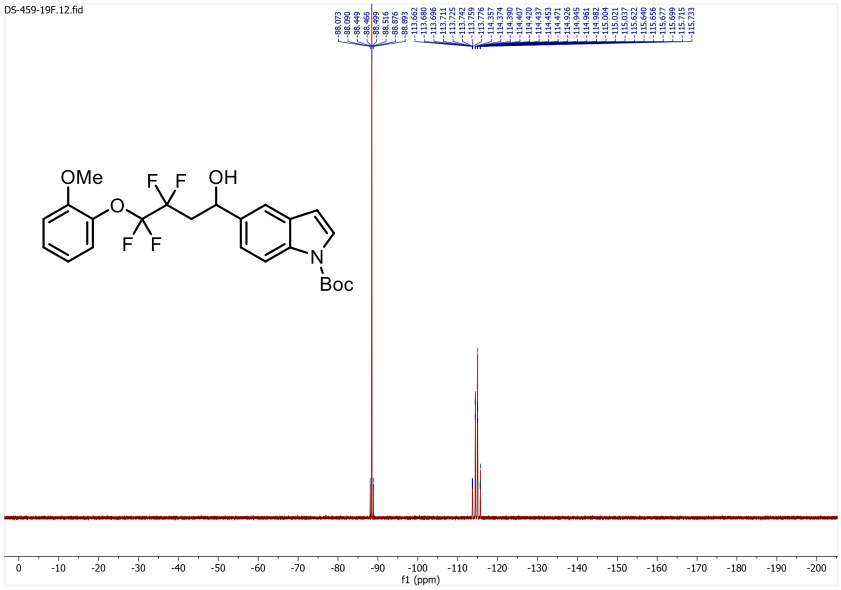


Compound 40. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

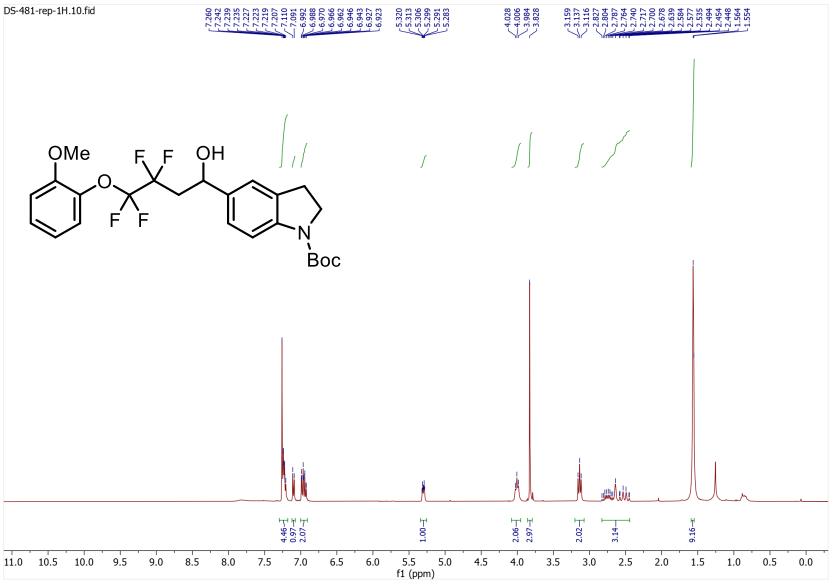


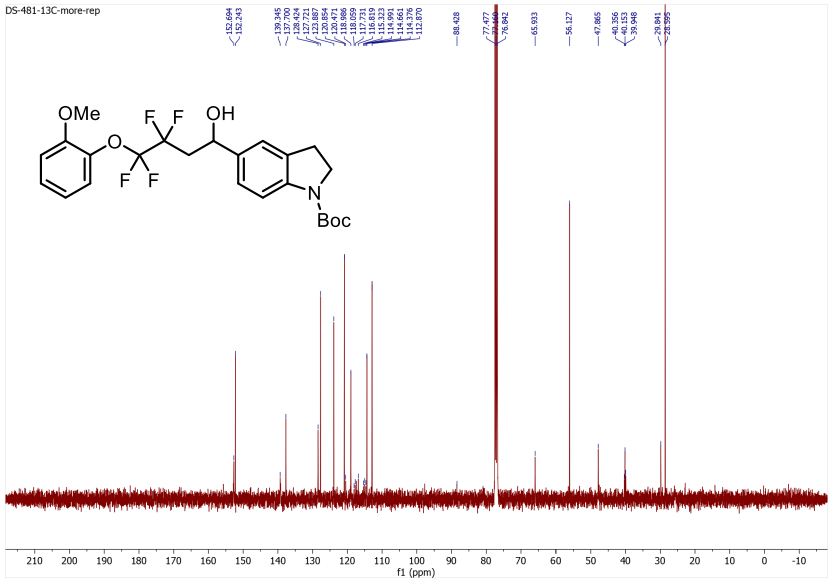


Compound 40. ^{19}F NMR ($CDCl_3$, 376 MHz)

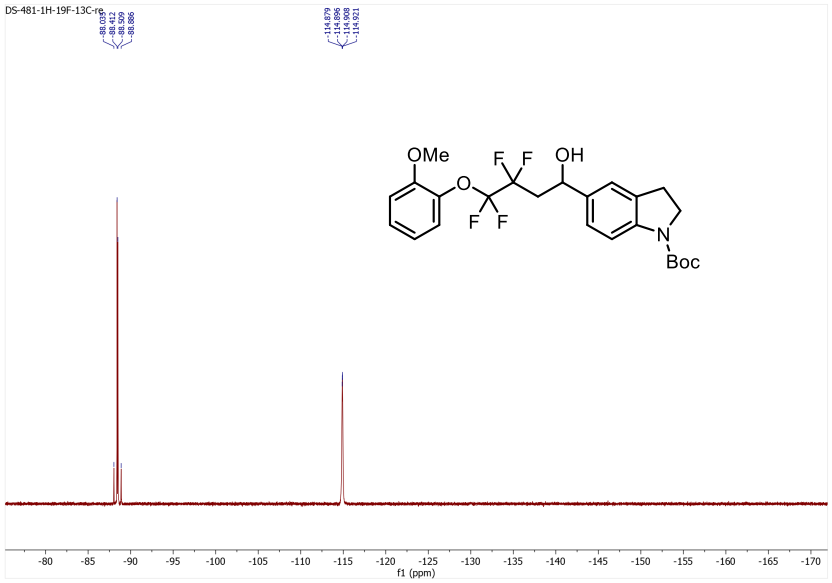


Compound 41. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

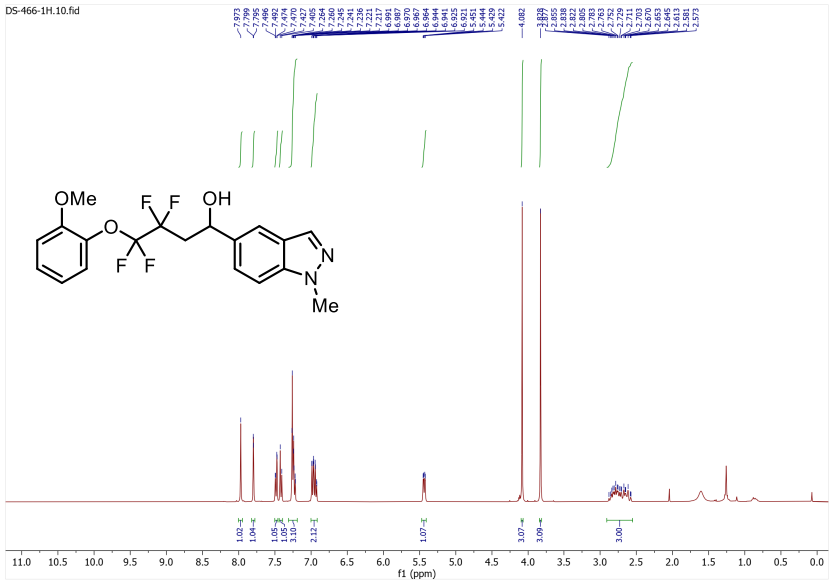


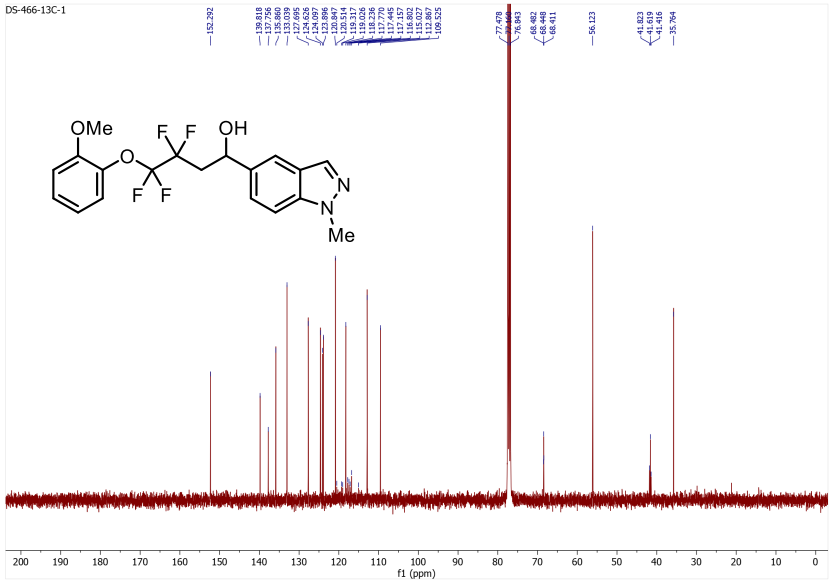


Compound 41. ^{19}F NMR ($CDCl_3$, 376 MHz)

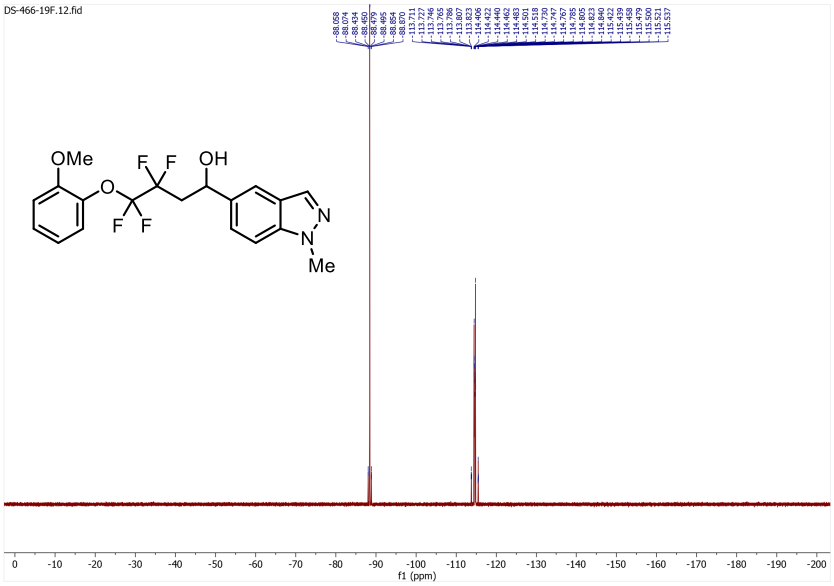


Compound 42. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

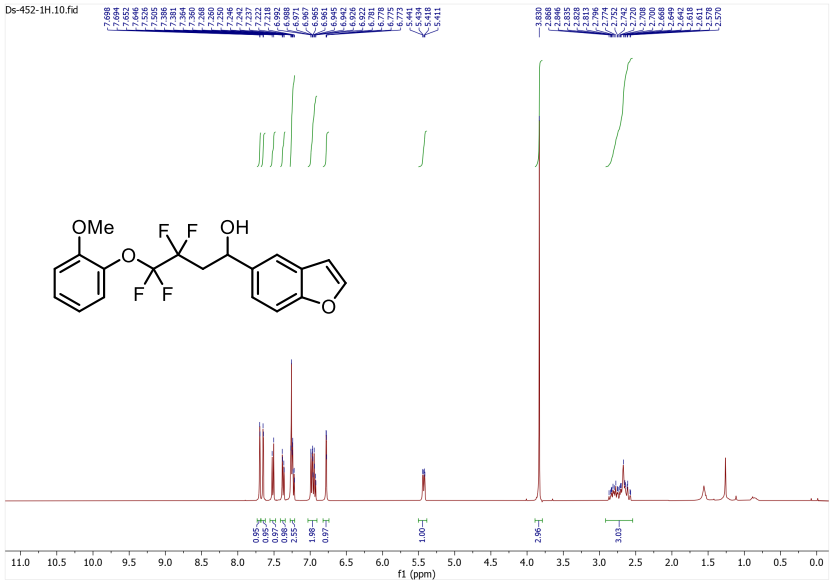


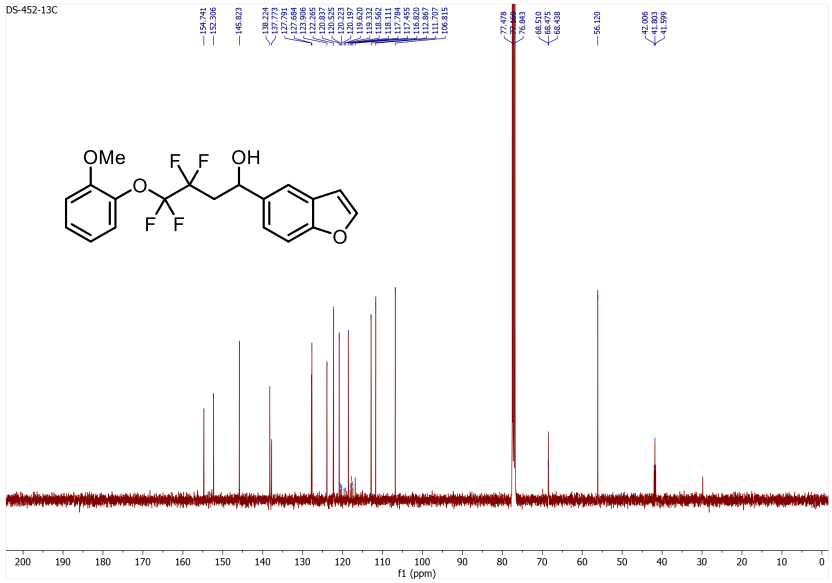


Compound 42. ^{19}F NMR ($CDCl_3$, 376 MHz)

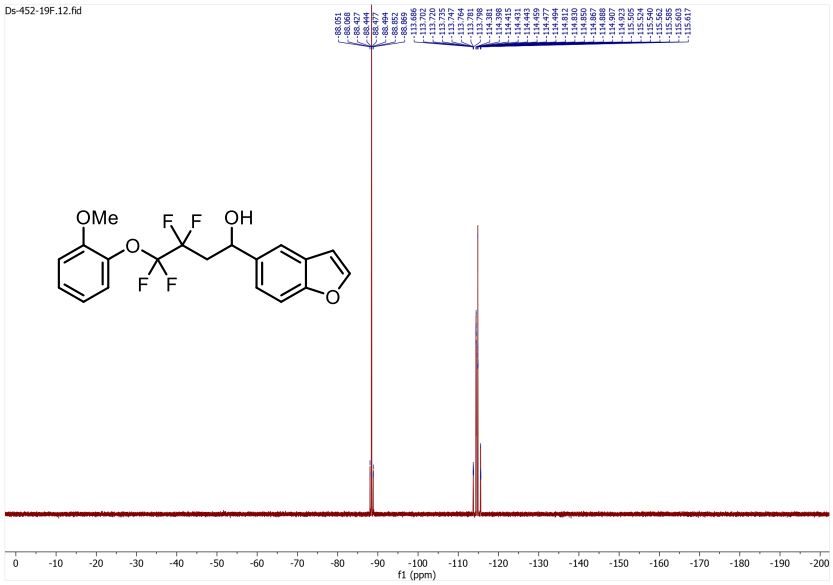


Compound 43. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

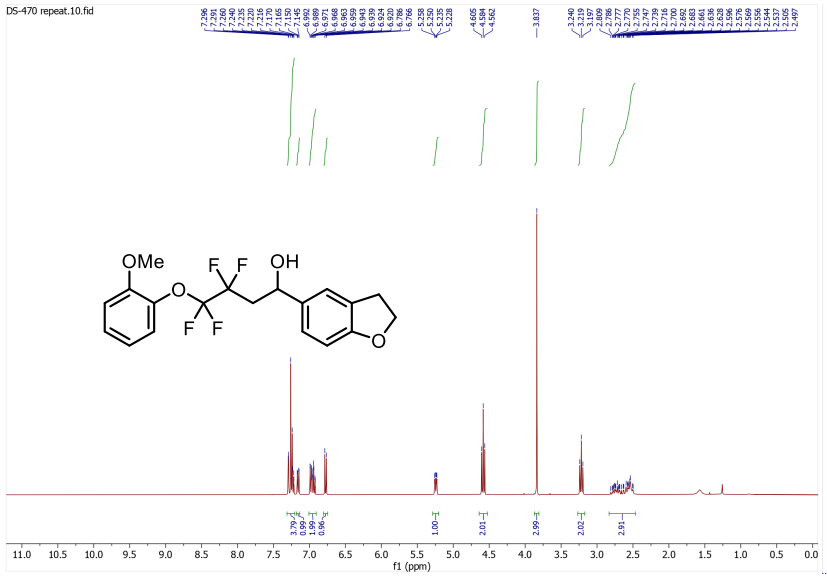


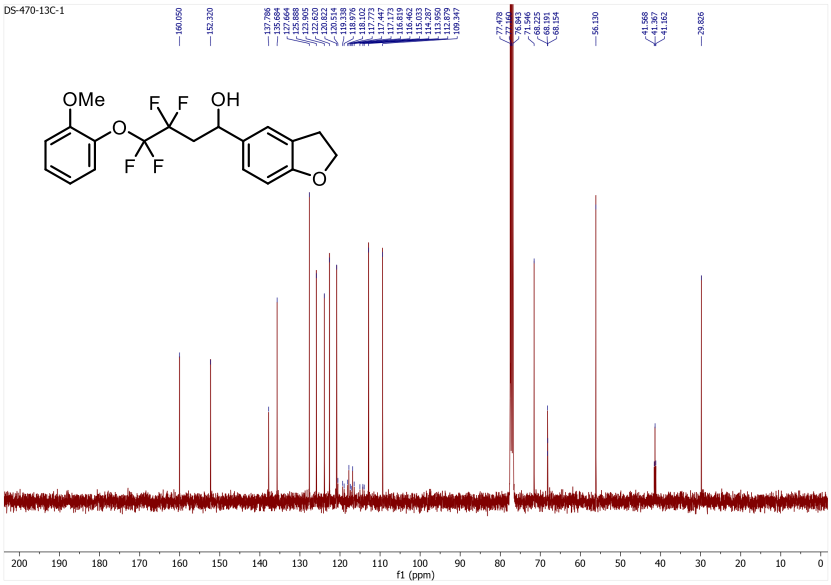


Compound 43. ^{19}F NMR ($CDCl_3$, 376 MHz)



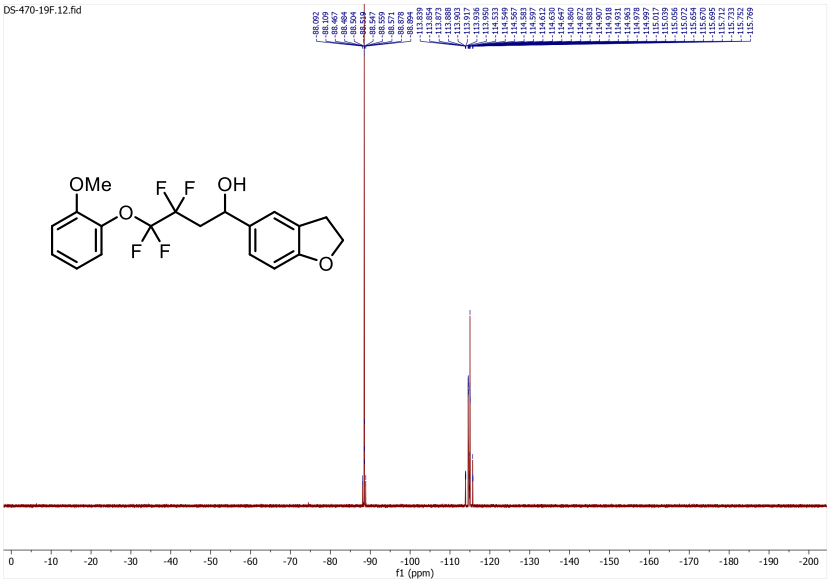
Compound 44. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)



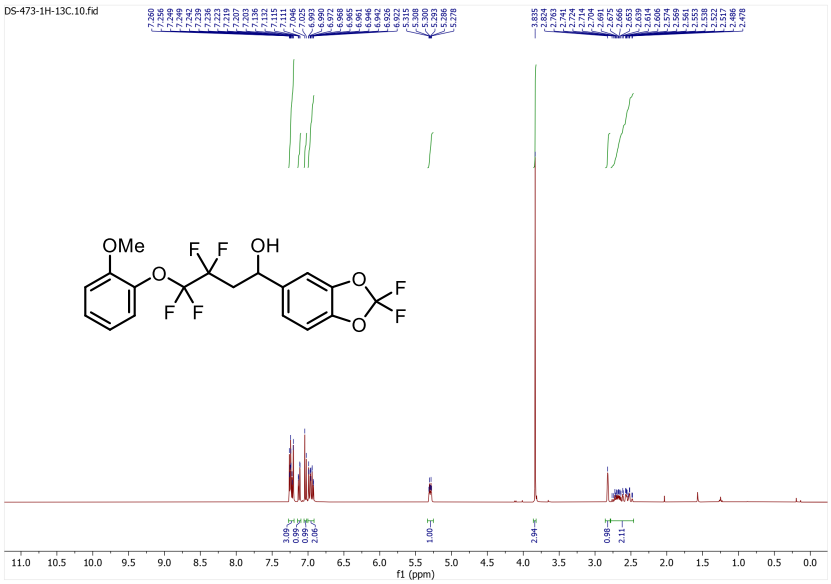


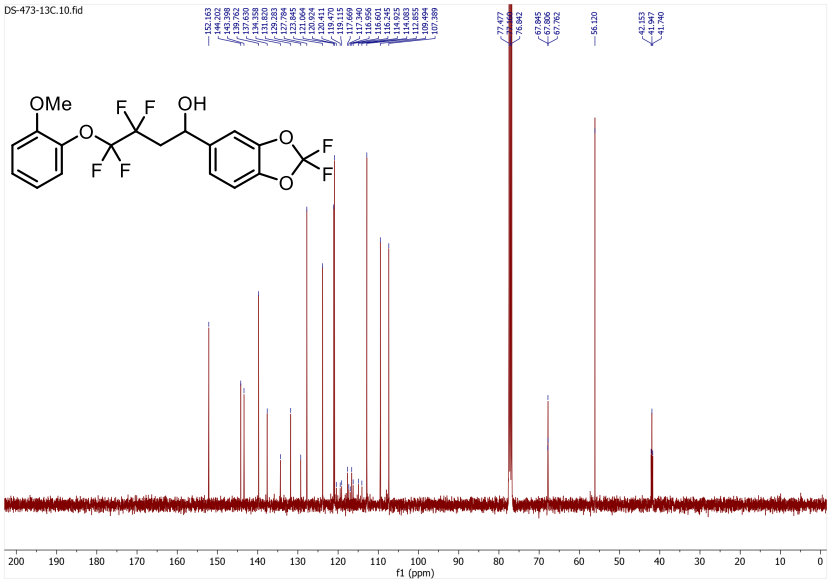
Commented [DS8]: Changed spectra

Compound 44. ^{19}F NMR ($CDCl_3$, 376 MHz)

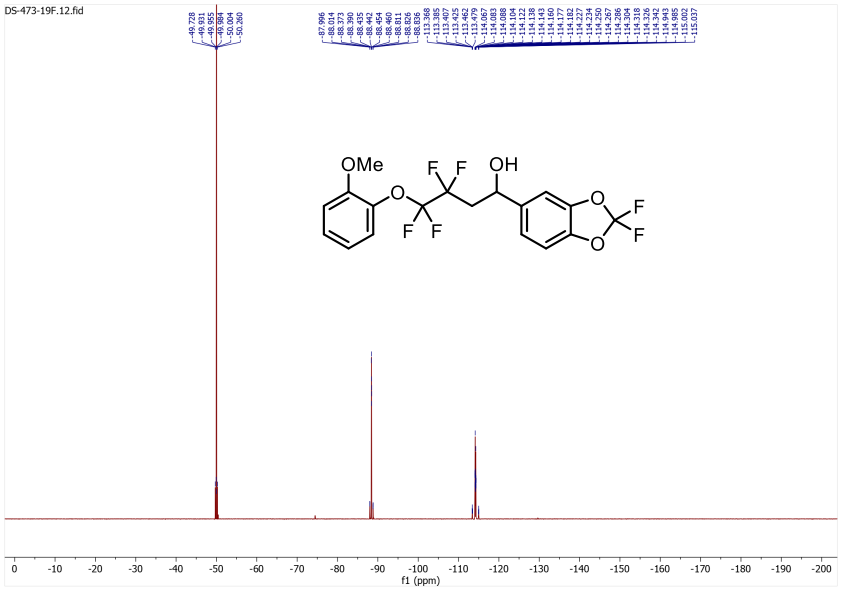


Compound 45. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

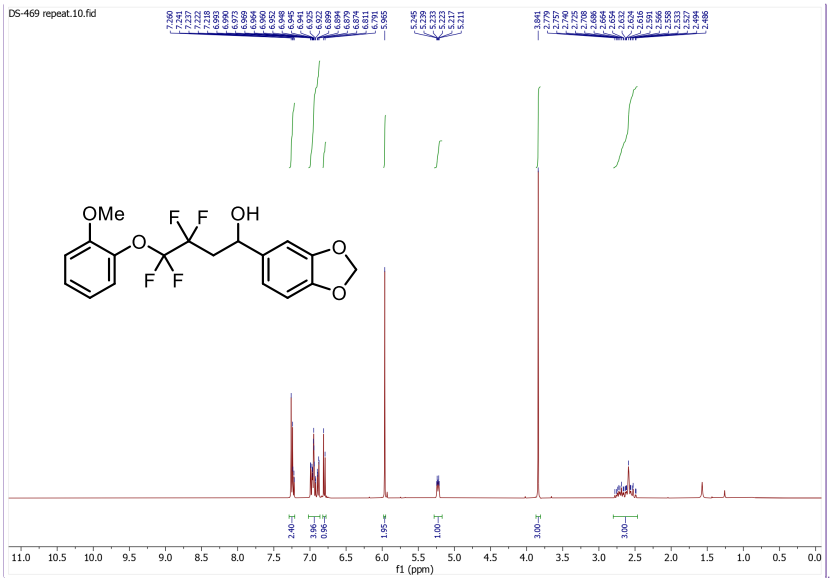


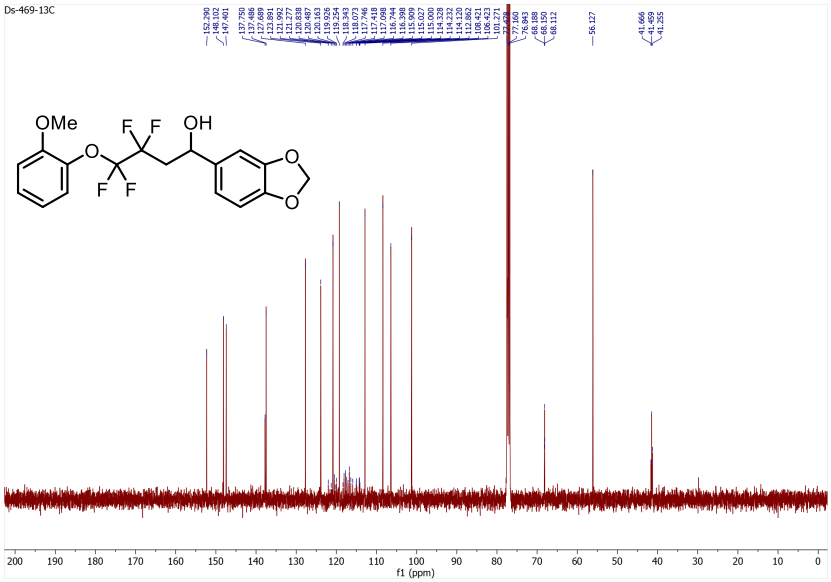


Compound 45. ^{19}F NMR ($CDCl_3$, 376 MHz)



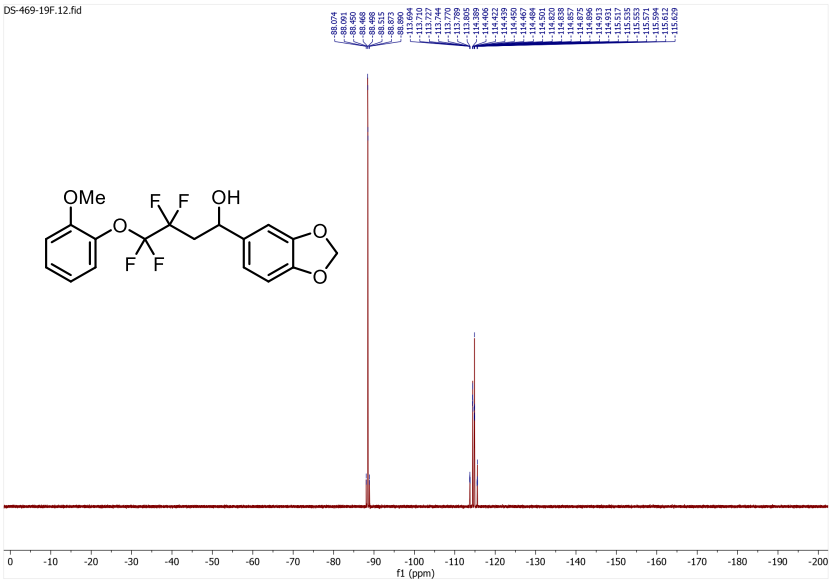
Compound 46. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)



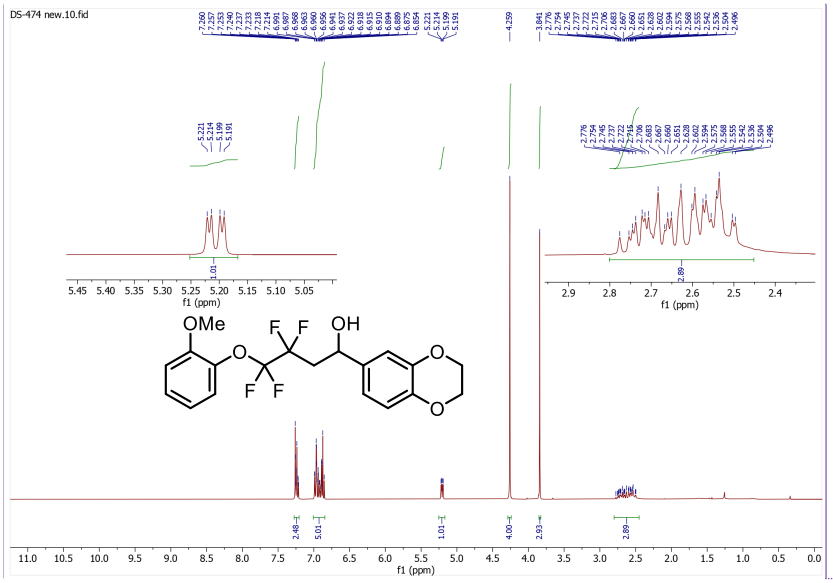


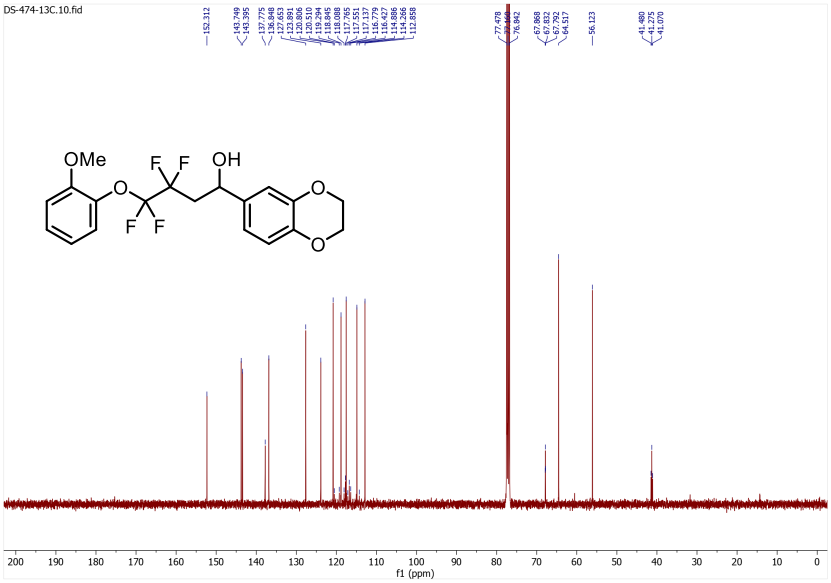
Commented [DS9]: Changed the spectra

Compound 46. ^{19}F NMR ($CDCl_3$, 376 MHz)



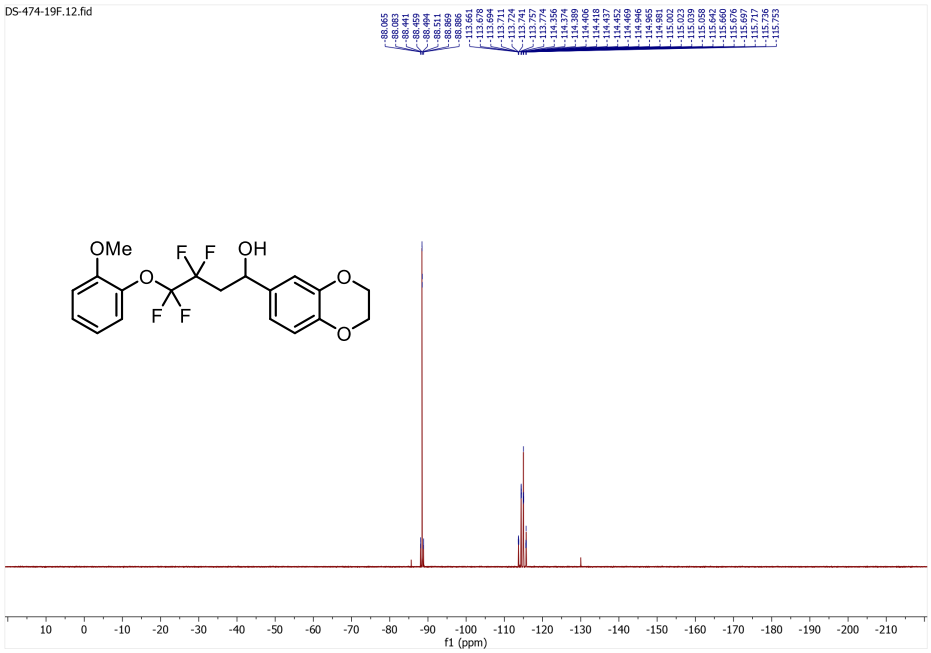
Compound 47. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)



