Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supplementary Information

Stereoselective Hydrodefluorination of CF_3-substituted alkenes and *gem*-Difluoroalkenes by H^-

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1, General Information

All chemicals were obtained from commercial sources and were used as received unless otherwise noted. All the reactions were carried out under argon atmosphere in a argon-filled glove box. The ^{1}H NMR spectra were recorded on a 400 MHz or 600 MHz NMR spectrometer. The ^{13}C NMR spectra were recorded at 101 MHz or 151 MHz. The ^{19}F NMR spectra were recorded at 376 MHz or 565 MHz. Chemical shifts were expressed in parts per million (δ) downfield from the internal standard tetramethylsilane, and were reported as s (singlet), d (doublet), t (triplet), dd (doublet of doublet), dt (doublet of triplet), m (multiplet), brs (broad single), etc. The residual solvent signals were used as references and the chemical shifts were converted to the TMS scale. High resolution mass spectra were obtained on an Agilent Q-TOF 6540 spectrometer. Column chromatography was performed on silica gel (300-400 mesh). Thin layer chromatography was performed on pre-coated glass back plates and visualized with UV light at 254 nm. Flash column chromatography was performed on silica gel *gem*-difluoroalkenes[1,2] and trifluoromethyl alkenes[3,4] were prepared according to literature reports.

2. General Synthetic Procedures and Characterization

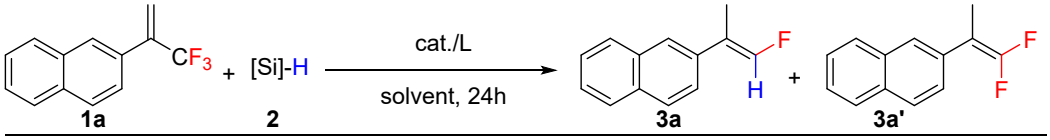
General procedure A: $Zn(OAc)_2$ (3.7 mg, 0.02 mmol) and Xantphos (11.6 mg, 0.02 mmol) in DMSO (2.0 mL) were charged into a 25 mL pressure tube under argon. The mixture was stirred for 30 min at room temperature. Then Ph_2SiH_2 (110.6 mg, 0.6 mmol) and trifluoromethyl alkene **1** (0.2 mmol, 1.0 equiv) were added sequentially to the reaction mixture. The reaction tube was then sealed and placed into an oil bath at 120 ℃. After stirred for 24 h, the reaction mixture was quenched with H_2O (2.0 mL) and extracted with dichloromethane. The organic layer was separated, dried over Na_2SO_4, concentrated, and purified by silica gel chromatography to give the monofluoride product **3a** – **3p**.

General procedure B: $Zn(OAc)_2$ (3.7 mg, 0.02 mmol) and PPh_3 (5.3 mg, 0.02 mmol) in DMSO (2.0 mL) were charged into a 25 mL pressure tube under argon. The mixture was stirred for 30 min at room temperature. Then Ph_2SiH_2 (36.8 mg, 0.2 mmol) and *gem*-difluoroalkene **4** (0.2 mmol, 1.0 equiv) were added sequentially to the reaction mixture. The reaction tube was then sealed and placed into an oil bath at 50 ℃. After stirred for 24 h, the reaction mixture was quenched with H_2O (2.0 mL) and extracted with dichloromethane. The organic layer was separated, dried over Na_2SO_4,

concentrated, and purified by silica gel chromatography to give the monofluoride product **3a**, **3m** and **5a** – **5z**.

