

Supporting Information For

Nickel-Catalyzed C-H (Poly)addition of Alkenes and Alkynes with Polyfluoroarenes Enabled by an Unsymmetric *N*-Heterocyclic Carbene

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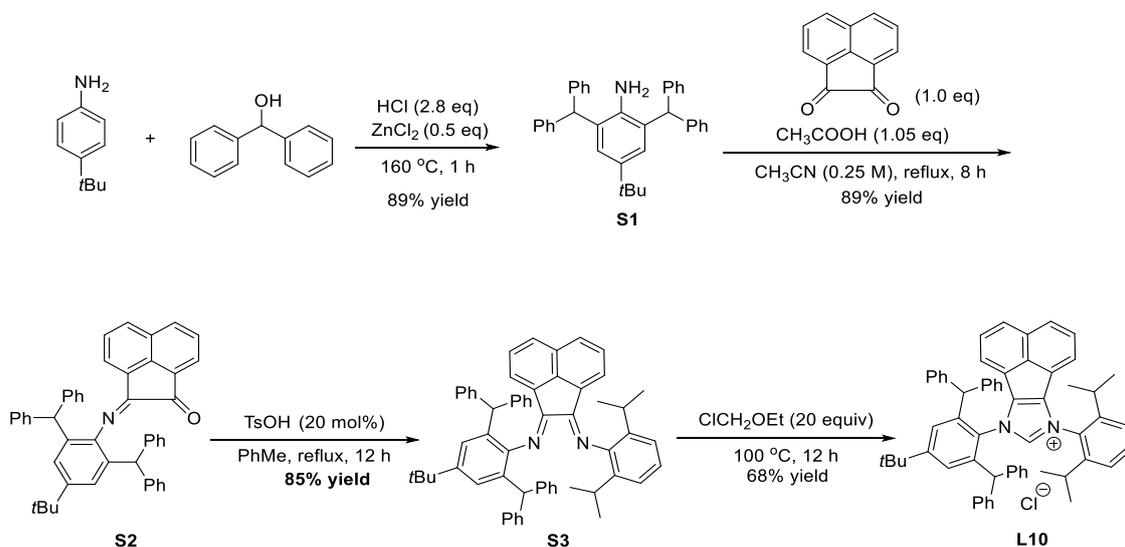
1. General Information

All the reactions were conducted under N₂ atmosphere with standard dry box or vacuum-line techniques, and the glassware was dried in oven (140 °C for 4 h) or flame-dried. Reaction solvents, including anhydrous heptane, THF, cyclohexane, *n*-hexane, etc., were purchased from Energy Chemical Co., Ltd. or J&K Chemical Co., Ltd. and used as received. Bis(1,5-cyclooctadiene) nickel was purchased from Strem Chemicals Inc. and stored under -20 °C. Octa-1,7-diene, deca-1,9-diene, dimethyldivynylsilane, 1,4-bis(dimethyl(vinyl)silyl) benzene, and 2,5-dimethylhexa-1,5-diene were purchased from TCI Chemical Co. Ltd. and used as received. 2,2',3,3',5,5',6,6'-octafluoro-1,1'-biphenyl and 1,2,4,5-tetrafluorobenzene were purchased from Aladdin Chemical Co., Ltd. and used as received. 1,4-bis((trimethylsilyl)ethynyl)benzene and 1,3-bis((trimethylsilyl)ethynyl)benzene were purchased from Alfa Chemical Co., Ltd. and used as received.

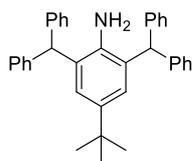
All new compounds were characterized by NMR spectroscopy, IR spectroscopy, high-resolution mass spectroscopy, and melting point (if solids). NMR spectra were recorded on a Bruker 400 MHz or 500 MHz spectrometer and were calibrated using the residual solvent as an internal reference (CDCl₃: 7.26 ppm for ¹H NMR and 77.16 ppm for ¹³C NMR). Melting points were measured on a SGW X-4 apparatus. All IR spectra were taken on a BRUKER TENSOR 27 FT-IR spectrometer. EI-HRMS spectra were obtained on a Waters Micromass G1540N/GCT Premier, ESI-HRMS spectra were obtained on an Agilent Technologies 6224 TOF LC/MS, and DART-HRMS spectra were obtained on a Thermo Fisher Scientific LTQ FT Ultra. GC analysis was performed on an Agilent 7890B using a DB-5MS column (30 m, 0.25 mm). GC-MS analyses were performed on a Shimadzu QP2010 SE using a DB-5MS column (30 m, 0.25 mm I.D.).

The molecular weights and molecular weight distributions of all copolymers were determined by gel permeation chromatography (GPC) using a Waters e2695 separation module with a 2414 refractive index detector and THF as the eluent. The instrument was calibrated with narrow-dispersity polystyrene standards between 589 and 96400 g/mol. All runs were performed at 0.6 mL/min flow rate and 35 °C. Differential scanning calorimetry (DSC) was performed on a DSC2A-01318 at a heating rate of 10 °C/min under a nitrogen atmosphere. Data was recorded from the second scan, and thermal history difference in the polymers was eliminated by first heating the specimen to 300 °C (or 250 °C), cooling at 10 °C/min to 20 °C (or -50 °C). Thermal gravimetric analysis (TGA) was performed on a TGA Q500 V6.7 Build 203 thermogravimetric analyzer at a heating rate of 10 °C/min under a nitrogen atmosphere. Fluorescence spectra were obtained on a F-4700 FL Spectrophotometer in DCM (1mg/mL).

2. Preparation of L10

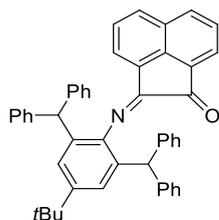


L1-L6 were synthesized according to references¹⁻².



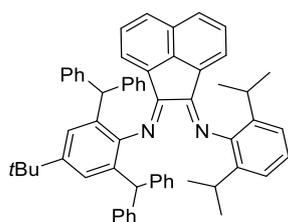
2,6-dibenzhydryl-4-(*tert*-butyl)aniline (S1)

A 500 mL round-bottom flask was charged with 4-(*tert*-butyl)aniline (14.9 g, 100 mmol), diphenylmethanol (36.8 g, 200 mmol), and a stir bar. Then the mixture was heated at 100 °C until all solid melts. A solution of ZnCl₂ (6.8 g) in concentrated HCl (8.5 mL) was added slowly to this mixture. The reaction mixture released white fume, and there was water on the wall of the flask. After finishing, the mixture was heated at 160 °C for another 1 h until the mixture became solid. Upon cooling to room temperature, the solid was dissolved in CH₂Cl₂ and washed with saturated NH₄Cl a.q. and saturated NaCl a.q. respectively. Then the organic layer was dried under anhydrous Na₂SO₄ and filtered. Solvent was removed under reduced pressure, and a grey solid was obtained. The crude product was washed with MeOH, giving pure product as a white powder in 89% yield (43.0 g) with matched spectra³. ¹H NMR (400 MHz, CDCl₃) δ 7.31 – 7.25 (m, 8H), 7.23 – 7.18 (m, 4H), 7.09 (m, 8H), 6.57 (s, 2H), 5.45 (s, 2H), 0.96 (d, *J* = 1.5 Hz, 9H). ¹³C NMR (101 MHz, CDCl₃) δ 143.0, 140.1, 139.6, 129.6, 128.6, 128.5, 126.7, 125.6, 52.8, 34.1, 31.4.



2-((2,6-dibenzhydryl-4-(*tert*-butyl)phenyl)imino)acenaphthylene-1(2*H*)-one (S2)

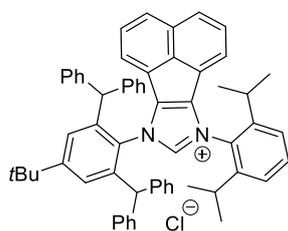
In a 250 mL round-bottom flask, acenaphthylene-1,2-dione (3.64 g, 20.0 mmol) and 80 mL acetonitrile were added. The flask was evacuated and backfilled with N₂ three times. Then the mixture was heated to reflux for 1 h, and 12 mL of acetic acid was added. After another 1 h, **S1** (9.63 g, 20.0 mmol) was added, and the reaction mixture was heated to reflux for 8 h. Upon cooling to room temperature, the solvent was removed in vacuo. Then 50 mL of ethanol was added, and the mixture was heated to reflux for 2 h. After cooling to room temperature, the mixture was filtered to get orange powder in 89% yield (11.46 g). **¹H NMR (400 MHz, CDCl₃)** δ 8.01 (t, *J* = 7.5 Hz, 2H), 7.74 – 7.64 (m, 2H), 7.23 (m, 4H), 7.16 (m, 2H), 7.03 (m, 5H), 6.99 (s, 2H), 6.84 (d, *J* = 7.5 Hz, 4H), 6.59 (t, *J* = 7.6 Hz, 4H), 6.42 (t, *J* = 7.3 Hz, 2H), 6.00 (d, *J* = 7.1 Hz, 1H), 5.44 (s, 2H), 1.16 (s, 9H). **¹³C NMR (101 MHz, CDCl₃)** δ 189.9, 162.5, 146.7, 146.0, 143.2, 142.6, 142.0, 131.9, 131.2, 130.2, 130.0, 129.8, 129.5, 128.5, 128.2, 127.9, 127.6, 127.4, 127.2, 126.3, 125.6, 125.2, 123.9, 121.6, 52.5, 34.6, 31.5. **HRMS (ESI)** calculated for C₄₈H₄₀NO [M+H]⁺ *m/z* 646.3104, found 646.3100. **Melting point:** 190–192 °C. **IR (neat, cm⁻¹)** 2960, 1730, 1654, 1598, 1492, 1447, 1028, 698, 605.



*N*¹-(2,6-dibenzhydryl-4-(*tert*-butyl)phenyl)-*N*²-(2,6-diisopropylphenyl)acenaphthylene-1,2-diimine (S3)

In a 250 mL round-bottom flask, **S2** (11.40 g, 17.6 mmol), 2,6-diisopropylaniline (3.13 g, 17.6 mmol), and TsOH · H₂O (0.67 g, 3.5 mmol) were added, then the flask was evacuated and backfilled with N₂ three times. Then 150 mL toluene was added, and the reaction mixture was heated to reflux for 12 h. Upon cooling to room temperature, the solvent was removed in vacuo. Then 50 mL of ethanol was added, and the mixture was heated to reflux for 2 h. After cooling to room temperature, the mixture was filtered to obtain a yellow solid in 85% yield (12.03 g). **¹H NMR (400 MHz, CDCl₃)**

δ 7.66 (d, $J = 8.2$ Hz, 1H), 7.49 (d, $J = 8.2$ Hz, 1H), 7.29 – 7.22 (m, 7H), 7.18 (m, 3H), 7.09 (d, $J = 7.5$ Hz, 4H), 7.00 (s, 2H), 6.91 (d, $J = 7.5$ Hz, 4H), 6.85 (t, $J = 7.7$ Hz, 1H), 6.56 (t, $J = 7.5$ Hz, 4H), 6.43 (d, $J = 7.2$ Hz, 1H), 6.37 (t, $J = 7.3$ Hz, 2H), 5.77 (d, $J = 7.1$ Hz, 1H), 5.66 (s, 2H), 3.17 (m, 2H), 1.29 (d, $J = 6.8$ Hz, 6H), 1.19 (s, 9H), 1.02 (d, $J = 6.8$ Hz, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 163.8, 162.2, 147.2, 146.9, 146.1, 143.9, 141.9, 140.1, 135.8, 131.7, 129.8, 129.7, 129.6, 128.7, 128.7, 128.6, 128.0, 127.8, 127.7, 127.00, 126.9, 126.1, 125.5, 125.3, 124.5, 124.3, 123.6, 122.9, 52.4, 34.5, 31.6, 28.6, 24.4, 23.8. **HRMS (ESI)** calculated for $\text{C}_{60}\text{H}_{57}\text{N}_2$ $[\text{M}+\text{H}]^+$ m/z 805.4516, found 805.4511. **Melting point:** 210–213 °C. **IR (neat, cm^{-1})** 2958, 2867, 1667, 1596, 1598, 1492, 1450, 906, 727, 699.



7-(2,6-dibenzhydryl-4-(tert-butyl)phenyl)-9-(2,6-diisopropylphenyl)-7H-acenaphtho[1,2-d]imidazol-9-ium chloride (L10)

A 150 mL nitrogen-flushed thick-walled reaction vessel was charged with **S3** (9.66 g, 12.0 mmol) and chloromethyl ethyl ether (21 mL, 240 mmol). The vessel was sealed, and the reaction mixture was stirred at 100 °C for 12 h. After cooling to room temperature, the solvent was removed in vacuo. The crude product was purified by column chromatography (0–20% EtOAc in hexanes to 10% methanol in CH_2Cl_2) to provide the title compound as a bright yellow powder in 68% yield (6.92 g). ^1H NMR (400 MHz, CDCl_3) δ 12.42 (s, 1H), 7.81 (d, $J = 8.2$ Hz, 1H), 7.64 (m, 2H), 7.45 – 7.37 (m, 3H), 7.28 (m, 8H), 7.20 – 7.15 (m, 2H), 7.13 (s, 2H), 7.08 (dd, $J = 8.3, 7.1$ Hz, 1H), 6.98 (d, $J = 6.9$ Hz, 1H), 6.79 (d, $J = 7.4$ Hz, 4H), 6.72 (t, $J = 7.6$ Hz, 4H), 6.62 (t, $J = 7.3$ Hz, 2H), 6.26 (d, $J = 6.9$ Hz, 1H), 5.60 (s, 2H), 2.71 (m, 2H), 1.34 (d, $J = 6.8$ Hz, 6H), 1.15 (s, 9H), 1.07 (d, $J = 6.8$ Hz, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 154.2, 145.0, 143.1, 141.6, 141.1, 140.8, 138.1, 137.0, 132.04, 130.0, 129.8, 129.5, 129.3, 129.1, 129.0, 128.9, 128.6, 128.3, 127.4, 127.2, 126.8, 126.6, 124.9, 124.1, 122.5, 122.1, 121.9, 52.2, 35.1, 31.0, 29.4, 24.6, 23.8. **HRMS (ESI)** calculated for $\text{C}_{61}\text{H}_{57}\text{N}_2^+$ $[\text{M}]^+$ m/z 817.4516, found 817.4508. **Melting point:** 292–295 °C. **IR (neat, cm^{-1})** 2960, 2868, 2657, 1515, 1443, 1031, 765, 700, 604.

3. Reaction Optimization

Table S1 Solvent Optimization

Entry	Solvent	Yield ^a /%	3:3a ^b
1	hexane	89	>99:1
2	DME	31	>99:1
3	cyclohexane	97	>99:1
4	toluene	95	>99:1
5	THF	67	>99:1
6	dioxane	82	>99:1
7	CPME	64	>99:1

^a Reactions run with 0.25 mmol **1** and 0.50 mmol **2**. Yields were determined by ¹H NMR using CHCl₂CHCl₂ as a standard. ^b

Determined by GC and NMR analysis.

Table S2 Control experiment

Entry	Variations from standard condition	Yield ^a /%	3:3a
1	No L10	N.R.	-
2	Only <i>t</i> BuOK	N.R.	-
3	1.0 equiv 2	61	>99:1
4	2.0 equiv 1	65	>99:1

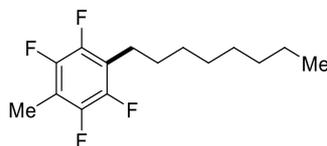
^a Reactions run with 0.25 mmol **1** and 0.50 mmol **2**. Yields were determined by ¹H NMR analysis using CHCl₂CHCl₂ as a standard.

^b Determined by GC and NMR analysis.

4. Nickel-Catalyzed Hydroarylation of Alkenes with Fluoroarenes.

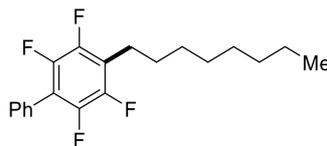
General Procedure A (GPA): In a nitrogen-filled glove box, bis(1,5-cyclooctadiene)nickel (2.8 mg, 10 μmol , 2 mol%), $t\text{BuOK}$ (2.2 mg, 20 μmol , 4 mol%), **L10** (8.5 mg, 10 μmol , 2 mol%) and heptane (1.0 mL) were added to an 8 mL vial equipped with a magnetic stirring bar. The reaction mixture was allowed to stir at room temperature overnight, and fluoroarene (0.5 mmol) and alkene (1.0 mmol) were added. The vial was taken out of the glovebox and stirred at 130 $^{\circ}\text{C}$ for 12 h. After cooling to room temperature, the resulting mixture was purified directly by silica gel column using a mixture of hexanes, petroleum ether, and ethyl acetate (EtOAc) as the eluent. Then concentrated in vacuo to give the pure product.

5. Characterization of Hydroarylation Products.



1,2,4,5-tetrafluoro-3-methyl-6-octylbenzene (3)

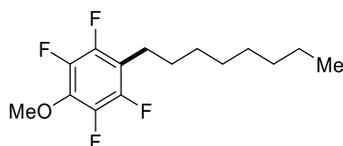
Following the GPA using 1,2,4,5-tetrafluoro-3-methylbenzene (82.0 mg, 0.5 mmol, 1.0 equiv) and oct-1-ene (112.2 mg, 1.0 mmol, 2.0 equiv). The crude product was purified by column chromatography (100% hexanes) to provide the title compound as a colorless oil in 97% yield (135.3 mg). **$^1\text{H NMR}$ (400 MHz, CDCl_3)** δ 2.68 (t, $J = 7.6$ Hz, 2H), 2.23 (t, $J = 2.0$ Hz, 3H), 1.56 (m, 2H), 1.38 – 1.19 (m, 10H), 0.88 (t, $J = 6.9$ Hz, 3H). **$^{13}\text{C NMR}$ (101 MHz, CDCl_3)** δ 145.1 (dm, $J_F = 243.4$), 144.7 (dm, $J_F = 243.4$), 118.0 (t, $J_F = 18.8$ Hz), 113.3 (t, $J_F = 19.2$ Hz), 32.0, 29.5, 29.4, 29.3, 22.8, 14.2, 7.6 – 7.0 (m). **$^{19}\text{F NMR}$ (377 MHz, CDCl_3)** δ -145.26 (ddd, $J = 22.1, 12.9, 2.0$ Hz, 2F), -146.72 (dd, $J = 22.1, 12.9$ Hz, 2F). **HRMS (EI)** calculated for $\text{C}_{15}\text{H}_{20}\text{F}_4$ $[\text{M}]^+$ m/z 276.1496, found 276.1494. **IR (neat, cm^{-1})** 2927, 2857, 1483, 1275, 1112, 1063, 898, 600.



2,3,5,6-tetrafluoro-4-octyl-1,1'-biphenyl (4)

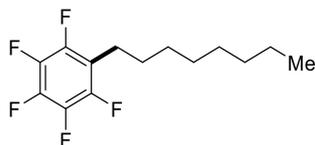
Following the GPA using 2,3,5,6-tetrafluoro-1,1'-biphenyl (113.1 mg, 0.5 mmol, 1.0 equiv) and oct-1-ene (112.2 mg, 1.0 mmol, 2.0 equiv). The crude product was purified by column

chromatography (100% hexanes) to provide the title compound as a white solid in 98% yield (165.0 mg). **¹H NMR (400 MHz, CDCl₃)** δ 7.48 (m, 5H), 2.78 (t, *J* = 7.0 Hz, 2H), 1.65 (m, 2H), 1.31 (m, 10H), 0.90 (t, *J* = 6.3 Hz, 3H). **¹³C NMR (101 MHz, CDCl₃)** δ 146.9 (dm, *J_F* = 256.5 Hz), 143.8 (dm, *J_F* = 257.6 Hz), 130.3, 129.0, 128.7, 128.0, 120.4 – 120.0 (m), 118.3–118.0 (m), 32.0, 29.5, 29.4, 29.3, 23.0, 22.8, 14.2. **¹⁹F NMR (377 MHz, CDCl₃)** δ -145.03 – -145.79 (m, 4F). **HRMS (EI)** calculated for C₂₀H₂₂F₄[M]⁺ *m/z* 338.1652, found 338.1650. **IR (neat, cm⁻¹)** 2914, 2848, 1476, 1436, 960, 914, 690, 672. **Melting point:** 47-48 °C.



1,2,4,5-tetrafluoro-3-methoxy-6-octylbenzene(5)

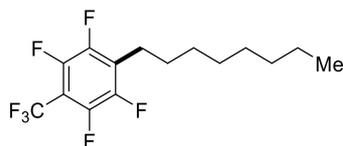
Following the GPA using 1,2,4,5-tetrafluoro-3-methoxybenzene (90.1 mg, 0.5 mmol, 1.0 equiv), oct-1-ene (112.2 mg, 1.0 mmol, 2.0 equiv) and 5 mol% catalyst. The crude product was purified by column chromatography (100% hexanes) to provide the title compound as a colorless oil in 68% yield (103.0 mg). **¹H NMR (400 MHz, CDCl₃)** δ 4.03 (t, *J* = 1.2 Hz, 3H), 2.71 – 2.61 (m, 2H), 1.56 (m, 2H), 1.28 (m, 10H), 0.88 (t, *J* = 6.9 Hz, 3H). **¹³C NMR (101 MHz, CDCl₃)** δ 145.5 (dm, *J_F* = 243.4 Hz), 141.2 (ddt, *J_F* = 247.5, 16.2, 4.0 Hz), 136.4–136.2 (m), 114.3 (t, *J_F* = 19.2 Hz), 62.3 (t, *J_F* = 3.5 Hz), 32.0, 29.6, 29.4, 29.3, 22.8, 22.5, 14.2. **¹⁹F NMR (377 MHz, CDCl₃)** δ -146.24 (dd, *J* = 21.7, 8.9 Hz, 2F), -158.97 (dd, *J* = 21.9, 9.0 Hz, 2F). **HRMS (EI)** calculated for C₁₅H₂₀F₄O[M]⁺ *m/z* 292.1445, found 292.1431. **IR (neat, cm⁻¹)** 2927, 2857, 1654, 1490, 1195, 1129, 1014, 972.



1,2,3,4,5-pentafluoro-6-octylbenzene (6)

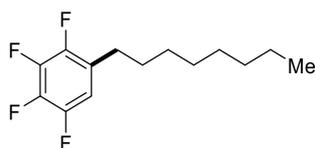
Following the GPA using 1,2,3,4,5-pentafluorobenzene (84.0 mg, 0.5 mmol, 1.0 equiv) and oct-1-ene (168.3 mg, 1.5 mmol, 3.0 equiv). The crude product was purified by column chromatography (100% hexanes) to provide the title compound as a colorless oil in 88% yield (119.4 mg) with matched spectra⁴. **¹H NMR (400 MHz, CDCl₃)** δ 2.68 (t, *J* = 7.6 Hz, 2H), 1.64 – 1.52 (m, 2H),

1.38 – 1.18 (m, 10H), 0.88 (t, $J = 6.9$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 145.2 (dm, $J_F = 245.4$ Hz), 139.5 (dm, $J_F = 252.5$ Hz), 137.5 (dm, $J_F = 250.5$ Hz), 115.7 (t, $J_F = 19.0$ Hz), 32.0, 29.5, 29.4, 29.3, 22.8, 22.5, 14.2. ^{19}F NMR (377 MHz, CDCl_3) δ -144.60 (dd, $J = 22.3, 8.0$ Hz, 2F), -158.58 (t, $J = 20.8$ Hz, 2F), -163.06 – -163.44 (m, 1F).



1,2,4,5-tetrafluoro-3-octyl-6-(trifluoromethyl)benzene (7)

Following the GPA using 1,2,4,5-tetrafluoro-3-(trifluoromethyl)benzene (109.0 mg, 0.5 mmol, 1.0 equiv), oct-1-ene (112.2 mg, 1.0 mmol, 2.0 equiv). The crude product was purified by column chromatography (100% hexanes) to provide the title compound as a colorless oil in 91% yield (154.0 mg) with matched spectra⁵. ^1H NMR (400 MHz, CDCl_3) δ 2.77 (t, $J = 7.6$ Hz, 2H), 1.68 – 1.56 (m, 2H), 1.41 – 1.19 (m, 10H), 0.88 (t, $J = 6.8$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 145.3 (dm, $J_F = 251.5$ Hz), 144.1 (ddm, $J_F = 259.6, 16.2$ Hz), 126.0 (t, $J_F = 18.5$ Hz), 121.1 (- CF_3 , $J_F = 274.7$ Hz), 107.6-107.1 (m), 32.0, 30.0, 29.4, 29.3, 29.2, 29.1 (m), 23.3, 22.8, 14.2. ^{19}F NMR (377 MHz, CDCl_3) δ -56.20 (td, $J = 21.5, 6.8$ Hz, 3F), -141.72 – -141.89 (m, 2F), -142.38 – -142.79 (m, 2F).



1,2,3,4-tetrafluoro-5-octylbenzene (8)

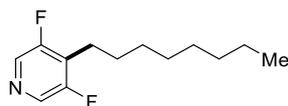
Following the GPA using 1,2,3,4-tetrafluorobenzene (75.0 mg, 0.5 mmol, 1.0 equiv), oct-1-ene (112.2 mg, 1.0 mmol, 2.0 equiv). The crude product was purified by column chromatography (100% hexanes) to provide the title compound as a colorless oil in 75% yield (98.5 mg). ^1H NMR (400 MHz, CDCl_3) δ 6.95 – 6.67 (m, 1H), 2.60 (t, $J = 7.7$ Hz, 2H), 1.66 – 1.49 (m, 2H), 1.28 (m, 10H), 0.88 (t, $J = 6.9$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 147.0 (ddm, $J_F = 246.4, 10.1$ Hz), 145.9 (ddm, $J_F = 246.4, 10.1$ Hz), 140.8 (dtm, $J_F = 252.5, 13.1$ Hz), 138.8 (dtm, $J_F = 251.5, 13.1$ Hz), 126.2 (dm, $J_F = 15.2$ Hz), 111.1 (dt, $J_F = 19.2, 4.0$ Hz), 32.0, 30.0, 29.5, 29.4, 29.3, 28.6, 22.8, 14.2. ^{19}F NMR (377 MHz, CDCl_3) δ -140.64 – -146.74 (m, 1F), -144.29 – -144.56 (m, 1F), -156.62 (td, $J = 5.0, 1.0$ Hz 1F), -159.83 (td, $J = 20.5, 7.9$ Hz, 1F). HRMS (EI) calculated for $\text{C}_{14}\text{H}_{18}\text{F}_4$ $[\text{M}]^+$ m/z

262.1339, found 262.1339. **IR (neat, cm⁻¹)** 2927, 2857, 1524, 1486, 1369, 1111, 930, 713.



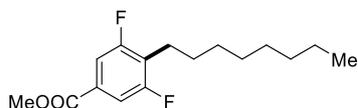
2,3,5,6-tetrafluoro-4-octylpyridine (9)

Following the GPA using 2,3,5,6-tetrafluoropyridine (75.6 mg, 0.5 mmol, 1.0 equiv), oct-1-ene (112.2 mg, 1.0 mmol, 2.0 equiv), and 5 mol% catalyst. The crude product was purified by column chromatography (100% hexanes) to provide the title compound as a colorless oil in 73% yield (90.0 mg) with matched spectra⁵. **¹H NMR (400 MHz, CDCl₃)** δ 2.80 (t, J = 7.7 Hz, 2H), 1.71 – 1.57 (m, 2H), 1.30 – 1.26 (m, 10H), 0.88 (t, J = 6.8 Hz, 3H). **¹³C NMR (101 MHz, CDCl₃)** δ 143.4 (dtm, J_F = 245.4, 16.2 Hz), 140.5 (dm, J_F = 256.5), 135.7 (t, J_F = 17.2 Hz), 31.9, 29.4, 29.3, 29.2, 28.7, 23.9, 22.8, 14.2. **¹⁹F NMR (377 MHz, CDCl₃)** δ -91.83 – -92.33 (m, 2F), -145.43 – -145.99 (m, 2F).



3,5-difluoro-4-octylpyridine (10)

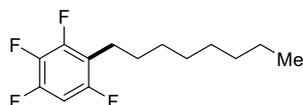
Following the GPA using 3,5-difluoropyridine (57.6 mg, 0.5 mmol, 1.0 equiv), oct-1-ene (112.2 mg, 1.0 mmol, 2.0 equiv), and 5 mol% catalyst. The crude product was purified by column chromatography (2% EtOAc in hexane) to provide the title compound as a pale-yellow oil in 68% yield (78.4 mg). **¹H NMR (400 MHz, CDCl₃)** δ 8.24 (s, 2H), 2.69 (t, J = 7.6 Hz, 2H), 1.61-1.55 (m, 2H), 1.38 – 1.18 (m, 10H), 0.86 (t, J = 6.8 Hz, 3H). **¹³C NMR (101 MHz, CDCl₃)** δ 158.3 (dd, J_F = 258.1, 4.1 Hz), 133.8 (dd, J_F = 22.4, 6.1 Hz), 126.90 (t, J_F = 17.5 Hz), 31.9, 29.4, 29.3, 29.2, 28.9, 22.7, 22.2, 14.2. **¹⁹F NMR (377 MHz, CDCl₃)** δ -130.91 (s, 2F). **HRMS (EI)** calculated for C₁₃H₁₉F₂N [M]⁺ m/z 227.1480, found 227.1479. **IR (neat, cm⁻¹)** 2926, 2856, 1570, 1420, 1280, 1229, 874, 574.



methyl 3,5-difluoro-4-octylbenzoate (11)

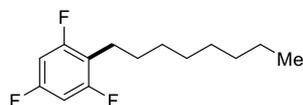
Following the GPA using methyl 3,5-difluorobenzoate (86.1 mg, 0.5 mmol, 1.0 equiv), oct-1-ene (112.2 mg, 1.0 mmol, 2.0 equiv), and 5 mol% catalyst. The crude product was purified by

column chromatography (2% EtOAc in hexane) to provide the title compound as a yellow oil in 71% yield (105.8 mg). **¹H NMR (400 MHz, CDCl₃)** δ 7.63 – 7.42 (m, 2H), 3.91 (s, 3H), 2.69 (t, *J* = 7.6 Hz, 2H), 1.69 – 1.49 (m, 3H), 1.39 – 1.17 (m, 10H), 0.87 (t, *J* = 6.9 Hz, 3H). **¹³C NMR (101 MHz, CDCl₃)** δ 165.4 (t, *J_F* = 3.4 Hz), 161.3 (dd, *J_F* = 247.3, 9.2 Hz), 129.8 (t, *J_F* = 9.7 Hz), 123.9 (t, *J_F* = 20.7 Hz), 112.4 (dd, *J_F* = 20.2, 8.1 Hz), 52.6, 32.0, 29.5, 29.40, 29.38, 29.3, 22.8, 14.2. **¹⁹F NMR (377 MHz, CDCl₃)** δ -114.65 (d, *J* = 7.1 Hz, 2F). **HRMS (EI)** calculated for C₁₆H₂₂F₂O₂ [M]⁺ *m/z* 284.1582, found 284.1582. **IR (neat, cm⁻¹)** 2926, 2856, 1730, 1581, 1426, 1325, 1230, 1001, 767.



1,2,3,5-tetrafluoro-4-octylbenzene (12)

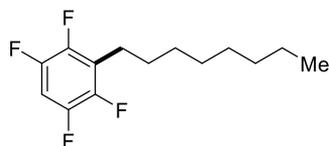
Following the GPA using 1,2,3,5-tetrafluorobenzene (225.0 mg, 1.5 mmol, 3.0 equiv), oct-1-ene (56.1 mg, 0.5 mmol, 1.0 equiv), and 5 mol% catalyst. The crude product was purified by column chromatography (100% hexane) to provide the title compound as a colorless oil in 63% yield (82.5 mg). **¹H NMR (400 MHz, CDCl₃)** δ 6.81 – 6.66 (m, 1H), 2.63 (t, *J* = 7.6 Hz, 2H), 1.59-1.52 (m, 2H), 1.36 – 1.22 (m, 10H), 0.88 (t, *J* = 6.8 Hz, 3H). **¹³C NMR (101 MHz, CDCl₃)** δ 155.5 (dm, *J_F* = 245.4 Hz), 150.2 (dm, *J_F* = 248.5 Hz), 148.9 (dm, *J_F* = 249.4 Hz), 137.2 (dm, *J_F* = 248.5 Hz), 115.8 (t, *J_F* = 22.4 Hz), 100.4 (ddd, *J_F* = 29.0, 21.2, 3.8 Hz), 32.0, 29.5, 29.4, 29.3, 22.8, 22.4, 14.2. **¹⁹F NMR (377 MHz, CDCl₃)** δ -119.85 (t, *J* = 11.3 Hz, 1F), -137.2 (d, *J* = 26.4 Hz, 1F), -136.62 (ddd, *J* = 21.9, 10.7, 4.8 Hz, 1F), -165.96 – -166.22 (m, 1F). **HRMS (EI)** calculated for C₁₄H₁₈F₄ [M]⁺ *m/z* 262.1339, found 262.1336. **IR (neat, cm⁻¹)** 2927, 2857, 1646, 1515, 1465, 1254, 1121, 834.



1,3,5-trifluoro-2-octylbenzene (13)

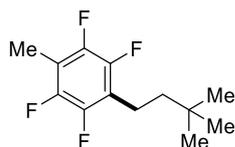
Following the GPA using 1,3,5-trifluorobenzene (198.1 mg, 1.5 mmol, 3.0 equiv), oct-1-ene (56.1 mg, 0.5 mmol, 1.0 equiv), and 5 mol% catalyst. The crude product was purified by column chromatography (100% hexane) to provide the title compound as a colorless oil in 67% yield (79.5 mg). **¹H NMR (400 MHz, CDCl₃)** δ 6.82 – 6.49 (m, 2H), 2.60 (t, *J* = 7.6 Hz, 2H), 1.58-1.51 (m, 2H), 1.43 – 1.19 (m, 10H), 0.88 (t, *J* = 6.8 Hz, 3H). **¹³C NMR (101 MHz, CDCl₃)** δ 161.8 (ddd, *J_F*

= 248.5, 15.2, 12.2 Hz), 160.9 (dt, $J_F = 247.5, 16.2$), 114.5 (td, $J_F = 21.0, 4.6$ Hz), 99.9 (ddd, $J_F = 29.9, 25.2, 1.5$ Hz), 32.0, 29.7, 29.5, 29.4, 29.4, 22.8, 22.1 (t, $J_F = 1.8$ Hz). **^{19}F NMR (377 MHz, CDCl_3)** δ -112.38 – -112.53 (m, 1F), -113.29 – -113.45 (m, 2F). **HRMS (EI)** calculated for $\text{C}_{14}\text{H}_{19}\text{F}_3$ $[\text{M}]^+$ m/z 244.1433, found 244.1434. **IR (neat, cm^{-1})** 2926, 2856, 1604, 1494, 1378, 1115, 997, 838.



1,2,4,5-tetrafluoro-3-octylbenzene (14)

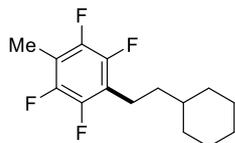
Following the GPA using 1,2,4,5-tetrafluorobenzene (225.0 mg, 1.5 mmol, 3.0 equiv), oct-1-ene (56.1 mg, 0.5 mmol, 1.0 equiv), and 5 mol% catalyst. The crude product was purified by column chromatography (100% hexane) to provide the title compound as a colorless oil in 85% yield (111.9 mg). **^1H NMR (400 MHz, CDCl_3)** δ 6.89 (ddd, $J = 9.8, 8.6, 4.9$ Hz, 1H), 2.78 – 2.65 (m, 2H), 1.68 – 1.56 (m, 2H), 1.37 – 1.21 (m, 10H), 0.88 (t, $J_F = 6.9$ Hz, 3H). **^{13}C NMR (101 MHz, CDCl_3)** δ 145.9 (dm, $J_F = 248.5$ Hz), 145.0 (dm, $J_F = 244.4$ Hz), 121.9 (t, $J_F = 18.5$ Hz), 103.4 (t, $J_F = 22.7$ Hz), 32.0, 29.38, 29.4, 29.3, 23.1, 22.8, 14.2. **^{19}F NMR (377 MHz, CDCl_3)** δ -140.06 – -140.53 (m, 2F), -144.83 – -145.35 (m, 2F). **HRMS (EI)** calculated for $\text{C}_{14}\text{H}_{18}\text{F}_4$ $[\text{M}]^+$ m/z 262.1339, found 262.1335. **IR (neat, cm^{-1})** 2927, 2857, 1499, 1290, 1250, 1170, 901, 837, 713.



1-(3,3-dimethylbutyl)-2,3,5,6-tetrafluoro-4-methylbenzene (15)

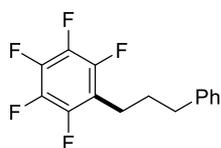
Following the GPA using 1,2,4,5-tetrafluoro-3-methylbenzene (82.0 mg, 0.5 mmol, 1.0 equiv) and 3,3-dimethylbut-1-ene (84.2 mg, 1.0 mmol, 2.0 equiv). The crude product was purified by column chromatography (100% hexane) to provide the title compound as a colorless oil in 94% yield (116.2 mg). **^1H NMR (400 MHz, CDCl_3)** δ 2.71 – 2.59 (m, 2H), 2.23 (t, $J = 2.1$ Hz, 3H), 1.49 – 1.38 (m, 2H), 0.97 (s, 9H). **^{13}C NMR (101 MHz, CDCl_3)** δ 145.2 (dddd, $J_F = 244.4, 14.6, 7.2, 3.8$ Hz), 144.8 (dddd, $J_F = 243.4, 14.2, 7.6, 3.8$ Hz), 118.77 (t, $J_F = 18.6$ Hz), 113.15 (t, $J_F = 19.2$ Hz), 43.8, 30.8, 29.1, 19.8 – 16.4 (m), 7.4. **^{19}F NMR (377 MHz, CDCl_3)** δ -145.25 (ddd, $J = 22.0, 12.8, 2.0$ Hz, 2F), -147.50 (dd, $J = 22.0, 12.9$ Hz, 2F). **HRMS (EI)** calculated for $\text{C}_{13}\text{H}_{16}\text{F}_4$ $[\text{M}]^+$ m/z

248.1183, found 248.1179. **IR (neat, cm⁻¹)** 2958, 2871, 1483, 1270, 1069, 885, 642, 605.



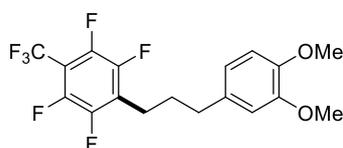
1-(2-cyclohexylethyl)-2,3,5,6-tetrafluoro-4-methylbenzene (16)

Following the GPA using 1,2,4,5-tetrafluoro-3-methylbenzene (82.0 mg, 0.5 mmol, 1.0 equiv) and vinylcyclohexane (110.2 mg, 1.0 mmol, 2.0 equiv). The crude product was purified by column chromatography (100% hexane) to provide the title compound as a colorless oil in 99% yield (140.3 mg). **¹H NMR (400 MHz, CDCl₃)** δ 2.79 – 2.58 (m, 2H), 2.23 (t, *J* = 2.0 Hz, 3H), 1.83 – 1.60 (m, 5H), 1.45 (dt, *J* = 10.1, 6.8 Hz, 2H), 1.30 – 1.12 (m, 4H), 0.99 – 0.85 (m, 2H). **¹³C NMR (101 MHz, CDCl₃)** δ 145.2 (dm, *J_F* = 244.4 Hz), 144.7 (dm, *J_F* = 244.4 Hz), 118.5 (t, *J_F* = 18.7 Hz), 113.2 (t, *J_F* = 19.2 Hz), 37.7, 37.2, 33.3, 26.8, 26.5, 20.3, 7.3. **¹⁹F NMR (377 MHz, CDCl₃)** δ -145.23 (ddd, *J* = 22.1, 12.8, 1.8 Hz, 2F), -146.98 (dd, *J* = 22.1, 12.8 Hz, 2F). **HRMS (EI)** calculated for C₁₅H₁₈F₄ [M]⁺ *m/z* 274.1339, found 274.1337. **IR (neat, cm⁻¹)** 2923, 2853, 1483, 1279, 1061, 936, 918, 603.



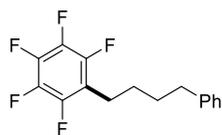
1,2,3,4,5-pentafluoro-6-(3-phenylpropyl)benzene (17)

Following the GPA using 1,2,3,4,5-pentafluorobenzene (84.1 mg, 0.5 mmol, 1.0 equiv), allylbenzene (177.3 mg, 1.5 mmol, 3.0 equiv), and 5 mol% catalyst. The crude product was purified by column chromatography (100% hexane) to provide the title compound as a colorless oil in 88% yield (126.4 mg) with matched spectra⁶. **¹H NMR (400 MHz, CDCl₃)** δ 7.35 – 7.27 (m, 2H), 7.26 – 7.15 (m, 3H), 2.84 – 2.61 (m, 4H), 1.95 (tt, *J* = 9.2, 6.9 Hz, 2H). **¹³C NMR (101 MHz, CDCl₃)** δ 145.3 (dm, *J_F* = 245.4 Hz), 141.3, 139.5 (dm, *J_F* = 251.5 Hz), 137.8 (dm, *J_F* = 250.5 Hz), 128.5, 128.4, 126.2, 115.3 (td, *J_F* = 18.9, 3.8 Hz), 35.5, 30.8, 22.2. **¹⁹F NMR (377 MHz, CDCl₃)** δ -144.25 (dd, *J* = 23.0, 8.9 Hz, 2F), -158.04 (t, *J* = 21.0 Hz, 1F), -160.38 – -166.23 (m, 2F).



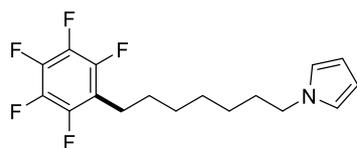
1-(3-(3,4-dimethoxyphenyl)propyl)-2,3,5,6-tetrafluoro-4-(trifluoromethyl)benzene (18)

Following the GPA using 1,2,4,5-tetrafluoro-3-(trifluoromethyl)benzene (109.1 mg, 0.5 mmol, 1.0 equiv), 4-allyl-1,2-dimethoxybenzene (178.2 mg, 1.0 mmol, 2.0 equiv), and 5 mol% catalyst. The crude product was purified by column chromatography (2-4% EtOAc in hexane) to provide the title compound as a colorless oil in 70% yield (143.2 mg). **¹H NMR (400 MHz, CDCl₃)** δ 6.70-6.70 (m, 3H), 3.87 (s, 3H), 3.86 (s, 3H), 2.80 (t, *J* = 7.7 Hz, 2H), 2.70 – 2.60 (m, 2H), 2.01 – 1.88 (m, 2H). **¹³C NMR (101 MHz, CDCl₃)** δ 148.9, 147.5, 145.1 (dm, *J_F* = 245.4 Hz), 143.8 (dm, *J_F* = 257.6 Hz), 125.4 (t, *J_F* = 18.2 Hz), 121.0 (-CF₃, *J_F* = 274.7 Hz), 107.9-106.8 (m) 133.4, 120.2, 111.5, 111.1, 55.8, 55.7, 34.9, 30.2, 22.7. **¹⁹F NMR (377 MHz, CDCl₃)** δ -56.23 (t, *J* = 21.5 Hz, 3F), -141.43 – -141.81 (m, 2F), -142.26 (td, *J* = 15.8, 6.1 Hz, 2F). **HRMS (EI)** calculated for C₁₈H₁₅F₇O [M]⁺ *m/z* 396.0955, found 396.0950. **IR (neat, cm⁻¹)** 2939, 1491, 1328, 1139, 1029, 960, 736, 713.



1,2,3,4,5-pentafluoro-6-(4-phenylbutyl)benzene (19)

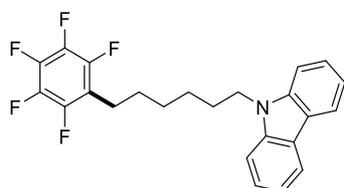
Following the GPA using 1,2,3,4,5-pentafluorobenzene (84.1 mg, 0.5 mmol, 1.0 equiv), but-3-en-1-ylbenzene (132.2 mg, 1.0 mmol, 2.0 equiv), and 5 mol% catalyst. The crude product was purified by column chromatography (100% hexane) to provide the title compound as a colorless oil in 79% yield (118.2 mg) with matched spectra⁷. **¹H NMR (400 MHz, CDCl₃)** δ 7.32-7.26 (m, 2H), 7.22-7.17 (m, 3H), 2.74 (t, *J* = 6.9 Hz, 2H), 2.66 (t, *J* = 7.1 Hz, 2H), 1.75 – 1.57 (m, 4H). **¹³C NMR (101 MHz, CDCl₃)** δ 145.2 (dm, *J_F* = 244.4 Hz), 142.1, 139.6 (dm, *J_F* = 252.5 Hz), 137.5 (dm, *J_F* = 250.5 Hz), 128.51, 128.50, 126.0, 115.4 (td, *J_F* = 18.9, 3.9 Hz), 35.6, 31.0, 28.9, 22.3. **¹⁹F NMR (377 MHz, CDCl₃)** δ -144.32 (dd, *J* = 22.5, 8.3 Hz, 2F), -158.18 (t, *J* = 20.8 Hz, 1F), -163.00 (ddd, *J* = 21.4, 8.4, 7.5 Hz, 2F).



1-(7-(perfluorophenyl)heptyl)-1H-pyrrole (20)

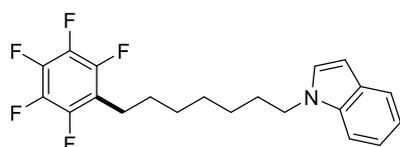
Following the GPA using 1,2,3,4,5-pentafluorobenzene (168.2 mg, 1.0 mmol, 2.0 equiv), 1-(hept-6-en-1-yl)-1H-pyrrole (156.6 mg, 0.5 mmol, 1.0 equiv), and 5 mol% catalyst. The crude

product was purified by column chromatography (100% hexane) to provide the title compound as a colorless oil in 92% yield (153.2 mg). **¹H NMR (400 MHz, CDCl₃)** δ 6.67 (t, *J* = 2.1 Hz, 2H), 6.16 (t, *J* = 2.1 Hz, 2H), 3.89 (t, *J* = 7.1 Hz, 2H), 2.70 (t, *J* = 7.6 Hz, 2H), 1.82-1.75 (m, 2H), 1.64 – 1.55 (m, 2H), 1.37-1.32 (m, 6H). **¹³C NMR (101 MHz, CDCl₃)** δ 145.1 (dm, *J_F* = 245.4 Hz), 139.5 (dm, *J_F* = 252.5 Hz), 137.5 (dm, *J_F* = 252.5 Hz), 120.5, 115.5 (td, *J_F* = 19.0, 3.7 Hz), 107.9, 49.6, 31.6, 29.3, 29.1, 28.9, 26.7, 22.4. **¹⁹F NMR (377 MHz, CDCl₃)** δ -144.47 (dd, *J* = 23.2, 9.1 Hz, 2F), -158.29 (t, *J* = 21.0 Hz, 1F), -163.08 (ddd, *J* = 24.5, 10.4, 1.4 Hz, 3F). **HRMS (ESI)** calculated for C₁₇H₁₉NF₅ [M+H]⁺ *m/z* 332.1432, found 332.1428. **IR (neat, cm⁻¹)** 2931, 2859, 1500, 1281, 1121, 962, 719, 615.



9-(6-(perfluorophenyl)hexyl)-9H-carbazole (21)

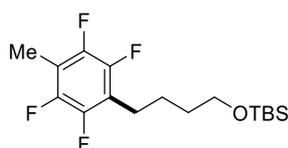
Following the GPA using 1,2,3,4,5-pentafluorobenzene (168.2 mg, 1.0 mmol, 2.0 equiv), 9-(hex-5-en-1-yl)-9H-carbazole (124.7 mg, 0.5 mmol, 1.0 equiv), and 5 mol% catalyst. The crude product was purified by column chromatography (100% hexane) to provide the title compound as a white solid in 54% yield (113.3 mg). **¹H NMR (400 MHz, CDCl₃)** δ 8.09 (d, *J* = 7.7 Hz, 2H), 7.44 (t, *J* = 7.2 Hz, 2H), 7.37 (d, *J* = 7.7 Hz, 2H), 7.21 (t, *J* = 7.2 Hz, 2H), 4.28 (t, *J* = 7.1 Hz, 2H), 2.61 (t, *J* = 7.4 Hz, 2H), 2.00 – 1.76 (m, 2H), 1.57 – 1.46 (m, 2H), 1.42-1.33 (m, 4H). **¹³C NMR (101 MHz, CDCl₃)** δ 145.1 (dm, *J_F* = 245.4 Hz), 139.5 (dm, *J_F* = 252.5 Hz), 137.5 (dm, *J_F* = 252.5 Hz), 140.5, 125.7, 123.0, 120.5, 118.9, 115.32 (t, *J_F* = 20.0 Hz), 108.7, 43.1, 29.2, 28.99, 28.95, 27.1, 22.3. **¹⁹F NMR (377 MHz, CDCl₃)** δ -144.47 (dd, *J* = 23.5, 9.3 Hz, 2F), -158.15 (t, *J* = 21.1 Hz, 1F), -162.37 – -167.29 (m, 2F). **HRMS (DART)** calculated for C₂₄H₂₁NF₅ [M+H]⁺ *m/z* 418.1589, found 418.1590. **IR (neat, cm⁻¹)** 2924, 2854, 1502, 1452, 999, 952, 747, 720. **Melting point:** 144-146 °C.



1-(7-(perfluorophenyl)heptyl)-1H-indole (22)

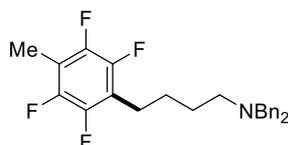
Following the GPA using 1,2,3,4,5-pentafluorobenzene (168.2 mg, 1.0 mmol, 2.0 equiv), 1-

(hept-6-en-1-yl)-1*H*-indole (106.7 mg, 0.5 mmol, 1.0 equiv), and 5 mol% catalyst. The crude product was purified by column chromatography (100% hexane) to provide the title compound as a colorless oil in 73% yield (142.3 mg). **¹H NMR (400 MHz, CDCl₃)** δ 7.62 (d, *J* = 7.9 Hz, 1H), 7.32 (dd, *J* = 8.2, 0.6 Hz, 1H), 7.23 – 7.15 (m, 1H), 7.14 – 7.02 (m, 2H), 6.47 (dd, *J* = 3.1, 0.7 Hz, 1H), 4.09 (t, *J* = 7.1 Hz, 2H), 2.64 (t, *J* = 7.6 Hz, 2H), 1.89 – 1.74 (m, 2H), 1.54-1.51 (m, 2H), 1.34 – 1.22 (m, 6H). **¹³C NMR (101 MHz, CDCl₃)** δ 145.1 (dm, *J_F* = 245.4 Hz), 139.5 (dm, *J_F* = 251.5 Hz), 137.5 (dm, *J_F* = 251.5 Hz), 136.1, 128.7, 127.8, 121.4, 121.0, 119.3, 109.4, 101.0, 46.4, 30.3, 29.3, 29.1, 29.0, 27.0, 22.3. **¹⁹F NMR (377 MHz, CDCl₃)** δ -144.47 (dd, *J* = 23.2, 9.1 Hz, 2F), -158.29 (t, *J* = 21.0 Hz, 1F), -163.08 (ddd, *J* = 24.5, 10.4, 1.4 Hz, 2F). **HRMS (DART)** calculated for C₂₁H₂₁NF₅ [M+H]⁺ *m/z* 382.1589, found 382.1587. **IR (neat, cm⁻¹)** 2931, 2858, 1500, 1462, 1314, 1121, 960, 737.



***tert*-butyldimethyl(4-(2,3,5,6-tetrafluoro-4-methylphenyl)butoxy)silane (23)**

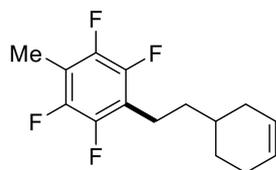
Following the GPA using 1,2,4,5-tetrafluoro-3-methylbenzene (82.0 mg, 0.5 mmol, 1.0 equiv), (but-3-en-1-yloxy)(*tert*-butyl)dimethylsilane (186.4 mg, 1.0 mmol, 2.0 equiv), and 5mol% catalyst. The crude product was purified by column chromatography (100% hexane) to provide the title compound as a colorless oil in 62% yield (104.2 mg). **¹H NMR (400 MHz, CDCl₃)** δ 3.63 (t, *J* = 6.2 Hz, 2H), 2.71 (t, *J* = 7.4 Hz, 2H), 2.23 (t, *J* = 2.1 Hz, 3H), 1.72 – 1.61 (m, 2H), 1.59 – 1.50 (m, 2H), 0.88 (s, 9H), 0.04 (s, 6H). **¹³C NMR (101 MHz, CDCl₃)** 145.1 (dm, *J_F* = 244.4 Hz), 144.7 (dm, *J_F* = 244.4 Hz), 117.8 (t, *J_F* = 18.7 Hz), 113.4 (t, *J_F* = 18.8 Hz), 62.7, 32.3, 26.1, 25.8, 22.6, 18.5, 7.5, -5.2. **¹⁹F NMR (377 MHz, CDCl₃)** δ -145.16 (ddd, *J* = 22.1, 12.9, 2.0 Hz, 2F), -146.57 (dd, *J* = 22.1, 12.9 Hz, 2F). **HRMS (DART)** calculated for C₁₇H₂₇OF₄Si [M+H]⁺ *m/z* 351.1762, found 351.1761. **IR (neat, cm⁻¹)** 2953, 2859, 1484, 1275, 1256, 1100, 835, 774.



***N,N*-dibenzyl-4-(2,3,5,6-tetrafluoro-4-methylphenyl)butan-1-amine (24)**

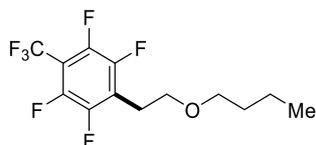
Following the GPA using 1,2,4,5-tetrafluoro-3-methylbenzene (164.0 mg, 1.0 mmol, 2.0 equiv),

N,N-dibenzylbut-3-en-1-amine (125.7 mg, 0.5 mmol, 1.0 equiv), and 5mol% catalyst. The crude product was purified by column chromatography (1% trimethylamine and 1% EtOAc in hexane) to provide the title compound as a yellow oil in 75% yield (164.7 mg). **¹H NMR (400 MHz, CDCl₃)** δ 7.39 – 7.28 (m, 8H), 7.25-7.21 (m, 2H), 3.55 (s, 4H), 2.62 (t, *J* = 6.9 Hz, 2H), 2.45 (t, *J* = 5.9 Hz, 2H), 2.24 (t, *J* = 2.0 Hz, 3H), 1.64 – 1.48 (m, 4H). **¹³C NMR (101 MHz, CDCl₃)** δ 145.1 (dddd, *J_F* = 244.4, 21.4, 14.2, 7.4, 3.8 Hz), 144.8 (dddd, *J_F* = 244.4, 21.5, 14.2, 7.4, 3.8 Hz), 139.9, 128.9, 128.3, 127.0, 117.8 (t, *J_F* = 18.8 Hz), 113.4 (t, *J_F* = 19.3 Hz), 58.6, 53.1, 27.0, 26.7 – 26.5 (m), 22.6, 7.5. **¹⁹F NMR (377 MHz, CDCl₃)** δ -145.07 (dd, *J* = 20.5, 12.9 Hz, 2F), -146.44 (dd, *J* = 22.1, 12.9 Hz, 2F). **HRMS (ESI)** calculated for C₂₅H₂₆NF₄ [M+H]⁺ *m/z* 416.1996, found 416.2006. **IR (neat, cm⁻¹)** 2937, 2795, 1484, 1273, 1115, 907, 734, 697.



1-(2-(cyclohex-3-en-1-yl)ethyl)-2,3,5,6-tetrafluoro-4-methylbenzene (25)

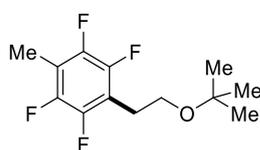
Following the GPA using 1,2,4,5-tetrafluoro-3-methylbenzene (82.0 mg, 0.5 mmol, 1.0 equiv), 4-vinylcyclohex-1-ene (108.2 mg, 1.0 mmol, 2.0 equiv), and 5 mol% catalyst at 90 °C for 12 h. The crude product was purified by column chromatography (100% hexane) to provide the title compound as a colorless oil in 99% yield (134.4 mg). **¹H NMR (400 MHz, CDCl₃)** δ 5.69-5.63 (m, 2H), 2.74 (t, *J* = 7.3 Hz, 2H), 2.23 (s, 3H), 2.17 (d, *J* = 17.1 Hz, 1H), 2.11 – 2.01 (m, 2H), 1.82-1.79 (m, 1H), 1.77 – 1.64 (m, 1H), 1.55 (m, 3H), 1.34 – 1.20 (m, 1H). **¹³C NMR (101 MHz, CDCl₃)** δ 145.1 (dm, *J_F* = 245.4 Hz), 144.6 (dm, *J_F* = 245.4 Hz), 127.2, 126.4, 118.1 (t, *J_F* = 18.5 Hz), 113.3 (t, *J_F* = 19.2 Hz), 36.2, 33.4, 31.7, 28.7, 25.2, 20.3, 7.5. **¹⁹F NMR (377 MHz, CDCl₃)** δ -145.12 (dd, *J* = 22.1, 12.9 Hz, 2F), -146.88 (dd, *J* = 22.0, 12.9 Hz, 2F). **HRMS (EI)** calculated for C₁₅H₁₆F₄ [M]⁺ *m/z* 272.1183, found 272.1181. **IR (neat, cm⁻¹)** 3025, 2916, 1483, 1277, 1091, 1058, 880, 651.



1-(2-butoxyethyl)-2,3,5,6-tetrafluoro-4-(trifluoromethyl)benzene (26)

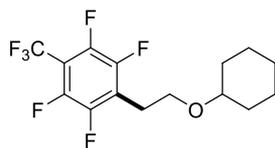
Following the GPA using 1,2,4,5-tetrafluoro-3-(trifluoromethyl)benzene (109.1 mg, 0.5 mmol,

1.0 equiv), 1-(vinylxy)butane (100.2 mg, 1.0 mmol, 2.0 equiv), and 5 mol% catalyst. The crude product was purified by column chromatography (1% EtOAc in hexane) to provide the title compound as a yellow oil in 88% yield (142.7 mg). **¹H NMR (400 MHz, CDCl₃)** δ 3.65 (t, *J* = 6.5 Hz, 2H), 3.42 (t, *J* = 6.6 Hz, 2H), 3.05 (t, *J* = 6.5 Hz, 2H), 1.55 – 1.45 (m, 2H), 1.35 – 1.23 (m, 2H), 0.88 (t, *J* = 7.4 Hz, 3H). **¹³C NMR (101 MHz, CDCl₃)** δ 145.8 (dm, *J_F* = 242.4 Hz), 144.2 (dm, *J_F* = 264.6 Hz), 122.9 (t, *J_F* = 17.2 Hz), 121.1 (-CF₃, *J_F* = 275.7 Hz), 108.5-107.7, 71.0, 68.4, 31.8, 24.1, 19.4, 13.8. **¹⁹F NMR (377 MHz, CDCl₃)** δ -51.57 – -59.88 (m, 3F), -141.19 – -142.65 (m, 4F). **HRMS (DART)** calculated for C₁₃H₁₄OF₇ [M+H]⁺ *m/z* 319.0927, found 319.0929. **IR (neat, cm⁻¹)** 2960, 2872, 1663, 1492, 1323, 1146, 956, 855, 714.



1-(2-(tert-butoxy)ethyl)-2,3,5,6-tetrafluoro-4-methylbenzene (27)

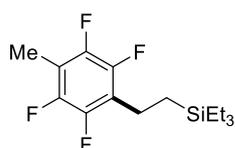
Following the GPA using 1,2,4,5-tetrafluoro-3-methylbenzene (82.0 mg, 0.5 mmol, 1.0 equiv), 2-methyl-2-(vinylxy)propane (100.2 mg, 1.0 mmol, 2.0 equiv), and 5 mol% catalyst. The crude product was purified by column chromatography (2% EtOAc in hexane) to provide the title compound as a yellow oil in 83% yield (111.6 mg). **¹H NMR (400 MHz, CDCl₃)** δ 3.52 (t, *J* = 6.5 Hz, 2H), 2.92 (s, 2H), 2.24 (s, 3H), 1.13 (s, 9H). **¹³C NMR (101 MHz, CDCl₃)** δ 145.2 (dm, *J_F* = 244.4 Hz), 144.8 (dm, *J_F* = 243.4 Hz), 114.8 (t, *J_F* = 18.6 Hz), 113.9 (t, *J_F* = 19.2 Hz), 73.3, 60.3, 27.5, 24.8, 7.5. **¹⁹F NMR (377 MHz, CDCl₃)** δ -145.18 (dd, *J* = 21.7, 13.0 Hz, 2F), -145.85 (dd, *J* = 21.7, 13.0 Hz, 2F). **HRMS (DART)** calculated for C₁₃H₁₇OF₄ [M+H]⁺ *m/z* 265.1210, found 265.1211. **IR (neat, cm⁻¹)** 2974, 2872, 1391, 1364, 1271, 1194, 1082, 897, 594.



1-(2-(cyclohexyloxy)ethyl)-2,3,5,6-tetrafluoro-4-(trifluoromethyl)benzene (28)

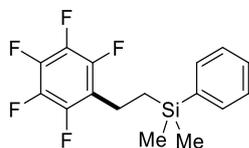
Following the GPA using 1,2,4,5-tetrafluoro-3-(trifluoromethyl)benzene (109.1 mg, 0.5 mmol, 1.0 equiv), (vinylxy)cyclohexane (126.2 mg, 1.0 mmol, 2.0 equiv), and 5 mol% catalyst. The crude product was purified by column chromatography (2% EtOAc in hexane) to provide the title compound as a yellow oil in 92% yield (159.4 mg). **¹H NMR (400 MHz, CDCl₃)** δ 3.67 (t, *J* = 6.6 Hz,

2H), 3.36 – 3.16 (m, 1H), 3.03 (t, $J = 6.6$ Hz, 2H), 1.84-1.81 (m, 2H), 1.68-1.67 (m, 2H), 1.35 – 1.10 (m, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 145.8 (dm, $J_F = 246.4$ Hz), 143.9 (dm, $J_F = 261.6$ Hz), 123.0 (t, $J_F = 18.1$ Hz), 121.1 ($-\text{CF}_3$, $J_F = 275.7$ Hz), 108.1-107.4 (m), 77.8, 65.4, 32.2, 25.9, 24.7, 24.0. ^{19}F NMR (377 MHz, CDCl_3) δ -56.29 (t, $J = 22.0$ Hz, 3F), -141.66 – -141.58 (m, 2F), -141.78 – -142.44 (m, 2F). HRMS (EI) calculated for $\text{C}_{15}\text{H}_{15}\text{F}_7\text{O} [\text{M}]^+$ m/z 344.1011, found 344.1012. IR (neat, cm^{-1}) 2934, 2860, 1492, 1323, 1144, 952, 855, 714.



triethyl(2,3,5,6-tetrafluoro-4-methylphenethyl)silane (29)

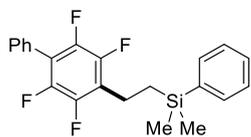
Following the GPA using 1,2,4,5-tetrafluoro-3-methylbenzene (82.0 mg, 0.5 mmol, 1.0 equiv) and triethyl(vinyl)silane (142.3 mg, 1.0 mmol, 2.0 equiv). The crude product was purified by column chromatography (100% hexane) to provide the title compound as a colorless oil in 66% yield (102.3 mg). ^1H NMR (400 MHz, CDCl_3) δ 2.76 – 2.57 (m, 2H), 2.23 (t, $J = 2.1$ Hz, 3H), 0.97 (t, $J = 7.9$ Hz, 9H), 0.87 – 0.79 (m, 2H), 0.58 (q, $J = 7.9$ Hz, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 145.2 (dddd, $J_F = 244.4$, 14.6, 7.2, 3.8 Hz), 144.5 (dddd, $J_F = 243.4$, 14.2, 7.7, 3.8 Hz), 121.0 (t, $J_F = 18.7$ Hz), 112.9 (t, $J_F = 19.3$ Hz), 17.3, 12.5, 7.4, 3.2. ^{19}F NMR (377 MHz, CDCl_3) δ -145.25 (dd, $J = 22.1$, 12.9 Hz, 2F), -147.86 (dd, $J = 22.0$, 12.9 Hz, 2F). HRMS (EI) calculated for $\text{C}_{13}\text{H}_{17}\text{F}_4\text{Si} [\text{M}-\text{C}_2\text{H}_5]^+$ m/z 277.1030, found $[\text{M}-\text{C}_2\text{H}_5]^+$ 277.1031. IR (neat, cm^{-1}) 2954, 2878, 1484, 1276, 1118, 857, 775, 727, 597.



dimethyl(2-(perfluorophenyl)ethyl)(phenyl)silane (30)

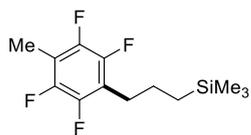
Following the GPA using 1,2,3,4,5-pentafluorobenzene (84.1 mg, 0.5 mmol, 1.0 equiv), dimethyl(phenyl)(vinyl)silane (162.3 mg, 1.0 mmol, 2.0 equiv). The crude product was purified by column chromatography (100% hexane) to provide the title compound as a colorless oil in 92% yield (149.2 mg) with matched spectra⁸. ^1H NMR (400 MHz, CDCl_3) δ 7.56 – 7.44 (m, 2H), 7.40 – 7.29 (m, 3H), 2.74 – 2.56 (m, 2H), 1.14 – 1.00 (m, 2H), 0.33 (s, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ

144.8 (dm, $J_F = 244.4$ Hz), 139.4 (dm, $J_F = 251.5$ Hz), 138.1, 137.5 (dm, $J_F = 252.5$ Hz), 133.6, 129.3, 128.0, 118.1 – 117.6 (m), 17.1, 16.3, -3.3. ^{19}F NMR (377 MHz, CDCl_3) δ -145.23 (dd, $J = 22.5, 8.3$ Hz, 2F), -158.93 (t, $J = 20.8$ Hz, 1F), -163.14 – -163.28 (m, 2F).



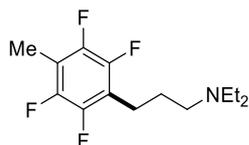
Dimethyl(phenyl)(2-(2,3,5,6-tetrafluoro-[1,1'-biphenyl]-4-yl)ethyl)silane (31)

Following the GPA using 1,2,4,5-tetrafluoro-3-(trifluoromethyl)benzene (113.1 mg, 0.5 mmol, 1.0 equiv) and dimethyl(phenyl)(vinyl)silane (162.3 mg, 1.0 mmol, 2.0 equiv). The crude product was purified by column chromatography (100% hexane) to provide the title compound as a white solid in 99% yield (192.1 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.67 – 7.31 (m, 10H), 2.90 – 2.68 (m, 2H), 1.19 (m, 7.0 Hz, 2H), 0.46 – 0.25 (m, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 144.9 (dm, $J_F = 237.4$ Hz), 143.7 (dm, $J_F = 232.3$ Hz), 138.2, 133.6, 130.3, 129.2, 128.9, 128.6, 128.0, 17.6, 16.2, -3.2. ^{19}F NMR (377 MHz, CDCl_3) δ -145.40 (dd, $J = 22.3, 12.2$ Hz, 2F), -145.96 (dd, $J = 22.3, 12.3$ Hz, 2F). HRMS (EI) calculated for $\text{C}_{22}\text{H}_{20}\text{F}_4\text{Si}$ $[\text{M}]^+$ m/z 388.1270, found 388.1275. IR (neat, cm^{-1}) 2952, 2893, 1481, 1436, 1061, 906, 756, 600. Melting point: 42-43 °C.



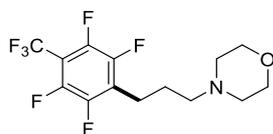
trimethyl(3-(2,3,5,6-tetrafluoro-4-methylphenyl)propyl)silane (32)

Following the GPA using 1,2,4,5-tetrafluoro-3-methylbenzene (82.0 mg, 0.5 mmol, 1.0 equiv), allyltrimethylsilane (114.3 mg, 1.0 mmol, 2.0 equiv), and 5mol% catalyst. The crude product was purified by column chromatography (100% hexane) to provide the title compound as a colorless oil in 69% yield (96.8 mg). ^1H NMR (400 MHz, CDCl_3) δ 2.70 (t, $J = 7.5$ Hz, 2H), 2.23 (t, $J = 2.1$ Hz, 3H), 1.64 – 1.53 (m, 2H), 0.61 – 0.45 (m, 2H), -0.03 (s, 9H). ^{13}C NMR (101 MHz, CDCl_3) δ 145.1 (dm, $J_F = 244.4$ Hz), 144.7 (dm, $J_F = 243.4$ Hz), 117.9 (t, $J_F = 18.8$ Hz), 113.3 (t, $J_F = 19.2$ Hz), 26.5, 24.2, 16.6, 7.5, -1.7. ^{19}F NMR (377 MHz, CDCl_3) δ -145.23 (ddd, $J = 22.2, 12.9, 2.0$ Hz, 2F), -146.59 (dd, $J = 22.2, 12.9$ Hz, 2F). HRMS (EI) calculated for $\text{C}_{13}\text{H}_{18}\text{F}_4\text{Si}$ $[\text{M}]^+$ m/z 278.1114, found 278.1120. IR (neat, cm^{-1}) 2954, 2878, 1483, 1272, 1116, 1061, 833, 692.



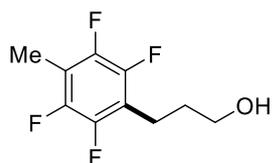
***N,N*-diethyl-3-(2,3,5,6-tetrafluoro-4-methylphenyl)propan-1-amine (33)**

Following the GPA using 1,2,4,5-tetrafluoro-3-methylbenzene (82.0 mg, 0.5 mmol, 1.0 equiv), *N,N*-diethylprop-2-en-1-amine (113.2 mg, 1.0 mmol, 2.0 equiv), and 5mol% catalyst. The crude product was purified by column chromatography (1% trimethylamine and 10% EtOAc in hexane) to provide the title compound as a colorless oil in 88% yield (127.1 mg). **¹H NMR (400 MHz, CDCl₃)** δ 2.69 (t, *J* = 7.7 Hz, 2H), 2.56 – 2.41 (m, 6H), 2.22 (s, 3H), 1.81 – 1.63 (m, 2H), 0.99 (t, *J* = 7.1 Hz, 6H). **¹³C NMR (101 MHz, CDCl₃)** δ 145.0 (dddd, *J_F* = 244.4, 21.4, 14.2, 7.4, 3.8 Hz), 144.6 (dddd, *J_F* = 244.4, 21.5, 14.2, 7.4, 3.8 Hz), 117.7 (t, *J_F* = 18.7 Hz), 113.3 (t, *J_F* = 19.2 Hz), 52.4, 46.9, 26.9, 22.4 – 20.5 (m), 11.7, 7.3. **¹⁹F NMR (377 MHz, CDCl₃)** δ -145.13 (dd, *J* = 22.1, 12.9 Hz, 2F), -146.57 (dd, *J* = 22.1, 12.9 Hz, 2F). **HRMS (ESI)** calculated for C₁₄H₂₀NF₄ [M+H]⁺ *m/z* 278.1526, found 278.1536. **IR (neat, cm⁻¹)** 2970, 2801, 1483, 1278, 1071, 932, 891, 600.

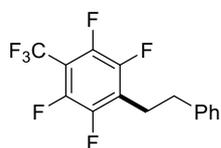


4-(3-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)propyl)morpholine (34)

Following the GPA using 1,2,4,5-tetrafluoro-3-(trifluoromethyl)benzene (109.1 mg, 0.5 mmol, 1.0 equiv), 4-allylmorpholine (127.2 mg, 1.0 mmol, 2.0 equiv), and 5mol% catalyst. The crude product was purified by column chromatography (1% trimethylamine and 10% EtOAc in hexane) to provide the title compound as a yellow oil in 91% yield (156.6 mg). **¹H NMR (400 MHz, CDCl₃)** δ 3.66 (t, *J* = 8.0 Hz, 4H), 2.83 (t, *J* = 7.6 Hz, 2H), 2.41 – 2.38 (m, 6H), 1.87 – 1.72 (m, 2H). **¹³C NMR (101 MHz, CDCl₃)** δ 145.3 (dm, *J_F* = 251.4 Hz), 144.0 (dm, *J_F* = 256.5 Hz), 125.6 (t, *J_F* = 18.4 Hz), 121.1 (-CF₃, *J_F* = 275.7 Hz), 108.4 – 106.7 (m), 67.0, 58.0, 53.7, 25.7, 21.1. **¹⁹F NMR (377 MHz, CDCl₃)** δ -54.69 – -58.45 (m, 3F), -141.19 – -142.08 (m, 2F), -142.23 – -142.99 (m, 2F). **HRMS (ESI)** calculated for C₁₄H₁₅NOF₇ [M+H]⁺ *m/z* 346.1036, found 346.1038. **IR (neat, cm⁻¹)** 2954, 2856, 1662, 1491, 1327, 1141, 1117, 970, 861, 713.

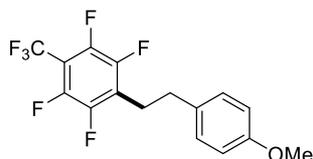


4,4,5,5-tetrafluoro-2-(3-(2,3,5,6-tetrafluoro-4-methylphenyl)propyl)-1,3,2-dioxaborolane (35) Following the GPA using 1,2,4,5-tetrafluoro-3-methylbenzene (82.0 mg, 0.5 mmol, 1.0 equiv), 2-allyl-4,4,5,5-tetrafluoro-1,3,2-dioxaborolane (252.0 mg, 1.5 mmol, 3.0 equiv), and 5mol% catalyst. The crude product was oxidized by using NaBO_3 (10 eq.) in THF/ H_2O (1/1) at room temperature for 2 h. And then purified by column chromatography (0-10% EtOAc in hexane) to provide the title compound as a yellow oil in 49% yield (53.0 mg). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 3.64 (t, $J = 6.3$ Hz, 2H), 2.77 (t, $J = 7.5$ Hz, 2H), 2.21 (t, $J = 2.0$ Hz, 3H), 1.93 (s, 1H), 1.87 – 1.75 (m, 2H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 145.1 (dm, $J_F = 244.4$ Hz), 144.6 (dm, $J_F = 244.4$ Hz), 117.1 (t, $J_F = 18.6$ Hz), 113.7 (t, $J_F = 19.2$ Hz), 61.9, 32.1, 19.2-19.0 (m), 7.4. $^{19}\text{F NMR}$ (377 MHz, CDCl_3) δ -144.88 (ddd, $J = 22.1, 12.8, 1.9$ Hz, 2F), -146.60 (dd, $J = 22.0, 12.9$ Hz, 2F). **HRMS (EI)** calculated for $\text{C}_{10}\text{H}_{10}\text{F}_4\text{O}$ $[\text{M}]^+$ m/z 222.0662, found 222.0662. **IR (neat, cm^{-1})** 3338, 2933, 2869, 1483, 1269, 1060, 927, 647, 597.



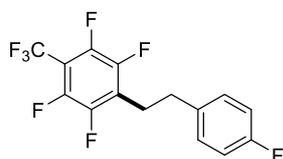
1,2,4,5-tetrafluoro-3-phenethyl-6-(trifluoromethyl)benzene (36)

Following the GPA using 1,2,4,5-tetrafluoro-3-(trifluoromethyl)benzene (109.1 mg, 0.5 mmol, 1.0 equiv), styrene (104.2 mg, 1.0 mmol, 2.0 equiv), and 5 mol% catalyst. The crude product was purified by column chromatography (100% hexane) to provide the title compound as a white solid in 76% yield (124.6 mg) with matched spectra⁵. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.31–7.21 (m, 3H), 7.18-7.16 (m, 2H), 3.07 (t, $J = 8.0$ Hz, 2H), 2.90 (t, $J = 8.0$ Hz, 2H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 145.3 (dm, $J_F = 247.5$ Hz), 144.0 (dm, $J_F = 259.6$ Hz), 139.8, 128.8, 128.4, 126.9, 124.8 (t, $J_F = 18.3$ Hz), 121.1 ($-\text{CF}_3$, $J_F = 274.7$ Hz), 108.8 – 107.0 (m), 35.1, 25.3. $^{19}\text{F NMR}$ (377 MHz, CDCl_3) δ -56.20 (t, $J = 21.6$ Hz, 3F), -141.18 – -141.69 (m, 2F), -142.22 – -142.51 (m, 2F).



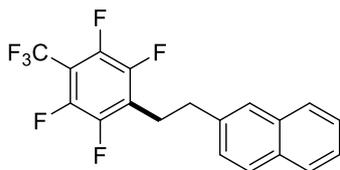
1,2,4,5-tetrafluoro-3-(4-methoxyphenethyl)-6-(trifluoromethyl)benzene (37)

Following the GPA using 1,2,4,5-tetrafluoro-3-(trifluoromethyl)benzene (109.1 mg, 0.5 mmol, 1.0 equiv), 1-methoxy-4-vinylbenzene (134.2 mg, 1.0 mmol, 2.0 equiv), and 5 mol% catalyst. The crude product was purified by column chromatography (100% hexane) to provide the title compound as a white solid in 69% yield (118.6 mg). **¹H NMR (400 MHz, CDCl₃)** δ 7.09 (d, *J* = 8.5 Hz, 2H), 6.93 – 6.76 (m, 2H), 3.80 (s, 3H), 3.04 (t, *J* = 7.8 Hz, 2H), 2.86 (t, *J* = 7.8 Hz, 2H). **¹³C NMR (101 MHz, CDCl₃)** δ 158.5, 145.3 (dm, *J_F* = 247.5 Hz), 144.1 (dm, *J_F* = 259.6 Hz), 131.9, 129.4, 124.9 (t, *J_F* = 18.4 Hz), 121.1 (-CF₃, *J_F* = 276.7 Hz), 114.1, 108.7 – 106.8 (m), 55.3, 34.2, 25.6. **¹⁹F NMR (377 MHz, CDCl₃)** δ -56.20 (td, *J* = 21.6, 2.9 Hz, 3F), -141.24 – -141.81 (m, 2F), -142.12 – -142.59 (m, 2F). **HRMS (EI)** calculated for C₁₆H₁₁F₇O [M]⁺ *m/z* 352.0693, found 352.0689. **IR (neat, cm⁻¹)** 2958, 2839, 1489, 1331, 1155, 1025, 937, 817, 714. **Melting point:** 60-62 °C.



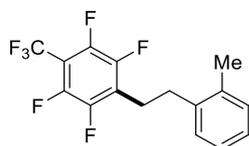
1,2,4,5-tetrafluoro-3-(4-fluorophenethyl)-6-(trifluoromethyl)benzene (38)

Following the GPA using 1,2,4,5-tetrafluoro-3-(trifluoromethyl)benzene (109.1 mg, 0.5 mmol, 1.0 equiv), 1-fluoro-4-vinylbenzene (122.1 mg, 1.0 mmol, 2.0 equiv) and 5 mol% cat. The crude product was purified by column chromatography (100% hexane) to provide the title compound as a white solid in 95% yield (163.7 mg). **¹H NMR (400 MHz, CDCl₃)** δ 7.17 – 7.09 (m, 2H), 7.02 – 6.93 (m, 2H), 3.05 (t, *J* = 7.7 Hz, 2H), 2.89 (t, *J* = 7.8 Hz, 2H). **¹³C NMR (101 MHz, CDCl₃)** δ 161.9 (d, *J_F* = 244.8 Hz), 145.4 (dm, *J_F* = 248.5 Hz), 144.1 (dm, *J_F* = 251.6 Hz), 135.4 (d, *J_F* = 3.3 Hz), 129.9 (d, *J_F* = 8.0 Hz), 124.4 (t, *J_F* = 18.3 Hz), 121.1 (-CF₃, *J_F* = 276.7 Hz), 115.6 (d, *J_F* = 21.3 Hz), 109.0 – 107.1 (m), 34.2, 25.4. **¹⁹F NMR (377 MHz, CDCl₃)** δ -56.22 (t, *J* = 21.9 Hz, 3F), -115.78 – -116.75 (m, 1F), -140.69 – -141.69 (m, 2F), -142.01 – -142.96 (m, 2F). **HRMS (EI)** calculated for C₁₅H₈F₈ [M]⁺ *m/z* 340.0943, found 340.0942. **IR (neat, cm⁻¹)** 2922, 2873, 1661, 1602, 1486, 1328, 1218, 1137, 1025, 939, 713, 524. **Melting point:** 68-71 °C.



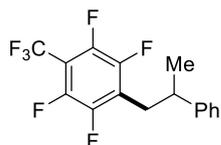
2-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenethyl)naphthalene (39)

Following the GPA using 1,2,4,5-tetrafluoro-3-(trifluoromethyl)benzene (109.1 mg, 0.5 mmol, 1.0 equiv), 2-vinylnaphthalene (154.2 mg, 1.0 mmol, 2.0 equiv) and 5 mol% cat. The crude product was purified by column chromatography (100% hexane) to provide the title compound as a white solid in 53% yield (97.3 mg). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.84 – 7.78 (m, 3H), 7.64 (s, 1H), 7.54 – 7.42 (m, 2H), 7.35 (dd, $J = 8.4, 1.6$ Hz, 1H), 3.22 – 3.13 (m, 2H), 3.13 – 3.04 (m, 2H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 145.4 (dm, $J_F = 248.5$ Hz), 144.0 (dm, $J_F = 258.6$ Hz), 137.3, 133.7, 132.5, 128.5, 127.8, 127.6, 126.8, 126.4, 125.8, 124.7 (t, $J_F = 18.3$ Hz), 121.1 (- CF_3 , $J_F = 273.7$ Hz), 108.7 – 107.0 (m), 35.2, 25.2. $^{19}\text{F NMR}$ (377 MHz, CDCl_3) δ -56.19 (t, $J = 22.0$ Hz, 3F), -139.73 – -141.26 (m, 2F), -141.80 – -143.42 (m, 2F). **HRMS (EI)** calculated for $\text{C}_{19}\text{H}_{11}\text{F}_7$ $[\text{M}]^+$ m/z 274.1339, found 274.1337. **IR (neat, cm^{-1})** 2944, 2875, 1663, 1488, 1326, 1142, 940, 713. **Melting point:** 154-156 °C.



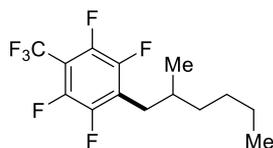
1,2,4,5-tetrafluoro-3-(2-methylphenethyl)-6-(trifluoromethyl)benzene (40)

Following the GPA using 1,2,4,5-tetrafluoro-3-(trifluoromethyl)benzene (109.1 mg, 0.5 mmol, 1.0 equiv), 1-methyl-2-vinylbenzene (118.2 mg, 1.0 mmol, 2.0 equiv), and 5 mol% catalyst. The crude product was purified by column chromatography (100% hexane) to provide the title compound as a white solid in 89% yield (148.4 mg). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.23 – 7.08 (m, 4H), 3.10 – 2.98 (m, 2H), 2.95 – 2.84 (m, 2H), 2.38 (s, 3H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 145.5 (dm, $J_F = 248.5$ Hz), 144.1 (dm, $J_F = 260.6$ Hz), 138.1, 136.1, 130.7, 129.0, 127.1, 126.4, 125.0 (t, $J_F = 18.4$ Hz), 121.2 (- CF_3 , $J_F = 275.7$ Hz), 109.2 – 106.8 (m), 32.7, 24.1, 19.0. $^{19}\text{F NMR}$ (377 MHz, CDCl_3) δ -56.20 (t, $J = 22.1$ Hz, 3F), -140.14 – -141.79 (m, 2F), -141.91 – -143.55 (m, 2F). **HRMS (EI)** calculated for $\text{C}_{16}\text{H}_{11}\text{F}_7$ $[\text{M}]^+$ m/z 336.0743, found 336.0741. **IR (neat, cm^{-1})** 2945, 2878, 1665, 1279, 1489, 1324, 1133, 939, 723. **Melting point:** 86-88 °C.



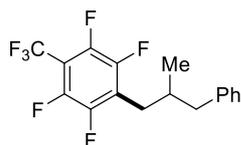
1,2,4,5-tetrafluoro-3-(2-phenylpropyl)-6-(trifluoromethyl)benzene (41)

Following the GPA using 1,2,4,5-tetrafluoro-3-(trifluoromethyl)benzene (109.1 mg, 0.5 mmol, 1.0 equiv), prop-1-en-2-ylbenzene (118.2 mg, 1.0 mmol, 2.0 equiv), and 5 mol% catalyst. The crude product was purified by column chromatography (100% hexane) to provide the title compound as a colorless oil in 93% yield (151.6 mg). **¹H NMR (400 MHz, CDCl₃)** δ 7.35 – 7.27 (m, 2H), 7.25 – 7.15 (m, 3H), 3.19 – 2.91 (m, 3H), 1.34 (d, *J* = 6.6 Hz, 3H). **¹³C NMR (101 MHz, CDCl₃)** δ 145.6 (dm, *J_F* = 244.4 Hz), 144.0(dm, *J_F* = 256.6 Hz), 145.0, 128.8, 127.0, 126.8, 124.30 (t, *J_F* = 18.2 Hz), 121.1 (-CF₃, *J_F* = 274.7 Hz), 108.5 – 107.2 (m), 39.8, 32.2, 21.0. **¹⁹F NMR (377 MHz, CDCl₃)** δ -56.24 (t, *J* = 21.7 Hz, 3F), -141.01 – -141.36 (m, 2F), -141.45 – -141.86 (m, 2F). **HRMS (EI)** calculated for C₁₆H₁₁F₇[M]⁺ *m/z* 336.0749, found 336.0756. **IR (neat, cm⁻¹)** 2923, 2853, 1483, 1279, 1061, 936, 918, 603.



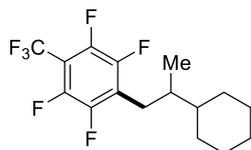
1,2,4,5-tetrafluoro-3-(2-methylhexyl)-6-(trifluoromethyl)benzene (42)

Following the GPA using 1,2,4,5-tetrafluoro-3-(trifluoromethyl)benzene (109.1 mg, 0.5 mmol, 1.0 equiv), 2-methylhex-1-ene (147.3 mg, 1.5 mmol, 3.0 equiv), and 5 mol% catalyst. The crude product was purified by column chromatography (100% hexane) to provide the title compound as a colorless oil in 73% yield (115.1 mg). **¹H NMR (400 MHz, CDCl₃)** δ 2.78 (dd, *J* = 13.1, 5.9 Hz, 1H), 2.58 (dd, *J* = 13.1, 8.6 Hz, 1H), 1.89 – 1.72 (m, 1H), 1.46 – 1.18 (m, 6H), 1.01 – 0.77 (m, 6H). **¹³C NMR (101 MHz, CDCl₃)** δ 145.6 (dm, *J_F* = 245.4 Hz), 144.2(dm, *J_F* = 259.6 Hz), 125.2 (t, *J_F* = 18.5 Hz), 121.2 (-CF₃, *J_F* = 275.7 Hz), 108.9 – 105.5 (m), 36.7, 33.7, 30.6, 29.4, 23.0, 19.3, 14.1. **¹⁹F NMR (377 MHz, CDCl₃)** δ -56.40 (t, *J* = 21.5 Hz, 3F), -141.18 – -141.64 (m, 2F), -141.86 – -142.31 (m, 2F). **HRMS (EI)** calculated for C₁₄H₁₅F₇[M]⁺ *m/z* 316.1056, found 316.1055. **IR (neat, cm⁻¹)** 2931, 2861, 1660, 1491, 1330, 1145, 971, 867, 714.



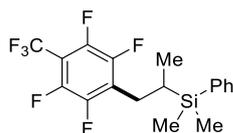
1,2,4,5-tetrafluoro-3-(2-methyl-3-phenylpropyl)-6-(trifluoromethyl)benzene (43)

Following the GPA using 1,2,4,5-tetrafluoro-3-(trifluoromethyl)benzene (109.1 mg, 0.5 mmol, 1.0 equiv), (2-methylallyl)benzene (132.2 mg, 1.0 mmol, 2.0 equiv), and 5 mol% catalyst. The crude product was purified by column chromatography (100% hexane) to provide the title compound as a colorless oil in 93% yield (164.5 mg). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.31 – 7.22 (m, 2H), 7.22 – 7.10 (m, 3H), 2.79 (dd, $J = 13.2, 5.9$ Hz, 1H), 2.71 – 2.53 (m, 3H), 2.26 – 2.08 (m, 1H), 0.90 (d, $J = 6.6$ Hz, 3H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 145.4 (dm, $J_F = 245.4$ Hz), 143.9 (dm, $J_F = 259.6$ Hz), 140.0, 129.1, 128.5, 126.4, 121.1 ($-\text{CF}_3$, $J_F = 271.7$ Hz), 108.8 – 106.6 (m), 43.6, 35.2, 30.4, 19.4. $^{19}\text{F NMR}$ (377 MHz, CDCl_3) δ -56.35 (t, $J = 22.0$ Hz, 3F), -140.79 – -141.31 (m, 2F), -141.53 – -142.29 (m, 2F). **HRMS (EI)** calculated for $\text{C}_{17}\text{H}_{13}\text{F}_7$ $[\text{M}]^+$ m/z 350.0900, found 350.0898. **IR (neat, cm^{-1})** 2964, 2921, 1661, 1491, 1329, 1142, 867, 814.



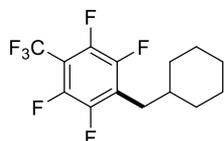
1-(2-cyclohexylpropyl)-2,3,5,6-tetrafluoro-4-(trifluoromethyl)benzene (44)

Following the GPA using 1,2,4,5-tetrafluoro-3-(trifluoromethyl)benzene (109.1 mg, 0.5 mmol, 1.0 equiv), prop-1-en-2-ylcyclohexane (124.2 mg, 1.0 mmol, 2.0 equiv), and 5 mol% catalyst. The crude product was purified by column chromatography (100% hexane) to provide the title compound as a colorless oil in 83% yield (136.5 mg). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 2.98 – 2.75 (m, 1H), 2.56 (dd, $J = 12.1, 10.7$ Hz, 1H), 1.85 – 1.63 (m, 6H), 1.32 – 1.05 (m, 6H), 0.82 (d, $J = 6.9$ Hz, 3H). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 145.6 (dm, $J_F = 245.4$ Hz), 144.2 (dm, $J_F = 256.5$ Hz), 125.9 (t, $J_F = 18.3$ Hz), 121.2 ($-\text{CF}_3$, $J_F = 275.7$ Hz), 108.5 – 106.5 (m), 43.2, 38.9, 30.6, 28.9, 27.9, 26.9, 26.9, 26.8, 15.7. $^{19}\text{F NMR}$ (377 MHz, CDCl_3) δ -56.23 (t, $J = 21.8$ Hz, 3F), -141.15 – -141.66 (m, 2F), -141.74 – -142.15 (m, 2F). **HRMS (EI)** calculated for $\text{C}_{16}\text{H}_{17}\text{F}_7$ $[\text{M}]^+$ m/z 342.1213, found 342.1216. **IR (neat, cm^{-1})** 2927, 2855, 1660, 1491, 1329, 1143, 969, 867, 714.



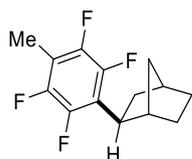
dimethyl(phenyl)(1-(2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl)propan-2-yl)silane (45)

Following the GPA using 1,2,4,5-tetrafluoro-3-(trifluoromethyl)benzene (109.1 mg, 0.5 mmol, 1.0 equiv), dimethyl(phenyl)(prop-1-en-2-yl)silane (176.3 mg, 1.0 mmol, 2.0 equiv), and 5 mol% catalyst. The crude product was purified by column chromatography (100% hexane) to provide the title compound as a colorless oil in 89% yield (175.8 mg). **¹H NMR (400 MHz, CDCl₃)** δ 7.56 – 7.47 (m, 2H), 7.43 – 7.32 (m, 3H), 2.94 – 2.79 (m, 1H), 2.56 (dd, *J* = 12.6, 12.1 Hz, 1H), 1.35 – 1.23 (m, 1H), 0.96 (d, *J* = 7.4 Hz, 3H), 0.39 (s, 3H), 0.35 (s, 3H). **¹³C NMR (101 MHz, CDCl₃)** δ 145.4 (dm, *J_F* = 253.5 Hz), 144.0 (dm, *J_F* = 252.6 Hz), 137.2, 133.9, 129.4, 128.0, 126.1 (t, *J_F* = 18.3 Hz), 121.1 (-CF₃, *J_F* = 275.7 Hz), 108.7 – 105.7 (m), 25.9, 20.3, 14.2, -4.5, -6.1. **¹⁹F NMR (377 MHz, CDCl₃)** δ -56.25 (t, *J* = 21.7 Hz, 3F), -141.34 – -141.79 (m, 2F), -141.83 – -142.30 (m, 2F). **HRMS (EI)** calculated for C₁₈H₁₇F₇Si [M]⁺ *m/z* 394.0988, found 394.0977. **IR (neat, cm⁻¹)** 2958, 2872, 1660, 1491, 1328, 1144, 965, 813, 712.



1-(cyclohexylmethyl)-2,3,5,6-tetrafluoro-4-(trifluoromethyl)benzene (46)

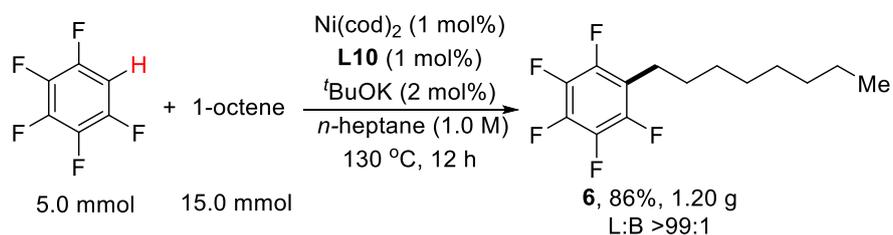
Following the GPA using 1,2,4,5-tetrafluoro-3-(trifluoromethyl)benzene (109.1 mg, 0.5 mmol, 1.0 equiv), methylenecyclohexane (96.2 mg, 1.0 mmol, 2.0 equiv), and 5 mol% catalyst. The crude product was purified by column chromatography (100% hexane) to provide the title compound as a colorless oil in 89% yield (138.0 mg). **¹H NMR (400 MHz, CDCl₃)** δ 2.66 (d, *J* = 7.0 Hz, 2H), 1.77 – 1.55 (m, 6H), 1.28 – 1.13 (m, 3H), 1.10 – 1.08 (dd, 2H). **¹³C NMR (101 MHz, CDCl₃)** δ 145.5 (dm, *J_F* = 245.4 Hz), 144.1 (dm, *J_F* = 259.6 Hz), 124.8 (t, *J_F* = 18.7 Hz), 121.2 (-CF₃, *J_F* = 275.7 Hz), 109.2 – 106.3 (m), 38.2, 33.0, 30.8, 26.3, 26.2. **¹⁹F NMR (377 MHz, CDCl₃)** δ -54.22 – -58.52 (m, 3F), -140.46 – -141.42 (m, 2F), -141.70 – -142.55 (m, 2F). **HRMS (EI)** calculated for C₁₄H₁₃F₇ [M]⁺ *m/z* 314.0900, found 314.0903. **IR (neat, cm⁻¹)** 2927, 2855, 1660, 1489, 1327, 1142, 980, 866, 713.



2-(2,3,5,6-tetrafluoro-4-methylphenyl)bicyclo[2.2.1]heptane (47)

Following the GPA using 1,2,4,5-tetrafluoro-3-methylbenzene (82.0 mg, 0.5 mmol, 1.0 equiv), bicyclo[2.2.1]hept-2-ene (94.2 mg, 1.0 mmol, 2.0 equiv), and 5 mol% catalyst. The crude product was purified by column chromatography (100% hexane) to provide the title compound as a colorless oil in 77% yield (98.9 mg). **¹H NMR (500 MHz, CDCl₃)** δ 3.06 – 2.92 (m, 1H), 2.49 (s, 1H), 2.36 (s, 1H), 2.21 (t, *J* = 2.0 Hz, 3H), 1.88 – 1.78 (m, 1H), 1.76 – 1.65 (m, 2H), 1.64 – 1.55 (m, 2H), 1.39 – 1.23 (m, 3H). **¹³C NMR (126 MHz, CDCl₃)** δ 145.4 (dm, *J_F* = 248.2 Hz), 144.8 (dm, *J_F* = 243.2 Hz), 122.0 (t, *J_F* = 15.5 Hz), 112.9 (t, *J_F* = 19.4 Hz), 41.7 (t, *J_F* = 2.2 Hz), 39.3 (t, *J_F* = 1.6 Hz), 39.0 (t, *J_F* = 2.1 Hz), 37.5 (t, *J_F* = 3.9 Hz), 36.7, 31.3, 28.5, 7.4. **¹⁹F NMR (471 MHz, CDCl₃)** δ -143.75 (dd, *J* = 21.5, 12.0 Hz, 2F), -145.35 (dd, *J* = 21.6, 11.9 Hz, 2F). **HRMS (EI)** calculated for C₁₄H₁₄F₄ [M]⁺ *m/z* 258.1026, found 258.1025. **IR (neat, cm⁻¹)** 2955, 2873, 1471, 1282, 1061, 906, 756, 600.

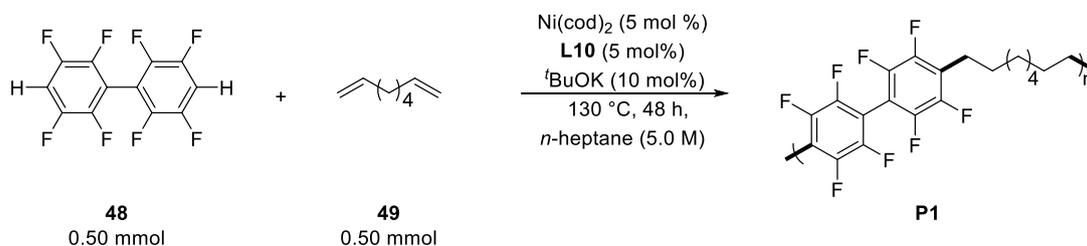
6. Gram-scale Synthesis of 1,2,3,4,5-pentafluoro-6-octylbenzene (6).



In a nitrogen-filled glove box, bis(1,5-cyclooctadiene)nickel (13.8 mg, 0.05 mmol, 1 mol%), $t\text{BuOK}$ (11.2 mg, 0.1 mmol, 2 mol%), **L10** (42.7 mg, 0.05 mmol, 1 mol%), and heptane (5.0 mL) were added to a Schlenk tube equipped with a magnetic stirring bar. The reaction mixture was allowed to stir at room temperature for 12 h, and then 1,2,3,4,5-pentafluorobenzene (840 mg, 5.0 mmol, 1.0 equiv) and oct-1-ene (2.35 mL, 15.0 mmol, 3.0 equiv) were added. The tube was taken out of the glovebox and stirred at 130 °C for 12 h. After cooling to room temperature, the resulting mixture was purified directly by silica gel column (100% hexanes) to provide the **2d** as a colorless oil in 86% yield with matched spectra. (1.20 g).

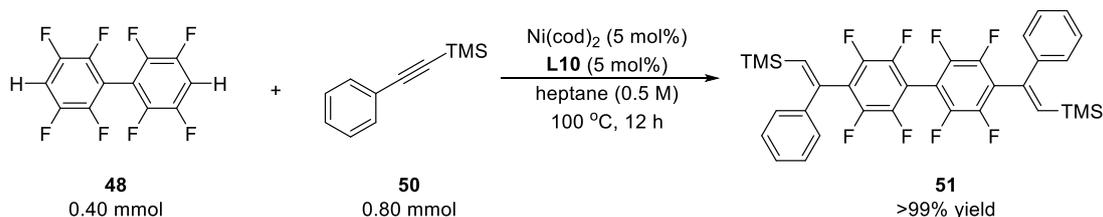
7. Nickel-catalyzed Copolymerization of Polyfluoroarenes with Dienes and Diynes.

7.1 Representative copolymerization of polyfluoroarenes with dienes



General procedure B (GPB): In a nitrogen-filled glove box, bis(1,5-cyclooctadiene)nickel (6.9 mg, 25 μmol , 5 mol%), $t\text{BuOK}$ (5.6 mg, 50 μmol , 10 mol%), **L10** (21.3 mg, 25 μmol , 1 mol%), and heptane (0.1 mL) were added to an 8 mL vial equipped with a magnetic stirring bar. The reaction mixture was allowed to stir at room temperature for 12 h, and then 2,2',3,3',5,5',6,6'-octafluoro-1,1'-biphenyl (149.1 mg, 0.50 mmol, 1.0 equiv) and octa-1,7-diene (55.1 mg, 0.50 mmol, 1.0 equiv) were added. The vial was taken out of the glovebox and stirred at 130 °C for 48 h. After cooling to room temperature, the resulting mixture was dissolved in DCM (5 mL) and then precipitated in methanol (100 mL) to provide a white solid. The precipitated polymer was dried under vacuum at 50 °C to constant weight.

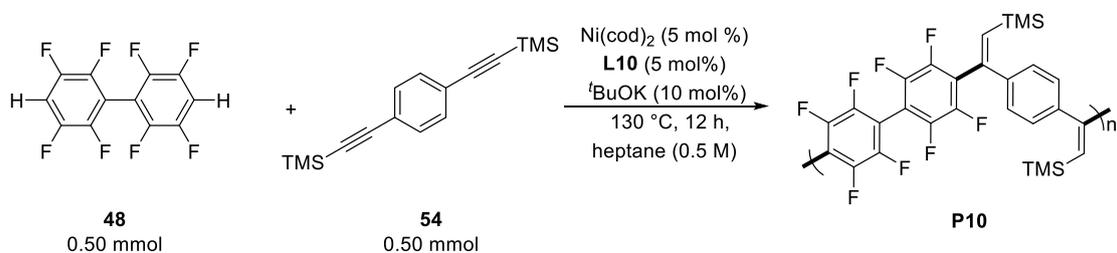
7.2 Model reaction of copolymerization of polyfluoroarenes with diynes



In a nitrogen-filled glove box, bis(1,5-cyclooctadiene)nickel (5.5 mg, 20 μmol , 5 mol%), $t\text{BuOK}$ (4.5 mg, 40 μmol , 10 mol%), **L10** (17.0 mg, 20 μmol , 5 mol%), and heptane (0.8 mL) were added to an 8 mL vial equipped with a magnetic stirring bar. The reaction mixture was allowed to stir at room temperature for 12 h, and then 2,2',3,3',5,5',6,6'-octafluoro-1,1'-biphenyl (119.2 mg, 0.40 mmol, 1.0 equiv) and trimethyl(phenylethynyl)silane (139.4 mg, 0.80 mmol, 2.0 equiv) were added. The vial was taken out of the glovebox and stirred at 100 °C for 12 h. After cooling to room

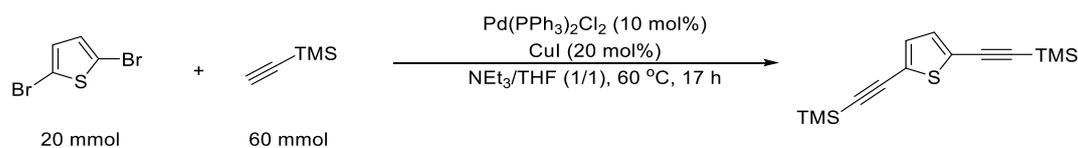
temperature, the resulting mixture was analyzed by GC analysis and then purified by silica gel column (100% PE) to provide the product as a white solid in quantitative yield (260.5 mg). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.42 – 7.28 (m, 10H), 6.17 (s, 2H), -0.01 (s, 18H). $^{19}\text{F NMR}$ (377 MHz, CDCl_3) δ -138.73 – -138.89 (m, 4F), -141.16 – -141.32 (m, 4F). $^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 144.2 (dm, $J_F = 322$ Hz), 143.5 (dm, $J_F = 308$ Hz), 143.0, 141.2, 140.9, 128.7, 128.3, 128.3, 126.6 (t, $J_F = 18.6$ Hz), 105.9, -0.1. **HRMS (EI)** calculated for $\text{C}_{33}\text{H}_{27}\text{F}_8\text{Si}_2$ $[\text{M}-\text{CH}_3]^+$ m/z 631.1518, found 631.1531. **IR (neat, cm^{-1})** 3023, 2959, 2899, 1594, 1461, 1251, 970, 866, 840, 697. **Melting point:** 145 - 146 °C.

7.3 Representative copolymerization of polyfluoroarenes with diynes

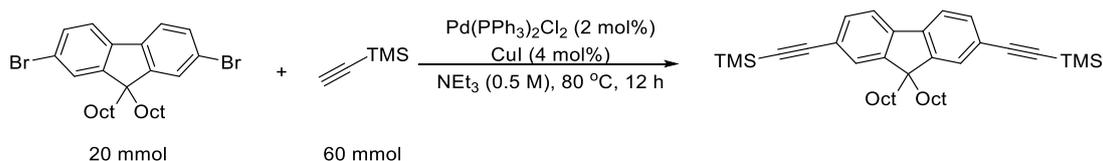


General procedure C (GPC): In a nitrogen-filled glove box, bis(1,5-cyclooctadiene)nickel (6.9 mg, 25 μmol , 5 mol%), $t\text{BuOK}$ (5.6 mg, 50 μmol , 10 mol%), **L10** (21.3 mg, 25 μmol , 1 mol%), and heptane (1.0 mL) were added to an 8 mL vial equipped with a magnetic stirring bar. The reaction mixture was allowed to stir at room temperature for 12 h, and then 2,2',3,3',5,5',6,6'-octafluoro-1,1'-biphenyl (149.1 mg, 0.50 mmol, 1.0 equiv) and 1,4-bis(trimethylsilyl)ethynylbenzene (135.3 mg, 0.50 mmol, 1.0 equiv) were added. The vial was taken out of the glovebox and stirred at 130 °C for 12 h. After cooling to room temperature, the resulting mixture was dissolved in DCM (5 mL) and then precipitated in methanol (100 mL) to provide a yellow solid. The crude product was dried under vacuo at 50 °C to constant weight.

7.4 Preparation of monomers

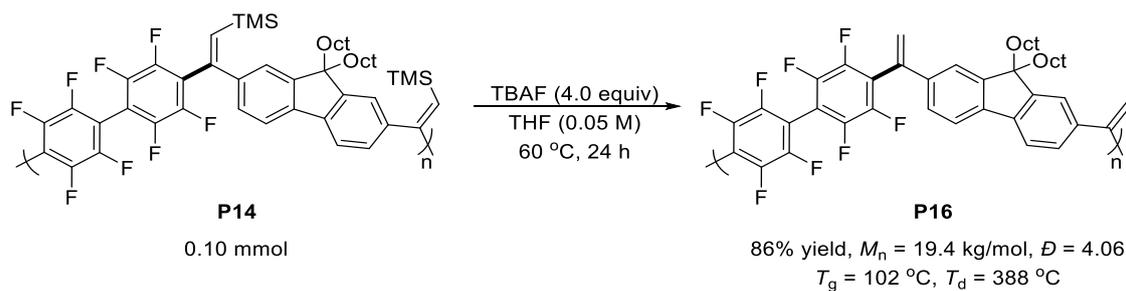


Synthesis of 2,5-bis((trimethylsilyl)ethynyl)thiophene: Pd(PPh₃)₂Cl₂ (1.40 g, 2.0 mmol, 10 mol%), CuI (0.76 g, 4.0 mmol, 20 mol%), triethylamine (40 mL), 2,5-dibromothiophene (4.84 g, 20 mmol, 1.0 equiv), ethynyltrimethylsilane (5.89 g, 60 mmol, 3.0 equiv) and THF (40 mL) was added to a 250 mL round bottom flask under nitrogen. The reaction mixture was stirred at 60 °C for 17 h. After cooling to room temperature, the resulting mixture was extracted with EtOAc and water, and dried over Na₂SO₄. Solvent was removed in vacuo and then purified by silica gel (100% PE). The resulting solid was recrystallized from hexane to provide pure product as a pale-yellow solid in 69% yield (3.82 g) with matched spectra¹⁸. ¹H NMR (400 MHz, CDCl₃) δ 7.04 (s, 2H), 0.24 (s, 18H).



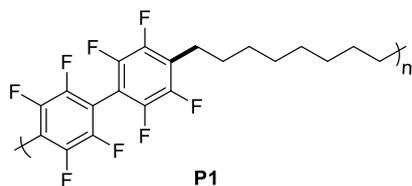
Synthesis of 1,1'-(2,7-bis((trimethylsilyl)ethynyl)-9H-fluorene-9,9-diyl)bis(octan-1-one): Pd(PPh₃)₂Cl₂ (1.40 g, 2.0 mmol, 10 mol%), CuI (0.76 g, 4.0 mmol, 20 mol%), triethylamine (40 mL), 1,1'-(2,7-dibromo-9H-fluorene-9,9-diyl)bis(octan-1-one) (10.97 g, 20 mmol, 1.0 equiv), ethynyltrimethylsilane (5.89 g, 60 mmol, 3.0 equiv) and THF (40 mL) was added to a 250 mL round bottom flask under nitrogen. The reaction mixture was stirred at 80 °C for 12 h. After cooling to room temperature, the resulting mixture was extracted with EtOAc and water, and dried over Na₂SO₄. Solvent was removed in vacuo and then purified by silica gel (0-10% EtOAc in PE). The resulting solid was recrystallized from hexane to provide pure product as a white solid in 58% yield (7.03 g) with matched spectra¹⁹. ¹H NMR (400 MHz, CDCl₃) δ 7.59 (d, *J* = 7.8 Hz, 2H), 7.45 (d, *J* = 8.1 Hz, 2H), 7.42 (s, 2H), 2.00 – 1.87 (m, 4H), 1.23 – 0.98 (m, 20H), 0.83 (t, *J* = 7.1 Hz, 6H), 0.58 – 0.45 (m, 4H), 0.29 (s, 18H).

7.5 Deprotection of P14

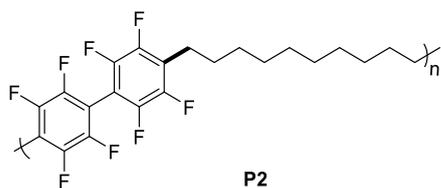


P14 (90.9 mg, 0.1 mmol, 1.0 equiv), NBu_4F (104.6 mg, 0.4 mmol, 4.0 equiv), and THF (4 mL) were added to an 8 mL vial equipped with a stir bar. The reaction mixture was stirred at 60 °C for 24 h. After cooling to room temperature, the resulting mixture was precipitated in methanol (20 mL) and washed with methanol (10 mL three times). The solid was dried under vacuo at 50 °C to constant weight to afford **P16** as a yellow solid in 86% yield ($M_n = 19.4$ kg/mol, $D = 4.06$, $T_g = 102$ °C, $T_d = 388$ °C). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.67 (d, $J = 7.8$ Hz, 2H), 7.36 (s, 2H), 7.28 (s, 2H), 6.17 (s, 2H), 5.60 (s, 2H), 1.97 (s, 4H), 1.19 (s, 4H), 1.14 – 0.98 (m, 16H), 0.80 (t, $J = 7.0$ Hz, 6H), 0.64 (s, 4H). $^{19}\text{F NMR}$ (377 MHz, CDCl_3) δ -138.06 – -138.58 (m, 4F), -139.29 – -139.81 (m, 4F). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 151.9, 145.9, 143.4, 143.3, 141.2, 137.7, 135.9, 125.5, 123.4, 123.2, 120.7, 120.5, 120.2, 106.6, 55.4, 40.4, 31.9, 30.0, 29.3, 23.8, 22.7, 14.2. IR (neat, cm^{-1}) 2926, 2854, 1612, 1464, 1311, 971, 915, 825, 718.

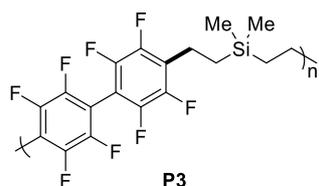
8. Characterization of Copolymers.



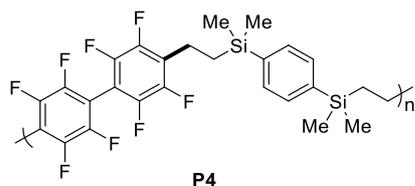
Following GPB using 2,2',3,3',5,5',6,6'-octafluoro-1,1'-biphenyl (149.1 mg, 0.50 mmol, 1.0 equiv) and octa-1,7-diene (55.1 mg, 0.50 mmol, 1.0 equiv) to give the product as a white solid in 99% yield ($M_n = 6.0$ kg/mol, $D = 1.70$, $T_m = 138.4$ °C, 145.7 °C, $T_d = 427$ °C). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 2.79 (t, $J = 7.7$ Hz, 4H), 1.66 (s, 4H), 1.39 (s, 8H). $^{19}\text{F NMR}$ (377 MHz, CDCl_3) δ -139.87 - -139.78 (m, 4F), -144.19 - -144.14 (m, 4F). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 145.1 (dm, $J_F = 243$ Hz), 143.9 (dm, $J_F = 252$ Hz), 123.0 (t, $J_F = 18.6$ Hz), 104.9 (t, $J_F = 17.3$ Hz), 29.4, 29.3, 29.2, 23.2. **IR (neat, cm^{-1})** 2931, 2860, 1466, 1252, 1142, 1106, 940, 721.



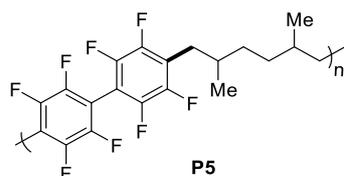
Following GPB using 2,2',3,3',5,5',6,6'-octafluoro-1,1'-biphenyl (149.1 mg, 0.50 mmol, 1.0 equiv) and deca-1,9-diene (69.1 mg, 0.50 mmol, 1.0 equiv) at 2.0 M to give the product as a white solid in 68% yield (148.0 mg, $M_n = 3.8$ kg/mol, $D = 1.19$, $T_m = 85.0$ °C, 93.4 °C, $T_d = 418$ °C). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 2.79 (t, $J = 7.8$ Hz, 4H), 1.67 – 1.63 (m, 4H), 1.44 – 1.24 (m, 12H). $^{19}\text{F NMR}$ (377 MHz, CDCl_3) δ -139.52 – -140.12 (m, 4F), -144.17 - -144.23 (m, 4F). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 145.1 (t, $J_F = 244$ Hz), 144.1 (dm, $J_F = 251$ Hz), 107.7 (t, $J_F = 21.9$ Hz), 104.7 (t, $J_F = 16.4$ Hz), 29.6, 29.4, 29.4, 29.3, 23.3. **IR (neat, cm^{-1})** 2928, 2855, 1470, 1250, 1177, 1141, 947, 740.



Following GPB using 2,2',3,3',5,5',6,6'-octafluoro-1,1'-biphenyl (149.1 mg, 0.50 mmol, 1.0 equiv) and dimethyldivynylsilane (56.1 mg, 0.50 mmol, 1.0 equiv) at 1.0 M for 24 h to give the product as a white solid in 68% yield (177.6 mg, $M_n = 19.1$ kg/mol, $D = 1.81$, $T_g = 56$ °C, $T_d = 419$ °C). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 2.81 (t, $J = 8.7$ Hz, 4H), 1.09 – 0.85 (m, 4H), 0.16 (s, 6H). $^{19}\text{F NMR}$ (377 MHz, CDCl_3) δ -139.63 (dd, $J = 17.3, 9.5$ Hz, 4F), -145.22 (dd, $J = 21.0, 10.2$ Hz, 4F). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 144.6 (dm, $J_F = 246$ Hz), 144.0 (dm, $J_F = 252$ Hz), 125.3 (t, $J_F = 18.4$ Hz), 104.72 (t, $J_F = 16.6$ Hz), 17.6, 15.5, -3.9. **IR** (neat, cm^{-1}) 2950, 2895, 1470, 1256, 1153, 974, 869, 720.

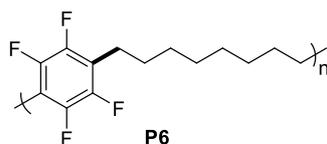


Following GPB using 2,2',3,3',5,5',6,6'-octafluoro-1,1'-biphenyl (149.1 mg, 0.50 mmol, 1.0 equiv) and 1,4-bis(dimethyl(vinyl)silyl)benzene (123.3 mg, 0.50 mmol, 1.0 equiv) to give the product as a white solid in 90% yield (245.6 mg, $M_n = 21.8$ kg/mol, $D = 1.54$, $T_g = 76$ °C, $T_d = 435$ °C). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.52 (s, 4H), 2.97 – 2.58 (m, 4H), 1.19 – 1.07 (m, 4H), 0.34 (s, 12H). $^{19}\text{F NMR}$ (377 MHz, CDCl_3) δ -139.62 – -139.90 (m, 4F), -144.80 – -145.07 (m, 4F). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 144.8 (dm, $J_F = 246$ Hz), 143.9 (dm, $J_F = 251$ Hz), 139.1, 133.0, 125.3 (t, $J_F = 18.4$ Hz), 104.6 (t, $J_F = 17.1$ Hz), 17.8, 16.1, -3.3. **IR** (neat, cm^{-1}) 3050, 2954, 2893, 1466, 1252, 1151, 886, 720.

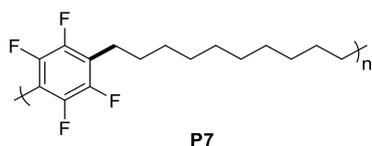


Following GPB using 2,2',3,3',5,5',6,6'-octafluoro-1,1'-biphenyl (149.1 mg, 0.50 mmol, 1.0 equiv) and 2,5-dimethylhexa-1,5-diene (55.1 mg, 0.50 mmol, 1.0 equiv) to give the product as a

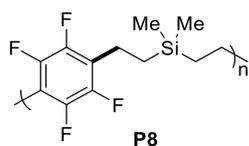
white solid in 56% yield (115.1 mg, $M_n = 3.0$ kg/mol, $D = 1.16$, $T_m = 39.1$ °C, 79.2 °C, 82.7 °C, $T_d = 388$ °C). **^1H NMR (400 MHz, CDCl_3)** δ 3.05 – 2.42 (m, 4H), 1.85 (s, 2H), 1.59 – 1.26 (m, 4H), 0.95 (d, $J = 6.6$ Hz, 6H). **^{19}F NMR (377 MHz, CDCl_3)** δ -139.38 – -139.95 (m, 4F), -142.74 (s, 4F). **^{13}C NMR (126 MHz, CDCl_3)** δ 145.3 (dm, $J_F = 246$ Hz), 144.0 (dm, $J_F = 252$ Hz), 122.0 (t, $J_F = 18.5$ Hz), 107.7 (t, $J_F = 22.4$ Hz), 34.2, 34.2, 33.8, 33.8, 30.7, 30.4, 19.5, 19.3. **IR (neat, cm^{-1})** 2963, 2932, 2876, 1472, 1253, 1107, 957, 720.



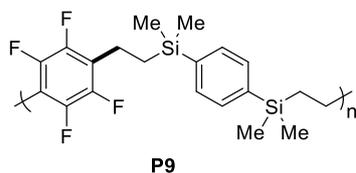
Following GPB using 1,2,4,5-tetrafluorobenzene (75.0 mg, 0.50 mmol, 1.0 equiv) and octa-1,7-diene (55.1 mg, 0.50 mmol, 1.0 equiv) to give the product as a white solid in 69% yield (89.6 mg, $M_n = 3.1$ kg/mol, $D = 1.21$, $T_m = 84.1$ °C, 92.5 °C, 94.4 °C, $T_d = 399$ °C). **^1H NMR (400 MHz, CDCl_3)** δ 2.67 (t, $J = 7.5$ Hz, 4H), 1.56 (t, $J = 7.3$ Hz, 4H), 1.31 (s, 8H). **^{19}F NMR (377 MHz, CDCl_3)** δ -146.41. **^{13}C NMR (126 MHz, CDCl_3)** δ 144.7 (dm, $J_F = 247$ Hz), 118.7 – 117.3 (m), 103.4 (t, $J_F = 22.5$ Hz), 29.4, 29.3, 29.3, 22.8. **IR (neat, cm^{-1})** 2931, 2859, 1479, 1260, 1127, 1014, 921, 609.



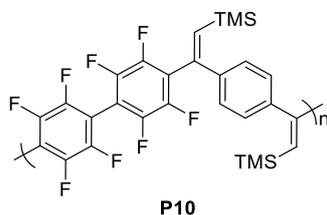
Following GPB using 1,2,4,5-tetrafluorobenzene (75.0 mg, 0.50 mmol, 1.0 equiv) and deca-1,9-diene (69.1 mg, 0.50 mmol, 1.0 equiv) to give the product as a white solid in 75% yield (107.5 mg, $M_n = 3.4$ kg/mol, $D = 1.24$, $T_m = 70.5$ °C, 81.0 °C, 88.1 °C, $T_d = 406$ °C). **^1H NMR (400 MHz, CDCl_3)** δ 2.67 (t, $J = 7.6$ Hz, 4H), 1.63 – 1.53 (m, 4H), 1.34 – 1.27 (m, 12H). **^{19}F NMR (377 MHz, CDCl_3)** δ -146.44 (s, 4F). **^{13}C NMR (126 MHz, CDCl_3)** δ 144.7 (dm, $J_F = 247$ Hz), 118.0 – 118.0 (m), 103.41 (t, $J_F = 22.7$ Hz), 29.6, 29.5, 29.4, 29.3, 22.8. **IR (neat, cm^{-1})** 2927, 2854, 1481, 1260, 1128, 943, 867, 610.



Following GPB using 1,2,4,5-tetrafluorobenzene (75.0 mg, 0.50 mmol, 1.0 equiv) and dimethyldivinylsilane (56.1 mg, 0.50 mmol, 1.0 equiv) to give the product as a white solid in 97% yield (127.1 mg, $M_n = 5.9$ kg/mol, $D = 1.26$, $T_m = 166$ °C, $T_d = 409$ °C). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 2.79 (t, $J = 7.7$ Hz, 4H), 1.66 (s, 4H), 1.39 (s, 8H). $^{19}\text{F NMR}$ (377 MHz, CDCl_3) δ -139.87 - -139.78 (m, 4F), -144.19 - -144.14 (m, 4F). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 145.1 (dm, $J_F = 243$ Hz), 143.9 (dm, $J_F = 252$ Hz), 123.0 (t, $J = 18.6$ Hz), 104.9 (t, $J = 17.3$ Hz), 29.4, 29.3, 29.2, 23.2. IR (neat, cm^{-1}) 2954, 2923, 2899, 1481, 1249, 1182, 1144, 863, 600.

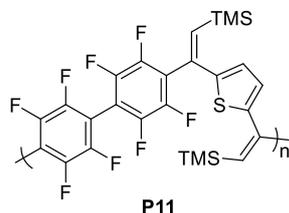


Following GPB using 1,2,4,5-tetrafluorobenzene (75.0 mg, 0.50 mmol, 1.0 equiv) and 1,4-bis(dimethyl(vinyl)silyl)benzene (123.3 mg, 0.50 mmol, 1.0 equiv) to give the product as a white solid in 83% yield (123.3 mg, $M_n = 6.7$ kg/mol, $D = 1.08$, $T_m = 197$ °C, $T_d = 421$ °C). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.49 (s, 4H), 2.65 (s, 4H), 1.06 (s, 4H), 0.30 (s, 12H). $^{19}\text{F NMR}$ (377 MHz, CDCl_3) δ -147.06 (s, 4F). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 144.4 (dm, $J_F = 256$ Hz), 139.3, 133.0, 120.2, 17.3, 16.2, -3.2. IR (neat, cm^{-1}) 3051, 2956, 2898, 1482, 1248, 1139, 858, 815, 798.