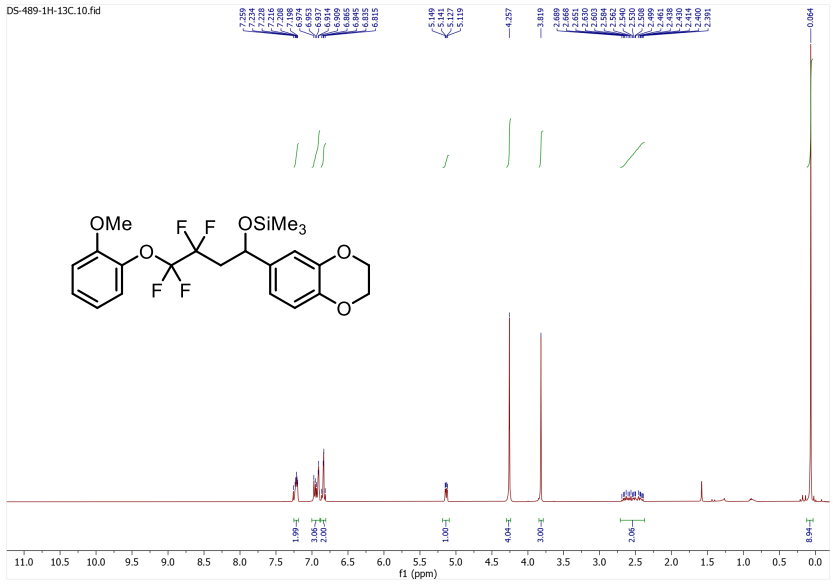


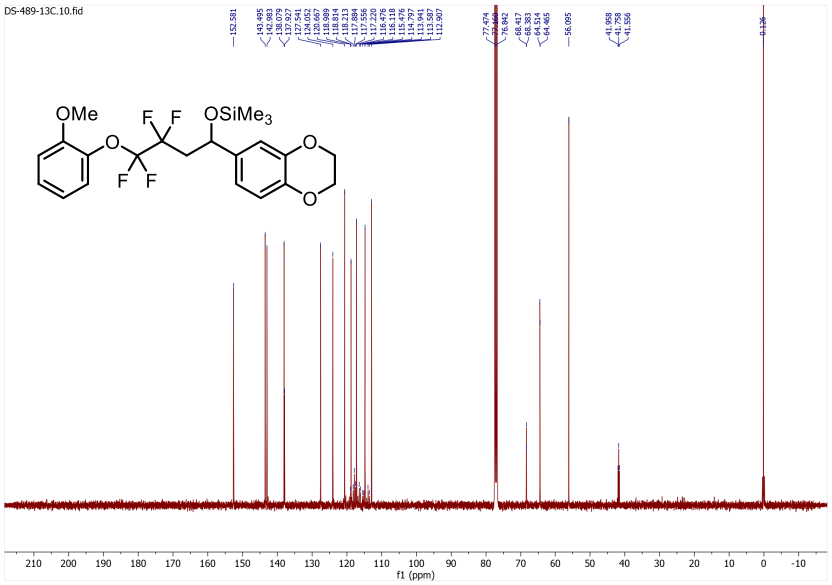
Commented [DS10]: Changed the spectra

Compound 47. ^{19}F NMR ($CDCl_3$, 376 MHz)

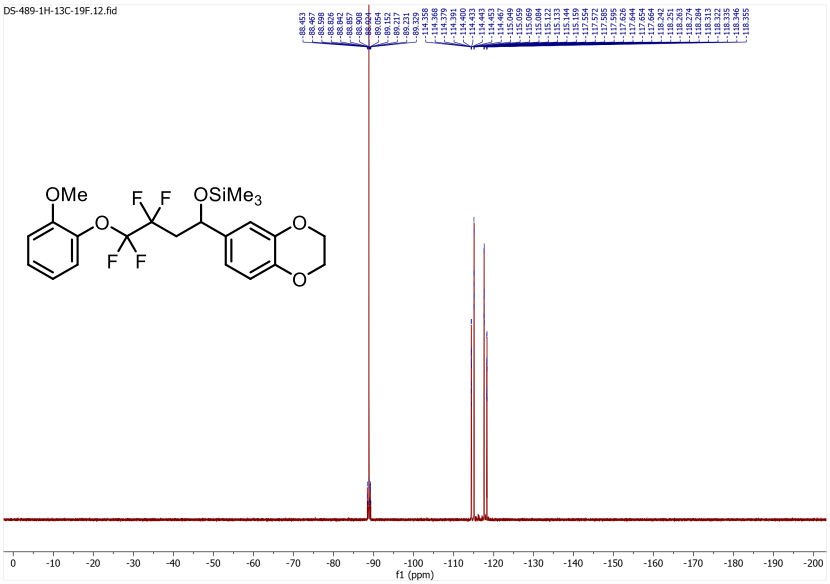


Compound 48. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

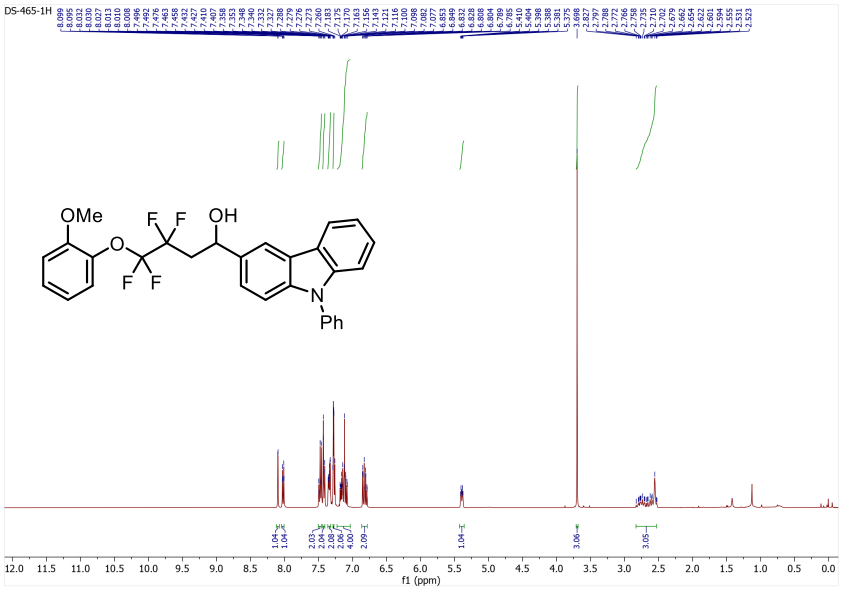


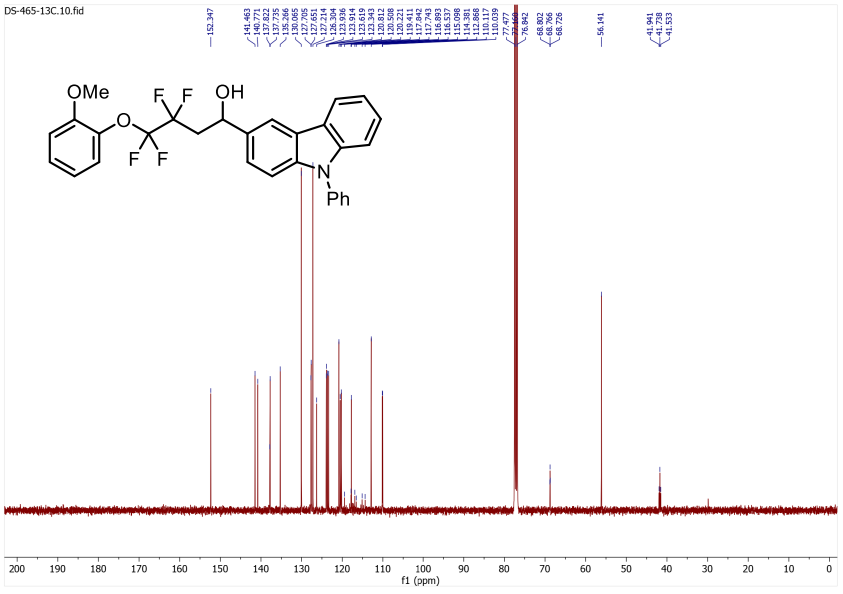


Compound 48. ^{19}F NMR ($CDCl_3$, 376 MHz)

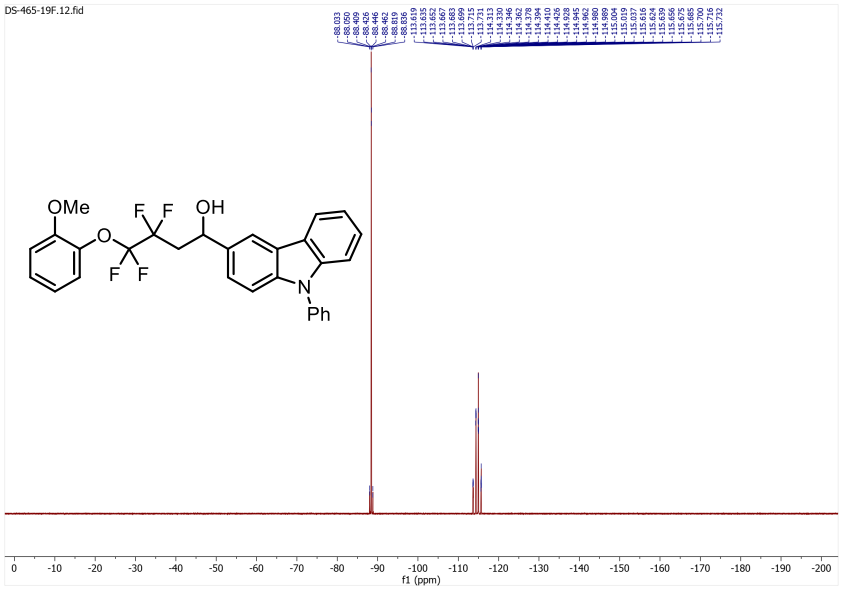


Compound 49. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

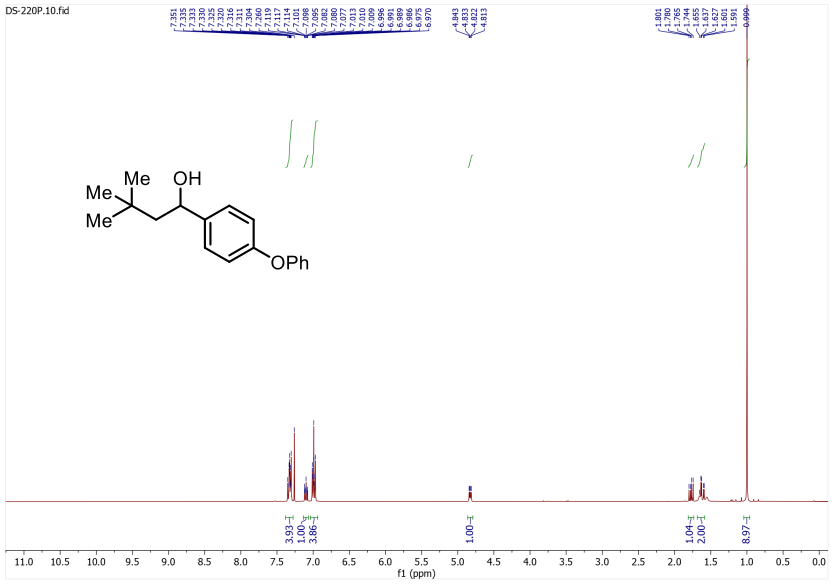


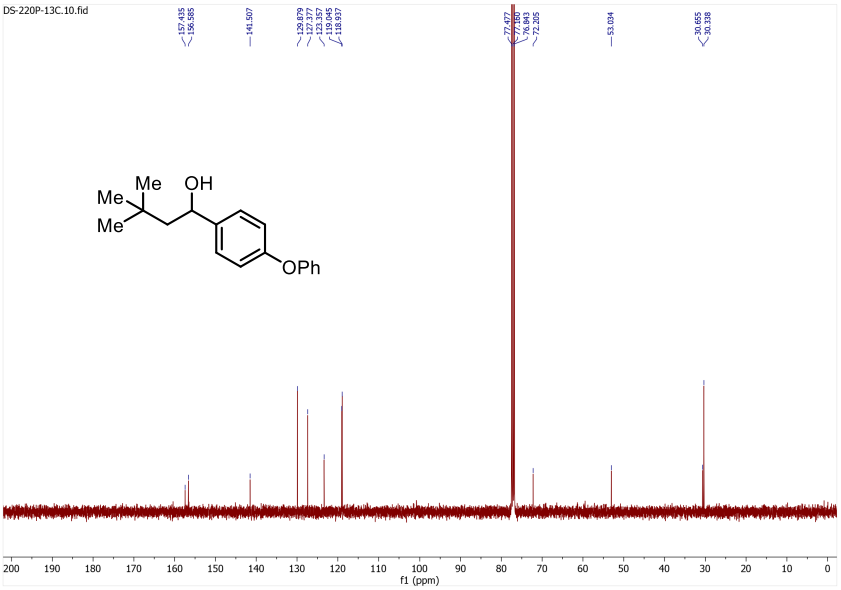


Compound 49. ^{19}F NMR ($CDCl_3$, 376 MHz)

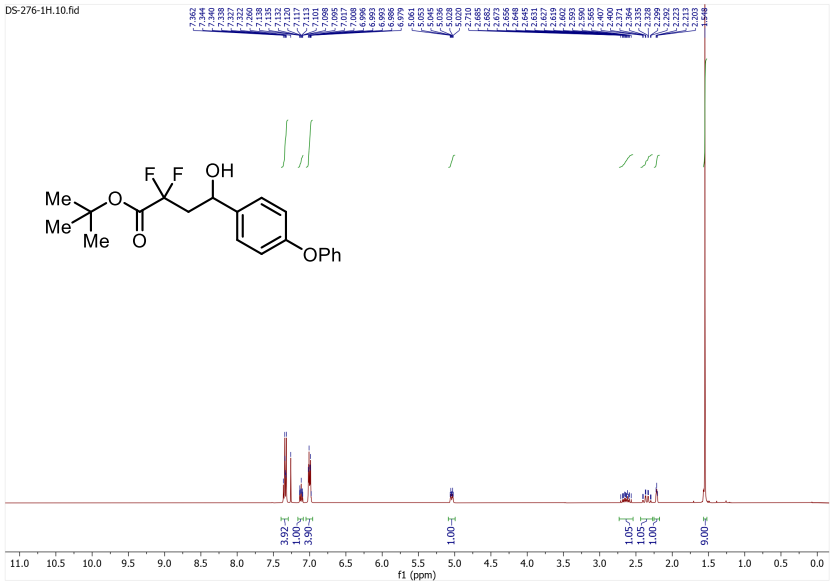


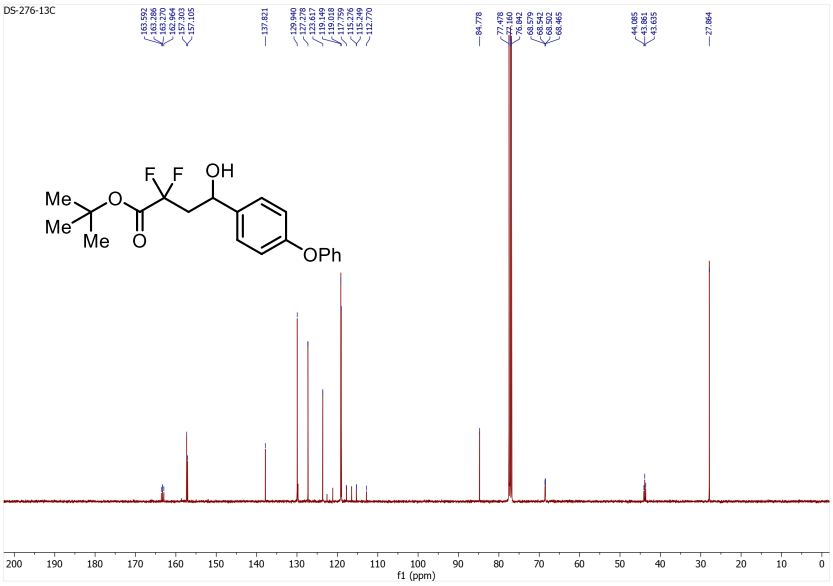
Compound 50. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)



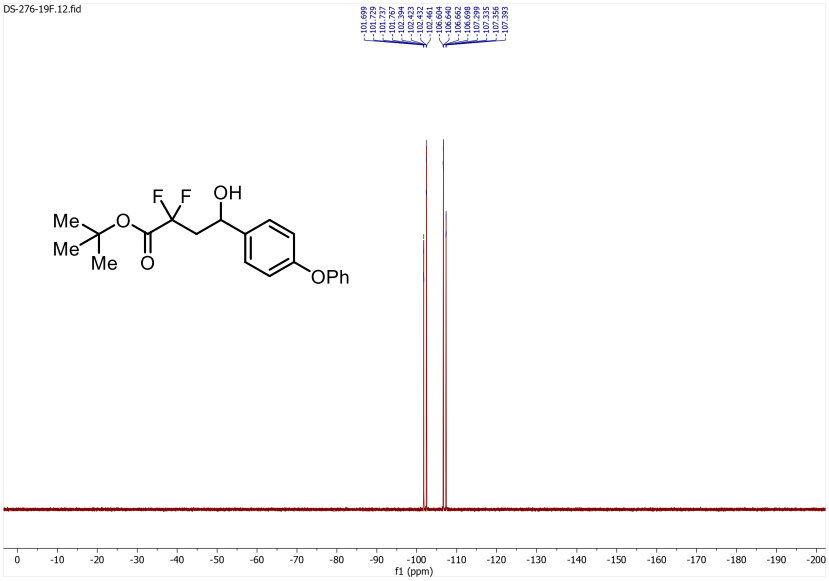


Compound 51. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

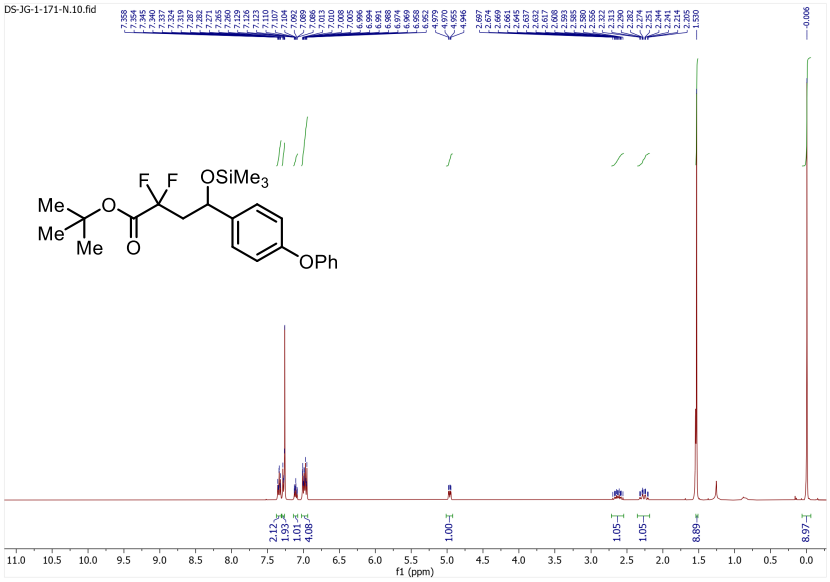


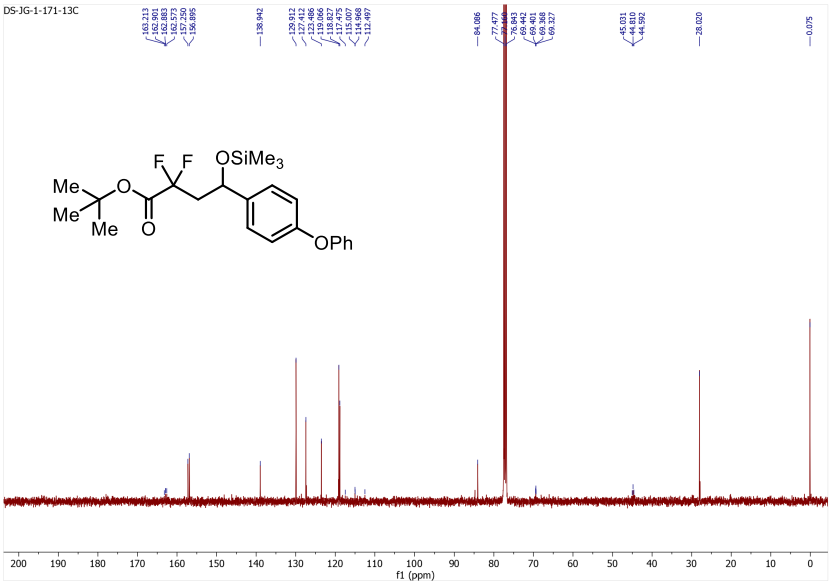


Compound 51. ^{19}F NMR ($CDCl_3$, 376 MHz)

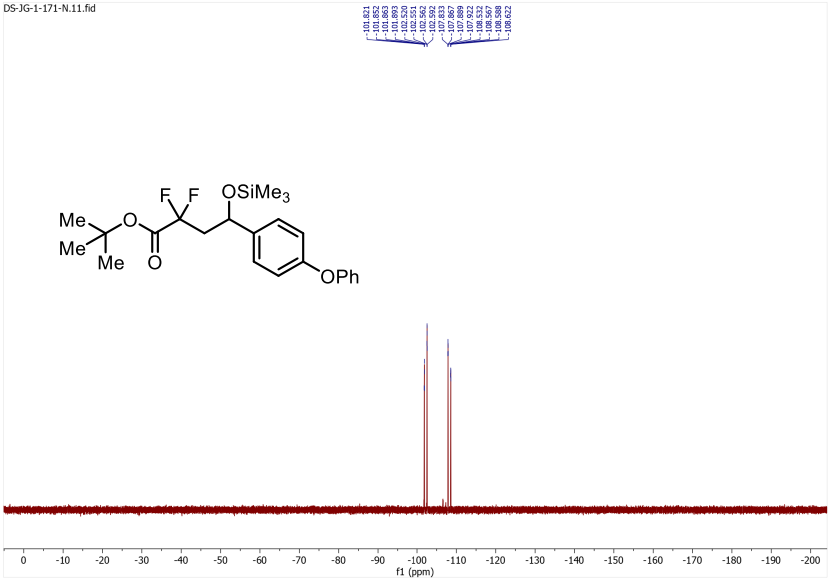


Compound 52. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

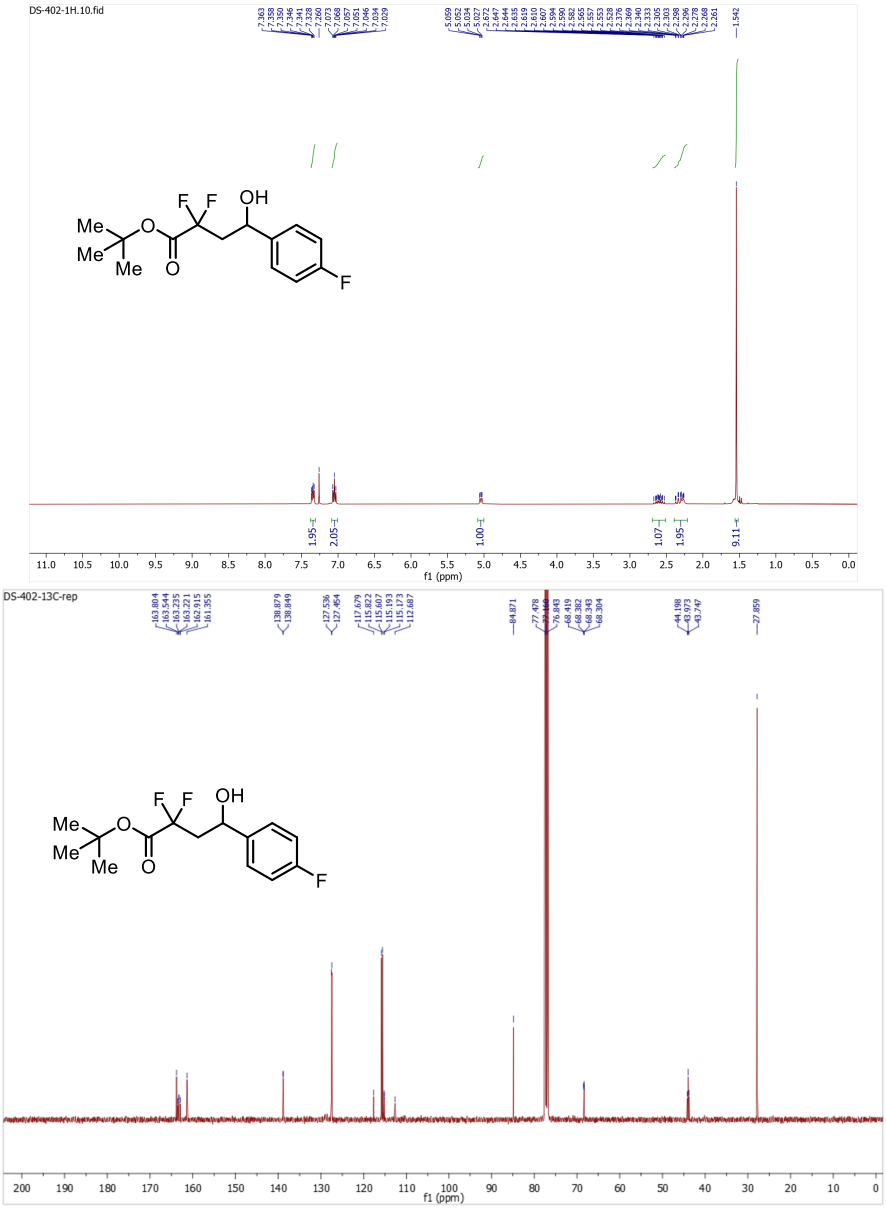




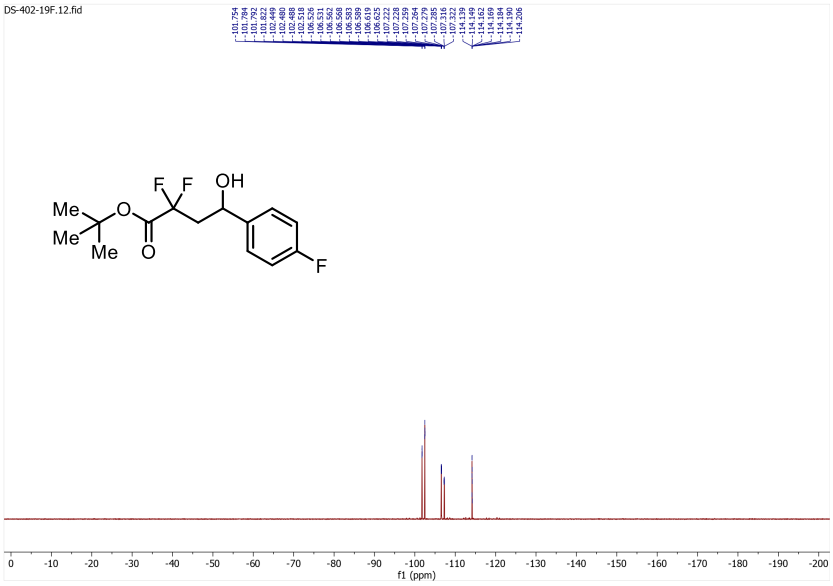
Compound 52. ^{19}F NMR ($CDCl_3$, 376 MHz)



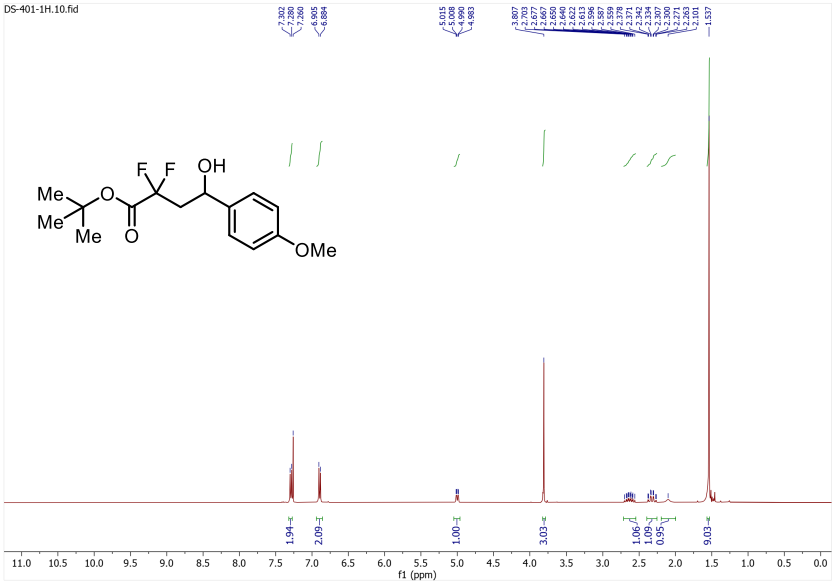
Compound 53. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

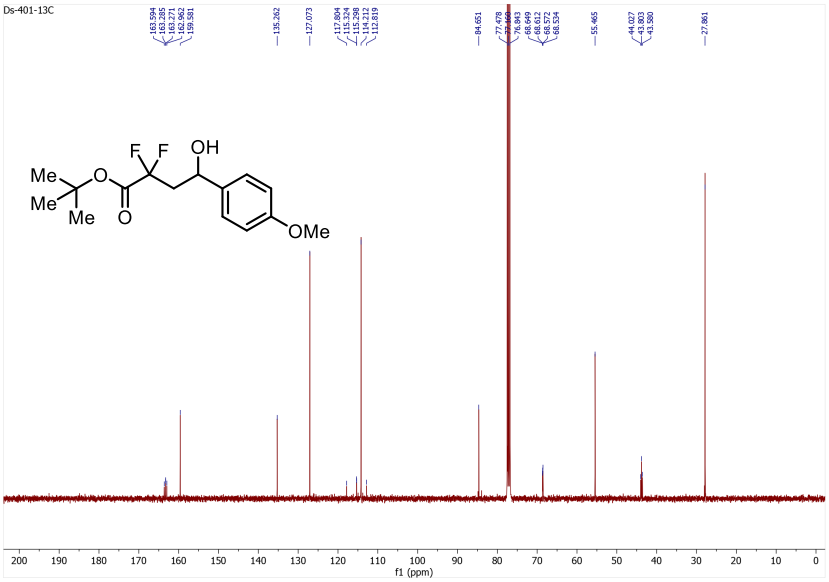


Compound 53. ^{19}F NMR ($CDCl_3$, 376 MHz)

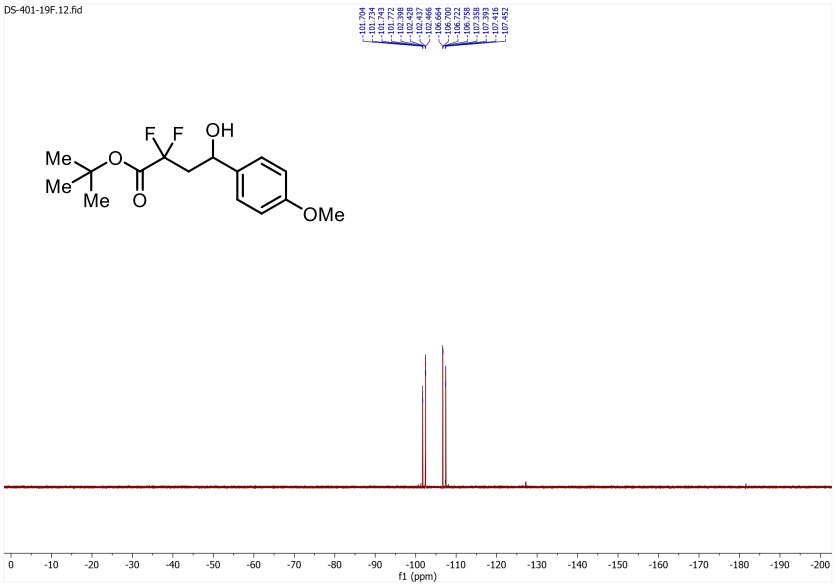


Compound 54. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

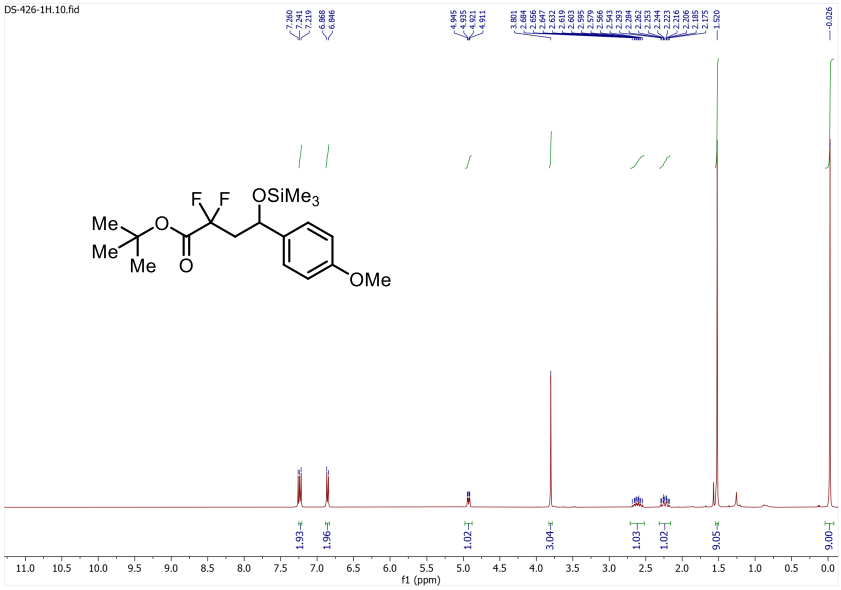


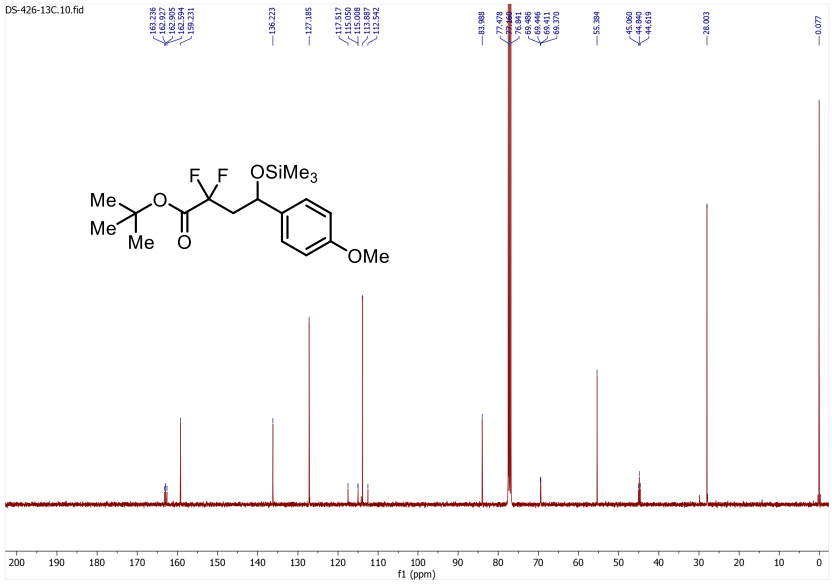


Compound 54. ^{19}F NMR ($CDCl_3$, 376 MHz)

