

Electronic Supplementary Information (ESI)

Nickel-catalysed enantioselective cross- electrophile coupling reaction with the retention of β -fluorine atom

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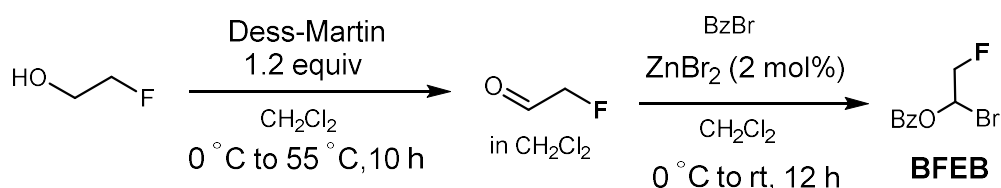
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1 General Information

^1H , ^{13}C and ^{19}F NMR spectra were recorded on Bruker AV 400 MHz instrument at 400 MHz (^1H NMR), 101 MHz (^{13}C NMR), and 376 MHz (^{19}F NMR), or Bruker AV 500 MHz instrument at 500 MHz (^1H NMR), 126 MHz (^{13}C NMR), 470 MHz (^{19}F NMR). Chemical shifts were reported in ppm downfield from internal Me_4Si and external CHCl_3 , respectively. Multiplicity was indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), qu (quintet), sex (sextet), sep (septet), m (multiplet), dd (doublet of doublet), and br (broad signal). Coupling constants were reported in Hertz (Hz). High resolution mass spectrometry (HRMS) spectra were obtained on a Bruker miorOTOF-QII instrument. Optical rotations were determined using an Autopol IV-T. HPLC analyses were carried out on Shimadzu Model LC-2030C 3D instrument or Shimadzu DGU-20A and was performed with Chiralpak® column (4.6 mm \times 250 mm \times 5 μm) using a Shimadzu HPLC system and was monitored using a UV-detector. X-ray structural analysis was conducted on the Bruker APEX-II CCD instrument.

Materials: Tetrahydrofuran (THF) was distilled from sodium/benzophenone prior to use; CH_2Cl_2 was distilled from calcium hydride. All purchased reagents were used without further purification. Thin-layer chromatography (TLC) was performed on precoated GF254 silica gel plates (Qingdao Marine Chemical Inc.) and compounds were visualized with a UV light at 254 nm. Flash chromatography separations were carried out using silica gel (200–300 mesh, Qingdao Marine Chemical Inc). The chiral ligands and the acid chlorides used in this study were purchased from commercial suppliers and used without further purification or were synthesized by ourselves from the reported literature.^[1-3] Other reagents used in this study were purchased from commercial suppliers and used without further purification.

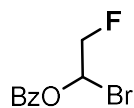
2 Synthesis of Brominated Fluoroethanol Benzoate (BFEB)



Dess-Martin reagent (30.54 g, 72 mmol, 1.2 equiv.) and DCM (150 mL) were added to a 250 mL Schlenk bottle containing a magnetic stirrer. The Schlenk bottle was placed in an ice water bath at 0 °C, the 2-fluoroethanol (3.84 g, 60 mmol, 1 equiv.) was slowly added while stirring. The reaction was stirred for 1 hour until the system turns milky white. Then the temperature of the system was raised to room temperature, and stirred for 9 hours. Then the temperature of the system was raised to 55 °C and reacted for 10 h. The DCM solution of fluoroacetaldehyde was obtained by low-temperature condensation at -17 °C and atmospheric distillation. Using trifluoromethoxybenzene as the internal standard, the concentration of fluoroacetaldehyde was determined by ¹⁹F-NMR (0.45 mol/L).

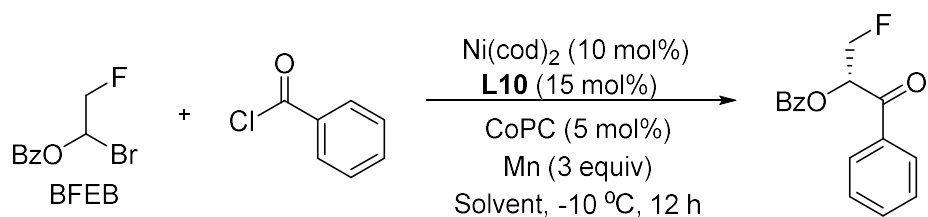
In a glove box, anhydrous zinc bromide (135.1 mg, 0.6 mmol, 0.02 equiv.) and DCM solvent (30 mL) were added to a 250 mL Schlenk bottle containing a magnetic stirrer, Then benzoyl bromide (5.55 g, 30 mmol, 1 equiv.) was added, and the system was sealed. The DCM solution of fluoroacetaldehyde (45 mmol, 1.5 equiv, DCM solution) was slowly add to the system under stirring conditions at 0 °C. Then the system was stirred at room temperature for 12 hours. The mixture was passed through a short column of diatomaceous earth to remove the inorganic salts. After evaporation under reduced pressure to remove the solvent, the residue was purified by flash chromatography on silica gel (PE : EA = 40: 1) to afford the brominated fluoroethanol benzoate (**BFEB**) (5.93 g, 80% yield). The reagent has stable properties and can be stored at room temperature for several months.

Brominated fluoroethanol benzoate (BFEB)

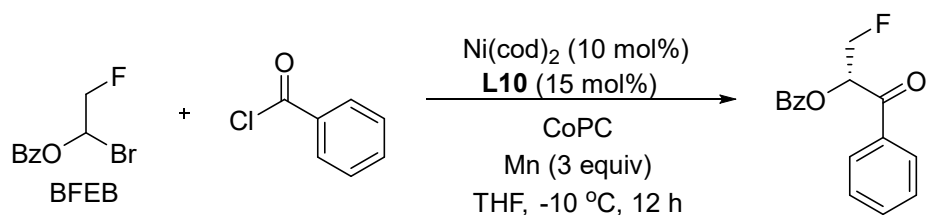


BFEB 5.93 g, 80% yield, PE : EA = 40: 1. White solid; m.p.: 65-66 °C; **¹H NMR** (400 MHz, CDCl₃) δ 8.13 – 8.06 (m, 2H), 7.63 (t, *J* = 7.5 Hz, 1H), 7.48 (t, *J* = 7.8 Hz, 2H), 7.00 (ddd, *J* = 11.0, 8.0, 3.1 Hz, 1H), 4.95 – 4.68 (m, 2H). **¹⁹F NMR** (376 MHz, Chloroform-*d*) δ -208.84 (td, *J* = 46.8, 10.3 Hz). **¹³C NMR** (101 MHz, CDCl₃) δ 164.1, 134.3, 130.3, 128.8, 128.4, 83.1 (d, *J* = 182.9 Hz), 70.9 (d, *J* = 23.6 Hz); **HRMS** (ESI) *m/z* calcd. for C₉H₈BrO₂FNa ([M+Na]⁺): 270.0526, found 270.0530.

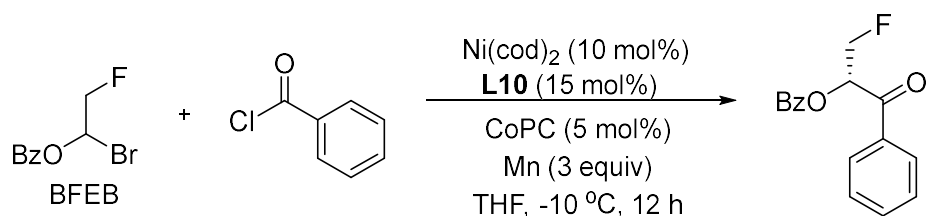
3 Selected reaction optimizations



Entry	Solvent	Yield (%)	ee (%)
1	DME	trace	-
2	MTBE	ND	-
3	Et ₂ O	ND	-
4	EtOAc	ND	-
5	CH ₃ OH	21	90
6	DCE	ND	-
7	toluene	ND	-

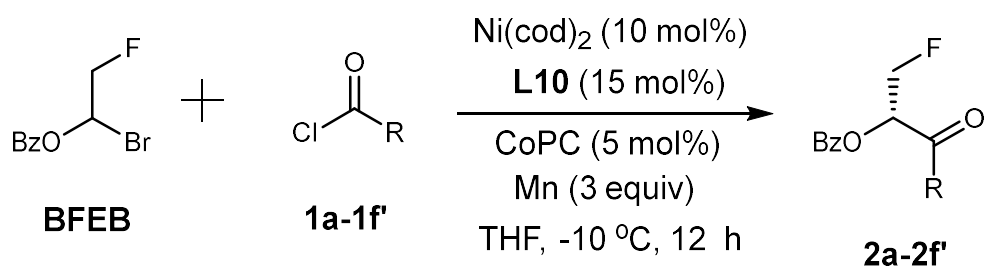


Entry	CoPC (mol%)	Yield (%)	ee (%)
1	2.5	76	91
2	5.0	81	93
3	7.5	82	92



Entry	THF (mL)	Yield (%)	ee (%)
1	0.5	82	93
2	1.0	81	93
3	1.5	78	92

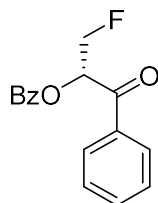
4 General Procedure for Synthesis of Products 2



In a glove box, $\text{Ni}(\text{cod})_2$ (2.8 mg, 0.01 mmol, 10 mol%), and **L10** (12.6 mg, 0.015 mmol, 15 mol%) were added into a 4 mL glass bottle in THF (1 mL). The mixture was stirred at room temperature for 30 mins, then brominated fluoroethanol benzoate (**BFEB**) (29.6 mg, 0.12 mmol, 1.2 equiv.), acid chlorides **1** (0.1 mmol, 1.0 equiv.), Mn (16.5 mg, 0.3 mmol, 3 equiv.), cobalt(II) phthalocyanine (CoPc) (2.9 mg, 0.005 mmol, 5 mol%) were added and keep stirring at $-10\text{ }^\circ\text{C}$ for 12 hours. After evaporation under reduced pressure to remove the solvent, the mixture was passed through a short column of silica gel to remove the metal complex. The residue was purified by flash chromatography on silica gel (PE : EA = 50: 1) to afford the desired chiral product **2**. The racemic products were obtained by employing **L1** as the ligand under otherwise identical conditions.

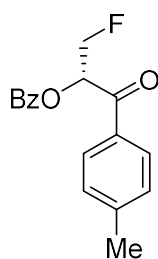
5 Characterization Data for New Compounds

(*S*)-3-fluoro-1-oxo-1-phenylpropan-2-yl benzoate (2a)



22.3 mg, 82% yield, 93% ee, PE : EA = 50: 1. White solid; m.p.: 104-105 °C; $[\alpha]_{\text{D}}^{25} = -60.8$ (*c* 1.0, CH₂Cl₂); **¹H NMR** (500 MHz, Chloroform-*d*) δ 7.92 (d, *J* = 7.7 Hz, 2H), 7.82 (d, *J* = 7.7 Hz, 2H), 7.41 (q, *J* = 7.2 Hz, 2H), 7.29 (dt, *J* = 15.4, 7.7 Hz, 4H), 6.19 (dt, *J* = 22.2, 4.5 Hz, 1H), 4.75 (dd, *J* = 47.0, 4.5 Hz, 2H). **¹⁹F NMR** (470 MHz, Chloroform-*d*) δ -228.36 (td, *J* = 46.9, 22.2 Hz). **¹³C NMR** (126 MHz, Chloroform-*d*) δ 193.3 (d, *J* = 6.6 Hz), 165.7, 134.7, 134.0, 133.7, 130.1, 128.9, 128.6, 128.5, 81.6 (d, *J* = 177.6 Hz), 74.9 (d, *J* = 20.2 Hz); **HRMS** (ESI) *m/z* calcd. for C₁₆H₁₃O₃FNa ([M+Na]⁺): 295.0746, found 295.0755; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IA, 0.8 mL/min, *n*-Hexane : *i*-PrOH =90:10, Rt (major) 12.03 min, Rt (minor) 15.28 min.

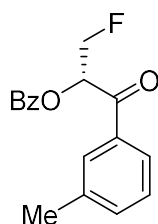
(*S*)-3-fluoro-1-oxo-1-(*p*-tolyl)propan-2-yl benzoate (2b)



22.3 mg, 78% yield, 88% ee, PE : EA = 50: 1. White solid; m.p.: 96-97 °C; $[\alpha]_{\text{D}}^{25} = -38.6$ (*c* 1.0, CH₂Cl₂); **¹H NMR** (500 MHz, Chloroform-*d*) δ 7.97 – 7.87 (m, 2H), 7.76 – 7.70 (m, 2H), 7.43 – 7.36 (m, 1H), 7.27 (t, *J* = 7.9 Hz, 2H), 7.10 (d, *J* = 8.0 Hz, 2H), 6.19 (dt, *J* = 21.8, 4.5 Hz, 1H), 4.74 (dd, *J* = 47.0, 4.5 Hz, 2H), 2.22 (s, 3H). **¹⁹F NMR** (470 MHz, Chloroform-*d*) δ -228.28 (td, *J* = 47.0, 21.9 Hz). **¹³C NMR** (126 MHz,

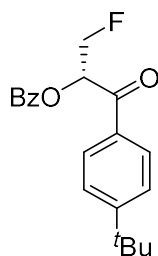
Chloroform-*d*) δ 193.3 (d, $J = 6.8$ Hz), 166.3, 145.8, 134.20, 132.7, 130.6, 130.2, 129.6, 129.3, 129.1, 82.3 (d, $J = 177.6$ Hz), 75.4 (d, $J = 20.2$ Hz), 22.3; **HRMS** (ESI) m/z calcd. for $C_{17}H_{15}O_3FNa$ ($[M+Na]^+$): 309.0903, found 309.0909; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, *n*-Hexane : *i*PrOH =90:10, Rt (major) 8.71 min, Rt (minor) 11.09 min.

(S)-3-fluoro-1-oxo-1-(*m*-tolyl)propan-2-yl benzoate (2c)



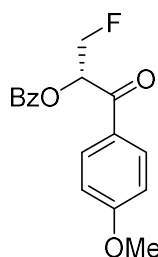
23.5 mg, 82% yield, 88% ee, PE : EA = 50: 1. White solid; m.p.: 102-103 °C; $[\alpha]_D^{25} = -38.4$ (*c* 1.0, CH_2Cl_2); **1H NMR** (500 MHz, Chloroform-*d*) δ 7.94 – 7.82 (m, 2H), 7.57 (d, $J = 8.4$ Hz, 2H), 7.35 (td, $J = 7.5, 1.4$ Hz, 1H), 7.22 (t, $J = 7.9$ Hz, 2H), 7.18 (d, $J = 7.8$ Hz, 1H), 7.14 (t, $J = 7.5$ Hz, 1H), 6.14 (dt, $J = 22.4, 4.5$ Hz, 1H), 4.69 (dd, $J = 47.0, 4.5$ Hz, 2H), 2.17 (s, 3H). **^{19}F NMR** (470 MHz, Chloroform-*d*) δ -228.19 (td, $J = 46.9, 22.4$ Hz). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 194.1 (d, $J = 6.6$ Hz), 166.4, 139.6, 135.6, 135.4, 134.4, 130.8, 129.8, 129.7, 129.5, 129.2, 126.5, 82.4 (d, $J = 177.6$ Hz), 75.7 (d, $J = 20.2$ Hz), 22.1; **HRMS** (ESI) m/z calcd. for $C_{17}H_{15}O_3FNa$ ($[M+Na]^+$): 309.0903, found 309.0910; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, *n*-Hexane : *i*PrOH =90:10, Rt (major) 8.03 min, Rt (minor) 9.56 min.

(S)-1-(4-(*tert*-butyl)phenyl)-3-fluoro-1-oxopropan-2-yl benzoate (2d)



25.3 mg, 77% yield, 91% ee, PE : EA = 50: 1. White solid; m.p.: 100-101 °C; $[\alpha]_D^{25} = -29.4$ (*c* 1.0, CH₂Cl₂); **¹H NMR** (500 MHz, Chloroform-*d*) δ 7.96 – 7.91 (m, 2H), 7.81 – 7.76 (m, 2H), 7.40 (dt, *J* = 7.7, 3.7 Hz, 1H), 7.35 – 7.30 (m, 2H), 7.30 – 7.23 (m, 2H), 6.22 (dt, *J* = 21.6, 4.6 Hz, 1H), 4.98 – 4.56 (m, 2H), 1.15 (s, 9H). **¹⁹F NMR** (470 MHz, Chloroform-*d*) δ -228.19 (td, *J* = 46.8, 21.6 Hz). **¹³C NMR** (126 MHz, Chloroform-*d*) δ 193.2 (d, *J* = 6.8 Hz), 166.4, 158.8, 134.3, 132.7, 130.8, 129.7, 129.3, 129.2, 126.7, 82.4 (d, *J* = 177.8 Hz), 75.4 (d, *J* = 20.2 Hz), 36.0, 31.7; **HRMS** (ESI) *m/z* calcd. for C₂₀H₂₁O₃FNa ([M+Na]⁺): 351.1372, found 351.1378; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, *n*-Hexane : ^tPrOH =90:10, R_t (major) 7.17 min, R_t (minor) 9.45 min.

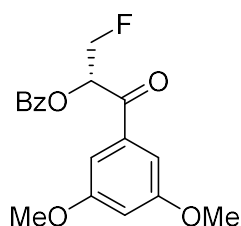
(S)-3-fluoro-1-(4-methoxyphenyl)-1-oxopropan-2-yl benzoate (2e)



20.3 mg, 67% yield, 92% ee, PE : EA = 50: 1. White solid; m.p.: 95-96 °C; $[\alpha]_D^{25} = -48.2$ (*c* 1.0, CH₂Cl₂); **¹H NMR** (500 MHz, Chloroform-*d*) δ 8.14 – 8.09 (m, 2H), 8.04 – 7.99 (m, 2H), 7.62 – 7.55 (m, 1H), 7.46 (ddt, *J* = 8.5, 6.5, 1.2 Hz, 2H), 6.99 – 6.93 (m, 2H), 6.37 (dt, *J* = 21.2, 4.7 Hz, 1H), 4.92 (dd, *J* = 47.0, 4.7 Hz, 2H), 3.86 (s, 3H). **¹⁹F NMR** (470 MHz, Chloroform-*d*) δ -228.14 (td, *J* = 46.9, 21.3 Hz). **¹³C NMR** (126 MHz, Chloroform-*d*) δ 191.4 (d, *J* = 7.3 Hz), 165.7, 164.3, 133.6, 131.1, 130.1, 129.0, 128.5, 127.5, 114.2, 81.8 (d, *J* = 177.7 Hz), 74.5 (d, *J* = 19.9 Hz), 55.6; **HRMS** (ESI)

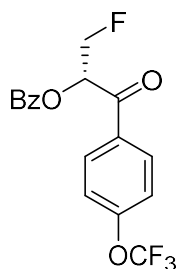
m/z calcd. for $C_{17}H_{15}O_4FNa$ ($[M+Na]^+$): 325.0852, found 325.0860; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, *n*-Hexane : *i*-PrOH =90:10, R_t (major) 13.12 min, R_t (minor) 16.75 min.

(*S*)-1-(3,5-dimethoxyphenyl)-3-fluoro-1-oxopropan-2-yl benzoate (2f)



27.9 mg, 84% yield, 96% ee, PE : EA = 50: 1. White solid; m.p.: 50-51 °C; $[\alpha]_D^{25} = -14.4$ (c 1.0, CH_2Cl_2); 1H NMR (500 MHz, Chloroform-*d*) δ 8.15 – 8.07 (m, 2H), 7.59 (ddt, $J = 8.8, 7.2, 1.3$ Hz, 1H), 7.52 – 7.40 (m, 2H), 7.13 (d, $J = 2.3$ Hz, 2H), 6.68 (t, $J = 2.3$ Hz, 1H), 6.32 (dt, $J = 22.3, 4.4$ Hz, 1H), 4.93 (dd, $J = 47.0, 4.4$ Hz, 2H), 3.81 (s, 6H). ^{19}F NMR (470 MHz, Chloroform-*d*) δ -228.41 (td, $J = 47.1, 22.2$ Hz). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 192.9 (d, $J = 6.8$ Hz), 165.7, 161.1, 136.4, 133.7, 130.1, 128.9, 128.5, 106.5, 106.2, 81.7 (d, $J = 177.8$ Hz), 74.9 (d, $J = 20.2$ Hz), 55.6; HRMS (ESI) m/z calcd. for $C_{18}H_{17}O_5FNa$ ($[M+Na]^+$): 355.0958, found 355.0965; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, *n*-Hexane : *i*-PrOH =90:10, R_t (major) 13.15 min, R_t (minor) 11.97 min.

(*S*)-3-fluoro-1-oxo-1-(4-(trifluoromethoxy)phenyl)propan-2-yl benzoate (2g)

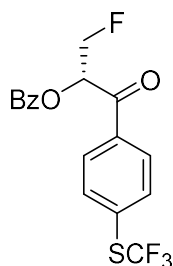


28.5 mg, 80% yield, 95% ee, PE : EA = 50: 1. White solid; m.p.: 63-64 °C; $[\alpha]_D^{25} = -44.0$ (c 1.0, CH_2Cl_2); 1H NMR (500 MHz, Chloroform-*d*) δ 7.95 – 7.85 (m, 4H), 7.46

- 7.38 (m, 1H), 7.28 (t, $J = 7.8$ Hz, 2H), 7.16 – 7.09 (m, 2H), 6.10 (ddd, $J = 22.4, 4.9, 3.9$ Hz, 1H), 4.91 – 4.57 (m, 2H). ^{19}F NMR (470 MHz, Chloroform- d) δ -57.60, -228.57 (tdd, $J = 47.2, 22.6, 4.3$ Hz). ^{13}C NMR (126 MHz, Chloroform- d) δ 193.0 (d, $J = 6.0$ Hz), 166.4, 154.0, 134.6, 133.6, 131.5, 130.8, 129.4, 129.3, 121.3, 121.0 (q, $J = 259.3$ Hz), 82.3 (d, $J = 177.3$ Hz), 75.6 (d, $J = 20.7$ Hz); HRMS (ESI) m/z calcd. for $\text{C}_{17}\text{H}_{12}\text{O}_4\text{F}_4\text{Na}$ ($[\text{M}+\text{Na}]^+$): 379.0569, found 379.0572; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, n -Hexane : i PrOH =90:10, Rt (major) 7.64 min, Rt (minor) 9.88 min.

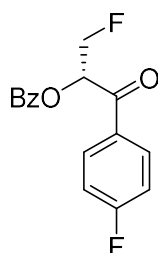
(*S*)-3-fluoro-1-oxo-1-(4-((trifluoromethyl)thio)phenyl)propan-2-yl

benzoate (2h)



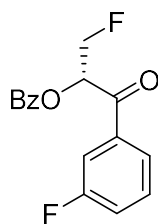
19.7 mg, 53% yield, 92% ee, PE : EA = 50: 1. White solid; m.p.: 66-67 °C; $[\alpha]_{\text{D}}^{25} = -33.4$ (c 1.0, CH_2Cl_2); ^1H NMR (500 MHz, Chloroform- d) δ 7.97 – 7.93 (m, 2H), 7.90 (d, $J = 8.4$ Hz, 2H), 7.63 (d, $J = 8.1$ Hz, 2H), 7.50 – 7.45 (m, 1H), 7.33 (t, $J = 7.8$ Hz, 2H), 6.14 (ddd, $J = 22.7, 5.1, 3.7$ Hz, 1H), 4.82 (ddd, $J = 46.9, 4.4, 2.9$ Hz, 2H). ^{19}F NMR (470 MHz, Chloroform- d) δ -41.48, -228.61 (td, $J = 46.9, 22.7$ Hz). ^{13}C NMR (126 MHz, Chloroform- d) δ 193.9 (d, $J = 6.0$ Hz), 166.4, 137.0, 136.4, 134.6, 131.9 (d, $J = 2.3$ Hz), 129.9 (q, $J = 309.96$ Hz), 130.8, 130.0, 129.3, 129.3, 82.2 (d, $J = 177.5$ Hz), 75.7 (d, $J = 20.7$ Hz); HRMS (ESI) m/z calcd. for $\text{C}_{17}\text{H}_{12}\text{O}_3\text{F}_4\text{NaS}$ ($[\text{M}+\text{Na}]^+$): 395.0341, found 395.0339; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, n -Hexane : i PrOH =90:10, Rt (major) 8.57 min, Rt (minor) 12.02 min.

(S)-3-fluoro-1-(4-fluorophenyl)-1-oxopropan-2-yl benzoate(2i)



12.8 mg, 44% yield, 90% ee, PE : EA = 50: 1. White solid; m.p.: 81-82 °C; $[\alpha]_D^{25} = -76.4$ (*c* 1.0, CH₂Cl₂); ¹H NMR (500 MHz, Chloroform-*d*) δ 7.89 – 7.79 (m, 4H), 7.36 (t, *J* = 7.5 Hz, 1H), 7.22 (t, *J* = 7.7 Hz, 2H), 6.92 (t, *J* = 8.4 Hz, 2H), 6.07 (dt, *J* = 22.3, 4.5 Hz, 1H), 4.70 (dd, *J* = 47.0, 4.6 Hz, 2H). ¹⁹F NMR (470 MHz, Chloroform-*d*) δ -103.02 (tt, *J* = 8.8, 5.1 Hz), -228.44 (td, *J* = 46.9, 22.4 Hz). ¹³C NMR (126 MHz, Chloroform-*d*) δ 192.8 (d, *J* = 6.3 Hz), 166.9 (d, *J* = 256.7 Hz), 166.4, 134.5, 132.1 (d, *J* = 9.6 Hz), 131.8 (d, *J* = 3.1 Hz), 130.8, 129.5, 129.3, 116.9 (d, *J* = 22.1 Hz), 82.3 (d, *J* = 177.3 Hz), 75.5 (d, *J* = 20.4 Hz). HRMS (ESI) *m/z* calcd. for C₁₆H₁₂O₃F₂Na ([M+Na]⁺): 313.0652, found 313.0661; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, *n*-Hexane : ⁱPrOH =90:10, Rt (major) 9.28 min, Rt (minor) 10.88 min.

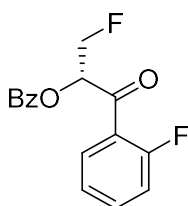
(S)-3-fluoro-1-(3-fluorophenyl)-1-oxopropan-2-yl benzoate (2j)



18.6 mg, 64% yield, 94% ee, PE : EA = 50: 1. White solid; m.p.: 56-57 °C; $[\alpha]_D^{25} = -57.8$ (*c* 1.0, CH₂Cl₂); ¹H NMR (500 MHz, Chloroform-*d*) δ 7.87 (d, *J* = 7.9 Hz, 2H), 7.57 (d, *J* = 7.7 Hz, 1H), 7.47 (dt, *J* = 9.1, 2.2 Hz, 1H), 7.37 (t, *J* = 7.5 Hz, 1H), 7.23 (td, *J* = 8.1, 2.6 Hz, 3H), 7.07 (td, *J* = 8.2, 2.8 Hz, 1H), 6.05 (dt, *J* = 22.6, 4.4 Hz, 1H), 4.83 – 4.60 (m, 2H). ¹⁹F NMR (470 MHz, Chloroform-*d*) δ -110.87 (td, *J* = 8.8, 5.4 Hz), -228.49 (td, *J* = 46.8, 22.5 Hz). ¹³C NMR (126 MHz, Chloroform-*d*) δ 193.2 (dd, *J* =

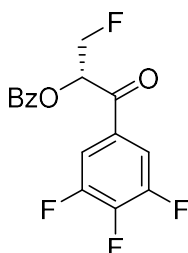
6.4, 2.3 Hz), 166.4, 163.6 (d, $J = 249.0$ Hz), 137.4 (d, $J = 6.5$ Hz), 134.5, 131.4 (d, $J = 7.4$ Hz), 130.8, 129.4, 129.3, 125.0 (d, $J = 3.2$ Hz), 121.8 (d, $J = 21.6$ Hz), 116.2 (d, $J = 22.8$ Hz), 82.2 (d, $J = 177.4$ Hz), 75.7 (d, $J = 20.7$ Hz); **HRMS** (ESI) m/z calcd. for $C_{16}H_{12}O_3F_2Na$ ($[M+Na]^+$): 313.0652, found 313.0660; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, *n*-Hexane : *i*PrOH =90:10, Rt (major) 8.61 min, Rt (minor) 10.01 min.

(*S*)-3-fluoro-1-(2-fluorophenyl)-1-oxopropan-2-yl benzoate (2k)



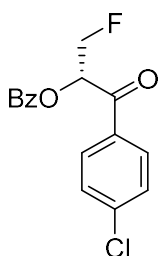
22.4 mg, 77% yield, 85% ee, PE : EA = 50: 1. White solid; m.p.: 48-49 °C; $[\alpha]_D^{25} = -89.0$ (c 1.0, CH_2Cl_2); **1H NMR** (500 MHz, Chloroform-*d*) δ 8.11 (d, $J = 7.8$ Hz, 2H), 7.92 (td, $J = 7.5, 1.8$ Hz, 1H), 7.59 (td, $J = 7.3, 5.4$ Hz, 2H), 7.46 (t, $J = 7.7$ Hz, 2H), 7.29 (t, $J = 7.6$ Hz, 1H), 7.18 (dd, $J = 11.3, 8.3$ Hz, 1H), 6.26 (dt, $J = 25.7, 3.8$ Hz, 1H), 5.08 – 4.83 (m, 2H). **^{19}F NMR** (470 MHz, Chloroform-*d*) δ -109.20 (dt, $J = 11.1, 6.0$ Hz), -229.63 (td, $J = 47.0, 25.4$ Hz). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 190.8 (dd, $J = 6.9, 3.8$ Hz), 165.8, 161.5 (d, $J = 253.6$ Hz), 135.7 (d, $J = 9.2$ Hz), 133.7, 131.3 (d, $J = 2.7$ Hz), 130.1, 129.1, 128.6, 125.2 (d, $J = 3.2$ Hz), 123.4 (d, $J = 13.7$ Hz), 116.7 (d, $J = 23.5$ Hz), 81.1 (dd, $J = 177.5, 2.7$ Hz), 78.2 (dd, $J = 19.6, 7.8$ Hz); **HRMS** (ESI) m/z calcd. for $C_{16}H_{12}O_3F_2Na$ ($[M+Na]^+$): 313.0652, found 313.0661; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, *n*-Hexane : *i*PrOH =90:10, Rt (major) 8.15 min, Rt (minor) 8.57 min.

(S)-3-fluoro-1-oxo-1-(3,4,5-trifluorophenyl)propan-2-yl benzoate (2l)



15.7 mg, 48% yield, 94% ee, PE : EA = 50: 1. White solid; m.p.: 48-49 °C; $[\alpha]_D^{25} = -45.4$ (*c* 1.0, CH₂Cl₂); **¹H NMR** (500 MHz, Chloroform-*d*) δ 7.89 (dd, *J* = 8.2, 1.4 Hz, 2H), 7.50 (t, *J* = 6.9 Hz, 2H), 7.43 (t, *J* = 7.6 Hz, 1H), 7.29 (t, *J* = 7.8 Hz, 2H), 5.90 (dt, *J* = 23.0, 4.3 Hz, 1H), 4.75 (dt, *J* = 47.0, 4.1 Hz, 2H). **¹⁹F NMR** (470 MHz, Chloroform-*d*) δ -131.33 – -131.48 (m), -150.46 (tt, *J* = 20.1, 6.3 Hz), -228.49 (td, *J* = 46.8, 23.2 Hz). **¹³C NMR** (126 MHz, Chloroform-*d*) δ 191.8, 166.2, 151.9 (ddd, *J* = 253.5, 10.2, 3.3 Hz), 144.3 (dt, *J* = 249.48, 15.12 Hz), 134.7, 130.9 (d, *J* = 4.2 Hz), 130.6, 129.3, 128.9, 114.1 (dd, *J* = 17.2, 5.7 Hz), 82.0 (d, *J* = 177.2 Hz), 75.4 (d, *J* = 21.1 Hz); **HRMS** (ESI) *m/z* calcd. for C₁₆H₁₀O₃F₄Na ([M+Na]⁺): 349.0464, found 349.0466; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, *n*-Hexane : *i*-PrOH = 90:10, Rt (major) 9.02 min, Rt (minor) 10.21 min.

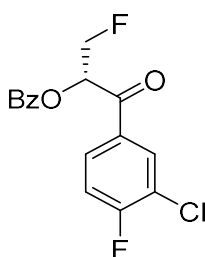
(S)-1-(4-chlorophenyl)-3-fluoro-1-oxopropan-2-yl benzoate (2m)



25.5 mg, 83% yield, 94% ee, PE : EA = 50: 1. White solid; m.p.: 53-54 °C; $[\alpha]_D^{25} = -37.0$ (*c* 1.0, CH₂Cl₂); **¹H NMR** (500 MHz, Chloroform-*d*) δ 7.90 (dd, *J* = 8.4, 1.4 Hz, 2H), 7.76 (d, *J* = 8.6 Hz, 2H), 7.41 (td, *J* = 7.4, 1.5 Hz, 1H), 7.32 – 7.22 (m, 4H), 6.08 (dt, *J* = 22.4, 4.4 Hz, 1H), 4.89 – 4.63 (m, 2H). **¹⁹F NMR** (470 MHz, Chloroform-*d*) δ -228.53 (td, *J* = 46.9, 22.5 Hz). **¹³C NMR** (126 MHz, Chloroform-*d*) δ 193.3 (d, *J* = 6.0 Hz), 166.4, 141.3, 134.5, 133.7, 130.8, 130.0, 129.4, 129.3, 82.3 (d, *J* = 177.3 Hz), 75.5

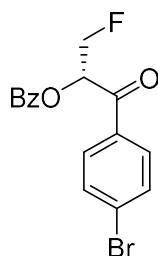
(d, $J = 20.6$ Hz); **HRMS** (ESI) m/z calcd. for $C_{16}H_{12}O_3FNaCl$ ($[M+Na]^+$): 329.0357, found 329.0364; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, *n*-Hexane : *i*PrOH =90:10, R_t (major) 9.36 min, R_t (minor) 11.67 min.

(S)-1-(3-chloro-4-fluorophenyl)-3-fluoro-1-oxopropan-2-yl benzoate
(2n)



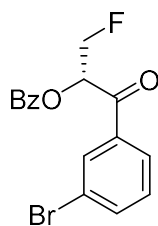
24.0 mg, 74% yield, 95% ee, PE : EA = 50: 1. White solid; m.p.: 69-70 °C; $[\alpha]_D^{25} = -71.4$ (c 1.0, CH_2Cl_2); **1H NMR** (500 MHz, Chloroform-*d*) δ 7.97 – 7.86 (m, 3H), 7.74 (ddd, $J = 8.6, 4.5, 2.3$ Hz, 1H), 7.42 (t, $J = 7.4$ Hz, 1H), 7.28 (t, $J = 7.7$ Hz, 2H), 7.06 (t, $J = 8.6$ Hz, 1H), 6.00 (ddd, $J = 22.7, 5.0, 3.7$ Hz, 1H), 4.75 (dt, $J = 46.9, 4.1$ Hz, 2H). **^{19}F NMR** (470 MHz, Chloroform-*d*) δ -105.54 (td, $J = 7.7, 4.4$ Hz), -228.46 (td, $J = 46.9, 22.7$ Hz). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 191.7 (d, $J = 5.9$ Hz), 165.6, 161.5 (d, $J = 258.8$ Hz), 133.9, 131.9 (d, $J = 3.8$ Hz), 131.8, 130.0, 129.1 (d, $J = 8.6$ Hz), 128.6, 128.5, 122.4 (d, $J = 18.3$ Hz), 117.2 (d, $J = 21.8$ Hz), 81.5 (d, $J = 177.2$ Hz), 74.8 (d, $J = 20.7$ Hz); **HRMS** (ESI) m/z calcd. for $C_{16}H_{11}O_3F_2NaCl$ ($[M+Na]^+$): 347.0262, found 347.0268; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, *n*-Hexane : *i*PrOH =90:10, R_t (major) 10.02 min, R_t (minor) 11.47 min.

(S)-1-(4-bromophenyl)-3-fluoro-1-oxopropan-2-yl benzoate (2o)



28.8 mg, 82% yield, 94% ee, PE : EA = 50: 1. White solid; m.p.: 61-62 °C; $[\alpha]_D^{25} = -85.8$ (*c* 1.0, CH₂Cl₂); ¹H NMR (500 MHz, Chloroform-*d*) δ 8.12 – 8.06 (m, 2H), 7.90 – 7.85 (m, 2H), 7.66 – 7.57 (m, 3H), 7.46 (t, *J* = 7.7 Hz, 2H), 6.26 (dt, *J* = 22.3, 4.3 Hz, 1H), 5.02 – 4.83 (m, 2H). ¹⁹F NMR (470 MHz, Chloroform-*d*) δ -228.58 (td, *J* = 46.9, 22.4 Hz). ¹³C NMR (126 MHz, Chloroform-*d*) δ 192.8 (d, *J* = 6.2 Hz), 165.6, 133.8, 133.5, 132.3, 130.1, 130.1, 129.4, 128.7, 128.6, 81.5 (d, *J* = 177.4 Hz), 74.8 (d, *J* = 20.5 Hz); HRMS (ESI) *m/z* calcd. for C₁₆H₁₂O₃FNaBr ([M+Na]⁺): 372.9852, found 372.9861; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, *n*-Hexane : ⁱPrOH = 90:10, Rt (major) 9.78 min, Rt (minor) 12.57 min.

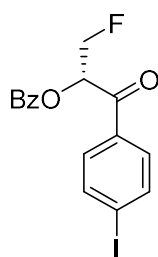
(S)-1-(3-bromophenyl)-3-fluoro-1-oxopropan-2-yl benzoate (2p)



17.2 mg, 49% yield, 87% ee, PE : EA = 50: 1. White solid; m.p.: 80-81 °C; $[\alpha]_D^{25} = -30.4$ (*c* 1.0, CH₂Cl₂); ¹H NMR (500 MHz, Chloroform-*d*) δ 7.95 (t, *J* = 1.8 Hz, 1H), 7.93 – 7.88 (m, 2H), 7.74 (dt, *J* = 7.8, 1.4 Hz, 1H), 7.53 (dd, *J* = 8.1, 2.0 Hz, 1H), 7.42 (tq, *J* = 7.2, 1.7 Hz, 1H), 7.31 – 7.24 (m, 2H), 7.18 (t, *J* = 7.9 Hz, 1H), 6.06 (ddd, *J* = 22.9, 5.1, 3.6 Hz, 1H), 4.75 (ddd, *J* = 47.0, 4.4, 2.8 Hz, 2H). ¹⁹F NMR (470 MHz, Chloroform-*d*) δ -228.43 (td, *J* = 46.8, 23.1 Hz). ¹³C NMR (126 MHz, Chloroform-*d*) δ 193.3 (d, *J* = 6.0 Hz), 166.3, 137.5, 137.2, 134.5, 132.3, 131.2, 130.8, 129.7, 129.3, 127.8, 123.9, 82.2 (d, *J* = 177.5 Hz), 75.7 (dd, *J* = 20.5, 11.6 Hz); HRMS (ESI) *m/z*

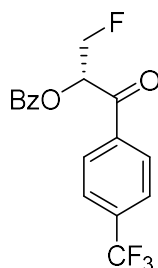
calcd. for $C_{16}H_{12}O_3FNaBr$ ($[M+Na]^+$): 372.9852, found 372.9848; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, *n*-Hexane : *i*-PrOH =90:10, Rt (major) 9.31 min, Rt (minor) 10.80 min.

(*S*)-3-fluoro-1-(4-iodophenyl)-1-oxopropan-2-yl benzoate (2q)



31.5 mg, 79% yield, 94% ee, PE : EA = 50: 1. White solid; m.p.: 72-73 °C; $[\alpha]_D^{25} = -52.8$ (*c* 1.0, CH_2Cl_2); 1H NMR (500 MHz, Chloroform-*d*) δ 8.11 – 8.06 (m, 2H), 7.86 (d, *J* = 8.5 Hz, 2H), 7.71 (d, *J* = 8.6 Hz, 2H), 7.64 – 7.57 (m, 1H), 7.47 (t, *J* = 7.8 Hz, 2H), 6.25 (ddd, *J* = 22.2, 4.9, 3.9 Hz, 1H), 5.05 – 4.75 (m, 2H). ^{19}F NMR (470 MHz, Chloroform-*d*) δ -228.62 (td, *J* = 47.1, 22.2 Hz). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 193.1 (d, *J* = 6.2 Hz), 165.6, 138.3, 134.0, 133.8, 130.1, 129.9, 128.7, 128.6, 102.3, 81.5 (d, *J* = 177.4 Hz), 74.7 (d, *J* = 20.6 Hz); HRMS (ESI) *m/z* calcd. for $C_{16}H_{12}O_3FNaI$ ($[M+Na]^+$): 420.9713, found 420.9717; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, *n*-Hexane : *i*-PrOH =90:10, Rt (major) 11.13 min, Rt (minor) 14.75 min.

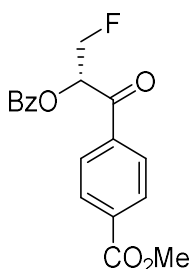
(*S*)-3-fluoro-1-oxo-1-(4-(trifluoromethyl)phenyl)propan-2-yl benzoate (2r)



17.4 mg, 51% yield, 76% ee, PE : EA = 50: 1. White solid; m.p.: 63-64 °C; $[\alpha]_D^{25} = -$

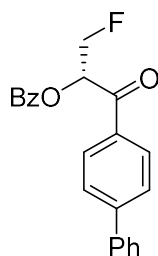
35.2 (*c* 1.0, CH₂Cl₂); **¹H NMR** (500 MHz, Chloroform-*d*) δ 7.87 (dd, *J* = 14.4, 7.9 Hz, 4H), 7.52 (d, *J* = 8.1 Hz, 2H), 7.38 (t, *J* = 7.4 Hz, 1H), 7.24 (t, *J* = 7.7 Hz, 2H), 6.05 (dt, *J* = 22.9, 4.3 Hz, 1H), 4.73 (dt, *J* = 46.9, 3.6 Hz, 2H). **¹⁹F NMR** (470 MHz, Chloroform-*d*) δ -63.31, -228.77 (td, *J* = 46.9, 22.8 Hz). **¹³C NMR** (126 MHz, Chloroform-*d*) δ 196.0 (d, *J* = 5.8 Hz), 168.4, 140.3, 137.8 (q, *J* = 33.0 Hz), 136.6, 132.8, 131.7, 131.3, 131.2, 128.7 (q, *J* = 3.8 Hz), 126.1 (q, *J* = 273.0 Hz), 84.2 (d, *J* = 177.4 Hz), 77.8 (d, *J* = 20.8 Hz); **HRMS** (ESI) *m/z* calcd. for C₁₇H₁₂O₃F₄Na ([M+Na]⁺): 363.0620, found 363.0624; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, *n*-Hexane : ⁱPrOH =90:10, Rt (major) 8.32 min, Rt (minor) 10.99 min.

methyl (*S*)-4-(2-(benzoyloxy)-3-fluoropropanoyl)benzoate (2s)



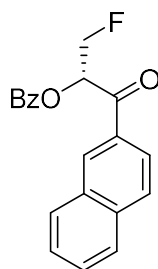
13.2 mg, 40% yield, 92% ee, PE : EA = 50: 1. White solid; m.p.: 95-96 °C; [α]_D²⁵ = -10.6 (*c* 1.0, CH₂Cl₂); **¹H NMR** (500 MHz, Chloroform-*d*) δ 8.14 (d, *J* = 8.4 Hz, 2H), 8.07 (dd, *J* = 16.7, 8.0 Hz, 4H), 7.60 (tq, *J* = 7.2, 1.5 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 2H), 6.30 (ddd, *J* = 23.1, 4.9, 3.7 Hz, 1H), 4.95 (ddd, *J* = 46.9, 4.3, 1.9 Hz, 2H), 3.94 (s, 3H). **¹⁹F NMR** (470 MHz, Chloroform-*d*) δ -228.66 (td, *J* = 46.9, 22.9 Hz). **¹³C NMR** (126 MHz, Chloroform-*d*) δ 193.6 (d, *J* = 6.2 Hz), 166.0, 165.6, 138.0, 134.6, 133.8, 130.0, 128.6, 128.5, 128.1, 81.5 (d, *J* = 177.4 Hz), 75.2 (d, *J* = 20.6 Hz), 52.6; **HRMS** (ESI) *m/z* calcd. for C₁₈H₁₅O₅FNa ([M+Na]⁺): 353.0801, found 353.0809; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, *n*-Hexane : ⁱPrOH =90:10, Rt (major) 16.69 min, Rt (minor) 18.29 min.

(S)-1-([1,1'-biphenyl]-4-yl)-3-fluoro-1-oxopropan-2-yl benzoate (2t)



28.6 mg, 82% yield, 94% ee, PE : EA = 50: 1. White solid; m.p.: 105-106 °C; $[\alpha]_D^{25} = -79.2$ (*c* 1.0, CH₂Cl₂); **¹H NMR** (500 MHz, Chloroform-*d*) δ 8.03 – 7.87 (m, 4H), 7.56 – 7.49 (m, 2H), 7.46 – 7.36 (m, 3H), 7.27 (td, *J* = 7.6, 3.9 Hz, 4H), 7.24 – 7.19 (m, 1H), 6.22 (dt, *J* = 22.0, 4.5 Hz, 1H), 4.78 (dd, *J* = 47.0, 4.5 Hz, 2H). **¹⁹F NMR** (470 MHz, Chloroform-*d*) δ -228.27 (td, *J* = 47.1, 22.0 Hz). **¹³C NMR** (126 MHz, Chloroform-*d*) δ 193.4 (d, *J* = 6.5 Hz), 166.3, 147.3, 140.1, 134.3, 133.9, 130.7, 129.8, 129.6, 129.5, 129.1, 129.1, 128.1, 127.9, 82.3 (d, *J* = 177.4 Hz), 75.4 (d, *J* = 20.3 Hz); **HRMS** (ESI) *m/z* calcd. for C₂₂H₁₇O₃FNa ([M+Na]⁺): 371.1059, found 371.1064; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, *n*-Hexane : ^{*i*}PrOH = 90:10, Rt (major) 13.04 min, Rt (minor) 16.67 min.

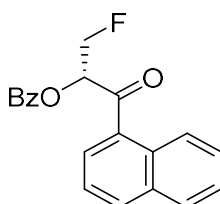
(S)-3-fluoro-1-(naphthalen-2-yl)-1-oxopropan-2-yl benzoate (2u)



26.1 mg, 81% yield, 91% ee, PE : EA = 50: 1. White solid; m.p.: 85-86 °C; $[\alpha]_D^{25} = -44.6$ (*c* 1.0, CH₂Cl₂); **¹H NMR** (500 MHz, Chloroform-*d*) δ 8.40 (s, 1H), 7.94 (d, *J* = 7.7 Hz, 2H), 7.84 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.78 (d, *J* = 8.1 Hz, 1H), 7.73 (d, *J* = 8.7 Hz, 1H), 7.68 (d, *J* = 8.1 Hz, 1H), 7.46 – 7.34 (m, 3H), 7.26 (t, *J* = 7.7 Hz, 2H), 6.35 (dt, *J* = 21.9, 4.5 Hz, 1H), 4.81 (dd, *J* = 47.0, 4.5 Hz, 2H). **¹⁹F NMR** (470 MHz, Chloroform-*d*) δ -228.11 (td, *J* = 46.9, 21.8 Hz). **¹³C NMR** (126 MHz, Chloroform-*d*) δ 193.8 (d, *J* = 6.6 Hz), 166.3, 136.6, 134.3, 133.0, 132.6, 131.2, 130.7, 130.4, 129.7,

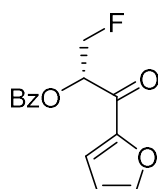
129.5, 129.5, 129.1, 128.4, 127.7, 124.5, 82.4 (d, $J = 177.8$ Hz), 75.5 (d, $J = 20.3$ Hz); **HRMS** (ESI) m/z calcd. for $C_{20}H_{15}O_3FNa$ ($[M+Na]^+$): 345.0903, found 345.0910; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, *n*-Hexane : *i*PrOH =90:10, R_t (major) 13.35 min, R_t (minor) 19.51 min.

(S)-3-fluoro-1-(naphthalen-1-yl)-1-oxopropan-2-yl benzoate (2v)



23.2 mg, 72% yield, 96% ee, PE : EA = 50: 1. White solid; m.p.: 94-95 °C; $[\alpha]_D^{25} = -24.8$ (c 1.0, CH_2Cl_2); **1H NMR** (500 MHz, Chloroform-*d*) δ 8.34 (d, $J = 8.4$ Hz, 1H), 8.02 (dd, $J = 8.0, 1.4$ Hz, 2H), 7.96 – 7.92 (m, 2H), 7.81 (dd, $J = 8.1, 1.4$ Hz, 1H), 7.55 – 7.43 (m, 4H), 7.37 (t, $J = 7.8$ Hz, 2H), 6.27 (ddd, $J = 26.9, 4.6, 2.7$ Hz, 1H), 4.97 – 4.74 (m, 2H). **^{19}F NMR** (470 MHz, Chloroform-*d*) δ -228.45 (td, $J = 47.2, 27.0$ Hz). **^{13}C NMR** (126 MHz, Acetonitrile-*d*₃) δ 198.6 (d, $J = 5.3$ Hz), 167.2, 135.5, 135.4, 134.7, 134.6, 131.5, 131.2, 130.7, 130.4, 130.2, 129.6, 129.2, 128.5, 126.5, 126.3, 83.9 (d, $J = 173.0$ Hz), 79.4 (d, $J = 19.1$ Hz); **HRMS** (ESI) m/z calcd. for $C_{20}H_{15}O_3FNa$ ($[M+Na]^+$): 345.0903, found 345.0910; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, *n*-Hexane : *i*PrOH =90:10, R_t (major) 12.17 min, R_t (minor) 15.19 min.

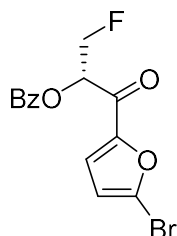
(S)-3-fluoro-1-(furan-2-yl)-1-oxopropan-2-yl benzoate (2w)



13.9 mg, 53% yield, 70% ee, PE : EA = 50: 1. White solid; m.p.: 69-70 °C; $[\alpha]_D^{25} = -37.0$ (c 1.0, CH_2Cl_2); **1H NMR** (500 MHz, Chloroform-*d*) δ 8.13 (ddd, $J = 11.6, 8.3, 1.4$ Hz, 2H), 7.66 (d, $J = 1.7$ Hz, 1H), 7.61 (tt, $J = 7.0, 1.4$ Hz, 1H), 7.48 (t, $J = 7.8$ Hz,

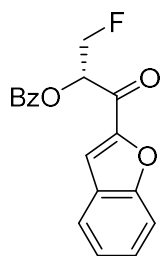
2H), 7.41 (d, $J = 3.6$ Hz, 1H), 6.60 (dd, $J = 3.7, 1.7$ Hz, 1H), 6.17 (ddd, $J = 22.9, 5.4, 3.0$ Hz, 1H), 5.08 – 4.86 (m, 2H). ^{19}F NMR (470 MHz, Chloroform- d) δ -228.97 (td, $J = 46.8, 22.9$ Hz). ^{13}C NMR (126 MHz, Chloroform- d) δ 180.92 (d, $J = 6.9$ Hz), 165.62, 150.67, 147.43, 133.70, 130.20, 130.09, 128.85, 128.56, 128.50, 119.64, 112.86, 81.39 (d, $J = 177.9$ Hz), 75.04 (d, $J = 20.2$ Hz); HRMS (ESI) m/z calcd. for $\text{C}_{14}\text{H}_{11}\text{O}_4\text{NaF}$ ($[\text{M}+\text{Na}]^+$): 285.0539, found 285.0543; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, n -Hexane : i PrOH =90:10, R_t (major) 13.07 min, R_t (minor) 17.35 min.

(*S*)-1-(5-bromofuran-2-yl)-3-fluoro-1-oxopropan-2-yl benzoate (2x)



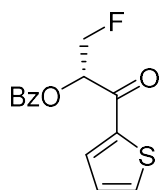
14.3 mg, 42% yield, 79% ee, PE : EA = 50: 1. White solid; m.p.: 62-63 °C; $[\alpha]_{\text{D}}^{25} = -36.8$ (c 1.0, CH_2Cl_2); ^1H NMR (500 MHz, Chloroform- d) δ 8.13 (d, $J = 7.7$ Hz, 2H), 7.62 (t, $J = 7.5$ Hz, 1H), 7.48 (t, $J = 7.7$ Hz, 2H), 7.33 (d, $J = 3.7$ Hz, 1H), 6.54 (d, $J = 3.6$ Hz, 1H), 6.09 (ddd, $J = 23.2, 5.2, 3.1$ Hz, 1H), 5.08 – 4.84 (m, 2H). ^{19}F NMR (470 MHz, Chloroform- d) δ -229.20 (td, $J = 46.8, 23.3$ Hz). ^{13}C NMR (126 MHz, Chloroform- d) δ 179.8 (d, $J = 6.7$ Hz), 165.6, 152.3, 133.8, 130.1, 129.9, 128.7, 128.6, 121.6, 115.0, 81.3 (d, $J = 177.9$ Hz), 74.8 (d, $J = 20.4$ Hz); HRMS (ESI) m/z calcd. for $\text{C}_{14}\text{H}_{10}\text{O}_4\text{FNaBr}$ ($[\text{M}+\text{Na}]^+$): 362.9644, found 362.9652; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, n -Hexane : i PrOH =99:1, R_t (major) 19.69 min, R_t (minor) 23.27 min.

(S)-1-(benzofuran-2-yl)-3-fluoro-1-oxopropan-2-yl benzoate (2y)



17.2 mg, 55% yield, 76% ee, PE : EA = 50: 1. White solid; m.p.: 91-92 °C; $[\alpha]_{\text{D}}^{25} = -113.8$ (*c* 1.0, CH₂Cl₂); **¹H NMR** (400 MHz, Chloroform-*d*) δ 8.16 (d, *J* = 7.7 Hz, 2H), 7.74 (t, *J* = 4.1 Hz, 2H), 7.61 (dd, *J* = 16.4, 8.3 Hz, 2H), 7.51 (dt, *J* = 15.2, 7.4 Hz, 3H), 7.34 (t, *J* = 7.5 Hz, 1H), 6.31 (ddd, *J* = 23.1, 5.5, 3.1 Hz, 1H), 5.06 (dddd, *J* = 46.7, 24.4, 10.5, 4.3 Hz, 2H). **¹⁹F NMR** (470 MHz, Chloroform-*d*) δ -228.94 (td, *J* = 46.8, 23.1 Hz). **¹³C NMR** (126 MHz, Chloroform-*d*) δ 183.1 (d, *J* = 6.9 Hz), 165.6, 155.9, 150.4, 133.8, 130.1, 129.2, 128.8, 128.6, 126.8, 124.3, 123.7, 115.3, 112.6, 81.3 (d, *J* = 177.9 Hz), 75.3 (d, *J* = 20.3 Hz); **HRMS** (ESI) *m/z* calcd. for C₁₈H₁₃O₄FNa ([M+Na]⁺): 335.0696, found 335.0704; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, *n*-Hexane : ⁱPrOH = 90:10, *R*_t (major) 12.28 min, *R*_t (minor) 14.42 min.

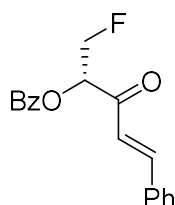
(S)-3-fluoro-1-oxo-1-(thiophen-2-yl)propan-2-yl benzoate (2z)



18.4 mg, 66% yield, 90% ee, PE : EA = 50: 1. White solid; m.p.: 56-57 °C; $[\alpha]_{\text{D}}^{25} = -28.0$ (*c* 1.0, CH₂Cl₂); **¹H NMR** (500 MHz, Chloroform-*d*) δ 8.14 (d, *J* = 7.6 Hz, 2H), 7.95 (d, *J* = 3.9 Hz, 1H), 7.73 (d, *J* = 4.9 Hz, 1H), 7.62 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.17 (t, *J* = 4.4 Hz, 1H), 6.16 (ddd, *J* = 21.4, 5.6, 3.4 Hz, 1H), 5.06 – 4.86 (m, 2H). **¹⁹F NMR** (470 MHz, Chloroform-*d*) δ -228.42 (tdd, *J* = 46.8, 21.3, 3.1 Hz). **¹³C NMR** (126 MHz, Chloroform-*d*) δ 185.8 (d, *J* = 6.7 Hz), 165.6, 140.8, 135.4, 133.8, 133.6, 130.1, 128.8, 128.6, 128.5, 81.9 (d, *J* = 178.3 Hz), 75.6 (d, *J* = 20.6 Hz); **HRMS**

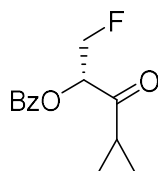
(ESI) m/z calcd. for $C_{14}H_{11}O_3FNaS$ ($[M+Na]^+$): 301.0311, found 301.0320; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, *n*-Hexane : *i*PrOH =90:10, R_t (major) 11.95 min, R_t (minor) 16.64 min.

(S)-1-fluoro-3-oxo-5-phenylpent-4-en-2-yl benzoate (2a')



20.0 mg, 67% yield, 71% ee, PE : EA = 50: 1. White solid; m.p.: 70-71 °C; $[\alpha]_D^{25} = -366.4$ (*c* 1.0, CH_2Cl_2); 1H NMR (500 MHz, Chloroform-*d*) δ 7.99 (dd, $J = 8.3, 1.4$ Hz, 2H), 7.63 (d, $J = 15.8$ Hz, 1H), 7.45 (td, $J = 7.3, 1.5$ Hz, 1H), 7.39 – 7.35 (m, 2H), 7.32 (t, $J = 7.8$ Hz, 2H), 7.24 – 7.19 (m, 3H), 6.84 (d, $J = 15.8$ Hz, 1H), 5.59 (ddd, $J = 25.3, 4.9, 2.9$ Hz, 1H), 4.87 – 4.63 (m, 2H). ^{19}F NMR (470 MHz, Chloroform-*d*) δ -230.41 (td, $J = 47.0, 25.3$ Hz). ^{13}C NMR (126 MHz, Acetonitrile-*d*₃) δ 192.5 (d, $J = 6.0$ Hz), 166.0, 145.1, 134.8, 134.3, 131.7, 130.2, 129.8, 129.6, 129.4, 129.4, 121.9, 82.5 (d, $J = 172.8$ Hz), 78.4 (d, $J = 19.1$ Hz); HRMS (ESI) m/z calcd. for $C_{18}H_{15}O_3FNa$ ($[M+Na]^+$): 321.0903, found 321.0911; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, *n*-Hexane : *i*PrOH =90:10, R_t (major) 12.50 min, R_t (minor) 16.39 min.

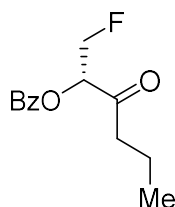
(S)-1-cyclopropyl-3-fluoro-1-oxopropan-2-yl benzoate (2b')



13.9 mg, 59% yield, 64% ee, PE : EA = 50: 1. White solid; m.p.: 63-64 °C; $[\alpha]_D^{25} = -23.0$ (*c* 1.0, CH_2Cl_2); 1H NMR (500 MHz, Chloroform-*d*) δ 8.08 (dt, $J = 8.5, 1.6$ Hz, 2H), 7.55 (td, $J = 7.2, 1.4$ Hz, 1H), 7.41 (t, $J = 7.8$ Hz, 2H), 5.56 (ddd, $J = 27.5, 4.6, 2.7$ Hz, 1H), 4.95 – 4.70 (m, 2H), 2.15 (ddd, $J = 7.9, 4.6, 3.3$ Hz, 1H), 1.19 – 1.11 (m, 1H),

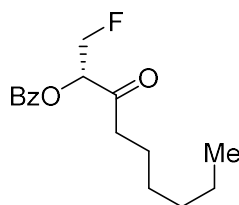
1.06 (dtd, $J = 10.6, 4.7, 2.1$ Hz, 1H), 1.01 – 0.87 (m, 2H). ^{19}F NMR (470 MHz, Chloroform- d) δ -230.29 (td, $J = 47.5, 27.6$ Hz). ^{13}C NMR (126 MHz, Chloroform- d) δ 203.2 (d, $J = 5.3$ Hz), 164.6, 132.7, 129.0, 127.9, 127.6, 80.7 (d, $J = 176.1$ Hz), 77.3 (d, $J = 19.6$ Hz), 16.7, 11.5, 11.0; HRMS (ESI) m/z calcd. for $\text{C}_{13}\text{H}_{13}\text{O}_3\text{FNa}$ ($[\text{M}+\text{Na}]^+$): 259.0746, found 259.0749; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, n -Hexane : i PrOH =90:10, R_t (major) 8.95 min, R_t (minor) 9.56 min.

(*S*)-1-fluoro-3-oxohexan-2-yl benzoate (2c')



9.1 mg, 38% yield, 66% ee, PE : EA = 50 : 1. White solid; m.p.: 95-96 °C; $[\alpha]_{\text{D}}^{25} = -17.4$ (c 1.0, CH_2Cl_2); ^1H NMR (500 MHz, Chloroform- d) δ 8.14 (dd, $J = 8.5, 1.3$ Hz, 2H), 7.67 – 7.60 (m, 1H), 7.50 (t, $J = 7.8$ Hz, 2H), 5.51 (ddd, $J = 28.7, 4.1, 2.7$ Hz, 1H), 5.02 – 4.71 (m, 2H), 2.70 – 2.47 (m, 2H), 1.66 (hd, $J = 7.3, 2.4$ Hz, 2H), 0.93 (t, $J = 7.4$ Hz, 3H). ^{19}F NMR (470 MHz, Chloroform- d) δ -231.05 – -231.40 (m). ^{13}C NMR (126 MHz, Chloroform- d) δ 204.0 (d, $J = 4.6$ Hz), 164.7, 132.8, 129.0, 127.9, 127.6, 81.0 (d, $J = 175.2$ Hz), 76.8 (d, $J = 19.8$ Hz), 40.5, 15.2, 12.5; HRMS (ESI) m/z calcd. for $\text{C}_{13}\text{H}_{15}\text{O}_3\text{FNa}$ ($[\text{M}+\text{Na}]^+$): 261.0903, found 261.0909; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, n -Hexane : i PrOH =90:10, R_t (major) 7.96 min, R_t (minor) 8.43 min.

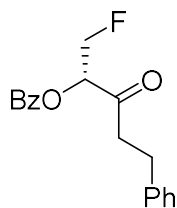
(*S*)-1-fluoro-3-oxononan-2-yl benzoate (2d')



10.9 mg, 39% yield, 54% ee, PE : EA = 50 : 1. White solid; m.p.: 43-44 °C; $[\alpha]_{\text{D}}^{25} = -$

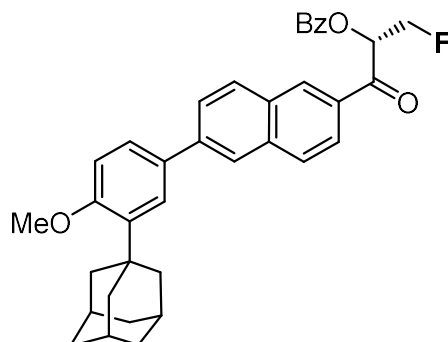
46.6 (*c* 1.0, CH₂Cl₂); **¹H NMR** (500 MHz, Chloroform-*d*) δ 8.17 – 8.11 (m, 2H), 7.63 (td, *J* = 7.3, 1.5 Hz, 1H), 7.57 – 7.43 (m, 2H), 5.51 (ddd, *J* = 28.7, 4.1, 2.6 Hz, 1H), 4.86 (dddd, *J* = 72.1, 47.8, 10.4, 3.4 Hz, 2H), 2.74 – 2.45 (m, 2H), 1.61 (dp, *J* = 10.8, 7.0 Hz, 2H), 1.33 – 1.23 (m, 6H), 0.86 (t, *J* = 6.8 Hz, 3H). **¹⁹F NMR** (470 MHz, Chloroform-*d*) δ -231.13 (td, *J* = 47.1, 28.7 Hz). **¹³C NMR** (126 MHz, Chloroform-*d*) δ 205.1 (d, *J* = 4.6 Hz), 165.7, 133.8, 130.0, 128.9, 128.7, 82.0 (d, *J* = 175.4 Hz), 77.8 (d, *J* = 19.8 Hz), 39.7, 31.6, 28.7, 22.8, 22.4, 14.0.; **HRMS** (ESI) *m/z* calcd. for C₁₆H₂₁O₃FNa ([M+Na]⁺): 303.1372, found 303.1380; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, *n*-Hexane : *i*PrOH =99:1, Rt (major) 7.17 min, Rt (minor) 7.68 min.

(*S*)-1-fluoro-3-oxo-5-phenylpentan-2-yl benzoate (2e')



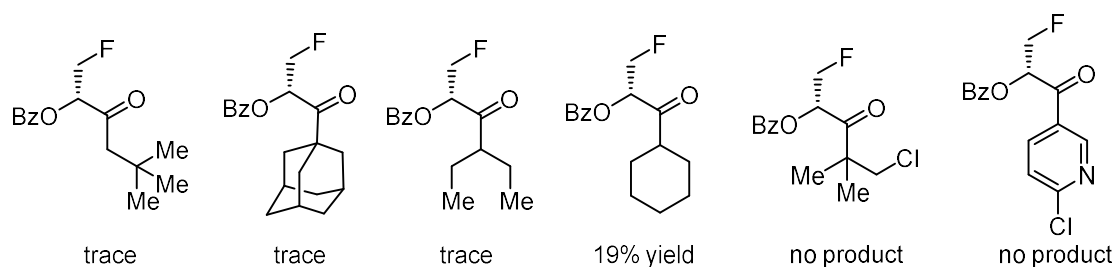
19.2 mg, 64% yield, 54% ee, PE : EA = 50: 1. White solid; m.p.: 47-48 °C; [α]_D²⁵ = -12.0 (*c* 1.0, CH₂Cl₂); **¹H NMR** (500 MHz, Chloroform-*d*) δ 7.98 (dd, *J* = 8.3, 1.5 Hz, 2H), 7.49 (td, *J* = 7.4, 1.5 Hz, 1H), 7.35 (t, *J* = 7.8 Hz, 2H), 7.13 (t, *J* = 7.5 Hz, 2H), 7.04 (dd, *J* = 7.2, 5.5 Hz, 3H), 5.38 (ddd, *J* = 28.5, 4.0, 2.6 Hz, 1H), 4.70 (dddd, *J* = 73.5, 47.8, 10.5, 3.3 Hz, 2H), 2.92 – 2.70 (m, 4H). **¹⁹F NMR** (470 MHz, Chloroform-*d*) δ -231.19 (td, *J* = 47.2, 28.6 Hz). **¹³C NMR** (126 MHz, Chloroform-*d*) δ 205.0 (d, *J* = 4.6 Hz), 166.4, 141.2, 134.6, 130.8, 129.5, 129.4, 129.3, 129.1, 127.0, 82.7 (d, *J* = 175.5 Hz), 78.6 (d, *J* = 19.8 Hz), 42.1, 29.6; **HRMS** (ESI) *m/z* calcd. for C₁₈H₁₇O₃FNa ([M+Na]⁺): 323.1059, found 323.1050; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, *n*-Hexane : *i*PrOH =90:10, Rt (major) 8.18 min, Rt (minor) 10.15 min.

(S)-1-(6-(3-adamantan-1-yl)-4-methoxyphenyl)naphthalen-2-yl)-3-fluoro-1-oxopropan-2-yl benzoate e (2f')

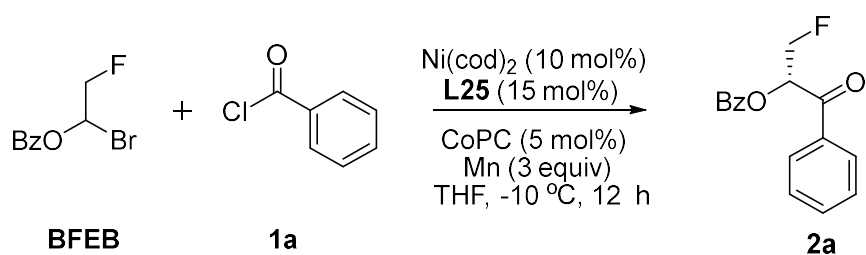


43.3 mg, 77% yield, 82% ee, PE : EA = 50: 1. White solid; m.p.: 302-303 °C; $[\alpha]_D^{25} = -65.2$ (*c* 1.0, CH₂Cl₂); **¹H NMR** (400 MHz, Chloroform-*d*) δ 8.58 (s, 1H), 8.14 (d, *J* = 7.7 Hz, 2H), 8.06 – 7.91 (m, 4H), 7.82 (dd, *J* = 8.5, 1.7 Hz, 1H), 7.65 – 7.51 (m, 3H), 7.46 (t, *J* = 7.7 Hz, 2H), 6.99 (d, *J* = 8.4 Hz, 1H), 6.55 (dt, *J* = 21.7, 4.6 Hz, 1H), 5.00 (dd, *J* = 47.0, 4.5 Hz, 2H), 3.90 (s, 3H), 2.18 (s, 6H), 2.10 (s, 3H), 1.80 (s, 6H). **¹⁹F NMR** (376 MHz, Chloroform-*d*) δ -227.82 (td, *J* = 46.8, 21.7 Hz). **¹³C NMR** (101 MHz, Chloroform-*d*) δ 191.9 (d, *J* = 6.8 Hz), 164.7, 158.1, 141.2, 138.0, 135.4, 132.6, 131.2, 130.4, 130.1, 129.4, 129.1, 129.0, 127.9, 127.9, 127.5, 125.8, 124.9, 124.7, 123.7, 123.2, 111.1, 80.8 (d, *J* = 177.6 Hz), 73.8 (d, *J* = 20.2 Hz), 54.1, 52.4, 39.6, 36.2, 36.08, 28.1; **HRMS** (ESI) *m/z* calcd. for C₃₇H₃₅O₄FN_a ([*M*+Na]⁺): 585.2417, found 585.2421; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IA, 0.8 mL/min, *n*-Hexane : *i*-PrOH =90:10, *R_t* (major) 13.89 min, *R_t* (minor) 17.65 min.

Selected results of unsuccessful substrates



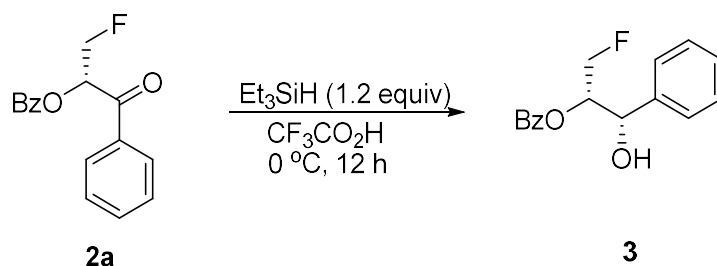
6 Gram-Scale Reaction



In a glove box, $\text{Ni}(\text{cod})_2$ (95.2 mg, 0.34 mmol, 10 mol%), and **L1** (0.43g, 0.51 mmol, 15 mol%) were added into a 100 mL Schlenk flask equipped with a stirring bar in 34 mL Tetrahydrofuran (THF). The mixture was stirred at room temperature for 30 mins, then brominated fluoroethanol benzoate (**BFEB**) (1.00 g, 4.08 mmol, 1.2 equiv.), benzoyl chloride **1a** (0.48 g, 3.4 mmol, 1.0 equiv.), Mn (0.56 g, 10.2 mmol, 3 equiv.), cobalt(II) phthalocyanine (CoPc) (98.6 mg, 0.17 mmol, 5 mol%) was added and keep stirring at $-10\text{ }^\circ\text{C}$ for 12 hours. After evaporation under reduced pressure to remove the solvent, the mixture was passed through a short column of silica gel to remove the metal complex. The residue was purified by flash chromatography on silica gel (PE : EA = 50: 1) to afford the desired product **2a** (0.66 g, 72% yield, 91% ee).

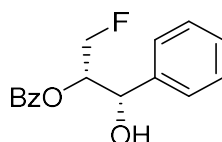
7 Synthesis Transformation

7.1 Reduction of ketone group

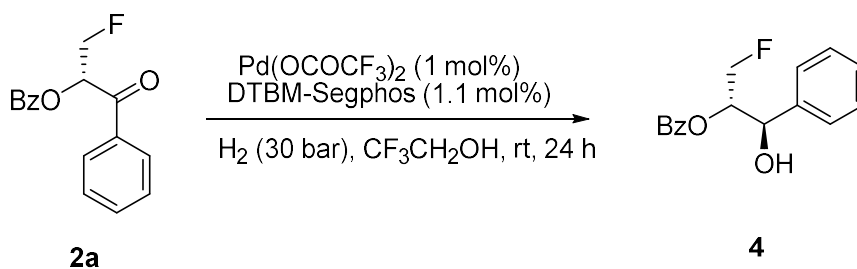


To a solution of **2a** (27.2 mg, 0.1 mmol, 1.0 equiv.) in 1 mL $\text{CF}_3\text{CO}_2\text{H}$, Et_3SiH (14.0 mg, 0.12 mmol, 1.2 equiv.) was added. The mixture was stirred at 0 °C for 12 hours. The reaction was quenched by water, and the aqueous phase was extracted with CH_2Cl_2 three times. The combined organic layers were washed with brine, dried over sodium sulfate and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (PE : EA = 20: 1) to give pure product **3** (17.6 mg, 64% yield, 37:1 dr, 95% ee).^[4]

(1*S*,2*S*)-3-fluoro-1-hydroxy-1-phenylpropan-2-yl benzoate (**3**)

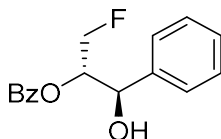


17.6 mg, 64% yield, 37:1 dr, 95% ee, PE : EA = 20: 1. White solid; m.p.: 63-64 °C; $[\alpha]_{\text{D}}^{25} = -33.6$ (c 1.0, CH_2Cl_2); **¹H NMR** (500 MHz, Chloroform-*d*) δ 7.90 (dd, $J = 8.3$, 1.4 Hz, 2H), 7.51 – 7.44 (m, 1H), 7.40 – 7.30 (m, 4H), 7.27 (dd, $J = 8.3$, 6.6 Hz, 2H), 7.23 – 7.19 (m, 1H), 5.38 (dddd, $J = 22.2$, 6.1, 5.1, 2.6 Hz, 1H), 5.06 (d, $J = 6.1$ Hz, 1H), 4.86 – 4.52 (m, 2H), 2.61 (s, 1H). **¹⁹F NMR** (470 MHz, Chloroform-*d*) δ -235.21 (td, $J = 47.4$, 22.4 Hz). **¹³C NMR** (126 MHz, Chloroform-*d*) δ 164.8, 138.5, 132.3, 128.7, 128.5, 127.8, 127.6, 127.4, 125.4, 80.3 (d, $J = 171.9$ Hz), 75.0 (d, $J = 18.1$ Hz), 71.4 (d, $J = 7.0$ Hz); **HRMS** (ESI) m/z calcd. for $\text{C}_{16}\text{H}_{15}\text{O}_3\text{FNa}$ ($[\text{M}+\text{Na}]^+$): 297.0903, found 297.0906; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IA, 0.4 mL/min, *n*-Hexane : *i*PrOH = 90:10, R_t (major) 23.77 min, R_t (minor) 26.26 min.



In a glove box, **2a** (27.2 mg, 0.1 mmol, 1.0 equiv.), (*R*)-DTBM-SegPHOS (1.3 mg, 1.1 mol%) and $\text{Pd}(\text{OCOCF}_3)_2$ (0.33 mg, 1.0 mol%) were added into a Teflon reaction tube in 1 mL trifluoroethanol (TFE). Then the tube was transferred into a stainless-steel autoclave which was attached to the high-pressure hydrogen cylinders, and the system was purged three times with hydrogen to remove argon. Then the autoclave was charged with hydrogen (30 bar). The reaction was stirred at room temperature for 24 h. The hydrogen gas was released slowly and carefully in a fume hood. After evaporation under reduced pressure to remove the solvent, the mixture was passed through a short column of silica gel to remove the metal complex. The residue was purified by flash chromatography on silica gel (PE : EA = 20 : 1) to afford the desired product **4** (13.4 mg, 50% yield, 5:1 dr, 96% ee).^[5]

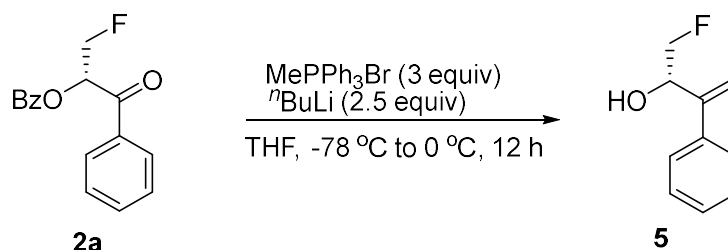
(1*R*,2*S*)-3-fluoro-1-hydroxy-1-phenylpropan-2-yl benzoate (**4**)



13.4 mg, 50% yield, 5:1 dr, 96% ee, PE : EA = 20: 1. White solid; m.p.: 63-64 °C; $[\alpha]_D^{25} = -12.8$ (*c* 1.0, CH_2Cl_2); **¹H NMR** (500 MHz, Chloroform-*d*) δ 8.01 (dd, *J* = 8.0, 1.6 Hz, 2H), 7.53 – 7.49 (m, 1H), 7.41 – 7.34 (m, 4H), 7.29 (dd, *J* = 8.2, 6.2 Hz, 2H), 7.27 – 7.24 (m, 1H), 5.41 – 5.30 (m, 1H), 5.04 (d, *J* = 7.3 Hz, 1H), 4.40 (dddd, *J* = 129.7, 46.8, 10.5, 3.6 Hz, 2H), 2.52 (s, 1H). **¹⁹F NMR** (470 MHz, Chloroform-*d*) δ -233.93 (tdd, *J* = 47.4, 23.9, 5.5 Hz). **¹³C NMR** (126 MHz, Chloroform-*d*) δ 164.8, 138.5, 132.3, 128.7, 128.5, 127.8, 127.6, 127.4, 125.4, 80.3 (d, *J* = 171.9 Hz), 75.0 (d, *J* = 18.1 Hz), 71.4 (d, *J* = 7.0 Hz); **HRMS** (ESI) *m/z* calcd. for $\text{C}_{16}\text{H}_{15}\text{O}_3\text{FNa}$ ($[\text{M}+\text{Na}]^+$): 297.0903, found 297.0906; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IA, 0.4 mL/min, *n*-Hexane : *i*PrOH = 90:10, *R*_t (major) 27.32 min, *R*_t (minor)

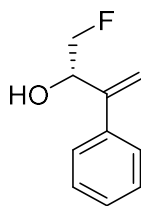
28.62 min.

7.2 Wittig reaction



An oven-dried flask was charged with methyltriphenylphosphonium bromide (107.2 mg, 0.30 mmol, 3.0 equiv.), and THF (0.50 mL) was added under N₂ atmosphere. The resulting suspension was cooled to -78 °C, and n-BuLi (0.11 mL, 0.25 mmol, 2.5 equiv, 2.5 M solution in hexanes) was added dropwise. After the resulting orange solution was stirred for 30 mins, a solution of **2a** (27.2 mg, 0.1 mmol, 1.0 equiv.) in THF (0.25 mL) was added to the reaction mixture. The reaction was stirred at 0 °C for 12 hours. The reaction was quenched with saturated aqueous NH₄Cl solution. The aqueous layer was extracted with ethyl acetate (3 × 2.0 mL) and the combined organic layers were washed with brine, dried over anhydrous Na₂SO₄ and concentrated in vacuo. The product was purified by flash column chromatography on silica (PE : EA = 20 : 1) to give compound **5** (11.1 mg, 67% yield, 91% ee).^[6]

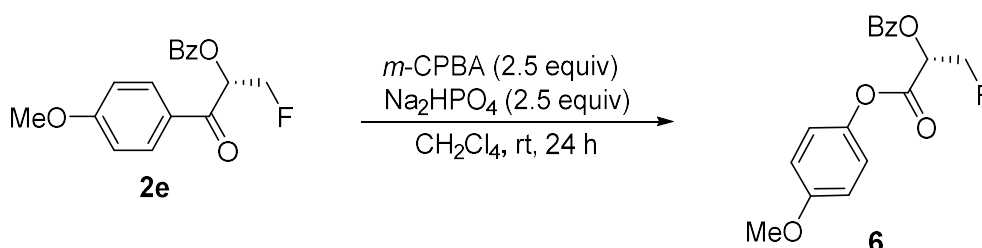
(*S*)-1-fluoro-3-phenylbut-3-en-2-ol (**5**)



11.1 mg, 67% yield, 91% ee, PE : EA = 20: 1. White solid; m.p.: 79-80 °C; $[\alpha]_D^{25} = -156.4$ (*c* 1.0, CH₂Cl₂); ¹H NMR (500 MHz, Chloroform-*d*) δ 7.33 – 7.21 (m, 5H), 5.43 (dt, *J* = 27.5, 1.2 Hz, 2H), 4.90 (dd, *J* = 16.7, 7.3 Hz, 1H), 4.45 – 4.11 (m, 2H), 2.32 (d, *J* = 3.7 Hz, 1H). ¹⁹F NMR (470 MHz, Chloroform-*d*) δ -224.34 (td, *J* = 47.7, 16.9 Hz). ¹³C NMR (126 MHz, Chloroform-*d*) δ 145.0 (d, *J* = 7.9 Hz), 138.0, 127.6, 127.1, 125.6, 114.1, 85.0 (d, *J* = 172.8 Hz), 71.4 (d, *J* = 19.8 Hz); HRMS (ESI) *m/z* calcd. for

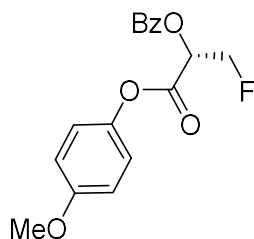
C₁₀H₁₁OFK ([M+K]⁺): 205.0431, found 205.0436; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IA, 0.8 mL/min, *n*-Hexane : *i*PrOH =90:10, Rt (major) 9.36 min, Rt (minor) 8.09 min.