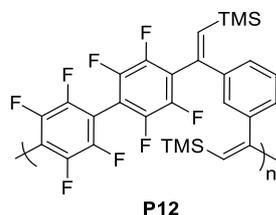


Following GPC using 2,2',3,3',5,5',6,6'-octafluoro-1,1'-biphenyl (149.1 mg, 0.50 mmol, 1.0 equiv) and 1,4-bis(trimethylsilyl)ethynylbenzene (135.3 mg, 0.50 mmol, 1.0 equiv) to give the product as a yellow solid in 89% yield (253.2 mg, $M_n = 16.4$ kg/mol, $D = 2.92$, $T_g = 189$ °C, $T_d = 410$ °C). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.30 (s, 4H), 6.17 (s, 2H), 0.03 (s, 18H). $^{19}\text{F NMR}$ (377 MHz, CDCl_3) δ -138.71 - -138.63 (m, 4F), -140.97 - -141.34 (m, 4F). $^{13}\text{C NMR}$ (126 MHz, CDCl_3)

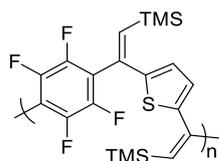
δ 144.2 (dm, $J_F = 252$ Hz), 143.7 (dm, $J_F = 244$ Hz), 142.3, 141.7, 140.7, 128.5, 126.49 (t, $J_F = 18.3$ Hz), 106.0 (t, $J_F = 20.2$ Hz), 0.13. **IR (neat, cm^{-1})** 2957, 2900, 1590, 1463, 973, 866, 837, 722.



Following GPC using 2,2',3,3',5,5',6,6'-octafluoro-1,1'-biphenyl (149.1 mg, 0.50 mmol, 1.0 equiv) and 2,5-bis((trimethylsilyl)ethynyl)thiophene (138.3 mg, 0.50 mmol, 1.0 equiv) to give the product as a brown solid in 94% yield (269.1 mg, $M_n = 16.3$ kg/mol, $D = 4.37$, $T_g = 150$ °C, $T_d = 365$ °C). **^1H NMR (400 MHz, CDCl_3)** δ 6.90 (s, 2H), 6.16 (s, 2H), 0.15 (s, 18H). **^{19}F NMR (377 MHz, CDCl_3)** δ -138.14 – -138.50 (m, 4F), -141.0 – -141.09 (m, 4F). **^{13}C NMR (126 MHz, CDCl_3)** δ 144.0 (dm, $J_F = 252$ Hz), 143.6 (dm, $J_F = 250$ Hz), 134.4, 127.7, 126.1 (t, $J_F = 18.1$ Hz), 106.3 (t, $J_F = 16.4$ Hz), -0.0. **IR (neat, cm^{-1})** 2956, 2900, 1579, 1464, 1248, 973, 860, 838, 719.

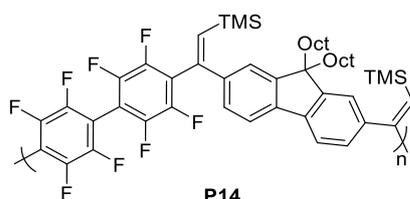


Following GPC using 2,2',3,3',5,5',6,6'-octafluoro-1,1'-biphenyl (149.1 mg, 0.50 mmol, 1.0 equiv) and 1,3-bis((trimethylsilyl)ethynyl)benzene (138.3 mg, 0.50 mmol, 1.0 equiv) to give the product as a yellow solid in 91% yield (257.3 mg, $M_n = 15.3$ kg/mol, $D = 2.76$, $T_g = 140$ °C, $T_d = 408$ °C). **^1H NMR (400 MHz, CDCl_3)** 7.34 (t, $J = 7.9$ Hz, 1H), 7.26 (s, 2H), 6.19 (s, 2H), -0.08 (s, 18H). **^{19}F NMR (377 MHz, CDCl_3)** δ -138.74 – -138.83 (m, 4F), -140.79 – -141.12 (m, 4F). **^{13}C NMR (126 MHz, CDCl_3)** δ 144.0 (dm, $J_F = 253$ Hz), 143.7 (dm, $J_F = 249$ Hz), 142.2, 141.9, 140.8, 126.4 (t, $J_F = 18.1$ Hz), 106.0 (t, $J_F = 17.0$ Hz). -0.3. **IR (neat, cm^{-1})** 2957, 2900, 1589, 1464, 1249, 973, 838, 711.



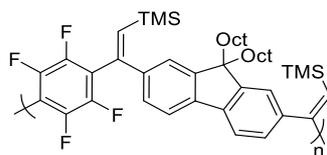
P13

Following GPC using 1,2,4,5-tetrafluorobenzene (75.0 mg, 0.50 mmol, 1.0 equiv) and 2,5-bis(trimethylsilyl)ethynylthiophene (138.3 mg, 0.50 mmol, 1.0 equiv) to give the product as a brown solid in 75% yield (160.9 mg, $M_n = 6.4$ kg/mol, $D = 1.39$, $T_g = 102$ °C, $T_d = 377$ °C). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 6.84 (s, 2H), 6.07 (s, 2H), 0.12 (s, 18H). $^{19}\text{F NMR}$ (377 MHz, CDCl_3) δ -142.37 (s, 4F). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 144.0 (dm, $J_F = 252$ Hz), 143.5 (dm, $J_F = 252$ Hz), 143.4, 142.3, 135.0, 127.3, 123.3, 105.0 (t, $J_F = 22.6$ Hz), 0.0. **IR** (neat, cm^{-1}) 2956, 2899, 1577, 1467, 1249, 982, 839, 752, 695.



P14

Following GPC using 2,2',3,3',5,5',6,6'-octafluoro-1,1'-biphenyl (149.1 mg, 0.50 mmol, 1.0 equiv) and 1,1'-(2,7-bis(trimethylsilyl)ethynyl)-9H-fluorene-9,9-diylbis(octan-1-one) (305.5 mg, 0.50 mmol, 1.0 equiv) to give the product as a yellow solid in 93% yield (424.3 mg, $M_n = 26.2$ kg/mol, $D = 3.96$, $T_g = 106.5$ °C, $T_d = 401$ °C). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.64 (d, $J = 7.8$ Hz, 2H), 7.31 (s, 2H), 7.19 (d, $J = 7.9$ Hz, 2H), 6.20 (s, 2H), 1.99 (s, 4H), 1.19 – 1.13 (m, 4H), 1.10 – 0.94 (m, 16H), 0.77 (t, $J = 7.1$ Hz, 6H), 0.59 (s, 4H), 0.01 (s, 18H). $^{19}\text{F NMR}$ (377 MHz, CDCl_3) δ -138.86 (s, 2F), -141.30 (s, 2F). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 151.0, 144.2 (dm, $J_F = 253$ Hz), 143.7 (dm, $J_F = 244$ Hz), 143.7, 140.8, 140.2, 127.4, 126.74 (t, $J_F = 17.9$ Hz), 123.3, 119.7, 105.8, 55.6, 40.7, 31.8, 30.1, 29.4, 29.3, 23.9, 22.7, 14.1, 0.2. **IR** (neat, cm^{-1}) 2927, 2854, 1591, 1463, 1263, 1248, 972, 837, 718.



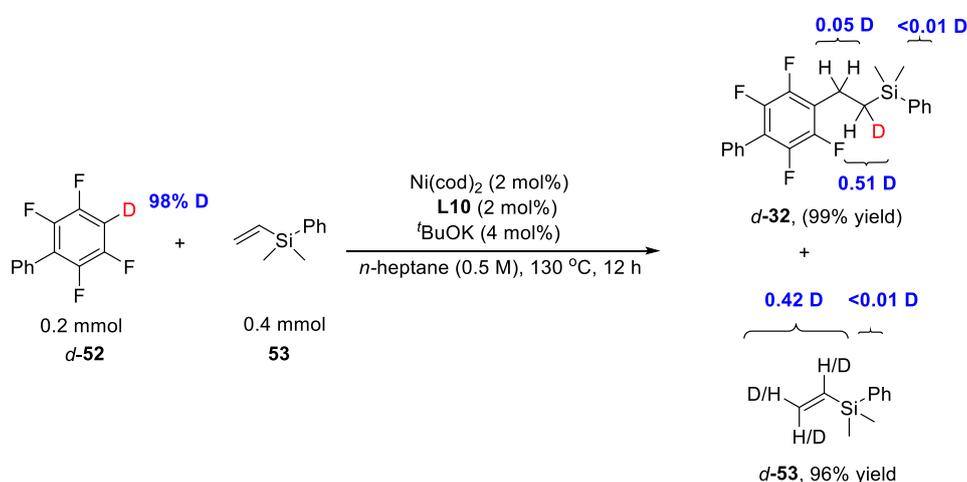
P15

Following GPC using 1,2,4,5-tetrafluorobenzene (75.0 mg, 0.50 mmol, 1.0 equiv) and 1,1'-

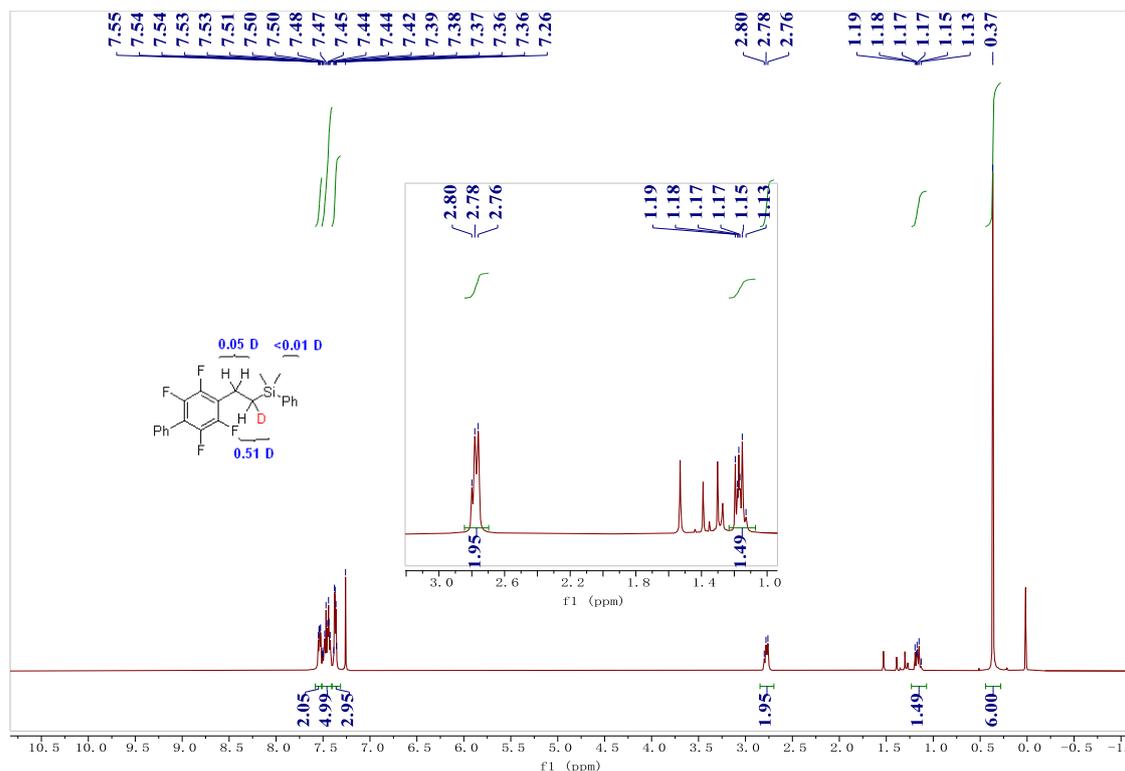
(2,7-bis(trimethylsilyl)ethynyl)-9*H*-fluorene-9,9-diylbis(octan-1-one) (305.5 mg, 0.50 mmol, 1.0 equiv) to give the product as a yellow solid in 60% yield (227.6 mg, $M_n = 11.9$ kg/mol, $D = 1.76$, $T_g = 77$ °C, $T_d = 404$ °C). **¹H NMR (400 MHz, CDCl₃)** δ 7.60 (d, $J = 7.9$ Hz, 2H), 7.28 (s, 2H), 7.14 (d, $J = 7.8$ Hz, 2H), 6.10 (s, 2H), 1.96 (s, 4H), 1.19 (q, $J = 7.2$ Hz, 4H), 1.13 – 0.95 (m, 16H), 0.83 – 0.79 (m, 6H), 0.58 (s, 4H), 0.00 (s, 18H). **¹⁹F NMR (377 MHz, CDCl₃)** δ -142.86 (s, 4F). **¹³C NMR (126 MHz, CDCl₃)** δ 150.8, 144.3, 143.7 (dm, $J_F = 249$ Hz), 140.7, 139.8, 127.3, 123.6, 123.3, 119.5, 55.5, 40.8, 31.9, 30.1, 29.4, 29.3, 23.8, 22.7, 14.2, 0.2. **IR (neat, cm⁻¹)** 2925, 2853, 1591, 1462, 1329, 1247, 979, 836, 752.

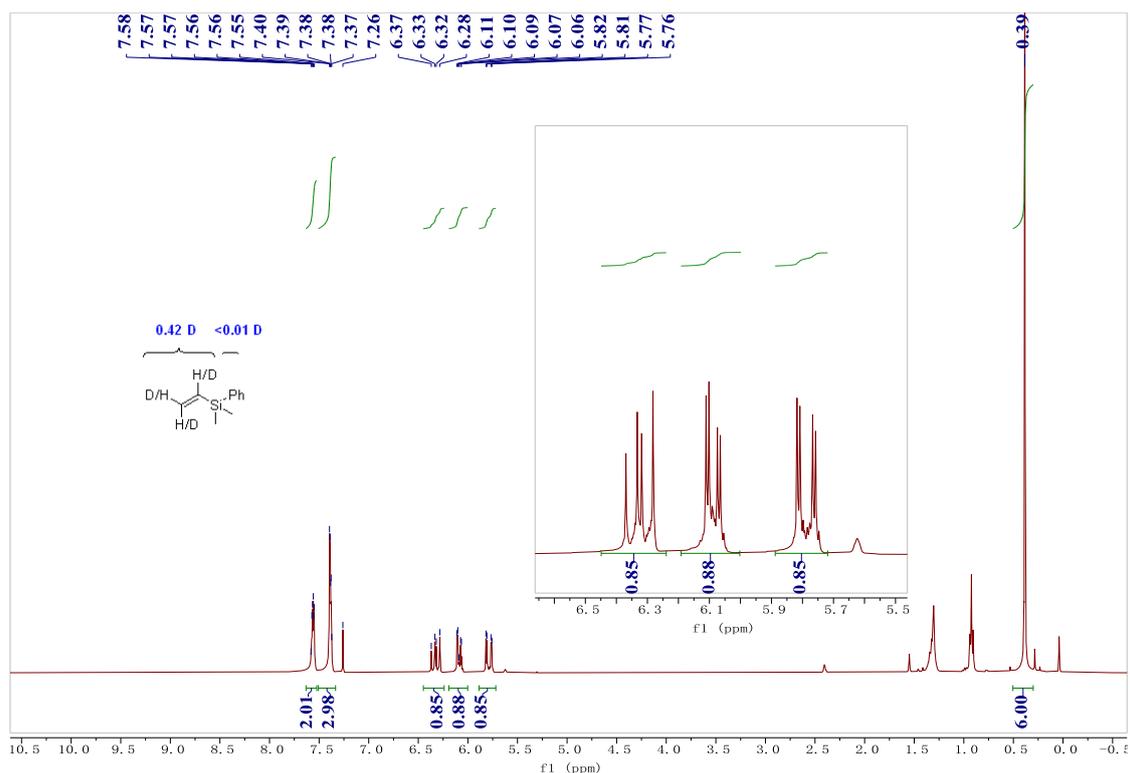
9. Mechanism Experiments.

9.1 Deuterium-labeling experiment.

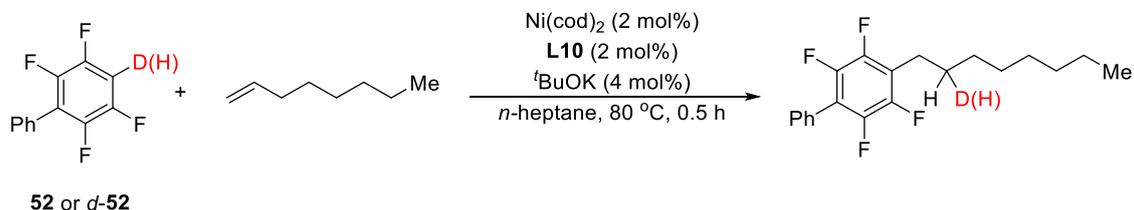


In a nitrogen-filled glove box, bis(1,5-cyclooctadiene)nickel (1.1 mg, 4 μmol , 2 mol%), $t\text{BuOK}$ (0.9 mg, 8 μmol , 4 mol%), **L10** (3.4 mg, 2 μmol , 2 mol%), and heptane (0.4 mL) were added to an 8 mL vial equipped with a magnetic stirring bar. The reaction mixture was allowed to stir at room temperature for 12 h, and *d*-52 (45.4 mg, 0.2 mmol) and dimethyl(phenyl)(vinyl)silane (64.9 mg, 0.4 mmol) were added. The vial was taken out of the glovebox and stirred at 130 °C for 12 h. After cooling to room temperature, the resulting mixture was purified directly by silica gel column (100% hexanes) to give the pure product *d*-32 in 99% yield (77.8 mg) and remaining alkene in 96% yield (31.0 mg, 1.9 mmol).

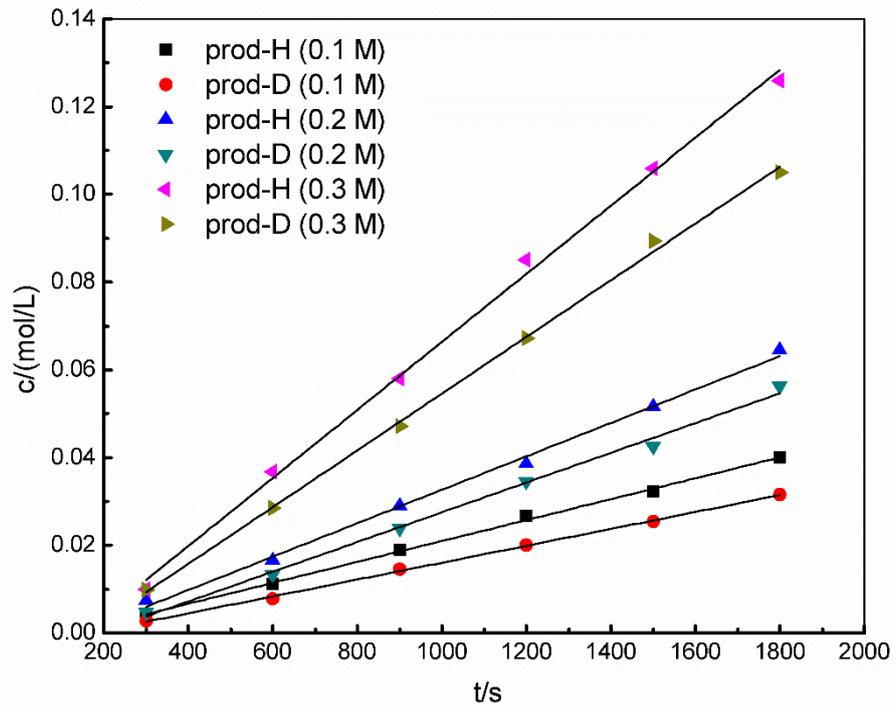




9.2 Intermolecular $^1\text{H}/^2\text{H}$ KIE measurement.



In a nitrogen-filled glove box, bis(1,5-cyclooctadiene)nickel (1.1 mg, 4 μmol , 2 mol%), *t*BuOK (0.9 mg, 8 μmol , 4 mol%), **L10** (3.4 mg, 2 μmol , 2 mol%), and heptane (2.0 mL) were added to an 8 mL vial equipped with a magnetic stirring bar. The reaction mixture was allowed to stir at room temperature for 12 h, and then **52** or *d*-**52** (0.2 mmol), oct-1-ene (44.9 mg, 0.4 mmol), and dodecane (34.1 mg, 0.2 mmol) were added. The vial was stirred at 80 $^\circ\text{C}$ for 30 min. 20 μL of the solution was taken out and analyzed by GC every 5 min. The experiment was conducted for 3 times at different concentrations of substrates to give an average KIE of 1.19 ± 0.05 .



10. DFT Calculation

10.1 Computational Details

All density functional theory (DFT) calculations were carried out using the Gaussian16 software package⁹. Geometry optimizations of all intermediates and transition states were carried out at the PBE0¹⁰ level of theory with additional Grimme's D3 dispersion correction (Becke–Johnson damping)¹¹ using a mixed basis set of LANL2DZ¹² (augmented with one f function,¹³ Ni(ζ_f) = 3.130) for nickel and 6-31G(d,p) for other atoms. The PBE0 functional has been shown to have a low mean absolute deviation over a variety of organometallic reactions and used in the theoretical study of mechanisms of nickel-catalyzed hydroarylation of alkenes with arenes.¹⁴ A solvation energy correction was calculated with an SMD solvent correction for heptane for all optimization and single-point energy calculations.¹⁵ Vibrational frequencies were computed at the same level to evaluate their zero-point vibrational energy (ZPVE) and thermal corrections at 403 K, as well as to check whether each optimized structure is a transition state or not. The single-point energies were computed at the same level of theory with a mixed basis set of LanL2TZ(f)¹⁶ for nickel and 6-31++G(d,p) for all other atoms. In addition, to correct the Gibbs free energies under pressure of 1 atm to the standard state in solution (1 mol/L), a correction of $RT\ln(c_s/c_g)$ (about 2.56 kcal/mol) is added to the energies of all species. c_s is the standard molar concentration in solution (1 mol/L), c_g is the standard molar concentration in the gas phase (0.040883 mol/L), and R is the gas constant. The 3D diagrams of molecules were generated using CYLview20¹⁷.

10.2 Ligand-to-ligand hydrogen transfer process vs oxidative addition

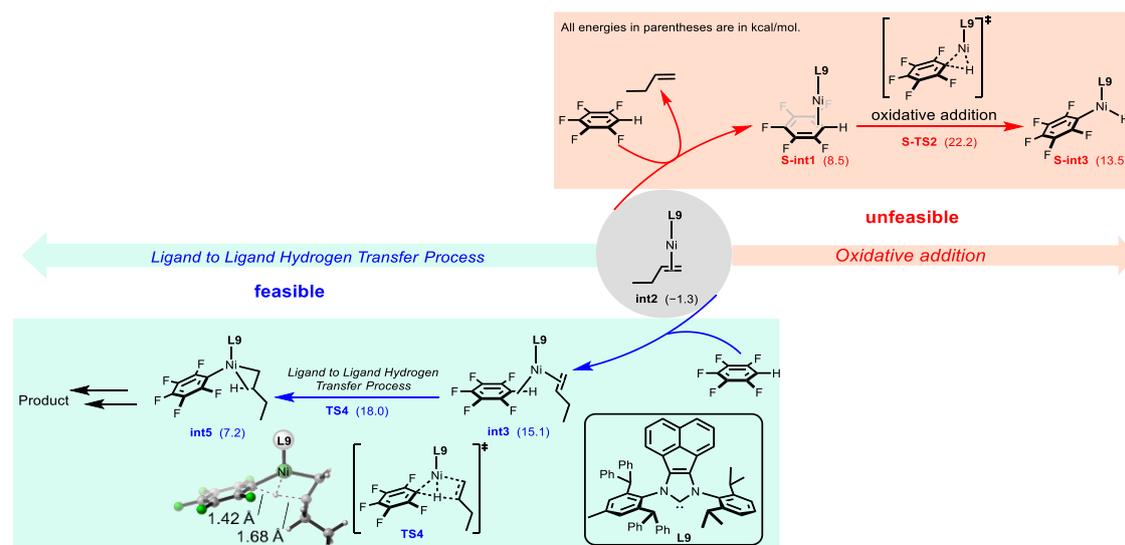


Figure S1. DFT-computed free energy changes of ligand-to-ligand hydrogen transfer process and oxidative addition.

10.3 Table of energies

Zero-point correction (*ZPE*), thermal correction to enthalpy (*TCH*), thermal correction to Gibbs free energy (*TCG*), energies (*E*), enthalpies (*H*), and Gibbs free energies (*G*) (in Hartree) of the structures calculated at the PBE0-D3(BJ)/6-31++G(d,p)-LanL2TZ(f)-SMD(Heptane)//PBE0-D3(BJ)/6-31G(d,p)-LanL2DZ-SMD(Heptane) level of theory.

Table S3. Energies for All Calculated Species

Structures	<i>ZPE</i>	<i>tcH</i>	<i>tcG</i>	<i>E</i>	<i>H</i>	<i>G</i>	Imaginary Frequency
int2(L9)	1.034528	1.139652	0.873328	-2673.716655	-2672.577004	-2672.843328	
pentafluoro- benzene	0.060450	0.076373	0.010267	-727.720119	-727.643746	-727.709852	
TS4(L9)	1.094384	1.215215	0.919011	-3401.437257	-3400.222042	-3400.518246	971.4i
int5(L9)	1.098865	1.219653	0.923069	-3401.458579	-3400.238926	-3400.535510	
TS6(L9)	1.097412	1.218219	0.918365	-3401.432020	-3400.213801	-3400.513655	335.8i
int7(L9)	1.100068	1.221777	0.918111	-3401.474205	-3400.252428	-3400.556094	
but-1-ene	0.109245	0.119212	0.069328	-157.042970	-156.923759	-156.973643	
P-l	0.174654	0.200383	0.109110	-884.813445	-884.613063	-884.704336	
TS8	1.094687	1.215213	0.920972	-3401.433064	-3400.217852	-3400.512093	1038.4i
int9	1.097923	1.219549	0.920601	-3401.448665	-3400.229117	-3400.528065	
TS10	1.098182	1.218517	0.923797	-3401.429836	-3400.211319	-3400.506039	308.7i
int11	1.099972	1.221495	0.919498	-3401.471247	-3400.249753	-3400.551750	
P-b	0.174545	0.200265	0.111827	-884.811958	-884.611693	-884.700131	
int1-L9	1.148453	1.262674	0.981138	-2830.791883	-2829.529210	-2829.810746	
int1-L7	0.907303	0.995299	0.771580	-2025.360725	-2024.365426	-2024.589145	
int1-L8	1.390372	1.530676	1.191101	-3636.225695	-3634.695019	-3635.034594	
int2-L7	0.793888	0.872283	0.668422	-1868.279208	-1867.406926	-1867.610787	
int2-L8	1.277296	1.407910	1.089301	-3479.155180	-3477.747271	-3478.065880	
int3-L9	1.096771	1.218627	0.914798	-3401.438025	-3400.219398	-3400.523227	
int3-L7	0.855908	0.951591	0.708395	-2596.005950	-2595.054359	-2595.297555	
TS4-L7	0.852705	0.947633	0.706876	-2596.002140	-2595.054508	-2595.295265	948.9i
TS4-L8	1.336269	1.483038	1.129543	-4206.861138	-4205.378100	-4205.731595	969.7i
int5-L7	0.857296	0.952125	0.712681	-2596.024186	-2595.072062	-2595.311506	
int5-L8	1.340331	1.487429	1.132204	-4206.882786	-4205.395357	-4205.750582	
TS6-L7	0.855861	0.950645	0.707762	-2595.994674	-2595.044030	-2595.286913	336.8i
TS6-L8	1.339569	1.486233	1.130480	-4206.864760	-4205.378528	-4205.734281	331.7i
int7-L7	0.858531	0.953870	0.709256	-2596.035473	-2595.081604	-2595.326218	
int7-L8	1.341941	1.489648	1.127490	-4206.899997	-4205.410350	-4205.772508	
S-int1	0.986114	1.097833	0.817842	-3244.381674	-3243.283841	-3243.563832	
S-TS2	0.981076	1.092688	0.812132	-3244.354179	-3243.261491	-3243.542047	542.3i

10.4 Cartesian Coordinates of the Structures

int2(L9)

C	0.03463800	-0.34183500	1.13560800
N	-0.09463400	0.02771600	-0.18645000
N	-1.25032800	-0.63584400	1.52354200
C	1.02653900	0.44186400	-0.96189300
C	3.25481800	1.24262200	-2.42233000
C	1.81510500	-0.53084200	-1.58410300
C	1.33166900	1.80507500	-1.03878300
C	2.44791300	2.18516900	-1.78211300
C	2.92924500	-0.10992500	-2.30737300
H	2.71494400	3.23774200	-1.82851200
H	3.56881900	-0.85733300	-2.76957100
C	-1.58357100	-1.06305300	2.84467200
C	-2.21817900	-1.87866700	5.39715900
C	-1.40042100	-2.41103100	3.18010300
C	-2.07435600	-0.10871900	3.74883400
C	-2.39253500	-0.54705800	5.03446900
C	-1.72423500	-2.79954800	4.48196900
H	-2.77158400	0.16151900	5.76433500
H	-1.58734600	-3.83445300	4.78165100
C	-2.16117100	1.35293300	3.35925100
H	-2.26177700	1.39836100	2.26927300
C	-0.82555000	-3.39903200	2.18703300
H	-0.87054700	-2.93373900	1.19712300
C	0.46058500	2.81568300	-0.31106100
H	0.08031300	2.30302800	0.57911300
C	1.42110200	-1.99348000	-1.47241100
H	0.95594600	-2.10615400	-0.48753200
C	4.48751100	1.67326000	-3.16298700
H	5.33802400	1.75858700	-2.47585400
C	-0.85144700	2.05726000	3.73118500
H	0.00961800	1.53297600	3.30155400
H	-0.72190100	2.07696400	4.81946400
H	-0.84751500	3.09203200	3.37042200
C	-1.62785600	-4.69686500	2.11689500
H	-1.22347500	-5.34812200	1.33479700
H	-2.68012800	-4.50175200	1.88659100
H	-1.58568200	-5.25584000	3.05758200
Ni	1.57880700	-0.65817200	2.16790500
H	4.76378100	0.95213800	-3.93723000
H	4.35184900	2.65077000	-3.63482000

C	1.27164100	3.99176100	0.20547300
C	2.06543800	3.78833100	1.33946900
C	1.27975300	5.24523900	-0.40518500
C	2.85776200	4.81106100	1.84608900
H	2.05365300	2.81308300	1.81919100
C	2.07639300	6.27202900	0.10073900
H	0.65292600	5.42550200	-1.27342300
C	2.86822600	6.05904500	1.22424400
H	3.46426900	4.63530100	2.73038100
H	2.07117400	7.24390900	-0.38520100
H	3.48550700	6.86129000	1.61845600
C	0.35974900	-2.35119800	-2.49624300
C	0.44429700	-1.93002400	-3.82617100
C	-0.74798700	-3.10631600	-2.10477000
C	-0.55178800	-2.26151800	-4.74086600
H	1.28678100	-1.32031300	-4.14145400
C	-1.75245200	-3.42660700	-3.01218500
H	-0.82833200	-3.43449400	-1.07136200
C	-1.65669600	-3.00527100	-4.33543500
H	-0.47072900	-1.92399100	-5.77056100
H	-2.61636400	-3.99571400	-2.68124800
H	-2.44390600	-3.24591300	-5.04383500
C	0.64686800	-3.66970300	2.49932000
C	-3.36957300	2.06985200	3.95357800
C	-5.90719900	-0.97037000	-0.03678400
C	-5.92686900	-0.62608000	-1.37325000
C	-4.72409000	-0.24988000	-2.03352600
C	-3.56612200	-0.24812300	-1.25828800
C	-3.53781100	-0.60926500	0.12214600
C	-4.71524300	-0.97150700	0.73549600
H	-5.43603000	0.13160900	-4.05613600
H	-6.83562500	-1.25600100	0.44932100
H	-6.86244600	-0.64402600	-1.92594400
C	-4.56915100	0.11543100	-3.40084100
C	-2.27574800	0.09677700	-1.75971800
H	-4.74878000	-1.25682500	1.78278900
C	-2.15438800	0.43737300	-3.08417200
C	-3.32339000	0.44116700	-3.89226900
H	-1.19660600	0.69666000	-3.51960700
H	-3.22166300	0.71307500	-4.93881700
C	-2.13533400	-0.47453700	0.48149800
C	-1.40382300	-0.05662200	-0.60272700
C	2.62927000	-2.91073200	-1.45527700
C	3.04382000	-3.65954500	-2.55549300

C	3.36909300	-2.98296700	-0.26942000
C	4.18495000	-4.45755900	-2.47553900
H	2.46745400	-3.62946100	-3.47560300
C	4.50533600	-3.77834400	-0.18831700
H	3.03728600	-2.40225300	0.59162200
C	4.91931800	-4.51810900	-1.29569700
H	4.49588400	-5.03746100	-3.34029500
H	5.06682200	-3.82374900	0.74103200
H	5.80651200	-5.14215900	-1.23550600
C	-0.75226100	3.21048700	-1.13186000
C	-2.00079800	3.29707000	-0.51231100
C	-0.66258300	3.49004500	-2.49756400
C	-3.13592700	3.64437500	-1.23690700
H	-2.08165000	3.07545700	0.54919900
C	-1.79432500	3.85280000	-3.22315800
H	0.29717800	3.40383800	-2.99999100
C	-3.03540100	3.92573800	-2.59670000
H	-4.10135300	3.68315300	-0.74082600
H	-1.70758700	4.06462100	-4.28542200
H	-3.92136300	4.18825700	-3.16731900
H	-3.30291000	2.15408200	5.04346500
H	-3.43132700	3.08841600	3.55661000
H	-4.30377300	1.55437200	3.70786600
H	0.76139700	-4.14560800	3.47974400
H	1.09353900	-4.32421500	1.74317000
H	1.23828000	-2.73672900	2.52454600
H	-2.46746600	-2.19967100	6.40473200
C	3.20949200	0.33512500	2.51234100
H	2.93520500	1.24080900	3.06310600
C	3.20175500	-0.88414200	3.21851600
H	3.82525200	-1.71364000	2.87641000
H	2.95606600	-0.90479200	4.28174400
C	4.06470600	0.58483300	1.29683700
H	3.50372300	1.17431500	0.56234400
H	4.29682000	-0.36927300	0.80924200
C	5.36257900	1.31761700	1.63419300
H	5.96220800	0.74687400	2.35181900
H	5.97069600	1.48317700	0.73737700
H	5.15633200	2.29817100	2.07866900

pentafluorobenzene

C	1.20548900	-0.42316000	-0.00000100
C	1.19139800	0.96624800	-0.00000300
C	0.00000400	1.67320300	-0.00000400

C	-1.19139800	0.96625100	-0.00000300
C	-1.20549100	-0.42315100	-0.00000200
C	0.00000000	-1.11431300	0.00000000
H	0.00000000	2.75661200	-0.00000300
F	-2.35608800	1.61193300	0.00000000
F	-2.35395500	-1.09260900	0.00000200
F	-0.00001200	-2.44164100	0.00000400
F	2.35395800	-1.09260700	0.00000300
F	2.35609600	1.61191600	0.00000100

TS4(L9)

C	-0.14640000	-0.72670200	-0.64932500
N	-0.75319600	0.08519200	0.28456500
N	-1.02192600	-0.73716600	-1.70895700
C	-0.09915300	0.50465100	1.48328800
C	1.26983700	1.26978900	3.78085500
C	0.57313500	1.73644500	1.49322800
C	-0.12890400	-0.33143600	2.60310900
C	0.54509200	0.07956000	3.75156000
C	1.26971800	2.08511300	2.64752900
H	0.54856000	-0.57148000	4.62129200
H	1.84927800	3.00425900	2.65403300
C	-0.81728600	-1.42656400	-2.94728100
C	-0.53158800	-2.67170000	-5.39403400
C	-0.02910500	-0.80411200	-3.93253700
C	-1.45193800	-2.66493300	-3.14954500
C	-1.29440100	-3.26873500	-4.39975200
C	0.10089100	-1.45680600	-5.15910100
H	-1.76743600	-4.22661200	-4.59175500
H	0.70676700	-1.01020500	-5.94022400
C	-2.27139500	-3.34720100	-2.06692600
H	-1.90574000	-2.96882500	-1.10576700
C	0.63020000	0.54030000	-3.68319500
H	0.94564300	0.54800800	-2.63326500
C	-0.90547000	-1.63584500	2.53694200
H	-0.76237600	-2.01799100	1.51922100
C	0.47816800	2.67305000	0.29963800
H	0.28820100	2.04875200	-0.57845600
C	2.10162100	1.63977300	4.97292500
H	3.15747400	1.42728100	4.76665300
C	-2.10415400	-4.86877900	-2.06753500
H	-1.05696100	-5.17866700	-2.11101000
H	-2.62813700	-5.32995900	-2.91185800
H	-2.53956900	-5.28629100	-1.15395300

C	-0.36246900	1.68841200	-3.89408500
H	0.12047800	2.64849000	-3.68057000
H	-1.24437400	1.60040700	-3.25582400
H	-0.70564200	1.71123600	-4.93470700
Ni	1.40536700	-1.76717800	-0.39121900
H	2.02453900	2.70631200	5.20607900
H	1.81327400	1.07021800	5.86029400
C	-0.34303700	-2.70855600	3.45400900
C	1.00077900	-3.07359900	3.29772700
C	-1.11015300	-3.37389800	4.40864800
C	1.56026800	-4.07717700	4.07778500
H	1.60910200	-2.54879700	2.56591100
C	-0.54878100	-4.38218600	5.19259400
H	-2.15463700	-3.10819400	4.53861300
C	0.78514600	-4.73797600	5.03085000
H	2.60506300	-4.34437700	3.94323100
H	-1.16253000	-4.88998200	5.93158400
H	1.22106600	-5.52350700	5.64153800
C	-0.70506900	3.62393300	0.42043700
C	-1.09925300	4.17792500	1.63947500
C	-1.39741800	3.99116200	-0.73611000
C	-2.15395300	5.08612600	1.69853600
H	-0.59003300	3.88398900	2.55293000
C	-2.45872800	4.88672200	-0.67866600
H	-1.10454600	3.56055600	-1.68993100
C	-2.83881400	5.44202600	0.54092300
H	-2.44671500	5.50760700	2.65642700
H	-2.99611300	5.14365900	-1.58696900
H	-3.67059000	6.13880200	0.58876600
C	1.87272400	0.78066800	-4.53693500
C	-3.76214000	-3.01387500	-2.17550300
C	-5.31150900	1.06774400	-3.33021600
C	-5.88572500	1.77745300	-2.29472100
C	-5.21184300	1.89680900	-1.04812500
C	-3.97052600	1.27024000	-0.95159100
C	-3.38263600	0.51417500	-2.00880500
C	-4.05376800	0.42066800	-3.20739600
H	-6.62491000	3.09040200	0.10196000
H	-5.83933600	0.99129700	-4.27631900
H	-6.85549500	2.24887100	-2.43048100
C	-5.66387800	2.58330800	0.11430700
C	-3.15117600	1.30551200	0.21470300
H	-3.64748900	-0.13805500	-4.04510200
C	-3.61546100	1.96800500	1.32367200

C	-4.88507800	2.60199900	1.25126700
H	-3.03978000	2.01584000	2.24006900
H	-5.24430500	3.12801000	2.13080300
C	-2.13196600	0.03678800	-1.43450600
C	-1.97662700	0.53160300	-0.16681600
C	3.85156100	-0.39446800	-1.34349900
C	4.89994700	0.51161300	-1.31638600
C	5.26881600	1.08487000	-0.10537400
C	4.59672100	0.73127400	1.05683400
C	3.56549300	-0.19278600	0.98147100
C	3.12968000	-0.75377700	-0.21220800
C	1.75505100	3.43856900	-0.00552300
C	2.08135800	4.63773900	0.63393200
C	2.61975800	2.94858900	-0.98491600
C	3.25538500	5.31423900	0.31624700
H	1.39978500	5.05955100	1.36717000
C	3.78704100	3.63072100	-1.31708800
H	2.37505200	2.01504000	-1.48494600
C	4.11241500	4.81375900	-0.66056600
H	3.49505200	6.24297400	0.82656200
H	4.44837900	3.22849600	-2.07907200
H	5.02557500	5.34486500	-0.91267500
C	-2.39159700	-1.37946500	2.69781300
C	-3.29258200	-1.90661800	1.77104700
C	-2.88946800	-0.61137300	3.75426900
C	-4.65861000	-1.66529700	1.88518000
H	-2.91484200	-2.50460300	0.94540700
C	-4.25600800	-0.37919500	3.87931300
H	-2.19741100	-0.18480800	4.47573700
C	-5.14465000	-0.90074800	2.94139000
H	-5.34136400	-2.06646200	1.14172200
H	-4.62716600	0.22047000	4.70596900
H	-6.20908600	-0.70371700	3.02874200
H	-4.15246700	-3.30958600	-3.15608300
H	-4.32618000	-3.56451100	-1.41433500
H	-3.96365300	-1.95092800	-2.03927400
H	1.61540100	0.94355500	-5.58950500
H	2.38364800	1.68545700	-4.19146800
H	2.58097500	-0.04743100	-4.47523100
F	6.25040100	1.98291100	-0.06744800
F	5.53138200	0.88016400	-2.43685100
F	3.53543500	-0.94908500	-2.52810300
F	4.94797000	1.27973300	2.22248200
H	-0.42008400	-3.16141800	-6.35739200

F	2.99068600	-0.56426300	2.13519300
H	2.83659100	-2.13961800	-0.12539500
C	2.14023200	-3.66908600	-0.25551100
H	2.50484400	-3.94911400	0.73643700
C	0.73282100	-3.60148300	-0.42767600
H	0.33450700	-3.80092400	-1.41879900
H	0.07227600	-3.84404400	0.40236400
C	3.02623600	-4.11880700	-1.40050700
H	4.04261000	-3.72223300	-1.27731000
H	2.64062000	-3.69635400	-2.33623000
C	3.08479000	-5.63952400	-1.50575400
H	3.73175700	-5.95657300	-2.33082300
H	3.47542900	-6.08452300	-0.58353100
H	2.08672200	-6.05670300	-1.67657200

int5(L9)

C	-0.05993400	-0.72862400	-0.61405100
N	-0.71528900	0.02770200	0.33041200
N	-0.88375900	-0.71373300	-1.71132600
C	-0.12367900	0.48263000	1.55247900
C	1.03707300	1.36343300	3.92484800
C	0.40988800	1.78005300	1.60605900
C	-0.10625900	-0.36884400	2.66042900
C	0.46229300	0.09625700	3.84378700
C	1.00444500	2.18617500	2.79874300
H	0.49507200	-0.56351500	4.70635300
H	1.47355500	3.16551800	2.84148200
C	-0.61300400	-1.29832800	-2.99293700
C	-0.21755600	-2.31917000	-5.52719500
C	0.20309000	-0.58092400	-3.88911200
C	-1.23727400	-2.51077800	-3.33452500
C	-1.02239700	-3.00085100	-4.62581200
C	0.39265000	-1.12597500	-5.15934500
H	-1.48734300	-3.93581700	-4.92251500
H	1.02498700	-0.60730600	-5.87173500
C	-2.11697300	-3.28855700	-2.36967600
H	-1.87495300	-2.94254000	-1.35945500
C	0.81125300	0.76028600	-3.51529600
H	1.11589700	0.69412200	-2.46425300
C	-0.73229500	-1.74651900	2.54753700
H	-0.52463700	-2.08531800	1.52687500
C	0.28409500	2.73423400	0.42879400
H	0.16082900	2.12255600	-0.47033800
C	1.73371900	1.81376800	5.17463500

H	2.81211100	1.63353000	5.09025400
C	-1.86193300	-4.79727900	-2.43035600
H	-0.79868300	-5.04714100	-2.39441800
H	-2.27881900	-5.23646800	-3.34308000
H	-2.35237900	-5.28927000	-1.58419900
C	-0.22430900	1.88286800	-3.64808800
H	0.22185600	2.84050300	-3.35804000
H	-1.10765100	1.71643100	-3.02826200
H	-0.55967200	1.97178100	-4.68767100
Ni	1.47408000	-1.73486800	-0.30072900
H	1.59604200	2.88480300	5.35037700
H	1.37602300	1.27065700	6.05363900
C	-0.07175300	-2.77454200	3.44788900
C	1.31844000	-2.93357500	3.36278700
C	-0.78949100	-3.60432300	4.30735800
C	1.97029200	-3.89948700	4.11902100
H	1.88878900	-2.27492000	2.71193200
C	-0.13493300	-4.57420500	5.06712800
H	-1.86729700	-3.49657200	4.38202200
C	1.24367900	-4.72667300	4.97573900
H	3.04926200	-4.00458400	4.04293100
H	-0.71069800	-5.21203900	5.73220300
H	1.75192000	-5.48195000	5.56841100
C	-0.96152500	3.60432200	0.53775900
C	-1.42599000	4.10098700	1.75699800
C	-1.64645300	3.95403600	-0.62836500
C	-2.54116100	4.93429700	1.80720100
H	-0.92448200	3.81996100	2.67831900
C	-2.76972400	4.77146300	-0.58016300
H	-1.29965900	3.56939300	-1.58320200
C	-3.21918900	5.27033800	0.63988100
H	-2.88649600	5.31145600	2.76607400
H	-3.29934600	5.01209600	-1.49748300
H	-4.09806500	5.90723200	0.68017800
C	2.04763300	1.12857600	-4.33171600
C	-3.60713500	-3.03223000	-2.61184200
C	-5.16726400	1.03377000	-3.40875300
C	-5.81797200	1.64208700	-2.35394100
C	-5.20351800	1.70442600	-1.07326700
C	-3.93850600	1.12900600	-0.96368100
C	-3.27553100	0.46895400	-2.03984600
C	-3.88811100	0.43365300	-3.27253700
H	-6.71846800	2.75028500	0.09009800
H	-5.64942200	1.00248700	-4.38135000

H	-6.80230500	2.07853100	-2.50115900
C	-5.73473000	2.28916700	0.11080400
C	-3.16638500	1.13252500	0.23453200
H	-3.42051800	-0.04593700	-4.12706700
C	-3.70615200	1.69601700	1.36384900
C	-5.00386600	2.26847800	1.27919800
H	-3.16769900	1.71429400	2.30400000
H	-5.42402500	2.71685900	2.17452000
C	-2.02951500	0.00895100	-1.44174000
C	-1.94085000	0.44263300	-0.14681700
C	3.67848800	-0.31087800	-1.41487400
C	4.79113900	0.51006600	-1.53459900
C	5.27297600	1.14518000	-0.39710400
C	4.64349000	0.94264200	0.82316000
C	3.52516700	0.11955200	0.87380200
C	2.98252000	-0.50372400	-0.23517200
C	1.52420900	3.58359400	0.18540300
C	1.70336400	4.83372400	0.78349600
C	2.50750700	3.11538700	-0.68864700
C	2.84495000	5.58755600	0.52512300
H	0.93258400	5.23271700	1.43654400
C	3.64089700	3.87504100	-0.96332300
H	2.38631400	2.13961800	-1.15116000
C	3.81630000	5.11293900	-0.35157500
H	2.96777600	6.55615700	1.00185100
H	4.39181400	3.49461500	-1.64955900
H	4.70227000	5.70524500	-0.56105200
C	-2.24098000	-1.65235100	2.66717800
C	-3.05143600	-2.20781500	1.67537500
C	-2.85009300	-0.98931700	3.73662600
C	-4.43739700	-2.09372900	1.73717400
H	-2.58676400	-2.72491600	0.83923500
C	-4.23584100	-0.88427500	3.80835300
H	-2.23146100	-0.54121600	4.50983900
C	-5.03378500	-1.42999000	2.80478400
H	-5.04922700	-2.51426500	0.94423200
H	-4.69423300	-0.36441000	4.64520400
H	-6.11425800	-1.33062100	2.85147400
H	-3.88445500	-3.29934800	-3.63800600
H	-4.20767700	-3.64919200	-1.93403300
H	-3.88256300	-1.99012000	-2.44789900
H	1.78958500	1.36557900	-5.37008600
H	2.50717800	2.02669700	-3.90638800
H	2.79638500	0.33558100	-4.32802500

F	6.32322100	1.96538200	-0.48620400
F	5.39932500	0.71115200	-2.71083600
F	3.28597300	-0.97608000	-2.52997100
F	5.11597600	1.54715500	1.91760900
H	-0.05971700	-2.72174000	-6.52382700
F	2.98326100	-0.07728400	2.09380100
H	2.69238000	-2.81679400	0.08918400
C	2.06167200	-3.79861800	-0.10591200
H	2.16945100	-4.28229200	0.87080400
C	0.65761700	-3.44135100	-0.42251200
H	0.36259600	-3.63486600	-1.45199400
H	-0.10125900	-3.74327900	0.29885700
C	2.85442600	-4.51071500	-1.19937200
H	3.92579400	-4.47161100	-0.96676900
H	2.71956600	-3.96518000	-2.14117700
C	2.41545000	-5.95826400	-1.36335800
H	2.98392500	-6.45833700	-2.15392200
H	2.56390000	-6.52240000	-0.43552000
H	1.35274600	-6.02209300	-1.62056600

TS6(L9)

C	-0.27486500	0.15320900	0.95344300
N	-0.94001000	0.15284400	-0.25114900
N	-1.22975200	-0.20538400	1.86879400
C	-0.24733000	0.37290500	-1.48003100
C	1.24627800	0.79520400	-3.78343100
C	0.25759600	-0.73662100	-2.17166800
C	-0.03325100	1.68359600	-1.91634200
C	0.70101600	1.87256200	-3.08535600
C	1.01314200	-0.50018100	-3.31639900
H	0.90012300	2.88559200	-3.42350900
H	1.45769300	-1.34464500	-3.83643100
C	-0.95044200	-0.40866400	3.25474700
C	-0.49402000	-0.83165500	5.93724200
C	-0.64567000	-1.70861600	3.68347900
C	-1.00102200	0.69264400	4.12259900
C	-0.76978600	0.45149900	5.47754600
C	-0.42596400	-1.89784600	5.04929000
H	-0.80173000	1.27742200	6.18149500
H	-0.18992400	-2.89178600	5.41808900
C	-1.31455300	2.08411600	3.60961400
H	-1.07466800	2.09548100	2.54049700
C	-0.55159700	-2.87036400	2.71448100
H	-0.57692200	-2.45809900	1.70070600

C	-0.58041000	2.84120800	-1.09562000
H	-0.42952000	2.55566200	-0.04695700
C	-0.04836800	-2.13948500	-1.67360000
H	-0.13532300	-2.06873000	-0.58478000
C	2.13917000	1.01772000	-4.96831000
H	3.18659500	0.88528100	-4.67210700
C	-0.45774400	3.16186700	4.26935100
H	0.60723700	2.91697700	4.20349400
H	-0.70983100	3.30091800	5.32602400
H	-0.61689700	4.12294800	3.76939400
C	-1.74953400	-3.81054600	2.86384600
H	-1.67613100	-4.64038100	2.15228400
H	-2.69545900	-3.29064000	2.68315000
H	-1.78838900	-4.24025900	3.87130600
Ni	1.46079600	0.75990700	1.33707000
H	1.93510800	0.30132900	-5.77014300
H	2.03147700	2.02805900	-5.37153300
C	0.22036800	4.11858900	-1.28207800
C	1.52588600	4.14465000	-0.77717100
C	-0.27400700	5.25459800	-1.92030900
C	2.32098100	5.27485500	-0.91318700
H	1.91461300	3.25485700	-0.28936500
C	0.52341000	6.39111200	-2.05816000
H	-1.28954900	5.25873200	-2.30403900
C	1.82063100	6.40596400	-1.55796700
H	3.33233200	5.27366300	-0.51548000
H	0.12245300	7.26910800	-2.55720400
H	2.43868100	7.29280900	-1.66556400
C	-1.39233500	-2.63473200	-2.18132700
C	-1.83092000	-2.38793900	-3.48393400
C	-2.21055200	-3.38072400	-1.32950700
C	-3.05428800	-2.88568000	-3.92659400
H	-1.21847700	-1.78725700	-4.15120300
C	-3.43867900	-3.86652500	-1.76369500
H	-1.88330700	-3.57069600	-0.31016800
C	-3.86369400	-3.62316100	-3.06736500
H	-3.38024900	-2.68482900	-4.94359600
H	-4.06887400	-4.42699700	-1.07923200
H	-4.82527500	-3.99652700	-3.40719100
C	0.76828300	-3.62861900	2.85815300
C	-2.80630500	2.39372700	3.75895300
C	-6.00627900	-1.25476800	2.42395500
C	-6.59892800	-1.17561600	1.17979700
C	-5.81976900	-0.85566100	0.03371800

C	-4.45923500	-0.64172700	0.24893500
C	-3.84063100	-0.71858100	1.53251600
C	-4.61937000	-1.02572100	2.62578700
H	-7.32643300	-0.87250000	-1.53869000
H	-6.61851100	-1.49869100	3.28726000
H	-7.66552000	-1.35487300	1.07342800
C	-6.27586200	-0.71756900	-1.30784800
C	-3.53592700	-0.30409200	-0.78415000
H	-4.19902400	-1.09335600	3.62471000
C	-4.00426600	-0.17138000	-2.06721800
C	-5.38837100	-0.38525800	-2.30851600
H	-3.34733500	0.08972800	-2.88792300
H	-5.75238700	-0.28180400	-3.32646600
C	-2.44680000	-0.40500400	1.25948500
C	-2.26574100	-0.17332400	-0.08261800
C	3.67825900	-1.03759300	1.49994400
C	4.60590800	-1.87924900	0.90653100
C	4.99277800	-1.66143400	-0.40947800
C	4.42697500	-0.60642500	-1.11544500
C	3.50985700	0.21853500	-0.48836400
C	3.08953100	0.04453900	0.83716100
C	1.06720800	-3.13868300	-1.92923200
C	1.13082200	-3.91861300	-3.08572600
C	2.06102000	-3.29419800	-0.96004100
C	2.17325000	-4.82294600	-3.27327100
H	0.34923500	-3.83504600	-3.83534700
C	3.09536900	-4.20767200	-1.13776100
H	2.01996000	-2.68651300	-0.05944700
C	3.15722100	-4.97208200	-2.30007400
H	2.20869600	-5.42108100	-4.17967600
H	3.85447800	-4.31903100	-0.36925600
H	3.96528700	-5.68370800	-2.44271100
C	-2.07486100	2.99986200	-1.28875700
C	-2.90783900	3.11101000	-0.17423200
C	-2.64982000	3.03224700	-2.56206500
C	-4.28461800	3.24705700	-0.32155700
H	-2.46904800	3.07609500	0.81995600
C	-4.02521000	3.18515300	-2.71378100
H	-2.01423200	2.92446300	-3.43740300
C	-4.84730400	3.28836900	-1.59408300
H	-4.91749700	3.30952500	0.55907500
H	-4.45782100	3.20931700	-3.71024600
H	-5.92229800	3.38624200	-1.71316500
H	-3.10451100	2.36631100	4.81317000

H	-3.03435700	3.39338800	3.37253300
H	-3.42404500	1.67124400	3.21691100
H	0.83200700	-4.15392500	3.81747600
H	0.85630900	-4.38091500	2.06713400
H	1.62458000	-2.95325500	2.78714500
F	5.85806400	-2.48677100	-1.00035600
F	5.10589300	-2.92820800	1.57000900
F	3.34588600	-1.28962300	2.78214000
F	4.75790200	-0.41331600	-2.39518400
H	-0.31922600	-0.99907400	6.99634500
F	3.00905100	1.23477200	-1.21227400
C	3.06720500	1.61530700	1.97564700
H	2.16343800	2.28398200	2.11290600
H	3.31049400	1.18734800	2.95401900
C	4.21110600	2.46394600	1.43786300
H	4.18677200	3.43191400	1.96020700
H	4.04885700	2.68918800	0.37769800
C	5.59935000	1.85972400	1.62575300
H	5.65891500	0.89437500	1.11181900
H	5.75713500	1.65084400	2.69249700
C	6.69882900	2.77645000	1.10983000
H	6.68360500	3.74621100	1.62095200
H	7.69055400	2.33787400	1.25935800
H	6.57931500	2.96681300	0.03691500

int7(L9)

C	0.12930000	-0.49895300	-0.28731200
N	-1.05140500	0.13965000	0.00716000
N	-0.25488200	-1.63967700	-0.94347600
C	-1.08522900	1.36529500	0.73697400
C	-1.10035000	3.74779900	2.17034900
C	-0.98384100	2.57546200	0.03977300
C	-1.17572300	1.31535300	2.13104000
C	-1.17818200	2.52209100	2.83043800
C	-1.00150600	3.75642300	0.77663900
H	-1.21317900	2.49871500	3.91643300
H	-0.90389100	4.70338100	0.25279700
C	0.67903200	-2.62557600	-1.38995500
C	2.48977200	-4.52195700	-2.22934700
C	1.26283400	-2.47497800	-2.65647800
C	0.97099300	-3.69594700	-0.53208200
C	1.89581000	-4.64195700	-0.97845100
C	2.17562700	-3.45146500	-3.05958300
H	2.15686500	-5.47867200	-0.33768000

H	2.65139900	-3.36919400	-4.03175300
C	0.34971200	-3.79005800	0.84732100
H	-0.53783900	-3.14836600	0.85311700
C	0.89439800	-1.31548800	-3.55949200
H	0.51684500	-0.51371500	-2.91619800
C	-1.27236100	-0.02413100	2.84229600
H	-0.74299500	-0.74733600	2.21243500
C	-0.85884800	2.56467300	-1.47539600
H	-0.22921600	1.70063400	-1.71986400
C	-1.06778600	5.03565800	2.94082600
H	-0.03793900	5.39769500	3.04221700
C	1.31346700	-3.24398100	1.90349000
H	1.60900200	-2.21512600	1.66810000
H	2.22170000	-3.85549100	1.95720100
H	0.84763300	-3.24574500	2.89505500
C	-0.23005200	-1.72016600	-4.51703100
H	-0.51103800	-0.87776200	-5.15895300
H	-1.12403800	-2.04828600	-3.97783200
H	0.09054200	-2.54227200	-5.16721400
Ni	1.90364100	-0.05307700	0.16112100
H	-1.63836900	5.81987400	2.43407100
H	-1.47367700	4.91098800	3.94825700
C	-0.51907400	-0.00671900	4.16113400
C	0.87662900	0.05082400	4.10009900
C	-1.14052500	-0.02496800	5.40814200
C	1.63880800	0.09775000	5.25908900
H	1.36284500	0.05587700	3.12911800
C	-0.37614300	0.02169900	6.57456800
H	-2.22315100	-0.08455100	5.47093800
C	1.01168200	0.08568900	6.50491500
H	2.72144000	0.14348800	5.18293100
H	-0.87217500	0.00516800	7.54128100
H	1.60312600	0.12164300	7.41551500
C	-2.20240100	2.32232100	-2.13469300
C	-3.34314700	3.03423200	-1.75481300
C	-2.31677600	1.36262300	-3.14194500
C	-4.56705400	2.79346700	-2.37298400
H	-3.27179100	3.77293500	-0.96061200
C	-3.54199200	1.10658400	-3.74970300
H	-1.43549700	0.80050600	-3.44048200
C	-4.67186300	1.82411600	-3.36752300
H	-5.44527500	3.35480500	-2.06588300
H	-3.61380400	0.33879700	-4.51476600
H	-5.63157900	1.62100900	-3.83345700

C	2.08896300	-0.74971200	-4.32231900
C	-0.11600700	-5.20316400	1.19010100
C	-4.16405900	-4.18995400	-2.51409400
C	-5.29403900	-3.47522700	-2.17092500
C	-5.17677000	-2.23537500	-1.48374000
C	-3.88222600	-1.80758000	-1.19412200
C	-2.70970200	-2.54054500	-1.54751100
C	-2.85231400	-3.73894500	-2.20950700
H	-7.26508000	-1.66277300	-1.25220200
H	-4.27489500	-5.13508300	-3.03759500
H	-6.27824000	-3.85976100	-2.42489900
C	-6.23353100	-1.38295700	-1.05567400
C	-3.58373300	-0.59345900	-0.50893700
H	-1.99287300	-4.33595500	-2.49985500
C	-4.62193300	0.20876000	-0.10536000
C	-5.94946100	-0.20895000	-0.39153000
H	-4.44987400	1.13955100	0.42212300
H	-6.76775400	0.42793500	-0.06869800
C	-1.62472500	-1.71101200	-1.04658100
C	-2.12973400	-0.58513100	-0.44151800
C	4.20177000	0.70524400	-0.99432400
C	4.18055700	2.05802300	-0.74938600
C	3.78476300	2.53707900	0.51217600
C	3.44720000	1.65194000	1.50787600
C	3.45623600	0.25166200	1.26193800
C	3.85060300	-0.26504100	-0.01671600
C	-0.10946200	3.78044000	-1.99382500
C	-0.68881000	4.75833000	-2.79989400
C	1.23474500	3.91656700	-1.63005700
C	0.06112300	5.85473000	-3.22700300
H	-1.72710400	4.66282100	-3.10247100
C	1.98325900	5.00693300	-2.05176100
H	1.68385400	3.15363300	-1.00030600
C	1.39430700	5.98416000	-2.85401400
H	-0.40374600	6.60863200	-3.85656000
H	3.02374800	5.08698200	-1.75449300
H	1.97524400	6.83915700	-3.18816700
C	-2.70767000	-0.50586800	2.93675900
C	-3.00573100	-1.83891400	2.64607800
C	-3.75228100	0.34793900	3.30041700
C	-4.31339600	-2.30953600	2.70506800
H	-2.20126100	-2.51056000	2.35681500
C	-5.06094300	-0.12216000	3.37192100
H	-3.54144700	1.39261000	3.51181100

C	-5.34684900	-1.45075300	3.06889400
H	-4.52565800	-3.34464000	2.45361200
H	-5.86154700	0.55614600	3.65419500
H	-6.37015700	-1.81251000	3.10687400
H	0.72336800	-5.90031600	1.28426000
H	-0.64213200	-5.20168000	2.15041500
H	-0.79944000	-5.59469200	0.42969100
H	2.46906600	-1.45071900	-5.07360600
H	1.79113900	0.16035600	-4.85322900
H	2.90890500	-0.49264300	-3.64702100
F	3.70161700	3.85629500	0.70577000
F	4.49722400	2.93761600	-1.70506100
F	4.63994300	0.28321500	-2.19115400
F	3.12395000	2.09760900	2.72300700
H	3.20784500	-5.26748600	-2.55942800
F	3.54946600	-0.54259200	2.36902100
C	4.26109400	-1.70176400	-0.20732200
H	3.72042700	-2.31838800	0.51493000
H	3.93074700	-2.02751800	-1.19952100
C	5.76486800	-1.93707100	-0.05795000
H	6.08640100	-1.60338200	0.93765800
H	6.30573300	-1.31917300	-0.78639900
C	6.13469300	-3.40196900	-0.25411400
H	5.80292800	-3.72498000	-1.25012600
H	5.57221500	-4.01287200	0.46508000
C	7.62533000	-3.66569200	-0.09812700
H	7.97502200	-3.38261800	0.90119700
H	7.86543000	-4.72378400	-0.24589600
H	8.20737000	-3.08867300	-0.82570800

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C	-1.85060100	0.01781700	-0.27948300
C	-0.71603800	-0.29417300	0.34248900
H	-1.94383200	0.92915900	-0.86712800
H	-2.72811300	-0.62065100	-0.22432300
H	-0.66538700	-1.22105600	0.91708300
C	0.53937700	0.52041200	0.30813700
H	0.80104300	0.82360200	1.33164600
H	0.36234100	1.44307800	-0.25697700
C	1.71450000	-0.24662000	-0.29559800
H	2.62798800	0.35644900	-0.28431400
H	1.91664700	-1.16698400	0.26339500
H	1.50588500	-0.52821500	-1.33265100

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C	-0.44839000	1.18423400	-0.33038400
C	-1.77855800	1.20104700	0.06718500
C	-2.44589000	-0.00019700	0.26722300
C	-1.77824600	-1.20124800	0.06708700
C	-0.44808000	-1.18402900	-0.33047400
C	0.24931200	0.00020000	-0.54694200
F	-3.71838000	-0.00036900	0.65029200
F	-2.41418700	2.35418800	0.25973000
F	0.16884000	2.35617100	-0.50774800
F	-2.41354600	-2.35458100	0.25952500
F	0.16945900	-2.35578900	-0.50797300
C	1.69857700	0.00036400	-0.93694200
H	1.90061000	-0.88091800	-1.55371200
H	1.90053400	0.88197600	-1.55325800
C	2.62857100	0.00007300	0.27955800
H	2.40881600	-0.87969200	0.89797300
H	2.40888300	0.87959500	0.89834400
C	4.10143300	0.00008700	-0.10977500
H	4.31009400	0.87809500	-0.73538700
H	4.31003400	-0.87777200	-0.73561600
C	5.02665400	-0.00010100	1.09856400
H	4.85993000	-0.88392900	1.72430400
H	6.07906500	-0.00014900	0.79782000
H	4.86006400	0.88362100	1.72448900

TS8

C	-0.25678300	0.39097100	0.93900100
N	-0.63134000	-0.03517600	-0.32086500
N	-1.08808800	-0.30120500	1.78994400
C	0.13361800	0.21206700	-1.50539700
C	1.66907500	0.70240900	-3.77867300
C	1.04411900	-0.76686300	-1.93794200
C	-0.05014000	1.40626300	-2.20974200
C	0.70738200	1.61984000	-3.35969800
C	1.82274000	-0.48168500	-3.05751000
H	0.58192500	2.54862100	-3.90849400
H	2.57921300	-1.19841100	-3.36565500
C	-1.02966800	-0.28191900	3.22203900
C	-1.02652800	-0.40156200	5.98171200
C	-0.10461400	-1.12808500	3.86088500
C	-1.94464800	0.51405300	3.93157600
C	-1.92458700	0.42936600	5.32604200
C	-0.12118900	-1.16527700	5.25581700

H	-2.61576600	1.03267900	5.90568500
H	0.58395600	-1.80129600	5.78044600
C	-2.91725000	1.44589200	3.23293700
H	-2.47009600	1.69875000	2.26566800
C	0.84229700	-2.00994200	3.06909000
H	1.07820000	-1.47288400	2.14338900
C	-1.07557400	2.41143100	-1.71469000
H	-0.99260200	2.40645200	-0.62088600
C	1.12173300	-2.12484600	-1.25820300
H	0.76164500	-1.99629300	-0.23270000
C	2.57141800	1.00362000	-4.93831200
H	2.73914900	0.12005000	-5.56182500
C	-3.13871400	2.74605400	4.00667600
H	-2.19986100	3.20192000	4.33084000
H	-3.75901200	2.58296400	4.89496400
H	-3.66780200	3.46728100	3.37599200
C	0.16637400	-3.33421500	2.69867000
H	0.84584500	-3.95132600	2.10039000
H	-0.75474700	-3.18629600	2.12984300
H	-0.08868000	-3.89823900	3.60310700
Ni	0.97449400	1.75292600	1.37394900
H	2.16700400	1.79990700	-5.56870400
H	3.55074200	1.33290300	-4.57069900
C	-0.77678800	3.83999600	-2.14070400
C	0.49101800	4.37251200	-1.86570000
C	-1.73371400	4.66949900	-2.72370900
C	0.79053600	5.69430500	-2.17039500
H	1.24767600	3.73652500	-1.41512900
C	-1.43342900	5.99690300	-3.03001600
H	-2.72479100	4.28107500	-2.93500000
C	-0.17326600	6.51462400	-2.75589200
H	1.77972300	6.08576400	-1.94899300
H	-2.19436200	6.62626500	-3.48337100
H	0.05885600	7.54874600	-2.99407300
C	0.19795000	-3.14099800	-1.91790700
C	-0.01723500	-3.17839700	-3.29649900
C	-0.42480000	-4.10288600	-1.11902700
C	-0.82447400	-4.16245400	-3.86312900
H	0.43479200	-2.42276900	-3.93226200
C	-1.24226400	-5.07740000	-1.67926900
H	-0.27422000	-4.07705600	-0.04371600
C	-1.44132000	-5.11391600	-3.05720700
H	-0.97967200	-4.17579800	-4.93858700
H	-1.73258000	-5.80287500	-1.03661700

H	-2.08280100	-5.87194500	-3.49716200
C	2.16082800	-2.29449400	3.78396400
C	-4.27385200	0.78560000	2.97174000
C	-4.76471200	-3.57880700	1.95886100
C	-5.15148300	-3.84074700	0.65973700
C	-4.47898800	-3.21730200	-0.42709700
C	-3.43365400	-2.35613100	-0.09795500
C	-3.04463400	-2.06169800	1.24236800
C	-3.70953200	-2.68360300	2.27572700
H	-5.56133200	-4.02748400	-2.13449500
H	-5.28769200	-4.06737300	2.77579000
H	-5.97209000	-4.52594000	0.46424000
C	-4.75566400	-3.37202300	-1.81486300
C	-2.63892000	-1.66751000	-1.06061300
H	-3.44982300	-2.49767100	3.31349700
C	-2.93141700	-1.83085100	-2.39180700
C	-4.00447300	-2.69130200	-2.74840900
H	-2.36632300	-1.32406600	-3.16476800
H	-4.22804500	-2.81925300	-3.80338000
C	-1.95621600	-1.10675400	1.08068700
C	-1.69043600	-0.91543800	-0.24842700
C	3.67088700	0.65548400	1.93437000
C	4.89223300	0.05529700	1.67179600
C	5.39967200	0.09824700	0.37859300
C	4.68558600	0.74217300	-0.62271400
C	3.47238400	1.33670000	-0.30778000
C	2.90792700	1.28481100	0.95910900
C	2.53283100	-2.68121400	-1.13771400
C	3.11672600	-3.47045900	-2.13211500
C	3.26350000	-2.42536900	0.02352100
C	4.40416200	-3.97566600	-1.97271800
H	2.55118200	-3.71372000	-3.02690100
C	4.54348300	-2.94453200	0.19506500
H	2.82084200	-1.80569400	0.79830100
C	5.12117900	-3.71780300	-0.80768900
H	4.84257300	-4.58480300	-2.75830400
H	5.09321800	-2.73490000	1.10815500
H	6.12174100	-4.12013500	-0.67923300
C	-2.47839200	1.93829900	-2.04447300
C	-3.42668100	1.79398300	-1.03087100
C	-2.84737700	1.62922300	-3.35712100
C	-4.71378200	1.34545700	-1.31503500
H	-3.14559300	2.02432900	-0.00631600
C	-4.13629400	1.19233200	-3.64664900

H	-2.11449500	1.72746300	-4.15397800
C	-5.07265800	1.04490200	-2.62512700
H	-5.43203600	1.22109500	-0.50972400
H	-4.40808900	0.95670200	-4.67200700
H	-6.07338500	0.68733000	-2.84902000
H	-4.72553700	0.44545700	3.91075100
H	-4.95970400	1.50882000	2.51634300
H	-4.19947500	-0.07291400	2.30366100
H	2.01969900	-2.94872500	4.65128600
H	2.83887500	-2.81813900	3.10202900
H	2.65383500	-1.37876800	4.11395700
F	6.55593700	-0.49863900	0.09988500
F	5.57182500	-0.59393100	2.62313700
F	3.22469400	0.64068400	3.20489500
F	5.17035600	0.77887100	-1.86576100
H	-1.02581200	-0.44846500	7.06710500
F	2.84895100	2.00281500	-1.29091100
H	2.31167200	2.46414000	1.45433300
C	1.37387000	3.55162500	2.20393400
H	1.69455500	4.36474100	1.54836300
C	-0.01517700	3.22501000	2.24185000
H	-0.38544500	2.83267700	3.18964600
H	1.96438800	3.46817500	3.11754400
C	-0.99842800	4.06860400	1.46594000
H	-0.59349900	4.28925800	0.47330200
H	-1.93218300	3.51725500	1.30013500
C	-1.31471600	5.39393900	2.15851200
H	-0.40762900	5.99915800	2.26302800
H	-2.04315400	5.97714200	1.58379000
H	-1.72304500	5.23807700	3.16256000

int9

C	0.17110800	-0.40580900	0.82751900
N	0.82452300	0.08776100	-0.27387800
N	1.09407300	-0.32474300	1.83482500
C	0.19117000	0.21526300	-1.54904200
C	-1.14433100	0.41492500	-3.97541800
C	-0.44276100	1.42305400	-1.87315400
C	0.19318400	-0.88237700	-2.41413800
C	-0.47238600	-0.75720200	-3.63217800
C	-1.11240100	1.49573800	-3.09105200
H	-0.51045700	-1.61279000	-4.30087800
H	-1.65049800	2.40614700	-3.34042400
C	0.80079900	-0.67422500	3.18984300

C	0.25940000	-1.32446600	5.80891100
C	0.38184300	0.34549300	4.05724200
C	0.94671000	-2.01271800	3.58852800
C	0.66738600	-2.31515500	4.92227700
C	0.11662500	-0.01070100	5.38111700
H	0.76325000	-3.33837500	5.27075600
H	-0.21402900	0.75081900	6.08113300
C	1.41890000	-3.08021000	2.61892800
H	1.12877800	-2.75683500	1.61146700
C	0.24172900	1.78294300	3.59563700
H	0.29430400	1.78631600	2.50200600
C	0.90563900	-2.16336900	-2.00925300
H	0.77893200	-2.25132300	-0.92384900
C	-0.36611100	2.60321300	-0.91599800
H	-0.38783100	2.18352700	0.09514100
C	-1.95551400	0.49672700	-5.23455600
H	-3.01694400	0.35106600	-5.00075200
C	0.77397700	-4.44275100	2.86154100
H	-0.31591800	-4.37208200	2.91923200
H	1.13376800	-4.90529900	3.78678600
H	1.02711400	-5.12257100	2.04176100
C	1.40142500	2.63399500	4.11937200
H	1.30663800	3.66761200	3.76868000
H	2.36970400	2.25089700	3.78418400
H	1.40695300	2.65439500	5.21508400
Ni	-1.49984200	-1.41075900	1.01439300
H	-1.85959800	1.47493000	-5.71556600
H	-1.66460200	-0.27320800	-5.95400100
C	0.25043400	-3.40412200	-2.59375100
C	-1.04307800	-3.71932000	-2.16176000
C	0.87267100	-4.24109400	-3.51812900
C	-1.70037600	-4.84344100	-2.64356400
H	-1.53635300	-3.05799400	-1.45442900
C	0.21242700	-5.36980500	-4.00485600
H	1.88039200	-4.01852500	-3.85508300
C	-1.07255400	-5.67515700	-3.57084700
H	-2.70411300	-5.07034900	-2.29471300
H	0.71132900	-6.01301800	-4.72461700
H	-1.58349800	-6.55583600	-3.94951400
C	0.95179100	3.34706500	-1.04762900
C	1.51006100	3.64743500	-2.29232000
C	1.61852300	3.76990100	0.10428800
C	2.69842800	4.36796500	-2.38084600
H	1.01915600	3.29877000	-3.19739400

C	2.81544300	4.47316400	0.01989600
H	1.19735100	3.53383400	1.07850000
C	3.35690100	4.77998000	-1.22560700
H	3.11876800	4.59471900	-3.35689900
H	3.32864700	4.77427600	0.92861400
H	4.29392000	5.32447900	-1.29508600
C	-1.10416000	2.39340100	3.98367900
C	2.94622200	-3.19590500	2.64733300
C	5.76605200	0.84200300	2.86090000
C	6.35499000	1.26981500	1.68784200
C	5.59959800	1.32421200	0.48456700
C	4.26258000	0.93835400	0.57270200
C	3.64860400	0.49322100	1.78077600
C	4.40578300	0.44187100	2.92997000
H	7.09302100	2.02579300	-0.93622000
H	6.36070900	0.80390900	3.76884100
H	7.40160800	1.56223000	1.68043100
C	6.06032800	1.71415100	-0.80462500
C	3.36816000	0.91982800	-0.53757600
H	3.98867900	0.10267300	3.87345400
C	3.84253100	1.28943900	-1.77104100
C	5.20197800	1.68820100	-1.88220000
H	3.20962700	1.27901000	-2.64980500
H	5.57061100	1.98213300	-2.86048100
C	2.28593500	0.18331300	1.37585500
C	2.11803800	0.43793900	0.03593900
C	-3.73885500	0.29037600	1.51020800
C	-4.85155500	1.05271000	1.17641300
C	-5.25518400	1.12470900	-0.15022100
C	-4.54155700	0.43133200	-1.11795400
C	-3.44361300	-0.32607400	-0.73415400
C	-2.99337600	-0.41288200	0.57561200
C	-1.56344400	3.53599500	-0.99986300
C	-1.61426500	4.63426400	-1.86130900
C	-2.65980800	3.28362400	-0.17360800
C	-2.74402400	5.44772700	-1.90421500
H	-0.75987400	4.86882500	-2.48907500
C	-3.78636200	4.09889100	-0.20675400
H	-2.62526500	2.43114000	0.49859700
C	-3.83331500	5.18346300	-1.07851400
H	-2.76758700	6.29758500	-2.58085700
H	-4.62710700	3.88242200	0.44587100
H	-4.71135600	5.82213000	-1.10960900
C	2.39815300	-2.06857600	-2.25789900

C	3.29223400	-2.44232000	-1.25332200
C	2.91090700	-1.61643500	-3.47678500
C	4.66692300	-2.36108400	-1.45203900
H	2.90348000	-2.78910600	-0.29908800
C	4.28565300	-1.54770600	-3.68474600
H	2.22698700	-1.30685300	-4.26266400
C	5.16806800	-1.91509100	-2.67146300
H	5.34482500	-2.63630300	-0.64923300
H	4.66875200	-1.19449300	-4.63826700
H	6.24027700	-1.84337000	-2.82826600
H	3.28988000	-3.48703300	3.64635700
H	3.28740100	-3.96056900	1.94077600
H	3.43318700	-2.25188800	2.38758000
H	-1.20112300	2.50876700	5.06871800
H	-1.20116600	3.39041900	3.54063300
H	-1.93618300	1.78082000	3.63016700
F	-6.29439200	1.89051200	-0.49164600
F	-5.52182800	1.74990400	2.10210900
F	-3.40848800	0.23886900	2.81961100
F	-4.91790600	0.50147700	-2.39866000
H	0.04388900	-1.58203800	6.84198700
F	-2.82597700	-1.02316000	-1.70733500
C	-2.59534400	-2.87224200	1.38946700
C	-3.72575200	-3.45363400	0.55457400
H	-3.70058500	-4.55219100	0.65079500
H	-3.54004100	-3.23884800	-0.50386600
C	-2.81952500	-2.92886200	2.88870700
H	-2.99493700	-3.96078200	3.23493000
H	-1.95895300	-2.54276600	3.44762900
H	-1.65104100	-3.43107300	1.12425200
H	-3.68812400	-2.33406100	3.18309000
C	-5.13121500	-2.98400000	0.91432700
H	-5.86716300	-3.44079800	0.24418300
H	-5.40545900	-3.26255900	1.93683000
H	-5.23006100	-1.89881500	0.82629000

TS10

C	-0.20486100	0.23103900	0.90381800
N	-0.92804300	0.09019900	-0.26021300
N	-1.06564300	-0.17769300	1.89149200
C	-0.31478600	0.27625600	-1.53679900
C	1.03540300	0.63978300	-3.93960300
C	0.23842600	-0.83961500	-2.17979800
C	-0.21639200	1.56537100	-2.07003400

C	0.44506100	1.72182900	-3.28628500
C	0.92106200	-0.63203400	-3.37524800
H	0.54698000	2.71893800	-3.70493700
H	1.40095700	-1.47841600	-3.85986700
C	-0.67953000	-0.25060700	3.26602400
C	0.13380900	-0.35860700	5.89508000
C	0.00072200	-1.39814300	3.70840200
C	-0.98327200	0.83012000	4.10495600
C	-0.55699400	0.75442100	5.43297700
C	0.40389700	-1.42472200	5.04375600
H	-0.76496700	1.57776200	6.10968500
H	0.94265500	-2.28767100	5.42140000
C	-1.70790500	2.05438400	3.58235600
H	-2.18653300	1.77420300	2.63836400
C	0.23725400	-2.57778300	2.78524300
H	0.31373400	-2.18119100	1.76711100
C	-0.81629400	2.73498800	-1.30518300
H	-0.57345000	2.54947800	-0.25004100
C	0.06003400	-2.22443400	-1.58149100
H	-0.02910500	-2.08616200	-0.49958600
C	1.84535400	0.84126600	-5.18643800
H	2.91460700	0.80099700	-4.94656800
C	-0.71146300	3.17572100	3.28034200
H	0.04076900	2.84380300	2.55546500
H	-0.18546900	3.48857400	4.18931100
H	-1.22260400	4.05194600	2.86595000
C	-0.96037100	-3.53261400	2.83316000
H	-0.80419800	-4.37471900	2.14984700
H	-1.89481800	-3.03650400	2.55570000
H	-1.08590900	-3.94150100	3.84229100
Ni	1.46487100	1.03510700	1.12368500
H	1.64937700	0.05998900	-5.92742900
H	1.64344200	1.81204900	-5.64667000
C	-0.17019400	4.06920100	-1.64187200
C	1.19843300	4.22430300	-1.38664900
C	-0.87939600	5.15212800	-2.15927900
C	1.83971700	5.42923800	-1.64293400
H	1.76042000	3.37825800	-1.00286400
C	-0.23634100	6.36290800	-2.41795400
H	-1.94232400	5.05469200	-2.35634400
C	1.12217300	6.50708100	-2.16121200
H	2.90264100	5.52743900	-1.43904900
H	-0.80608000	7.19590900	-2.82067100
H	1.62097700	7.45092800	-2.36237500

C	-1.23750800	-2.87267600	-2.03715500
C	-1.71959700	-2.74012600	-3.34103300
C	-1.96576600	-3.64635800	-1.13017600
C	-2.89784100	-3.37372900	-3.72972000
H	-1.17785900	-2.12307700	-4.05272600
C	-3.14867000	-4.26914500	-1.51109400
H	-1.60465000	-3.74839000	-0.11008800
C	-3.61848900	-4.13648100	-2.81547300
H	-3.25853300	-3.25998600	-4.74847900
H	-3.70992200	-4.84956700	-0.78452000
H	-4.54560500	-4.61710600	-3.11389000
C	1.53100200	-3.33482500	3.07185200
C	-2.81164200	2.53319600	4.52328100
C	-5.67308700	-1.66144300	2.77819900
C	-6.33628900	-1.71294300	1.56883300
C	-5.65518200	-1.38634500	0.36367100
C	-4.31552700	-1.02213900	0.48741500
C	-3.62489800	-0.96297600	1.73466100
C	-4.30759100	-1.28666000	2.88546800
H	-7.23037100	-1.65689900	-1.11570400
H	-6.21014500	-1.91586300	3.68734000
H	-7.38298900	-2.00334700	1.53469700
C	-6.19115600	-1.38261600	-0.95506800
C	-3.48594200	-0.66212100	-0.61515400
H	-3.82709900	-1.26390000	3.85904600
C	-4.02937400	-0.66609100	-1.87578900
C	-5.39423100	-1.03236300	-2.02358200
H	-3.44348900	-0.40296300	-2.74815500
H	-5.81741100	-1.03673300	-3.02376600
C	-2.28476100	-0.53681700	1.36308600
C	-2.20016800	-0.36477000	0.00239500
C	3.85138300	-0.53516600	1.42668900
C	4.81130000	-1.37319300	0.87821200
C	5.14636300	-1.26177700	-0.46362900
C	4.48602500	-0.31993000	-1.24448700
C	3.53714300	0.49942900	-0.66274400
C	3.17334500	0.44481700	0.69166500
C	1.26018800	-3.13603300	-1.77876300
C	1.36545800	-4.02052500	-2.85389100
C	2.28925600	-3.10189800	-0.83425800
C	2.48044900	-4.84507800	-2.98554600
H	0.56081400	-4.08092700	-3.58100200
C	3.39507000	-3.93785100	-0.95341600
H	2.21851200	-2.40838700	0.00013000

C	3.49609000	-4.80970300	-2.03471700
H	2.54766500	-5.52670100	-3.82904200
H	4.17892700	-3.90603100	-0.20279800
H	4.35992500	-5.46098200	-2.13131100
C	-2.32811400	2.73594500	-1.41185100
C	-3.10939400	2.87771800	-0.26391800
C	-2.96890000	2.60338900	-2.64679800
C	-4.49909900	2.87372500	-0.34039600
H	-2.61832900	2.98447900	0.70022500
C	-4.35827800	2.61523700	-2.72890700
H	-2.37187000	2.48087400	-3.54693000
C	-5.12801200	2.74369400	-1.57512300
H	-5.08956200	2.96264900	0.56699300
H	-4.84181000	2.50959400	-3.69624200
H	-6.21210700	2.73062700	-1.63741900
H	-2.41017900	2.91128000	5.46946000
H	-3.36943400	3.35255100	4.05796600
H	-3.51945000	1.73044100	4.75216500
H	1.48775200	-3.87369300	4.02493300
H	1.69772800	-4.08213600	2.28928100
H	2.39388700	-2.66587200	3.09223900
F	6.04584900	-2.08489200	-1.00536000
F	5.38707100	-2.32733500	1.61987500
F	3.56945200	-0.71964500	2.73288500
F	4.75766900	-0.23330400	-2.54952500
H	0.46337500	-0.39850300	6.92951500
F	2.93805300	1.39738800	-1.46932900
C	2.98907600	2.17734300	1.55665500
C	4.15413000	2.94105900	0.92904400
H	4.06892000	3.97935400	1.28408100
H	4.02098400	2.98019800	-0.15581800
C	3.05936900	2.10180500	3.07259800
H	3.11722900	3.11740700	3.48779800
H	2.17484500	1.61808200	3.50085000
H	2.06747900	2.75918900	1.24960300
H	3.93565100	1.54733800	3.41266000
C	5.55308000	2.43383400	1.25573100
H	6.30375700	3.08603600	0.79803300
H	5.74314300	2.42461900	2.33340500
H	5.71911800	1.42177800	0.87710600
int11			
C	-0.07393800	0.76402200	-0.02368000
N	0.93167800	-0.17581200	0.01357300

N	0.57609200	1.94383800	-0.27568800
C	0.66418700	-1.56083300	0.24057200
C	0.02995400	-4.23390000	0.68170500
C	0.36701900	-2.37861300	-0.85712800
C	0.66461500	-2.05067000	1.55398900
C	0.34493300	-3.39254900	1.74955000
C	0.05097700	-3.71367000	-0.61260100
H	0.31364700	-3.78107400	2.76361400
H	-0.21027900	-4.35265500	-1.45155300
C	-0.07836200	3.20538900	-0.42027900
C	-1.25899900	5.67487000	-0.71629400
C	-0.55323100	3.57040100	-1.68718400
C	-0.17374500	4.03875000	0.70515700
C	-0.78024200	5.28303300	0.52978600
C	-1.15095200	4.82702600	-1.81122000
H	-0.87683700	5.95589100	1.37593000
H	-1.53950000	5.14023600	-2.77569200
C	0.32552900	3.57416700	2.05867200
H	1.11183500	2.83286800	1.87744400
C	-0.47176700	2.62420900	-2.86672800
H	0.18683200	1.79800700	-2.58060600
C	1.01846000	-1.13259800	2.71634100
H	0.56593800	-0.16020500	2.49008300
C	0.41607700	-1.81365300	-2.26983900
H	0.03487000	-0.78790500	-2.20677500
C	-0.37894800	-5.65683500	0.92646900
H	-1.46199100	-5.71830600	1.08680700
C	-0.79975900	2.87169500	2.82473100
H	-1.20948500	2.03689400	2.24374100
H	-1.61600300	3.57137200	3.03818500
H	-0.43468900	2.47699100	3.77964600
C	0.13616700	3.28328800	-4.10305400
H	0.23958100	2.54992300	-4.90982500
H	1.12831300	3.69276700	-3.88677000
H	-0.49081800	4.09680900	-4.48324600
Ni	-1.95095200	0.62511300	0.17503400
H	-0.13795700	-6.29730400	0.07337900
H	0.10666000	-6.06764500	1.81624500
C	0.40111200	-1.59128000	4.03053700
C	-0.96301600	-1.36319900	4.23147700
C	1.12521600	-2.24117000	5.03095300
C	-1.59215400	-1.78299500	5.39716600
H	-1.53452200	-0.85256100	3.46580200
C	0.49530500	-2.66416400	6.20060900

H	2.19008900	-2.40942900	4.90559400
C	-0.86448800	-2.43957900	6.38785200
H	-2.65383200	-1.59353400	5.52977500
H	1.07566900	-3.16702900	6.96946800
H	-1.35335800	-2.76790300	7.30081900
C	1.84012400	-1.72462600	-2.78551300
C	2.74365800	-2.77847100	-2.62519500
C	2.26247900	-0.58041000	-3.46482200
C	4.03349300	-2.69258700	-3.14210700
H	2.43497300	-3.66802400	-2.08228000
C	3.55686900	-0.48290900	-3.96545700
H	1.56910300	0.24661000	-3.59587800
C	4.44618500	-1.54222300	-3.80922500
H	4.72283300	-3.52209800	-3.00982600
H	3.87204600	0.42519200	-4.47110500
H	5.45900900	-1.46660200	-4.19364700
C	-1.84978700	2.02707800	-3.15821600
C	0.94460000	4.69569700	2.88814200
C	4.96553900	3.96978600	-1.15715100
C	5.90782700	2.96149800	-1.11654100
C	5.51318700	1.62174000	-0.84911000
C	4.15255200	1.40698700	-0.63559300
C	3.17470400	2.44439000	-0.67629000
C	3.58301300	3.73250400	-0.93863700
H	7.42252600	0.57791000	-0.93703600
H	5.28731700	4.98631800	-1.36415300
H	6.95599800	3.18966400	-1.29094800
C	6.35228400	0.47385900	-0.77948100
C	3.58366700	0.12799300	-0.35954800
H	2.87807200	4.55750900	-0.98145800
C	4.41653400	-0.96107800	-0.30312700
C	5.80783000	-0.76404500	-0.51654600
H	4.03782100	-1.95537600	-0.10178300
H	6.46048200	-1.63088100	-0.46936600
C	1.92985300	1.74600900	-0.40501600
C	2.15917200	0.40506900	-0.22013600
C	-4.41500000	0.36883000	-0.82654400
C	-4.47734900	-0.97271800	-1.11796200
C	-3.97913900	-1.92661500	-0.20983400
C	-3.44471500	-1.51261700	0.98118500
C	-3.33549800	-0.12327400	1.27709700
C	-3.88949700	0.87376300	0.39797800
C	-0.51657000	-2.55325200	-3.21639700
C	-0.06879900	-3.47566400	-4.16261000

C	-1.89008400	-2.31614400	-3.10815200
C	-0.97642400	-4.15567600	-4.97319600
H	0.99490700	-3.65980200	-4.27576400
C	-2.79739500	-2.99495100	-3.91271500
H	-2.23953700	-1.58979300	-2.37896700
C	-2.34137000	-3.92126700	-4.84871600
H	-0.60990600	-4.86947500	-5.70597000
H	-3.85828600	-2.79987200	-3.80338100
H	-3.04826700	-4.45271500	-5.47957900
C	2.51566800	-0.91068900	2.81813900
C	3.01516100	0.37485200	3.03432800
C	3.41820600	-1.97461700	2.73897500
C	4.38257300	0.59754100	3.16336200
H	2.32158400	1.21006700	3.09641500
C	4.78525800	-1.75856200	2.88927400
H	3.04443300	-2.97793500	2.55052000
C	5.27234900	-0.47090800	3.09764400
H	4.75282900	1.60801800	3.31044900
H	5.47314100	-2.59754200	2.82850200
H	6.34026300	-0.29915300	3.19447000
H	0.19838000	5.43155100	3.20619300
H	1.39395800	4.28211900	3.79679000
H	1.72766900	5.22207800	2.33289800
H	-2.56557200	2.80204900	-3.45358300
H	-1.79101600	1.28936700	-3.96600000
H	-2.24938100	1.52405900	-2.26970500
F	-4.00032400	-3.21613000	-0.54956300
F	-4.98445100	-1.39022400	-2.28568500
F	-4.93893700	1.21285200	-1.72814100
F	-2.99806000	-2.40430600	1.86784400
H	-1.72681400	6.64849000	-0.83186600
F	-3.24883900	0.16956700	2.61304800
C	-4.25840200	2.23712600	0.96550400
C	-5.65844100	2.22800000	1.60718300
H	-5.80817600	3.20889100	2.07818300
H	-5.65509000	1.49354100	2.42178900
C	-4.05377500	3.38734000	-0.01603900
H	-4.16963800	4.34261100	0.50648900
H	-3.04476200	3.35828200	-0.43513400
H	-3.55390000	2.40028400	1.78726500
H	-4.76164600	3.36674500	-0.84642600
C	-6.82417900	1.93404400	0.67328300
H	-7.77215400	1.99735800	1.21744000
H	-6.87621700	2.64174700	-0.15972900

H	-6.76125100	0.92571600	0.25177900
P-b			
C	0.04695800	1.11799100	-0.11347600
C	-1.32091600	1.26438100	0.07285900
C	-2.13598500	0.14050800	0.08346900
C	-1.57175600	-1.11444100	-0.09184300
C	-0.19928800	-1.22758100	-0.27588000
C	0.65054200	-0.12443400	-0.29891300
F	-3.44643200	0.26752200	0.26122600
F	-1.85314900	2.47187500	0.24397100
F	0.78700100	2.23324900	-0.10536300
F	-2.34342000	-2.19852200	-0.07963000
F	0.29718100	-2.45901400	-0.43271100
C	2.14154100	-0.28995700	-0.49532100
C	2.92729900	0.12534300	0.75737800
H	2.79028800	1.19890500	0.93015300
H	3.99266600	-0.02031400	0.54022900
C	2.63116900	0.44419100	-1.74447600
H	3.69309100	0.23519800	-1.90834000
H	2.08344500	0.12032900	-2.63450100
H	2.31087300	-1.36134900	-0.64707200
H	2.51136600	1.52613500	-1.64580900
C	2.54712700	-0.65948300	2.00389000
H	3.17373000	-0.37416800	2.85439500
H	1.50499700	-0.48259900	2.29011100
H	2.66876700	-1.73723600	1.84727600
int1-L9			
C	-0.48807000	-0.51722700	0.60272800
N	0.22148400	0.06707700	-0.43152000
N	0.27848200	-1.61900300	0.93488400
C	-0.05625000	1.36178600	-0.96530600
C	-0.60927100	3.89585300	-1.99165000
C	0.72418300	2.45012700	-0.54860000
C	-1.12463300	1.52102500	-1.86020200
C	-1.36783800	2.78844600	-2.37855500
C	0.41007100	3.71043500	-1.06233300
H	-2.19213200	2.92380400	-3.07206900
H	0.95924800	4.57582400	-0.70310600
C	0.03460600	-2.56882900	1.97898100
C	-0.22691200	-4.45525000	3.98484700
C	0.27749000	-2.18179000	3.30909300
C	-0.35686500	-3.87318300	1.63311900

C	-0.46968200	-4.80865000	2.66568200
C	0.13120600	-3.14988100	4.30247200
H	-0.77069600	-5.82481500	2.42768800
H	0.30438300	-2.88124600	5.33914000
C	-0.70618900	-4.28304300	0.21405200
H	-0.72918400	-3.37713600	-0.39881700
C	0.71779400	-0.76985600	3.64375000
H	0.17714000	-0.10467400	2.95885900
C	-2.02159900	0.33308400	-2.17013200
H	-2.28798600	-0.08604000	-1.18548500
C	1.86301900	2.27806300	0.44900900
H	1.70292600	1.31963800	0.95108200
C	-0.89810900	5.25395600	-2.56154600
H	-1.97483000	5.42631200	-2.65126500
C	-2.08961200	-4.93748500	0.14439300
H	-2.85674100	-4.33849700	0.63969400
H	-2.08472100	-5.92923400	0.60945300
H	-2.38508200	-5.07547200	-0.90164400
C	2.22157200	-0.60353200	3.40070900
H	2.53419100	0.42667600	3.60354700
H	2.49884100	-0.84888000	2.37184200
H	2.79187200	-1.26445400	4.06337100
Ni	-2.18393700	0.02901000	1.33823000
H	-0.47620000	6.04645900	-1.93756200
H	-0.46915100	5.35840000	-3.56557600
C	-3.33068000	0.74824400	-2.81682400
C	-4.27842100	1.41340900	-2.03015800
C	-3.62097000	0.51439000	-4.16042600
C	-5.48790900	1.83107300	-2.57139000
H	-4.05368800	1.60022900	-0.98301100
C	-4.83362700	0.93394800	-4.70624100
H	-2.89854500	-0.00542200	-4.78253200
C	-5.77006800	1.59184600	-3.91580000
H	-6.21337100	2.33956800	-1.94230500
H	-5.04549300	0.74044900	-5.75426200
H	-6.71618300	1.91387500	-4.34158700
C	3.23128300	2.19572600	-0.21256400
C	3.57755500	2.95112900	-1.33413900
C	4.19532900	1.35382800	0.34782000
C	4.85956900	2.87480200	-1.87449100
H	2.83560100	3.58881100	-1.80545900
C	5.47012500	1.26318900	-0.19805200
H	3.93552200	0.75384000	1.21609500
C	5.80928100	2.02895300	-1.31101200

H	5.11037500	3.47127500	-2.74758500
H	6.19654300	0.58568300	0.24129300
H	6.80407300	1.95801500	-1.74120600
C	0.36373900	-0.34258100	5.06451100
C	0.33113300	-5.23510200	-0.38576900
C	4.51795400	-3.94675000	0.01722500
C	5.09708900	-3.34772200	-1.08263300
C	4.45935500	-2.24438900	-1.71540800
C	3.24575400	-1.83239700	-1.16804000
C	2.62655400	-2.46537600	-0.04990500
C	3.27457400	-3.51848900	0.55460200
H	5.87017600	-1.77823000	-3.30765800
H	5.02417300	-4.78108500	0.49397800
H	6.04714800	-3.71255700	-1.46397900
C	4.93105100	-1.50350700	-2.83501700
C	2.49706200	-0.71594400	-1.64373300
H	2.85424300	-4.02511900	1.41808300
C	2.97789500	-0.01826100	-2.72472000
C	4.20198300	-0.43476600	-3.31204500
H	2.45478100	0.84483300	-3.12038900
H	4.58021700	0.12676500	-4.16112200
C	1.40103600	-1.70203700	0.13989400
C	1.34980100	-0.66140000	-0.74567900
C	1.85718800	3.32994400	1.55134500
C	2.46906500	4.57708300	1.40020000
C	1.23709500	3.03927600	2.76936300
C	2.42502100	5.51981200	2.42348800
H	3.00707700	4.80465100	0.48427500
C	1.19404300	3.97717700	3.79661100
H	0.78581500	2.06188600	2.91283300
C	1.78260700	5.22651900	3.62348200
H	2.90480200	6.48473500	2.28487000
H	0.70194800	3.72853900	4.73291900
H	1.75201800	5.96200600	4.42214200
C	-1.29858200	-0.76020000	-2.92819900
C	-1.62986600	-2.09634800	-2.69037300
C	-0.32268700	-0.47099900	-3.88283200
C	-0.98707800	-3.12064100	-3.37758200
H	-2.39604000	-2.32935900	-1.95489400
C	0.32182500	-1.49456100	-4.57359400
H	-0.05959900	0.56554300	-4.07605300
C	-0.00383500	-2.82297900	-4.31877200
H	-1.25122400	-4.15479100	-3.17447400
H	1.09043100	-1.25270200	-5.30212300

H	0.50714600	-3.62250100	-4.84713400
H	0.42251500	-6.14434200	0.21992900
H	0.02667300	-5.53759600	-1.39333700
H	1.31792300	-4.77618900	-0.46157200
H	0.95428100	-0.88059900	5.81462700
H	0.58055200	0.72260200	5.19569800
H	-0.69636000	-0.50169000	5.28440700
H	-0.32705900	-5.19619200	4.77304500
C	-1.93451300	2.02074600	1.40645500
H	-2.12759700	2.43308000	0.41851700
C	-2.99609800	1.65775900	2.23582100
H	-4.01434500	1.83665500	1.89141800
C	-3.02296300	-1.77178900	1.35031000
H	-3.06742200	-2.17535300	0.33944100
H	-2.51325200	-2.39507900	2.07849200
C	-3.97443200	-0.83302100	1.76078300
H	-4.16738500	-0.73999300	2.83079300
H	-0.97488700	2.29656100	1.83033900
C	-5.13644500	-0.45873900	0.87699700
H	-5.43005400	0.58753600	1.03589300
H	-4.83749600	-0.53864200	-0.17493000
C	-2.82780500	1.60881400	3.73329600
H	-3.50421500	0.86421600	4.17281500
H	-1.80868100	1.27791100	3.96885300
C	-3.08190700	2.96657600	4.38753300
H	-4.09969000	3.31730200	4.18156600
H	-2.95968300	2.91794800	5.47582000
H	-2.38881300	3.71988100	3.99833700
C	-6.35132900	-1.35282900	1.12107400
H	-7.19002600	-1.07437700	0.47280900
H	-6.10588600	-2.40255800	0.92730100
H	-6.69240200	-1.28025900	2.16035500

int1-L7

C	0.41272800	0.00842300	-0.02188900
N	-0.45376300	1.08042500	0.05554400
N	-0.42438600	-1.08291000	-0.13613600
C	-0.07763100	2.45671400	0.16839800
C	0.48982800	5.14586600	0.43755700
C	-0.15982700	3.27851900	-0.96878600
C	0.29885900	2.94382900	1.43188200
C	0.58487400	4.30507600	1.54055600
C	0.12456500	4.63655000	-0.80093200
H	0.88417000	4.71327500	2.50035200

H	0.07002400	5.30065400	-1.65829800
C	-0.02437300	-2.45759700	-0.11840800
C	0.57558200	-5.15303500	-0.11964100
C	0.43541600	-3.04506400	-1.30848600
C	-0.16329300	-3.17878600	1.08012700
C	0.13731400	-4.54310900	1.04749200
C	0.73493100	-4.40756100	-1.28231300
H	0.03838700	-5.12992900	1.95577600
H	1.09837300	-4.89240200	-2.18227500
C	-0.59859400	-2.53086900	2.38337800
H	-0.52366100	-1.44582100	2.25428100
C	0.58078400	-2.22064700	-2.57238800
H	0.92961200	-1.23071600	-2.25865900
C	0.35325800	2.02380600	2.63552300
H	0.67476500	1.04411300	2.26841100
C	-0.52979400	2.74524100	-2.34216000
H	-0.44602300	1.65382500	-2.30451100
C	0.30578100	-2.92119000	3.55554500
H	1.36297300	-2.76130000	3.33310200
H	0.17198700	-3.97202400	3.83435000
H	0.04882700	-2.32045400	4.43461000
C	-0.76862500	-2.05022800	-3.27699900
H	-0.65677500	-1.42241100	-4.16781500
H	-1.51541300	-1.58178600	-2.63075500
H	-1.16332900	-3.02151500	-3.59676300
Ni	2.31282700	0.02355100	-0.01316300
C	1.36371000	2.46706300	3.68911800
C	-1.97133000	3.10261200	-2.71474100
C	1.61463600	-2.78272700	-3.54338200
C	-2.05003800	-2.87446500	2.72860400
C	-5.14532400	-2.45737500	-0.50280300
C	-5.92439200	-1.33295300	-0.32588800
C	-5.31201400	-0.06576800	-0.11189700
C	-3.91926900	-0.04545800	-0.09921500
C	-3.10665400	-1.20716400	-0.25976700
C	-3.72496500	-2.41828400	-0.47012800
H	-7.05036500	1.22917500	0.09919900
H	-5.62913200	-3.41561200	-0.66775200
H	-7.00787200	-1.41141800	-0.34959200
C	-5.96480100	1.18211900	0.09586400
C	-3.14300400	1.13775600	0.08428800
H	-3.15494700	-3.33324500	-0.60005100
C	-3.80058100	2.32813400	0.29503300
C	-5.22196500	2.32662200	0.29756400

H	-3.26039300	3.25708400	0.45119900
H	-5.73603600	3.26917200	0.46129100
C	-1.74764800	-0.69512400	-0.14547200
C	-1.76717400	0.66355000	0.00424200
C	0.41204200	3.25111700	-3.43808600
C	-1.03496500	1.86414600	3.26362700
H	-2.16923500	-3.95632600	2.85893200
H	-2.34032700	-2.39091400	3.66762700
H	-2.74759900	-2.55055700	1.95446700
H	1.26913300	-3.70704800	-4.02041900
H	1.80281600	-2.05894200	-4.34283400
H	2.56720200	-2.99201600	-3.04720300
H	0.80789500	-6.21433500	-0.12186000
C	2.51149900	1.11829200	-1.65429400
H	2.18778700	2.12473700	-1.40413000
C	3.77377000	0.67366500	-1.24470700
H	4.40659600	1.38050600	-0.70667500
C	2.56278400	-1.04896300	1.63559300
H	2.09422500	-0.58292100	2.50206900
H	2.23811500	-2.06365700	1.42158900
C	3.81012100	-0.60370900	1.18153100
H	4.43076300	-1.31559200	0.63564400
H	2.01898500	0.67181000	-2.51797800
C	4.57131300	0.48088500	1.90085200
H	5.26564400	0.97777500	1.21205200
H	3.86908500	1.25214400	2.24134000
C	4.51867400	-0.39796500	-1.99894500
H	5.21324500	-0.92033700	-1.32932400
H	3.80619500	-1.15208800	-2.35524800
H	-2.10398400	4.19036700	-2.74382300
H	-2.21350300	2.71021100	-3.70828200
H	-2.69503400	2.69404600	-2.00773400
H	1.46313100	3.08657700	-3.19119300
H	0.19888300	2.72864700	-4.37666200
H	0.27009000	4.32076600	-3.62668900
H	0.71113100	6.20423100	0.54361700
H	2.34812100	2.65831600	3.25154200
H	1.04121600	3.37460000	4.21194600
H	1.47818700	1.68425200	4.44594000
H	-1.39999300	2.82414900	3.64663300
H	-1.77014900	1.48928600	2.54660900
H	-0.99588100	1.15985000	4.10211000
C	5.35588400	-0.05541400	3.09706900
H	6.07574600	-0.82010200	2.78300200

H	5.91374700	0.74071400	3.60360000
H	4.68397100	-0.51782500	3.82818500
C	5.29903300	0.16332500	-3.18650000
H	6.03040000	0.91079800	-2.85788500
H	5.84335400	-0.62442100	-3.72008800
H	4.62603100	0.65345700	-3.89836600

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C	-0.15041800	0.40970100	0.38574100
N	0.24393400	0.66185700	-0.91740400
N	-0.25619700	-0.97603300	0.40981200
C	0.68295900	1.92225700	-1.42302300
C	1.57571300	4.36286600	-2.42832300
C	2.06135200	2.15867800	-1.51028700
C	-0.26099300	2.89002200	-1.79840800
C	0.20941100	4.08822300	-2.32729800
C	2.48096100	3.40259600	-1.98662400
H	-0.50672200	4.85054400	-2.61859200
H	3.54257500	3.63431100	-1.98805500
C	-0.64246800	-1.81175200	1.50385700
C	-1.31789500	-3.59645600	3.54543700
C	0.31118200	-2.13904500	2.47451600
C	-1.93619300	-2.36430300	1.52875400
C	-2.23973200	-3.25994700	2.55353200
C	-0.05139100	-3.01934900	3.49390800
H	-3.23932900	-3.68293500	2.59920100
H	0.67899100	-3.25586800	4.26330400
C	-2.96695900	-2.01583300	0.46680400
H	-2.66143000	-1.05385400	0.03698400
C	1.72014500	-1.57910000	2.41870100
H	1.67253800	-0.67398400	1.80308200
C	-1.73678300	2.67813400	-1.49466000
H	-1.75938200	2.27076200	-0.47044400
C	3.07228300	1.10719300	-1.07466000
H	2.52257100	0.35519600	-0.50289900
C	2.04745700	5.67560100	-2.98234700
H	1.45437900	6.50749400	-2.59040300
Ni	-0.56880300	1.74002400	1.74866200
H	3.09671900	5.85898300	-2.73594600
H	1.95333100	5.69761400	-4.07474800
C	-2.48919600	3.99833400	-1.44067400
C	-2.37323900	4.79431300	-0.29783400
C	-3.25691000	4.46521200	-2.50876300
C	-3.01146300	6.02673400	-0.21918900

H	-1.77421700	4.43428900	0.53312700
C	-3.89485000	5.70181900	-2.43391500
H	-3.36172900	3.85431000	-3.40073900
C	-3.77578800	6.48589700	-1.29008300
H	-2.91479800	6.62696700	0.68142400
H	-4.49080800	6.05020600	-3.27305500
H	-4.27844500	7.44714000	-1.23124600
C	3.69998500	0.36387200	-2.24548200
C	4.08286600	0.98969900	-3.43356300
C	3.90860900	-1.01181700	-2.12116000
C	4.67270400	0.25960800	-4.46354600
H	3.89901900	2.05063000	-3.57194700
C	4.48887200	-1.74461600	-3.14943200
H	3.59968700	-1.51700300	-1.21145600
C	4.87846600	-1.10957400	-4.32599800
H	4.96264200	0.76509500	-5.38085300
H	4.62287800	-2.81600400	-3.03077000
H	5.32725000	-1.67974600	-5.13440200
C	0.53236600	-5.08874400	-2.18569600
C	0.89974300	-4.71584800	-3.46179200
C	0.98748600	-3.33828800	-3.80594700
C	0.69025500	-2.42696800	-2.79359700
C	0.30433200	-2.80713800	-1.47469600
C	0.22479200	-4.14464100	-1.17096800
H	1.59420200	-3.44784900	-5.89359400
H	0.46191800	-6.14483600	-1.94225000
H	1.12071600	-5.47341700	-4.20903400
C	1.34849100	-2.78723400	-5.06635100
C	0.74223300	-1.01193800	-2.96194300
H	-0.08598800	-4.48726000	-0.19036800
C	1.09525300	-0.50738200	-4.19085200
C	1.39449000	-1.41891000	-5.23686500
H	1.17269300	0.56012000	-4.36693400
H	1.68384200	-1.01496500	-6.20248400
C	0.09296500	-1.53193100	-0.80117900
C	0.37693800	-0.49790400	-1.64853000
C	4.11439300	1.66006000	-0.11269000
C	5.32718800	2.20384900	-0.53910100
C	3.85648300	1.60303400	1.26078800
C	6.24500400	2.70066100	0.38382100
H	5.56818000	2.21562200	-1.59841300
C	4.77367900	2.08993800	2.18659400
H	2.92154100	1.17120000	1.60770000
C	5.97251600	2.64702000	1.74807200

H	7.18391400	3.12039300	0.03318600
H	4.54993500	2.02379700	3.24787100
H	6.69412800	3.02723600	2.46539300
C	-2.44160800	1.67661700	-2.38642900
C	-3.67297400	1.15904700	-1.96416000
C	-1.96046200	1.31513300	-3.64333700
C	-4.41451900	0.32390200	-2.79021800
H	-4.05864600	1.43201900	-0.98461600
C	-2.69416400	0.46172200	-4.46790600
H	-1.00848100	1.71138700	-3.98369100
C	-3.92744200	-0.02649100	-4.04977800
H	-5.36802000	-0.06400100	-2.44399800
H	-2.29660700	0.18281600	-5.43979700
H	-4.50147000	-0.68788500	-4.69219800
C	0.71602100	3.23854500	1.34643100
H	0.42354900	3.72226200	0.41996600
C	0.03607000	3.53026200	2.53068100
H	-0.79029000	4.24129200	2.48835700
C	-2.04502900	0.69517700	2.58573400
H	-2.75580300	0.38807600	1.82315300
H	-1.61053100	-0.10686900	3.17644100
C	-2.10480400	1.99137600	3.09232500
H	-1.70634500	2.17227600	4.09085400
H	1.75431400	2.92229100	1.38212500
C	-3.18680900	2.94658400	2.65797800
H	-2.85412700	3.98669100	2.76489700
H	-3.40257100	2.79982800	1.59251900
C	0.73420200	3.48283500	3.86546600
H	0.03898100	3.18749700	4.66282200
H	1.52135700	2.72208800	3.83688600
C	-2.94270400	-3.01734700	-0.67970400
C	-3.17384100	-4.37809200	-0.46255000
C	-2.71956900	-2.57539800	-1.98318500
C	-3.17341200	-5.27500000	-1.52549800
H	-3.35602700	-4.74028900	0.54508500
C	-2.72234900	-3.46962600	-3.05049600
H	-2.53290700	-1.52211700	-2.16484300
C	-2.94652400	-4.82318400	-2.82474600
H	-3.35122700	-6.33073500	-1.33931500
H	-2.53477900	-3.10201800	-4.05491200
H	-2.93850000	-5.52513000	-3.65367000
C	-4.39107100	-1.80930100	0.98853200
C	-4.66339600	-1.39505700	2.29673600
C	-5.47000500	-1.94933300	0.10778600

C	-5.96771700	-1.13200800	2.70882000
H	-3.85218600	-1.26970100	3.00480200
C	-6.77285300	-1.68002800	0.51566600
H	-5.28531200	-2.27490000	-0.91096900
C	-7.02970200	-1.27058400	1.82083500
H	-6.14837500	-0.81504700	3.73231600
H	-7.58996900	-1.79710900	-0.19104600
H	-8.04634100	-1.06428300	2.14299600
C	2.71584000	-2.50952900	1.74384000
C	2.42658000	-3.83708700	1.43062500
C	3.98370600	-2.00941200	1.42107600
C	3.37075400	-4.64218300	0.79477300
H	1.45272600	-4.24577000	1.67832700
C	4.92946000	-2.81187700	0.79401300
H	4.22954200	-0.97911400	1.66339500
C	4.62372600	-4.13387600	0.47260200
H	3.11818800	-5.66922500	0.54624500
H	5.90117800	-2.39690800	0.54206600
H	5.35828000	-4.75995900	-0.02583000
C	2.16581100	-1.12171000	3.79816200
C	3.10247600	-1.81837600	4.56135900
C	1.58148600	0.03172700	4.33033100
C	3.45150700	-1.36830200	5.83385300
H	3.57012100	-2.71024800	4.15485800
C	1.93227900	0.48357600	5.59733600
H	0.84634900	0.57270700	3.73409600
C	2.86997100	-0.21717700	6.35500900
H	4.18457600	-1.92006200	6.41593400
H	1.47558500	1.38675400	5.99207200
H	3.14608400	0.13548200	7.34470900
C	-1.69881400	-4.52594400	4.66055500
H	-0.82293500	-5.03043100	5.07765200
H	-2.17948500	-3.97510100	5.47784000
H	-2.40652300	-5.28829900	4.32192600
C	1.35800900	4.83070400	4.22441600
H	0.59714200	5.61846600	4.27127400
H	1.86080100	4.79360900	5.19775600
H	2.09563200	5.12661100	3.47112700
C	-4.47318500	2.75255700	3.45965700
H	-5.24385800	3.46987800	3.15552500
H	-4.87175000	1.74346500	3.31236600
H	-4.29325900	2.88742100	4.53261700

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C	-0.38923100	-0.49638500	0.02614700
N	-0.39253500	0.87880500	0.10579300
N	0.94869200	-0.82530800	0.01951700
C	-1.58012100	1.67075600	0.15933000
C	-3.87964400	3.19198600	0.25488600
C	-2.25490300	1.78924100	1.38082900
C	-2.01322200	2.30868000	-1.01458500
C	-3.17764000	3.07406600	-0.94005000
C	-3.42265900	2.55613900	1.40082600
H	-3.54702300	3.57592000	-1.82870600
H	-3.97813600	2.65575200	2.32909200
C	1.42304700	-2.17081000	-0.06020200
C	2.38254800	-4.75292400	-0.21162600
C	1.47107900	-2.93912800	1.11153700
C	1.82970700	-2.66441800	-1.30965800
C	2.31537600	-3.97151400	-1.35946600
C	1.95719300	-4.24426200	1.00867700
H	2.63250500	-4.38801700	-2.31063900
H	2.00049400	-4.86946300	1.89563000
C	1.65026100	-1.84889500	-2.57325200
H	1.55366400	-0.79748500	-2.28513100
C	0.95755900	-2.40778400	2.43307100
H	0.83436600	-1.32453200	2.33442600
C	-1.28794800	2.10419600	-2.32935800
H	-0.24336200	1.86760300	-2.10145800
C	-1.76516300	1.11238500	2.64389400
H	-0.79297000	0.65951200	2.42669800
C	0.33927700	-2.26333000	-3.24906000
H	-0.50113300	-2.16344600	-2.55267400
H	0.38589700	-3.30878600	-3.57514400
H	0.14090900	-1.64115100	-4.12852900
C	1.93099600	-2.65392700	3.58430800
H	1.56012400	-2.17894200	4.49848400
H	2.91973700	-2.23876900	3.36446100
H	2.05298300	-3.72085600	3.79895300
Ni	-1.78922300	-1.74783800	0.02238000
C	-1.88335000	0.89489800	-3.05621800
C	-1.56056600	2.11805500	3.77696100
C	-0.42032500	-3.00383300	2.72797900
C	2.83482100	-1.95156900	-3.53022900
C	5.50684900	1.04857100	0.15539000
C	5.39239700	2.42123400	0.23003800
C	4.10612100	3.03076000	0.25883700
C	3.01207900	2.17009500	0.20767600

C	3.12266600	0.74901100	0.13009800
C	4.37784600	0.18683500	0.10436000
H	4.62574600	5.14271500	0.37304400
H	6.49628500	0.60119100	0.13410800
H	6.28417800	3.04111400	0.26601200
C	3.81339400	4.42223300	0.33101000
C	1.65458000	2.61097600	0.22322100
H	4.52018900	-0.88815600	0.04668900
C	1.40044500	3.96099700	0.29307100
C	2.50373800	4.85518700	0.34674600
H	0.38660800	4.34969000	0.30705400
H	2.29988500	5.92056000	0.40167500
C	1.73907900	0.29801300	0.09651000
C	0.89050300	1.37443200	0.15023600
C	-2.71223200	-0.01652000	3.05102400
C	-1.28519600	3.34365600	-3.21916400
H	2.95092600	-2.96254100	-3.93514700
H	2.68670600	-1.27875800	-4.38110800
H	3.77278500	-1.67262200	-3.03924300
H	-0.36748500	-4.09523400	2.80912900
H	-0.82395600	-2.60922800	3.66634700
H	-1.14188500	-2.76872600	1.92798500
H	2.76134700	-5.76943700	-0.27128700
C	-3.48550900	-1.77683000	-0.90959800
H	-3.27756900	-1.80144500	-1.98410900
C	-3.29733300	-2.96189300	-0.16926600
H	-3.84677800	-3.11112600	0.76332100
H	-2.98522200	-3.88020200	-0.66968500
C	-4.43441000	-0.68218600	-0.49505200
H	-3.98319400	0.29689900	-0.69665700
H	-4.59444400	-0.72799800	0.58893700
H	-2.76972700	-0.76859900	2.25430700
H	-2.35741600	-0.50578700	3.96467900
H	-3.72268300	0.36162100	3.24300500
H	-1.14206300	1.61741700	4.65655400
H	-0.87089100	2.91512000	3.48063900
H	-2.50316100	2.58501500	4.08253200
H	-0.89924600	4.22059200	-2.68924000
H	-0.64914500	3.17122800	-4.09328200
H	-2.28583000	3.58459700	-3.59335900
H	-2.93385300	1.07642200	-3.31104500
H	-1.33800300	0.69521600	-3.98531700
H	-1.83706200	0.00226900	-2.42518800
H	-4.78959100	3.78443400	0.29045000

C	-5.77933700	-0.77038600	-1.21570500
H	-6.27468200	-1.72529000	-1.00857500
H	-6.45237900	0.03729900	-0.90585400
H	-5.64794200	-0.69545700	-2.30168400

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C	0.13345800	-0.12992000	-0.61640900
N	-0.10659300	-0.82502600	0.55910300
N	0.37610200	1.15659500	-0.17576600
C	-0.53925900	-2.18298500	0.60894200
C	-1.37826900	-4.83583300	0.76636800
C	0.41056800	-3.20574800	0.51100300
C	-1.90494300	-2.45704600	0.76978400
C	-2.29958800	-3.79228600	0.85125500
C	-0.02925500	-4.52514900	0.59083100
H	-3.35784900	-4.02129400	0.94149400
H	0.69710100	-5.32768000	0.49462900
C	0.60560200	2.27512400	-1.02669800
C	1.09484700	4.50710200	-2.62145600
C	1.92929000	2.61637100	-1.34070200
C	-0.47565100	3.03538600	-1.47813200
C	-0.20504800	4.14796800	-2.27814900
C	2.15391100	3.72997700	-2.14032700
H	-1.03558200	4.75355200	-2.63042800
H	3.17533400	4.00832300	-2.38472000
C	-1.90397400	2.68737100	-1.10045100
H	-1.84787700	1.85597000	-0.38875600
C	3.05409600	1.72809300	-0.84707500
H	2.72188300	1.32076300	0.11568600
C	-2.91869100	-1.32302900	0.82606600
H	-2.50732100	-0.51611200	0.21049300
C	1.88246600	-2.85428800	0.36712300
H	1.93045200	-1.96752500	-0.27759400
C	-1.83473100	-6.26543900	0.80182300
H	-2.00417100	-6.64069800	-0.21462500
Ni	0.31478200	-0.75005000	-2.39193000
H	-1.08681900	-6.91422500	1.26707900
H	-2.77420800	-6.37346100	1.35094000
C	-4.24700000	-1.70014700	0.18744700
C	-4.39216700	-1.54782700	-1.19362500
C	-5.32281900	-2.20380500	0.92198500
C	-5.57604300	-1.90558400	-1.82978500
H	-3.57131000	-1.13419500	-1.77106500
C	-6.50754900	-2.56797500	0.28604500

H	-5.24149800	-2.29665000	2.00095100
C	-6.63781100	-2.42352400	-1.09224400
H	-5.66773900	-1.76852500	-2.90352100
H	-7.33429500	-2.95765200	0.87372800
H	-7.56375800	-2.70312000	-1.58689000
C	2.45423400	-2.45532600	1.71452300
C	2.33429500	-3.28024700	2.83696700
C	3.09433300	-1.22433800	1.85949900
C	2.85915000	-2.88736500	4.06491500
H	1.81668500	-4.23192100	2.74761000
C	3.60899000	-0.82042200	3.08779400
H	3.17603600	-0.57599800	0.99349900
C	3.49624100	-1.65485800	4.19530900
H	2.75915400	-3.54135500	4.92695000
H	4.08854400	0.15030300	3.17774100
H	3.88844500	-1.34178200	5.15840100
C	1.16411800	3.93034600	3.81417700
C	1.02483200	3.11804900	4.92172000
C	0.67055600	1.74894500	4.76603300
C	0.47330000	1.30404100	3.46057500
C	0.62578900	2.13491600	2.30987500
C	0.97116700	3.45664500	2.48878900
H	0.65988700	1.06095800	6.83303100
H	1.43449800	4.97318900	3.95263900
H	1.18929100	3.52251300	5.91697600
C	0.51494300	0.77609600	5.79431800
C	0.12500500	-0.03667100	3.12059000
H	1.08968300	4.13446300	1.64883100
C	-0.01142900	-0.95466000	4.13159700
C	0.19006300	-0.52340100	5.47126300
H	-0.25898600	-1.99006300	3.92897000
H	0.08162400	-1.25523300	6.26650600
C	0.34678700	1.23614300	1.20099800
C	0.05047300	-0.01736000	1.66484000
C	2.65795400	-3.93164300	-0.36933900
C	3.70313700	-4.65800000	0.19729100
C	2.30728000	-4.18518300	-1.70095300
C	4.37837600	-5.62665200	-0.54708700
H	4.00098700	-4.46292400	1.22276800
C	2.97235400	-5.15355800	-2.44079000
H	1.51693800	-3.59161700	-2.15515100
C	4.01354500	-5.88158000	-1.86410800
H	5.19311200	-6.18175400	-0.09004200
H	2.68512300	-5.33397200	-3.47334900