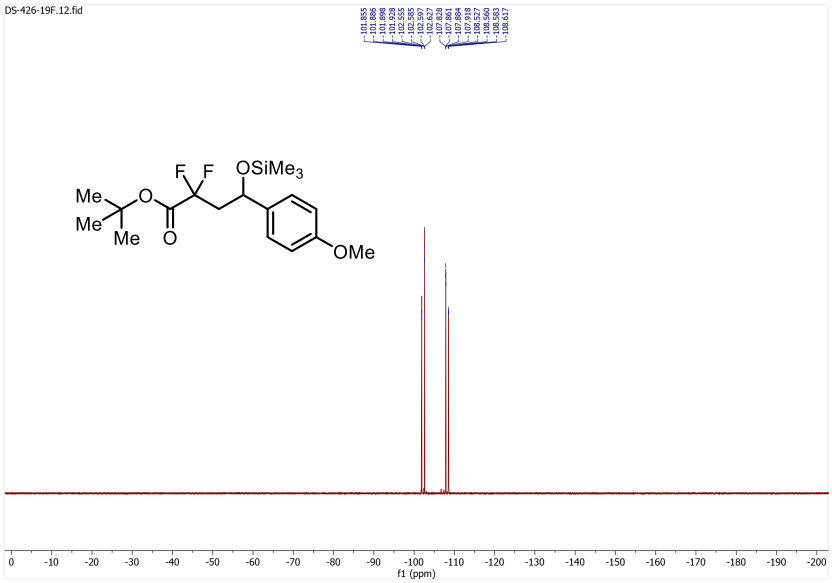


Compound 55. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

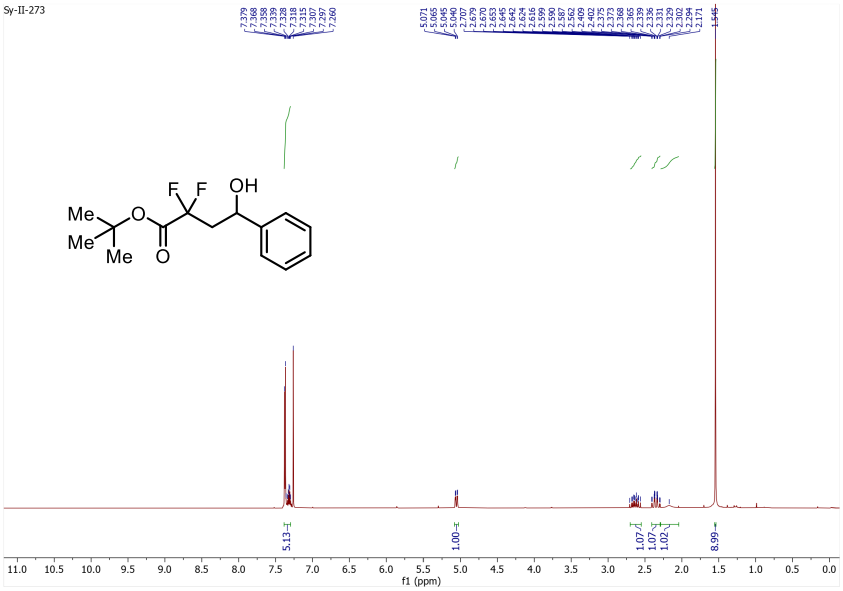


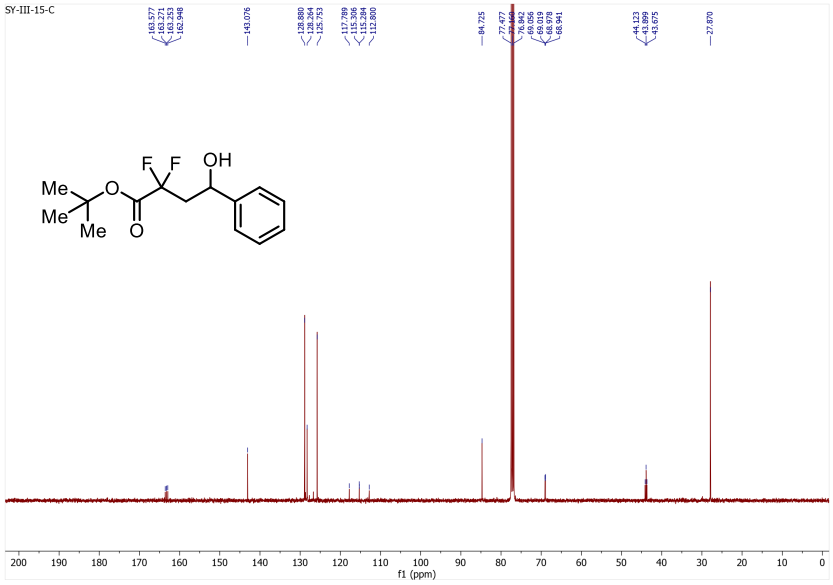


Compound 55. ^{19}F NMR ($CDCl_3$, 376 MHz)

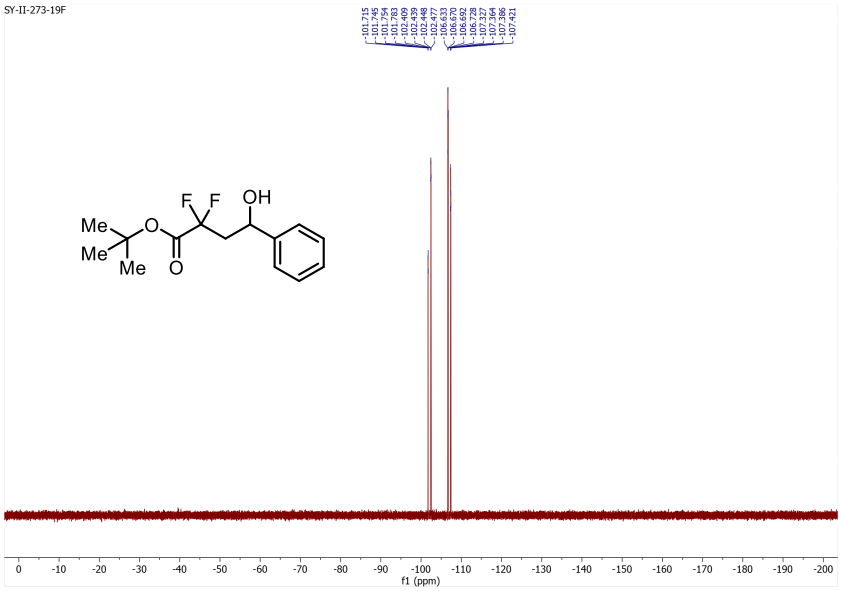


Compound 56. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

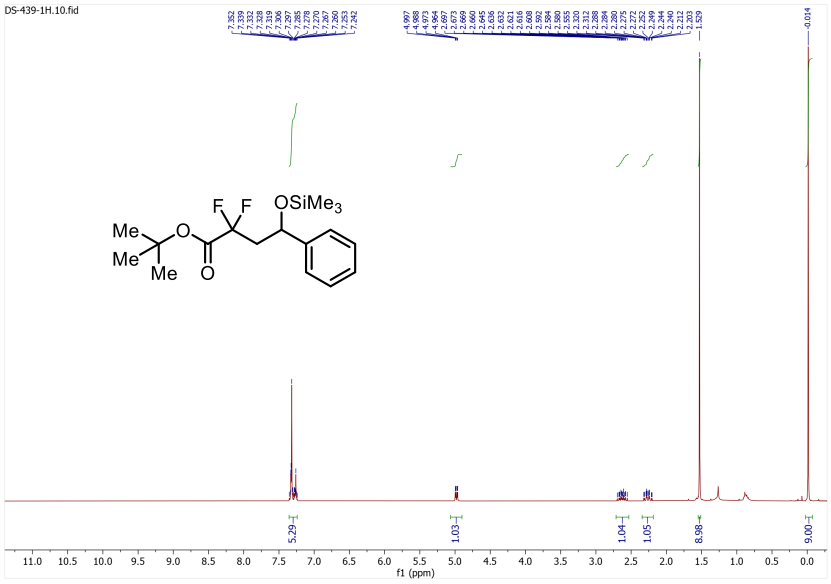


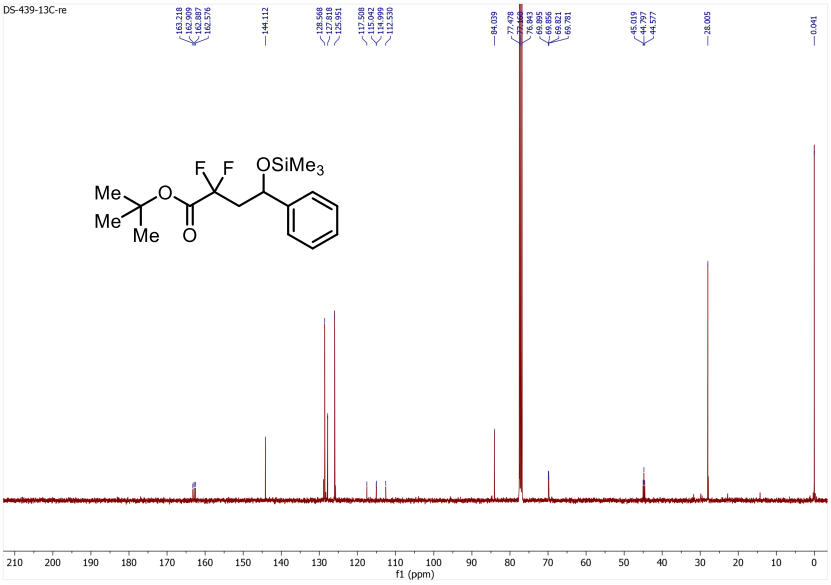


Compound 56. ^{19}F NMR ($CDCl_3$, 376 MHz)

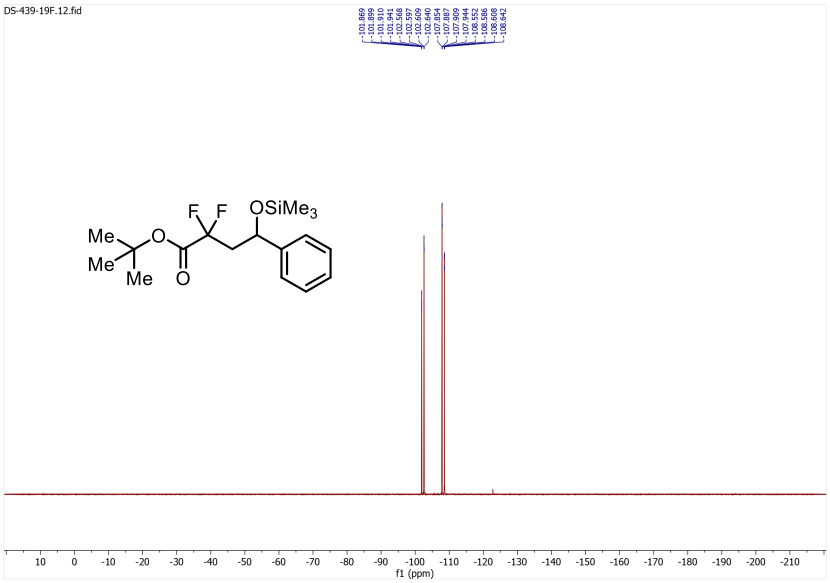


Compound 57. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

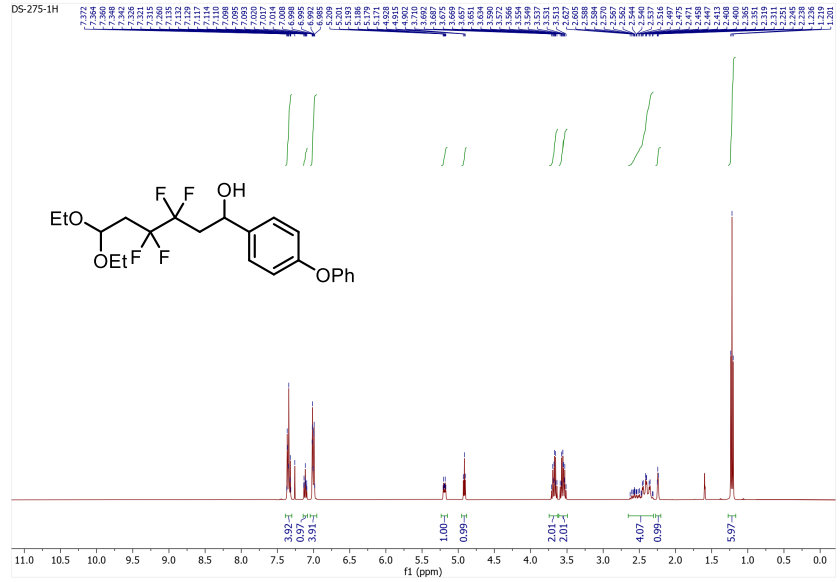


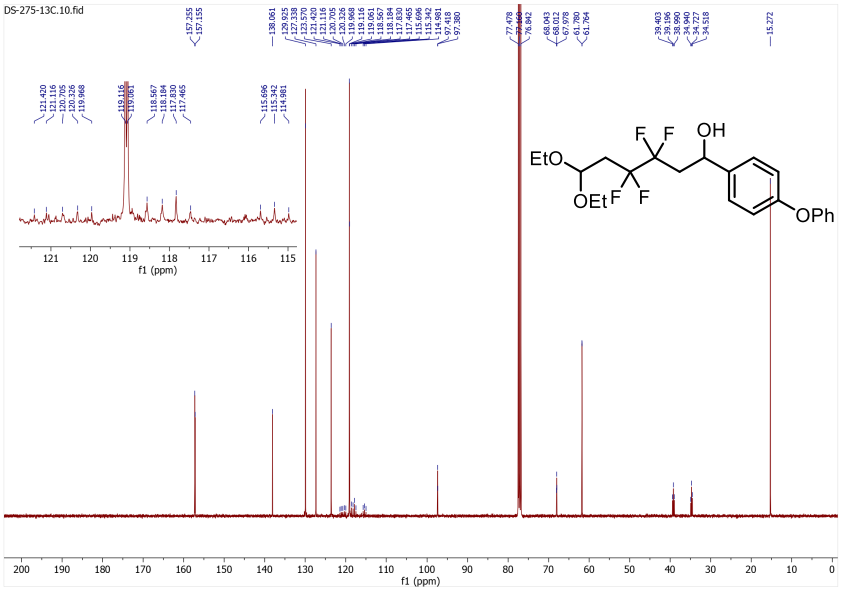


Compound 57. ^{19}F NMR ($CDCl_3$, 376 MHz)

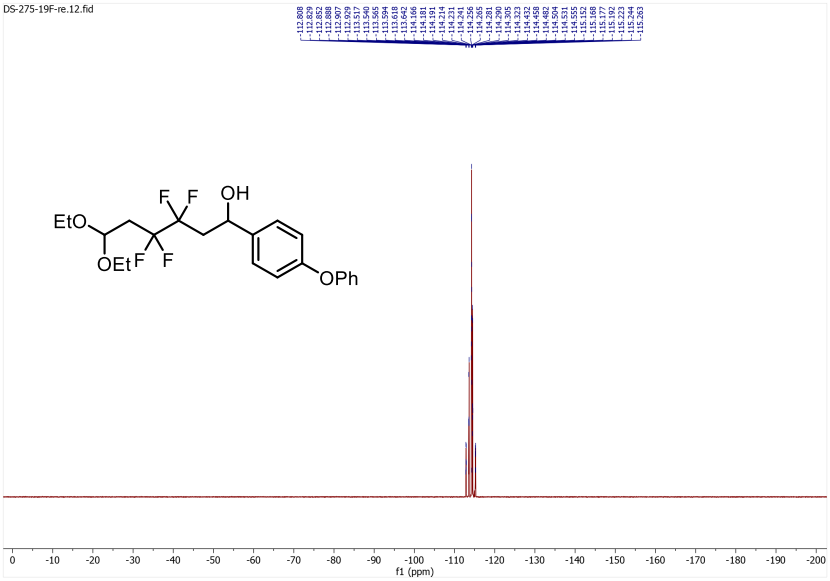


Compound 58. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

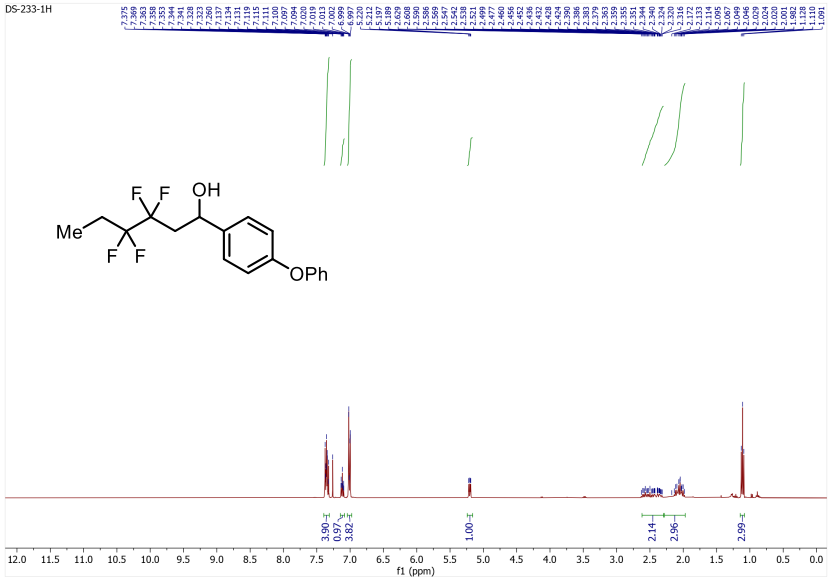


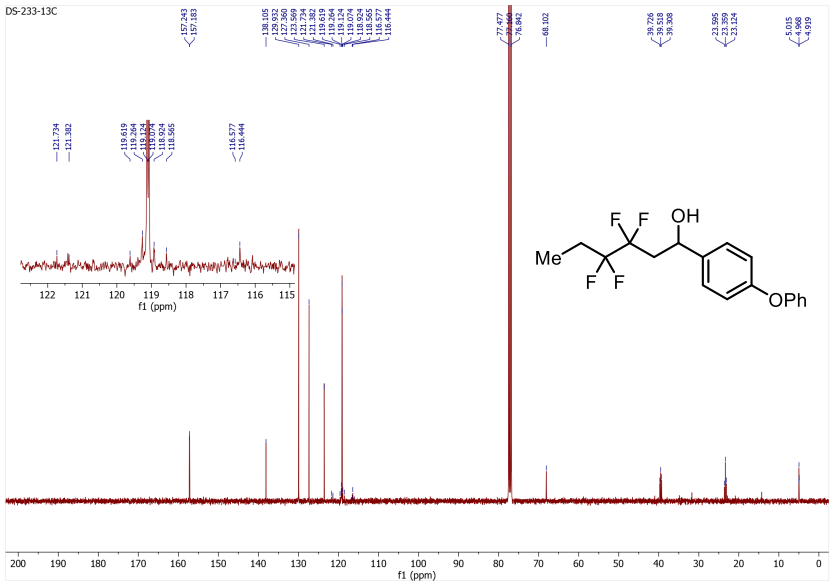


Compound 58. ^{19}F NMR ($CDCl_3$, 376 MHz)

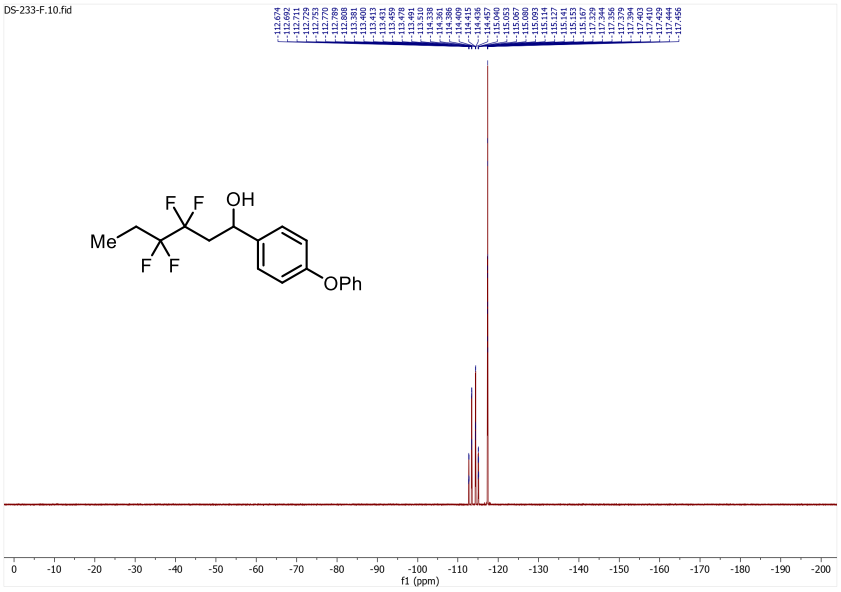


Compound 59. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

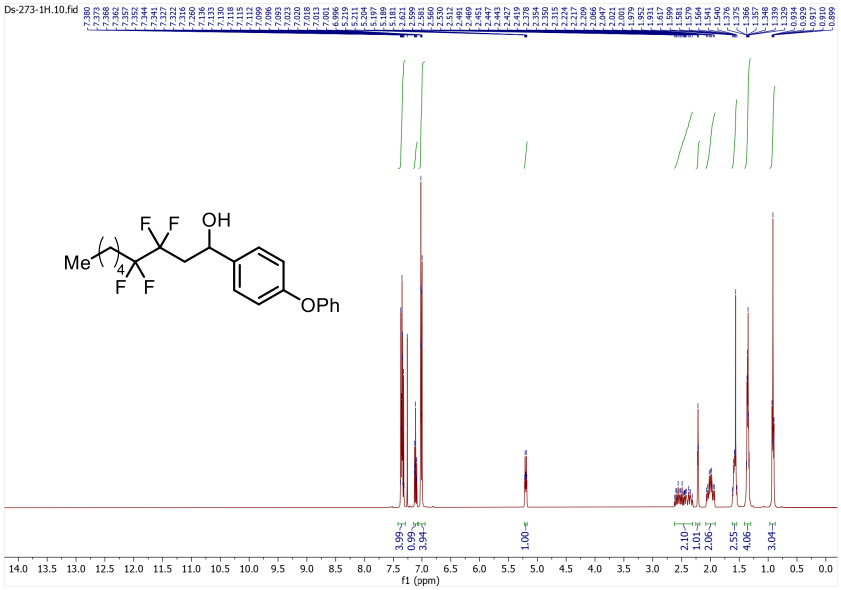


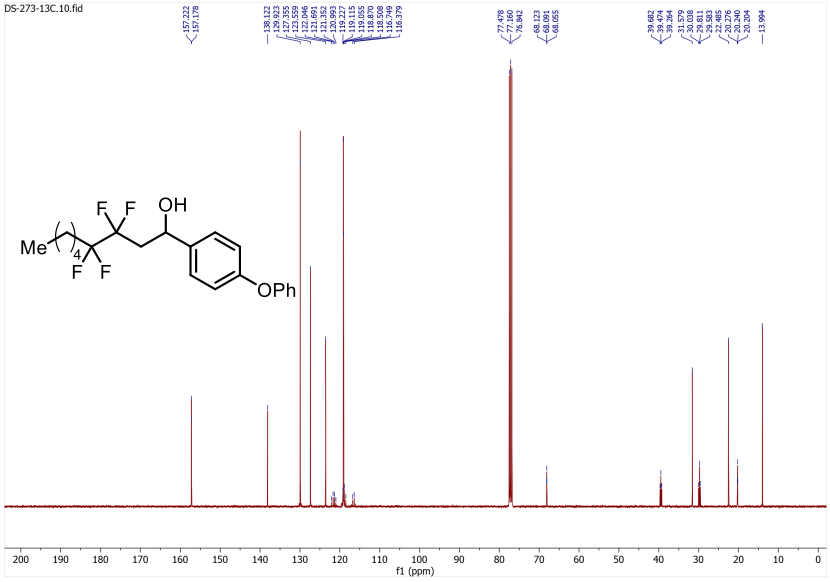


Compound 59. ^{19}F NMR ($CDCl_3$, 376 MHz)

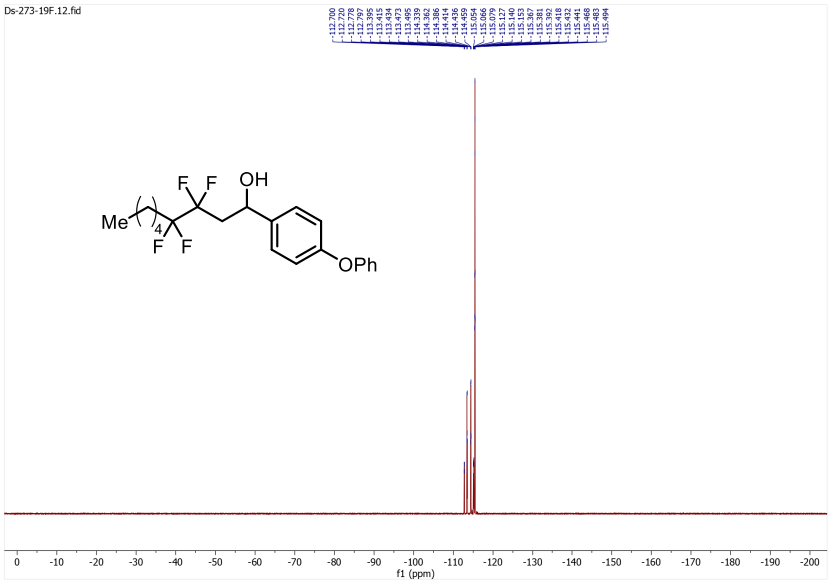


Compound 60. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

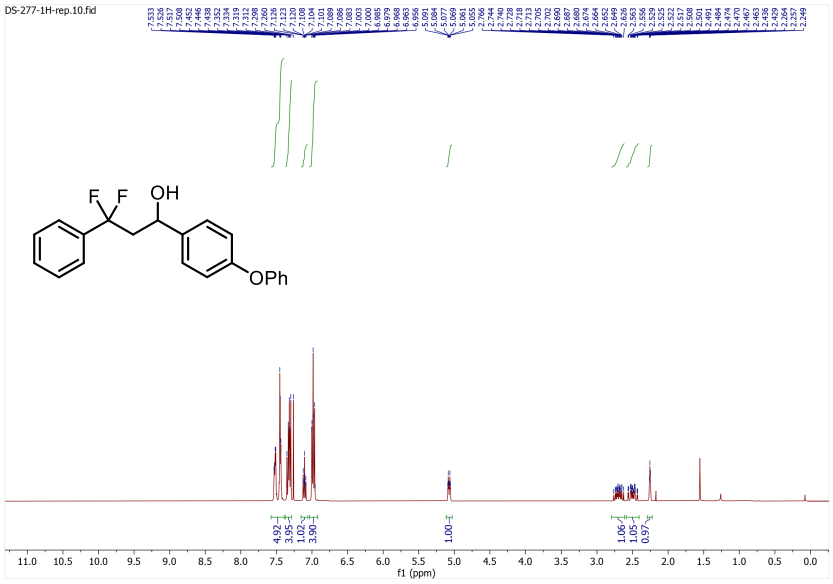


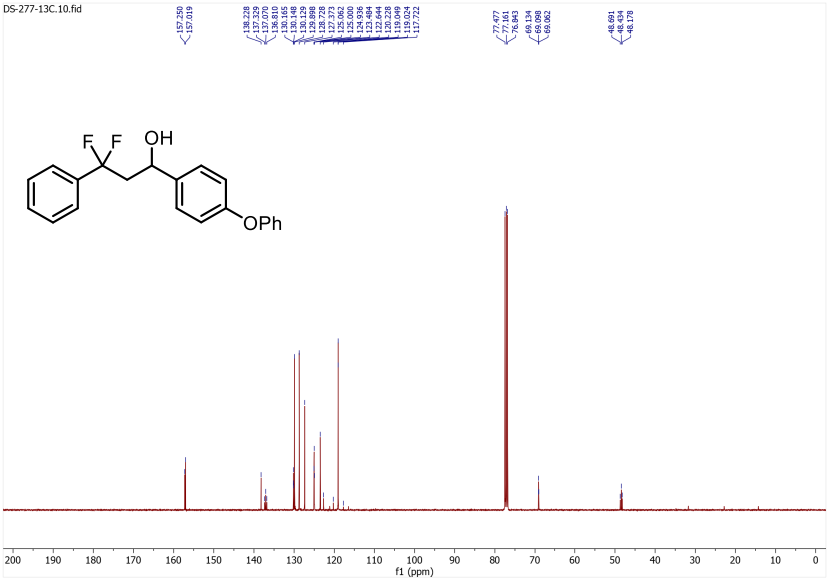


Compound 60. ^{19}F NMR ($CDCl_3$, 376 MHz)

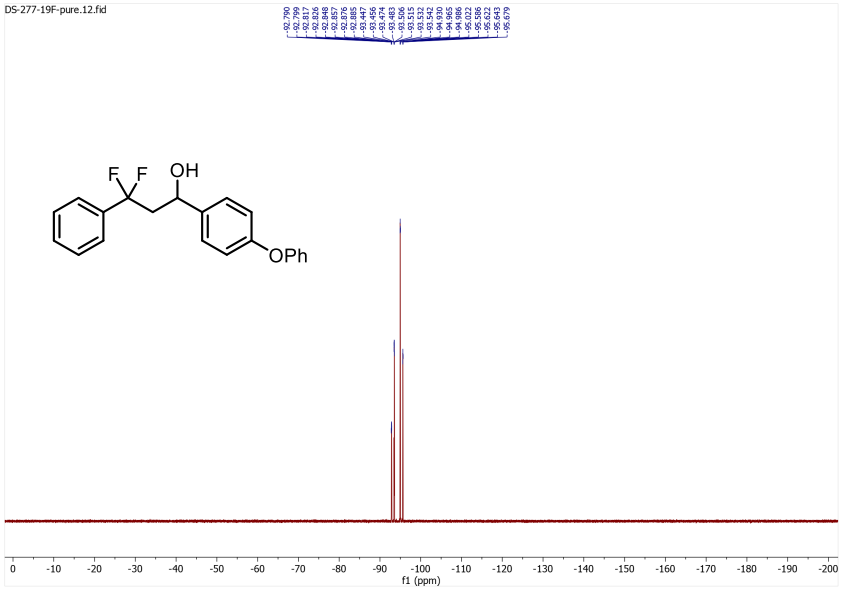


Compound 61. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

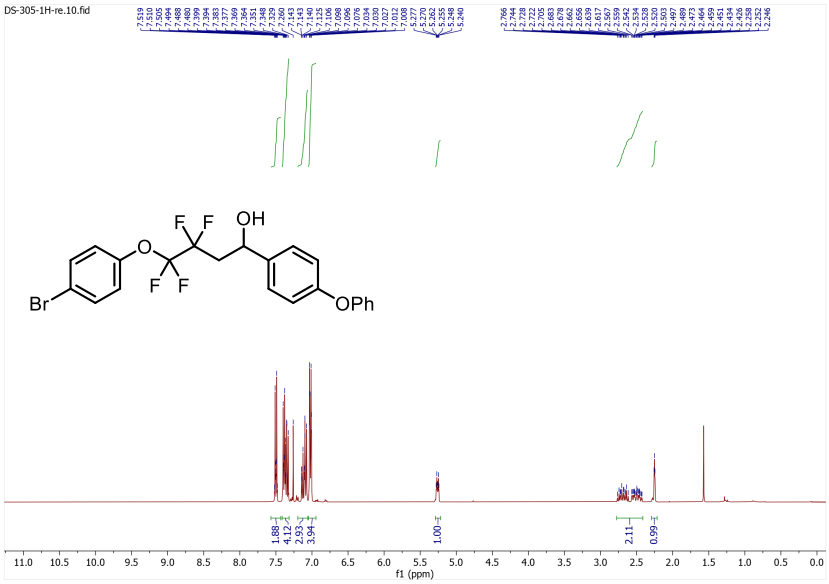


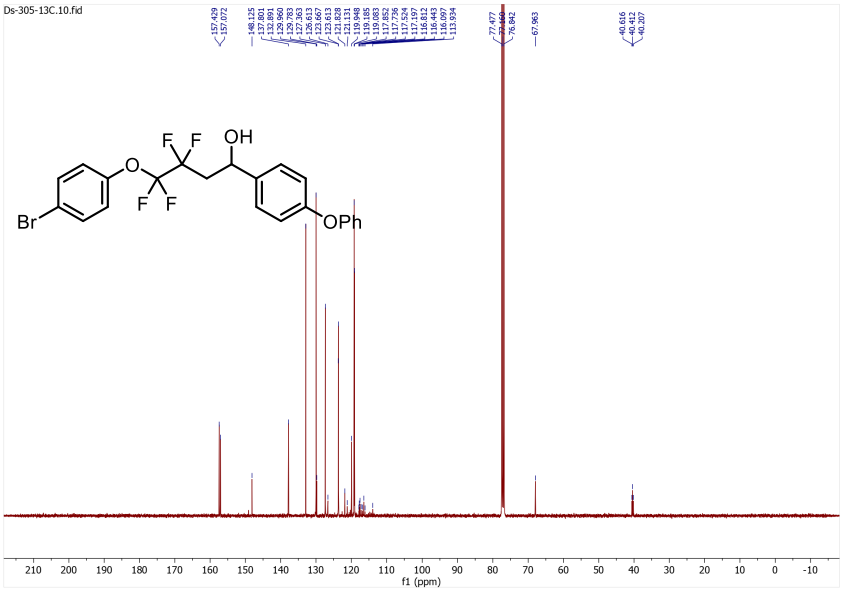


Compound 61. ^{19}F NMR ($CDCl_3$, 376 MHz)