7.3 Baeyer-Villiger oxidation



To a solid of **2e** (30.2 mg, 0.1 mmol, 1.0 equiv.) in CH₂Cl₂ (1 mL), was added *m*-CPBA (43.1 mg, 0.25 mmol, 2.5 equiv.) and Na₂HPO₄ (35.6 mg, 0.25 mmol, 2.5 equiv.) at room temperature. After being stirred at room temperature for 24 h, the mixture was poured into water (3.0 mL) and saturated sodium hydrogen carbonate (3.0 mL), the organic layer was separated and the aqueous phase was extracted with CH₂Cl₂ (3 × 2.0 mL). The combined organic layers were washed with saturated brine, dried over MgSO₄ and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (eluting with petroleum ether/ethyl acetate) to give product **6** (26.7 mg, 84% yield, 88% ee).^[7]

(*S*)-3-fluoro-1-(4-methoxyphenoxy)-1-oxopropan-2-yl benzoate(**6**)

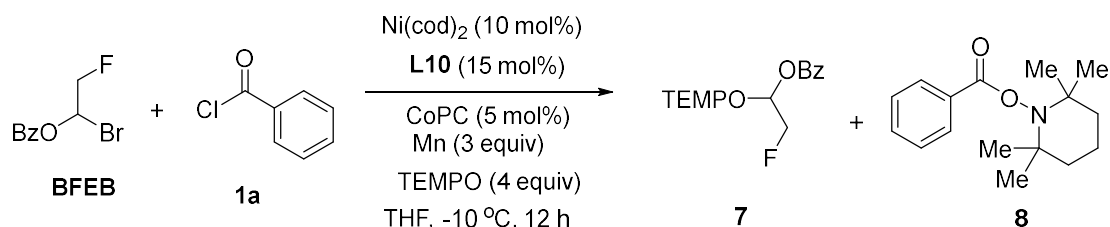


26.7 mg, 84% yield, 88% ee, PE : EA = 20: 1. White solid; m.p.: 97-98 °C; [α]_D²⁵ = -57.3 (*c* 1.0, CH₂Cl₂); ¹H NMR (500 MHz, Chloroform-*d*) δ 8.19 – 8.13 (m, 2H), 7.65 – 7.58 (m, 1H), 7.48 (t, *J* = 7.8 Hz, 2H), 7.07 – 7.04 (m, 2H), 6.90 – 6.87 (m, 2H), 5.76 (ddd, *J* = 27.4, 4.5, 2.4 Hz, 1H), 5.20 – 4.87 (m, 2H), 3.79 (s, 3H). ¹⁹F NMR (470 MHz, Chloroform-*d*) δ -229.26 (td, *J* = 46.9, 27.1 Hz). ¹³C NMR (126 MHz, Chloroform-*d*) δ 164.66, 164.62 (d, *J* = 7.9 Hz), 156.63, 142.58, 132.74, 129.09, 127.73, 127.53, 121.01, 113.51, 80.77 (d, *J* = 177.6 Hz), 70.94 (d, *J* = 20.2 Hz), 54.58. ; HRMS (ESI)

m/z calcd. For $C_{17}H_{15}O_5FNa$ ($[M+Na]^+$): 341.0801, found 341.0795; The enantiomeric excess was determined by Chiral HPLC (Chiralpak IB, 0.8 mL/min, *n*-Hexane : *i*-PrOH = 90:10, Rt (major) 10.71 min, Rt (minor) 12.25 min.

8 Mechanistic Studies

8.1 Radical Trapping Experiment



In a glove box, $\text{Ni}(\text{cod})_2$ (2.8 mg, 0.01 mmol, 10 mol%), and **L10** (12.6 mg, 0.015 mmol, 15 mol%) were added into a 4 mL glass bottle in 1 mL Tetrahydrofuran (THF). The mixture was stirred at room temperature for 30 mins, then brominated fluoroethanol benzoate (**BFEb**) (29.6 mg, 0.12 mmol, 1.2 equiv.), benzoyl chloride **1a** (14.1 mg, 0.1 mmol, 1.0 equiv.), Mn (16.5 mg, 0.3 mmol, 3 equiv.), cobalt(II) phthalocyanine (CoPc) (2.9 mg, 0.005 mmol, 5 mol%) and TEMPO (62.5 mg, 0.4 mmol, 4.0 equiv) was added and keep stirring at $-10\text{ }^\circ\text{C}$ for 12 hours. After evaporation under reduced pressure to remove the solvent, the mixture was passed through a short column of silica gel to remove the metal complex. The residue was purified by flash chromatography on silica gel (PE : EA = 50: 1) to afford the desired product **8** (11.5 mg, 44% yield). Product **7** was evidently detected by HRMS and GCMS.



Figure S1. GC-MS data for **7**

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1321 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 18-18 H: 27-27 N: 0-100 O: 0-100 F: 1-4 Na: 0-1

37

240117-9-287-1 10 (0.072)

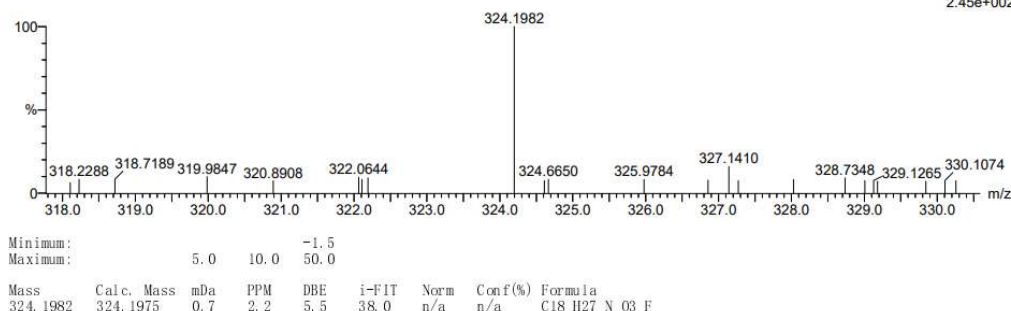
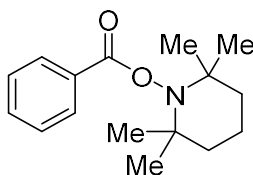
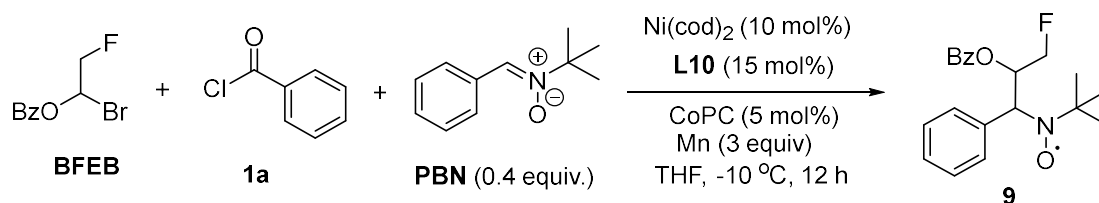
1: TOF MS ES+
2.45e+002

Figure S2. HRMS data for 7.

2,2,6,6-tetramethylpiperidin-1-yl benzoate (8)

11.5 mg, 44% yield, PE : EA = 50: 1. White solid; m.p.: 83-84 °C; $^1\text{H NMR}$ (500 MHz, Chloroform-*d*) δ 8.00 (d, $J = 8.0$ Hz, 2H), 7.53 – 7.46 (m, 1H), 7.39 (t, $J = 7.6$ Hz, 2H), 1.70 (dt, $J = 14.9, 12.0$ Hz, 2H), 1.62 (d, $J = 13.3$ Hz, 1H), 1.51 (dt, $J = 12.5, 2.8$ Hz, 2H), 1.39 (dt, $J = 13.2, 3.4$ Hz, 1H), 1.20 (s, 6H), 1.05 (s, 6H). $^{13}\text{C NMR}$ (126 MHz, Chloroform-*d*) δ 165.4, 131.8, 128.7, 128.5, 127.4, 59.4, 38.1, 31.0, 19.8, 16.0; **HRMS** (ESI) m/z calcd. for $\text{C}_{16}\text{H}_{23}\text{NO}_2\text{Na}$ ($[\text{M}+\text{Na}]^+$): 284.1626, found 284.1631.

8.2 EPR Experiment



In a glove box, $\text{Ni}(\text{cod})_2$ (2.8 mg, 0.01 mmol, 10 mol%), and **L10** (12.6 mg, 0.015 mmol, 15 mol%) were added into a 4 mL glass bottle in 1 mL Tetrahydrofuran (THF). The mixture was stirred at room temperature for 30 mins, then brominated fluoroethanol benzoate (**BFEB**) (29.6 mg, 0.12 mmol, 1.2 equiv.), benzoyl chloride **1a** (14.1 mg, 0.1 mmol, 1.0 equiv.), Mn (16.5 mg, 0.3 mmol, 3 equiv.), cobalt(II) phthalocyanine (CoPc) (2.9 mg, 0.005 mmol, 5 mol%) and *N*-benzylidene-tertbutylamineoxide (**PBN**) (7.1 mg, 0.04 mmol, 0.4 equiv.) was added and keep stirring at $-10\text{ }^\circ\text{C}$ for 1 hours and then analyzed by EPR (Figure S3).

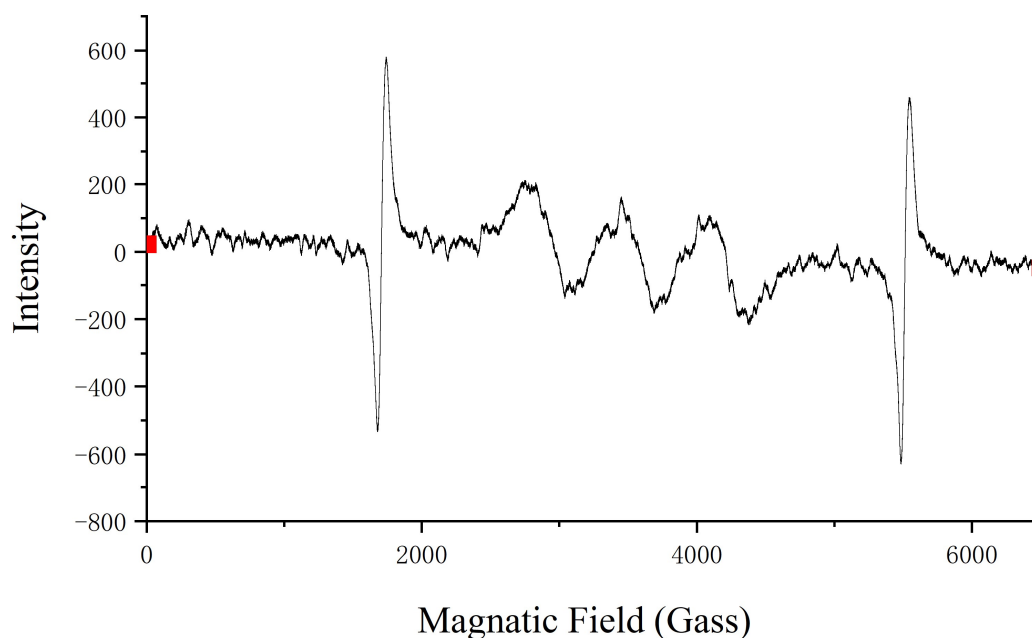


Figure S3. The EPR spectrum of **9**.

MEASUREMENT CONDITIONS

MAGNET FIELD

Sweep time Center field mT Sweep width +/- x mT

AMP

	CH1	CH2
Mod. freq.	<input type="text" value="100.00"/> kHz	<input type="text" value="2nd"/> Mode
Mod. width +/-	<input type="text" value="1.0"/> x <input type="text" value="0.1"/> mT	<input type="text" value="2.000"/> x <input type="text" value="1"/> Amplitude
Phase	<input type="text" value="0"/> deg	<input type="text" value="0"/> deg
	<input type="text" value="10.00"/> x <input type="text" value="100"/> s	<input type="text" value="0.03"/> s

MICRO WAVE

Frequency MHz Power mW Phase Coupling

Accumulation Date Mn ESR data

Total waves Tempe UCR2M Length

SEQUENTIAL CONTROL

- + (From To)

Index

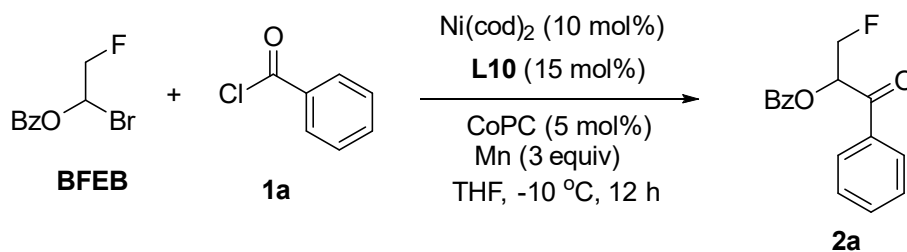
CLOSE

PX CONDITIONS

LOOK

PRINT

Figure S4. The measurement conditions of EPR.



In a glove box, Ni(cod)_2 (2.8 mg, 0.01 mmol, 10 mol%), and **L10** (12.6 mg, 0.015 mmol, 15 mol%) were added into a 4 mL glass bottle in 1 mL Tetrahydrofuran (THF). The mixture was stirred at room temperature for 30 mins, then brominated fluoroethanol benzoate (**BFEB**) (29.6 mg, 0.12 mmol, 1.2 equiv.), benzoyl chloride **1a** (14.1 mg, 0.1 mmol, 1.0 equiv.), Mn (16.5 mg, 0.3 mmol, 3 equiv.), cobalt(II) phthalocyanine (CoPc) (2.9 mg, 0.005 mmol, 5 mol%) was added and keep stirring at $-10\text{ }^\circ\text{C}$ for 1 hours and then analyzed by EPR (Figure S5).

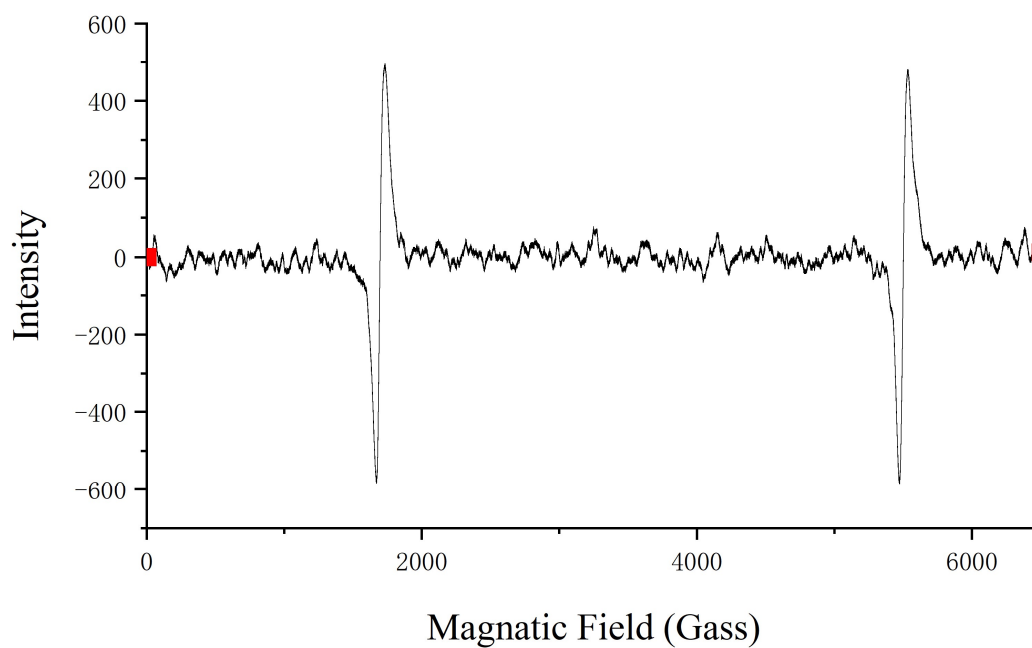


Figure S5. The EPR spectrum of **2a**.

N-benzylidene-tertbutylamineoxide (**PBN**) (7.1 mg, 0.04 mmol, 0.4 equiv.) was added into a 4 mL glass bottle in 1 mL Tetrahydrofuran (THF) and then analyzed by EPR (Figure S6).

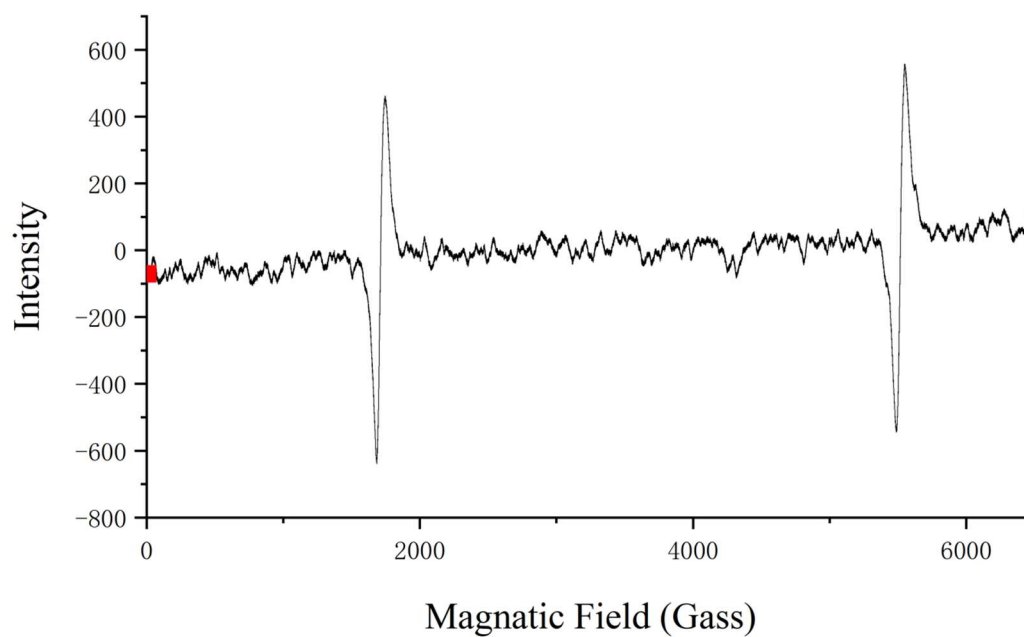
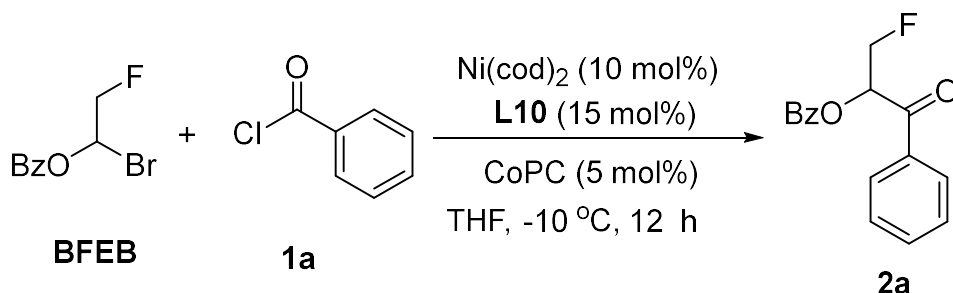
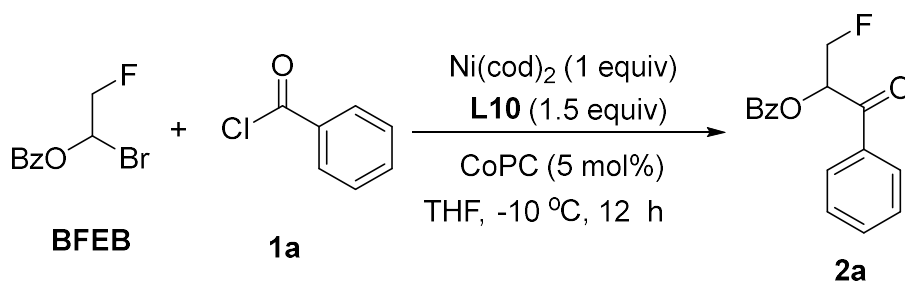


Figure S6. The EPR spectrum of PBN in THF

8.3 Stoichiometric reaction

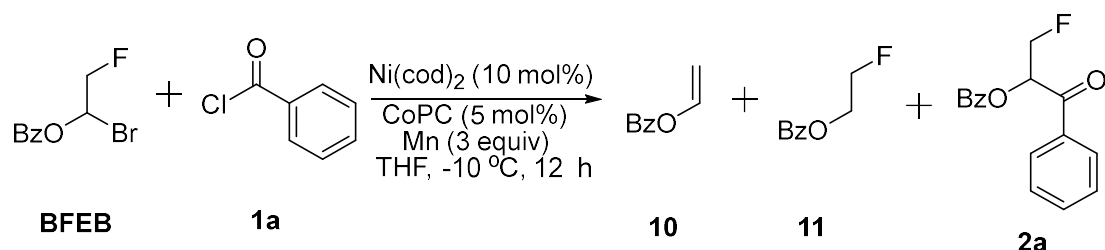


In a glove box, $\text{Ni}(\text{cod})_2$ (2.8 mg, 0.01 mmol, 10 mol%), and **L1** (12.6 mg, 0.015 mmol, 15 mol%) were added into a 4 mL glass bottle in 1 mL Tetrahydrofuran (THF). The mixture was stirred at room temperature for 30 mins, then brominated fluoroethanol benzoate (**BFEB**) (29.6 mg, 0.12 mmol, 1.2 equiv.), benzoyl chloride **1a** (14.1 mg, 0.1 mmol, 1.0 equiv.), cobalt(II) phthalocyanine (CoPc) (2.9 mg, 0.005 mmol, 5 mol%) was added and keep stirring at $-10\text{ }^\circ\text{C}$ for 12 hours. Detected **2a** (trace) through TLC.



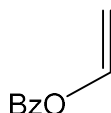
In a glove box, $\text{Ni}(\text{cod})_2$ (27.5 mg, 0.1 mmol, 1.0 equiv.), and **L10** (125.8 mg, 0.15 mmol, 1.5 equiv.) were added into a 4 mL glass bottle in 1 mL Tetrahydrofuran (THF). The mixture was stirred at room temperature for 30 mins, then brominated fluoroethanol benzoate (**BFEB**) (29.6 mg, 0.12 mmol, 1.2 equiv.), benzoyl chloride **1a** (14.1 mg, 0.1 mmol, 1.0 equiv.), cobalt(II) phthalocyanine (CoPc) (2.9 mg, 0.005 mmol, 5 mol%) was added and keep stirring at $-10\text{ }^\circ\text{C}$ for 12 hours. After evaporation under reduced pressure to remove the solvent, the mixture was passed through a short column of silica gel to remove the metal complex. The residue was purified by flash chromatography on silica gel (PE : EA = 50: 1) to afford the desired product **2a** (21.8 mg, 80% yield, 93% ee).

8.4 Ligand effect and side-products examination



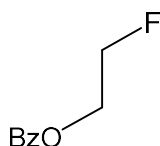
In a glove box, Ni(cod)₂ (27.5 mg, 0.1 mmol, 10 mol%), brominated fluoroethanol benzoate (**BFEB**) (0.30 g, 1.2 mmol, 1.2 equiv.), benzoyl chloride **1a** (0.14 g, 1 mmol, 1.0 equiv.), Mn (0.16 g, 3 mmol, 3 equiv.), cobalt(II) phthalocyanine (CoPc) (28.6 mg, 0.05 mmol, 5 mol%) were added into 50 mL Schlenk flask equipped with a stirring bar in 10 mL Tetrahydrofuran (THF). The mixture was stirred at -10 °C for 12 hours. After evaporation under reduced pressure to remove the solvent, the mixture was passed through a short column of silica gel to remove the metal complex. The residue was purified by flash chromatography on silica gel (PE : EA = 50: 1) to afford the product **10** (78.5 mg, 53% yield), product **11** (30.3 mg, 18% yield), product **2a** (trace).

vinyl benzoate(**10**)



78.5 mg, 53% yield, PE : EA = 100: 1. Yellow oil; ¹H NMR (500 MHz, Chloroform-*d*) δ 8.03 (d, *J* = 7.6 Hz, 2H), 7.56 – 7.47 (m, 1H), 7.44 (dd, *J* = 14.0, 6.3 Hz, 1H), 7.38 (t, *J* = 7.7 Hz, 2H), 5.05 – 4.58 (m, 2H). ¹³C NMR (126 MHz, Chloroform-*d*) δ 163.7, 141.5, 133.6, 130.0, 129.0, 128.6, 98.3; HRMS (ESI) *m/z* calcd. for C₉H₉O₂ ([M+H]⁺): 149.0603, found 149.0598.

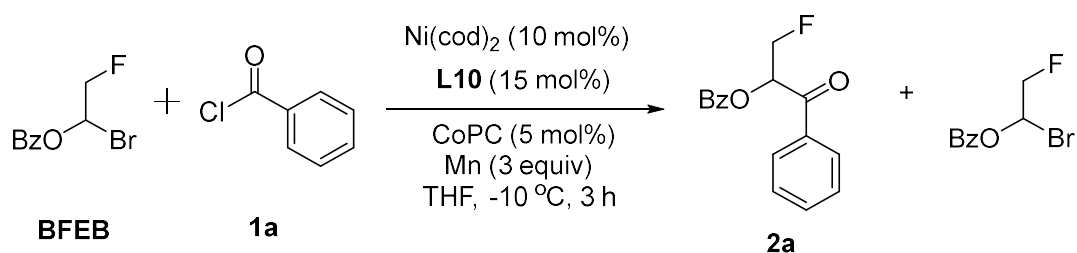
2-fluoroethyl benzoate (**11**)



30.3 mg, 18% yield, PE : EA = 50: 1. Yellow oil; ¹H NMR (500 MHz, Chloroform-*d*)

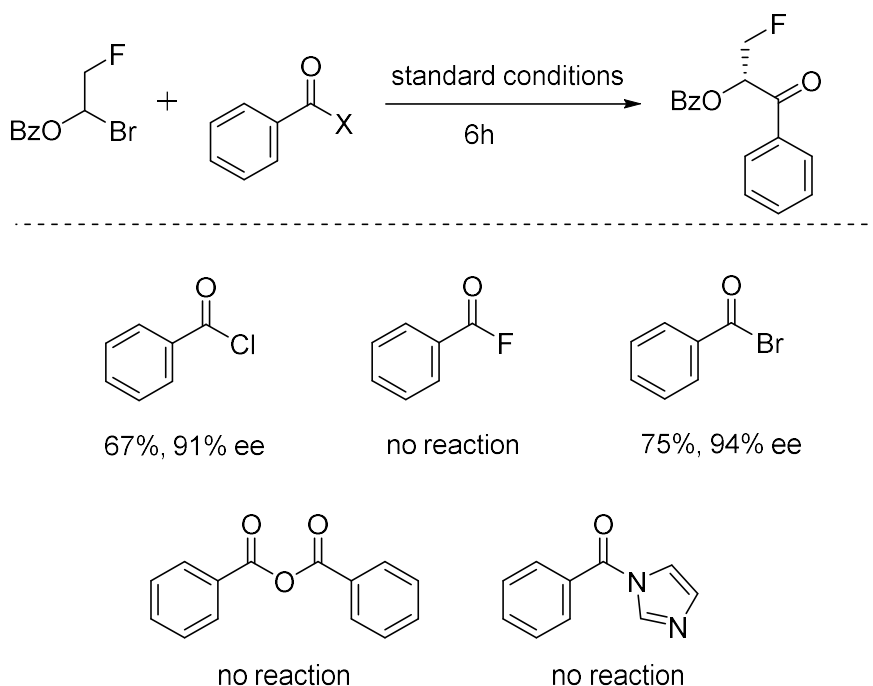
δ 8.12 – 8.04 (m, 2H), 7.61 – 7.54 (m, 1H), 7.45 (t, $J = 7.8$ Hz, 2H), 4.85 – 4.48 (m, 2H), 4.71 – 4.57 (m, 2H). ^{19}F NMR (470 MHz, Chloroform- d) δ -224.31 – -224.68 (m). ^{13}C NMR (126 MHz, Chloroform- d) δ 165.4, 132.2, 128.7, 128.7, 127.4, 80.4 (d, $J = 170.8$ Hz), 62.8 (d, $J = 20.2$ Hz); HRMS (ESI) m/z calcd. for $\text{C}_9\text{H}_9\text{O}_2\text{NaF}$ ($[\text{M}+\text{Na}]^+$): 191.0484, found 191.0487.

8.5 Probing the kinetic resolution of starting material



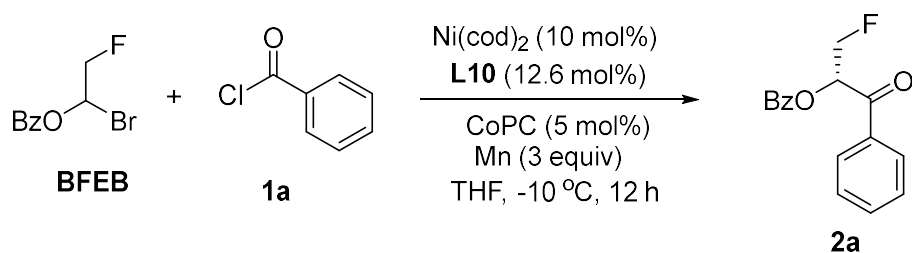
In a glove box, $\text{Ni}(\text{cod})_2$ (2.8 mg, 0.01 mmol, 10 mol%), and **L10** (12.6 mg, 0.015 mmol, 15 mol%) were added into a 4 mL glass bottle in 1 mL Tetrahydrofuran (THF). The mixture was stirred at room temperature for 30 mins, then brominated fluoroethanol benzoate (**BFEB**) (29.6 mg, 0.12 mmol, 1.2 equiv.), benzoyl chloride **1a** (14.1 mg, 0.1 mmol, 1.0 equiv.), Mn (16.5 mg, 0.3 mmol, 3 equiv.), cobalt(II) phthalocyanine (CoPc) (2.9 mg, 0.005 mmol, 5 mol%) and keep stirring at -10°C for 3 hours. After evaporation under reduced pressure to remove the solvent, the mixture was passed through a short column of silica gel to remove the metal complex. The residue was purified by flash chromatography on silica gel (PE : EA = 50: 1) to afford the desired product **2a** (14.2 mg, 52% yield, 92% ee) and the recovered **BFEB** (14.6 mg, 59% yield, 1.5% ee).

8.6 Comparing experiments with various acyl donors



In a glove box, Ni(cod)₂ (2.8 mg, 0.01 mmol, 10 mol%), and **L10** (12.6 mg, 0.015 mmol, 15 mol%) were added into a 4 mL glass bottle in 1 mL Tetrahydrofuran (THF). The mixture was stirred at room temperature for 30 mins, then brominated fluoroethanol benzoate (**BFEB**) (29.6 mg, 0.12 mmol, 1.2 equiv.), acyl donors (0.1 mmol, 1.0 equiv.), Mn (16.5 mg, 0.3 mmol, 3 equiv.), cobalt(II) phthalocyanine (CoPc) (2.9 mg, 0.005 mmol, 5 mol%) and keep stirring at -10 °C for 6 hours. After evaporation under reduced pressure to remove the solvent, the mixture was passed through a short column of silica gel to remove the metal complex. The residue was purified by flash chromatography on silica gel (PE : EA = 50: 1) to afford the desired product **2a**. Acyl donors = benzoyl chloride, afford the desired product **2a** (18.2 mg, 67% yield, 91% ee). Acyl donors = benzoyl bromide, afford the desired product **2a** (20.4 mg, 75% yield, 94% ee).

8.7 Nonlinear Effect Study



In a glove box, Ni(cod)₂ (2.8 mg, 0.01 mmol, 10 mol%), (4*S*,4'*S*,5*R*,5'*R*)-**L10** and (4*R*,4'*R*,5*S*,5'*S*)-**L10** (Table S1) were added into a 4 mL glass bottle in 1 mL Tetrahydrofuran (THF). The mixture was stirred at room temperature for 30 mins, then brominated fluoroethanol benzoate (**BFEB**) (29.6 mg, 0.12 mmol, 1.2 equiv.), benzoyl chloride **1a** (14.1 mg, 0.1 mmol, 1.0 equiv.), Mn (16.5 mg, 0.3 mmol, 3 equiv.), cobalt(II) phthalocyanine (CoPc) (2.9 mg, 0.005 mmol, 5 mol%) and keep stirring at -10 °C for 12 hours. After evaporation under reduced pressure to remove the solvent, the mixture was passed through a short column of silica gel to remove the metal complex. The residue was purified by flash chromatography on silica gel (PE : EA = 50: 1) to afford the desired product **2a**. The enantiomeric excess was determined by Chiral HPLC (Table S1, Figure S7).

entry	ee of L10 (%)	(4 <i>S</i> ,4' <i>S</i> ,5 <i>R</i> ,5' <i>R</i>)- L10 (mol%)	(4 <i>R</i> ,4' <i>R</i> ,5 <i>S</i> ,5' <i>S</i>)- L10 (mol%)	ee of 2a (%)
1	20	7.6	5	11
2	40	8.8	3.8	32
3	60	10.1	2.5	54
4	80	11.3	1.3	79
5	99	12.6	0	93

Table S1. The amount of chiral ligand **L10** and ee of **2a**

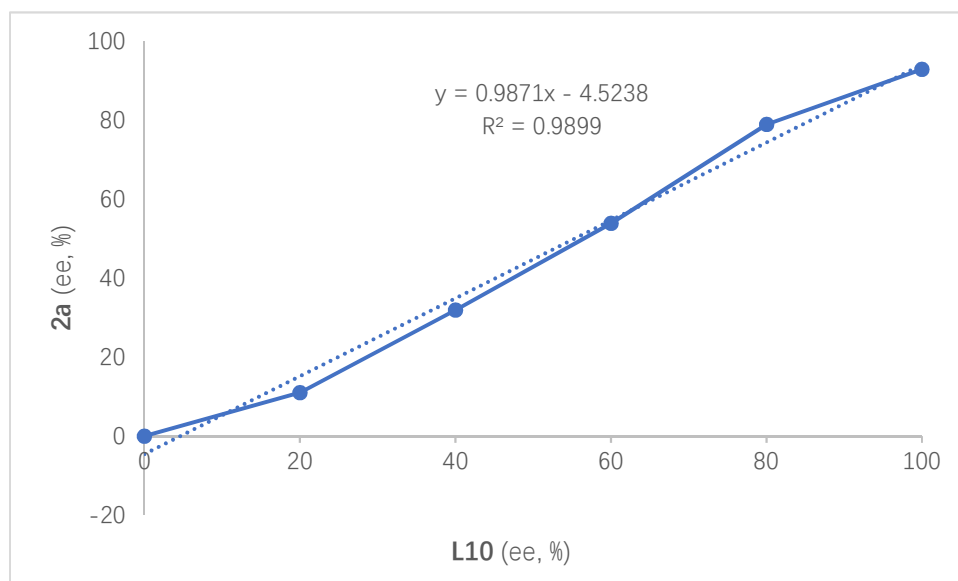


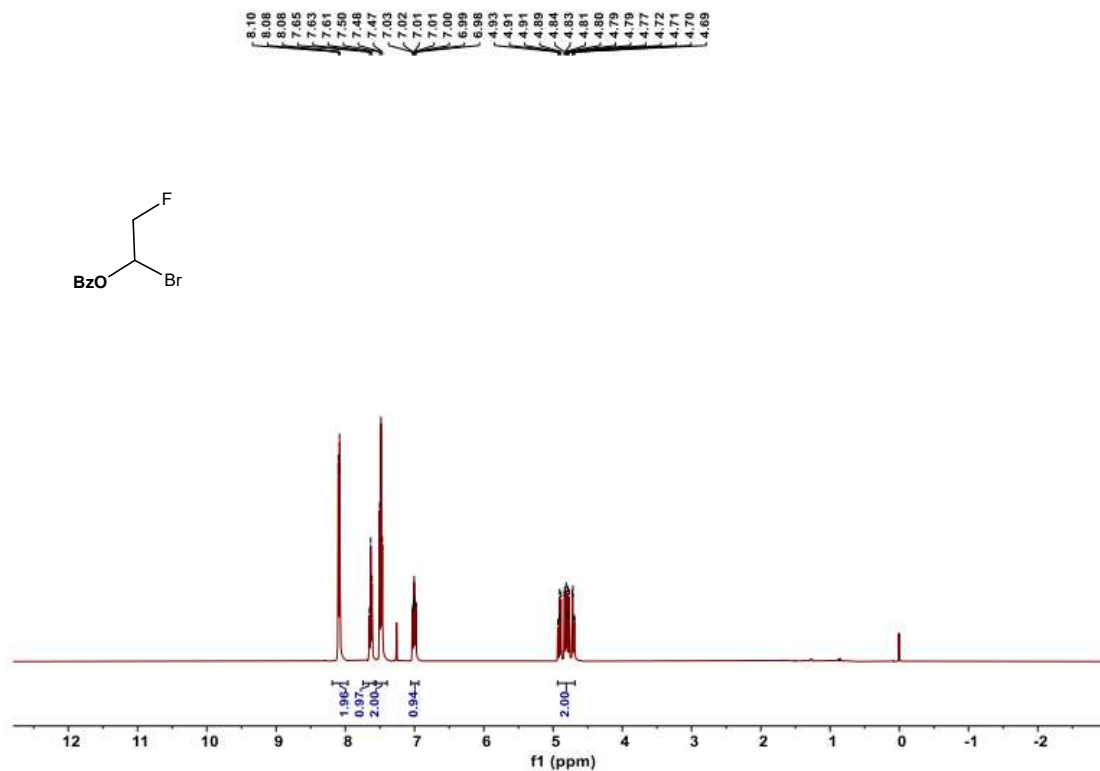
Figure S7. The ee of **2a** correlates linearly with the ee of the chiral ligand **L10**.

9 References

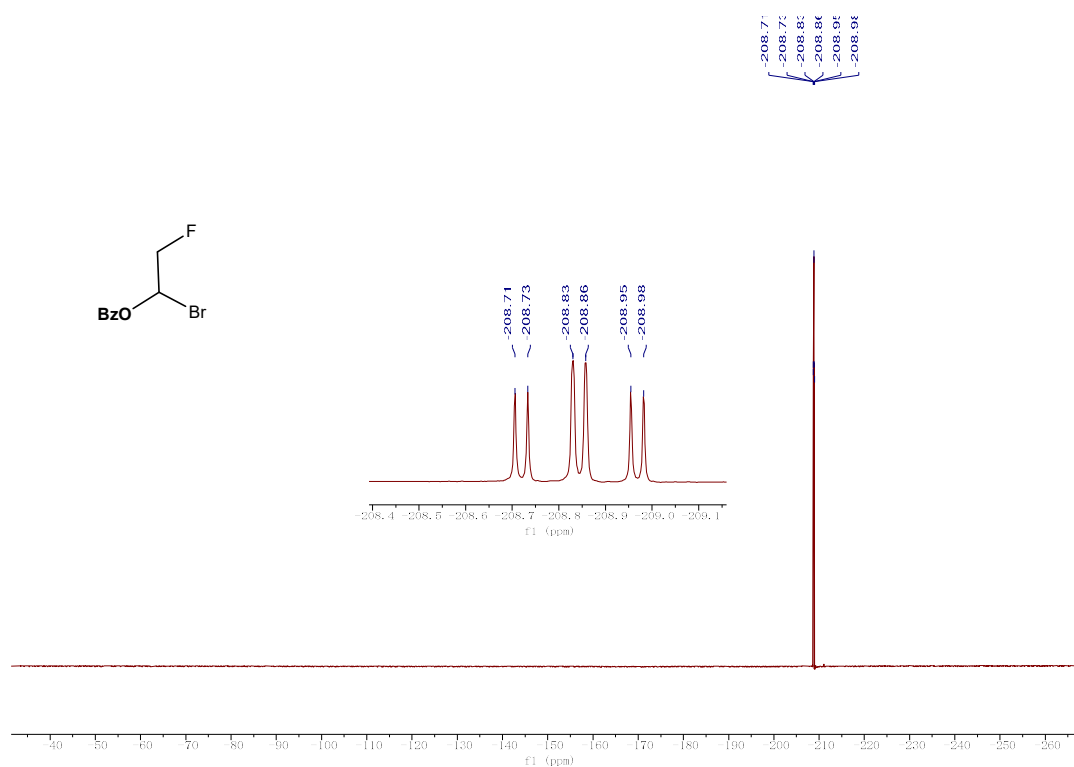
- [1] X.-Q. Mou, F.-M. Rong, H. Zhang, G. Chen, G. He, *Org. Lett.*, 2019, **21**, 4657–4661.
- [2] J. Wu, H. Wu, X. Liu, Y. Zhang, G. Huang, C. Zhang, *Org. Lett.*, 2022, **24**, 4322–4327.
- [3] B. Roh, A. O. Farah, B. Kim, T. Feoktistova, F. Moeller, K. D. Kim, P. H-Y. Cheong, H. G. Lee, *J. Am. Chem. Soc.*, 2023, **145**, 13, 7075–7083.
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- [5] J. Chen, D. Liu, N. Butt, C. Li, D. Fan, Y. Liu, W. Zhang, *Angew. Chem. Int. Ed.*, 2013, **52**, 11632–11636.
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- [7] H-X. Zhang, J. Nie, H. Cai, J-A. Ma, *Org. Lett.*, 2014, **16**, 2542–2545.

10 NMR spectra of the related compound

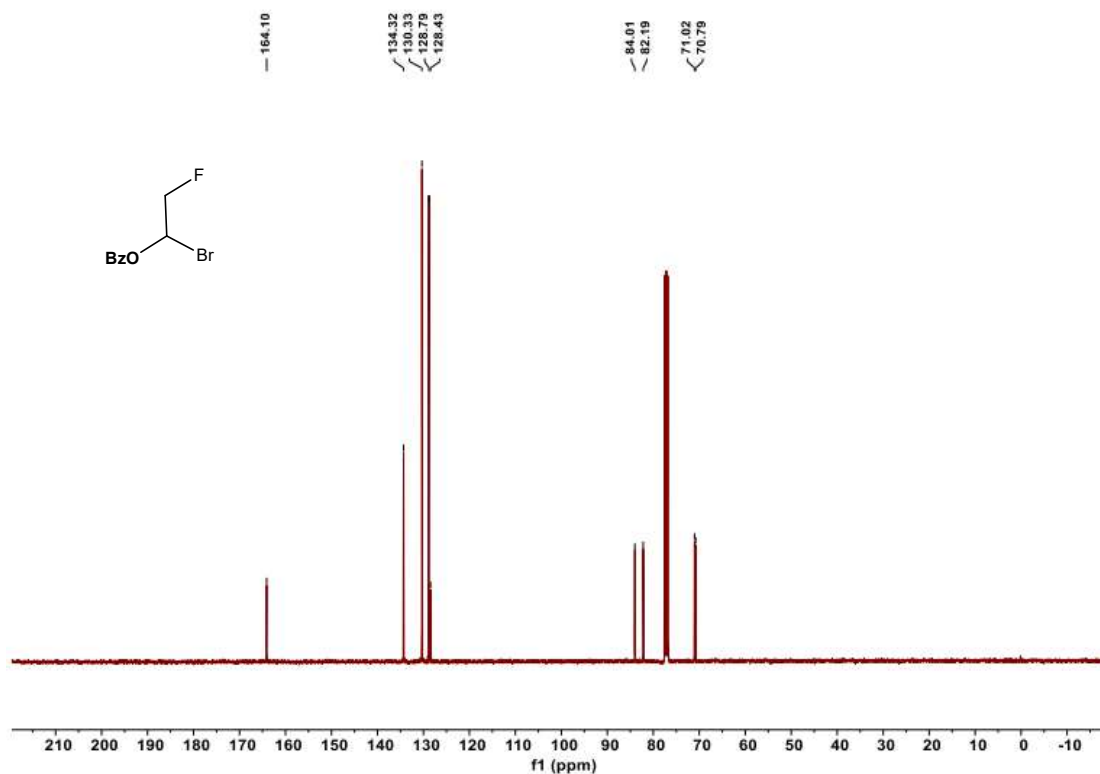
^1H , ^{13}C , and ^{19}F NMR spectra of **BFEB**



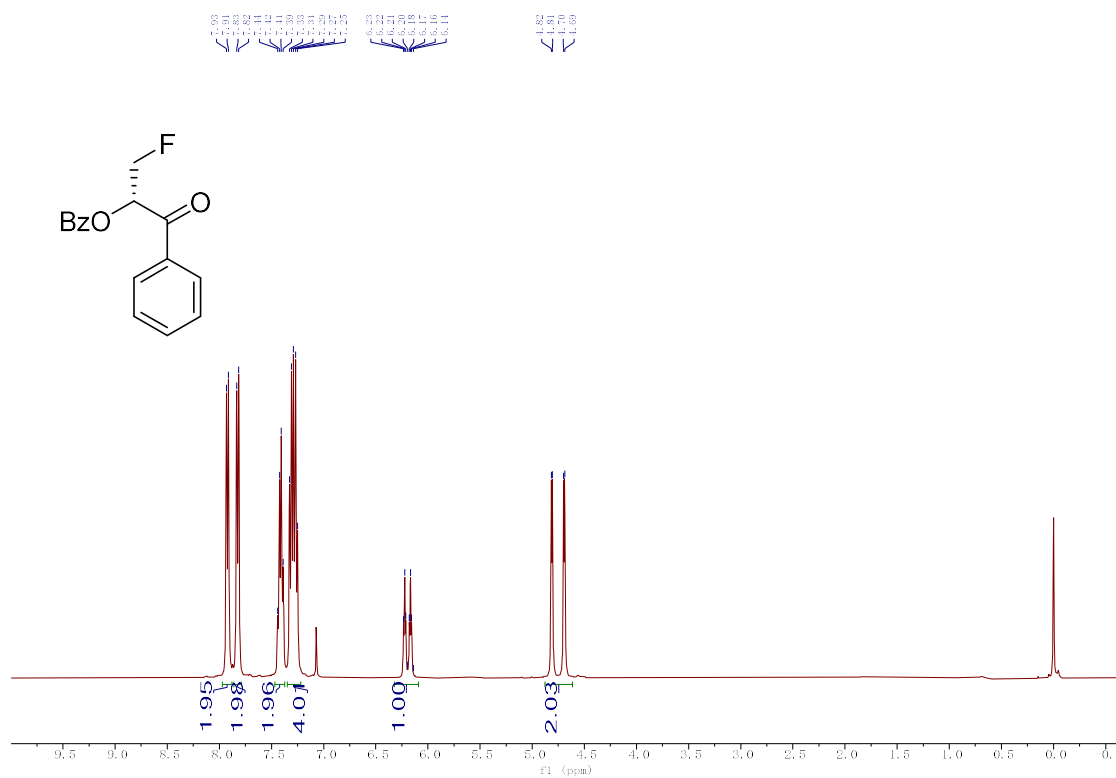
^1H NMR (400 MHz, Chloroform-*d*) of **BFEB**



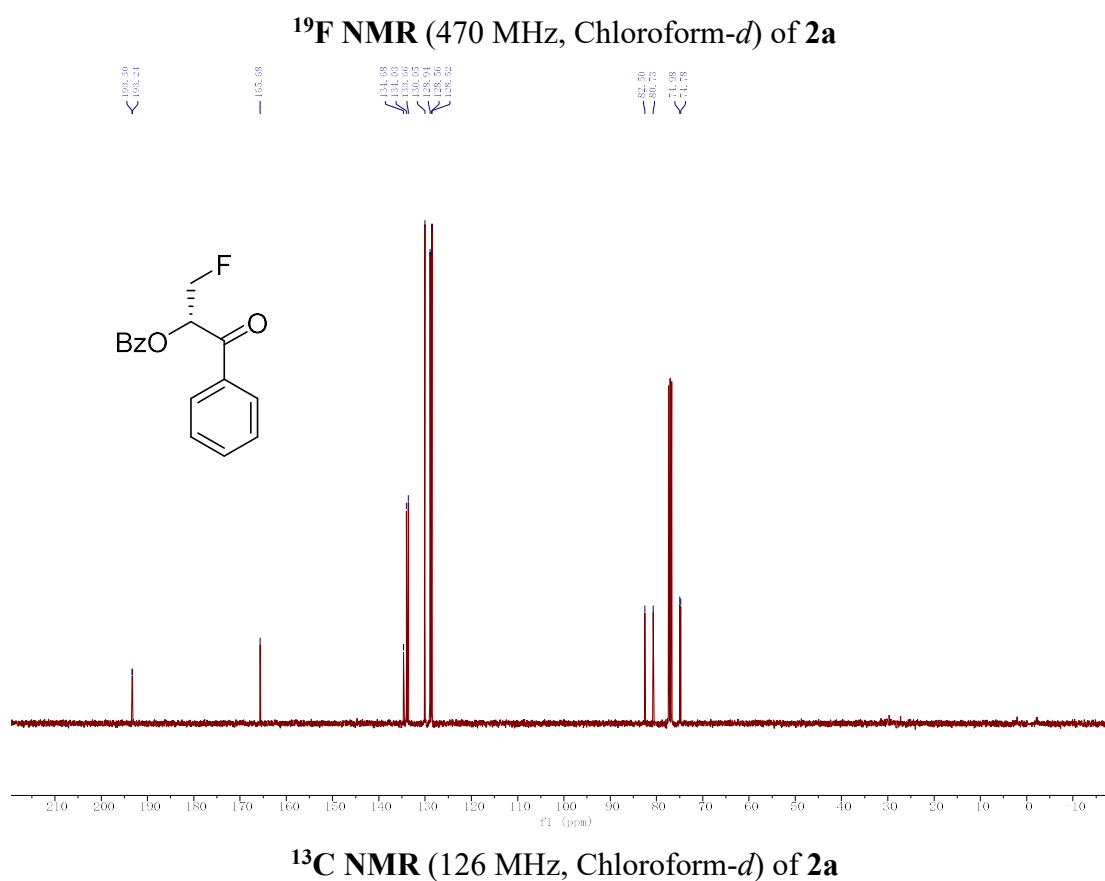
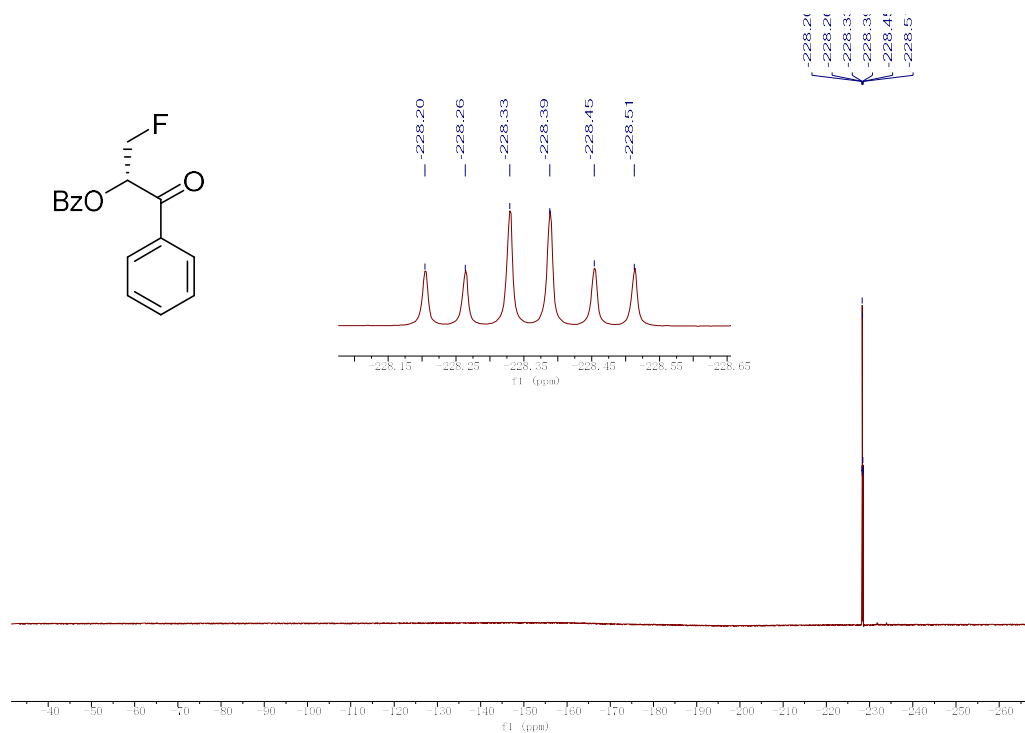
^{19}F NMR (376 MHz, Chloroform-*d*) of **BFEB**



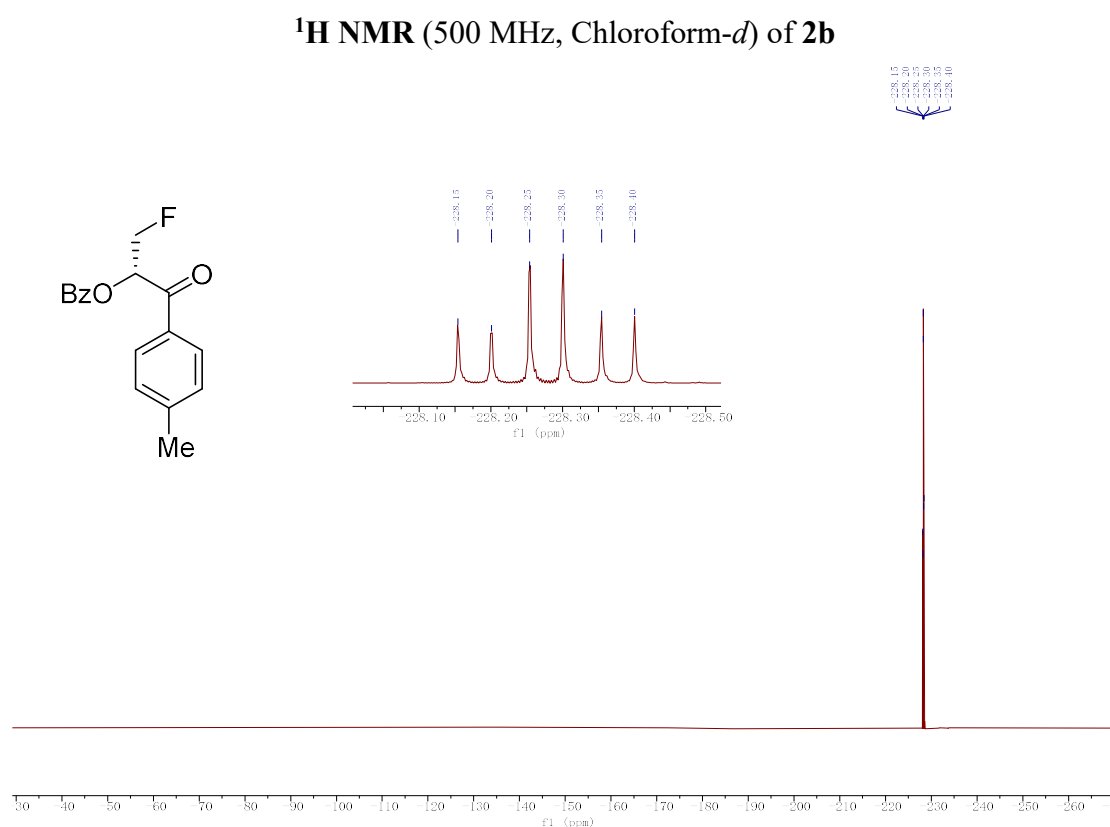
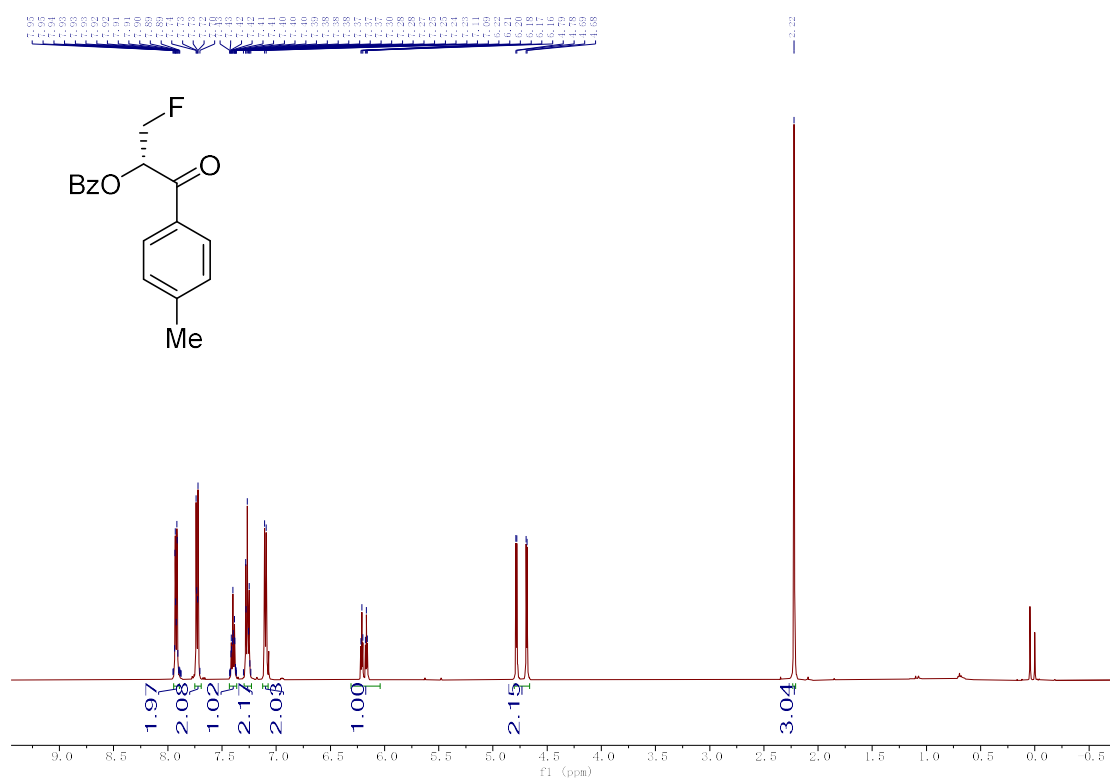
^{13}C NMR (101 MHz, Chloroform-*d*) of BFEb
 ^1H , ^{13}C , and ^{19}F NMR spectra of **2a**

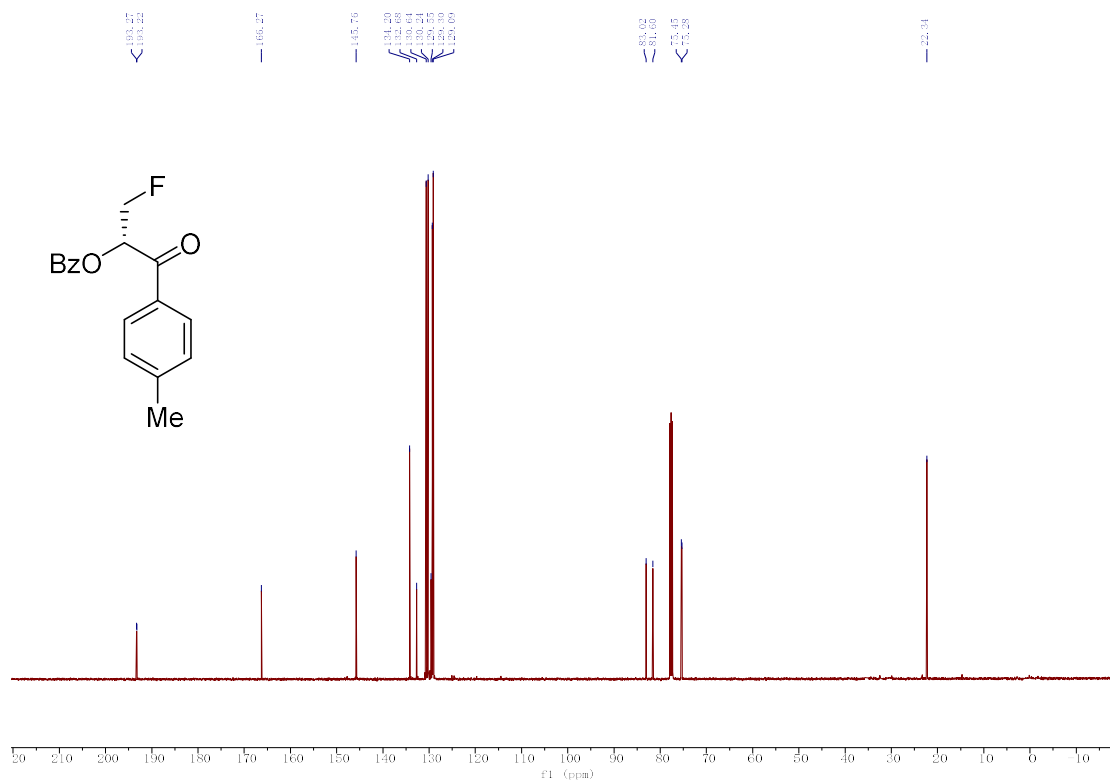


^1H NMR (500 MHz, Chloroform-*d*) of **2a**

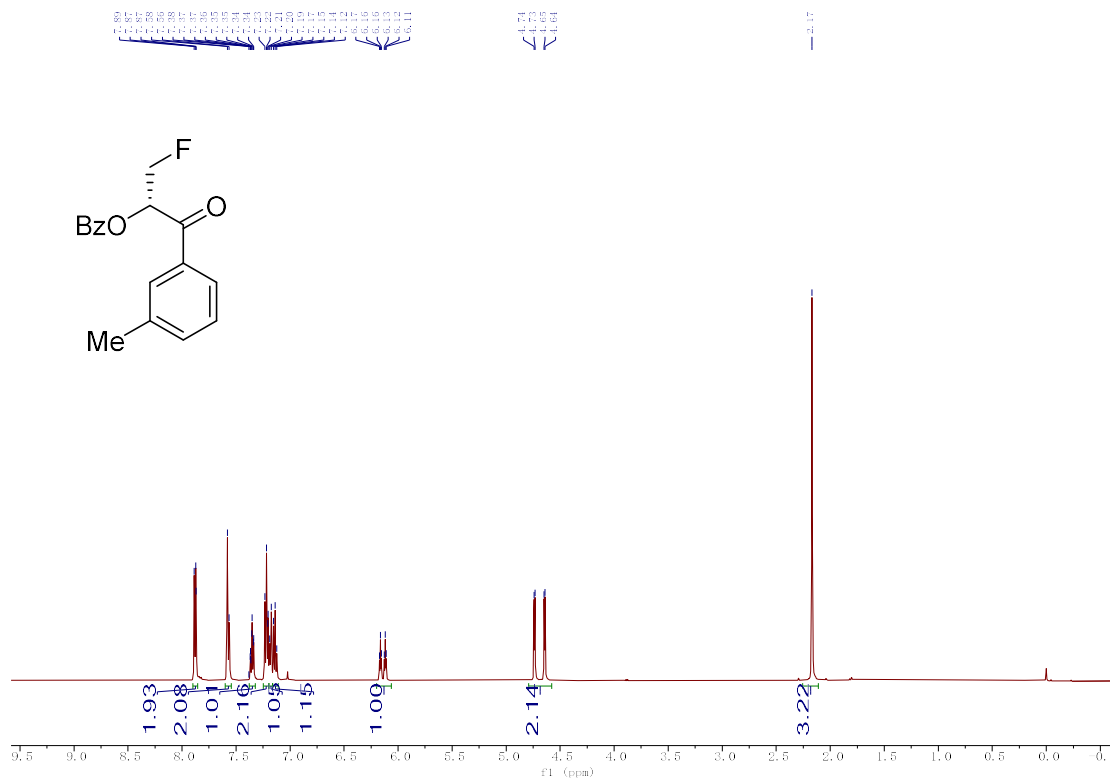


^1H , ^{13}C , and ^{19}F NMR spectra of **2b**

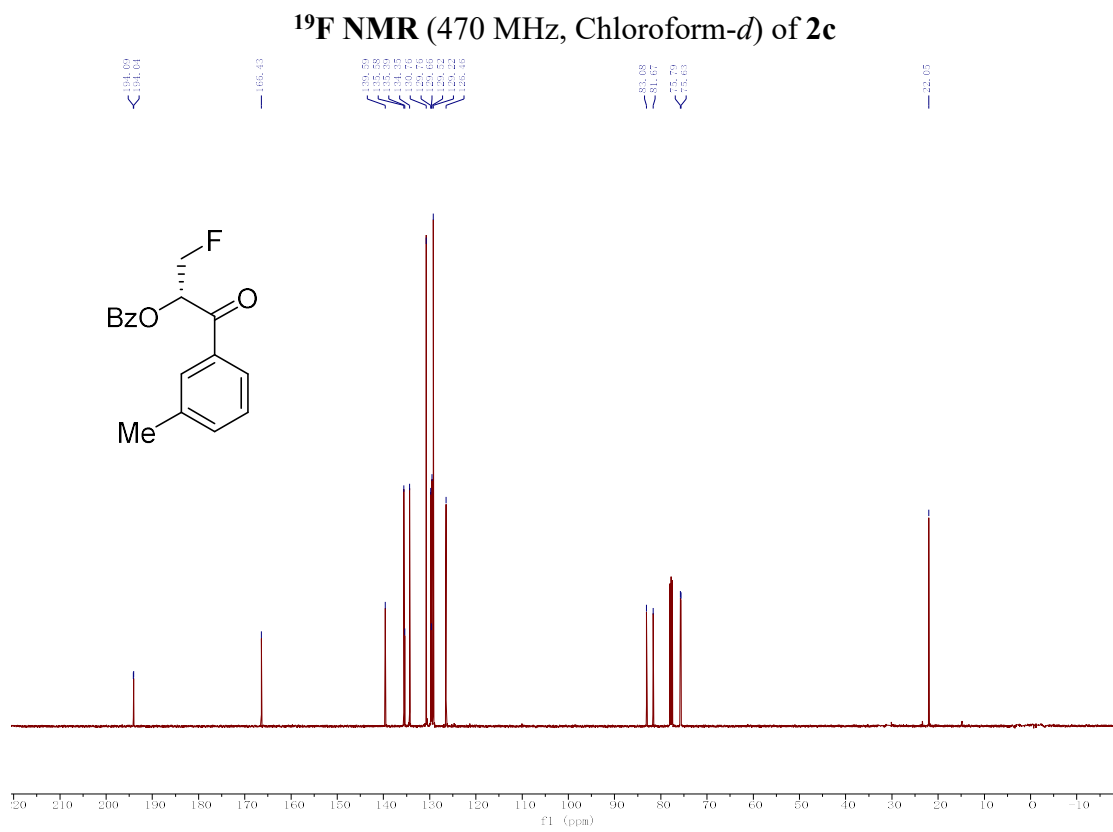
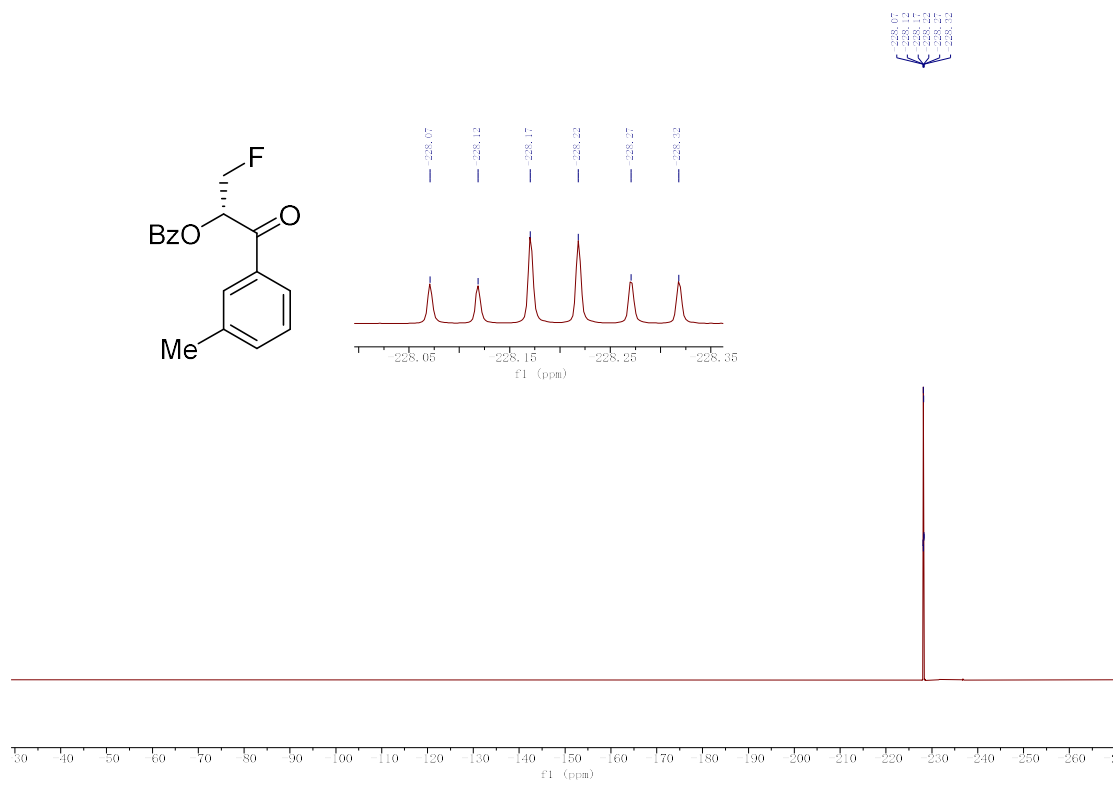




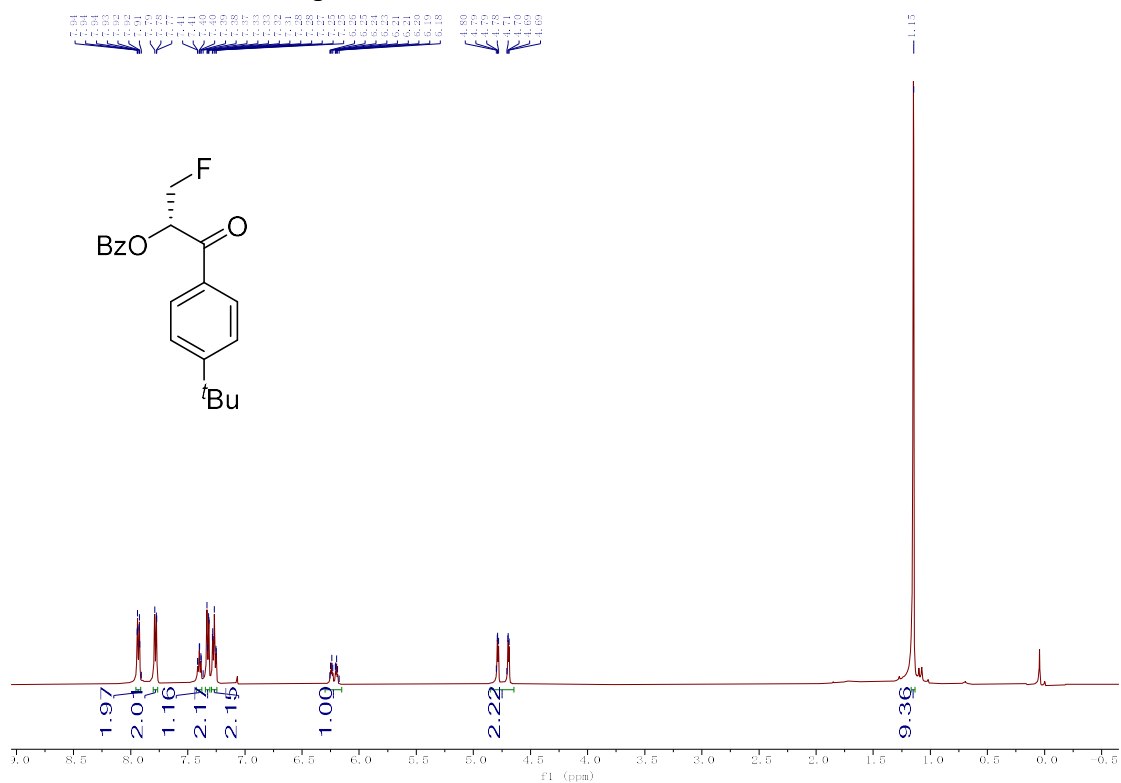
¹³C NMR (126 MHz, Chloroform-*d*) of **2b**
¹H, ¹³C, and ¹⁹F NMR spectra of **2c**



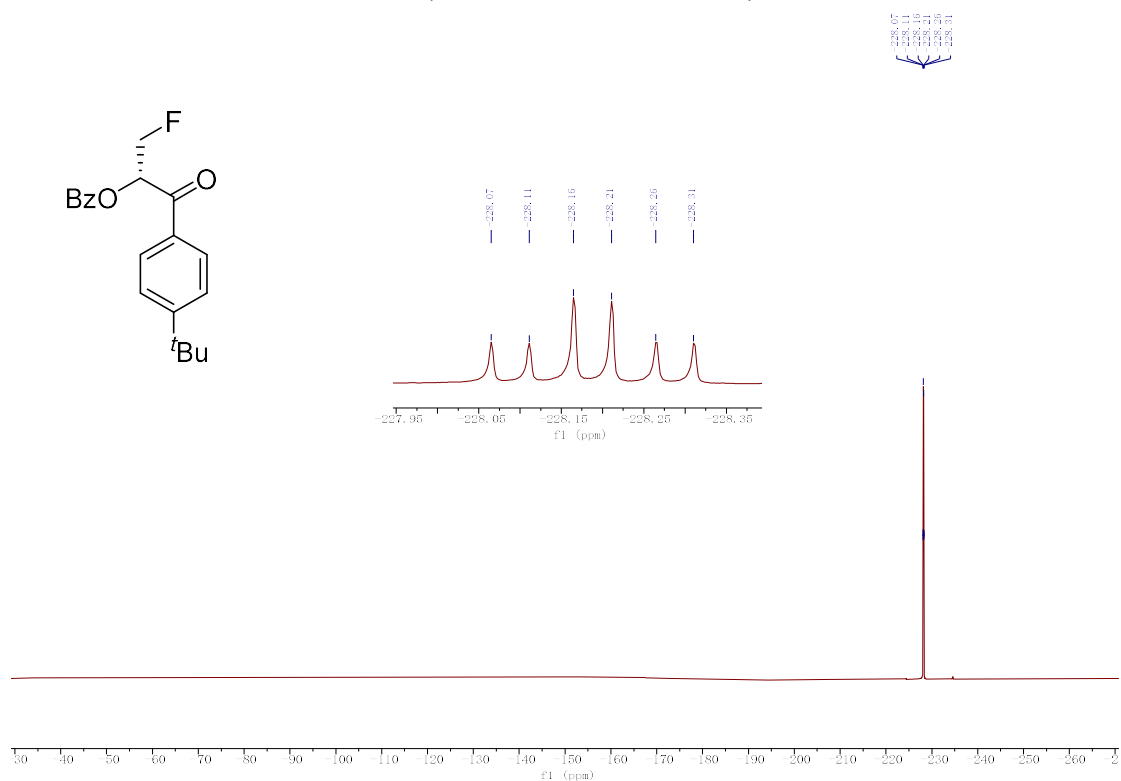
¹H NMR (500 MHz, Chloroform-*d*) of **2c**



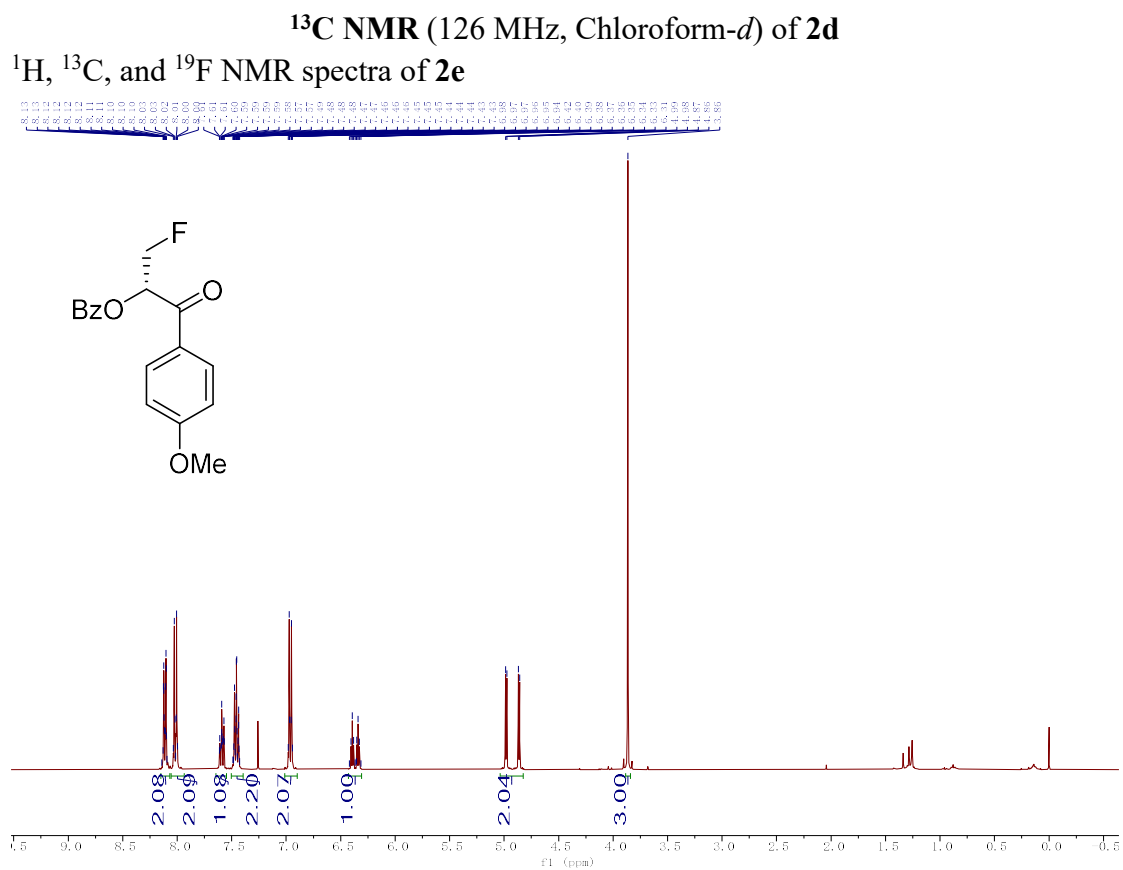
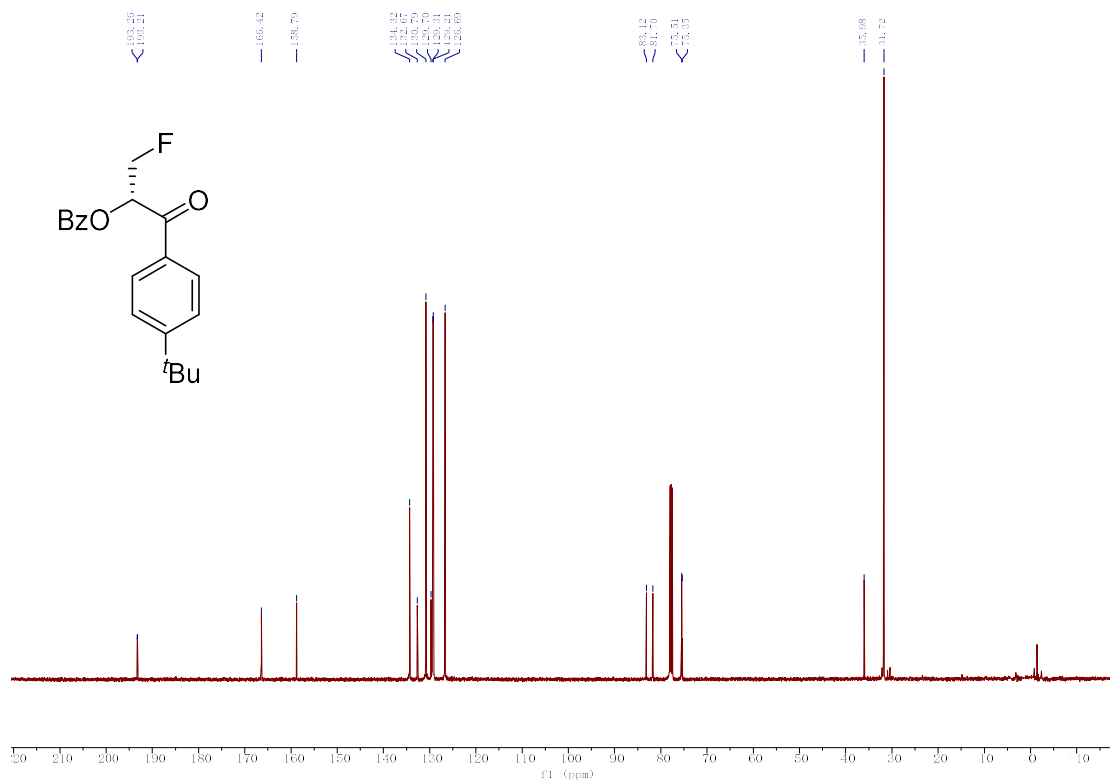
^1H , ^{13}C , and ^{19}F NMR spectra of **2d**