H	4.53787000	-6.63805300	-2.44132500
C	-3.08781400	-0.76246000	2.22602200
C	-3.21231100	0.61761200	2.39713200
C	-3.14934500	-1.58418600	3.35297300
C	-3.37850400	1.16902200	3.66244400
H	-3.17211200	1.26794100	1.52733600
C	-3.33297000	-1.03698300	4.62055500
H	-3.03105800	-2.65861500	3.23901300
C	-3.44086500	0.34116400	4.78068900
H	-3.45654000	2.24696100	3.77239400
H	-3.37380400	-1.69031500	5.48786500
H	-3.56339000	0.76867400	5.77148900
C	-1.19650300	-1.67639200	-3.21565000
H	-2.03752400	-0.97959400	-3.22121300
C	-0.16743400	-1.46344700	-4.15846100
H	0.42320300	-2.31712900	-4.49759400
H	-0.23921300	-0.64650100	-4.88037700
C	-1.53102200	-3.06148800	-2.72298100
H	-1.91956900	-3.02021100	-1.70199800
H	-0.61947800	-3.66961200	-2.67626300
C	-2.52683000	3.85548800	-0.34978300
C	-2.28659000	3.98148200	1.02114900
C	-3.28266200	4.84067600	-0.98966500
C	-2.78008700	5.06733000	1.73718500
H	-1.69894200	3.22378300	1.53147400
C	-3.77893400	5.92797600	-0.27498200
H	-3.49879500	4.74677100	-2.05015500
C	-3.52904000	6.04678900	1.08972300
H	-2.57550400	5.14539200	2.80161700
H	-4.36710100	6.68389600	-0.78801000
H	-3.91935700	6.89480600	1.64511100
C	-2.74029900	2.18296000	-2.26743700
C	-2.18177200	1.86395900	-3.50605100
C	-4.10785600	1.95508000	-2.07399500
C	-2.97104200	1.34339400	-4.53018900
H	-1.11886400	2.00445900	-3.66973100
C	-4.89720300	1.43824900	-3.09495700
H	-4.55856400	2.18350400	-1.11203300
C	-4.33113200	1.13206300	-4.33123700
H	-2.51318400	1.09328700	-5.48294300
H	-5.95453800	1.26380500	-2.91812900
H	-4.94525500	0.72603700	-5.13004700
C	4.31990000	2.50882400	-0.55228100
C	4.48410600	3.08343400	0.71078500

C	5.31511700	2.70090600	-1.51366700
C	5.61386300	3.83920500	1.00716100
H	3.71562800	2.93541800	1.46656500
C	6.44493800	3.45988200	-1.21999500
H	5.20894700	2.24052900	-2.49210900
C	6.59780200	4.03177400	0.04035200
H	5.72781200	4.27386300	1.99637900
H	7.21106800	3.59926400	-1.97766600
H	7.48258000	4.61853500	0.27025600
C	3.28039600	0.52871000	-1.75594300
C	2.52290900	0.31018000	-2.91571800
C	4.27065000	-0.39651800	-1.41587800
C	2.79143500	-0.79388000	-3.73458500
H	1.78524500	1.04440300	-3.23458700
C	4.50694900	-1.51534500	-2.20960600
H	4.87231300	-0.23223600	-0.52630800
C	3.77761300	-1.71140900	-3.37736000
H	2.25299800	-0.90704900	-4.66670200
H	5.26618400	-2.23388600	-1.91527200
H	3.97440700	-2.57458700	-4.00505400
C	1.36782100	5.71007800	-3.47691900
H	1.97896600	6.44386700	-2.93983400
H	1.91849800	5.43437000	-4.38289700
H	0.44102300	6.20226600	-3.78212900
C	-2.55443400	-3.76043400	-3.61701400
H	-2.17588900	-3.86332700	-4.64009800
H	-2.79866800	-4.76027600	-3.23929400
H	-3.48790000	-3.18879900	-3.66521400

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C	-0.25631500	-0.76990500	-0.65866600
N	-0.71372800	0.10258200	0.31041600
N	-1.23959200	-0.73567300	-1.62289600
C	0.09950200	0.49468800	1.41620800
C	1.79350800	1.17663900	3.51621100
C	0.81902400	1.69694000	1.34232100
C	0.18532700	-0.35417400	2.52728100
C	1.02096000	0.01623600	3.57648900
C	1.68056000	2.00133000	2.39686900
H	1.10993600	-0.64157800	4.43643400
H	2.29455000	2.89497000	2.33561600
C	-1.22569400	-1.47866900	-2.84643300
C	-1.33880300	-2.79504700	-5.27083400
C	-0.47937800	-0.97210700	-3.92468900

C	-1.99321500	-2.65278600	-2.93888000
C	-2.04143900	-3.29094000	-4.18106100
C	-0.55341600	-1.65615000	-5.13881500
H	-2.62490600	-4.19970400	-4.28955600
H	0.01277400	-1.29577800	-5.99131500
C	-2.71922400	-3.24466300	-1.74303900
H	-2.20074600	-2.87690600	-0.85081800
C	0.36377800	0.28071800	-3.77451200
H	0.76345800	0.26743400	-2.75379500
C	-0.64795200	-1.62515600	2.55696900
H	-0.59624600	-2.03753100	1.54023000
C	0.60414700	2.64625600	0.17433000
H	0.26668100	2.03733600	-0.66965500
C	2.78488100	1.48893400	4.59754300
H	3.73458500	0.98403400	4.38755900
C	-2.66492700	-4.77403200	-1.71824500
H	-1.65579000	-5.16017700	-1.87919500
H	-3.32321100	-5.21229800	-2.47646100
H	-3.01249100	-5.13750700	-0.74559600
C	-0.48862400	1.54291400	-3.94020500
H	0.12220600	2.44029600	-3.79009700
H	-1.32143100	1.57516300	-3.23275100
H	-0.90975400	1.59065800	-4.95091400
Ni	1.17354100	-1.99886200	-0.53909700
H	2.99035000	2.56114000	4.66110100
H	2.43699200	1.14395500	5.57542900
C	-0.05642300	-2.69163800	3.46187000
C	1.19504700	-3.21903300	3.12020600
C	-0.69923500	-3.17595600	4.59972500
C	1.78971300	-4.20300500	3.89882400
H	1.69968600	-2.84053600	2.23510600
C	-0.10311500	-4.16468700	5.38298900
H	-1.67444700	-2.78540100	4.87329800
C	1.14061100	-4.68069000	5.03733700
H	2.76063400	-4.60095400	3.61606100
H	-0.61913200	-4.53213300	6.26583800
H	1.60252100	-5.45188100	5.64727600
C	-0.50544300	3.65270500	0.45329700
C	-0.71614100	4.20501800	1.71720200
C	-1.31005700	4.07723300	-0.60703300
C	-1.70373400	5.16820700	1.91386700
H	-0.11865100	3.86673700	2.55916300
C	-2.30395900	5.02815900	-0.41104100
H	-1.15851600	3.64822000	-1.59435100

C	-2.50203500	5.58116400	0.85213700
H	-1.85465300	5.58796100	2.90482200
H	-2.93236800	5.32971700	-1.24402500
H	-3.28122100	6.32153200	1.00830000
C	1.55525100	0.32311900	-4.72735500
C	-4.18266800	-2.80056400	-1.66763300
C	-5.54696800	1.31576300	-2.84805200
C	-5.97434500	2.06695600	-1.77169500
C	-5.17496200	2.15694400	-0.59878200
C	-3.96768900	1.46092200	-0.61604900
C	-3.53144900	0.66262500	-1.71463200
C	-4.32297500	0.59651600	-2.83961200
H	-6.40089000	3.43625000	0.66759400
H	-6.16946500	1.26177400	-3.73646800
H	-6.92431500	2.59281600	-1.81811000
C	-5.47261300	2.87616300	0.59305300
C	-3.03495000	1.46041200	0.46274100
H	-4.03610500	0.00460000	-3.70361600
C	-3.35266800	2.15512600	1.60342700
C	-4.58627400	2.85882500	1.64808700
H	-2.68689100	2.18079000	2.45726600
H	-4.82685500	3.41152100	2.55142000
C	-2.26054600	0.11703500	-1.25849000
C	-1.94670400	0.62024900	-0.02263400
C	3.81040800	-0.52020400	-1.45622100
C	4.64297400	0.58557200	-1.51839300
C	5.03979300	1.20421500	-0.33799800
C	4.60558400	0.71538500	0.88782500
C	3.79789100	-0.41258500	0.91851100
C	3.37044000	-1.03100400	-0.24545100
C	1.84051000	3.38213800	-0.31627800
C	2.34998000	4.50724600	0.33920700
C	2.44410300	2.97868400	-1.50889400
C	3.44980000	5.19045700	-0.16973000
H	1.85897200	4.87484600	1.23557200
C	3.52977600	3.67447700	-2.03461700
H	2.05005300	2.11141800	-2.03344500
C	4.04197300	4.77840900	-1.36050500
H	3.83303200	6.05981500	0.35707300
H	3.98271800	3.34457600	-2.96381700
H	4.89322800	5.31839500	-1.76442200
C	-2.10314000	-1.30177200	2.83469900
C	-3.10578500	-1.85990200	2.03989600
C	-2.47308700	-0.44653700	3.87662800

C	-4.44632000	-1.56378500	2.26799800
H	-2.82672100	-2.52592100	1.22791400
C	-3.81397300	-0.16124300	4.11836100
H	-1.70141200	0.00559200	4.49445800
C	-4.80471000	-0.71398900	3.31036800
H	-5.21016200	-1.99051700	1.62431100
H	-4.08494700	0.50550900	4.93247200
H	-5.84947800	-0.47501400	3.48589800
H	-4.71714800	-3.07697500	-2.58390300
H	-4.68316800	-3.29966000	-0.83024400
H	-4.28758500	-1.72448500	-1.52816100
H	1.24275500	0.49629400	-5.76318400
H	2.22142200	1.14769600	-4.45330900
H	2.13678100	-0.60106900	-4.69165600
F	5.82934900	2.26889400	-0.38321900
F	5.05218600	1.06711900	-2.69253200
F	3.44098100	-1.10047900	-2.60167300
F	4.98504100	1.31874200	2.01377300
H	-1.38877900	-3.30960200	-6.22637000
F	3.46443700	-0.91910000	2.10594100
H	2.90435900	-2.06032300	-0.19749400
C	1.91372800	-3.86491800	-0.52398100
H	2.30282900	-4.18055100	0.44880200
C	0.51075100	-3.80663100	-0.67801800
H	0.08725500	-3.94246800	-1.67286300
H	-0.15071500	-4.07506900	0.14562900
C	2.80730600	-4.20685900	-1.69609500
H	3.79830500	-3.74673100	-1.57511400
H	2.38125300	-3.77605000	-2.61137900
C	2.98057600	-5.71385600	-1.87695900
H	3.63487800	-5.94770200	-2.72484300
H	3.41804600	-6.16907200	-0.98082500
H	2.01241800	-6.19561400	-2.05109100

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C	0.62196000	-0.36336300	-0.18185500
N	0.35350900	0.97279000	-0.39525400
N	1.93896800	-0.37878400	0.21080200
C	-0.93768000	1.47890600	-0.74176400
C	-3.41890100	2.49008600	-1.41390300
C	-1.62566200	2.25802100	0.20272800
C	-1.46851700	1.17755600	-2.01069400
C	-2.71809800	1.70914200	-2.32681500
C	-2.88109700	2.75288200	-0.16261100

H	-3.16076200	1.49206300	-3.29191500
H	-3.44500500	3.34610600	0.55139000
C	2.67881600	-1.57021500	0.48434100
C	4.11370000	-3.86206800	1.00887700
C	2.69550800	-2.06168900	1.79770400
C	3.37695700	-2.17647900	-0.56901900
C	4.08877300	-3.34265800	-0.27944900
C	3.42881200	-3.22526900	2.03777700
H	4.62916300	-3.84945600	-1.07353800
H	3.45869800	-3.64213400	3.03968400
C	3.33955400	-1.61694200	-1.97746900
H	2.92779800	-0.60429600	-1.92445000
C	1.89194300	-1.39460400	2.89521000
H	1.71680100	-0.35651700	2.59225400
C	-0.70577000	0.32057900	-3.00514700
C	-1.08434700	2.53829600	1.59443200
H	-0.03885200	2.22124800	1.62793300
Ni	-0.42530100	-1.81132700	-0.82011700
C	5.91671500	2.43673100	0.92338700
C	5.56967100	3.73666200	0.61899500
C	4.24290600	4.04420200	0.20499800
C	3.35134700	2.97561000	0.13968100
C	3.70506300	1.62760600	0.44670600
C	4.99505500	1.35818600	0.84095300
H	4.37775200	6.19168600	-0.12964500
H	6.93408000	2.22059200	1.23605900
H	6.30944100	4.52923300	0.69160600
C	3.72955700	5.32015900	-0.16154700
C	1.98790600	3.10359600	-0.26267200
H	5.31806100	0.35096300	1.08629100
C	1.52285200	4.34610900	-0.62635800
C	2.41652800	5.44928600	-0.56437900
H	0.50052000	4.49552000	-0.95992700
H	2.04418500	6.42907700	-0.84865200
C	2.47264600	0.88902900	0.21498000
C	1.47570800	1.74256400	-0.18145200
C	-3.68023000	-0.92560200	1.34991200
C	-4.68864300	-0.17874800	1.94374400
C	-5.66508800	0.39907800	1.14172600
C	-5.63434700	0.22224600	-0.23542500
C	-4.61376200	-0.53145500	-0.79940600
C	-3.62080800	-1.09697900	-0.02096700
F	-6.62682700	1.13301700	1.69446500
F	-4.71422000	0.01151300	3.26155500

F	-2.74370300	-1.46421000	2.13573900
F	-6.56237800	0.79635600	-0.99962300
F	-4.60203100	-0.68468700	-2.12588200
H	-2.78041900	-1.62593000	-0.46975000
C	-0.73834400	-3.64435300	-0.27374600
H	-1.39878700	-3.61693300	0.59943400
C	-1.30229400	-3.39655800	-1.54340600
H	-0.79174900	-3.76814000	-2.43528800
H	-2.38085600	-3.28908900	-1.66748300
C	0.50951900	-4.46317000	-0.07654100
H	1.11827700	-4.03175700	0.72558900
H	1.12221700	-4.42083100	-0.98432300
C	0.19789600	-5.92116100	0.26055600
H	1.11680700	-6.50046500	0.40634800
H	-0.39203200	-5.99445100	1.18176200
H	-0.38023600	-6.39472900	-0.54047200
H	-0.24062100	-0.51289000	-2.44412300
H	-4.40032900	2.87578000	-1.67559700
H	4.67261100	-4.77076800	1.21425800
C	-1.12007400	4.02719100	1.94012100
H	-2.14618400	4.40515600	2.00385500
H	-0.64997700	4.19555300	2.91447300
H	-0.58279100	4.62931100	1.20231800
C	-1.83471600	1.72362400	2.64939600
H	-1.41641000	1.91665600	3.64332800
H	-2.89612300	1.99168100	2.67978100
H	-1.75774000	0.65217700	2.45568600
C	2.62525900	-1.36136500	4.23377300
H	2.75010300	-2.36287600	4.65897700
H	3.61700900	-0.90721100	4.13897400
H	2.05196100	-0.77406500	4.95827500
C	0.52404200	-2.07153800	3.02197800
H	0.63761300	-3.12009200	3.32125300
H	-0.08643400	-1.56736000	3.77915000
H	-0.01311800	-2.04347700	2.06905100
C	4.73304000	-1.50782500	-2.59413300
H	5.19303700	-2.49044400	-2.74374400
H	4.67281500	-1.02370600	-3.57443500
H	5.40283100	-0.91309900	-1.96486700
C	2.39773800	-2.44207700	-2.85553600
H	2.74651300	-3.47709400	-2.94696900
H	1.38824300	-2.45670700	-2.42325100
H	2.33711200	-2.01596000	-3.86331700
C	0.43352600	1.11250100	-3.65102100

H	1.00933200	0.47234100	-4.32780000
H	0.03379800	1.94940100	-4.23522800
H	1.12210000	1.52338300	-2.90748000
C	-1.59155500	-0.32444400	-4.06407700
H	-1.00505300	-1.04887900	-4.63746100
H	-2.43314100	-0.85567300	-3.61102900
H	-1.98711500	0.41060300	-4.77433600

TS4-L7

C	0.27772000	0.28661200	0.30823300
N	0.58519200	-1.04487800	0.46224100
N	1.42459500	0.84032900	-0.21596600
C	-0.30705400	-2.04899700	0.95282900
C	-1.97773900	-4.02449300	1.90752100
C	-0.85024100	-2.96588900	0.03973100
C	-0.56278600	-2.10446300	2.33229300
C	-1.40387900	-3.11781300	2.79044500
C	-1.70449800	-3.94736500	0.54862200
H	-1.62673000	-3.18924300	3.85015200
H	-2.16167300	-4.65888200	-0.13309700
C	1.64734800	2.23933900	-0.42773800
C	2.18384900	4.90912900	-0.87328900
C	1.17063200	2.83130500	-1.60924200
C	2.36603300	2.95315600	0.54689900
C	2.63148000	4.30078300	0.29118100
C	1.45345700	4.18388700	-1.80751900
H	3.18489100	4.88202400	1.02249400
H	1.09553100	4.67807300	-2.70421600
C	2.83870200	2.31619200	1.84204700
H	2.26708700	1.39252300	1.98292500
C	0.39146200	2.02510400	-2.63118800
H	-0.27381900	1.35885600	-2.07075200
C	0.08505400	-1.12451900	3.28991800
H	0.29661000	-0.21197700	2.72490500
C	-0.56178200	-2.91212900	-1.44934300
H	0.22254900	-2.16901900	-1.61993500
C	2.58629600	3.20406200	3.06257000
H	1.55476500	3.56001700	3.11011400
H	3.24719800	4.07753900	3.07118500
H	2.79242600	2.63818400	3.97723100
C	1.32621800	1.16178800	-3.48461100
H	0.74534800	0.56666500	-4.19756000
H	1.92151900	0.47083200	-2.88302400
H	2.01814100	1.79110600	-4.05611700

Ni	-1.30954700	1.17899500	0.79574000
C	-0.83109100	-0.72206500	4.44199100
C	-0.05019400	-4.25093200	-1.98178700
C	-0.48470900	2.88759200	-3.53436900
C	4.32530100	1.95510200	1.77678700
C	5.91822100	-0.26313300	-1.93120400
C	6.13384800	-1.60690600	-1.70604700
C	5.13050900	-2.39600200	-1.07657400
C	3.95691200	-1.73575800	-0.71902800
C	3.73302300	-0.34253900	-0.93255400
C	4.71827600	0.39476400	-1.54859800
H	6.07964100	-4.35553700	-1.03403800
H	6.69284600	0.32282200	-2.41696800
H	7.06924600	-2.06744600	-2.01194500
C	5.18990500	-3.78673000	-0.77812600
C	2.84276800	-2.37796600	-0.10187100
H	4.59825300	1.45655400	-1.74101800
C	2.93056700	-3.72061300	0.18441900
C	4.12300800	-4.41051300	-0.16555000
H	2.11724700	-4.25436600	0.66669000
H	4.18780300	-5.47108800	0.05894500
C	2.39805400	-0.12078200	-0.39092500
C	1.87492300	-1.30253400	0.05909000
C	-3.36575700	0.81837600	-1.35390000
C	-4.34266200	0.14030400	-2.06941800
C	-4.96165000	-0.96027900	-1.48899500
C	-4.60672800	-1.35317800	-0.20399900
C	-3.63572000	-0.63429600	0.47708000
C	-2.95594500	0.44360000	-0.07994400
C	-1.79550700	-2.45487100	-2.22640600
C	1.41482500	-1.68257700	3.80385800
H	4.93318800	2.85505300	1.62817100
H	4.64397400	1.48647100	2.71412100
H	4.54696300	1.26217900	0.96331800
H	0.11437900	3.48618600	-4.23017400
H	-1.13690600	2.24731800	-4.13487400
H	-1.12217500	3.56405500	-2.95861800
F	-5.89566100	-1.63335600	-2.15963200
F	-4.69242200	0.52367800	-3.29972900
F	-2.80735700	1.89124200	-1.94147600
F	-5.20557600	-2.40846800	0.35229900
H	2.39597000	5.95968400	-1.05132600
F	-3.36911400	-1.00122000	1.73941200
H	-2.76848100	1.51514300	0.83965900

C	-2.13003200	2.71294900	1.85625900
H	-2.81617600	2.40223700	2.64907400
C	-0.74170000	2.53265900	2.08910100
H	-0.04459800	3.22421500	1.62131400
H	-0.40305600	2.08374600	3.02081600
C	-2.61195300	3.88740100	1.02732000
H	-3.58788000	3.66454100	0.57678000
H	-1.91421000	4.04149400	0.19492900
H	2.09611700	-1.92237900	2.98120700
H	1.91366400	-0.95424500	4.45294300
H	1.25569600	-2.59894900	4.38385800
H	-1.79518200	-0.36166500	4.07062600
H	-1.01926200	-1.55064500	5.13350600
H	-0.36655600	0.08125700	5.02353300
H	0.21260300	-4.15711800	-3.04061700
H	0.84097400	-4.58669700	-1.44452000
H	-0.81089900	-5.03492900	-1.90129800
H	-2.12113600	-1.46958900	-1.88945400
H	-1.57191000	-2.39323000	-3.29706100
H	-2.62919900	-3.15368700	-2.09708100
H	-2.64495200	-4.79570900	2.28175800
C	-2.71380600	5.16406000	1.85616400
H	-3.06854000	6.00505300	1.25059000
H	-3.41040100	5.03676000	2.69262300
H	-1.73864100	5.43397600	2.27492800

TS4-L8

C	0.13983500	0.28289900	-0.37819400
N	0.26934900	0.58914600	0.96443400
N	0.87468900	-0.87968500	-0.52511000
C	-0.54041300	1.55276900	1.64810800
C	-2.20177400	3.39684700	2.92217900
C	-1.73654300	1.10852000	2.23548700
C	-0.13412400	2.88794500	1.73953900
C	-0.96829300	3.78668500	2.40511100
C	-2.56967500	2.05483100	2.82600600
H	-0.66973700	4.82947600	2.46546100
H	-3.53690700	1.73658800	3.20713700
C	1.06052300	-1.65102700	-1.72010700
C	1.55185200	-3.30963700	-3.92420900
C	0.17494300	-2.70377100	-2.00568500
C	2.20380500	-1.43173300	-2.50869700
C	2.42812400	-2.27755100	-3.59501400
C	0.43049400	-3.50118500	-3.12146200

H	3.30488300	-2.11129200	-4.21410100
H	-0.27064900	-4.29648900	-3.36008400
C	3.21790500	-0.36011600	-2.14492200
H	2.66795200	0.42025500	-1.60506100
C	-1.01532300	-3.03711400	-1.12374600
H	-1.26441700	-2.13258400	-0.55691800
C	1.18242900	3.34187900	1.13855700
H	1.35169300	2.70581600	0.26190500
C	-2.06662200	-0.37183700	2.30855300
H	-1.45518600	-0.87873800	1.55687000
C	-3.15128300	4.40172100	3.50332800
H	-3.94057300	4.62690300	2.77626700
Ni	-0.61087400	1.46470800	-1.66596800
H	-3.64016400	4.02338800	4.40648800
H	-2.64660000	5.33940000	3.75033300
C	1.10930500	4.77064100	0.61521300
C	0.14109900	5.07672800	-0.34889000
C	1.96811500	5.78164000	1.04411400
C	0.04117900	6.35715000	-0.87717000
H	-0.54907900	4.30039800	-0.66430200
C	1.86772200	7.06878600	0.51546000
H	2.72275700	5.56548100	1.79366600
C	0.90863600	7.36105100	-0.44728600
H	-0.71784600	6.57437000	-1.62407100
H	2.54584100	7.84385700	0.86191100
H	0.83274900	8.36347100	-0.85890100
C	-1.64912500	-0.95742600	3.65401800
C	-1.83623500	-0.29001000	4.86705500
C	-1.04901200	-2.21801600	3.67972400
C	-1.45143900	-0.87776600	6.07042700
H	-2.26439800	0.70739200	4.87625500
C	-0.66172300	-2.80772300	4.87699200
H	-0.86303400	-2.73892100	2.74707500
C	-0.86453200	-2.13952200	6.08135400
H	-1.60547100	-0.33996200	7.00210200
H	-0.18262300	-3.78253600	4.86016000
H	-0.55533700	-2.59205400	7.01925700
C	3.69325400	-4.12831500	1.88030600
C	3.78091700	-3.71879100	3.19415800
C	3.11086100	-2.53856900	3.62031000
C	2.37968700	-1.85590400	2.64896500
C	2.27990600	-2.27941700	1.29080100
C	2.94665100	-3.41660900	0.90483500
H	3.65841600	-2.46287600	5.72561100

H	4.21883600	-5.02640500	1.56910700
H	4.36608200	-4.29376700	3.90704900
C	3.10776700	-1.97444900	4.92594400
C	1.65564600	-0.65444100	2.90325300
H	2.92820000	-3.76711100	-0.12030100
C	1.66692200	-0.13379000	4.17492500
C	2.40651500	-0.81326000	5.17721800
H	1.11794600	0.76568100	4.42630900
H	2.40756300	-0.40047200	6.18167500
C	1.43804500	-1.26119000	0.67754300
C	1.06785000	-0.33077800	1.61043200
C	-3.52037300	1.03329500	-2.61818200
C	-4.88907700	0.95108900	-2.40754600
C	-5.44842200	1.60915600	-1.31956100
C	-4.63750000	2.37019300	-0.48878900
C	-3.27773400	2.42956500	-0.75204800
C	-2.65984000	1.71374600	-1.76864000
C	-3.50683300	-0.69307100	1.94067400
C	-4.52369200	-0.80846700	2.89022500
C	-3.82027600	-0.90568800	0.59435400
C	-5.82546400	-1.11444800	2.49956800
H	-4.29224400	-0.68140400	3.94388000
C	-5.11346600	-1.23952100	0.20473300
H	-3.04169600	-0.80303600	-0.15721100
C	-6.12412300	-1.33542000	1.15821300
H	-6.60579400	-1.19606700	3.25128100
H	-5.32725600	-1.42640800	-0.84368100
H	-7.13618300	-1.58955800	0.85704600
C	2.35852900	3.11324400	2.06859900
C	3.61816600	2.86266900	1.51702200
C	2.24208000	3.19423600	3.45661100
C	4.73048900	2.67166300	2.33056900
H	3.72600200	2.82656600	0.43527000
C	3.35386000	3.00606200	4.27476700
H	1.27103000	3.39690000	3.89972200
C	4.59966700	2.73728600	3.71619900
H	5.69783900	2.46791300	1.88008700
H	3.24254600	3.06336800	5.35406100
H	5.46406800	2.58209200	4.35524000
F	-6.75416600	1.51500100	-1.08408000
F	-5.67664800	0.23630400	-3.21826400
F	-3.02909000	0.42939400	-3.71912400
F	-5.17051500	3.02699600	0.54408500
F	-2.54655300	3.24453400	0.01963700

H	-1.57106900	2.34753800	-2.45682000
C	-0.21537700	2.82881600	-3.14673000
H	-0.48049600	3.86882300	-2.93636100
C	0.94168600	2.31900200	-2.48946400
H	1.55531000	1.60907600	-3.03424000
H	1.49298000	2.96743600	-1.81095100
C	-0.52686500	2.38567400	-4.56330500
H	-1.59551300	2.50765800	-4.77902200
H	-0.31819700	1.31248200	-4.65439600
C	-2.24188100	-3.36818300	-1.96682900
C	-2.81199700	-4.63988500	-2.02252700
C	-2.80615300	-2.34441700	-2.72848300
C	-3.93449800	-4.87439300	-2.81621200
H	-2.38776700	-5.44949400	-1.43728700
C	-3.92819900	-2.57204100	-3.51598600
H	-2.34591200	-1.36361300	-2.70646700
C	-4.49974400	-3.84325700	-3.55859700
H	-4.36942300	-5.86967600	-2.84652100
H	-4.35741000	-1.75415500	-4.08468400
H	-5.37961300	-4.02661000	-4.16880100
C	-0.73807700	-4.12852900	-0.10346900
C	0.30218500	-5.04862200	-0.22303300
C	-1.62823900	-4.26147300	0.96813900
C	0.46446700	-6.06475000	0.71749800
H	0.99364900	-4.97267100	-1.05625400
C	-1.47190700	-5.27663700	1.90501500
H	-2.46010300	-3.56620500	1.05746100
C	-0.41825100	-6.18109300	1.78545900
H	1.28904700	-6.76451600	0.61346500
H	-2.16977600	-5.35338800	2.73395000
H	-0.28975800	-6.97171100	2.51913600
C	3.86891200	0.32431500	-3.34542800
C	3.17421700	0.52015000	-4.54536600
C	5.15648500	0.85801400	-3.23829100
C	3.75021300	1.21825600	-5.60274800
H	2.17202900	0.11819900	-4.65970200
C	5.73269800	1.56087800	-4.29288600
H	5.71621200	0.72143000	-2.31836300
C	5.03389100	1.74288100	-5.48187300
H	3.18882500	1.35142800	-6.52328100
H	6.73513500	1.96487500	-4.18175300
H	5.48446000	2.28705900	-6.30685100
C	4.24986100	-0.91114300	-1.17248600
C	5.05596700	-2.00289500	-1.50698500

C	4.42070800	-0.31202400	0.07421200
C	6.00500400	-2.48204500	-0.61043100
H	4.93994200	-2.48112700	-2.47545600
C	5.36599300	-0.79084100	0.97759000
H	3.79014900	0.52555000	0.35486800
C	6.16210800	-1.87864300	0.63666500
H	6.62278200	-3.33297400	-0.88444800
H	5.46017400	-0.31882600	1.95112400
H	6.89377700	-2.26335600	1.34111600
C	1.79472100	-4.17237100	-5.12770900
H	1.41451800	-5.18663800	-4.97631300
H	1.28469500	-3.76209900	-6.00745900
H	2.86000300	-4.23528300	-5.36721400
C	0.29525900	3.16330300	-5.58593900
H	0.07544000	2.83333800	-6.60737000
H	0.08078900	4.23653300	-5.52852800
H	1.36656600	3.03051300	-5.40428800

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C	0.24302600	0.28000700	0.27914600
N	0.43790700	-1.07300400	0.40265900
N	1.42403300	0.75572700	-0.24627400
C	-0.50217100	-2.03622300	0.89135800
C	-2.17735500	-4.01186900	1.84157300
C	-1.12894700	-2.88627600	-0.03514500
C	-0.68786000	-2.15156100	2.27641600
C	-1.53775000	-3.16037400	2.73170800
C	-1.97575600	-3.87239800	0.47437800
H	-1.70393800	-3.27447100	3.79909300
H	-2.48501800	-4.54020200	-0.21446000
C	1.79981700	2.12766000	-0.43428200
C	2.65380700	4.71983500	-0.84649100
C	1.41640800	2.78055200	-1.61658600
C	2.59554200	2.73953800	0.55173800
C	3.01876100	4.04889700	0.31278200
C	1.85566000	4.09403100	-1.79583900
H	3.63230300	4.55249800	1.05344800
H	1.56949900	4.63320800	-2.69235300
C	2.98515300	2.04387600	1.84497800
H	2.31434400	1.18763700	1.97474600
C	0.58960300	2.07529700	-2.67376300
H	-0.11766300	1.42222500	-2.15405000
C	0.00480700	-1.24024300	3.26901400
H	0.54004100	-0.47161800	2.70430700

C	-0.92410000	-2.77499900	-1.53510300
H	-0.28665700	-1.90687400	-1.73069600
C	2.82524400	2.94823500	3.07000100
H	1.84110100	3.42031200	3.11287600
H	3.58304900	3.73867800	3.08791400
H	2.95761300	2.35738600	3.98245100
C	1.48015200	1.20362900	-3.56570900
H	0.87265100	0.68586300	-4.31556400
H	2.02344000	0.44508600	-2.99633300
H	2.21746600	1.81848600	-4.09473700
Ni	-1.27466400	1.22315700	0.78150900
C	-1.00803700	-0.52170900	4.16065000
C	-0.22360800	-4.01317500	-2.09958800
C	-0.22977800	3.03446100	-3.53179600
C	4.42480400	1.52477300	1.79122700
C	5.84397200	-0.64847700	-1.91958600
C	5.97078500	-2.00143000	-1.68123400
C	4.90705600	-2.72283400	-1.07062800
C	3.76652000	-1.99009800	-0.74765700
C	3.63613200	-0.58729900	-0.97272800
C	4.67910700	0.08479200	-1.56796700
H	5.74125200	-4.73176900	-0.97729500
H	6.66459300	-0.11470400	-2.38958600
H	6.88377900	-2.52038100	-1.96003600
C	4.88023700	-4.10922000	-0.74994100
C	2.60428300	-2.55726300	-0.14628200
H	4.63125300	1.15139100	-1.76481000
C	2.61012000	-3.89748100	0.16469200
C	3.76778000	-4.66006600	-0.14853300
H	1.75726600	-4.37684300	0.63562000
H	3.76706900	-5.71830000	0.09515700
C	2.30929700	-0.27995300	-0.45437100
C	1.70013700	-1.42326800	-0.01706900
C	-3.22412600	0.88528800	-1.43379900
C	-4.38743800	0.44374300	-2.05399600
C	-5.18926200	-0.47932400	-1.39545700
C	-4.82093300	-0.92390800	-0.13193000
C	-3.65202700	-0.43508400	0.43756800
C	-2.79855100	0.45956600	-0.18806000
C	-2.24805600	-2.54324100	-2.26201600
C	1.03138100	-2.01186100	4.10004400
H	5.12606500	2.35526800	1.65067900
H	4.68247200	1.02506600	2.73118900
H	4.58024400	0.81357300	0.97876100

H	0.40481000	3.63286500	-4.19513200
H	-0.91682700	2.46539000	-4.16376500
H	-0.82840600	3.71490300	-2.91964400
F	-6.31003700	-0.92691300	-1.96649800
F	-4.74945700	0.89008900	-3.26261800
F	-2.50366900	1.80600200	-2.11491300
F	-5.60171500	-1.79878300	0.51206000
H	2.98820200	5.74057900	-1.00933300
F	-3.38072700	-0.85764900	1.69162900
H	-2.51906000	2.19364300	1.38052400
C	-1.82192700	2.92191400	1.99304600
H	-2.32374900	2.86349800	2.96585700
C	-0.43395000	2.39873200	2.00265800
H	0.30704400	3.05687100	1.55517500
H	-0.08739400	1.93744400	2.92706500
C	-2.02019100	4.27650400	1.31629400
H	-3.08751600	4.44486800	1.12828300
H	-1.52975400	4.24820800	0.33512000
H	1.78246900	-2.49133700	3.46416700
H	1.55197400	-1.33748800	4.78872900
H	0.55135600	-2.79415300	4.69826100
H	-1.74040200	0.02307800	3.55877100
H	-1.55507300	-1.22597900	4.79649400
H	-0.49855200	0.19012300	4.81944500
H	-0.07059000	-3.90049800	-3.17818600
H	0.75285200	-4.17928300	-1.63889400
H	-0.82969600	-4.91263000	-1.94329200
H	-2.75604700	-1.66016200	-1.87655600
H	-2.06941800	-2.39667600	-3.33256100
H	-2.92252600	-3.39945600	-2.15346500
H	-2.84097400	-4.78692600	2.21414800
C	-1.45291400	5.41998100	2.14436800
H	-1.61066800	6.38312000	1.64861400
H	-1.92982000	5.46958000	3.13000800
H	-0.37612900	5.29668000	2.30146800

int5-L8

C	0.02481100	0.41347100	-0.03519500
N	0.29387500	-0.14154100	1.20061900
N	0.97356200	-0.13699100	-0.87159500
C	-0.61480600	-0.17853300	2.30991200
C	-2.38384400	-0.32711400	4.45977800
C	-1.42707400	-1.31348400	2.44878500
C	-0.65212200	0.86773700	3.23524900

C	-1.52892800	0.76481900	4.31290000
C	-2.32487500	-1.34838400	3.51414600
H	-1.57455400	1.57908600	5.03067900
H	-3.01735100	-2.18323300	3.58544000
C	1.11400900	-0.01573500	-2.29436900
C	1.66033300	-0.08611100	-5.03883000
C	0.34815100	-0.84841900	-3.12905900
C	2.14372900	0.78969300	-2.81285700
C	2.39584800	0.73159500	-4.18392200
C	0.63554300	-0.85492400	-4.49342100
H	3.17103300	1.36823800	-4.60073200
H	0.03492700	-1.48408300	-5.14458700
C	2.98134800	1.69544600	-1.92434800
H	2.40880300	1.84204700	-1.00324800
C	-0.75731300	-1.75957400	-2.61450000
H	-1.08056600	-1.36776000	-1.64223100
C	0.26209800	2.06372400	3.06539800
H	0.37285600	2.20307800	1.98441500
C	-1.33361000	-2.48156200	1.48367300
H	-0.78765000	-2.13487800	0.60116600
C	-3.38959800	-0.36871900	5.57215000
H	-4.33861600	0.06968500	5.24092100
Ni	-1.10245800	1.90733200	-0.23299300
H	-3.59746600	-1.39430000	5.89050600
H	-3.05075500	0.20097600	6.44203100
C	-0.36238700	3.35236700	3.57822800
C	-1.65158900	3.68958000	3.14324900
C	0.31149800	4.23324600	4.42210400
C	-2.24440700	4.88262400	3.53700600
H	-2.19643500	2.99407600	2.50928300
C	-0.28381600	5.43119100	4.81801800
H	1.30924200	3.98552100	4.77093400
C	-1.55969000	5.76181700	4.37615100
H	-3.24530000	5.12508600	3.19028100
H	0.25676100	6.10586100	5.47619000
H	-2.02221800	6.69483000	4.68523300
C	-0.51581800	-3.63533800	2.04456600
C	-0.65438800	-4.09854800	3.35551900
C	0.41831000	-4.25995100	1.21503600
C	0.11292400	-5.16447400	3.81910400
H	-1.35234400	-3.61466700	4.03090400
C	1.18749900	-5.32300900	1.67505600
H	0.55777800	-3.89828800	0.20115400
C	1.03667500	-5.78146500	2.98038400

H	-0.00887700	-5.50766500	4.84297300
H	1.91502100	-5.77924200	1.01049700
H	1.64229200	-6.60616700	3.34553700
C	4.84264500	-3.18534700	-1.00482600
C	5.06462700	-3.63912500	0.27941500
C	4.22755100	-3.20701600	1.34431800
C	3.19859700	-2.32848300	1.00704500
C	2.96215100	-1.85988600	-0.31830200
C	3.79202000	-2.28783200	-1.32713200
H	5.09679000	-4.26147600	3.03851800
H	5.49913900	-3.51513900	-1.80460000
H	5.88344400	-4.32459100	0.48137500
C	4.31839200	-3.57544000	2.71529800
C	2.26776600	-1.80266400	1.95000300
H	3.67584400	-1.93732800	-2.34700100
C	2.37858000	-2.17472200	3.26774400
C	3.41976300	-3.06861000	3.63077300
H	1.68941900	-1.81133500	4.02131000
H	3.49956200	-3.36699700	4.67181800
C	1.81538300	-0.97489700	-0.16491400
C	1.40226500	-0.95871900	1.13807400
C	-3.67537100	1.97640200	-1.49565500
C	-5.04244500	1.95120700	-1.72973300
C	-5.88611500	1.54048400	-0.70633900
C	-5.33955900	1.19083200	0.52077700
C	-3.95953800	1.23794200	0.68710000
C	-3.06714500	1.59478200	-0.31009100
C	-2.70251300	-2.88495800	0.95701000
C	-3.31023900	-4.10475800	1.24603900
C	-3.34593600	-1.99710600	0.08832500
C	-4.53875100	-4.43212300	0.67092600
H	-2.81141900	-4.81176100	1.90201200
C	-4.56483700	-2.32386800	-0.49165000
H	-2.87441200	-1.04613400	-0.14443100
C	-5.16655500	-3.54834000	-0.20110100
H	-4.99968000	-5.38910700	0.90038500
H	-5.03367000	-1.62925000	-1.18238600
H	-6.11669600	-3.81145200	-0.65697600
C	1.65444800	1.78649900	3.60157700
C	2.76765500	2.28036700	2.91624200
C	1.86363100	1.05483500	4.77265000
C	4.05864700	2.03609000	3.37629500
H	2.62083300	2.86662900	2.01210000
C	3.15317800	0.80993800	5.23715800

H	1.00872900	0.66144800	5.31556400
C	4.25552700	1.29376500	4.53774800
H	4.90954800	2.42153100	2.82141200
H	3.29658100	0.23180000	6.14582300
H	5.26141200	1.09399200	4.89540900
F	-7.20639100	1.50364700	-0.89393000
F	-5.55910400	2.31356200	-2.91201000
F	-2.90630700	2.42518900	-2.52352700
F	-6.14685500	0.81946700	1.51941900
F	-3.51286300	0.92186800	1.91748300
H	-1.77831600	3.47177100	-0.15862800
C	-0.77431000	4.06952600	-0.24756100
H	-0.76632200	4.58962200	0.71544100
C	0.34899600	3.11125400	-0.39579600
H	0.75790300	3.06552400	-1.40452000
H	1.13155500	3.14555200	0.36064700
C	-1.02000800	5.02712600	-1.41156600
H	-2.03236000	5.44412500	-1.34476700
H	-0.97609700	4.46153600	-2.34944800
C	-1.97248100	-1.66063200	-3.53030100
C	-2.36539000	-2.67680800	-4.40172500
C	-2.69790700	-0.46919600	-3.51788600
C	-3.47606500	-2.50586000	-5.22724700
H	-1.81332200	-3.61105400	-4.42922500
C	-3.80756600	-0.29546300	-4.33573100
H	-2.37200500	0.33091500	-2.86493800
C	-4.20393600	-1.32070400	-5.19306000
H	-3.77330200	-3.30852600	-5.89668600
H	-4.36251900	0.63691500	-4.29572700
H	-5.07385900	-1.19418700	-5.83133400
C	-0.31792100	-3.19741000	-2.38358300
C	0.96892900	-3.65320100	-2.66384900
C	-1.25221400	-4.10939400	-1.87164300
C	1.32316300	-4.98248100	-2.43116000
H	1.70466000	-2.96739300	-3.06815700
C	-0.90590800	-5.43620500	-1.65280500
H	-2.25998800	-3.77306200	-1.64904500
C	0.38664700	-5.87960600	-1.93110800
H	2.33718300	-5.31018600	-2.64253400
H	-1.64531600	-6.11990600	-1.24648200
H	0.66066300	-6.91508500	-1.75041600
C	3.19765200	3.08651500	-2.51991600
C	2.25829800	3.66991800	-3.37880300
C	4.30911400	3.84759100	-2.14615300

C	2.43348700	4.96384400	-3.86045000
H	1.38112400	3.10679900	-3.68282900
C	4.48256600	5.14449100	-2.62179800
H	5.04986300	3.41937200	-1.47798000
C	3.54847200	5.70798300	-3.48569500
H	1.68974000	5.39058200	-4.52747900
H	5.35656900	5.71348600	-2.31712900
H	3.68646100	6.71750600	-3.86185500
C	4.28606600	1.04371100	-1.49464600
C	5.25180000	0.64135600	-2.42083900
C	4.54341700	0.85517600	-0.13665600
C	6.43853600	0.05350500	-1.99555900
H	5.07661900	0.78756000	-3.48250300
C	5.72771200	0.26317400	0.29379100
H	3.79687100	1.15049500	0.59511000
C	6.67923200	-0.14122600	-0.63634400
H	7.17808600	-0.25680300	-2.72863500
H	5.89131000	0.10549400	1.35593200
H	7.60113300	-0.61156300	-0.30694100
C	1.93365000	-0.10276500	-6.51405500
H	1.70611100	-1.07914800	-6.95094100
H	1.31196500	0.63794200	-7.03095300
H	2.97821800	0.13776800	-6.73090600
C	0.00485300	6.15193400	-1.42161100
H	-0.14938100	6.82262700	-2.27323800
H	-0.06514900	6.75234100	-0.50729200
H	1.02304100	5.75657700	-1.48606500

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C	0.49113900	0.23175500	0.30088400
N	0.97859100	-1.05010000	0.25605000
N	1.59228400	1.02257200	0.07296400
C	0.16230700	-2.20756100	0.44545600
C	-1.46756000	-4.39687300	0.81549300
C	-0.33435800	-2.86880000	-0.68684400
C	-0.10800600	-2.62612200	1.75506300
C	-0.93390900	-3.73922000	1.91651600
C	-1.16787100	-3.96787000	-0.47185700
H	-1.17415500	-4.08443600	2.91810500
H	-1.59108800	-4.49081100	-1.32468400
C	1.52507300	2.44821100	-0.00473900
C	1.41845600	5.19780800	-0.16120700
C	1.50466700	3.04581700	-1.27229400
C	1.47757700	3.18612100	1.19049100

C	1.42339200	4.57564700	1.08320900
C	1.45682700	4.44128300	-1.32416800
H	1.38234500	5.18097400	1.98304100
H	1.43630000	4.93701700	-2.29060900
C	1.52369400	2.49544500	2.53987000
H	1.05891000	1.51035700	2.41605200
C	1.50125200	2.23252200	-2.55148800
H	1.53299400	1.17374500	-2.27839500
C	0.44563900	-1.89357200	2.96016600
H	1.14678600	-1.13449900	2.59880500
C	-0.00177400	-2.41545100	-2.09472300
H	0.76105000	-1.63401700	-2.02503300
C	0.73145600	3.22772300	3.61877400
H	-0.29146800	3.43946200	3.29088500
H	1.20019600	4.17543900	3.90501500
H	0.67690200	2.61027700	4.52128700
C	2.73341600	2.52815100	-3.40740800
H	2.72766100	1.90713700	-4.30941000
H	3.66034000	2.32173400	-2.86378900
H	2.75509000	3.57587200	-3.72725800
Ni	-1.21982800	0.84879400	0.76130500
C	-0.67021900	-1.16428200	3.70990300
C	0.58937300	-3.55293700	-2.92823700
C	0.21091300	2.46026300	-3.34053200
C	2.97420700	2.27801600	2.98000100
C	6.45841000	0.91276400	-0.70771300
C	6.84894800	-0.41022700	-0.72144500
C	5.88719800	-1.44221900	-0.53154900
C	4.56847100	-1.03360600	-0.34412100
C	4.15661200	0.33282500	-0.33169800
C	5.10845700	1.31033700	-0.50995300
H	7.13285400	-3.22474900	-0.64570800
H	7.20657600	1.68685000	-0.85061100
H	7.89336800	-0.66793200	-0.87456000
C	6.12452700	-2.84550500	-0.50395000
C	3.48267000	-1.93388400	-0.12732500
H	4.85068000	2.36510300	-0.49989800
C	3.74148100	-3.28458900	-0.09858900
C	5.07969800	-3.72129400	-0.29372300
H	2.95385000	-4.01260600	0.07091800
H	5.28035900	-4.78839700	-0.27285000
C	2.72224000	0.25729800	-0.09437400
C	2.33304500	-1.05393100	0.02264600
C	-3.19786900	1.12373700	-1.27538700

C	-4.06728900	0.57288200	-2.20366600
C	-4.59742500	-0.69163200	-1.97908400
C	-4.23729700	-1.38272100	-0.82700800
C	-3.37184400	-0.79785500	0.08144800
C	-2.80823700	0.47215700	-0.10018600
C	-1.22234600	-1.79828900	-2.77726000
C	1.22645000	-2.83030800	3.88157300
H	3.48406100	3.23820800	3.11838700
H	3.01102700	1.73481100	3.93058900
H	3.54009500	1.70210800	2.24183100
H	0.13786900	3.49415000	-3.69601900
H	0.18324200	1.80539900	-4.21829700
H	-0.67066700	2.25302600	-2.72950000
F	-5.43016200	-1.24354900	-2.86461600
F	-4.39798700	1.24040900	-3.31262200
F	-2.71496200	2.35498000	-1.53715500
F	-4.71336400	-2.61465200	-0.62393900
H	1.37661600	6.28168900	-0.22205400
F	-3.06233600	-1.50808600	1.18041200
C	-2.83344000	1.69831900	1.39647600
H	-1.97478200	1.84255300	2.12085300
H	-2.97966000	2.65274600	0.88093800
C	-4.06751000	1.29226100	2.18956400
H	-4.08065100	1.87798500	3.12066900
H	-3.98809100	0.24298900	2.49496300
C	-5.39025900	1.52833900	1.46591100
H	-5.40816000	0.96538200	0.52638500
H	-5.45888900	2.58917200	1.18890300
H	-2.12311700	-5.25070900	0.96075800
H	-1.18652000	-0.46446400	3.04298100
H	-1.41452000	-1.86737400	4.09983200
H	-0.26060800	-0.60005800	4.55553000
H	0.58263800	-3.60222900	4.31646100
H	2.03654000	-3.33181700	3.34213200
H	1.66923000	-2.26640500	4.70945100
H	0.88730000	-3.18224600	-3.91465200
H	1.47444700	-3.98332700	-2.44896800
H	-0.13441900	-4.35976600	-3.08619700
H	-1.59224800	-0.94218300	-2.20841200
H	-0.96323900	-1.45363200	-3.78441800
H	-2.03649200	-2.52533800	-2.87007000
C	-6.59181300	1.13730700	2.31360600
H	-6.61856800	1.70092300	3.25353800
H	-7.53286500	1.32524600	1.78680800

H	-6.56214400	0.07174600	2.56878500
TS6-L8			
C	-0.08650900	0.29115800	0.20110100
N	-0.58789000	-0.19178200	-0.98606900
N	-1.14219800	0.19363900	1.07874100
C	0.20487700	-0.21214300	-2.17556500
C	1.92458800	-0.10637300	-4.35937000
C	1.03382400	-1.31451700	-2.43873500
C	0.17234100	0.90689400	-3.01254900
C	1.04533300	0.94109000	-4.10066300
C	1.89004000	-1.23170900	-3.53219000
H	1.07176800	1.83024800	-4.72526000
H	2.57564300	-2.05114100	-3.72612700
C	-1.01869000	0.34808900	2.49470500
C	-0.83276400	0.57424000	5.26851700
C	-0.89913300	-0.81300500	3.26921500
C	-1.00107300	1.62740800	3.07409800
C	-0.93695500	1.71059900	4.46200300
C	-0.78358100	-0.67271900	4.65358600
H	-0.92807400	2.69147700	4.92720900
H	-0.61612600	-1.56035400	5.25770000
C	-0.97986900	2.87322300	2.20210900
H	-0.22746500	2.67044500	1.42189300
C	-0.84652000	-2.18885400	2.62744600
H	-0.65524500	-2.03406700	1.56034000
C	-0.81372000	2.02998600	-2.75516000
H	-1.09198700	1.97860800	-1.69739100
C	0.93227700	-2.57249400	-1.59409300
H	0.64667900	-2.25575900	-0.58564000
C	2.94306900	-0.01416200	-5.45627200
H	3.93585500	0.15572700	-5.02359600
Ni	1.55882100	1.18637200	0.48027400
H	2.99660400	-0.94025900	-6.03740500
H	2.72824800	0.81094600	-6.14027000
C	-0.19631300	3.40827400	-2.93168000
C	1.00804100	3.68704700	-2.27265200
C	-0.81758400	4.42617500	-3.65369300
C	1.57332000	4.95475600	-2.33332800
H	1.50432300	2.89273600	-1.71838900
C	-0.24909900	5.69864800	-3.71625200
H	-1.75377400	4.22592700	-4.16581000
C	0.94475600	5.96820000	-3.05676100
H	2.50875900	5.15146300	-1.81681500

H	-0.74612300	6.48022800	-4.28441600
H	1.38603800	6.95959500	-3.10546700
C	-0.16588700	-3.50660700	-2.08803100
C	-0.66909500	-3.46848400	-3.38783600
C	-0.65111200	-4.48218000	-1.21019000
C	-1.65064400	-4.37137000	-3.79599100
H	-0.29640900	-2.72455500	-4.08598400
C	-1.63792600	-5.37469400	-1.61091700
H	-0.23790900	-4.54606500	-0.20628500
C	-2.14563200	-5.31967800	-2.90824900
H	-2.03337000	-4.32405600	-4.81194300
H	-2.00917600	-6.11578500	-0.90845000
H	-2.91772900	-6.01545400	-3.22357800
C	-5.88212600	-1.07201700	1.46385100
C	-6.30272600	-1.50749300	0.22348500
C	-5.39586500	-1.53131900	-0.87157100
C	-4.09582300	-1.10034100	-0.60898700
C	-3.65957500	-0.63941100	0.66734800
C	-4.55697800	-0.62841900	1.70869700
H	-6.66214000	-2.29291900	-2.47022700
H	-6.58491200	-1.07294800	2.29177200
H	-7.32806000	-1.83861200	0.08162000
C	-5.66632300	-1.94770700	-2.20499700
C	-3.05993700	-1.06872000	-1.58887300
H	-4.26890700	-0.31363600	2.70603000
C	-3.35290300	-1.46500300	-2.87115800
C	-4.67059200	-1.90760200	-3.15856100
H	-2.61222000	-1.43032100	-3.66095500
H	-4.89588800	-2.21800500	-4.17446500
C	-2.26053200	-0.30472300	0.44895300
C	-1.91133200	-0.54992800	-0.85708700
C	3.98555500	-0.09446900	1.31517600
C	5.08274000	-0.90259400	1.06656200
C	5.55576500	-1.04588100	-0.23123300
C	4.91398600	-0.36847200	-1.26145400
C	3.83083300	0.44306700	-0.97306500
C	3.30604600	0.60646500	0.31466300
C	2.23480100	-3.33710900	-1.43845200
C	2.69455100	-4.22130100	-2.41970800
C	2.97667400	-3.19072600	-0.26735300
C	3.88840300	-4.91372200	-2.24436700
H	2.10150600	-4.38348700	-3.31596200
C	4.16185500	-3.89710900	-0.08088400
H	2.61854500	-2.52001100	0.50810200

C	4.62751100	-4.75232600	-1.07435600
H	4.23593900	-5.59186300	-3.01888500
H	4.72327700	-3.76958200	0.83986100
H	5.55622800	-5.29783500	-0.93443800
C	-2.10226300	1.81490700	-3.53301000
C	-3.32607400	1.93891400	-2.87294000
C	-2.10676100	1.49609200	-4.89396900
C	-4.52739500	1.75720100	-3.55087300
H	-3.33646400	2.16720900	-1.81225900
C	-3.30675500	1.31095000	-5.57507300
H	-1.16598700	1.38019200	-5.42361800
C	-4.52206700	1.44120600	-4.90585700
H	-5.46536900	1.84216500	-3.00958700
H	-3.29126600	1.06093000	-6.63246300
H	-5.45748500	1.28940100	-5.43703000
F	6.58305400	-1.85539700	-0.48765700
F	5.66427100	-1.59071200	2.05862100
F	3.57992300	0.01704100	2.59752300
F	5.33625600	-0.52215200	-2.51975300
F	3.27931300	1.11605900	-1.99767000
C	2.96946800	2.44928800	0.88965300
H	3.20440100	2.37426900	1.95631900
C	4.02640600	3.25531800	0.14845900
H	3.83117400	4.31933100	0.35035000
H	3.91127600	3.12675100	-0.93344800
C	5.46628700	2.95799700	0.55590600
H	5.70015900	1.90489500	0.36753400
H	5.56772100	3.10642200	1.63966200
C	0.34749900	-2.99421000	3.12657900
C	0.25225400	-4.33558700	3.49437100
C	1.60550400	-2.38060200	3.13551900
C	1.39369800	-5.05003700	3.85913400
H	-0.71552200	-4.82782700	3.49003000
C	2.74317100	-3.09156500	3.49652800
H	1.69468700	-1.33676900	2.85096700
C	2.64036200	-4.43437800	3.85883500
H	1.30284200	-6.09562200	4.14051000
H	3.70908600	-2.59543200	3.47831200
H	3.52801900	-4.99533100	4.13710200
C	-2.17343800	-2.92678100	2.70212200
C	-2.91037200	-3.04152500	3.88365300
C	-2.68041500	-3.52033700	1.54433200
C	-4.12007800	-3.73088200	3.90190800
H	-2.54810100	-2.58037700	4.79677600

C	-3.88756600	-4.21081700	1.55749600
H	-2.13491100	-3.42026200	0.61111200
C	-4.61395400	-4.31793600	2.73956000
H	-4.68057300	-3.80530500	4.82986500
H	-4.26496900	-4.64484200	0.63609800
H	-5.56229100	-4.84745000	2.75463800
C	-2.27628000	3.14930800	1.47066100
C	-2.23685000	3.93109100	0.31064200
C	-3.51163300	2.71458000	1.94744500
C	-3.40926500	4.27960300	-0.34944400
H	-1.27810100	4.27582800	-0.07031800
C	-4.68775900	3.04814200	1.27745300
H	-3.55213800	2.10965600	2.84854900
C	-4.64105800	3.83550500	0.13176600
H	-3.35797400	4.88287600	-1.25114200
H	-5.64092900	2.68656600	1.65255700
H	-5.55707000	4.09685700	-0.39034200
C	-0.47454000	4.09514300	2.95539800
C	-1.29783600	5.17531000	3.27331700
C	0.86449400	4.13145200	3.36141400
C	-0.79276400	6.27022900	3.97313900
H	-2.33918200	5.16468400	2.96697300
C	1.37104600	5.22320000	4.05580300
H	1.50656700	3.28416400	3.14079700
C	0.54176700	6.30087700	4.36319000
H	-1.44883800	7.10314900	4.21033800
H	2.41456700	5.23215800	4.35857500
H	0.93490500	7.15681100	4.90429400
C	-0.76123000	0.70490100	6.76188200
H	-0.33086100	-0.18944500	7.22041800
H	-0.15564700	1.56681900	7.05727600
H	-1.76049600	0.84838900	7.19052700
H	1.98612000	2.99068400	0.79367800
C	6.46541600	3.83722300	-0.18161200
H	6.27737600	4.90081900	0.00635900
H	7.49355300	3.62201900	0.12642300
H	6.40377900	3.67766700	-1.26427100

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C	-0.45671400	0.00312000	0.12400200
N	-1.37227300	1.02322200	0.16503600
N	-1.21523000	-1.13835000	0.03925900
C	-0.99702000	2.39454900	0.31741500
C	-0.16804000	5.00273000	0.60807500

C	-0.91031500	3.19830400	-0.82854300
C	-0.72029400	2.86631600	1.60787900
C	-0.29330500	4.19023800	1.72746200
C	-0.48232600	4.51501300	-0.65511200
H	-0.05423900	4.58788500	2.70907600
H	-0.38749100	5.16541800	-1.51882500
C	-0.63184700	-2.44415700	0.02166700
C	0.51522200	-4.94912800	-0.00812800
C	-0.42757300	-3.07167800	-1.21502600
C	-0.26854400	-3.02897200	1.24639400
C	0.30701200	-4.29939400	1.20325400
C	0.15531900	-4.34073800	-1.20351200
H	0.60191500	-4.78511600	2.12802600
H	0.34023300	-4.85249100	-2.14312100
C	-0.52208000	-2.32172800	2.56287100
H	-0.54273700	-1.24713100	2.35559500
C	-0.74283200	-2.37103000	-2.52063200
H	-1.42170400	-1.54047000	-2.30161400
C	-0.85313100	1.97826800	2.82963600
H	-1.43600900	1.09719800	2.53912300
C	-1.21653900	2.64008500	-2.20452800
H	-1.90196000	1.79510200	-2.07457800
C	0.58519500	-2.55266100	3.58741200
H	1.56703800	-2.30411900	3.17402700
H	0.61474200	-3.58936500	3.93958700
H	0.41676900	-1.92043600	4.46520100
C	-1.44407100	-3.27843500	-3.52832500
H	-1.72800800	-2.70273400	-4.41517100
H	-2.35340800	-3.71916600	-3.10683300
H	-0.79706600	-4.09457600	-3.86698200
Ni	1.41990300	0.04199900	0.20780200
C	0.51898300	1.48690600	3.29519000
C	-1.91212200	3.64867100	-3.11528700
C	0.54264900	-1.77224400	-3.09696000
C	-1.88653400	-2.72199500	3.13079900
C	-5.84968600	-2.80366500	-0.20518000
C	-6.68896600	-1.70955200	-0.16437100
C	-6.14849000	-0.39666600	-0.06289000
C	-4.75963900	-0.30116200	-0.00949700
C	-3.88510300	-1.42839000	-0.05186500
C	-4.43469800	-2.68590600	-0.14967300
H	-7.95510100	0.81899900	-0.05148200
H	-6.27993200	-3.79775900	-0.28320300
H	-7.76574000	-1.84771700	-0.21040800

C	-6.86923700	0.82981400	-0.01302000
C	-4.05364400	0.93496200	0.08951500
H	-3.81601000	-3.57767400	-0.18460800
C	-4.77476800	2.10508900	0.13589200
C	-6.19268200	2.02822800	0.08263900
H	-4.28691500	3.07217700	0.21197000
H	-6.75957800	2.95384200	0.11894200
C	-2.55730100	-0.83660600	0.02945800
C	-2.65572600	0.53073900	0.10895500
C	3.60320000	-0.90667500	-0.80139400
C	3.60495700	-0.31729200	-2.04530600
C	3.32689300	1.05652700	-2.16964300
C	3.05107600	1.80846000	-1.05489000
C	2.98422200	1.19743900	0.22694600
C	3.34549700	-0.18210500	0.39752600
C	0.06160700	2.09884300	-2.84868800
C	-1.61242600	2.66651500	3.96336100
H	-1.91225400	-3.79352700	3.35983900
H	-2.09459600	-2.17373100	4.05616200
H	-2.69660600	-2.51111800	2.42616400
H	1.27368800	-2.55506200	-3.32621200
H	0.33659000	-1.21639400	-4.01791000
H	0.99871200	-1.08804100	-2.37466300
F	3.26959400	1.59888700	-3.38892900
F	3.81242800	-1.03899200	-3.15242600
F	3.93283400	-2.20316000	-0.71321900
F	2.79203100	3.11256000	-1.17227600
H	0.96918300	-5.93604800	-0.01983600
F	3.08575200	2.04352700	1.28720800
C	3.79293100	-0.72124500	1.73406900
H	3.11059300	-0.35832000	2.50879400
H	3.70013800	-1.81239800	1.71311300
C	5.22683400	-0.32246500	2.10163400
H	5.45203500	-0.73214300	3.09561700
H	5.27651000	0.76961600	2.19752300
C	6.28504000	-0.79358600	1.11077500
H	6.10028200	-0.33351200	0.13171400
H	6.18879700	-1.87691900	0.96143600
H	0.17302500	6.02800300	0.72044000
H	1.01166700	0.92139200	2.49427400
H	1.16891700	2.32673000	3.56295500
H	0.41725700	0.83858800	4.17300800
H	-1.05413200	3.51456700	4.37368100
H	-2.58740500	3.03380100	3.62721200

H	-1.78053800	1.96111800	4.78387900
H	-2.21938100	3.15953900	-4.04519000
H	-2.80596300	4.06995900	-2.64357100
H	-1.25079100	4.47677900	-3.39132500
H	0.50932400	1.32434700	-2.21908900
H	-0.15368000	1.66563100	-3.83156200
H	0.80045400	2.89530000	-2.97973300
C	7.69817000	-0.45622200	1.56471700
H	7.93196800	-0.93250000	2.52386000
H	8.44480300	-0.79051300	0.83712800
H	7.82316700	0.62481900	1.69539500

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C	0.02583000	0.13736700	0.05905200
N	-0.91637300	-0.34563100	-0.81937800
N	-0.68987700	0.40734300	1.20283400
C	-0.54081400	-0.69986700	-2.14968400
C	0.51750500	-1.26130100	-4.65434700
C	-0.07916200	-1.99492300	-2.41043900
C	-0.56104300	0.29721800	-3.13061700
C	-0.00545000	0.00201300	-4.37309000
C	0.44917800	-2.25236400	-3.67338600
H	0.04235700	0.78357300	-5.12748400
H	0.84288200	-3.24208800	-3.88692700
C	-0.09157200	0.86846700	2.41472800
C	1.02318800	1.73788100	4.81712400
C	0.41807700	-0.07828900	3.31298100
C	-0.02824100	2.24243000	2.67670200
C	0.52836000	2.65315500	3.88760500
C	0.97422700	0.37847800	4.50607200
H	0.60072800	3.71757100	4.09397600
H	1.40213100	-0.34518100	5.19465100
C	-0.53658500	3.25106800	1.66232200
H	-0.39913900	2.79021100	0.67606600
C	0.34166700	-1.55908900	2.98621700
H	0.37577800	-1.63525400	1.89328600
C	-1.25495800	1.61526100	-2.84228100
H	-1.28422800	1.72108000	-1.75463200
C	-0.26153200	-3.08289600	-1.37150800
H	-0.39781400	-2.56850700	-0.41502400
C	1.18039800	-1.53559500	-5.97150900
H	2.23533200	-1.24150500	-5.92922400
Ni	1.87789400	0.37095700	-0.29697700
H	1.14546100	-2.59856700	-6.22578600

H	0.71417100	-0.97046100	-6.78382900
C	-0.48081800	2.82271800	-3.33941200
C	0.59625200	3.26561700	-2.56468100
C	-0.79565100	3.50796500	-4.51205000
C	1.34525900	4.36892300	-2.95295800
H	0.85192900	2.72048900	-1.65730600
C	-0.03962800	4.61070500	-4.90756900
H	-1.64606700	3.19065800	-5.10900000
C	1.02949200	5.04517800	-4.13024000
H	2.17108000	4.70584900	-2.33245100
H	-0.29625900	5.13718600	-5.82282600
H	1.61091600	5.91035900	-4.43602800
C	-1.54072400	-3.88425900	-1.59962600
C	-2.32282300	-3.77169800	-2.74842200
C	-1.95424600	-4.77061300	-0.59703000
C	-3.49838700	-4.51073800	-2.88557400
H	-2.01872200	-3.09698900	-3.54251600
C	-3.12908000	-5.49985100	-0.72703000
H	-1.33858100	-4.89455900	0.28997400
C	-3.91133100	-5.36917100	-1.87422500
H	-4.09337200	-4.40570100	-3.78882000
H	-3.43230700	-6.17677300	0.06701100
H	-4.83070500	-5.93816300	-1.97783800
C	-5.15139800	0.08042100	3.26009000
C	-6.02167100	-0.39703800	2.30244000
C	-5.55145300	-0.69499100	0.99317500
C	-4.19526700	-0.47240200	0.75731500
C	-3.29636800	0.04104800	1.73783700
C	-3.77498000	0.30916800	2.99707000
H	-7.36920800	-1.39931500	0.02482000
H	-5.52573900	0.29159300	4.25754000
H	-7.06876200	-0.55440700	2.54754600
C	-6.30698600	-1.20532600	-0.09888900
C	-3.55468900	-0.74269600	-0.48770500
H	-3.12769600	0.67804900	3.78432800
C	-4.31091400	-1.22562200	-1.52871700
C	-5.69454000	-1.45326400	-1.31017000
H	-3.87928800	-1.42483000	-2.50252700
H	-6.28630500	-1.83679900	-2.13591800
C	-2.02201700	0.09830000	1.03708300
C	-2.16789000	-0.36891200	-0.24725800
C	4.39545300	-0.17119100	0.32103100
C	4.62667900	-1.43501000	-0.16275700
C	4.22770700	-1.76890100	-1.47223400

C	3.56708800	-0.84742000	-2.23916400
C	3.23338800	0.43244700	-1.71242900
C	3.76301700	0.85198400	-0.44232900
C	0.93938300	-3.98883600	-1.17249800
C	1.13978800	-5.13318600	-1.94784600
C	1.84053100	-3.70656700	-0.14329200
C	2.22524200	-5.96990400	-1.70335300
H	0.42331100	-5.38612600	-2.72503400
C	2.91436300	-4.55180200	0.11685700
H	1.69685000	-2.81621600	0.46415800
C	3.11086600	-5.68533000	-0.66709100
H	2.36904300	-6.85661500	-2.31468800
H	3.59424900	-4.31807300	0.92961100
H	3.94901400	-6.34709000	-0.46830000
C	-2.70995500	1.56196800	-3.28801300
C	-3.69595800	2.07337800	-2.44100900
C	-3.10765700	0.99071100	-4.50028400
C	-5.04072000	2.02428000	-2.79150000
H	-3.40892700	2.48460200	-1.47829700
C	-4.45301800	0.94539400	-4.85806600
H	-2.36372900	0.55668300	-5.16133800
C	-5.42513000	1.46075100	-4.00483500
H	-5.78919800	2.40543600	-2.10259700
H	-4.74151500	0.49569000	-5.80429300
H	-6.47518600	1.41310800	-4.27894200
F	4.51194500	-2.97783500	-1.95139400
F	5.24209900	-2.35975600	0.58336500
F	4.87885000	0.13883900	1.53715700
F	3.26937600	-1.13080600	-3.50766500
F	2.99319300	1.38260400	-2.65828400
C	4.09549600	2.30440100	-0.19474800
H	4.19898900	2.46573100	0.88368500
C	5.36264800	2.76827200	-0.92382600
H	5.50393900	3.83749600	-0.71287900
H	5.19445300	2.68804600	-2.00511800
C	6.63155100	2.01143300	-0.55067800
H	6.51978100	0.95437800	-0.82255600
H	6.76675500	2.03536100	0.53862100
C	1.55565000	-2.32827600	3.48037400
C	1.45934900	-3.50431100	4.22165000
C	2.82516600	-1.86452400	3.11463500
C	2.60903700	-4.20077800	4.59433300
H	0.48229100	-3.88395600	4.50377300
C	3.97141600	-2.55574600	3.48573500

H	2.91140500	-0.94884200	2.53698800
C	3.86595000	-3.73085300	4.22994300
H	2.51615400	-5.11717000	5.17064300
H	4.94223800	-2.17908200	3.18069200
H	4.75973300	-4.27566600	4.52057700
C	-0.99774300	-2.13557300	3.40481700
C	-1.50144400	-1.97508000	4.69853000
C	-1.76706600	-2.82941500	2.47105300
C	-2.74492800	-2.49732100	5.04266000
H	-0.92221700	-1.42733100	5.43694200
C	-3.01465000	-3.34536100	2.80630000
H	-1.39416700	-2.94541400	1.45811200
C	-3.50776800	-3.17963200	4.09668600
H	-3.12445200	-2.36174000	6.05177600
H	-3.60252100	-3.85691200	2.04979300
H	-4.48610400	-3.56919700	4.36236600
C	-2.01856700	3.54078900	1.79661200
C	-2.73189600	3.92801100	0.65830200
C	-2.68694200	3.48672300	3.01911600
C	-4.08821400	4.22442700	0.73293700
H	-2.20831700	4.00828500	-0.29165400
C	-4.04537900	3.78749900	3.09807900
H	-2.14396100	3.19648700	3.91410900
C	-4.75205100	4.14801300	1.95577600
H	-4.62591800	4.51665200	-0.16487800
H	-4.55403100	3.72913200	4.05631400
H	-5.81330700	4.37051100	2.01646500
C	0.31647800	4.51137900	1.65150600
C	-0.18385500	5.78153800	1.92932600
C	1.67160400	4.37554900	1.33641600
C	0.65588100	6.89517500	1.88275400
H	-1.23374600	5.90655900	2.17532000
C	2.50871300	5.48153400	1.28484200
H	2.05981300	3.38182400	1.13656400
C	2.00013400	6.75152000	1.55851900
H	0.25080200	7.87984800	2.09909900
H	3.55825000	5.35436300	1.03257900
H	2.64966400	7.62129600	1.51898700
C	1.59532400	2.20473400	6.12390000
H	2.40459100	1.55066200	6.46081000
H	1.98652100	3.22282100	6.04656800
H	0.82888600	2.20619800	6.90852700
H	3.25729200	2.91666300	-0.53519800
C	7.86663900	2.57709200	-1.23754900

H	8.03386800	3.62347700	-0.95716000
H	8.76733800	2.01422700	-0.97218900
H	7.76214400	2.54143900	-2.32798500

S-int1

C	0.40284900	0.12894800	0.48721600
N	-0.80807100	0.10419500	-0.16031600
N	0.12326200	-0.26989000	1.76491800
C	-0.85711100	0.34915300	-1.56523300
C	-0.75503800	0.82853800	-4.30112400
C	-0.73964700	-0.73572500	-2.43659700
C	-0.90769800	1.67361300	-2.02291200
C	-0.86387300	1.89050600	-3.39547800
C	-0.68553500	-0.47218000	-3.80705800
H	-0.88442900	2.91129800	-3.76729800
H	-0.55474600	-1.30255900	-4.49624600
C	1.12832800	-0.43759600	2.76959600
C	3.06428100	-0.74602400	4.70219300
C	1.94116100	-1.58343800	2.72369500
C	1.26076400	0.55759600	3.74762200
C	2.24334700	0.37346100	4.72250900
C	2.91900000	-1.70972100	3.71110000
H	2.38052200	1.12374100	5.49453200
H	3.57998400	-2.56969900	3.70248800
C	0.43083300	1.82526800	3.68826200
H	-0.52102200	1.58054800	3.20356000
C	1.74164400	-2.64950400	1.66306600
H	1.48057500	-2.13006100	0.73340900
C	-1.00522000	2.79873000	-1.00608500
H	-0.32659100	2.52283800	-0.19093500
C	-0.66990100	-2.14801400	-1.88677500
H	-0.30775800	-2.06457300	-0.85716600
C	-0.69230900	1.10016800	-5.77629700
H	-1.59947700	1.60694100	-6.12401800
C	1.14538500	2.86062300	2.81358700
H	1.32539900	2.47501900	1.80624000
H	2.11901600	3.12173700	3.24120800
H	0.55308300	3.77953200	2.73357000
C	0.57814400	-3.57202500	2.04042800
H	0.41621500	-4.31938900	1.25568000
H	-0.35565600	-3.02274700	2.18919200
H	0.80062500	-4.10703000	2.97071900
Ni	2.00514800	0.61471500	-0.36699100
H	0.15325300	1.75246300	-6.01964200

H	-0.58088100	0.17607400	-6.34895100
C	-0.48547300	4.11880500	-1.54277000
C	0.88604500	4.37360400	-1.45039900
C	-1.30805100	5.06977500	-2.14817100
C	1.42664800	5.54731400	-1.96356000
H	1.52883500	3.64792400	-0.95828700
C	-0.76694800	6.24475300	-2.66619700
H	-2.37904600	4.89804500	-2.20408000
C	0.60094700	6.48612300	-2.57892000
H	2.49376600	5.73194100	-1.87456100
H	-1.42018800	6.97669700	-3.13334100
H	1.02035900	7.40493600	-2.97889200
C	-2.04242800	-2.79020500	-1.78978300
C	-3.02787300	-2.60354400	-2.76169500
C	-2.33896300	-3.59051500	-0.68336400
C	-4.27892500	-3.20169300	-2.62826300
H	-2.82324800	-1.97101100	-3.62055300
C	-3.58891700	-4.18281200	-0.54321800
H	-1.58379100	-3.73420300	0.08467700
C	-4.56543800	-3.98925800	-1.51690600
H	-5.03442500	-3.04303600	-3.39302300
H	-3.80431300	-4.78434200	0.33513300
H	-5.54565500	-4.44384700	-1.40616700
C	2.98887200	-3.48005800	1.37675000
C	0.09958700	2.39875800	5.06273000
C	-3.51847700	-1.66706200	4.76659800
C	-4.68862000	-1.67045700	4.03460000
C	-4.67553400	-1.30271200	2.66030100
C	-3.43901300	-0.94336000	2.12705100
C	-2.22505700	-0.94172700	2.87747400
C	-2.26533200	-1.30656400	4.20360800
H	-6.77276900	-1.53760200	2.12379400
H	-3.54893600	-1.95325400	5.81384800
H	-5.62441700	-1.95697400	4.50702700
C	-5.78273000	-1.26701100	1.76660800
C	-3.24423300	-0.55475200	0.76910200
H	-1.36894000	-1.32634000	4.81615500
C	-4.32891000	-0.53623100	-0.07339300
C	-5.59840600	-0.89800500	0.45076900
H	-4.23422900	-0.26392700	-1.11803600
H	-6.45221400	-0.88519200	-0.22020400
C	-1.22400800	-0.52451600	1.90793900
C	-1.81407700	-0.29384300	0.68799300
C	4.30024100	0.90081500	1.11505600

C	4.90344200	-0.29191400	0.81794500
C	4.88053200	-0.80009600	-0.49980800
C	4.27508600	-0.08093500	-1.50042300
C	3.63527000	1.16325100	-1.25768000
C	3.58119400	1.61078000	0.10693800
H	3.47371100	1.84885100	-2.08581100
C	0.37543800	-2.98173700	-2.60848400
C	0.06149600	-4.05118000	-3.44439200
C	1.72048800	-2.64928800	-2.41054500
C	1.07638700	-4.77629400	-4.06964800
H	-0.97794100	-4.32655900	-3.59817000
C	2.73308000	-3.37308000	-3.02658900
H	1.96926900	-1.80949100	-1.76180900
C	2.41070300	-4.44326700	-3.86119900
H	0.81861700	-5.60987400	-4.71727700
H	3.76866100	-3.09857800	-2.85108200
H	3.19842600	-5.01427900	-4.34438500
C	-2.39784800	2.87455300	-0.40802700
C	-2.54691800	3.06583000	0.96730000
C	-3.54517700	2.74980700	-1.19542800
C	-3.81025800	3.12940300	1.54567800
H	-1.65884700	3.15387000	1.58823700
C	-4.81159600	2.82893400	-0.62144700
H	-3.44390700	2.57134300	-2.26301700
C	-4.94810900	3.01427300	0.75124400
H	-3.90566500	3.25990500	2.61985200
H	-5.69397900	2.72953300	-1.24768200
H	-5.93537900	3.05569900	1.20171300
H	0.98904000	2.78338300	5.57289500
H	-0.59671300	3.23688500	4.95685300
H	-0.36897800	1.65071900	5.71047700
H	3.22404000	-4.15890400	2.20432400
H	2.81962100	-4.09750400	0.48921400
H	3.86844900	-2.86082700	1.18970700
F	5.43731800	-1.99356500	-0.74099500
F	5.48711700	-1.02371900	1.77041600
F	4.34394100	1.39618700	2.35122500
F	4.33374200	-0.54923600	-2.75337100
F	3.39052200	2.93730500	0.36348800
H	3.83320500	-0.86525500	5.46022900
S-TS2			
C	-0.32229900	-0.35223300	1.01616100
N	-0.80046500	0.02701900	-0.21550900

N	-1.39368700	-0.91743400	1.64268700
C	0.09959700	0.68854400	-1.10706300
C	2.08738600	1.95562700	-2.57623800
C	0.94708200	-0.08816200	-1.90737700
C	0.20321600	2.08442700	-1.04228900
C	1.20039400	2.69835400	-1.79392900
C	1.93701100	0.56936300	-2.63645500
H	1.32537600	3.77503900	-1.71893800
H	2.63071900	-0.01971700	-3.22964400
C	-1.36092300	-1.44329400	2.97123600
C	-1.31151600	-2.45806700	5.52760600
C	-1.06405000	-2.80270100	3.14213800
C	-1.63447300	-0.57634800	4.03630100
C	-1.60111800	-1.11460000	5.32454800
C	-1.04502300	-3.29351400	4.44816700
H	-1.79922200	-0.47073300	6.17669700
H	-0.81362700	-4.33951700	4.62378200
C	-1.91046700	0.89644900	3.81473900
H	-2.02537200	1.05599800	2.73790100
C	-0.70883400	-3.68003300	1.95914700
H	-1.11856500	-3.20471300	1.06084700
C	-0.74476700	2.86776000	-0.15051700
H	-0.93051900	2.23608400	0.72508100
C	0.75982700	-1.59730200	-1.95507600
H	0.49329900	-1.90786400	-0.93824600
C	3.23590700	2.63210300	-3.26486400
H	4.05943200	2.77869400	-2.55537900
C	-0.71477800	1.73419200	4.27310300
H	0.19816000	1.41490200	3.76006700
H	-0.55157700	1.63009900	5.35174800
H	-0.88032500	2.79496100	4.05570500
C	-1.31379000	-5.07840900	2.04601500
H	-1.10677700	-5.63293300	1.12481300
H	-2.39954100	-5.03786600	2.18037800
H	-0.88973800	-5.65848700	2.87241100
Ni	1.55043200	-0.12430300	1.29318300
H	3.61782400	2.03450000	-4.09687500
H	2.95502700	3.61852300	-3.64539000
C	-0.11812700	4.14161000	0.39122700
C	0.80512200	4.02731400	1.43567400
C	-0.41340200	5.40851200	-0.11148700
C	1.42412600	5.15433900	1.96212300
H	1.04576000	3.04073300	1.82281200
C	0.20851700	6.53988400	0.41488300

H	-1.14200200	5.51482600	-0.90970400
C	1.12783000	6.41724200	1.45155200
H	2.13895300	5.04620300	2.77316300
H	-0.03307400	7.52049400	0.01403500
H	1.60941600	7.29989300	1.86276400
C	-0.41259700	-1.98125300	-2.83920100
C	-0.65745700	-1.34458800	-4.05840500
C	-1.27414300	-3.00168600	-2.43032100
C	-1.73388900	-1.72892800	-4.85438000
H	-0.00833400	-0.53347300	-4.37806200
C	-2.35776700	-3.37832400	-3.21644300
H	-1.09374300	-3.49920400	-1.48020400
C	-2.58949900	-2.74354100	-4.43393900
H	-1.91025500	-1.22498700	-5.80080200
H	-3.02763400	-4.16108000	-2.87268400
H	-3.43880800	-3.03126700	-5.04661400
C	0.81313600	-3.73499300	1.79861900
C	-3.20940300	1.34693500	4.48109300
C	-6.14895000	-2.05773700	1.11880500
C	-6.53943800	-1.66217200	-0.14478700
C	-5.60743300	-1.04031900	-1.02090700
C	-4.31526600	-0.86494400	-0.52776100
C	-3.90538600	-1.27258700	0.77682500
C	-4.82736800	-1.87249700	1.60391700
H	-6.83359700	-0.68915500	-2.78536100
H	-6.87563300	-2.53063100	1.77294500
H	-7.56219900	-1.82556100	-0.47379400
C	-5.84573500	-0.57893100	-2.34609000
C	-3.26005400	-0.25859100	-1.27126700
H	-4.56690300	-2.20174100	2.60538100
C	-3.51749900	0.17642700	-2.54750300
C	-4.82739300	0.00448600	-3.06933700
H	-2.75163900	0.64303700	-3.15481400
H	-5.02562300	0.35123700	-4.07916600
C	-2.50363500	-0.88935800	0.82775300
C	-2.12805200	-0.29590400	-0.35549700
C	4.25703300	-0.97958100	1.44250400
C	5.56605000	-0.96229300	0.98724800
C	6.06304000	0.18370900	0.37927800
C	5.23960400	1.29423300	0.24138200
C	3.93830200	1.24452200	0.71713300
C	3.38359100	0.09974400	1.29534200
C	2.04715200	-2.33098900	-2.28333200
C	2.38453100	-2.74369000	-3.57239900

C	2.94977200	-2.56653400	-1.24336900
C	3.60957800	-3.36300600	-3.81505000
H	1.68439600	-2.58957900	-4.38834400
C	4.17316000	-3.18154600	-1.48128500
H	2.68488900	-2.25840000	-0.23591600
C	4.50852400	-3.57885400	-2.77430100
H	3.85976900	-3.67990000	-4.82381400
H	4.86233600	-3.34312100	-0.65725900
H	5.46301600	-4.05998300	-2.96763600
C	-2.08973900	3.08703400	-0.81812200
C	-3.25924500	2.96894300	-0.06339600
C	-2.19601700	3.42167800	-2.17031000
C	-4.50652100	3.17464400	-0.64273600
H	-3.18827400	2.70306000	0.98872000
C	-3.44309800	3.64126200	-2.75055200
H	-1.29554800	3.49861700	-2.77394500
C	-4.60223400	3.51415500	-1.98973600
H	-5.40513400	3.05847500	-0.04389800
H	-3.50830600	3.90222400	-3.80338400
H	-5.57560800	3.66869300	-2.44599600
H	-3.16167500	1.25462500	5.57139200
H	-3.40706700	2.39925700	4.25063000
H	-4.06170600	0.75654100	4.12920900
H	1.27815900	-4.22490100	2.66140000
H	1.09245100	-4.29433500	0.89872100
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S-int3

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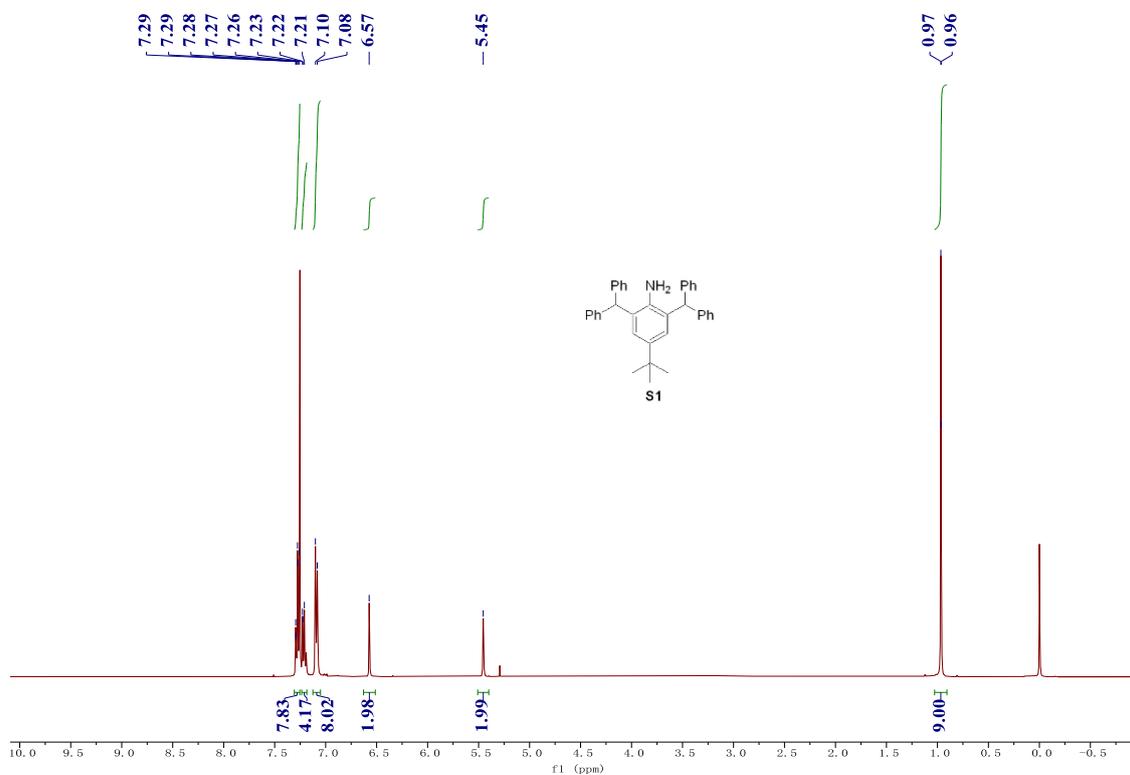
11. References

1. Lan, X.-B.; Li, Y.; Li, Y.-F.; Shen, D.-S.; Ke, Z.; Liu, F.-S. *J. Org. Chem.* **2017**, *82*, 2914.
2. Zhang, F. Y.; Lan, X. B.; Xu, C.; Yao, H. G.; Li, T.; Liu, F. S. *Org. Chem. Front.* **2019**, *6*, 3292.
3. Bakhoda, A.; Jiang, Q.; Badiei, Y. M.; Bertke, J. A.; Cundari, T. R.; Warren, T. H. *Angew. Chem., Int. Ed.* **2019**, *58*, 3421.
4. Dua, S. S.; Howells, R. D.; Gilman, H. *J. Fluor. Chem.* **1974**, *4*, 381.
5. Sun, Y.; Sun, H.; Jia, J.; Du, A.; Li, X. *Organometallics*, **2014**, *33*, 1079.
6. Xu, S.; Wu, G.; Ye, F.; Wang, X.; Li, H.; Zhao, X.; Zhang, Y.; Wang, J. *Angew. Chem. Int. Ed.* **2015**, *54*, 4669.
7. Filler, R.; Choe, E.W. *Can. J. Chem.* **1975**, *53*, 1491.
8. Blomeyer, S.; Linnemannstöns, M.; Nissen, J. H.; Paulus, J.; Neumann, B.; Stammler, H.-G.; Mitzel, N. W. *Angew. Chem. Int. Ed.* **2017**, *56*, 13259.
9. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 16, Revision A.03*; Gaussian Inc., Wallingford, CT, **2016**.
10. Adamo, C.; Barone, V. *J. Chem. Phys.* **1999**, *110*, 6158.
11. Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. *J. Chem. Phys.* **2010**, *132*, 154104.
12. Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 299.

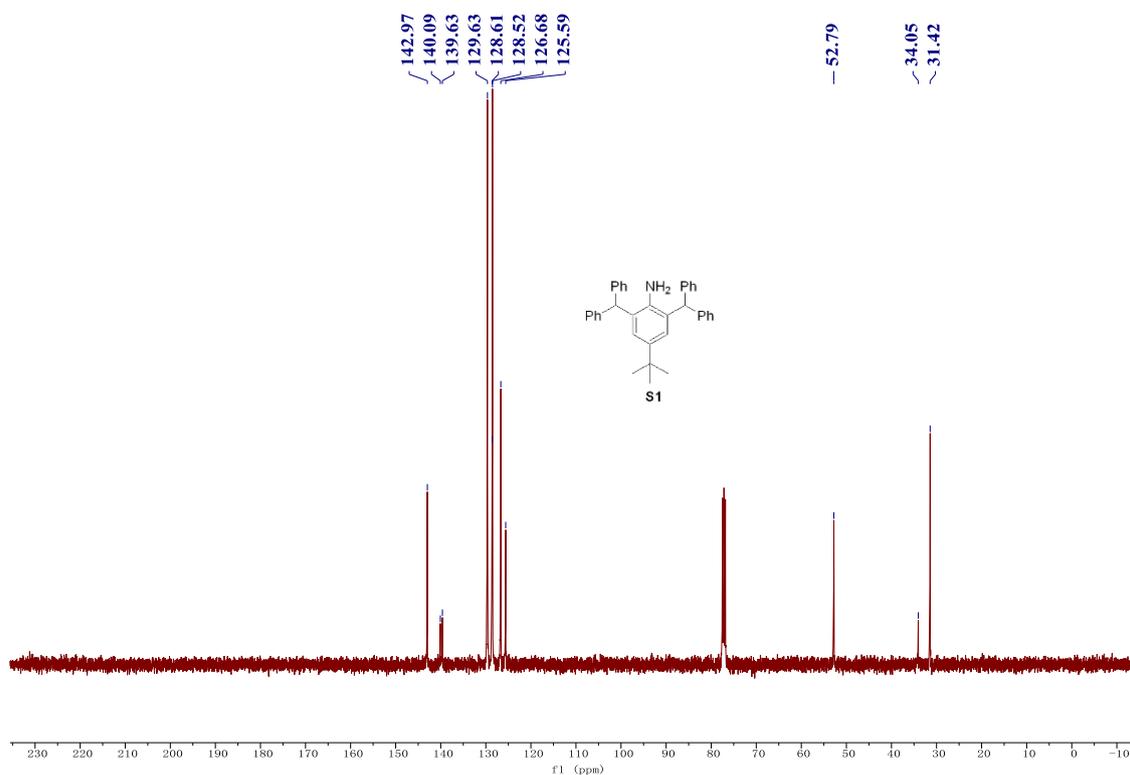
13. Ehlers, A. W.; Böhme, M.; Dapprich, S.; Gobbi, A.; Höllwarth, A.; Jonas, V.; Köhler, K. F.; Stegmann, R.; Veldkamp, A.; Frenking, G. *Chem. Phys. Lett.* **1993**, *208*, 111.
14. a) Steinmetz, M.; Grimme, S. *ChemistryOpen* **2013**, *2*, 115. b) Dohm, S.; Hansen, A.; Steinmetz, M.; Grimme, S.; Checinski, M. P. *J. Chem. Theory Comput.* **2018**, *14*, 2596. c) Saper, N. I.; Ohgi, A.; Small, D. W.; Semba, K.; Nakao, Y.; Hartwig, J. F. *Nat. Chem.* **2020**, *12*, 276.
15. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2009**, *113*, 6378–6396.
16. Roy, L. E.; Hay, P. J.; Martin, R. L. *J. Chem. Theory Comput.* **2008**, *4*, 1029–1031.
17. CYLview, 20; Legault, C. Y. Université de Sherbrooke, **2020** (<http://www.cylview.org>).
18. Seidler, A.; Svoboda, J.; Dekoj, V.; Chocholousova, J. V.; Vacek, J.; Stara, I. G.; Stary, I. *Tetrahedron Lett.* **2013**, *54*, 2795.
19. Liu, S.; Zhang, K.; Lu, J.; Zhang, J.; Yip, H.-L.; Huang, F.; Cao, Y. *J. Am. Chem. Soc.* **2013**, *135*, 15326.

12. NMR Spectra.

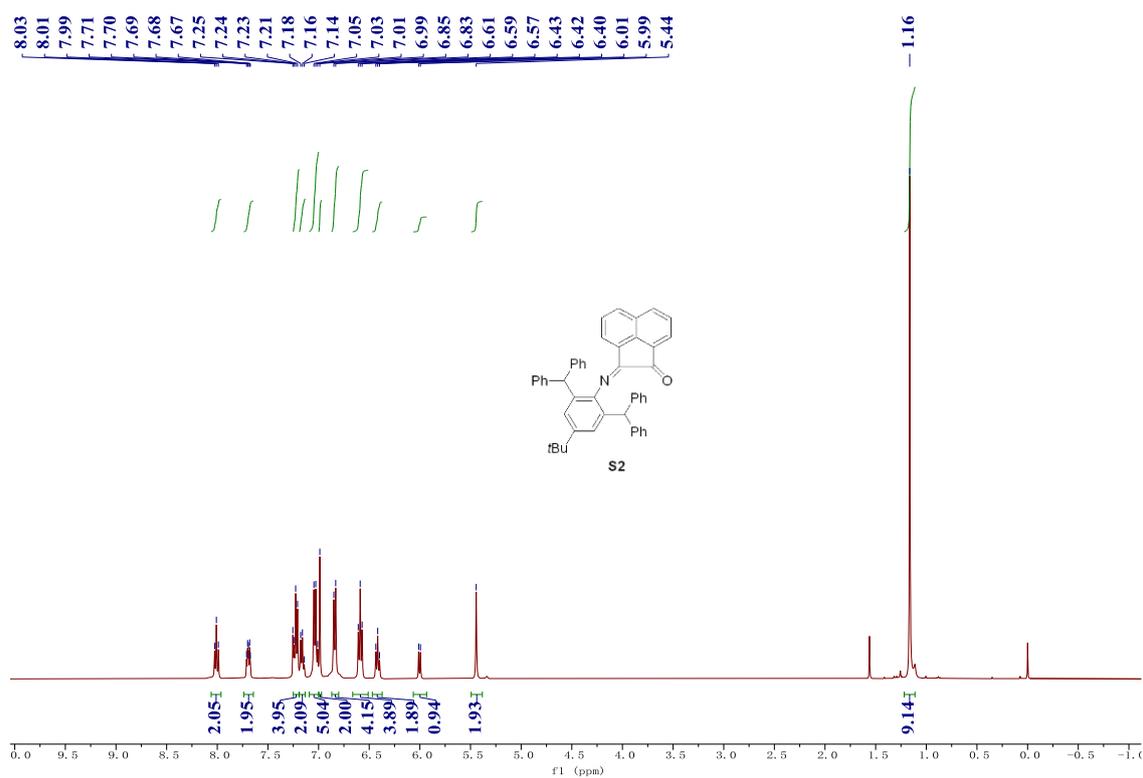
¹H NMR spectra of S1



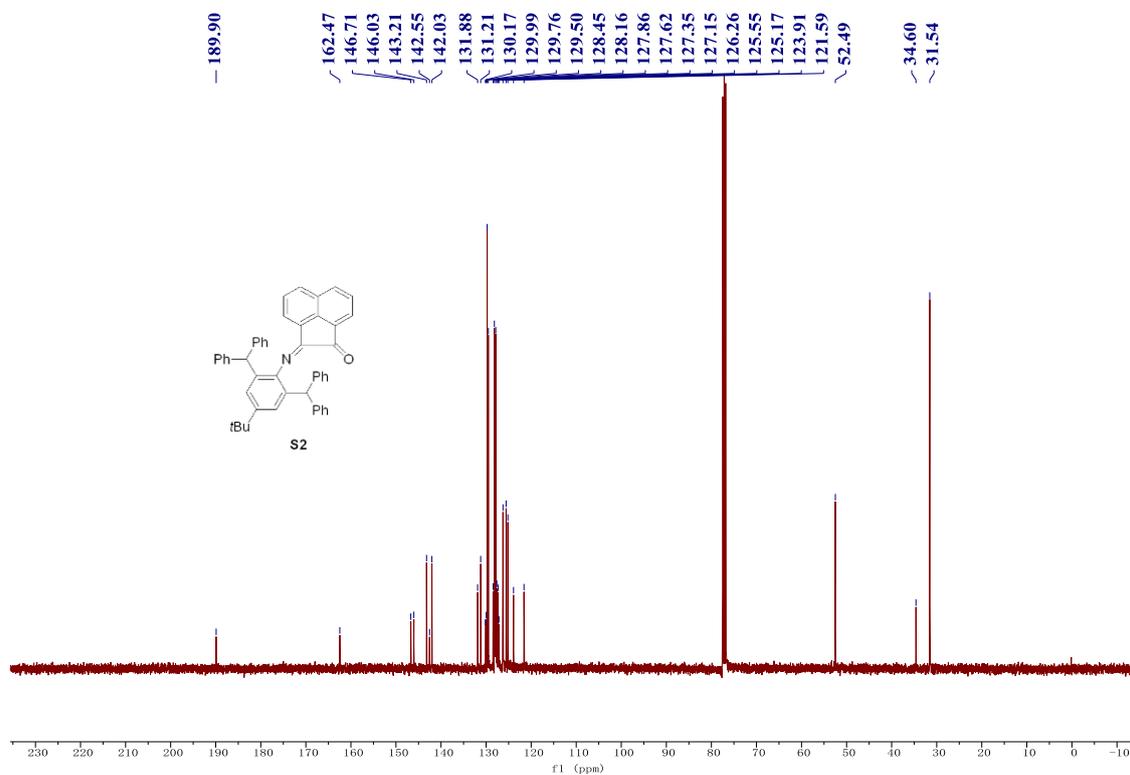
¹³C NMR spectrum of S1



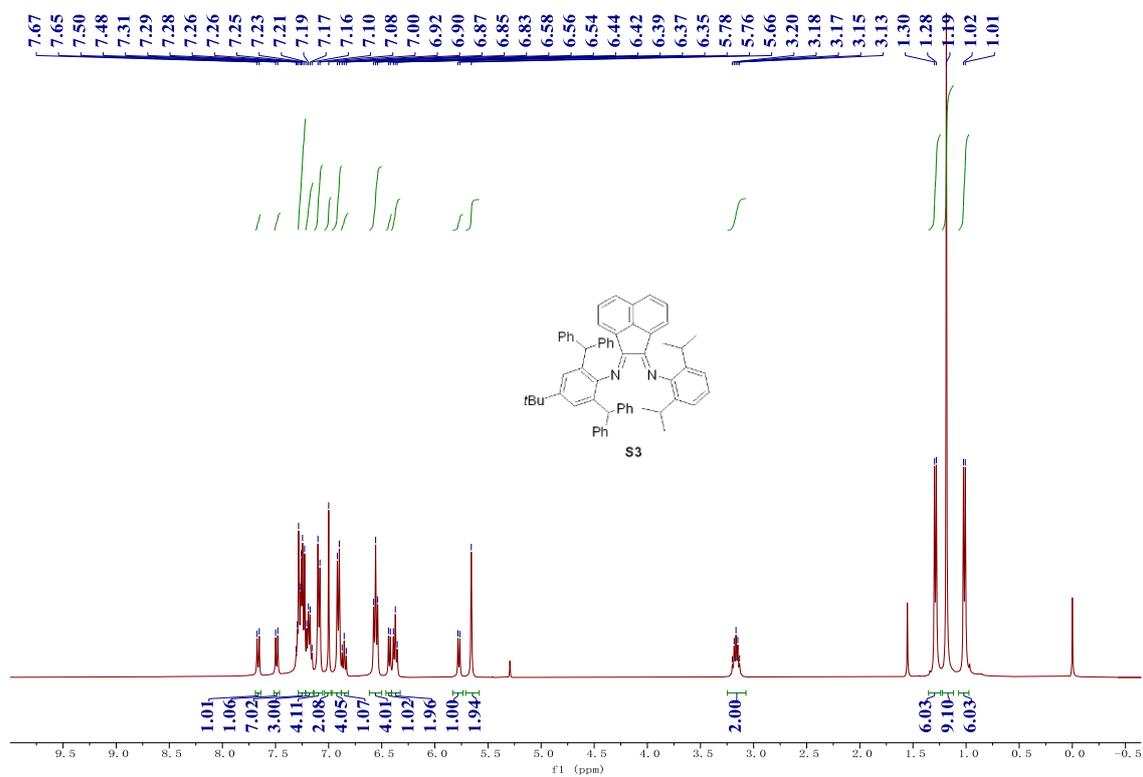
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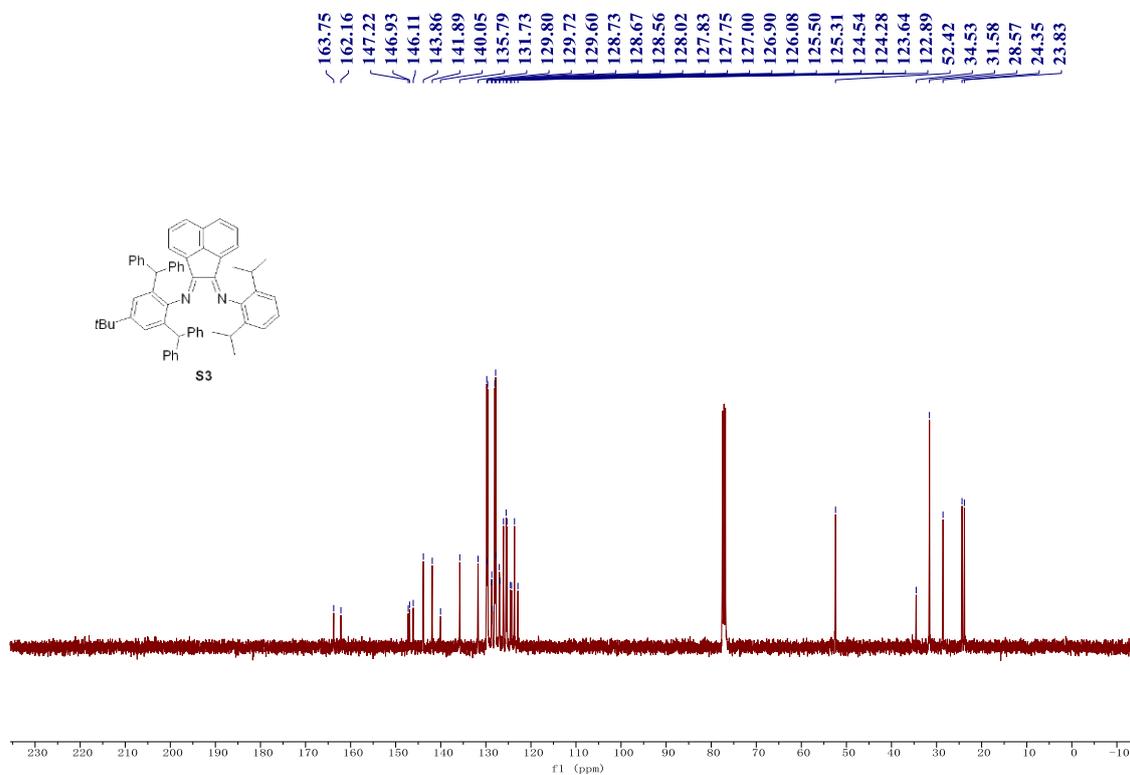
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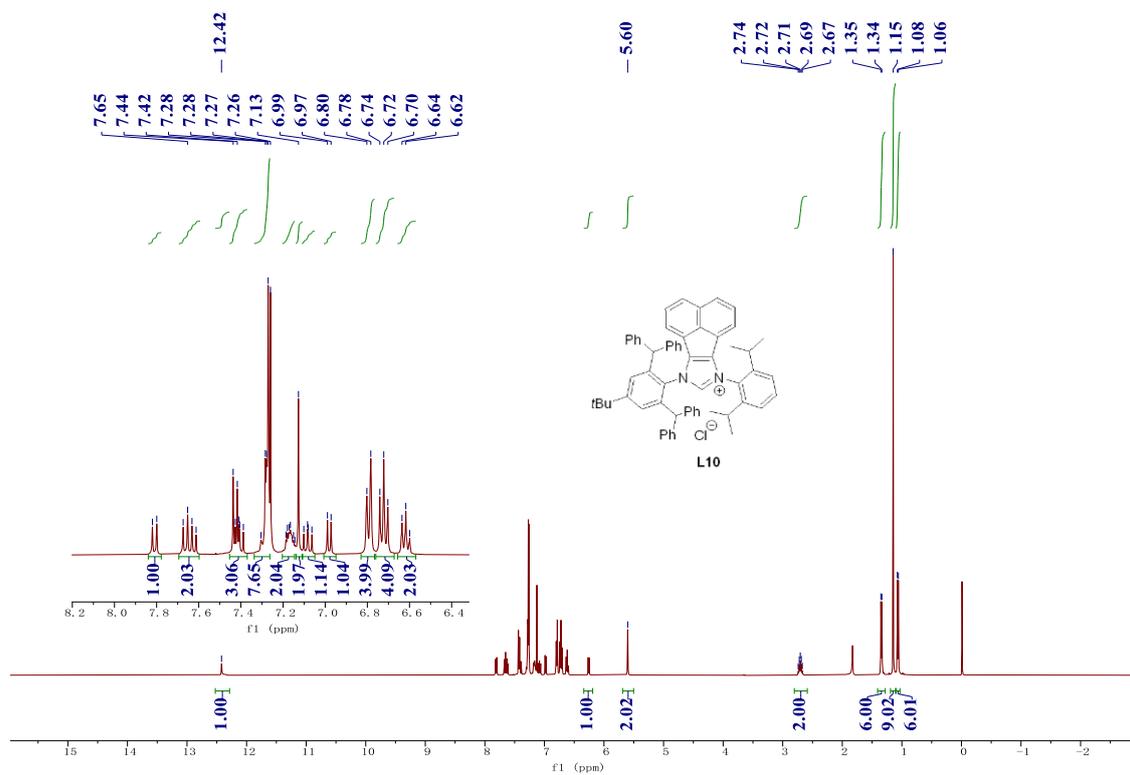
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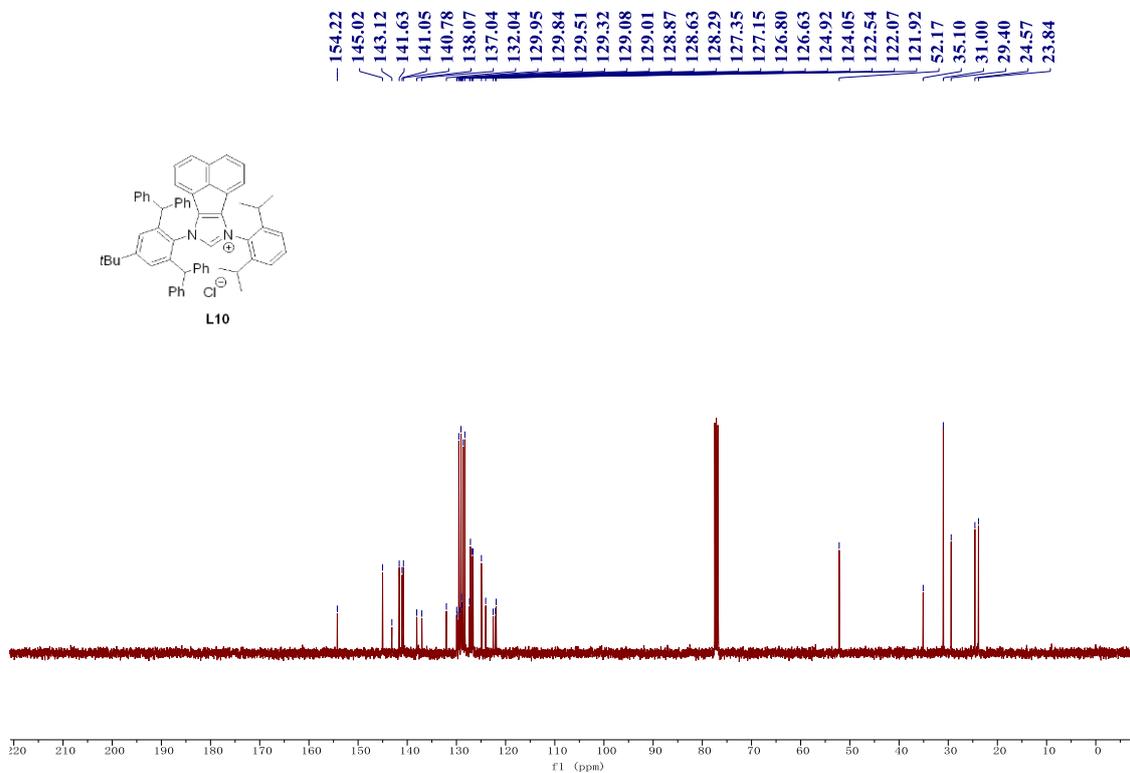
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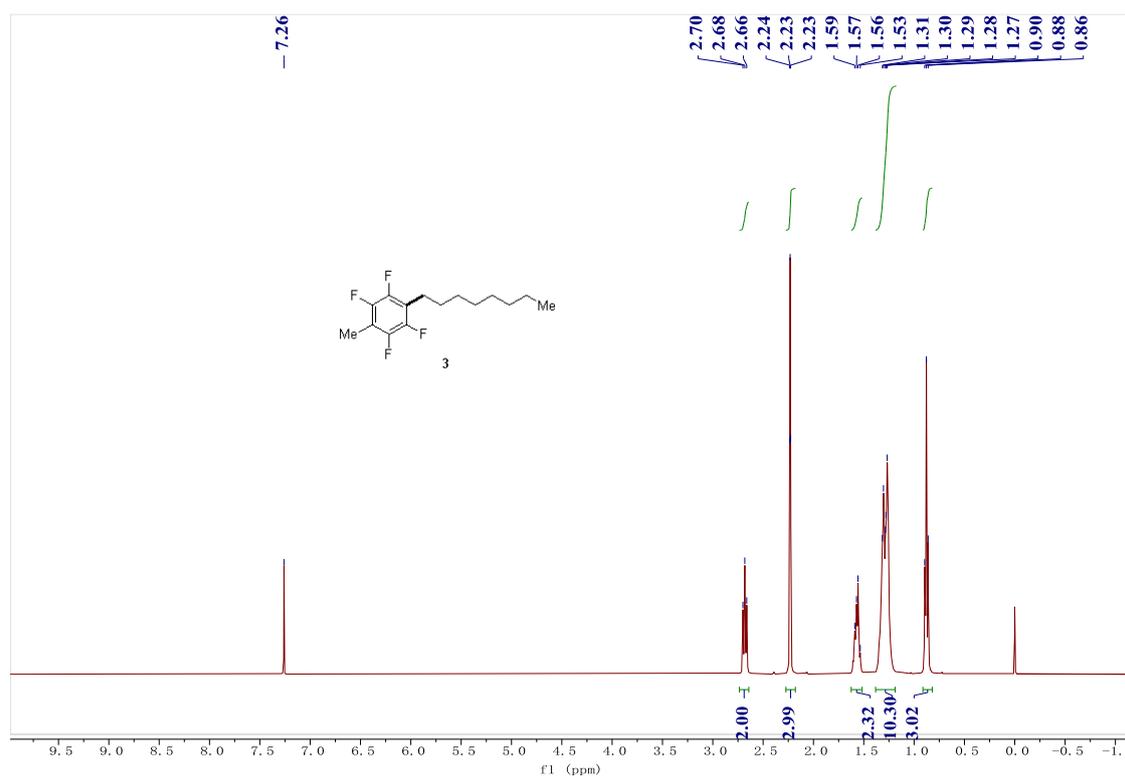
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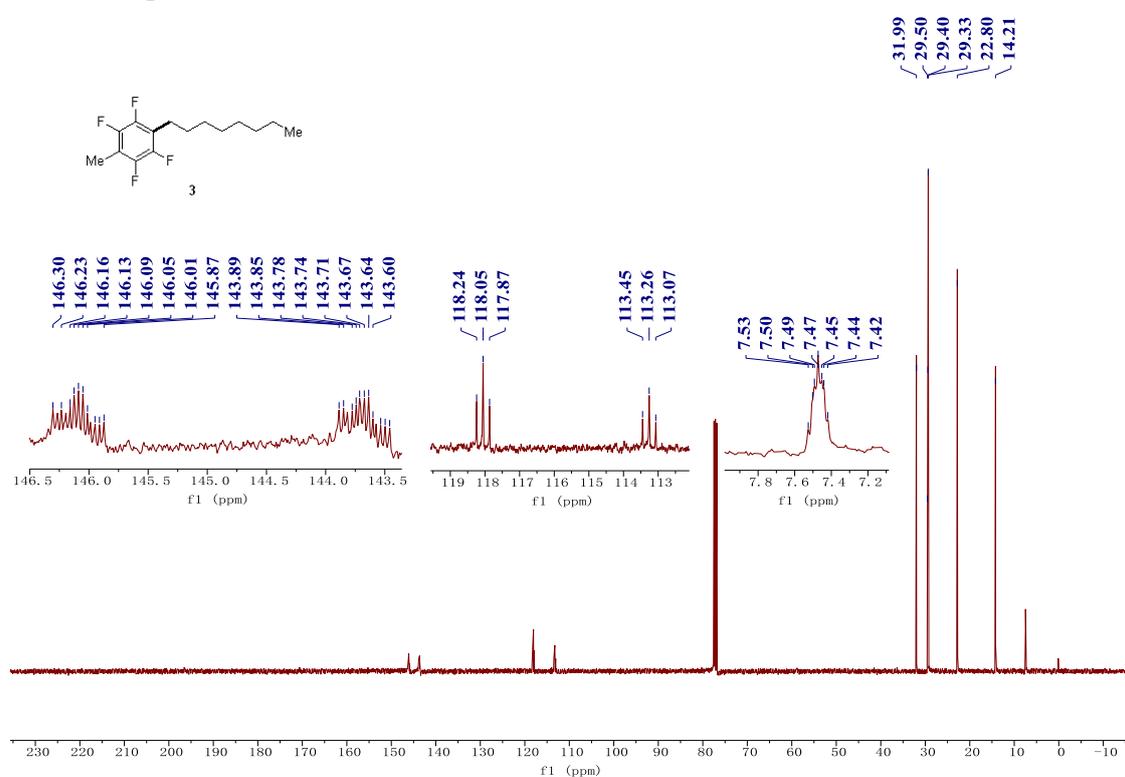
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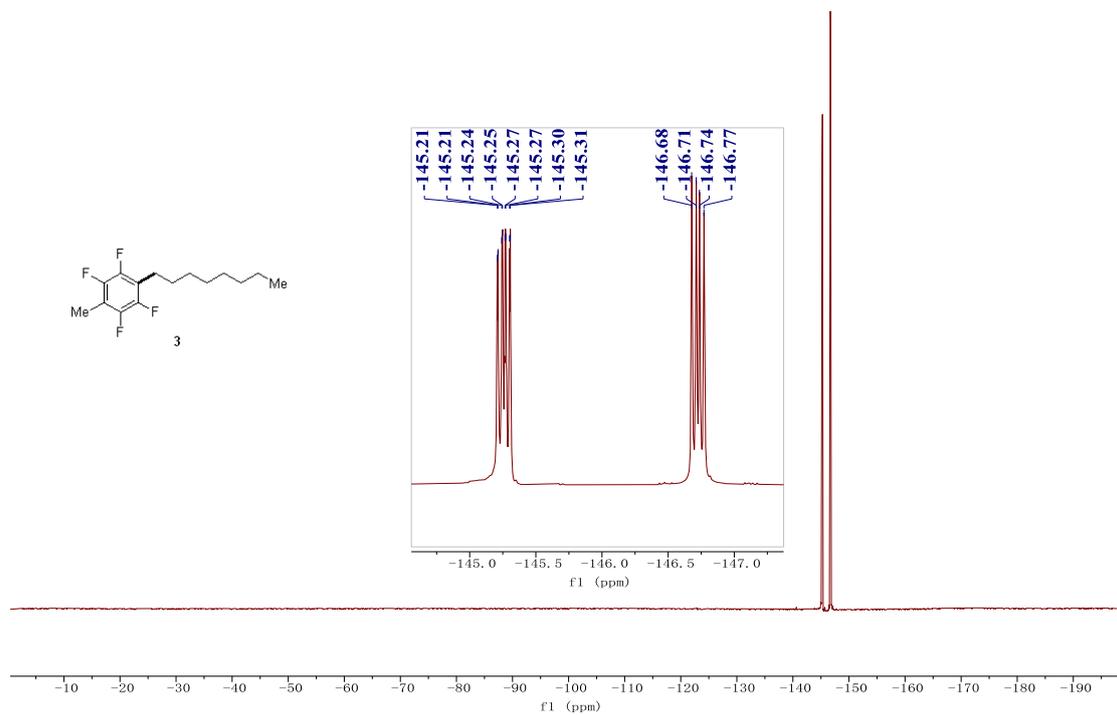
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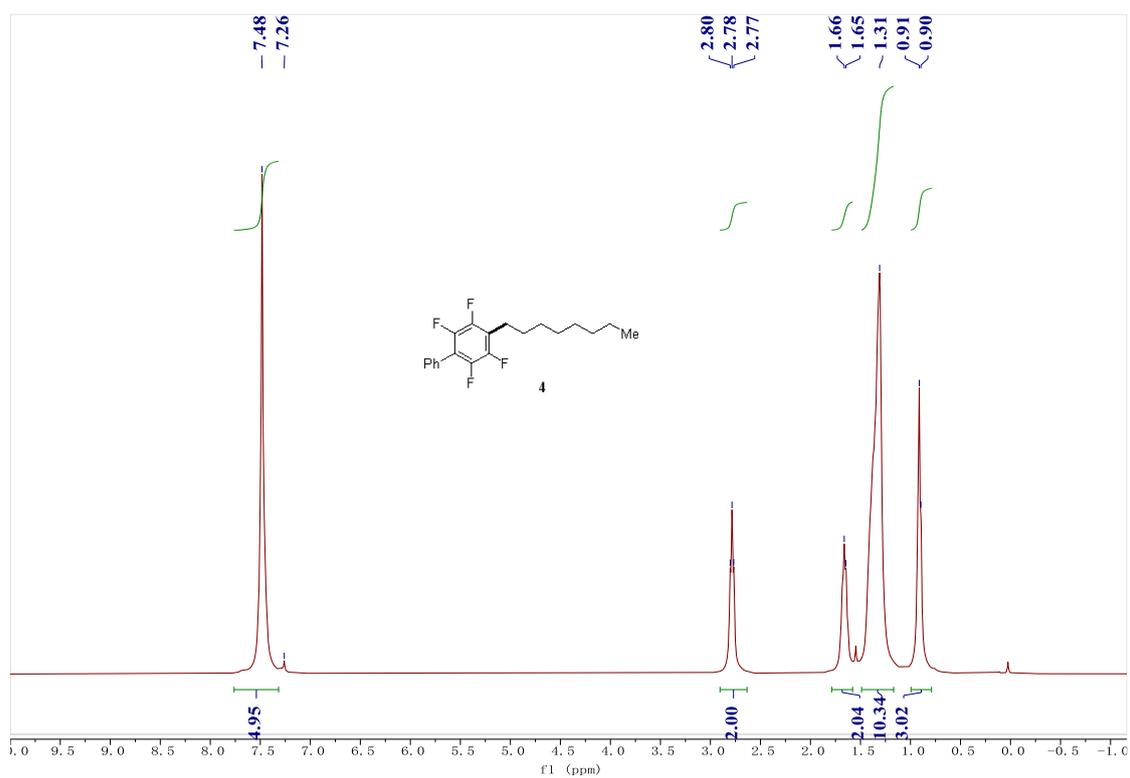
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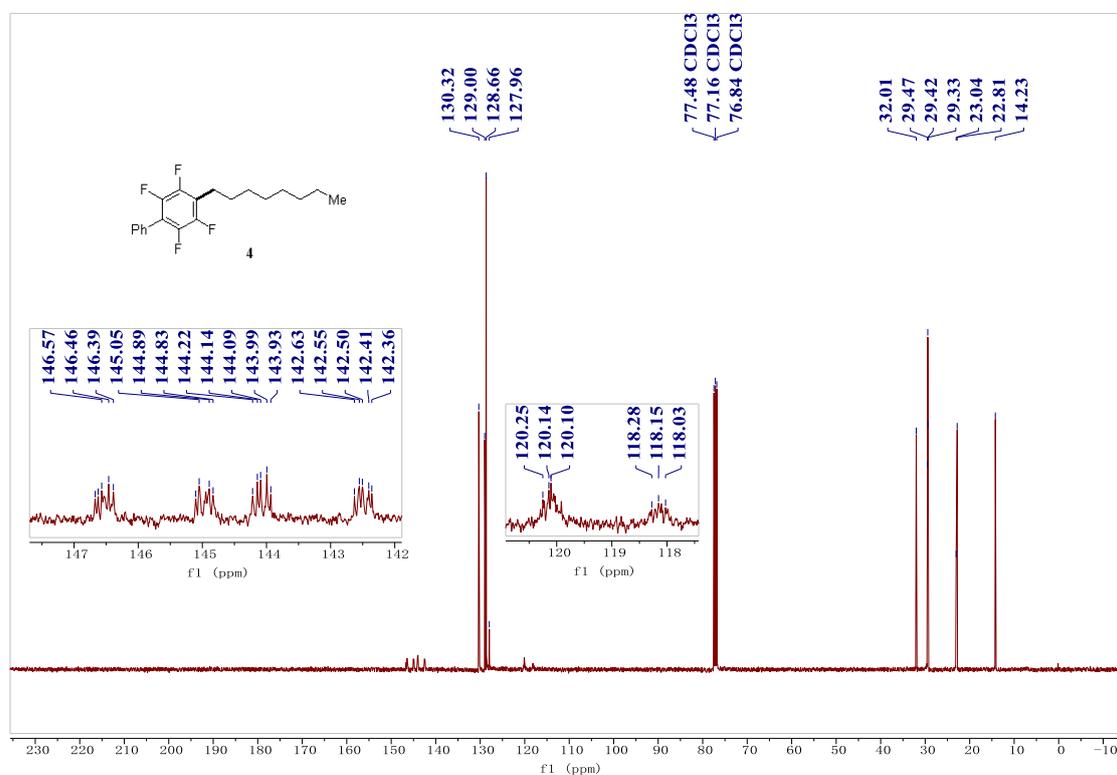
¹⁹F NMR Spectrum of 3