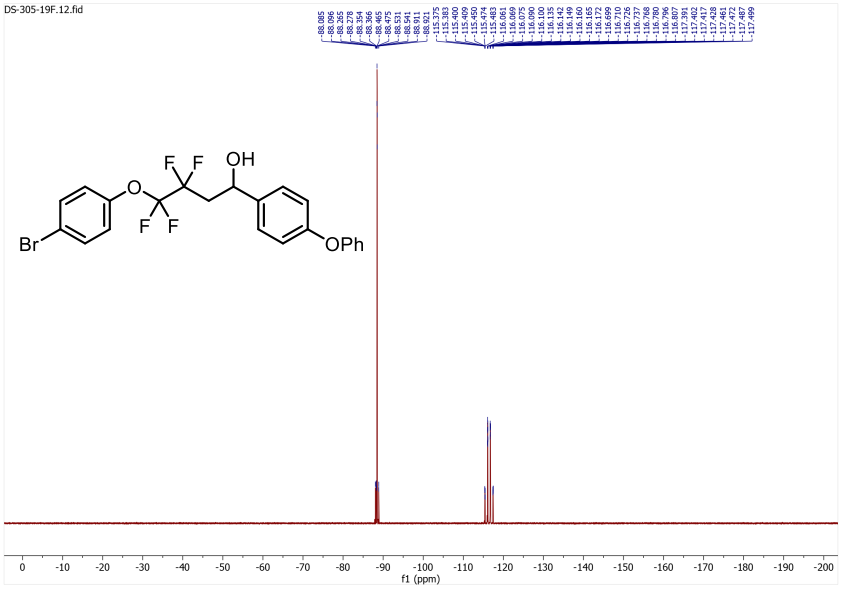


Compound 62. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

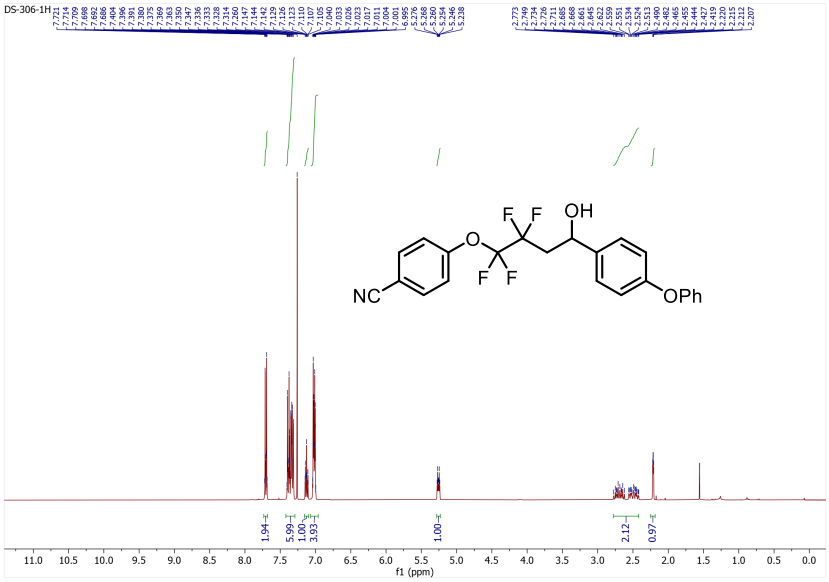


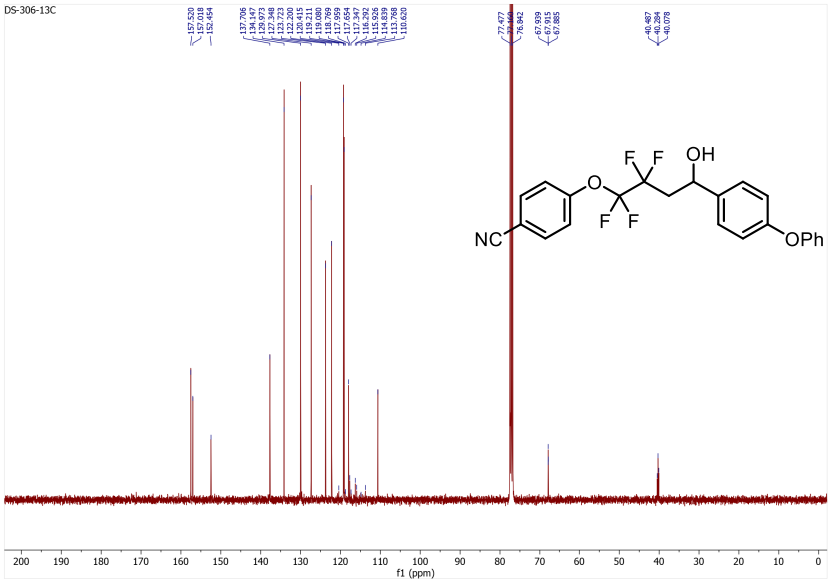


Compound 62. ^{19}F NMR ($CDCl_3$, 376 MHz)

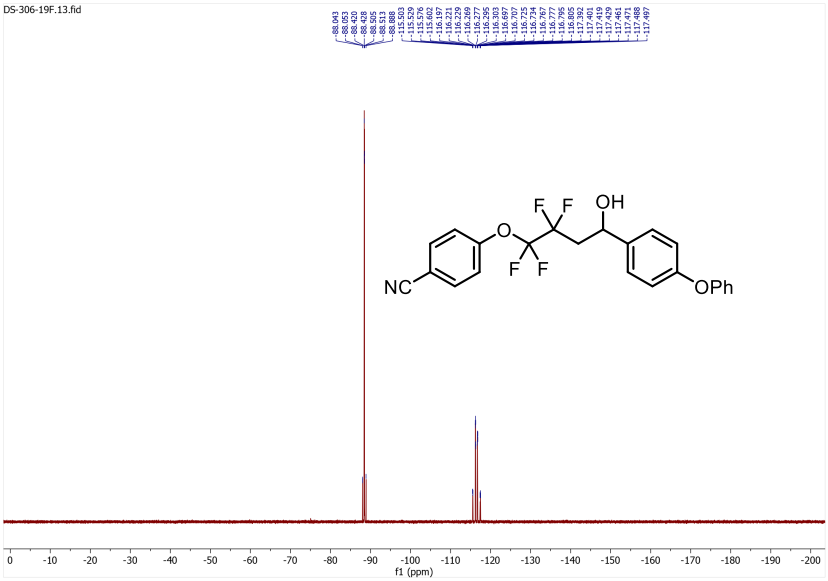


Compound 63. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

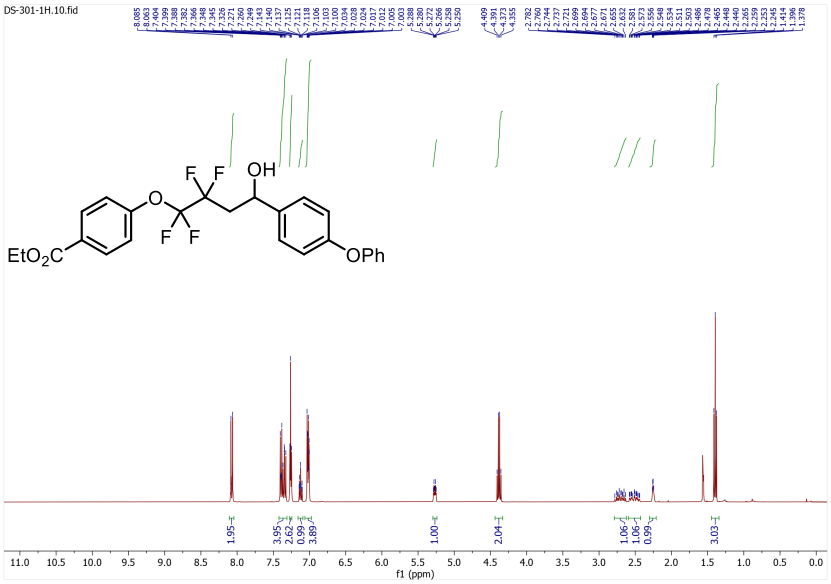


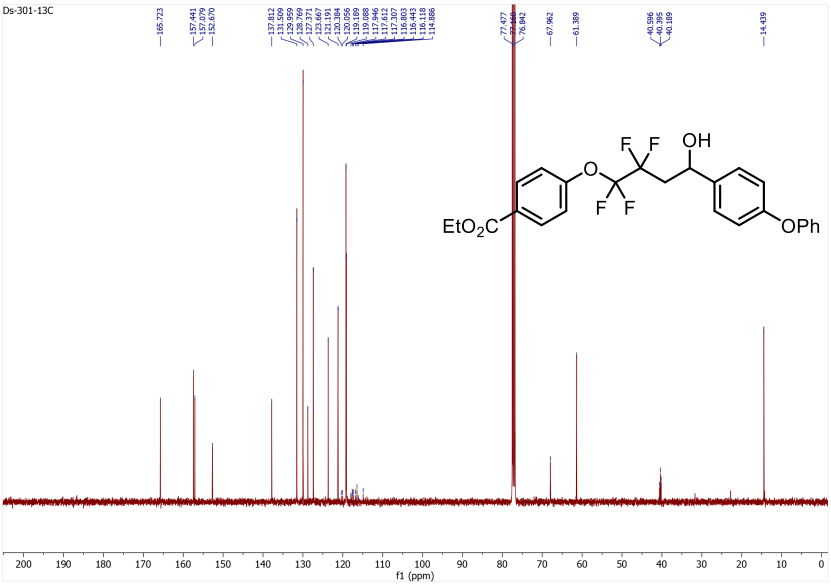


Compound 63. ^{19}F NMR ($CDCl_3$, 376 MHz)

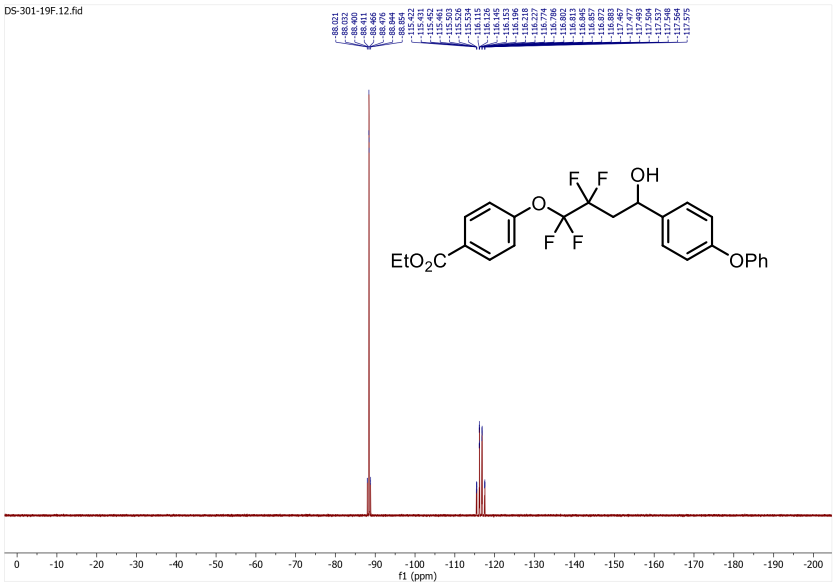


Compound 64. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

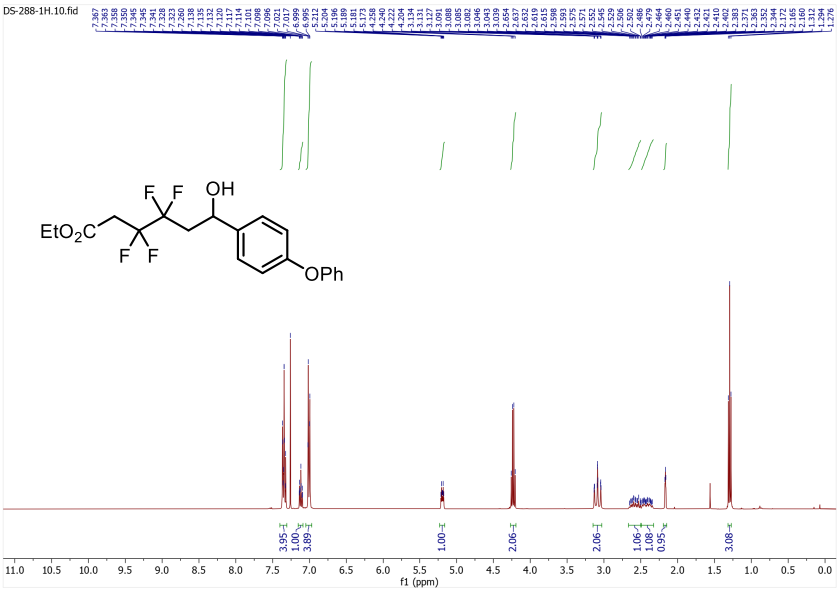


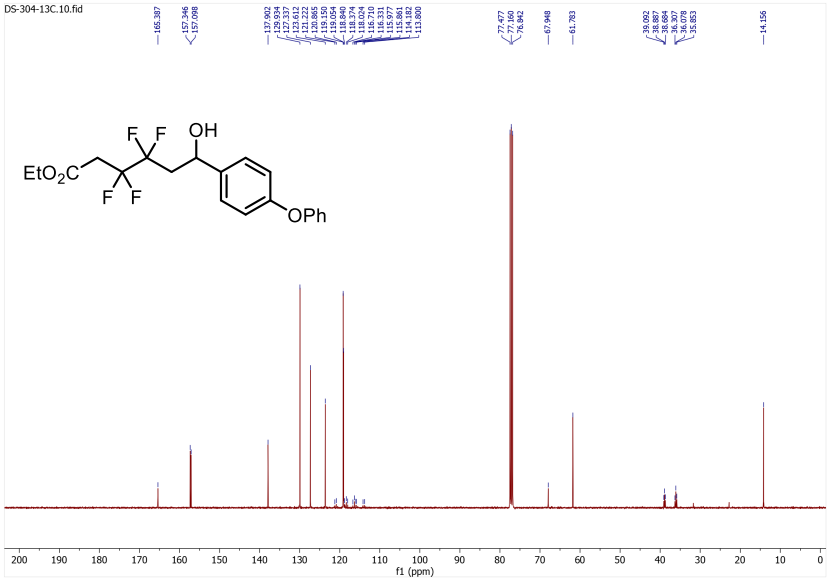


Compound 64. ^{19}F NMR ($CDCl_3$, 376 MHz)

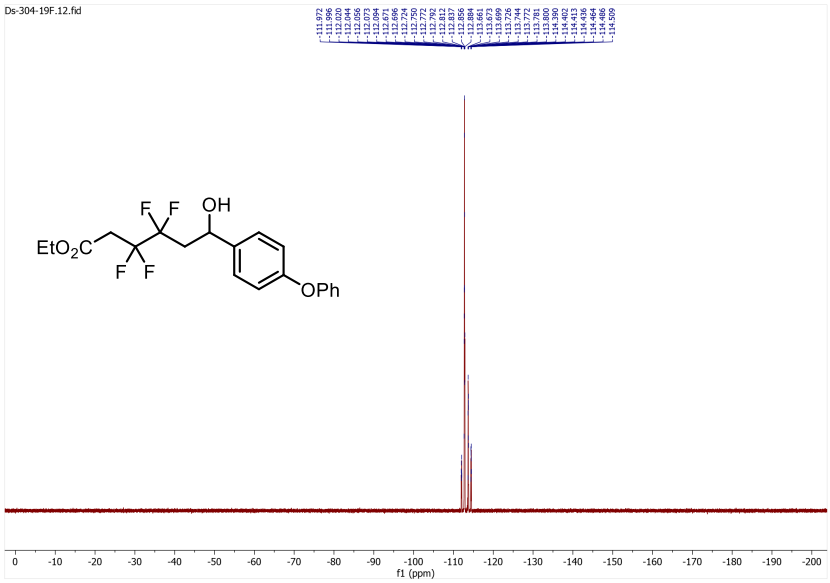


Compound 65. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

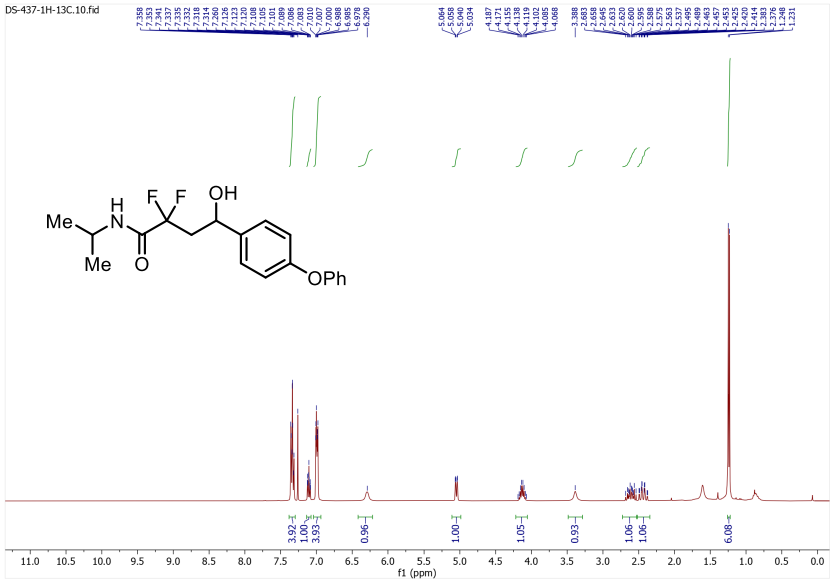


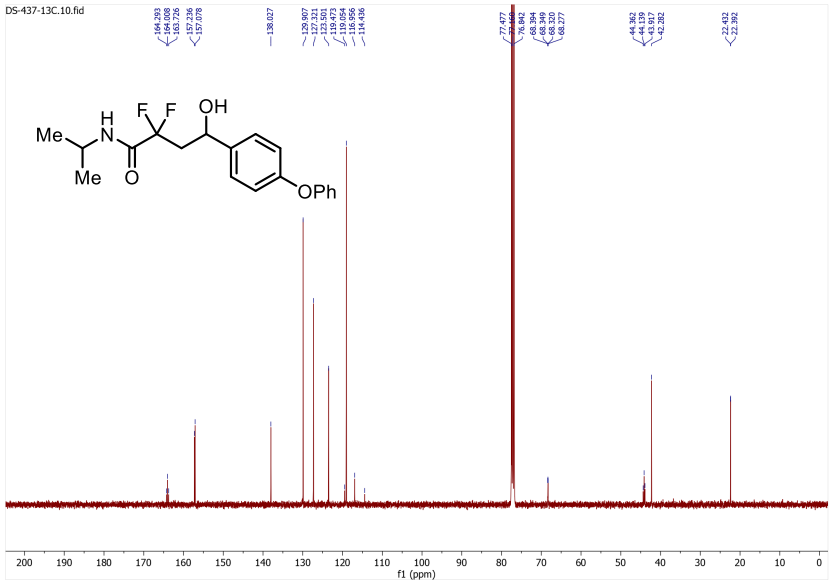


Compound 65. ^{19}F NMR ($CDCl_3$, 376 MHz)

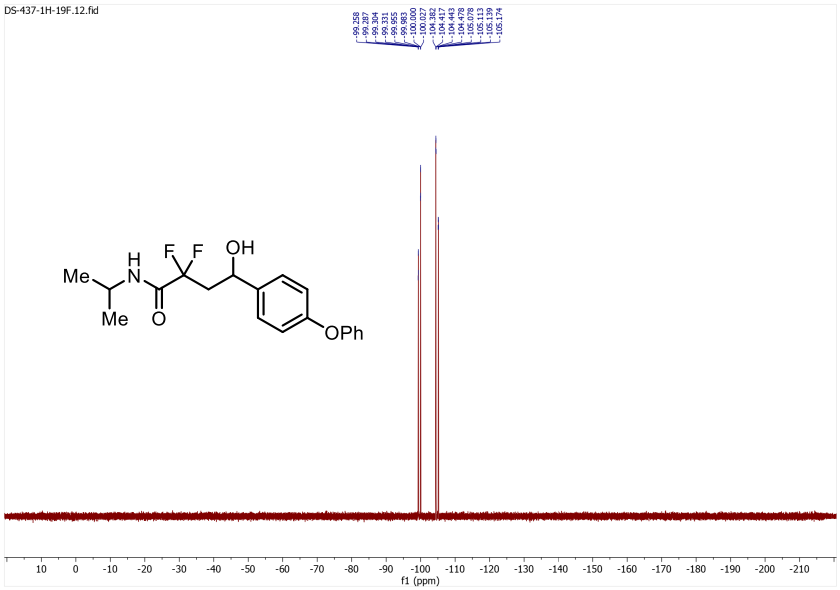


Compound 66. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

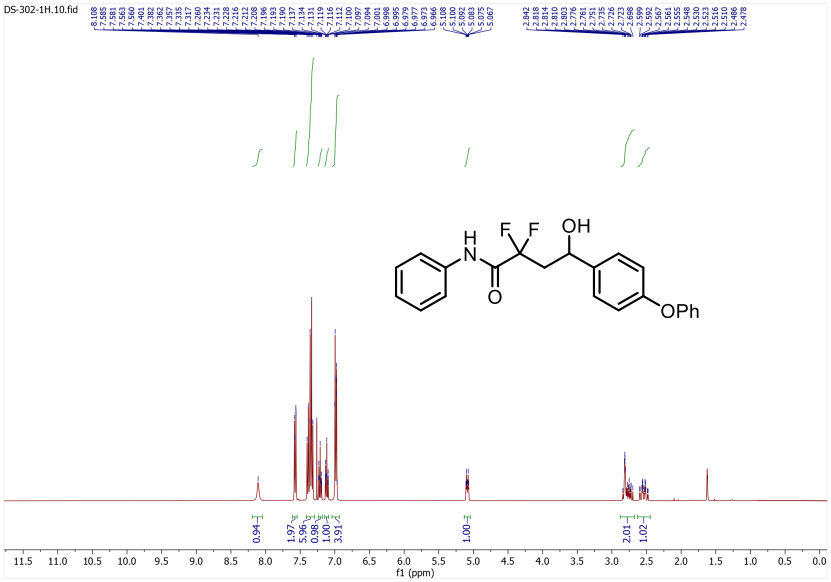


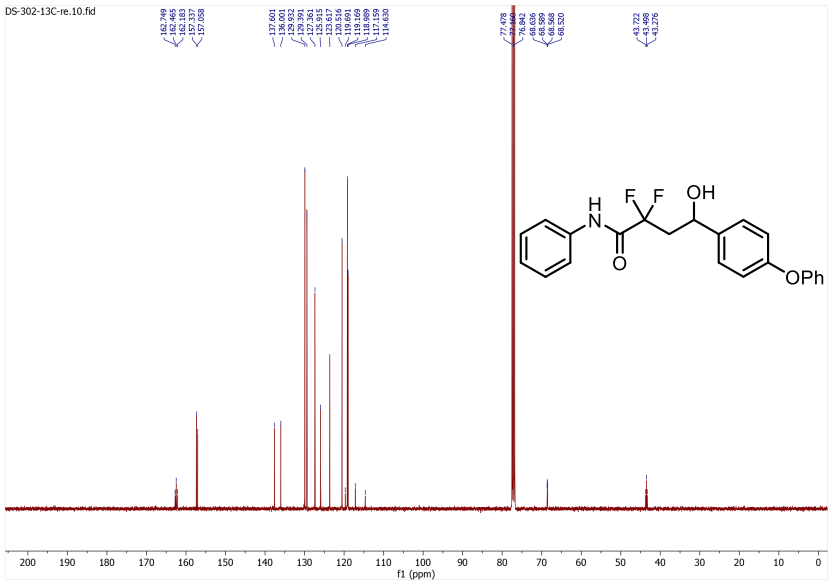


Compound 66. ^{19}F NMR ($CDCl_3$, 376 MHz)

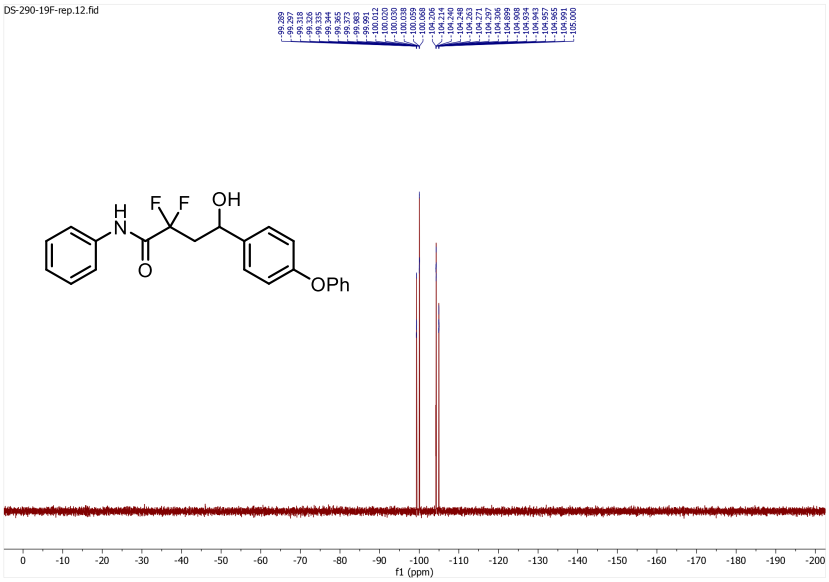


Compound 67. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

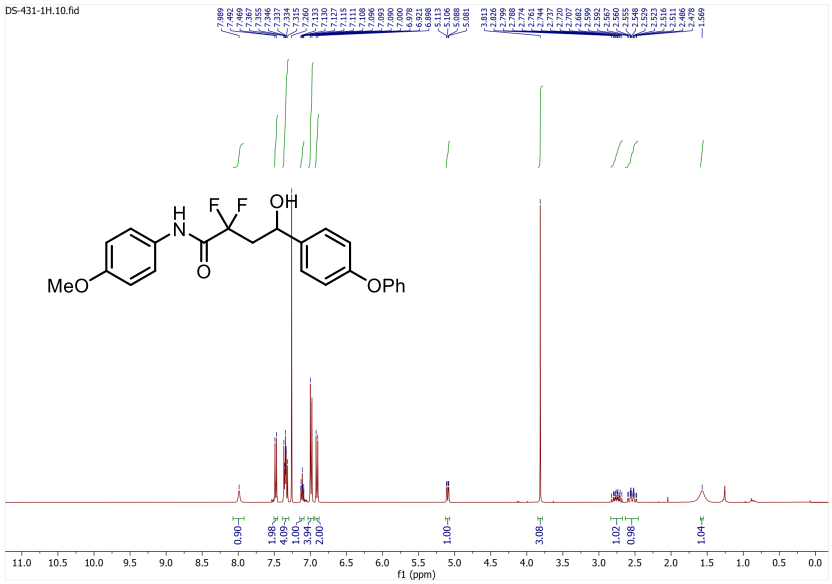


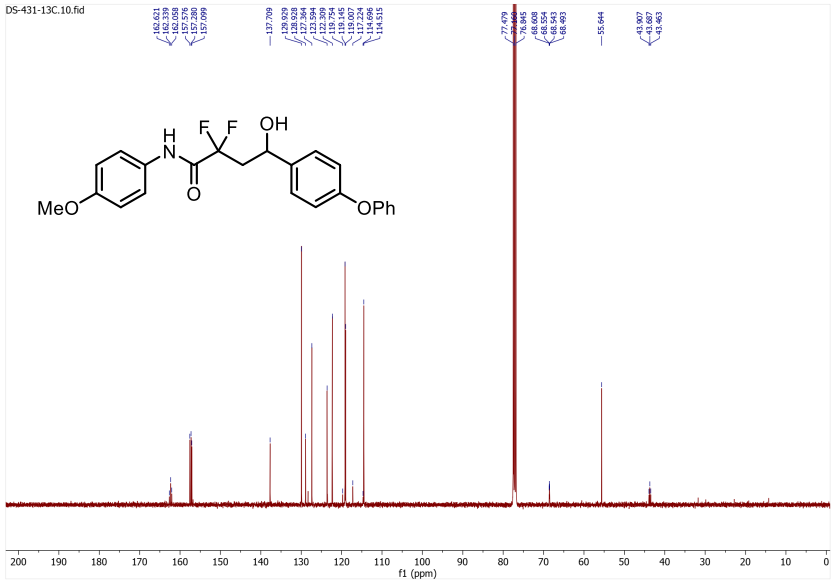


Compound 67. ^{19}F NMR ($CDCl_3$, 376 MHz)

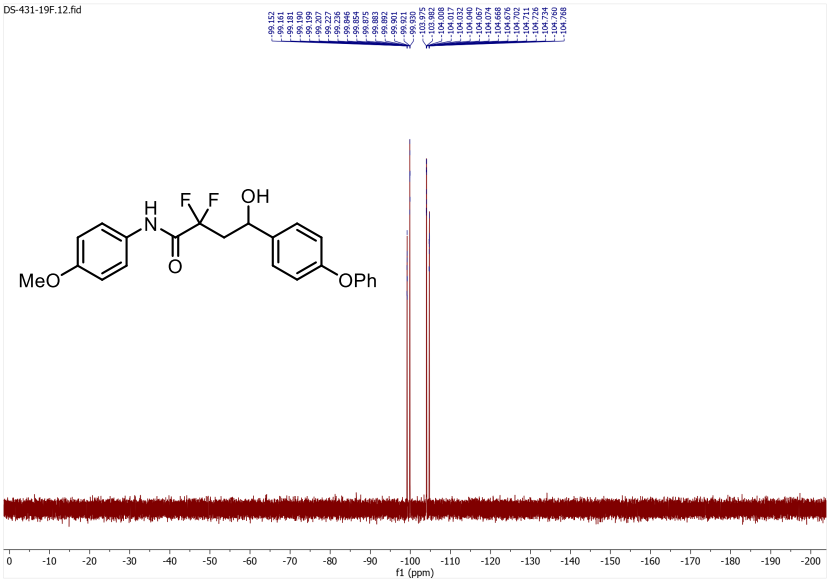


Compound 68. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

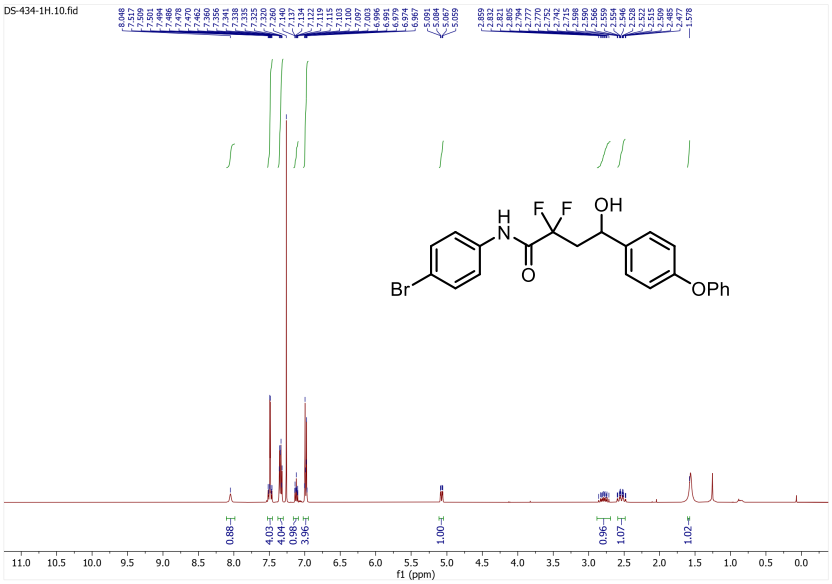


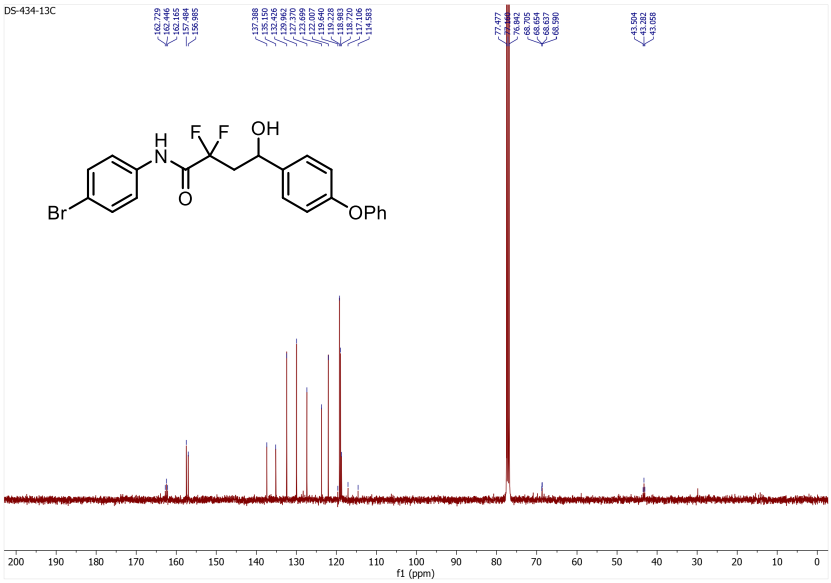


Compound 68. ^{19}F NMR ($CDCl_3$, 376 MHz)

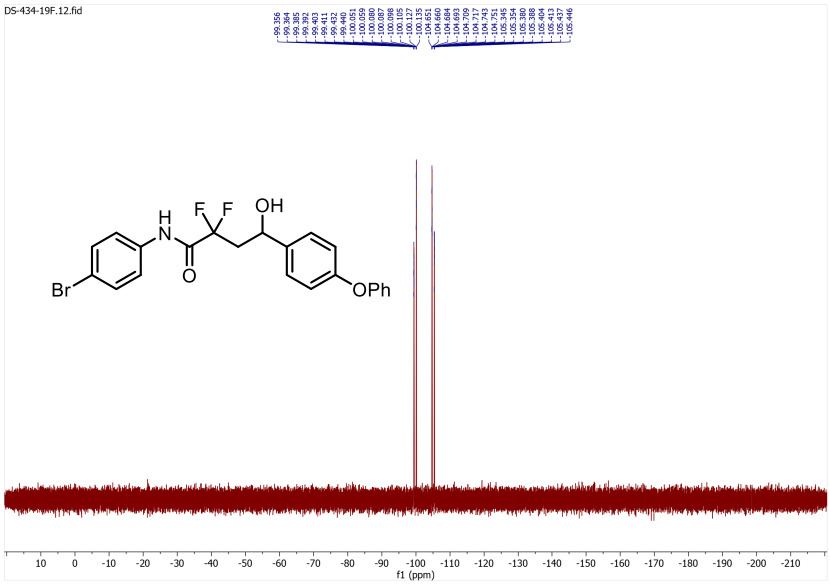


Compound 69. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

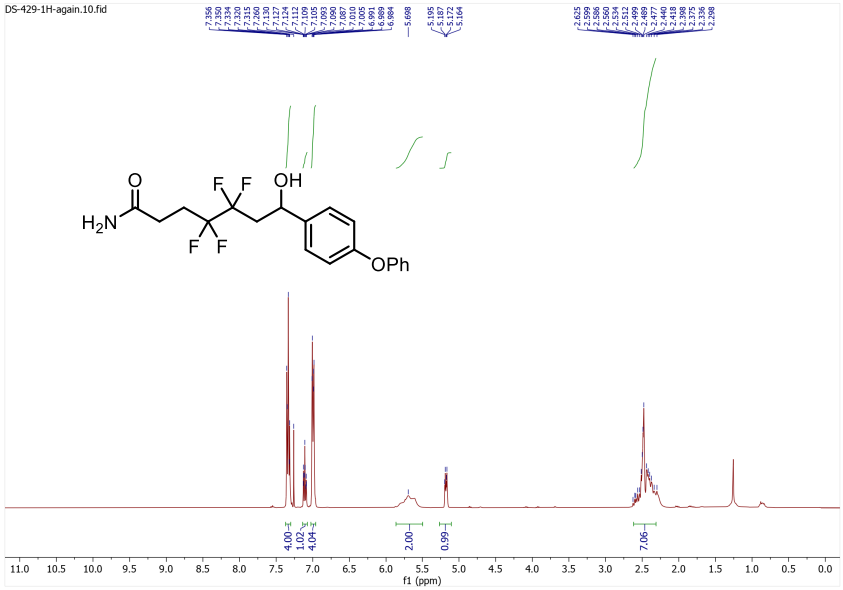


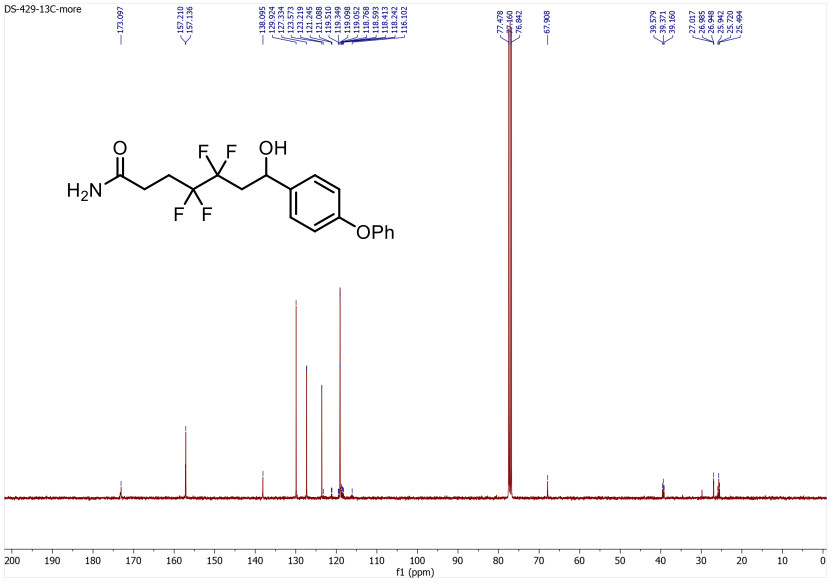


Compound 69. ^{19}F NMR ($CDCl_3$, 376 MHz)