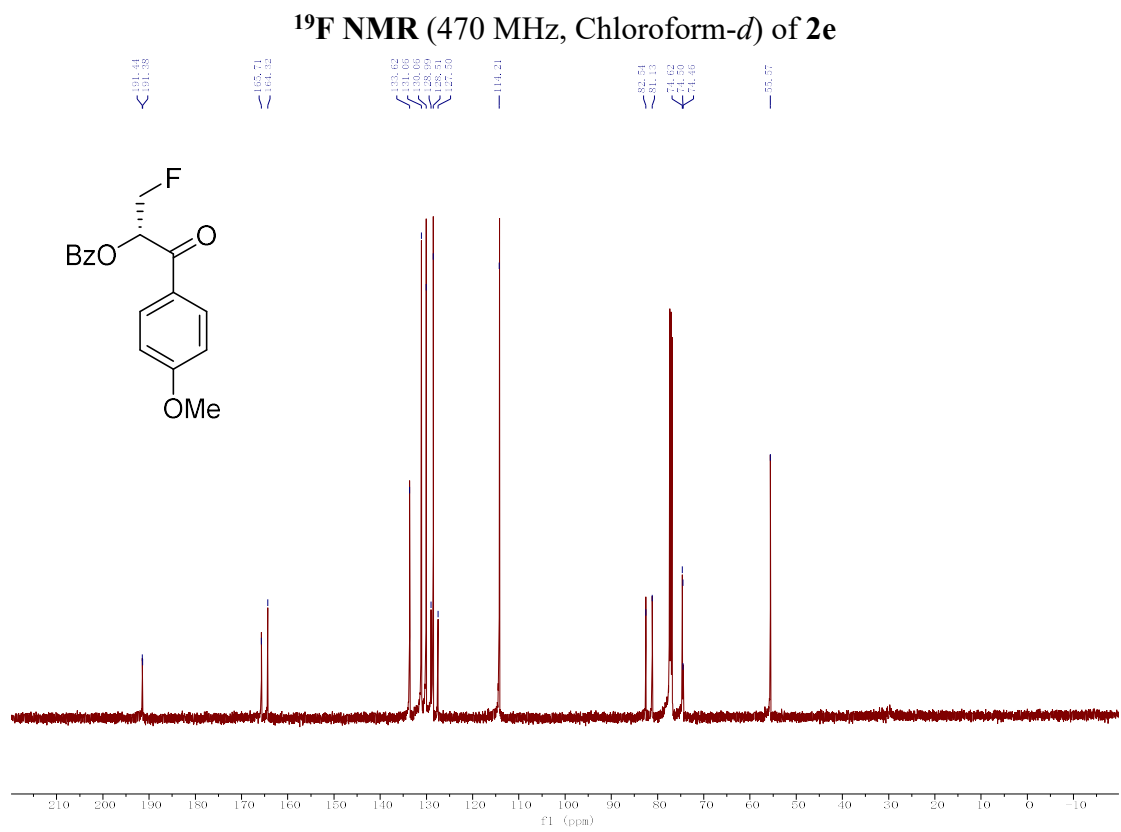
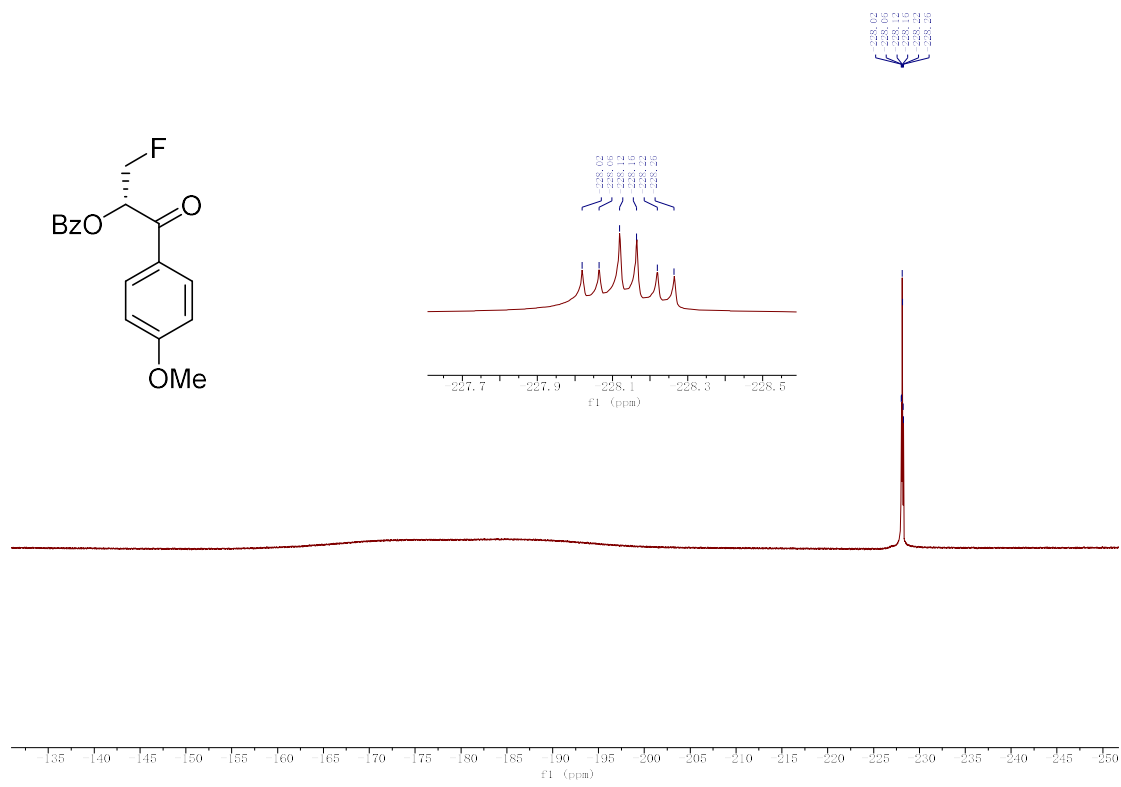


^1H NMR (500 MHz, Chloroform-*d*) of **2d**

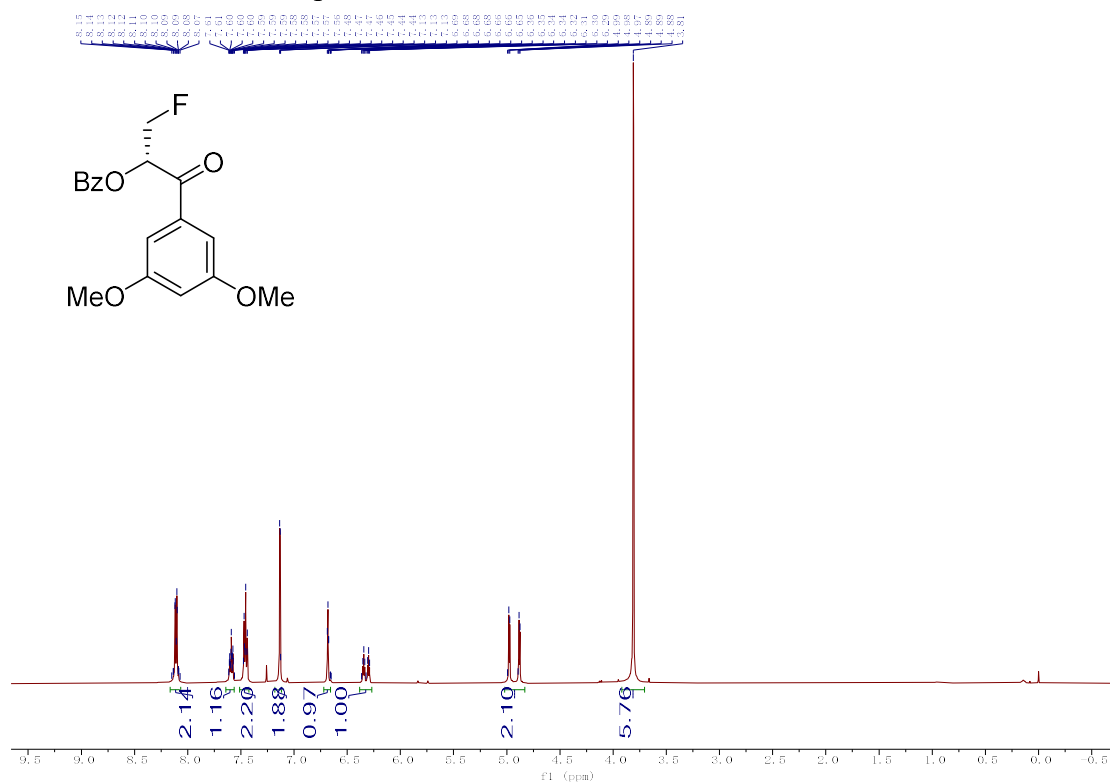


^{19}F NMR (470 MHz, Chloroform-*d*) of **2d**

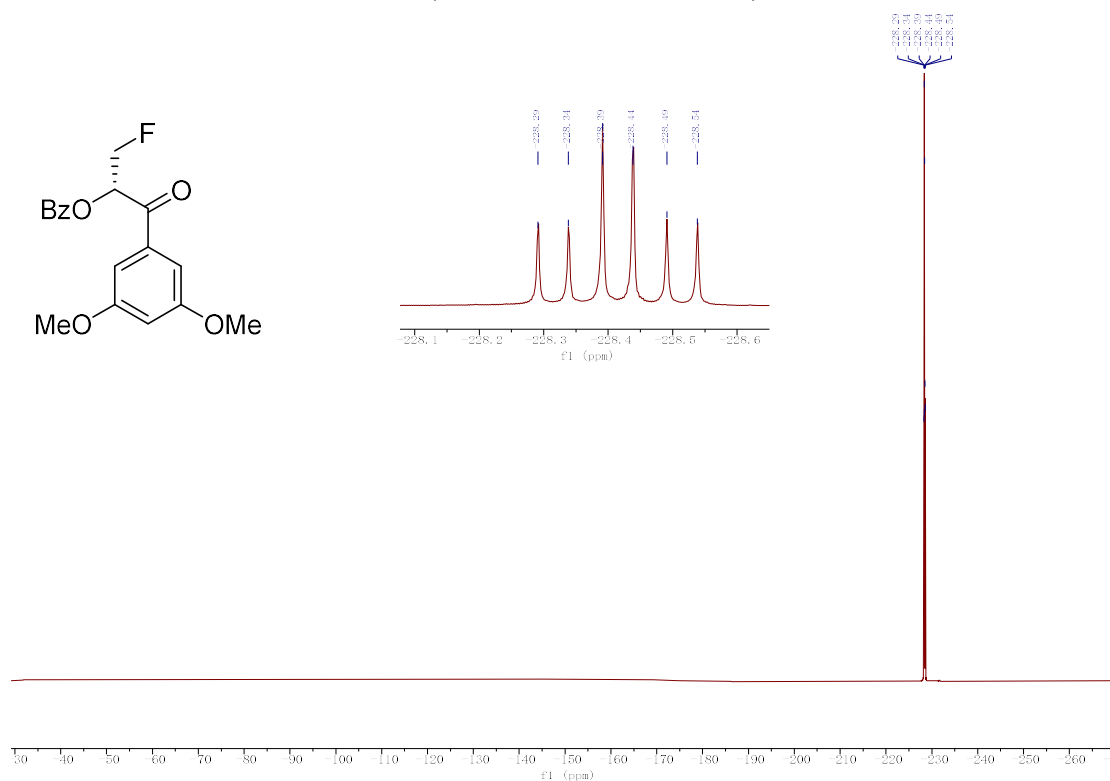




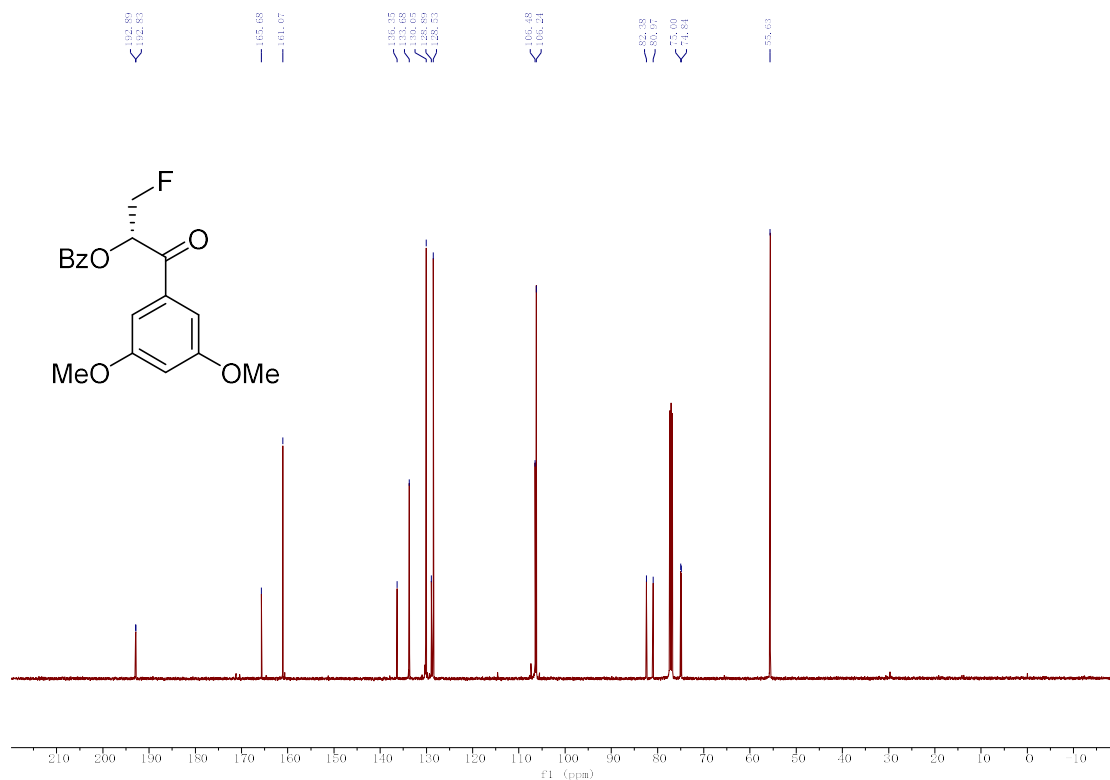
^1H , ^{13}C , and ^{19}F NMR spectra of **2f**



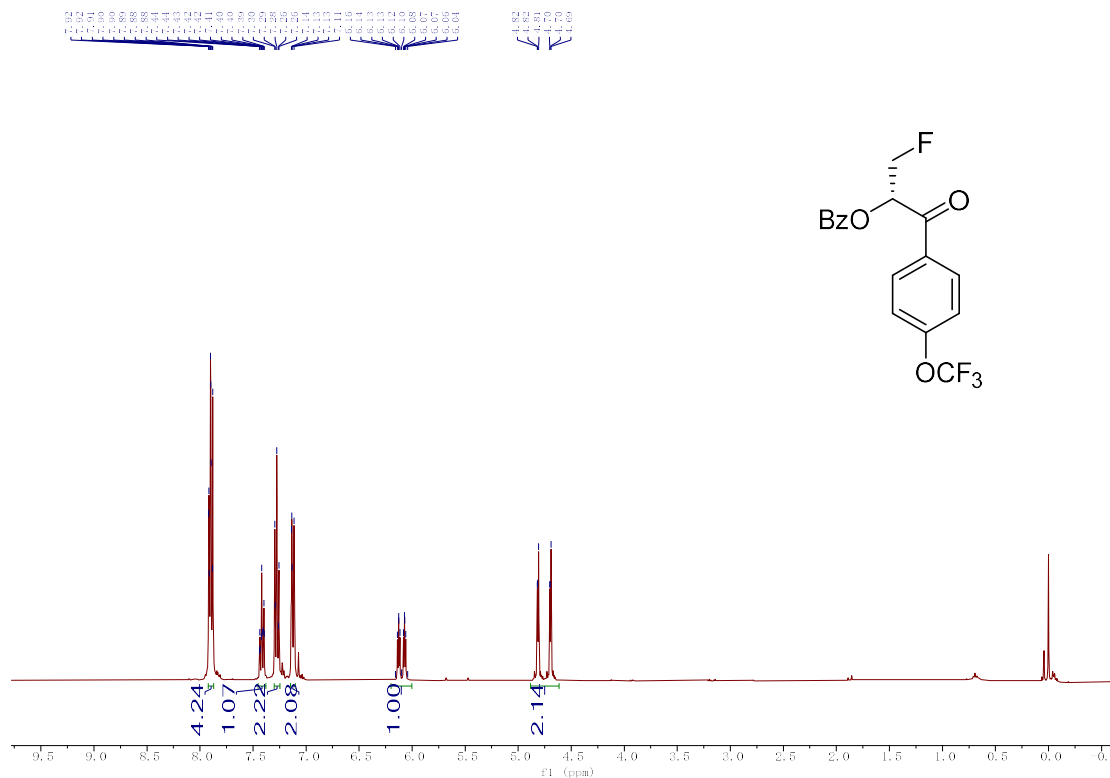
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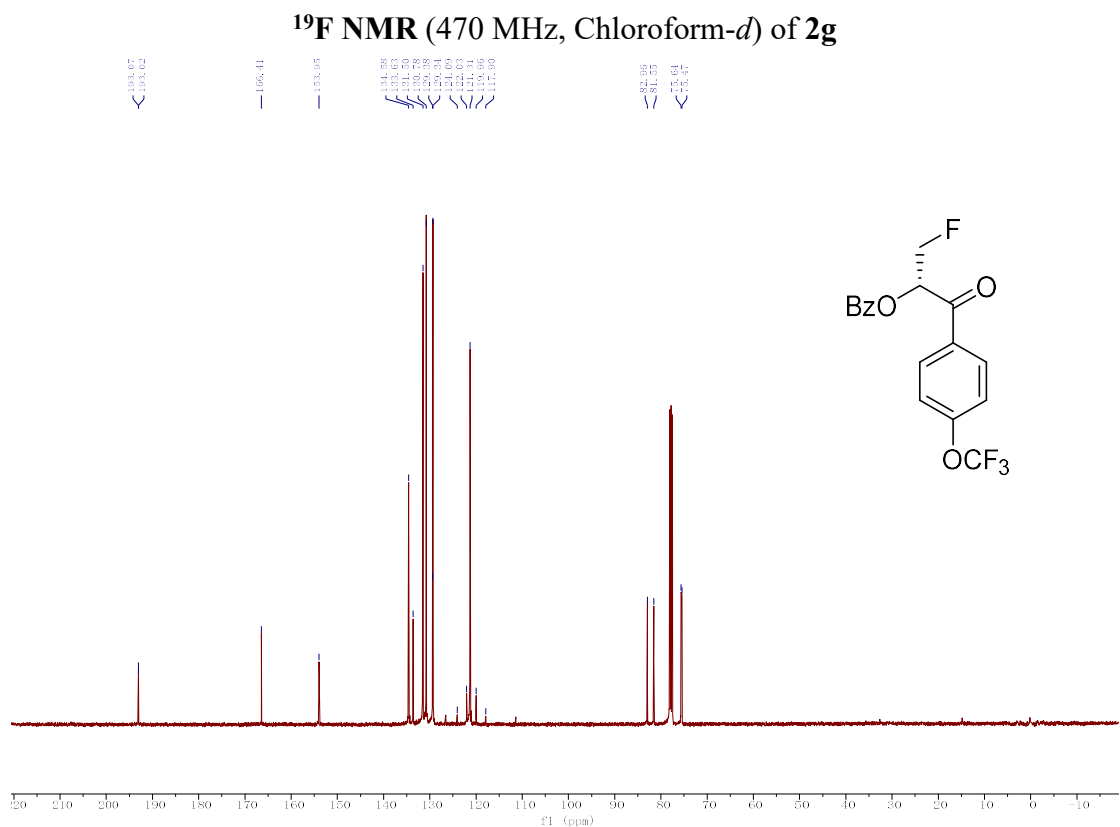
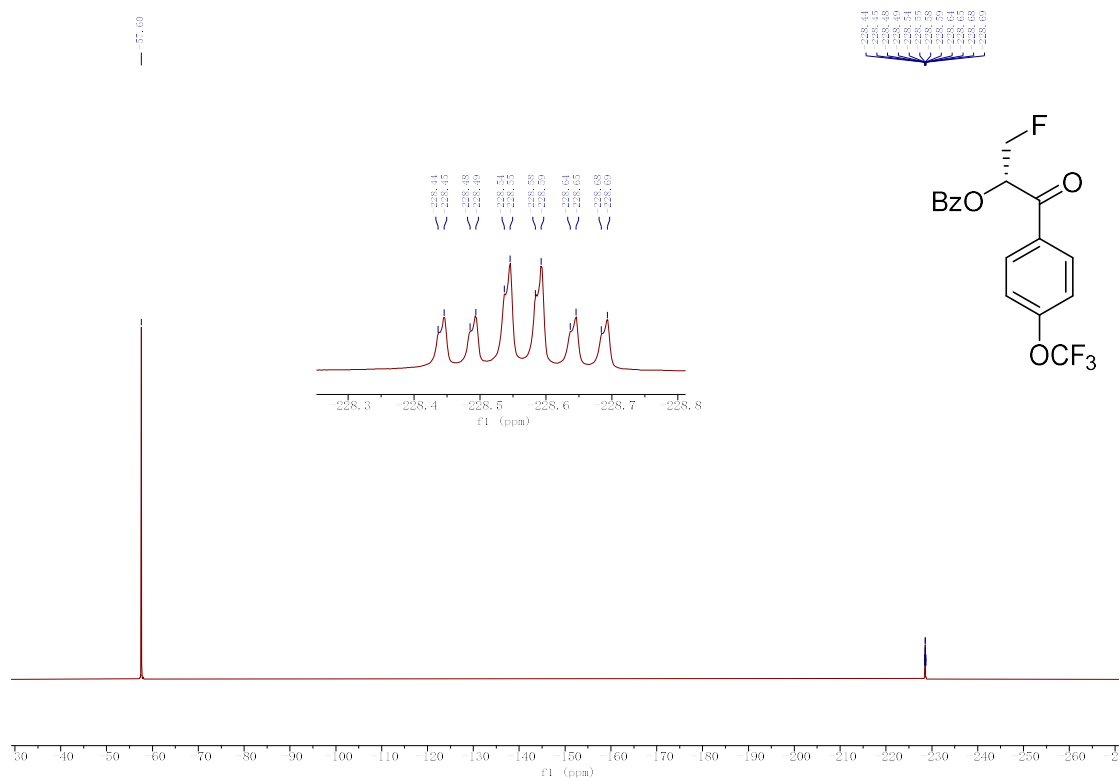
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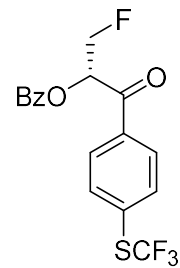
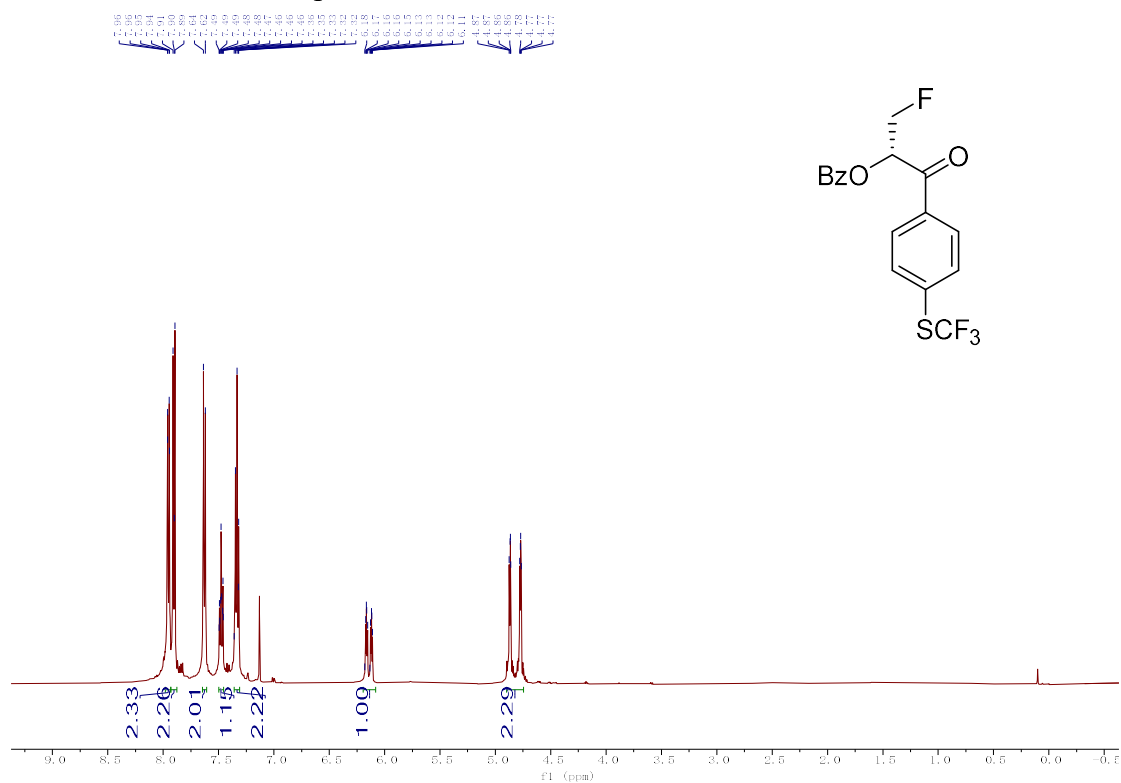
^{13}C NMR (126 MHz, Chloroform-*d*) of **2f**
 ^1H , ^{13}C , and ^{19}F NMR spectra of **2g**



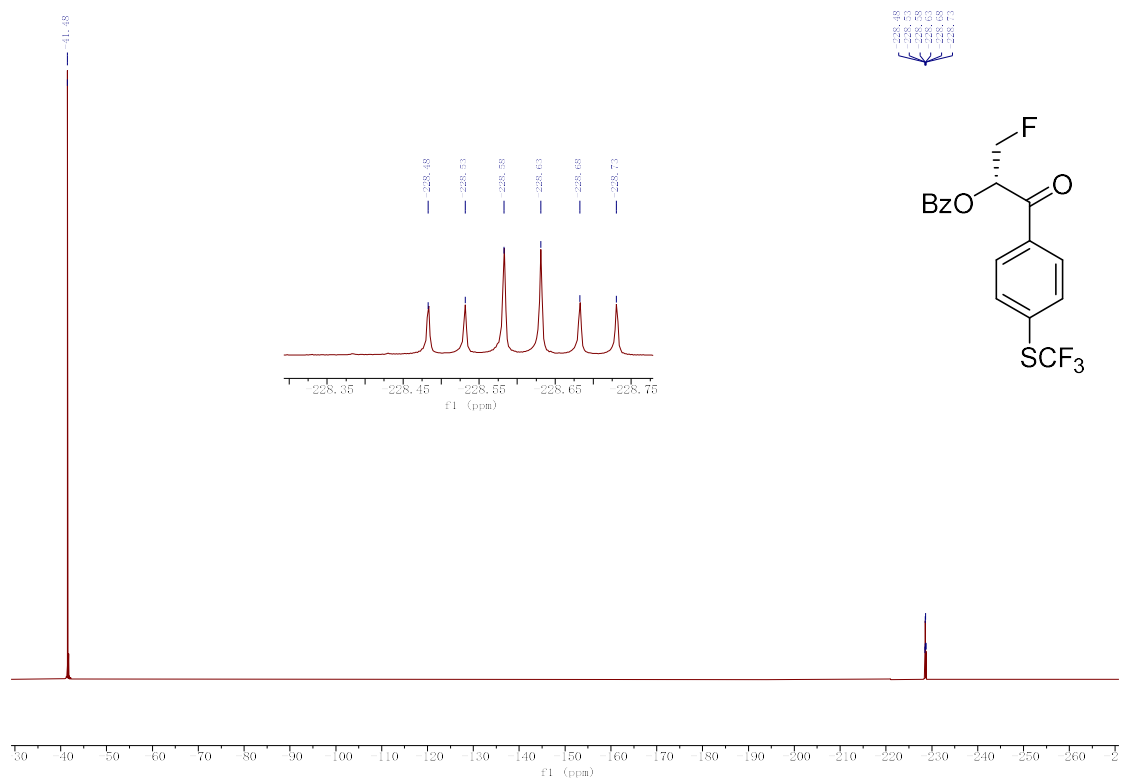
^1H NMR (500 MHz, Chloroform-*d*) of **2g**



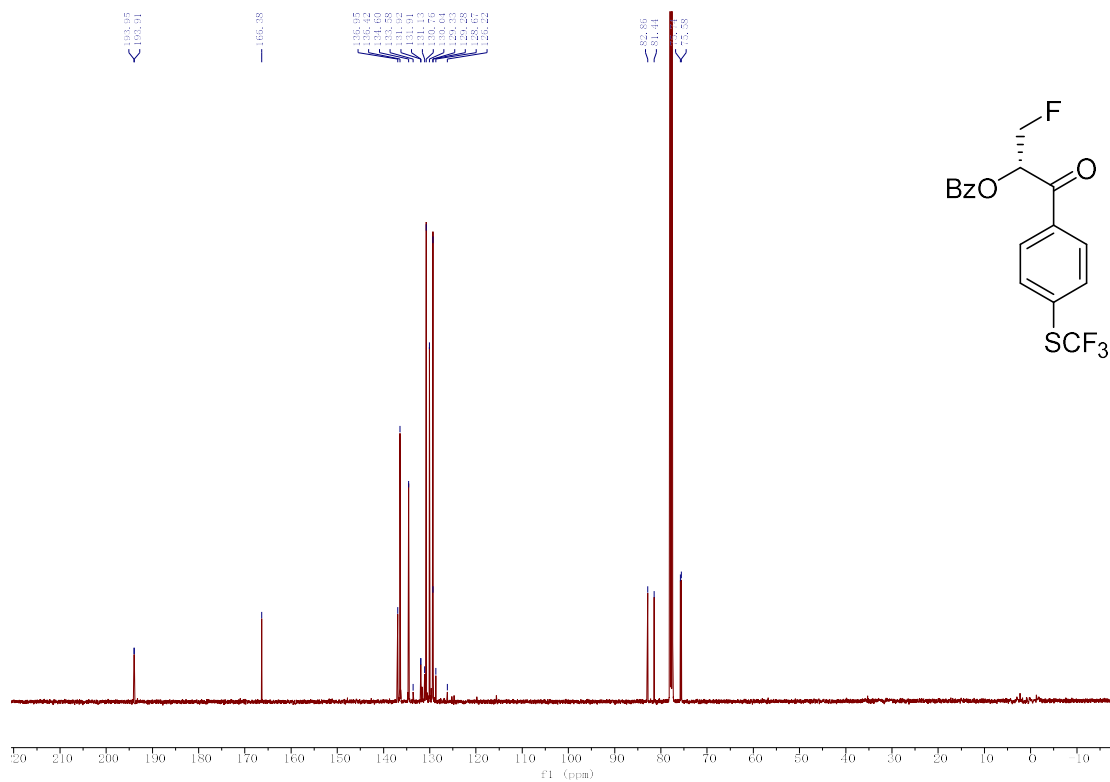
^1H , ^{13}C , and ^{19}F NMR spectra of **2h**



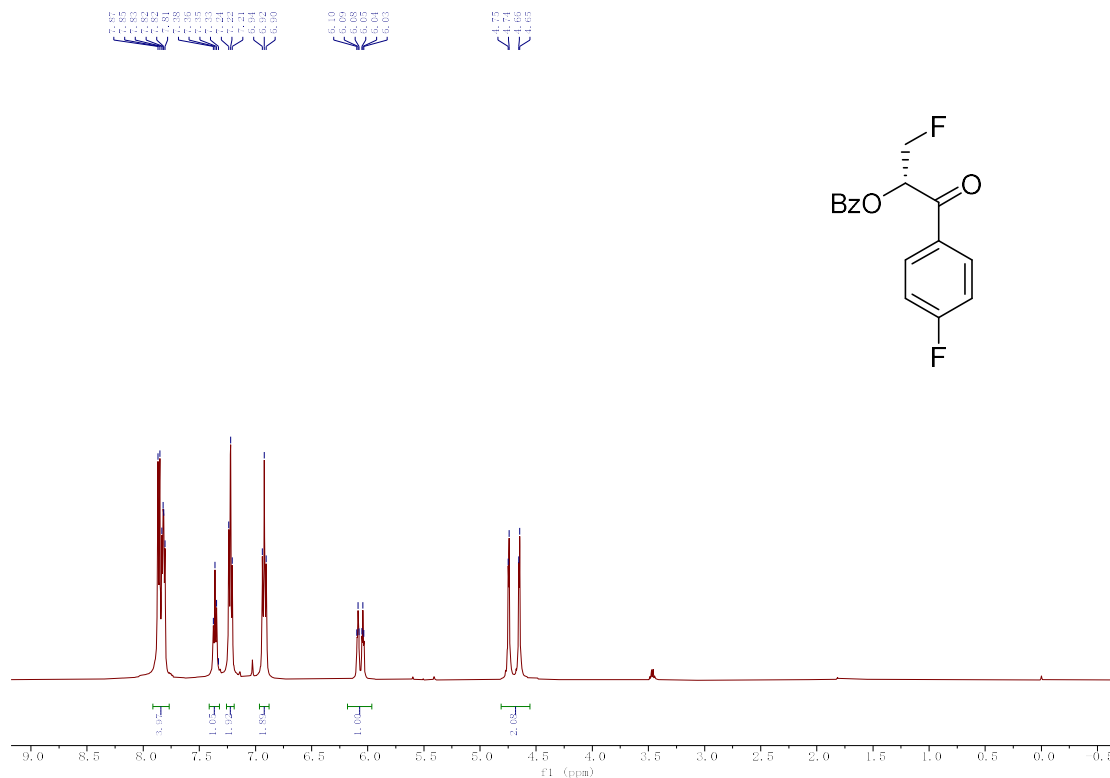
^1H NMR (500 MHz, Chloroform-*d*) of **2h**



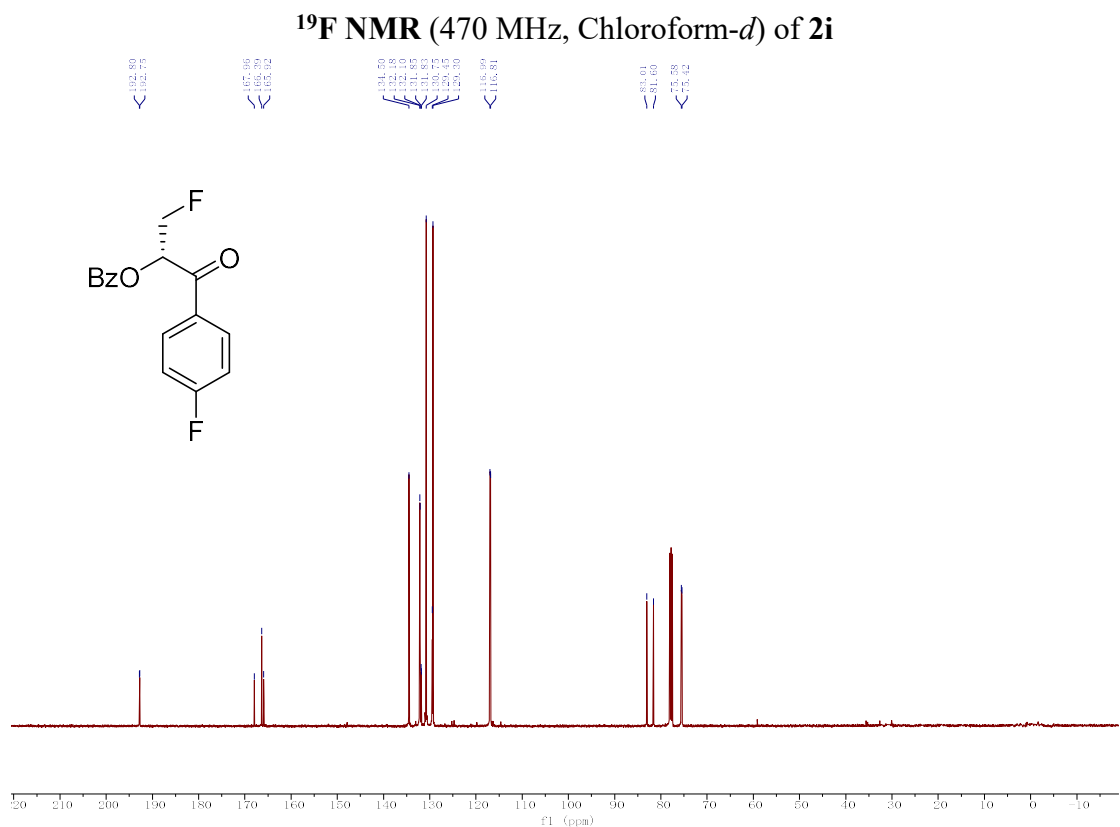
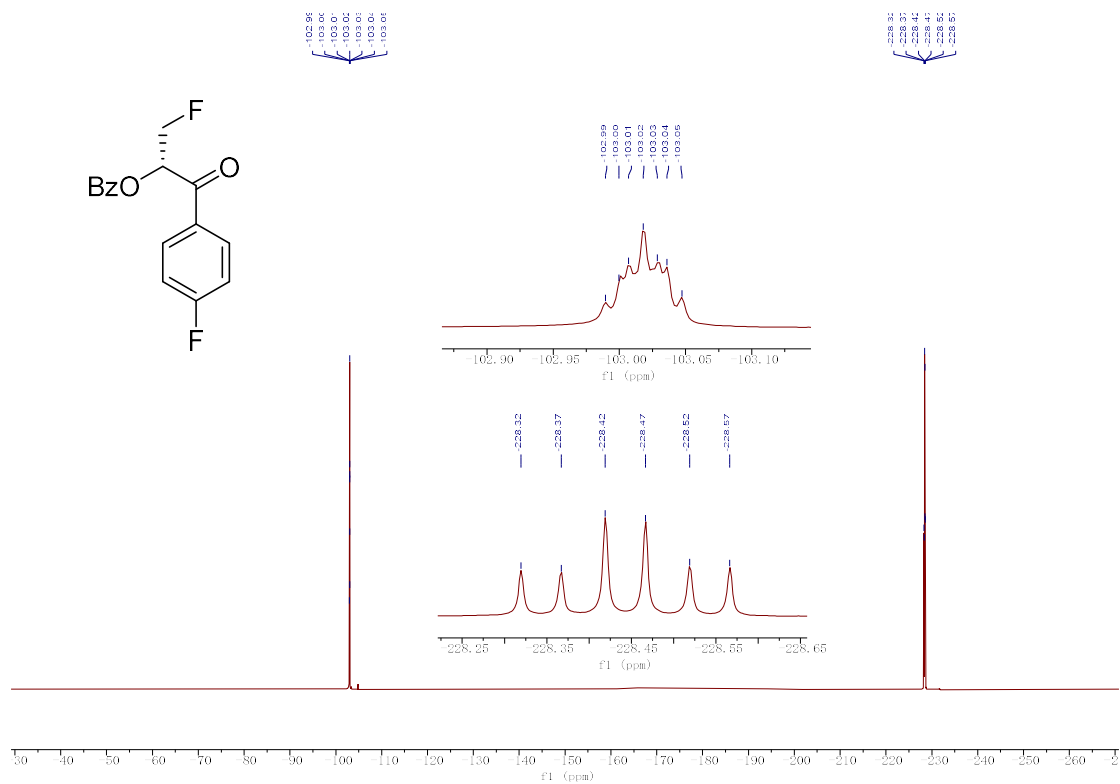
^{19}F NMR (470 MHz, Chloroform-*d*) of **2h**



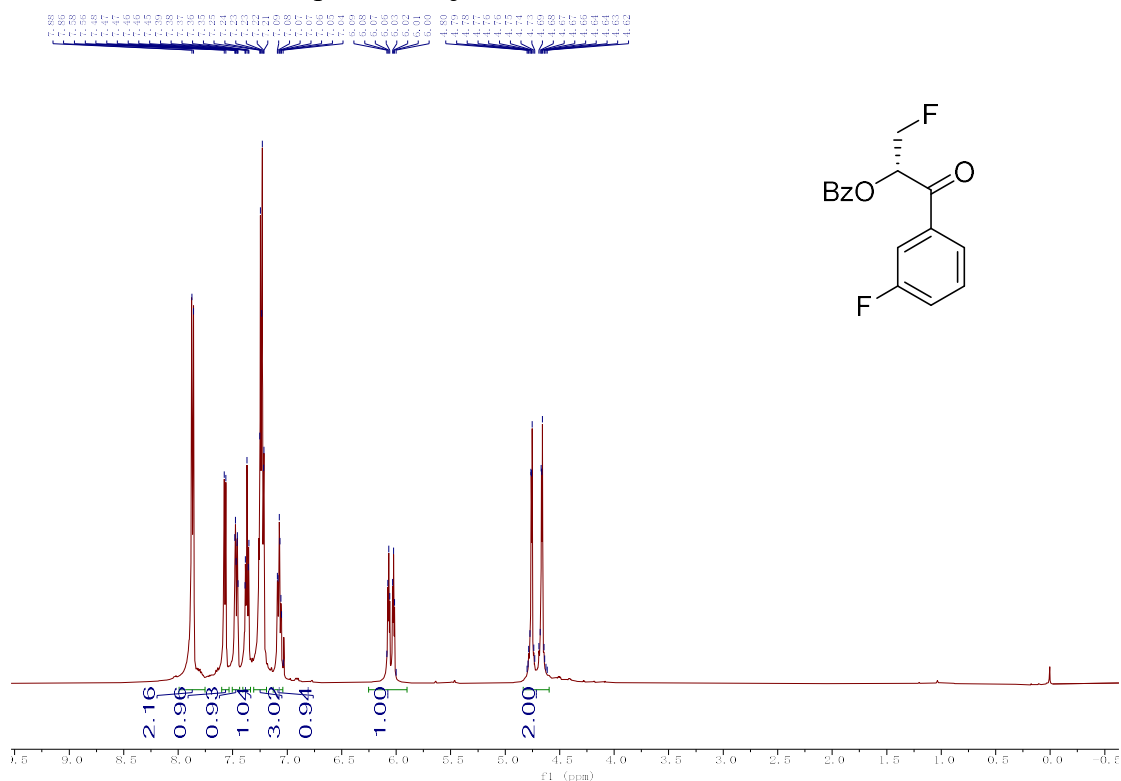
¹³C NMR (126 MHz, Chloroform-*d*) of **2h**
¹H, ¹³C, and ¹⁹F NMR spectra of **2i**



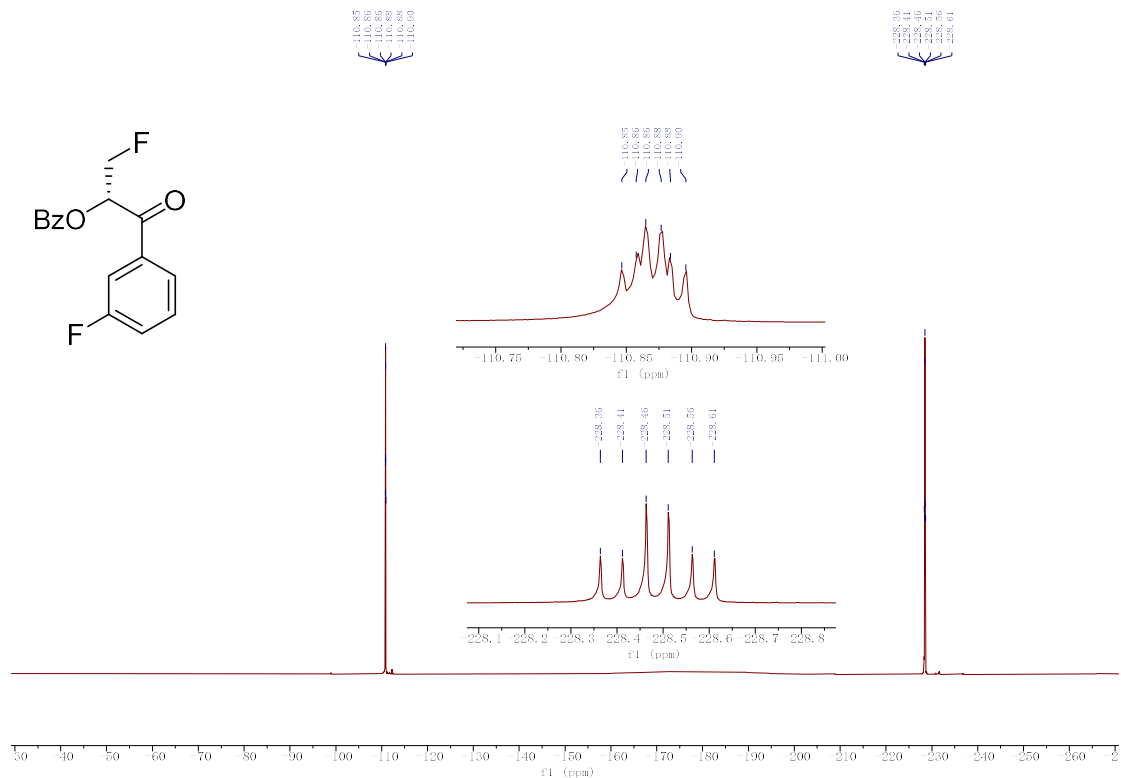
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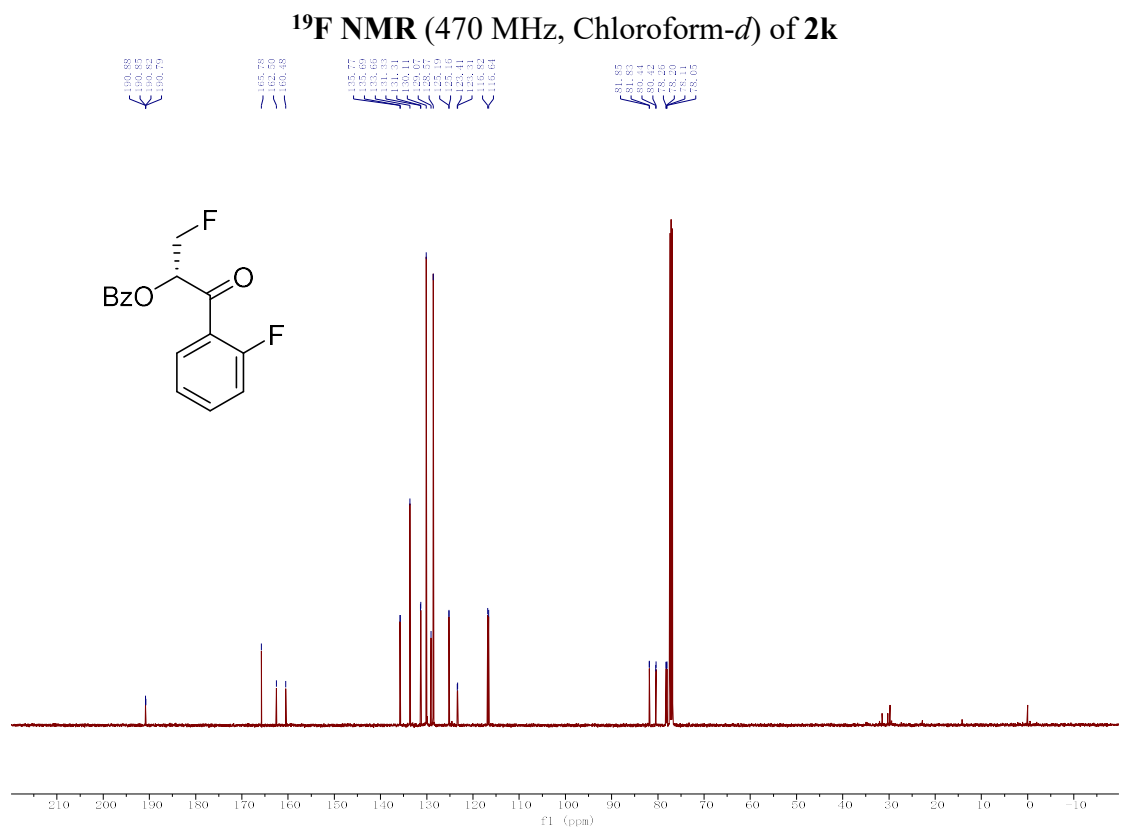
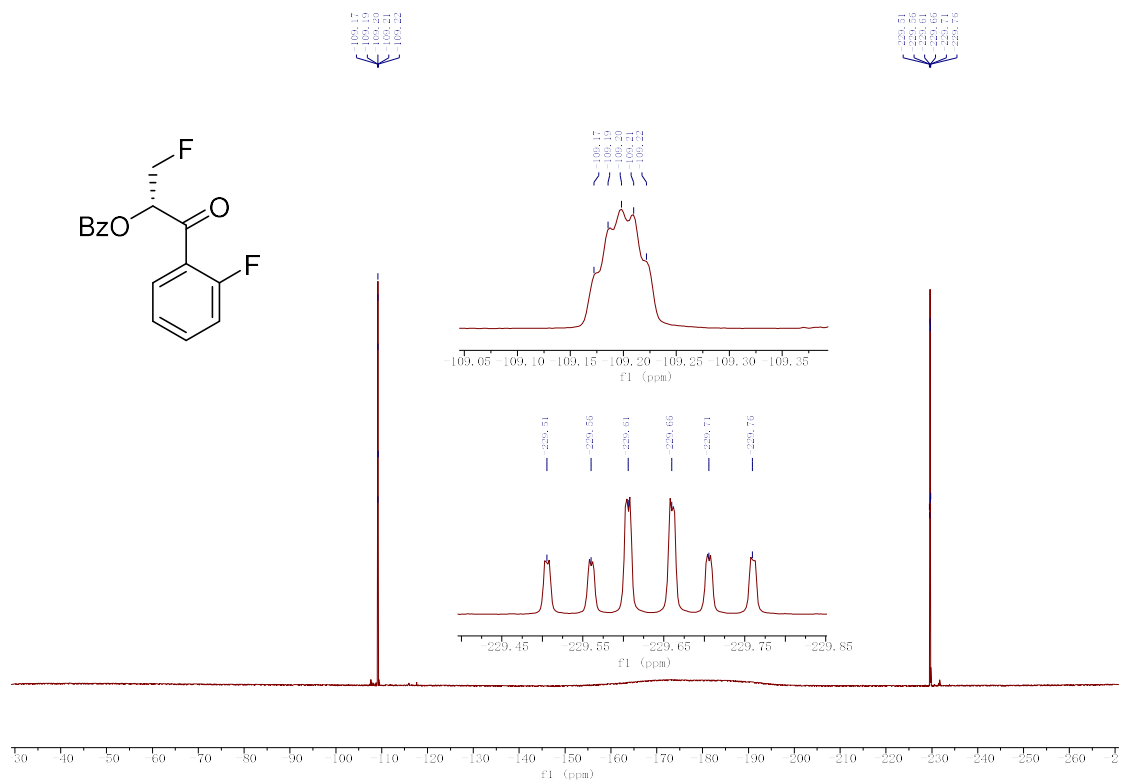
^1H , ^{13}C , and ^{19}F NMR spectra of **2j**



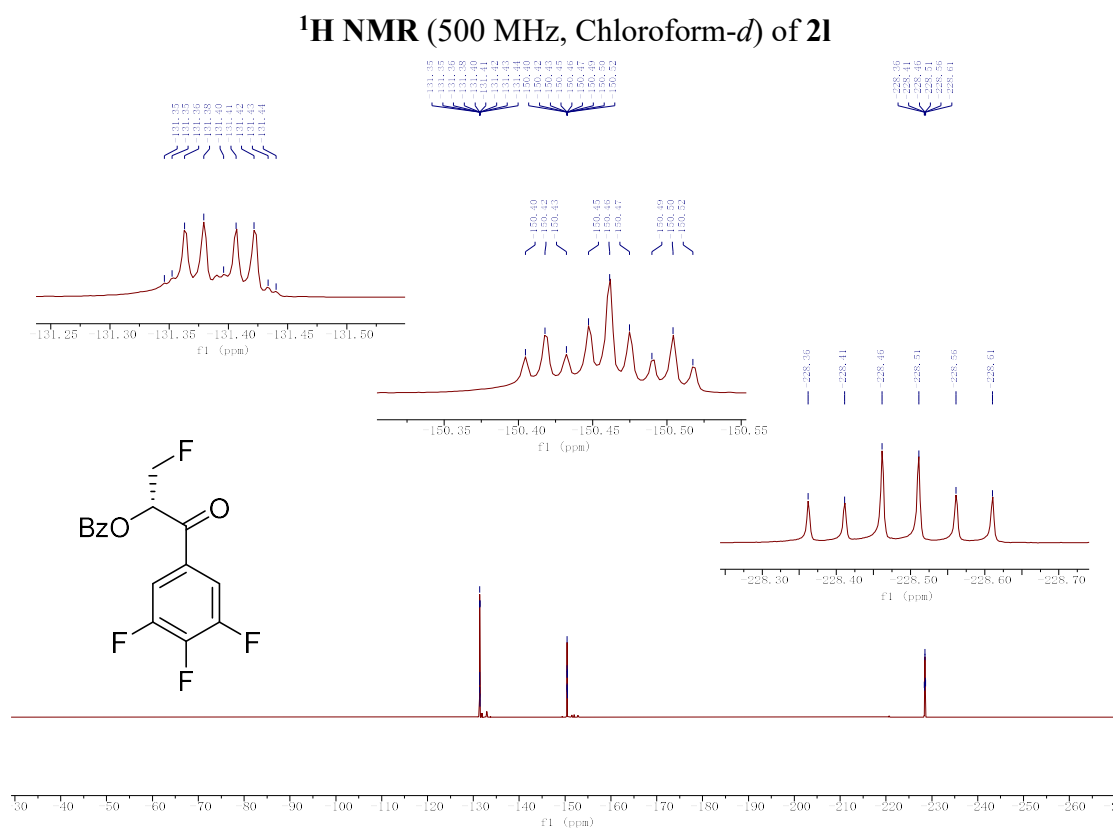
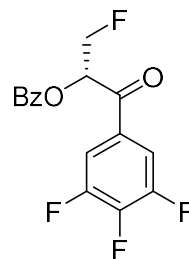
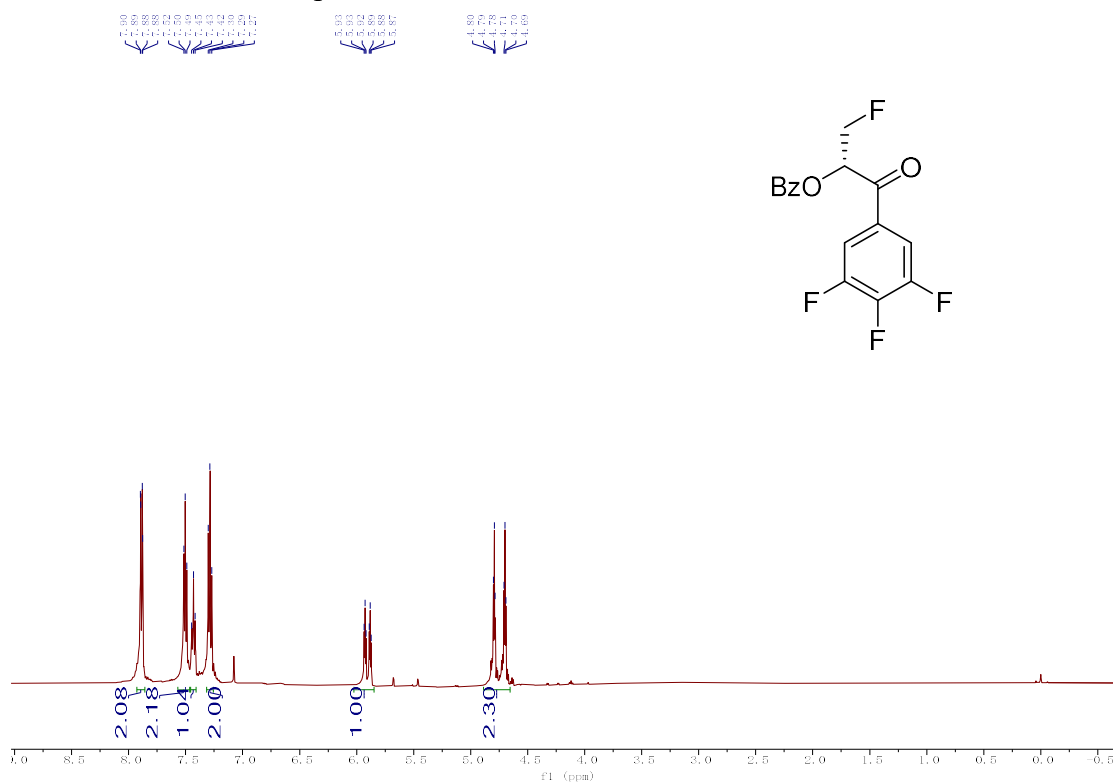
^{13}C NMR (100 MHz, Chloroform-*d*) of **2j**



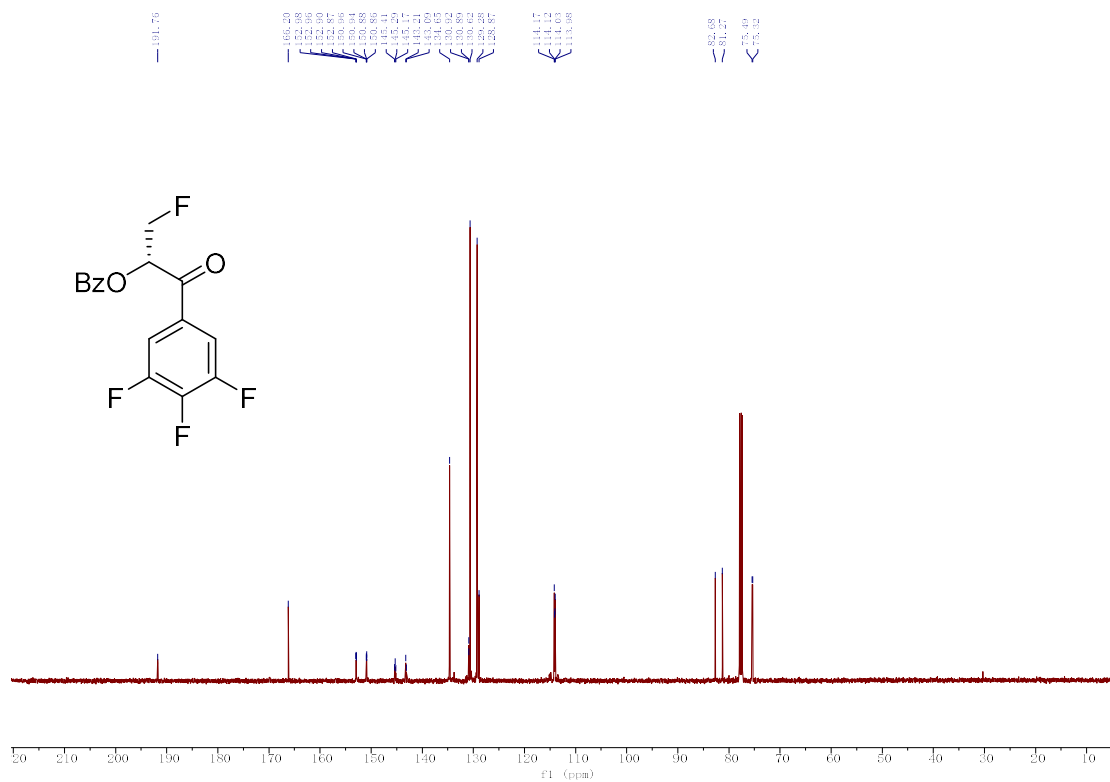
^{19}F NMR (470 MHz, Chloroform-*d*) of **2j**



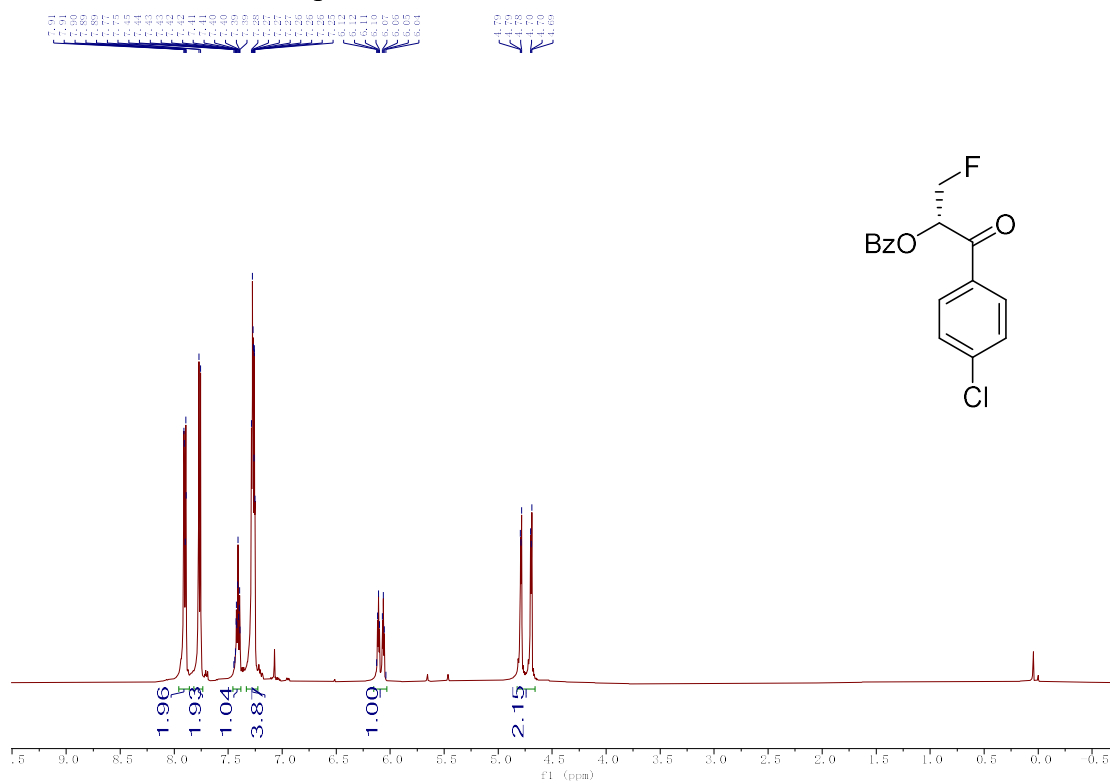
^1H , ^{13}C , and ^{19}F NMR spectra of **21**



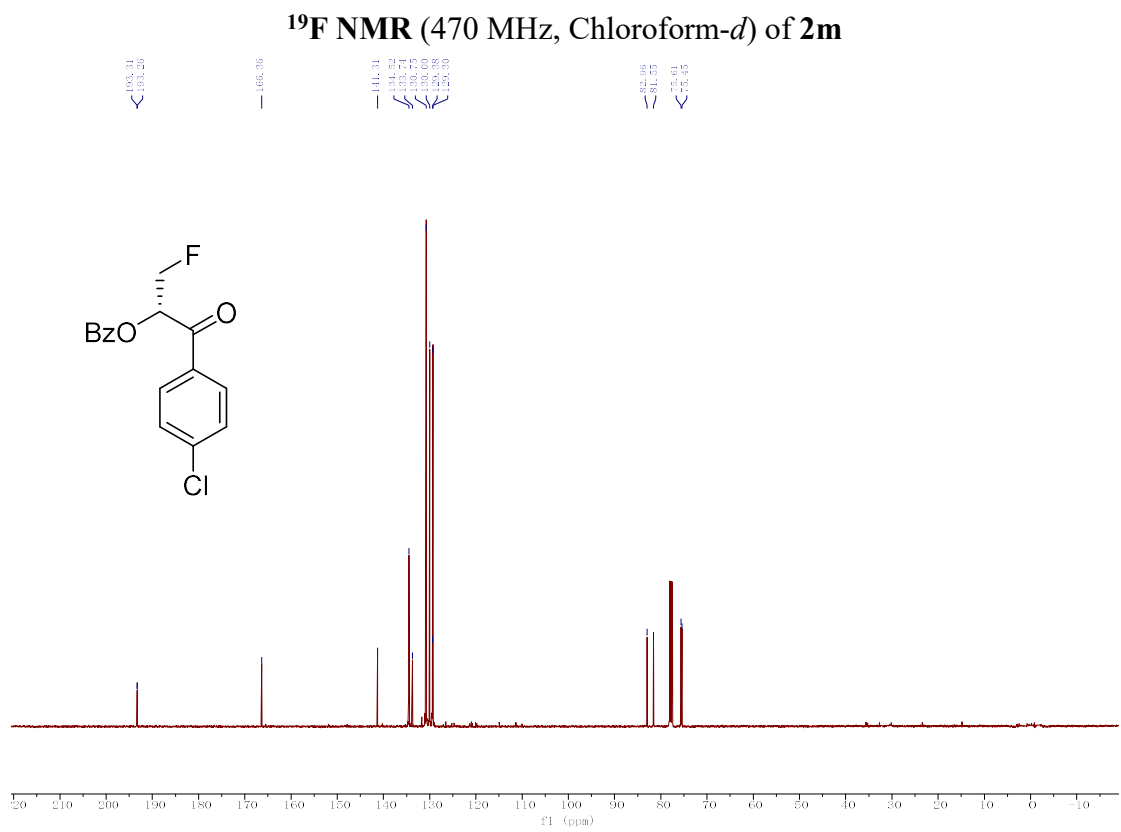
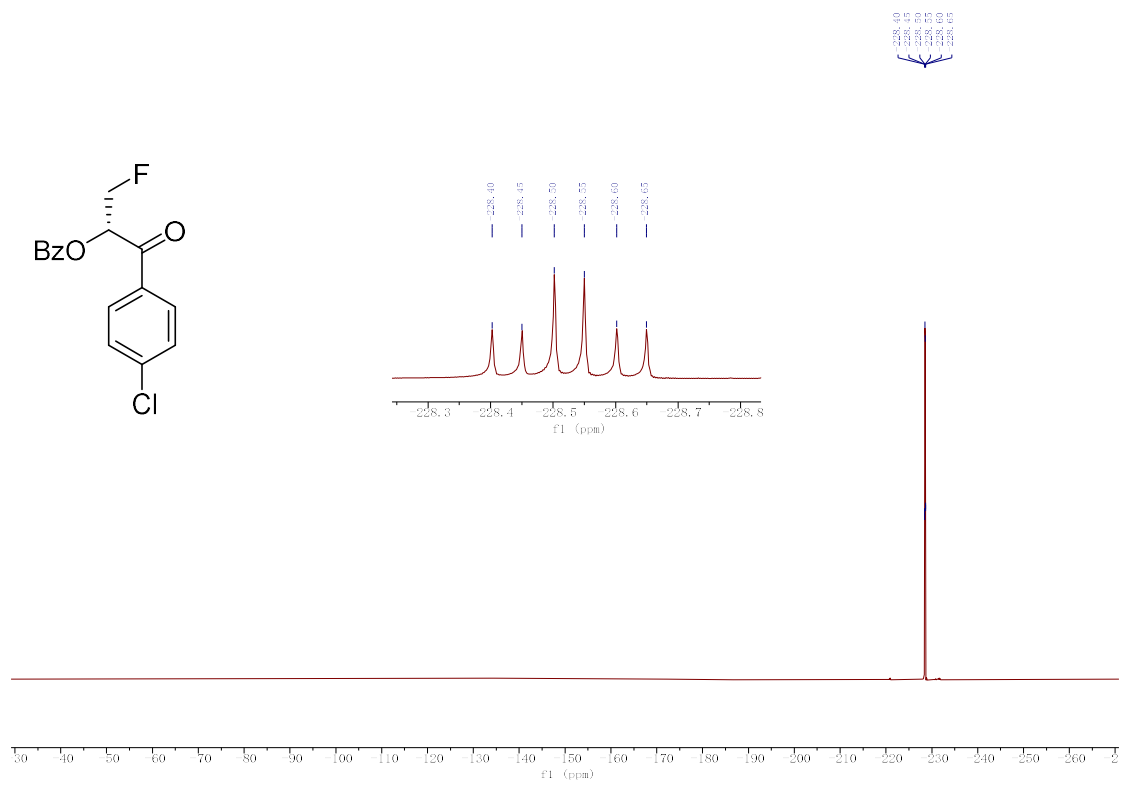
^{19}F NMR (470 MHz, Chloroform-*d*) of **21**



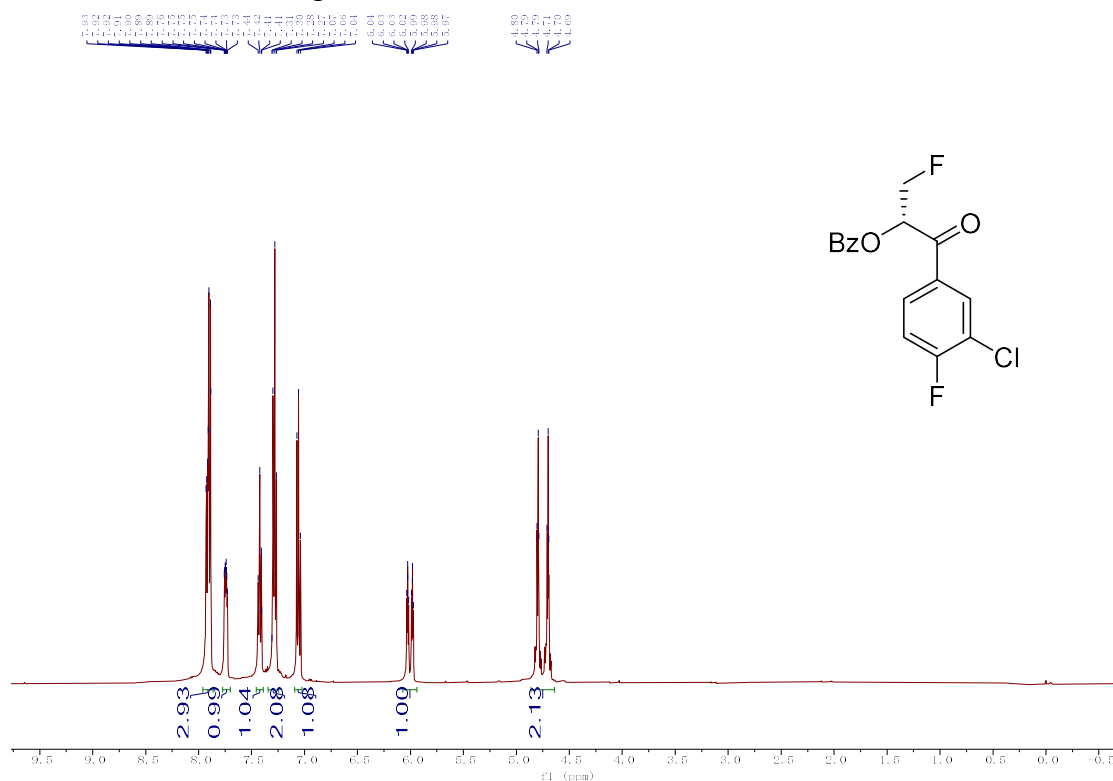
^{13}C NMR (126 MHz, Chloroform-*d*) of **2l**
 ^1H , ^{13}C , and ^{19}F NMR spectra of **2m**



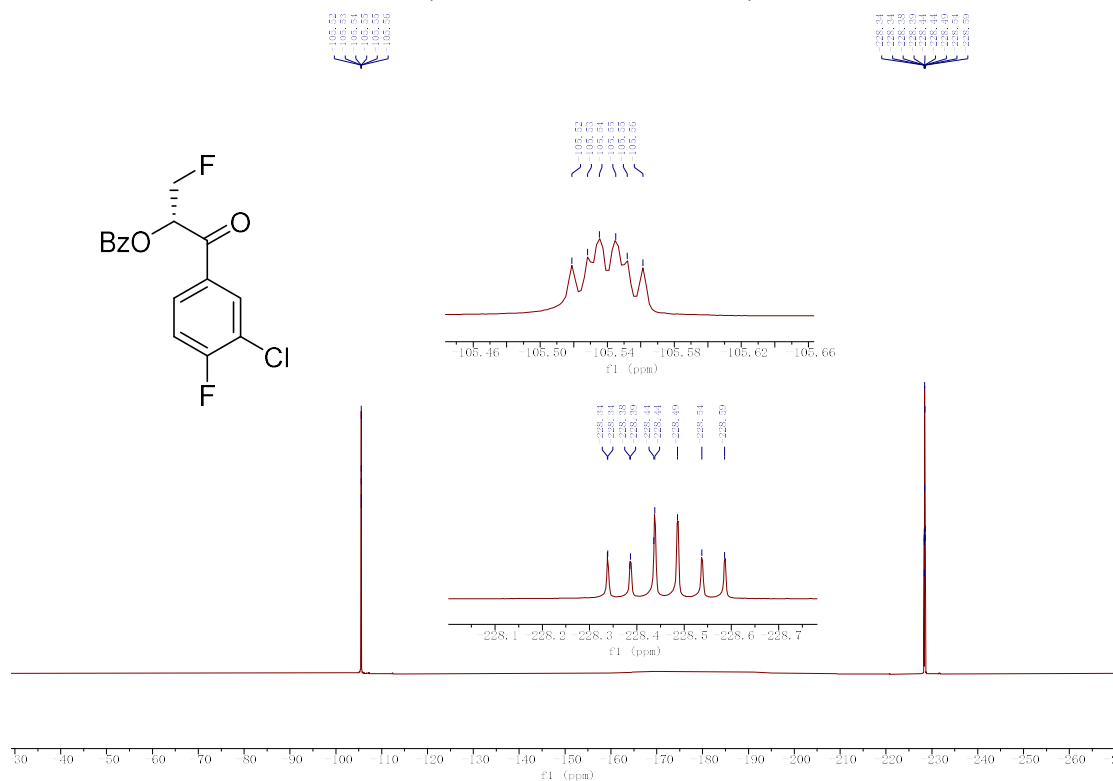
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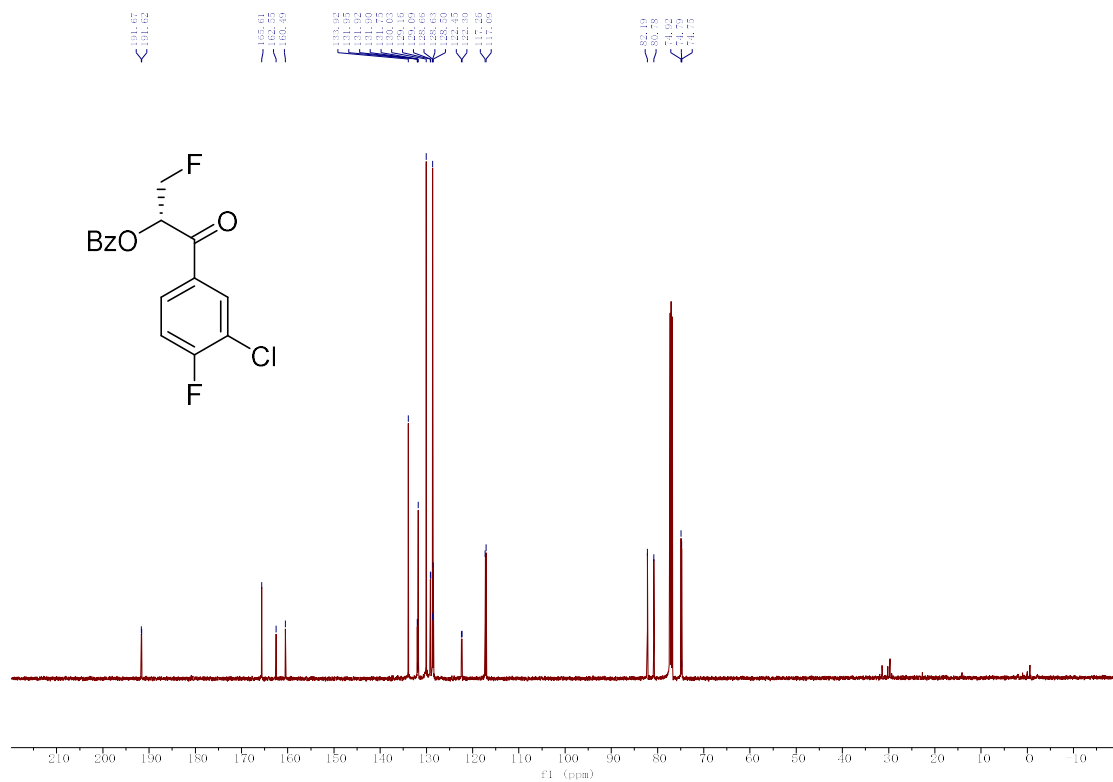
^1H , ^{13}C , and ^{19}F NMR spectra of **2n**



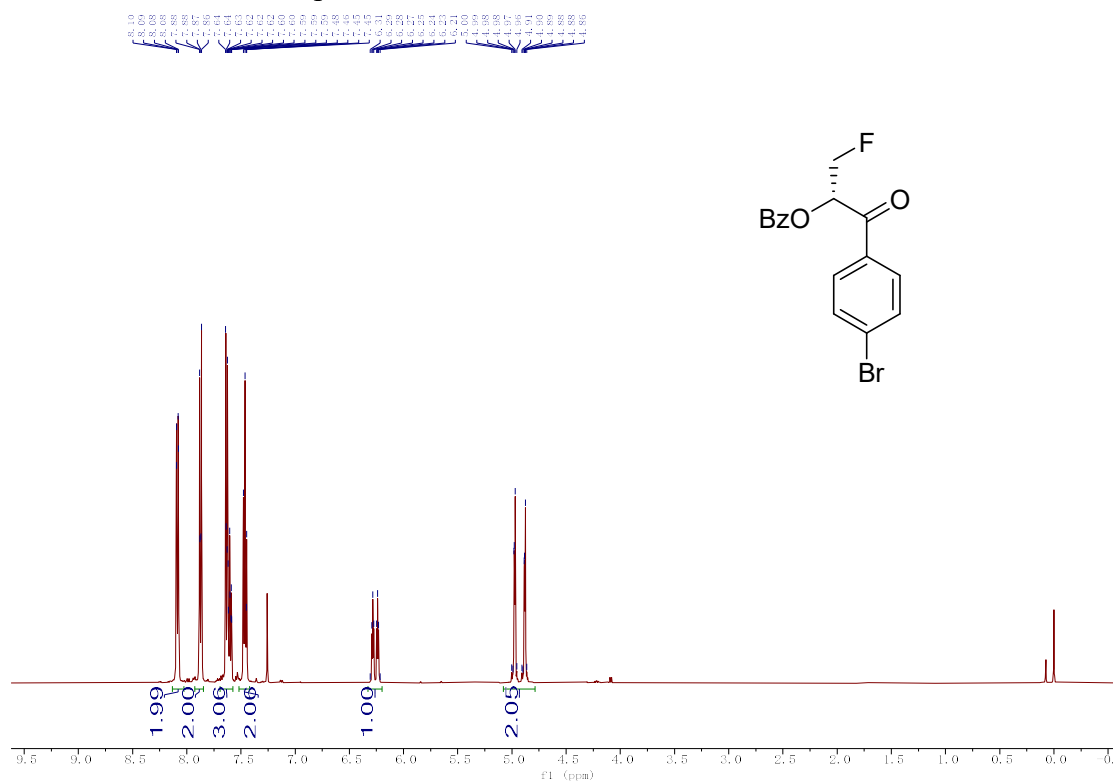
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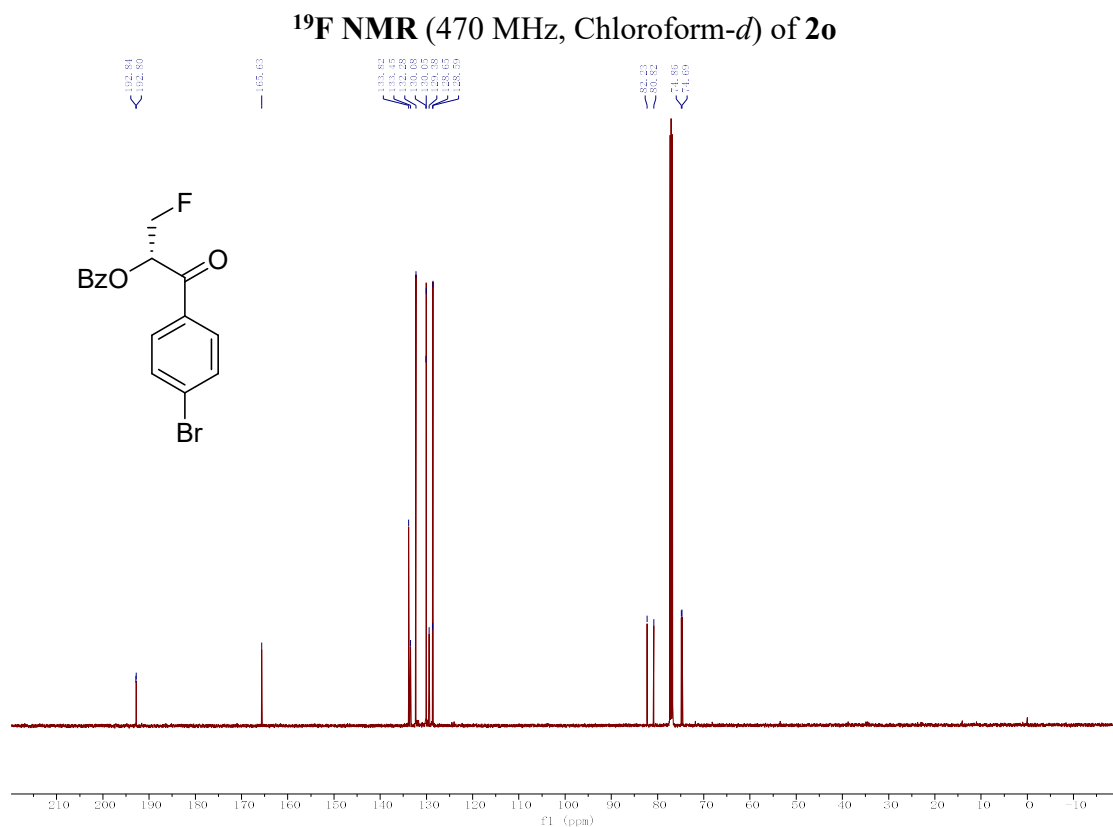
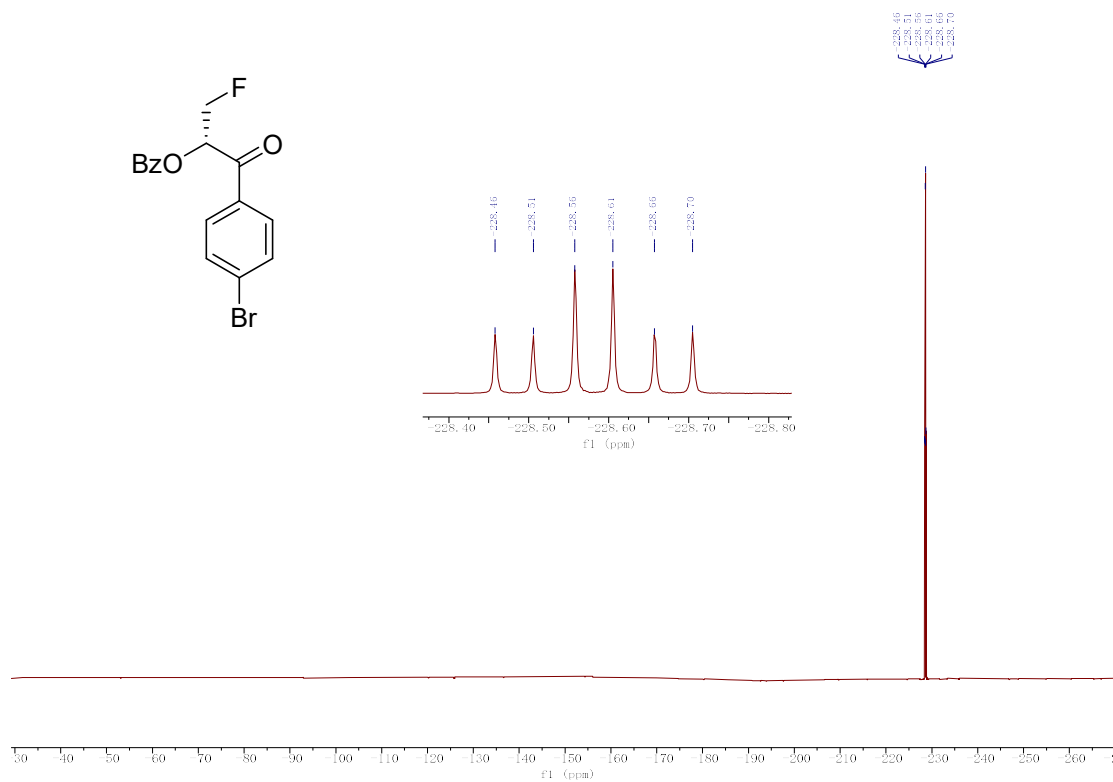
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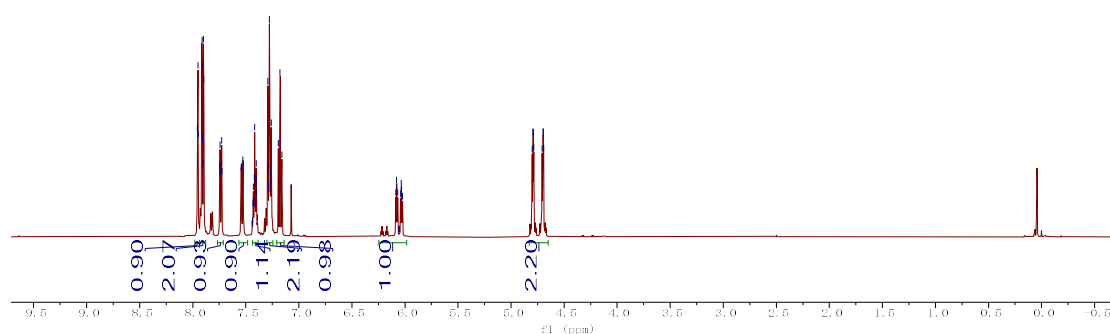
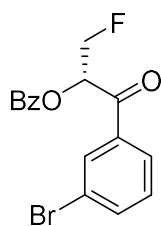
^{13}C NMR (126 MHz, Chloroform-*d*) of **2n**
 ^1H , ^{13}C , and ^{19}F NMR spectra of **2o**