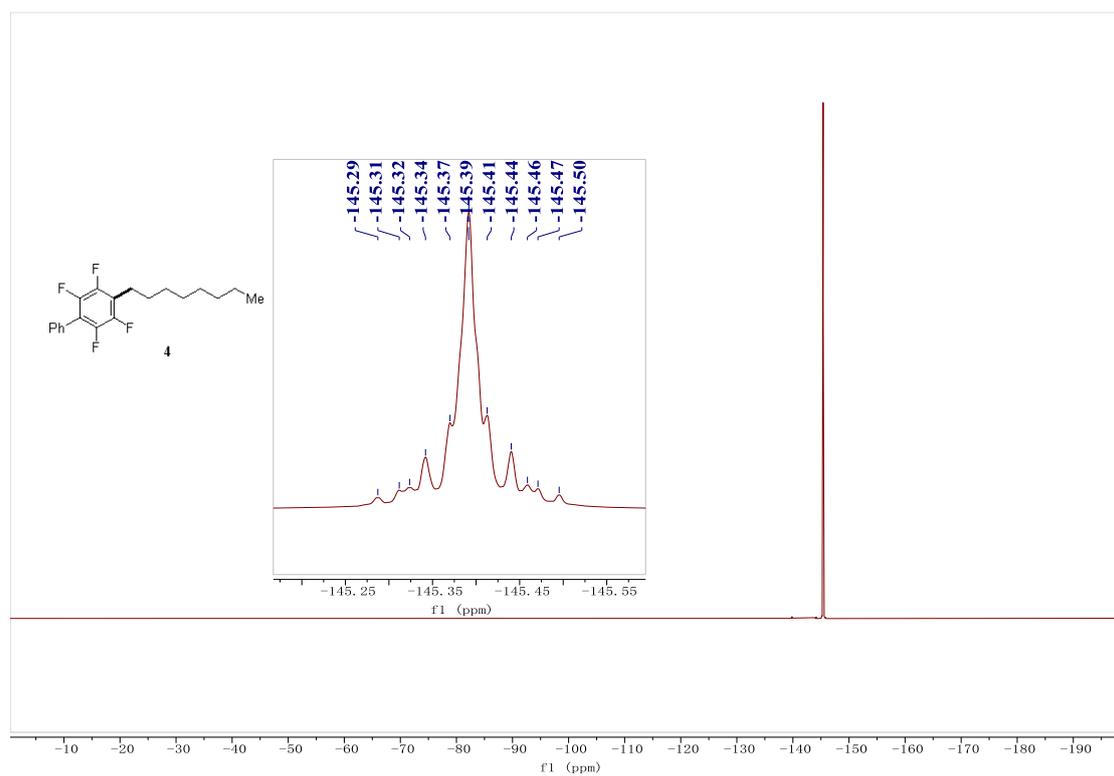
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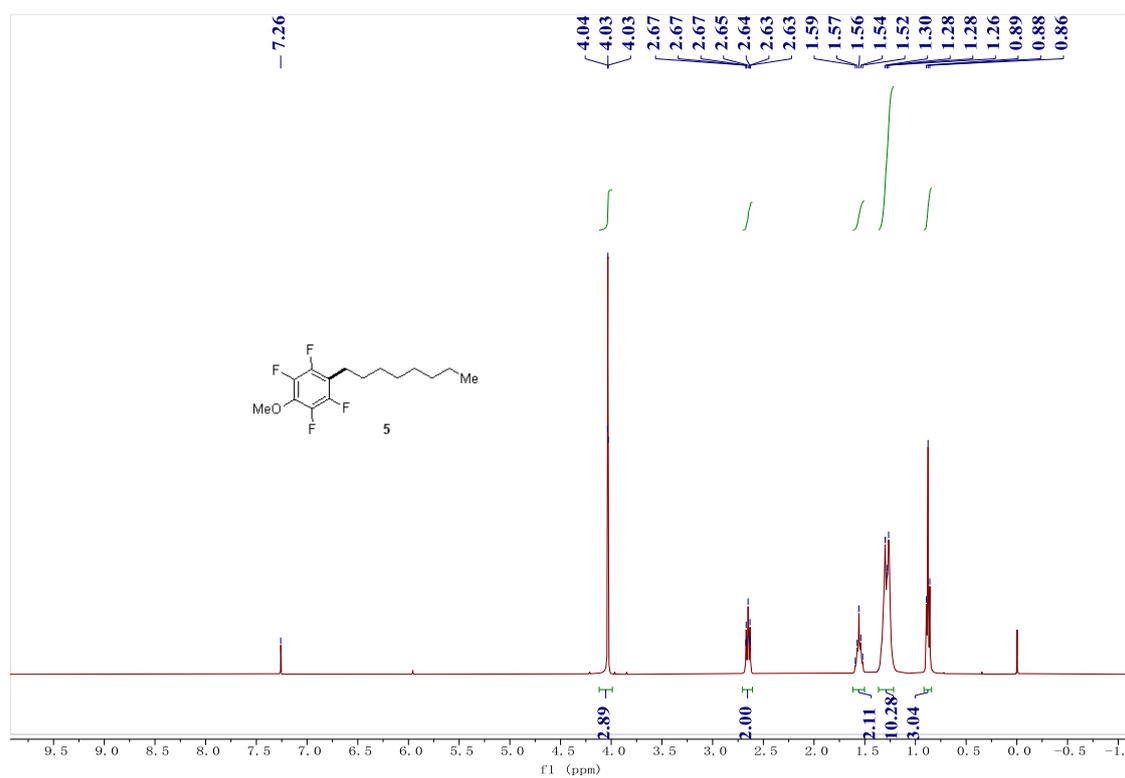
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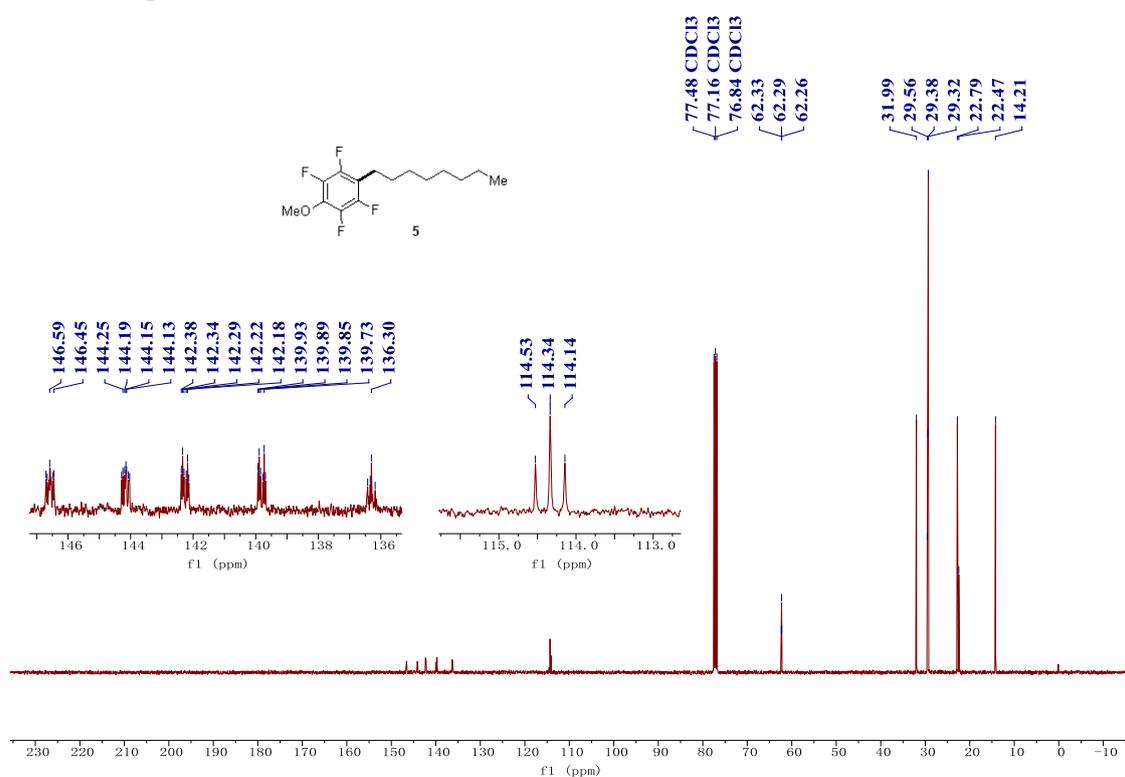
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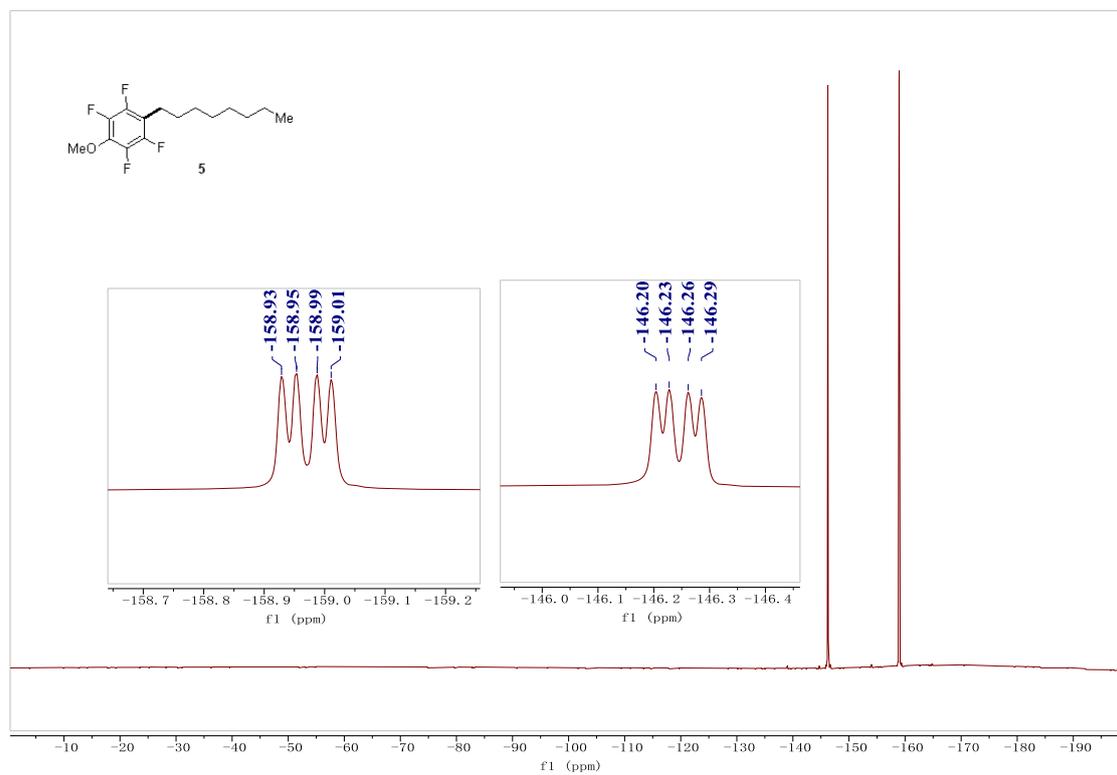
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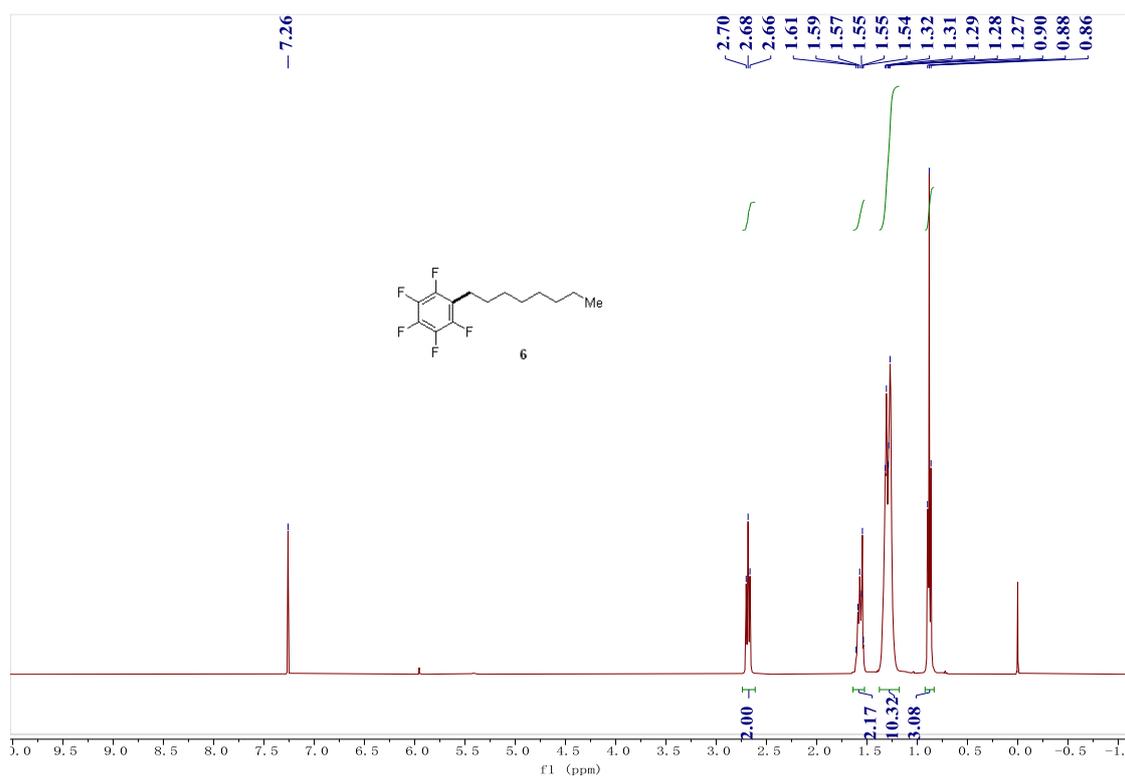
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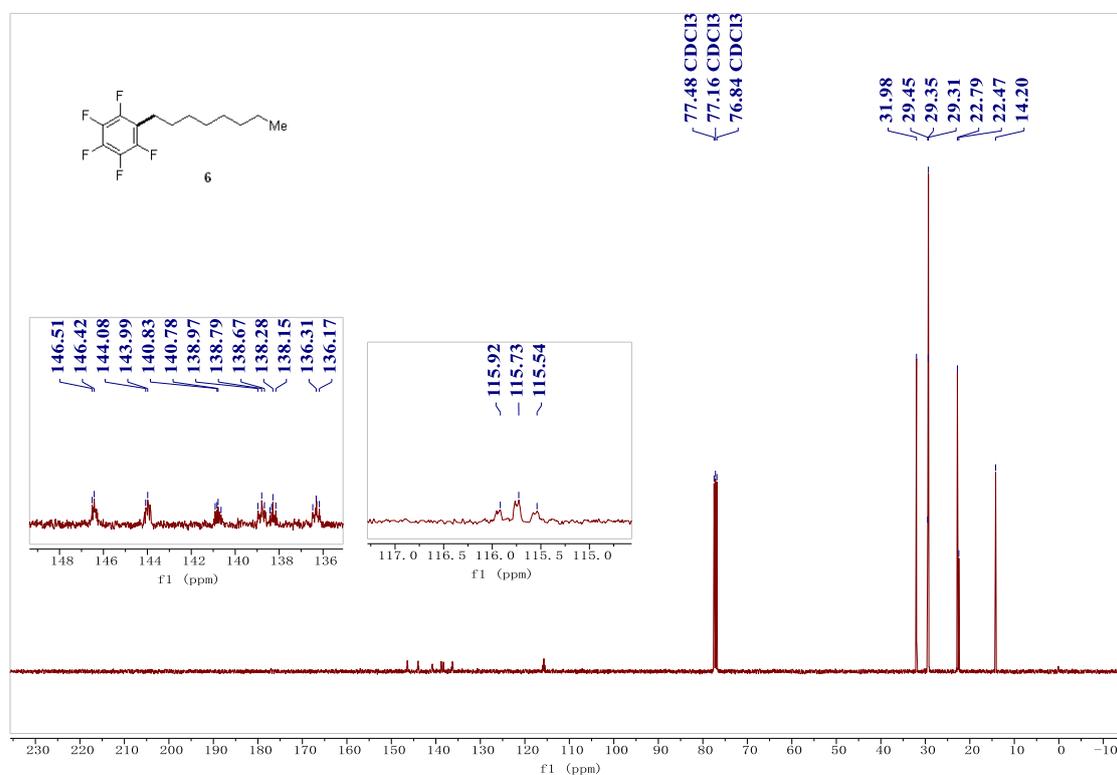
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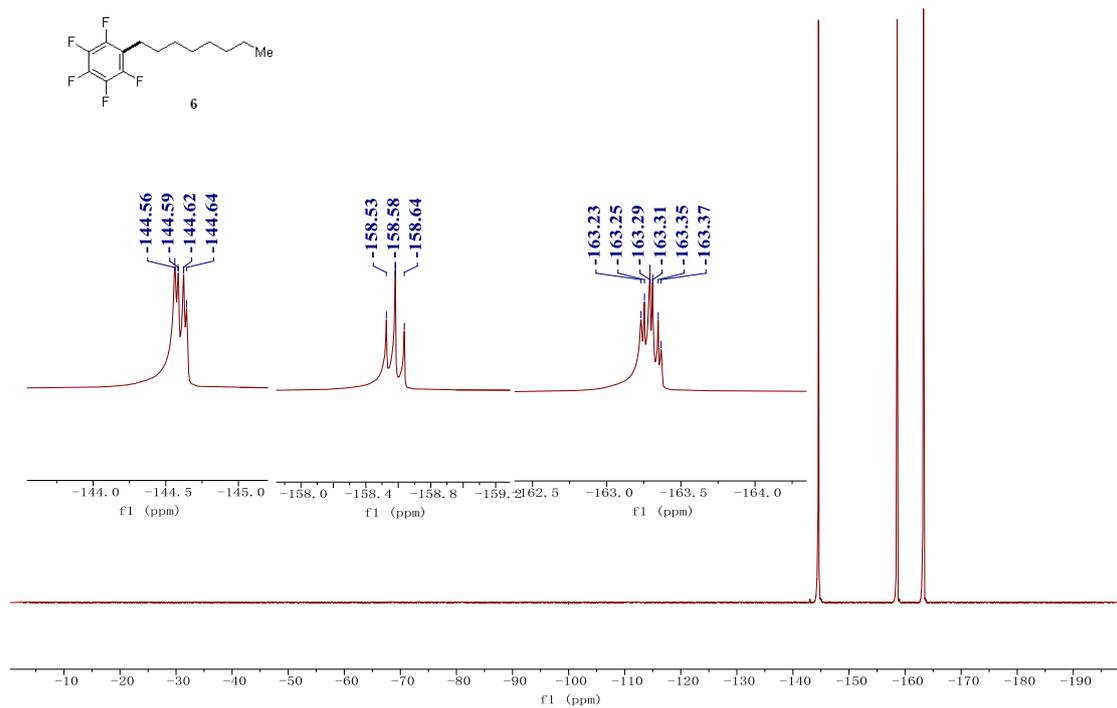
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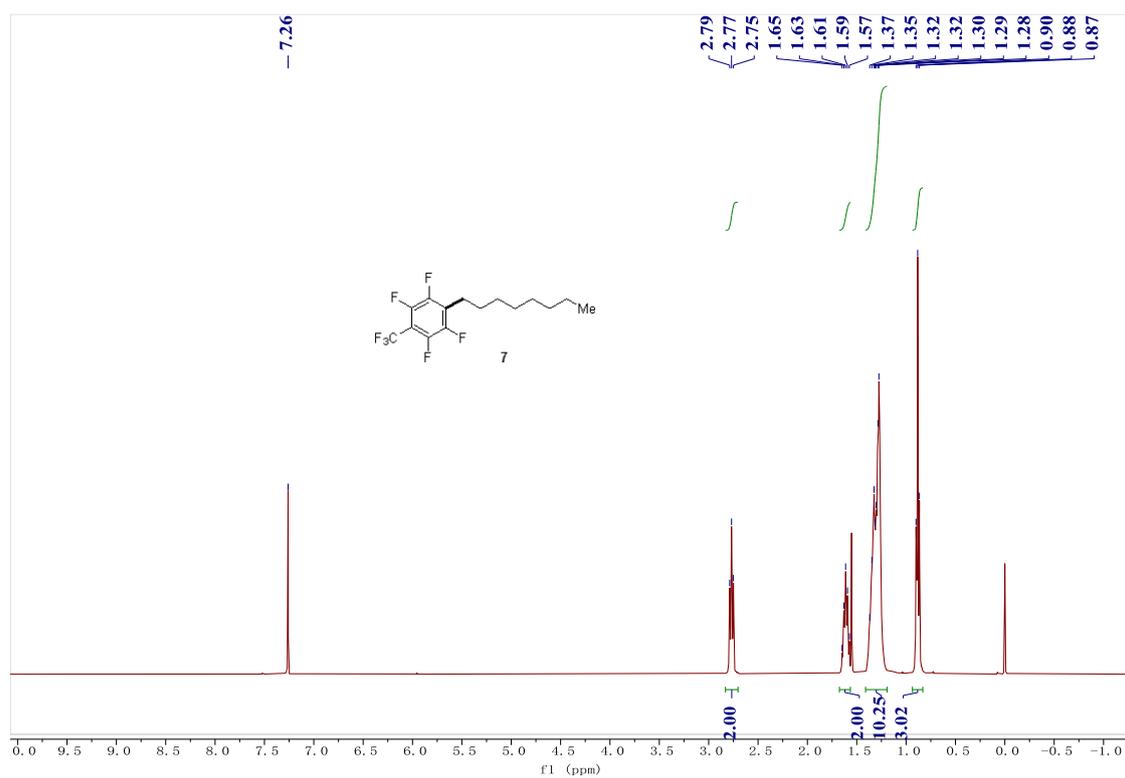
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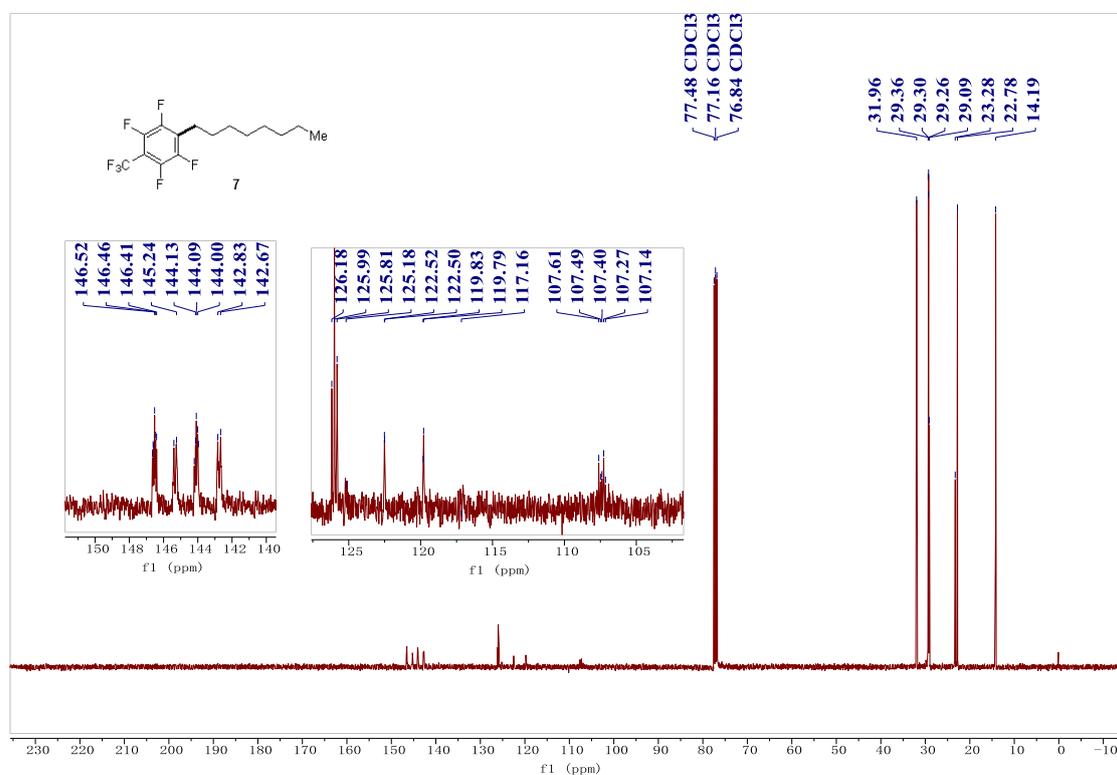
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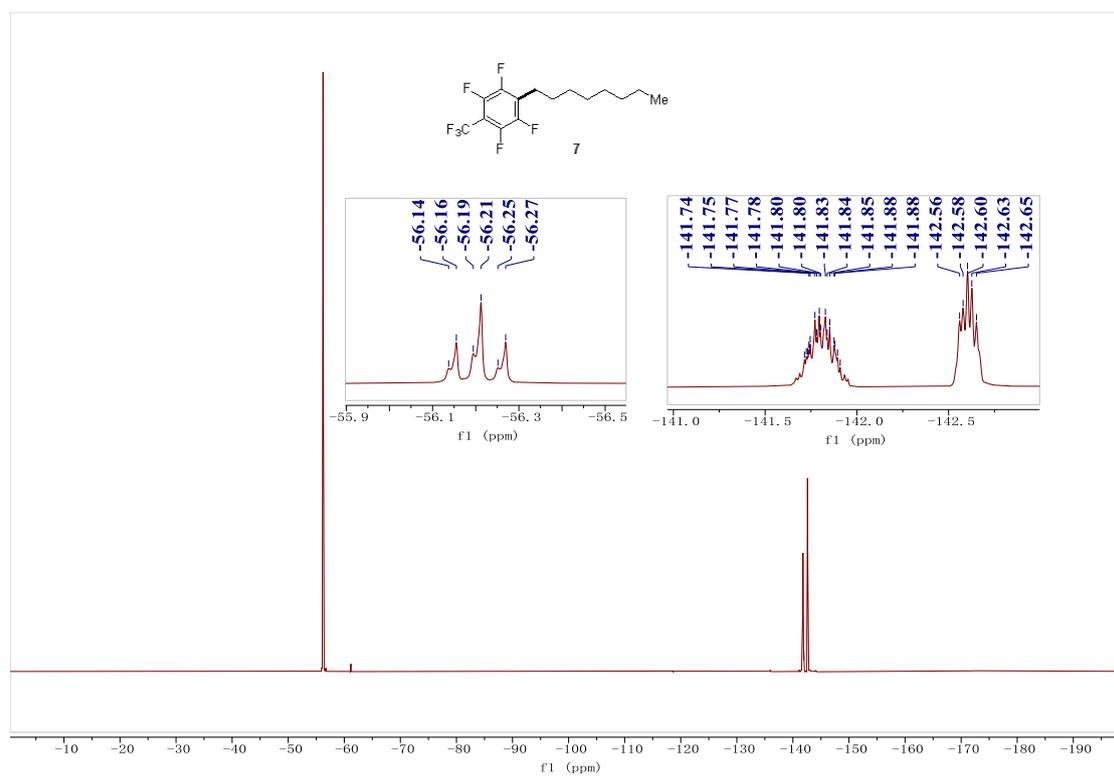
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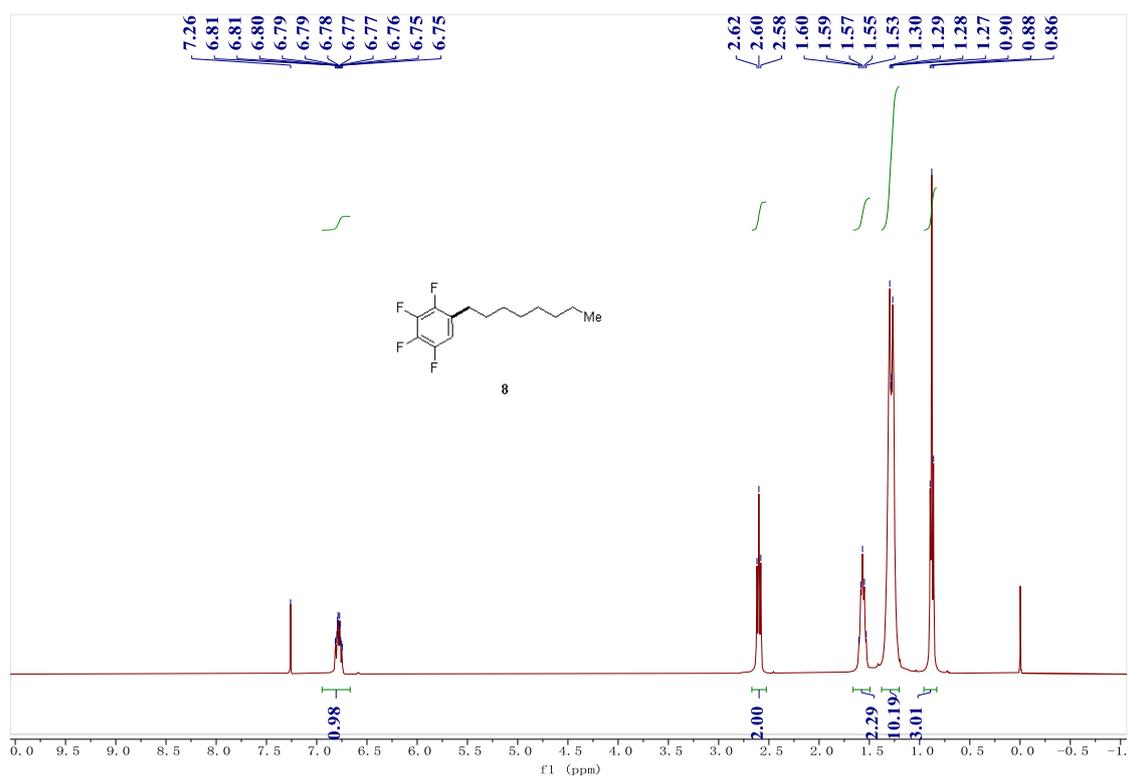
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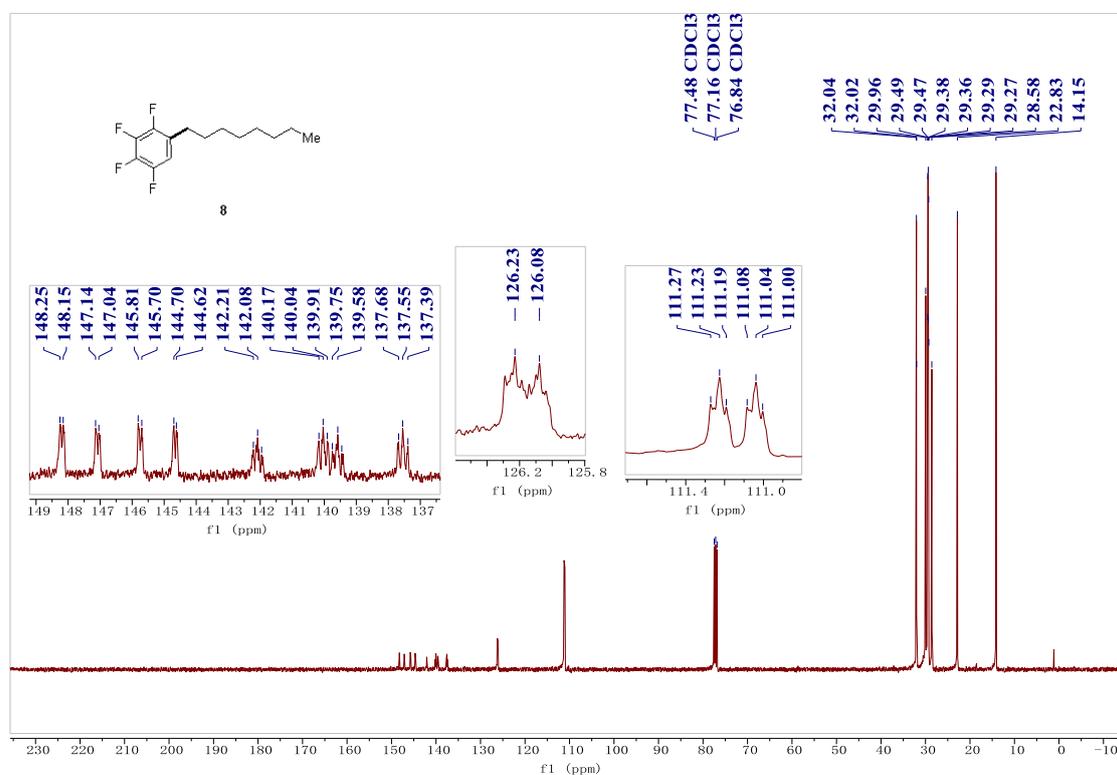
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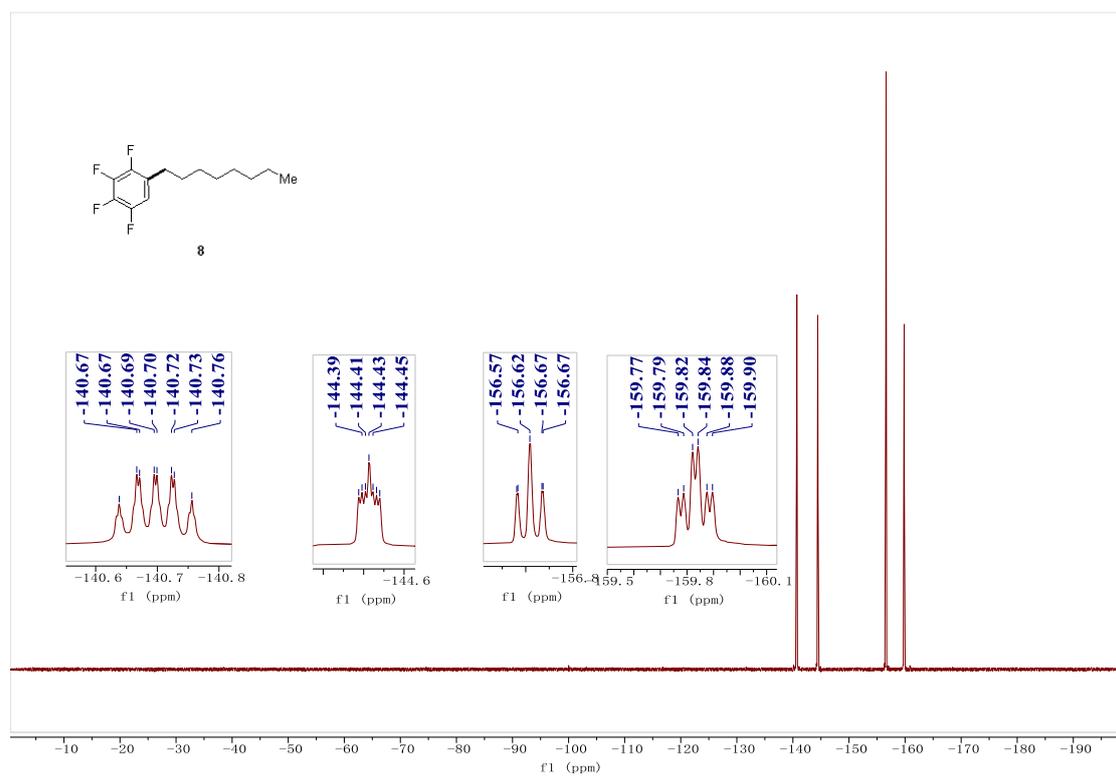
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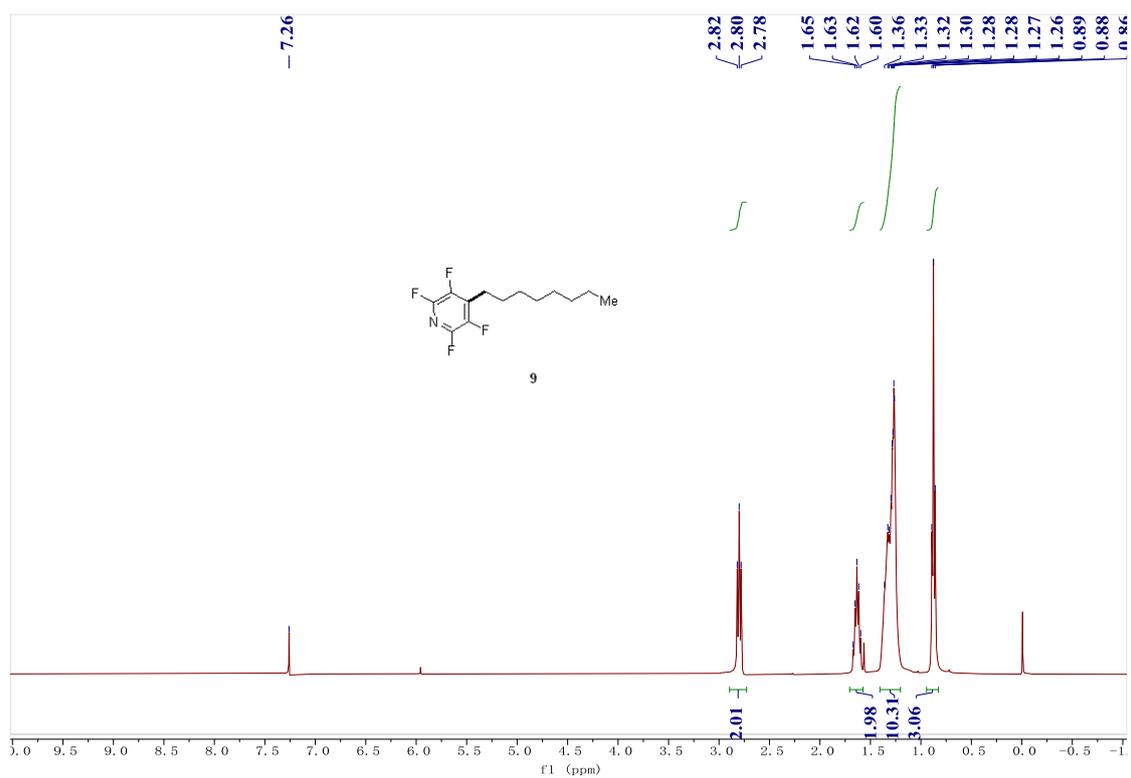
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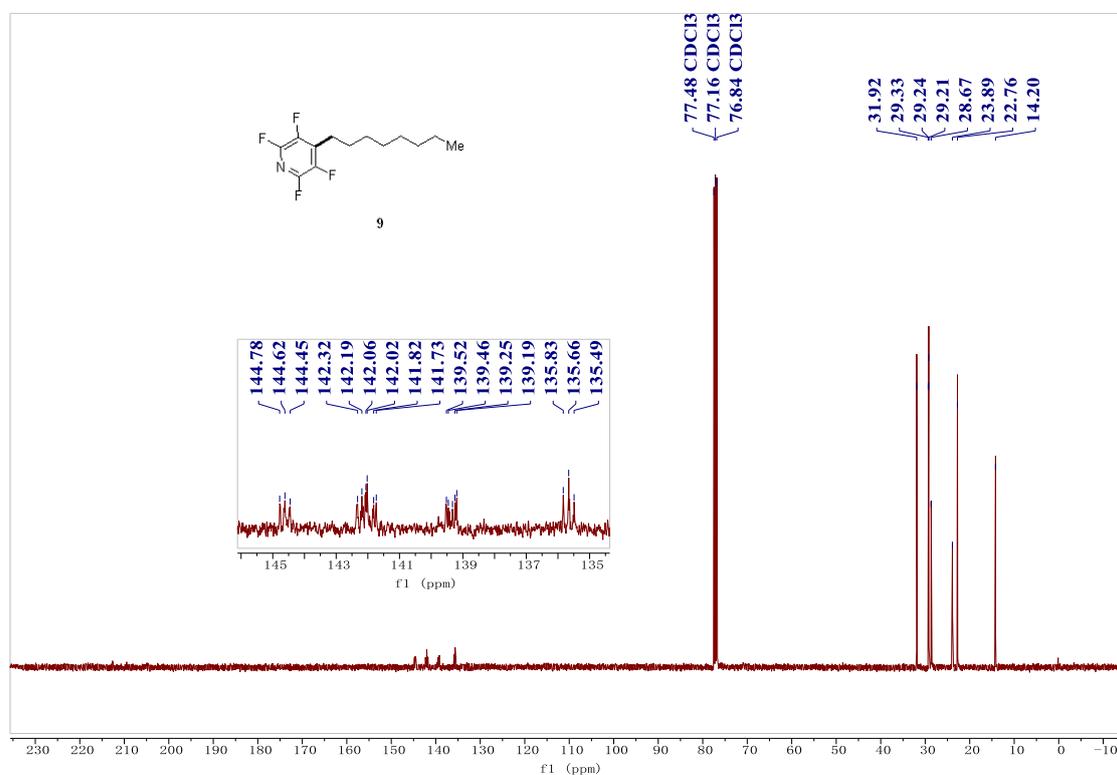
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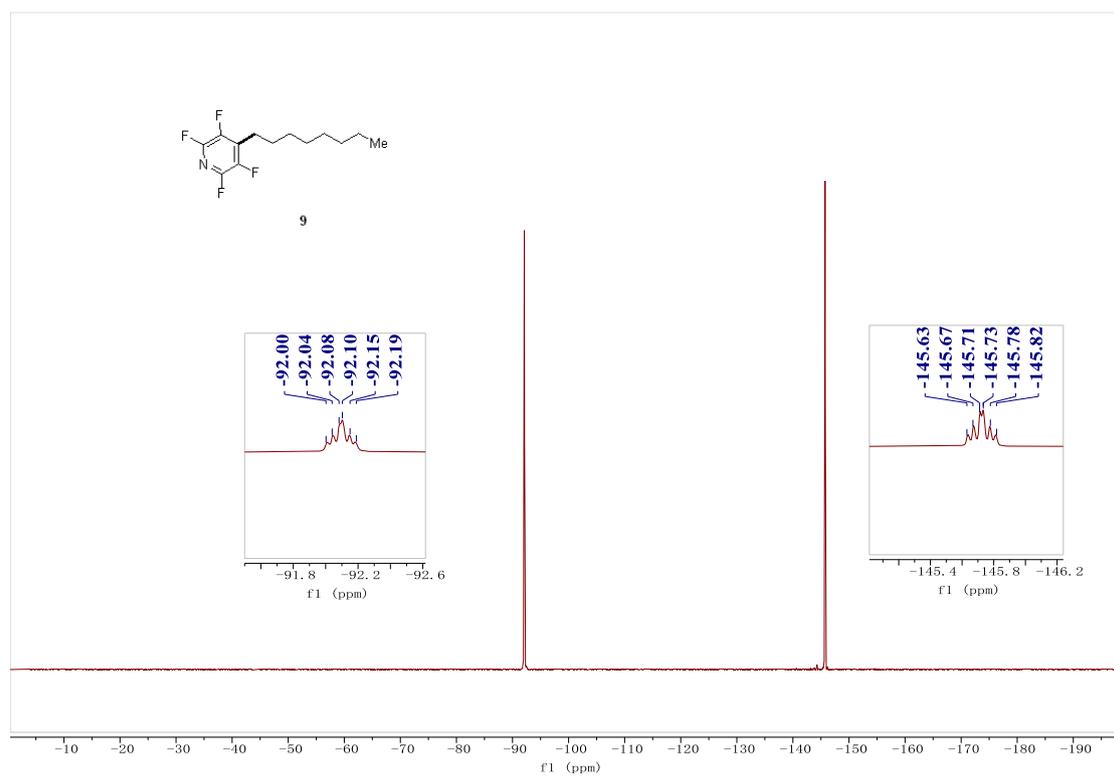
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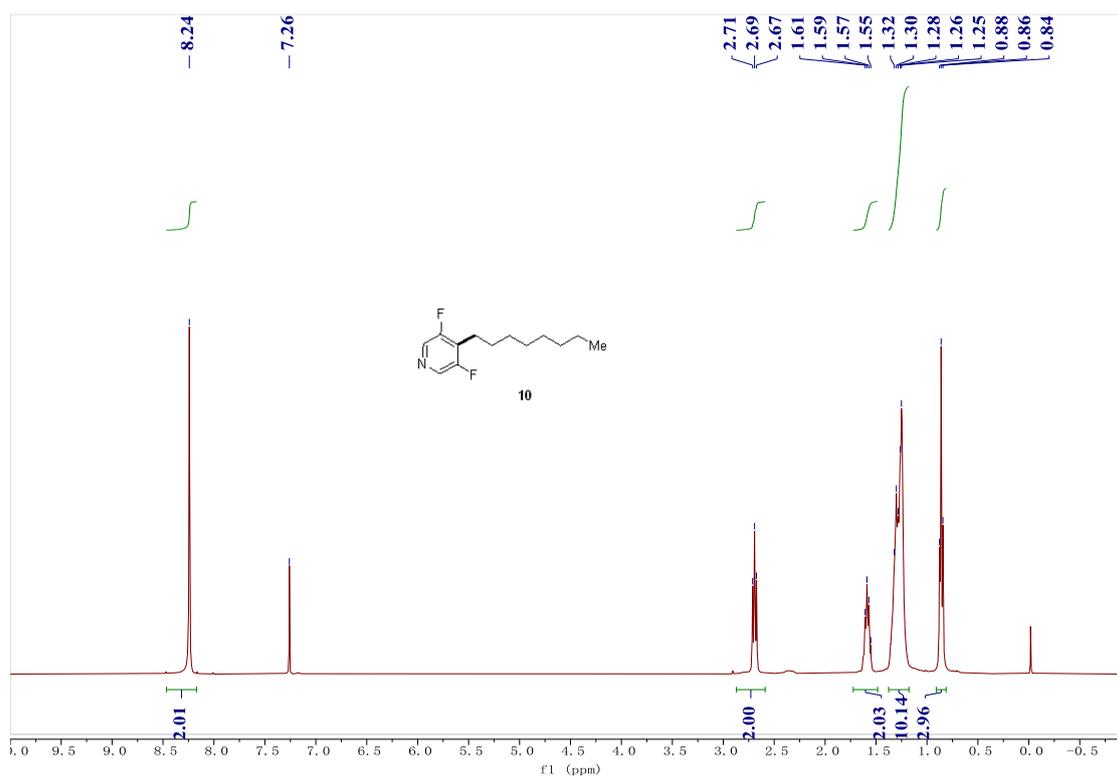
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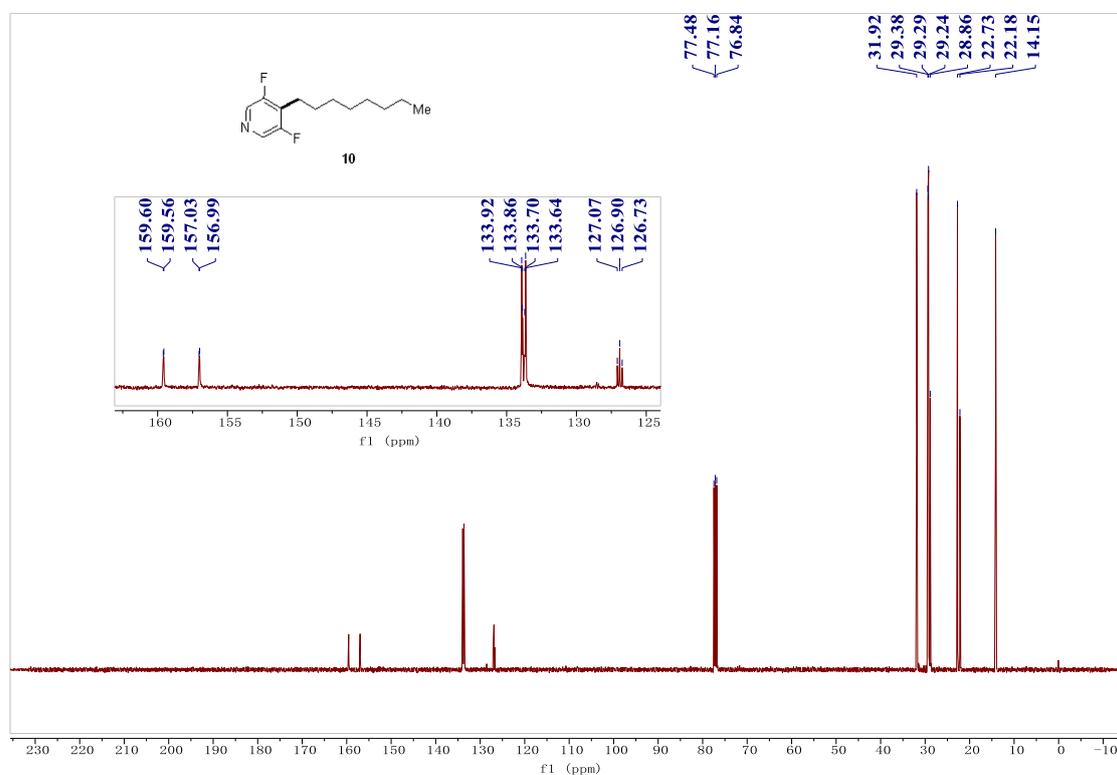
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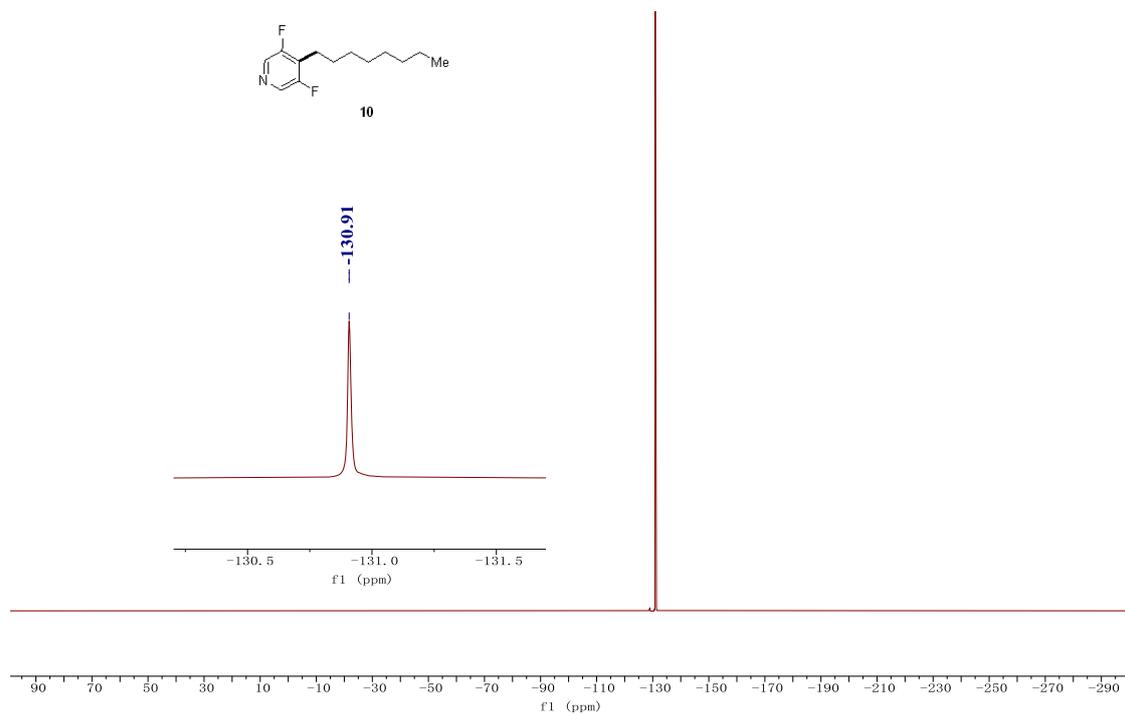
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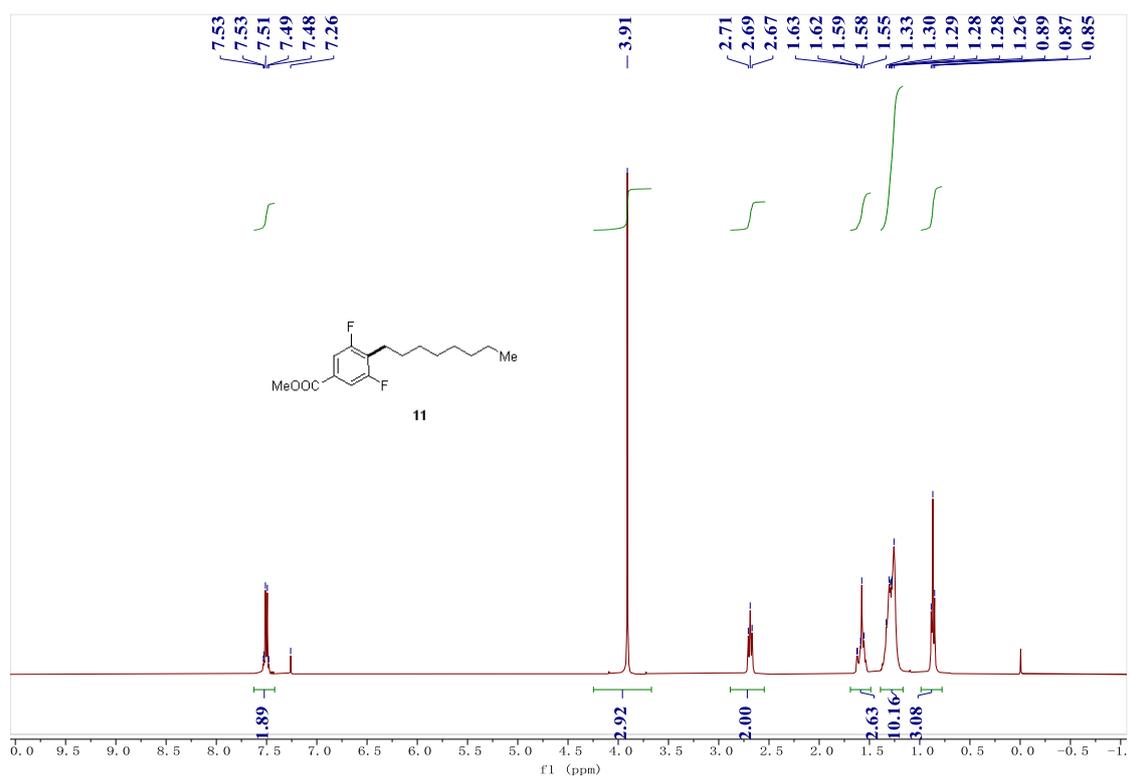
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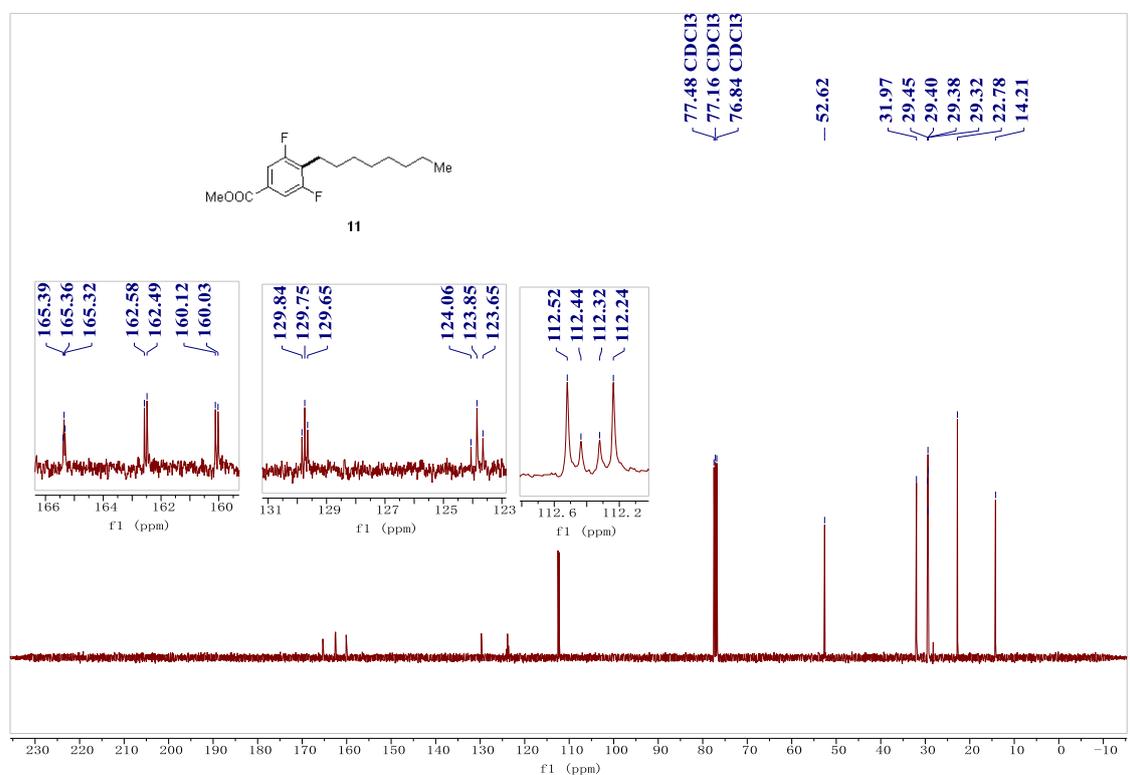
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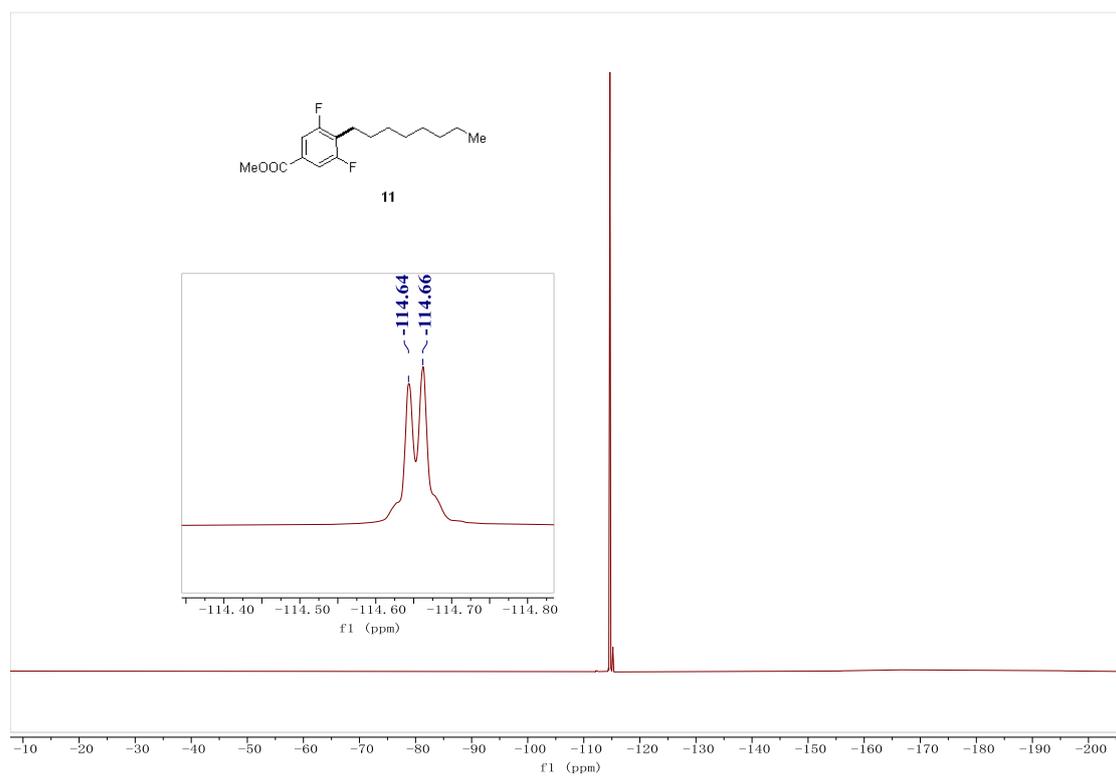
¹H NMR Spectrum of 11



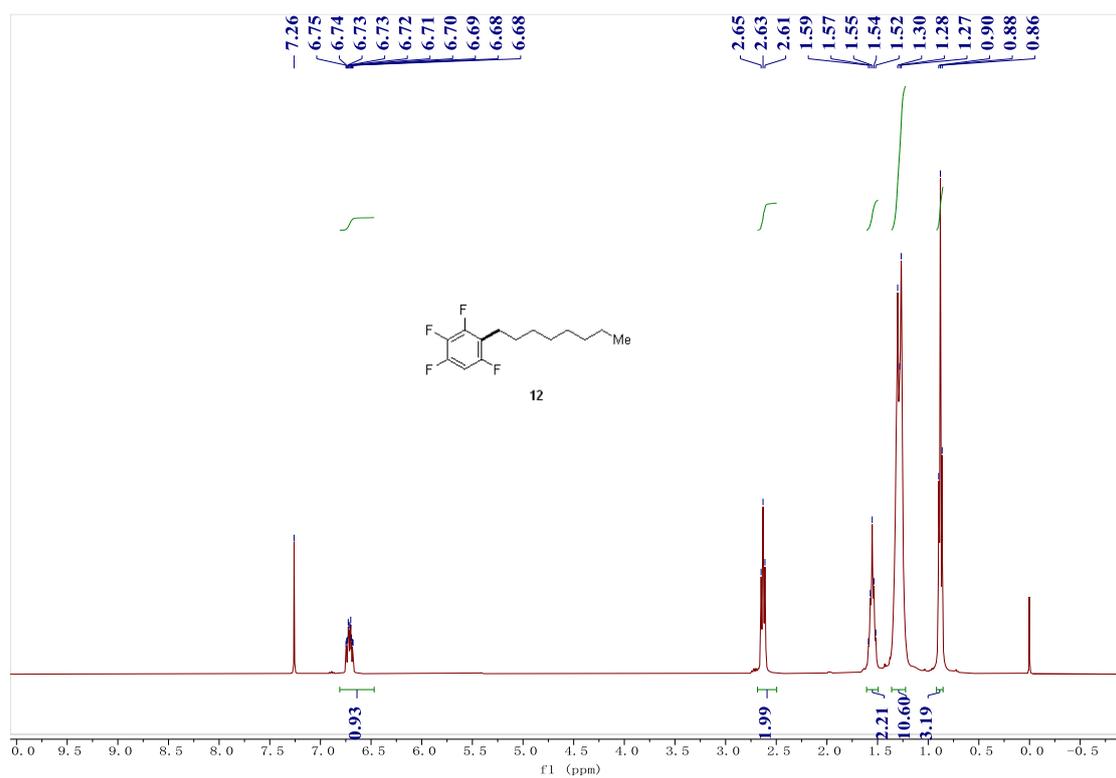
¹³C NMR Spectrum of 11



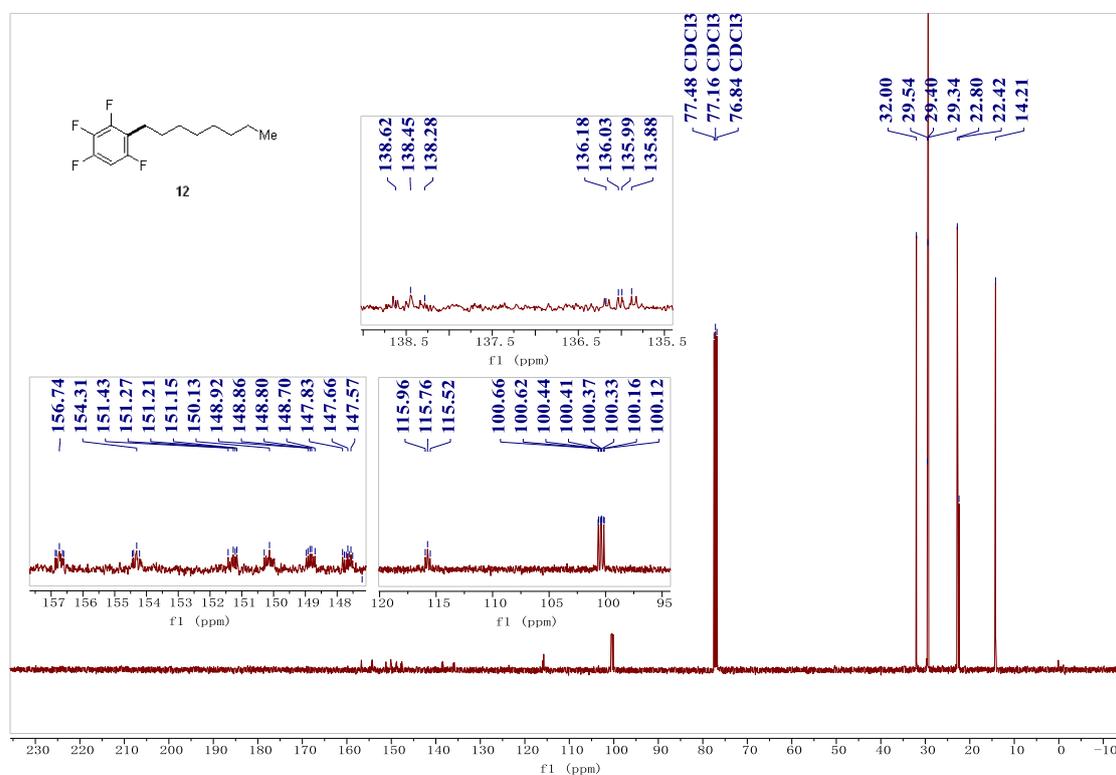
¹⁹F NMR Spectrum of 11



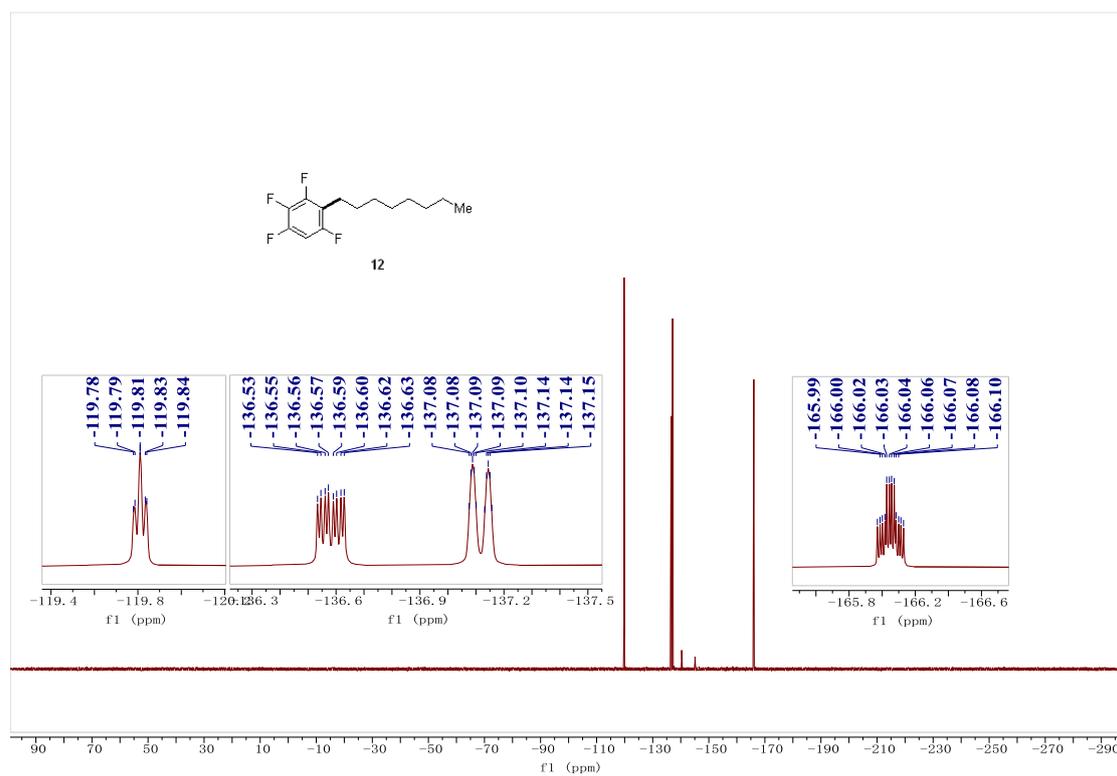
¹H NMR Spectrum of 12



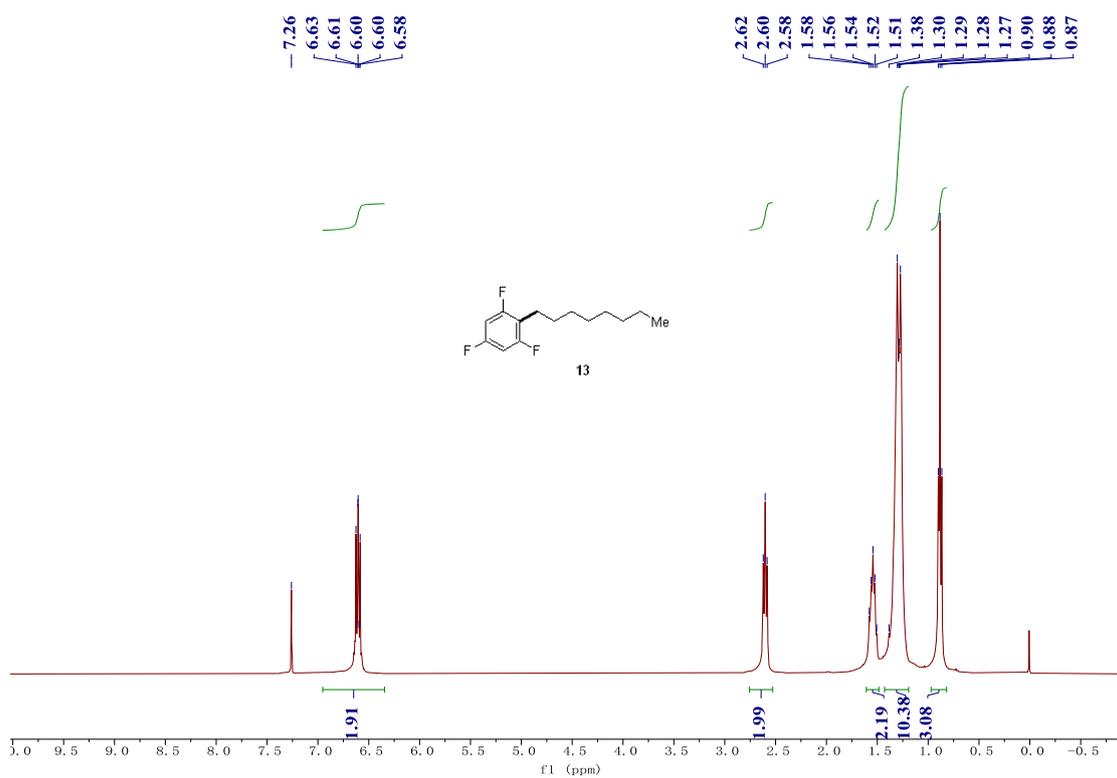
¹³C NMR Spectrum of 12



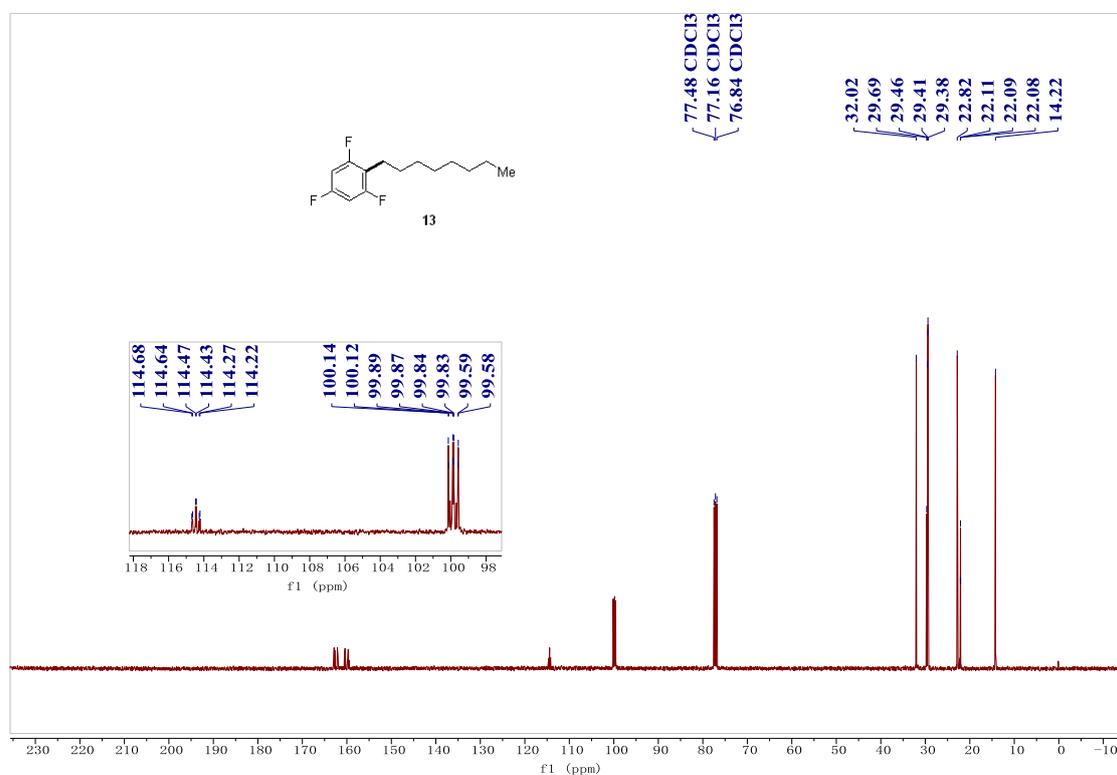
¹⁹F NMR Spectrum of 12



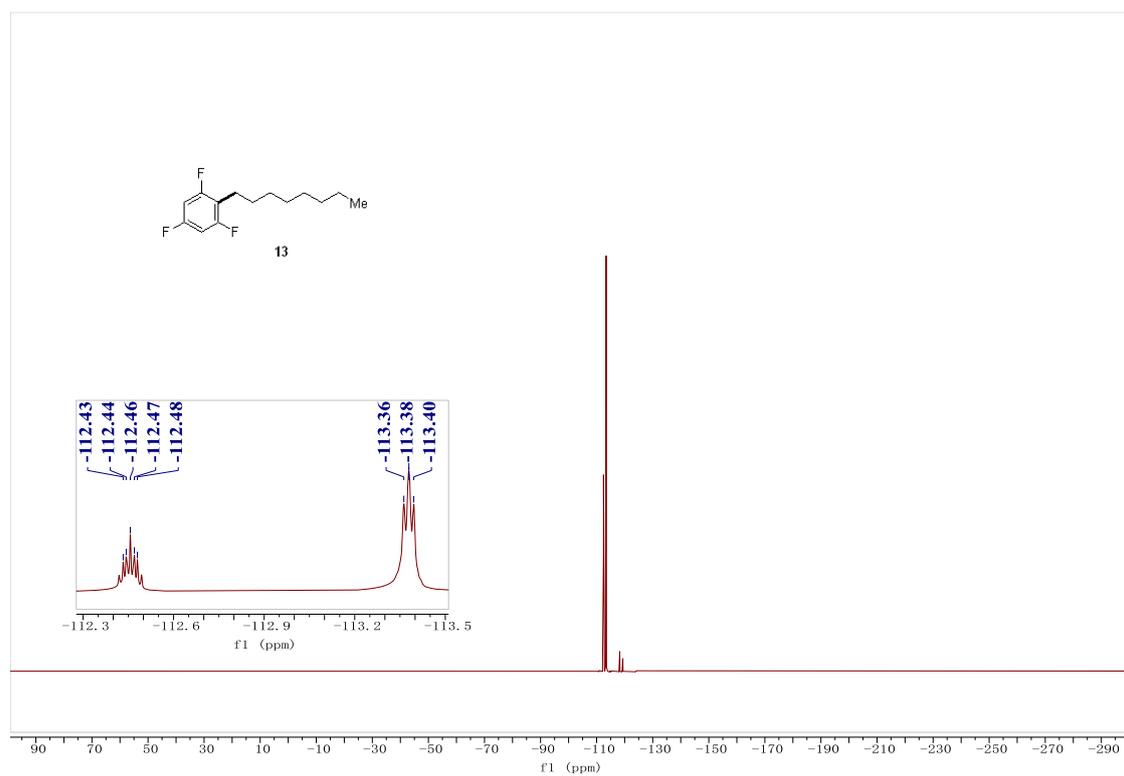
¹H NMR Spectrum of 13



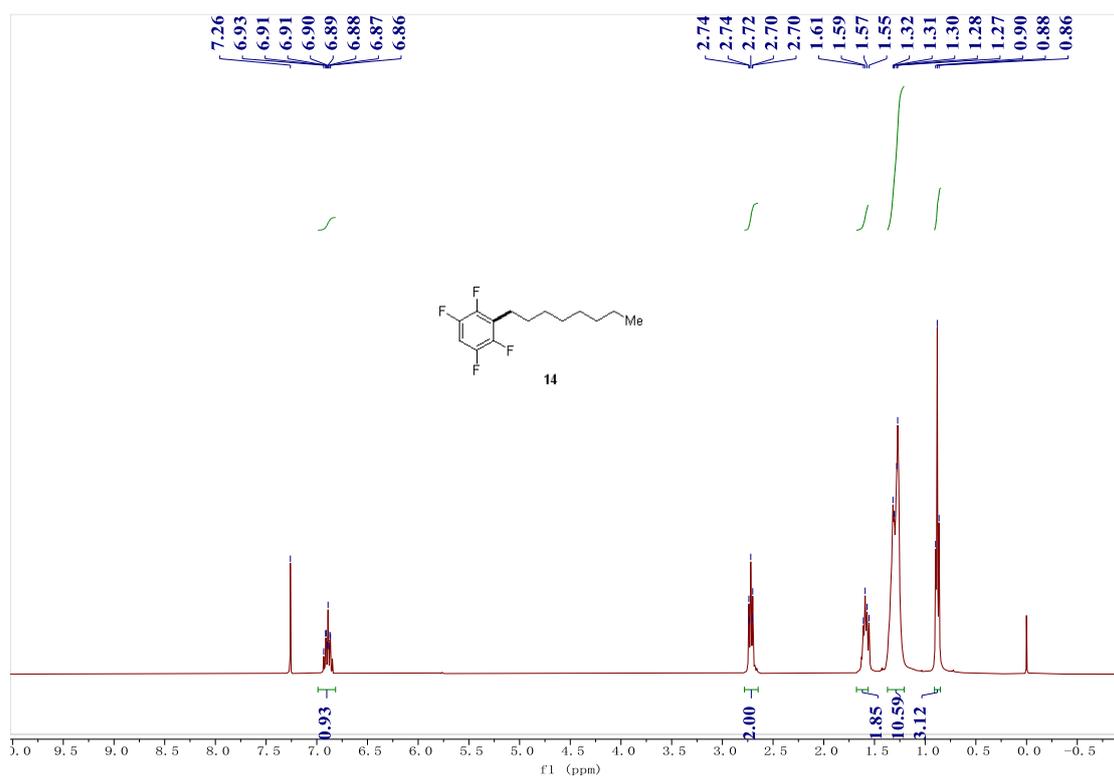
¹³C NMR Spectrum of 13



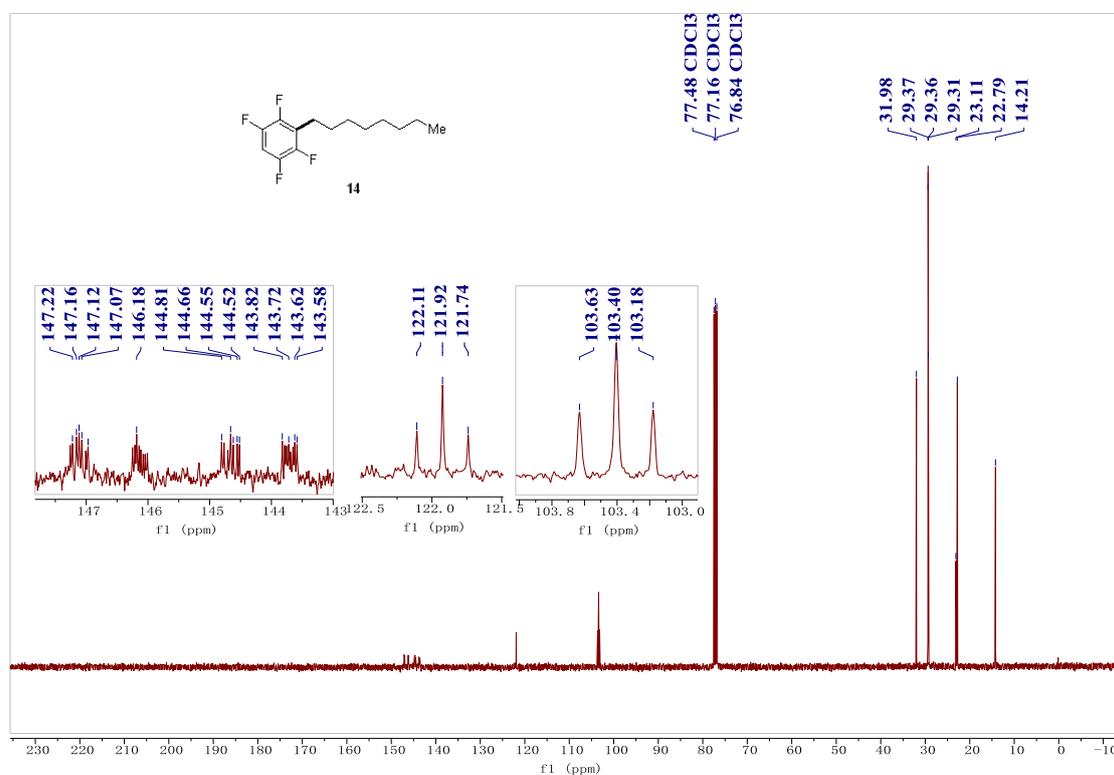
¹⁹F NMR Spectrum of 13



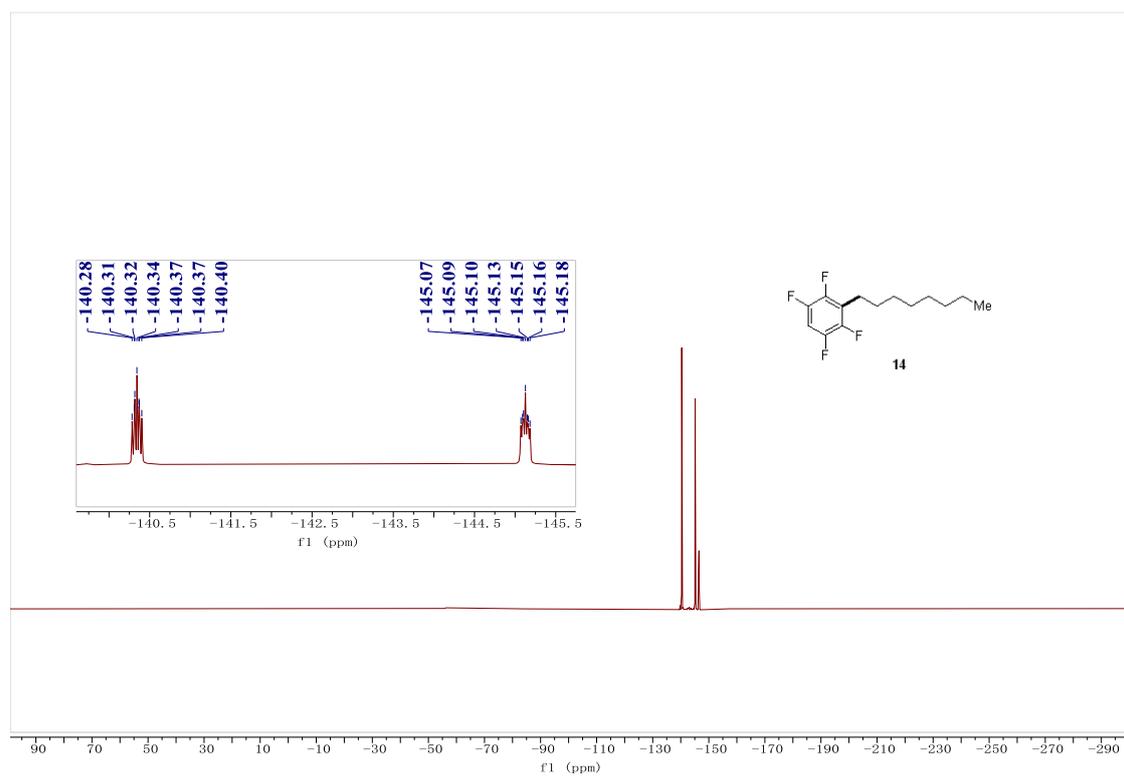
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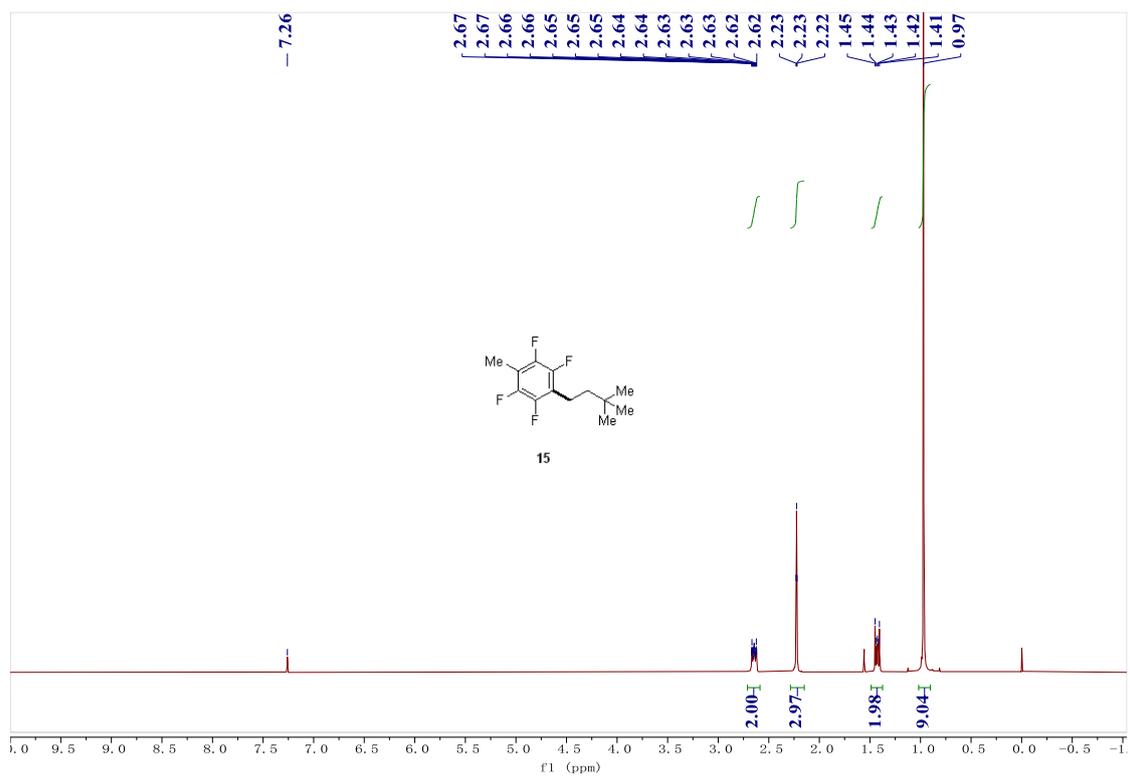
¹³C NMR Spectrum of 14



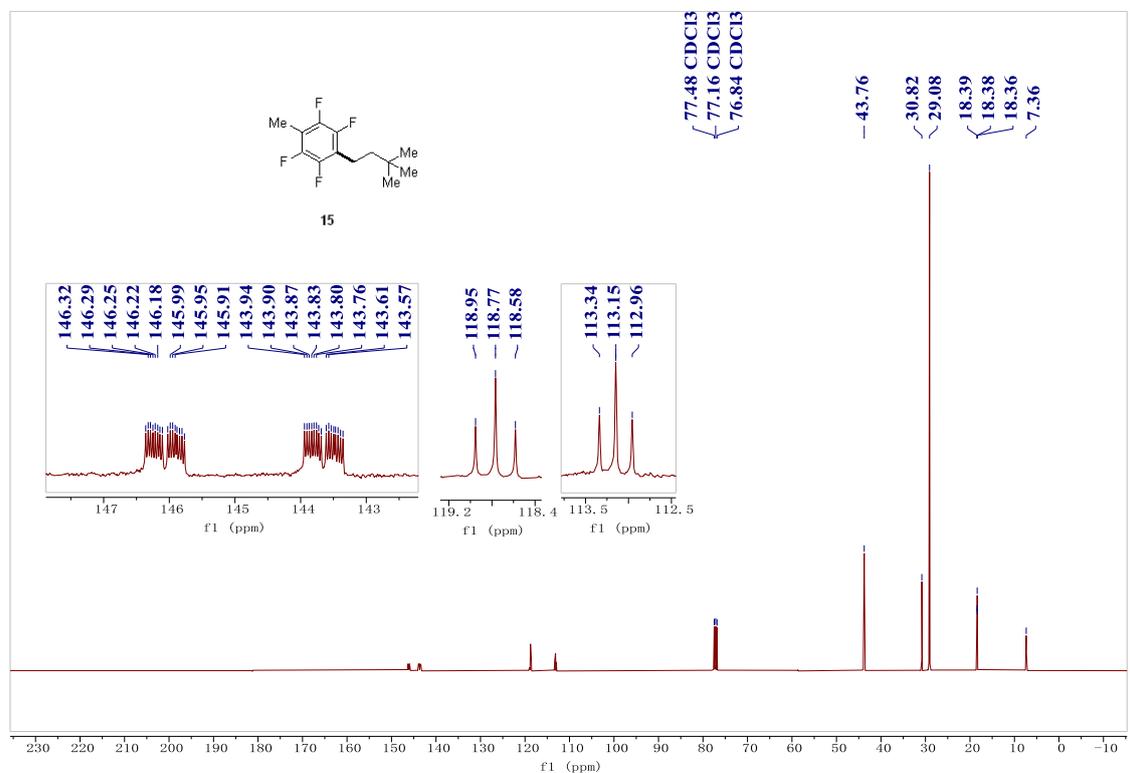
¹⁹F NMR Spectrum of 14



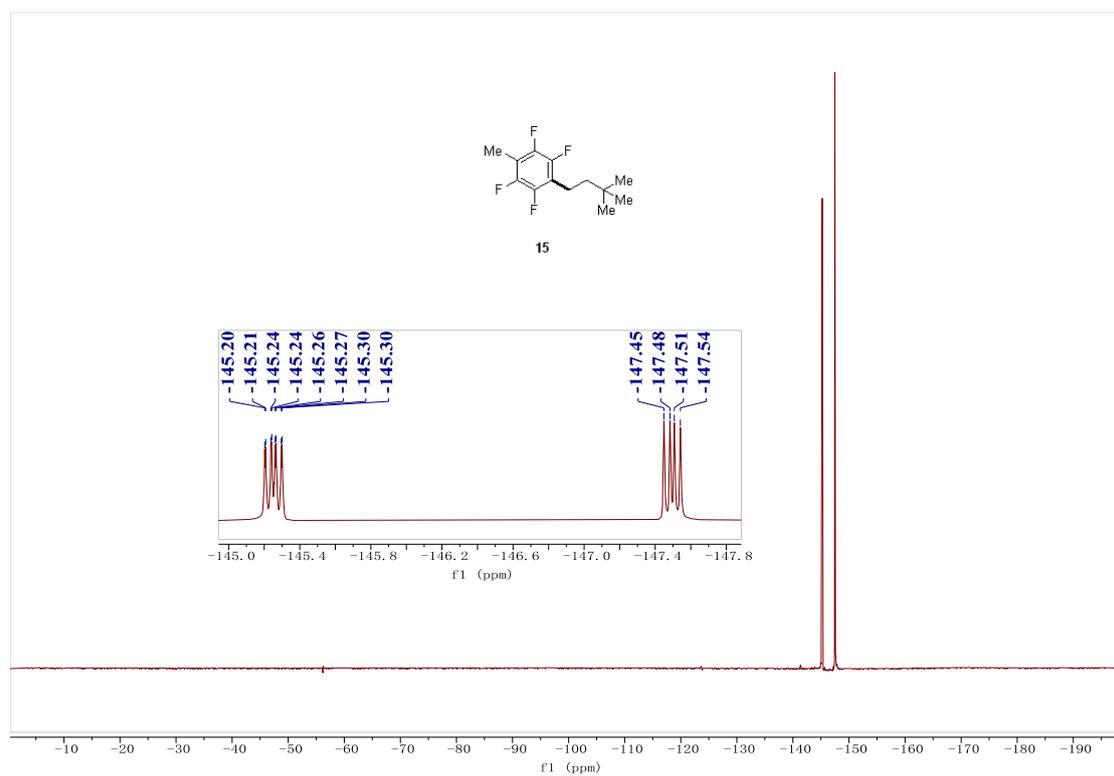
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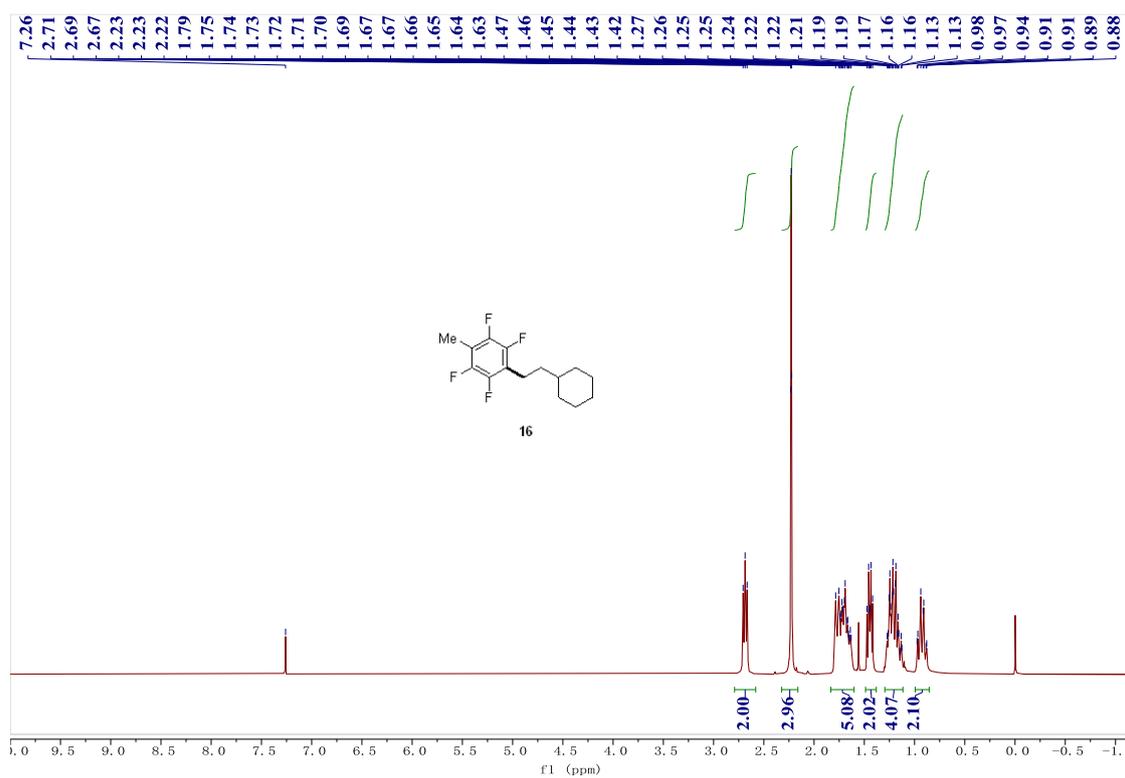
¹³C NMR Spectrum of 15



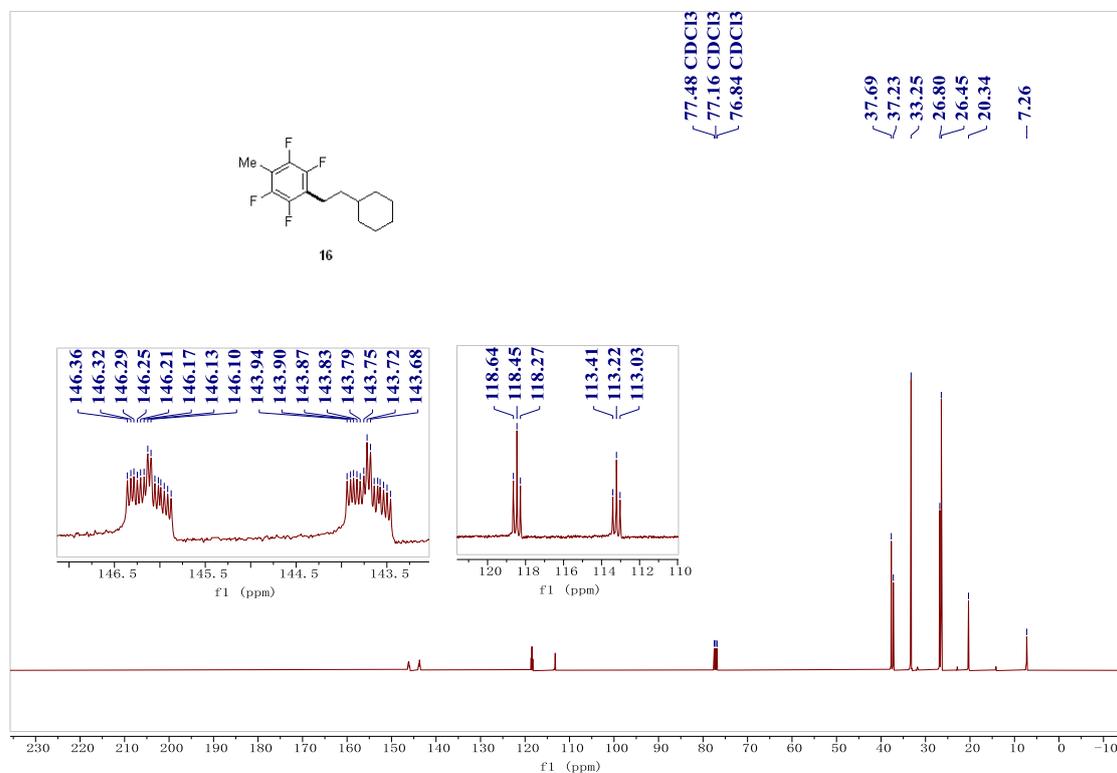
¹⁹F NMR Spectrum of 15



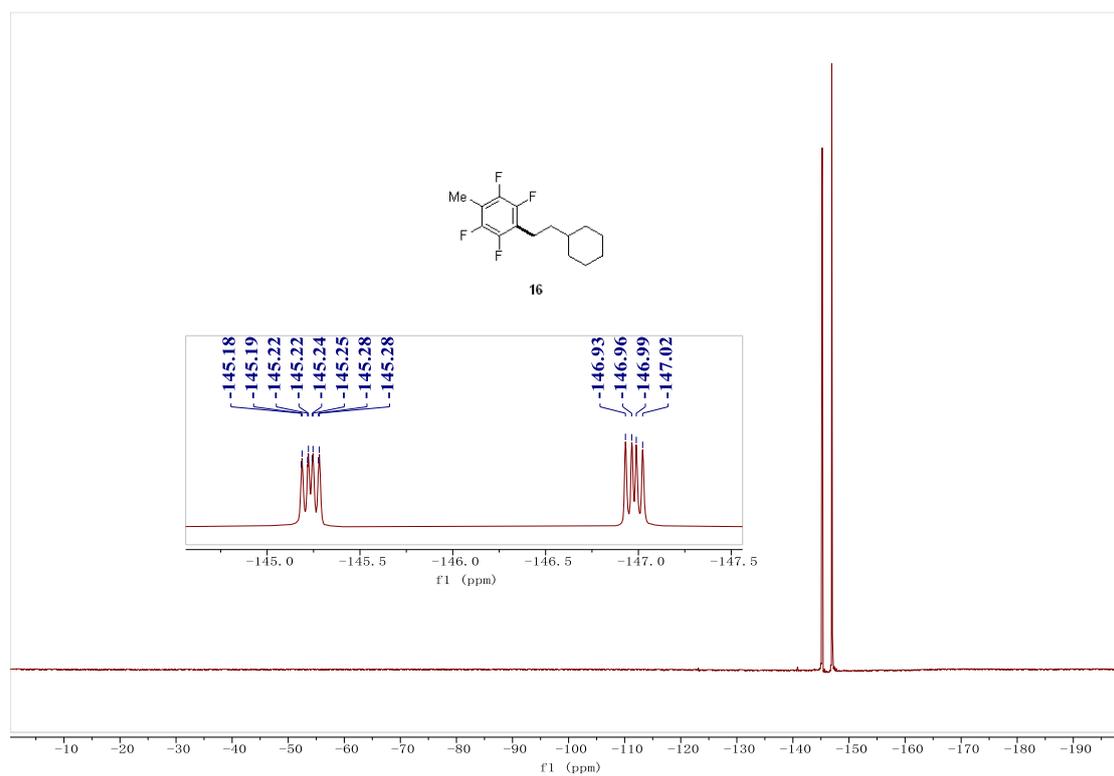
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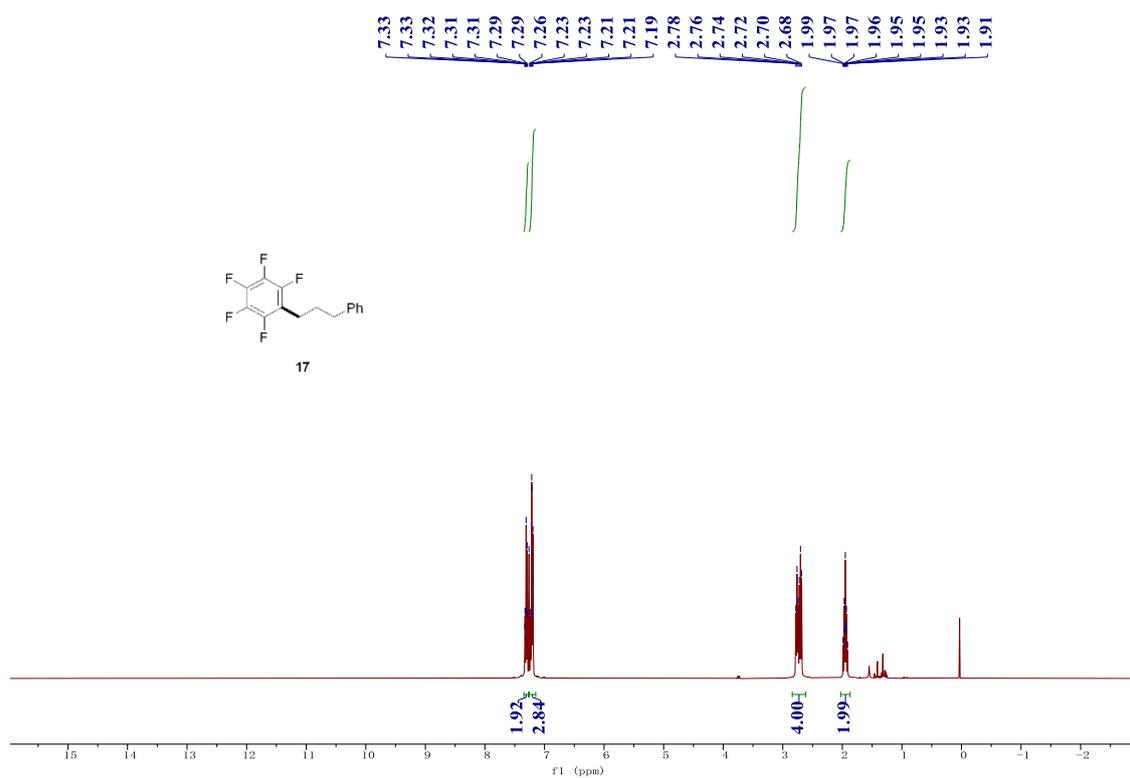
¹³C NMR Spectrum of 16



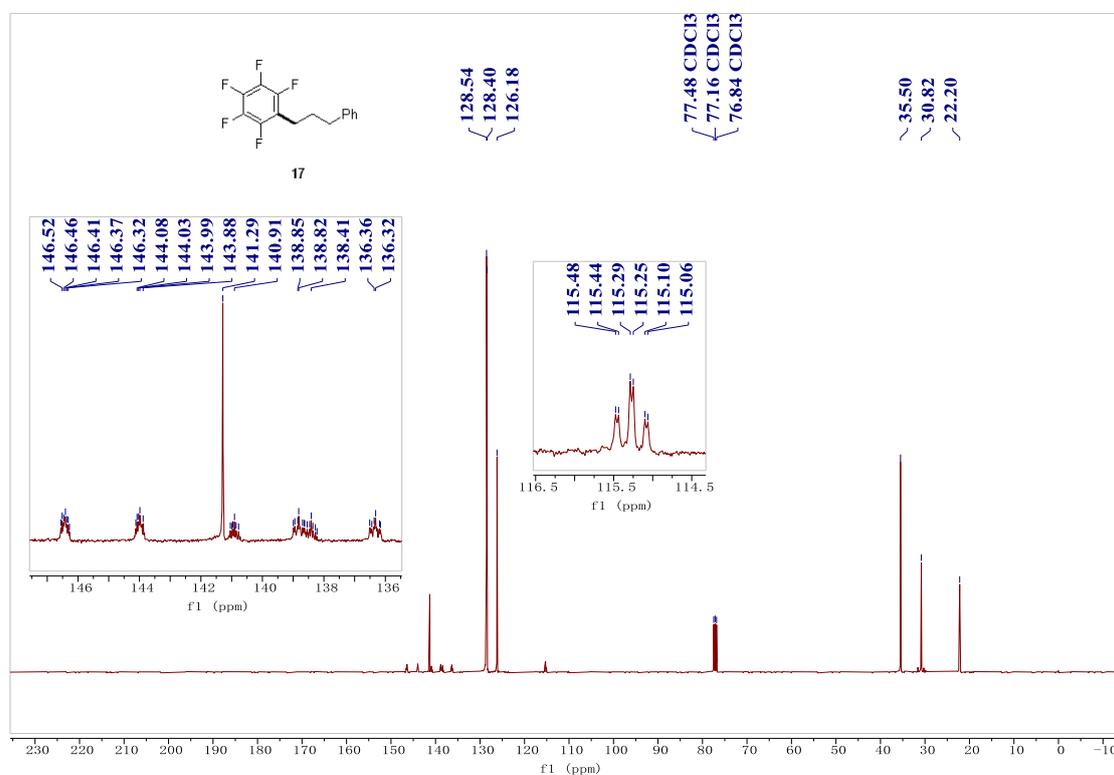
¹⁹F NMR Spectrum of 16



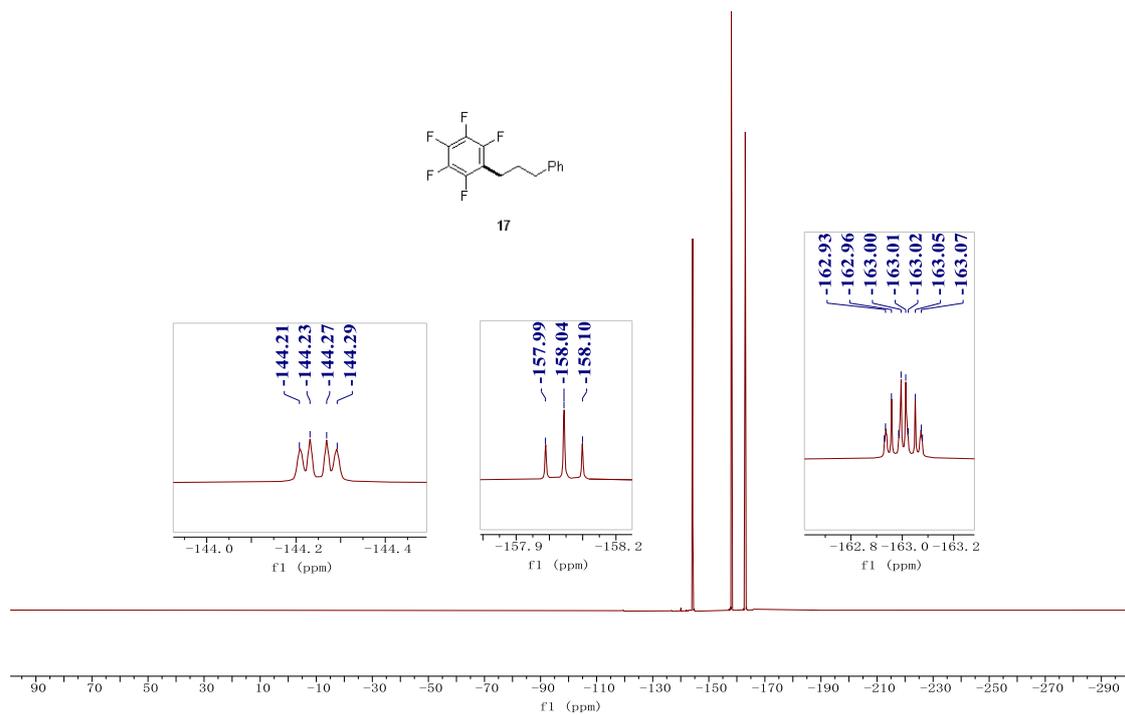
¹H NMR Spectrum of 17



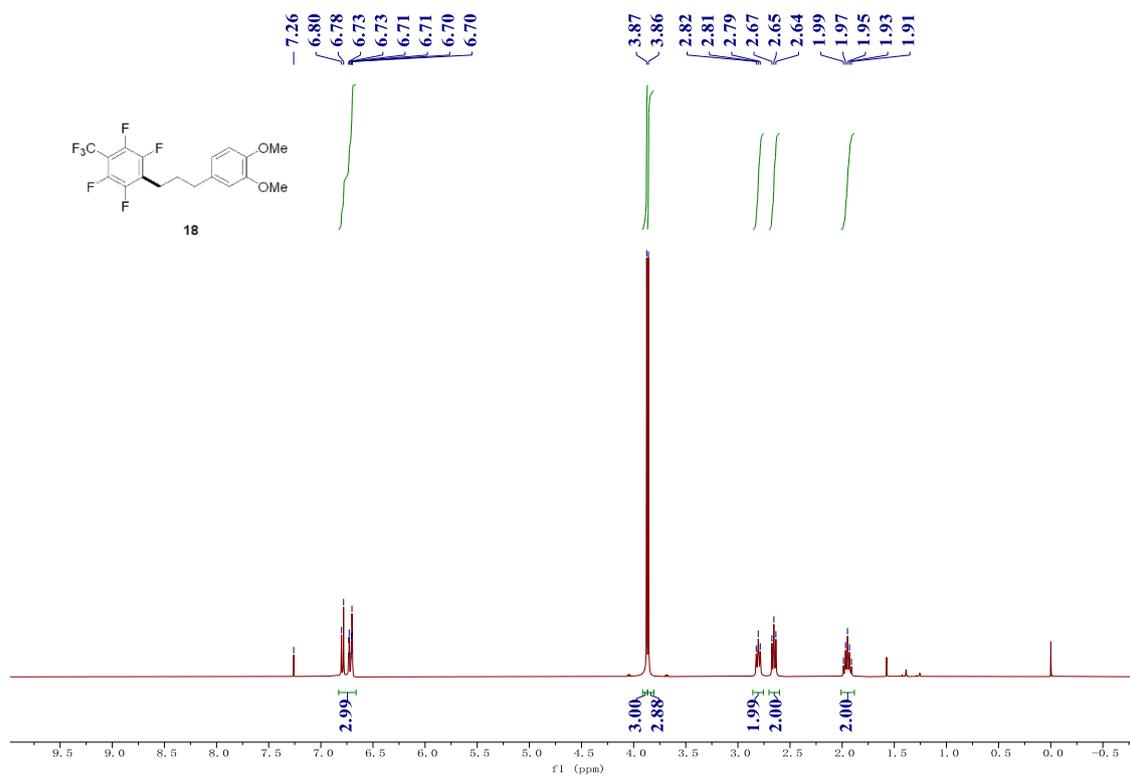
¹³C NMR Spectrum of 17



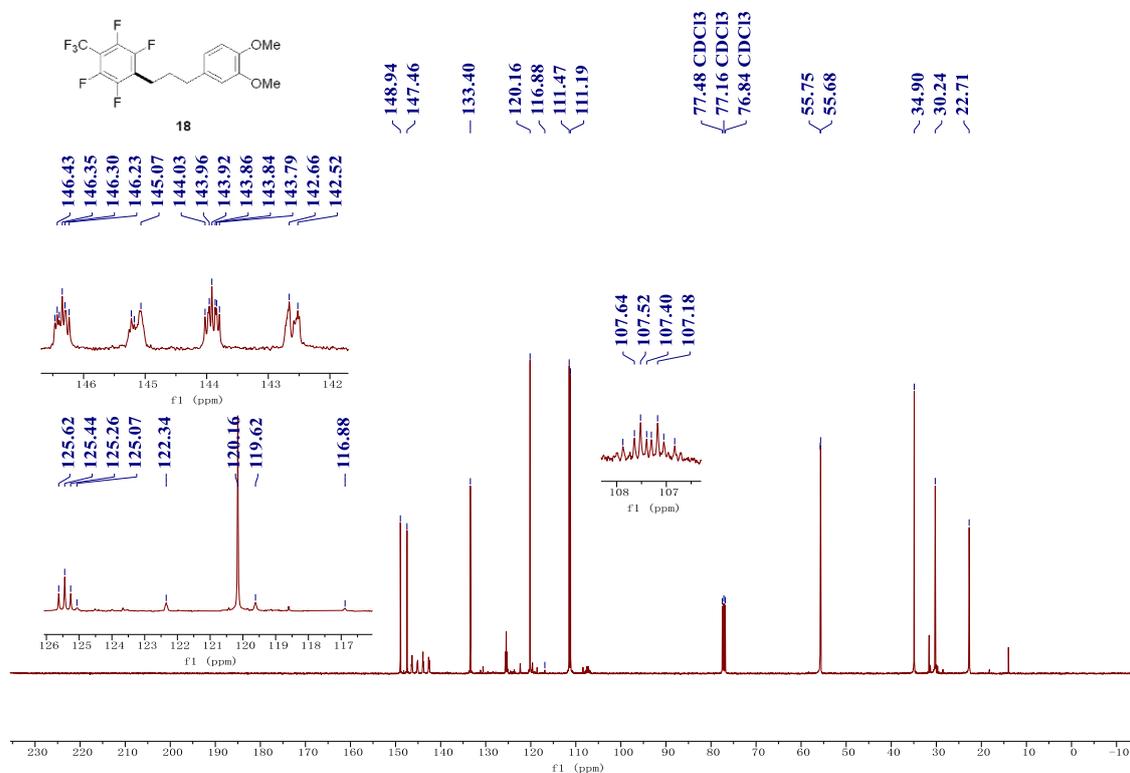
¹⁹F NMR Spectrum of 17



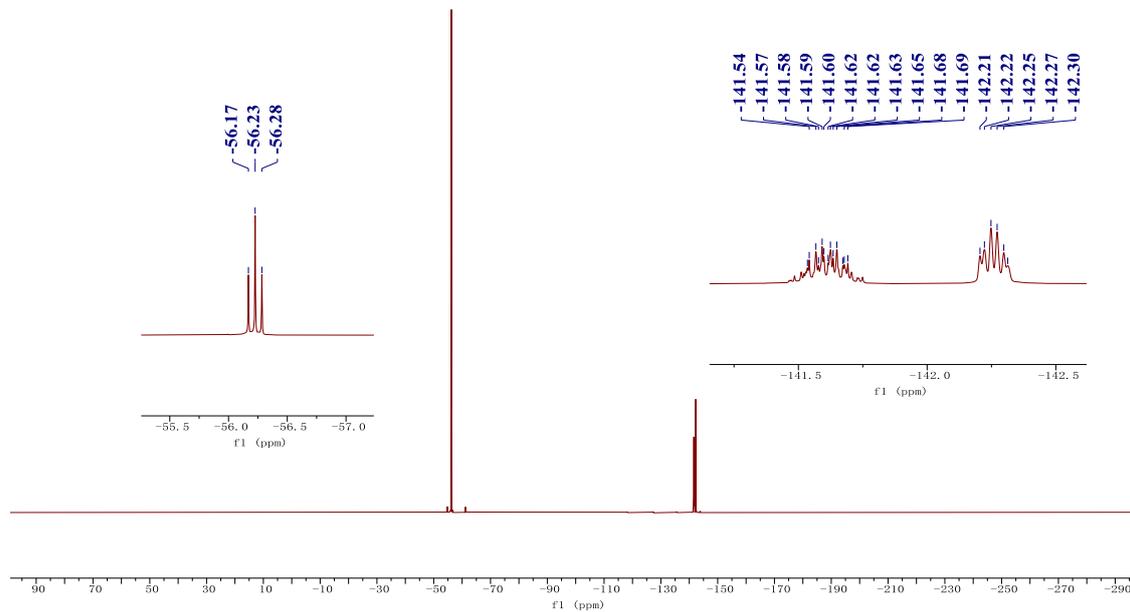
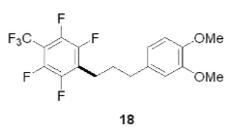
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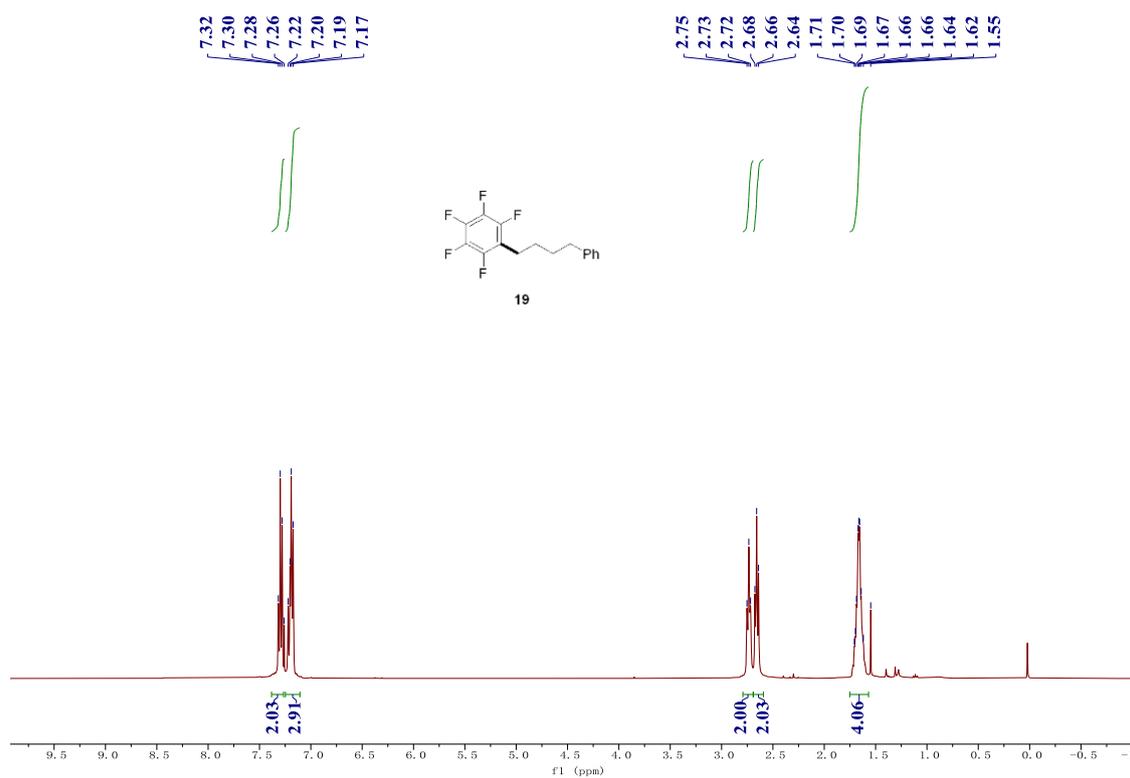
¹³C NMR Spectrum of 18