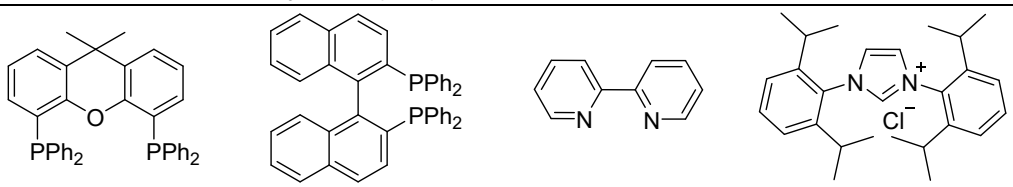
General procedure C: $Zn(OAc)_2$ (3.7 mg, 0.02 mmol) and PPh_3 (5.3 mg, 0.02 mmol) in DMSO (2.0 mL) were charged into a 25 mL pressure tube under argon. The mixture was stirred for 30 min at room temperature. Then Ph_2SiH_2 (36.8 mg, 0.2 mmol) and perfluoroaromatic product **6** (0.2 mmol, 1.0 equiv) were added sequentially to the reaction mixture. The reaction tube was then sealed and placed into an oil bath at 50 ℃. After stirred for 24 h, the reaction mixture was quenched with H_2O and extracted with dichloromethane. The organic layer was separated, dried over Na_2SO_4, concentrated, and purified by silica gel chromatography to give the product **7a**, **7b**.

2.1 Supplementary Table S1, Optimization of reaction conditions of **1a**. [a]



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

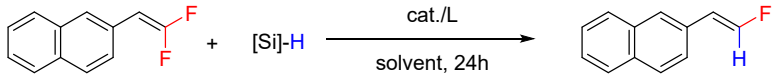
Entry	solvent	[Si]-H	cat.	L(mol %)	T(°C)	**3a** yield(%)	**3a'** yield(%)	**3a** *E/Z*
1	DMSO	Ph_2SiH_2	$Zn(OAc)_2$	PPh_3	50	21	52	85/15
2[b]	DMSO	Ph_2SiH_2	$Zn(OAc)_2$	PPh_3	100	45	31	85/15
3	DMSO	Ph_2SiH_2	$Zn(OAc)_2$	PPh_3	100	63	11	85/15
4[c]	DMSO	Ph_2SiH_2	$Zn(OAc)_2$	PPh_3	100	63	11	85/15
5	DMSO	Ph_2SiH_2	$Zn(OAc)_2$	PPh_3	120	66	9	85/15
6	DMSO	Ph_2SiH_2	$Zn(OAc)_2$	Xantphos	120	87	trace	85/15
7	DMSO	Ph_2SiH_2	$Zn(OAc)_2$	*rac*-BINAP	120	66	11	85/15
8	DMSO	Ph_2SiH_2	$Zn(OAc)_2$	Bpy	120	77	trace	84/16
9[e]	DMSO	Ph_2SiH_2	$Zn(OAc)_2$	**L1**	120	69	trace	83/17
10	DMSO	Ph_2SiH_2	$Zn(OAc)_2$	--	120	63	11	85/15
11	DMSO	Ph_2SiH_2	--	Xantphos	120	--	--	--
12	DMSO	Ph_2SiH_2	--	--	120	--	--	--
13	DMSO	Ph_2SiH_2	CsOAc	Xantphos	120	49	19	73/27
14	DMSO	Ph_2SiH_2	NaOAc	Xantphos	120	67	6	74/26
15	DMSO	Ph_2SiH_2	$ZnCl_2$	Xantphos	120	--	38	--
16	DMSO	Ph_2SiH_2	$ZnBr_2$	Xantphos	120	--	25	--
17	DMSO	Ph_2SiH_2	$Zn(acac)_2$	Xantphos	120	76	--	81/19
18	DMSO	Ph_2SiH_2	$Zn_3(PO_4)_2$	Xantphos	120	--	11	--
19	DMSO	Ph_2SiH_2	CsF	Xantphos	120	78	--	75/25
20	DMSO	Ph_2SiH_2	KF	Xantphos	120	10	60	--
21	DMSO	Ph_2SiH_2	BPh_3	Xantphos	120	--	--	--
22	DMF	Ph_2SiH_2	$Zn(OAc)_2$	Xantphos	120	--	trace	--
23	THF	Ph_2SiH_2	$Zn(OAc)_2$	Xantphos	120	trace	56	--
24	toluene	Ph_2SiH_2	$Zn(OAc)_2$	Xantphos	120	trace	61	--
25	DCE	Ph_2SiH_2	$Zn(OAc)_2$	Xantphos	120	trace	53	--
26	DMSO	$(MeO)_2SiHMe$	$Zn(OAc)_2$	Xantphos	120	12	41	80/20
27	DMSO	$PhSiH_3$	$Zn(OAc)_2$	Xantphos	120	38	29	84/16
28[d]	DMSO	$PhSiH_3$	$Zn(OAc)_2$	Xantphos	120	17	45	84/16