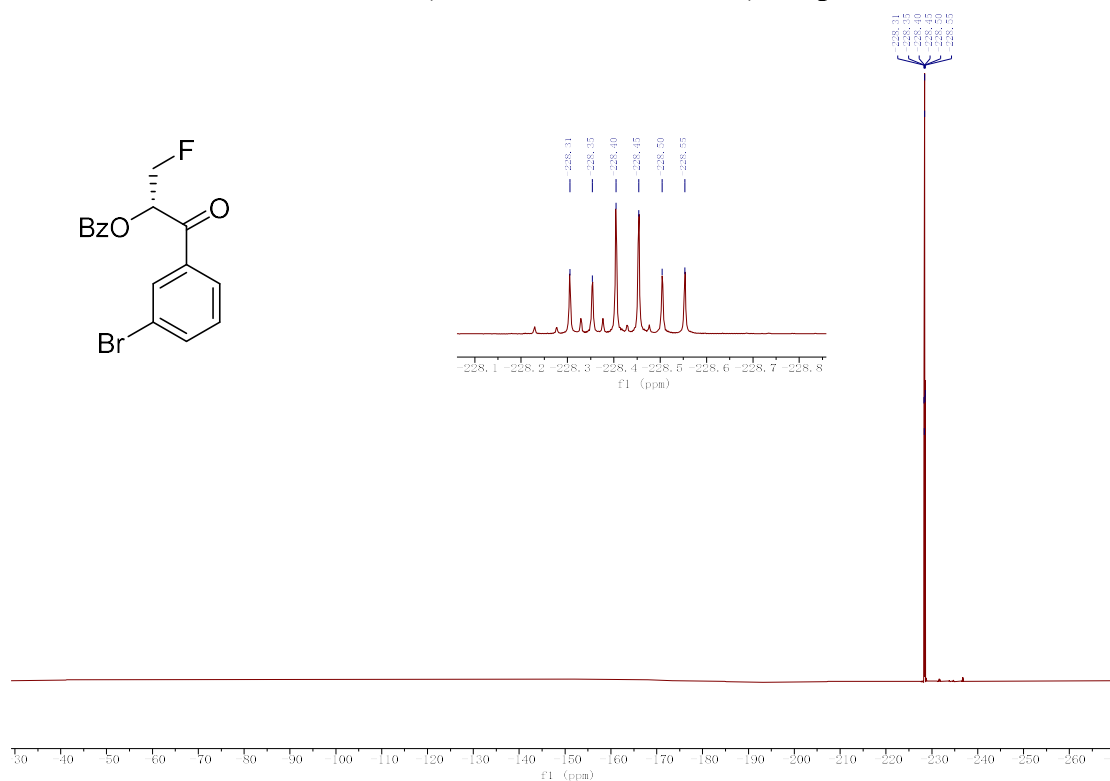
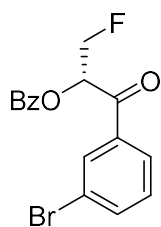
^1H NMR (500 MHz, Chloroform-*d*) of **2o**



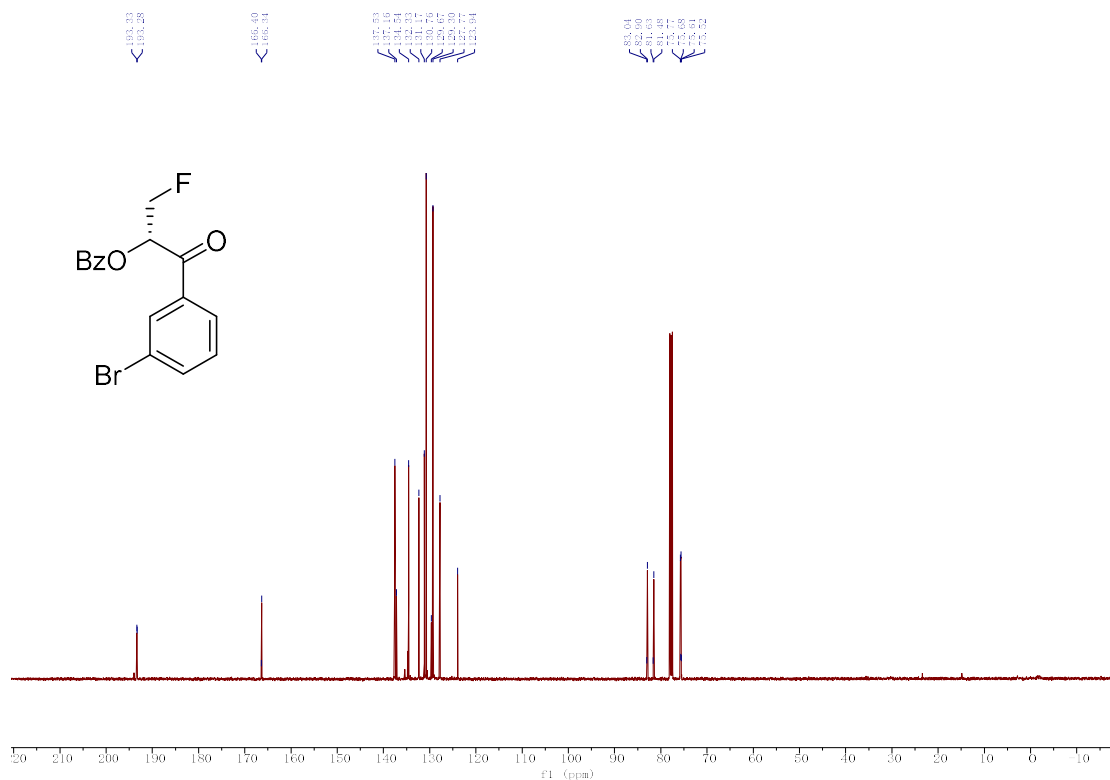
^1H , ^{13}C , and ^{19}F NMR spectra of **2p**



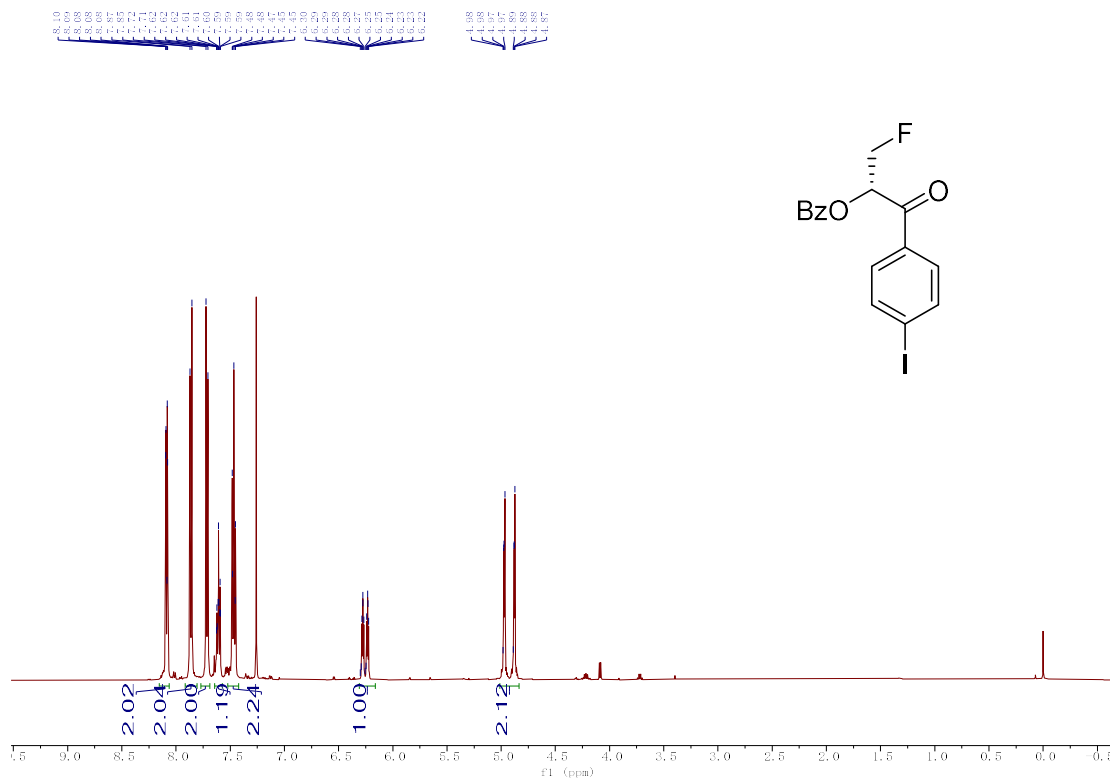
^1H NMR (500 MHz, Chloroform-*d*) of **2p**



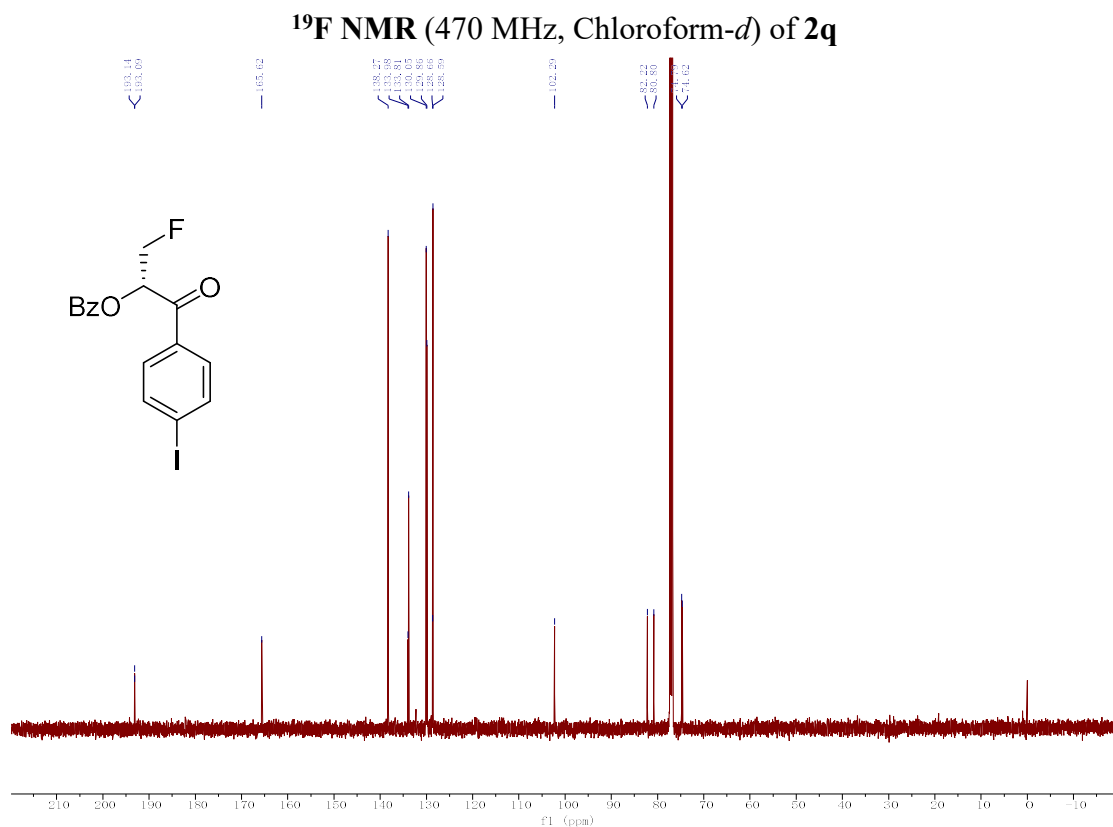
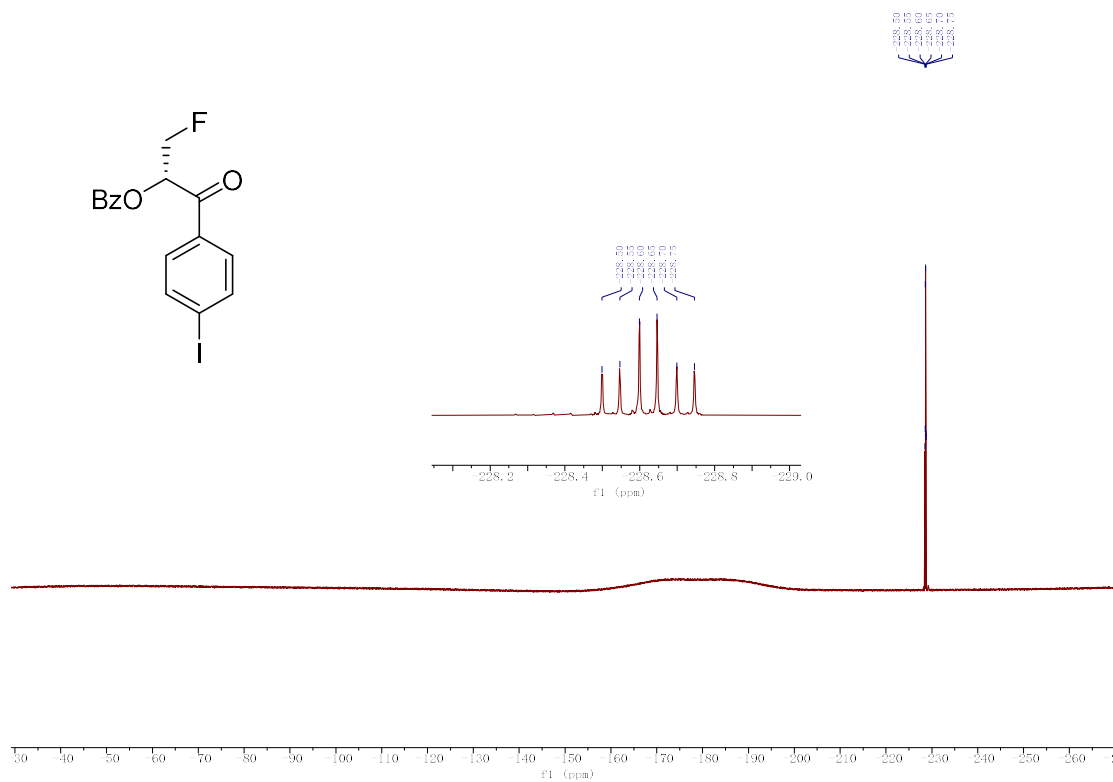
^{19}F NMR (470 MHz, Chloroform-*d*) of **2p**



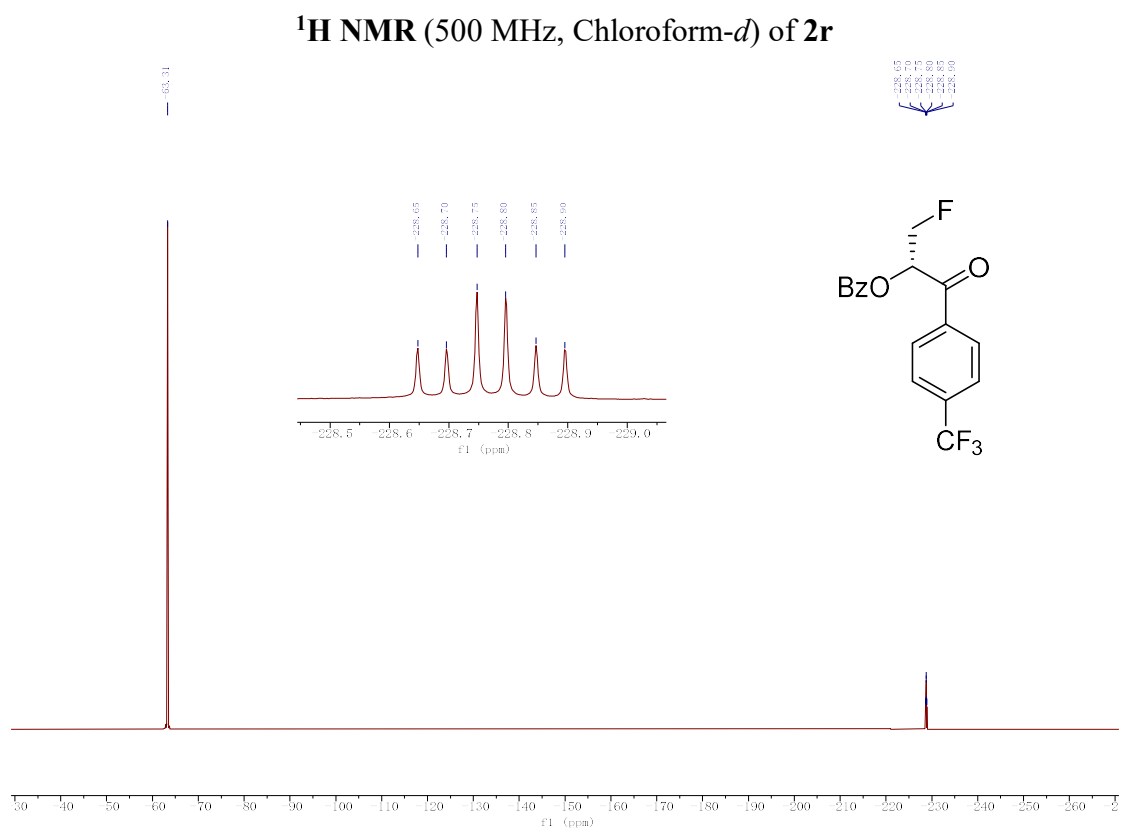
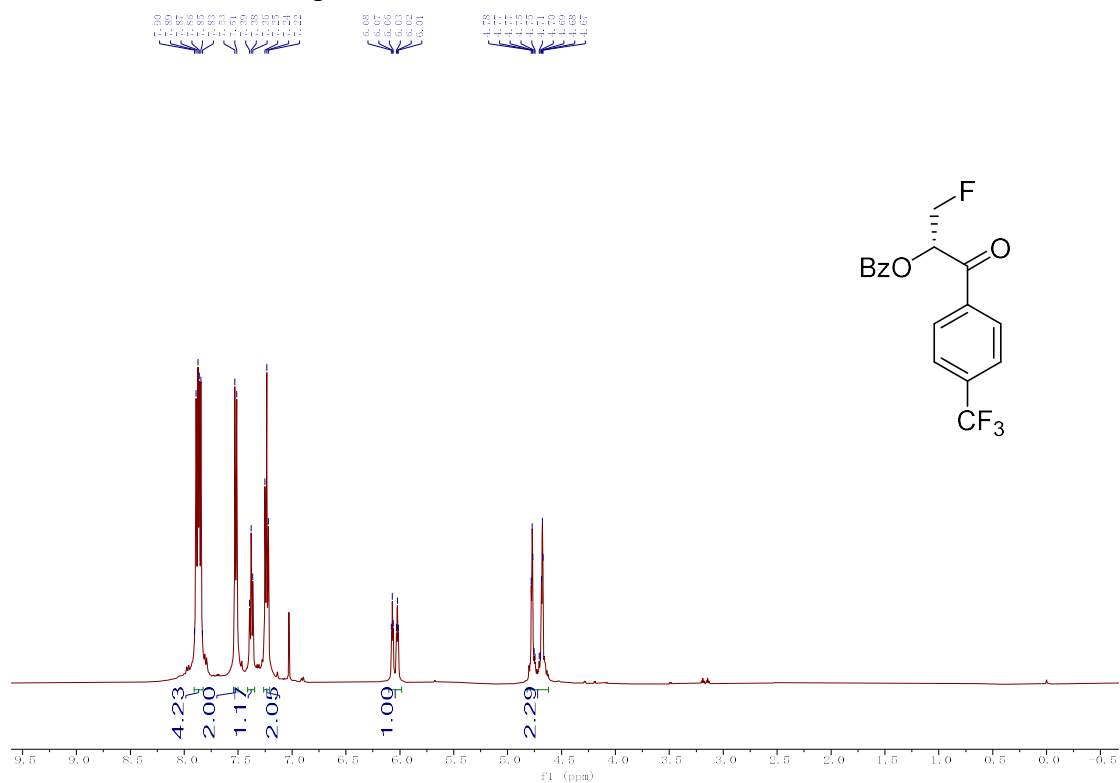
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¹H, ¹³C, and ¹⁹F NMR spectra of 2q

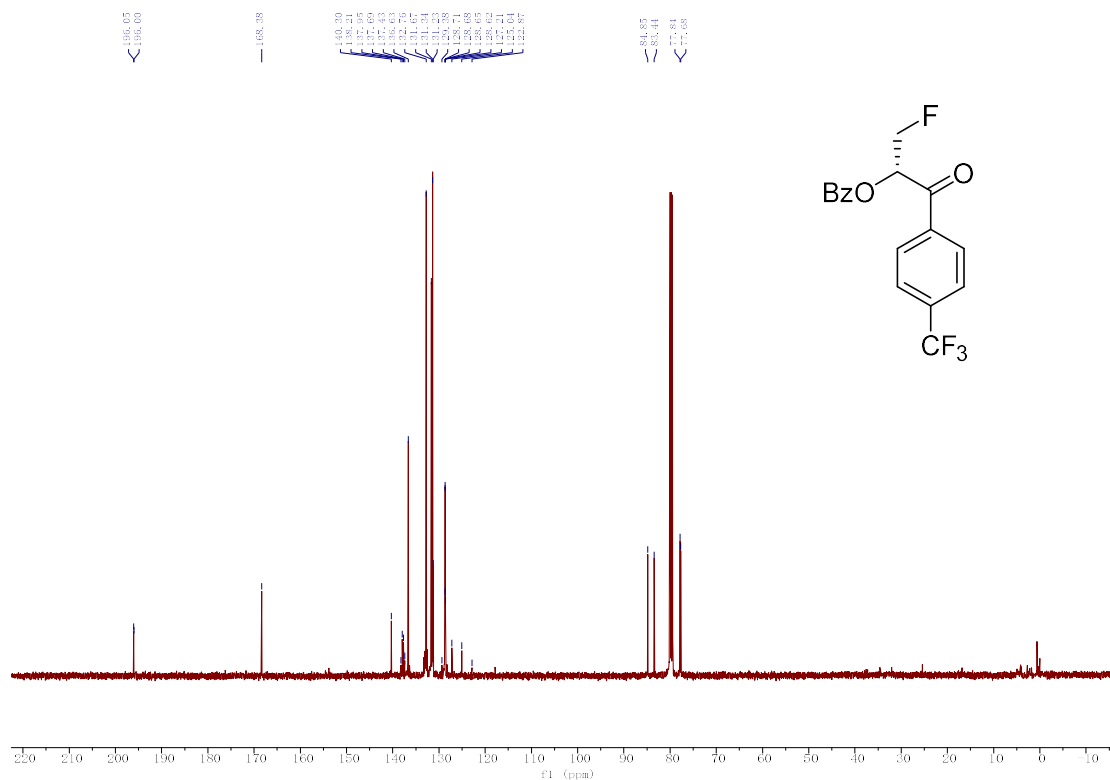


¹H NMR (500 MHz, Chloroform-*d*) of 2q

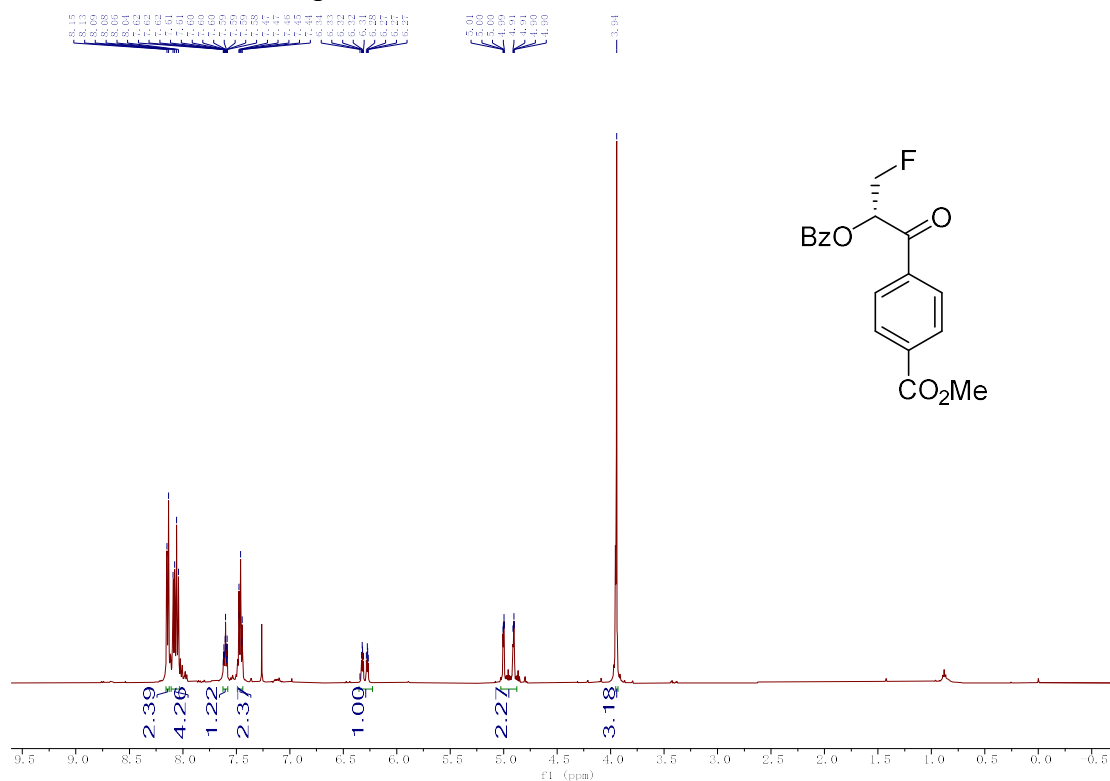


^1H , ^{13}C , and ^{19}F NMR spectra of **2r**

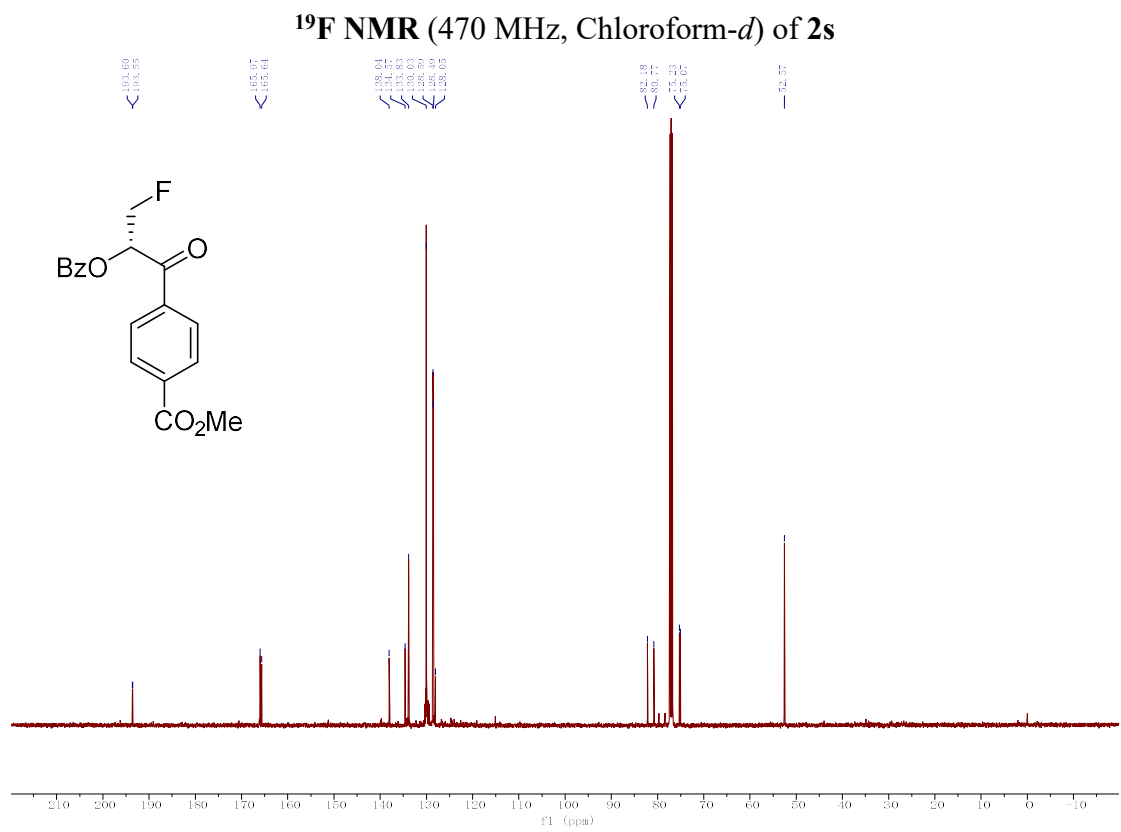
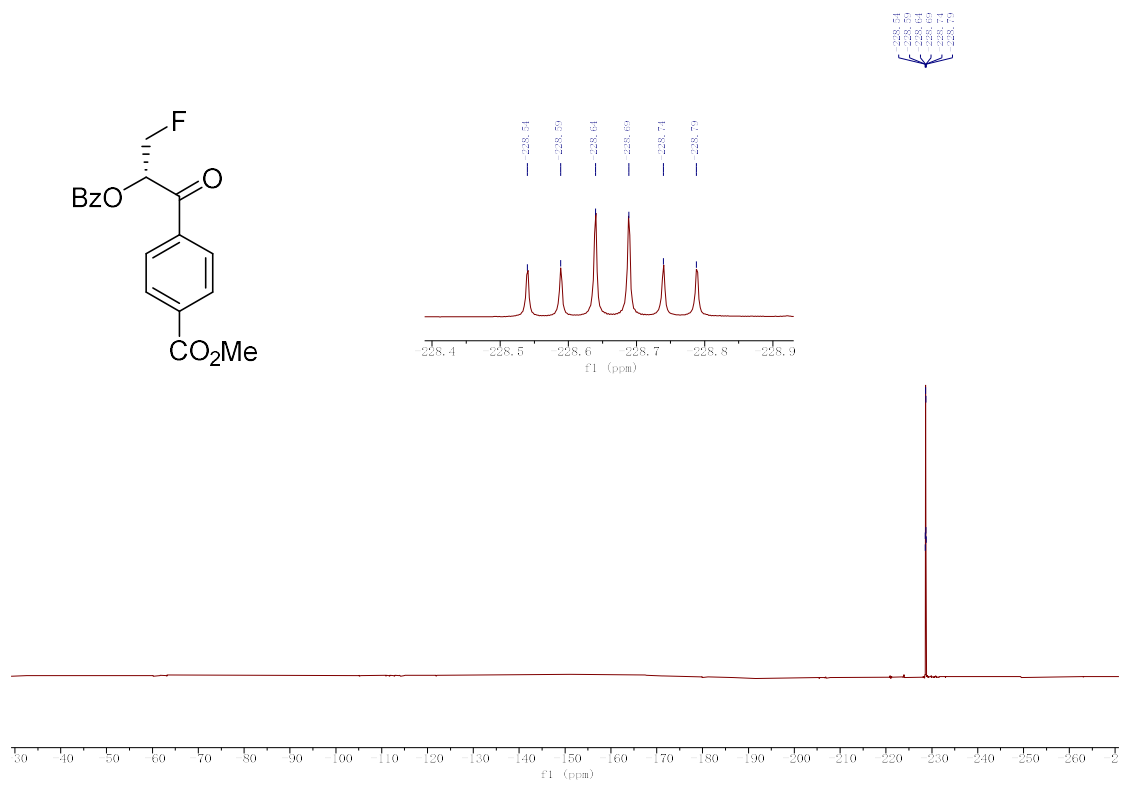




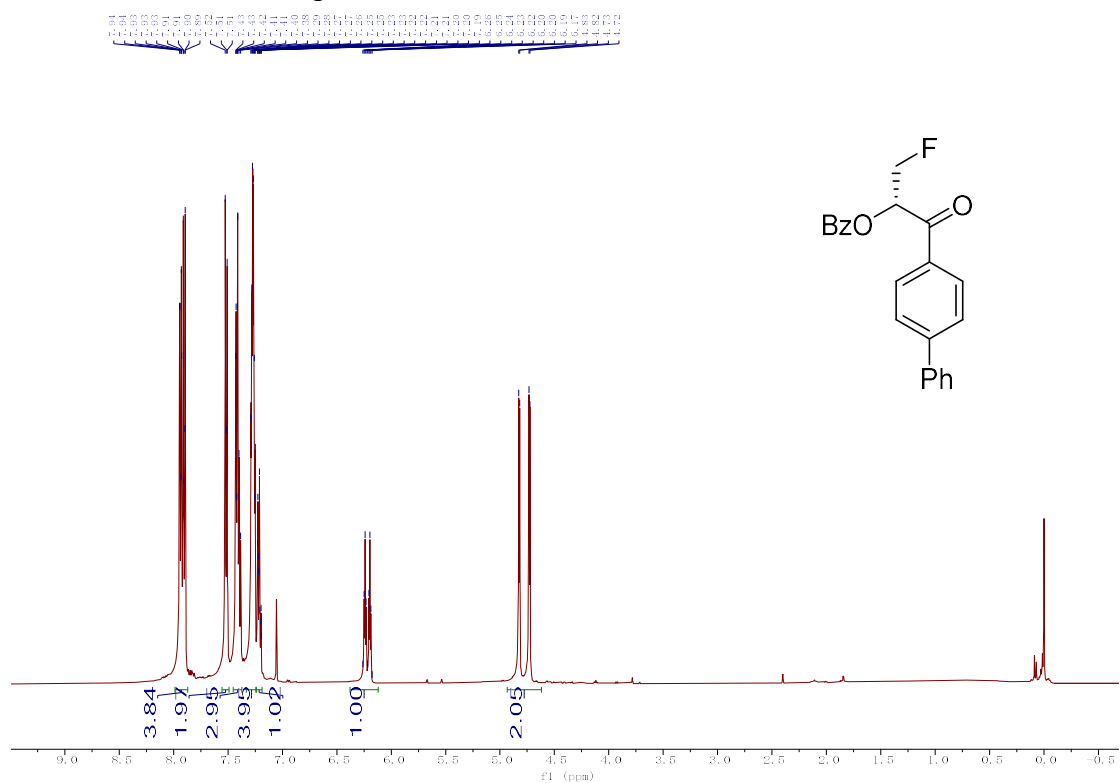
¹³C NMR (126 MHz, Chloroform-*d*) of **2r**
¹H, ¹³C, and ¹⁹F NMR spectra of **2s**



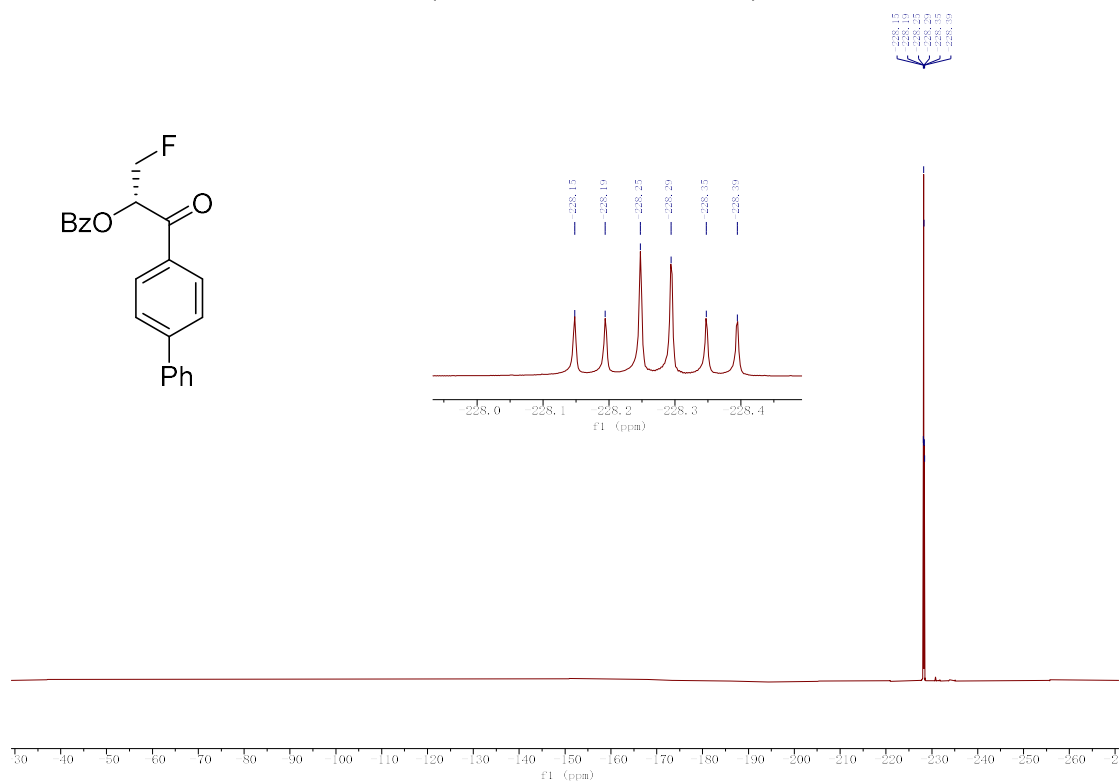
¹H NMR (500 MHz, Chloroform-*d*) of **2s**



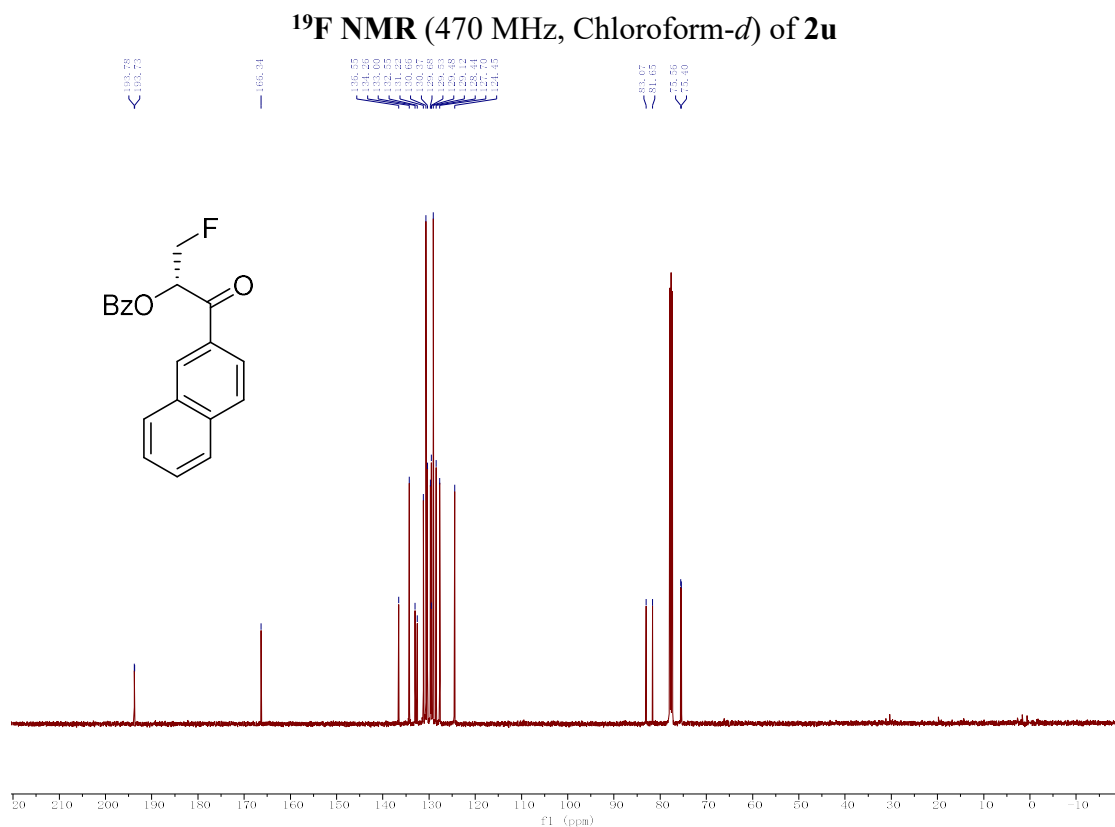
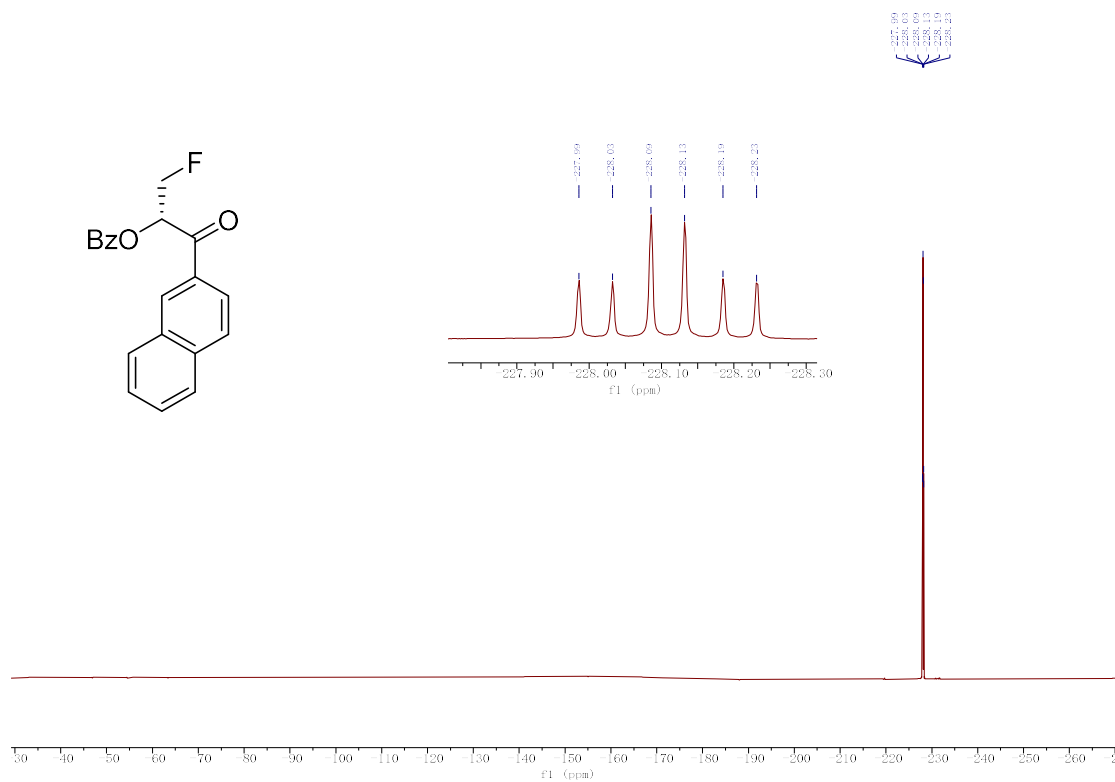
^1H , ^{13}C , and ^{19}F NMR spectra of **2t**



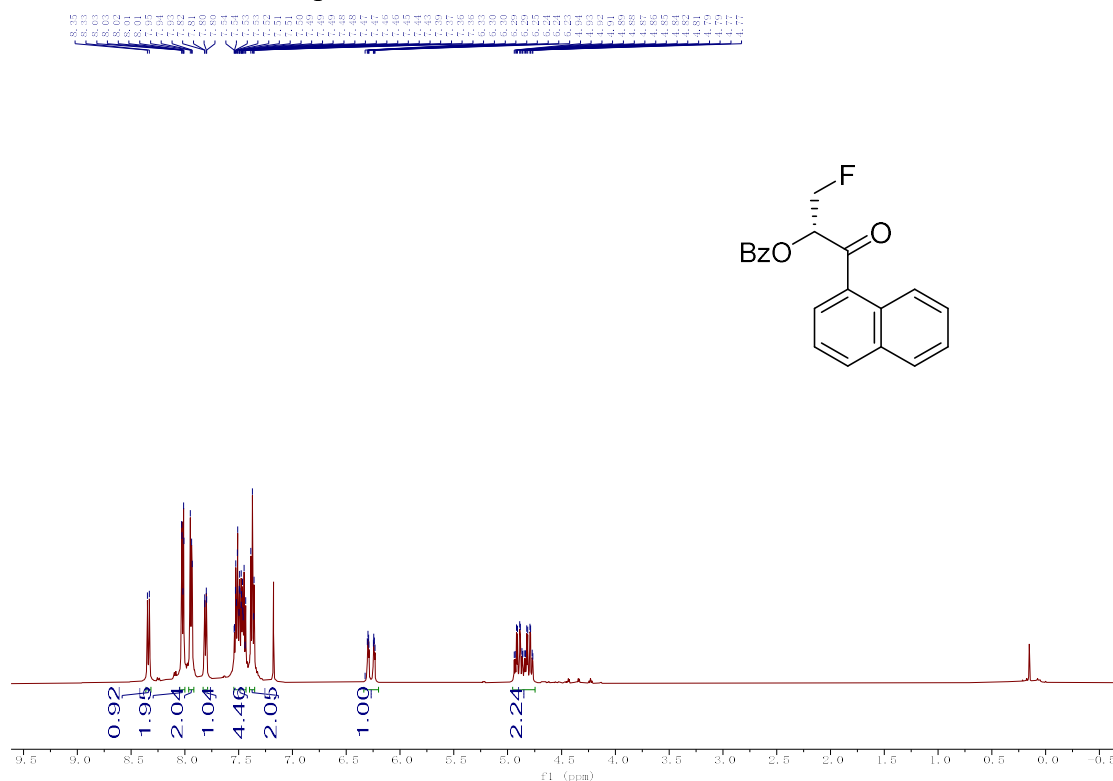
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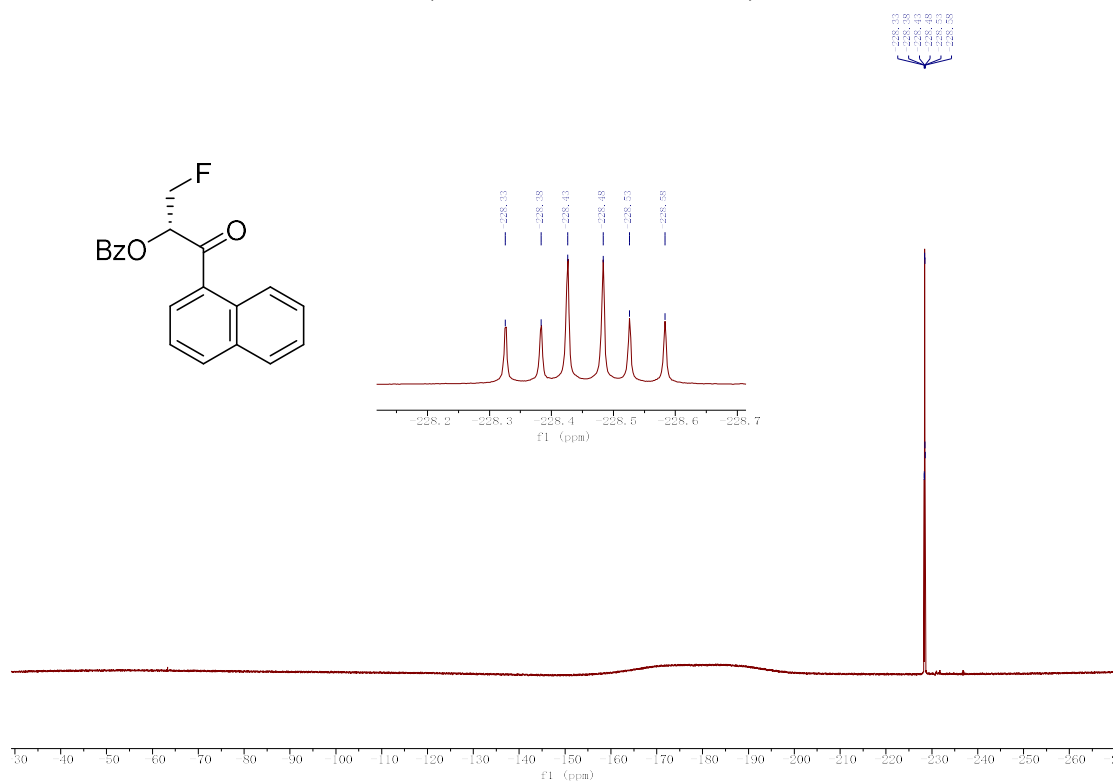
^{19}F NMR (470 MHz, Chloroform-*d*) of **2t**



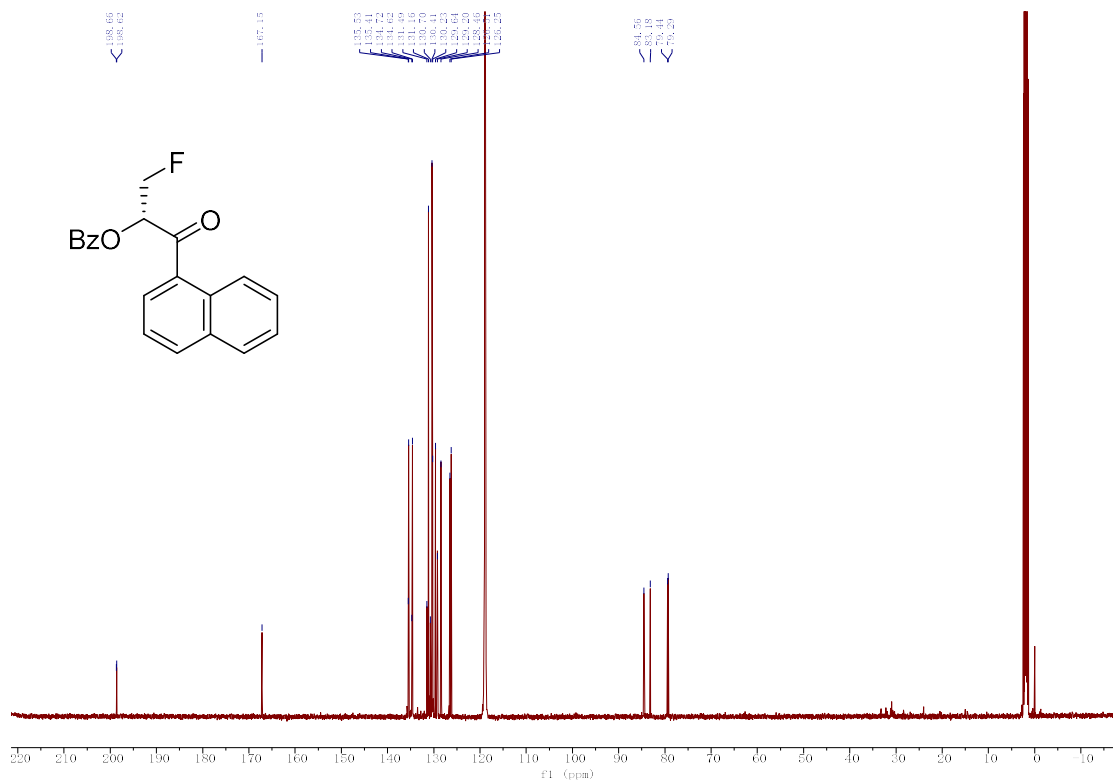
¹H, ¹³C, and ¹⁹F NMR spectra of **2v**



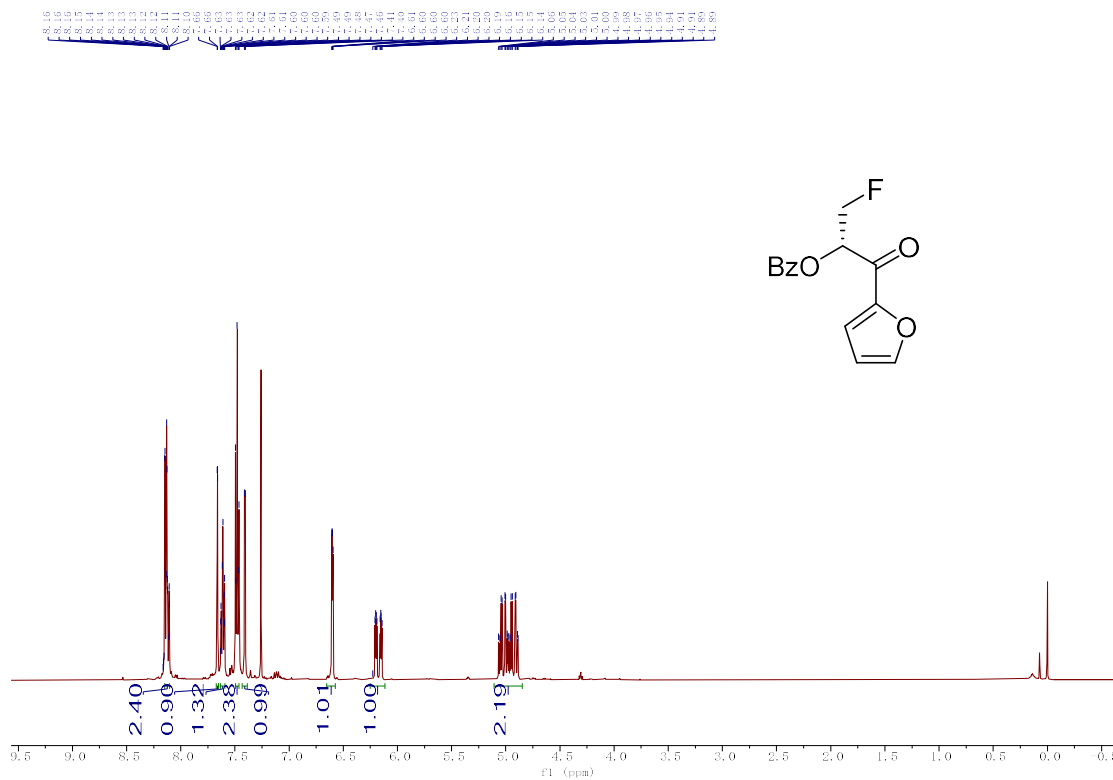
¹H NMR (500 MHz, Chloroform-d) of **2v**



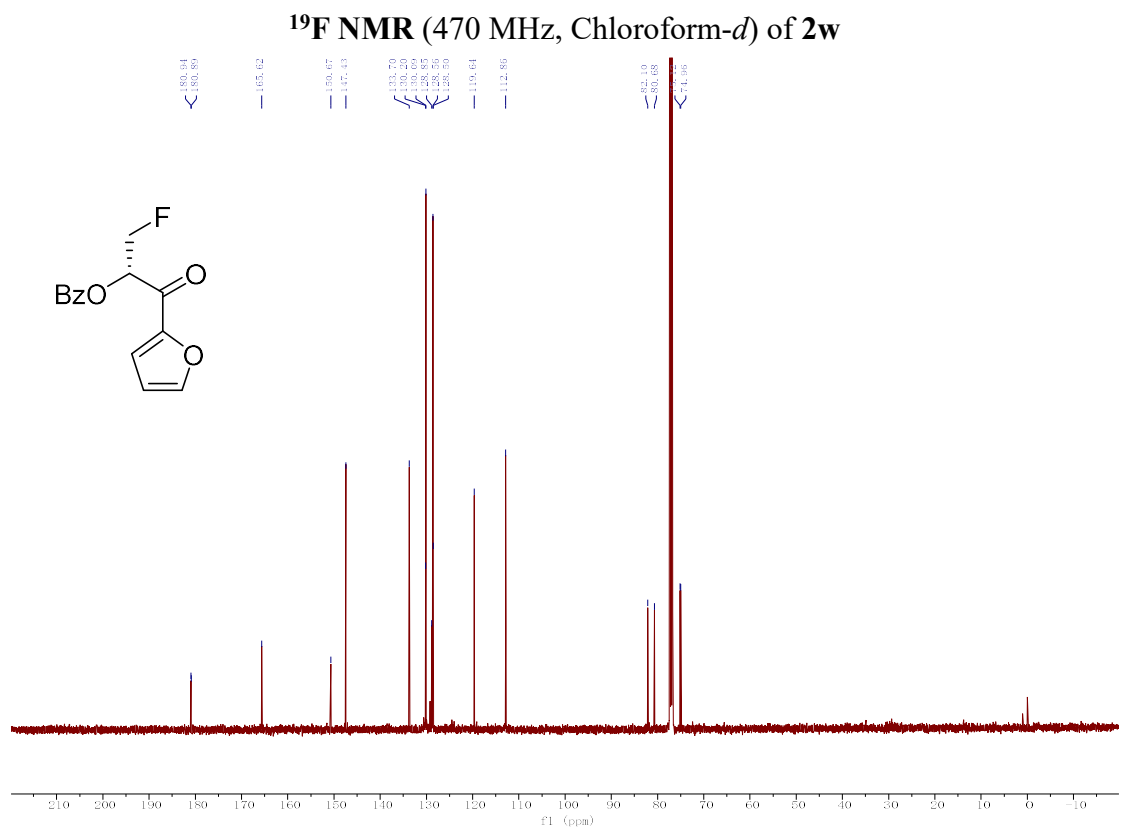
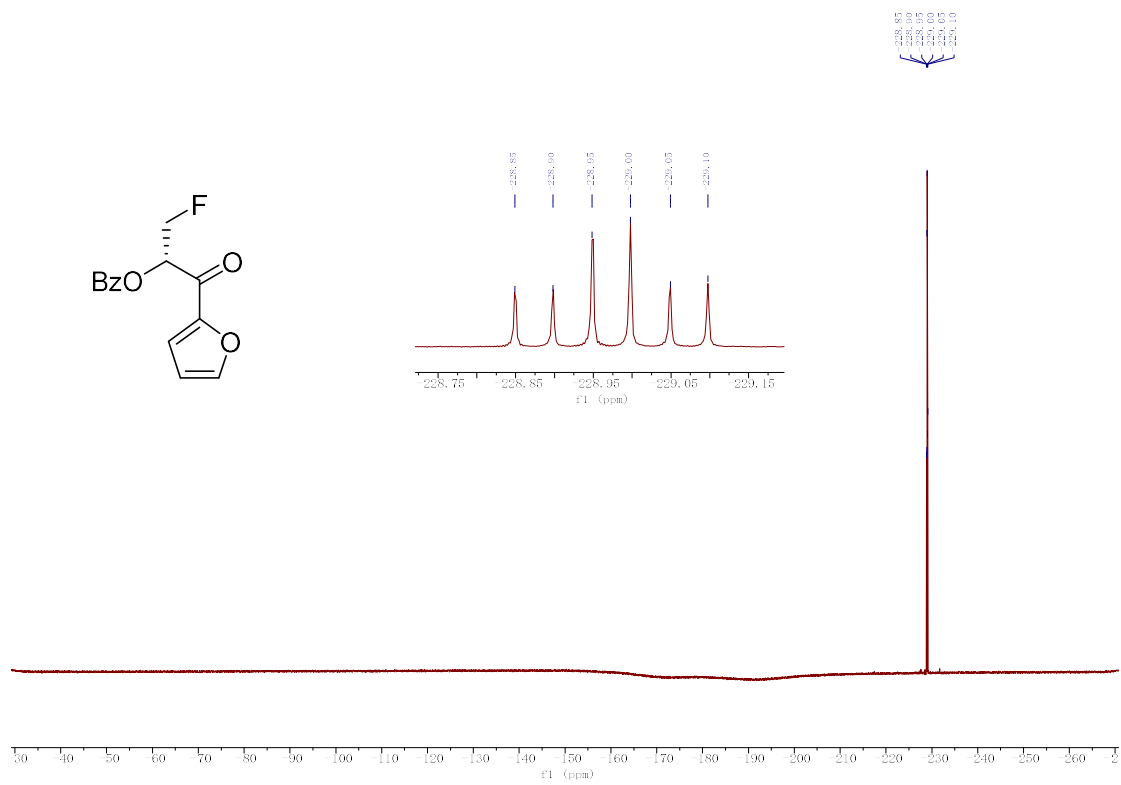
¹⁹F NMR (470 MHz, Chloroform-d) of **2v**



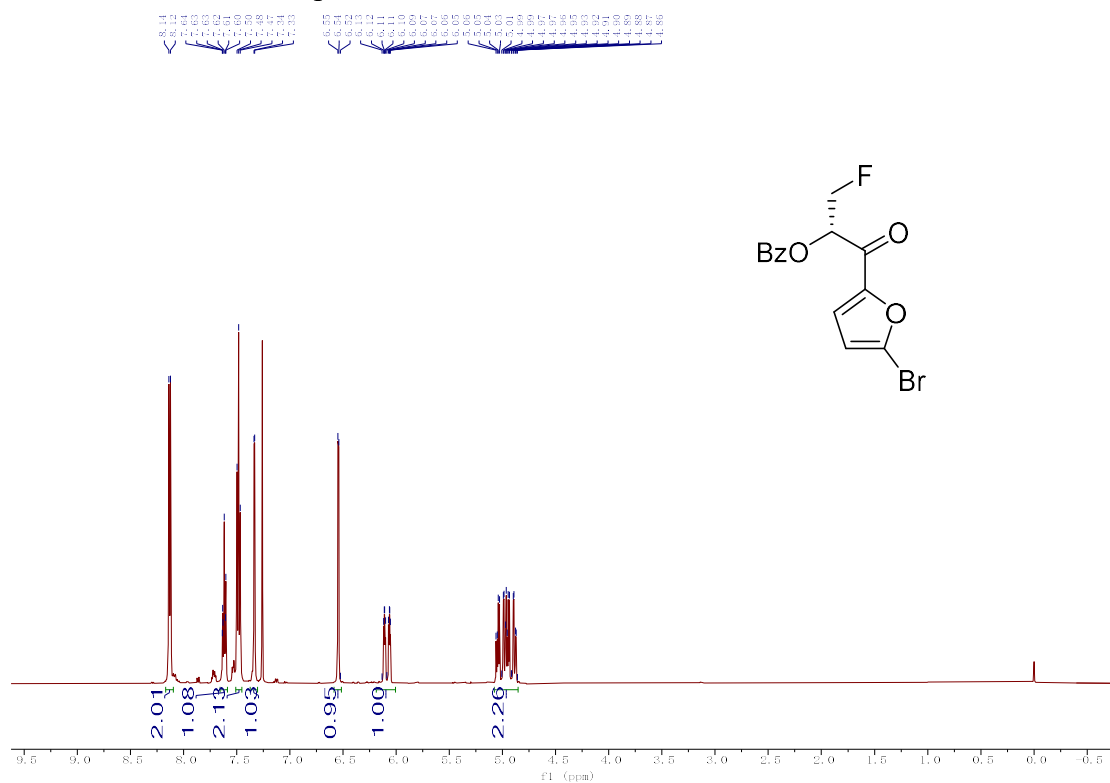
^{13}C NMR (126 MHz, Acetonitrile- d_3) of 2v
 ^1H , ^{13}C , and ^{19}F NMR spectra of 2w



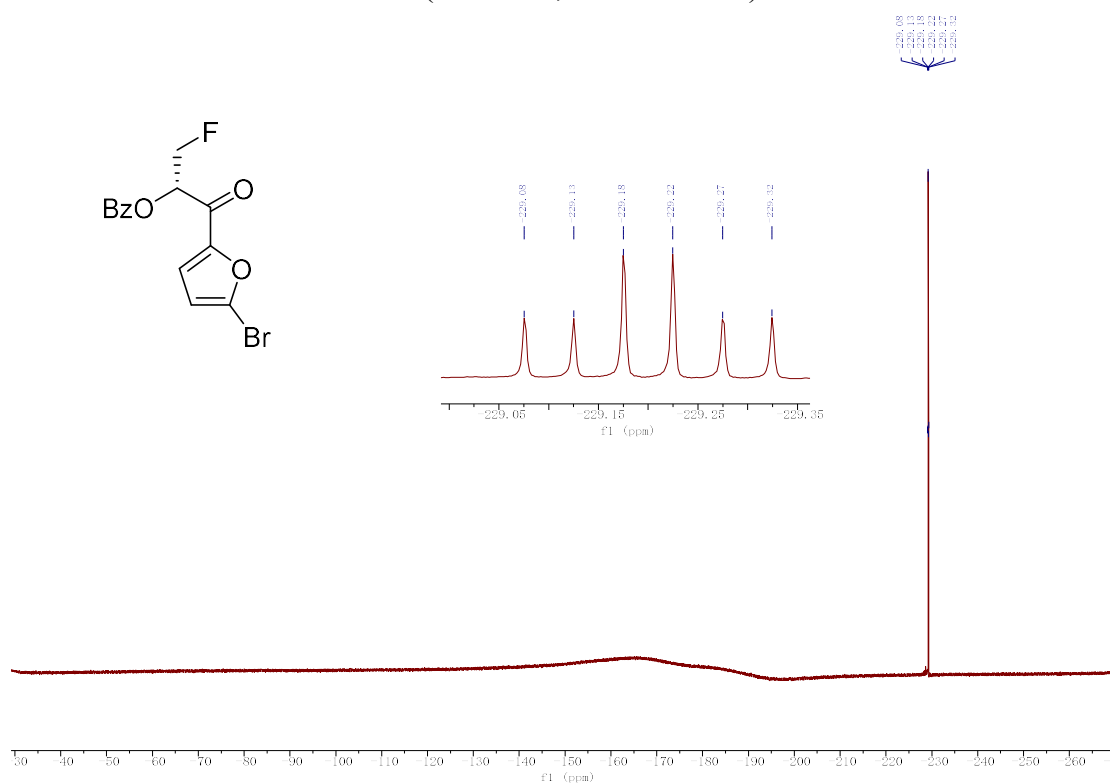
^1H NMR (500 MHz, Chloroform- d) of 2w



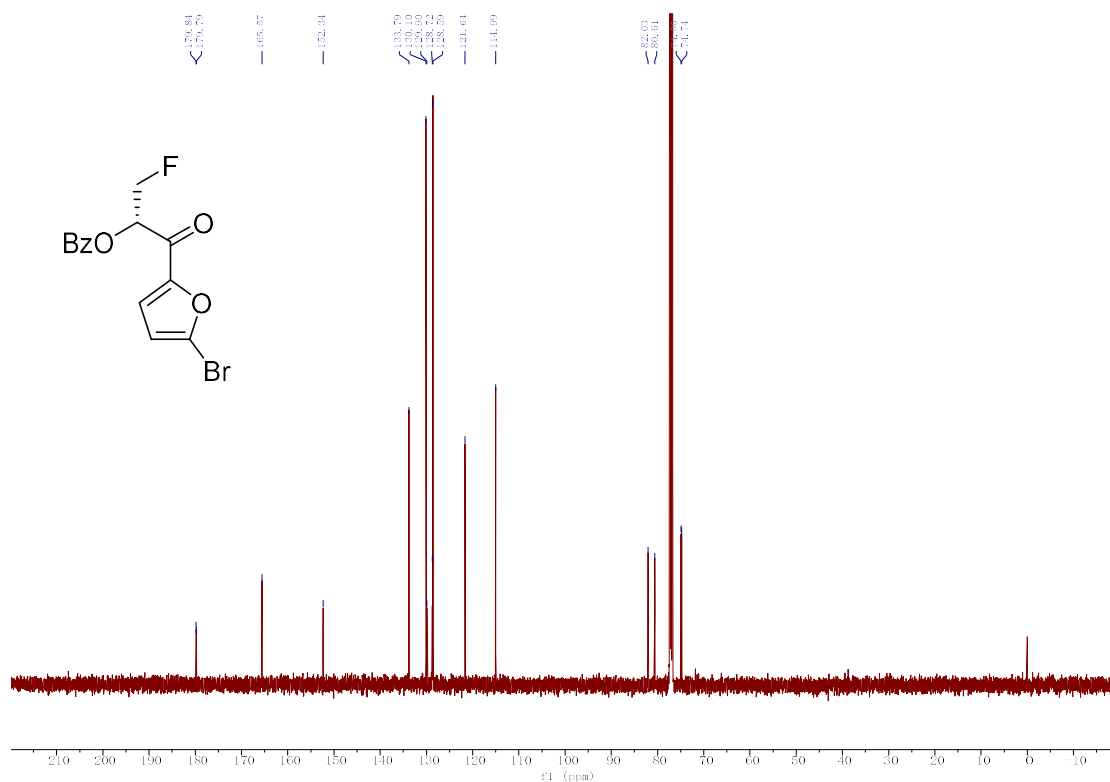
^1H , ^{13}C , and ^{19}F NMR spectra of **2x**



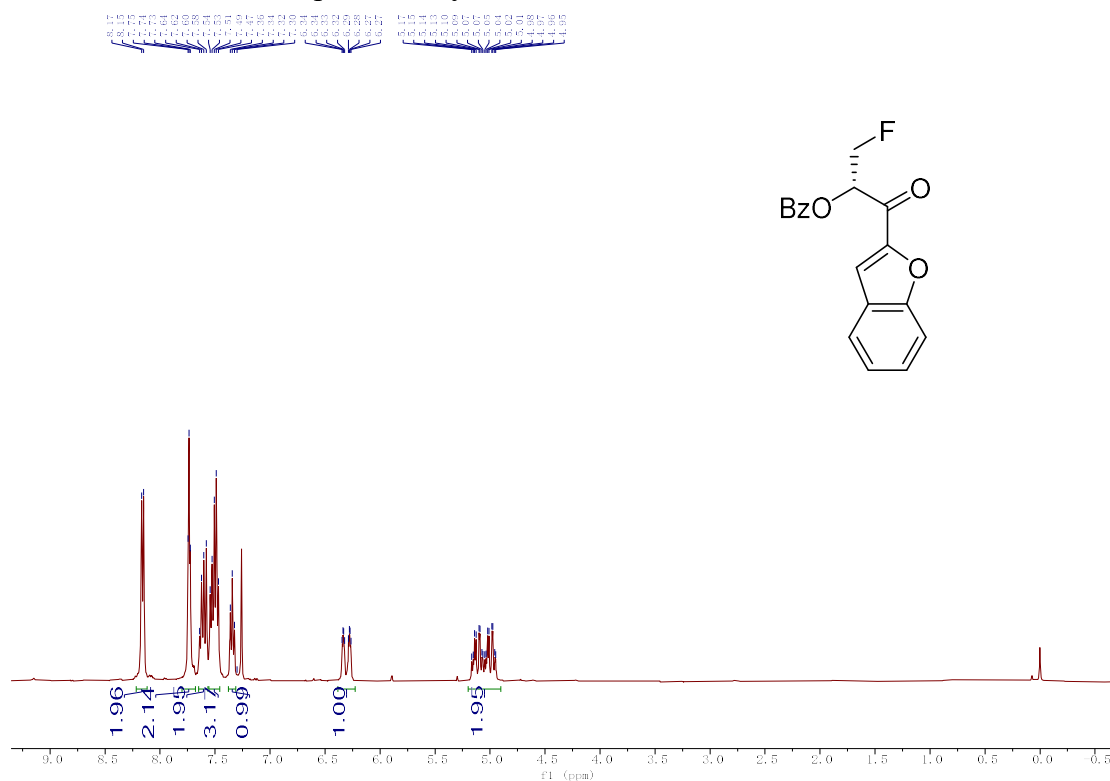
^1H NMR (500 MHz, Chloroform-*d*) of **2x**



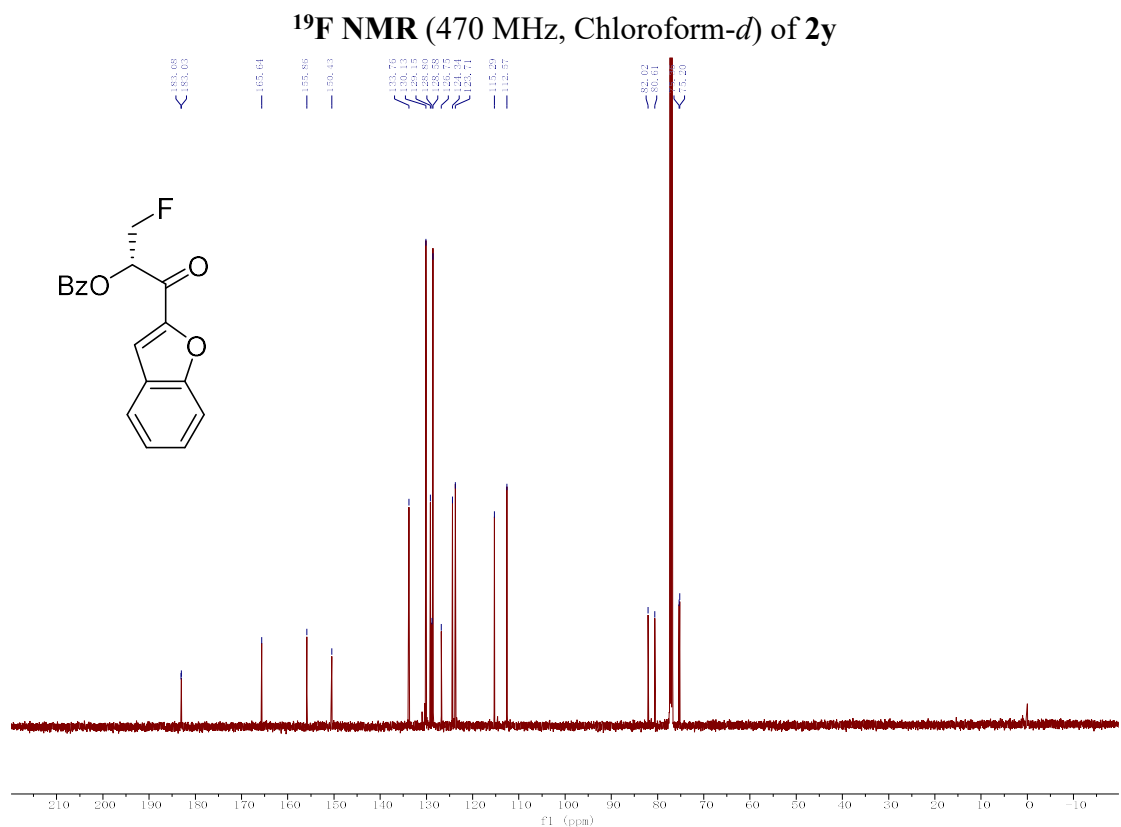
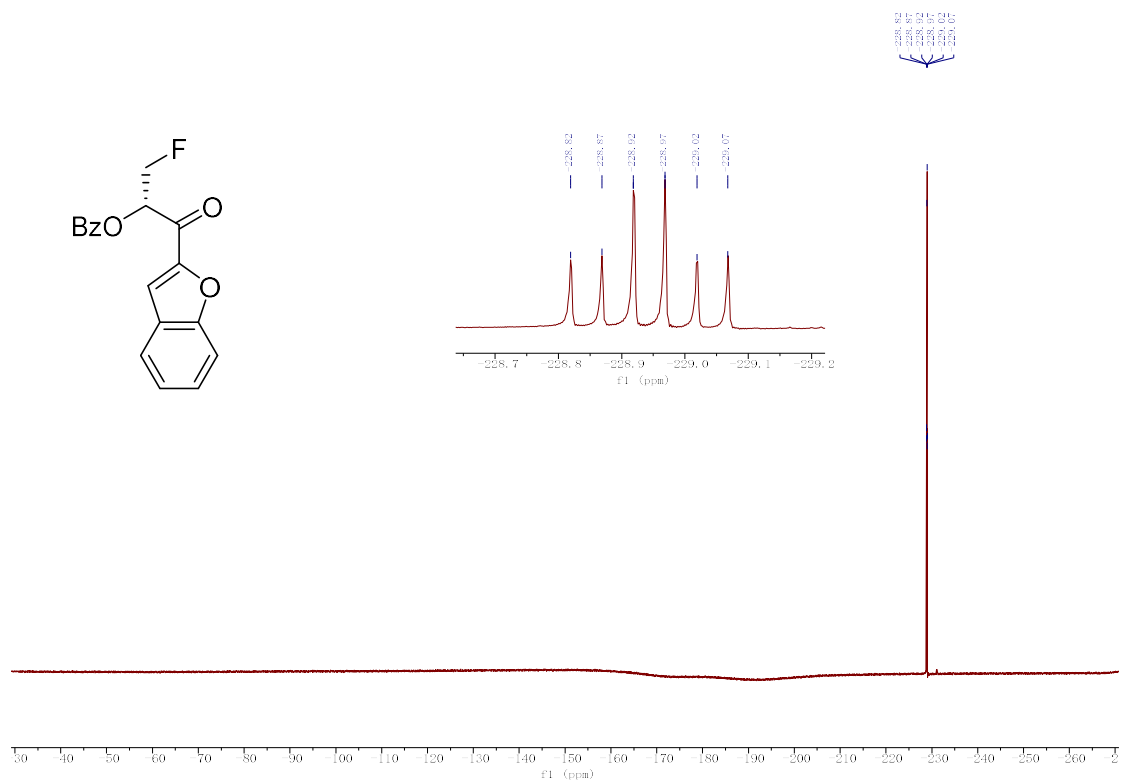
^{19}F NMR (470 MHz, Chloroform-*d*) of **2x**