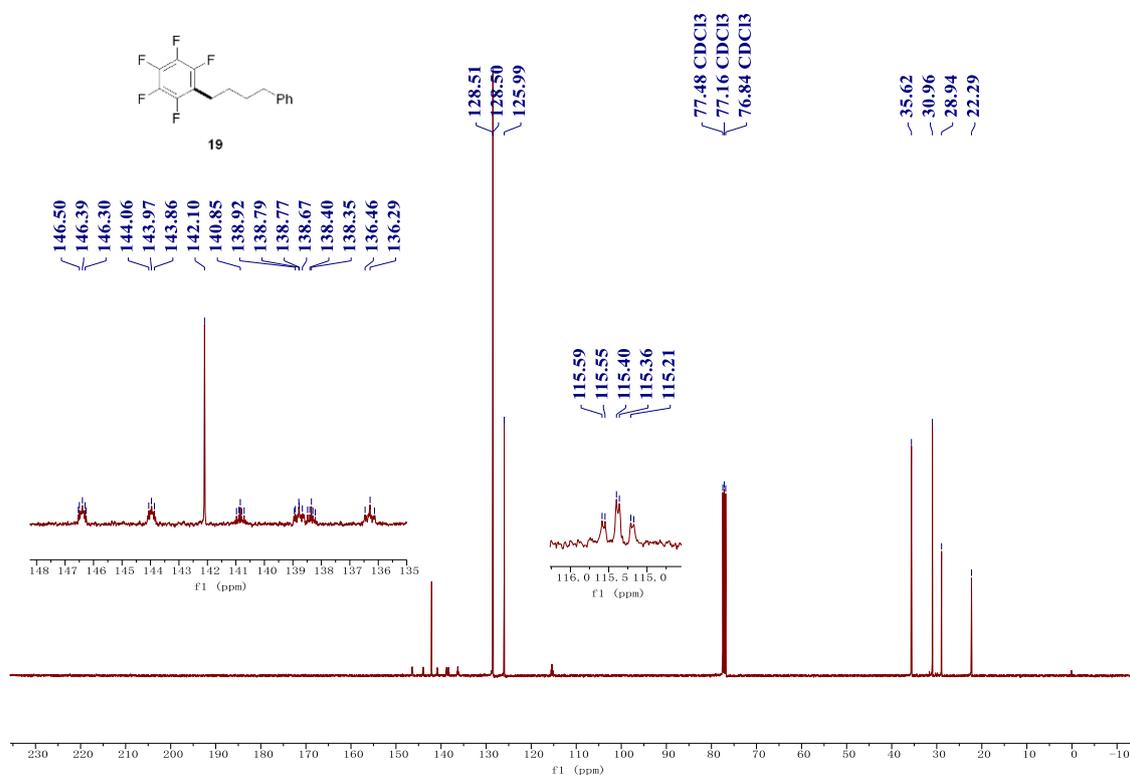
¹⁹F NMR Spectrum of 18



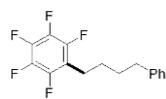
¹H NMR Spectrum of 19



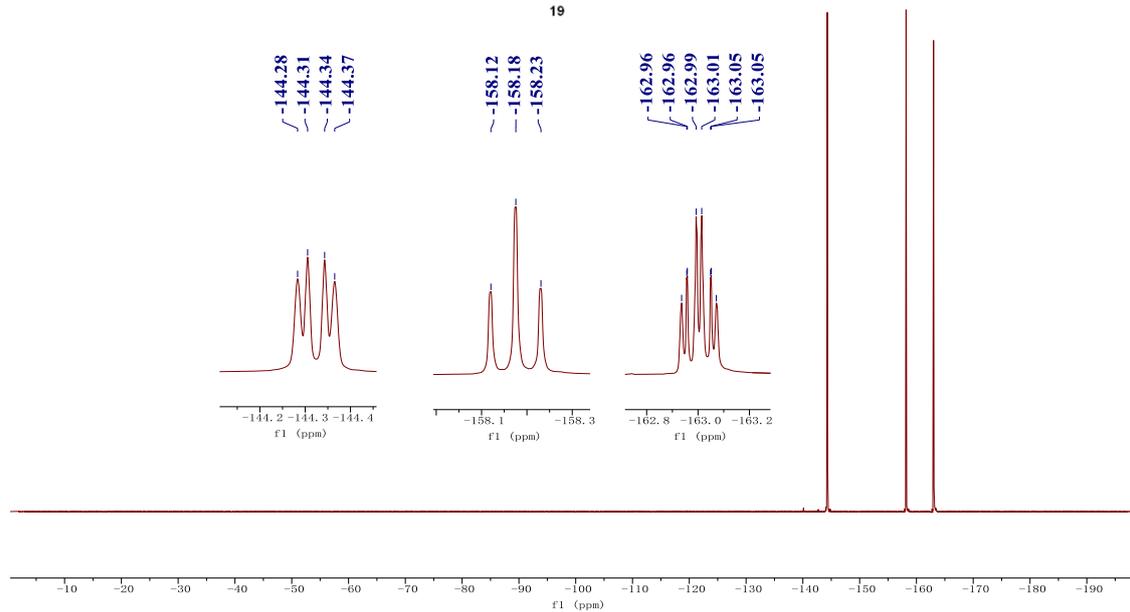
¹³C NMR Spectrum of 19



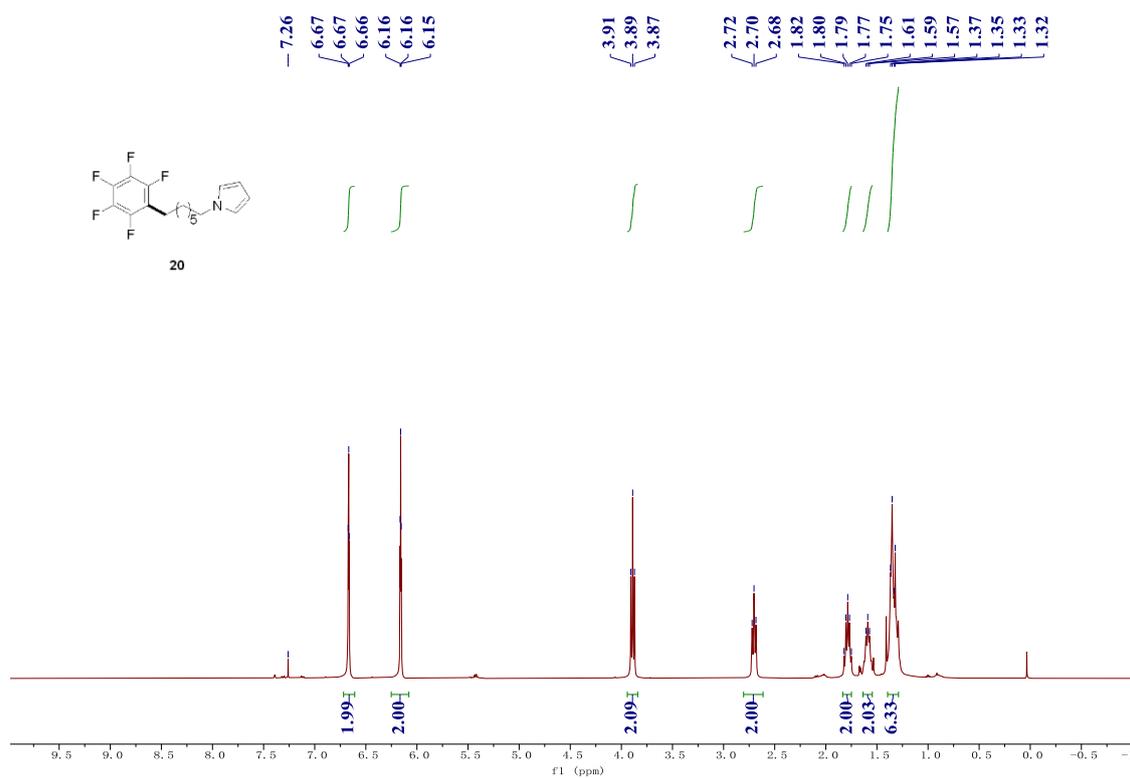
¹⁹F NMR Spectrum of 19



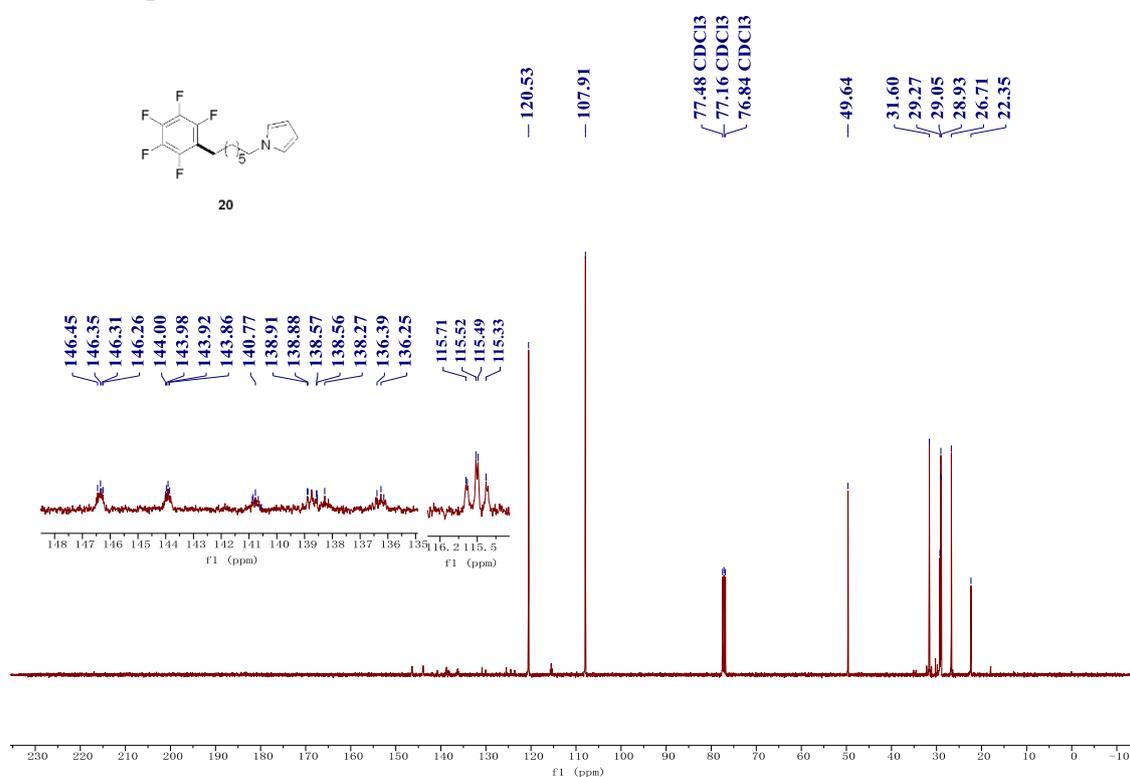
19



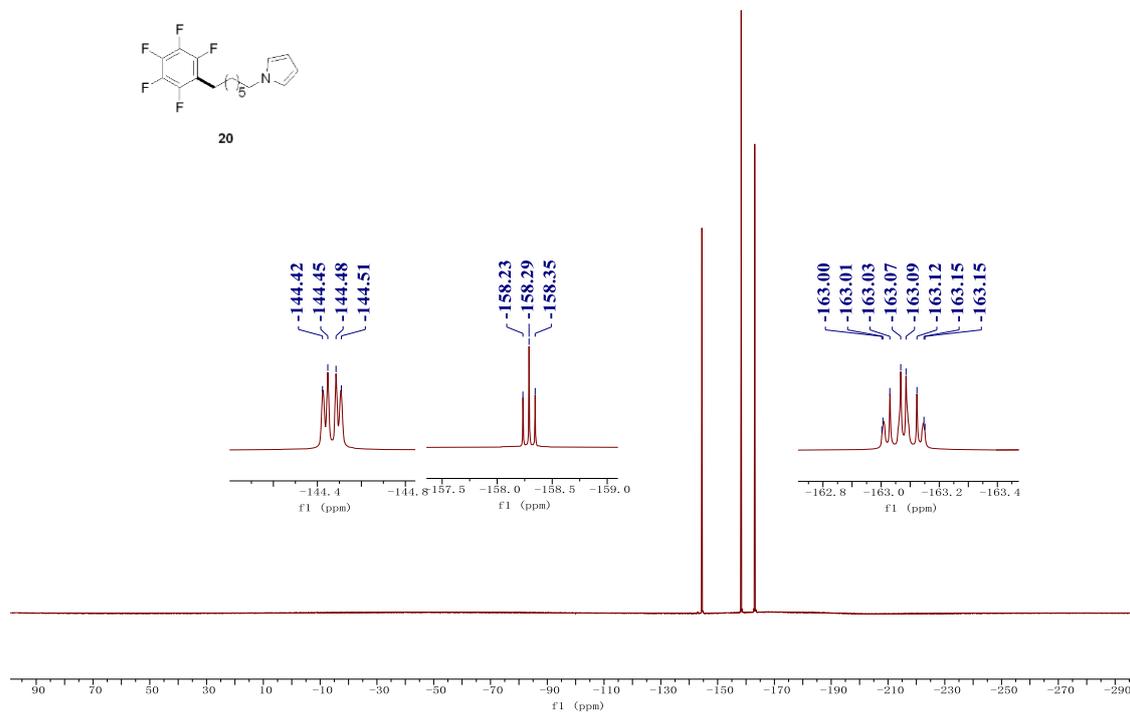
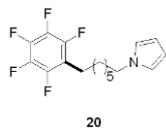
¹H NMR Spectrum of 20



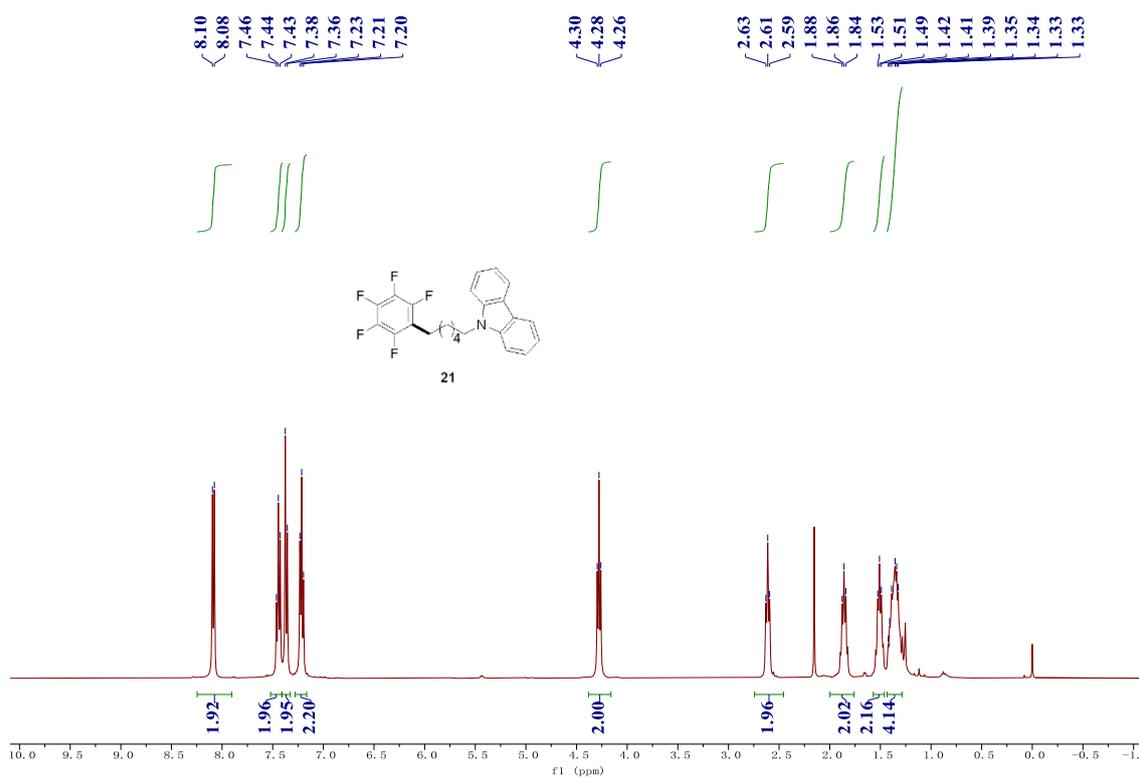
¹³C NMR Spectrum of 20



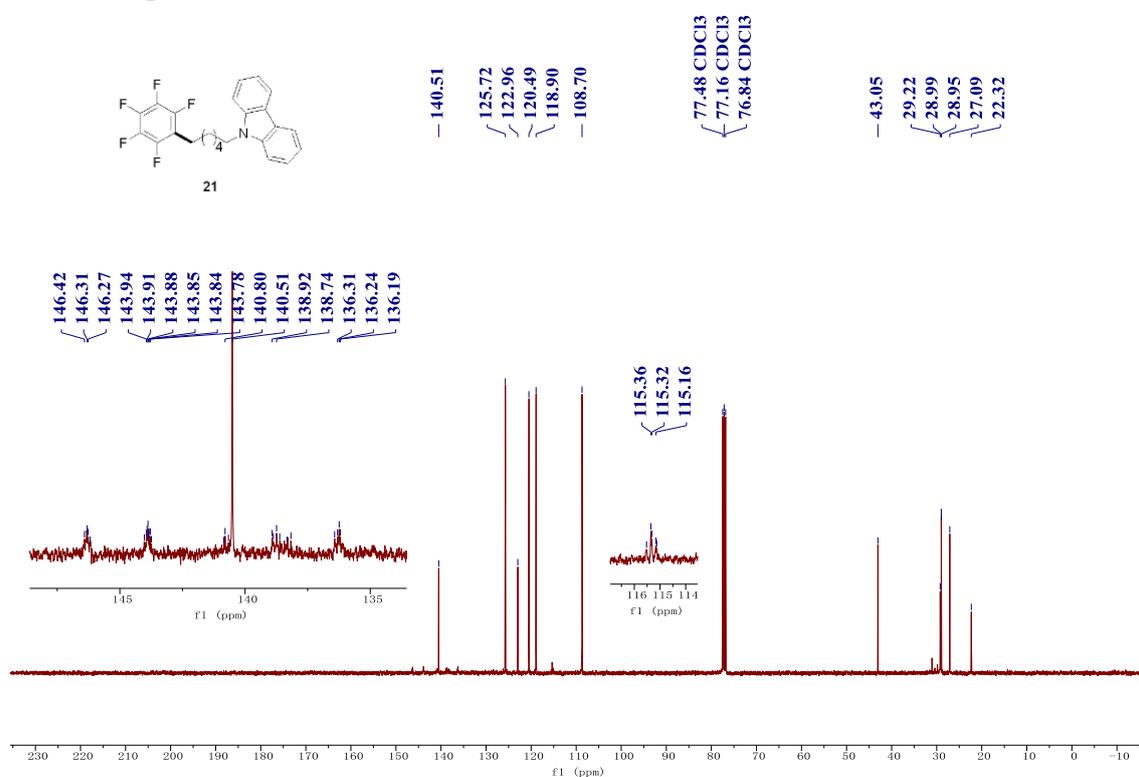
¹⁹F NMR Spectrum of 20



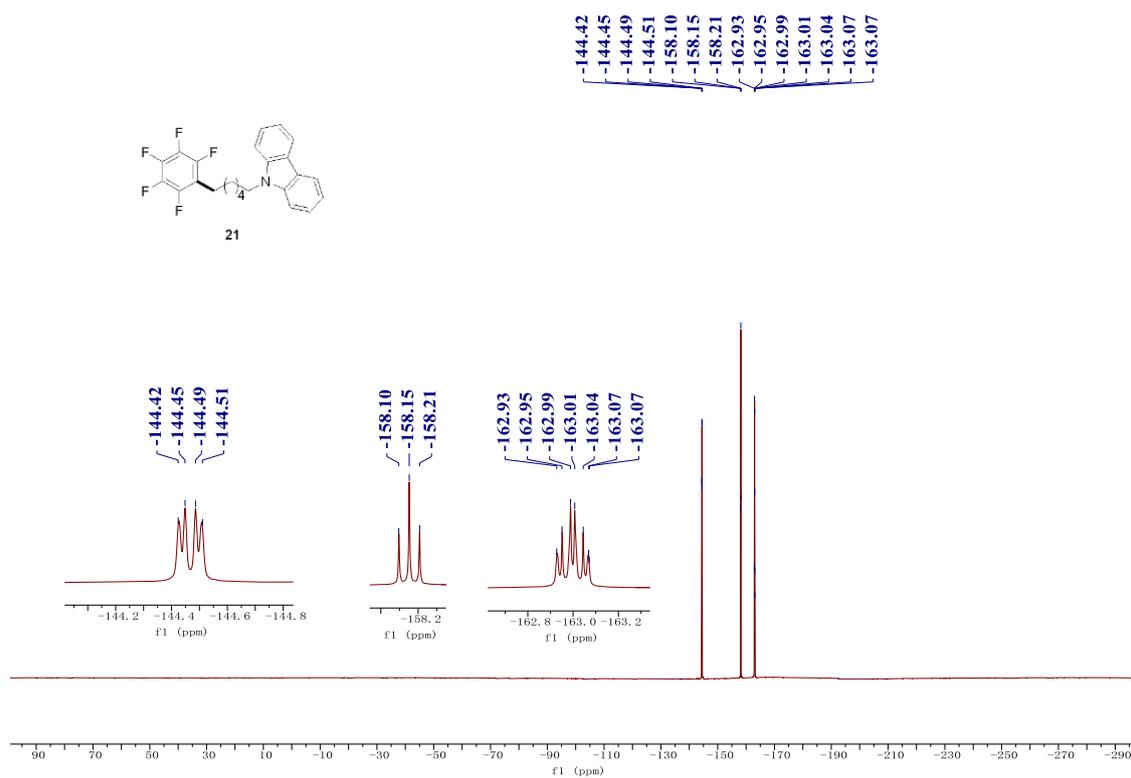
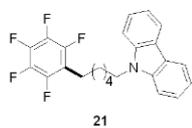
¹H NMR Spectrum of 21



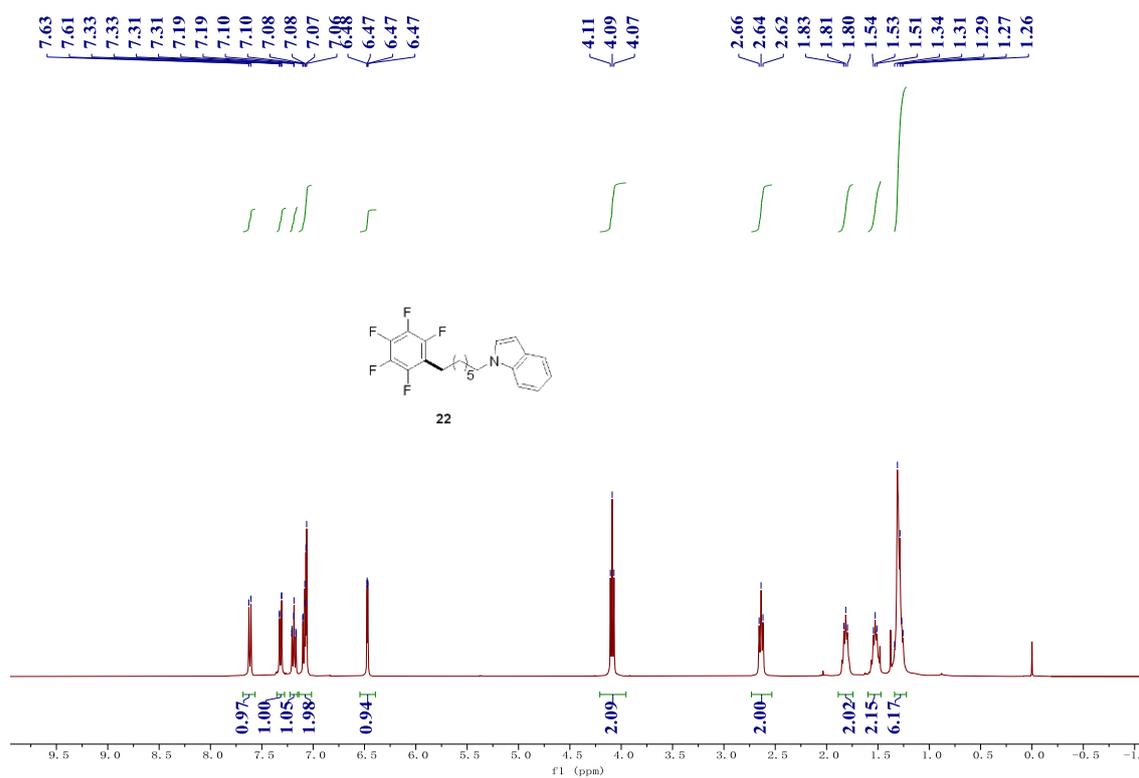
¹³C NMR Spectrum of 21



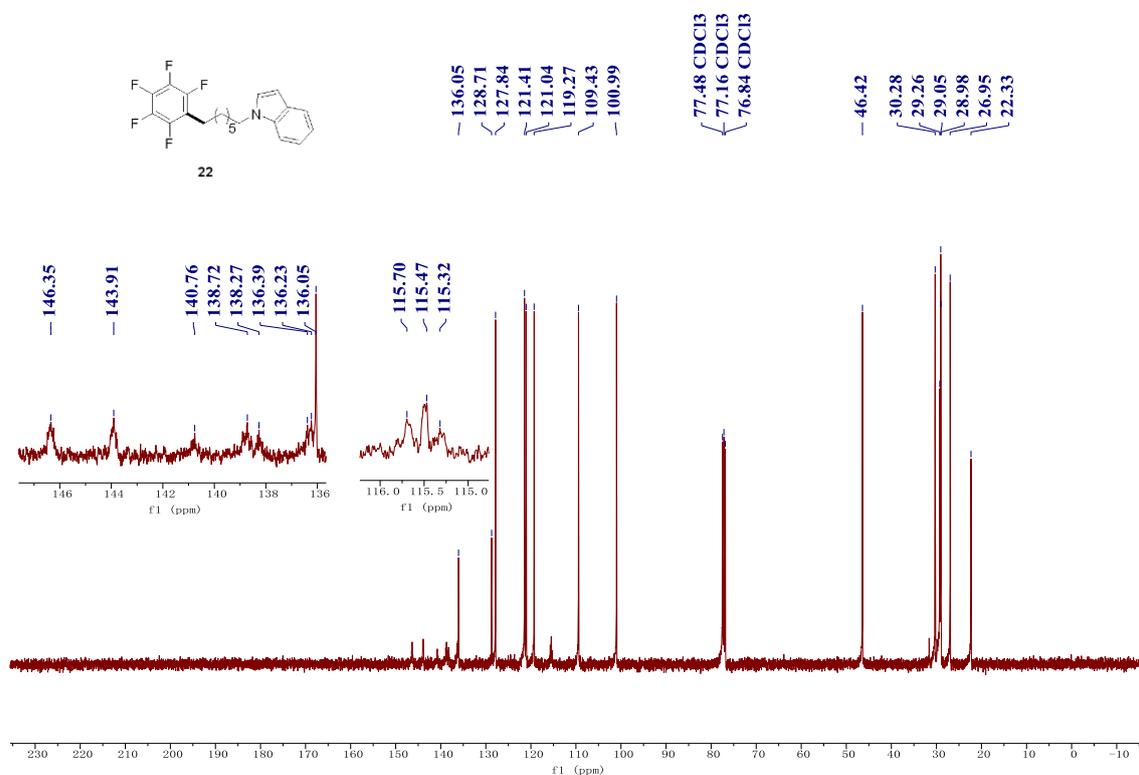
¹⁹F NMR Spectrum of 21



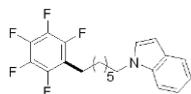
¹H NMR Spectrum of 22



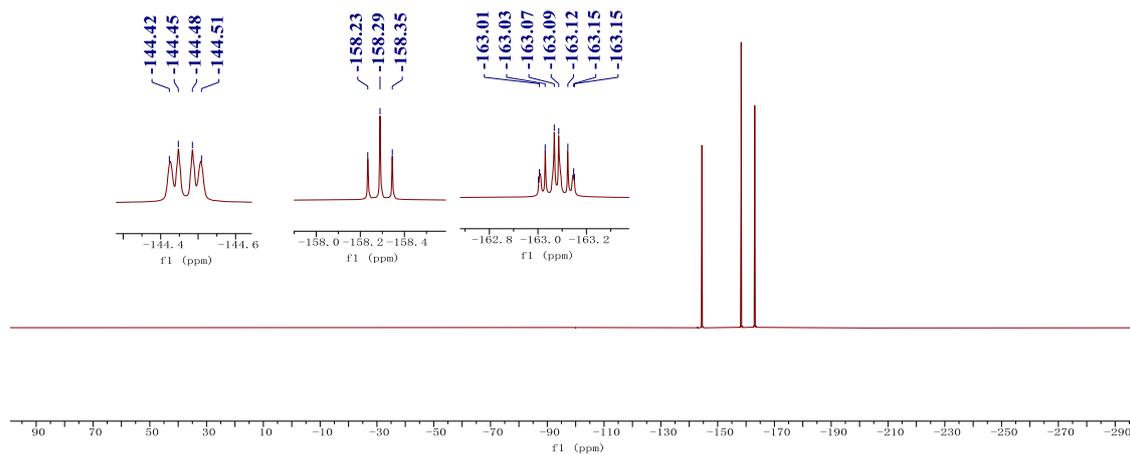
¹³C NMR Spectrum of 22



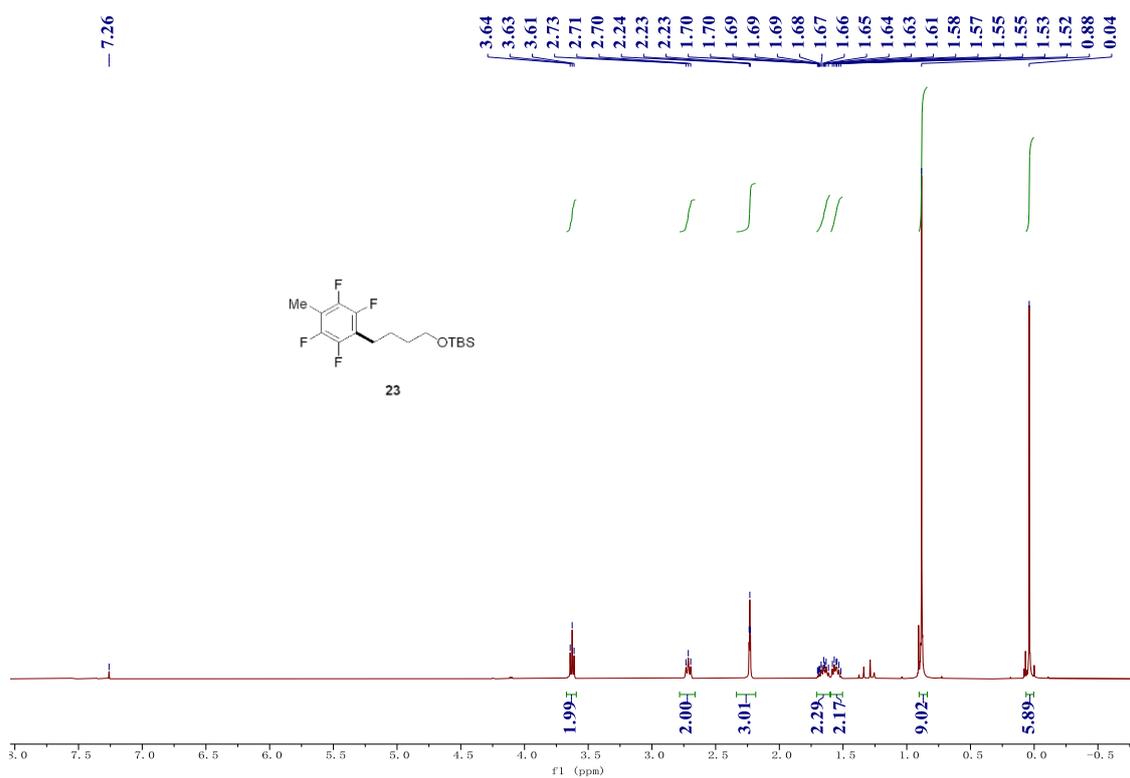
¹⁹F NMR Spectrum of 22



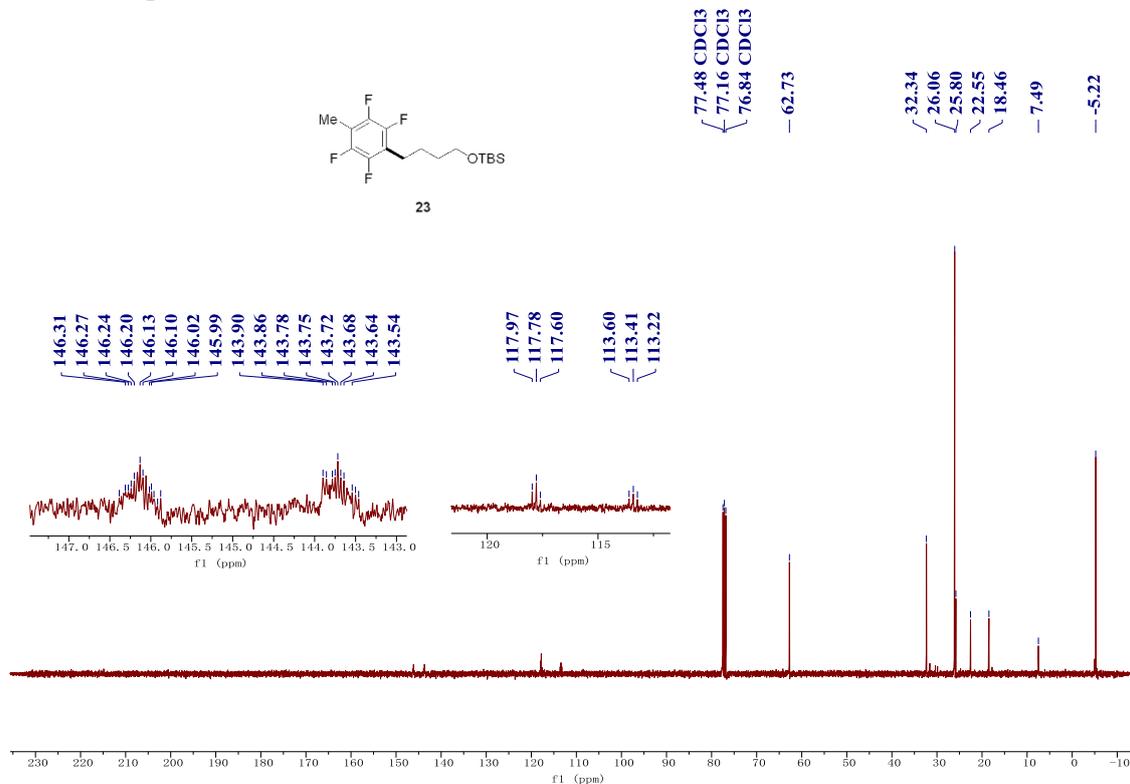
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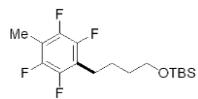
¹H NMR Spectrum of 23



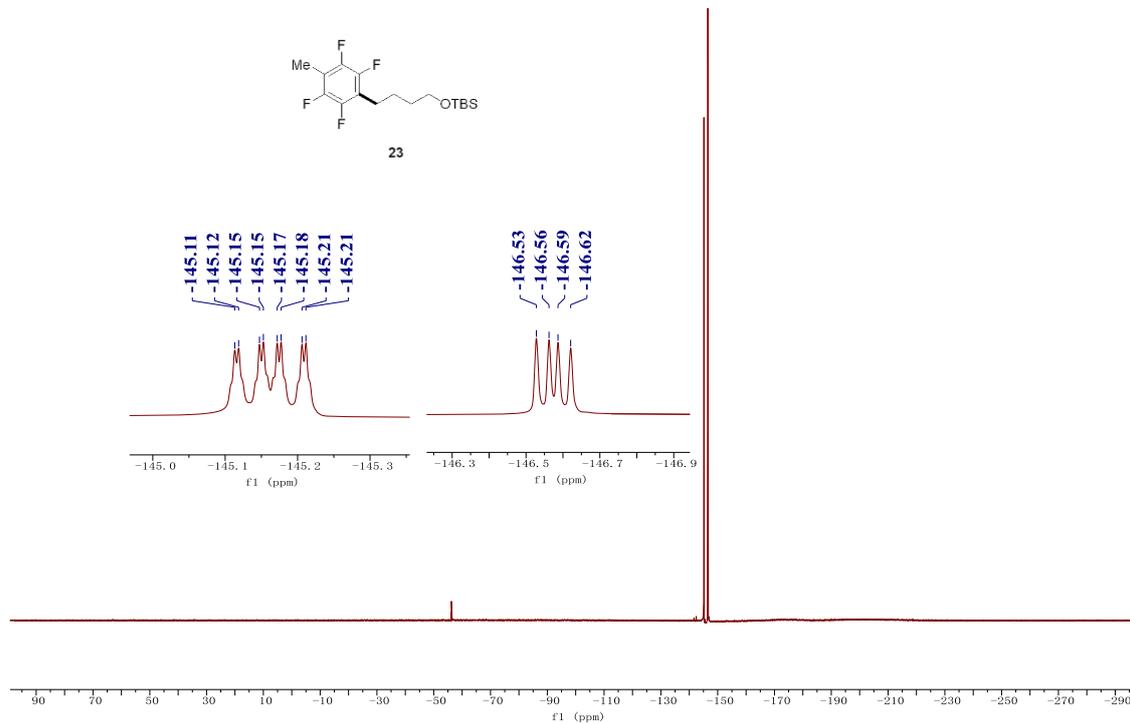
¹³C NMR Spectrum of 23



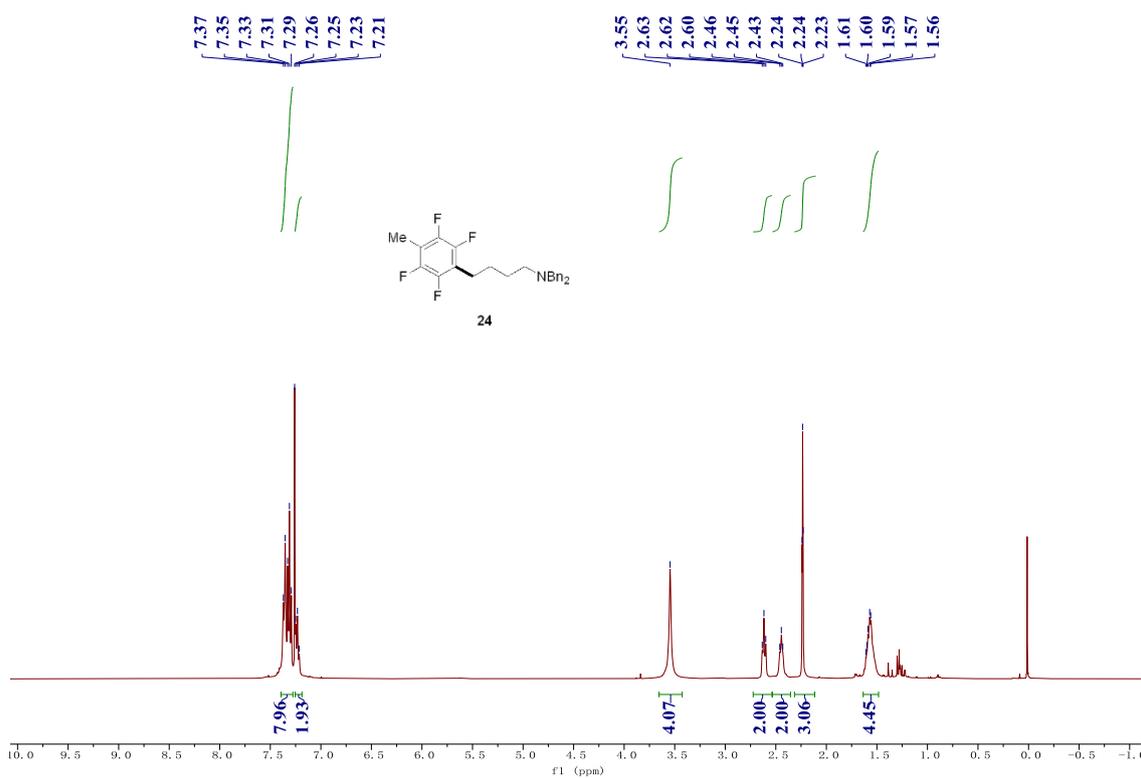
¹⁹F NMR Spectrum of 23



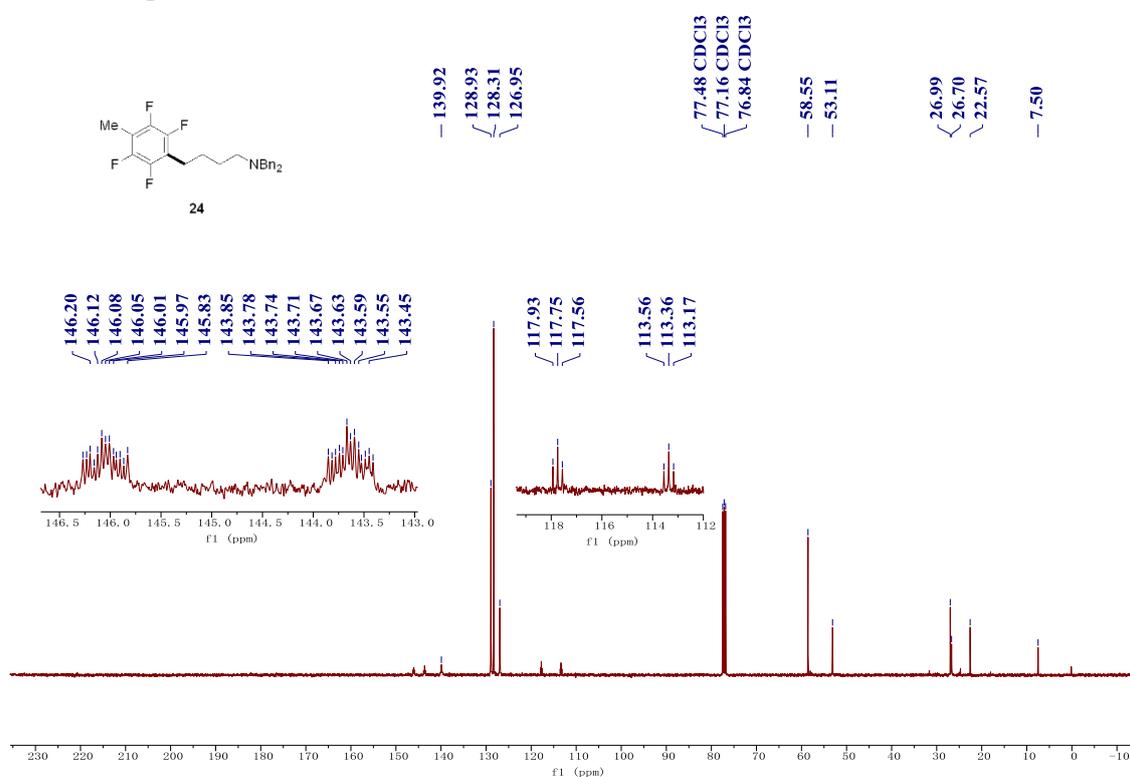
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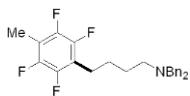
¹H NMR Spectrum of 24



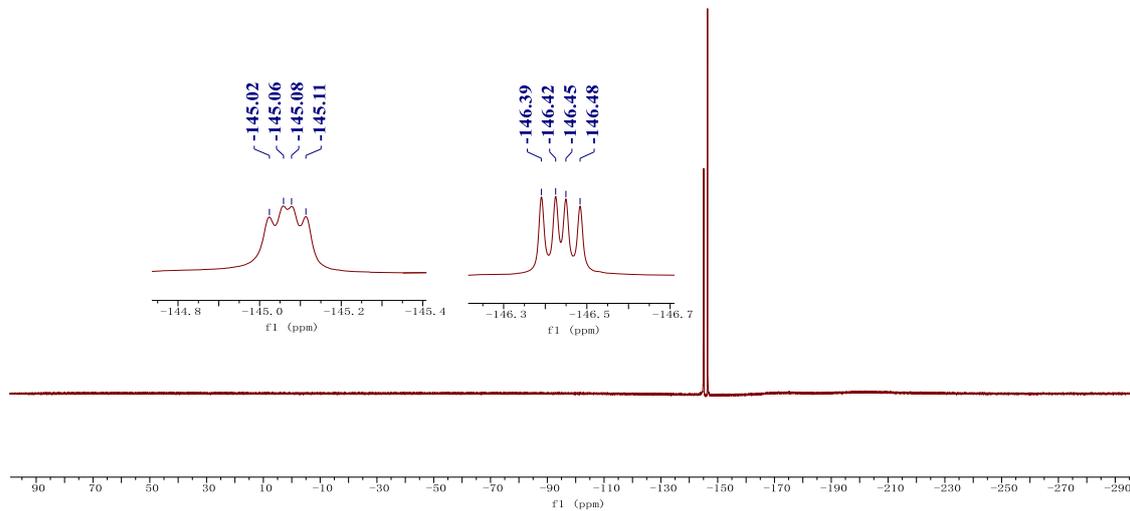
¹³C NMR Spectrum of 24



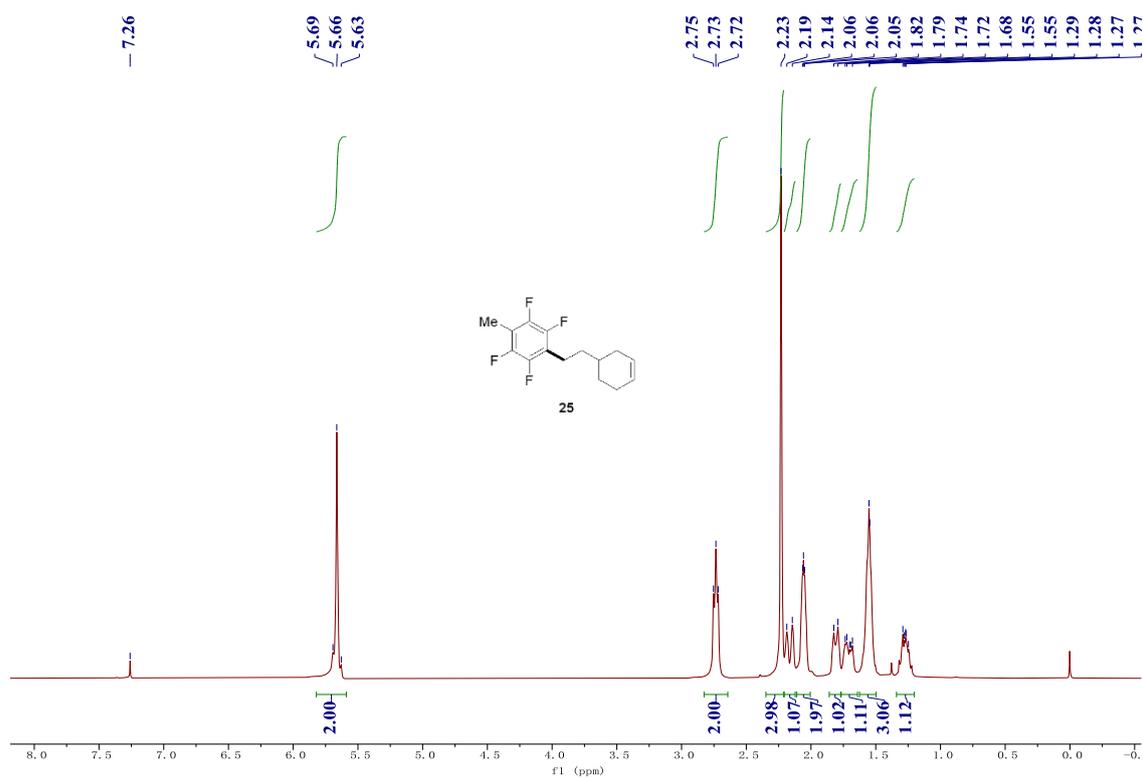
¹⁹F NMR Spectrum of 24



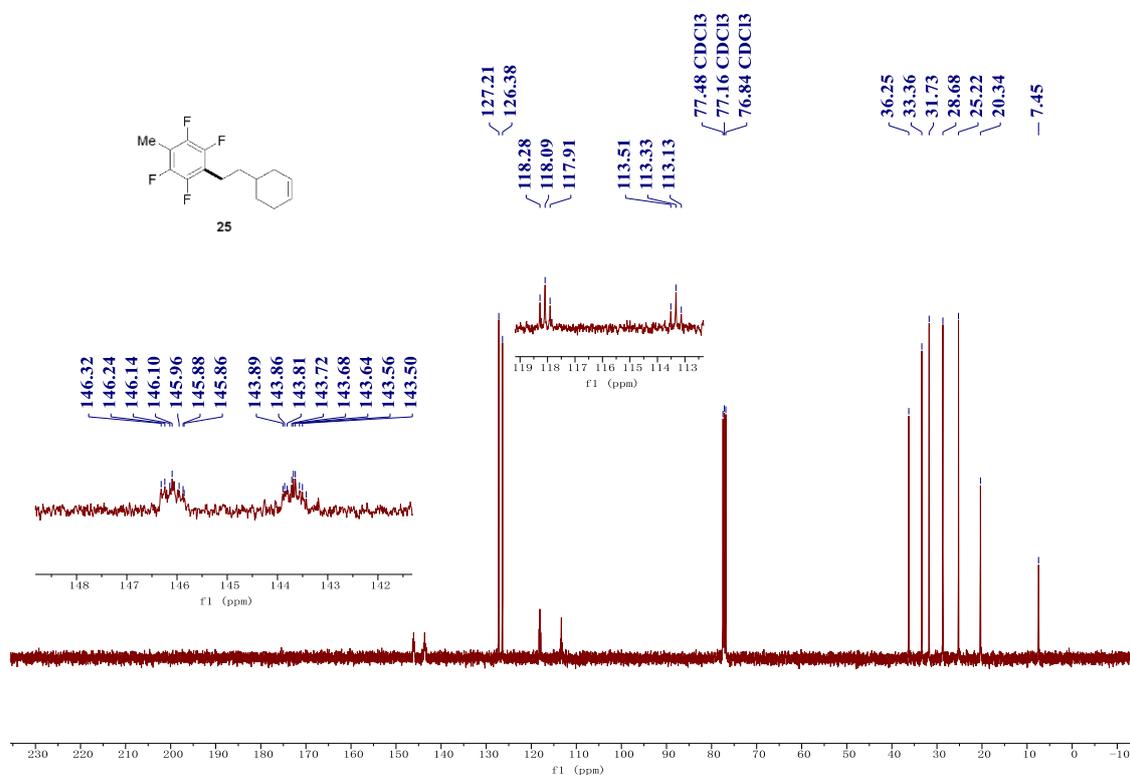
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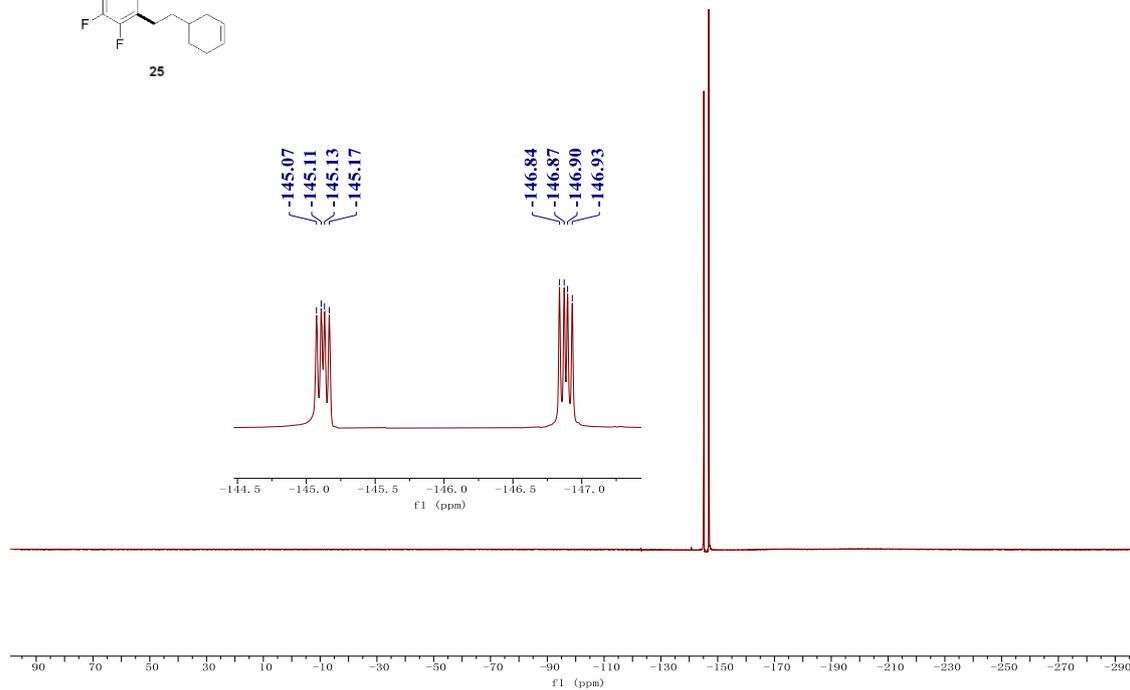
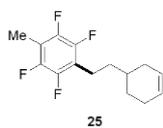
¹H NMR Spectrum of 25



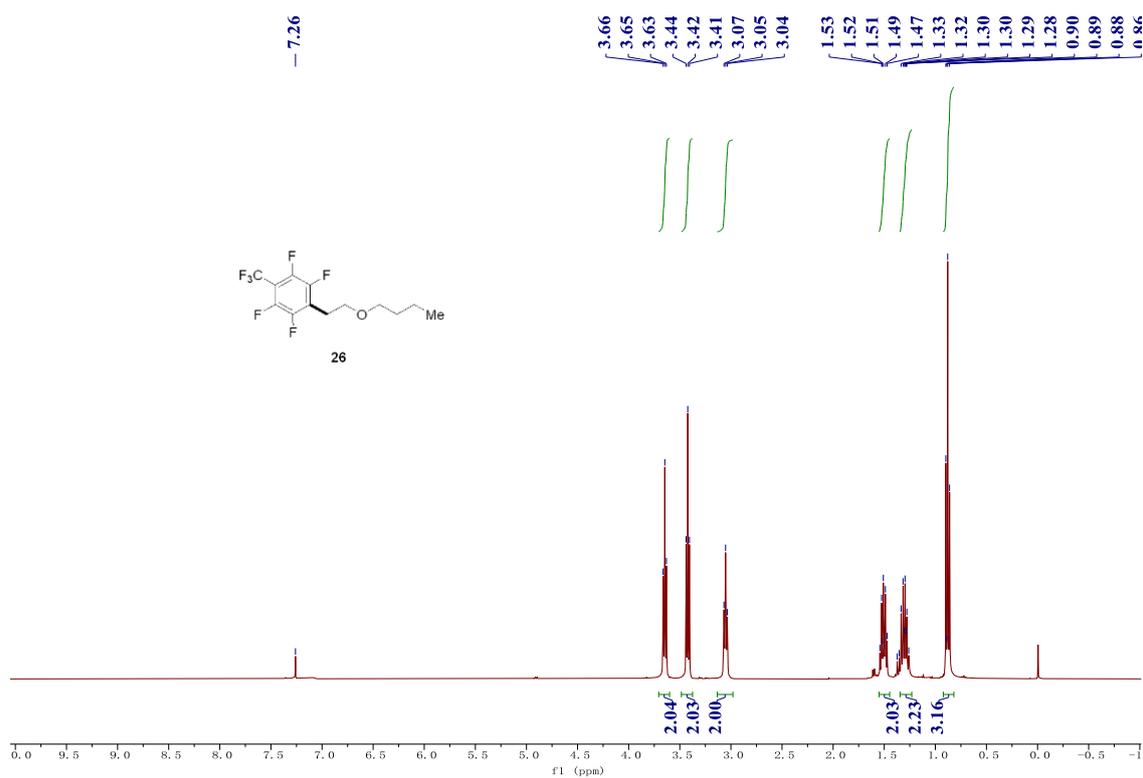
¹³C NMR Spectrum of 25



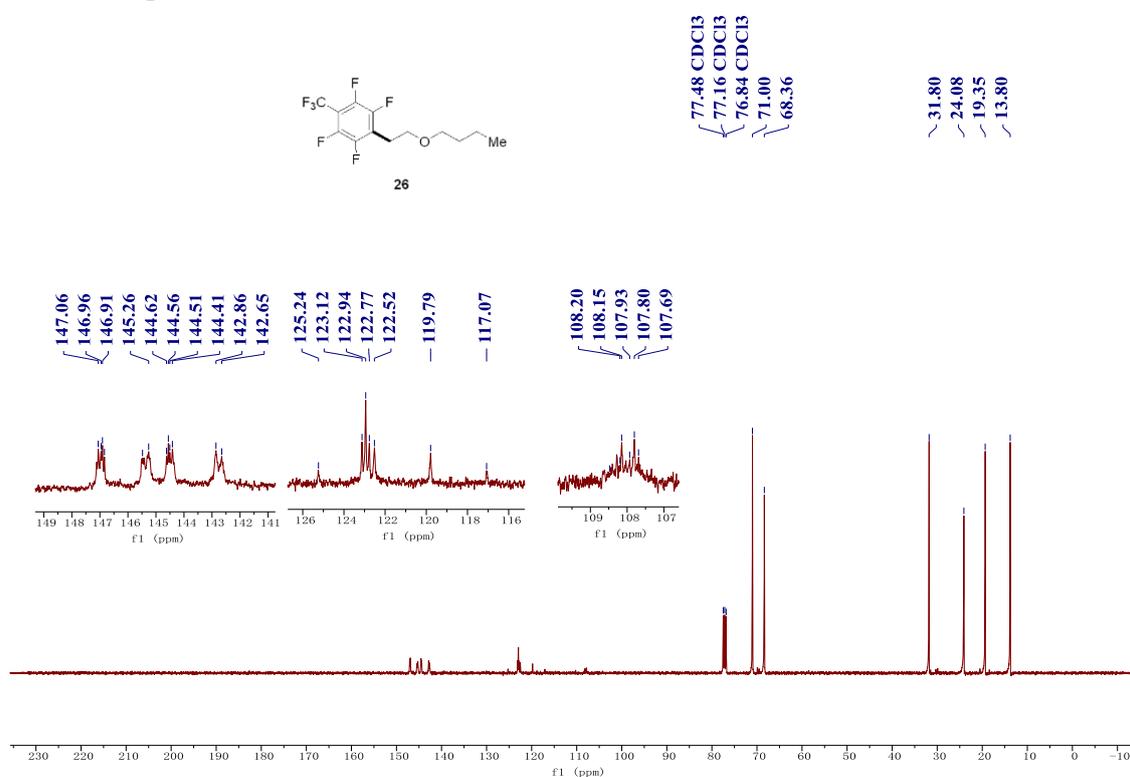
¹⁹F NMR Spectrum of 25



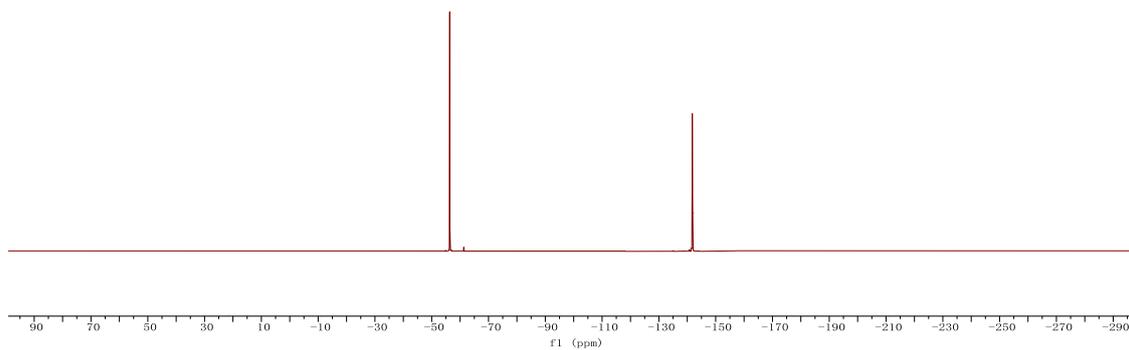
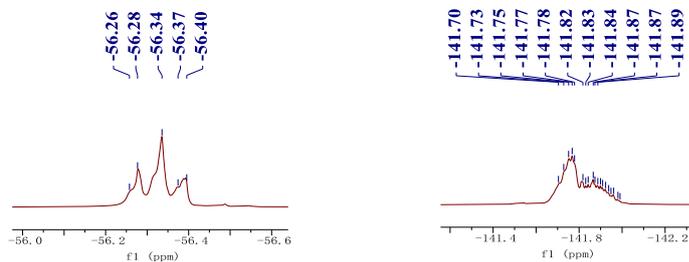
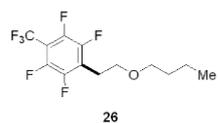
¹H NMR Spectrum of 26



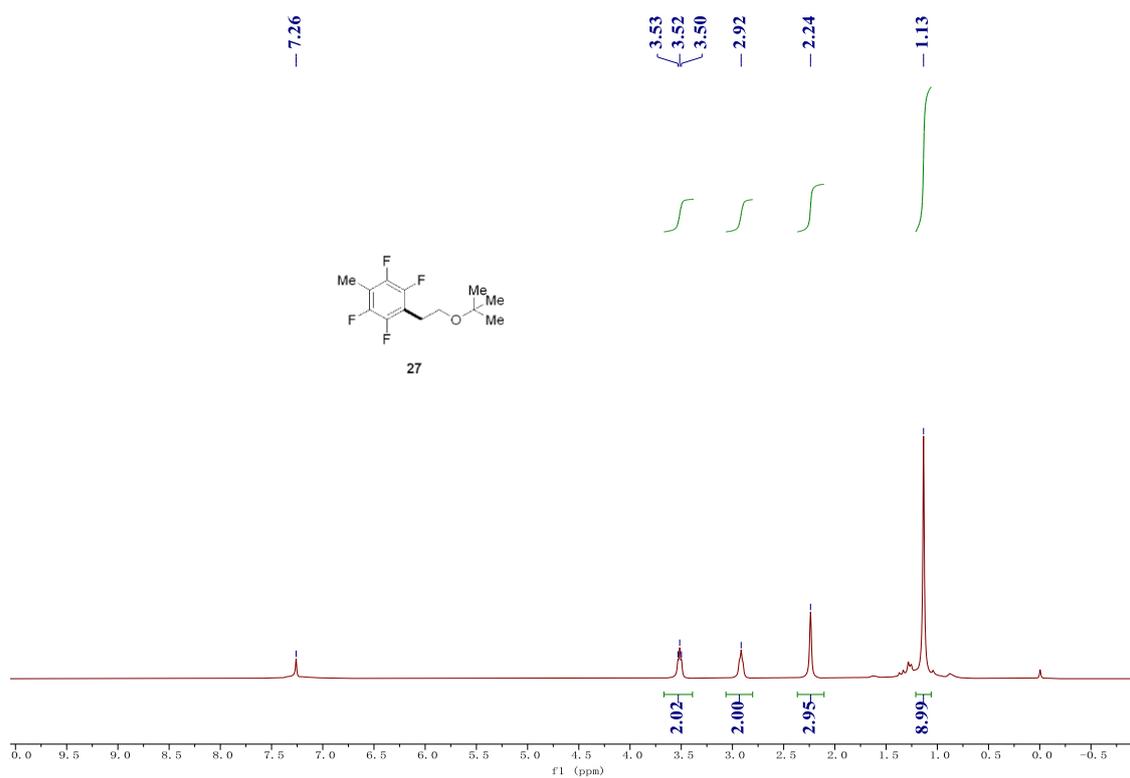
¹³C NMR Spectrum of 26



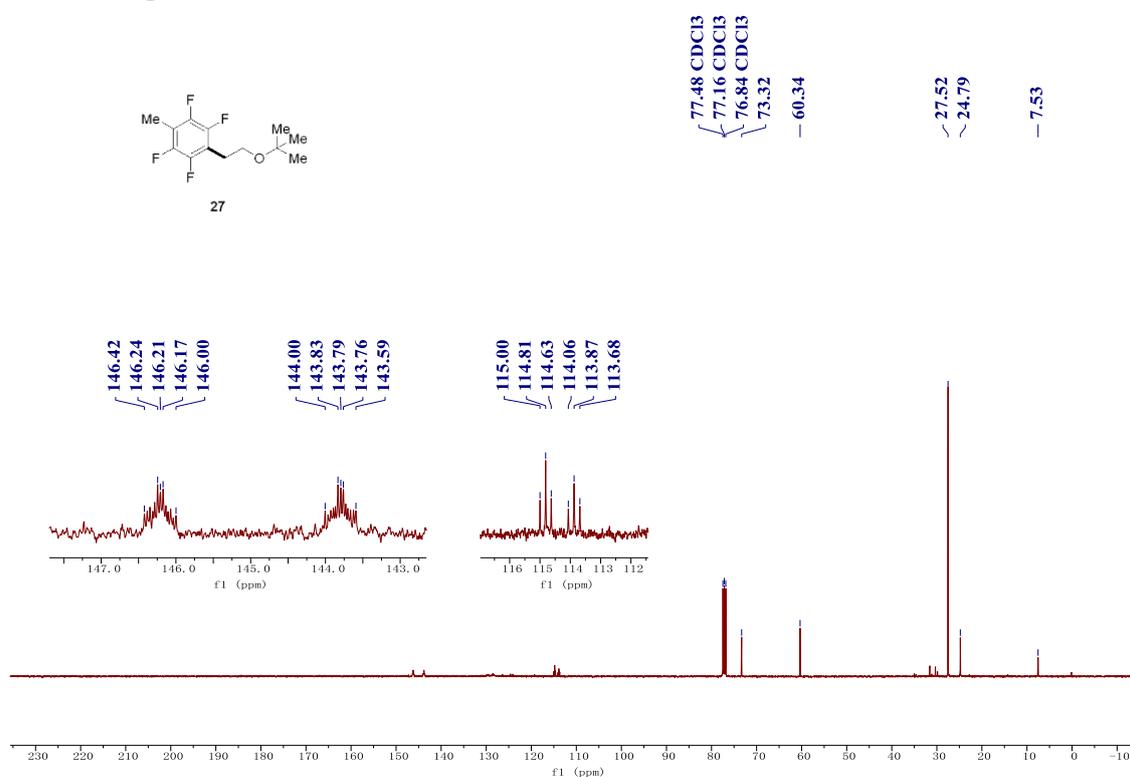
¹⁹F NMR Spectrum of 26



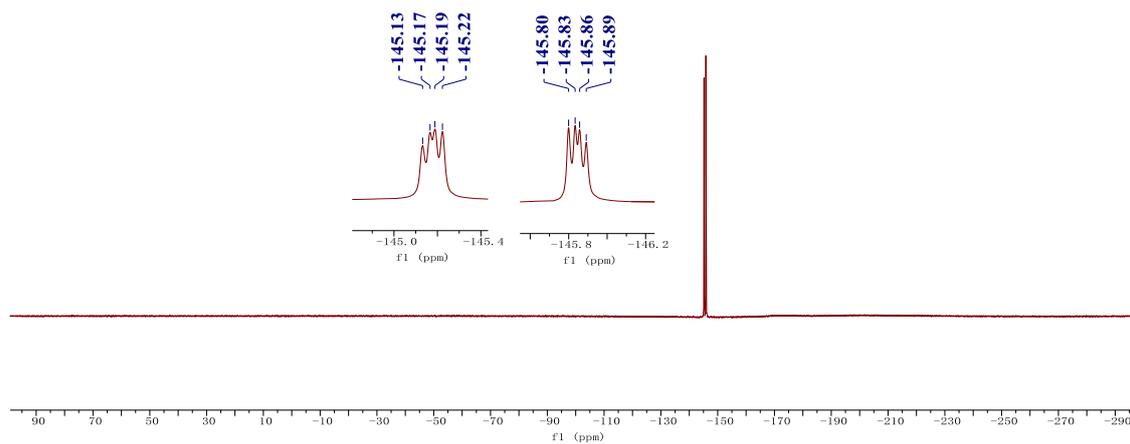
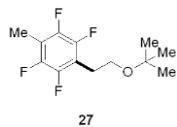
¹H NMR Spectrum of 27



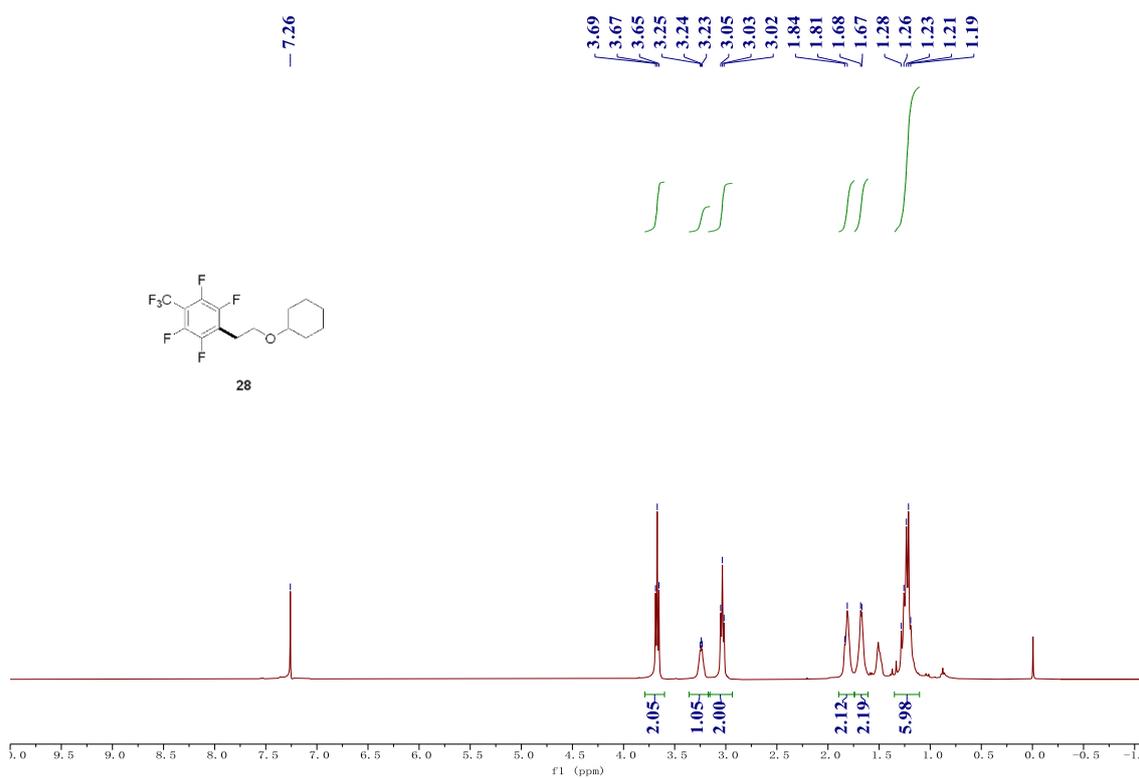
¹³C NMR Spectrum of 27



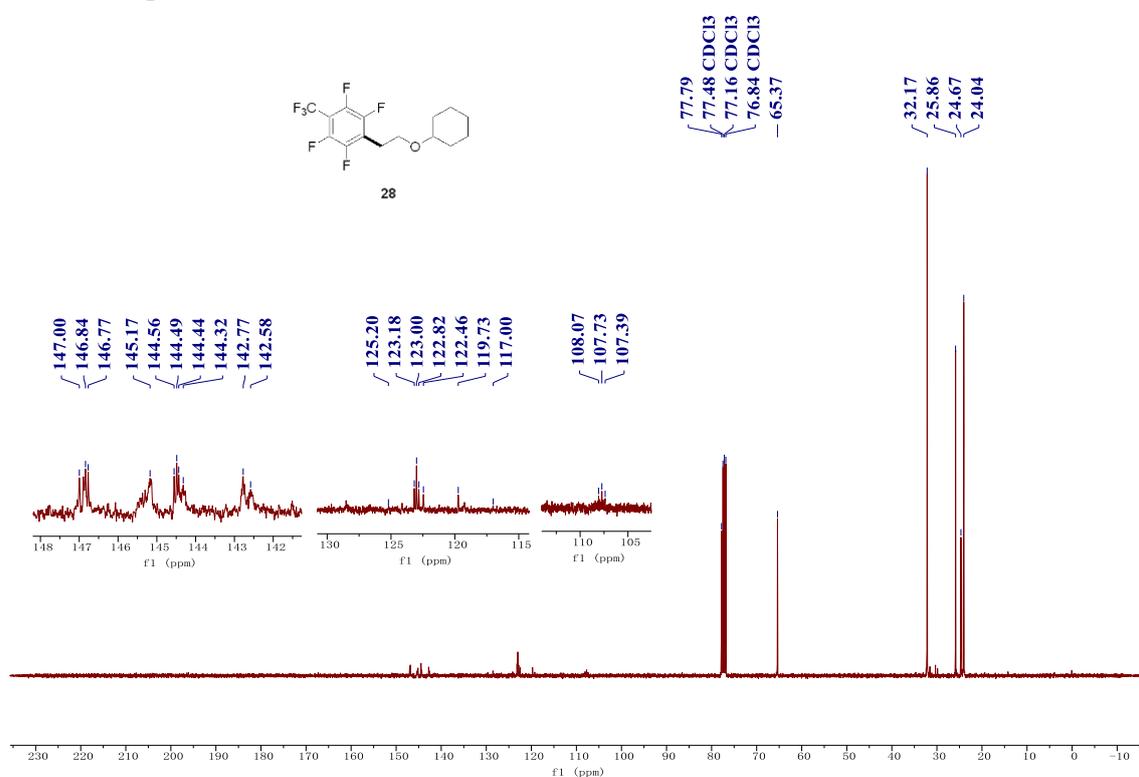
¹⁹F NMR Spectrum of 27



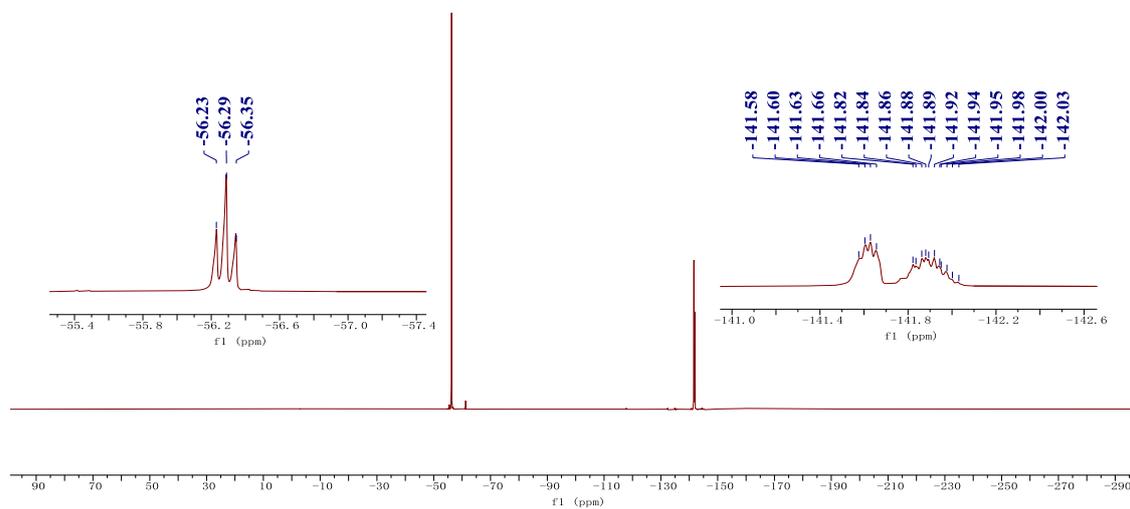
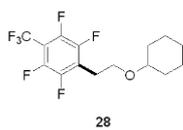
¹H NMR Spectrum of 28



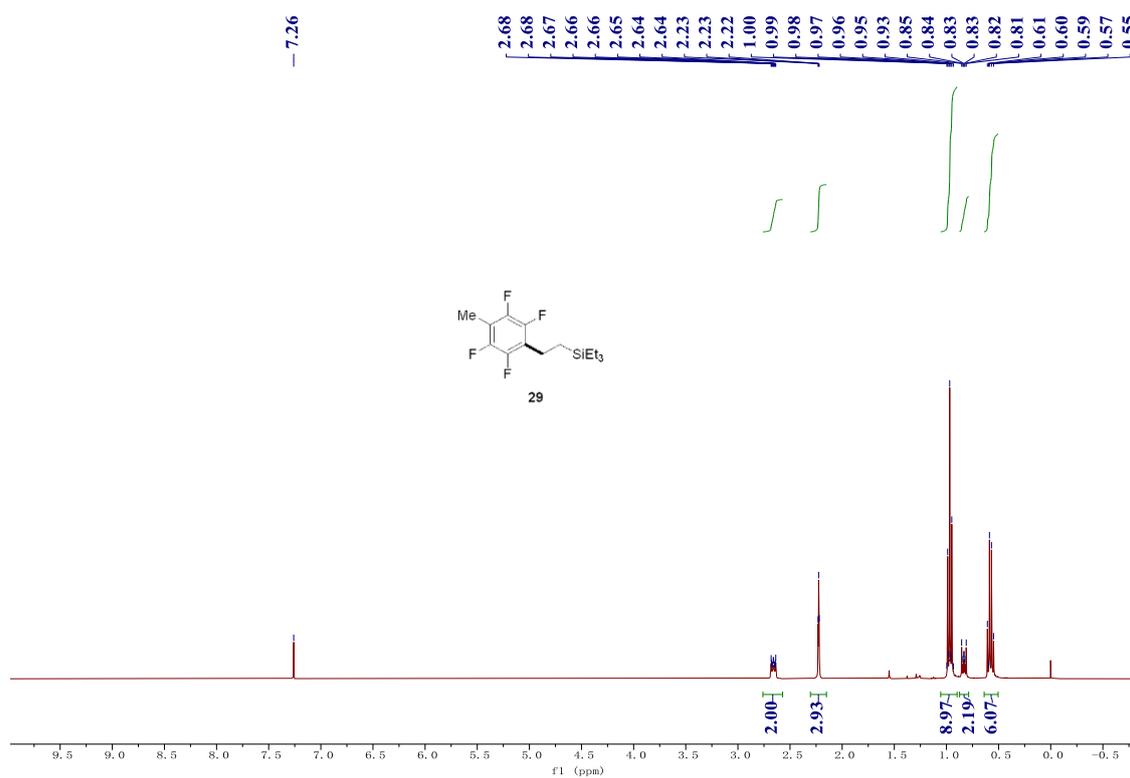
¹³C NMR Spectrum of 28



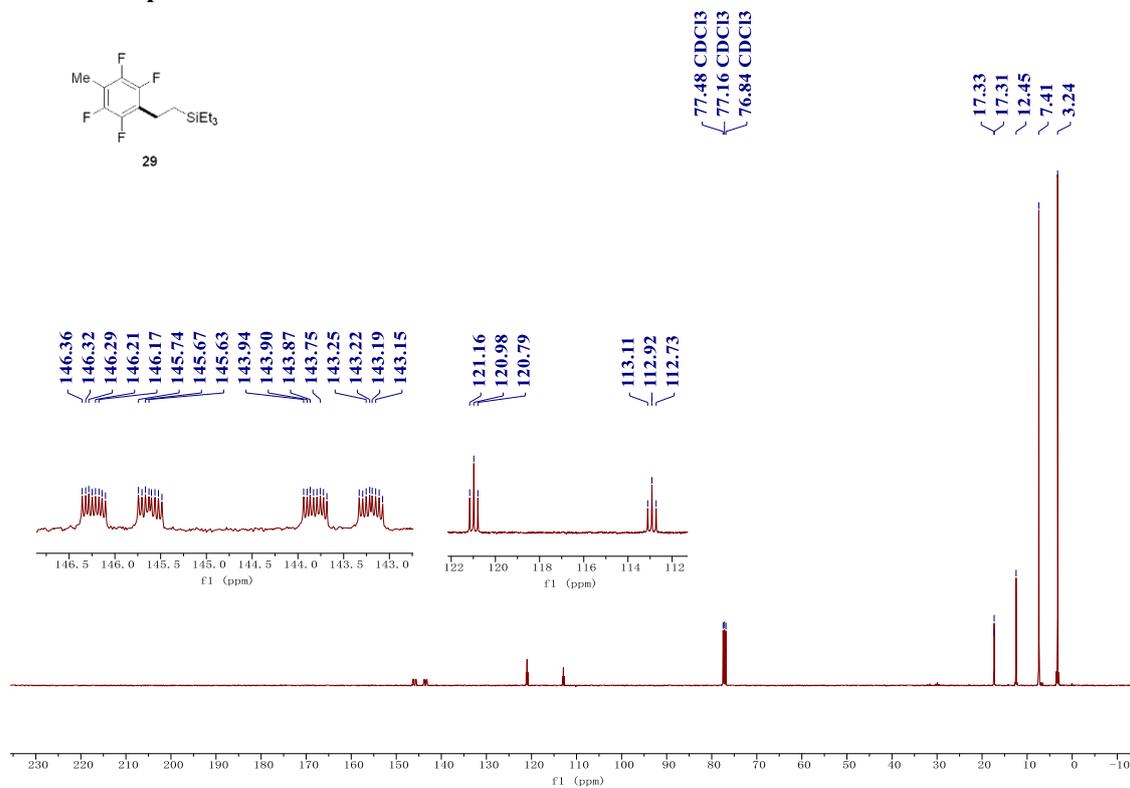
¹⁹F NMR Spectrum of 28



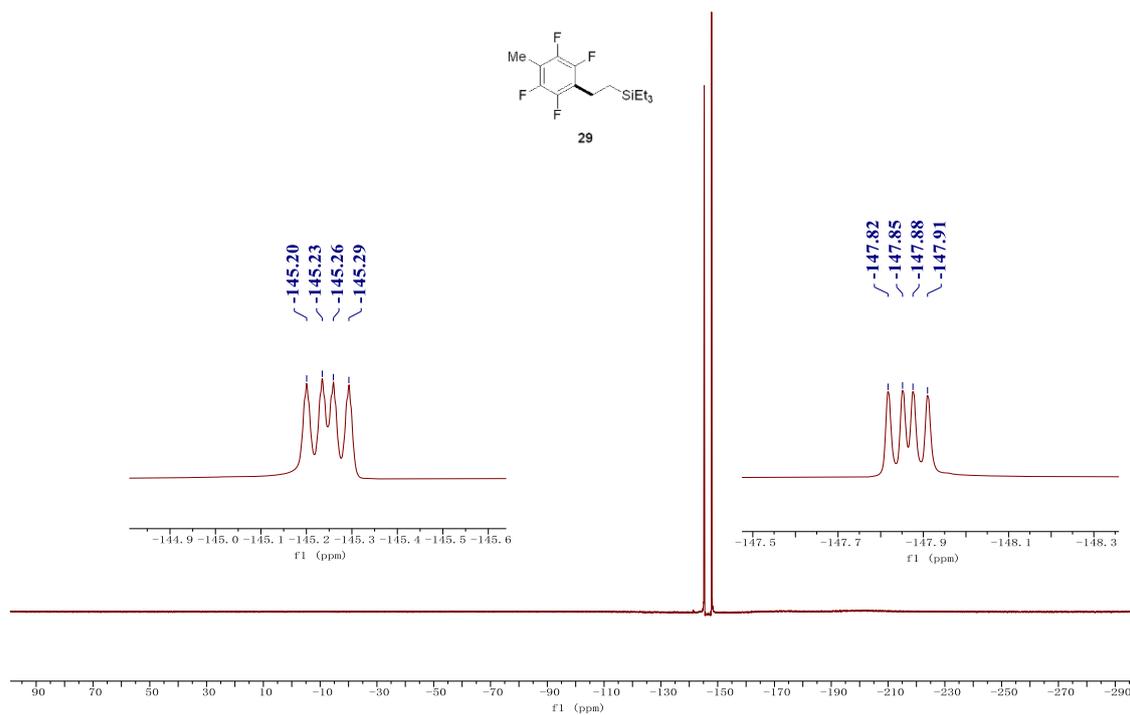
¹H NMR Spectrum of 29



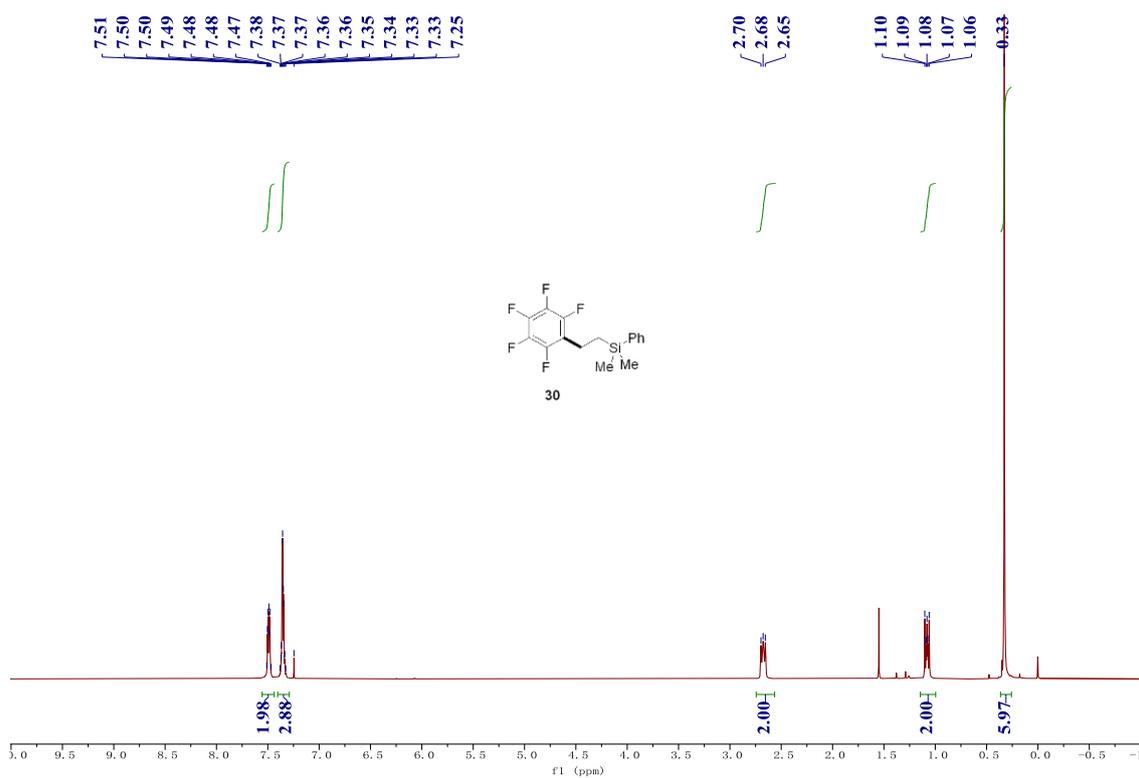
¹³C NMR Spectrum of 29



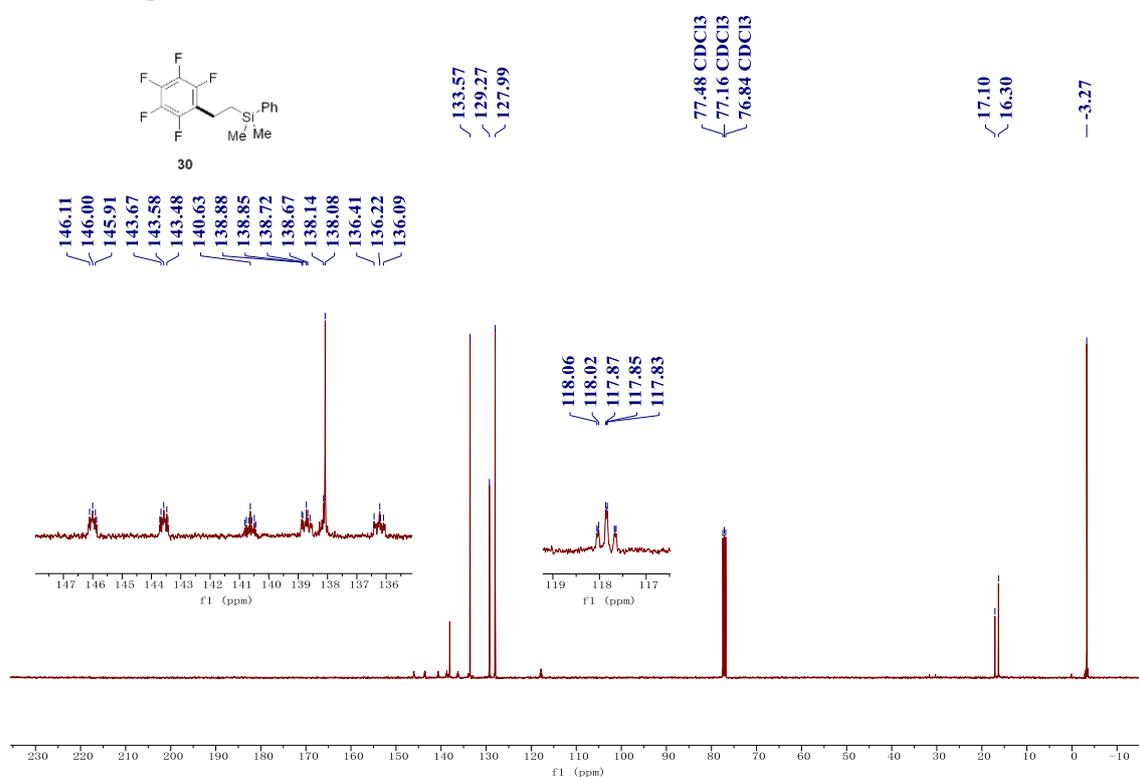
¹⁹F NMR Spectrum of 29



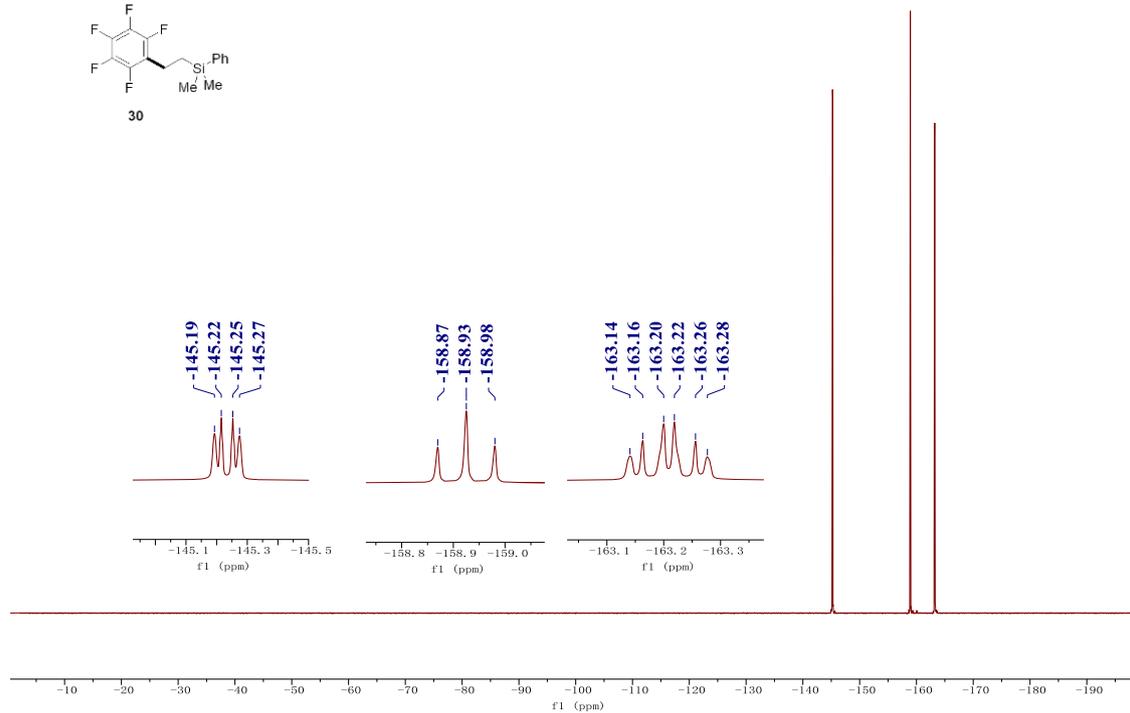
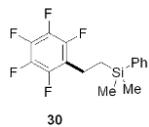
¹H NMR Spectrum of 30



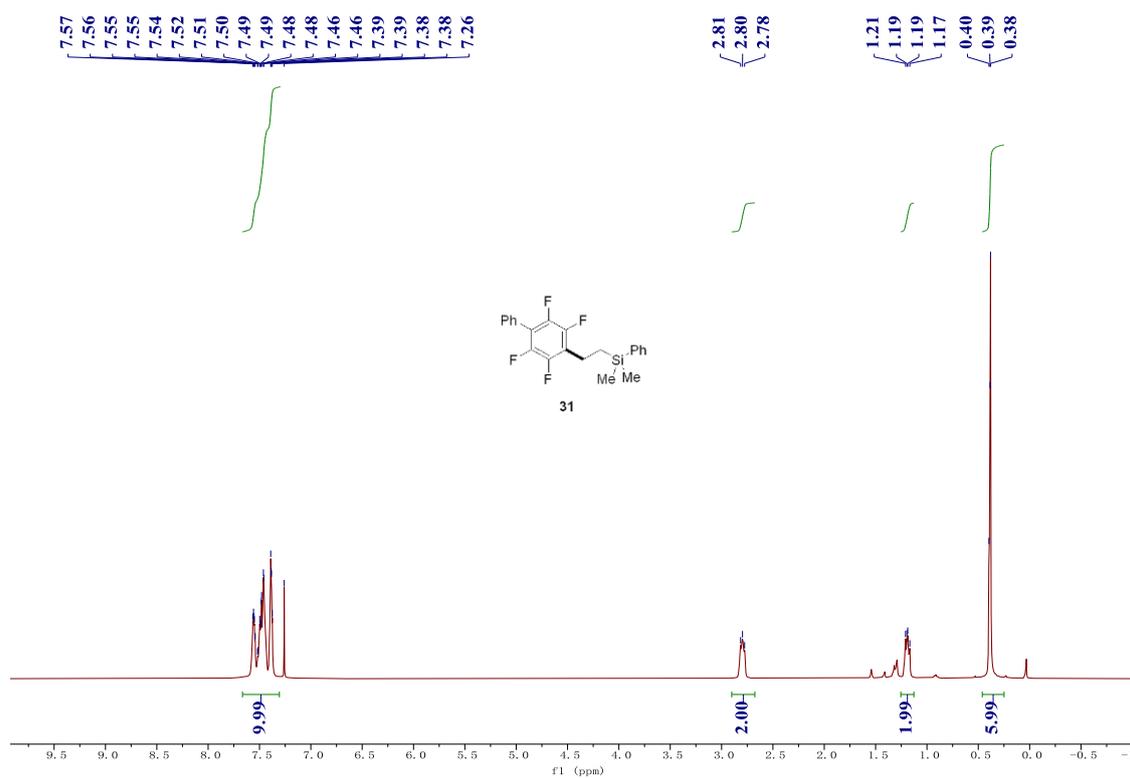
¹³C NMR Spectrum of 30



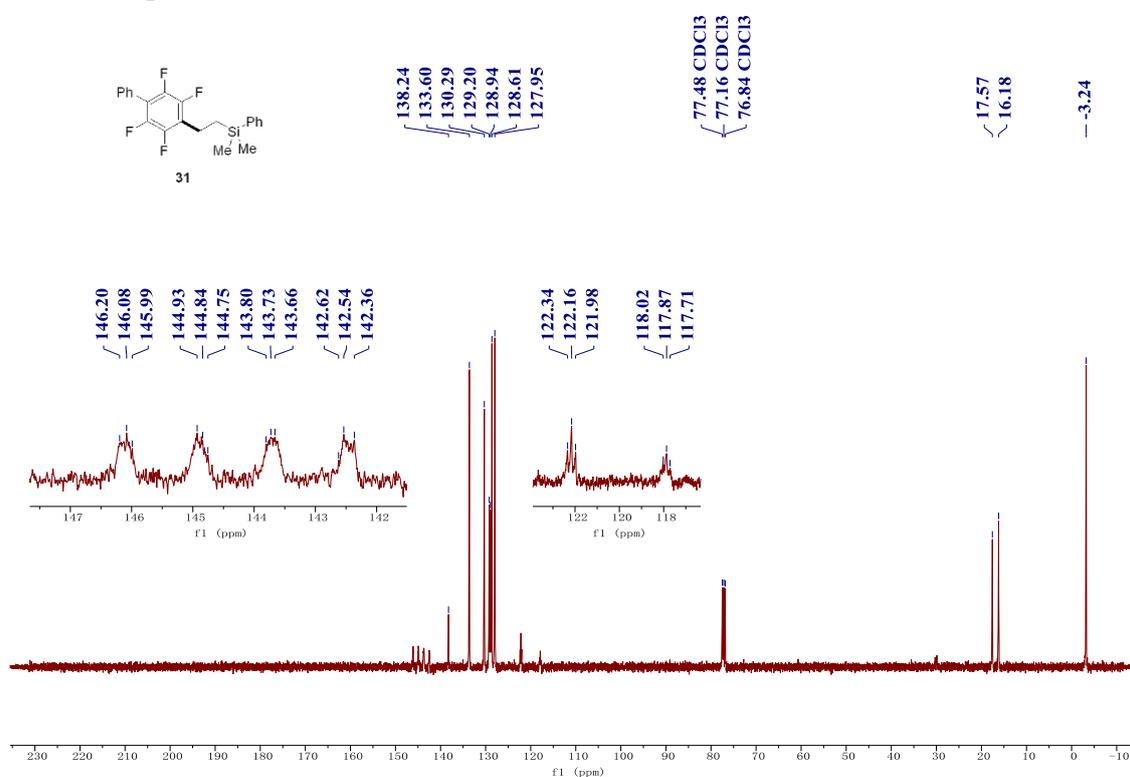
¹⁹F NMR Spectrum of 30



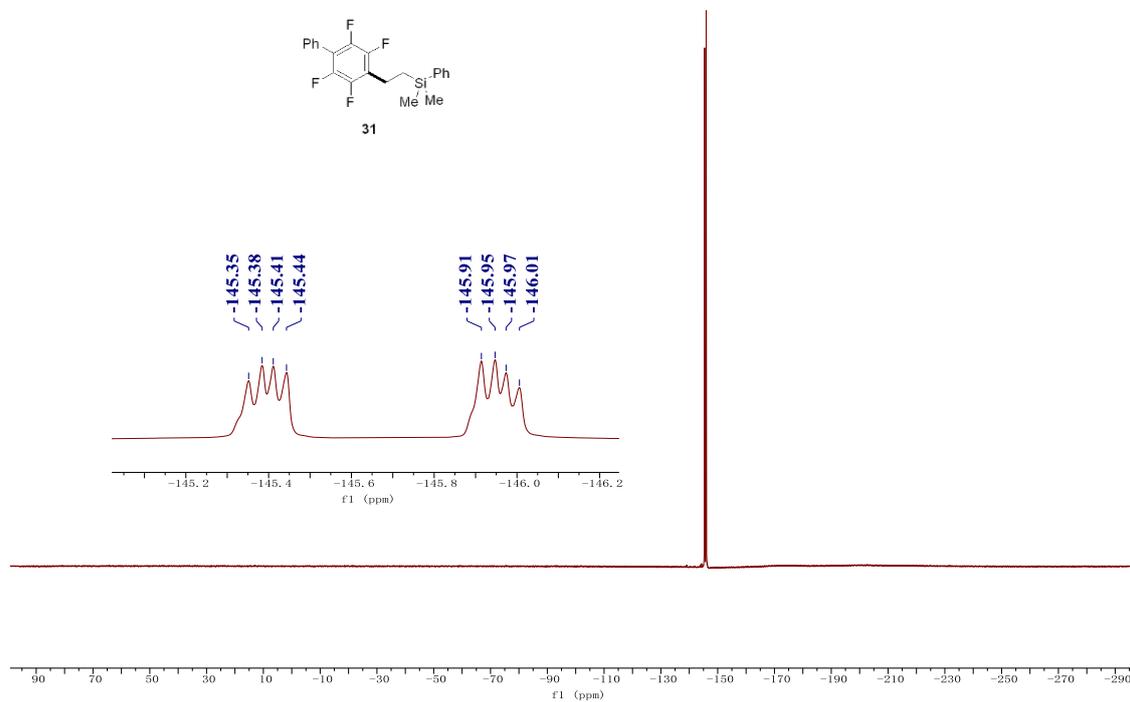
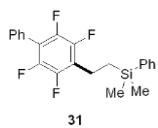
¹H NMR Spectrum of 31



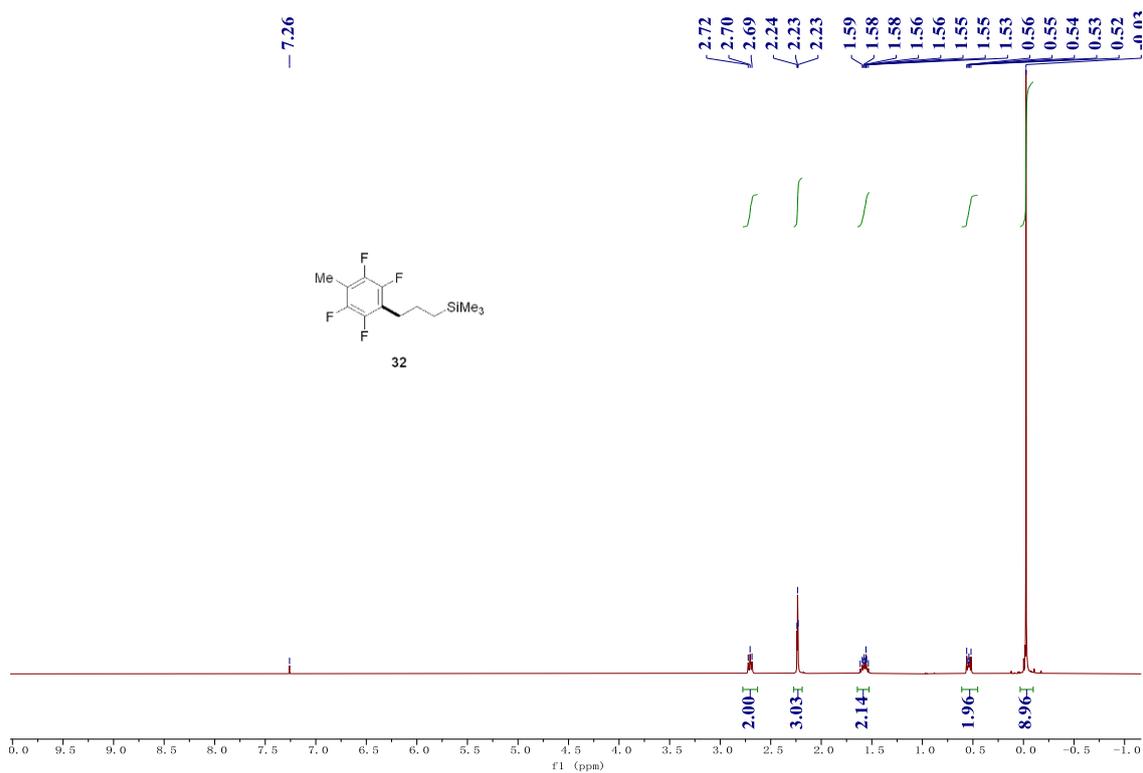
¹³C NMR Spectrum of 31



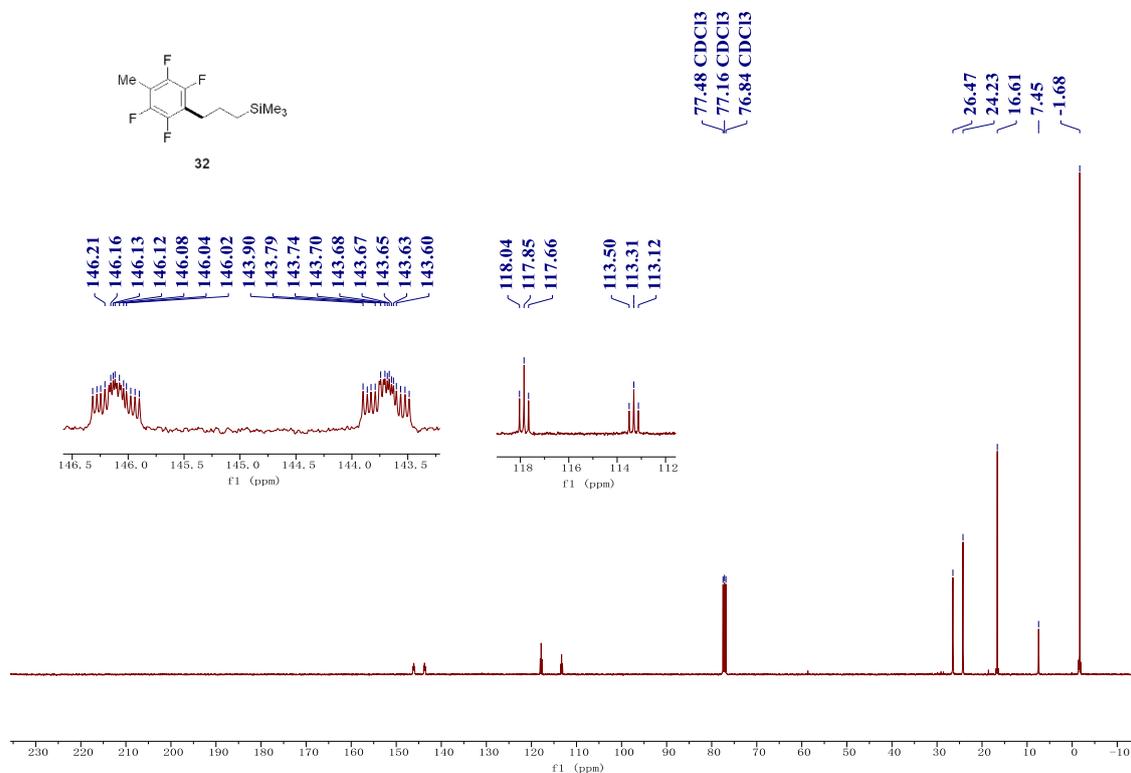
¹⁹F NMR Spectrum of 31



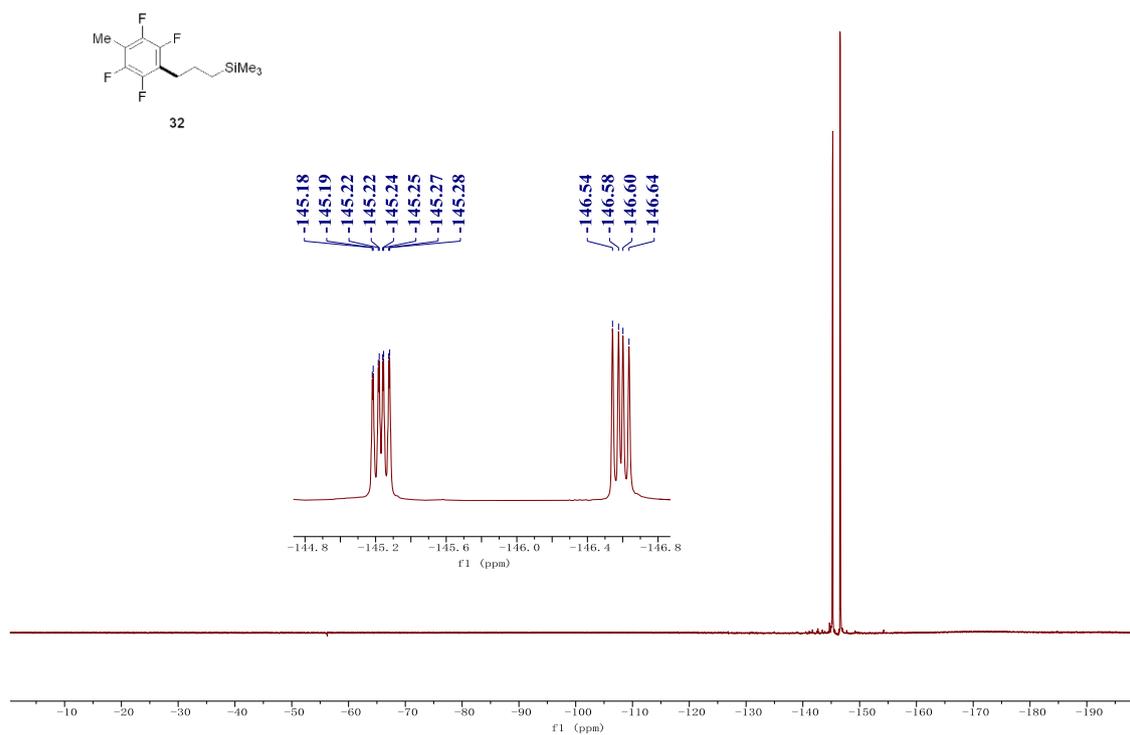
¹H NMR Spectrum of 32



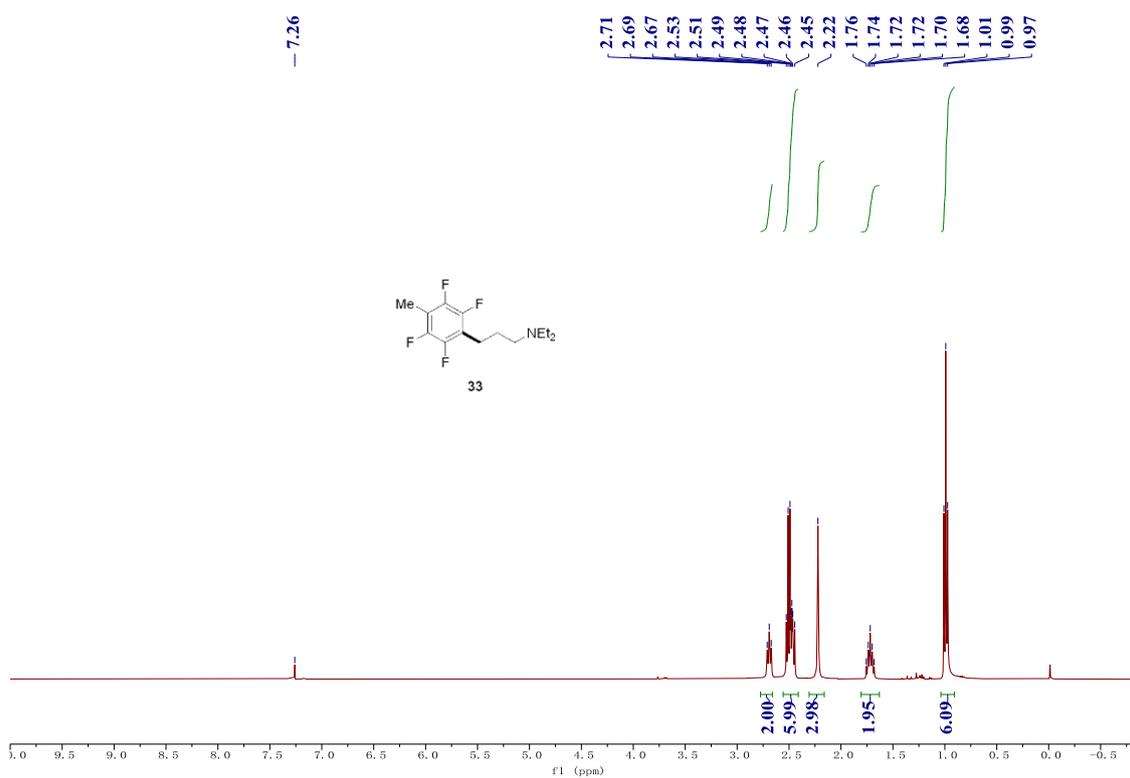
¹³C NMR Spectrum of 32



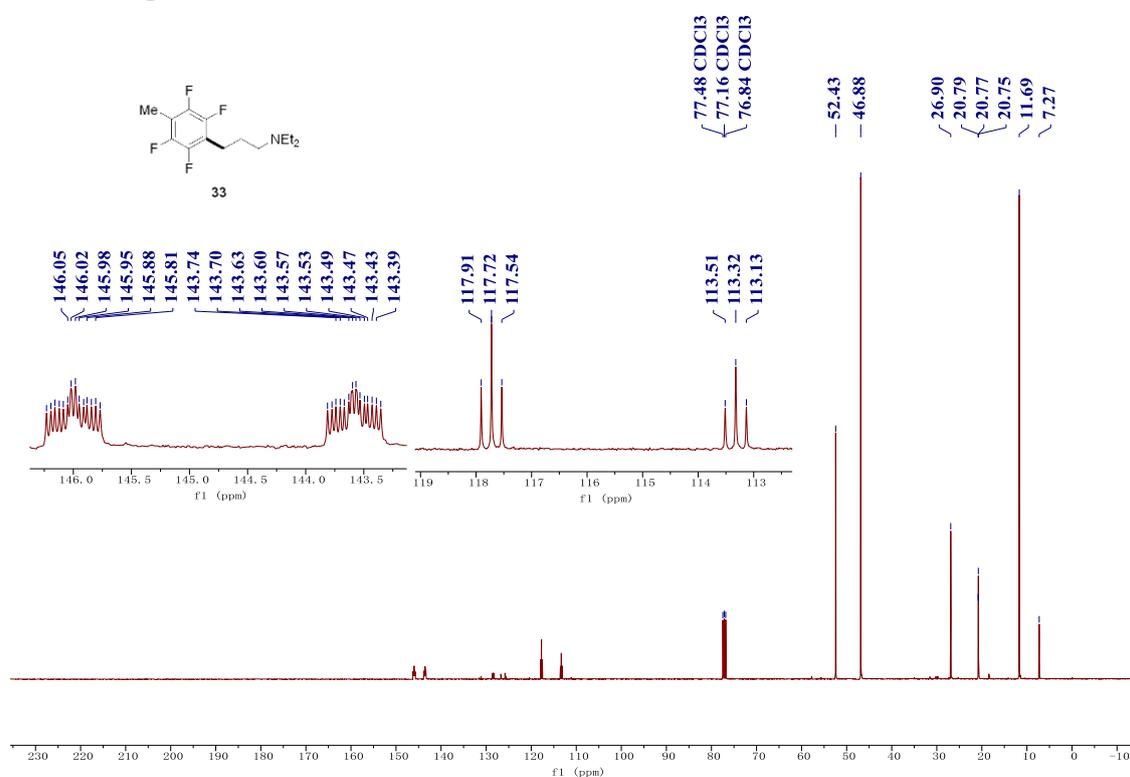
¹⁹F NMR Spectrum of 32



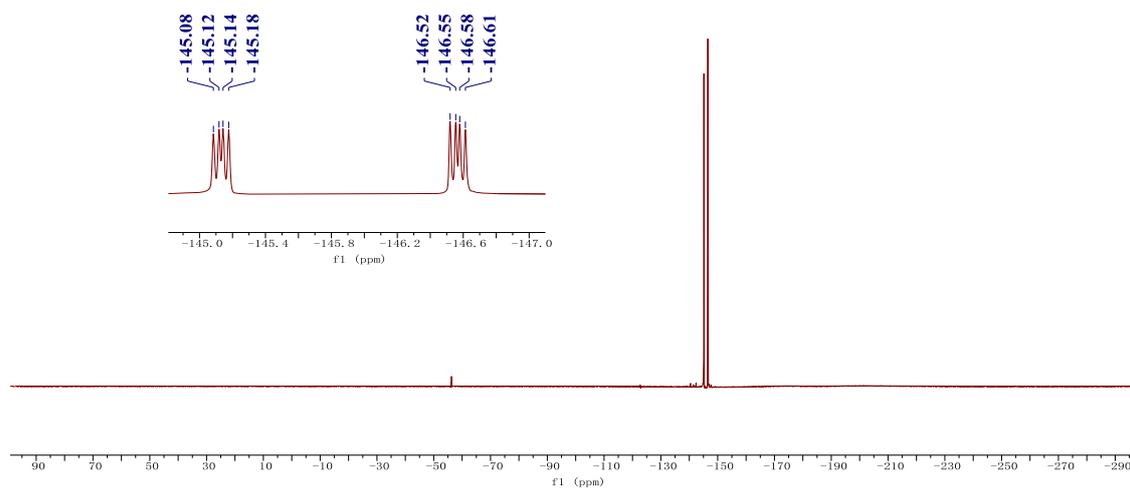
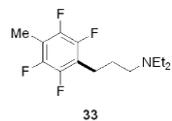
¹H NMR Spectrum of 33



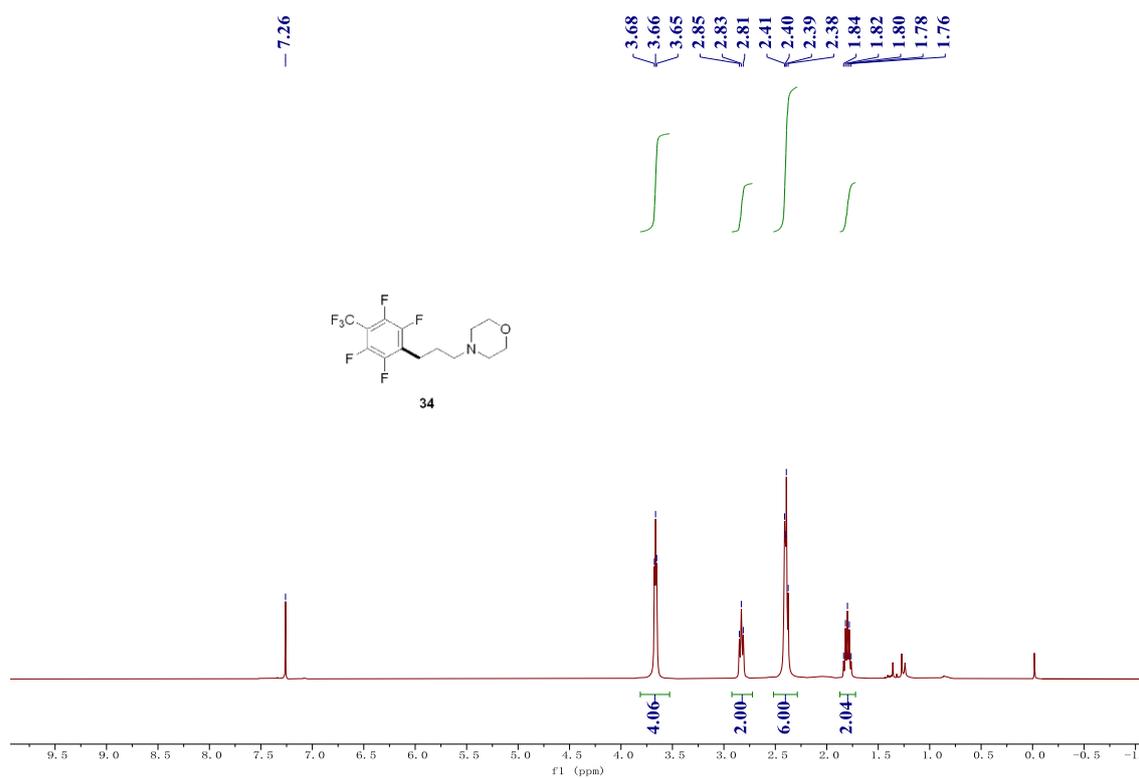
¹³C NMR Spectrum of 33



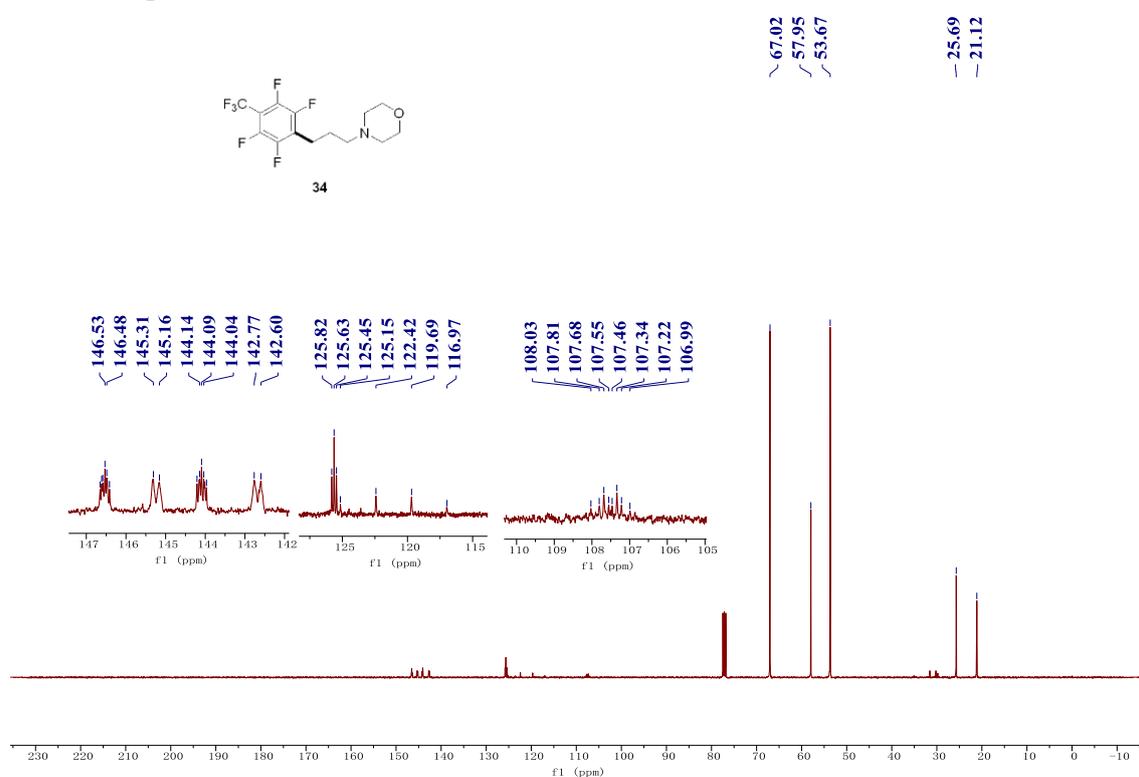
¹⁹F NMR Spectrum of 33



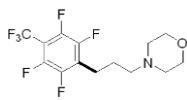
¹H NMR Spectrum of 34



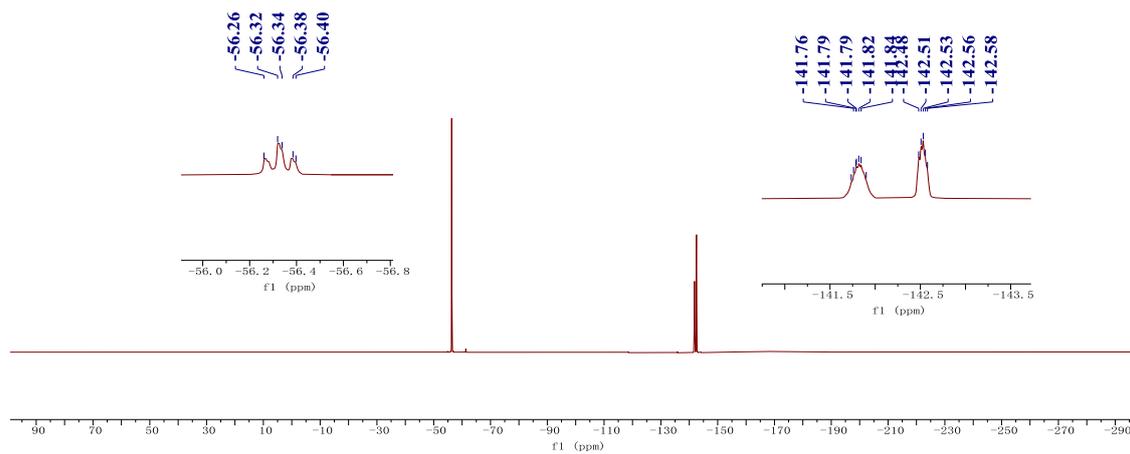
¹³C NMR Spectrum of 34



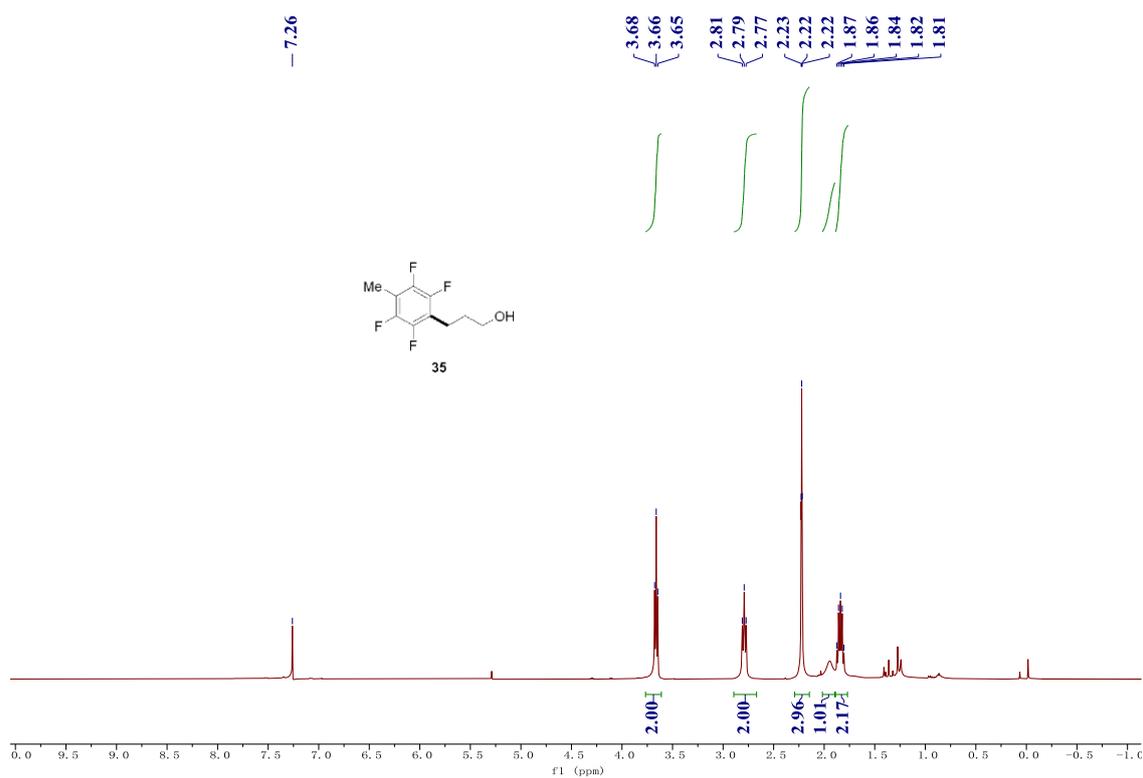
¹⁹F NMR Spectrum of 34



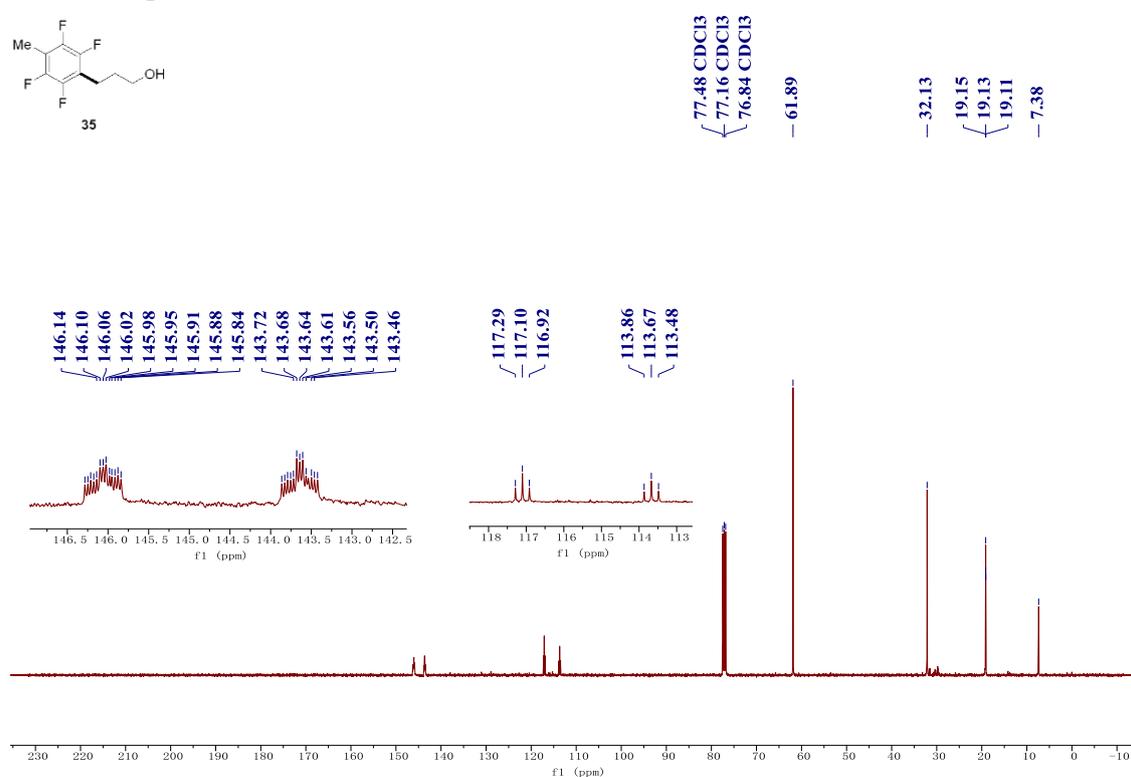
34



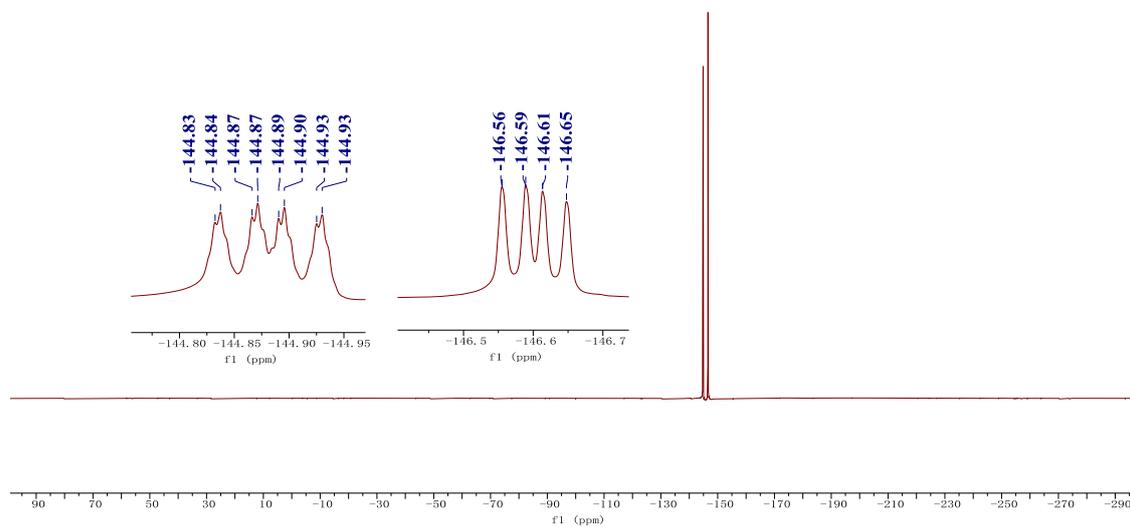
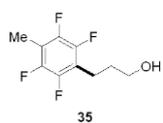
¹H NMR Spectrum of 35



