

Nickel-catalysed asymmetric hydromonofluoromethylation of 1,3-enynes for enantioselective construction of monofluoromethyl-tethered chiral allenes

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Supplementary Information

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1. General information

Reactions were monitored by thin layer chromatography (TLC) using UV light or KMnO_4 to visualize the course of reaction. Purification of reaction products was carried out by flash chromatography on silica gel. Chemical yields refer to pure isolated substances. The optical rotation $[\alpha]_D$ was measured using Anton Paar MCP 5500. Infrared (IR) spectra were obtained using a SHIMADZU TRTracer-100. The HRMS spectra were measured on Waters Premier GC-TOF MS (EI) or Bruker maXis impact spectrometer using electron spray ionization (ESI) method. Chiral HPLC analysis was performed on a Shimadzu LC-20AD instrument using Daicel chiral columns at 25 °C and a mixture of HPLC -grade hexanes and isopropanol as eluent. ^1H , ^{13}C , and ^{19}F NMR were recorded using a Bruker DPX-400 or 500 MHz spectrometer. Chemical shifts were reported in ppm from tetramethylsilane with the solvent resonance as the internal standard. The following abbreviations were used to designate chemical shift multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet.

Unless mentioned, all reactions were performed under N_2 atmosphere. Anhydrous CH_2Cl_2 , and THF were prepared by Innovative Technology PS-MD-5. Anhydrous toluene was prepared by distillation over sodium-benzophenone ketyl prior to use. Absolute MeOH, EtOH and i PrOH were prepared by first dried over anhydrous Na_2SO_4 , then treated by Mg chips, distilled and stored under N_2 atmosphere. $\text{Ni}(\text{COD})_2$ was purchased from Sigma-Aldrich and used as received. The 1,3-enynes **1a-1x**^[1] and **1aa-1ac**^[1b] were prepared according to the corresponding literatures. FBSM **2** were prepared following the reported methods.^[2] Diethyl fluoromalonate **4** was commercially available and distillation before use.

List of abbreviation:

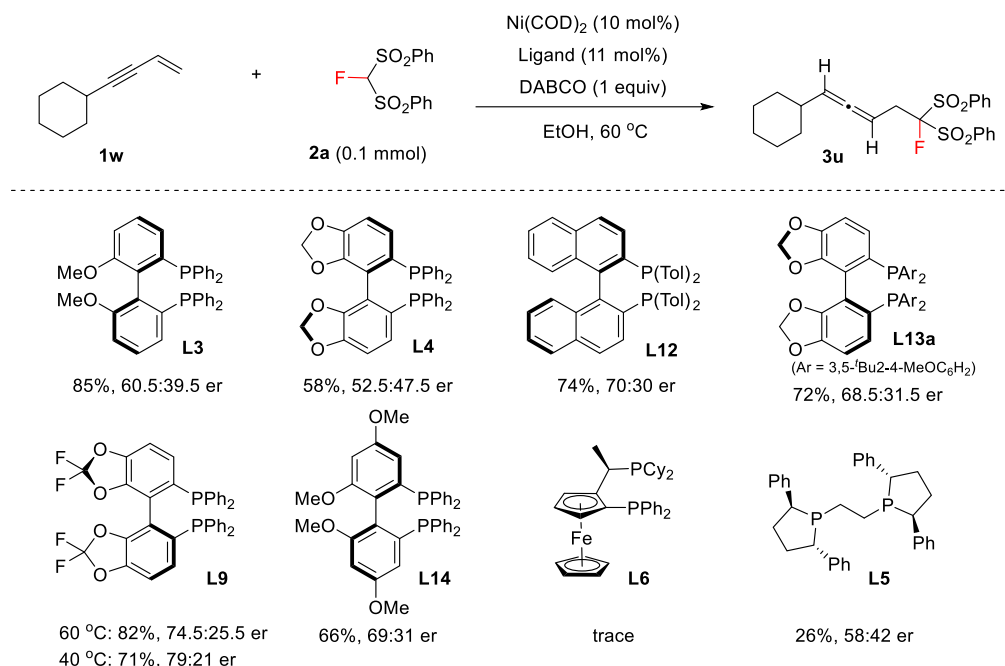
Entry	Chemical name	Abbreviation
1	Petroleum ether	PE
2	Ethyl acetate	EtOAc
3	Tetrahydrofuran	THF
4	Ethanol	EtOH
5	Methanol	MeOH
6	Dichloromethane	CH_2Cl_2

¹ (a) Yang, S.-Q.; Wang, Y.-F.; Zhao, W.-C.; Lin, G.-Q.; He, Z.-T. *J. Am. Chem. Soc.* **2021**, *143*, 7285. (b) Adamson, N. J.; Jeddi, H.; Malcolmson, S. J. *J. Am. Chem. Soc.* **2019**, *141*, 8574.

² (a) Sankar, U.; Mahalakshmi, S.; Balasubramanian, K. K. *Synlett*, **2013**, *24*, 1533. (b) Urban, M.; Franc, M.; Hofmanová M.; Čisárováb, I.; Veselý J. *Org. Biomol. Chem.* **2017**, *15*, 9071.

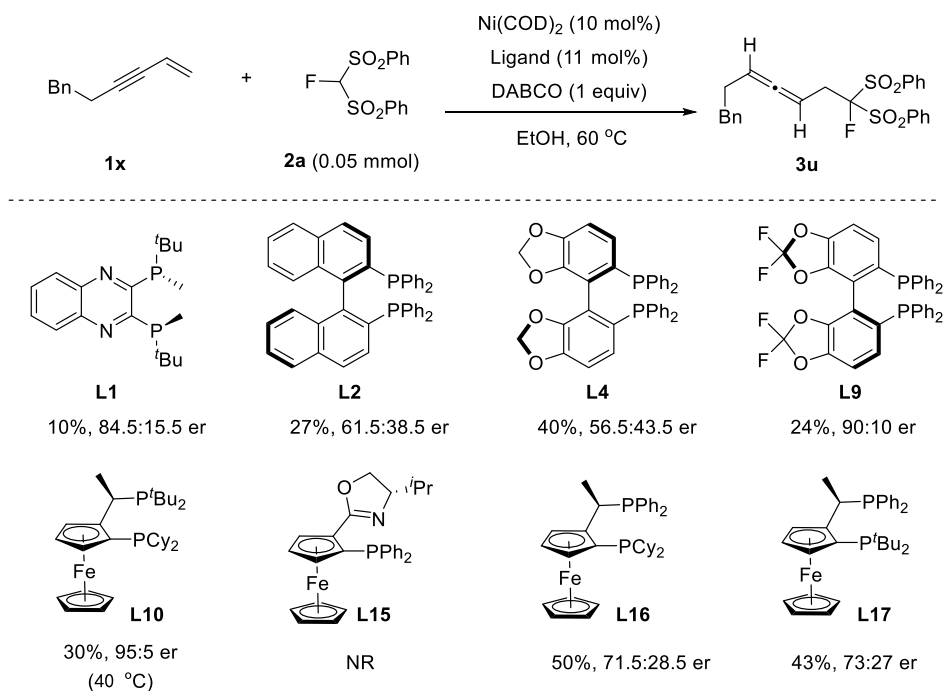
2. Selected conditions for reaction optimization

Table S1: Selected optimization of chiral ligands for hydromonofluoromethylation of **1w** and **2a**.^a



^a Conditions: **1w** (0.15 mmol), **2a** (0.10 mmol), Ni(COD)_2 (10 mol%), ligand (11 mol%), and DABCO (1.0 equiv), at 25 °C for 3 d in EtOH (1.0 mL), unless otherwise noted. The yield was determined by ¹H NMR analysis of the crude product using 1,3,5-trimethoxybenzene as internal standard. er was determined by chiral HPLC analysis.

Table S2: Selected optimization of chiral ligands for hydromonofluoromethylation of **1x** and **2a**.^a



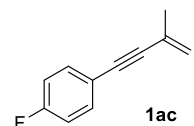
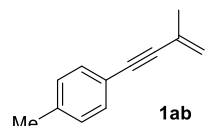
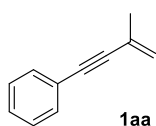
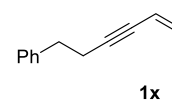
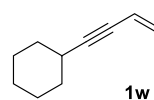
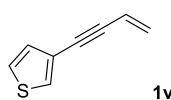
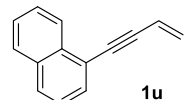
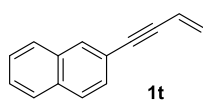
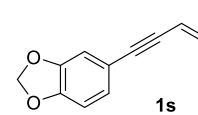
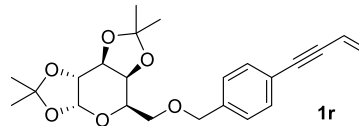
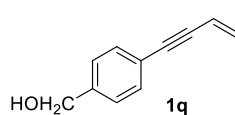
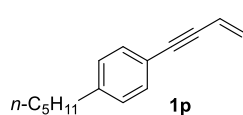
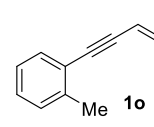
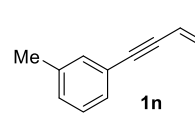
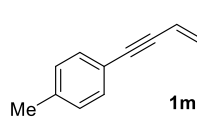
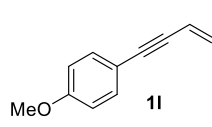
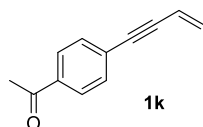
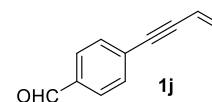
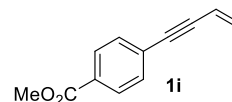
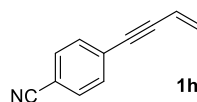
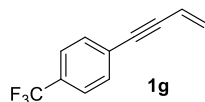
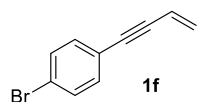
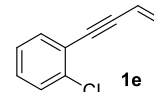
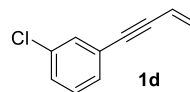
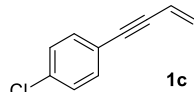
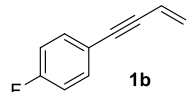
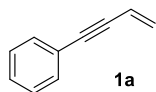
^a Conditions: **1x** (0.075 mmol), **2a** (0.05 mmol), Ni(COD)_2 (10 mol%), ligand (11 mol%), and DABCO (1.0 equiv), at 60 °C for 2 d in EtOH (0.5 mL), unless otherwise noted. The yield was determined by ¹H NMR analysis of the crude product using 1,3,5-trimethoxybenzene as internal standard. er was determined by chiral HPLC analysis.

Table S3: Selected conditions for optimization of hydromonofluoroalkylation.^a

$\text{EtO}_2\text{C}-\text{C}(\text{F})_2-\text{CO}_2\text{Et}$ (4, 0.05 mmol) + $\text{Ph}-\text{C}\equiv\text{C}-\text{CH}(\text{Me})-\text{CH}_2\text{OH}$ (1aa, 1.5 equivs) $\xrightarrow[\text{EtOH, } T\text{ }^\circ\text{C, 2 d}]{\text{Ni(COD)}_2\text{ (x mol\%)} \\ \text{Ligand (1.1x mol\%)} \\ \text{DABCO (1.0 equiv)}}$ $\text{Ph}-\text{CH}=\text{C}(\text{Me})-\text{CH}_2-\text{C}(\text{F})(\text{CO}_2\text{Et})_2$ (3aa)					
 L1 L4 L9 L18 L13b L11 L19 L10 L7 <i>ent</i>-L8					
Entry	Ligand	x	T (°C)	yield (%) ^b	er ^c
1	L1	10	60	trace	-
2	L4	10	60	22	92:8
3	L9	10	60	trace	-
4	L18	10	60	10	84:16
5	L13b	10	60	20	85:15
6	L11	10	60	14	95:5
7	L19	10	60	NR ^d	-
8	L10	10	60	5	85:15
9	L7	10	60	5	79:21
10	<i>ent</i> - L8	10	60	4	90.5:9.5
11	L11	20	60	30	95:5
12 ^e	L11	20	60	43	95:5
13	L11	20	80	50	92:8

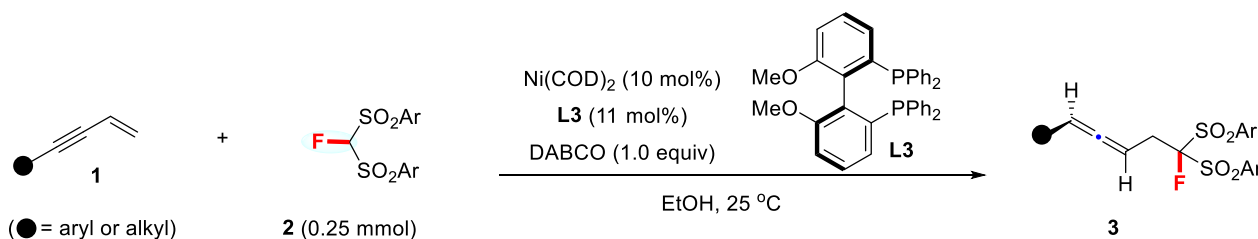
^a Conditions: **1aa** (0.075 mmol), **4** (0.05 mmol), Ni(COD)₂ (10 mol%), ligand (11 mol%), and DABCO (1.0 equiv), at 25 °C for 2 d in EtOH (0.25 mL), unless otherwise noted. ^b The yield was determined by ¹H NMR analysis of the crude product using 1,3,5-trimethoxybenzene as internal standard. ^c Determined by chiral HPLC analysis. ^d No reaction. ^e 2.0 equivs DABCO was used.

3. The structure of 1,3-enynes **1** used in this hydromonofluoromethylation

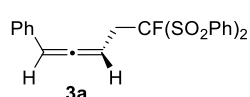


4. Enantioselective hydromonofluoromethylation of 1,3-enynes **1** with FBSM **2**

4.1 Procedure for enantioselective hydromonofluoromethylation of 1,3-enynes **1** with **2**

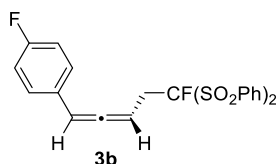


In a glove box, to a Schlenk tube equipped with a stirring bar were successively added Ni(COD)_2 (6.9 mg, 10 mol%), and (*R*)-MeO-BIPHEP **L3** (16.0 mg, 11 mol%), followed by the addition of absolute EtOH (2.5 mL). The resulting mixture was stirred at room temperature for 15 min, and then added DABCO (28.0 mg, 1.0 equiv) and FBSM **2** (0.25 mmol, 1.0 equiv). After being stirred for another 5 min, to the mixture was added 1,3-enynes **1** (0.375 mmol, 1.5 equivs). After it take out from the glove box, the reaction mixture was stirred at 25 °C until full conversion. The reaction was monitored by TLC analysis. After full consumption of **2**, the reaction mixture was concentrated under vacuum. The crude residue was purified by silica gel column chromatography using PE/EtOAc (6:1, v/v) as the eluent to afford the desired products **3**. (Note: 20 mol% of Ni catalyst was used in the case of products **3t-3u**, and **3aa-3ac**)



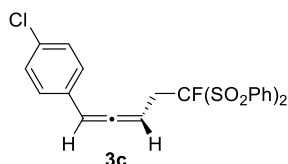
Product **3a** was obtained in 94% yield as a yellow oil (3 days). HPLC analysis (Chiralcel AD-H, *i*PrOH/hexane = 20/80, 1.0 mL/min, 254 nm; t_r

(major) = 23.16 min, t_r (minor) = 25.49 min) gave the isomeric composition of the product: 96:4 er; $[\alpha]_D^{20} = -67.9$ ($c = 0.1$, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ 7.94 (d, $J = 8.0$ Hz, 4H), 7.74-7.66 (m, 2H), 7.57-7.51 (m, 4H), 7.30-7.26 (m, 2H), 7.23-7.18 (m, 3H), 6.16 (dt, $J = 6.4, 2.4$ Hz, 1H), 5.69-5.63 (m, 1H), 3.27-3.20 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 207.7, 135.3 (d, $J = 1.9$ Hz), 135.1, 134.9, 133.2, 130.87, 130.85, 130.83, 129.0 (d, $J = 2.3$ Hz), 128.6, 127.3, 127.1, 114.0 (d, $J = 266.0$ Hz), 95.9, 85.4 (d, $J = 8.1$ Hz), 30.8 (d, $J = 18.9$ Hz); ^{19}F NMR (376 MHz, CDCl_3): δ -141.58 (s, 1F); IR (neat): 1448, 1348, 1265, 1151, 1078, 732, 721, 682, 667, 597; HRMS (ESI): Exact mass calcd for $\text{C}_{23}\text{H}_{19}\text{FNaO}_4\text{S}_2$ $[\text{M}+\text{Na}]^+$: 465.0601, Found: 465.0599.



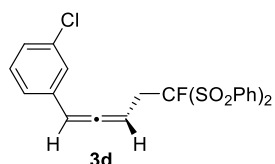
Product **3b** was obtained in 88% yield as a yellow oil (3 days). HPLC analysis (Chiralcel AD-H, *i*PrOH/hexane = 20/80, 1.0 mL/min, 254 nm; *t_r* (major) = 24.68 min, *t_r* (minor) = 28.19 min) gave the isomeric composition

of the product: 96:4 er; $[\alpha]_D^{20} = 1.2$ (*c* = 0.3, CHCl₃); ¹H NMR (300 MHz, CDCl₃): δ 7.96-7.92 (m, 4H), 7.76-7.67 (m, 2H), 7.59-7.51 (m, 4H), 7.23-7.19 (m, 2H), 7.01-6.94 (m, 2H), 6.14 (dt, *J* = 6.3, 2.7 Hz, 1H), 5.72-5.64 (m, 1H), 3.27-3.24 (m, 1H), 3.20 (dt, *J* = 7.5, 2.4 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 207.6 (d, *J* = 2.4 Hz), 162.0 (d, *J* = 245.1 Hz), 135.3 (d, *J* = 1.4 Hz), 135.1, 134.9, 130.87, 130.85, 129.06, 129.04, 128.6 (d, *J* = 4.0 Hz), 115.6 (d, *J* = 30.0 Hz), 114.0 (d, *J* = 265.8 Hz), 95.0, 85.7 (d, *J* = 8.1 Hz), 30.9 (d, *J* = 18.9 Hz); ¹⁹F NMR (376 MHz, CDCl₃): δ -114.67 (s, 1F), -141.45 (s, 1F); IR (neat): 1730, 1697, 1599, 1338, 1155, 1080, 910, 837, 752, 559 cm⁻¹; HRMS (ESI): Exact mass calcd for C₂₃H₁₈F₂NaO₄S₂ [M+Na]⁺: 483.0512, Found: 483.0505.



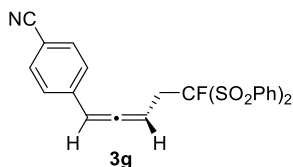
Product **3c** was obtained in 93% yield as a yellow oil (3 days). HPLC analysis (Chiralcel AD-H, *i*PrOH/hexane = 20/80, 1.0 mL/min, 254 nm; *t_r* (major) = 30.99 min, *t_r* (minor) = 33.83 min) gave the isomeric composition

of the product: 95.5:4.5 er; $[\alpha]_D^{20} = -67.2$ (*c* = 0.03, CHCl₃); ¹H NMR (400 MHz, CDCl₃): δ 7.93 (d, *J* = 8.4 Hz, 4H), 7.75-7.68 (m, 2H), 7.58-7.52 (m, 4H), 7.25-7.16 (m, 4H), 6.13 (dt, *J* = 6.8, 2.4 Hz, 1H), 5.72-5.69 (m, 1H), 3.26-3.24 (m, 1H), 3.23-3.19 (m, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 207.8, 135.3 (d, *J* = 1.7 Hz), 135.0, 134.9, 132.9, 131.8, 130.8, 129.0 (d, *J* = 1.7 Hz), 128.7, 128.3, 114.0 (d, *J* = 266.0 Hz), 95.0, 85.8 (d, *J* = 8.2 Hz), 30.8 (d, *J* = 18.9 Hz); ¹⁹F NMR (376 MHz, CDCl₃): δ -141.24 (s, 1F); IR (neat): 1583, 1491, 1448, 1336, 1151, 1080, 908, 835, 727, 557 cm⁻¹; HRMS (ESI): Exact mass calcd for C₂₃H₁₈FCINaO₄S₂ [M+Na]⁺: 499.0211, Found: 499.0208.



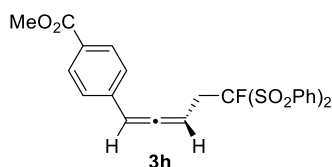
Product **3d** was obtained in 94% yield as a yellow oil (3 days). HPLC analysis (Chiralcel AD-H, *i*PrOH/hexane = 20/80, 1.0 mL/min, 254 nm; *t_r* (major) = 46.15 min, *t_r* (minor) = 34.72 min) gave the isomeric composition

of the product: 93:7 er; $[\alpha]_D^{20} = -270.4$ (*c* = 0.17, CHCl₃); ¹H NMR (400 MHz, CDCl₃): δ 7.96-7.92 (m, 4H), 7.74-7.66 (m, 2H), 7.58-7.51 (m, 4H), 7.23-7.15 (m, 3H), 7.12-7.10 (m, 1H), 6.11 (dt, *J* = 6.4, 2.4 Hz, 1H), 5.73-5.68 (m, 1H), 3.26 (dd, *J* = 7.6, 2.4 Hz, 1H), 3.22 (dd, *J* = 7.6, 2.8 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 207.9, 135.4 (d, *J* = 3.5 Hz), 135.3, 135.0, 134.8, 134.4, 130.87,



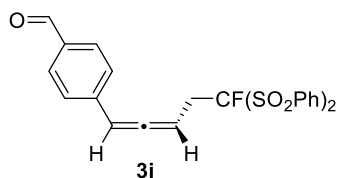
Product **3g** was obtained in 94% yield as a orange oil (3 days). HPLC analysis (Chiralcel AD-H, *i*PrOH/hexane = 50/50, 0.8 mL/min, 254 nm; *t_r* (major) = 33.24 min, *t_r* (minor) = 29.29 min) gave the isomeric composition

of the product: 95:5 er; $[\alpha]_D^{20} = -131.1$ (*c* = 0.3, CHCl₃); ¹H NMR (400 MHz, CDCl₃): δ 7.93-7.90 (m, 4H), 7.76-7.69 (m, 2H), 7.58-7.52 (m, 6H), 7.37-7.45 (m, 2H), 6.21 (dt, *J* = 6.4, 2.4 Hz, 1H), 5.86-5.81 (m, 1H), 3.33-3.16 (m, 2H); ¹³C NMR (100 MHz, CDCl₃): δ 208.8, 138.5, 135.4 (d, *J* = 1.5 Hz), 134.9, 134.7, 132.3, 130.8, 129.1, 127.6, 118.9, 113.8 (d, *J* = 266.1 Hz), 110.4, 95.2, 86.5 (d, *J* = 8.1 Hz), 30.6 (d, *J* = 19.0 Hz); ¹⁹F NMR (376 MHz, CDCl₃): δ -141.04 (s, 1F); IR (neat): 1726, 1448, 1336, 1163, 1151, 1080, 910, 752, 727, 682, 557 cm⁻¹; HRMS (ESI): Exact mass calcd for C₂₄H₁₈FNNaO₄S₂ [M+Na]⁺: 490.0553, Found: 490.0549.



Product **3h** was obtained in 91% yield as a yellow oil (3 days). HPLC analysis (Chiralcel AD-H, *i*PrOH/hexane = 50/50, 0.8 mL/min, 254 nm; *t_r* (major) = 32.78 min, *t_r* (minor) = 27.09 min) gave the isomeric composition

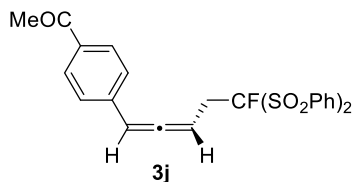
of the product: 95:5 er; $[\alpha]_D^{20} = -31.2$ (*c* = 0.02, CHCl₃); ¹H NMR (300 MHz, CDCl₃): δ 7.94-7.89 (m, 6H), 7.70-7.63 (m, 2H), 7.55-7.47 (m, 4H), 7.29 (d, *J* = 8.4 Hz, 2H), 6.20-6.17 (m, 1H), 5.78-5.70 (m, 1H), 3.87 (s, 3H), 3.30-3.21 (m, 2H); ¹³C NMR (125 MHz, CDCl₃): δ 208.6, 166.7, 138.2, 135.3 (d, *J* = 3.4 Hz), 134.9, 134.7, 130.74, 130.73, 129.8, 129.0 (d, *J* = 2.1 Hz), 128.7, 126.9, 113.8 (d, *J* = 265.9 Hz), 95.4, 85.9 (d, *J* = 8.1 Hz), 52.0, 30.6 (d, *J* = 18.9 Hz); ¹⁹F NMR (282 MHz, CDCl₃): δ -141.21 (s, 1F); IR (neat): 1716, 1448, 1348, 1280, 1153, 1080, 906, 723, 682, 557, 511 cm⁻¹; HRMS (ESI): Exact mass calcd for C₂₅H₂₁FNaO₆S₂ [M+Na]⁺: 523.0656, Found: 523.0654.



Product **3i** was obtained in 53% yield as a yellow oil (4 days). HPLC analysis (Chiralcel AD-H, *i*PrOH/hexane = 50/50, 0.8 mL/min, 254 nm; *t_r* (major) = 38.77 min, *t_r* (minor) = 32.39 min) gave the isomeric composition of the product: 93:7 er; $[\alpha]_D^{20} = 3.3$ (*c* = 0.1, CHCl₃); ¹H

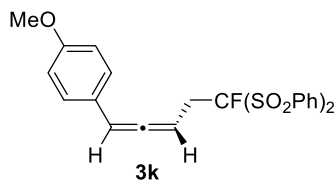
NMR (300 MHz, CDCl₃): δ 9.96 (s, 1H), 7.93 (d, *J* = 8.1 Hz, 4H), 7.80 (d, *J* = 8.1 Hz, 2H), 7.76-7.67 (m, 2H), 7.58-7.51 (m, 4H), 7.41 (d, *J* = 8.1 Hz, 2H), 6.25-6.23 (m, 1H), 5.84-5.76 (m, 1H), 3.31-3.21 (m, 2H); ¹³C NMR (125 MHz, CDCl₃): δ 209.0, 191.6, 140.0, 135.4 (d, *J* = 2.9 Hz), 135.2, 135.0, 134.8, 130.8, 130.1, 129.1 (d, *J* = 1.8 Hz), 127.6, 113.9 (d, *J* = 265.9 Hz), 95.5, 86.2 (d, *J* =

8.1 Hz), 30.6 (d, $J = 18.9$ Hz); ^{19}F NMR (282 MHz, CDCl_3): δ -141.24 (s, 1F); IR (neat): 1693, 1602, 1448, 1348, 1165, 1080, 912, 750, 729, 684 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{24}\text{H}_{19}\text{FNaO}_5\text{S}_2$ $[\text{M}+\text{Na}]^+$: 493.0550, Found: 493.0556.



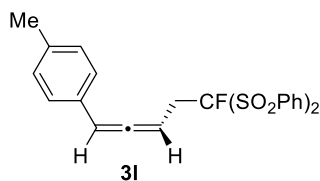
Product **3j** was obtained in 92% yield as a yellow oil (3 days). HPLC analysis (Chiralcel AD-H, $i\text{PrOH}$ /hexane = 40/60, 1.0 mL/min, 254 nm; t_r (major) = 35.93 min, t_r (minor) = 33.28 min) gave the isomeric

composition of the product: 96.5:3.5 er. $[\alpha]_{\text{D}}^{20} = -9.5$ ($c = 0.03$, CHCl_3); ^1H NMR (500 MHz, CDCl_3): δ 7.95 (d, $J = 8.5$ Hz, 4H), 7.91-7.89 (m, 2H), 7.77-7.70 (m, 2H), 7.59-7.54 (m, 4H), 7.36 (d, $J = 8.5$ Hz, 2H), 6.24 (dt, $J = 6.0, 2.5$ Hz, 1H), 5.81-5.77 (m, 1H), 3.34-3.21 (m, 2H), 2.60 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 208.8, 197.5, 138.5, 135.8, 135.4 (d, $J = 2.8$ Hz), 135.0, 134.8, 130.8, 129.1 (d, $J = 2.0$ Hz), 128.7, 127.2, 113.9 (d, $J = 265.6$ Hz), 95.4, 86.0 (d, $J = 8.1$ Hz), 30.6 (d, $J = 19.0$ Hz), 26.5; ^{19}F NMR (376 MHz, CDCl_3): δ -142.26 (s, 1F); IR (neat): 1732, 1682, 1448, 1340, 1267, 1153, 1080, 754, 684, 592, 563 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{25}\text{H}_{21}\text{FNaO}_5\text{S}_2$ $[\text{M}+\text{Na}]^+$: 507.0707, Found: 507.0711.



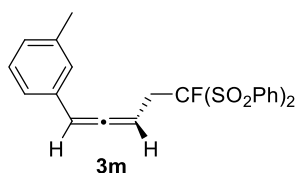
Product **3k** was obtained in 91% yield as a yellow oil (3 days). HPLC analysis (Chiralcel AD-H, $i\text{PrOH}$ /hexane = 30/70, 1.0 mL/min, 254 nm; t_r (major) = 23.12 min, t_r (minor) = 26.74 min) gave the isomeric

composition of the product: 95.5:4.5 er; $[\alpha]_{\text{D}}^{20} = -4.4$ ($c = 0.2$, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ 7.96-7.93 (m, 4H), 7.74-7.67 (m, 2H), 7.57-7.52 (m, 4H), 7.18-7.14 (m, 2H), 6.84-6.81 (m, 2H), 6.12 (dt, $J = 6.4, 2.4$ Hz, 1H), 5.65-5.60 (m, 1H), 3.79 (s, 3H), 3.25-3.22 (m, 1H), 3.21-3.18 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 207.3, 159.0, 135.3, 135.2, 135.0, 130.9, 129.03, 129.01, 128.2, 125.4, 114.13 (d, $J = 266.0$ Hz), 114.09, 95.3, 85.2 (d, $J = 8.1$ Hz), 55.3, 31.1 (d, $J = 18.7$ Hz); ^{19}F NMR (376 MHz, CDCl_3): δ -141.56 (s, 1F); IR (neat): 1732, 1599, 1512, 1448, 1249, 1151, 835, 754, 684, 559 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{24}\text{H}_{21}\text{FNaO}_5\text{S}_2$ $[\text{M}+\text{Na}]^+$: 495.0706, Found: 495.0711.



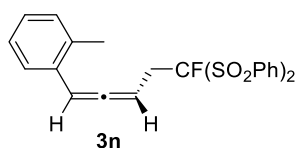
Product **3l** was obtained in 90% yield as a yellow oil (3 days). HPLC analysis (Chiralcel AS-H, *i*PrOH/hexane = 30/70, 1.0 mL/min, 254 nm; *t_r* (major) = 28.74 min, *t_r* (minor) = 24.65 min) gave the isomeric composition of the product: 93.5:6.5 er; $[\alpha]_D^{20} = -0.4$ (*c* = 0.01, CHCl₃);

¹H NMR (400 MHz, CDCl₃): δ 7.94 (d, *J* = 6.8 Hz, 4H), 7.73-7.66 (m, 2H), 7.56-7.51 (m, 4H), 7.13-7.07 (m, 4H), 6.13 (dt, *J* = 6.4, 2.8 Hz, 1H), 5.65-5.60 (m, 1H), 3.26-3.18 (m, 2H), 2.32 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 207.5, 137.1, 135.3 (d, *J* = 1.8 Hz), 135.2, 135.0, 130.8, 130.2, 129.3, 129.0 (d, *J* = 2.3 Hz), 127.0, 114.1 (d, *J* = 266.0 Hz), 95.7, 85.2 (d, *J* = 8.1 Hz), 30.9 (d, *J* = 18.9 Hz), 21.2; ¹⁹F NMR (376 MHz, CDCl₃): δ -141.57 (s, 1F); IR (neat): 1734, 1343, 1238, 1155, 1043, 756, 684, 592, 559 cm⁻¹; HRMS (ESI): Exact mass calcd for C₂₄H₂₁FNaO₄S₂ [M+Na]⁺: 479.0757, Found: 479.0763.



Product **3m** was obtained in 88% yield as a yellow oil (3 days). HPLC analysis (Chiralcel AD-H, *i*PrOH/hexane = 20/80, 1.0 mL/min, 254 nm; *t_r*(major) = 16.61 min, *t_r*(minor) = 17.56 min) gave the isomeric composition

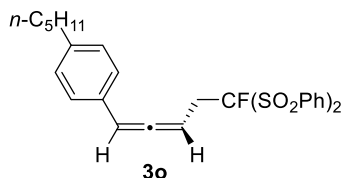
of the product: 95.5:4.5 er; $[\alpha]_D^{20} = -115.3$ (*c* = 0.2, CHCl₃); ¹H NMR (400 MHz, CDCl₃): δ 7.93 (d, *J* = 8.0 Hz, 4H), 7.72-7.65 (m, 2H), 7.55-7.49 (m, 4H), 7.16 (t, *J* = 7.6 Hz, 1H), 7.07 (s, 1H), 7.03-7.00 (m, 2H), 6.12 (dt, *J* = 6.4, 2.4 Hz, 1H), 5.67-5.62 (m, 1H), 3.32-3.15 (m, 2H), 2.30 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 207.7, 138.1, 135.3 (d, *J* = 2.4 Hz), 135.1, 134.9, 133.0, 130.8, 129.0 (d, *J* = 2.6 Hz), 128.4, 128.1, 127.7, 124.2, 114.0 (d, *J* = 265.9 Hz), 95.9, 85.2 (d, *J* = 8.2 Hz), 30.8 (d, *J* = 18.9 Hz), 21.2; ¹⁹F NMR (376 MHz, CDCl₃): δ -141.47 (s, 1F); IR (neat): 1583, 1448, 1346, 1153, 1080, 908, 773, 752, 725, 682, 599, 559 cm⁻¹; HRMS (ESI): Exact mass calcd for C₂₄H₂₁FNaO₄S₂ [M+Na]⁺: 479.0757, Found: 479.0755.



Product **3n** was obtained in 72% yield as a yellow oil (3 days). HPLC analysis (Chiralcel OD-H, *i*PrOH/hexane = 25/75, 1.0 mL/min, 254 nm; *t_r*(major) = 16.17 min, *t_r*(minor) = 18.46 min) gave the isomeric

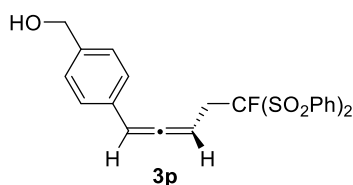
composition of the product: 95.5:4.5 er; $[\alpha]_D^{20} = -203.5$ (*c* = 0.2, CHCl₃); ¹H NMR (400 MHz, CDCl₃): δ 7.95 (d, *J* = 8.0 Hz, 4H), 7.74-7.68 (m, 2H), 7.57-7.52 (m, 4H), 7.26-7.24 (m, 1H), 7.12 (s, 3H), 6.34 (d, *J* = 6.4 Hz, 1H), 5.64-5.59 (m, 1H), 3.26 (d, *J* = 6.8 Hz, 1H), 3.21 (d, *J* = 7.6 Hz, 1H),

2.31 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 208.3, 135.3 (d, $J = 1.0$ Hz), 135.1, 134.9, 131.5, 130.9, 130.4, 129.0 (d, $J = 2.0$ Hz), 127.7, 127.2, 126.1, 114.0 (d, $J = 266.2$ Hz), 93.2, 84.5 (d, $J = 8.2$ Hz), 30.9 (d, $J = 18.9$ Hz), 19.8; ^{19}F NMR (376 MHz, CDCl_3): δ -141.75 (s, 1F); IR (neat): 1450, 1342, 1157, 1080, 732, 686, 563 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{24}\text{H}_{21}\text{FNaO}_4\text{S}_2$ $[\text{M}+\text{Na}]^+$: 497.0758, Found: 497.0765.



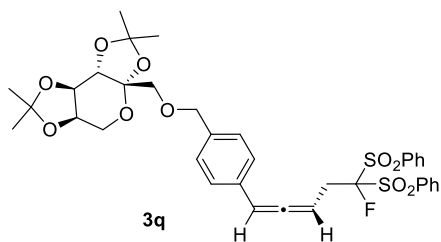
Product **3o** was obtained in 91% yield as a yellow oil (3 days). HPLC analysis (Chiralcel AD-H, i PrOH/hexane = 20/80, 1.0 mL/min, 254 nm; t_r (major) = 15.99 min, t_r (minor) = 18.34 min) gave the isomeric

composition of the product: 95.5:4.5 er; $[\alpha]_{\text{D}}^{20} = -23.8$ ($c = 0.04$, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ 7.94 (d, $J = 8.0$ Hz, 4H), 7.72-7.65 (m, 2H), 7.55-7.50 (m, 4H), 7.15-7.08 (m, 4H), 6.15-6.12 (m, 1H), 5.65-5.60 (m, 1H), 3.26-3.18 (m, 2H), 2.56 (t, $J = 7.6$ Hz, 2H), 1.62-1.55 (m, 2H), 1.36-1.26 (m, 4H), 0.88 (t, $J = 6.8$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 207.6, 142.2, 135.3 (d, $J = 2.3$ Hz), 135.2, 135.0, 130.8, 130.4, 129.0 (d, $J = 2.2$ Hz), 128.7, 127.0, 114.1 (d, $J = 266.1$ Hz), 95.7, 85.1 (d, $J = 8.1$ Hz), 35.6, 31.4, 31.1, 30.9 (d, $J = 18.9$ Hz), 22.5, 14.0; ^{19}F NMR (376 MHz, CDCl_3): δ -141.54 (s, 1F); IR (neat): 1448, 1348, 1313, 1153, 1080, 908, 752, 727, 682, 596, 555 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{28}\text{H}_{30}\text{FO}_4\text{S}_2$ $[\text{M}+\text{H}]^+$: 513.1564, Found: 513.1563.



Product **3p** was obtained in 71% yield as a yellow oil (3 days). HPLC analysis (Chiralcel AS-H, i PrOH/hexane = 40/60, 1.0 mL/min, 254 nm; t_r (major) = 51.38 min, t_r (minor) = 37.21 min) gave the isomeric

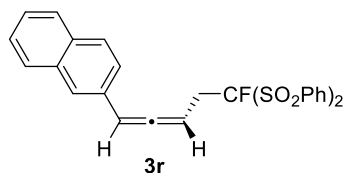
composition of the product: 95:5 er; $[\alpha]_{\text{D}}^{20} = -50.2$ ($c = 0.04$, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ 7.94 (d, $J = 7.6$ Hz, 4H), 7.74-7.68 (m, 2H), 7.57-7.52 (m, 4H), 7.29-7.22 (m, 4H), 6.17-6.16 (m, 1H), 5.69-5.64 (m, 1H), 4.66 (s, 2H), 3.26-3.20 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 207.7, 140.1, 135.3 (d, $J = 1.4$ Hz), 134.9, 134.7, 132.3, 130.7, 129.0 (d, $J = 2.0$ Hz), 127.2, 127.1, 114.0 (d, $J = 266.3$ Hz), 95.6, 85.3 (d, $J = 8.1$ Hz), 64.6, 30.7 (d, $J = 18.8$ Hz); ^{19}F NMR (376 MHz, CDCl_3): δ -141.36 (s, 1F); IR (neat): 1448, 1348, 1165, 1155, 1080, 902, 721, 682, 596, 557 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{24}\text{H}_{21}\text{FNaO}_5\text{S}_2$ $[\text{M}+\text{Na}]^+$: 495.0707, Found: 495.0703.



Product **3q** was obtained in 60% yield as a yellow oil (3 days).

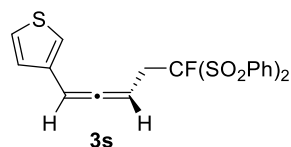
^9F NMR analysis of the crude mixture revealed that the dr value was $>20:1$; $[\alpha]_{\text{D}}^{20} = -17.5$ ($c = 0.3$, CHCl_3); ^1H NMR (400 MHz, CDCl_3): 7.94 (d, $J = 7.6$ Hz, 4H), 7.75-7.67 (m, 2H), 7.58-7.52 (m, 4H), 7.26 (d, $J = 8.0$ Hz, 2H), 7.19 (d, $J = 8.0$ Hz, 2H), 6.15

(dt, $J = 6.4, 2.4$ Hz, 1H), 5.68-5.63 (m, 1H), 4.66-4.54 (m, 3H), 4.43 (d, $J = 2.4$ Hz, 1H), 4.23 (dd, $J = 8.0, 1.6$ Hz, 1H), 3.92 (dd, $J = 12.8, 2.0$ Hz, 1H), 3.73 (d, $J = 12.8$ Hz, 1H), 3.25 (dd, $J = 7.6, 2.4$ Hz, 1H), 3.21 (dt, $J = 7.2, 2.0$ Hz, 1H), 1.54 (s, 3H), 1.42-1.41 (m, 6H), 1.33 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 207.8, 137.3, 135.3, 135.2, 135.0, 132.5, 130.91, 130.9 (t, $J = 1.9$ Hz), 129.0, 127.9, 127.0, 114.1 (d, $J = 266.1$ Hz), 108.9, 108.5, 102.7, 95.6, 85.4 (d, $J = 7.8$ Hz), 73.4, 71.5, 71.0, 70.2, 70.1, 61.0, 30.8 (d, $J = 18.7$ Hz), 26.6, 25.8, 25.4, 24.0; ^{19}F NMR (376 MHz, CDCl_3): δ -141.58 (s, 1F); IR (neat): 1448, 1350, 1251, 1165, 1112, 1070, 910, 731, 684 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{36}\text{H}_{39}\text{FNaO}_{10}\text{S}_2$ $[\text{M}+\text{Na}]^+$: 737.1861, Found: 737.1867.



Product **3r** was obtained in 93% yield as a yellow solid (3 days). m.p. = 115-116 $^{\circ}\text{C}$; HPLC analysis (Chiralcel AS-H, $i\text{PrOH}$ /hexane = 40/60, 1.0 mL/min, 254 nm; t_{r} (major) = 33.17 min, t_{r} (minor) = 28.41 min)

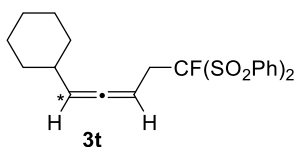
gave the isomeric composition of the product: 93:7 er; $[\alpha]_{\text{D}}^{20} = -163.6$ ($c = 0.3$, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ 7.95-7.93 (m, 4H), 7.78-7.68 (m, 4H), 7.66-7.62 (m, 2H), 7.56-7.48 (m, 4H), 7.46-7.40 (m, 3H), 6.34-6.32 (m, 1H), 5.77-5.72 (m, 1H), 3.31-3.25 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 208.3, 135.3 (d, $J = 3.3$ Hz), 135.1, 134.9, 133.5, 132.7, 130.87, 130.86, 130.84, 130.83, 130.76, 129.0 (d, $J = 3.0$ Hz), 128.2, 127.7, 127.6, 126.2, 126.0, 125.8, 124.8, 114.0 (d, $J = 265.9$ Hz), 96.2, 85.6 (d, $J = 8.2$ Hz), 30.9 (d, $J = 18.8$ Hz); ^{19}F NMR (376 MHz, CDCl_3): δ -141.39 (s, 1F); IR (neat): 1448, 1336, 1151, 1078, 906, 821, 723, 682, 599, 557 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{27}\text{H}_{21}\text{FNaO}_4\text{S}_2$ $[\text{M}+\text{Na}]^+$: 515.0757, Found: 515.0751.



Product **3s** was obtained in 69% yield as a yellow solid (3 days). m.p. = 120 -122 $^{\circ}\text{C}$; HPLC analysis (Chiralcel AD-H, $i\text{PrOH}$ /hexane = 30/70, 1.0 mL/min, 254 nm; t_{r} (major) = 23.33 min, t_{r} (minor) = 25.27 min) gave the

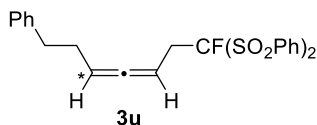
isomeric composition of the product: 93:7 er; $[\alpha]_{\text{D}}^{20} = -209.1$ ($c = 0.2$, CHCl_3); ^1H NMR (400 MHz,

CDCl₃): δ 7.94-7.92 (m, 4H), 7.74-7.67 (m, 2H), 7.57-7.51 (m, 4H), 7.26-7.23 (m, 1H), 7.09-7.08 (m, 1H), 7.04 (dd, J = 4.8, 1.2 Hz, 1H), 6.24 (dt, J = 6.8, 2.4 Hz, 1H), 5.63-5.58 (m, 1H), 3.28-3.13 (m, 2H); ¹³C NMR (100 MHz, CDCl₃): δ 208.1, 135.3 (d, J = 3.0 Hz), 135.1, 134.9, 134.3, 130.84, 130.82, 130.81, 129.0 (d, J = 2.5 Hz), 126.5, 125.9, 121.6, 114.0 (d, J = 266.1 Hz), 90.4, 84.6 (d, J = 8.2 Hz), 31.0 (d, J = 18.8 Hz); ¹⁹F NMR (376 MHz, CDCl₃): δ -141.40 (s, 1F); IR (neat): 1448, 1346, 1313, 1151, 1080, 908, 750, 682, 559 cm⁻¹; HRMS (ESI): Exact mass calcd for C₂₁H₁₇FN₄O₄S₃ [M+Na]⁺: 471.0165, Found: 471.0176.



The reaction (0.25 mmol) was carried out at 40 °C for 4 days using Ni(COD)₂ (6.8 mg, 10 mol%), (*S*)-difluorophos (**L9**, 18.8 mg, 11 mol%), and DABCO (28.0 mg, 1.0 equivs). Product **3t** was obtained in 67% yield

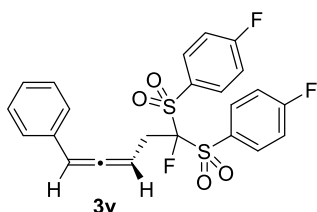
as a yellow oil. HPLC analysis (Chiralcel AD-H, ⁱPrOH/hexane = 30/70, 1.0 mL/min, 230 nm; t_r (major) = 7.70 min, t_r (minor) = 10.37 min) gave the isomeric composition of the product: 76.5:23.5 er. [α]_D²⁰ = -86.9 (c = 0.2, CHCl₃); ¹H NMR (400 MHz, CDCl₃): δ 7.94 (d, J = 8.4 Hz, 4H), 7.74-7.70 (m, 2H), 7.56 (t, J = 7.2 Hz, 4H), 5.14-5.07 (m, 2H), 3.21-3.05 (m, 2H), 1.94-1.85 (m, 1H), 1.69-1.58 (m, 5H), 1.29-1.06 (m, 3H), 1.02-0.91 (m, 2H); ¹³C NMR (100 MHz, CDCl₃): δ 205.6, 135.4, 135.2, 135.1, 130.9 (d, J = 1.4 Hz), 129.0, 128.9, 114.3 (d, J = 266.2 Hz), 98.4, 81.9 (d, J = 7.9 Hz), 36.8, 32.7 (d, J = 2.5 Hz), 31.3 (d, J = 18.7 Hz), 26.0, 25.9; ¹⁹F NMR (376 MHz, CDCl₃): δ -142.32 (s, 1F); IR (neat): 1448, 1346, 1313, 1153, 1080, 754, 736, 684, 567 cm⁻¹; HRMS (ESI): Exact mass calcd for C₂₃H₂₆FO₄S₂ [M+H]⁺: 449.1251, Found: 449.1241.



The reaction (0.25 mmol) was carried out at 40 °C for 4 days using Ni(COD)₂ (13.8 mg, 20 mol%), Josiphos SL-009-1 (**L10**, 37.6 mg, 22 mol%), and DABCO (56.0 mg, 2.0 equivs). Product **3u** was obtained in 43% yield as a yellow oil.

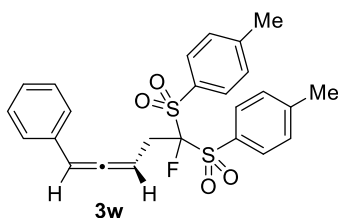
HPLC analysis (Chiralcel AD-H, ⁱPrOH/hexane = 20/80, 1.0 mL/min, 254 nm; t_r (major) = 15.52 min, t_r (minor) = 22.30 min) gave the isomeric composition of the product: 95:5 er; [α]_D²⁰ = -33.4 (c = 0.1, CHCl₃); ¹H NMR (400 MHz, CDCl₃): δ 7.94-7.89 (m, 4H), 7.73-7.68 (m, 2H), 7.58-7.52 (m, 4H), 7.30-7.26 (m, 2H), 7.21-7.14 (m, 3H), 5.19-5.08 (m, 2H), 3.21-2.95 (m, 2H), 2.64 (t, J = 8.0, 2H), 2.29-2.23 (m, 2H); ¹³C NMR (100 MHz, CDCl₃): δ 206.7, 141.4, 135.3, 135.2 (d, J = 1.7 Hz), 130.86, 130.85, 130.83, 128.9 (d, J = 1.7 Hz), 128.4, 128.3, 125.9, 114.3 (d, J = 266.1 Hz), 91.7,

81.6 (d, $J = 8.2$ Hz), 35.1, 31.0 (d, $J = 18.5$ Hz), 29.7; ^{19}F NMR (376 MHz, CDCl_3): δ -141.95 (s, 1F); IR (neat): 1450, 1342, 1157, 1080, 1026, 995, 871, 732, 678 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{25}\text{H}_{24}\text{FO}_4\text{S}_2$ $[\text{M}+\text{H}]^+$: 471.1095, Found: 471.1083.



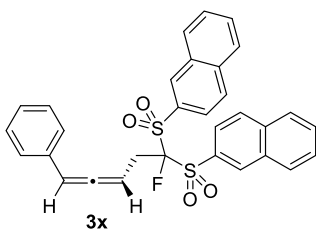
Product **3v** was obtained in 82% yield as a yellow oil (3 days). HPLC analysis (Chiralcel AD-H, $i\text{PrOH}$ /hexane = 20/80, 1.0 mL/min, 254 nm; t_r (major) = 24.07 min, t_r (minor) = 29.00 min) gave the isomeric composition of the product: 95.5:4.5 er; $[\alpha]_{\text{D}}^{20} = -294.9$ ($c = 0.3$, CHCl_3);

^1H NMR (400 MHz, CDCl_3): δ 7.99-7.96 (m, 4H), 7.32-7.18 (m, 9H), 6.18 (dt, $J = 6.8, 2.8$ Hz, 1H), 5.69-5.63 (m, 1H), 3.23 (dd, $J = 7.6, 2.4$ Hz, 1H), 3.19 (dd, $J = 7.6, 2.4$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 207.8, 168.3 (d, $J = 2.0$ Hz), 134.09-134.04 (m), 133.99-133.95 (m), 133.1, 131.0 (d, $J = 3.0$ Hz), 130.7 (d, $J = 3.0$ Hz), 128.7, 127.5, 127.1, 116.7 (d, $J = 1.0$ Hz), 116.5 (d, $J = 2.0$ Hz), 113.9 (d, $J = 265.0$ Hz), 96.1, 85.2 (d, $J = 9.0$ Hz), 31.0 (d, $J = 19.0$ Hz); ^{19}F NMR (376 MHz, CDCl_3): δ -99.65 (s, 1F), -99.69 (s, 1F), -141.15 (s, 1F); IR (neat): 1589, 1491, 1348, 1242, 1149, 1080, 906, 837, 729, 650 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{23}\text{H}_{17}\text{F}_3\text{NaO}_4\text{S}_2$ $[\text{M}+\text{Na}]^+$: 501.0413, Found: 501.0401.



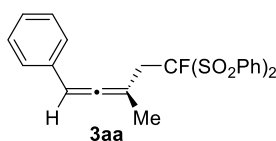
Product **3w** was obtained in 85% yield as a yellow oil (3 days). HPLC analysis (Chiralcel AD-H, $i\text{PrOH}$ /hexane = 20/80, 1.0 mL/min, 254 nm; t_r (major) = 25.44 min, t_r (minor) = 31.64 min) gave the isomeric composition of the product: 96:4 er; $[\alpha]_{\text{D}}^{20} = -130.3$ ($c = 0.3$, CHCl_3);

^1H NMR (400 MHz, CDCl_3): δ 7.83-7.80 (m, 4H), 7.34-7.17 (m, 9H), 6.15 (dt, $J = 6.4, 2.4$ Hz, 1H), 5.68-5.62 (m, 1H), 3.23 (dd, $J = 7.6, 2.4$ Hz, 1H), 3.19 (dd, $J = 7.6, 2.4$ Hz, 1H), 2.45 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 207.6, 146.7, 133.3, 132.1, 131.9, 130.9 (d, $J = 1.0$ Hz), 130.8 (d, $J = 1.0$ Hz), 129.6, 128.5, 127.2, 127.0, 113.8 (d, $J = 265.3$ Hz), 95.8, 85.6 (d, $J = 8.0$ Hz), 30.9 (d, $J = 19.1$ Hz), 21.8 (d, $J = 3.6$ Hz); ^{19}F NMR (376 MHz, CDCl_3): δ -142.03 (s, 1F); IR (neat): 1450, 1342, 1265, 1157, 1080, 732, 686, 648, 594 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{25}\text{H}_{24}\text{FO}_4\text{S}_2$ $[\text{M}+\text{H}]^+$: 471.1095, Found: 471.1086.



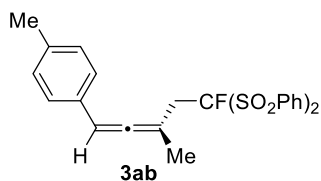
Product **3x** was obtained in 98% yield as a yellow solid (3 days). m.p. = 108-109 °C; HPLC analysis (Chiralcel OD-H, *i*PrOH/hexane = 10/90, 1.0 mL/min, 254 nm; *t_r* (major) = 34.90 min, *t_r* (minor) = 40.53 min) gave the isomeric composition of the product: 95.5:4.5 er; $[\alpha]_D^{20} = -366.4$ (*c* =

0.4, CHCl₃); ¹H NMR (400 MHz, CDCl₃): δ 8.42 (d, *J* = 9.6 Hz, 2H), 7.84-7.79 (m, 7H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.67-7.62 (m, 2H), 7.57-7.53 (m, 2H), 7.25-7.21 (m, 4H), 7.20-7.17 (m, 1H), 6.12 (dt, *J* = 6.4, 2.4 Hz, 1H), 5.82-5.76 (m, 1H), 3.41 (dd, *J* = 7.6, 2.4 Hz, 1H), 3.37 (dd, *J* = 7.2, 2.4 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 207.8, 135.8, 133.4, 133.35, 133.3, 131.9, 131.8, 131.7, 131.6, 130.0 (d, *J* = 3.0 Hz), 129.6, 129.0, 128.5, 127.88, 127.86, 127.73, 127.7, 127.3, 127.1, 124.5, 114.6 (d, *J* = 265.7 Hz), 95.9, 85.6 (d, *J* = 8.4 Hz), 30.7 (d, *J* = 18.8 Hz); ¹⁹F NMR (376 MHz, CDCl₃): δ -140.60 (s, 1F); IR (neat): 1496, 1334, 1149, 1072, 856, 817, 740, 686, 640 cm⁻¹; HRMS (ESI): Exact mass calcd for C₃₁H₂₃FO₄NaS₂ [M+Na]⁺: 565.0914, Found: 565.0902.



The reaction (0.25 mmol) was carried out at 60 °C for 6 days using Ni(COD)₂ (13.8 mg, 20 mol%), (*S,S*)-Benzp* (**L11**, 15.5 mg, 22 mol%), and DABCO (56.0 mg, 2.0 equivs). Product **3aa** was obtained in 43% yield as a

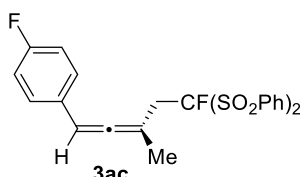
colorless oil. HPLC analysis (Chiralcel AD-H, *i*PrOH/hexane = 20/80, 1.0 mL/min, 254 nm; *t_r* (major) = 16.14 min, *t_r* (minor) = 13.55 min) gave the isomeric composition of the product: 91.5:8.5 er; $[\alpha]_D^{20} = -120.2$ (*c* = 0.1, CHCl₃); ¹H NMR (400 MHz, CDCl₃): δ 7.94-7.88 (m, 4H), 7.72-7.67 (m, 1H), 7.66-7.62 (m, 1H), 7.56-7.46 (m, 4H), 7.29-7.16 (m, 5H), 5.90-5.87 (m, 1H), 3.37-3.22 (m, 2H), 1.79 (dd, *J* = 2.8, 1.6 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 206.2, 135.3, 135.2, 135.12, 135.11, 134.2, 131.0 (d, *J* = 1.4 Hz), 130.8 (d, *J* = 1.3 Hz), 128.9, 128.5, 127.1, 127.0, 115.3 (d, *J* = 269.5 Hz), 94.8 (d, *J* = 3.3 Hz), 94.2, 34.1 (d, *J* = 17.2 Hz), 19.6 (d, *J* = 2.0 Hz); IR (neat): 1450, 1342, 1265, 1149, 1080, 825, 732, 686, 624, 601 cm⁻¹; HRMS (ESI): Exact mass calcd for C₂₄H₂₂FO₄S₂ [M+H]⁺: 457.0938, Found: 457.0932.



The reaction (0.25 mmol) was carried out at 60 °C for 4 days using Ni(COD)₂ (13.8 mg, 20 mol%), (*S,S*)-Benzp* (**L11**, 15.5 mg, 22 mol%), and DABCO (56.0 mg, 2.0 equivs). Product **3ab** was obtained in 39%

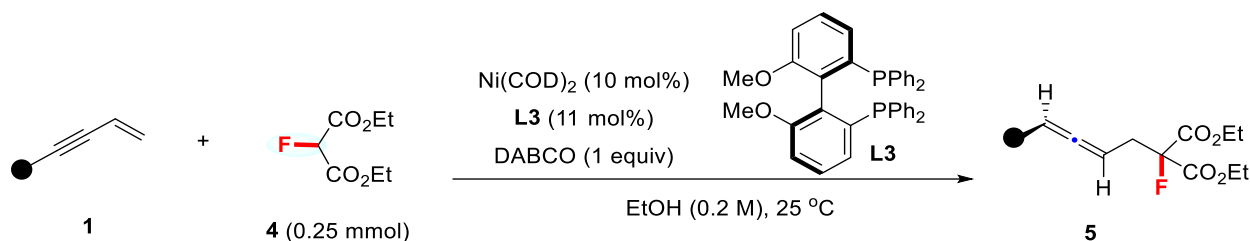
yield as a yellow oil. HPLC analysis (Chiralcel AD-H, *i*PrOH/hexane = 20/80, 1.0 mL/min, 254 nm;

$t_r(\text{major}) = 15.80 \text{ min}$, $t_r(\text{minor}) = 13.28 \text{ min}$) gave the isomeric composition of the product: 94.5:5.5 er; $[\alpha]_D^{20} = -134.4$ ($c = 0.1$, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ 7.94-7.89 (m, 4H), 7.71-7.62 (m, 2H), 7.54-7.46 (m, 4H), 7.12-7.07 (m, 4H), 5.87-5.84 (m, 1H), 3.36-3.21 (m, 2H), 2.32 (s, 3H), 1.77 (dd, $J = 3.2, 1.6 \text{ Hz}$, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 206.0, 136.7, 135.3, 135.15, 135.13, 135.1, 131.2, 130.9 (d, $J = 1.5 \text{ Hz}$), 130.8 (d, $J = 1.3 \text{ Hz}$), 129.2, 128.9, 127.0, 115.3 (d, $J = 269.3 \text{ Hz}$), 94.6 (d, $J = 3.2 \text{ Hz}$), 94.0, 34.2 (d, $J = 17.3 \text{ Hz}$), 21.2, 19.6 (d, $J = 2.2 \text{ Hz}$); ^{19}F NMR (376 MHz, CDCl_3): δ -144.16 (s, 1F); IR (neat): 1342, 1265, 1157, 1080, 732, 609, 547, 532, 462 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{25}\text{H}_{24}\text{FO}_4\text{S}_2$ $[\text{M}+\text{H}]^+$: 471.1095, Found: 471.1088.

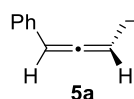


The reaction (0.25 mmol) was carried out at 60 °C for 5 days using $\text{Ni}(\text{COD})_2$ (13.8 mg, 20 mol%), (*S,S*)-Benzp* (**L11**, 15.5 mg, 22 mol%), and DABCO (56.0 mg, 2.0 equivs). Product **3ac** was obtained in 44% yield as a yellow solid. m.p. = 105-106 °C; HPLC analysis (Chiralcel AD-H, $i\text{PrOH}$ /hexane = 20/80, 1.0 mL/min, 254 nm; $t_r(\text{major}) = 17.57 \text{ min}$, $t_r(\text{minor}) = 15.76 \text{ min}$) gave the isomeric composition of the product: 94:6 er; $[\alpha]_D^{20} = -89.9$ ($c = 0.1$, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ 7.92-7.88 (m, 4H), 7.72-7.63 (m, 2H), 7.55-7.47 (m, 4H), 7.21-7.18 (m, 2H), 6.99-6.93 (m, 2H), 5.91-5.88 (m, 1H), 3.30 (t, $J = 2.0 \text{ Hz}$, 1H), 3.25 (dd, $J = 3.6, 2.0 \text{ Hz}$, 1H), 1.79 (dd, $J = 2.8, 1.6 \text{ Hz}$, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 206.0 (d, $J = 2.5 \text{ Hz}$), 161.9 (d, $J = 244.6 \text{ Hz}$), 135.23, 135.18, 135.14, 130.9 (d, $J = 1.4 \text{ Hz}$), 130.8 (d, $J = 1.3 \text{ Hz}$), 130.2 (d, $J = 3.2 \text{ Hz}$), 128.96, 128.95, 128.6 (d, $J = 7.9 \text{ Hz}$), 115.4 (d, $J = 21.5 \text{ Hz}$), 115.3 (d, $J = 269.5 \text{ Hz}$), 95.1 (d, $J = 3.0 \text{ Hz}$), 93.3, 34.3 (d, $J = 17.4 \text{ Hz}$), 19.6 (d, $J = 2.2 \text{ Hz}$); ^{19}F NMR (376 MHz, CDCl_3): δ -115.21 (s, 1F), -144.18 (s, 1F); IR (neat): 1504, 1450, 1342, 1157, 1080, 848, 732, 686, 609, 547, 532 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{24}\text{H}_{21}\text{FO}_4\text{S}_2$ $[\text{M}+\text{H}]^+$: 475.0849, Found: 475.0838.

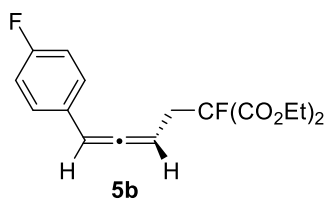
5. Enantioselective hydromonofluoroalkylation of 1,3-enynes **1** with **4**



In a glove box, to a Schlenk tube equipped with a stirring bar were successively added $\text{Ni}(\text{COD})_2$ (6.9 mg, 10 mol%), and (*R*)-MeO-BIPHEP **L3** (16.0 mg, 11 mol%), followed by the addition of absolute EtOH (1.25 mL). The resulting mixture was stirred at room temperature for 15 min, and then added DABCO (28.0 mg, 1.0 equiv) and diethyl fluoromalonate **4** (0.25 mmol, 1.0 equiv). After being stirred for another 5 min, to the mixture was added 1,3-enynes **1** (0.375 mmol, 1.5 equivs). After it take out from the glove box, the reaction mixture was stirred at 25 °C until full conversion. The reaction was monitored by TLC analysis. After full consumption of **4**, the reaction mixture was concentrated under vacuum. The crude residue was purified by silica gel column chromatography using PE/EtOAc (25:1-20:1, v/v) as the eluent to afford the desired products **5**. (Note: 20 mol% of Ni catalyst was used in the case of products **5v-5w**, and **5aa-5ac**)



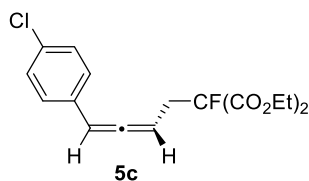
Product **5a** was obtained in 98% yield as a colorless oil (3 days). HPLC analysis (Chiralcel OJ-H, $i\text{PrOH}$ /hexane = 2/98, 1.0 mL/min, 254 nm; t_r (major) = 25.87 min, t_r (minor) = 32.16 min) gave the isomeric composition of the product: 95.5:4.5 er; $[\alpha]_D^{20} = -174.5$ ($c = 0.02$, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ 7.31-7.26 (m, 4H), 7.21-7.17 (m, 1H), 6.19 (dt, $J = 6.8, 2.0$ Hz, 1H), 5.56-5.50 (m, 1H), 4.32-4.20 (m, 4H), 3.03 (dt, $J = 7.6, 2.4$ Hz, 1H), 2.97 (dt, $J = 7.6, 2.0$ Hz, 1H), 1.30 (t, $J = 7.2$ Hz, 3H), 1.26 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 207.4, 165.7 (d, $J = 25.5$ Hz), 165.6 (d, $J = 25.3$ Hz), 133.6, 128.5, 127.1, 126.9, 95.3, 93.9 (d, $J = 198.7$ Hz), 86.6 (d, $J = 3.7$ Hz), 62.7, 62.67, 34.5, 34.2, 13.9, 13.8; ^{19}F NMR (376 MHz, CDCl_3): δ -166.40 (s, 1F); IR (neat): 1749, 1460, 1369, 1199, 1084, 1012, 873, 752, 692, 628 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{17}\text{H}_{20}\text{FO}_4$ $[\text{M}+\text{H}]^+$: 307.1340, Found: 307.1337



Product **5b** was obtained in 94% yield as a colorless oil (3 days). HPLC analysis (Chiralcel OD-H, *i*PrOH/hexane = 20/80, 1.0 mL/min, 254 nm; *t_r* (major) = 9.29 min, *t_r* (minor) = 8.17 min) gave the isomeric composition

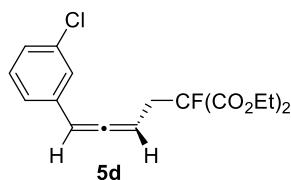
of the product: 96.5:3.5 er; $[\alpha]_D^{20} = -102.5$ (*c* = 0.2, CHCl₃); ¹H NMR

(400 MHz, CDCl₃): δ 7.26-7.21 (m, 2H), 7.01-6.96 (m, 2H), 6.16 (dt, *J* = 6.4, 2.4 Hz, 1H), 5.56-5.50 (m, 1H), 4.33-4.19 (m, 4H), 3.08-3.01 (m, 1H), 3.00-2.91 (m, 1H), 1.31 (t, *J* = 7.2 Hz, 3H), 1.27 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 207.2 (d, *J* = 2.3 Hz), 165.6 (d, *J* = 26 Hz), 165.5 (d, *J* = 26 Hz), 162.0 (d, *J* = 244.9 Hz), 129.6 (d, *J* = 3.3 Hz), 128.3 (d, *J* = 7.9 Hz), 115.5 (d, *J* = 21.5 Hz), 94.4, 93.8 (d, *J* = 198.9 Hz), 86.8 (d, *J* = 3.6 Hz), 62.72, 62.7, 34.3 (d, *J* = 21.0 Hz), 13.9, 13.8; ¹⁹F NMR (376 MHz, CDCl₃): δ -115.02 (s, 1F), -166.41 (s, 1F); IR (neat): 1747, 1508, 1300, 1222, 1157, 1093, 1012, 839, 698, 536 cm⁻¹; HRMS (ESI): Exact mass calcd for C₁₇H₁₈F₂NaO₄ [M+Na]⁺: 347.1065, Found: 347.1062.



Product **5c** was obtained in 95% yield as a yellow oil (3 days). HPLC analysis (Chiralcel OJ-H, *i*PrOH/hexane = 2/98, 1.0 mL/min, 254 nm; *t_r* (major) = 27.11 min, *t_r* (minor) = 25.81 min) gave the isomeric composition

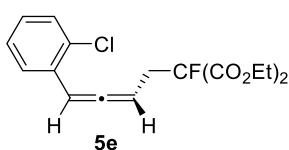
of the product: 97.5:2.5 er; $[\alpha]_D^{20} = -23.1$ (*c* = 0.03, CHCl₃); ¹H NMR (400 MHz, CDCl₃): δ 7.27-7.24 (m, 2H), 7.21-7.18 (m, 2H), 6.15 (dt, *J* = 6.4, 2.4 Hz, 1H), 5.57-5.52 (m, 1H), 4.33-4.23 (m, 4H), 3.04-3.01 (m, 1H), 2.99-2.95 (m, 1H), 1.31 (t, *J* = 7.2 Hz, 3H), 1.27 (t, *J* = 6.8 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 207.4, 165.6 (d, *J* = 25 Hz), 165.5 (d, *J* = 25 Hz), 132.7, 132.2, 128.7, 128.1, 94.5, 93.8 (d, *J* = 199.0 Hz), 87.0 (d, *J* = 3.6 Hz), 62.8, 62.7, 34.2 (d, *J* = 21.0 Hz), 14.0, 13.9; ¹⁹F NMR (376 MHz, CDCl₃): δ -166.43 (s, 1F); IR (neat): 1593, 1477, 1336, 1151, 1078, 908, 790, 752, 682, 555 cm⁻¹; HRMS (ESI): Exact mass calcd for C₁₇H₁₈FCINaO₄ [M+Na]⁺: 363.0769, Found: 363.0764.



Product **5d** was obtained in 97% yield as a yellow oil (3 days). HPLC analysis (Chiralcel OJ-H, *i*PrOH/hexane = 2/98, 1.0 mL/min, 254 nm; *t_r* (major) = 20.46 min, *t_r* (minor) = 24.13 min) gave the isomeric composition

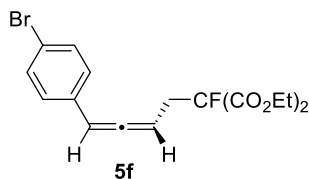
of the product: 98:2 er; $[\alpha]_D^{20} = -270.5$ (*c* = 0.3, CHCl₃); ¹H NMR (400 MHz, CDCl₃): δ 7.26-7.24 (m, 1H), 7.21 (d, *J* = 7.6 Hz, 1H), 7.17-7.12 (m, 2H), 6.14 (dt, *J* = 6.4, 2.4 Hz, 1H),

5.60-5.55 (m, 1H), 4.36-4.22 (m, 4H), 3.04 (dd, $J = 7.6, 2.4$ Hz, 1H), 2.98 (dd, $J = 7.6, 2.4$ Hz, 1H), 1.31 (t, $J = 7.2$ Hz, 3H), 1.28 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 207.5, 165.6 (d, $J = 25$ Hz), 165.5 (d, $J = 25$ Hz), 135.7, 134.5, 129.7, 127.1, 126.7, 125.1, 94.4, 93.8 (d, $J = 199.1$ Hz), 87.2 (d, $J = 3.8$ Hz), 62.8, 62.7, 34.2 (d, $J = 20.0$ Hz), 13.93, 13.88; ^{19}F NMR (376 MHz, CDCl_3): δ -166.37 (s, 1F); IR (neat): 1749, 1508, 1307, 1278, 1259, 1082, 763, 750 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{17}\text{H}_{18}\text{FClNaO}_4$ $[\text{M}+\text{Na}]^+$: 363.0769, Found: 363.0772.



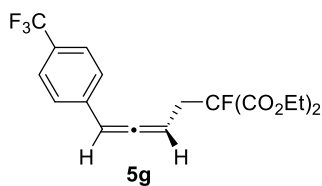
Product **5e** was obtained in 95% yield as a yellow oil (3 days). HPLC analysis (Chiralcel OJ-H, $i\text{PrOH}$ /hexane = 5/95, 1.0 mL/min, 254 nm; t_r (major) = 10.97 min, t_r (minor) = 11.81 min) gave the isomeric composition

of the product: 97.5:2.5 er; $[\alpha]_D^{20} = -23.1$ ($c = 0.06$, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ 7.43 (d, $J = 8.0$ Hz, 1H), 7.32 (d, $J = 8.0$ Hz, 1H), 7.20 (t, $J = 7.2$ Hz, 1H), 7.12 (t, $J = 7.6$ Hz, 1H), 6.66-6.64 (m, 1H), 5.60-5.55 (m, 1H), 4.33-4.19 (m, 4H), 3.06-3.03 (m, 1H), 3.00-2.97 (m, 1H), 1.31 (t, $J = 6.8$ Hz, 3H), 1.26 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 208.1, 165.6 (d, $J = 25$ Hz), 165.5 (d, $J = 25$ Hz), 132.0, 131.4, 129.5, 128.5, 128.2, 126.8, 93.8 (d, $J = 198.8$ Hz), 91.7, 86.8 (d, $J = 3.6$ Hz), 62.7, 34.2 (d, $J = 21$ Hz), 13.9, 13.8; ^{19}F NMR (376 MHz, CDCl_3): δ -166.31 (s, 1F); IR (neat): 1749, 1477, 1306, 1288, 1082, 875, 763, 742, 623 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{17}\text{H}_{18}\text{FClNaO}_4$ $[\text{M}+\text{Na}]^+$: 363.0769, Found: 363.0769.



Product **5f** was obtained in 91% yield as a yellow oil (3 days). HPLC analysis (Chiralcel AD-H, $i\text{PrOH}$ /hexane = 5/95, 0.8 mL/min, 254 nm; t_r (major) = 11.06 min, t_r (minor) = 10.07 min) gave the isomeric composition

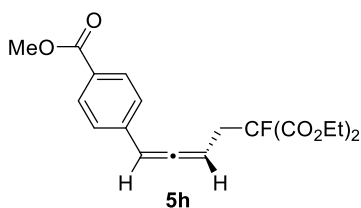
of the product: 97:3 er. $[\alpha]_D^{20} = -184.2$ ($c = 0.2$, CHCl_3); ^1H NMR (500 MHz, CDCl_3): δ 7.42-7.40 (m, 2H), 7.14 (d, $J = 8.0$ Hz, 2H), 6.14-6.13 (m, 1H), 5.55-5.52 (m, 1H), 4.32-4.22 (m, 4H), 3.03-3.00 (m, 1H), 2.99-2.96 (m, 1H), 1.32-1.29 (m, 3H), 1.28-1.26 (m, 3H); ^{13}C NMR (125 MHz, CDCl_3): δ 207.5, 165.6 (d, $J = 20$ Hz), 165.5 (d, $J = 20$ Hz), 132.7, 131.7, 128.4, 120.8, 94.6, 93.8 (d, $J = 199.0$ Hz), 87.1 (d, $J = 3.7$ Hz), 62.81, 62.77, 34.2 (d, $J = 21.0$ Hz), 14.0, 13.9; ^{19}F NMR (376 MHz, CDCl_3): δ -166.43 (s, 1F); IR (neat): 1747, 1489, 1302, 1242, 1068, 1008, 856, 833, 501 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{17}\text{H}_{18}\text{BrFNaO}_4$ $[\text{M}+\text{Na}]^+$: 407.0264, Found: 407.0271.



Product **5g** was obtained in 96% yield as a colorless oil (3 days). HPLC analysis (Chiralcel OJ-H, *i*PrOH/hexane = 2/98, 1.0 mL/min, 254 nm; *t_r* (major) = 22.79 min, *t_r* (minor) = 19.24 min) gave the isomeric

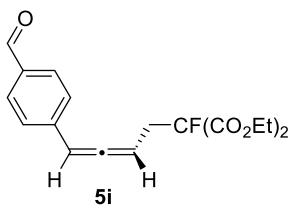
composition of the product: 98:2 er; $[\alpha]_D^{20} = -106.1$ (*c* = 0.1, CHCl₃); ¹H

NMR (400 MHz, CDCl₃): δ 7.54 (d, *J* = 8.0 Hz, 2H), 7.37 (d, *J* = 8.4 Hz, 2H), 6.24-6.21 (m, 1H), 5.63-5.58 (m, 1H), 4.33-4.25 (m, 4H), 3.07-3.03 (m, 1H), 3.01-2.98 (m, 1H), 1.31 (t, *J* = 6.8 Hz, 3H), 1.27 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 208.1, 165.6 (d, *J* = 25 Hz), 165.5 (d, *J* = 25 Hz), 137.6 (d, *J* = 1.5 Hz), 129.0 (q, *J* = 32.1 Hz), 127.0, 125.5 (q, *J* = 3.9 Hz), 124.1 (q, *J* = 270.2 Hz), 94.5, 93.7 (d, *J* = 199.2 Hz), 87.3 (d, *J* = 3.7 Hz), 62.83, 62.81, 34.1 (d, *J* = 21 Hz), 14.0, 13.9; ¹⁹F NMR (376 MHz, CDCl₃): δ -62.48 (s, 3F), -166.39 (s, 1F); IR (neat): 1749, 1323, 1244, 1182, 1064, 1053, 1016, 877, 846 cm⁻¹; HRMS (ESI): Exact mass calcd for C₁₈H₁₈F₄NaO₄ [M+Na]⁺: 397.1033, Found: 397.1033.



Product **5h** was obtained in 94% yield as a yellow oil (3 days). HPLC analysis (Chiralcel OJ-H, *i*PrOH/hexane = 10/90, 1.0 mL/min, 254 nm; *t_r* (major) = 44.21 min, *t_r* (minor) = 39.83 min) gave the isomeric composition of the product: 96.5:3.5 er; $[\alpha]_D^{20} = -49.0$ (*c* = 0.06,

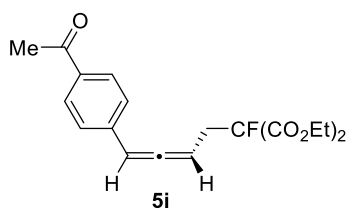
CHCl₃); ¹H NMR (400 MHz, CDCl₃): δ 7.97 (d, *J* = 8.4 Hz, 2H), 7.33 (d, *J* = 8.4 Hz, 2H), 6.23 (dt, *J* = 6.4, 2.0 Hz, 1H), 5.63-5.57 (m, 1H), 4.33-4.22 (m, 4H), 3.91 (s, 3H), 3.07-3.04 (m, 1H), 3.01-2.98 (m, 1H), 1.31 (t, *J* = 7.2 Hz, 3H), 1.27 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 208.3, 166.8, 165.6 (d, *J* = 26 Hz), 165.5 (d, *J* = 26 Hz), 138.7, 129.9, 128.7, 126.7, 94.9, 93.8 (d, *J* = 199.3 Hz), 87.1 (d, *J* = 3.7 Hz), 62.80, 62.76, 52.0, 34.1 (d, *J* = 21.1 Hz), 13.95, 13.89; ¹⁹F NMR (376 MHz, CDCl₃): δ -166.37 (s, 1F); IR (neat): 2924, 1751, 1718, 1608, 1437, 1278, 1111, 1018, 738 cm⁻¹; HRMS (ESI): Exact mass calcd for C₁₉H₂₁FN₂O₆ [M+Na]⁺: 387.1214, Found: 387.1209.



Product **5i** was obtained in 62% yield as a yellow oil (3 days). HPLC analysis (Chiralcel AD-H, *i*PrOH/hexane = 10/90, 1.0 mL/min, 254 nm; *t_r* (major) = 14.01 min, *t_r* (minor) = 13.09 min) gave the isomeric composition of the product: 96:4 er; $[\alpha]_D^{20} = -5.0$ (*c* = 0.01, CHCl₃); ¹H NMR (400 MHz,

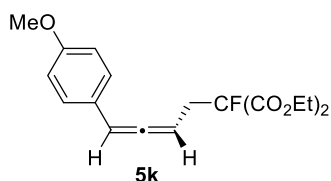
CDCl₃): δ 9.97 (s, 1H), 7.82 (d, *J* = 7.6 Hz, 2H), 7.43 (d, *J* = 7.6 Hz, 2H), 6.27-6.26 (m, 1H), 5.66-

5.60 (m, 1H), 4.34-4.22 (m, 4H), 3.08-3.05 (m, 1H), 3.02-3.00 (m, 1H), 1.34-1.26 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 208.6, 191.6, 165.5 (d, $J = 25$ Hz), 165.4 (d, $J = 25$ Hz), 140.4, 135.1, 130.0, 127.3, 94.9, 93.7 (d, $J = 199.1$ Hz), 87.3 (d, $J = 3.6$ Hz), 62.84, 62.81, 33.9 (d, $J = 21.1$ Hz), 14.0, 13.9; ^{19}F NMR (376 MHz, CDCl_3): δ -166.42 (s, 1F); IR (neat): 1747, 1693, 1602, 1303, 1209, 1082, 1012, 854, 837, 790 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{18}\text{H}_{19}\text{FNaO}_5$ $[\text{M}+\text{Na}]^+$: 357.1109, Found: 357.1100.



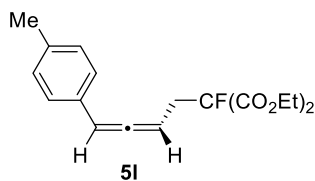
Product **5j** was obtained in 98% yield as a yellow oil (3 days). HPLC analysis (Chiralcel OD-H, $i\text{PrOH}$ /hexane = 10/90, 1.0 mL/min, 230 nm; t_r (major) = 13.86 min, t_r (minor) = 12.88 min) gave the isomeric composition of the product: 95:5 er; $[\alpha]_{\text{D}}^{20} = -17.1$ ($c = 0.04$, CHCl_3);

^1H NMR (400 MHz, CDCl_3): δ 7.90 (d, $J = 8.4$ Hz, 2H), 7.35 (d, $J = 8.4$ Hz, 2H), 6.26-6.23 (m, 1H), 5.63-5.58 (m, 1H), 4.36-4.21 (m, 4H), 3.07-3.04 (m, 1H), 3.01-2.98 (m, 1H), 2.59 (s, 3H), 1.33-1.26 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 208.4, 197.5, 165.5 (d, $J = 26$ Hz), 165.4 (d, $J = 26$ Hz), 138.9, 135.7, 128.7, 126.9, 94.9, 93.7 (d, $J = 199.3$ Hz), 87.1 (d, $J = 3.6$ Hz), 62.81, 62.77, 34.0 (d, $J = 21.1$ Hz), 26.5, 14.0, 13.9; ^{19}F NMR (376 MHz, CDCl_3): δ -166.36 (s, 1F); IR (neat): 2926, 1749, 1682, 1303, 1267, 1084, 1051, 1014, 854, 501 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{19}\text{H}_{21}\text{FNaO}_5$ $[\text{M}+\text{Na}]^+$: 371.1265, Found: 371.1258.



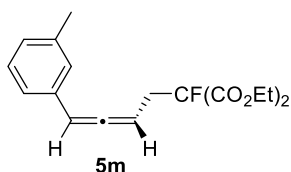
Product **5k** was obtained in 85% yield as a yellow oil (3 days). HPLC analysis (Chiralcel AD-H, $i\text{PrOH}$ /hexane = 5/95, 1.0 mL/min, 254 nm; t_r (major) = 12.37 min, t_r (minor) = 11.41 min) gave the isomeric composition of the product: 96.5:3.5 er; $[\alpha]_{\text{D}}^{20} = -56.6$ ($c = 0.2$, CHCl_3);

^1H NMR (400 MHz, CDCl_3): δ 7.20 (d, $J = 8.4$ Hz, 2H), 6.84 (d, $J = 8.8$ Hz, 2H), 6.17-6.14 (m, 1H), 5.52-5.47 (m, 1H), 4.33-4.19 (m, 4H), 3.80 (s, 3H), 3.03-3.00 (m, 1H), 2.98-2.94 (m, 1H), 1.33-1.26 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 207.0, 165.8 (d, $J = 25$ Hz), 165.7 (d, $J = 25$ Hz), 158.9, 128.1, 125.9, 114.1, 94.8, 94.0 (d, $J = 198.6$ Hz), 86.5 (d, $J = 3.7$ Hz), 62.8, 62.7, 55.3, 34.6 (d, $J = 21.1$ Hz), 14.0, 13.9; ^{19}F NMR (376 MHz, CDCl_3): δ -166.49 (s, 1F); IR (neat): 2924, 1749, 1599, 1512, 1246, 1026, 854, 825, 607, 597 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{18}\text{H}_{21}\text{FNaO}_5$ $[\text{M}+\text{Na}]^+$: 359.1265, Found: 359.1261.



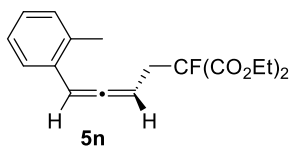
Product **5l** was obtained in 92% yield as a yellow oil (3 days). HPLC analysis (Chiralcel AD-H, *i*PrOH/hexane = 5/95, 1.0 mL/min, 230 nm; *t_r* (major) = 7.38 min, *t_r* (minor) = 6.66 min) gave the isomeric composition of the product: 96.5:3.5 er; $[\alpha]_D^{20} = -20.6$ (*c* = 0.03, CHCl₃); ¹H NMR

(400 MHz, CDCl₃): δ 7.16 (d, *J* = 8.0 Hz, 2H), 7.10 (d, *J* = 8.0 Hz, 2H), 6.16 (dt, *J* = 6.4, 2.4 Hz, 1H), 5.53-5.48 (m, 1H), 4.34-4.21 (m, 4H), 3.02 (dt, *J* = 7.6, 2.0 Hz, 1H), 2.98-2.95 (m, 1H), 2.32 (s, 3H), 1.30 (t, *J* = 7.2 Hz, 3H), 1.26 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 207.2, 165.7 (d, *J* = 25 Hz), 165.6 (d, *J* = 25 Hz), 136.9, 130.6, 129.3, 126.8, 95.1, 94.0 (d, *J* = 198.7 Hz), 86.4 (d, *J* = 3.7 Hz), 62.72, 62.67, 34.5 (d, *J* = 21.0 Hz), 21.1, 14.0, 13.9; ¹⁹F NMR (376 MHz, CDCl₃): δ -166.48 (s, 1F); IR (neat): 1749, 1514, 1369, 1305, 1201, 1084, 1012, 856, 732, 702 cm⁻¹; HRMS (ESI): Exact mass calcd for C₁₈H₂₁FN₂O₄ [M+Na]⁺: 343.1316, Found: 343.1312.



Product **5m** was obtained in 93% yield as a yellow oil (3 days). HPLC analysis (Chiralcel OJ-H, *i*PrOH/hexane = 5/95, 1.0 mL/min, 254 nm; *t_r* (major) = 12.27 min, *t_r* (minor) = 15.08 min) gave the isomeric composition

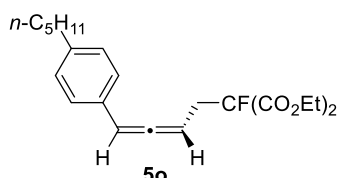
of the product: 97.5:2.5 er; $[\alpha]_D^{20} = -88.2$ (*c* = 0.1, CHCl₃); ¹H NMR (400 MHz, CDCl₃): δ 7.18 (t, *J* = 7.6 Hz, 1H), 7.09-7.06 (m, 2H), 7.01 (d, *J* = 7.2 Hz, 1H), 6.16 (dt, *J* = 6.8, 2.4 Hz, 1H), 5.54-5.51 (m, 1H), 4.32-4.21 (m, 4H), 3.04-3.02 (m, 1H), 2.99-2.96 (m, 1H), 2.33 (s, 3H), 1.31 (t, *J* = 7.2 Hz, 3H), 1.26 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 207.4, 165.7 (d, *J* = 25 Hz), 165.6 (d, *J* = 25 Hz), 138.2, 133.5, 128.4, 128.0, 127.5, 124.1, 95.3, 94.0 (d, *J* = 198.7 Hz), 86.5 (d, *J* = 3.7 Hz), 62.73, 62.7, 34.4 (d, *J* = 21 Hz), 21.3, 14.0, 13.9; ¹⁹F NMR (376 MHz, CDCl₃): δ -166.45 (s, 1F); IR (neat): 2984, 1749, 1368, 1290, 1242, 1082, 848, 790, 690 cm⁻¹; HRMS (ESI): Exact mass calcd for C₁₈H₂₁FN₂O₄ [M+Na]⁺: 343.1316, Found: 343.1312.



Product **5n** was obtained in 98% yield as a colorless oil (3 days). HPLC analysis (Chiralcel OJ-3, *i*PrOH/hexane = 2/98, 1.0 mL/min, 254 nm; *t_r* (major) = 26.72 min, *t_r* (minor) = 25.68 min) gave the isomeric composition

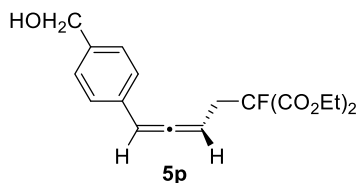
of the product: 97.5:2.5 er; $[\alpha]_D^{20} = -203.5$ (*c* = 0.3, CHCl₃); ¹H NMR (400 MHz, CDCl₃): δ 7.33 (d, *J* = 7.2 Hz, 1H), 7.16-7.09 (m, 3H), 6.38 (dt, *J* = 6.4, 2.4 Hz, 1H), 5.52-5.47 (m, 1H), 4.31-4.19 (m, 4H), 3.05-3.02 (m, 1H), 2.99-2.96 (m, 1H), 2.34 (s, 3H), 1.30 (t, *J* = 6.8 Hz, 3H), 1.26 (t, *J* = 7.2 Hz,

3H); ^{13}C NMR (100 MHz, CDCl_3): δ 208.0, 165.7 (d, $J = 26$ Hz), 165.6 (d, $J = 25$ Hz), 135.0, 131.8, 130.4, 127.4, 127.0, 126.1, 94.0 (d, $J = 198.7$ Hz), 92.5, 85.7 (d, $J = 3.7$ Hz), 62.72, 62.66, 34.5 (d, $J = 21.2$ Hz), 19.7, 14.0, 13.9; ^{19}F NMR (376 MHz, CDCl_3): δ -166.30 (s, 1F); IR (neat): 1751, 1465, 1372, 1242, 1080, 910, 763, 732, 702, 624 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{18}\text{H}_{21}\text{FNaO}_4$ $[\text{M}+\text{Na}]^+$: 343.1316, Found: 343.1306.



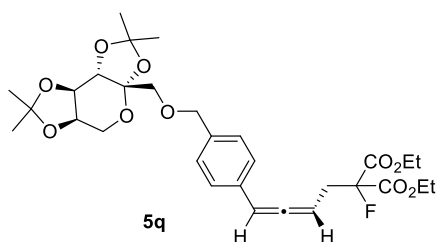
Product **5o** was obtained in 96% yield as a colorless oil (3 days). HPLC analysis (Chiralcel OJ-H, $i\text{PrOH}$ /hexane = 5/95, 1.0 mL/min, 254 nm; t_r (major) = 15.09 min, t_r (minor) = 11.78 min) gave the isomeric composition of the product: 97:3 er; $[\alpha]_{\text{D}}^{20} = -52.7$ ($c = 0.08$, CHCl_3); ^1H NMR (400 MHz, CDCl_3):

δ 7.18 (d, $J = 7.6$ Hz, 2H), 7.10 (d, $J = 8.0$ Hz, 2H), 6.18-6.15 (m, 1H), 5.53-5.48 (m, 1H), 4.33-4.21 (m, 4H), 3.02 (dt, $J = 7.2$, 2.4 Hz, 1H), 2.96 (dt, $J = 7.6$, 2.0 Hz, 1H), 2.57 (t, $J = 7.6$ Hz, 2H), 1.62-1.55 (m, 2H), 1.32-1.24 (m, 10H), 0.88 (t, $J = 6.4$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 207.3, 165.7 (d, $J = 25$ Hz), 165.6 (d, $J = 25$ Hz), 142.1, 130.8, 128.6, 126.8, 95.1, 94.0 (d, $J = 198.8$ Hz), 86.4 (d, $J = 3.7$ Hz), 62.7, 62.6, 35.6, 34.5 (d, $J = 21$ Hz), 31.4, 31.1, 14.0, 13.96, 13.88; ^{19}F NMR (376 MHz, CDCl_3): δ -166.43 (s, 1F); IR (neat): 2930, 1749, 1512, 1303, 1242, 1199, 1082, 875, 854, 736, 536 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{22}\text{H}_{29}\text{FNaO}_4$ $[\text{M}+\text{Na}]^+$: 399.1942, Found: 399.1941.



Product **5p** was obtained in 82% yield as a yellow oil (3 days). HPLC analysis (Chiralcel OJ-H, $i\text{PrOH}$ /hexane = 20/80, 1.0 mL/min, 254 nm; t_r (major) = 22.41 min, t_r (minor) = 25.80 min) gave the isomeric composition of the product: 97:3 er; $[\alpha]_{\text{D}}^{20} = -22.2$ ($c = 0.02$, CHCl_3); ^1H NMR (400 MHz, CDCl_3):

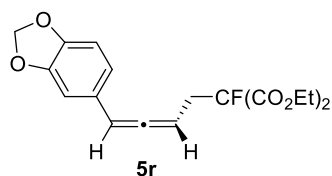
δ 7.30-7.25 (m, 4H), 6.19 (dt, $J = 6.4$, 2.4 Hz, 1H), 5.56-5.50 (m, 1H), 4.65 (s, 2H), 4.32-4.21 (m, 4H), 3.03 (dt, $J = 7.6$, 2.4 Hz, 1H), 2.97 (dt, $J = 7.6$, 2.0 Hz, 1H), 1.86 (s, br, 1H), 1.31 (t, $J = 7.2$ Hz, 3H), 1.27 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 207.5, 165.7 (d, $J = 25$ Hz), 165.6 (d, $J = 25$ Hz), 139.9, 133.0, 127.2, 127.0, 95.0, 93.9 (d, $J = 198.9$ Hz), 86.63 (d, $J = 3.7$ Hz), 65.0, 62.8, 62.7, 34.4 (d, $J = 21$ Hz), 14.0, 13.9; ^{19}F NMR (376 MHz, CDCl_3): δ -166.42 (s, 1F); IR (neat): 1747, 1390, 1303, 1244, 1084, 1011, 856, 829, 777, 538 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{18}\text{H}_{21}\text{FNaO}_5$ $[\text{M}+\text{Na}]^+$: 359.1265, Found: 359.1262.



Product **5q** was obtained in 94% yield as a yellow oil (3 days).

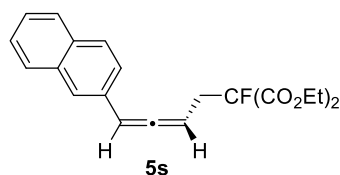
^{19}F NMR analysis of the crude mixture revealed that the dr value was >20:1; $[\alpha]_{\text{D}}^{20} = -261.58$ ($c = 0.46$, CHCl_3); ^1H NMR (400 MHz, CDCl_3): 7.21-7.15 (m, 4H), 6.1-6.10 (m, 1H), 5.48-5.42

(m, 1H), 4.58-4.46 (m, 3H), 4.35 (s, 1H), 4.22-4.15 (m, 5H), 3.84 (d, $J = 12.8$ Hz, 1H), 3.65 (d, $J = 13.2$ Hz, 1H), 3.56-3.49 (m, 2H), 2.95 (d, $J = 6.4$ Hz, 1H), 2.90 (d, $J = 6.4$ Hz, 1H), 1.47 (s, 3H), 1.34 (s, 6H), 1.26 (s, 3H), 1.23-1.17 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 207.3, 165.6 (d, $J = 25$ Hz), 165.5 (d, $J = 25$ Hz), 137.0, 132.8, 127.7, 126.7, 108.8, 108.4, 102.6, 95.0, 93.8 (d, $J = 198.6$ Hz), 86.5 (d, $J = 3.8$ Hz), 73.3, 71.3, 70.9, 70.0, 69.97, 62.7, 62.6, 60.9, 34.3 (d, $J = 20.9$ Hz), 26.5, 25.7, 25.3, 23.9, 13.9, 13.8; ^{19}F NMR (376 MHz, CDCl_3): δ -166.53 (s, 1F); IR (neat): 1751, 1381, 1249, 1203, 1112, 1068, 908, 756, 727, 648 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{30}\text{H}_{39}\text{FNaO}_{10}$ $[\text{M}+\text{Na}]^+$: 601.2419, Found: 601.2421.



Product **5r** was obtained in 64% yield as a yellow oil (3 days). HPLC analysis (Chiralcel OD-H, $i\text{PrOH}$ /hexane = 5/95, 1.0 mL/min, 230 nm; t_{r} (major) = 11.56 min, t_{r} (minor) = 9.66 min) gave the isomeric

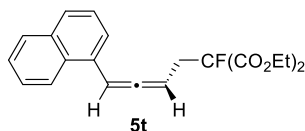
composition of the product: 95.5:4.5 er; $[\alpha]_{\text{D}}^{20} = -95.5$ ($c = 0.1$, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ 6.79 (d, $J = 1.6$ Hz, 1H), 6.75-6.69 (m, 2H), 6.12 (dt, $J = 6.4$, 2.4 Hz, 1H), 5.94 (s, 2H), 5.54-5.49 (m, 1H), 4.35-4.22 (m, 4H), 3.02 (dt, $J = 7.6$, 2.4 Hz, 1H), 2.97-2.94 (m, 1H), 1.31 (t, $J = 7.2$ Hz, 3H), 1.28 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 206.9, 165.7 (d, $J = 26$ Hz), 165.6 (d, $J = 25$ Hz), 148.0, 146.9, 127.6, 120.7, 108.3, 106.7, 101.0, 95.2, 93.9 (d, $J = 198.9$ Hz), 86.8 (d, $J = 3.7$ Hz), 62.8, 62.7, 34.5 (d, $J = 21.0$ Hz), 14.0, 13.9; ^{19}F NMR (376 MHz, CDCl_3): δ -166.46 (s, 1F); IR (neat): 1747, 1505, 1489, 1305, 1246, 1203, 1096, 1037, 929, 877 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{18}\text{H}_{20}\text{FO}_6$ $[\text{M}+\text{H}]^+$: 351.1238, Found: 351.1234.



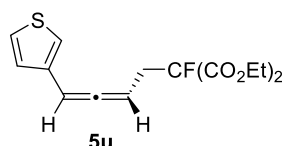
Product **5s** was obtained in 96% yield as a yellow oil (3 days). HPLC analysis (Chiralcel OJ-H, $i\text{PrOH}$ /hexane = 20/80, 1.0 mL/min, 254 nm; t_{r} (major) = 30.94 min, t_{r} (minor) = 40.29 min) gave the isomeric

composition of the product: 95:5 er. $[\alpha]_{\text{D}}^{20} = -89.5$ ($c = 0.07$, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ 7.80-7.76 (m, 3H), 7.65 (s, 1H), 7.47-7.41 (m, 3H), 6.38-6.37 (m, 1H), 5.64-5.59 (m, 1H), 4.35-4.20 (m, 4H), 3.08 (d, $J = 7.6$ Hz, 1H), 3.03 (d, $J = 7.6$ Hz, 1H), 1.32 (t, $J = 6.8$ Hz, 3H), 1.26 (t, $J =$

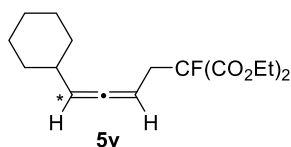
7.6 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 207.9, 165.7 (d, $J = 26$ Hz), 165.6 (d, $J = 25$ Hz), 133.5, 132.7, 131.1, 128.2, 127.6, 126.2, 125.8, 125.7, 124.7, 95.7, 93.9 (d, $J = 198.7$ Hz), 86.9 (d, $J = 3.8$ Hz), 62.8, 62.7, 34.4 (d, $J = 21$ Hz), 14.0, 13.9; ^{19}F NMR (376 MHz, CDCl_3): δ -166.35 (s, 1F); IR (neat): 1747, 1303, 1242, 1201, 1143, 1128, 1082, 906, 856, 754, 538 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{21}\text{H}_{21}\text{FNaO}_4$ $[\text{M}+\text{Na}]^+$: 379.1316, Found: 379.1311.



Product **5t** was obtained in 83% yield as a yellow oil (3 days). HPLC analysis (Chiralcel OJ-3, $i\text{PrOH}$ /hexane = 5/95, 1.0 mL/min, 230 nm; t_r (major) = 37.60 min, t_r (minor) = 36.52 min) gave the isomeric composition of the product: 95:5 er; $[\alpha]_D^{20} = -56.4$ ($c = 0.2$, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ 8.15 (d, $J = 8.4$ Hz, 1H), 7.85-7.82 (m, 1H), 7.74 (d, $J = 8.4$ Hz, 1H), 7.56-7.41 (m, 4H), 6.89 (dt, $J = 6.4, 2.4$ Hz, 1H), 5.62-5.56 (m, 1H), 4.31-4.11 (m, 4H), 3.10-3.08 (m, 1H), 3.05-3.02 (m, 1H), 1.29 (t, $J = 7.2$ Hz, 3H), 1.19 (t, $J = 6.8$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 208.7, 165.7 (d, $J = 25$ Hz), 165.6 (d, $J = 25$ Hz), 133.8, 130.7, 129.8, 128.6, 127.7, 126.1, 125.7, 125.6, 125.5, 123.4, 94.0 (d, $J = 198.8$ Hz), 91.8, 85.6 (d, $J = 3.7$ Hz), 62.72, 62.71, 34.5 (d, $J = 21.1$ Hz), 14.0, 13.8; ^{19}F NMR (376 MHz, CDCl_3): δ -166.21 (s, 1F); IR (neat): 1751, 1465, 1373, 1303, 1249, 1149, 1087, 856, 779, 748, 547 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{21}\text{H}_{22}\text{FO}_4$ $[\text{M}+\text{H}]^+$: 357.1497, Found: 357.1484.

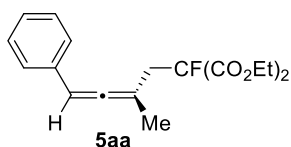


Product **5u** was obtained in 55% yield as a yellow oil (3 days). HPLC analysis (Chiralcel OJ-H, $i\text{PrOH}$ /hexane = 10/90, 1.0 mL/min, 254 nm; t_r (major) = 21.00 min, t_r (minor) = 28.48 min) gave the isomeric composition of the product: 95.5:4.5 er; $[\alpha]_D^{20} = -49.7$ ($c = 0.2$, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ 7.27-7.25 (m, 1H), 7.09 (d, $J = 2.8$ Hz, 1H), 7.06 (d, $J = 5.2$ Hz, 1H), 6.26 (dt, $J = 6.4, 2.4$ Hz, 1H), 5.49-5.43 (m, 1H), 4.33-4.22 (m, 4H), 3.06-2.90 (m, 2H), 1.31 (t, $J = 7.2$ Hz, 3H), 1.27 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 207.8, 165.7 (d, $J = 25$ Hz), 165.6 (d, $J = 25$ Hz), 134.8, 126.4, 125.9, 121.2, 93.9 (d, $J = 198.8$ Hz), 89.9, 85.8 (d, $J = 3.7$ Hz), 62.8, 62.7, 34.5 (d, $J = 21.1$ Hz), 14.0, 13.9; ^{19}F NMR (376 MHz, CDCl_3): δ -166.51 (s, 1F); IR (neat): 1749, 1369, 1269, 1244, 1201, 1149, 1084, 1012, 856, 788 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{15}\text{H}_{17}\text{FNaO}_4\text{S}$ $[\text{M}+\text{Na}]^+$: 335.0724, Found: 335.0714.



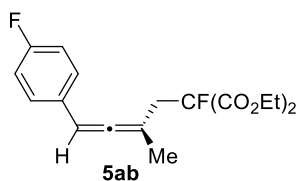
The reaction (0.25 mmol) was carried out at 40 °C for 4 days using Ni(COD)₂ (6.9 mg, 10 mol%), (S)-difluorophos (**L9**, 18.8 mg, 11 mol%), and DABCO (28.0 mg, 1.0 equivs). Product **5v** was obtained in 47% yield as a

yellow oil. HPLC analysis (Chiralcel AS-3, *i*PrOH/hexane = 0.5/99.5, 1.0 mL/min, 230 nm; *t_r* (major) = 6.37 min, *t_r* (minor) = 6.85 min) gave the isomeric composition of the product: 87.5:12.5 er; $[\alpha]_D^{20}$ = -40.3 (*c* = 0.1, CHCl₃); ¹H NMR (400 MHz, CDCl₃): 5.15-5.04 (m, 2H), 4.35-4.23 (m, 4H), 2.91-2.88 (m, 1H), 2.85-2.82 (m, 1H), 2.00-1.91 (m, 1H), 1.75-1.68 (m, 4H), 1.64-1.60 (m, 1H), 1.31 (td, *J* = 6.8, 1.6 Hz, 6H), 1.29-1.04 (m, 5H); ¹³C NMR (100 MHz, CDCl₃): δ 205.2, 165.8 (d, *J* = 25 Hz), 165.7 (d, *J* = 25 Hz), 96.7, 94.2 (d, *J* = 198.6 Hz), 83.2 (d, *J* = 3.8 Hz), 62.6, 62.5, 36.9, 35.0 (d, *J* = 20.9 Hz), 32.84, 32.8, 26.1, 25.9, 14.0, 13.9; ¹⁹F NMR (376 MHz, CDCl₃): δ -166.57 (s, 1F); IR (neat): 1751, 1450, 1303, 1242, 1087, 1049, 748, 493 cm⁻¹; HRMS (ESI): Exact mass calcd for C₁₇H₂₆FO₄ [M+H]⁺: 313.1810, Found: 313.1802.



The reaction (0.25 mmol) was carried out at 60 °C for 4 days using Ni(COD)₂ (13.8 mg, 20 mol%), (S,S)-Benzp* (**L11**, 15.5 mg, 22 mol%), and DABCO (56.0 mg, 2.0 equivs). Product **5aa** was obtained in 26% yield

as a colorless oil. HPLC analysis (Chiralcel OJ-H, *i*PrOH/hexane = 2/98, 1.0 mL/min, 254 nm; *t_r*(major) = 16.74 min, *t_r*(minor) = 22.59 min) gave the isomeric composition of the product: 97:3 er; $[\alpha]_D^{20}$ = -55.4 (*c* = 0.05, CHCl₃); ¹H NMR (400 MHz, CDCl₃): δ 7.30-7.23 (m, 4H), 7.20-7.15 (m, 1H), 6.09-6.06 (m, 1H), 4.25-4.11 (m, 4H), 3.08-2.92 (m, 2H), 1.87 (dd, *J* = 2.8, 1.0 Hz, 3H), 1.24 (t, *J* = 7.2 Hz, 3H), 1.21 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 204.2, 165.9 (d, *J* = 26 Hz), 165.8 (d, *J* = 26 Hz), 134.6, 128.5, 126.94, 126.89, 96.5, 94.7, 94.4 (d, *J* = 200.4 Hz), 62.7, 62.6, 38.5 (d, *J* = 20.4 Hz), 19.8 (d, *J* = 1.5 Hz), 13.9, 13.8; ¹⁹F NMR (376 MHz, CDCl₃): δ -165.67 (s, 1F); IR (neat): 1751, 1450, 1373, 1303, 1249, 1165, 1049, 856, 748, 694 cm⁻¹; HRMS (ESI): Exact mass calcd for C₁₈H₂₂FO₄ [M+H]⁺: 321.1497, Found: 321.1492.



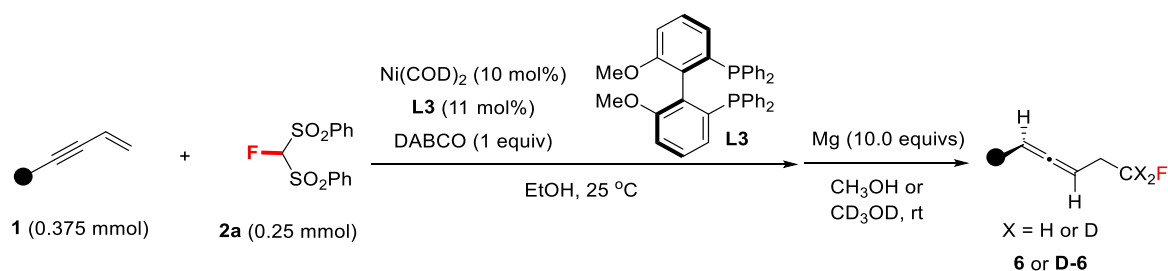
The reaction (0.25 mmol) was carried out at 60 °C for 4 days using Ni(COD)₂ (13.8 mg, 20 mol%), (S,S)-Benzp* (**L11**, 15.5 mg, 22 mol%), and DABCO (56.0 mg, 2.0 equivs). Product **5ab** was obtained in 45%

yield as a yellow oil (3 days). HPLC analysis (Chiralcel AD-H, *i*PrOH/hexane = 2/98, 1.0 mL/min,

230 nm; t_r (major) = 9.86 min, t_r (minor) = 9.00 min) gave the isomeric composition of the product: 99:1 er; $[\alpha]_D^{20} = -58.9$ ($c = 0.1$, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ 7.24-7.18 (m, 2H), 7.00-6.95 (m, 2H), 6.07-6.03 (m, 1H), 4.23-4.12 (m, 4H), 3.02-3.01 (m, 1H), 2.96 (d, $J = 2.4$ Hz, 1H), 1.86 (dd, $J = 2.8, 1.0$ Hz, 3H), 1.26-1.20 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 203.8 (d, $J = 2.4$ Hz), 165.8 (d, $J = 25$ Hz), 165.7 (d, $J = 26$ Hz), 161.9 (d, $J = 244.3$ Hz), 130.6 (d, $J = 3.3$ Hz), 128.3 (d, $J = 7.9$ Hz), 115.5, 115.3, 96.7, 94.3 (d, $J = 200.5$ Hz), 93.8, 62.7, 62.6, 38.5 (d, $J = 20.4$ Hz), 19.8, 13.9, 13.8; ^{19}F NMR (376 MHz, CDCl_3): δ -115.47 (s, 1F), -165.79 (s, 1F); IR (neat): 1751, 1512, 1303, 1257, 1226, 1157, 1087, 1049, 848, 732, 702, 570 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{18}\text{H}_{21}\text{FO}_4$ $[\text{M}+\text{H}]^+$: 339.1402, Found: 339.1398.

6. Synthetic utility

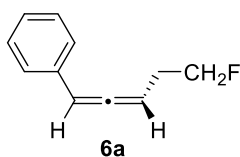
6.1 Procedure for the tandem synthesis of fluoromethyl-tethered allenes 6 and D-6



In a glove box, to a Schlenk tube equipped with a stirring bar were successively added $\text{Ni}(\text{COD})_2$ (6.9 mg, 10 mol%), and (*R*)-MeO-BIPHEP **L3** (16.0 mg, 11 mol%), followed by the addition of absolute EtOH (2.5 mL). The resulting mixture was stirred at rt for 15 min, and then added DABCO (28.0 mg, 1.0 equiv) and FBSM **2a** (0.25 mmol, 1.0 equiv). After being stirred for another 5 min, to the mixture was added 1,3-enynes **1** (0.375 mmol, 1.5 equivs). After it take out from the glove box, the reaction mixture was stirred at 25 °C until full conversion. The reaction was monitored by TLC analysis. After full consumption of **2a**, the reaction mixture was concentrated under vacuum, and the residue was filtrated over a short pad of silica gel to give the crude product **3**, which was used for the next reductive desulfonylation step.

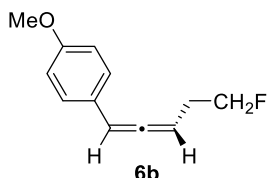
To a solution of above crude products **3** in absolute **MeOH** (2.5 mL) or **CD₃OD** (2.5 mL) was added activated Mg (60.0 mg, 10 equivs) in one portion at 0 °C under N_2 atmosphere. The reaction was stirred at rt until full consumption of **3** monitored by TLC or GC-MS analysis. After adding

water (3 mL) and dilute HCl (3 mL, 2 N), the reaction mixture was extracted with CH₂Cl₂ (10 mL × 2). The combined organic layers were dried over Na₂SO₄, and concentrated under reduced pressure. The obtained residue was purified by flash chromatography with PE as the eluent to provide the desired **CH₂F**- or **CD₂F**-tethered allenes **6** or **D-6**. (In the case of **6b** and **D-6b**, PE/CH₂Cl₂ (10:1, v/v) was used as the eluent). The products **D-6** have 100% deuterium incorporation at monofluoromethyl group according to the ¹H NMR analysis.



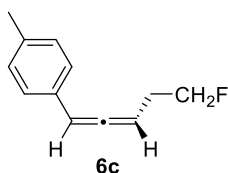
Product **6a** was obtained in 82% yield as a colorless oil. HPLC analysis (Chiralcel OD-H, *i*PrOH/hexane = 0.1/99.9, 1.0 mL/min, 254 nm; *t_r* (major) = 11.11 min, *t_r* (minor) = 12.54 min) gave the isomeric composition of the

product: 95.5:4.5 er; $[\alpha]_D^{20} = 0.7$ (*c* = 0.08, CHCl₃); ¹H NMR (400 MHz, CDCl₃): δ 7.33-7.28 (m, 4H), 7.23-7.17 (m, 1H), 6.19 (dt, *J* = 6.4, 2.8 Hz, 1H), 5.62-5.56 (m, 1H), 4.61 (t, *J* = 6.0 Hz, 1H), 4.50 (t, *J* = 6.0 Hz, 1H), 2.59-2.47 (m, 2H); ¹³C NMR (100 MHz, CDCl₃): δ 205.9, 134.2, 128.6, 127.0, 126.7, 95.3, 90.0 (d, *J* = 7.6 Hz), 82.8 (d, *J* = 166.7 Hz), 29.9 (d, *J* = 20.6 Hz); ¹⁹F NMR (376 MHz, CDCl₃): δ -217.85 (s, 1F); IR (neat): 1722, 1452, 1271, 1176, 1070, 1028, 1001, 713, 700 cm⁻¹; HRMS (EI-GCQTOF): Exact mass calcd for C₁₁H₁₁F [M]⁺: 162.0839, Found: 162.0841.



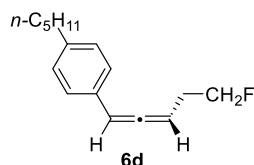
Product **6b** was obtained in 82% yield as a yellow oil. HPLC analysis (Chiralcel OD-H, *i*PrOH/hexane = 1/99, 1.0 mL/min, 254 nm; *t_r* (major) = 8.82 min, *t_r* (minor) = 9.64 min) gave the isomeric composition of the product:

95:5 er; $[\alpha]_D^{20} = -7.4$ (*c* = 0.1, CHCl₃); ¹H NMR (400 MHz, CDCl₃): δ 7.23-7.20 (m, 2H), 6.87-6.83 (m, 2H), 6.16 (dt, *J* = 6.4, 2.8 Hz, 1H), 5.59-5.54 (m, 1H), 4.61 (t, *J* = 6.0 Hz, 1H), 4.49 (t, *J* = 6.4 Hz, 1H), 3.80 (s, 3H), 2.57-2.52 (m, 1H), 2.51-2.46 (m, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 205.4, 158.8, 127.8, 126.5, 114.1, 94.7, 89.9 (d, *J* = 7.5 Hz), 82.9 (d, *J* = 166.6 Hz), 55.3, 30.1 (d, *J* = 20.5 Hz); ¹⁹F NMR (376 MHz, CDCl₃): δ -217.82 (s, 1F); IR (neat): 1743, 1600, 1577, 1512, 1302, 1249, 1172, 1161, 1031, 835 cm⁻¹; HRMS (GC-TOF MS): Exact mass calcd for C₁₂H₁₃FO [M]⁺: 192.0945, Found: 192.0948.



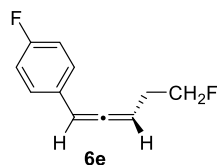
Product **6c** was obtained in 68% yield as a colorless oil. HPLC analysis (Chiralcel OD-H, *i*PrOH/hexane = 0.1/99.9, 1.0 mL/min, 254 nm; *t_r* (major) =

10.53 min, t_r (minor) = 12.53 min) gave the isomeric composition of the product: 93:7 er; $[\alpha]_D^{20} = -22.4$ ($c = 0.07$, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ 7.18 (d, $J = 8.0$ Hz, 2H), 7.11 (d, $J = 8.0$ Hz, 2H), 6.17 (dt, $J = 6.4, 3.2$ Hz, 1H), 5.59-5.54 (m, 1H), 4.61 (t, $J = 6.4$ Hz, 1H), 4.49 (t, $J = 6.0$ Hz, 1H), 2.58-2.52 (m, 1H), 2.52-2.46 (m, 1H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 205.7, 136.8, 131.2, 129.3, 126.6, 95.1, 89.9 (d, $J = 7.7$ Hz), 82.9 (d, $J = 166.6$ Hz), 30.0 (d, $J = 20.5$ Hz), 21.2; ^{19}F NMR (376 MHz, CDCl_3): δ -217.80 (s, 1F); IR (neat): 1724, 1670, 1604, 1512, 1178, 1111, 1066, 1037, 910, 879, 844, 732, 505 cm^{-1} ; HRMS (EI-GCQTOF): Exact mass calcd for $\text{C}_{12}\text{H}_{13}\text{F}$ $[\text{M}]^+$: 176.0996, Found: 176.0998.



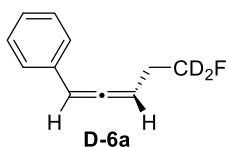
Product **6d** was obtained in 75% yield as a yellow oil. HPLC analysis (Chiralcel OD-H, $i\text{PrOH}$ /hexane = 0.1/99.9, 1.0 mL/min, 254 nm; t_r (major) = 9.25 min, t_r (minor) = 14.48 min) gave the isomeric composition of the

product: 93:7 er; $[\alpha]_D^{20} = -25.9$ ($c = 0.1$, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ 7.18 (d, $J = 8.0$ Hz, 2H), 7.11 (d, $J = 8.0$ Hz, 2H), 6.17 (dt, $J = 6.4, 3.2$ Hz, 1H), 5.59-5.54 (m, 1H), 4.61 (t, $J = 6.4$ Hz, 1H), 4.49 (t, $J = 6.0$ Hz, 1H), 2.59-2.46 (m, 4H), 1.63-1.56 (m, 2H), 1.37-1.26 (m, 4H), 0.88 (t, $J = 6.8$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 205.7, 141.9, 131.4, 128.7, 126.6, 95.1, 89.9 (d, $J = 7.7$ Hz), 82.9 (d, $J = 166.7$ Hz), 35.6, 31.4, 31.2, 30.0 (d, $J = 20.6$ Hz), 22.5, 14.0; ^{19}F NMR (376 MHz, CDCl_3): δ -217.79 (s, 1F); IR (neat): 1512, 1458, 1381, 1219, 1080, 1041, 1018, 972, 879, 841, 771 cm^{-1} ; HRMS (EI-GCQTOF): Exact mass calcd for $\text{C}_{16}\text{H}_{21}\text{F}$ $[\text{M}]^+$: 232.1622, Found: 232.1626.



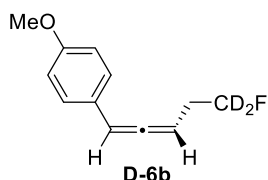
Product **6e** was obtained in 68% yield as a yellow oil. HPLC analysis (Chiralcel OD-H, $i\text{PrOH}$ /hexane = 0.1/99.9, 1.0 mL/min, 254 nm; t_r (major) = 7.34 min, t_r (minor) = 7.71 min) gave the isomeric composition of the product: 93.5:6.5 er;

$[\alpha]_D^{20} = -0.4$ ($c = 0.06$, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ 7.27-7.22 (m, 2H), 7.02-6.96 (m, 2H), 6.18-6.15 (m, 1H), 5.62-5.57 (m, 1H), 4.61 (td, $J = 6.4, 0.8$ Hz, 1H), 4.49 (td, $J = 6.4, 0.8$ Hz, 1H), 2.58-2.53 (m, 1H), 2.52-2.47 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 205.7 (d, $J = 2.3$ Hz), 161.9 (d, $J = 244.5$ Hz), 130.2 (d, $J = 3.4$ Hz), 128.1 (d, $J = 8.0$ Hz), 115.5 (d, $J = 21.6$ Hz), 94.4, 90.4 (d, $J = 7.1$ Hz), 82.7 (d, $J = 166.8$ Hz), 30.0 (d, $J = 20.6$ Hz); ^{19}F NMR (376 MHz, CDCl_3): δ -115.38 (s, 1F), -218.00 (s, 1F); IR (neat): 1728, 1597, 1512, 1265, 1234, 1157, 1018, 841, 756, 462 cm^{-1} ; HRMS (EI-GCQTOF): Exact mass calcd for $\text{C}_{11}\text{H}_{10}\text{F}_2$ $[\text{M}]^+$: 180.0745, Found: 180.0746.



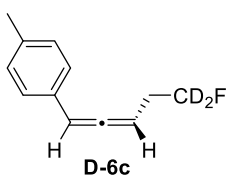
Product **D-6a** was obtained in 63% yield as a colorless oil. HPLC analysis (Chiralcel OD-H, *i*PrOH/hexane = 0.1/99.9, 1.0 mL/min, 254 nm; *t_r* (major) = 9.49 min, *t_r* (minor) = 10.99 min) gave the isomeric composition of the product:

95.4:4.5 er; $[\alpha]_D^{20} = -46.4$ ($c = 0.06$, CHCl₃); ¹H NMR (400 MHz, CDCl₃): δ 7.30-7.29 (m, 4H), 7.21-7.17 (m, 1H), 6.21-6.17 (m, 1H), 5.61-5.56 (m, 1H), 2.54 (dd, $J = 7.2, 2.8$ Hz, 1H), 2.48 (dd, $J = 7.2, 2.8$ Hz, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 205.9, 134.2, 128.6, 127.0, 126.7, 95.3, 90.0 (d, $J = 7.6$ Hz), 83.4-80.8 (m, CD₂F), 29.7 (d, $J = 20.6$ Hz); ¹⁹F NMR (376 MHz, CDCl₃): δ -219.06~-219.15 (m, 1F); IR (neat): 1952, 1599, 1496, 1149, 1087, 1072, 949, 877, 775, 731, 690, 628 cm⁻¹; HRMS (EI-GCQTOF): Exact mass calcd for C₁₁H₉D₂F [M]⁺: 164.0965, Found: 164.0966.



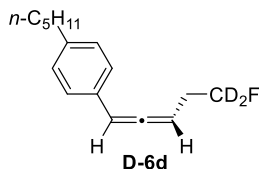
Product **D-6b** was obtained in 67% yield as a colorless oil. HPLC analysis (Chiralcel OD-H, *i*PrOH/hexane = 2/98, 1.0 mL/min, 254 nm; *t_r* (major) = 6.48 min, *t_r* (minor) = 6.87 min) gave the isomeric composition of the product:

95:5 er; ¹H NMR (500 MHz, CDCl₃): δ 7.23-7.20 (m, 2H), 6.86-6.84 (m, 2H), 6.16 (dt, $J = 6.5, 3.0$ Hz, 1H), 5.58-5.54 (m, 1H), 3.80 (s, 3H), 2.53 (dd, $J = 7.0, 2.5$ Hz, 1H), 2.48 (dd, $J = 7.0, 2.5$ Hz, 1H); ¹³C NMR (125 MHz, CDCl₃): δ 205.4, 158.8, 127.8, 126.5, 114.1, 94.7, 89.9 (d, $J = 7.7$ Hz), 83.2-81.2 (m, CD₂F), 55.3, 29.9 (d, $J = 20.5$ Hz); ¹⁹F NMR (376 MHz, CDCl₃): δ -219.05~-219.13 (m, 1F); IR (neat): 1728, 1604, 1512, 1465, 1249, 1165, 1033, 910, 833, 732, 462 cm⁻¹; HRMS (EI-GCQTOF): Exact mass calcd for C₁₂H₁₁D₂FO [M]⁺: 194.1070, Found: 194.1071.



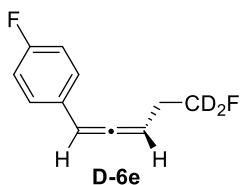
Product **D-6c** was obtained in 74% yield as a colorless oil. HPLC analysis (Chiralcel OD-H, *i*PrOH/hexane = 0.1/99.9, 1.0 mL/min, 254 nm; *t_r* (major) = 10.41 min, *t_r* (minor) = 12.13 min) gave the isomeric composition of the product:

93:7 er; $[\alpha]_D^{20} = -54.8$ ($c = 0.08$, CHCl₃); ¹H NMR (400 MHz, CDCl₃): δ 7.18 (d, $J = 8.0$ Hz, 2H), 7.11 (d, $J = 8.0$ Hz, 2H), 6.18-6.15 (m, 1H), 5.59-5.54 (m, 1H), 2.54 (dd, $J = 7.2, 2.8$ Hz, 1H), 2.48 (dd, $J = 7.2, 2.8$ Hz, 1H), 2.32 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 205.6, 136.7, 131.2, 129.3, 126.6, 95.1, 89.9 (d, $J = 7.6$ Hz), 83.2-81.1 (m, CD₂F), 29.8 (d, $J = 20.5$ Hz), 21.2; ¹⁹F NMR (376 MHz, CDCl₃): δ -219.01~-219.10 (m, 1F); IR (neat): 1952, 1512, 1448, 1149, 1087, 949, 910, 879, 839, 821, 732, 592, 557 cm⁻¹; HRMS (GC-TOF MS): Exact mass calcd for C₁₂H₁₁FD₂ [M]⁺: 178.1121, Found: 178.1124.



Product **D-6d** was obtained in 82% yield as a colorless oil. HPLC analysis (Chiralcel OD-H, *i*PrOH/hexane = 0.1/99.9, 1.0 mL/min, 254 nm; *t_r* (major) = 9.28 min, *t_r* (minor) = 14.43 min) gave the isomeric composition of the

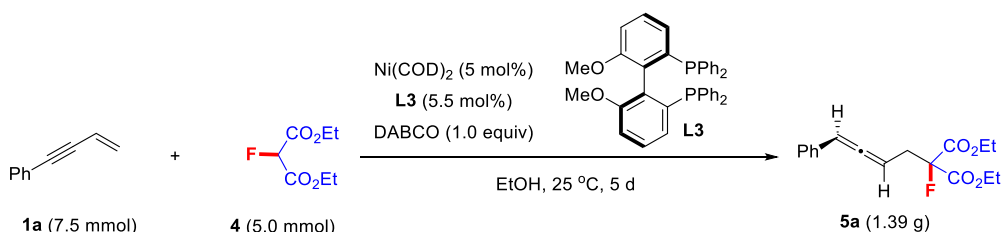
product: 92.5:7.5 er; $[\alpha]_D^{20} = -13.7$ (*c* = 0.04, CHCl₃); ¹H NMR (400 MHz, CDCl₃): δ 7.20 (d, *J* = 8.0 Hz, 2H), 7.11 (d, *J* = 8.4 Hz, 2H), 6.17 (dt, *J* = 6.4, 2.8 Hz, 1H), 5.59-5.54 (m, 1H), 2.58-2.55 (m, 2H), 2.53-2.46 (m, 2H), 1.63-1.55 (m, 2H), 1.37-1.25 (m, 4H), 0.88 (t, *J* = 6.0 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 205.7, 141.9, 131.4, 128.7, 126.6, 95.1, 89.8 (d, *J* = 7.7 Hz), 83.5-82.6 (m), 81.9-80.9 (m), 35.6, 31.4, 31.2, 29.8 (d, *J* = 20.6 Hz), 22.5, 14.0; ¹⁹F NMR (376 MHz, CDCl₃): δ -219.01~-219.09 (m, 1F); IR (neat): 1724, 1697, 1672, 1604, 1089, 950, 908, 729, 648 cm⁻¹; HRMS (GC-TOF MS): Exact mass calcd for C₁₆H₁₉D₂F [M]⁺: 234.1747, Found: 234.1751.



Product **D-6e** was obtained in 54% yield as a colorless oil. HPLC analysis (Chiralcel OD-3, *i*PrOH/hexane = 0.1/99.9, 1.0 mL/min, 254 nm; *t_r* (major) = 7.44 min, *t_r* (minor) = 7.85 min) gave the isomeric composition of the product:

93:7 er; $[\alpha]_D^{20} = -9.6$ (*c* = 0.02, CHCl₃); ¹H NMR (500 MHz, CDCl₃): δ 7.26-7.23 (m, 2H), 7.01-6.97 (m, 2H), 6.18-6.15 (m, 1H), 5.61-5.57 (m, 1H), 2.54 (dd, *J* = 6.5, 2.5 Hz, 1H), 2.49 (dd, *J* = 6.5, 2.5 Hz, 1H); ¹³C NMR (125 MHz, CDCl₃): δ 205.7 (d, *J* = 2.4 Hz), 161.9 (d, *J* = 244.1 Hz), 130.2 (d, *J* = 3.2 Hz), 128.1 (d, *J* = 8.0 Hz), 115.4 (d, *J* = 21.6 Hz), 94.4, 90.3 (d, *J* = 7.0 Hz), 83.1-81.0 (m, CD₂F), 29.7 (d, *J* = 20.5 Hz); ¹⁹F NMR (376 MHz, CDCl₃): δ -115.39 (s, 1F), -219.23~-219.31 (m, 1F); IR (neat): 1512, 1226, 1157, 1087, 949, 910, 841, 732, 478, 447 cm⁻¹; HRMS (EI-GCQTOF): Exact mass calcd for C₁₁H₈D₂F₂ [M]⁺: 182.0871, Found: 182.0870.

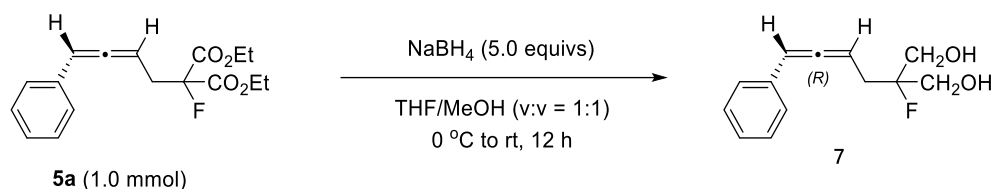
6.2 Gram-scale synthesis of functionalized monofluoroalkylated allene 5a



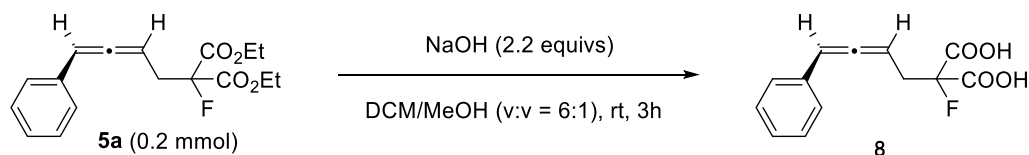
In a glove box, to a Schlenk tube equipped with a stirring bar were successively added Ni(COD)₂ (68.7 mg, 5 mol%), (*R*)-MeO-BIPHEP **L3** (145.5 mg, 5.5 mol%), followed by the addition of absolute EtOH (25 mL). The resulting mixture was stirred at room temperature for 15

min, and then added (560.0 mg, 1.0 equiv) and **4** (890.5 mg, 5.0 mmol). After being stirred for another 5 min, to the mixture was added 1,3-enyne **1a** (1440 mg, 7.5 mmol, 1.5 equivs). After it take out from the glove box, the reaction mixture was stirred at 25 °C until full conversion. The reaction was monitored by TLC analysis. After full consumption of **4**, the reaction mixture was concentrated under vacuum. The crude residue was purified by silica gel column chromatography using PE/EtOAc (6:1, v/v) as the eluent to afford the desired product **5a** (1.39 g, 91%) as yellow oil. HPLC analysis (Chiralcel OJ-H, *i*PrOH/hexane = 2/98, 1.0 mL/min, 254 nm; *t_r* (major) = 20.31 min, *t_r* (minor) = 22.64 min) gave the isomeric composition of the product: 97:3 er.

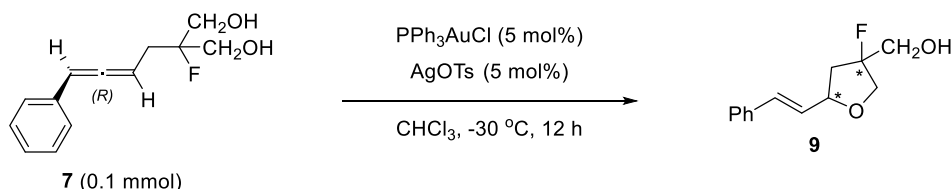
6.3 Transformations of product **5a**



To a stirred solution of **5a** (308.5 mg, 1.0 mmol, 1.0 equiv) in a mixed solvent of THF (5 mL) and MeOH (5 mL) was slowly added NaBH₄ at 0 °C. The resulting suspension was stirred at rt for overnight. After quenching with H₂O (20 mL), the solution was extracted with CH₂Cl₂ (20 mL × 3). The combined organic layers were successively washed with saturated NH₄Cl (aq., 10 mL) and brine (10 mL), and then dried over Na₂SO₄ and concentrated under reduced pressure. The obtained residue was purified by flash column chromatography using PE/EtOAc (1/1, v/v) as the eluent to afford fluorinated allene diol **7** (197.1 mg, 89% yield) as a white solid, m.p. = 65-66 °C. The absolute configuration and structure of **7** were confirmed by its X-ray diffraction. HPLC analysis (Chiralcel OJ-H, *i*PrOH/hexane = 30/70, 1.0 mL/min, 254 nm; *t_r* (major) = 13.05 min, *t_r* (minor) = 14.13 min) gave the isomeric composition of the product: 96.5:3.5 er; [α]_D²⁰ = -8.97 (*c* = 0.01, CHCl₃); ¹H NMR (400 MHz, CDCl₃): δ 7.33-7.25 (m, 4H), 7.22-7.18 (m, 1H), 6.18 (dt, *J* = 6.8, 2.0 Hz, 1H), 5.58-5.53 (m, 1H), 3.91-3.86 (m, 2H), 3.84-3.78 (m, 2H), 2.57 (dd, *J* = 8.0, 2.4 Hz, 1H), 2.52 (dd, *J* = 7.6, 2.4 Hz, 1H), 2.37 (s, br, 2H); ¹³C NMR (100 MHz, CDCl₃): δ 206.9, 134.0, 128.7, 127.1, 126.7, 97.40 (d, *J* = 173.2 Hz), 94.7, 88.1 (d, *J* = 7.9 Hz), 64.4 (d, *J* = 16.8 Hz), 64.2 (d, *J* = 17.0 Hz), 32.3 (d, *J* = 21.8 Hz); ¹⁹F NMR (376 MHz, CDCl₃): δ -172.23 (s, 1F); IR (neat): 3354, 2931, 1494, 1452, 1049, 968, 881, 767, 694, 628 cm⁻¹; HRMS (ESI): Exact mass calcd for C₁₃H₁₅FN₂O₂ [M+Na]⁺: 245.0948, Found: 245.0947.

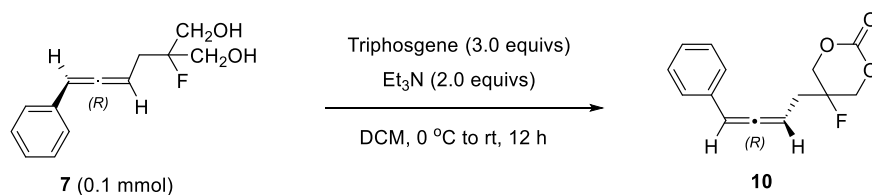


Compound **5a** (61.2 mg, 0.2 mmol, 1.0 equiv) was dissolved in a mixed solvent of MeOH (0.2 mL) and CH₂Cl₂ (1.2 mL), followed by the addition of NaOH (17.6 mg, 0.44 mmol, 2.2 equivs). The reaction mixture was stirred at room temperature (rt) until full conversion of **5a** (ca. 3 h). Then water and HCl (2 N) were added, the resulting mixture was extracted with EtOAc (10 mL $\times$ 3). The combined organic phases were successively washed with brine and water (10 mL, each), and then dried over Na₂SO₄, filtrated, and concentrated under vacuum to afford the analytically pure product **8** (47.3 mg, 95% yield) as white solid; m.p. = 86-88 °C; $[\alpha]_{\text{D}}^{20} = -13.6$ ($c = 0.1$, CHCl₃); ¹H NMR (400 MHz, CD₃OD): δ 7.30-7.25 (m, 4H), 7.21-7.15 (m, 1H), 6.23 (dt, $J = 6.4, 2.4$ Hz, 1H), 5.57-5.51 (m, 1H), 2.98 (dt, $J = 8.0, 2.4$ Hz, 1H), 2.94-2.91 (m, 1H); ¹³C NMR (100 MHz, CD₃OD): δ 208.3, 169.2 (d, $J = 25.6$ Hz), 169.0 (d, $J = 25.3$ Hz), 135.2, 129.6, 128.1, 127.9, 95.9, 95.2 (d, $J = 195.0$ Hz), 87.9 (d, $J = 3.7$ Hz), 35.6 (d, $J = 21.2$ Hz); ¹⁹F NMR (376 MHz, CD₃OD): δ -166.73 (s, 1F); IR (neat): 1743, 1325, 1269, 1163, 1118, 1064, 970, 848, 692 cm⁻¹; HRMS (ESI): Exact mass calcd for C₁₃H₁₁FO₄Na [M+Na]⁺: 273.0534, Found: 273.0534.

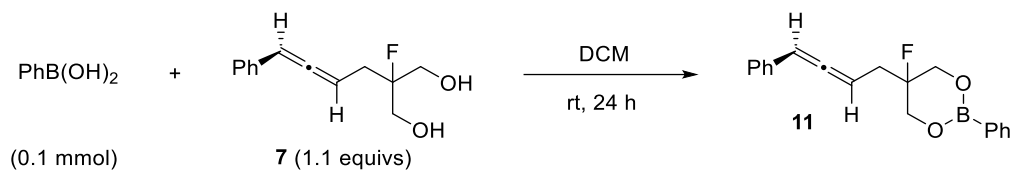


To a stirred solution of PPh₃AuCl (2.5 mg, 5 mol%) and silver *p*-toluenesulfonate (1.4 mg, 5 mol%, AgOTs) in CHCl₃ (1 mL) was added **7** (22.2 mg, 0.1 mmol) at -30 °C. After full consumption of **7** by TLC analysis, the reaction mixture was directly purified by flash column chromatography using PE/EtOAc (2/1, v/v) as the eluent to afford **9** (16.8 mg, 75% yield) as a yellow oil; ¹⁹F NMR analysis of the crude mixture revealed that the dr value was 2:1. Major isomer of **9**: HPLC analysis (Chiralcel AD-3, ⁱPrOH/hexane = 5/95, 1.0 mL/min, 254 nm; t_{r} (major) = 27.63 min, t_{r} (minor) = 25.37 min) gave the isomeric composition of the product: 98:2 er; $[\alpha]_{\text{D}}^{20} = -16.3$ ($c = 0.1$, CHCl₃); ¹H NMR (400 MHz, CDCl₃): δ 7.39-7.37 (m, 2H), 7.33-7.29 (m, 2H), 7.27-7.22 (m, 1H), 6.65 (d, $J = 16.0$ Hz, 1H), 6.18 (dd, $J = 16.0, 6.8$ Hz, 1H), 4.81-4.75 (m, 1H), 4.15-3.97 (m, 2H), 3.89-3.75 (m, 2H), 2.43-2.34 (m, 1H), 2.19 (s, 1H), 1.91-1.77 (m, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 136.3, 132.2, 128.5, 128.0, 127.9, 126.5, 105.0 (d, $J = 177.1$ Hz), 79.6, 74.3 (d, $J = 27.0$ Hz), 65.4 (d, $J =$

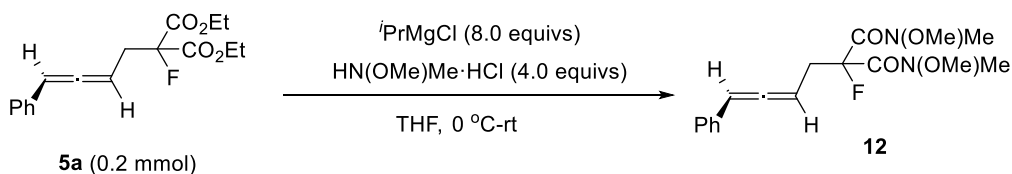
26.4 Hz), 41.5 (d, $J = 21.8$ Hz); ^{19}F NMR (376 MHz, CDCl_3): δ -155.85 (s, 1F); IR (neat): 1496, 1450, 1373, 1219, 1041, 964, 887, 756, 694, 671 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{13}\text{H}_{16}\text{FO}_2$ $[\text{M}+\text{H}]^+$: 223.1129, Found: 223.1124. Minor isomer of **9**: HPLC analysis (Chiralcel AD-H, i PrOH/hexane = 15/85, 1.0 mL/min, 254 nm; t_r (major) = 9.84 min, t_r (minor) = 8.79 min) gave the isomeric composition of the product: 98:2 er; $[\alpha]_{\text{D}}^{20} = -3.0$ ($c = 0.03$, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ 7.41-7.39 (m, 2H), 7.34-7.30 (m, 2H), 7.27-7.23 (m, 1H), 6.61 (d, $J = 16.0$ Hz, 1H), 6.32 (dd, $J = 16.0$, 7.2 Hz, 1H), 4.58 (dd, $J = 14.4$, 7.2 Hz, 1H), 4.21 (dd, $J = 20.0$, 11.2 Hz, 1H), 3.91-3.77 (m, 3H), 2.44-2.33 (m, 1H), 2.19-2.07 (m, 1H), 2.04-2.01 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 136.3, 132.0, 128.8, 128.6, 127.9, 126.6, 105.0 (d, $J = 179.0$ Hz), 80.2, 74.4 (d, $J = 26.4$ Hz), 65.2 (d, $J = 26.9$ Hz), 41.0 (d, $J = 22.5$ Hz); ^{19}F NMR (376 MHz, CDCl_3): δ -153.79 (s, 1F); IR (neat): 1489, 1450, 1373, 1040, 946, 910, 802, 732, 694, 648 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{13}\text{H}_{16}\text{FO}_2$ $[\text{M}+\text{H}]^+$: 223.1129, Found: 223.1124.



To a stirred solution of **7** (22.2 mg, 0.1 mmol, 1.0 equiv) in CH_2Cl_2 (1 mL) was successively added Et_3N (20.2 mg, 0.2 mmol) and triphosgene (44.5 mg, 0.15 mmol) at -30 °C. The reaction mixture was naturally warmed to rt and stirred for overnight. After full consumption of **7** by TLC analysis, the reaction mixture was directly purified by flash column chromatography using PE/EtOAc (2/1, v/v) as the eluent to afford 1,3-dioxan-2-one **10** in 65% yield (16.1 mg) as a yellow oil; HPLC analysis (Chiralcel OD-H, i PrOH/hexane = 30/70, 1.0 mL/min, 254 nm; t_r (major) = 39.47 min, t_r (minor) = 32.91 min) gave the isomeric composition of the product: 96.5:3.5 er; $[\alpha]_{\text{D}}^{20} = -18.0$ ($c = 0.04$, CHCl_3); ^1H NMR (400 MHz, acetone- d_6): δ 7.22 (s, 2H), 7.21 (d, $J = 1.2$ Hz, 2H), 7.13-7.08 (m, 1H), 6.24 (dt, $J = 6.4$, 2.4 Hz, 1H), 5.58-5.52 (m, 1H), 4.69-4.65 (m, 1H), 4.61-4.55 (m, 1H), 4.49-4.40 (m, 2H), 2.61 (dd, $J = 7.6$, 2.4 Hz, 1H), 2.55 (dd, $J = 7.6$, 2.4 Hz, 1H); ^{13}C NMR (125 MHz, acetone- d_6): δ 208.1, 147.6, 134.9, 129.7, 128.2, 127.9, 95.9, 89.2 (d, $J = 177.1$ Hz), 87.4 (d, $J = 4.9$ Hz), 73.2 (d, $J = 12.7$ Hz), 73.0 (d, $J = 12.9$ Hz), 32.7 (d, $J = 21.2$ Hz); ^{19}F NMR (376 MHz, acetone- d_6): δ -168.88 (s, 1F); IR (neat): 1774, 1458, 1259, 1242, 1147, 1072, 910, 841, 766, 684 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{14}\text{H}_{13}\text{FNaO}_3$ $[\text{M}+\text{Na}]^+$: 271.0741, Found: 271.0740.

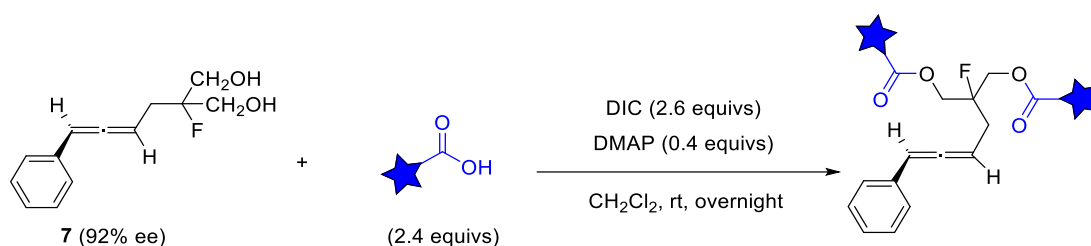


To a solution of **7** (24.3 mg, 0.11 mmol) in CH₂Cl₂ (2 mL) was added phenylboronic acid (12.1 mg, 0.1 mmol). The resulting mixture was stirred at room temperature for overnight. After then, the reaction mixture was concentrated under vacuo, and the crude residue was purified by flash column chromatography (hexane/ethyl acetate = 5/1) to afford **11** in 90% yield (27.5 mg) as a white solid. m.p. = 79-80 °C; HPLC analysis (Chiralcel AS-3, *i*PrOH/hexane = 10/90, 0.5 mL/min, 254 nm; *t_r* (major) = 35.51 min, *t_r* (minor) = 44.47 min) gave the isomeric composition of the product: 96.5:3.5 er; [α]_D²⁰ = -1.1 (*c* = 0.01, CHCl₃); ¹H NMR (400 MHz, CDCl₃): δ 7.83-7.81 (m, 2H), 7.46-7.41 (m, 1H), 7.37-7.27 (m, 6H), 7.24-7.20 (m, 1H), 6.22 (dt, *J* = 6.8, 2.4 Hz, 1H), 5.60-5.54 (m, 1H), 4.33-4.23 (m, 2H), 4.17-4.04 (m, 2H), 2.51 (dd, *J* = 7.6, 2.4 Hz, 1H), 2.46 (dd, *J* = 8.0, 2.4 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 207.0, 133.9, 133.6, 130.9, 128.7, 127.6, 127.3, 126.8, 95.2, 91.6 (d, *J* = 176.7 Hz), 86.8 (d, *J* = 5.9 Hz), 66.9 (d, *J* = 9.5 Hz), 66.7 (d, *J* = 9.5 Hz), 33.4 (d, *J* = 21.3 Hz); ¹⁹F NMR (376 MHz, CDCl₃): δ -169.17 (s, 1F); IR (neat): 1597, 1465, 1350, 1311, 1249, 1172, 1095, 879, 817, 694 cm⁻¹; HRMS (GC-TOF MS): Exact mass calcd for C₁₉H₁₈F¹⁰BO₂ [M]⁺: 307.1415, Found: 307.1413.

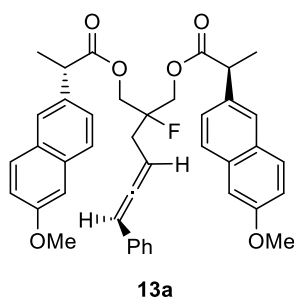


To a stirred solution of **5a** (61.2 mg, 0.2 mmol) and HN(OMe)Me·HCl (78.5 mg, 0.8 mmol), in THF (2 mL) was added *i*PrMgBr (0.7 mL, 2.5M in THF) at 0 °C. The reaction mixture was allowed to stir at room temperature until full conversion of **5a**. After quenching with H₂O (10 mL), the solution was extracted with CH₂Cl₂ (10 mL $\times$ 3). The combined organic layers were successively washed with sat. NH₄Cl (aq., 10 mL) and brine (10 mL), and then dried over Na₂SO₄ and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (PE/EtOAc = 4:1, v/v) to afford **12** (51.9 mg, 77% yield) as a yellow oil; HPLC analysis (Chiralcel OD-H, *i*PrOH/hexane = 40/60, 1.0 mL/min, 254 nm; *t_r* (major) = 6.53 min, *t_r* (minor) = 8.14 min)

gave the isomeric composition of the product: 97:3 er; $[\alpha]_{\text{D}}^{20} = -33.6$ ($c = 0.1$, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ 7.29 (d, $J = 4.0$ Hz, 4H), 7.21-7.16 (m, 1H), 6.17-6.14 (m, 1H), 5.68-5.62 (m, 1H), 3.66 (s, 3H), 3.57 (s, 3H), 3.18 (s, 3H), 3.13 (s, 3H), 3.07-2.83 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 207.2, 167.8 (d, $J = 23.6$ Hz), 167.5 (d, $J = 24.4$ Hz), 134.0, 128.4, 126.89, 126.87, 94.6, 93.8 (d, $J = 188.0$ Hz), 87.5 (d, $J = 4.3$ Hz), 61.6 (d, $J = 2.4$ Hz), 61.3 (d, $J = 1.5$ Hz), 34.3 (d, $J = 21.9$ Hz), 33.1; ^{19}F NMR (376 MHz, CDCl_3): δ -158.89 (s, 1F); IR (neat): 1668, 1458, 1381, 1201, 1112, 985, 912, 727, 692, 520 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{17}\text{H}_{22}\text{FN}_2\text{O}_4$ $[\text{M}+\text{H}]^+$: 337.1558, Found: 337.1551.

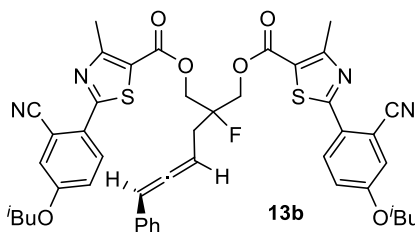


To a solution of **7** (11.2 mg, 0.01 mmol) and carboxylic acid-based drug (0.24 mmol, 2.4 equivalents) in CH_2Cl_2 (1.2 mL) were added DMAP (12.2 mg, 0.04 mmol) and DIC (32.0 mg, 0.26 mmol). The resulting suspension was stirred at rt for overnight. After adding H_2O (5 mL), the reaction mixture was extracted with CH_2Cl_2 (10 mL $\times$ 3). The combined organic layers were dried over Na_2SO_4 , and concentrated under reduced pressure to give the residue, which was purified by flash column chromatography (PE/EtOAc, 4/1, v/v) to afford the corresponding drug derivatives **13a-13c**.



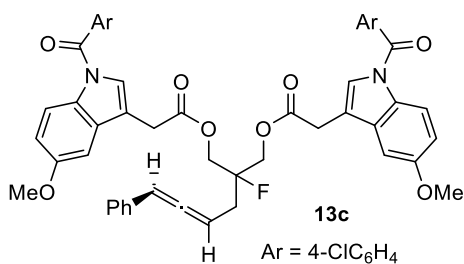
Product **13a** was obtained in 99% yield as a colorless oil from (S)-naproxen (55.2 mg) (12 h). ^{19}F NMR analysis of the crude mixture revealed that the dr value was >20:1; $[\alpha]_{\text{D}}^{20} = -36.1$ ($c = 0.2$, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ 7.56-7.50 (m, 5H), 7.48 (s, 1H), 7.23-7.14 (m, 4H), 7.12-7.08 (m, 1H), 7.04-7.00 (m, 4H), 6.96 (s, 2H), 5.85-5.83 (m, 1H), 5.20-5.15 (m, 1H), 4.18-3.97 (m, 4H), 3.80 (s, 3H), 3.79 (s, 3H), 3.73-3.66 (m, 2H), 2.23-2.06 (m, 2H), 1.44 (dd, $J = 7.2, 1.2$ Hz, 3H), 1.41 (dd, $J = 7.2, 1.6$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 207.1, 173.63, 173.61, 157.6, 135.0, 133.74, 133.69, 133.67, 129.24, 129.21, 128.83, 128.81, 128.6, 127.2, 127.1, 127.0, 126.7, 126.1, 126.0, 125.9, 119.0, 105.54, 94.7, 94.2 (d, $J = 178.1$ Hz), 87.0 (d, $J = 7.1$ Hz), 64.0 (d, $J = 20.7$ Hz), 63.7 (d, $J = 21.0$ Hz), 55.2, 45.21, 45.19, 32.6 (d, $J = 21.6$

Hz), 18.09, 18.07; ^{19}F NMR (376 MHz, CDCl_3): δ -167.66 (s, 1F); IR (neat): 1736, 1604, 1263, 1149, 1064, 852, 810, 732, 692 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{41}\text{H}_{39}\text{FNaO}_6$ $[\text{M}+\text{Na}]^+$: 669.2623, Found: 669.2629.



Product **13b** was obtained in 94% yield as a foam solid from febuxostat (75.9 mg) (72 h). m.p. = 107-108 °C; HPLC analysis (Chiralcel IA, i PrOH/hexane = 15/85, 1.0 mL/min, 254 nm; t_r (major) = 74.38 min, t_r (minor) = 70.63 min) gave the isomeric

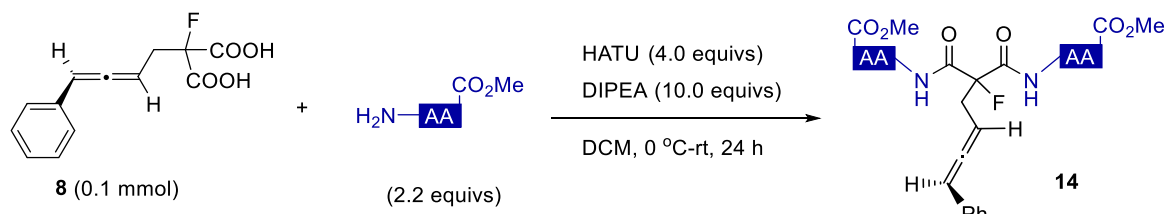
composition of the product: 96:4 er; $[\alpha]_D^{20}$ = -26.8 (c = 0.2, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ 8.11 (dd, J = 9.2, 2.4 Hz, 2H), 8.06-8.02 (m, 2H), 7.30-7.23 (m, 4H), 7.20-7.15 (m, 1H), 6.99 (dd, J = 8.8, 1.6 Hz, 2H), 6.23 (dt, J = 6.4, 2.4 Hz, 1H), 5.65-5.60 (m, 1H), 4.68-4.53 (m, 4H), 3.90 (d, J = 6.4 Hz, 4H), 2.77-2.74 (m, 8H), 2.26-2.16 (m, 2H), 1.10 (s, 6H), 1.09 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 207.5, 167.83, 167.80, 162.60, 162.59, 162.26, 162.24, 161.07, 161.05, 133.5, 132.6, 132.1, 128.7, 127.3, 126.8, 125.7, 120.5, 120.4, 115.3, 112.6, 102.97, 102.95, 95.3, 94.1 (d, J = 179.0 Hz), 87.1 (d, J = 7.6 Hz), 75.7, 64.9 (d, J = 5.1 Hz), 64.7 (d, J = 4.3 Hz), 33.3 (d, J = 21.8 Hz), 28.1, 19.0, 17.58, 17.56; ^{19}F NMR (376 MHz, CDCl_3): δ -166.74 (s, 1F); IR (neat): 2922, 2852, 1720, 1604, 1508, 1460, 1255, 1085, 1010 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{45}\text{H}_{43}\text{FN}_4\text{NaO}_6\text{S}_2$ $[\text{M}+\text{Na}]^+$: 841.2500, Found: 841.2518.



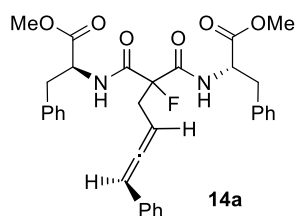
Product **13c** was obtained in 99% yield as a foam solid from indomethacin (83.8 mg) (11 h). m.p. = 71-72 °C; HPLC analysis (Chiralcel AD-H, i PrOH/hexane = 50/50, 1.0 mL/min, 254 nm; t_r (major) = 37.59 min, t_r (minor) = 43.97 min) gave the isomeric composition of the product: 95:5 er; $[\alpha]_D^{20}$ = -86.8

(c = 0.3, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ 7.63-7.59 (m, 4H), 7.44-7.40 (m, 4H), 7.28-7.24 (m, 2H), 7.20-7.15 (m, 3H), 6.91 (t, J = 2.8 Hz, 2H), 6.83 (d, J = 9.2 Hz, 2H), 6.64 (dd, J = 9.2, 2.4 Hz, 2H), 6.06 (dt, J = 6.4, 2.0 Hz, 1H), 5.34-5.32 (m, 1H), 4.30-4.15 (m, 4H), 3.78 (s, 6H), 3.65 (s, 2H), 3.63 (s, 2H), 2.46-2.36 (m, 2H), 2.33 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 207.1, 169.9, 168.2, 156.0, 139.2, 136.0, 133.8, 133.5, 131.1, 130.7, 130.3, 129.1, 128.7, 127.2, 126.8, 115.0, 111.9, 111.78, 111.76, 101.1, 95.0, 94.2 (d, J = 192.8 Hz), 87.0 (d, J = 7.7 Hz), 64.3 (d,

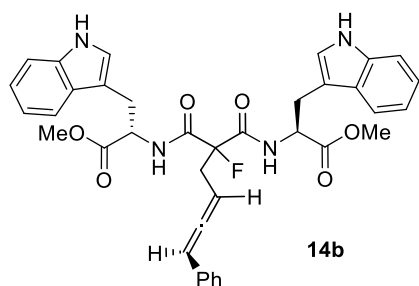
$J = 20.6$ Hz), 64.0 (d, $J = 20.3$ Hz), 55.6, 32.9 (d, $J = 20.6$ Hz), 30.0, 13.2; ^{19}F NMR (376 MHz, CDCl_3): δ -167.20 (s, 1F); IR (neat): 2957, 1743, 1682, 1591, 1477, 1317, 1222, 1141, 1087, 925, 833, 754, 736, 692 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{51}\text{H}_{43}\text{Cl}_2\text{FN}_2\text{NaO}_8$ $[\text{M}+\text{Na}]^+$: 923.2273, Found: 923.2283.



To a solution of carboxylic acid **8** (31.4 mg, 0.1 mmol) and amino acid or dipeptide (2.4 equiv) in anhydrous CH_2Cl_2 (3.0 mL) was added HATU (4.0 equivalents) at 0 °C. After being stirred for 10 min, DIPEA (10.0 equiv) was added to the reaction mixture. The resulting solution was warmed to rt and stirred for 24 hours. After adding H_2O (5 mL), the reaction mixture was extracted with CH_2Cl_2 (5 mL $\times$ 2). The organic phases were dried over anhydrous Na_2SO_4 and concentrated in vacuo to give the residue, which was purified by flash column chromatography (PE/EtOAc = 2/1, v/v) to furnish the desired products.



Product **14a** was obtained in 85% yield as a white solid from methyl *L*-phenylalaninate (47.5 mg). m.p. = 97-98 °C; ^{19}F NMR analysis of the crude mixture revealed that the dr value was $>20:1$; $[\alpha]_{\text{D}}^{20} = -63.8$ ($c = 0.1$, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ 7.30-7.16 (m, 13H), 7.09-7.03 (m, 4H), 6.13 (dt, $J = 6.4, 2.4$ Hz, 1H), 5.33-5.27 (m, 1H), 4.89-4.83 (m, 1H), 4.82-4.77 (m, 1H), 3.69 (s, 3H), 3.68 (s, 3H), 3.17-3.03 (m, 4H), 2.94-2.72 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 207.4, 170.85, 170.80, 165.9 (d, $J = 22$ Hz), 165.6 (d, $J = 23$ Hz), 135.30, 135.26, 133.7, 129.12, 129.10, 128.64, 128.63, 128.5, 127.3, 127.2, 127.1, 126.9, 95.6 (d, $J = 199.9$ Hz), 95.3, 86.5 (d, $J = 2.9$ Hz), 53.35, 53.29, 52.4, 37.8, 37.7, 36.5 (d, $J = 21.6$ Hz); ^{19}F NMR (376 MHz, CDCl_3): δ -170.50 (s, 1F); IR (neat): 3418, 3340, 3001, 1743, 1697, 1512, 1180, 910, 725, 702, 648 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{33}\text{H}_{34}\text{O}_6\text{FN}_2$ $[\text{M}+\text{H}]^+$: 573.2395, Found: 573.2392.

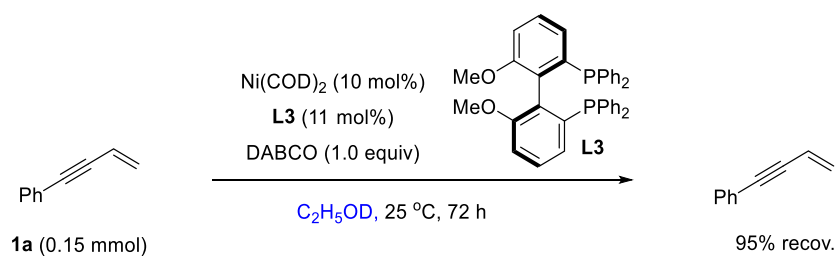


Product **14b** was obtained in 99% yield as a white solid from methyl *L*-tryptophanate 56.0 mg). m.p. = 101-102 °C; ^{19}F NMR analysis of the crude mixture revealed that the dr value was >20:1; $[\alpha]_{\text{D}}^{20} = -6.1$ ($c = 0.05$, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ 8.10 (s, 1H), 7.99 (s, 1H), 7.49 (d, $J = 8.0$ Hz, 2H), 7.30-7.11 (m,

11H), 7.09-7.04 (m, 2H), 6.76 (t, $J = 2.4$ Hz, 2H), 6.09 (dt, $J = 6.4, 2.4$ Hz, 1H), 5.38-5.33 (m, 1H), 4.91-4.86 (m, 1H), 4.81-4.76 (m, 1H), 3.63 (s, 3H), 3.59 (s, 3H), 3.32-3.19 (m, 4H), 2.96-2.74 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 207.3, 171.4, 171.3, 166.2 (d, $J = 21.9$ Hz), 165.5 (d, $J = 22.8$ Hz), 136.1, 133.7, 128.5, 127.09, 127.06, 126.9, 123.3, 123.1, 122.2, 122.1, 119.6, 119.5, 118.4, 118.2, 111.4, 111.3, 109.0, 108.9, 95.9 (d, $J = 200.0$ Hz), 95.2, 86.5 (d, $J = 2.9$ Hz), 52.8, 52.7, 52.52, 52.48, 36.4 (d, $J = 21.1$ Hz), 27.5, 27.4; ^{19}F NMR (376 MHz, CDCl_3): δ -170.03 (s, 1F); IR (neat): 3410, 3348, 1743, 1689, 1512, 1435, 1350, 1211, 910, 732 cm^{-1} ; HRMS (ESI): Exact mass calcd for $\text{C}_{37}\text{H}_{36}\text{O}_6\text{N}_4\text{F}$ $[\text{M}+\text{H}]^+$: 651.2613, Found: 651.2598.

7. Experiments and DFT mechanistic studies

7.1 Deuterium labeling study



In a glove box, to a Schlenk tube equipped with a stirring bar were successively added $\text{Ni}(\text{COD})_2$ (2.8 mg, 10 mol%), and (*R*)-MeO-BIPHEP **L3** (6.4 mg, 11 mol%), followed by the addition of absolute EtOD (1.0 mL). The resulting mixture was stirred at room temperature for 15 min, and then added DABCO (11.2 mg, 1.0 equiv). After being stirred for another 5 min, to the mixture was added 1,3-enyne **1a** (0.15 mmol). After it take out from the glove box, the resulting mixture was stirred at 25 °C for 3 days. The reaction mixture was concentrated under vacuum to give the crude residue, which was purified by silica gel column chromatography to recovery 1,3-enyne **1a** (18.2 mg, 95% recovery).

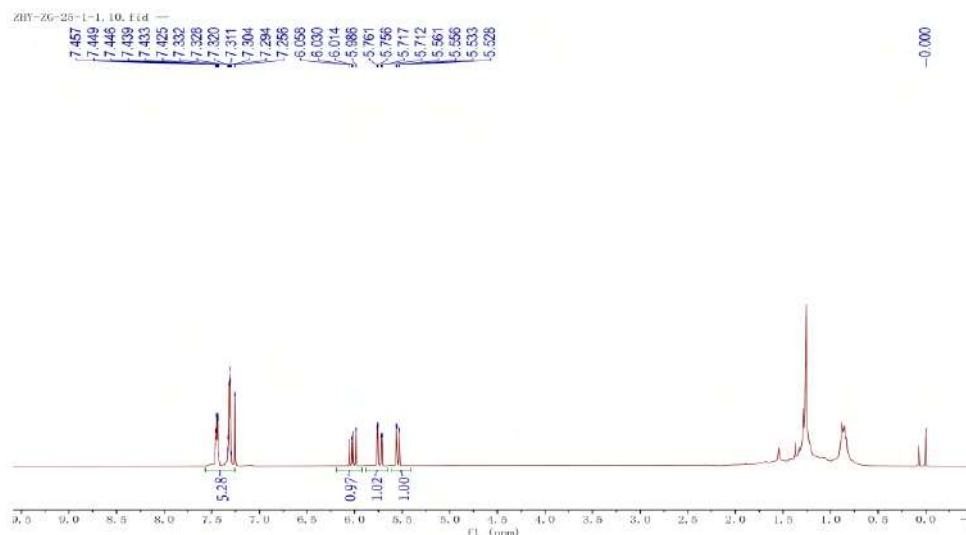
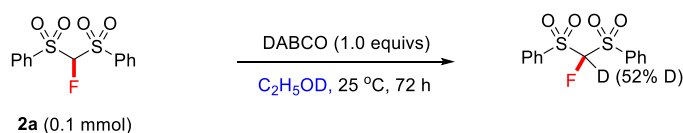


Fig. S1 The deuterium incorporation ratio of the recovered 1,3-enyne **1a**.



In a glove box, to a Schlenk tube equipped with a stirring bar were successively added $\text{Ni}(\text{COD})_2$ (2.8 mg, 10 mol%), and (*R*)-MeO-BIPHEP **L3** (6.4 mg, 11 mol%), followed by the addition of absolute EtOD (1.0 mL). The resulting mixture was stirred at room temperature for 15 min, and then added DABCO (11.2 mg, 1.0 equiv) and FBSM **2a** (0.1 mmol, 1.0 equiv). After it take out from the glove box, the resulting mixture was stirred at 25 °C for 3 days. The reaction mixture was concentrated under vacuum to give the residue, which was directly analyzed by ^1H NMR analysis with CDCl_3 .

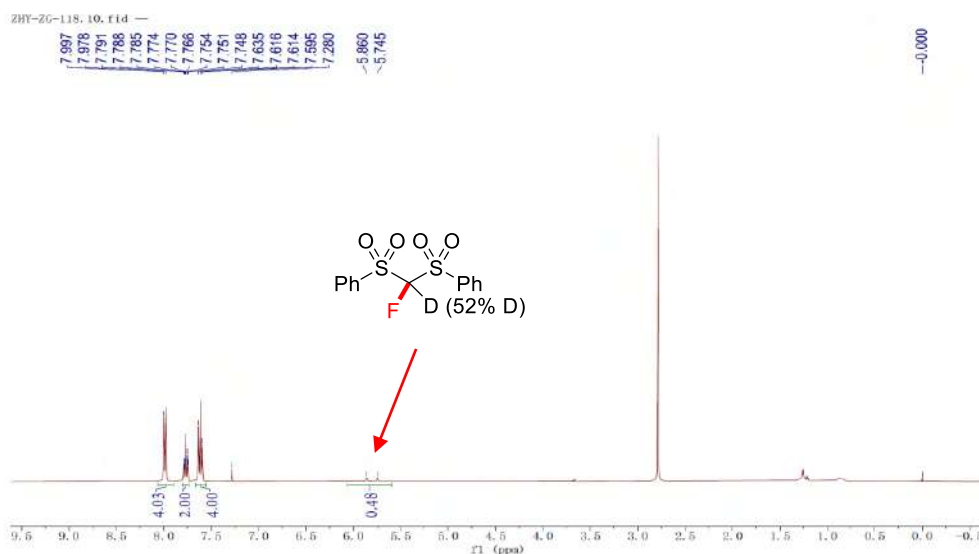
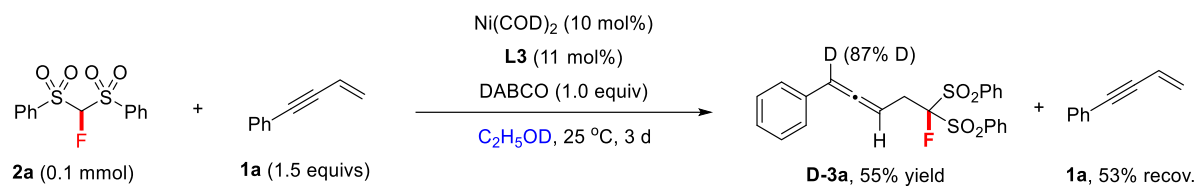


Fig. S2 The recovered FBSM **2a** with 52% D incorporation.



In a glove box, to a Schlenk tube equipped with a stirring bar were successively added Ni(COD)₂ (2.8 mg, 10 mol%), and (*R*)-MeO-BIPHEP **L3** (6.4 mg, 11 mol%), followed by the addition of absolute EtOD (1.0 mL). The resulting mixture was stirred at room temperature for 15 min, and then added DABCO (11.2 mg, 1.0 equiv) and FBSM **2a** (0.1 mmol, 1.0 equiv). After being stirred for another 5 min, to the mixture was added 1,3-enyne **1a** (0.15 mmol, 1.5 equivs). After it take out from the glove box, the reaction mixture was stirred at 25 °C for 3 days. The reaction was monitored by TLC analysis. After full consumption of **2a**, the reaction mixture was concentrated under vacuum. The crude residue was purified by silica gel column chromatography using PE/EtOAc (6:1, v/v) as the eluent to afford the desired products **D-3a** with 55% yield, along with the recovery of **1a** (53% recov.).

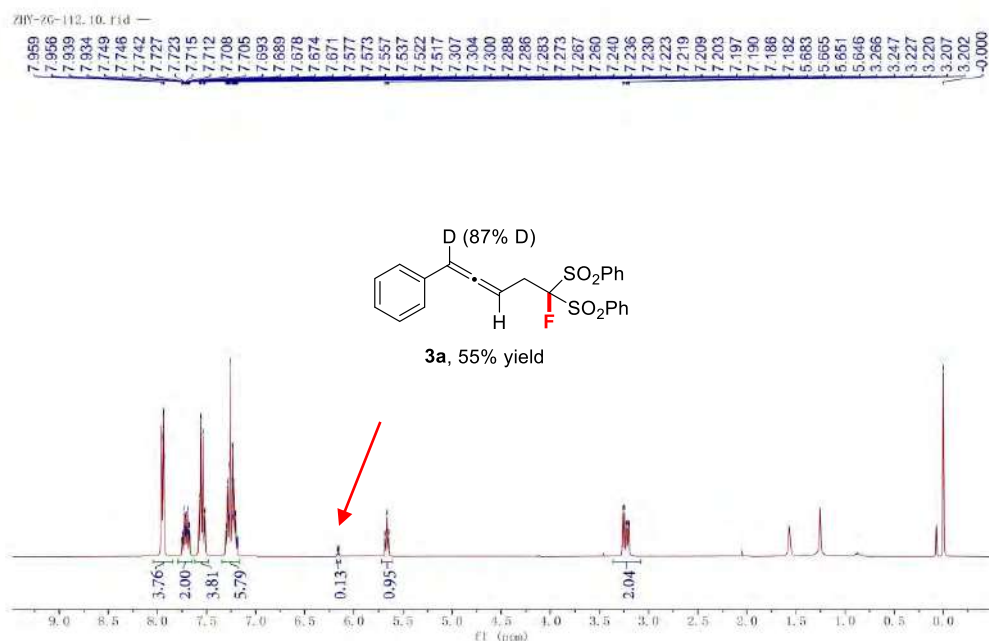


Fig. S3 The product **3a** with 87% D (0.87 D) incorporation at the methyl group (in EtOD).