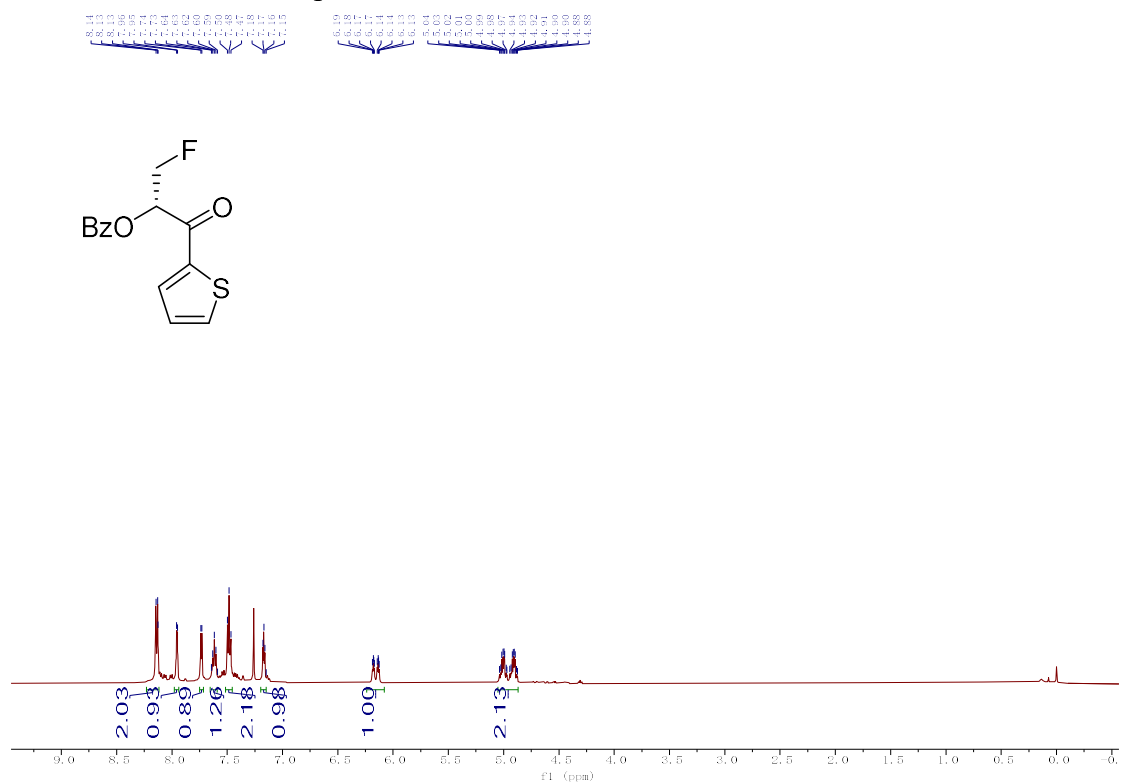
^{13}C NMR (126 MHz, Chloroform-*d*) of **2x**
 ^1H , ^{13}C , and ^{19}F NMR spectra of **2y**



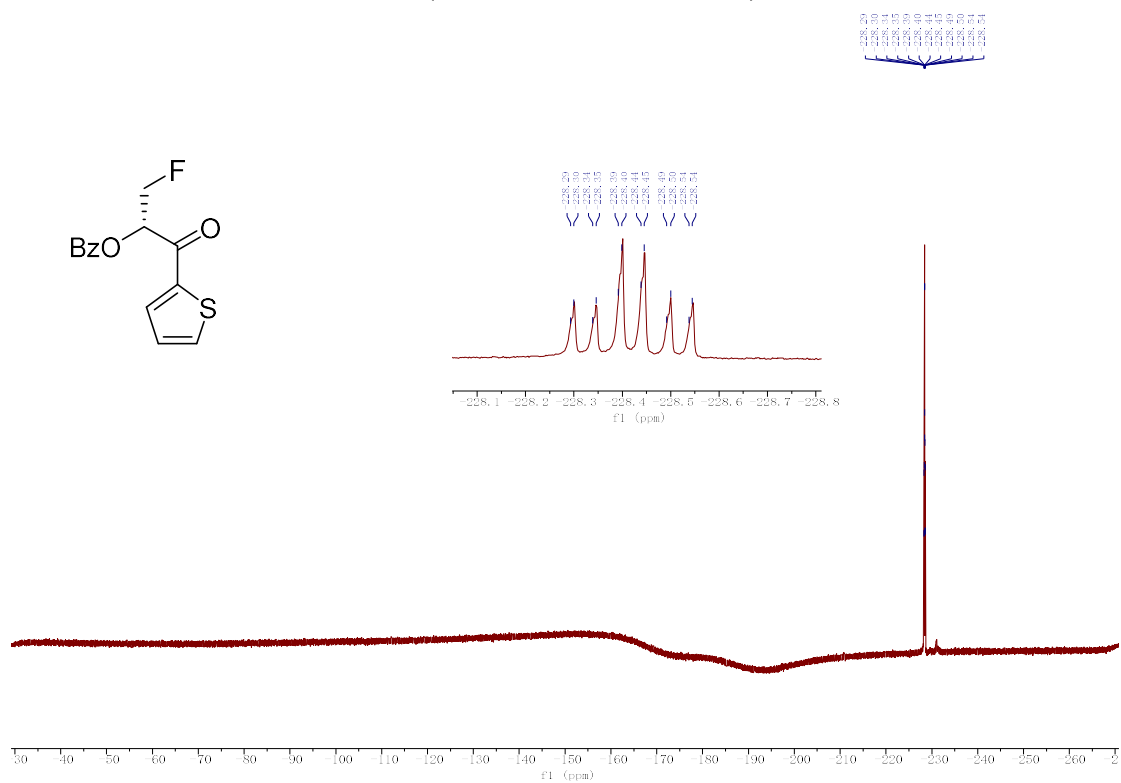
^1H NMR (500 MHz, Chloroform-*d*) of **2y**



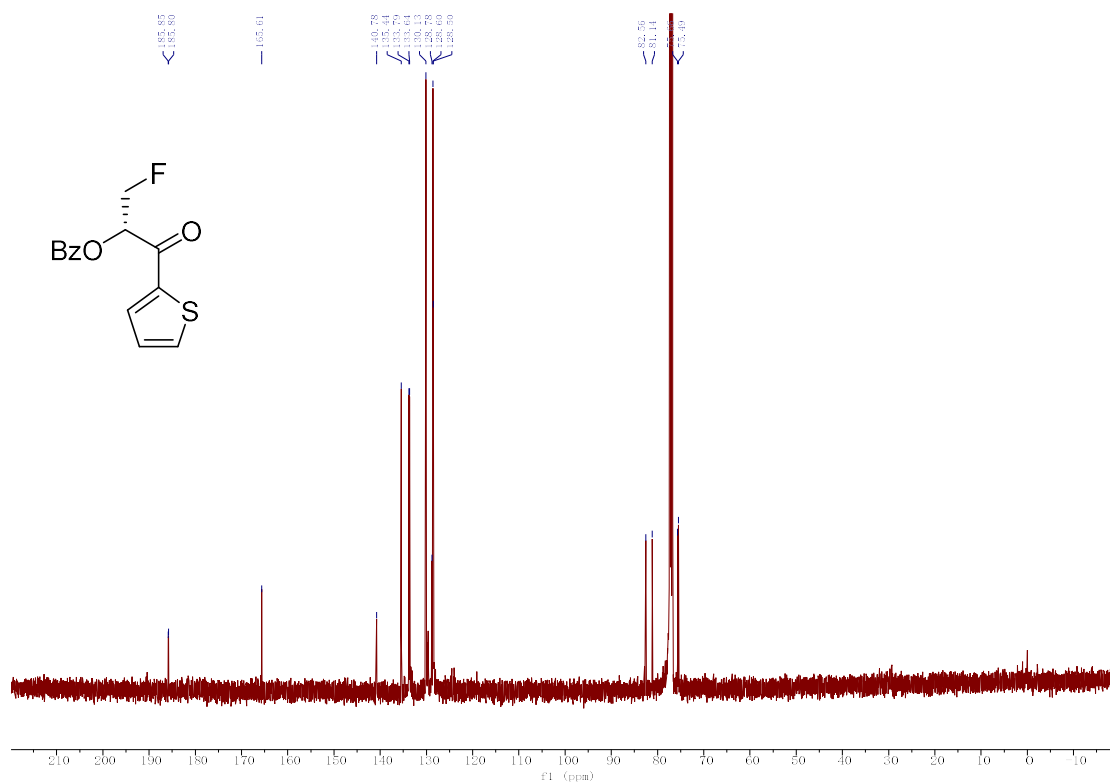
^1H , ^{13}C , and ^{19}F NMR spectra of **2z**



^1H NMR (500 MHz, Chloroform-*d*) of **2z**

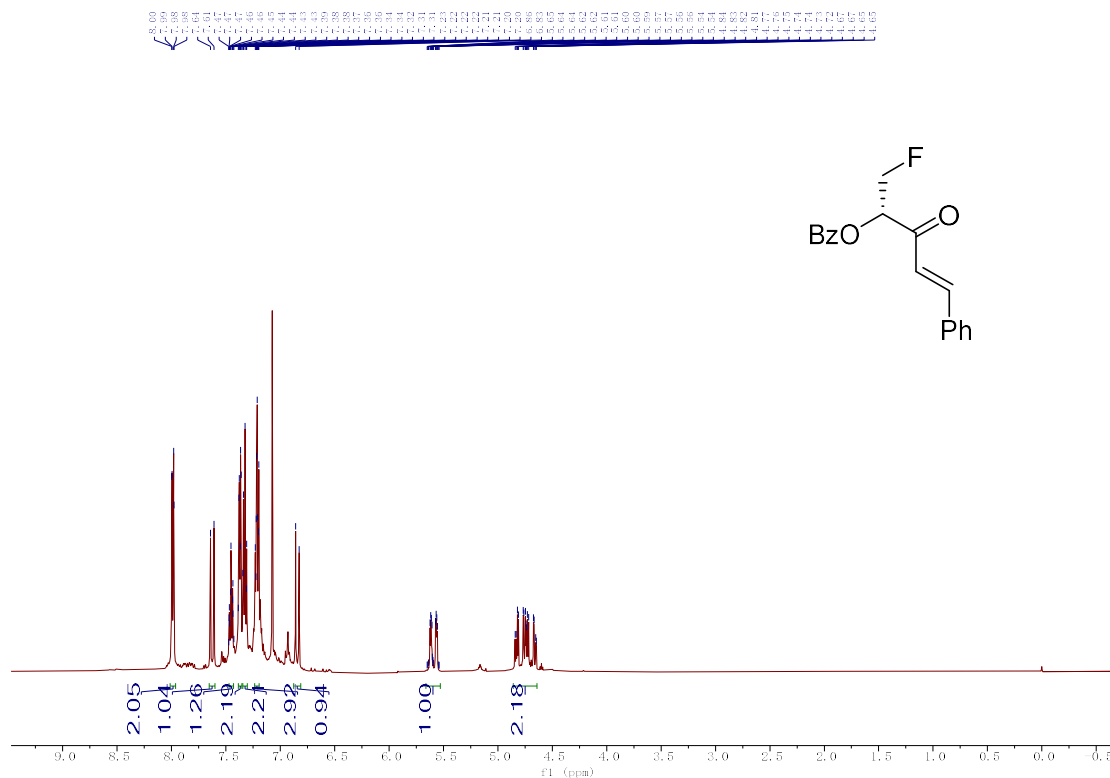


^{19}F NMR (470 MHz, Chloroform-*d*) of **2z**

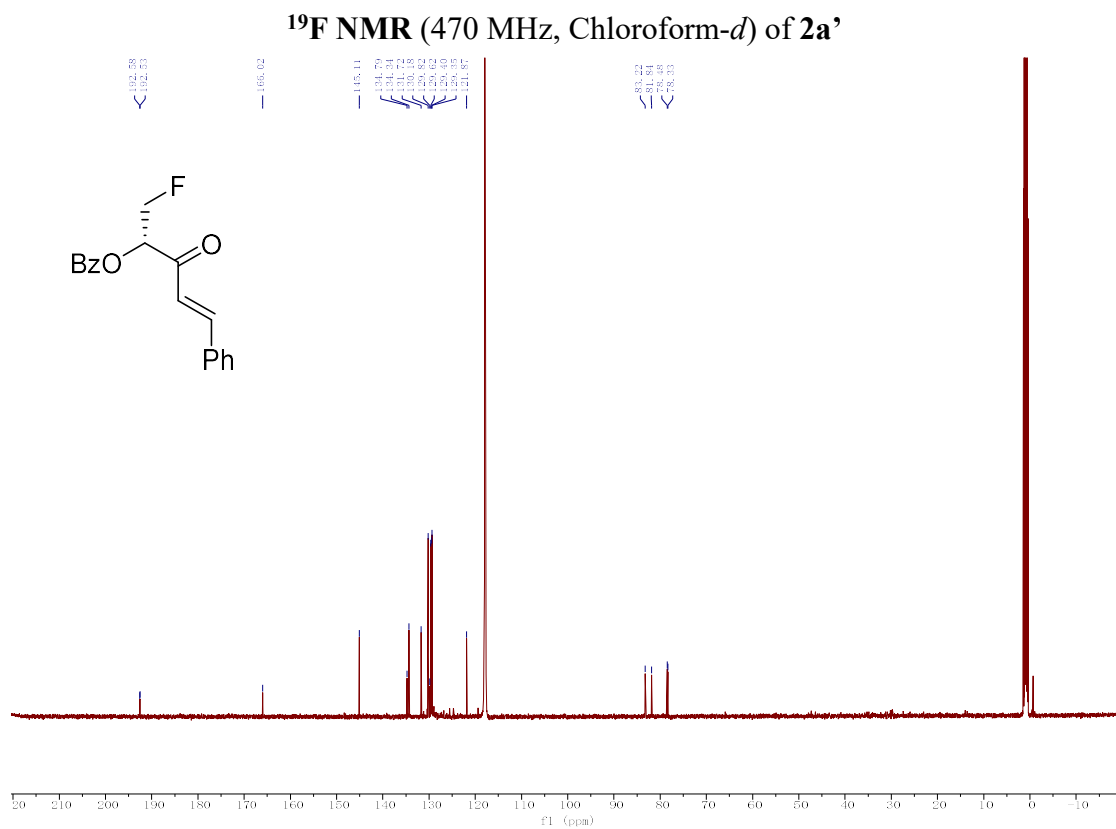
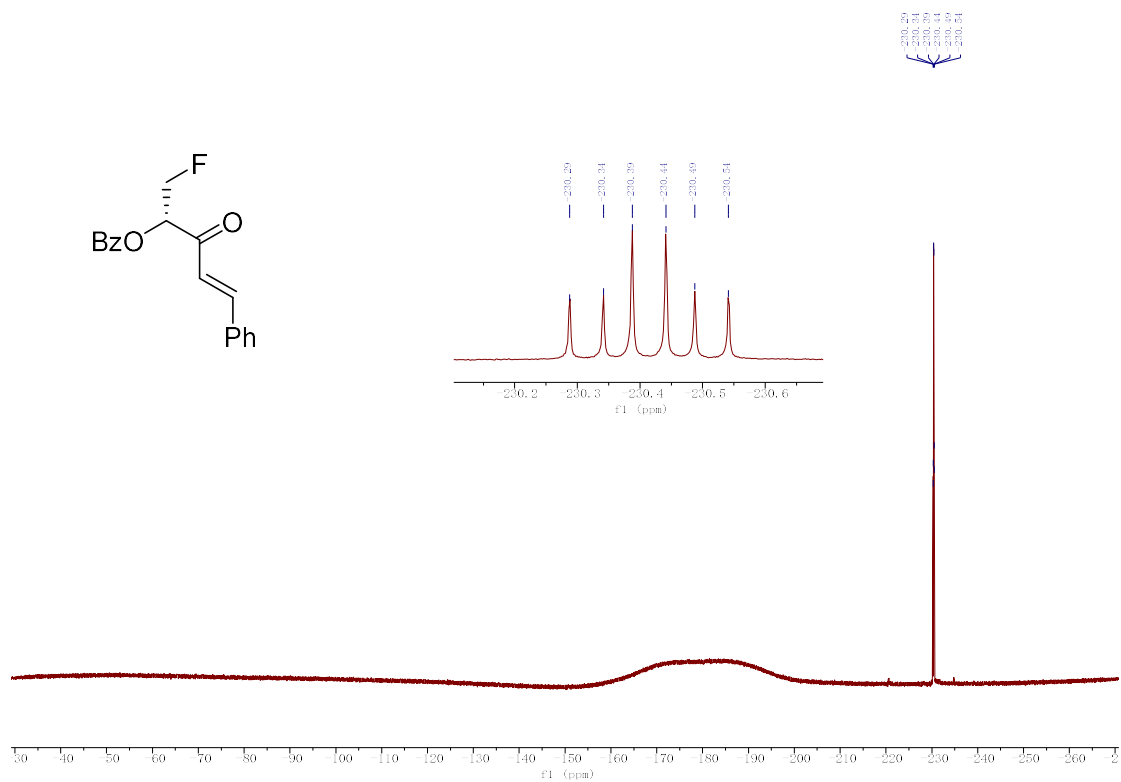


¹³C NMR (126 MHz, Chloroform-*d*) of **2z**

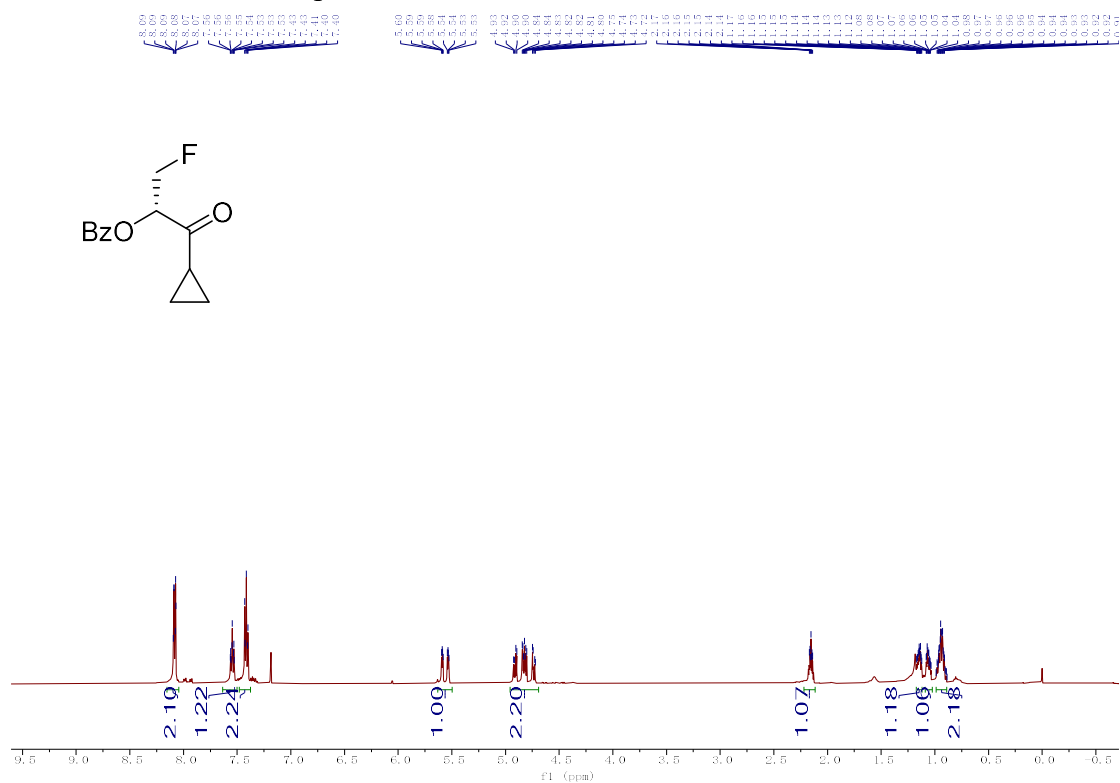
¹H, ¹³C, and ¹⁹F NMR spectra of **2a'**



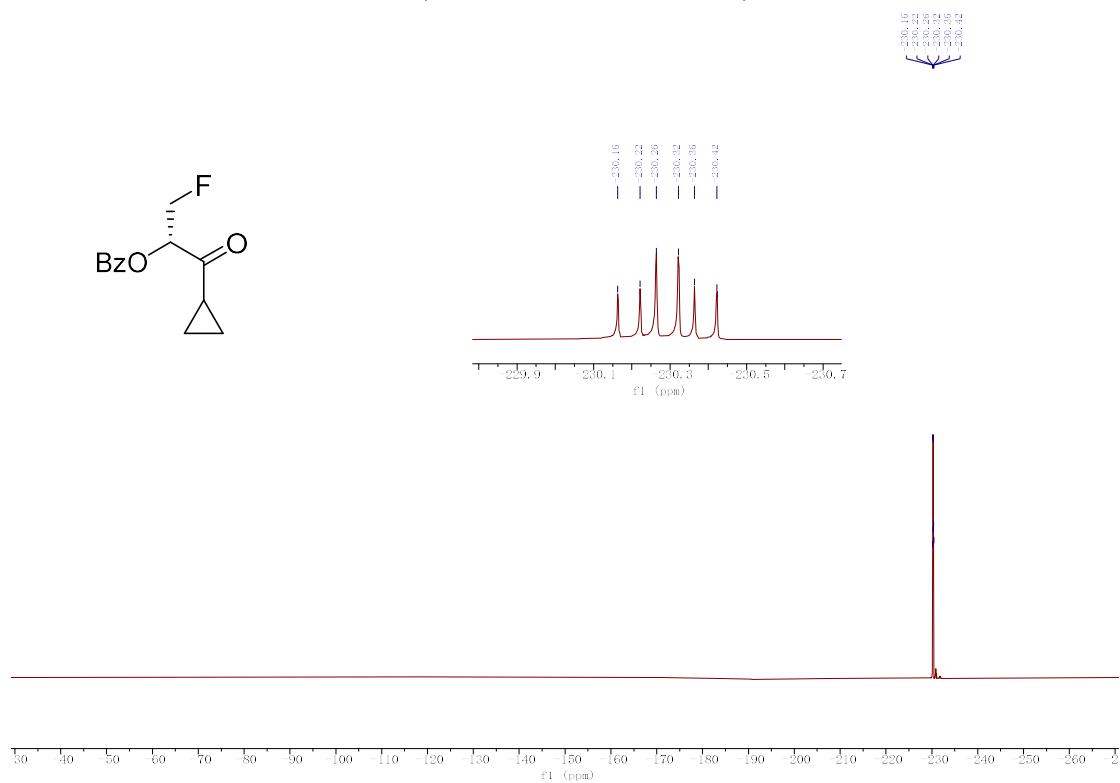
¹H NMR (500 MHz, Chloroform-*d*) of **2a'**



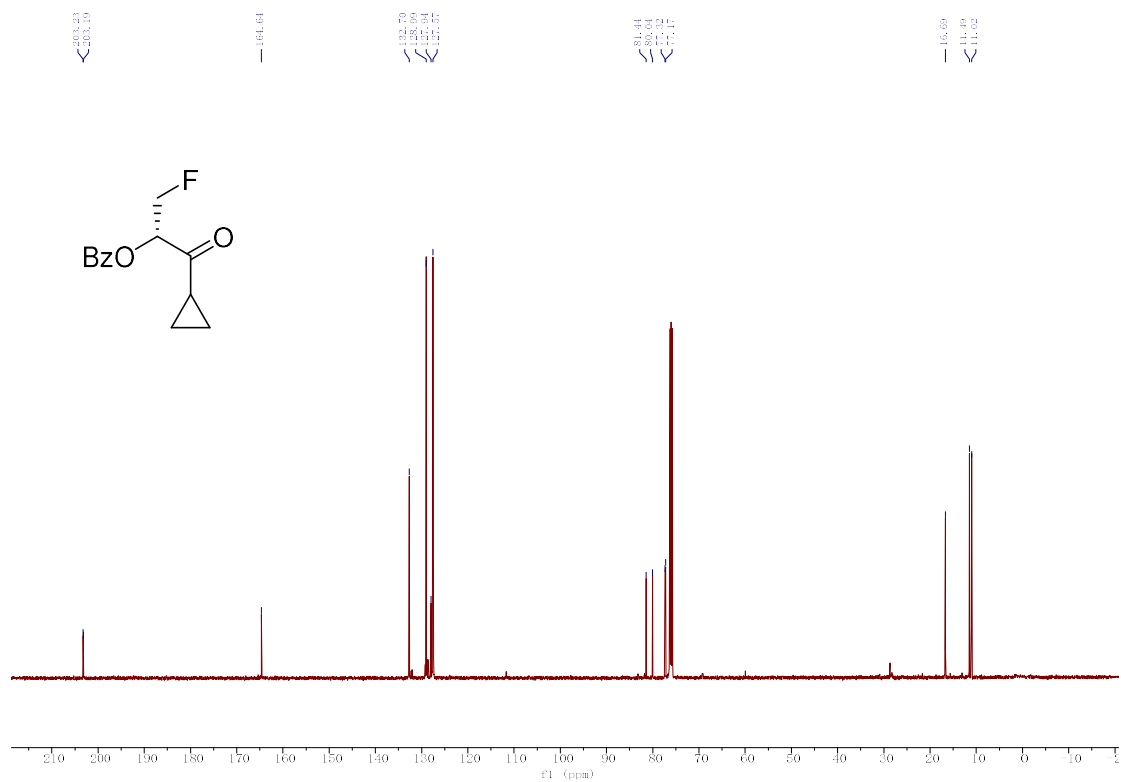
^1H , ^{13}C , and ^{19}F NMR spectra of **2b'**



^1H NMR (500 MHz, Chloroform-*d*) of **2b'**

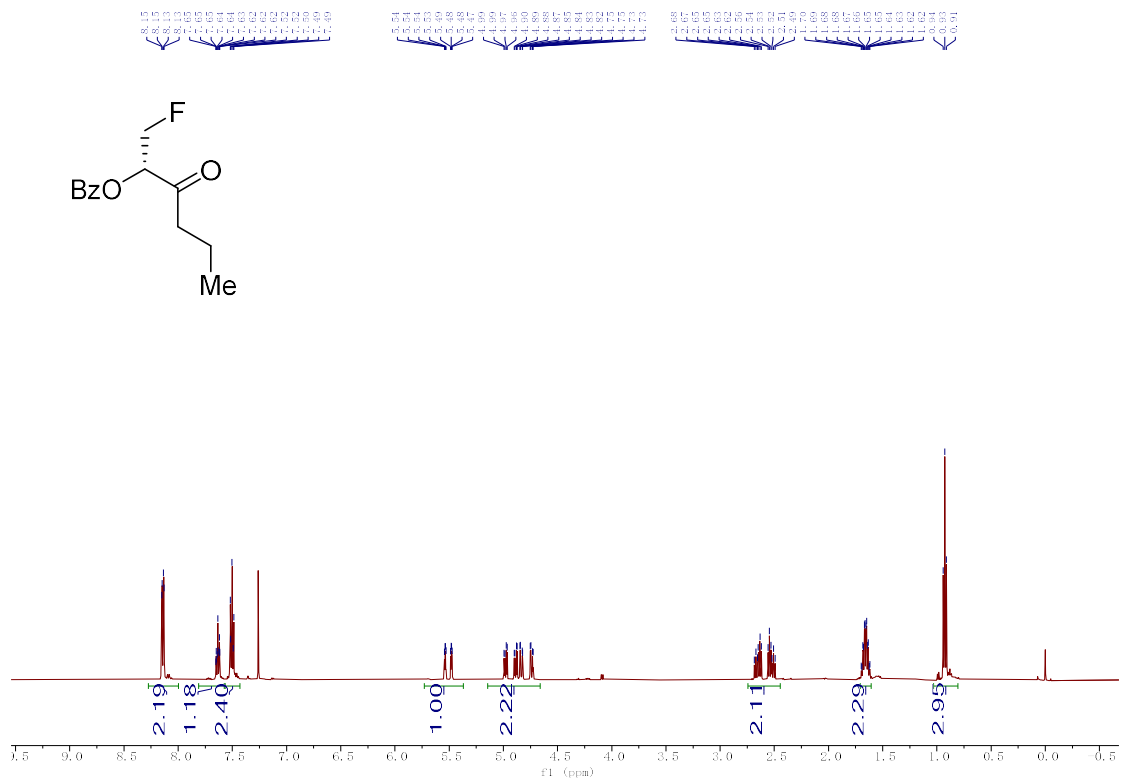


^{19}F NMR (470 MHz, Chloroform-*d*) of **2b'**

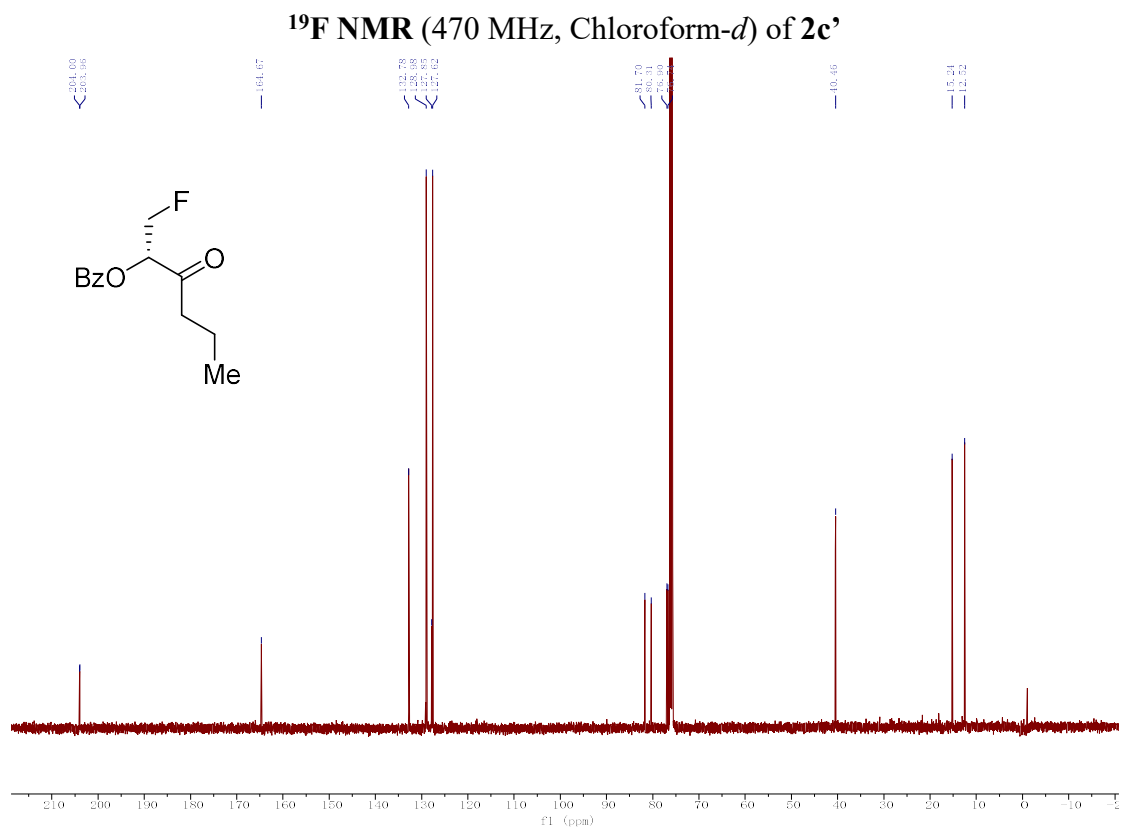
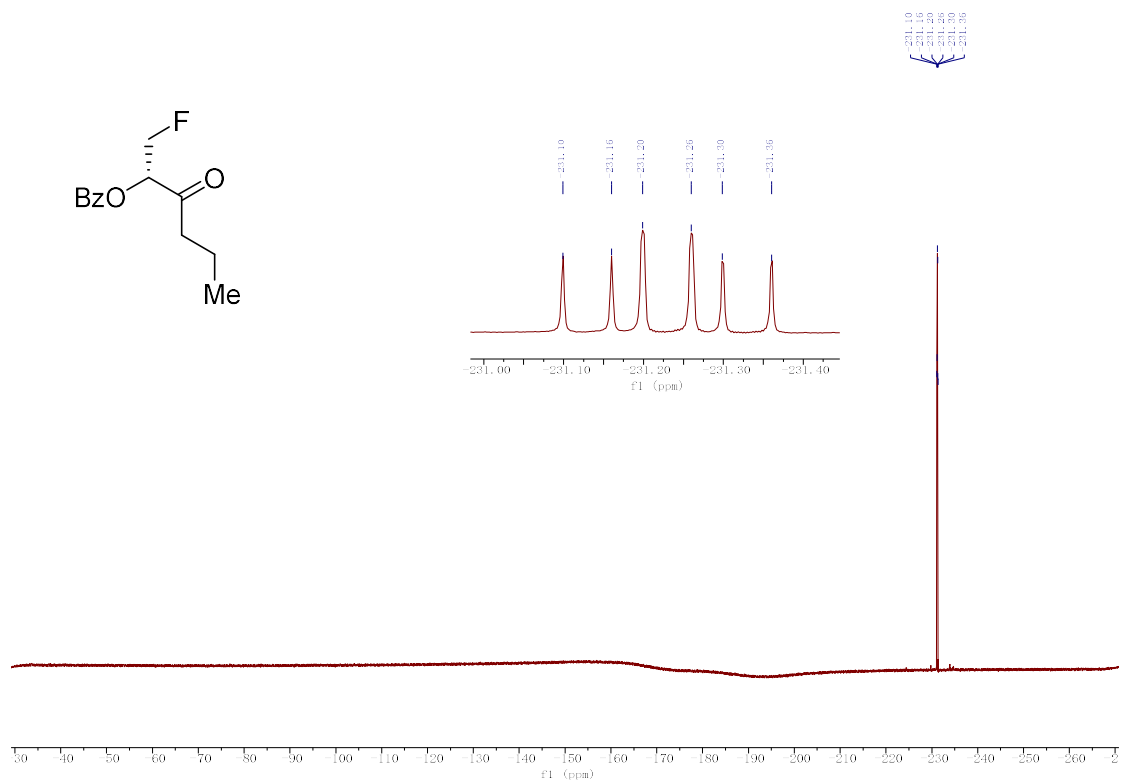


¹³C NMR (126 MHz, Chloroform-*d*) of **2b'**

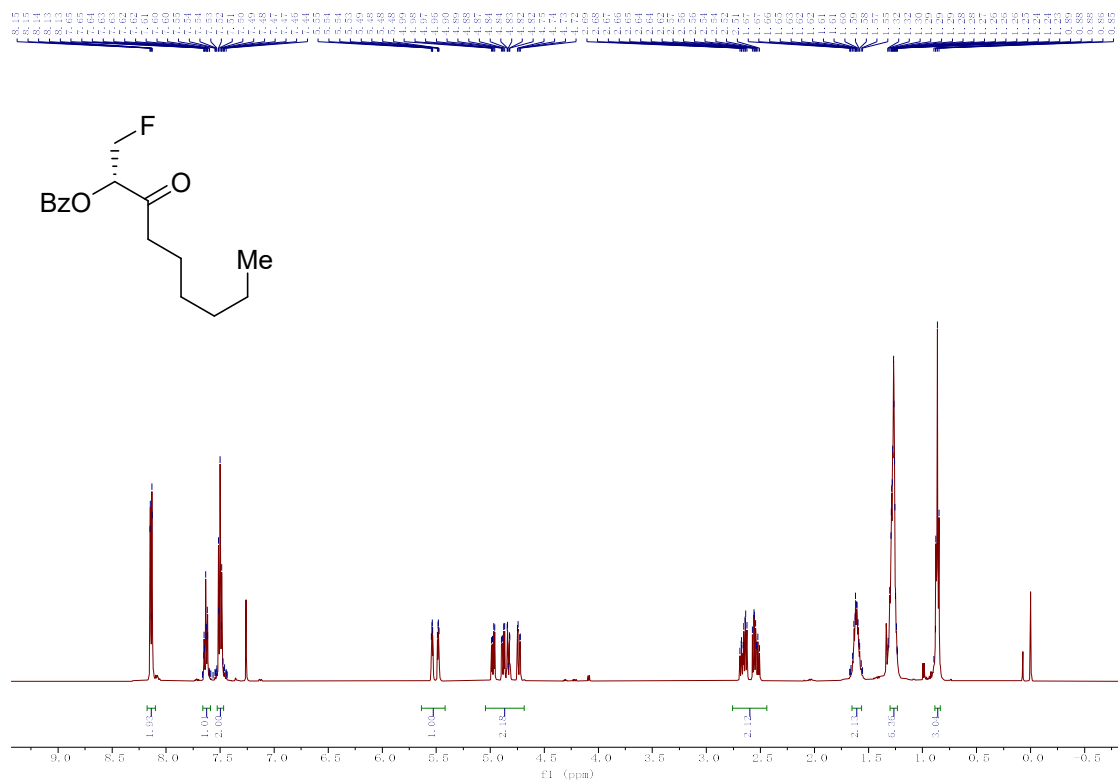
¹H, ¹³C, and ¹⁹F NMR spectra of **2c'**



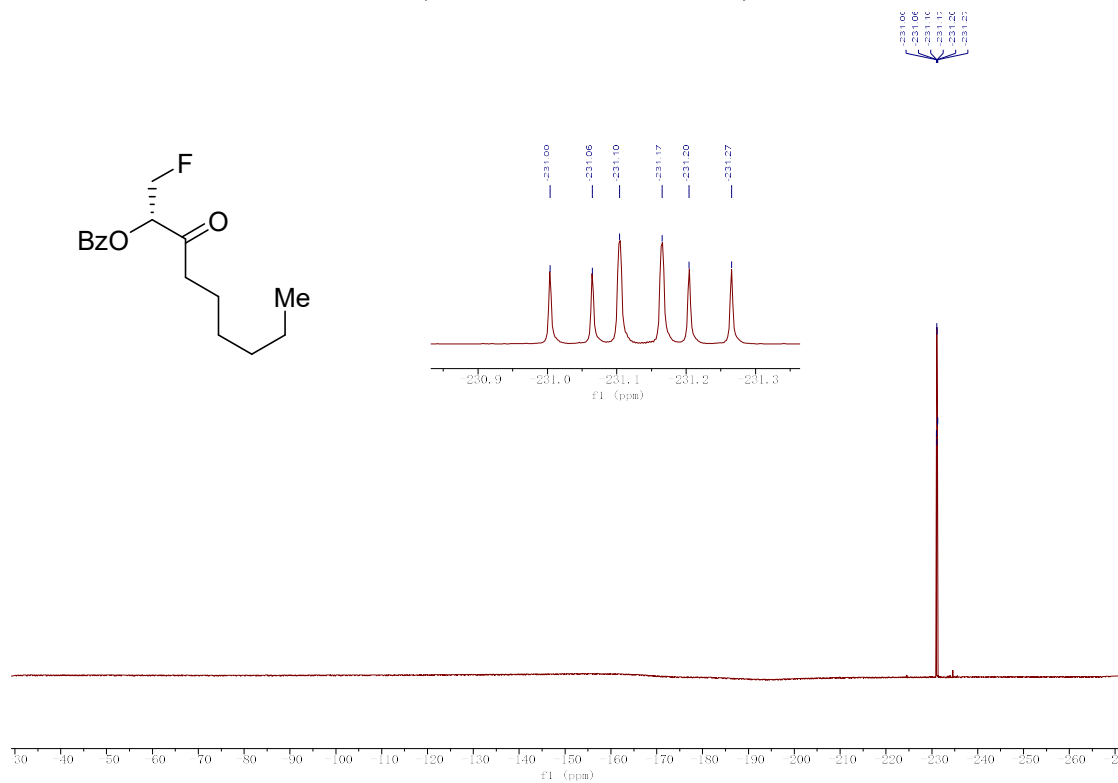
¹H NMR (500 MHz, Chloroform-*d*) of **2c'**



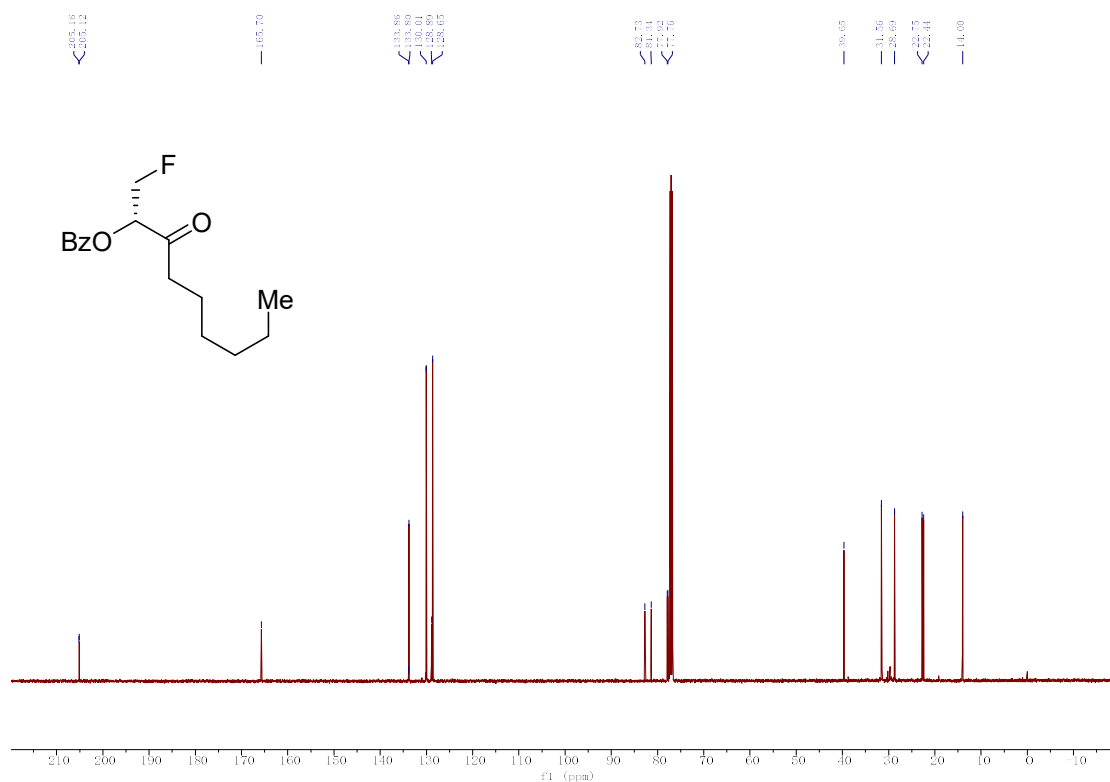
^1H , ^{13}C , and ^{19}F NMR spectra of **2d'**



^1H NMR (500 MHz, Chloroform-*d*) of **2d'**

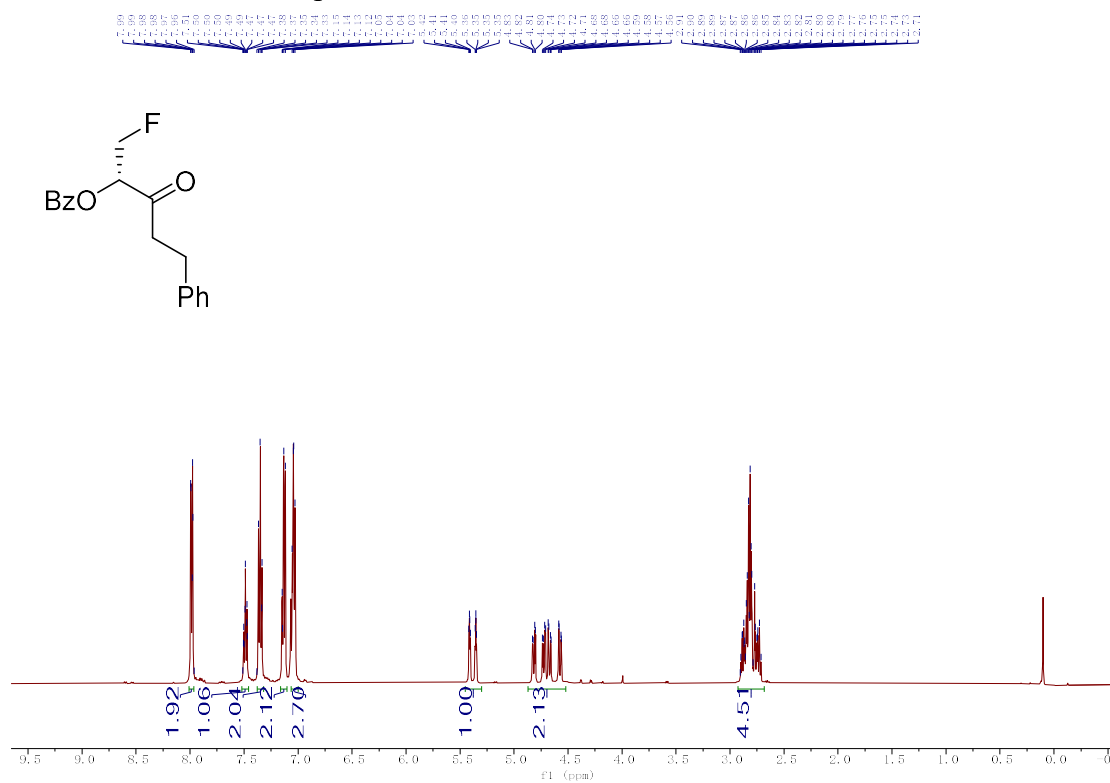


^{19}F NMR (470 MHz, Chloroform-*d*) of **2d'**

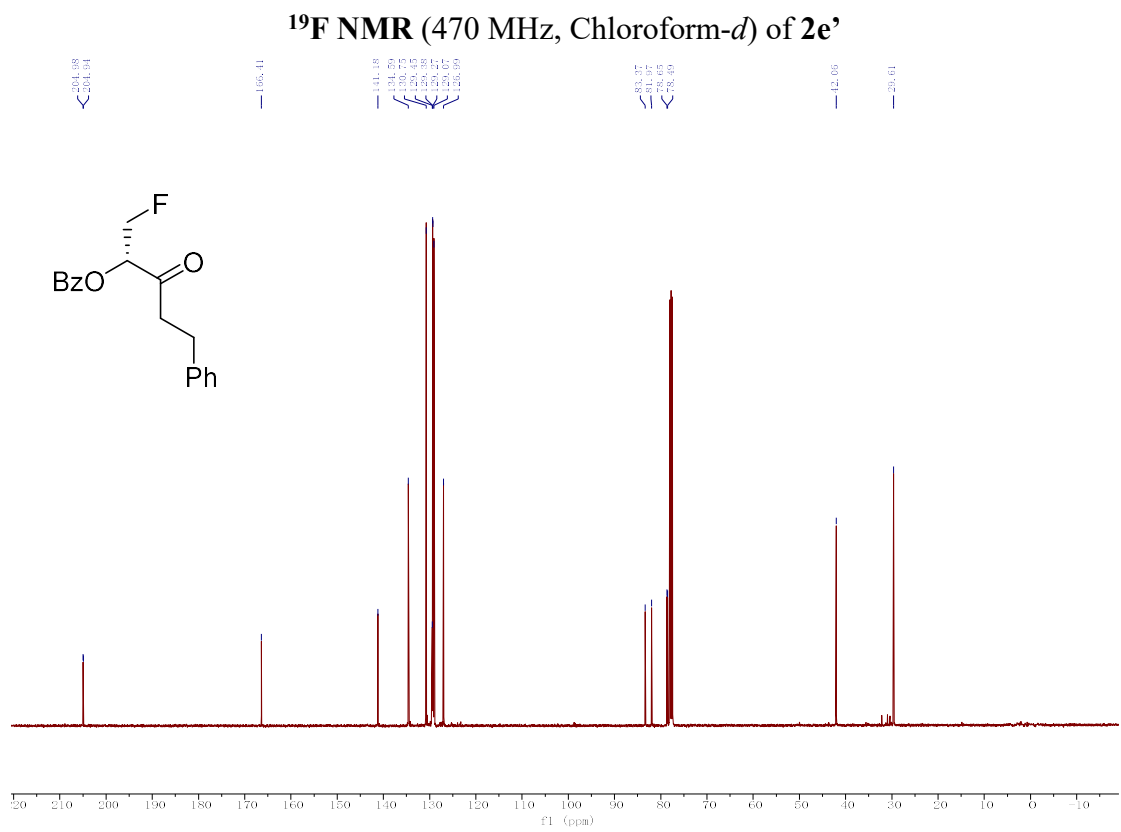
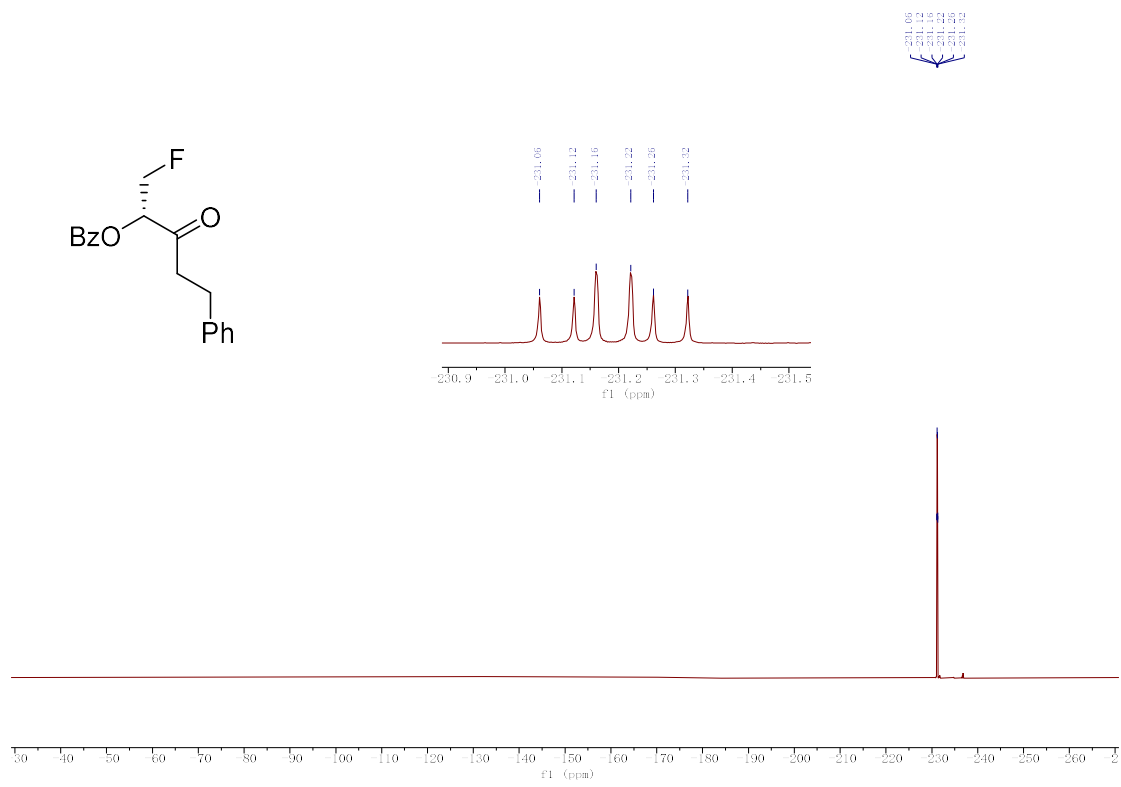


¹³C NMR (126 MHz, Chloroform-*d*) of **2d'**

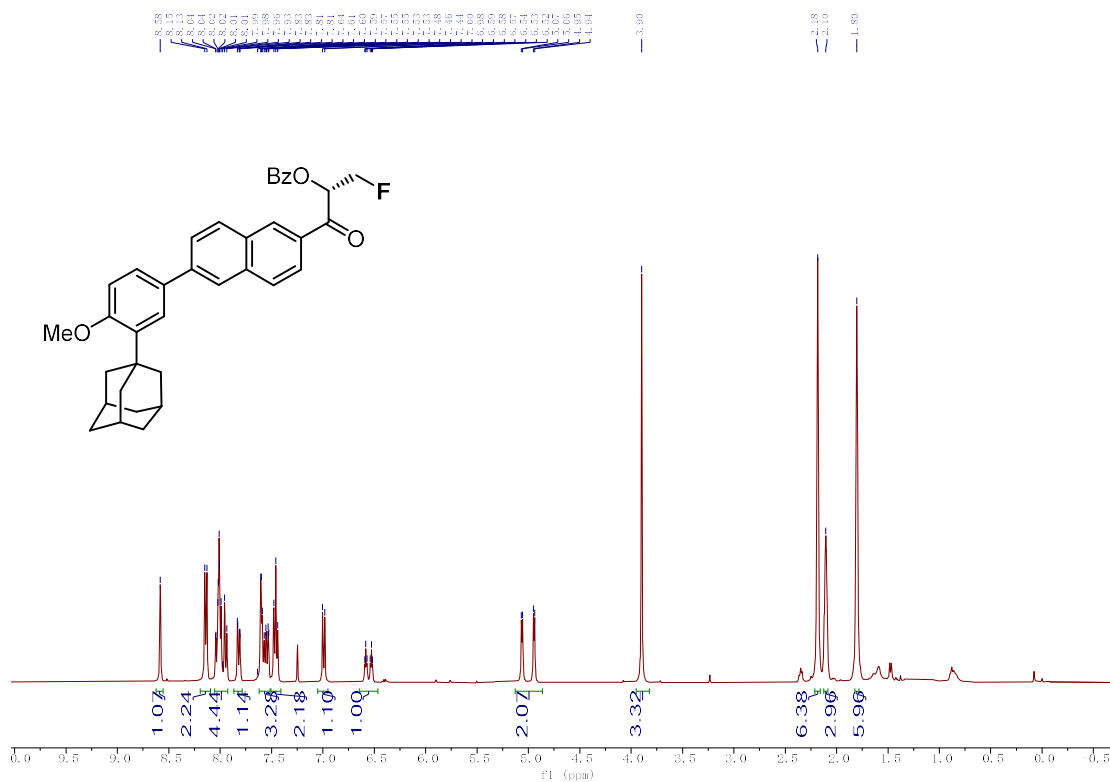
¹H, ¹³C, and ¹⁹F NMR spectra of **2e'**



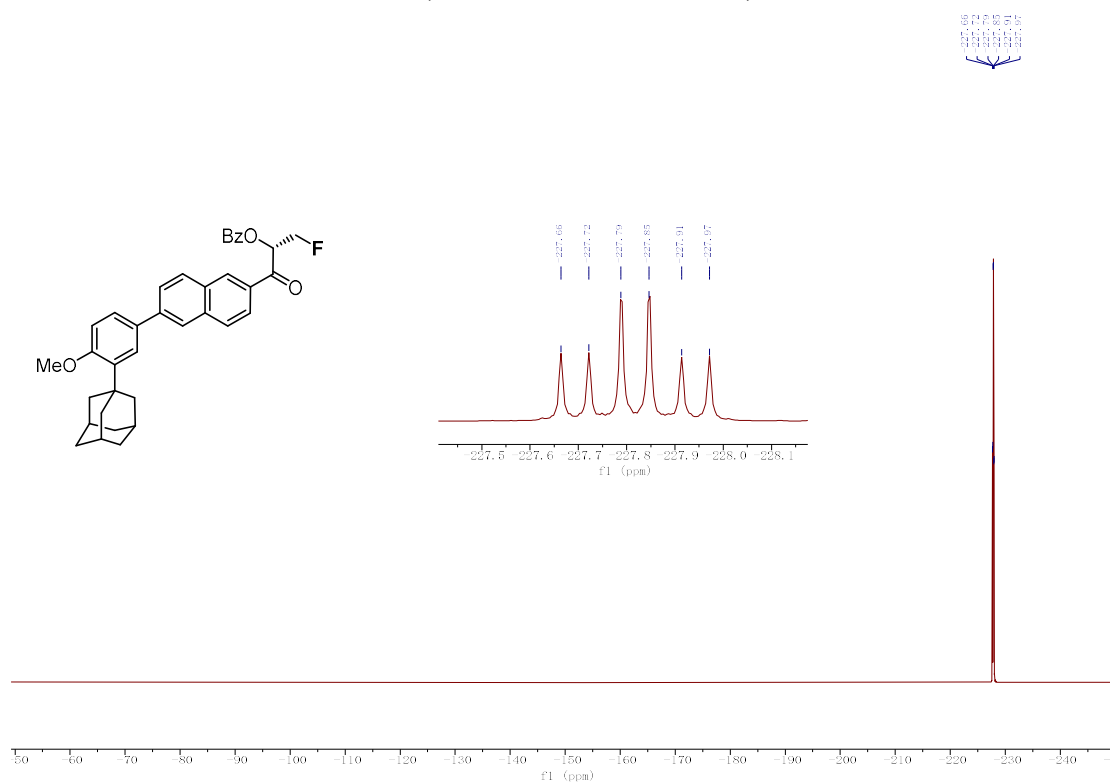
¹H NMR (500 MHz, Chloroform-*d*) of **2e'**



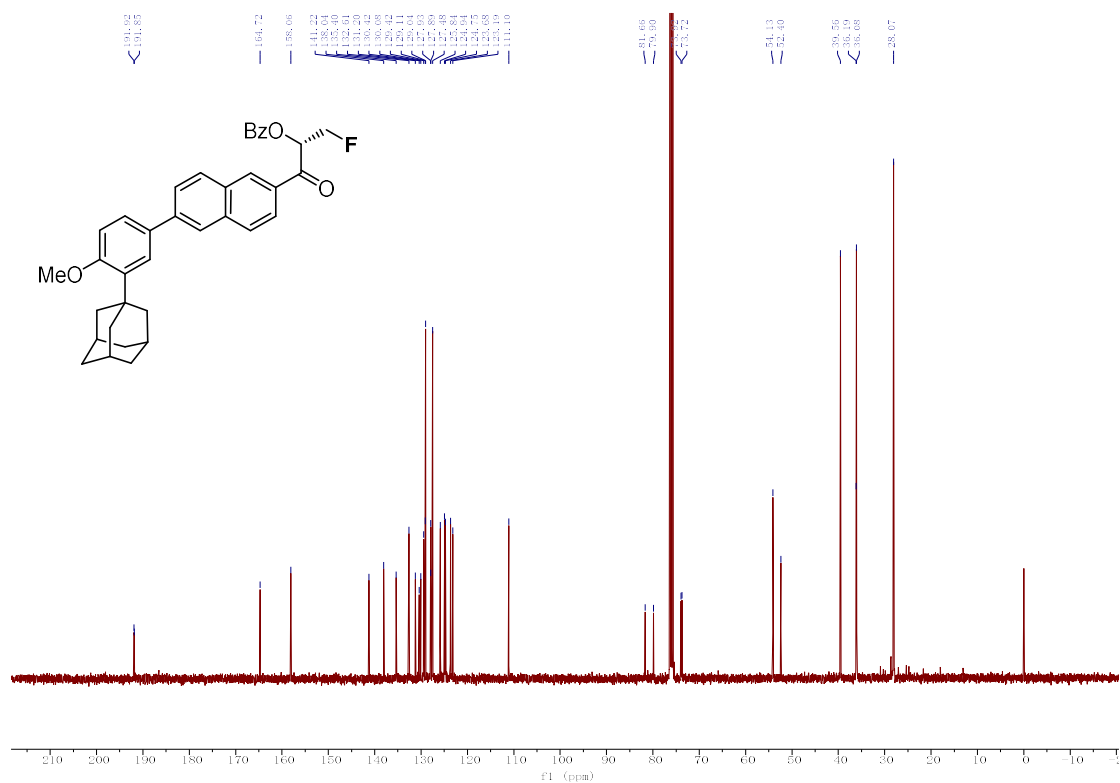
^1H , ^{13}C , and ^{19}F NMR spectra of **2f**



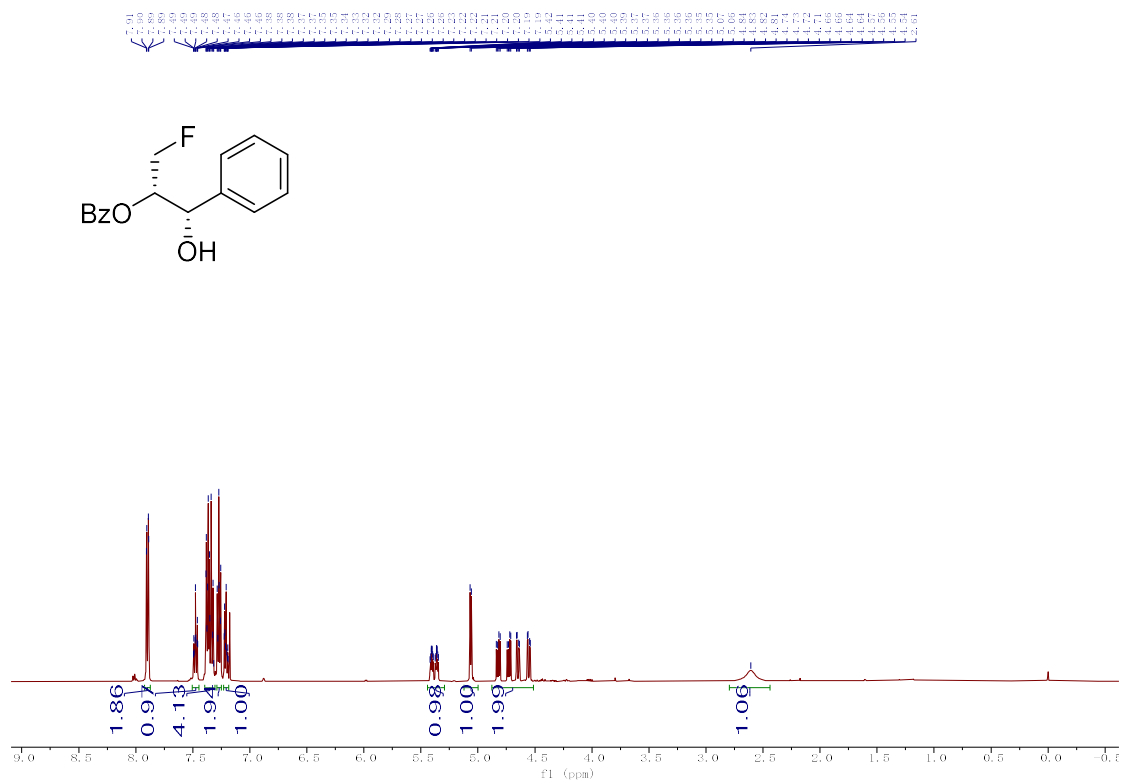
^1H NMR (400 MHz, Chloroform-*d*) of **2f**



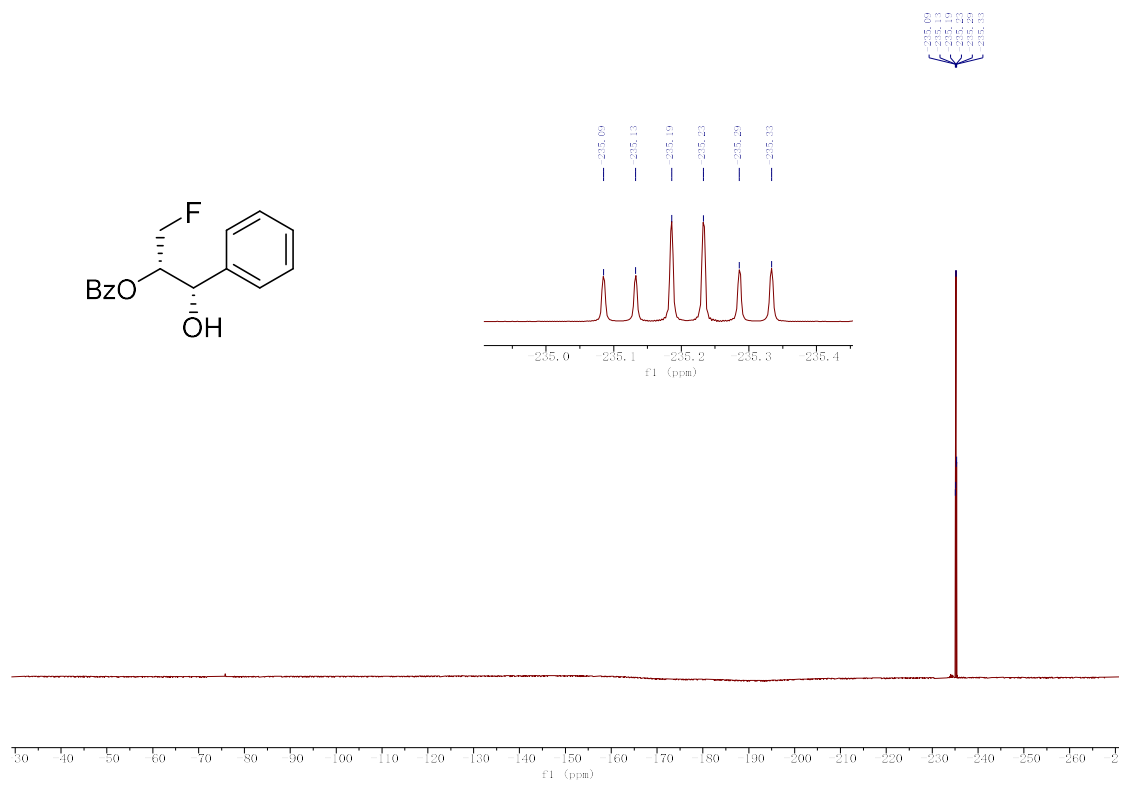
^{19}F NMR (376 MHz, Chloroform-*d*) of **2f**



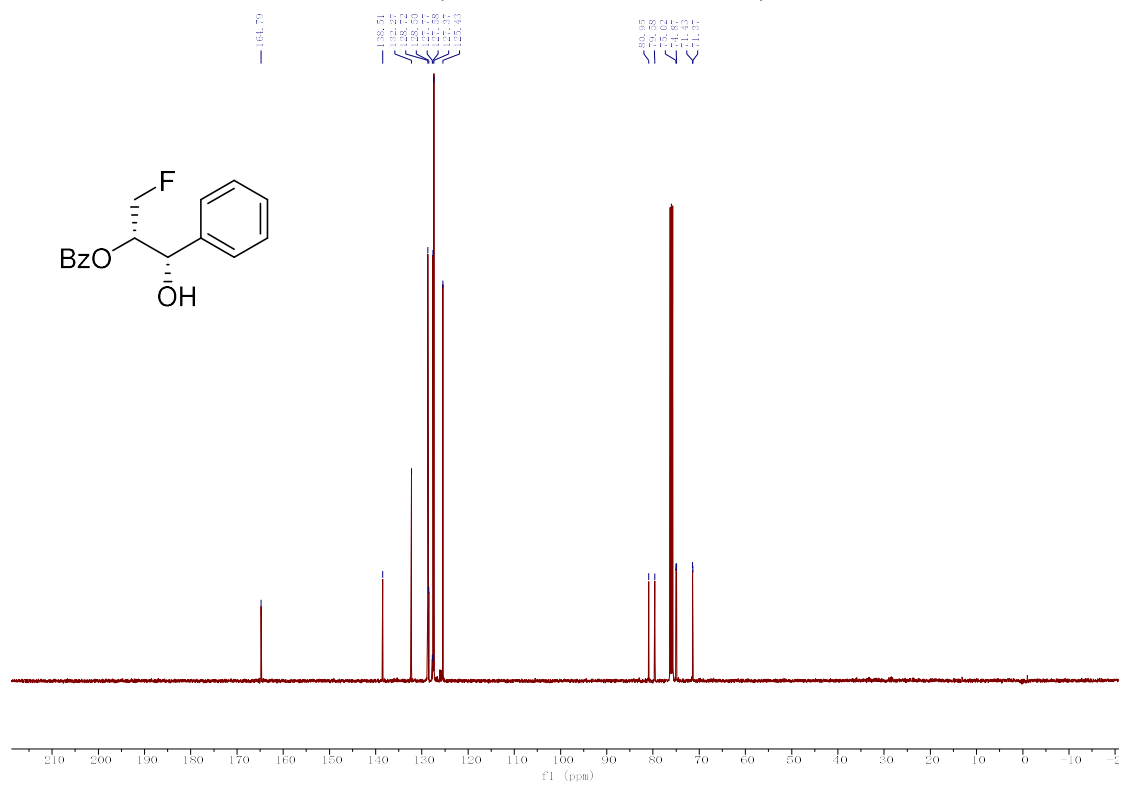
¹³C NMR (101 MHz, Chloroform-*d*) of **2f**
¹H, ¹³C, and ¹⁹F NMR spectra of **3**



¹H NMR (500 MHz, Chloroform-*d*) of **3**

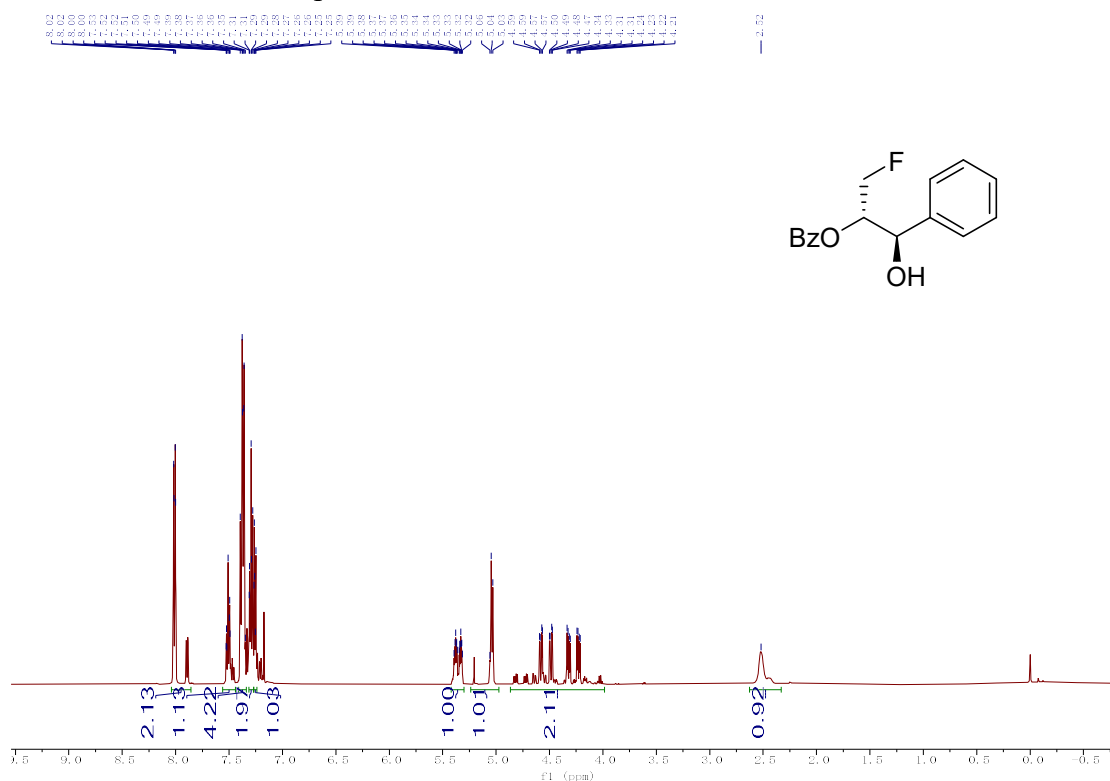


^{19}F NMR (470 MHz, Chloroform- d) of **3**

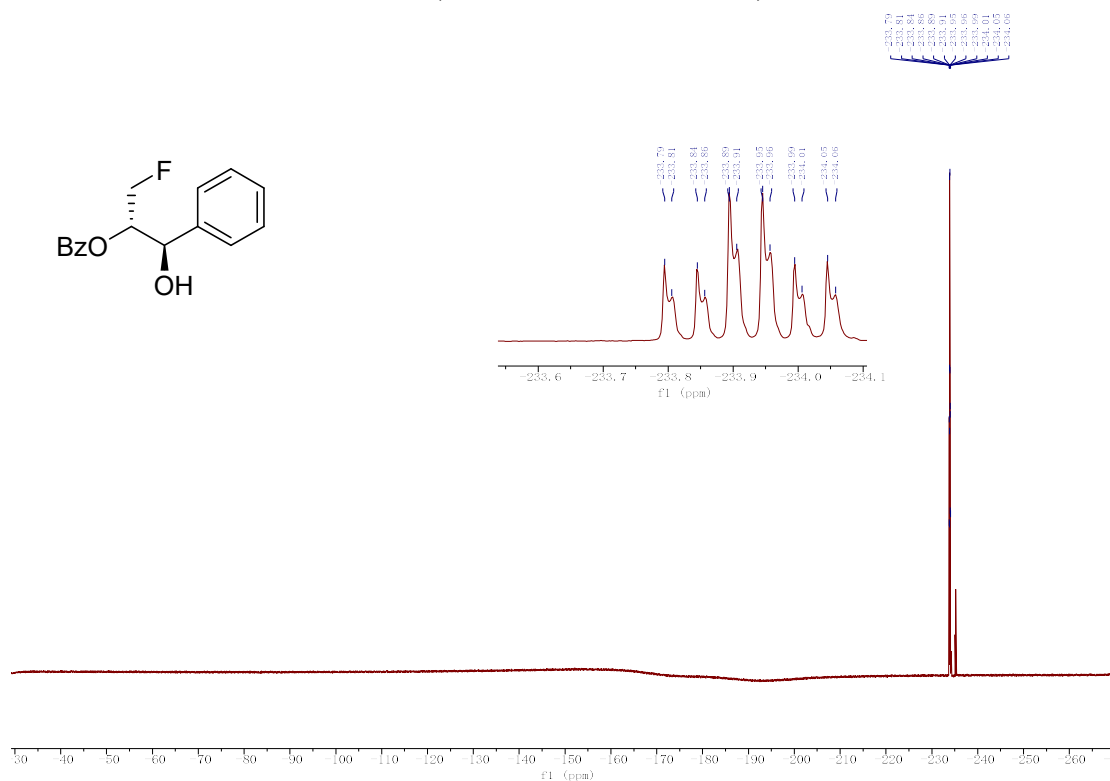


^{13}C NMR (126 MHz, Chloroform- d) of **3**

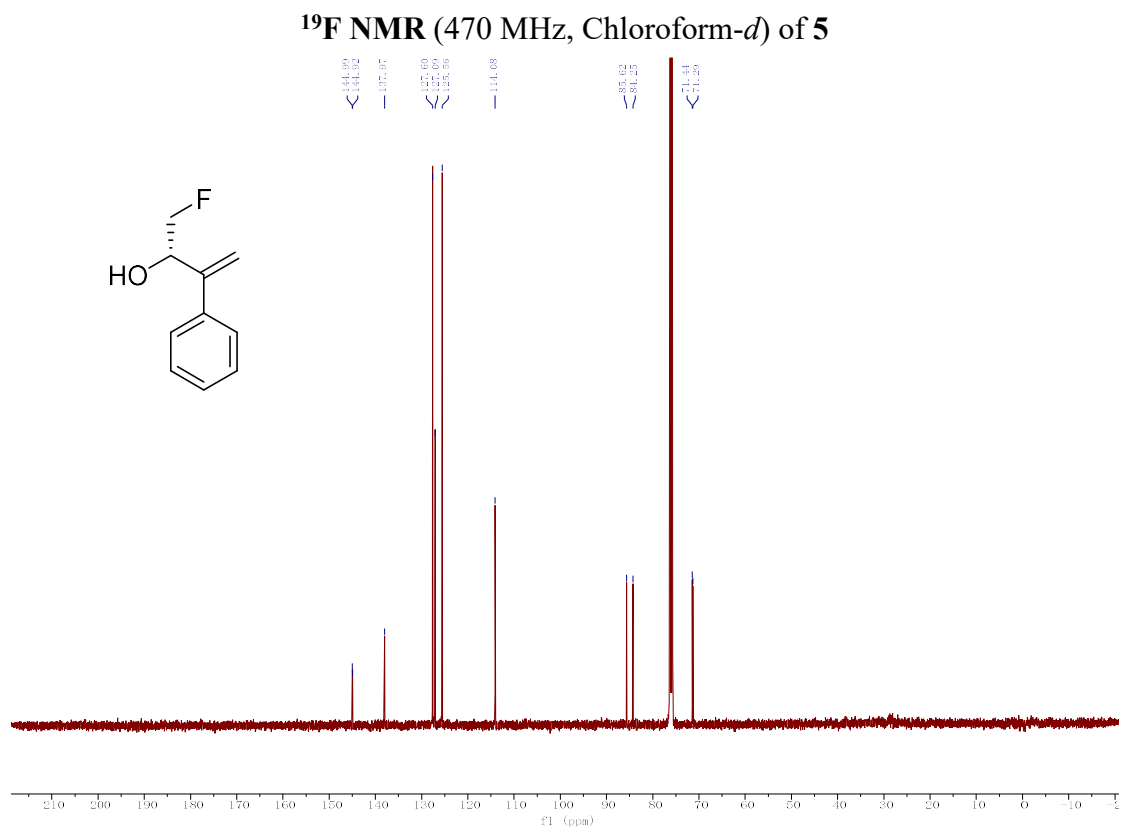
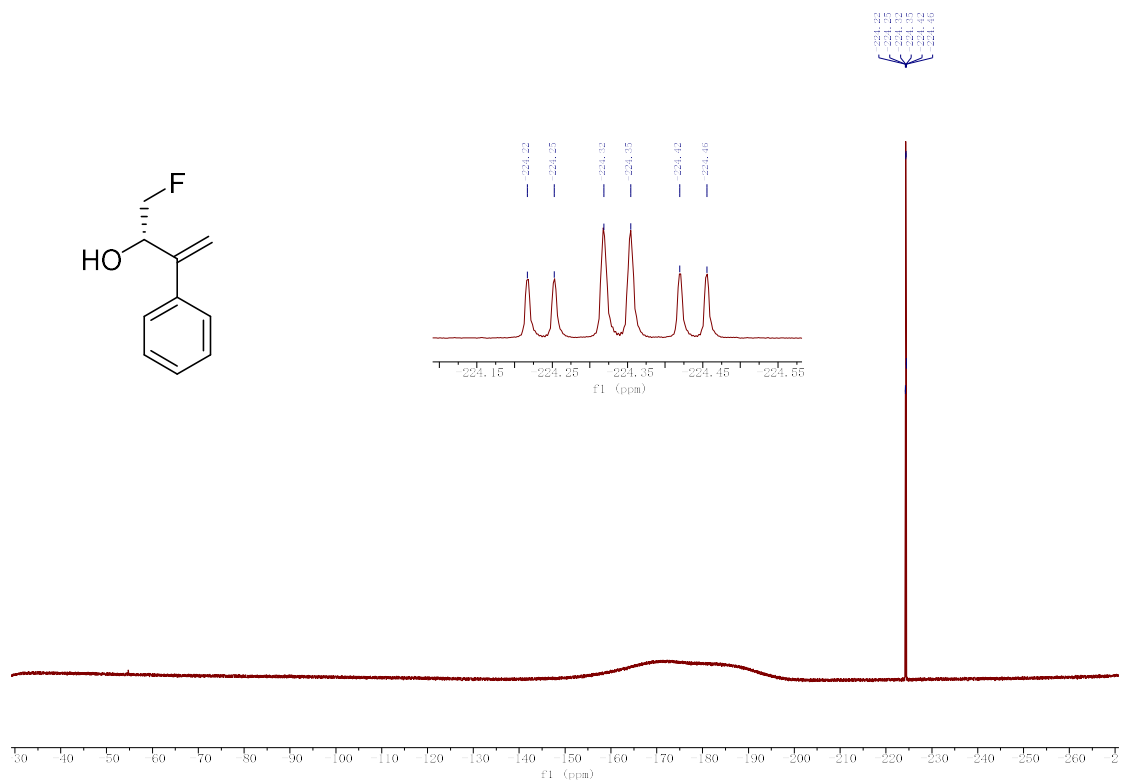
^1H , ^{13}C , and ^{19}F NMR spectra of 4