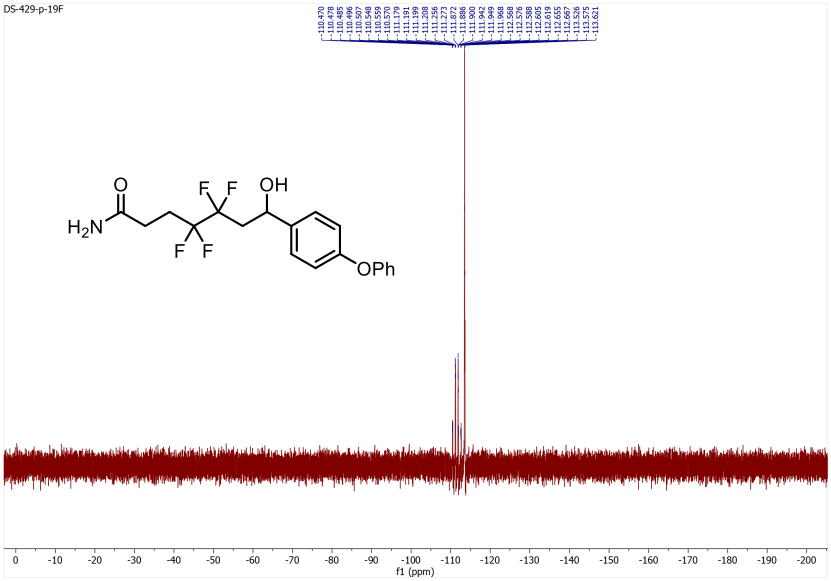


Compound 70. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

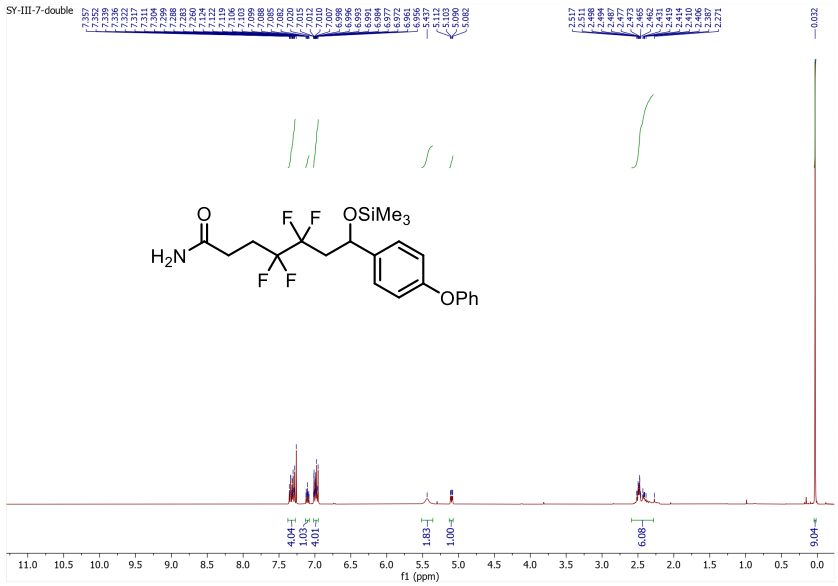


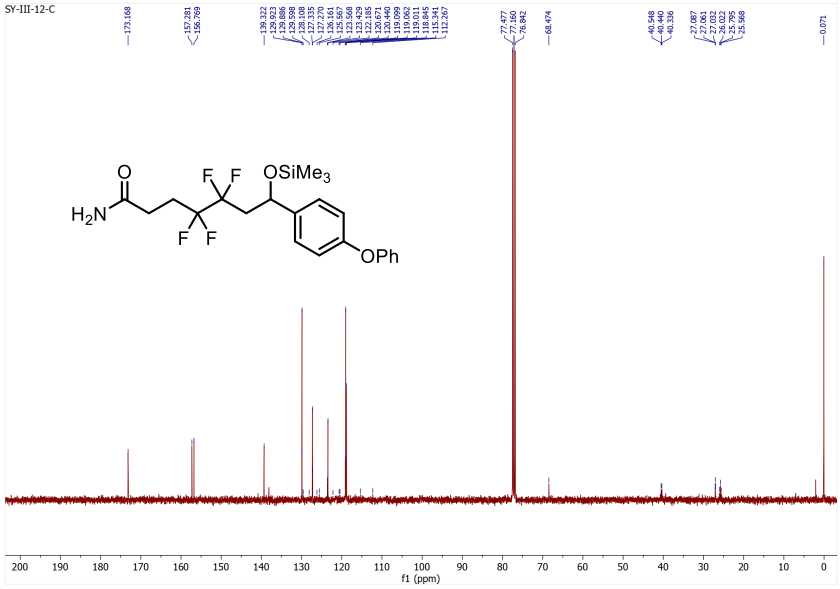


Compoud 70. ^{19}F NMR ($CDCl_3$, 376 MHz)

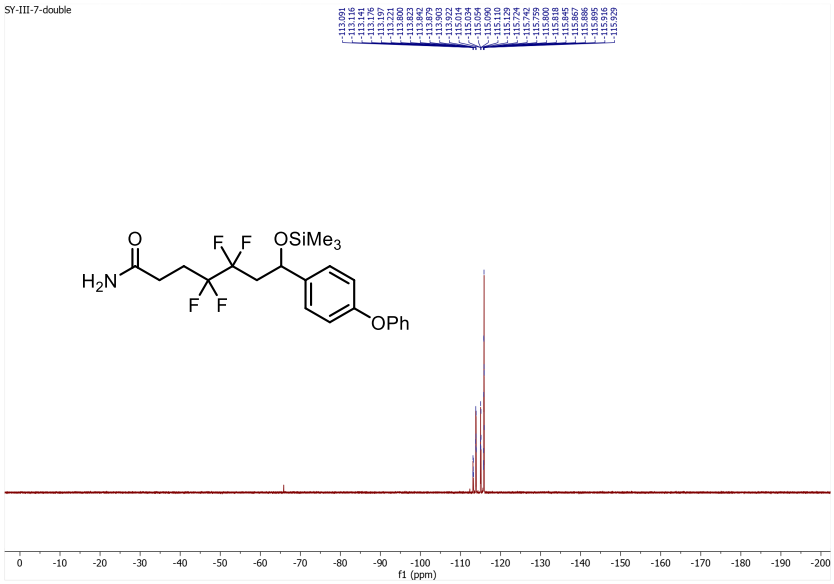


Compound 71. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

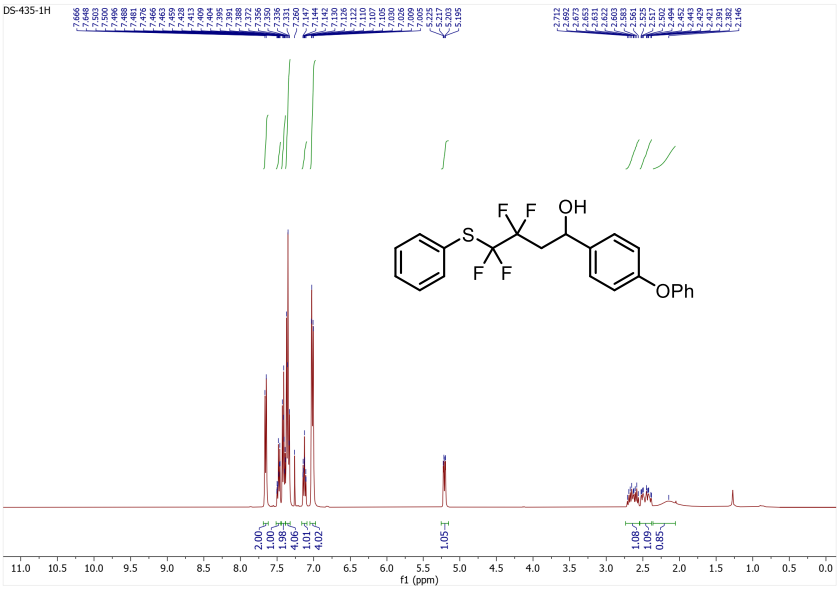


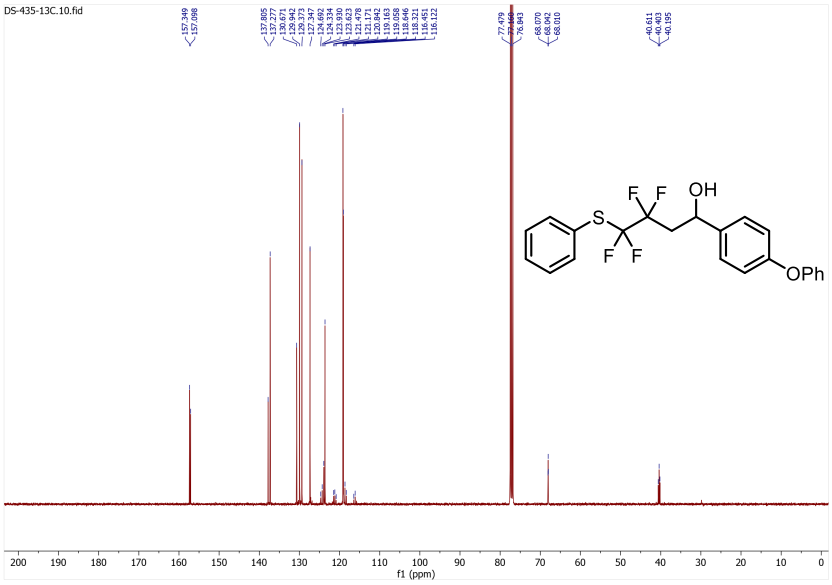


Compound 71. ^{19}F NMR ($CDCl_3$, 376 MHz)

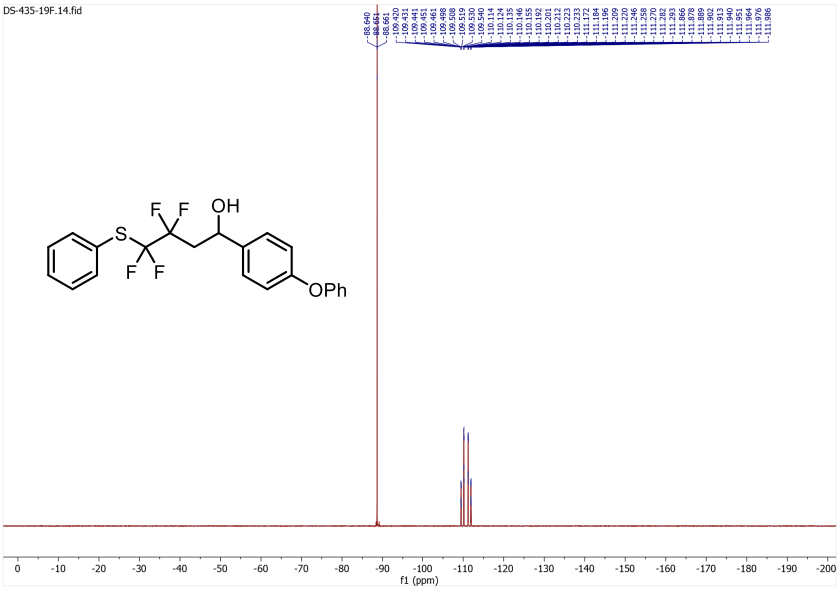


Compound 72. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

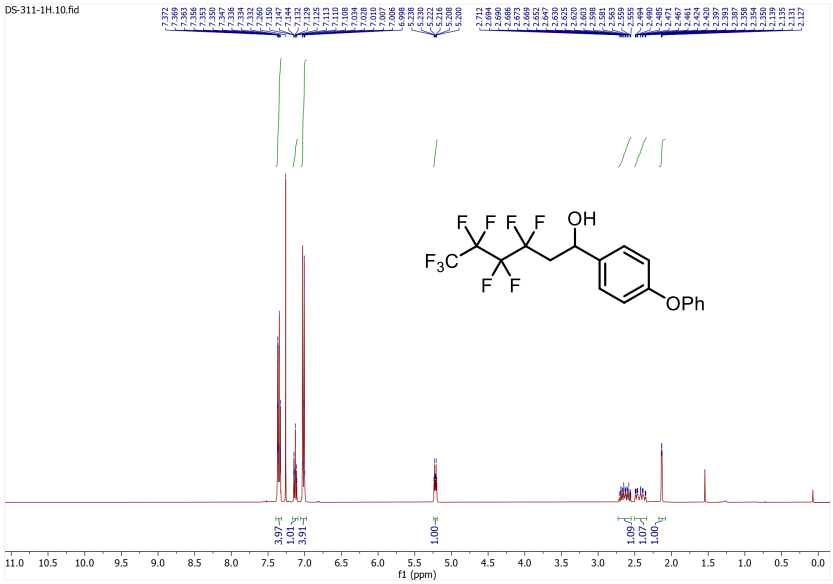


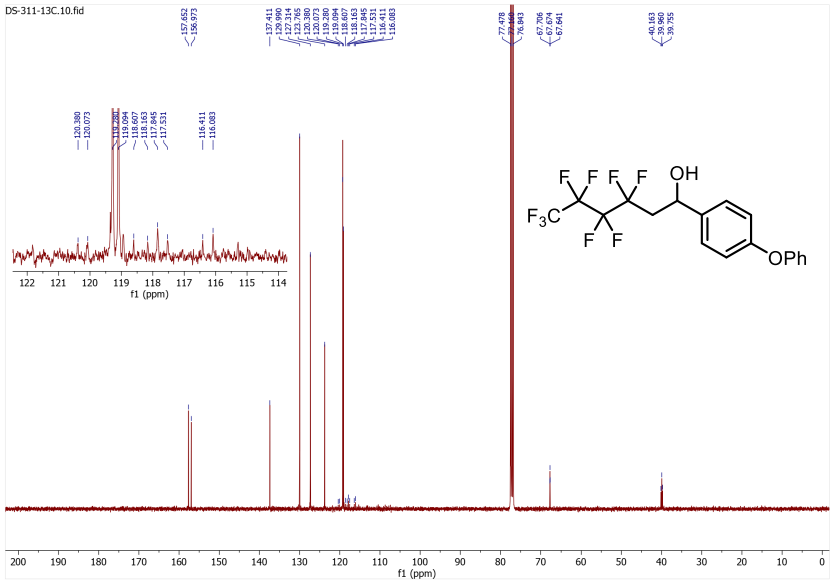


Compound 72. ^{19}F NMR ($CDCl_3$, 376 MHz)

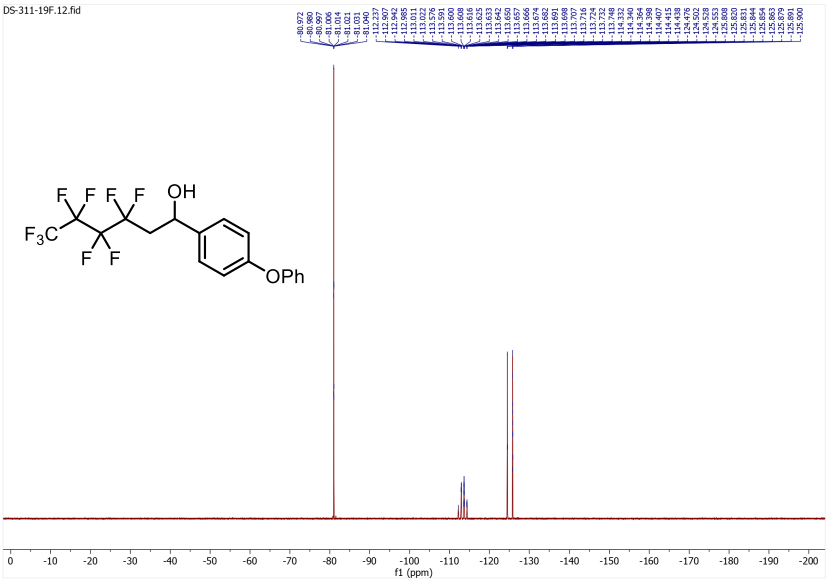


Compound 73. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

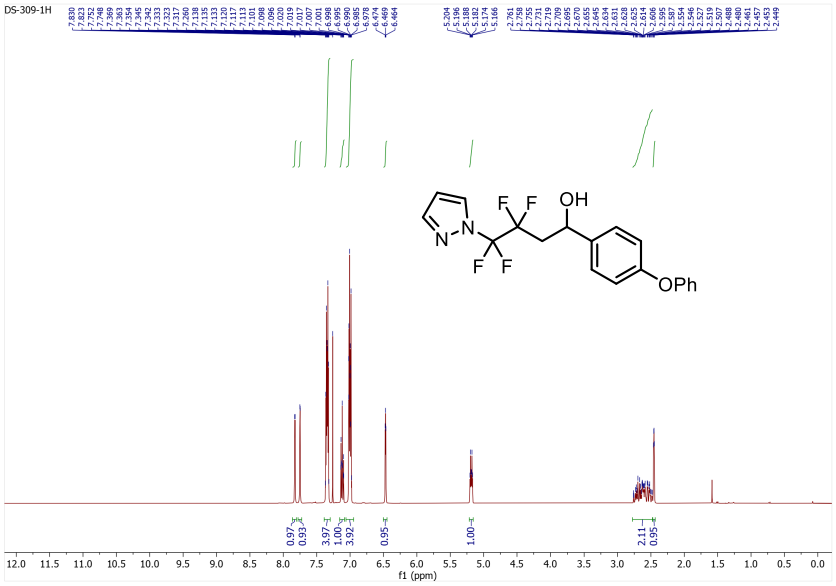


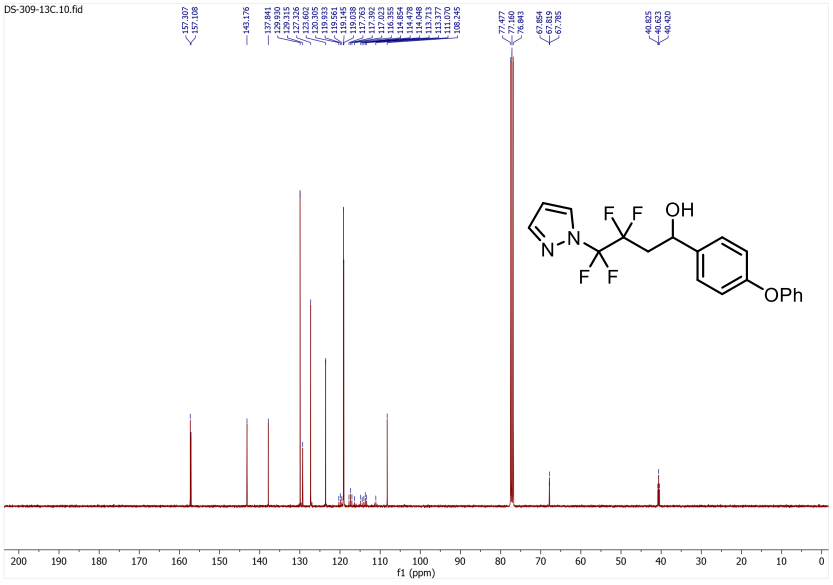


Compound 73. ^{19}F NMR ($CDCl_3$, 376 MHz)

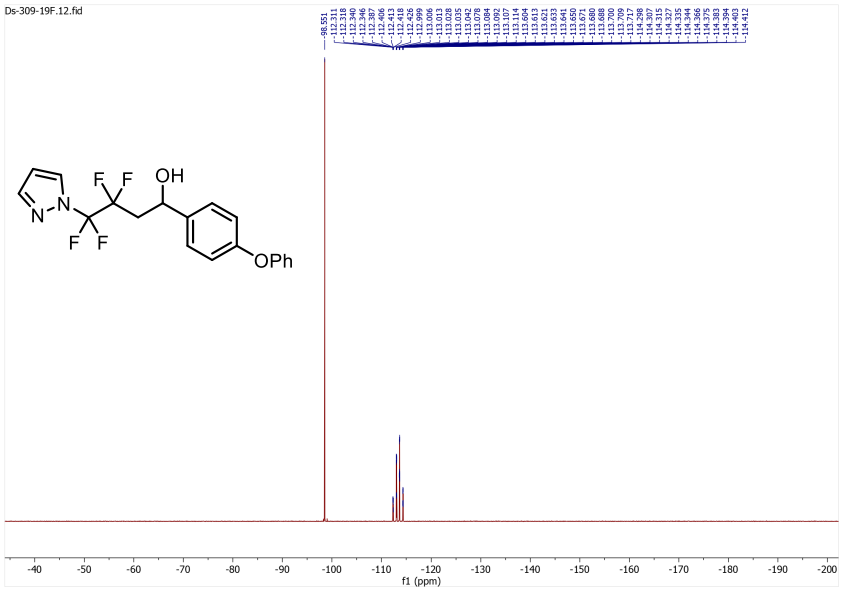


Compound 74. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

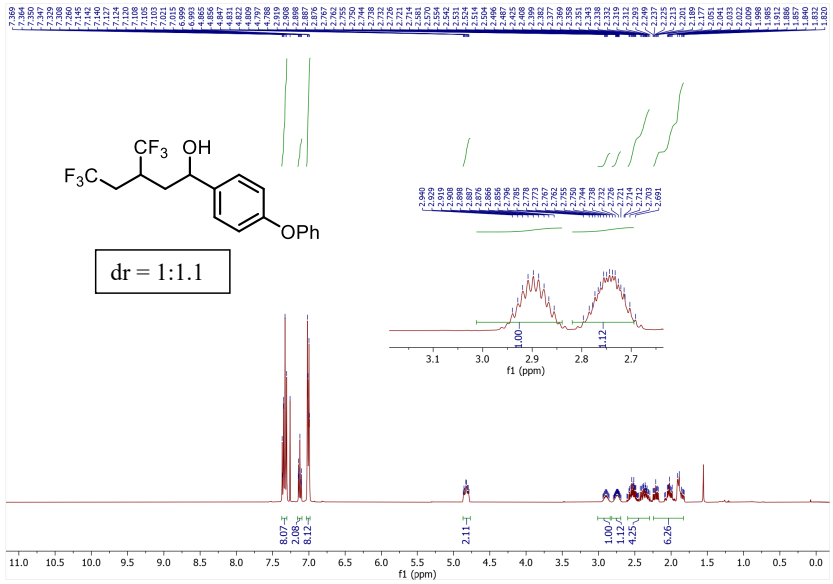


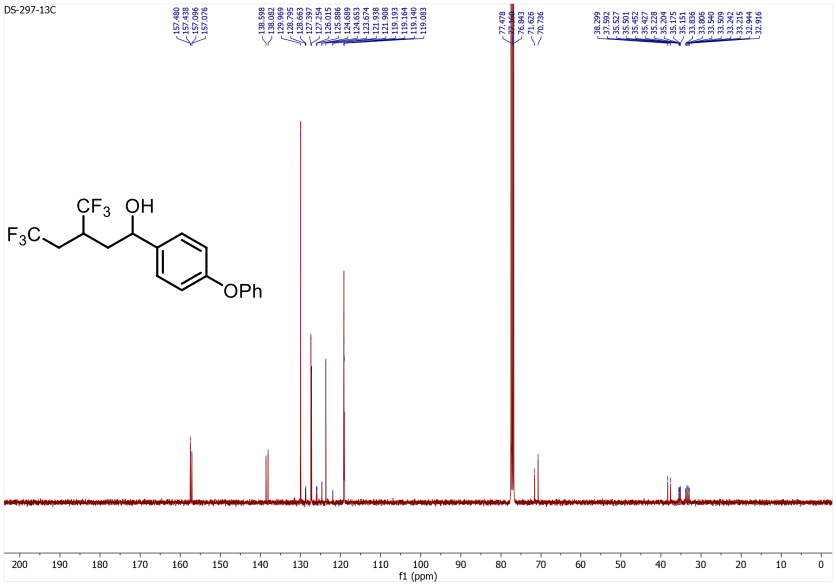


Compound 74. ^{19}F NMR ($CDCl_3$, 376 MHz)

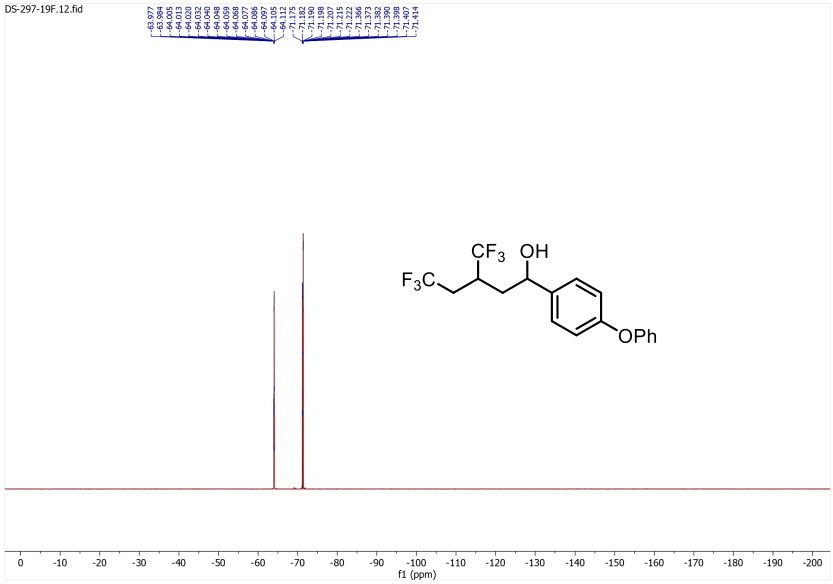


Compound 75. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

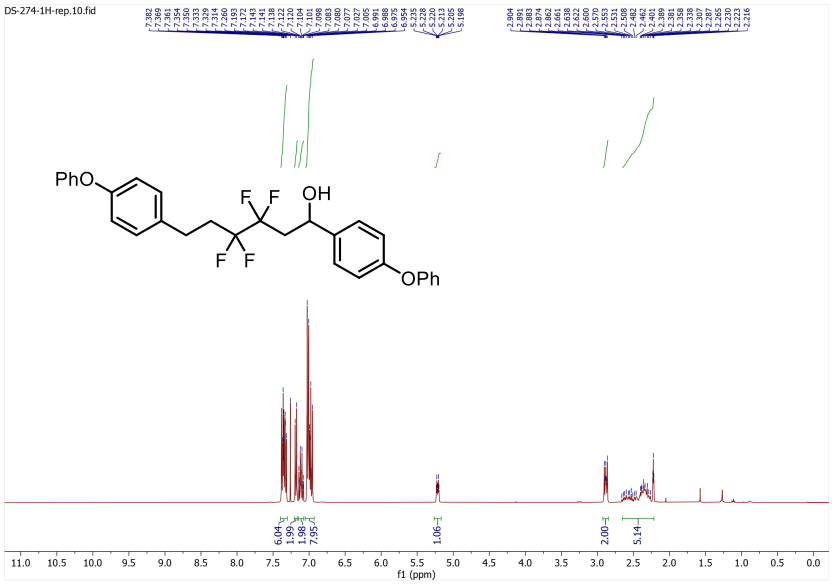


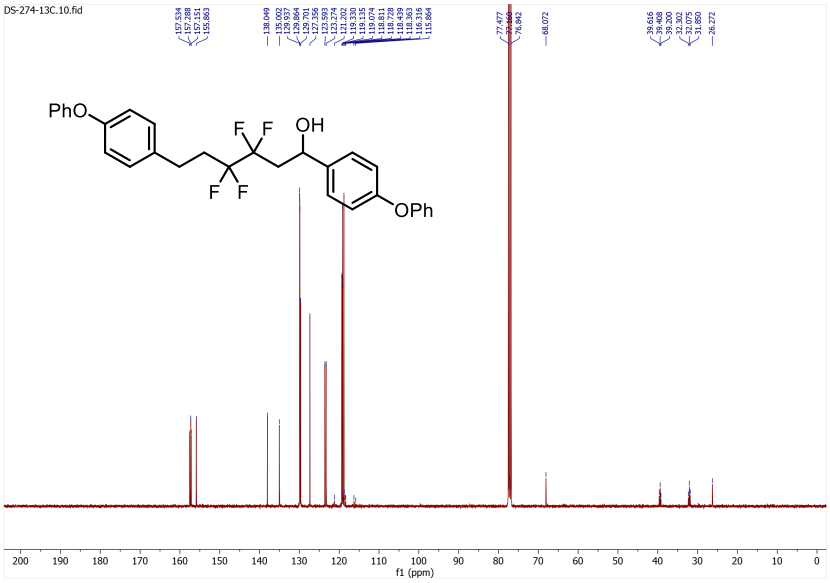


Compound 75. ^{19}F NMR ($CDCl_3$, 376 MHz)

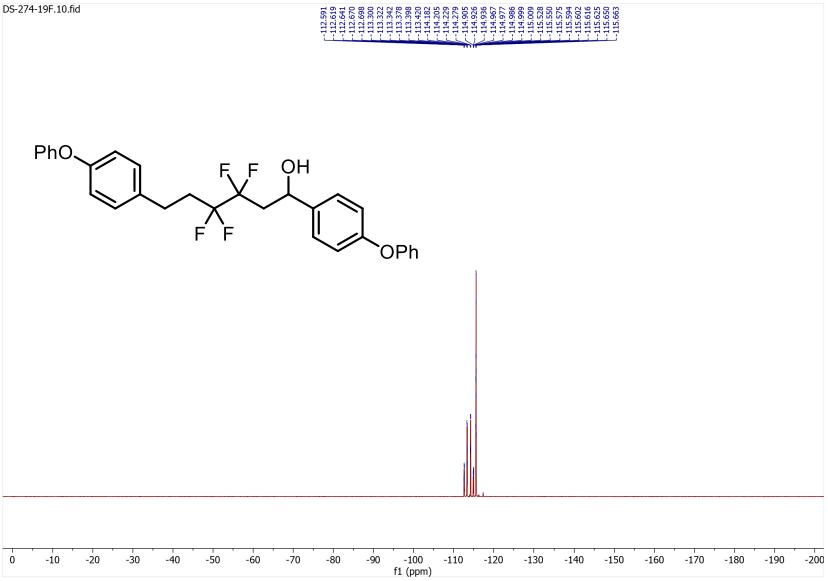


Compound 76. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

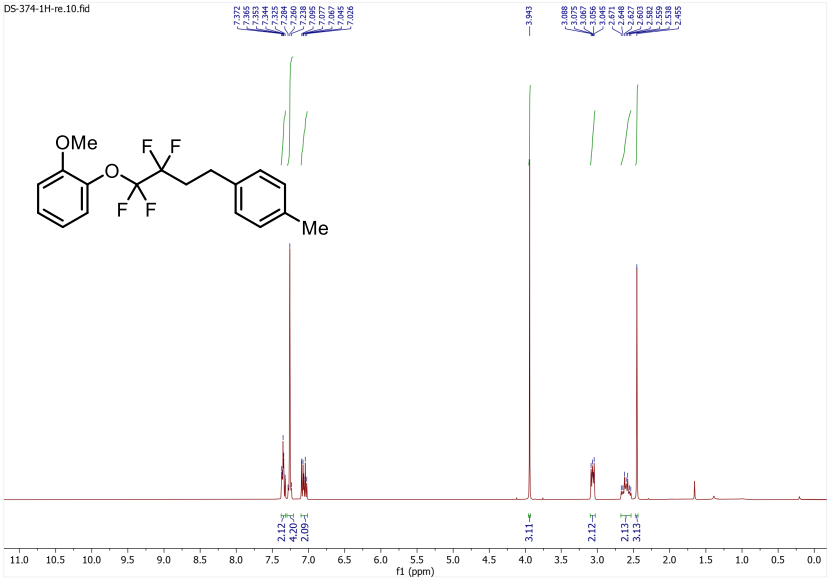


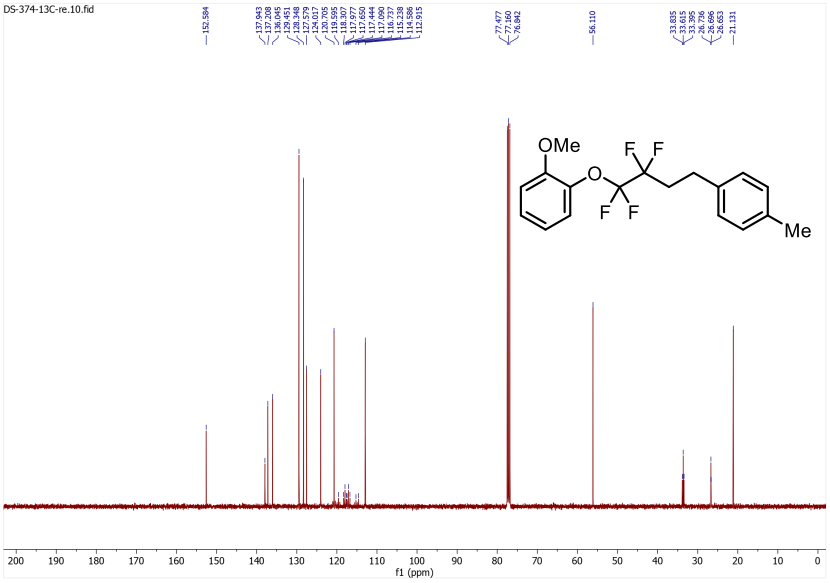


Compound 76. ^{19}F NMR ($CDCl_3$, 376 MHz)