7.2 DFT calculations

All the DFT calculations were performed with the Gaussian 16^[3] programs. Geometry optimization and frequency calculations were carried out at the PBE0-D3(BJ)^[4]/def2-SVP^[5] level of theory. All the transition states have only one imaginary frequency, while the stationary points do not. Single-point energy was calculated at the level of PBE0-D3(BJ)/def2-TZVP/PCM^[6] (ethanol). The reported free energy in solution includes Gibbs free energy correction at temperature of 298.15 K and pressure of 1 atm. Considering the overestimation of the entropy contribution, the free energies were corrected by +2.6 (or -2.6) kcal/mol for one-to-two (or two-to-one) molecular conversions, based on the free-volume theory.^[7] The 3D plots for the molecules were created with CYLview 20.^[8]

For the initial transformation of Ni(COD)₂, the ligand exchange between **L3** and one COD molecule, followed by the ligand exchange between **1a** and the other COD molecule forming intermediate **A**, which is the active species in the catalytic cycle, is the most favorable pathway. Such a process is highly exergonic by 26.8 kcal/mol. While all other pathways for the transformation of Ni(COD)₂ are significantly endergonic (Fig. S4).

For the protonation of intermediate **A**, various proton sources were considered, including ethanol, **2a**, and protonated DABCO by **2a** (**BH**⁺), corresponding to **TSb1**, **TSc1**, and **TS1**, respectively (Fig. S5). The results indicate that the most favorable pathway for protonation is the case of **BH**⁺ as proton source with the lowest energy barrier of 25.2 kcal/mol. In addition, the direct oxidative addition of ethanol by Ni(0) is also unfavorable with the energy barrier over 60 kcal/mol. The above results demonstrate that the successful reaction needs the presence of both DABCO (**B**) and **2a**. Notably, this step is completely distinct with the traditional Pd-catalyzed hydrofunctionalizations of 1,3-enynes,^[1b] as well as Ni-catalyzed hydrofunctionalization of 1,3-dienes.^[9]

³ Frisch, M. J. *et al.* Gaussian 16 Rev. C.02 (Wallingford, CT, **2019**).

⁴ (a) Adamo, C. & Barone, V. *J. Chem. Phys.* **1999**, *110*, 6158. (b) Grimme, S., Antony, J., Ehrlich, S. & Krieg, H. *J. Chem. Phys.* **2010**, *132*, 154104.

⁵ Weigend, F. & Ahlrichs, R. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297–3305.

⁶ (a) Miertuš, S., Scrocco, E. & Tomasi, J. *Chem. Phys.* **1981**, *55*, 117. (b) Mennucci, B., Cancè, E. & Tomasi, J. *J. Phys. Chem. B* **1997**, *101*, 10506. (c) Tomasi, J., Mennucci, B. & Cammi, R. *Chem. Rev.* **2005**, *105*, 2999.

⁷ Benson, S. W. *The Foundations of Chemical Kinetics*; Krieger: Malabar, FL (**1982**).

⁸ Legault, C. Y. CYLview20 (Université Sherbrooke, **2020**).

⁹ Cheng, L.; Li, M.-M.; Xiao, L.-J.; Xie, J.-H.; Zhou, Q.-L. *J. Am. Chem. Soc.* **2018**, *140*, 11627. (b) Flaget, A.; Zhang, C.; Mazet, C. *ACS Catal.* **2022**, *12*, 15638.

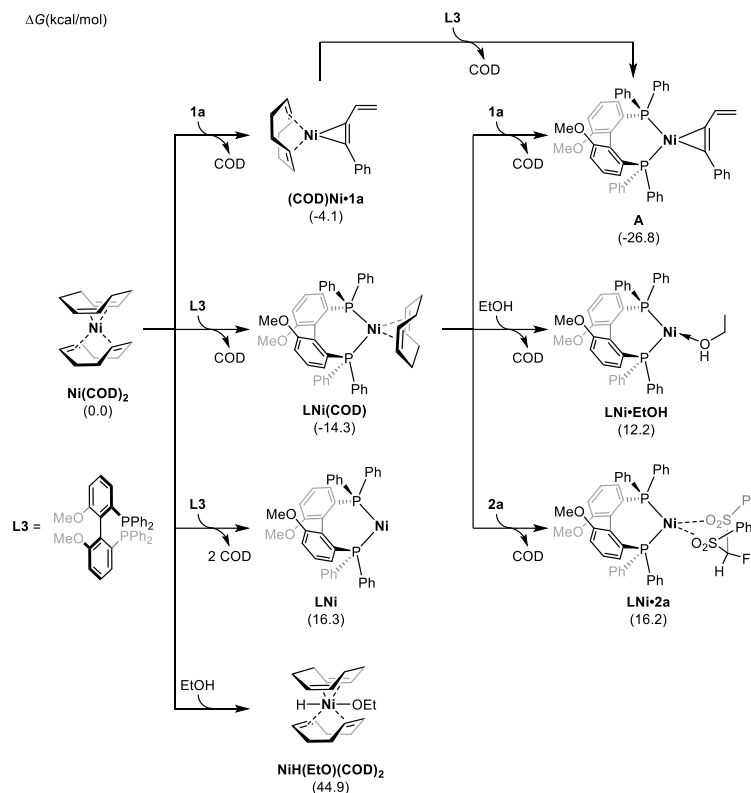


Fig. S4 Free energy profile for transformation of $\text{Ni}(\text{COD})_2$ at the PBE0-D3(BJ)/def2-TZVP/PCM(EtOH)//PBE0-D3(BJ)/def2-SVP level.

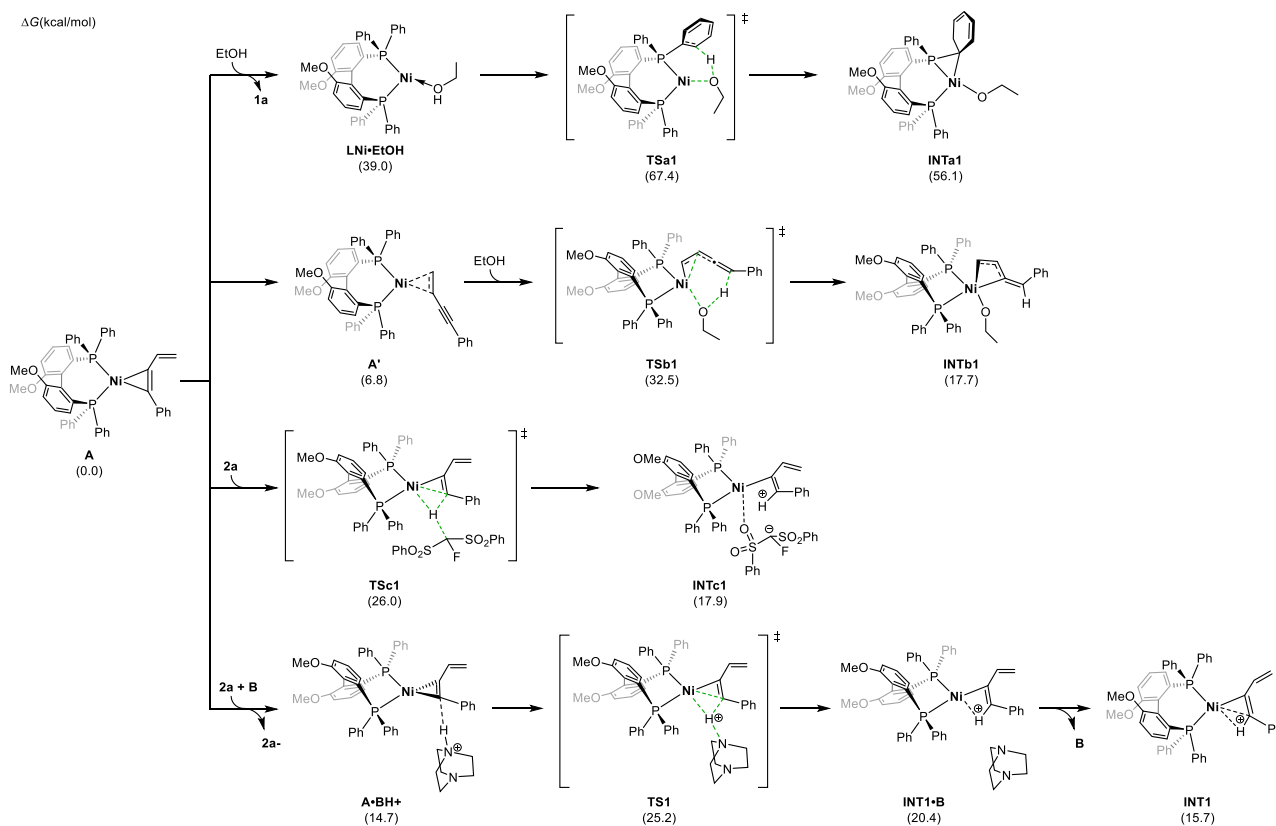


Fig. S5 Free energy profile for transformation of **A** at the PBE0-D3(BJ)/def2-TZVP/PCM(EtOH)//PBE0-D3(BJ)/def2-SVP level.

For the nucleophilic attack step after protonation, the direct nucleophilic attack of **INT1** by **2a⁻** is unfavorable by the energy barrier of 29.8 kcal/mol, indicating the transformation to η^3 -coordinated isomer **INT2** is an essential step (Fig. S6). Besides, the nucleophilic attack to the 2-position of butadienyl ligand of **INT2^R** via **TSe1** yielding 1,3-butadiene compound is also unfavorable than which needs to overcome the high energy barrier of 29.9 kcal/mol, while the case of 4-position via **TS3^R** only needs the energy barrier of 9.4 kcal/mol, indicating that this reaction also has excellent regioselectivity.

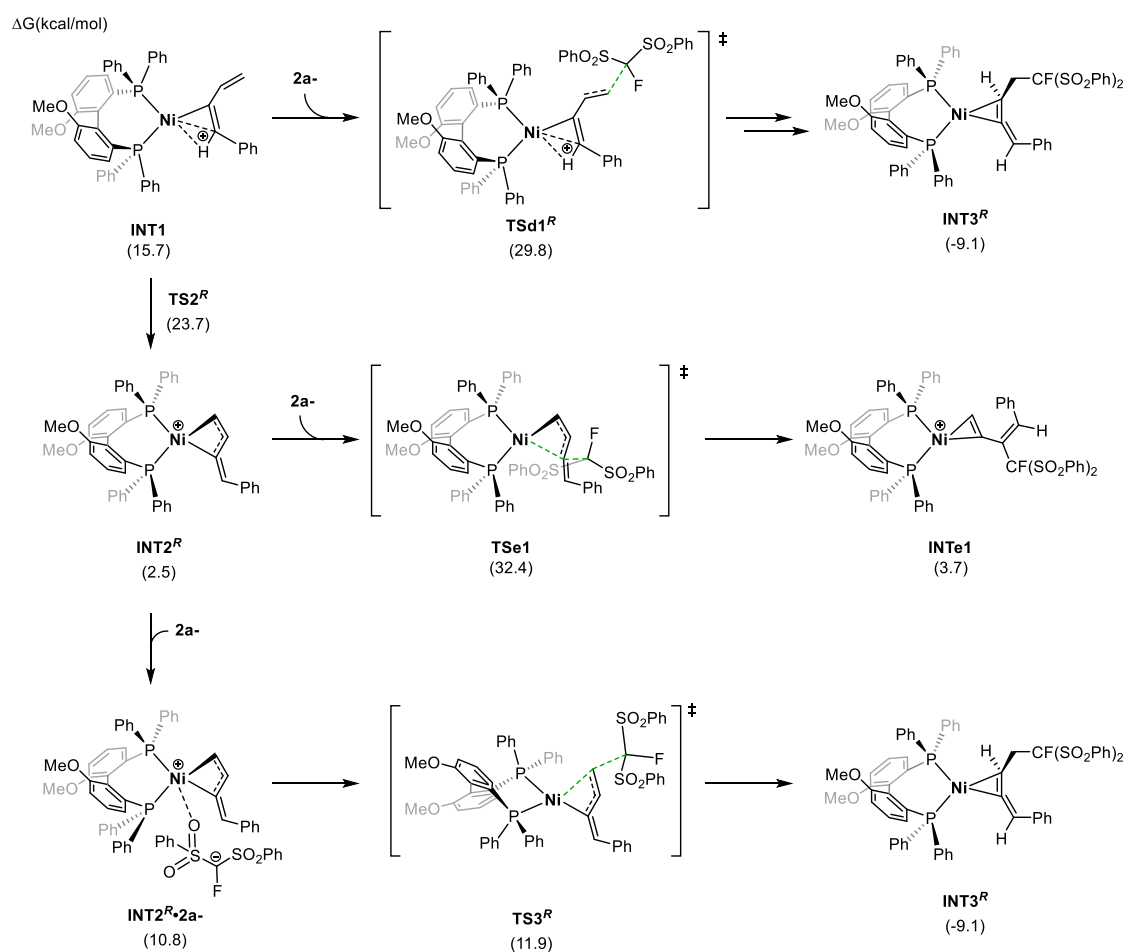


Fig. S6 Free energy profile for transformation of **INT1** at the PBE0-D3(BJ)/def2-TZVP/PCM(EtOH)//PBE0-D3(BJ)/def2-SVP level.

3D plots, thermochemistry information, and optimized Cartesian coordinates for all of the stationary point

Ni(COD)₂

Thermal Correction to Free Energy = 0.325422
a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-
TZVP/PCM(ethanol) Level = -2131.72451186
a.u.

Cartesian Coordinates (Angstroms):

Ni	0.000017	-0.000018	0.000004
C	-1.456759	0.406638	-1.455887
H	-0.942074	0.463592	-2.418782
C	-1.310302	1.508153	-0.624644
H	-0.720655	2.343260	-1.017768
C	-2.572772	-0.615936	-1.383364
H	-3.484657	-0.147302	-0.984832
H	-2.832304	-0.935136	-2.404729
C	-1.310295	-1.508139	0.624718
C	-1.456779	-0.406602	1.455922
C	-2.187939	-1.844703	-0.552359
H	-3.093172	-2.391053	-0.222639
H	-1.635114	-2.551261	-1.193237
H	-0.720624	-2.343230	1.017840
H	-0.942073	-0.463456	2.418812
C	-2.572847	0.615899	1.383327
H	-2.832546	0.935022	2.404674
H	-3.484642	0.147243	0.984626
C	-2.187936	1.844708	0.552439
H	-1.635069	2.551176	1.193382
H	-3.093121	2.391150	0.222739
C	1.456783	0.406597	1.455912
H	0.942089	0.463464	2.418808
C	1.310300	1.508136	0.624703
H	0.720646	2.343232	1.017841
C	2.572834	-0.615927	1.383339
H	3.484675	-0.147268	0.984756
H	2.832440	-0.935113	2.404691
C	1.310291	-1.508136	-0.624695
C	1.456711	-0.406598	-1.455927
C	2.187979	-1.844696	0.552357
H	3.093195	-2.391061	0.222613
H	1.635171	-2.551242	1.193266
H	0.720658	-2.343257	-1.017816
H	0.942000	-0.463520	-2.418810
C	2.572736	0.615964	-1.383429
H	2.832239	0.935179	-2.404798
H	3.484630	0.147324	-0.984940
C	2.187927	1.844713	-0.552391
H	1.635087	2.551276	-1.193252
H	3.093163	2.391065	-0.222685

L3

Thermal Correction to Free Energy = 0.525665
a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-
TZVP/PCM(ethanol) Level = -2299.00078768
a.u.

Cartesian Coordinates (Angstroms):

C	-0.479482	-1.582130	-0.115820
C	-1.708331	-1.061673	-0.546826
C	-2.272914	-1.504246	-1.750461
C	-1.610956	-2.457533	-2.514971
C	-0.394855	-2.993500	-2.094589
C	0.167791	-2.565401	-0.888932
C	0.144154	-1.114016	1.151711
C	1.210082	-0.202174	1.160748
C	1.734907	0.247935	2.381878
C	1.205300	-0.217021	3.577931
C	0.151291	-1.130393	3.585363
C	-0.377447	-1.583493	2.375592
H	-3.228183	-1.096984	-2.086297
H	-2.047123	-2.796715	-3.457941
H	0.105252	-3.746138	-2.704112
H	2.550729	0.973141	2.387334
H	1.613795	0.136047	4.528132
H	-0.254000	-1.479392	4.535134
P	-2.513652	0.193947	0.539304
P	1.847031	0.383146	-0.468984
C	-4.228266	0.159648	-0.126845
C	-4.768261	1.130043	-0.977976
C	-5.042686	-0.904884	0.287804
C	-6.091390	1.032593	-1.410432
H	-4.148167	1.966057	-1.309658
C	-6.357291	-1.009483	-0.156157
H	-4.631077	-1.662957	0.961385
C	-6.887231	-0.036896	-1.005703
H	-6.500144	1.798251	-2.074758
H	-6.976038	-1.849861	0.168490
H	-7.922036	-0.112412	-1.348467
C	-1.881848	1.766651	-0.171998
C	-2.101160	2.935696	0.571710
C	-1.213832	1.860516	-1.399212
C	-1.697384	4.176195	0.081992
H	-2.600582	2.867818	1.542670
C	-0.793079	3.100745	-1.878789
H	-1.014938	0.957219	-1.978595
C	-1.041510	4.260300	-1.146788
H	-1.884864	5.079588	0.667755
H	-0.259596	3.157862	-2.830424
H	-0.708246	5.229335	-1.525644
C	2.625521	1.974291	0.022780
C	3.989643	2.250708	-0.123037
C	1.776072	2.988529	0.491914
C	4.493647	3.512032	0.197425
H	4.667154	1.473358	-0.483615
C	2.283063	4.241484	0.820073
H	0.707675	2.791178	0.610063
C	3.644792	4.509847	0.671085
H	5.561929	3.711483	0.080276
H	1.605059	5.015494	1.188520
H	4.042477	5.495711	0.924183
C	3.330065	-0.679382	-0.716252

C	4.000469	-1.351552	0.312823
C	3.800822	-0.811353	-2.028785
C	5.123686	-2.127045	0.033885
H	3.631765	-1.274083	1.337939
C	4.931429	-1.579506	-2.307565
H	3.269659	-0.305041	-2.840260
C	5.594894	-2.240377	-1.275255
H	5.637503	-2.647184	0.846499
H	5.290407	-1.667014	-3.336137
H	6.477692	-2.847634	-1.490153
O	1.322991	-3.040979	-0.386765
O	-1.398872	-2.456596	2.281119
C	2.085418	-3.930783	-1.152392
H	2.364206	-3.492172	-2.125891
H	3.002662	-4.123762	-0.582939
H	1.553951	-4.884045	-1.321217
C	-2.085886	-2.822115	3.443013
H	-2.907152	-3.478704	3.128149
H	-1.441298	-3.376485	4.148137
H	-2.507530	-1.941295	3.958147

COD

Thermal Correction to Free Energy = 0.149525 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -311.773511342 a.u.

Cartesian Coordinates (Angstroms):

C	-0.028787	1.689305	-0.219352
H	-0.322147	2.616775	-0.725598
C	1.198583	1.232395	-0.498463
H	1.794428	1.845598	-1.185768
C	-1.085966	1.086411	0.665789
H	-0.655348	0.702368	1.600104
H	-1.778514	1.885929	0.972488
C	-1.198582	-1.232396	-0.498462
C	0.028788	-1.689305	-0.219349
C	-1.913543	-0.004698	-0.019660
H	-2.730109	-0.317242	0.658886
H	-2.429624	0.438981	-0.890039
H	-1.794427	-1.845601	-1.185767
H	0.322148	-2.616777	-0.725592
C	1.085965	-1.086410	0.665792
H	1.778513	-1.885928	0.972493
H	0.655346	-0.702366	1.600106
C	1.913543	0.004698	-0.019657
H	2.429626	-0.438982	-0.890034
H	2.730108	0.317244	0.658890

Ethanol

Thermal Correction to Free Energy = 0.055056 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -154.928619084 a.u.

Cartesian Coordinates (Angstroms):

C	-1.215948	-0.216988	-0.000006
C	0.092409	0.537478	0.000007
H	-1.286266	-0.860759	0.889596
H	-2.071247	0.474902	0.000043
H	-1.286298	-0.860678	-0.889664
H	0.137187	1.199643	-0.889201
H	0.137178	1.199641	0.889215
O	1.142020	-0.395222	0.000014
H	1.974517	0.086083	-0.000099

1a

Thermal Correction to Free Energy = 0.109218 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -385.483426238 a.u.

Cartesian Coordinates (Angstroms):

C	-3.282008	0.163761	-0.000186
C	-2.691079	-1.100076	-0.000126
C	-1.306645	-1.227139	-0.000010
C	-0.487450	-0.083015	0.000046
C	-1.093507	1.186966	-0.000005
C	-2.478768	1.304503	-0.000122
H	-4.370256	0.259833	-0.000277
H	-3.316101	-1.996197	-0.000171
H	-0.839952	-2.214027	0.000040
H	-0.460823	2.076590	0.000048
H	-2.937107	2.296276	-0.000163
C	0.931278	-0.207738	0.000194
C	2.146705	-0.305165	0.000267
C	3.557771	-0.451705	0.000048
C	4.433986	0.565888	0.000001
H	3.933663	-1.482207	-0.000074
H	5.509533	0.375845	-0.000155
H	4.099349	1.606212	0.000106

2a

Thermal Correction to Free Energy = 0.177773 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -1698.22449671 a.u.

Cartesian Coordinates (Angstroms):

C	-1.509564	-1.283825	0.468668
H	-2.381899	-1.935758	0.281660
F	-0.974467	-1.508018	1.683880
S	-2.209158	0.413548	0.393042
O	-3.066297	0.428548	-0.782150
O	-2.722869	0.633964	1.738741
S	-0.299765	-1.784020	-0.829161
O	-0.271471	-3.237575	-0.723431
O	-0.676762	-1.101293	-2.059384
C	1.259385	-1.154256	-0.264980
C	1.863940	-1.721747	0.857962

C	1.880655	-0.161383	-1.017097
C	3.102778	-1.234981	1.261925
H	1.368552	-2.528348	1.399477
C	3.127775	0.303734	-0.609312
H	1.382084	0.230713	-1.904422
C	3.730703	-0.224327	0.531266
H	3.588403	-1.656540	2.144592
H	3.628914	1.083584	-1.186402
H	4.707174	0.147417	0.850693
C	-0.837121	1.500441	0.132453
C	0.001221	1.791310	1.208618
C	-0.669463	2.077440	-1.123543
C	1.054950	2.676635	1.006836
H	-0.182461	1.334108	2.182600
C	0.380156	2.975416	-1.303769
H	-1.355267	1.811681	-1.929993
C	1.237859	3.269912	-0.243650
H	1.729955	2.914155	1.831556
H	0.527404	3.448796	-2.277006
H	2.059660	3.974541	-0.392236

NiH(EtO)(COD)₂

Thermal Correction to Free Energy = 0.395235 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -2286.59223884 a.u.

Cartesian Coordinates (Angstroms):

Ni	0.241069	-0.034372	0.034112
C	2.006878	-1.166710	1.412094
H	1.431670	-1.457384	2.298580
C	2.298617	0.145670	1.270954
H	1.933849	0.836104	2.035795
C	2.519953	-2.278637	0.537520
H	3.514004	-2.007136	0.155920
H	2.673913	-3.176373	1.156255
C	0.908813	-1.451636	-1.276352
C	1.487896	-0.202594	-1.535076
C	1.584430	-2.631634	-0.628751
H	2.146452	-3.206944	-1.389064
H	0.800352	-3.319230	-0.271257
H	0.050232	-1.718863	-1.903968
H	1.014870	0.392168	-2.323018
C	2.920614	0.181484	-1.215861
H	3.253608	0.929773	-1.950697
H	3.572517	-0.692118	-1.373128
C	3.129453	0.769659	0.188189
H	2.868327	1.836008	0.169539
H	4.198966	0.715076	0.463994
C	-3.222662	-0.434584	-1.344618
H	-3.296066	-0.681917	-2.410265
C	-2.944104	0.840798	-1.037646
H	-2.846673	1.532223	-1.883933
C	-3.409875	-1.580248	-0.394099
H	-3.976113	-1.263807	0.492190

H	-4.035033	-2.341517	-0.886662
C	-1.141534	-1.513832	0.902642
C	-1.271748	-0.290442	1.522619
C	-2.118162	-2.271373	0.045677
H	-2.398185	-3.170386	0.625352
H	-1.590449	-2.664793	-0.841050
H	-0.362111	-2.167796	1.303327
H	-0.562835	-0.100067	2.335759
C	-2.462732	0.645709	1.531789
H	-2.293613	1.359302	2.350880
H	-3.360142	0.077265	1.823133
C	-2.733371	1.495521	0.290396
H	-1.866341	2.164633	0.188514
H	-3.603261	2.146687	0.496600
C	0.595996	4.161013	-0.010957
C	0.442626	2.761873	-0.588696
H	1.476120	4.206402	0.650381
H	0.713639	4.918672	-0.803108
H	-0.284714	4.423958	0.596118
H	-0.427449	2.771416	-1.293415
H	1.326529	2.565643	-1.245258
O	0.299253	1.839943	0.418128
H	-0.762547	0.255643	-0.886642

2a⁻

Thermal Correction to Free Energy = 0.164479 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -1697.74218518 a.u.

Cartesian Coordinates (Angstroms):

C	-1.892810	-0.578210	0.490375
F	-1.511221	-0.903174	1.779512
S	-1.871808	1.133700	0.251297
O	-2.501948	1.475238	-1.023739
O	-2.360130	1.716834	1.507077
S	-1.110873	-1.636269	-0.625405
O	-1.487751	-3.011744	-0.281011
O	-1.287814	-1.130379	-1.989444
C	0.651422	-1.566843	-0.279847
C	1.137081	-2.108471	0.912030
C	1.505719	-0.929225	-1.176526
C	2.491445	-1.988315	1.212367
H	0.444787	-2.615092	1.585775
C	2.860552	-0.821636	-0.871457
H	1.084048	-0.525318	-2.098476
C	3.354688	-1.346299	0.322505
H	2.879068	-2.403851	2.146720
H	3.533458	-0.313641	-1.567099
H	4.417284	-1.252763	0.562732
C	-0.172743	1.703650	0.113181
C	0.676723	1.582308	1.214965
C	0.290674	2.214539	-1.096232
C	2.004376	1.980248	1.097412
H	0.283817	1.171769	2.147031

C	1.618431	2.628570	-1.199063
H	-0.409346	2.271074	-1.932504
C	2.475197	2.512730	-0.105202
H	2.680377	1.872940	1.949649
H	1.988386	3.038754	-2.143029
H	3.518615	2.827932	-0.190804

B

Thermal Correction to Free Energy = 0.154450 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -345.067638732 a.u.

Cartesian Coordinates (Angstroms):

C	0.778117	1.252503	-0.559730
C	-0.778012	1.252425	-0.560049
H	1.184395	2.083712	0.039323
H	1.184782	1.361056	-1.578390
H	-1.184636	2.083858	0.038460
H	-1.184254	1.360478	-1.578930
C	0.778060	-0.141498	1.364600
H	1.184275	-1.075940	1.784897
H	1.184758	0.686376	1.967967
C	-0.778139	-0.141148	1.364591
H	-1.184797	-1.075210	1.785304
H	-1.184453	0.687187	1.967584
C	-0.778097	-1.111208	-0.804563
H	-1.184415	-2.047538	-0.388612
H	-1.184697	-1.008664	-1.823875
C	0.778071	-1.111074	-0.804773
H	1.184681	-2.047516	-0.389358
H	1.184361	-1.007997	-1.824154
N	-1.266937	0.000052	-0.000081
N	1.266937	-0.000024	-0.000016

BH⁺

Thermal Correction to Free Energy = 0.169438 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -345.526583440 a.u.

Cartesian Coordinates (Angstroms):

C	0.732706	-0.592512	-1.294455
C	-0.816451	-0.572547	-1.250218
H	1.155301	0.016181	-2.105555
H	1.155571	-1.604113	-1.363916
H	-1.217617	0.017368	-2.085983
H	-1.217253	-1.590881	-1.349125
C	0.734149	1.416600	0.133659
H	1.157652	1.814224	1.066135
H	1.157042	1.982237	-0.707883
C	-0.814987	1.369739	0.129751
H	-1.215136	1.798921	1.058790
H	-1.215771	1.965024	-0.702383
C	-0.815035	-0.796538	1.121844

H	-1.214847	-0.373211	2.053713
H	-1.216157	-1.815334	1.029183
C	0.734134	-0.824701	1.159525
H	1.158003	-0.379100	2.069885
H	1.156664	-1.831441	1.037381
N	-1.270603	0.000388	0.000765
N	1.212428	-0.000317	-0.000705
H	2.236676	-0.000621	-0.001301

(COD)Ni-1a

Thermal Correction to Free Energy = 0.281413 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -2205.43725681 a.u.

Cartesian Coordinates (Angstroms):

Ni	-0.815247	0.229927	-0.009119
C	-2.671963	0.754603	-0.793092
H	-2.430218	1.596650	-1.450966
C	-2.651112	0.997225	0.565255
H	-2.428174	2.019182	0.890194
C	-3.281367	-0.456334	-1.461344
H	-4.124259	-0.829627	-0.862579
H	-3.714317	-0.154441	-2.427316
C	-1.232589	-1.705810	-0.603321
C	-1.477964	-1.597471	0.749948
C	-2.251109	-1.572957	-1.704546
H	-2.766885	-2.536495	-1.878405
H	-1.702971	-1.357528	-2.635320
H	-0.258993	-2.102319	-0.911528
H	-0.667546	-1.883966	1.429383
C	-2.835783	-1.407529	1.385454
H	-2.865574	-1.951528	2.341997
H	-3.611681	-1.868766	0.758207
C	-3.154203	0.074474	1.643926
H	-2.679553	0.382573	2.589074
H	-4.241576	0.210877	1.798499
C	4.809025	-1.463037	0.039847
C	3.655584	-2.162397	0.393944
C	2.419586	-1.522976	0.385261
C	2.310309	-0.167053	0.033412
C	3.484463	0.525876	-0.318333
C	4.717142	-0.116976	-0.319154
H	5.779263	-1.965503	0.043390
H	3.720180	-3.215926	0.677066
H	1.516362	-2.070189	0.662694
H	3.409627	1.577970	-0.601836
H	5.616999	0.436100	-0.600042
C	1.029978	0.502400	0.018750
C	0.402304	1.635323	-0.086616
C	0.431821	3.072241	-0.155920
C	1.458200	3.840311	0.246453
H	-0.470452	3.565044	-0.539418
H	1.403550	4.930718	0.191518
H	2.369210	3.399732	0.661166

L3·Ni(COD)

Thermal Correction to Free Energy = 0.707554
a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-
TZVP/PCM(ethanol) Level = -4118.98062991
a.u.

Cartesian Coordinates (Angstroms):

P	-1.618320	0.347071	-0.104731
P	1.618260	0.347155	0.104736
O	1.063493	-3.915333	-1.045512
O	-1.063272	-3.915469	1.045364
C	-0.299530	-2.052705	-0.683361
C	0.299595	-2.052712	0.683282
C	-1.279431	-1.149885	-1.132349
C	1.279438	-1.149848	1.132298
C	0.110619	-3.100496	-1.538274
C	-0.110470	-3.100566	1.538159
C	-0.447261	-3.252987	-2.807473
C	0.447415	-3.253052	2.807357
C	-1.858690	-1.335749	-2.395611
C	1.858698	-1.335696	2.395561
C	-1.444101	-2.373603	-3.218490
C	1.444180	-2.373601	3.218410
C	1.516070	-4.981946	-1.825042
C	-1.515728	-4.982171	1.824842
C	-2.113233	-0.453361	1.478583
C	-3.230179	0.990099	-0.713264
C	2.113395	-0.453209	-1.478547
C	3.229978	0.990306	0.713489
C	-1.501220	-0.044367	2.665642
C	-3.341854	1.460584	-2.031825
C	1.501534	-0.044203	-2.665680
C	3.341458	1.460561	2.032148
C	-3.065106	-1.479698	1.514387
C	-4.320378	1.175540	0.147221
C	3.065266	-1.479553	-1.514248
C	4.320224	1.176066	-0.146866
C	-1.837247	-0.645923	3.876444
C	-4.520965	2.041105	-2.489870
C	1.837722	-0.645733	-3.876451
C	4.520432	2.041191	2.490403
C	-3.409764	-2.072797	2.725668
C	-5.492895	1.780432	-0.304738
C	3.410075	-2.072639	-2.725493
C	5.492602	1.781071	0.305307
C	-2.795275	-1.657637	3.908658
C	-5.604335	2.203441	-1.626751
C	2.795751	-1.657448	-3.908559
C	5.603851	2.203863	1.627407
H	-2.653157	-0.674734	-2.736245
H	2.653101	-0.674615	2.736222
H	-1.905526	-2.503355	-4.200582
H	1.905605	-2.503344	4.200503
H	2.275641	-5.504688	-1.229513

H	0.701672	-5.688033	-2.066293
H	-2.275254	-5.504959	1.229296
H	-0.701253	-5.688188	2.066041
H	-0.730897	0.727940	2.616594
H	-2.484865	1.394109	-2.704350
H	0.731212	0.728108	-2.616735
H	2.484420	1.393803	2.704585
H	-3.529941	-1.819497	0.585344
H	-4.255429	0.844986	1.185186
H	3.529971	-1.819380	-0.585151
H	4.255419	0.845693	-1.184897
H	-1.340961	-0.329063	4.796614
H	-4.585278	2.388339	-3.524010
H	1.341557	-0.328851	-4.796677
H	4.584600	2.388242	3.524613
H	-4.158947	-2.868526	2.747287
H	-6.327987	1.916713	0.386898
H	4.159247	-2.868381	-2.747024
H	6.327734	1.917615	-0.386228
H	-3.062425	-2.128588	4.858164
H	-6.526804	2.668953	-1.981692
H	3.063024	-2.128384	-4.858037
H	6.526211	2.669465	1.982514
H	-0.117961	-4.052093	-3.470645
H	0.118174	-4.052206	3.470501
Ni	-0.000066	1.772323	-0.000024
H	1.978043	-4.632835	-2.765189
H	-1.977719	-4.633163	2.765017
C	0.996803	3.173807	-1.153795
H	1.762457	2.662273	-1.747290
C	-0.322211	3.071840	-1.594002
H	-0.501767	2.510785	-2.519679
C	1.493475	4.322110	-0.297423
H	0.924206	5.230627	-0.553424
H	2.538668	4.543639	-0.563240
C	0.322102	3.072130	1.593624
C	-0.996930	3.173979	1.153407
C	1.410391	4.045234	1.212246
H	1.287396	4.996751	1.766637
H	2.370996	3.632533	1.547607
H	0.501655	2.511290	2.519434
H	-1.762551	2.662569	1.747056
C	-1.493673	4.322101	0.296829
H	-2.538903	4.543558	0.562560
H	-0.924513	5.230718	0.552724
C	-1.410495	4.045021	-1.212802
H	-2.371093	3.632317	-1.548173
H	-1.287429	4.996462	-1.767308

LNi

Thermal Correction to Free Energy = 0.526680
a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-
TZVP/PCM(ethanol) Level = -3807.13110430
a.u.

Cartesian Coordinates (Angstroms):

P	1.775577	-0.036127	-1.038180
P	-1.775627	0.036091	-1.038159
O	-0.992859	1.115598	3.162858
O	0.992993	-1.115499	3.162821
C	0.325255	0.672019	1.284825
C	-0.325221	-0.671955	1.284847
C	1.323208	1.066820	0.372814
C	-1.323204	-1.066788	0.372882
C	-0.062373	1.571868	2.299103
C	0.062467	-1.571786	2.299119
C	0.486953	2.853771	2.371417
C	-0.486830	-2.853698	2.371478
C	1.880373	2.350613	0.462620
C	-1.880356	-2.350582	0.462749
C	1.454441	3.233680	1.445621
C	-1.454369	-3.233629	1.445744
C	-1.359769	1.914079	4.247851
C	1.359845	-1.913899	4.247893
C	2.252640	-1.595750	-0.206168
C	3.367116	0.677468	-1.629261
C	-2.252661	1.595756	-0.206203
C	-3.367172	-0.677555	-1.629156
C	1.753911	-2.785997	-0.745789
C	3.244521	1.612643	-2.666427
C	-1.753973	2.785978	-0.745918
C	-3.244560	-1.612992	-2.666087
C	3.048471	-1.646295	0.944504
C	4.647130	0.348469	-1.170556
C	-3.048431	1.646359	0.944509
C	-4.647204	-0.348344	-1.170650
C	2.061746	-4.011943	-0.162077
C	4.365876	2.238351	-3.204358
C	-2.061796	4.011956	-0.162264
C	-4.365914	-2.238748	-3.203962
C	3.370268	-2.873913	1.518892
C	5.773156	0.959386	-1.721247
C	-3.370219	2.874008	1.518838
C	-5.773227	-0.959309	-1.721295
C	2.878712	-4.057417	0.966748
C	5.636375	1.910917	-2.730974
C	-2.878711	4.057486	0.966595
C	-5.636431	-1.911101	-2.730773
H	2.655352	2.655744	-0.242087
H	-2.655368	-2.655737	-0.241911
H	1.888430	4.235130	1.501755
H	-1.888344	-4.235082	1.501911
H	-2.088602	1.335792	4.830704
H	-0.493913	2.151939	4.891084
H	2.088551	-1.335521	4.830813
H	0.493935	-2.151812	4.891033
H	1.093344	-2.724069	-1.615061
H	2.242655	1.831545	-3.050498
H	-1.093450	2.724006	-1.615220
H	-2.242681	-1.832064	-3.050027

H	3.389930	-0.719143	1.410921
H	4.772254	-0.398243	-0.384767
H	-3.389847	0.719229	1.410999
H	-4.772344	0.398576	-0.385063
H	1.656148	-4.934262	-0.584542
H	4.249529	2.971518	-4.006390
H	-1.656227	4.934254	-0.584802
H	-4.249550	-2.972120	-4.005803
H	4.001993	-2.907226	2.410392
H	6.767406	0.688229	-1.357171
H	-4.001895	2.907365	2.410371
H	-6.767490	-0.687981	-1.357380
H	3.126687	-5.018471	1.424482
H	6.521545	2.388632	-3.158112
H	-3.126681	5.018563	1.424282
H	-6.521600	-2.388853	-3.157872
H	0.164601	3.556038	3.139434
H	-0.164402	-3.555958	3.139470
Ni	-0.000027	-0.000002	-2.066554
H	-1.832606	2.857586	3.923387
H	1.832801	-2.857379	3.923521

L3Ni·EtOH

Thermal Correction to Free Energy = 0.602297 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -3962.08272942 a.u.

Cartesian Coordinates (Angstroms):

P	1.660100	0.699775	-0.133479
P	-1.667882	0.550732	-0.246746
O	-0.821426	-3.393811	1.697513
O	1.279152	-3.674332	-0.399540
C	0.403615	-1.544520	0.962782
C	-0.158646	-1.831797	-0.390365
C	1.319950	-0.506694	1.217417
C	-1.154538	-1.053943	-1.011352
C	0.038110	-2.404781	2.017827
C	0.336171	-2.970684	-1.059347
C	0.541908	-2.213780	3.306539
C	-0.128214	-3.313713	-2.331107
C	1.842827	-0.339739	2.507146
C	-1.622464	-1.414072	-2.282840
C	1.445480	-1.180494	3.538581
C	-1.106184	-2.527529	-2.933589
C	-1.181738	-4.321933	2.675882
C	1.792060	-4.834230	-0.982558
C	2.365565	-0.379301	-1.436507
C	3.119970	1.647505	0.464999
C	-2.280448	-0.006163	1.394826
C	-3.227103	0.919897	-1.170615
C	1.907009	-0.204241	-2.745693
C	2.866298	2.625917	1.446827
C	-2.018273	0.815192	2.496219
C	-3.093318	1.827337	-2.230599

C	3.308070	-1.379020	-1.166834
C	4.401078	1.596819	-0.099131
C	-2.968712	-1.209168	1.592931
C	-4.499485	0.415018	-0.879990
C	2.390054	-1.007486	-3.776346
C	3.865590	3.496522	1.872530
C	-2.447066	0.453631	3.771136
C	-4.190455	2.194052	-3.005781
C	3.800089	-2.174007	-2.198922
C	5.396315	2.483474	0.313364
C	-3.411280	-1.564986	2.864993
C	-5.604065	0.797106	-1.640703
C	3.340992	-1.989818	-3.504570
C	5.138435	3.431496	1.301571
C	-3.150236	-0.735871	3.956341
C	-5.452794	1.679663	-2.709451
H	2.569244	0.449558	2.703376
H	-2.395561	-0.813331	-2.764626
H	1.851279	-1.037493	4.543312
H	-1.472401	-2.794500	-3.928231
H	-1.857440	-5.040343	2.193485
H	-0.303414	-4.864839	3.068352
H	2.521467	-5.245932	-0.272733
H	1.003224	-5.586637	-1.161505
H	1.141449	0.552697	-2.937397
H	1.862381	2.689811	1.881436
H	-1.454254	1.738539	2.334985
H	-2.103908	2.255095	-2.424866
H	3.643520	-1.542391	-0.139365
H	4.622192	0.859293	-0.873497
H	-3.130304	-1.885929	0.750538
H	-4.635708	-0.276479	-0.046559
H	2.015035	-0.872753	-4.793677
H	3.649764	4.234317	2.649998
H	-2.226230	1.098805	4.625044
H	-4.063164	2.895436	-3.834401
H	4.541678	-2.947815	-1.983446
H	6.388022	2.428468	-0.143305
H	-3.956934	-2.501505	3.007468
H	-6.592658	0.399998	-1.395879
H	3.723077	-2.619705	-4.312128
H	5.922692	4.120480	1.623674
H	-3.490589	-1.021432	4.955002
H	-6.320385	1.974687	-3.304951
H	0.239315	-2.864612	4.126229
H	0.270215	-4.181808	-2.855261
Ni	-0.061455	1.841686	-0.325786
H	-1.712305	-3.845855	3.519340
H	2.305735	-4.620995	-1.936486
C	-1.827567	4.663081	-0.084510
C	-0.405515	4.796865	0.389562
H	-1.909855	4.901634	-1.155152
H	-2.493593	5.331811	0.479322
H	-2.148837	3.618020	0.053012
H	-0.346512	4.654042	1.484312

H	0.000517	5.797635	0.158502
O	0.382034	3.808121	-0.266098
H	1.313728	3.905770	-0.027516

L3Ni-2a

Thermal Correction to Free Energy = 0.729400 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -5505.37652780 a.u.

Cartesian Coordinates (Angstroms):

P	1.008836	-1.671896	-0.186781
P	0.926565	1.627079	0.013416
O	5.386792	0.903273	-0.481559
O	4.942998	-1.195899	1.605375
C	3.444831	-0.390329	-0.418330
C	3.197468	0.204358	0.930288
C	2.608316	-1.354599	-1.003844
C	2.226490	1.178642	1.239584
C	4.629960	-0.029248	-1.091111
C	4.041459	-0.260782	1.965254
C	4.957733	-0.605175	-2.320333
C	3.917673	0.220486	3.268506
C	2.947785	-1.942438	-2.228806
C	2.123812	1.667287	2.549061
C	4.115074	-1.563533	-2.877317
C	2.959648	1.190319	3.547702
C	6.600907	1.279417	-1.061804
C	5.814431	-1.707901	2.569964
C	1.494049	-2.372693	1.427253
C	0.249288	-3.049284	-1.112310
C	1.878701	1.925670	-1.518597
C	0.361397	3.335160	0.423698
C	0.815465	-1.937924	2.571567
C	-0.285244	-2.753257	-2.376739
C	1.409106	1.412200	-2.729791
C	-0.412087	3.546890	1.578401
C	2.540602	-3.295323	1.545992
C	0.053785	-4.325036	-0.574479
C	3.049915	2.694451	-1.496635
C	0.544207	4.408717	-0.460707
C	1.181159	-2.426455	3.823897
C	-0.966795	-3.726609	-3.101308
C	2.112467	1.656371	-3.909050
C	-0.941411	4.804674	1.858399
C	2.895091	-3.788029	2.799115
C	-0.644834	-5.293362	-1.295834
C	3.740775	2.946598	-2.677156
C	0.001160	5.661693	-0.181631
C	2.217349	-3.351707	3.939114
C	-1.150944	-5.000636	-2.560494
C	3.276183	2.421726	-3.884693
C	-0.734679	5.869057	0.982624
H	2.296008	-2.696300	-2.671919
H	1.377752	2.422245	2.791277

H	4.378913	-2.019639	-3.834543
H	2.861658	1.574868	4.565551
H	7.051040	2.023838	-0.392581
H	7.290184	0.422163	-1.159906
H	6.450889	-2.441293	2.058134
H	6.454731	-0.919460	3.003740
H	0.013310	-1.201697	2.479110
H	-0.183666	-1.743913	-2.784875
H	0.481588	0.835939	-2.740613
H	-0.648435	2.705055	2.233377
H	3.088345	-3.612255	0.654850
H	0.441910	-4.561037	0.418501
H	3.424822	3.085157	-0.547541
H	1.107650	4.269363	-1.383648
H	0.654648	-2.074270	4.713758
H	-1.372678	-3.483146	-4.086280
H	1.744397	1.247489	-4.852889
H	-1.536722	4.944480	2.764181
H	3.708460	-4.512821	2.888178
H	-0.794480	-6.285153	-0.862111
H	4.648873	3.554538	-2.656252
H	0.154465	6.481325	-0.887877
H	2.501283	-3.734759	4.922716
H	-1.694635	-5.762549	-3.124476
H	3.823300	2.614750	-4.810908
H	-1.159671	6.852325	1.198148
H	5.864699	-0.310837	-2.847528
H	4.557695	-0.156507	4.065409
Ni	-0.409601	-0.024142	0.066008
H	6.456474	1.735214	-2.057153
H	5.268487	-2.216006	3.383914
C	-2.828101	1.717975	-0.076769
H	-2.032311	2.479596	-0.056741
F	-4.036866	2.282390	0.157730
S	-2.907696	1.071467	-1.794557
O	-1.624662	0.439888	-2.128810
O	-3.404201	2.196058	-2.578318
S	-2.270750	0.406094	1.194256
O	-1.688883	0.954384	2.458033
O	-2.037835	-1.017060	0.626561
C	-3.965851	0.106597	1.841648
C	-4.528704	1.033053	2.721101
C	-4.674244	-1.031856	1.469583
C	-5.815172	0.827661	3.208544
H	-3.948952	1.905944	3.025087
C	-5.960723	-1.237854	1.969060
H	-4.210702	-1.758102	0.802921
C	-6.535172	-0.308056	2.831665
H	-6.257434	1.554134	3.894758
H	-6.512956	-2.135209	1.679029
H	-7.543860	-0.469545	3.219949
C	-4.142475	-0.194476	-1.762815
C	-5.484754	0.178776	-1.698238
C	-3.744037	-1.526824	-1.847325
C	-6.452228	-0.820793	-1.695143

H	-5.756193	1.234076	-1.648290
C	-4.725453	-2.514096	-1.858285
H	-2.684607	-1.778499	-1.885808
C	-6.072973	-2.161682	-1.777340
H	-7.508460	-0.551440	-1.631343
H	-4.428367	-3.563210	-1.923536
H	-6.838797	-2.941188	-1.779326

A

Thermal Correction to Free Energy = 0.661691 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -4192.70487378 a.u.

Cartesian Coordinates (Angstroms):

P	-1.118755	1.512974	-0.128722
P	0.921183	-1.075286	0.049409
O	-2.859106	-3.271289	-0.811490
O	-4.044189	-1.535665	1.299531
C	-2.176877	-1.050390	-0.571136
C	-1.762298	-1.429670	0.810267
C	-2.044471	0.247812	-1.093143
C	-0.421682	-1.578602	1.206368
C	-2.757403	-2.052490	-1.376451
C	-2.782797	-1.686111	1.749697
C	-3.171179	-1.770477	-2.679817
C	-2.471916	-2.054521	3.059941
C	-2.475610	0.526999	-2.396860
C	-0.118034	-1.966251	2.518051
C	-3.027107	-0.479104	-3.179097
C	-1.137902	-2.193051	3.432639
C	-3.473011	-4.302466	-1.527005
C	-5.109418	-1.821951	2.157088
C	-2.049514	1.603071	1.442602
C	-1.538119	3.078369	-0.992944
C	0.582652	-2.085766	-1.436596
C	2.428383	-1.833352	0.773013
C	-1.321403	1.779536	2.623727
C	-0.695417	3.463697	-2.044954
C	0.706880	-1.474048	-2.688041
C	3.068213	-1.118352	1.796074
C	-3.444243	1.492180	1.501261
C	-2.611688	3.905402	-0.647134
C	0.196571	-3.429757	-1.360409
C	3.023784	-3.003989	0.294108
C	-1.979495	1.851410	3.849679
C	-0.940316	4.634408	-2.757000
C	0.454705	-2.197394	-3.851979
C	4.261299	-1.576199	2.344113
C	-4.100288	1.576551	2.726578
C	-2.846972	5.085955	-1.351205
C	-0.041518	-4.154337	-2.525081
C	4.228272	-3.454510	0.834313
C	-3.369037	1.753310	3.902011
C	-2.017572	5.449679	-2.410490

C	0.084194	-3.538574	-3.771549
C	4.847925	-2.745104	1.860037
H	-2.374605	1.535890	-2.798909
H	0.922024	-2.090928	2.821423
H	-3.355103	-0.257317	-4.197544
H	-0.893766	-2.488092	4.456028
H	-3.466340	-5.184462	-0.873639
H	-4.518044	-4.055088	-1.784592
H	-6.029023	-1.653095	1.581990
H	-5.088223	-2.871969	2.498649
H	-0.231126	1.848715	2.569581
H	0.174677	2.845701	-2.283607
H	0.987512	-0.417980	-2.735630
H	2.639911	-0.171242	2.135205
H	-4.013812	1.312506	0.586265
H	-3.263521	3.636326	0.185938
H	0.063026	-3.901175	-0.383709
H	2.559878	-3.560808	-0.521753
H	-1.403449	1.980338	4.768987
H	-0.272956	4.921201	-3.573071
H	0.542996	-1.709342	-4.825358
H	4.753097	-0.997779	3.129215
H	-5.189817	1.498209	2.765613
H	-3.683945	5.727688	-1.065079
H	-0.332504	-5.205956	-2.460559
H	4.688563	-4.364328	0.441013
H	-3.885477	1.811828	4.863456
H	-2.203194	6.376339	-2.959119
H	-0.110583	-4.107511	-4.684173
H	5.797839	-3.093087	2.272726
H	-3.600809	-2.549704	-3.308556
H	-3.260228	-2.232944	3.790579
Ni	0.984919	1.074892	-0.080650
H	-2.923571	-4.541549	-2.454315
H	-5.114344	-1.159342	3.040240
C	6.752042	0.212967	-0.014313
C	6.392123	1.327150	0.744874
C	5.093983	1.825605	0.688374
C	4.121449	1.208053	-0.118858
C	4.500614	0.088594	-0.878820
C	5.801188	-0.399139	-0.832088
H	7.771423	-0.177954	0.032005
H	7.131776	1.813167	1.386727
H	4.806557	2.692988	1.287616
H	3.745558	-0.401495	-1.497211
H	6.072393	-1.275010	-1.426515
C	2.754387	1.674412	-0.116128
C	1.939224	2.682110	0.012343
C	1.804639	4.116330	0.093679
C	2.822162	4.986303	-0.022294
H	0.793155	4.507868	0.252394
H	2.653992	6.064729	0.043892
H	3.845834	4.642242	-0.197317

A'

Thermal Correction to Free Energy = 0.662550 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -4192.69483552 a.u.

Cartesian Coordinates (Angstroms):

P	-1.738386	1.462477	-0.275056
P	0.845864	-0.659163	0.008360
O	-2.382313	-3.623695	-0.801005
C	-2.781876	2.840192	-0.892184
C	-4.120088	2.704314	-1.285187
H	-4.588548	1.717465	-1.301980
C	-4.856169	3.820144	-1.676521
C	-4.268407	5.085235	-1.672865
C	-2.938361	5.229578	-1.283007
C	-2.198364	4.111917	-0.902115
H	-1.149969	4.214198	-0.612126
C	-2.384291	1.312287	1.439187
C	-1.476410	1.418794	2.496220
H	-0.411917	1.530771	2.275593
C	-1.919082	1.358646	3.816235
C	-3.275650	1.199358	4.088915
C	-4.188882	1.098131	3.037891
C	-3.746722	1.153971	1.719772
H	-4.466462	1.064041	0.904535
C	1.306311	-2.069203	-1.069008
C	0.761673	-3.347531	-0.918985
H	0.015793	-3.534754	-0.144795
C	1.162220	-4.383844	-1.763669
C	2.113759	-4.155328	-2.755087
C	2.265620	-1.843911	-2.066670
H	2.711467	-0.851734	-2.172699
C	2.338197	-0.476575	1.051933
C	3.226443	-1.528132	1.305022
H	3.043624	-2.510824	0.863244
C	4.343940	-1.321932	2.110917
C	4.585681	-0.067109	2.668434
C	3.708847	0.985634	2.414265
C	2.595462	0.783920	1.602612
H	1.927891	1.616976	1.364375
C	-2.183041	-1.300010	-0.623935
C	-2.327309	-0.019633	-1.183282
C	-2.695549	0.119923	-2.531249
H	-2.758937	1.113589	-2.977738
C	-2.965079	-1.002954	-3.299436
H	-3.247619	-0.888970	-4.348663
C	-2.876623	-2.279827	-2.748680
C	-2.493118	-2.427503	-1.414578
C	-2.616466	-4.789590	-1.537160
H	-3.652764	-4.834372	-1.915747
H	-2.454167	-5.630559	-0.850716
C	-0.380442	-1.396967	1.171946
C	-0.014383	-1.690241	2.492556
H	1.022873	-1.573658	2.807461
C	-0.971102	-2.110572	3.406690

H	-0.678184	-2.331557	4.435899	O	5.186498	-0.093507	-0.128176
C	-2.305417	-2.240167	3.032905	C	2.818806	-0.055439	1.090372
C	-2.678929	-1.956987	1.718081	C	2.996592	-0.898707	-0.126571
C	-1.720851	-1.539349	0.772294	C	2.134782	1.171906	1.102682
Ni	0.285386	1.238473	-0.894665	C	1.999125	-1.713188	-0.686366
O	-3.946406	-2.029689	1.268768	C	3.457700	-0.492670	2.271425
H	-1.919026	-4.881853	-2.388150	C	4.281716	-0.896106	-0.712990
C	-4.954071	-2.441435	2.145827	C	3.413866	0.280003	3.434255
H	-4.776280	-3.464233	2.522495	C	4.553822	-1.677651	-1.837538
H	-5.051939	-1.755676	3.005598	C	2.121561	1.955026	2.264331
H	-5.890813	-2.431414	1.574008	C	2.286432	-2.512915	-1.799755
C	1.624945	1.645601	-2.312572	C	2.756483	1.505765	3.415800
H	1.491030	0.955114	-3.156881	C	3.553865	-2.486432	-2.367039
C	0.666525	2.690622	-2.133808	C	4.797514	-2.155693	3.294949
H	0.985729	3.614157	-1.634217	C	6.497991	-0.066050	-0.621579
H	-3.096976	-3.150833	-3.365082	C	2.337943	1.610721	-1.734547
H	-3.046910	-2.549707	3.768815	C	0.705015	3.384539	-0.166266
C	2.668885	-2.882769	-2.900222	C	0.462843	-1.876222	1.738348
C	2.930819	1.665739	-1.753922	C	-0.562749	-3.054307	-0.718303
C	4.038215	1.598641	-1.238622	C	1.988404	1.007394	-2.946382
H	0.732291	-5.380843	-1.636159	C	-0.179622	3.754068	0.857845
H	2.428123	-4.969169	-3.413173	C	-0.111926	-0.957617	2.622740
H	3.421144	-2.696309	-3.670607	C	-0.921864	-3.025059	-2.074879
H	5.039547	-2.144382	2.294115	C	3.600212	2.199279	-1.586345
H	5.474925	0.098082	3.280618	C	1.106422	4.358181	-1.086732
H	3.909068	1.976605	2.826987	C	1.194955	-2.954700	2.248224
H	-5.255092	0.980336	3.248154	C	-0.942709	-4.153486	0.058240
H	-1.197970	1.431930	4.633560	C	2.896466	0.986391	-4.002671
H	-3.624823	1.155754	5.123536	C	-0.634113	5.063480	0.974294
H	-5.897119	3.700754	-1.987081	C	0.020537	-1.118386	3.999112
H	-4.848060	5.959067	-1.980205	C	-1.607676	-4.088888	-2.650229
H	-2.469687	6.216576	-1.283682	C	4.499144	2.187588	-2.648592
H	-0.089195	2.845788	-2.912639	C	0.638517	5.669046	-0.979325
C	5.280480	1.455730	-0.567039	C	1.313833	-3.125340	3.625623
C	5.821917	2.509084	0.195893	C	-1.652179	-5.209344	-0.516078
C	5.981772	0.235097	-0.614059	C	4.150307	1.576802	-3.854688
C	7.012806	2.339903	0.892815	C	-0.228748	6.027096	0.049197
H	5.286231	3.459640	0.236517	C	0.727509	-2.210740	4.501362
C	7.173445	0.075740	0.083229	C	-1.977668	-5.184544	-1.870153
H	5.564361	-0.591243	-1.192729	H	1.633470	2.929005	2.266509
C	7.695118	1.123388	0.843237	H	1.521332	-3.163217	-2.222625
H	7.415523	3.168425	1.481257	H	2.747580	2.124035	4.316548
H	7.699478	-0.881335	0.038357	H	3.771127	-3.110107	-3.237134
H	8.631712	0.994149	1.390798	H	5.242115	-3.111190	2.990352
A·BH⁺				H	5.603455	-1.461161	3.587319
Thermal Correction to Free Energy = 0.854016				H	7.055169	0.634162	0.013051
a.u.				H	6.974067	-1.059885	-0.564707
Electronic Energy at the PBE0-D3(BJ)/def2-				H	1.002228	0.546976	-3.051302
TZVP/PCM(ethanol) Level = -4538.25183007				H	-0.513118	3.000433	1.573312
a.u.				H	-0.619981	-0.086198	2.199981
Cartesian Coordinates (Angstroms):				H	-0.683144	-2.145078	-2.678431
P	1.128934	1.613317	-0.370581	H	3.881328	2.654628	-0.633560
P	0.279726	-1.571653	-0.052411	H	1.780335	4.092324	-1.902994
O	4.081892	-1.678672	2.188765	H	1.689670	-3.649127	1.564974
				H	-0.696451	-4.188524	1.120873

H	2.624322	0.505159	-4.944569
H	-1.310473	5.337199	1.788211
H	-0.409550	-0.383026	4.683425
H	-1.878595	-4.050442	-3.707548
H	5.479808	2.656061	-2.535431
H	0.958733	6.415412	-1.709894
H	1.877727	-3.974132	4.019826
H	-1.946117	-6.060607	0.102630
H	4.860654	1.563800	-4.684798
H	-0.589452	7.054718	0.132077
H	0.833122	-2.343628	5.580628
H	-2.529397	-6.014502	-2.317336
H	3.900359	-0.060545	4.347697
H	5.540494	-1.663811	-2.299189
Ni	-0.602672	0.323395	-0.683193
H	4.137727	-2.327930	4.162822
H	6.532097	0.290854	-1.665106
C	-5.552480	-2.510381	-2.313504
C	-5.289769	-1.418534	-3.143736
C	-4.227251	-0.563768	-2.867304
C	-3.391726	-0.789341	-1.756693
C	-3.653066	-1.911567	-0.949445
C	-4.727258	-2.754954	-1.215437
H	-6.390200	-3.176458	-2.531772
H	-5.921921	-1.231785	-4.015203
H	-4.018933	0.284174	-3.523166
H	-2.975582	-2.130114	-0.121327
H	-4.905097	-3.623765	-0.577170
C	-2.310243	0.116894	-1.425509
C	-1.892254	1.359917	-1.536606
C	-2.228851	2.704725	-1.942704
C	-3.397671	3.081068	-2.494060
H	-1.465085	3.471139	-1.771014
H	-3.580164	4.123861	-2.766762
H	-4.194468	2.362200	-2.705583
C	-4.955510	1.107678	0.448325
C	-5.939429	1.554103	1.555987
H	-4.712551	1.899002	-0.273445
C	-3.912922	-0.336653	2.121668
C	-3.085101	1.938420	1.773928
H	-6.793007	0.864204	1.620471
H	-6.345161	2.551207	1.333188
H	-2.933575	-0.664191	2.497011
H	-4.368165	-1.175844	1.580720
C	-4.836117	0.254093	3.215592
C	-4.126586	2.479540	2.780957
H	-2.151352	1.610784	2.250853
H	-2.825301	2.644719	0.973955
H	-4.313762	0.307187	4.181827
H	-5.718121	-0.386122	3.359287
H	-3.683566	2.574107	3.782879
N	-3.676616	0.739598	1.122021
H	-2.991312	0.425188	0.385498
H	-4.472179	3.479811	2.482710
H	-5.291350	0.227644	-0.115285

N	-5.269562	1.588767	2.844677
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TS1

Thermal Correction to Free Energy = 0.849984 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -4538.23103774 a.u.

Imaginary Frequency = 1207.0517i cm⁻¹

Cartesian Coordinates (Angstroms):

P	1.111341	1.573301	0.469419
P	0.057183	-1.391325	-0.569793
O	4.237940	-2.472098	0.428303
O	4.960257	0.019673	-1.022827
C	2.880686	-0.580644	0.551606
C	2.743695	-0.697921	-0.926775
C	2.281697	0.440422	1.307220
C	1.574485	-1.129880	-1.574915
C	3.702284	-1.521986	1.209195
C	3.879677	-0.387837	-1.706391
C	3.905678	-1.443845	2.589366
C	3.836390	-0.492712	-3.098428
C	2.498560	0.520862	2.688642
C	1.543922	-1.250726	-2.969337
C	3.305568	-0.420490	3.316549
C	2.669709	-0.928908	-3.717322
C	5.115846	-3.409399	0.991149
C	6.149557	0.288305	-1.715589
C	2.079272	2.282181	-0.900234
C	0.852797	2.952362	1.642654
C	0.613806	-2.569860	0.710562
C	-1.060543	-2.361900	-1.648794
C	1.495259	2.393376	-2.166577
C	0.004534	2.733795	2.737167
C	0.342911	-2.330144	2.061652
C	-1.668535	-1.688208	-2.718794
C	3.399050	2.707488	-0.700808
C	1.378128	4.231339	1.438408
C	1.338344	-3.713541	0.348705
C	-1.381459	-3.705813	-1.423567
C	2.223253	2.931025	-3.225337
C	-0.295594	3.764839	3.620590
C	0.765862	-3.228840	3.037665
C	-2.540087	-2.357246	-3.573442
C	4.117454	3.255906	-1.759235
C	1.066767	5.268070	2.318496
C	1.750133	-4.617236	1.324154
C	-2.276251	-4.365641	-2.265334
C	3.532004	3.365480	-3.021564
C	0.233775	5.038850	3.410164
C	1.462675	-4.378322	2.668585
C	-2.847579	-3.698519	-3.347517
H	2.052758	1.328335	3.269944
H	0.646977	-1.608506	-3.473721
H	3.479557	-0.353727	4.392945

H	2.641897	-1.024741	-4.805047
H	5.445887	-4.058715	0.171001
H	5.997137	-2.920539	1.439912
H	6.892269	0.573222	-0.960301
H	6.511476	-0.601146	-2.258724
H	0.471912	2.040940	-2.321607
H	-0.429263	1.744315	2.894261
H	-0.172223	-1.414436	2.356116
H	-1.476408	-0.622727	-2.873300
H	3.868387	2.592999	0.279299
H	2.023275	4.429576	0.580818
H	1.592773	-3.887701	-0.699576
H	-0.938489	-4.244326	-0.584087
H	1.767176	3.007243	-4.214714
H	-0.951940	3.577844	4.473742
H	0.562598	-3.024156	4.091160
H	-3.000782	-1.817931	-4.403889
H	5.143059	3.596896	-1.599288
H	1.479969	6.264154	2.144388
H	2.305454	-5.511966	1.033173
H	-2.521378	-5.413270	-2.075922
H	4.100569	3.791821	-3.851432
H	-0.007782	5.853105	4.096982
H	1.790682	-5.087307	3.432346
H	-3.539735	-4.221898	-4.011065
H	4.532811	-2.173718	3.100314
H	4.707504	-0.240867	-3.702249
Ni	-0.733681	0.641284	-0.161183
H	4.614820	-4.025875	1.757003
H	6.025193	1.121420	-2.428136
C	-6.110724	0.983784	-3.149275
C	-5.534218	2.221964	-2.859040
C	-4.403057	2.301448	-2.054344
C	-3.817385	1.139162	-1.522505
C	-4.407895	-0.098138	-1.825054
C	-5.540316	-0.177446	-2.631230
H	-7.000805	0.926299	-3.779781
H	-5.973246	3.136497	-3.264738
H	-3.958584	3.273139	-1.832571
H	-3.950005	-1.013333	-1.446906
H	-5.975164	-1.153304	-2.861070
C	-2.615661	1.198957	-0.680227
C	-1.742040	2.166771	-0.414349
C	-1.576363	3.596151	-0.414774
C	-2.438027	4.454892	0.155110
H	-0.640050	3.985479	-0.831964
H	-2.227649	5.526516	0.187865
H	-3.360989	4.105200	0.626587
C	-4.839855	-0.133443	1.510733
C	-5.272757	-0.753064	2.870024
H	-4.957066	0.959711	1.481494
C	-3.227569	-1.897911	1.227744
C	-2.635311	0.111606	2.420350
H	-6.123979	-1.436397	2.734485
H	-5.594665	0.026912	3.576089

H	-2.160844	-2.088928	1.051604
H	-3.774703	-2.268543	0.349860
C	-3.727216	-2.531644	2.552585
C	-3.065713	-0.587249	3.732317
H	-1.571664	-0.033637	2.166060
H	-2.810679	1.197710	2.434238
H	-2.925867	-3.113167	3.033089
H	-4.564704	-3.220700	2.368684
H	-2.235154	-1.164518	4.166879
N	-3.416267	-0.442269	1.306348
H	-2.820569	0.202143	0.239799
H	-3.377969	0.151367	4.485567
H	-5.402250	-0.543066	0.660955
N	-4.169118	-1.491015	3.464300

INT1-B

Thermal Correction to Free Energy = 0.853696 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -4538.24242553 a.u.

Cartesian Coordinates (Angstroms):

P	1.114452	1.463796	0.755290
P	0.112941	-1.282860	-0.813628
O	4.303737	-2.457589	-0.055345
O	4.977320	0.270520	-1.039524
C	2.906838	-0.652535	0.415322
C	2.773146	-0.487156	-1.058303
C	2.271061	0.180644	1.350670
C	1.604550	-0.811566	-1.766445
C	3.735775	-1.693144	0.887885
C	3.893782	-0.017194	-1.775746
C	3.908395	-1.893055	2.260360
C	3.829234	0.142664	-3.162727
C	2.451273	-0.020042	2.725128
C	1.547669	-0.661562	-3.156551
C	3.266794	-1.054867	3.166810
C	2.658915	-0.183128	-3.841044
C	5.189274	-3.476825	0.326470
C	6.155666	0.679065	-1.682243
C	2.076721	2.435161	-0.441835
C	0.798319	2.540865	2.191064
C	0.661610	-2.673026	0.223906
C	-1.058765	-1.985270	-2.028694
C	1.507220	2.786393	-1.670784
C	-0.161383	2.115696	3.119925
C	0.334707	-2.706725	1.583407
C	-1.774221	-1.087019	-2.835263
C	3.392612	2.815652	-0.147042
C	1.409769	3.785969	2.357870
C	1.421496	-3.710884	-0.332117
C	-1.324881	-3.355099	-2.132219
C	2.244306	3.523521	-2.593789
C	-0.486872	2.912987	4.211367
C	0.743395	-3.775415	2.376898

C	-2.721717	-1.552189	-3.742389
C	4.118801	3.564986	-1.068171
C	1.072308	4.588865	3.447304
C	1.818922	-4.783014	0.461775
C	-2.281927	-3.816345	-3.034564
C	3.546912	3.917645	-2.291169
C	0.129157	4.154595	4.375334
C	1.479384	-4.817549	1.815003
C	-2.978665	-2.919320	-3.842150
H	1.967129	0.639070	3.446305
H	0.642947	-0.928198	-3.703788
H	3.412571	-1.210686	4.238019
H	2.617890	-0.067037	-4.926362
H	5.544169	-3.943814	-0.600300
H	6.053905	-3.074569	0.880890
H	6.904953	0.825755	-0.894762
H	6.518960	-0.088332	-2.386432
H	0.489483	2.466494	-1.909228
H	-0.669496	1.159205	2.976112
H	-0.225880	-1.882259	2.026865
H	-1.600002	-0.010363	-2.752083
H	3.855415	2.507209	0.793447
H	2.138931	4.144629	1.629390
H	1.715121	-3.670420	-1.383862
H	-0.797393	-4.068054	-1.496454
H	1.800074	3.787813	-3.555729
H	-1.233795	2.571003	4.931304
H	0.491703	-3.790476	3.439615
H	-3.272689	-0.839269	-4.359501
H	5.140775	3.870421	-0.832040
H	1.549633	5.564046	3.566447
H	2.400868	-5.596215	0.021783
H	-2.484671	-4.887465	-3.103710
H	4.121722	4.501334	-3.014024
H	-0.133520	4.787343	5.226075
H	1.794385	-5.659588	2.435705
H	-3.728418	-3.285504	-4.547127
H	4.540797	-2.700791	2.627417
H	4.688364	0.517138	-3.718328
Ni	-0.683489	0.656058	-0.055976
H	4.686330	-4.240594	0.943589
H	6.013842	1.629601	-2.224000
C	-6.129052	2.140038	-2.893827
C	-5.317746	3.220118	-2.539381
C	-4.186752	3.024201	-1.755467
C	-3.848098	1.735531	-1.311393
C	-4.668706	0.655914	-1.674032
C	-5.799534	0.857104	-2.459703
H	-7.017819	2.301123	-3.508089
H	-5.570527	4.226913	-2.879803
H	-3.556836	3.872695	-1.484550
H	-4.403328	-0.344149	-1.325458
H	-6.428661	0.006837	-2.733476
C	-2.645399	1.475380	-0.514757
C	-1.646054	2.239260	-0.047769

C	-1.446506	3.642545	0.218575
C	-2.277053	4.385495	0.967249
H	-0.512802	4.090912	-0.141276
H	-2.049388	5.429711	1.194154
H	-3.195095	3.963084	1.385391
C	-5.030369	-1.001166	1.443284
C	-5.244544	-1.793945	2.765167
H	-5.298825	0.061874	1.547818
C	-3.269989	-2.484577	0.824707
C	-2.805509	-0.546880	2.132767
H	-6.008848	-2.577344	2.645992
H	-5.584116	-1.134920	3.579474
H	-2.211903	-2.526354	0.528689
H	-3.852275	-2.855224	-0.033452
C	-3.531745	-3.309101	2.114534
C	-2.993392	-1.400231	3.415945
H	-1.752796	-0.532412	1.785821
H	-3.094110	0.504890	2.289111
H	-2.616697	-3.820319	2.454529
H	-4.294110	-4.086281	1.950220
H	-2.055849	-1.895098	3.718434
N	-3.624153	-1.087499	1.056699
H	-2.582780	0.351104	-0.307942
H	-3.317918	-0.778008	4.264920
H	-5.640492	-1.405745	0.620609
N	-3.995187	-2.423446	3.171888

INT1

Thermal Correction to Free Energy = 0.674531 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -4193.16165684 a.u.

Cartesian Coordinates (Angstroms):

P	-0.475592	1.630291	-0.263447
P	0.202567	-1.602862	-0.059351
O	-4.170161	-1.910164	-0.403832
O	-4.219996	0.278253	1.656667
C	-2.561740	-0.224008	-0.406692
C	-2.213259	-0.683791	0.965898
C	-1.920073	0.842284	-1.057423
C	-1.047245	-1.408550	1.260301
C	-3.608842	-0.894491	-1.074952
C	-3.127410	-0.416139	2.006545
C	-3.989959	-0.507035	-2.362618
C	-2.863088	-0.850430	3.308687
C	-2.313142	1.234670	-2.343099
C	-0.794038	-1.856839	2.561556
C	-3.342478	0.555895	-2.983894
C	-1.702862	-1.571080	3.573866
C	-5.254673	-2.595083	-0.973452
C	-5.209333	0.533112	2.618753
C	-1.043798	2.146659	1.379453
C	-0.154889	3.143302	-1.224865
C	-0.661692	-2.378965	-1.450093

C	1.414065	-2.825032	0.548241
C	-0.221737	1.930371	2.490553
C	0.547819	3.011477	-2.430858
C	-0.442339	-1.896417	-2.744096
C	2.328569	-2.408557	1.529155
C	-2.298769	2.747787	1.542197
C	-0.513661	4.415945	-0.773591
C	-1.541701	-3.448542	-1.239928
C	1.522345	-4.113482	0.014194
C	-0.649357	2.317677	3.757862
C	0.862941	4.134805	-3.186713
C	-1.098245	-2.480150	-3.824937
C	3.315210	-3.276059	1.986273
C	-2.714120	3.145244	2.809734
C	-0.183156	5.541970	-1.527698
C	-2.185291	-4.035625	-2.325215
C	2.521170	-4.975189	0.466977
C	-1.892753	2.927999	3.916927
C	0.499302	5.404082	-2.733673
C	-1.966908	-3.550270	-3.615723
C	3.413651	-4.561894	1.453871
H	-1.823133	2.073501	-2.837787
H	0.103678	-2.434996	2.782027
H	-3.651594	0.861316	-3.985927
H	-1.509011	-1.920590	4.590366
H	-5.559168	-3.356084	-0.244722
H	-6.104914	-1.918768	-1.164199
H	-6.008646	1.081447	2.105515
H	-5.622461	-0.402617	3.031537
H	0.748839	1.444431	2.359641
H	0.866819	2.022406	-2.772353
H	0.231715	-1.049932	-2.899921
H	2.278481	-1.393343	1.933917
H	-2.957382	2.885020	0.681259
H	-1.038993	4.536687	0.175539
H	-1.734153	-3.808068	-0.226142
H	0.832995	-4.445351	-0.764387
H	-0.010319	2.139510	4.625291
H	1.407550	4.022316	-4.126749
H	-0.933098	-2.096412	-4.833900
H	4.021379	-2.939793	2.748297
H	-3.688195	3.623657	2.935334
H	-0.460618	6.534184	-1.165049
H	-2.863695	-4.876623	-2.163710
H	2.600687	-5.978005	0.041412
H	-2.225100	3.236044	4.911016
H	0.756694	6.288363	-3.321022
H	-2.477525	-4.010825	-4.464683
H	4.194274	-5.240509	1.804898
H	-4.791225	-1.029486	-2.884252
H	-3.560899	-0.635391	4.117343
Ni	1.229875	0.342143	-0.246638
H	-4.969462	-3.093414	-1.915479
H	-4.821496	1.153204	3.444700
C	7.299489	-0.719111	0.286409

C	6.938794	0.596100	0.587428
C	5.630346	1.026216	0.402828
C	4.658846	0.137361	-0.085146
C	5.029816	-1.182336	-0.384045
C	6.341370	-1.607280	-0.199580
H	8.330456	-1.049949	0.430137
H	7.687679	1.293567	0.969313
H	5.351173	2.054074	0.640447
H	4.278302	-1.884319	-0.756857
H	6.616074	-2.637533	-0.436148
C	3.270482	0.556290	-0.261579
C	2.526800	1.640543	-0.054109
C	2.696464	3.045698	0.210954
C	3.510026	3.853224	-0.486612
H	2.050271	3.478340	0.983895
H	3.555357	4.923856	-0.274084
H	4.131080	3.470549	-1.301338
H	2.682034	-0.390723	-0.616430

TS2^R

Thermal Correction to Free Energy = 0.675257 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -4193.14971893 a.u.

Imaginary Frequency = 32.0001i cm⁻¹

Cartesian Coordinates (Angstroms):

P	0.452860	-1.316553	0.094331
P	-0.917391	1.731572	-0.031647
O	-4.462580	-0.442983	1.275209
O	-3.729144	-2.426391	-0.862274
C	-2.233187	-0.938046	0.811368
C	-2.538097	-0.446473	-0.561315
C	-0.981763	-1.425266	1.229717
C	-2.113842	0.800274	-1.043892
C	-3.303916	-0.937012	1.733595
C	-3.356450	-1.249152	-1.383942
C	-3.124725	-1.411803	3.034907
C	-3.719944	-0.809528	-2.660460
C	-0.819165	-1.927017	2.528251
C	-2.483754	1.242097	-2.318631
C	-1.886206	-1.914416	3.417129
C	-3.285187	0.431849	-3.115105
C	-5.593247	-0.453477	2.106850
C	-4.582780	-3.264251	-1.596234
C	-0.130459	-2.091236	-1.441341
C	1.747583	-2.405066	0.766547
C	-1.708433	1.975554	1.579115
C	-0.747001	3.368790	-0.806818
C	-0.024406	-1.413246	-2.659347
C	2.348890	-2.074818	1.991258
C	-0.955281	1.766264	2.738870
C	0.084830	3.454359	-1.933627
C	-0.719444	-3.361789	-1.394871
C	2.256298	-3.475885	0.024982

C	-3.054298	2.351016	1.675541
C	-1.358261	4.525960	-0.313472
C	-0.495497	-2.005173	-3.827838
C	3.419000	-2.818461	2.474800
C	-1.541066	1.935399	3.990327
C	0.278685	4.673707	-2.575242
C	-1.175783	-3.953804	-2.568562
C	3.334928	-4.214705	0.510799
C	-3.631629	2.531403	2.929333
C	-1.152959	5.747217	-0.953378
C	-1.065156	-3.276689	-3.784099
C	3.915455	-3.891601	1.733798
C	-2.877657	2.321241	4.084944
C	-0.341368	5.822786	-2.084133
H	0.132919	-2.350068	2.843253
H	-2.153821	2.216298	-2.682148
H	-1.753299	-2.308671	4.426931
H	-3.582970	0.772942	-4.109137
H	-6.415831	-0.030081	1.517848
H	-5.860428	-1.478813	2.413275
H	-4.765685	-4.146642	-0.971088
H	-5.545226	-2.771050	-1.813385
H	0.407940	-0.411513	-2.687755
H	1.987675	-1.220518	2.569436
H	0.088120	1.450684	2.653906
H	0.584537	2.557249	-2.313172
H	-0.829999	-3.881652	-0.440100
H	1.819117	-3.734015	-0.940996
H	-3.653035	2.480896	0.770745
H	-1.988972	4.478346	0.576270
H	-0.422079	-1.467847	-4.775617
H	3.877401	-2.552309	3.429726
H	-0.954144	1.763235	4.894978
H	0.923047	4.729308	-3.455503
H	-1.624862	-4.949045	-2.533722
H	3.724093	-5.048401	-0.077717
H	-4.678189	2.835410	3.006219
H	-1.630817	6.648051	-0.562102
H	-1.428019	-3.743366	-4.702901
H	4.761935	-4.470465	2.109357
H	-3.335990	2.459208	5.066992
H	-0.184201	6.782903	-2.580627
H	-3.947901	-1.400964	3.748507
H	-4.344565	-1.429777	-3.302551
Ni	1.055474	0.700324	-0.204316
H	-5.439571	0.165987	3.006709
H	-4.117790	-3.585541	-2.543627
C	7.872183	1.005242	0.627375
C	7.263586	0.805660	-0.613102
C	5.887966	0.629298	-0.703418
C	5.089646	0.641413	0.453179
C	5.717399	0.840169	1.694582
C	7.093373	1.022110	1.783176
H	8.953269	1.147617	0.691432
H	7.870360	0.790176	-1.521390

H	5.426830	0.481214	-1.679916
H	5.109115	0.848654	2.603444
H	7.561148	1.176212	2.758167
C	3.640541	0.427829	0.445784
C	2.787223	0.247389	-0.580951
C	2.953160	0.179036	-2.022240
C	2.997073	1.242768	-2.845845
H	2.962226	-0.829236	-2.460987
H	3.063722	1.116805	-3.929502
H	3.018583	2.263190	-2.451577
H	3.212737	0.386719	1.455282

TS2^s

Thermal Correction to Free Energy = 0.675232 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -4193.14487429 a.u.

Imaginary Frequency = 35.6309i cm⁻¹

Cartesian Coordinates (Angstroms):

P	0.360926	-1.387802	0.087696
P	-0.784046	1.730700	-0.120084
O	-4.413172	-0.060299	1.445691
O	-3.965940	-2.190301	-0.627564
C	-2.259813	-0.766928	0.901783
C	-2.604346	-0.305784	-0.472872
C	-1.032687	-1.341246	1.284173
C	-2.112786	0.883692	-1.028730
C	-3.280456	-0.636996	1.871751
C	-3.537193	-1.063058	-1.212225
C	-3.082360	-1.076976	3.182139
C	-3.950733	-0.630759	-2.476260
C	-0.857267	-1.809879	2.593504
C	-2.529047	1.318268	-2.291207
C	-1.875946	-1.674239	3.527525
C	-3.449035	0.556044	-3.002648
C	-5.499255	0.060318	2.326527
C	-4.924667	-2.981711	-1.278576
C	-0.379004	-2.139179	-1.393010
C	1.577755	-2.586074	0.717075
C	-1.473971	2.137722	1.503894
C	-0.460320	3.294453	-0.990165
C	-0.343569	-1.471438	-2.619636
C	2.224945	-2.341534	1.938314
C	-0.691507	1.917649	2.642297
C	0.331311	3.229106	-2.148217
C	-1.033602	-3.373364	-1.286496
C	1.986533	-3.674902	-0.060966
C	-2.775380	2.638544	1.633236
C	-0.909975	4.537294	-0.531889
C	-0.942435	-2.038903	-3.740526
C	3.234096	-3.187746	2.385797
C	-1.204140	2.201031	3.905061
C	0.643625	4.388834	-2.851461
C	-1.619482	-3.942682	-2.413009

C	3.004050	-4.515390	0.387288
C	-3.278703	2.931526	2.897697
C	-0.587081	5.696035	-1.235695
C	-1.573628	-3.277663	-3.639350
C	3.625747	-4.278601	1.610542
C	-2.495966	2.710679	4.031961
C	0.183951	5.624094	-2.394933
H	0.065500	-2.306731	2.884582
H	-2.141200	2.248177	-2.709956
H	-1.729425	-2.045005	4.544315
H	-3.786565	0.890922	-3.986046
H	-6.309368	0.532224	1.757429
H	-5.839138	-0.925153	2.686978
H	-5.133434	-3.827906	-0.612834
H	-5.859345	-2.422940	-1.454397
H	0.132939	-0.492426	-2.685497
H	1.949063	-1.475897	2.545164
H	0.314337	1.502684	2.533493
H	0.704644	2.264393	-2.507923
H	-1.091941	-3.883621	-0.321974
H	1.517032	-3.868675	-1.026726
H	-3.399282	2.777737	0.746966
H	-1.506970	4.602961	0.379874
H	-0.922261	-1.507374	-4.694138
H	3.726194	-2.987160	3.339992
H	-0.595537	2.020701	4.793658
H	1.255013	4.329199	-3.754569
H	-2.119258	-4.910696	-2.332134
H	3.312759	-5.361906	-0.229915
H	-4.289922	3.332280	2.999890
H	-0.940111	6.663844	-0.872846
H	-2.037414	-3.726882	-4.520681
H	4.422915	-4.939215	1.958095
H	-2.896579	2.937343	5.022757
H	0.434382	6.535896	-2.941702
H	-3.866742	-0.967681	3.930228
H	-4.666596	-1.215155	-3.053531
Ni	1.115660	0.571038	-0.263329
H	-5.249914	0.697356	3.192038
H	-4.545627	-3.366828	-2.240410
C	7.888384	1.050755	0.618300
C	7.299084	0.749039	-0.609498
C	5.944941	0.439874	-0.683432
C	5.150416	0.426507	0.476737
C	5.765113	0.709643	1.709473
C	7.116553	1.026087	1.780205
H	8.951997	1.293694	0.671240
H	7.904510	0.745130	-1.518805
H	5.506257	0.171400	-1.645278
H	5.163394	0.686631	2.622298
H	7.573779	1.250458	2.746550
C	3.721108	0.114318	0.467853
C	2.858467	0.134604	-0.571065
C	3.100186	0.581272	-1.941156
C	2.763652	-0.080522	-3.063255

H	3.586357	1.563298	-2.045435
H	2.968396	0.342295	-4.049957
H	2.316403	-1.076789	-3.024305
H	3.328581	-0.179178	1.446403

INT2^R

Thermal Correction to Free Energy = 0.677294 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -4193.18555889 a.u.

Cartesian Coordinates (Angstroms):

P	0.591881	-1.159462	0.232061
P	-1.151064	1.645398	-0.006974
O	-4.524364	-1.129558	0.558338
O	-3.157029	-2.819666	-1.485612
C	-2.198209	-1.250909	0.479760
C	-2.312409	-0.725859	-0.907092
C	-0.974571	-1.563749	1.091941
C	-1.961797	0.585946	-1.262543
C	-3.394519	-1.461849	1.199211
C	-2.846951	-1.580496	-1.894462
C	-3.358074	-1.965186	2.502147
C	-3.009527	-1.130743	-3.207285
C	-0.945185	-2.080926	2.393439
C	-2.146446	1.038115	-2.575017
C	-2.134202	-2.274540	3.086036
C	-2.663598	0.176145	-3.534450
C	-5.761048	-1.363260	1.179155
C	-3.758358	-3.710563	-2.387978
C	0.485425	-1.954045	-1.394344
C	1.864053	-2.076373	1.163897
C	-2.264631	1.650652	1.423468
C	-1.205329	3.332178	-0.703001
C	0.996363	-1.287970	-2.513032
C	2.335804	-1.520268	2.362011
C	-1.730942	1.489597	2.705833
C	-0.350417	3.630023	-1.776851
C	-0.081841	-3.227328	-1.534335
C	2.421020	-3.270366	0.696343
C	-3.646085	1.812373	1.254850
C	-1.994496	4.348527	-0.157322
C	0.938057	-1.890661	-3.767361
C	3.333649	-2.158851	3.089651
C	-2.571653	1.492257	3.815888
C	-0.309789	4.913472	-2.311221
C	-0.125040	-3.829234	-2.788290
C	3.431240	-3.901908	1.422789
C	-4.480103	1.827235	2.368625
C	-1.942501	5.637538	-0.689495
C	0.379514	-3.160497	-3.904643
C	3.886476	-3.350576	2.617941
C	-3.944685	1.664257	3.647488
C	-1.107163	5.921599	-1.766431
H	0.002866	-2.343506	2.862305

H	-1.903351	2.064365	-2.847611
H	-2.109894	-2.679345	4.100179
H	-2.807804	0.529758	-4.557708
H	-6.531803	-1.043112	0.467552
H	-5.903377	-2.433075	1.407022
H	-3.947021	-4.636869	-1.831783
H	-4.716444	-3.316754	-2.766986
H	1.441733	-0.296357	-2.397250
H	1.935741	-0.567035	2.717596
H	-0.655059	1.344120	2.831160
H	0.288548	2.850025	-2.201428
H	-0.506880	-3.736194	-0.666066
H	2.081652	-3.704624	-0.245655
H	-4.067311	1.910507	0.251422
H	-2.648019	4.141168	0.691852
H	1.331639	-1.367105	-4.641178
H	3.695374	-1.716455	4.020262
H	-2.153869	1.356681	4.815662
H	0.351748	5.131342	-3.152719
H	-0.557272	-4.826770	-2.896109
H	3.865859	-4.830510	1.046234
H	-5.556099	1.964549	2.238560
H	-2.561934	6.424749	-0.254068
H	0.338982	-3.634179	-4.888266
H	4.680093	-3.845401	3.182178
H	-4.603289	1.671905	4.519106
H	-1.070828	6.931533	-2.180694
H	-4.278956	-2.120049	3.063436
H	-3.411197	-1.791305	-3.975006
Ni	0.947607	1.000620	0.235918
H	-5.864881	-0.777964	2.108519
H	-3.095658	-3.932798	-3.241596
C	8.049831	1.183863	-0.148824
C	7.093565	2.184581	0.036584
C	5.744010	1.860498	0.100463
C	5.323338	0.526179	-0.028751
C	6.296876	-0.471743	-0.201206
C	7.647649	-0.146083	-0.264742
H	9.110184	1.442062	-0.194739
H	7.407128	3.225794	0.140675
H	5.005730	2.647442	0.269322
H	5.979518	-1.514336	-0.289506
H	8.391856	-0.933455	-0.403630
C	3.917554	0.125948	0.005144
C	2.859568	0.937499	0.086819
C	2.487974	2.285264	-0.069464
C	1.600645	2.826838	0.862332
H	2.599680	2.772616	-1.049963
H	1.095577	3.773704	0.659109
H	1.667667	2.526827	1.916014
H	3.747023	-0.954145	-0.012054

INT2^s

Thermal Correction to Free Energy = 0.676312
a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -4193.18627199
a.u.

Cartesian Coordinates (Angstroms):

P	0.631825	-1.160750	0.241949
P	-1.148388	1.628402	-0.073365
O	-4.478251	-1.142385	0.669464
O	-3.137594	-2.903206	-1.346140
C	-2.153835	-1.261040	0.541031
C	-2.311109	-0.779735	-0.858342
C	-0.916811	-1.561839	1.133519
C	-1.988458	0.523407	-1.266419
C	-3.333144	-1.452349	1.294403
C	-2.866868	-1.670595	-1.800778
C	-3.267489	-1.918643	2.609786
C	-3.086428	-1.261730	-3.118615
C	-0.858946	-2.046738	2.446608
C	-2.229017	0.934735	-2.583005
C	-2.031164	-2.217514	3.172469
C	-2.772781	0.039562	-3.496219
C	-5.700088	-1.360118	1.324499
C	-3.759352	-3.828889	-2.198241
C	0.477253	-1.892379	-1.409743
C	1.937035	-2.120881	1.086019
C	-2.255358	1.703721	1.362428
C	-1.195071	3.276586	-0.852907
C	0.901210	-1.157768	-2.521653
C	2.413660	-1.650806	2.319152
C	-1.714334	1.612095	2.648982
C	-0.349254	3.513684	-1.948363
C	-0.037930	-3.184447	-1.577669
C	2.526230	-3.252392	0.514677
C	-3.639130	1.839997	1.192681
C	-1.987880	4.318106	-0.363441
C	0.808426	-1.710182	-3.797123
C	3.440581	-2.315215	2.979267
C	-2.550654	1.657387	3.761350
C	-0.319919	4.763352	-2.558324
C	-0.116772	-3.735175	-2.852953
C	3.567140	-3.908722	1.172952
C	-4.468716	1.898847	2.308519
C	-1.947395	5.573250	-0.971821
C	0.301776	-2.998176	-3.962097
C	4.022933	-3.445759	2.403942
C	-3.926551	1.803643	3.591232
C	-1.120670	5.797002	-2.069393
H	0.098258	-2.305649	2.898323
H	-2.005338	1.954340	-2.894634
H	-1.983839	-2.597172	4.195477
H	-2.961116	0.361329	-4.522812
H	-6.487342	-1.064660	0.620298
H	-5.833509	-2.422694	1.588717
H	-3.909200	-4.742128	-1.609611
H	-4.738612	-3.461598	-2.548734
H	1.301519	-0.149253	-2.385012

H	1.986685	-0.746822	2.761497	C	-2.462147	-1.368396	-1.401991
H	-0.635709	1.489372	2.776378	C	-3.612625	-1.227285	-0.471757
H	0.292335	2.713602	-2.330757	C	-1.712112	-0.286357	-1.899436
H	-0.395334	-3.748131	-0.712738	C	-3.483856	-0.856197	0.872434
H	2.187140	-3.620556	-0.454931	C	-2.167114	-2.672577	-1.858168
H	-4.065813	1.883615	0.187742	C	-4.900170	-1.492229	-0.986178
H	-2.636702	4.156324	0.499278	C	-1.150029	-2.894017	-2.786364
H	1.132876	-1.132636	-4.665285	C	-6.027089	-1.399711	-0.169598
H	3.801053	-1.940856	3.939817	C	-0.717738	-0.519437	-2.859057
H	-2.127391	1.575576	4.764684	C	-4.621974	-0.739291	1.682443
H	0.336133	4.934727	-3.414633	C	-0.443698	-1.807887	-3.291602
H	-0.509423	-4.746254	-2.983760	C	-5.878420	-1.012132	1.159241
H	4.024704	-4.787847	0.713863	C	-2.613557	-4.987359	-1.644058
H	-5.546813	2.016674	2.176793	C	-6.177417	-2.164336	-2.865143
H	-2.569252	6.381384	-0.580417	C	-3.402640	1.887071	-0.691432
H	0.233578	-3.432328	-4.962254	C	-1.267404	2.583742	-2.389137
H	4.839560	-3.960227	2.915173	C	-1.147075	-2.293283	1.656088
H	-4.581851	1.844619	4.464427	C	-2.180128	-0.192660	3.312773
H	-1.093311	6.780548	-2.543517	C	-3.561576	2.773440	0.378358
H	-4.175451	-2.055852	3.196130	C	0.034625	2.632487	-2.907396
H	-3.507042	-1.950093	-3.850980	C	0.225445	-2.473457	1.854938
Ni	0.924060	1.002488	0.378051	C	-2.606954	1.106950	3.618865
H	-5.785735	-0.746099	2.237034	C	-4.510976	1.532009	-1.466005
H	-3.128377	-4.064415	-3.072156	C	-2.213167	3.507823	-2.857149
C	7.979711	1.256554	-0.208158	C	-1.995272	-3.408057	1.617248
C	7.058279	2.185239	0.280785	C	-2.025814	-1.121395	4.345319
C	5.703460	1.878835	0.310068	C	-4.819996	3.285271	0.686928
C	5.245720	0.631816	-0.145363	C	0.368691	3.561122	-3.891600
C	6.180129	-0.289971	-0.642553	C	0.742967	-3.756698	2.022419
C	7.536670	0.018473	-0.670606	C	-2.884829	1.467415	4.933471
H	9.043736	1.502170	-0.232479	C	-5.769620	2.035456	-1.147866
H	7.401950	3.159308	0.636259	C	-1.869299	4.440704	-3.833015
H	4.986610	2.615345	0.680178	C	-1.469226	-4.688402	1.774321
H	5.832280	-1.262861	-1.000156	C	-2.294257	-0.753773	5.664393
H	8.252658	-0.710769	-1.056186	C	-5.927116	2.908535	-0.071127
C	3.834303	0.245610	-0.107311	C	-0.579363	4.468139	-4.358597
C	2.845341	0.937715	0.452506	C	-0.100001	-4.865721	1.979217
C	2.441485	1.978242	1.287183	C	-2.724311	0.537095	5.961584
C	1.512815	2.896427	0.769046	H	-0.112339	0.298483	-3.241087
H	2.564824	1.868665	2.375560	H	-4.523197	-0.451276	2.728396
H	0.964228	3.562903	1.441137	H	0.358195	-1.972292	-4.014294
H	1.628253	3.260750	-0.256972	H	-6.761017	-0.926321	1.797242
H	3.596118	-0.711376	-0.583554	H	-3.322074	-5.611632	-1.084663
INT2^R·2a⁻				H	-2.727978	-5.196708	-2.722191
Thermal Correction to Free Energy = 0.866940				H	-5.975253	-2.401220	-3.917251
a.u.				H	-6.595677	-3.057601	-2.369234
Electronic Energy at the PBE0-D3(BJ)/def2-				H	-2.681777	3.072599	0.955320
TZVP/PCM(ethanol) Level = -5890.93552931				H	0.814354	1.959638	-2.540786
a.u.				H	0.915938	-1.630928	1.855752
Cartesian Coordinates (Angstroms):				H	-2.728193	1.836484	2.815412
P	-1.701016	1.364162	-1.081853	H	-4.387016	0.855376	-2.315145
P	-1.800514	-0.590795	1.562674	H	-3.228299	3.510788	-2.460405
O	-2.923078	-3.659187	-1.335384	H	-3.066363	-3.277436	1.455630
O	-4.955771	-1.784531	-2.300085	H	-1.686691	-2.134529	4.120434
				H	-4.936037	3.978445	1.523342

H	1.390189	3.575285	-4.278750
H	1.818034	-3.869761	2.178129
H	-3.220541	2.482490	5.158674
H	-6.636137	1.742946	-1.745757
H	-2.621372	5.152293	-4.182190
H	-2.136470	-5.553476	1.742524
H	-2.162099	-1.485391	6.464942
H	-6.917117	3.300087	0.174400
H	-0.312762	5.200475	-5.124584
H	0.307990	-5.871591	2.108131
H	-2.930764	0.822239	6.995803
H	-0.903789	-3.902156	-3.118103
H	-7.021411	-1.604964	-0.565827
Ni	-0.501720	1.026617	0.730414
H	-1.587259	-5.247994	-1.331804
H	-6.923988	-1.351274	-2.821847
C	4.546577	5.864064	1.229823
C	4.318540	4.611643	1.800759
C	3.227895	3.844788	1.403708
C	2.344224	4.324111	0.423796
C	2.600159	5.570295	-0.168450
C	3.685599	6.339734	0.240015
H	5.406365	6.462299	1.541921
H	5.007904	4.209261	2.546893
H	3.093602	2.840407	1.810259
H	1.931426	5.935993	-0.952831
H	3.866570	7.313636	-0.222121
C	1.199291	3.521732	-0.025031
C	0.572825	2.639002	0.744931
C	0.385271	2.263049	2.080997
C	0.656852	0.944112	2.438833
H	-0.233213	2.897208	2.732375
H	1.496477	0.414691	1.984583
H	0.299873	0.567721	3.400225
H	0.904562	3.639999	-1.069601
C	3.383790	0.614242	0.096811
F	4.349043	1.315767	-0.569789
S	4.062687	-0.309949	1.385715
O	3.016184	-1.239386	1.851610
O	4.699995	0.616979	2.321009
S	2.265340	-0.126819	-0.982614
O	2.252786	0.734780	-2.176695
O	0.988811	-0.393639	-0.274679
C	2.789102	-1.726348	-1.571013
C	3.900147	-1.773778	-2.415045
C	2.129178	-2.882994	-1.168444
C	4.353653	-3.010118	-2.862033
H	4.395710	-0.846494	-2.709819
C	2.593210	-4.116018	-1.624022
H	1.258637	-2.801928	-0.517994
C	3.700620	-4.180665	-2.469098
H	5.226844	-3.061972	-3.516088
H	2.080967	-5.031033	-1.315344
H	4.062150	-5.149423	-2.822673
C	5.371840	-1.317327	0.715065

C	6.529397	-0.691067	0.248816
C	5.198567	-2.695259	0.608292
C	7.517685	-1.465139	-0.352818
H	6.642521	0.388268	0.360537
C	6.200973	-3.460115	0.017120
H	4.278094	-3.145668	0.981444
C	7.355589	-2.847062	-0.467739
H	8.426458	-0.987431	-0.726761
H	6.073813	-4.541461	-0.072298
H	8.137599	-3.449595	-0.936362

TS3^R

Thermal Correction to Free Energy = 0.864455 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -5890.93124724 a.u.

Imaginary Frequency = 146.0799i cm⁻¹

Cartesian Coordinates (Angstroms):

P	-2.151790	1.381670	-0.684121
P	-1.797397	-1.299504	1.243202
O	-4.377986	-3.112672	-1.808038
O	-6.030601	-0.619678	-1.539094
C	-3.359452	-1.048787	-1.417375
C	-4.176613	-0.992409	-0.173353
C	-2.464104	-0.037504	-1.806798
C	-3.621035	-1.180890	1.102398
C	-3.492572	-2.191892	-2.232611
C	-5.566232	-0.787868	-0.287954
C	-2.719731	-2.335426	-3.386452
C	-6.373674	-0.748173	0.851302
C	-1.699479	-0.182782	-2.970862
C	-4.436243	-1.156924	2.240483
C	-1.826252	-1.329850	-3.742959
C	-5.801251	-0.935770	2.106378
C	-4.576202	-4.267404	-2.572198
C	-7.406752	-0.473035	-1.739784
C	-3.802121	2.034233	-0.282893
C	-1.361755	2.663039	-1.716014
C	-1.348128	-2.747462	0.237118
C	-1.486707	-1.804233	2.972139
C	-4.080510	2.382341	1.042176
C	0.004042	2.505601	-1.992997
C	-0.164332	-2.739222	-0.507565
C	-1.562365	-0.808648	3.958356
C	-4.781821	2.205952	-1.268643
C	-2.009536	3.839339	-2.107812
C	-2.160108	-3.891262	0.245686
C	-1.093290	-3.095373	3.334827
C	-5.330132	2.895473	1.382096
C	0.707826	3.501260	-2.661065
C	0.212827	-3.874408	-1.223178
C	-1.286005	-1.110116	5.287888
C	-6.024068	2.732848	-0.927416
C	-1.299459	4.836517	-2.777201

C	-1.780448	-5.017894	-0.476344
C	-0.800031	-3.389895	4.666244
C	-6.300862	3.073125	0.397722
C	0.056902	4.670860	-3.052521
C	-0.591972	-5.010259	-1.211042
C	-0.901751	-2.403686	5.643974
H	-0.996619	0.595514	-3.267001
H	-4.002075	-1.314218	3.228474
H	-1.216426	-1.445580	-4.641678
H	-6.436936	-0.912787	2.994683
H	-5.335129	-4.862356	-2.048200
H	-4.945045	-4.027723	-3.584980
H	-7.556929	-0.379524	-2.822845
H	-7.967369	-1.351110	-1.374233
H	-3.309601	2.240259	1.804333
H	0.544958	1.617083	-1.661146
H	0.490932	-1.868685	-0.544272
H	-1.831022	0.214055	3.677007
H	-4.574017	1.909769	-2.299540
H	-3.064046	3.994388	-1.873057
H	-3.095530	-3.891075	0.810592
H	-0.997896	-3.871550	2.573351
H	-5.546472	3.156516	2.420424
H	1.778499	3.363374	-2.824515
H	1.156615	-3.856281	-1.770612
H	-1.352440	-0.327519	6.047307
H	-6.783447	2.876200	-1.700120
H	-1.811127	5.756099	-3.071528
H	-2.411037	-5.910529	-0.460025
H	-0.480211	-4.398854	4.936331
H	-7.279439	3.480466	0.663637
H	0.612762	5.464130	-3.558290
H	-0.290424	-5.900612	-1.768771
H	-0.666975	-2.637679	6.684959
H	-2.801550	-3.229999	-4.002899
H	-7.445613	-0.571968	0.767108
Ni	-0.888873	0.671025	0.909174
H	-3.651210	-4.863337	-2.657458
H	-7.797835	0.433159	-1.245247
C	3.432326	6.135593	2.114751
C	3.623737	4.753202	2.157958
C	2.600132	3.885181	1.796493
C	1.352674	4.387162	1.388758
C	1.180336	5.779601	1.325196
C	2.205911	6.646229	1.691003
H	4.242197	6.812829	2.397221
H	4.590398	4.343717	2.461741
H	2.780214	2.809627	1.786308
H	0.221152	6.179558	0.984391
H	2.049231	7.726816	1.640560
C	0.240772	3.515474	1.006246
C	0.154270	2.202253	1.236615
C	0.746951	1.187157	2.021454
C	1.051949	-0.033745	1.410184
H	0.788821	1.263839	3.115687

H	0.981346	-0.144279	0.323359
H	1.257358	-0.926933	2.003220
H	-0.566898	4.004535	0.451427
C	3.330052	-0.100127	0.657880
F	4.097103	0.722690	1.429458
S	3.729706	-1.779831	0.906125
O	3.067687	-2.543961	-0.157465
O	3.460045	-2.072961	2.316065
S	3.162002	0.501733	-0.976395
O	3.178648	1.963250	-0.861652
O	1.992028	-0.160786	-1.583249
C	4.569260	0.037113	-1.959040
C	5.791243	0.657521	-1.694945
C	4.442416	-0.951640	-2.930679
C	6.909841	0.272708	-2.425998
H	5.850140	1.431238	-0.926808
C	5.568768	-1.316454	-3.666282
H	3.466546	-1.413013	-3.090102
C	6.797591	-0.707500	-3.414334
H	7.875599	0.742269	-2.226641
H	5.486199	-2.083389	-4.440257
H	7.678621	-1.000910	-3.990221
C	5.488463	-1.951973	0.685349
C	6.349305	-1.344235	1.601190
C	5.972166	-2.655171	-0.414648
C	7.722060	-1.422813	1.385882
H	5.939218	-0.819065	2.464879
C	7.348333	-2.735689	-0.611828
H	5.262415	-3.122967	-1.098039
C	8.221093	-2.115922	0.281481
H	8.408868	-0.947028	2.089924
H	7.740065	-3.281671	-1.473073
H	9.300081	-2.176197	0.119595

TS3^s

Thermal Correction to Free Energy = 0.864305 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -5890.92481586 a.u.

Imaginary Frequency = 254.2622i cm⁻¹

Cartesian Coordinates (Angstroms):

P	-3.031960	1.385525	-0.112067
P	-1.326435	-1.453687	0.529040
O	-4.455315	-3.222401	-1.891580
O	-6.377355	-1.540191	-0.244398
C	-3.897149	-1.070817	-1.180548
C	-4.086784	-1.606224	0.196726
C	-3.558628	0.262594	-1.474106
C	-3.020179	-1.915255	1.052578
C	-4.121396	-1.968833	-2.246400
C	-5.403870	-1.868559	0.625105
C	-3.991726	-1.550428	-3.572187
C	-5.643749	-2.417328	1.886529
C	-3.463816	0.680886	-2.808062

C	-3.263980	-2.483913	2.308864	H	-0.133803	-4.866273	-3.884934
C	-3.674089	-0.223113	-3.840825	H	2.163123	-3.084788	4.734303
C	-4.569565	-2.726548	2.716085	H	-4.144144	-2.248732	-4.394438
C	-4.654794	-4.183410	-2.889125	H	-6.661665	-2.606659	2.226073
C	-7.706551	-1.826616	0.082961	Ni	-1.003665	0.710002	0.230484
C	-4.361116	1.252430	1.127924	H	-3.743843	-4.336218	-3.492966
C	-3.215162	3.088865	-0.763987	H	-8.033279	-1.278874	0.984129
C	-0.992320	-2.538740	-0.895427	C	3.032932	6.496608	0.308044
C	-0.260148	-2.071973	1.870650	C	3.285479	5.179107	-0.079594
C	-4.020932	1.080585	2.472190	C	2.280707	4.220448	-0.027437
C	-2.320148	3.530287	-1.752008	C	0.992292	4.567334	0.413007
C	-0.145713	-2.090129	-1.914703	C	0.748119	5.895486	0.798096
C	-0.262714	-1.367463	3.085128	C	1.758090	6.852184	0.747188
C	-5.709776	1.336945	0.758114	H	3.828384	7.244988	0.267190
C	-4.126960	4.004170	-0.226473	H	4.277183	4.883112	-0.429571
C	-1.533888	-3.829011	-0.958350	H	2.511831	3.201583	-0.342724
C	0.630706	-3.131991	1.694782	H	-0.253730	6.174376	1.137394
C	-5.018006	0.988640	3.441059	H	1.548918	7.881006	1.051372
C	-2.364061	4.839922	-2.216745	C	-0.109771	3.602053	0.467485
C	0.162863	-2.926869	-2.984673	C	-0.046503	2.322840	0.100645
C	0.589018	-1.744145	4.115776	C	0.773101	1.325517	-0.452805
C	-6.702746	1.259382	1.729627	C	1.221414	0.271665	0.353024
C	-4.157725	5.322618	-0.682109	H	0.914881	1.256439	-1.540141
C	-1.226517	-4.659235	-2.032628	H	1.253310	0.355046	1.442239
C	1.491383	-3.497989	2.728585	H	1.489320	-0.689810	-0.080569
C	-6.358197	1.080728	3.070606	H	-1.066087	3.995223	0.829585
C	-3.283220	5.742015	-1.680707	C	3.633393	0.389243	0.327352
C	-0.379249	-4.208856	-3.047024	F	4.208420	1.494839	0.886923
C	1.468110	-2.812814	3.937421	S	3.976824	-1.033287	1.267888
H	-3.231441	1.718412	-3.043396	O	3.513753	-2.193746	0.496747
H	-2.430023	-2.735190	2.964583	O	3.459803	-0.765813	2.613712
H	-3.589141	0.110957	-4.877412	S	3.837007	0.385598	-1.410739
H	-4.758728	-3.166597	3.698047	O	3.754923	1.801222	-1.791802
H	-4.900065	-5.120758	-2.373894	O	2.901583	-0.577909	-2.005076
H	-5.491861	-3.912206	-3.556021	C	5.474927	-0.173205	-1.827033
H	-8.316026	-1.502918	-0.770292	C	6.563199	0.622971	-1.466875
H	-7.862293	-2.907403	0.245825	C	5.644052	-1.404370	-2.454107
H	-2.967017	1.007877	2.753358	C	7.847641	0.170382	-1.748296
H	-1.554760	2.854242	-2.137060	H	6.392729	1.580855	-0.971867
H	0.299865	-1.095588	-1.874463	C	6.936315	-1.838352	-2.745264
H	-0.929767	-0.510174	3.218631	H	4.759927	-1.996013	-2.698226
H	-5.978299	1.450440	-0.294868	C	8.033954	-1.054000	-2.393584
H	-4.812303	3.696094	0.564370	H	8.710453	0.776962	-1.464325
H	-2.201554	-4.178067	-0.167366	H	7.086557	-2.797520	-3.246850
H	0.680550	-3.654969	0.738490	H	9.045554	-1.400912	-2.617874
H	-4.745947	0.842063	4.488614	C	5.744311	-1.169983	1.440635
H	-1.655043	5.164158	-2.981496	C	6.419051	-0.230705	2.222488
H	0.842634	-2.568565	-3.760336	C	6.424583	-2.174821	0.757427
H	0.589387	-1.183477	5.052982	C	7.807302	-0.294640	2.300021
H	-7.753507	1.336193	1.439325	H	5.852762	0.533340	2.757084
H	-4.870847	6.025649	-0.245184	C	7.812660	-2.233675	0.852451
H	-1.644635	-5.668178	-2.074743	H	5.854167	-2.890370	0.163443
H	2.209582	-4.303626	2.566090	C	8.503000	-1.293806	1.617003
H	-7.140098	1.012969	3.830922	H	8.350610	0.435864	2.904253
H	-3.305747	6.775889	-2.033029	H	8.358819	-3.015338	0.319487

H 9.592734 -1.340517 1.683627

INT3^R

Thermal Correction to Free Energy = 0.868711
a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-
TZVP/PCM(ethanol) Level = -5890.96895937
a.u.

Cartesian Coordinates (Angstroms):

P	-1.792690	1.485723	-0.772265
P	-1.467326	-1.305341	0.973394
O	-5.411078	-2.147627	-0.976045
O	-6.113925	0.593458	-0.144089
C	-3.801109	-0.454419	-1.000995
C	-4.053625	-0.324725	0.464300
C	-2.890082	0.349574	-1.707576
C	-3.155248	-0.748329	1.461109
C	-4.550499	-1.415795	-1.710851
C	-5.294642	0.221305	0.858273
C	-4.370981	-1.589039	-3.084643
C	-5.618202	0.367589	2.208108
C	-2.720593	0.176259	-3.087249
C	-3.497290	-0.617752	2.813382
C	-3.453852	-0.790373	-3.762353
C	-4.714245	-0.057921	3.176914
C	-6.231013	-3.078107	-1.618597
C	-7.378189	1.101658	0.164726
C	-2.985577	2.570123	0.094757
C	-1.075861	2.562042	-2.074991
C	-1.832538	-2.612611	-0.259990
C	-0.872558	-2.296843	2.411898
C	-2.670390	3.014689	1.382943
C	0.153048	2.167162	-2.622385
C	-1.090148	-2.658738	-1.444088
C	-0.407072	-1.596283	3.535647
C	-4.192484	2.965829	-0.495530
C	-1.653782	3.764760	-2.495736
C	-2.830285	-3.570457	-0.032274
C	-0.758976	-3.693001	2.407278
C	-3.550043	3.847421	2.071416
C	0.776371	2.948881	-3.591400
C	-1.333548	-3.660668	-2.382543
C	0.134407	-2.268525	4.627431
C	-5.063355	3.808624	0.190370
C	-1.021028	4.550999	-3.457872
C	-3.061445	-4.575955	-0.966072
C	-0.201936	-4.365688	3.495324
C	-4.745218	4.247696	1.476116
C	0.192143	4.143645	-4.010633
C	-2.313194	-4.621886	-2.144029
C	0.244032	-3.658854	4.609157
H	-2.008581	0.801228	-3.628324
H	-2.810280	-0.961160	3.586754
H	-3.314587	-0.926449	-4.837582
H	-4.969410	0.047059	4.234127

H	-6.859960	-3.531510	-0.841529
H	-6.881257	-2.598445	-2.371478
H	-7.870866	1.318162	-0.791981
H	-7.987318	0.369514	0.723864
H	-1.726465	2.699625	1.834855
H	0.634955	1.255769	-2.264697
H	-0.324848	-1.901560	-1.625174
H	-0.459423	-0.506562	3.540353
H	-4.461141	2.591263	-1.486119
H	-2.594602	4.103505	-2.058542
H	-3.436537	-3.516734	0.875369
H	-1.097388	-4.264266	1.541480
H	-3.298572	4.185787	3.079312
H	1.736858	2.627927	-4.001749
H	-0.753684	-3.685067	-3.308127
H	0.487104	-1.700754	5.491780
H	-5.998891	4.121595	-0.280405
H	-1.478133	5.492875	-3.771297
H	-3.833980	-5.325714	-0.776696
H	-0.118686	-5.455384	3.469418
H	-5.432251	4.904791	2.015444
H	0.688608	4.764752	-4.760414
H	-2.499101	-5.408942	-2.879349
H	0.682649	-4.187713	5.458496
H	-4.935344	-2.346100	-3.628168
H	-6.567414	0.809605	2.508939
Ni	-0.363256	0.509820	0.506366
H	-5.642675	-3.872865	-2.109853
H	-7.312378	2.034745	0.751055
C	4.163148	5.713321	2.080246
C	3.961201	4.452298	2.645298
C	2.941593	3.628602	2.183555
C	2.098107	4.037301	1.135992
C	2.311341	5.311238	0.582514
C	3.329081	6.139526	1.047196
H	4.966386	6.358738	2.444084
H	4.610020	4.103330	3.452653
H	2.791376	2.647468	2.634406
H	1.664209	5.644241	-0.234158
H	3.474696	7.125110	0.596984
C	1.033140	3.193115	0.589827
C	0.767736	1.922860	0.916971
C	1.103907	0.833614	1.747472
C	2.401363	0.043177	1.729385
H	0.761212	0.930558	2.789291
H	2.231680	-1.020898	1.959454
H	3.054532	0.412250	2.541645
H	0.430849	3.669537	-0.191677
C	3.282043	0.115112	0.503917
F	3.496308	1.376491	0.073151
S	4.958152	-0.514724	1.061833
O	4.777562	-1.903501	1.478897
O	5.409053	0.505442	2.003619
S	2.643484	-0.754450	-1.019178
O	3.512387	-0.346488	-2.118463

O	1.204242	-0.463167	-1.090546
C	2.812335	-2.492772	-0.754188
C	3.709052	-3.188663	-1.560462
C	1.989031	-3.135076	0.169239
C	3.807256	-4.569113	-1.407347
H	4.307090	-2.641956	-2.291447
C	2.109340	-4.511113	0.320417
H	1.262664	-2.572498	0.757724
C	3.018166	-5.224321	-0.462418
H	4.502666	-5.135748	-2.030569
H	1.483244	-5.024353	1.052139
H	3.104971	-6.306507	-0.340434
C	6.015117	-0.462025	-0.354373
C	6.344554	0.771818	-0.914904
C	6.536276	-1.661337	-0.831287
C	7.192864	0.789665	-2.016212
H	5.934744	1.692681	-0.498138
C	7.396805	-1.623746	-1.925727
H	6.263787	-2.596114	-0.338115
C	7.714274	-0.403121	-2.520537
H	7.453279	1.742323	-2.482026
H	7.823051	-2.551498	-2.314104
H	8.383342	-0.378776	-3.383937

INT3^s

Thermal Correction to Free Energy = 0.868164
a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-
TZVP/PCM(ethanol) Level = -5890.97137747
a.u.

Cartesian Coordinates (Angstroms):

P	-2.792223	1.638929	0.087675
P	-1.685569	-1.504511	0.180739
O	-5.638797	-2.375649	-1.422756
O	-6.666058	-0.501672	0.709412
C	-4.444340	-0.465704	-0.805506
C	-4.410827	-1.084111	0.551632
C	-3.882608	0.782160	-1.131959
C	-3.271227	-1.705459	1.087351
C	-5.121669	-1.193297	-1.808387
C	-5.613445	-1.113012	1.286435
C	-5.222565	-0.697069	-3.109143
C	-5.670746	-1.734371	2.535554
C	-4.010960	1.282403	-2.434836
C	-3.343410	-2.353888	2.326642
C	-4.669793	0.544133	-3.408923
C	-4.534330	-2.358671	3.041478
C	-6.328927	-3.153684	-2.356390
C	-7.907969	-0.540560	1.348526
C	-3.825655	1.710828	1.593019
C	-2.741189	3.380697	-0.490764
C	-2.012657	-2.373043	-1.392288
C	-0.496868	-2.572221	1.063182
C	-3.241410	1.365554	2.815301
C	-1.926180	3.668630	-1.596767

C	-1.570692	-1.787721	-2.582653
C	-0.099421	-2.190804	2.355411
C	-5.174024	2.087486	1.554678
C	-3.384035	4.437519	0.163264
C	-2.704038	-3.589542	-1.432334
C	0.199031	-3.598579	0.416287
C	-3.993548	1.394769	3.987623
C	-1.793466	4.973033	-2.062415
C	-1.817053	-2.411331	-3.803818
C	0.956648	-2.834370	2.990525
C	-5.919771	2.131646	2.729168
C	-3.236273	5.746907	-0.294314
C	-2.941235	-4.215054	-2.653100
C	1.269771	-4.229306	1.049653
C	-5.332071	1.781125	3.945646
C	-2.449043	6.017597	-1.411134
C	-2.501191	-3.625119	-3.839710
C	1.649831	-3.851866	2.334063
H	-3.595156	2.257449	-2.688124
H	-2.466045	-2.858908	2.730851
H	-4.757264	0.941531	-4.422987
H	-4.583501	-2.860108	4.011104
H	-6.657988	-4.057428	-1.827522
H	-7.215676	-2.627471	-2.751969
H	-8.613185	-0.009750	0.696113
H	-8.261695	-1.576952	1.491056
H	-2.191640	1.059859	2.834785
H	-1.361131	2.864197	-2.072525
H	-1.039573	-0.833709	-2.541972
H	-0.595079	-1.351397	2.851667
H	-5.642865	2.327787	0.597443
H	-3.996504	4.244479	1.045407
H	-3.065423	-4.038290	-0.503759
H	-0.066957	-3.880043	-0.604200
H	-3.533076	1.111278	4.936765
H	-1.150559	5.176197	-2.921887
H	-1.473731	-1.945410	-4.730179
H	1.275678	-2.505429	3.981299
H	-6.968968	2.436071	2.695241
H	-3.739988	6.561243	0.232321
H	-3.474766	-5.168617	-2.680420
H	1.830765	-4.999701	0.516892
H	-5.921895	1.807832	4.865301
H	-2.332733	7.044522	-1.765873
H	-2.691414	-4.116872	-4.797131
H	2.513366	-4.320068	2.809539
H	-5.728570	-1.268547	-3.886529
H	-6.594836	-1.740401	3.112811
Ni	-0.940854	0.534201	0.023105
H	-5.680421	-3.450332	-3.198937
H	-7.880244	-0.035281	2.329885
C	4.411845	5.021705	-1.208269
C	4.088706	3.797852	-1.798040
C	2.921321	3.128611	-1.446692
C	2.047110	3.666311	-0.487678

C	2.370494	4.910803	0.078278
C	3.542644	5.577422	-0.269562
H	5.328697	5.546302	-1.489111
H	4.748948	3.360905	-2.552843
H	2.683552	2.173003	-1.915771
H	1.686936	5.353308	0.808641
H	3.776985	6.540741	0.191390
C	0.795598	2.998794	-0.110214
C	0.494124	1.699931	-0.236213
C	0.959702	0.393873	-0.490781
C	1.866213	-0.324081	0.488282
H	1.034037	0.046168	-1.530936
H	1.717220	0.068293	1.504629
H	1.635949	-1.398844	0.524011
H	0.023878	3.667457	0.289189
C	3.350087	-0.236855	0.225722
F	3.818202	1.032627	0.179982
S	4.232926	-1.073899	1.660972
O	4.416122	-2.485735	1.330303
O	3.494812	-0.669825	2.856322
S	3.737630	-1.012664	-1.417251
O	3.413312	0.010325	-2.410787
O	3.090657	-2.318564	-1.440498
C	5.497889	-1.220135	-1.463359
C	6.298405	-0.092366	-1.648174
C	6.024577	-2.506526	-1.396447
C	7.674788	-0.266747	-1.749100
H	5.843711	0.898059	-1.709355
C	7.403229	-2.665129	-1.516539
H	5.350047	-3.350792	-1.245223
C	8.222629	-1.549313	-1.690137
H	8.322737	0.602090	-1.881426
H	7.839859	-3.665535	-1.475040
H	9.303667	-1.680294	-1.781167
C	5.830498	-0.297596	1.748349
C	5.931905	1.054822	2.079639
C	6.953522	-1.102051	1.582528
C	7.198827	1.617314	2.192649
H	5.034872	1.655015	2.234120
C	8.215147	-0.528606	1.717582
H	6.824080	-2.158834	1.345614
C	8.336651	0.828355	2.011132
H	7.297875	2.678161	2.432311
H	9.106230	-1.146326	1.586892
H	9.328165	1.277271	2.107391

3a^R

Thermal Correction to Free Energy = 0.311749

a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -2083.75296017

a.u.

Cartesian Coordinates (Angstroms):

C	-8.201116	0.462215	0.393920
C	-7.213630	-0.152134	1.167547

C	-5.930502	-0.321862	0.662540
C	-5.606733	0.120470	-0.629864
C	-6.605510	0.735101	-1.397312
C	-7.891772	0.904810	-0.890296
H	-9.209213	0.594367	0.793631
H	-7.448799	-0.502293	2.175602
H	-5.159132	-0.803854	1.268673
H	-6.366229	1.083341	-2.405773
H	-8.657274	1.386231	-1.503655
C	-4.259200	-0.042342	-1.193609
C	-3.230789	-0.593160	-0.587155
C	-2.217325	-1.141128	0.032375
C	-1.256418	-0.355690	0.884059
H	-2.035238	-2.217322	-0.075502
H	-1.063474	-0.874345	1.835997
H	-1.659667	0.641613	1.111097
H	-4.107244	0.332801	-2.213616
C	0.089739	-0.127529	0.219812
F	-0.025332	0.556763	-0.943092
S	1.091376	0.920434	1.396256
O	1.654811	0.013244	2.391325
O	0.187706	2.002500	1.776280
S	0.842917	-1.782473	-0.191342
O	0.308647	-2.096130	-1.512407
O	0.589418	-2.636239	0.963440
C	2.589071	-1.552897	-0.367094
C	3.072192	-1.023521	-1.563709
C	3.431102	-1.995269	0.649563
C	4.448553	-0.916509	-1.732585
H	2.373445	-0.715684	-2.343459
C	4.806974	-1.895077	0.457782
H	2.998086	-2.403880	1.563913
C	5.310720	-1.356879	-0.726739
H	4.851124	-0.498189	-2.657284
H	5.489276	-2.243044	1.236445
H	6.391341	-1.282037	-0.870339
C	2.407184	1.638354	0.446492
C	2.113573	2.539059	-0.578946
C	3.714161	1.366792	0.840165
C	3.169619	3.134082	-1.261066
H	1.078199	2.764665	-0.834762
C	4.759290	1.986477	0.160711
H	3.892825	0.676188	1.665276
C	4.487834	2.857644	-0.892821
H	2.962357	3.830812	-2.076112
H	5.790873	1.783078	0.455454
H	5.311284	3.336250	-1.428108

3a^S

Thermal Correction to Free Energy = 0.311755

a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -2083.75295775 a.u.

Cartesian Coordinates (Angstroms):

C	8.201348	0.462389	0.393569
C	7.213950	-0.151703	1.167517
C	5.930762	-0.321595	0.662713
C	5.606847	0.120298	-0.629805
C	6.605532	0.734680	-1.397573
C	7.891853	0.904560	-0.890759
H	9.209494	0.594667	0.793116
H	7.449238	-0.501532	2.175660
H	5.159456	-0.803374	1.269100
H	6.366135	1.082588	-2.406124
H	8.657282	1.385781	-1.504367
C	4.259262	-0.042743	-1.193370
C	3.230855	-0.593209	-0.586596
C	2.217330	-1.140892	0.033094
C	1.256348	-0.355216	0.884485
H	2.035308	-2.217140	-0.074377
H	1.063258	-0.873683	1.836494
H	1.659595	0.642125	1.111361
H	4.107251	0.331976	-2.213526
C	-0.089712	-0.127139	0.219994
F	0.025571	0.557160	-0.942892
S	-1.091652	0.920670	1.396228
O	-1.654910	0.013353	2.391290
O	-0.188258	2.002956	1.776293
S	-0.842614	-1.782178	-0.191367
O	-0.308287	-2.095580	-1.512478
O	-0.588940	-2.636030	0.963332
C	-2.588804	-1.552884	-0.367059
C	-3.072035	-1.023515	-1.563636
C	-3.430745	-1.995483	0.649574
C	-4.448417	-0.916784	-1.732508
H	-2.373360	-0.715496	-2.343380
C	-4.806639	-1.895561	0.457801
H	-2.997649	-2.404087	1.563891
C	-5.310494	-1.357399	-0.726689
H	-4.851070	-0.498495	-2.657185
H	-5.488869	-2.243722	1.236441
H	-6.391131	-1.282787	-0.870285
C	-2.407579	1.638244	0.446346
C	-2.114153	2.538866	-0.579213
C	-3.714507	1.366471	0.840050
C	-3.170317	3.133588	-1.261415
H	-1.078825	2.764647	-0.835061
C	-4.759756	1.985877	0.160525
H	-3.893038	0.675924	1.665236
C	-4.488477	2.856949	-0.893129
H	-2.963192	3.830249	-2.076555
H	-5.791299	1.782321	0.455302
H	-5.312018	3.335333	-1.428475

TSa1

Thermal Correction to Free Energy = 0.601176
a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -3962.03632786

a.u.

Imaginary Frequency = 365.6466i cm⁻¹

Cartesian Coordinates (Angstroms):

P	1.668178	-0.528036	0.059833
P	-1.516887	-0.480916	0.514928
O	-1.112637	3.249808	-1.958488
O	1.165930	3.841001	-0.096466
C	0.254137	1.546010	-1.134250
C	-0.184225	1.963407	0.230368
C	1.179619	0.512475	-1.357282
C	-1.048769	1.211066	1.045444
C	-0.231850	2.270801	-2.241811
C	0.326877	3.182566	0.725152
C	0.183788	1.954756	-3.536825
C	-0.015119	3.635046	2.001484
C	1.622897	0.224036	-2.654037
C	-1.382802	1.669167	2.327158
C	1.117785	0.938733	-3.731487
C	-0.868991	2.871979	2.793353
C	-1.624296	4.024755	-3.002539
C	1.723436	5.050717	0.326705
C	2.395859	0.639299	1.251856
C	2.916482	-1.700841	-0.360688
C	-2.267134	-0.180992	-1.135443
C	-2.935787	-0.913719	1.596732
C	2.002478	0.554137	2.590544
C	2.603837	-2.813728	-1.287376
C	-1.942678	-1.073411	-2.162898
C	-2.797129	-2.082861	2.352423
C	3.320225	1.614630	0.859610
C	4.076299	-1.827842	0.445890
C	-3.112793	0.899893	-1.408892
C	-4.122252	-0.175721	1.697098
C	2.530522	1.433592	3.533177
C	3.696367	-3.736680	-1.580635
C	-2.468215	-0.900646	-3.440870
C	-3.820239	-2.508281	3.198842
C	3.851191	2.488261	1.804503
C	4.998527	-2.826832	0.234876
C	-3.649195	1.064142	-2.683352
C	-5.145379	-0.601173	2.539771
C	3.455640	2.399551	3.140891
C	4.822411	-3.775402	-0.818644
C	-3.328626	0.164759	-3.700971
C	-4.995961	-1.767485	3.292605
H	2.371191	-0.554193	-2.808975
H	-2.040881	1.073527	2.961868
H	1.456373	0.708705	-4.744624
H	-1.130490	3.224044	3.794263
H	-2.302728	4.757135	-2.546281
H	-0.825329	4.564273	-3.541226
H	2.368681	5.400093	-0.489531
H	0.948612	5.813255	0.521341
H	1.260624	-0.196082	2.877209
H	2.002187	-2.537194	-2.169965

H	-1.247958	-1.889322	-1.945919
H	-1.874247	-2.662723	2.251648
H	3.614385	1.689514	-0.189989
H	4.270723	-1.078822	1.217402
H	-3.320467	1.642096	-0.635104
H	-4.250247	0.740320	1.117837
H	2.212102	1.369120	4.576185
H	3.557440	-4.453146	-2.395540
H	-2.198668	-1.597618	-4.237797
H	-3.698003	-3.424259	3.781783
H	4.580685	3.242556	1.498437
H	5.904494	-2.858676	0.844923
H	-4.314872	1.906882	-2.886999
H	-6.067777	-0.019366	2.609778
H	3.872104	3.088659	3.880007
H	5.600183	-4.517525	-1.014512
H	-3.745435	0.300274	-4.702168
H	-5.802034	-2.098969	3.951870
H	-0.208370	2.499429	-4.395126
H	0.390424	4.569653	2.387488
Ni	0.075486	-1.833193	0.432140
H	-2.192824	3.412959	-3.724791
H	2.335934	4.920717	1.235957
C	-1.711710	-4.619828	-0.382398
C	-0.285177	-4.433053	-0.860018
H	-1.719927	-5.028491	0.639810
H	-2.268058	-5.308621	-1.038074
H	-2.235696	-3.651622	-0.358671
H	-0.303341	-4.050432	-1.906123
H	0.215303	-5.422093	-0.907848
O	0.426411	-3.584092	-0.019711
H	1.725004	-3.415813	-0.680944

INTa1

Thermal Correction to Free Energy = 0.602178
a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-
TZVP/PCM(ethanol) Level = -3962.05532297
a.u.

Cartesian Coordinates (Angstroms):

P	-0.965840	-1.345793	-0.038013
P	1.430854	0.678563	-0.537095
O	-1.526367	3.291799	1.880910
O	-3.514147	2.090638	-0.066874
C	-1.364300	1.094911	1.108793
C	-1.232709	1.633837	-0.278362
C	-1.407675	-0.286282	1.359359
C	-0.061266	1.606195	-1.061033
C	-1.580866	1.980192	2.181423
C	-2.423335	2.133265	-0.854899
C	-1.824203	1.485749	3.465585
C	-2.443976	2.604402	-2.168846
C	-1.685771	-0.783049	2.637854
C	-0.096895	2.078014	-2.382337
C	-1.886155	0.110383	3.682428

C	-1.275278	2.573334	-2.922992
C	-1.745133	4.231109	2.894055
C	-4.747934	2.497032	-0.585743
C	-2.301202	-1.242635	-1.249792
C	-0.185923	-2.929989	0.258115
C	1.834349	1.237130	1.153999
C	2.816652	1.362635	-1.506771
C	-1.972214	-1.158523	-2.607330
C	0.250552	-3.343780	1.654177
C	2.526521	0.326811	1.961702
C	3.744963	0.434653	-1.993790
C	-3.641453	-1.188240	-0.850002
C	-0.654855	-4.046367	-0.570213
C	1.540479	2.516651	1.633207
C	3.021831	2.735006	-1.701796
C	-2.979174	-1.031713	-3.560719
C	-0.664840	-4.372013	2.253511
C	2.911459	0.696354	3.248790
C	4.865628	0.888470	-2.691621
C	-4.643835	-1.057902	-1.807288
C	-1.108283	-5.187475	0.002662
C	1.924302	2.877760	2.922386
C	4.137595	3.175997	-2.406131
C	-4.314279	-0.980138	-3.161793
C	-1.252842	-5.276847	1.447304
C	2.605945	1.968301	3.732035
C	5.058945	2.251461	-2.904229
H	-1.750412	-1.859948	2.801771
H	0.804968	2.037054	-2.994745
H	-2.097131	-0.264094	4.686822
H	-1.290258	2.932883	-3.954585
H	-1.662230	5.220735	2.427167
H	-2.751176	4.127978	3.337182
H	-5.485108	2.352325	0.214276
H	-4.740829	3.562475	-0.875582
H	-0.919717	-1.167455	-2.903295
H	0.389533	-2.473185	2.310854
H	2.769779	-0.660503	1.553619
H	3.585992	-0.631449	-1.774913
H	-3.894220	-1.234491	0.212007
H	-0.693612	-3.926759	-1.656947
H	0.984258	3.221450	1.010795
H	2.305323	3.459784	-1.306425
H	-2.718946	-0.959974	-4.619245
H	-0.783894	-4.424486	3.340433
H	3.452538	-0.014875	3.877569
H	5.594253	0.166760	-3.069154
H	-5.690635	-1.020147	-1.495466
H	-1.458579	-6.013532	-0.621416
H	1.692054	3.877787	3.297922
H	4.294246	4.245974	-2.563967
H	-5.103933	-0.876861	-3.910147
H	-1.867449	-6.079351	1.865227
H	2.904217	2.254865	4.743619
H	5.936031	2.601009	-3.454971

H	-1.977114	2.167819	4.301625
H	-3.365996	2.979672	-2.611458
Ni	1.036077	-1.479978	-0.476552
H	-0.991468	4.150085	3.696999
H	-5.041500	1.887261	-1.457916
C	4.038765	-3.536186	0.835626
C	3.171057	-3.411001	-0.409409
H	4.896462	-2.848226	0.767655
H	4.421976	-4.561429	0.970773
H	3.465764	-3.261773	1.737159
H	2.323430	-4.127077	-0.330258
H	3.765435	-3.766175	-1.281414
O	2.756495	-2.111550	-0.614876
H	1.256862	-3.798460	1.557765

TSb1

Thermal Correction to Free Energy = 0.736875 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -4347.59769388 a.u.

Imaginary Frequency = 1110.0593i cm⁻¹

Cartesian Coordinates (Angstroms):

P	-0.758564	1.646255	-0.458433
P	0.075656	-1.519528	0.017391
O	-4.317545	-2.070356	-0.241490
C	-0.846930	3.281676	-1.287961
C	-2.035468	3.895437	-1.705751
H	-2.987055	3.366856	-1.615438
C	-2.011949	5.174301	-2.257375
C	-0.804367	5.859115	-2.392288
C	0.382290	5.256678	-1.979378
C	0.360800	3.973102	-1.437755
H	1.289364	3.490503	-1.124098
C	-1.313468	2.082008	1.241756
C	-0.537159	1.675185	2.331804
H	0.367202	1.089143	2.148606
C	-0.924536	2.005341	3.628211
C	-2.084764	2.745213	3.847192
C	-2.862793	3.151837	2.762611
C	-2.480503	2.821370	1.465478
H	-3.101810	3.138084	0.626551
C	-0.838703	-2.565648	-1.184276
C	-1.601843	-3.661481	-0.757596
H	-1.675390	-3.884971	0.309594
C	-2.275489	-4.452685	-1.683613
C	-2.208592	-4.149744	-3.044970
C	-0.787752	-2.262772	-2.547753
H	-0.235140	-1.383701	-2.879532
C	1.315380	-2.666411	0.724109
C	1.476852	-3.995807	0.315654
H	0.796945	-4.430186	-0.419212
C	2.512065	-4.772206	0.835476
C	3.395762	-4.234075	1.768231
C	3.249461	-2.906472	2.170079

C	2.227523	-2.121883	1.643602
H	2.149534	-1.066256	1.918688
C	-2.762654	-0.334763	-0.406443
C	-2.151551	0.682667	-1.157454
C	-2.488663	0.857404	-2.509237
H	-1.983896	1.621926	-3.101832
C	-3.463833	0.063025	-3.093860
H	-3.723298	0.205849	-4.145608
C	-4.117740	-0.919432	-2.353864
C	-3.765740	-1.121322	-1.019181
C	-5.330534	-2.877501	-0.766425
H	-6.207442	-2.282329	-1.076907
H	-5.631467	-3.562615	0.036444
C	-1.198348	-1.334726	1.329009
C	-0.949312	-1.707757	2.655501
H	-0.021073	-2.220581	2.910982
C	-1.883286	-1.424416	3.643845
H	-1.684705	-1.718452	4.677448
C	-3.070982	-0.765033	3.337927
C	-3.330069	-0.397558	2.015879
C	-2.399019	-0.680411	0.997274
Ni	1.012651	0.475616	-0.675348
O	-4.442994	0.251459	1.623268
H	-4.974657	-3.470261	-1.626895
C	-5.412258	0.572510	2.577268
H	-5.825579	-0.330016	3.061421
H	-5.010504	1.245060	3.355238
H	-6.219280	1.089917	2.042671
C	2.136292	-0.250833	-2.219765
H	1.874978	-1.276368	-2.508647
C	1.283634	0.848923	-2.575004
H	1.741004	1.836716	-2.700867
H	-4.878491	-1.538218	-2.828395
H	-3.783173	-0.535800	4.129900
C	-1.469428	-3.049848	-3.474103
C	3.221806	-0.079315	-1.404102
C	4.089047	0.075164	-0.471951
O	2.176853	0.908055	0.974650
C	2.487823	2.253142	1.209673
H	1.565119	2.861039	1.197345
C	3.187449	2.449852	2.541262
H	3.415768	3.513120	2.717162
H	4.134191	1.889217	2.574443
H	2.551007	2.093354	3.366423
H	-2.860029	-5.310314	-1.340689
H	-2.739366	-4.770763	-3.771079
H	-1.428893	-2.794564	-4.535550
H	2.628195	-5.806958	0.503507
H	4.207658	-4.844273	2.171308
H	3.952124	-2.468328	2.883196
H	-3.772637	3.734822	2.926943
H	-0.315025	1.674503	4.472434
H	-2.384838	3.007432	4.864959
H	-2.945064	5.639514	-2.584569
H	-0.789128	6.862436	-2.824817

H	1.333232	5.783990	-2.085689
H	3.129819	2.644838	0.390639
H	0.478716	0.651727	-3.293201
H	3.236270	0.412378	0.492654
C	5.540560	0.111856	-0.380303
C	6.360604	0.135783	-1.522481
C	6.157357	0.120116	0.880505
C	7.745275	0.170123	-1.403720
H	5.889913	0.129904	-2.508648
C	7.544546	0.149834	0.999395
H	5.526314	0.094077	1.772030
C	8.344102	0.177071	-0.142065
H	8.366353	0.190759	-2.302965
H	8.005035	0.152961	1.990548
H	9.432689	0.203594	-0.050915

INTb1

Thermal Correction to Free Energy = 0.741672 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -4347.62601041 a.u.

Cartesian Coordinates (Angstroms):

P	-0.587594	1.699421	-0.349588
P	-0.017854	-1.618639	0.173143
O	-4.233351	-1.869838	-1.066798
C	-0.362114	3.320532	-1.176772
C	-1.364398	4.008910	-1.873131
H	-2.345540	3.551710	-2.018483
C	-1.112362	5.272354	-2.402386
C	0.139258	5.866056	-2.238475
C	1.142072	5.188379	-1.548305
C	0.894672	3.920254	-1.026257
H	1.682224	3.380524	-0.492474
C	-1.555414	2.168337	1.138688
C	-1.099099	1.766366	2.398100
H	-0.188811	1.157826	2.449529
C	-1.804818	2.135855	3.541070
C	-2.961552	2.905225	3.436820
C	-3.420756	3.302153	2.179812
C	-2.722718	2.933988	1.033447
H	-3.097641	3.240754	0.055957
C	-0.727878	-2.717120	-1.117028
C	-1.734040	-3.649853	-0.829865
H	-2.137801	-3.712272	0.183396
C	-2.230547	-4.481993	-1.829787
C	-1.743042	-4.381936	-3.133626
C	-0.247471	-2.624198	-2.427918
H	0.522073	-1.889529	-2.668990
C	0.990202	-2.762723	1.189255
C	0.959667	-4.157326	1.063046
H	0.287769	-4.629640	0.344056
C	1.793880	-4.952172	1.847264
C	2.663268	-4.364480	2.764987
C	2.703918	-2.976015	2.886796

C	1.884094	-2.171487	2.097614
H	1.933605	-1.075939	2.173061
C	-2.591519	-0.224864	-0.828674
C	-1.782629	0.776367	-1.391485
C	-1.787225	0.983030	-2.780622
H	-1.137655	1.740269	-3.221602
C	-2.618692	0.229976	-3.596303
H	-2.615238	0.394948	-4.676389
C	-3.467323	-0.731597	-3.052241
C	-3.458114	-0.954635	-1.675335
C	-5.155689	-2.594450	-1.826873
H	-5.888486	-1.930685	-2.318631
H	-5.685313	-3.255119	-1.128620
C	-1.505170	-1.292208	1.198905
C	-1.554060	-1.644707	2.552983
H	-0.717093	-2.179741	3.004199
C	-2.667764	-1.313194	3.314204
H	-2.703784	-1.589621	4.370818
C	-3.743847	-0.631474	2.750695
C	-3.699581	-0.271909	1.402370
C	-2.576049	-0.591525	0.615042
Ni	1.324062	0.548131	-0.148733
O	-4.680230	0.403286	0.772865
H	-4.657486	-3.212547	-2.593624
C	-5.830018	0.750144	1.487414
H	-6.359397	-0.141132	1.868465
H	-5.596429	1.419177	2.333758
H	-6.486833	1.280950	0.786228
C	2.534335	-0.218206	-1.576936
H	2.492738	-1.301336	-1.761228
C	1.586871	0.642621	-2.166016
H	1.834375	1.699351	-2.306391
H	-4.117440	-1.312207	-3.705760
H	-4.602882	-0.371246	3.368247
C	-0.752817	-3.448023	-3.431836
C	3.204205	0.230619	-0.448139
C	4.324005	0.313569	0.263001
O	1.629257	0.814339	1.690338
C	2.084407	2.060245	2.077239
H	1.320441	2.857804	1.911222
C	2.452956	2.056242	3.551724
H	2.812406	3.045090	3.879128
H	3.242983	1.313950	3.749513
H	1.581085	1.784766	4.167872
H	-3.007203	-5.212783	-1.589784
H	-2.136570	-5.033413	-3.918004
H	-0.372170	-3.357092	-4.451872
H	1.764230	-6.039181	1.737296
H	3.316759	-4.990079	3.378349
H	3.393147	-2.507674	3.594186
H	-4.327331	3.906249	2.091035
H	-1.445409	1.813033	4.521186
H	-3.509344	3.198653	4.336183
H	-1.900600	5.797540	-2.947308
H	0.333213	6.857755	-2.654214

H	2.126483	5.644034	-1.418756
H	2.973867	2.384737	1.490974
H	0.867750	0.233304	-2.880483
H	4.220185	0.530615	1.331445
C	5.687612	0.151153	-0.245382
C	5.969835	-0.062735	-1.605377
C	6.764357	0.202734	0.654285
C	7.278213	-0.230802	-2.042597
H	5.145990	-0.088562	-2.322512
C	8.074868	0.034775	0.216014
H	6.559726	0.373220	1.714766
C	8.338735	-0.184171	-1.135084
H	7.476305	-0.395961	-3.104743
H	8.896846	0.075662	0.935123
H	9.366509	-0.314318	-1.482139

TSc1

Thermal Correction to Free Energy = 0.860133 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -5890.90451436 a.u.

Imaginary Frequency = 825.6938i cm⁻¹

Cartesian Coordinates (Angstroms):

P	1.742959	-0.216059	1.700255
P	1.352888	0.349486	-1.543391
O	4.909733	-2.342328	-1.728033
O	5.979585	-0.672429	0.443152
C	3.478855	-1.470649	-0.101182
C	3.937191	-0.124379	-0.548112
C	2.554087	-1.668568	0.937215
C	3.133833	0.772715	-1.276275
C	4.024852	-2.599802	-0.747859
C	5.269984	0.234868	-0.255242
C	3.633196	-3.887939	-0.377235
C	5.784945	1.466581	-0.661860
C	2.157100	-2.961912	1.299125
C	3.668114	1.994811	-1.702656
C	2.697271	-4.058283	0.639867
C	4.977865	2.334729	-1.390215
C	5.499748	-3.409693	-2.410363
C	7.326874	-0.419191	0.713048
C	3.158476	0.805139	2.255152
C	0.971061	-0.864625	3.227561
C	1.512123	-1.264051	-2.393853
C	0.776236	1.487071	-2.854823
C	3.103284	2.189392	2.056903
C	-0.418937	-1.025680	3.213442
C	0.779716	-2.375415	-1.970675
C	0.700725	2.856204	-2.561296
C	4.295501	0.241355	2.847368
C	1.687193	-1.176868	4.390527
C	2.394916	-1.386977	-3.475478
C	0.303851	1.031309	-4.090510
C	4.159287	3.000787	2.464755

C	-1.083684	-1.499312	4.342863
C	0.919708	-3.593748	-2.631779
C	0.234405	3.759715	-3.510919
C	5.342666	1.056506	3.268521
C	1.019466	-1.650355	5.517020
C	2.521584	-2.602330	-4.141063
C	-0.187235	1.936329	-5.029899
C	5.276474	2.436988	3.078629
C	-0.366959	-1.813141	5.495030
C	1.782316	-3.709038	-3.719627
C	-0.207353	3.301548	-4.751196
H	1.424217	-3.100699	2.095502
H	3.061539	2.680854	-2.292526
H	2.387468	-5.067938	0.920064
H	5.382524	3.293198	-1.724054
H	6.177518	-2.969502	-3.152950
H	6.083370	-4.056370	-1.731344
H	7.706932	-1.293021	1.257846
H	7.912017	-0.292806	-0.214860
H	2.231413	2.621204	1.558303
H	-0.998183	-0.771919	2.324437
H	0.113428	-2.285374	-1.113650
H	0.978995	3.216839	-1.567970
H	4.379783	-0.843396	2.943049
H	2.768466	-1.038010	4.429050
H	2.989336	-0.526447	-3.792740
H	0.301591	-0.036283	-4.313418
H	4.110262	4.078904	2.295657
H	-2.171084	-1.592609	4.306302
H	0.348233	-4.459505	-2.289092
H	0.179795	4.821531	-3.261935
H	6.221916	0.609070	3.738860
H	1.585542	-1.884974	6.421889
H	3.204428	-2.687302	-4.990223
H	-0.560845	1.566264	-5.987717
H	6.102761	3.074342	3.403302
H	-0.887500	-2.175025	6.385520
H	1.882230	-4.664353	-4.241649
H	-0.589494	4.008007	-5.492118
H	4.041399	-4.759836	-0.887386
H	6.808090	1.751198	-0.418725
Ni	0.377490	0.808255	0.397229
H	4.746962	-4.023112	-2.934775
H	7.456923	0.478036	1.343197
C	-2.552952	5.893140	-1.191839
C	-1.908412	5.900138	0.047656
C	-1.428025	4.716288	0.594819
C	-1.573480	3.496876	-0.088724
C	-2.209529	3.505630	-1.338869
C	-2.700280	4.690577	-1.880076
H	-2.936413	6.823711	-1.617750
H	-1.785112	6.838426	0.594818
H	-0.934386	4.722168	1.568737
H	-2.304080	2.573947	-1.897419
H	-3.191226	4.672662	-2.856371

C	-1.043156	2.246810	0.462010
C	-0.418314	1.950708	1.605473
C	-0.392431	2.329363	2.989581
C	-1.505947	2.689879	3.654919
H	0.554062	2.221336	3.532750
H	-1.473189	2.899408	4.727656
H	-2.473754	2.728790	3.144616
C	-3.087195	0.483218	-0.296799
H	-1.765389	1.280246	-0.019854
F	-3.890231	0.997032	-1.274582
S	-2.365127	-1.024197	-0.841215
O	-1.338938	-1.360792	0.161365
O	-1.982551	-0.775247	-2.232745
S	-3.972920	0.500547	1.246508
O	-4.138798	1.908790	1.604285
O	-3.313425	-0.435396	2.159880
C	-5.594617	-0.133504	0.882123
C	-6.473337	0.641208	0.123699
C	-5.950153	-1.392348	1.358694
C	-7.724198	0.117977	-0.190101
H	-6.172524	1.635726	-0.208493
C	-7.209100	-1.898619	1.046341
H	-5.238072	-1.953522	1.964854
C	-8.089979	-1.149086	0.267661
H	-8.422880	0.707234	-0.788407
H	-7.500992	-2.885702	1.411539
H	-9.075032	-1.552080	0.020125
C	-3.548361	-2.345398	-0.836140
C	-4.564465	-2.332152	-1.792353
C	-3.464734	-3.334727	0.140539
C	-5.521002	-3.341587	-1.762690
H	-4.593173	-1.540138	-2.542907
C	-4.419685	-4.349469	0.145244
H	-2.659807	-3.289434	0.876484
C	-5.444476	-4.350799	-0.800831
H	-6.329088	-3.344380	-2.497348
H	-4.365383	-5.141586	0.895755
H	-6.194473	-5.145303	-0.788183

INTc1

Thermal Correction to Free Energy = 0.863657 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -5890.92096493 a.u.

Cartesian Coordinates (Angstroms):

P	1.767206	0.514509	1.636855
P	1.475563	-0.155801	-1.602803
O	4.580398	-3.103148	-0.698181
O	5.927507	-0.887244	0.790175
C	3.319182	-1.518787	0.462521
C	3.967253	-0.505355	-0.416643
C	2.375662	-1.203680	1.454874
C	3.283536	0.139785	-1.460253
C	3.673657	-2.870894	0.267483

C	5.336406	-0.231672	-0.225848
C	3.082615	-3.877260	1.034242
C	5.999511	0.681941	-1.048132
C	1.784565	-2.216998	2.220180
C	3.958439	1.036327	-2.296681
C	2.139684	-3.541736	2.002121
C	5.304587	1.304291	-2.081108
C	4.970778	-4.419662	-0.964644
C	7.299409	-0.718386	1.001478
C	3.273078	1.532285	1.762505
C	0.976629	0.575736	3.279311
C	1.390068	-1.950258	-1.910910
C	0.964252	0.629511	-3.170506
C	3.323700	2.750879	1.077948
C	-0.397493	0.310718	3.337649
C	0.471166	-2.735831	-1.211221
C	1.007267	2.029866	-3.257573
C	4.369314	1.123395	2.532490
C	1.666241	0.919904	4.448725
C	2.243866	-2.543471	-2.850217
C	0.389386	-0.100931	-4.214159
C	4.455942	3.557271	1.168601
C	-1.068264	0.366557	4.557297
C	0.391261	-4.103682	-1.462732
C	0.520986	2.682377	-4.385257
C	5.493119	1.938793	2.631220
C	0.988587	0.977586	5.664289
C	2.157616	-3.909806	-3.100561
C	-0.105533	0.557859	-5.338625
C	5.538984	3.154566	1.948157
C	-0.377397	0.697637	5.720860
C	1.228899	-4.690926	-2.408773
C	-0.035062	1.945765	-5.430929
H	1.045582	-1.961619	2.980932
H	3.433057	1.518873	-3.120835
H	1.675416	-4.332369	2.596181
H	5.828159	2.008092	-2.732474
H	5.701976	-4.368760	-1.781382
H	5.447035	-4.890266	-0.086561
H	7.566924	-1.360228	1.850536
H	7.888289	-1.026031	0.119716
H	2.471133	3.054700	0.464073
H	-0.968233	0.082648	2.433975
H	-0.165657	-2.268845	-0.460712
H	1.397689	2.619717	-2.423675
H	4.353852	0.151372	3.030669
H	2.729270	1.163346	4.415482
H	2.979462	-1.933624	-3.380877
H	0.303609	-1.185711	-4.137637
H	4.492700	4.503573	0.624255
H	-2.143642	0.178150	4.559879
H	-0.335445	-4.707341	-0.913874
H	0.548056	3.773012	-4.432350
H	6.342057	1.620058	3.241086
H	1.531413	1.253670	6.571651

H	2.818364	-4.368607	-3.840430
H	-0.562425	-0.022741	-6.143395
H	6.425158	3.789710	2.021909
H	-0.906218	0.755033	6.675769
H	1.159979	-5.762935	-2.611171
H	-0.432934	2.458628	-6.309696
H	3.342569	-4.922899	0.872577
H	7.053715	0.908461	-0.891612
Ni	0.465827	0.975584	0.022764
H	4.116483	-5.038320	-1.288997
H	7.549483	0.327489	1.251498
C	-3.075065	5.194237	-2.890355
C	-2.472438	5.651167	-1.716185
C	-1.766655	4.772644	-0.902505
C	-1.653586	3.419396	-1.255610
C	-2.263640	2.965402	-2.434036
C	-2.969368	3.849788	-3.243365
H	-3.631851	5.887474	-3.525731
H	-2.556289	6.703039	-1.431820
H	-1.299186	5.125965	0.018479
H	-2.194251	1.906650	-2.696921
H	-3.444890	3.481940	-4.155752
C	-0.898492	2.480412	-0.430364
C	-0.314688	2.487383	0.761765
C	-0.399556	3.262358	1.971371
C	-1.571198	3.567810	2.553466
H	0.540847	3.528084	2.469842
H	-1.592913	4.109297	3.503025
H	-2.526910	3.246017	2.125565
C	-3.395746	0.657531	-0.144411
H	-0.766410	1.510681	-1.043979
F	-4.280223	0.920643	-1.158420
S	-2.355135	-0.644013	-0.528757
O	-1.246829	-0.664743	0.460056
O	-1.997818	-0.487992	-1.950655
S	-4.192447	0.693118	1.395438
O	-4.669133	2.058809	1.622626
O	-3.328597	0.032225	2.383372
C	-5.647961	-0.321178	1.211939
C	-6.700612	0.137168	0.418277
C	-5.676205	-1.585252	1.797062
C	-7.787887	-0.702332	0.192077
H	-6.656887	1.139602	-0.009798
C	-6.772769	-2.412811	1.568923
H	-4.838434	-1.898545	2.421087
C	-7.823512	-1.975625	0.763010
H	-8.617543	-0.358089	-0.430115
H	-6.803506	-3.406860	2.021082
H	-8.680233	-2.629414	0.581863
C	-3.128547	-2.242784	-0.383676
C	-4.108794	-2.585032	-1.316576
C	-2.824734	-3.074643	0.692540
C	-4.785507	-3.791400	-1.170870
H	-4.327946	-1.905776	-2.142616
C	-3.499504	-4.288011	0.817498

H	-2.069860	-2.756704	1.413972
C	-4.477607	-4.645552	-0.110117
H	-5.558862	-4.068718	-1.890713
H	-3.265150	-4.954684	1.651127
H	-5.009160	-5.594231	-0.003768

TSd1^R

Thermal Correction to Free Energy = 0.866336 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -5890.90467182 a.u.

Imaginary Frequency = 51.5531i cm⁻¹

Cartesian Coordinates (Angstroms):

P	-2.438035	-0.922078	1.474031
P	-1.893888	1.425632	-0.823072
O	-5.428450	-0.476814	-2.668351
O	-4.039688	-3.058667	-2.055287
C	-4.166798	-0.717186	-0.721143
C	-3.003328	-1.015948	-1.603959
C	-4.079217	-0.708553	0.681857
C	-1.936388	-0.121335	-1.801999
C	-5.413389	-0.451093	-1.324137
C	-2.976400	-2.259221	-2.266528
C	-6.533987	-0.159522	-0.542128
C	-1.883845	-2.615609	-3.060376
C	-5.205789	-0.417795	1.461640
C	-0.847434	-0.479415	-2.603126
C	-6.420125	-0.143085	0.845169
C	-0.824973	-1.725851	-3.214894
C	-6.638994	-0.278984	-3.340143
C	-4.101572	-4.291856	-2.712225
C	-1.835898	-2.510905	0.826325
C	-2.830636	-1.202649	3.240435
C	-3.500970	2.222403	-1.129825
C	-0.653183	2.520171	-1.589390
C	-0.487293	-2.610682	0.477886
C	-2.723156	-0.109752	4.108552
C	-4.203376	2.767322	-0.050685
C	0.699866	2.222057	-1.361780
C	-2.681287	-3.619508	0.675885
C	-3.235751	-2.440608	3.751667
C	-4.036230	2.309678	-2.421032
C	-0.995679	3.686226	-2.284156
C	0.026793	-3.818943	0.012381
C	-3.041134	-0.241609	5.457785
C	-5.429270	3.395443	-0.257297
C	1.690764	3.064876	-1.855963
C	-2.160737	-4.825937	0.217675
C	-3.542347	-2.574692	5.104001
C	-5.255713	2.948616	-2.626017
C	0.003296	4.532307	-2.762048
C	-0.806080	-4.928036	-0.110139
C	-3.452017	-1.476026	5.957740
C	-5.954320	3.488954	-1.545075

C	1.345400	4.221950	-2.551977
H	-5.128948	-0.410841	2.550082
H	-0.007274	0.203094	-2.726978
H	-7.298815	0.085319	1.452998
H	0.038051	-2.014307	-3.818821
H	-6.419810	-0.366655	-4.411833
H	-7.387602	-1.041868	-3.063578
H	-5.048832	-4.758620	-2.413108
H	-4.092632	-4.169731	-3.809582
H	0.168353	-1.740873	0.533051
H	-2.367995	0.848094	3.720223
H	-3.791617	2.678255	0.958098
H	0.996152	1.331995	-0.797595
H	-3.750066	-3.529862	0.884241
H	-3.296503	-3.311260	3.097163
H	-3.500351	1.862891	-3.261886
H	-2.043783	3.945351	-2.444037
H	1.086443	-3.872260	-0.243947
H	-2.950233	0.619788	6.123353
H	-5.978709	3.808671	0.591477
H	2.735255	2.821951	-1.655325
H	-2.817458	-5.693218	0.111680
H	-3.847380	-3.548404	5.494397
H	-5.665781	3.023808	-3.636198
H	-0.273158	5.444464	-3.296513
H	-0.402832	-5.878770	-0.468111
H	-3.689779	-1.585783	7.018485
H	-6.914060	3.985381	-1.708353
H	2.126120	4.893425	-2.917292
H	-7.493753	0.061886	-1.007962
H	-1.845479	-3.590003	-3.546314
Ni	-1.209833	0.827782	1.182509
H	-7.057440	0.723128	-3.141750
H	-3.268730	-4.953514	-2.418009
C	2.592367	5.347247	0.791515
C	3.160527	4.141379	1.197901
C	2.356744	3.096884	1.642593
C	0.964008	3.238288	1.700763
C	0.403772	4.460087	1.285441
C	1.205149	5.499890	0.831762
H	3.225291	6.166130	0.440700
H	4.241686	3.986829	1.173842
H	2.831362	2.158332	1.917545
H	-0.683603	4.580536	1.300620
H	0.744663	6.434722	0.503136
C	0.044359	2.177746	2.132619
C	0.157854	0.824886	2.385361
C	1.088439	-0.149459	2.799140
C	2.346030	0.109348	3.250227
H	0.829296	-1.193860	2.608145
H	3.051580	-0.704471	3.432658
H	2.678276	1.118365	3.499839
H	-0.964292	2.593984	2.355283
C	3.766614	0.211995	0.814212
F	3.750340	1.217355	-0.130161

S	2.988465	-1.192891	0.172062
O	2.858154	-2.228019	1.200378
O	1.772904	-0.669902	-0.485436
S	5.312262	0.167771	1.598099
O	5.525648	1.519989	2.124829
O	5.348778	-1.000934	2.478123
C	6.532315	-0.069155	0.320979
C	6.870379	1.006931	-0.500133
C	7.053467	-1.342943	0.103158
C	7.738699	0.793454	-1.567326
H	6.456943	1.994216	-0.289030
C	7.925318	-1.542134	-0.964007
H	6.769255	-2.153342	0.776642
C	8.263621	-0.478386	-1.800296
H	8.013890	1.626886	-2.218266
H	8.340041	-2.536127	-1.146102
H	8.945187	-0.640805	-2.638836
C	3.965876	-1.906231	-1.139166
C	4.243983	-1.142547	-2.274499
C	4.471963	-3.194801	-0.987013
C	5.048742	-1.687082	-3.269845
H	3.836717	-0.134330	-2.365692
C	5.258389	-3.736850	-2.001975
H	4.243761	-3.745023	-0.071830
C	5.549549	-2.983941	-3.138253
H	5.286793	-1.096030	-4.157144
H	5.654162	-4.750233	-1.899227
H	6.176533	-3.406861	-3.926865

TSe1

Thermal Correction to Free Energy = 0.867326 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -5890.90145084 a.u.

Imaginary Frequency = 270.4078i cm⁻¹

Cartesian Coordinates (Angstroms):

P	1.193541	0.876065	-1.259869
P	1.811182	-0.550459	1.751211
O	5.809263	-1.009711	-0.050630
O	4.357104	-1.906492	-2.458945
C	3.765233	-0.035036	-0.623684
C	3.207805	-1.412576	-0.490448
C	3.010728	1.092356	-0.998602
C	2.385991	-1.823864	0.573111
C	5.152285	0.112219	-0.402544
C	3.580556	-2.365097	-1.463110
C	5.769714	1.356678	-0.531458
C	3.134957	-3.685243	-1.372522
C	3.644151	2.333690	-1.142659
C	1.931112	-3.145394	0.654274
C	5.006604	2.459010	-0.904540
C	2.310026	-4.063558	-0.315900
C	7.194603	-0.960129	0.123844
C	4.772445	-2.784504	-3.464855

C	1.278076	-0.283079	-2.690106
C	0.637926	2.437380	-2.018289
C	3.382474	0.184176	2.329921
C	1.165296	-1.434014	3.221705
C	0.683835	-1.546255	-2.648485
C	0.708727	3.613251	-1.253851
C	3.557697	1.570001	2.383591
C	-0.119610	-1.992349	3.118869
C	2.000792	0.090405	-3.832231
C	-0.027541	2.476674	-3.248025
C	4.434762	-0.655702	2.720902
C	1.824433	-1.473193	4.456241
C	0.770544	-2.403064	-3.744563
C	0.202912	4.813108	-1.741281
C	4.759717	2.109881	2.834456
C	-0.708423	-2.611614	4.217318
C	2.082086	-0.762324	-4.928853
C	-0.552614	3.676939	-3.726606
C	5.629616	-0.113607	3.185221
C	1.223870	-2.084540	5.556421
C	1.455933	-2.009380	-4.891502
C	-0.424564	4.849054	-2.985584
C	5.794052	1.270592	3.243771
C	-0.038797	-2.660892	5.439852
H	3.071478	3.203726	-1.462800
H	1.286752	-3.452298	1.478553
H	5.489020	3.432655	-1.020564
H	1.959355	-5.096403	-0.251680
H	7.515332	-1.979461	0.374570
H	7.710602	-0.638030	-0.797712
H	5.377881	-2.192988	-4.163144
H	5.389819	-3.606093	-3.060109
H	0.183023	-1.874814	-1.740088
H	1.154044	3.588734	-0.256827
H	2.760348	2.228924	2.041882
H	-0.658644	-1.926647	2.171971
H	2.502563	1.060835	-3.861744
H	-0.155090	1.562335	-3.828770
H	4.320550	-1.739763	2.645076
H	2.808568	-1.016009	4.568720
H	0.300232	-3.388066	-3.692570
H	0.259112	5.714390	-1.127579
H	4.889798	3.194077	2.857252
H	-1.708642	-3.041198	4.120865
H	2.639165	-0.452412	-5.816502
H	-1.072636	3.689434	-4.687506
H	6.440437	-0.777078	3.496071
H	1.749338	-2.103793	6.514272
H	1.513210	-2.677298	-5.755137
H	-0.842486	5.786424	-3.359467
H	6.734406	1.695838	3.603159
H	-0.507185	-3.136431	6.304909
H	6.836614	1.472387	-0.343670
H	3.413580	-4.417189	-2.130081
Ni	0.142524	0.555170	0.847389

H	7.479321	-0.283864	0.948901
H	3.915018	-3.208873	-4.013817
C	-3.130247	6.734073	0.896034
C	-2.548749	5.928077	1.876584
C	-2.173224	4.620060	1.591248
C	-2.374539	4.069697	0.310630
C	-2.971991	4.893935	-0.663865
C	-3.342183	6.202450	-0.376916
H	-3.418754	7.763079	1.123399
H	-2.382509	6.326847	2.881160
H	-1.715965	4.008064	2.370605
H	-3.150753	4.478530	-1.658222
H	-3.807748	6.814194	-1.154636
C	-1.995414	2.717966	-0.064976
C	-1.610097	1.744130	0.784435
C	-1.093593	1.563474	2.071826
C	0.260955	1.923023	2.264440
H	-1.631087	0.971510	2.819786
H	0.646317	2.825221	1.774302
H	0.717050	1.698309	3.234953
H	-2.133848	2.452084	-1.115563
C	-2.897070	0.028252	0.604256
F	-2.871528	-0.646517	1.791803
S	-4.524725	0.653315	0.303993
O	-4.553088	1.181313	-1.054747
O	-4.844407	1.463751	1.473132
S	-2.050017	-0.877555	-0.605353
O	-0.787881	-1.244946	0.124322
O	-1.958095	-0.110629	-1.842054
C	-2.811701	-2.432803	-0.967396
C	-3.079388	-3.335832	0.064655
C	-3.175592	-2.694913	-2.287180
C	-3.728661	-4.525513	-0.243154
H	-2.794045	-3.101419	1.090911
C	-3.808542	-3.900769	-2.580413
H	-2.954266	-1.952557	-3.056460
C	-4.087491	-4.811402	-1.562381
H	-3.957410	-5.237001	0.553118
H	-4.090341	-4.126316	-3.611514
H	-4.592655	-5.751495	-1.795721
C	-5.561872	-0.791497	0.361414
C	-5.902358	-1.332114	1.601371
C	-5.960803	-1.387518	-0.833903
C	-6.645312	-2.509176	1.637787
H	-5.591561	-0.820407	2.513778
C	-6.709310	-2.559973	-0.782339
H	-5.683210	-0.919378	-1.780125
C	-7.045868	-3.122015	0.449601
H	-6.923485	-2.945803	2.599952
H	-7.030546	-3.038907	-1.709857
H	-7.631297	-4.043970	0.484273

INTe1

Thermal Correction to Free Energy = 0.870244 a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -5890.95008059 a.u.

Cartesian Coordinates (Angstroms):

P	1.585458	1.271751	-0.760437
P	1.516822	-1.295828	1.487447
O	5.641906	-1.775294	-0.052983
O	4.412515	-1.358287	-2.738487
C	3.873162	-0.279347	-0.356295
C	3.100484	-1.474083	-0.811439
C	3.369054	1.034906	-0.342722
C	2.102190	-2.110979	-0.049478
C	5.221932	-0.495470	-0.000357
C	3.447897	-2.015429	-2.067247
C	6.042364	0.564942	0.386346
C	2.802378	-3.151013	-2.561394
C	4.211613	2.096508	0.011812
C	1.459116	-3.250674	-0.552715
C	5.528800	1.857892	0.381004
C	1.809025	-3.757810	-1.796957
C	6.982937	-2.060686	0.210106
C	4.809469	-1.822877	-3.994617
C	1.658580	0.755662	-2.530914
C	1.334429	3.080990	-0.931138
C	3.077889	-1.100350	2.427066
C	0.647358	-2.630985	2.409028
C	0.824178	-0.247822	-3.026201
C	1.607744	3.953365	0.135815
C	3.337295	0.126396	3.046038
C	-0.691454	-2.851492	2.048712
C	2.586599	1.356048	-3.393722
C	0.677171	3.598427	-2.056679
C	4.020204	-2.132068	2.532450
C	1.172434	-3.351098	3.488745
C	0.890960	-0.624336	-4.367593
C	1.279788	5.303964	0.058820
C	4.512343	0.318704	3.769270
C	-1.468266	-3.796302	2.712657
C	2.649454	0.985712	-4.732856
C	0.345229	4.949222	-2.129154
C	5.186728	-1.944749	3.269157
C	0.389696	-4.288441	4.163261
C	1.794335	-0.002733	-5.225671
C	0.653294	5.809422	-1.078073
C	5.435314	-0.718852	3.887893
C	-0.927735	-4.522598	3.774070
H	3.842258	3.120345	-0.017942
H	0.688008	-3.744443	0.040065
H	6.173279	2.694458	0.662256
H	1.304589	-4.647985	-2.181634
H	7.105177	-3.143512	0.077090
H	7.657207	-1.535081	-0.489194
H	5.587649	-1.135106	-4.349694
H	5.230120	-2.842997	-3.940091
H	0.142373	-0.757485	-2.348809

H	2.072451	3.572906	1.046847
H	2.618439	0.939107	2.929076
H	-1.121812	-2.247684	1.249753
H	3.263084	2.123320	-3.008528
H	0.412040	2.936110	-2.882358
H	3.846485	-3.078080	2.014025
H	2.197905	-3.175193	3.817410
H	0.233910	-1.415110	-4.737895
H	1.495416	5.961130	0.904227
H	4.710835	1.286407	4.235803
H	-2.509317	-3.947544	2.413328
H	3.371696	1.467996	-5.396472
H	-0.166216	5.328804	-3.017282
H	5.911624	-2.758549	3.354125
H	0.816706	-4.838772	5.005550
H	1.840631	-0.291531	-6.279121
H	0.385976	6.866803	-1.132486
H	6.355384	-0.570522	4.458916
H	-1.536119	-5.257231	4.307363
H	7.076010	0.391393	0.683712
H	3.060527	-3.556888	-3.538981
Ni	0.229173	0.389963	0.714530
H	7.264478	-1.795119	1.244358
H	3.974424	-1.812456	-4.715596
C	-1.665624	6.699801	1.952210
C	-1.452265	5.642502	2.840286
C	-1.746086	4.336701	2.469023
C	-2.261368	4.049550	1.190666
C	-2.490097	5.128002	0.318114
C	-2.192448	6.434797	0.690113
H	-1.432777	7.725115	2.249971
H	-1.060764	5.841461	3.841259
H	-1.593794	3.522513	3.177872
H	-2.903520	4.924285	-0.672874
H	-2.374337	7.252366	-0.011912
C	-2.669763	2.719351	0.757239
C	-2.290601	1.485743	1.198599
C	-1.143986	1.070253	2.013450
C	0.067149	1.801509	2.043613
H	-1.344030	0.309590	2.775867
H	0.095426	2.791684	1.583840
H	0.703935	1.706656	2.930628
H	-3.416193	2.744333	-0.042295
C	-3.050210	0.325618	0.630672
F	-2.953450	-0.794259	1.391690
S	-4.890730	0.635184	0.430177
O	-5.091925	1.192001	-0.907557
O	-5.319465	1.332787	1.632205
S	-2.204939	-0.123203	-0.982565
O	-0.978805	-0.814116	-0.493735
O	-2.105220	1.052509	-1.830211
C	-3.128240	-1.376113	-1.813296
C	-3.082337	-2.689048	-1.342135
C	-3.828859	-1.017614	-2.963292
C	-3.781349	-3.666420	-2.042247

H	-2.495524	-2.938504	-0.457276
C	-4.511724	-2.012221	-3.658119
H	-3.827733	0.024042	-3.288331
C	-4.490539	-3.328736	-3.196293
H	-3.763722	-4.699758	-1.690203
H	-5.061676	-1.757245	-4.566606
H	-5.029313	-4.104165	-3.746064
C	-5.615709	-0.989244	0.475716
C	-5.622713	-1.709208	1.671766
C	-6.256321	-1.455566	-0.667758
C	-6.240727	-2.954840	1.695007
H	-5.149299	-1.296797	2.563477
C	-6.885547	-2.697394	-0.625037
H	-6.254571	-0.843082	-1.570064
C	-6.867146	-3.448802	0.548421
H	-6.246015	-3.538546	2.618143
H	-7.391285	-3.077530	-1.515082
H	-7.356251	-4.425398	0.576511

F2₀

Thermal Correction to Free Energy = 0.119051
a.u.