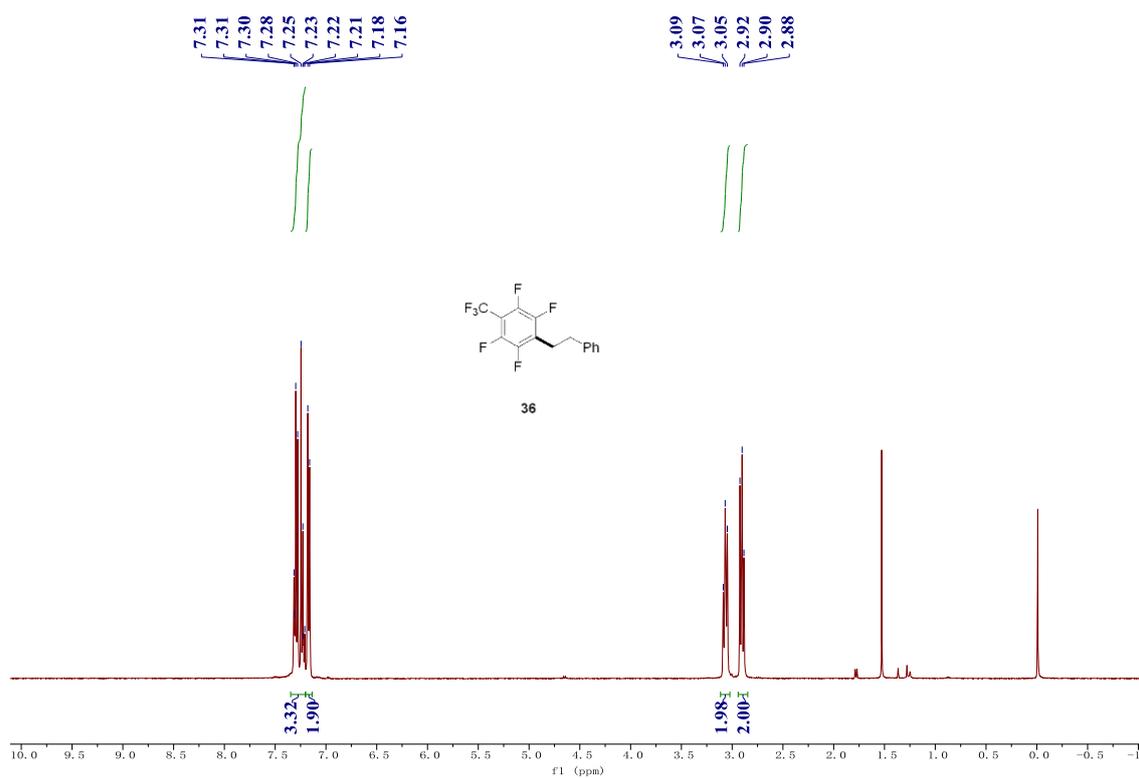
¹³C NMR Spectrum of 35



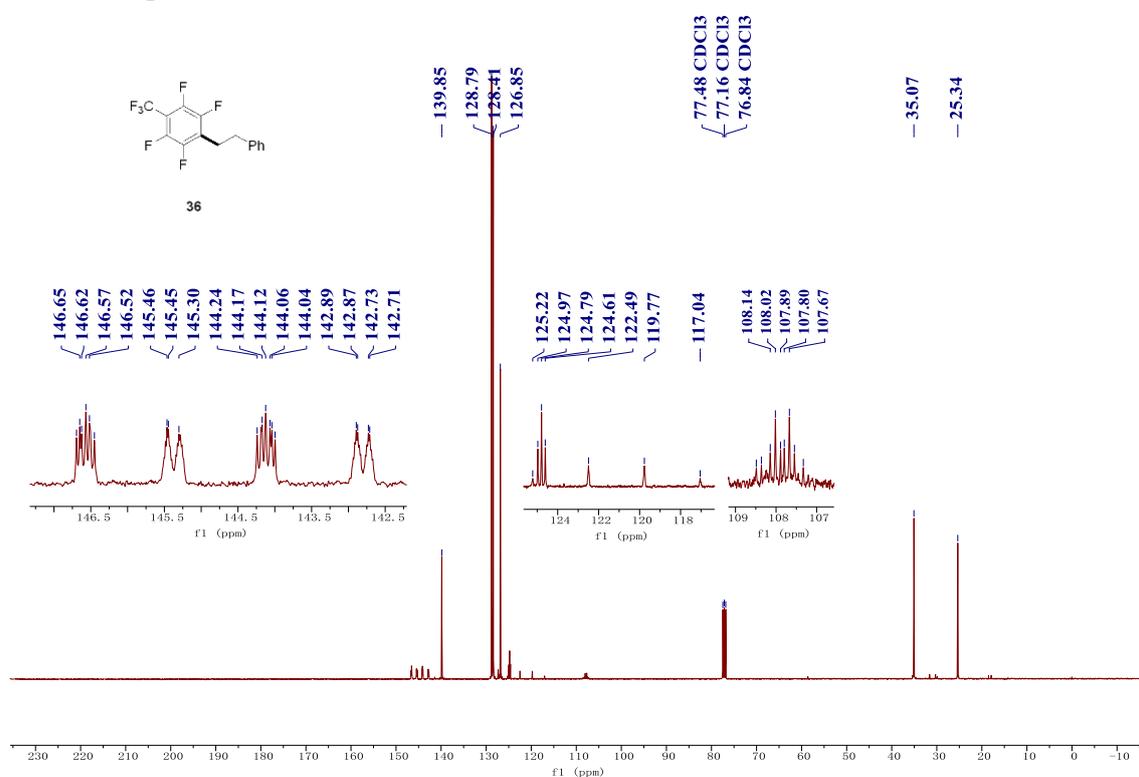
¹⁹F NMR Spectrum of 35



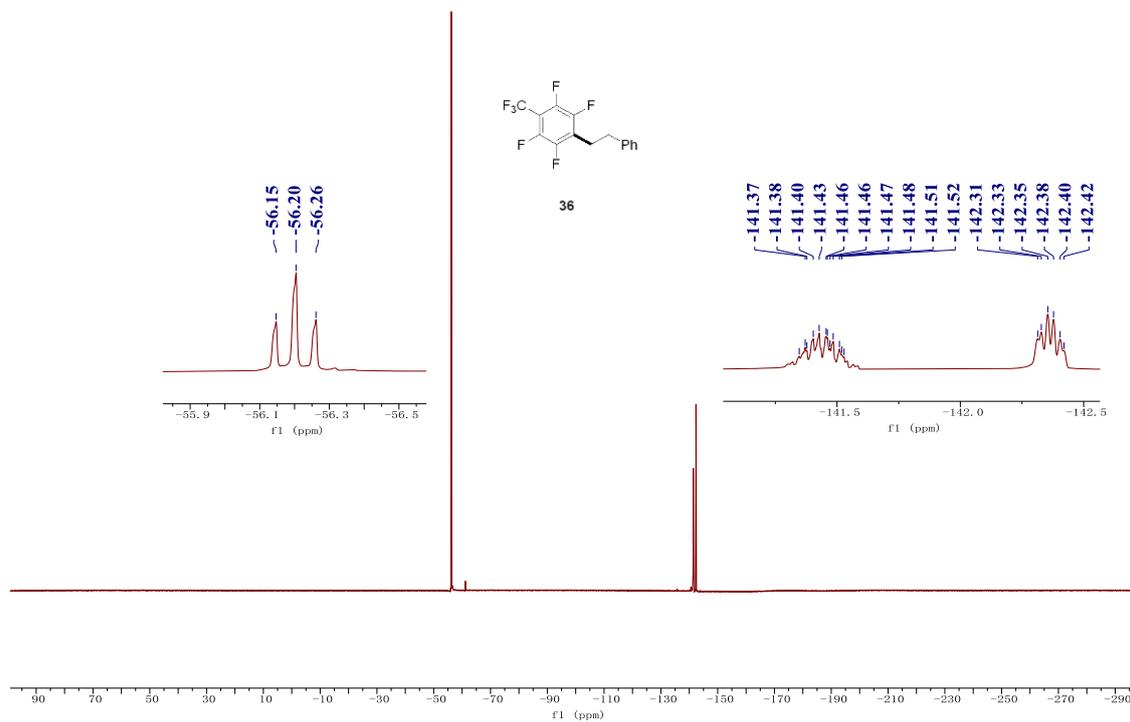
¹H NMR Spectrum of 36



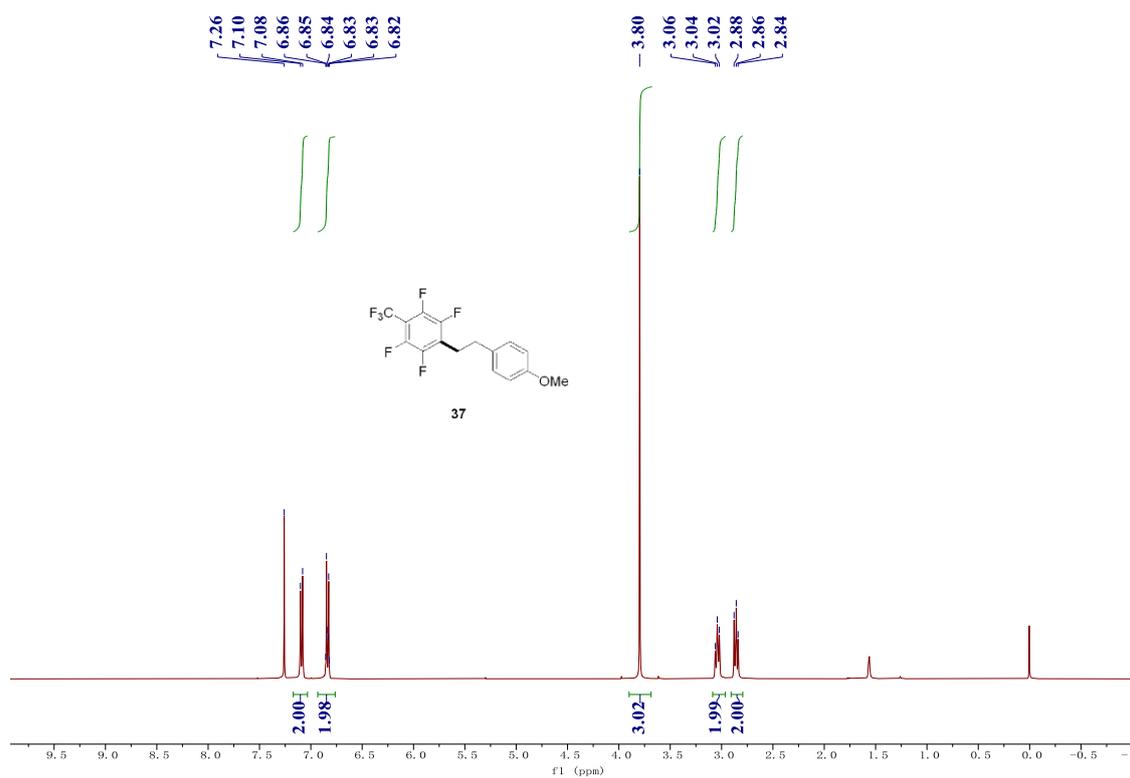
¹³C NMR Spectrum of 36



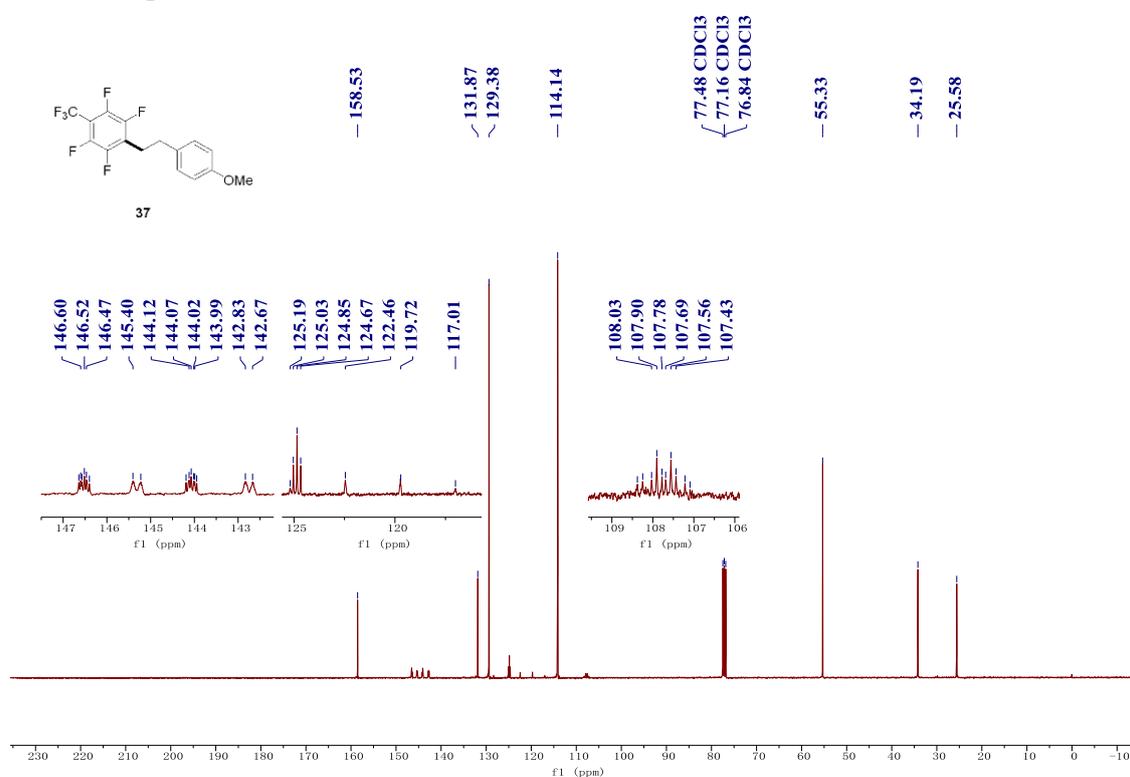
¹⁹F NMR Spectrum of 36



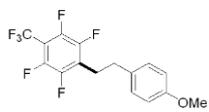
¹H NMR Spectrum of 37



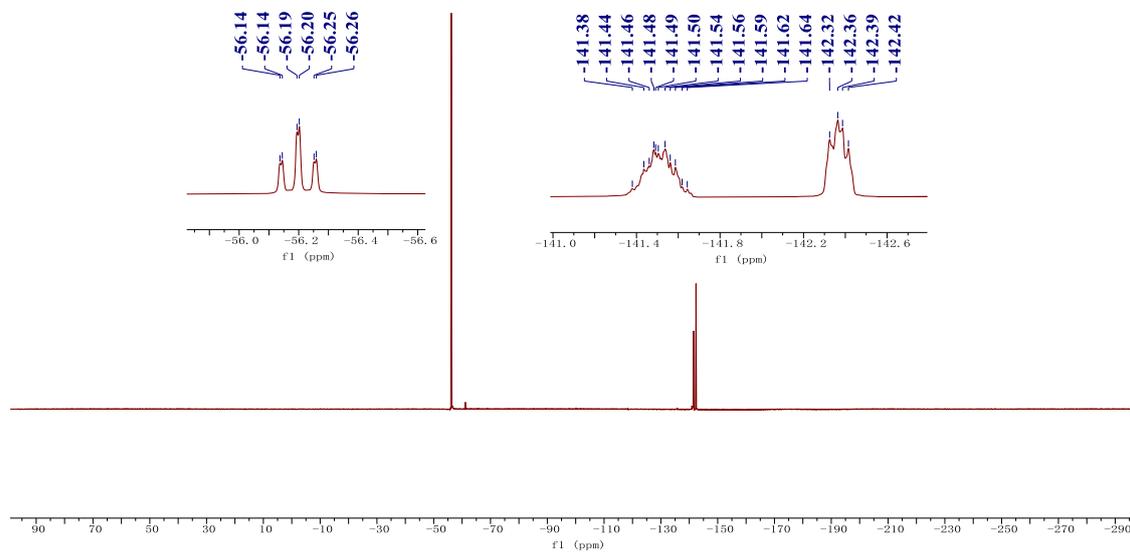
¹³C NMR Spectrum of 37



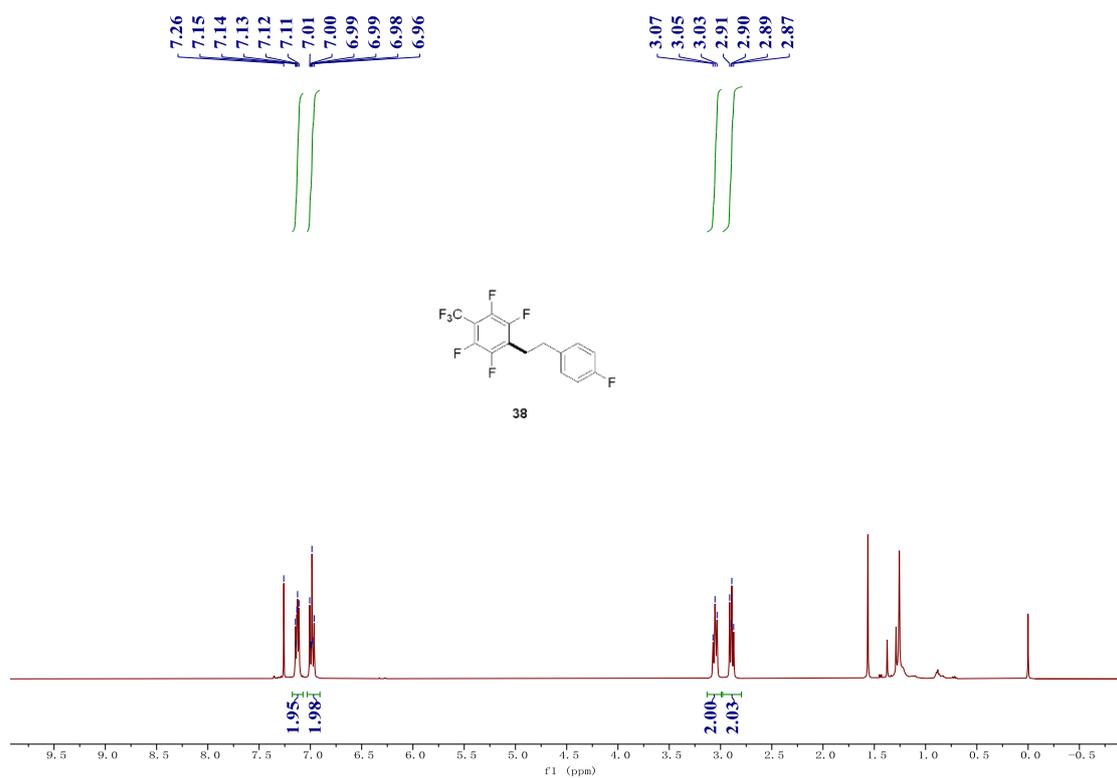
¹⁹F NMR Spectrum of 37



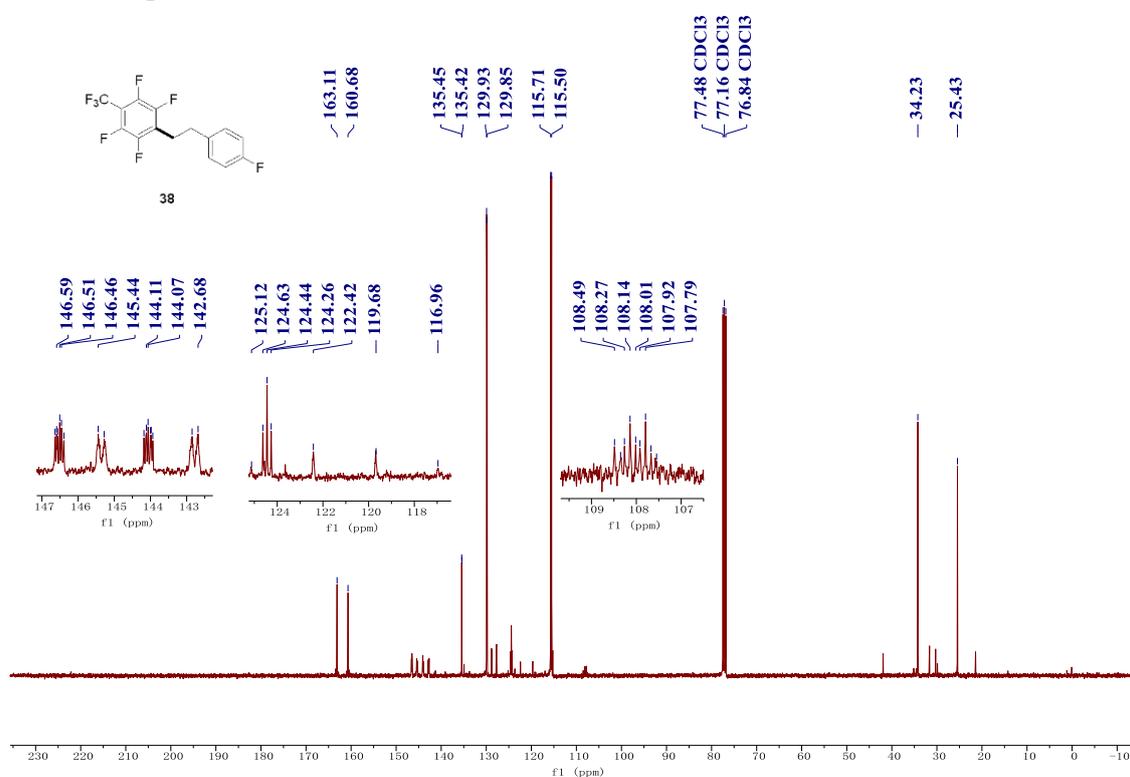
37



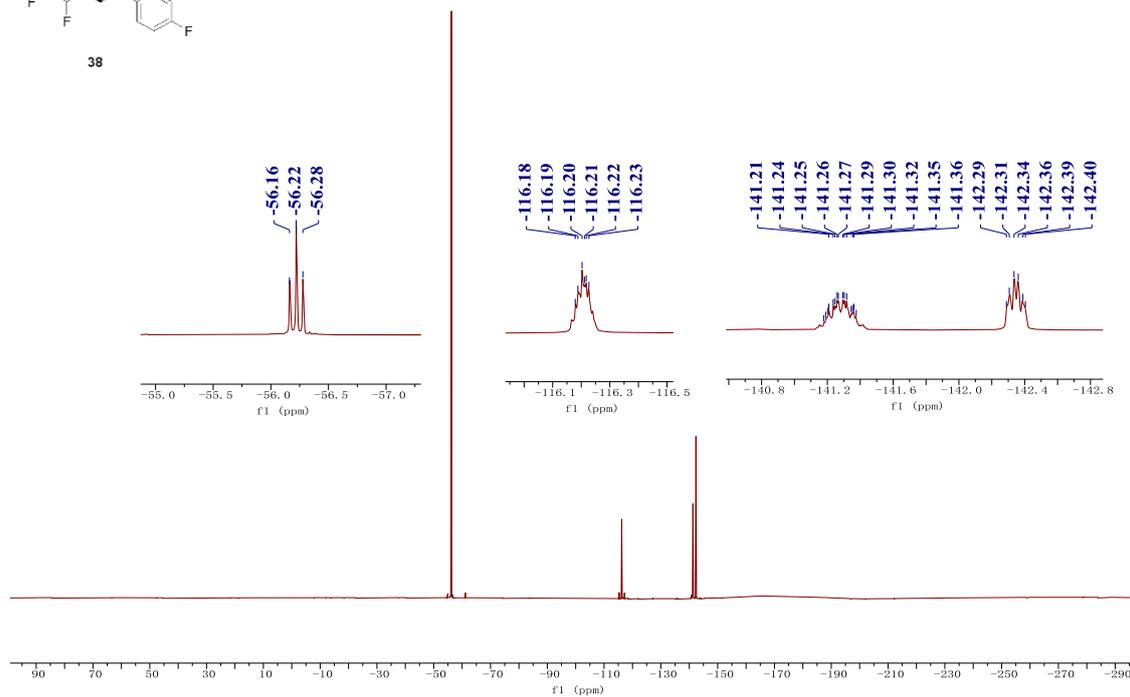
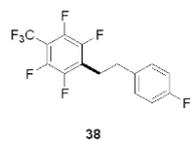
¹H NMR Spectrum of 38



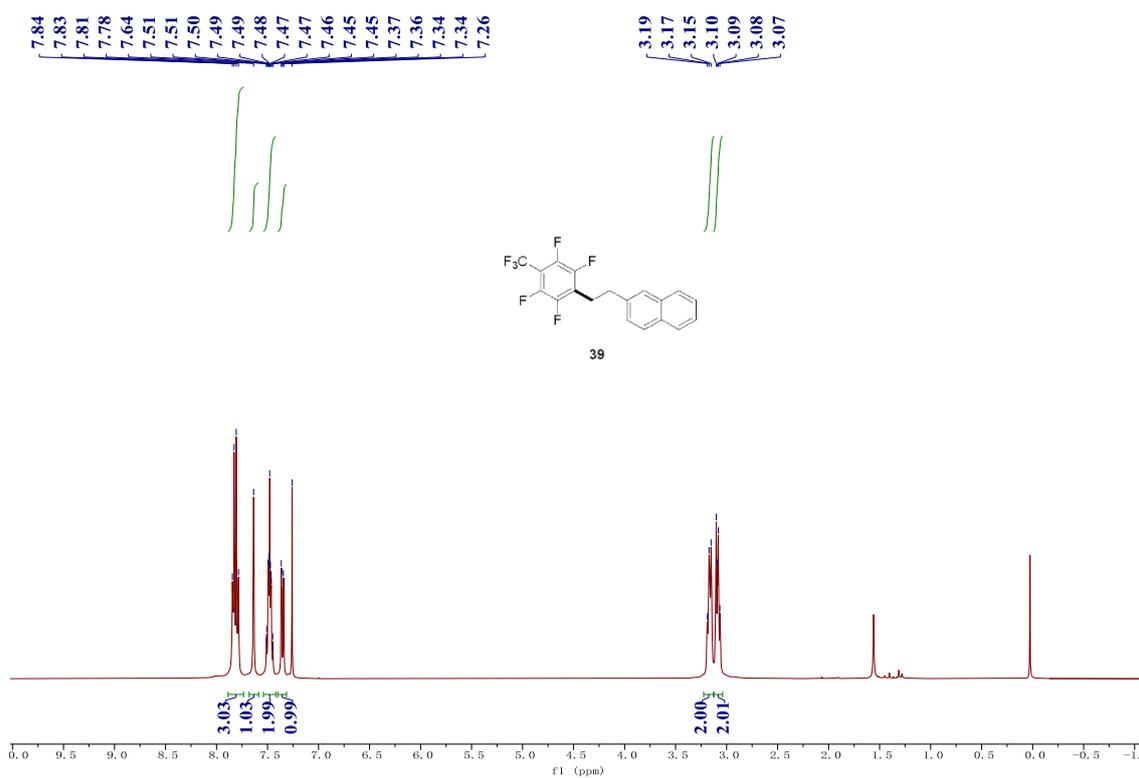
¹³C NMR Spectrum of 38



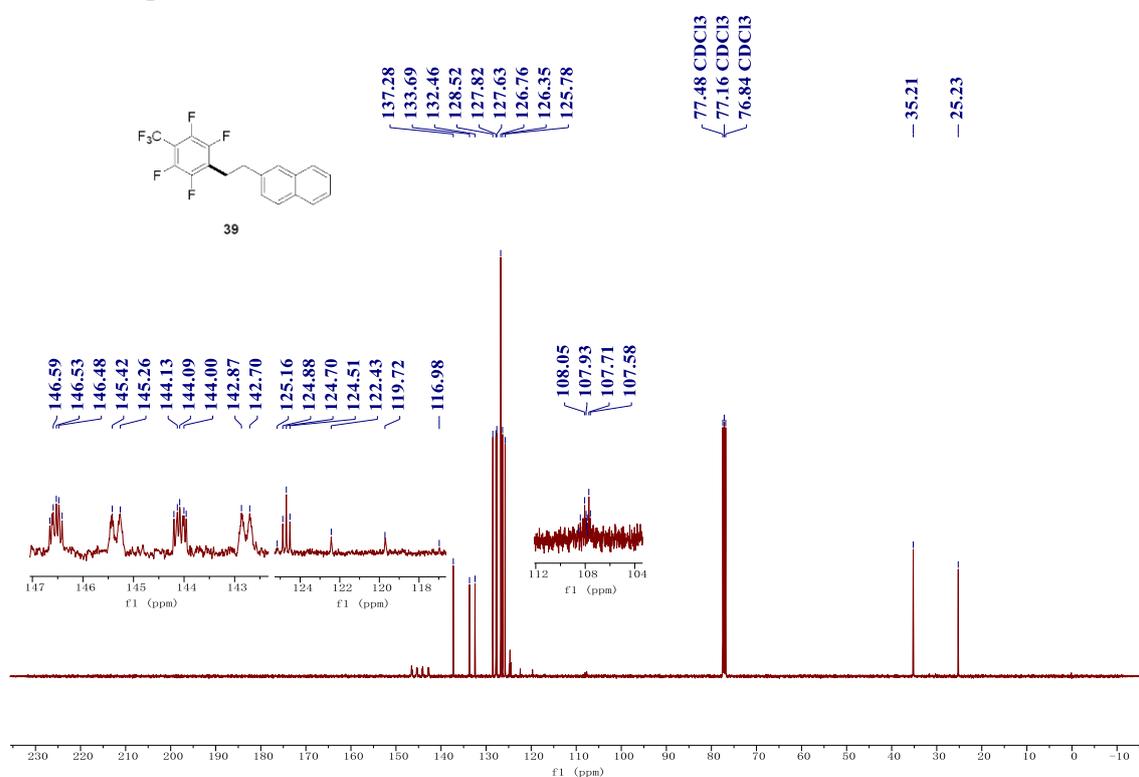
¹⁹F NMR Spectrum of 38



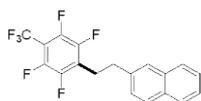
¹H NMR Spectrum of 39



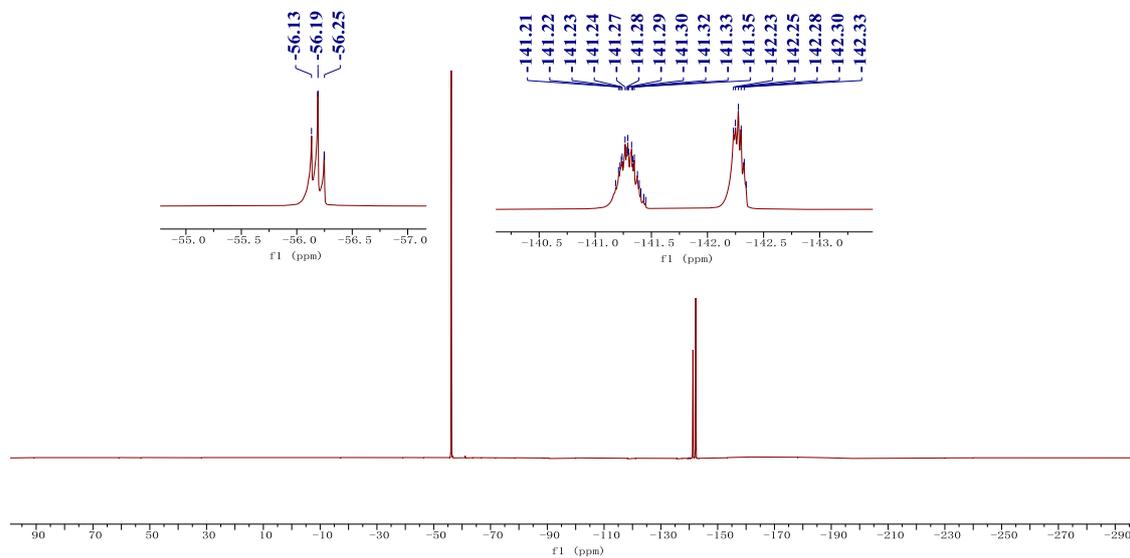
¹³C NMR Spectrum of 39



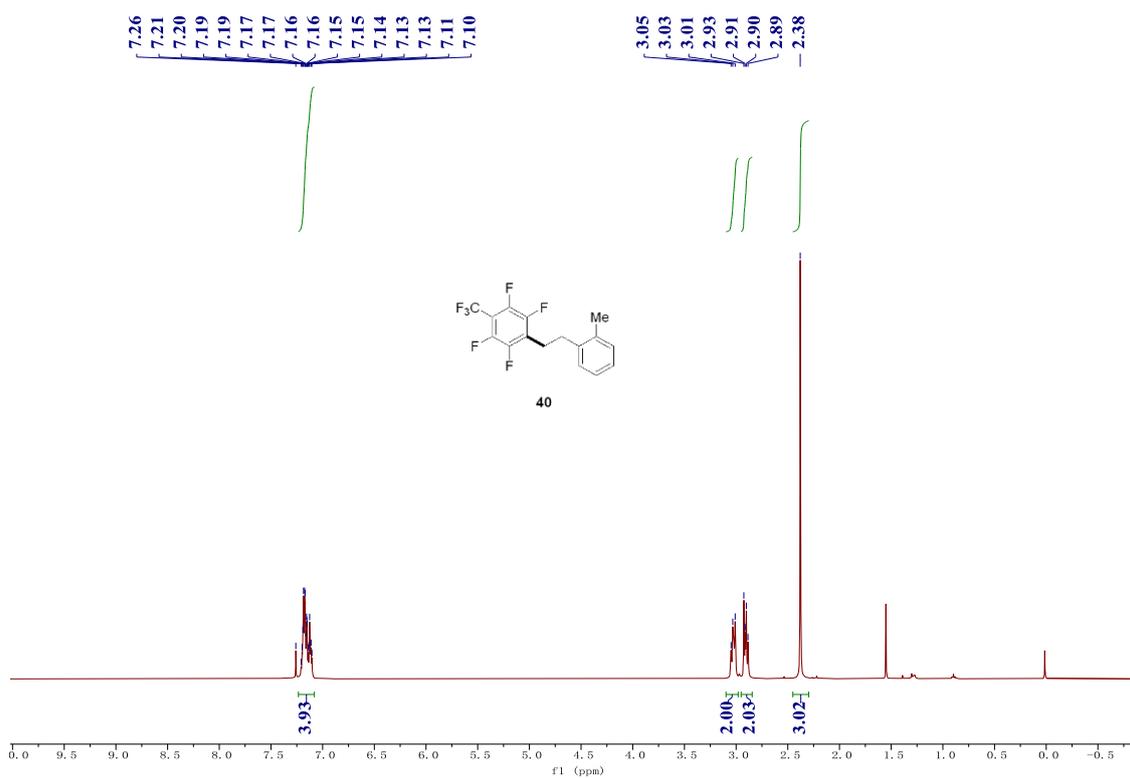
¹⁹F NMR Spectrum of 39



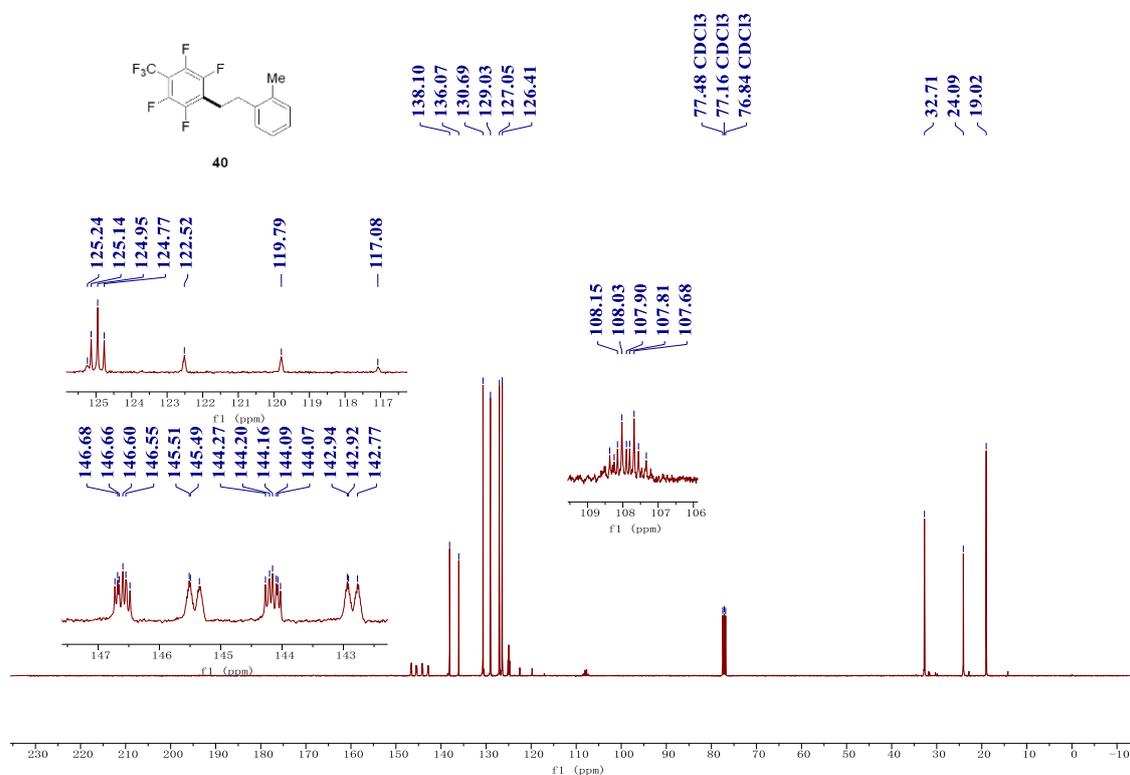
39



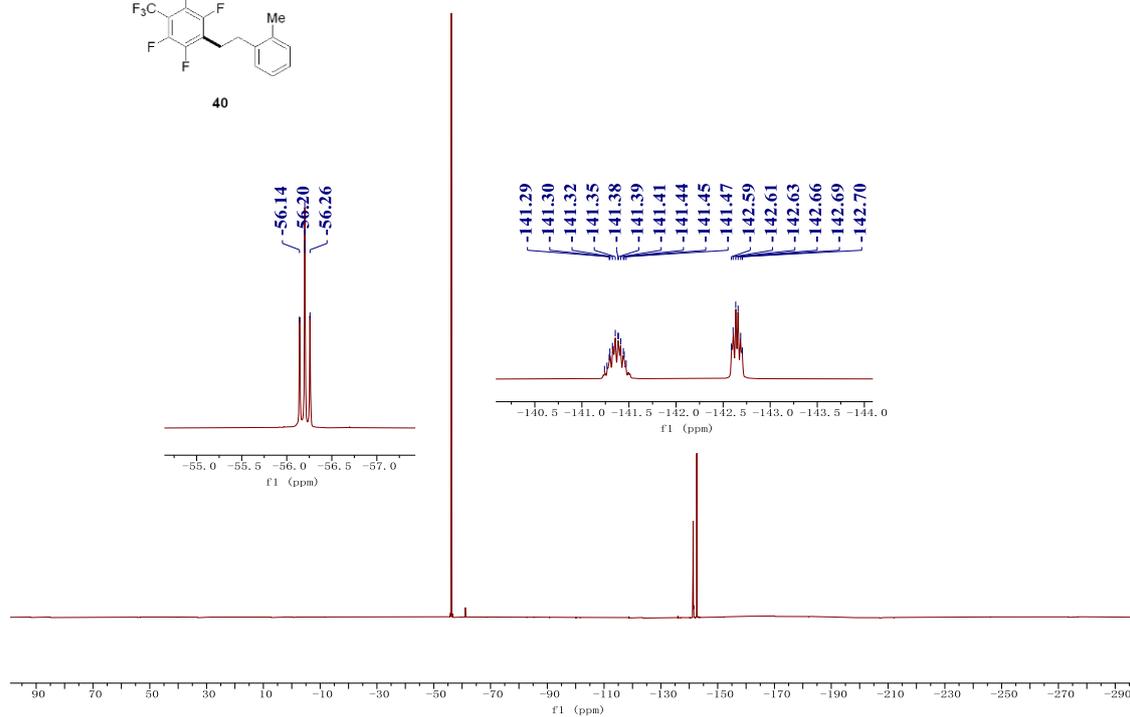
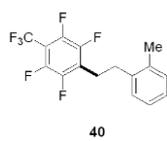
¹H NMR Spectrum of 40



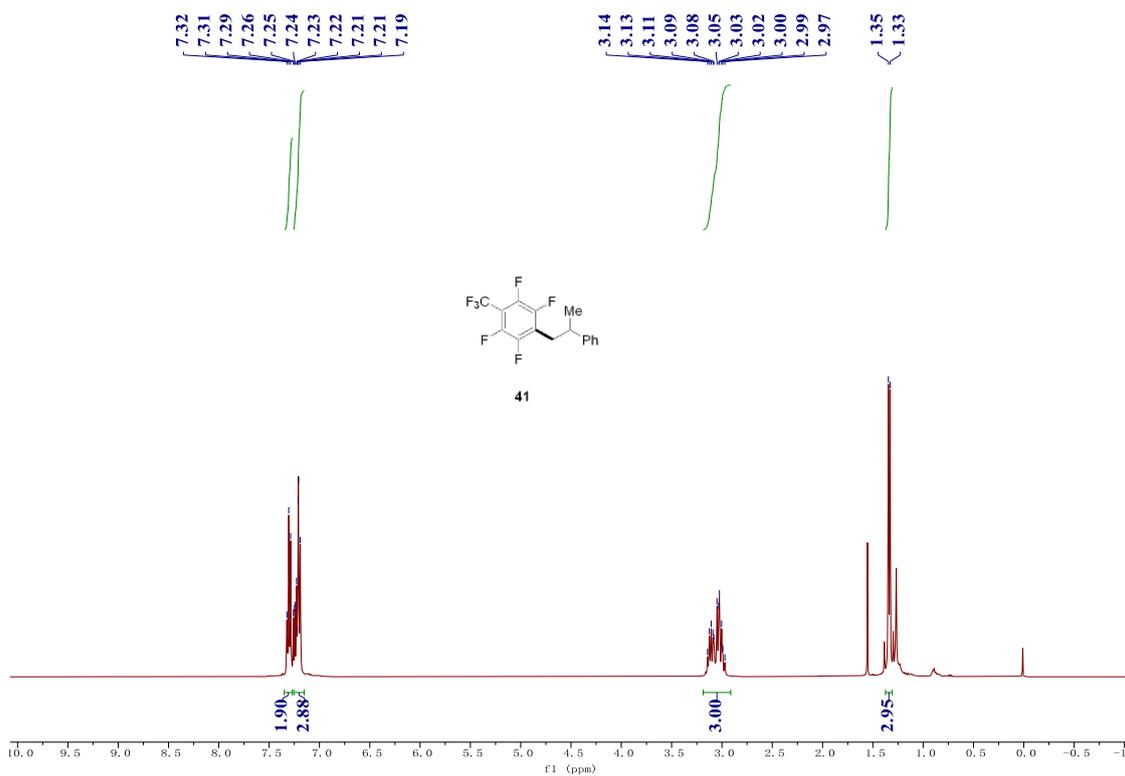
¹³C NMR Spectrum of 40



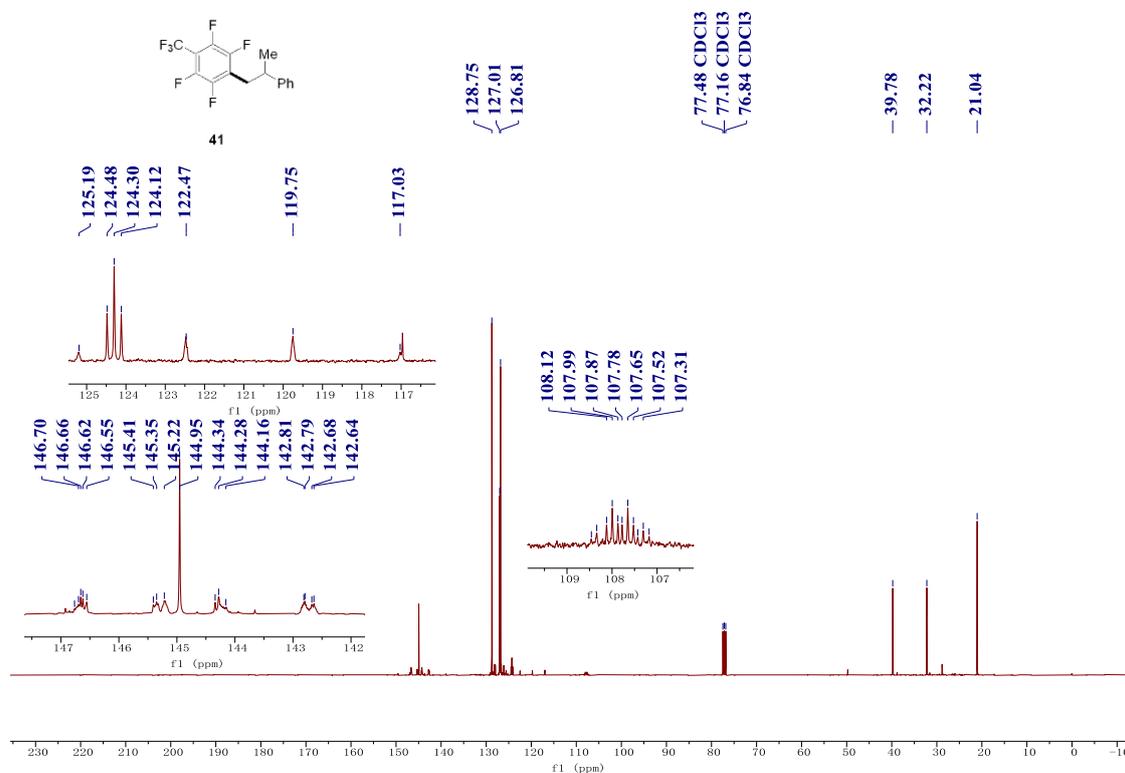
¹⁹F NMR Spectrum of 40



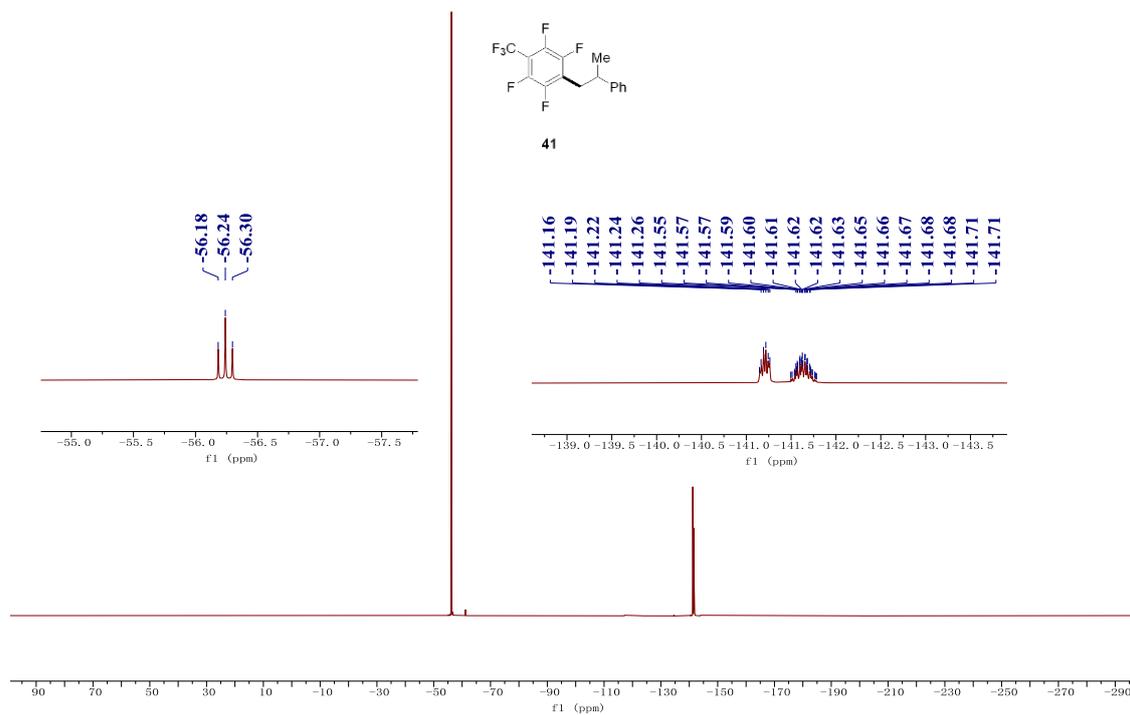
¹H NMR Spectrum of 41



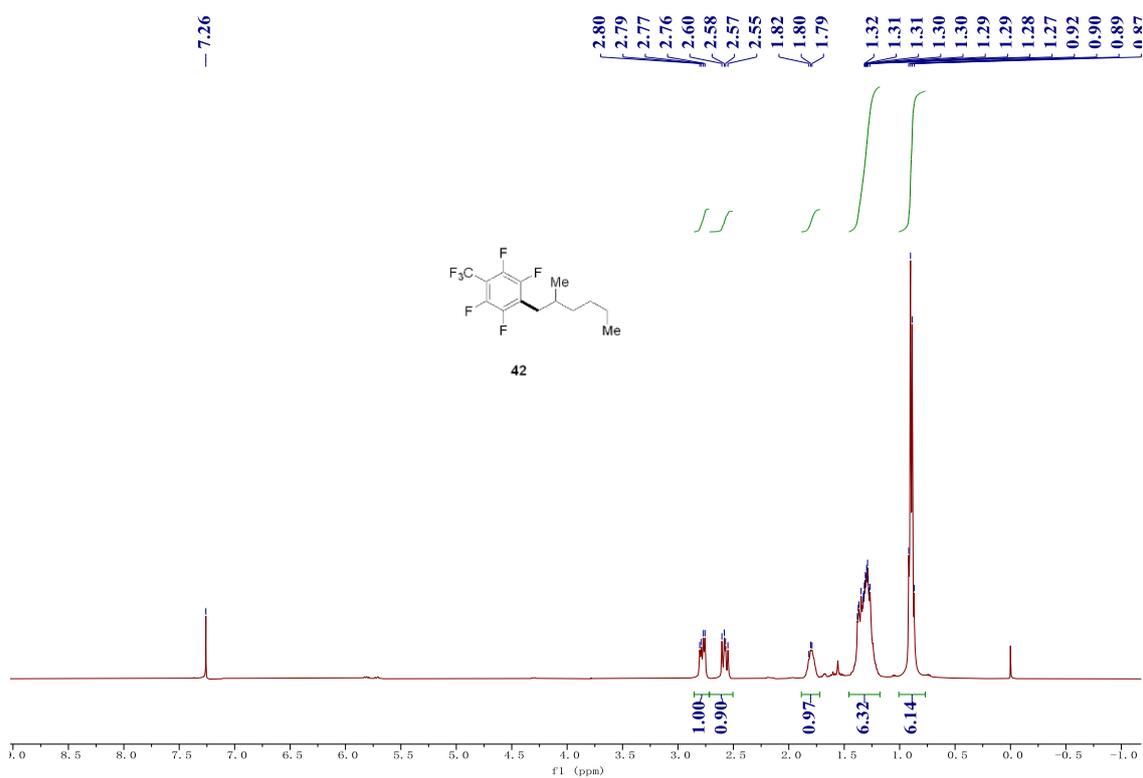
¹³C NMR Spectrum of 41



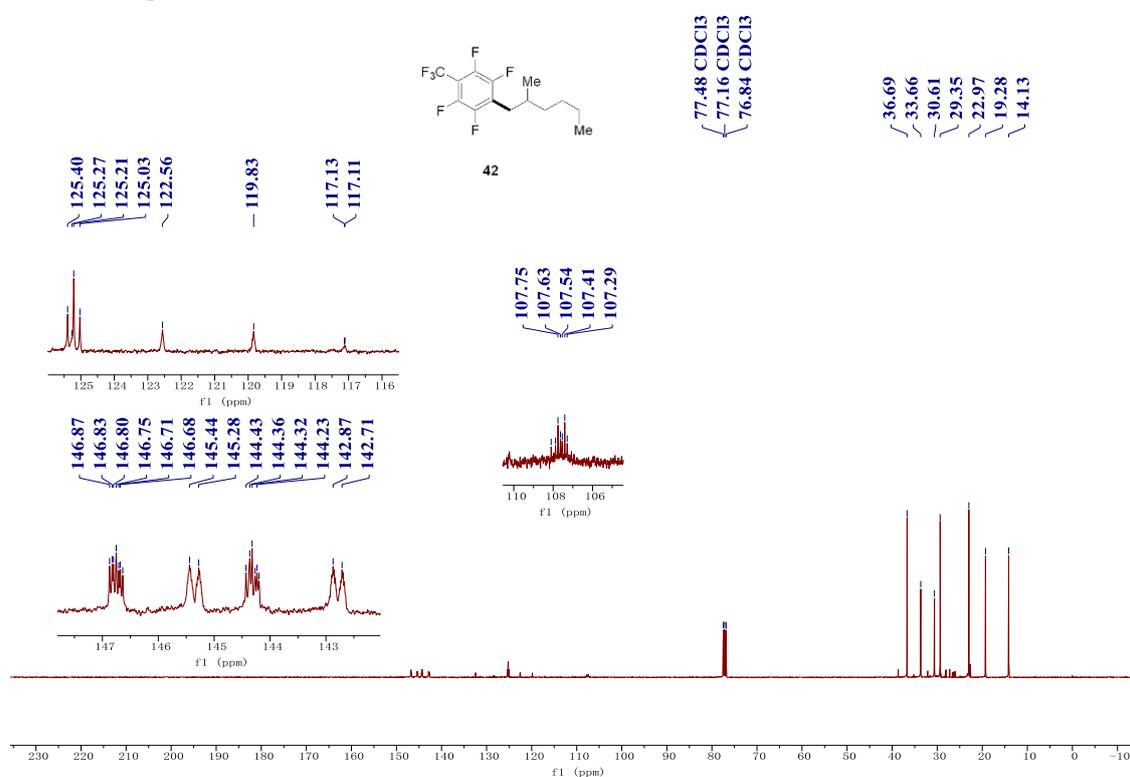
¹⁹F NMR Spectrum of 41



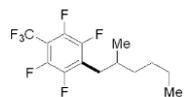
¹H NMR Spectrum of 42



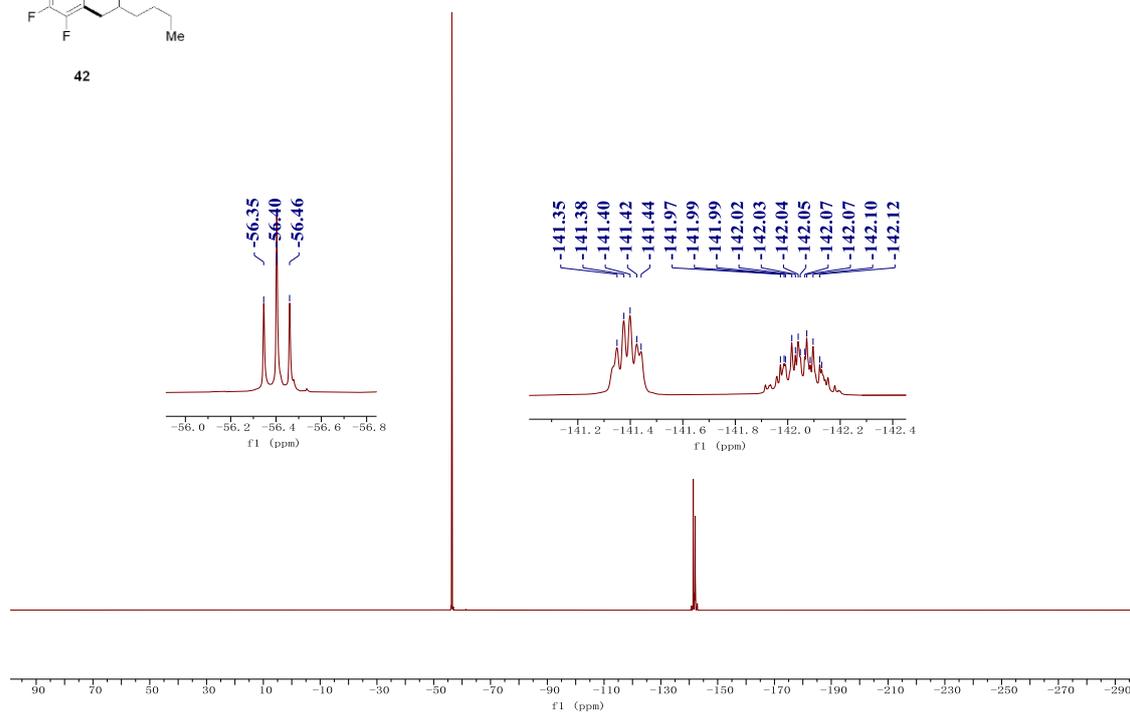
¹³C NMR Spectrum of 42



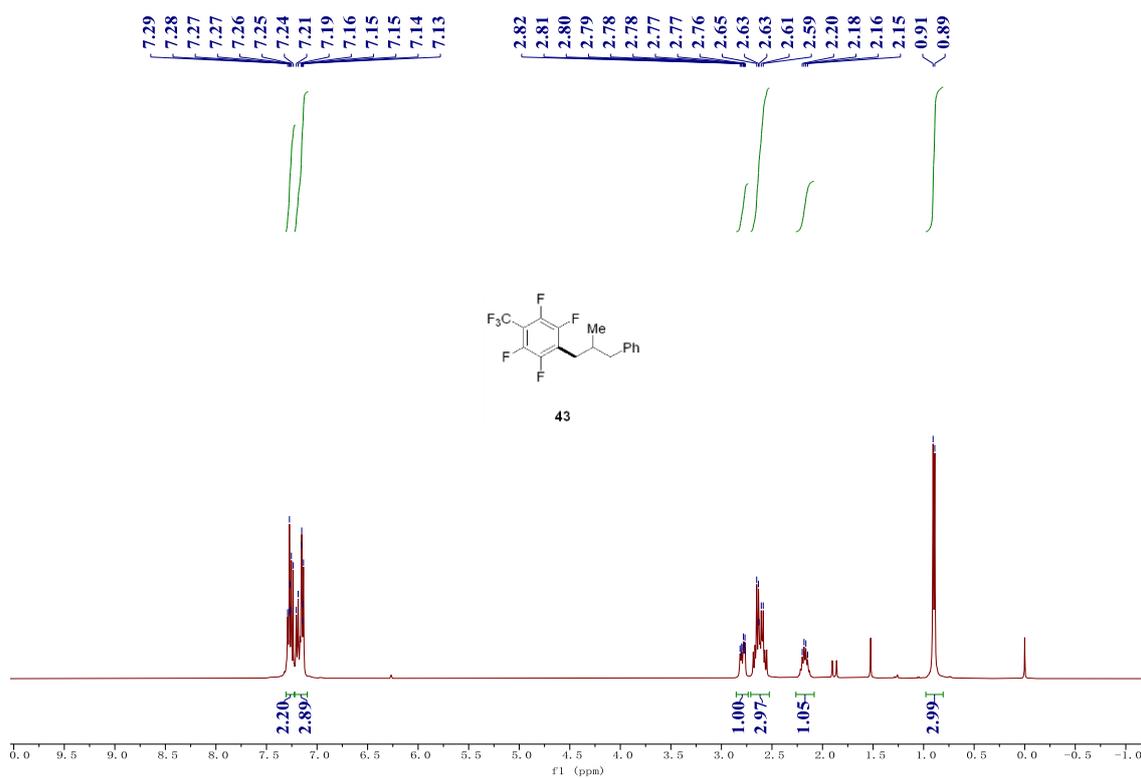
¹⁹F NMR Spectrum of 42



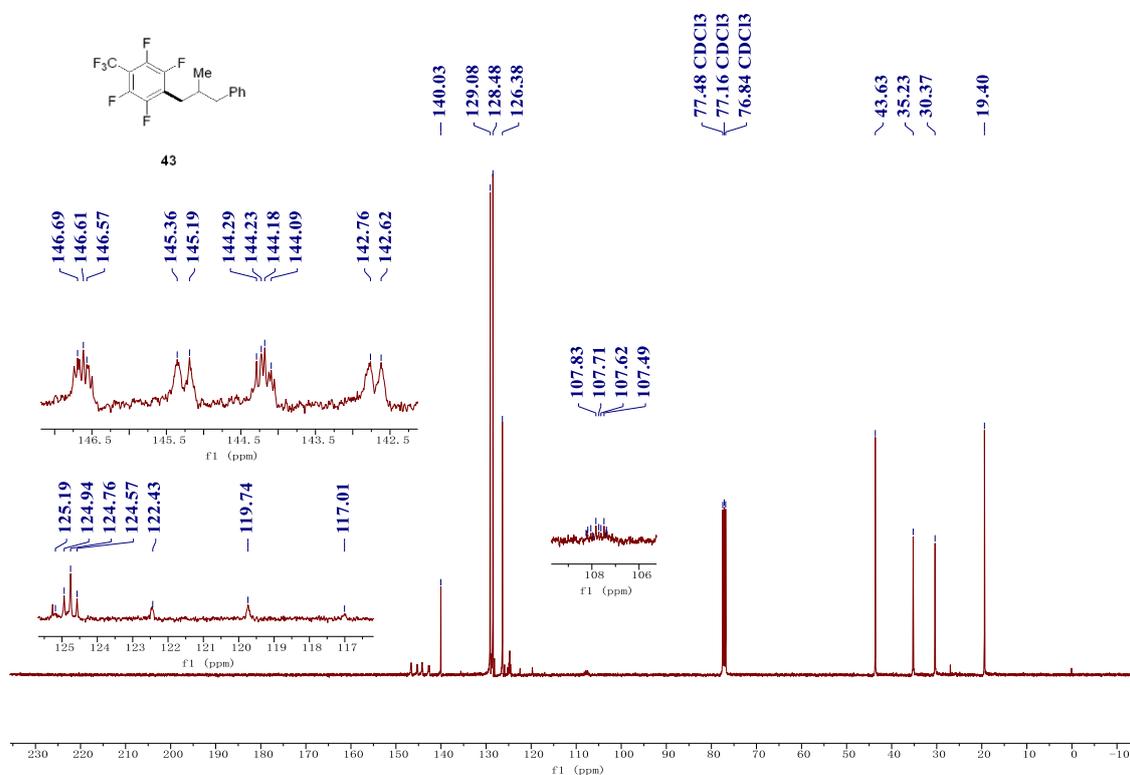
42



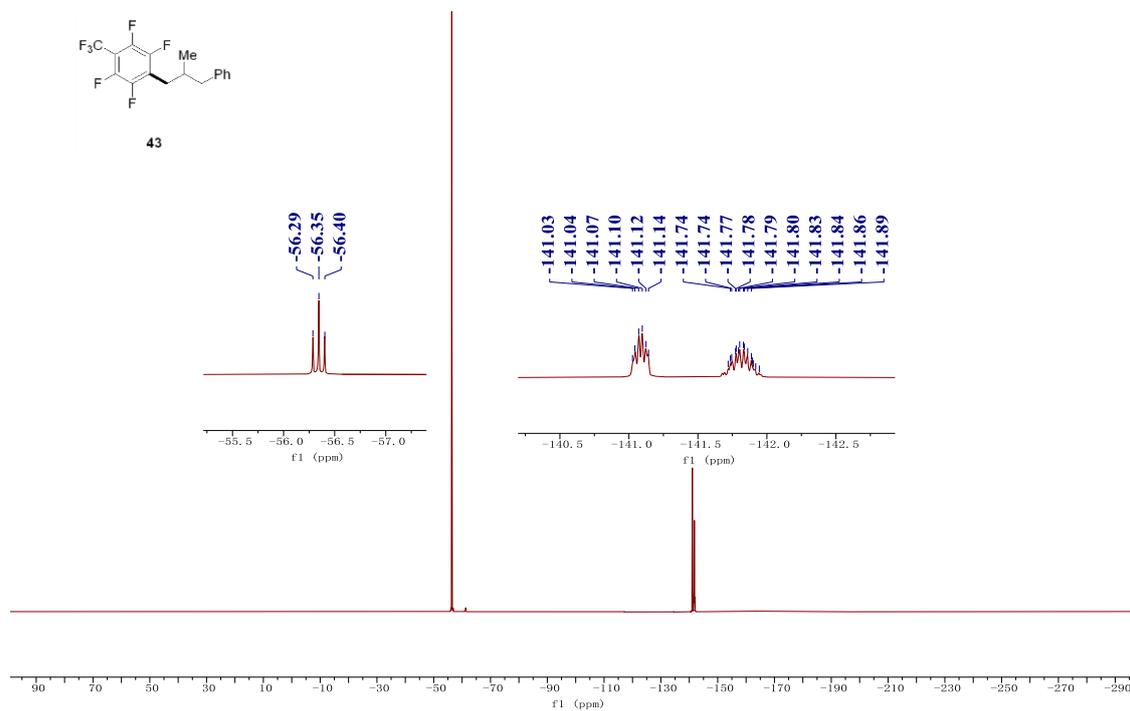
¹H NMR Spectrum of 43



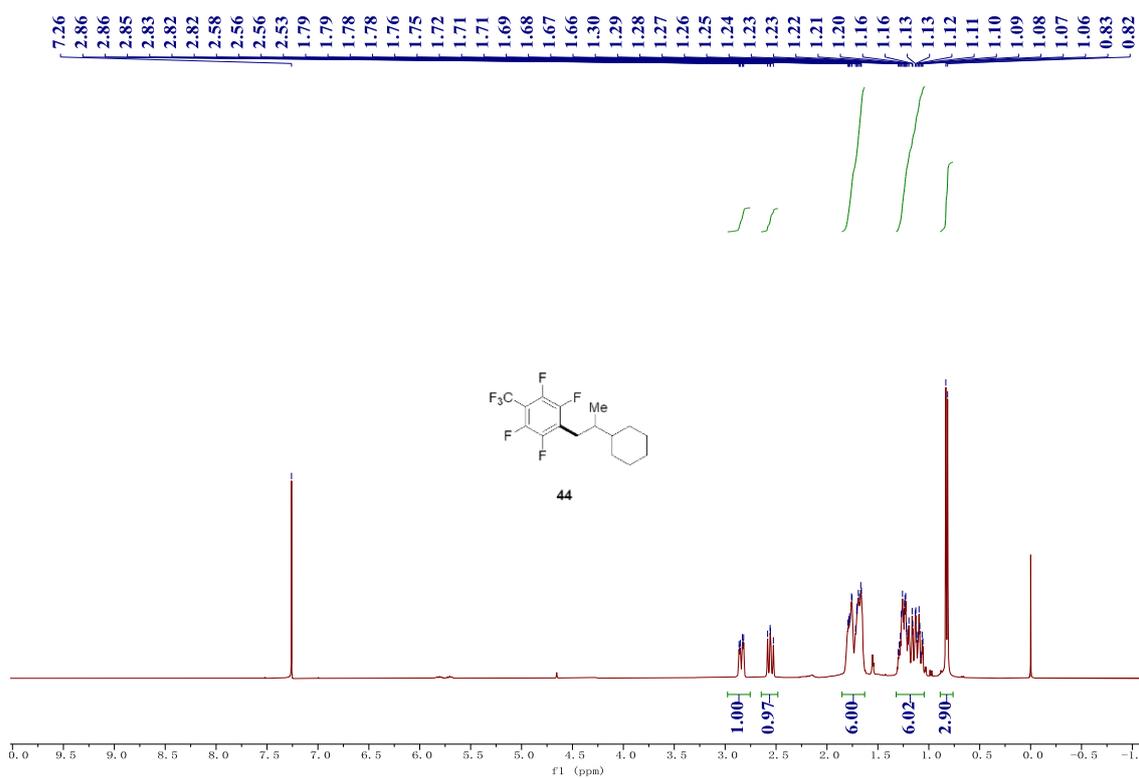
¹³C NMR Spectrum of 43



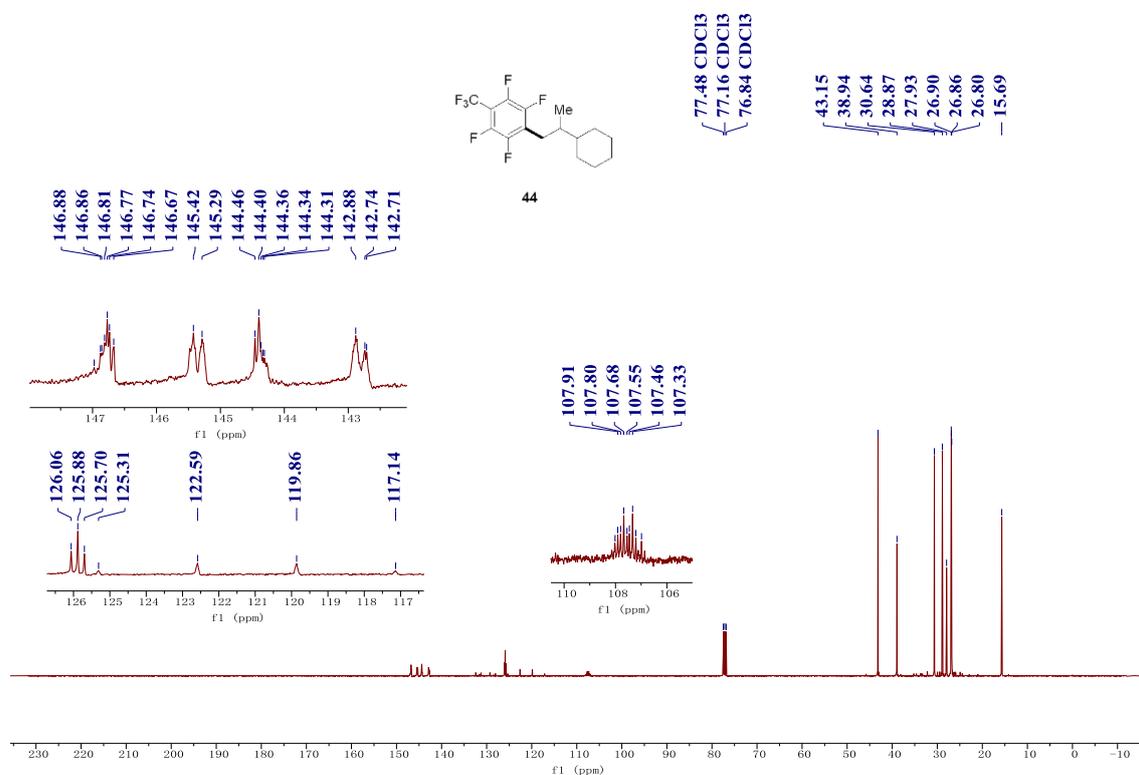
¹⁹F NMR Spectrum of 43



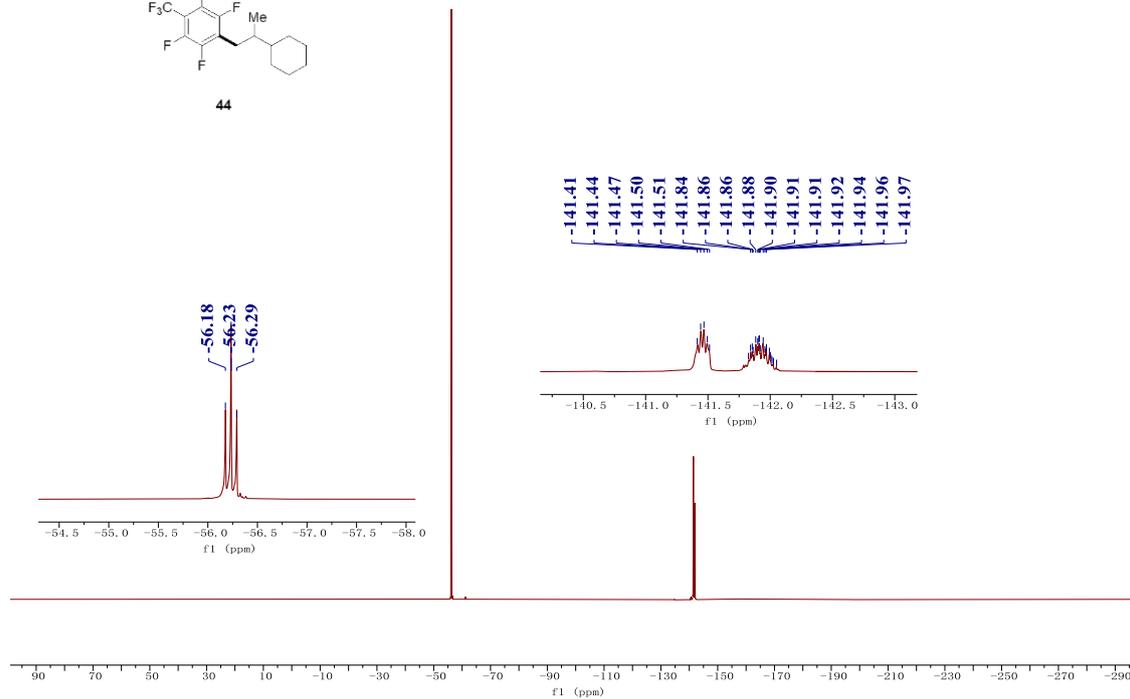
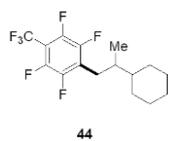
¹H NMR Spectrum of 44