Xantphos *rac*-BINAP Bpy **L1**

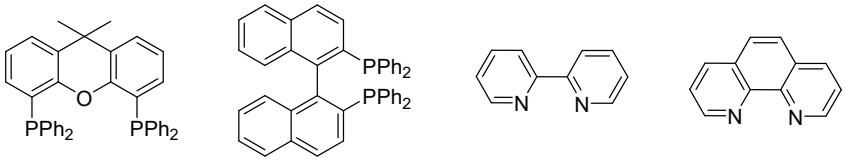
[a]Reaction conditions: **1a** (0.20 mmol), **2** (0.60 mmol), cat. (10 mmol%), **L** (10 mmol%), solvent (2.0 mL), 24 h under argon, yield and *E/Z* ratio determined by ^{19}F NMR with trifluoromethylbenzene (0.1 mmol) as internal standard. [b] **2a** (0.40 mmol). [c] **2a** (0.80 mmol). [d] $PhSiH_3$ (0.20 mmol). [e] CsOAc (0.02 mmol) was added.

2.2 Supplementary Table S2, Optimization of reaction conditions of **4a**. [a]



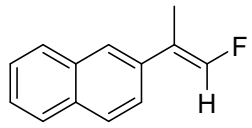
4a **2** **5a**

Entry	solvent	[Si]-H	cat.	L(mol %)	T(°C)	**5a** yield(%)	**5a** *E/Z*
1	DMSO	Ph_2SiH_2	--	--	30	--	--
2	DMSO	Ph_2SiH_2	$Zn(OAc)_2$	--	30	45	93/7
3	DMSO	Ph_2SiH_2	$Zn(OAc)_2$	PPh_3	30	62	96/4
4	DMSO	Ph_2SiH_2	$Zn(OAc)_2$	Xantphos	30	57	94/6
5	DMSO	Ph_2SiH_2	$Zn(OAc)_2$	*rac*-BINAP	30	60	96/4
6	DMSO	Ph_2SiH_2	$Zn(OAc)_2$	Bpy	30	39	95/5
7	DMSO	Ph_2SiH_2	$Zn(OAc)_2$	1,10-phen	30	42	93/7
8	THF	Ph_2SiH_2	$Zn(OAc)_2$	PPh_3	30	--	--
9	toluene	Ph_2SiH_2	$Zn(OAc)_2$	PPh_3	30	--	--
10	tBuOMe	Ph_2SiH_2	$Zn(OAc)_2$	PPh_3	30	--	--
11	1,4-Dioxane	Ph_2SiH_2	$Zn(OAc)_2$	PPh_3	30	--	--
12	DME	Ph_2SiH_2	$Zn(OAc)_2$	PPh_3	30	--	--
13	MeOH	Ph_2SiH_2	$Zn(OAc)_2$	PPh_3	30	--	--
14	DCE	Ph_2SiH_2	$Zn(OAc)_2$	PPh_3	30	--	--
15	DMA	Ph_2SiH_2	$Zn(OAc)_2$	PPh_3	30	--	--
16	DMSO	Ph_2SiH_2	$Zn(OAc)_2$	PPh_3	50	81	95/5
17[b]	DMSO	Ph_2SiH_2	$Zn(OAc)_2$	PPh_3	50	84	95/5
18[b]	DMSO	$PhSiH_3$	$Zn(OAc)_2$	PPh_3	50	53	95/5
19[b]	DMSO	$(MeO)_3SiH$	$Zn(OAc)_2$	PPh_3	50	23	94/6
20[c]	DMSO	Ph_2SiH_2	$Zn(OAc)_2$	PPh_3	50	63	94/6
21[d]	DMSO	Ph_2SiH_2	$Zn(OAc)_2$	PPh_3	50	--	--
22[b]	DMSO	Ph_2SiH_2	$ZnCl_2$	PPh_3	50	--	--
23[b]	DMSO	Ph_2SiH_2	$ZnBr_2$	PPh_3	50	--	--
24[b]	DMSO	Ph_2SiH_2	BPh_3	PPh_3	50	--	--
25[b]	DMSO	Ph_2SiH_2	$Cu(OAc)_2$	PPh_3	30	9	68/32
26[b]	DMSO	Ph_2SiH_2	NaOAc	PPh_3	30	17	90/10
27[b]	DMSO	Ph_2SiH_2	^{t}BuOK	PPh_3	30	23	89/11
28[b]	DMSO	Ph_2SiH_2	Na_2CO_3	PPh_3	30	12	90/10