Electronic Energy at the PBE0-D3(BJ)/def2-TZVP/PCM(ethanol) Level = -385.870272651
a.u.

Cartesian Coordinates (Angstroms):

C	-3.063490	0.609797	-0.095915
C	-1.986364	1.486521	0.065162
C	-0.693286	0.992046	0.146137
C	-0.474226	-0.393957	0.065662
C	-1.555810	-1.272152	-0.095254
C	-2.848286	-0.765090	-0.175667
H	-4.079552	1.005444	-0.158719
H	-2.160786	2.562471	0.128888
H	0.146590	1.679744	0.274726
H	-1.385896	-2.349694	-0.156303
H	-3.691242	-1.447508	-0.300387
C	0.873550	-0.953170	0.151325
C	2.041889	-0.412084	0.278106
C	3.305764	0.106989	0.452665
C	4.036844	0.459426	-0.649154
H	3.705965	0.244049	1.465486
H	5.039785	0.889985	-0.548018
H	3.636537	0.322035	-1.659485
H	0.969091	-2.056479	0.095411

8. X-ray crystallographic data of 3s, 3ac, and 7

Data intensity of **3s**^[10] was collected using a 'Bruker APEX-II CCD' diffractometer at 297.82(10) K. Data collection and reduction were done by using Olex2 and the structure was solved with the ShelXS structure solution program using direct methods and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for non-H atoms using SHELX-97. Hydrogen atoms were added at their geometrically ideal positions and refined isotropically. Crystal data for (**3s**)₂: C₄₂H₃₄F₂O₈S₆, $T = 297.82(10)$ K, triclinic, P1, $a = 9.6128(3)$ Å, $b = 10.2795(3)$ Å, $c = 12.5045(3)$ Å, $\alpha = 103.159(2)^\circ$, $\beta = 96.871(2)^\circ$, $\gamma = 116.633(3)^\circ$, $V = 1040.05(6)$ Å³. $Z = 1$, $\rho_{\text{calc}} = 1.432$ g/cm³. 23484 reflections collected, 6878 [$R_{\text{int}} = 0.0751$, $R_{\text{sigma}} = 0.0557$] independent reflections, $R_1 = 0.0531$, $wR_2 = 0.1504$ ($I \geq 2\sigma(I)$), $R_1 = 0.0555$, $wR_2 = 0.1541$ (all data), GOF = 1.054, and 0.060(16) parameters.

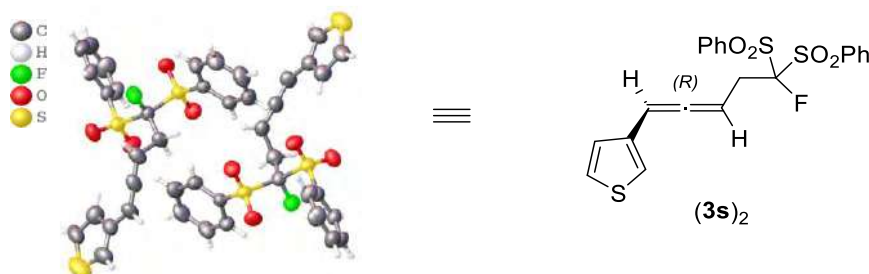


Table S4. Crystal data and structure refinement for **3s**.

Identification code	3s
Empirical formula	C ₄₂ H ₃₄ F ₂ O ₈ S ₆
Formula weight	897.05
Temperature/K	297.82(10)
Crystal system	triclinic
Space group	P1
$a/\text{\AA}$	9.6128(3)
$b/\text{\AA}$	10.2795(3)
$c/\text{\AA}$	12.5045(3)
$\alpha/^\circ$	103.159(2)
$\beta/^\circ$	96.871(2)
$\gamma/^\circ$	116.633(3)
Volume/Å ³	1040.05(6)
Z	1
$\rho_{\text{calc}}/\text{g cm}^{-3}$	1.432

¹⁰ Supplementary crystallographic data have been deposited at Cambridge Crystallographic Data Center (CCDC number: 2275115).

μ/mm^{-1}	3.562
F(000)	464.0
Crystal size/ mm^3	$0.39 \times 0.32 \times 0.26$
Radiation	Cu K α ($\lambda = 1.54184$)
2 Θ range for data collection/ $^\circ$	7.508 to 134.15
Index ranges	$-11 \leq h \leq 11, -12 \leq k \leq 12, -14 \leq l \leq 14$
Reflections collected	23484
Independent reflections	6878 [$R_{\text{int}} = 0.0751, R_{\text{sigma}} = 0.0557$]
Data/restraints/parameters	6878/3/523
Goodness-of-fit on F^2	1.054
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0531, wR_2 = 0.1504$
Final R indexes [all data]	$R_1 = 0.0555, wR_2 = 0.1541$
Largest diff. peak/hole / $e \text{ \AA}^{-3}$	0.40/-0.45
Flack parameter	0.060(16)

Table S5. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3s**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U(eq)
S4	9462.9(14)	2387.8(13)	8309.6(10)	46.4(3)
S5	7599.2(15)	2805.8(14)	6333.4(11)	49.2(3)
S2	12418.1(17)	6918.1(16)	13474.1(11)	54.5(4)
S3	10673.5(14)	7609.8(14)	11614.0(10)	48.0(3)
S6	3883(3)	7189(3)	6939(2)	88.0(6)
S1	16292(3)	2581(3)	13013(3)	109.2(9)
F1	13593(4)	9340(4)	12838(3)	65.3(9)
O8	5957(5)	2089(6)	5703(4)	64.1(11)
F2	6886(5)	294(4)	6796(3)	63.7(9)
O5	10255(5)	4021(5)	8867(4)	61.5(11)
O6	10188(6)	1733(6)	7587(4)	64.4(11)
O1	11447(7)	5305(5)	12928(4)	75.3(14)
C9	12577(7)	7792(6)	12321(5)	46.5(12)
O3	10276(6)	8513(6)	12431(4)	69.1(12)
O7	8457(6)	4419(5)	6907(4)	61.9(11)
O4	9587(5)	6000(5)	11086(4)	60.0(10)
C27	8300(8)	-146(7)	9001(6)	57.9(14)
C33	10221(8)	3405(8)	5513(6)	64.2(16)
C22	8973(7)	1445(7)	9338(5)	47.0(12)

Atom	x	y	z	U(eq)
C4	15805(8)	4449(8)	12226(6)	63.1(15)
C8	13267(7)	7135(8)	11450(5)	58.6(14)
C10	11446(8)	7588(7)	14369(5)	51.8(13)
C23	9288(9)	2312(8)	10442(5)	59.1(15)
C3	16532(9)	3549(10)	12098(8)	81(2)
O2	14052(6)	7554(7)	14097(4)	73.0(13)
C1	14979(10)	4268(10)	13105(7)	77.5(19)
C37	5555(8)	3924(8)	8572(5)	61.2(14)
C29	8009(8)	813(7)	4725(5)	56.7(13)
C2	15107(10)	3280(9)	13699(8)	81(2)
C31	10423(10)	1545(10)	4113(6)	74.0(18)
C16	11190(7)	8482(6)	10560(5)	48.1(12)
C12	11444(12)	9571(9)	15775(6)	78(2)
C28	8687(7)	2285(7)	5459(5)	48.8(12)
C20	12443(10)	10774(9)	10037(7)	77(2)
C25	8282(9)	-1(10)	10930(7)	72.8(19)
C32	11064(9)	3010(10)	4822(7)	76.7(19)
C17	10751(8)	7592(7)	9436(5)	57.0(14)
C38	4543(8)	4458(8)	8472(6)	62.2(15)
C7	14930(8)	7454(8)	11920(6)	65.8(16)
C24	8976(11)	1592(10)	11249(6)	74(2)
C5	15897(9)	5440(9)	11538(6)	68.2(17)
C11	12253(9)	9090(8)	15067(6)	61.9(15)
C18	11142(10)	8288(10)	8618(6)	71.6(19)
C30	8911(10)	438(9)	4072(6)	68.4(17)
C35	6221(7)	1858(7)	8037(5)	58.5(14)
C34	7473(7)	1811(6)	7416(5)	46.0(12)
C41	5219(8)	6679(7)	6391(7)	69.1(18)
C36	6582(7)	3434(7)	8718(5)	57.8(13)
C26	7972(9)	-848(8)	9827(7)	67.8(17)
C6	15395(7)	6443(8)	11720(5)	62.6(15)
C39	4532(8)	5415(7)	7773(6)	59.0(14)
C21	12028(9)	10092(8)	10883(6)	65.6(17)
C19	11979(10)	9867(11)	8926(7)	80(2)
C15	9888(9)	6572(9)	14370(6)	70.7(18)
C13	9936(12)	8587(12)	15794(7)	85(2)

Atom	x	y	z	U(eq)
C40	5438(9)	5724(9)	6948(6)	69.7(17)
C42	3650(8)	6139(9)	7837(7)	71.3(18)
C14	9168(11)	7093(12)	15113(8)	91(2)

Table S6. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^{-3}$) for **3s**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
S4	50.6(7)	49.4(7)	44.7(7)	16.4(6)	16.5(6)	27.3(6)
S5	55.7(7)	49.2(7)	46.8(7)	20.0(6)	16.5(6)	26.0(6)
S2	70.3(9)	58.2(8)	46.3(7)	22.8(7)	18.3(7)	37.0(7)
S3	52.3(7)	55.7(7)	43.9(7)	16.2(6)	15.7(6)	32.1(6)
S6	72.3(11)	74.5(11)	121.3(17)	44.5(12)	19.2(11)	34.4(9)
S1	83.7(13)	90.5(15)	153(2)	64.2(17)	8.7(15)	35.5(12)
F1	62.0(19)	51.9(19)	67(2)	22.4(17)	2.5(17)	17.4(16)
O8	54(2)	73(3)	68(3)	33(2)	13(2)	30(2)
F2	74(2)	44.4(17)	61(2)	16.3(15)	9.8(17)	21.4(16)
O5	59(2)	45(2)	67(3)	17(2)	8(2)	16.7(19)
O6	72(3)	86(3)	60(3)	27(2)	34(2)	54(3)
O1	114(4)	52(2)	61(3)	20(2)	27(3)	39(3)
C9	49(3)	51(3)	40(3)	16(2)	10(2)	24(2)
O3	90(3)	93(3)	52(2)	21(2)	27(2)	67(3)
O7	83(3)	47(2)	58(3)	20(2)	26(2)	31(2)
O4	52(2)	55(2)	63(3)	17(2)	14.5(19)	18.8(18)
C27	66(3)	50(3)	54(3)	14(3)	7(3)	28(3)
C33	58(3)	62(4)	55(4)	13(3)	19(3)	16(3)
C22	51(3)	56(3)	41(3)	18(2)	12(2)	32(3)
C4	62(3)	67(4)	59(4)	21(3)	6(3)	32(3)
C8	65(3)	85(4)	52(3)	33(3)	27(3)	50(3)
C10	61(3)	56(3)	38(3)	17(3)	12(2)	28(3)
C23	75(4)	63(3)	50(3)	17(3)	19(3)	43(3)
C3	66(4)	83(5)	95(6)	26(4)	8(4)	42(4)
O2	73(3)	105(4)	61(3)	38(3)	16(2)	55(3)
C1	80(4)	90(5)	67(4)	28(4)	24(4)	43(4)
C37	62(3)	78(4)	49(3)	22(3)	20(3)	37(3)
C29	60(3)	54(3)	46(3)	12(3)	8(3)	23(3)
C2	79(4)	72(4)	82(5)	29(4)	-8(4)	34(4)
C31	77(4)	94(5)	56(4)	18(4)	20(3)	48(4)

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
C16	54(3)	50(3)	46(3)	15(2)	13(2)	30(3)
C12	114(6)	74(5)	45(4)	11(3)	10(4)	52(5)
C28	54(3)	52(3)	38(3)	14(2)	10(2)	24(3)
C20	75(4)	60(4)	83(5)	33(4)	8(4)	21(3)
C25	76(4)	93(5)	74(5)	53(4)	28(4)	46(4)
C32	62(4)	87(5)	71(5)	25(4)	25(4)	27(4)
C17	73(4)	56(3)	49(3)	15(3)	11(3)	39(3)
C38	60(3)	82(4)	58(4)	28(3)	24(3)	41(3)
C7	59(3)	83(4)	77(4)	47(4)	28(3)	41(3)
C24	96(5)	98(5)	55(4)	35(4)	33(4)	63(5)
C5	70(4)	97(5)	65(4)	35(4)	26(3)	58(4)
C11	71(4)	61(3)	46(3)	12(3)	10(3)	29(3)
C18	95(5)	90(5)	46(4)	23(4)	19(4)	58(5)
C30	90(5)	72(4)	42(3)	5(3)	14(3)	46(4)
C35	56(3)	63(3)	61(4)	28(3)	19(3)	28(3)
C34	47(3)	44(3)	45(3)	17(2)	12(2)	19(2)
C41	63(4)	48(3)	82(5)	22(3)	4(3)	19(3)
C36	58(3)	74(4)	44(3)	17(3)	15(2)	34(3)
C26	64(4)	57(4)	77(5)	30(4)	6(3)	24(3)
C6	57(3)	89(4)	59(3)	39(3)	23(3)	41(3)
C39	57(3)	59(3)	57(3)	15(3)	9(3)	28(3)
C21	76(4)	57(4)	57(4)	18(3)	0(3)	31(3)
C19	79(5)	97(6)	72(5)	50(5)	21(4)	39(4)
C15	66(4)	64(4)	61(4)	13(3)	17(3)	17(3)
C13	108(6)	117(7)	59(4)	30(5)	38(5)	74(6)
C40	80(4)	70(4)	64(4)	26(3)	22(4)	38(4)
C42	54(3)	76(4)	90(5)	30(4)	18(3)	35(3)
C14	75(5)	113(7)	79(5)	27(5)	37(4)	39(5)

Table S7. Bond Lengths for 3s

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S4	O5	1.442(4)	C8	C7	1.492(8)
S4	O6	1.431(4)	C10	C11	1.378(9)
S4	C22	1.766(5)	C10	C15	1.390(9)
S4	C34	1.852(6)	C23	C24	1.367(10)
S5	O8	1.432(5)	C1	C2	1.426(11)
S5	O7	1.427(5)	C37	C38	1.321(9)

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S5	C28	1.756(6)	C37	C36	1.306(8)
S5	C34	1.858(5)	C29	C28	1.378(8)
S2	O1	1.426(5)	C29	C30	1.376(9)
S2	C9	1.852(5)	C31	C32	1.366(11)
S2	C10	1.754(6)	C31	C30	1.372(11)
S2	O2	1.434(5)	C16	C17	1.385(8)
S3	C9	1.842(6)	C16	C21	1.405(9)
S3	O3	1.425(4)	C12	C11	1.394(10)
S3	O4	1.433(5)	C12	C13	1.353(13)
S3	C16	1.756(6)	C20	C21	1.399(10)
S6	C41	1.744(8)	C20	C19	1.374(13)
S6	C42	1.695(8)	C25	C24	1.394(12)
S1	C3	1.653(9)	C25	C26	1.368(12)
S1	C2	1.799(10)	C17	C18	1.372(10)
F1	C9	1.375(7)	C38	C39	1.460(9)
F2	C34	1.381(6)	C7	C6	1.291(9)
C9	C8	1.524(8)	C5	C6	1.309(10)
C27	C22	1.394(8)	C18	C19	1.379(12)
C27	C26	1.378(10)	C35	C34	1.520(8)
C33	C28	1.387(8)	C35	C36	1.506(9)
C33	C32	1.368(10)	C41	C40	1.400(10)
C22	C23	1.374(8)	C39	C40	1.428(10)
C4	C3	1.381(10)	C39	C42	1.354(9)
C4	C1	1.430(10)	C15	C14	1.374(11)
C4	C5	1.456(9)	C13	C14	1.366(13)

Table S8. Bond Angles for **3s**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O5	S4	C22	108.8(3)	C4	C3	S1	113.1(7)
O5	S4	C34	107.6(3)	C2	C1	C4	116.1(8)
O6	S4	O5	120.5(3)	C36	C37	C38	177.5(7)
O6	S4	C22	109.4(3)	C30	C29	C28	118.8(6)
O6	S4	C34	105.8(3)	C1	C2	S1	104.1(7)
C22	S4	C34	103.4(3)	C32	C31	C30	120.6(7)
O8	S5	C28	108.9(3)	C17	C16	S3	120.3(4)
O8	S5	C34	103.0(3)	C17	C16	C21	121.2(6)
O7	S5	O8	119.7(3)	C21	C16	S3	118.5(5)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O7	S5	C28	110.3(3)	C13	C12	C11	121.1(7)
O7	S5	C34	108.1(3)	C33	C28	S5	118.1(5)
C28	S5	C34	105.7(3)	C29	C28	S5	120.5(5)
O1	S2	C9	105.6(3)	C29	C28	C33	121.5(6)
O1	S2	C10	110.2(3)	C19	C20	C21	119.7(7)
O1	S2	O2	120.3(3)	C26	C25	C24	120.9(6)
C10	S2	C9	107.8(3)	C31	C32	C33	120.9(7)
O2	S2	C9	104.4(3)	C18	C17	C16	119.7(6)
O2	S2	C10	107.8(3)	C37	C38	C39	125.7(6)
O3	S3	C9	106.9(3)	C6	C7	C8	124.1(7)
O3	S3	O4	120.6(3)	C23	C24	C25	119.6(7)
O3	S3	C16	108.8(3)	C6	C5	C4	124.8(7)
O4	S3	C9	106.4(3)	C10	C11	C12	117.6(7)
O4	S3	C16	109.3(3)	C17	C18	C19	119.6(7)
C16	S3	C9	103.5(3)	C31	C30	C29	119.9(7)
C42	S6	C41	92.9(4)	C36	C35	C34	115.4(5)
C3	S1	C2	95.4(4)	S4	C34	S5	113.4(3)
S3	C9	S2	114.2(3)	F2	C34	S4	104.2(4)
F1	C9	S2	105.8(3)	F2	C34	S5	104.7(4)
F1	C9	S3	105.5(3)	F2	C34	C35	106.7(5)
F1	C9	C8	110.6(5)	C35	C34	S4	116.6(4)
C8	C9	S2	110.3(4)	C35	C34	S5	110.1(4)
C8	C9	S3	110.3(4)	C40	C41	S6	108.2(6)
C26	C27	C22	117.5(6)	C37	C36	C35	121.8(6)
C32	C33	C28	118.3(7)	C25	C26	C27	120.6(6)
C27	C22	S4	118.7(4)	C7	C6	C5	178.6(8)
C23	C22	S4	118.6(5)	C40	C39	C38	125.3(6)
C23	C22	C27	122.6(5)	C42	C39	C38	123.4(6)
C3	C4	C1	111.1(7)	C42	C39	C40	111.2(6)
C3	C4	C5	123.0(7)	C20	C21	C16	118.0(7)
C1	C4	C5	125.9(7)	C20	C19	C18	121.7(7)
C7	C8	C9	113.8(5)	C14	C15	C10	118.2(7)
C11	C10	S2	119.4(5)	C12	C13	C14	120.4(7)
C11	C10	C15	121.8(6)	C41	C40	C39	114.2(7)
C15	C10	S2	118.8(5)	C39	C42	S6	113.4(6)
C24	C23	C22	118.7(6)	C13	C14	C15	120.8(8)

Table S9. Hydrogen Atom Coordinates ($\text{\AA} \times 10^{-4}$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^{-3}$) for **3s**.

Atom	x	y	z	U(eq)
H27	8081.29	-712.96	8247.17	70
H33	10665.56	4398.48	6006.77	77
H8A	12564.55	6033.5	11137.91	70
H8B	13275.67	7560.89	10831.8	70
H23	9704.62	3367.98	10636.36	71
H3	17097.95	3494.05	11551.5	97
H1	14391.83	4765.3	13279.24	93
H29	6960.27	85.88	4671.19	68
H2	14676.97	3049.87	14303.1	97
H31	11017.09	1294.34	3653.42	89
H12	11950.01	10585.23	16242.65	94
H20	13030.61	11836.71	10226.13	93
H25	8027.44	-493.35	11474.21	87
H32	12086.44	3749.51	4835.26	92
H17	10193.05	6527.24	9236.08	68
H38	3768.5	4201.51	8883	75
H7	15678.27	8442.59	12385.54	79
H24	9225.78	2161.39	12007.06	88
H5	16345.17	5353.34	10924.66	82
H11	13299	9758.41	15065.83	74
H18	10844.38	7697.45	7860.95	86
H30	8496.5	-564.92	3604.09	82
H35A	5194.8	1374.2	7483.08	70
H35B	6106.81	1250.17	8544.92	70
H41	5701.1	6989.01	5825.23	83
H36	7561.75	4076.35	9255.91	69
H26	7535.6	-1906.29	9633.07	81
H21	12298.07	10686.93	11636.26	79
H19	12236.84	10330.6	8366.3	96
H15	9348.46	5567.91	13881.59	85
H13	9417.85	8930.2	16274.02	102
H40	6116.81	5324.04	6795.35	84
H42	2981.69	6067.24	8326.57	86
H14	8145.85	6420.07	15152.44	109

Data intensity of **3ac**^[11] was collected using a 'Bruker APEX-II CCD' diffractometer at 297.96(14) K. Data collection and reduction were done by using Olex2 and the structure was solved with the ShelXS structure solution program using direct methods and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for non-H atoms using SHELX-97. Hydrogen atoms were added at their geometrically ideal positions and refined isotropically. Crystal data for **3ac**: C₂₄H₂₀F₂O₄S₂, $T = 297.96(14)$ K, monoclinic, P2₁, $a = 9.1305(2)$ Å, $b = 10.80990(10)$ Å, $c = 23.0760(3)$ Å, $\alpha = 90^\circ$, $\beta = 97.4390(10)^\circ$, $\gamma = 90^\circ$, $V = 2258.43(6)$ Å³. $Z = 4$, $\rho_{\text{calc}} = 1.396$ g/cm³. 52769 reflections measured ($7.728^\circ \leq 2\theta \leq 134.096^\circ$), 8033 unique ($R_{\text{int}} = 0.0811$, $R_{\text{sigma}} = 0.0523$) which were used in all calculations. The final R_1 was 0.0359 ($I \geq 2\sigma(I)$) and wR_2 was 0.0968 (all data).

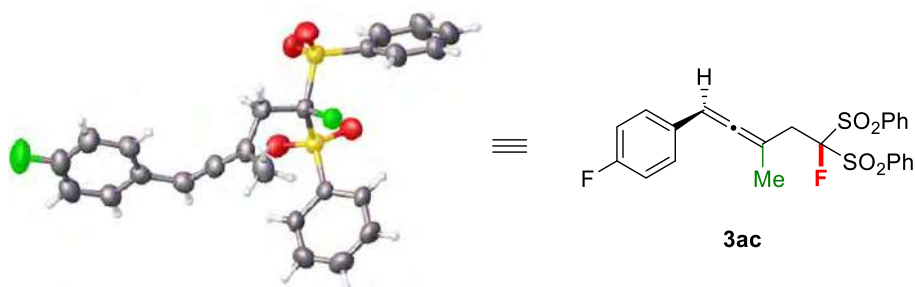


Table S10 Crystal data and structure refinement for 3ac.

Identification code	3ac
Empirical formula	C ₂₄ H ₂₀ F ₂ O ₄ S ₂
Formula weight	474.52
Temperature/K	297.96(14)
Crystal system	monoclinic
Space group	P2 ₁
$a/\text{\AA}$	9.1305(2)
$b/\text{\AA}$	10.80990(10)
$c/\text{\AA}$	23.0760(3)
$\alpha/^\circ$	90
$\beta/^\circ$	97.4390(10)
$\gamma/^\circ$	90
Volume/Å ³	2258.43(6)
Z	4
$\rho_{\text{calc}}/\text{g/cm}^3$	1.396
μ/mm^{-1}	2.537
$F(000)$	984.0

¹¹ Supplementary crystallographic data have been deposited at Cambridge Crystallographic Data Center (CCDC number: 2277305).

Crystal size/mm ³	0.42 × 0.36 × 0.26
Radiation	Cu K α (λ = 1.54184)
2 Θ range for data collection/°	7.728 to 134.096
Index ranges	-10 ≤ h ≤ 10, -12 ≤ k ≤ 12, -27 ≤ l ≤ 27
Reflections collected	52769
Independent reflections	8033 [R_{int} = 0.0811, R_{sigma} = 0.0523]
Data/restraints/parameters	8033/1/579
Goodness-of-fit on F^2	1.034
Final R indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0359, wR_2 = 0.0942
Final R indexes [all data]	R_1 = 0.0397, wR_2 = 0.0968
Largest diff. peak/hole / e Å ⁻³	0.28/-0.17
Flack parameter	0.009(9)

Table S11 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 3ac. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	x	y	z	$U(\text{eq})$
S1	2672.8(9)	7427.7(7)	-4327.2(3)	42.9(2)
S2	495.2(10)	6141.5(8)	-3624.4(3)	52.1(2)
F1	-3870(4)	5747(3)	-8079.0(13)	105.4(10)
F2	2641(2)	5078.4(16)	-4071.6(7)	50.0(4)
O1	1710(3)	8253(2)	-4680.5(11)	61.2(7)
O2	3294(3)	7787(2)	-3751.6(9)	59.4(7)
O3	-303(3)	7270(3)	-3719.3(11)	72.2(8)
O4	-291(3)	4996(3)	-3631.6(11)	72.9(8)
C1	-1682(4)	5573(3)	-6670.7(15)	56.5(9)
C2	-2769(5)	5316(4)	-7126.1(18)	64.6(10)
C3	-2818(5)	6015(4)	-7627.6(17)	66.8(11)
C4	-1841(5)	6942(4)	-7689.7(17)	69.9(11)
C5	-783(5)	7202(3)	-7224.4(14)	58.5(9)
C6	-678(4)	6519(3)	-6714.2(13)	46.3(8)
C7	526(4)	6785(3)	-6238.4(14)	51.7(8)
C8	878(4)	6099(3)	-5776.1(14)	50.5(8)
C9	1246(4)	5389(3)	-5324.6(13)	47.3(8)
C10	558(4)	5624(3)	-4771.4(13)	48.9(8)
C11	1618(3)	5997(3)	-4239.8(12)	41.3(7)
C12	4123(4)	6966(3)	-4708.5(14)	47.1(8)
C13	4091(4)	7279(4)	-5291.7(14)	61.0(10)
C14	5258(6)	6886(5)	-5582.0(19)	83.8(15)

Table S11 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 3ac. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	x	y	z	U(eq)
C15	6391(6)	6198(6)	-5288(2)	92.5(16)
C16	6425(5)	5915(5)	-4717(2)	80.3(13)
C17	5289(4)	6303(4)	-4418.0(18)	60.4(9)
C18	1708(4)	6223(4)	-2967.2(13)	51.9(8)
C19	2513(5)	5191(4)	-2761.9(15)	64.7(10)
C20	3390(5)	5284(5)	-2227.9(17)	74.8(12)
C21	3462(5)	6358(5)	-1912.1(17)	74.6(12)
C22	2645(5)	7358(4)	-2119.9(15)	68.6(11)
C23	1765(5)	7316(4)	-2652.9(15)	60.4(9)
C24	2244(5)	4297(4)	-5351.6(16)	64.3(10)
S3	2667.0(9)	4858.6(6)	599.5(3)	42.9(2)
S4	610.3(10)	3463.6(8)	1320.5(3)	49.4(2)
F3	-4525(3)	3210(3)	-2962.0(13)	107.4(10)
F4	2773(2)	2499.2(15)	848.4(7)	49.0(4)
O5	1681(3)	5619(2)	217.9(11)	60.0(6)
O6	3209(3)	5277(2)	1173.7(10)	59.3(6)
O7	-307(3)	4534(3)	1222.7(12)	66.7(8)
O8	-51(3)	2268(3)	1326.0(11)	68.7(7)
C25	-1886(5)	2908(3)	-1672.2(15)	57.2(9)
C26	-3077(5)	2656(4)	-2083.3(17)	67.2(10)
C27	-3352(5)	3452(4)	-2546.4(17)	70.7(11)
C28	-2522(5)	4469(4)	-2615.1(17)	71.0(12)
C29	-1344(5)	4718(4)	-2188.2(15)	58.3(9)
C30	-1004(4)	3933(3)	-1716.5(14)	48.7(8)
C31	292(5)	4198(3)	-1281.3(15)	54.6(9)
C32	786(4)	3488(3)	-840.2(14)	52.3(8)
C33	1265(4)	2789(3)	-397.1(14)	50.0(8)
C34	627(4)	2984(3)	169.7(14)	52.9(8)
C35	1699(3)	3385(3)	695.6(13)	41.9(7)
C36	4184(4)	4418(3)	249.7(13)	42.4(7)
C37	4162(4)	4609(4)	-345.4(14)	53.9(9)
C38	5333(5)	4198(5)	-608.6(17)	73.1(12)
C39	6508(5)	3585(5)	-286.4(19)	75.4(12)
C40	6524(4)	3413(4)	301.8(18)	68.1(10)
C41	5370(4)	3844(4)	573.9(15)	53.8(8)

Table S11 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 3ac. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	x	y	z	U(eq)
C42	1822(4)	3640(3)	1977.3(14)	48.1(8)
C43	2817(5)	2714(4)	2164.8(16)	60.4(10)
C44	3672(5)	2839(4)	2697.6(16)	67.1(11)
C45	3518(5)	3845(5)	3041.3(16)	69.7(11)
C46	2527(6)	4756(5)	2848.3(17)	77.2(13)
C47	1669(5)	4671(4)	2307.8(16)	64.0(10)
C48	2315(5)	1736(4)	-443.0(17)	67.9(11)

Table S12 Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 3ac. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S1	39.4(5)	47.2(4)	42.1(4)	-3.9(3)	5.1(3)	-2.1(3)
S2	41.7(5)	73.3(6)	41.6(4)	4.7(4)	6.8(3)	0.2(4)
F1	86(2)	133(2)	83.1(17)	-12.1(16)	-42.5(15)	-0.1(18)
F2	47.5(12)	53.2(10)	47.5(9)	4.5(8)	-0.8(8)	9.5(9)
O1	55.3(16)	52.4(13)	76.0(16)	14.8(12)	8.3(12)	10.0(12)
O2	60.7(17)	74.9(15)	42.7(12)	-18.7(11)	7.4(11)	-15.7(13)
O3	57.3(18)	101(2)	59.4(15)	6.1(14)	10.6(12)	29.1(16)
O4	66.4(19)	96(2)	57.5(14)	5.2(14)	12.0(13)	-32.6(16)
C1	63(3)	56(2)	50.5(19)	4.6(15)	7.2(17)	-7.4(18)
C2	53(2)	71(2)	68(2)	-2.5(19)	-0.7(19)	-8.6(19)
C3	55(3)	83(3)	57(2)	-7.8(19)	-14.0(18)	9(2)
C4	81(3)	75(3)	50(2)	10.9(18)	-5.0(19)	5(2)
C5	69(3)	58(2)	47.0(18)	6.7(15)	0.0(16)	-6.9(18)
C6	54(2)	47.1(17)	38.2(15)	0.4(12)	5.6(14)	2.1(14)
C7	59(2)	53.4(18)	41.3(17)	-2.7(14)	1.9(15)	-6.7(16)
C8	49(2)	59(2)	42.7(17)	-7.8(14)	2.3(14)	-2.4(16)
C9	48(2)	51.5(17)	40.1(16)	-5.9(13)	-3.0(14)	-7.7(15)
C10	40(2)	58.6(19)	45.6(17)	-0.8(14)	-2.6(14)	-9.0(15)
C11	36.4(18)	48.9(17)	38.1(14)	1.9(12)	3.0(12)	2.8(13)
C12	38(2)	56.2(18)	47.0(17)	-7.0(14)	4.3(14)	-8.7(15)
C13	55(2)	86(3)	43.1(17)	-2.4(17)	9.1(15)	-17(2)
C14	78(4)	123(4)	54(2)	-18(2)	23(2)	-24(3)
C15	61(3)	125(4)	98(4)	-37(3)	30(3)	-11(3)
C16	43(3)	95(3)	104(4)	-9(3)	14(2)	3(2)
C17	41(2)	77(2)	62(2)	-3.0(18)	3.8(17)	0.8(18)

Table S12 Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 3ac. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
C18	50(2)	70(2)	36.6(15)	4.4(15)	8.5(14)	-1.2(17)
C19	80(3)	69(2)	43.8(18)	7.0(16)	3.6(17)	6(2)
C20	81(3)	89(3)	53(2)	17(2)	2(2)	12(2)
C21	74(3)	106(3)	44(2)	3(2)	5.8(19)	-12(3)
C22	81(3)	84(3)	42.8(18)	-10.0(19)	14.7(18)	-12(2)
C23	64(3)	71(2)	49.4(18)	1.3(17)	18.7(17)	5(2)
C24	72(3)	62(2)	54(2)	-10.7(16)	-7.0(18)	10.3(19)
S3	40.1(5)	41.2(4)	46.6(4)	-2.7(3)	3.1(3)	-0.7(3)
S4	38.3(5)	63.8(5)	45.9(4)	3.5(3)	4.7(3)	1.8(4)
F3	87(2)	136(2)	87.5(18)	-16.6(17)	-33.1(15)	-0.1(18)
F4	47.3(11)	46.5(10)	52.0(10)	4.1(8)	2.1(8)	9.4(8)
O5	54.2(16)	49.4(13)	76.1(16)	13.0(11)	7.2(13)	11.1(11)
O6	63.6(17)	65.3(15)	49.4(13)	-19.1(11)	8.5(11)	-13.4(12)
O7	49.9(17)	90(2)	58.9(15)	1.2(13)	1.7(12)	25.8(14)
O8	63.4(19)	79.1(17)	64.8(15)	3.4(13)	13.5(13)	-24.5(15)
C25	64(3)	59(2)	49.3(18)	2.2(15)	8.4(17)	-1.8(17)
C26	61(3)	73(2)	65(2)	-7(2)	0.6(19)	-8(2)
C27	64(3)	88(3)	56(2)	-10(2)	-8.8(19)	8(2)
C28	79(3)	82(3)	51(2)	8.6(18)	2(2)	18(2)
C29	64(3)	57(2)	54.0(19)	7.1(16)	8.7(17)	2.8(18)
C30	55(2)	50.1(17)	42.3(16)	-1.1(13)	10.4(15)	4.3(15)
C31	60(2)	53.1(19)	51.2(19)	-1.5(15)	9.8(17)	0.4(17)
C32	52(2)	53.6(19)	49.7(18)	-9.6(15)	1.1(15)	-4.7(16)
C33	52(2)	48.0(17)	46.7(17)	-7.2(14)	-6.3(15)	-5.5(15)
C34	47(2)	62(2)	47.5(18)	-4.9(14)	-1.6(15)	-12.4(16)
C35	35.8(18)	44.5(15)	44.3(15)	0.9(13)	1.0(12)	3.8(13)
C36	36.8(19)	49.3(16)	40.0(16)	-3.0(12)	1.2(13)	-5.8(14)
C37	43(2)	75(2)	42.2(16)	5.7(15)	-2.8(14)	-1.5(17)
C38	66(3)	112(4)	42.4(19)	-2(2)	10.9(18)	-2(3)
C39	50(3)	106(4)	72(3)	-16(2)	18(2)	1(2)
C40	38(2)	91(3)	74(3)	7(2)	3.5(18)	5(2)
C41	39(2)	72(2)	48.5(18)	5.4(15)	-1.5(15)	-2.8(17)
C42	44(2)	60(2)	40.5(16)	5.4(13)	7.1(14)	4.3(15)
C43	66(3)	66(2)	48.9(18)	3.3(16)	3.5(17)	13.8(19)
C44	62(3)	83(3)	55(2)	13.1(19)	1.1(18)	16(2)

Table S12 Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 3ac. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C45	63(3)	104(3)	40.9(18)	3.0(19)	3.8(17)	9(2)
C46	89(3)	91(3)	50(2)	-19(2)	6(2)	13(3)
C47	68(3)	73(2)	51.0(19)	-1.8(17)	8.0(18)	20(2)
C48	80(3)	60(2)	60(2)	-13.8(17)	-6.1(19)	9(2)

Table S13 Bond Lengths for 3ac.

Atom	Atom	Length/ $\text{\AA}$	Atom	Atom	Length/ $\text{\AA}$
S1	O1	1.431(2)	S3	O5	1.434(2)
S1	O2	1.429(2)	S3	O6	1.427(2)
S1	C11	1.847(3)	S3	C35	1.849(3)
S1	C12	1.755(3)	S3	C36	1.757(3)
S2	O3	1.424(3)	S4	O7	1.429(3)
S2	O4	1.430(3)	S4	O8	1.428(3)
S2	C11	1.862(3)	S4	C35	1.857(3)
S2	C18	1.761(3)	S4	C42	1.767(3)
F1	C3	1.354(4)	F3	C27	1.367(5)
F2	C11	1.384(3)	F4	C35	1.383(3)
C1	C2	1.377(5)	C25	C26	1.374(5)
C1	C6	1.386(5)	C25	C30	1.382(5)
C2	C3	1.377(6)	C26	C27	1.369(6)
C3	C4	1.361(6)	C27	C28	1.357(6)
C4	C5	1.377(5)	C28	C29	1.387(6)
C5	C6	1.382(4)	C29	C30	1.383(5)
C6	C7	1.477(5)	C30	C31	1.478(5)
C7	C8	1.305(5)	C31	C32	1.307(5)
C8	C9	1.302(5)	C32	C33	1.301(5)
C9	C10	1.515(5)	C33	C34	1.514(5)
C9	C24	1.498(5)	C33	C48	1.501(5)
C10	C11	1.516(4)	C34	C35	1.520(4)
C12	C13	1.384(5)	C36	C37	1.386(4)
C12	C17	1.383(5)	C36	C41	1.382(5)
C13	C14	1.396(6)	C37	C38	1.370(6)
C14	C15	1.379(7)	C38	C39	1.392(6)
C15	C16	1.349(7)	C39	C40	1.368(6)
C16	C17	1.384(6)	C40	C41	1.376(5)

Table S13 Bond Lengths for 3ac.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C18	C19	1.385(5)	C42	C43	1.383(5)
C18	C23	1.385(5)	C42	C47	1.367(5)
C19	C20	1.383(6)	C43	C44	1.375(5)
C20	C21	1.368(7)	C44	C45	1.364(6)
C21	C22	1.364(7)	C45	C46	1.372(6)
C22	C23	1.380(5)	C46	C47	1.388(6)

Table S14 Bond Angles for 3ac.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	S1	C11	107.07(15)	O5	S3	C35	107.21(14)
O1	S1	C12	109.86(16)	O5	S3	C36	110.06(15)
O2	S1	O1	120.04(17)	O6	S3	O5	120.21(16)
O2	S1	C11	106.03(14)	O6	S3	C35	105.98(14)
O2	S1	C12	108.00(15)	O6	S3	C36	108.28(15)
C12	S1	C11	104.75(15)	C36	S3	C35	103.80(14)
O3	S2	O4	119.61(18)	O7	S4	C35	106.05(15)
O3	S2	C11	106.03(15)	O7	S4	C42	109.70(17)
O3	S2	C18	110.01(18)	O8	S4	O7	119.61(18)
O4	S2	C11	104.09(16)	O8	S4	C35	103.60(16)
O4	S2	C18	108.17(17)	O8	S4	C42	108.00(16)
C18	S2	C11	108.30(15)	C42	S4	C35	109.41(15)
C2	C1	C6	120.8(3)	C26	C25	C30	121.6(4)
C1	C2	C3	118.2(4)	C27	C26	C25	117.6(4)
F1	C3	C2	118.2(4)	F3	C27	C26	118.4(4)
F1	C3	C4	119.0(4)	C28	C27	F3	118.2(4)
C4	C3	C2	122.8(4)	C28	C27	C26	123.5(4)
C3	C4	C5	118.1(4)	C27	C28	C29	117.9(4)
C4	C5	C6	121.3(4)	C30	C29	C28	120.9(4)
C1	C6	C7	121.7(3)	C25	C30	C29	118.5(3)
C5	C6	C1	118.8(3)	C25	C30	C31	121.9(3)
C5	C6	C7	119.5(3)	C29	C30	C31	119.6(3)
C8	C7	C6	125.3(3)	C32	C31	C30	125.5(4)
C9	C8	C7	178.3(4)	C33	C32	C31	179.2(4)
C8	C9	C10	118.9(3)	C32	C33	C34	118.1(3)
C8	C9	C24	121.8(3)	C32	C33	C48	122.6(3)
C24	C9	C10	119.2(3)	C48	C33	C34	119.2(3)

Table S14 Bond Angles for 3ac.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C9	C10	C11	115.8(3)	C33	C34	C35	116.7(3)
S1	C11	S2	111.05(16)	S3	C35	S4	111.46(16)
F2	C11	S1	106.8(2)	F4	C35	S3	107.0(2)
F2	C11	S2	105.34(18)	F4	C35	S4	105.49(19)
F2	C11	C10	111.9(3)	F4	C35	C34	111.6(3)
C10	C11	S1	114.9(2)	C34	C35	S3	114.7(2)
C10	C11	S2	106.4(2)	C34	C35	S4	106.2(2)
C13	C12	S1	119.7(3)	C37	C36	S3	120.2(3)
C17	C12	S1	119.2(3)	C41	C36	S3	118.9(2)
C17	C12	C13	121.1(3)	C41	C36	C37	120.9(3)
C12	C13	C14	118.1(4)	C38	C37	C36	118.6(4)
C15	C14	C13	119.9(4)	C37	C38	C39	120.6(4)
C16	C15	C14	121.6(4)	C40	C39	C38	120.2(4)
C15	C16	C17	119.6(5)	C39	C40	C41	119.8(4)
C12	C17	C16	119.7(4)	C40	C41	C36	119.9(3)
C19	C18	S2	120.1(3)	C43	C42	S4	120.2(3)
C23	C18	S2	118.1(3)	C47	C42	S4	117.9(3)
C23	C18	C19	121.8(3)	C47	C42	C43	121.7(3)
C20	C19	C18	117.8(4)	C44	C43	C42	118.8(4)
C21	C20	C19	121.2(4)	C45	C44	C43	120.6(4)
C22	C21	C20	119.9(4)	C44	C45	C46	119.8(4)
C21	C22	C23	121.1(4)	C45	C46	C47	121.1(4)
C22	C23	C18	118.2(4)	C42	C47	C46	118.0(4)

Table S15 Torsion Angles for 3ac.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
S1	C12	C13	C14	-179.5(3)	S3	C36	C37	C38	-176.8(3)
S1	C12	C17	C16	178.9(3)	S3	C36	C41	C40	175.5(3)
S2	C18	C19	C20	-176.6(3)	S4	C42	C43	C44	-175.4(3)
S2	C18	C23	C22	176.0(3)	S4	C42	C47	C46	174.3(3)
F1	C3	C4	C5	179.8(4)	F3	C27	C28	C29	179.2(4)
O1	S1	C11	S2	-84.74(19)	O5	S3	C35	S4	-89.07(18)
O1	S1	C11	F2	160.91(18)	O5	S3	C35	F4	156.06(19)
O1	S1	C11	C10	36.1(3)	O5	S3	C35	C34	31.7(3)
O1	S1	C12	C13	-8.2(3)	O5	S3	C36	C37	-12.0(3)
O1	S1	C12	C17	171.2(3)	O5	S3	C36	C41	170.1(3)

Table S15 Torsion Angles for 3ac.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O2	S1	C11	S2	44.5(2)	O6	S3	C35	S4	40.5(2)
O2	S1	C11	F2	-69.8(2)	O6	S3	C35	F4	-74.4(2)
O2	S1	C11	C10	165.4(2)	O6	S3	C35	C34	161.2(2)
O2	S1	C12	C13	-140.8(3)	O6	S3	C36	C37	-145.2(3)
O2	S1	C12	C17	38.6(3)	O6	S3	C36	C41	36.9(3)
O3	S2	C11	S1	50.5(2)	O7	S4	C35	S3	53.0(2)
O3	S2	C11	F2	165.8(2)	O7	S4	C35	F4	168.8(2)
O3	S2	C11	C10	-75.2(3)	O7	S4	C35	C34	-72.6(2)
O3	S2	C18	C19	174.8(3)	O7	S4	C42	C43	179.7(3)
O3	S2	C18	C23	-1.8(3)	O7	S4	C42	C47	4.2(4)
O4	S2	C11	S1	177.57(17)	O8	S4	C35	S3	179.79(17)
O4	S2	C11	F2	-67.2(2)	O8	S4	C35	F4	-64.4(2)
O4	S2	C11	C10	51.8(3)	O8	S4	C35	C34	54.2(2)
O4	S2	C18	C19	42.5(4)	O8	S4	C42	C43	47.8(3)
O4	S2	C18	C23	-134.1(3)	O8	S4	C42	C47	-127.7(3)
C1	C2	C3	F1	178.9(4)	C25	C26	C27	F3	179.5(4)
C1	C2	C3	C4	0.0(7)	C25	C26	C27	C28	-0.6(7)
C1	C6	C7	C8	8.7(6)	C25	C30	C31	C32	3.9(6)
C2	C1	C6	C5	-0.1(6)	C26	C25	C30	C29	0.2(6)
C2	C1	C6	C7	-178.0(4)	C26	C25	C30	C31	-179.0(4)
C2	C3	C4	C5	-1.4(7)	C26	C27	C28	C29	-0.8(7)
C3	C4	C5	C6	2.1(6)	C27	C28	C29	C30	1.8(6)
C4	C5	C6	C1	-1.4(6)	C28	C29	C30	C25	-1.5(6)
C4	C5	C6	C7	176.6(4)	C28	C29	C30	C31	177.6(4)
C5	C6	C7	C8	-169.2(4)	C29	C30	C31	C32	-175.2(4)
C6	C1	C2	C3	0.8(6)	C30	C25	C26	C27	0.9(6)
C8	C9	C10	C11	-116.5(4)	C32	C33	C34	C35	-117.7(4)
C9	C10	C11	S1	59.5(4)	C33	C34	C35	S3	59.3(4)
C9	C10	C11	S2	-177.1(2)	C33	C34	C35	S4	-177.2(2)
C9	C10	C11	F2	-62.6(4)	C33	C34	C35	F4	-62.7(4)
C11	S1	C12	C13	106.5(3)	C35	S3	C36	C37	102.5(3)
C11	S1	C12	C17	-74.1(3)	C35	S3	C36	C41	-75.5(3)
C11	S2	C18	C19	-69.8(3)	C35	S4	C42	C43	-64.3(3)
C11	S2	C18	C23	113.7(3)	C35	S4	C42	C47	120.2(3)
C12	S1	C11	S2	158.62(16)	C36	S3	C35	S4	154.45(16)

Table S15 Torsion Angles for 3ac.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C12	S1	C11	F2	44.3(2)	C36	S3	C35	F4	39.6(2)
C12	S1	C11	C10	-80.5(3)	C36	S3	C35	C34	-84.8(3)
C12	C13	C14	C15	0.6(7)	C36	C37	C38	C39	1.0(7)
C13	C12	C17	C16	-1.7(6)	C37	C36	C41	C40	-2.4(5)
C13	C14	C15	C16	-1.7(8)	C37	C38	C39	C40	-1.7(7)
C14	C15	C16	C17	1.1(8)	C38	C39	C40	C41	0.3(7)
C15	C16	C17	C12	0.6(7)	C39	C40	C41	C36	1.8(6)
C17	C12	C13	C14	1.1(6)	C41	C36	C37	C38	1.0(6)
C18	S2	C11	S1	-67.5(2)	C42	S4	C35	S3	-65.2(2)
C18	S2	C11	F2	47.8(2)	C42	S4	C35	F4	50.6(2)
C18	S2	C11	C10	166.7(2)	C42	S4	C35	C34	169.2(2)
C18	C19	C20	C21	0.0(7)	C42	C43	C44	C45	1.5(6)
C19	C18	C23	C22	-0.5(6)	C43	C42	C47	C46	-1.2(6)
C19	C20	C21	C22	0.8(7)	C43	C44	C45	C46	-1.6(7)
C20	C21	C22	C23	-1.5(7)	C44	C45	C46	C47	0.3(7)
C21	C22	C23	C18	1.3(6)	C45	C46	C47	C42	1.1(7)
C23	C18	C19	C20	-0.2(6)	C47	C42	C43	C44	-0.1(6)
C24	C9	C10	C11	67.7(4)	C48	C33	C34	C35	67.5(4)

Table S16 Hydrogen Atom Coordinates ($\text{\AA} \times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 3ac.

Atom	x	y	z	U(eq)
H1	-1621.97	5106.55	-6329.83	68
H2	-3451.19	4688.39	-7095.99	78
H4	-1886.95	7386.53	-8036.47	84
H5	-126.16	7849.42	-7254.04	70
H7	1076.97	7499.41	-6271.07	62
H10A	46.12	4878.91	-4676.93	59
H10B	-177.3	6270.9	-4850.53	59
H13	3314.49	7736.82	-5484.53	73
H14	5270.73	7088.67	-5973.06	101
H15	7150.14	5923.42	-5488.35	111
H16	7208.6	5461.65	-4525.8	96
H17	5309.27	6117.92	-4023.44	72
H19	2465.32	4459.49	-2975.88	78
H20	3940.21	4603.23	-2080.85	90

Table S16 Hydrogen Atom Coordinates ($\text{\AA} \times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for 3ac.

Atom	x	y	z	U(eq)
H21	4066.7	6406.93	-1556.17	89
H22	2682.1	8078.81	-1898.78	82
H23	1224.17	8004.57	-2797.04	72
H24A	2427.15	4170.34	-5747.77	96
H24B	1783.32	3573.23	-5215.53	96
H24C	3162.94	4446.21	-5108.84	96
H25	-1669.3	2374.76	-1356.42	69
H26	-3674.03	1970.63	-2048.18	81
H28	-2735.67	4983.32	-2938.11	85
H29	-775.77	5423.07	-2219.52	70
H31	799.82	4931.29	-1324.85	66
H34A	165.32	2217.42	268.2	64
H34B	-145.27	3602.85	102.43	64
H37	3368.57	5007.32	-561.51	65
H38	5342.61	4330.35	-1006.27	88
H39	7285.44	3291.53	-471.46	90
H40	7312.07	3005.85	516.9	82
H41	5388.93	3748.61	975.38	65
H43	2905.52	2018.81	1934.59	73
H44	4361.09	2232.49	2824.71	81
H45	4082.49	3913.05	3405.33	84
H46	2429.8	5441.86	3083.53	93
H47	1009.83	5295.45	2174.45	77
H48A	2477.44	1634.9	-843.06	102
H48B	1902.63	988.97	-307.62	102
H48C	3237.89	1909.78	-207.51	102

Data intensity of **7**^[12] was collected using a 'Bruker APEX-II CCD' diffractometer at 297.75(10) K. Data collection and reduction were done by using Olex2 and the structure was solved with the ShelXS structure solution program using direct methods and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for non-H atoms using SHELX-97. Hydrogen atoms were added at their geometrically ideal positions and refined isotropically. Crystal data for **7**: C₁₃H₁₅FO₂, $T = 297.75(10)$ K, monoclinic, $P2_1$, $a = 5.7657(2)$ Å, $b = 8.4827(4)$ Å, $c = 12.1582(5)$ Å, $\alpha = 90^\circ$, $\beta = 99.606(4)^\circ$, $\gamma = 90^\circ$, $V = 586.30(4)$ Å³. $Z = 2$, $\rho_{\text{calc}} = 1.259$ g/cm³. 10142 reflections collected, 1977 [$R_{\text{int}} = 0.0642$, $R_{\text{sigma}} = 0.0404$] independent reflections, $R_1 = 0.0387$, $wR_2 = 0.1043$ ($I \geq 2\sigma(I)$), $R_1 = 0.0419$, $wR_2 = 0.1069$ (all data), GOF = 1.128, and 0.0(2) parameters.



Table S17. Crystal data and structure refinement for **7**.

Identification code	7
Empirical formula	C ₁₃ H ₁₅ FO ₂
Formula weight	222.25
Temperature/K	297.75(10)
Crystal system	monoclinic
Space group	$P2_1$
$a/\text{\AA}$	5.7657(2)
$b/\text{\AA}$	8.4827(4)
$c/\text{\AA}$	12.1582(5)
$\alpha/^\circ$	90
$\beta/^\circ$	99.606(4)
$\gamma/^\circ$	90
Volume/Å ³	586.30(4)
Z	2
$\rho_{\text{calc}}/\text{g/cm}^3$	1.259
μ/mm^{-1}	0.779

¹² Supplementary crystallographic data have been deposited at Cambridge Crystallographic Data Center (CCDC number: 2275110).

F(000)	236.0
Crystal size/mm ³	0.33 × 0.26 × 0.22
Radiation	CuKα (λ = 1.54184)
2θ range for data collection/°	7.374 to 134.132
Index ranges	-6 ≤ h ≤ 6, -10 ≤ k ≤ 9, -14 ≤ l ≤ 14
Reflections collected	10142
Independent reflections	1977 [R _{int} = 0.0642, R _{sigma} = 0.0404]
Data/restraints/parameters	1977/1/146
Goodness-of-fit on F ²	1.128
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0387, wR ₂ = 0.1043
Final R indexes [all data]	R ₁ = 0.0419, wR ₂ = 0.1069
Largest diff. peak/hole / e Å ⁻³	0.11/-0.13
Flack parameter	0.0(2)

Table S18. Fractional atomic coordinates (×10⁴) and equivalent isotropic displacement parameters (Å²×10³) for **7**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U(eq)
F1	-5714(3)	-6181(2)	-8837.6(13)	52.0(5)
O1	-7721(4)	-3285(3)	-9448.6(19)	57.9(6)
O2	-1270(4)	-5485(3)	-9449.0(18)	58.8(6)
C1	-10226(6)	-6583(5)	-3874(3)	58.6(9)
C2	-10592(6)	-5990(5)	-2853(3)	68.0(10)
C3	-9044(7)	-4938(5)	-2284(3)	69.9(10)
C4	-7129(7)	-4452(5)	-2728(3)	65.8(9)
C5	-6770(6)	-5006(4)	-3747(3)	56.1(8)
C6	-8300(5)	-6091(4)	-4334(2)	48.8(7)
C7	-7876(7)	-6744(5)	-5410(3)	60.6(9)
C8	-6299(6)	-6199(5)	-5968(2)	60.9(8)
C9	-4708(6)	-5622(5)	-6483(3)	62.0(9)
C10	-5126(5)	-4356(4)	-7352(2)	50.8(7)
C11	-4484(5)	-4783(3)	-8475(2)	42.2(6)
C12	-5261(5)	-3544(4)	-9350(3)	52.9(7)
C13	-1879(5)	-5136(4)	-8390(3)	53.3(8)

Table S19. Anisotropic Displacement Parameters (Å²×10⁻³) for **7**. The Anisotropic displacement factor exponent takes the form: -2π²[h²a²U₁₁+2hka*b*U₁₂+...].

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
F1	51.5(10)	49.8(11)	55.6(9)	-6.6(8)	11.9(7)	-8.8(8)
O1	45.3(12)	62.0(17)	66.9(14)	16.4(11)	10.6(9)	3.9(10)
O2	43.8(11)	70.9(16)	66.0(13)	-16.7(11)	22.3(9)	-12.6(10)
C1	52.5(18)	63(2)	58.6(19)	9.6(16)	3.8(14)	-9.7(15)
C2	64(2)	79(3)	65(2)	13(2)	23.9(16)	-2.6(19)
C3	93(3)	67(3)	54.1(19)	2.0(17)	24.0(18)	0(2)
C4	75(2)	66(3)	55.6(18)	-2.5(17)	8.5(16)	-14.7(19)
C5	53.5(18)	60(2)	55.3(18)	3.8(15)	10.1(14)	-7.5(15)
C6	49.4(16)	50.6(19)	45.2(14)	9.3(13)	4.4(12)	3.1(13)
C7	76(2)	56(2)	49.4(18)	2.8(15)	9.9(15)	-2.7(17)
C8	75(2)	63(2)	45.3(16)	3.2(16)	12.1(14)	13.2(18)
C9	60.2(19)	81(3)	45.3(16)	5.4(16)	10.8(13)	20.6(18)
C10	47.6(15)	60(2)	45.0(15)	-5.1(14)	6.7(12)	2.5(14)
C11	38.0(14)	43.9(17)	44.7(14)	-3.0(12)	7.2(10)	-7.9(11)
C12	45.8(16)	55(2)	58.7(17)	10.7(15)	12.3(13)	-2.7(14)
C13	42.0(16)	66(2)	52.3(16)	-3.3(15)	10.6(12)	1.0(14)

Table S20. Bond Lengths for 7

Atom	Atom	Length/Å	Atom	Atom	Length/Å
F1	C11	1.413(3)	C5	C6	1.388(5)
O1	C12	1.421(4)	C6	C7	1.478(4)
O2	C13	1.421(4)	C7	C8	1.306(5)
C1	C2	1.387(5)	C8	C9	1.291(5)
C1	C6	1.389(4)	C9	C10	1.497(5)
C2	C3	1.366(6)	C10	C11	1.517(4)
C3	C4	1.370(5)	C11	C12	1.510(4)
C4	C5	1.373(5)	C11	C13	1.518(4)

Table S21. Bond Angles for 7.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	C1	C6	120.2(3)	C8	C9	C10	124.8(3)
C3	C2	C1	120.4(3)	C9	C10	C11	115.4(3)
C2	C3	C4	119.9(4)	F1	C11	C10	107.2(2)
C3	C4	C5	120.3(4)	F1	C11	C12	106.8(2)
C4	C5	C6	120.9(3)	F1	C11	C13	107.2(2)
C1	C6	C7	120.4(3)	C10	C11	C13	111.9(2)
C5	C6	C1	118.3(3)	C12	C11	C10	112.3(3)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C5	C6	C7	121.3(3)	C12	C11	C13	111.0(2)
C8	C7	C6	124.0(4)	O1	C12	C11	110.0(2)
C9	C8	C7	177.5(4)	O2	C13	C11	111.8(2)

Table S22. Hydrogen Atom Coordinates ($\text{\AA} \times 10^{-4}$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^{-3}$) for **7**.

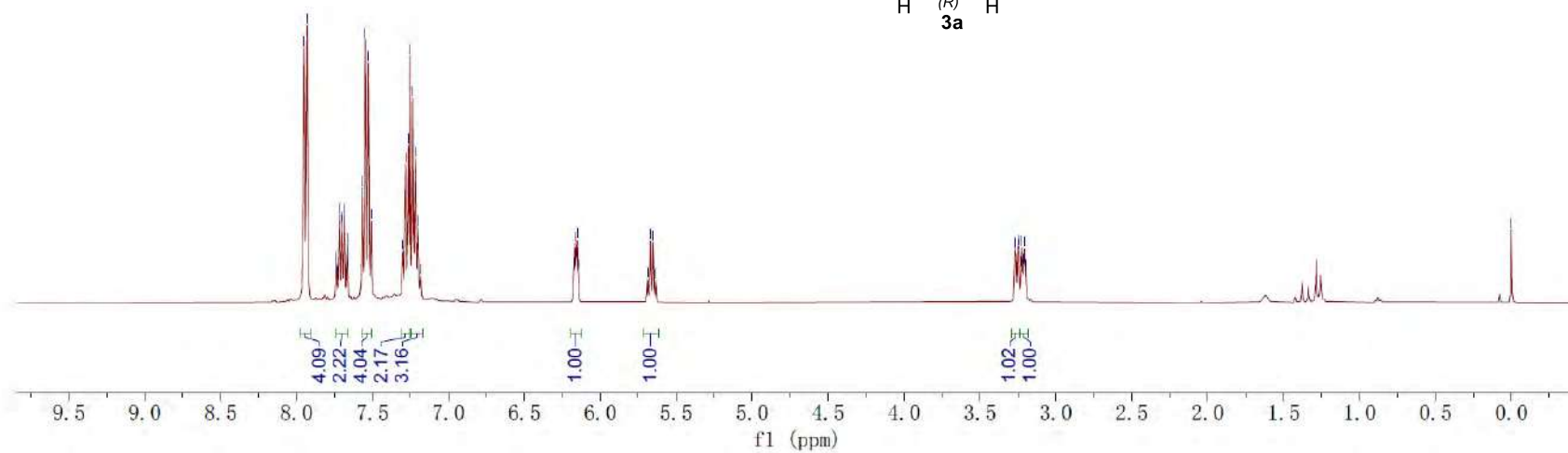
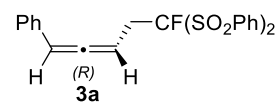
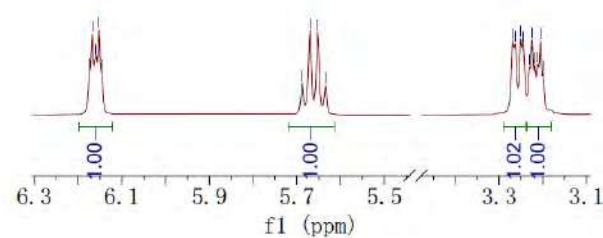
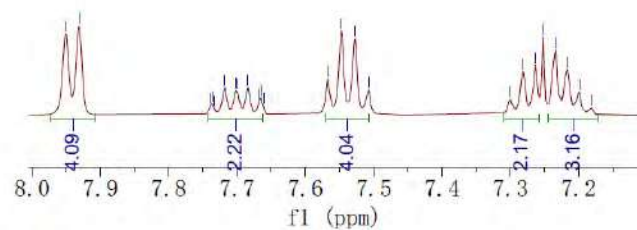
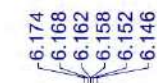
Atom	x	y	z	U(eq)
H1	-8076.85	-2470.63	-9799.53	87
H2	61.83	-4881.73	-9548.72	71
H1A	-11272.87	-7312.61	-4250.5	70
H2A	-11899.26	-6311.31	-2554.96	82
H3	-9289.52	-4551.26	-1597.01	84
H4	-6067.46	-3744.07	-2335.95	79
H5	-5484.67	-4648.53	-4047.32	67
H7	-8788.35	-7594.47	-5708.22	73
H9	-3189.96	-6021.12	-6301.53	74
H10A	-4229.04	-3431.82	-7069.37	61
H10B	-6777.7	-4070.19	-7462.71	61
H12A	-4423.93	-2567.72	-9144.97	63
H12B	-4890.92	-3887.09	-10062.26	63
H13B	-1470.86	-6025.8	-7894.72	64

9. NMR spectra

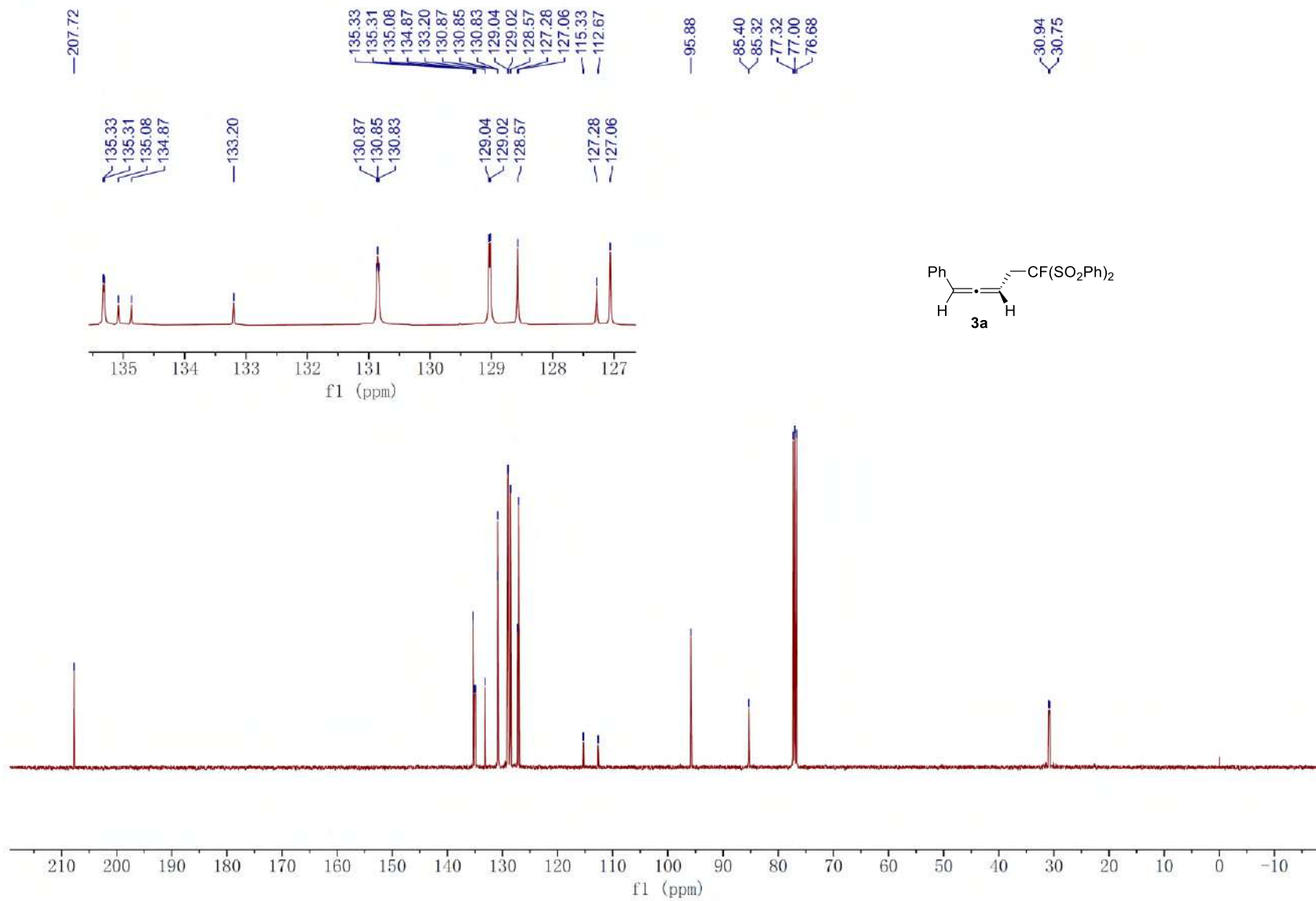
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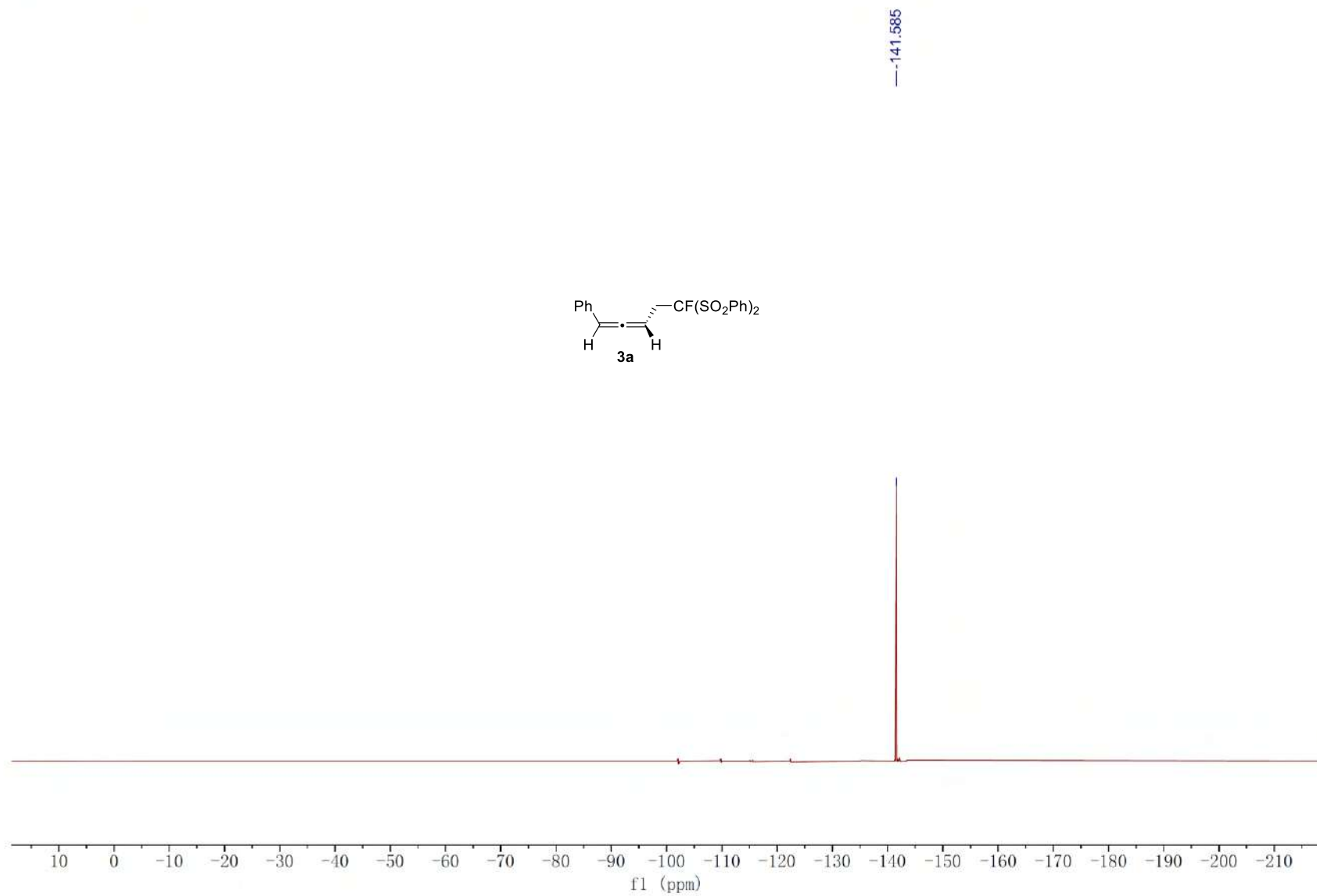
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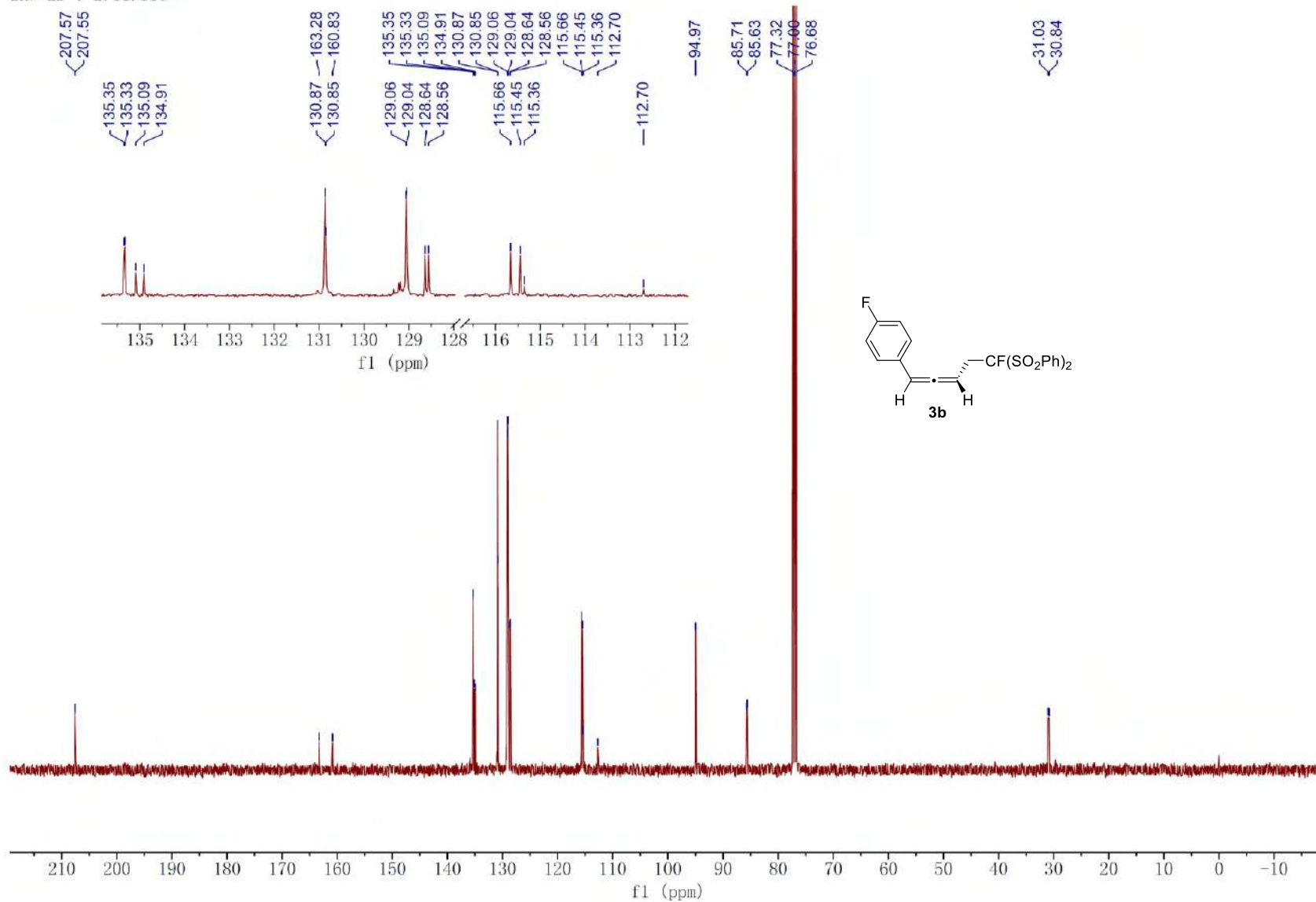
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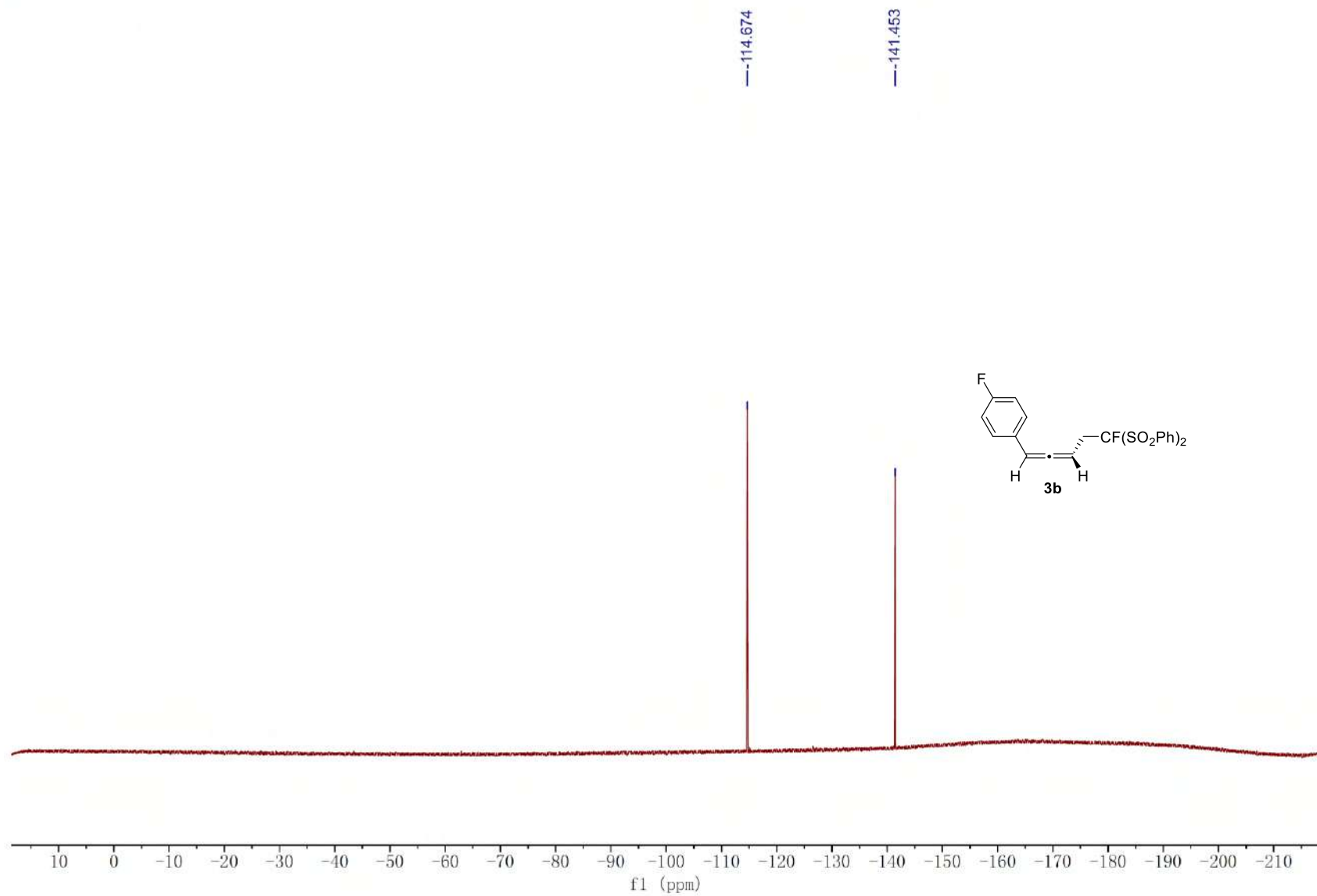
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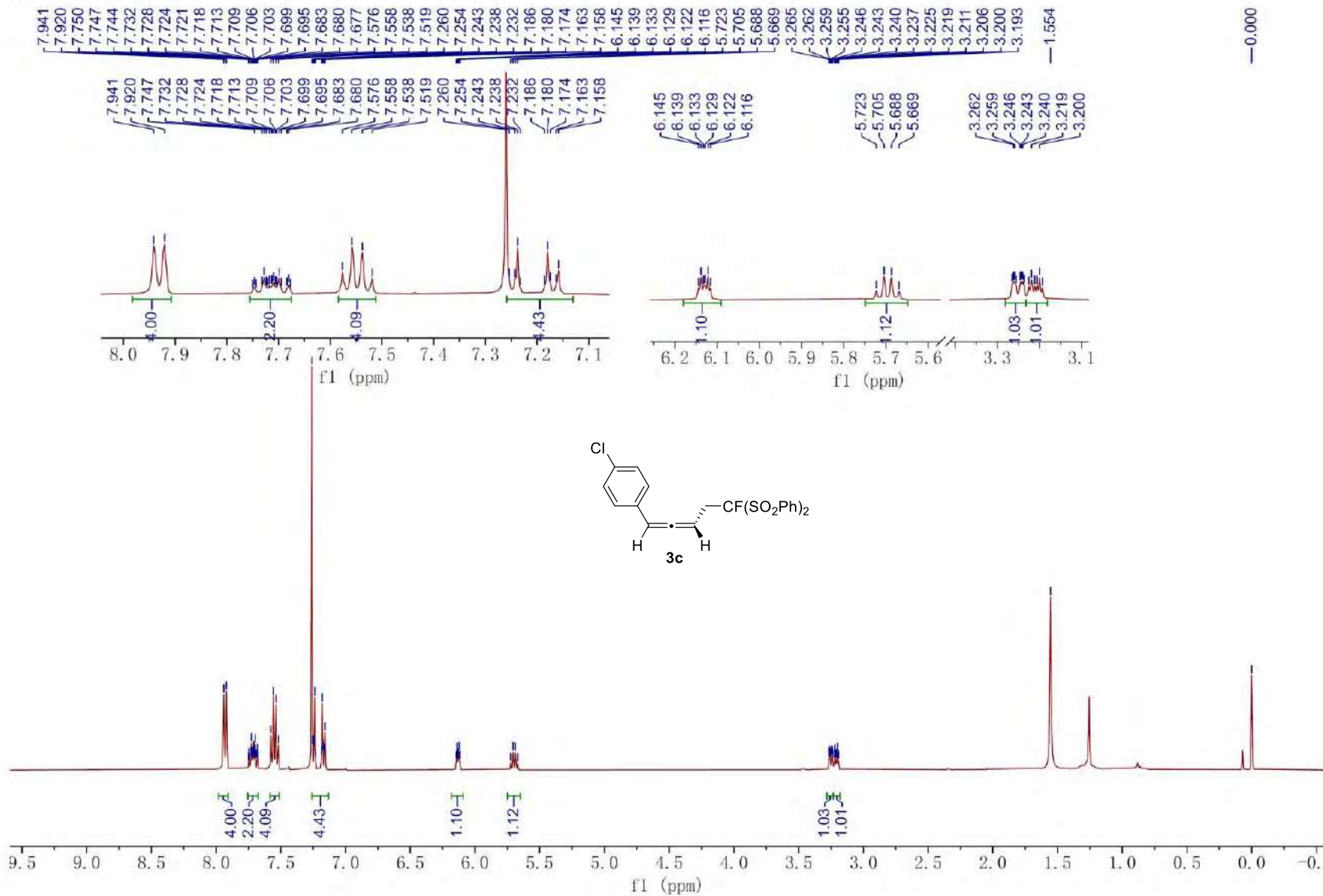
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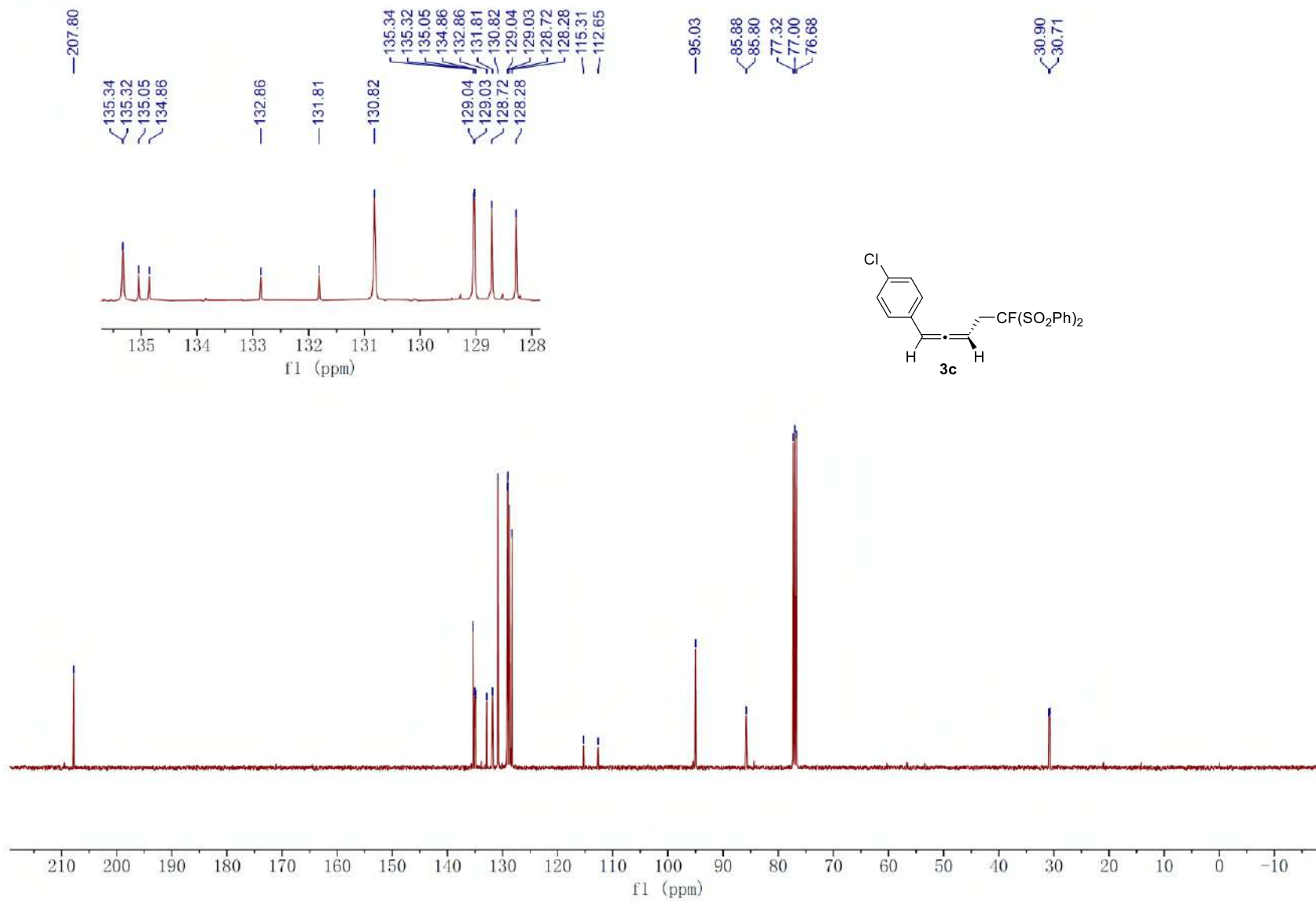
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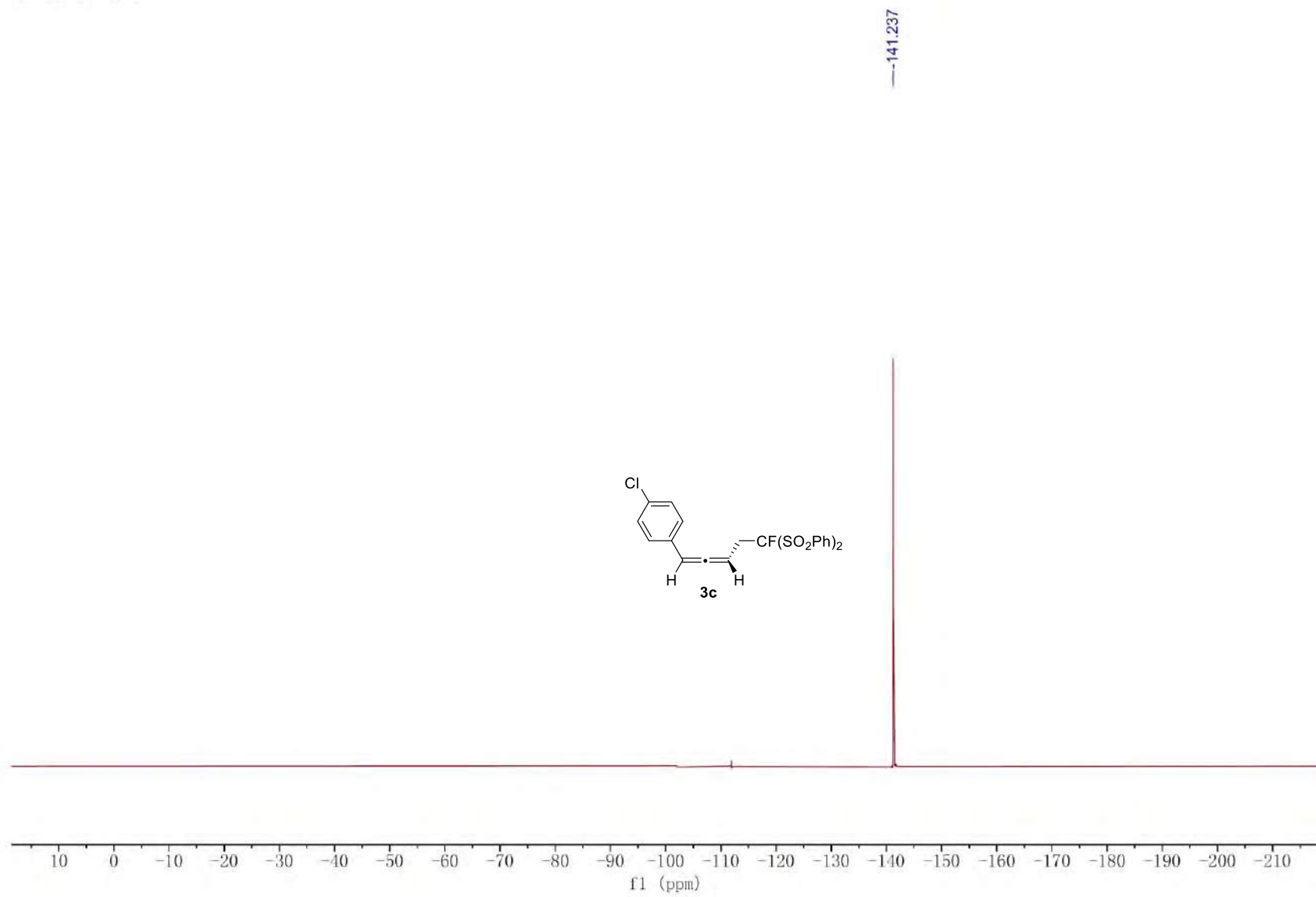
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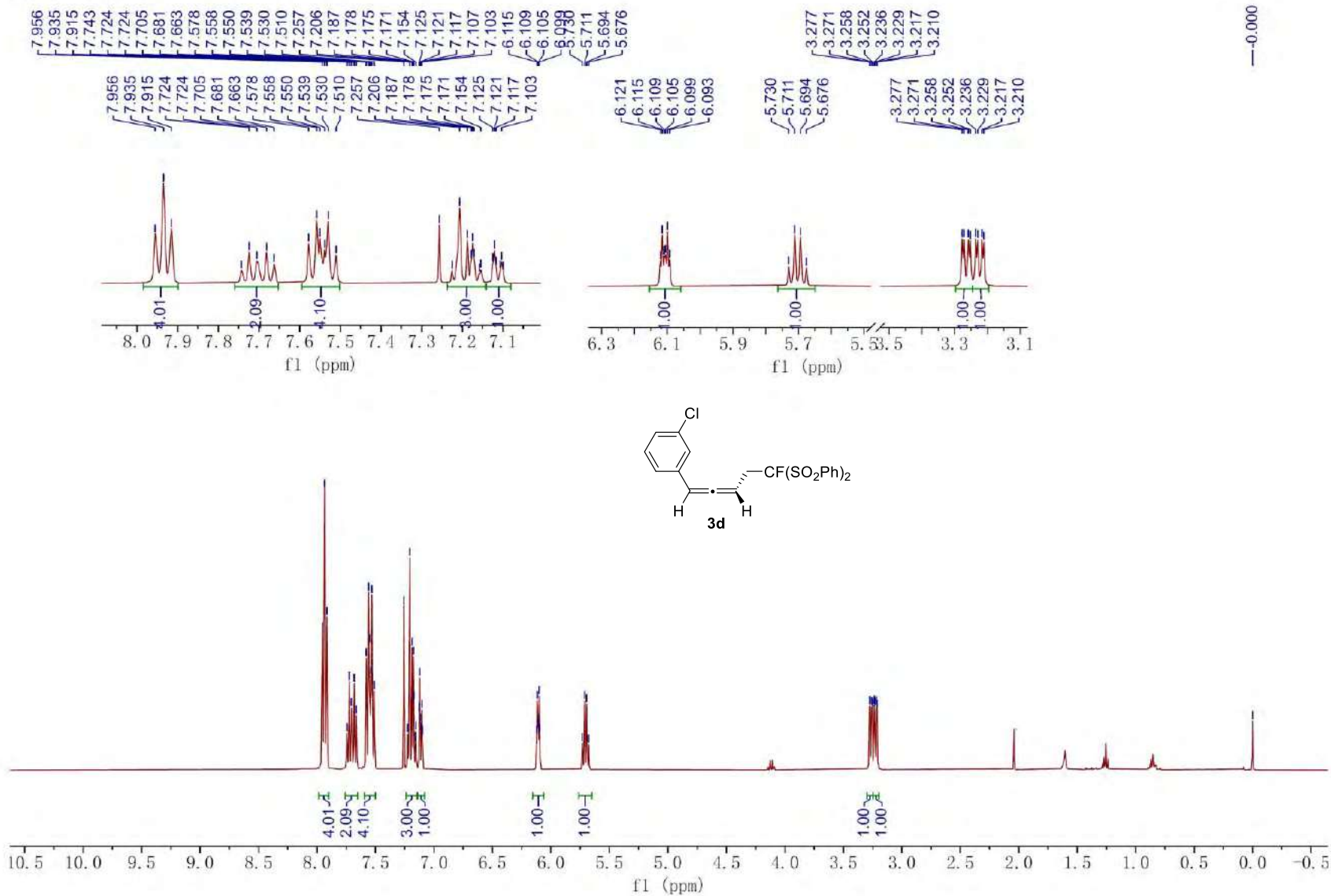
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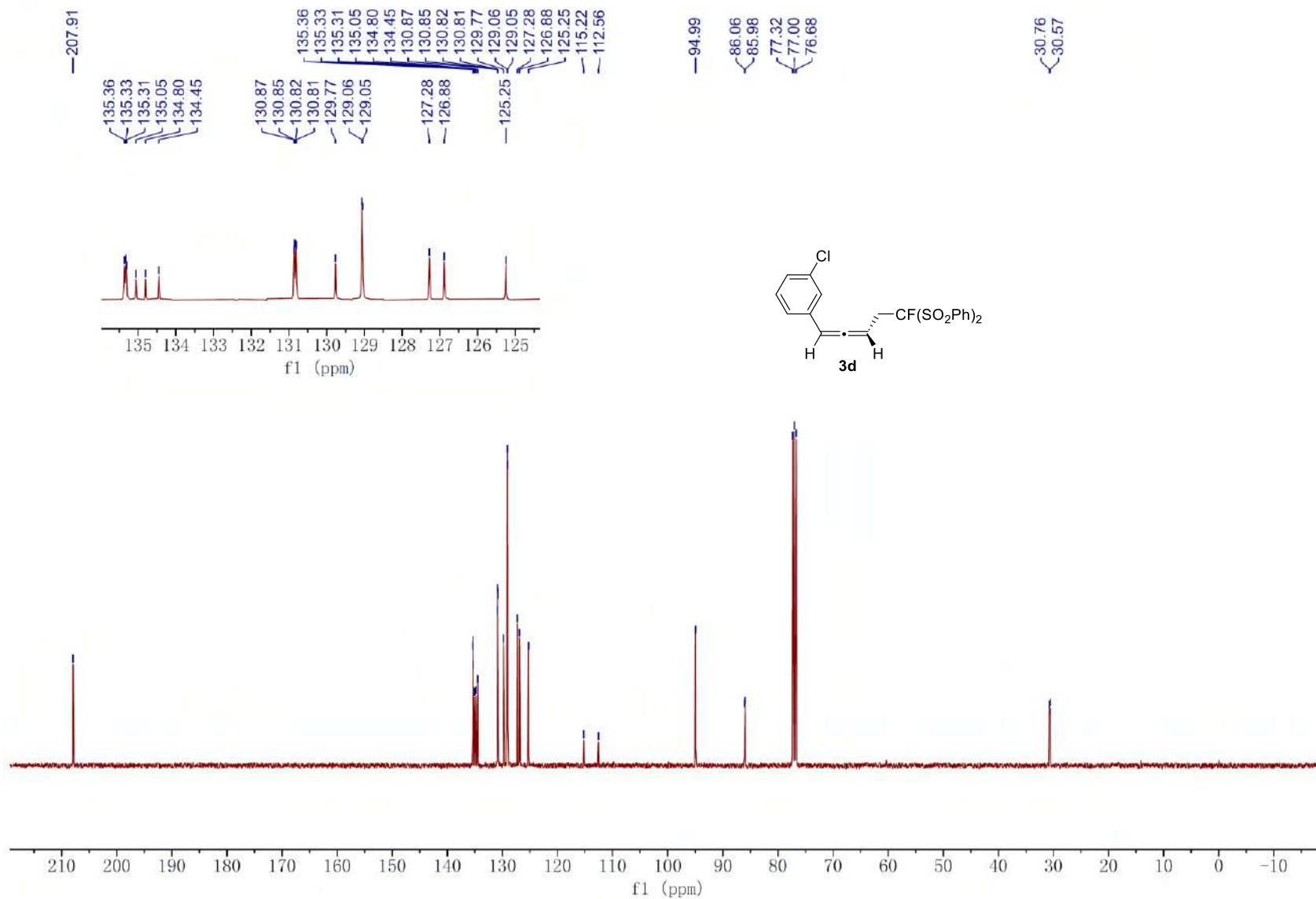
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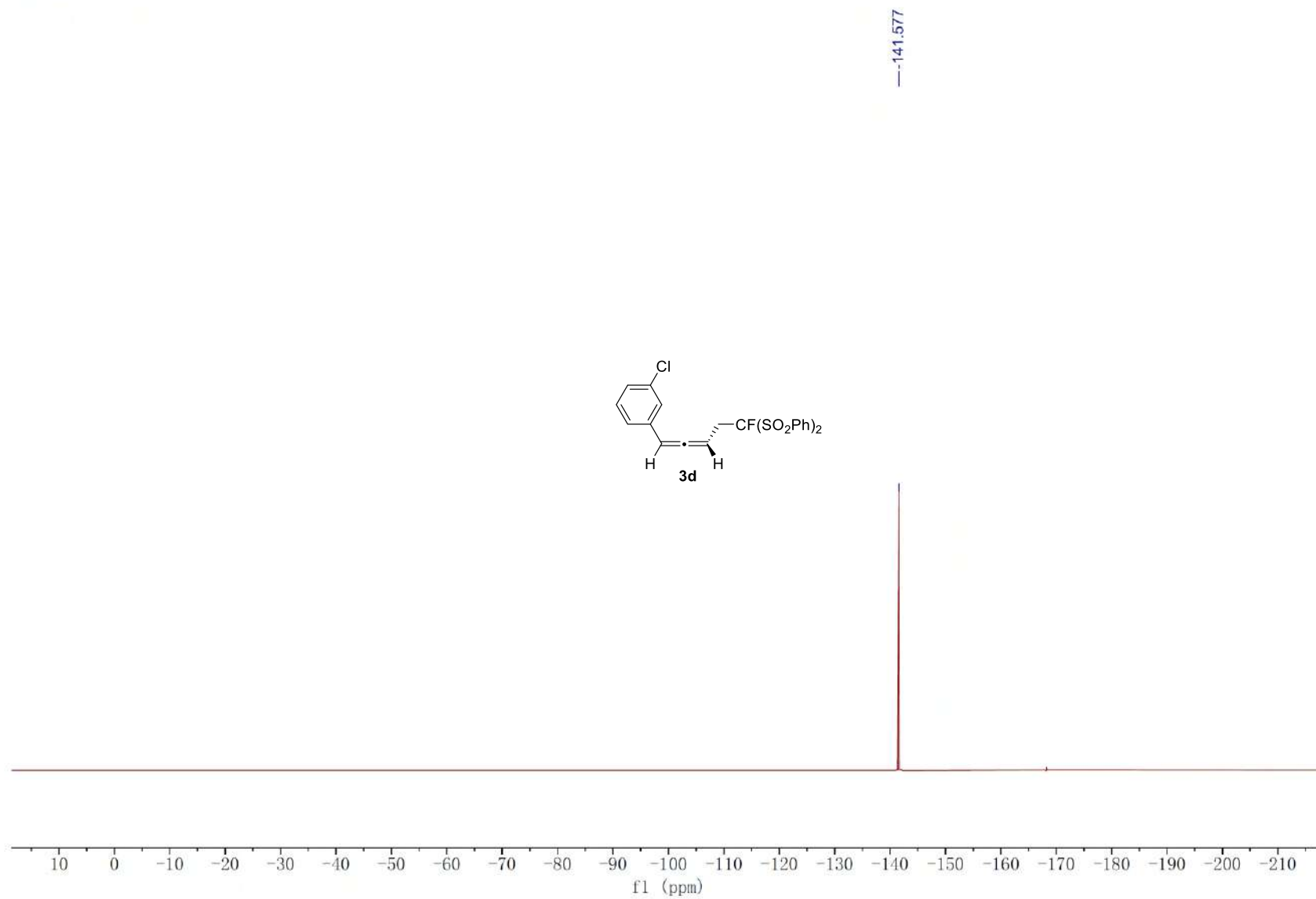
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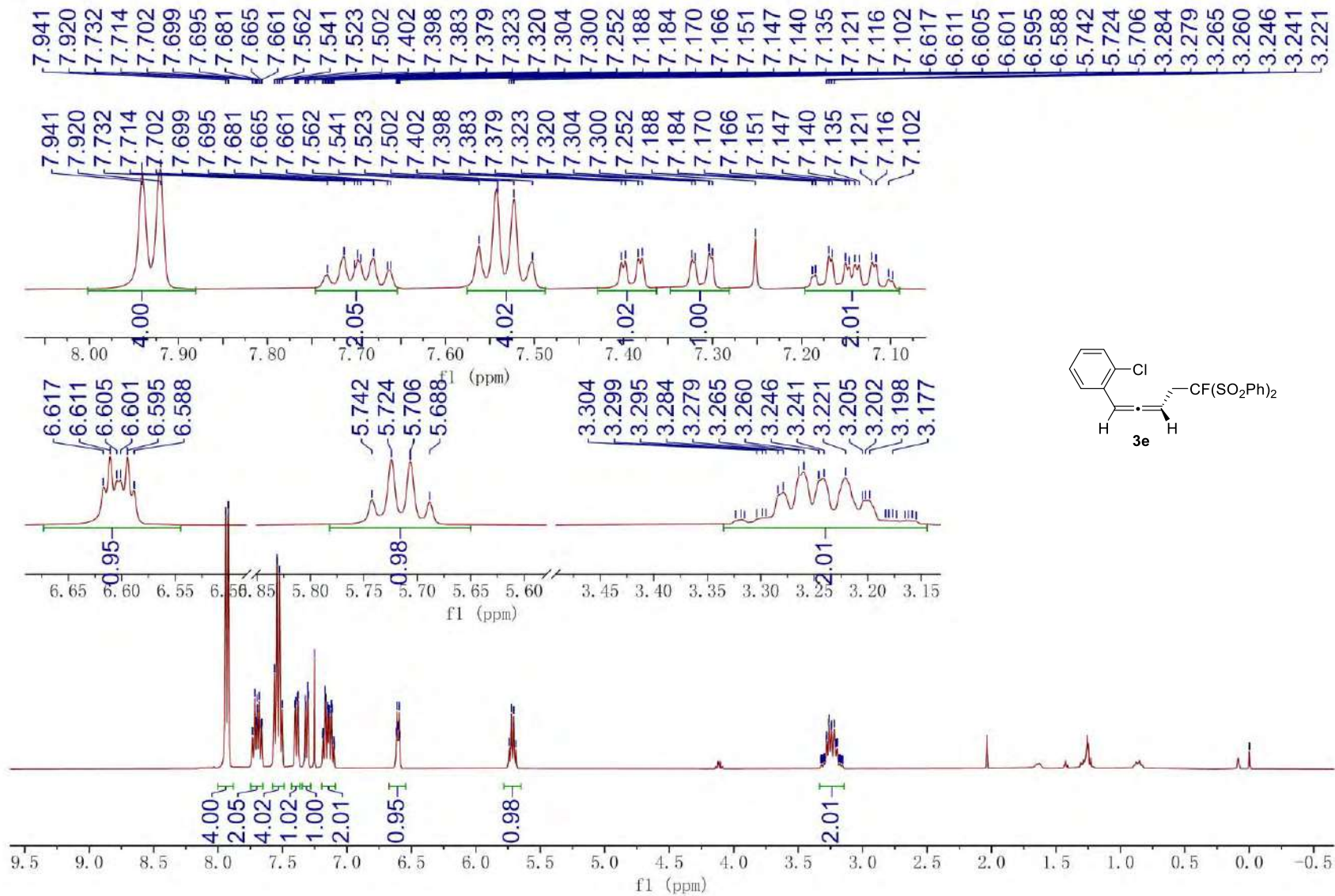
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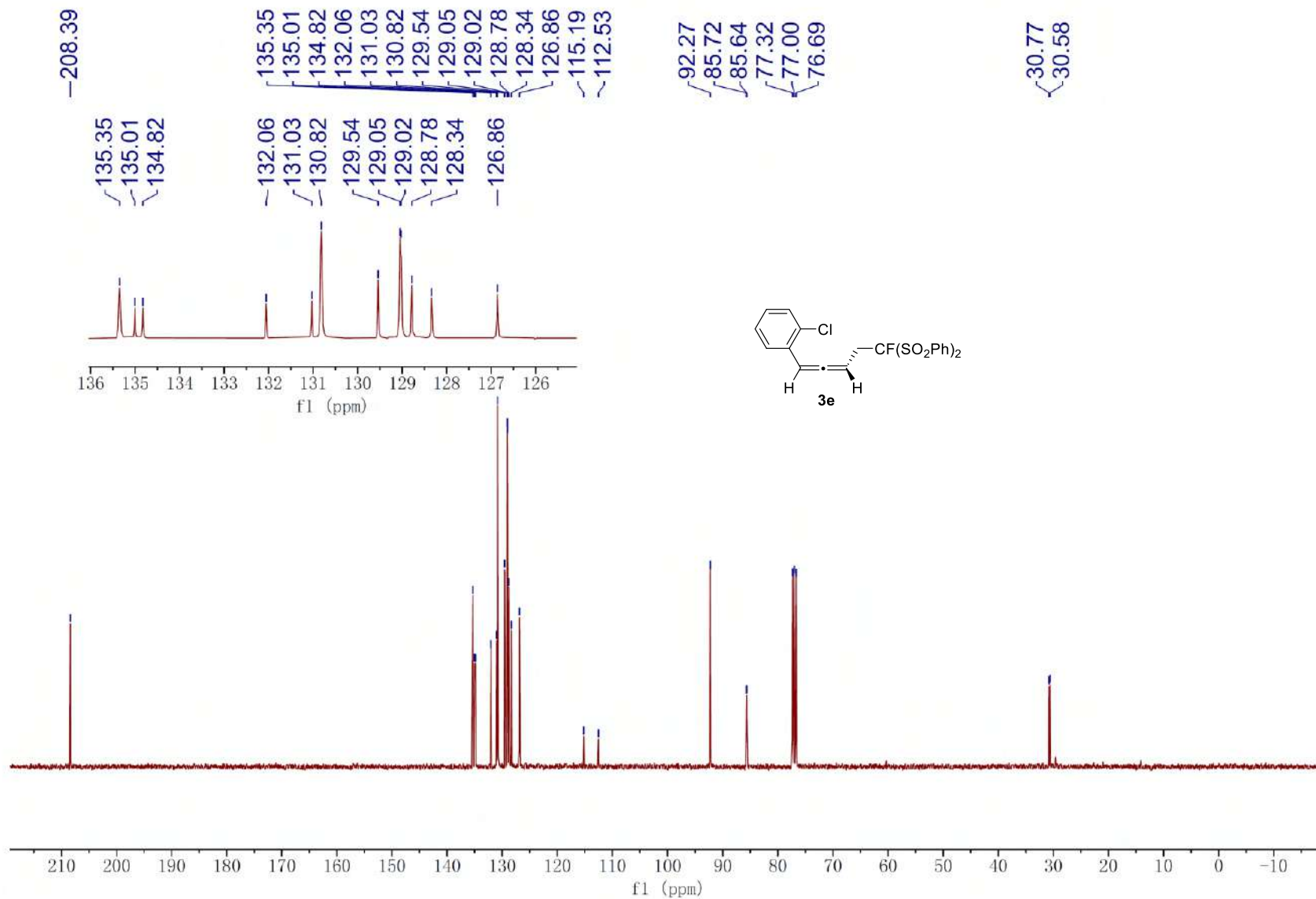
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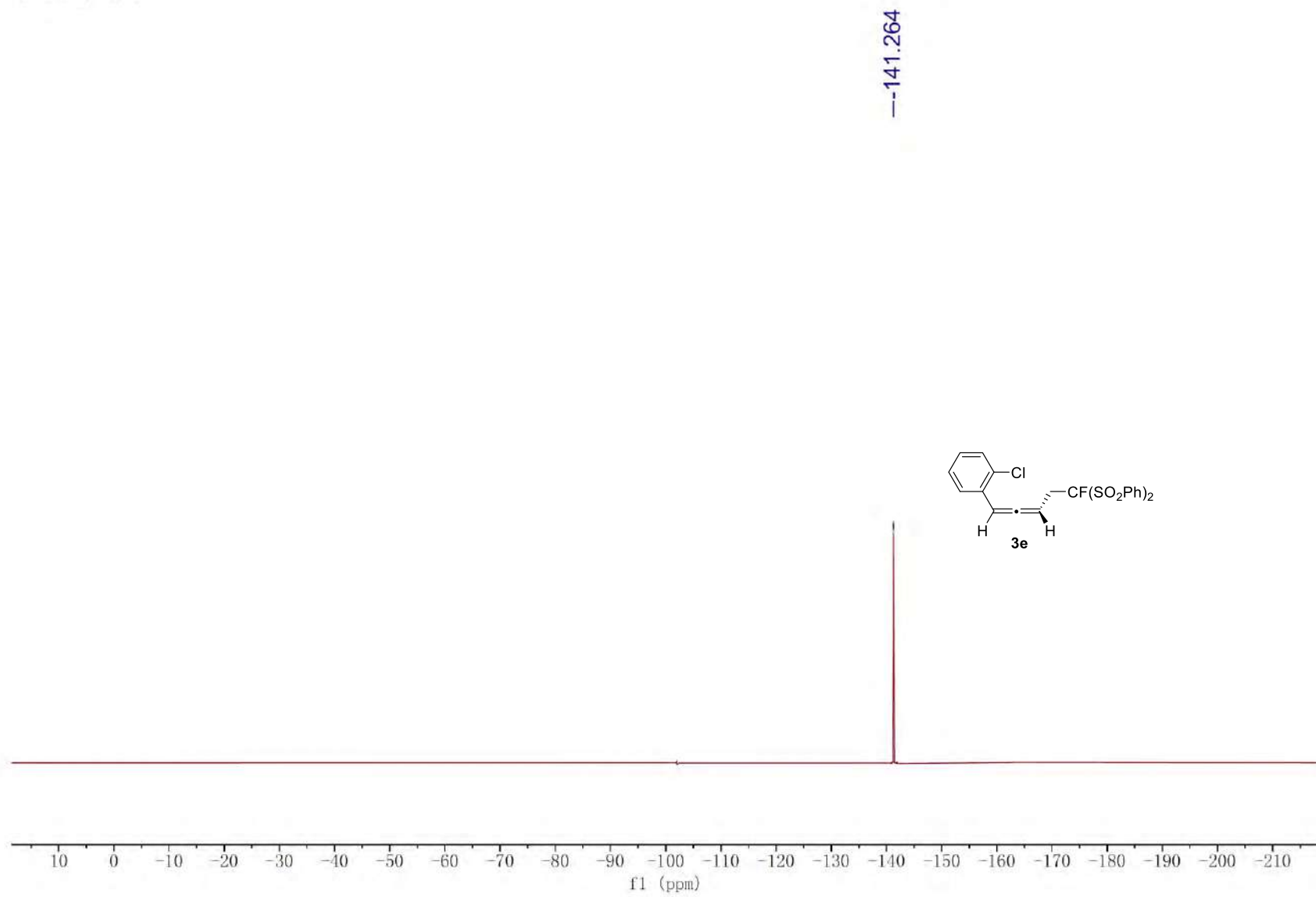
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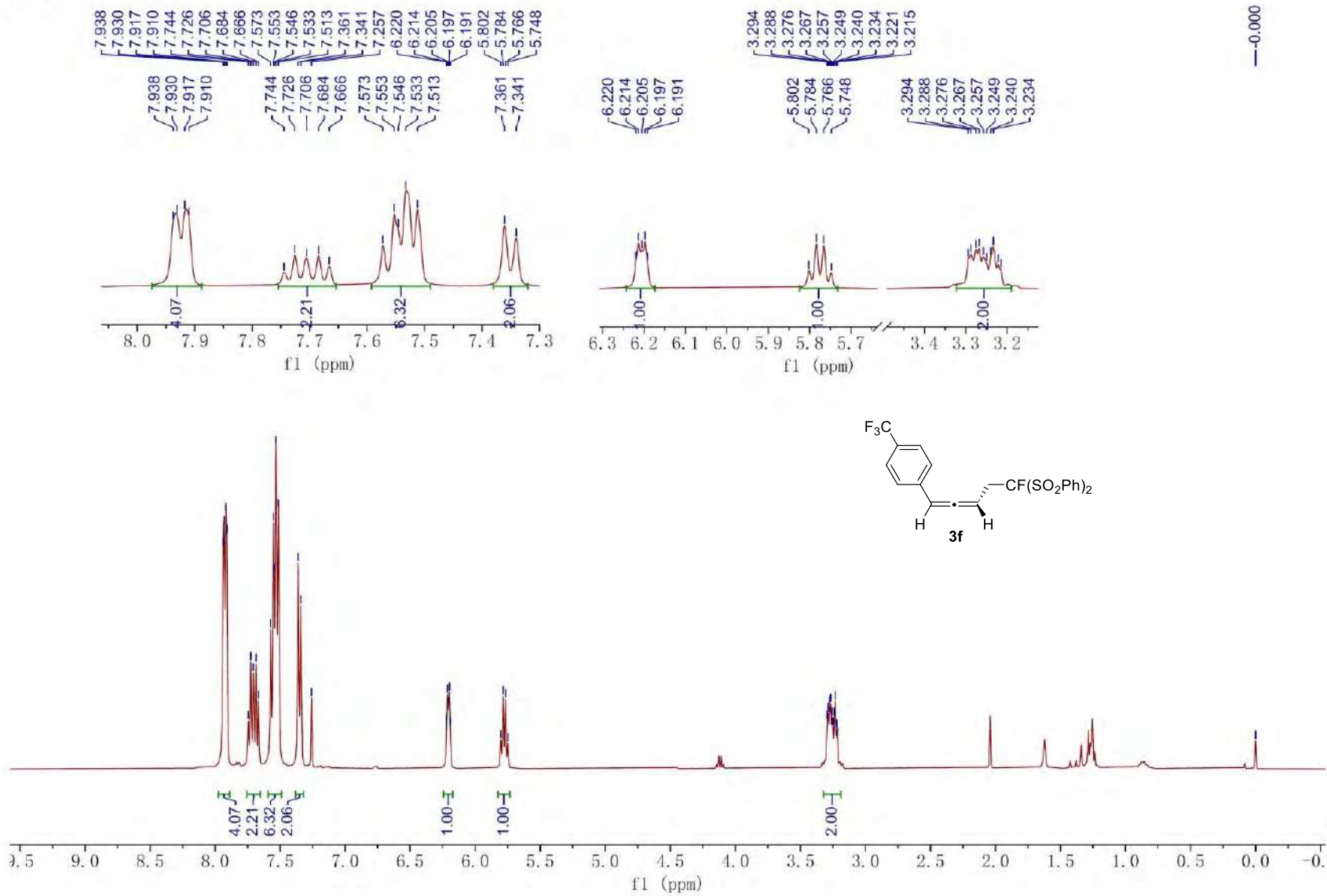
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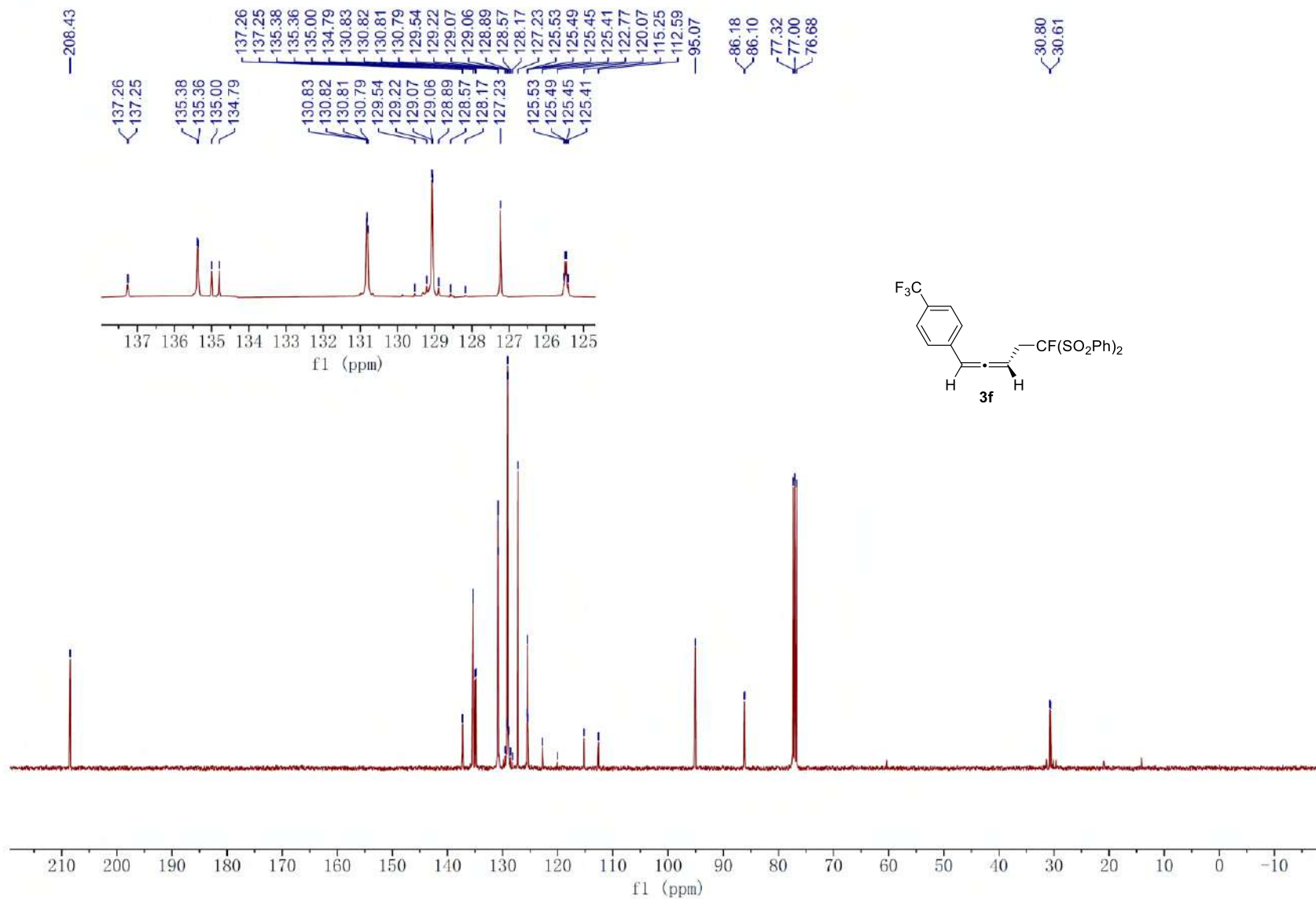
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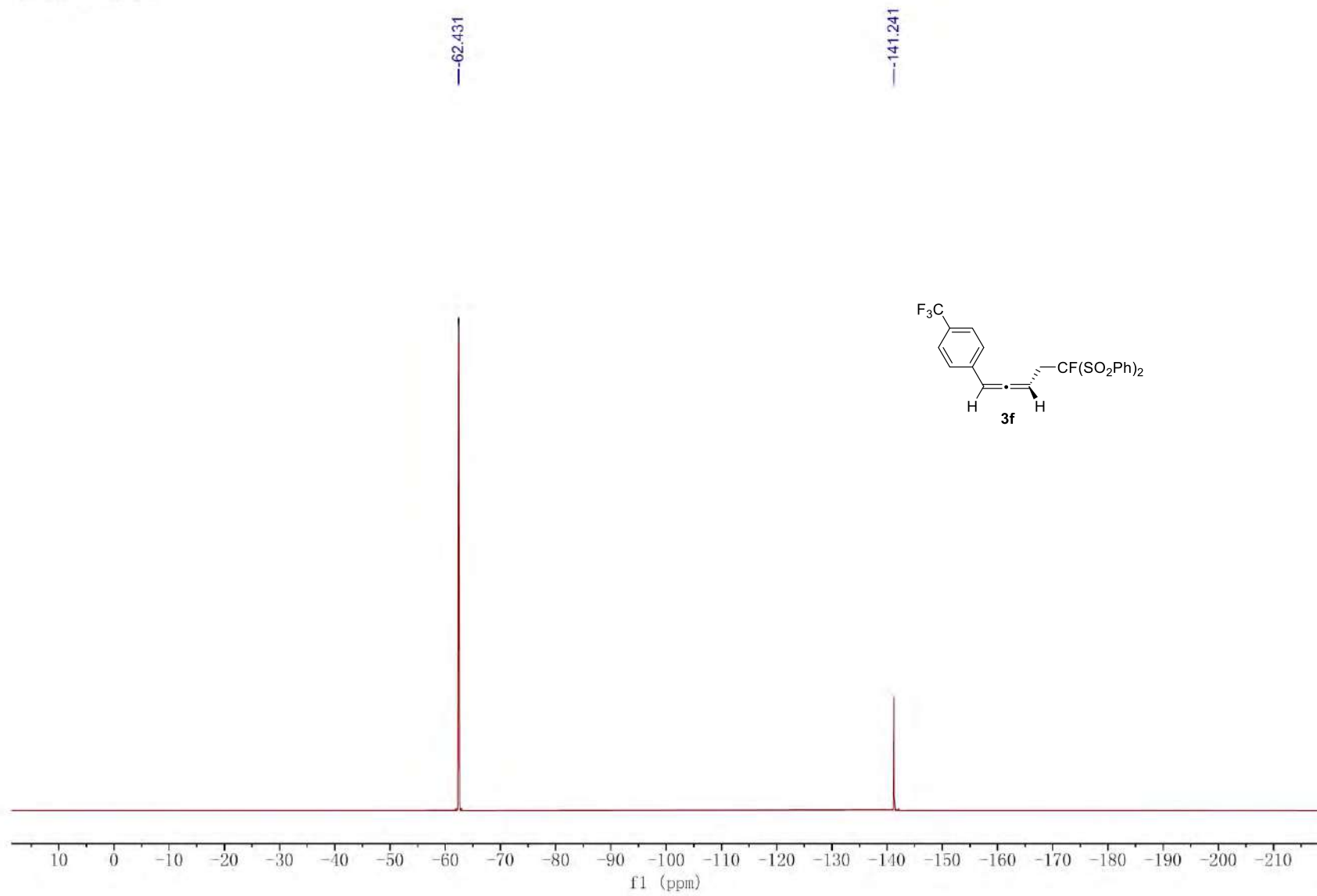
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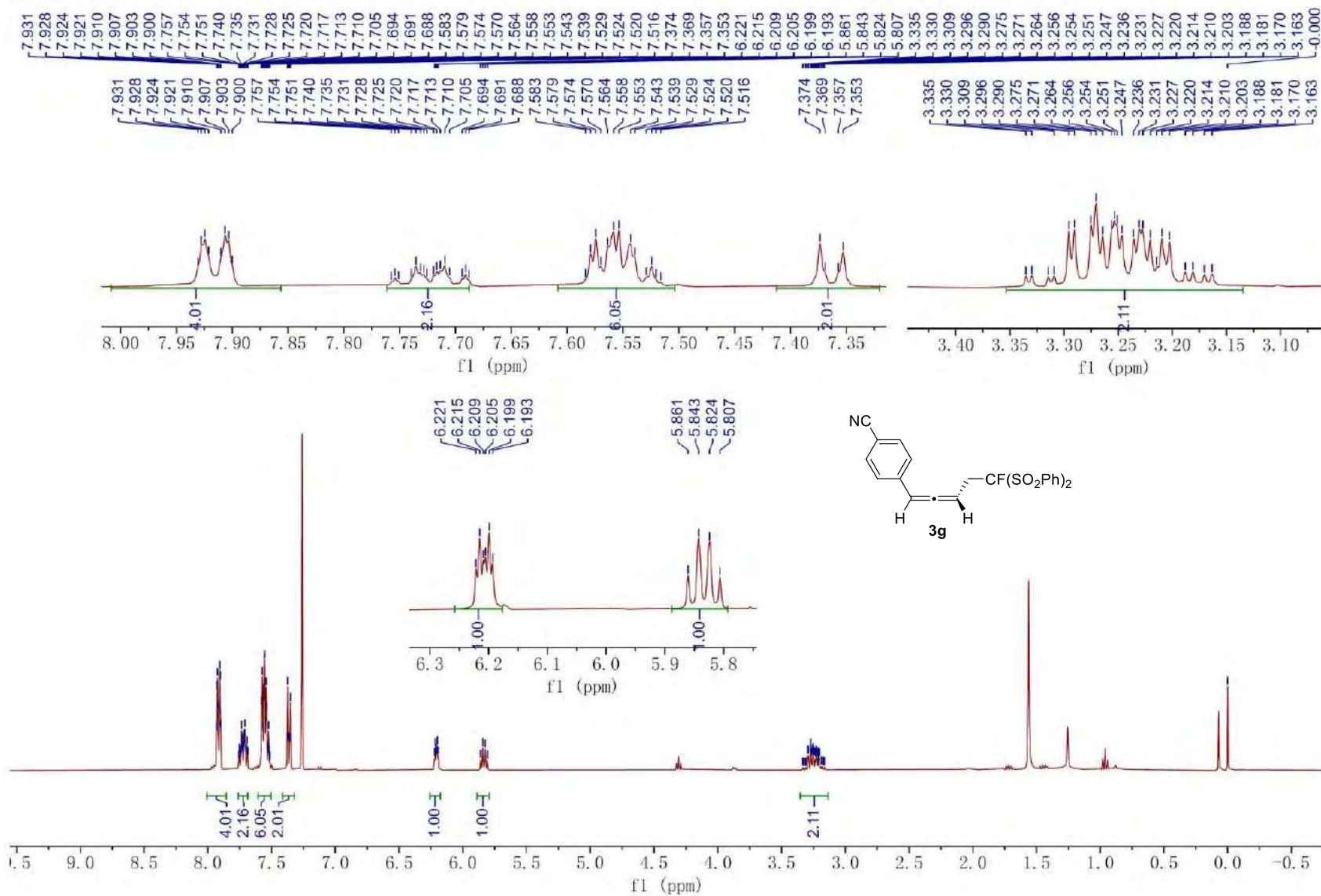
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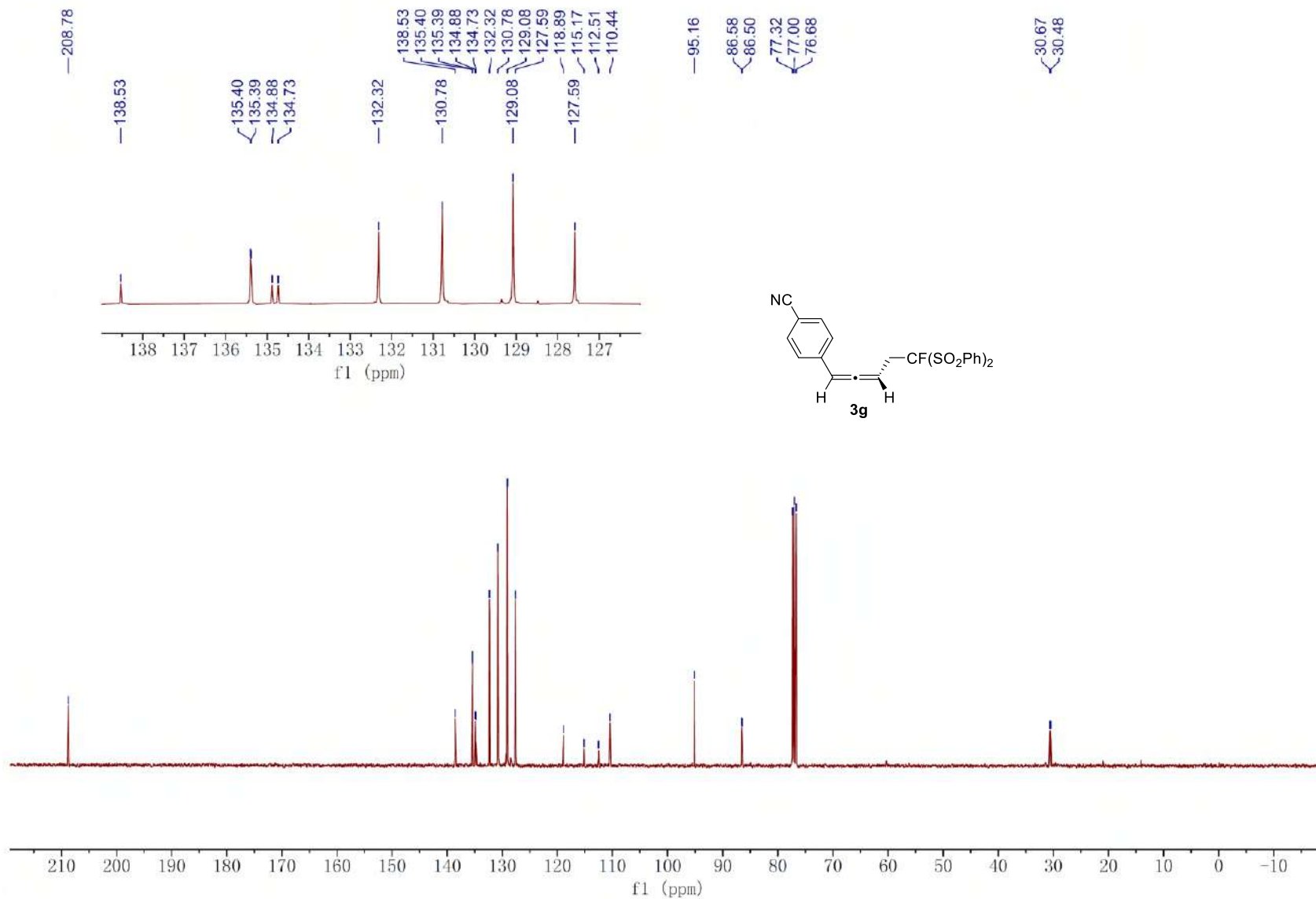
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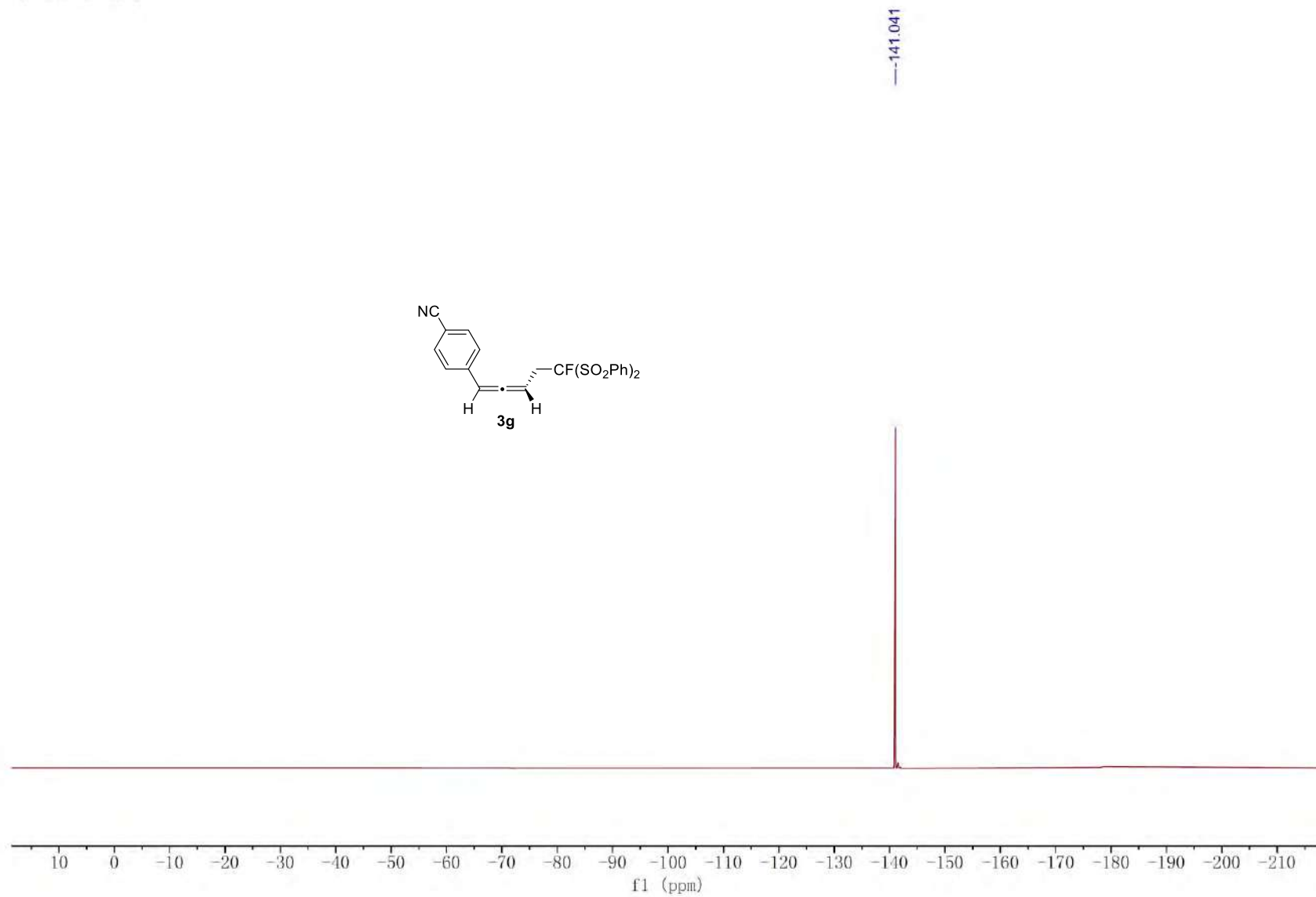
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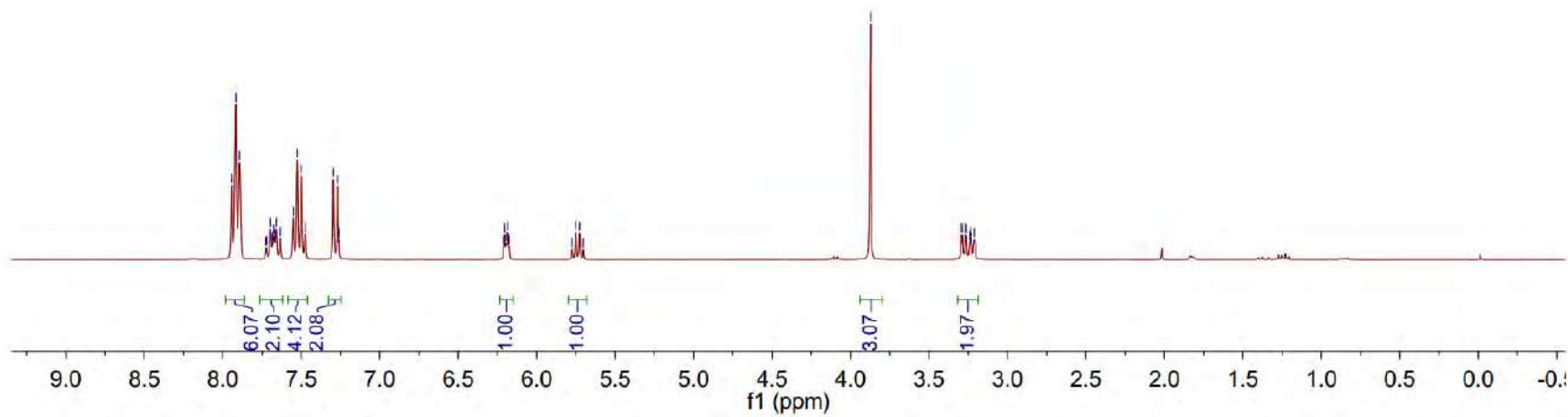
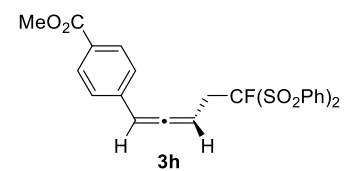
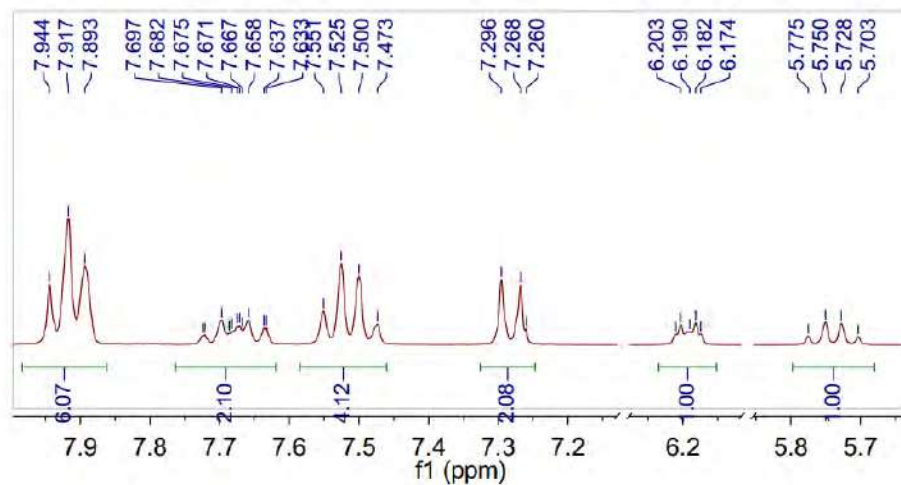
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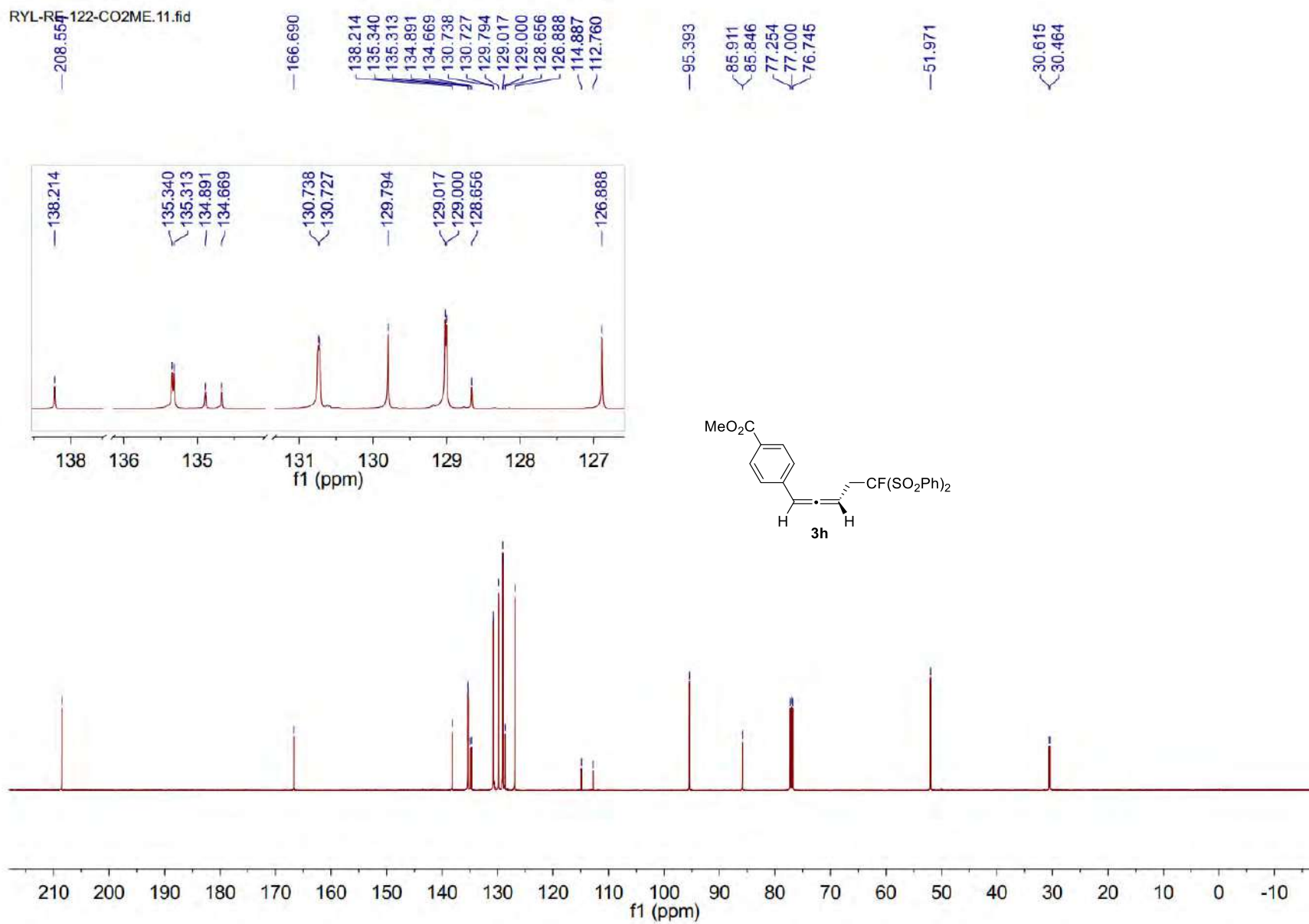
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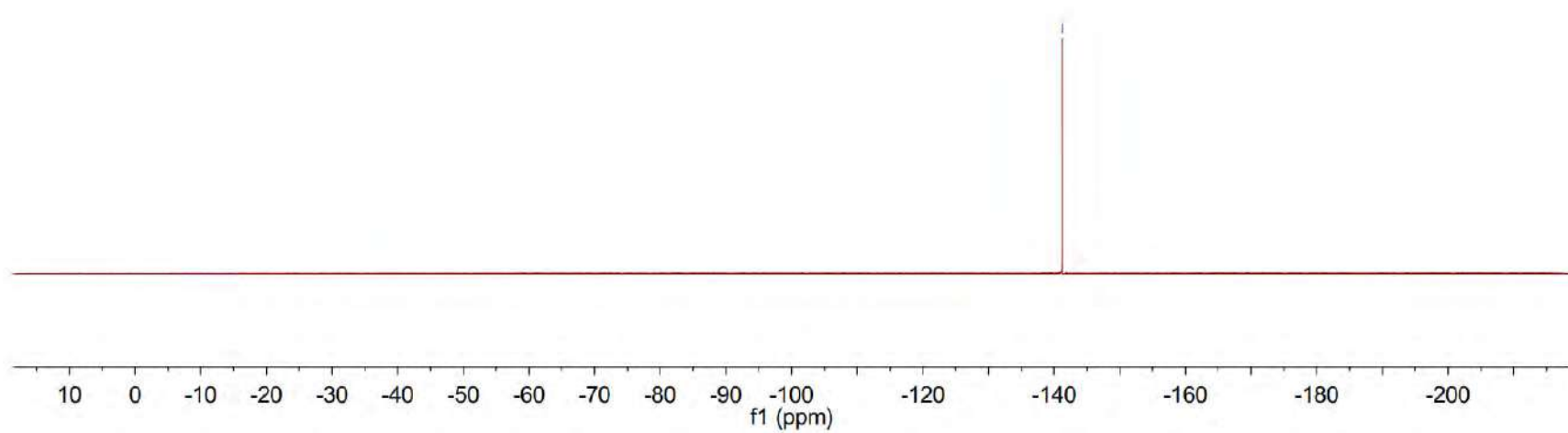
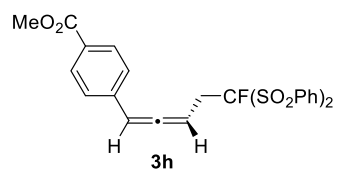


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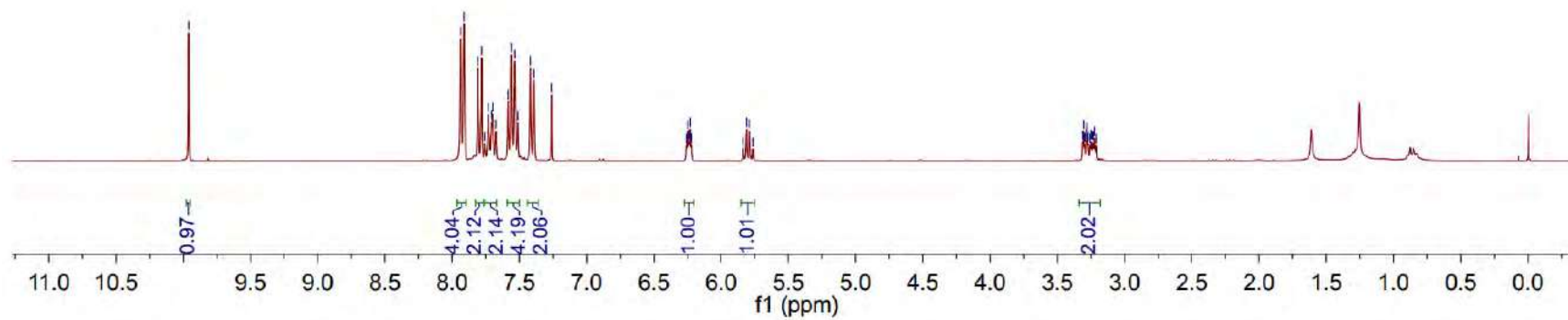
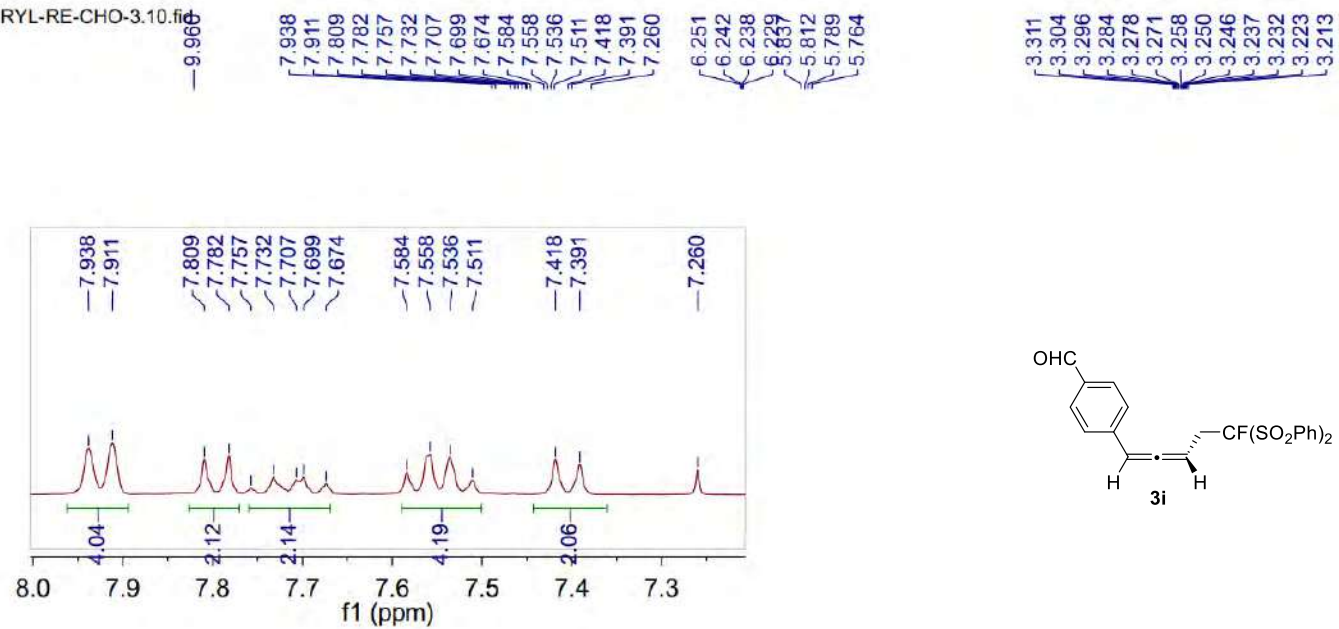


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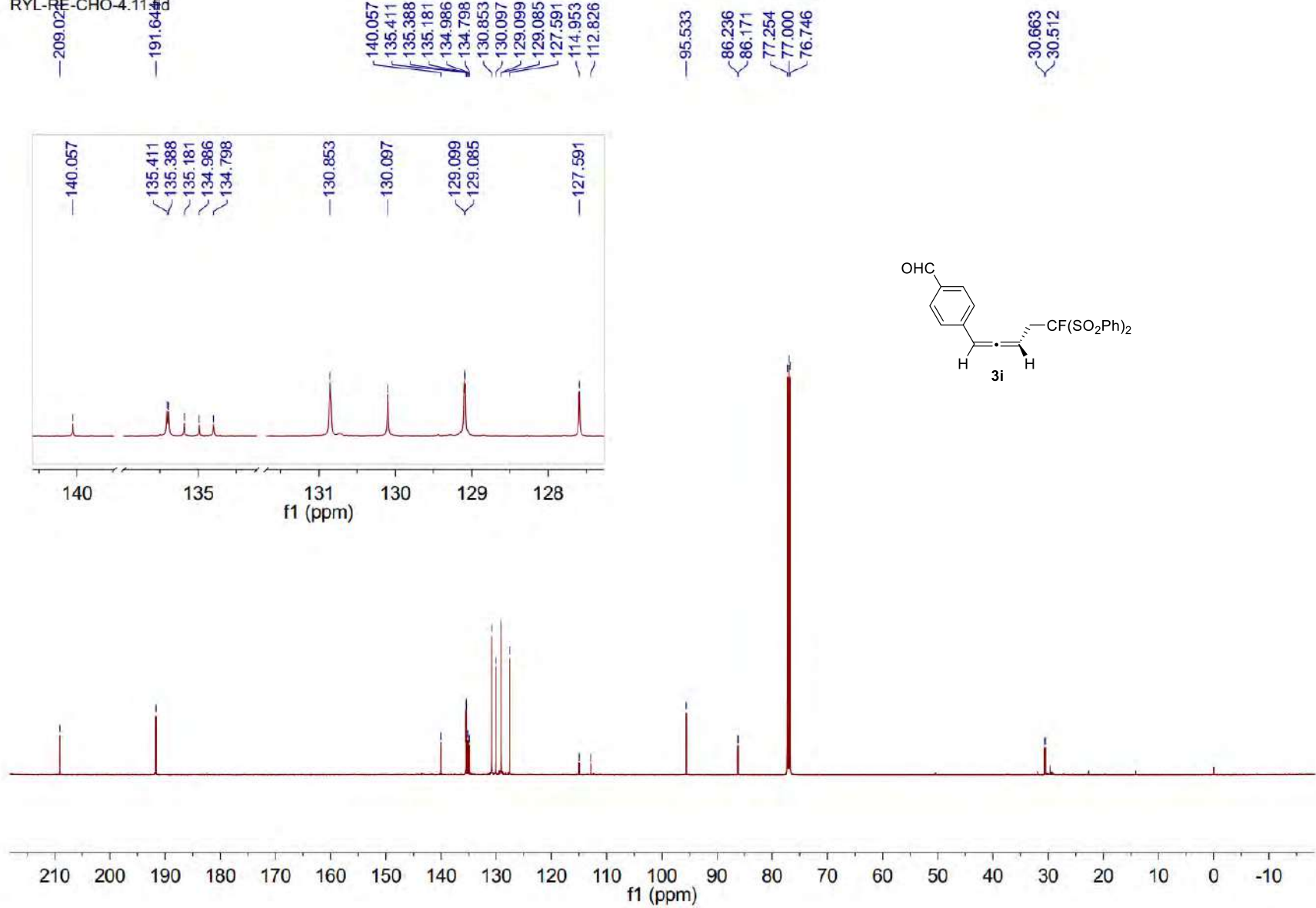
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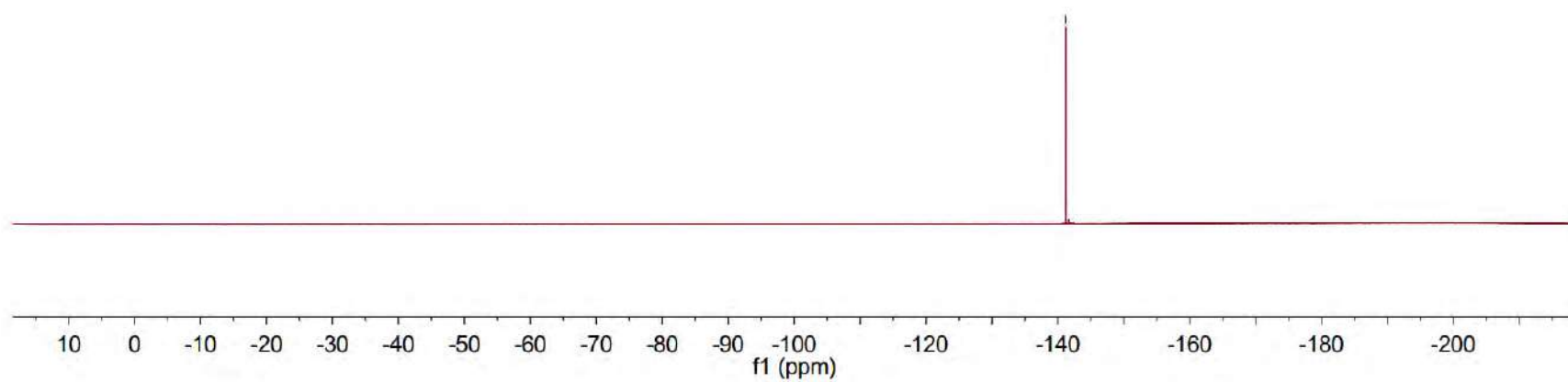
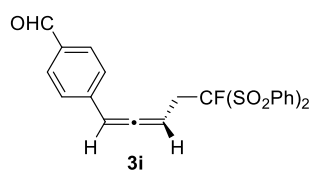


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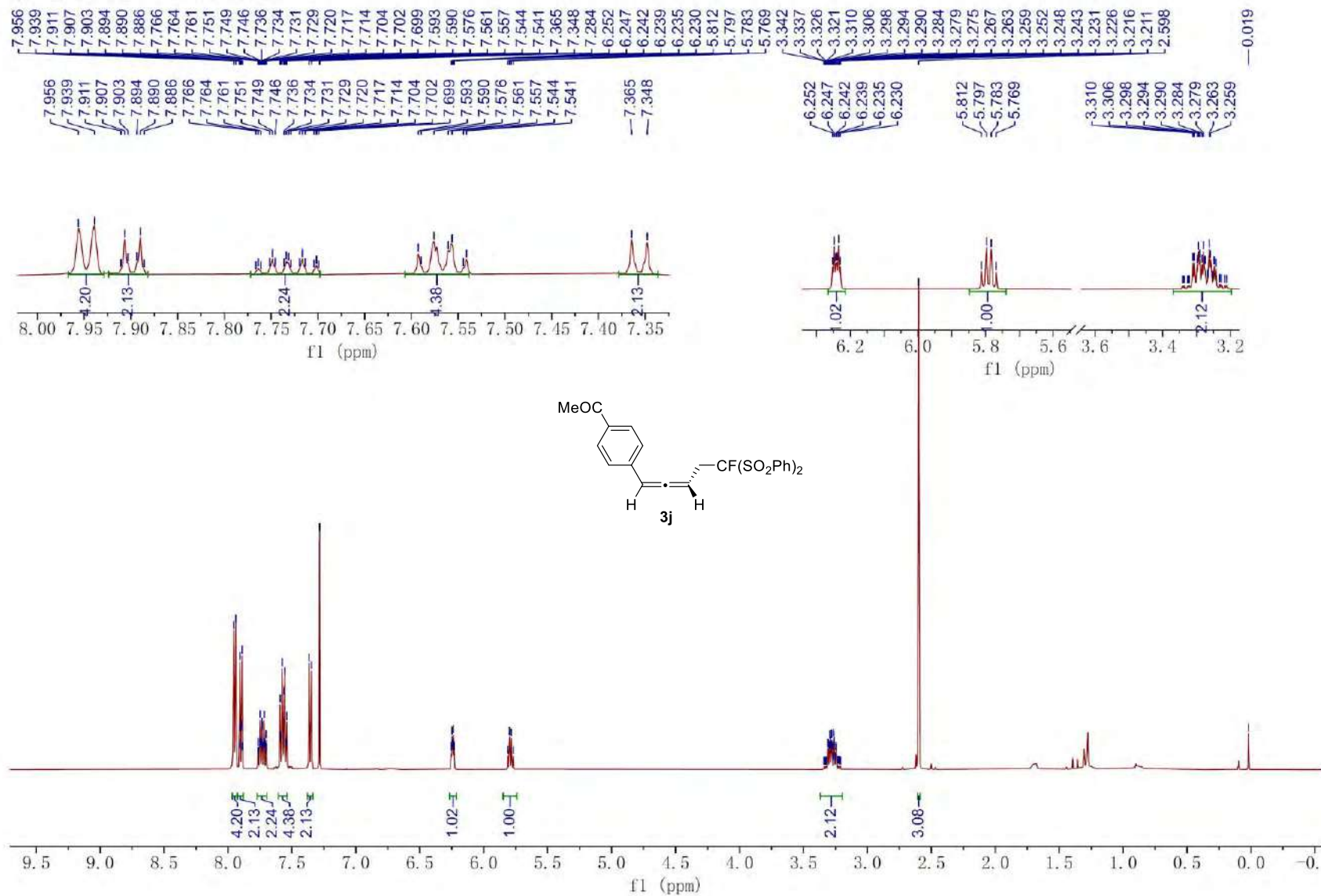


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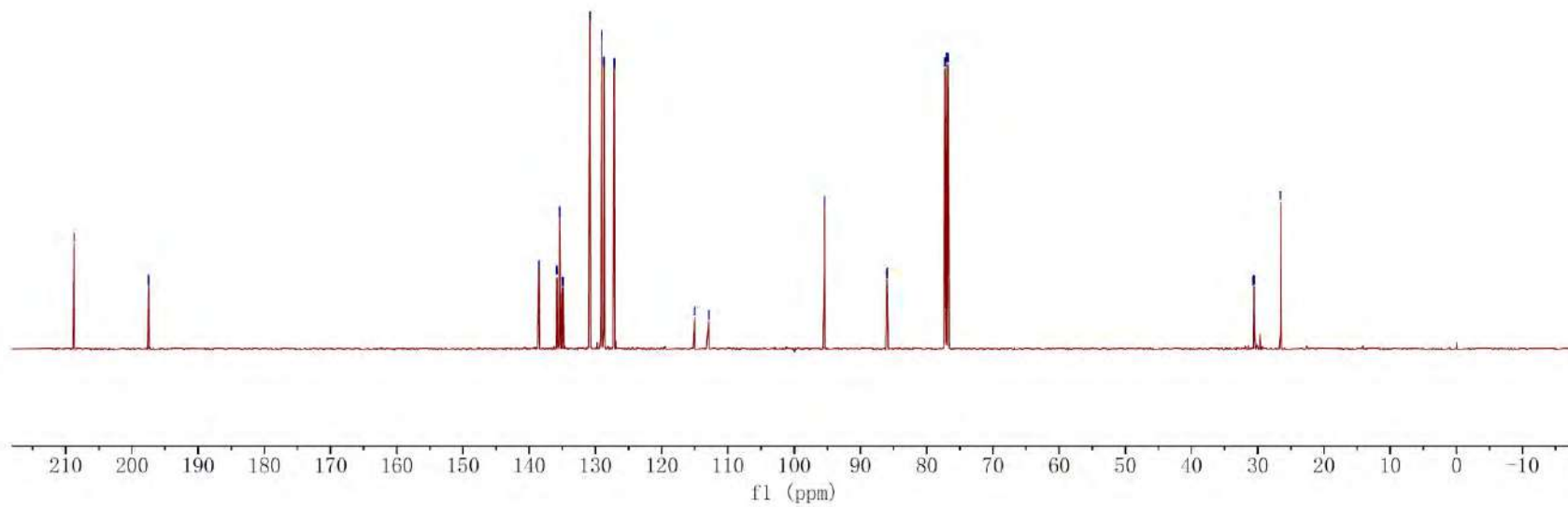
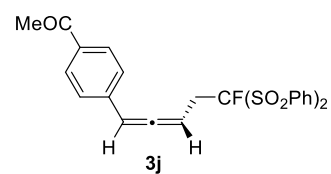
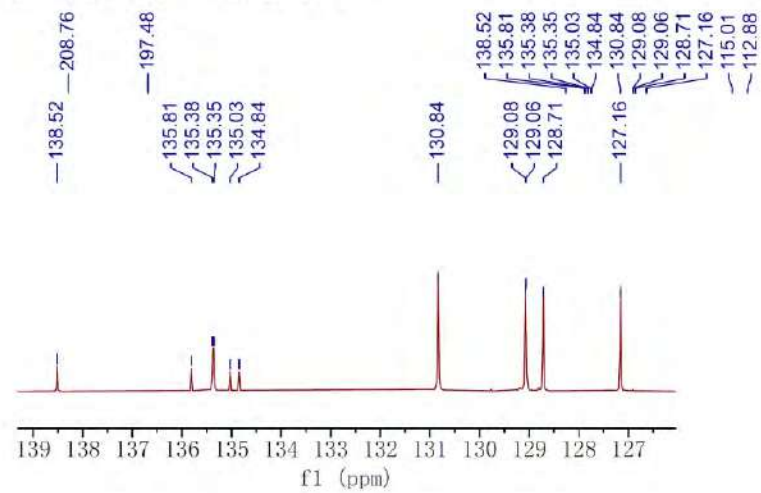
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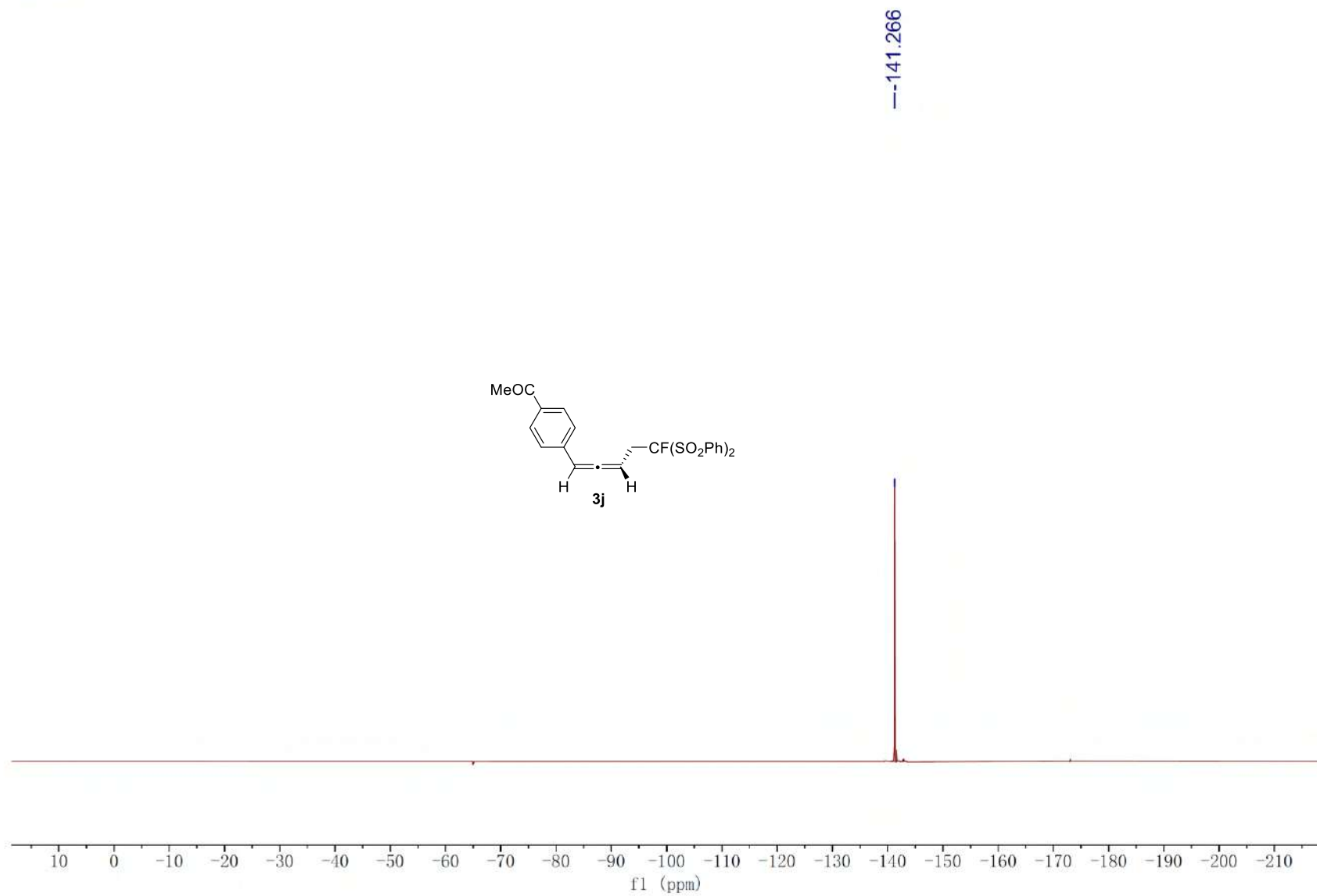
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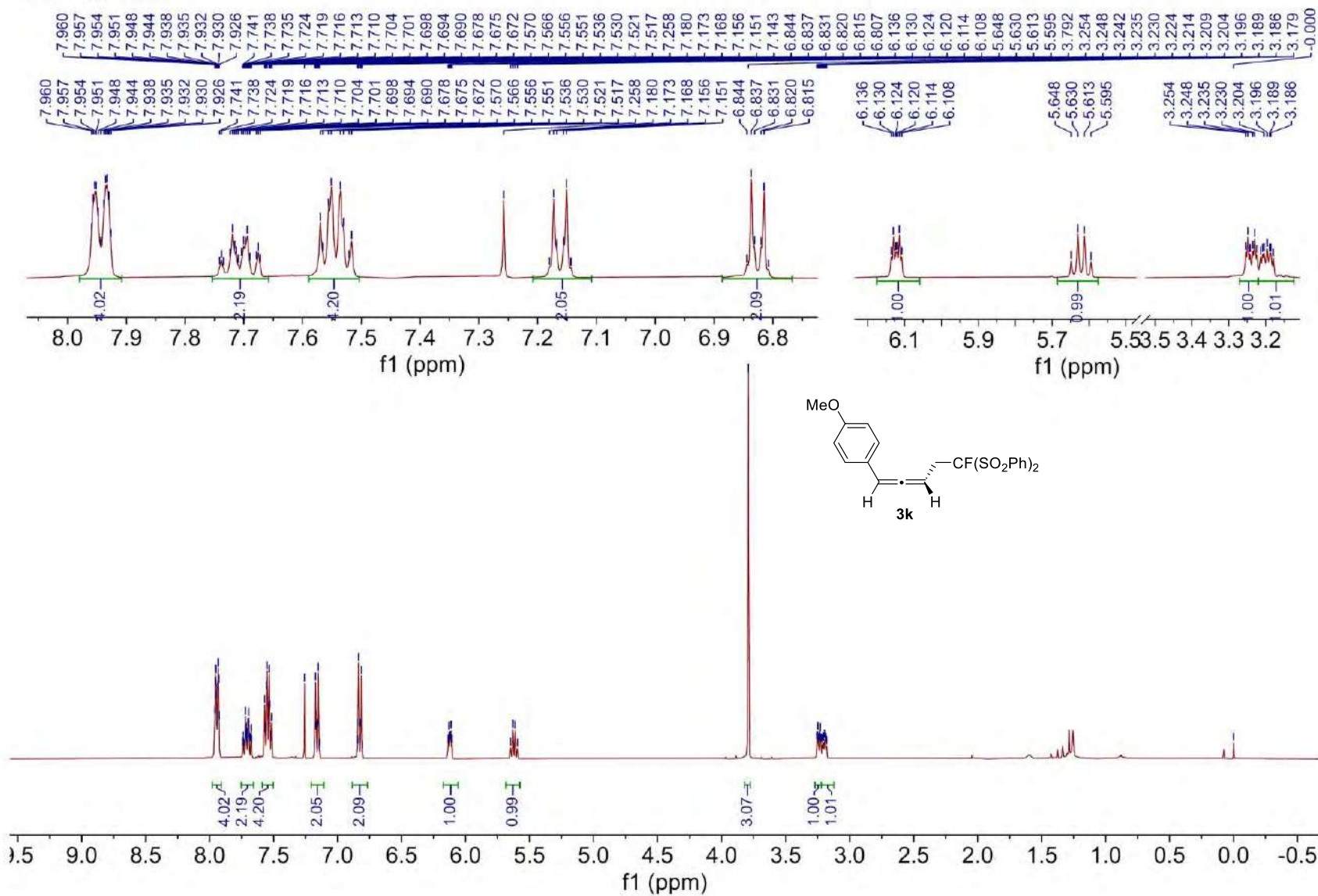
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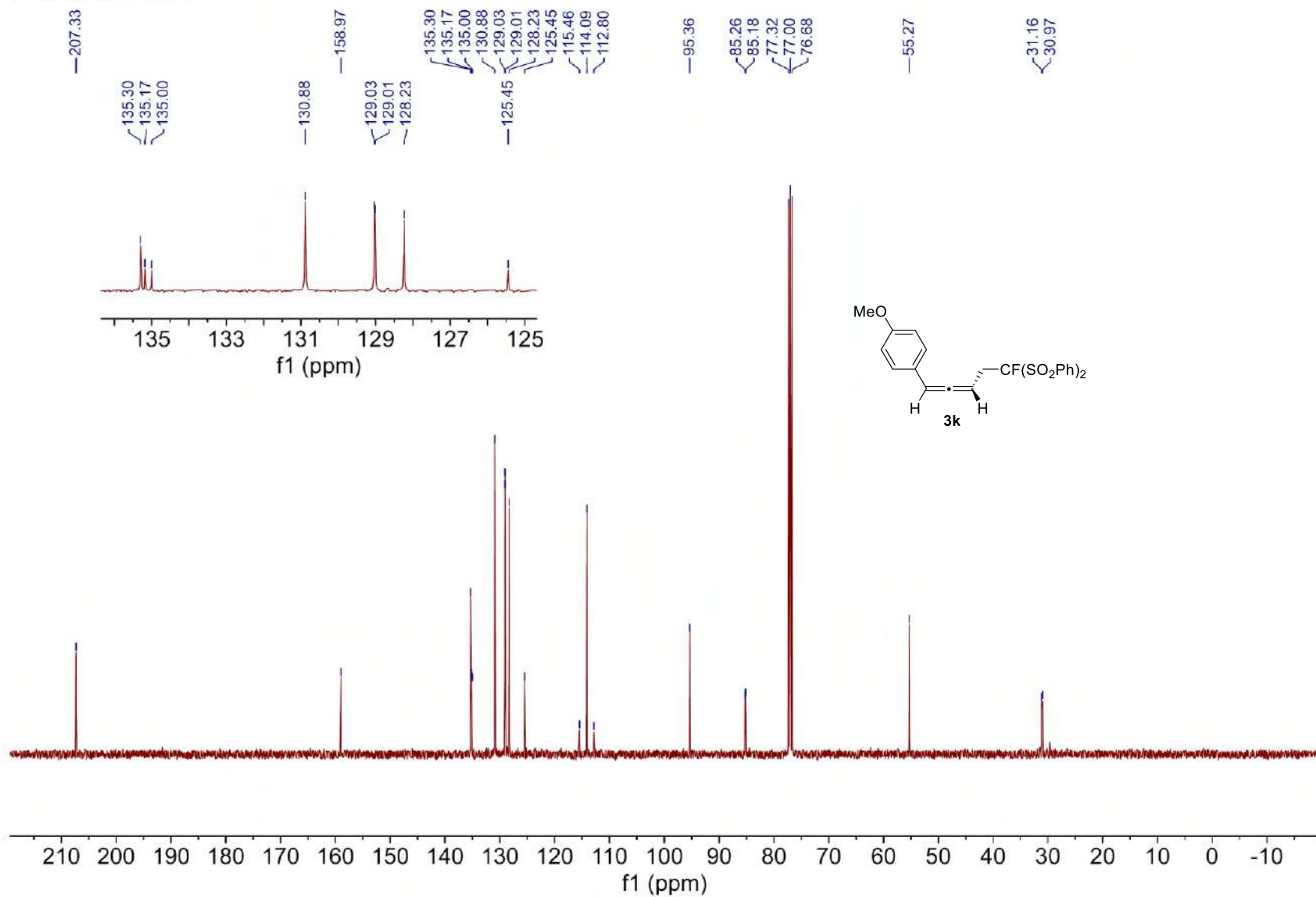
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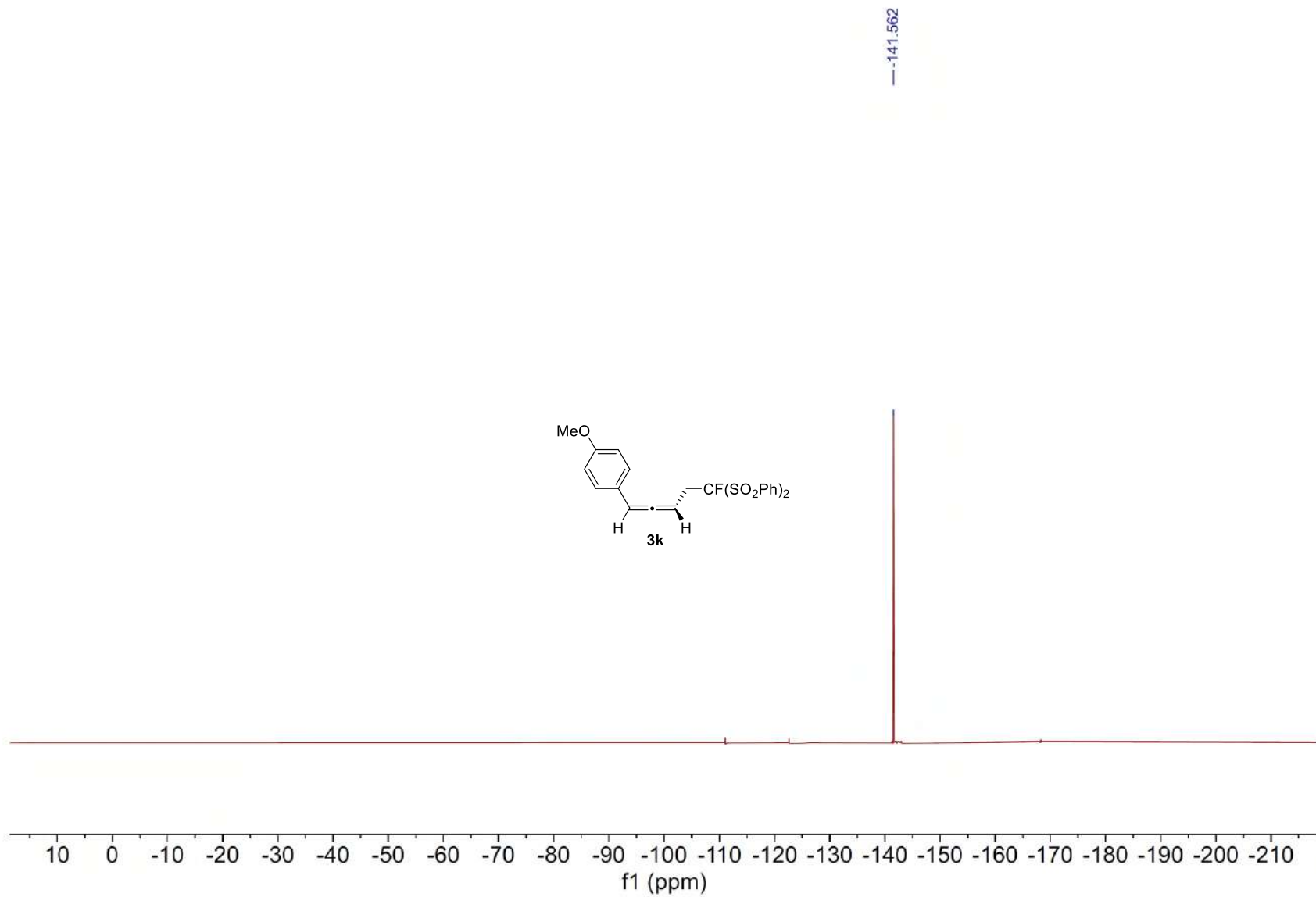