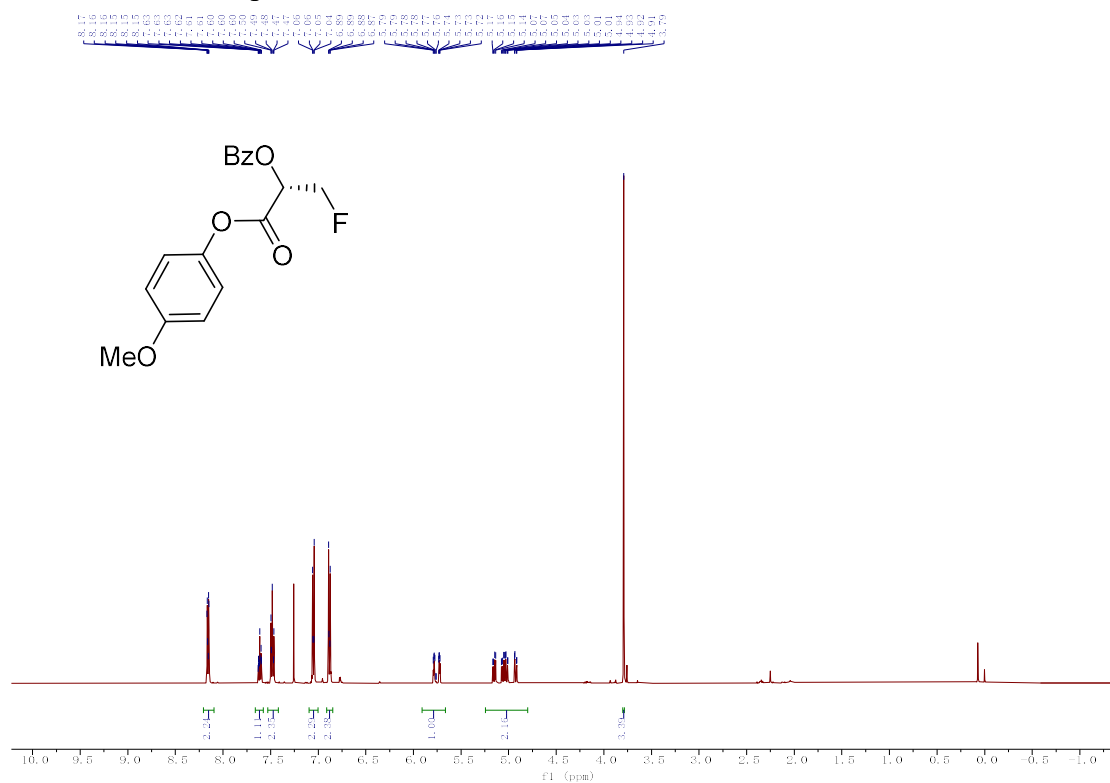
^1H NMR (500 MHz, Chloroform- d) of 4



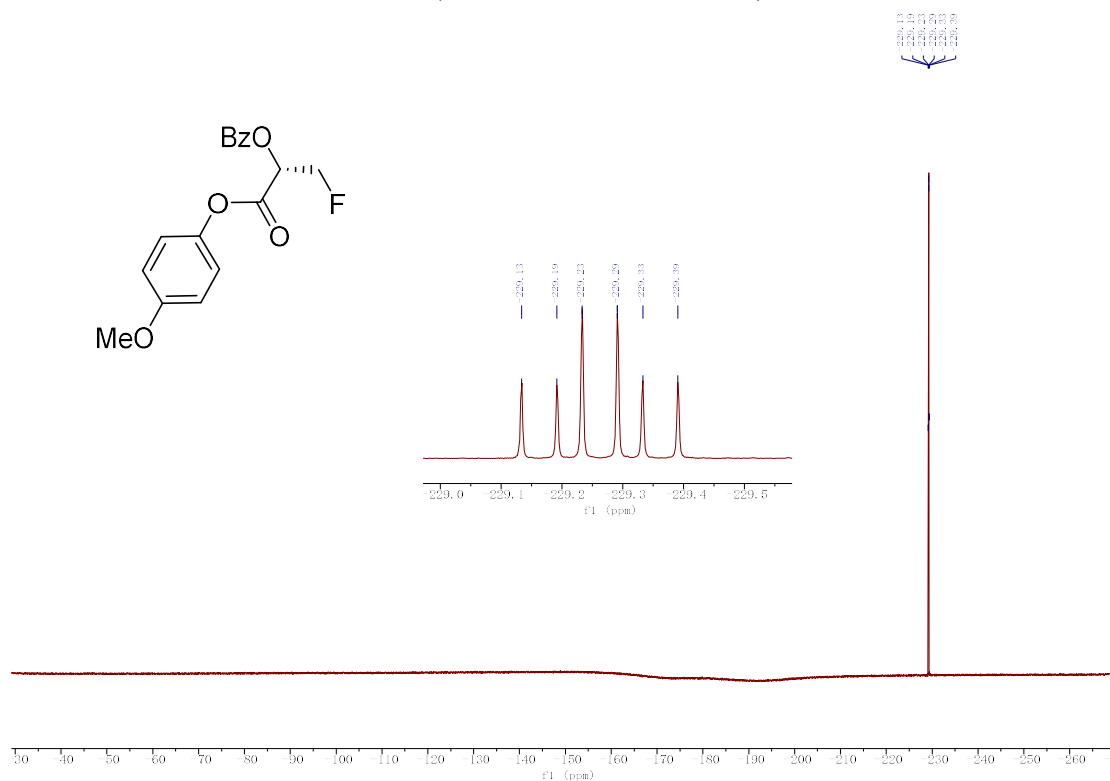
^{19}F NMR (470 MHz, Chloroform- d) of 4



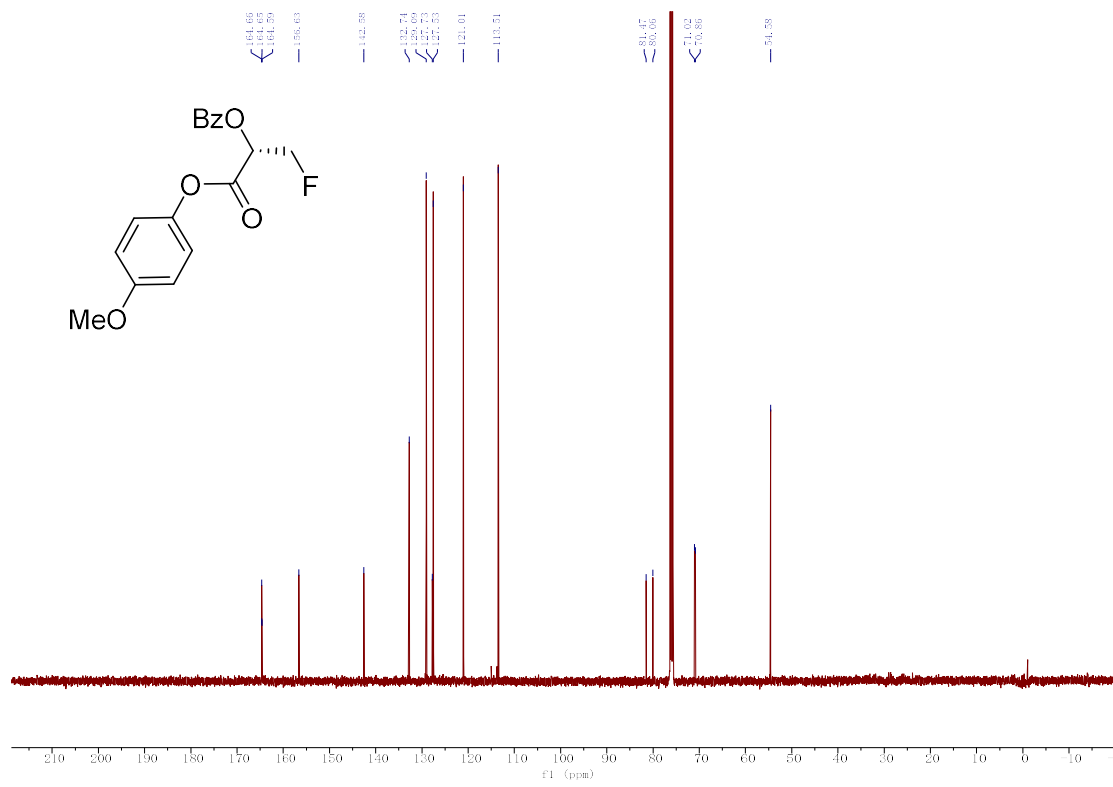
^1H and ^{13}C NMR spectra of 6



^1H NMR (500 MHz, Chloroform-*d*) of 6

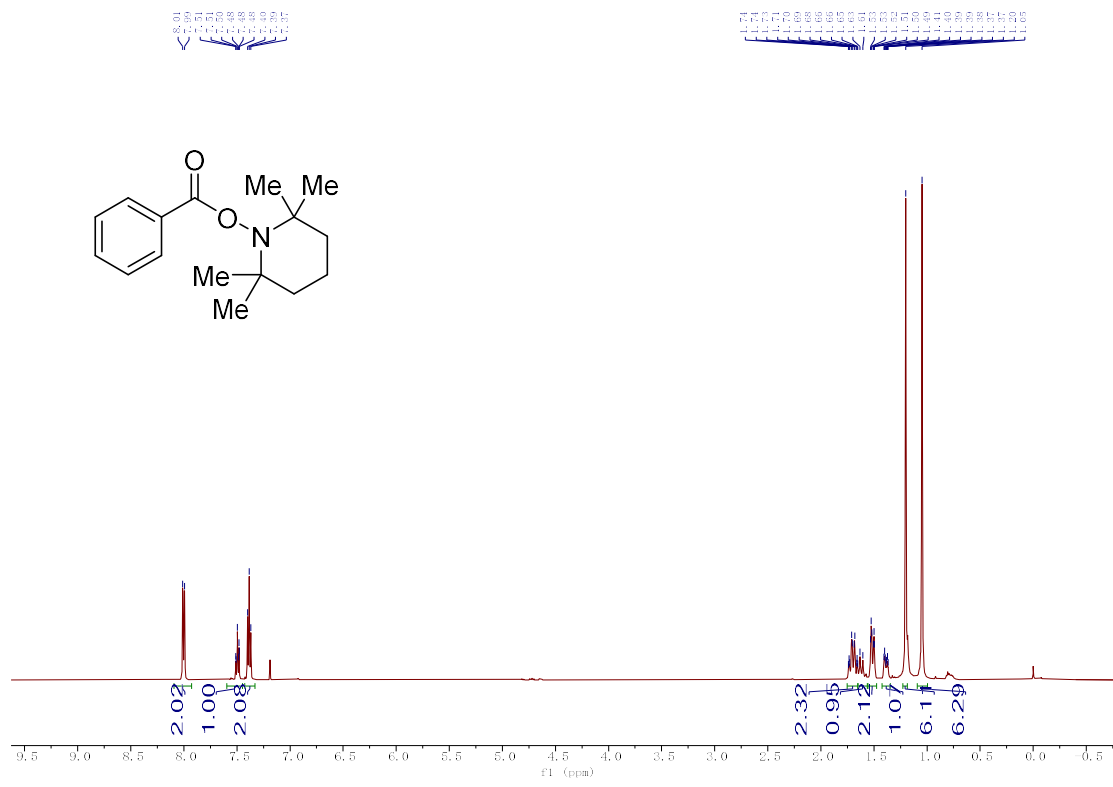


^{19}F NMR (470 MHz, Chloroform-*d*) of 6

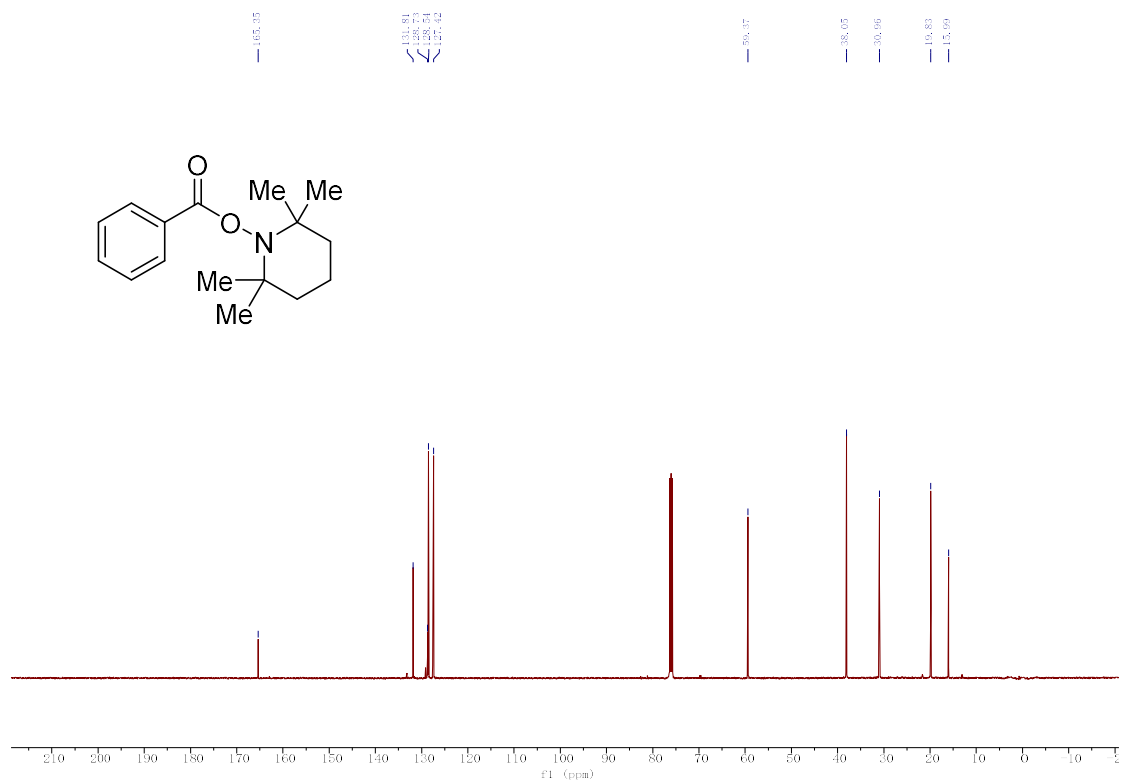


^{13}C NMR (126 MHz, Chloroform-*d*) of **6**

^1H and ^{13}C NMR spectra of **8**

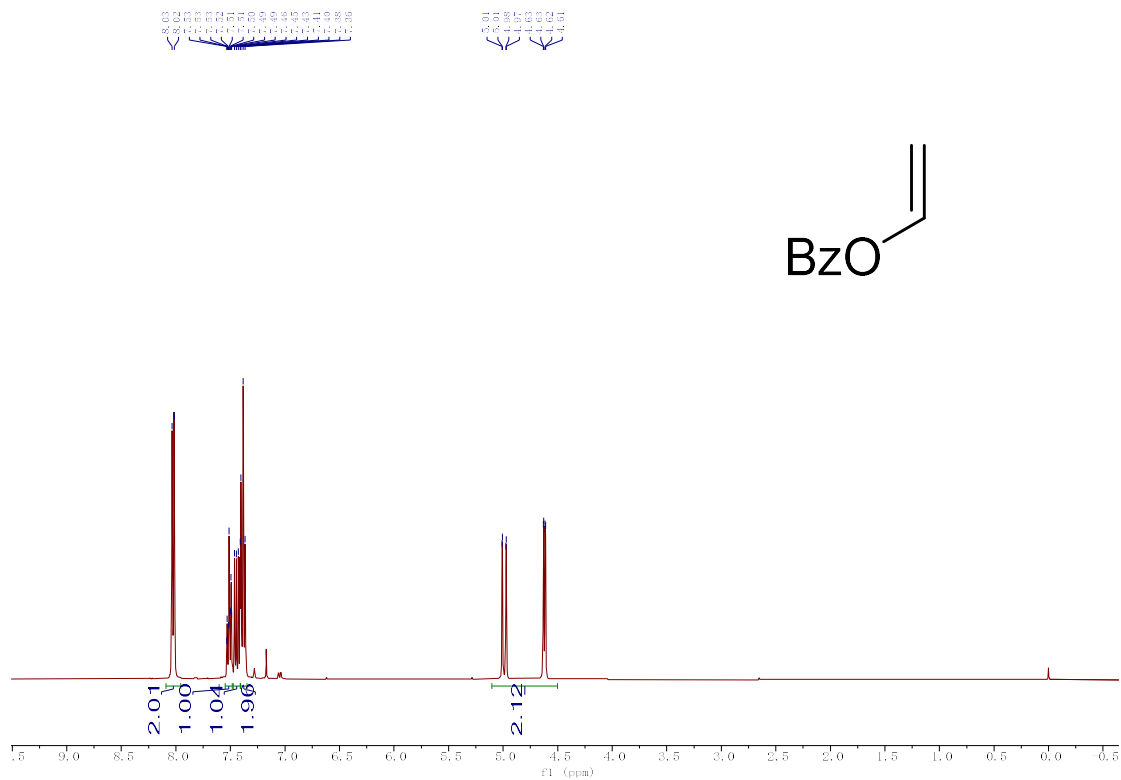


^1H NMR (500 MHz, Chloroform-*d*) of **8**

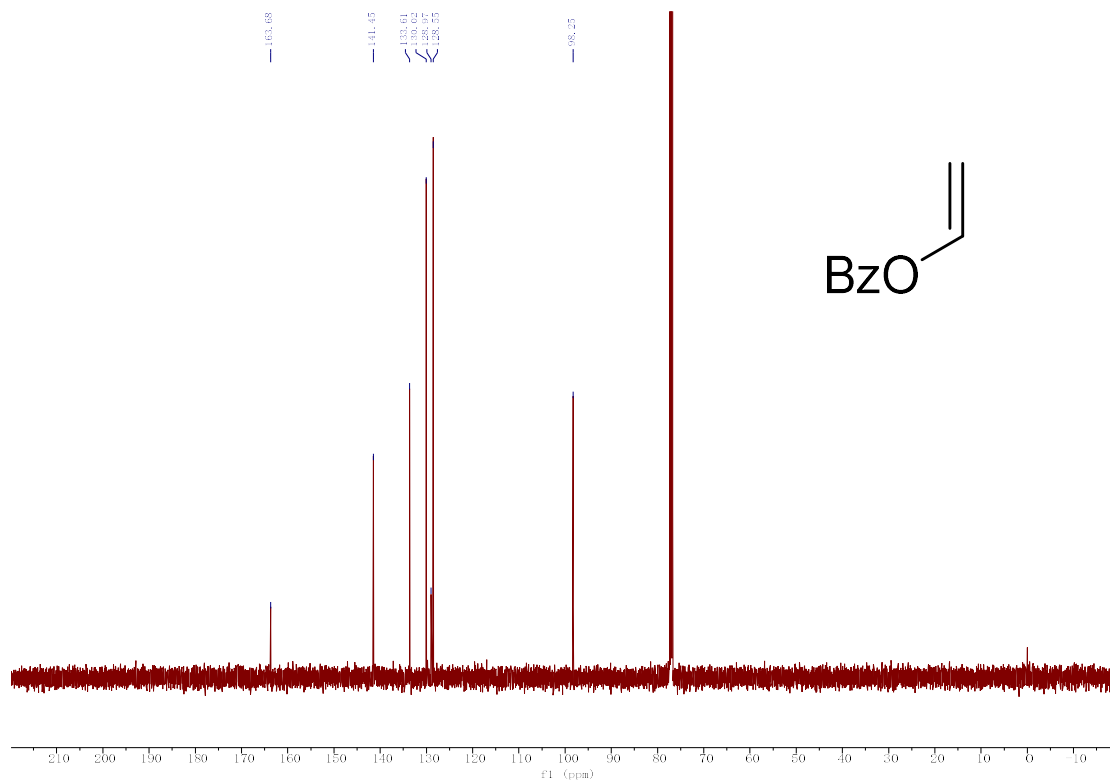


^{13}C NMR (126 MHz, Chloroform-*d*) of **8**

^1H and ^{13}C NMR spectra of **10**

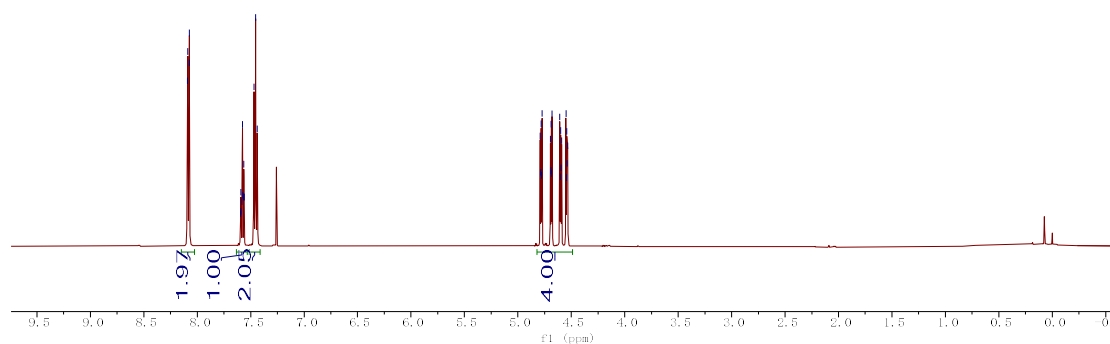
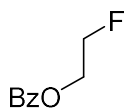
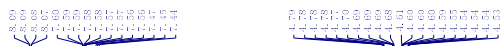


^1H NMR (500 MHz, Chloroform-*d*) of **10**

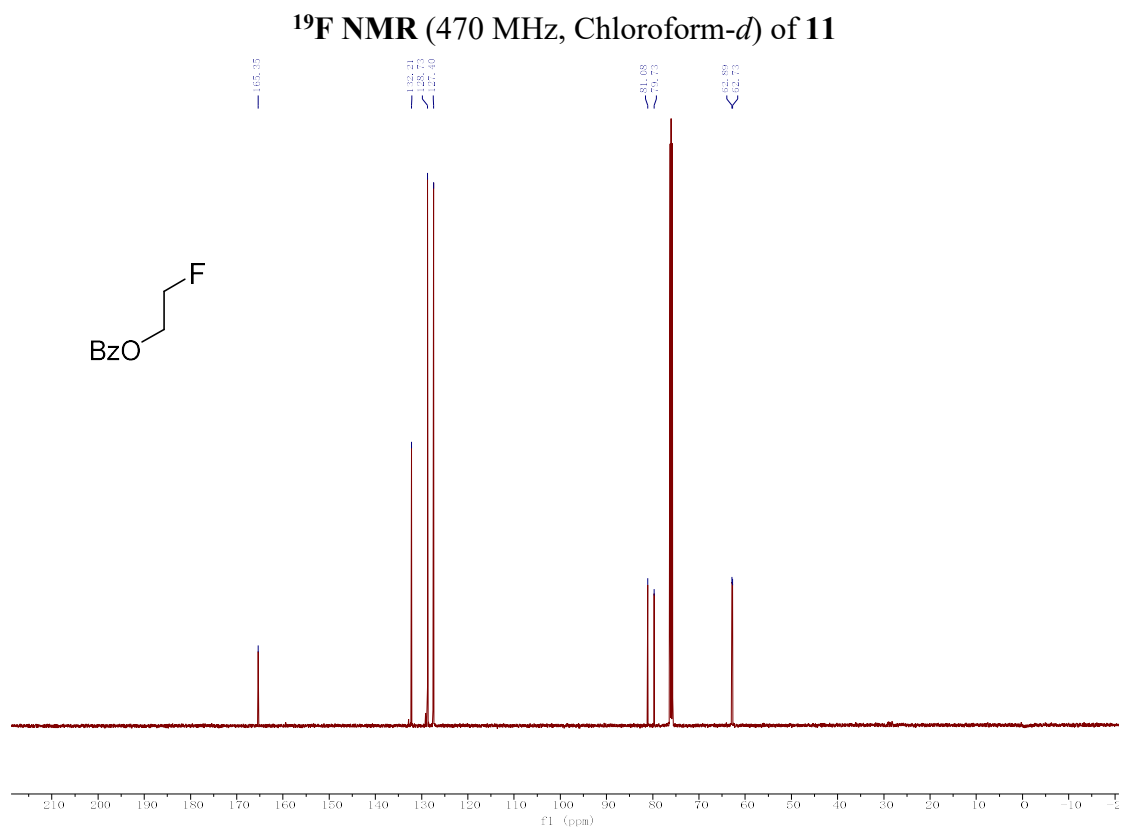
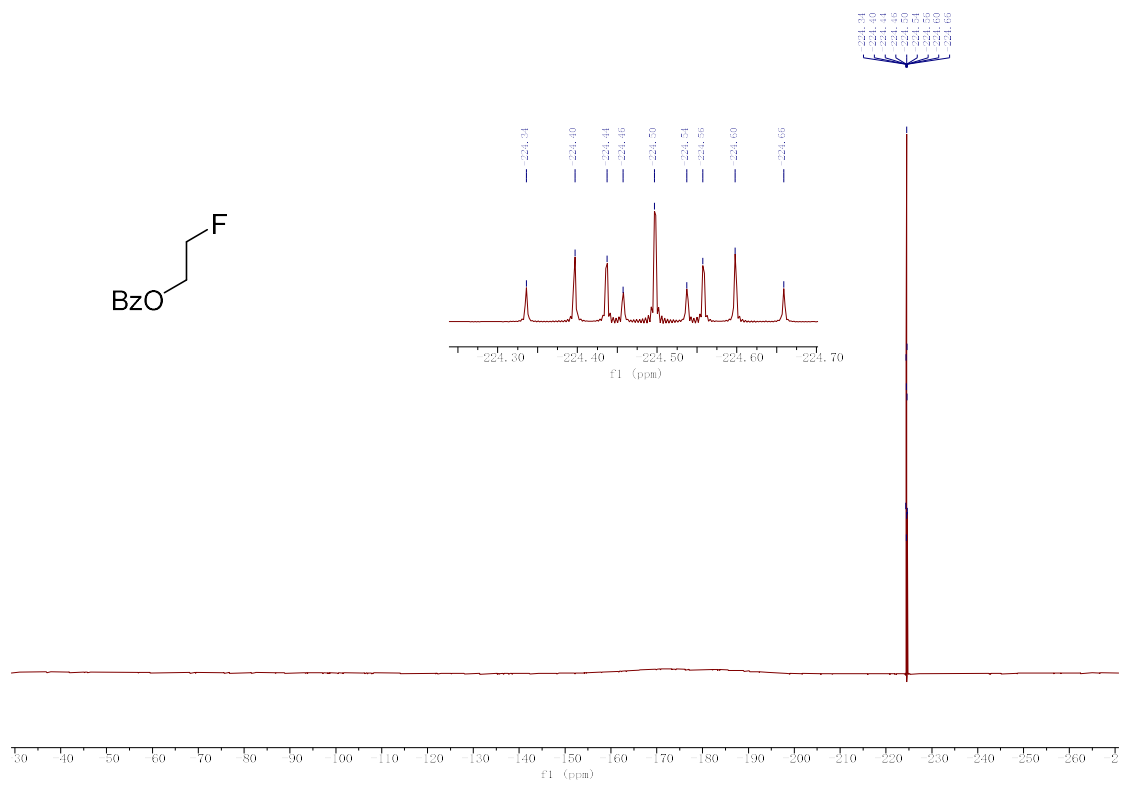


¹³C NMR (126 MHz, Chloroform-*d*) of **10**

¹H, ¹³C, and ¹⁹F NMR spectra of **11**

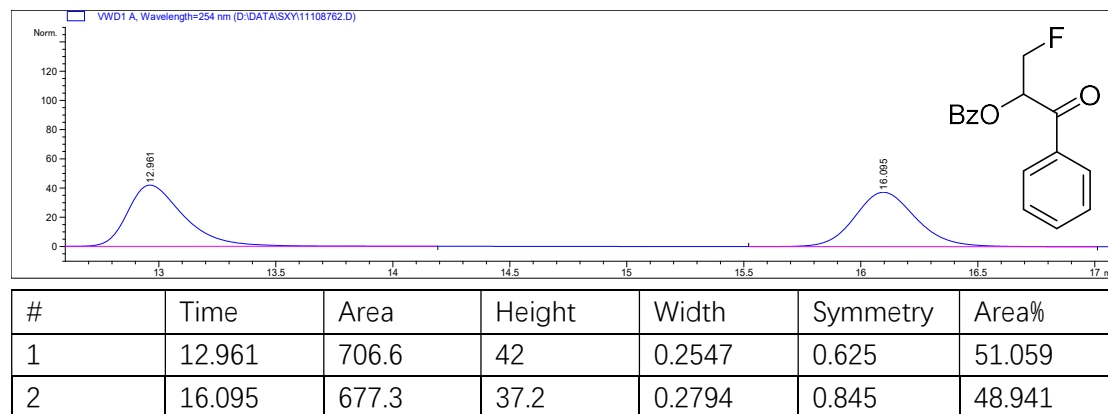


¹H NMR (500 MHz, Chloroform-*d*) of **11**

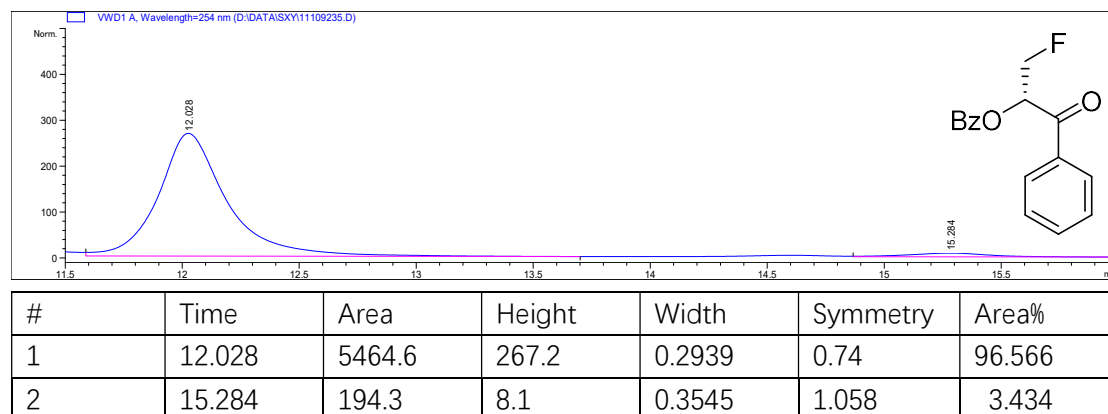


11 HPLC charts of the related compounds

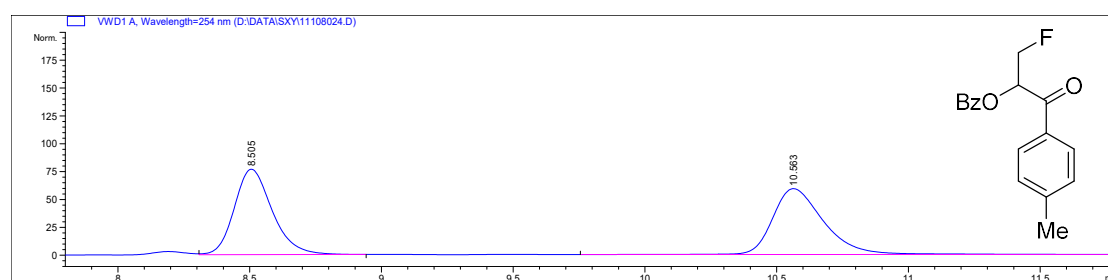
2a 254nm, IA, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



2a 254nm, IA, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min

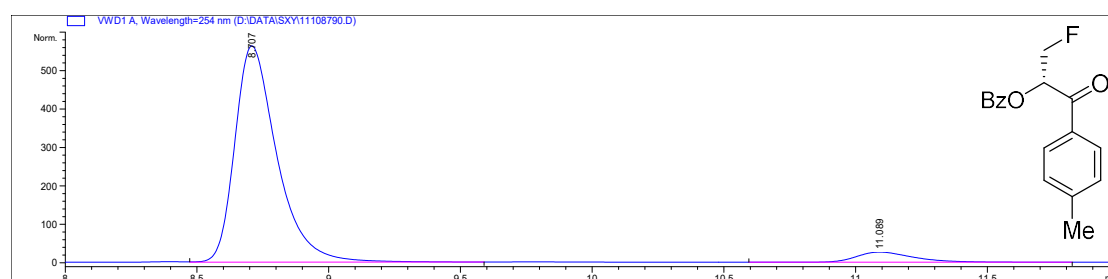


2b 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



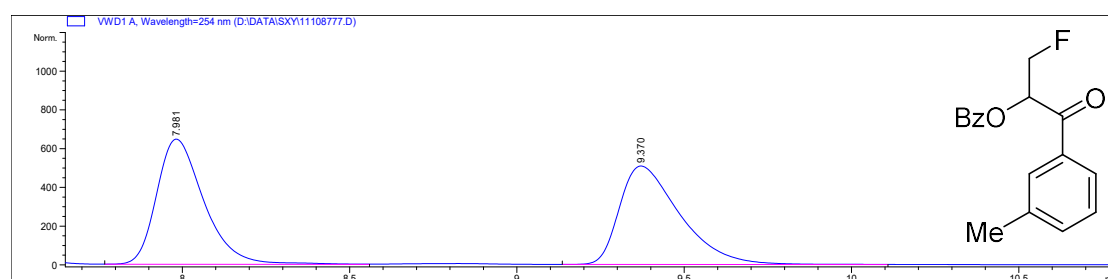
#	Time	Area	Height	Width	Symmetry	Area%
1	8.505	767.4	76.7	0.1516	0.772	48.884
2	10.563	802.5	59.1	0.2064	0.643	51.116

2b 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



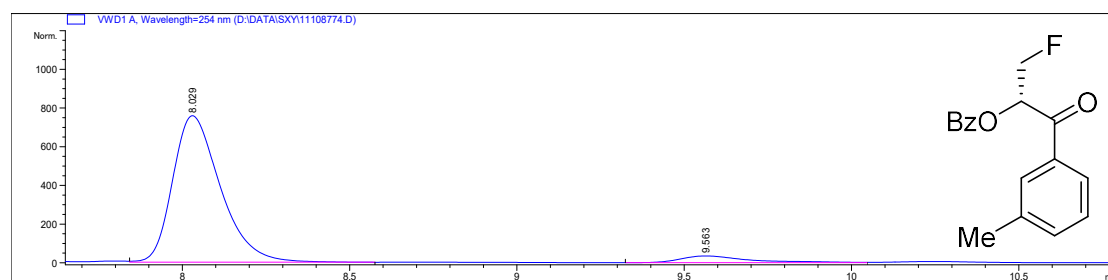
#	Time	Area	Height	Width	Symmetry	Area%
1	8.707	6245.1	563.1	0.1687	0.631	94.087
2	11.089	392.5	26.3	0.225	0.651	5.913

2c 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



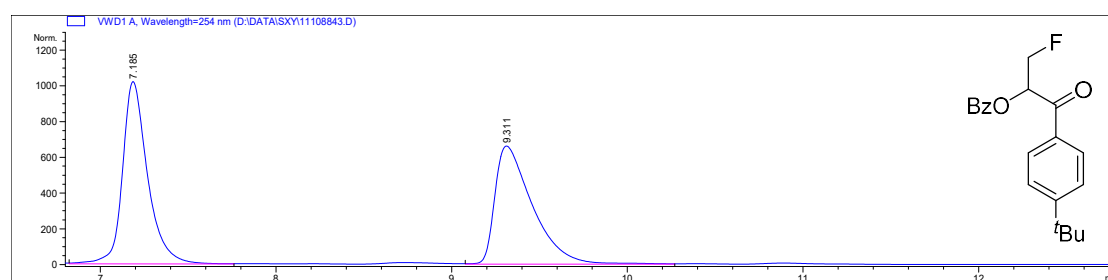
#	Time	Area	Height	Width	Symmetry	Area%
1	7.981	6359.6	646.6	0.1497	0.663	49.909
2	9.37	6382.8	508.3	0.1887	0.517	50.091

2c 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



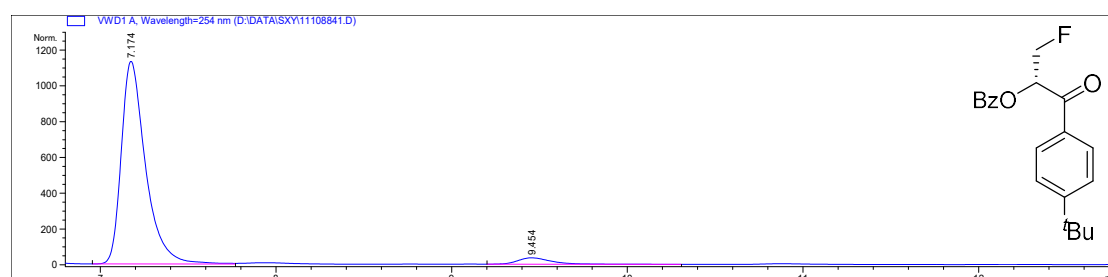
#	Time	Area	Height	Width	Symmetry	Area%
1	8.029	7500.8	757.2	0.1505	0.664	93.873
2	9.563	489.6	34.6	0.2072	0.516	6.127

2d 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



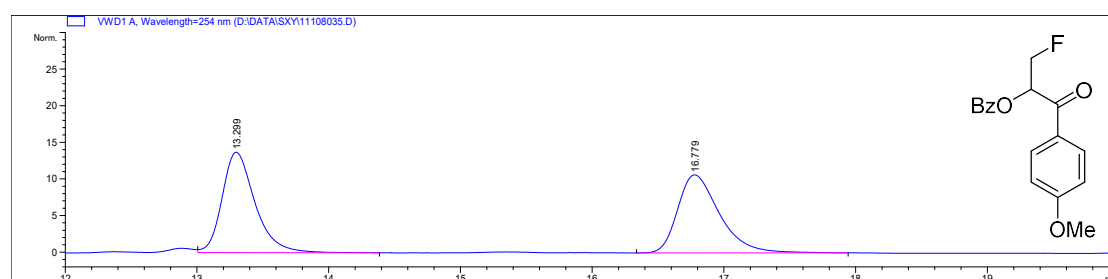
#	Time	Area	Height	Width	Symmetry	Area%
1	7.185	10137.9	1020.5	0.1479	0.696	50.827
2	9.311	9807.9	660.9	0.2212	0.413	49.173

2d 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



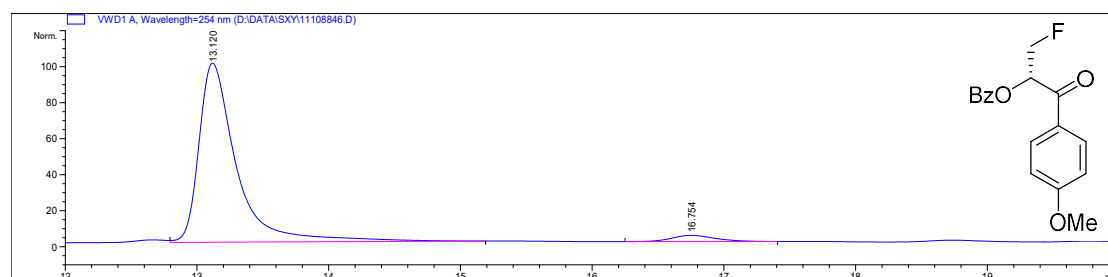
#	Time	Area	Height	Width	Symmetry	Area%
1	7.174	10875.6	1133.3	0.144	0.609	95.646
2	9.454	495.1	36	0.2054	0.624	4.354

2e 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



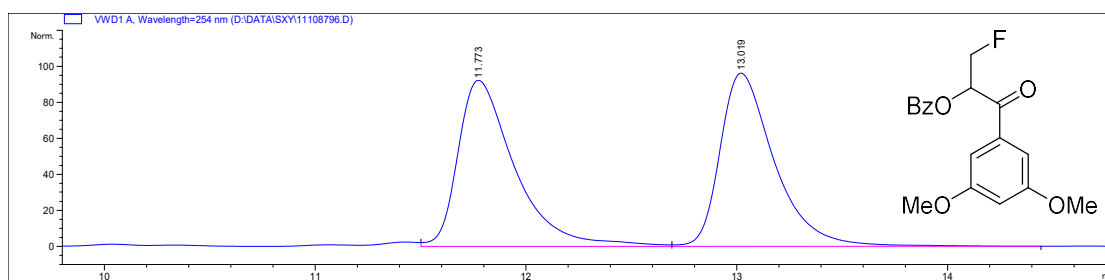
#	Time	Area	Height	Width	Symmetry	Area%
1	13.299	238.3	13.7	0.264	0.7	50.368
2	16.779	234.8	10.7	0.3371	0.634	49.632

2e 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



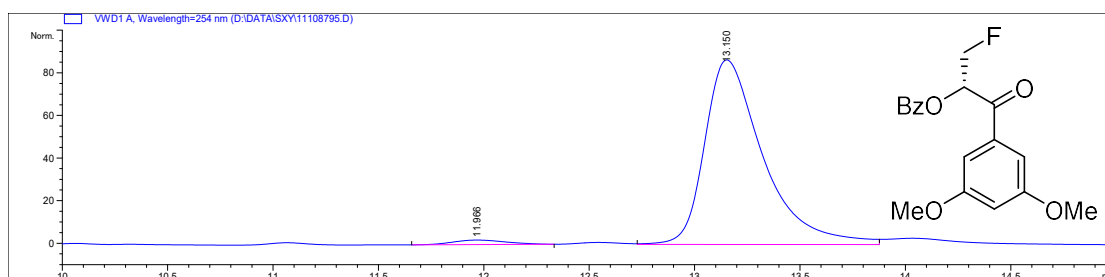
#	Time	Area	Height	Width	Symmetry	Area%
1	13.120	1968.5	99.5	0.2921	0.515	96.126
2	16.754	79.3	3.4	0.3517	0.789	3.874

2f 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



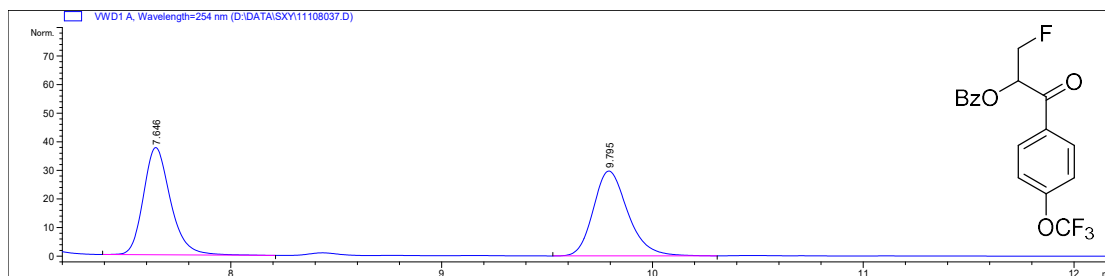
#	Time	Area	Height	Width	Symmetry	Area%
1	11.773	1729.4	92.3	0.2799	0.523	50.042
2	13.019	1726.4	96.2	0.2691	0.585	49.958

2f 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



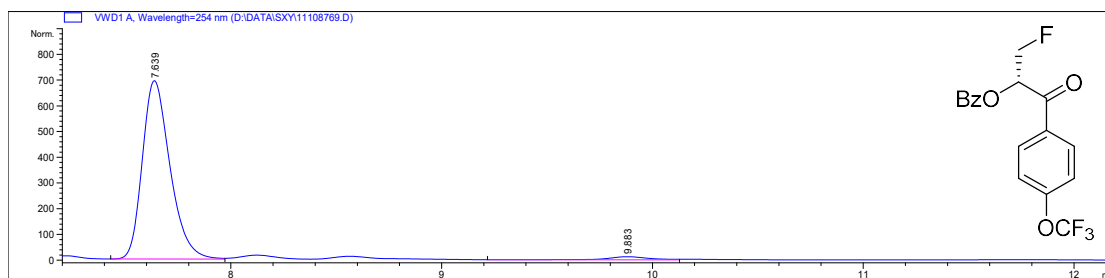
#	Time	Area	Height	Width	Symmetry	Area%
1	11.966	36.3	2.1	0.2715	0.819	2.123
2	13.15	1674.1	86.6	0.2881	0.566	97.877

2g 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



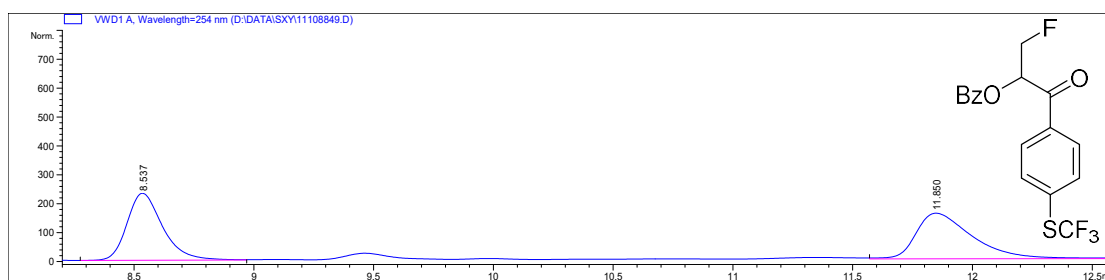
#	Time	Area	Height	Width	Symmetry	Area%
1	7.646	335.5	37.5	0.1363	0.773	49.827
2	9.795	337.8	29.7	0.1735	0.772	50.173

2g 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



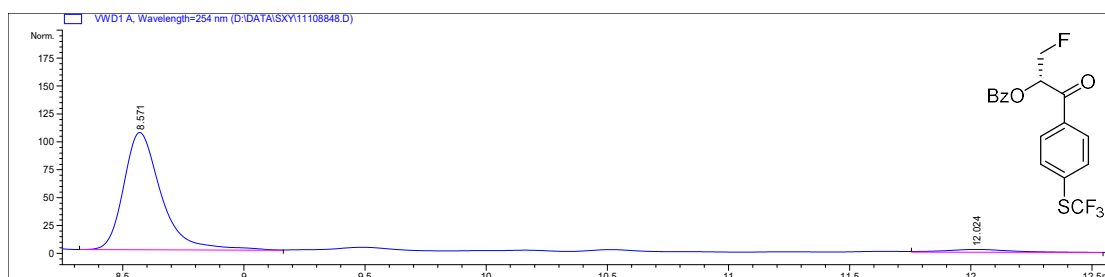
#	Time	Area	Height	Width	Symmetry	Area%
1	7.639	6326.8	693.5	0.1399	0.715	97.494
2	9.883	162.6	11.9	0.2018	0.936	2.506

2h 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



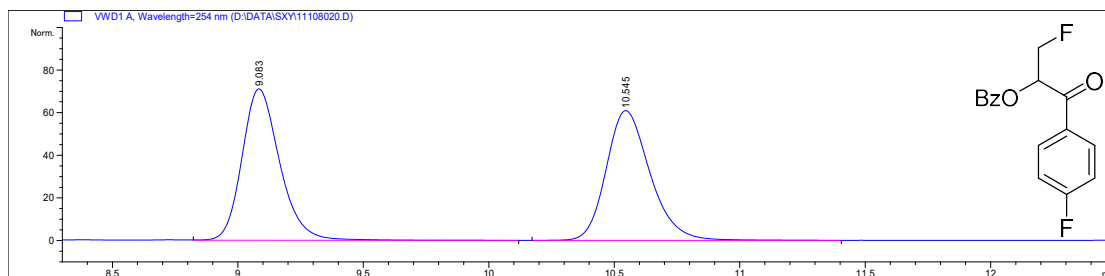
#	Time	Area	Height	Width	Symmetry	Area%
1	8.537	2397.6	231.9	0.157	0.716	47.453
2	11.85	2655.1	158	0.2499	0.498	52.547

2h 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



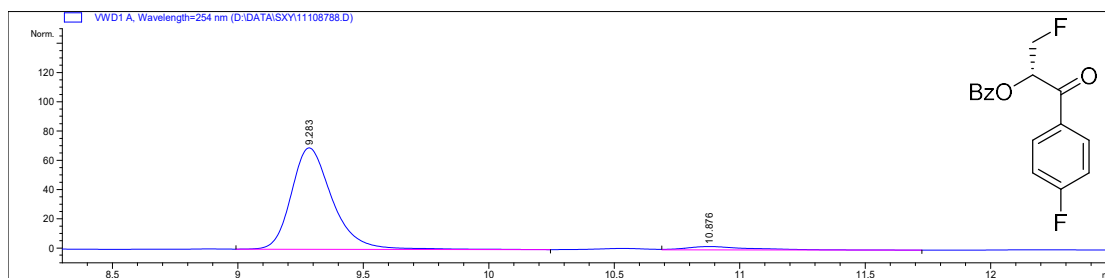
#	Time	Area	Height	Width	Symmetry	Area%
1	8.571	1132	105.1	0.162	0.685	95.913
2	12.024	48.2	2.5	0.2813	0.91	4.087

2i 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



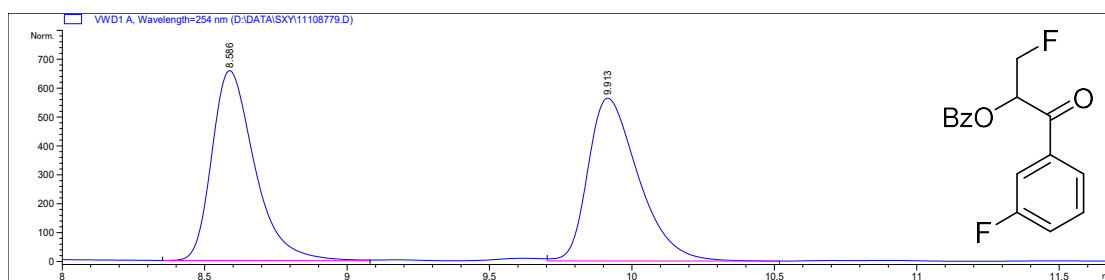
#	Time	Area	Height	Width	Symmetry	Area%
1	9.083	741.5	71.1	0.1596	0.769	50.042
2	10.545	740.2	60.9	0.1855	0.76	49.958

2i 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



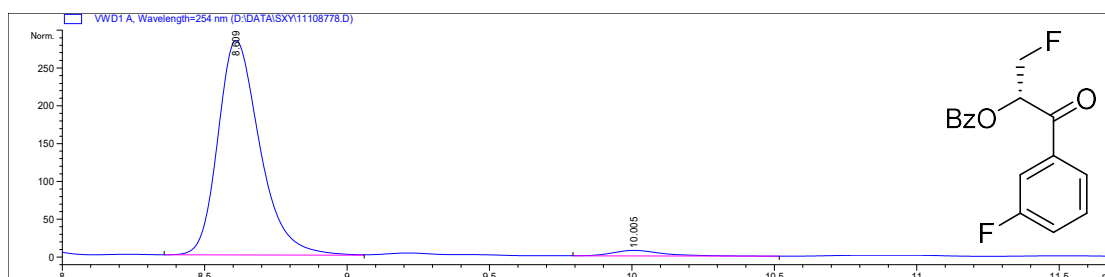
#	Time	Area	Height	Width	Symmetry	Area%
1	9.283	789.4	69.4	0.1735	0.718	95.189
2	10.876	39.9	2.3	0.2483	0.487	4.811

2j 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



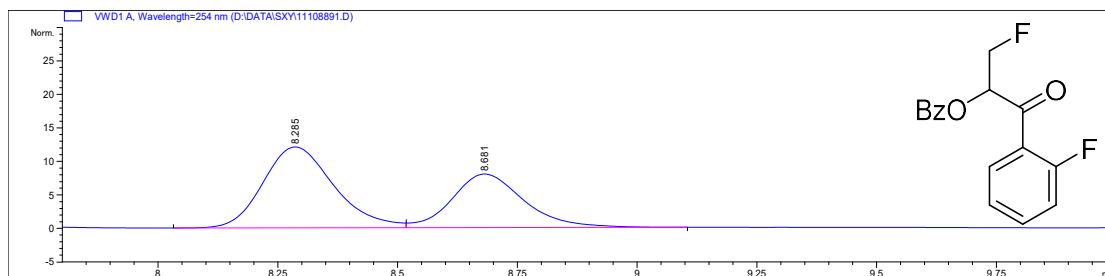
#	Time	Area	Height	Width	Symmetry	Area%
1	8.586	6863.8	657.4	0.1597	0.66	49.827
2	9.913	6911.4	563.2	0.1883	0.609	50.173

2j 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



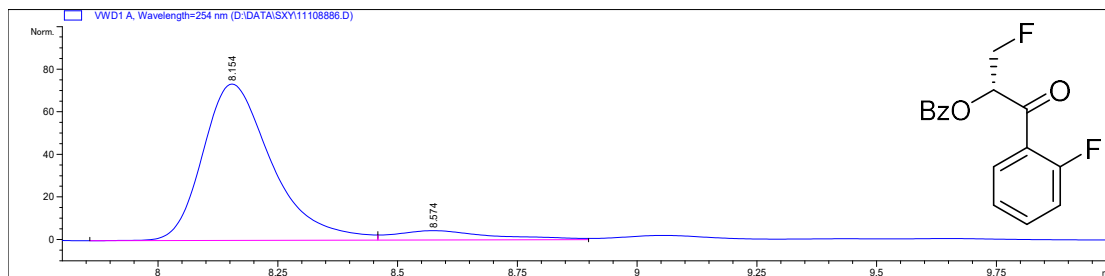
#	Time	Area	Height	Width	Symmetry	Area%
1	8.609	2904	284.4	0.1555	0.715	97.056
2	10.005	88.1	7.3	0.1822	0.694	2.944

2k 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



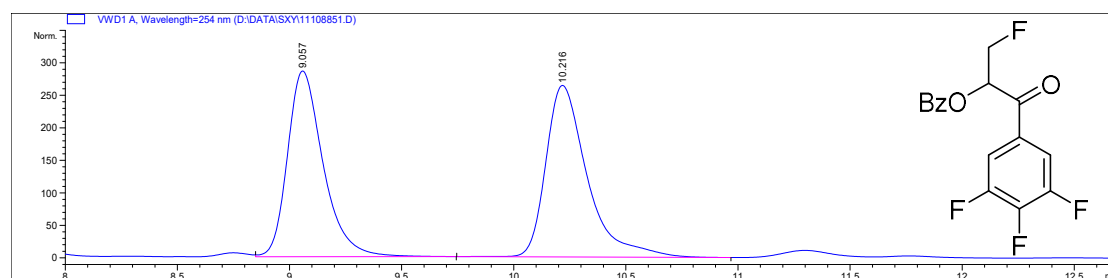
#	Time	Area	Height	Width	Symmetry	Area%
1	8.285	124.3	12.1	0.1594	0.789	59.908
2	8.681	83.2	8	0.1593	0.79	40.092

2k 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



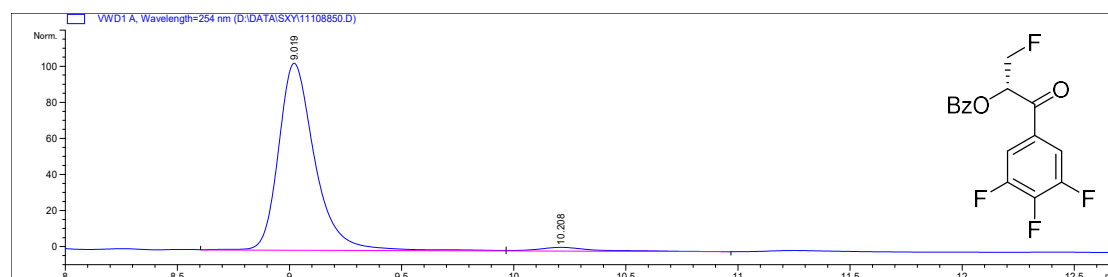
#	Time	Area	Height	Width	Symmetry	Area%
1	8.154	737.2	73.5	0.1534	0.686	92.420
2	8.574	60.5	4.4	0.1964	0.578	7.580

2l 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



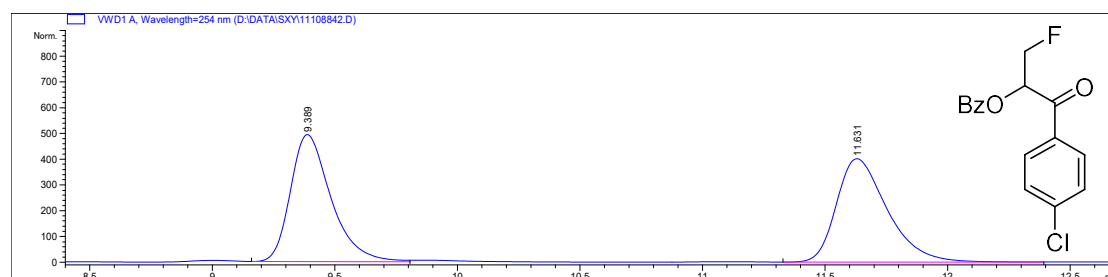
#	Time	Area	Height	Width	Symmetry	Area%
1	9.057	3152.7	285.6	0.1681	0.691	48.263
2	10.216	3379.6	263.9	0.1946	0.622	51.737

2l 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



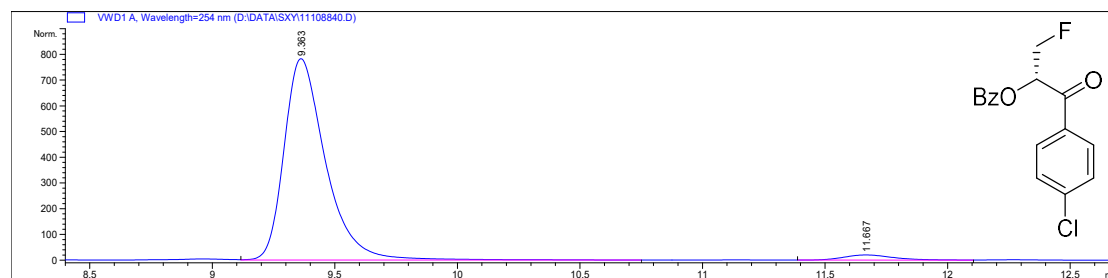
#	Time	Area	Height	Width	Symmetry	Area%
1	9.019	1168.1	103.7	0.1707	0.702	97.070
2	10.208	35.3	2.1	0.247	0.624	2.930

2m 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



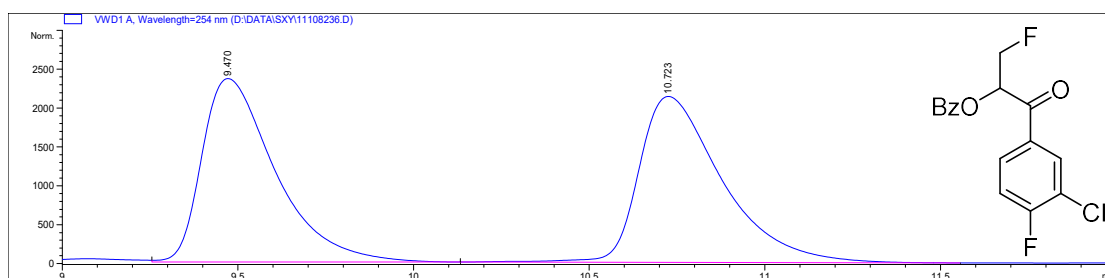
#	Time	Area	Height	Width	Symmetry	Area%
1	9.389	5679	493.5	0.175	0.665	49.490
2	11.631	5796.1	401.8	0.2192	0.633	50.510

2m 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



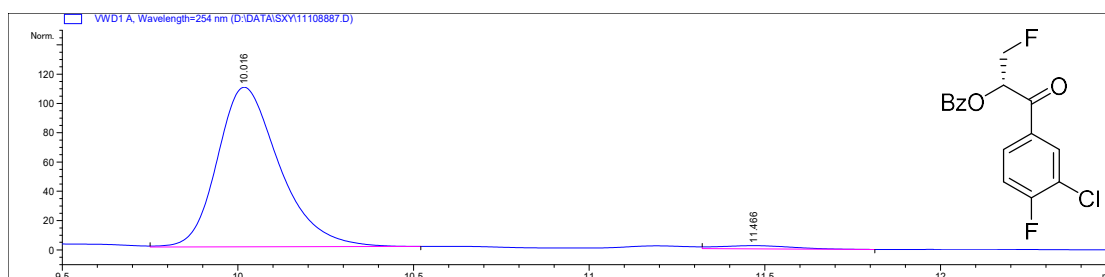
#	Time	Area	Height	Width	Symmetry	Area%
1	9.363	9223.2	782.9	0.1768	0.633	97.004
2	11.667	284.9	20.1	0.2167	0.739	2.996

2n 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



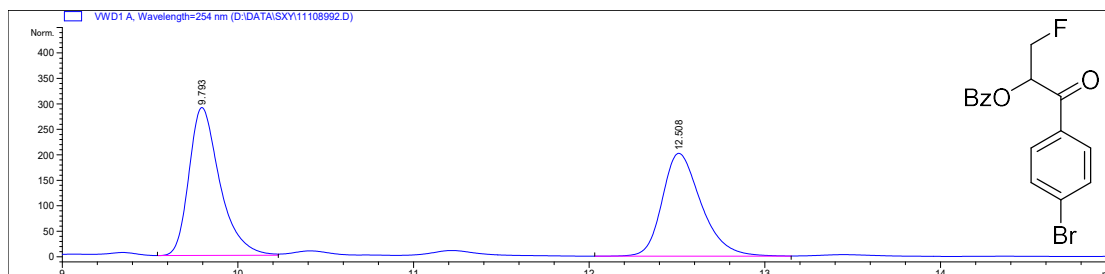
#	Time	Area	Height	Width	Symmetry	Area%
1	9.47	34215.2	2359	0.2187	0.514	49.359
2	10.723	35104.3	2133.6	0.2487	0.519	50.641

2n 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



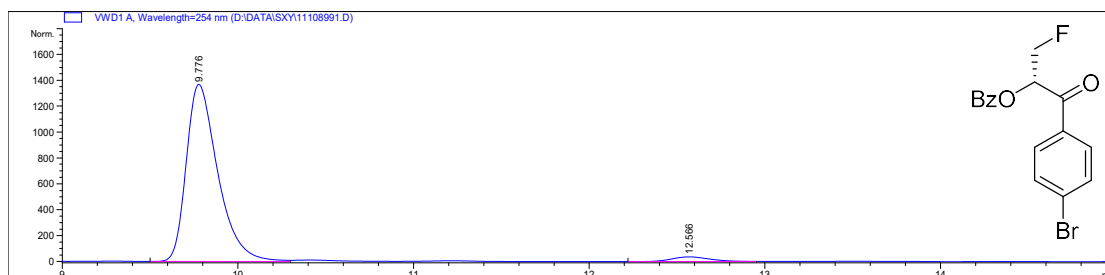
#	Time	Area	Height	Width	Symmetry	Area%
1	10.016	1341.2	109	0.1872	0.721	97.724
2	11.466	31.2	2.2	0.2189	0.845	2.276

2o 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



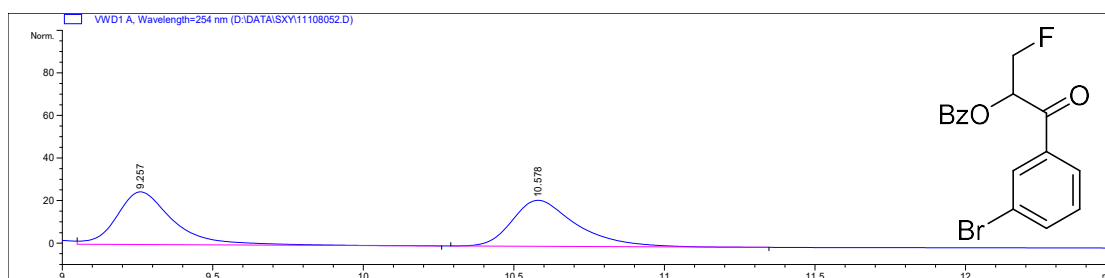
#	Time	Area	Height	Width	Symmetry	Area%
1	9.793	3541.5	290.5	0.1845	0.67	53.213
2	12.508	3113.8	201.9	0.2353	0.704	46.787

2o 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



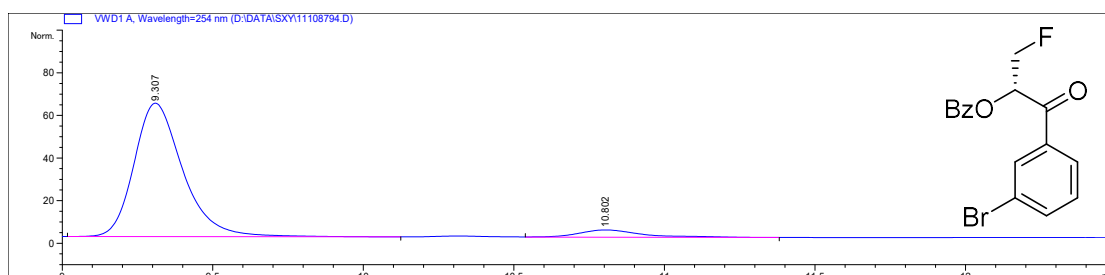
#	Time	Area	Height	Width	Symmetry	Area%
1	9.776	17058.1	1369.7	0.189	0.616	97.014
2	12.566	525	35.8	0.2265	0.831	2.986

2p 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



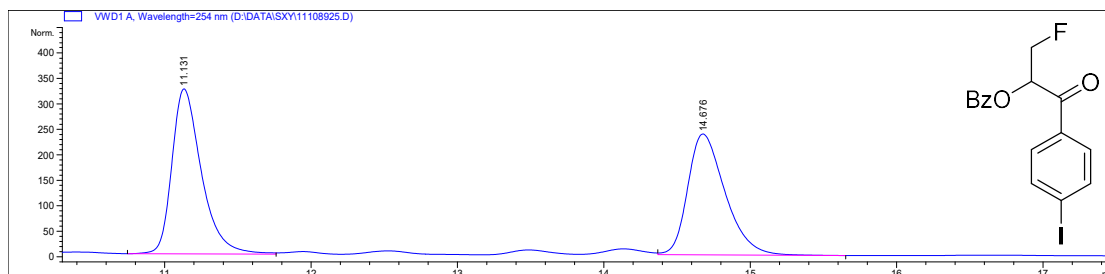
#	Time	Area	Height	Width	Symmetry	Area%
1	9.257	321.5	24.7	0.1939	0.679	50.112
2	10.578	320	21.6	0.2192	0.636	49.888

2p 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



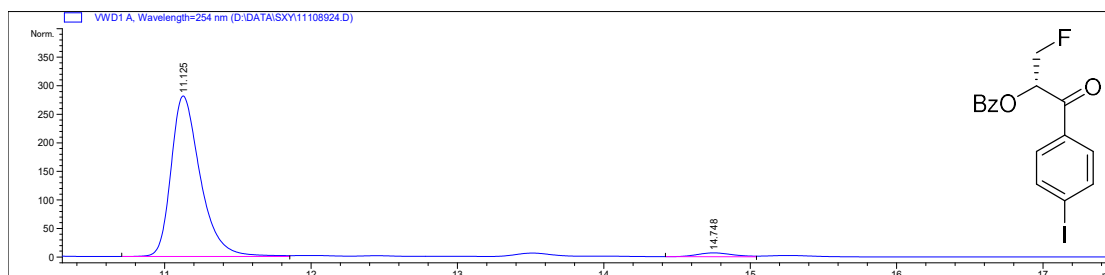
#	Time	Area	Height	Width	Symmetry	Area%
1	9.307	705.1	62.6	0.1721	0.723	93.422
2	10.802	49.6	3.4	0.2179	0.679	6.578

2q 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



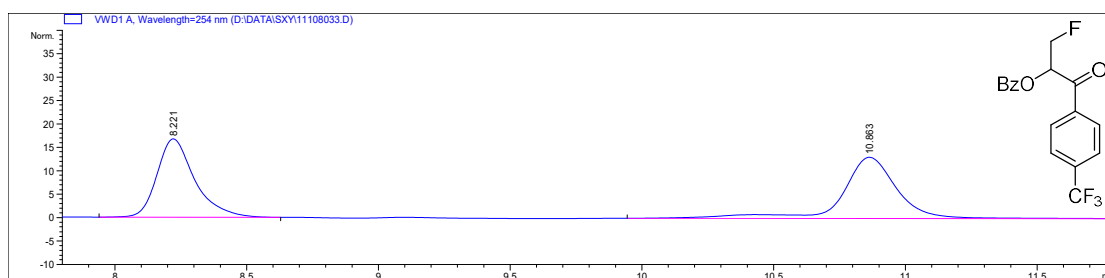
#	Time	Area	Height	Width	Symmetry	Area%
1	11.131	4532.7	323.8	0.2128	0.651	51.860
2	14.676	4207.6	237.3	0.2694	0.649	48.140

2q 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



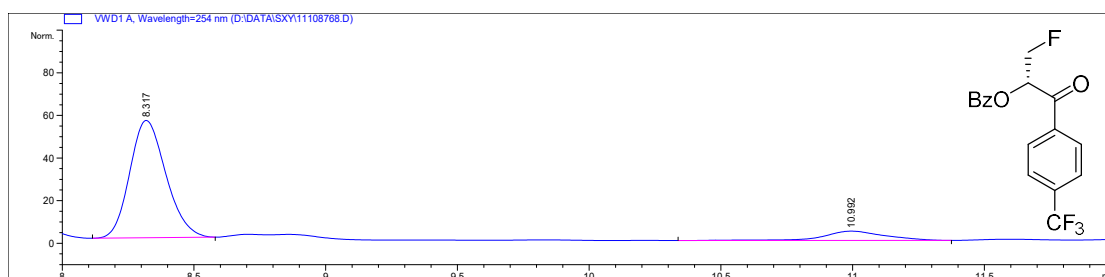
#	Time	Area	Height	Width	Symmetry	Area%
1	11.125	3895.2	281.1	0.2097	0.658	97.163
2	14.748	113.7	6.7	0.2615	0.809	2.837

2r 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



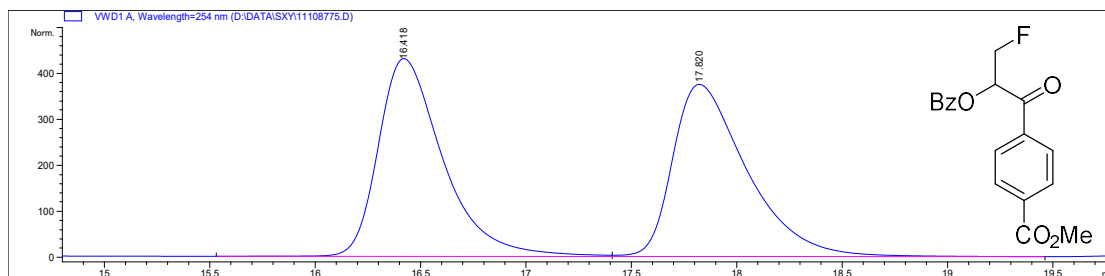
#	Time	Area	Height	Width	Symmetry	Area%
1	8.221	166.6	16.7	0.1482	0.71	46.678
2	10.863	190.3	13.1	0.2147	1.005	53.322

2r 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



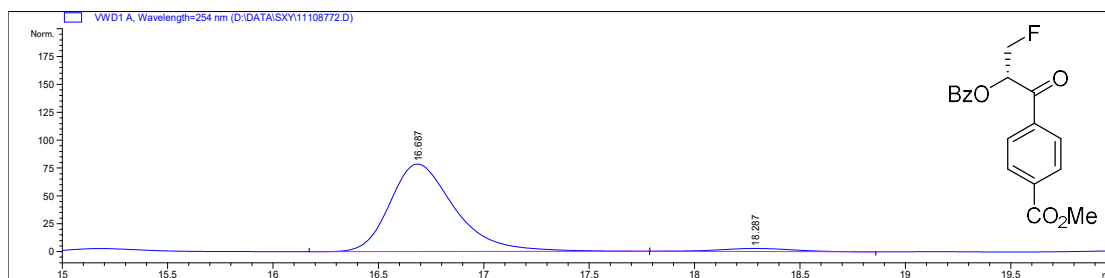
#	Time	Area	Height	Width	Symmetry	Area%
1	8.317	525.8	55.1	0.1477	0.801	87.959
2	10.992	72	4.4	0.2364	0.872	12.041

2s 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



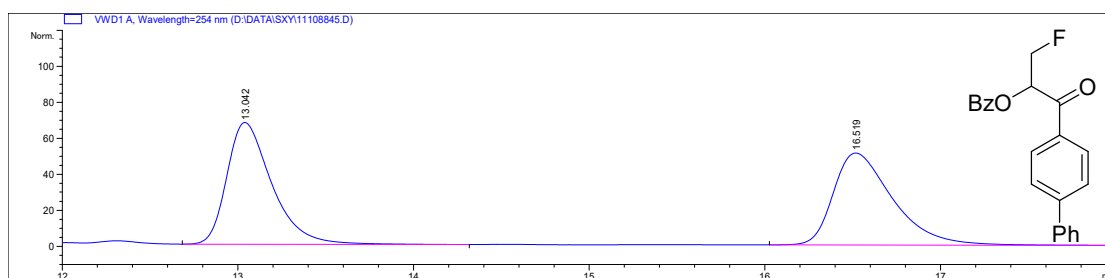
#	Time	Area	Height	Width	Symmetry	Area%
1	16.418	9200	430.4	0.3222	0.609	50.091
2	17.82	9166.5	374.5	0.3685	0.524	49.909

2s 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



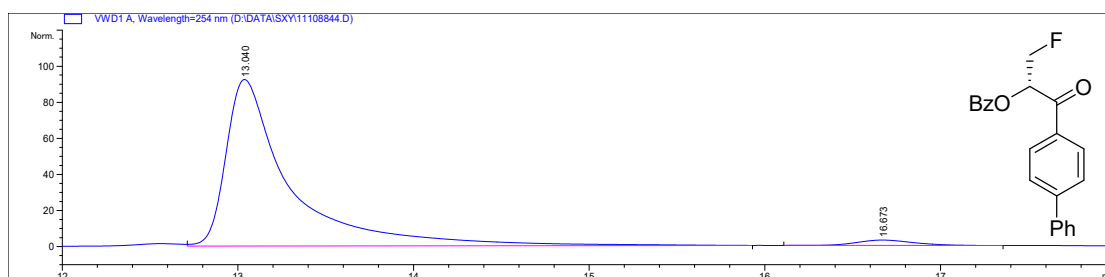
#	Time	Area	Height	Width	Symmetry	Area%
1	16.687	1672.6	78.5	0.3229	0.701	96.242
2	18.287	65.3	2.7	0.3667	0.88	3.758

2t 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



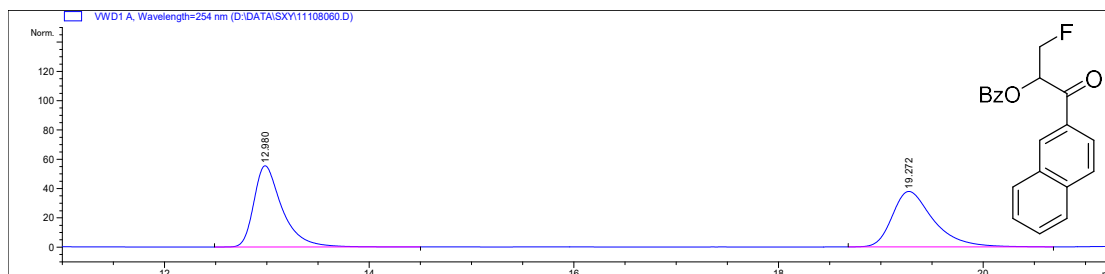
#	Time	Area	Height	Width	Symmetry	Area%
1	13.042	1204.2	67.6	0.2689	0.622	49.986
2	16.519	1204.9	51.1	0.3553	0.56	50.014

2t 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



#	Time	Area	Height	Width	Symmetry	Area%
1	13.04	2339.4	92.3	0.3567	0.362	97.167
2	16.673	68.2	3	0.3462	0.794	2.833

2u 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



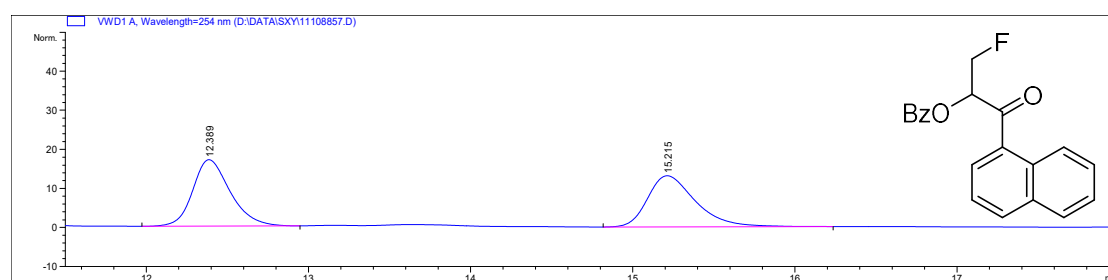
#	Time	Area	Height	Width	Symmetry	Area%
1	12.98	1063.3	55.5	0.2863	0.609	50.198
2	19.272	1055	37.8	0.4186	0.636	49.802

2u 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



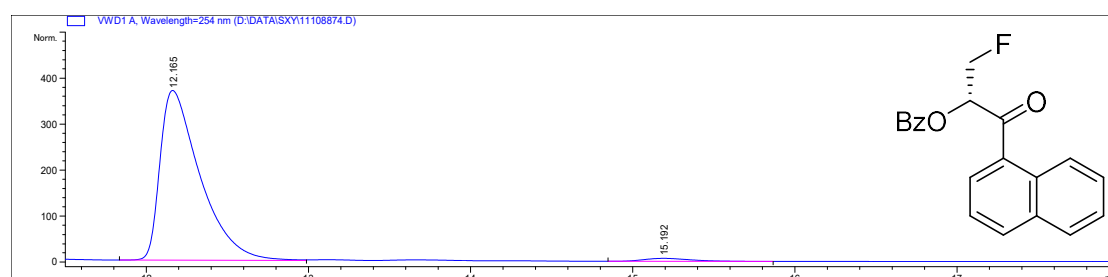
#	Time	Area	Height	Width	Symmetry	Area%
1	13.346	5727.2	318.4	0.2725	0.671	95.432
2	19.51	274.1	11	0.3787	0.787	4.568

2v 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



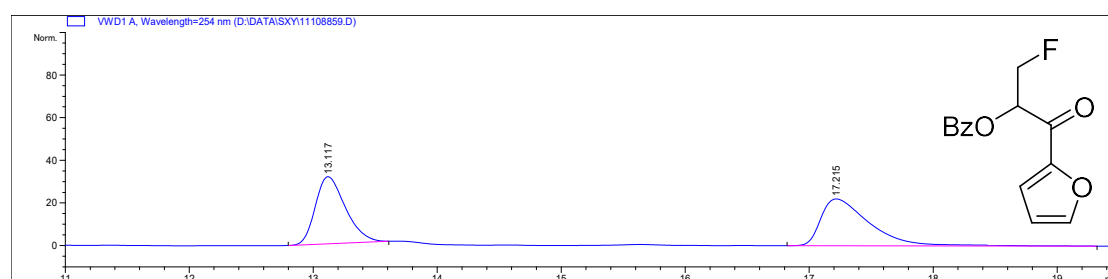
#	Time	Area	Height	Width	Symmetry	Area%
1	12.389	273.9	17	0.2429	0.736	50.459
2	15.215	268.9	13.1	0.3106	0.646	49.541

2v 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



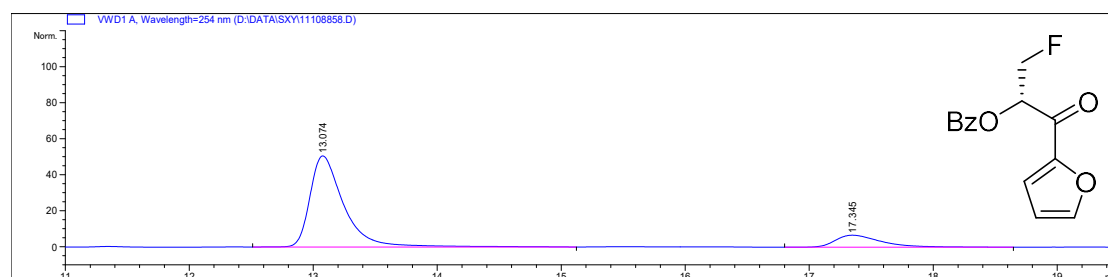
#	Time	Area	Height	Width	Symmetry	Area%
1	12.165	6330.3	369.4	0.2538	0.425	97.941
2	15.192	133.1	6.5	0.3099	0.673	2.059

2w 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



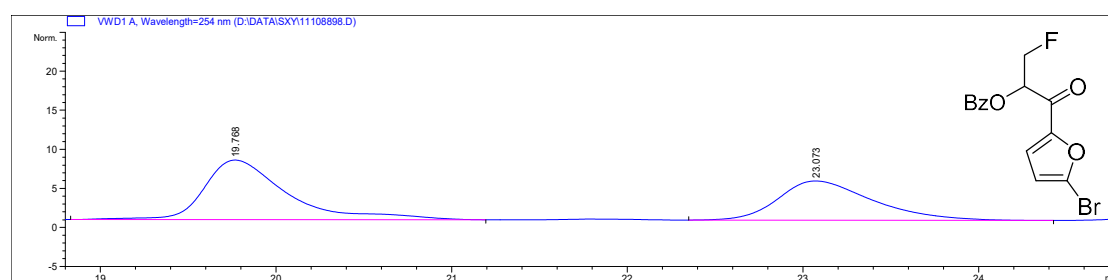
#	Time	Area	Height	Width	Symmetry	Area%
1	13.117	530.4	31.5	0.2576	0.69	47.060
2	17.215	596.7	22	0.4118	0.422	52.940

2w 254nm, IB, *n*-Hexane : *i*PrOH 90:10, 0.8 mL/min



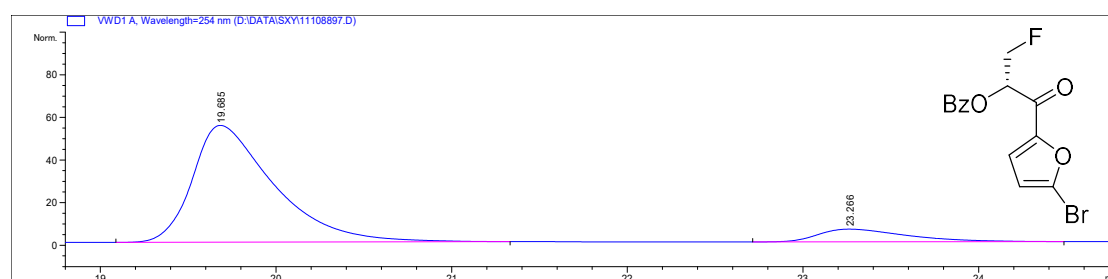
#	Time	Area	Height	Width	Symmetry	Area%
1	13.074	961.2	50.6	0.2843	0.552	84.849
2	17.345	171.6	6.7	0.3885	0.552	15.151

2x 254nm, IB, *n*-Hexane : *i*PrOH = 99:1, 0.8 mL/min



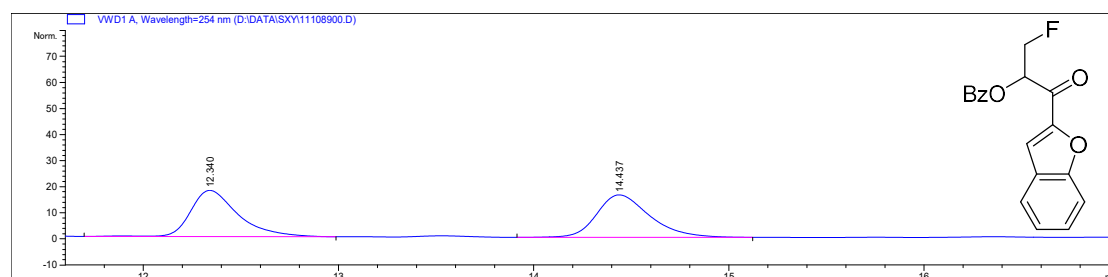
#	Time	Area	Height	Width	Symmetry	Area%
1	19.768	250.2	7.6	0.4874	0.562	57.141
2	23.073	187.7	5	0.548	0.632	42.859