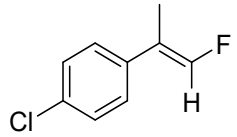
Xantphos *rac*-BINAP Bpy 1,10-phen

[a]Reaction conditions: **4a** (0.20 mmol), **2** (0.40 mmol), cat. (10 mmol%), **L** (10 mmol%), solvent (2.0 mL), 24 h under argon, NMR yield with trifluoromethylbenzene (0.1 mmol) as internal standard, *E/Z* ratio determined by ^{1}H NMR. [b] [Si]-H (0.20 mmol). [c] **2a** (0.20 mmol), $Zn(OAc)_2$ (5 mmol%). [d] In the air.

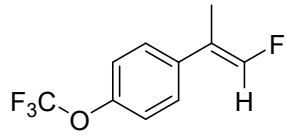


3a[5], General procedure A, (from trifluoromethyl alkene), purified by silica gel chromatography (PE). Colorless oil, 32.4 mg (87% yield, *E/Z* = 85/15); ^{1}H NMR (400 MHz, $CDCl_3$) δ (*E* isomer) 7.85 – 7.79 (m, 3H), 7.74 (s, 1H), 7.49 – 7.44 (m, 3H), 7.06 (dq, *J* = 84.8, 1.6 Hz, 1H), 2.16 (dd, *J* = 3.8, 1.6 Hz, 3H). HRMS (ESI, m/z): calcd for $C_{13}H_{12}F^+$ $[M + H]^+$: 187.0918, found 187.0946.

3a General procedure B, (from *gem*-difluoroalkene), Ph_2SiH_2 (73.7 mg, 0.40 mmol), 100 ℃, purified by silica gel chromatography (PE). Colorless oil, 24.2 mg (65% yield, *E/Z* = 89/11); ^{1}H NMR (400 MHz, $CDCl_3$) δ (*E* isomer) 7.84 – 7.80 (m, 3H), 7.75 (s, 1H), 7.50 – 7.44 (m, 3H), 7.07 (dq, *J* = 84.8, 1.6 Hz, 1H), 2.16 (dd, *J* = 3.8, 1.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (*E* isomer) 146.6 (d, *J* = 258.0 Hz), 135.0 (d, *J* = 8.7 Hz), 133.6, 132.8, 128.3, 128.1, 127.7, 126.5, 126.0, 124.7 (d, *J* = 4.4 Hz), 124.1 (d, *J* = 2.4 Hz), 12.3 (d, *J* = 6.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -128.33 (dq, *J* = 84.6, 5.2 Hz); (*E* isomer) -130.34 (dq, *J* = 84.8, 3.6 Hz). HRMS (ESI, m/z): calcd for $C_{13}H_{12}F^+$ $[M + H]^+$: 187.0918, found 187.0891.