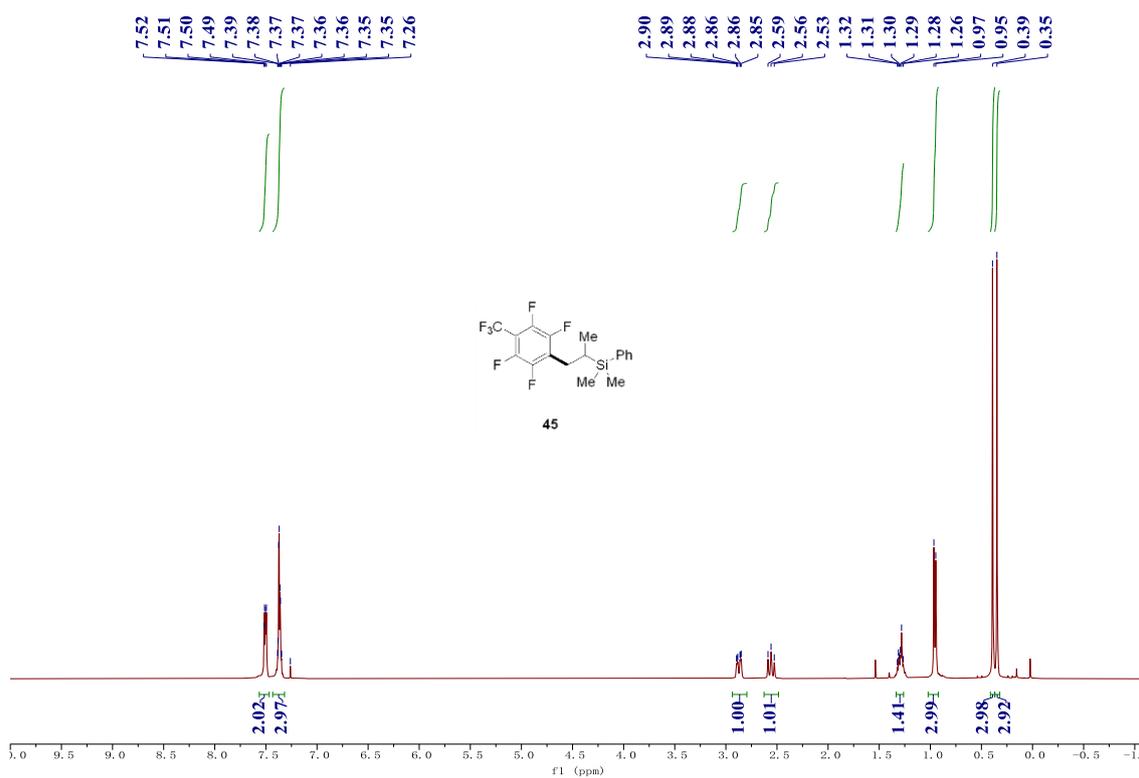
¹³C NMR Spectrum of 44



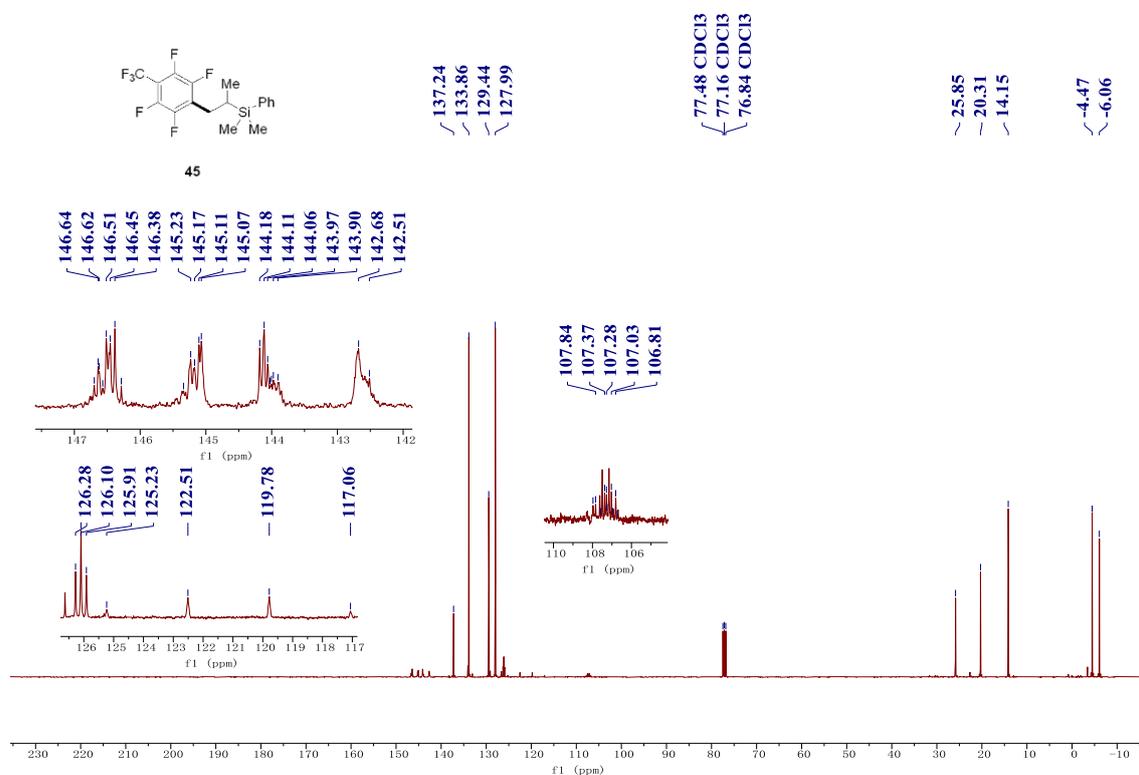
¹⁹F NMR Spectrum of 44



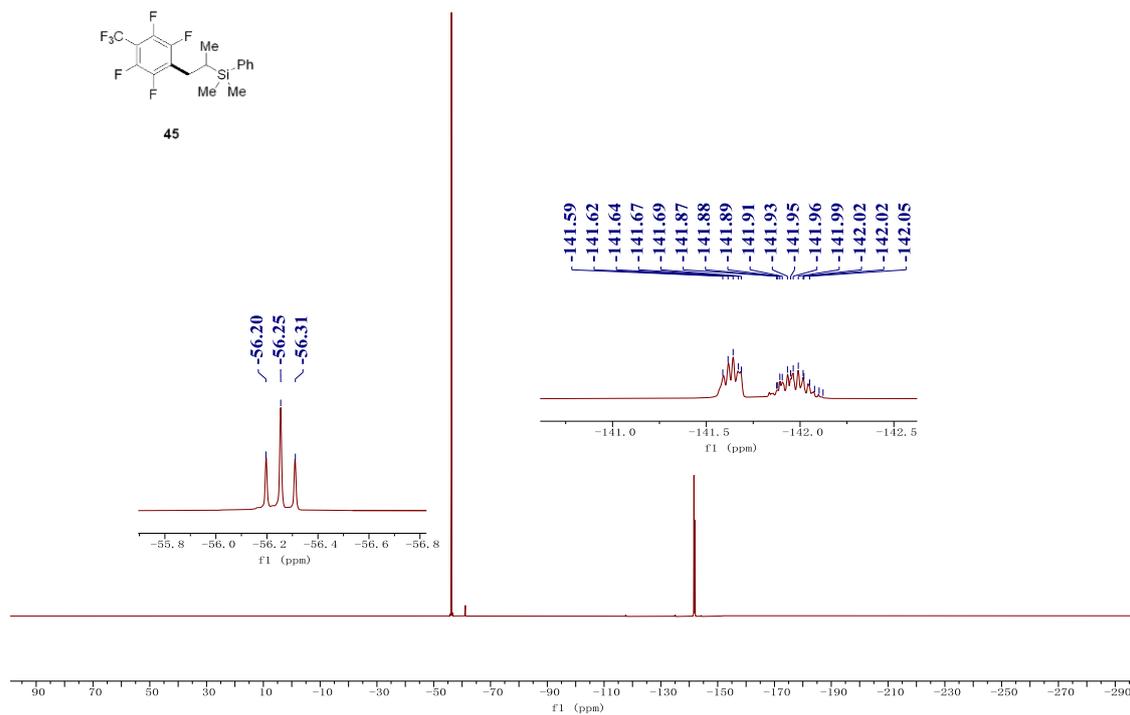
¹H NMR Spectrum of 45



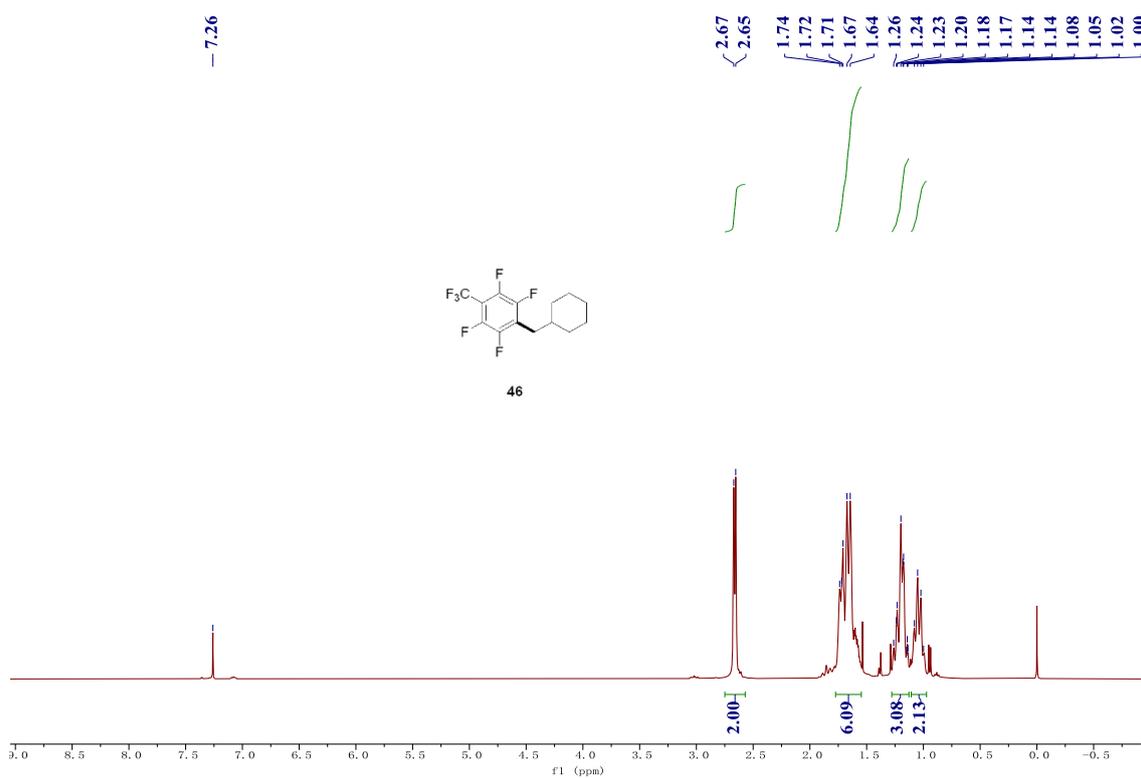
¹³C NMR Spectrum of 45



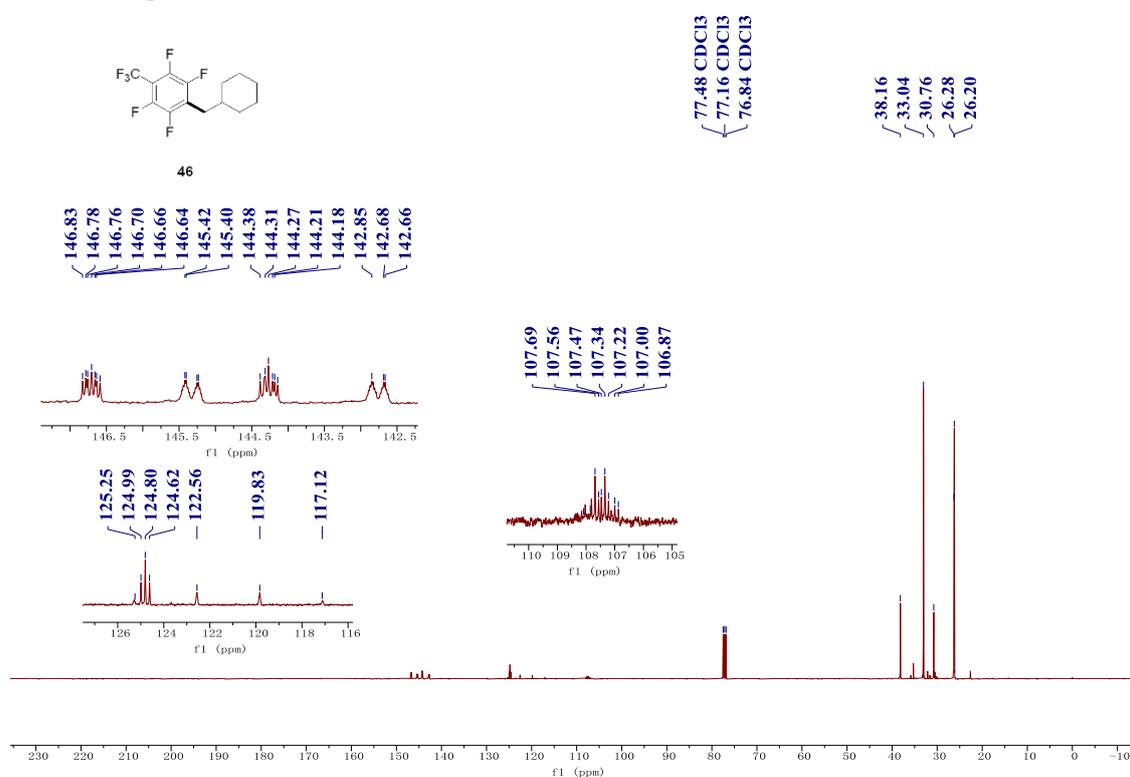
¹⁹F NMR Spectrum of 45



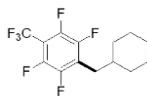
¹H NMR Spectrum of 46



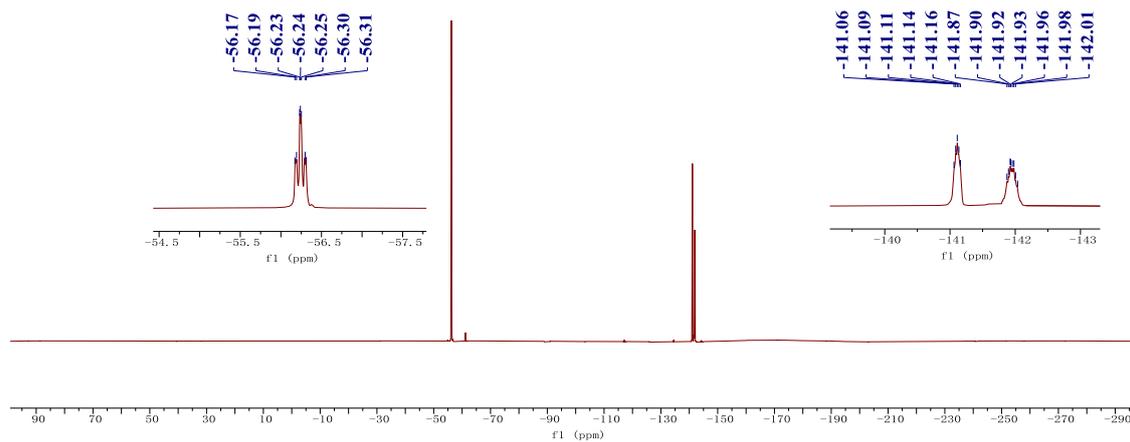
¹³C NMR Spectrum of 46



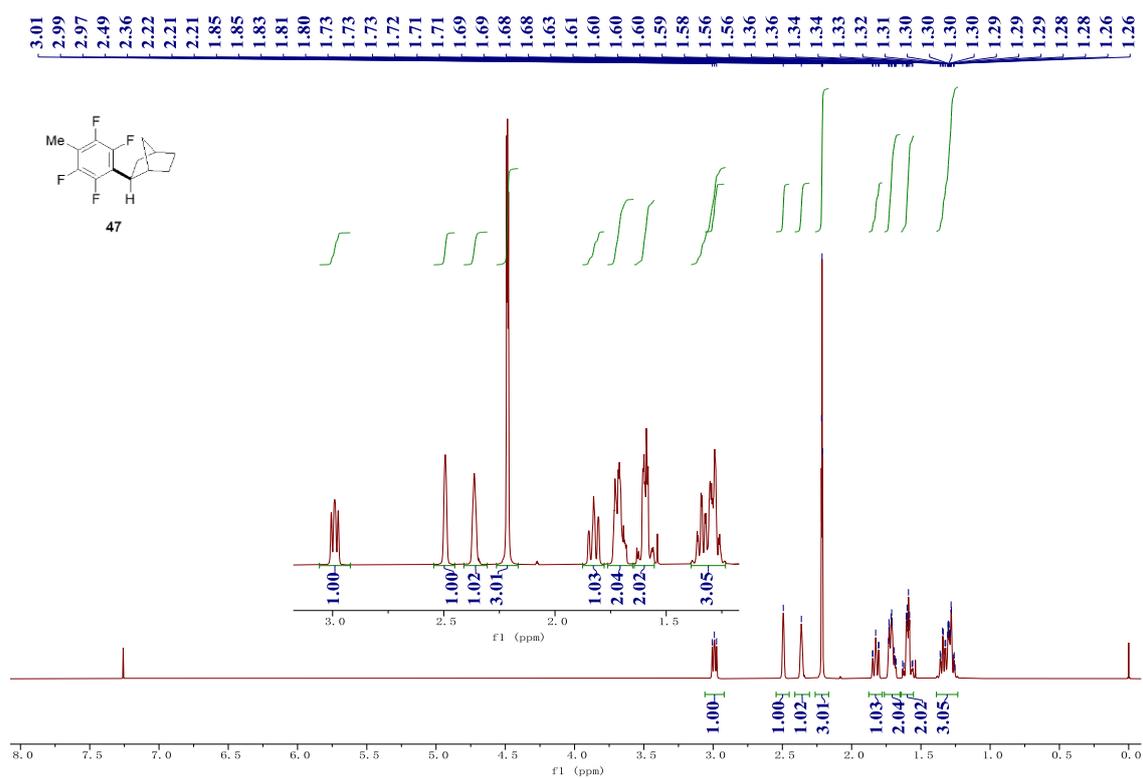
¹⁹F NMR Spectrum of 46



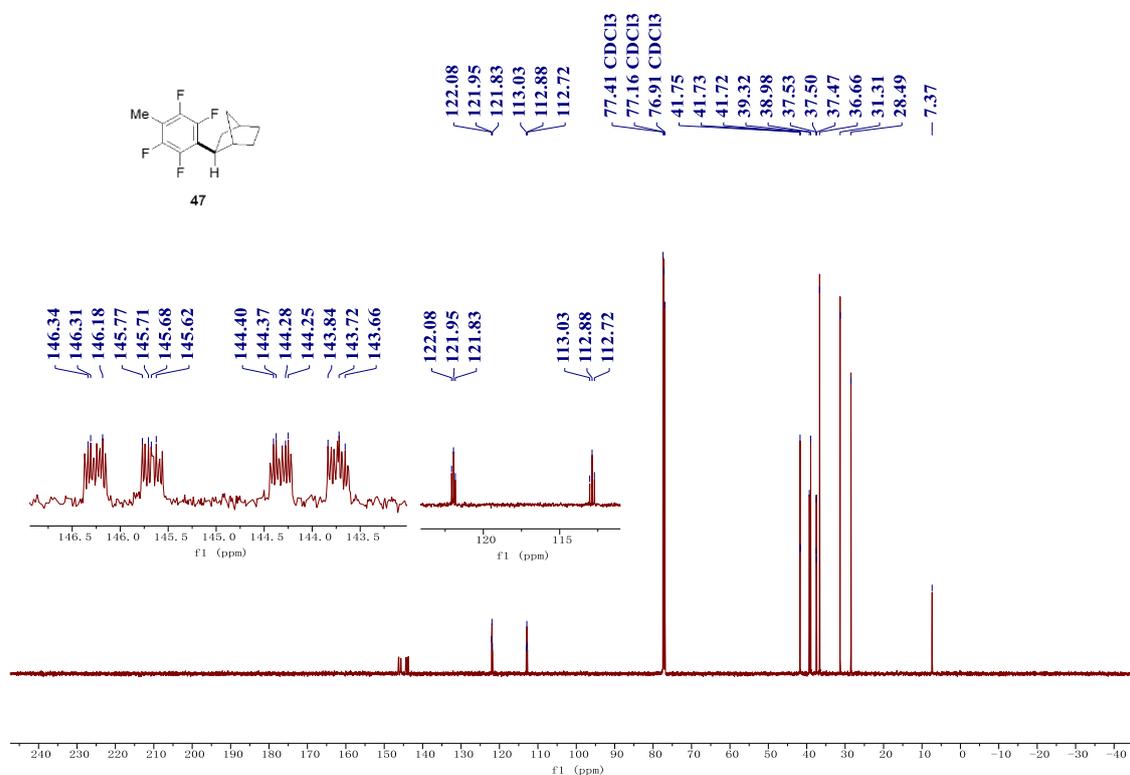
46



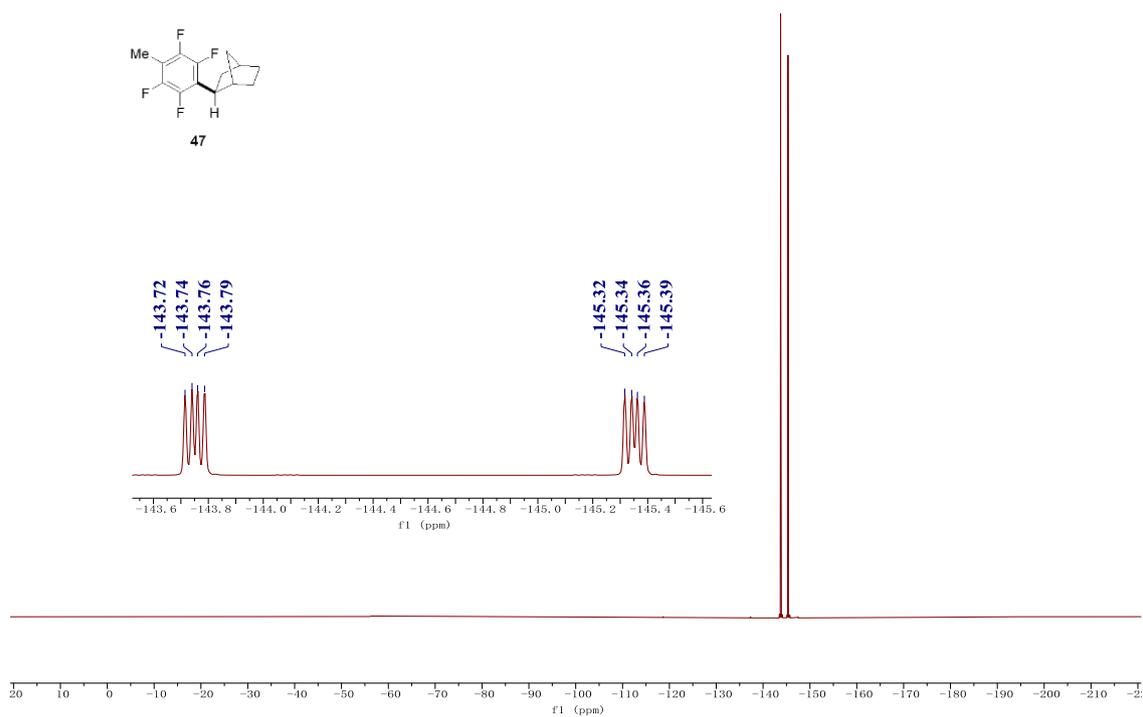
¹H NMR Spectrum of 47



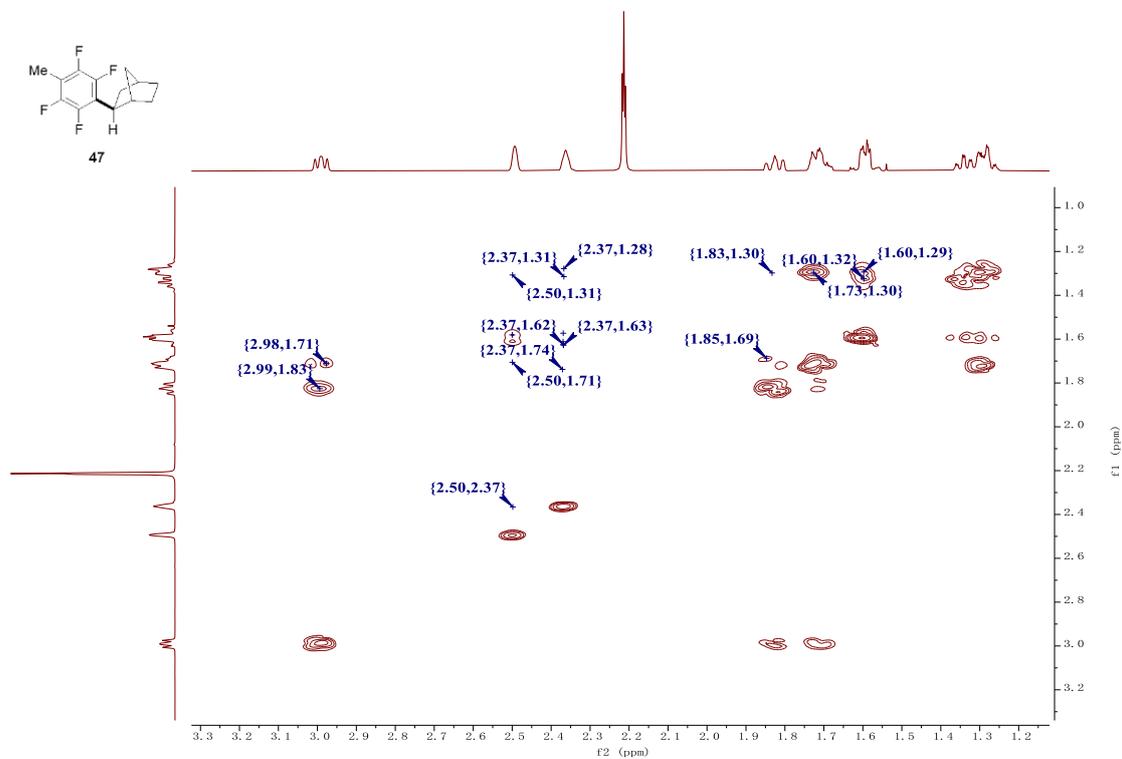
¹³C NMR Spectrum of 47



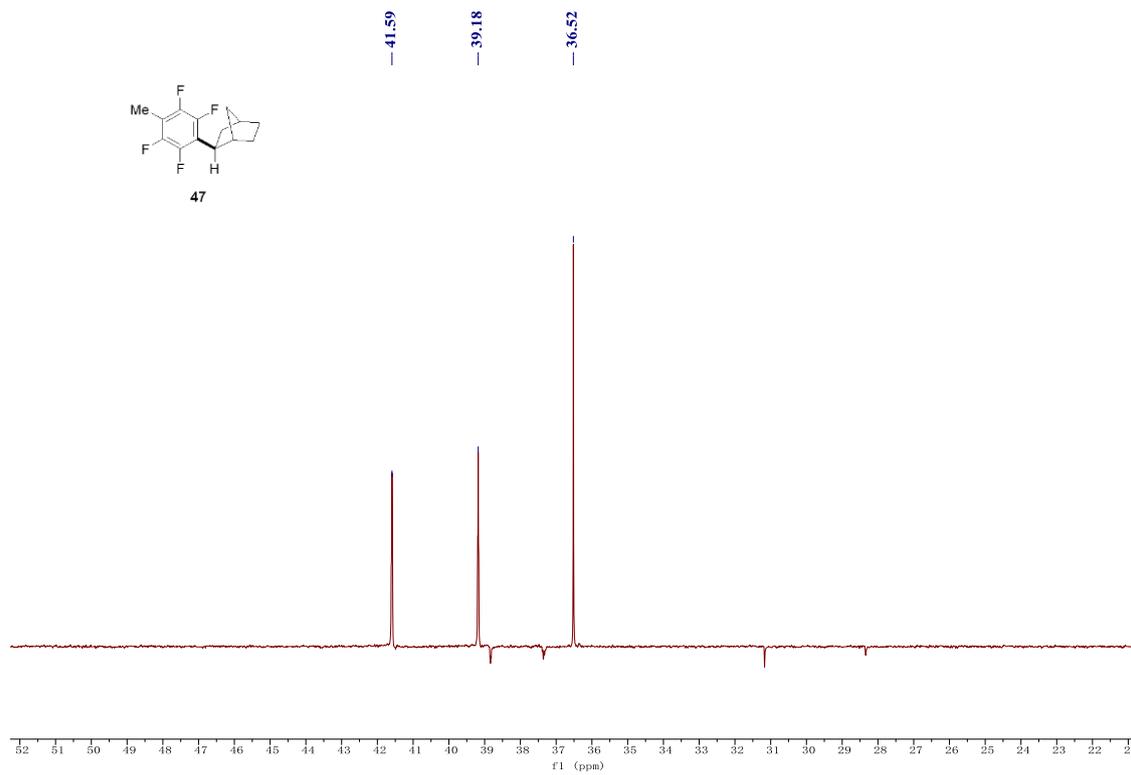
¹⁹F NMR Spectrum of 47



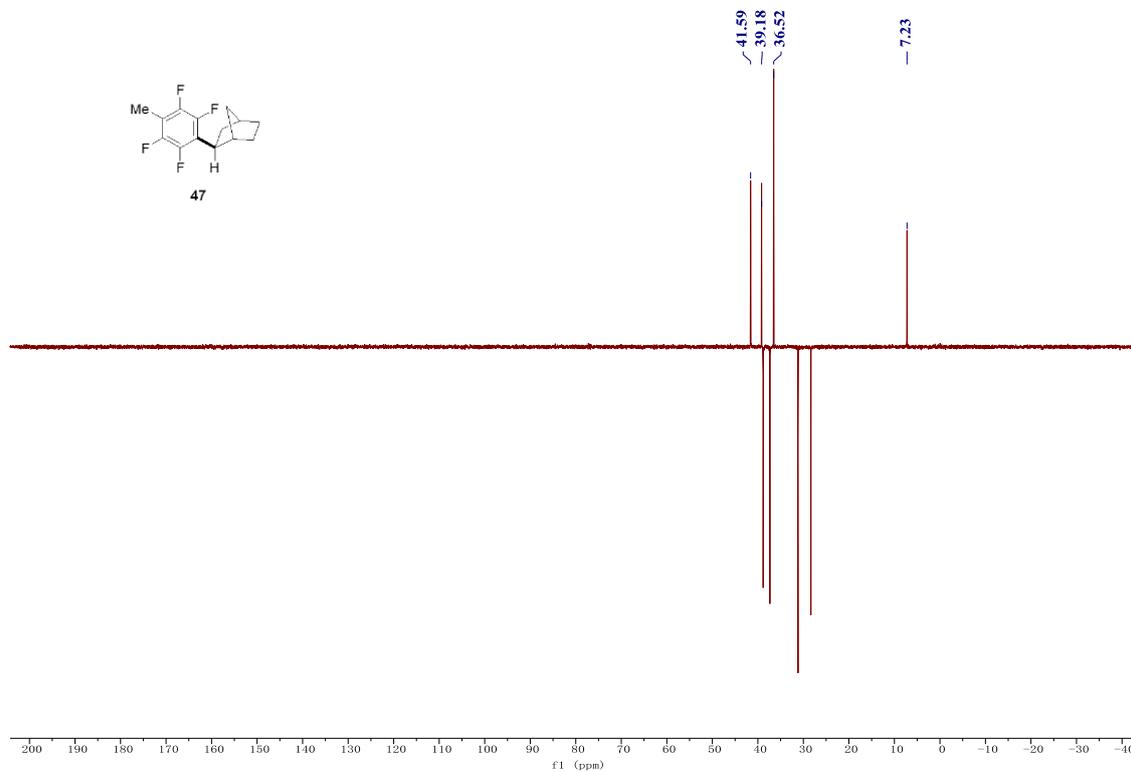
H-H COSY Spectrum of 47



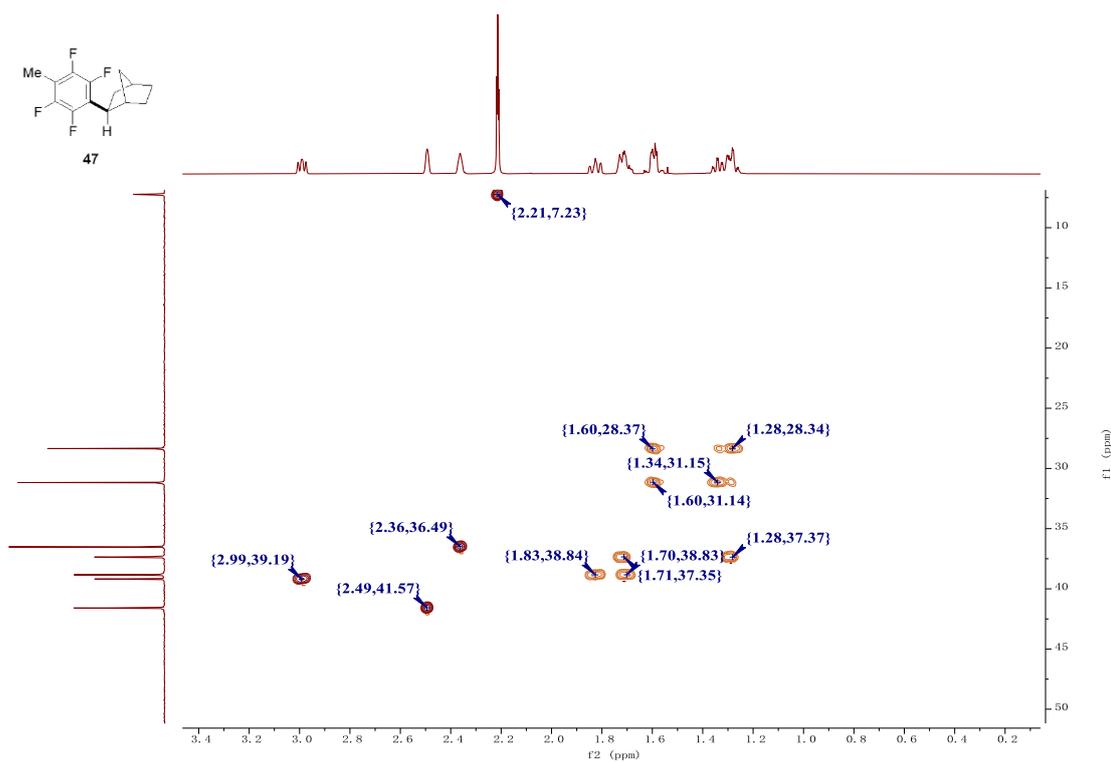
DEPT90 Spectrum of 47



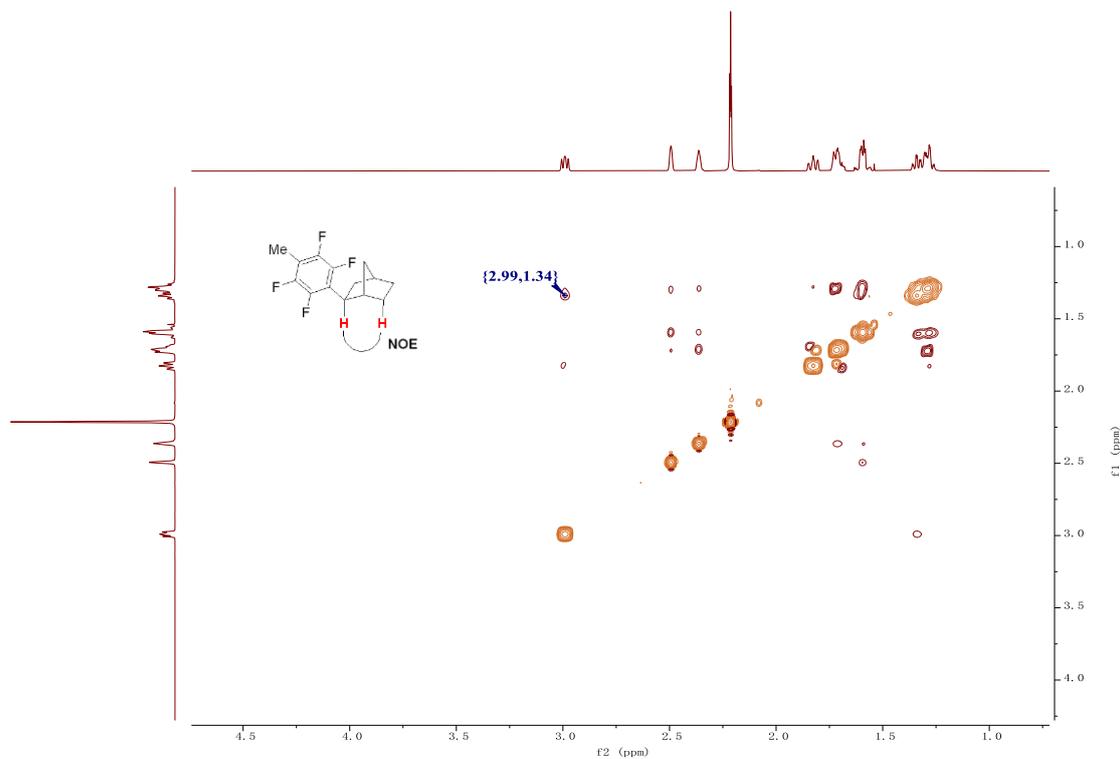
DEPT135 Spectrum of 47



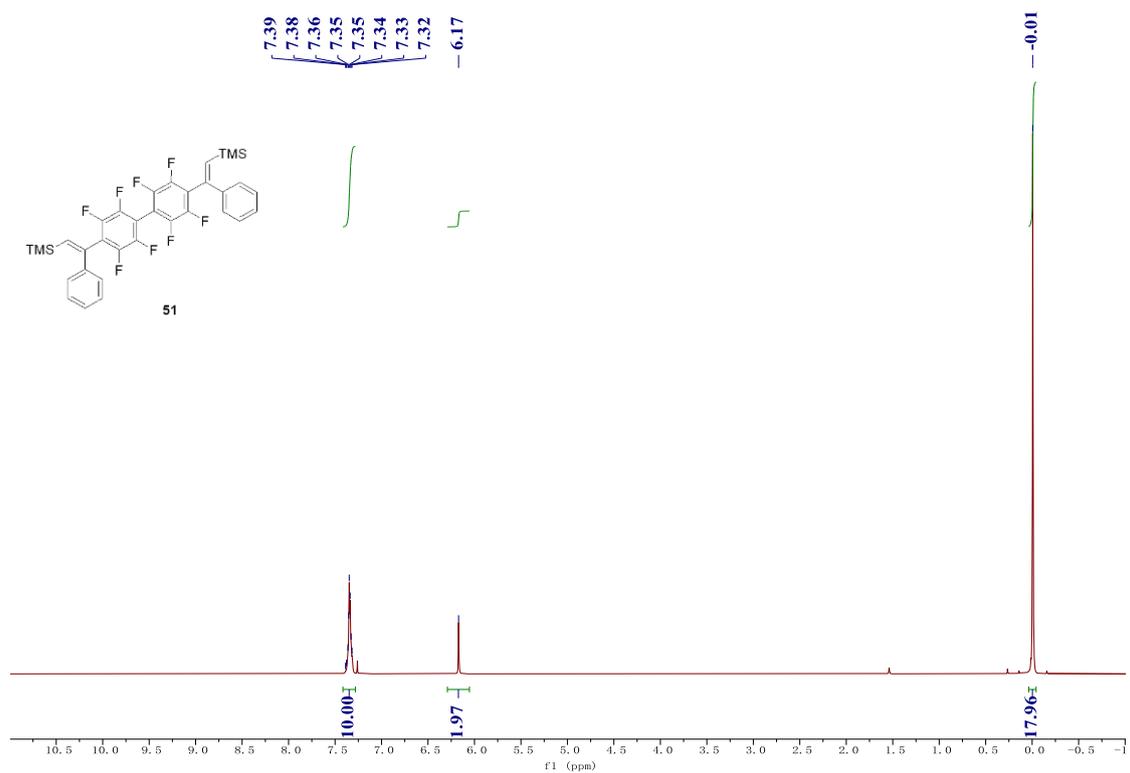
HSQC Spectrum of 47



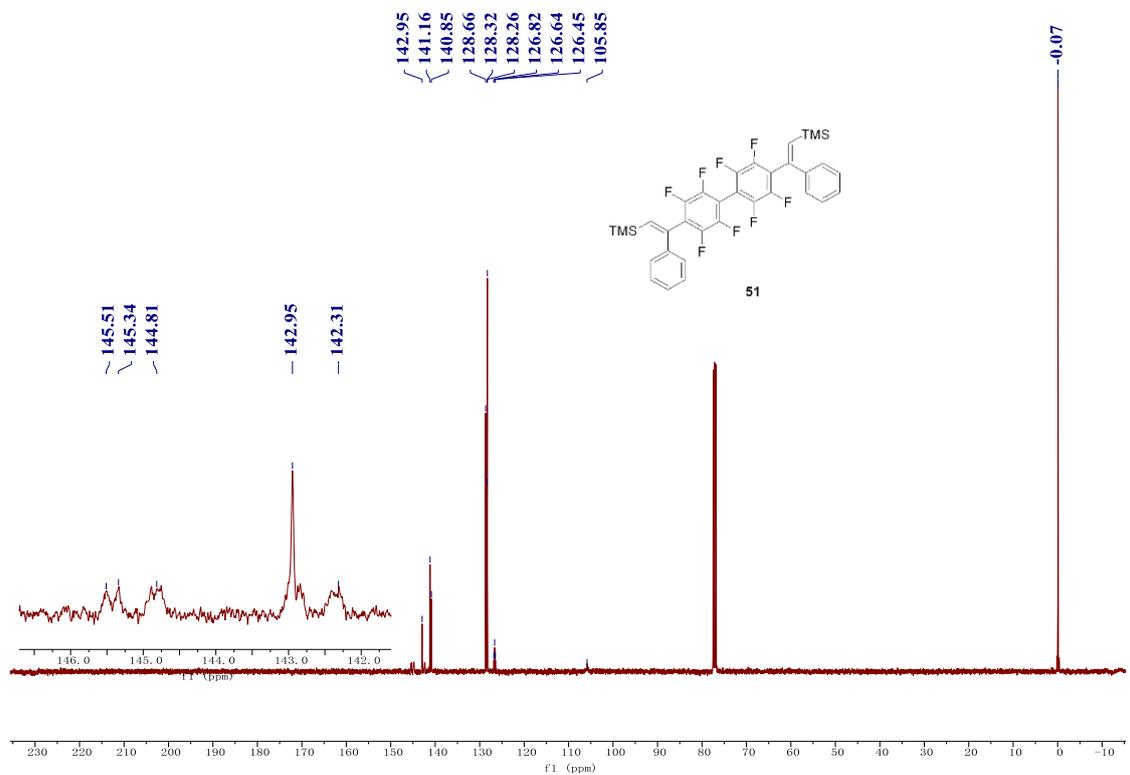
H-H NOESY Spectrum of 47



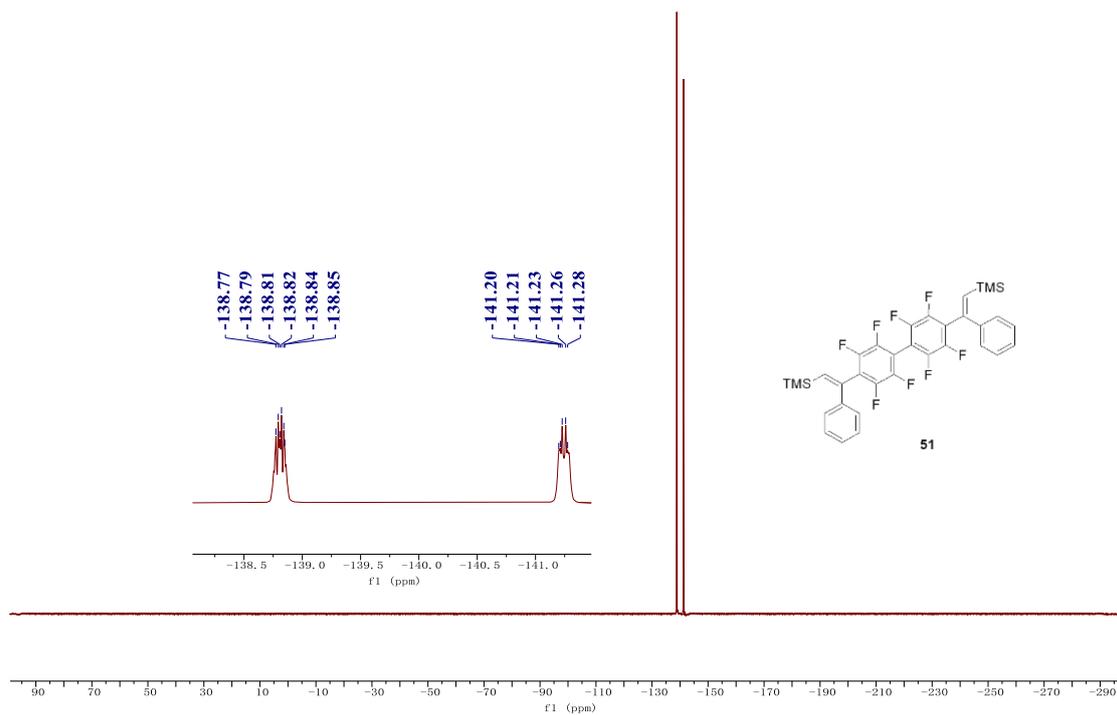
¹H NMR Spectrum of 51



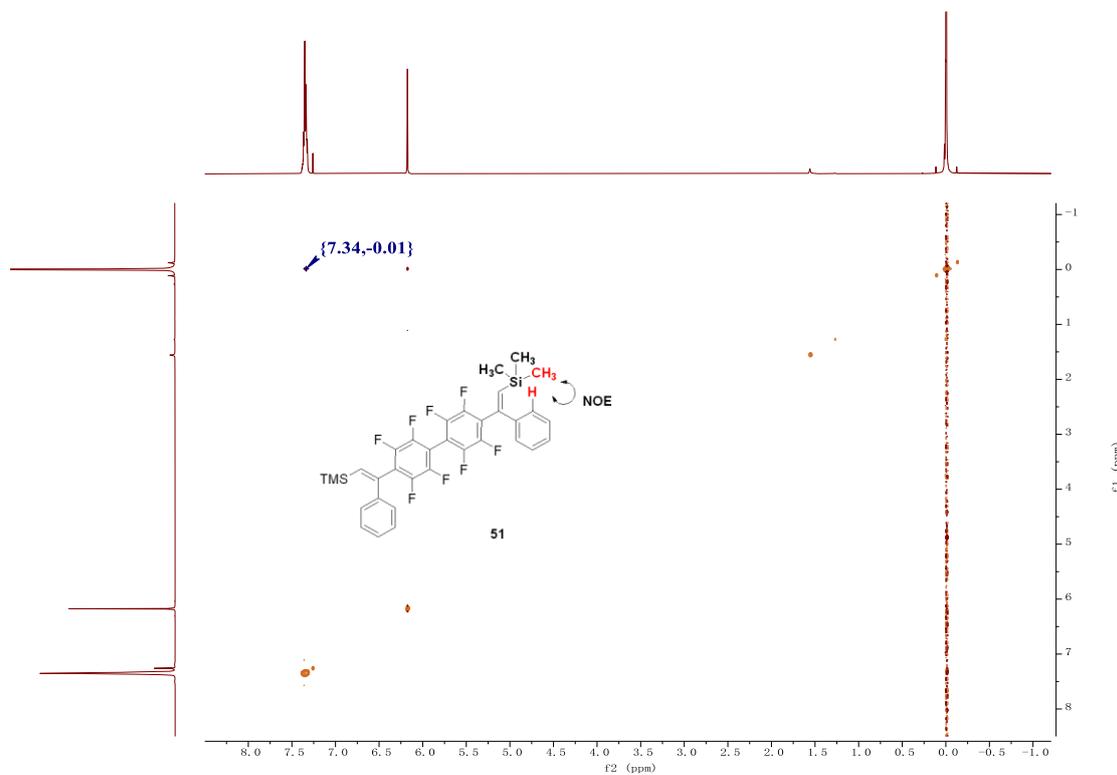
¹³C NMR Spectrum of 51



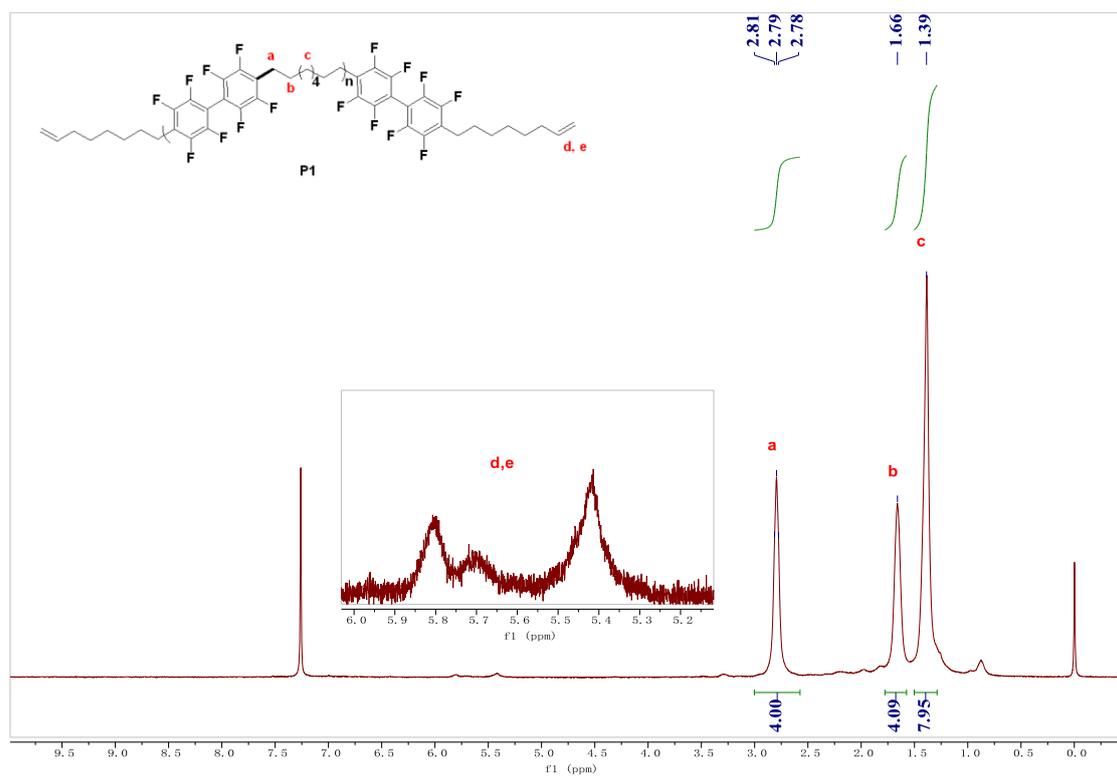
¹⁹F NMR Spectrum of 51



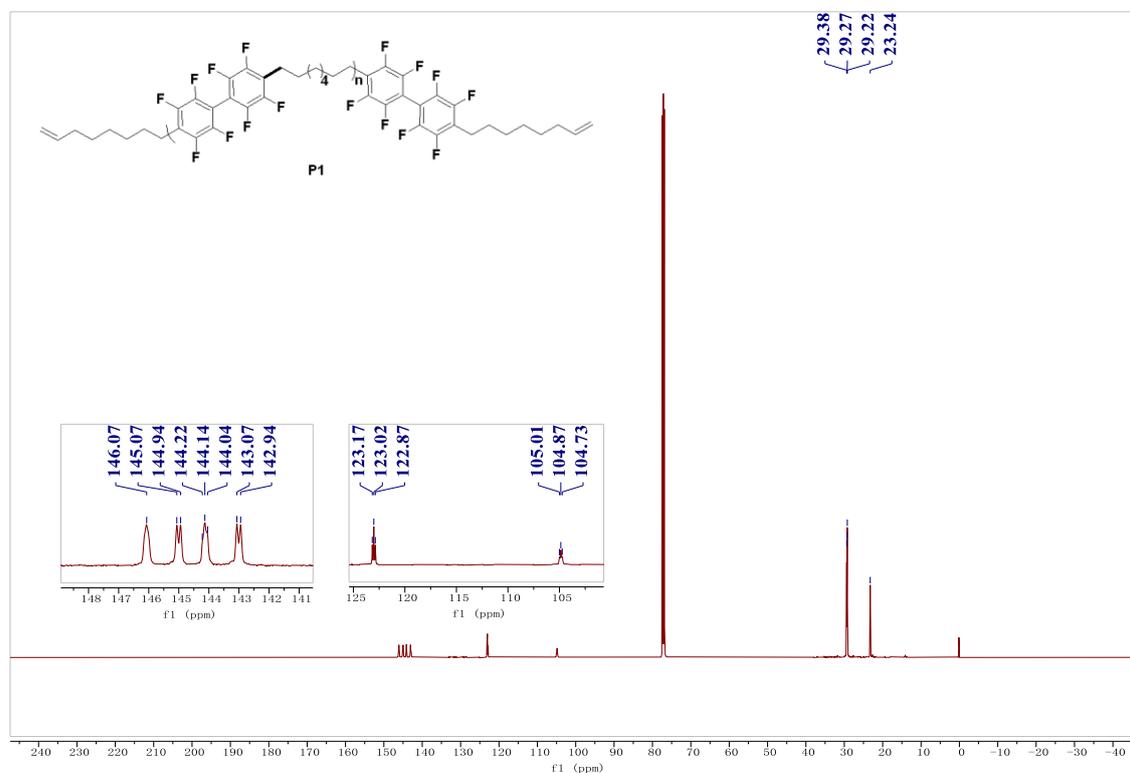
H-H NOESY Spectrum of 51



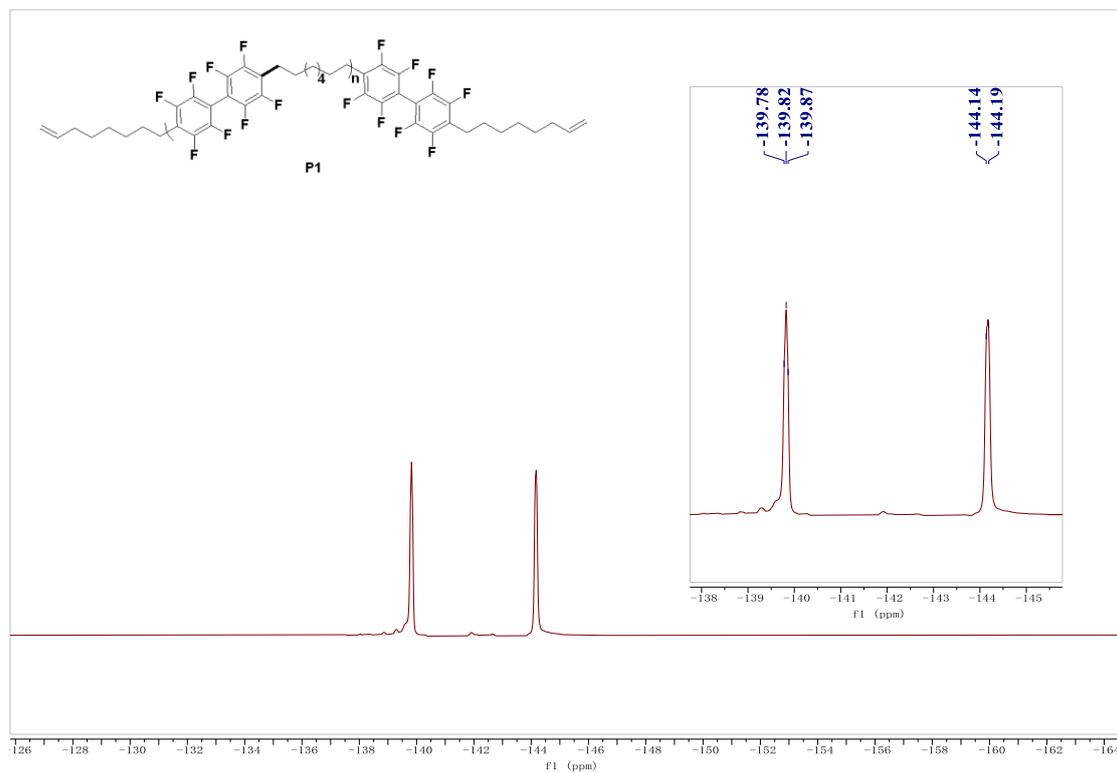
¹H NMR Spectrum of P1



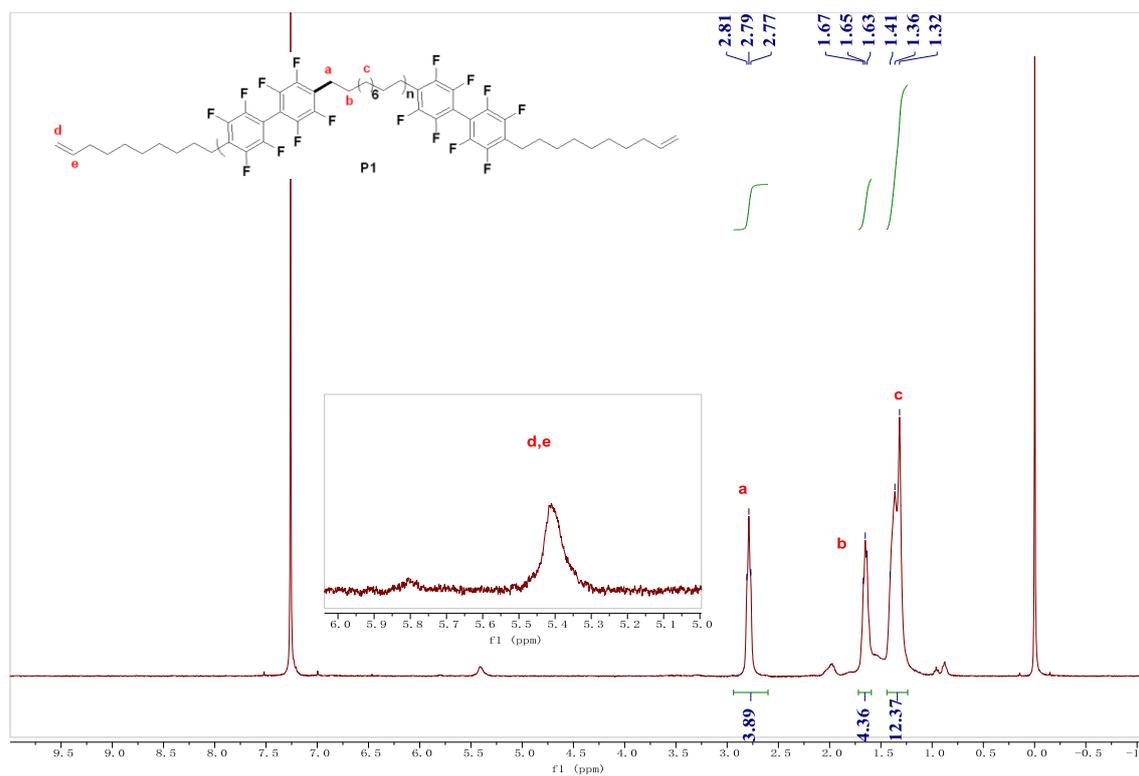
¹³C NMR Spectrum of P1



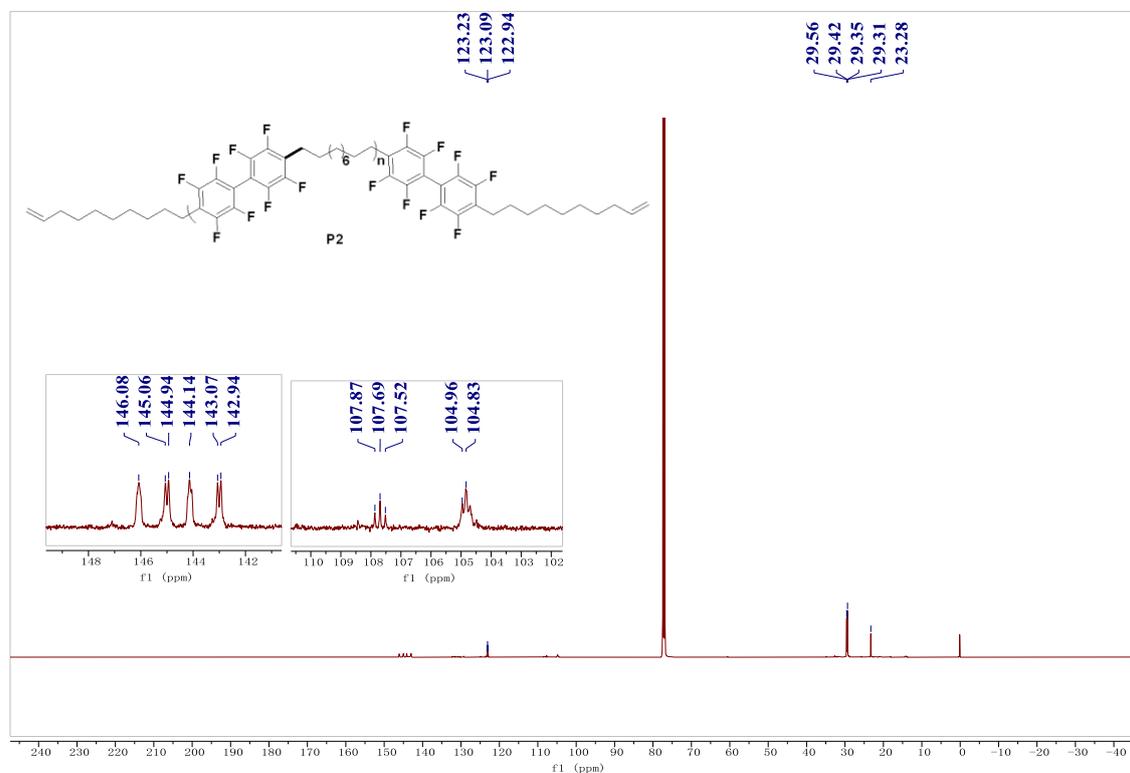
¹⁹F NMR Spectrum of P1



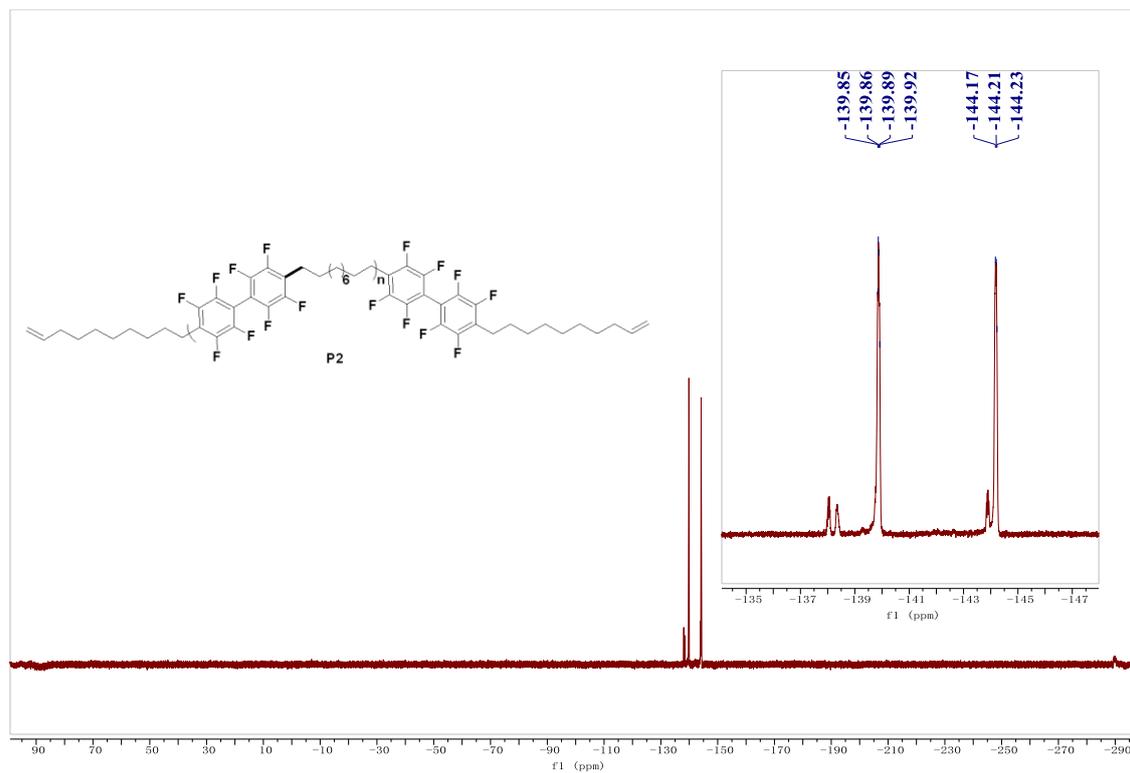
¹H NMR Spectrum of P2



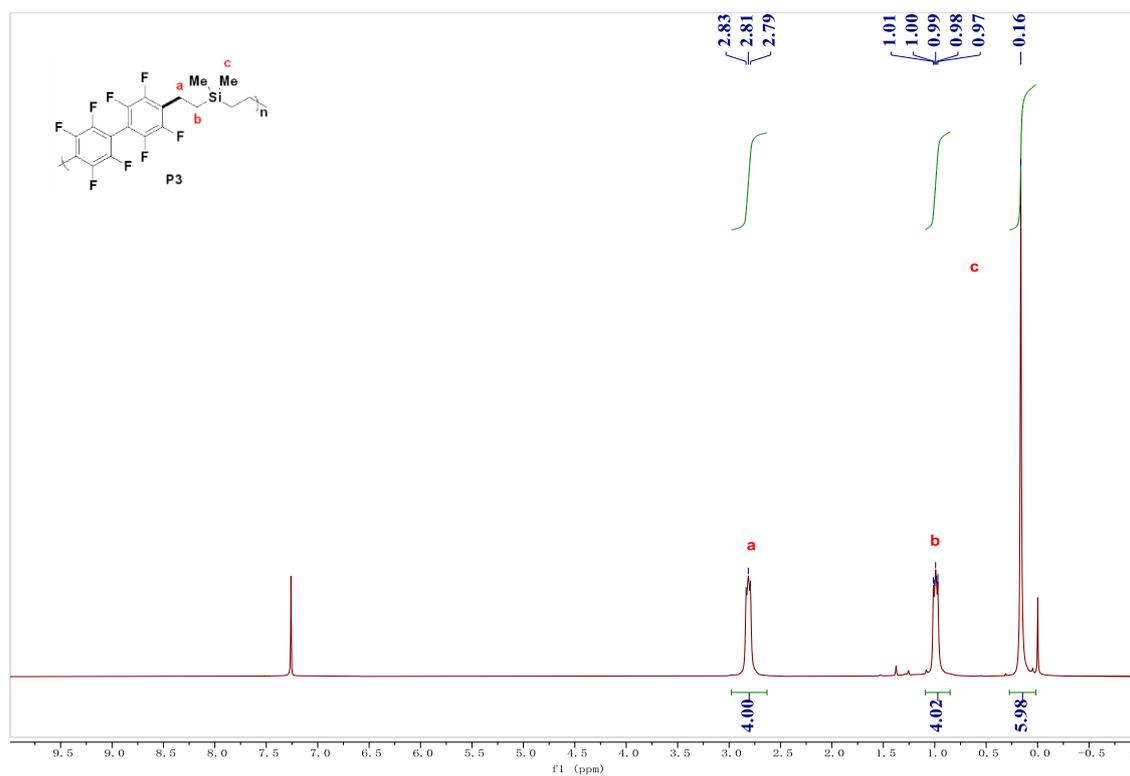
¹³C NMR Spectrum of P2



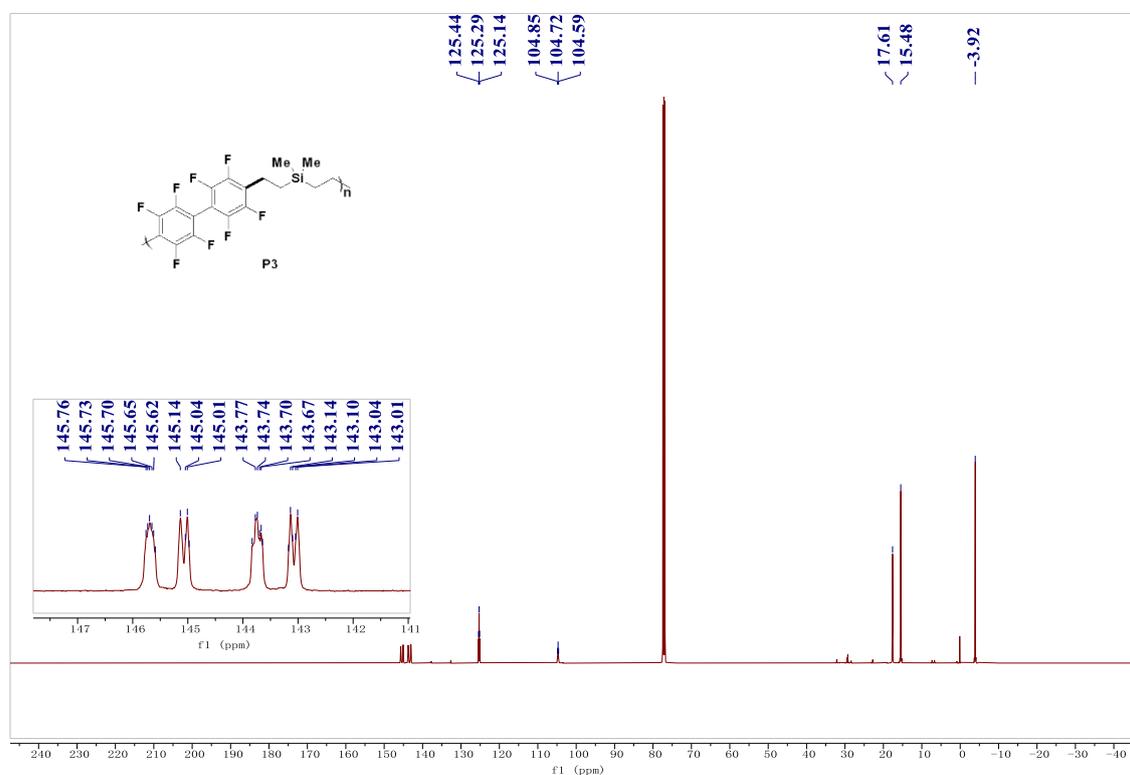
¹⁹F NMR Spectrum of P2



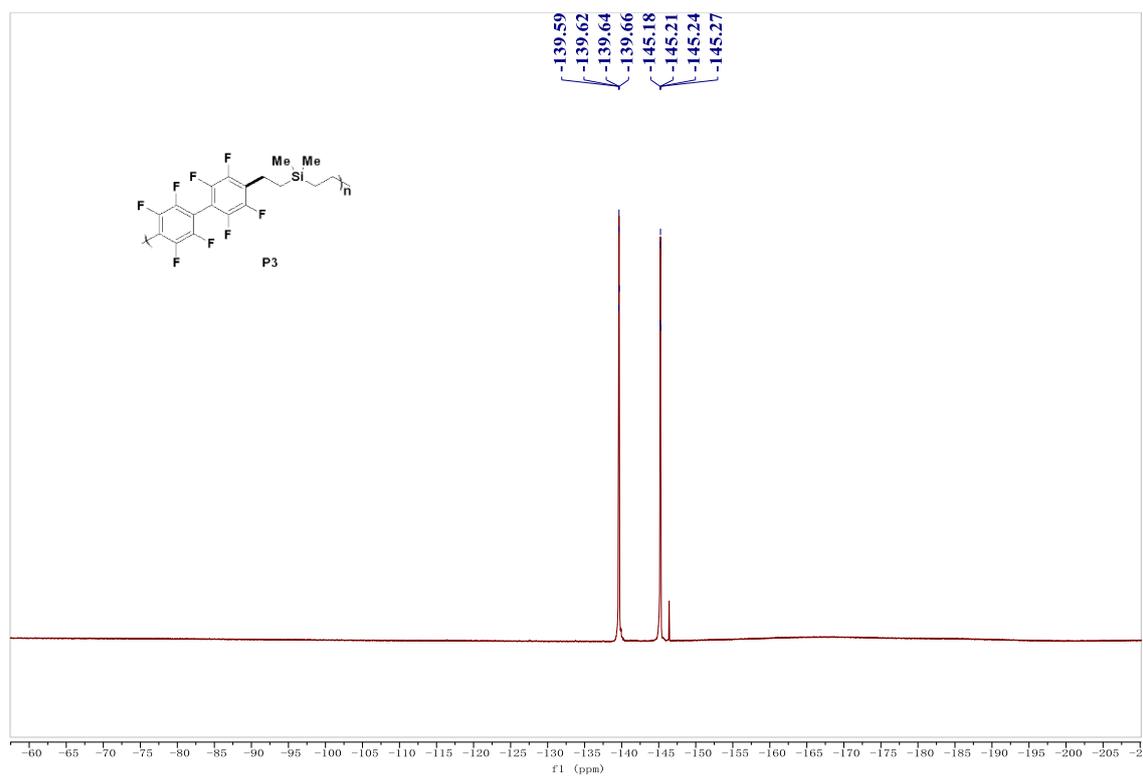
¹H NMR Spectrum of P3



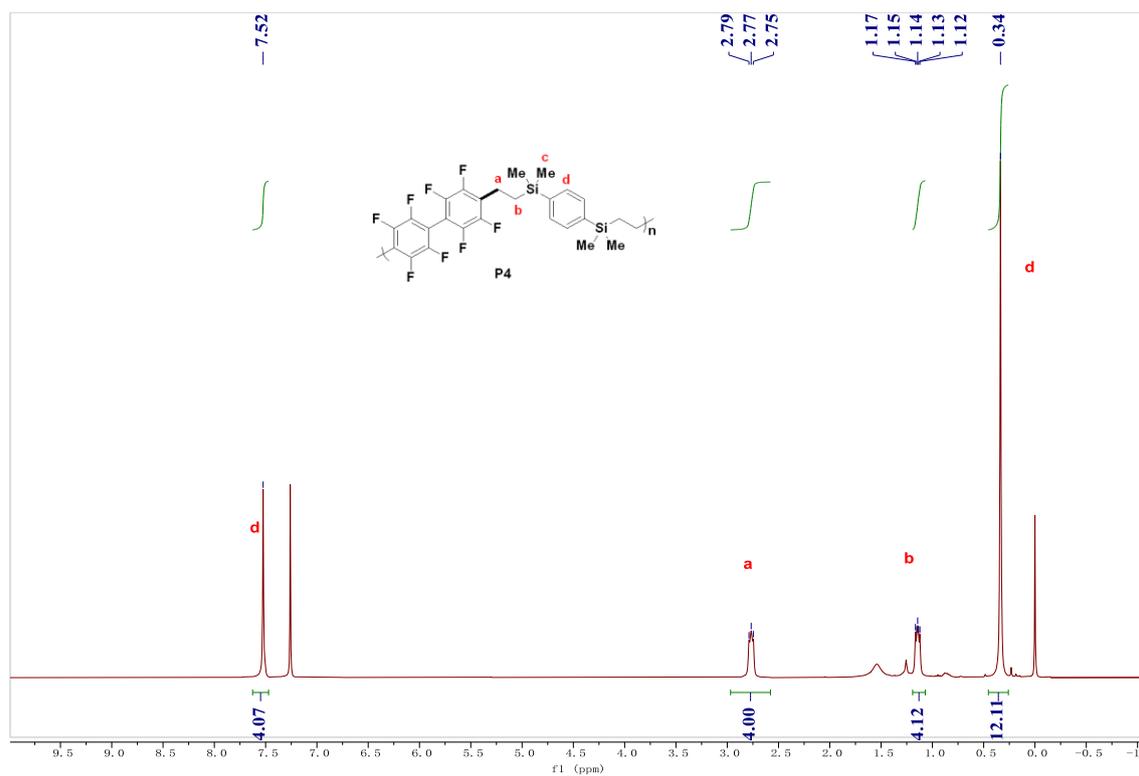
¹³C NMR Spectrum of P3



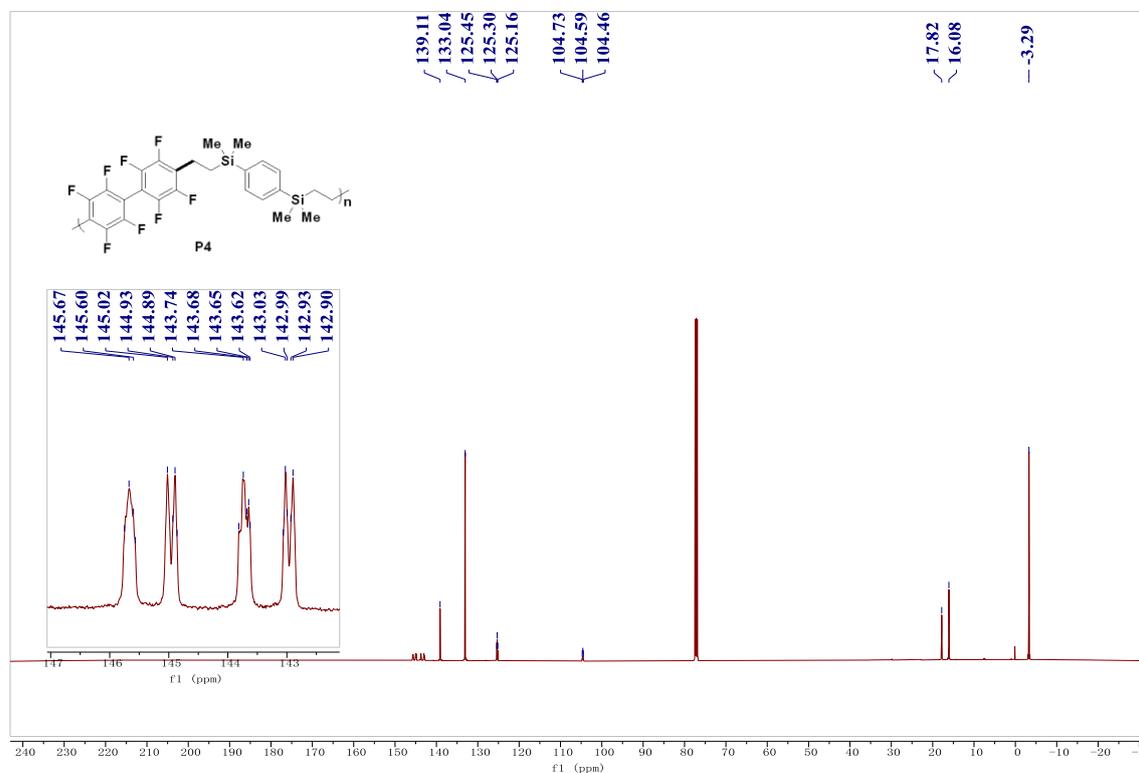
¹⁹F NMR Spectrum of P3



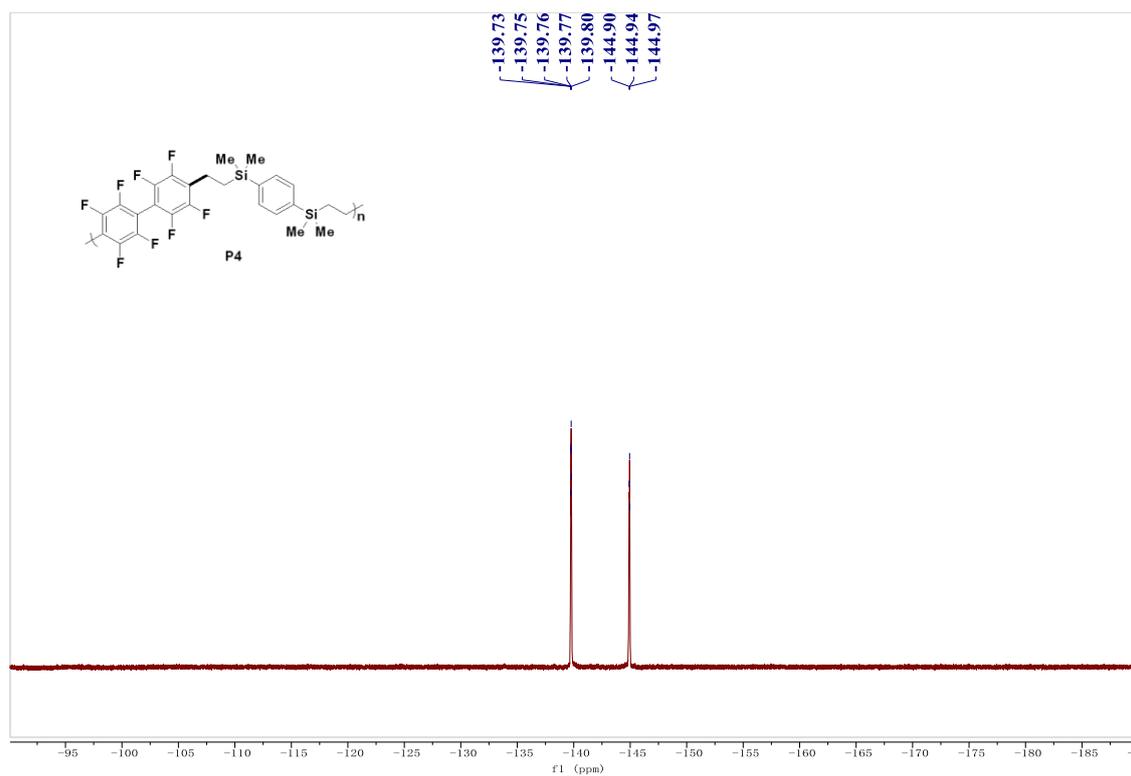
¹H NMR Spectrum of P4



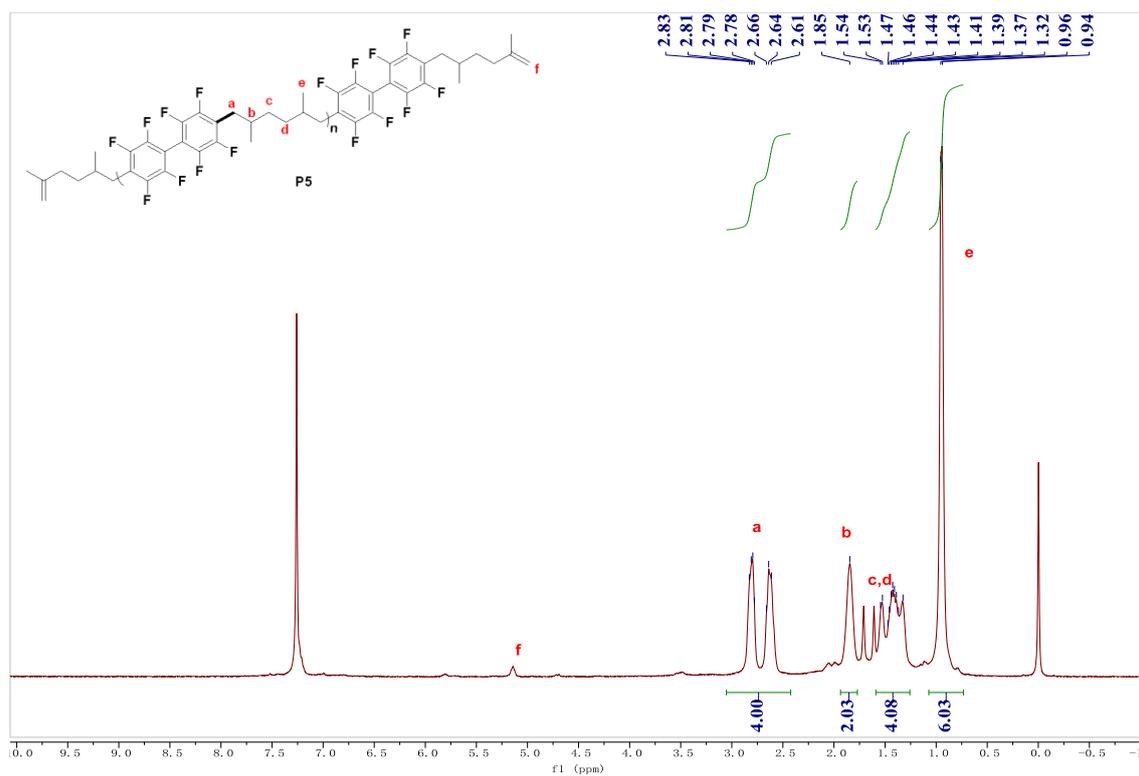
¹³C NMR Spectrum of P4



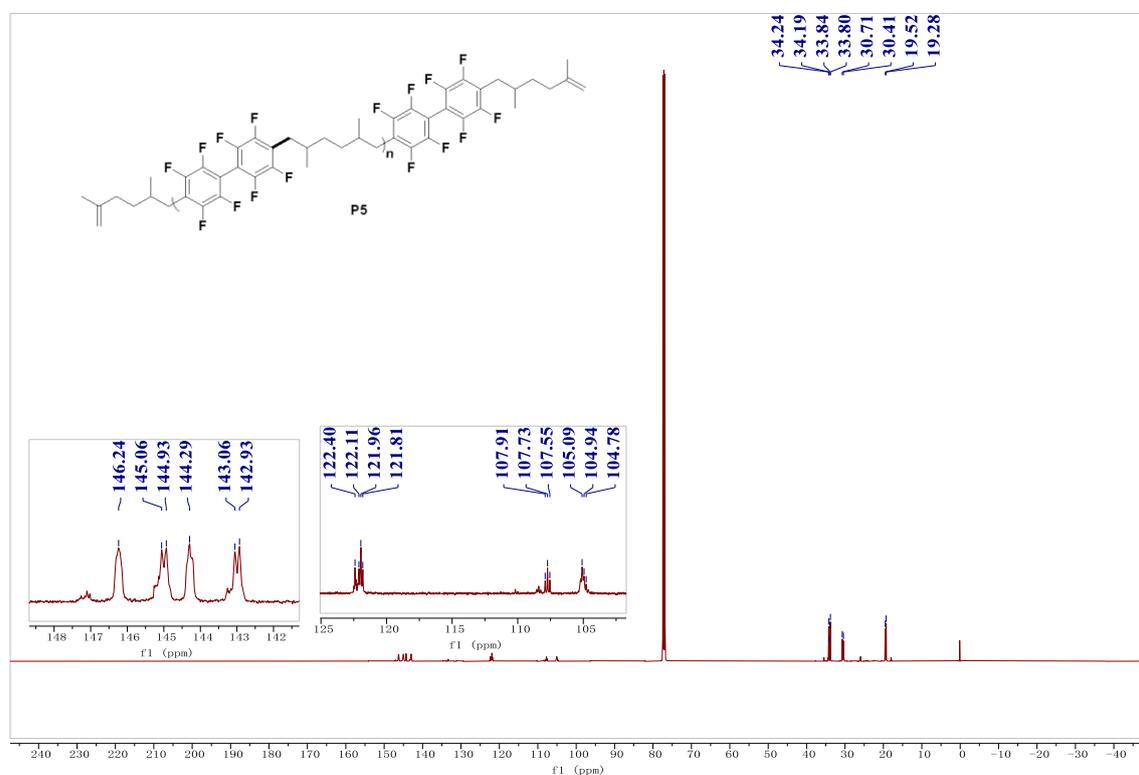
¹⁹F NMR Spectrum of P4



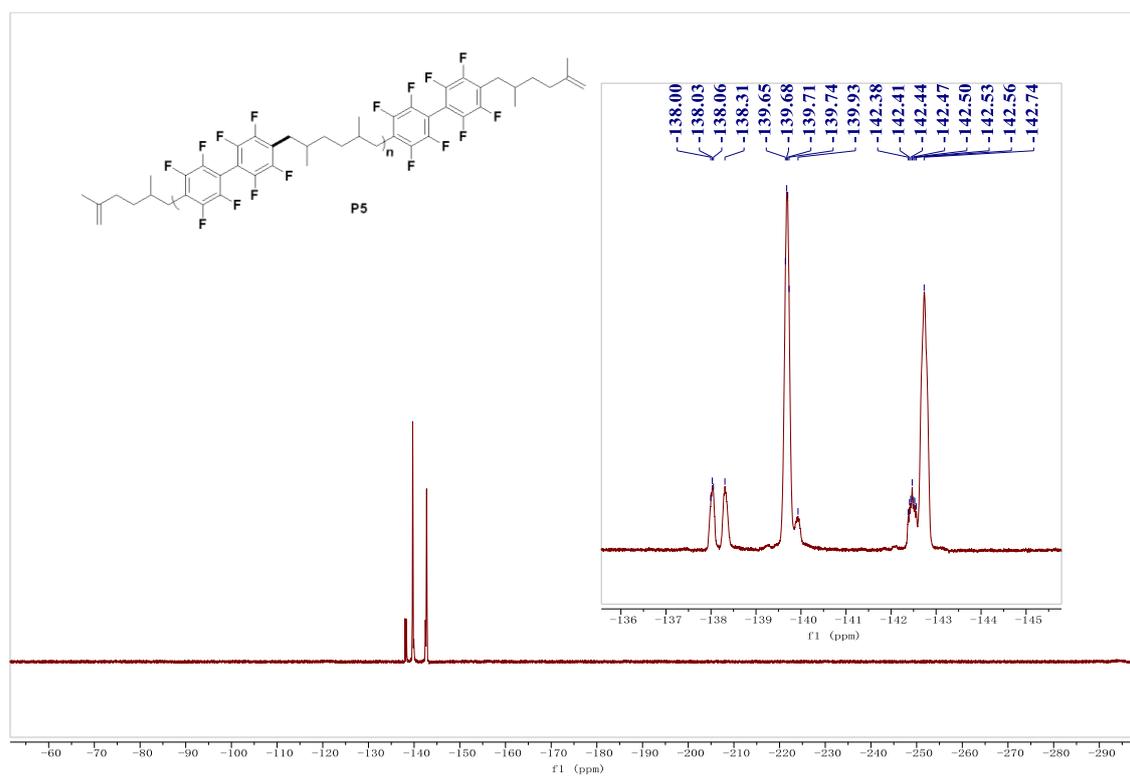
¹H NMR Spectrum of P5



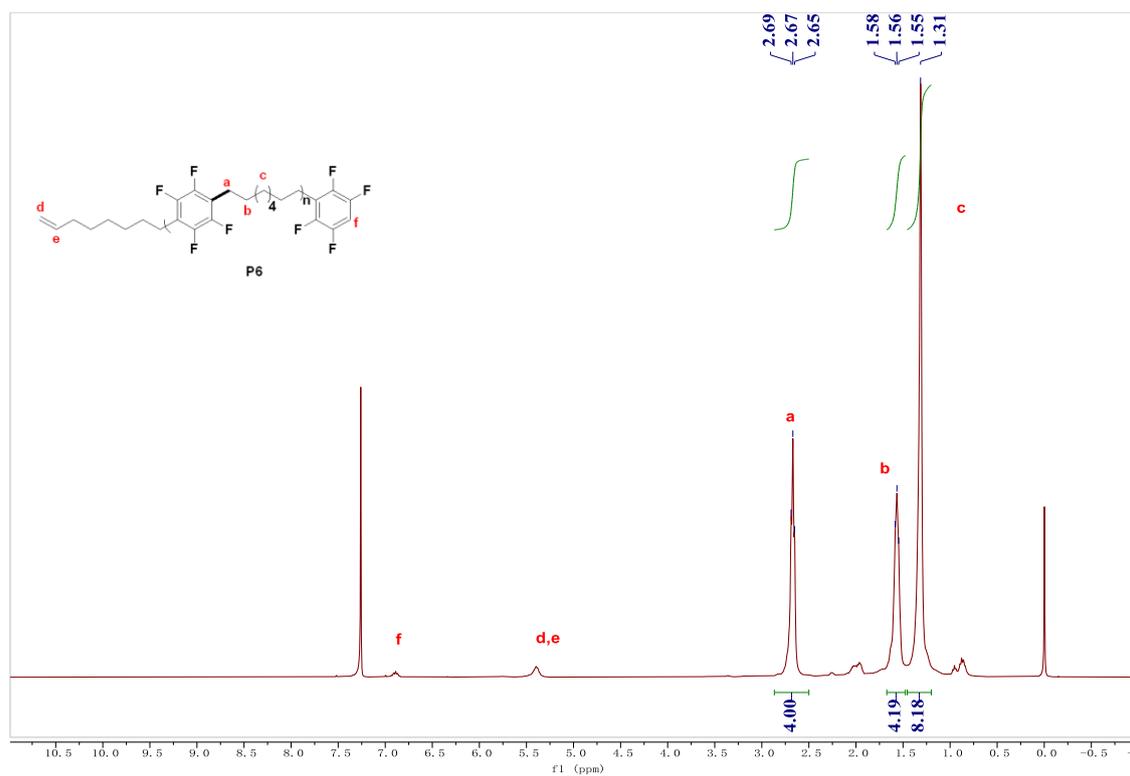
¹³C NMR Spectrum of P5



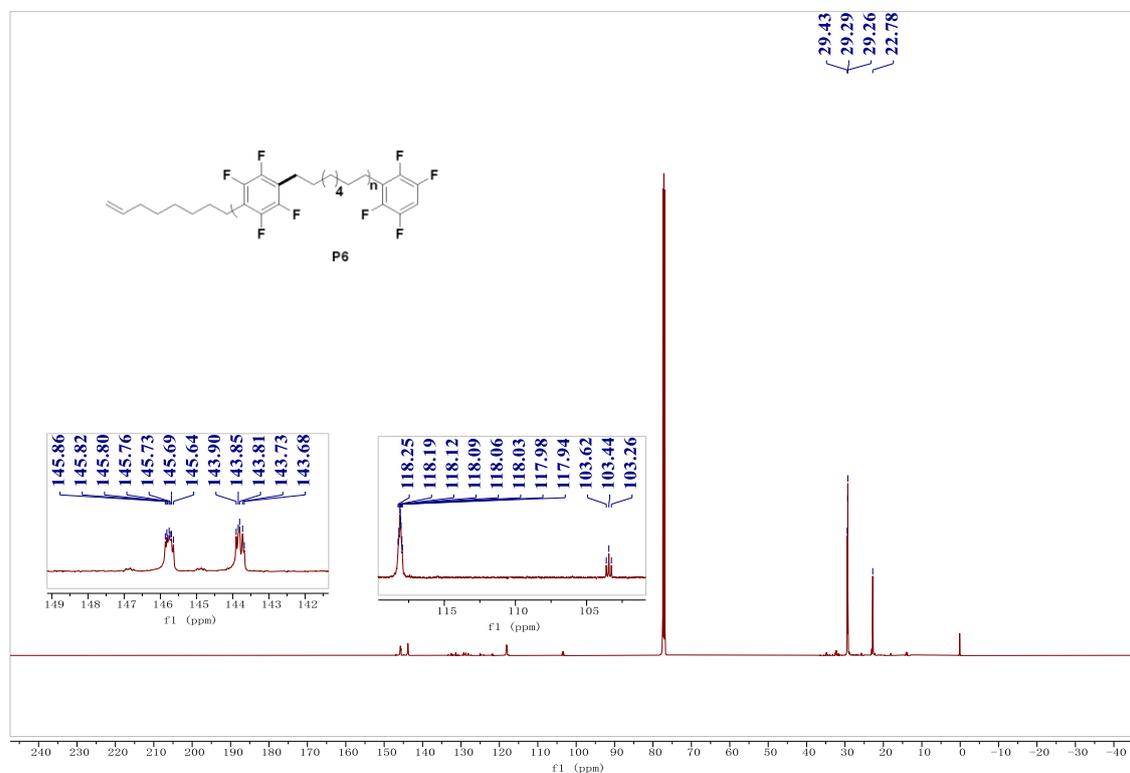
¹⁹F NMR Spectrum of P5



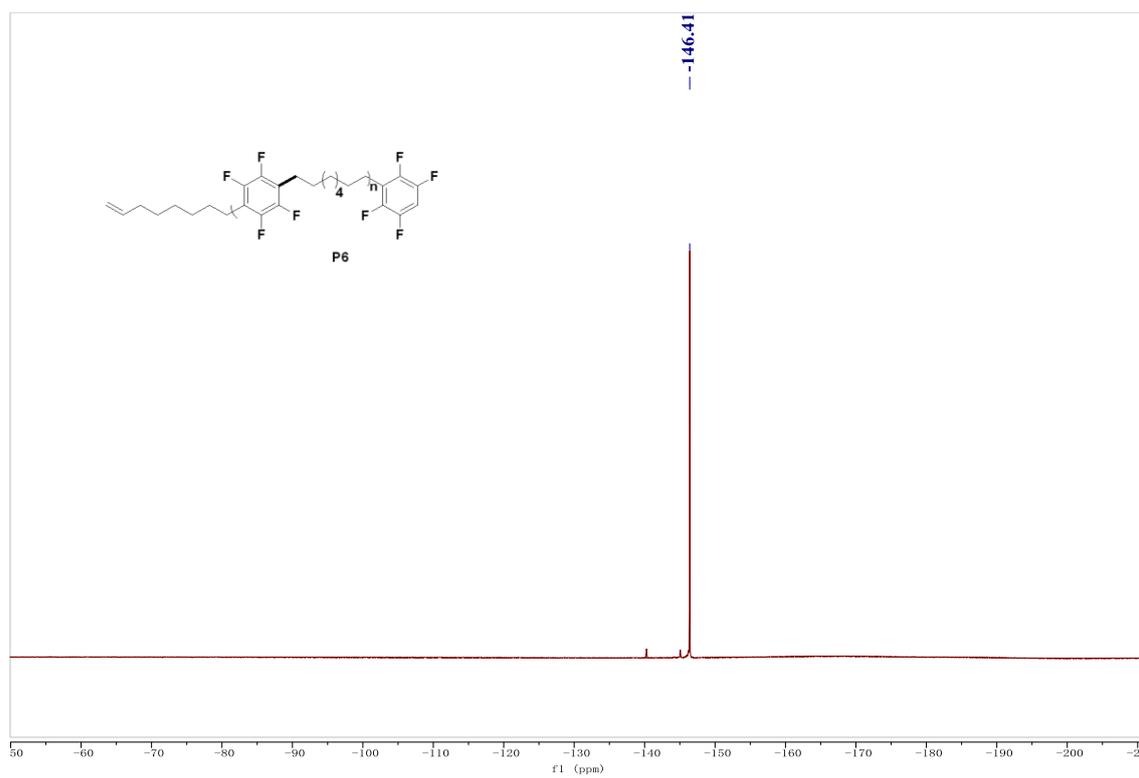
¹H NMR Spectrum of P6



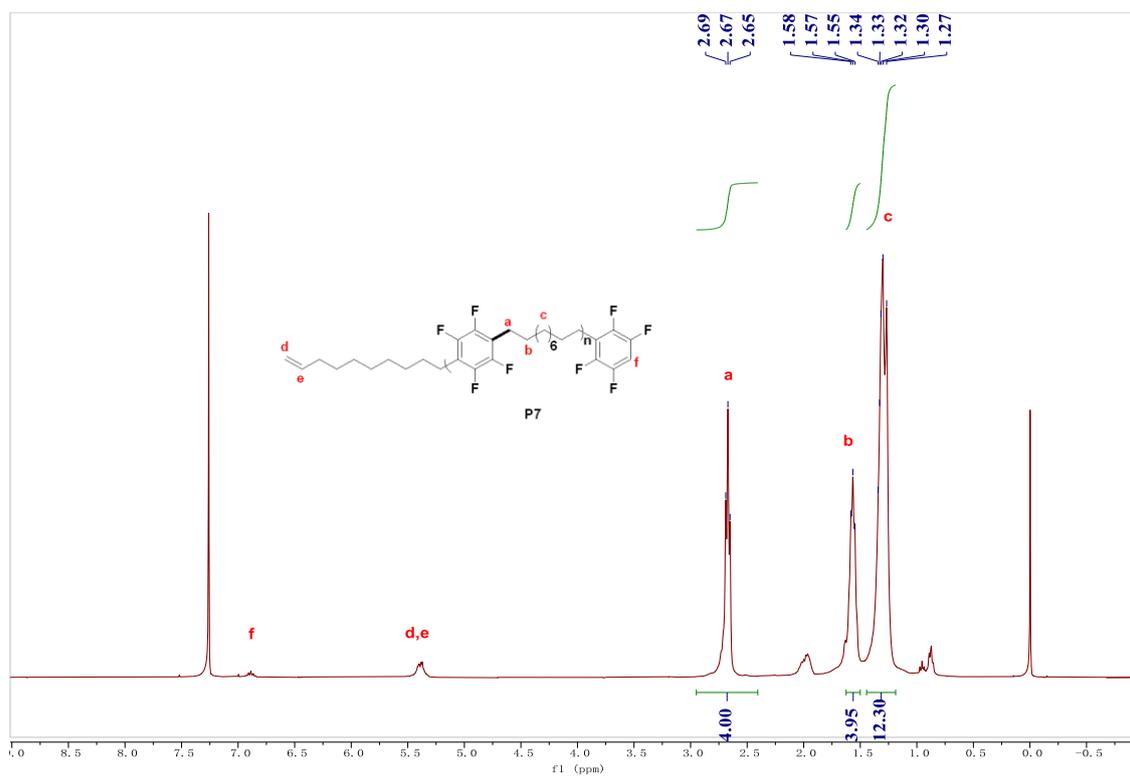
¹³C NMR Spectrum of P6



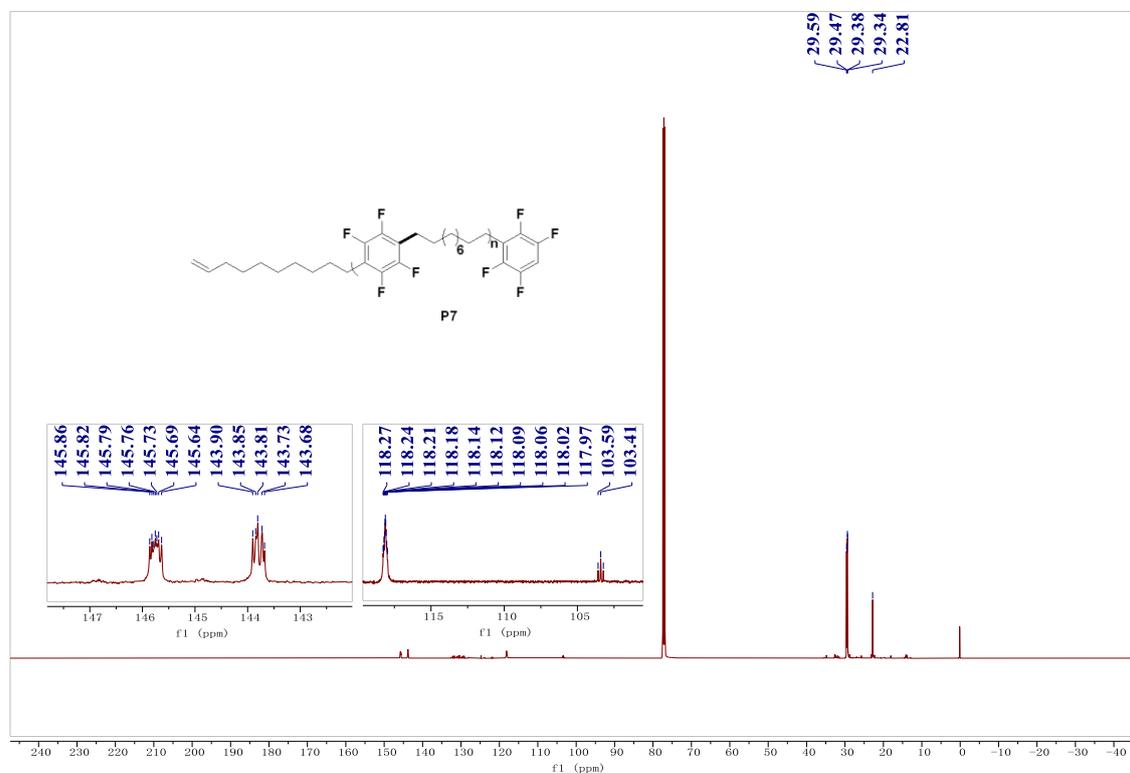
¹⁹F NMR Spectrum of P6



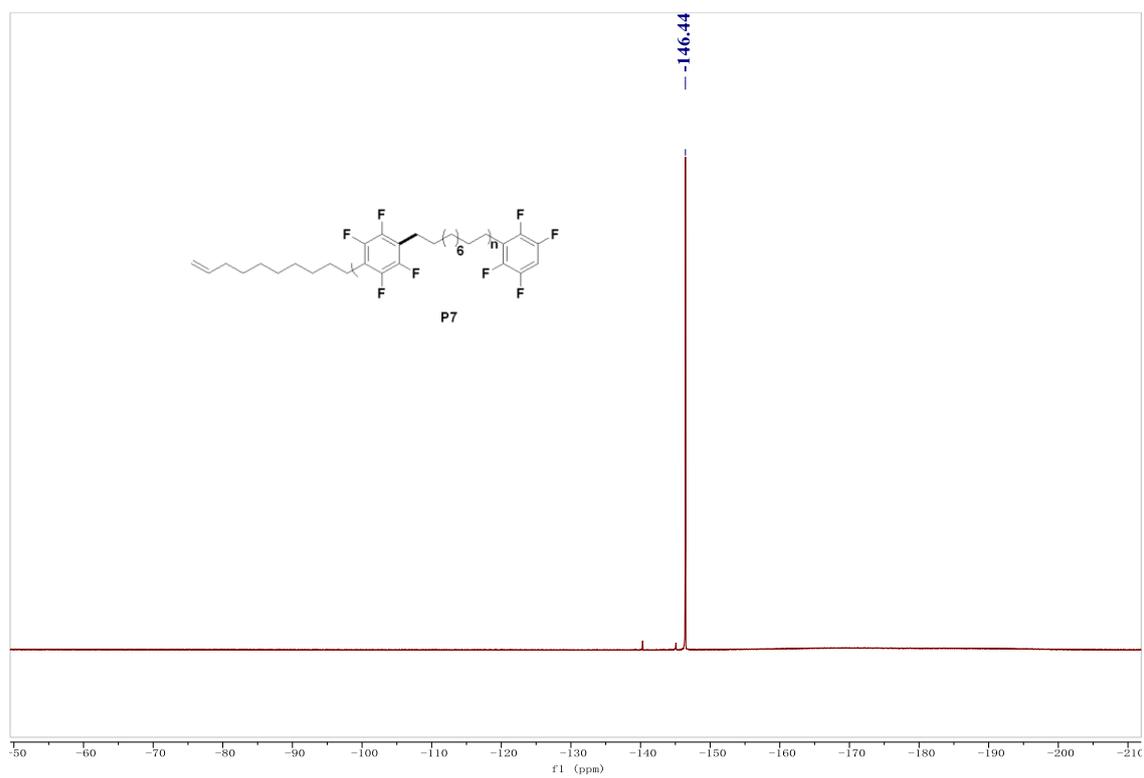
¹H NMR Spectrum of P7



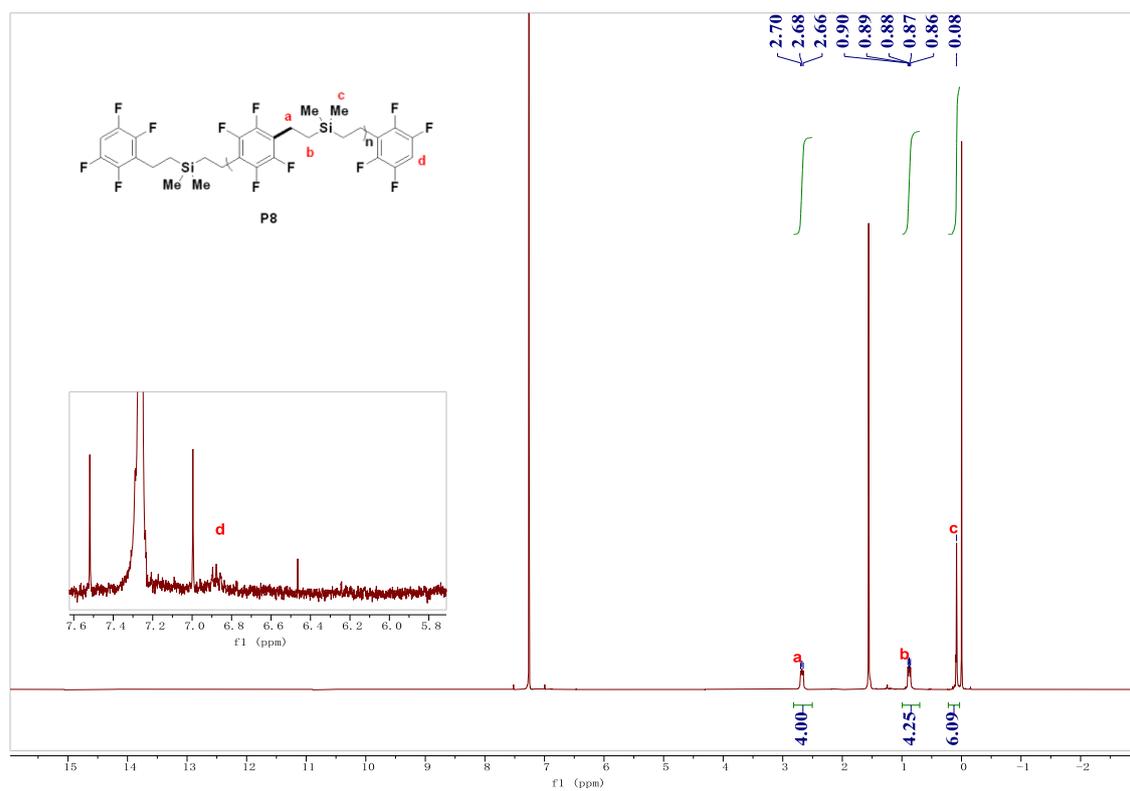
¹³C NMR Spectrum of P7



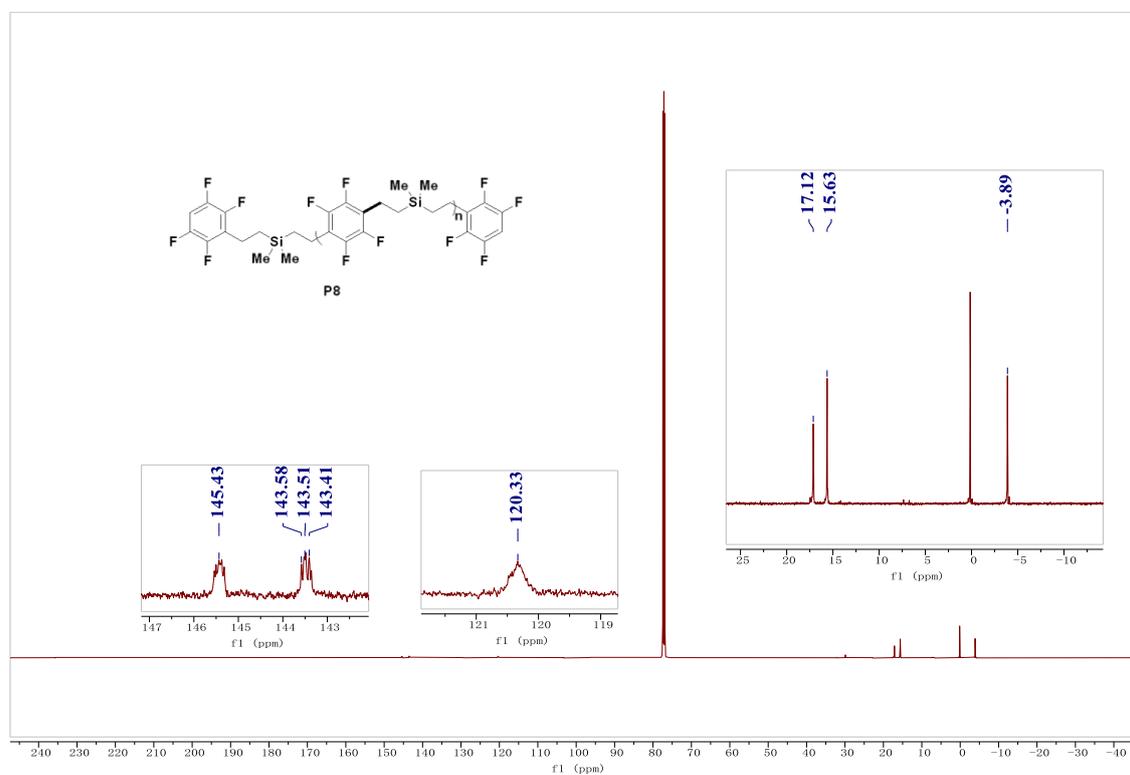
¹⁹F NMR Spectrum of P7



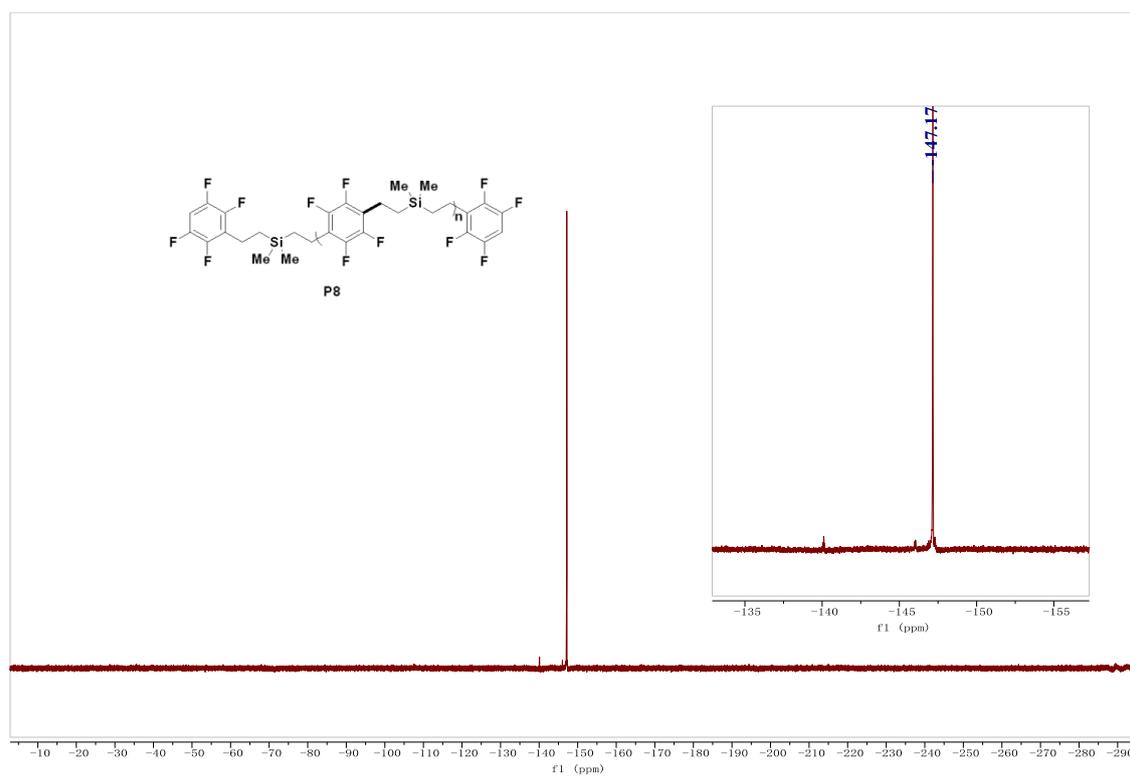
¹H NMR Spectrum of P8



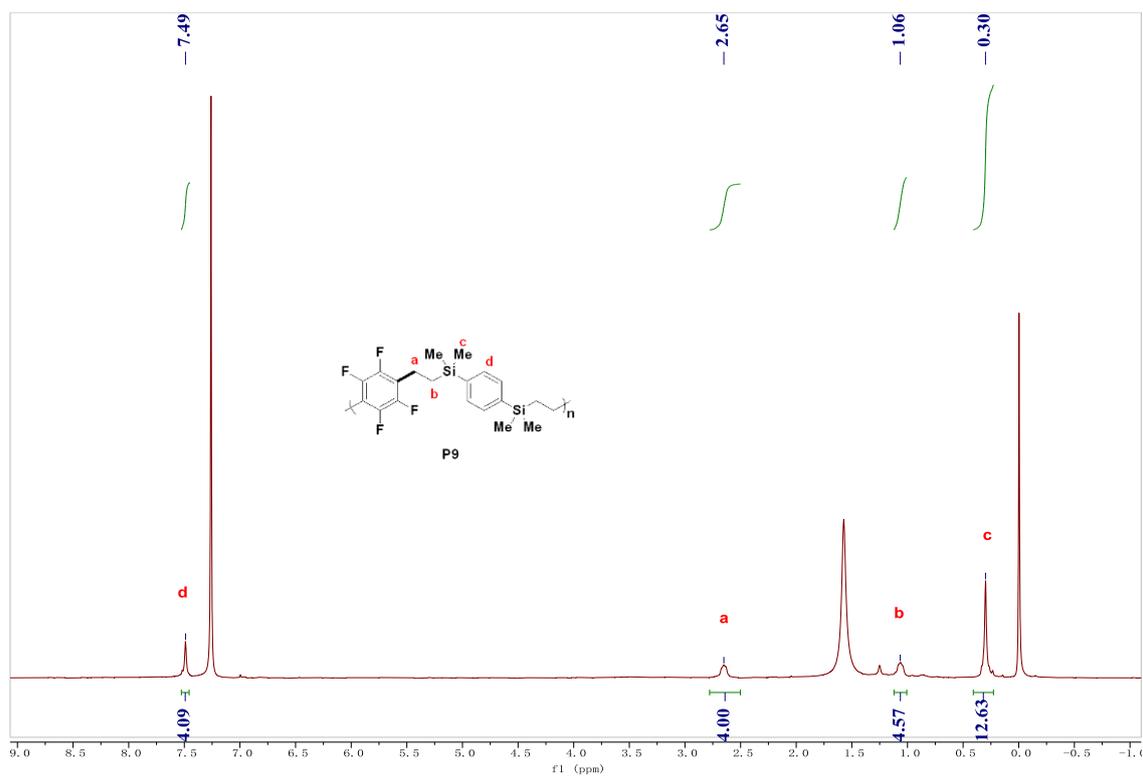
¹³C NMR Spectrum of P8



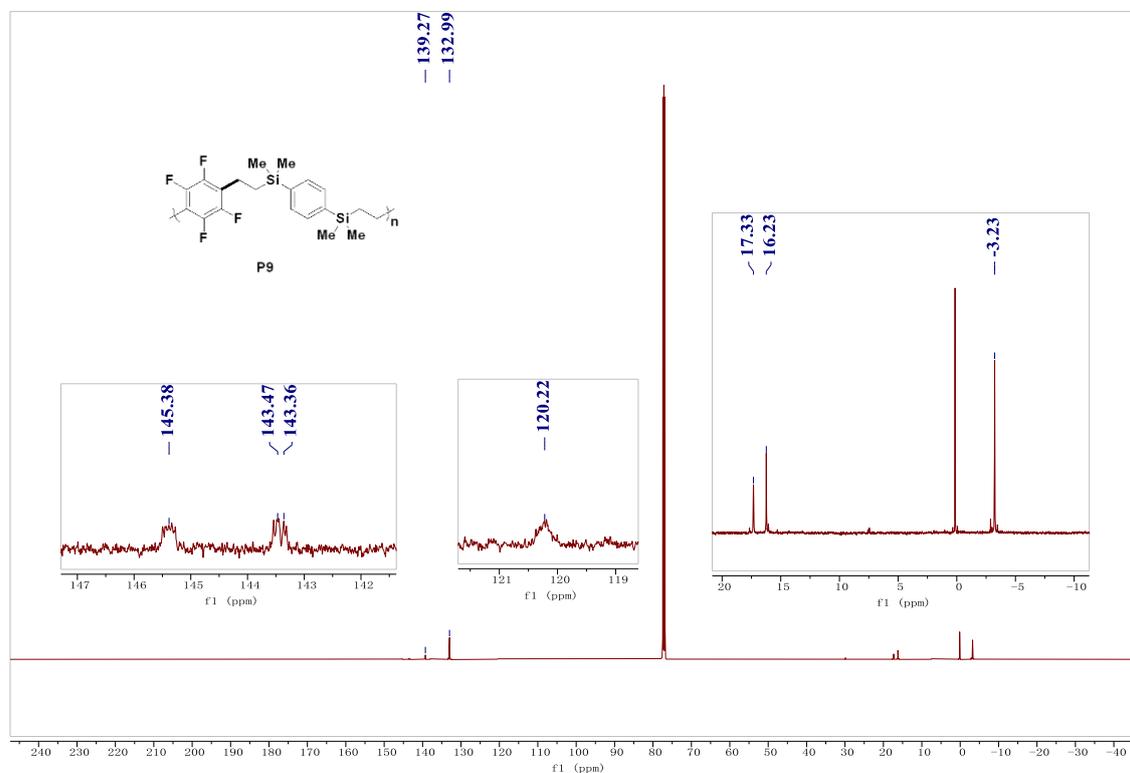
¹⁹F NMR Spectrum of P8



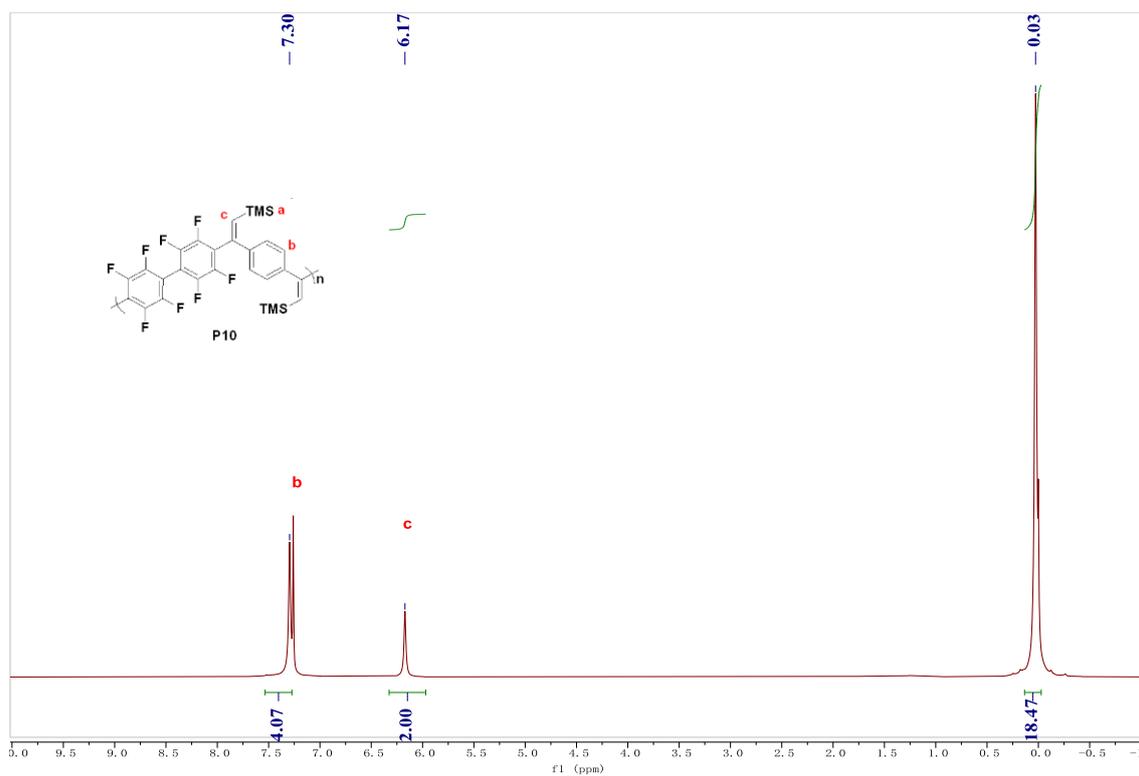
¹H NMR Spectrum of P9



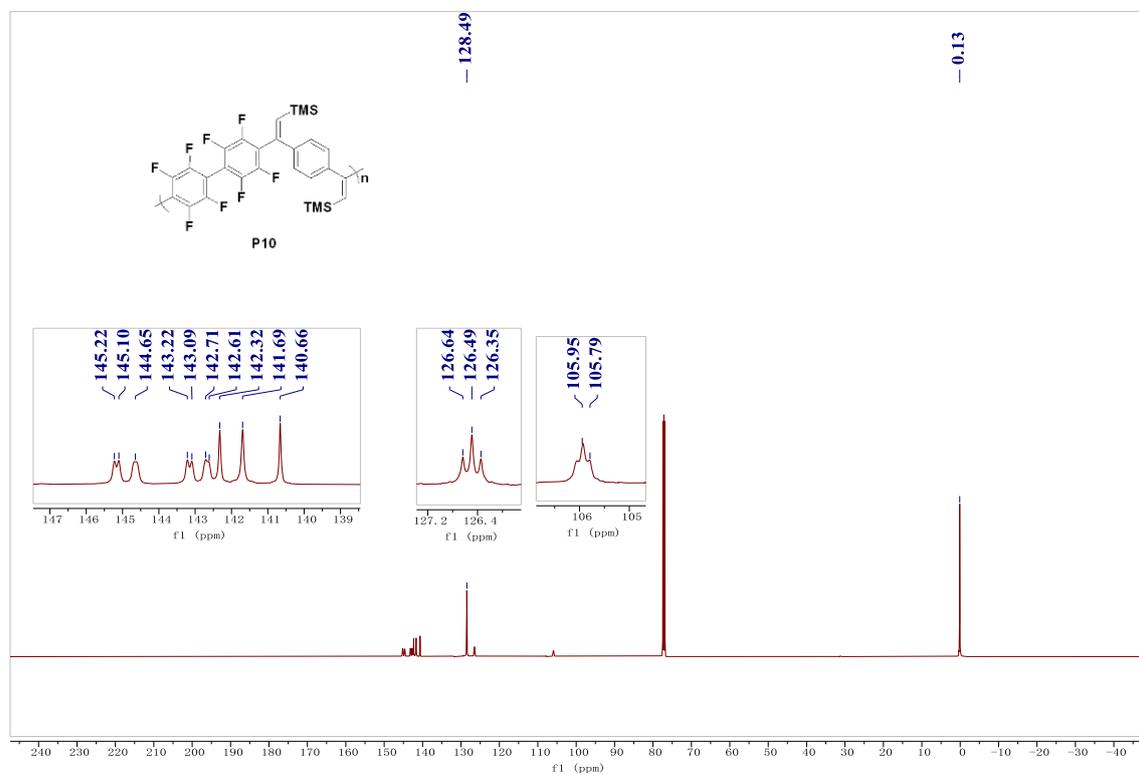
¹³C NMR Spectrum of P9



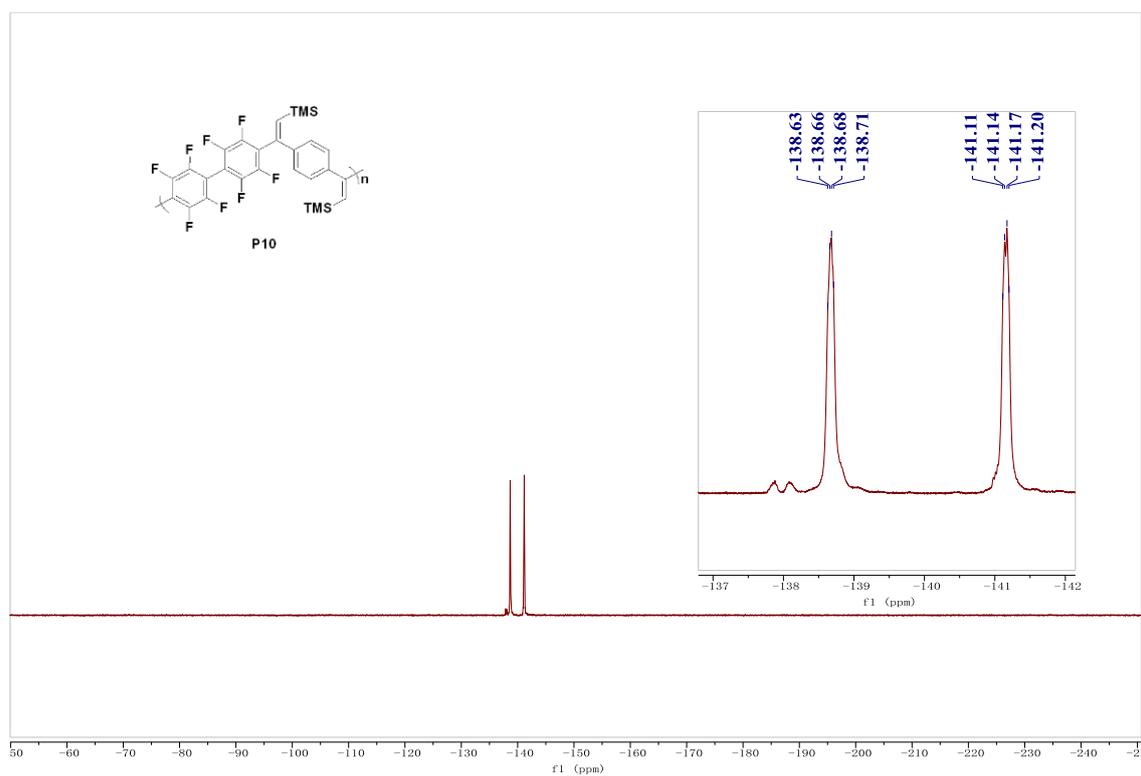
¹H NMR Spectrum of P10



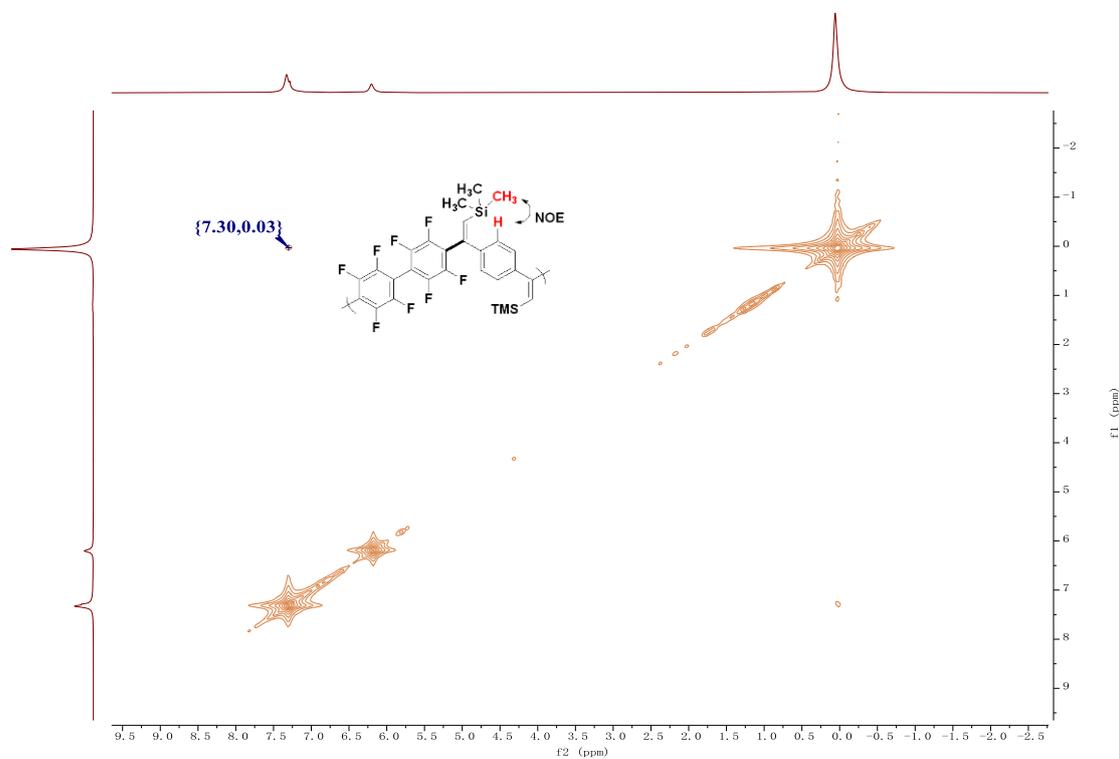
¹³C NMR Spectrum of P10



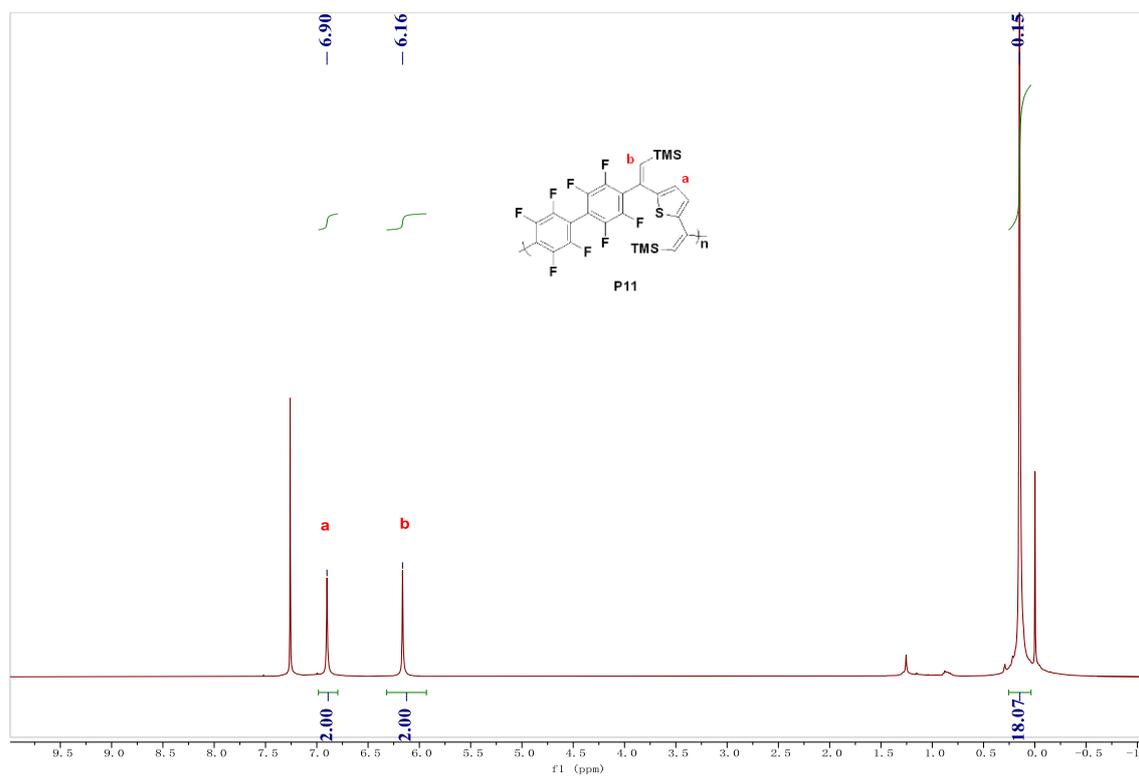
¹⁹F NMR Spectrum of P10



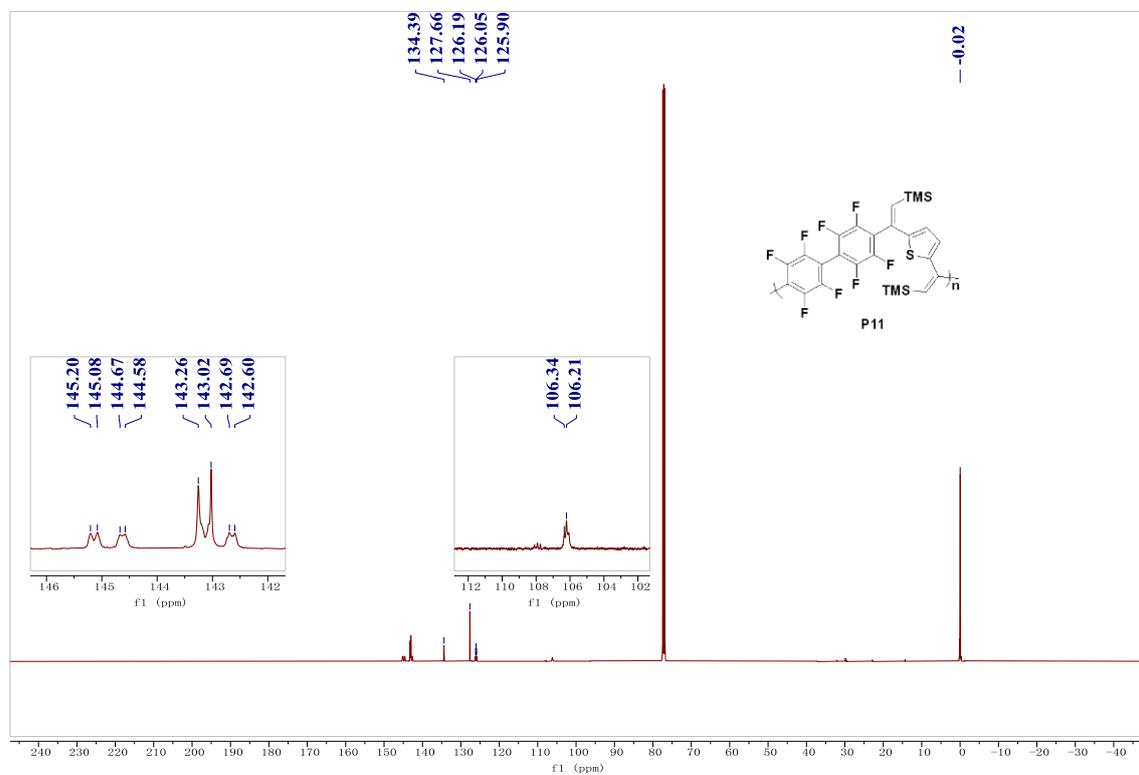
H-H NOESY Spectrum of P10



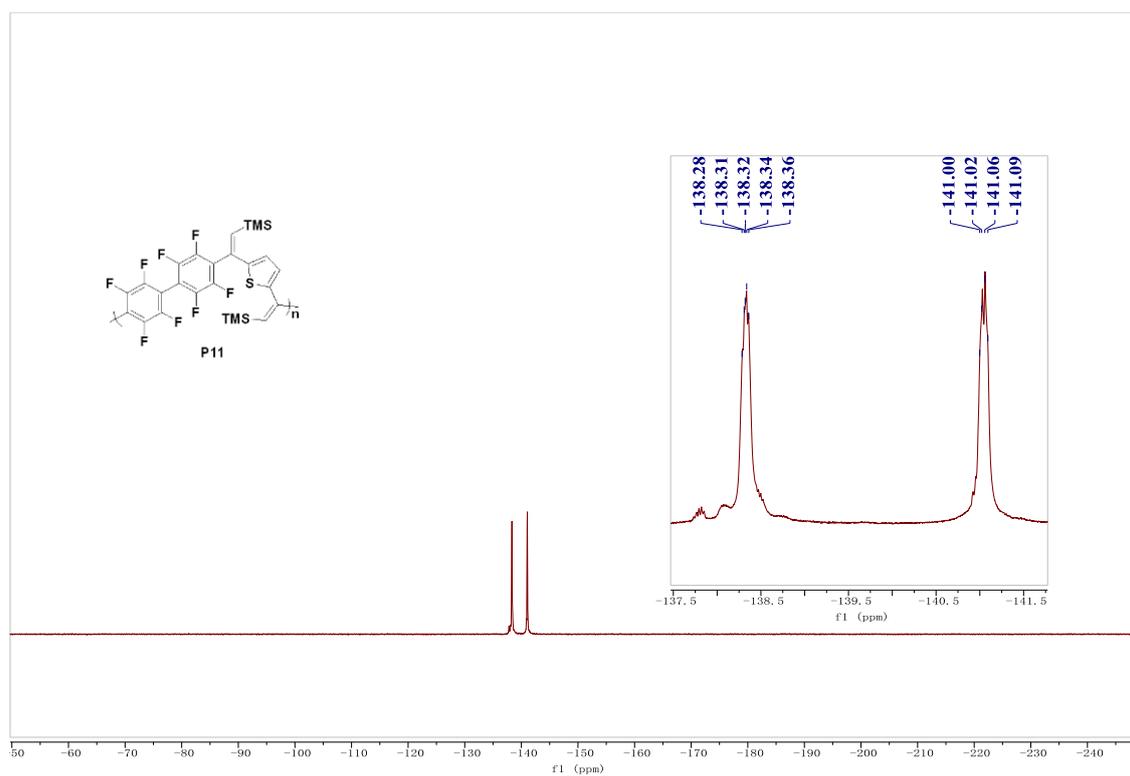
¹H NMR Spectrum of P11



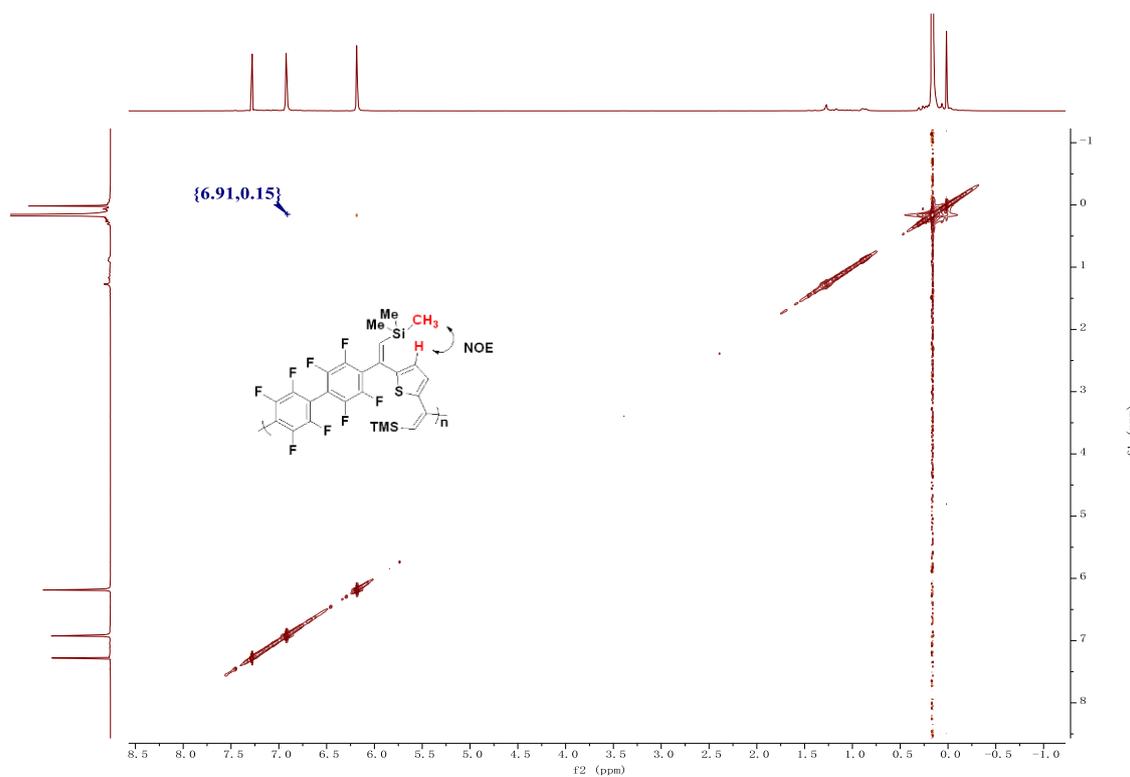
¹³C NMR Spectrum of P11



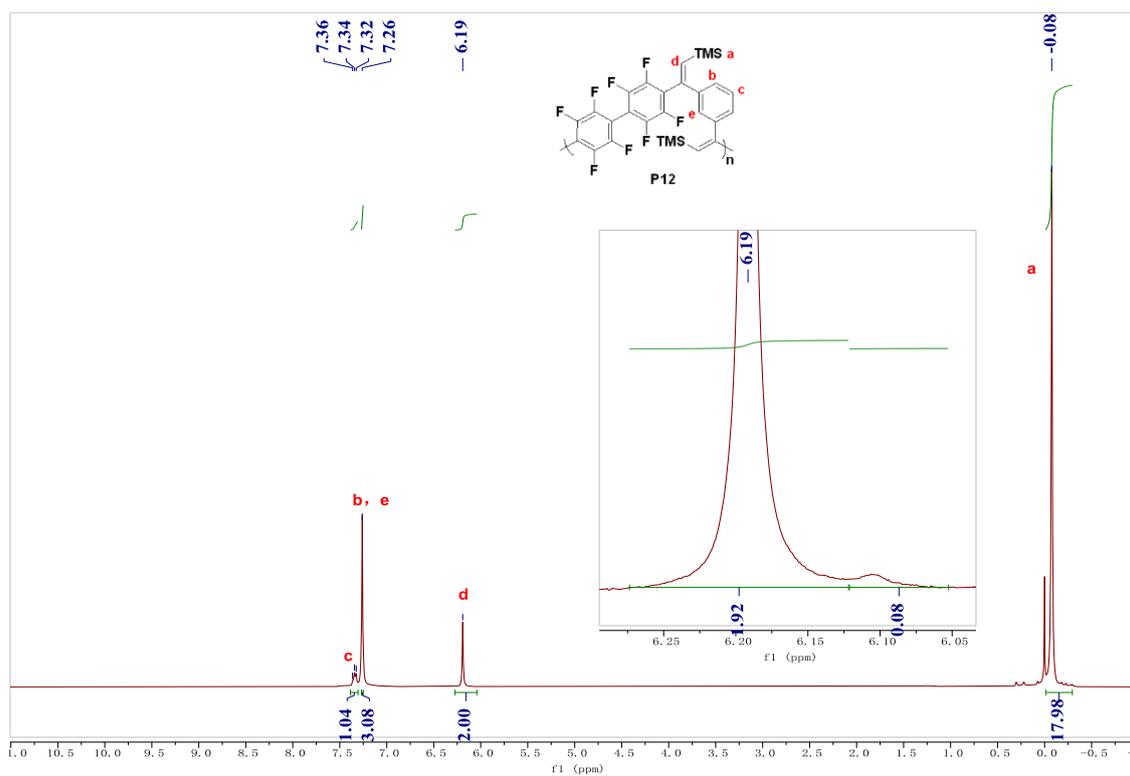
¹⁹F NMR Spectrum of P11



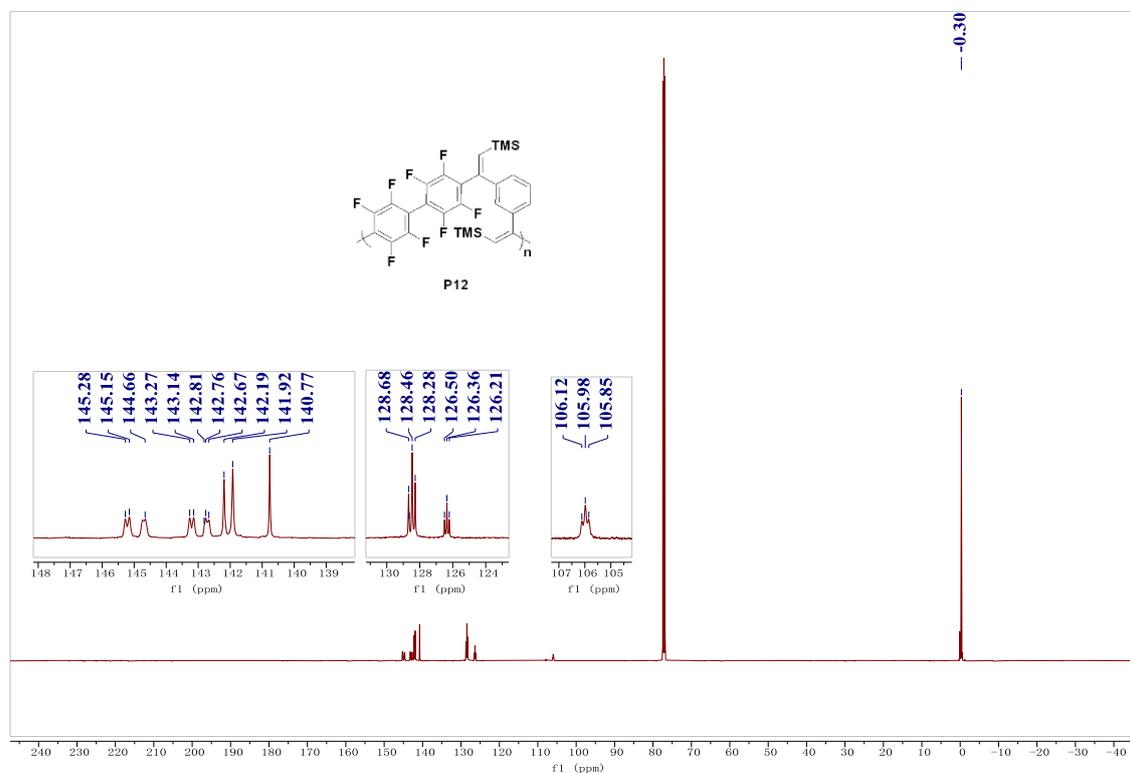
H-H NOESY Spectrum of P11



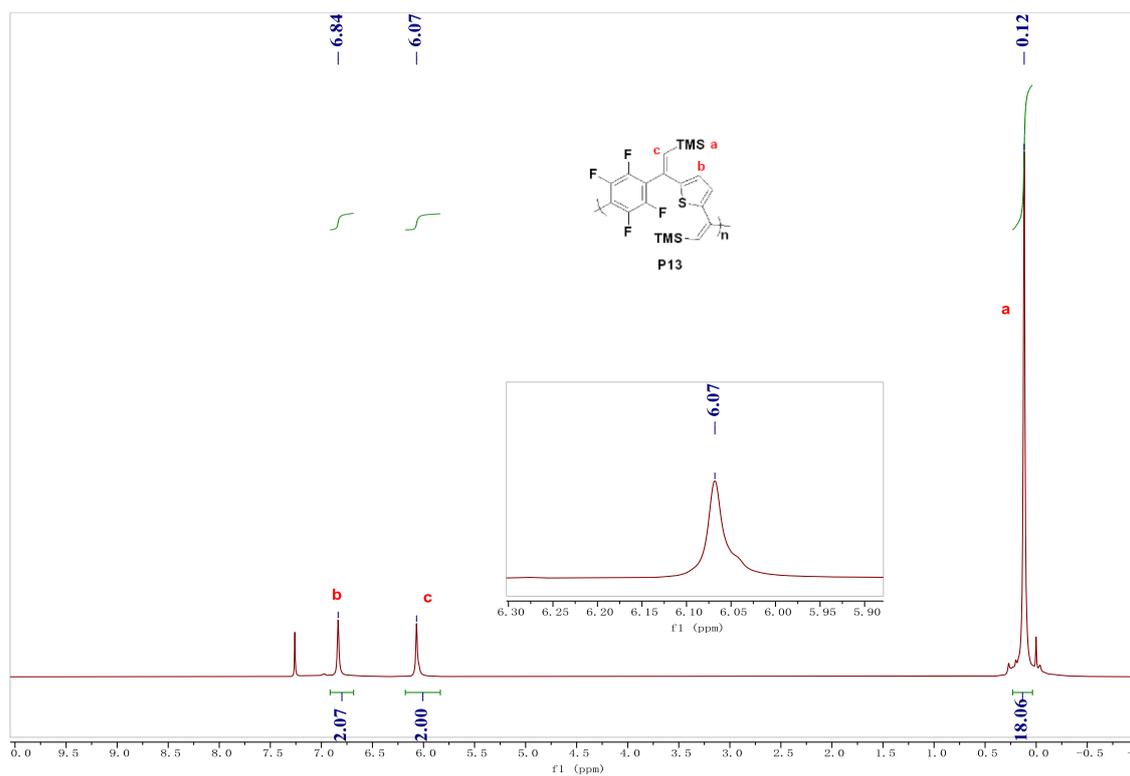
¹H NMR Spectrum of P12



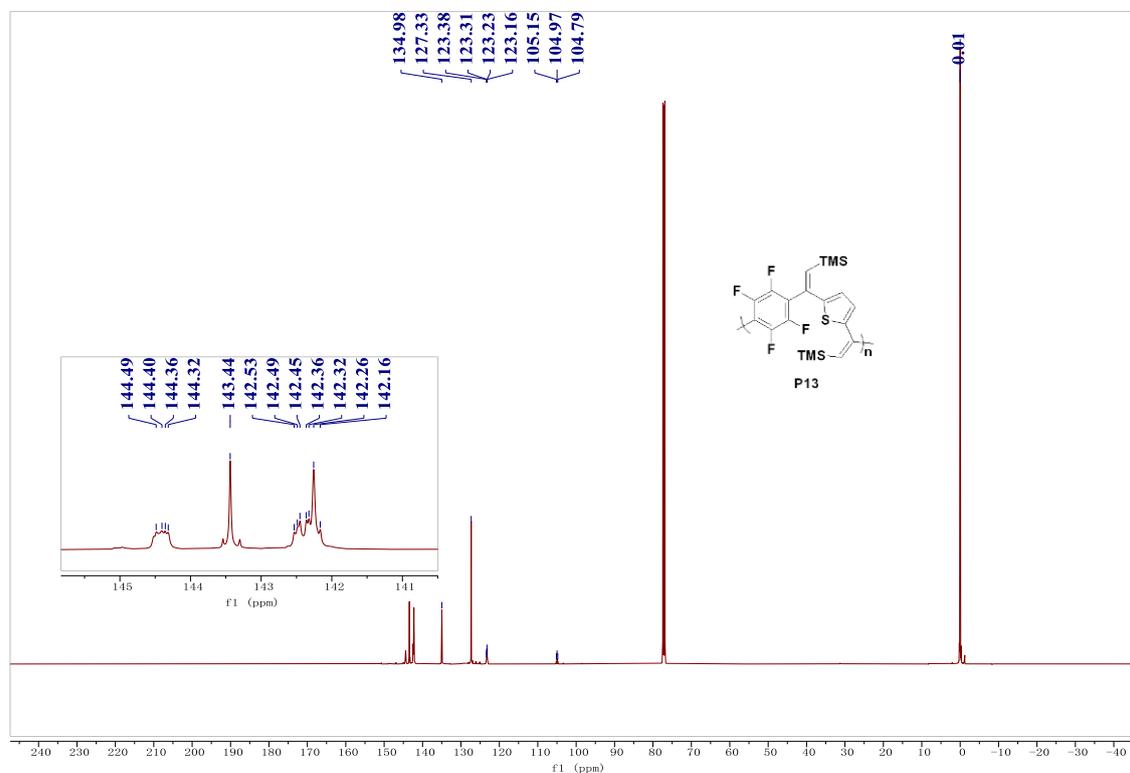
¹³C NMR Spectrum of P12



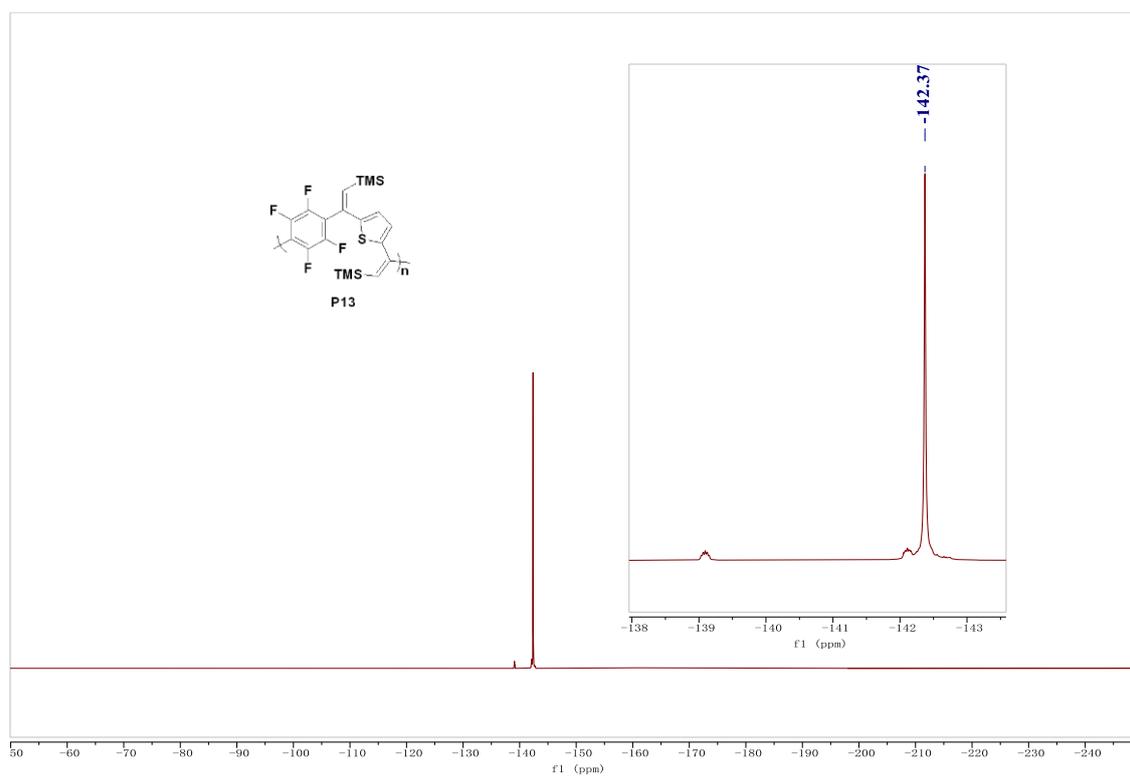
¹H NMR Spectrum of P13



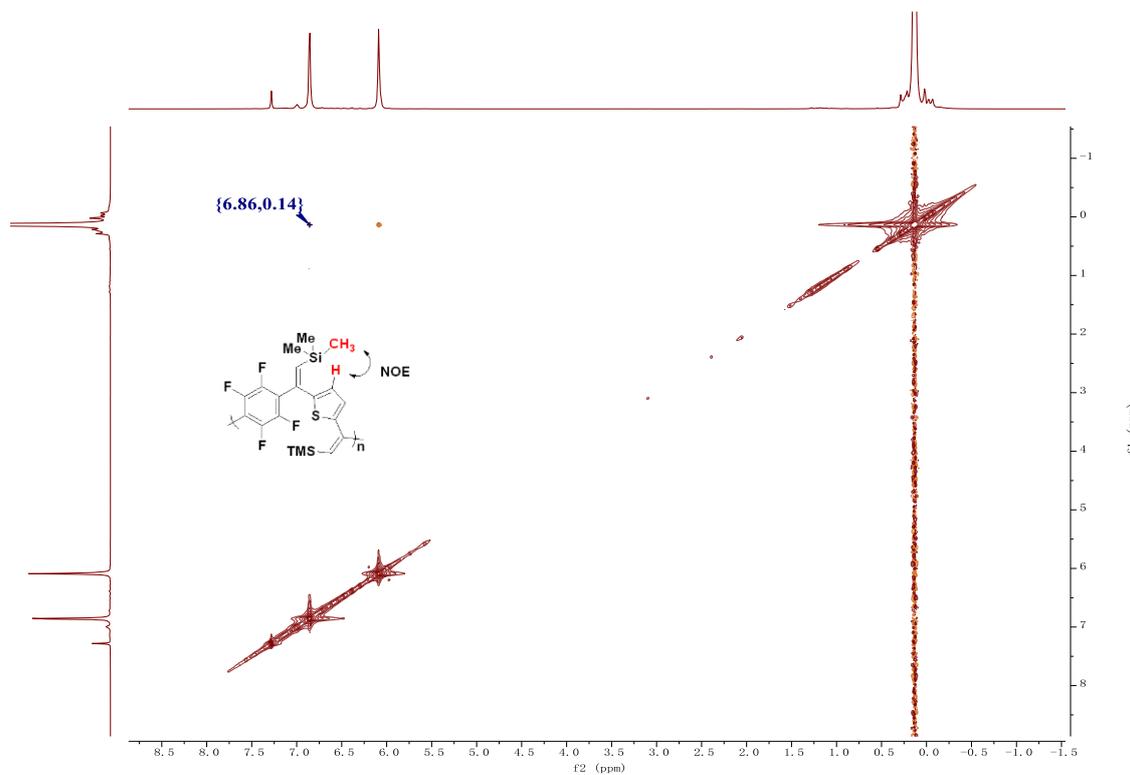
¹³C NMR Spectrum of P13



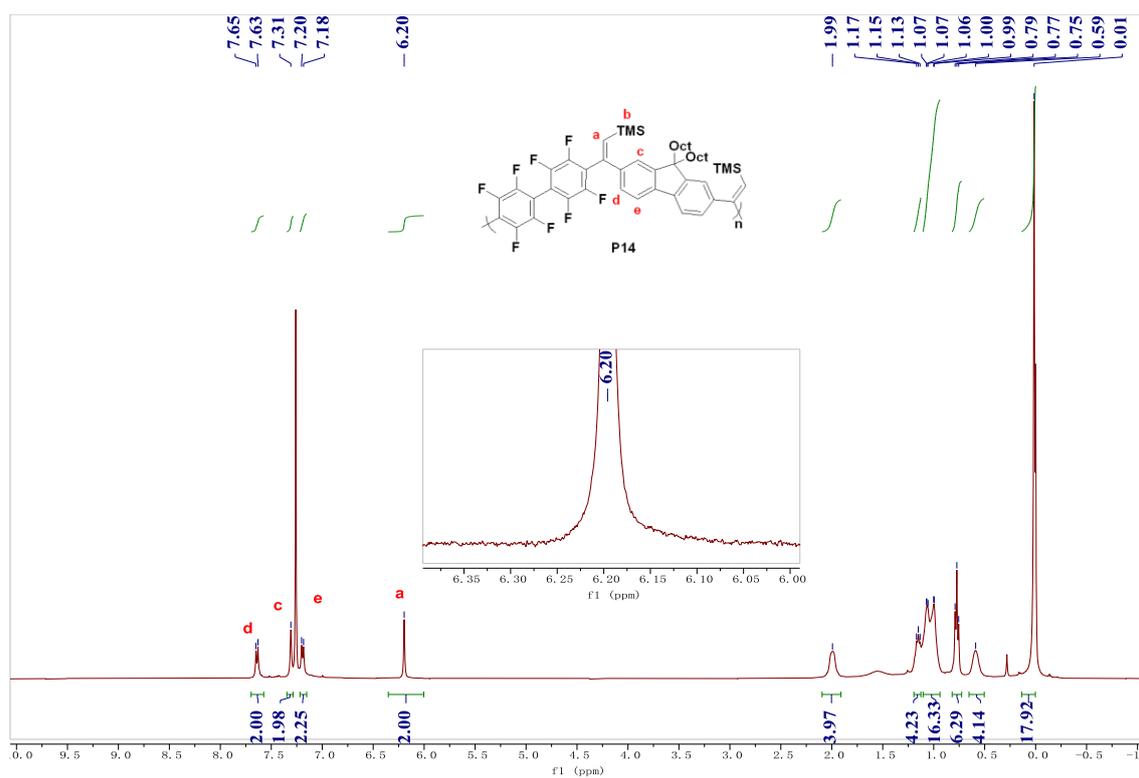
^{19}F NMR Spectrum of P13



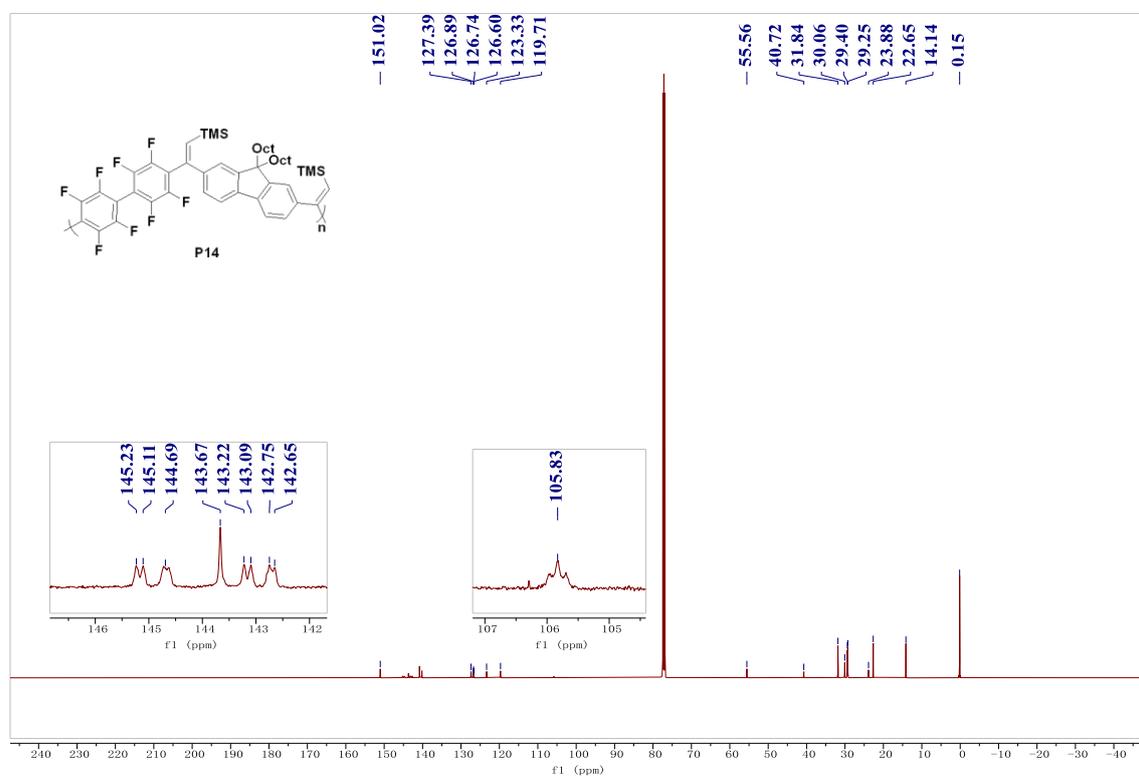
H-H NOESY Spectrum of P13



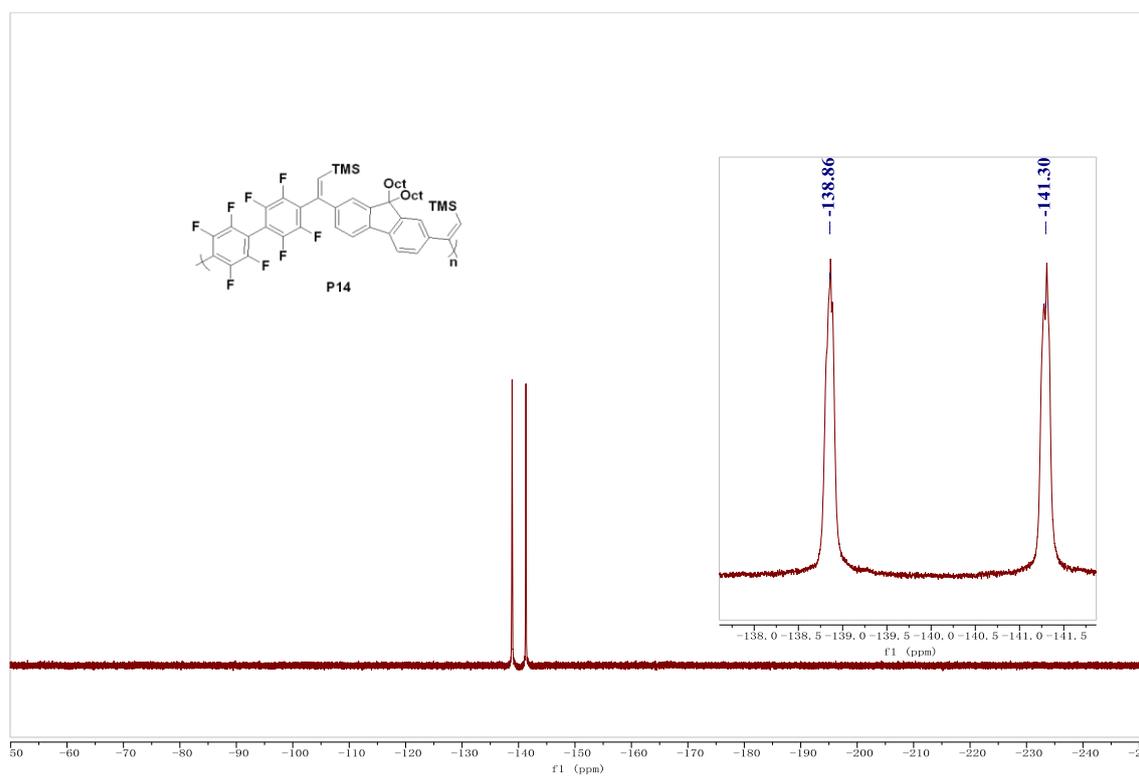
¹H NMR Spectrum of P14



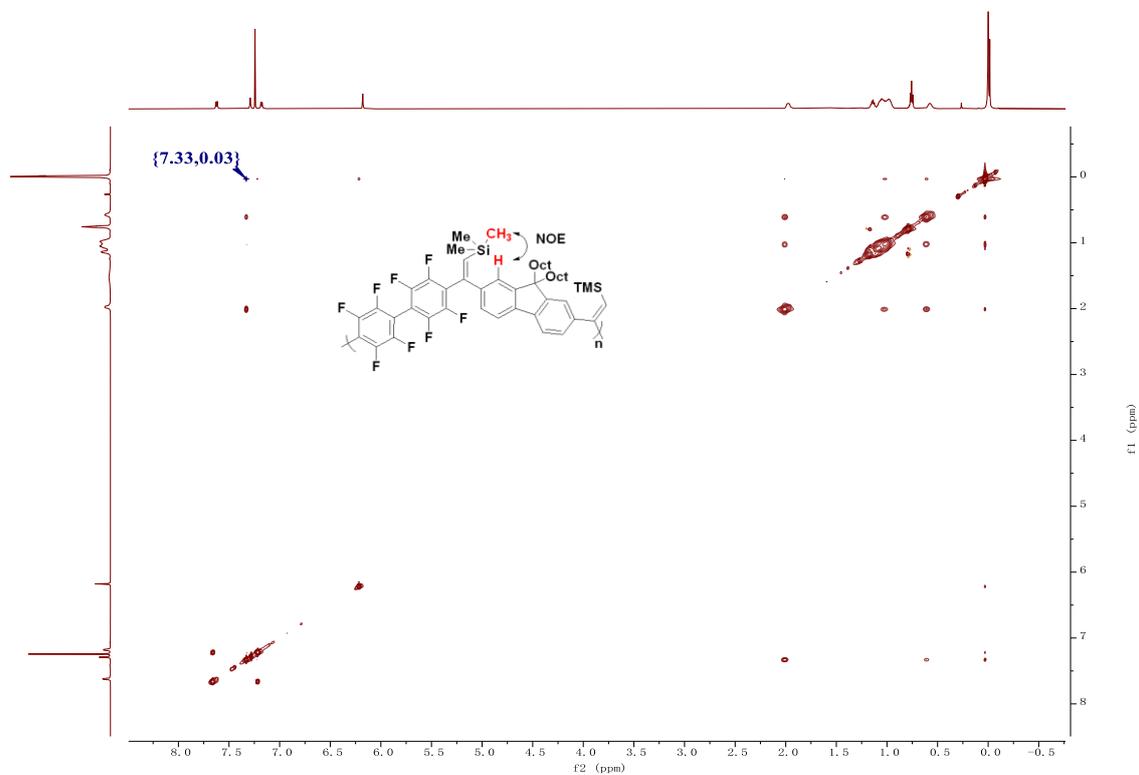
¹³C NMR Spectrum of P14



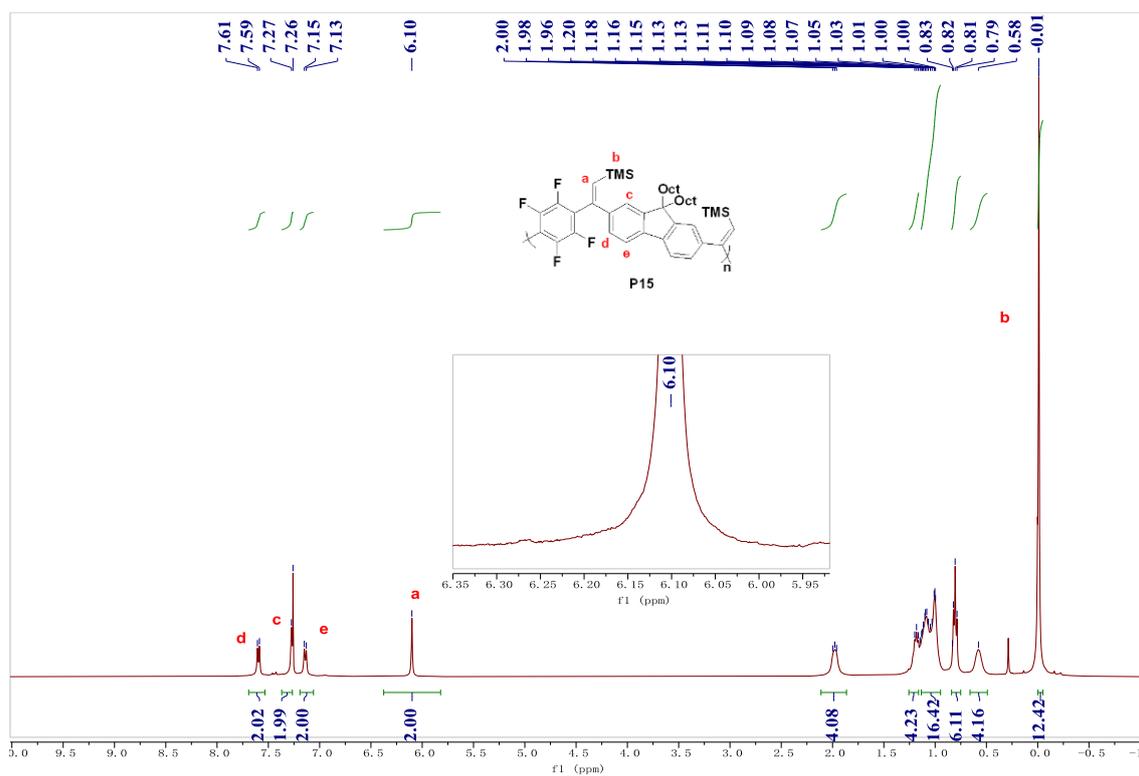
¹⁹F NMR Spectrum of P14



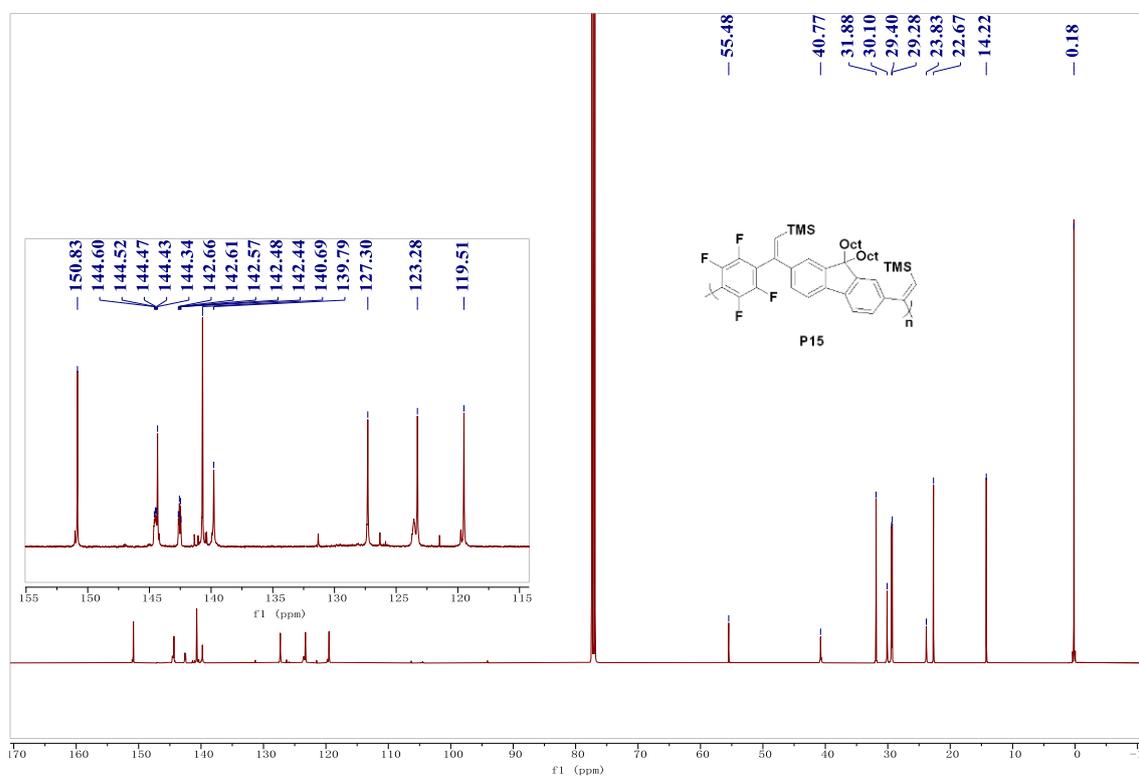
H-H NOESY Spectrum of P14



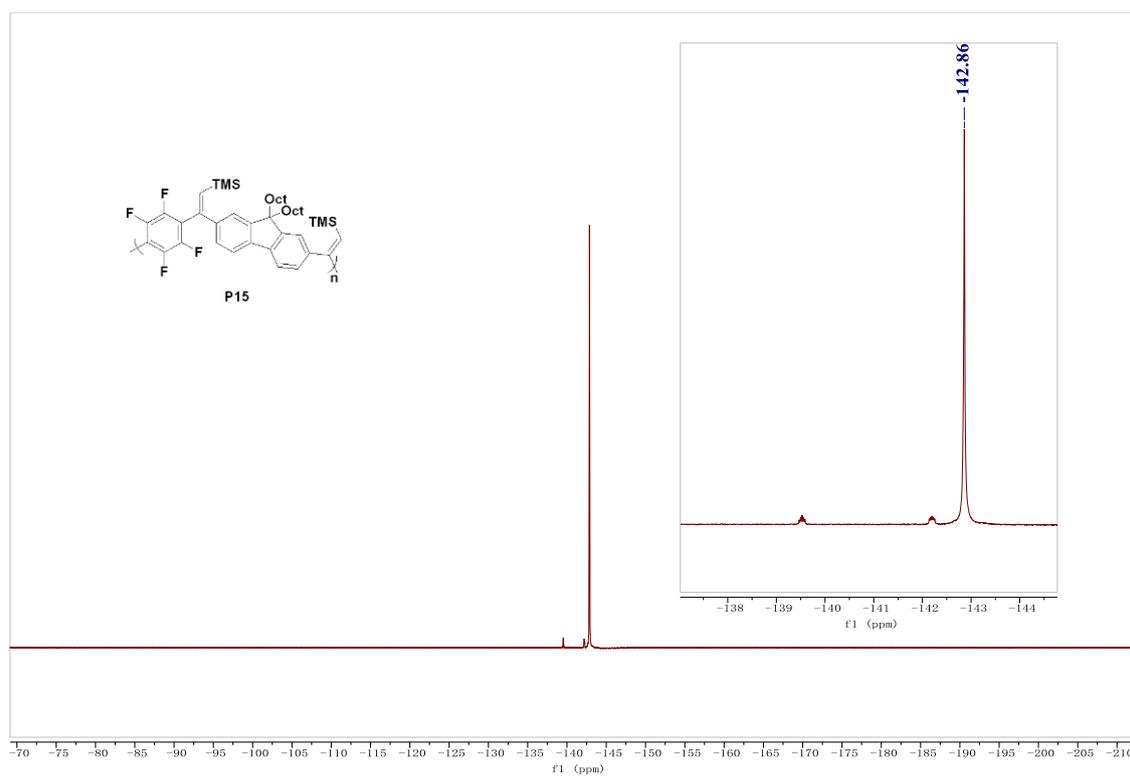
¹H NMR Spectrum of P15



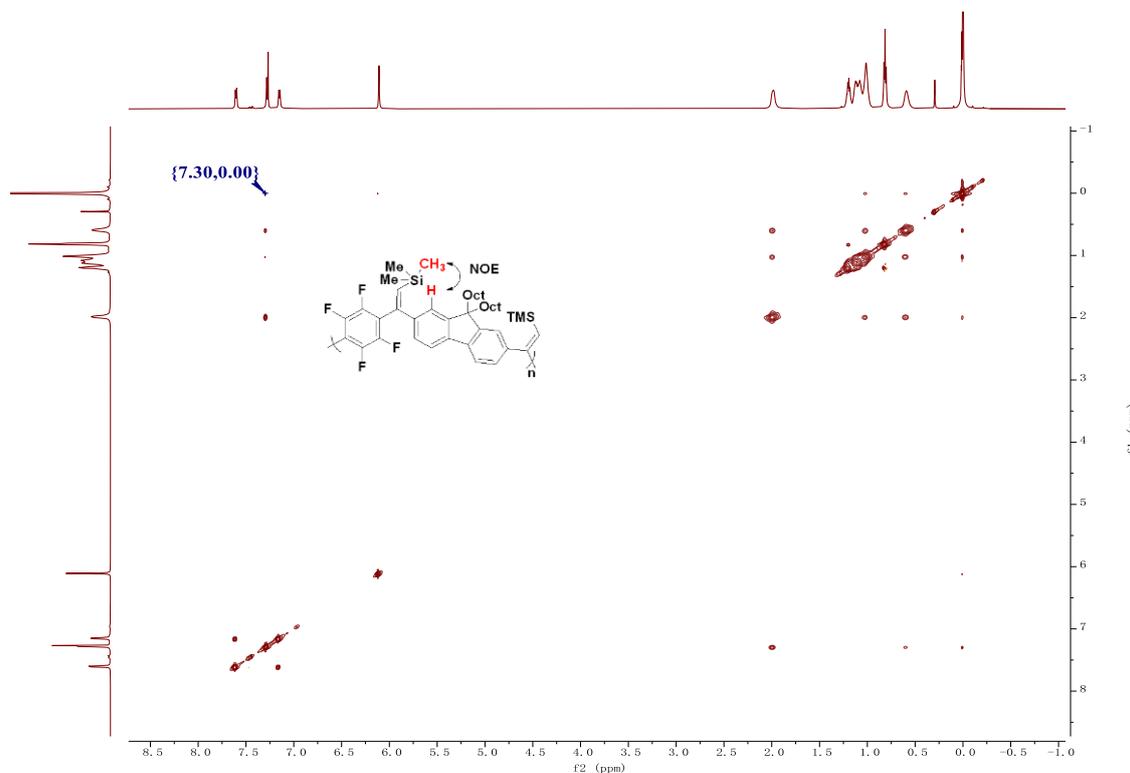
¹³C NMR Spectrum of P15



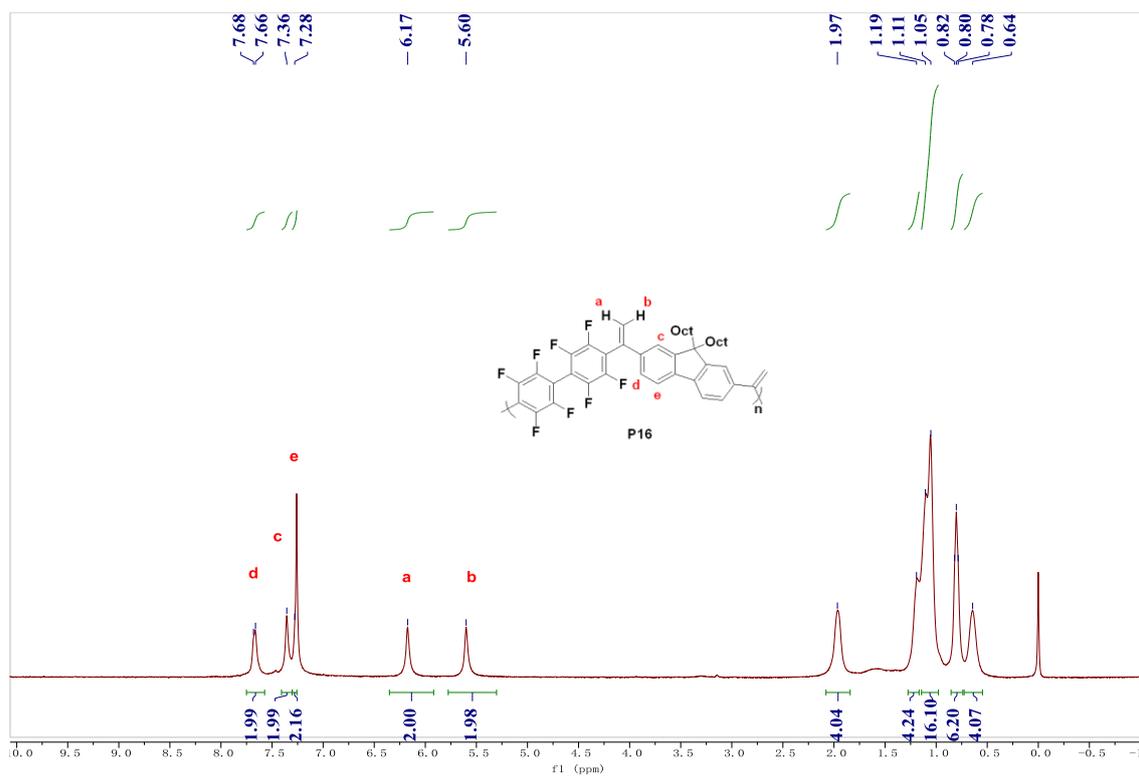
¹⁹F NMR Spectrum of P15



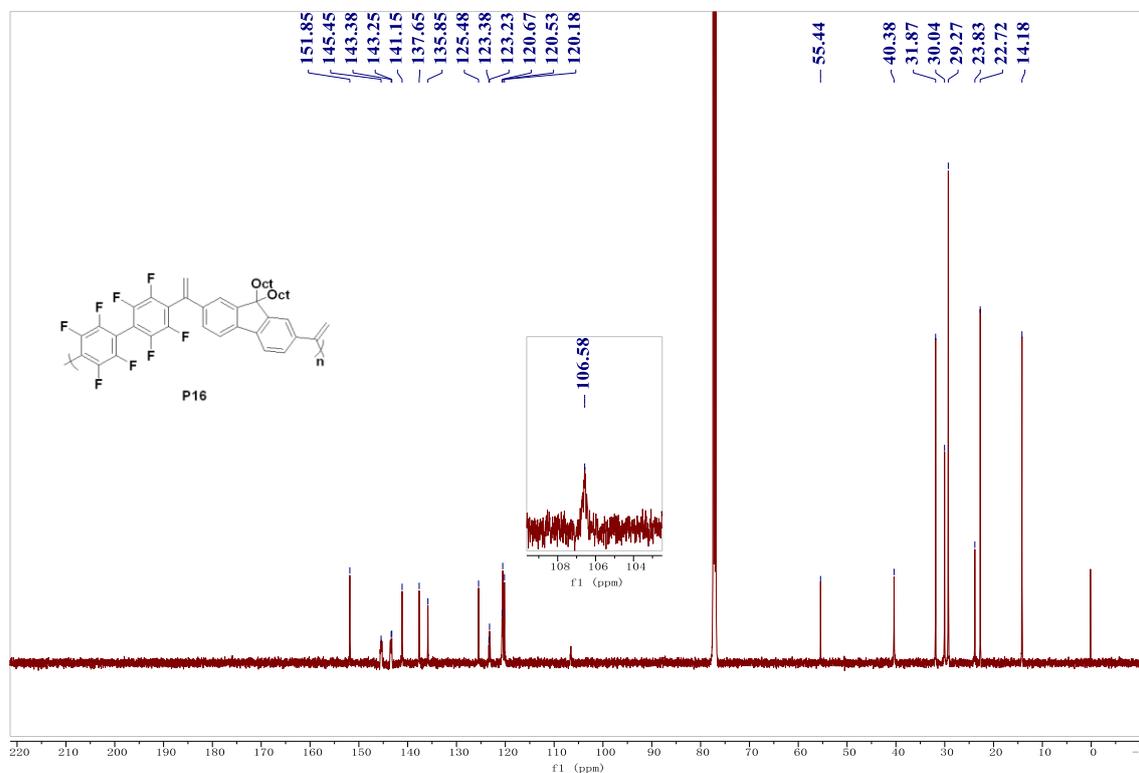
H-H NOESY Spectrum of P15