2x 254nm, IB, *n*-Hexane : *i*PrOH = 99:1, 0.8 mL/min



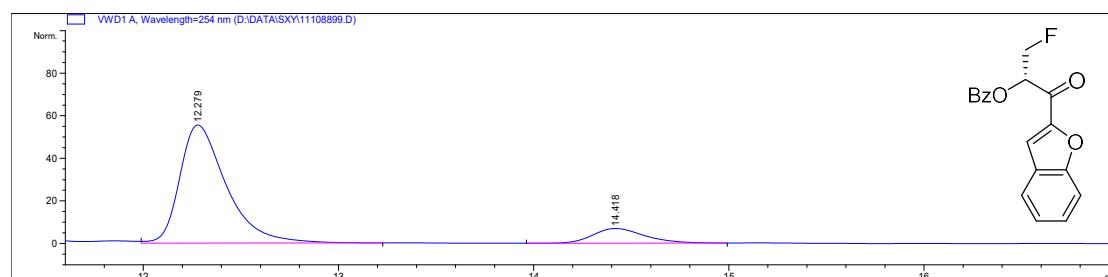
#	Time	Area	Height	Width	Symmetry	Area%
1	19.685	1769.9	54.8	0.4713	0.498	89.581
2	23.266	205.9	6	0.5201	0.519	10.419

2y 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



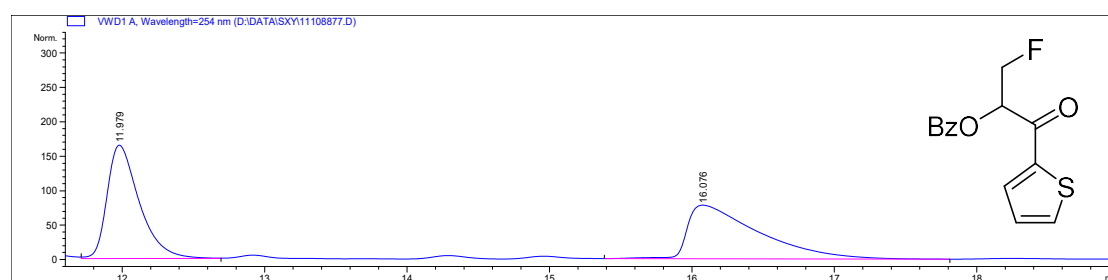
#	Time	Area	Height	Width	Symmetry	Area%
1	12.34	300.4	17.8	0.2527	0.648	49.401
2	14.437	307.7	16.3	0.2842	0.709	50.599

2y 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



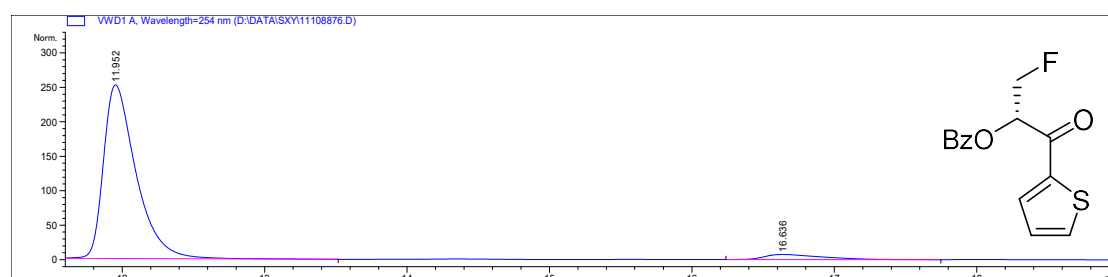
#	Time	Area	Height	Width	Symmetry	Area%
1	12.279	918.7	55.5	0.2499	0.597	87.927
2	14.418	126.1	6.9	0.2784	0.749	12.073

2z 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



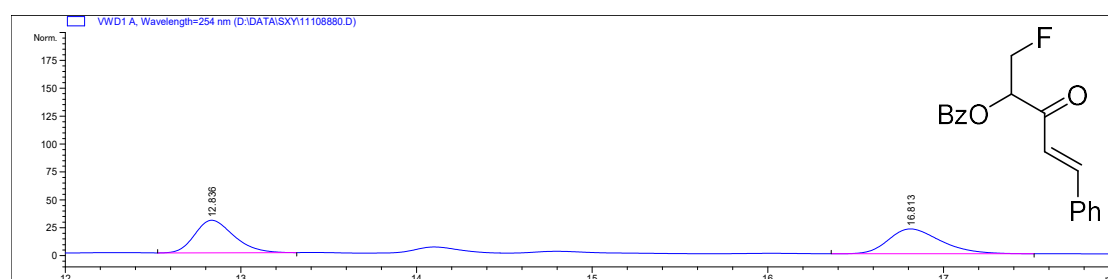
#	Time	Area	Height	Width	Symmetry	Area%
1	11.979	2586.9	164.7	0.2371	0.574	49.020
2	16.076	2690.4	77.8	0.498	0.261	50.980

2z 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



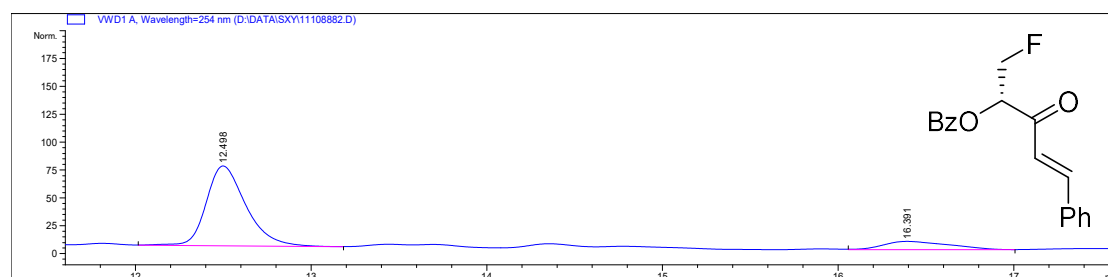
#	Time	Area	Height	Width	Symmetry	Area%
1	11.952	4012	252	0.2381	0.541	95.133
2	16.636	205.2	7.3	0.4126	0.424	4.867

2a' 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



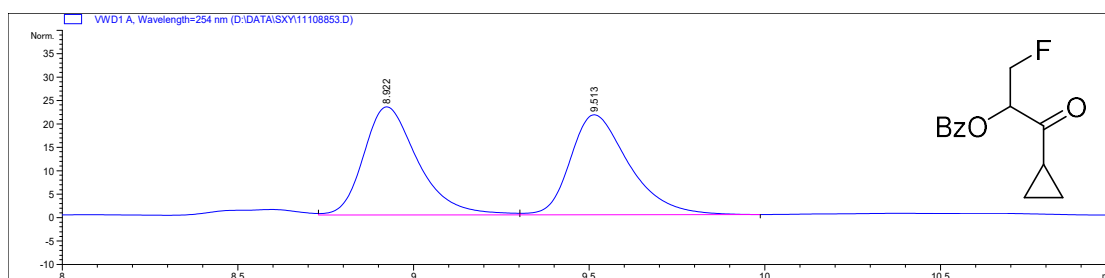
#	Time	Area	Height	Width	Symmetry	Area%
1	12.836	448.3	29.2	0.2347	0.739	49.397
2	16.813	459.2	22.2	0.3165	0.693	50.603

2a' 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



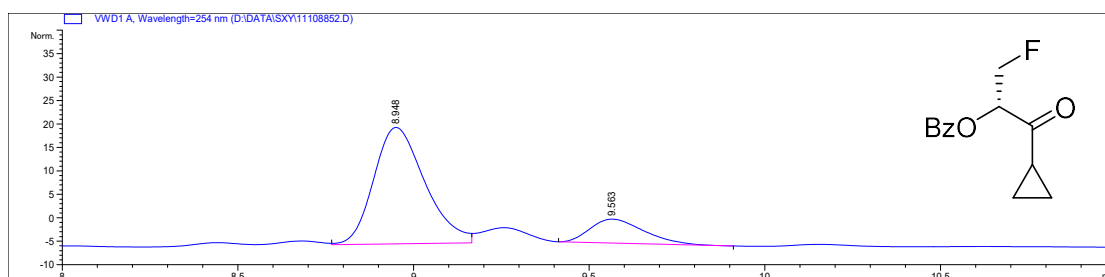
#	Time	Area	Height	Width	Symmetry	Area%
1	12.498	1129	71.7	0.2391	0.7	85.333
2	16.391	194.1	7.4	0.3725	0.546	14.667

2b' 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



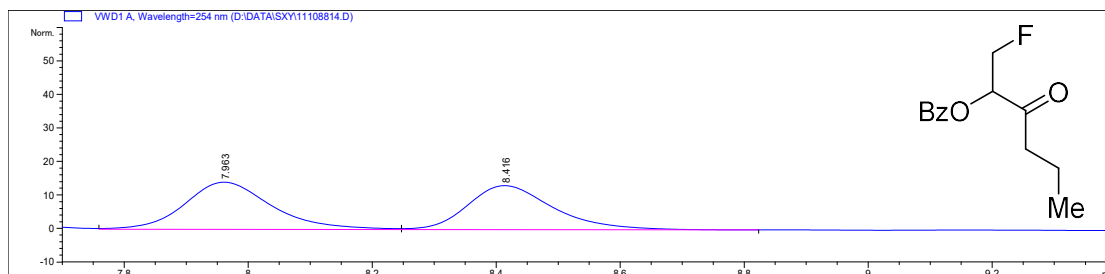
#	Time	Area	Height	Width	Symmetry	Area%
1	8.922	248.3	23.1	0.1617	0.696	50.074
2	9.513	247.6	21.4	0.1745	0.653	49.926

2b' 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



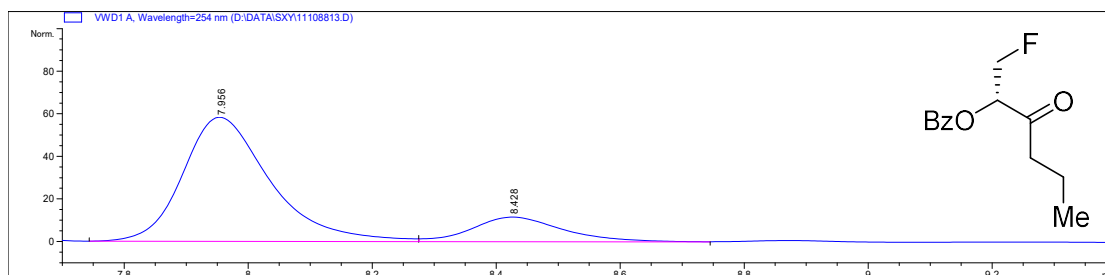
#	Time	Area	Height	Width	Symmetry	Area%
1	8.948	251.9	24.9	0.1561	0.731	82.225
2	9.563	54.4	5.1	0.1668	0.641	17.775

2c' 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



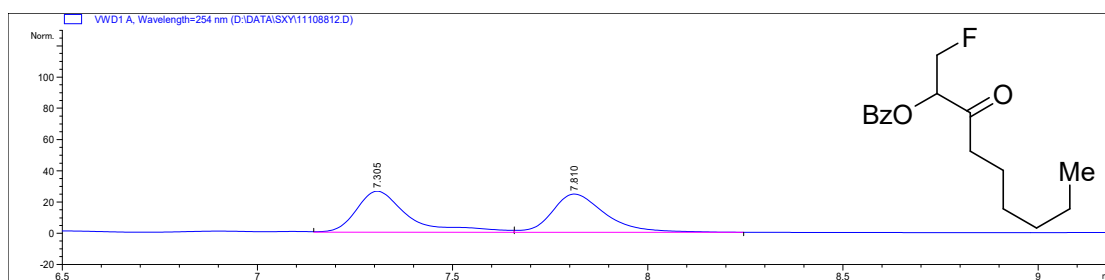
#	Time	Area	Height	Width	Symmetry	Area%
1	7.963	138.1	14.1	0.1478	0.797	52.301
2	8.416	125.9	13.2	0.1452	0.72	47.699

2c' 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



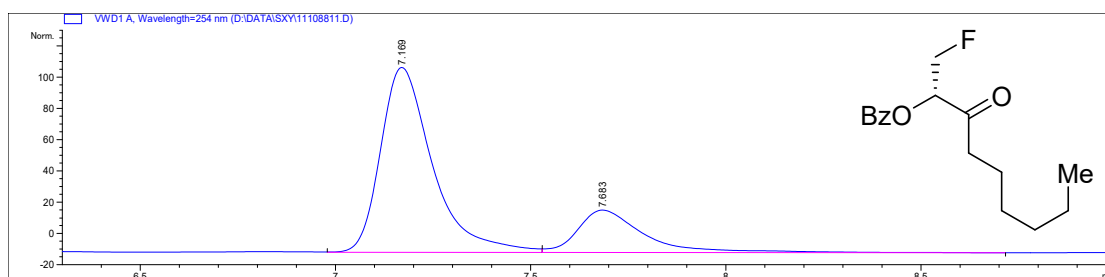
#	Time	Area	Height	Width	Symmetry	Area%
1	7.956	571	58.3	0.1477	0.694	82.879
2	8.428	118	11.6	0.154	0.767	17.121

2d' 254nm, IB, *n*-Hexane : *i*PrOH = 99:1, 0.8 mL/min



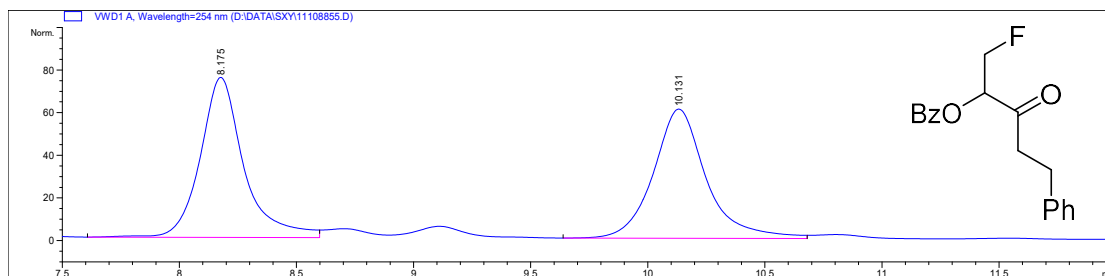
#	Time	Area	Height	Width	Symmetry	Area%
1	7.305	243.8	26.3	0.1386	0.607	51.423
2	7.81	230.3	24.5	0.1417	0.679	48.577

2d' 254nm, IB, *n*-Hexane : *i*PrOH = 99:1, 0.8 mL/min



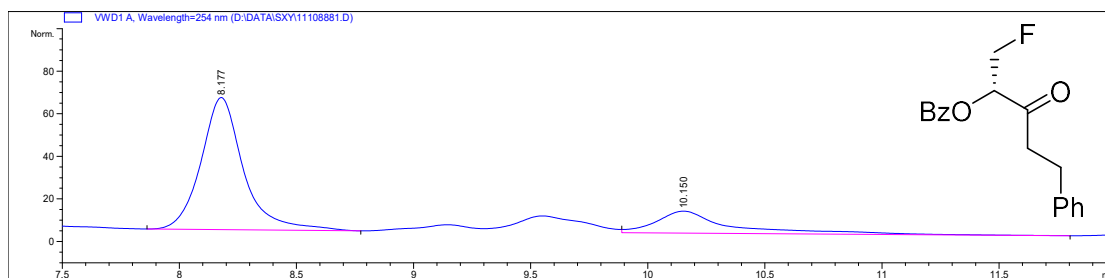
#	Time	Area	Height	Width	Symmetry	Area%
1	7.169	1095.4	118.4	0.14	0.636	77.189
2	7.683	323.7	27.1	0.1758	0.541	22.811

2e' 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



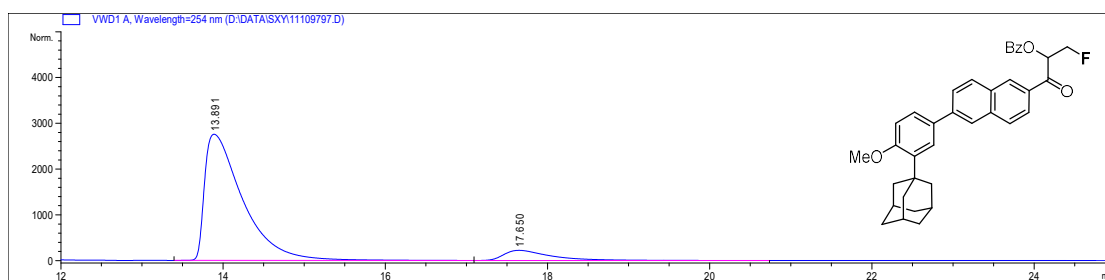
#	Time	Area	Height	Width	Symmetry	Area%
1	8.175	974.1	75.1	0.1892	0.829	50.478
2	10.131	955.7	60.7	0.2304	0.867	49.522

2e' 254nm, IB, *n*-Hexane : *i*PrOH = 90:10, 0.8 mL/min



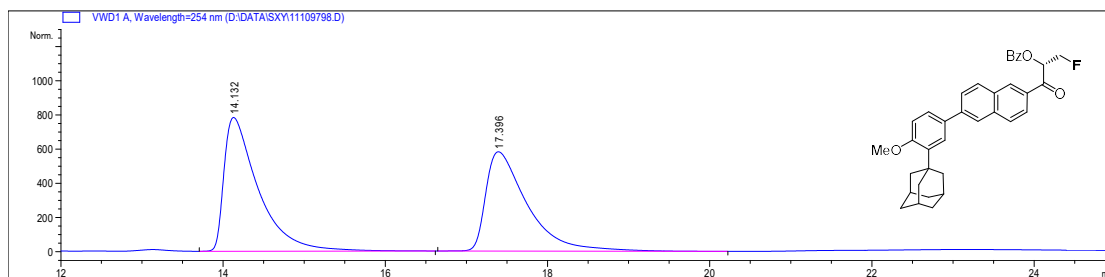
#	Time	Area	Height	Width	Symmetry	Area%
1	8.177	784.4	62.1	0.1867	0.843	77.064
2	10.15	233.5	10.3	0.315	0.497	22.936

2f 254nm, IA, n-hexane:i-PrOH= 90:10, 0.8 mL/min



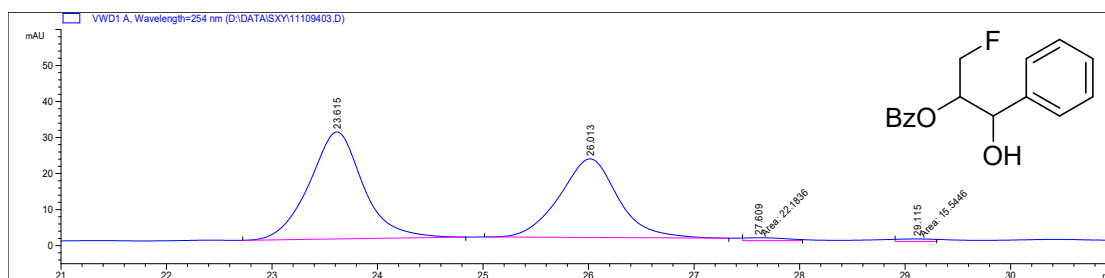
#	Time	Area	Height	Width	Symmetry	Area%
1	13.891	89989.3	2756.5	0.4843	0.298	90.939
2	17.65	8966.4	221.1	0.5941	0.425	9.061

2f 254nm, IA, n-hexane:i-PrOH= 90:10, 0.8 mL/min



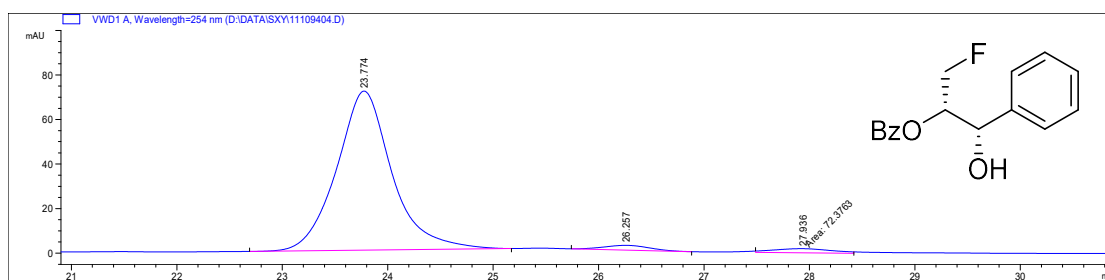
#	Time	Area	Height	Width	Symmetry	Area%
1	14.132	22935.9	782.1	0.4266	0.354	52.721
2	17.396	20568.6	580.4	0.5256	0.399	47.279

3 254nm, IA, n-Hexane : i-PrOH = 90:10, 0.4 mL/min



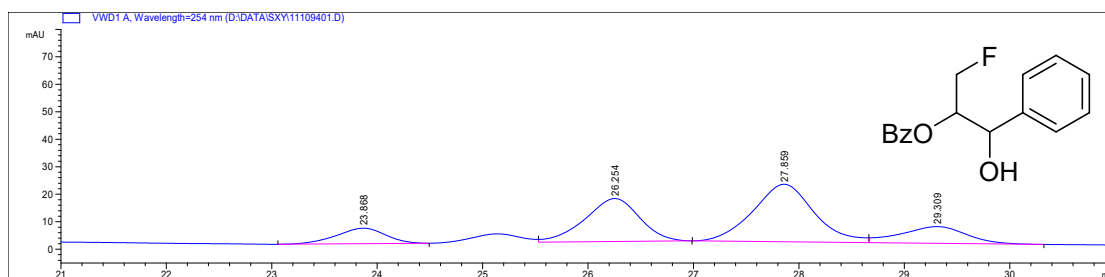
#	Time	Area	Height	Width	Symmetry	Area%
1	23.615	1054.2	29.7	0.5261	1.006	54.507
2	26.013	842.1	21.8	0.5709	1.036	43.542
3	27.609	22.2	8E-1	0.4644	0.447	1.147
4	29.115	15.5	7E-1	0.3686	1.129	0.804

3 254nm, IA, n-hexane:i-PrOH= 90:10, 0.4 mL/min



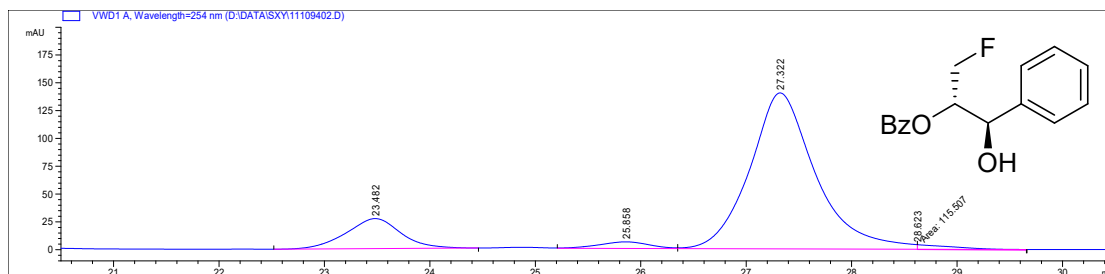
#	Time	Area	Height	Width	Symmetry	Area%
1	23.774	2607.4	71.4	0.5322	0.932	95.050
2	26.257	63.4	2.1	0.4437	0.906	2.312
3	27.936	72.4	1.9	0.6429	0	2.638

4 254nm, IA, n-hexane:i-PrOH= 90:10, 0.4 mL/min



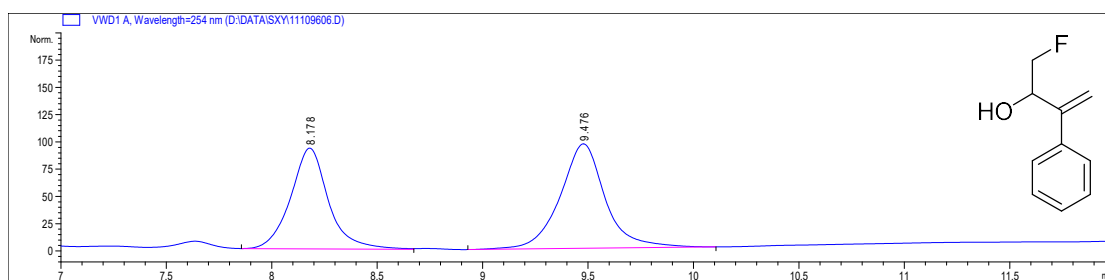
#	Time	Area	Height	Width	Symmetry	Area%
1	23.868	182.7	5.6	0.4787	1.204	9.840
2	26.254	565.5	15.7	0.5422	1.197	30.459
3	27.859	844.6	20.9	0.5931	0.992	45.492
4	29.309	263.8	6.1	0.6268	1.203	14.210

4 254nm, IA, n-hexane:i-PrOH= 90:10, 0.4 mL/min



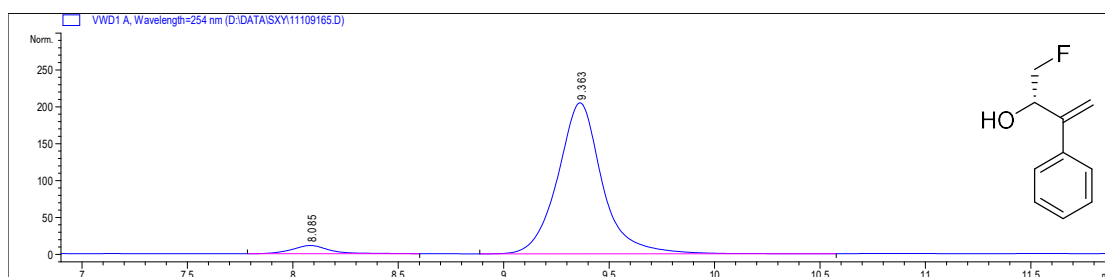
#	Time	Area	Height	Width	Symmetry	Area%
1	23.482	972.8	27	0.528	1.105	13.259
2	25.858	193.5	5.9	0.5002	1.132	2.637
3	27.322	6054.9	140.2	0.6239	0	82.530
4	28.623	115.5	4.3	0.3156	0	1.574

5 254nm, IA, n-hexane:i-PrOH= 90:10, 0.8 mL/min



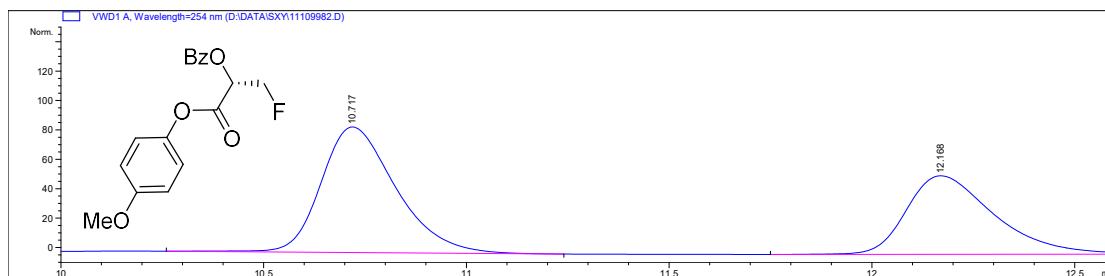
#	Time	Area	Height	Width	Symmetry	Area%
1	8.178	1154.9	92.4	0.1851	0.952	44.697
2	9.476	1428.9	95.9	0.2176	1.024	55.303

5 254nm, IA, n-hexane:i-PrOH= 90:10, 0.8 mL/min



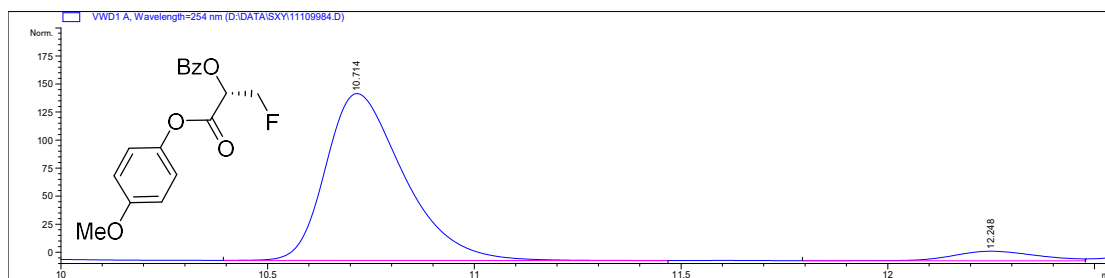
#	Time	Area	Height	Width	Symmetry	Area%
1	8.085	136	11.1	0.1811	0.936	4.339
2	9.363	2998.7	204.6	0.2161	0.944	95.661

6 254nm, IB, n-Hexane : iPrOH = 90:10, 0.8 mL/min



#	Time	Area	Height	Width	Symmetry	Area%
1	8.085	136	11.1	0.1811	0.936	4.339
2	9.363	2998.7	204.6	0.2161	0.944	95.661

6 254nm, IB, n-Hexane : iPrOH = 90:10, 0.8 mL/min



#	Time	Area	Height	Width	Symmetry	Area%
1	8.085	136	11.1	0.1811	0.936	4.339
2	9.363	2998.7	204.6	0.2161	0.944	95.661

12 X-Ray Crystallographic Data

The X-ray crystallographic structure for (Brominated fluoroethanol benzoate (**BFEB**)). Crystal data has been deposited to CCDC, number 2250621.

In a 5 mL glass vial, **BFEB** (50.0 mg) was dissolved in 1 mL of DCM, and 2 mL of hexane was slowly added along the inner wall of the glass vial, and the interface between the two phases was obvious. A needle-like solid was precipitated after 24 h of standing at room temperature and subjected to X-ray analysis.

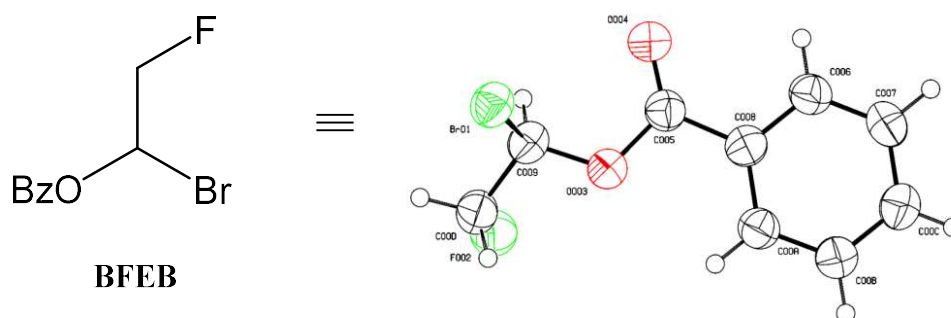


Table S2. Crystal data and structure refinement for **BFEB**.

Empirical formula	C ₉ H ₈ BrFO ₂
Formula weight	247.26
Temperature/K	150.00
Crystal system	monoclinic
Space group	P2 ₁
a/Å	4.3286(2)
b/Å	11.3274(6)
c/Å	9.4733(5)
α/°	90
β/°	91.124(2)
γ/°	90
Volume/Å ³	464.40(4)
Z	2
ρ _{calc} /cm ³	1.767
μ/mm ⁻¹	5.909

F(000)	244.0
Crystal size/mm ³	0.2 × 0.15 × 0.1
Radiation	CuKα (λ = 1.54178)
2θ range for data collection/°	12.18 to 144.178
Index ranges	-5 ≤ h ≤ 5, -9 ≤ k ≤ 13, -11 ≤ l ≤ 10
Reflections collected	3009
Independent reflections	1296 [Rint = 0.0382, Rsigma = 0.0568]
Data/restraints/parameters	1296/1/118
Goodness-of-fit on F ²	1.161
Final R indexes [I ≥ 2σ (I)]	R1 = 0.0418, wR2 = 0.0906
Final R indexes [all data]	R1 = 0.0419, wR2 = 0.0907
Largest diff. peak/hole / e Å ⁻³	0.66/-0.40

The X-ray crystallographic structure for (*S*)-3-fluoro-1-oxo-1-phenylpropan-2-yl benzoate (**2a**). Crystal data has been deposited to CCDC, number 2336970.

The compound **2a** (20.0 mg) was dissolved in CH₂Cl₂ (0.3 mL), then n-Hexane (1.2 mL) was added slowly, and the mixture was allowed to stand at -20°C. The single crystal of the target compound was obtained after several days and subjected to X-ray analysis.

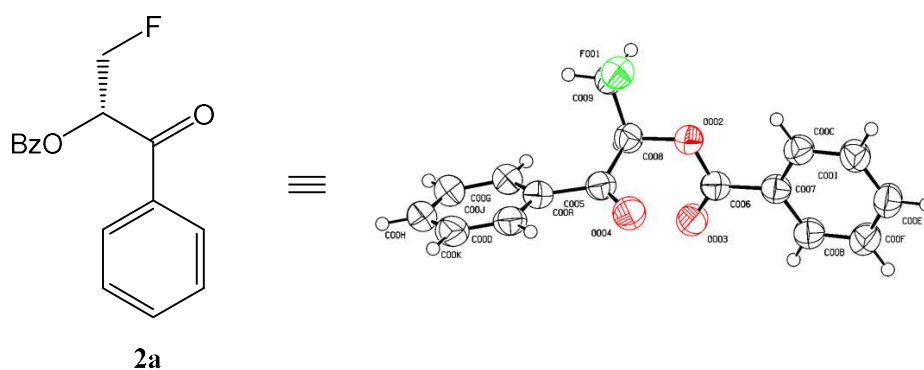


Table S3. Crystal data and structure refinement for **2a**.

Identification code	cu_0103_6_0m
Empirical formula	C ₁₆ H ₁₃ FO ₃
Formula weight	272.26
Temperature/K	150.00
Crystal system	orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
a/Å	6.65300(10)
b/Å	13.5440(3)
c/Å	15.3370(4)

$\alpha/^\circ$	90
$\beta/^\circ$	90
$\gamma/^\circ$	90
Volume/ \AA^3	1381.99(5)
Z	4
$\rho_{\text{calc}}/\text{g/cm}^3$	1.309
μ/mm^{-1}	0.827
F(000)	568.0
Crystal size/ mm^3	$0.2 \times 0.15 \times 0.1$
Radiation	CuK α ($\lambda = 1.54178$)
2θ range for data collection/ $^\circ$	8.71 to 149.06
Index ranges	$-8 \leq h \leq 8, -16 \leq k \leq 16, -18 \leq l \leq 15$
Reflections collected	16491
Independent reflections	2812 [$R_{\text{int}} = 0.0296, R_{\text{sigma}} = 0.0219$]
Data/restraints/parameters	2812/0/181
Goodness-of-fit on F^2	1.147
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0585, wR_2 = 0.1284$
Final R indexes [all data]	$R_1 = 0.0592, wR_2 = 0.1296$
Largest diff. peak/hole / $e \text{\AA}^{-3}$	0.37/-0.14
Flack parameter	-0.01(5)

The X-ray crystallographic structure for (1*S*,2*S*)-3-fluoro-1-hydroxy-1-phenylpropan-2-yl benzoate (**3**). Crystal data has been deposited to CCDC, number 2336972.

The compound **3** (17.0 mg) was dissolved in CH_2Cl_2 (0.3 mL), then n-Hexane (1.2 mL) was added slowly, and the mixture was allowed to stand at -20°C . The single crystal of the target compound was obtained after several days and subjected to X-ray analysis.

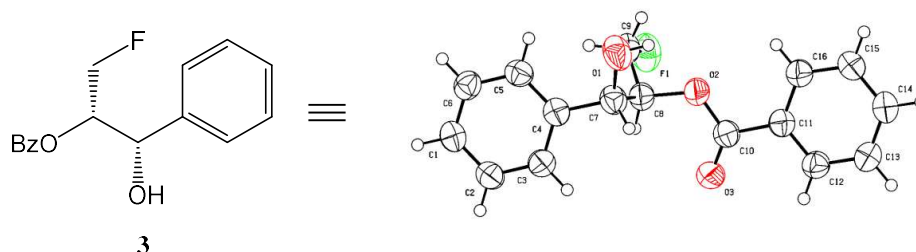


Table S4. Crystal data and structure refinement for **3**.

Identification code	cu_0117_3_0m
Empirical formula	$\text{C}_{16}\text{H}_{15}\text{FO}_3$
Formula weight	274.28

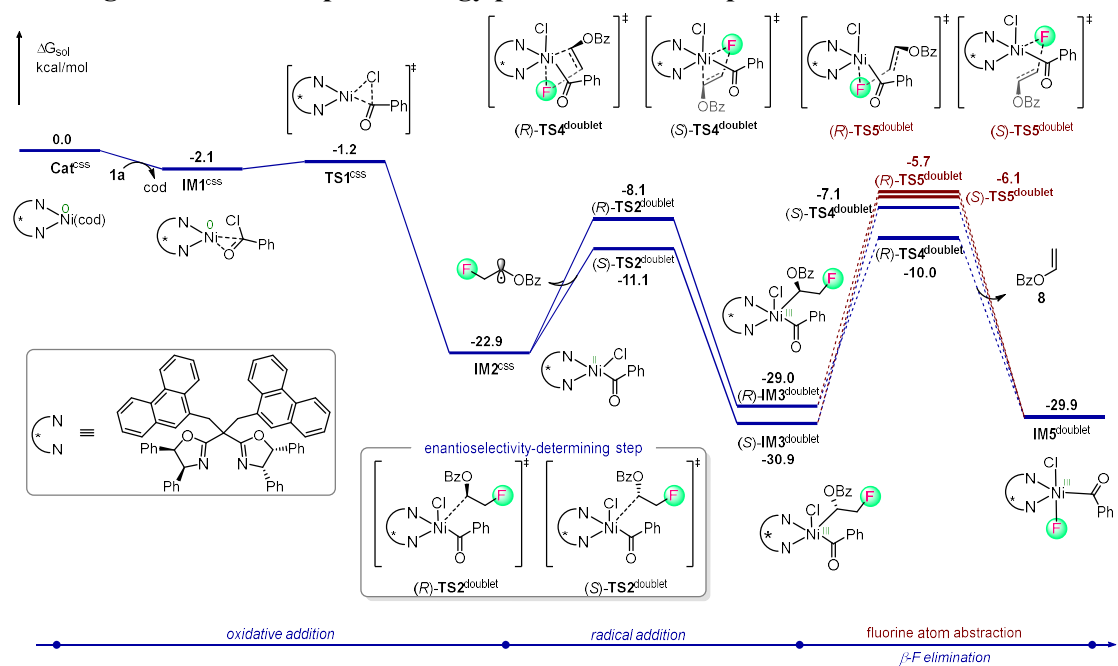
Temperature/K	150.00
Crystal system	orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
a/Å	5.6714(2)
b/Å	7.3732(2)
c/Å	32.2276(8)
α /°	90
β /°	90
γ /°	90
Volume/Å ³	1347.64(7)
Z	4
ρ_{calc} /cm ³	1.352
μ /mm ⁻¹	0.848
F(000)	576.0
Crystal size/mm ³	0.2 × 0.15 × 0.1
Radiation	CuK α (λ = 1.54178)
2 Θ range for data collection/°	10.982 to 149.236
Index ranges	-6 ≤ h ≤ 7, -9 ≤ k ≤ 9, -31 ≤ l ≤ 40
Reflections collected	10963
Independent reflections	2739 [R _{int} = 0.0276, R _{sigma} = 0.0254]
Data/restraints/parameters	2739/0/182
Goodness-of-fit on F ²	1.113
Final R indexes [I ≥ 2 σ (I)]	R ₁ = 0.0649, wR ₂ = 0.1442
Final R indexes [all data]	R ₁ = 0.0659, wR ₂ = 0.1461
Largest diff. peak/hole / e Å ⁻³	0.37/-0.22
Flack parameter	0.06(6)

13 Computational Results

13.1 Computational Details: All the calculations were performed using Gaussian 09 package^[1]. The geometry optimizations were carried out using (u)B3LYP-D3(BJ)^[2] functional with a mixed basis set of SDD for Ni and Br and 6-31G(*d*) for all other atoms. Frequencies were computed analytically at the same level of theory to confirm whether the structures are minima (no imaginary frequencies) or transition states (only one imaginary frequency). Selected transition-state structures were confirmed to connect the correct reactants and products by intrinsic reaction coordinate (IRC) calculations.^[3] To obtain better accuracy, solution-phase single-point energies for the optimized geometries were recalculated using (u)TPSS-D3(BJ)^[4] functional with a larger basis set of def2-TZVPP^[5,6]. Solvation effects (solvent=THF) were taken into account by performing single-point calculations with the SMD model^[7]. The final free energies reported in the article are the large basis set single-point energies corrected by gas-phase Gibbs free energy correction (at 298.15 K). The 3D diagrams of molecules were generated using CYLView^[8]. Non-covalent interactions^[9] were performed with Multiwfn^[10], and were visualized with visual molecular dynamics (VMD)^[11].

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13.2. Figure S8 DFT-computed energy profiles of the competitive fluorine elimination



13.3 Table S5 of Calculated Energies and Energy Corrections

Stationary point	Single-point energy-(u)TPSS-D3(BJ)-SMD def2-TZVPP (a.u.)	Thermal correction to Gibbs free energy at 298.15 K (a.u.)
1a	-805.446056	0.068432
radical	-598.381081	0.112394
cod	-312.232002	0.149973
(<i>R</i>)- 2	-943.636490	0.208580
(<i>S</i>)- 2	-943.636490	0.208580
Cat^{css}	-4434.608418	0.995710
IM1^{css}	-4927.825472	0.913791
IM2^{css}	-4927.858167	0.913415
(<i>R</i>)- IM3^{doublet}	-5526.274827	1.051548
(<i>S</i>)- IM3^{doublet}	-5526.281251	1.055094
IM4^{doublet}	-4582.640173	0.818450
IM5^{doublet}	-5027.728981	0.911238
TS1^{css}	-4927.823528	0.913334
(<i>R</i>)- TS2^{doublet}	-5526.241520	1.051679
(<i>S</i>)- TS2^{doublet}	-5526.246315	1.051611
(<i>R</i>)- TS3^{doublet}	-5526.261407	1.051925
(<i>S</i>)- TS3^{doublet}	-5526.263208	1.055483
(<i>R</i>)- TS4^{doublet}	-5526.242464	1.049579
(<i>S</i>)- TS4^{doublet}	-5526.238836	1.050565
(<i>R</i>)- TS5^{doublet}	-5526.237198	1.051056
(<i>S</i>)- TS5^{doublet}	-5526.238194	1.051425

13.4 Cartesian coordinates

1a

C	1.08690400	0.39512300	-0.04968800
C	2.45935600	0.40690500	0.20751100
C	3.14939300	1.61480400	0.27611300
C	2.46117300	2.82049900	0.08625800
C	1.07902500	2.80571600	-0.17228500
C	0.39730200	1.59618700	-0.23944800
H	0.55392800	-0.54986400	-0.10252300
H	2.99409300	-0.52628600	0.35503300
H	4.21362300	1.62680700	0.47566300
H	0.56354700	3.74864800	-0.31608700
H	-0.66982600	1.58727900	-0.43935800
C	3.09980300	4.15430600	0.13939900
O	2.55384300	5.20505200	-0.01527200
Cl	4.90065600	4.14300800	0.47662700

radical

C	2.24180000	-1.71164100	0.34841100
C	1.38143600	-0.86889900	-0.49931900
H	3.29537600	-1.50362700	0.13414500
H	2.04211100	-1.52490400	1.40984900
H	1.58087000	-0.60120900	-1.52832700
F	2.02247200	-3.08489100	0.11804700
O	0.09753400	-0.71948900	-0.06409800
C	-0.80399700	-0.08292300	-0.89184200
O	-0.49320600	0.34684400	-1.98119400
C	-2.14764800	-0.00347600	-0.27900800
C	-2.43312500	-0.54363500	0.98328700
C	-3.15701800	0.63825600	-1.01105800
C	-3.72023900	-0.43882100	1.50499800
H	-1.65062900	-1.04131500	1.54359700
C	-4.44081900	0.74013000	-0.48436400
H	-2.91292900	1.04670000	-1.98567000
C	-4.72367800	0.20187300	0.77403100
H	-3.94180000	-0.85780000	2.48203800
H	-5.22133900	1.23749200	-1.05236200
H	-5.72626500	0.28111100	1.18471700

cod

C	-1.57280000	0.61698000	-0.27206200
C	0.67855000	1.79766200	-0.04200400
C	1.57325400	0.69233700	-0.54300300
C	1.57336400	-0.61702600	-0.26887600
C	0.64787000	-1.39770500	0.63553900
C	-1.57216500	-0.69241800	-0.54600800
H	-2.31886500	1.22013100	-0.78977800
H	2.33789600	1.04095000	-1.23863600
H	2.32049600	-1.22021900	-0.78500100
H	-2.33540800	-1.04111900	-1.24313100
C	-0.64908500	1.39774400	0.63408900
C	-0.67847900	-1.79767400	-0.04304200
H	1.25170900	2.43270500	0.65225600
H	0.44617800	2.44790300	-0.89790400
H	-0.44945100	0.85928900	1.56285600
H	-1.15684200	2.32285400	0.93326100
H	-1.25300700	-2.43254000	0.65024900
H	-0.44449400	-2.44811500	-0.89834800
H	1.15503100	-2.32280300	0.93575500
H	0.44647600	-0.85918300	1.56389300

(R)-2

C	1.68077300	1.84158700	0.10158400
C	0.77496000	0.68623400	-0.29468000
H	2.73183700	1.55471700	-0.01351900
H	1.48966600	2.11606900	1.14455400
H	0.82488600	0.52486500	-1.37392900
F	1.42579500	2.93555900	-0.70809500
O	-0.55066500	1.06884800	0.05722300
C	-1.52540900	0.24912500	-0.41566700
O	-1.28564700	-0.70956300	-1.12342100
C	-2.87967700	0.67195000	0.01637500
C	-3.97154500	-0.08870400	-0.42158100
C	-3.08648900	1.78892100	0.83652200
C	-5.26299800	0.26618500	-0.04305900
H	-3.78429500	-0.95010600	-1.05344900
C	-4.38114200	2.14036500	1.21234500
H	-2.23579300	2.36965000	1.17289700
C	-5.46871900	1.38113900	0.77393900
H	-6.10895200	-0.32426200	-0.38246100
H	-4.54255100	3.00585700	1.84823400
H	-6.47684000	1.65781800	1.06981800
C	1.17980800	-0.59282700	0.46316700
O	0.58634200	-0.89443000	1.48310200
C	2.33495300	-1.38772900	-0.04169900
C	3.00633200	-1.09779700	-1.23970400
C	2.76254700	-2.47465300	0.73771100
C	4.08688200	-1.87914800	-1.64614700
H	2.69101700	-0.27201200	-1.86841400
C	3.83903000	-3.25392600	0.33009400
H	2.22944200	-2.68508200	1.65845600
C	4.50444400	-2.95636800	-0.86318000
H	4.59870100	-1.64949900	-2.57587000
H	4.16234400	-4.09336000	0.93861700
H	5.34548900	-3.56498800	-1.18296400

(S)-2

C	1.68077300	1.84158700	-0.10158400
C	0.77496000	0.68623400	0.29468000
H	2.73183700	1.55471700	0.01351900
H	1.48966600	2.11606900	-1.14455400
H	0.82488600	0.52486500	1.37392900
F	1.42579500	2.93555900	0.70809500
O	-0.55066500	1.06884800	-0.05722300
C	-1.52540900	0.24912500	0.41566700

O	-1.28564700	-0.70956300	1.12342100
C	-2.87967700	0.67195000	-0.01637500
C	-3.97154500	-0.08870400	0.42158100
C	-3.08648900	1.78892100	-0.83652200
C	-5.26299800	0.26618500	0.04305900
H	-3.78429500	-0.95010600	1.05344900
C	-4.38114200	2.14036500	-1.21234500
H	-2.23579300	2.36965000	-1.17289700
C	-5.46871900	1.38113900	-0.77393900
H	-6.10895200	-0.32426200	0.38246100
H	-4.54255100	3.00585700	-1.84823400
H	-6.47684000	1.65781800	-1.06981800
C	1.17980800	-0.59282700	-0.46316700
O	0.58634200	-0.89443000	-1.48310200
C	2.33495300	-1.38772900	0.04169900
C	3.00633200	-1.09779700	1.23970400
C	2.76254700	-2.47465300	-0.73771100
C	4.08688200	-1.87914800	1.64614700
H	2.69101700	-0.27201200	1.86841400
C	3.83903000	-3.25392600	-0.33009400
H	2.22944200	-2.68508200	-1.65845600
C	4.50444400	-2.95636800	0.86318000
H	4.59870100	-1.64949900	2.57587000
H	4.16234400	-4.09336000	-0.93861700
H	5.34548900	-3.56498800	1.18296400

Cat^{css}

C	-0.40746400	1.18956800	-0.54689500
C	-1.73755100	0.56485500	-0.88337600
Ni	-1.78932700	-1.39179300	1.33824000
N	0.05574900	-0.73887700	1.00186400
N	-2.39558700	-0.31424300	-0.21340900
C	0.43527500	0.26909000	0.30193900
C	1.27085100	-1.33561600	1.59608600
C	2.29745700	-0.16297100	1.47621200
O	1.75462000	0.58977600	0.34825600
C	-3.72903700	-0.44046300	-0.83429900
C	-3.54648300	0.29919200	-2.20730400
O	-2.36256300	1.10348300	-1.97711300
C	-0.74798200	2.53034400	0.24994100
H	-1.53209000	2.29264000	0.97001600
H	-1.17913300	3.21836000	-0.48390000
C	0.37711200	1.57444200	-1.84162900
H	-0.32981400	2.07630700	-2.50689600

H	1.11852900	2.31019200	-1.55160900
H	1.08504500	-1.54668400	2.65041100
H	2.17554100	0.48017500	2.34949700
H	-3.93537300	-1.49499400	-1.01781300
H	-3.28014800	-0.44067700	-2.97274400
C	1.67516100	-2.60730100	0.88329800
C	2.60309200	-4.89227900	-0.44832900
C	2.53062400	-3.50611000	1.52912500
C	1.74041900	-4.00580600	-1.09498000
C	2.99577200	-4.64162900	0.86799200
H	2.84957600	-3.30238300	2.54834000
H	1.42503200	-4.19435600	-2.11564100
H	3.66407400	-5.32838500	1.37993400
H	2.96415100	-5.77672700	-0.96611400
H	-8.13850000	-0.31908500	0.67010200
C	-7.14403900	0.11288700	0.73596500
C	-4.58377300	1.19916400	0.90408900
C	-6.90159100	1.18859600	1.59114100
C	-5.61688200	1.72971600	1.67384700
C	-4.81845000	0.12079800	0.04808100
H	-7.70644900	1.59832300	2.19461700
H	-5.41741900	2.56031600	2.34518400
H	-3.58097900	1.60013400	0.98970200
C	4.70745800	1.25883900	-2.38978700
C	3.34187000	1.32862500	-2.20995100
C	2.47150400	0.33153600	-2.71669600
C	3.04559100	-0.78390200	-3.40542900
C	4.44958900	-0.82247800	-3.57622600
C	5.26772800	0.17703200	-3.08856100
C	1.03107200	0.41554100	-2.56516100
C	2.18982200	-1.84775800	-3.90625000
C	0.78247400	-1.72067800	-3.74918100
C	0.24729500	-0.56861800	-3.09581500
C	-0.07353700	-2.74352400	-4.21769700
H	-1.14584300	-2.62706600	-4.08013200
C	0.43631400	-3.87304200	-4.82630300
C	1.82930700	-4.00602800	-4.98315100
C	2.68276100	-3.01496500	-4.53314700
H	5.34504400	2.03406800	-1.97589500
H	2.94494400	2.15556700	-1.63658600
H	4.90131800	-1.65169400	-4.10803800
H	6.34233600	0.11798700	-3.23489400
H	-0.83251800	-0.49316400	-3.02685100
H	-0.22959800	-4.65612800	-5.17664900

H	2.23844600	-4.89453100	-5.45530000
H	3.75022700	-3.15532600	-4.65668600
C	-6.10528100	-0.41757000	-0.02880700
H	-6.29421100	-1.25934500	-0.69009700
C	-4.69456600	1.13714800	-2.68343100
C	-4.88542600	2.44317100	-2.22127000
C	-5.63684300	0.57083300	-3.54642800
C	-6.00924300	3.16735600	-2.61272200
H	-4.15255600	2.88528000	-1.55611000
C	-6.76646300	1.29232400	-3.93252200
H	-5.48708100	-0.44153600	-3.91492700
C	-6.95519700	2.59320800	-3.46484300
H	-6.14941900	4.18105400	-2.24840600
H	-7.49314000	0.84126400	-4.60214700
H	-7.83216300	3.15896900	-3.76603600
C	1.27929200	-2.86896100	-0.43073300
H	0.60396200	-2.18629700	-0.93050500
C	3.74762600	-0.47935000	1.29479900
C	4.24913200	-1.04867100	0.11890800
C	4.61590000	-0.23938500	2.36529400
C	5.59733400	-1.38261100	0.02555100
H	3.58754000	-1.23014500	-0.71781700
C	5.96549900	-0.58107700	2.27435700
H	4.22754500	0.22122700	3.27056800
C	6.45803600	-1.15567600	1.10211200
H	5.97299100	-1.81877900	-0.89459700
H	6.63011100	-0.39217200	3.11290300
H	7.50894700	-1.42139400	1.02548100
C	4.54815600	5.73144800	0.31371500
C	3.29155000	5.34406500	-0.10652400
C	2.48783900	4.49742800	0.69132300
C	2.96940600	4.04597700	1.95178100
C	4.26035100	4.45694700	2.35294200
C	5.03469200	5.27905700	1.55438100
C	1.21740100	4.04319400	0.22006000
C	2.11473400	3.19084900	2.76066500
C	0.85446200	2.75325000	2.24685800
C	0.44632600	3.15670100	0.91546300
C	0.04336400	1.91863400	3.05364500
H	-0.90495300	1.55342000	2.67938800
C	0.44298100	1.52712500	4.31828100
C	1.68560800	1.94769800	4.81933200
C	2.49916300	2.76106600	4.05165600
H	0.89125400	4.38638200	-0.75889300

H	5.16015000	6.37695900	-0.30945100
H	2.90381400	5.67630000	-1.06633000
H	4.66844400	4.12020500	3.29895000
H	6.02553100	5.57370900	1.88764400
H	-0.20479300	0.89179900	4.91366000
H	2.00731800	1.64058300	5.81022600
H	3.44901900	3.08228300	4.46300500
C	-3.00360100	-3.04501900	1.16043800
C	-4.20561900	-1.69346300	2.99556200
C	-2.90138800	-0.92189800	3.03473500
C	-1.67351000	-1.49842700	3.37653400
C	-1.51180300	-2.93710000	3.85313200
C	-1.69210500	-3.48186500	1.36471500
H	-3.35977800	-3.07070800	0.12994000
H	-3.00409800	0.16101700	3.10374700
H	-0.86681900	-0.82307400	3.65520000
H	-1.12020200	-3.80574600	0.49764800
C	-4.09593800	-3.03949700	2.22608600
C	-1.12476500	-3.90286200	2.70439100
H	-4.58744800	-1.88500400	4.01298100
H	-4.95537700	-1.06512000	2.50773600
H	-3.92582200	-3.86243000	2.93003300
H	-5.06271500	-3.25211900	1.75244300
H	-1.42721100	-4.93092700	2.96775900
H	-0.03368100	-3.93076600	2.60780300
H	-0.74264900	-2.98187800	4.63564700
H	-2.43790500	-3.27442100	4.33124800

IM1^{CSS}

C	-0.38217800	0.96998300	-0.85152100
C	-1.72690500	0.44412400	-1.28487500
N	0.08849400	-1.20661900	0.34080000
N	-2.34274500	-0.58715200	-0.84339000
C	0.45748300	-0.07704800	-0.15210300
C	1.28784300	-1.87530600	0.89660200
C	2.29331400	-0.68664900	0.99703200
O	1.75059300	0.25652700	0.00696100
C	-3.77350400	-0.47131200	-1.23188600
C	-3.69648000	0.58285100	-2.37300900
O	-2.43237400	1.26847300	-2.09955900
C	-0.75325200	2.15682100	0.15180500
H	-1.63315100	1.85574800	0.72354300
H	-1.05742700	2.99665400	-0.47911500
C	0.41925000	1.56225800	-2.04880400

H	-0.27717900	2.17372900	-2.62975300
H	1.15900900	2.23667200	-1.62756500
H	1.04946100	-2.22666500	1.90223600
H	2.14759800	-0.20155100	1.96160100
H	-4.11113900	-1.43553000	-1.61466500
H	-3.53889000	0.05148900	-3.32110900
C	1.72642100	-3.03793500	0.03801200
C	2.69447700	-5.14578400	-1.52836700
C	2.51981500	-4.03627400	0.61015300
C	1.89448900	-4.15787800	-2.10274500
C	3.00595600	-5.08364700	-0.16828100
H	2.76378700	-3.98566900	1.66833500
H	1.63842700	-4.20115100	-3.15606300
H	3.62136100	-5.85442900	0.28703200
H	3.06776100	-5.96628700	-2.13507900
H	-6.42545100	-1.63556300	2.41825900
C	-5.89125700	-0.84369300	1.90146100
C	-4.48836100	1.16732000	0.57550200
C	-5.82185200	0.43489200	2.45385100
C	-5.11929100	1.44182400	1.78652200
C	-4.55586900	-0.11592100	0.01541200
H	-6.31121000	0.64840700	3.39994000
H	-5.06498200	2.44155700	2.20804900
H	-3.95597100	1.95917800	0.05936300
C	4.75330400	1.26086900	-2.62960000
C	3.38805600	1.32945800	-2.44575100
C	2.50407400	0.43100700	-3.09285100
C	3.06108800	-0.58592700	-3.93181300
C	4.46514000	-0.62736600	-4.09901200
C	5.29772700	0.27821600	-3.47229600
C	1.06505800	0.51938500	-2.93876700
C	2.18902300	-1.54903100	-4.58478900
C	0.78316000	-1.42249700	-4.41457800
C	0.26600700	-0.36368100	-3.60674300
C	-0.08784800	-2.35537700	-5.02228900
H	-1.15820900	-2.24599000	-4.86708800
C	0.40682600	-3.39362600	-5.78546300
C	1.79771500	-3.52142400	-5.96337200
C	2.66576400	-2.61946600	-5.37557500
H	5.40383800	1.95656800	-2.10872800
H	3.00004100	2.07320700	-1.76243100
H	4.90588700	-1.38232900	-4.73922200
H	6.37189000	0.22051300	-3.62160600
H	-0.81415500	-0.28251300	-3.52775100

H	-0.26958700	-4.11048400	-6.24102200
H	2.19381900	-4.33841200	-6.55937900
H	3.73101400	-2.75654900	-5.51914600
C	-5.25870400	-1.11790800	0.68764600
H	-5.26832800	-2.12591000	0.28761800
C	-4.82194600	1.57010500	-2.51730300
C	-4.57915200	2.93769800	-2.66834500
C	-6.14043900	1.09993500	-2.52649000
C	-5.64520700	3.82696900	-2.81487300
H	-3.55856600	3.30323800	-2.66153700
C	-7.20249900	1.98834600	-2.67754100
H	-6.33869500	0.03998900	-2.39546000
C	-6.95778600	3.35604900	-2.81984800
H	-5.44666900	4.88923800	-2.92522900
H	-8.22167900	1.61331600	-2.67479800
H	-7.78639200	4.04915100	-2.93192900
C	1.41518700	-3.10676700	-1.32146900
H	0.79178500	-2.34479200	-1.77170800
C	3.75175300	-0.93667900	0.78526000
C	4.27469300	-1.34511800	-0.44708600
C	4.60939600	-0.79162200	1.88111800
C	5.63452300	-1.61584800	-0.57124600
H	3.62287900	-1.45285300	-1.30407100
C	5.97106300	-1.06859200	1.75757900
H	4.20279200	-0.45929800	2.83311500
C	6.48516000	-1.48361900	0.52880700
H	6.02696200	-1.92893600	-1.53338800
H	6.62725900	-0.95473300	2.61587500
H	7.54516000	-1.69999500	0.42705500
C	4.44000100	5.20065400	1.63418700
C	3.27342700	4.90994600	0.95566300
C	2.40012400	3.89696300	1.41273200
C	2.71693900	3.16753700	2.59324600
C	3.91862200	3.48719500	3.26459000
C	4.76245200	4.47897700	2.79828500
C	1.21874800	3.56757900	0.67742100
C	1.79908700	2.13394700	3.04802300
C	0.61635000	1.85398900	2.29613900
C	0.37147300	2.56984300	1.06034700
C	-0.26054500	0.84141100	2.75600400
H	-1.16543400	0.60871000	2.20836500
C	0.02024100	0.09698000	3.88557500
C	1.19365000	0.35714700	4.61201700
C	2.05386900	1.36197100	4.20594100

H	1.02103100	4.12205100	-0.23734700
H	5.10606200	5.97853500	1.27261500
H	3.01096300	5.45421000	0.05176100
H	4.19725900	2.95072000	4.16429000
H	5.67991700	4.70039900	3.33579300
H	-0.65957300	-0.68533200	4.19991400
H	1.42125800	-0.23116200	5.49607600
H	2.94586800	1.55195200	4.79189900
Ni	-1.65617600	-1.98509900	0.39631300
Cl	-1.09382700	-5.08351500	0.90430100
C	-1.85869300	-3.45978300	1.52925600
O	-3.00425300	-3.15410800	0.99015800
C	-1.64096700	-3.29964200	2.99674200
C	-2.61862400	-2.61781000	3.74214900
C	-0.46521400	-3.71147000	3.64337600
C	-2.42779800	-2.36881400	5.10021600
H	-3.52071300	-2.29324500	3.23465300
C	-0.27210700	-3.44636900	4.99898000
H	0.28250700	-4.25867400	3.07924600
C	-1.25218100	-2.77819000	5.73744300
H	-3.19944900	-1.85062900	5.66420900
H	0.64364100	-3.77558800	5.48368100
H	-1.10416200	-2.58192700	6.79585200

IM2^{CSS}

C	-0.41131400	1.15216200	-0.72874800
C	-1.74281800	0.56646000	-1.11343900
N	0.02327200	-0.79967900	0.81645800
N	-2.36328800	-0.41963300	-0.58230700
C	0.40628900	0.22005800	0.12999800
C	1.23722100	-1.39278900	1.43842400
C	2.25706400	-0.22223200	1.32817500
O	1.70662400	0.54536900	0.20362500
C	-3.75069400	-0.40920200	-1.10064800
C	-3.60523800	0.49086300	-2.37339500
O	-2.39733700	1.26200100	-2.06922100
C	-0.77971500	2.47821300	0.07775200
H	-1.62967200	2.25715500	0.72543500
H	-1.13278900	3.19144300	-0.67194500
C	0.41438800	1.54485400	-1.99287300
H	-0.26448500	2.07855600	-2.66318300
H	1.16573000	2.25675900	-1.66612700
H	1.03536100	-1.58246500	2.49205200
H	2.13398300	0.42065900	2.19934700

H	-4.03302400	-1.42581400	-1.37411300
H	-3.34757400	-0.14373600	-3.22983800
C	1.64151900	-2.67741900	0.75322300
C	2.52368800	-5.02279100	-0.49247200
C	2.44526100	-3.58586800	1.44773900
C	1.71620900	-4.12349900	-1.18869700
C	2.88594200	-4.75188600	0.82913400
H	2.71278600	-3.38438600	2.48070000
H	1.42328000	-4.32609200	-2.21342400
H	3.49960200	-5.45587300	1.38333600
H	2.86268000	-5.93617300	-0.97367700
H	-8.10211500	0.31758800	0.37709700
C	-7.04393400	0.47069900	0.56871600
C	-4.32683400	0.83670000	1.05231800
C	-6.63118400	1.19969400	1.68647500
C	-5.26958300	1.37318500	1.93015100
C	-4.73284600	0.11927700	-0.07390600
H	-7.36651400	1.61667100	2.36867600
H	-4.93534300	1.91615000	2.80968900
H	-3.27108600	0.93888600	1.27338100
C	4.73967100	1.13373800	-2.55254600
C	3.37608300	1.23549500	-2.37086900
C	2.48363700	0.25349600	-2.86710400
C	3.03090900	-0.88131000	-3.54642600
C	4.43307500	-0.95233800	-3.71912600
C	5.27393700	0.03348500	-3.24218700
C	1.04597300	0.37103200	-2.71557800
C	2.15135100	-1.93165700	-4.03455800
C	0.74761200	-1.77272800	-3.87655200
C	0.24021400	-0.59987200	-3.23792000
C	-0.13238000	-2.78419900	-4.32459200
H	-1.20100400	-2.64616600	-4.18025400
C	0.35190100	-3.93207400	-4.91922300
C	1.74106800	-4.09467400	-5.08226800
C	2.61751800	-3.11639600	-4.64889500
H	5.39657700	1.89796600	-2.14886200
H	2.99672000	2.07919900	-1.80961100
H	4.86536000	-1.79585800	-4.24433300
H	6.34652400	-0.05014500	-3.39059400
H	-0.83863900	-0.50624700	-3.16989300
H	-0.33137900	-4.70699700	-5.25338300
H	2.12934300	-4.99730300	-5.54498400
H	3.68114300	-3.28080300	-4.77517200
C	-6.10008700	-0.06964200	-0.29993900

H	-6.42670300	-0.63454100	-1.16850900
C	-4.73747800	1.40375200	-2.72883900
C	-4.97164800	2.58284200	-2.01221400
C	-5.61716200	1.03337300	-3.74880700
C	-6.07813400	3.37325200	-2.30968700
H	-4.29504700	2.86703000	-1.21428300
C	-6.73231700	1.82005300	-4.04063300
H	-5.43365400	0.12171800	-4.31263800
C	-6.96419700	2.99179500	-3.32060900
H	-6.25505500	4.28438900	-1.74574900
H	-7.41282400	1.52047000	-4.83231000
H	-7.82999300	3.60758800	-3.54647900
C	1.27844300	-2.95366100	-0.56689000
H	0.64712700	-2.26189500	-1.11019700
C	3.70761200	-0.53289800	1.14323000
C	4.20876500	-1.13356500	-0.01718000
C	4.57726200	-0.25117600	2.20238500
C	5.56011800	-1.45560700	-0.10623600
H	3.54731900	-1.34974800	-0.84576700
C	5.92981900	-0.58124800	2.11549600
H	4.18720500	0.22936100	3.09624900
C	6.42263500	-1.18623900	0.95893000
H	5.93671200	-1.91679400	-1.01352600
H	6.59573400	-0.36081300	2.94499100
H	7.47570600	-1.44386100	0.88566300
C	4.35218500	5.88091800	0.78600000
C	3.17209400	5.44104200	0.22065600
C	2.35703600	4.49599000	0.88417000
C	2.74697000	3.99270300	2.15705900
C	3.96093500	4.46041600	2.70858000
C	4.74730600	5.38205400	2.04102200
C	1.16120600	4.00773300	0.27062400
C	1.88461400	3.02813100	2.82417400
C	0.68421800	2.58625700	2.18610400
C	0.36567700	3.06700100	0.85608600
C	-0.13624100	1.64690700	2.85656000
H	-1.04574600	1.28455900	2.39562300
C	0.20930800	1.12673800	4.08994000
C	1.39672800	1.55112900	4.70908400
C	2.20732700	2.48670800	4.09013000
H	0.90597300	4.39042500	-0.71505600
H	4.97296400	6.60517600	0.26688800
H	2.85369100	5.81243100	-0.75026400
H	4.29431700	4.09682700	3.67359200

H	5.67575700	5.72175400	2.49072700
H	-0.42711400	0.37438000	4.54190300
H	1.68055700	1.14730500	5.67667200
H	3.11247000	2.80541000	4.59383800
Ni	-1.73994700	-1.59608400	0.95683300
Cl	-3.57600400	-2.81677100	0.96383100
C	-1.31854000	-2.35627200	2.61042300
O	-1.41245500	-1.61663400	3.58406900
C	-0.77342200	-3.74687200	2.76242900
C	-0.14010400	-4.09759900	3.96322500
C	-0.80255300	-4.66187700	1.70367500
C	0.46273200	-5.34528700	4.10120400
H	-0.13126500	-3.37194000	4.77091600
C	-0.21024900	-5.91407100	1.84612300
H	-1.29511400	-4.38137100	0.78022300
C	0.42648100	-6.25613200	3.04116100
H	0.95775100	-5.61195400	5.03160600
H	-0.23130200	-6.61815600	1.01953100
H	0.89778400	-7.23004200	3.14637400

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C	-1.79550700	0.43957700	-0.11281500
C	-0.76425800	-0.42915000	-0.79927900
N	-0.15759800	1.30528800	1.55961700
N	0.49622600	-0.52402400	-0.58294200
C	-1.34087900	0.94267200	1.23232800
C	-0.22524100	1.90353000	2.91669100
C	-1.64244000	1.45658700	3.39818500
O	-2.31690600	1.12620900	2.14012800
C	1.07938400	-1.39290000	-1.63775400
C	-0.17567800	-1.81171100	-2.49776400
O	-1.27186500	-1.13364300	-1.81792100
C	-3.12443000	-0.34361300	-0.01688400
H	-3.47792400	-0.45398400	-1.04191400
H	-3.85078400	0.28551700	0.50870500
C	-2.01808300	1.76320500	-0.97275600
H	-2.87110900	2.27199000	-0.51260100
H	-1.14509000	2.39937400	-0.81841400
H	0.53020900	1.42513900	3.54151600
H	-1.54559500	0.50946200	3.93786600
H	1.71297000	-0.75194800	-2.25189200
H	-0.10819200	-1.35605100	-3.48796300
C	0.00987600	3.39616900	2.86693500
C	0.45704500	6.16213600	2.83621800

C	0.76947300	4.00079900	3.87303100
C	-0.29933700	5.56450000	1.82676800
C	0.99065100	5.37674500	3.85788000
H	1.22620700	3.38226400	4.63932800
H	-0.71330400	6.16859200	1.02406400
H	1.59702400	5.83165000	4.63547600
H	0.63868800	7.23292100	2.81910800
H	4.73797000	-4.25802200	-1.86651900
C	3.82597400	-3.98739200	-1.34281200
C	1.50780900	-3.25069900	0.02520700
C	3.42356400	-4.70349500	-0.21392000
C	2.26430900	-4.33217600	0.46928800
C	1.90609400	-2.53015300	-1.10180300
H	4.01737600	-5.54320200	0.13669200
H	1.94176300	-4.87808000	1.35073700
H	0.62001100	-2.95575000	0.56656500
C	1.19225100	1.41520000	-3.89436900
C	0.15110900	1.61005800	-3.00593100
C	-1.19719600	1.40219000	-3.38317500
C	-1.48128400	1.01933500	-4.73072200
C	-0.39522200	0.82437600	-5.61465200
C	0.91441100	1.00752500	-5.20948400
C	-2.28684400	1.54050100	-2.43680800
C	-2.86143100	0.83781600	-5.15694400
C	-3.90466800	1.05950700	-4.21510200
C	-3.57374800	1.40343200	-2.86754300
C	-5.25342200	0.90660000	-4.60840900
H	-6.03354100	1.08143200	-3.87162100
C	-5.57819800	0.53641300	-5.89787500
C	-4.55139400	0.30960800	-6.83291900
C	-3.22536200	0.45793300	-6.46852100
H	2.21182700	1.56410900	-3.55655200
H	0.39808000	1.91200900	-1.99643100
H	-0.58499100	0.52452300	-6.63860900
H	1.72550100	0.84504500	-5.91343900
H	-4.39233900	1.53302100	-2.16300300
H	-6.61748100	0.41880200	-6.19004100
H	-4.79966000	0.01636400	-7.84878300
H	-2.45965100	0.27715600	-7.21392700
C	3.06810100	-2.90442200	-1.78248000
H	3.39111500	-2.33026300	-2.64731300
C	-0.45811300	-3.28299200	-2.60908300
C	-1.24508600	-3.94905700	-1.66667500
C	0.14268200	-4.00929100	-3.64117600

C	-1.42369200	-5.32836800	-1.75040400
H	-1.71698300	-3.38995600	-0.87177800
C	-0.02915100	-5.39048300	-3.72144200
H	0.75421700	-3.49338500	-4.37770300
C	-0.81261900	-6.05325700	-2.77432400
H	-2.03399000	-5.83009900	-1.00576100
H	0.44551000	-5.94779200	-4.52408100
H	-0.94710300	-7.12949300	-2.83713900
C	-0.52114700	4.18842300	1.84376100
H	-1.10613100	3.73050500	1.05274300
C	-2.42865000	2.44960800	4.19742200
C	-2.23939300	2.48928000	5.58227100
C	-3.27960600	3.37826000	3.59249700
C	-2.88315400	3.45571300	6.35371700
H	-1.58044000	1.76542500	6.05562400
C	-3.93192500	4.33744800	4.36552000
H	-3.43211000	3.34374000	2.51956500
C	-3.73182000	4.38244400	5.74620800
H	-2.72611500	3.48062200	7.42811600
H	-4.59427200	5.05371200	3.88770800
H	-4.23742800	5.13357200	6.34616900
C	-0.61855500	-5.08626400	3.17808500
C	-0.78075200	-3.78806500	2.73515500
C	-1.89518100	-3.43521200	1.93845100
C	-2.86859400	-4.41465700	1.60253700
C	-2.67271700	-5.73413700	2.07126300
C	-1.57086000	-6.06529600	2.83917800
C	-2.01857000	-2.10032900	1.42894800
C	-4.00592600	-4.01471400	0.78848300
C	-4.09624800	-2.67216600	0.30741700
C	-3.04832500	-1.71728300	0.61839000
C	-5.21633800	-2.30999100	-0.47907900
H	-5.31178600	-1.29290000	-0.84028700
C	-6.20581400	-3.22063500	-0.79492800
C	-6.11089600	-4.54233300	-0.33076600
C	-5.03259300	-4.92287600	0.44476100
H	-1.21001600	-1.42422300	1.68839600
H	0.24246500	-5.34946600	3.78587300
H	-0.04738000	-3.02191200	2.96989900
H	-3.38966600	-6.51025900	1.82833000
H	-1.44352700	-7.08827300	3.18202000
H	-7.05339400	-2.91286200	-1.40033100
H	-6.88359100	-5.26500200	-0.57641300
H	-4.98413500	-5.94503000	0.80169700

Ni	1.62114100	0.54755700	0.79484600
Cl	1.49294500	-0.97453400	2.62095100
C	3.20122100	0.35665800	-0.24841100
O	3.07727500	1.01341400	-1.27496300
C	4.39954200	-0.47740800	0.01409300
C	5.52161500	-0.28720800	-0.81086800
C	4.42563800	-1.45223500	1.01673100
C	6.65888100	-1.06675600	-0.62905200
H	5.47860400	0.47153300	-1.58550500
C	5.56187700	-2.23991300	1.18288500
H	3.55561800	-1.59314400	1.64531000
C	6.67731000	-2.04937700	0.36723000
H	7.52881000	-0.91484300	-1.26226000
H	5.57549900	-2.99940400	1.95809800
H	7.56429400	-2.66173100	0.50693900
C	2.98835700	3.14821300	0.86197700
C	2.74461600	1.92401900	1.70175000
H	3.80447600	3.00353800	0.14988700
H	2.07394600	3.41548400	0.31944700
H	2.10101800	2.17859100	2.53315400
F	3.32786900	4.22695900	1.68691800
O	3.97789800	1.46574200	2.24609900
C	4.03882800	1.27267600	3.58366000
O	3.14884100	1.56627300	4.36051100
C	5.33430500	0.66553400	3.98891900
C	6.36645800	0.42994700	3.07171300
C	5.50468200	0.32128000	5.33587900
C	7.55768500	-0.14951600	3.50338300
H	6.22859700	0.69111200	2.03015900
C	6.69580500	-0.25890400	5.76273800
H	4.68965500	0.51270600	6.02533800
C	7.72445600	-0.49491400	4.84602700
H	8.35174800	-0.33845100	2.78691400
H	6.82383200	-0.52935700	6.80703700
H	8.65409400	-0.94899200	5.17880600

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C	0.71917100	-1.46253000	0.23493700
C	0.95800200	-0.12346100	-0.42628700
N	-1.37838800	-0.68109000	1.34345500
N	0.22026800	0.92604300	-0.48086600
C	-0.34566800	-1.42731600	1.29881900
C	-2.22082200	-1.13500700	2.46989900
C	-1.22607700	-2.03467500	3.27334800

O	-0.21714900	-2.36394100	2.27034900
C	0.91286100	1.92718300	-1.33623800
C	2.18751200	1.14925200	-1.84484300
O	2.11804000	-0.09471900	-1.09176600
C	2.07006100	-1.96606600	0.80143300
H	2.68582100	-2.19070300	-0.06640400
H	1.88704300	-2.91112400	1.32344100
C	0.17313600	-2.48982100	-0.85588400
H	0.12016900	-3.45629800	-0.34436000
H	-0.84688500	-2.18762200	-1.09587600
H	-2.48695100	-0.26074700	3.06561800
H	-0.71706700	-1.41304200	4.01791600
H	0.26922000	2.12039900	-2.19640800
H	2.05501500	0.87572500	-2.89283100
C	-3.46988200	-1.83531900	1.97838300
C	-5.80601400	-3.12700900	1.11618200
C	-4.69692000	-1.56600500	2.59021400
C	-4.58284100	-3.40779500	0.50460000
C	-5.86062700	-2.20595100	2.16215700
H	-4.74355000	-0.83671300	3.39472800
H	-4.53577400	-4.10757700	-0.32437900
H	-6.80864600	-1.97446800	2.63878300
H	-6.71198300	-3.61489600	0.76886500
H	1.80846300	6.48710000	-1.41786500
C	1.72748200	5.58804600	-0.81384800
C	1.48199400	3.27896200	0.73048800
C	1.98841400	5.63539000	0.55793400
C	1.86054800	4.48012200	1.32815100
C	1.22332600	3.22641500	-0.63790300
H	2.28305000	6.57225000	1.02307800
H	2.05667000	4.50070600	2.39526600
H	1.36246600	2.39112600	1.33367100
C	-0.29688600	0.11392200	-4.31724400
C	-0.18119400	-0.78519300	-3.27300600
C	0.87419800	-1.72623500	-3.21843000
C	1.81882700	-1.76541900	-4.28952100
C	1.67702400	-0.82857900	-5.33977200
C	0.64925200	0.09787900	-5.35594300
C	1.03058700	-2.62360300	-2.08988400
C	2.89070400	-2.75026900	-4.27357300
C	2.96150100	-3.66631900	-3.18671600
C	2.01748300	-3.56542000	-2.11723900
C	3.98233400	-4.64321800	-3.15506600
H	4.01638500	-5.33299500	-2.31529100

C	4.92219900	-4.72029900	-4.16322100
C	4.86157200	-3.81381000	-5.23776500
C	3.86783900	-2.85290700	-5.28921700
H	-1.11397100	0.82857000	-4.31074300
H	-0.91787900	-0.74392100	-2.48456400
H	2.38728700	-0.83094400	-6.15845200
H	0.57267600	0.80439000	-6.17765500
H	2.12307800	-4.25698600	-1.28399000
H	5.70433400	-5.47297500	-4.12826600
H	5.59906100	-3.86724800	-6.03336500
H	3.84851300	-2.17079300	-6.13128000
C	1.34645500	4.38774100	-1.40704900
H	1.12936800	4.35300400	-2.47162600
C	3.52734000	1.79048300	-1.63614600
C	4.13633800	1.79610500	-0.37692900
C	4.15973100	2.42143500	-2.70946700
C	5.36198100	2.42962600	-0.19438100
H	3.65604000	1.30050800	0.45551100
C	5.38280000	3.06759300	-2.52511700
H	3.69306200	2.40540600	-3.69176500
C	5.98553600	3.07222000	-1.26654000
H	5.82337800	2.42027700	0.78835800
H	5.86695900	3.55832000	-3.36478900
H	6.94038600	3.57034900	-1.12301400
C	-3.42328800	-2.76785600	0.93572100
H	-2.48240700	-2.97584100	0.43951900
C	-1.79479400	-3.26702200	3.90888800
C	-2.42126200	-3.14673900	5.15356900
C	-1.77796000	-4.50667700	3.26510300
C	-3.03697900	-4.24985300	5.74250200
H	-2.43025500	-2.18437000	5.65991300
C	-2.38488900	-5.61263200	3.85921400
H	-1.28424500	-4.60089600	2.30464100
C	-3.01981300	-5.48684900	5.09556900
H	-3.52364000	-4.14479000	6.70782900
H	-2.36422500	-6.57363900	3.35311200
H	-3.49498800	-6.34878700	5.55500300
C	2.81542600	2.87097000	4.67628100
C	2.15034400	1.92250800	3.92405300
C	2.87238100	0.93211000	3.21797600
C	4.29147300	0.90129000	3.28212700
C	4.94165700	1.88969000	4.05658500
C	4.22155200	2.85350100	4.73897000
C	2.17352000	-0.02426000	2.41152900