RYL-RB-OME-PH.10.fid —

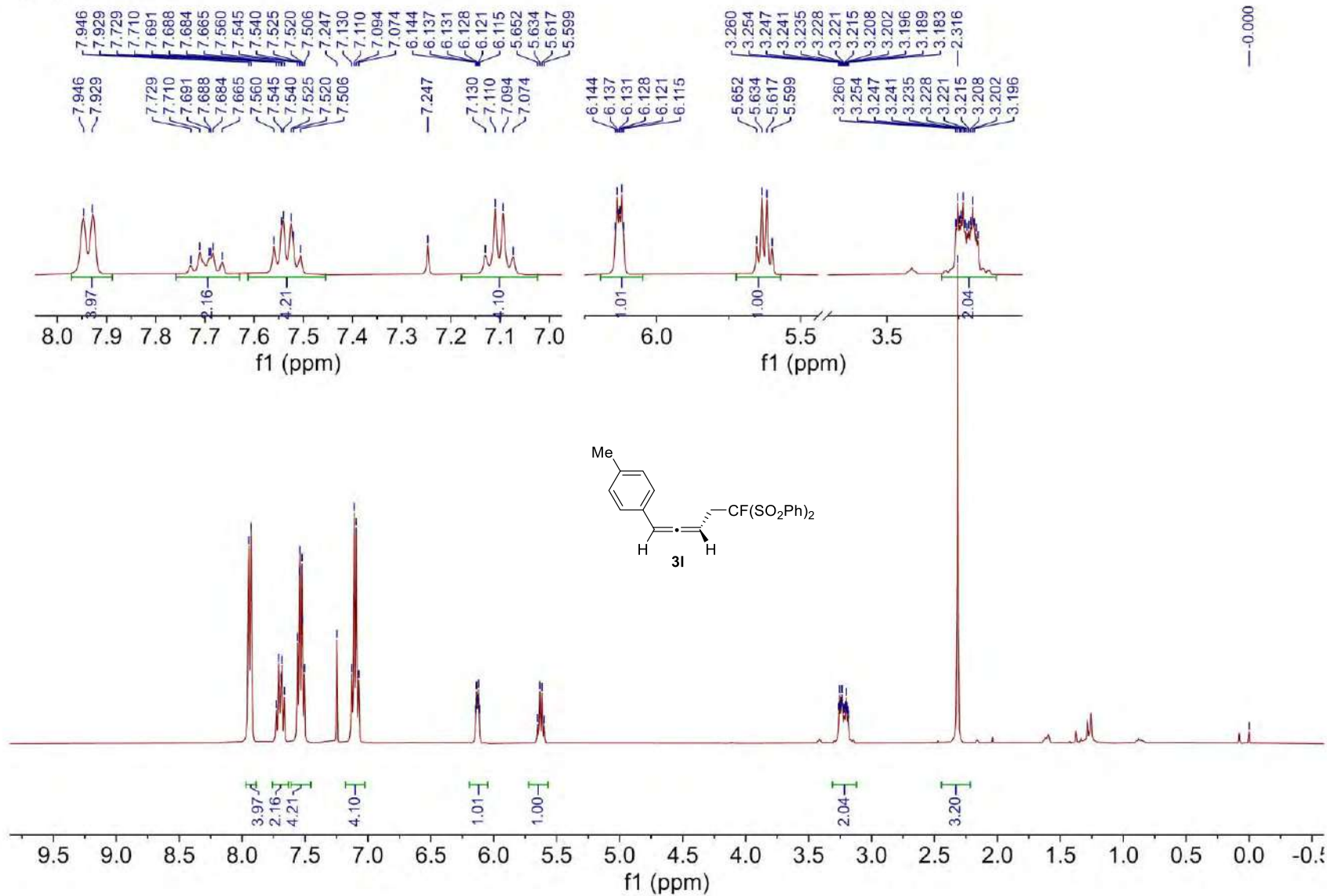


RYL-RB-OME-PH.11.fid —

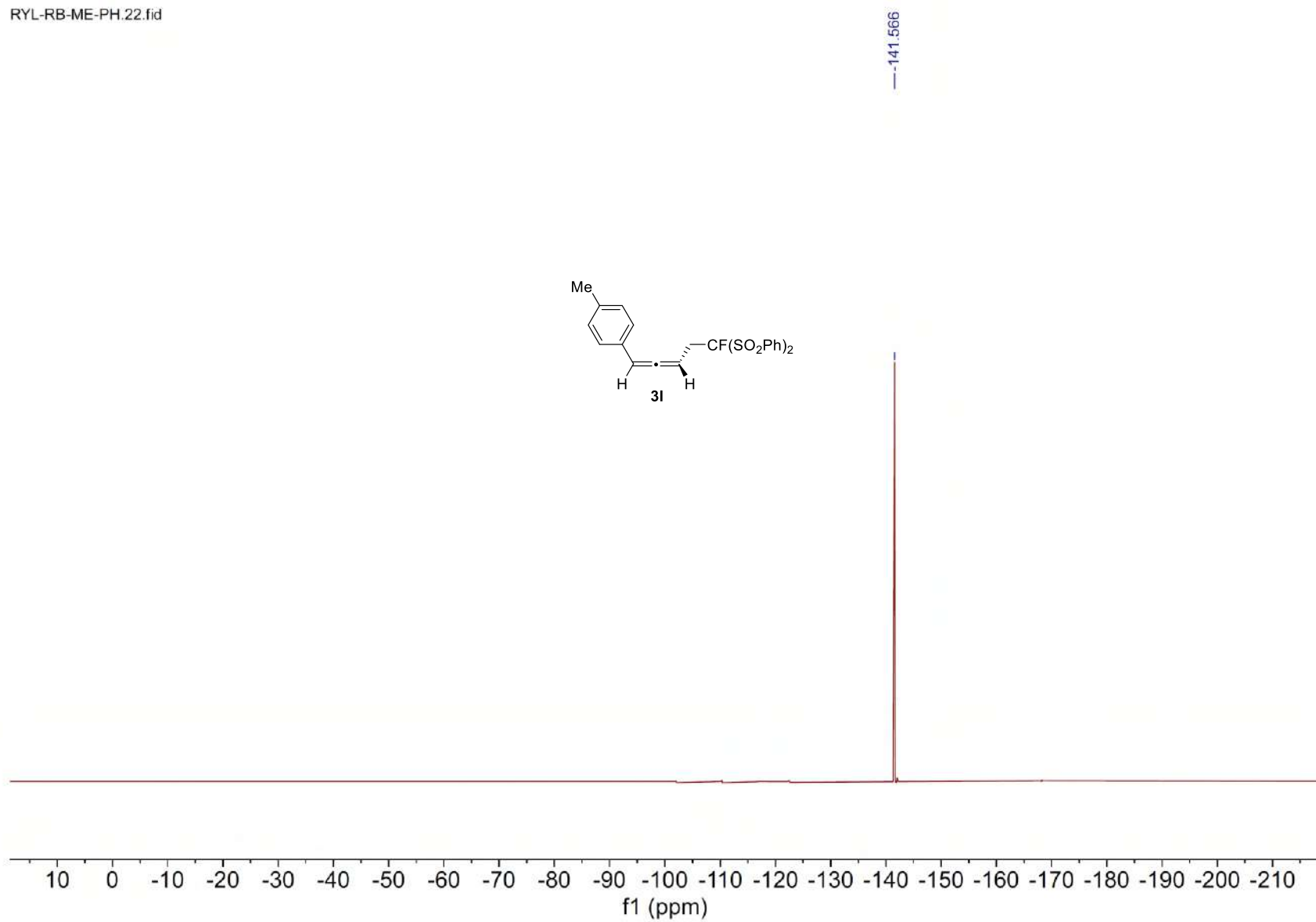




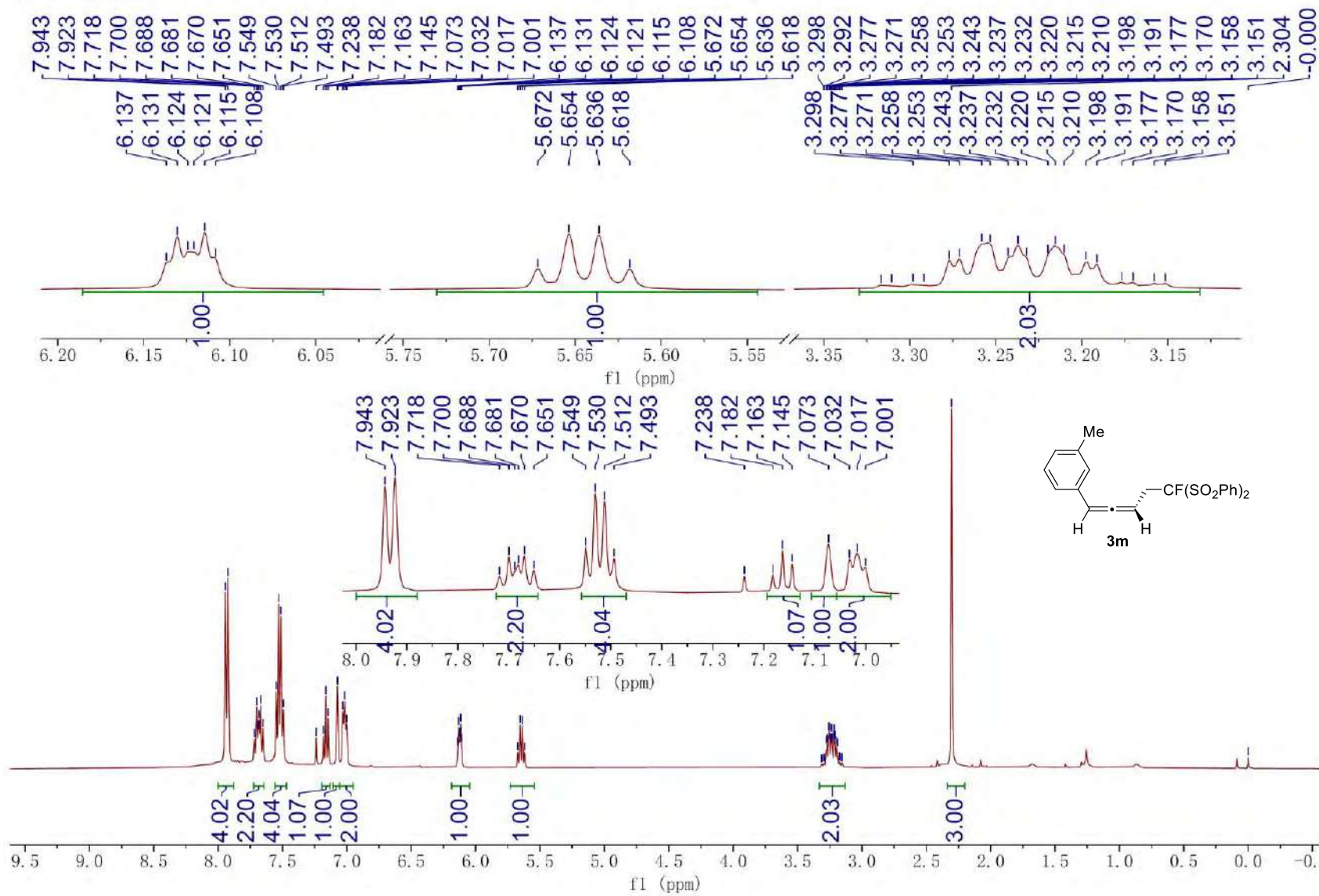
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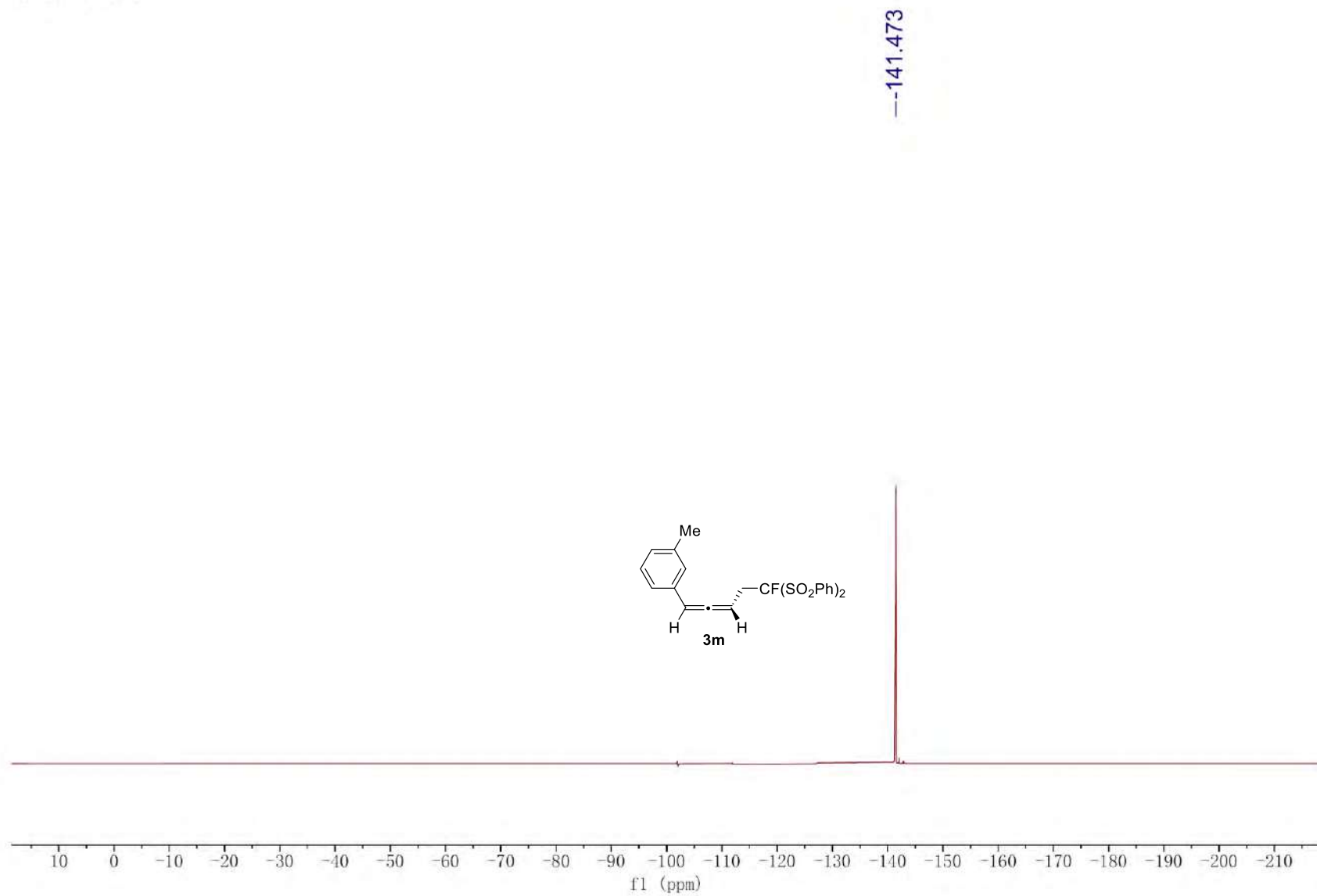
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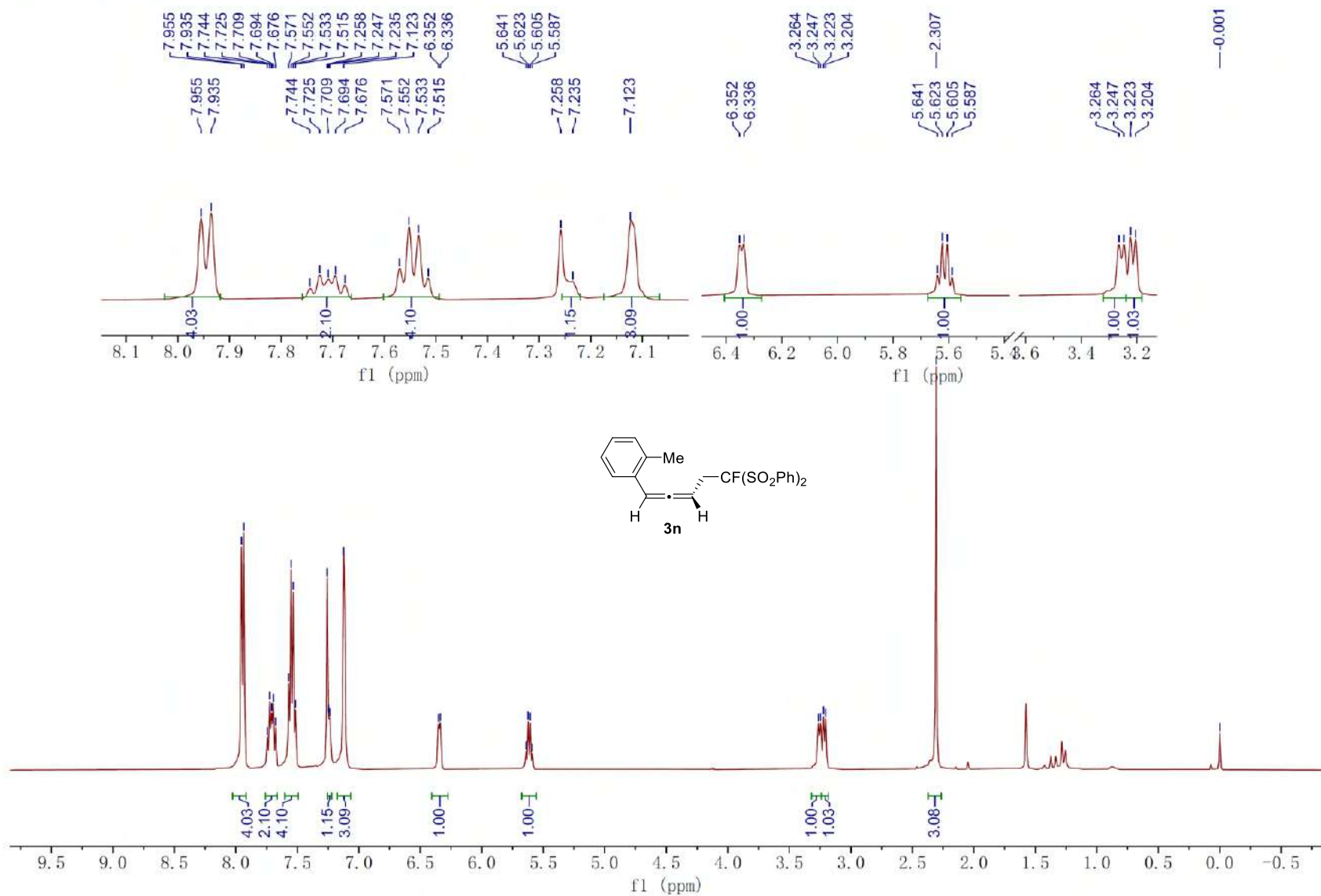
ZHY-ZG-38-400M-H



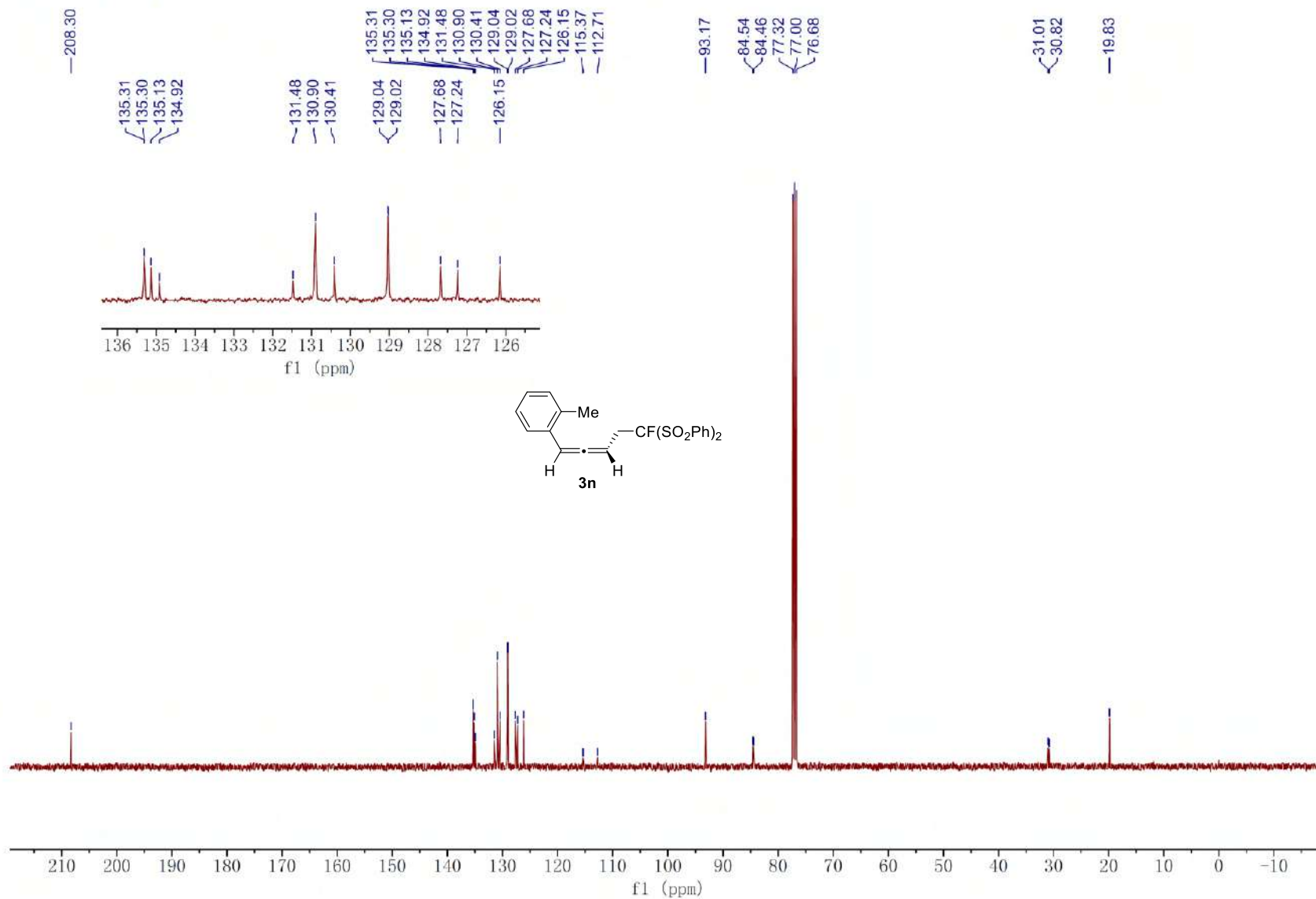
ZHY-ZG-38-376M-F



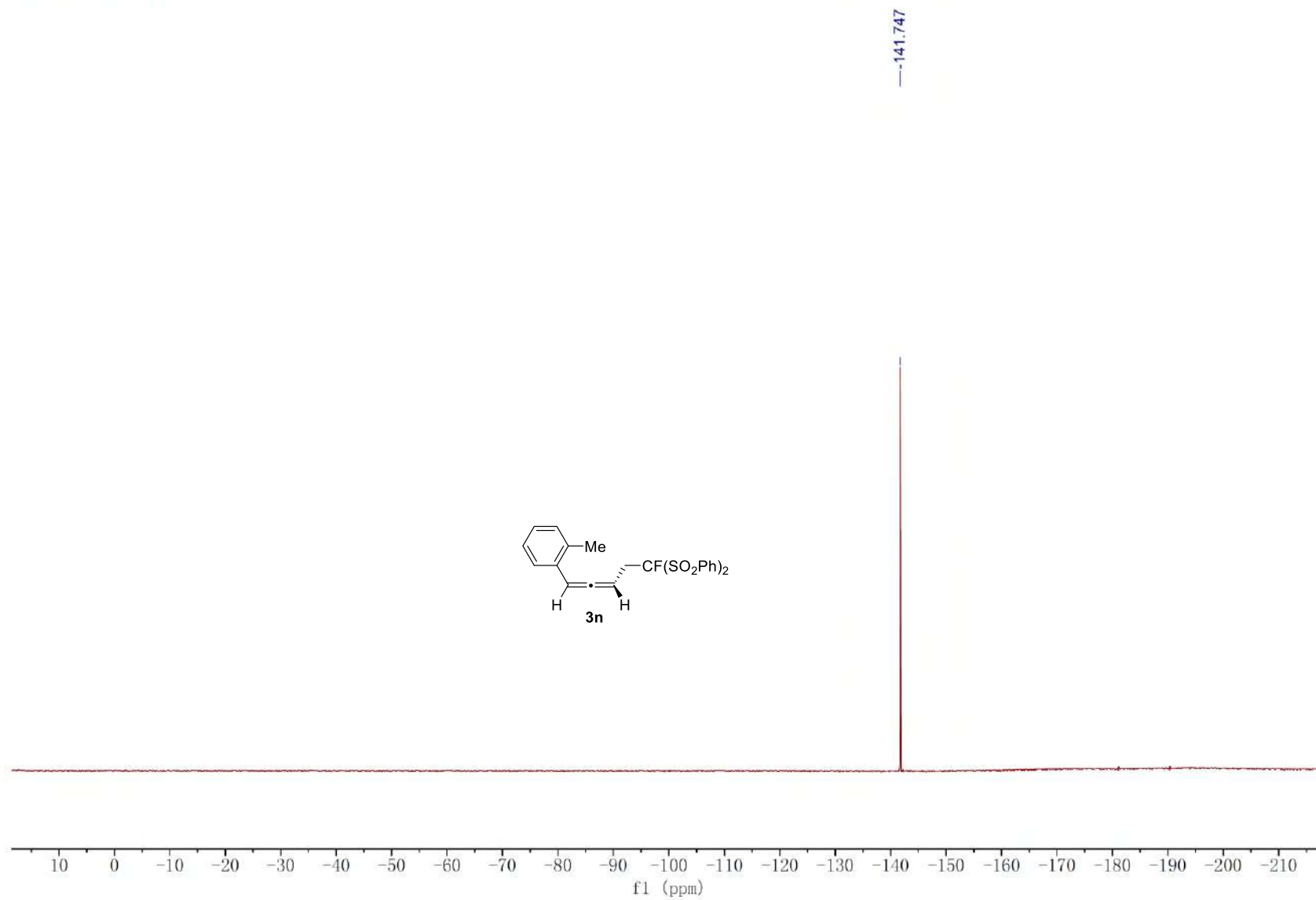
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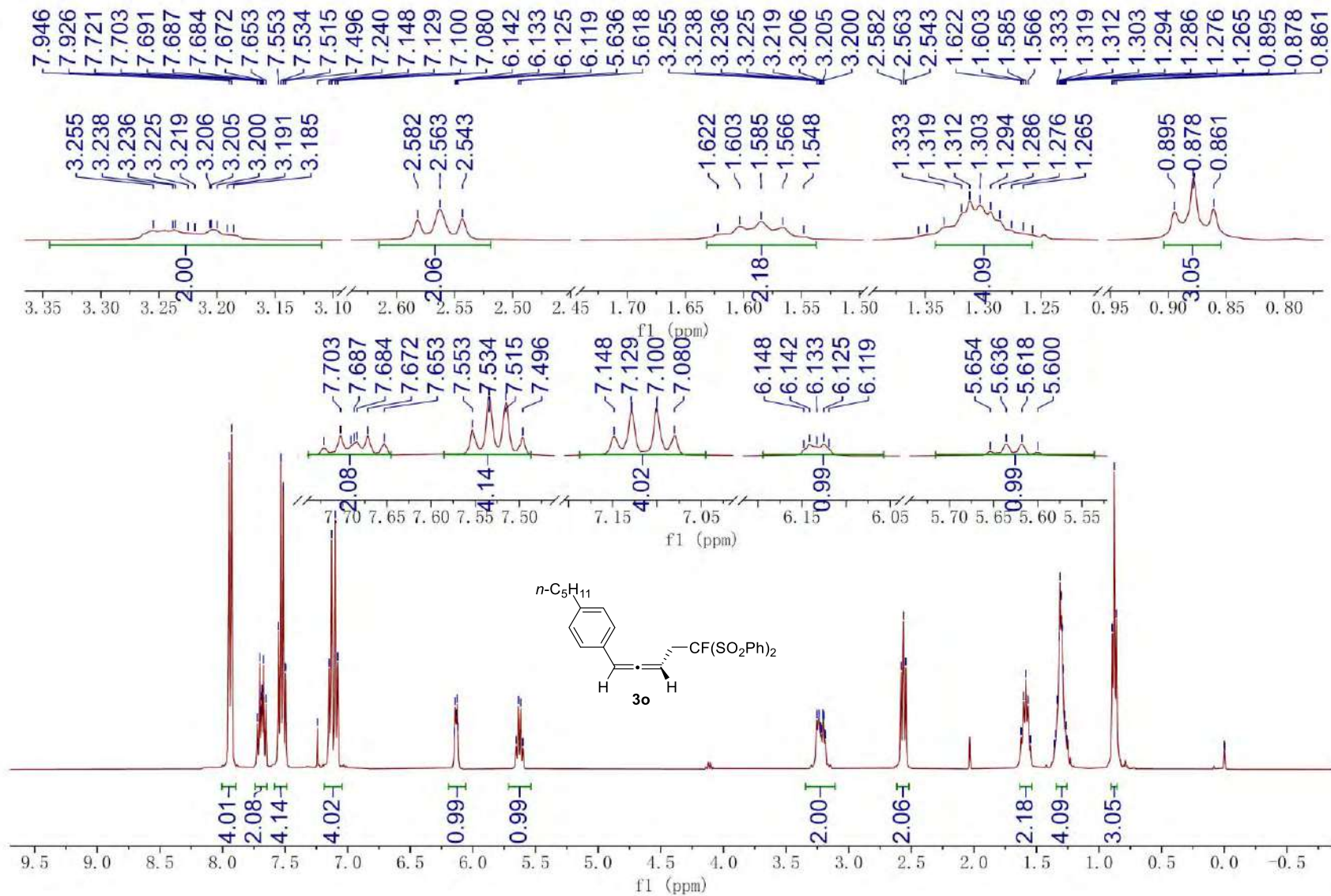


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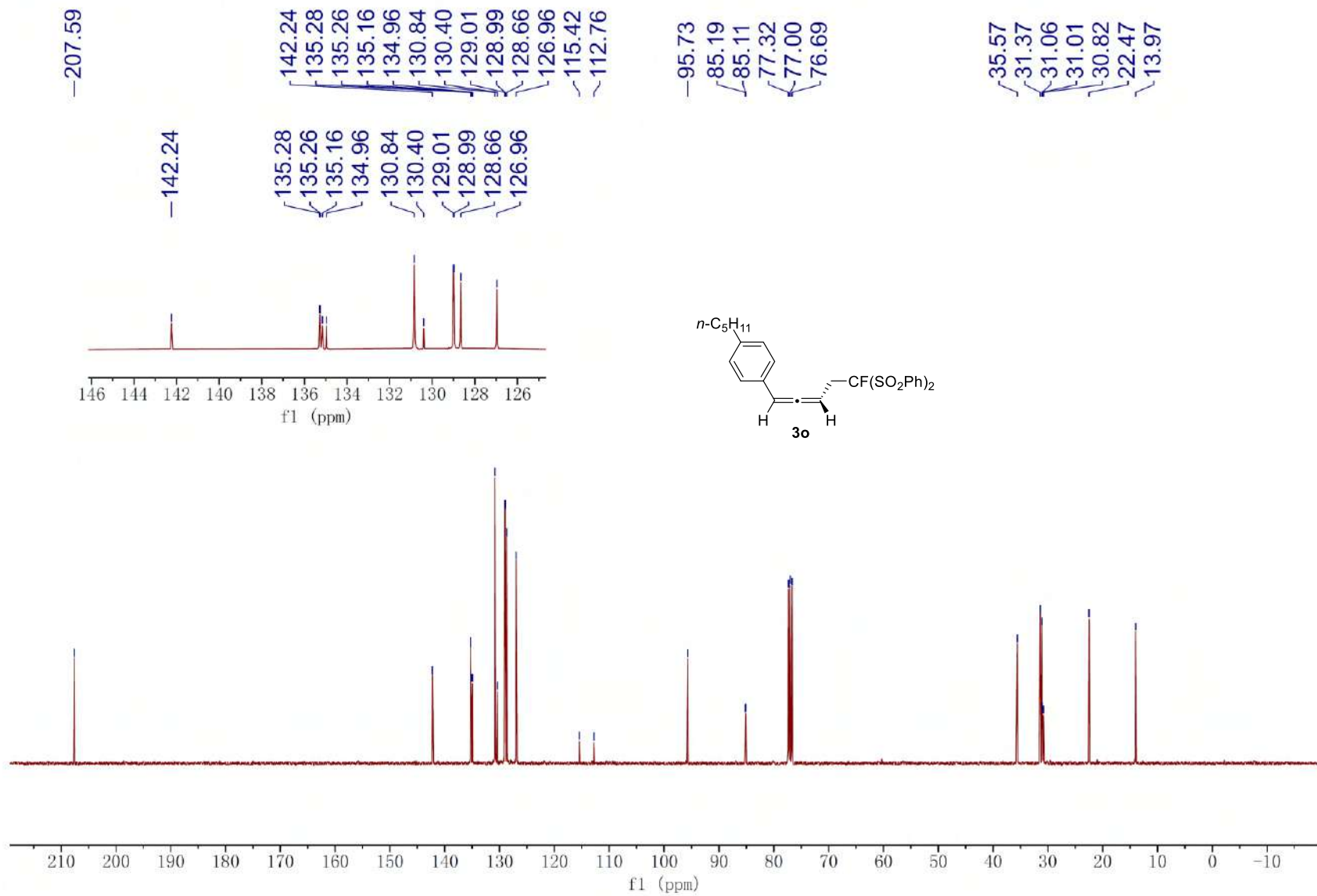


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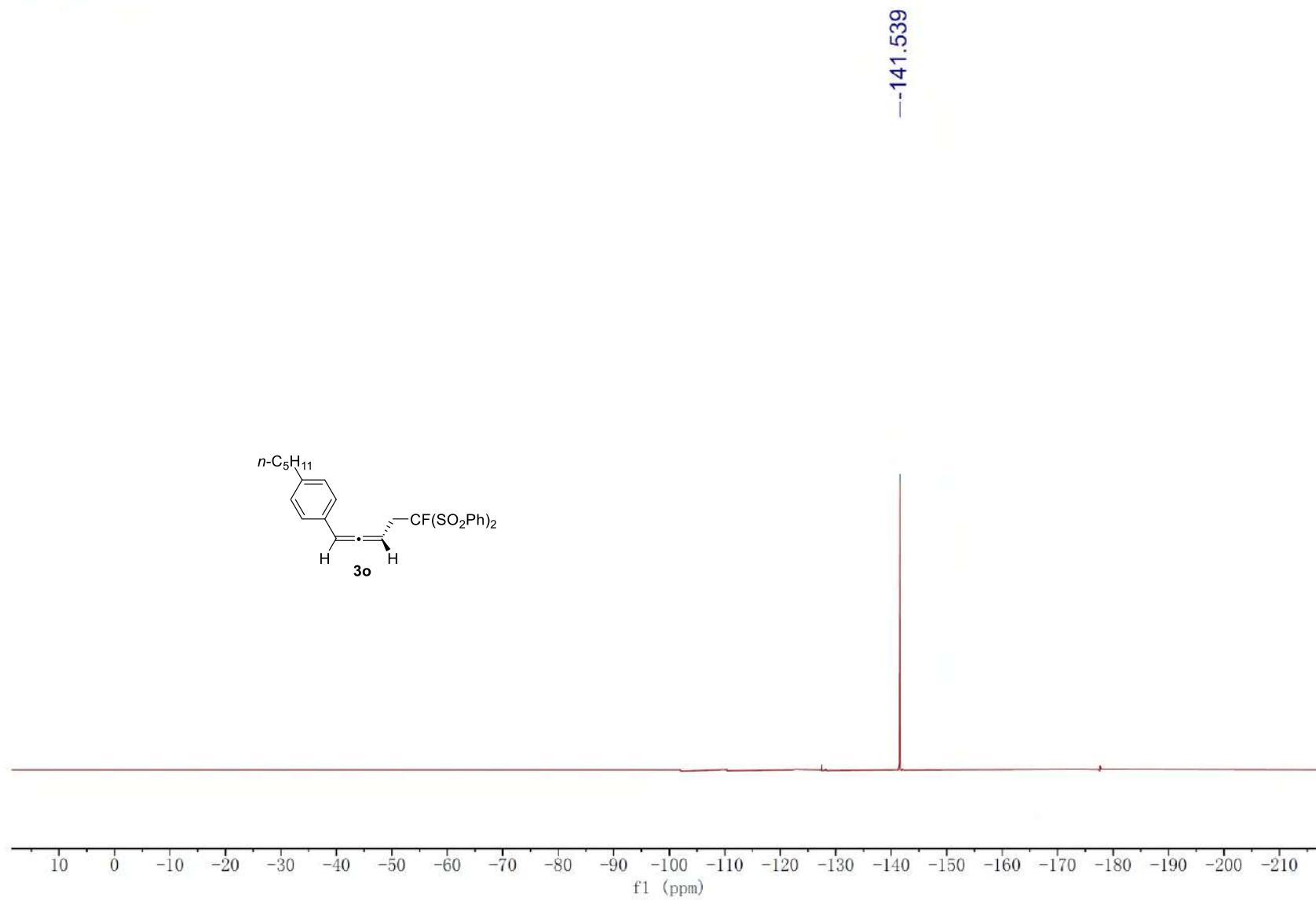




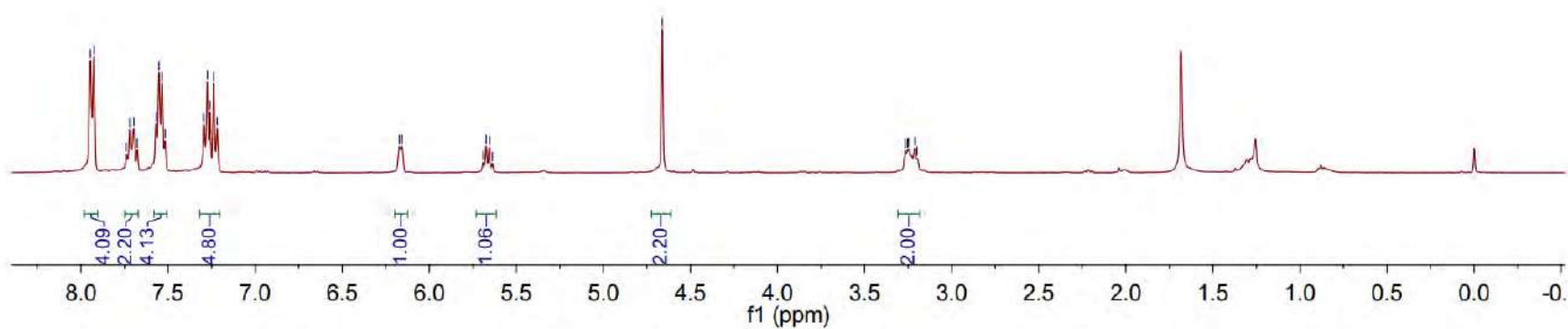
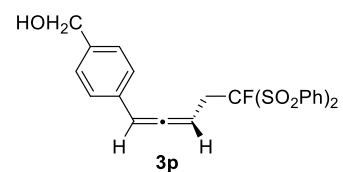
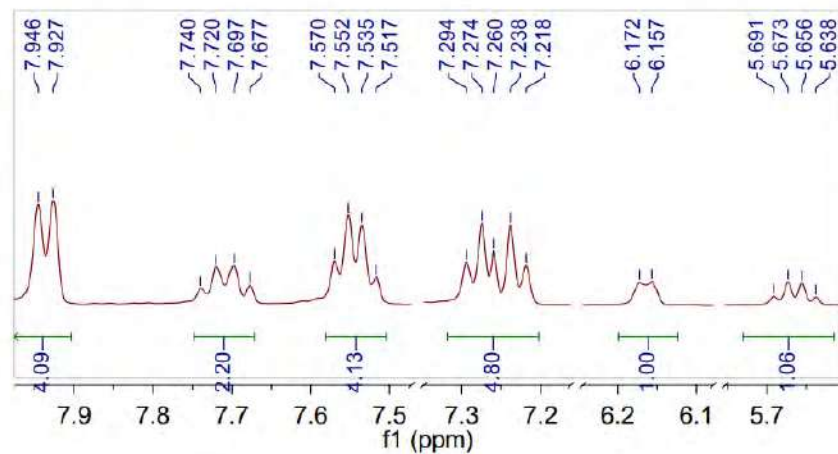
ZHY-ZG-42-100M-C



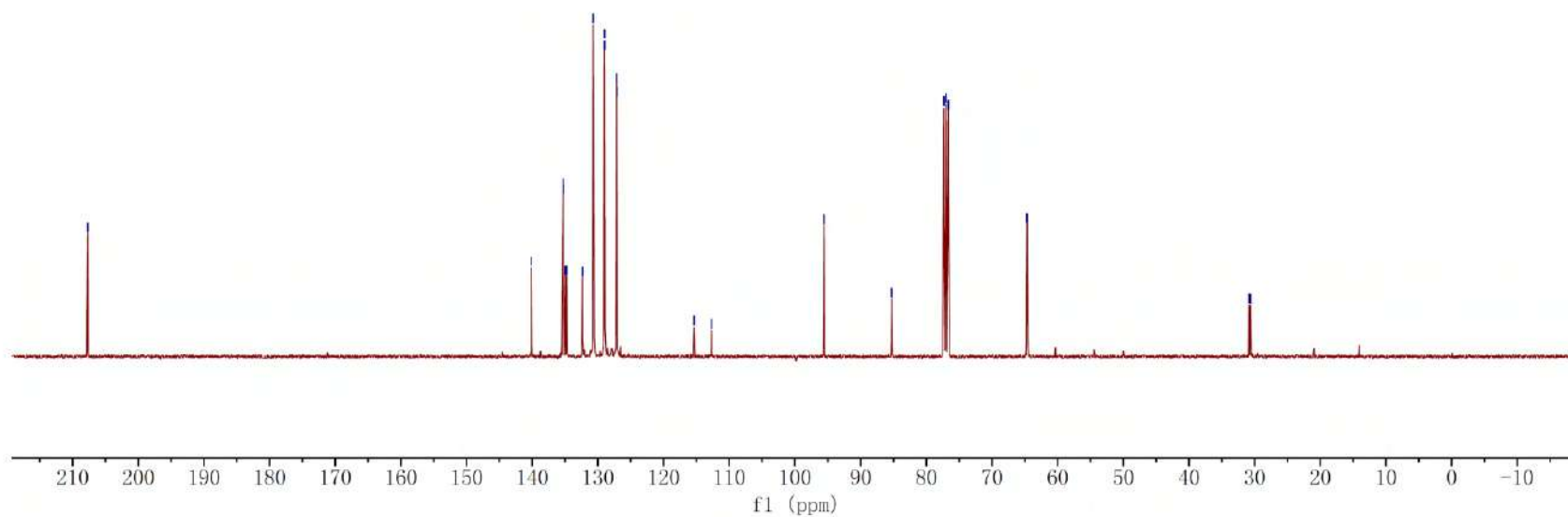
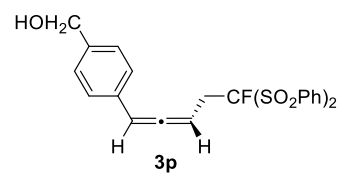
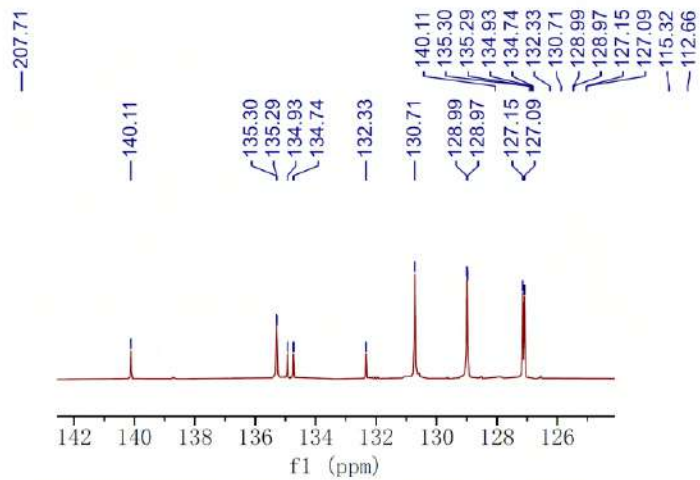
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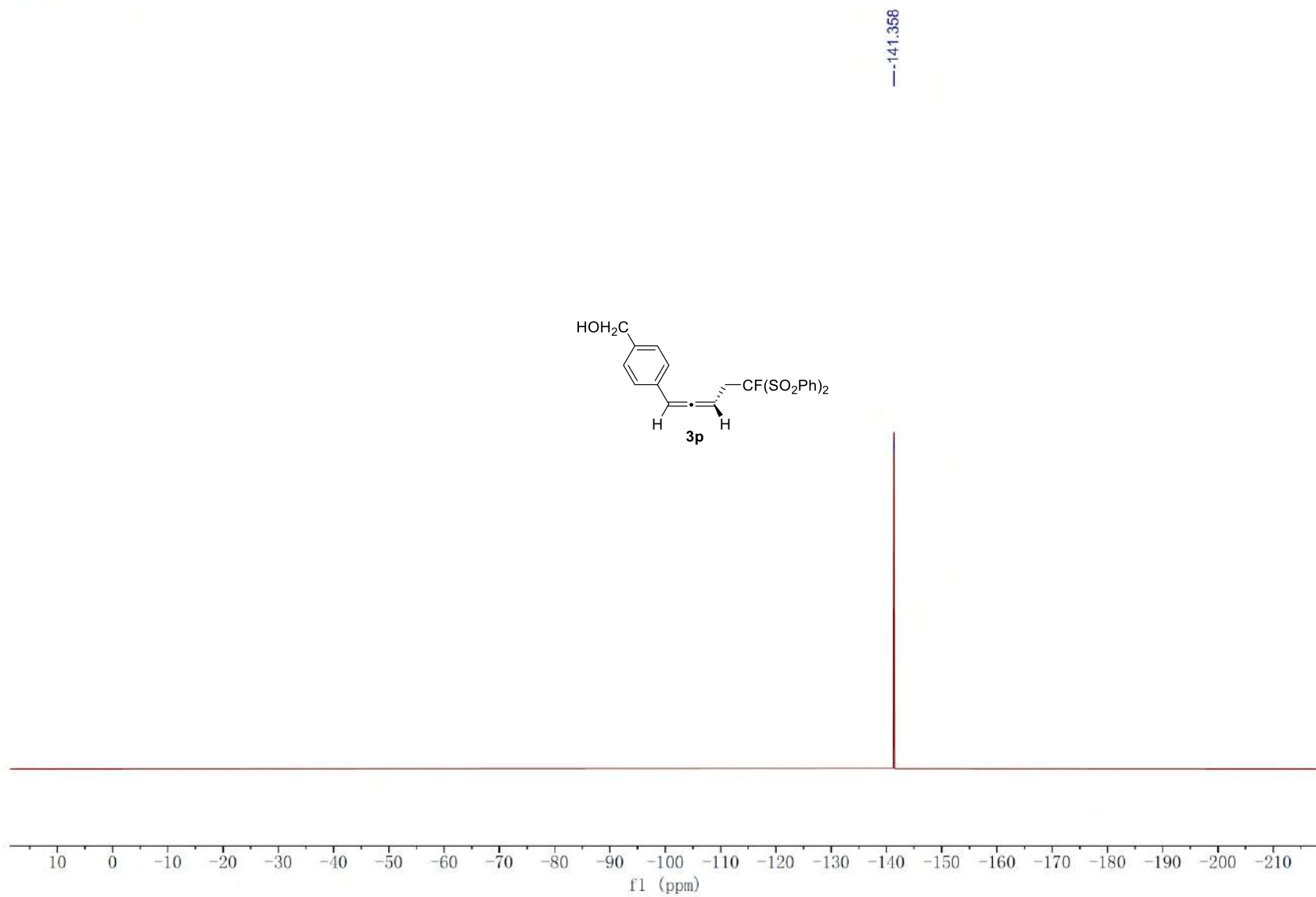
7.946
7.927
7.740
7.720
7.697
7.677
7.570
7.552
7.535
7.517
7.294
7.274
7.260
7.238
7.218
6.172
6.157
5.691
5.673
5.656
5.638
-4.662
3.264
3.253
3.247
3.212
3.199



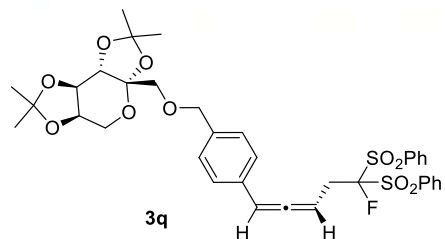
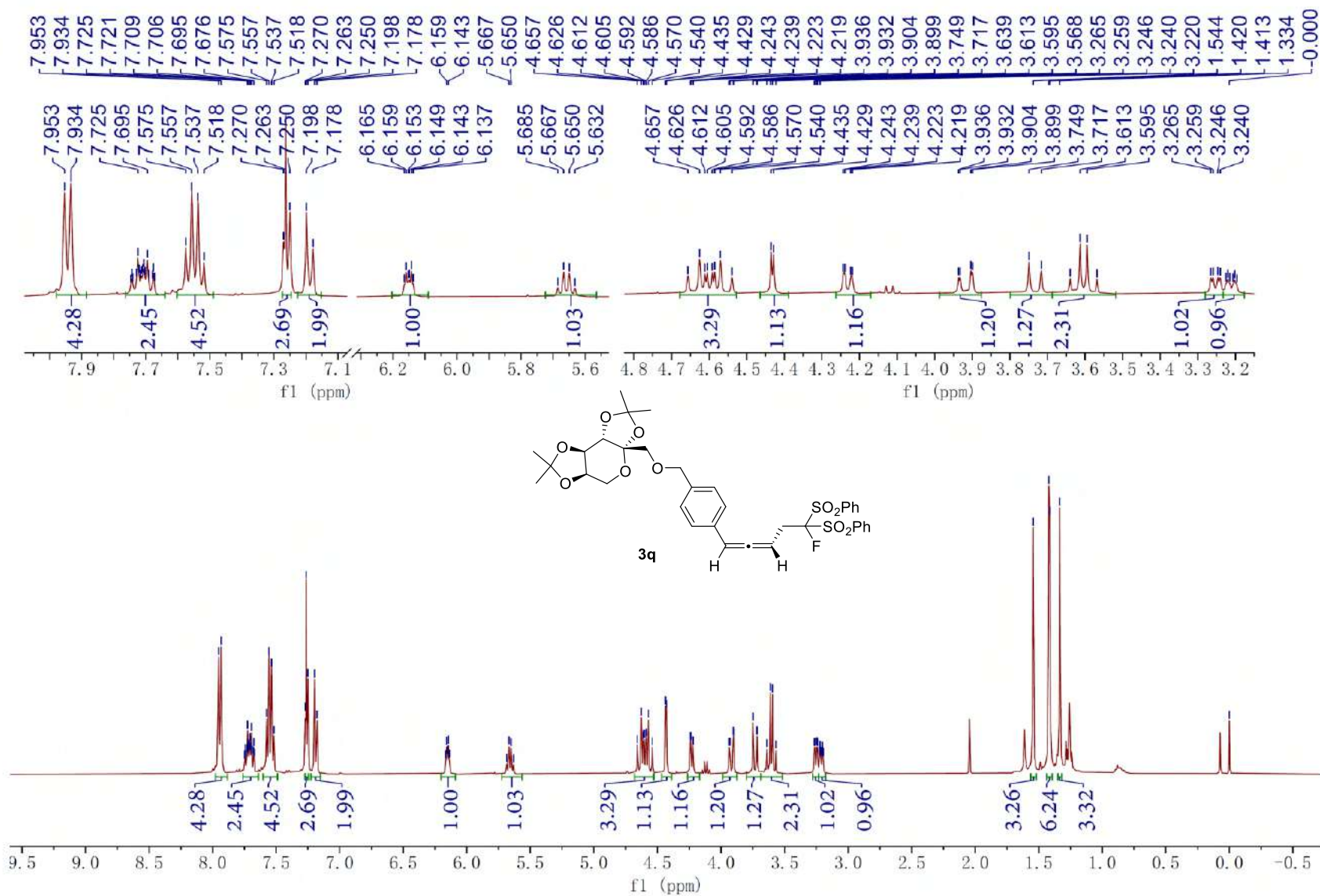
ZHY-ZG-72-100M-C



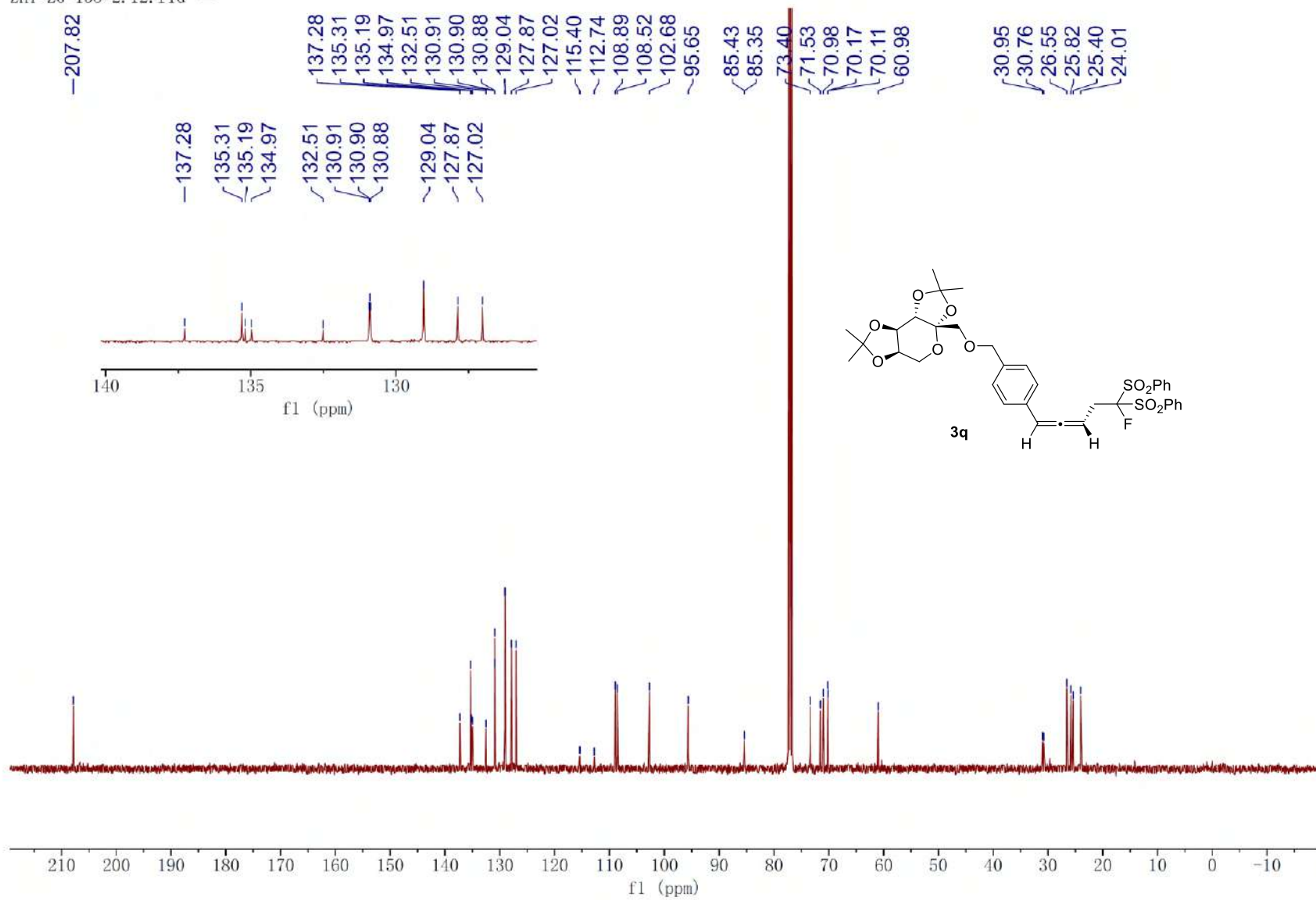
ZHY-ZG-72-376M-H



ZHY-ZG-138-2.10.fid —



ZHY-ZG-138-2.12.fid —



ZHY-ZG-138-2.11.fid —

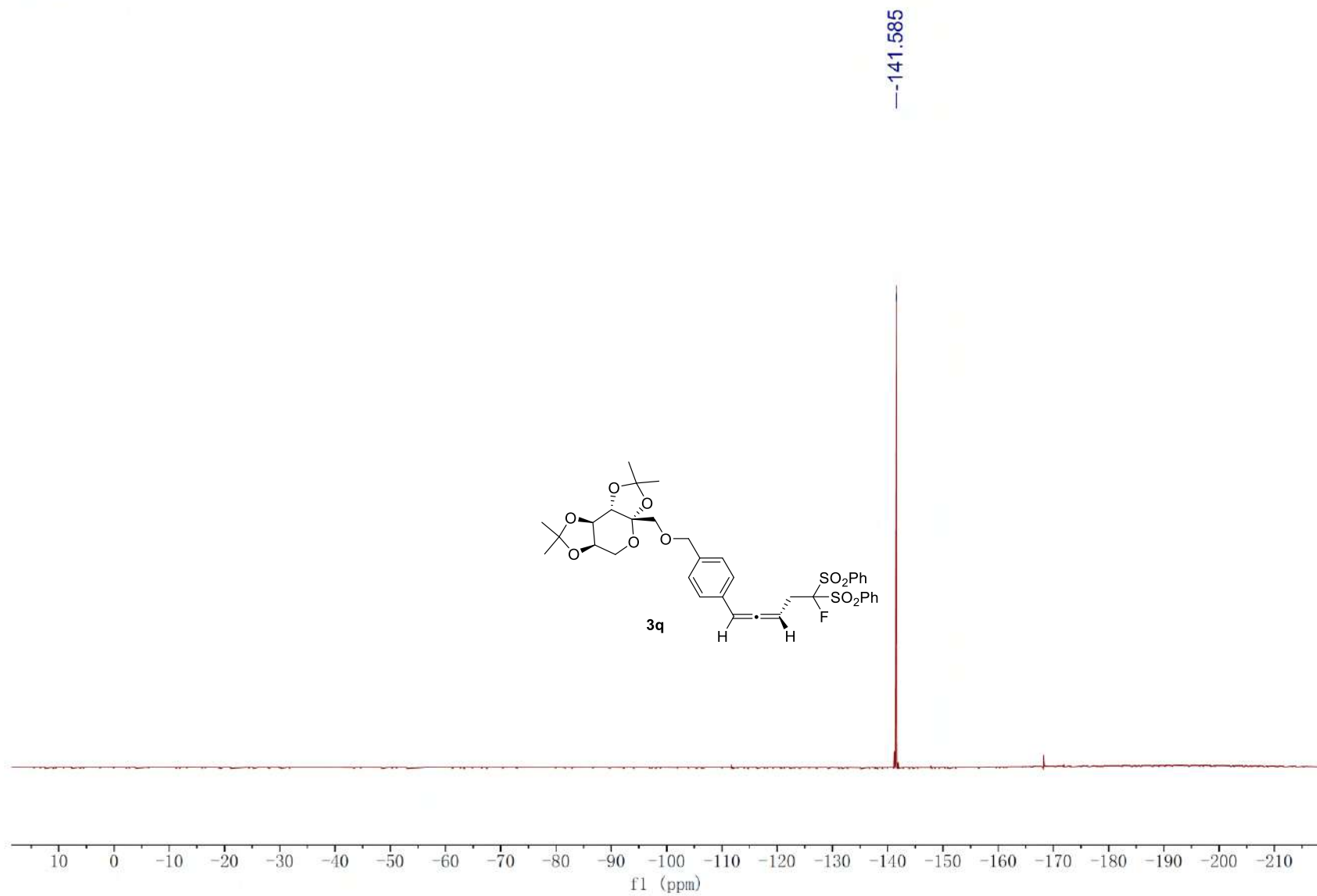
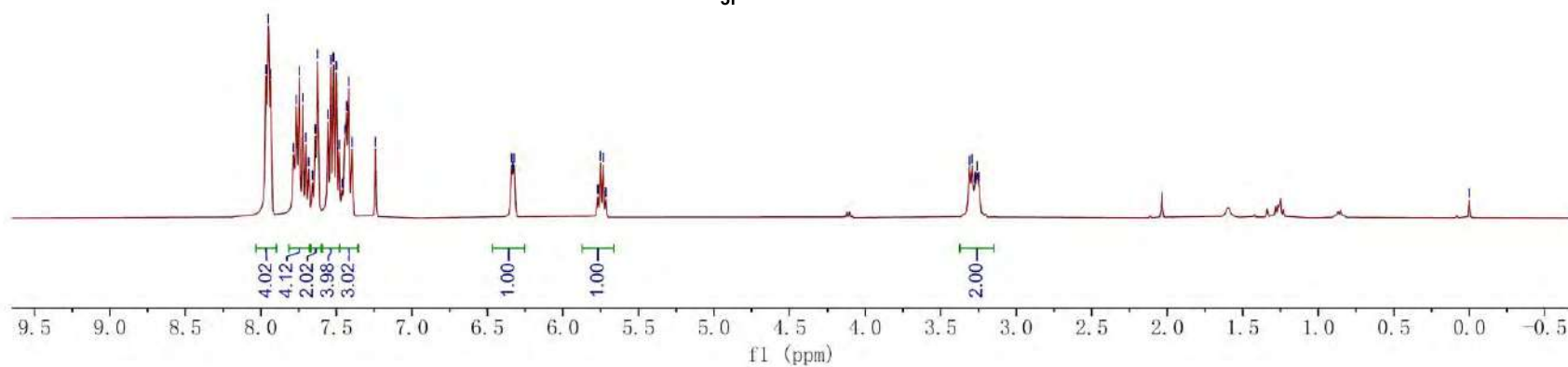
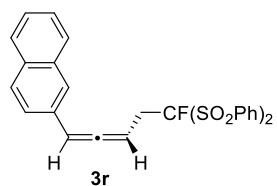
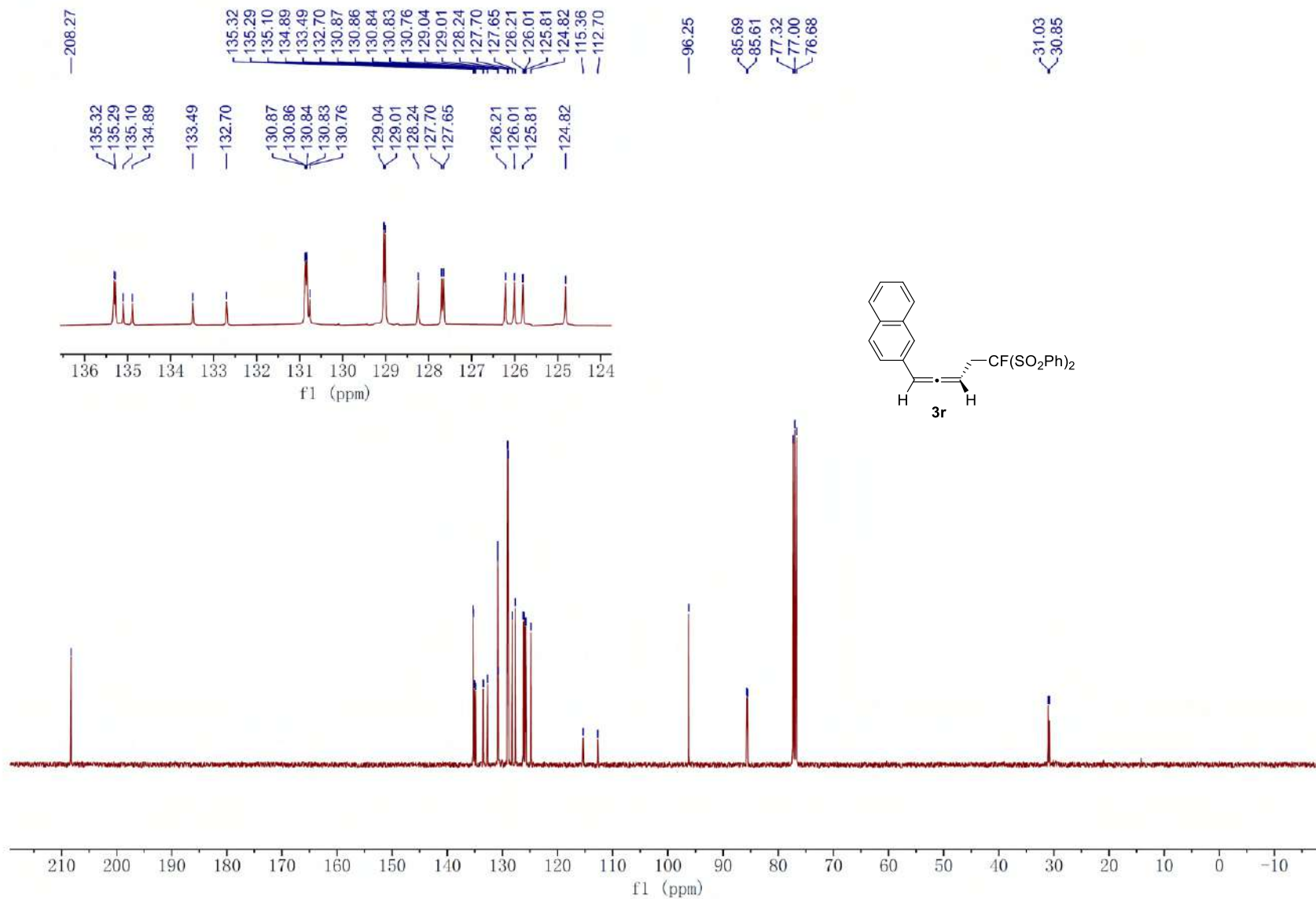


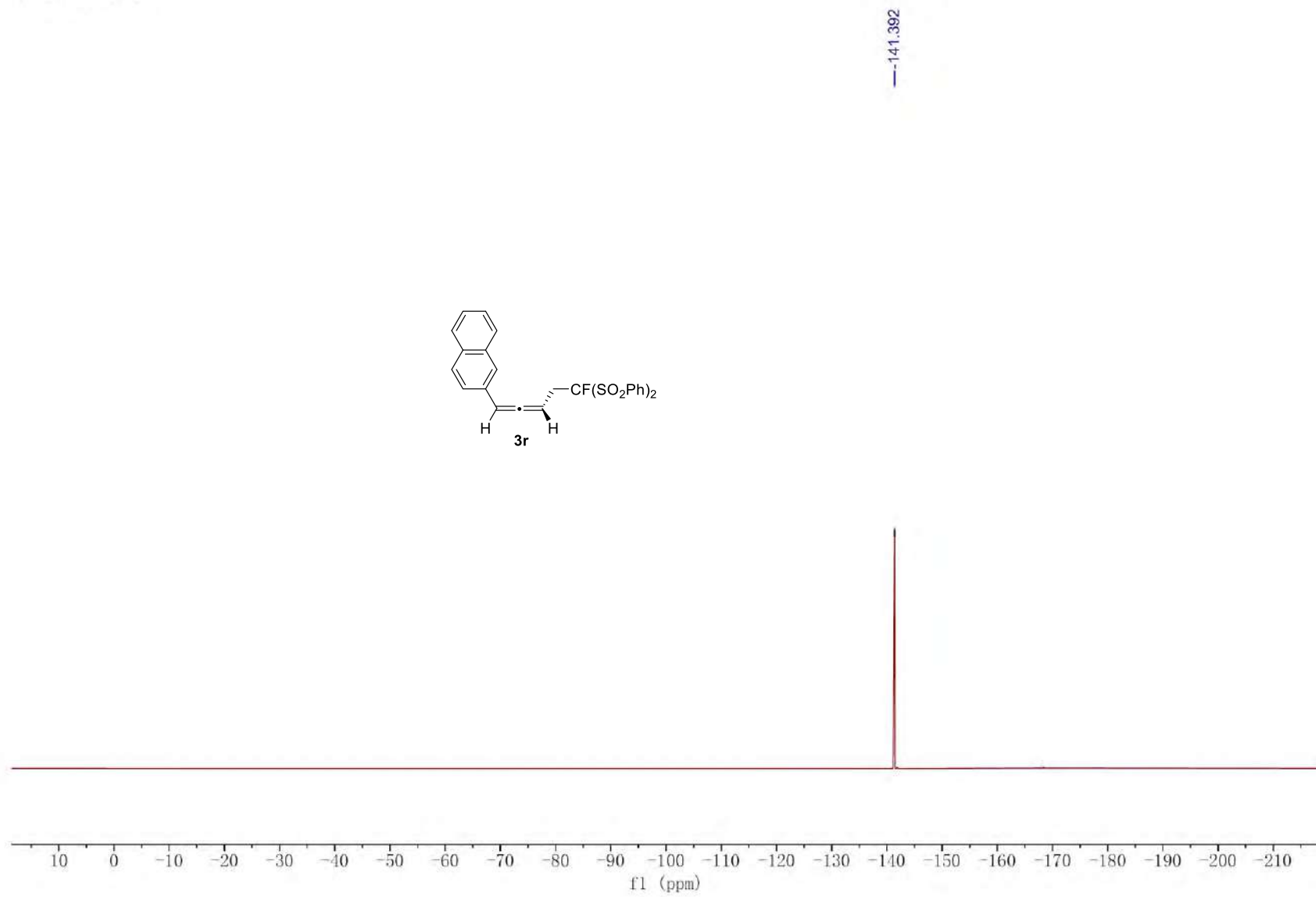
Figure 1 displays two ^1H NMR spectra of compound **1**. The top spectrum, recorded in CDCl_3 , shows peaks in the aromatic region (7.4–8.1 ppm) with integration values of 4.02, 4.12, 2.02, 3.98, and 3.02. The bottom spectrum, recorded in $\text{DMSO}-d_6$, shows peaks in the aliphatic region (3.1–6.5 ppm) with integration values of 1.00, 1.00, and 2.00. Chemical shift labels (ppm) are provided for each peak.



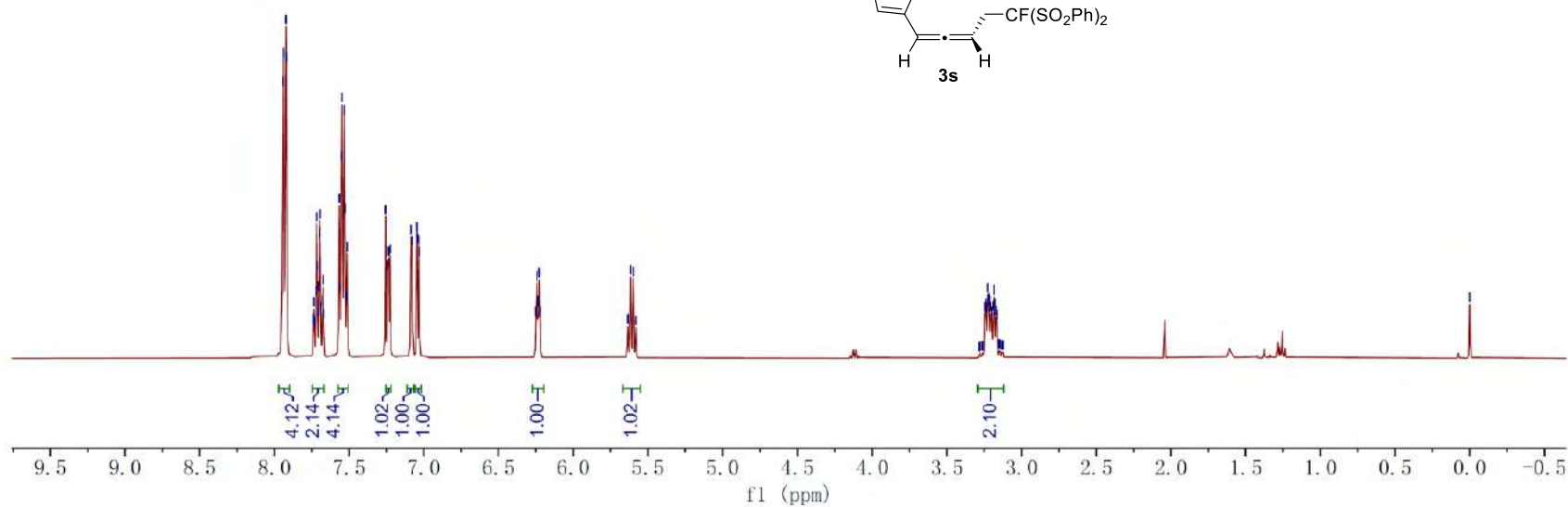
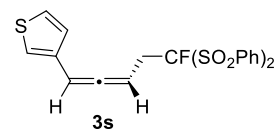
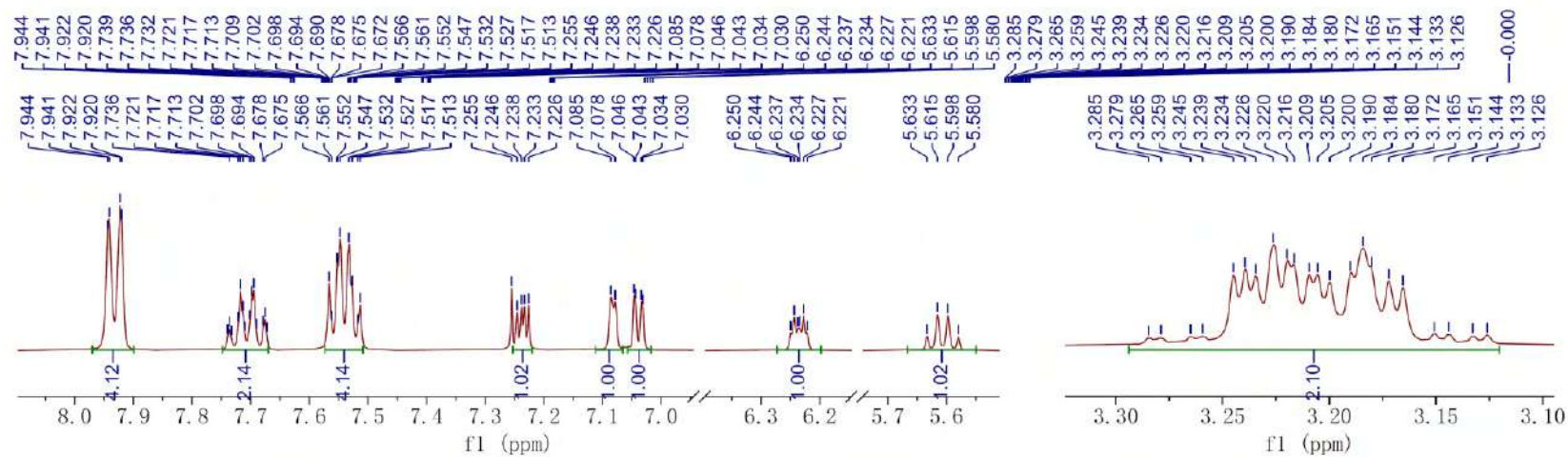
ZHY-ZG-62-100M-C



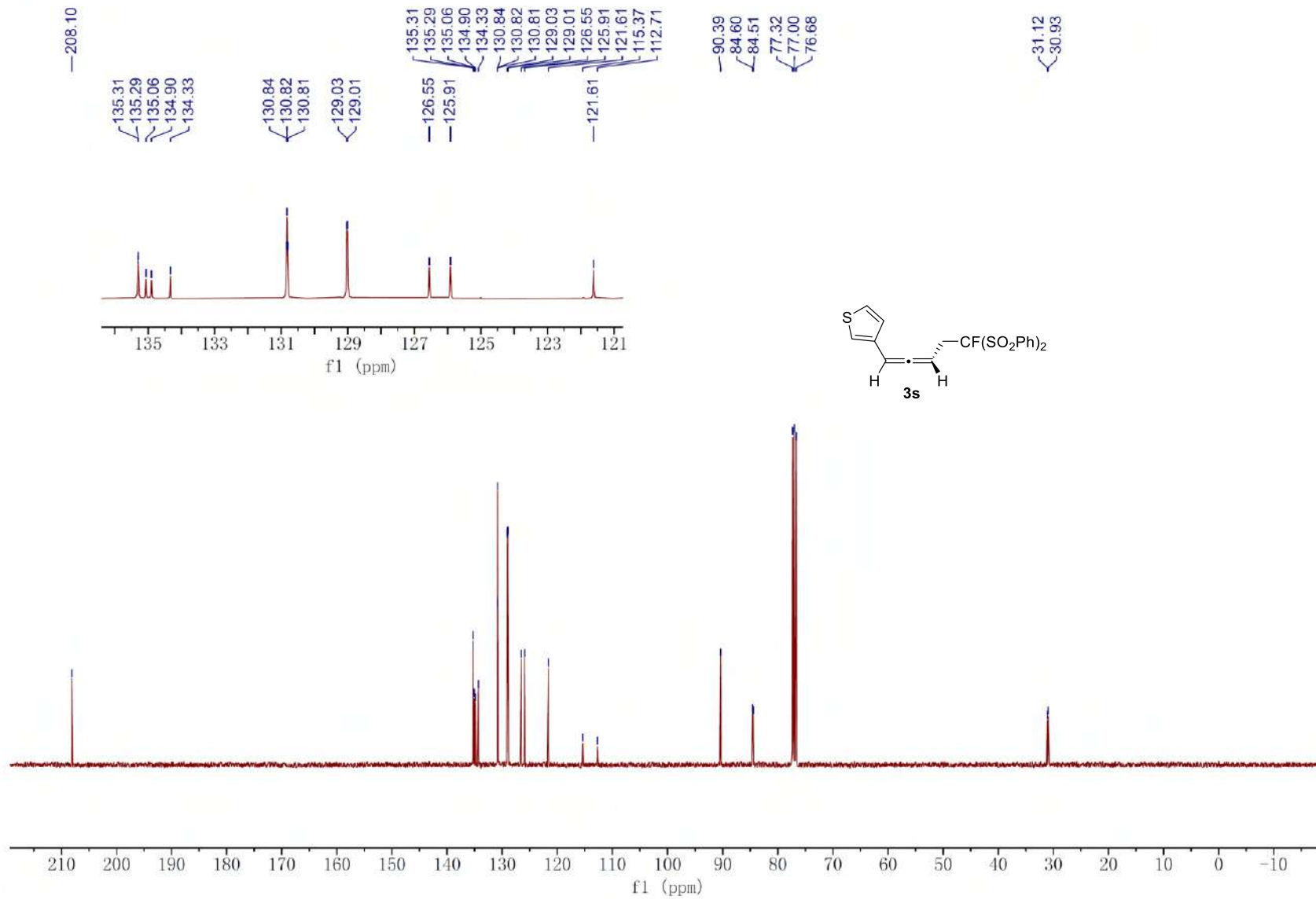
ZHYY-ZG-62-376M-F



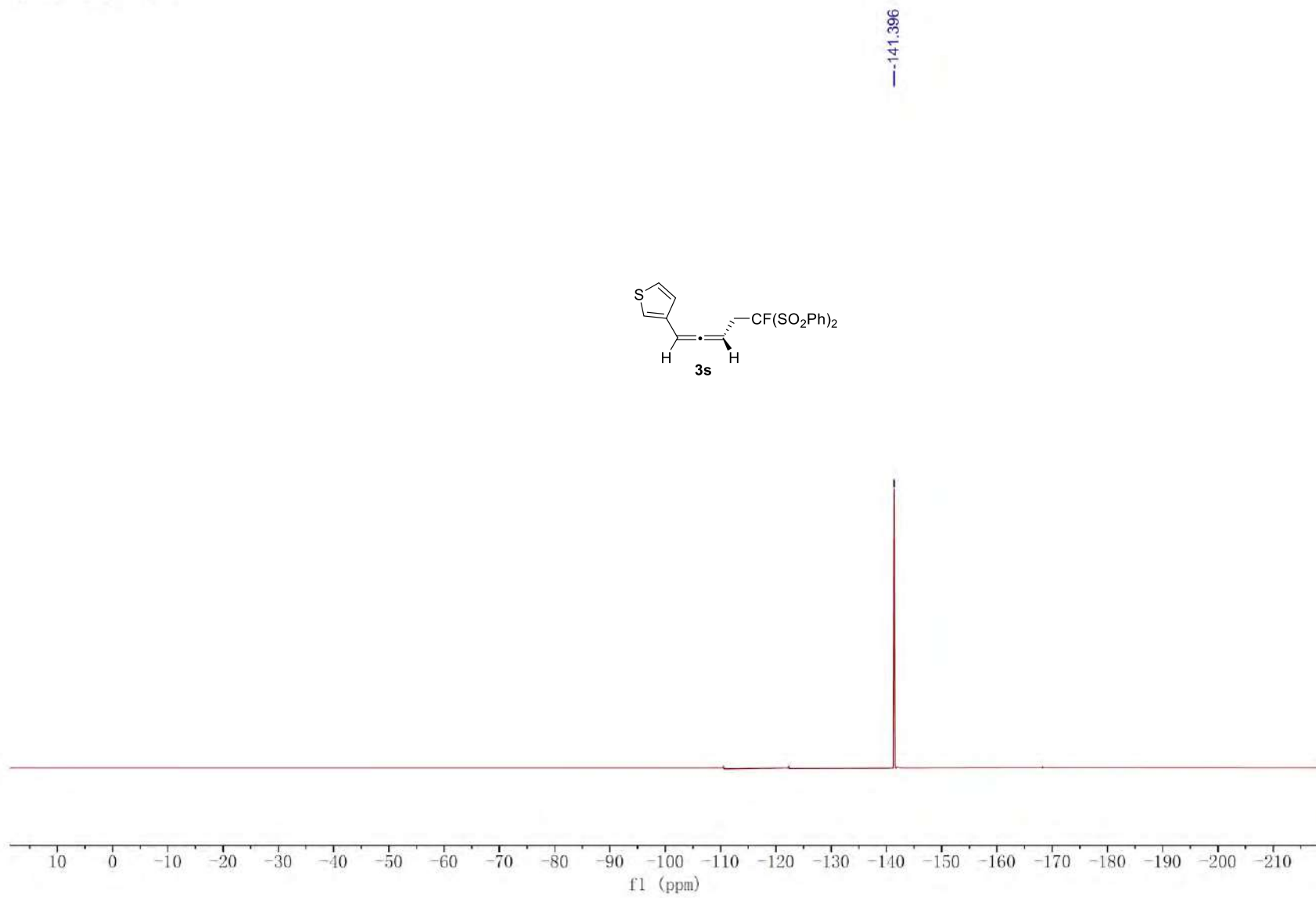
ZHY-ZH-10.10.fid —



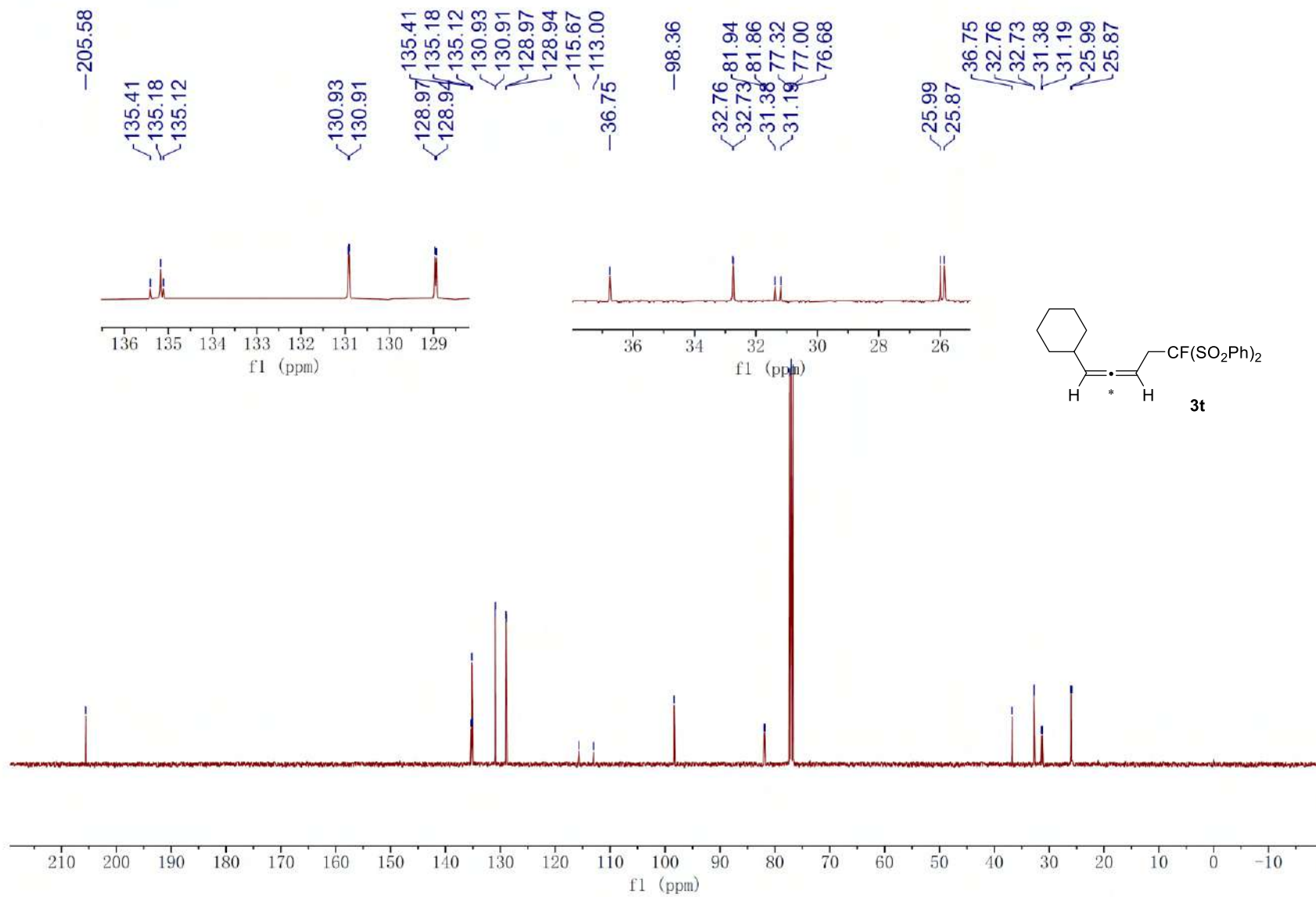
ZHY-ZH-10. 12. fid —



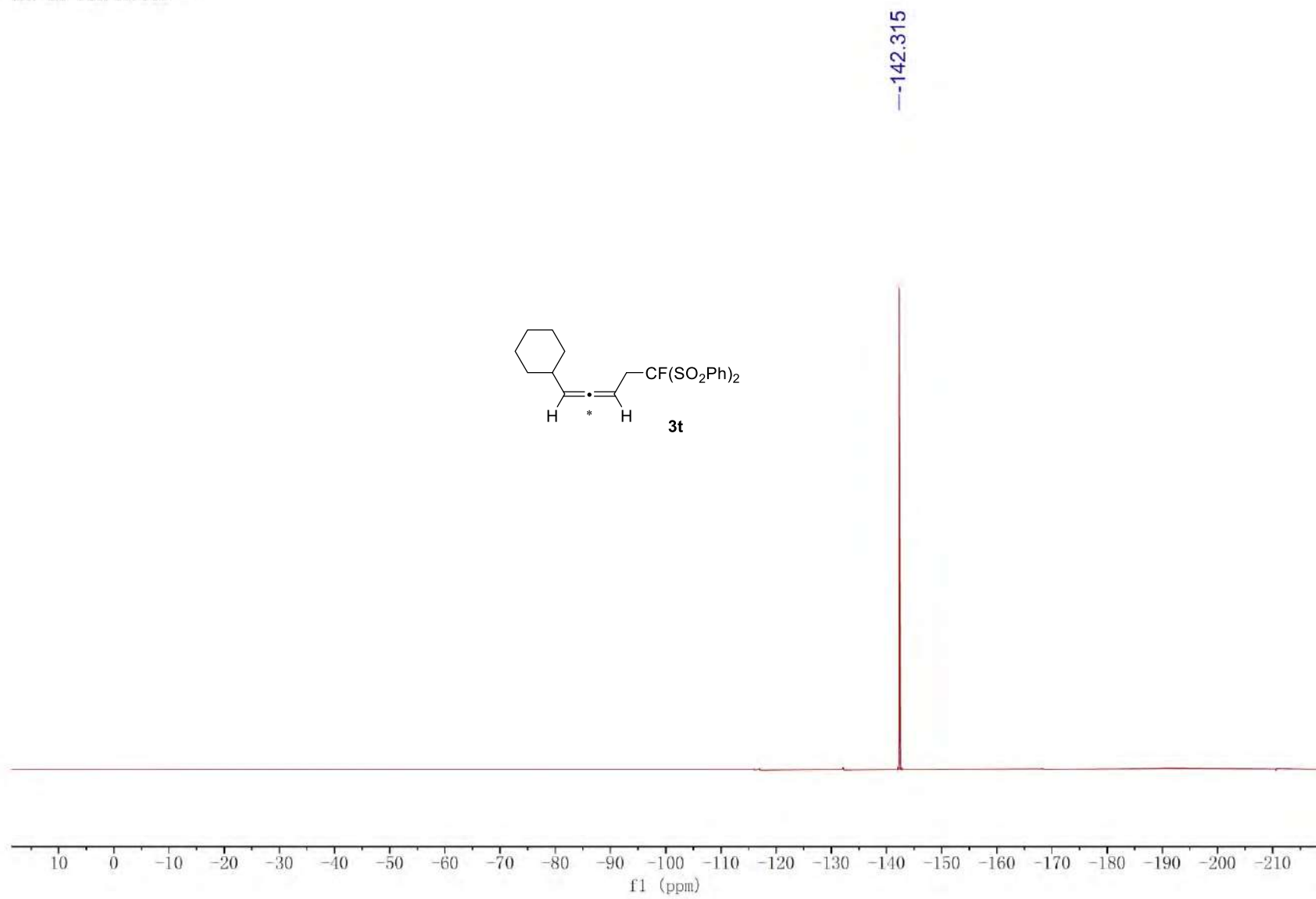
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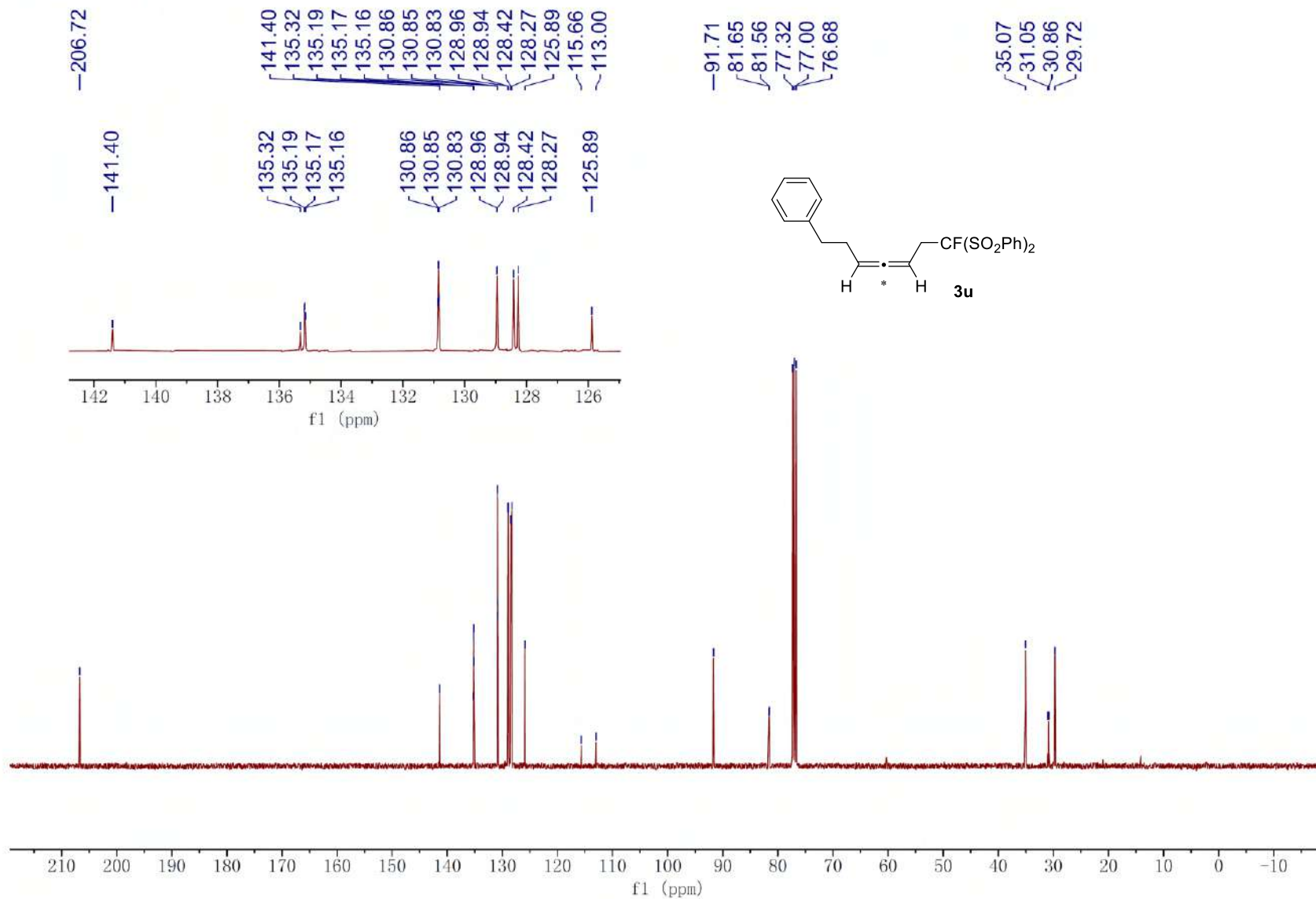
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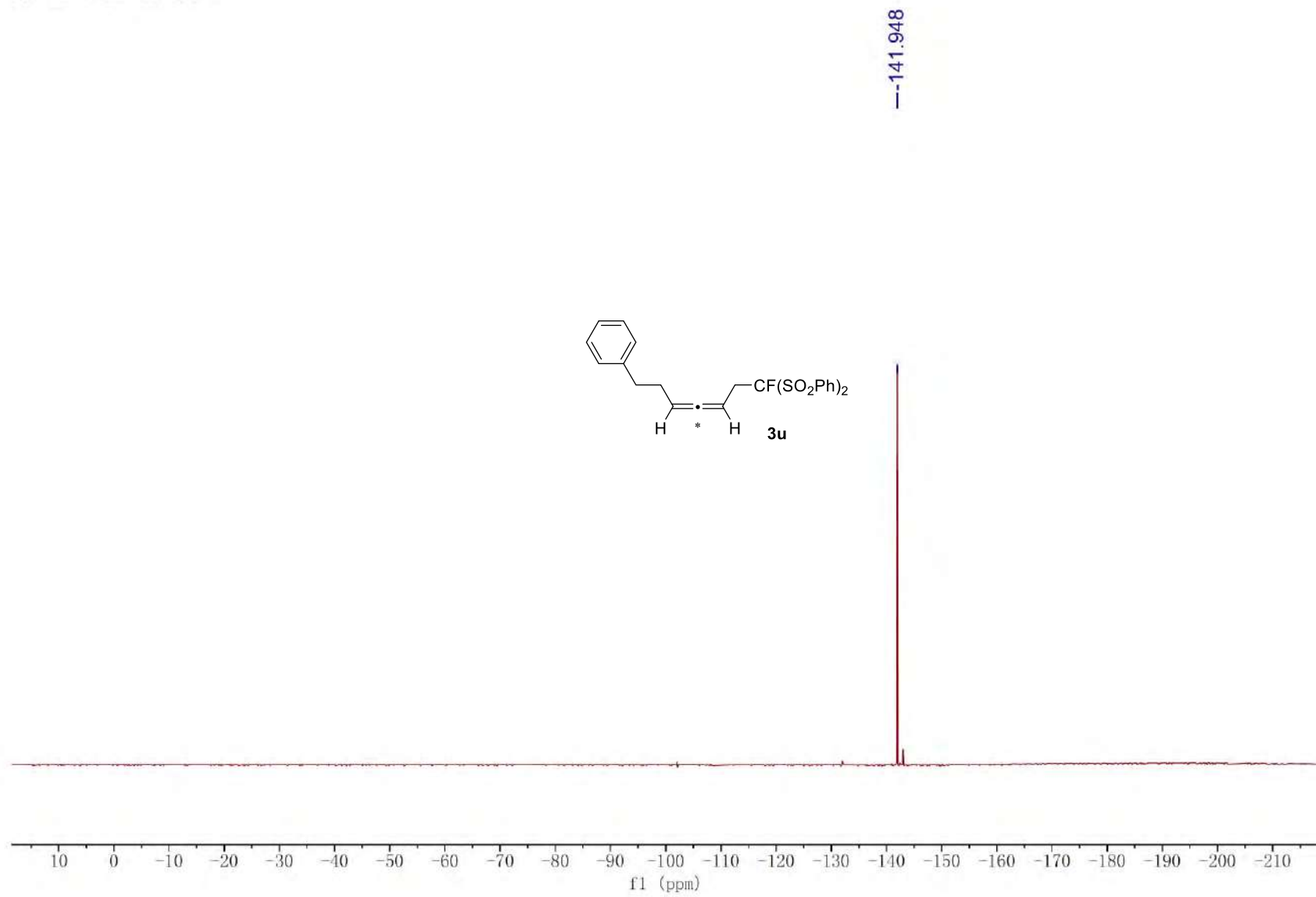
ZHY-ZG-146.13.fid —

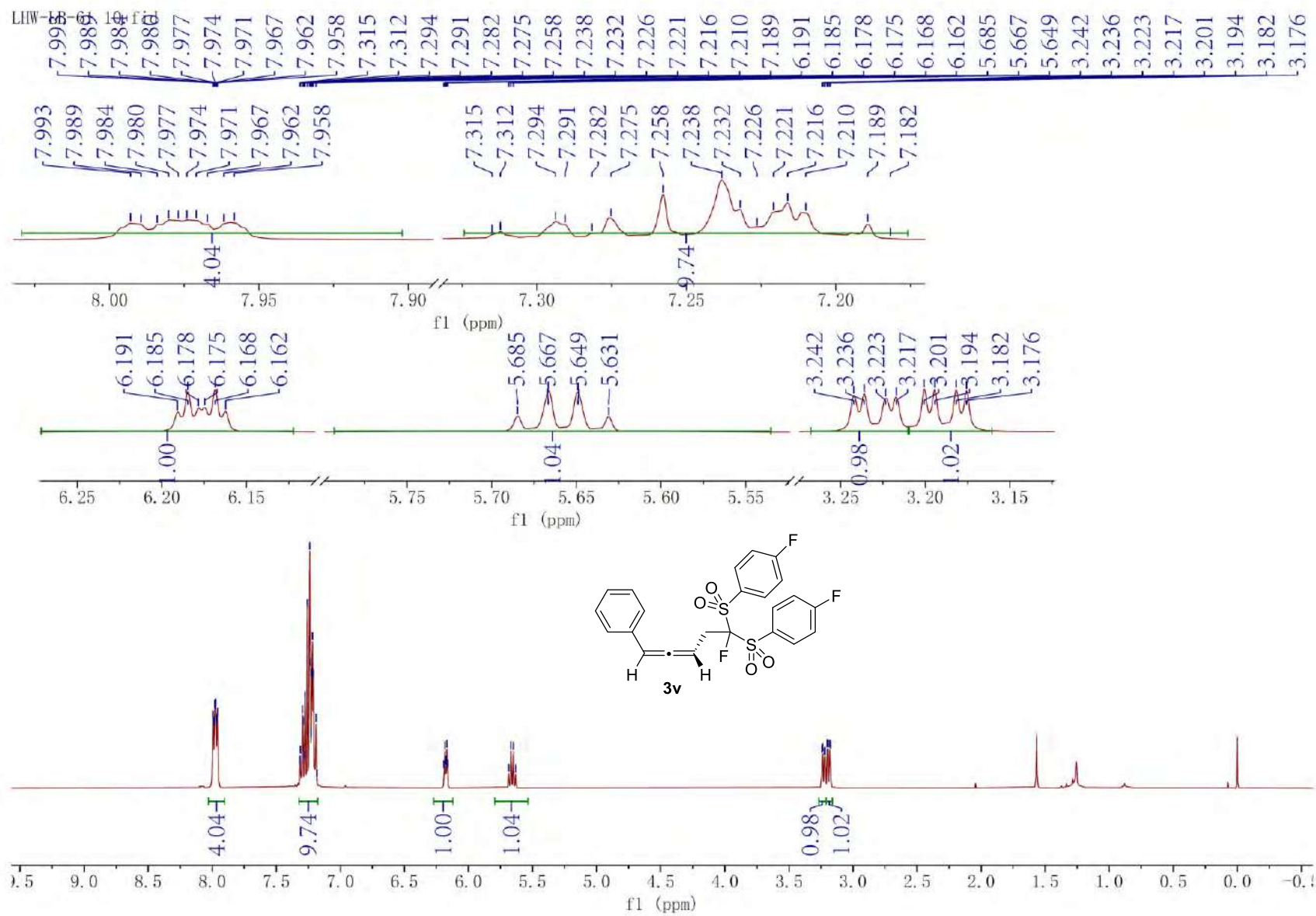


ZHY-ZH-29.13.fid —

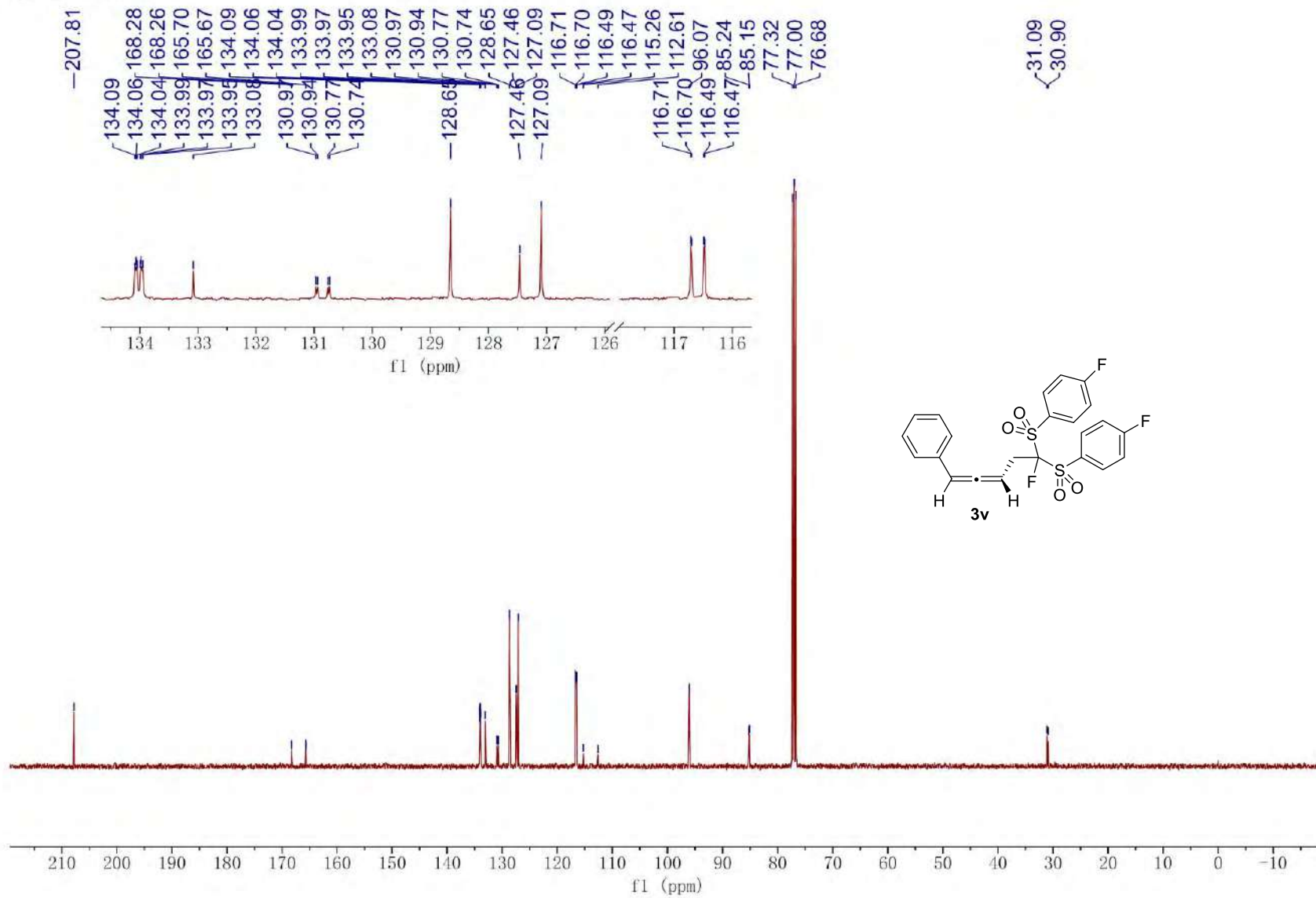


LIL-LL-55-HCF.21.fid —

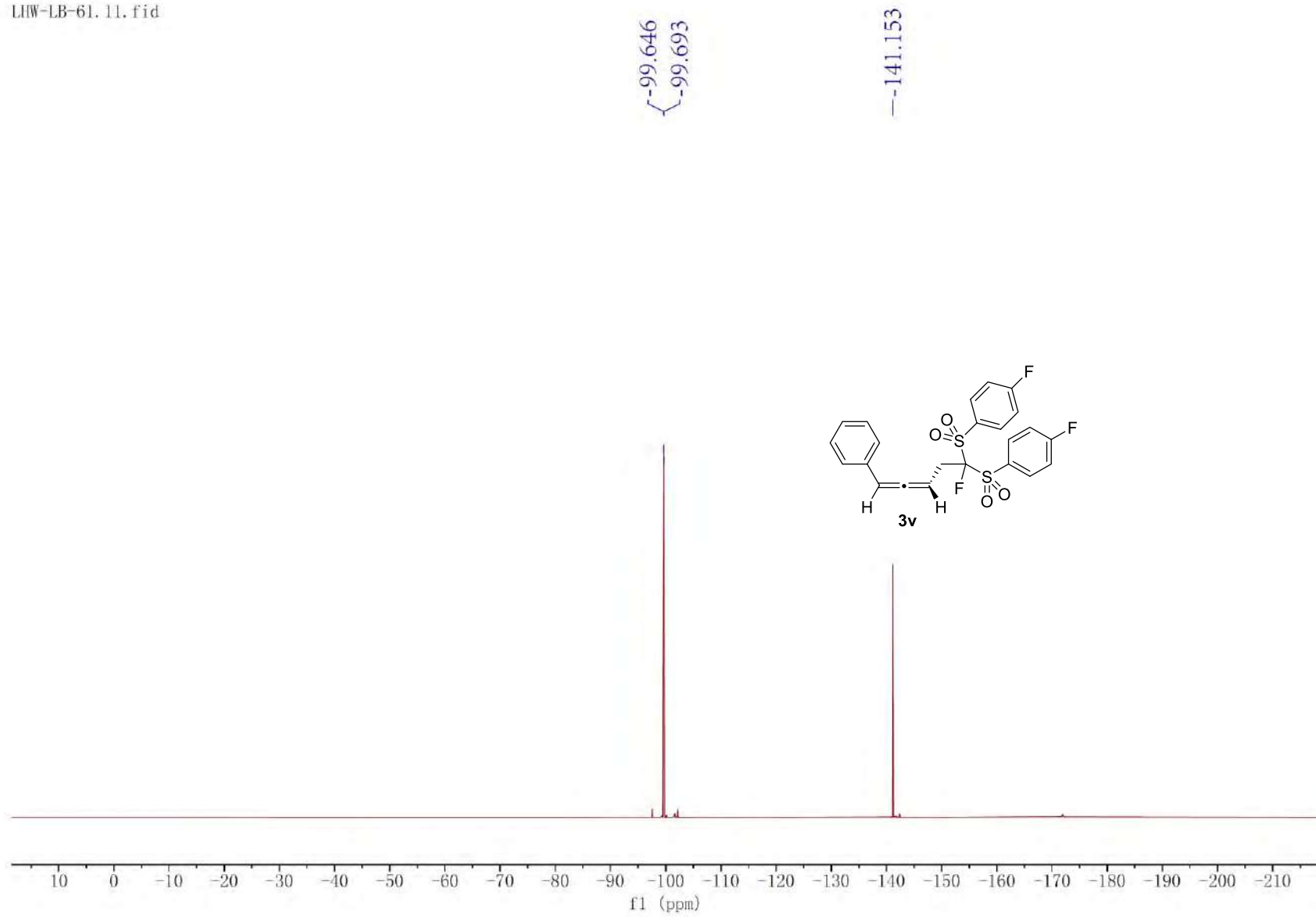




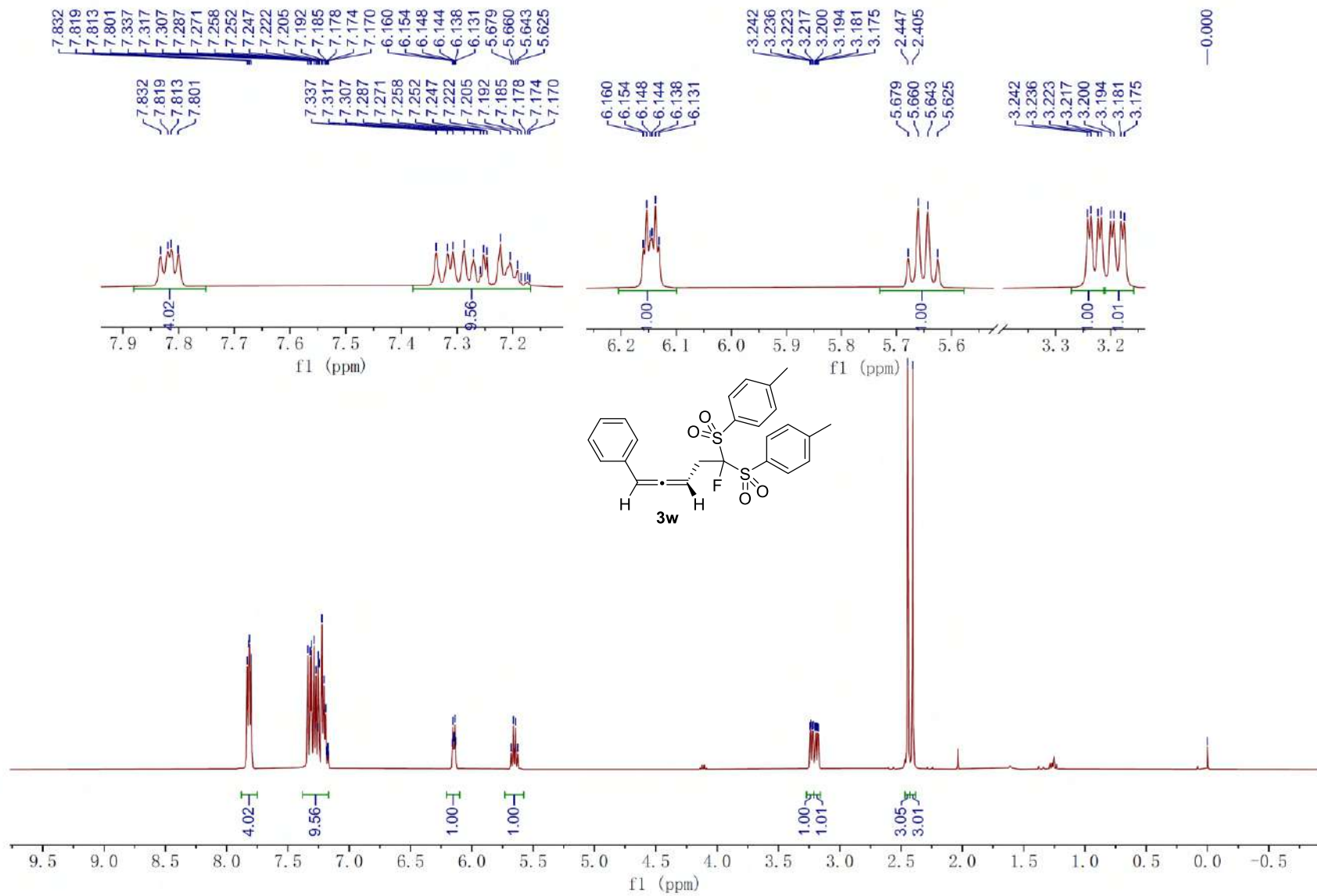
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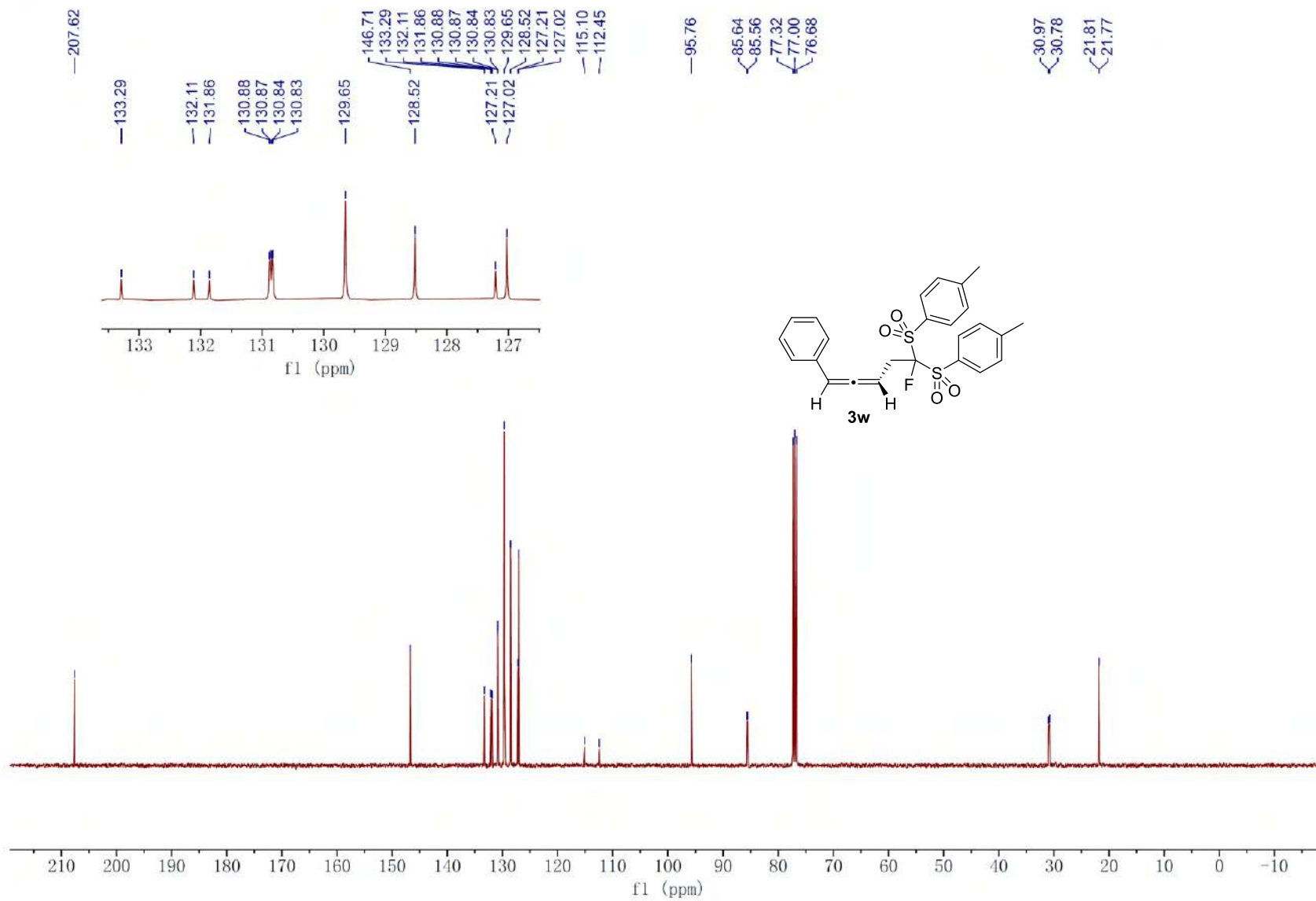
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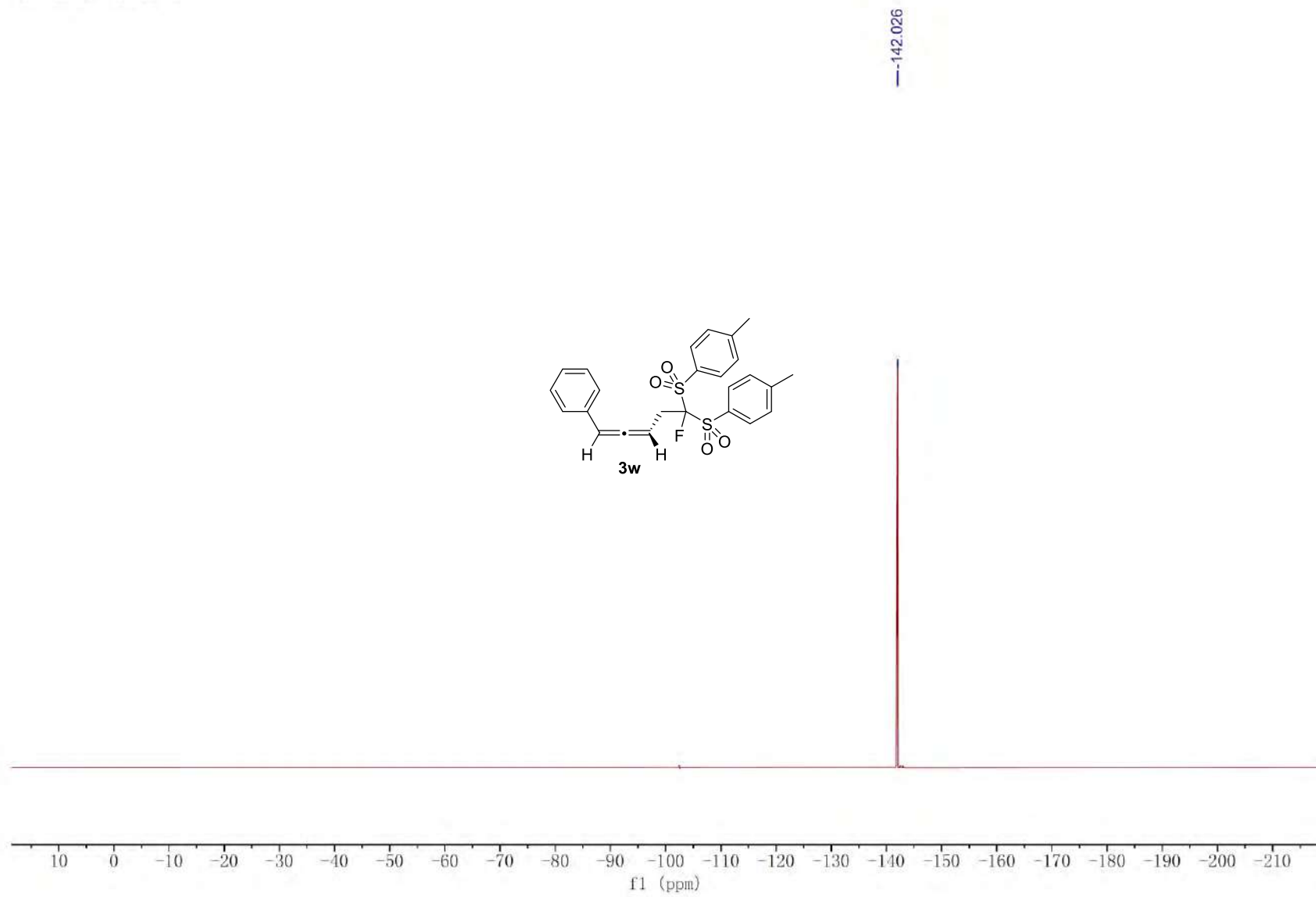
ZHY-ZH-35.10.fid —



ZHY-ZH-35.12.fid —

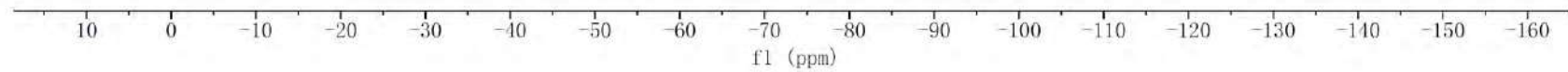
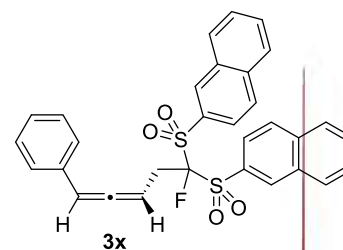


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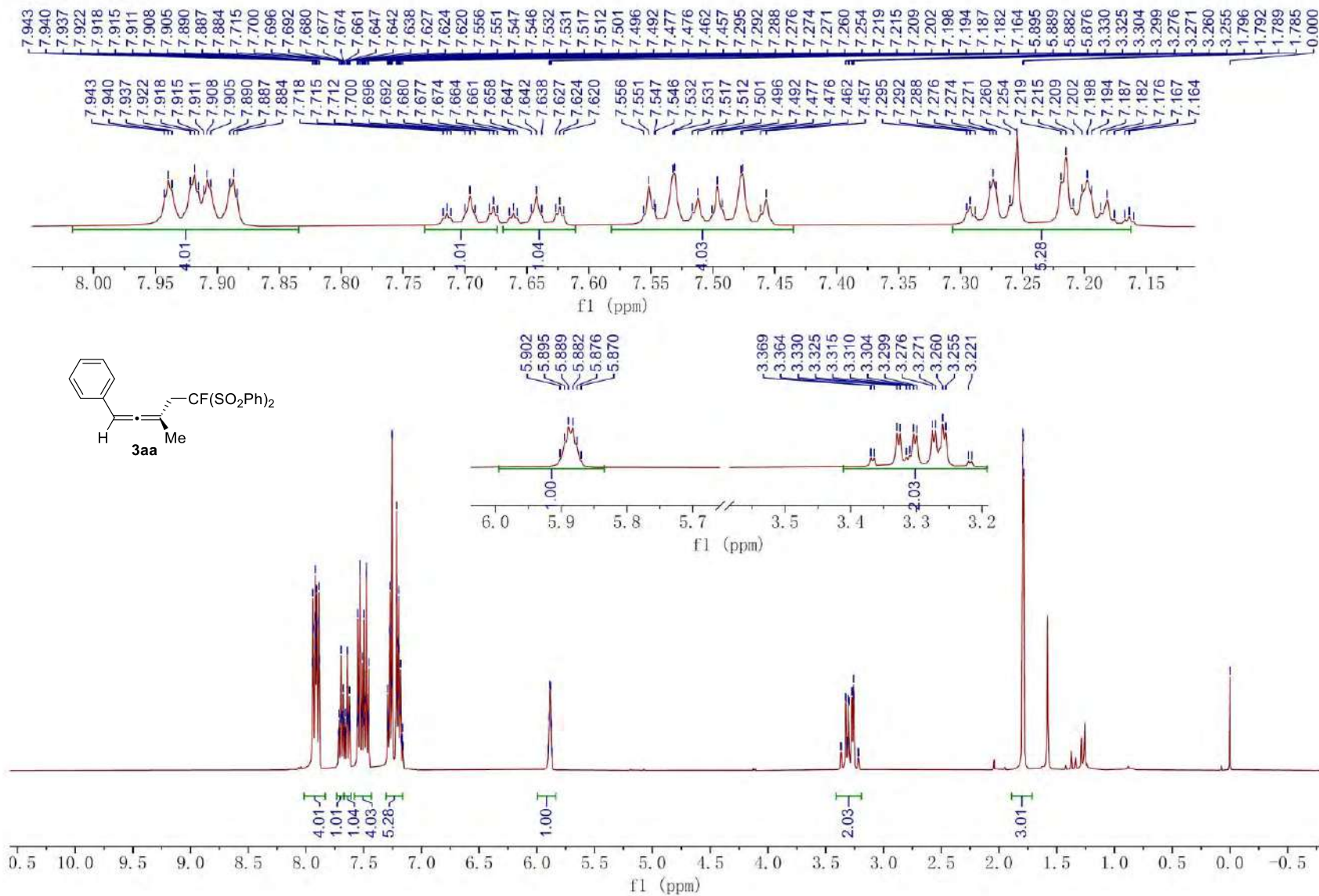


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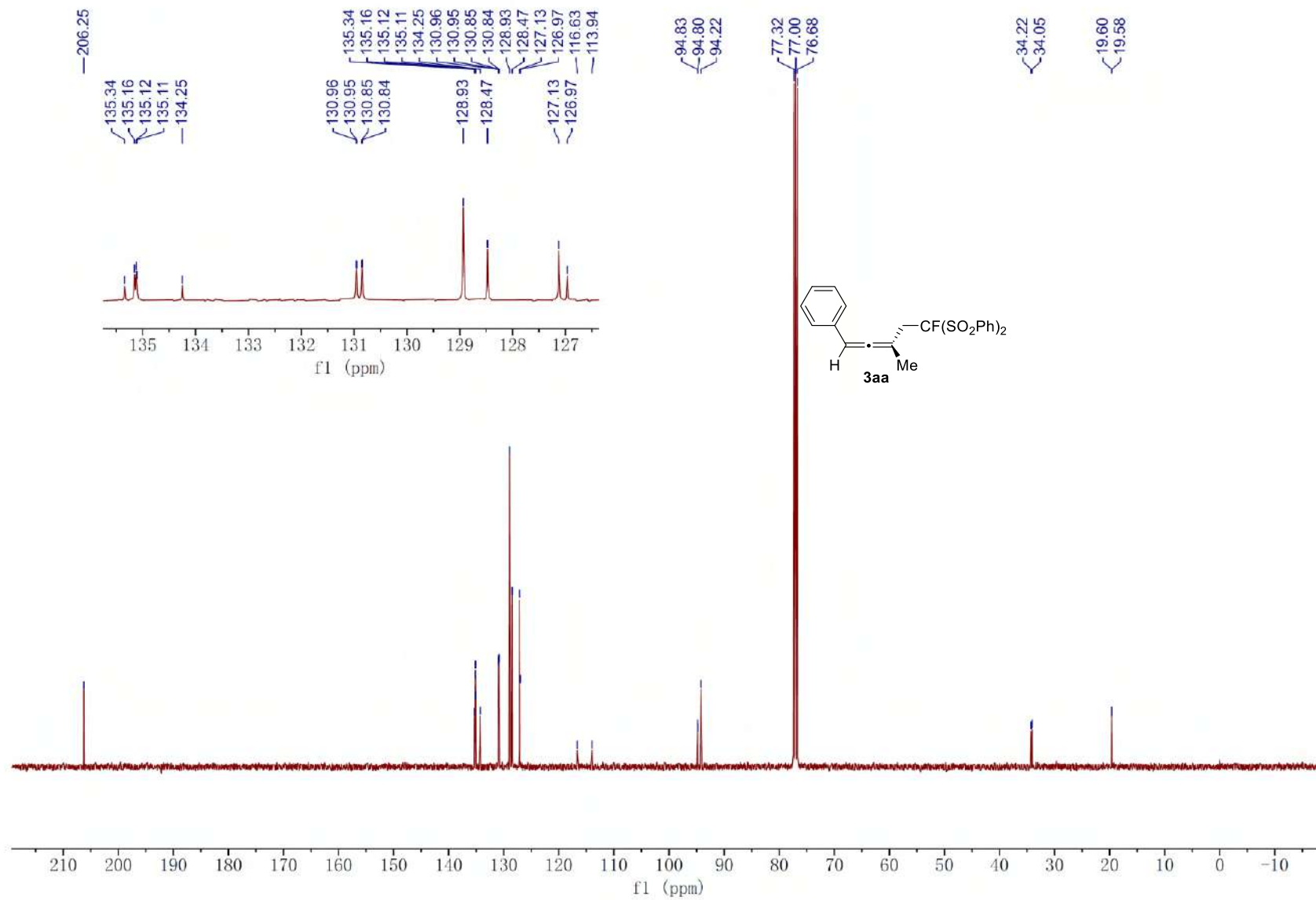
—140.596



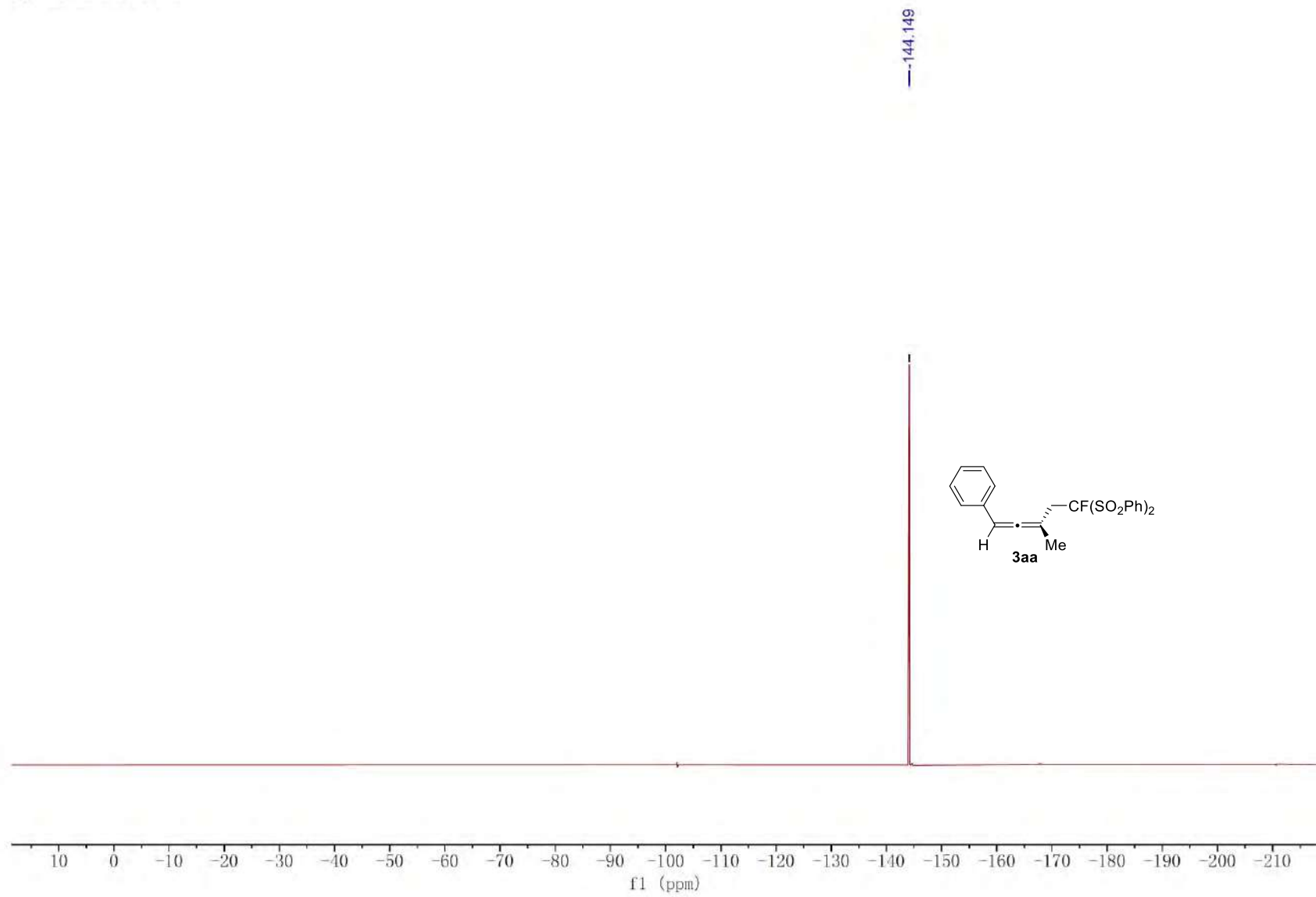
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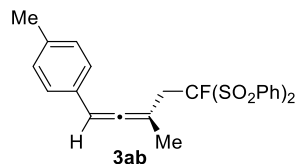


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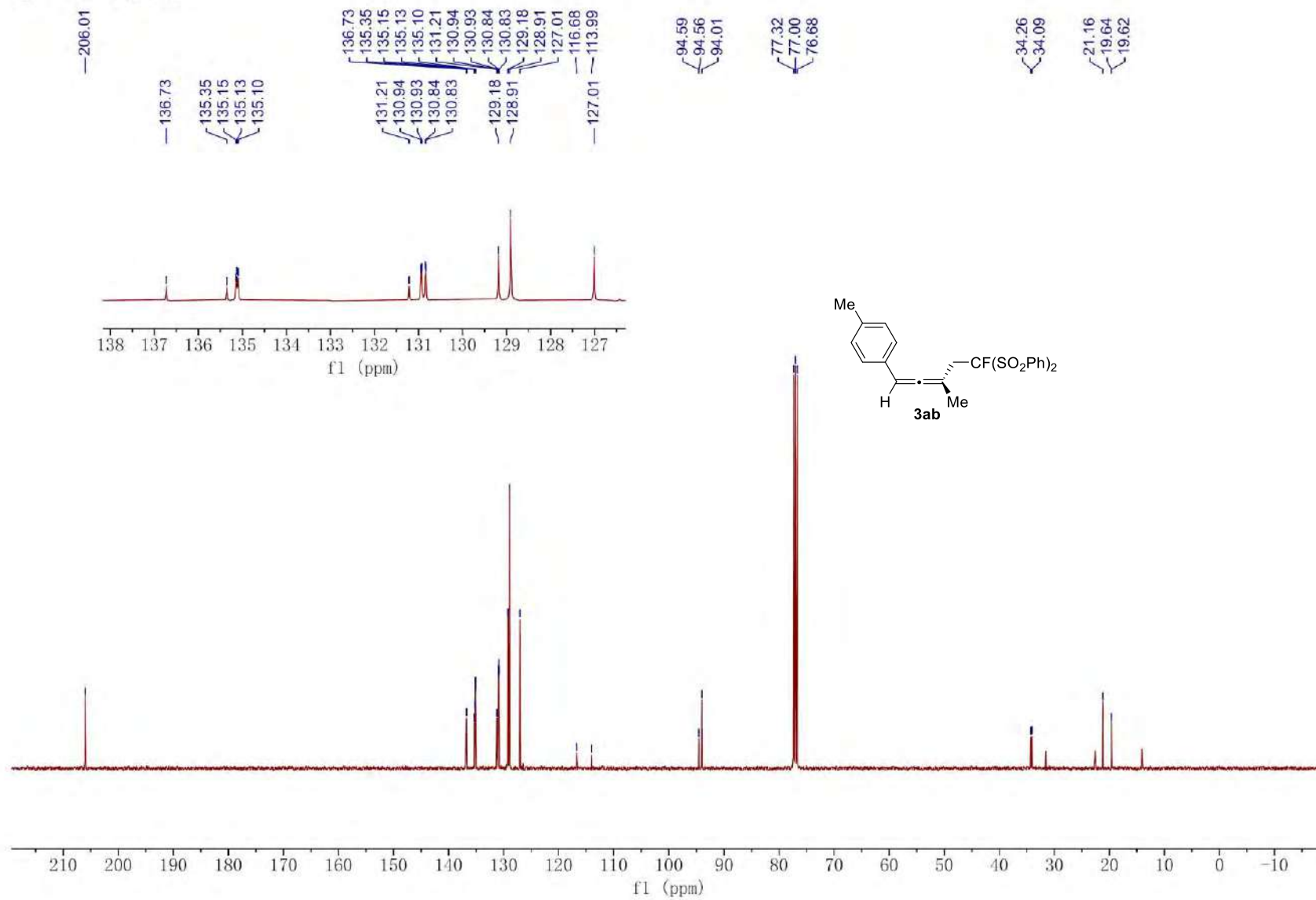


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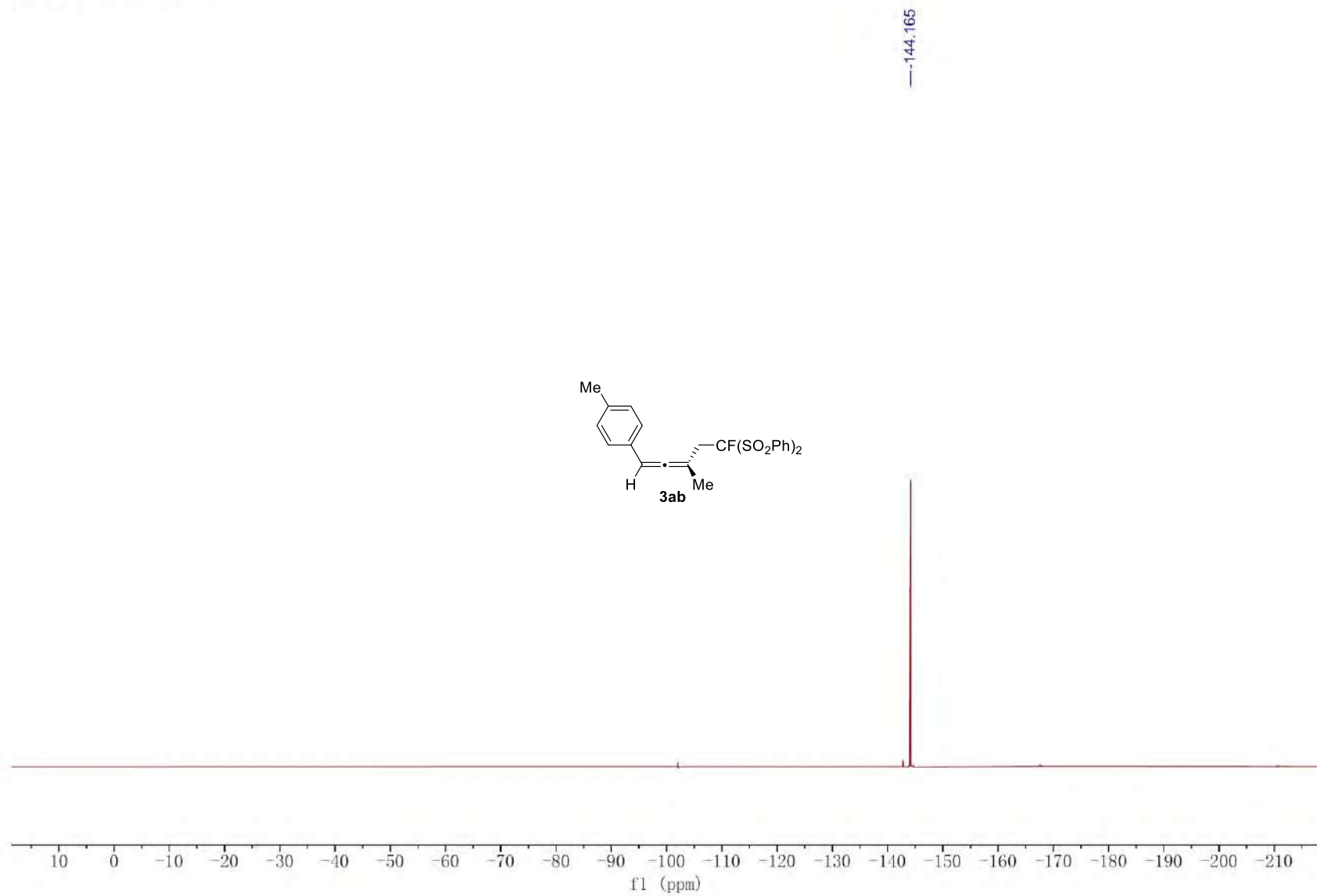




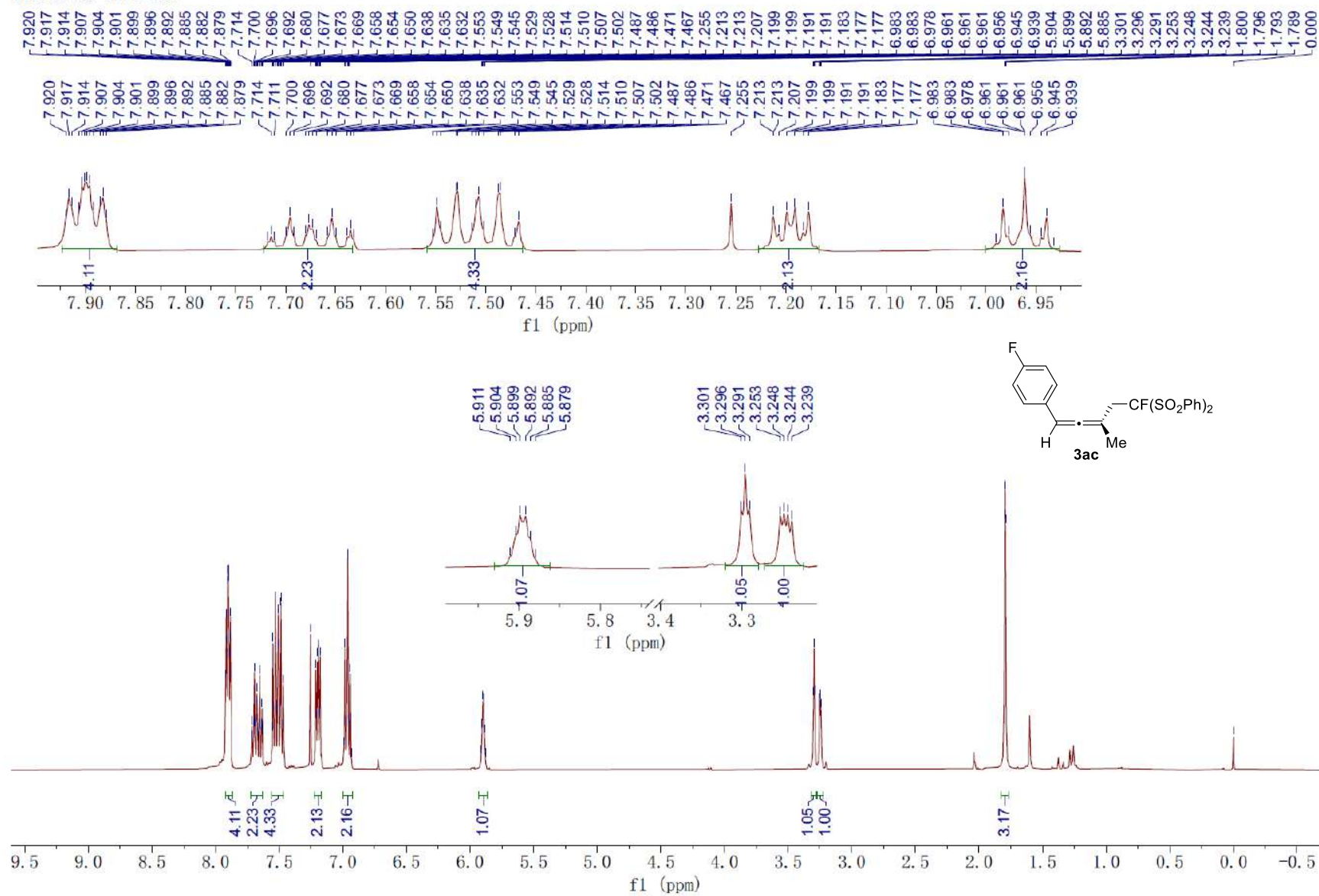
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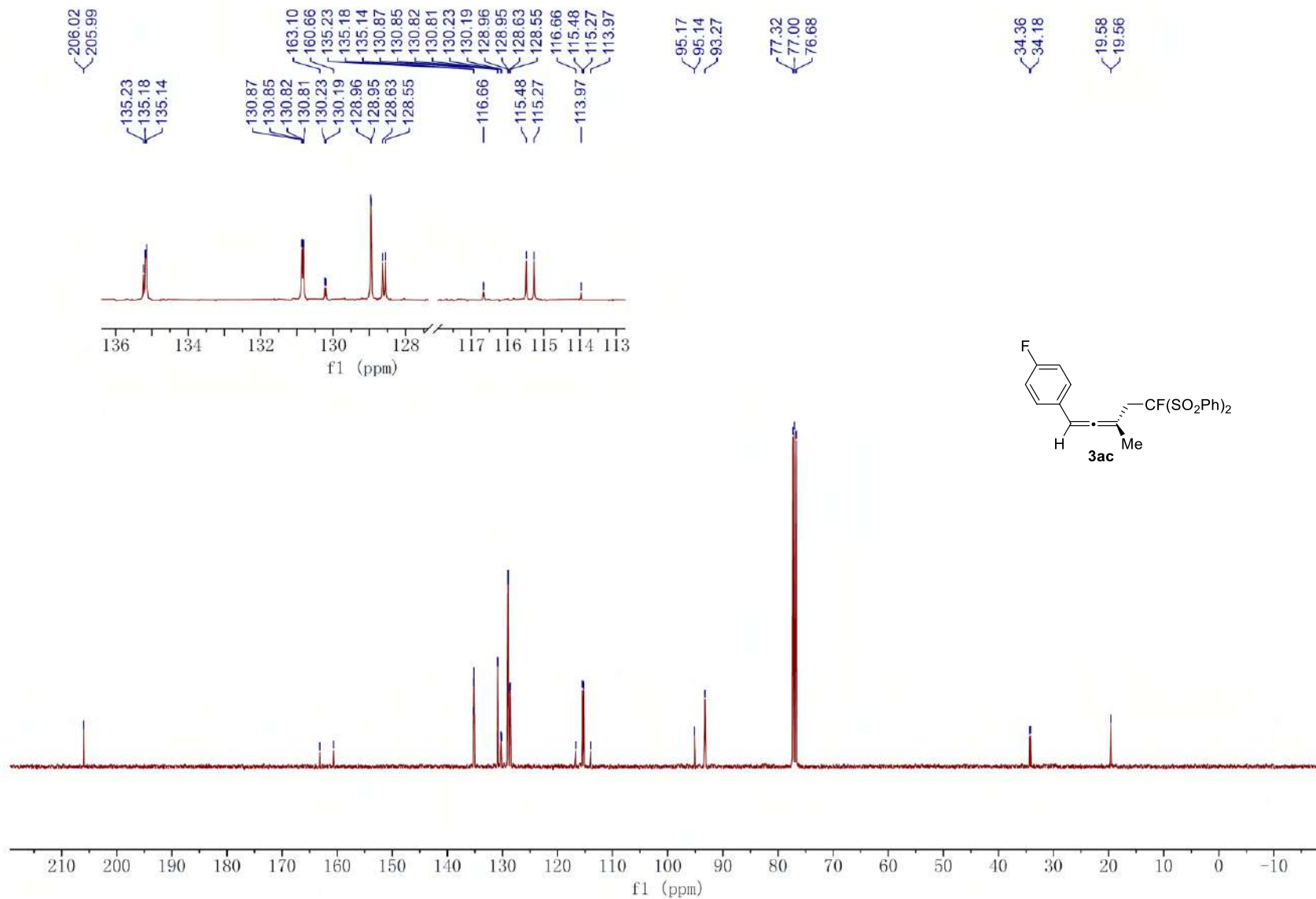
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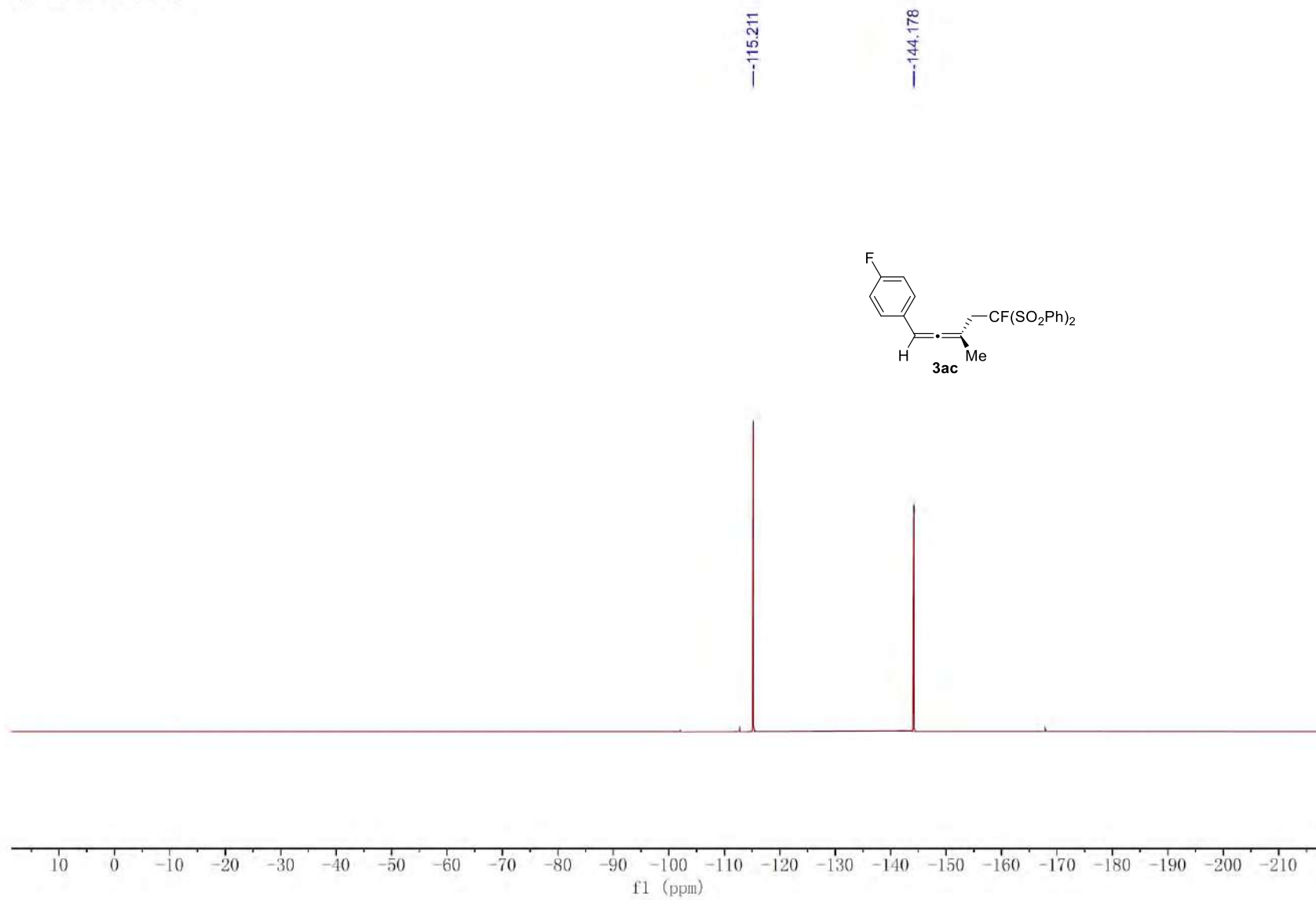
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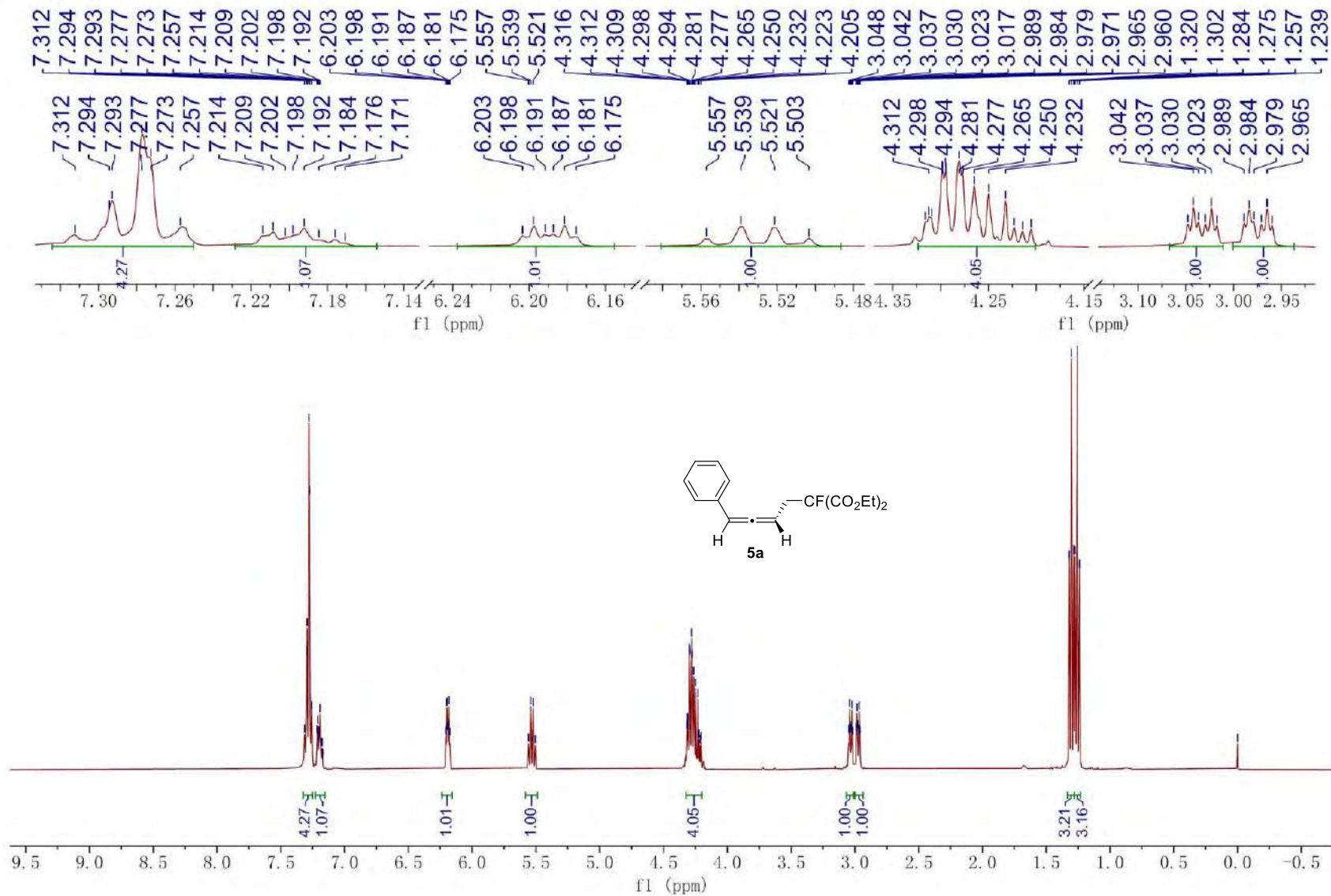
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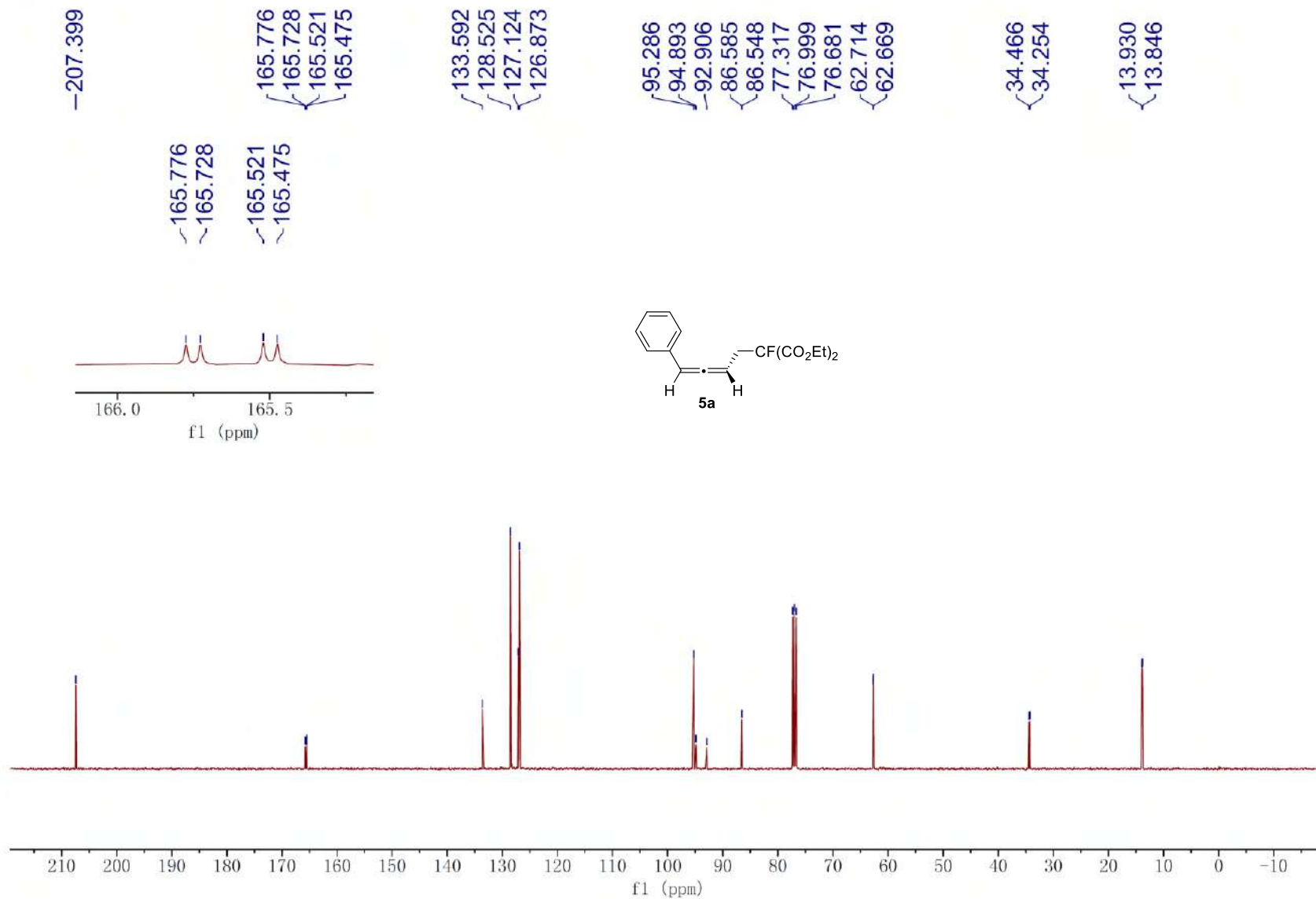
LIL-LL-69-C. 11. fid —



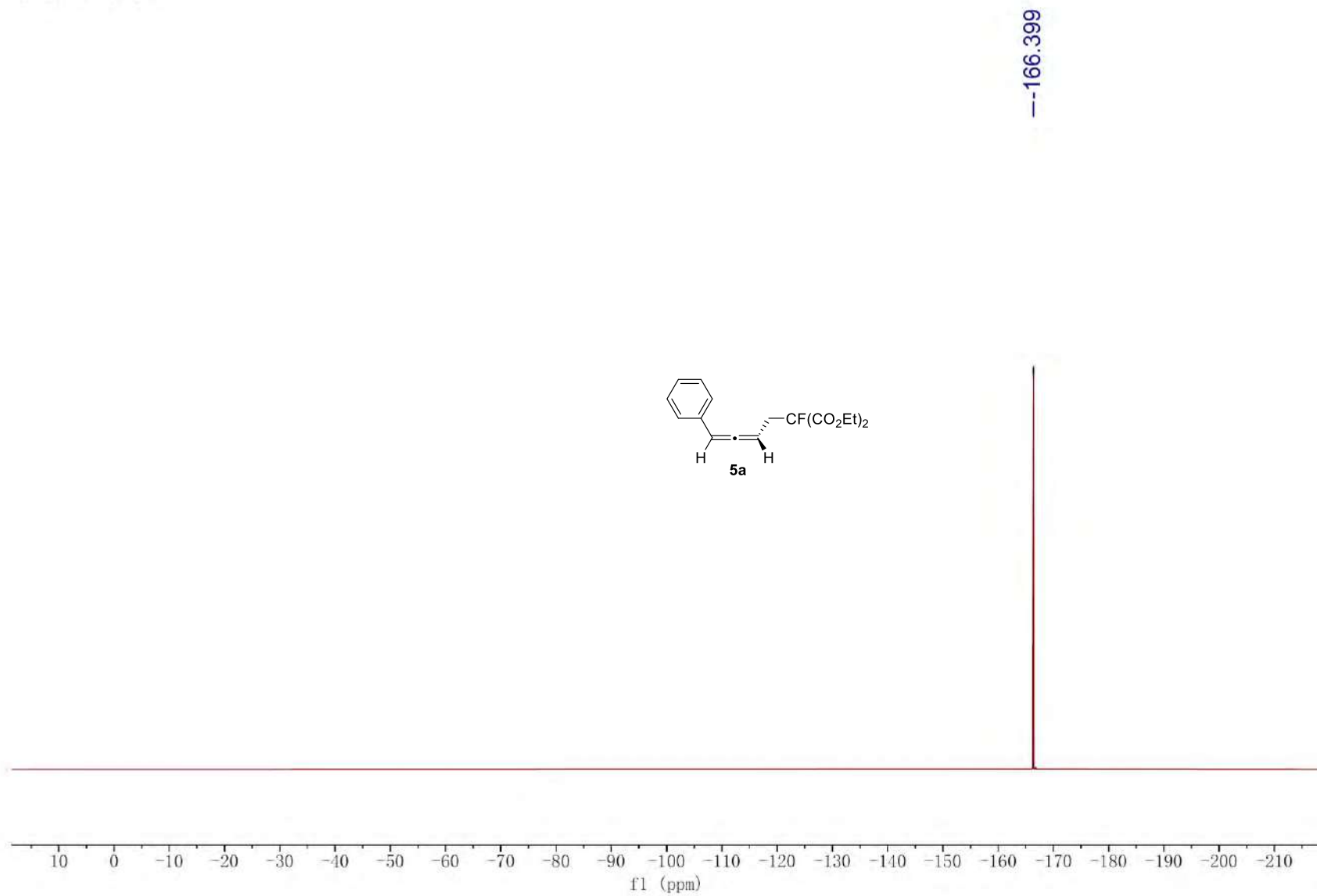
ZHY-ZG-36-400M-H



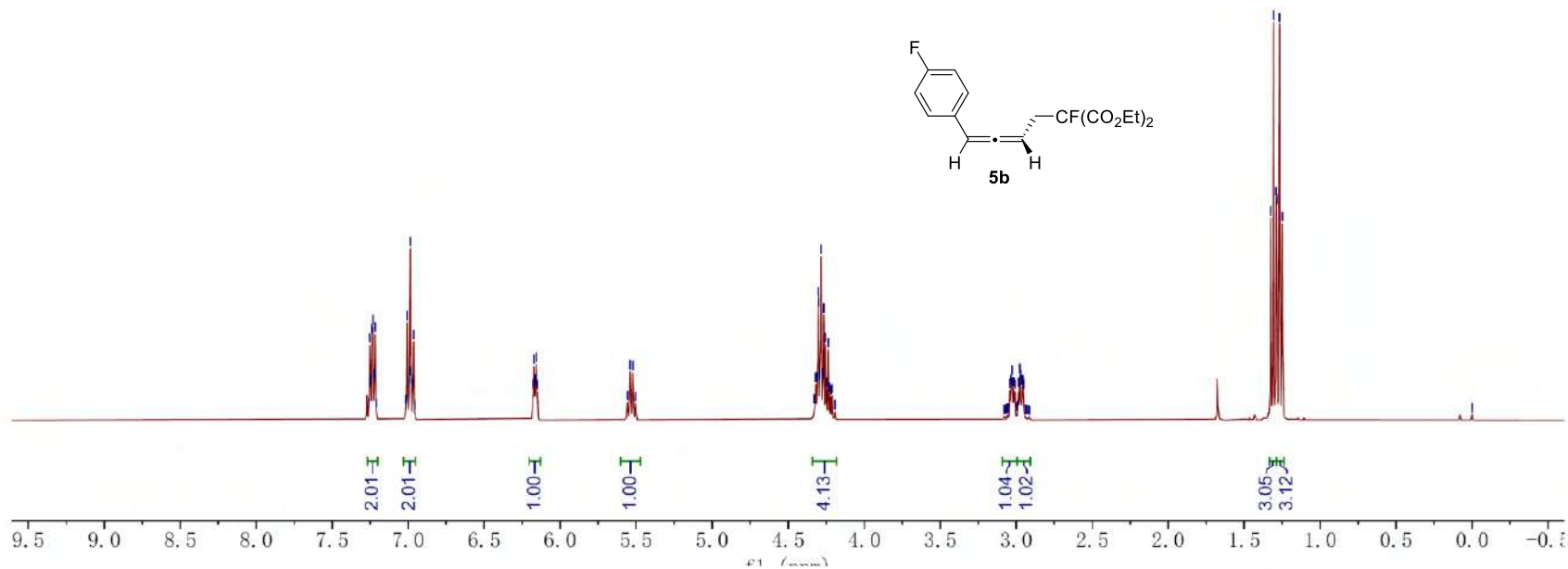
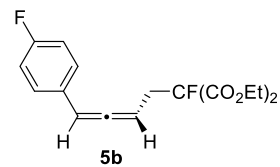
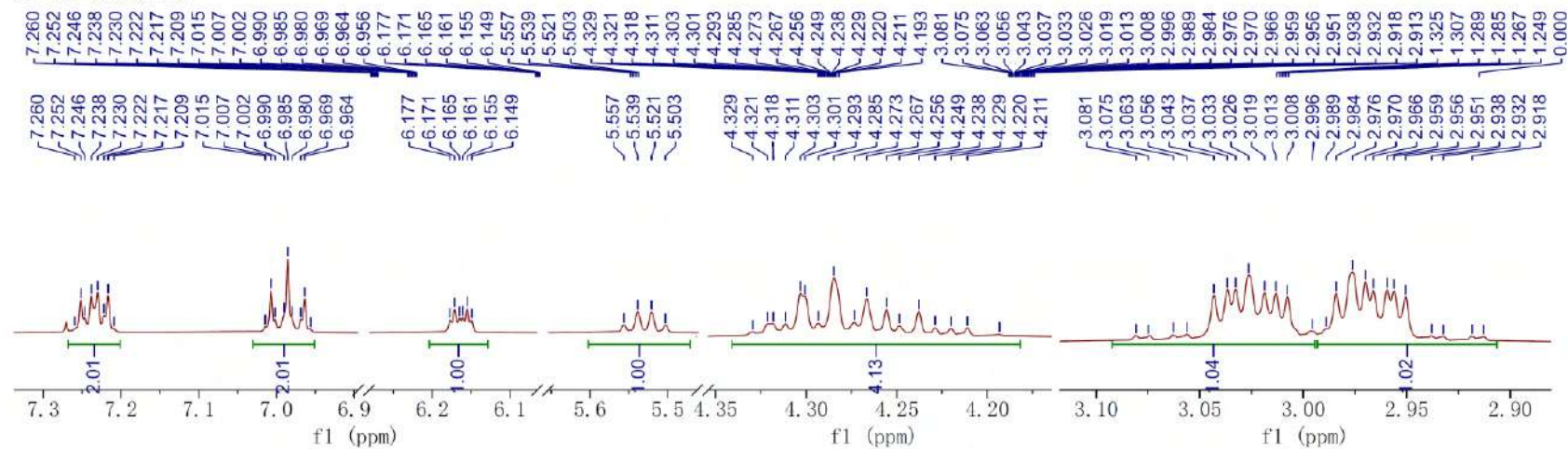
ZHY-ZG-36-100M-C



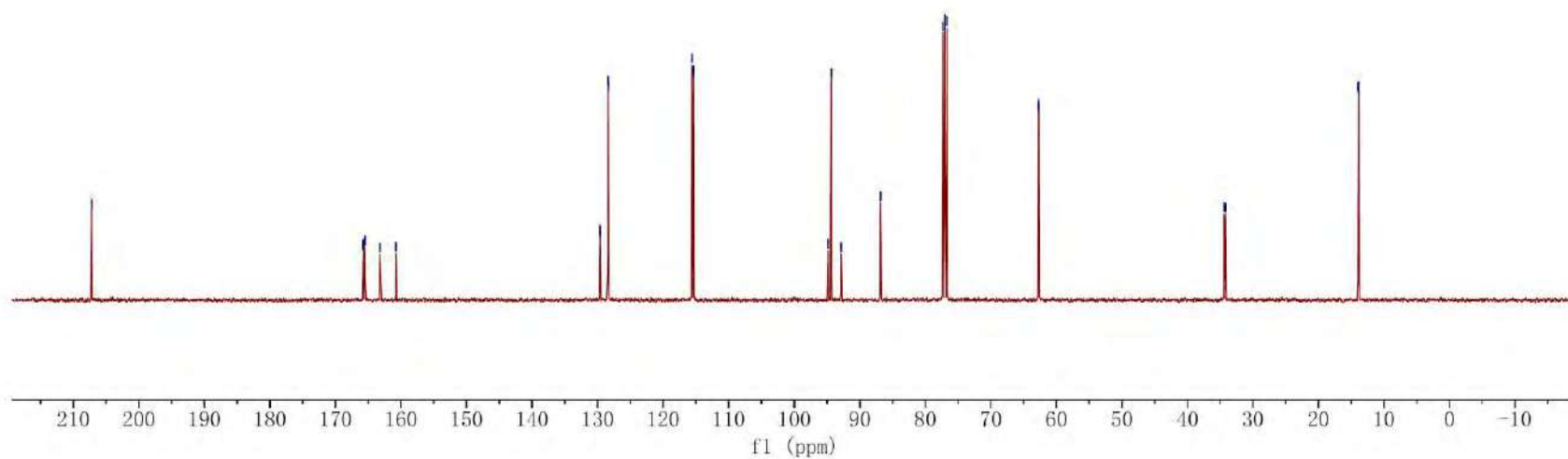
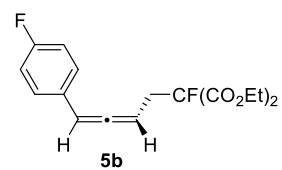
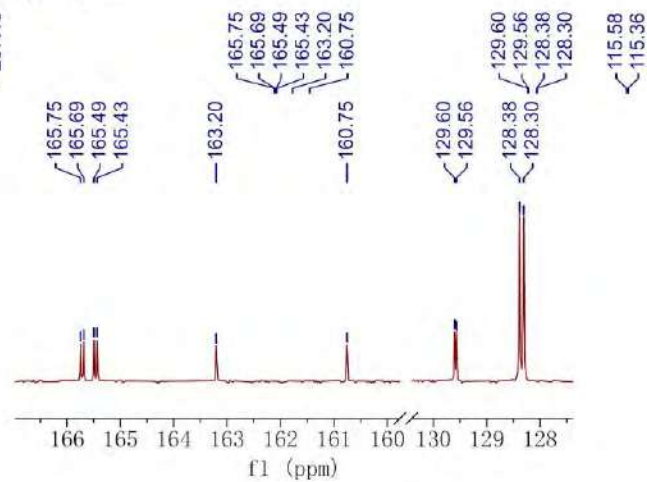
ZHYY-ZG-36-376M-F