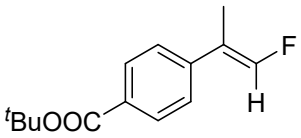


3b, General procedure A, purified by silica gel chromatography (PE). Colorless oil, NMR yield 84%, *E/Z* = 86/14; ^{1}H NMR (400 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.31 – 7.29 (m, 2H), 7.26 – 7.22 (m, 2H), 6.88 (dq, *J* = 84.6, 1.6 Hz, 1H), 2.02 (dd, *J* = 3.8, 1.6 Hz, 3H); (*Z* isomer) 6.66 (dq, *J* = 84.4, 1.6 Hz, 1H), 1.89 (dd, *J* = 5.0, 1.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) (mixture of isomers) δ 146.3 (d, *J* = 258.8 Hz), 136.2 (d, *J* = 9.4 Hz), 133.4, 128.9, 127.3 (d, *J* = 3.0 Hz), 119.4 (d, *J* = 10.2 Hz), 12.3 (d, *J* = 5.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomer) δ (*Z* minor) -127.75 (dq, *J* = 84.4, 5.0 Hz); (*E* major) -129.92 – -130.17 (m). HRMS (ESI, m/z): calcd for $C_9H_8ClFK^+$ $[M + K]^+$: 208.9930, found 208.9919.

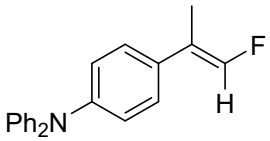


3c, General procedure A, purified by silica gel chromatography (PE). Colorless oil, NMR yield 62%, *E/Z* = 84/16; ^{1}H NMR (400 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.33 – 7.30 (m, 2H),

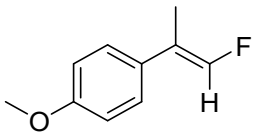
7.19 – 7.17 (m, 2H), 6.88 (dq, *J* = 84.4, 1.6 Hz, 1H), 2.03 (dd, *J* = 3.8, 1.6 Hz, 3H); (*Z* isomer) 1.91 (dd, *J* = 4.8, 1.6 Hz, 3H). ^{13}C NMR (101 MHz, CD_2Cl_2) (mixture of isomers) *δ* 148.9, 146.8 (d, *J* = 258.1 Hz), 136.9 (d, *J* = 9.0 Hz), 127.7 (d, *J* = 3.5 Hz), 121.5, 121.0 (q, *J* = 256.5 Hz), 119.6 (d, *J* = 10.2 Hz), 12.4 (d, *J* = 6.3 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) *δ* (*Z* isomer) -57.83 (s, 3F), -128.03 (dq, *J* = 84.8, 4.8 Hz, 1F) (*E* isomer) -57.92 (s, 3F), -129.52 – -129.77 (m, 1F). HRMS (ESI, m/z): calcd for $C_{10}H_7OF_4^+$ $[M + H]^+$: 219.0428, found 219.0459.



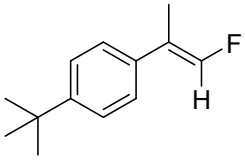
3d, General procedure A, purified by silica gel chromatography (PE : EA = 15:1). Colorless oil, 46.7 mg (99% yield, *E/Z* = 84/16); ^{1}H NMR (400 MHz, $CDCl_3$) (mixture of isomers) *δ* (*E* isomer) 7.96 – 7.93 (m, 2H), 7.36 – 7.32 (m, 2H), 6.97 (dq, *J* = 84.4, 1.6 Hz, 1H), 2.05 (dd, *J* = 3.8, 1.6 Hz, 3H), 1.59 (s, 9H); (*Z* isomer) 6.69 (dq, *J* = 84.0, 1.6 Hz, 1H), 1.92 (dd, *J* = 4.8, 1.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) (mixture of isomers) δ 165.6, 147.1 (d, *J* = 260.6 Hz), 141.8 (d, *J* = 8.9 Hz), 129.8, 129.4, 125.6 (d, *J* = 3.4 Hz), 119.8 (d, *J* = 10.2 Hz), 81.2, 28.3, 12.1 (d, *J* = 5.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) *δ* (*Z* isomer) -126.30 (dq, *J* = 84.0, 4.8 Hz); (*E* isomer) -128.45 (dq, *J* = 84.4, 3.8 Hz). HRMS (ESI, m/z): calcd for $C_{14}H_{17}FNaO_2^+$ $[M + Na]^+$: 259.1105, found 259.1106.