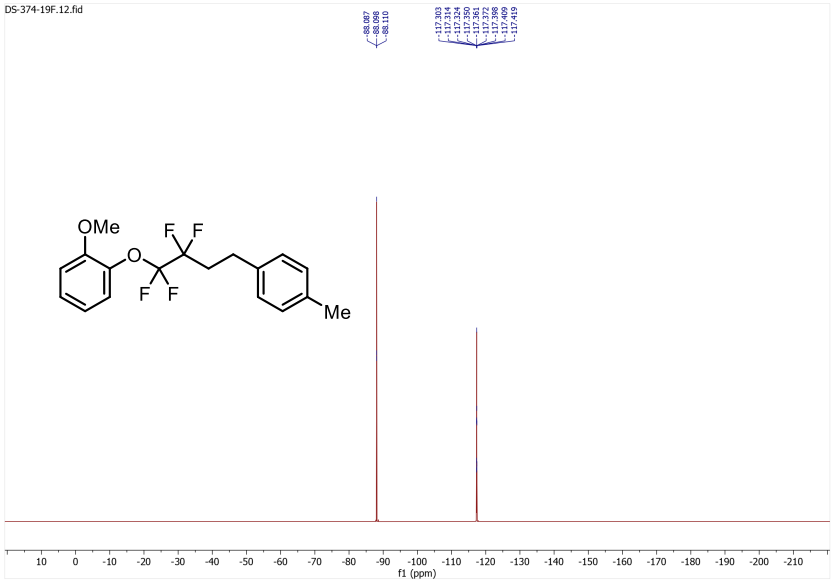


Compound 78. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

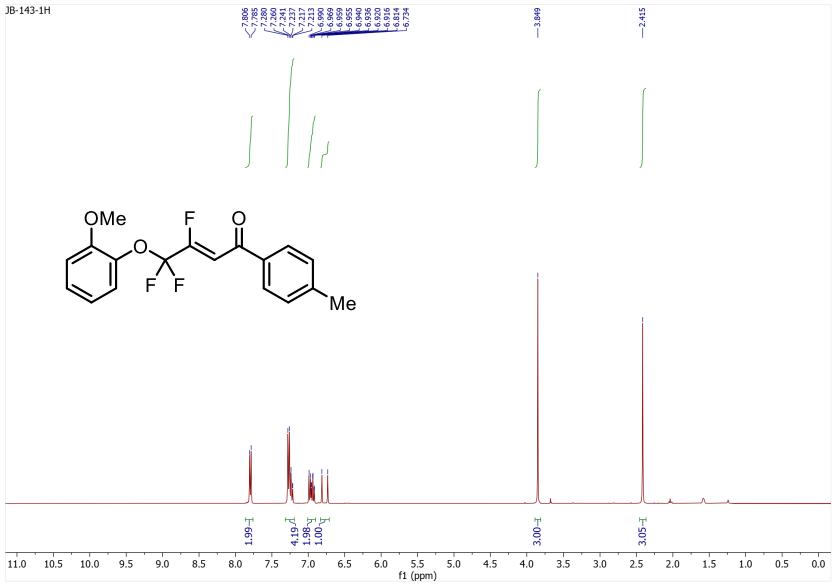


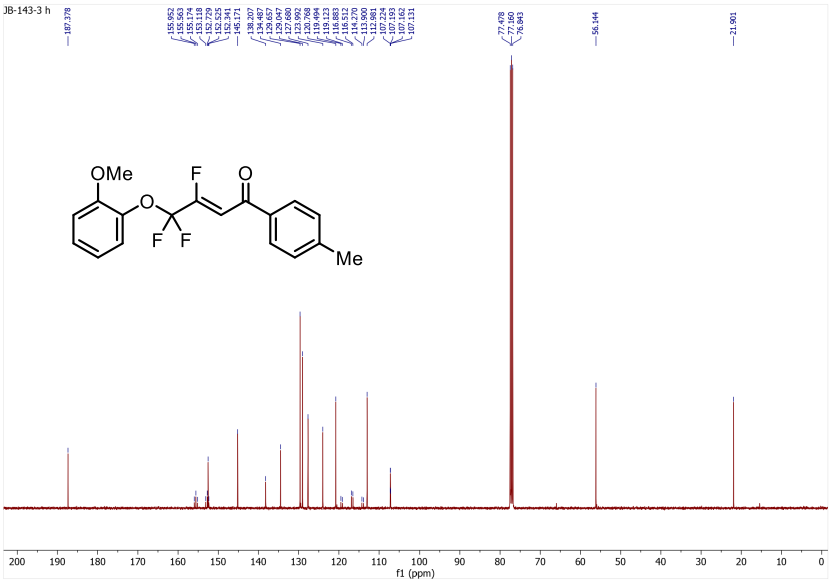


Compound 78. ^{19}F NMR ($CDCl_3$, 376 MHz)

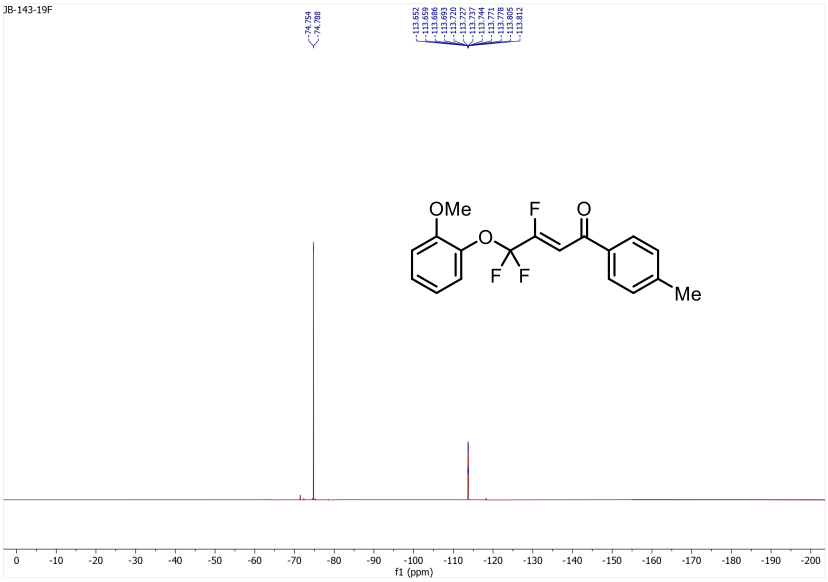


Compound 79. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

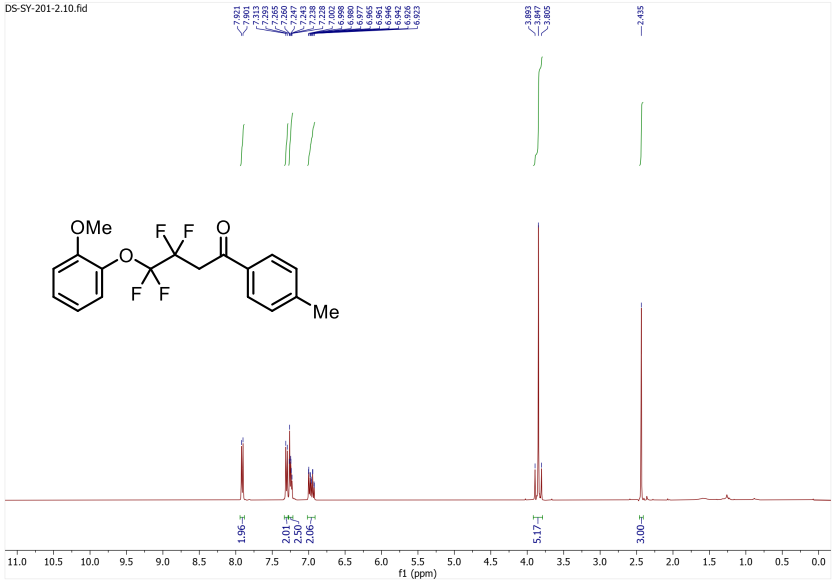


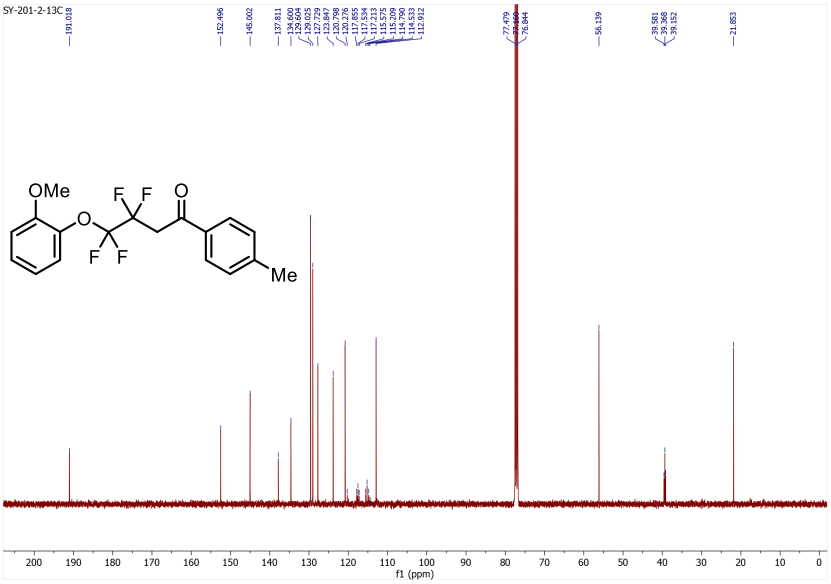


Compound 79. ^{19}F NMR ($CDCl_3$, 376 MHz)

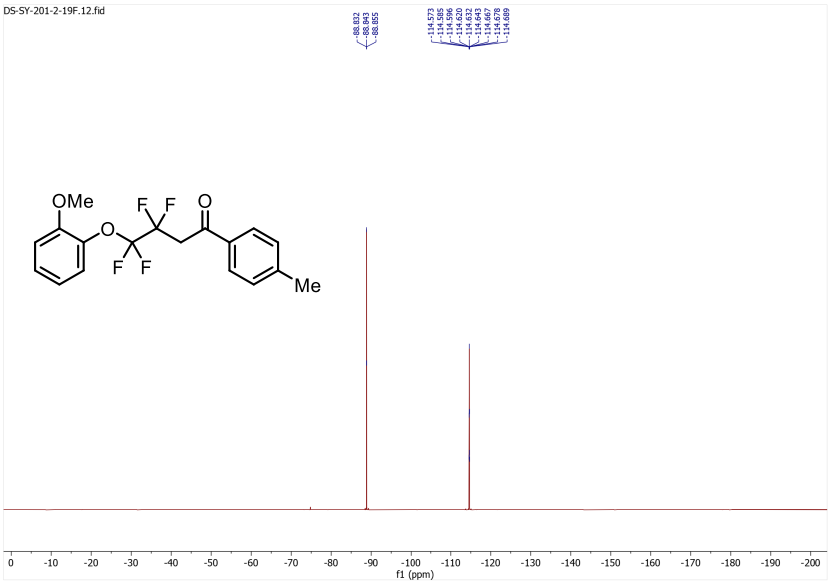


Compound 80. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

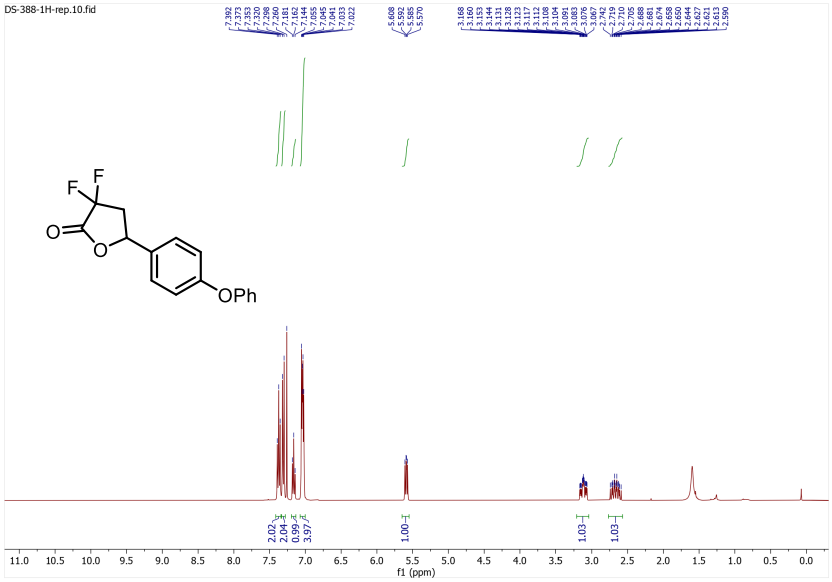


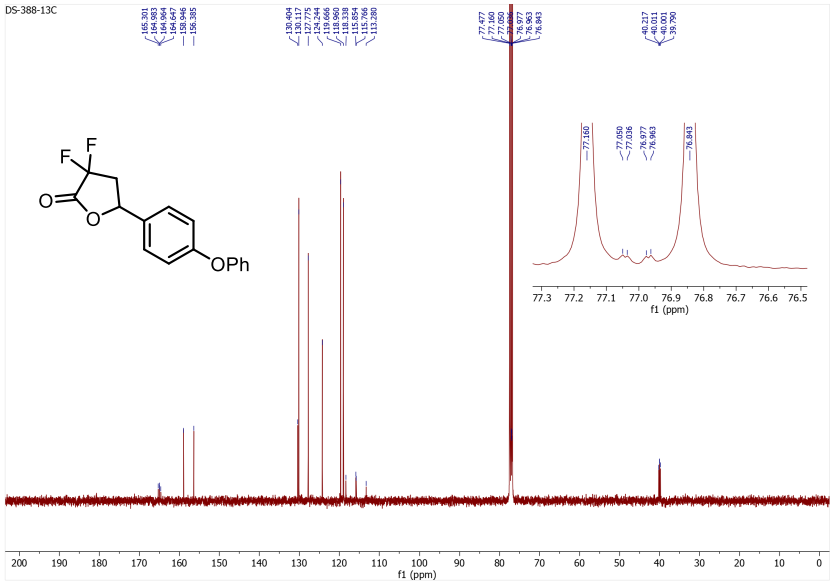


Compound 80. ^{19}F NMR ($CDCl_3$, 376 MHz)

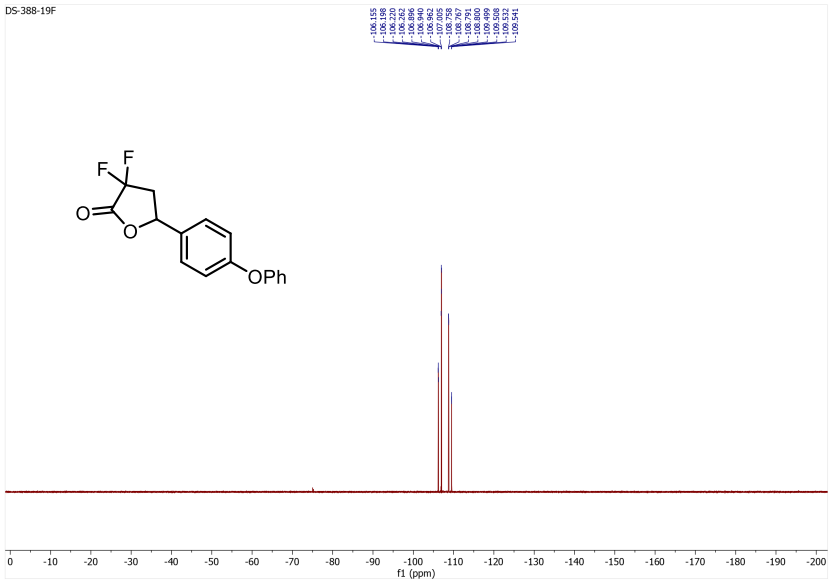


Compound 81. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

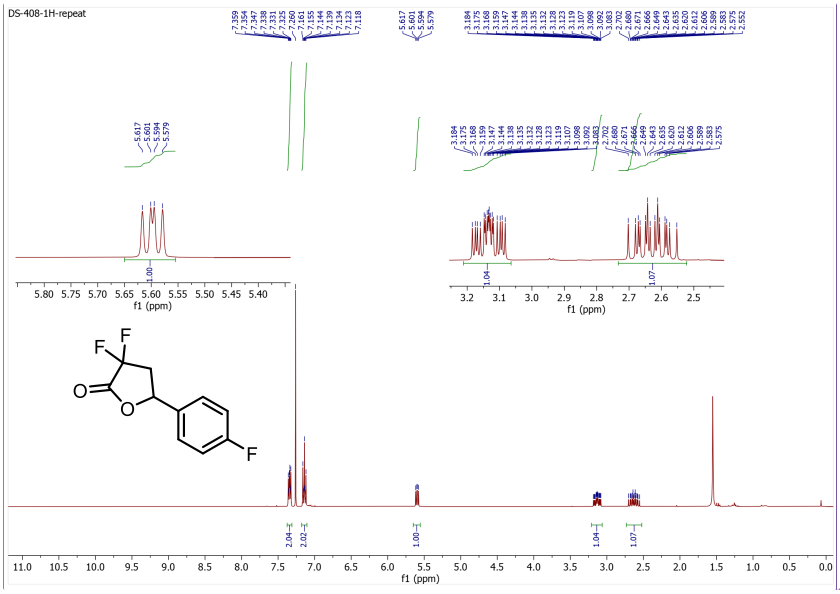


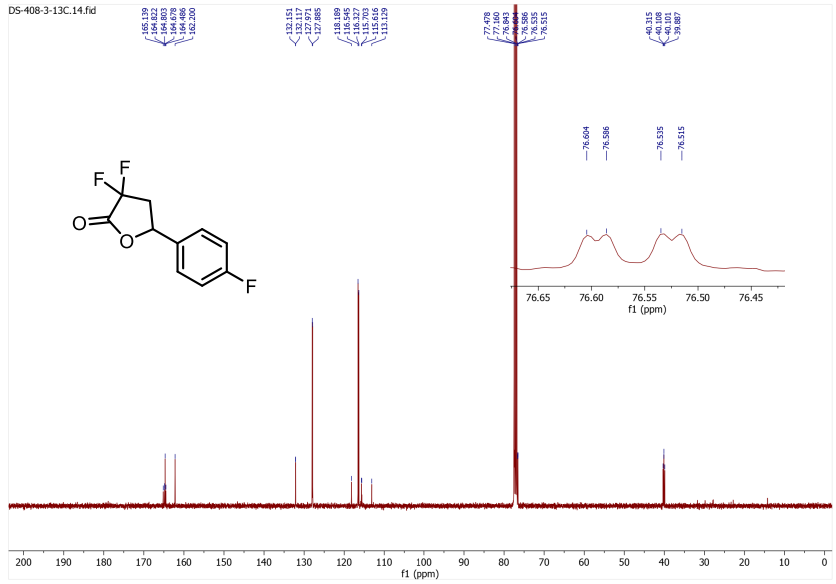


Compound 81. ^{19}F NMR ($CDCl_3$, 376 MHz)



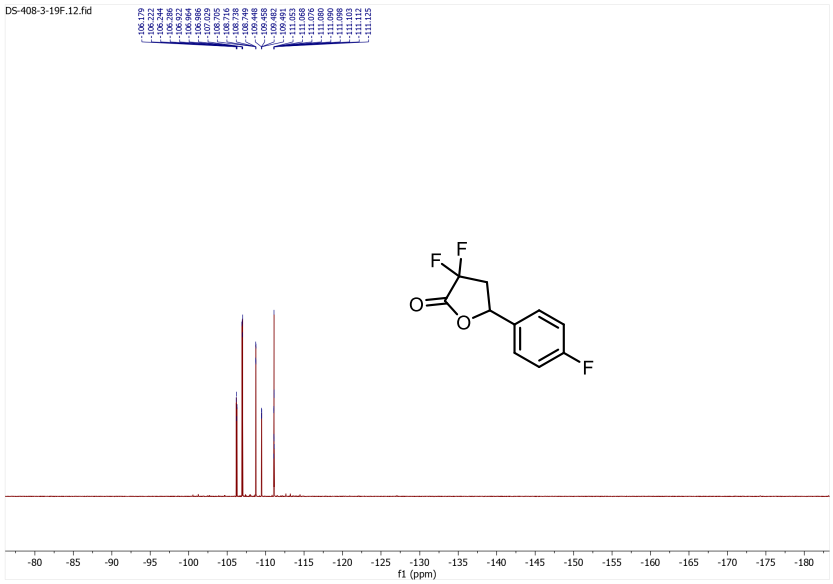
Compound 82. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)



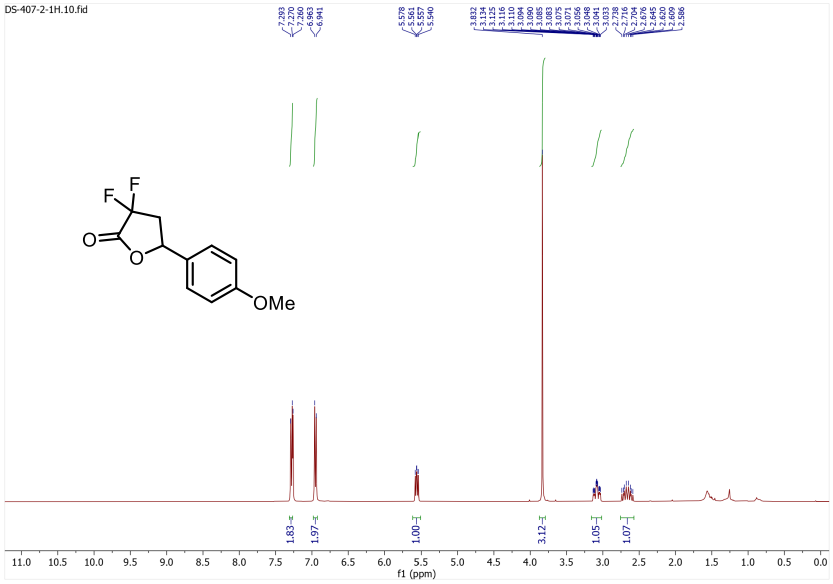


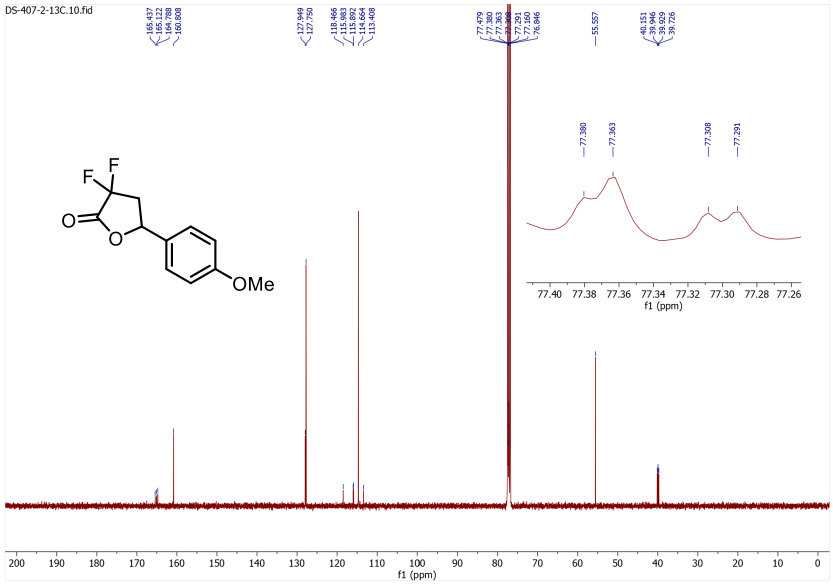
Commented [DS11]: Updated spectra

Compound 82. ^{19}F NMR ($CDCl_3$, 376 MHz)

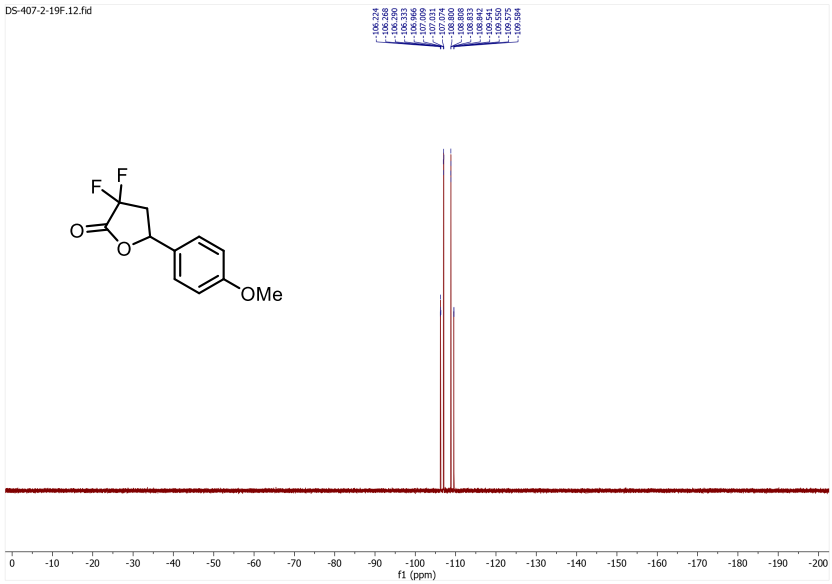


Compound 83. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

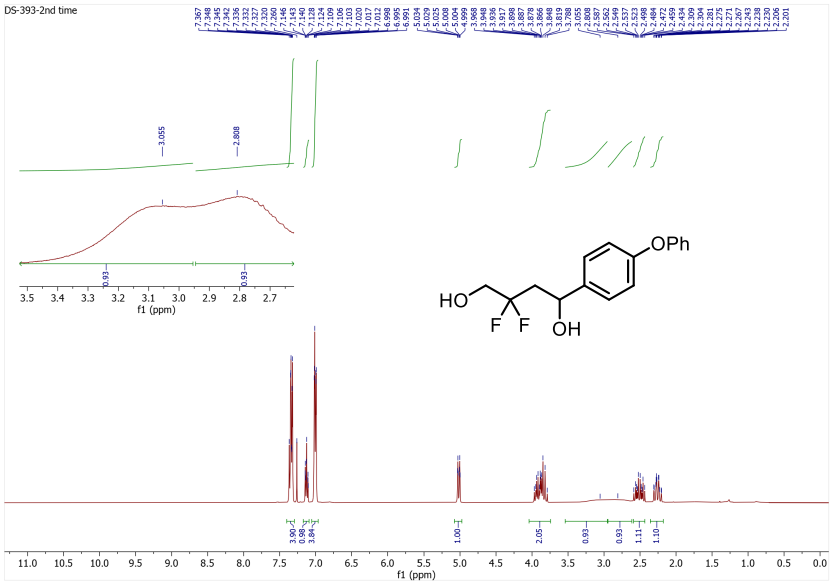


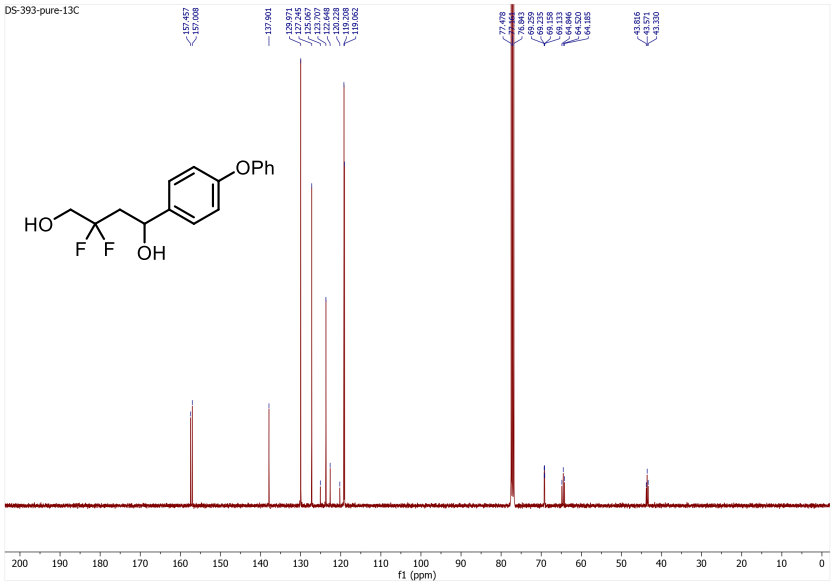


Compound 83. ^{19}F NMR ($CDCl_3$, 376 MHz)

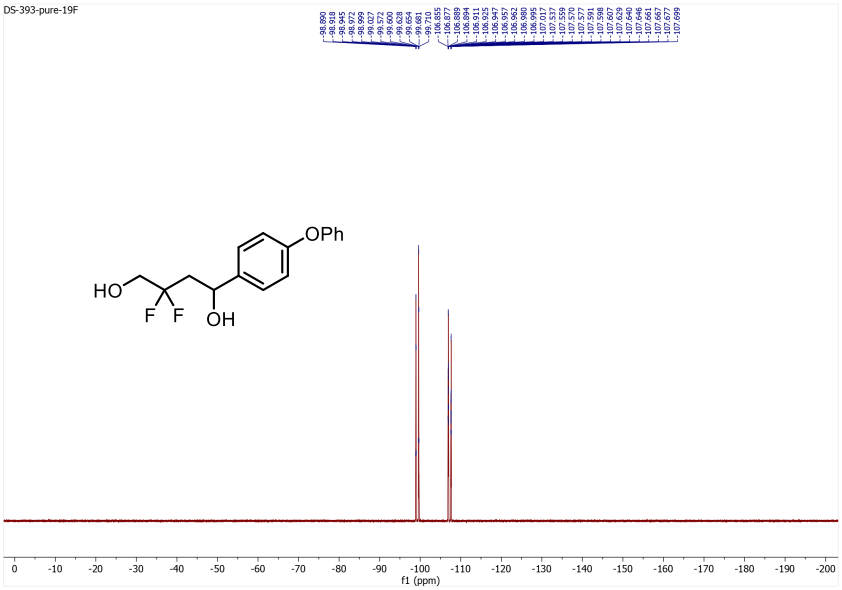


Compound 84. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

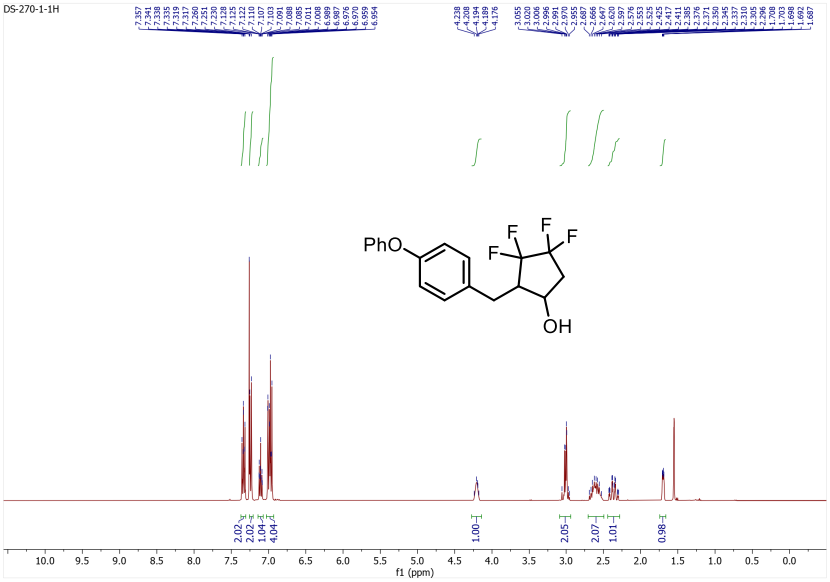


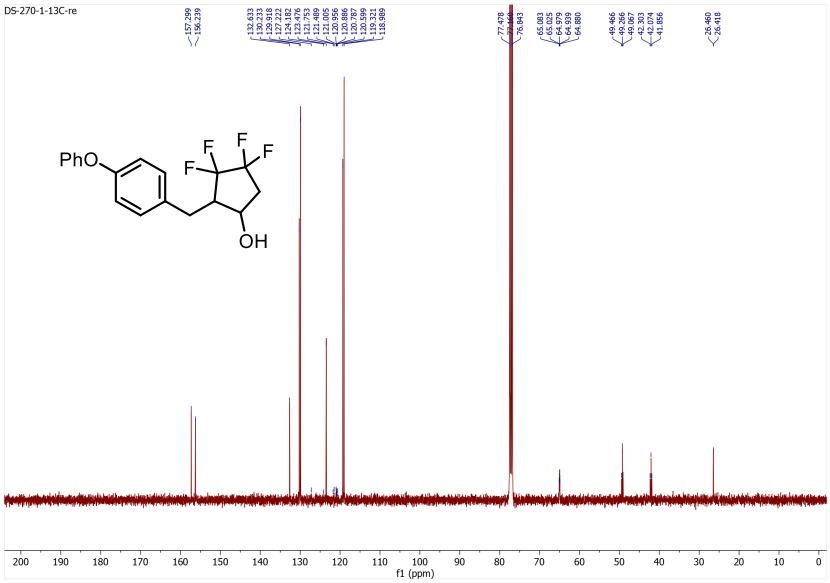


Compound 84. ^{19}F NMR ($CDCl_3$, 376 MHz)