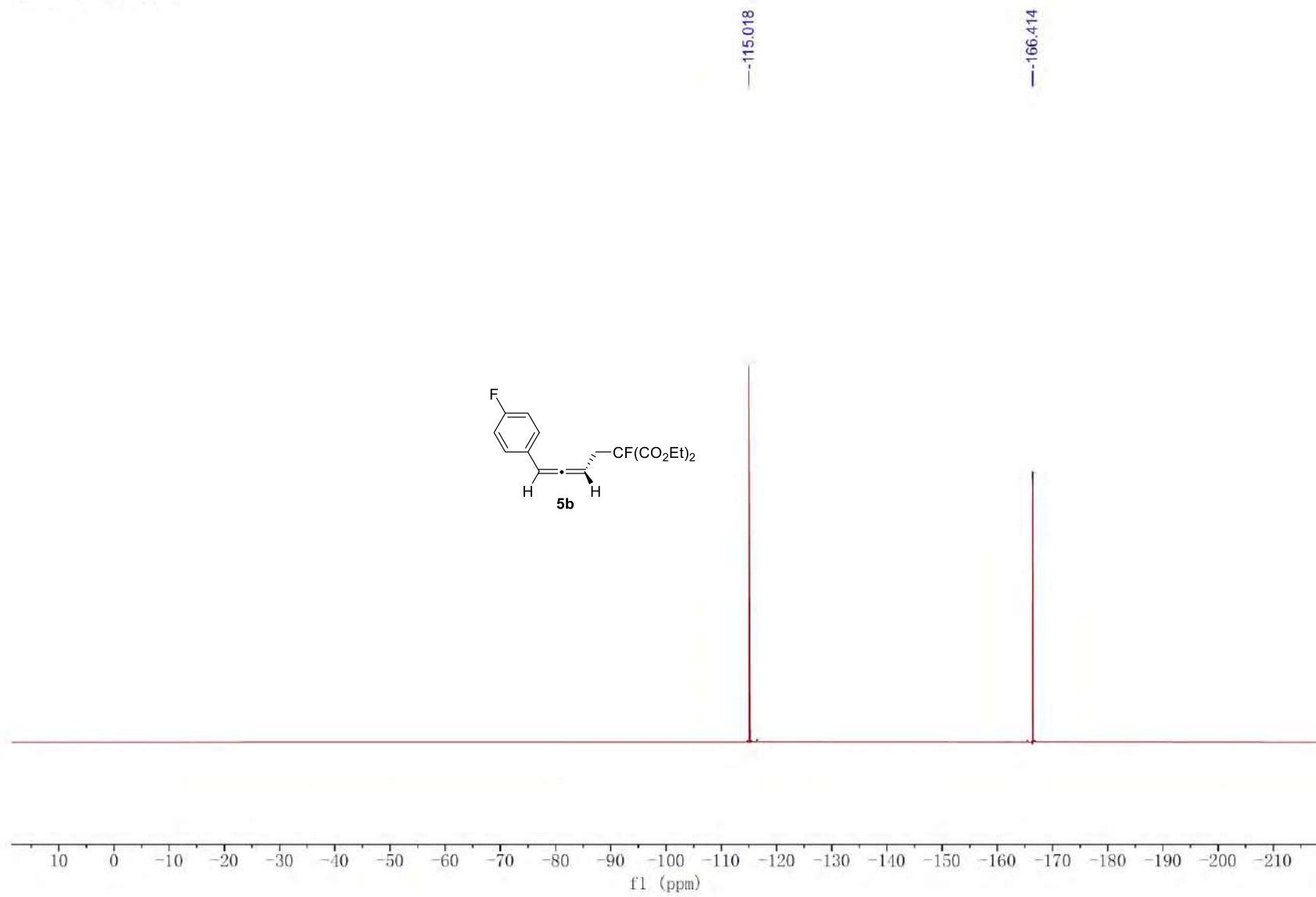
ZHY-ZF-42.20.fid —



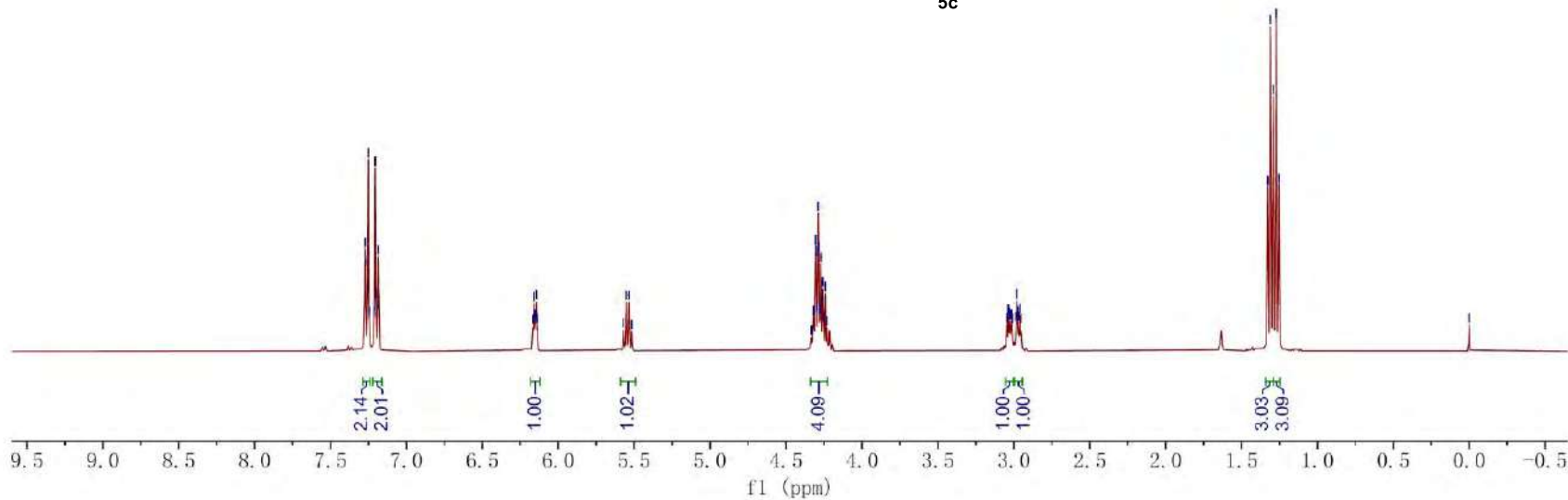
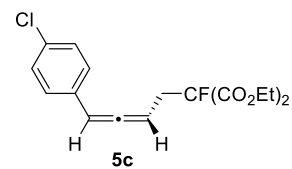
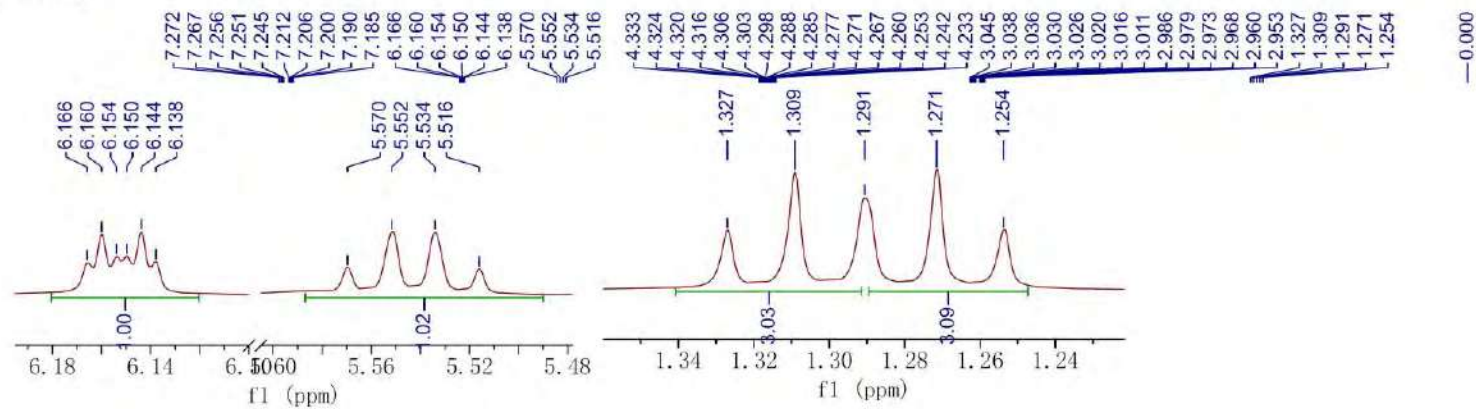
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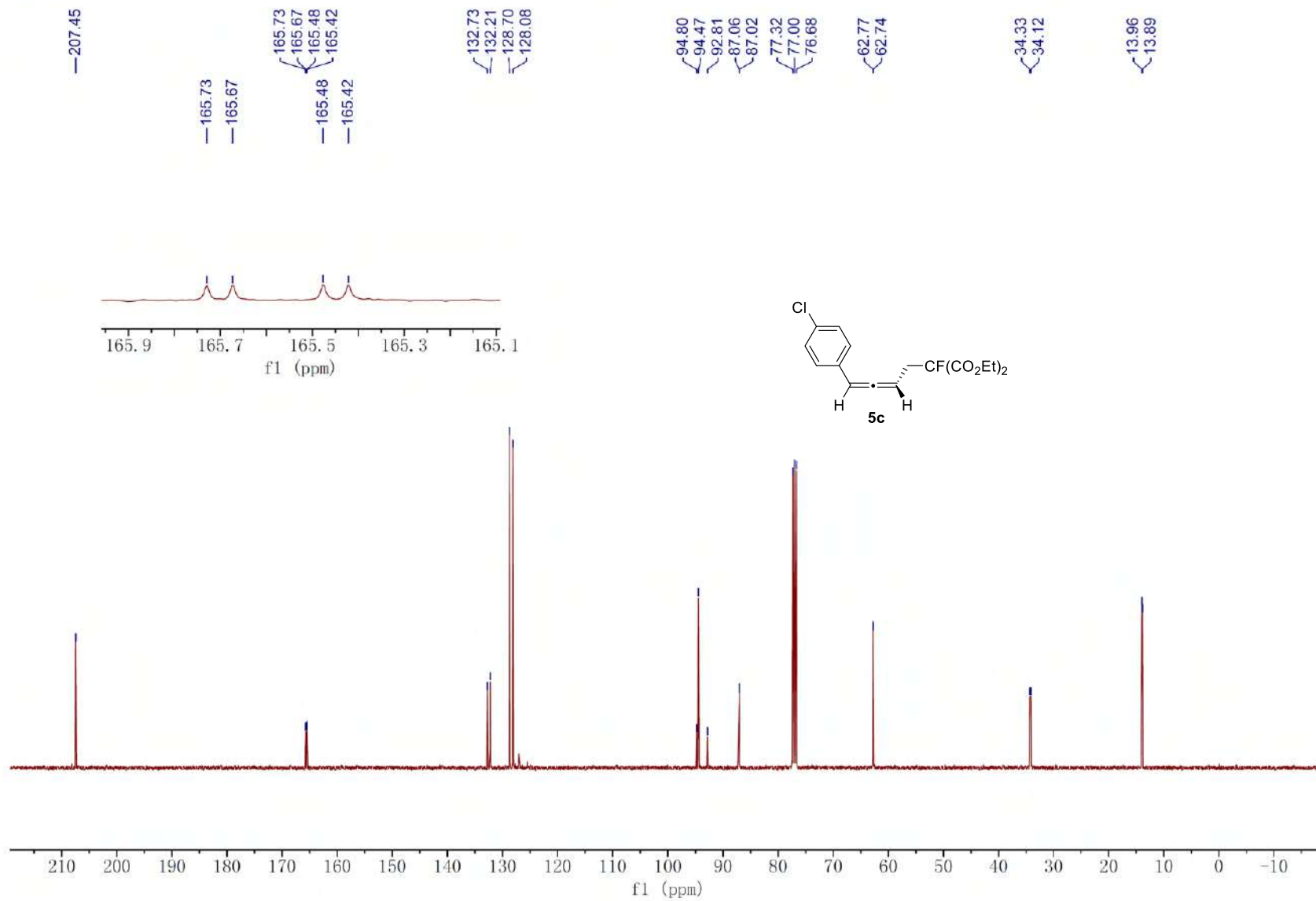
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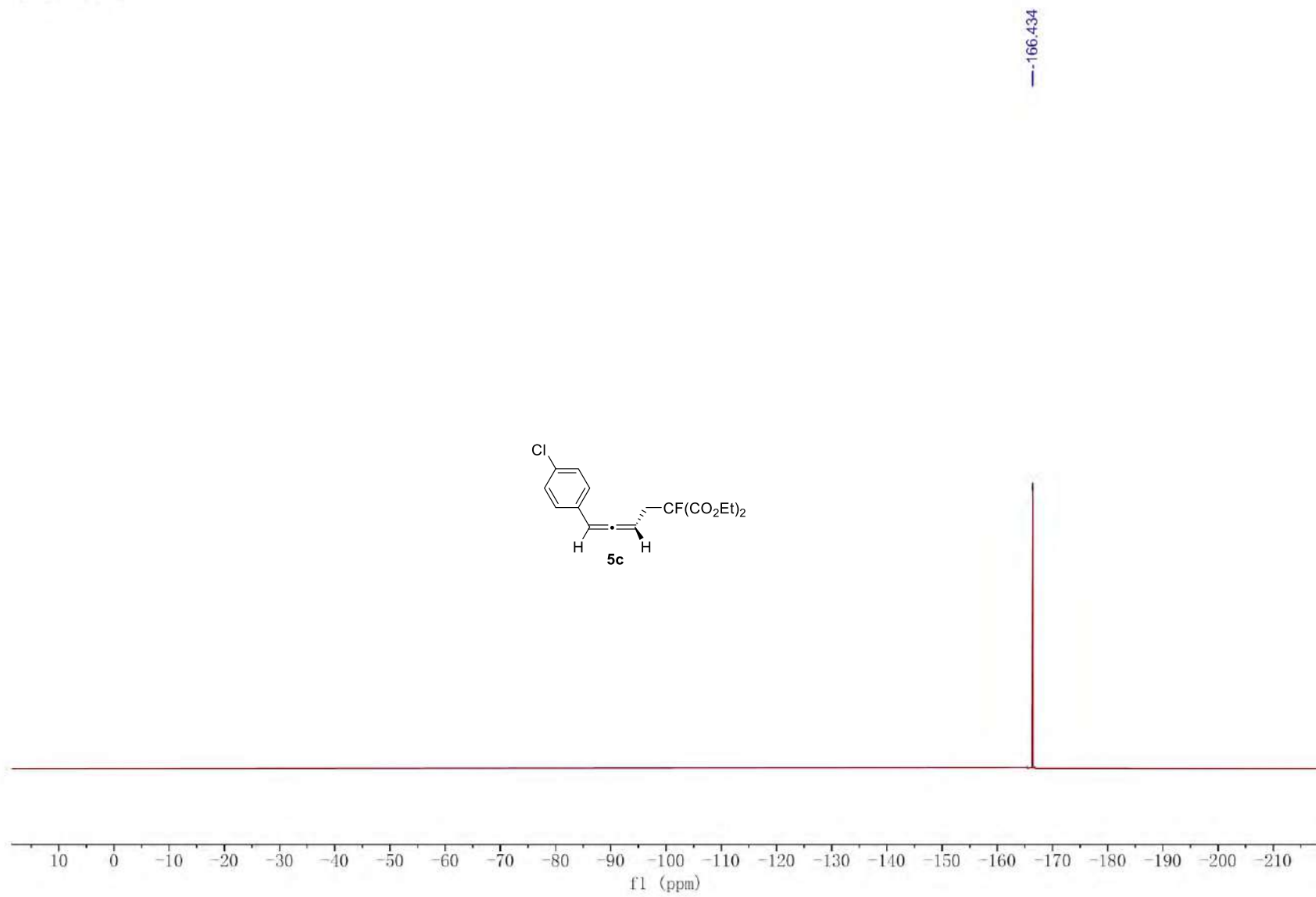
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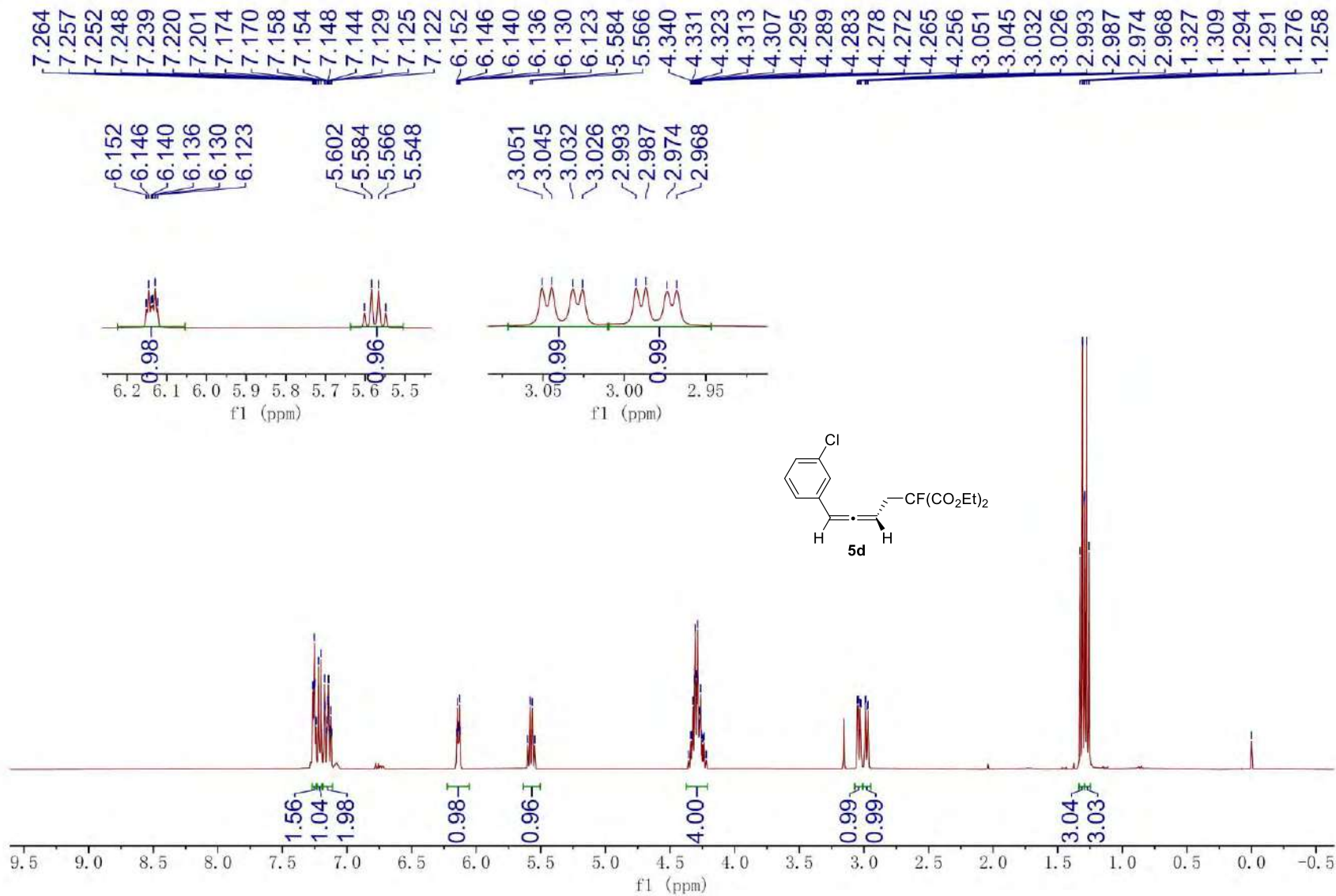
ZHY-ZG-100M-C



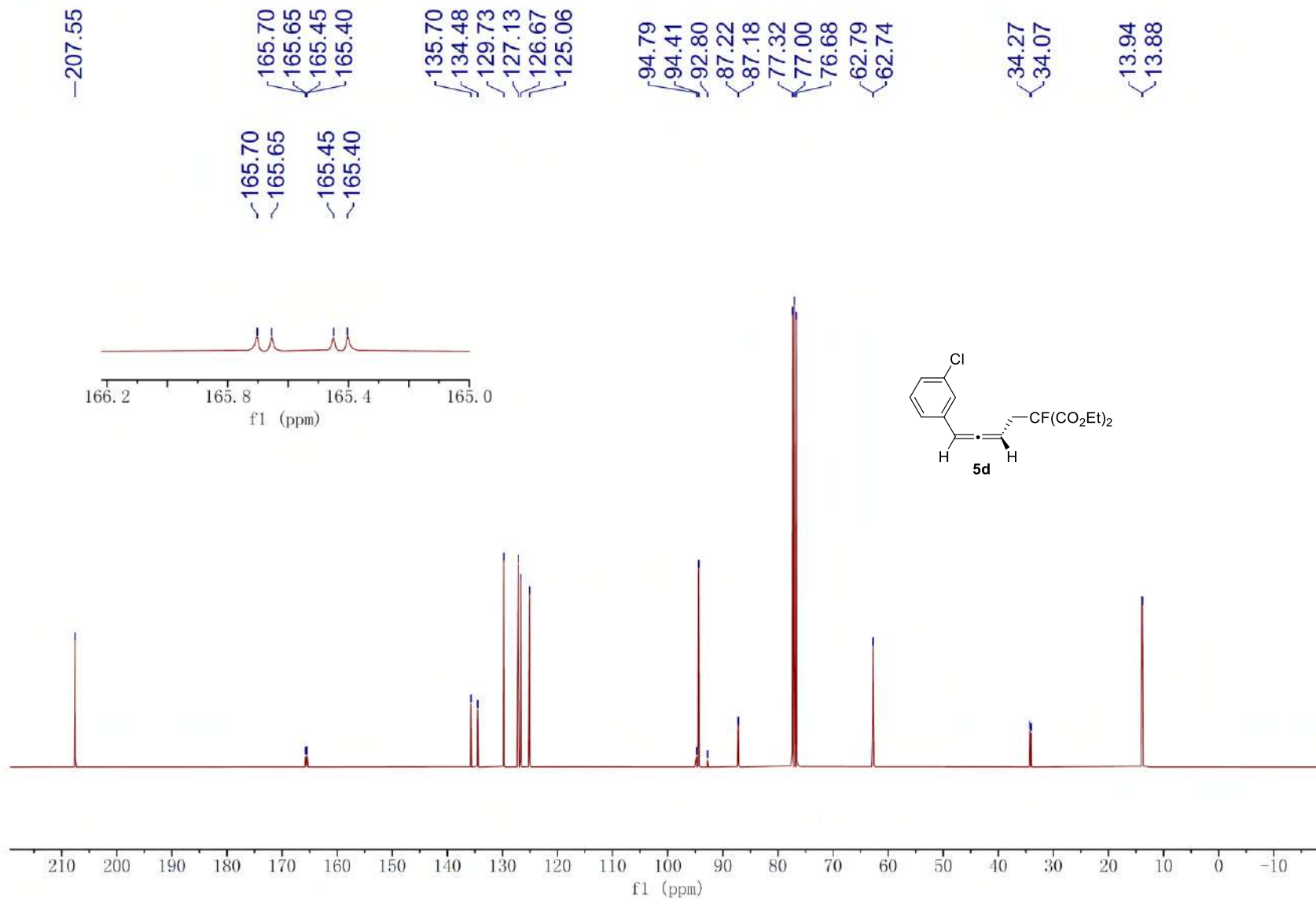
ZHYY-ZG-376M-F



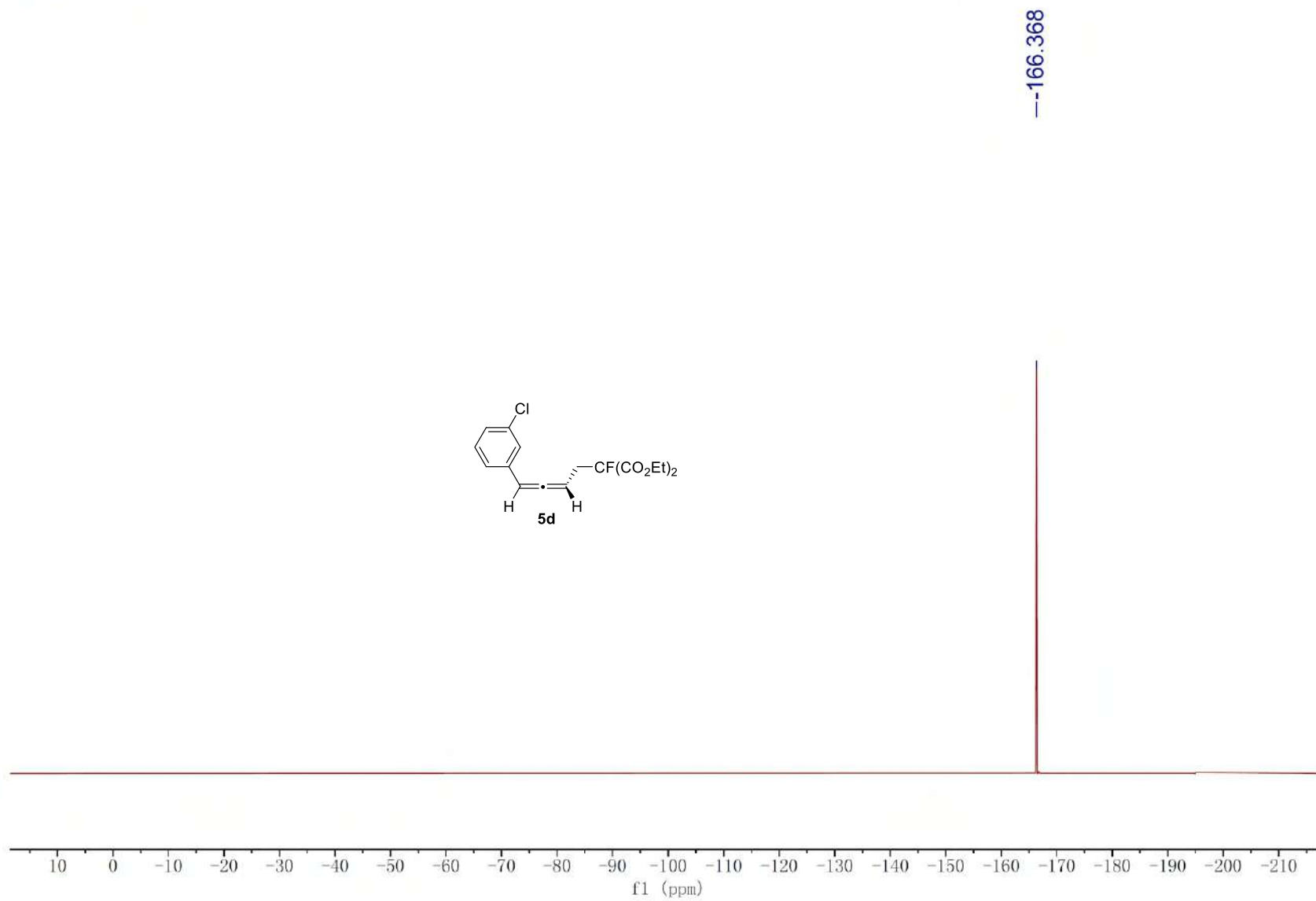
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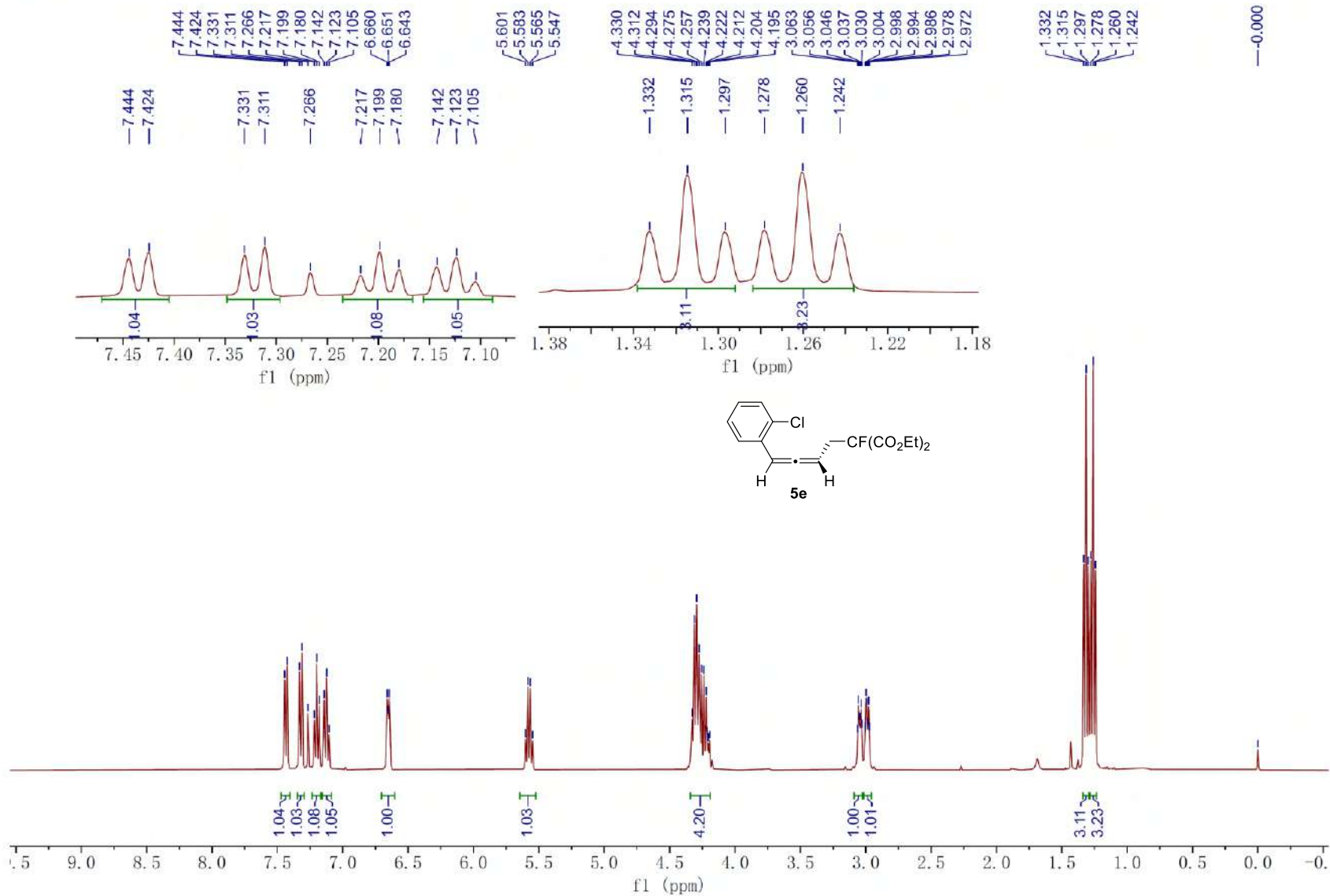
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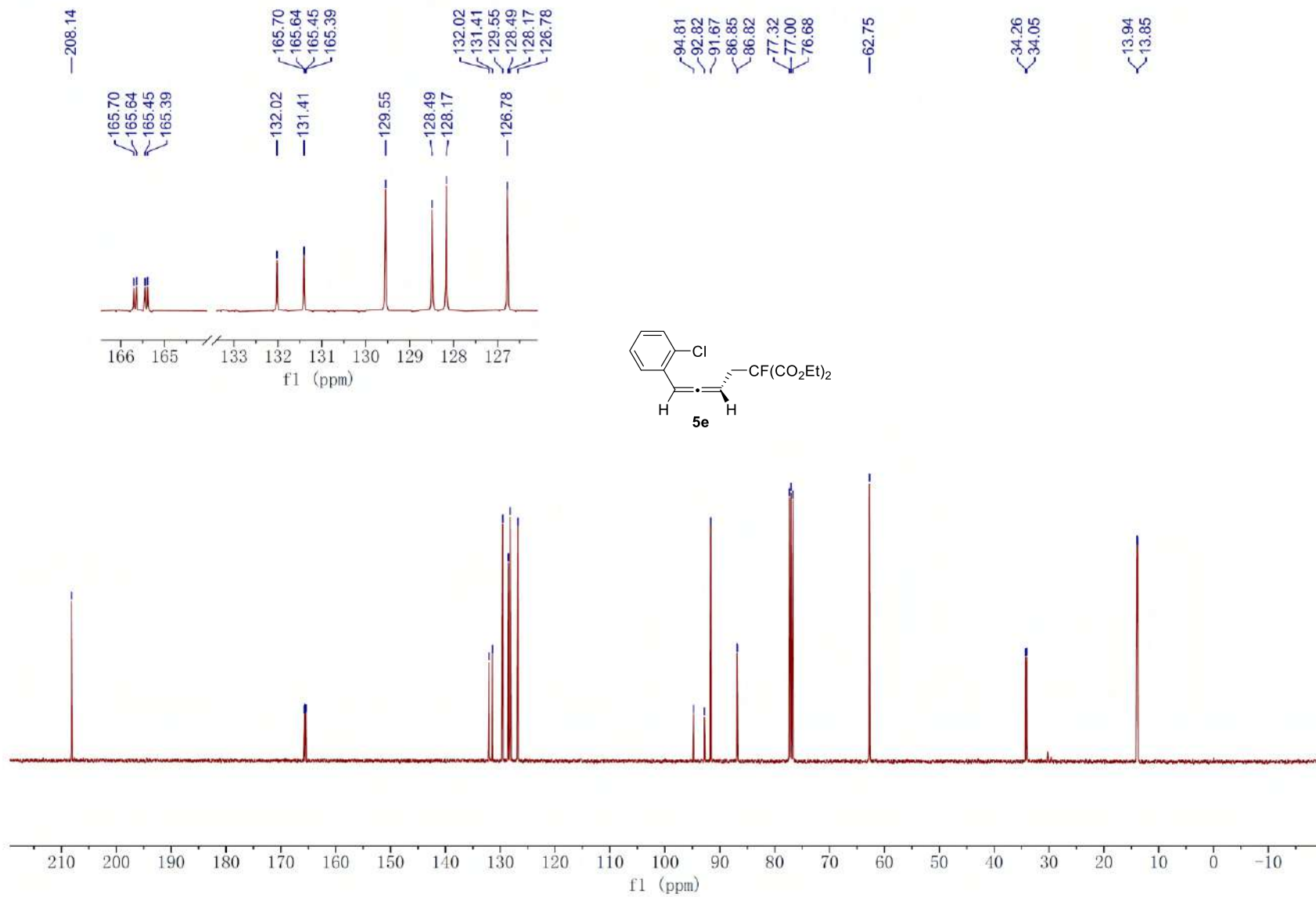
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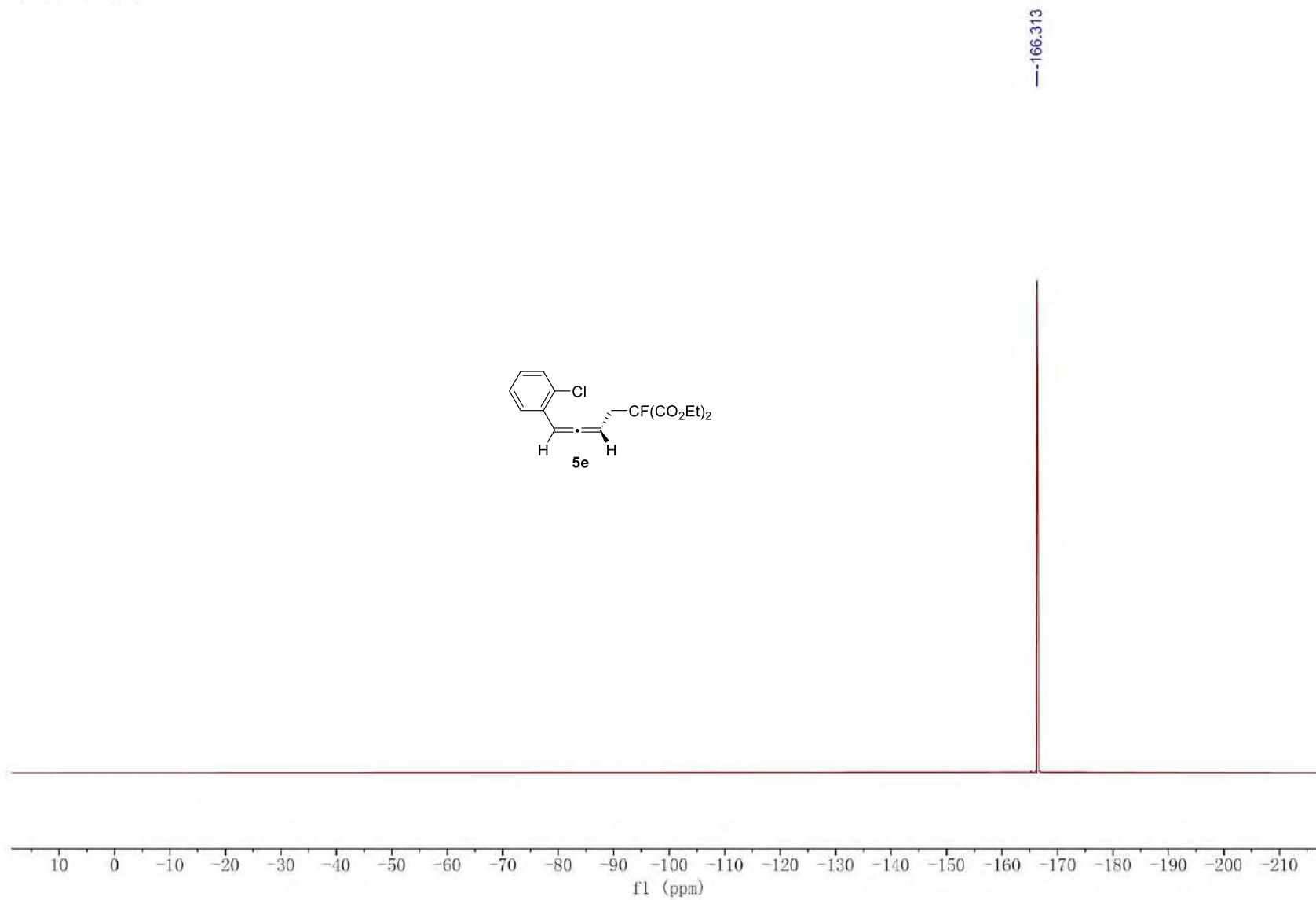
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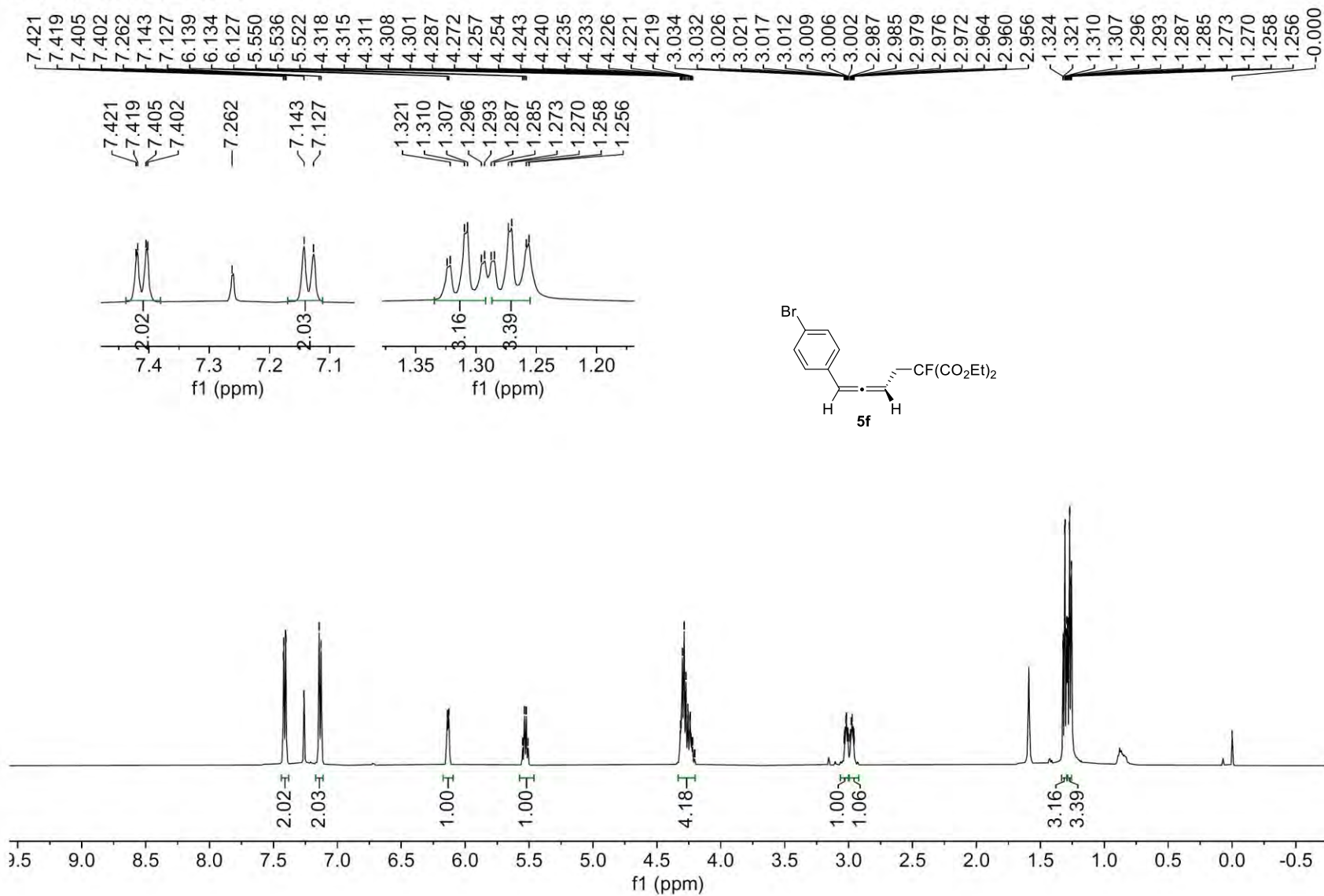
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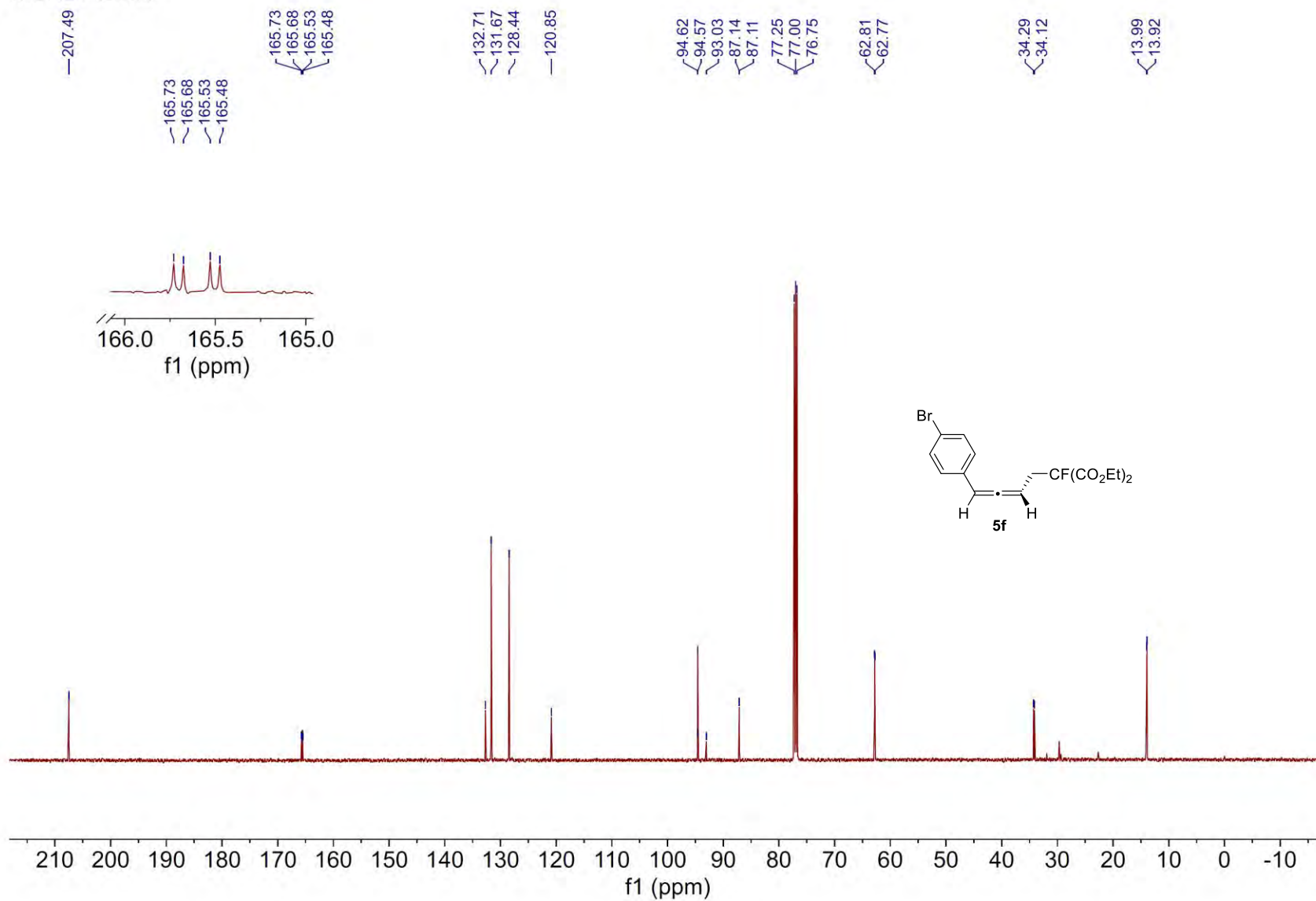
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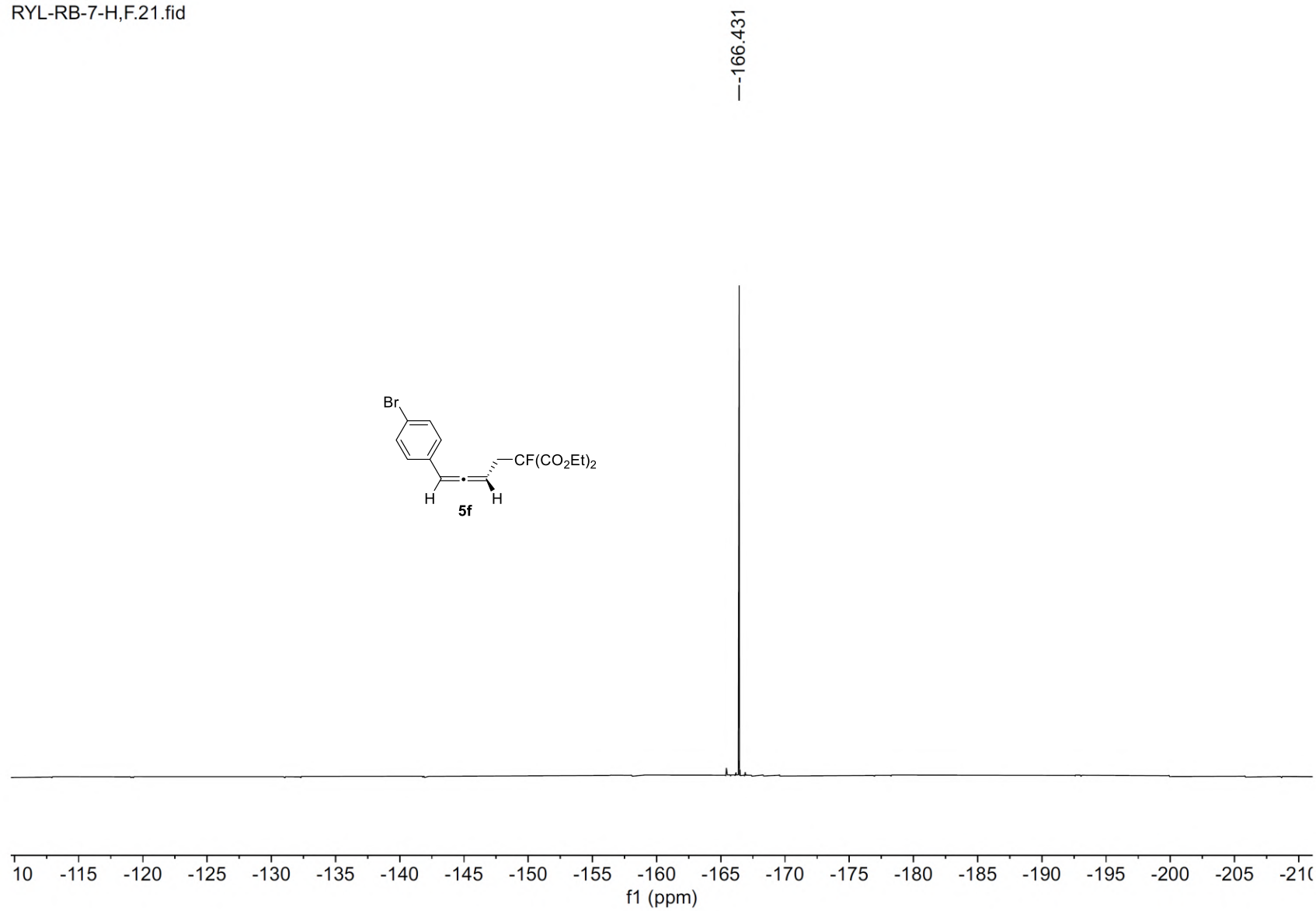
RYL-RB-7-3.10.fid — 500M



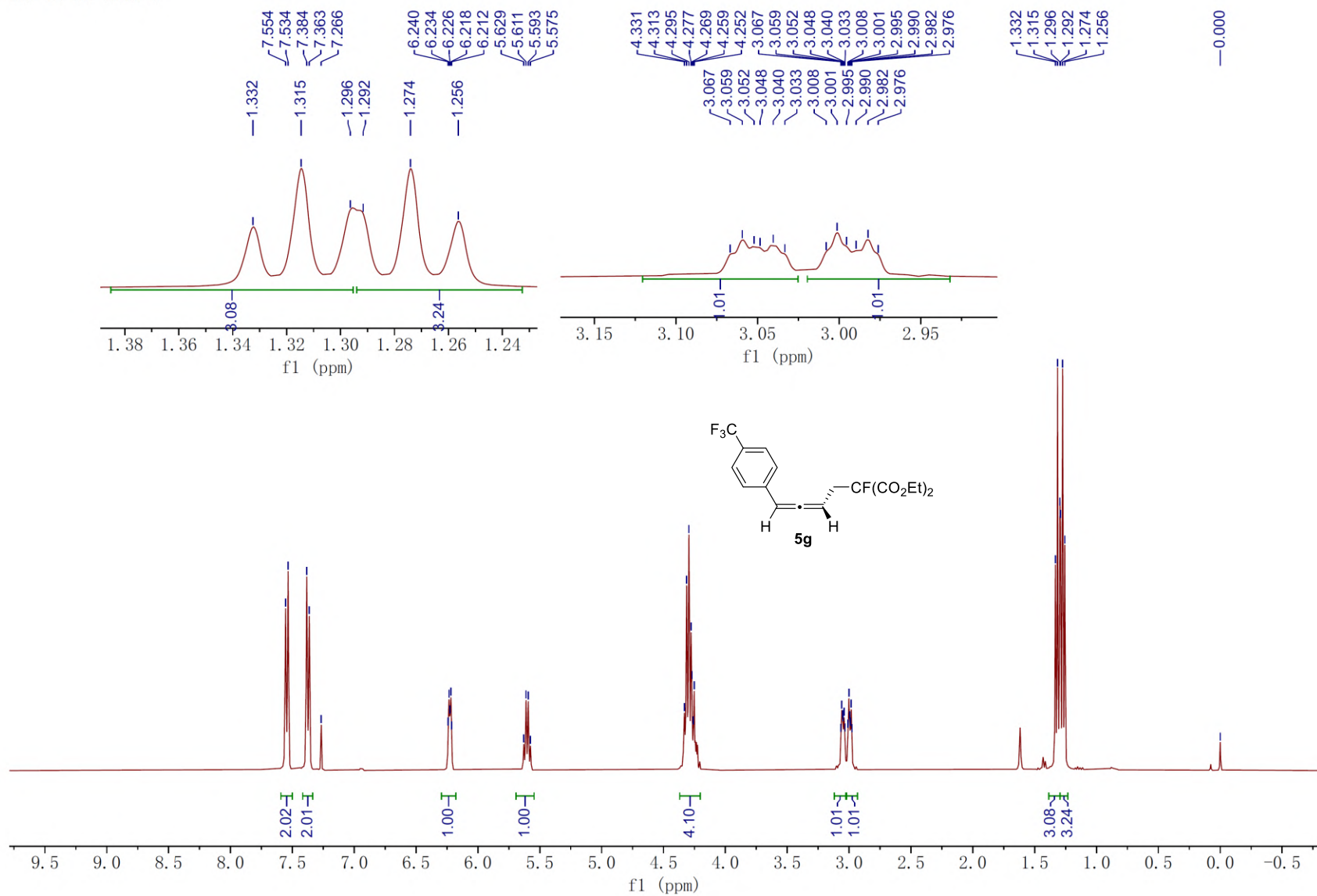
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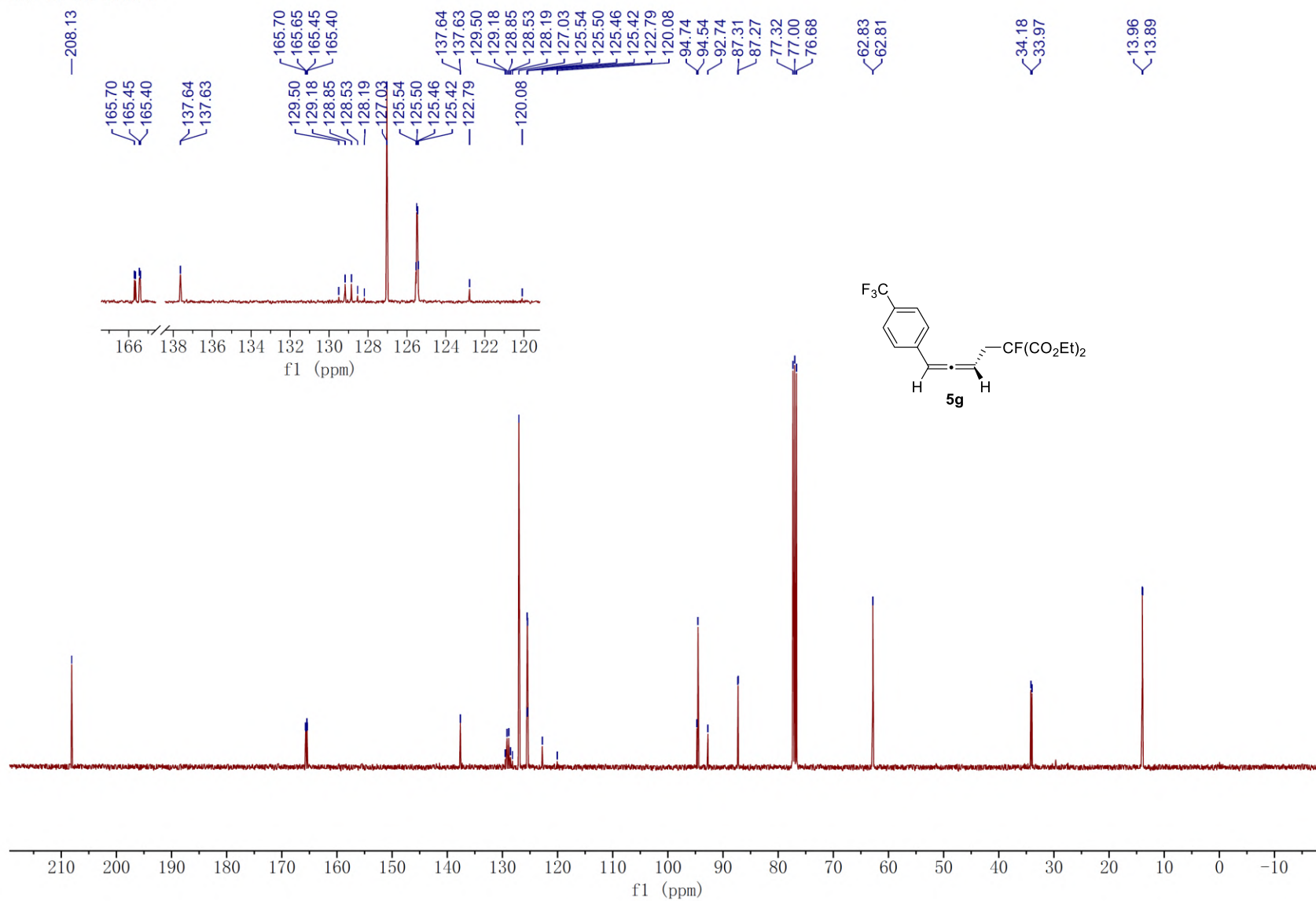
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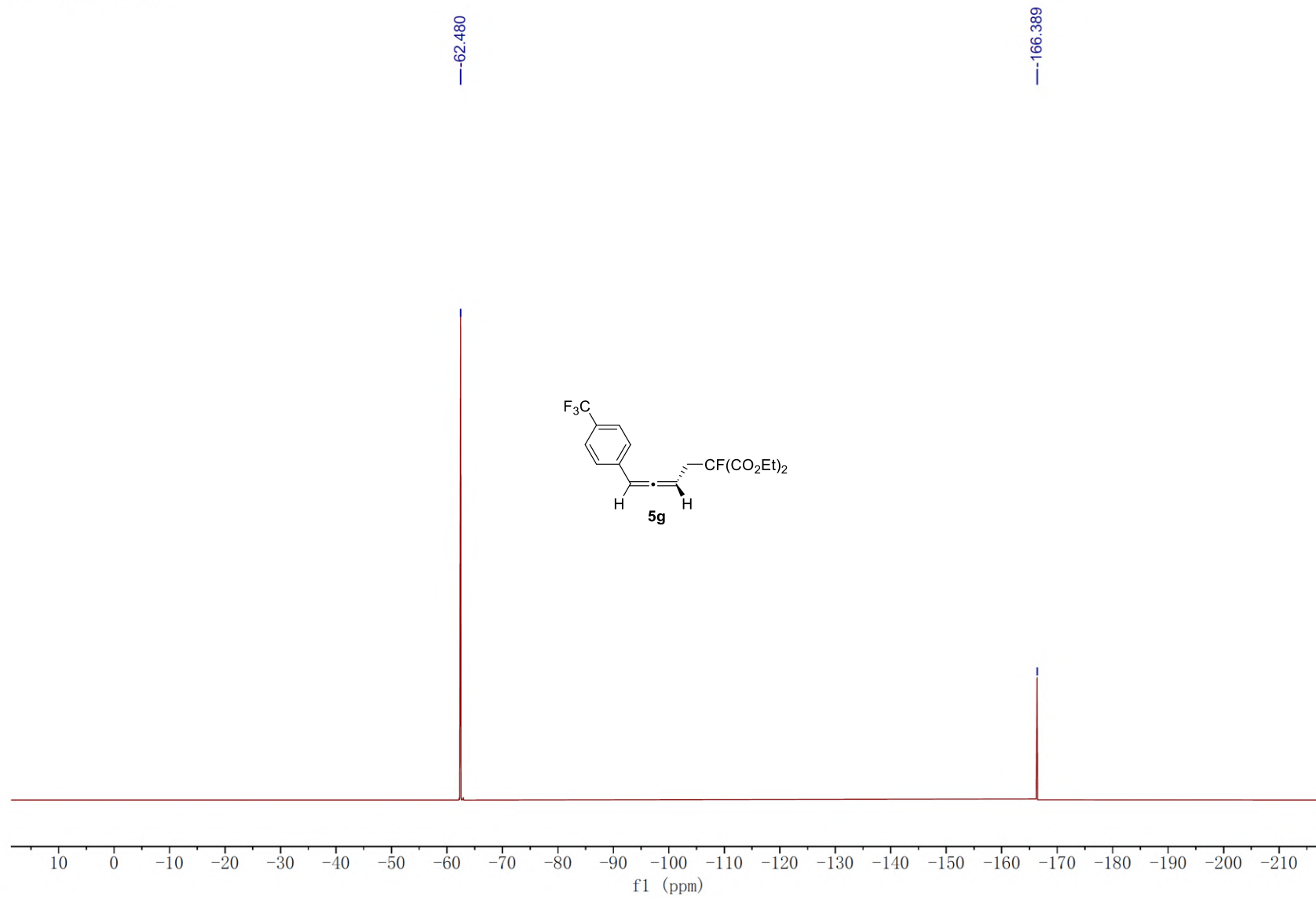
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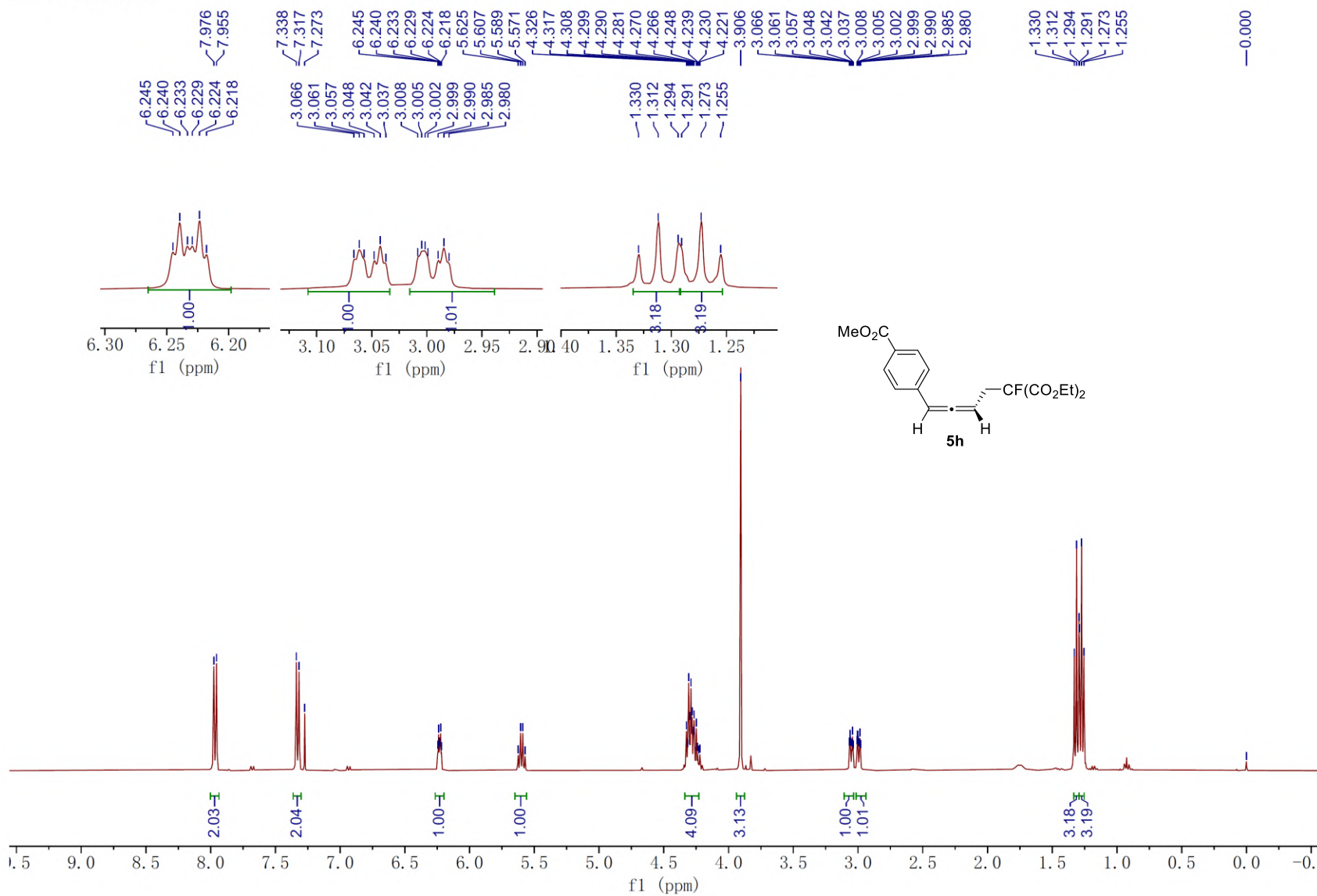
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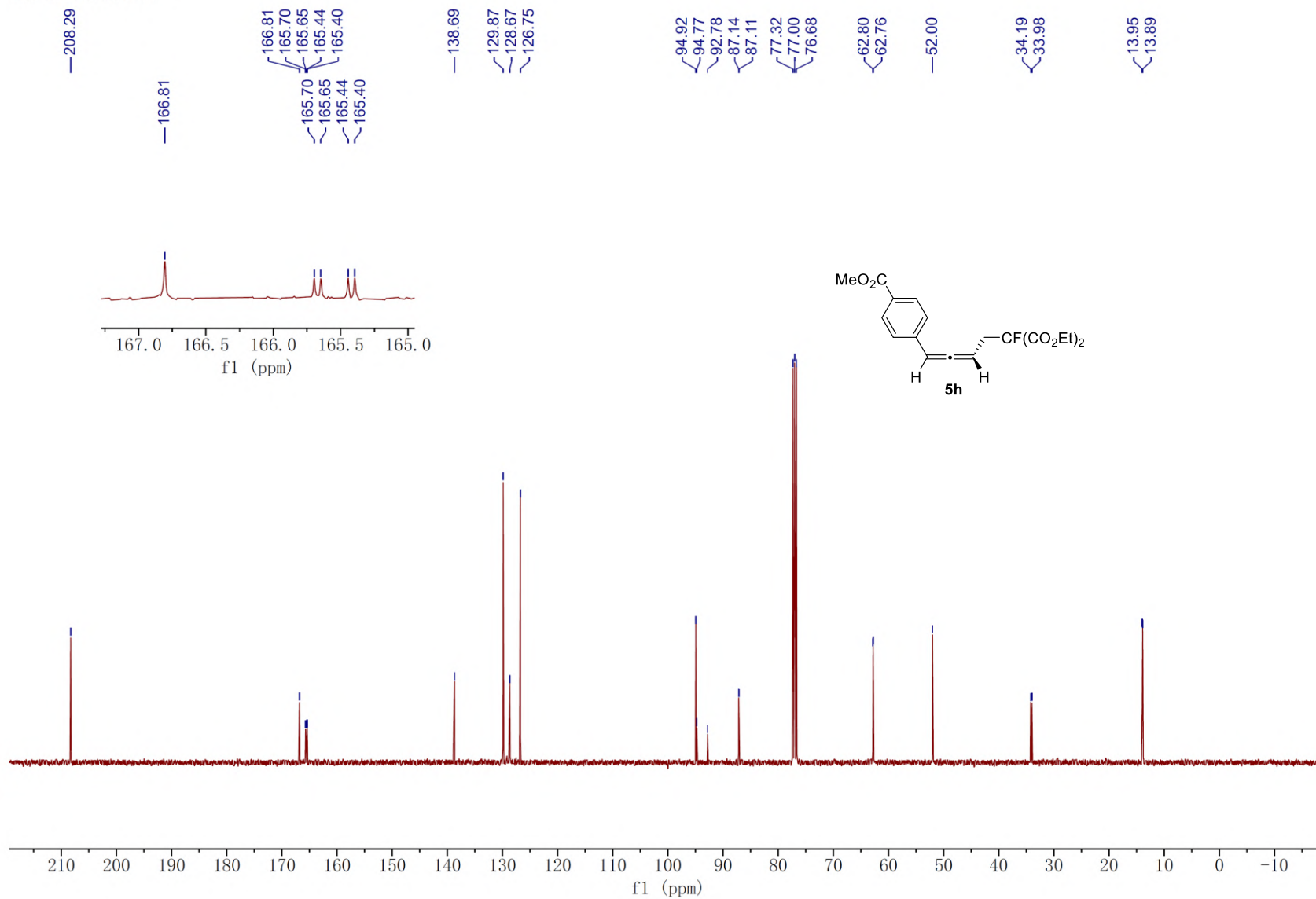
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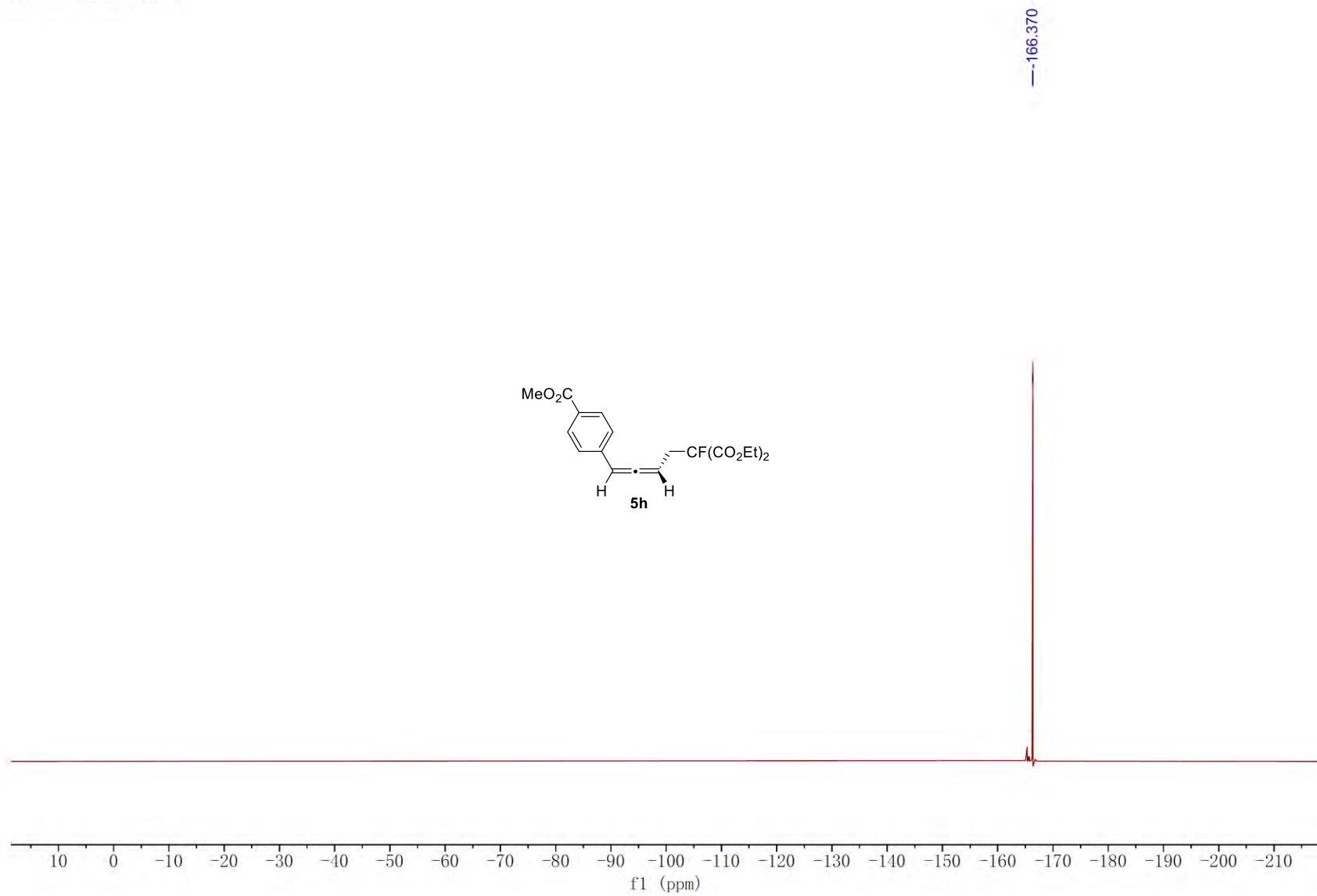
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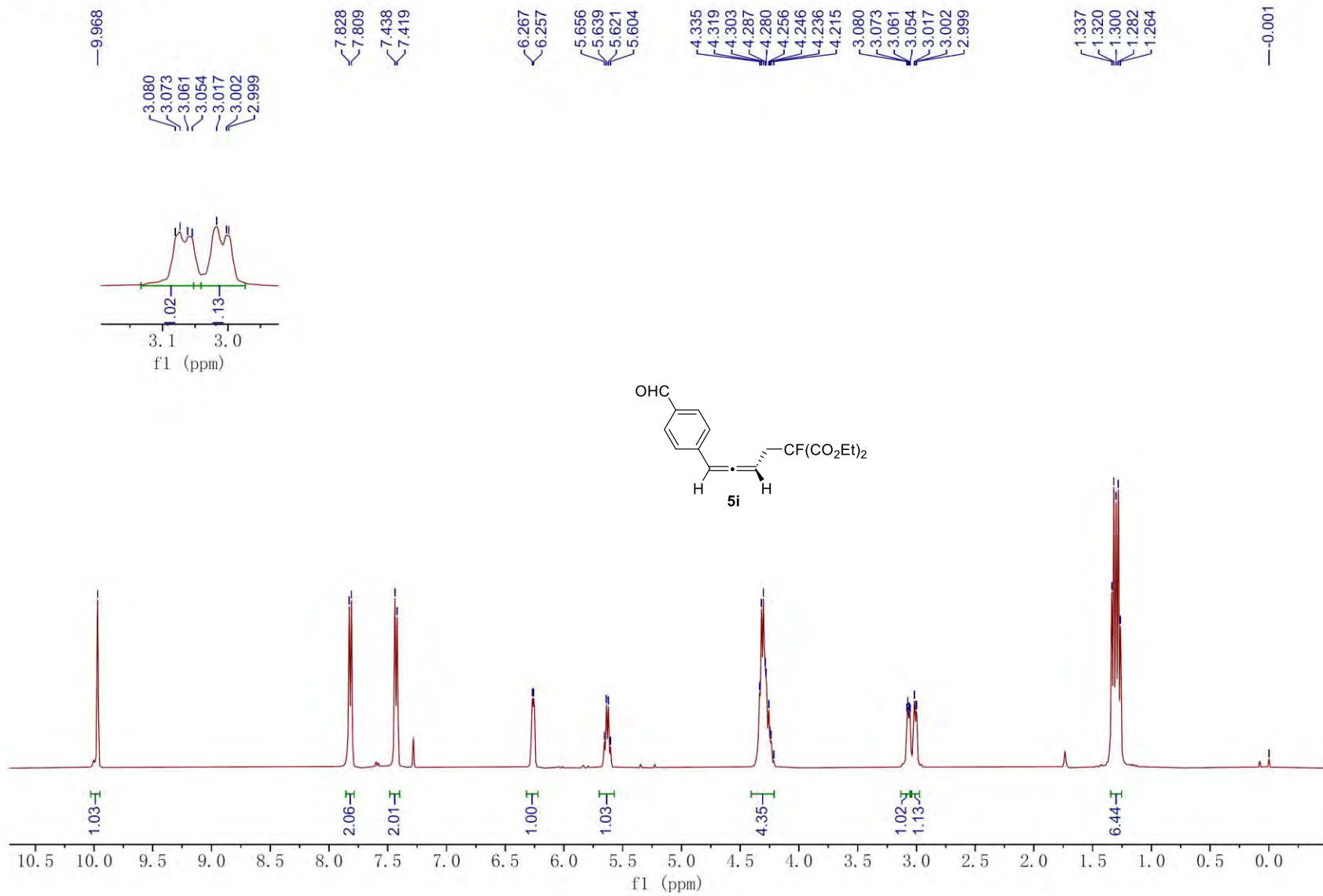
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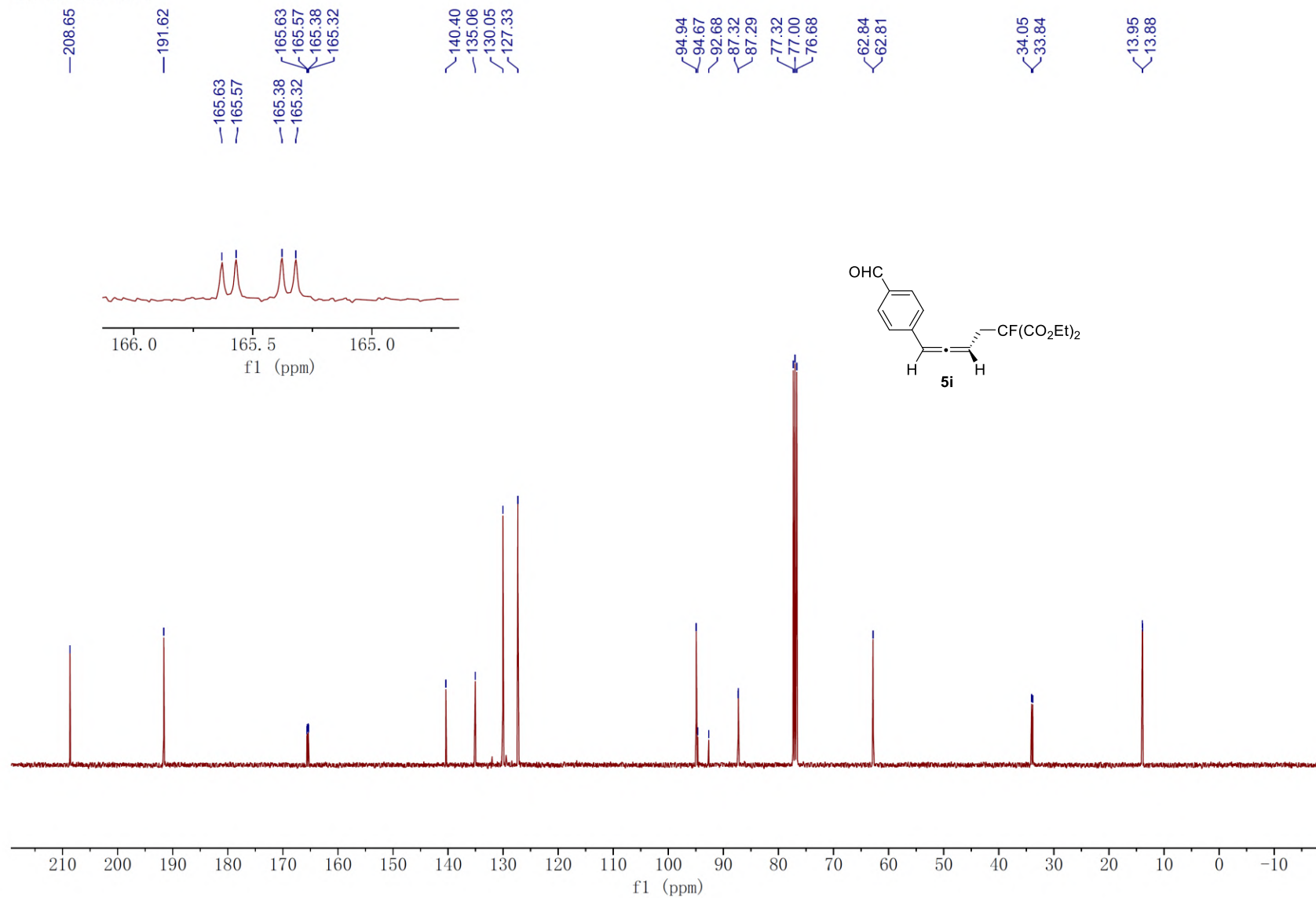
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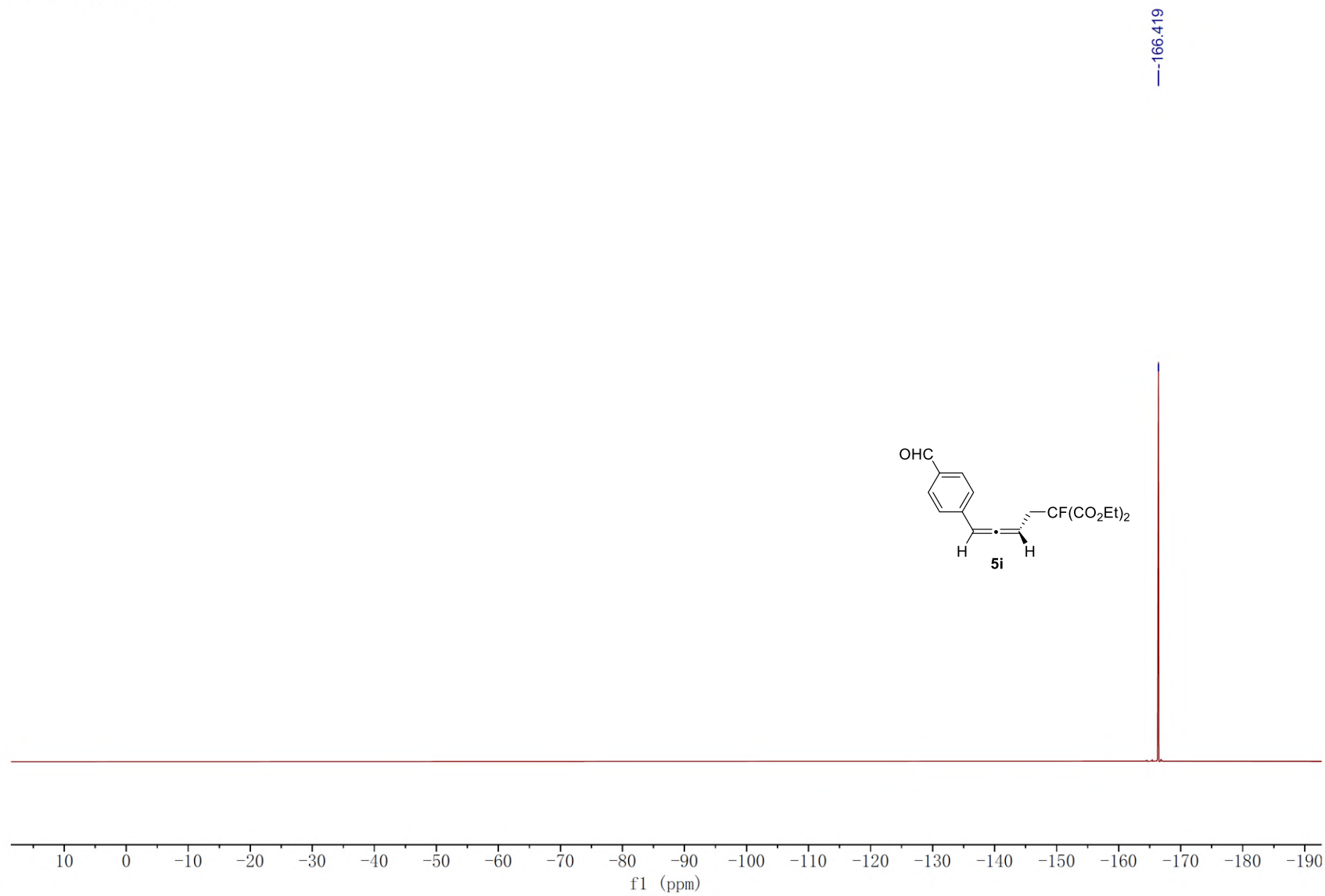
ZHY-ZG-128-400M-H



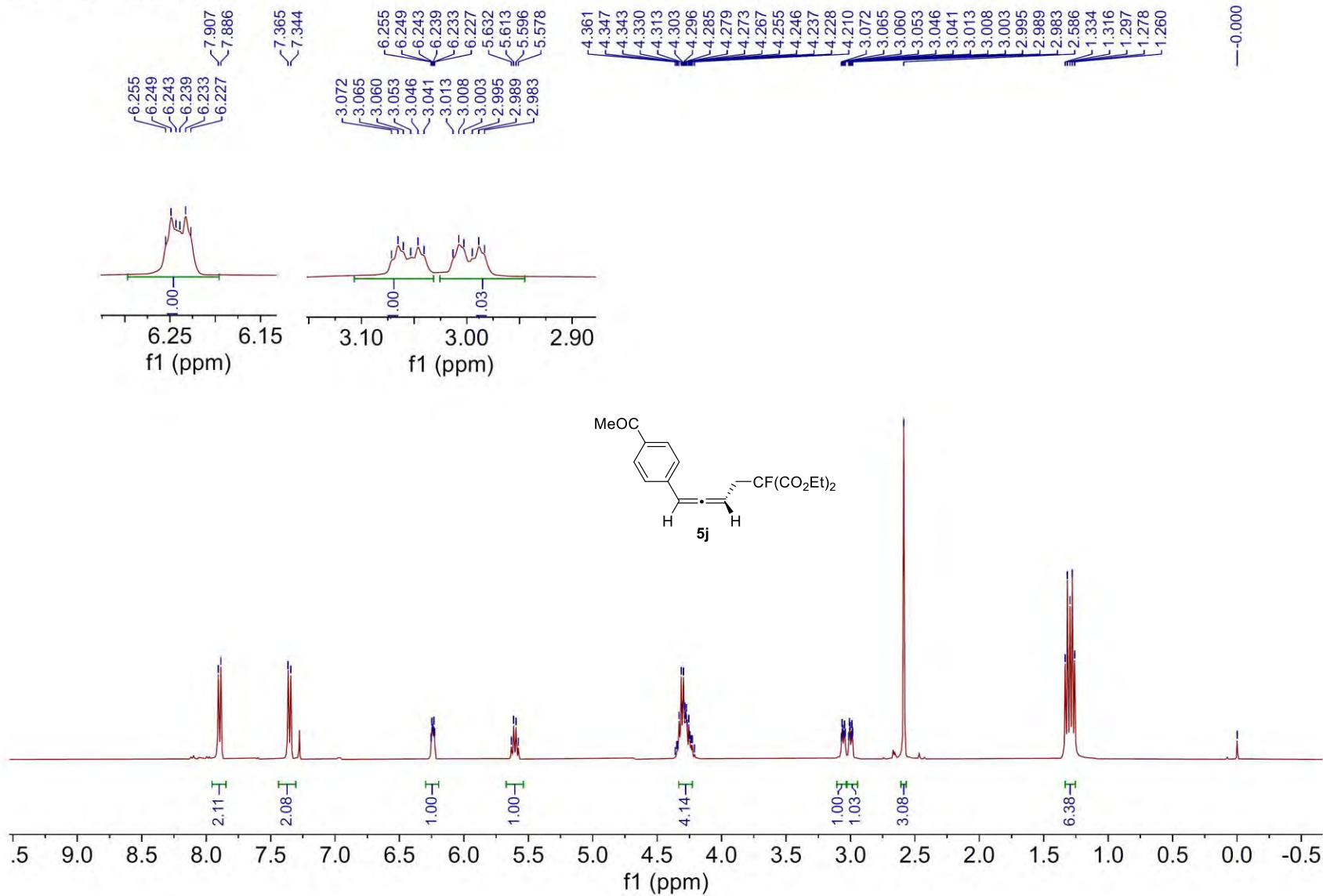
ZHY-ZG-128-100M-C



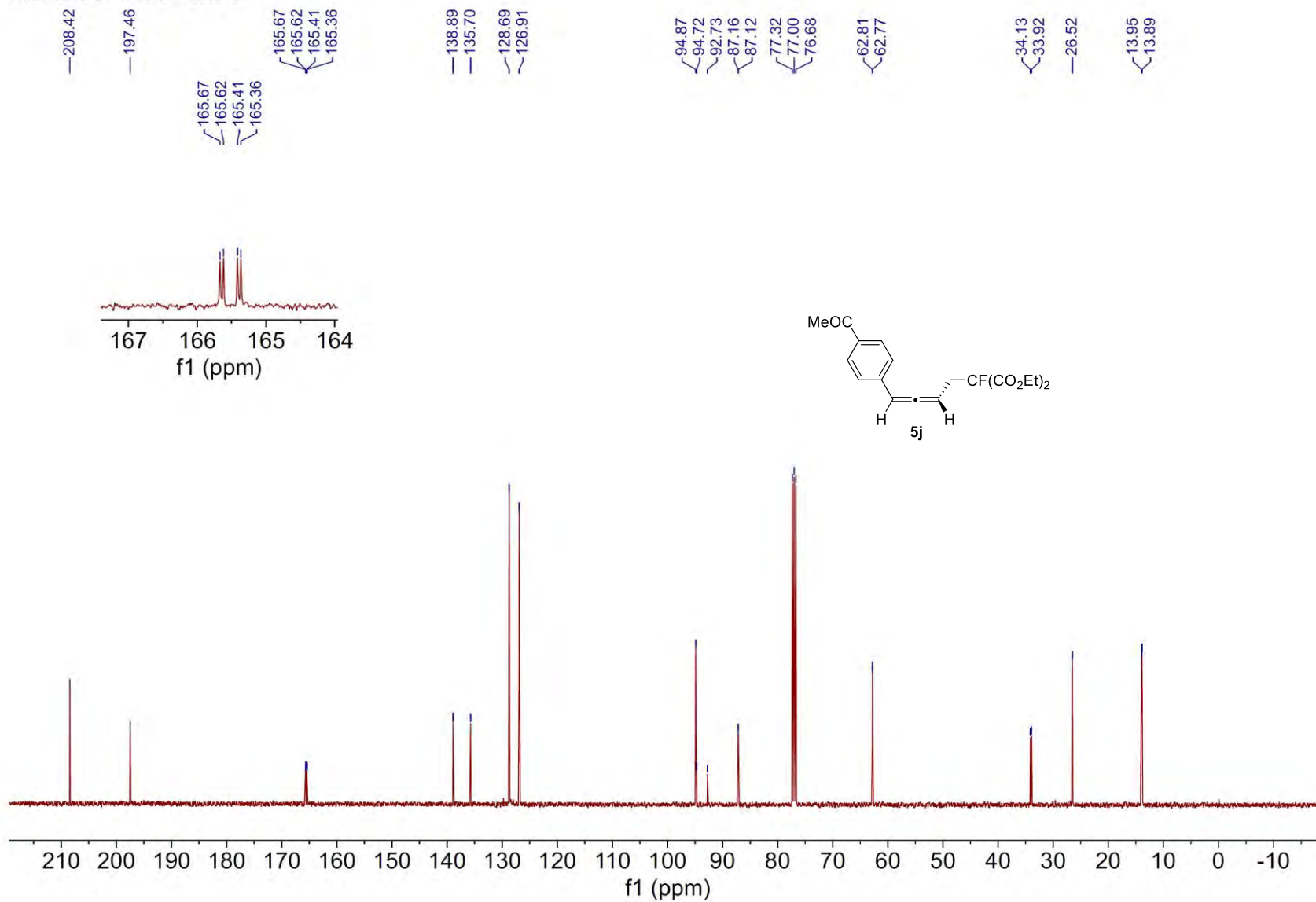
ZHY-ZG-128-376M-F

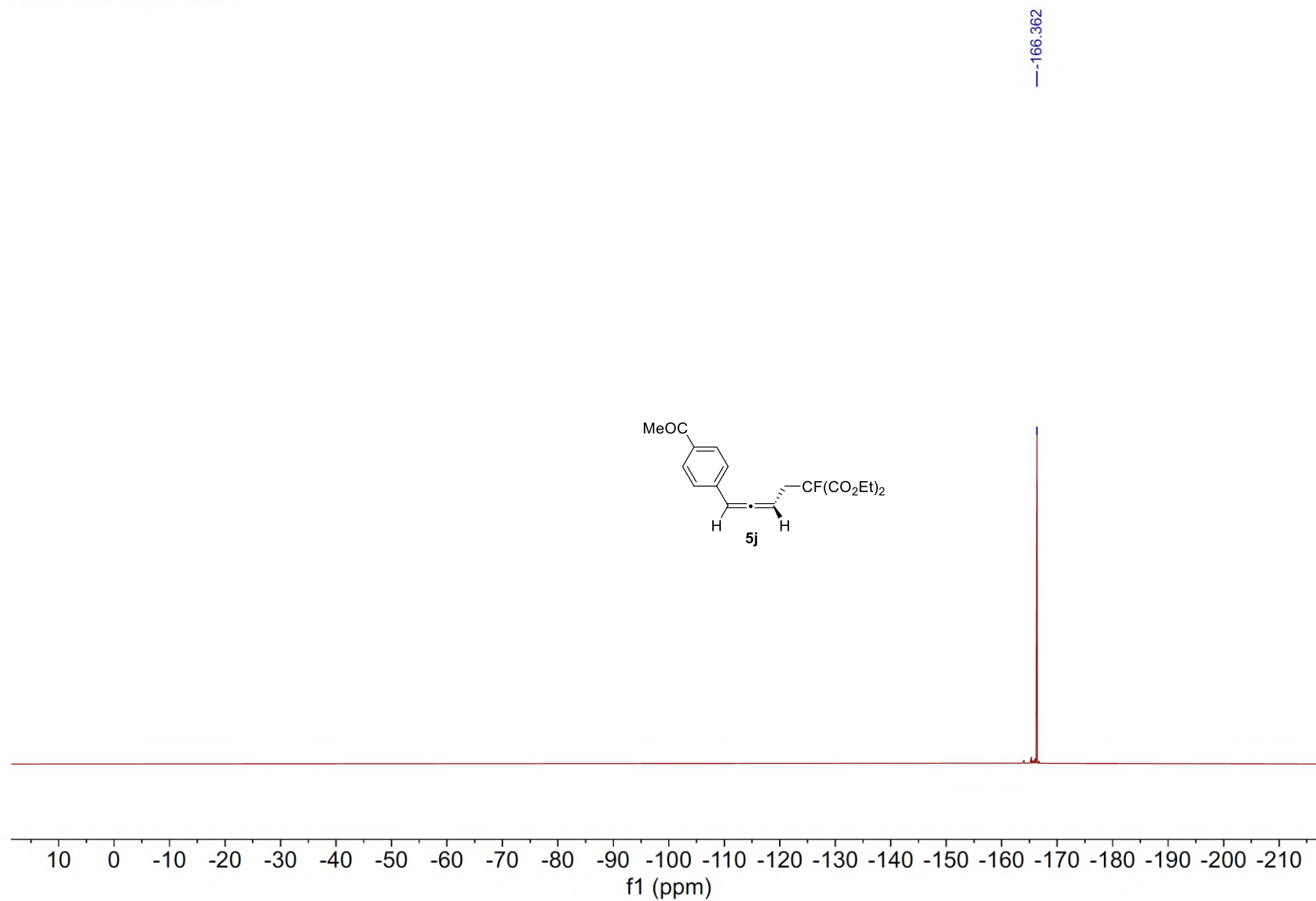


RYL-RB-15-ET-1.10.fid — boss ZF

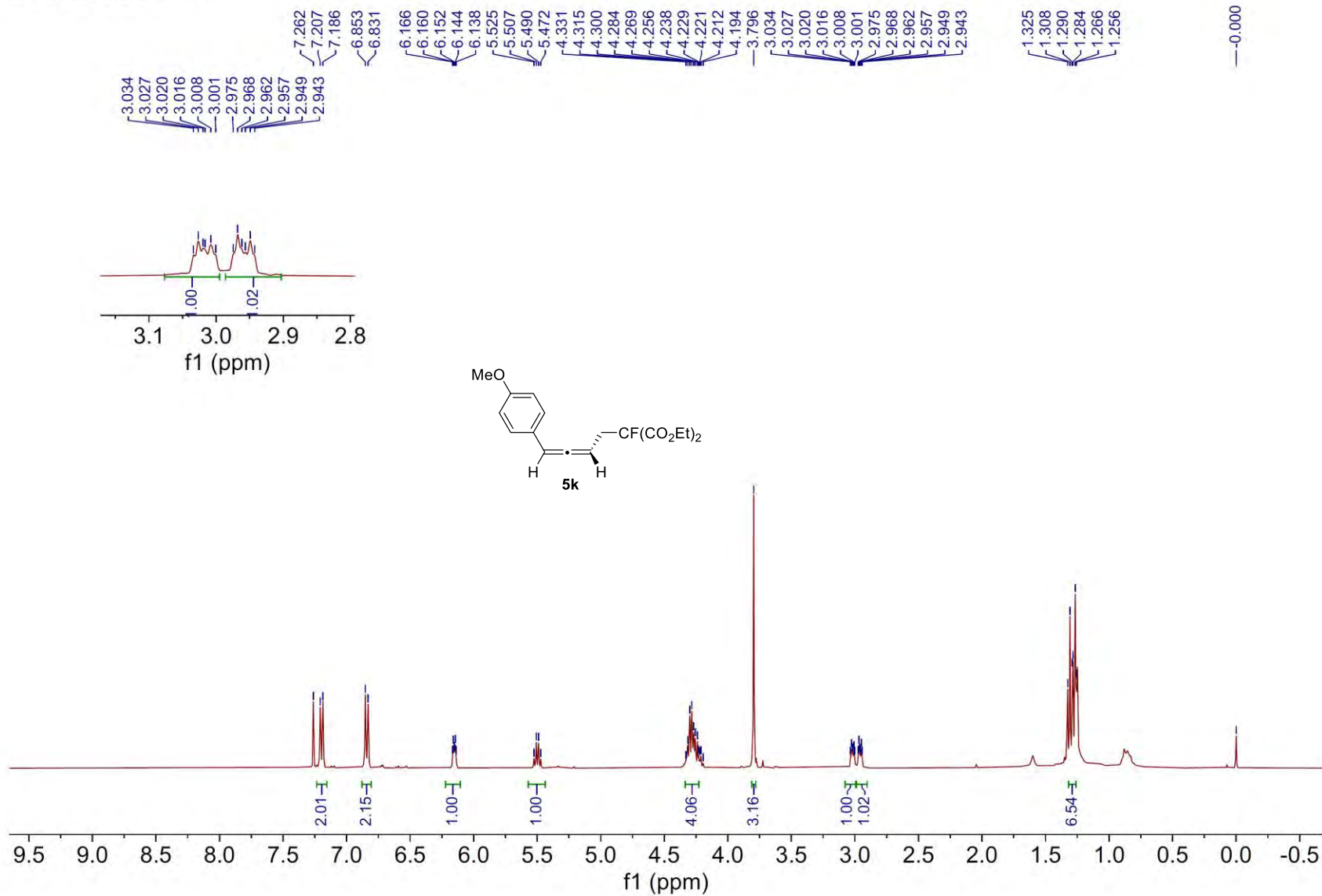


RYL-RB-15-ET-1.11.fid — boss ZF

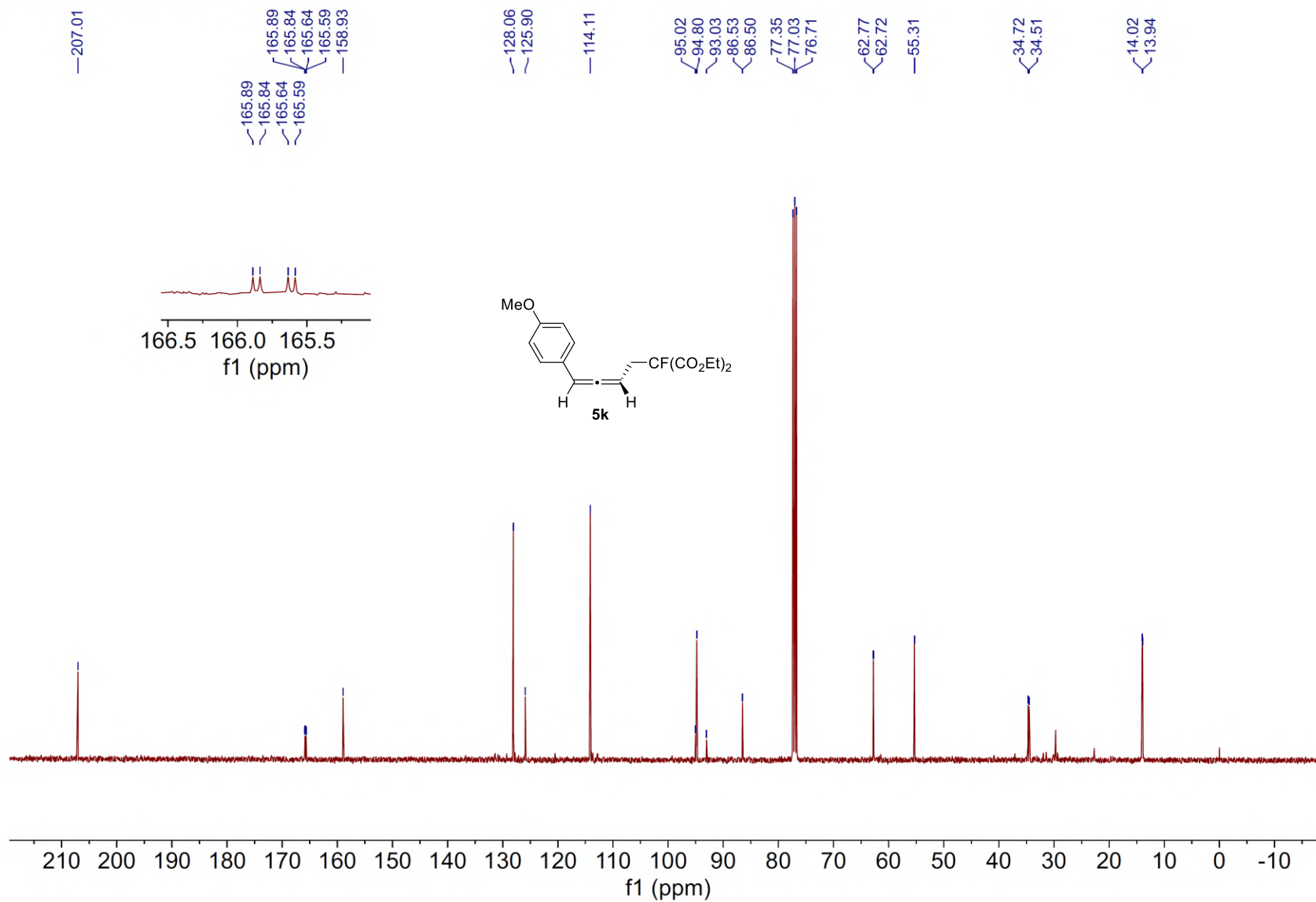


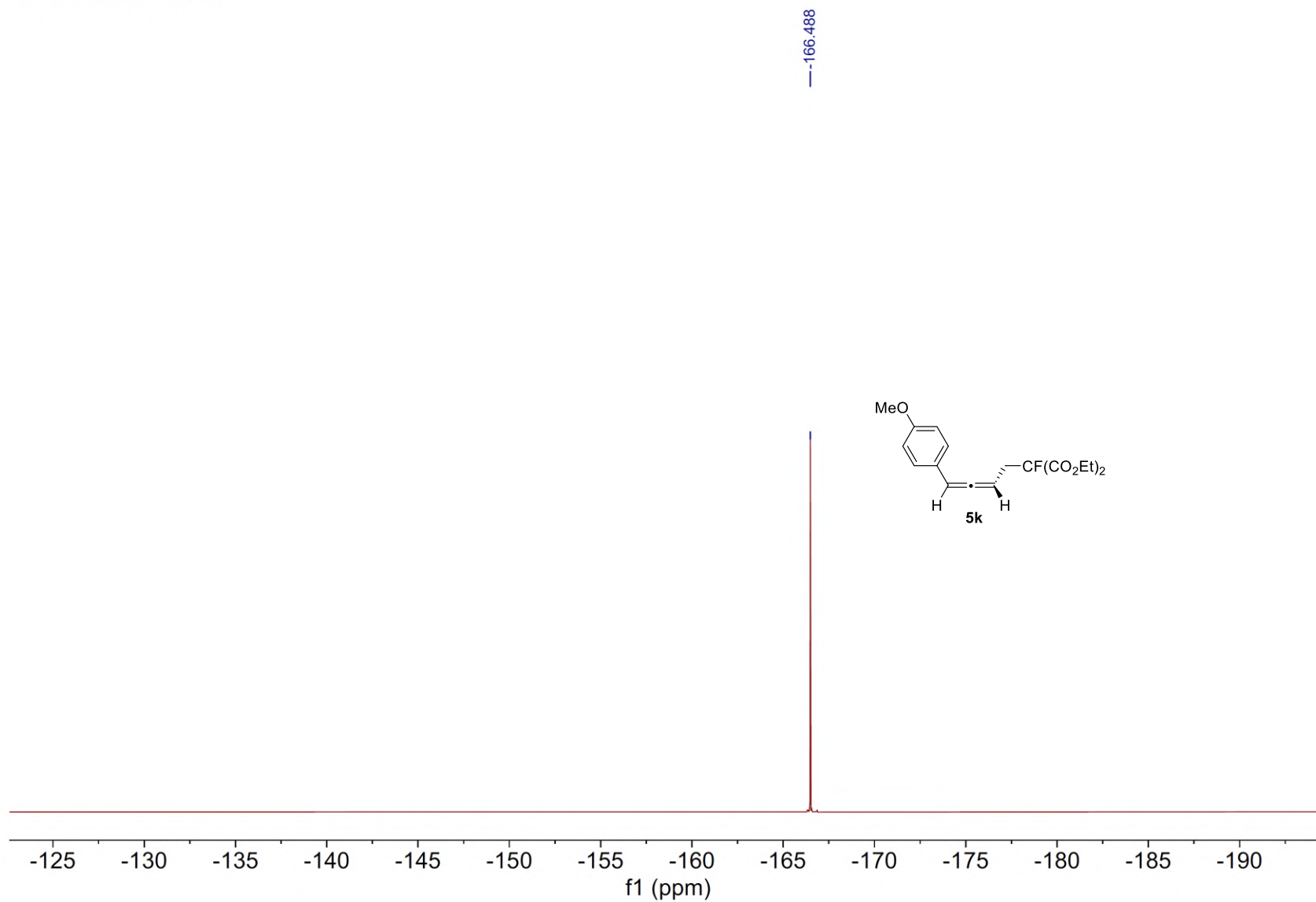


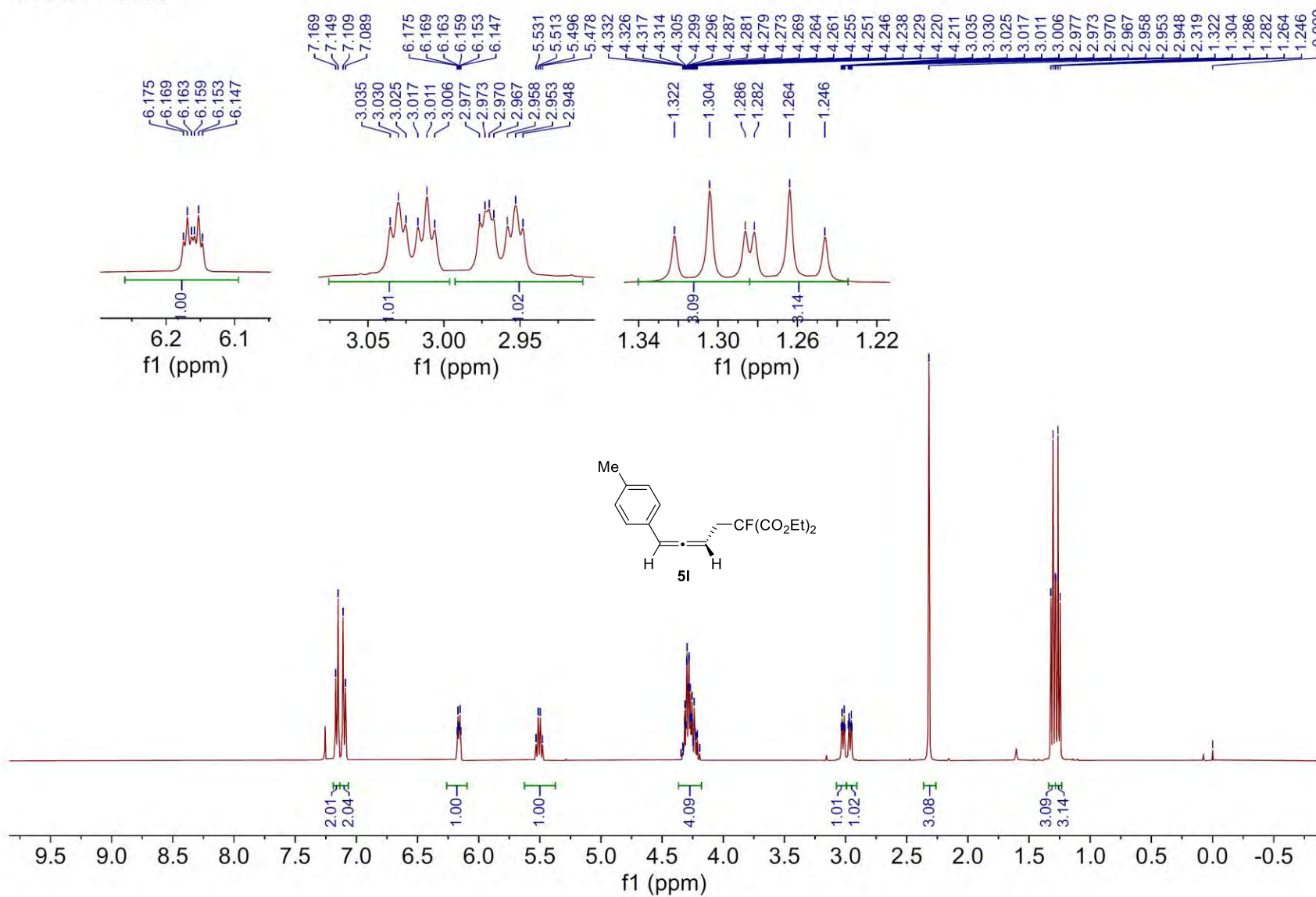
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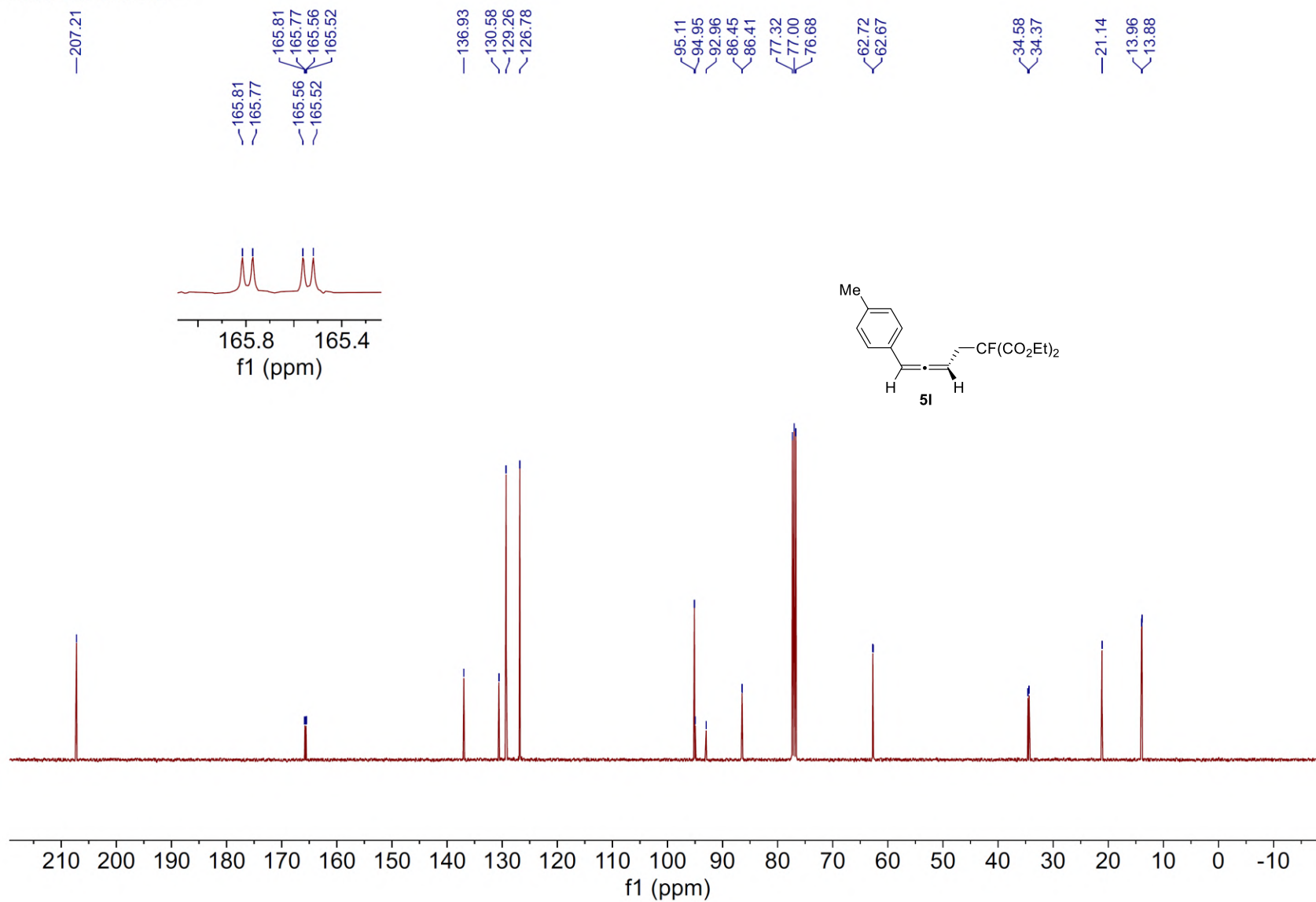
RYL-RB-23-Et.11.fid — boss ZF





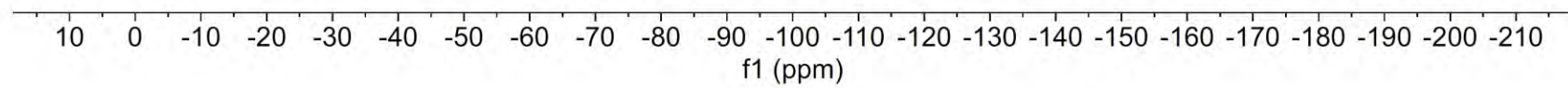
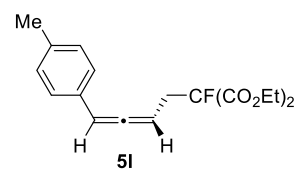


RYL-ME-ET-1.10.11.fid —

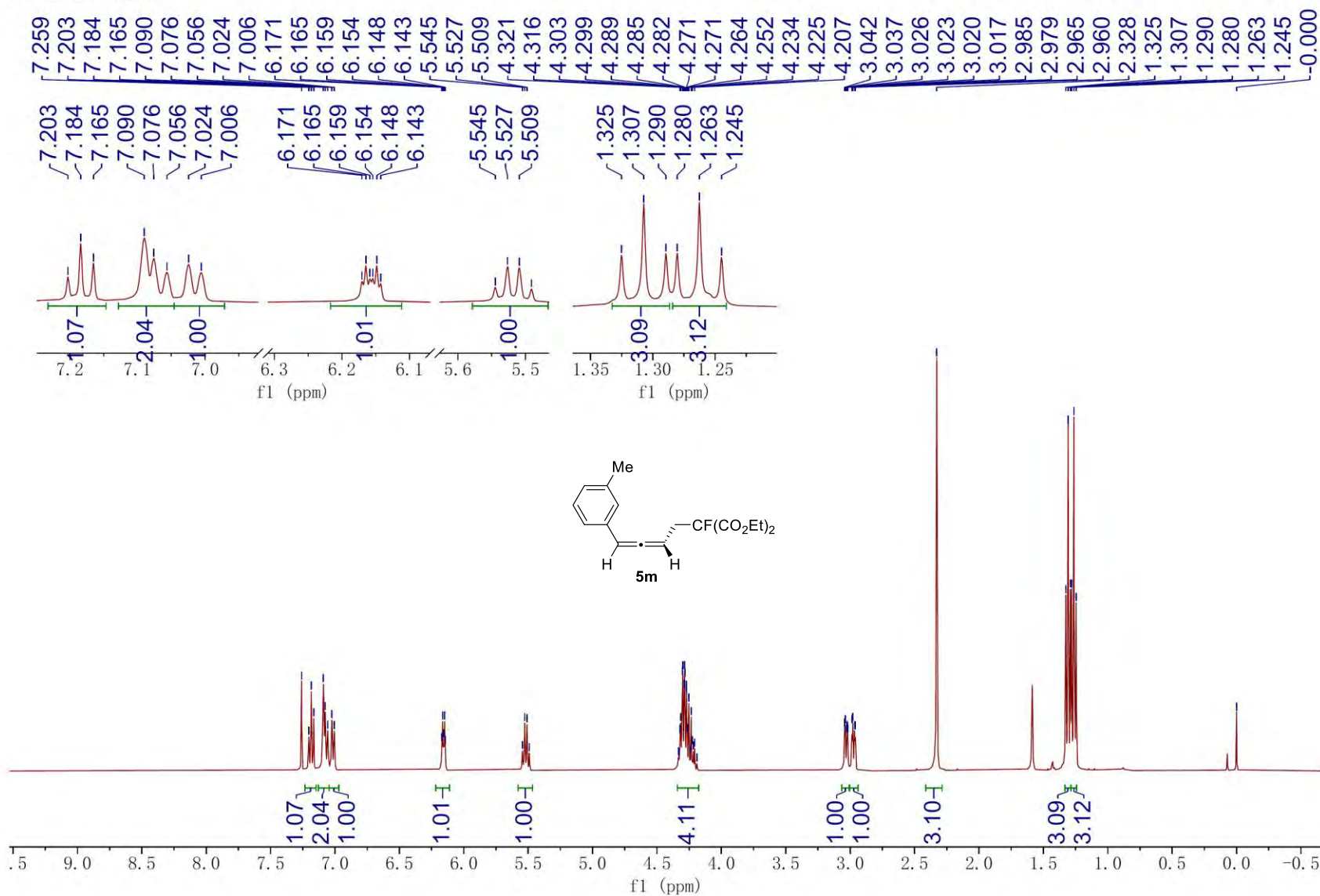


RYL-ME-ET-1.10.12.fid —

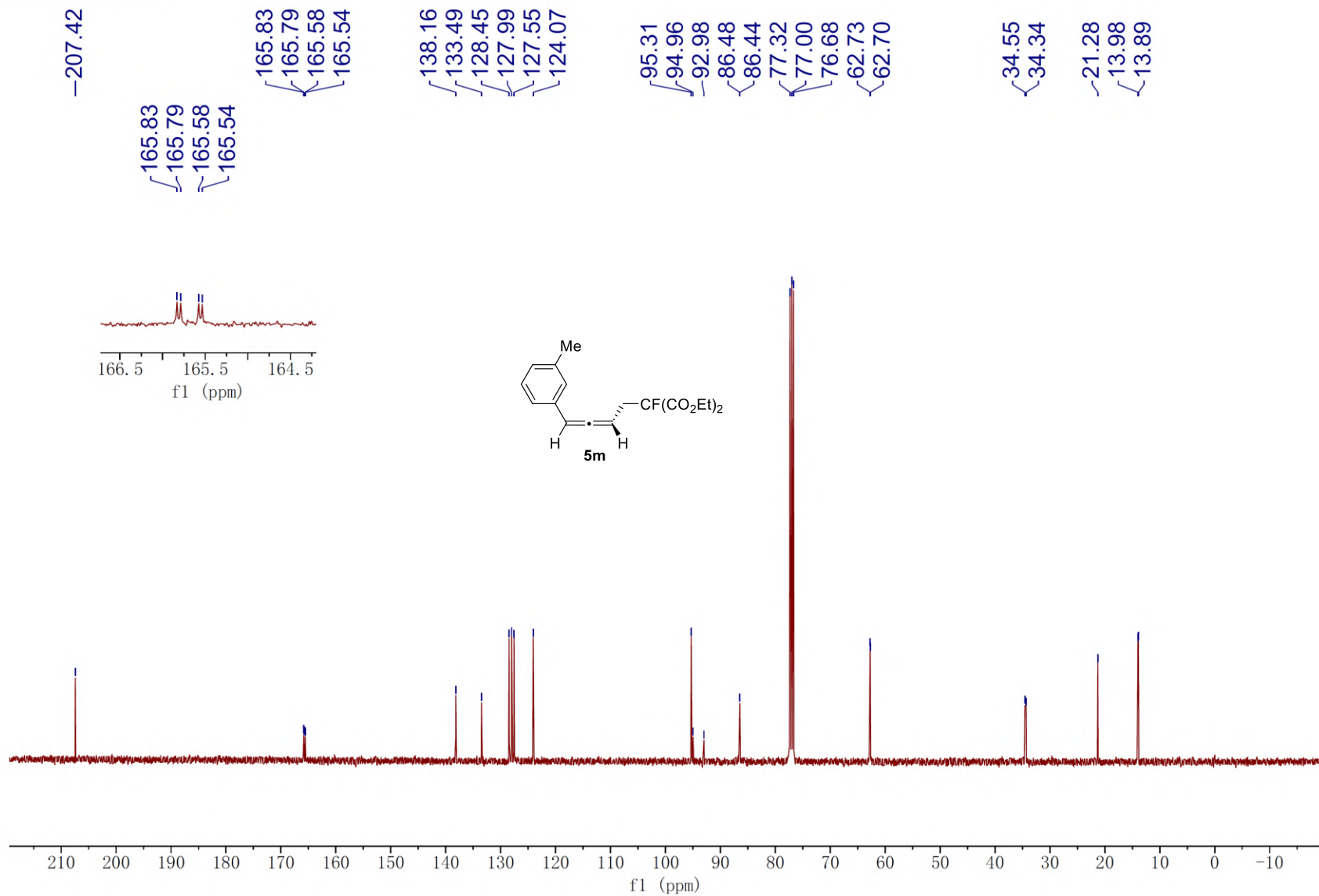
— -166.478



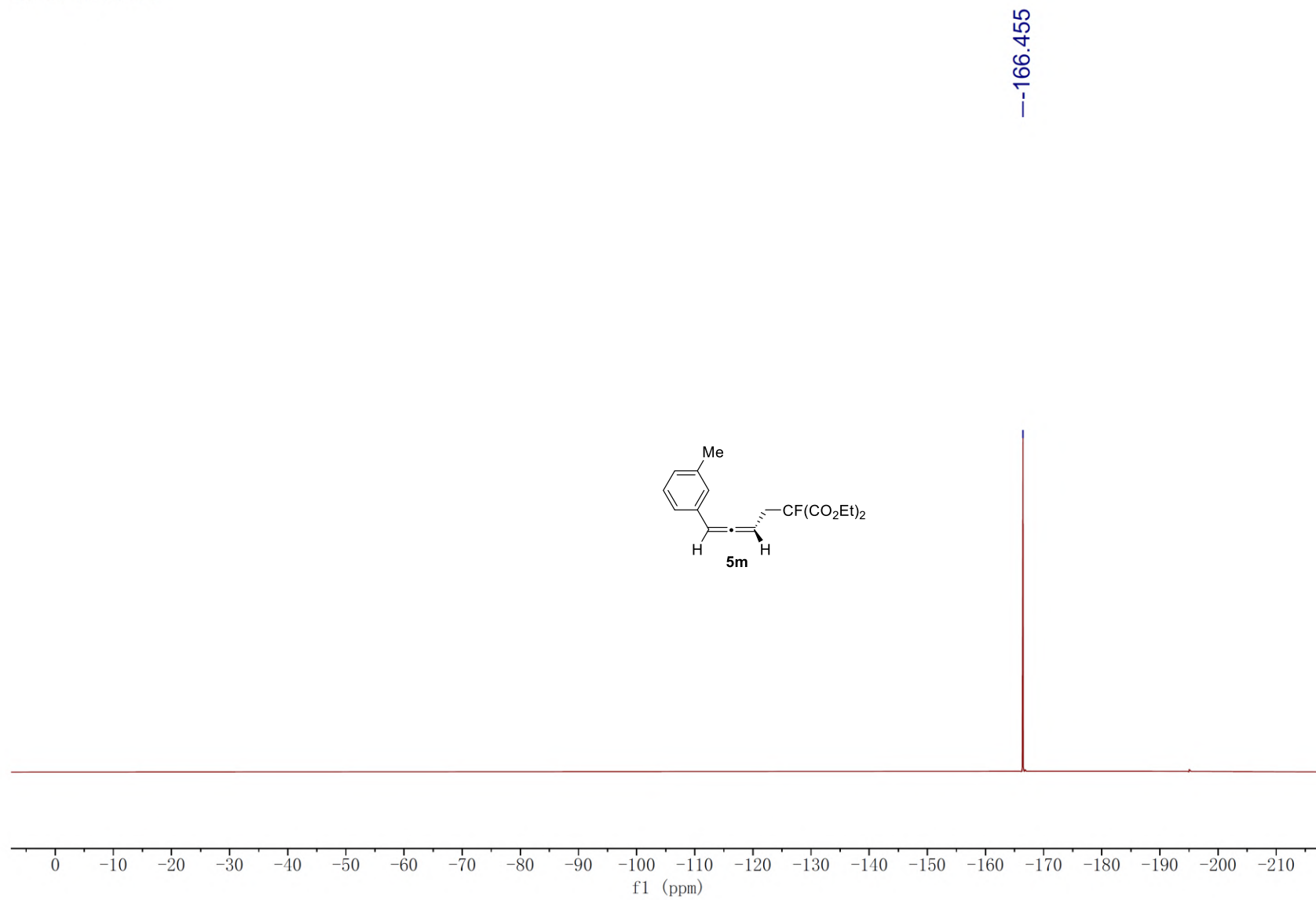
ZHY-ZG-58-400M-H



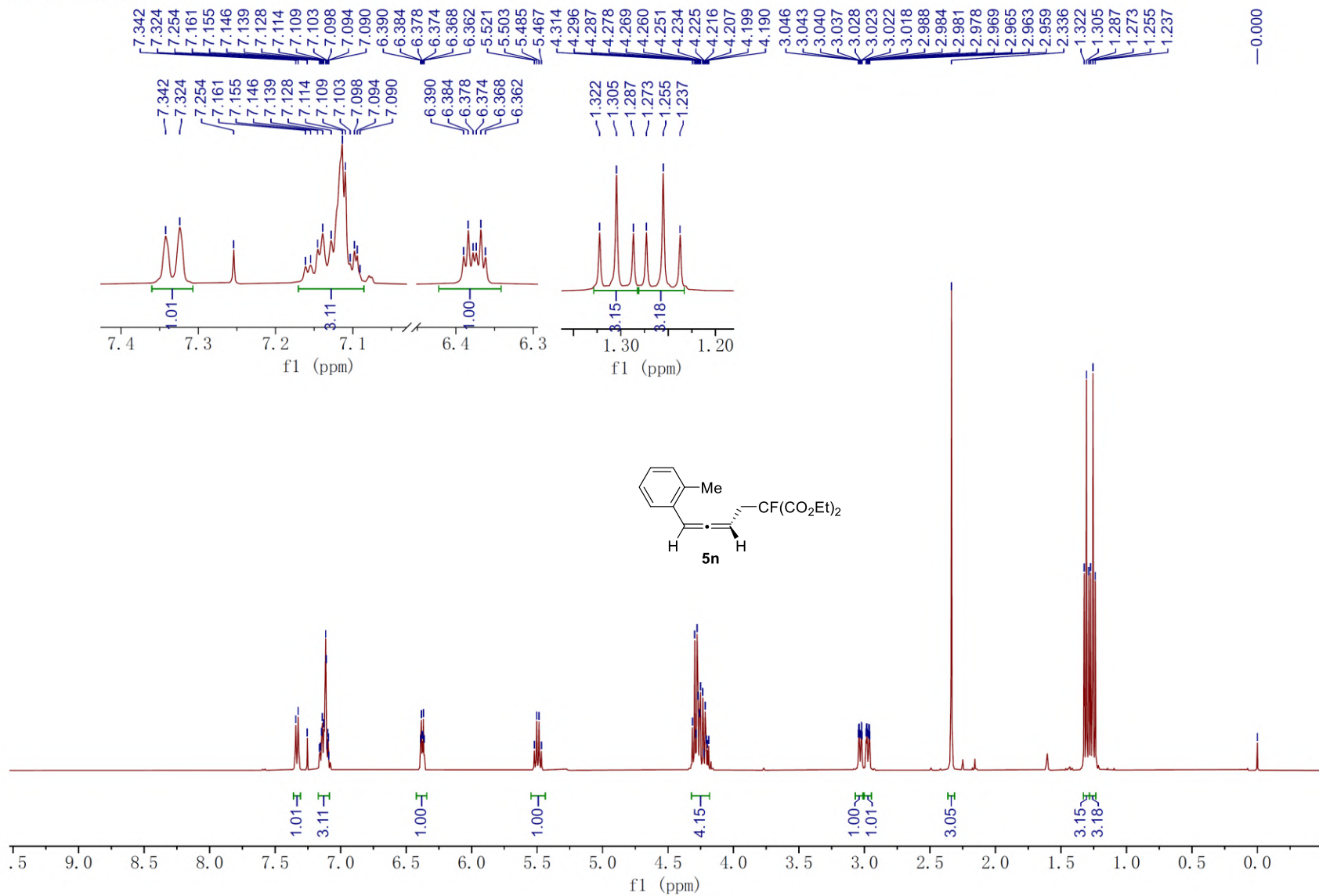
ZHY-ZG-58-100M-C



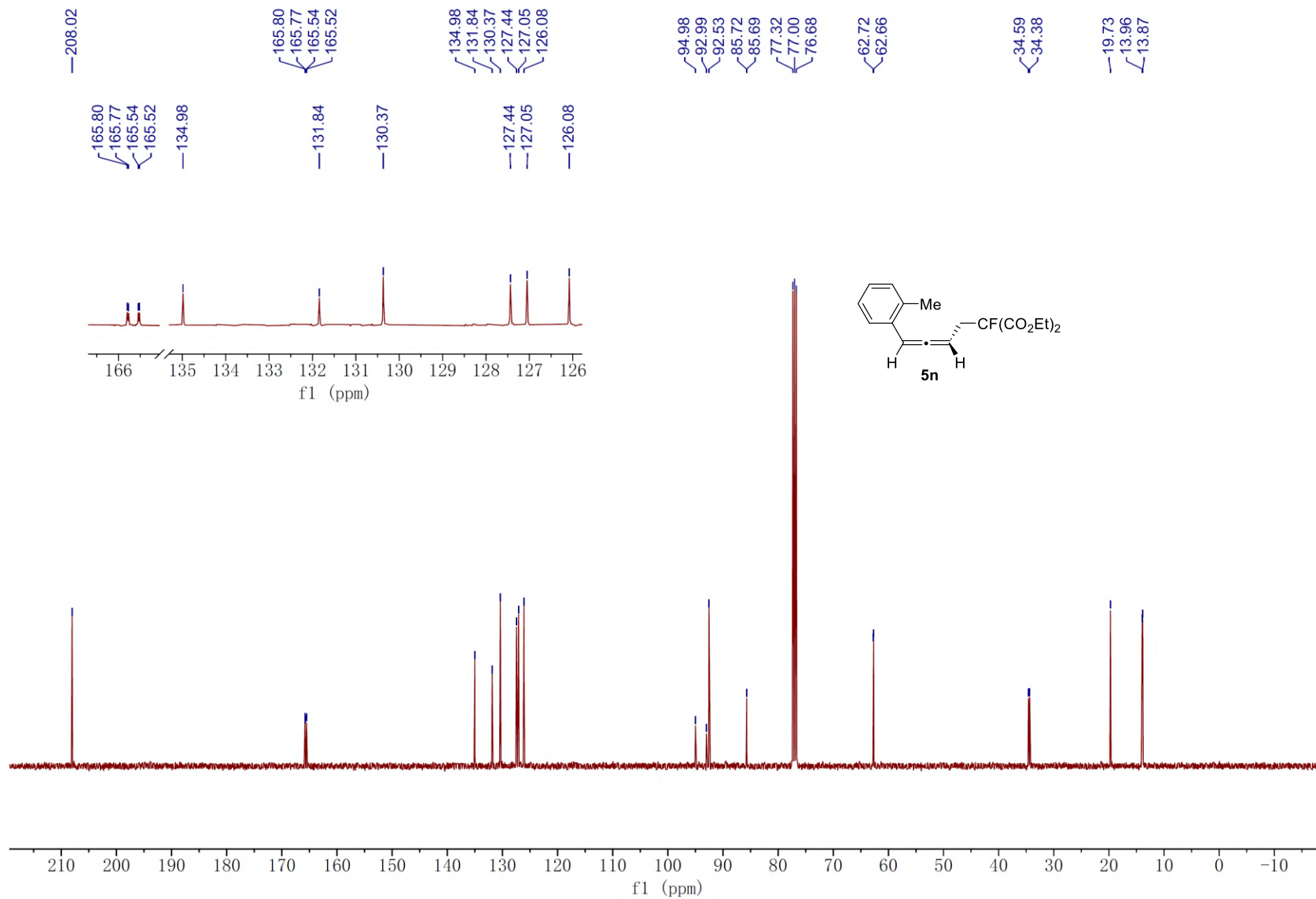
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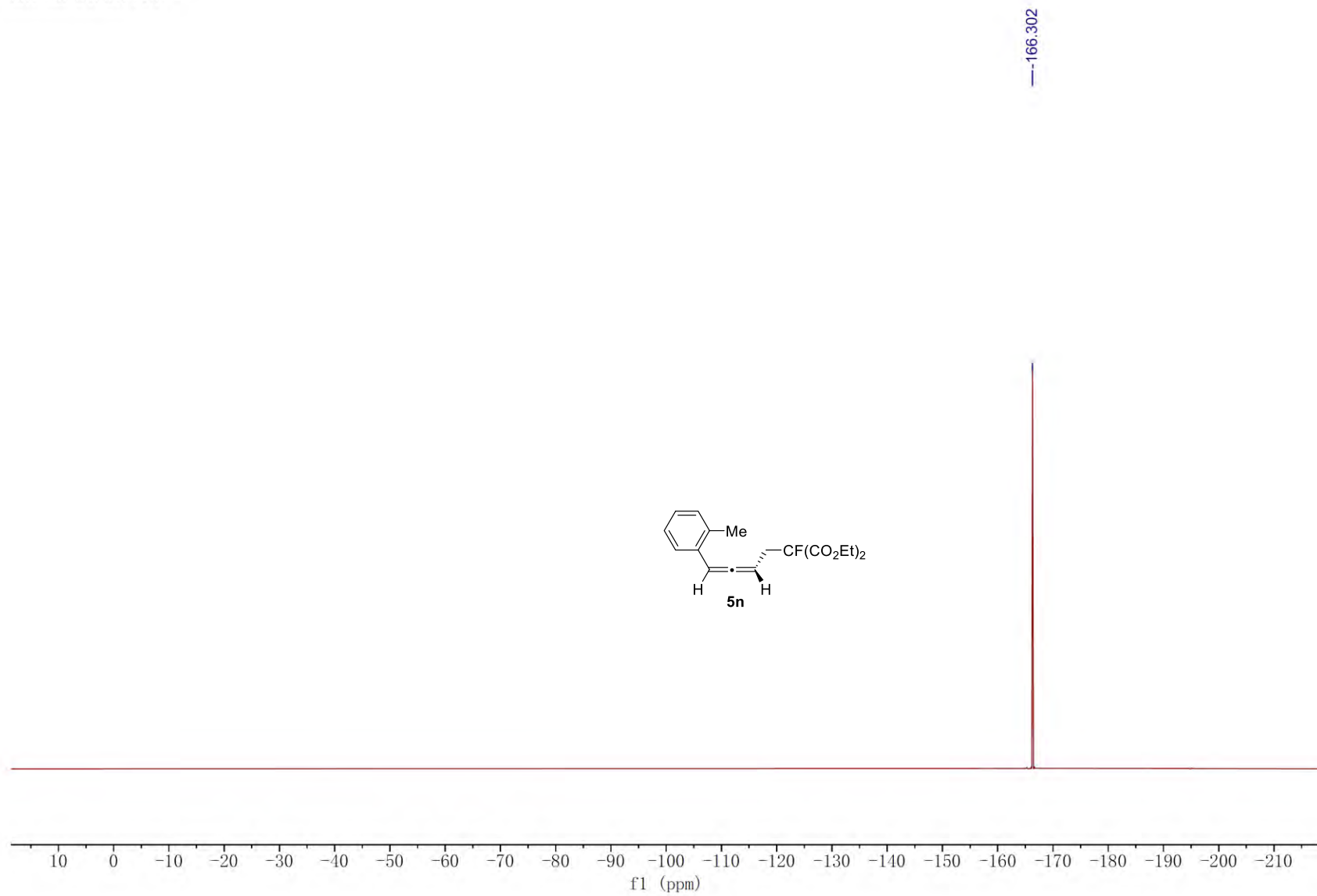
ZHY-ZH-54. 20. fid —



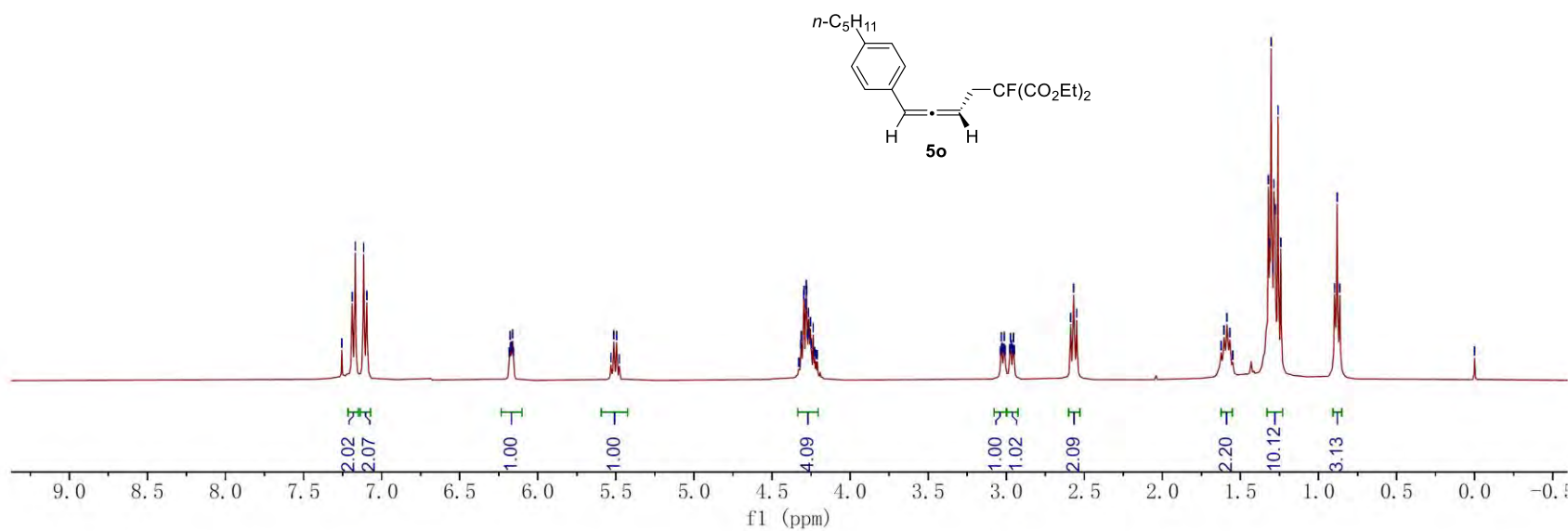
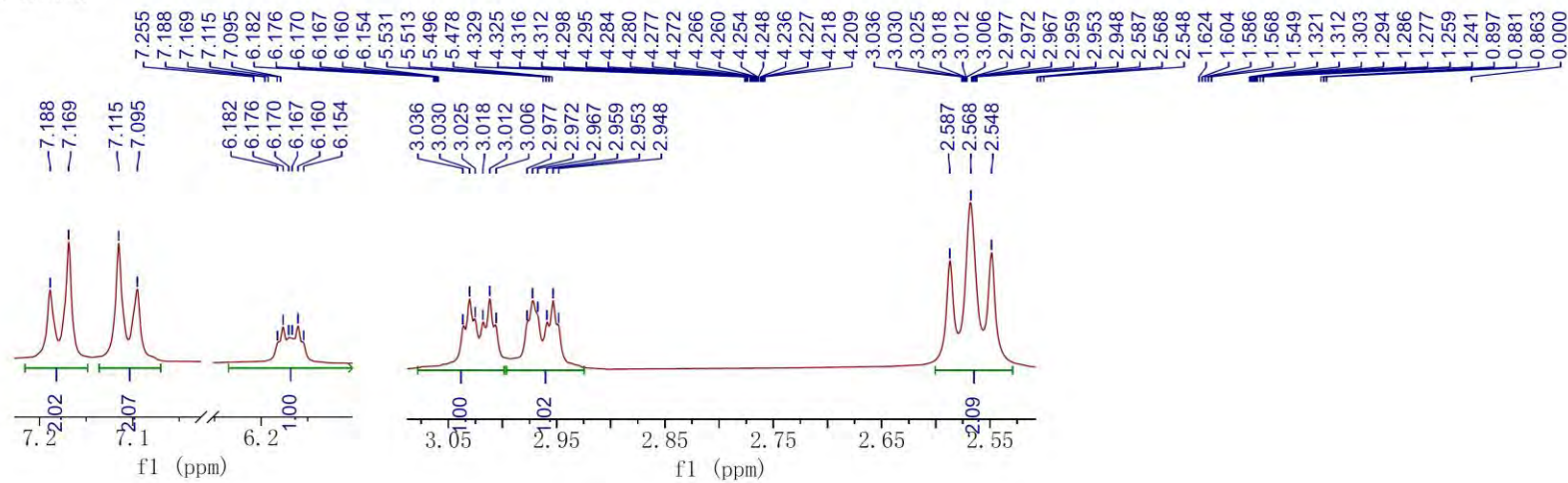
ZHY-ZH-54. 22. fid —



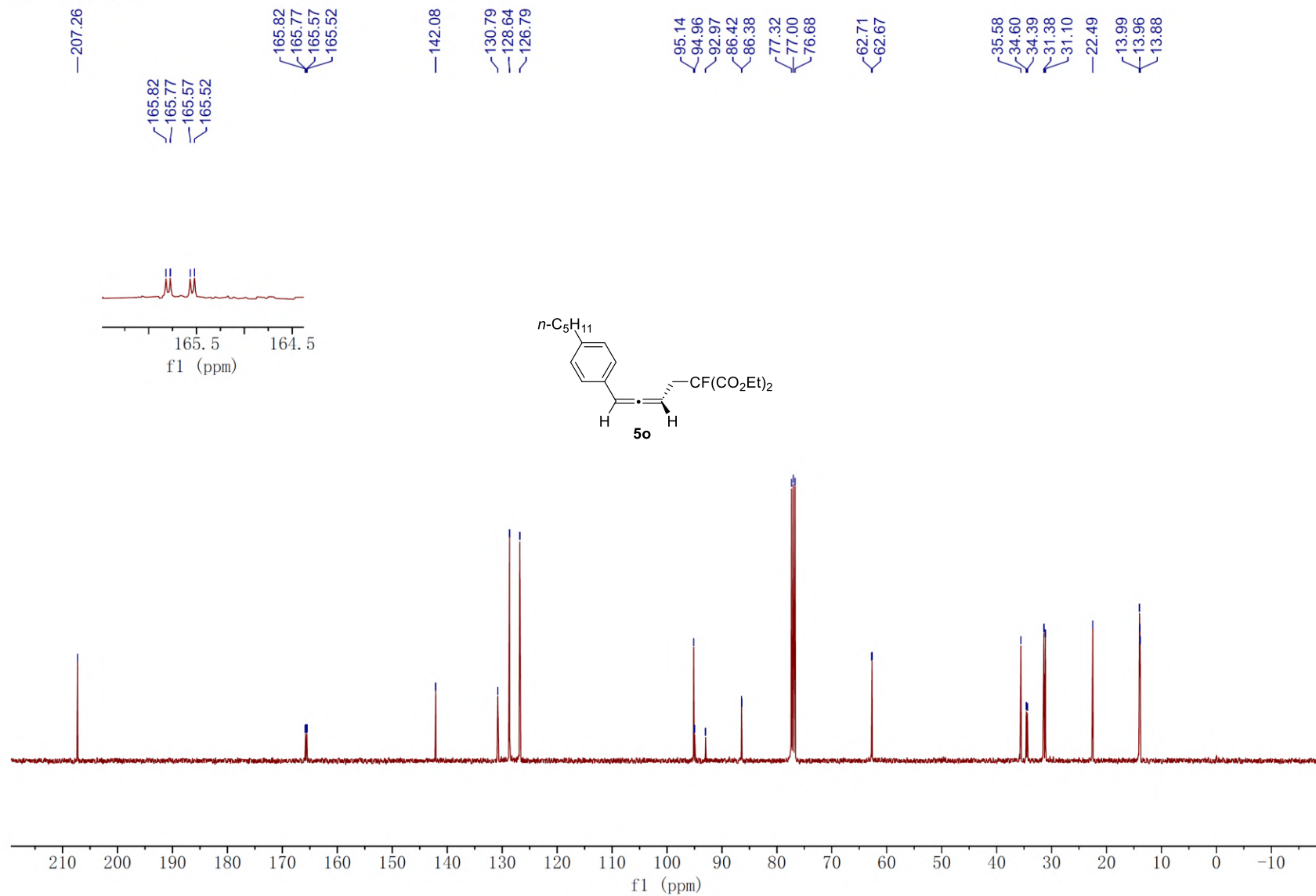
ZHY-ZH-54. 21. fid —



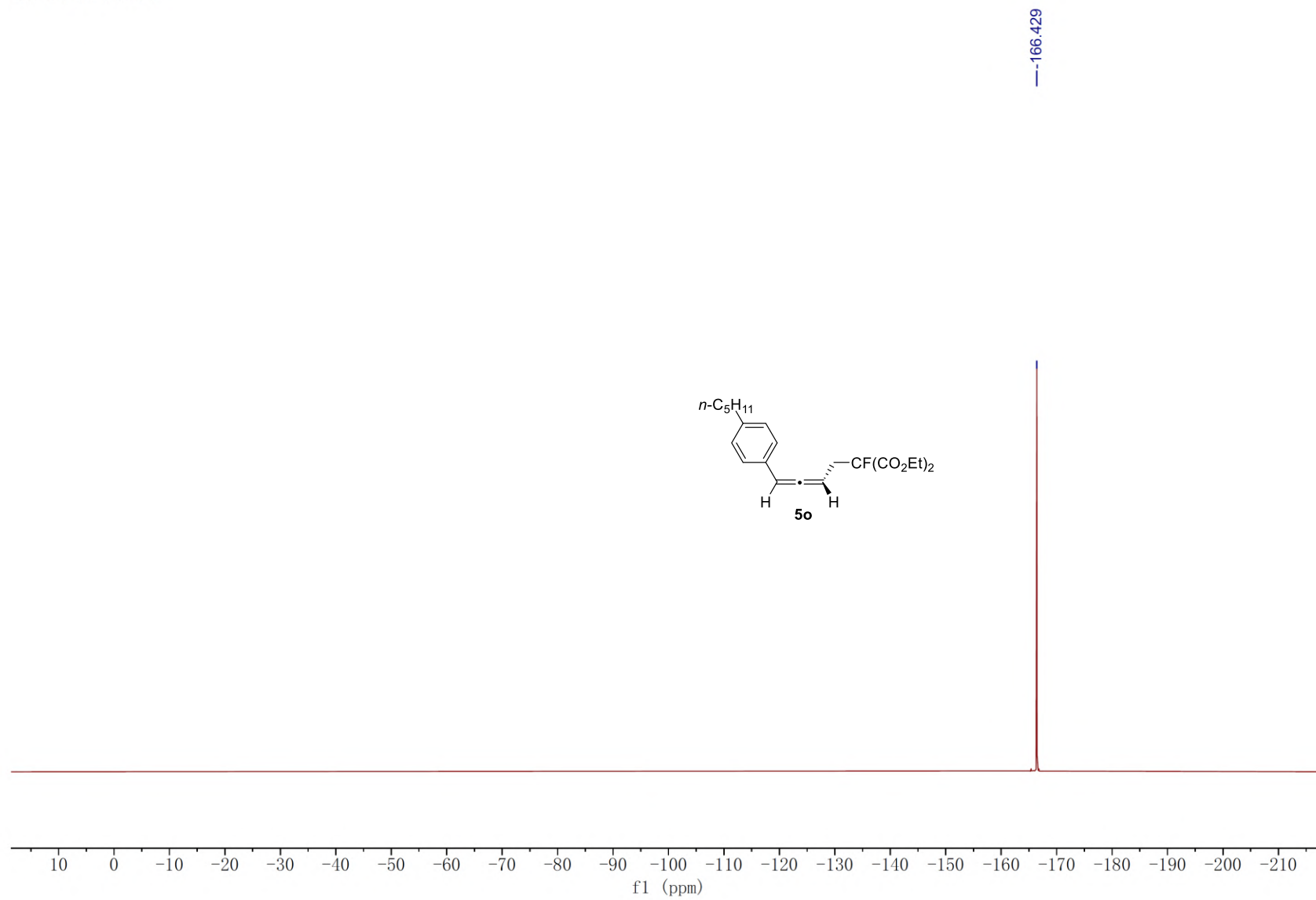
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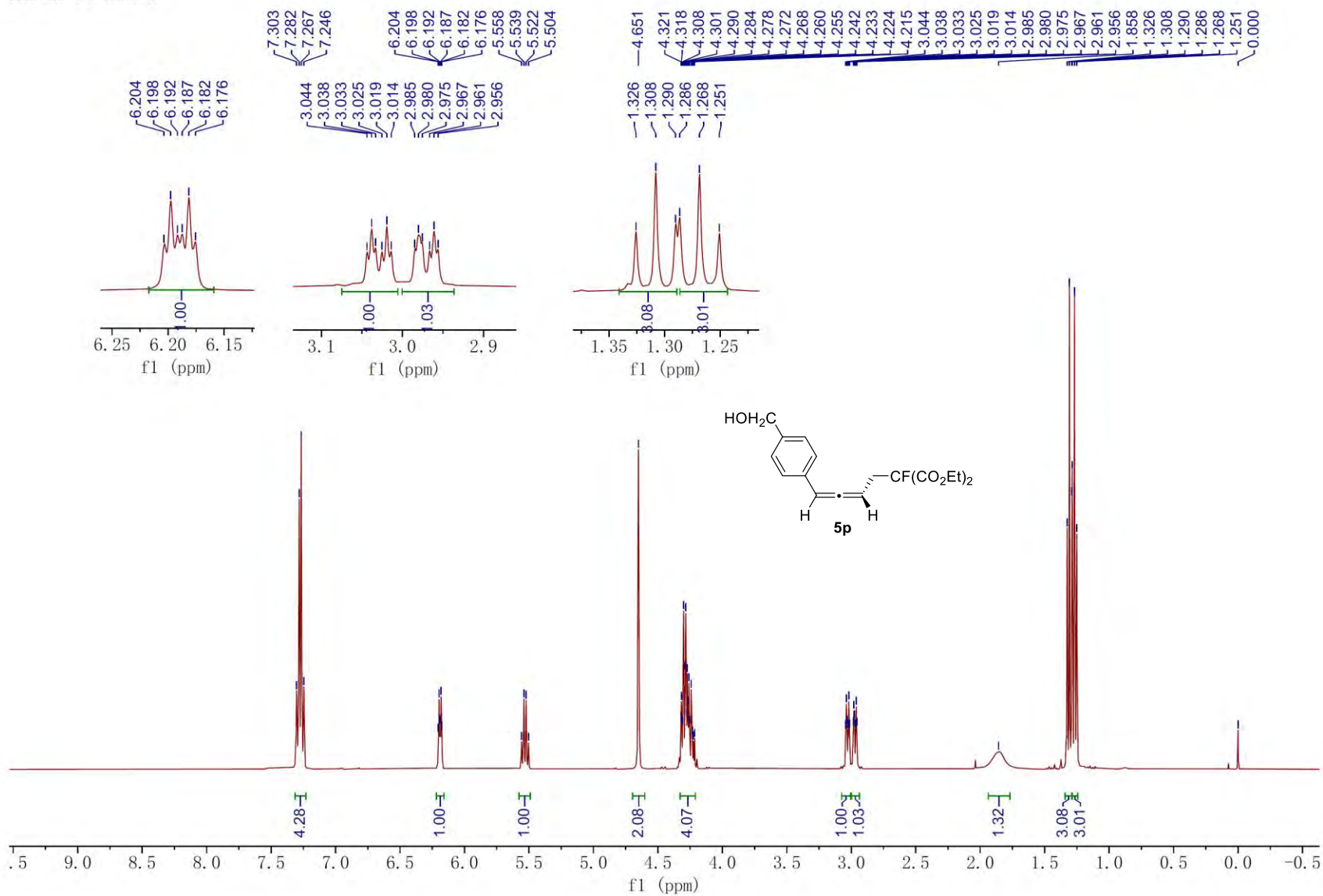
ZHY-ZG-55-100M-C



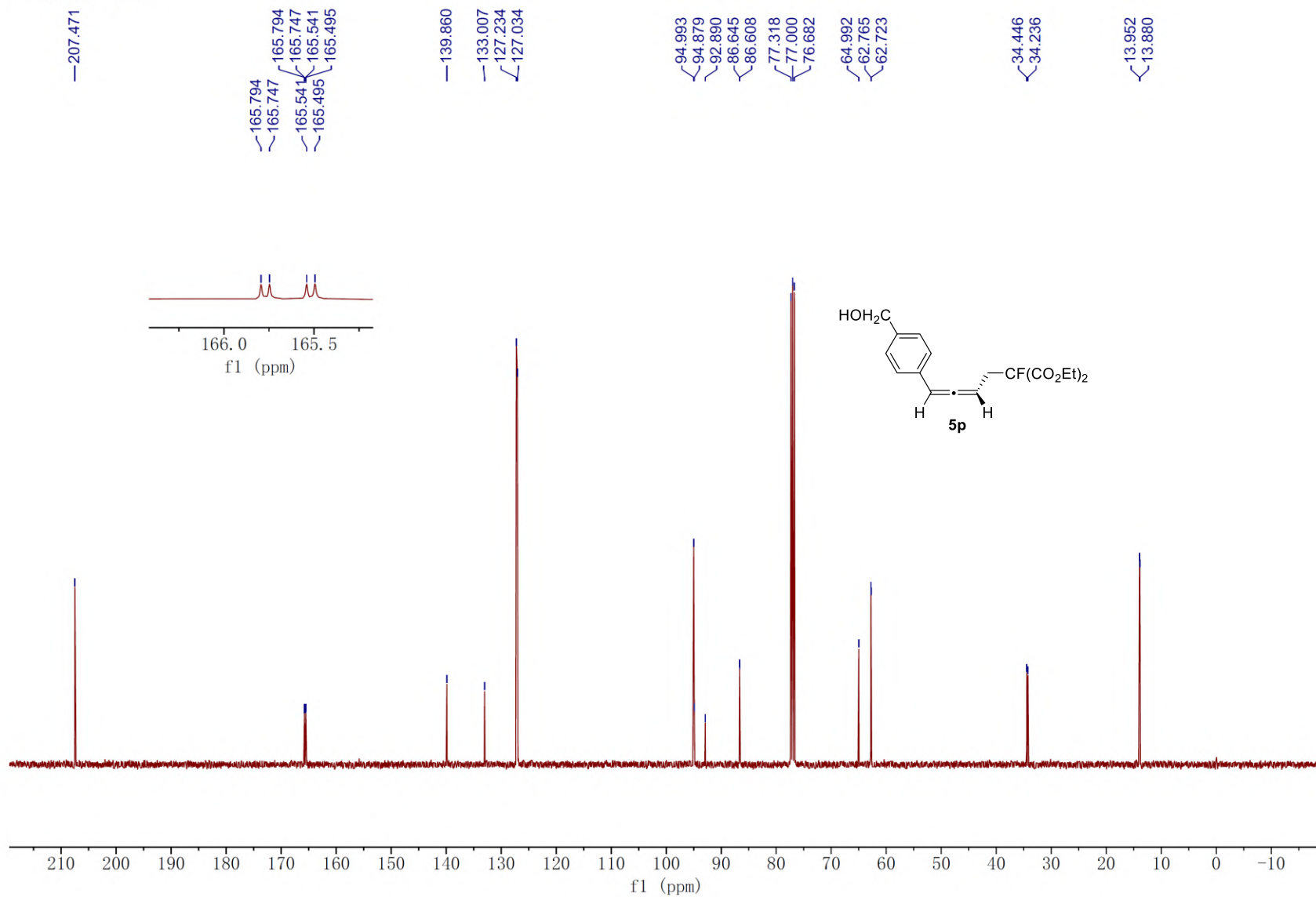
ZHY-ZG-55-376M-F



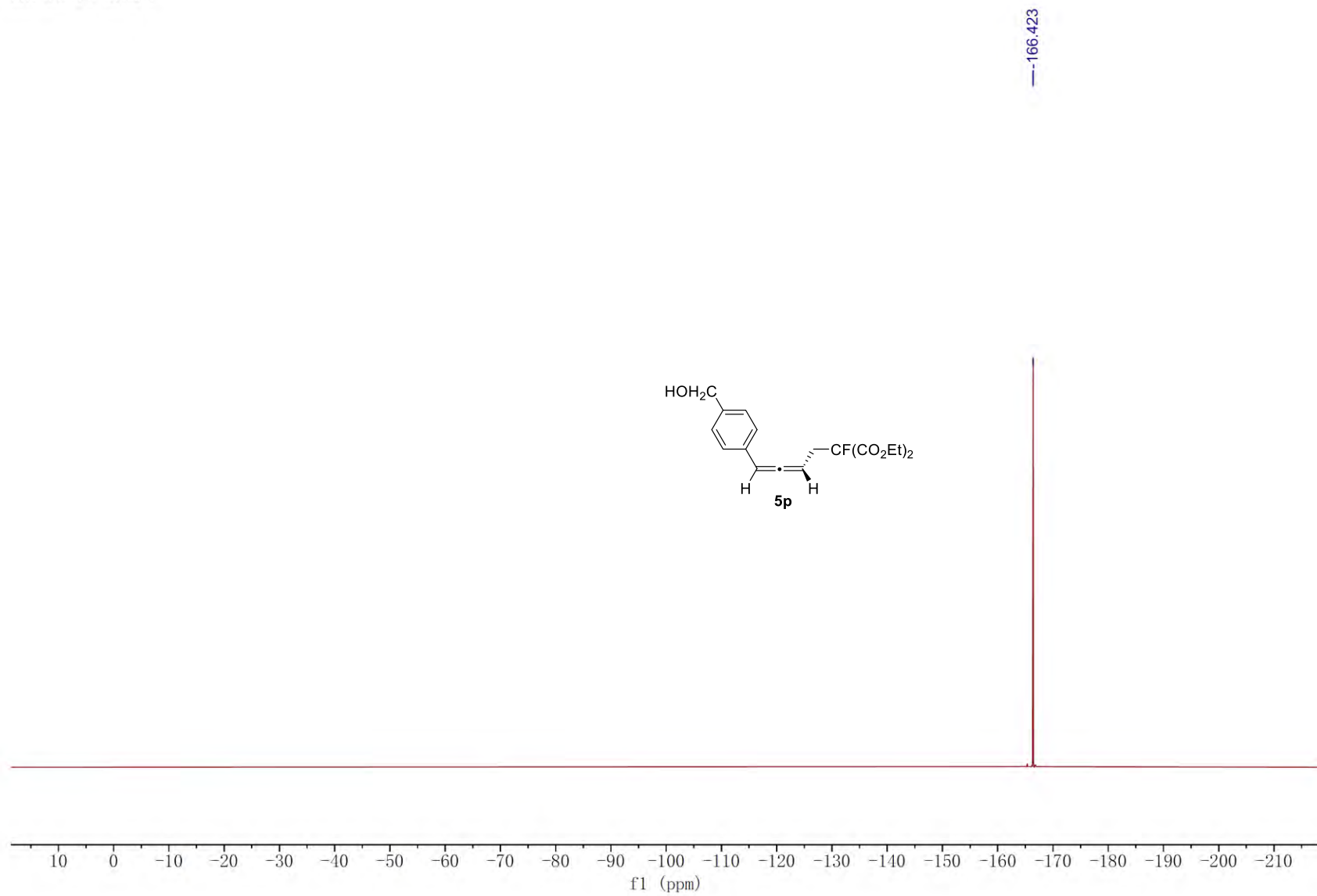
ZHY-ZG-71-400M-H



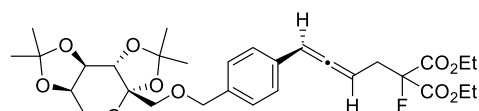
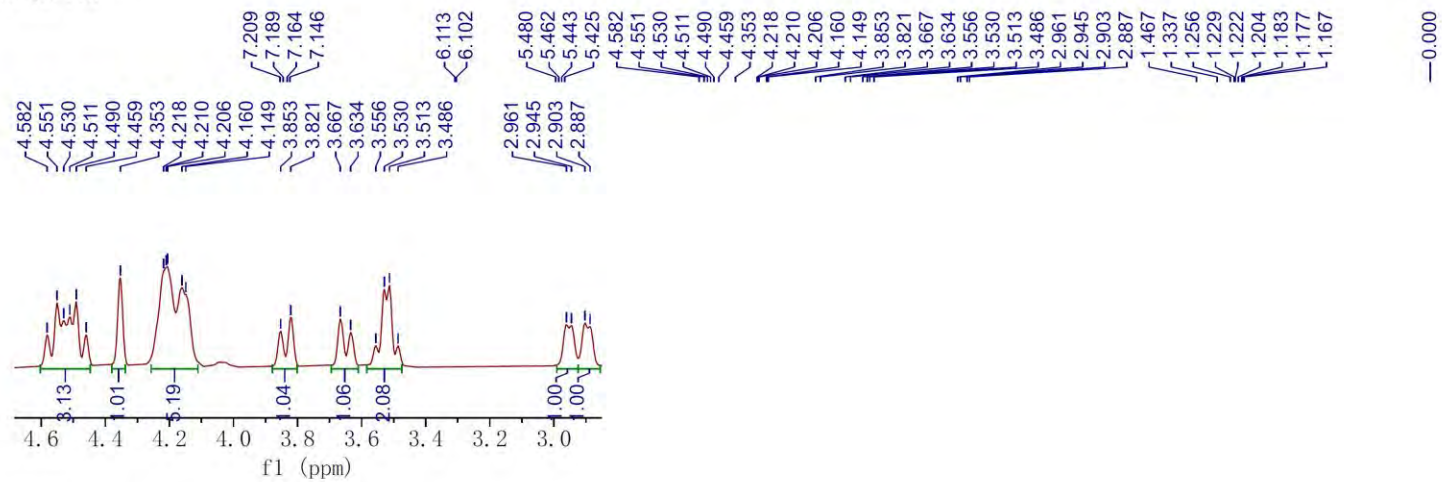
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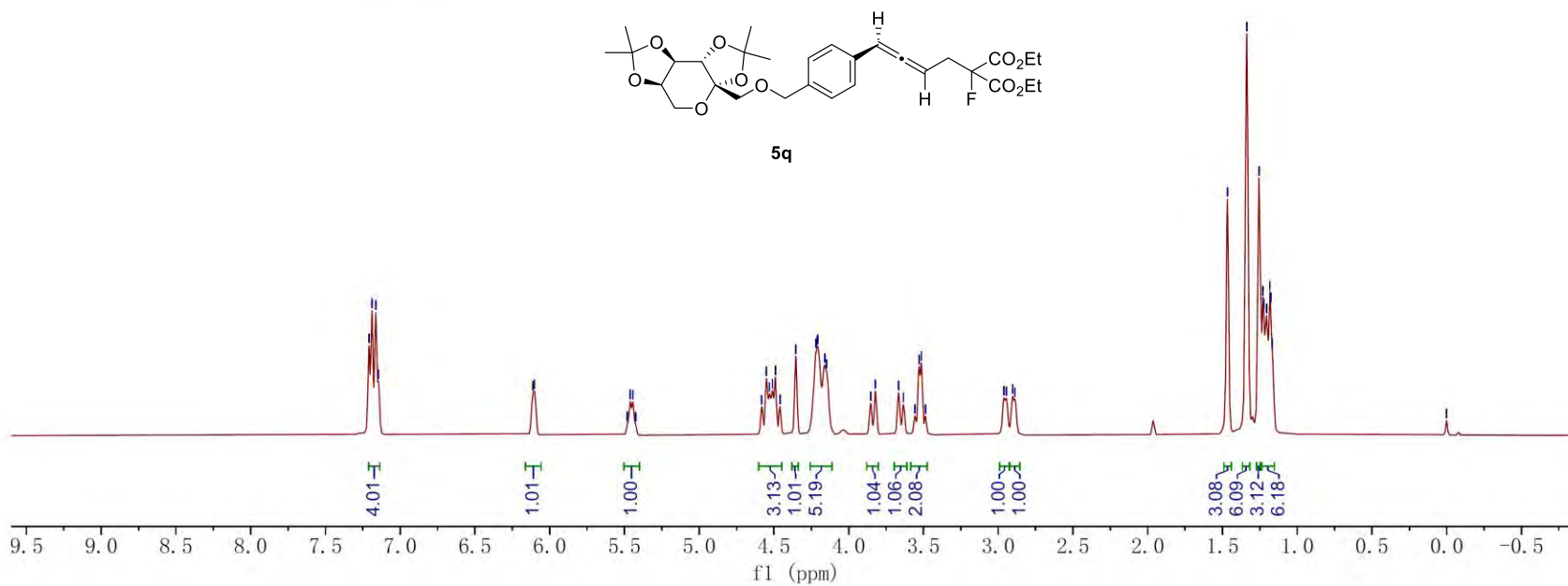
ZHY-ZG-71-376M-F