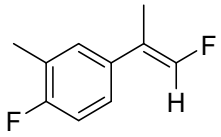
3e, General procedure A, purified by silica gel chromatography (PE : Acetone = 30:1). Colorless oil, 21.8 mg (36% yield, *E/Z* = 85/15); ^{1}H NMR (400 MHz, $CDCl_3$) *δ* (*E* isomer) 7.28 – 7.23 (m, 4H), 7.19 – 7.15 (m, 2H), 7.11 – 7.08 (m, 4H), 7.01 – 6.79 (m, 5H), 2.02 (dd, *J* = 3.8, 1.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (*E* isomer) 147.8, 147.3, 145.7 (d, *J* = 257.1 Hz), 131.6 (d, *J* = 9.0 Hz), 129.4, 126.7 (d, *J* = 3.5 Hz), 124.5, 123.9, 123.1, 119.7 (d, *J* = 10.2 Hz), 12.3 (d, *J* = 5.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) *δ* (*Z* isomer) -129.02 – -129.25 (m); (*E* isomer) -132.60 (dq, *J* = 84.8, 3.8 Hz). HRMS (ESI, m/z): calcd for $C_{21}H_{18}FKN^+$ $[M + K]^+$: 342.1055, found 342.1036.



3f[5], General procedure A, after adding $Zn(OAc)_2$ (7.3mg, 0.04 mmol) and Xantphos (23.1mg, 0.04 mmol), add NaOAc (16.4 mg, 0.2 mmol) and use $PhSiH_3$ as silane, 130℃, purified by silica gel chromatography (PE : DCM = 8:1). Colorless oil, NMR yield 56%, *E/Z* = 83/17; ^{1}H NMR (400 MHz, $CDCl_3$) δ (*E* isomer) 7.25 – 7.21 (m, 2H), 6.89 – 6.85 (m, 2H), 6.85 (dq, *J* = 86.0, 1.6 Hz, 1H), 3.81 (s, 3H), 2.01 (dd, *J* = 3.8, 1.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (*E* isomer) 159.2, 145.3 (d, *J* = 256.4 Hz), 130.1 (d, *J* = 8.7 Hz), 127.1 (d, *J* = 3.0 Hz), 119.6 (d, *J* = 9.6 Hz), 114.1, 55.4, 12.5 (d, *J* = 5.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -130.31 (dq, *J* = 84.6, 4.8 Hz); (*E* isomer) -133.01 (dq, *J* = 86.0, 3.8 Hz). HRMS (ESI, m/z): calcd for $C_{10}H_{12}FO^+$ $[M + H]^+$: 167.0867, found 167.0876.

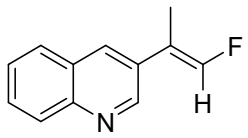


3g[5], General procedure A, after adding $Zn(OAc)_2$ (7.3mg, 0.04 mmol) and Xantphos (23.1mg, 0.04 mmol), add NaOAc (16.4 mg, 0.2 mmol) and use $PhSiH_3$ as silane, 130℃, purified by silica gel chromatography (PE). Colorless oil, NMR yield 51%, *E/Z* = 77/23; ^{1}H NMR (400 MHz, $CDCl_3$) δ (*E* isomer) 7.38 – 7.34 (m, 2H), 7.26 – 7.23 (m, 2H), 6.90 (dq, *J* = 86.0, 1.6 Hz, 1H), 2.03 (dd, *J* = 3.8, 1.6 Hz, 3H), 1.32 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (*E* isomer) 150.6, 145.9 (d, *J* = 257.2 Hz), 134.7 (d, *J* = 8.8 Hz), 125.7 (d, *J* = 3.5 Hz), 125.6, 119.9 (d, *J* = 9.9 Hz), 34.6, 31.4, 12.3 (d, *J* = 6.0 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ (*E* isomer) -132.15 (dq, *J* = 86.0, 3.8 Hz). HRMS (ESI, m/z): calcd for $C_{13}H_{17}FK^+$ $[M + K]^+$: 231.0946, found 231.0951.