C	4.99801900	-0.13695000	2.54765800
C	4.26172800	-1.08670500	1.77285000
C	2.81446600	-0.99643000	1.69835000
C	4.97940200	-2.08845300	1.07560900
H	4.44281500	-2.82797800	0.49368600
C	6.35853000	-2.15418900	1.11458200
C	7.08106400	-1.21176600	1.86321900
C	6.40802800	-0.22974600	2.56418900
H	1.09613800	0.09866900	2.37067500
H	2.25426600	3.63038500	5.21333000
H	1.06723700	1.93845300	3.83589600
H	6.02340300	1.90218600	4.12723600
H	4.74777800	3.60093400	5.32610400
H	6.87968400	-2.93182900	0.56388700
H	8.16596500	-1.25345400	1.89478000
H	6.98414800	0.48380100	3.14170700
Ni	-1.71036800	1.08902100	0.20710700
Cl	-1.22482500	2.05082200	2.46753600
C	-2.10275600	2.44988300	-1.16115500
O	-2.35300900	1.98424500	-2.25680800
C	-1.98731300	3.92793400	-0.97875800
C	-2.21370900	4.73322200	-2.11033400
C	-1.64141600	4.52399300	0.23850200
C	-2.09671600	6.11476700	-2.01970800
H	-2.47982700	4.25251600	-3.04560900
C	-1.52604300	5.91008900	0.32300300
H	-1.44155700	3.90377100	1.10365300
C	-1.75175200	6.70619600	-0.79954600
H	-2.27419300	6.73339500	-2.89529100
H	-1.24148000	6.36336000	1.26734000
H	-1.65553000	7.78650200	-0.72927200
C	-3.65575300	1.22436700	0.54213500
H	-3.73223000	0.64646800	1.46205600
C	-4.36613700	2.52542800	0.74865000
H	-4.52279700	3.06817700	-0.18821400
H	-3.78830600	3.13713100	1.44532700
F	-5.63145500	2.29198500	1.31221100
O	-4.40274200	0.47471200	-0.46662400
C	-3.73957400	-0.40134900	-1.19996000
O	-2.51349500	-0.53374500	-1.15578200
C	-4.59800000	-1.23673500	-2.06791900
C	-3.98885300	-2.06448600	-3.01935100
C	-5.98956400	-1.25107900	-1.90920500
C	-4.76959700	-2.90471000	-3.80854900

H	-2.91076900	-2.03602900	-3.13360100
C	-6.76543200	-2.09670900	-2.69817500
H	-6.44309900	-0.61627200	-1.15733400
C	-6.15761300	-2.92421200	-3.64583300
H	-4.29827300	-3.54321400	-4.54995100
H	-7.84399700	-2.11409500	-2.57205900
H	-6.76563000	-3.58364400	-4.25900400

IM4^{doublet}

C	-0.35470000	0.54895900	1.37980700
C	-0.72749300	1.07878000	0.01048000
Ni	-0.14480900	-1.37605000	-1.44844700
N	0.75860500	-1.42564900	0.30684900
N	-0.58756400	0.51586700	-1.13549800
C	0.50899300	-0.68811100	1.31594100
C	1.59109600	-2.56456500	0.73257500
C	1.87257000	-2.24294900	2.25478200
O	1.04915000	-1.06133500	2.50372900
C	-0.98496200	1.47726600	-2.18338100
C	-1.27877400	2.79481200	-1.36474300
O	-1.23578900	2.33001000	0.02516000
C	-1.67398300	0.23822700	2.19536600
H	-2.09114700	1.20778100	2.48035200
H	-1.36704500	-0.26060000	3.11892600
C	0.40885100	1.64386900	2.18329600
H	-0.22940700	2.53282500	2.21544700
H	0.47721500	1.26566700	3.20626600
H	0.95377300	-3.44973800	0.65898200
H	1.45684200	-3.03895600	2.87855900
H	-0.10313500	1.65646000	-2.80685000
H	-0.42807600	3.47498400	-1.46473100
C	2.78795400	-2.75640800	-0.16277700
C	5.02322300	-3.15469900	-1.79962400
C	3.67845200	-1.70635300	-0.41053500
C	4.13105800	-4.20131000	-1.56785200
C	4.79153600	-1.90343300	-1.22210200
H	3.50987000	-0.73767400	0.04220900
H	4.29290800	-5.17071100	-2.03031000
H	5.47453400	-1.07810100	-1.39928800
H	5.89171000	-3.30978300	-2.43402300
H	-4.52209100	-1.39090700	-3.29631000
C	-3.92373000	-0.53094500	-3.57374400
C	-2.35663000	1.66241700	-4.26717900
C	-4.19472900	0.17200900	-4.74596700

C	-3.40604400	1.27180100	-5.09394300
C	-2.09369000	0.97200800	-3.07786900
H	-5.01097400	-0.13872500	-5.39218300
H	-3.60532200	1.82086700	-6.00992600
H	-1.74757800	2.52231500	-4.53618500
C	3.08840500	3.72345100	4.81385200
C	2.24190000	3.10005000	3.91714500
C	2.68087600	2.70920600	2.62946700
C	4.03122200	2.99133400	2.25333300
C	4.87272800	3.62546100	3.19516700
C	4.41964200	3.98266600	4.45124000
C	1.79808000	2.01706500	1.70682500
C	4.50525100	2.62103200	0.92878500
C	3.59511200	1.99663600	0.03533800
C	2.26085500	1.70290400	0.46275600
C	4.01738400	1.63199600	-1.26360700
H	3.30825300	1.13817500	-1.92265600
C	5.31260500	1.87199200	-1.67782900
C	6.22190500	2.48409600	-0.79472300
C	5.82532700	2.84930700	0.47916800
H	2.72289200	4.01060400	5.79532500
H	1.21579500	2.91482700	4.21217600
H	5.90083300	3.84518600	2.93177400
H	5.09266100	4.46778800	5.15204300
H	1.64067500	1.17389000	-0.24888600
H	5.62958700	1.58505400	-2.67609300
H	7.24336400	2.67048500	-1.11344700
H	6.55071000	3.31681600	1.13502400
C	-2.88027600	-0.12988500	-2.73840500
H	-2.67688700	-0.68432400	-1.83037500
C	-2.54857700	3.54014600	-1.64523300
C	-2.48104200	4.85483200	-2.11288900
C	-3.80060400	2.93086300	-1.49493200
C	-3.64550600	5.55401600	-2.43686300
H	-1.51162000	5.33381300	-2.22830600
C	-4.96172700	3.62636200	-1.81557100
H	-3.86187300	1.90421200	-1.16148900
C	-4.88815100	4.93957300	-2.28893400
H	-3.57957100	6.57489600	-2.80173300
H	-5.92502100	3.13506900	-1.71473200
H	-5.79611100	5.47829600	-2.54475800
C	3.01490600	-3.99964600	-0.75449000
H	2.30015600	-4.80292300	-0.60139200
C	3.30622500	-1.97761800	2.63919400

C	4.20555800	-3.05007900	2.66007700
C	3.76984500	-0.69129800	2.91851100
C	5.55411000	-2.83209700	2.93006600
H	3.85565000	-4.05355500	2.43235400
C	5.12079200	-0.47209800	3.19083700
H	3.08035900	0.14031400	2.91483300
C	6.01723500	-1.53986100	3.19172600
H	6.24508600	-3.67015900	2.92980900
H	5.46301400	0.53792900	3.39646500
H	7.07054200	-1.37020800	3.39652700
C	-6.84176100	-0.32905700	-1.17954000
C	-5.88805700	0.26389300	-0.37697600
C	-4.79037700	-0.47704300	0.11679300
C	-4.66892900	-1.85927000	-0.20004400
C	-5.66279600	-2.43935500	-1.02139900
C	-6.72400500	-1.69340600	-1.50290000
C	-3.78183100	0.15220800	0.91199700
C	-3.55935500	-2.61293300	0.36220500
C	-2.63951600	-1.96607800	1.24275100
C	-2.73103100	-0.53606400	1.44665500
C	-1.66965500	-2.75217300	1.90641400
H	-1.01866800	-2.28957300	2.63731000
C	-1.53935900	-4.10244400	1.64976500
C	-2.37521200	-4.71696500	0.70336000
C	-3.37150000	-3.98583900	0.08864900
H	-3.85771700	1.22393200	1.07682100
H	-7.67954700	0.25027800	-1.55624300
H	-5.96893500	1.31352300	-0.10782600
H	-5.60578500	-3.49029000	-1.27935200
H	-7.47181000	-2.16726800	-2.13215400
H	-0.78950800	-4.68653700	2.17659900
H	-2.24836400	-5.76745500	0.46201300
H	-4.01486200	-4.48447800	-0.62581700
Cl	-0.38138900	-3.28580600	-2.47859200

IM5^{doublet}

C	-2.08813000	1.30102100	-0.05671000
C	-1.58847400	-0.11456900	-0.26306700
N	0.16393000	2.15859400	0.64522600
N	-0.38928100	-0.55796500	-0.32146700
C	-1.10846200	2.22984000	0.61660400
C	0.67377700	3.26912400	1.47143100
C	-0.58222500	4.20293700	1.59683800
O	-1.67614700	3.30904100	1.19437900

C	-0.42530500	-1.97143800	-0.75059300
C	-1.96866800	-2.28074400	-0.82742500
O	-2.57349800	-0.99654500	-0.49543500
C	-3.40396900	1.23175600	0.75500700
H	-4.12931300	0.72134200	0.12135600
H	-3.76819200	2.25259300	0.90742400
C	-2.31444600	1.96626800	-1.48562400
H	-2.76948800	2.94159200	-1.28996700
H	-1.32070800	2.13840700	-1.90479500
H	0.90237100	2.83855800	2.45225300
H	-0.77221400	4.46466700	2.63834400
H	-0.02723100	-1.99693200	-1.76585900
H	-2.24663100	-2.48490700	-1.86335000
C	1.91875500	3.93767300	0.94506900
C	4.19241500	5.30446100	0.04716100
C	2.32834700	3.81466300	-0.38569500
C	3.78179500	5.42868000	1.37651800
C	3.46825800	4.49227800	-0.82488500
H	1.78493000	3.16825300	-1.06956000
H	4.34414700	6.05111500	2.06708200
H	3.78601700	4.38044300	-1.85788700
H	5.07589200	5.83215600	-0.30160600
H	1.23714100	-3.40880900	3.37114500
C	1.21479000	-3.55706800	2.29567100
C	1.14841000	-3.90301400	-0.46629100
C	1.96050400	-4.57870300	1.70345100
C	1.92359800	-4.75425300	0.31948000
C	0.40531100	-2.87465300	0.12132100
H	2.57449900	-5.23162600	2.31750400
H	2.51497200	-5.53514700	-0.14937300
H	1.13792100	-4.01901500	-1.54742600
C	-0.70737600	-1.05519000	-4.17973200
C	-1.22654000	-0.03572700	-3.40105200
C	-2.62672200	0.13984700	-3.27066500
C	-3.50700000	-0.72954300	-3.98826600
C	-2.93903300	-1.76684900	-4.76266600
C	-1.56942200	-1.93610500	-4.85339500
C	-3.18828100	1.16566000	-2.41326500
C	-4.94734800	-0.53208200	-3.90928600
C	-5.45059900	0.54169400	-3.12286500
C	-4.53830700	1.36006800	-2.38680500
C	-6.84381600	0.76687500	-3.04675500
H	-7.20426800	1.59428300	-2.44033700
C	-7.73220500	-0.04677000	-3.72072500

C	-7.24221800	-1.11498800	-4.49466200
C	-5.88198200	-1.34906900	-4.58520100
H	0.36930100	-1.16658900	-4.25056100
H	-0.52151900	0.60900200	-2.88472300
H	-3.58473200	-2.44710400	-5.30593700
H	-1.16445900	-2.74289200	-5.45821900
H	-4.95447600	2.14818900	-1.76293400
H	-8.80119300	0.13332100	-3.65415200
H	-7.93513800	-1.76084900	-5.02626100
H	-5.53861200	-2.17903400	-5.19191400
C	0.44000600	-2.71047000	1.50813800
H	-0.12290500	-1.91041500	1.96981400
C	-2.47562100	-3.36256400	0.08360200
C	-2.90285900	-3.08647000	1.38397600
C	-2.44300800	-4.68714900	-0.36303600
C	-3.28646600	-4.12352500	2.23248000
H	-2.93889900	-2.06355700	1.72885800
C	-2.81873400	-5.72581100	0.48731700
H	-2.11343500	-4.90596700	-1.37599300
C	-3.24066900	-5.44566600	1.78872400
H	-3.61128300	-3.89038700	3.24182100
H	-2.78568200	-6.75221700	0.13293400
H	-3.53456000	-6.25498000	2.45127000
C	2.65453200	4.74229600	1.82207100
H	2.34499300	4.82792300	2.86156500
C	-0.59282600	5.43703500	0.73908800
C	-0.59481400	5.34646300	-0.65883100
C	-0.56251700	6.69623100	1.34135500
C	-0.57131100	6.50085300	-1.43638900
H	-0.59689700	4.37490600	-1.14059800
C	-0.53082200	7.85473000	0.56346100
H	-0.55987700	6.77122200	2.42607000
C	-0.53751400	7.75826500	-0.82736600
H	-0.56904600	6.41924900	-2.51942400
H	-0.50562500	8.82835200	1.04429600
H	-0.51480800	8.65743500	-1.43637400
C	-0.54406200	-1.64198500	5.49551100
C	-0.68619500	-0.81672300	4.39712500
C	-1.96838800	-0.55219200	3.86122200
C	-3.12504600	-1.12375700	4.45548000
C	-2.94531800	-1.96147500	5.58015400
C	-1.68396500	-2.21799700	6.08766900
C	-2.09591200	0.25061400	2.68312400
C	-4.42308400	-0.83359500	3.86516300

C	-4.50416800	-0.02902700	2.68584600
C	-3.29537900	0.49214700	2.07628700
C	-5.77894700	0.22961000	2.12820400
H	-5.85883100	0.84593600	1.24046100
C	-6.93246700	-0.28089000	2.69131800
C	-6.85213600	-1.07686200	3.84540800
C	-5.62140000	-1.34201600	4.41491400
H	-1.16332500	0.61017600	2.26616300
H	0.44321100	-1.84593900	5.89991100
H	0.18262100	-0.37562500	3.91430500
H	-3.80230000	-2.42173800	6.05902900
H	-1.57543900	-2.87014700	6.94967400
H	-7.89718500	-0.06669300	2.24081400
H	-7.75461900	-1.48326600	4.29266100
H	-5.58277000	-1.95254800	5.30969600
Ni	1.31367200	0.57834700	-0.15006600
Cl	2.08834200	0.28787200	2.01108000
C	2.59494900	-1.06712800	-1.29874200
O	2.14066500	-1.13586700	-2.40021400
C	3.73003700	-1.87279600	-0.79732900
C	4.38717200	-2.69430600	-1.73654200
C	4.11005600	-1.89356100	0.54682800
C	5.41620400	-3.52765700	-1.32196000
H	4.07182100	-2.66777300	-2.77407900
C	5.14121400	-2.74032700	0.95278900
H	3.58709200	-1.26698500	1.25783500
C	5.79258200	-3.55354500	0.02689200
H	5.92556000	-4.16004500	-2.04347800
H	5.42989500	-2.76397100	1.99917500
H	6.59519200	-4.21086500	0.35026800
F	1.16421200	1.38433300	-1.84435900

TS1^{css}

C	-0.41451400	1.06618700	-0.80143200
C	-1.75359600	0.53906800	-1.25233200
N	-0.01751200	-1.06919500	0.49047700
N	-2.42163200	-0.40760800	-0.71302800
C	0.39223900	0.01644300	-0.06499800
C	1.16607300	-1.76917800	1.04274700
C	2.21551400	-0.61552300	1.08761900
O	1.69812100	0.30315200	0.06085100
C	-3.78135300	-0.43520300	-1.29704100
C	-3.63723700	0.55965100	-2.50299300
O	-2.36939200	1.23539800	-2.23481300

C	-0.77505300	2.27457500	0.17504200
H	-1.64500100	1.98014700	0.76561700
H	-1.08991100	3.09999700	-0.47059500
C	0.42004100	1.60592200	-2.00077700
H	-0.24977400	2.21752300	-2.61186600
H	1.16796400	2.27335100	-1.58406400
H	0.94042400	-2.08247900	2.06265800
H	2.09515400	-0.08449200	2.03143200
H	-3.97221300	-1.44617200	-1.66250500
H	-3.47397700	-0.01862700	-3.41978700
C	1.55912700	-2.96706400	0.21138100
C	2.49737100	-5.11125600	-1.32266900
C	2.41140000	-3.92146700	0.77728000
C	1.63600100	-4.17058800	-1.88675100
C	2.88073200	-4.98818500	0.01464400
H	2.72094100	-3.81555800	1.81402500
H	1.31876200	-4.26518700	-2.91958000
H	3.54484600	-5.72179300	0.46310400
H	2.86100200	-5.94381200	-1.91866200
H	-7.36234900	-1.52007900	1.48648600
C	-6.64460100	-0.76483100	1.18087200
C	-4.76632000	1.14784600	0.41556400
C	-6.61996900	0.47754700	1.81252100
C	-5.67654900	1.43481400	1.42847300
C	-4.79408100	-0.09471300	-0.22976200
H	-7.32767600	0.70001300	2.60600500
H	-5.65165700	2.40394800	1.91869700
H	-4.04005800	1.89801500	0.11809700
C	4.75544100	1.25333300	-2.53875900
C	3.38920600	1.33609400	-2.36715400
C	2.50309800	0.42478100	-2.99275800
C	3.06024000	-0.62187700	-3.79477600
C	4.46463700	-0.67394200	-3.95493700
C	5.29929800	0.24439600	-3.34987800
C	1.06304100	0.52556400	-2.85059600
C	2.18852400	-1.60659600	-4.41547500
C	0.78289100	-1.46633100	-4.25992800
C	0.26572300	-0.37721900	-3.49380900
C	-0.08977000	-2.41455900	-4.84056400
H	-1.16041500	-2.29501600	-4.69559700
C	0.40389000	-3.48269900	-5.56211800
C	1.79533300	-3.62671500	-5.72192500
C	2.66474000	-2.70968100	-5.16009600
H	5.40656700	1.96052200	-2.03419900

H	3.00261700	2.10461500	-1.71071300
H	4.90405900	-1.44916400	-4.57147000
H	6.37390300	0.17631500	-3.49135000
H	-0.81380100	-0.28776100	-3.43186000
H	-0.27378200	-4.21168800	-5.99591800
H	2.19077000	-4.46869400	-6.28252400
H	3.73018400	-2.85979500	-5.28865500
C	-5.73230400	-1.04915300	0.16374300
H	-5.72899100	-2.02903500	-0.30533300
C	-4.74422000	1.55668400	-2.71082500
C	-4.53382000	2.93247700	-2.60433500
C	-6.02615900	1.07674600	-3.00369900
C	-5.59778700	3.81969200	-2.77840500
H	-3.54041900	3.30571000	-2.38272600
C	-7.08662400	1.96240600	-3.17532600
H	-6.19873900	0.00636300	-3.07970800
C	-6.87541500	3.33861200	-3.06114600
H	-5.42463900	4.88859500	-2.69160000
H	-8.07871500	1.57835700	-3.39352700
H	-7.70273300	4.02972200	-3.19300700
C	1.16701100	-3.10452300	-1.12041200
H	0.48489600	-2.38761300	-1.55794600
C	3.66157900	-0.92424000	0.87347500
C	4.15713700	-1.38521400	-0.35143000
C	4.53272000	-0.78381600	1.95896400
C	5.50443400	-1.71018500	-0.47925200
H	3.49225200	-1.49377500	-1.19816500
C	5.88161200	-1.11660900	1.83231800
H	4.14695700	-0.41246300	2.90527300
C	6.36876300	-1.58212600	0.61064600
H	5.87634600	-2.06305100	-1.43566300
H	6.54907800	-1.00689800	2.68243800
H	7.41882100	-1.84156600	0.50657200
C	4.48230600	5.30350200	1.43450900
C	3.29389900	5.00763800	0.79741000
C	2.41908400	4.02441100	1.31299100
C	2.75688700	3.33179200	2.50931300
C	3.98034300	3.65606200	3.13760200
C	4.82540600	4.61796700	2.61447100
C	1.21572200	3.68510700	0.61930200
C	1.83630100	2.32884200	3.02337500
C	0.63132200	2.03795000	2.31114500
C	0.36588400	2.71101100	1.05471100
C	-0.24826200	1.05791100	2.83293900

H	-1.16826300	0.81709200	2.31439500
C	0.05177900	0.35317400	3.98350700
C	1.24720300	0.62173700	4.66998400
C	2.10966100	1.59759300	4.20308300
H	1.00328100	4.20953100	-0.30965600
H	5.14974400	6.05777200	1.02833600
H	3.01518700	5.52385700	-0.11796100
H	4.27553800	3.14674300	4.04759800
H	5.76016400	4.84376600	3.11925500
H	-0.62509900	-0.41581000	4.34049200
H	1.49306600	0.06463500	5.56920300
H	3.01904300	1.79589100	4.75848800
Ni	-1.85064200	-1.57185200	0.75639800
Cl	-1.88747100	-4.44071900	0.38988500
C	-2.04515000	-2.72274400	2.12038900
O	-3.21641100	-2.29381100	2.07269500
C	-1.35446500	-3.27082200	3.29917000
C	-1.78290500	-2.84328700	4.56650900
C	-0.21228400	-4.07598300	3.18553000
C	-1.05776600	-3.19555600	5.70473000
H	-2.67616300	-2.23060600	4.64015700
C	0.50309100	-4.42713100	4.32751900
H	0.07117400	-4.43557400	2.20317400
C	0.09017500	-3.98251900	5.58764800
H	-1.39325600	-2.86188600	6.68311700
H	1.38264500	-5.05858900	4.23484400
H	0.65253800	-4.25995100	6.47511900

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C	0.35443800	-1.83582900	-0.55724700
C	0.56301000	-0.35290700	-0.75904600
N	-0.41024500	-1.39570400	1.79293600
N	0.48102700	0.62489900	0.07535200
C	-0.07539000	-2.18110600	0.83966600
C	-1.05283200	-2.22619200	2.84130700
C	-0.55192600	-3.65552800	2.47107600
O	-0.22526200	-3.50923000	1.05116900
C	0.77218900	1.87793600	-0.68037500
C	0.67380600	1.39981000	-2.16106700
O	0.89786400	-0.04137400	-2.02351300
C	1.66386500	-2.58775100	-0.95647400
H	1.70644800	-2.57246300	-2.04199100
H	1.53195800	-3.63148900	-0.65514900
C	-0.83174500	-2.41442000	-1.46154000

H	-0.67347300	-3.49513000	-1.47781700
H	-1.77246600	-2.25422300	-0.93316300
H	-0.66113900	-1.92115000	3.81052100
H	0.39836500	-3.84559900	2.98306300
H	-0.03205600	2.57964400	-0.46075100
H	-0.36107300	1.50403200	-2.48755500
C	-2.55798200	-2.07376300	2.82974800
C	-5.35470600	-1.87301700	2.88104700
C	-3.26101400	-2.27321900	4.02184300
C	-4.65836200	-1.65847400	1.69059500
C	-4.65105100	-2.17873000	4.04739700
H	-2.71430000	-2.47708100	4.93688900
H	-5.19320900	-1.40083500	0.78062900
H	-5.18225500	-2.32494800	4.98310000
H	-6.43755500	-1.78904300	2.90310500
H	3.53189400	5.59074000	-0.25908800
C	3.44299400	4.51156900	-0.17279700
C	3.19073100	1.74791700	0.08683200
C	4.54007100	3.74671400	0.22997100
C	4.41119500	2.36553600	0.35746400
C	2.09315600	2.50683300	-0.31671500
H	5.48461800	4.22964400	0.46304300
H	5.24824100	1.76677100	0.69754700
H	3.08178800	0.67995300	0.22317400
C	-3.04125200	1.18937900	-2.42117200
C	-2.38073400	0.00391600	-2.15834400
C	-1.65331800	-0.67903600	-3.16057800
C	-1.60239300	-0.12127000	-4.47384400
C	-2.29884000	1.08502400	-4.71555000
C	-3.00406300	1.73181300	-3.71583000
C	-0.91789400	-1.89222500	-2.86874700
C	-0.82770100	-0.78610700	-5.51106100
C	-0.18242900	-2.01634100	-5.20194200
C	-0.26030900	-2.53893900	-3.87262800
C	0.56199500	-2.68915700	-6.19705700
H	1.04459000	-3.62875700	-5.93960200
C	0.68594600	-2.16292200	-7.46748400
C	0.06269800	-0.93958800	-7.77491400
C	-0.67682000	-0.26951500	-6.81709000
H	-3.55752900	1.69539900	-1.61328200
H	-2.40260800	-0.37154400	-1.14465200
H	-2.28381500	1.52265500	-5.70695500
H	-3.52284500	2.66068400	-3.93466100
H	0.26242000	-3.46951900	-3.66317900

H	1.26438500	-2.68536900	-8.22373700
H	0.16350800	-0.51553600	-8.76973000
H	-1.13787200	0.67428900	-7.08417700
C	2.22717500	3.89243000	-0.44484500
H	1.36650100	4.48633000	-0.73989700
C	1.58155700	1.97958000	-3.20008300
C	1.03016500	2.80611200	-4.18388500
C	2.95559000	1.71548200	-3.21611900
C	1.84282500	3.38007100	-5.16219900
H	-0.04098700	2.98969100	-4.18603400
C	3.76452500	2.27747500	-4.19963800
H	3.39072100	1.07125800	-2.46565000
C	3.21266200	3.11563200	-5.17171600
H	1.40472100	4.02296300	-5.92055600
H	4.82832100	2.05844800	-4.20151100
H	3.84692300	3.55618700	-5.93610000
C	-3.26861500	-1.76201400	1.66773200
H	-2.73067800	-1.54897700	0.75381400
C	-1.50711300	-4.78686000	2.69600500
C	-2.49260500	-5.11196200	1.75872900
C	-1.46359100	-5.47129500	3.91396000
C	-3.42591900	-6.10677600	2.04197700
H	-2.52769500	-4.58189500	0.81383800
C	-2.40440200	-6.45998700	4.20162100
H	-0.69547200	-5.22303200	4.64265900
C	-3.38826500	-6.77939600	3.26528200
H	-4.18827000	-6.35303800	1.30848700
H	-2.36438900	-6.98276800	5.15281900
H	-4.12018100	-7.55109600	3.48569200
C	5.32001400	-0.84834600	3.74517200
C	4.20689300	-1.33959800	3.09365000
C	4.18306400	-1.43261700	1.68278500
C	5.29821600	-0.99738000	0.91633100
C	6.42703800	-0.50894700	1.61481500
C	6.43963500	-0.43795000	2.99608000
C	3.03515700	-1.95771500	1.01611400
C	5.21024200	-1.04791100	-0.53506700
C	4.02487500	-1.54869000	-1.16495900
C	2.92801900	-2.02370700	-0.34380100
C	3.96468500	-1.55252100	-2.58026700
H	3.06728300	-1.88631800	-3.08516300
C	5.01330800	-1.09303400	-3.35243400
C	6.17345000	-0.59976900	-2.73422600
C	6.26057800	-0.57814600	-1.35556300

H	2.22726100	-2.30914100	1.64840900
H	5.32724800	-0.76804500	4.82786700
H	3.31831700	-1.62346500	3.65045600
H	7.30433800	-0.17929200	1.07005800
H	7.31987700	-0.05549200	3.50488400
H	4.92641800	-1.09398700	-4.43462000
H	6.99900500	-0.22949400	-3.33516200
H	7.15889700	-0.18046300	-0.89850700
Ni	0.29528800	0.51512500	2.05202900
Cl	0.74596100	0.03719500	4.19573100
C	0.74279600	2.34800900	2.29759900
O	-0.09645800	3.14820900	1.89294000
C	1.98857300	2.88938000	2.94715300
C	2.09315300	4.27626200	3.13228700
C	3.05567700	2.07082700	3.32601700
C	3.22781300	4.82973000	3.71779900
H	1.26856900	4.90079800	2.80485700
C	4.19611800	2.62272200	3.90519000
H	2.98937900	1.00434700	3.16567400
C	4.28224300	4.00026600	4.11092500
H	3.29668400	5.90535900	3.86057500
H	5.01854600	1.97281500	4.18817300
H	5.17039600	4.42917600	4.56840700
C	-2.86470100	1.91922600	1.82204800
C	-2.29897300	1.23985700	3.01096600
H	-3.96468500	1.95352000	1.84112100
H	-2.45197800	2.92421300	1.73515700
H	-2.62810900	0.26330700	3.32871900
F	-2.53605000	1.20466600	0.64642500
O	-1.90791800	2.08644900	4.00801100
C	-1.83155700	1.58140800	5.28672900
O	-2.39943300	0.56405000	5.62379500
C	-1.00434500	2.44349800	6.15711500
C	-0.24343700	3.50020500	5.64071800
C	-0.94800700	2.14030000	7.52345300
C	0.57556100	4.24151000	6.48806400
H	-0.27805900	3.71420100	4.58107500
C	-0.13925400	2.89347500	8.36911800
H	-1.53405100	1.30709300	7.89622900
C	0.62622500	3.94260600	7.85134400
H	1.19018400	5.03593500	6.07633100
H	-0.09561400	2.65865600	9.42895600
H	1.26848300	4.52103900	8.51018300

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C	0.84057200	-1.56111700	0.37908500
C	1.02149900	-0.24865300	-0.33959700
N	-0.96713000	-0.56264900	1.81341400
N	0.23061800	0.75948800	-0.38373700
C	-0.09104600	-1.46048700	1.55858600
C	-1.69524000	-0.98123600	3.04703600
C	-0.75866500	-2.09711400	3.60679400
O	0.02371900	-2.48078800	2.43601600
C	0.80867100	1.76244500	-1.31247300
C	2.12628500	1.06578700	-1.82034000
O	2.14120400	-0.18544600	-1.07343700
C	2.23090100	-2.07725600	0.82729400
H	2.78200200	-2.28863400	-0.08817300
H	2.08767000	-3.03085400	1.34575900
C	0.15479400	-2.59968600	-0.61303500
H	0.11758800	-3.54783600	-0.06798500
H	-0.87536300	-2.27394900	-0.77163800
H	-1.72498300	-0.12510200	3.71845000
H	-0.03982700	-1.64455600	4.30095500
H	0.11748200	1.85522500	-2.14869900
H	2.00818300	0.78800900	-2.86951500
C	-3.10713500	-1.41541600	2.73391800
C	-5.73634700	-2.16733400	2.13439000
C	-4.18497100	-0.75748400	3.33480500
C	-4.66468100	-2.83738900	1.54283600
C	-5.49496900	-1.12631100	3.03188500
H	-3.99188200	0.07747600	4.00007000
H	-4.84489600	-3.63799000	0.83164200
H	-6.32514400	-0.58148800	3.46930500
H	-6.75658900	-2.44194500	1.88348500
H	0.69939900	6.41928200	-1.39994600
C	0.92075600	5.52506100	-0.82491900
C	1.43929700	3.22149800	0.65530400
C	1.37576900	5.63057200	0.48983600
C	1.63421500	4.47452200	1.23024700
C	0.98414900	3.10927800	-0.66144700
H	1.52268000	6.60920900	0.93812100
H	1.99415700	4.54179900	2.25232500
H	1.64421900	2.32693000	1.22954000
C	-0.49947700	-0.05828900	-4.09572900
C	-0.32433500	-0.92594300	-3.03390700
C	0.67959400	-1.92130200	-3.04799100
C	1.50803700	-2.04836100	-4.20613900

C	1.30709400	-1.14361400	-5.27370200
C	0.33094800	-0.16400700	-5.22249300
C	0.89533000	-2.79803400	-1.91258100
C	2.52270000	-3.09070400	-4.25987400
C	2.65886900	-3.97215000	-3.15088300
C	1.83038200	-3.78812700	-1.99980100
C	3.62695700	-5.00135500	-3.18410100
H	3.71202700	-5.66311900	-2.32552500
C	4.45145300	-5.16541600	-4.27910500
C	4.32496700	-4.29504300	-5.37755100
C	3.38201800	-3.28302400	-5.36532700
H	-1.28845000	0.68414600	-4.04644300
H	-0.98142500	-0.82980900	-2.18282700
H	1.92582500	-1.21507500	-6.16081400
H	0.20021500	0.51227200	-6.06260100
H	1.97878400	-4.46128600	-1.15792600
H	5.19304200	-5.95874400	-4.29430200
H	4.97107800	-4.41709500	-6.24211200
H	3.31017100	-2.63049900	-6.22777900
C	0.72523700	4.26795700	-1.39581400
H	0.34575500	4.18440000	-2.41082400
C	3.41078100	1.81689200	-1.61032000
C	4.16651500	1.66145900	-0.44617700
C	3.81893200	2.74060900	-2.57688200
C	5.31509300	2.42495000	-0.24678100
H	3.85893300	0.94066700	0.29743000
C	4.96291600	3.51132400	-2.37438500
H	3.23533100	2.86198700	-3.48641500
C	5.71385900	3.35532300	-1.20733800
H	5.88959500	2.29161800	0.66493700
H	5.26992100	4.22980700	-3.12914500
H	6.60646700	3.95447500	-1.05076200
C	-3.35675300	-2.45972900	1.83815200
H	-2.53160400	-2.96121700	1.34564800
C	-1.41451700	-3.29035900	4.24051700
C	-2.10805100	-3.10652300	5.44202700
C	-1.37588000	-4.55751100	3.65662500
C	-2.76569100	-4.17554800	6.04537600
H	-2.14427600	-2.12079500	5.89910600
C	-2.03130900	-5.62943200	4.26454600
H	-0.83551400	-4.70051400	2.72783500
C	-2.72968100	-5.44180000	5.45672700
H	-3.30814400	-4.02006600	6.97335200
H	-1.99707800	-6.61169200	3.80180100

H	-3.24292500	-6.27586100	5.92640000
C	3.31729200	2.89940100	4.43734200
C	2.58821600	1.93292600	3.77314900
C	3.23961500	0.86786800	3.10862900
C	4.65662600	0.77455200	3.13101100
C	5.37531800	1.78057600	3.81662100
C	4.72275600	2.82118900	4.45300600
C	2.47553700	-0.09405800	2.37525700
C	5.28869800	-0.34122600	2.44260500
C	4.48494800	-1.28694500	1.73229900
C	3.04379500	-1.12424600	1.68289900
C	5.12702100	-2.36287800	1.07402200
H	4.53337600	-3.09505400	0.53961900
C	6.50029300	-2.50958000	1.09741800
C	7.29010900	-1.57554800	1.78688200
C	6.69064000	-0.51804300	2.44394200
H	1.40609700	0.07183400	2.35894000
H	2.80996600	3.71533600	4.94368700
H	1.50235600	1.98530300	3.73977000
H	6.45841200	1.74900400	3.84909700
H	5.30113900	3.58185100	4.96924900
H	6.96547000	-3.34455700	0.58188800
H	8.37064700	-1.68295000	1.80722700
H	7.31894300	0.18590400	2.97720600
Ni	-1.37339500	1.13613100	0.71535400
Cl	-2.34215800	2.10312000	2.49320400
C	-2.08991200	2.24852500	-0.64451000
O	-2.16381000	1.69760900	-1.74432400
C	-2.59789200	3.64999600	-0.51786100
C	-3.57331200	4.09026100	-1.42645300
C	-2.09568400	4.53709400	0.43944900
C	-4.06103000	5.39235900	-1.35970100
H	-3.93406600	3.39299100	-2.17603100
C	-2.56252200	5.84932800	0.48528000
H	-1.33453900	4.19812100	1.12872700
C	-3.55211600	6.27590700	-0.40269000
H	-4.82987600	5.72289800	-2.05321900
H	-2.15549800	6.53805500	1.22023600
H	-3.92623600	7.29519700	-0.35195900
C	-4.35412100	0.51896600	0.13525900
H	-3.84293200	-0.21243100	0.73663400
C	-5.29399800	1.51930800	0.66703700
H	-5.45208700	2.33459300	-0.04608600
H	-4.90238400	1.91530700	1.60513800

F	-6.55859800	0.93321200	0.92457300
O	-4.47978600	0.23969900	-1.19442500
C	-3.68868300	-0.72988500	-1.72797200
O	-2.98236700	-1.45712400	-1.04935000
C	-3.79789800	-0.79326900	-3.19945900
C	-3.29720600	-1.92751600	-3.85158200
C	-4.31555600	0.27287800	-3.94750200
C	-3.31472900	-1.99832700	-5.24088600
H	-2.88311800	-2.73271100	-3.25523500
C	-4.31922700	0.20314000	-5.33839500
H	-4.68654900	1.15079700	-3.43328700
C	-3.82035200	-0.93061000	-5.98603100
H	-2.92087100	-2.87669400	-5.74326400
H	-4.70767800	1.03471600	-5.91918100
H	-3.82350700	-0.97999600	-7.07139000

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C	-1.87417000	0.34946100	0.04047300
C	-0.82665000	-0.44760400	-0.70984300
N	-0.19389300	1.25675400	1.64517300
N	0.44134500	-0.50075100	-0.53340800
C	-1.38641900	0.89998200	1.35706400
C	-0.20139900	1.93429400	2.95471100
C	-1.67061200	1.68723900	3.45655200
O	-2.34643100	1.17400600	2.26004500
C	1.03898500	-1.28362100	-1.63924900
C	-0.22140800	-1.72302900	-2.48554800
O	-1.33165100	-1.13402900	-1.74307300
C	-3.14680700	-0.51619400	0.19385800
H	-3.55670300	-0.60932300	-0.81152400
H	-3.87167300	0.05210700	0.78682200
C	-2.24071500	1.66024200	-0.79564500
H	-3.12091800	2.08443800	-0.30323700
H	-1.42492100	2.37184100	-0.66000100
H	0.50240900	1.41515900	3.60932300
H	-1.67262200	0.86362700	4.17559200
H	1.62639200	-0.57892900	-2.23252000
H	-0.20621300	-1.21886800	-3.45382400
C	0.23061000	3.37909200	2.81821600
C	1.08610100	6.04055500	2.61145700
C	0.84801600	4.01080700	3.90253800
C	0.47280100	5.41702300	1.52502600
C	1.26845900	5.33464300	3.80134200
H	1.03390900	3.44809900	4.81055900

H	0.33173200	5.95671000	0.59254300
H	1.76066900	5.80807000	4.64567600
H	1.43010400	7.06741500	2.52795400
H	4.77847300	-3.99699700	-2.17426800
C	3.88828600	-3.78103600	-1.59104400
C	1.62435400	-3.18438700	-0.07391200
C	3.56880500	-4.56069900	-0.47776900
C	2.43810000	-4.25711600	0.28171200
C	1.93740700	-2.40333200	-1.18701100
H	4.20491000	-5.39650200	-0.19887600
H	2.18086100	-4.85084900	1.15367300
H	0.75836500	-2.94483900	0.52687500
C	0.91949400	1.59339000	-3.78035800
C	-0.11500300	1.69702300	-2.86896700
C	-1.45291600	1.40835400	-3.22821900
C	-1.73779000	1.03997900	-4.57925300
C	-0.65892000	0.94291600	-5.48796600
C	0.64347300	1.20339300	-5.10122000
C	-2.52824900	1.44314000	-2.25653700
C	-3.11039300	0.76884800	-4.98178900
C	-4.14529700	0.88525000	-4.01212400
C	-3.81079500	1.21925900	-2.66270500
C	-5.48724300	0.64019500	-4.38101500
H	-6.26078600	0.73435400	-3.62287600
C	-5.81316000	0.28143600	-5.67348300
C	-4.79438300	0.15997700	-6.63641200
C	-3.47520700	0.39901700	-6.29595000
H	1.93297600	1.79870000	-3.45336300
H	0.13425600	1.98258700	-1.85550600
H	-0.84803100	0.65585000	-6.51577000
H	1.44950400	1.11284800	-5.82377500
H	-4.62090500	1.27015600	-1.93846600
H	-6.84705700	0.09227700	-5.94666700
H	-5.04344500	-0.12310600	-7.65498400
H	-2.71553800	0.29818900	-7.06236700
C	3.07516700	-2.70506700	-1.94066200
H	3.33499700	-2.08209800	-2.79280100
C	-0.44155300	-3.19761200	-2.66134700
C	-1.10994600	-3.95348300	-1.69490200
C	0.08972300	-3.83388700	-3.78628100
C	-1.24147900	-5.33154400	-1.84870900
H	-1.52842500	-3.46355300	-0.82743400
C	-0.03382600	-5.21467800	-3.93746800
H	0.60730100	-3.24767300	-4.54206600

C	-0.69988500	-5.96647200	-2.96768100
H	-1.76086900	-5.90310400	-1.08567300
H	0.38549500	-5.70166400	-4.81337700
H	-0.79797800	-7.04199200	-3.08606500
C	0.04443300	4.09398900	1.63082800
H	-0.41690300	3.60935000	0.77732400
C	-2.39740400	2.87492000	4.01065100
C	-2.38313600	3.09433800	5.39058400
C	-3.01535200	3.80803700	3.17255700
C	-2.96936400	4.23962500	5.92919000
H	-1.90582900	2.36859600	6.04461600
C	-3.61069500	4.94675800	3.71081900
H	-3.02947800	3.63918500	2.10121700
C	-3.58516900	5.16816500	5.08946800
H	-2.94987000	4.40209000	7.00290100
H	-4.09038700	5.66578900	3.05292100
H	-4.04567900	6.05903200	5.50665800
C	-0.21499100	-5.17893900	3.13086400
C	-0.48722300	-3.87973500	2.74889500
C	-1.64202600	-3.58115400	1.98852700
C	-2.54167800	-4.61985700	1.62478200
C	-2.23362000	-5.93871500	2.03077600
C	-1.09451500	-6.21473100	2.76520400
C	-1.88023800	-2.23925800	1.54055600
C	-3.72222700	-4.27796100	0.84697200
C	-3.92923700	-2.92732800	0.42916900
C	-2.95348400	-1.90618300	0.76503800
C	-5.09046800	-2.62363700	-0.32179000
H	-5.27666000	-1.60283100	-0.63350600
C	-6.00750600	-3.59762400	-0.66596600
C	-5.79586700	-4.92692000	-0.26698400
C	-4.67669300	-5.25157800	0.47519700
H	-1.12430400	-1.50950700	1.81424900
H	0.67755900	-5.39881800	3.70963500
H	0.19300100	-3.07116400	2.99862400
H	-2.89221200	-6.75794300	1.76514400
H	-0.88064500	-7.23834300	3.05977100
H	-6.88826700	-3.33343200	-1.24400600
H	-6.51037900	-5.69924800	-0.53654700
H	-4.53759700	-6.28156100	0.78220300
Ni	1.54910800	0.53264300	0.82624300
Cl	1.69235300	-1.03722500	2.55174600
C	3.13383200	0.76444300	-0.13489300
O	2.72865900	1.45452600	-1.08283900

C	4.35214700	-0.07404400	-0.20987500
C	5.23163500	0.14139800	-1.28382300
C	4.61489300	-1.09201900	0.71549600
C	6.36980700	-0.64651100	-1.42315100
H	5.00251100	0.92800400	-1.99585100
C	5.75391300	-1.87949800	0.56756100
H	3.91553200	-1.27269100	1.52199300
C	6.63300100	-1.65798800	-0.49411400
H	7.05164800	-0.47488400	-2.25159900
H	5.94721200	-2.67453200	1.28123000
H	7.52000300	-2.27643000	-0.60392900
C	3.64251200	3.11915600	1.00511300
C	3.09172700	1.86227800	1.62500100
H	4.59988000	2.93704200	0.50543800
H	2.91970600	3.51920900	0.28971300
H	2.24878900	2.14545600	2.25388000
F	3.85600300	4.07419400	2.00102700
O	4.06476700	1.23420500	2.43543100
C	3.79432900	1.09729300	3.75768700
O	2.83552400	1.59935700	4.31201000
C	4.82143400	0.27283800	4.44316700
C	5.96449000	-0.19511500	3.78233900
C	4.61671600	-0.04036700	5.79234400
C	6.89126900	-0.97590700	4.46990700
H	6.11480000	0.04660300	2.73816600
C	5.54408900	-0.82240700	6.47510800
H	3.72298100	0.33235300	6.28047300
C	6.68276500	-1.29150300	5.81448700
H	7.77613500	-1.33929700	3.95493900
H	5.38045900	-1.06914600	7.52025900
H	7.40616500	-1.90265900	6.34748900

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C	-1.87613300	0.38002900	-0.11730200
C	-0.73410000	-0.42394700	-0.70458600
N	-0.51386200	1.10883500	1.85083200
N	0.49880400	-0.49016700	-0.36008600
C	-1.62893500	0.86742500	1.28912800
C	-0.77306900	1.57134800	3.22953100
C	-2.34204700	1.72299000	3.26316600
O	-2.75537200	1.13595000	1.99619000
C	1.21819700	-1.33620100	-1.34152700
C	0.09032400	-1.71970200	-2.37700700
O	-1.10255300	-1.11967100	-1.78847600

C	-3.15455300	-0.49345500	-0.18908300
H	-3.38140000	-0.59999600	-1.24855400
H	-3.97757500	0.06813800	0.26492600
C	-2.07072700	1.70968800	-0.97102200
H	-2.98219600	2.17415400	-0.58312000
H	-1.23742100	2.36992800	-0.72438200
H	-0.47194300	0.74852900	3.88160400
H	-2.75659100	1.08239700	4.04524100
H	1.94686300	-0.69417900	-1.84132700
H	0.25928000	-1.19227100	-3.31759200
C	0.06259300	2.77804400	3.57870400
C	1.75624000	4.92780500	4.18062900
C	0.93052300	2.71225500	4.67247500
C	0.88393900	5.00548000	3.09170100
C	1.77731600	3.78079500	4.97200200
H	0.97562400	1.79982000	5.26024800
H	0.87147700	5.89163500	2.46396900
H	2.46996000	3.70360900	5.80408200
H	2.42588800	5.75383600	4.40172100
H	4.60910000	-4.52032000	-1.33806000
C	3.71615800	-4.14334100	-0.84823200
C	1.45054500	-3.13574000	0.42547900
C	3.22134300	-4.77361700	0.29585300
C	2.09085900	-4.26415600	0.93372900
C	1.93637000	-2.50649300	-0.71975800
H	3.72297600	-5.65234200	0.69229300
H	1.69712100	-4.73866600	1.82697100
H	0.58587600	-2.73385000	0.93319200
C	1.36682100	1.49391500	-3.64045300
C	0.25475800	1.63473800	-2.83088600
C	-1.05420900	1.42131400	-3.32404100
C	-1.22470100	1.08330500	-4.70175400
C	-0.06787200	0.94136400	-5.50268300
C	1.20211200	1.13401300	-4.98846600
C	-2.21424700	1.50736600	-2.45833000
C	-2.56338800	0.89153800	-5.23995200
C	-3.67965900	1.05022100	-4.37175900
C	-3.46060800	1.35267600	-2.99134000
C	-4.99052200	0.88376700	-4.87309800
H	-5.82812600	1.01009400	-4.19142700
C	-5.20814900	0.56317300	-6.19809500
C	-4.10871600	0.40116000	-7.06127000
C	-2.81808400	0.56228000	-6.59042800
H	2.35205200	1.64839000	-3.21283800

H	0.41282900	1.89759400	-1.79489900
H	-0.16968700	0.67403400	-6.54820200
H	2.06878000	1.01251500	-5.63218000
H	-4.33359900	1.43900900	-2.34789100
H	-6.21936800	0.43555800	-6.57316600
H	-4.27248000	0.14818100	-8.10480200
H	-1.99372300	0.43254900	-7.28212900
C	3.07571400	-3.01396600	-1.35147100
H	3.47035900	-2.51213900	-2.23108900
C	-0.15026100	-3.17906200	-2.62872300
C	-0.84757600	-3.96478000	-1.70538200
C	0.36665500	-3.77059600	-3.78338400
C	-1.02262000	-5.32642400	-1.93431900
H	-1.25664800	-3.51016500	-0.81374200
C	0.20139600	-5.13769500	-4.00908500
H	0.90076700	-3.15897600	-4.50696200
C	-0.49429500	-5.91755700	-3.08429400
H	-1.56890700	-5.92116700	-1.20864200
H	0.60856600	-5.59006000	-4.90900000
H	-0.62777600	-6.98122200	-3.26116000
C	0.04429100	3.93633100	2.79124200
H	-0.61126300	3.99103800	1.93047400
C	-2.88481400	3.12247700	3.40209800
C	-2.78613500	3.75696700	4.64586500
C	-3.43523500	3.81713400	2.32342300
C	-3.21197900	5.07317200	4.80283600
H	-2.35032400	3.22535300	5.48767700
C	-3.86625800	5.13567300	2.48109000
H	-3.52985500	3.32441900	1.36273600
C	-3.75190000	5.76867600	3.71827700
H	-3.12061500	5.55730300	5.77077200
H	-4.29125200	5.66680900	1.63396700
H	-4.08344800	6.79585700	3.83953600
C	-0.74979000	-4.97101500	3.43077700
C	-0.95831200	-3.69946200	2.93362900
C	-1.94641400	-3.46891000	1.94811000
C	-2.74011700	-4.54389000	1.46551100
C	-2.49796500	-5.83376500	1.99159400
C	-1.52486900	-6.04422200	2.95204600
C	-2.12072200	-2.15530400	1.40507800
C	-3.74838700	-4.26350100	0.45458000
C	-3.90048700	-2.93394800	-0.04924800
C	-3.03644200	-1.87208400	0.43267700
C	-4.89310000	-2.69289100	-1.02929900

H	-5.03487300	-1.69019800	-1.41443900
C	-5.69712500	-3.70693600	-1.51239800
C	-5.53854300	-5.01447100	-1.02647000
C	-4.58475800	-5.27846600	-0.06235500
H	-1.44273100	-1.39969500	1.78488000
H	0.01390200	-5.14222400	4.18400300
H	-0.34777600	-2.86353400	3.26618800
H	-3.07710700	-6.68160400	1.64361800
H	-1.35879900	-7.04661300	3.33657500
H	-6.44751100	-3.49086500	-2.26727000
H	-6.16439900	-5.81793600	-1.40392000
H	-4.48448500	-6.29305700	0.30542700
Ni	1.43686300	0.59840400	1.06150900
Cl	1.47336700	-0.83702700	2.99815400
C	3.22728800	0.64559600	0.20234300
O	3.19214400	1.29441500	-0.84367300
C	4.31840500	-0.36700700	0.39425400
C	5.35110700	-0.35412100	-0.56149600
C	4.34727700	-1.32222700	1.41688500
C	6.39329700	-1.27216000	-0.48906000
H	5.31283600	0.38714900	-1.35193400
C	5.39118400	-2.24299700	1.48148300
H	3.53826400	-1.36409300	2.13470400
C	6.41559500	-2.22263400	0.53517900
H	7.18792600	-1.24817400	-1.23015900
H	5.38950000	-2.99127100	2.26835400
H	7.22492500	-2.94597100	0.59007000
C	4.30722700	1.81144600	2.49070300
C	2.99390600	1.94953900	1.78771800
H	5.15228400	1.90540400	1.80199600
H	4.34143900	0.84119500	2.99062600
H	2.20212800	1.97834000	2.54125900
F	4.43827900	2.81549400	3.46047000
O	2.98357000	3.18545900	1.07030800
C	1.95156100	3.42305000	0.27057700
O	1.00700200	2.64220500	0.13265200
C	2.01079000	4.74217500	-0.39363700
C	2.95122900	5.70647100	-0.00488900
C	1.08637000	5.03038500	-1.40607400
C	2.96204300	6.95171800	-0.62829300
H	3.65434300	5.47237600	0.78585500
C	1.10828300	6.27349200	-2.03224900
H	0.37072800	4.27243700	-1.70193300
C	2.04321600	7.23568500	-1.64206100

H	3.68685900	7.70128200	-0.32472500
H	0.39784700	6.49247500	-2.82382800
H	2.05631400	8.20706100	-2.12844400
(R)-TS4^{doublet}			
C	-1.78205000	1.17430000	-0.42252400
C	-1.33485900	-0.27047100	-0.50619600
N	0.51143000	2.05085700	0.06242000
N	-0.15097600	-0.75579200	-0.51551200
C	-0.75642100	2.08035700	0.21353100
C	1.08436500	3.20799000	0.78835500
C	-0.12068000	3.66232400	1.67366700
O	-1.26088000	3.07553600	0.97868400
C	-0.24925100	-2.21101100	-0.78269100
C	-1.80349800	-2.45809900	-0.87599900
O	-2.35545800	-1.12797900	-0.66793600
C	-3.12166900	1.23252000	0.34479100
H	-3.84913300	0.71247700	-0.27762800
H	-3.43885100	2.27945400	0.40036300
C	-1.95704100	1.73019900	-1.90485500
H	-2.34172100	2.75009800	-1.79493800
H	-0.95628500	1.79570400	-2.33484000
H	1.88534400	2.83868000	1.42895500
H	-0.05786100	3.14280200	2.63567400
H	0.18096900	-2.37666800	-1.77082200
H	-2.06645500	-2.73757900	-1.89843100
C	1.61391300	4.25505800	-0.16171800
C	2.62786200	6.21734200	-1.88950700
C	0.87512300	4.66851000	-1.27718400
C	3.36798500	5.81295700	-0.77843800
C	1.37822500	5.64309900	-2.13656300
H	-0.08640100	4.21111000	-1.48702300
H	4.34325500	6.24907900	-0.58299600
H	0.79808400	5.95151500	-3.00168400
H	3.02237800	6.97332100	-2.56232700
H	1.04537600	-3.33272500	3.56120100
C	1.10724700	-3.56753200	2.50286300
C	1.25495000	-4.13683300	-0.21822600
C	1.87328100	-4.64708200	2.05759400
C	1.94316000	-4.93502800	0.69420200
C	0.49631100	-3.04897300	0.22149900
H	2.41993000	-5.25828700	2.77038400
H	2.55077400	-5.76223700	0.33950300
H	1.32983700	-4.33935600	-1.28387100

C	-0.63939100	-1.66276300	-4.30487900
C	-1.06621900	-0.52858600	-3.63847700
C	-2.44292100	-0.22144000	-3.52013500
C	-3.39962000	-1.07804500	-4.14848600
C	-2.92837600	-2.23354700	-4.81339300
C	-1.57939900	-2.53118900	-4.88447300
C	-2.90209200	0.92690600	-2.76253900
C	-4.81608600	-0.74725200	-4.09293100
C	-5.21636500	0.43744300	-3.41365300
C	-4.23056800	1.23858400	-2.75743800
C	-6.58374300	0.79106900	-3.36070800
H	-6.86592900	1.70036500	-2.83544400
C	-7.54506700	-0.00063100	-3.95613700
C	-7.15691200	-1.17584300	-4.62588200
C	-5.82346000	-1.53757600	-4.69137700
H	0.42451400	-1.87115600	-4.36516000
H	-0.31159500	0.11641400	-3.20568300
H	-3.63514600	-2.90694500	-5.28425000
H	-1.25112500	-3.42866700	-5.40142900
H	-4.57445500	2.11290900	-2.20876300
H	-8.59352100	0.27866900	-3.90786900
H	-7.90796900	-1.80426500	-5.09578300
H	-5.55819800	-2.44725700	-5.21757700
C	0.42158700	-2.77355900	1.58887800
H	-0.15531600	-1.92798200	1.93614500
C	-2.38312200	-3.43797200	0.10628500
C	-2.93073500	-3.02644500	1.32259900
C	-2.30037200	-4.80379600	-0.18344700
C	-3.37647000	-3.96966800	2.24764100
H	-3.00736000	-1.97217700	1.54397600
C	-2.74010800	-5.74731200	0.74282200
H	-1.87678300	-5.12914500	-1.13061600
C	-3.27709500	-5.33170800	1.96356900
H	-3.79027200	-3.63067600	3.19249100
H	-2.66431900	-6.80613500	0.51171600
H	-3.61797800	-6.06744200	2.68667100
C	2.86092200	4.83649900	0.08029600
H	3.44323200	4.51137400	0.93856800
C	-0.29819500	5.13720500	1.87193800
C	-1.17210600	5.89096900	1.08511900
C	0.48596800	5.77894300	2.83631100
C	-1.25700400	7.27230100	1.25849300
H	-1.78833400	5.39217200	0.34557100
C	0.40802300	7.16046300	3.00268600

H	1.16183100	5.19418900	3.45587800
C	-0.46487100	7.91136500	2.21285100
H	-1.94256800	7.84977000	0.64472100
H	1.02370200	7.64893300	3.75241900
H	-0.53029000	8.98754100	2.34461500
C	-0.77261200	-1.41966700	5.48757300
C	-0.77805200	-0.69944800	4.30904900
C	-1.99818000	-0.38236700	3.66692900
C	-3.23220000	-0.79287400	4.23941600
C	-3.19202200	-1.52767700	5.44680800
C	-1.98990500	-1.83786200	6.05695000
C	-1.98724800	0.31410100	2.41425500
C	-4.46604900	-0.44938500	3.54988500
C	-4.41124200	0.24665800	2.30274100
C	-3.12913300	0.60318300	1.72387600
C	-5.62726500	0.56305800	1.65020700
H	-5.60577200	1.09758700	0.70793000
C	-6.85051200	0.21121900	2.18673600
C	-6.90357500	-0.47724900	3.40953700
C	-5.73316000	-0.79598100	4.07104600
H	-1.00303900	0.55020800	2.02303000
H	0.16853700	-1.66284300	5.97257100
H	0.15038300	-0.37988800	3.84415900
H	-4.11262500	-1.86365100	5.91063000
H	-1.98886200	-2.40803900	6.98173200
H	-7.76678300	0.46665800	1.66245300
H	-7.86148800	-0.75839800	3.83748900
H	-5.79739500	-1.32086200	5.01716600
Ni	1.62880400	0.33137400	-0.46069400
Cl	1.84318200	0.27006400	1.94263700
C	2.69941400	-1.32128300	-1.14493800
O	2.36425200	-1.58674900	-2.26844800
C	3.75378600	-2.08377400	-0.42192900
C	4.44061000	-3.05794200	-1.17184700
C	4.07040700	-1.88979600	0.92372200
C	5.43551700	-3.82063700	-0.57721200
H	4.18297100	-3.19480200	-2.21623800
C	5.06789700	-2.66478600	1.51380600
H	3.53943700	-1.14218500	1.49739700
C	5.75304900	-3.62377400	0.77064600
H	5.97479600	-4.55874700	-1.16366100
H	5.31242900	-2.50577800	2.55966600
H	6.53950300	-4.21340400	1.23330800
C	2.89533100	1.89748600	-2.18824600

C	3.50586000	1.44702000	-1.01481000
H	2.35582600	2.83252800	-2.17090200
H	3.30184700	1.58693000	-3.14431300
H	3.58552900	2.06994700	-0.13360600
F	1.33588000	0.95493800	-2.40295500
O	4.65775900	0.64688800	-1.23625500
C	5.58402300	0.59262400	-0.25389900
O	5.49362400	1.20067700	0.79563000
C	6.71990900	-0.29763800	-0.61480900
C	7.68307000	-0.55651600	0.36776800
C	6.84316300	-0.88168300	-1.88130100
C	8.75722300	-1.39636100	0.08883400
H	7.56295300	-0.09577500	1.34209000
C	7.92432700	-1.71521700	-2.16042800
H	6.09021000	-0.68400600	-2.63481500
C	8.87952400	-1.97683200	-1.17650900
H	9.49919800	-1.60015500	0.85565500
H	8.01787700	-2.16613700	-3.14433000
H	9.71912300	-2.63121000	-1.39504600

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C	-1.95093700	-0.13063300	1.45325700
C	-0.92786500	0.97457900	1.31236400
N	-0.54620300	-1.80454400	0.25375100
N	0.20142800	0.99014200	0.70143000
C	-1.68686100	-1.28822300	0.52740400
C	-0.78980600	-3.04195000	-0.52279200
C	-2.28522300	-2.87405300	-0.94410000
O	-2.77799000	-1.90784100	0.04323300
C	0.80801000	2.33303000	0.91378500
C	-0.21553200	3.05111300	1.87478900
O	-1.30207000	2.08388700	1.96414500
C	-3.36904700	0.46883900	1.28263300
H	-3.52741100	1.05827100	2.17938300
H	-4.08983100	-0.35568800	1.31706200
C	-1.84345300	-0.79261600	2.90592200
H	-2.43588000	-1.71113600	2.84531700
H	-0.80434100	-1.09795700	3.04499600
H	-0.15886500	-3.02242300	-1.40929700
H	-2.31264800	-2.35449300	-1.90573300
H	1.73664800	2.18016600	1.45973100
H	0.20928300	3.11507100	2.87838500
C	-0.50082400	-4.28565500	0.28645900
C	-0.08411800	-6.67418200	1.70247700

C	-0.66677400	-4.32732300	1.67476300
C	0.08821500	-6.63951700	0.31710800
C	-0.45706500	-5.51304100	2.38013200
H	-0.94573200	-3.42583600	2.20862000
H	0.38615100	-7.53680200	-0.21773500
H	-0.58577500	-5.52805200	3.45890600
H	0.07734400	-7.59830100	2.25000800
H	0.04634300	3.51160500	-3.55746900
C	0.62907100	3.67713900	-2.65720300
C	2.10800300	4.06416000	-0.33118400
C	1.62217700	4.65470100	-2.62359600
C	2.36447300	4.84736800	-1.45463500
C	1.10151100	3.09184300	-0.35719500
H	1.82342200	5.26061700	-3.50288700
H	3.14551000	5.60217700	-1.42038000
H	2.69551000	4.20103500	0.57327600
C	0.66253800	1.86948300	5.32518500
C	-0.13854300	1.01707400	4.59021000
C	-1.52819200	0.92075800	4.82685500
C	-2.10803800	1.72451500	5.85772900
C	-1.26233400	2.58916900	6.58953300
C	0.09337100	2.66538400	6.33331700
C	-2.36667600	0.01976600	4.06524300
C	-3.53425000	1.63680900	6.13102300
C	-4.31380000	0.69900200	5.39785100
C	-3.68826900	-0.09734700	4.39063700
C	-5.70050200	0.58313200	5.64898400
H	-6.27454100	-0.14087900	5.07598600
C	-6.31743600	1.37608300	6.59525300
C	-5.55382800	2.31046300	7.32003700
C	-4.19529200	2.43514100	7.09210200
H	1.72365600	1.90720700	5.10620400
H	0.33323700	0.43045900	3.81328800
H	-1.67908100	3.20575100	7.37736700
H	0.71630000	3.33771600	6.91658800
H	-4.31541400	-0.79641700	3.84186900
H	-7.38382500	1.28333900	6.77878100
H	-6.03362100	2.94090000	8.06313000
H	-3.63846600	3.16894500	7.66316700
C	0.36659500	2.90291900	-1.52627400
H	-0.39206000	2.13515200	-1.56498900
C	-0.75288200	4.38444200	1.44500700
C	-1.71768800	4.48171800	0.43713700
C	-0.24817000	5.54883700	2.02789400

C	-2.16793100	5.72914300	0.01523100
H	-2.11691300	3.58271800	-0.01172200
C	-0.69041900	6.80095800	1.59862800
H	0.49397800	5.47482500	2.81949400
C	-1.65147000	6.89235500	0.59101100
H	-2.91858300	5.78607100	-0.76693100
H	-0.29065800	7.70161900	2.05623800
H	-2.00010700	7.86633300	0.25873900
C	-0.11405600	-5.45168400	-0.38285200
H	0.02390300	-5.42461900	-1.46010700
C	-3.13018000	-4.10886800	-0.96600900
C	-3.25869300	-4.81205800	-2.16739800
C	-3.72039400	-4.61868700	0.19466100
C	-3.95424100	-6.02043900	-2.20708900
H	-2.80904400	-4.41212000	-3.07304900
C	-4.42327900	-5.82080000	0.15354100
H	-3.62655600	-4.07101400	1.12564100
C	-4.53761700	-6.52770700	-1.04551900
H	-4.04672300	-6.55961200	-3.14549100
H	-4.87978000	-6.20864300	1.05974800
H	-5.08367400	-7.46626800	-1.07483200
C	-2.65225900	2.79752600	-4.46910700
C	-2.47729300	1.92810100	-3.41025000
C	-3.19787300	2.10492400	-2.20580000
C	-4.12228000	3.17784800	-2.08370300
C	-4.27285300	4.05445400	-3.18321500
C	-3.55366700	3.87149500	-4.35018300
C	-2.97765900	1.22087500	-1.09773600
C	-4.86291800	3.32193700	-0.83993600
C	-4.63152500	2.40748700	0.23398600
C	-3.63760400	1.35686000	0.08773800
C	-5.37950500	2.56796200	1.42659300
H	-5.24154600	1.87962700	2.25138000
C	-6.29860300	3.58822900	1.57607200
C	-6.51107000	4.49614100	0.52690600
C	-5.80728100	4.35661700	-0.65358400
H	-2.22621000	0.45197900	-1.24333700
H	-2.09211200	2.65451300	-5.38893900
H	-1.76762600	1.10918900	-3.47213500
H	-4.96286900	4.88845000	-3.12368500
H	-3.68901500	4.56145600	-5.17844300
H	-6.85088000	3.68498100	2.50628800
H	-7.22795100	5.30454300	0.63852100
H	-5.99333500	5.06200700	-1.45510100

Ni	1.15117000	-0.66890100	-0.28791500
Cl	0.02691300	-0.43592400	-2.35705400
C	2.75680400	0.40560200	-0.92236600
O	3.25674100	1.13113800	-0.10755300
C	3.18106100	0.37150500	-2.34393900
C	3.66220500	1.57939100	-2.87535400
C	3.11392300	-0.78078100	-3.13389100
C	4.06630600	1.62945600	-4.20538200
H	3.68343300	2.46492900	-2.25072900
C	3.55705100	-0.72633900	-4.45285900
H	2.72667900	-1.69457800	-2.70336400
C	4.02134800	0.47568300	-4.99242200
H	4.41702900	2.56731100	-4.62666900
H	3.52021900	-1.62067800	-5.06795600
H	4.34428800	0.51488900	-6.02939900
C	2.50799500	-2.65752700	0.87831200
C	2.34678300	-1.42840800	1.52009700
H	3.51128200	-3.00893700	0.66214100
H	1.75608500	-3.41981700	1.02589300
H	1.57876900	-1.26081100	2.26375000
F	2.07687700	-2.41137200	-0.84954700
O	3.56130900	-0.75728900	1.77564800
C	3.53378800	0.36269000	2.50738300
O	2.53116100	0.76585700	3.08299700
C	4.84650300	1.05196700	2.55133800
C	4.95873400	2.20585000	3.33674900
C	5.94819100	0.60187700	1.81230200
C	6.16375800	2.90117100	3.38923400
H	4.09128500	2.54396300	3.89318700
C	7.15231100	1.29955000	1.86740800
H	5.84903700	-0.28271900	1.19484900
C	7.26269900	2.44805700	2.65519300
H	6.24752000	3.79594700	3.99936200
H	8.00430800	0.95110800	1.29095700
H	8.20297600	2.99095700	2.69435600

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C	0.70465100	-1.57656300	0.72348800
C	0.78635000	-0.24727600	0.01266400
N	-1.11713400	-0.72229100	2.22124800
N	-0.03651500	0.74126500	0.02967900
C	-0.16265600	-1.52605400	1.95803300
C	-1.83576500	-1.23537600	3.41318200
C	-0.76792300	-2.20575000	4.01212000

O	0.05026600	-2.53193900	2.84779300
C	0.55068100	1.82363600	-0.79830100
C	1.60435900	1.04441200	-1.63901200
O	1.85776000	-0.12222200	-0.78436600
C	2.14566700	-2.05210900	1.08261000
H	2.60503800	-2.38287000	0.15806100
H	2.04467500	-2.93025900	1.72523200
C	-0.01051800	-2.62826100	-0.24159500
H	0.07479300	-3.59734000	0.26098000
H	-1.06677500	-2.35341700	-0.27794400
H	-2.03227600	-0.40136600	4.08578400
H	-0.11447400	-1.63671800	4.68745000
H	-0.21309600	2.21139000	-1.47251100
H	1.10571300	0.64816000	-2.52226700
C	-3.14538300	-1.90735600	3.05768100
C	-5.55013100	-3.26828600	2.58101500
C	-4.31093600	-1.54412700	3.73413700
C	-4.39002700	-3.62699300	1.88927700
C	-5.50997600	-2.21763300	3.49839200
H	-4.28615800	-0.71063000	4.42803300
H	-4.41384600	-4.43894300	1.16729000
H	-6.41256000	-1.90480900	4.01331500
H	-6.48178300	-3.79537700	2.39504400
H	1.93144500	6.22875700	-0.21632900
C	1.82057900	5.24586400	0.23224900
C	1.50154700	2.72616700	1.37896300
C	2.23178200	5.02321900	1.54844200
C	2.07020800	3.76159900	2.12165800
C	1.09548700	2.94249300	0.05968200
H	2.67220700	5.83154900	2.12576400
H	2.38723900	3.57486900	3.14237700
H	1.37862400	1.74935700	1.82962600
C	-1.27444300	-0.08363500	-3.55207800
C	-0.93051300	-0.98099500	-2.55660100
C	0.20532700	-1.81854300	-2.68303500
C	0.98127000	-1.75724000	-3.88285000
C	0.59926900	-0.82985600	-4.88008300
C	-0.49817100	-0.00189500	-4.72011800
C	0.61759200	-2.70676700	-1.61144600
C	2.13538800	-2.62852700	-4.04711900
C	2.44374700	-3.55680800	-3.01368700
C	1.66103200	-3.56270300	-1.81678100
C	3.54916200	-4.42661500	-3.15516300
H	3.76580000	-5.12711200	-2.35236100

C	4.34528600	-4.38479600	-4.28232900
C	4.05083800	-3.46355100	-5.30447000
C	2.97068200	-2.60738800	-5.18680900
H	-2.13259500	0.56389400	-3.40293400
H	-1.55044700	-1.01362500	-1.66790300
H	1.17309000	-0.76224900	-5.79717300
H	-0.76012900	0.70335300	-5.50413500
H	1.95069000	-4.25523400	-1.02948600
H	5.19414900	-5.05520900	-4.38001900
H	4.67478400	-3.42257900	-6.19264500
H	2.77280800	-1.90913800	-5.99187200
C	1.25660600	4.20999700	-0.50696400
H	0.92991900	4.38623100	-1.52752400
C	2.87035300	1.72664900	-2.04817700
C	3.83676600	2.14097600	-1.12498200
C	3.06359600	1.98839200	-3.40904800
C	4.97275100	2.81700400	-1.56053000
H	3.70409500	1.93447900	-0.07164600
C	4.19891800	2.67242700	-3.84438200
H	2.32025700	1.64884600	-4.12589600
C	5.15549900	3.08920700	-2.91829900
H	5.71753800	3.12612400	-0.83437300
H	4.33806500	2.87208000	-4.90316300
H	6.04262700	3.61989700	-3.25312900
C	-3.19835900	-2.94476200	2.12194800
H	-2.30726100	-3.22558400	1.57373700
C	-1.26566900	-3.44335200	4.69859800
C	-1.87200600	-3.30684600	5.95209600
C	-1.18258800	-4.70628400	4.10965100
C	-2.40067900	-4.41857800	6.60389300
H	-1.94041500	-2.32461100	6.41372400
C	-1.70549500	-5.82074000	4.76641800
H	-0.70989200	-4.81159800	3.14005900
C	-2.31850200	-5.68053200	6.01133700
H	-2.87588000	-4.30000600	7.57330100
H	-1.63631200	-6.79970300	4.30064400
H	-2.72894800	-6.54864700	6.51886400
C	3.41246700	2.19451500	5.43944700
C	2.76737600	1.14803000	4.81081800
C	3.28715700	0.58308000	3.62380200
C	4.49354500	1.08728300	3.06753700
C	5.12833300	2.16319300	3.72918200
C	4.60286200	2.70586800	4.88790500
C	2.59081100	-0.47106500	2.95680200

C	5.00217400	0.48194800	1.84659100
C	4.24501400	-0.53458800	1.18121200
C	3.00043900	-0.99908400	1.76581400
C	4.74970200	-1.06070900	-0.03357400
H	4.18019400	-1.79772200	-0.58437600
C	5.95265500	-0.63945500	-0.56180400
C	6.70996100	0.33411000	0.10892500
C	6.23642700	0.88216800	1.28444000
H	1.69247900	-0.84345300	3.43452900
H	3.00223800	2.62585500	6.34771700
H	1.83982100	0.74957100	5.21457900
H	6.03759900	2.59060900	3.32271600
H	5.11045400	3.53559000	5.37122400
H	6.30492400	-1.05704300	-1.50003900
H	7.66055400	0.66446200	-0.29936200
H	6.83445300	1.63303800	1.78753100
Ni	-1.77582800	0.89061100	1.00374600
Cl	-3.33549700	1.50709400	2.48683900
C	-2.40799500	2.18718400	-0.23116100
O	-2.94246000	1.79585700	-1.25638500
C	-2.16104600	3.65657600	-0.03017000
C	-2.30072500	4.50570900	-1.13905800
C	-1.74665900	4.18523800	1.19673400
C	-2.03675400	5.86699000	-1.01958500
H	-2.62227600	4.07376700	-2.08169200
C	-1.49430500	5.55004900	1.31802400
H	-1.64335200	3.52616000	2.04936000
C	-1.63721300	6.39163000	0.21387300
H	-2.14186300	6.52029700	-1.88199800
H	-1.17345400	5.95443100	2.27316700
H	-1.43076800	7.45435300	0.30995700
C	-5.31073400	-0.56435100	0.23232500
H	-5.67914700	-1.09133500	1.10082600
O	-5.59367800	0.75984800	0.16745800
C	-6.32168200	1.31274000	1.20388900
O	-6.87864300	0.63544700	2.03927600
C	-6.33558900	2.78841800	1.13318700
C	-7.07688200	3.47599100	2.10365300
C	-5.60321400	3.49985900	0.17353700
C	-7.08417000	4.86699400	2.11649400
H	-7.62542600	2.90163200	2.84221800
C	-5.60601600	4.89242200	0.19804000
H	-5.01980700	2.96349400	-0.56327500
C	-6.34445500	5.57636100	1.16568800

H	-7.65617000	5.39953800	2.87100000
H	-5.01078300	5.44117900	-0.52450200
H	-6.33884700	6.66296800	1.18375200
C	-4.47720300	-1.10540100	-0.72525600
H	-4.42861500	-2.18428700	-0.78520700
H	-4.27246500	-0.53453100	-1.62109300
F	-2.72369700	-0.94286600	-0.09495600

(S)-TS5^{doublet}

C	-1.88779900	-0.22112200	0.95153200
C	-1.04275800	1.02606100	0.88869800
N	-0.31985200	-1.40104600	-0.60300700
N	0.14260600	1.17272700	0.40965200
C	-1.48134500	-1.22475900	-0.09984400
C	-0.33977000	-2.69117100	-1.34095400
C	-1.86898300	-2.87982000	-1.56525000
O	-2.44201800	-2.11441800	-0.46163300
C	0.48759100	2.61513400	0.53288100
C	-0.52191600	3.08687300	1.61577600
O	-1.60199200	2.10250400	1.45765800
C	-3.39389400	0.15436000	0.81585400
H	-3.69861700	0.57289500	1.76775500
H	-3.94718200	-0.77896500	0.68511600
C	-1.61769900	-0.94043900	2.35363300
H	-2.34897500	-1.75311000	2.41905600
H	-0.62145800	-1.38082600	2.29380100
H	0.18940500	-2.56466600	-2.28406300
H	-2.15821800	-2.34503000	-2.48064400
H	1.49288700	2.71038100	0.93772000
H	-0.08856100	2.87804700	2.59326400
C	0.30477800	-3.80739700	-0.54525600
C	1.42173000	-5.97236700	0.84647500
C	-0.14545600	-4.13573700	0.73766800
C	1.88106800	-5.64634300	-0.42974900
C	0.40385000	-5.21337700	1.42813000
H	-0.93010700	-3.55122800	1.20346900
H	2.67913700	-6.22366700	-0.88750600
H	0.03885700	-5.45938000	2.42164900
H	1.85513900	-6.80949300	1.38643500
H	-1.25255500	3.23336500	-3.77563000
C	-0.57410400	3.58576500	-3.00560300
C	1.15380500	4.47610800	-1.00687800
C	0.18293100	4.74087200	-3.20334900
C	1.04995100	5.18317600	-2.20162100

C	0.39700300	3.31928300	-0.80124400
H	0.10195800	5.29208100	-4.13624200
H	1.65313100	6.07329700	-2.35426300
H	1.83746500	4.81289400	-0.23311200
C	1.71194800	1.34490500	4.03268600
C	0.66369000	0.55668600	3.59105500
C	-0.66497900	0.78277500	4.02664300
C	-0.91644800	1.83645500	4.96085200
C	0.17678200	2.62334000	5.39148400
C	1.46344800	2.39074200	4.93688800
C	-1.77615500	-0.01005600	3.53193100
C	-2.27081200	2.08084500	5.43301500
C	-3.31044100	1.20520700	5.01222800
C	-3.01756400	0.16792900	4.07226400
C	-4.63208400	1.40910300	5.47108500
H	-5.41013100	0.72732600	5.13623000
C	-4.93611600	2.45921900	6.31456900
C	-3.91497900	3.33675600	6.72387100
C	-2.61414800	3.14864800	6.29256300
H	2.71338800	1.15110200	3.66228600
H	0.89322800	-0.23516300	2.88964000
H	0.01325700	3.42261300	6.10537600
H	2.28099100	3.01367100	5.28889100
H	-3.84323500	-0.45812400	3.74126000
H	-5.95568400	2.61076700	6.65676000
H	-4.14805900	4.16936900	7.38134800
H	-1.85264100	3.84706800	6.61969600
C	-0.46401300	2.87713300	-1.80890400
H	-1.05251300	1.97995500	-1.66217100
C	-1.03150200	4.49161500	1.58698700
C	-1.84299500	4.97926200	0.55658100
C	-0.64228400	5.35055700	2.62081900
C	-2.24831400	6.31086100	0.55986600
H	-2.16025000	4.32094800	-0.24094500
C	-1.04173400	6.68707800	2.61875100
H	-0.02698400	4.96379700	3.42915600
C	-1.84592900	7.16925700	1.58568200
H	-2.88532400	6.67430200	-0.24011900
H	-0.73197100	7.34599700	3.42501200
H	-2.16275100	8.20867100	1.58201600
C	1.32161800	-4.57081500	-1.12119300
H	1.69509800	-4.30285600	-2.10362600
C	-2.39887700	-4.28341600	-1.59380000
C	-2.03687600	-5.10578300	-2.66684600

C	-3.20881400	-4.79536200	-0.57882300
C	-2.47196400	-6.42773200	-2.71885000
H	-1.40385000	-4.71286900	-3.45883800
C	-3.64890400	-6.11865100	-0.63465900
H	-3.49105600	-4.15811000	0.25119800
C	-3.28047100	-6.93850300	-1.70080800
H	-2.17948600	-7.05906400	-3.55280700
H	-4.27888900	-6.50839700	0.15985400
H	-3.62097600	-7.96906700	-1.74060700
C	-3.48723100	2.02241700	-5.11045200
C	-3.34039800	1.17437900	-4.03073400
C	-3.67904500	1.59614100	-2.72461100
C	-4.18925800	2.90575900	-2.51252800
C	-4.32183100	3.75387300	-3.63556900
C	-3.97930000	3.32565700	-4.90534500
C	-3.48156200	0.72779600	-1.60716300
C	-4.53370800	3.30809100	-1.15777100
C	-4.26633800	2.42902300	-0.06065200
C	-3.71383700	1.11153000	-0.31730800
C	-4.56512000	2.87919200	1.24927900
H	-4.32875500	2.26062900	2.10496500
C	-5.13005800	4.11645600	1.47912000
C	-5.42452600	4.96386700	0.39887900
C	-5.12503600	4.56440800	-0.88841200
H	-3.12477200	-0.27442500	-1.81642800
H	-3.21870700	1.69128100	-6.10924200
H	-2.94925100	0.16912800	-4.16780300
H	-4.68311200	4.76786200	-3.50996400
H	-4.08682500	4.00233800	-5.74808600
H	-5.33560500	4.43279700	2.49716600
H	-5.87539000	5.93624200	0.57388500
H	-5.35799500	5.23248700	-1.70935400
Ni	1.31931000	-0.23149400	-0.29645900
Cl	2.67848300	-1.49385000	-1.56297700
C	2.80330200	0.88441000	0.02925200
O	3.24833400	0.94264900	1.16283800
C	3.33805900	1.79292800	-1.03739400
C	4.32591500	2.72362800	-0.68528400
C	2.83355200	1.77900900	-2.34240200
C	4.80619300	3.62581300	-1.62880200
H	4.71352800	2.70734700	0.32737900
C	3.30886700	2.68741000	-3.28470100
H	2.07270800	1.05485300	-2.60704300
C	4.29496900	3.61062900	-2.92989500

H	5.58166100	4.33596700	-1.35471400
H	2.90382100	2.68235900	-4.29222300
H	4.66459000	4.31933100	-3.66666200
C	2.68986900	-2.66289200	2.02383200
C	3.74126700	-1.93488900	2.56838500
H	2.83288000	-3.10302200	1.04396600
H	2.05907000	-3.21453100	2.70868700
F	1.47176200	-1.49576100	1.49247800
O	4.66983700	-1.45833000	1.69862100
C	5.48794800	-0.42939200	2.09799900
O	5.55036100	-0.04979100	3.24849700
C	6.24660200	0.12266400	0.95501900
C	5.99898900	-0.28326100	-0.36412000
C	7.18915400	1.12606900	1.21816100
C	6.69682500	0.31655100	-1.40963200
H	5.23535900	-1.02386100	-0.57062100
C	7.88559000	1.71727000	0.16816000
H	7.35149200	1.43082800	2.24663100
C	7.63845700	1.31303500	-1.14748200
H	6.48151000	0.02129300	-2.43187500
H	8.61575500	2.49557300	0.37175100
H	8.17234800	1.78420300	-1.96824700
H	3.78830300	-1.55110600	3.57914600