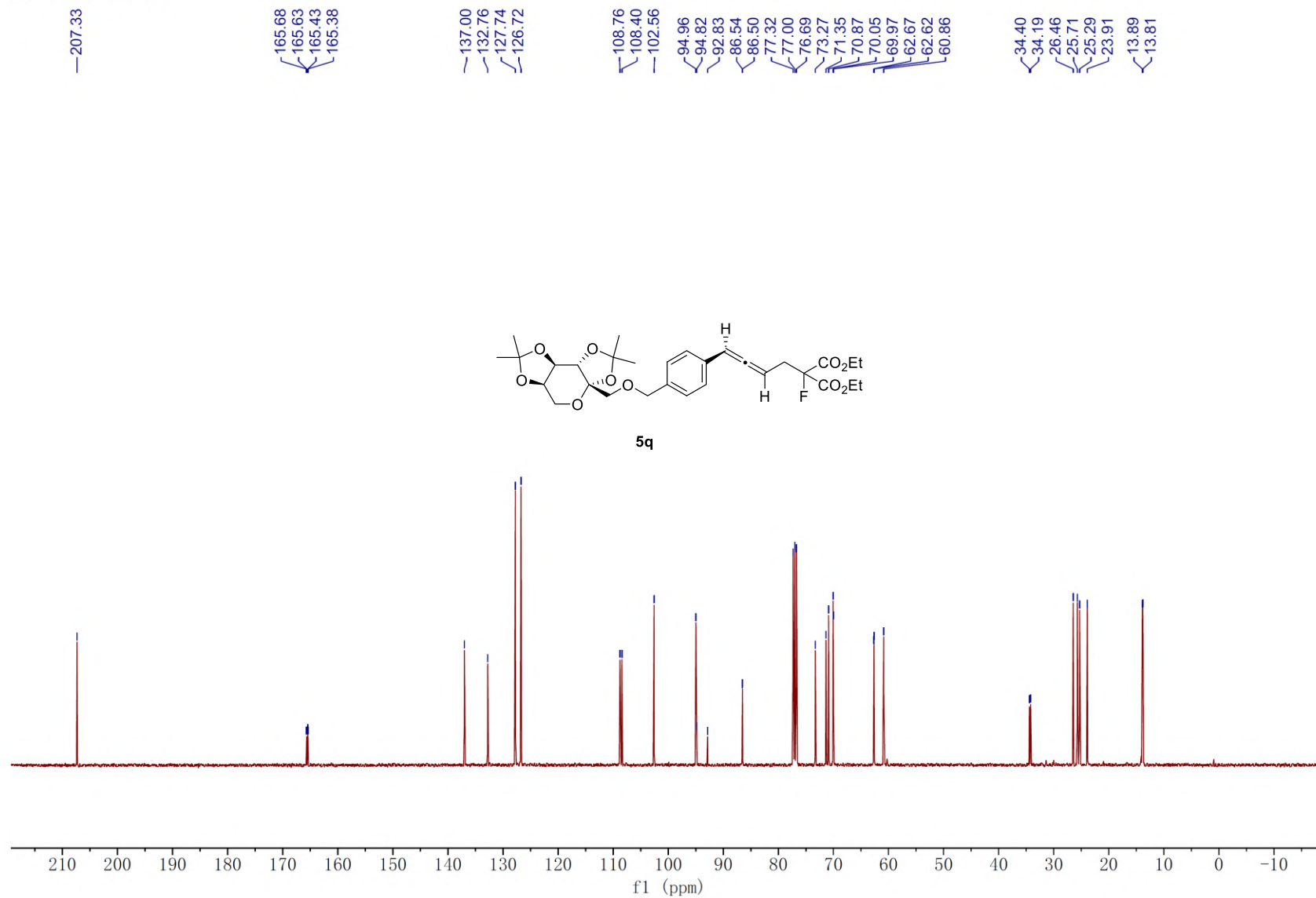
ZHY-ZG-133. 10. fid —



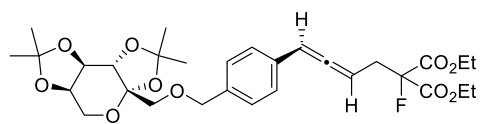
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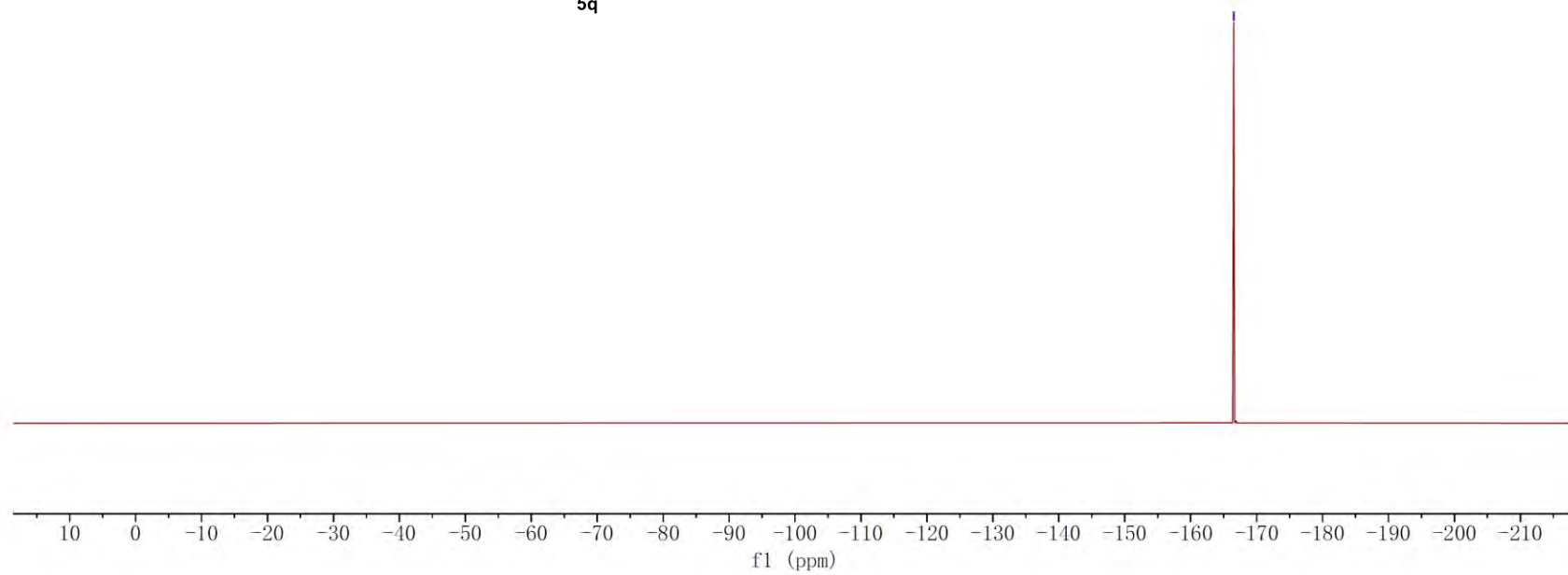
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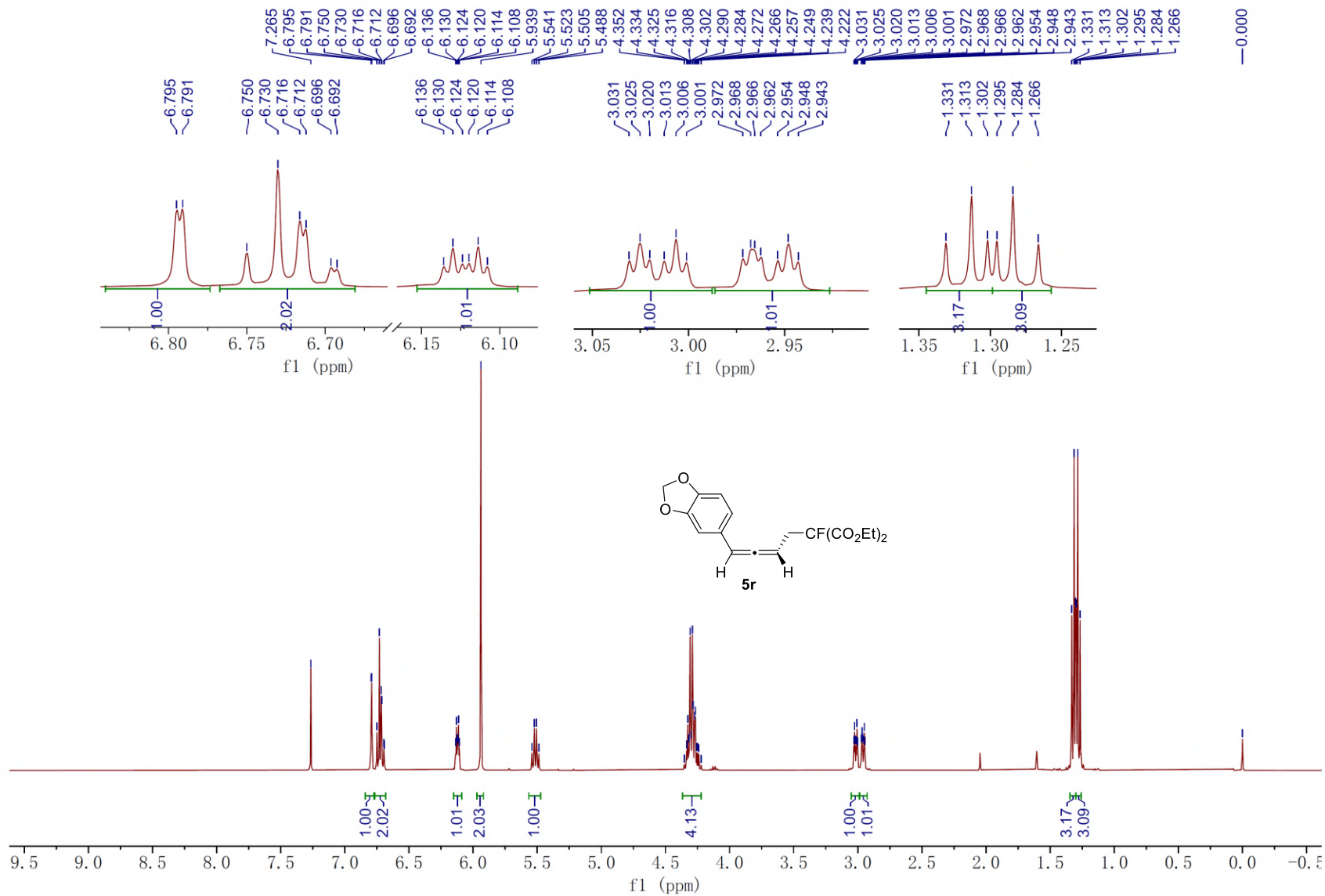
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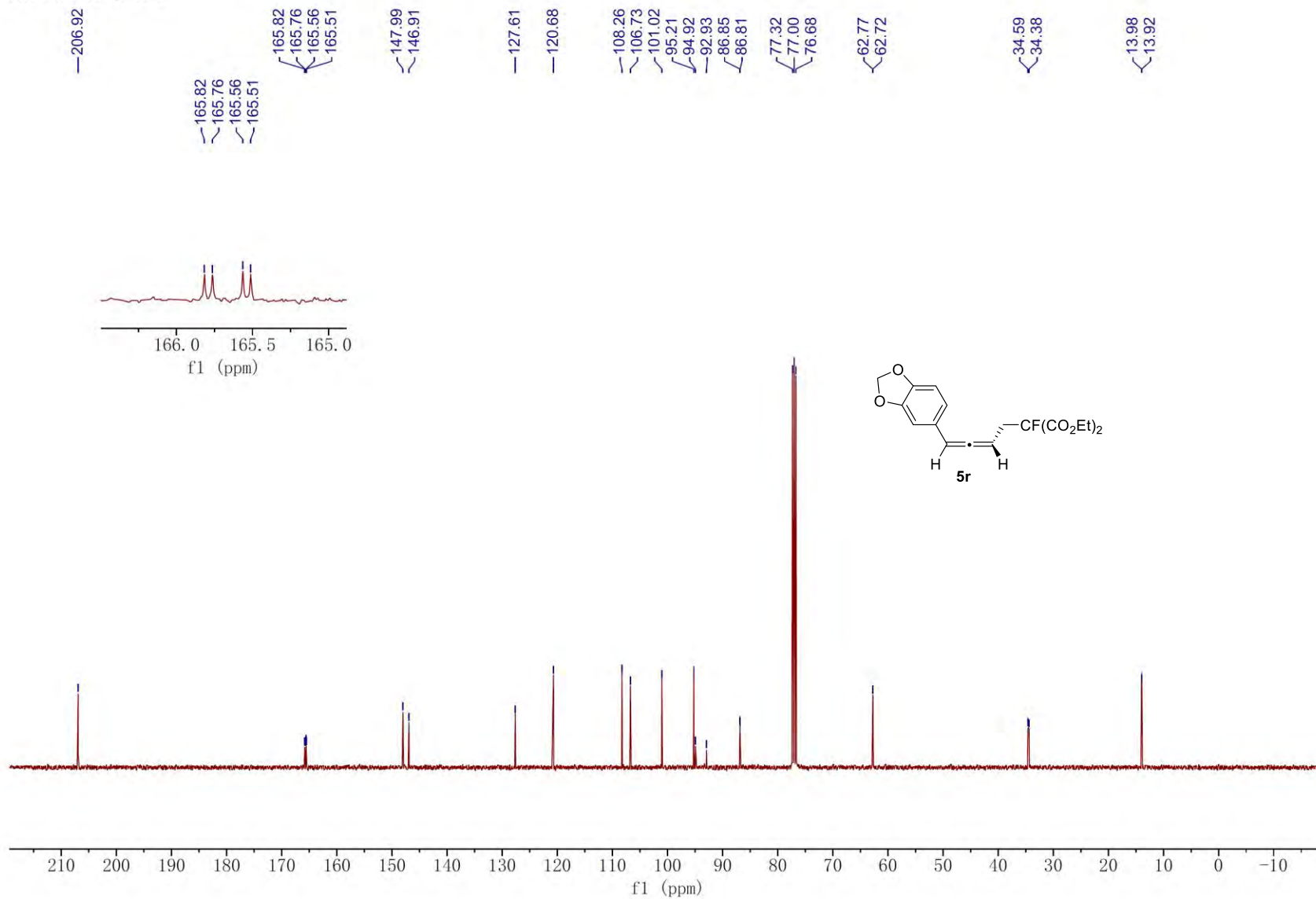
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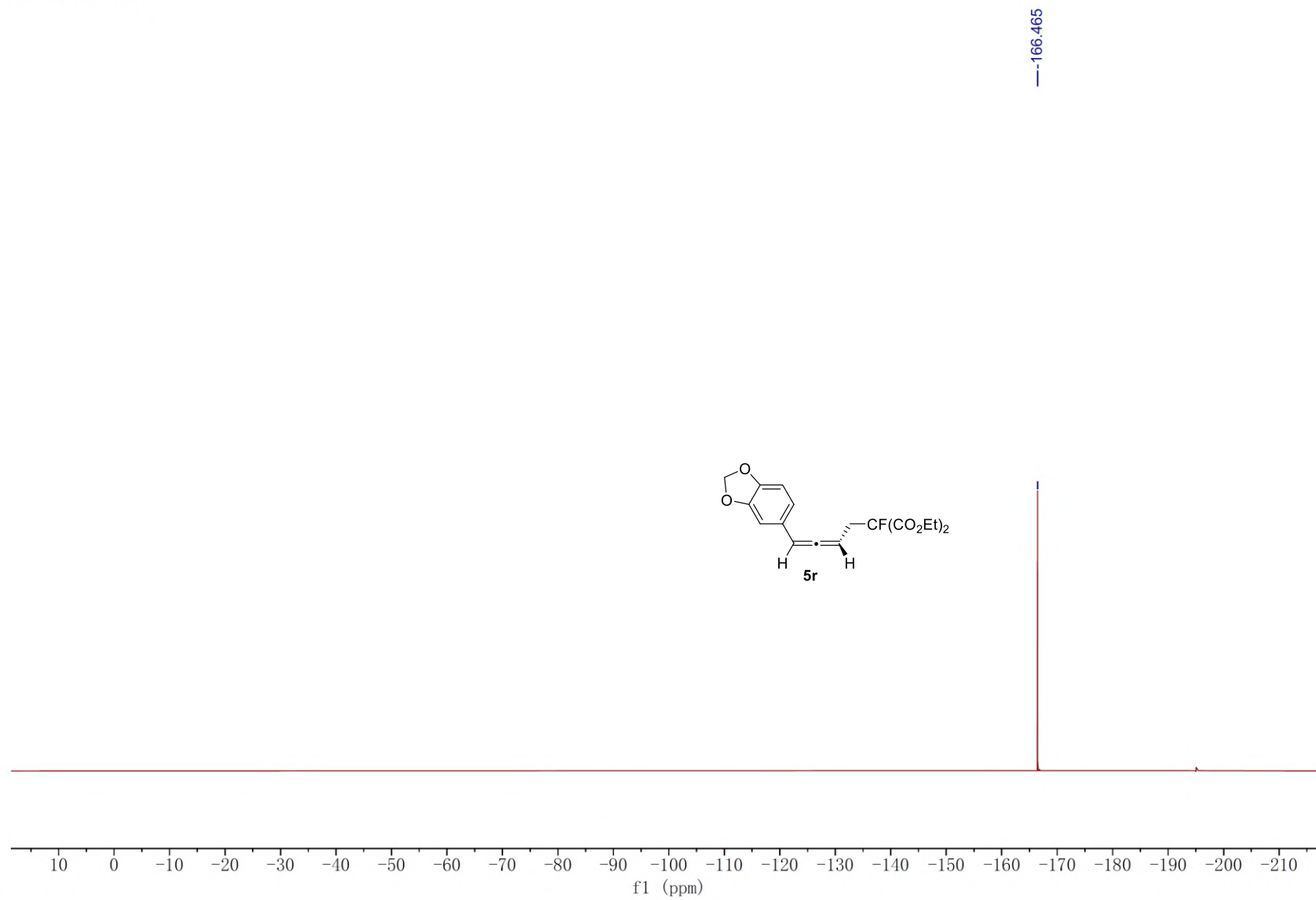
ZHY-ZG-110-400M-H



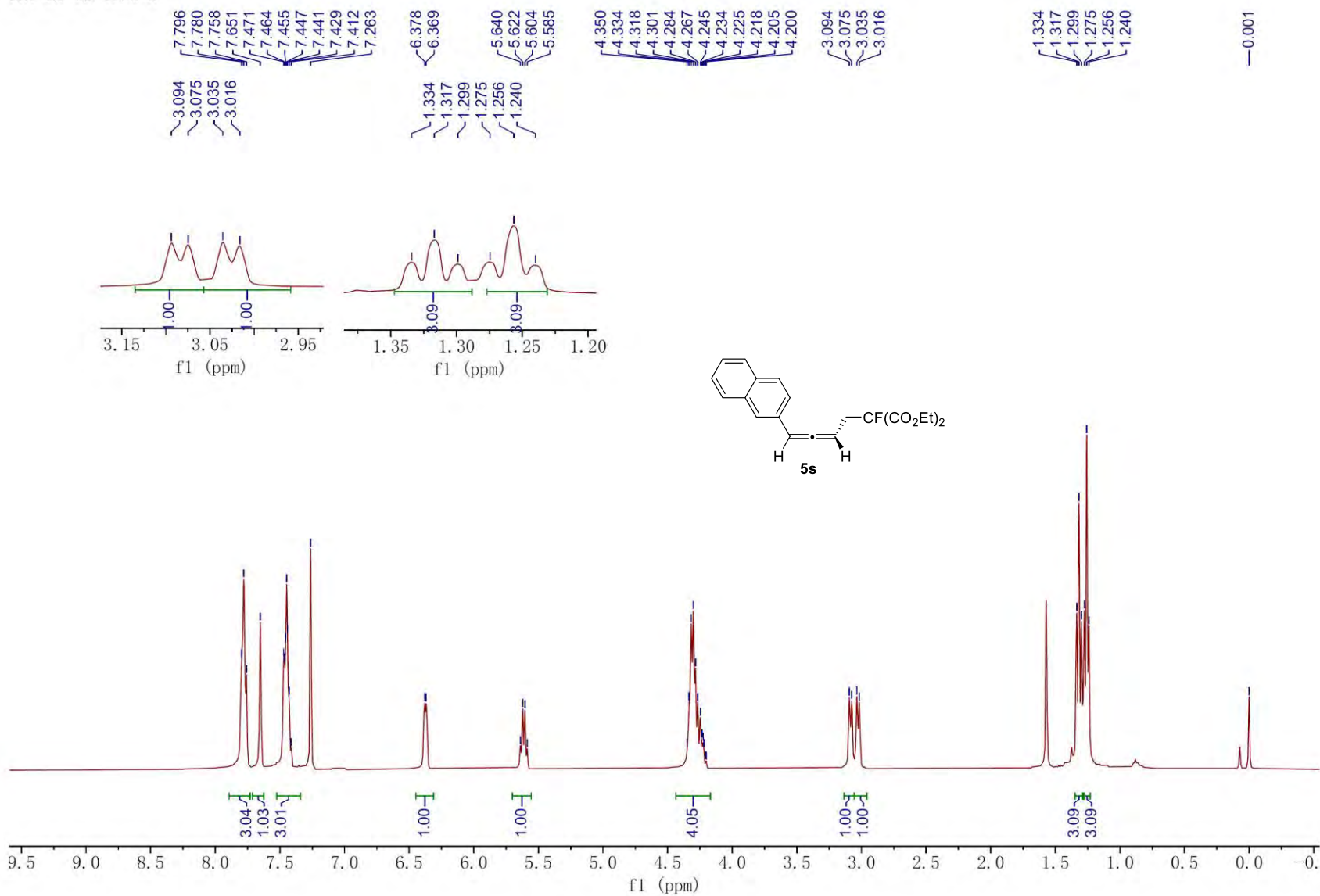
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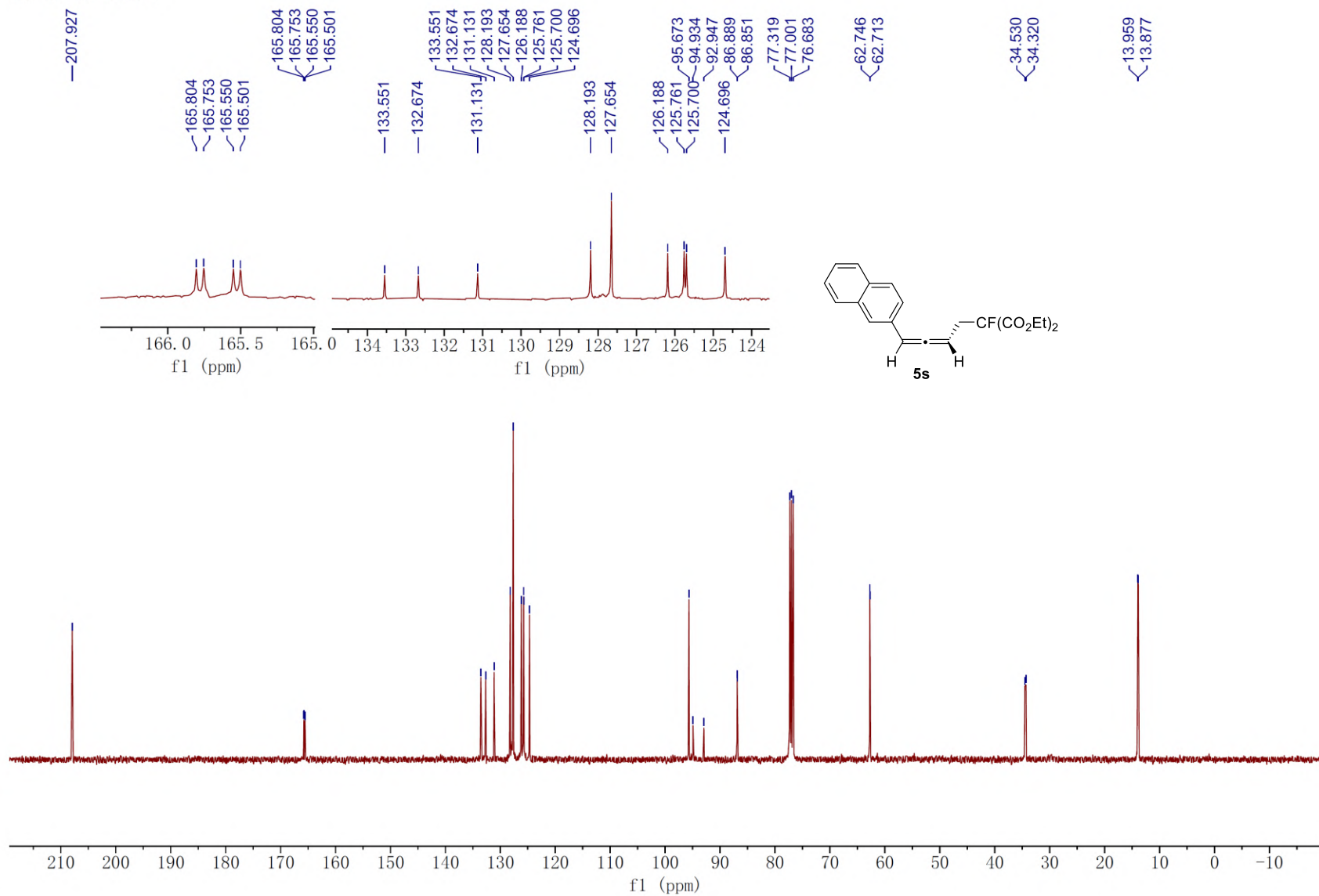
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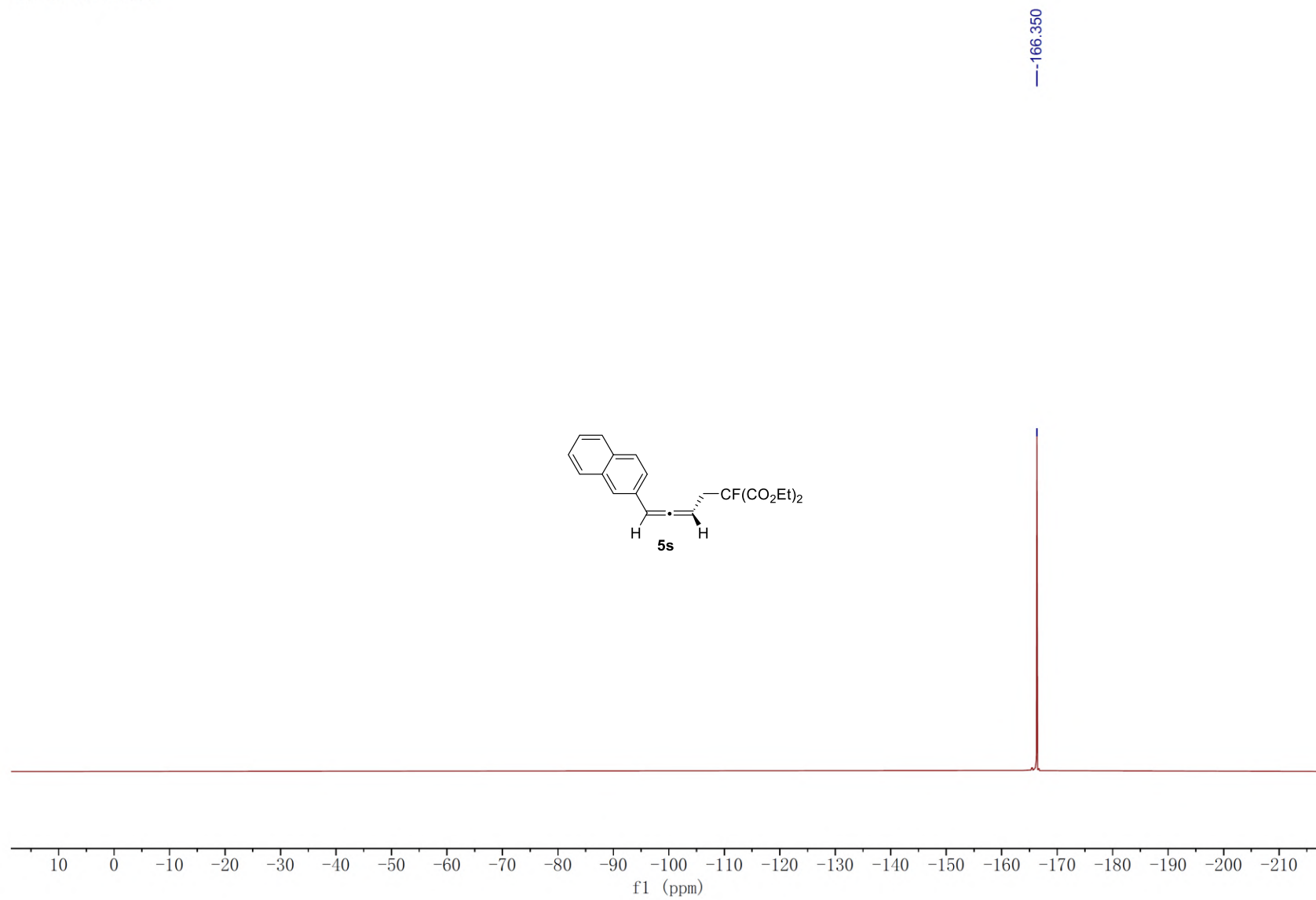
ZHY-ZG-63-400M-H



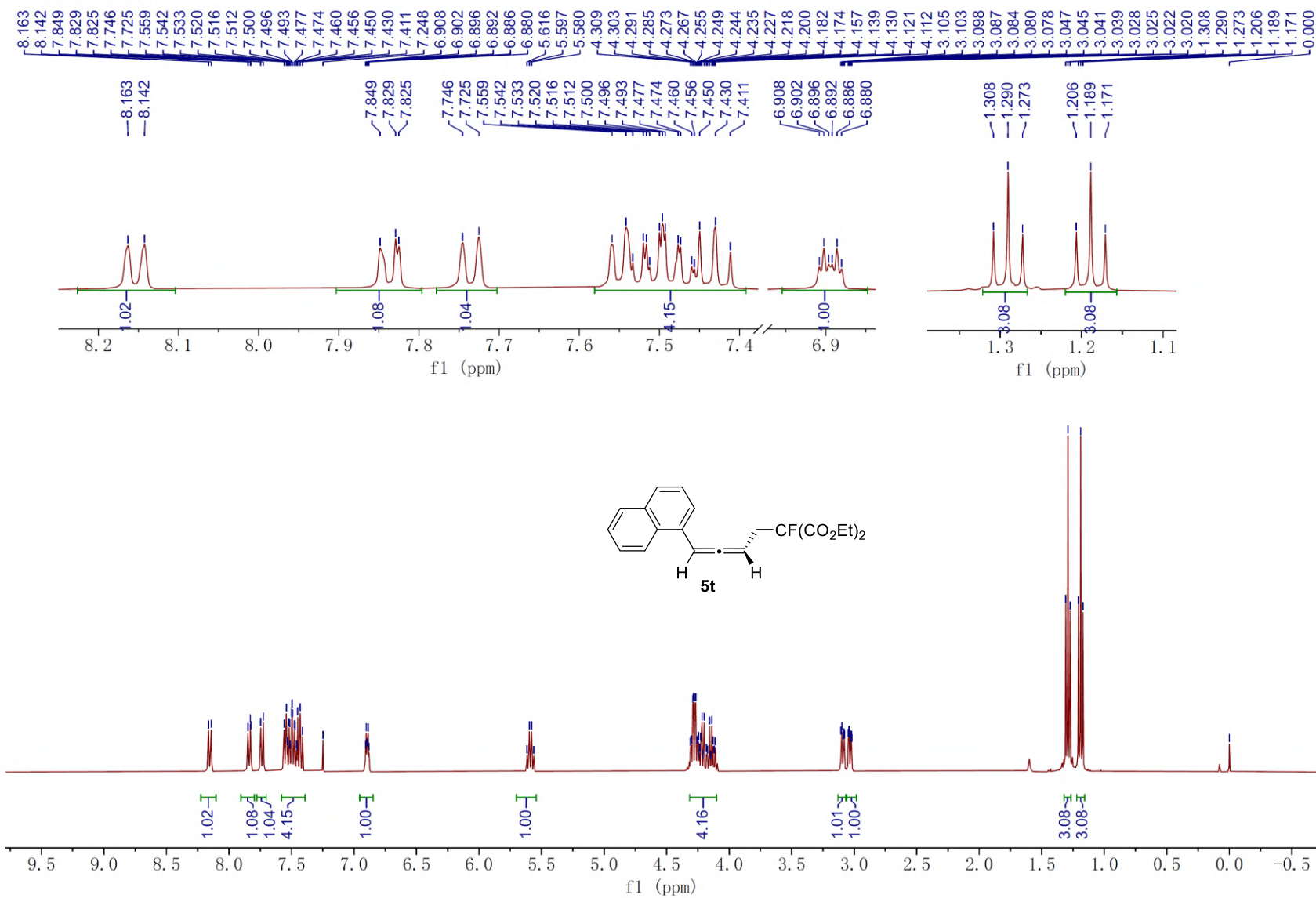
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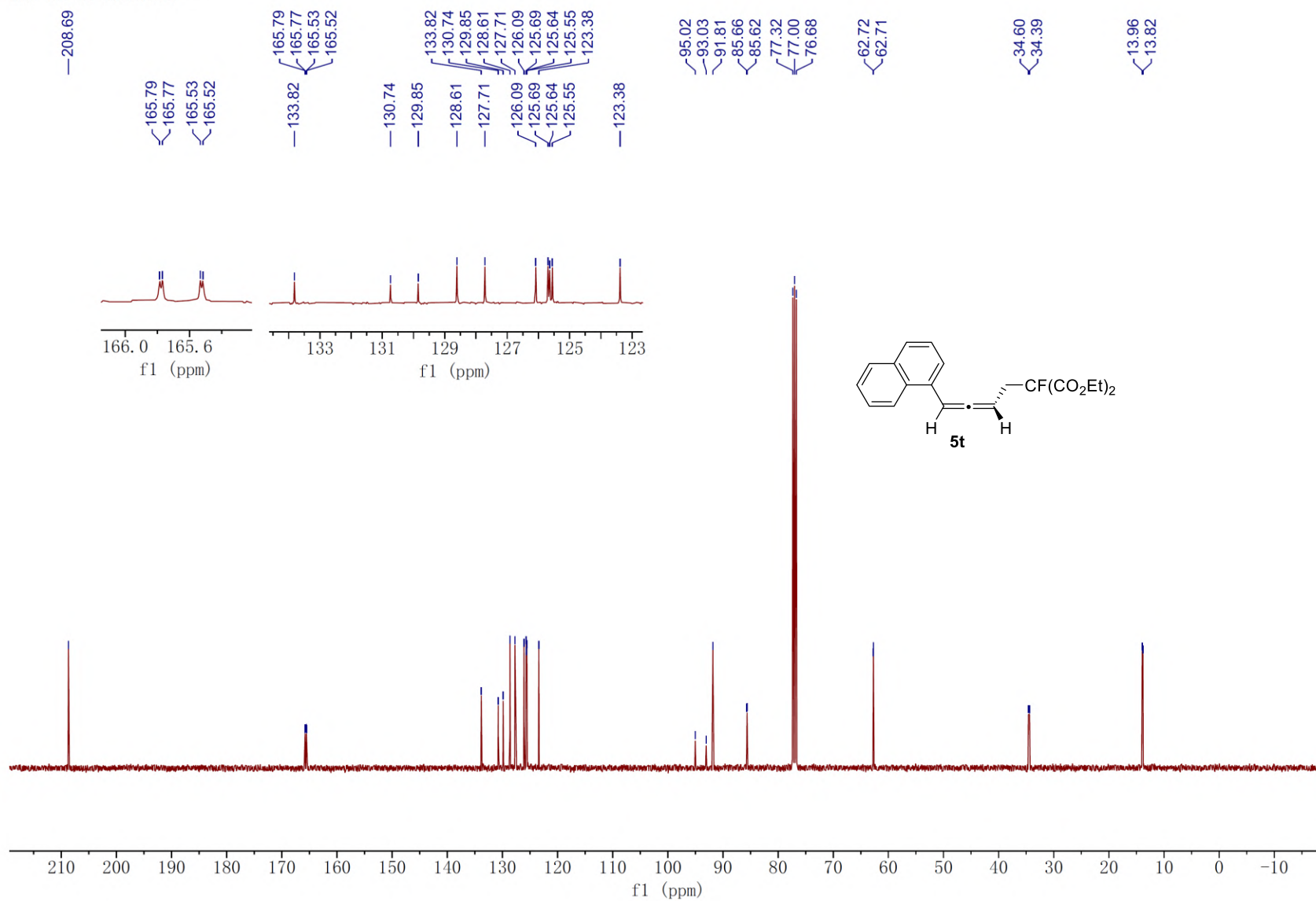
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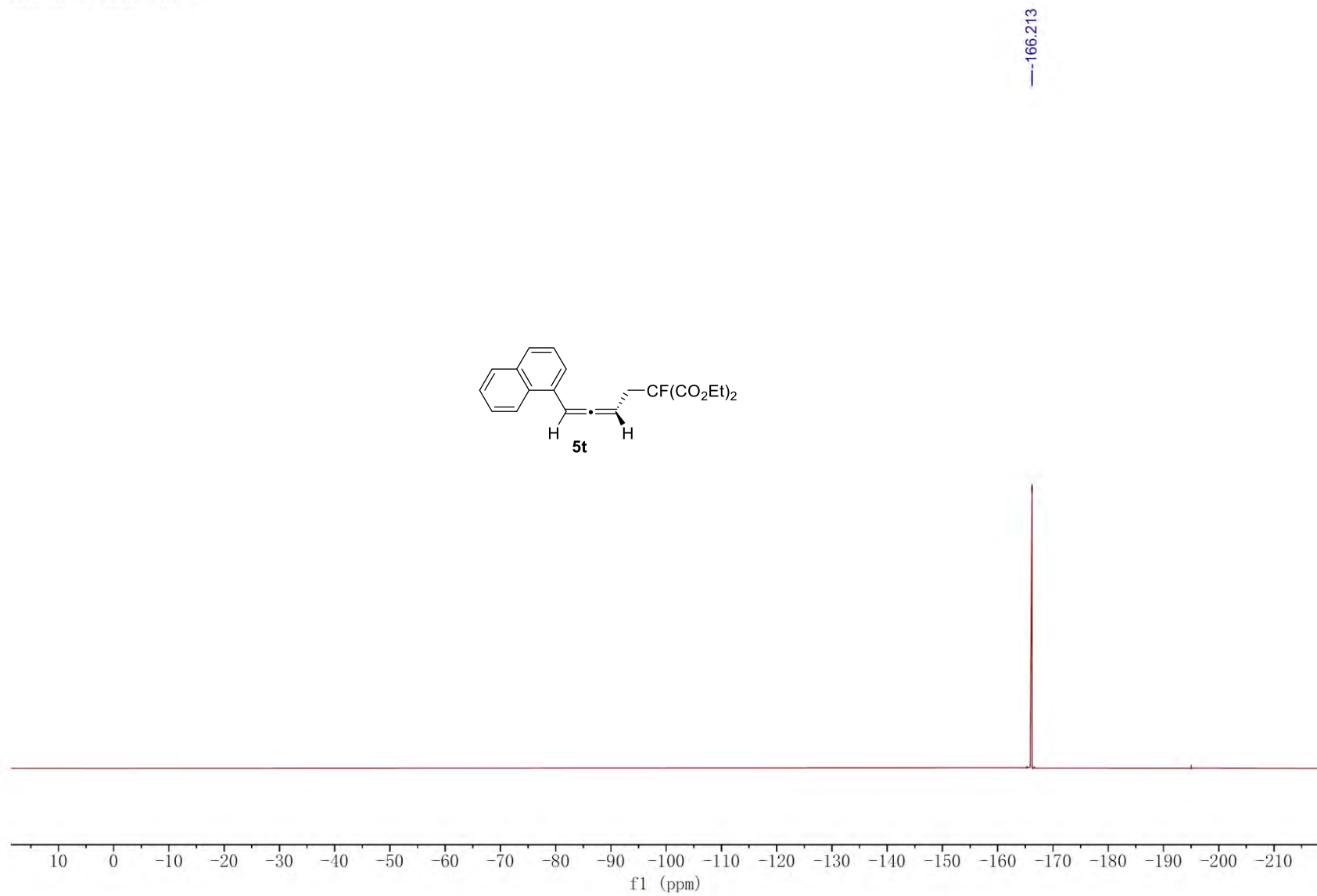
ZHY-ZH-48-C.20. fid —



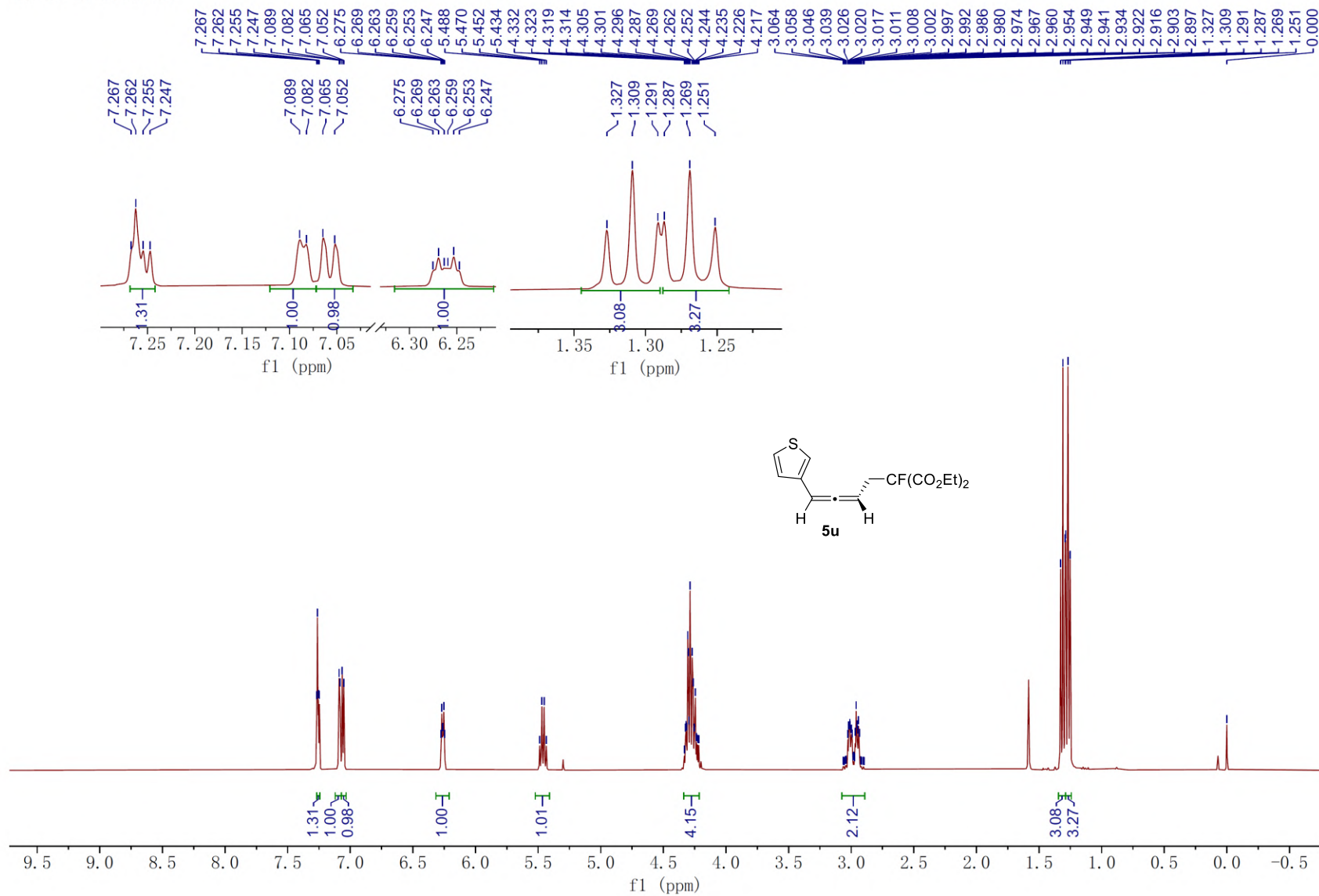
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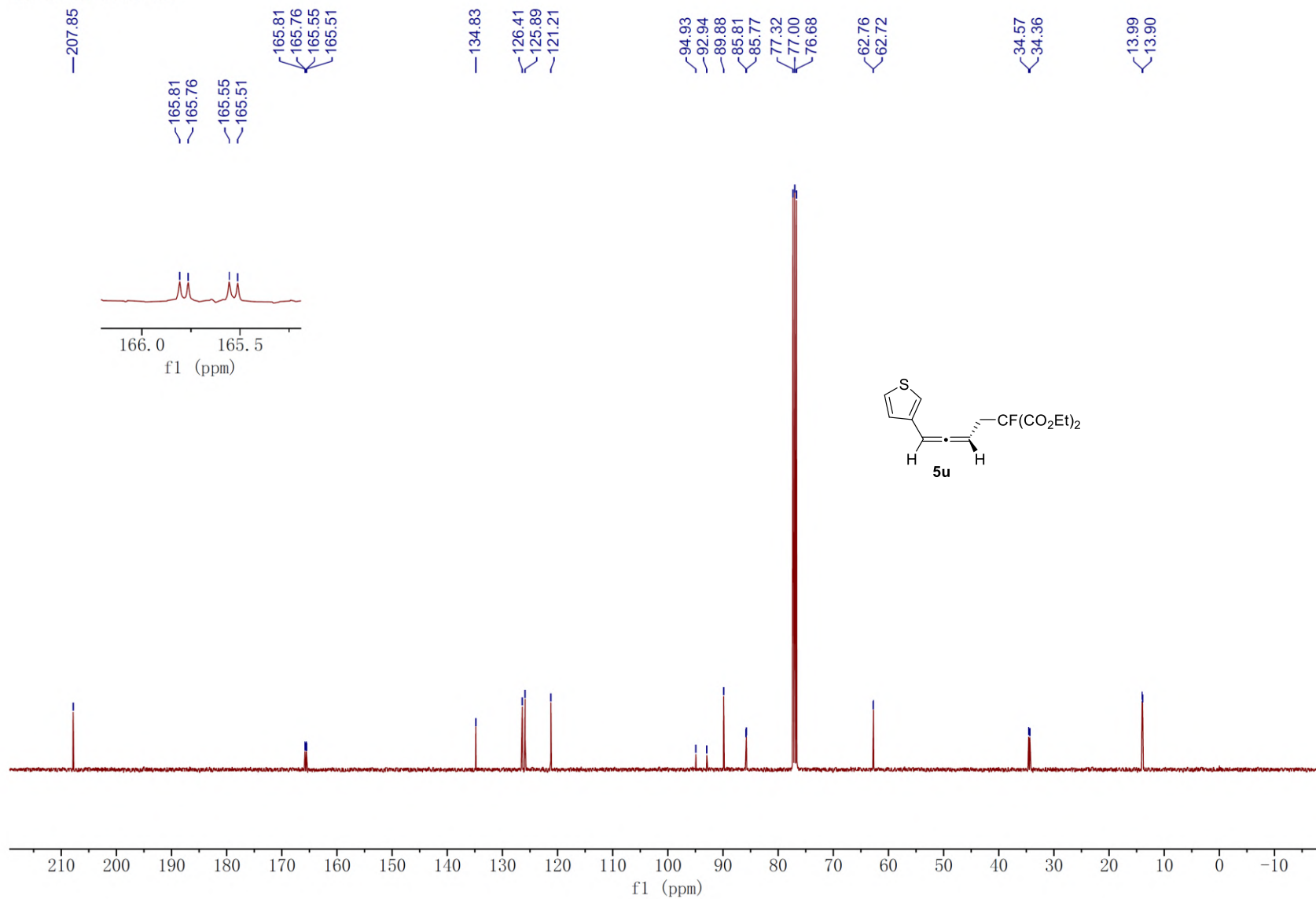
ZHY-ZII-48-C. 21. fid —



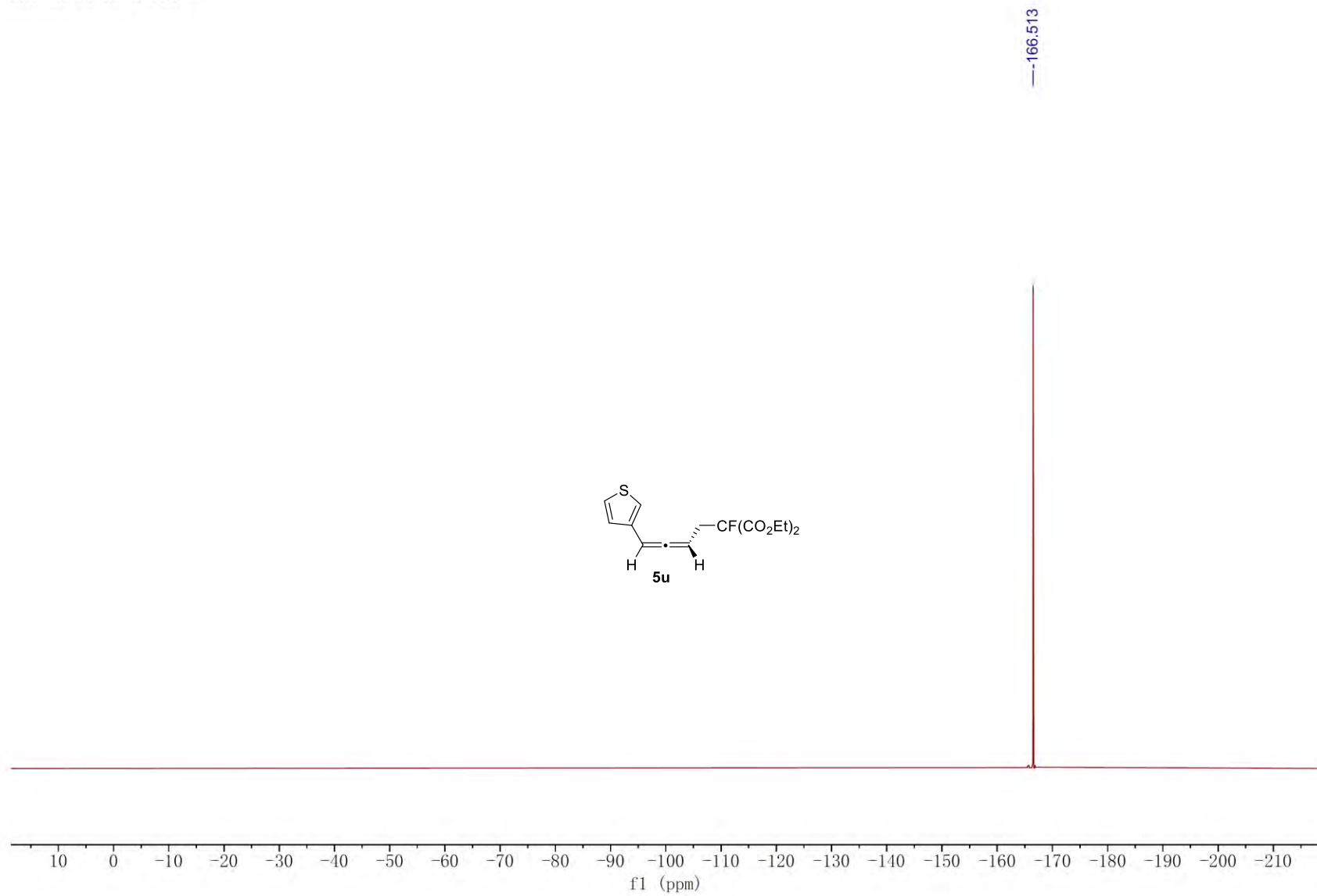
ZHY-ZH-11-2. 11. fid —



ZHY-ZH-11-2.10.fid —



ZHY-ZH-11-2. 12. fid —



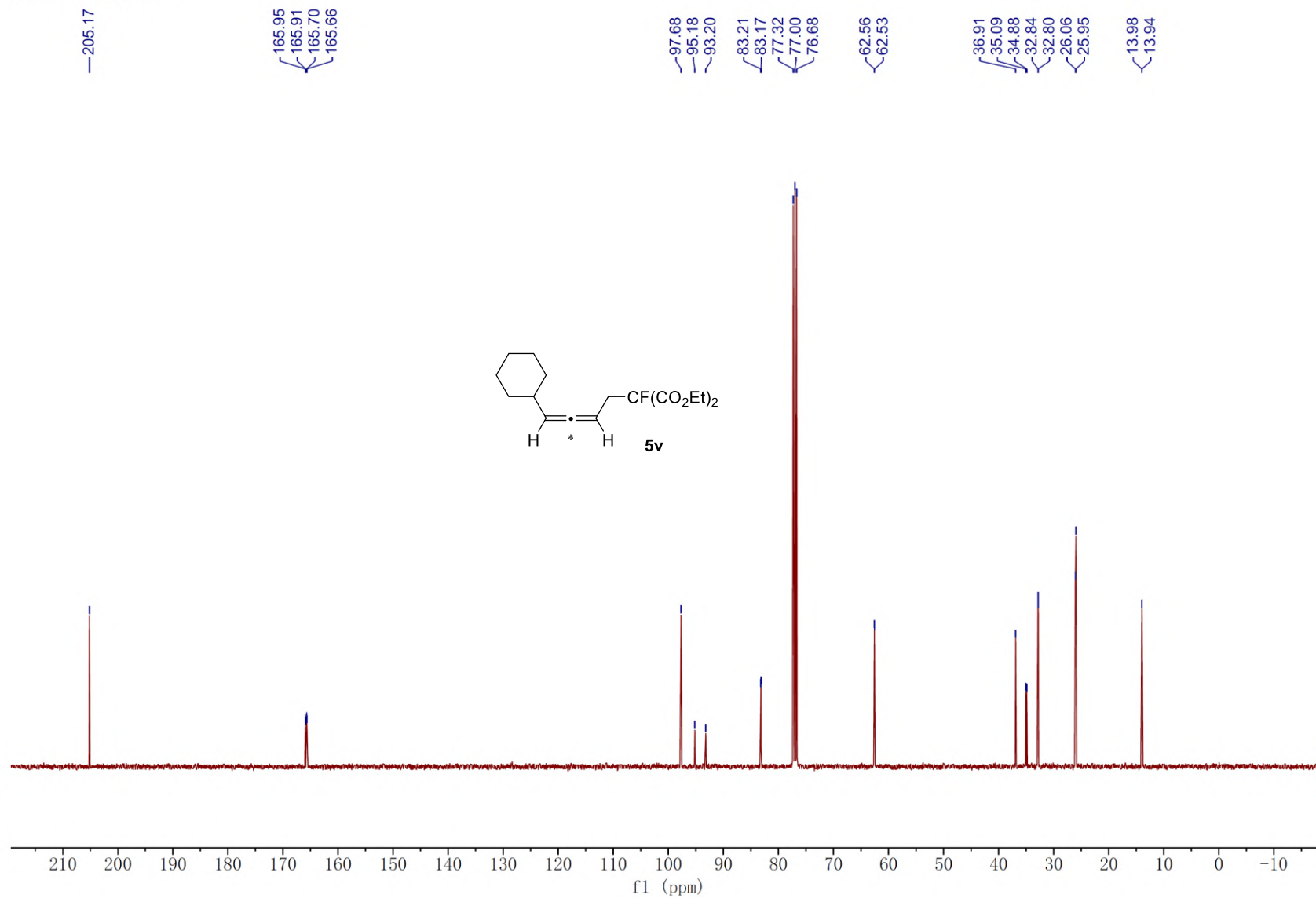
¹H NMR spectrum of compound 5v in CDCl₃.

Chemical structure of 5v: CCOC(=O)C(C(F)(F)F)C=Cc1ccccc1

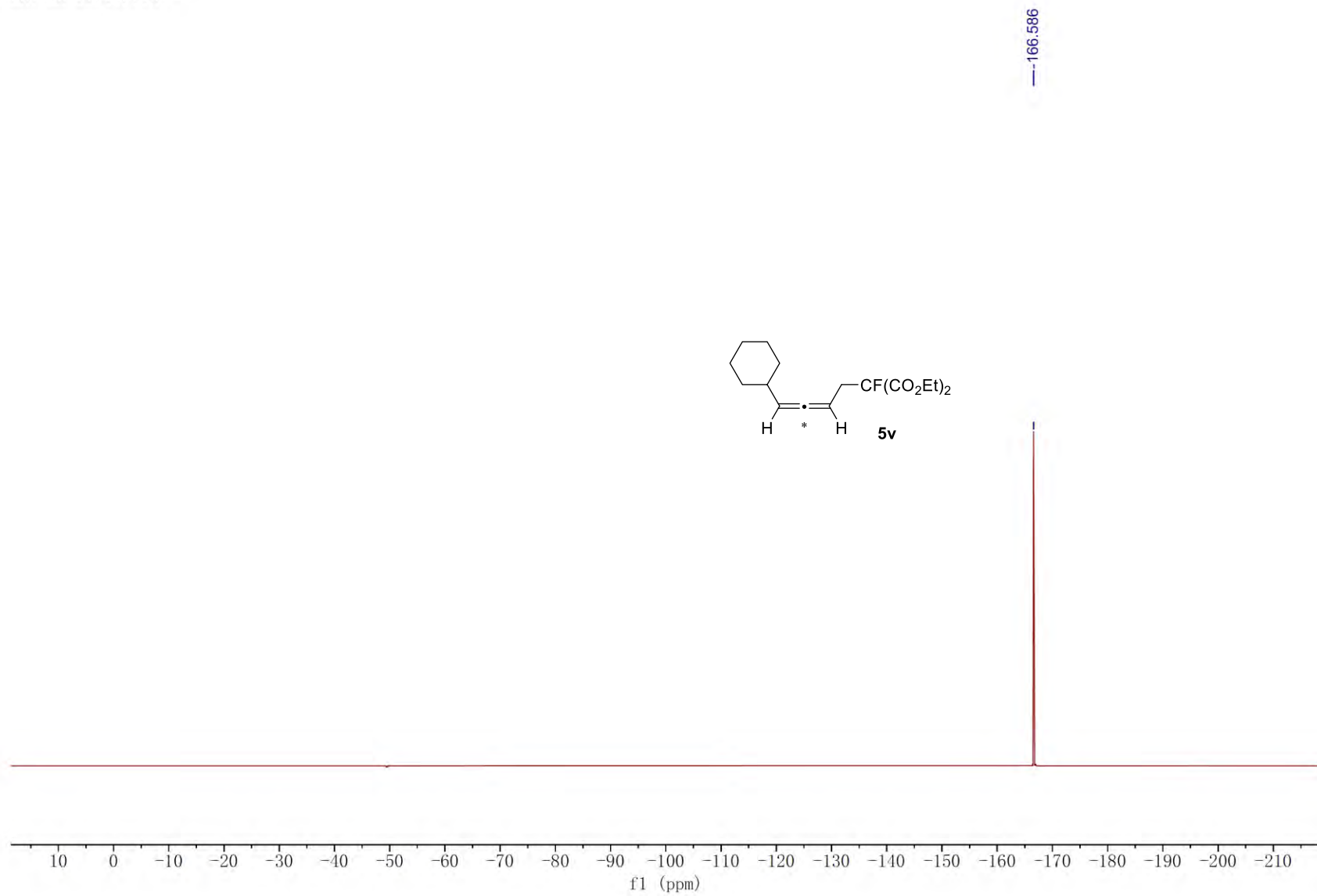
Peak list (ppm): 1.045, 1.051, 1.057, 1.064, 1.078, 1.084, 1.089, 1.108, 1.110, 1.115, 1.126, 1.132, 1.137, 1.149, 1.163, 1.170, 1.178, 1.193, 1.199, 1.207, 1.215, 1.222, 1.238, 1.245, 1.253, 1.269, 1.271, 1.276, 1.286, 1.293, 1.311, 1.315, 1.329, 1.333, 1.605, 1.611, 1.626, 1.631, 1.637, 1.641, 1.645, 1.679, 1.685, 1.694, 1.712, 1.718, 1.728, 1.742, 1.746, 1.750, 1.902, 1.911, 1.918, 1.926, 1.930, 1.933, 1.938, 1.946, 1.953, 1.961, 1.966, 1.974, 1.981, 1.989, 1.997, 2.818, 2.822, 2.824, 2.828, 2.836, 2.840, 2.843, 2.846, 2.877, 2.882, 2.888, 2.896, 2.902, 2.906.

Integration values: 1.03, 1.06, 4.31, 1.00, 1.01, 1.06, 4.35, 1.23, 6.28, 5.41.

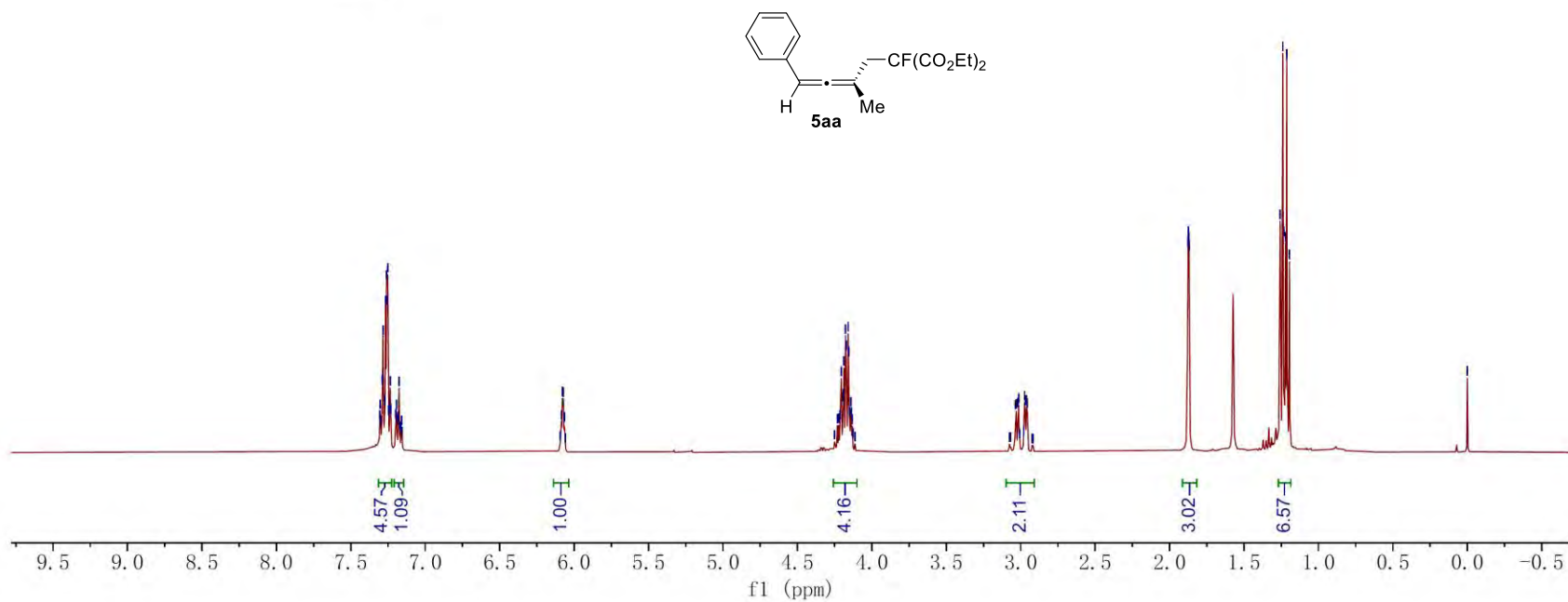
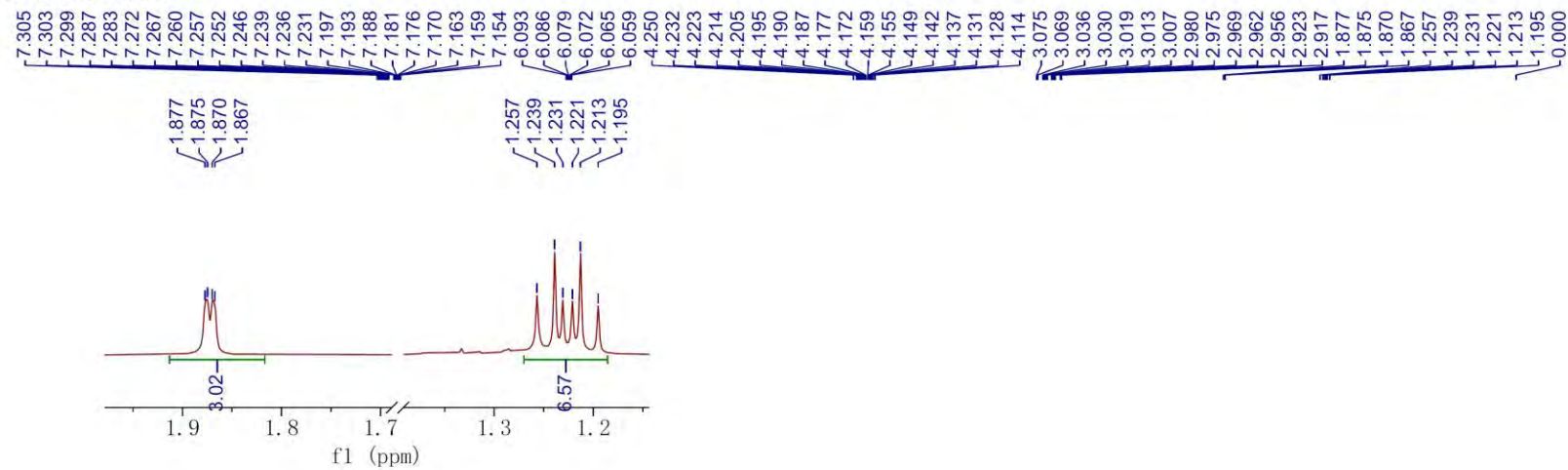
ZHY-ZH-67.12.fid —



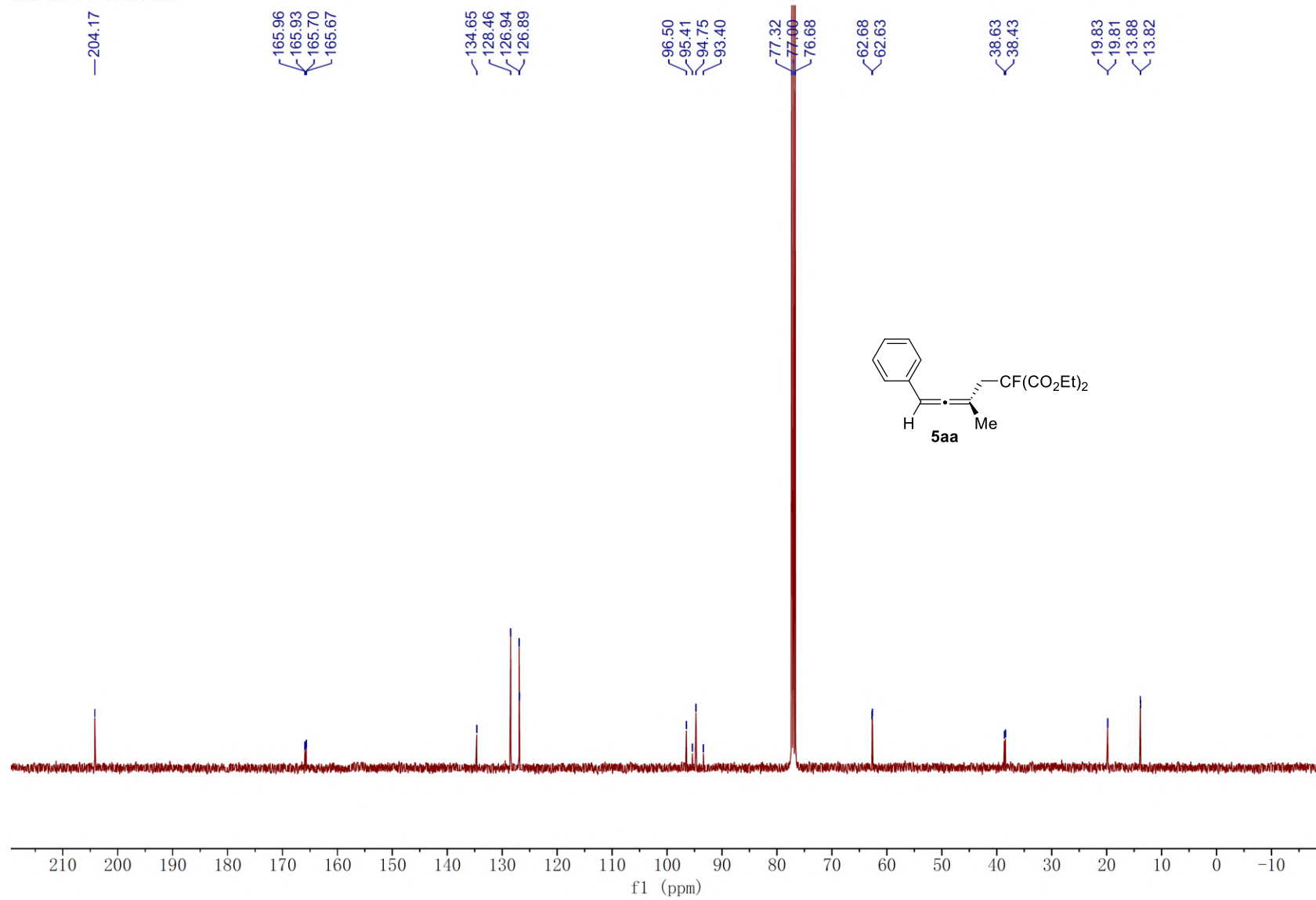
ZHY-ZH-67.11.fid —



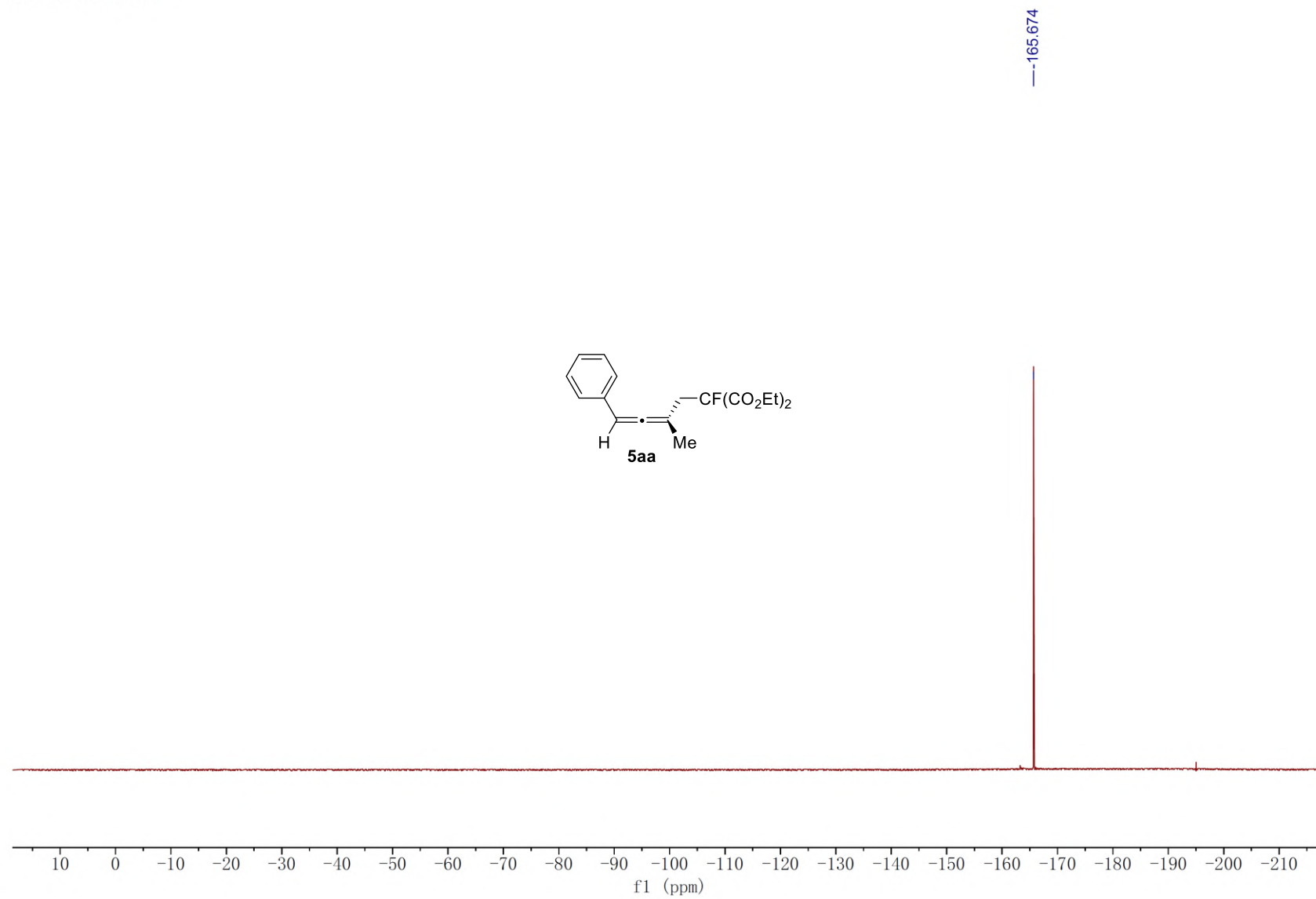
L1L-LL-78.10.fid —



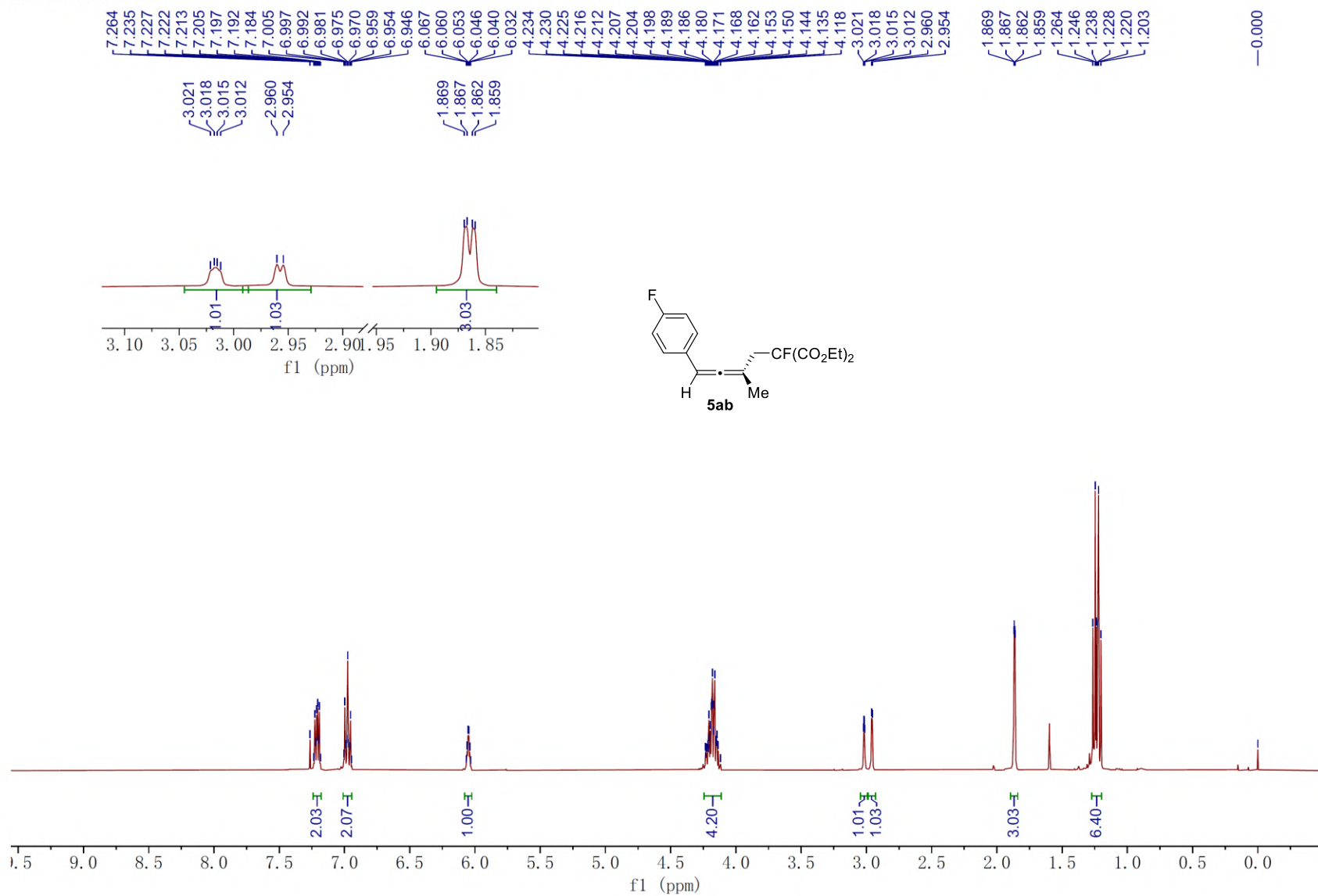
LIL-LL-78-C.10. fid —



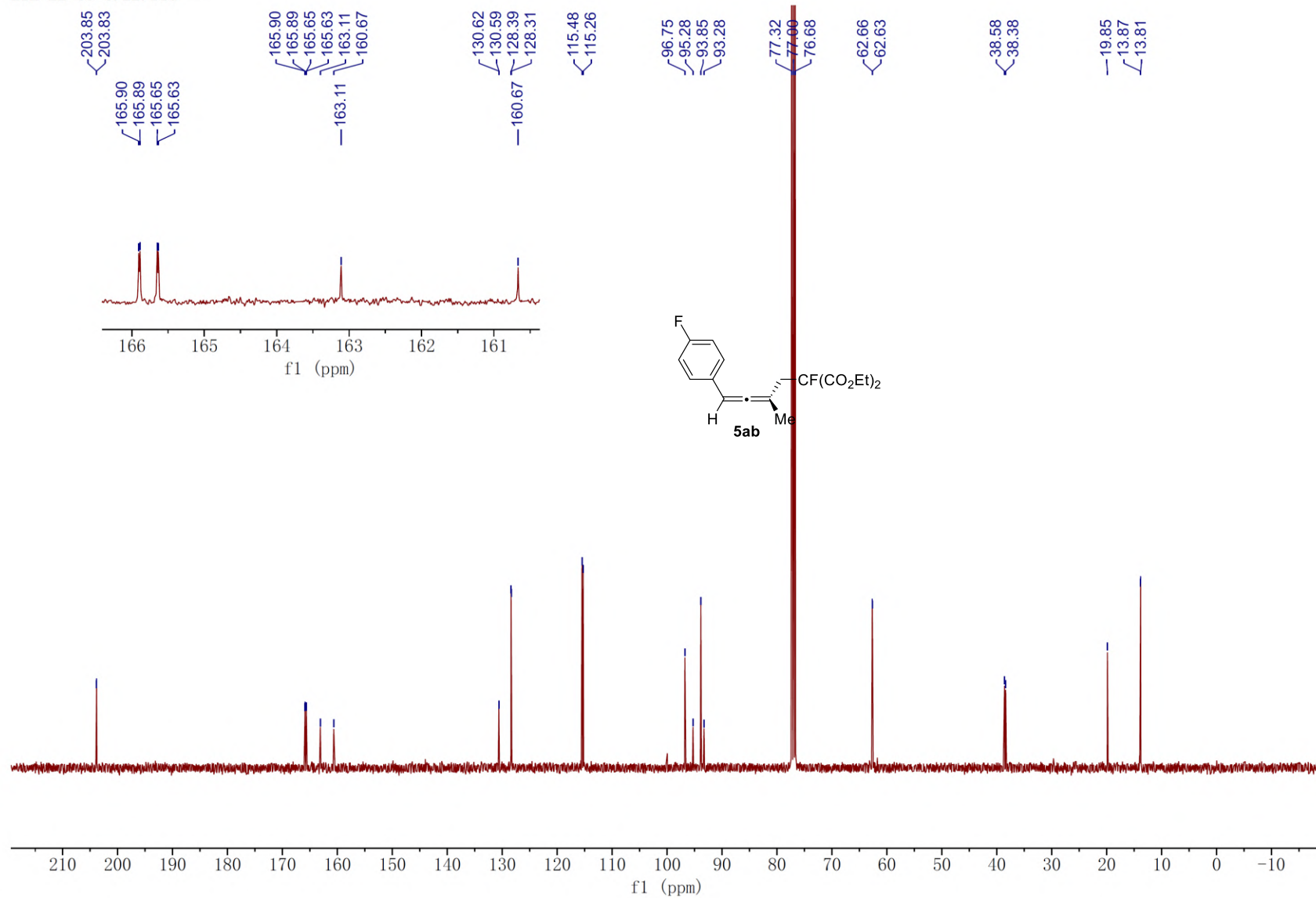
LIL-LL-78.11.fid —



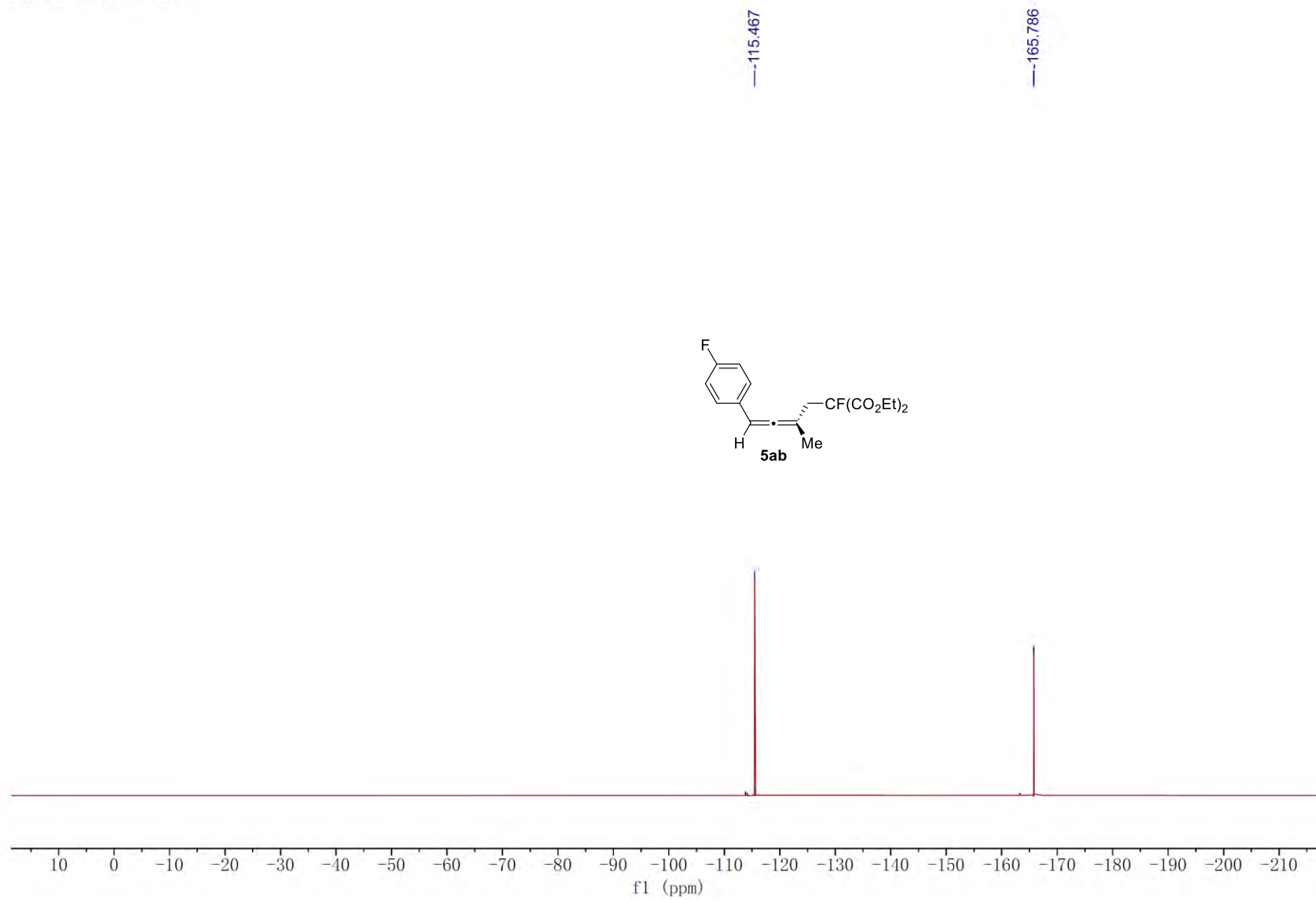
LIL-LL-63-C.20. fid —



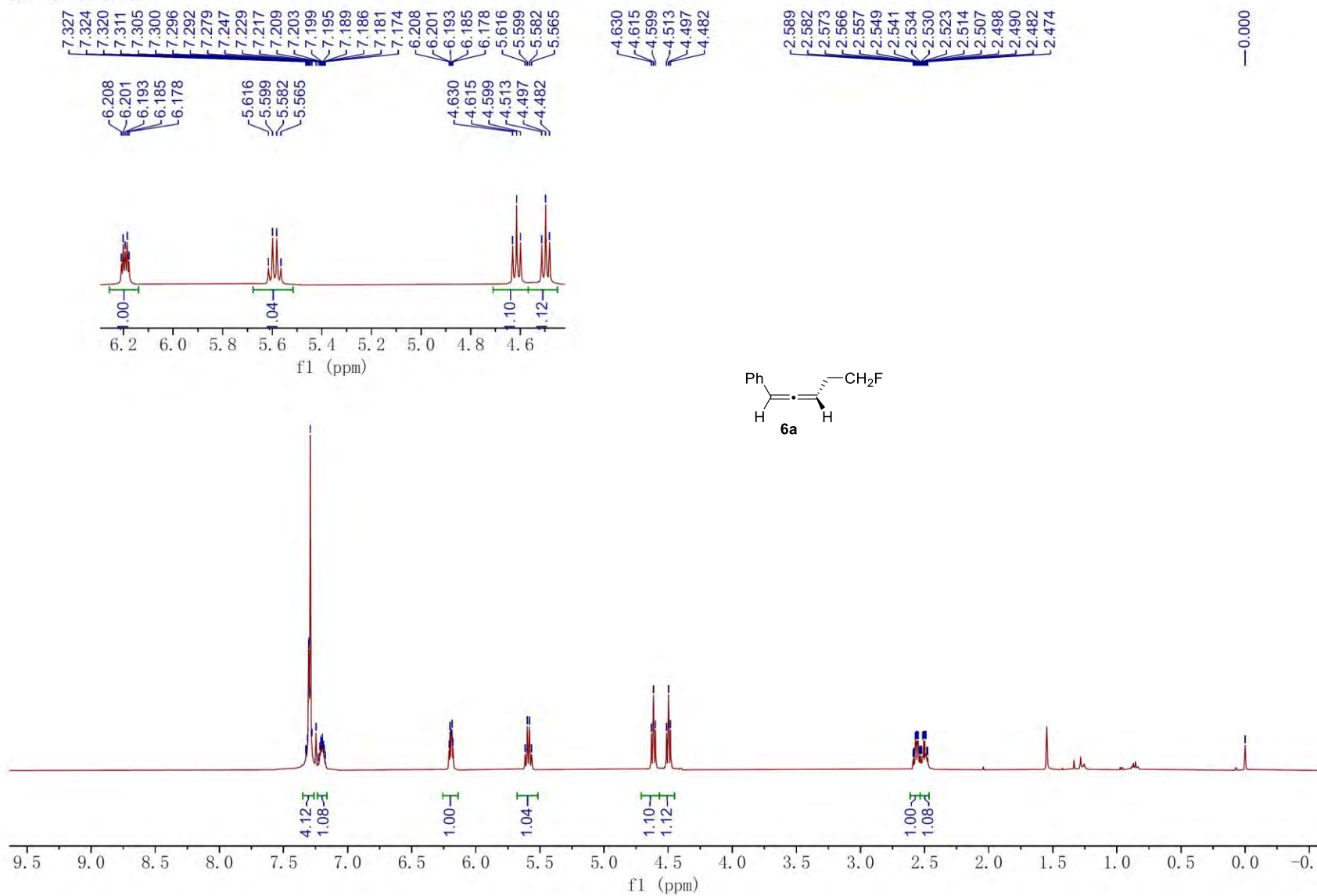
LIL-LL-63-C.22. fid —



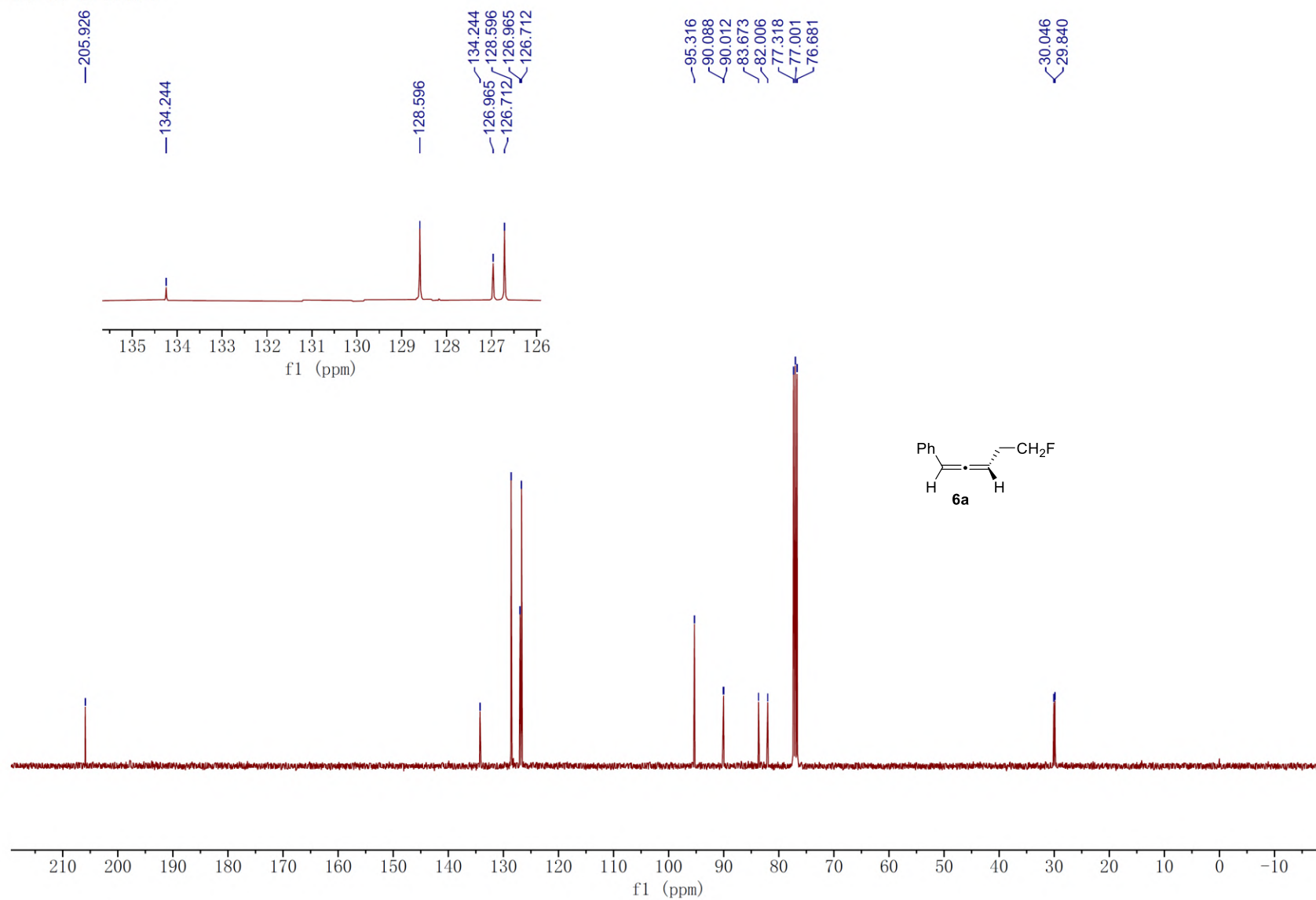
LIL-LL-63-C. 21. fid —



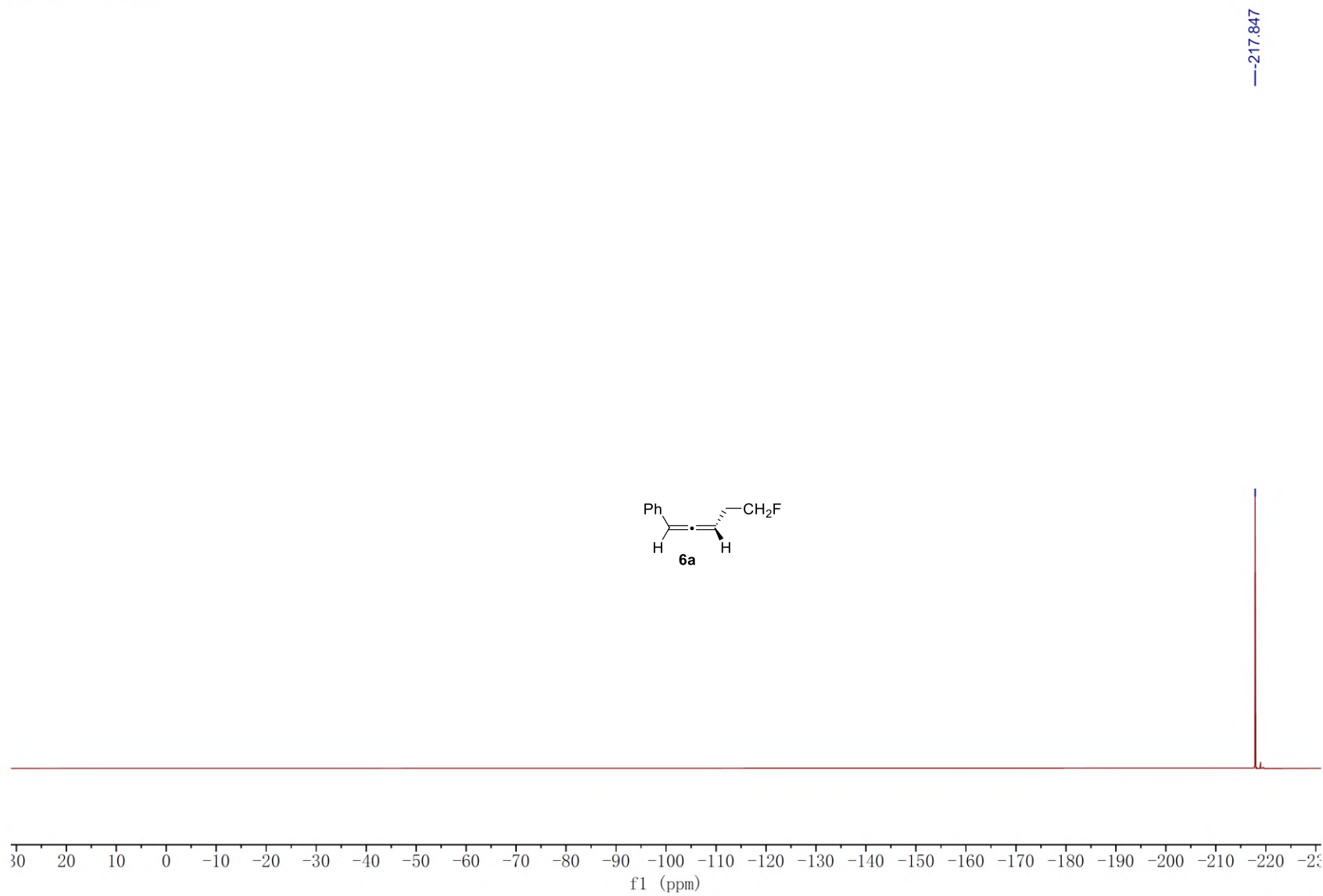
ZHY-ZG-92-400M-H



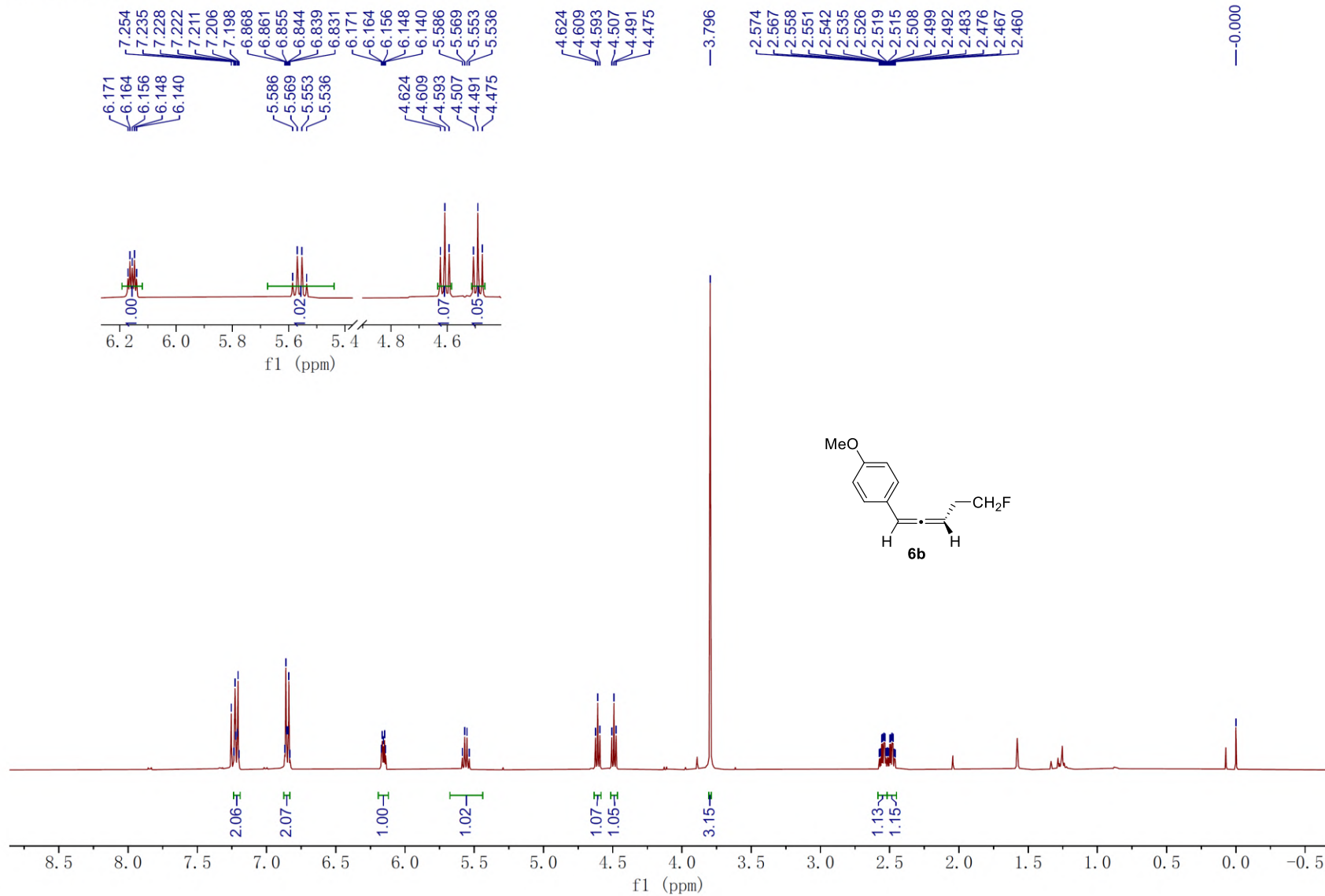
ZHY-ZG-92-100M-C



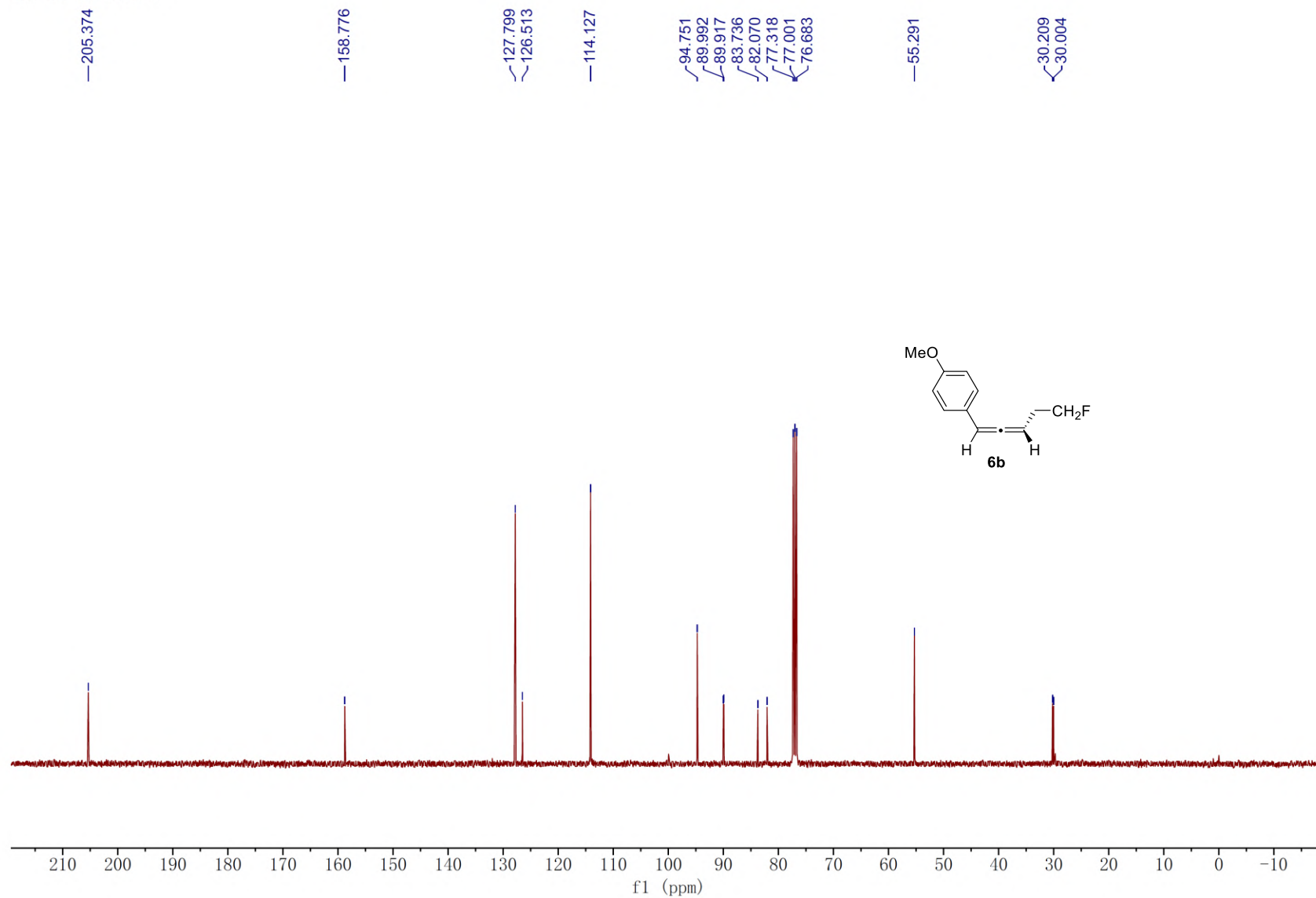
ZHY-ZG-92-376M-F



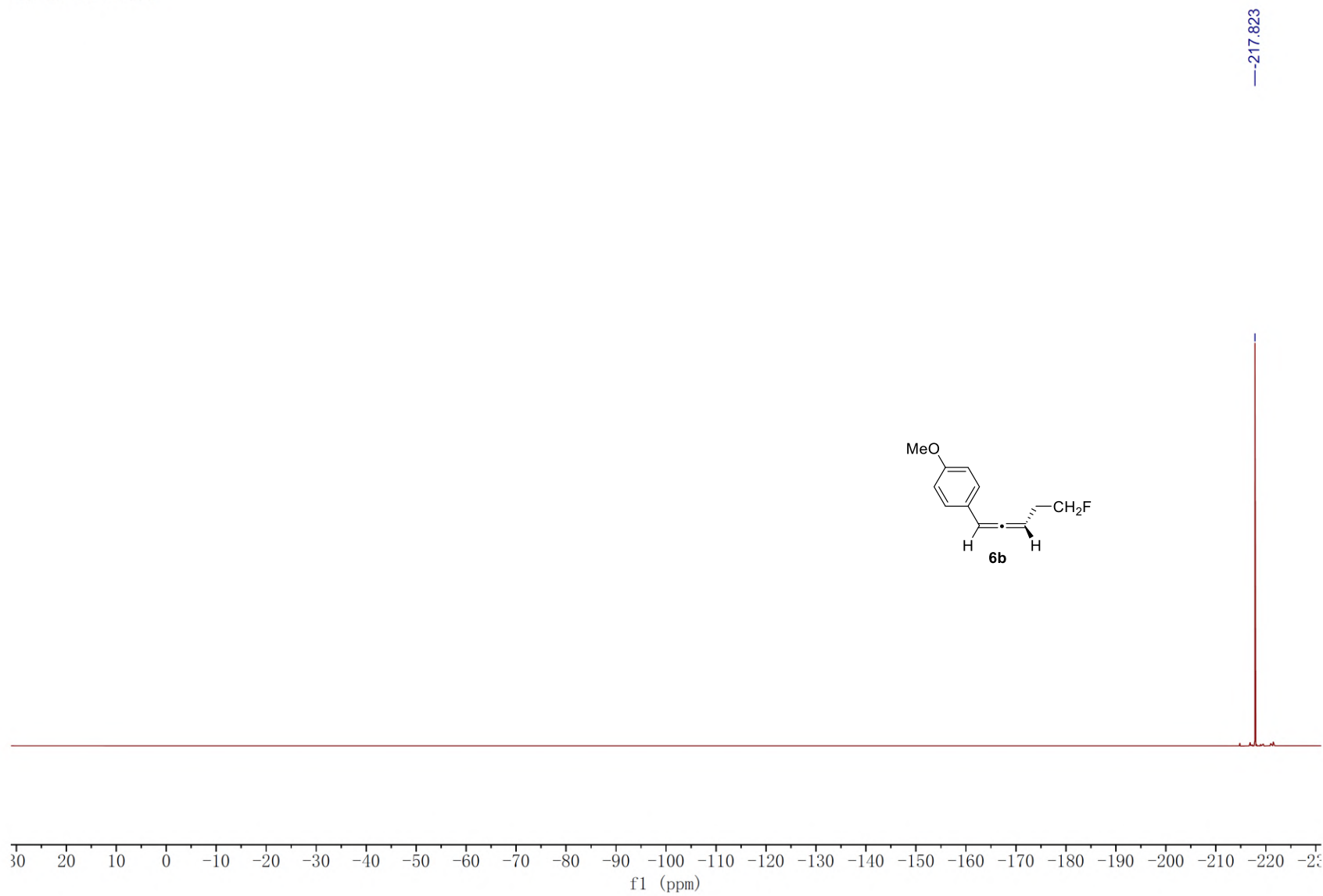
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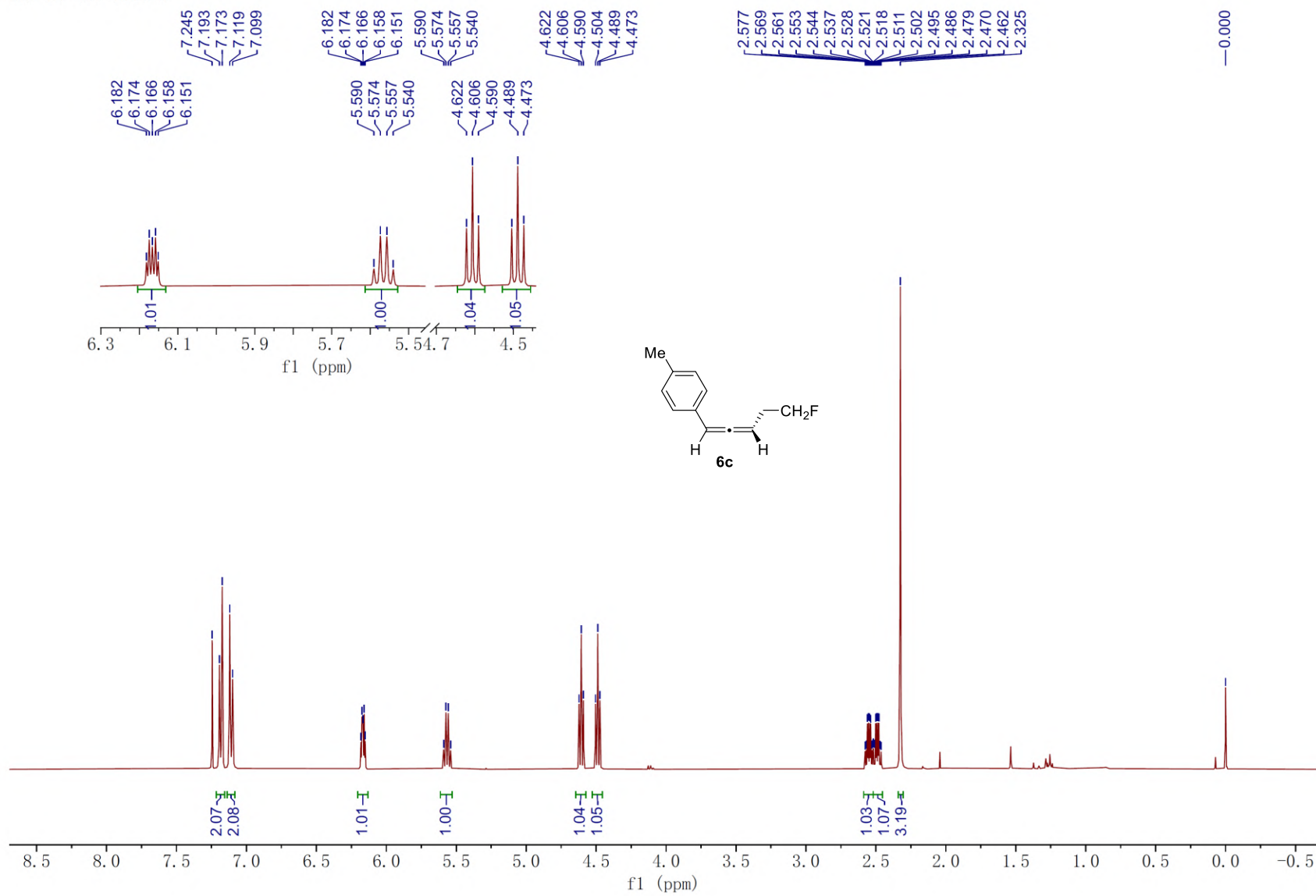
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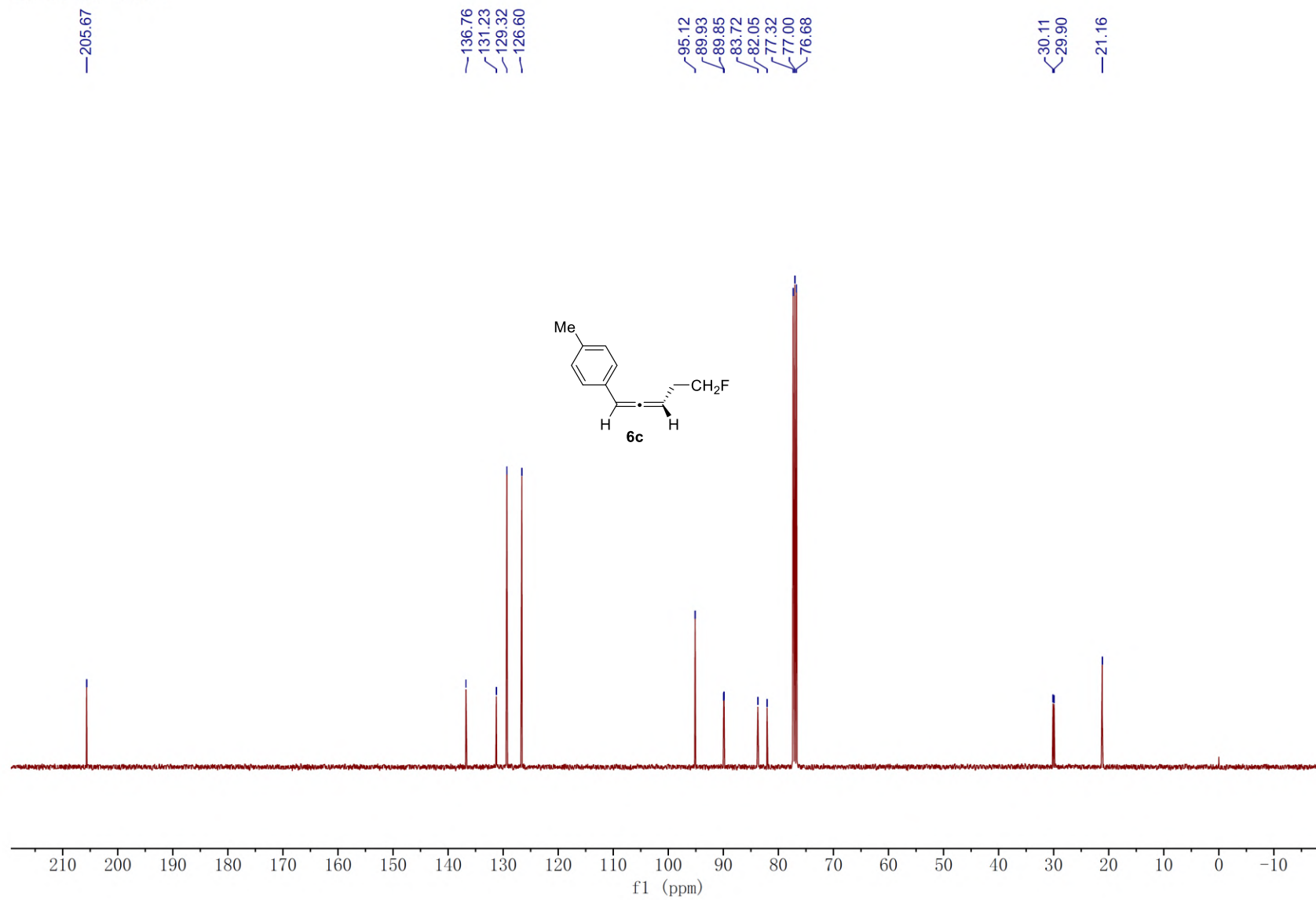
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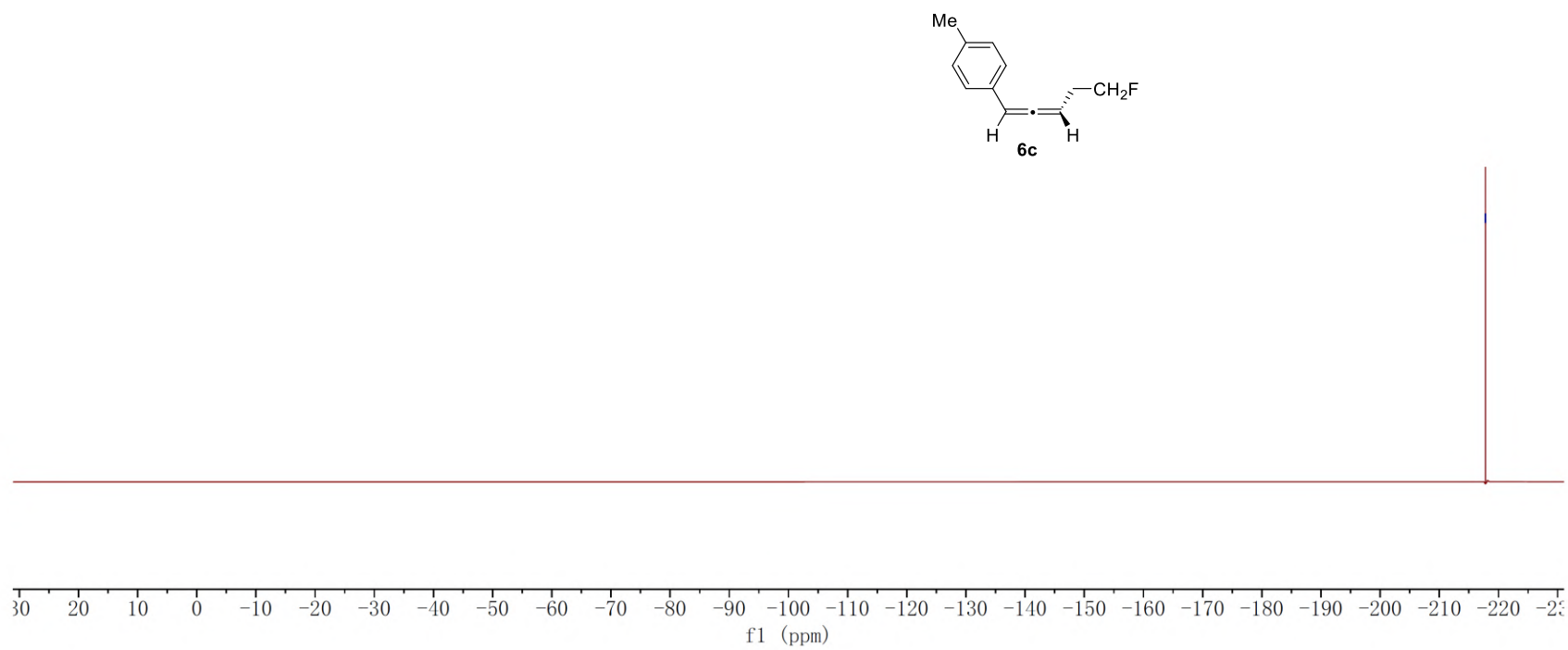
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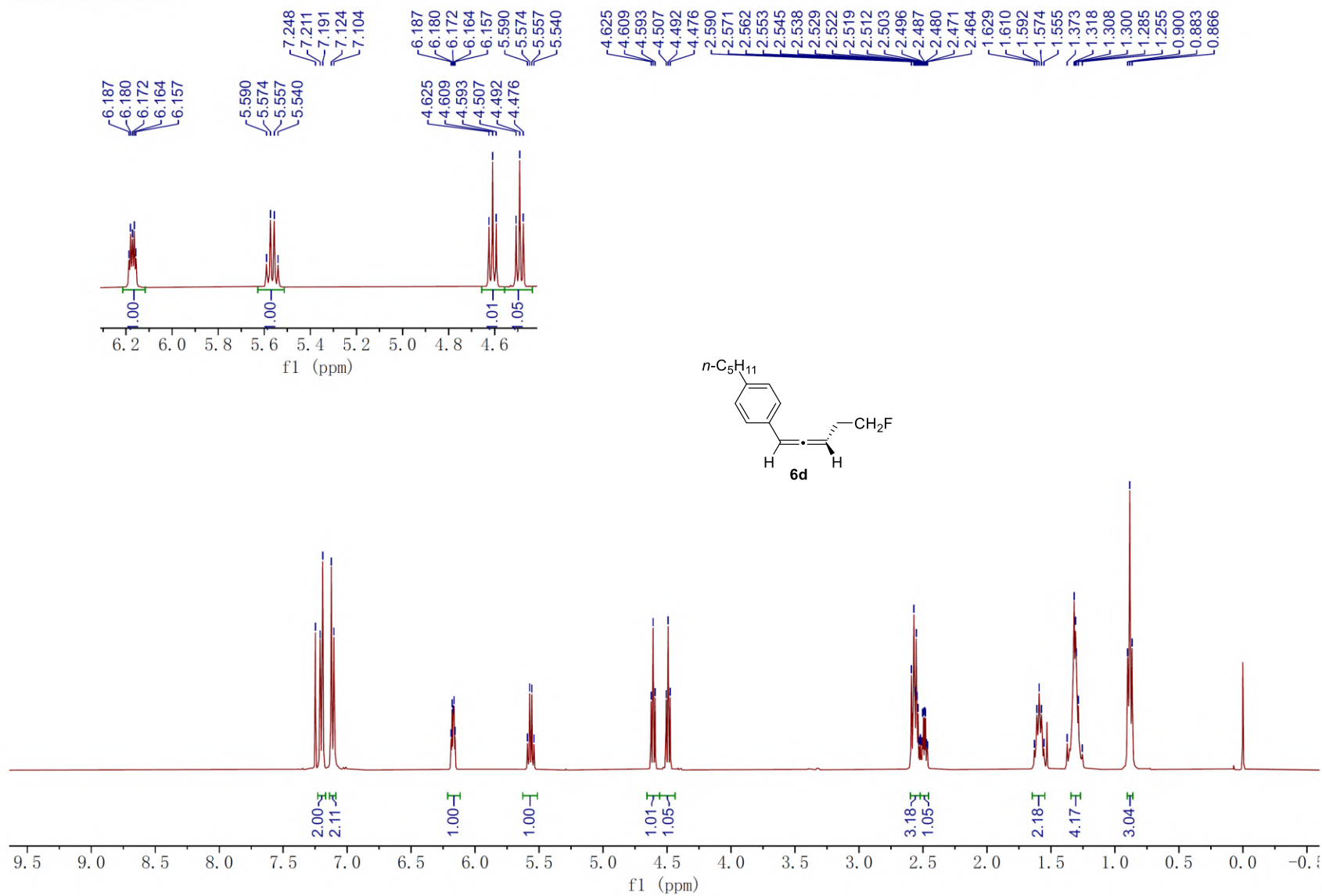
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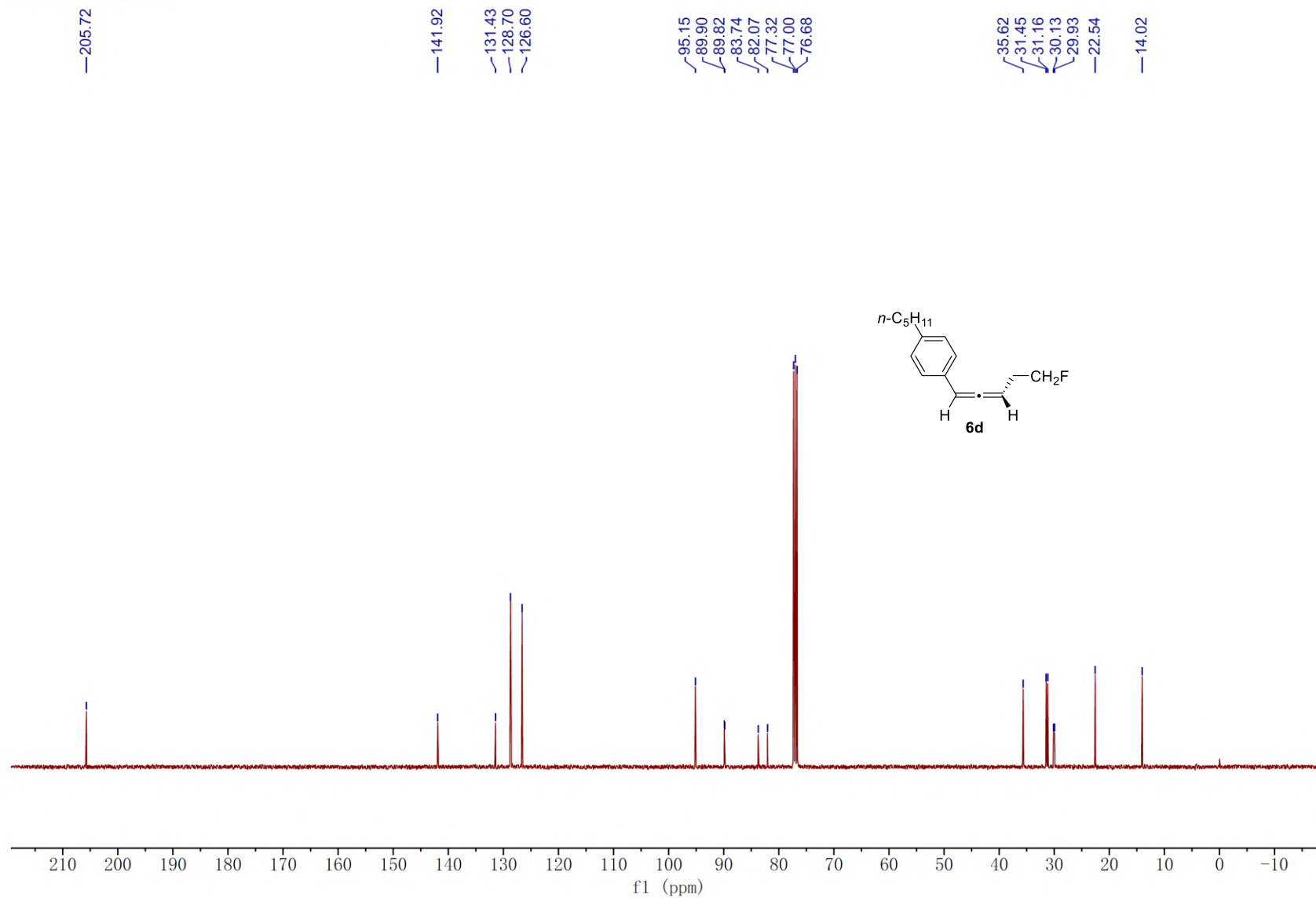
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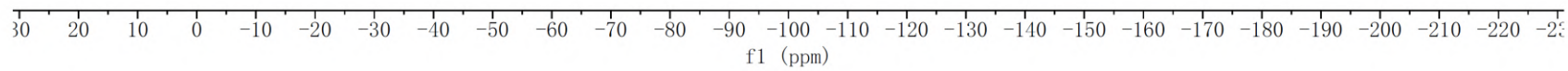
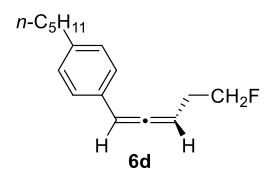


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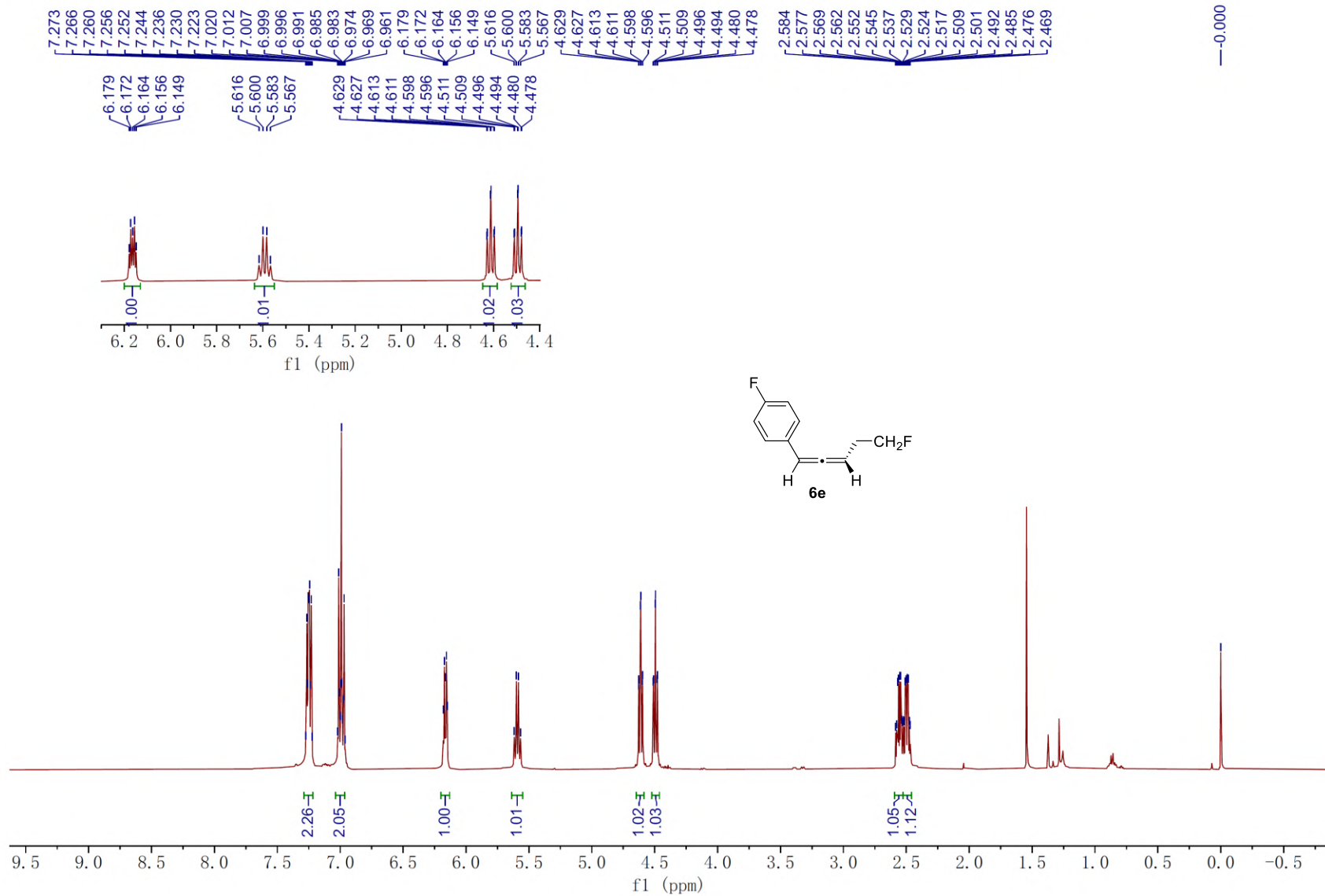


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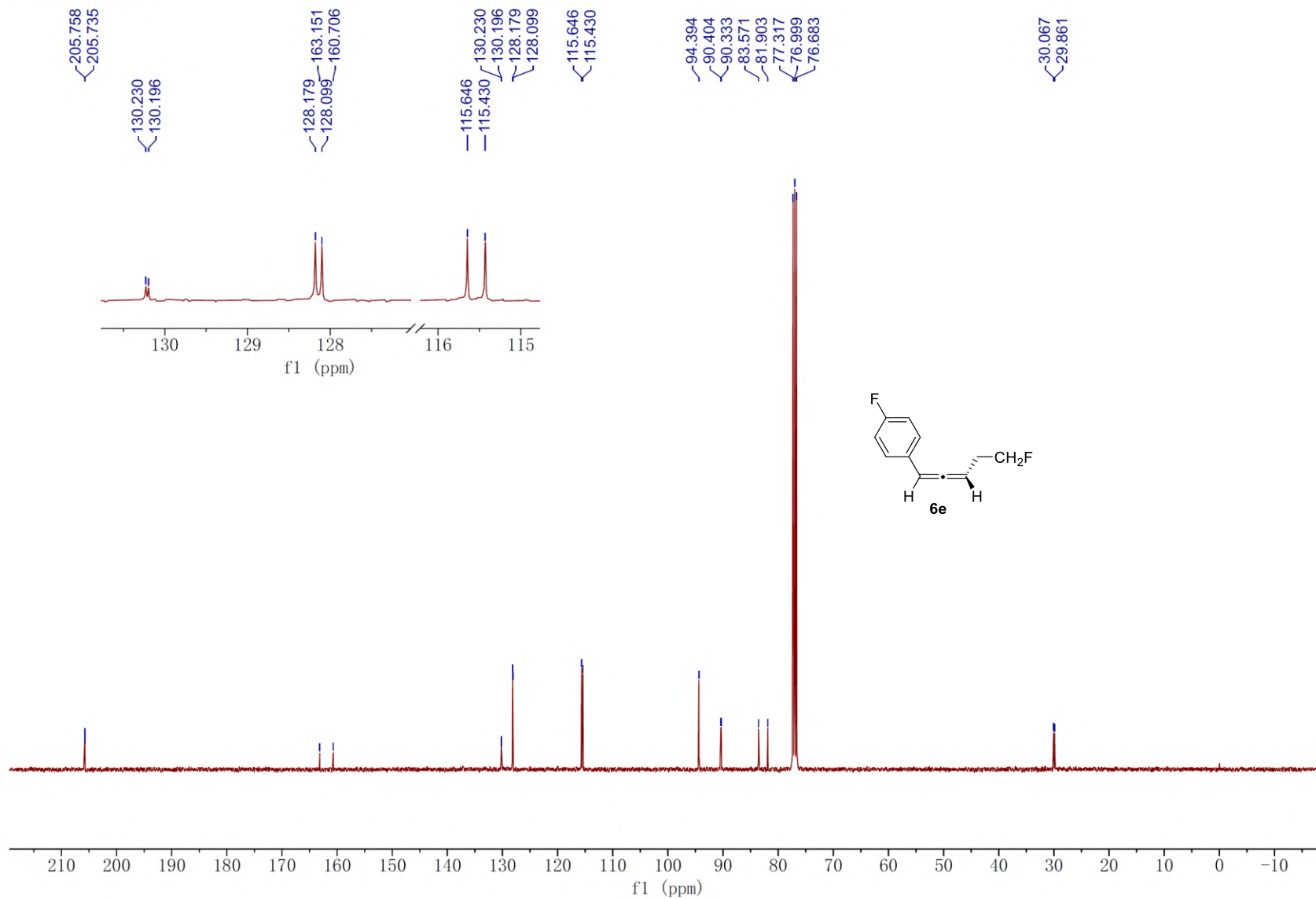
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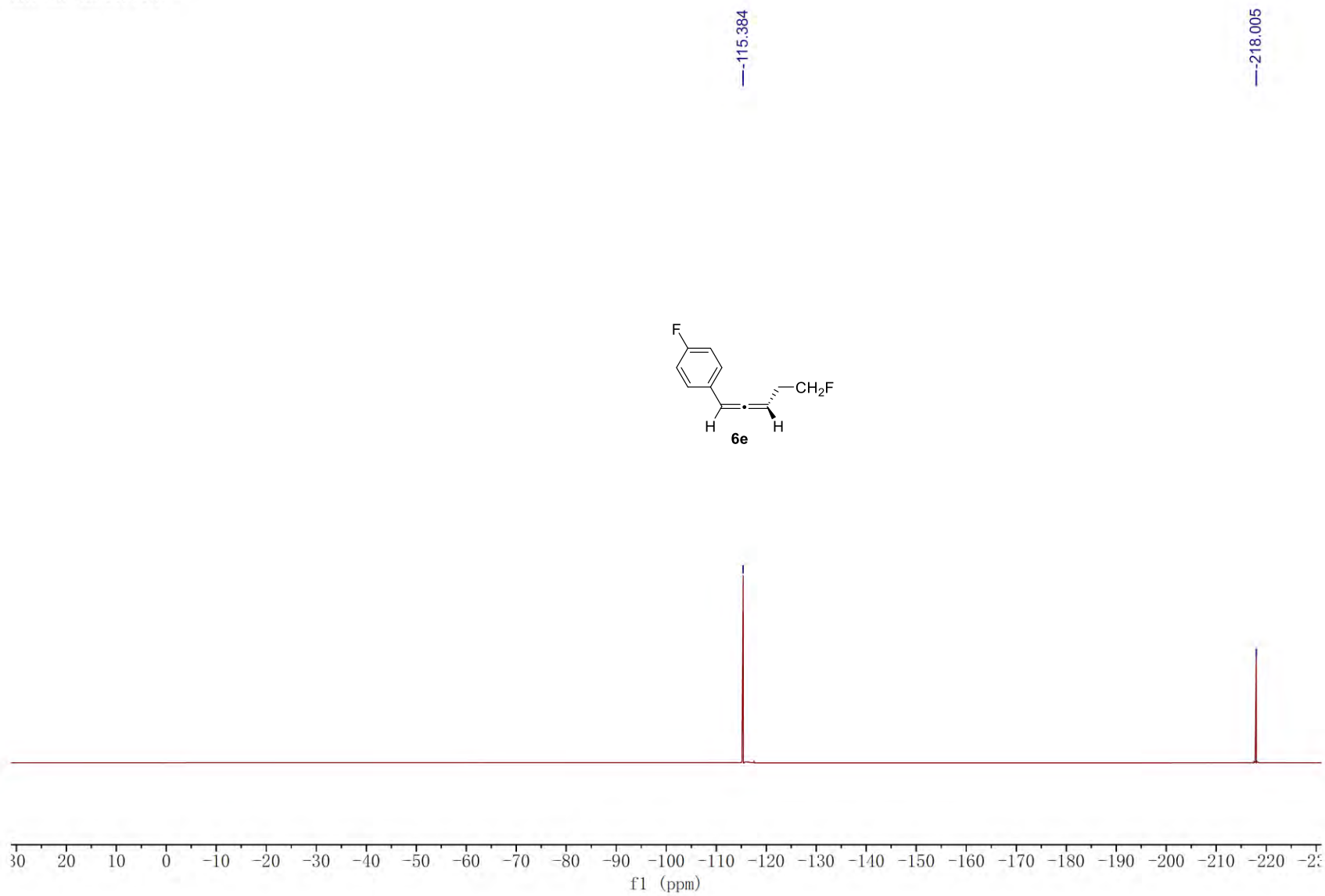
ZHY-ZH-43. 20. fid —



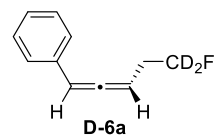
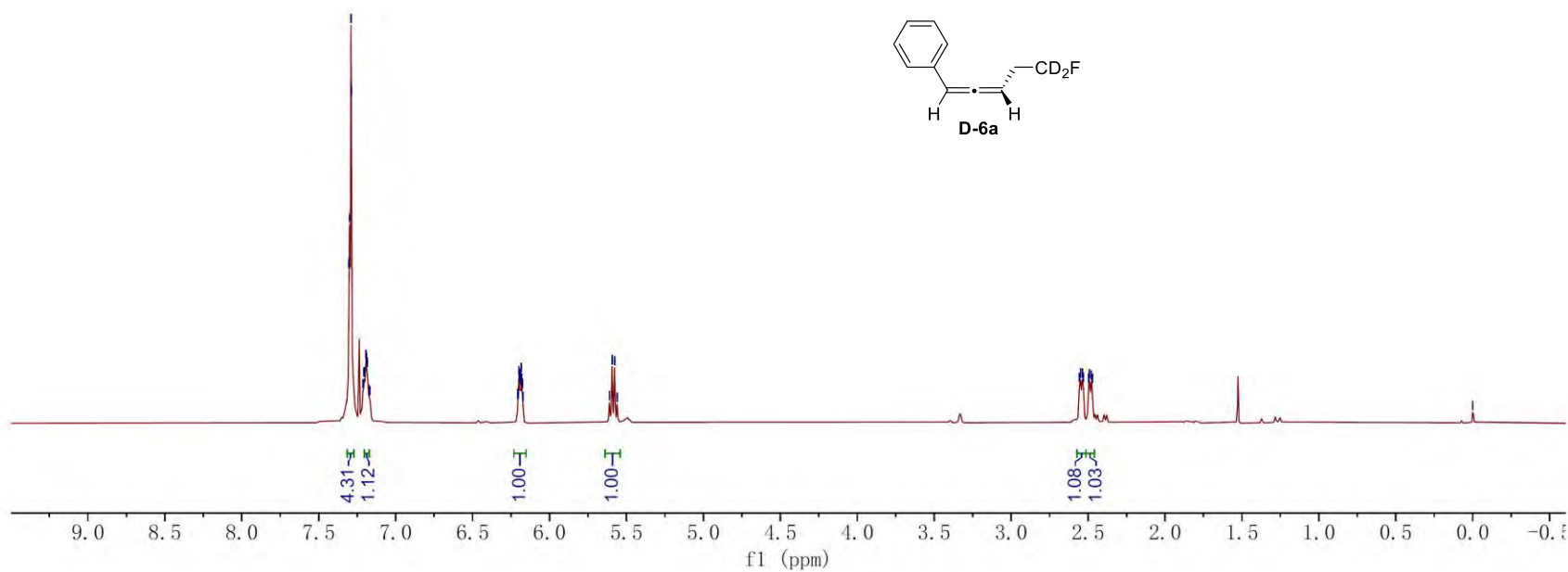
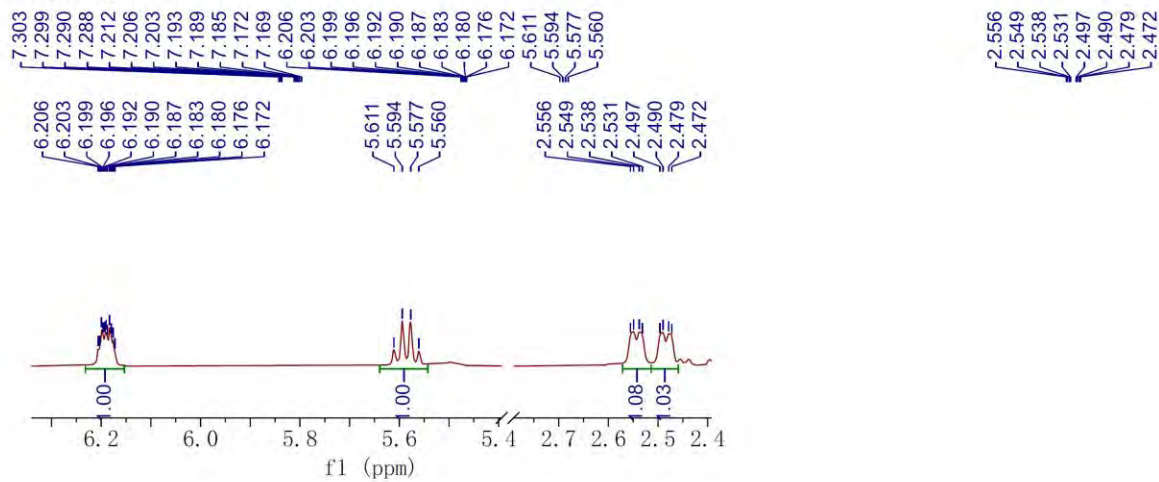
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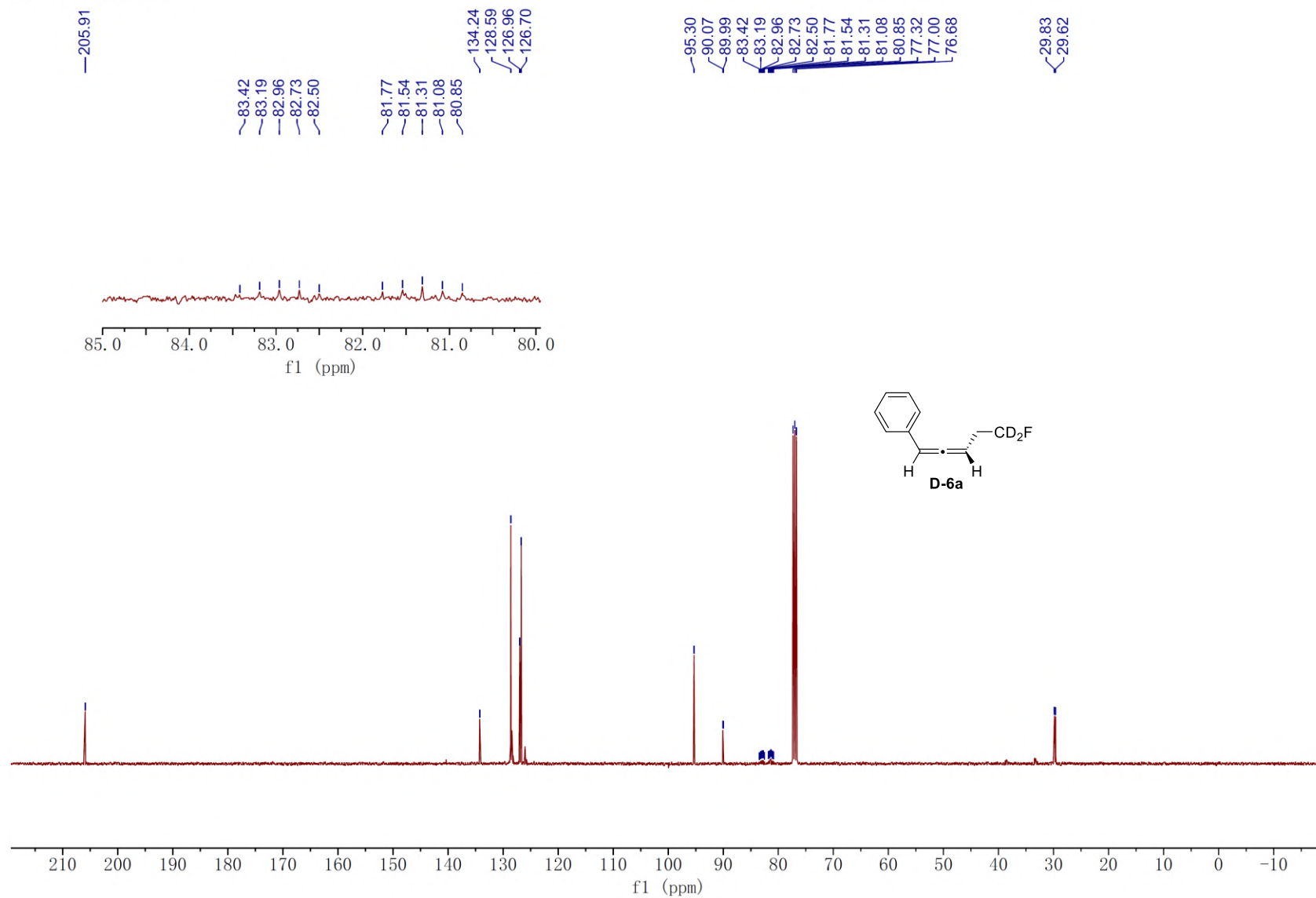
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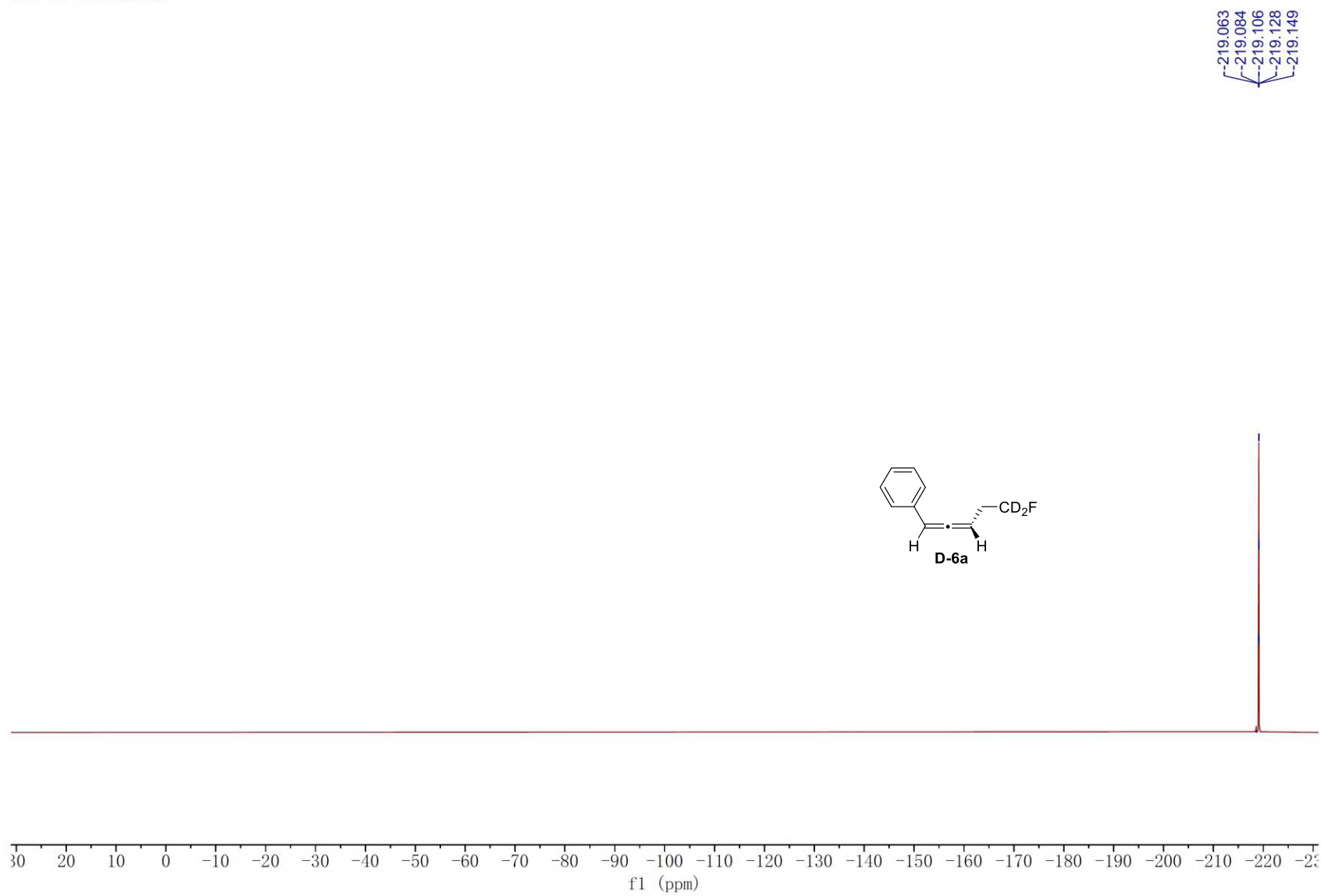
ZHY-ZG-116. 10. fid —



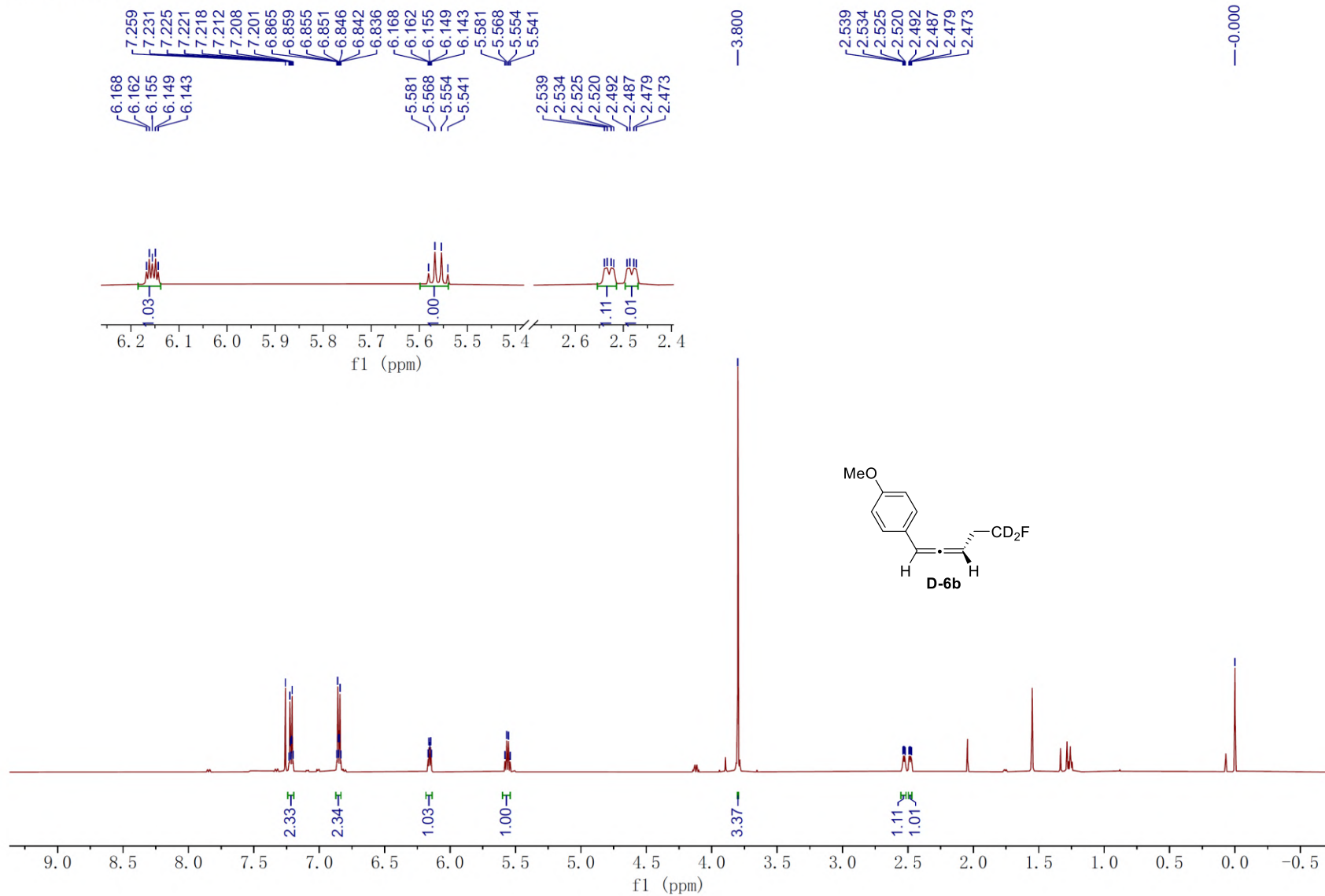
ZHY-ZG-116. 12. fid —



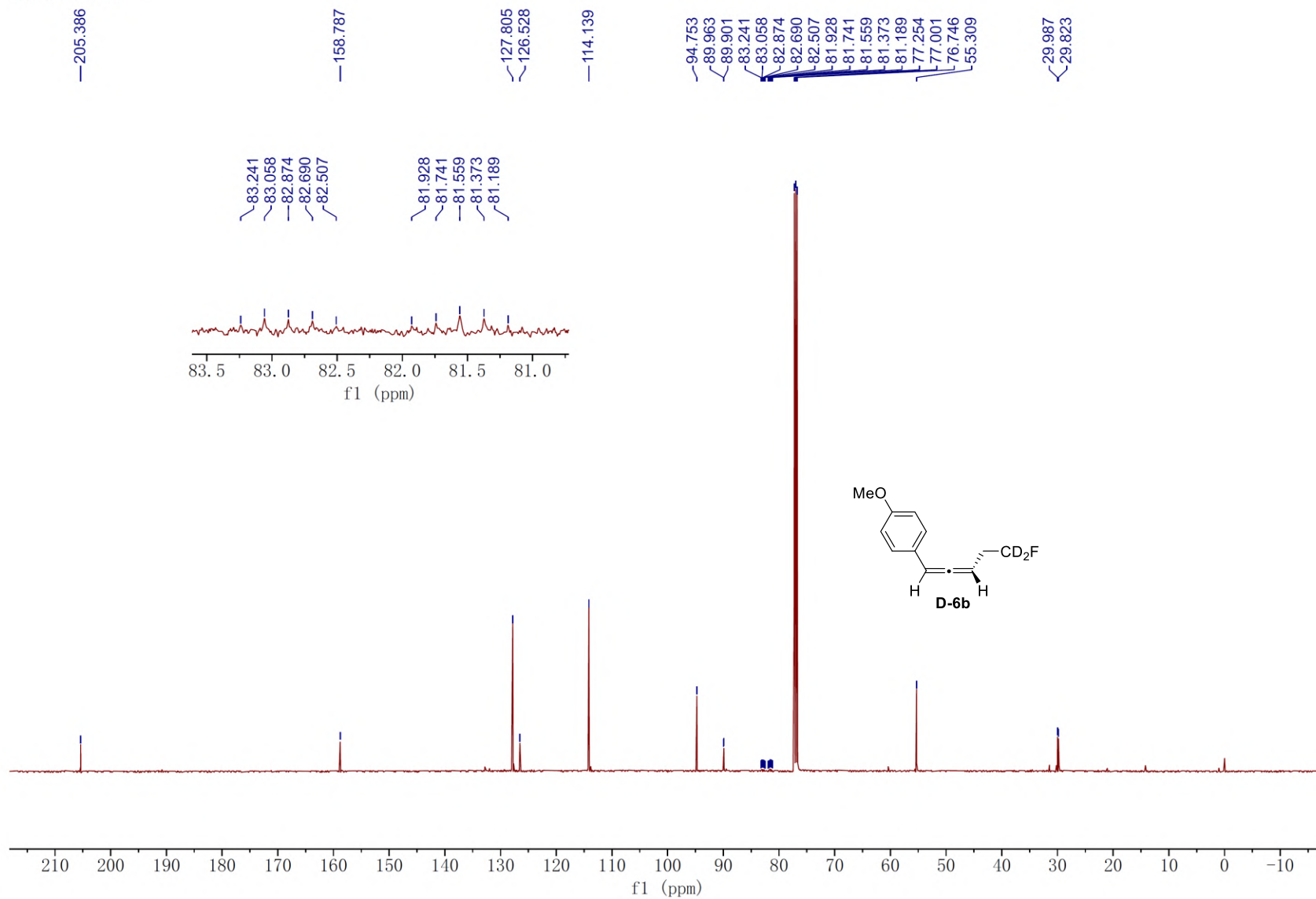
ZHY-ZG-116.20.fid —



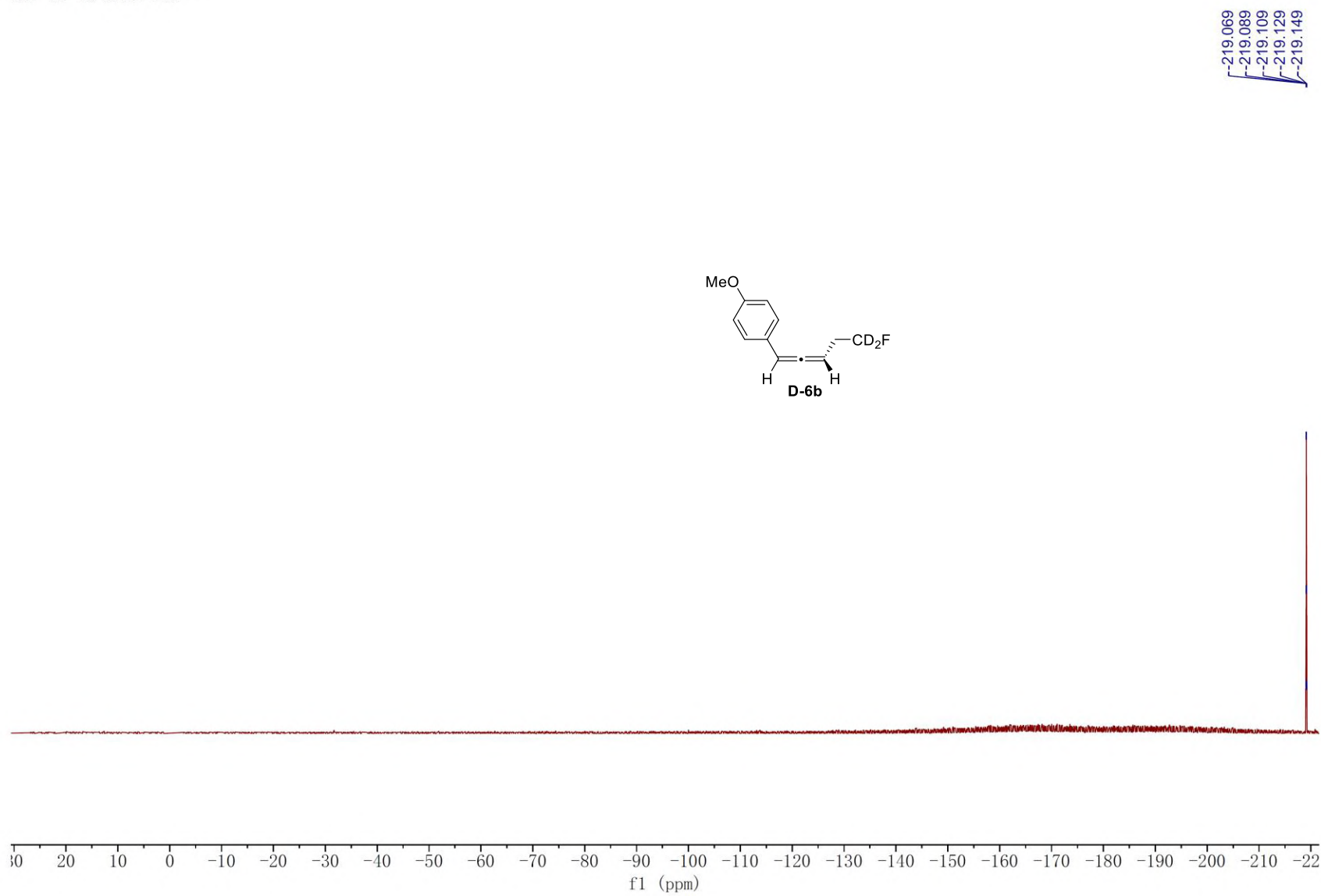
ZHY-ZH-78/10 —



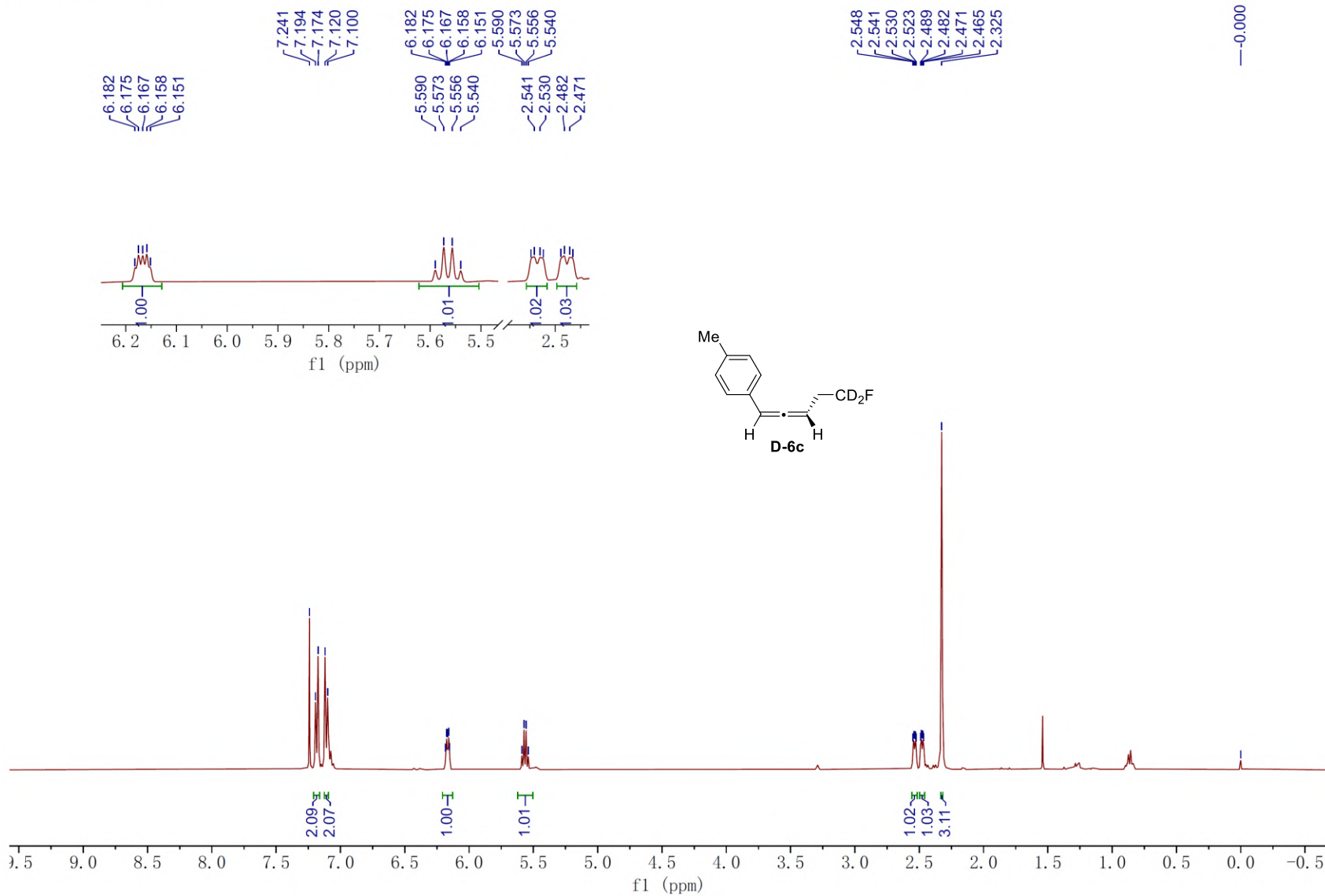
ZHY-ZH-78/11 —



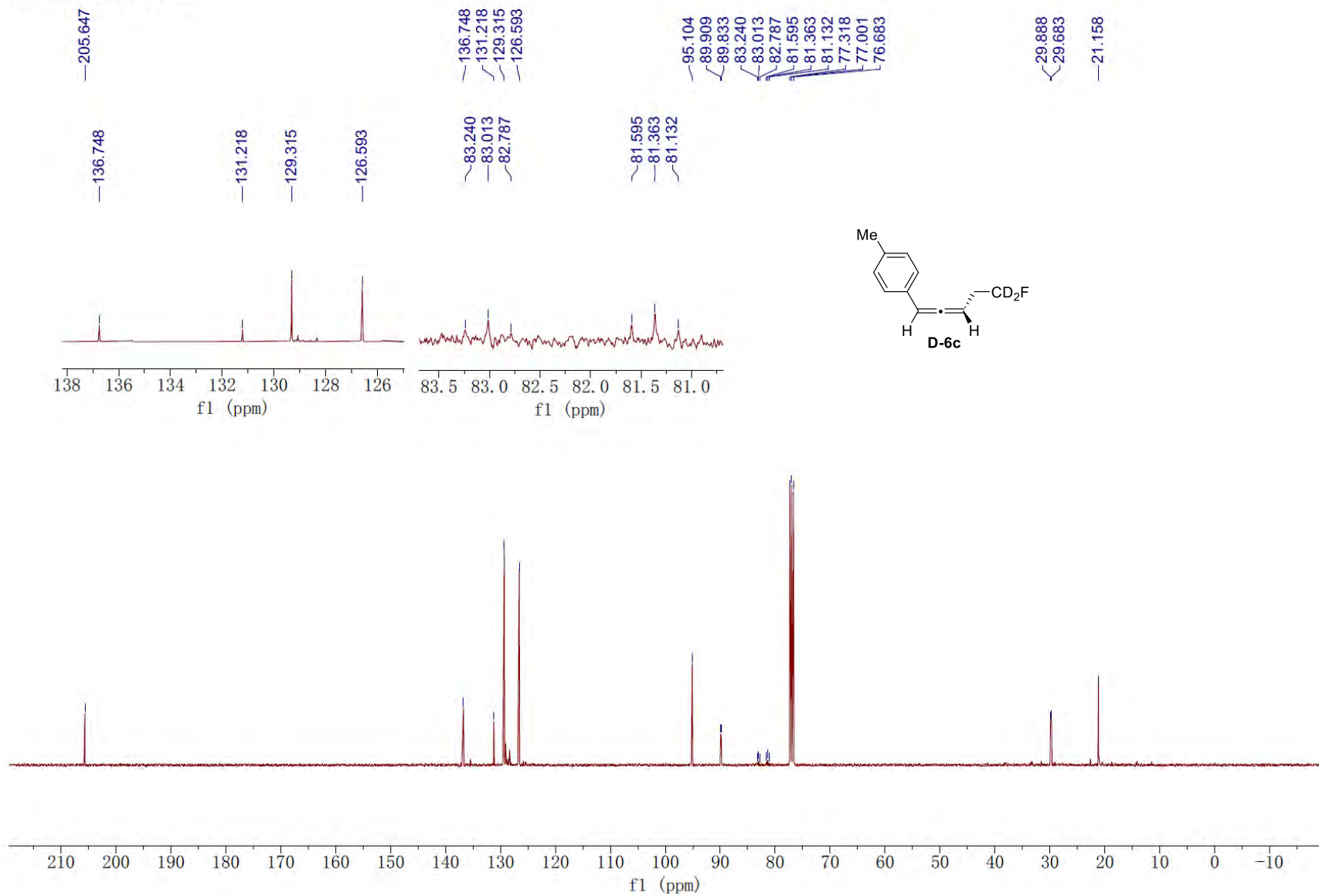
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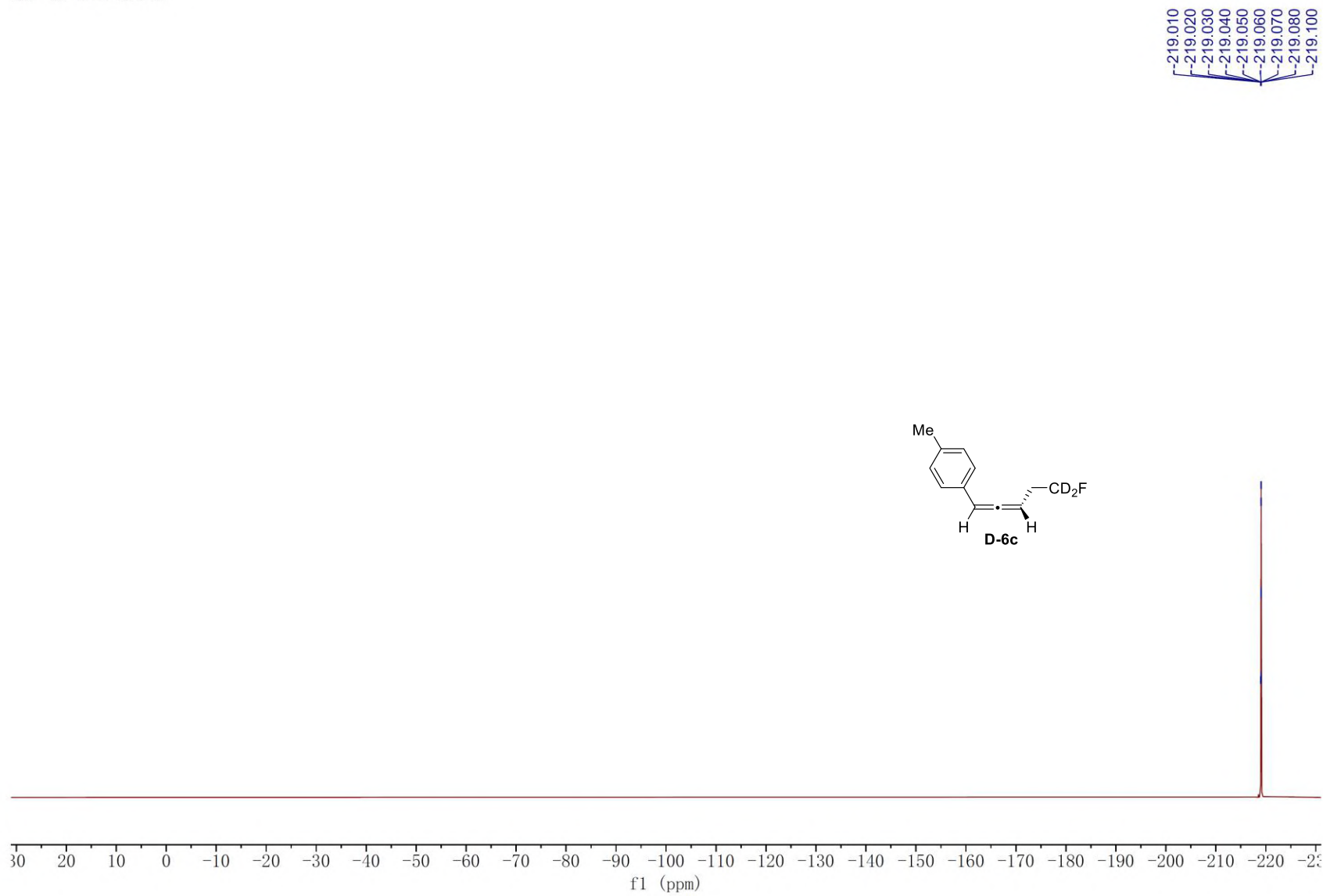
ZHY-ZG-117. 10. fid —



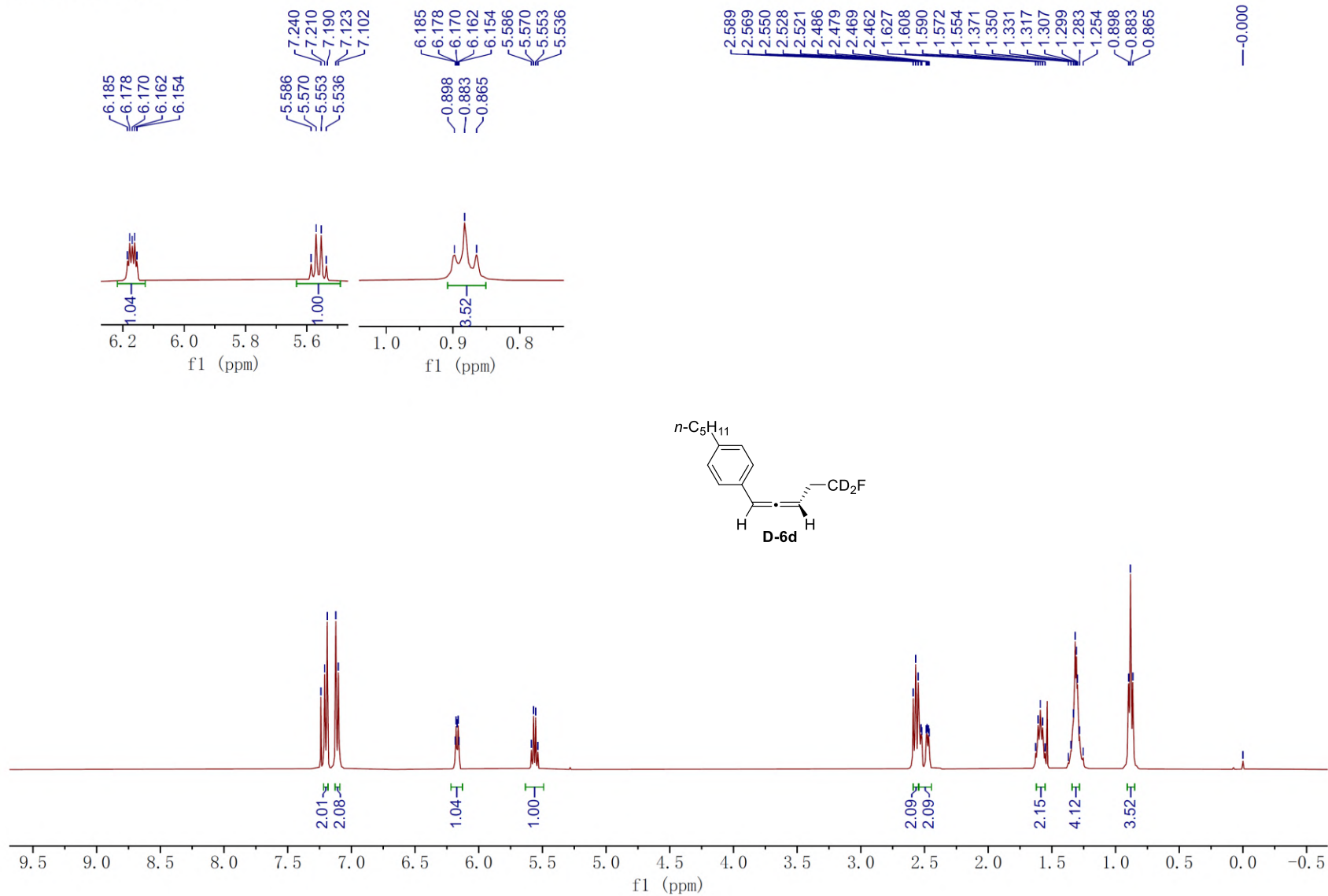
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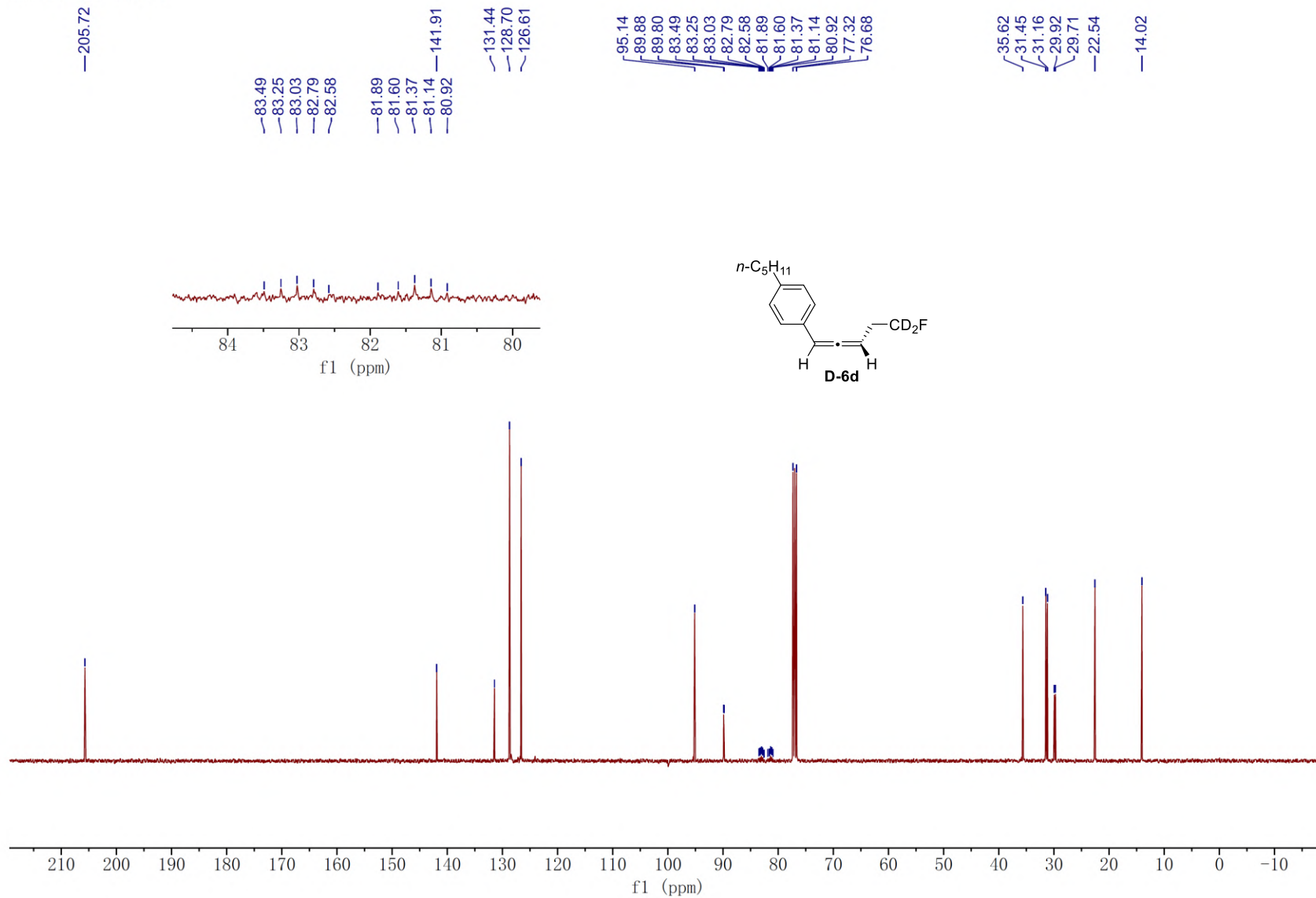
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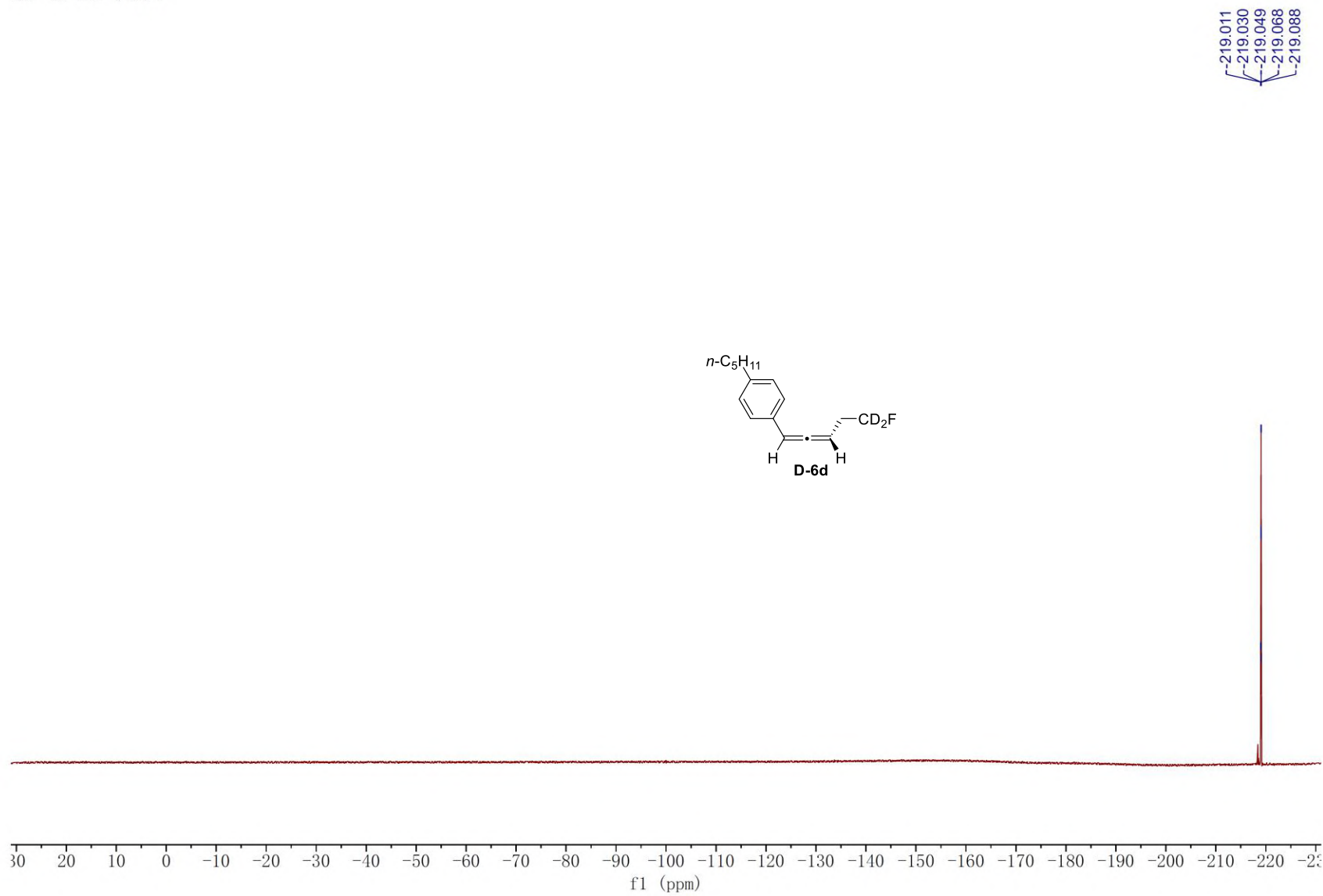
ZHY-ZG-122-400M-H