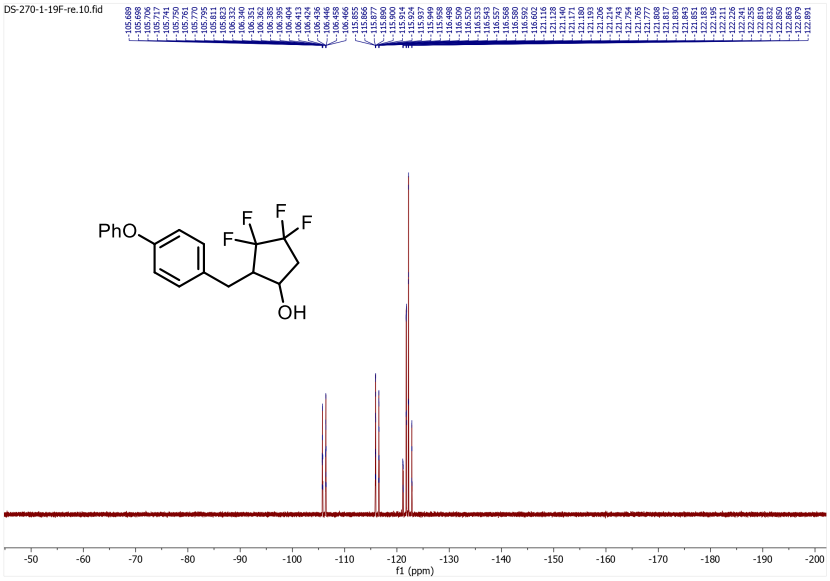


Compound 85. Top: (major) ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

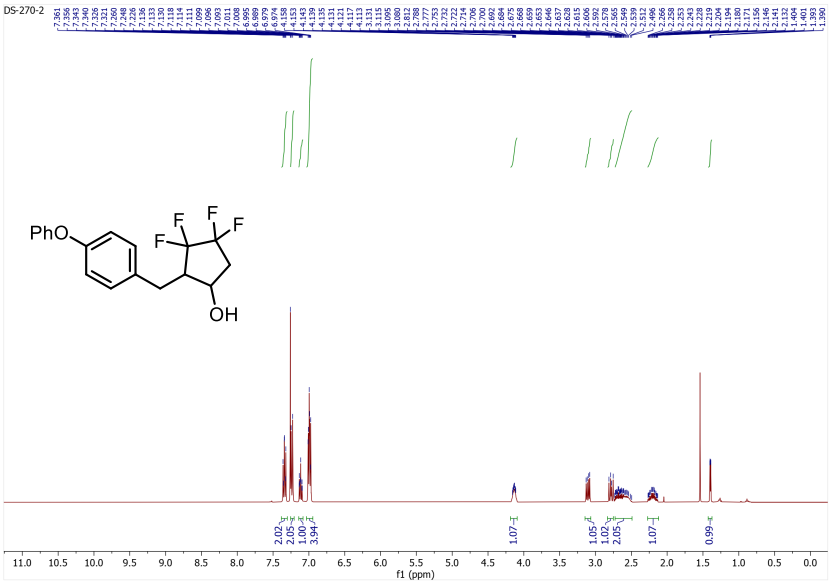


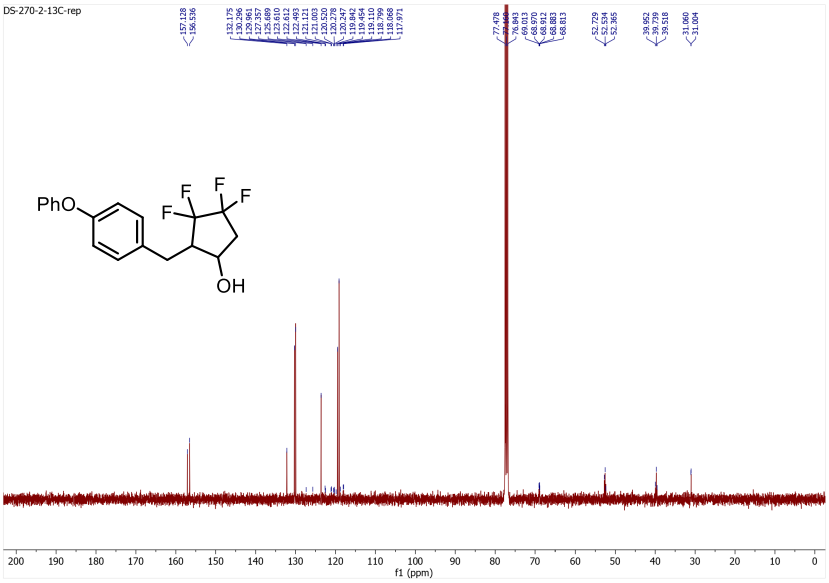


Compound 85. (major) ^{19}F NMR ($CDCl_3$, 376 MHz)

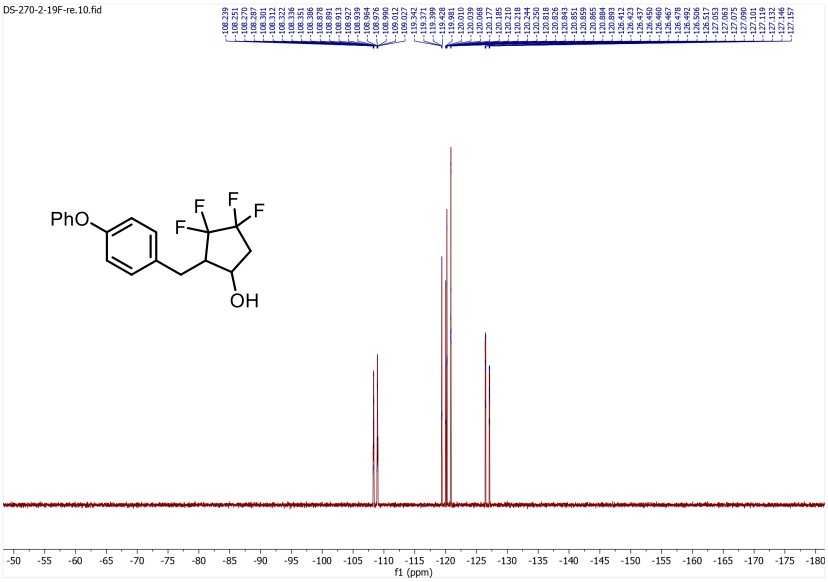


Compound 85. Top: (minor) ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

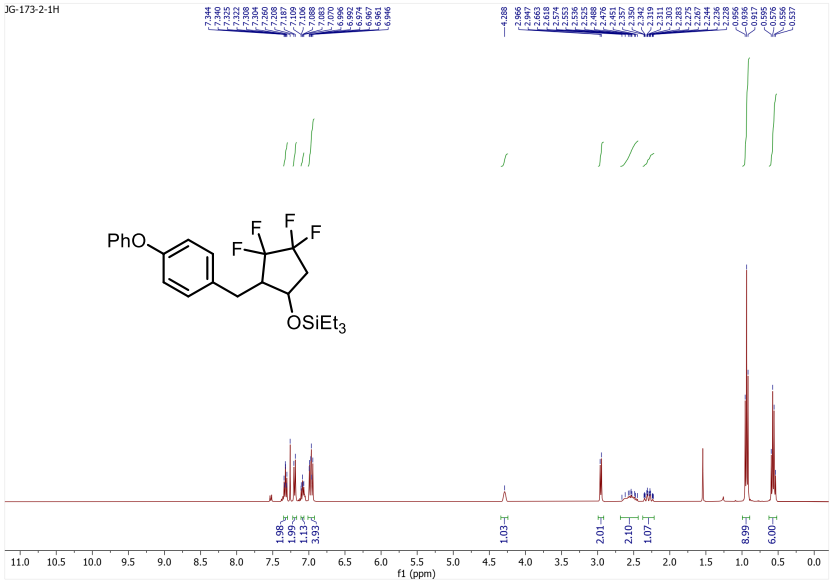


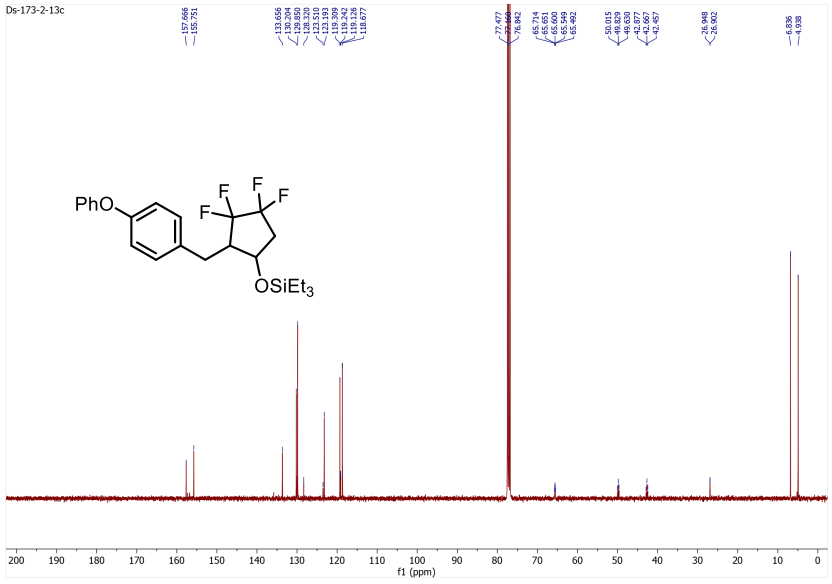


Compound 85. (minor) ^{19}F NMR ($CDCl_3$, 376 MHz)

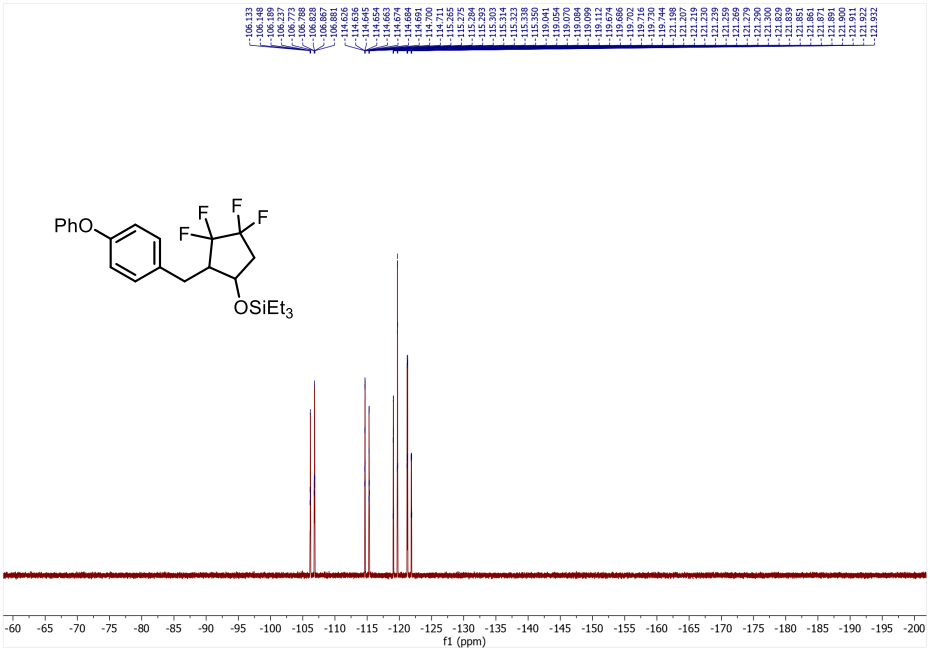


Compound 86. Top: (major) ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

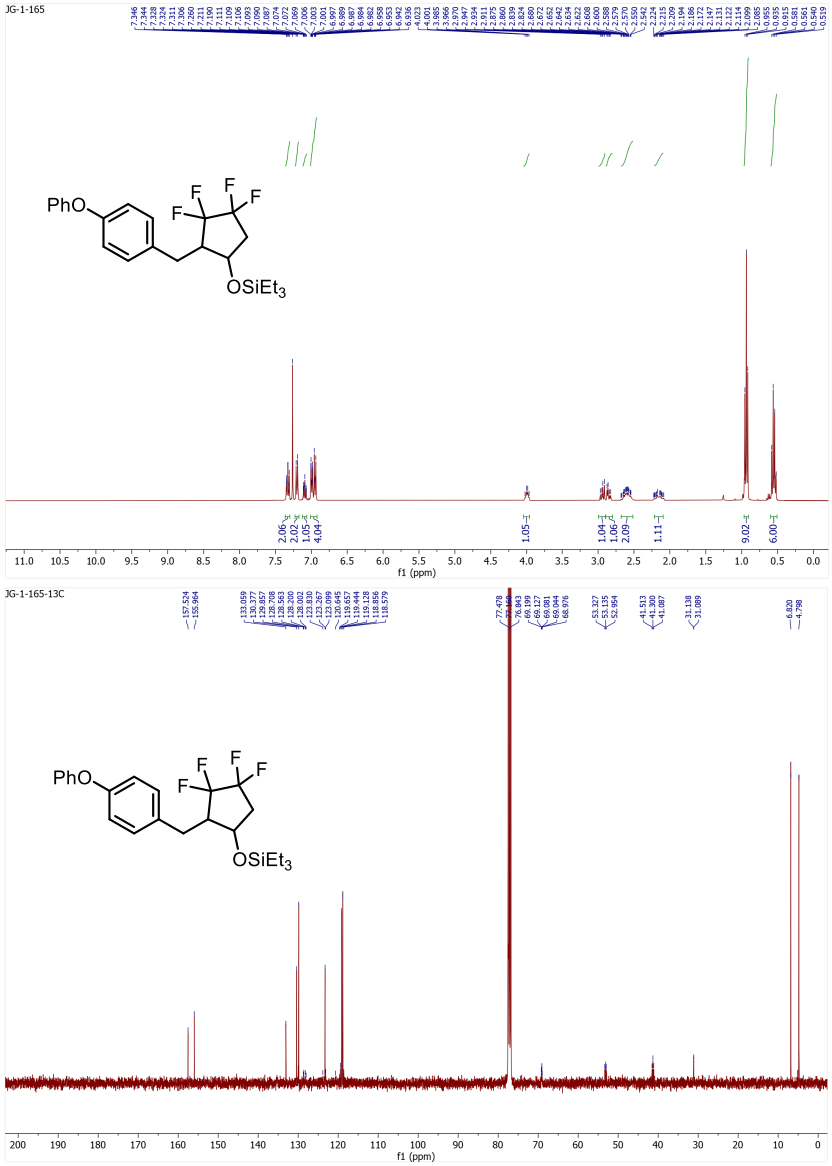




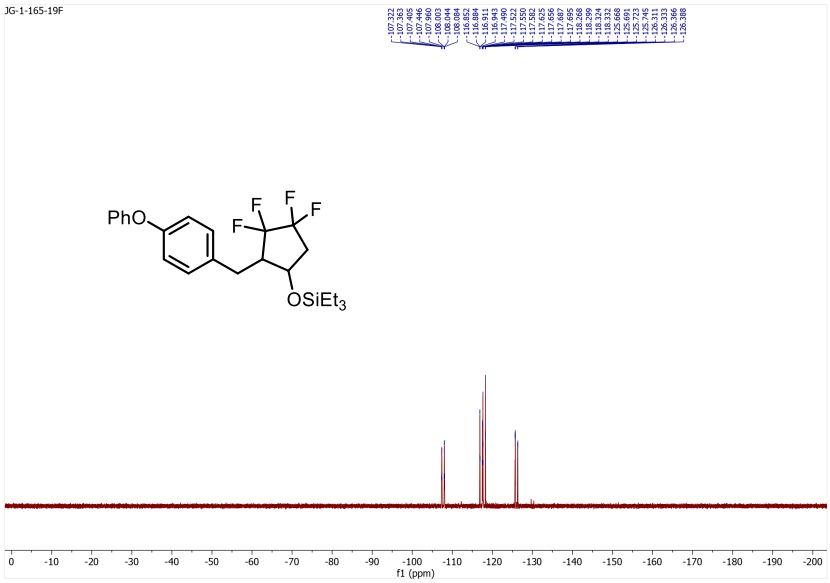
Compound 86. (major) ^{19}F NMR ($CDCl_3$, 376 MHz)



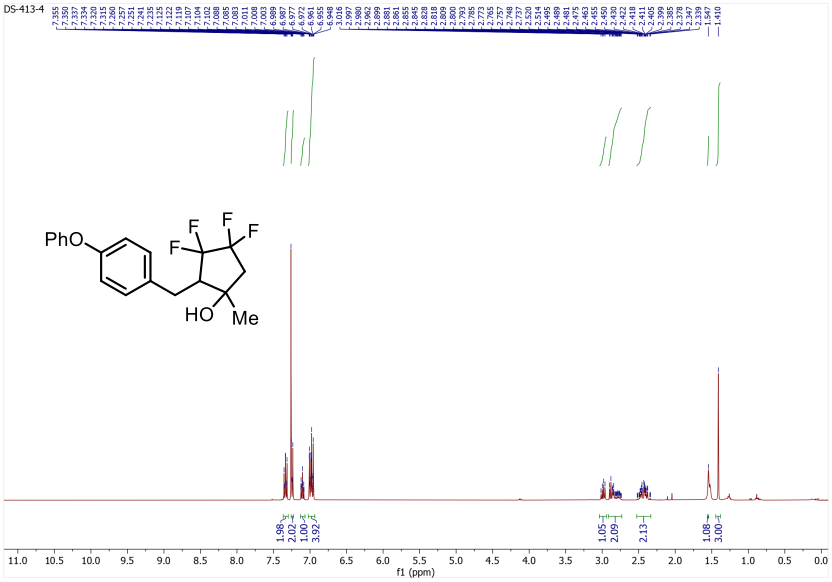
Compound 86. Top: (minor) ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

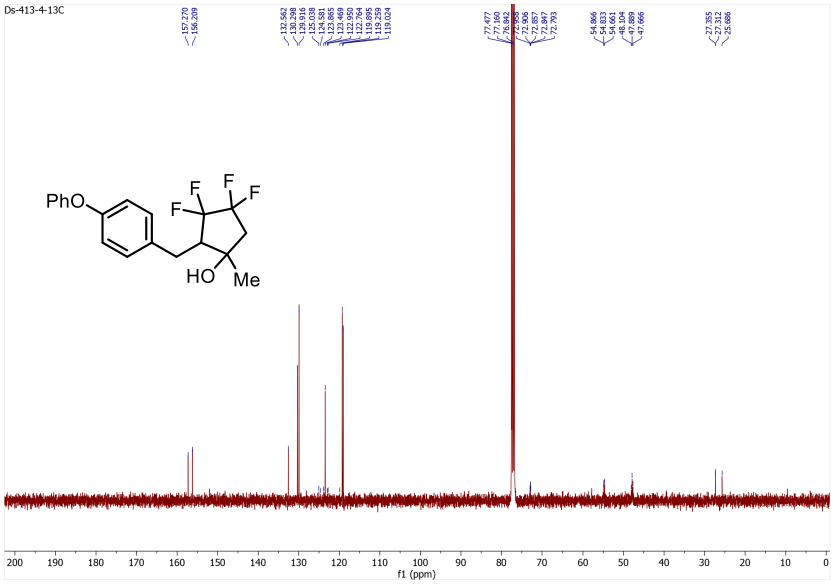


Compound 86. (minor) ^{19}F NMR ($CDCl_3$, 376 MHz)

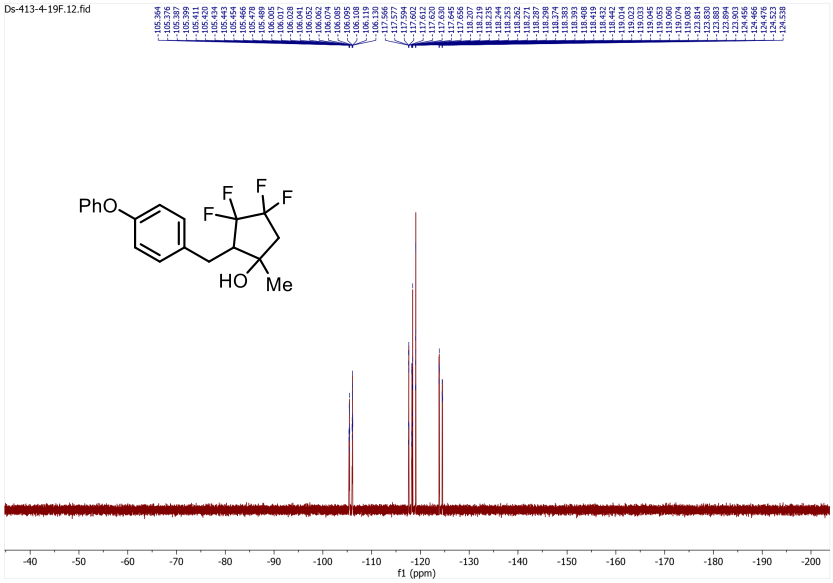


Compound 87. Top: (major) ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

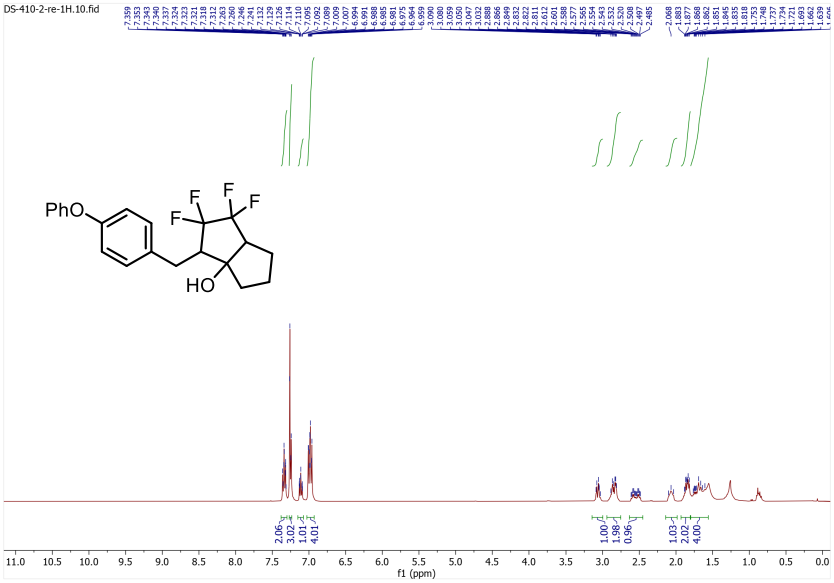


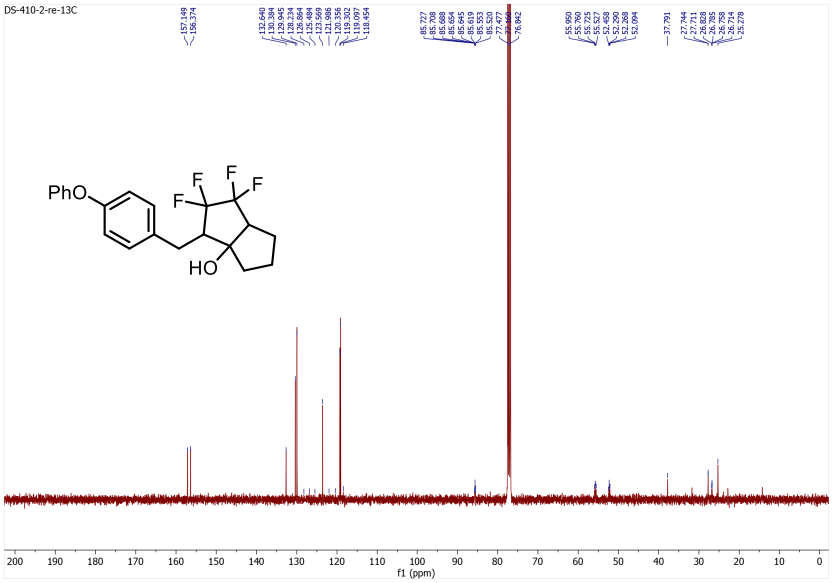


Compound 87. (major) ^{19}F NMR ($CDCl_3$, 376 MHz)

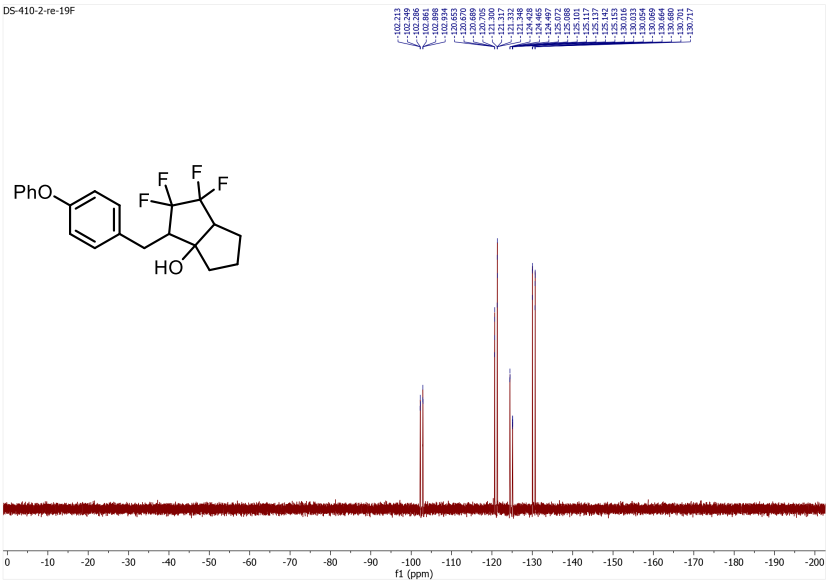


Compound 88. Top: (major) ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

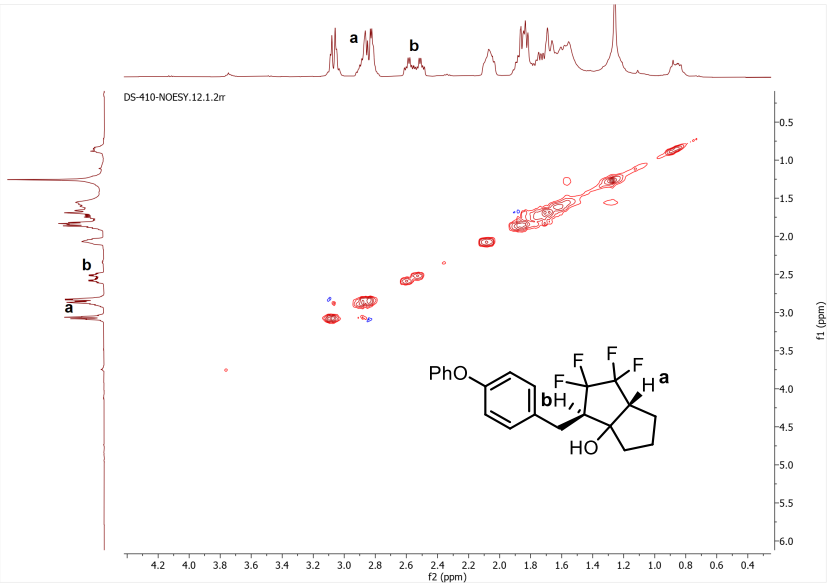




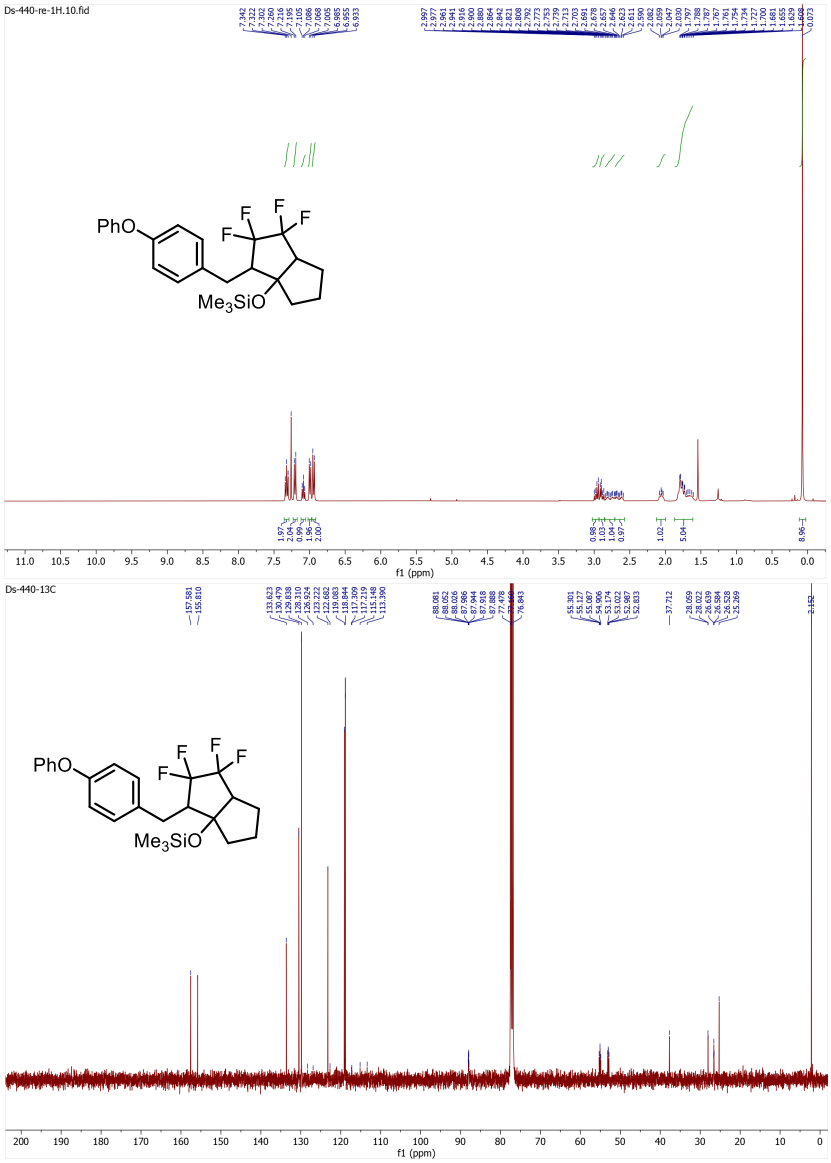
Compound 88. (major) ^{19}F NMR ($CDCl_3$, 376 MHz).



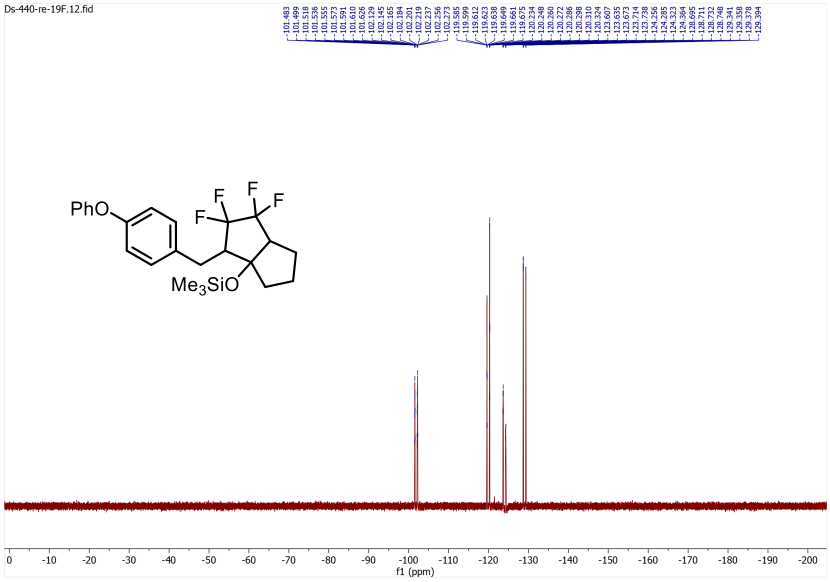
Compound 88. (major) NOESY ($CDCl_3$, 400 MHz)



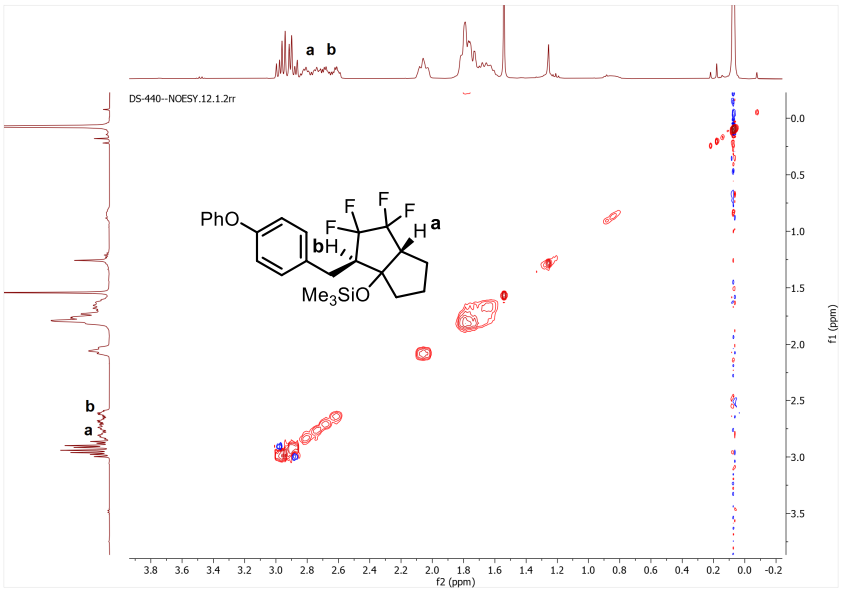
Compound 89. Top: (major) ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)



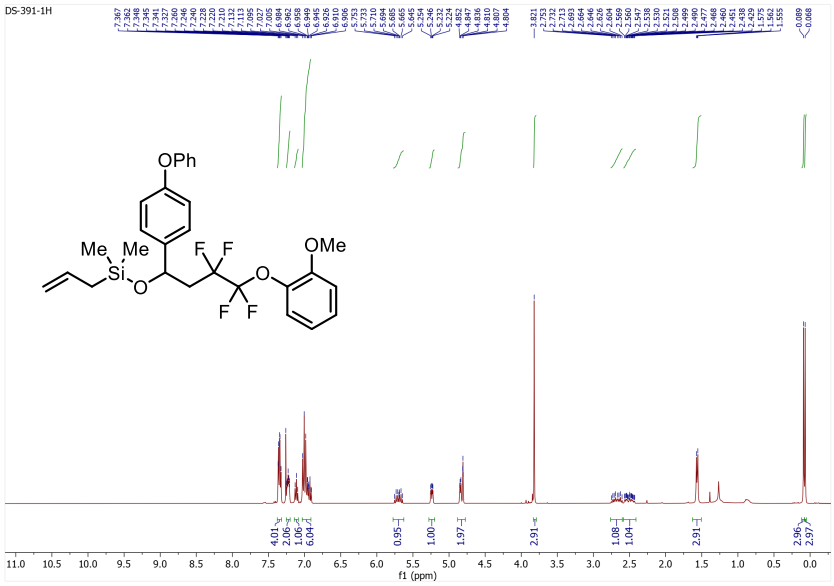
Compound 89. (major) ^{19}F NMR ($CDCl_3$, 376 MHz)

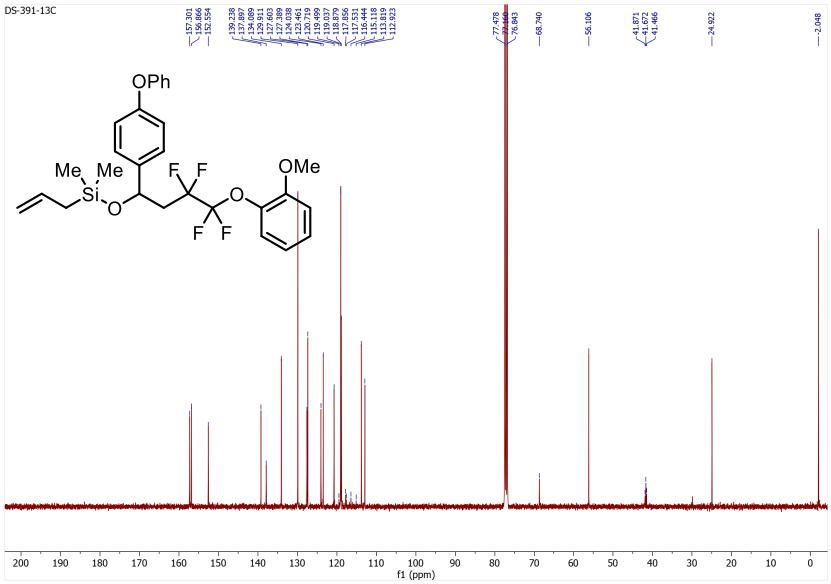


Compound 89. (major) NOESY ($CDCl_3$, 400 MHz)