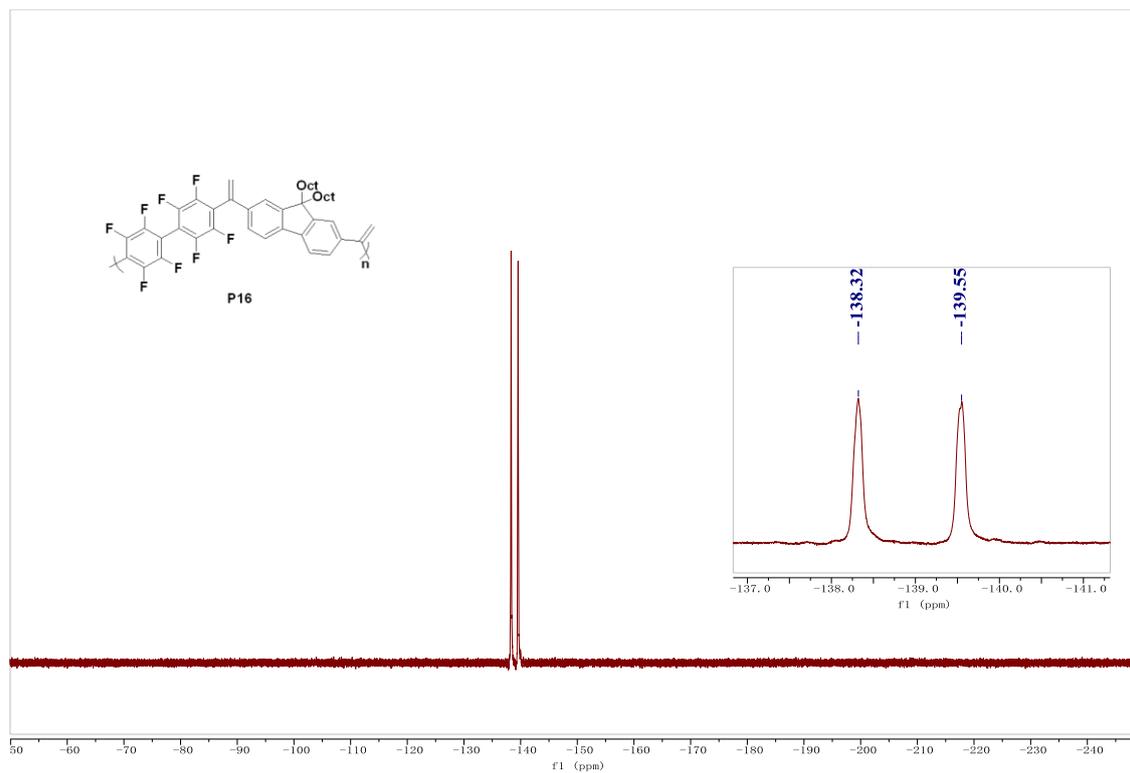
¹H NMR Spectrum of P16



¹³C NMR Spectrum of P16



¹⁹F NMR Spectrum of P16



13. GPC Curves.

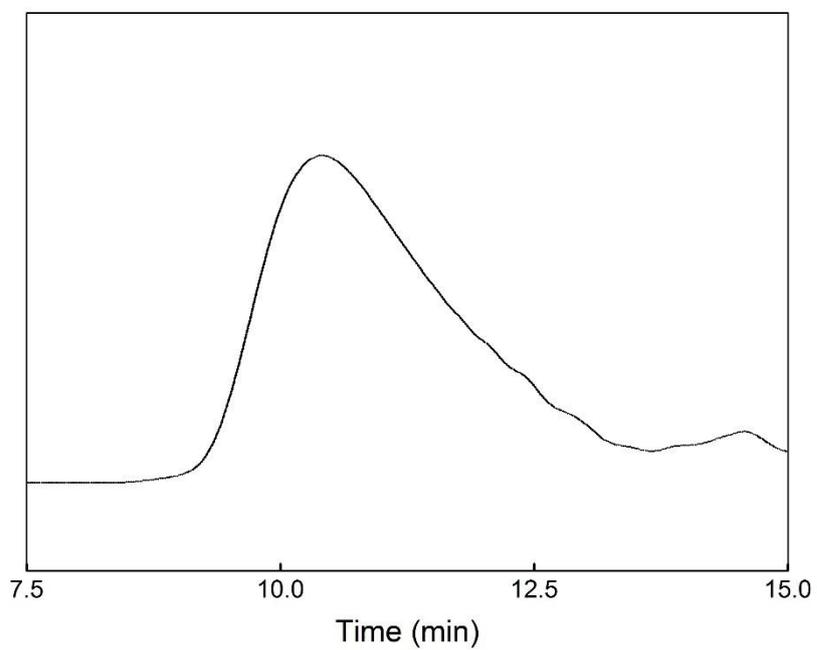


Figure S1. GPC curve of P1

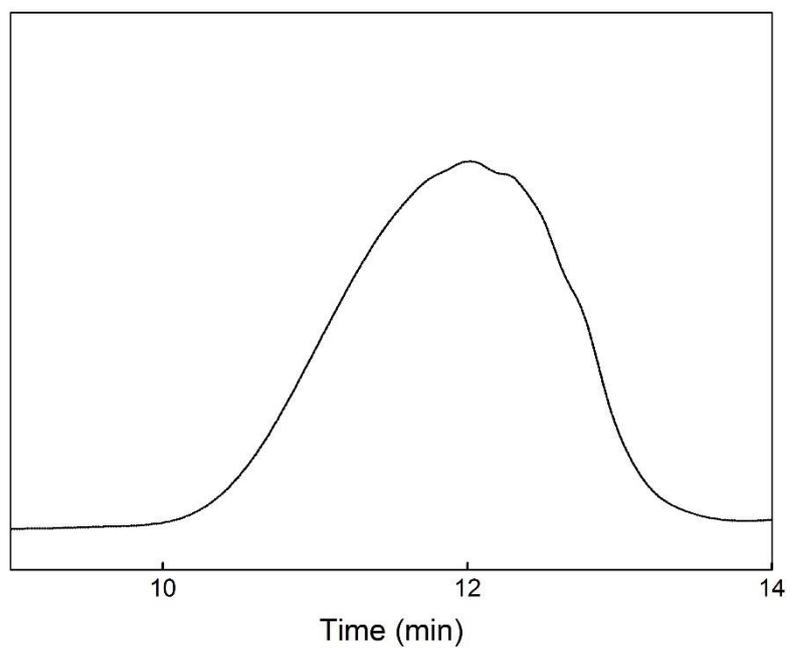


Figure S2. GPC curve of P2

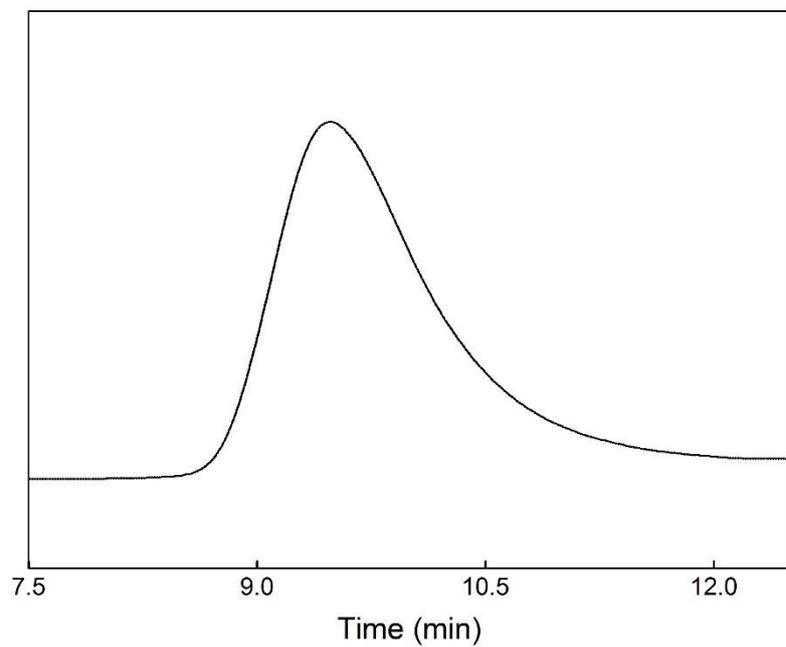


Figure S3. GPC curve of **P3**

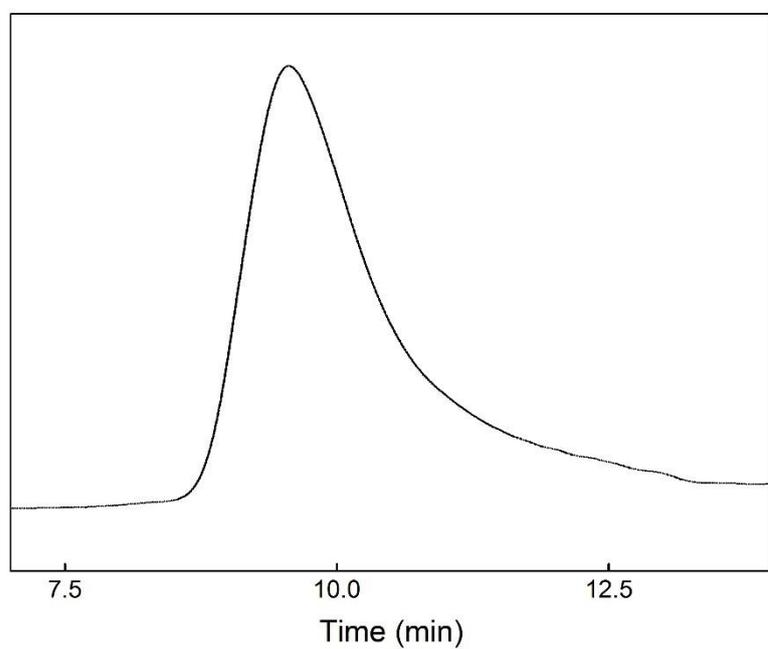


Figure S4. GPC curve of **P4**

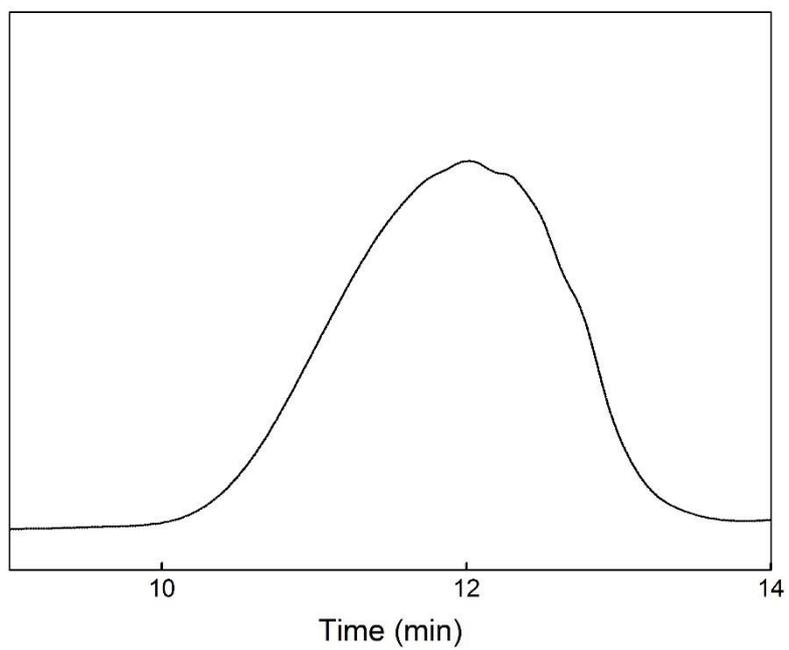


Figure S5. GPC curve of **P5**

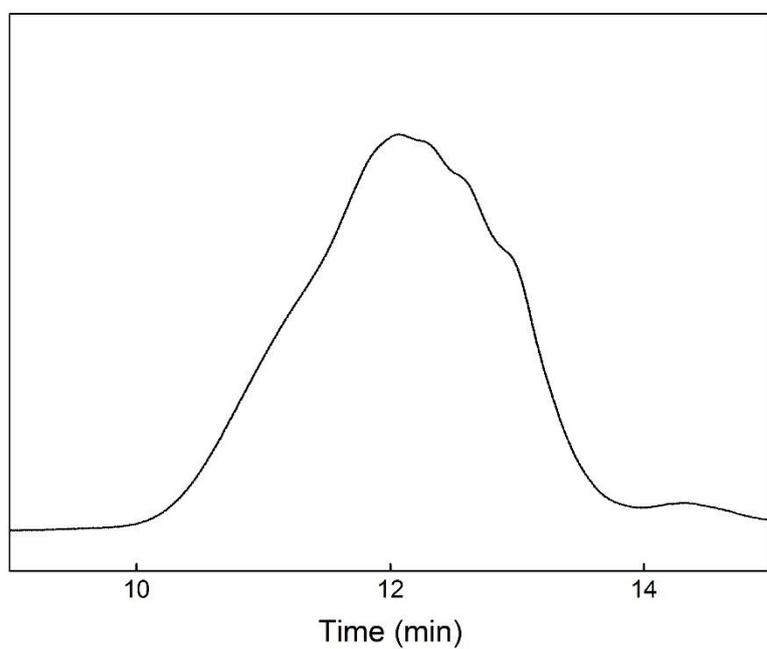


Figure S6. GPC curve of **P6**

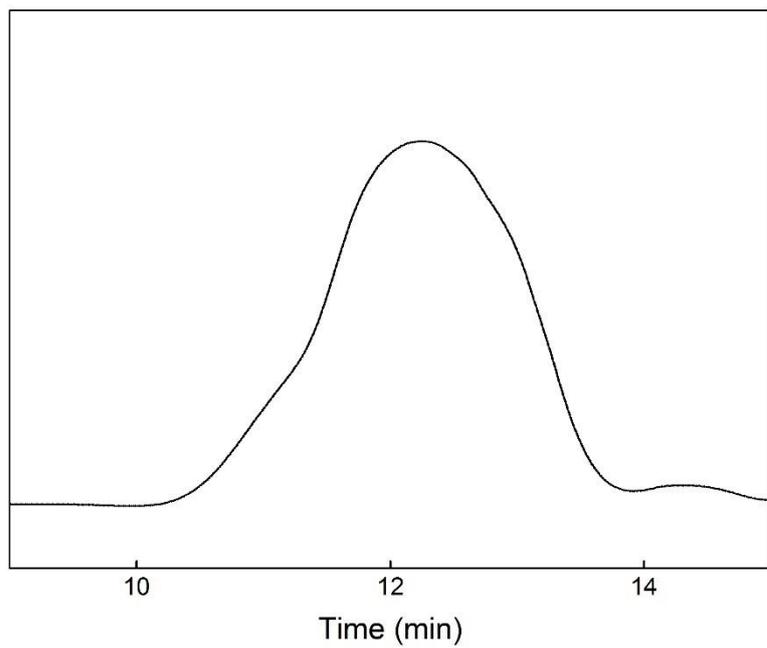


Figure S7. GPC curve of **P7**

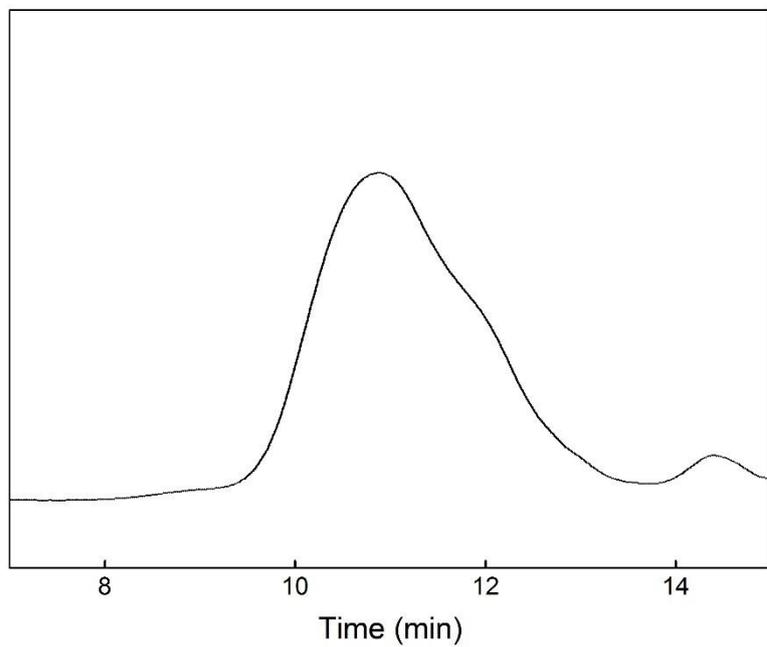


Figure S8. GPC curve of **P8**

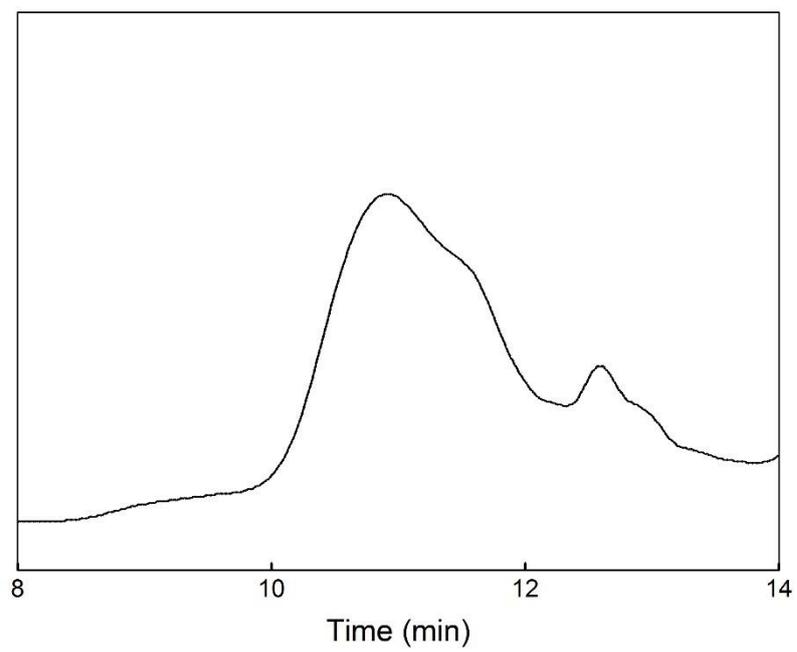


Figure S9. GPC curve of **P9**

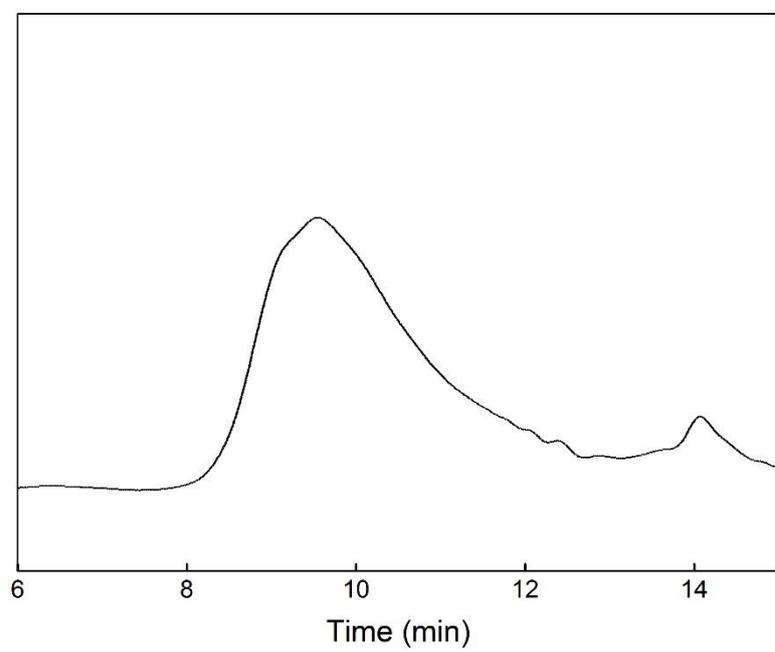


Figure S10. GPC curve of **P10**

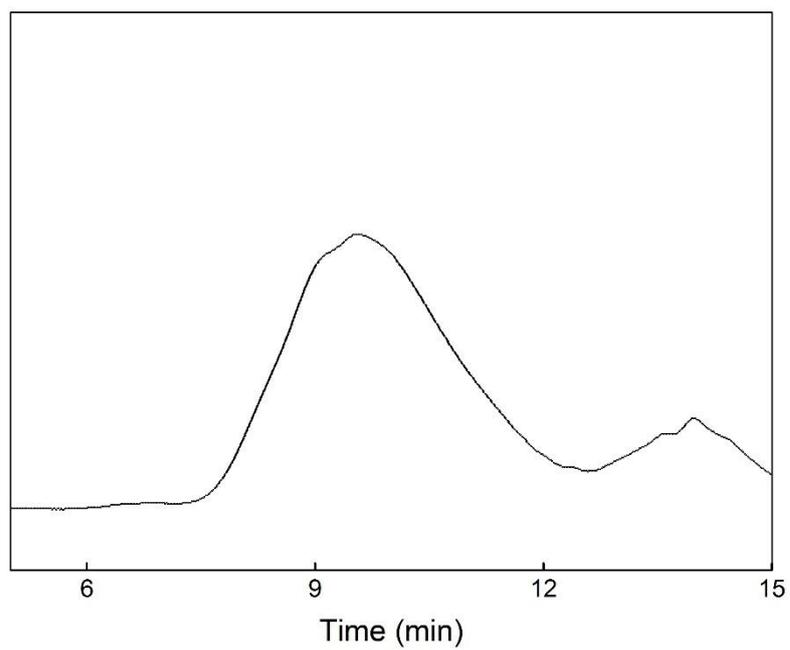


Figure S11. GPC curve of P11

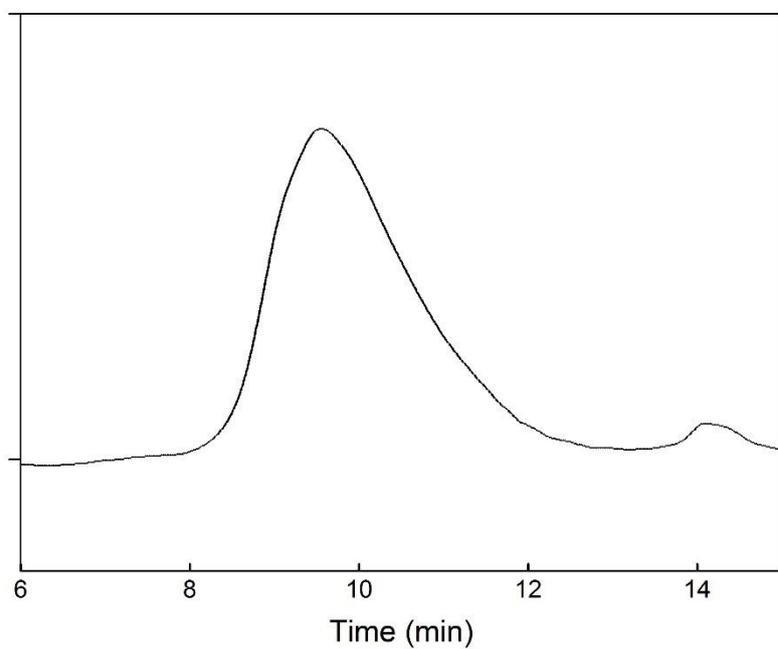


Figure S12. GPC curve of P12

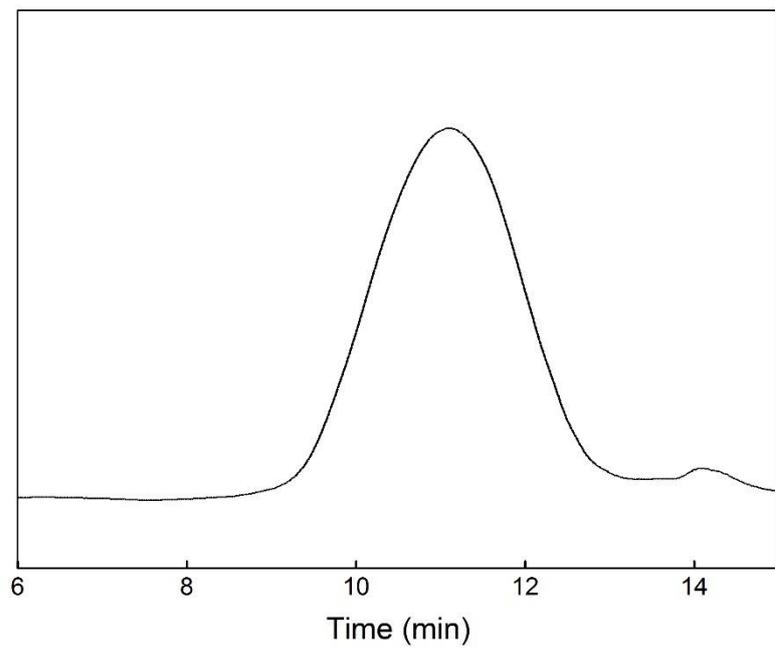


Figure S13. GPC curve of **P13**

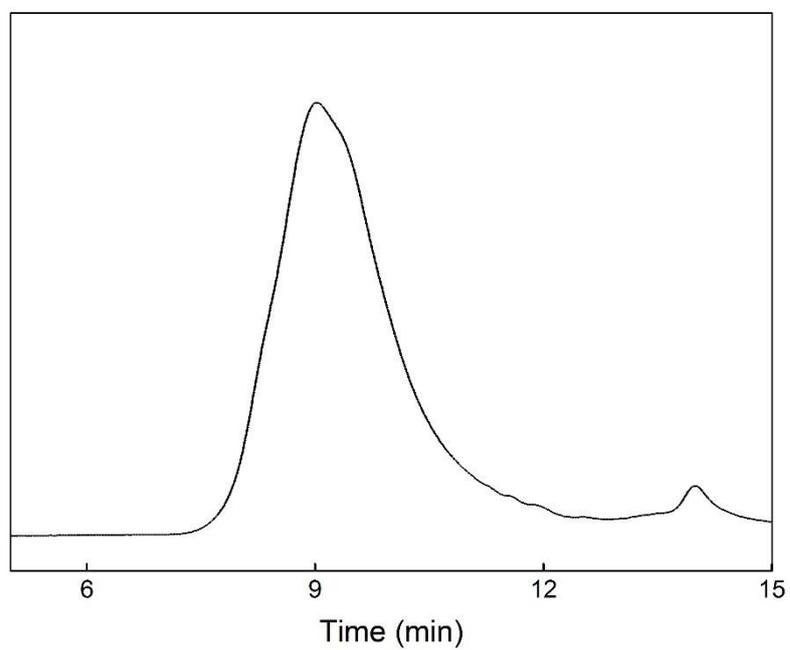


Figure S14. GPC curve of **P14**

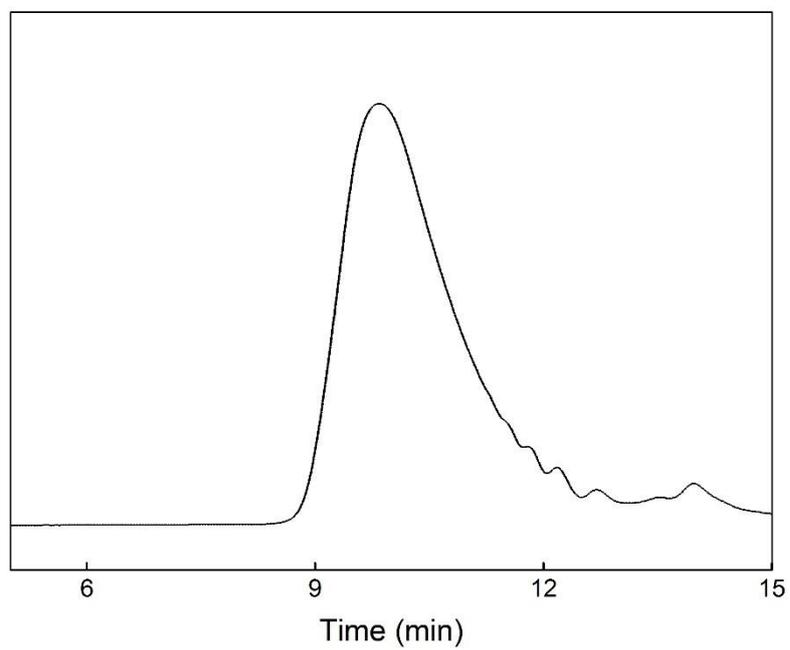


Figure S15. GPC curve of **P15**

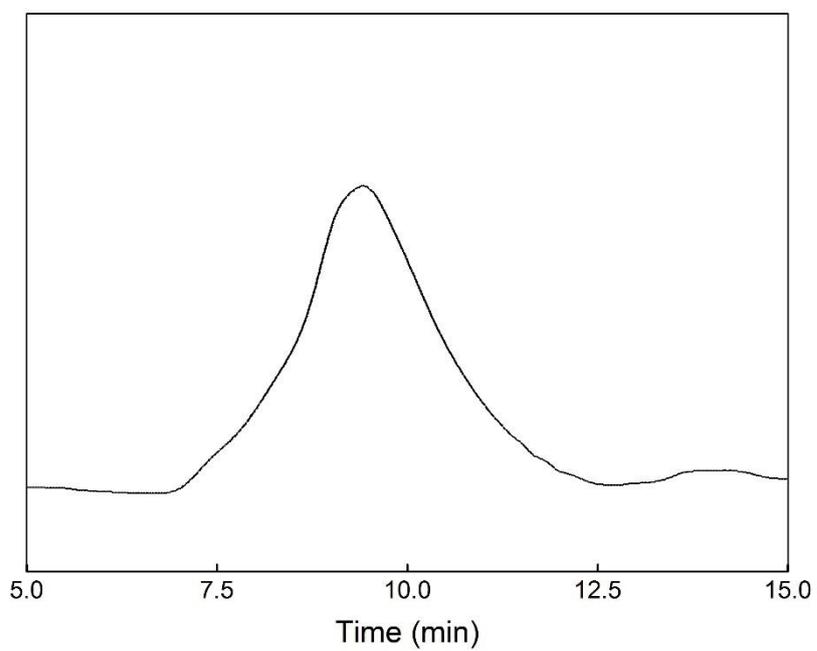


Figure S16. GPC curve of **P16**

14. TGA Curves.

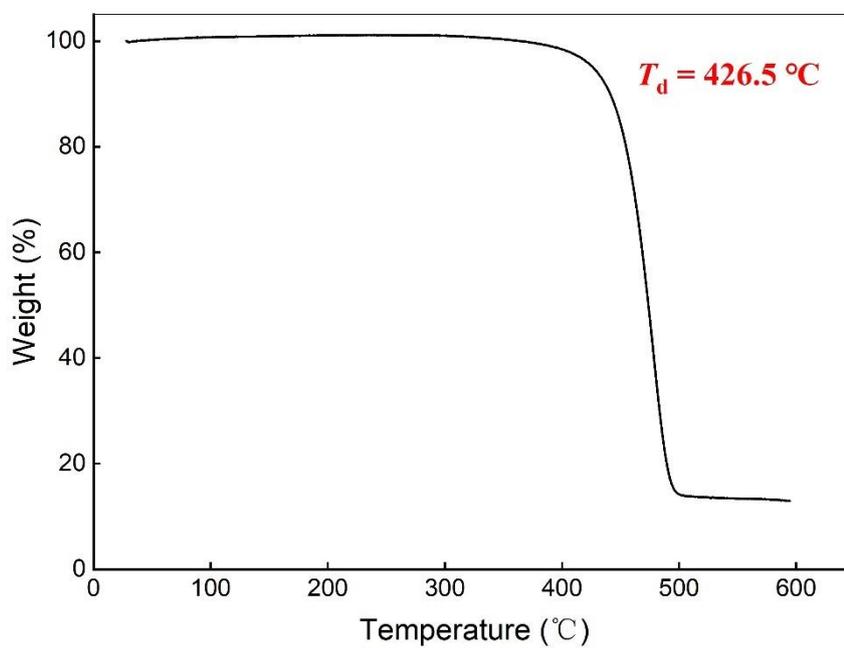


Figure S17. TGA curve of P1

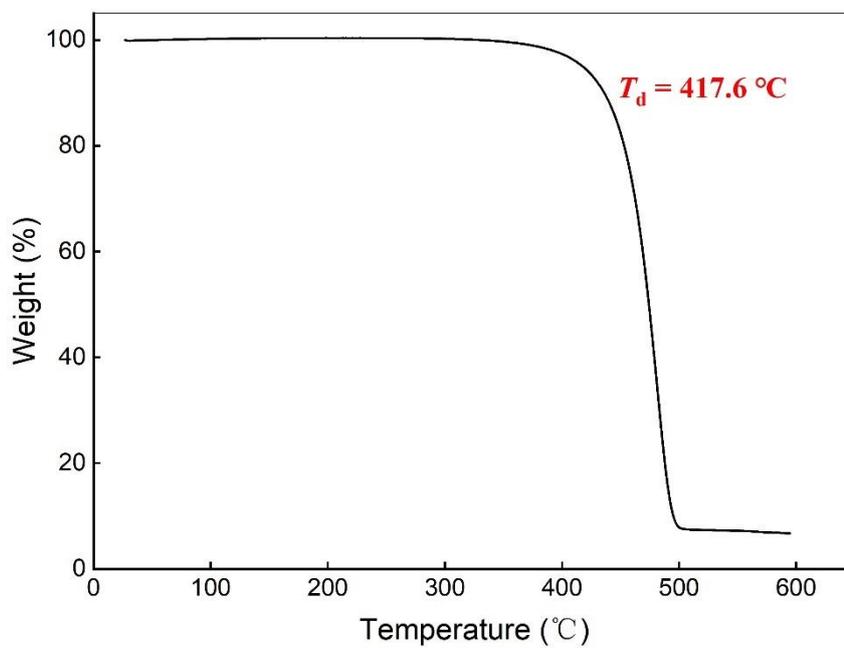


Figure S18. TGA curve of P2

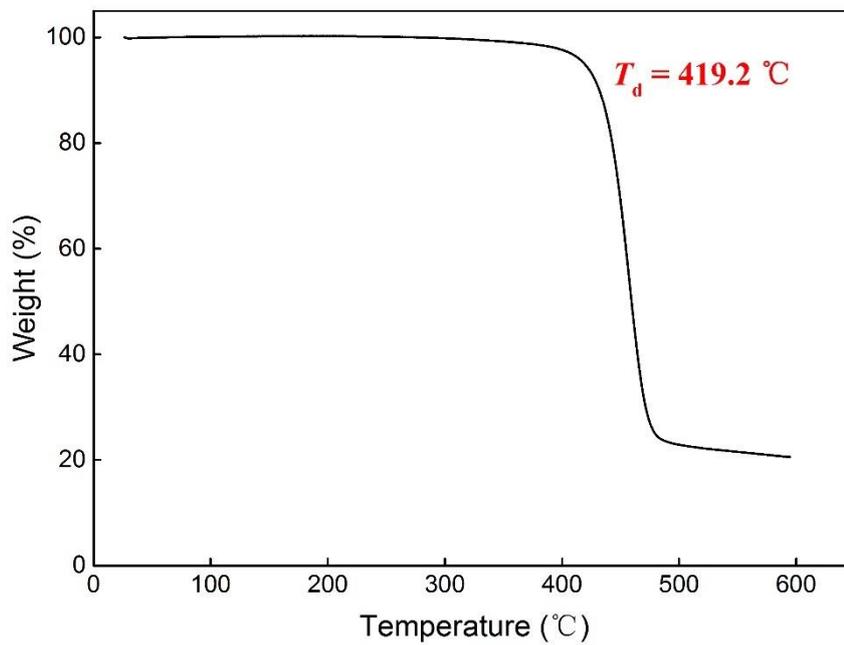


Figure S19. TGA curve of P3

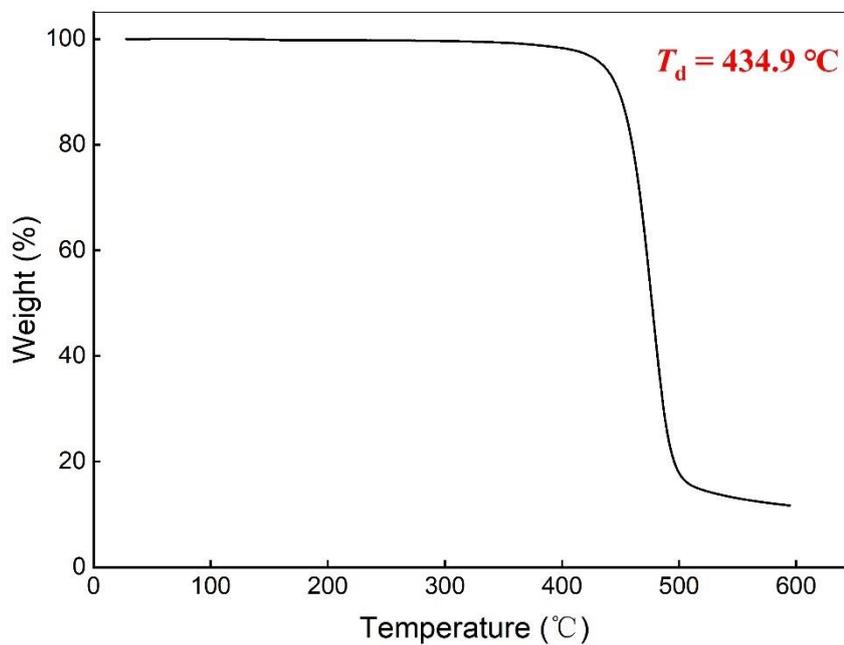


Figure S20. TGA curve of P4

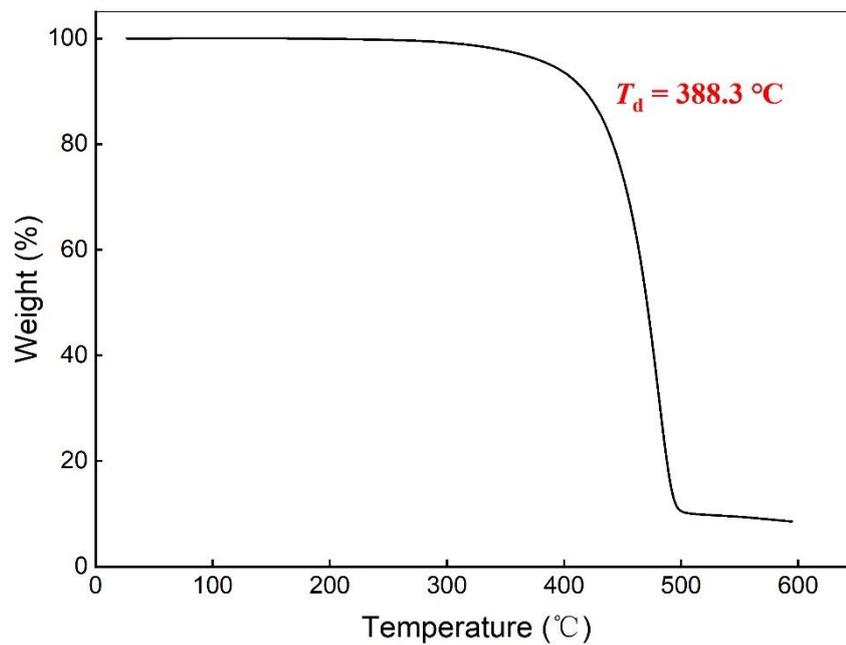


Figure S21. TGA curve of P5

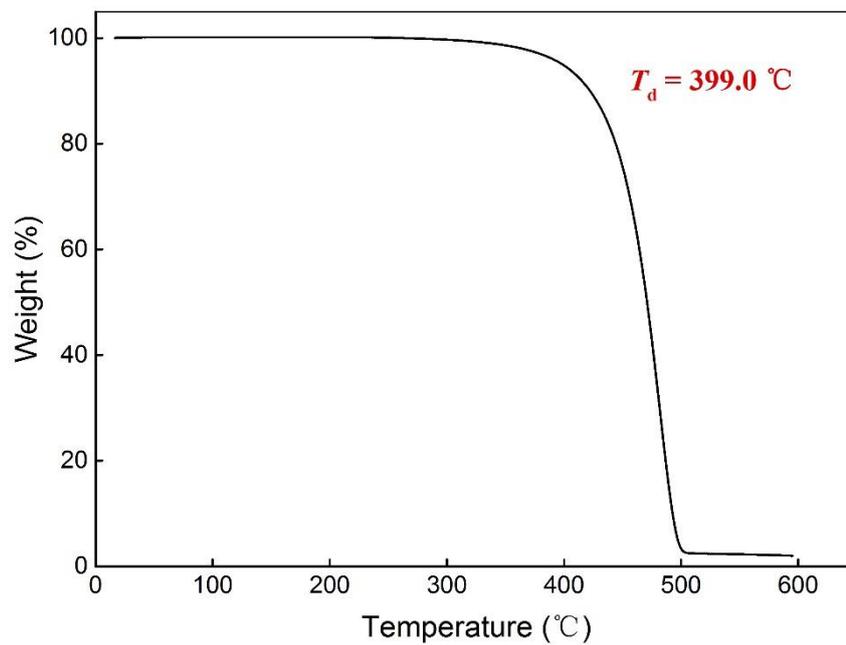


Figure S22. TGA curve of P6

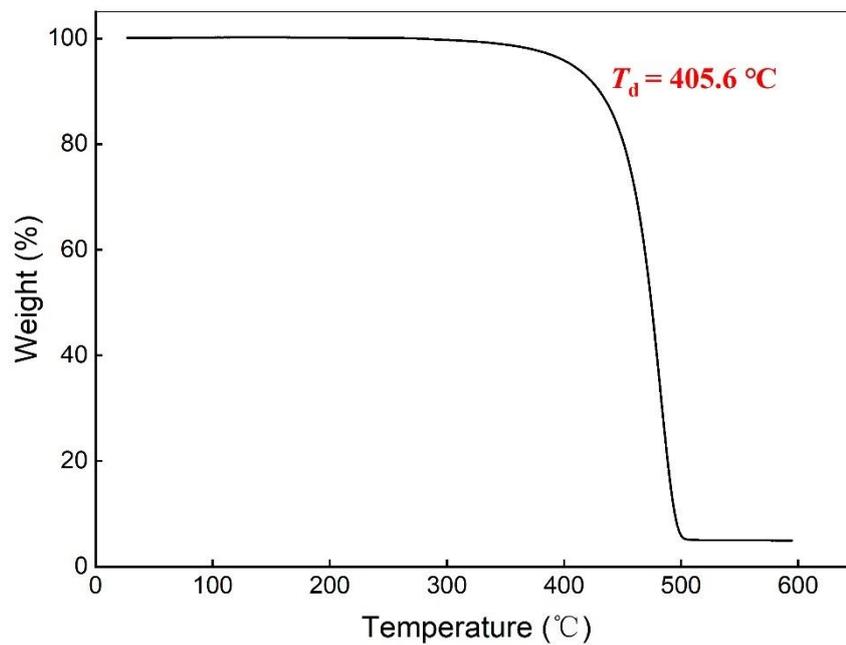


Figure S23. TGA curve of P7

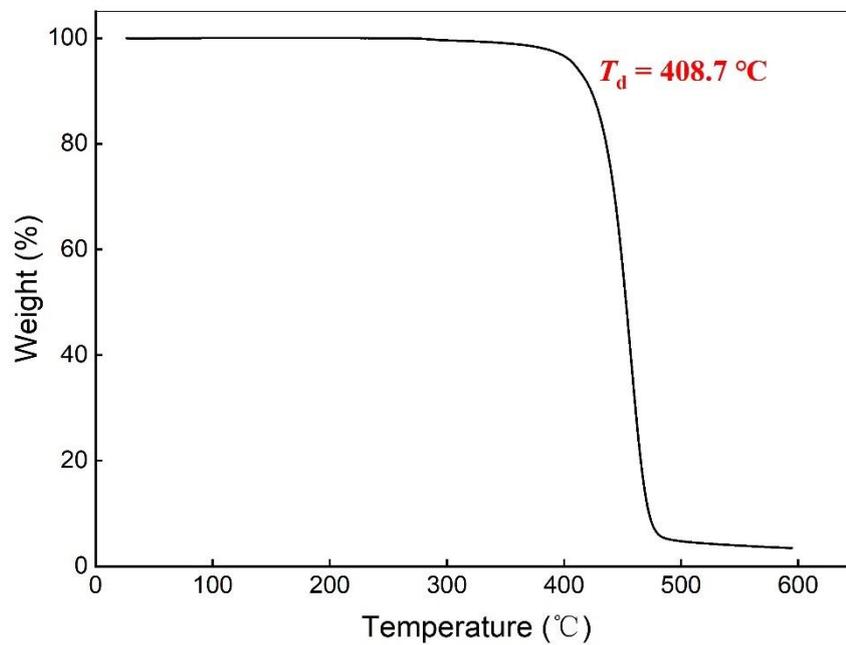


Figure S24. TGA curve of P8

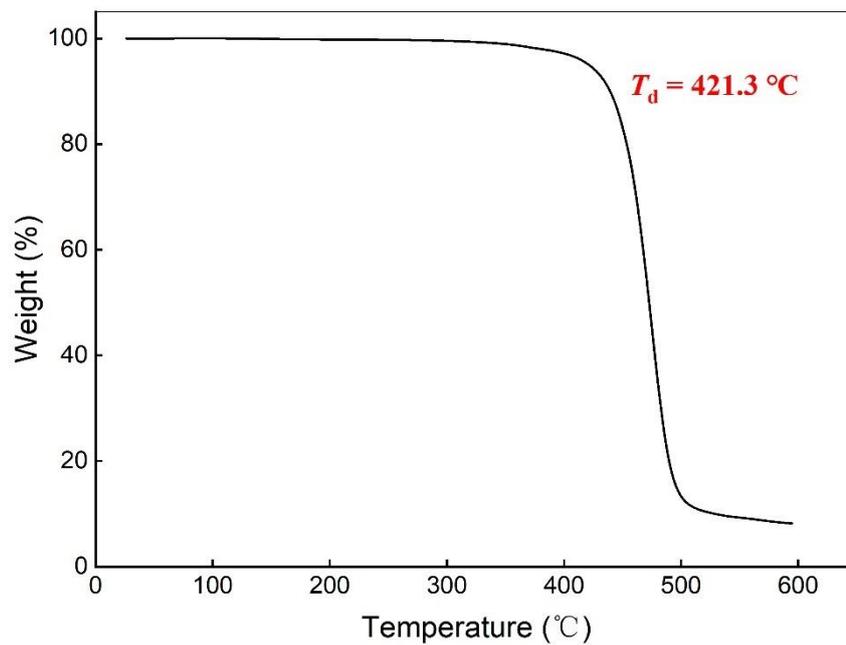


Figure S25. TGA curve of **P9**

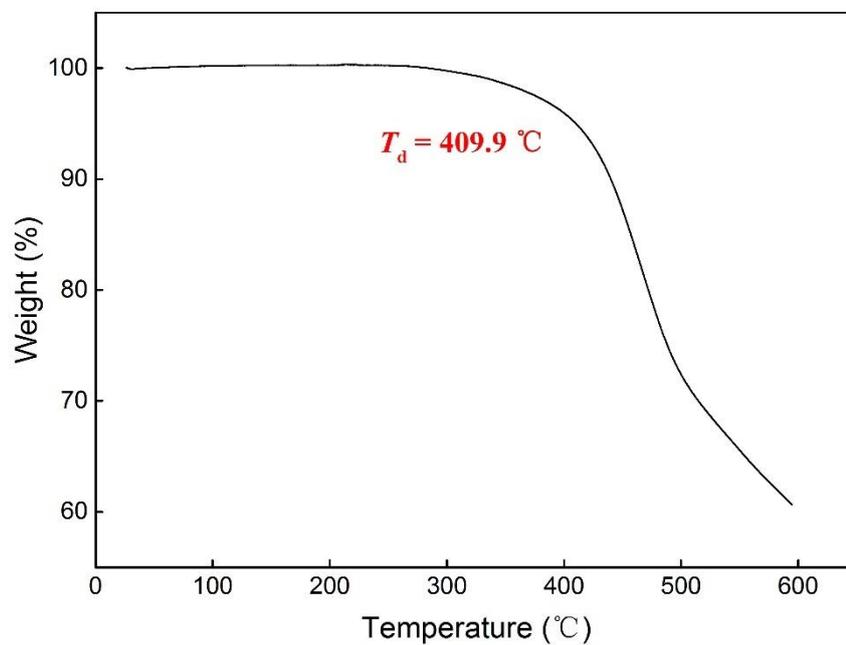


Figure S26. TGA curve of **P10**

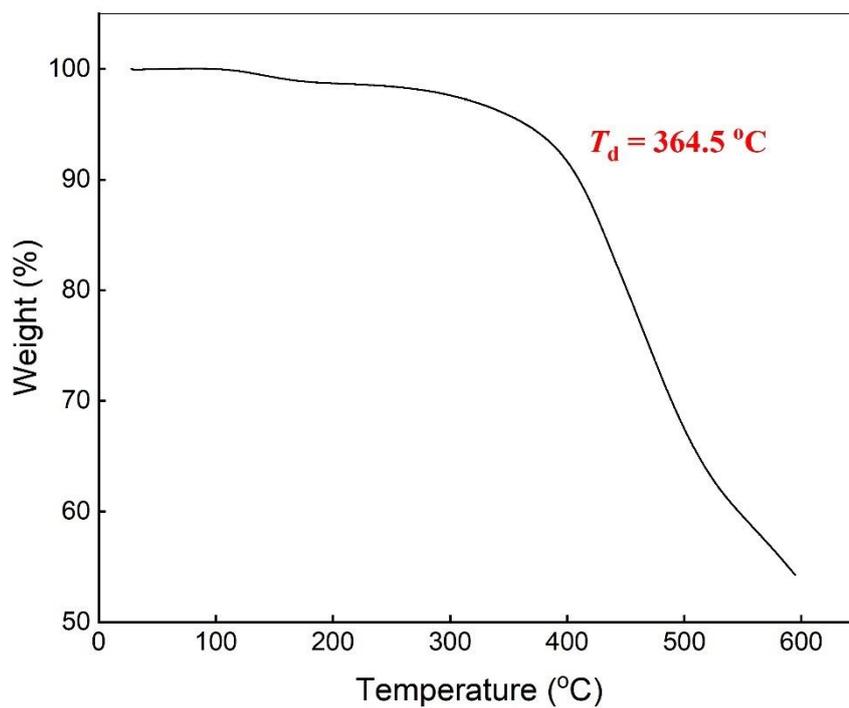


Figure S27. TGA curve of **P11**

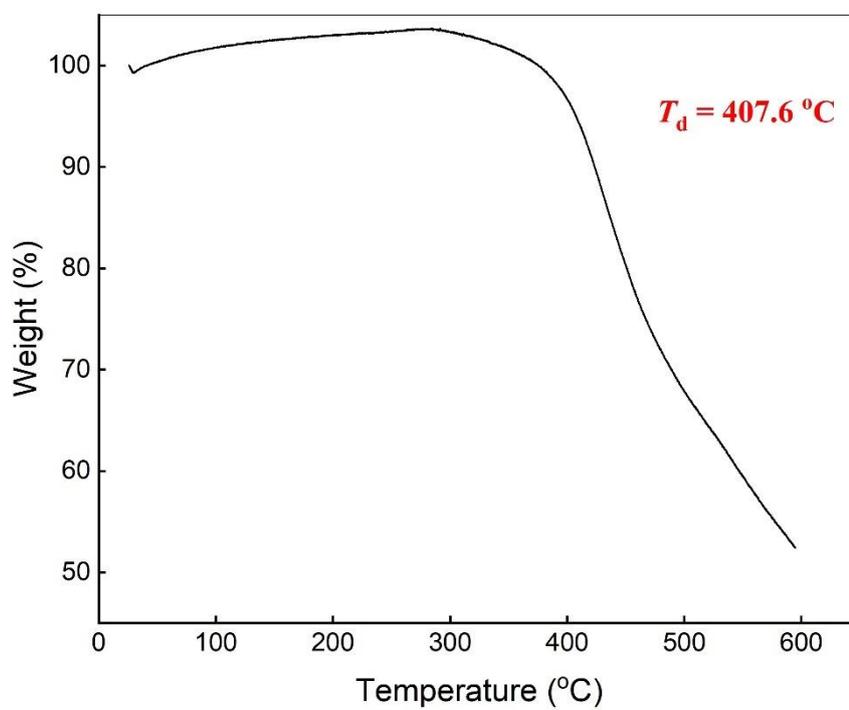


Figure S28. TGA curve of **P12**

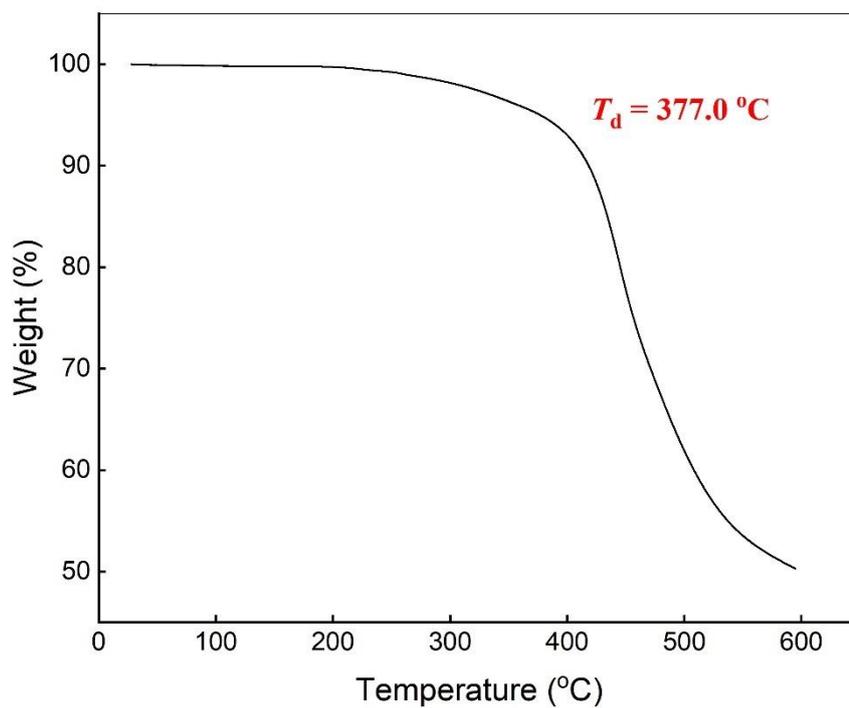


Figure S29. TGA curve of P13

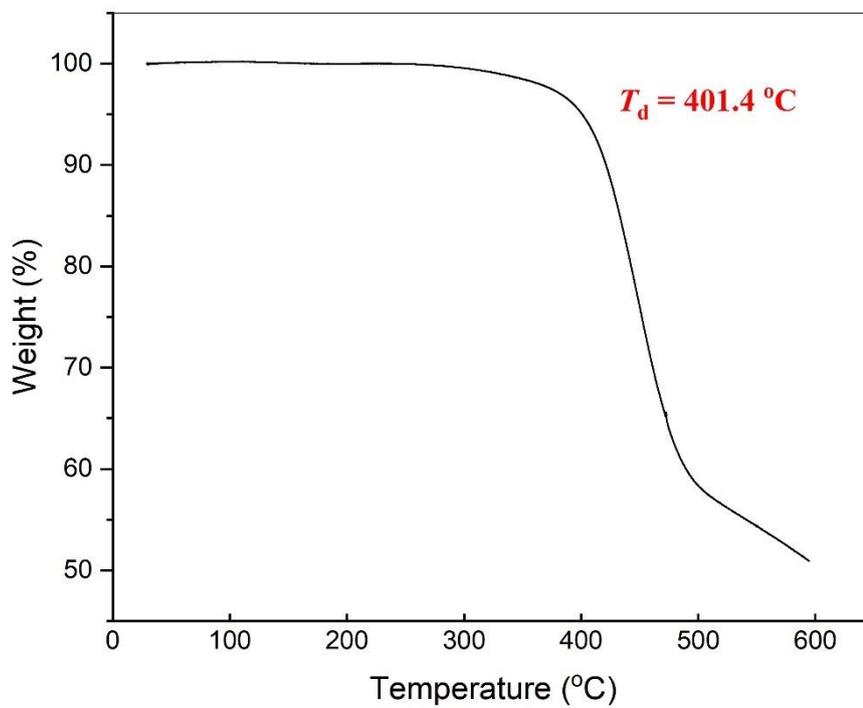


Figure S30. TGA curve of P14

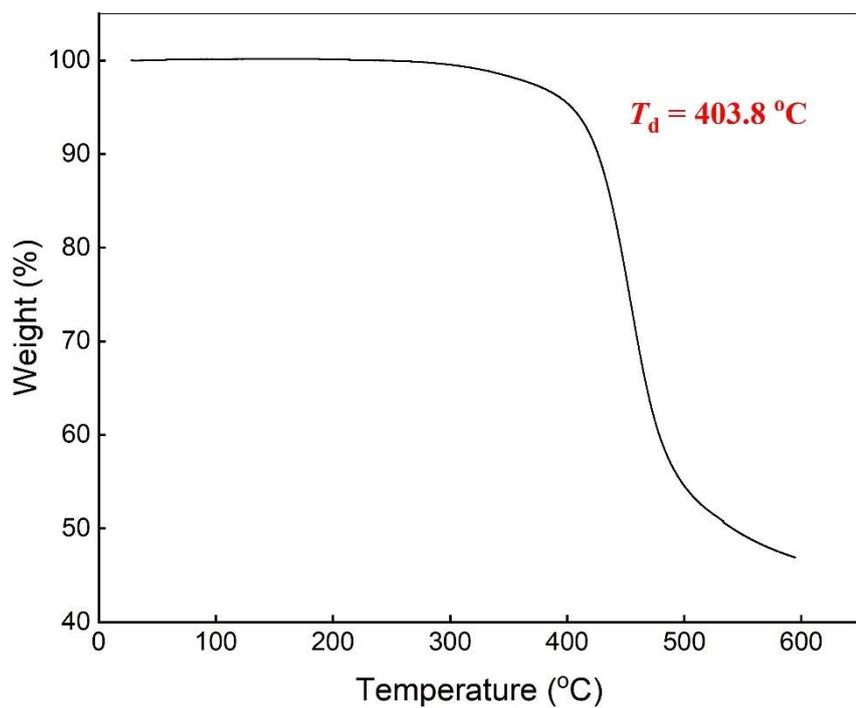


Figure S31. TGA curve of P15

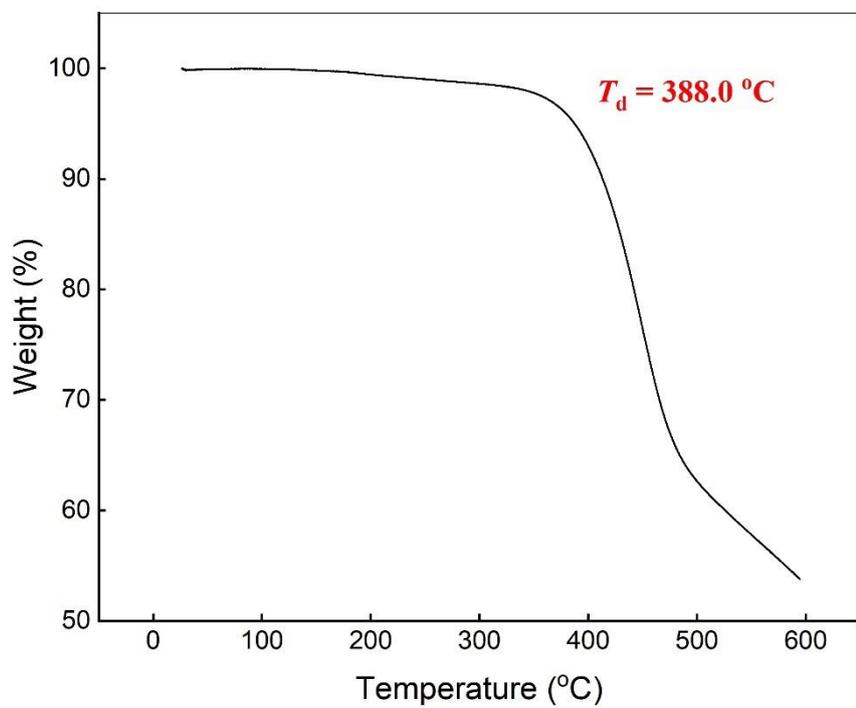


Figure S32. TGA curve of P16

15. DSC Curves.

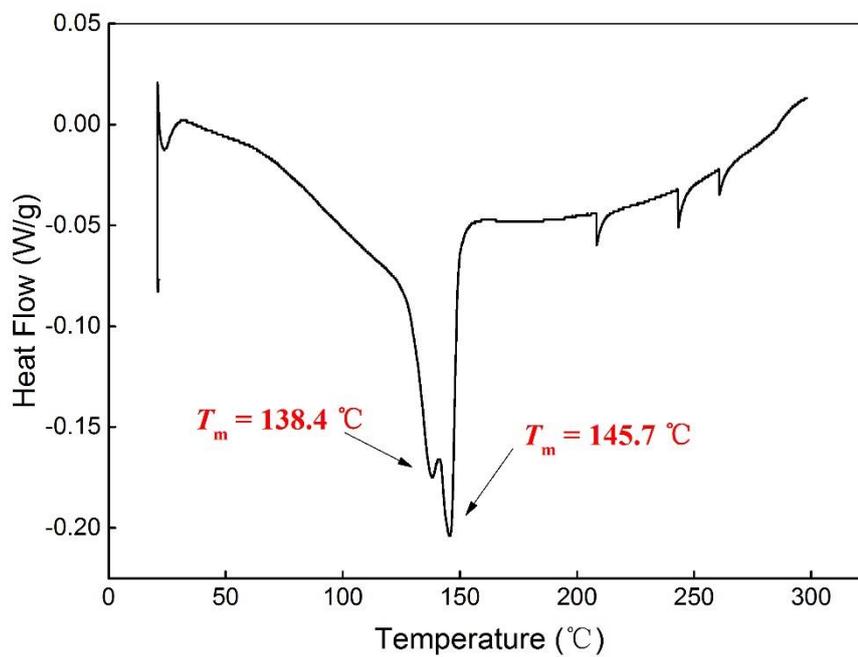


Figure S33. DSC curve of P1

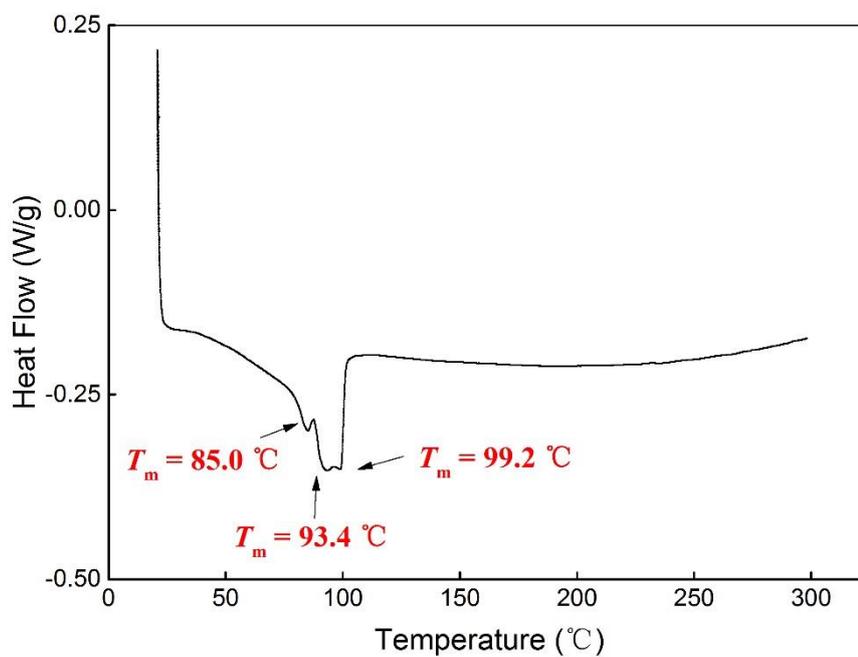


Figure S34. DSC curve of P2

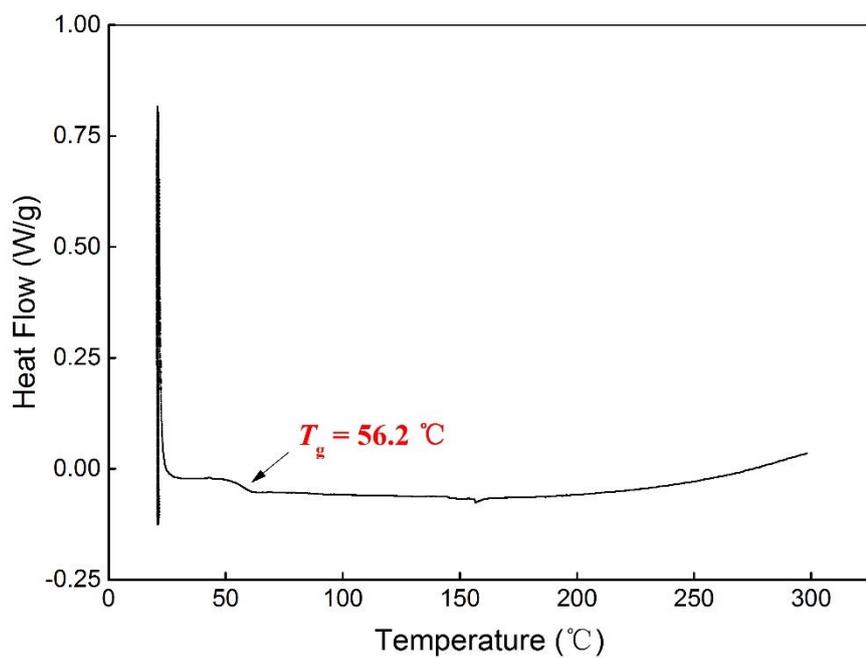


Figure S35. DSC curve of P3

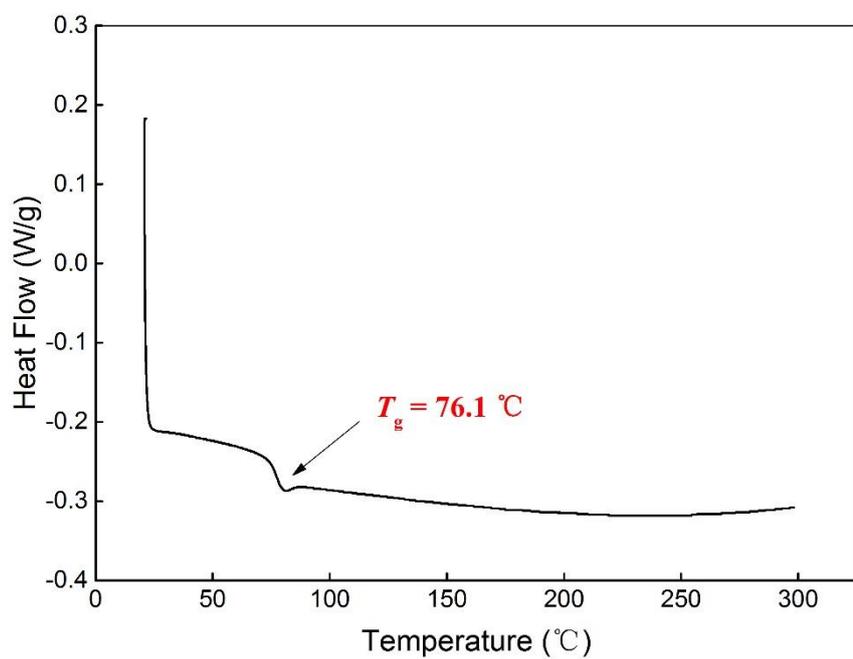


Figure S36. DSC curve of P4

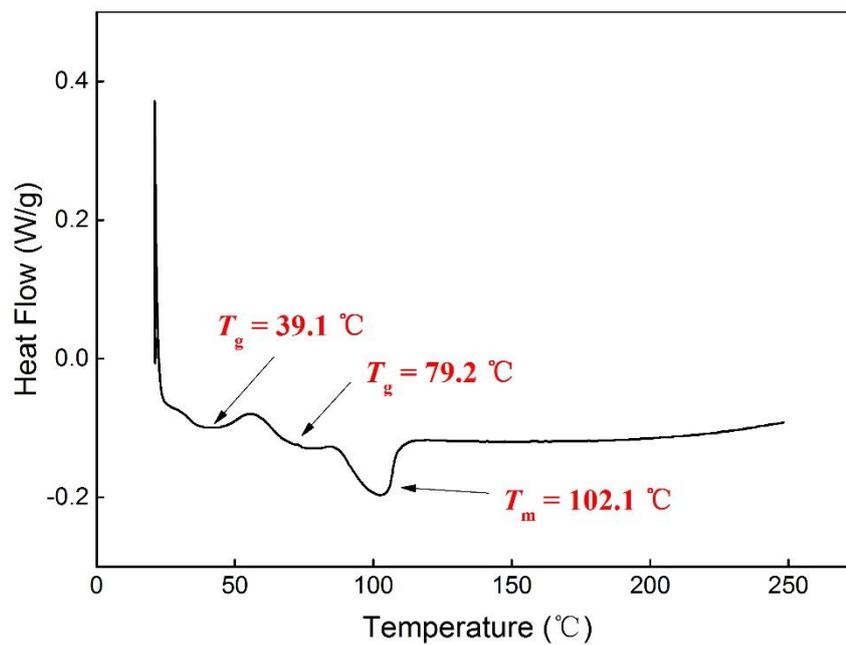


Figure S37. DSC curve of P5

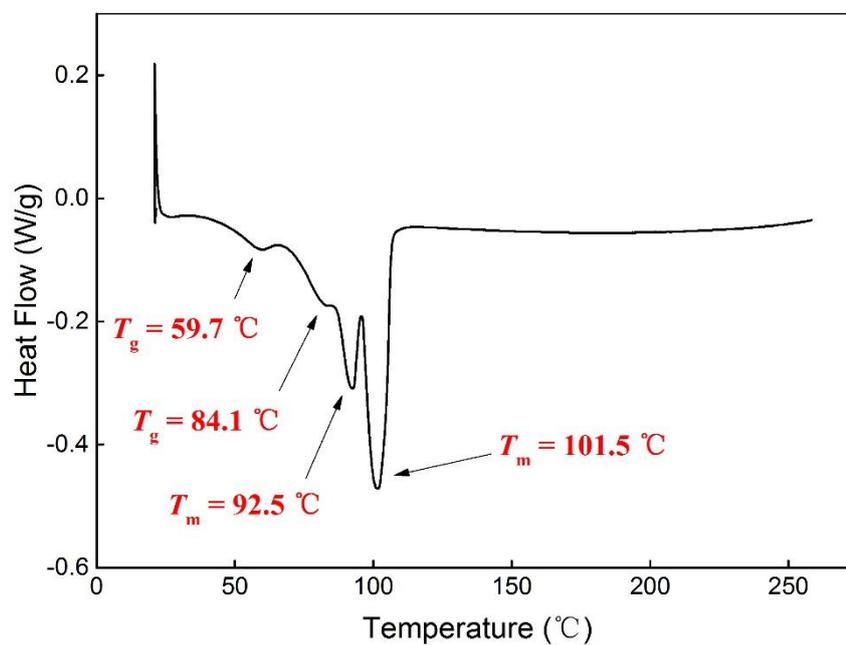


Figure S38. DSC curve of P6

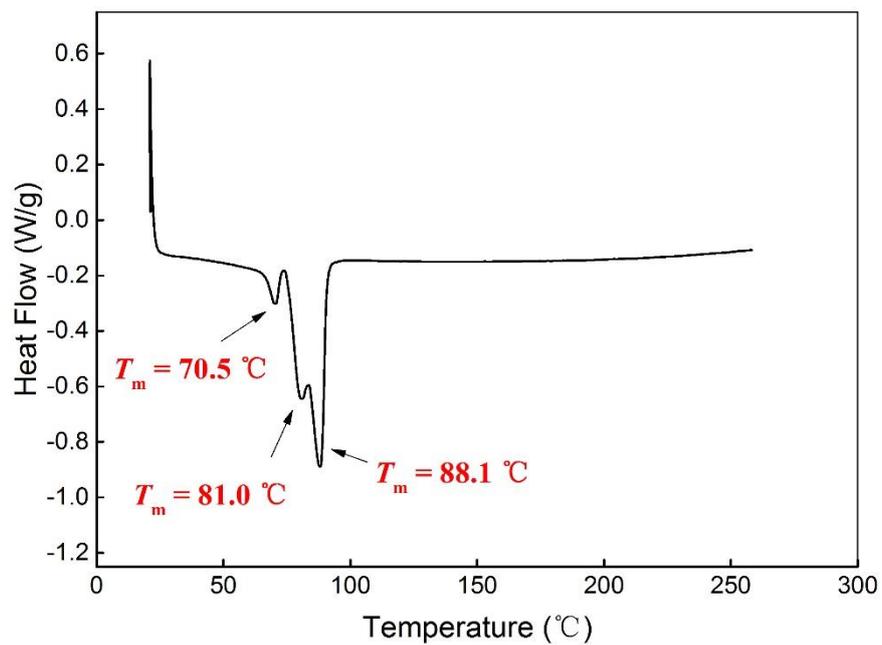


Figure S39. DSC curve of **P7**

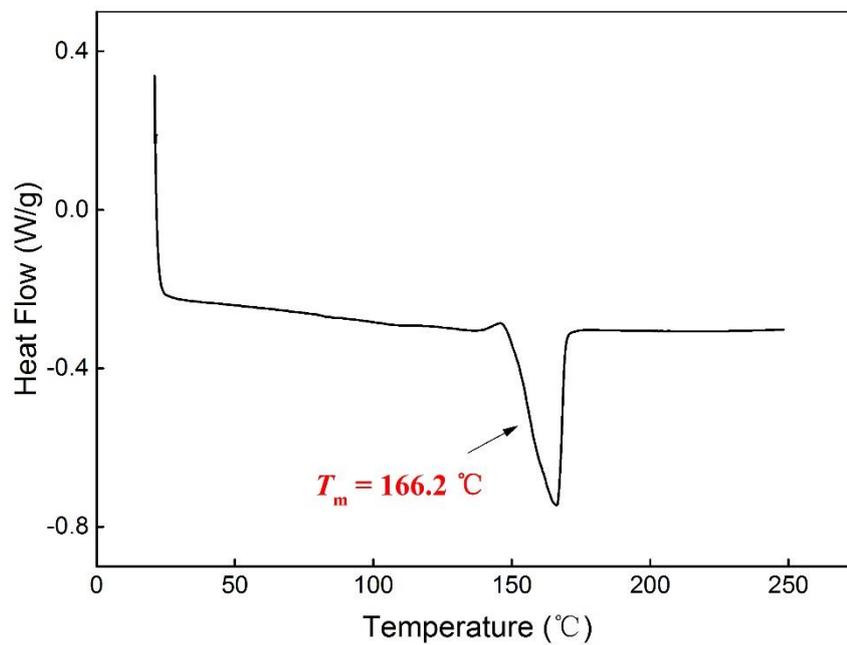


Figure S40. DSC curve of **P8**

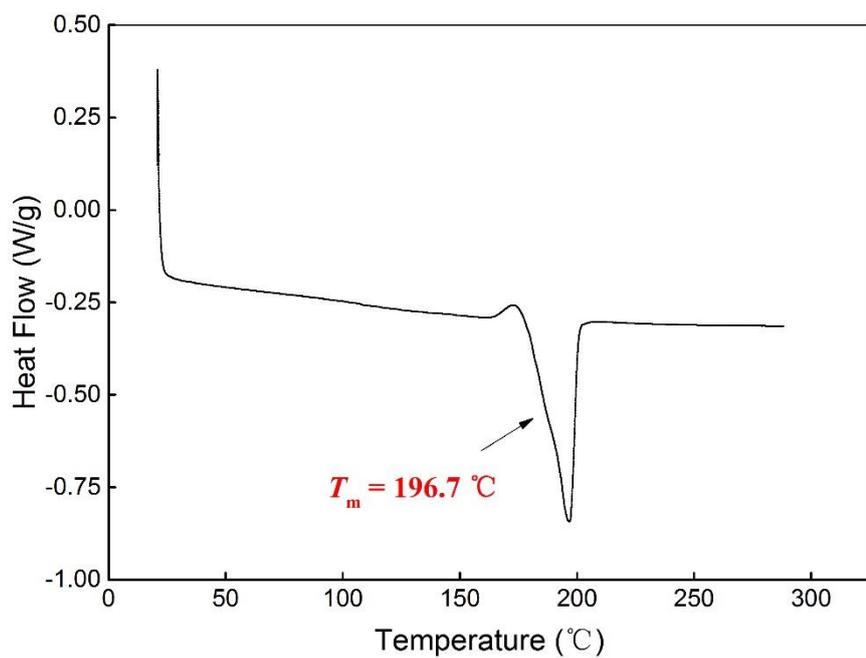


Figure S41. DSC curve of **P9**

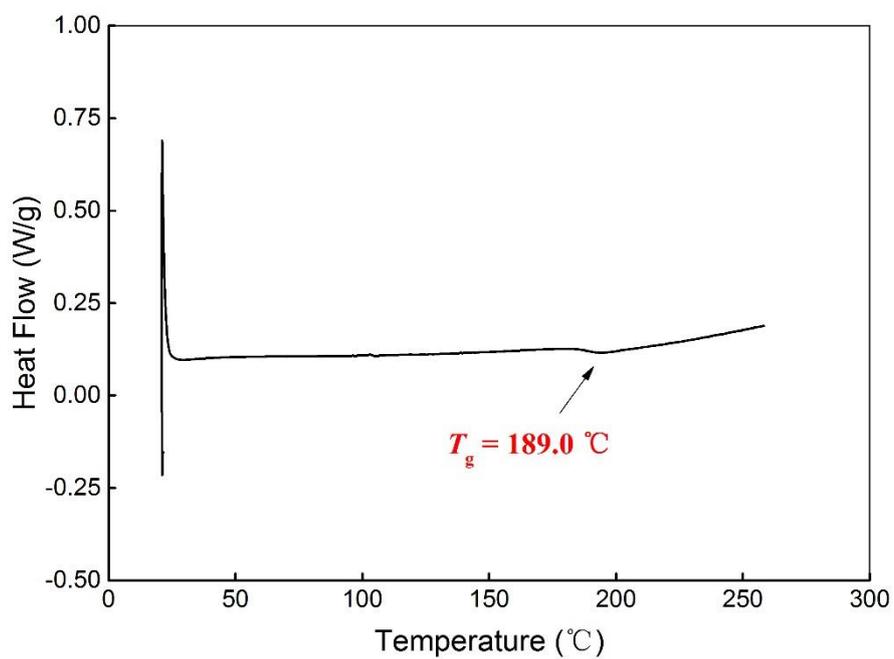


Figure S42. DSC curve of **P10**

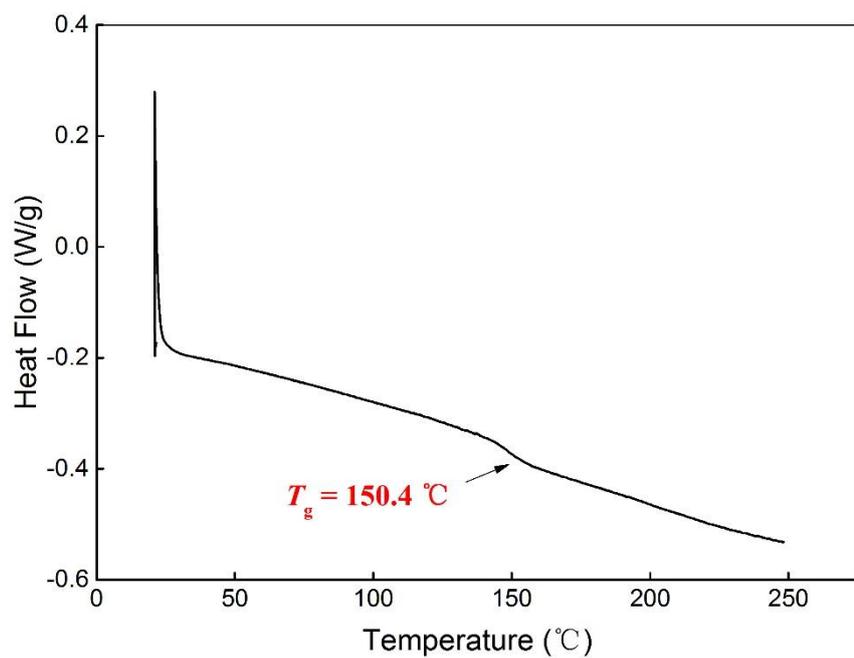


Figure S43. DSC curve of P11

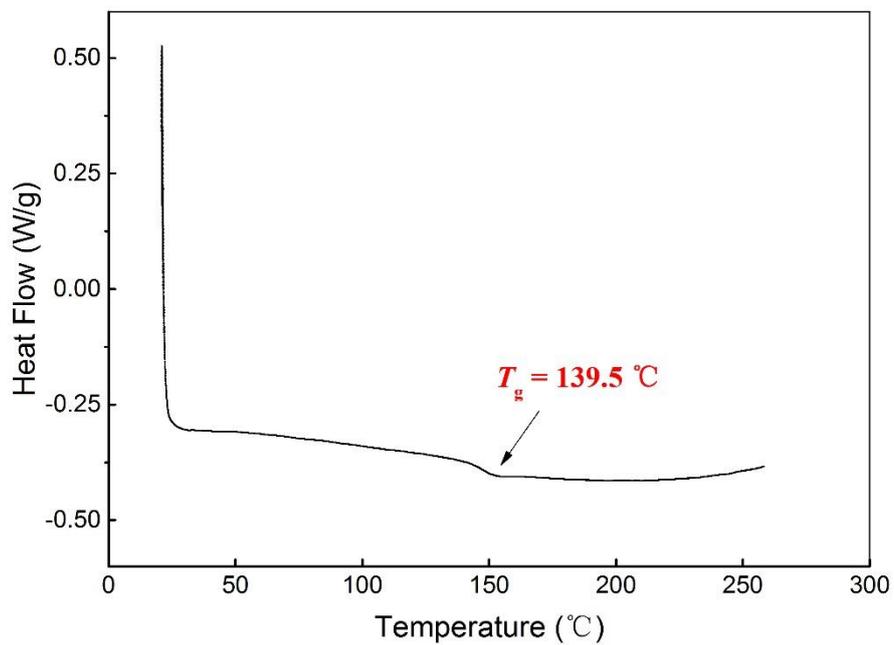


Figure S44. DSC curve of P12

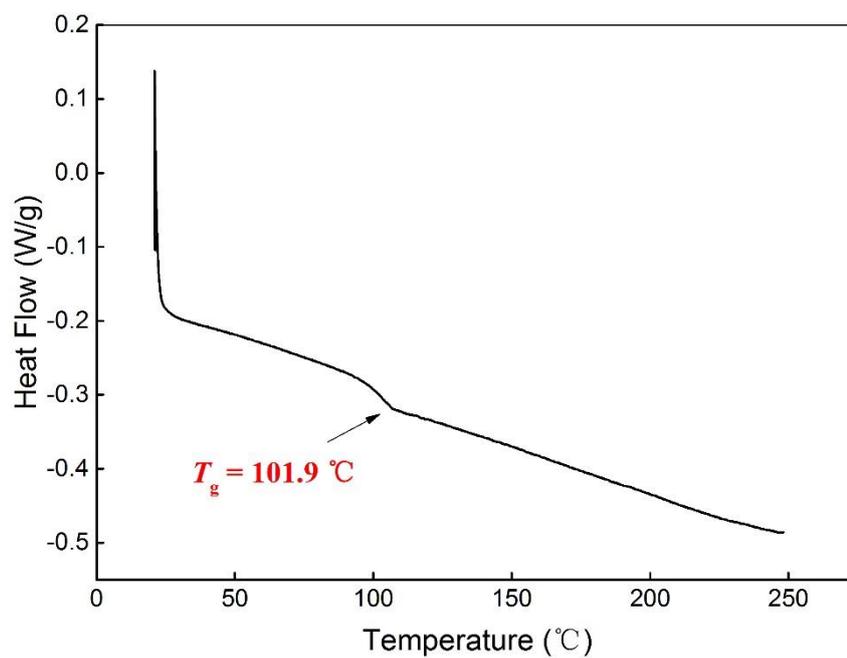


Figure S45. DSC curve of P13

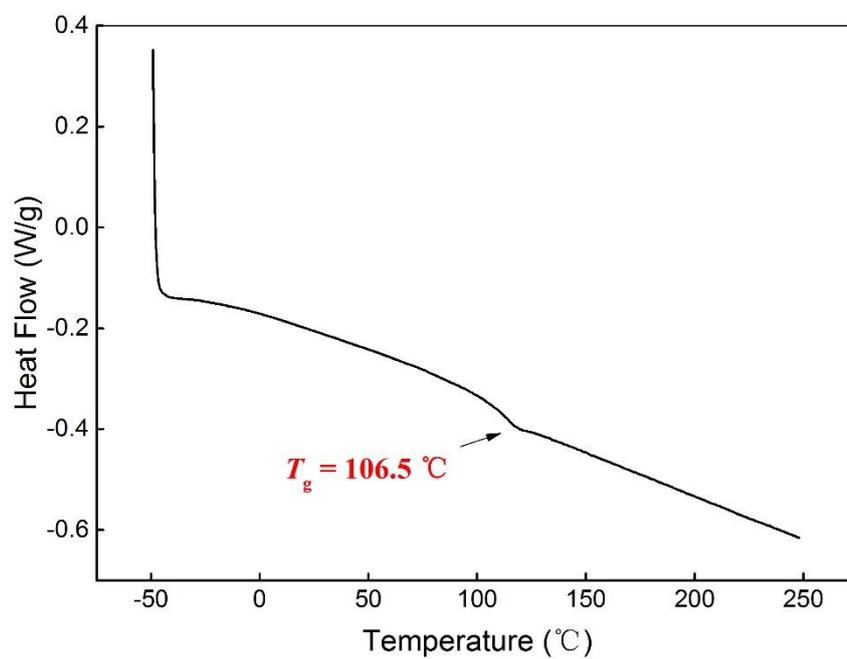


Figure S46. DSC curve of P14

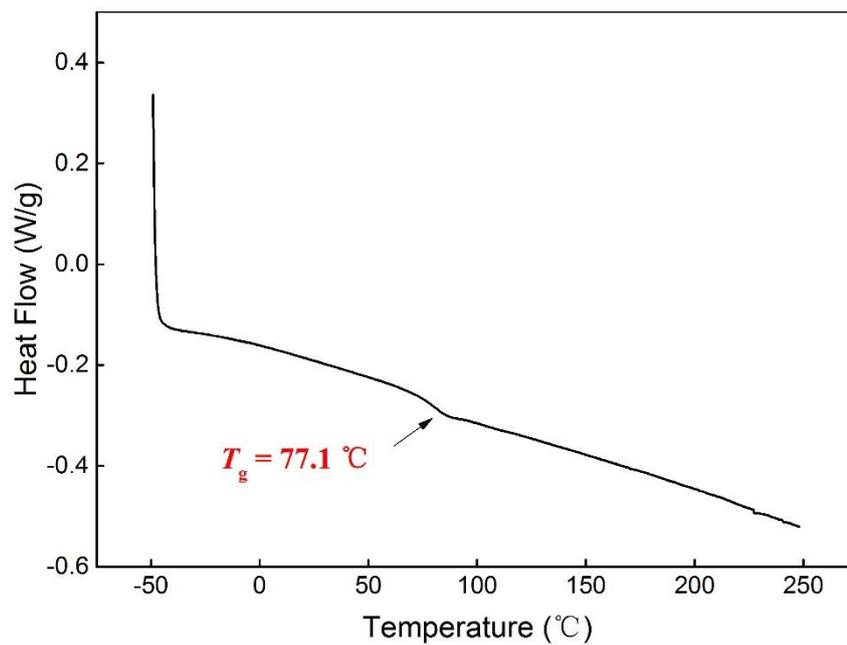


Figure S47. DSC curve of **P15**

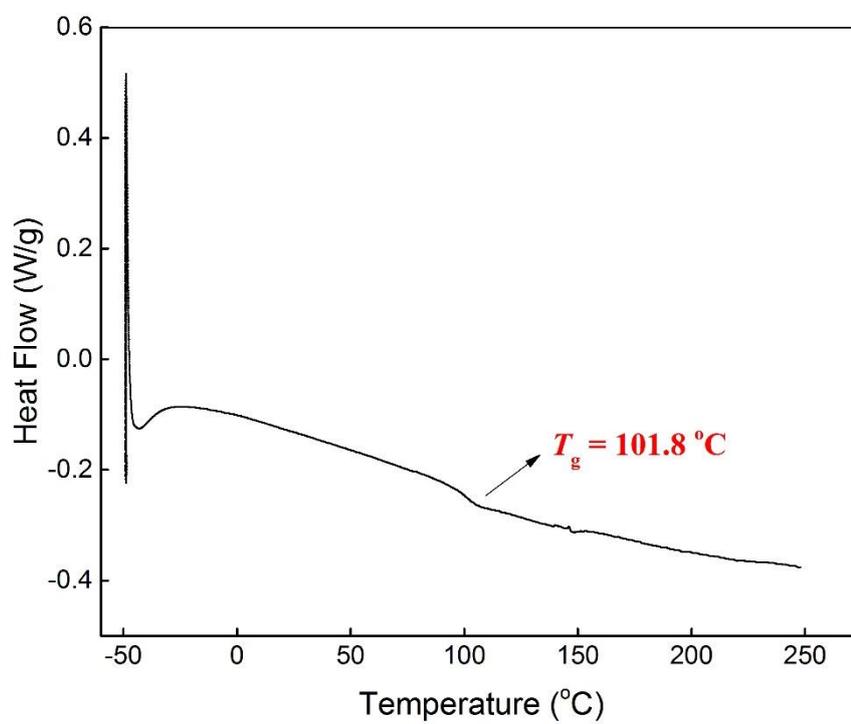


Figure S48. DSC curve of **P16**

16. Fluorescence Spectra.

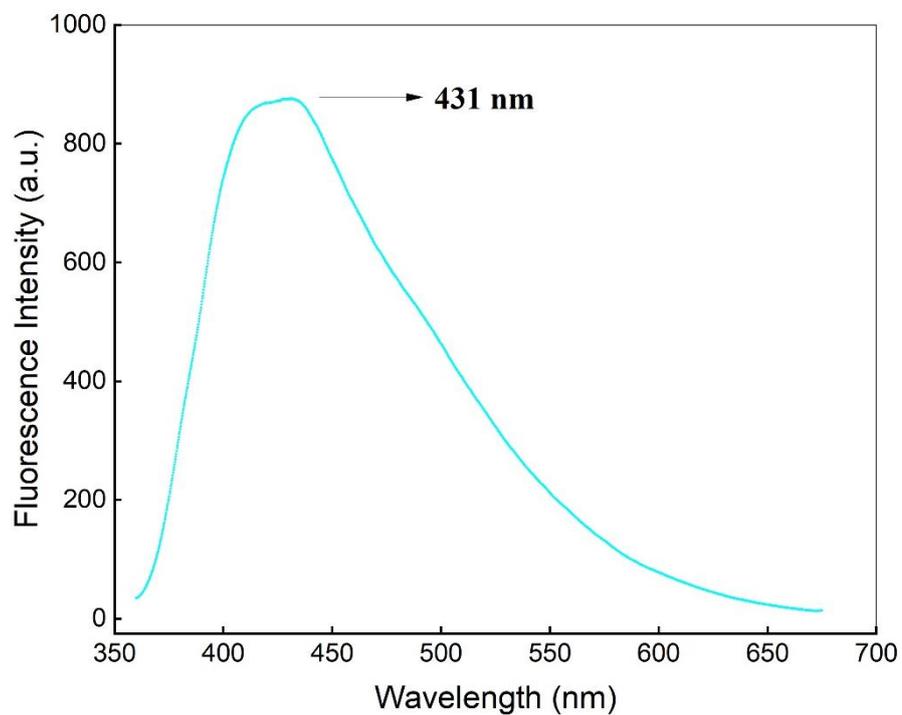


Figure S49. Fluorescence spectrum of **P10** ($\lambda_{\text{ex}} = 340$ nm).

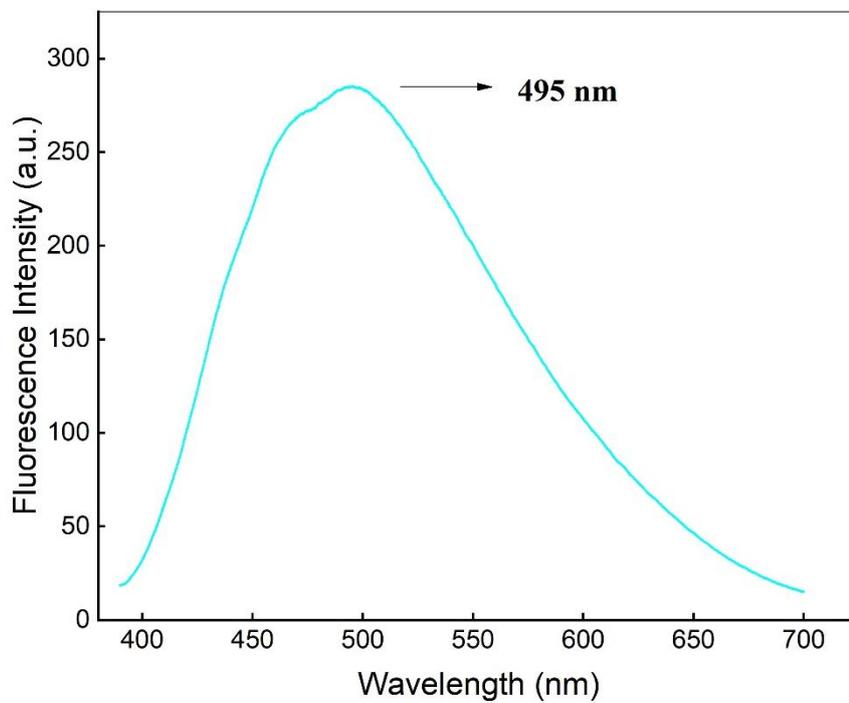


Figure S50. Fluorescence spectrum of **P11** ($\lambda_{\text{ex}} = 365$ nm).

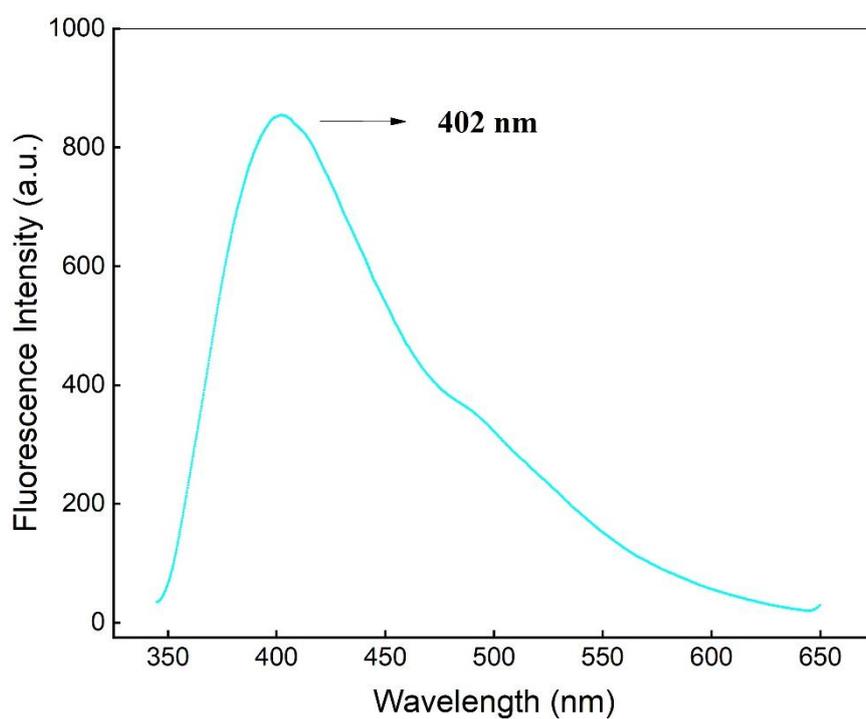


Figure S51. Fluorescence spectrum of **P12** ($\lambda_{\text{ex}} = 326$ nm).

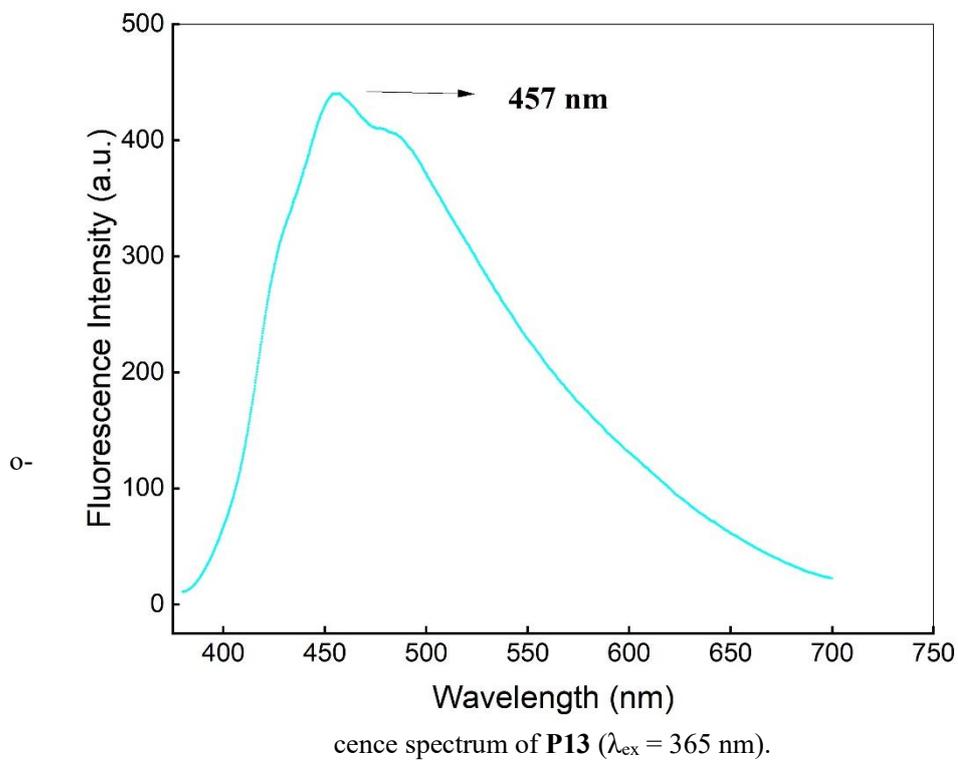


Figure S52. Fluorescence spectrum of **P13** ($\lambda_{\text{ex}} = 365$ nm).

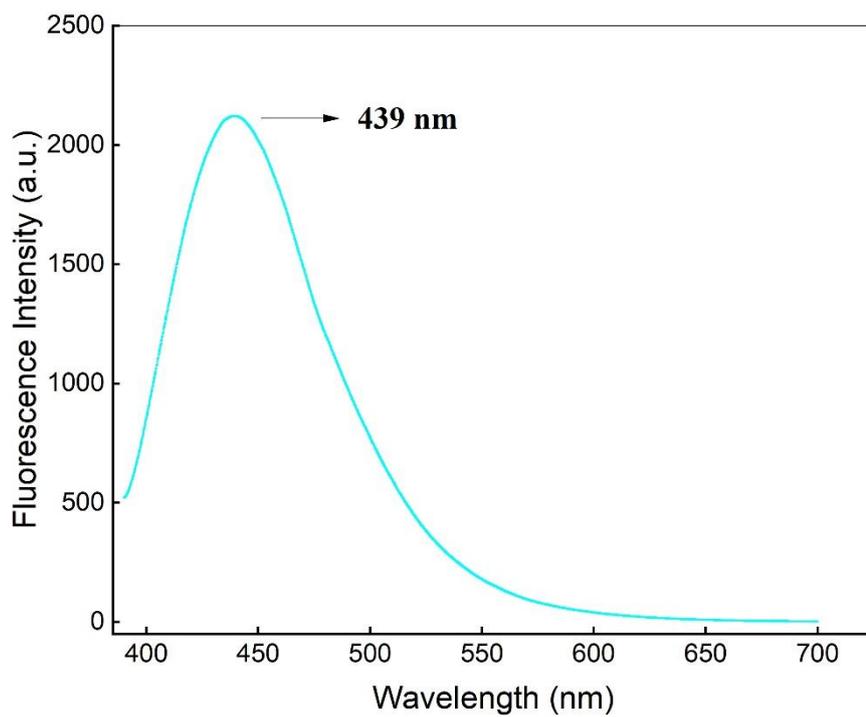


Figure S53. Fluorescence spectrum of **P14** ($\lambda_{\text{ex}} = 365$ nm).

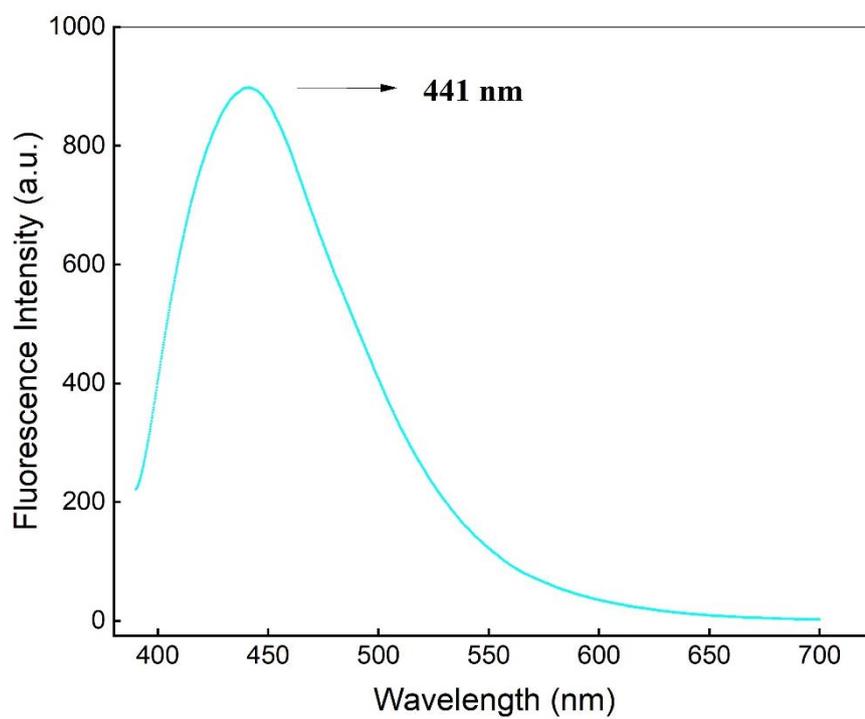


Figure S54. Fluorescence spectrum of **P15** ($\lambda_{\text{ex}} = 365$ nm).

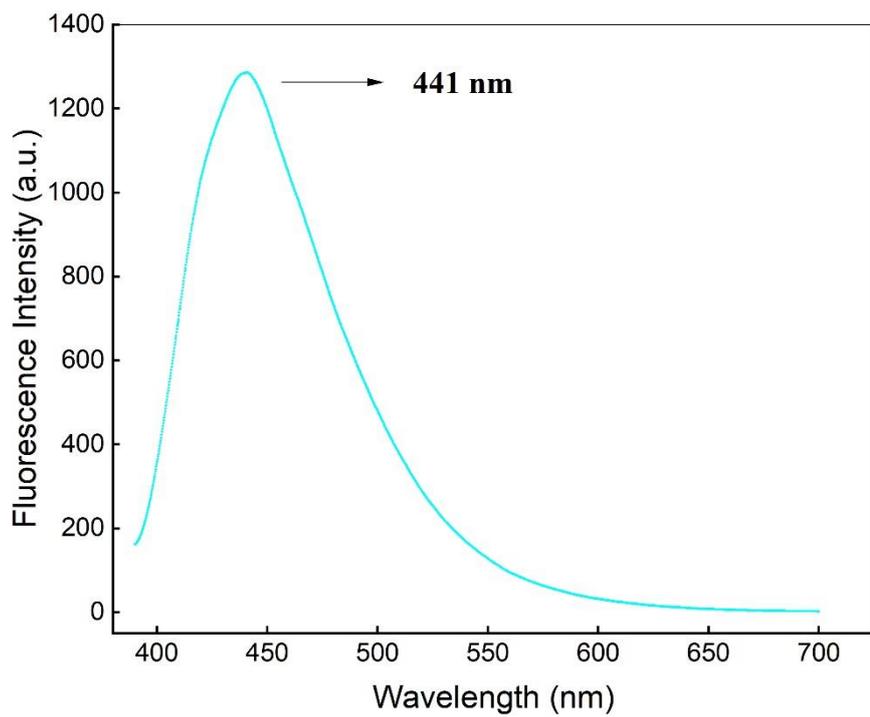


Figure S55. Fluorescence spectrum of **P16** ($\lambda_{\text{ex}} = 365$ nm).