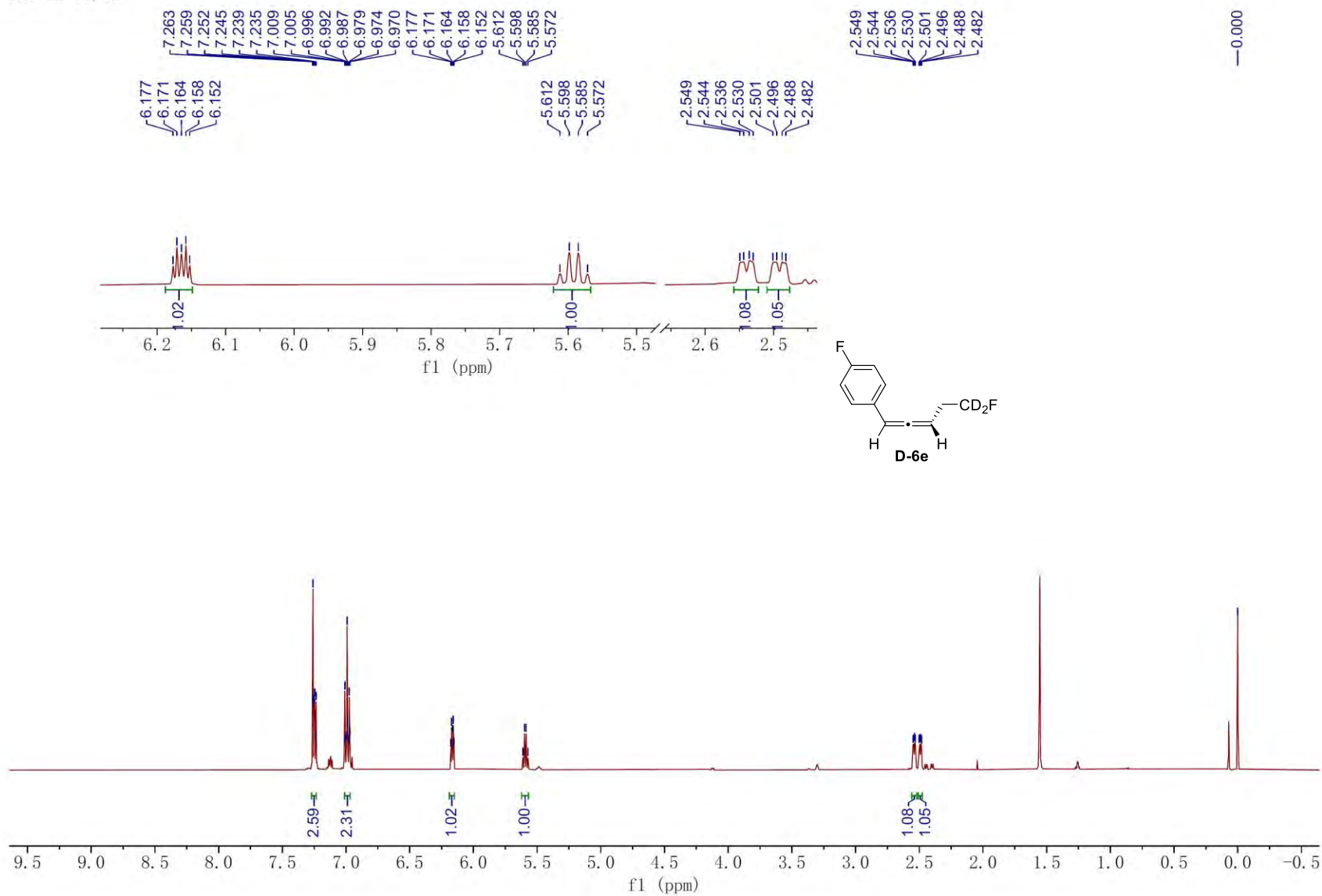
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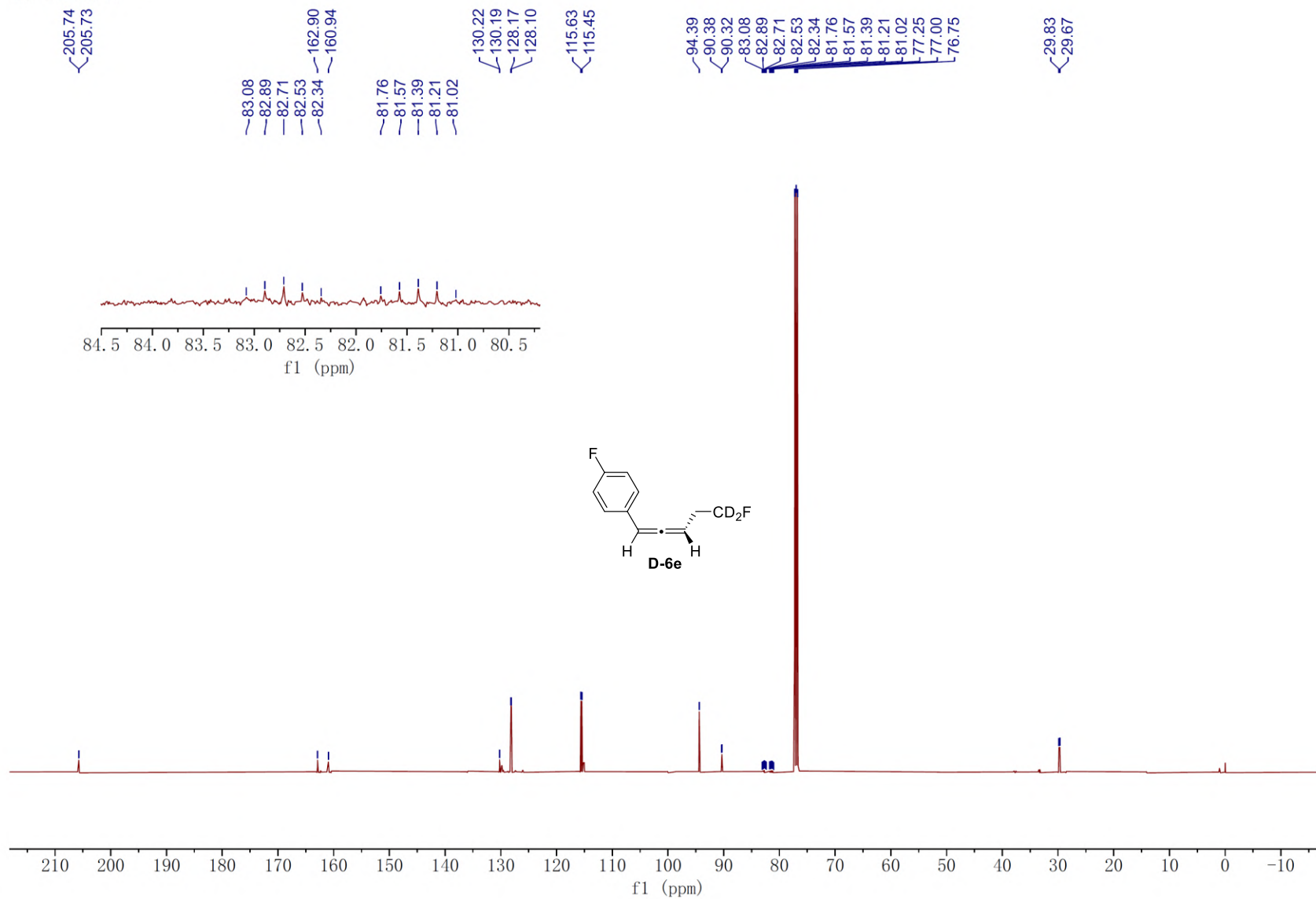
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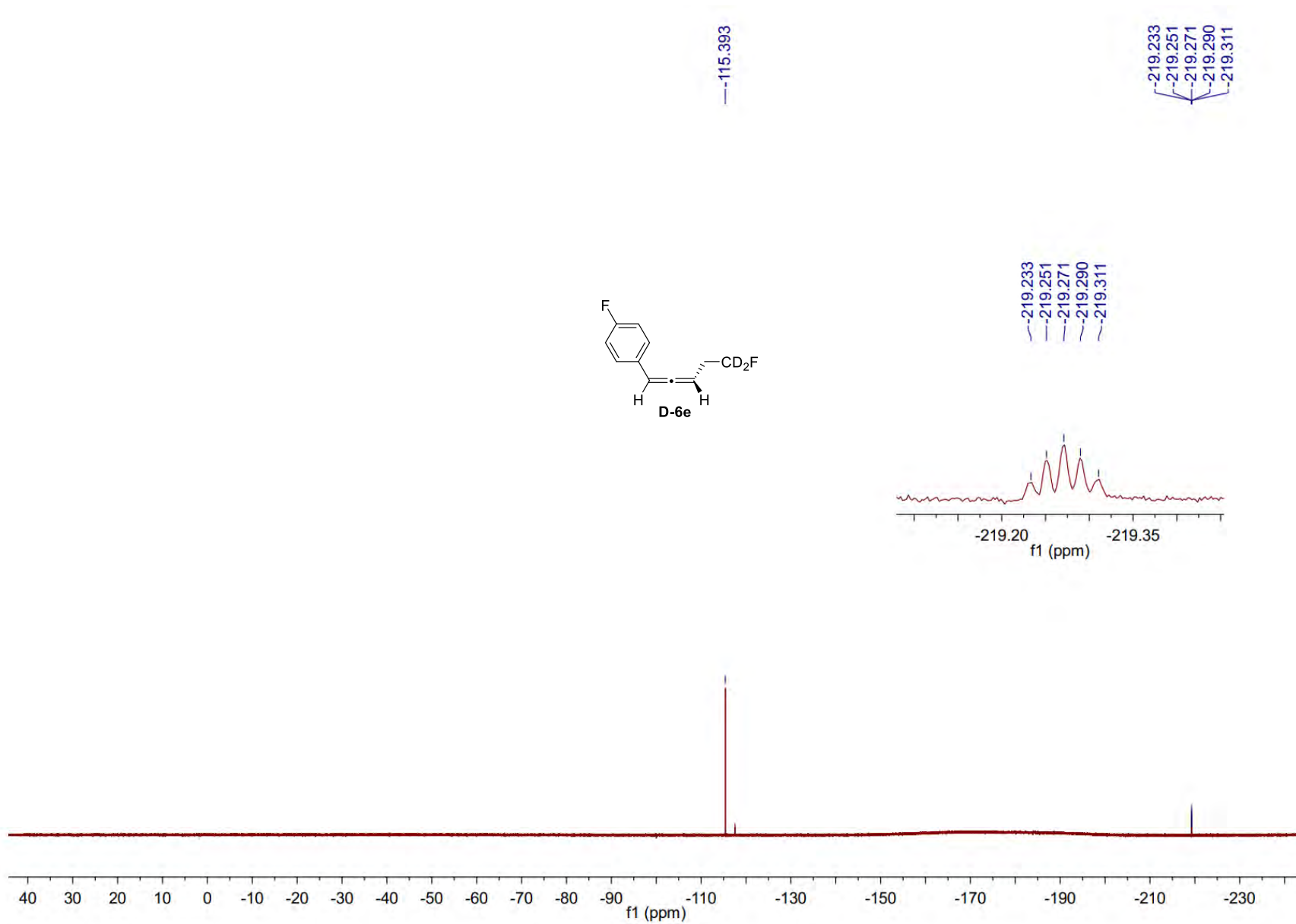


ZHY-ZH-77/10 —

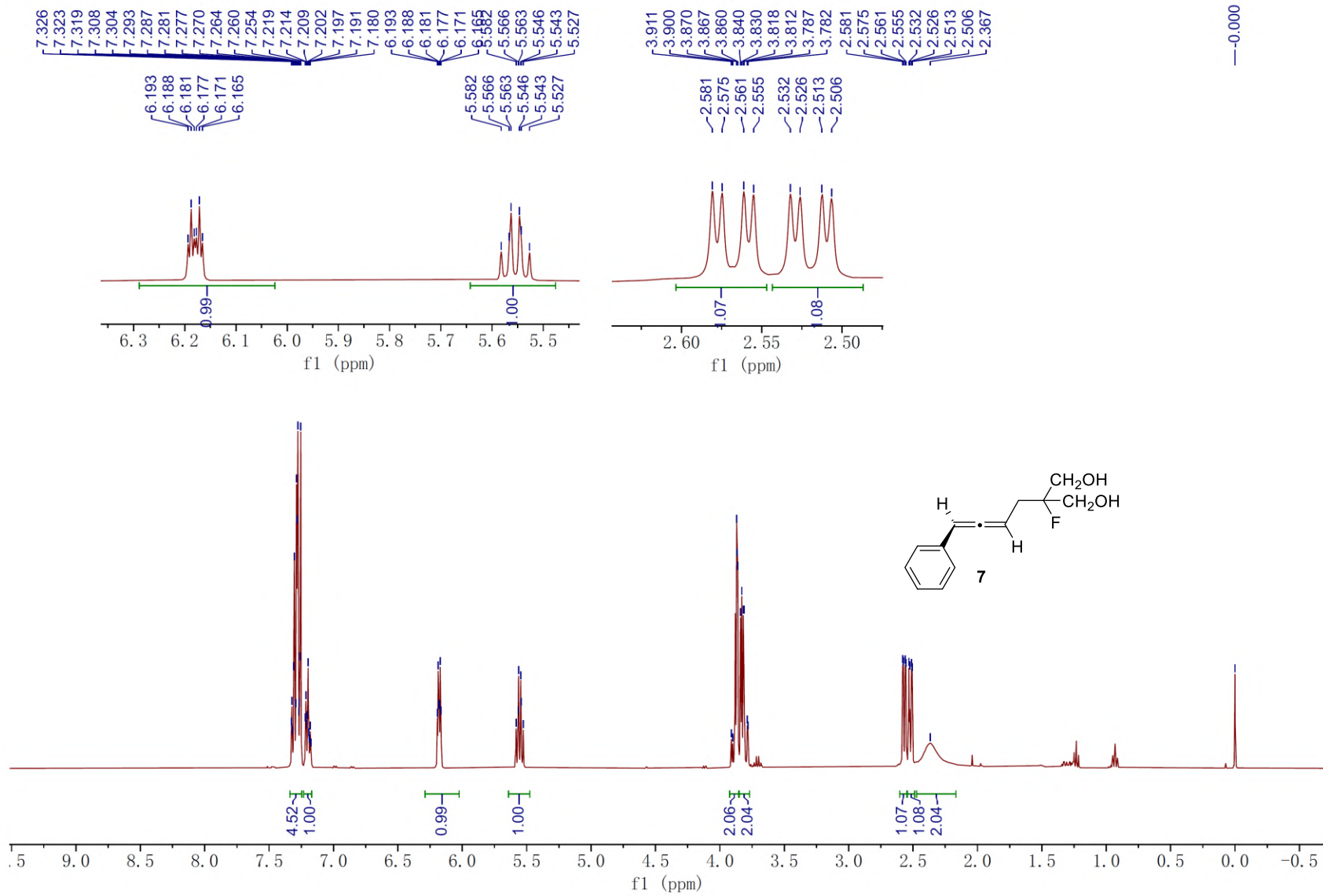


ZHY-ZH-77/11 —

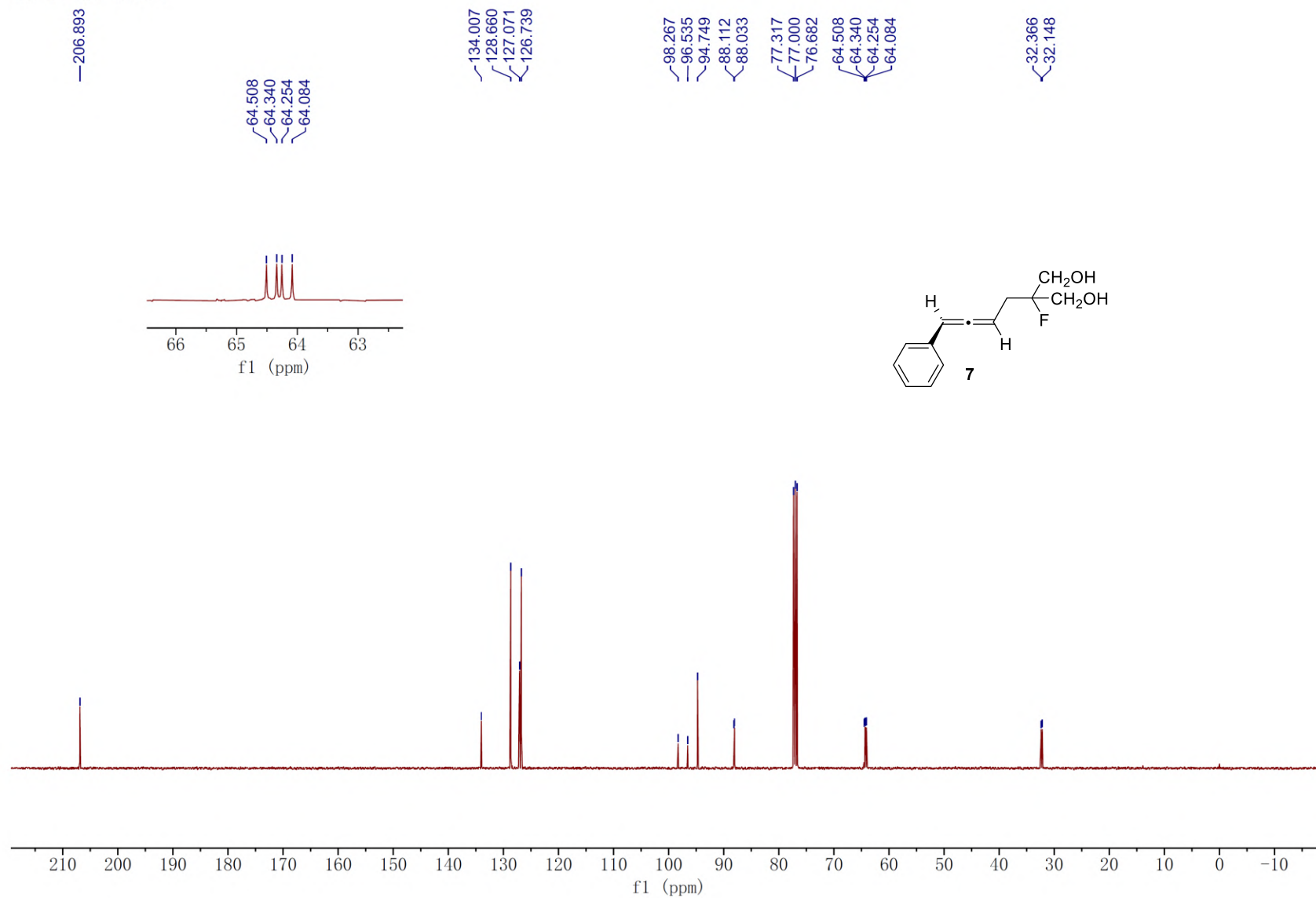




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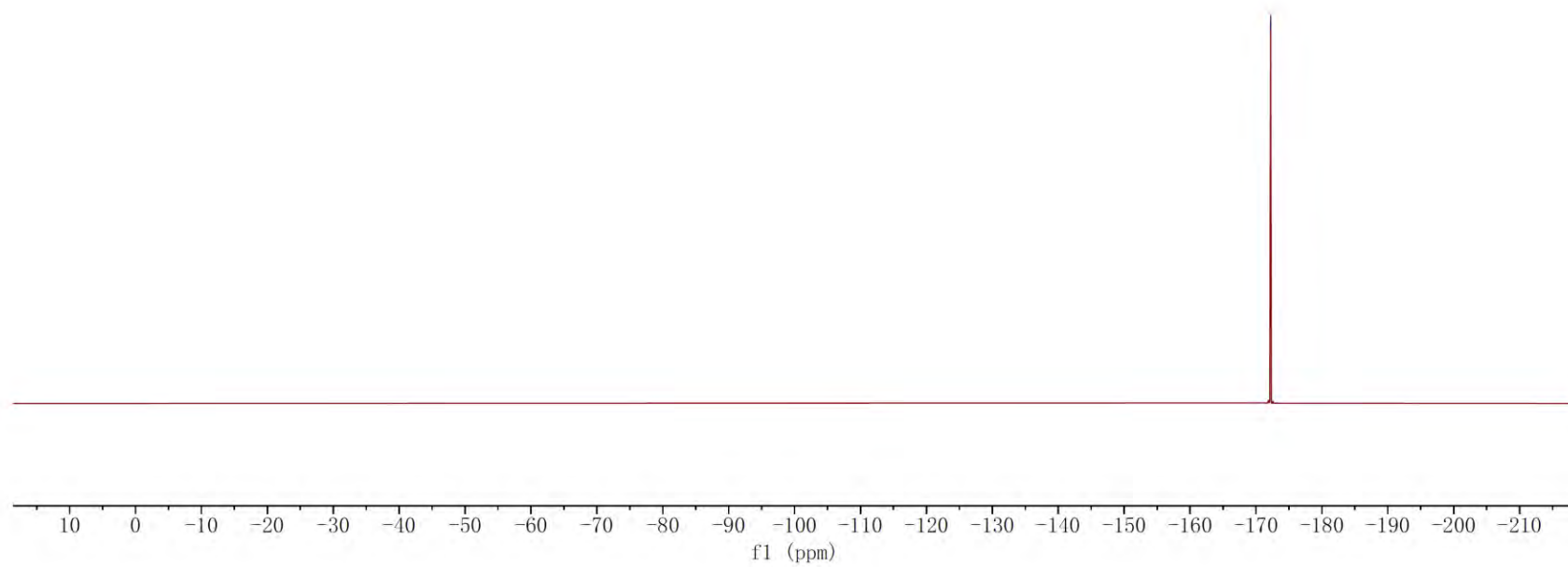
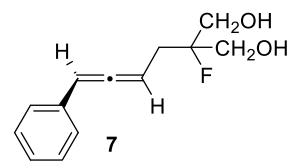


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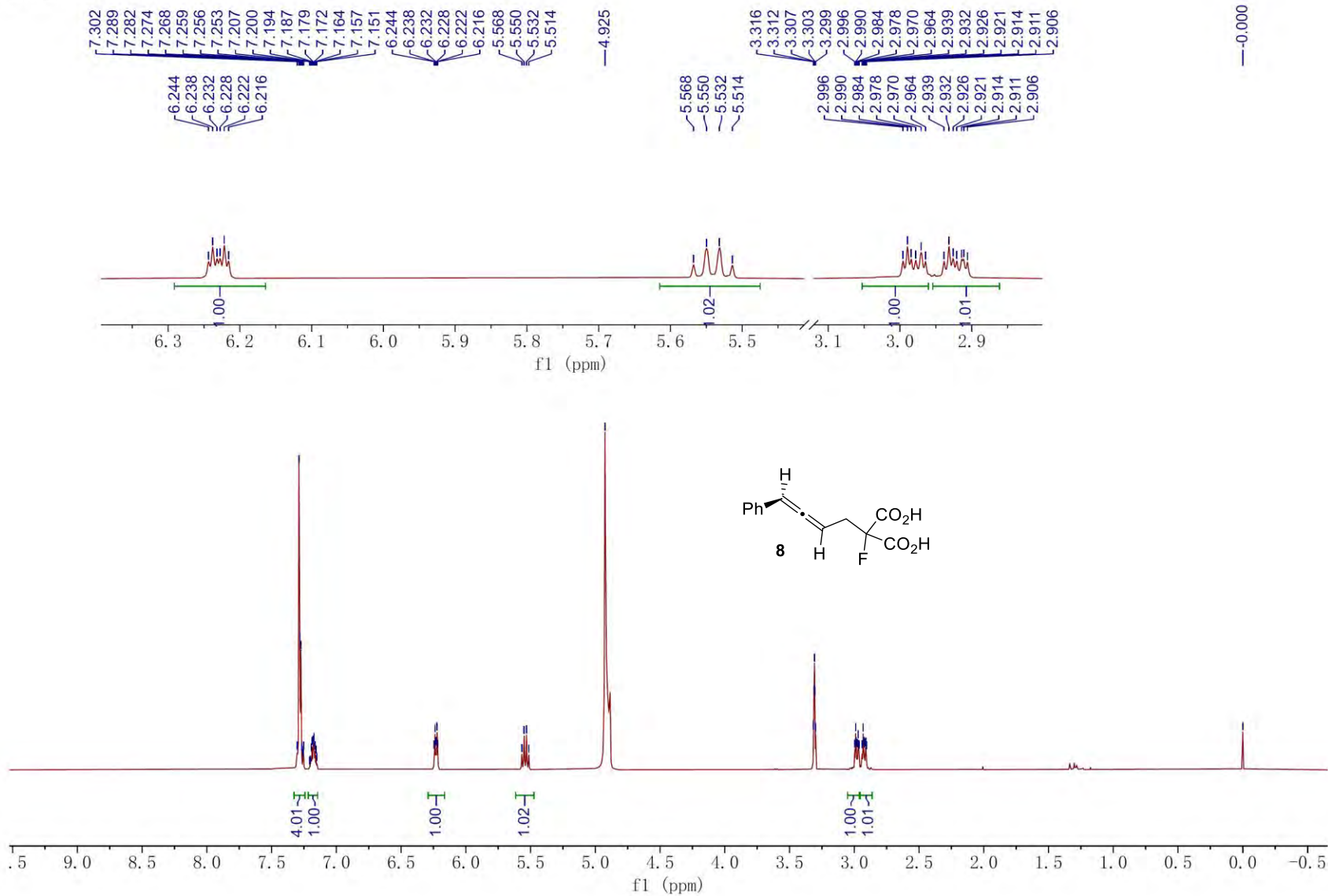


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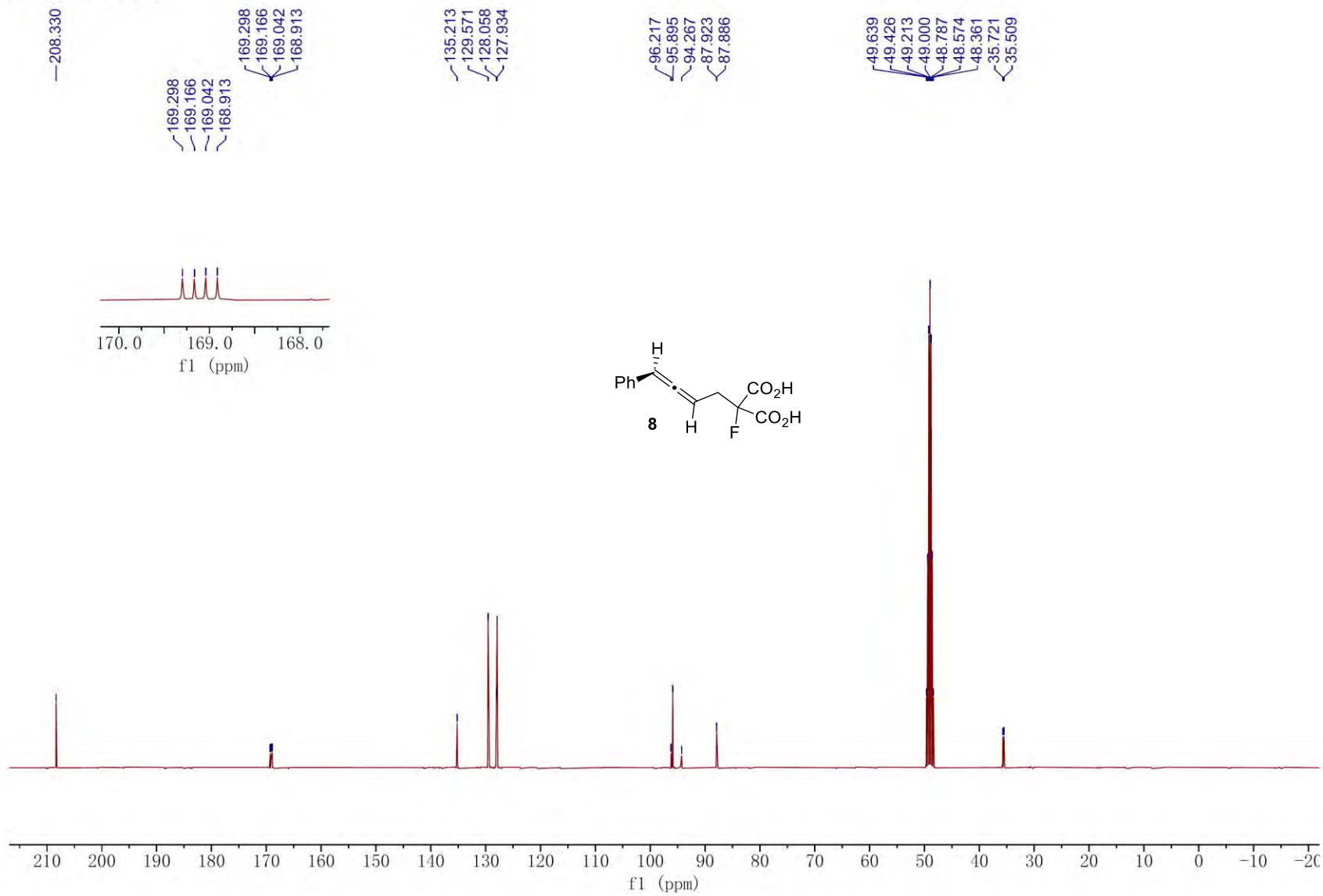
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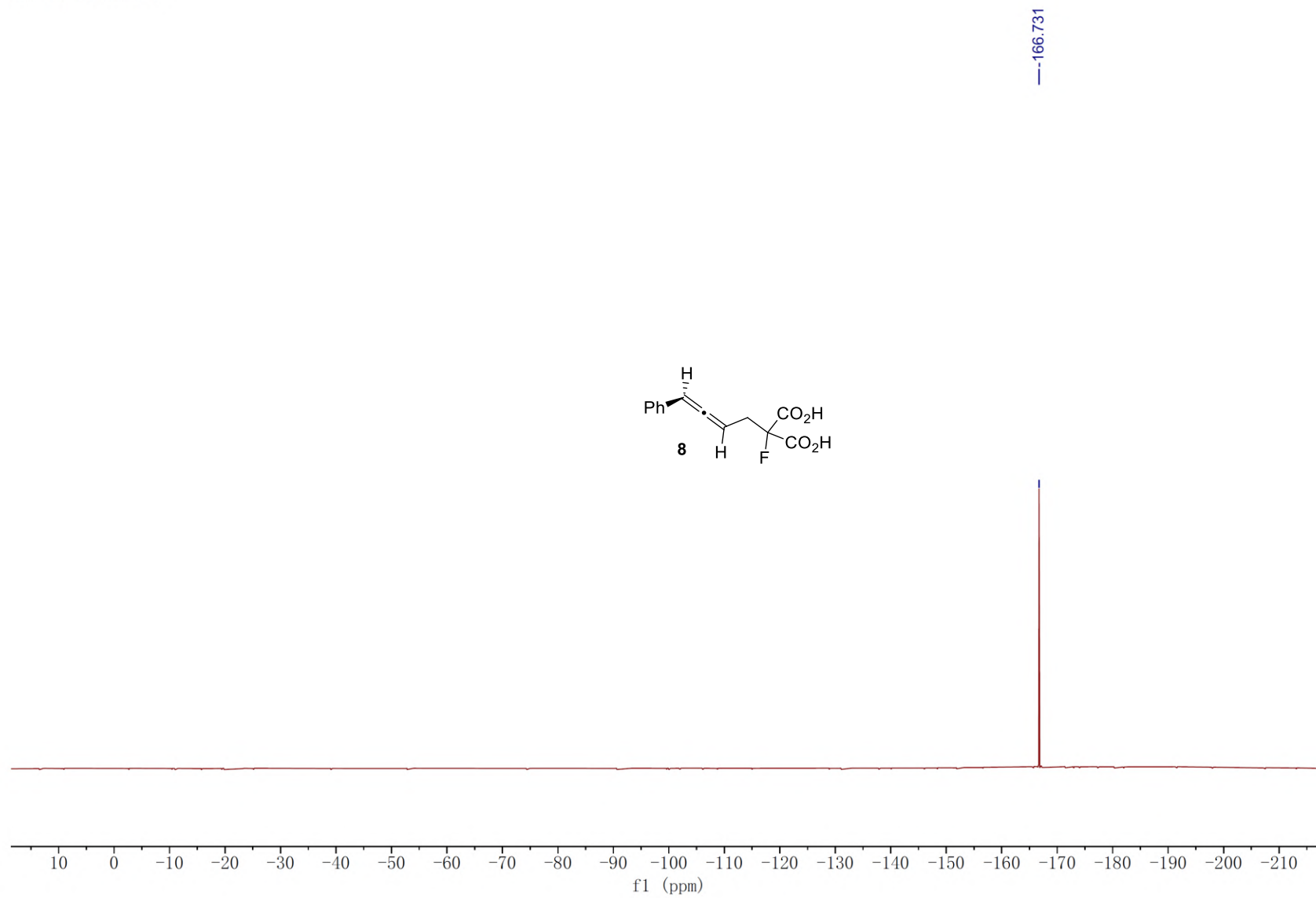
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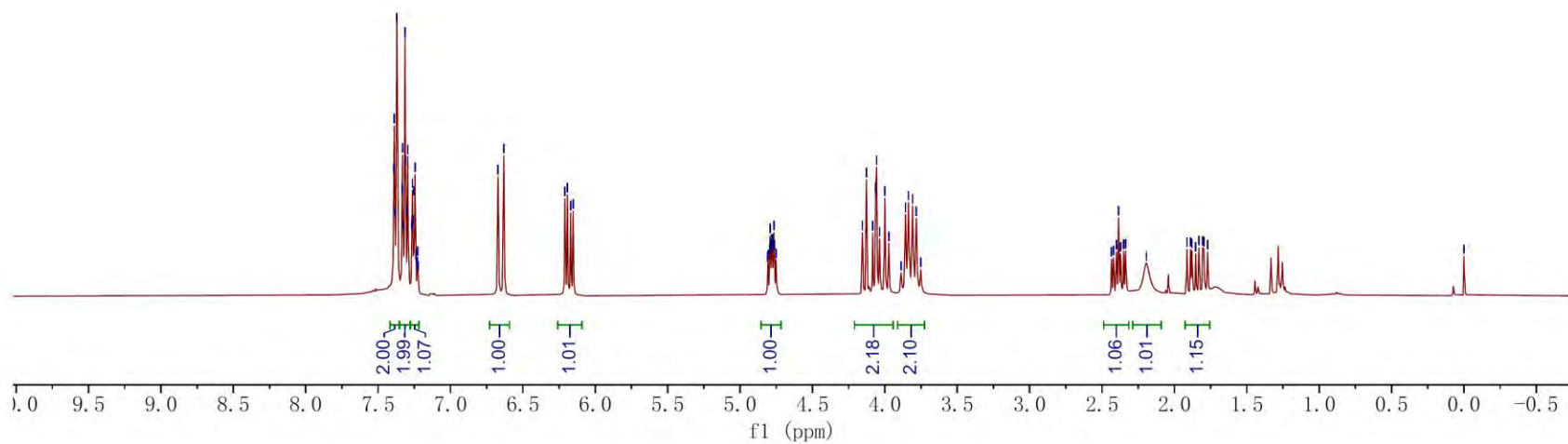
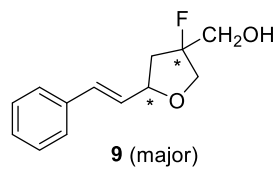
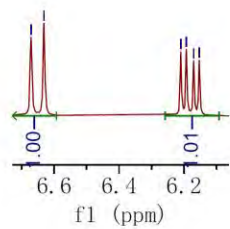
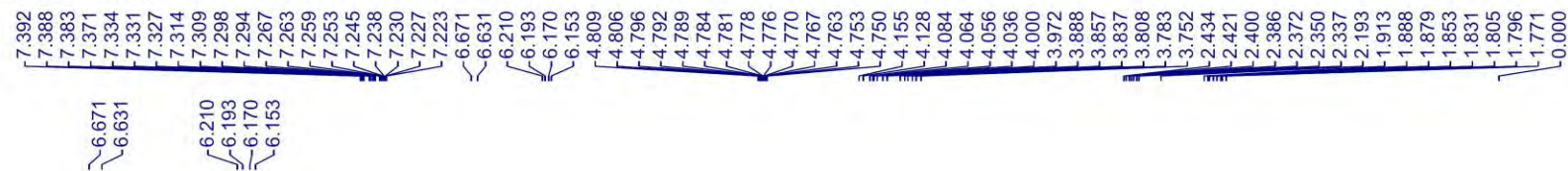
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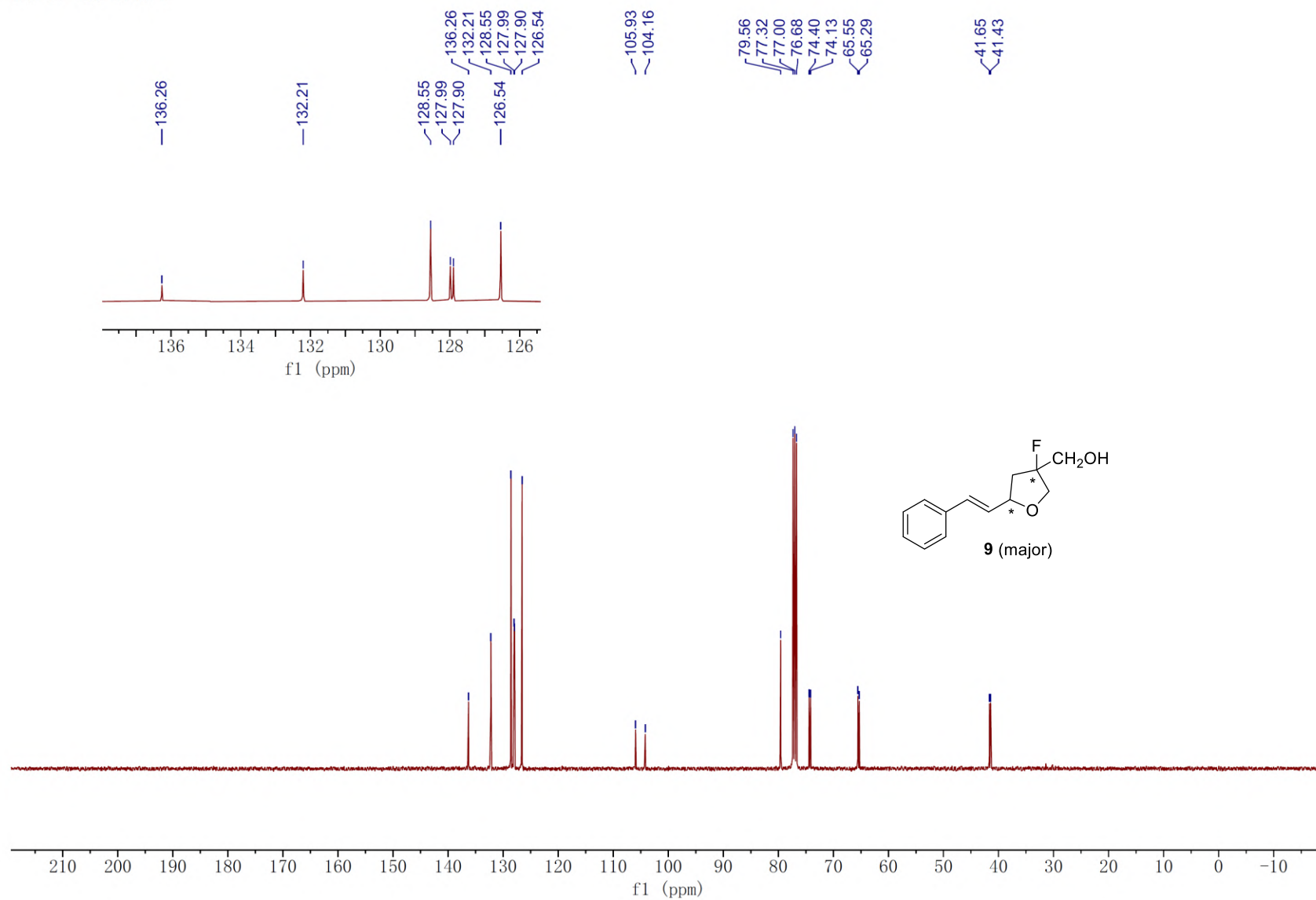
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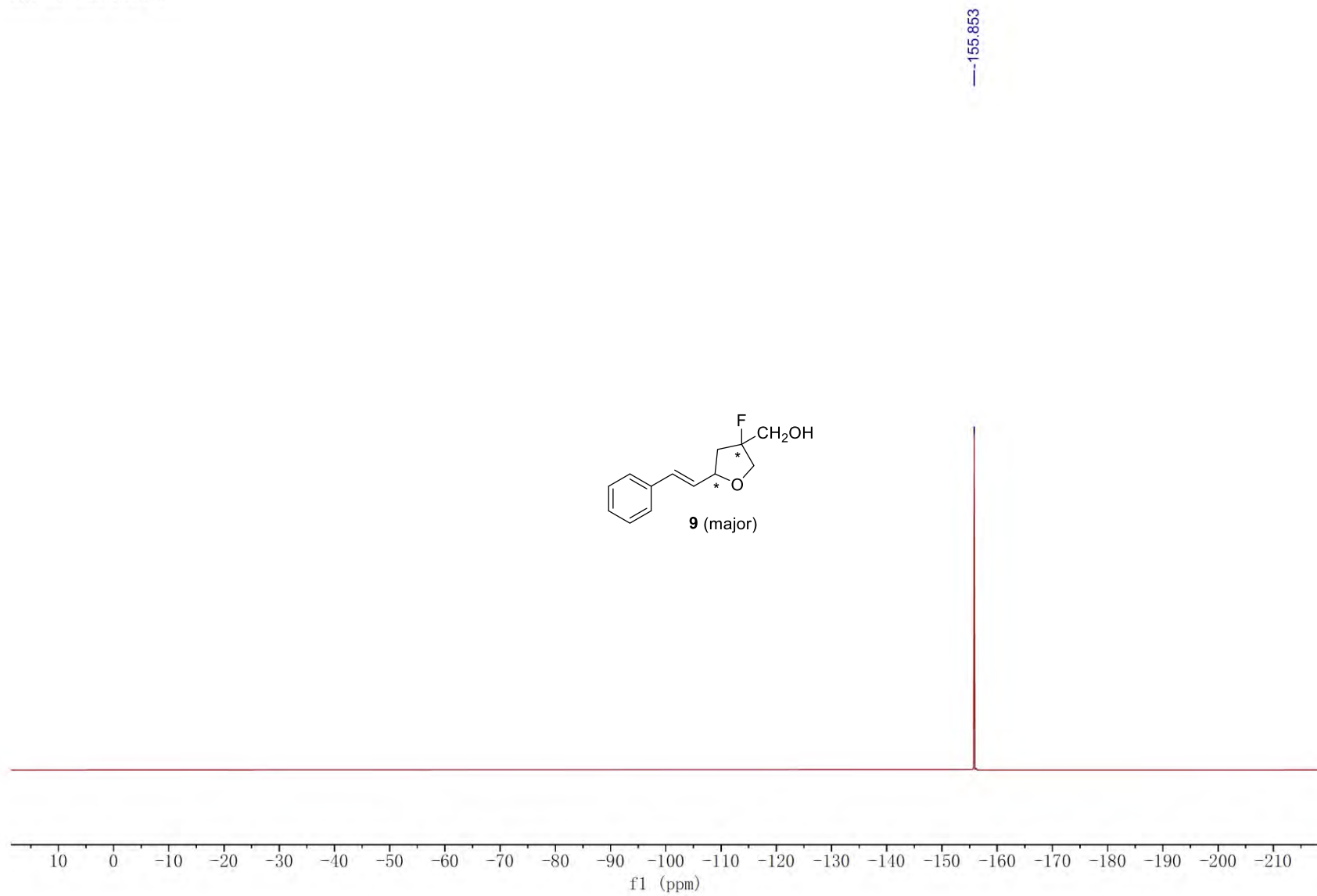
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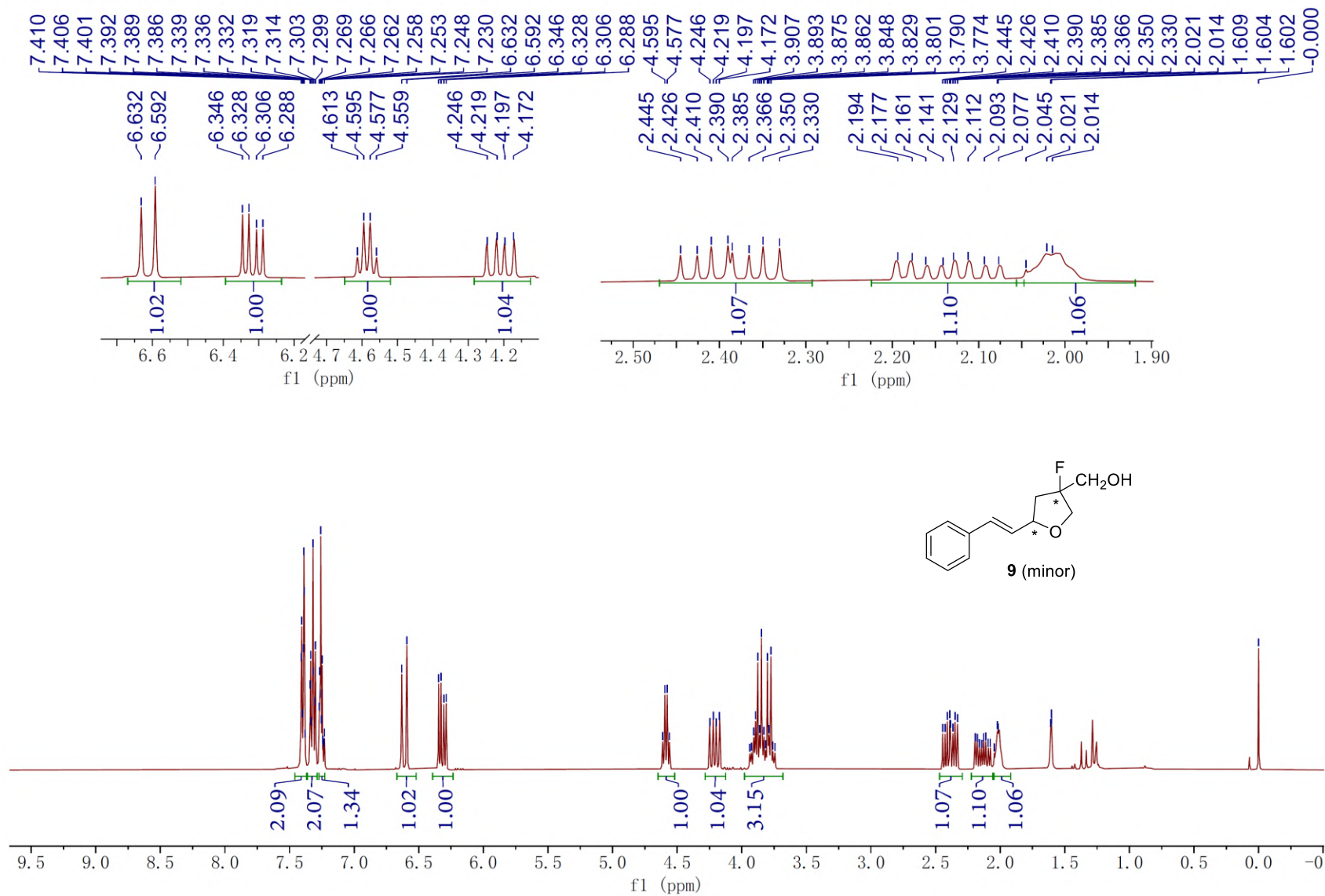
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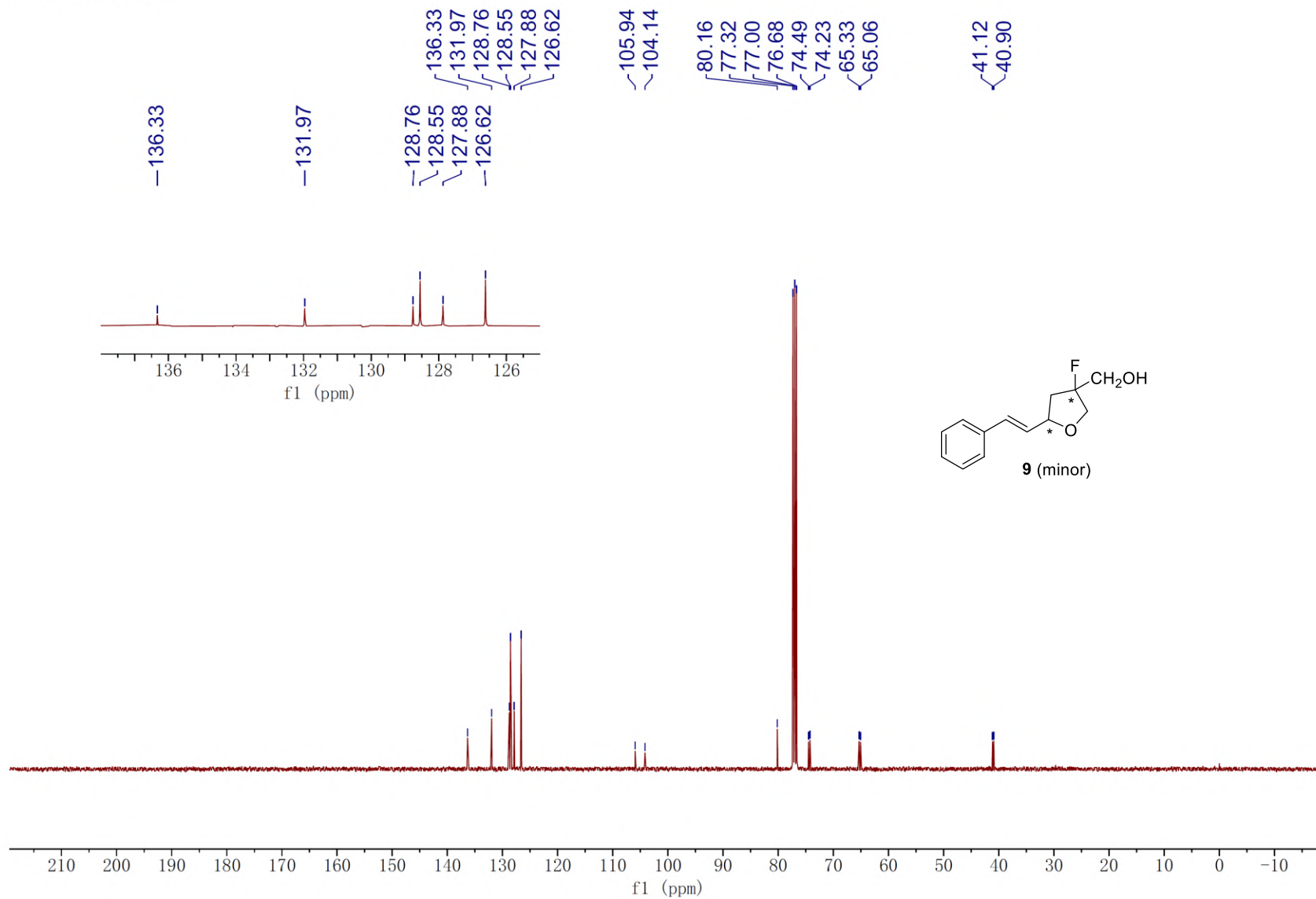
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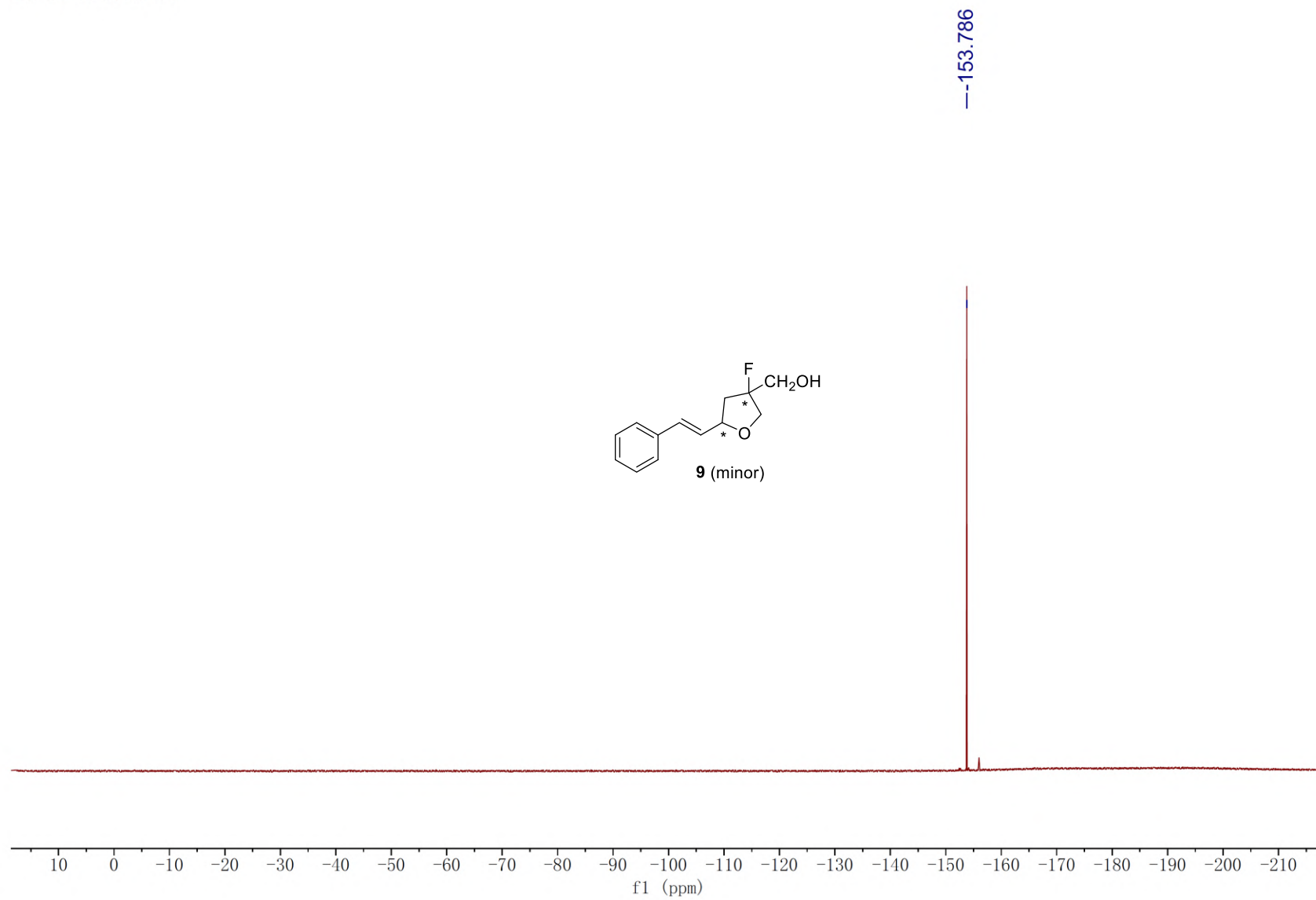
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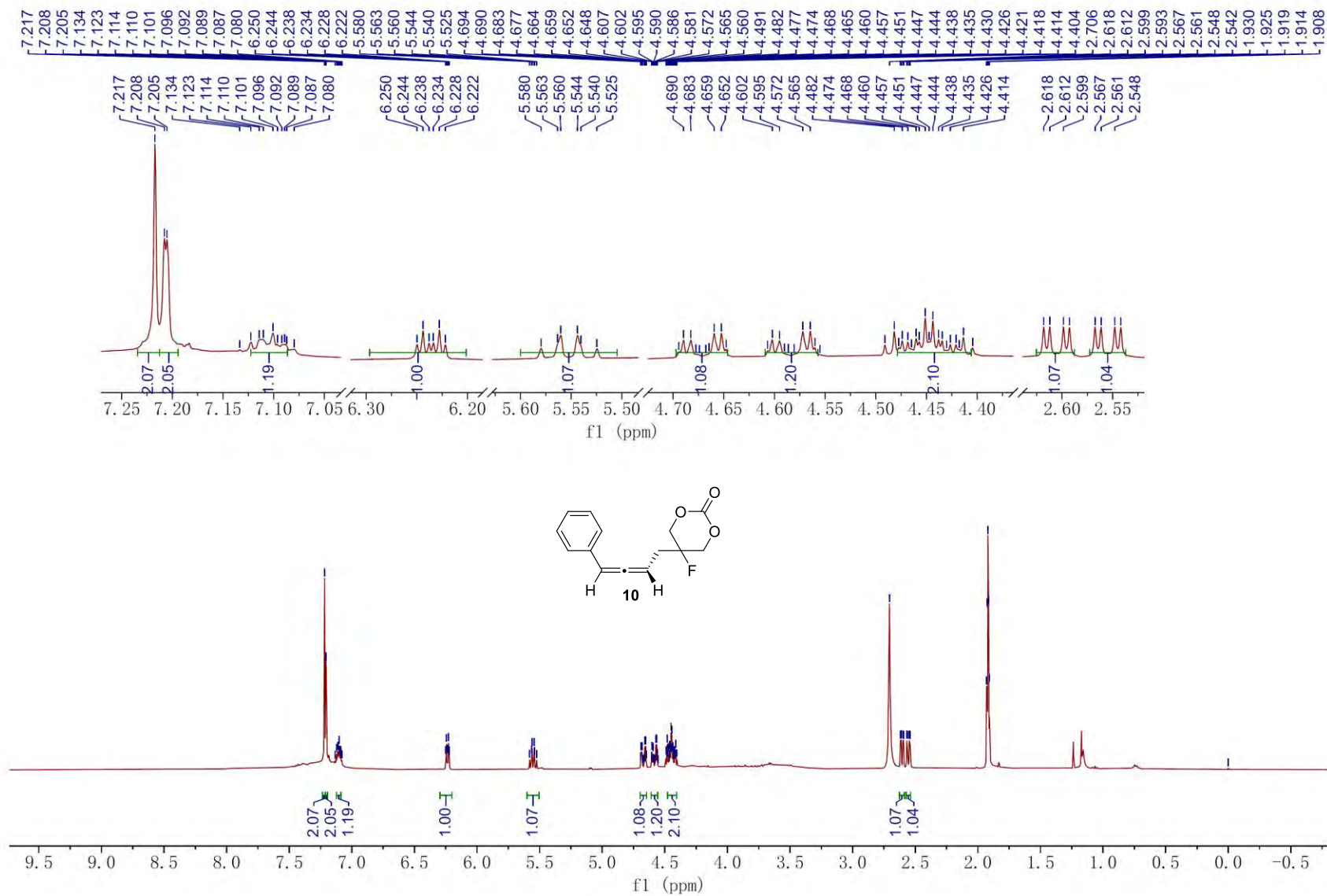
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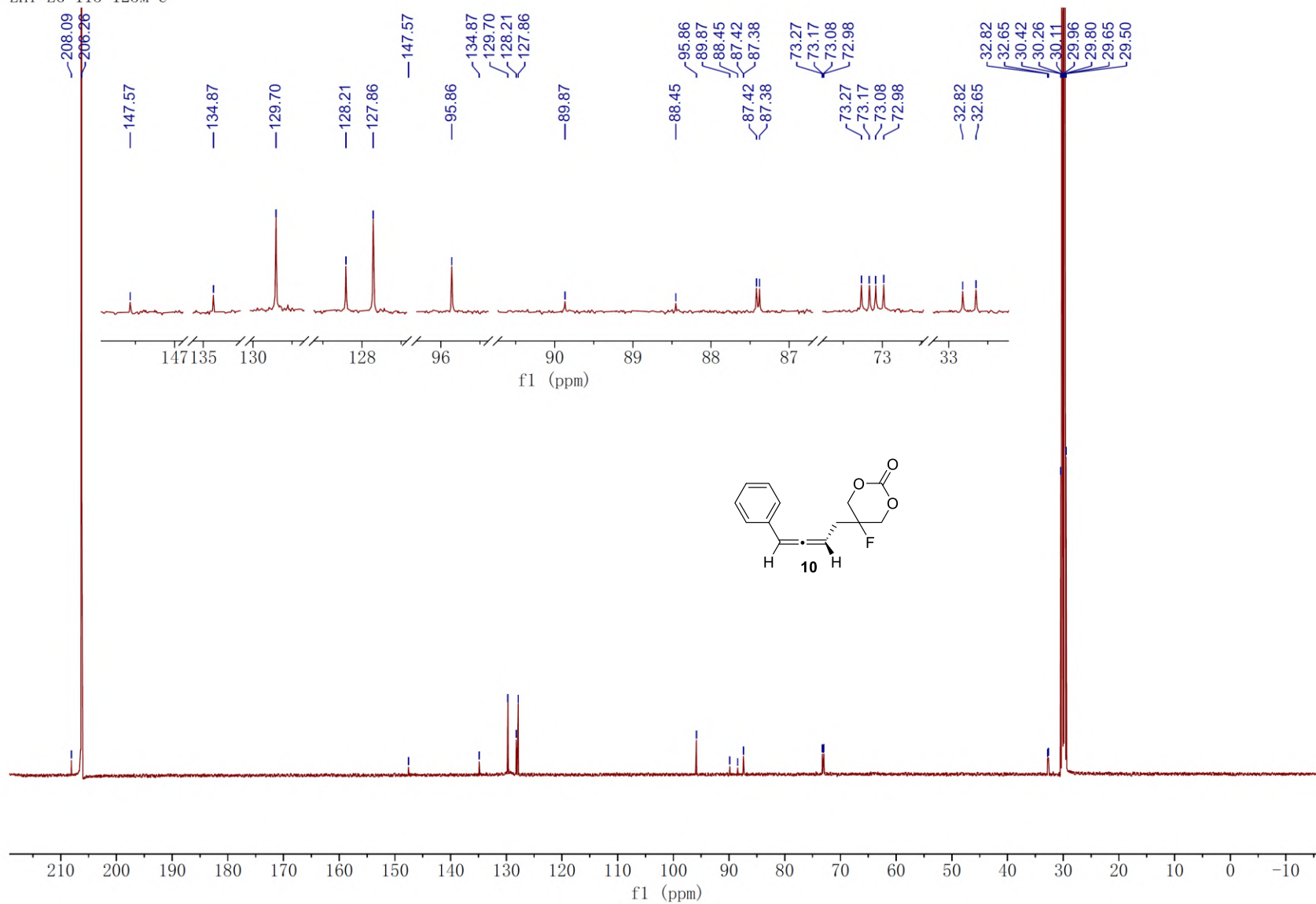
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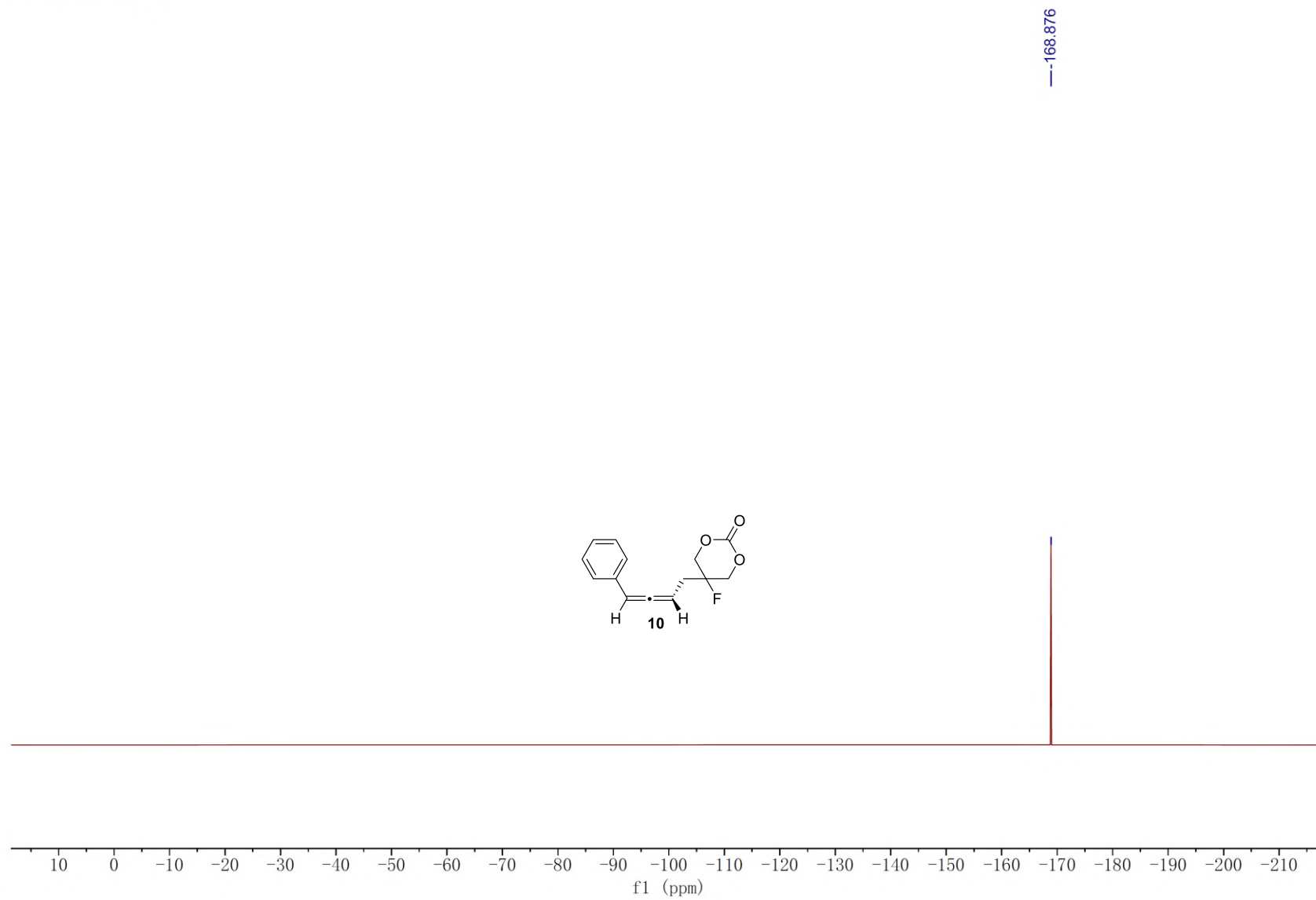
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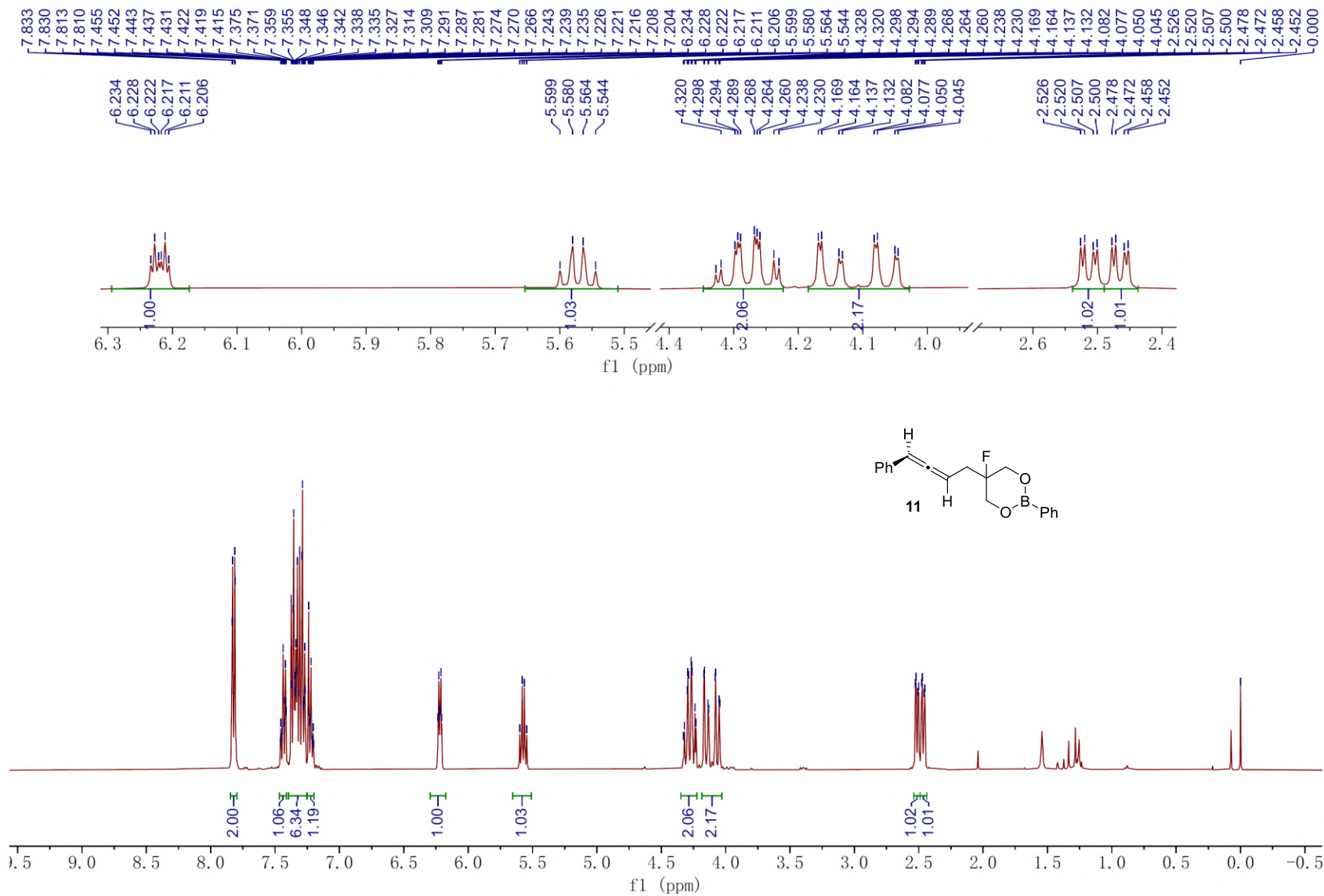
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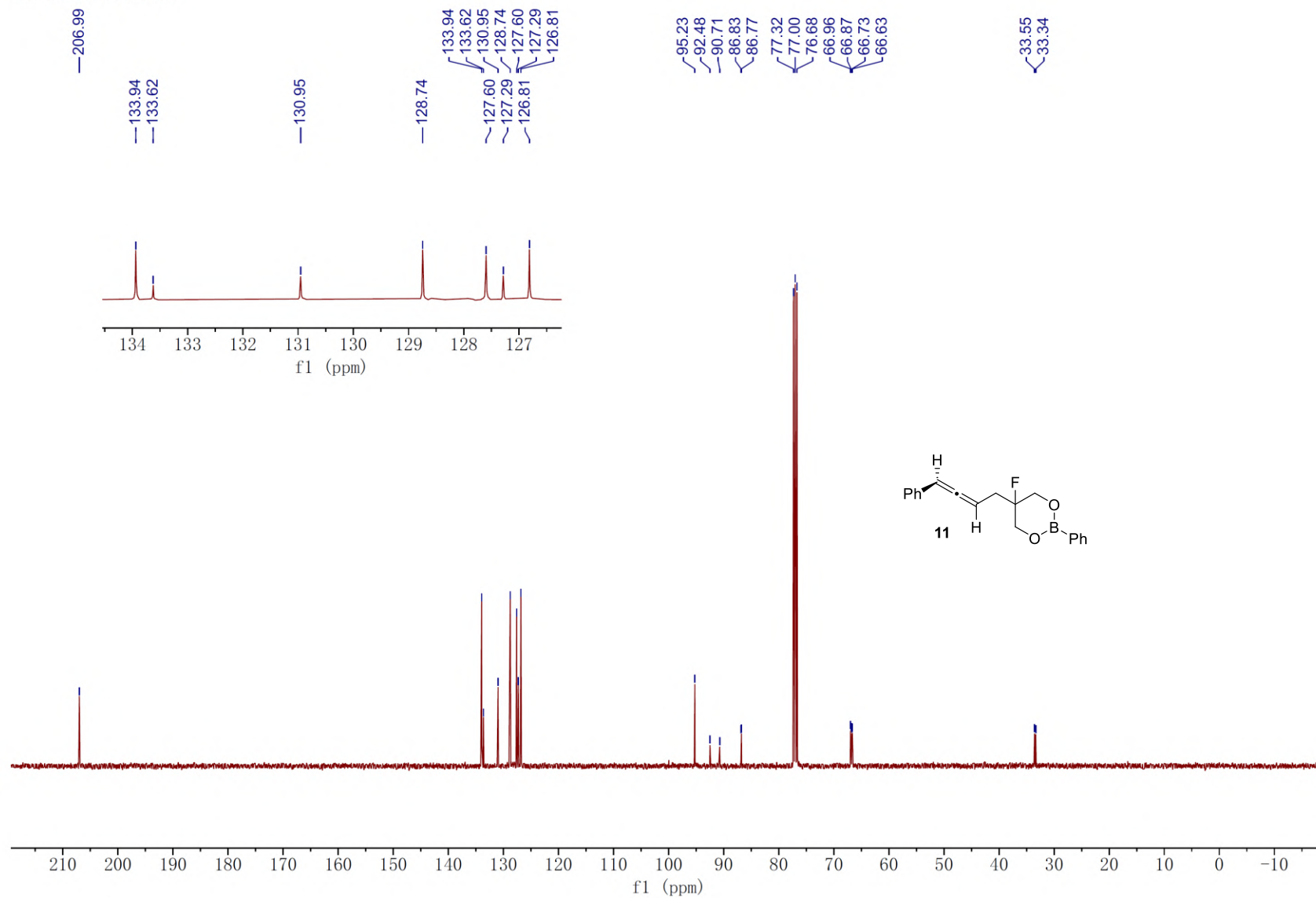
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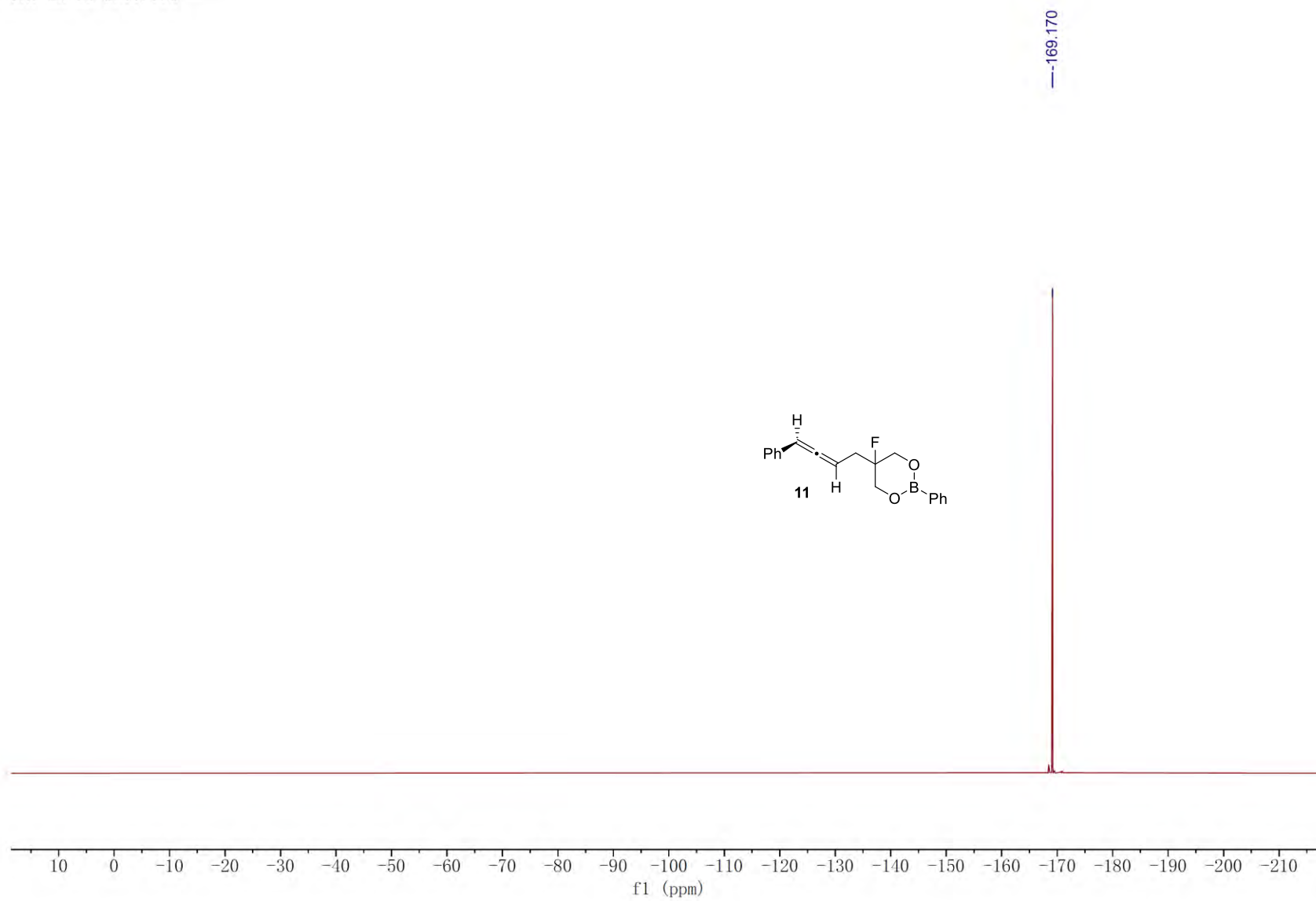
ZHY-ZH-36-C.10. fid —



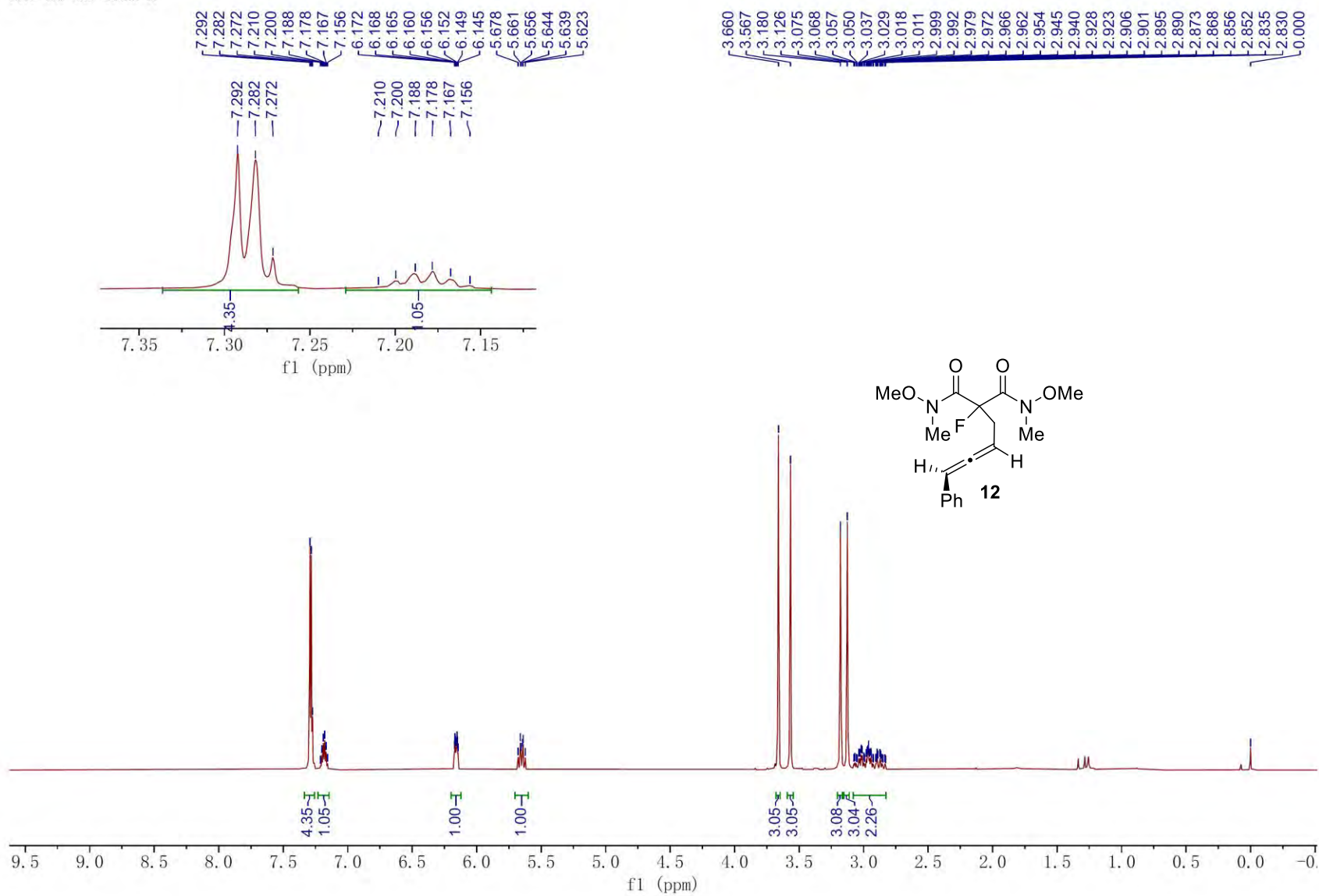
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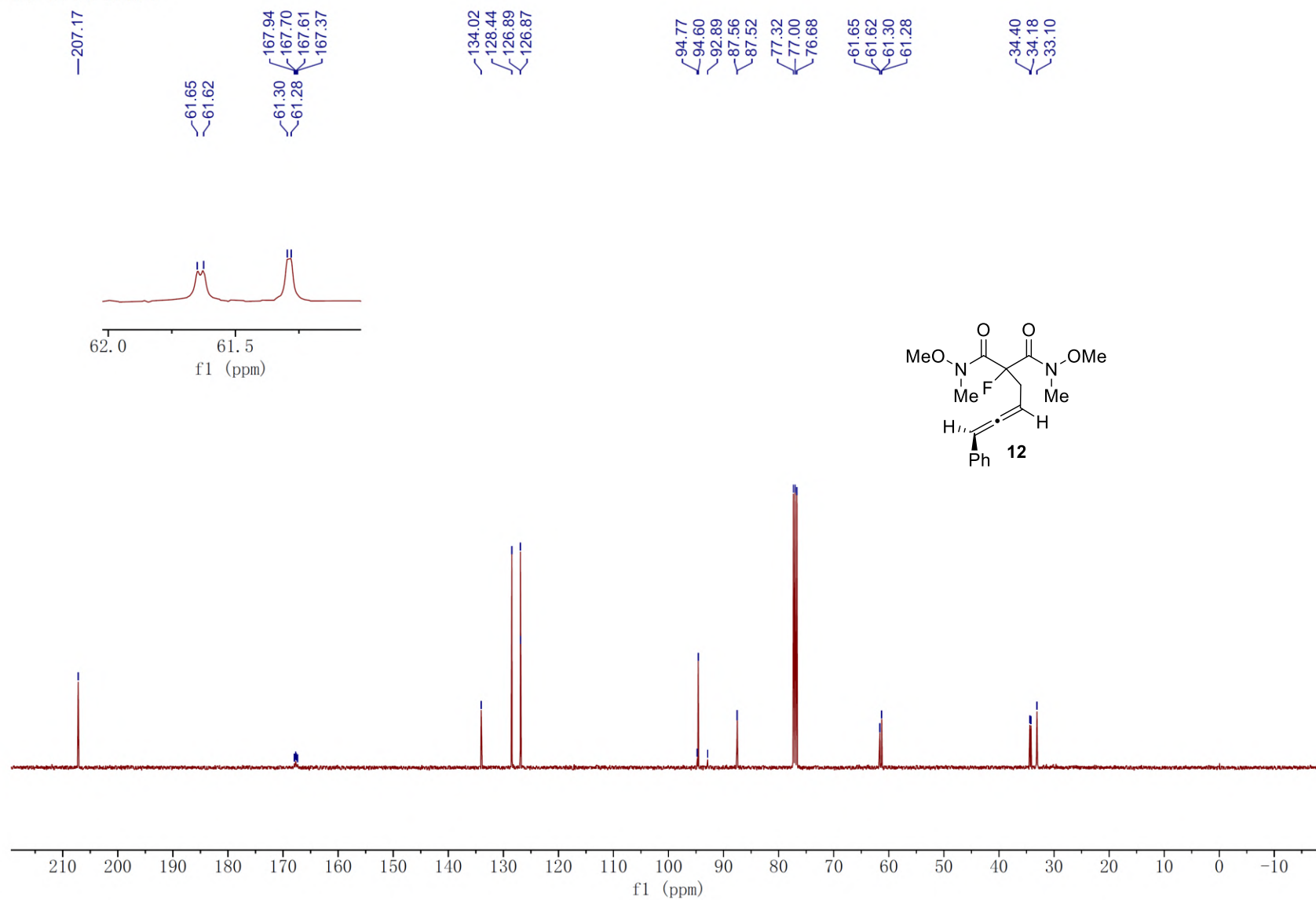
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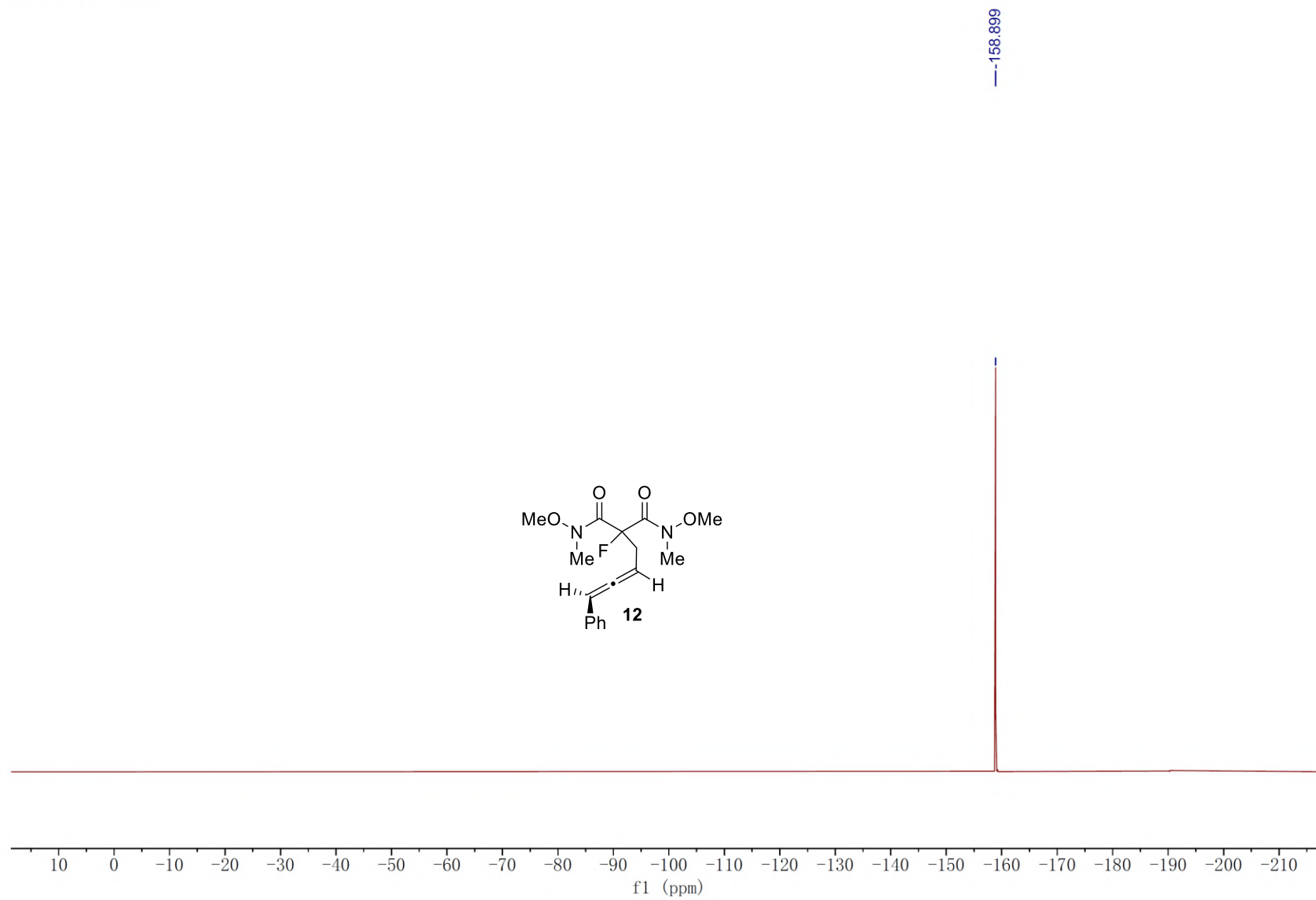
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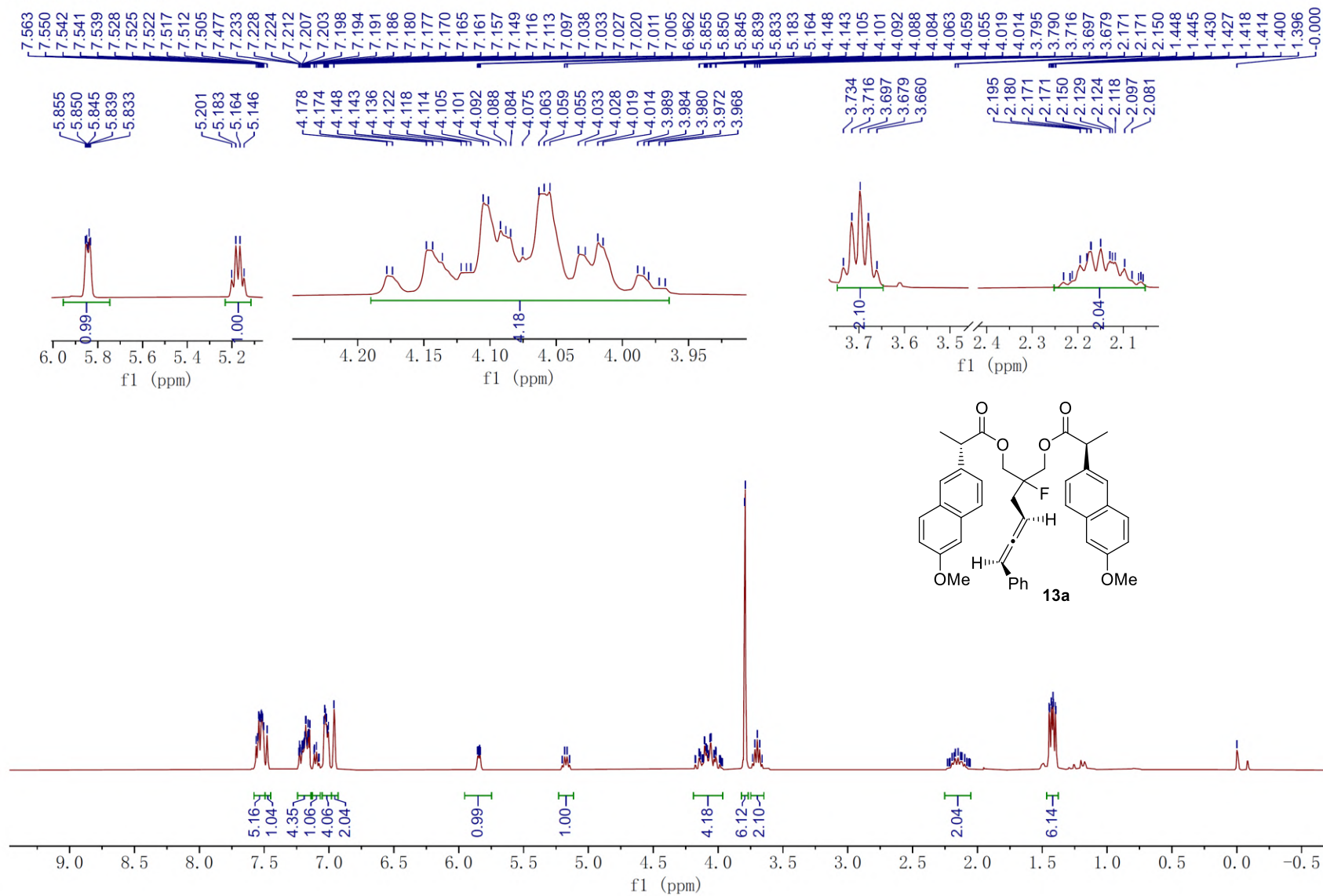
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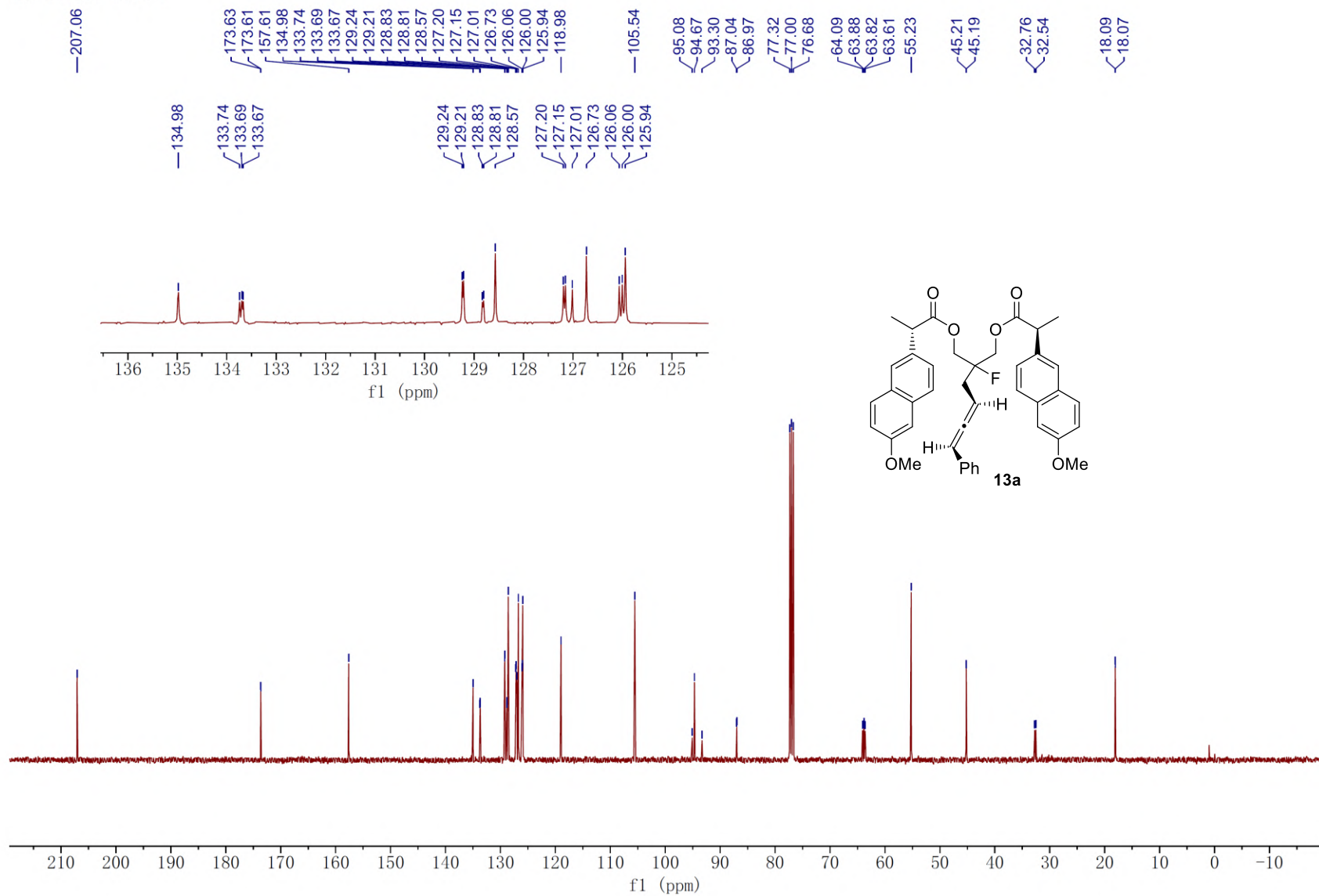
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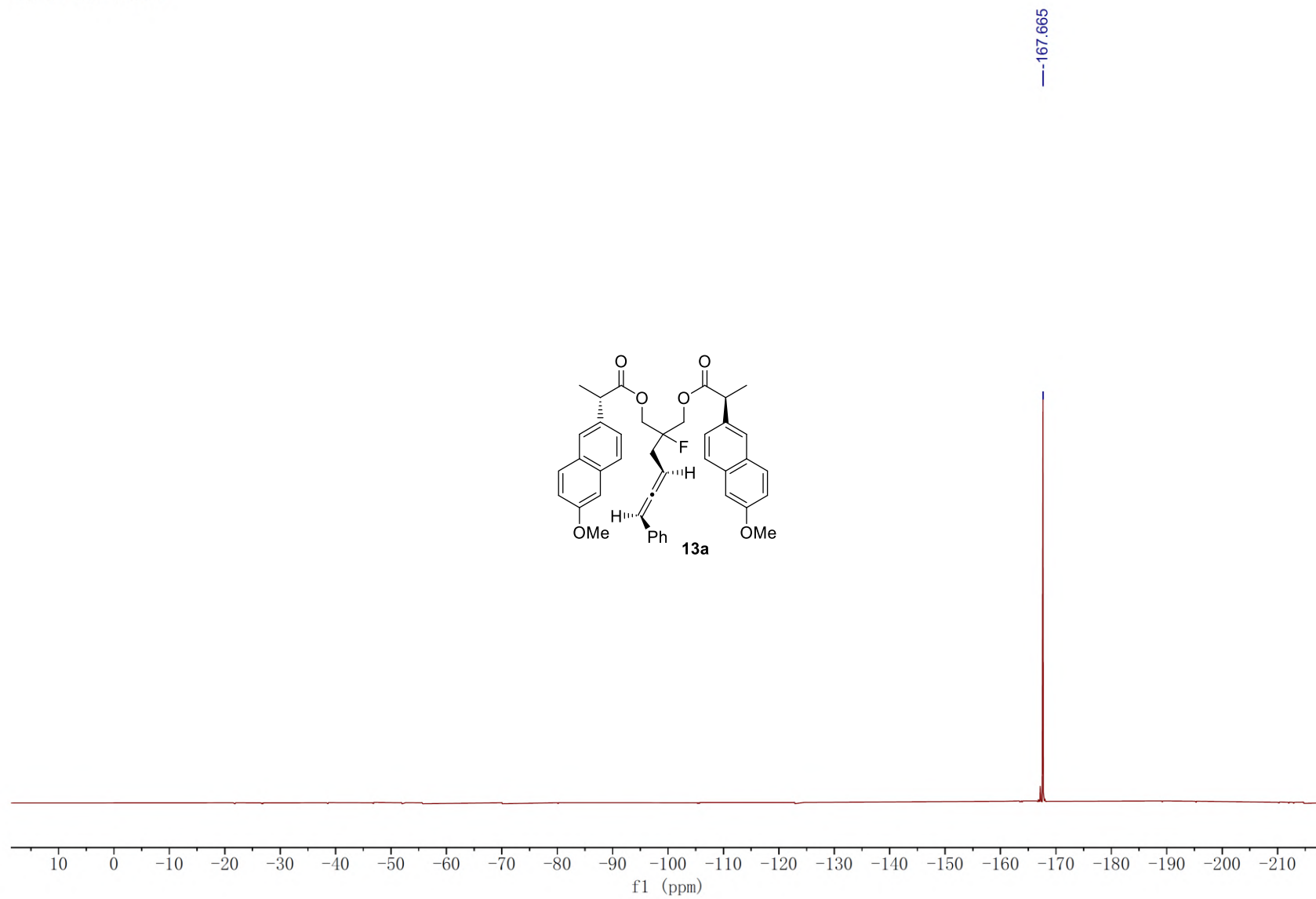
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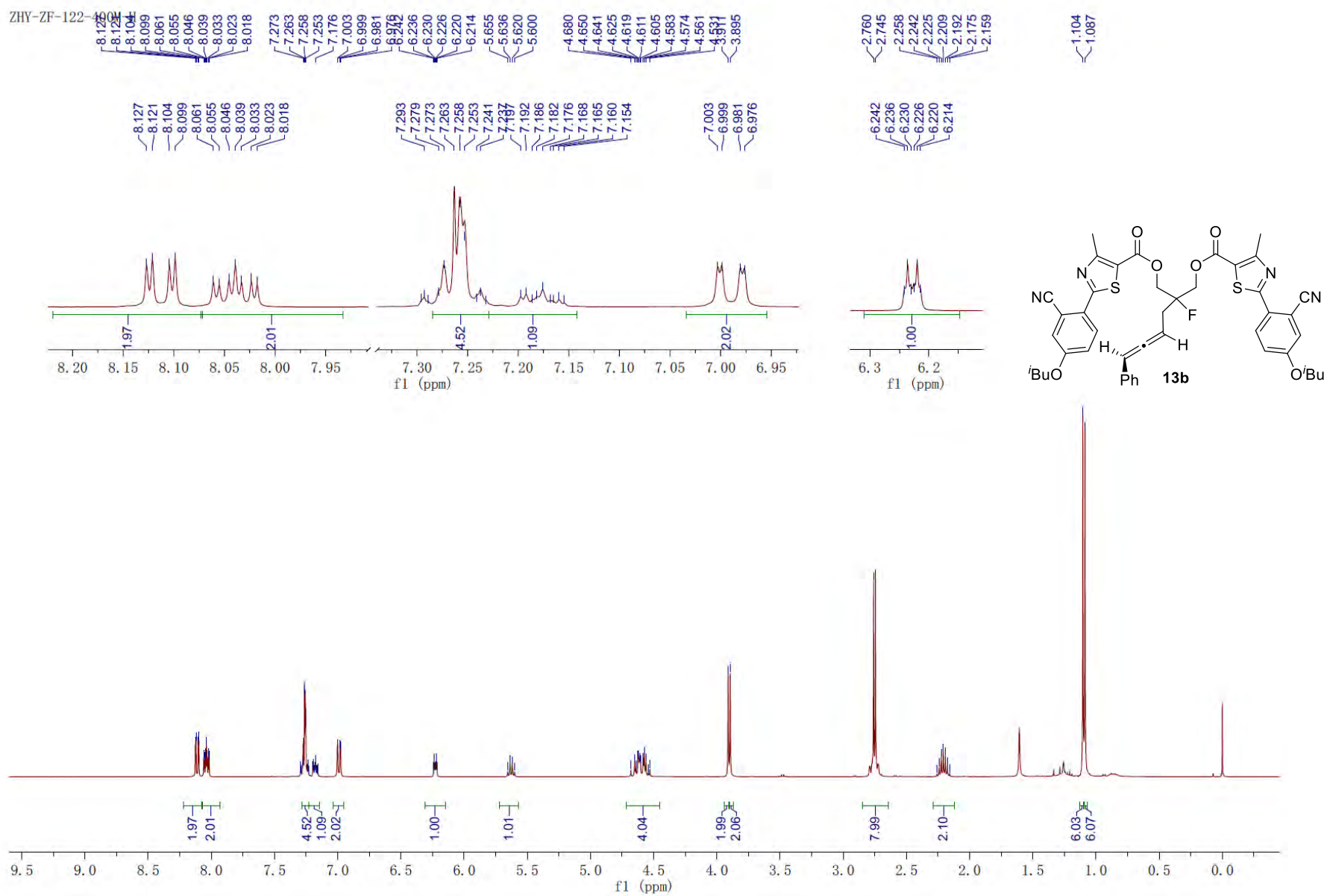
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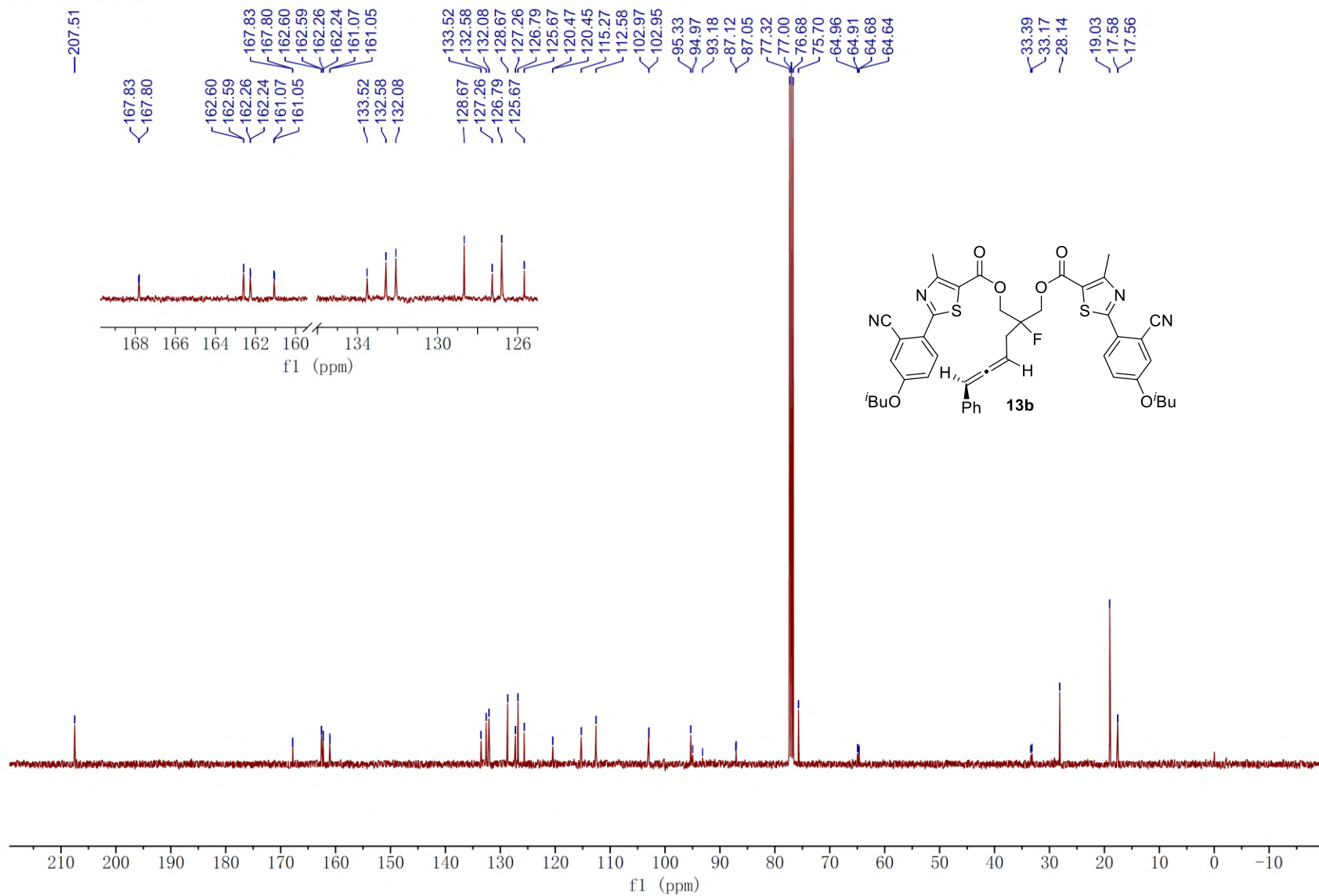
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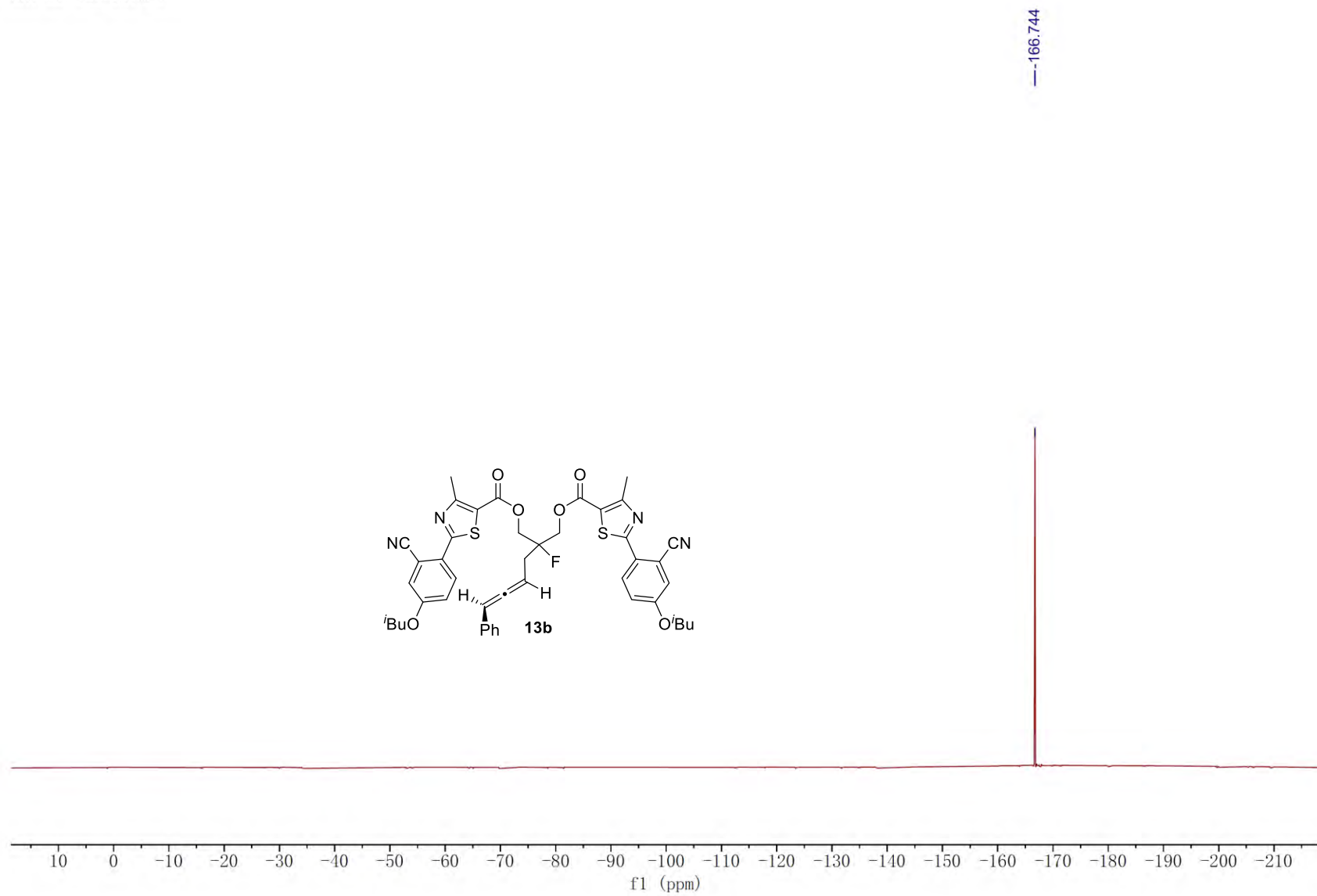
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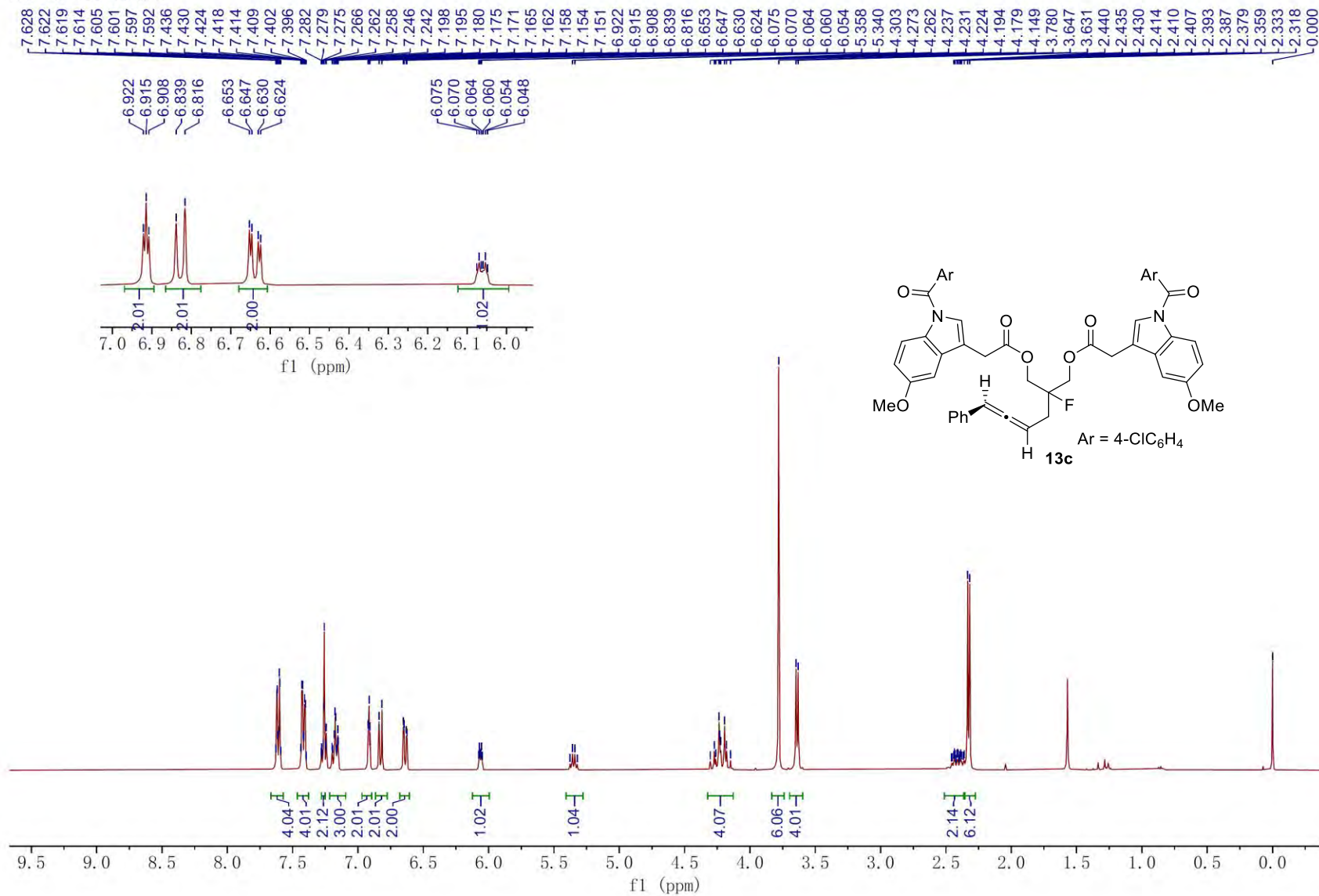
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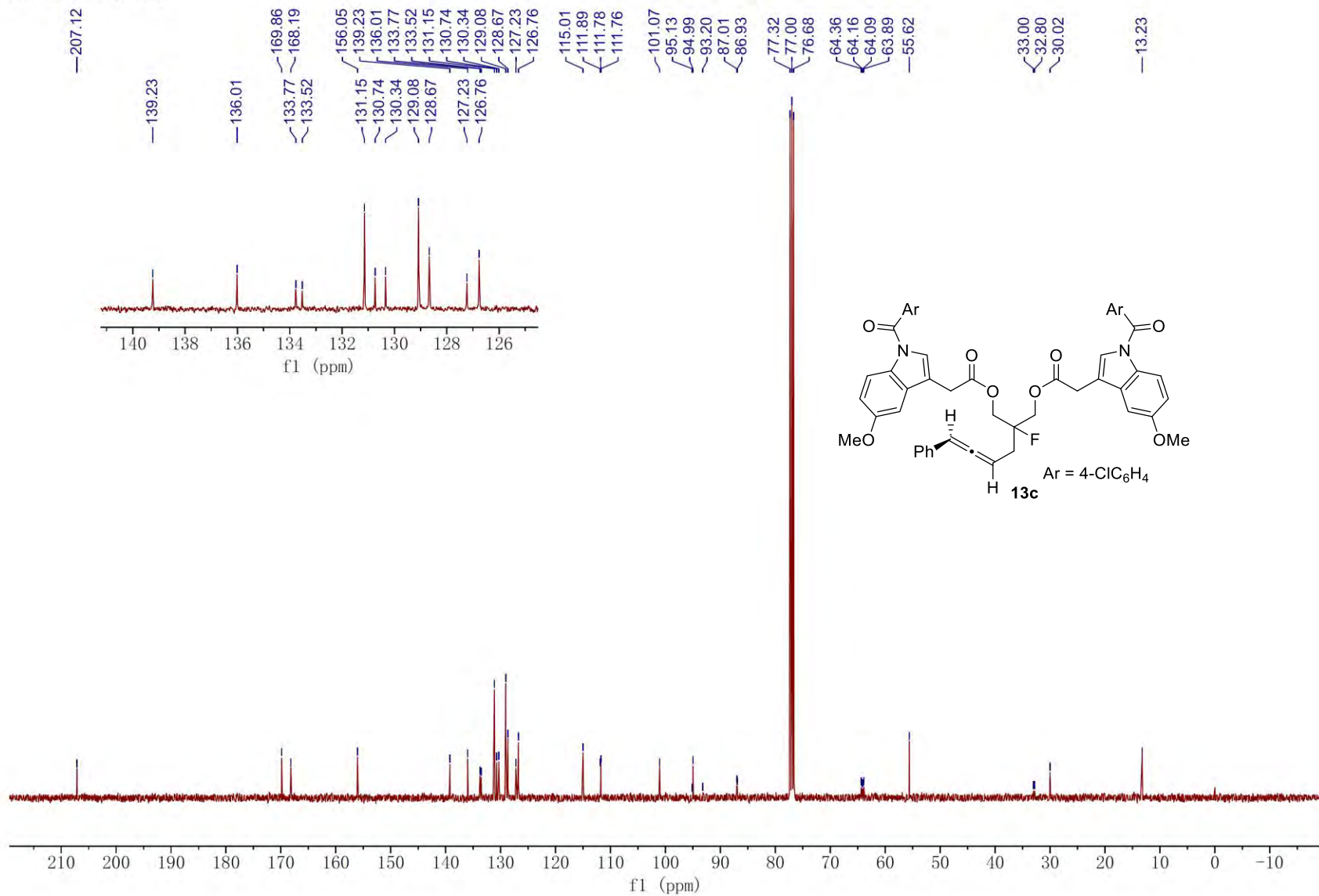
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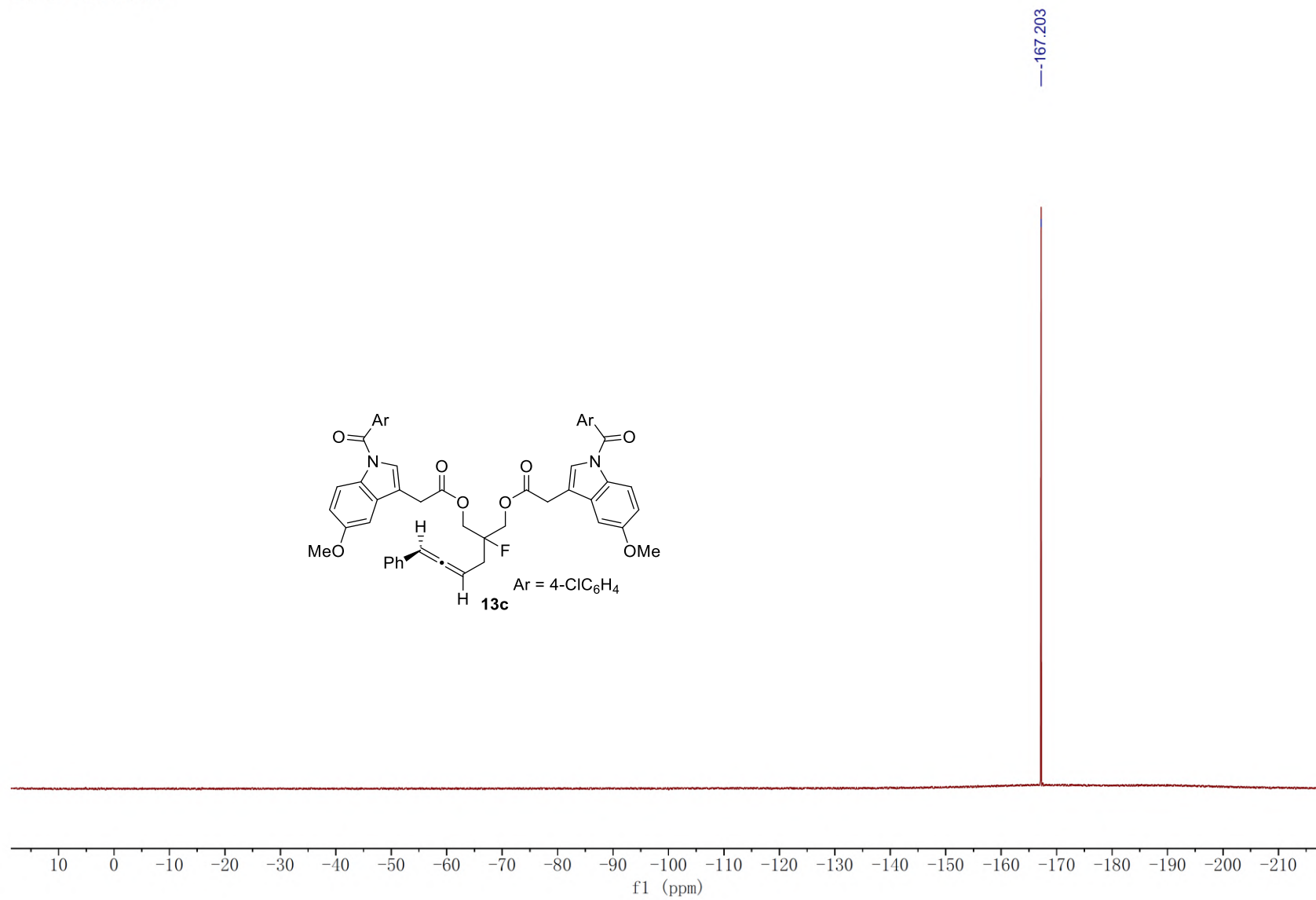
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ZHY-ZF-123-100M-C

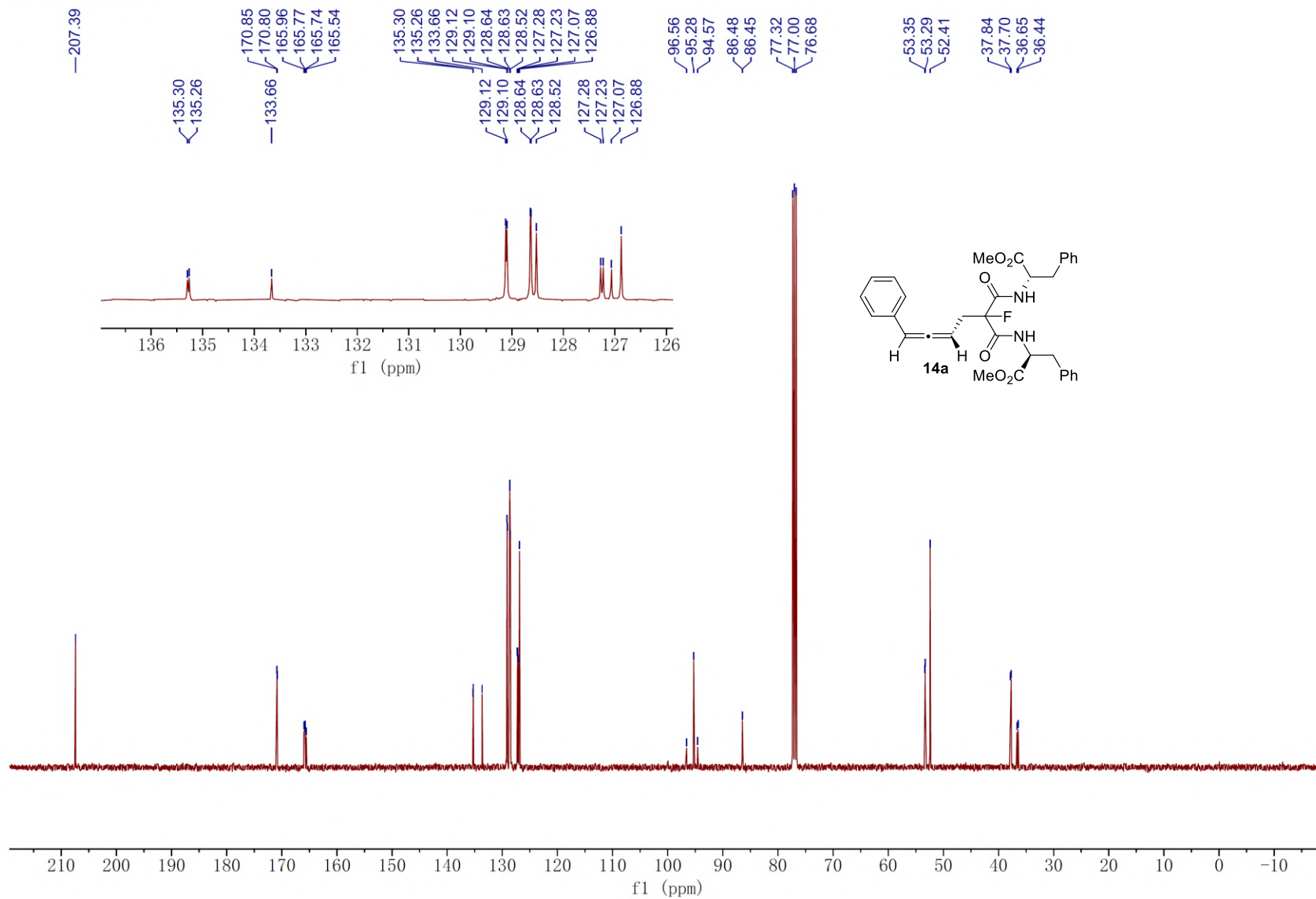


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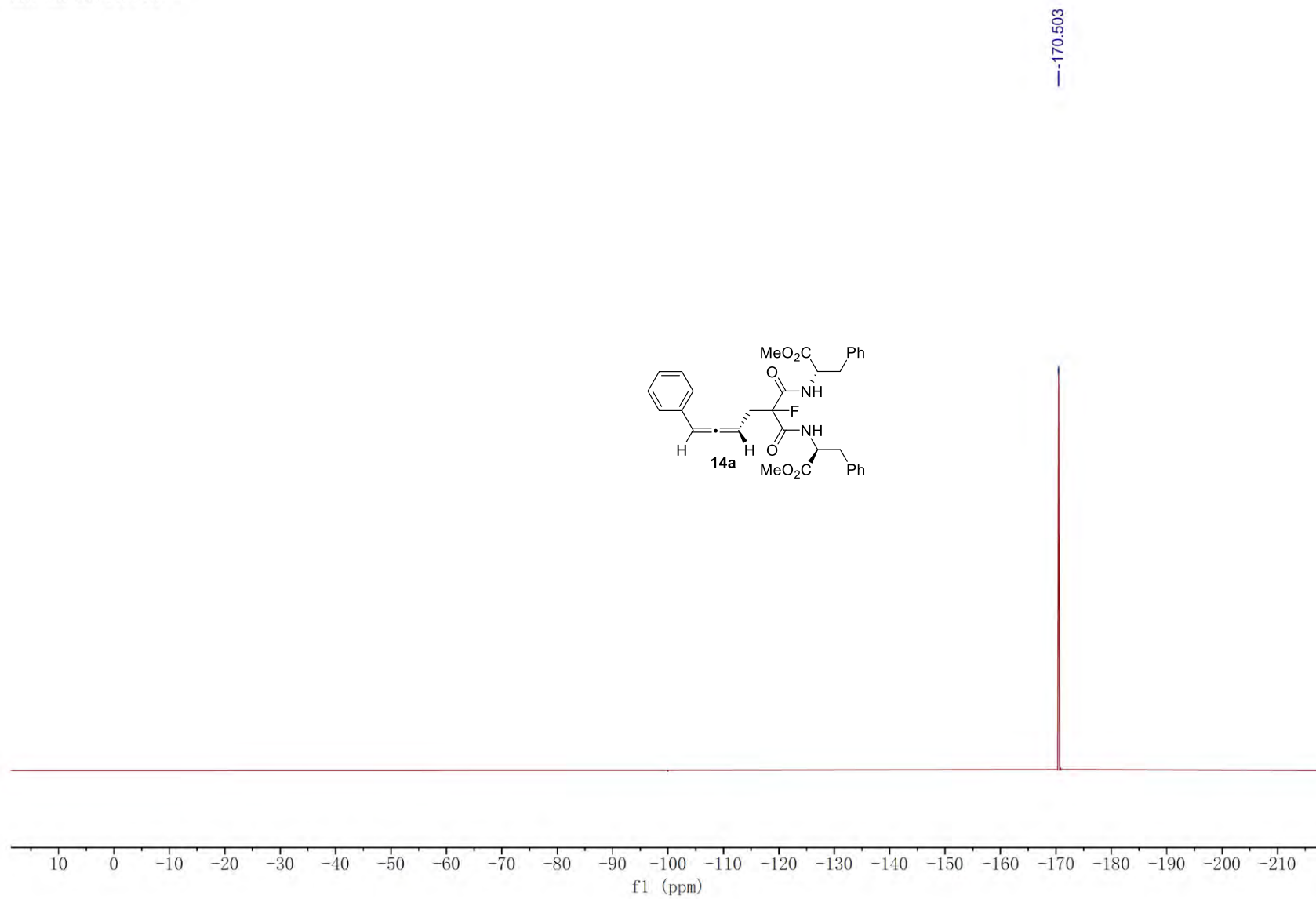


Chemical structure of **14a** is shown, featuring a central chiral core with two benzyl groups and a vinylic system.

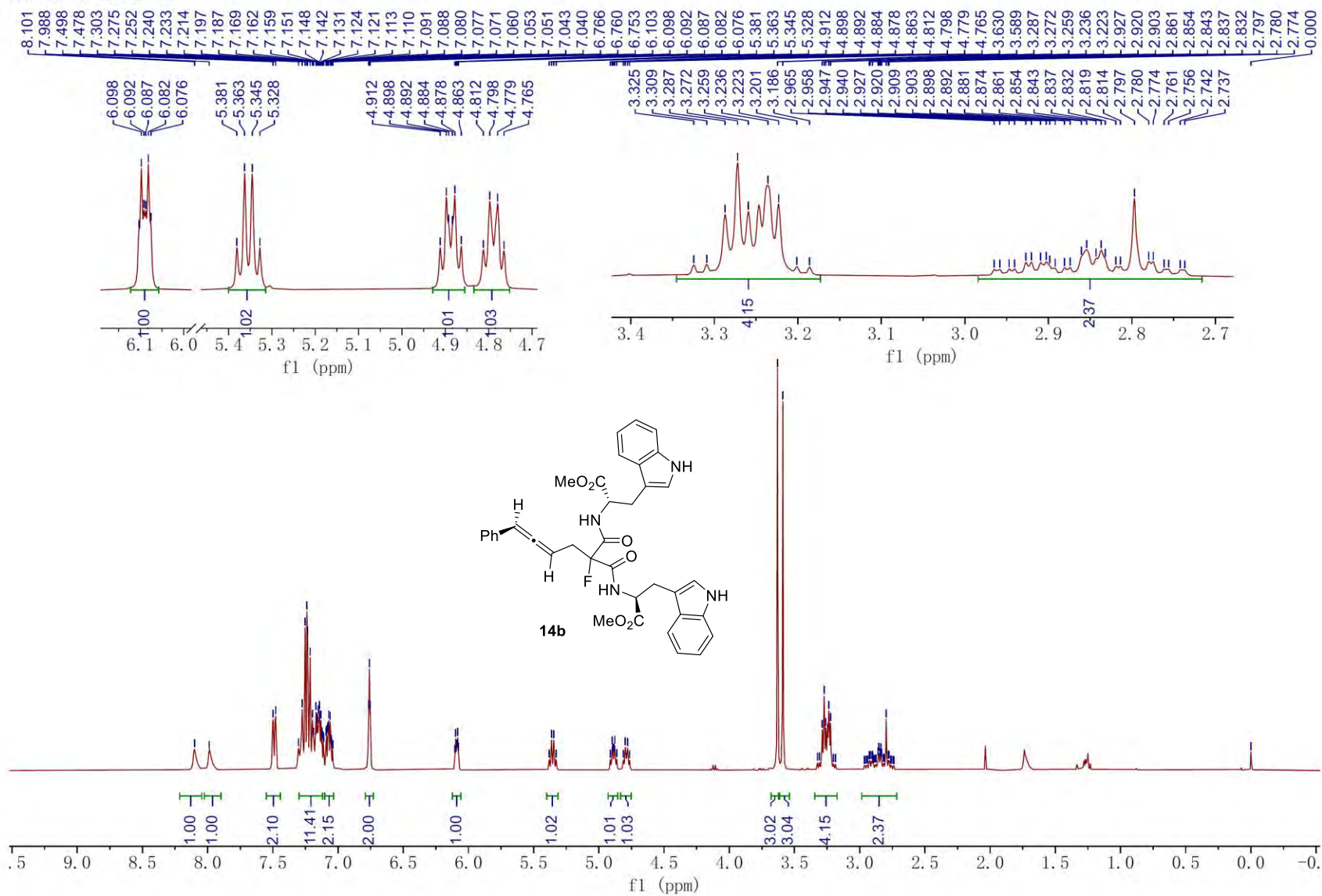
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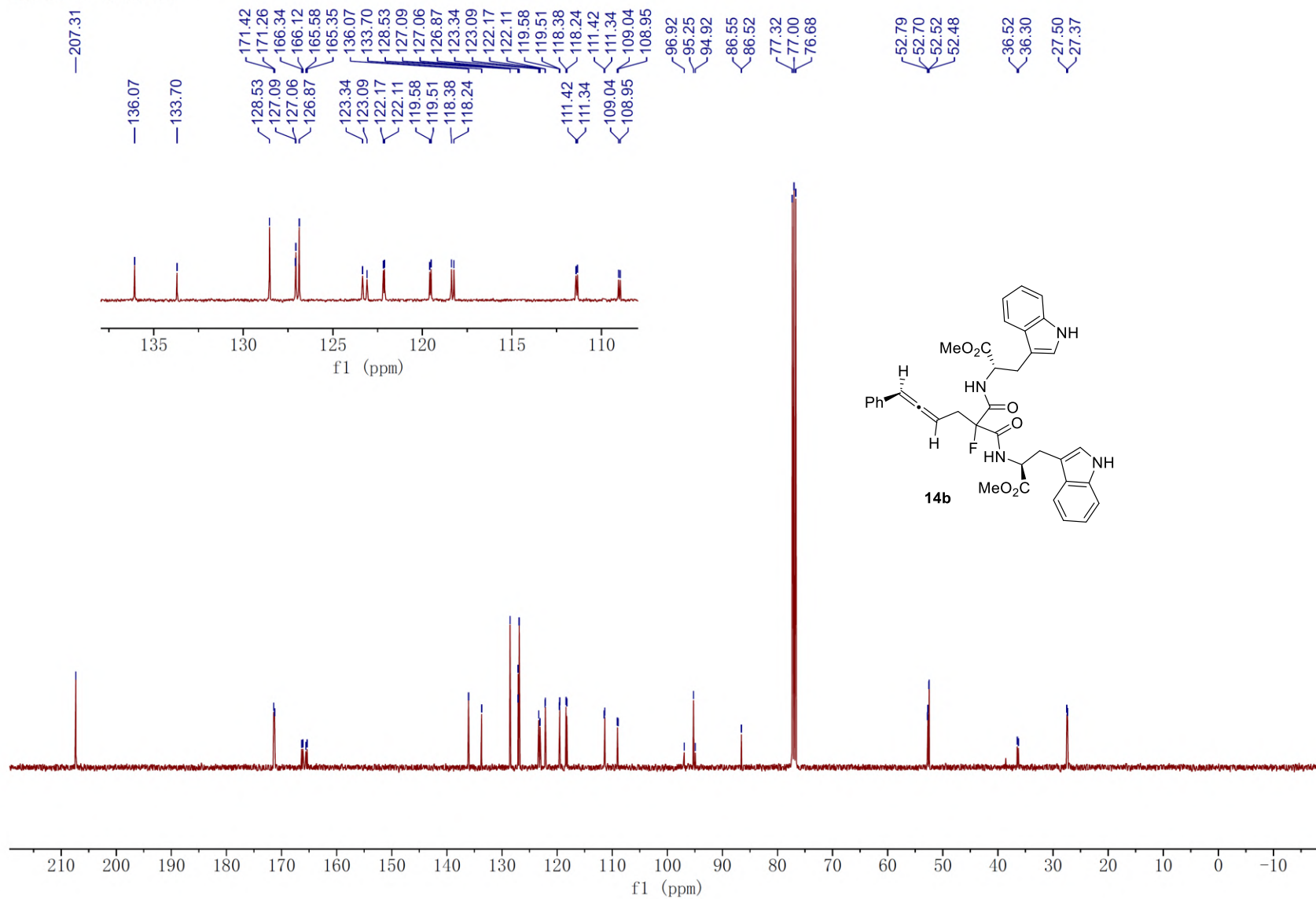
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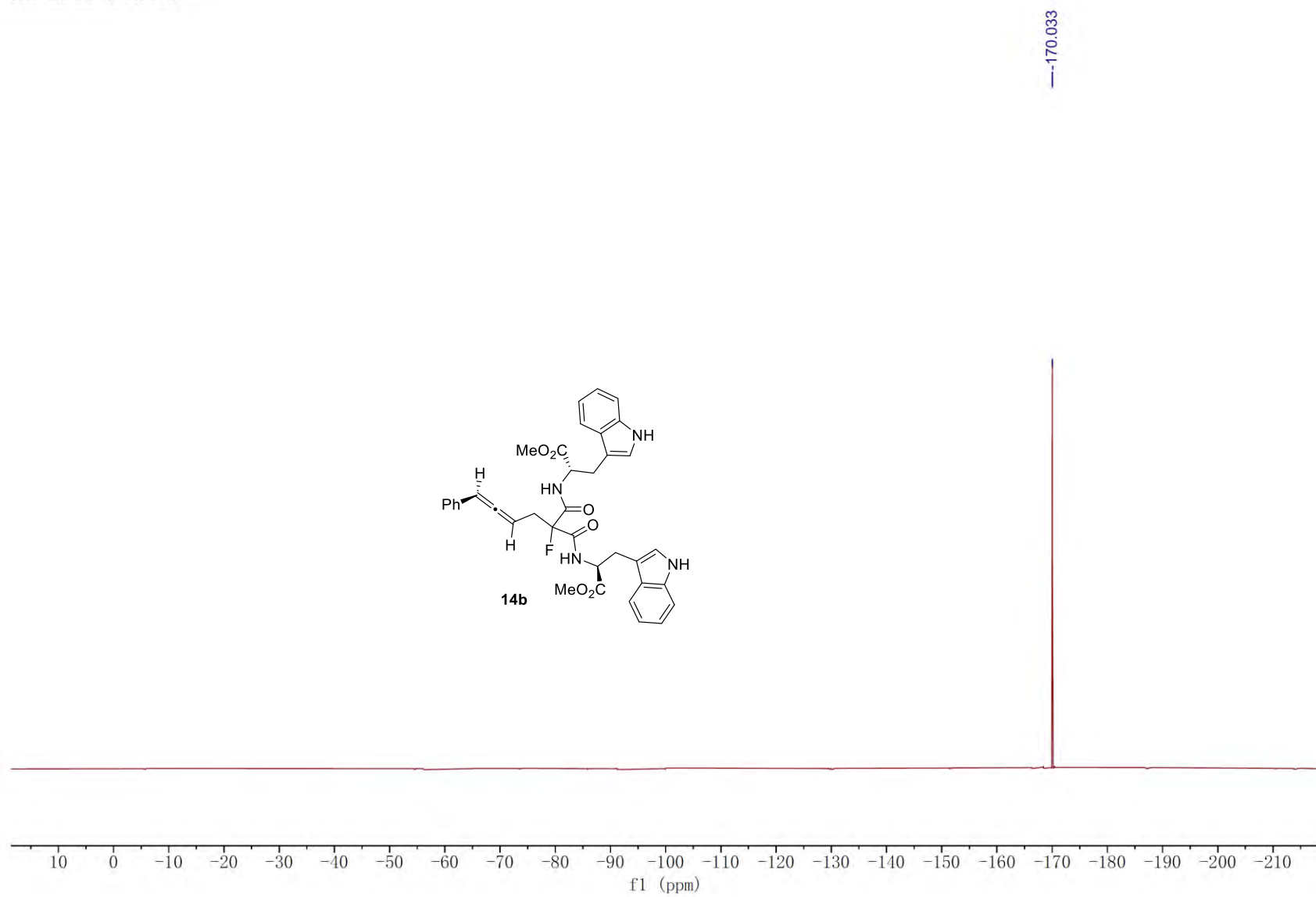
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ZHY-ZH-57-3. 12. fid —



ZHY-ZH-57-3. 11. fid —



10. HPLC spectra

3/30/2023 8:34:23 PM Page

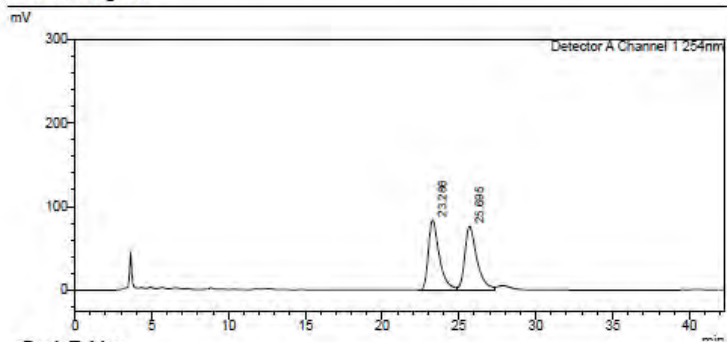
3/14/2023 9:56:56 PM Page 1

Analysis Report

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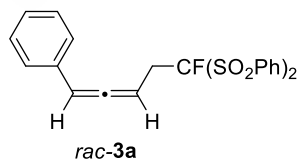
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 Data Filename : ZHY-ZH-19-RAC-ADH-80-20-1.0-254-230-1.lod
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
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 Date Processed : 3/14/2023 10:39:45 PM
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<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	23.288	4134953	83049	49.631
2	25.695	4196444	76110	50.369
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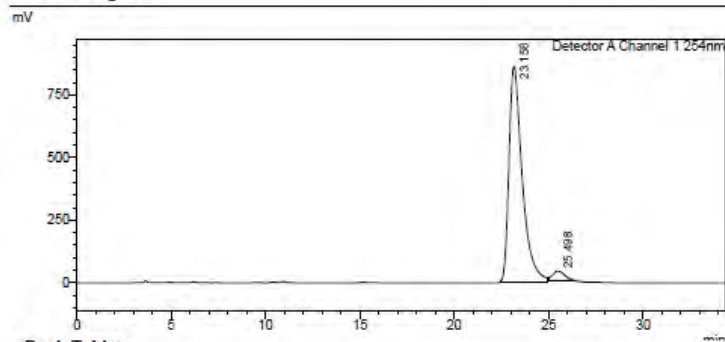
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Analysis Report

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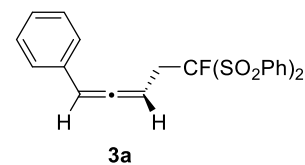
Sample Name : ZHY-ZH-19-ASY-ADH-80-20-1.0-254-230-1
 Sample ID :
 Data Filename : ZHY-ZH-19-ASY-ADH-80-20-1.0-254-230-1.lod
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
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 Date Processed : 3/14/2023 9:52:03 PM
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<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	23.158	41881899	860996	96.320
2	25.498	1599529	36555	3.680
Total		43481228	897551	



C:\data\ZHY\ZH\ZHY-ZH-19-ASY-ADH-80-20-1.0-254-230-1.l

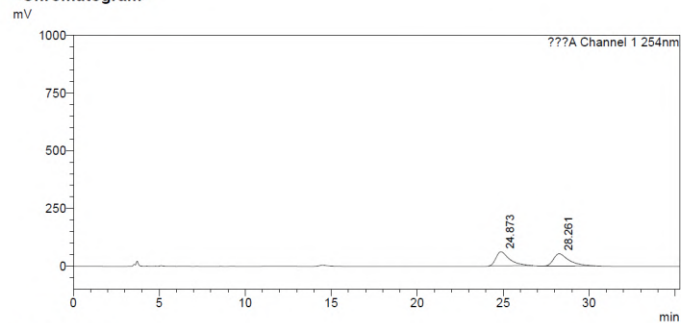


Analysis Report

<Sample Information>

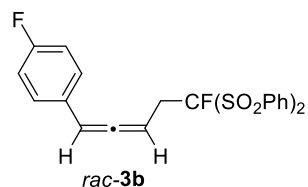
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 Sample ID :
 Data Filename : LHW-LB-7(F)-RAC-AD-H-80-20-254-230-1.0-1.lcd
 Method Filename : GY-1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
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<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	24.873	3348240	61064	50.151
2	28.261	3328021	53156	49.849
Total		6676261	114219	



F:\Data\LHW\LHW-LB-7(F)-RAC-AD-H-80-20-254-230-1.0-1.lcd

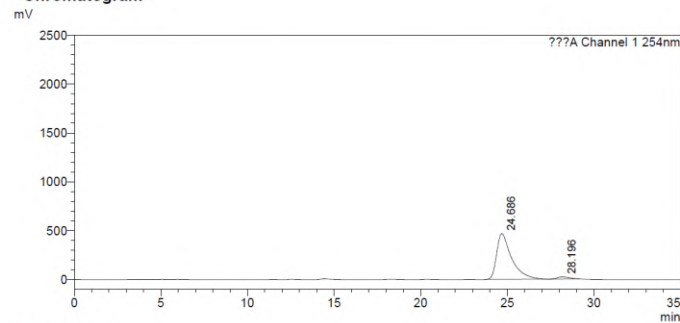


Analysis Report

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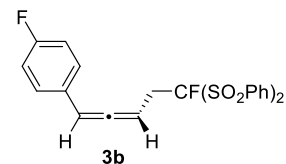
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 Method Filename : GY-1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
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<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	24.686	27904340	467530	96.366
2	28.196	1052241	21471	3.634
Total		28956581	489001	



F:\Data\LHW\LHW-LB-7(F)-ASY-AD-H-80-20-254-230-1.0-1.lcd

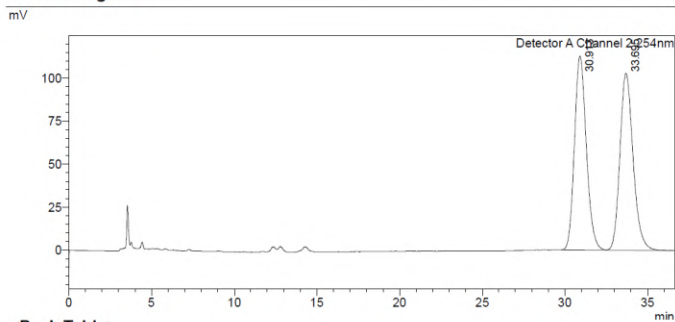
Analysis Report

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 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/11/10 8:57:32
 Date Processed : 2022/11/10 9:34:10

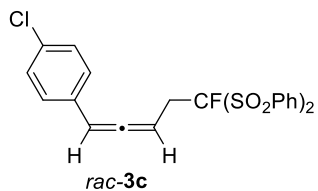
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 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	30.913	5635747	112730	49.723
2	33.695	5698475	102933	50.277
Total		11334222	215663	



D:\Data\ZHY\ZG\zhy-zg-49-rac-adh-80-20-1.0-254-2.lcd

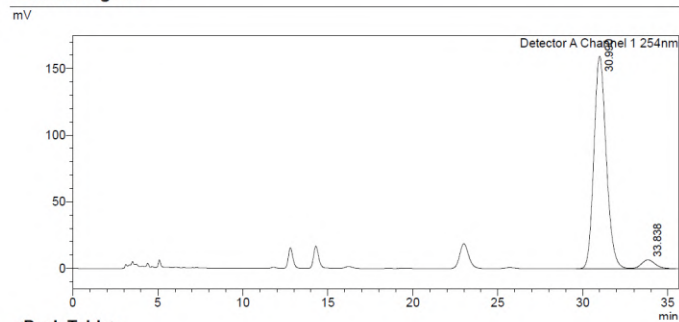
Analysis Report

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Sample Name : zhy-zg-49-asy-ash-80-20-1.0-254-2
 Sample ID :
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 Method Filename : xsl-230-254-1.0.lcm
 Batch Filename :
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 Injection Volume : 20 uL
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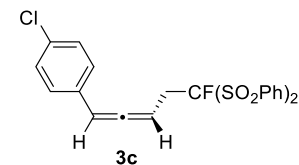
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 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	30.990	8055080	159694	95.677
2	33.838	363944	6599	4.323
Total		8419024	166294	



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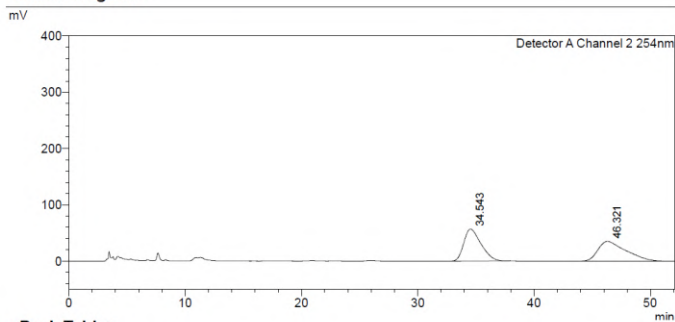
Analysis Report

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 Sample ID :
 Data Filename : zhy-zg-50-rac-ash-80-20-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
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 Injection Volume : 10 uL
 Date Acquired : 2023/1/10 22:07:15
 Date Processed : 2023/1/18 15:08:10

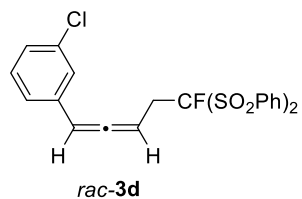
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<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	34.543	5859334	57035	49.998
2	46.321	5859842	34956	50.002
Total		11719176	91991	



D:\Data\ZHY\ZG\zhy-zg-50-rac-ash-80-20-1.0-254-230-1.lcd

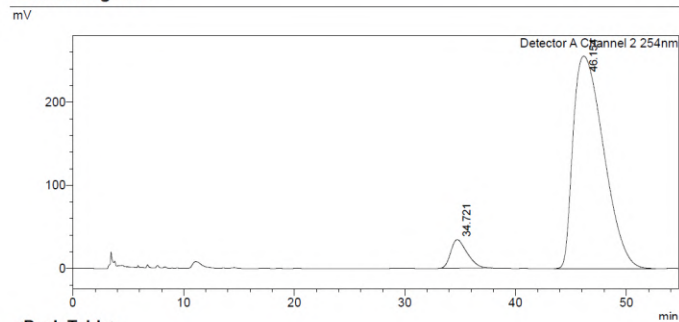
Analysis Report

<Sample Information>

Sample Name : zhy-zg-50-asy-adh-80-20-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zg-50-asy-ash-80-20-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 10 uL
 Date Acquired : 2023/1/10 23:00:22
 Date Processed : 2023/1/10 23:55:04

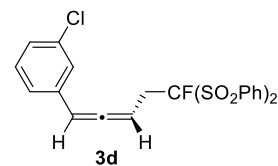
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 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	34.721	3535327	34467	6.721
2	46.154	49065733	255679	93.279
Total		52601060	290146	



D:\Data\ZHY\ZG\zhy-zg-50-asy-ash-80-20-1.0-254-230-1.lcd

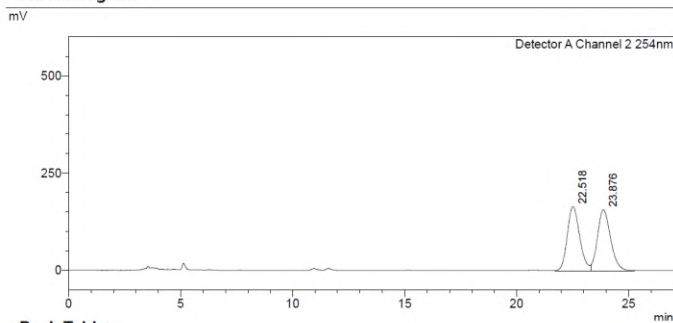
Analysis Report

<Sample Information>

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 Sample ID :
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 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/11/5 11:40:24
 Date Processed : 2023/1/18 15:04:45

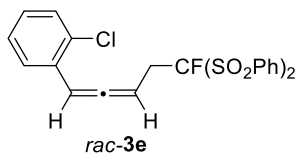
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 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	22.518	6396840	165828	49.839
2	23.876	6438181	157547	50.161
Total		12835021	323374	



D:\Data\ZHY\ZG\zhy-zg-43-2-rac-adh-85-15-1.0-254-2.lcd

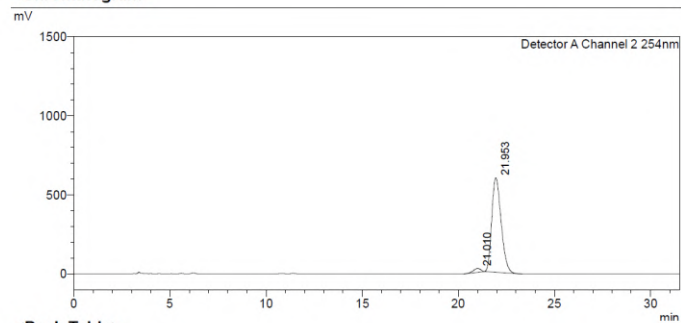
Analysis Report

<Sample Information>

Sample Name : zhy-zg-37-asy-adh-85-15-1.0-254-2
 Sample ID :
 Data Filename : zhy-zg-37-asy-adh-85-15-1.0-254-11.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/11/3 20:01:34
 Date Processed : 2023/1/18 15:05:03

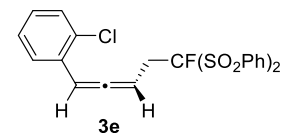
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	21.010	640275	23869	3.060
2	21.953	20286936	598284	96.940
Total		20927210	622154	



D:\Data\ZHY\ZG\zhy-zg-37-asy-adh-85-15-1.0-254-11.lcd

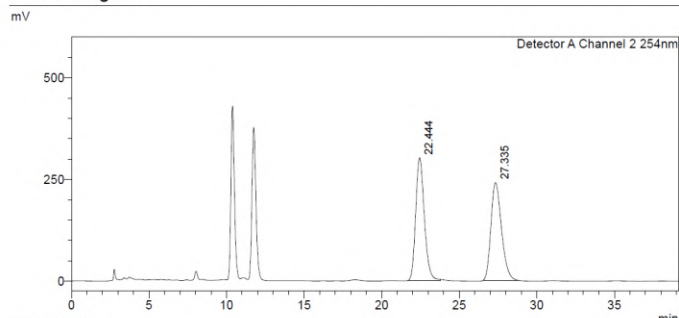
Analysis Report

<Sample Information>

Sample Name : ZHY-ZG-52-rac-adh-80-20-1.0-254-230-2
 Sample ID :
 Data Filename : ZHY-ZG-52-rac-adh-80-20-1.0-254-230-2.lcd
 Method Filename : 1.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 1 uL
 Date Acquired : 1/18/2023 4:23:28 PM
 Date Processed : 1/18/2023 5:02:39 PM

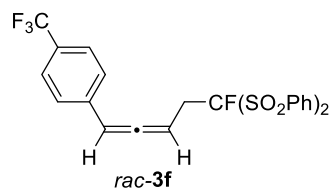
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	22.444	11724720	302515	50.495
2	27.335	11494849	241478	49.505
Total		23219569	543992	



C:\data\ZHY\ZHY-ZG-52-rac-adh-80-20-1.0-254-230-2.lcd

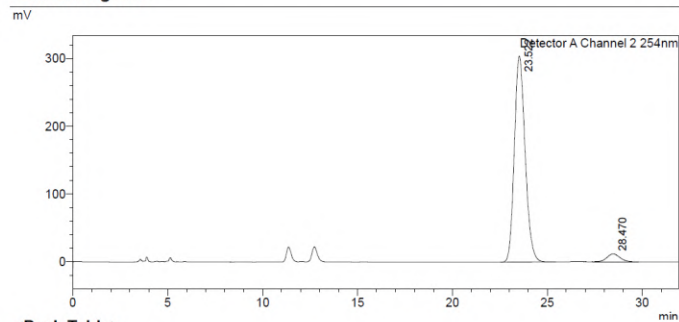
Analysis Report

<Sample Information>

Sample Name : zhy-zg-29-1-asy-adh-80-20-1.0-254-1
 Sample ID :
 Data Filename : zhy-zg-29-1-asy-adh-80-20-1.0-254-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/10/27 9:48:59
 Date Processed : 2022/10/27 10:20:55

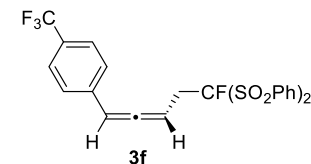
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	23.522	12032646	304368	95.604
2	28.470	553299	11649	4.396
Total		12585945	316017	



D:\Data\ZHY\ZG\zhy-zg-29-1-asy-adh-80-20-1.0-254-1.lcd

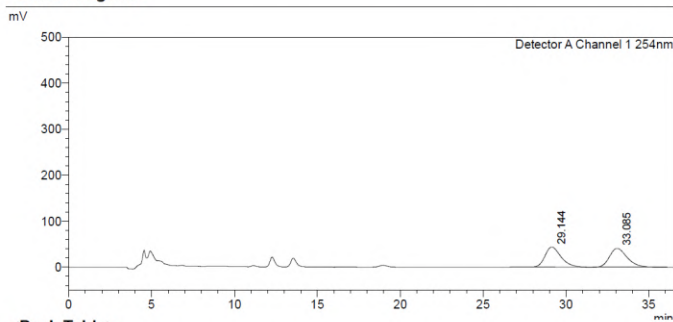
Analysis Report

<Sample Information>

Sample Name : zhy-zg-66-rac-adh-50-50-0.8-254-230-1
 Sample ID :
 Data Filename : zhy-zg-66-rac-adh-50-50-0.8-254-230-3.lcd
 Method Filename : 202209025.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/11/19 10:36:54
 Date Processed : 2023/1/18 16:36:34

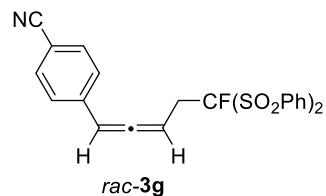
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	29.144	2929456	43682	49.089
2	33.085	3038153	41010	50.911
Total		5967609	84691	



D:\Data\ZHY\ZG\zhy-zg-66-rac-adh-50-50-0.8-254-230-3.lcd

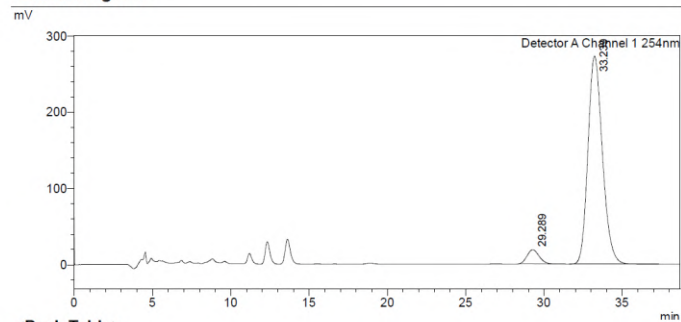
Analysis Report

<Sample Information>

Sample Name : zhy-zg-66-asy-adh-50-50-0.8-254-230-1
 Sample ID :
 Data Filename : zhy-zg-66-asy-adh-50-50-0.8-254-230-2.lcd
 Method Filename : 202209025.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/11/19 9:57:49
 Date Processed : 2022/11/19 12:17:22

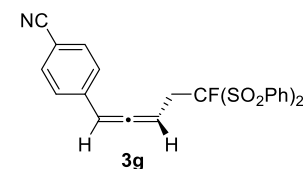
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	29.289	947858	18254	5.118
2	33.239	17572304	272827	94.882
Total		18520162	291081	



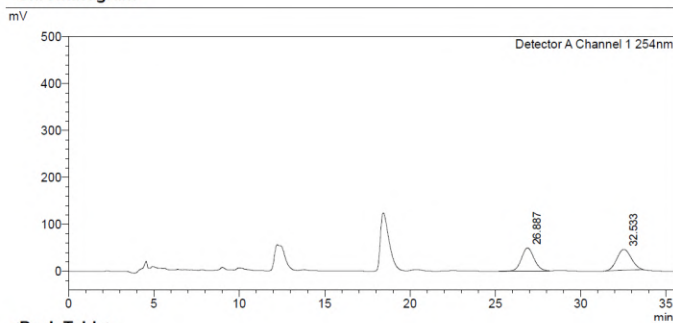
D:\Data\ZHY\ZG\zhy-zg-66-asy-adh-50-50-0.8-254-230-2.lcd

Analysis Report

<Sample Information>

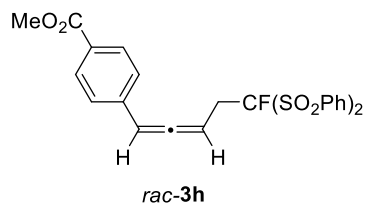
Sample Name : zhy-zg-57-rac-adh-50-50-0.8-254-230-1
 Sample ID :
 Data Filename : zhy-zg-57-rac-adh-50-50-0.8-254-230-5.lcd
 Method Filename : 202209025.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/11/19 11:52:33
 Date Processed : 2023/1/18 16:24:57
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	26.887	2578377	49581	49.601
2	32.533	2619902	44696	50.399
Total		5198280	94277	



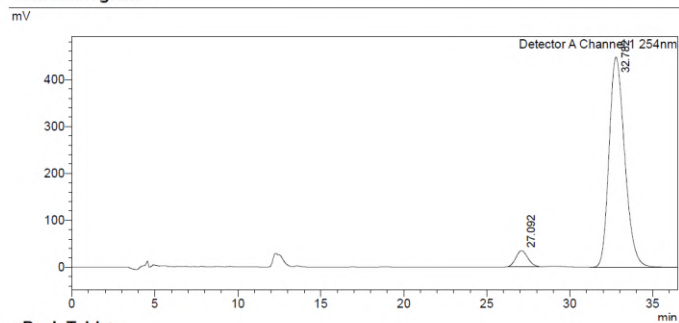
D:\Data\ZHY\ZG\zhy-zg-57-rac-adh-50-50-0.8-254-230-5.lcd

Analysis Report

<Sample Information>

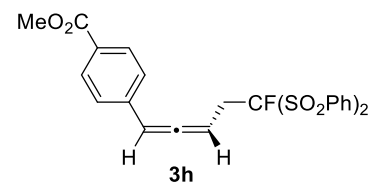
Sample Name : zhy-zg-57-asy-adh-50-50-0.8-254-230-1
 Sample ID :
 Data Filename : zhy-zg-57-asy-adh-50-50-0.8-254-230-4.lcd
 Method Filename : 202209025.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/11/19 11:14:30
 Date Processed : 2022/11/19 11:50:59
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	27.092	1643049	33722	5.314
2	32.782	29275494	447564	94.686
Total		30918543	481286	



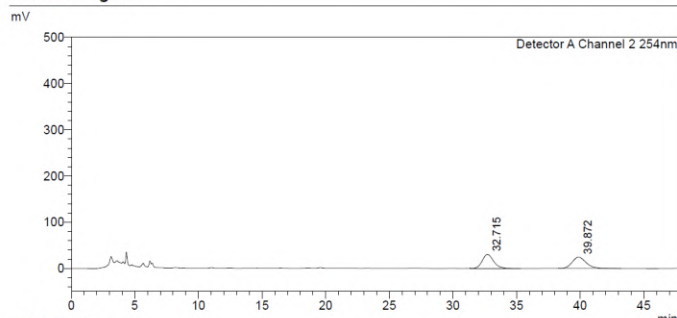
D:\Data\ZHY\ZG\zhy-zg-57-asy-adh-50-50-0.8-254-230-4.lcd

Analysis Report

<Sample Information>

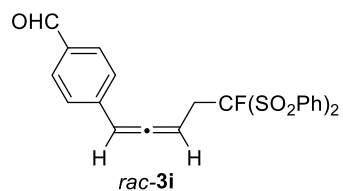
Sample Name : ZHY-ZG132-rac-adh-50-50-0.8-254-230-4
 Sample ID :
 Data Filename : ZHY-ZG132-rac-adh-50-50-0.8-254-230-4.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 1 uL
 Date Acquired : 1/18/2023 1:58:55 PM
 Date Processed : 1/18/2023 5:35:12 PM
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	32.715	1849723	30128	50.055
2	39.872	1845628	24174	49.945
Total		3695351	54301	



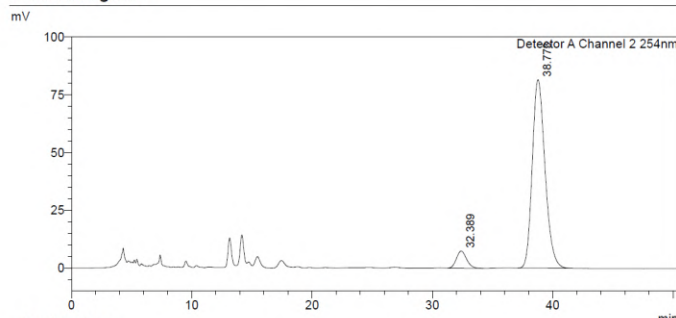
C:\date\ZHY\ZHY-ZG132-rac-adh-50-50-0.8-254-230-4.lcd

Analysis Report

<Sample Information>

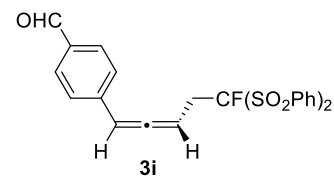
Sample Name : ZHY-ZG132-asy-adh-50-50-0.8-254-230-1
 Sample ID :
 Data Filename : ZHY-ZG132-asy-adh-50-50-0.8-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 1 uL
 Date Acquired : 1/18/2023 12:17:57 PM
 Date Processed : 1/18/2023 1:08:28 PM
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	32.389	445494	7505	6.882
2	38.773	6027777	81678	93.118
Total		6473270	89182	



C:\date\ZHY\ZHY-ZG132-asy-adh-50-50-0.8-254-230-1.lcd

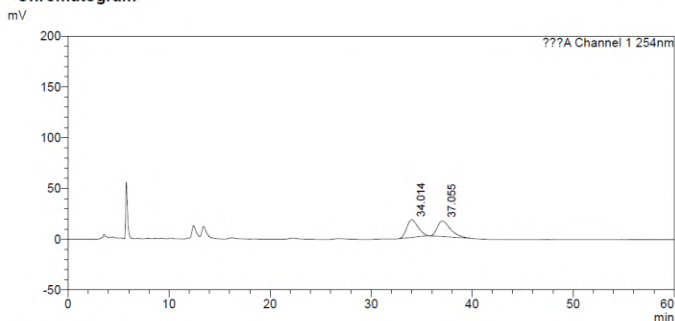


Analysis Report

<Sample Information>

Sample Name : RYL-RB-15-Ph-RAC-1.0-ADH-60-40-254-230-1.0
 Sample ID :
 Data Filename : RYL-RB-15-Ph-RAC-1.0-ADH-60-40-254-230-1.0.lcd
 Method Filename : RYL-1.0-254-230.lcm
 Batch Filename :
 Vial # : 1-1
 Sample Type : Unknown
 Injection Volume : 20 uL
 Date Acquired : 11/17/2022 5:18:23 PM
 Acquired by : System Administrator
 Date Processed : 11/17/2022 11:02:31 PM
 Processed by : System Administrator