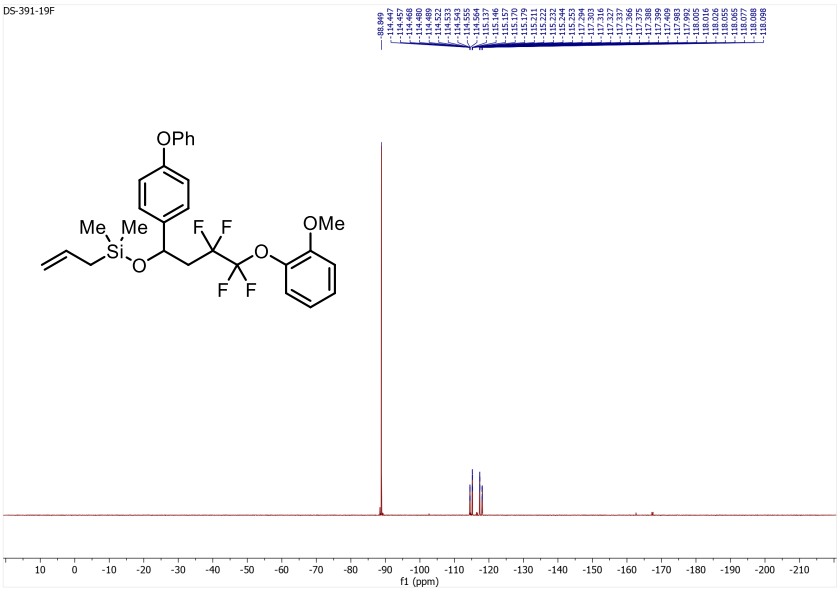


Compound 90. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

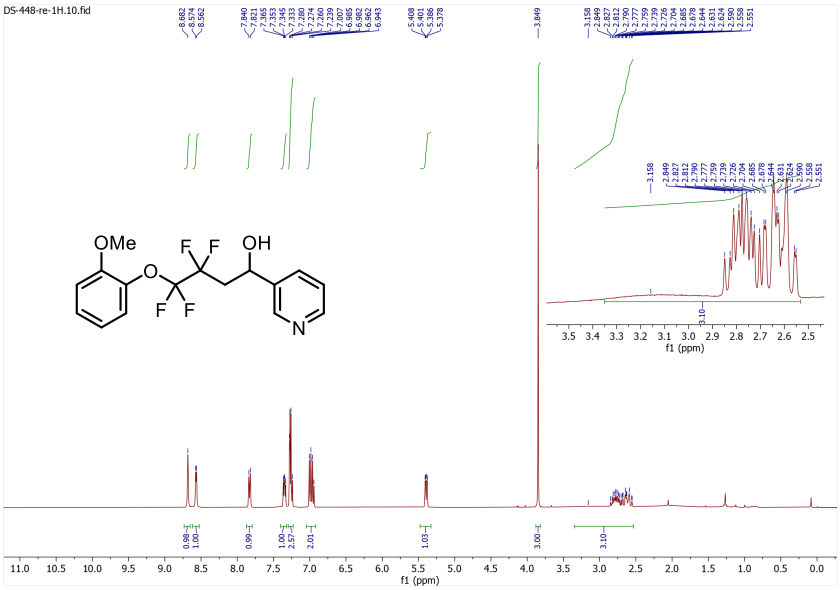


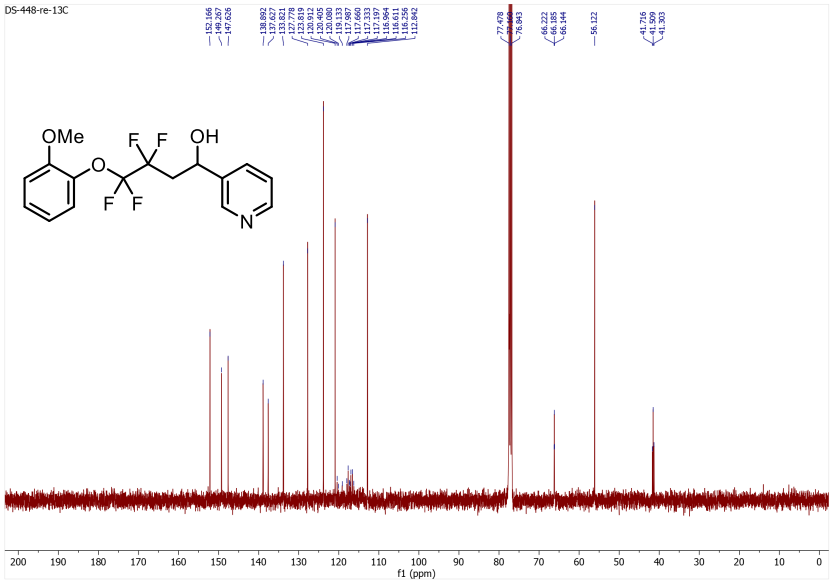


Compound 90. ^{19}F NMR ($CDCl_3$, 376 MHz)

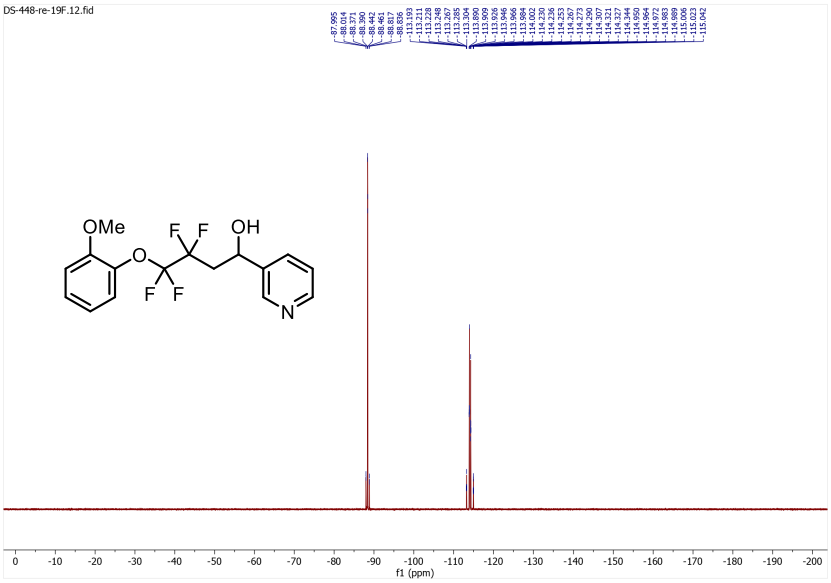


Compound P1. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

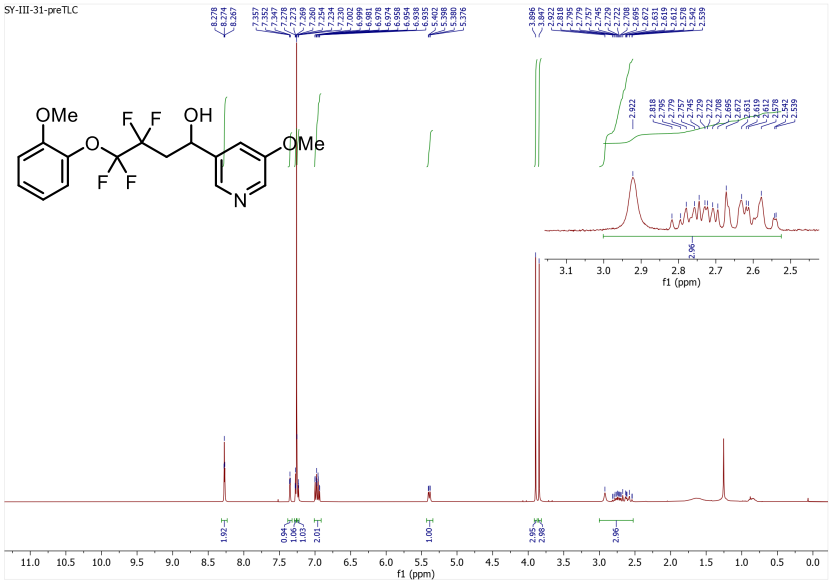


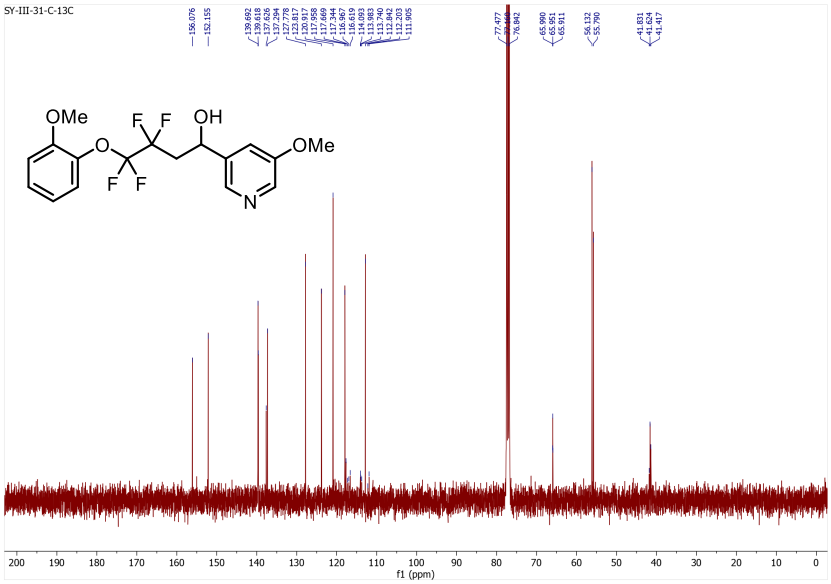


Compound P1. ^{19}F NMR ($CDCl_3$, 376 MHz)

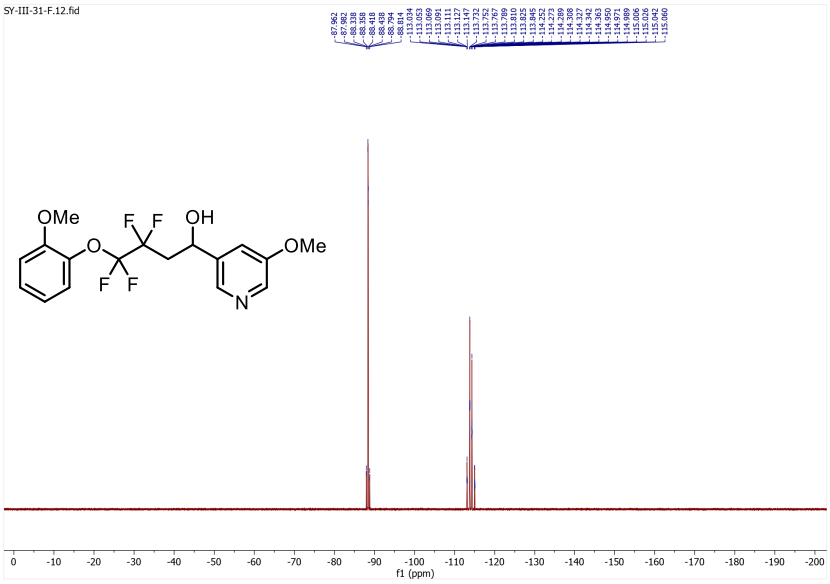


Compound P2. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

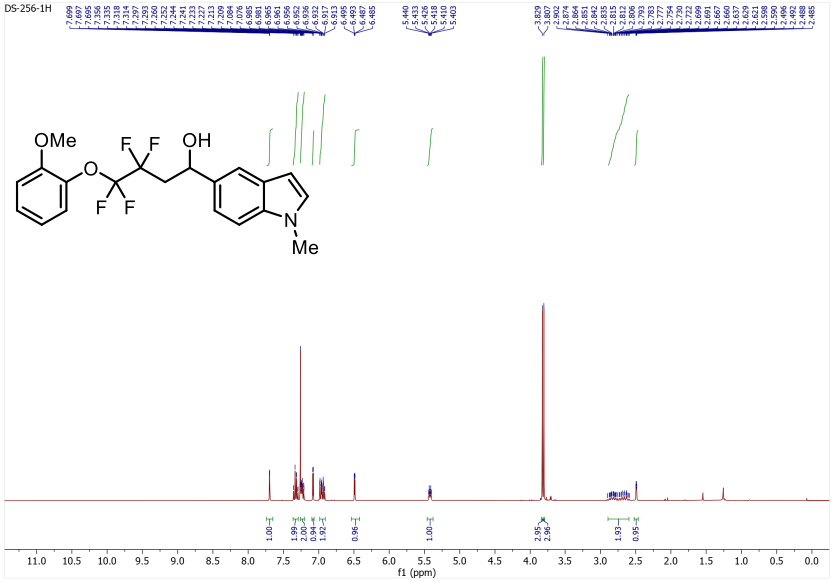


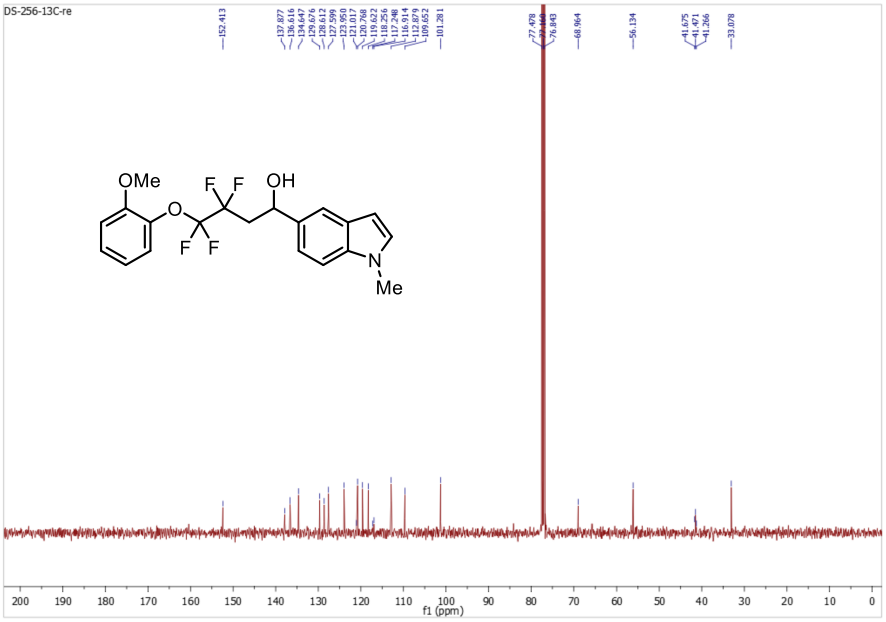


Compound P2. ^{19}F NMR ($CDCl_3$, 376 MHz)

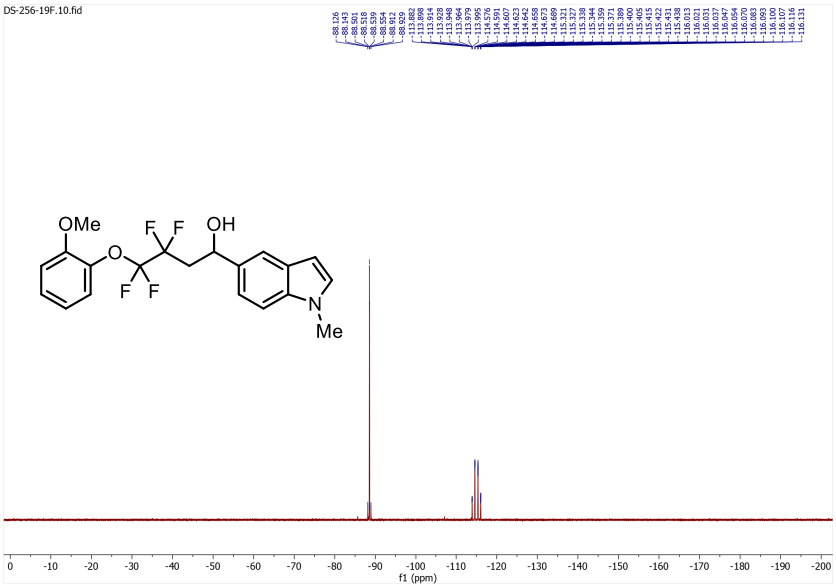


Compound P3. Top: ^{1}H NMR ($CDCl_3$, 400 MHz). Bottom: ^{13}C NMR ($CDCl_3$, 100 MHz)

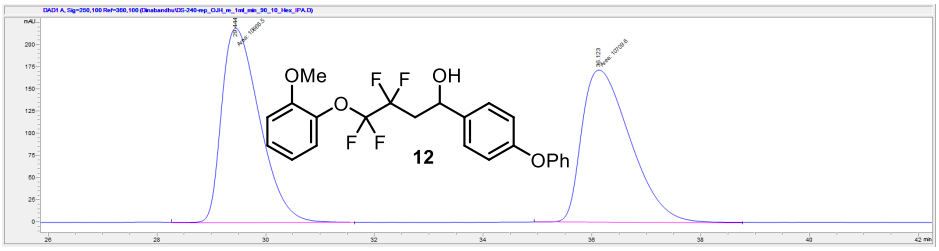




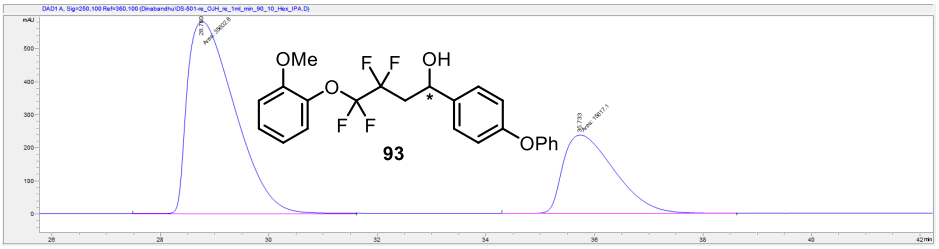
Compound P3. ^{19}F NMR ($CDCl_3$, 376 MHz)



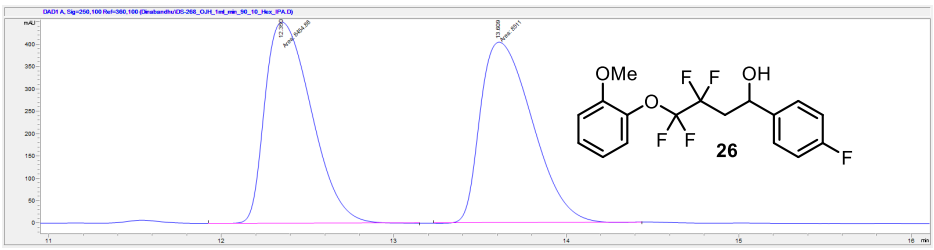
10. Chiral HPLC Traces



#	Time	Type	Area	Height	Width	Area%	Symmetry
1	29.444	MM	10666.5	219.7	0.8091	49.899	0.575
2	36.123	MM	10709.6	171.9	1.0382	50.101	0.531

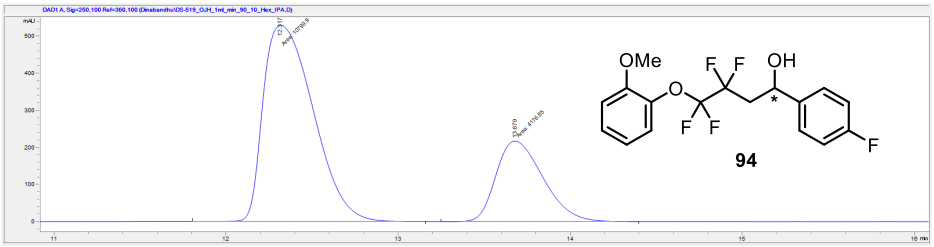


#	Time	Type	Area	Height	Width	Area%	Symmetry
1	28.76	MM	35602.8	582.5	1.0186	69.510	0.437
2	35.733	MM	15617.1	236.9	1.0989	30.490	0.486



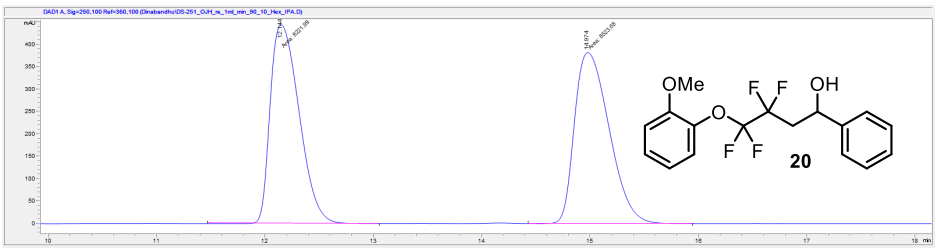
26

#	Time	Type	Area	Height	Width	Area%	Symmetry
1	12.35	MM	8454.9	451	0.3125	49.835	0.567
2	13.609	MM	8511	404.8	0.3504	50.165	0.55

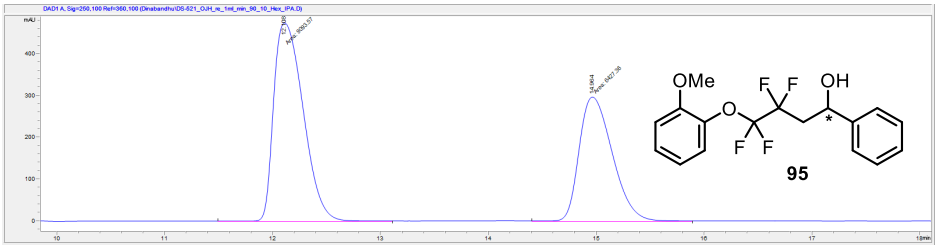


94

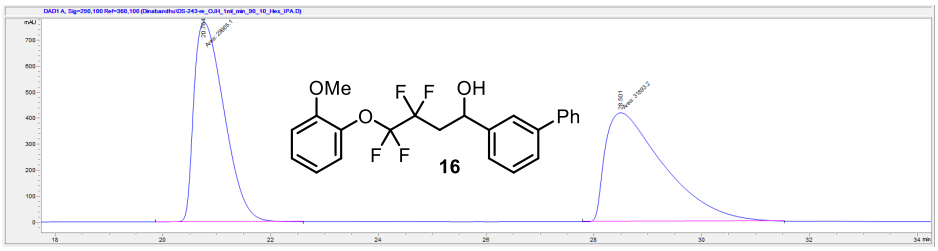
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	12.317	MM	10799.9	531.9	0.3384	72.111	0.53
2	13.679	MM	4176.9	218.4	0.3188	27.889	0.66



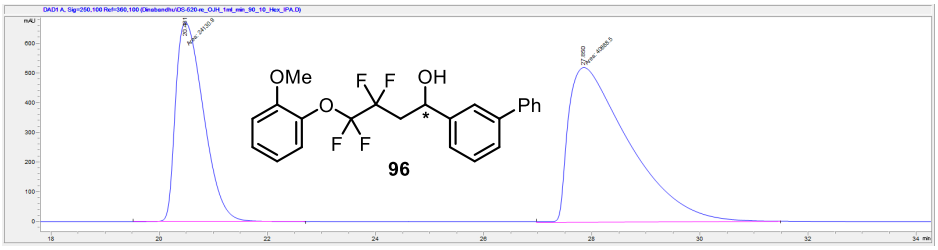
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	12.144	MM	8222	443.4	0.3091	49.099	0.581
2	14.974	MM	8523.7	382	0.3719	50.901	0.609



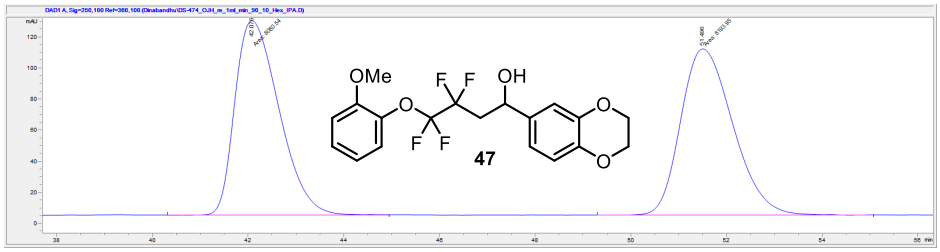
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	12.108	MM	9093.6	475.8	0.3185	58.589	0.57
2	14.964	MM	6427.4	298.2	0.3593	41.411	0.652



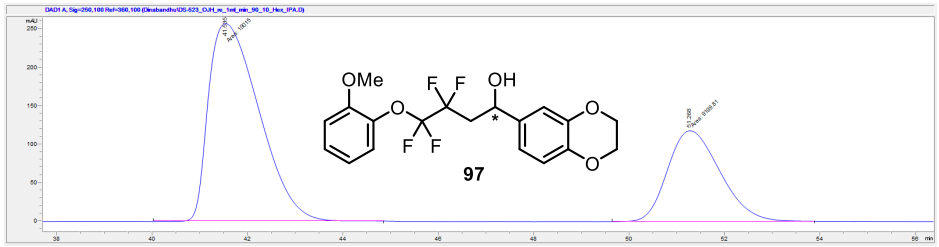
#	Time	Type	Area	Height	Width	Area%	Symmetry
1	20.764	MM	29965.1	768.3	0.6501	48.442	0.487
2	28.501	MM	31893.2	419	1.2687	51.558	0.346



#	Time	Type	Area	Height	Width	Area%	Symmetry
1	20.481	MM	24130.9	669.7	0.6005	37.113	0.525
2	27.85	MM	40888.5	520	1.3105	62.887	0.328



#	Time	Type	Area	Height	Width	Area%	Symmetry
1	42.076	MM	8080.5	125.6	1.0723	49.652	0.616
2	51.496	MM	8193.9	107.4	1.2715	50.348	0.716



#	Time	Type	Area	Height	Width	Area%	Symmetry
1	41.535	MM	19015	257.8	1.2294	67.394	0.498
2	51.268	MM	9199.8	118.8	1.2901	32.606	0.728

11. Crystallographic data

Compound 51.

The single crystal of **51** (**CCDC 2170253**) was prepared by recrystallization in chloroform. ORTEP diagram of **51** with 50% ellipsoid (crystal size 0.118 x 0.103 x 0.082 mm^3). Hydrogen atoms are omitted for clarity.

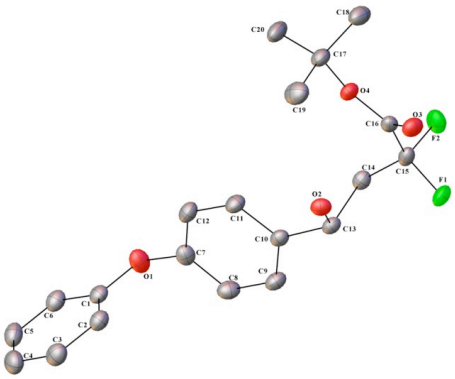


Table S7. Crystal data and structure refinement for 51

Identification code	ds276	
Empirical formula	C_{20} H_{22} F_2 O_4	
Formula weight	364.37	
Temperature	110.00 K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.4592(6) Å	α = 67.082(3)°.
	b = 11.1811(9) Å	β = 73.561(3)°.
	c = 12.5405(10) Å	γ = 80.326(4)°.
Volume	921.98(13) $Å^3$	
Z	2	
Density (calculated)	1.313 Mg/m^3	
Absorption coefficient	0.873 mm^{-1}	
F(000)	384	

Crystal size	0.118 x 0.103 x 0.082 mm^3
Theta range for data collection	3.942 to 70.282°.
Index ranges	-9<=h<=9, -13<=k<=13, -15<=l<=15
Reflections collected	13544
Independent reflections	3493 [R(int) = 0.0405]
Completeness to theta = 67.679°	99.8 %
Absorption correction	Semi-empirical from equiv. alents
Max. and min. transmission	0.4684 and 0.3684
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3493 / 19 / 249
Goodness-of-fit on F^2	1.052
Final R indices [I>2sigma(I)]	R1 = 0.0348, wR2 = 0.0862
R indices (all data)	R1 = 0.0370, wR2 = 0.0877
Extinction coefficient	n/a
Largest diff. peak and hole	0.250 and -0.208 e.$Å^{-3}$

Compound 81.

The single crystal of **81** (**CCDC 2213284**) was prepared by recrystallization in mixture of hexane and chloroform. ORTEP diagram of **81** with 50% ellipsoid (crystal size 0.129 x 0.104 x 0.008 mm^3). Hydrogen atoms are omitted for clarity.

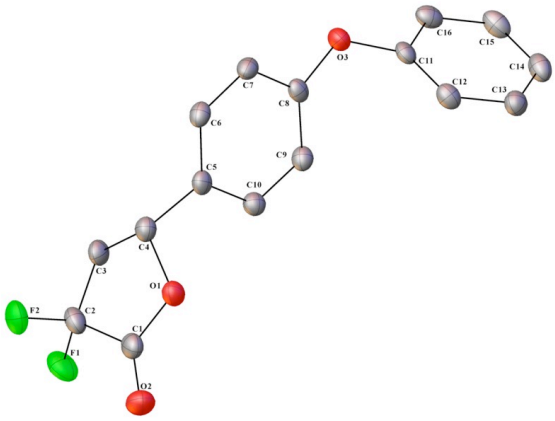


Table S8. Crystal data and structure refinement for 81

Identification code	og388	
Empirical formula	C_{16} H_{12} F_2 O_3	
Formula weight	290.26	
Temperature	110.00 K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$Pna2_1$	
Unit cell dimensions	a = 29.2415(18) Å	α = 90°.
	b = 7.5874(5) Å	β = 90°.
	c = 6.0208(4) Å	γ = 90°.
Volume	1335.82(15) $Å^3$	
Z	4	
Density (calculated)	1.443 Mg/m^3	
Absorption coefficient	1.004 mm^{-1}	
F(000)	600	
Crystal size	0.129 x 0.104 x 0.008 mm^3	
Theta range for data collection	3.022 to 62.574°.	
Index ranges	-33<=h<=33, -8<=k<=8, -6<=l<=6	
Reflections collected	13669	
Independent reflections	2091 [R(int) = 0.0576]	
Completeness to theta = 62.574°	99.6 %	
Absorption correction	Semi-empirical from equiv. alents	
Max. and min. transmission	0.7522 and 0.6696	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2091 / 1 / 191	
Goodness-of-fit on F^2	1.051	
Final R indices [I>2sigma(I)]	R1 = 0.0334, wR2 = 0.0804	
R indices (all data)	R1 = 0.0374, wR2 = 0.0820	
Absolute structure parameter	0.3(2)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.165 and -0.154 e.$Å^{-3}$	

Compound 84.

The single crystal of **84** (**CCDC 2211073**) was prepared by recrystallization in chloroform. ORTEP diagram of **84** with 50% ellipsoid (crystal size 0.086 x 0.067 x 0.035 mm^3). Hydrogen atoms are omitted for clarity.

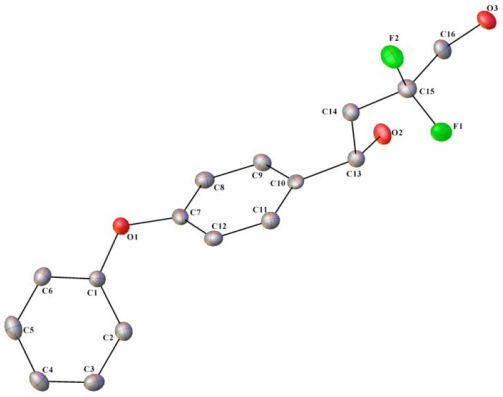
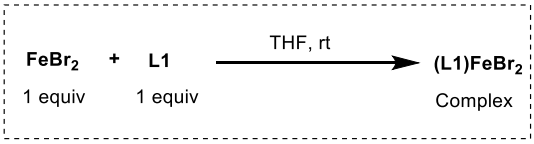


Table S9. Crystal data and structure refinement for 84

Identification code	ds393a	
Empirical formula	C_{16} H_{16} F_2 O_3	
Formula weight	294.29	
Temperature	110.00 K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$Pna2_1$	
Unit cell dimensions	a = 31.826(3) Å	α = 90°.
	b = 5.2173(4) Å	β = 90°.
	c = 8.1338(7) Å	γ = 90°.
Volume	1350.59(19) $Å^3$	
Z	4	
Density (calculated)	1.447 Mg/m^3	
Absorption coefficient	0.994 mm^{-1}	
F(000)	616	
Crystal size	0.086 x 0.067 x 0.035 mm^3	

Theta range for data collection	2.777 to 70.258°.
Index ranges	-38<=h<=38, -6<=k<=6, -9<=l<=9
Reflections collected	18270
Independent reflections	2561 [R(int) = 0.0485]
Completeness to theta = 67.679°	99.7 %
Absorption correction	Semi-empirical from equiv. alents
Max. and min. transmission	0.7533 and 0.6375
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2561 / 1 / 192
Goodness-of-fit on F^2	1.139
Final R indices [I>2sigma(I)]	R1 = 0.0390, wR2 = 0.1057
R indices (all data)	R1 = 0.0392, wR2 = 0.1058
Absolute structure parameter	0.08(3)
Extinction coefficient	n/a
Largest diff. peak and hole	0.292 and -0.217 e.Å^{-3}

(L1)$FeBr_2$ Complex.



The single crystal of **(L1)$FeBr_2$ Complex** (**CCDC 2254575**) was prepared by recrystallization in tetrahydrofuran (THF). ORTEP diagram of **(L1)$FeBr_2$ Complex** with 50% ellipsoid (crystal size 0.27×0.15×0.09 mm^3). Hydrogen atoms are omitted for clarity. Only one of the molecules from the asymmetric unit is shown.

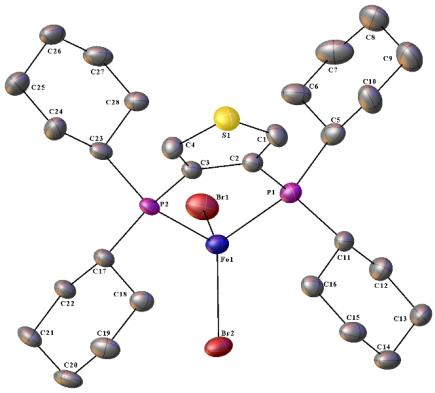


Table S10. Crystal data and structure refinement for (L1)FeBr$_2$.

Identification code	OG-DSFeBr2	
Empirical formula	$C_{28}H_{46}Br_2FeP_2S$	
Formula weight	692.32	
Temperature	110.00 K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 17.1165(5) Å	α = 89.485°.
	b = 19.8953(6) Å	β = 71.022°.
	c = 20.7440(7) Å	γ = 89.930°.
Volume	6679.9(4) Å^3	
Z	8	
Density (calculated)	1.377 g/cm^3	
Absorption coefficient	8.009 mm^{-1}	
F(000)	2848	
Crystal size	0.27×0.15×0.09 mm^3	
Theta range for data collection	2.221 to 70.316°	
Index ranges	-20<=h<=20, -24<=k<=24, -25<=l<=25	
Reflections collected	231826	
Independent reflections	25346 [R(int) = 0.0601]	

Completeness to theta = 70.316°	99.5 %
Absorption correction	Semi-empirical from equiv. alents
Max. and min. transmission	0.189 and 0.322
Refinement method	Full-matrix least-squares minimization on F^2
Data / restraints / parameters	25346/932/1387
Goodness-of-fit on F^2	1.024
Final R indices [I>2sigma(I)]	R1 = 0.0481, wR2 = 0.1266
R indices (all data)	R1 = 0.0525, wR2 = 0.1266
Extinction coefficient	n/a
Largest diff. peak and hole	1.642 and -1.171 e.$Å^{-3}$