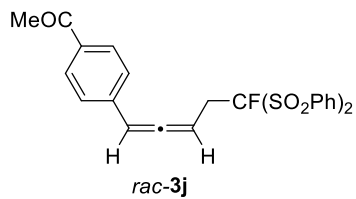
<Chromatogram>



<Peak Table>

???A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	34.014	1333563	17269	48.868
2	37.055	1395351	15473	51.132
Total		2728914	32741	



F:\Data\RYL\RYL-RB-15-Ph-RAC-1.0-ADH-60-40-254-230-1.0.lcd

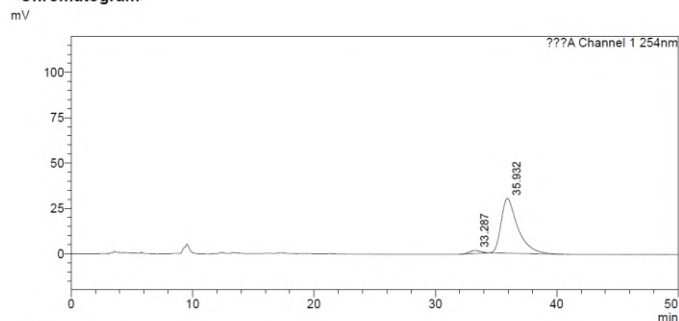


Analysis Report

<Sample Information>

Sample Name : RYL-RB-15-Ph-ASY-1.0-60-40-ADH-254-230-2.0
 Sample ID :
 Data Filename : RYL-RB-15-Ph-ASY-1.0-60-40-ADH-254-230-2.0.lcd
 Method Filename : RYL-1.0-254-230.lcm
 Batch Filename :
 Vial # : 1-1
 Sample Type : Unknown
 Injection Volume : 20 uL
 Date Acquired : 11/17/2022 9:12:24 PM
 Acquired by : System Administrator
 Date Processed : 11/17/2022 11:02:17 PM
 Processed by : System Administrator

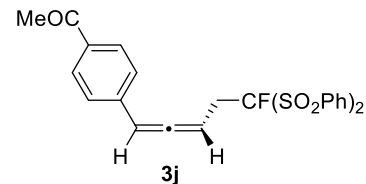
<Chromatogram>



<Peak Table>

???A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	33.287	106636	1680	3.577
2	35.932	2874819	30137	96.423
Total		2981455	31817	



F:\Data\RYL\RYL-RB-15-Ph-ASY-1.0-60-40-ADH-254-230-2.0.lcd

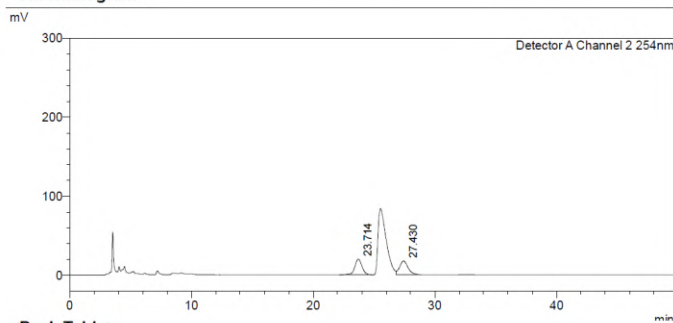
Analysis Report

<Sample Information>

Sample Name : zhy-zg-147-rac-adh-70-30-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zg-147-rac-adh-70-30-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/3/22 21:01:12
 Date Processed : 2023/3/22 22:55:36

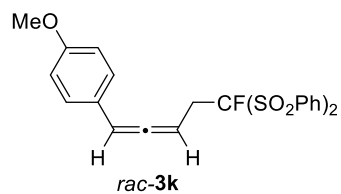
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	23.714	844530	20092	49.267
2	27.430	869659	17602	50.733
Total		1714189	37694	



D:\Data\ZHY\ZG\zhy-zg-147-rac-adh-70-30-1.0-254-230-1.lcd

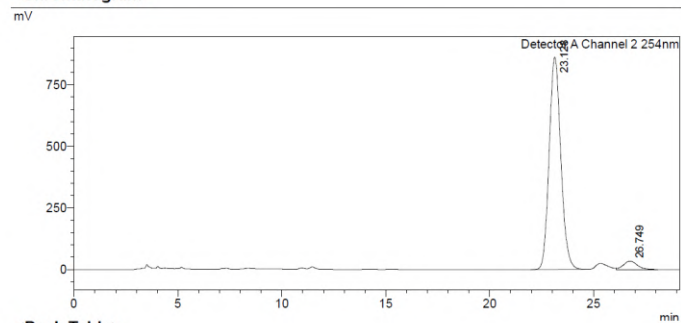
Analysis Report

<Sample Information>

Sample Name : zhy-zg-147-asy-adh-70-30-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zg-147-asy-adh-70-30-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/3/22 21:52:34
 Date Processed : 2023/3/22 22:21:42

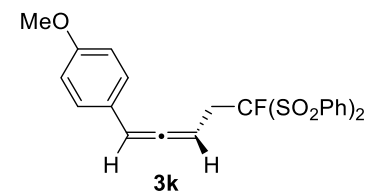
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	23.128	33585789	861213	95.479
2	26.749	1590303	34668	4.521
Total		35176092	895881	



D:\Data\ZHY\ZG\zhy-zg-147-asy-adh-70-30-1.0-254-230-1.lcd

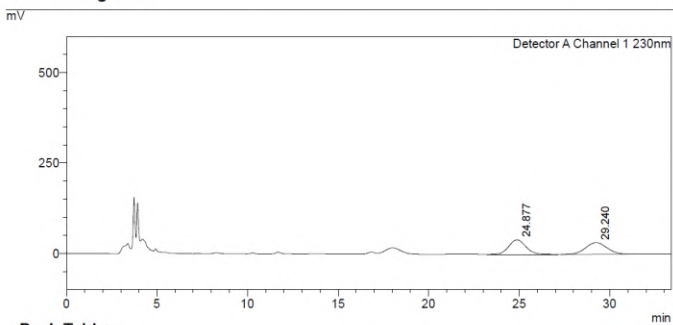
Analysis Report

<Sample Information>

Sample Name : zhy-zh-20-RAC-aSh-70-30-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zh-20-RAC-aSh-70-30-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/3/15 10:25:11
 Date Processed : 2023/6/5 16:17:24

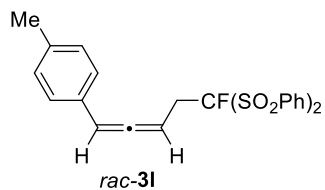
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	24.877	2627825	40336	49.371
2	29.240	2694752	32420	50.629
Total		5322577	72757	



D:\Data\ZHY\ZH\zhy-zh-20-RAC-aSh-70-30-1.0-254-230-1.lcd

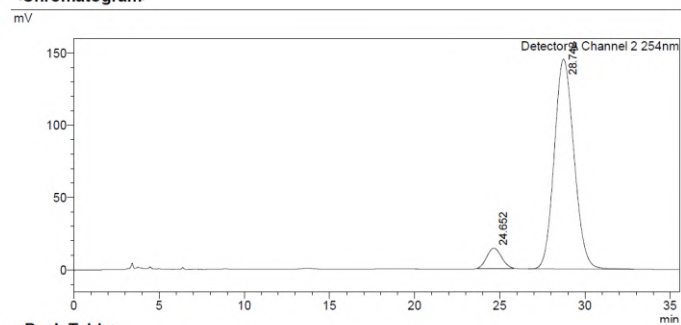
Analysis Report

<Sample Information>

Sample Name : zhy-zh-20-ASY-aSh-70-30-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zh-20-ASY-aSh-70-30-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/3/15 10:58:59
 Date Processed : 2023/3/15 11:34:33

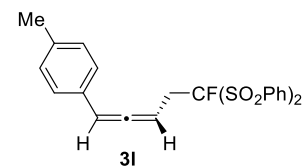
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	24.652	849736	14138	6.745
2	28.742	11748903	145361	93.255
Total		12598639	159499	



D:\Data\ZHY\ZH\zhy-zh-20-ASY-aSh-70-30-1.0-254-230-1.lcd

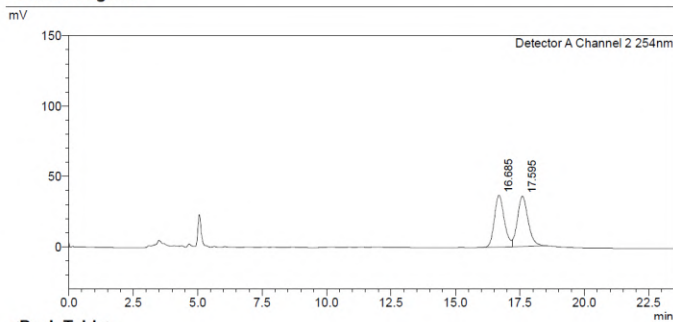
Analysis Report

<Sample Information>

Sample Name : zhy-zg-43-3-rac-adh-80-20-1.0-254-1
 Sample ID :
 Data Filename : zhy-zg-43-3-rac-adh-80-20-1.0-254-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/11/3 18:07:58
 Date Processed : 2022/11/3 18:31:26

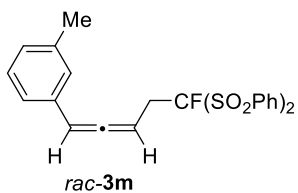
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	16.685	987565	36880	49.044
2	17.595	1026048	35678	50.956
Total		2013613	72558	



D:\Data\ZHY\ZG\zhy-zg-43-3-rac-adh-80-20-1.0-254-1.lcd

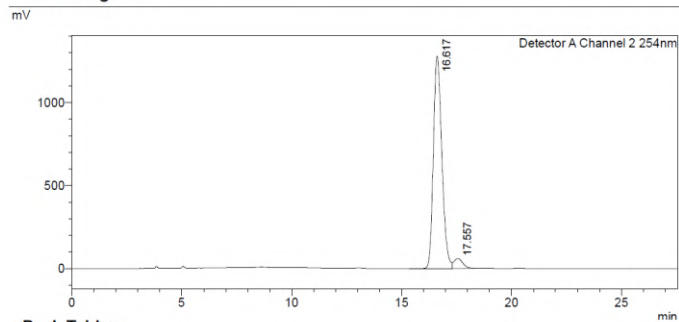
Analysis Report

<Sample Information>

Sample Name : zhy-zg-38-asy-adh-80-20-1.0-254-1
 Sample ID :
 Data Filename : zhy-zg-38-asy-adh-80-20-1.0-254-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/11/3 18:51:30
 Date Processed : 2022/11/3 19:19:04

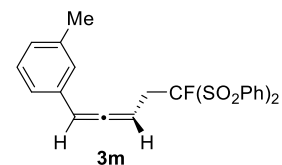
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	16.617	34301693	1280363	95.273
2	17.557	1702049	60054	4.727
Total		36003743	1340417	



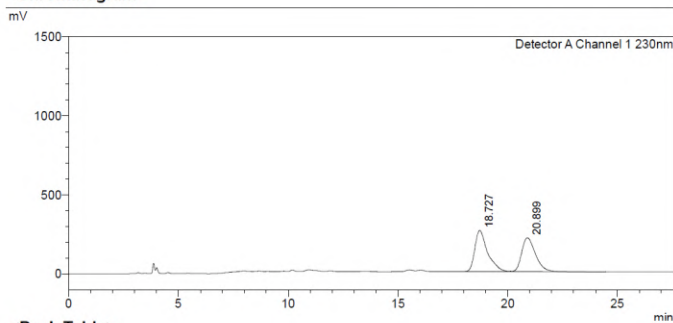
D:\Data\ZHY\ZG\zhy-zg-38-asy-adh-80-20-1.0-254-1.lcd

Analysis Report

<Sample Information>

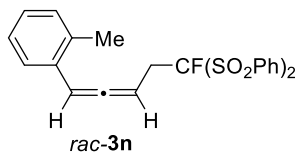
Sample Name : zhy-zg-124-rac-odh-75-25-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zg-124-rac-odh-75-25-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 10 uL
 Date Acquired : 2023/1/18 14:47:32
 Date Processed : 2023/1/18 16:56:03
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	18.727	10501836	259827	52.740
2	20.899	9410589	214729	47.260
Total		19912425	474556	



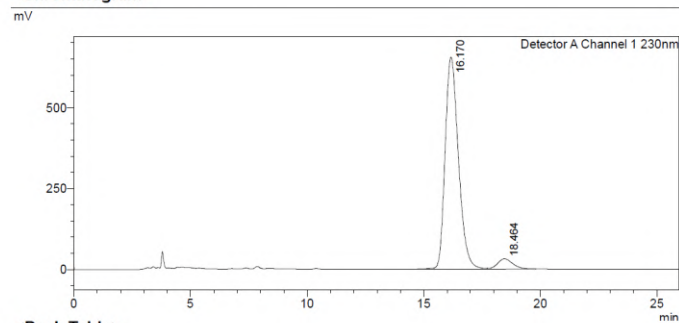
D:\Data\ZHY\ZG\zhy-zg-124-rac-odh-75-25-1.0-254-230-1.0-254-230-1.lcd

Analysis Report

<Sample Information>

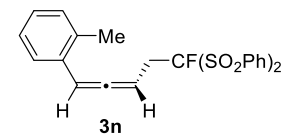
Sample Name : zhy-zg-124-asy-odh-75-25-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zg-124-asy-odh-75-25-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 10 uL
 Date Acquired : 2023/1/18 15:15:32
 Date Processed : 2023/1/18 15:41:30
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	16.170	25999666	654845	94.739
2	18.464	1443886	31602	5.261
Total		27443551	686447	



D:\Data\ZHY\ZG\zhy-zg-124-asy-odh-75-25-1.0-254-230-1.0-254-230-1.lcd

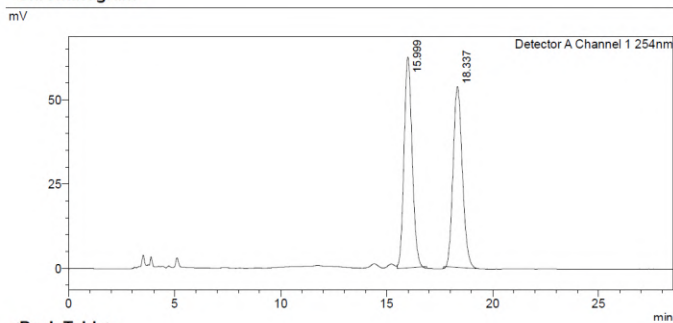
Analysis Report

<Sample Information>

Sample Name : zhy-zg-43-1-rac-adh-80-20-1.0-254-1
 Sample ID :
 Data Filename : zhy-zg-43-1-rac-adh-80-20-1.0-254-1.lcd
 Method Filename : xsl-230-254-1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/11/4 15:13:20
 Date Processed : 2022/11/4 15:44:08

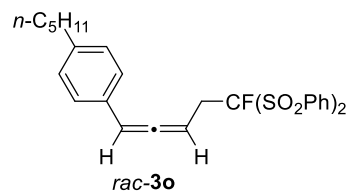
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	15.999	1654814	62490	50.440
2	18.337	1625937	53580	49.560
Total		3280751	116069	



D:\Data\ZHY\ZG\zhy-zg-43-1-rac-adh-80-20-1.0-254-1.lcd

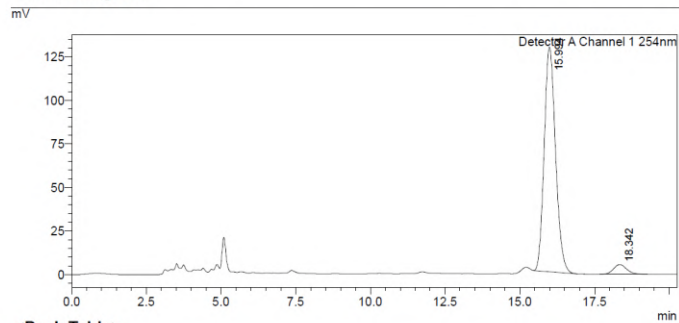
Analysis Report

<Sample Information>

Sample Name : zhy-zg-42-asy-adh-80-20-1.0-254-1
 Sample ID :
 Data Filename : zhy-zg-42-asy-adh-80-20-1.0-254-1.lcd
 Method Filename : xsl-230-254-1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/11/4 15:42:56
 Date Processed : 2022/11/4 16:03:13

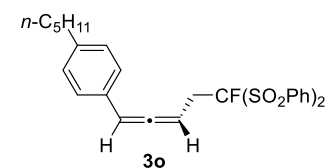
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	15.994	3410456	128950	95.288
2	18.342	168661	5519	4.712
Total		3579117	134469	



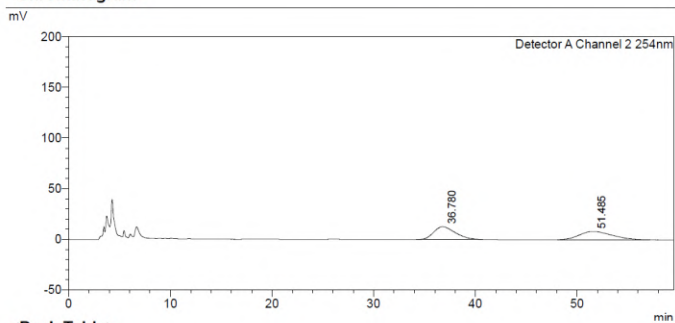
D:\Data\ZHY\ZG\zhy-zg-42-asy-adh-80-20-1.0-254-1.lcd

Analysis Report

<Sample Information>

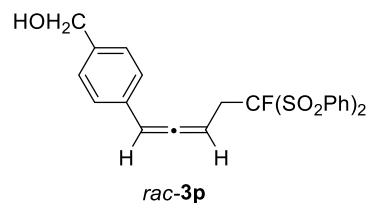
Sample Name : zhy-zg-72-rac-ash-60-40-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zg-72-rac-ash-60-40-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 10 uL
 Date Acquired : 2023/1/11 20:12:43
 Date Processed : 2023/1/18 16:45:29
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	36.780	1856526	12586	50.573
2	51.485	1814481	8107	49.427
Total		3671007	20692	



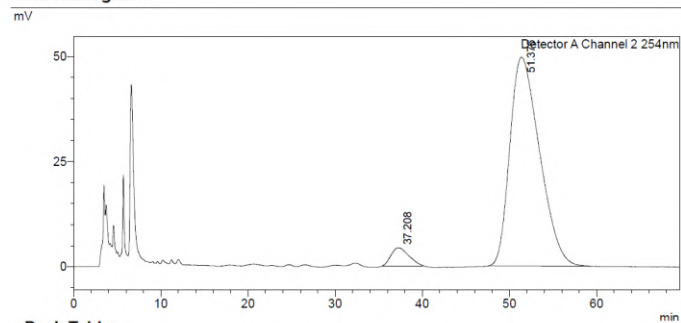
D:\Data\ZHY\ZG\zhy-zg-72-rac-ash-60-40-1.0-254-230-1.lcd

Analysis Report

<Sample Information>

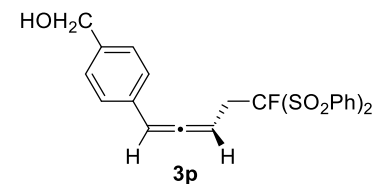
Sample Name : zhy-zg-72-asy-ash-60-40-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zg-72-asy-ash-60-40-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 10 uL
 Date Acquired : 2023/1/11 21:12:36
 Date Processed : 2023/1/11 22:22:06
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	37.208	627145	4400	5.050
2	51.376	11791355	49668	94.950
Total		12418500	54069	



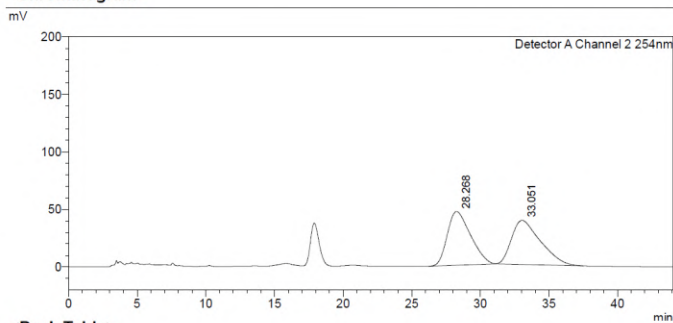
D:\Data\ZHY\ZG\zhy-zg-72-asy-ash-60-40-1.0-254-230-1.lcd

Analysis Report

<Sample Information>

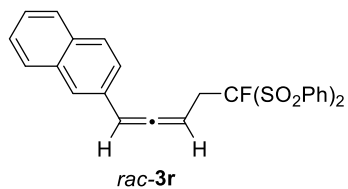
Sample Name : ZHY-ZG-143-RAC-ASH-60-40-1.0-254-230-1
 Sample ID :
 Data Filename : ZHY-ZG-143-RAC-ASH-60-40-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/2/6 21:04:35
 Date Processed : 2023/2/6 21:48:40
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	28.268	5491934	46707	49.377
2	33.051	5630475	38290	50.623
Total		11122409	84997	



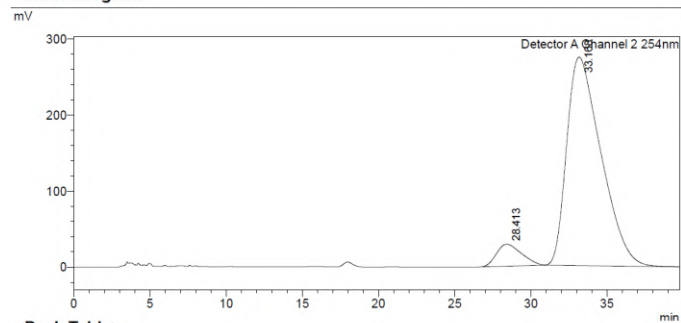
D:\Data\ZHY\ZG\ZHY-ZG-143-RAC-ASH-60-40-1.0-254-230-1.lcd

Analysis Report

<Sample Information>

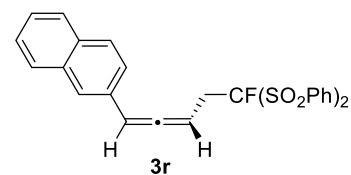
Sample Name : ZHY-ZG-143-ASY-ASH-60-40-1.0-254-230-1
 Sample ID :
 Data Filename : ZHY-ZG-143-ASY-ASH-60-40-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/2/6 20:22:07
 Date Processed : 2023/2/6 21:01:53
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	28.413	3266209	28812	7.085
2	33.168	42832390	274108	92.915
Total		46098599	302920	



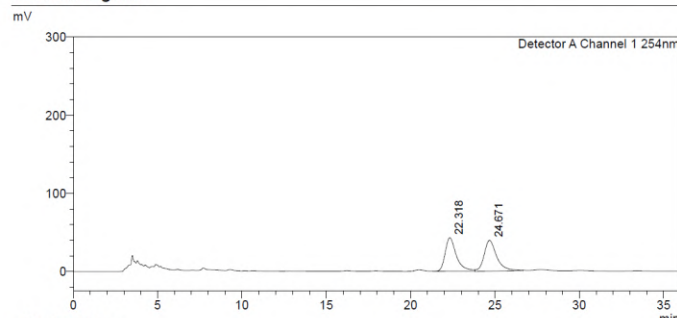
D:\Data\ZHY\ZG\ZHY-ZG-143-ASY-ASH-60-40-1.0-254-230-1.lcd

Analysis Report

<Sample Information>

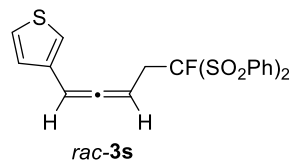
Sample Name : zhy-zh-10-rac-adh-70-30-1.0-254-230-4
 Sample ID :
 Data Filename : zhy-zh-10-rac-adh-70-30-1.0-254-230-6.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2/25/2023 4:10:00 PM
 Date Processed : 3/30/2023 8:22:59 PM
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	22.318	1975115	42921	49.439
2	24.671	2019944	39317	50.561
Total		3995060	82238	



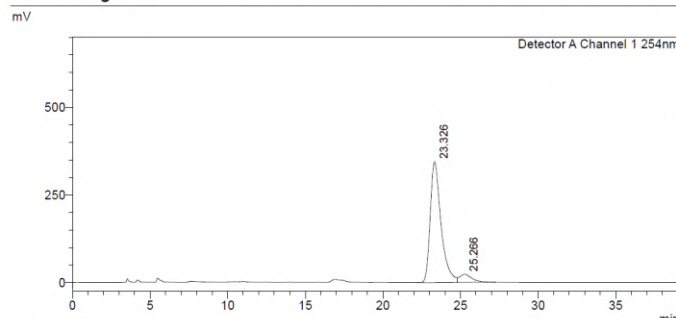
C:\date\ZHY\zhy-zh-10-rac-adh-70-30-1.0-254-230-6.lcd

Analysis Report

<Sample Information>

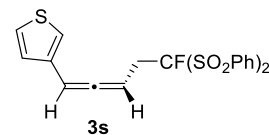
Sample Name : zhy-zh-10-asy-adh-70-30-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zh-10-asy-adh-70-30-1.0-254-230-2.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2/24/2023 8:20:55 PM
 Date Processed : 2/25/2023 7:42:37 PM
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	23.326	16701337	344818	92.784
2	25.266	1298944	23351	7.216
Total		18000282	368169	



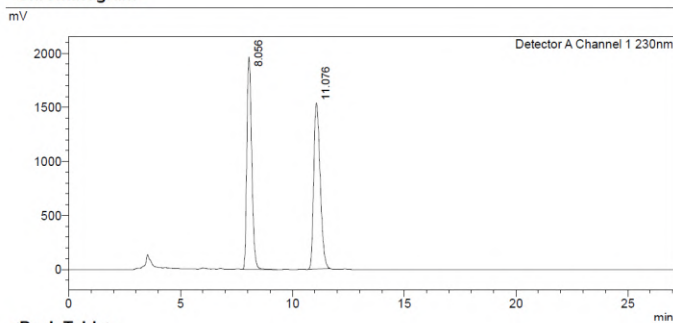
C:\date\ZHY\zhy-zh-10-asy-adh-70-30-1.0-254-230-2.lcd

Analysis Report

<Sample Information>

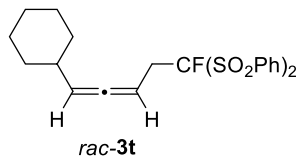
Sample Name : zhy-zh-51-2-rac-adh-70-30-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zh-51-2-rac-adh-70-30-1.0-254-230-4.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/4/20 16:07:59
 Date Processed : 2023/4/20 16:35:03
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	8.056	29615158	1962021	49.104
2	11.076	30695781	1535820	50.896
Total		60310940	3497841	



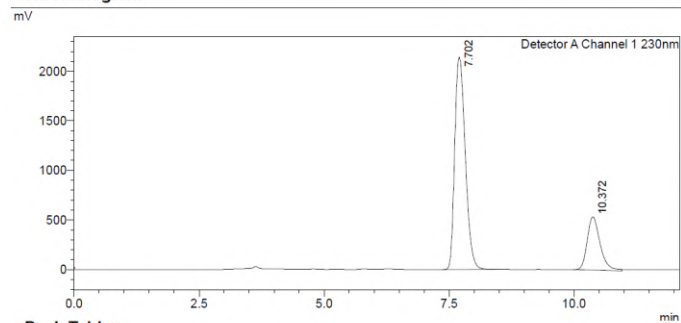
D:\Data\ZHY\ZH\zhy-zh-51-2-rac-adh-70-30-1.0-254-230-4.lcd

Analysis Report

<Sample Information>

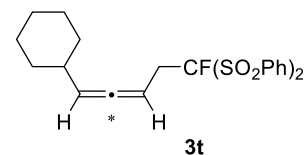
Sample Name : ZHY-ZH-66-ASY-ADH-70-30-254-230-1
 Sample ID :
 Data Filename : ZHY-ZH-66-ASY-ADH-70-30-254-230-2.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/5/3 22:44:24
 Date Processed : 2023/5/3 22:56:30
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	7.702	31470212	2140845	76.563
2	10.372	9633563	537799	23.437
Total		41103775	2678644	



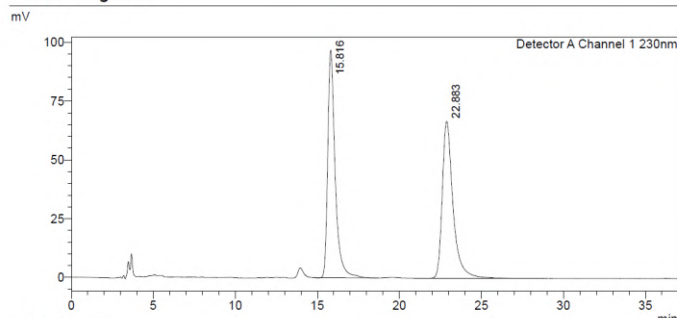
D:\Data\ZHY\ZH\ZHY-ZH-66-ASY-ADH-70-30-254-230-2.lcd

Analysis Report

<Sample Information>

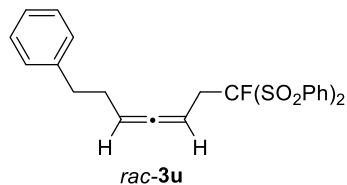
Sample Name : LIL-LL-84-rac-adh-80-20-254-230-1.0-1
 Sample ID :
 Data Filename : LIL-LL-84-rac-adh-80-20-254-230-1.0-1.lcd
 Method Filename : 254-230-1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 5/19/2023 9:27:45 AM
 Date Processed : 5/19/2023 12:16:13 PM
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	15.816	3032494	96867	49.897
2	22.883	3045068	66781	50.103
Total		6077562	163648	



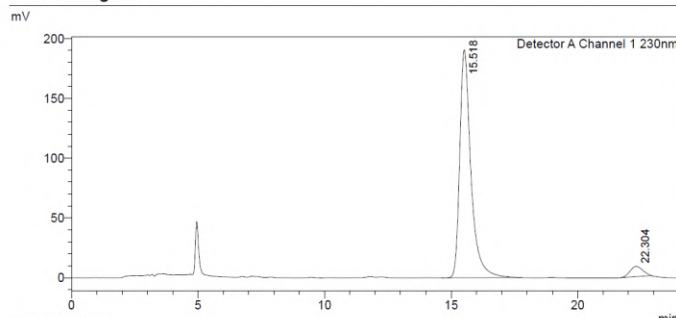
C:\data\LIL\LL-84-rac-adh-80-20-254-230-1.0-1.lcd

Analysis Report

<Sample Information>

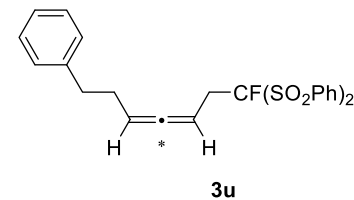
Sample Name : LIL-LL-84-asy-adh-80-20-254-230-1.0-2
 Sample ID :
 Data Filename : LIL-LL-84-asy-adh-80-20-254-230-1.0-2.lcd
 Method Filename : 254-230-1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 5/19/2023 11:49:28 AM
 Date Processed : 5/19/2023 12:13:30 PM
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	15.518	5829605	190518	95.113
2	22.304	2995550	8586	4.887
Total		6129155	199103	



C:\data\LIL\LL-84-asy-adh-80-20-254-230-1.0-2.lcd

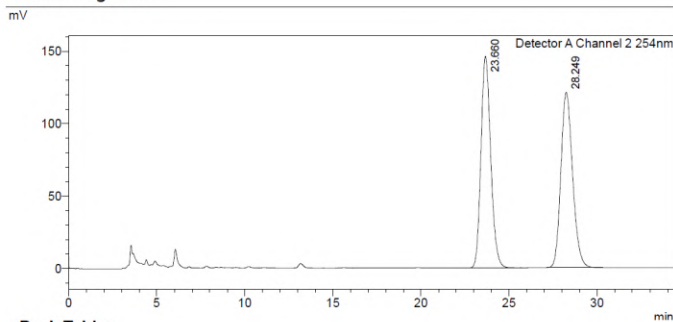
Analysis Report

<Sample Information>

Sample Name : zhy-zh-34-rac-adh-80-20-1.0-254-230-2
 Sample ID :
 Data Filename : zhy-zh-34-rac-adh-80-20-1.0-254-230-2.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/4/15 9:08:23
 Date Processed : 2023/4/15 9:42:45

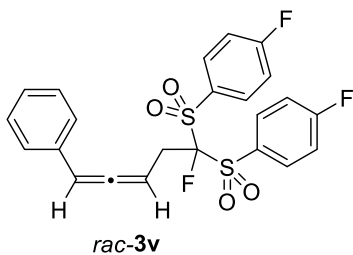
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	23.660	5623947	145949	50.085
2	28.249	5604870	120955	49.915
Total		11228817	266904	



D:\Data\ZHY\ZH\zhy-zh-34-rac-adh-80-20-1.0-254-230-2.lcd

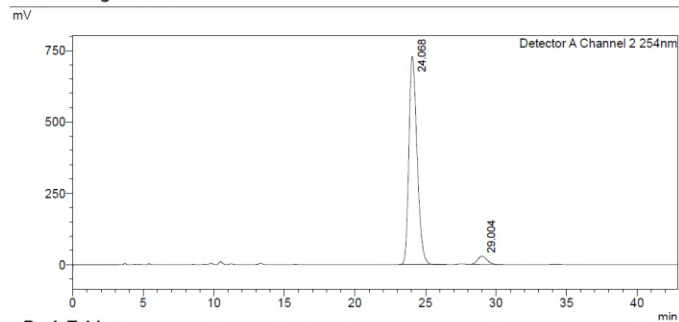
Analysis Report

<Sample Information>

Sample Name : zhy-zh-34-asy-adh-80-20-1.0-254-230-3
 Sample ID :
 Data Filename : zhy-zh-34-asy-adh-80-20-1.0-254-230-3.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/4/12 9:02:05
 Date Processed : 2023/4/15 9:42:38

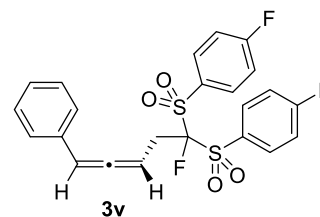
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	24.068	29374880	728758	95.676
2	29.004	1327608	28715	4.324
Total		30702489	757473	



D:\Data\ZHY\ZH\zhy-zh-34-asy-adh-80-20-1.0-254-230-3.lcd

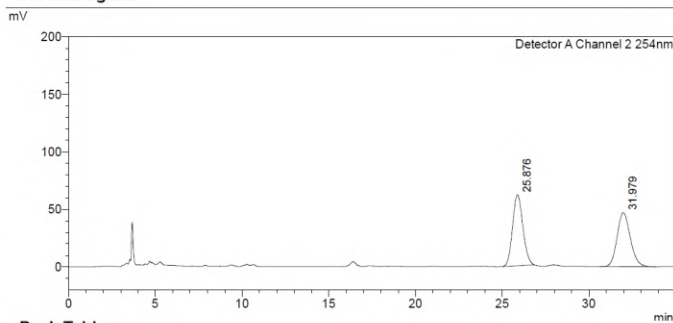
Analysis Report

<Sample Information>

Sample Name : zhy-zh-35-rac-adh-80-20-1.0-254-230-3
 Sample ID :
 Data Filename : zhy-zh-35-rac-adh-80-20-1.0-254-230-3.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/4/11 22:21:22
 Date Processed : 2023/4/11 22:56:15

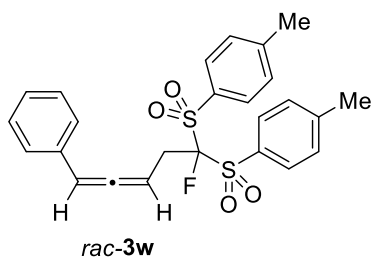
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	25.876	2560052	61788	50.700
2	31.979	2489341	47086	49.300
Total		5049392	108874	



D:\Data\ZHY\ZH\zhy-zh-35-rac-adh-80-20-1.0-254-230-3.lcd

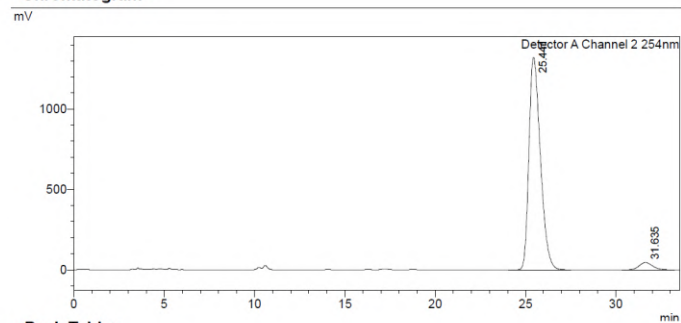
Analysis Report

<Sample Information>

Sample Name : zhy-zh-35-asy-adh-80-20-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zh-35-asy-adh-80-20-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/4/11 21:10:19
 Date Processed : 2023/4/11 22:17:29

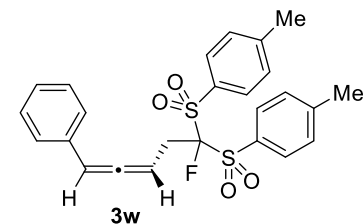
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	25.441	58342166	1322496	96.115
2	31.635	2357932	45308	3.885
Total		60700098	1367804	



D:\Data\ZHY\ZH\zhy-zh-35-asy-adh-80-20-1.0-254-230-1.lcd

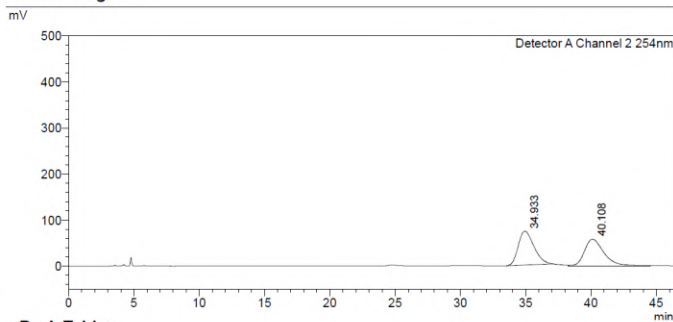
Analysis Report

<Sample Information>

Sample Name : ZHY-ZH-62-RAC-ODH-90-10-1.0-254-230-4
 Sample ID :
 Data Filename : ZHY-ZH-62-Rc-ODH-90-10-1.0-254-230-4.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/4/25 20:15:27
 Date Processed : 2023/4/25 21:01:47

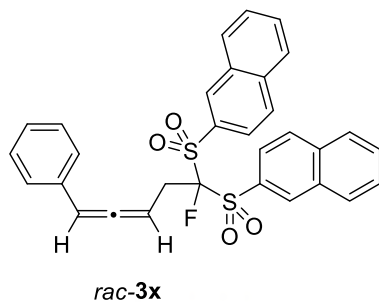
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	34.933	6140091	73492	50.496
2	40.108	6019431	58067	49.504
Total		12159523	131559	



D:\Data\ZHY\ZH\ZHY-ZH-62-Rc-ODH-90-10-1.0-254-230-4.lcd

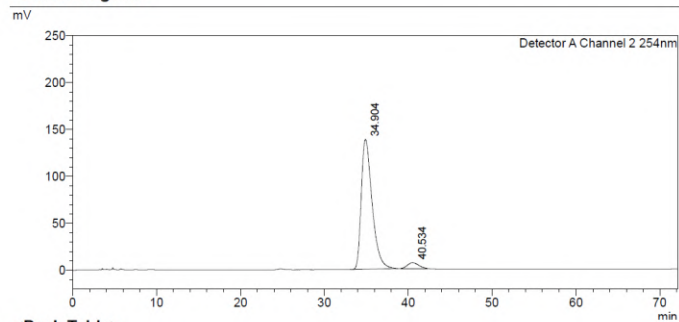
Analysis Report

<Sample Information>

Sample Name : ZHY-ZH-62-ASY-ODH-90-10-1.0-254-230-3
 Sample ID :
 Data Filename : ZHY-ZH-62-ASY-ODH-90-10-1.0-254-230-5.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/4/25 18:41:41
 Date Processed : 2023/4/25 19:54:27

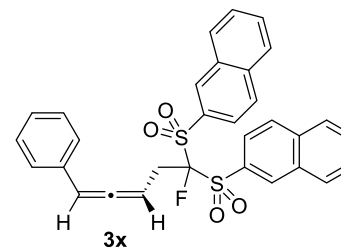
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	34.904	12488974	138788	95.684
2	40.534	563344	6162	4.316
Total		13052318	144950	



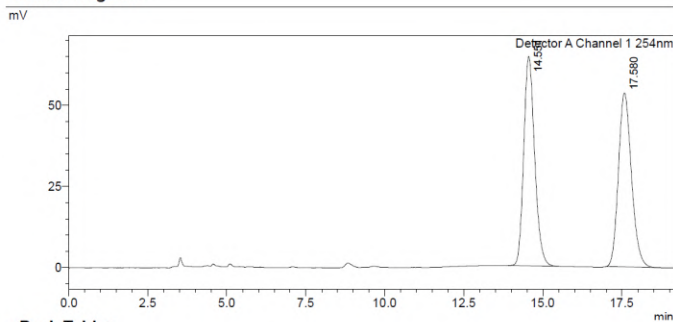
D:\Data\ZHY\ZH\ZHY-ZH-62-ASY-ODH-90-10-1.0-254-230-5.lcd

Analysis Report

<Sample Information>

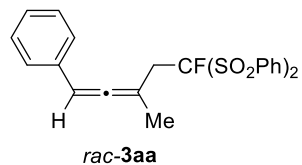
Sample Name : III-II-4-h-rac-adh-80-20-254-230-1.0-1
 Sample ID :
 Data Filename : III-II-4-h-rac-adh-80-20-254-230-1.0-1.lcd
 Method Filename : 1.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/5/19 22:26:59
 Date Processed : 2023/5/19 22:46:07
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	14.551	1552951	64566	50.302
2	17.580	1534298	53611	49.698
Total		3087249	118177	



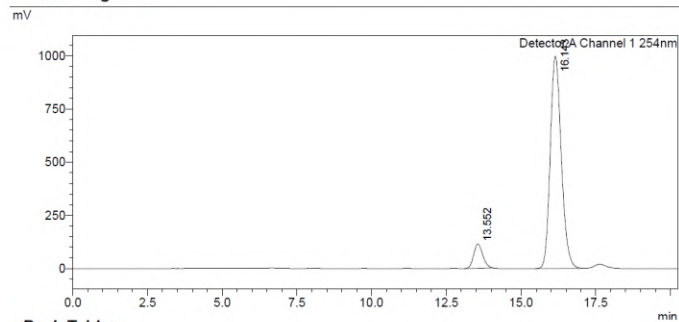
D:\Data\II\III-II-4-h-rac-adh-80-20-254-230-1.0-1.lcd

Analysis Report

<Sample Information>

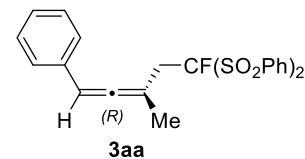
Sample Name : III-II-57-asy-adh-80-20-254-230-1.0-1
 Sample ID :
 Data Filename : III-II-57-asy-adh-80-20-254-230-1.0-1.lcd
 Method Filename : 1.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/5/15 22:02:41
 Date Processed : 2023/5/15 22:22:57
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	13.552	2405559	113940	8.587
2	16.143	25608086	997784	91.413
Total		28013645	1111724	



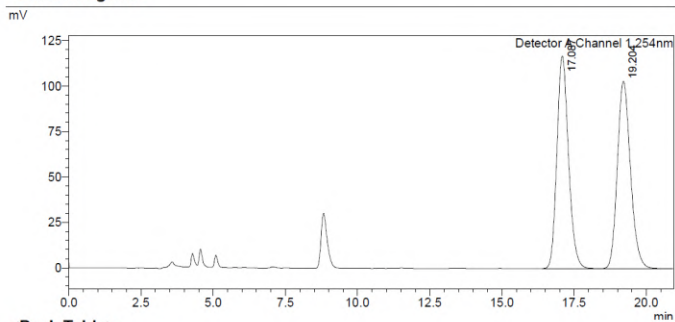
D:\Data\II\III-II-57-asy-adh-80-20-254-230-1.0-1.lcd

Analysis Report

<Sample Information>

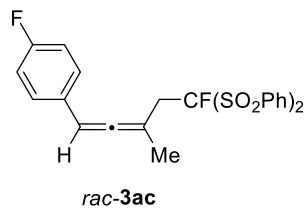
Sample Name : III-II-4-f-rac-adh-80-20-254-230-1.0-1
 Sample ID :
 Data Filename : III-II-4-f-rac-adh-80-20-254-230-1.0-1.lcd
 Method Filename : 1.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/5/19 22:05:34
 Date Processed : 2023/5/19 22:26:31
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	17.087	3264222	116796	50.057
2	19.204	3256851	102966	49.943
Total		6521074	219762	



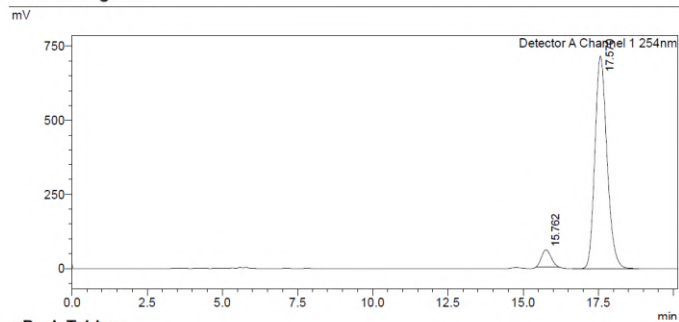
D:\Data\III\LL\III-II-4-f-rac-adh-80-20-254-230-1.0-1.lcd

Analysis Report

<Sample Information>

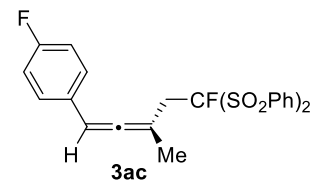
Sample Name : III-II-69-asy-adh-80-20-254-230-1.0-1
 Sample ID :
 Data Filename : III-II-69-asy-adh-80-20-254-230-1.0-1.lcd
 Method Filename : 1.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/5/15 21:14:20
 Date Processed : 2023/5/15 21:34:29
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	15.762	1298750	58367	6.091
2	17.570	20023948	716552	93.909
Total		21322698	774919	



D:\Data\III\LL\III-II-69-asy-adh-80-20-254-230-1.0-1.lcd

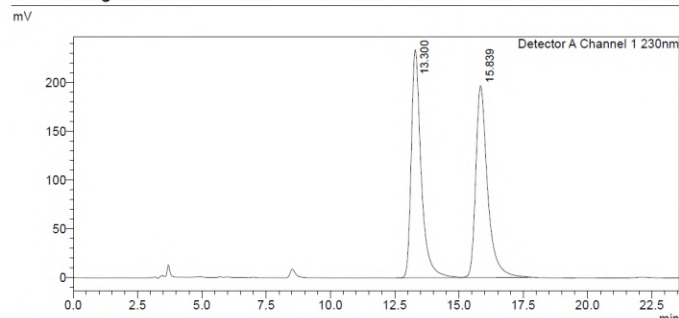
Analysis Report

<Sample Information>

Sample Name : LIL-LL-79-rac-adh-80-20-254-230-1.0-2
 Sample ID :
 Data Filename : LIL-LL-79-rac-adh-80-20-254-230-1.0-2.lcd
 Method Filename : 254-230-1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 5/19/2023 3:42:40 PM
 Date Processed : 5/19/2023 4:06:18 PM

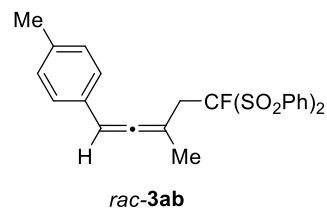
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	13.300	6266615	233906	50.016
2	15.839	6262602	196891	49.984
Total		12529217	430797	



C:\data\LIL\LL-79-rac-adh-80-20-254-230-1.0-2.lcd

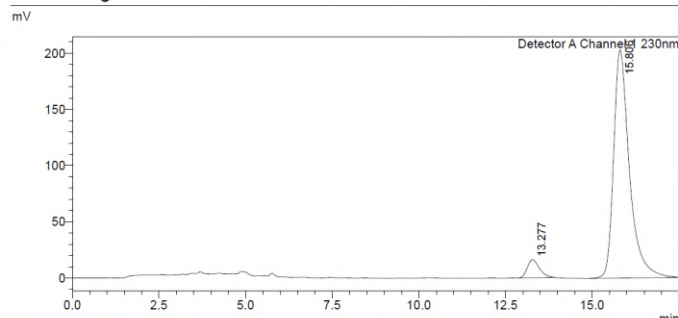
Analysis Report

<Sample Information>

Sample Name : LIL-LL-79-asy-adh-80-20-254-230-1.0-2
 Sample ID :
 Data Filename : LIL-LL-79-asy-adh-80-20-254-230-1.0-2.lcd
 Method Filename : 254-230-1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 5/19/2023 3:24:35 PM
 Date Processed : 5/19/2023 3:42:10 PM

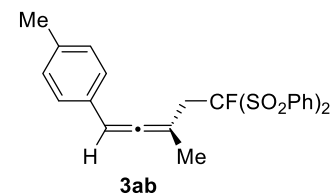
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	13.277	387971	16167	5.698
2	15.806	6420884	202990	94.302
Total		6808855	219157	



C:\data\LIL\LL-79-asy-adh-80-20-254-230-1.0-2.lcd

2023/3/30 22:50:45 Pa

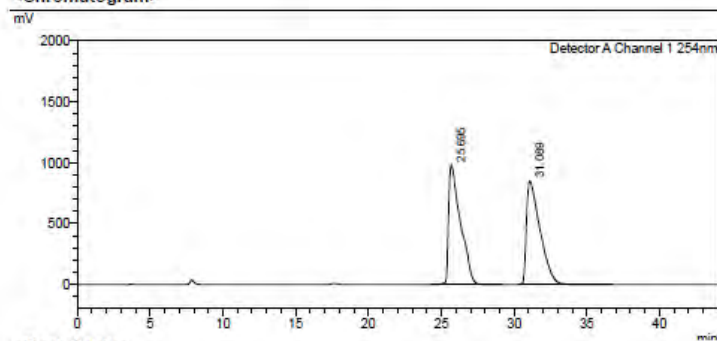
Analysis Report

<Sample Information>

Sample Name : ZHY-ZG-36-RAC-OJH-98-2-1.0-254-230-1
 Sample ID :
 Data Filename : ZHY-ZG-36-RAC-OJH-98-2-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/3/30 21:25:19
 Date Processed : 2023/3/30 22:09:20

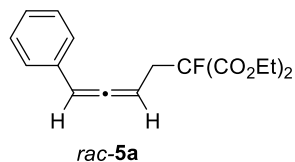
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	25.865	55396221	982318	50.206
2	31.089	54944683	852237	49.794
Total		110344204	1834555	



D:\Data\ZHY\ZG\ZHY-ZG-36-RAC-OJH-98-2-1.0-254-230-1.lcd

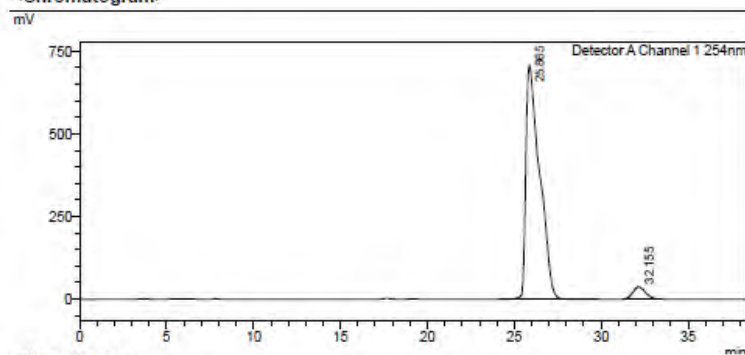
Analysis Report

<Sample Information>

Sample Name : ZHY-ZG-36-ASY-OJH-98-2-1.0-254-230-1
 Sample ID :
 Data Filename : ZHY-ZG-36-ASY-OJH-98-2-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/3/30 22:11:00
 Date Processed : 2023/3/30 22:49:22

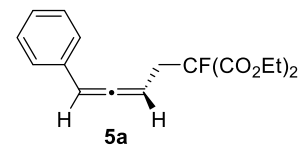
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	25.865	38996389	709343	95.561
2	32.155	1805316	35921	4.439
Total		40871705	744264	



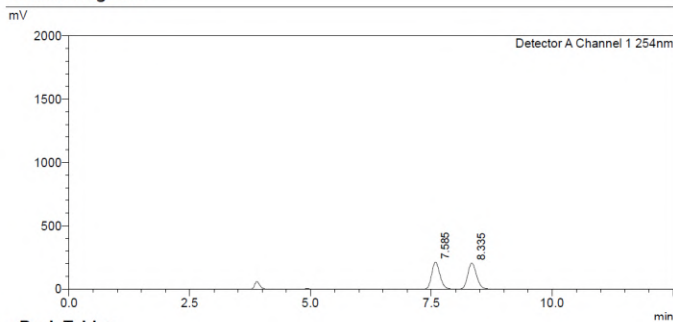
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Analysis Report

<Sample Information>

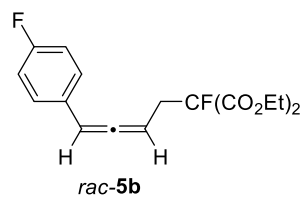
Sample Name : LHW-LA-137-RAC-OD-H-98-2-1.0-230-254-1
 Sample ID :
 Data Filename : LHW-LA-137(F)-RAC-OD-H-98-2-1.0-230-254-1.lcd
 Method Filename : LHW-230-254-1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/11/22 21:51:17
 Date Processed : 2022/11/22 22:03:49
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	7.585	2514712	213497	49.490
2	8.335	2566583	205352	50.510
Total		5081295	418848	



D:\Data\LHW\LHW-LA-137(F)-RAC-OD-H-98-2-1.0-230-254-1.lcd

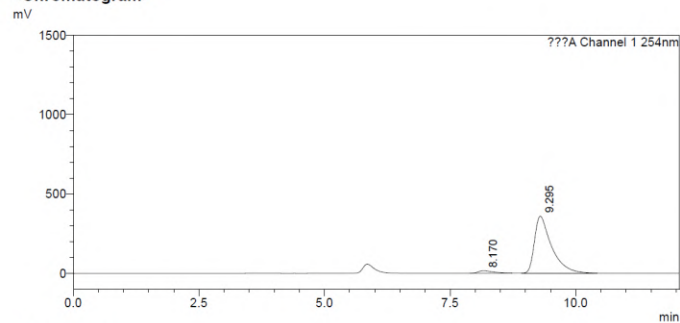


Analysis Report

<Sample Information>

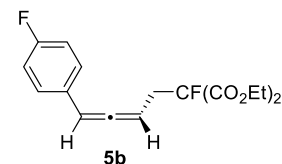
Sample Name : LHW-LB-7(F)-ASY-OD-H-80-20-254-230-1.0-1
 Sample ID :
 Data Filename : LHW-LB-7(F)-ASY-OD-H-80-20-254-230-1.0-1.lcd
 Method Filename : GY-1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 11/28/2022 10:17:27 PM
 Date Processed : 11/28/2022 10:29:33 PM
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	8.170	316727	16043	3.614
2	9.295	8447142	358893	96.386
Total		8763869	374936	



F:\Data\LHW\LHW-LB-7(F)-ASY-OD-H-80-20-254-230-1.0-1.lcd

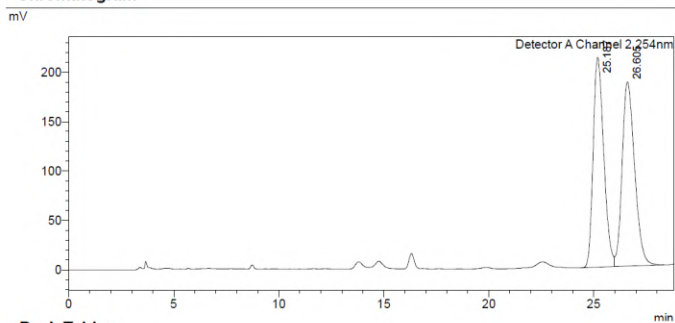
Analysis Report

<Sample Information>

Sample Name : zhy-zg-54-rac-ojh-98-2-1.0-254-3
 Sample ID :
 Data Filename : zhy-zg-54-rac-ojh-98-2-1.0-254-7.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/11/9 10:27:05
 Date Processed : 2022/11/9 10:55:53

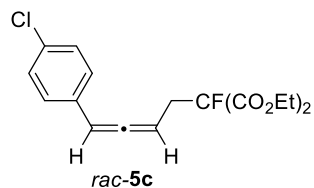
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	25.187	7460571	212612	49.129
2	26.605	7725061	186615	50.871
Total		15185631	399227	



D:\Data\ZHY\ZG\zhy-zg-54-rac-ojh-98-2-1.0-254-7.lcd

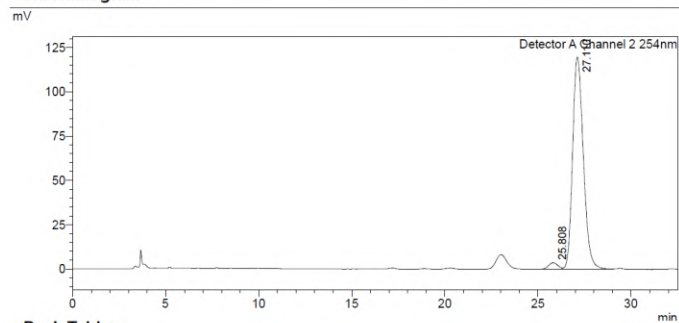
Analysis Report

<Sample Information>

Sample Name : zhy-zg-54-asy-ojh-98-2-1.0-254-3
 Sample ID :
 Data Filename : zhy-zg-54-asy-ojh-98-2-1.0-254-6.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/11/9 9:54:08
 Date Processed : 2022/11/9 10:54:44

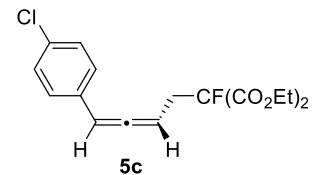
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	25.808	131064	3746	2.650
2	27.110	4814207	119730	97.350
Total		4945271	123476	



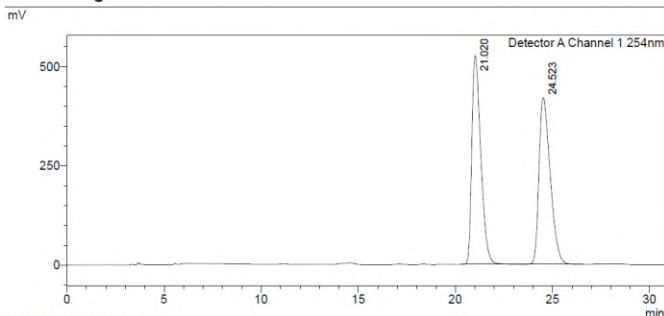
D:\Data\ZHY\ZG\zhy-zg-54-asy-ojh-98-2-1.0-254-6.lcd

Analysis Report

<Sample Information>

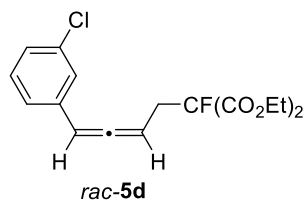
Sample Name : ZHY-ZG-51-RAC-OJH-98-2-1.0-254-1
 Sample ID :
 Data Filename : ZHY-ZG-51-RAC-OJH-98-2-1.0-254-3.lcd
 Method Filename : PPY-230-254-1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/11/7 22:18:44
 Date Processed : 2022/11/7 22:49:30
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	21.020	16997923	526603	50.056
2	24.523	16959913	420324	49.944
Total		33957836	946927	



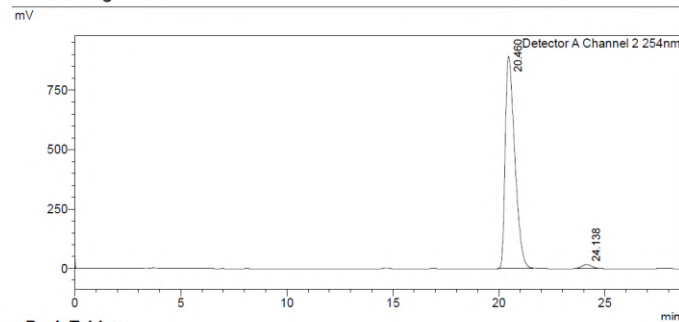
D:\Data\ZHY\ZG\ZHY-ZG-51-RAC-OJH-98-2-1.0-254-3.lcd

Analysis Report

<Sample Information>

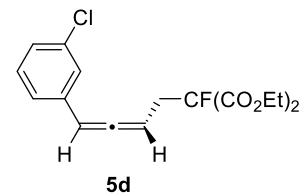
Sample Name : zhy-zg-51-asy-ojh-98-2-1.0-254-3
 Sample ID :
 Data Filename : zhy-zg-51-asy-ojh-98-2-1.0-254-4.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/11/9 8:46:31
 Date Processed : 2022/11/9 9:15:05
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	20.460	27949157	891537	97.887
2	24.138	603426	17330	2.113
Total		28552584	908866	



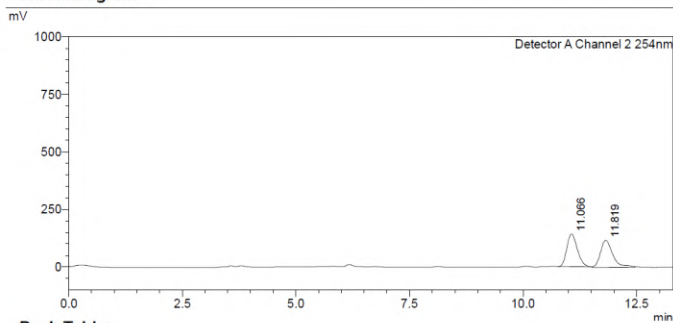
D:\Data\ZHY\ZG\zhy-zg-51-asy-ojh-98-2-1.0-254-4.lcd

Analysis Report

<Sample Information>

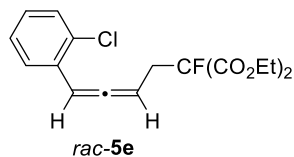
Sample Name : zhy-zg-68-rac-ogh-95-5-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zg-68-rac-ogh-95-5-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 10 uL
 Date Acquired : 2023/1/6 18:18:38
 Date Processed : 2023/1/18 16:40:19
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	11.066	2273317	142400	50.332
2	11.819	2243284	118174	49.668
Total		4516601	260574	



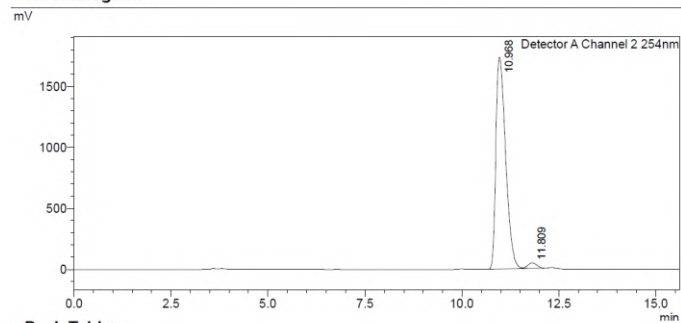
D:\Data\ZHY\ZG\zhy-zg-68-rac-ogh-95-5-1.0-254-230-1.lcd

Analysis Report

<Sample Information>

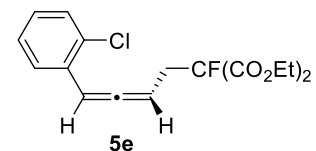
Sample Name : zhy-zg-68-asy-ogh-95-5-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zg-68-asy-ogh-95-5-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 10 uL
 Date Acquired : 2023/1/6 18:02:38
 Date Processed : 2023/1/10 15:09:31
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	10.968	30406213	1738109	97.578
2	11.809	754777	46529	2.422
Total		31160990	1784638	



D:\Data\ZHY\ZG\zhy-zg-68-asy-ogh-95-5-1.0-254-230-1.lcd

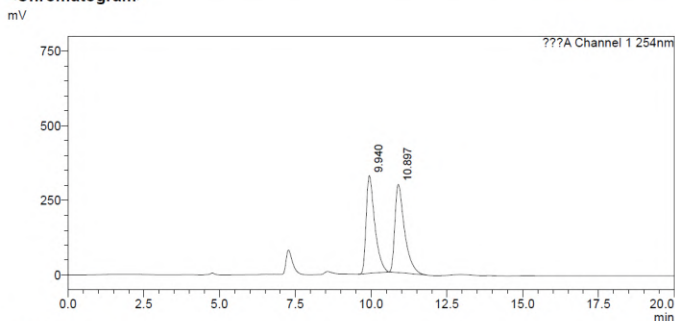


Analysis Report

<Sample Information>

Sample Name : RYL-RB-7-RAC-ADH-0.8-95-5-254-230-1.0
 Sample ID :
 Data Filename : RYL-RB-7-RAC-ADH-0.8-95-5-254-230-1.0.lcd
 Method Filename : RYL-0.8-254-230-1.lcm
 Batch Filename :
 Vial # : 1-1
 Sample Type : Unknown
 Injection Volume : 20 uL
 Date Acquired : 11/11/2022 5:14:37 PM
 Acquired by : System Administrator
 Date Processed : 11/11/2022 6:14:38 PM
 Processed by : System Administrator

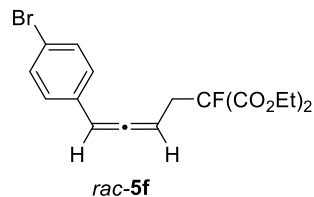
<Chromatogram>



<Peak Table>

??A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	9.940	6460801	327312	49.851
2	10.897	6499419	295231	50.149
Total		12960219	622543	



F:\Data\RYL\RYL-RB-7-RAC-ADH-0.8-95-5-254-230-1.0.lcd

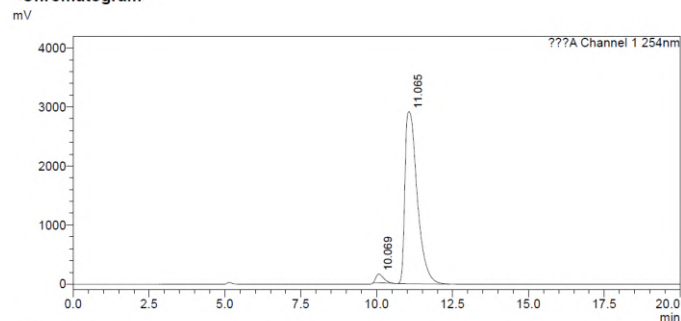


Analysis Report

<Sample Information>

Sample Name : RYL-RB-7-ASY-ADH-0.8-95-5-254-230-1
 Sample ID :
 Data Filename : RYL-RB-7-ASY-ADH-0.8-95-5-254-230-1.lcd
 Method Filename : RYL-0.8-254-230-1.lcm
 Batch Filename :
 Vial # : 1-1
 Sample Type : Unknown
 Injection Volume : 20 uL
 Date Acquired : 11/12/2022 10:35:59 AM
 Acquired by : System Administrator
 Date Processed : 11/12/2022 10:58:07 AM
 Processed by : System Administrator

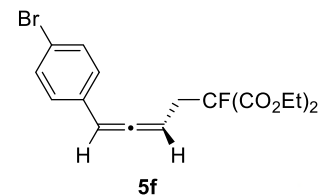
<Chromatogram>



<Peak Table>

??A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	10.069	2676367	152482	3.159
2	11.065	82041839	2912139	96.841
Total		84718206	3064621	



F:\Data\RYL\RYL-RB-7-ASY-ADH-0.8-95-5-254-230-1.lcd

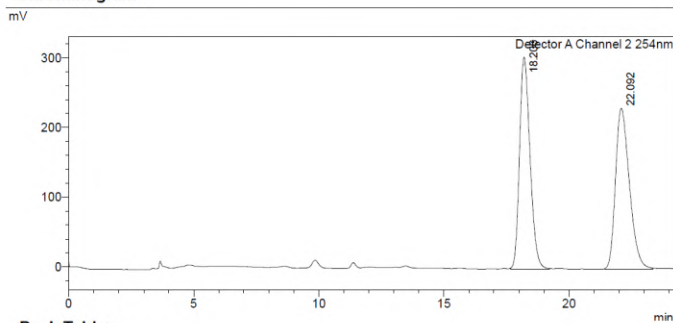
Analysis Report

<Sample Information>

Sample Name : zhy-zg-53-rac-ojh-98-2-1.0-254-3
 Sample ID :
 Data Filename : zhy-zg-53-rac-ojh-98-2-1.0-254-8.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/11/9 10:56:12
 Date Processed : 2022/11/9 11:20:24

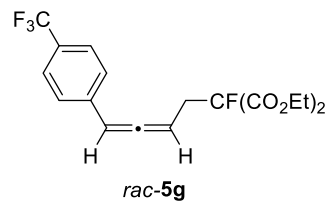
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	18.206	8827382	303699	49.853
2	22.092	8879321	230268	50.147
Total		17706703	533966	



D:\Data\ZHY\ZG\zhy-zg-53-rac-ojh-98-2-1.0-254-8.lcd

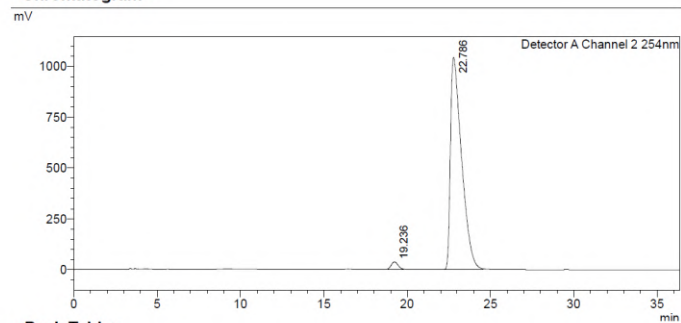
Analysis Report

<Sample Information>

Sample Name : zhy-zg-53-asy-ojh-98-2-1.0-254-3
 Sample ID :
 Data Filename : zhy-zg-53-asy-ojh-98-2-1.0-254-5.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/11/9 9:16:18
 Date Processed : 2022/11/9 10:14:04

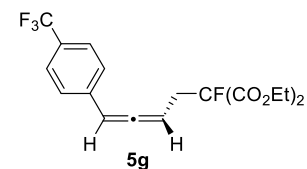
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	19.236	1008649	36045	2.044
2	22.786	48348792	1042864	97.956
Total		49357441	1078908	



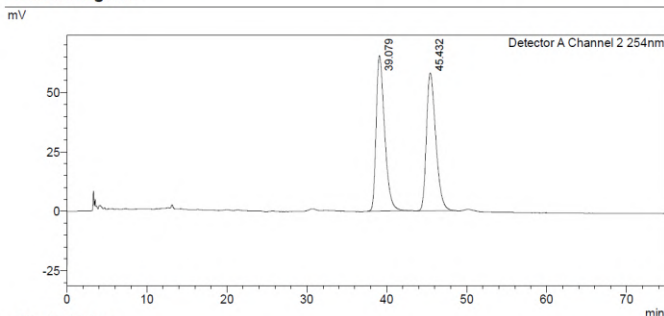
D:\Data\ZHY\ZG\zhy-zg-53-asy-ojh-98-2-1.0-254-5.lcd

Analysis Report

<Sample Information>

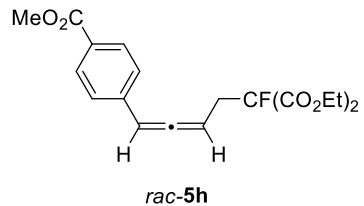
Sample Name : zhy-zg-56-rac-ogh-90-10-1.0-254-1
 Sample ID :
 Data Filename : zhy-zg-56-rac-ogh-90-10-1.0-254-2.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/11/16 16:21:05
 Date Processed : 2023/1/18 18:13:57
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	39.079	4829153	65444	50.591
2	45.432	4716312	58103	49.409
Total		9545465	123547	



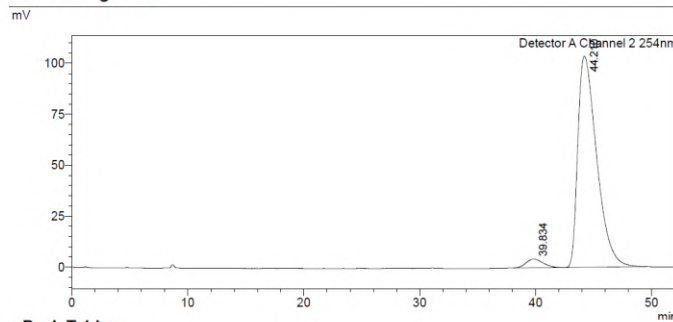
D:\Data\ZHY\ZG\zhy-zg-56-rac-ogh-90-10-1.0-254-2.lcd

Analysis Report

<Sample Information>

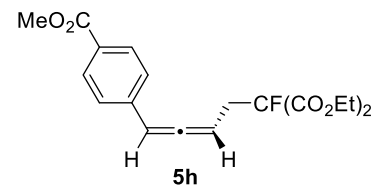
Sample Name : zhy-zg-56-asy-ogh-90-10-1.0-254-230-3
 Sample ID :
 Data Filename : zhy-zg-56-asy-ogh-90-10-1.0-254-230-3.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 10 uL
 Date Acquired : 2023/1/18 17:20:33
 Date Processed : 2023/1/18 18:12:47
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	39.834	447236	4301	3.678
2	44.210	11711976	103610	96.322
Total		12159213	107911	



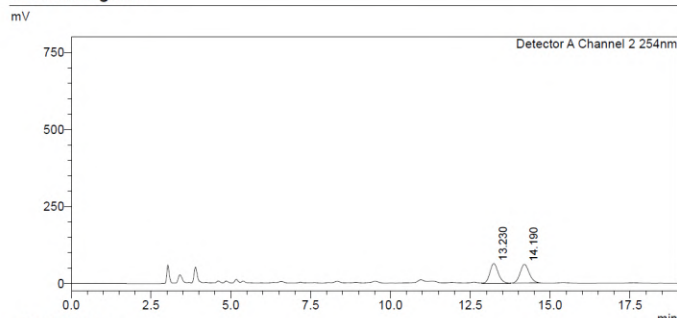
D:\Data\ZHY\ZG\zhy-zg-56-asy-ogh-90-10-1.0-254-230-3.lcd

Analysis Report

<Sample Information>

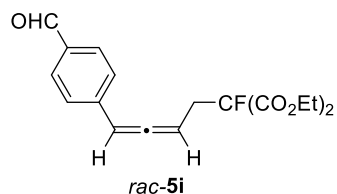
Sample Name : ZHY-ZG128-rac-adh-90-10-1.0-254-230-1
 Sample ID :
 Data Filename : ZHY-ZG128-rac-adh-90-10-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 1 uL
 Date Acquired : 1/17/2023 5:53:28 PM
 Date Processed : 1/18/2023 6:25:01 PM
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	13.230	1197602	64743	50.059
2	14.190	1194785	60641	49.941
Total		2392387	125384	



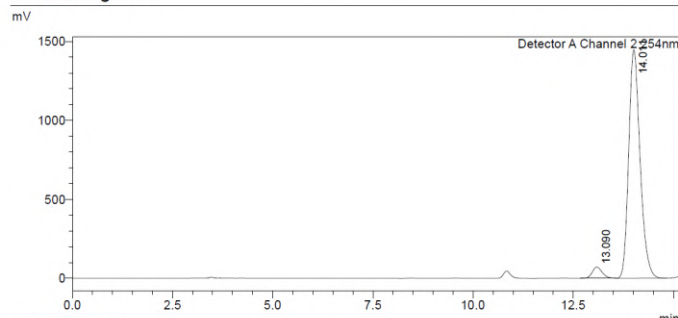
C:\date\ZHY\ZHY-ZG128-rac-adh-90-10-1.0-254-230-1.lcd

Analysis Report

<Sample Information>

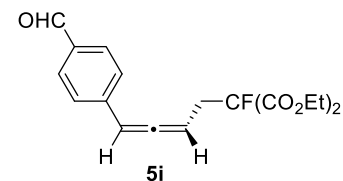
Sample Name : ZHY-ZG128-asy-adh-90-10-1.0-254-230-2
 Sample ID :
 Data Filename : ZHY-ZG128-asy-adh-90-10-1.0-254-230-2.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 1 uL
 Date Acquired : 1/17/2023 9:39:50 PM
 Date Processed : 1/18/2023 5:29:30 PM
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	13.090	1254614	71318	4.175
2	14.011	28793350	1446102	95.825
Total		30047964	1517420	



C:\date\ZHY\ZHY-ZG128-asy-adh-90-10-1.0-254-230-2.lcd

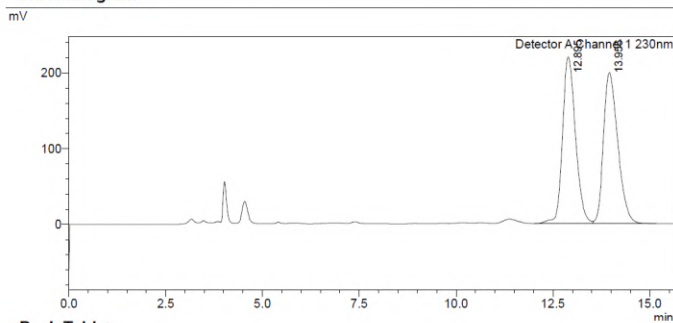
Analysis Report

<Sample Information>

Sample Name : zhy-zg-come(co2et)-rac-odh-90-10-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zg-come(co2et)-rac-odh-90-10-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 10 uL
 Date Acquired : 2023/1/18 11:34:42
 Date Processed : 2023/1/18 11:50:19

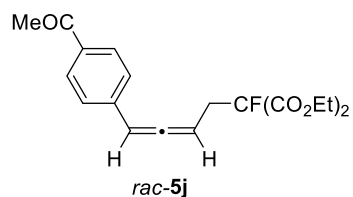
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	12.895	5140871	219751	50.020
2	13.956	5136742	199441	49.980
Total		10277613	419192	



D:\Data\ZHY\ZG\zhy-zg-come(co2et)-rac-odh-90-10-1.0-254-230-1.lcd

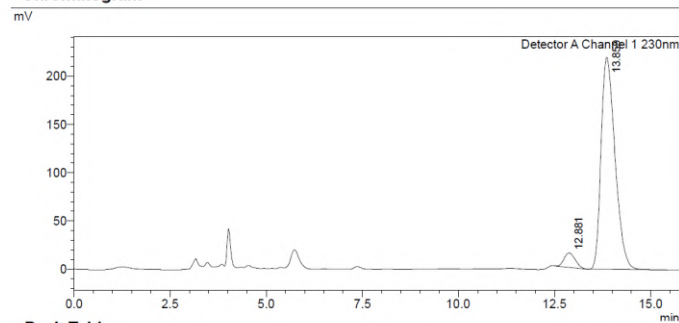
Analysis Report

<Sample Information>

Sample Name : zhy-zg-come(co2et)-asy-odh-90-10-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zg-come(co2et)-asy-odh-90-10-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 10 uL
 Date Acquired : 2023/1/18 11:50:45
 Date Processed : 2023/1/18 12:06:32

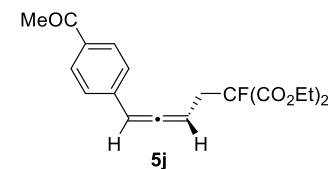
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	12.881	297287	14893	5.093
2	13.859	5539698	219538	94.907
Total		5836985	234431	



D:\Data\ZHY\ZG\zhy-zg-come(co2et)-asy-odh-90-10-1.0-254-230-1.lcd

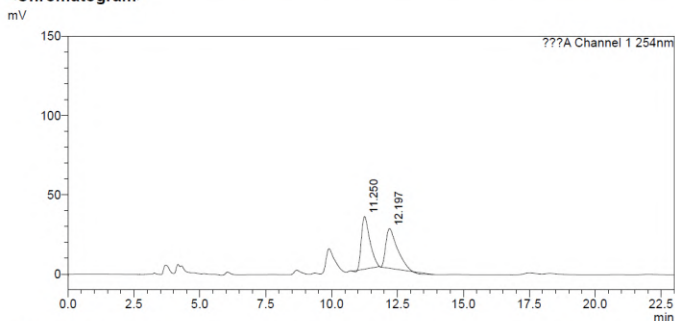


Analysis Report

<Sample Information>

Sample Name : RYL-RB-23-ET-RAC-ADH-1.0-95-5-254-230-3.0
 Sample ID :
 Data Filename : RYL-RB-23-ET-RAC-ADH-1.0-95-5-254-230-3.0.lcd
 Method Filename : RYL-1.0-254-230.lcm
 Batch Filename :
 Vial # : 1-1
 Sample Type : Unknown
 Injection Volume : 20 uL
 Date Acquired : 11/21/2022 5:08:40 PM
 Acquired by : System Administrator
 Date Processed : 11/21/2022 6:56:43 PM
 Processed by : System Administrator

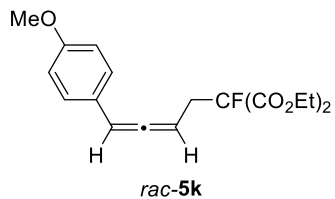
<Chromatogram>



<Peak Table>

??A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	11.250	736004	33133	49.713
2	12.197	744495	24977	50.287
Total		1480499	58110	



F:\Data\RYL\RYL-RB-23-ET-RAC-ADH-1.0-95-5-254-230-3.0.lcd

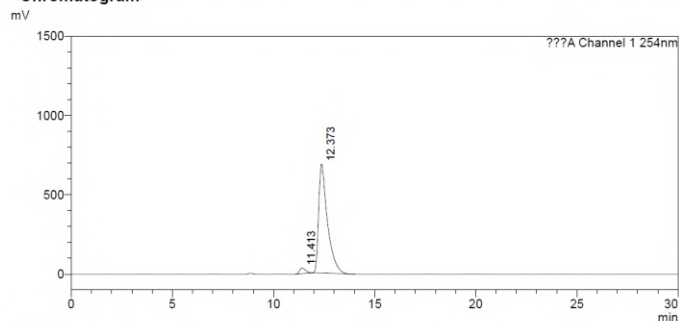


Analysis Report

<Sample Information>

Sample Name : RYL-RB-23-ET-ASY-ADH-1.0-95-5-254-230-1.0
 Sample ID :
 Data Filename : RYL-RB-23-ET-ASY-ADH-1.0-95-5-254-230-1.0.lcd
 Method Filename : RYL-1.0-254-230.lcm
 Batch Filename :
 Vial # : 1-1
 Sample Type : Unknown
 Injection Volume : 20 uL
 Date Acquired : 11/20/2022 12:47:33 PM
 Acquired by : System Administrator
 Date Processed : 11/20/2022 1:24:18 PM
 Processed by : System Administrator

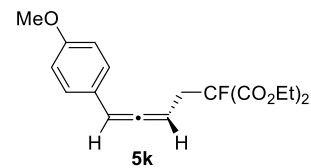
<Chromatogram>



<Peak Table>

??A Channel 1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	11.413	742177	35472	3.481
2	12.373	20576902	687490	96.519
Total		21319079	722962	



F:\Data\RYL\RYL-RB-23-ET-ASY-ADH-1.0-95-5-254-230-1.0.lcd

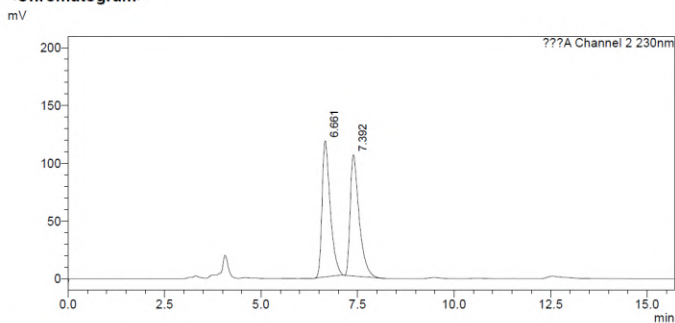


Analysis Report

<Sample Information>

Sample Name : RYL-RB-37-RAC-1.0-ET-ADH-95-5-254-230-1.0
 Sample ID :
 Data Filename : RYL-RB-37-RAC-1.0-ET-ADH-95-5-254-230-1.0.lcd
 Method Filename : GY-1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 11/26/2022 1:20:12 PM
 Date Processed : 11/26/2022 1:35:55 PM
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

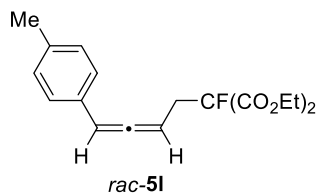
<Chromatogram>



<Peak Table>

???A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	6.661	1735048	117896	50.639
2	7.392	1691279	105088	49.361
Total		3426327	222984	



F:\Data\RYL\RYL-RB-37-RAC-1.0-ET-ADH-95-5-254-230-1.0.lcd

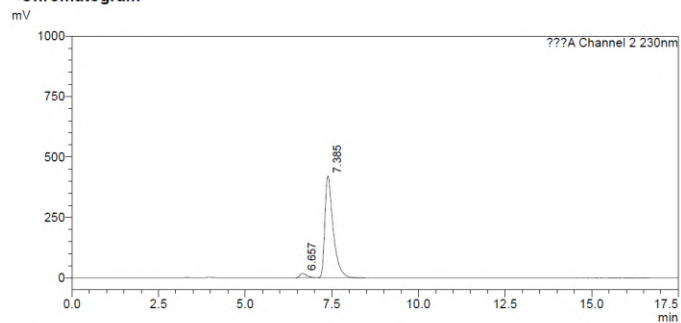


Analysis Report

<Sample Information>

Sample Name : RYL-RB-37-ASY-1.0-ET-ADH-95-5-254-230-3.0
 Sample ID :
 Data Filename : RYL-RB-37-ASY-1.0-ET-ADH-95-5-254-230-3.0.lcd
 Method Filename : GY-1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 11/26/2022 2:56:19 PM
 Date Processed : 11/26/2022 3:14:17 PM
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

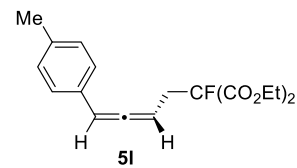
<Chromatogram>



<Peak Table>

???A Channel 2 230nm

Peak#	Ret. Time	Area	Height	Conc.
1	6.657	244134	17907	3.374
2	7.385	6992010	420764	96.626
Total		7236144	438671	



F:\Data\RYL\RYL-RB-37-ASY-1.0-ET-ADH-95-5-254-230-3.0.lcd

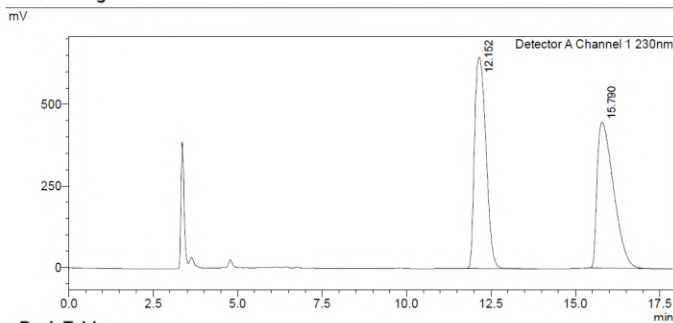
Analysis Report

<Sample Information>

Sample Name : zhy-zg-58-rac-ogh-95-5-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zg-58-rac-ogh-95-5-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 10 uL
 Date Acquired : 2023/1/6 17:43:30
 Date Processed : 2023/1/6 18:01:25

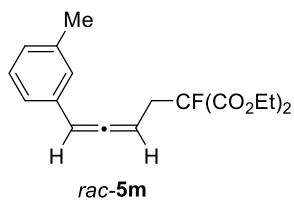
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	12.153	28902822	1228782	50.146
2	15.792	28734929	848966	49.854
Total		57637751	2077748	



D:\Data\ZHY\ZG\zhy-zg-58-rac-ogh-95-5-1.0-254-230-1.lcd

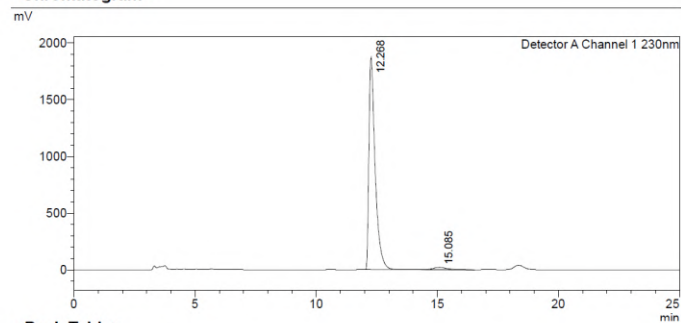
Analysis Report

<Sample Information>

Sample Name : zhy-zg-58-asy-ogh-95-5-1.0-254-1
 Sample ID :
 Data Filename : zhy-zg-58-asy-ogh-95-5-1.0-254-5.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/11/11 11:17:24
 Date Processed : 2023/1/6 18:01:09

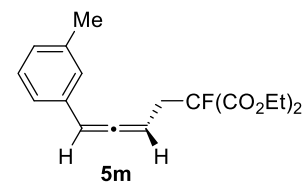
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	12.268	33449893	1870886	97.600
2	15.085	822594	20633	2.400
Total		34272487	1891519	



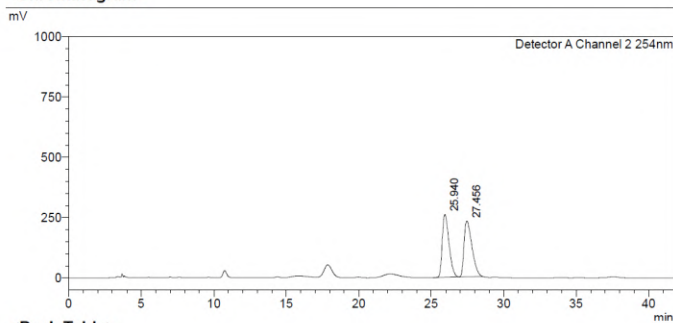
D:\Data\ZHY\ZG\zhy-zg-58-asy-ogh-95-5-1.0-254-5.lcd

Analysis Report

<Sample Information>

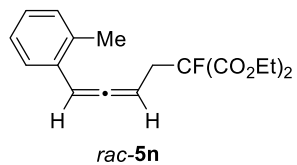
Sample Name : zhy-zh-54-rac-oj3-98-2-1.0-254-230-5
 Sample ID :
 Data Filename : zhy-zh-54-rac-oj3-98-2-1.0-254-230-10.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/5/2 19:57:37
 Date Processed : 2023/5/2 20:39:21
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	25.940	8472487	261623	49.140
2	27.456	8769039	231727	50.860
Total		17241526	493350	



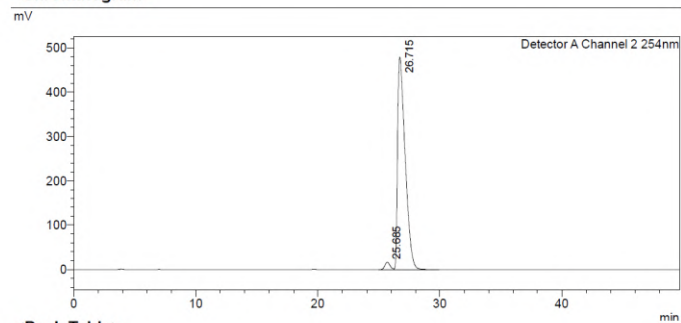
D:\Data\ZHY\ZH\zhy-zh-54-rac-oj3-98-2-1.0-254-230-10.lcd

Analysis Report

<Sample Information>

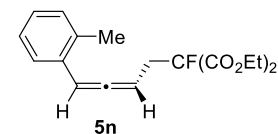
Sample Name : zhy-zh-54-asy-oj3-98-2-1.0-254-230-6
 Sample ID :
 Data Filename : zhy-zh-54-asy-oj3-98-2-1.0-254-230-12.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/5/2 21:56:14
 Date Processed : 2023/5/2 22:46:23
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	25.685	482092	16650	2.283
2	26.715	20638441	478948	97.717
Total		21120533	495598	



D:\Data\ZHY\ZH\zhy-zh-54-asy-oj3-98-2-1.0-254-230-12.lcd

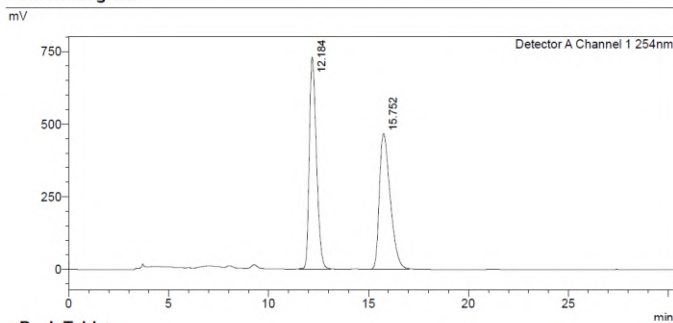
Analysis Report

<Sample Information>

Sample Name : zhy-ze-102-4-asy-ojh-80-20-1.0-254-1
 Sample ID :
 Data Filename : zhy-ze-102-4-rac-ojh-95-5-1.0-254-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/7/18 8:53:09
 Date Processed : 2022/8/18 21:17:42

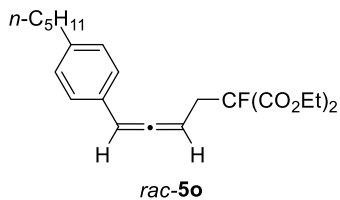
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	12.184	18010369	729459	50.491
2	15.752	17660157	466065	49.509
Total		35670526	1195523	



D:\Data\ZHY\ZE\zhy-ze-102-4-rac-ojh-95-5-1.0-254-1.lcd

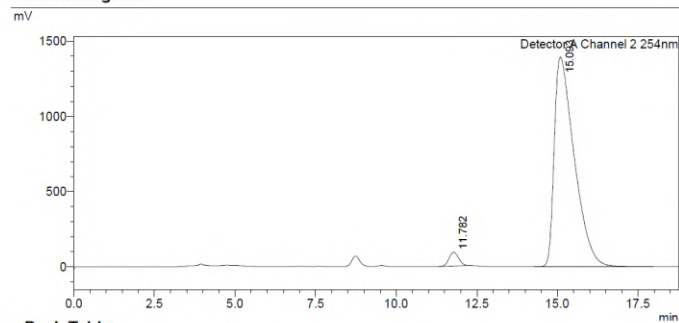
Analysis Report

<Sample Information>

Sample Name : zhy-zg-55-asy-ojh-95-5-1.0-254-1
 Sample ID :
 Data Filename : zhy-zg-55-asy-ojh-95-5-1.0-254-2.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/11/11 9:15:03
 Date Processed : 2022/11/11 10:07:32

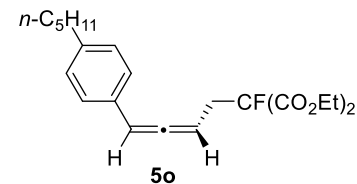
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	11.782	1929122	92370	3.118
2	15.093	59947311	1393309	96.882
Total		61876434	1485679	



D:\Data\ZHY\ZG\zhy-zg-55-asy-ojh-95-5-1.0-254-2.lcd

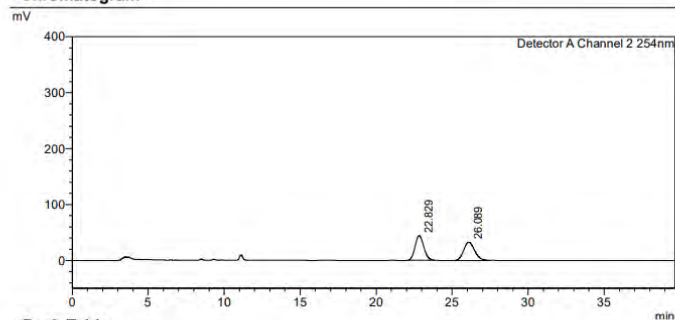
Analysis Report

<Sample Information>

Sample Name : zhy-zg-149-rac-ogh-80-20-1.0-254-230-5
 Sample ID :
 Data Filename : zhy-zg-149-rac-ogh-80-20-1.0-254-230-5.lcd
 Method Filename : LUOHUI-1.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/2/13 21:21:27
 Date Processed : 2023/2/13 22:02:06

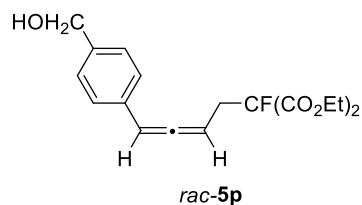
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	22.829	1729103	43811	50.530
2	26.089	1692833	32988	49.470
Total		3421935	76799	



D:\Data\ZHY\ZG\zhy-zg-149-rac-ogh-80-20-1.0-254-230-5.lcd

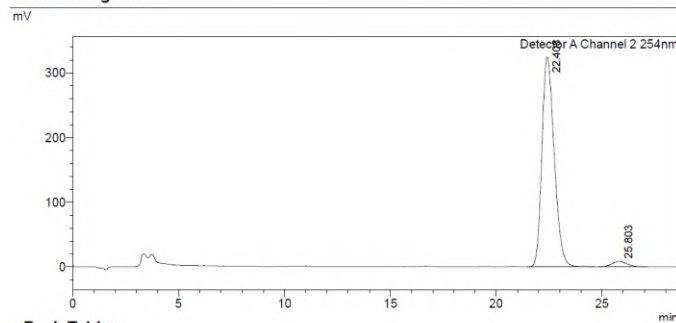
Analysis Report

<Sample Information>

Sample Name : zhy-zg-149-asy-ogh-80-20-1.0-254-230-5
 Sample ID :
 Data Filename : zhy-zg-149-asy-ogh-80-20-1.0-254-230-5.lcd
 Method Filename : LUOHUI-1.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/2/13 20:39:57
 Date Processed : 2023/2/13 21:08:34

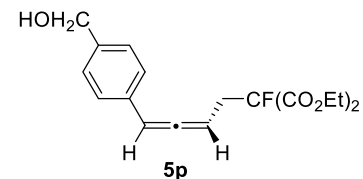
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	22.408	13102201	324260	96.944
2	25.803	413043	8312	3.056
Total		13515244	332572	



D:\Data\ZHY\ZG\zhy-zg-149-asy-ogh-80-20-1.0-254-230-5.lcd

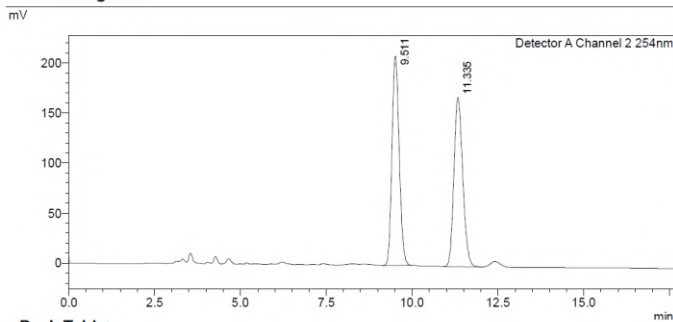
Analysis Report

<Sample Information>

Sample Name : zhy-zg-110-rac-odh-95-5-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zg-110-rac-odh-95-5-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 10 uL
 Date Acquired : 2023/1/10 17:15:57
 Date Processed : 2023/1/10 17:39:02

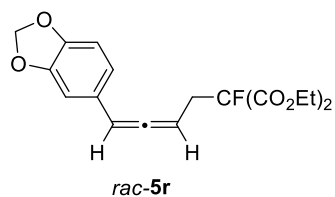
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	9.511	3056818	209094	50.214
2	11.335	3030749	169260	49.786
Total		6087568	378354	



D:\Data\ZHY\ZG\zhy-zg-110-rac-odh-95-5-1.0-254-230-1.lcd

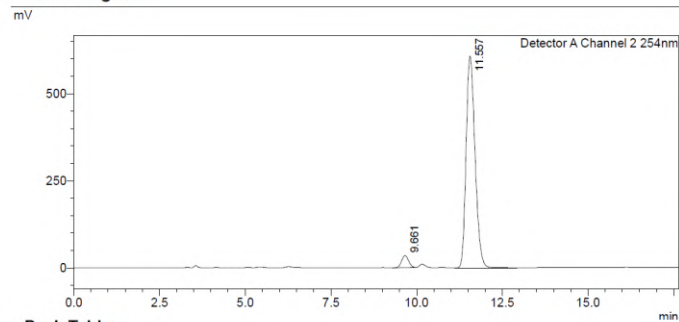
Analysis Report

<Sample Information>

Sample Name : zhy-zg-110-asy-odh-95-5-1.0-254-230-2
 Sample ID :
 Data Filename : zhy-zg-110-asy-odh-95-5-1.0-254-230-2.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 10 uL
 Date Acquired : 2023/1/10 20:08:43
 Date Processed : 2023/1/10 20:26:22

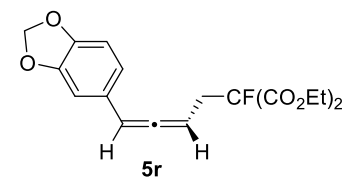
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	9.661	490877	34592	4.280
2	11.557	10979138	607237	95.720
Total		11470015	641829	



D:\Data\ZHY\ZG\zhy-zg-110-asy-odh-95-5-1.0-254-230-2.lcd

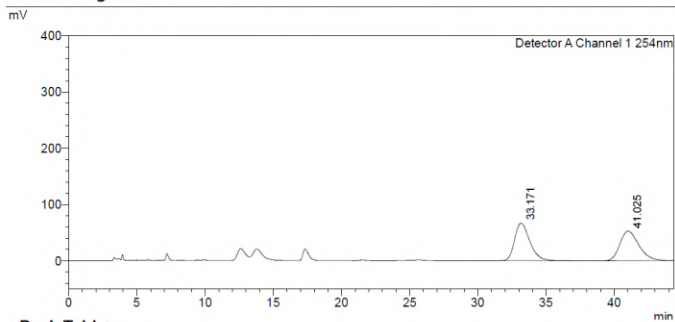
Analysis Report

<Sample Information>

Sample Name : zhy-zg-63-rac-ogh-80-20-1.0-254-1
 Sample ID :
 Data Filename : zhy-zg-63-rac-ogh-80-20-1.0-254-1.lcd
 Method Filename : xsl-230-254-1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/11/14 10:30:03
 Date Processed : 2023/1/18 16:32:19

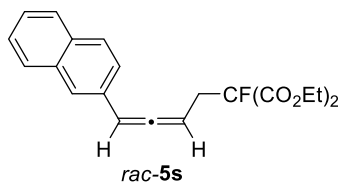
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	33.171	5193100	66888	50.301
2	41.025	5131039	52802	49.699
Total		10324139	119690	



D:\Data\ZHY\ZG\zhy-zg-63-rac-ogh-80-20-1.0-254-1.lcd

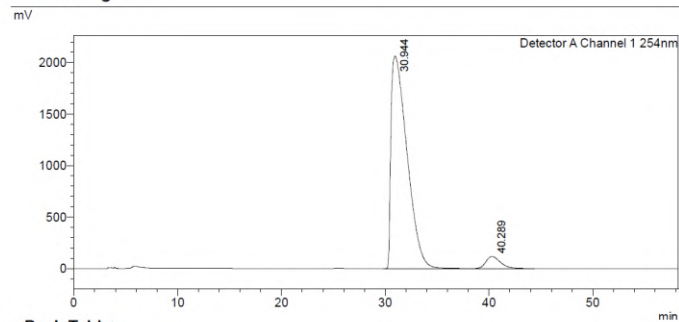
Analysis Report

<Sample Information>

Sample Name : zhy-zg-63-asy-ogh-80-20-1.0-254-2
 Sample ID :
 Data Filename : zhy-zg-63-asy-ogh-80-20-1.0-254-2.lcd
 Method Filename : xsl-230-254-1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/11/14 11:15:35
 Date Processed : 2022/11/14 12:13:50

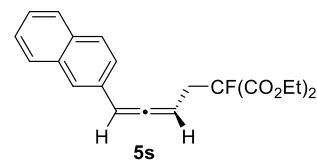
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	30.944	221867868	2062034	95.166
2	40.289	11269447	116649	4.834
Total		233137316	2178683	



D:\Data\ZHY\ZG\zhy-zg-63-asy-ogh-80-20-1.0-254-2.lcd

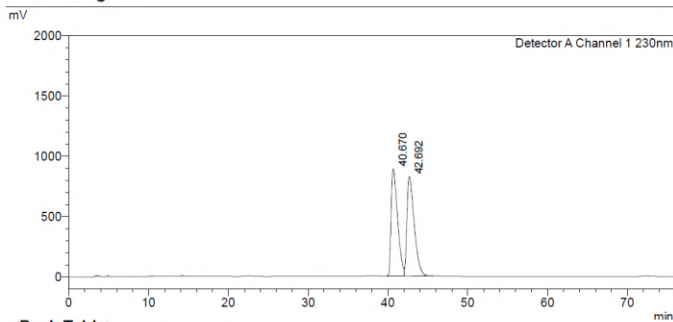
Analysis Report

<Sample Information>

Sample Name : zhy-zh-48-rac-oj3-95-5-1.0-254-230-2
 Sample ID :
 Data Filename : zhy-zh-48-rac-oj3-95-5-1.0-254-230-3.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/5/2 10:17:33
 Date Processed : 2023/5/2 11:33:21

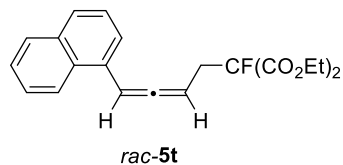
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	40.670	50630994	890312	49.117
2	42.692	52452143	825689	50.883
Total		103083137	1716001	



D:\Data\ZHY\ZH\zhy-zh-48-rac-oj3-95-5-1.0-254-230-3.lcd

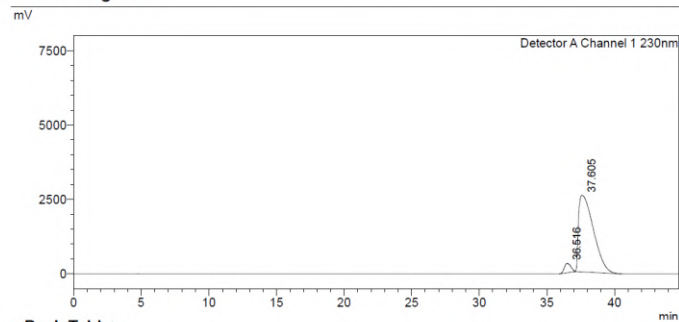
Analysis Report

<Sample Information>

Sample Name : zhy-zh-48-asy-oj3-95-5-1.0-254-230-2
 Sample ID :
 Data Filename : zhy-zh-48-asy-oj3-95-5-1.0-254-230-3.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/5/2 14:18:16
 Date Processed : 2023/5/4 15:20:20

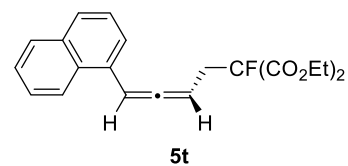
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	36.516	10459731	314627	5.062
2	37.605	196160248	2568952	94.938
Total		206619979	2883580	



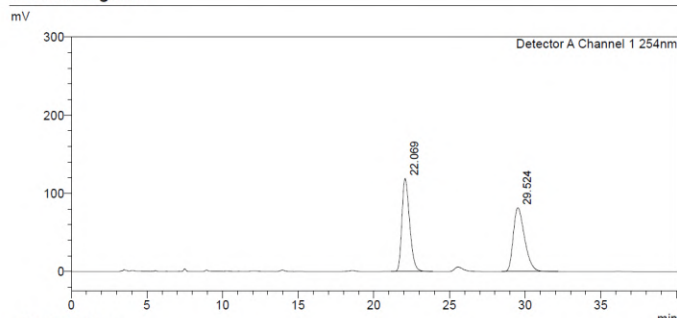
D:\Data\ZHY\ZH\zhy-zh-48-asy-oj3-95-5-1.0-254-230-3.lcd

Analysis Report

<Sample Information>

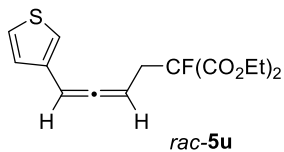
Sample Name : zhy-zh-11-rac-objh-90-10-1.0-254-230-2
 Sample ID :
 Data Filename : zhy-zh-11-rac-objh-90-10-1.0-254-230-3.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2/25/2023 9:38:32 AM
 Date Processed : 2/25/2023 10:18:41 AM
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	22.069	4242786	119085	49.930
2	29.524	4254691	81775	50.070
Total		8497477	200860	



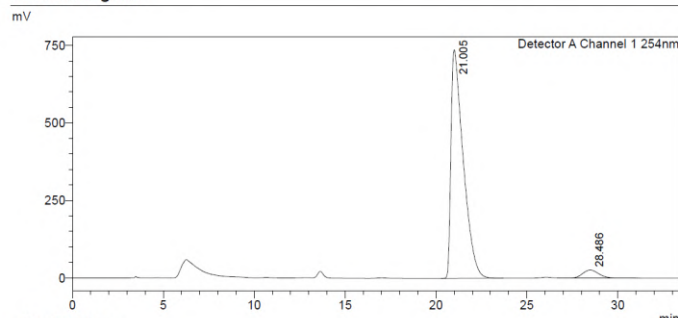
C:\date\ZHY\zhy-zh-11-rac-objh-90-10-1.0-254-230-3.lcd

Analysis Report

<Sample Information>

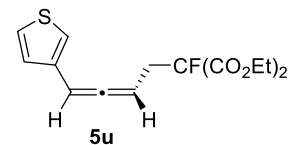
Sample Name : zhy-zh-11-asy-objh-90-10-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zh-11-asy-objh-90-10-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2/24/2023 9:56:46 PM
 Date Processed : 2/24/2023 11:03:54 PM
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	21.005	34555216	736798	95.693
2	28.486	1555300	25629	4.307
Total		36110515	762427	



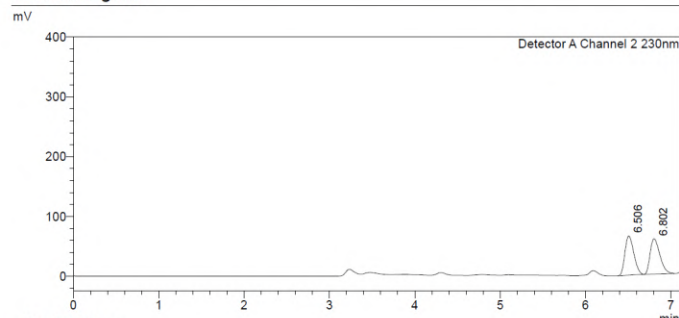
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Analysis Report

<Sample Information>

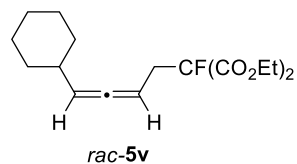
Sample Name : zhy-zh-67-rac-as-3-99.5-0.5-1.0-230-205-3
 Sample ID :
 Data Filename : zhy-zh-67-rac-as-3-99.5-0.5-1.0-230-205-3.lcd
 Method Filename : 1.0-205.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 5/16/2023 10:45:35 PM
 Date Processed : 5/16/2023 10:53:56 PM
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	6.506	474242	65562	50.365
2	6.802	467361	59117	49.635
Total		941604	124678	



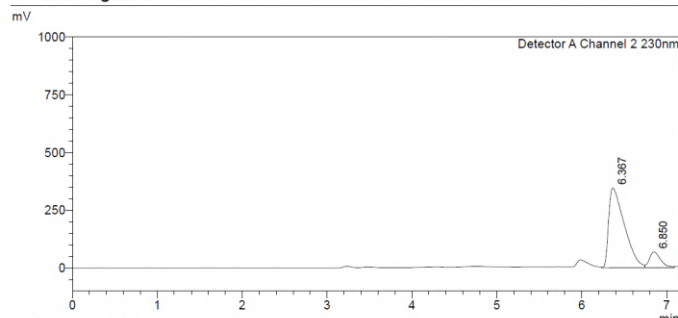
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Analysis Report

<Sample Information>

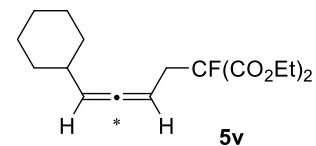
Sample Name : zhy-zh-67-asy-as-3-99.5-0.5-1.0-230-205-3
 Sample ID :
 Data Filename : zhy-zh-67-asy-as-3-99.5-0.5-1.0-230-205-3.lcd
 Method Filename : 1.0-205.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 5/16/2023 11:02:08 PM
 Date Processed : 5/16/2023 11:09:49 PM
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	6.367	4421687	345387	87.651
2	6.850	622991	68295	12.349
Total		5044677	413681	



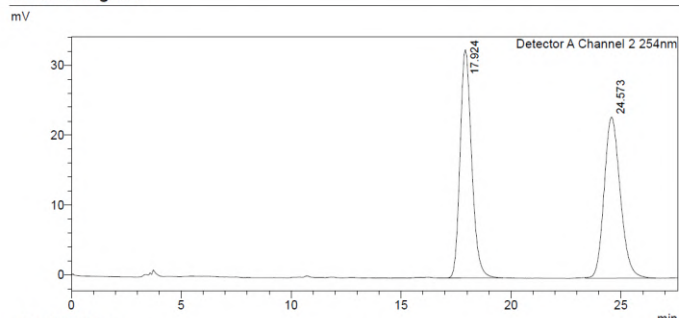
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Analysis Report

<Sample Information>

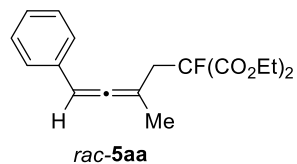
Sample Name : LIL-LL-78RAC-QJH-98-2-254-230-1.0-1
 Sample ID :
 Data Filename : LIL-LL-78-RAC-QJH-98-2-254-230-1.0-1.lcd
 Method Filename : 254-230-1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 5/18/2023 2:37:03 PM
 Date Processed : 5/19/2023 3:45:02 PM
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	17.924	1196083	32660	50.368
2	24.573	1178601	23060	49.632
Total		2374684	55719	



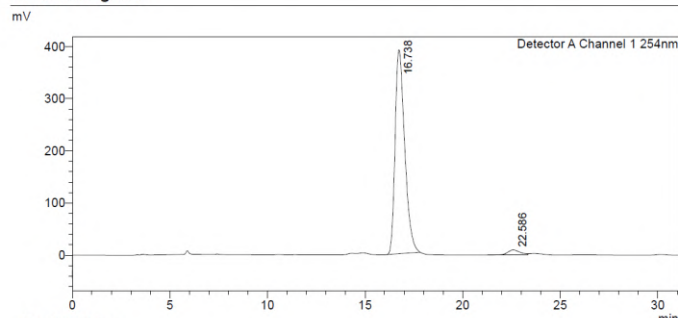
C:\data\LIL\LL-78-RAC-QJH-98-2-254-230-1.0-1.lcd

Analysis Report

<Sample Information>

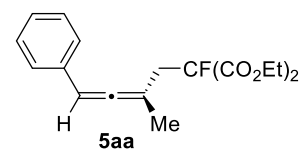
Sample Name : lil-ll-97-asy-qjh-98-2-254-230-1
 Sample ID :
 Data Filename : lil-ll-97-asy-qjh-98-2-254-230-1.lcd
 Method Filename : 254-230-1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 5/25/2023 9:01:43 AM
 Date Processed : 5/25/2023 9:32:51 AM
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	16.738	13354306	390506	96.737
2	22.586	450507	9709	3.263
Total		13804812	400215	



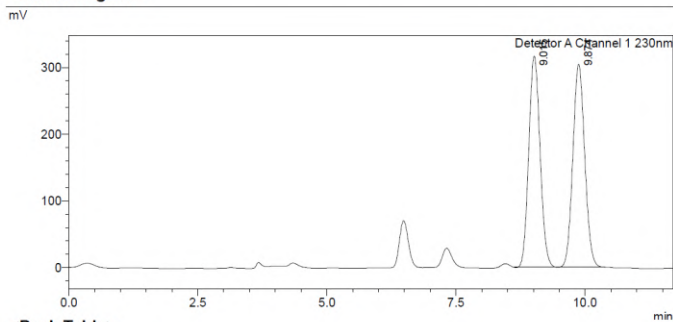
C:\data\LIL\ll-97-asy-qjh-98-2-254-230-1.lcd

Analysis Report

<Sample Information>

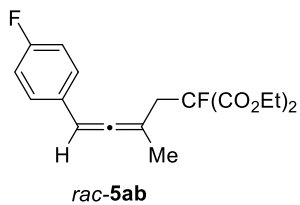
Sample Name	LIL-LL-64-RAC-ADH-98-2-254-230-1.0-2		
Sample ID			
Data Filename	LIL-LL-64-RAC-ADH-98-2-254-230-1.0-2.lcd		
Method Filename	LUOHUI-1.lcm		
Batch Filename			
Vial #	1-1	Sample Type	Unknown
Injection Volume	20 uL		
Date Acquired	2023/5/12 17:10:16	Acquired by	System Administrator
Date Processed	2023/5/12 17:22:00	Processed by	System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	9.015	4821477	316532	49.737
2	9.874	4872526	304199	50.263
Total		9694003	620731	



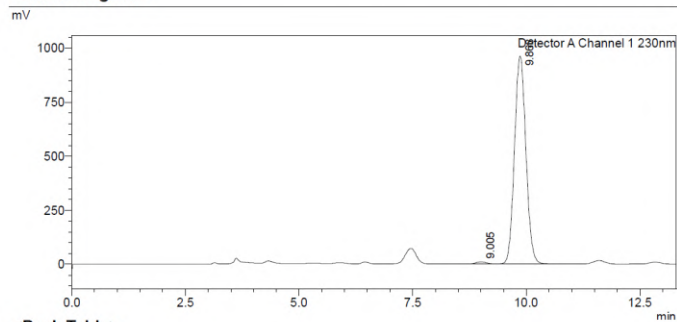
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Analysis Report

<Sample Information>

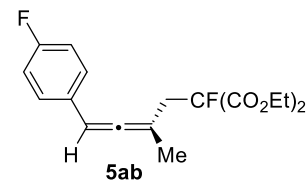
Sample Name	LIL-LL-64-ASY-ADH-98-2-254-230-1.0-1		
Sample ID			
Data Filename	LIL-LL-64-ASY-ADH-98-2-254-230-1.0-1.lcd		
Method Filename	LUOHUI-1.lcm		
Batch Filename			
Val #	1-1	Sample Type	Unknown
Injection Volume	20 uL		
Date Acquired	2023/5/12 16:36:49	Acquired by	System Administrator
Date Processed	2023/5/12 16:50:08	Processed by	System Administrator

<Chromatogram>



<Peak Table>

Detector A Channel 1 230nm				
Peak#	Ret. Time	Area	Height	Conc.
1	9.005	147238	9573	0.86
2	9.863	16794871	961216	99.13
Total		16942110	970789	



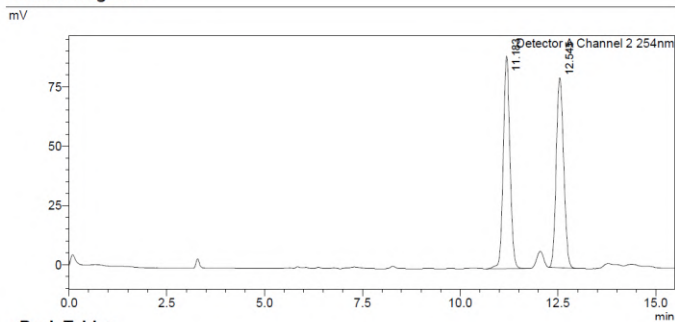
D:\Data\lil\LL\LIL-LL-64-ASY-ADH-98-2-254-230-1.0-1.lcd

Analysis Report

<Sample Information>

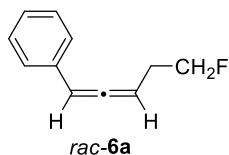
Sample Name : zhy-zg-92-rac-odh-99.9-0.1-1.0-254-205-1
 Sample ID :
 Data Filename : zhy-zg-92-rac-odh-99.9-0.1-1.0-254-205-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 10 uL
 Date Acquired : 2023/1/5 17:38:40
 Date Processed : 2023/1/5 17:54:10
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	11.183	1077642	89494	50.637
2	12.545	1050522	80043	49.363
Total		2128165	169537	



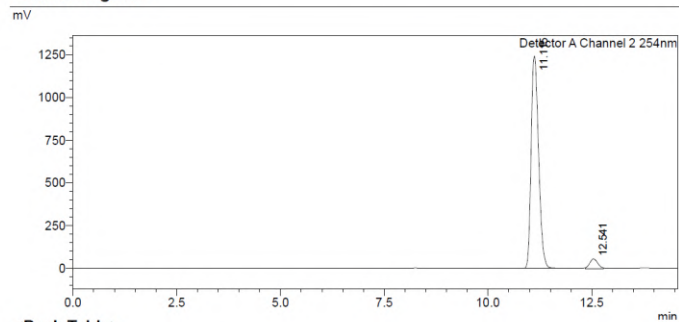
D:\Data\ZHY\ZG\zhy-zg-92-rac-odh-99.9-0.1-1.0-254-205-1.lcd

Analysis Report

<Sample Information>

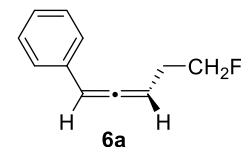
Sample Name : zhy-zg-92-asy-odh-99.9-0.1-1.0-254-205-1
 Sample ID :
 Data Filename : zhy-zg-92-asy-odh-99.9-0.1-1.0-254-205-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 10 uL
 Date Acquired : 2023/1/5 20:23:20
 Date Processed : 2023/1/5 20:37:54
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	11.115	15390110	1241664	95.448
2	12.541	734003	55617	4.552
Total		16124114	1297282	



D:\Data\ZHY\ZG\zhy-zg-92-asy-odh-99.9-0.1-1.0-254-205-1.lcd

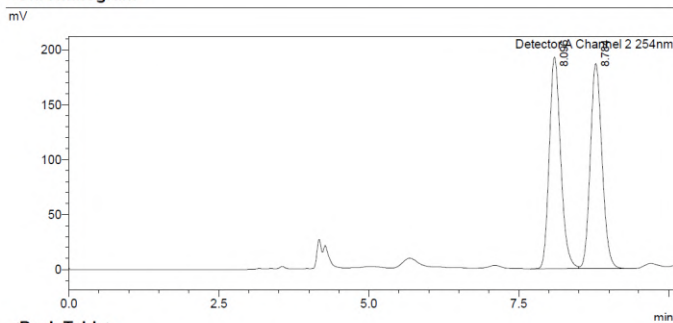
Analysis Report

<Sample Information>

Sample Name : zhy-zg-93-rac-odh-99-1-1.0-254-205-2
 Sample ID :
 Data Filename : zhy-zg-93-rac-odh-99-1-1.0-254-205-2.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 10 uL
 Date Acquired : 2023/1/6 11:41:08
 Date Processed : 2023/1/6 11:57:49

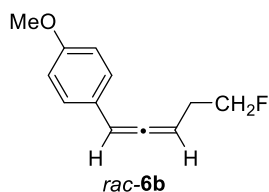
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	8.096	2576705	192588	50.123
2	8.784	2564051	186639	49.877
Total		5140756	379227	



D:\Data\ZHY\ZG\zhy-zg-93-rac-odh-99-1-1.0-254-205-2.lcd

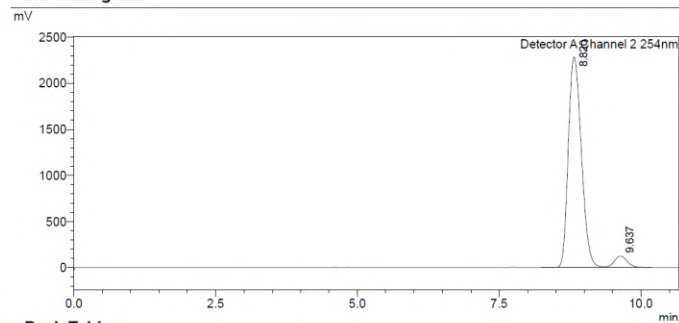
Analysis Report

<Sample Information>

Sample Name : ZHY-ZG-93-ASY-ODH-99-1-1.0-254-230-2
 Sample ID :
 Data Filename : ZHY-ZG-93-ASY-ODH-99-1-1.0-254-230-2.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/3/24 14:40:32
 Date Processed : 2023/3/24 14:51:13

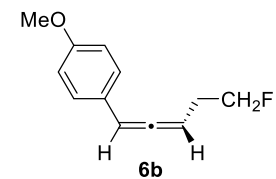
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	8.820	36487150	2283967	94.850
2	9.637	1981050	124744	5.150
Total		38468200	2408711	



D:\Data\ZHY\ZG\ZHY-ZG-93-ASY-ODH-99-1-1.0-254-230-2.lcd

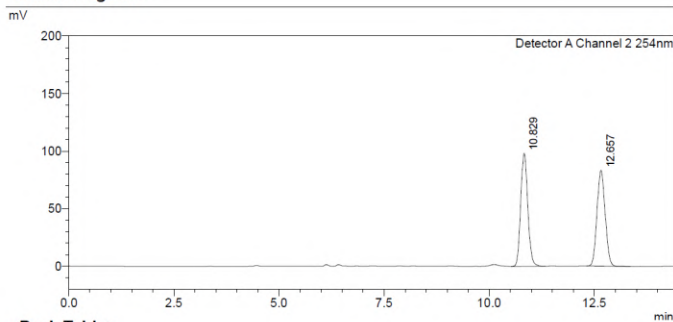
Analysis Report

<Sample Information>

Sample Name : ZHY-ZH-63-RAC-ODH-99.9-0.1-1.0-254-230-2
 Sample ID :
 Data Filename : ZHY-ZH-63-RAC-ODH-99.9-0.1-1.0-254-230-4.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/4/25 16:03:02
 Date Processed : 2023/4/25 16:17:26

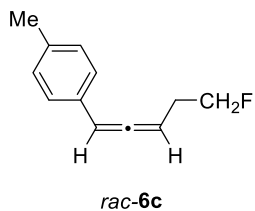
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	10.829	1157184	98239	50.769
2	12.657	1122120	83270	49.231
Total		2279304	181509	



D:\Data\ZHY\ZH\ZHY-ZH-63-RAC-ODH-99.9-0.1-1.0-254-230-4.lcd

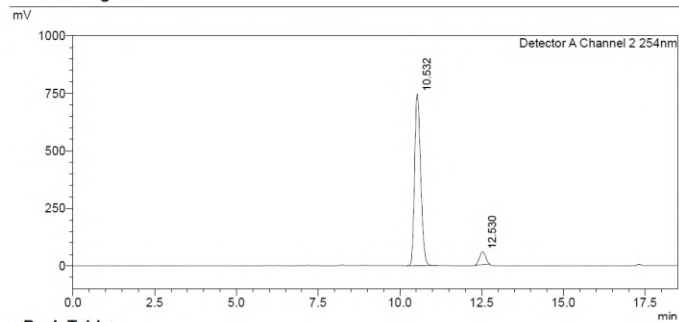
Analysis Report

<Sample Information>

Sample Name : ZHY-ZH-63-ASY-ODH-99.9-0.1-1.0-254-230-2
 Sample ID :
 Data Filename : ZHY-ZH-63-ASY-ODH-99.9-0.1-1.0-254-230-3.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/4/25 15:43:13
 Date Processed : 2023/4/25 16:17:20

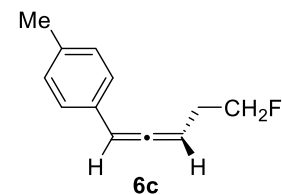
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	10.532	9614899	747061	92.938
2	12.530	730581	56216	7.062
Total		10345480	803277	



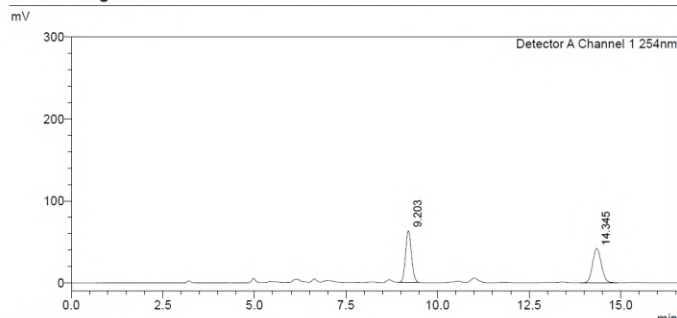
D:\Data\ZHY\ZH\ZHY-ZH-63-ASY-ODH-99.9-0.1-1.0-254-230-3.lcd

Analysis Report

<Sample Information>

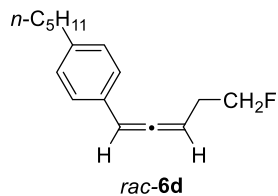
Sample Name : ZHY-ZG-105-RAC-ODH-99.9-0.1-1.0-254-230-1
 Sample ID :
 Data Filename : ZHY-ZG-105-RAC-ODH-99.9-0.1-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 3/29/2023 9:16:14 AM
 Date Processed : 3/30/2023 8:28:20 PM
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	9.203	716384	63450	50.808
2	14.345	693591	42024	49.192
Total		1409975	105474	



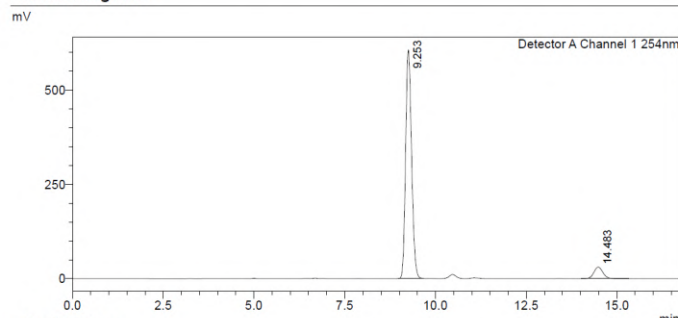
C:\date\ZHY\ZG\ZHY-ZG-105-RAC-ODH-99.9-0.1-1.0-254-230-1.lcd

Analysis Report

<Sample Information>

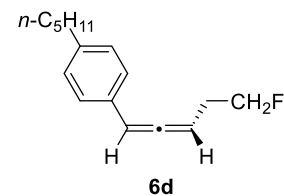
Sample Name : ZHY-ZG-105-ASY-ODH-99.9-0.1-1.0-254-230-2
 Sample ID :
 Data Filename : ZHY-ZG-105-ASY-ODH-99.9-0.1-1.0-254-230-2.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 3/29/2023 9:55:20 AM
 Date Processed : 3/29/2023 10:12:07 AM
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	9.253	6895321	606179	92.929
2	14.483	524692	30612	7.071
Total		7420012	636791	



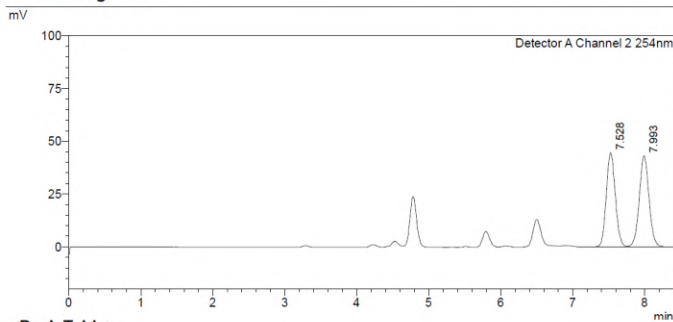
C:\date\ZHY\ZG\ZHY-ZG-105-ASY-ODH-99.9-0.1-1.0-254-230-2.lcd

Analysis Report

<Sample Information>

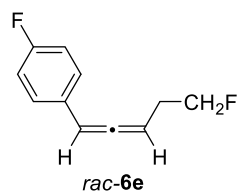
Sample Name : ZHY-ZH-43-RAC-ODH-99.9-0.1-1.0-254-230-1
 Sample ID :
 Data Filename : ZHY-ZH-43-RAC-ODH-99.9-0.1-1.0-254-230-2.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/4/21 16:17:03
 Date Processed : 2023/4/25 15:36:36
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	7.528	389765	44661	48.926
2	7.993	406877	43192	51.074
Total		796642	87853	



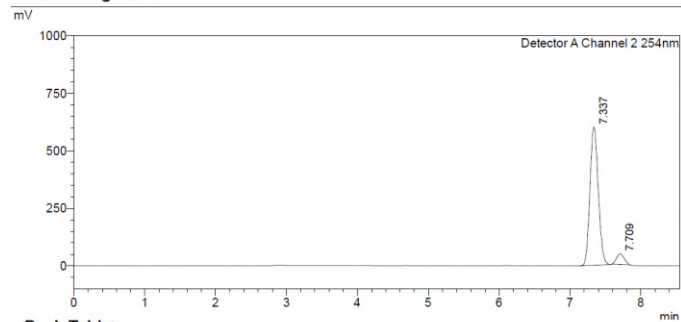
D:\Data\ZHY\ZH\ZHY-ZH-43-RAC-ODH-99.9-0.1-1.0-254-230-2.lcd

Analysis Report

<Sample Information>

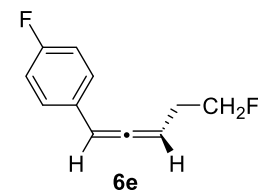
Sample Name : ZHY-ZH-60-ASY-ODH-99.9-0.1-1.0-254-230-2
 Sample ID :
 Data Filename : ZHY-ZH-60-ASY-ODH-99.9-0.1-1.0-254-230-2.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/4/25 15:34:02
 Date Processed : 2023/4/25 15:42:35
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	7.337	4900461	599790	93.394
2	7.709	346613	45831	6.606
Total		5247073	645621	



D:\Data\ZHY\ZH\ZHY-ZH-60-ASY-ODH-99.9-0.1-1.0-254-230-2.lcd

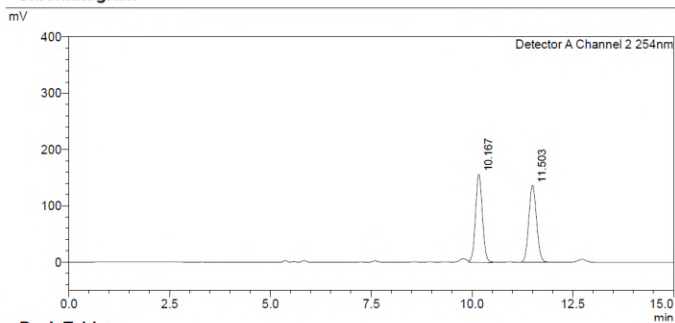
Analysis Report

<Sample Information>

Sample Name : ZHY-ZH-27-RAC-ODH-99.9-0.1-1.0-254-230-1
 Sample ID :
 Data Filename : ZHY-ZH-27-RAC-ODH-99.9-0.1-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/3/24 15:07:57
 Date Processed : 2023/3/24 20:26:14

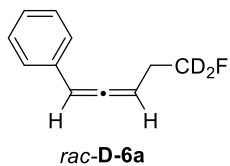
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	10.167	1864450	156681	50.406
2	11.503	1834381	136533	49.594
Total		3698831	293215	



D:\Data\ZHY\ZH\ZHY-ZH-27-RAC-ODH-99.9-0.1-1.0-254-230-1.lcd

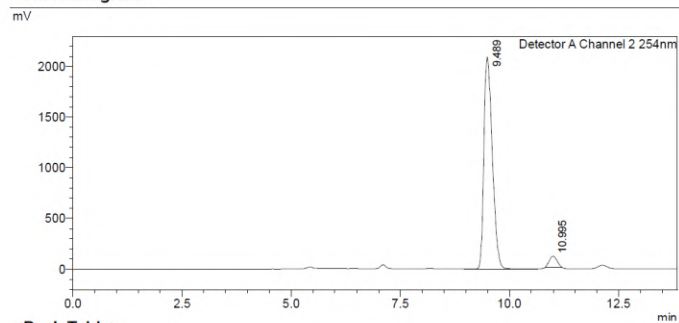
Analysis Report

<Sample Information>

Sample Name : ZHY-ZG-116-ASY-ODH-99.9-0.1-1.0-254-230-2
 Sample ID :
 Data Filename : ZHY-ZG-116-ASY-ODH-99.9-0.1-1.0-254-230-2.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/3/24 20:14:56
 Date Processed : 2023/3/24 20:28:47

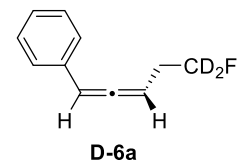
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	9.489	28027898	2090667	95.465
2	10.995	1331368	109395	4.535
Total		29359266	2200062	



D:\Data\ZHY\ZG\ZHY-ZG-116-ASY-ODH-99.9-0.1-1.0-254-230-2.lcd

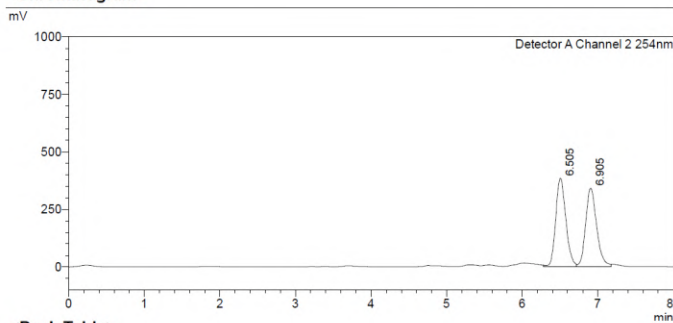
Analysis Report

<Sample Information>

Sample Name : ZHY-ZG-94-RAC-ODH-98-2-1.0-254-230-1
 Sample ID :
 Data Filename : ZHY-ZG-94-RAC-ODH-98-2-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/3/25 22:23:34
 Date Processed : 2023/3/25 22:38:19

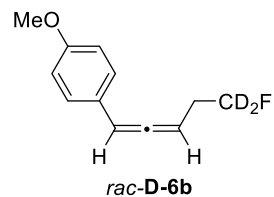
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	6.505	3564084	383794	50.884
2	6.905	3440285	340929	49.116
Total		7004369	724723	



D:\Data\ZHY\ZG\ZHY-ZG-94-RAC-ODH-98-2-1.0-254-230-1.lcd

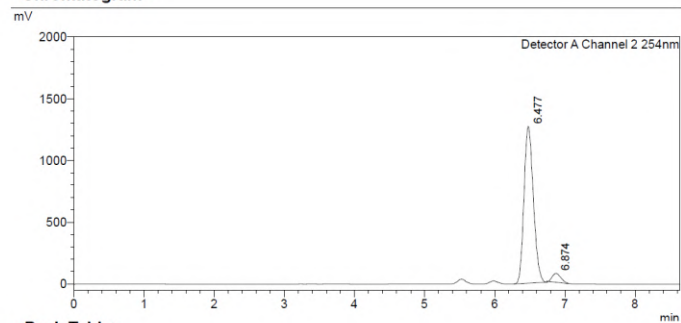
Analysis Report

<Sample Information>

Sample Name : ZHY-ZG-94-ASY-ODH-98-2-1.0-254-230-1
 Sample ID :
 Data Filename : ZHY-ZG-94-ASY-ODH-98-2-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/3/25 22:14:32
 Date Processed : 2023/3/25 22:23:11

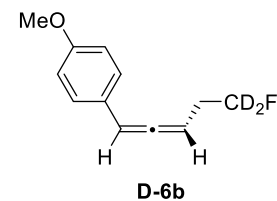
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	6.477	11812858	1271020	95.098
2	6.874	608890	72311	4.902
Total		12421747	1343332	



D:\Data\ZHY\ZG\ZHY-ZG-94-ASY-ODH-98-2-1.0-254-230-1.lcd

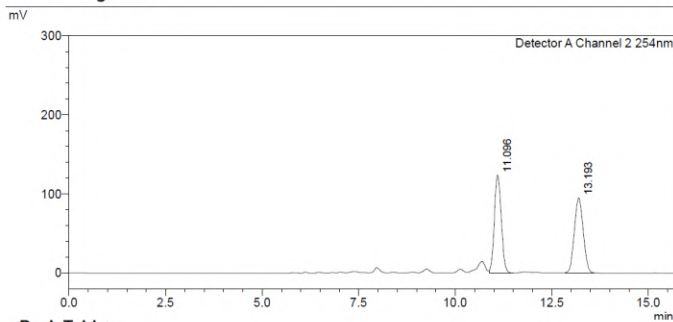
Analysis Report

<Sample Information>

Sample Name : ZHY-ZG-117-RAC-ODH-99.9-0.1-1.0-254-230-2
 Sample ID :
 Data Filename : ZHY-ZG-117-RAC-ODH-99.9-0.1-1.0-254-230-2.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/3/24 20:36:28
 Date Processed : 2023/3/24 20:52:08

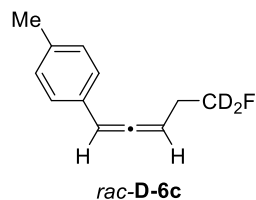
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	11.096	1531150	123352	50.395
2	13.193	1507136	94563	49.605
Total		3038286	217915	



D:\Data\ZHY\ZG\ZHY-ZG-117-RAC-ODH-99.9-0.1-1.0-254-230-2.lcd

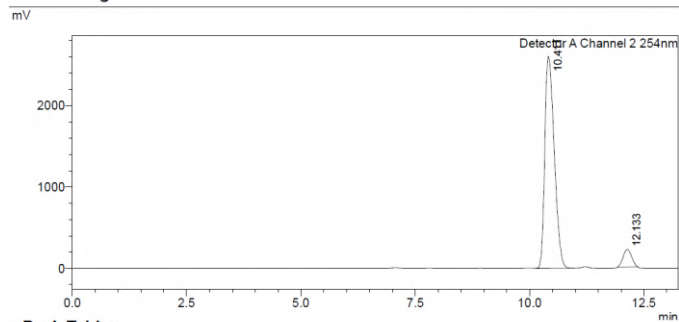
Analysis Report

<Sample Information>

Sample Name : ZHY-ZG-117-ASY-ODH-99.9-0.1-1.0-254-230-3
 Sample ID :
 Data Filename : ZHY-ZG-117-ASY-ODH-99.9-0.1-1.0-254-230-3.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/3/28 18:01:39
 Date Processed : 2023/3/28 18:14:55

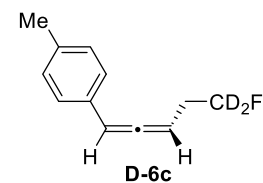
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	10.411	37499409	2606316	92.989
2	12.133	2827367	218538	7.011
Total		40326777	2824855	



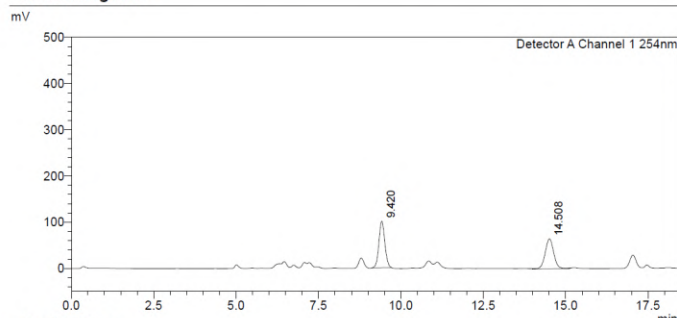
D:\Data\ZHY\ZG\ZHY-ZG-117-ASY-ODH-99.9-0.1-1.0-254-230-3.lcd

Analysis Report

<Sample Information>

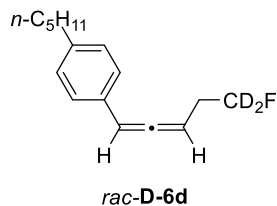
Sample Name : ZHY-ZG-122-RAC-ODH-99.9-0.1-1.0-254-230-2
 Sample ID :
 Data Filename : ZHY-ZG-122-RAC-ODH-99.9-0.1-1.0-254-230-2.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 3/29/2023 10:12:43 AM
 Date Processed : 3/30/2023 8:31:37 PM
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	9.420	1262076	101035	51.520
2	14.508	1187595	65063	48.480
Total		2449671	166098	



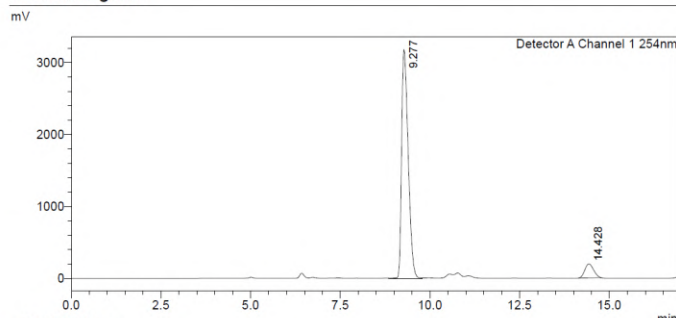
C:\date\ZHY\ZG\ZHY-ZG-122-RAC-ODH-99.9-0.1-1.0-254-230-2.lcd

Analysis Report

<Sample Information>

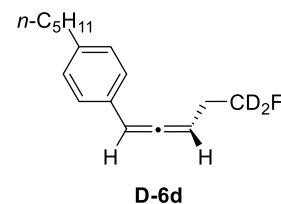
Sample Name : ZHY-ZG-122-ASY-ODH-99.9-0.1-1.0-254-230-2
 Sample ID :
 Data Filename : ZHY-ZG-122-ASY-ODH-99.9-0.1-1.0-254-230-2.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 3/29/2023 10:31:37 AM
 Date Processed : 3/29/2023 10:48:36 AM
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	9.277	40504620	3175871	92.412
2	14.428	3325783	195746	7.588
Total		43830403	3371617	



C:\date\ZHY\ZG\ZHY-ZG-122-ASY-ODH-99.9-0.1-1.0-254-230-2.lcd

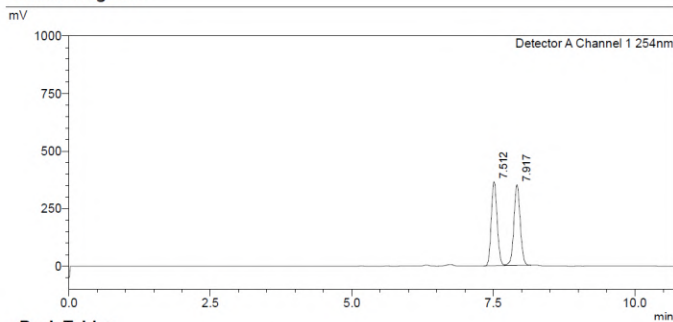
Analysis Report

<Sample Information>

Sample Name : zhy-zh-77-rac-od3-99.9-0.1-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zh-77-rac-od3-99.9-0.1-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/5/25 9:52:46
 Date Processed : 2023/5/25 10:03:27

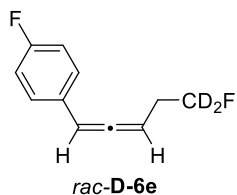
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	7.512	2640650	365393	49.059
2	7.917	2741966	351712	50.941
Total		5382617	717105	



D:\Data\ZHY\ZH\zhy-zh-77-rac-od3-99.9-0.1-1.0-254-230-1.lcd

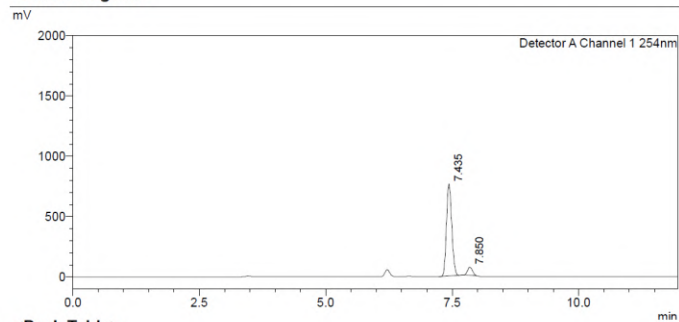
Analysis Report

<Sample Information>

Sample Name : zhy-zh-77-asy-od3-99.9-0.1-1.0-254-230-2
 Sample ID :
 Data Filename : zhy-zh-77-asy-od3-99.9-0.1-1.0-254-230-2.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/5/25 10:42:04
 Date Processed : 2023/5/25 10:58:47

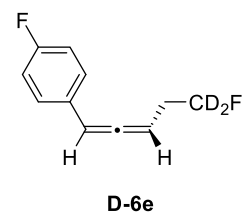
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	7.435	5602004	763941	92.635
2	7.850	445387	65994	7.365
Total		6047392	829935	



D:\Data\ZHY\ZH\zhy-zh-77-asy-od3-99.9-0.1-1.0-254-230-2.lcd

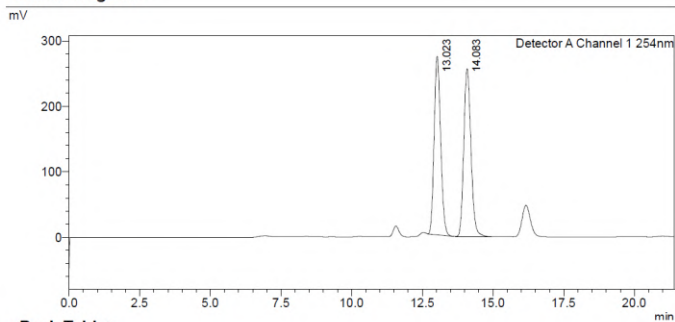
Analysis Report

<Sample Information>

Sample Name : zhy-zf-119-rac-ojh-70-30-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zf-119-rac-ojh-70-30-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/9/23 9:03:40
 Date Processed : 2022/9/23 9:25:07

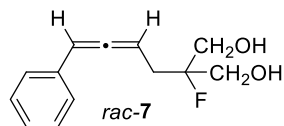
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	13.023	4376061	272430	49.141
2	14.083	4529107	256244	50.859
Total		8905168	528675	



D:\Data\ZHY\ZF\zhy-zf-119-rac-ojh-70-30-1.0-254-230-1.lcd

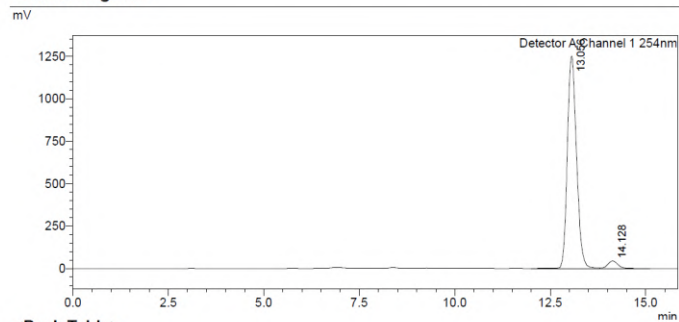
Analysis Report

<Sample Information>

Sample Name : zhy-zf-119-asy-ojh-70-30-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zf-119-asy-ojh-70-30-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/9/23 9:26:38
 Date Processed : 2022/9/23 9:42:29

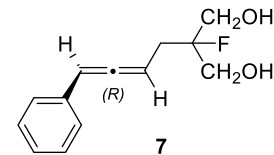
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	13.056	20862408	1250955	96.255
2	14.128	811792	44407	3.745
Total		21674200	1295362	



D:\Data\ZHY\ZF\zhy-zf-119-asy-ojh-70-30-1.0-254-230-1.lcd

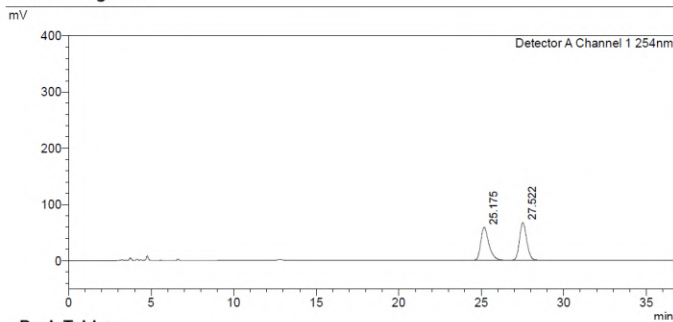
Analysis Report

<Sample Information>

Sample Name : zhy-zh-74-1-rac-ad-3-95-5-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zh-74-1-rac-ad-3-95-5-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/5/16 21:23:36
 Date Processed : 2023/5/16 22:03:13

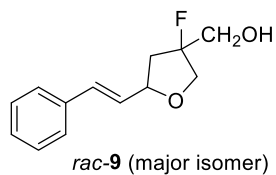
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	25.175	1991958	58639	49.563
2	27.522	2027085	66701	50.437
Total		4019043	125340	



D:\Data\ZHY\ZH\zhy-zh-74-1-rac-ad-3-95-5-1.0-254-230-1.lcd

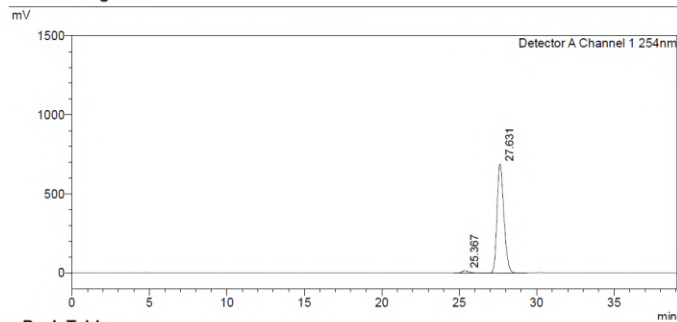
Analysis Report

<Sample Information>

Sample Name : zhy-zh-74-1-asy-ad-3-95-5-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zh-74-1-asy-ad-3-95-5-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/5/16 22:02:23
 Date Processed : 2023/5/16 22:41:28

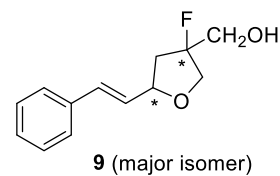
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	25.367	463480	13699	2.131
2	27.631	21288911	689969	97.869
Total		21752391	703668	



D:\Data\ZHY\ZH\zhy-zh-74-1-asy-ad-3-95-5-1.0-254-230-1.lcd

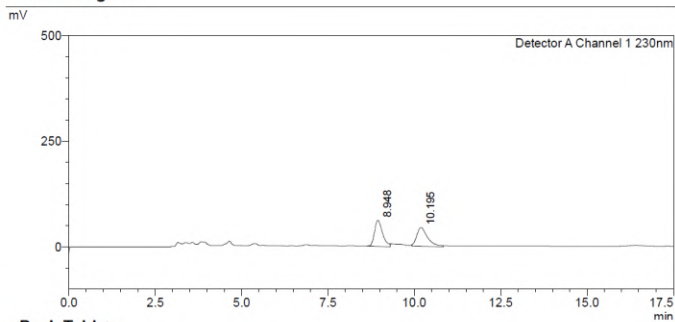
Analysis Report

<Sample Information>

Sample Name : zhy-zh-26-2-rac-adh-85-15-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zh-26-2-rac-adh-85-15-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/3/25 15:12:44
 Date Processed : 2023/3/30 20:34:56

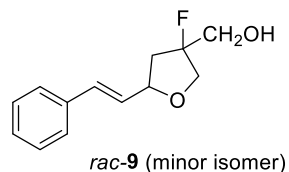
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	8.948	1000945	62064	50.868
2	10.195	966777	44335	49.132
Total		1967723	106399	



D:\Data\ZHY\ZH\zhy-zh-26-2-rac-adh-85-15-1.0-254-230-1.lcd

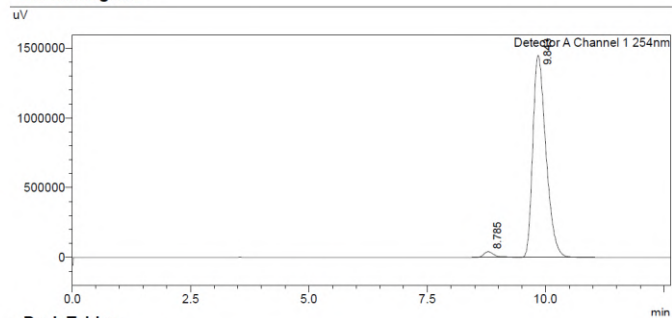
Analysis Report

<Sample Information>

Sample Name : zhy-zh-74-2-asy-adh-85-15-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zh-74-2-asy-adh-85-15-1.0-254-230-1.lcd
 Method Filename : 1.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/5/16 8:56:49
 Date Processed : 2023/5/16 14:15:07

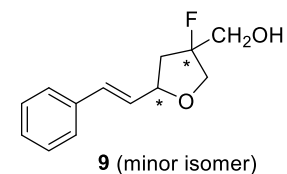
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	8.785	650183	41198	2.269
2	9.843	28010996	1448254	97.731
Total		28661179	1489452	



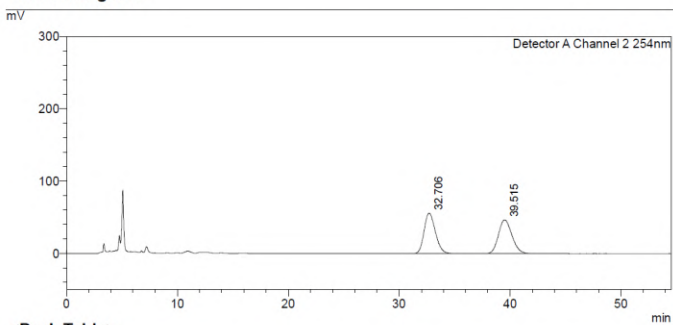
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Analysis Report

<Sample Information>

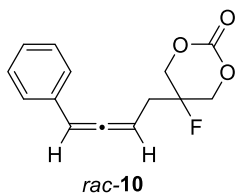
Sample Name : zhy-zg-115-rac-odh-70-30-1.0-254-230-2
 Sample ID :
 Data Filename : zhy-zg-115-rac-odh-70-30-1.0-254-230-2.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 10 uL
 Date Acquired : 2023/1/13 14:28:20
 Date Processed : 2023/1/18 16:52:45
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	32.706	3944264	55956	50.037
2	39.515	3938464	46664	49.963
Total		7882728	102619	



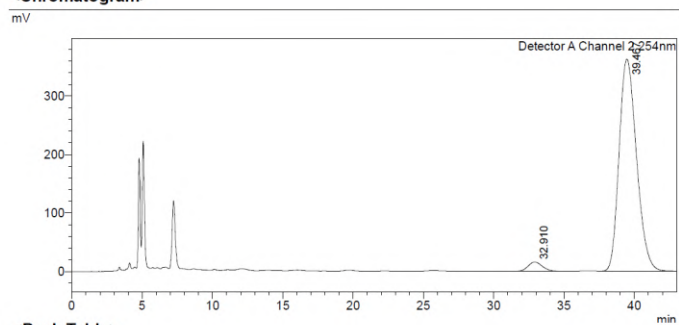
D:\Data\ZHY\ZG\zhy-zg-115-rac-odh-70-30-1.0-254-230-2.lcd

Analysis Report

<Sample Information>

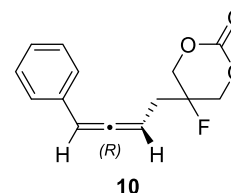
Sample Name : zhy-zg-115-asy-odh-70-30-1.0-254-230-2
 Sample ID :
 Data Filename : zhy-zg-115-asy-odh-70-30-1.0-254-230-2.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 10 uL
 Date Acquired : 2023/1/13 15:24:11
 Date Processed : 2023/1/13 16:07:11
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	32.910	1109008	15774	3.432
2	39.467	31203701	362848	96.568
Total		32312709	378623	



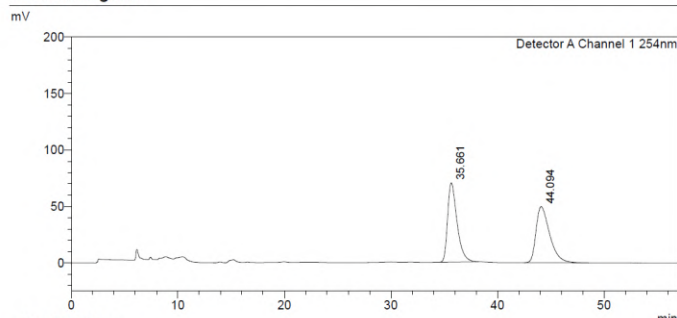
D:\Data\ZHY\ZG\zhy-zg-115-asy-odh-70-30-1.0-254-230-2.lcd

Analysis Report

<Sample Information>

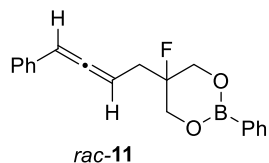
Sample Name : zhy-zh-36-rac-as-3-90-10-0.5-254-230-1
 Sample ID :
 Data Filename : zhy-zh-36-rac-as-3-90-10-0.5-254-230-1.lcd
 Method Filename : 1.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 4/25/2023 4:25:46 PM
 Date Processed : 4/25/2023 5:22:44 PM
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	35.661	4323313	70201	49.644
2	44.094	4385375	49588	50.356
Total		8708689	119789	



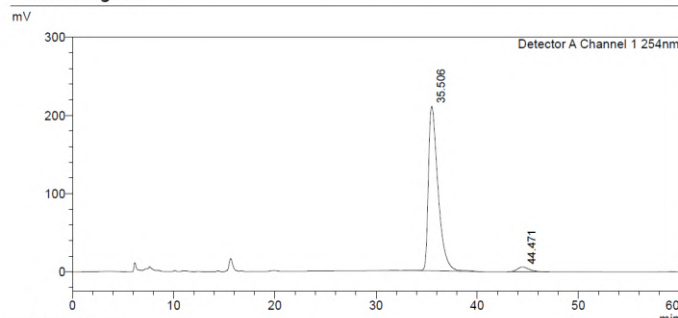
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Analysis Report

<Sample Information>

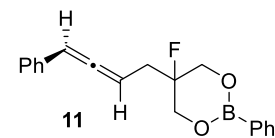
Sample Name : zhy-zh-36-asy-as-3-90-10-0.5-254-230-1
 Sample ID :
 Data Filename : zhy-zh-36-asy-as-3-90-10-0.5-254-230-1.lcd
 Method Filename : 1.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 4/25/2023 5:23:45 PM
 Date Processed : 4/25/2023 6:43:53 PM
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	35.506	13882133	210360	96.504
2	44.471	502921	6038	3.496
Total		14385054	216398	



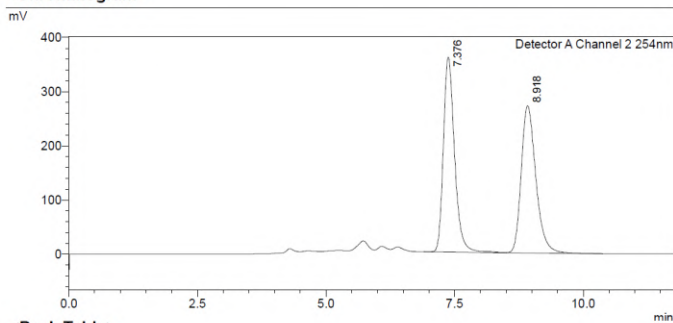
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Analysis Report

<Sample Information>

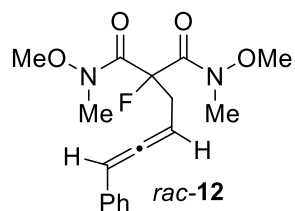
Sample Name : zhy-zg-83-racodh-60-40-1.0-254-230-2
 Sample ID :
 Data Filename : zhy-zg-83-racodh-60-40-1.0-254-230-2.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 10 uL
 Date Acquired : 2023/1/14 10:31:13
 Date Processed : 2023/1/14 10:43:00
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Detector A Channel 2 254nm				
Peak#	Ret. Time	Area	Height	Conc.
1	7.376	5453617	359930	50.392
2	8.918	5368675	271681	49.608
Total		10822292	631611	



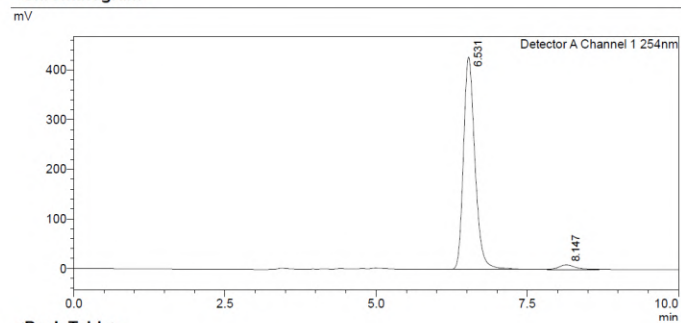
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Analysis Report

<Sample Information>

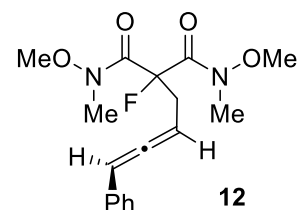
Sample Name : zhy-zh-79-asy-odh-60-40-1.0-254-230-5
 Sample ID :
 Data Filename : zhy-zh-79-asy-odh-60-40-1.0-254-230-5.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2023/5/18 21:49:37
 Date Processed : 2023/5/18 22:18:09
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Detector A Channel 1 254nm				
Peak#	Ret. Time	Area	Height	Conc.
1	6.531	5653968	427899	96.945
2	8.147	178181	9221	3.055
Total		5832149	437120	



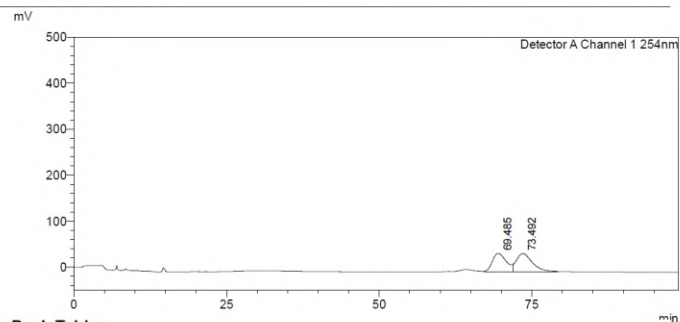
D:\Data\ZHY\ZH\zhy-zh-79-asy-odh-60-40-1.0-254-230-5.lcd

Analysis Report

<Sample Information>

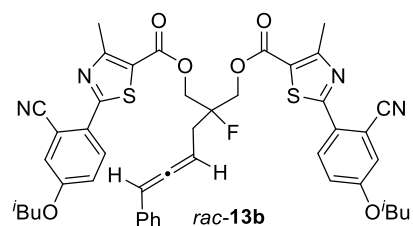
Sample Name : zhy-zf-122-rac-ia-85-15-0.5-254-230-1
 Sample ID :
 Data Filename : zhy-zf-122-rac-ia-85-15-0.5-254-230-1.lcd
 Method Filename : 0.5.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 10 uL
 Date Acquired : 2023/1/12 19:07:29
 Date Processed : 2023/1/18 17:04:07
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	69.485	6413481	40166	47.070
2	73.492	7212002	39868	52.930
Total		13625483	80034	



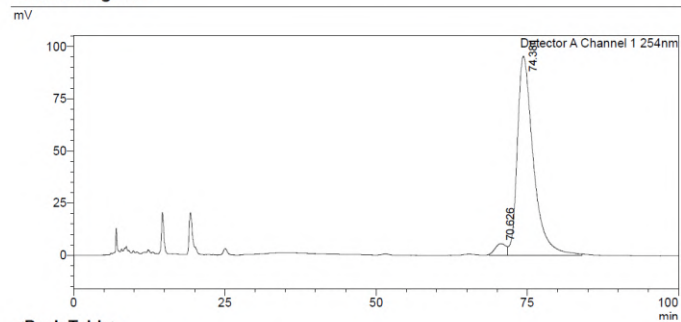
D:\Data\ZHY\ZF\zhy-zf-122-rac-ia-85-15-0.5-254-230-1.lcd

Analysis Report

<Sample Information>

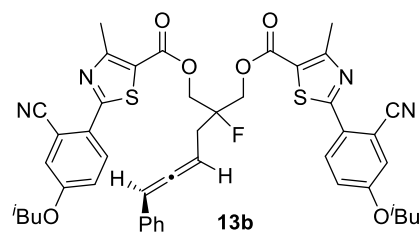
Sample Name : zhy-zf-122-asy-ia-85-15-0.5-254-230-1
 Sample ID :
 Data Filename : zhy-zf-122-asy-ia-85-15-0.5-254-230-1.lcd
 Method Filename : 0.5.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 10 uL
 Date Acquired : 2023/1/12 20:47:48
 Date Processed : 2023/1/12 23:03:56
 Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	70.626	698008	5558	3.809
2	74.381	17628224	95447	96.191
Total		18326232	101006	



D:\Data\ZHY\ZF\zhy-zf-122-asy-ia-85-15-0.5-254-230-1.lcd

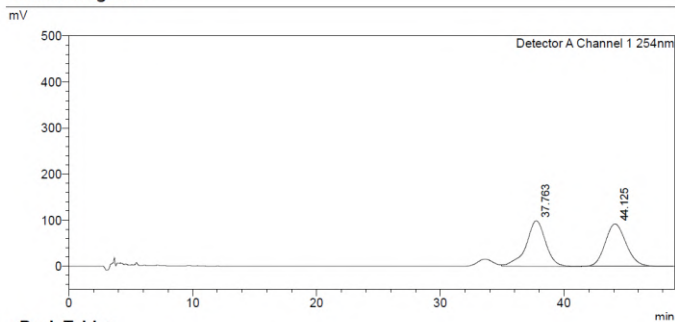
Analysis Report

<Sample Information>

Sample Name : zhy-zf-107-rac-adh-50-50-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zf-107-rac-adh-50-50-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/9/22 11:21:17
 Date Processed : 2023/1/18 17:05:01

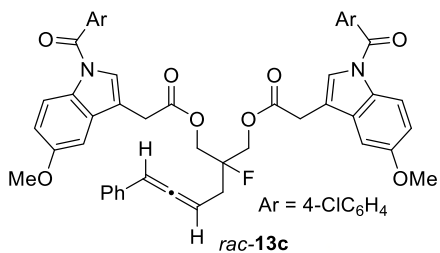
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	37.763	10965966	99205	50.423
2	44.125	10781974	92046	49.577
Total		21747940	191250	



D:\Data\ZHY\ZF\zhy-zf-107-rac-adh-50-50-1.0-254-230-1.lcd

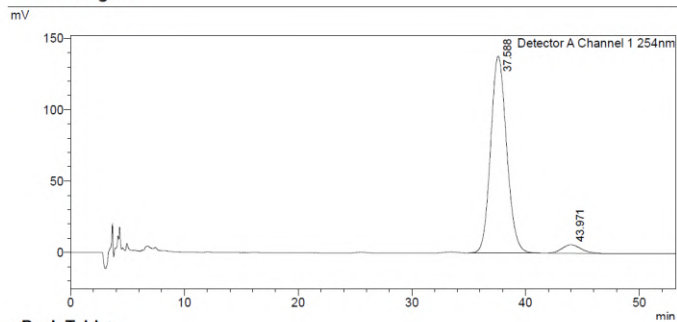
Analysis Report

<Sample Information>

Sample Name : zhy-zf-123-asy-adh-50-50-1.0-254-230-1
 Sample ID :
 Data Filename : zhy-zf-123-asy-adh-50-50-1.0-254-230-1.lcd
 Method Filename : 1.0.lcm
 Batch Filename :
 Vial # : 1-1
 Injection Volume : 20 uL
 Date Acquired : 2022/9/22 12:21:05
 Date Processed : 2022/9/22 13:14:16

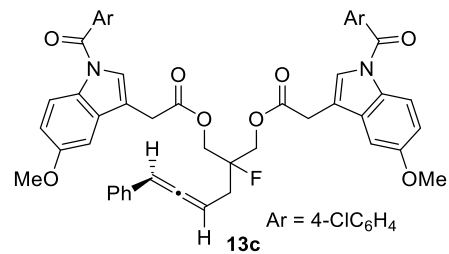
Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.
1	37.588	13503261	137866	95.214
2	43.971	678733	5939	4.786
Total		14181995	143805	



D:\Data\ZHY\ZF\zhy-zf-123-asy-adh-50-50-1.0-254-230-1.lcd