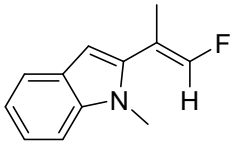


3h, General procedure A, purified by silica gel chromatography (PE). Colorless oil, NMR yield 77%, *E/Z* = 83/17; ^{1}H NMR (400 MHz, CD_2Cl_2) δ (*E* isomer) 7.18 – 7.13 (m, 1H), 7.02 – 7.00 (m, 1H), 6.97 (dd, *J* = 11.2, 1.8 Hz, 1H), 6.94 (dq, *J* = 84.8, 1.6 Hz, 1H), 2.25 (d, *J* = 2.0 Hz, 3H), 2.00 (dd, *J* = 3.8, 1.6 Hz, 3H). ^{13}C NMR (101 MHz, CD_2Cl_2) δ (*E* isomer) 161.8 (d, *J* = 243.8 Hz), 146.6 (d, *J* = 257.8 Hz), 137.5 (dd, *J* = 9.3, 8.0 Hz), 131.9 (d, *J* = 5.8 Hz), 124.3 (d, *J* = 17.4 Hz), 121.5 (dd, *J* =

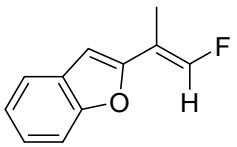
3.6, 2.8 Hz), 119.7 (dd, J = 10.8, 2.1 Hz), 112.6 (dd, J = 23.3, 3.5 Hz), 14.3 (d, J = 3.6 Hz), 12.2 (d, J = 6.1 Hz). ^{19}F NMR (376 MHz, CD_2Cl_2) (mixture of isomers) δ (*Z* isomer) -128.32 (dq, J = 84.6, 5.0 Hz, 1F); (*E* isomer) -118.19 – -118.26 (m, 1F), -131.73 (dq, J = 84.8, 3.8 Hz, 1F). HRMS (ESI, m/z): calcd for $C_{10}H_{11}F_2^+$ $[M + H]^+$: 169.0823, found 169.0837.



3i[5], General procedure A, purified by silica gel chromatography (PE : EA = 10:1). Colorless oil, 17.2 mg (46% yield, *E/Z* = 75/25); ^{1}H NMR (400 MHz, $CDCl_3$) δ (*E* isomer) 8.90 (d, J = 2.3 Hz, 1H), 8.09 (d, J = 8.4 Hz, 1H), 8.01 (d, J = 2.3 Hz, 1H), 7.81 (d, J = 8.1 Hz, 1H), 7.71 – 7.67 (m, 1H), 7.57 – 7.53 (m, 1H), 7.09 (dq, J = 83.6, 1.6 Hz, 1H), 2.16 (dd, J = 3.8, 1.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (*E* isomer) 148.5 (d, J = 2.2 Hz), 147.5, 147.1 (d, J = 261.0 Hz), 132.3 (d, J = 4.5 Hz), 130.6 (d, J = 9.0 Hz), 129.5, 129.3, 128.0, 127.9, 127.2, 117.7 (d, J = 11.0 Hz), 12.2 (d, J = 5.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ (*E* isomer) -127.07 (dq, J = 83.6, 3.8 Hz). HRMS (ESI, m/z): calcd for $C_{12}H_{11}NF^+$ $[M + H]^+$: 188.0870, found 188.0871.

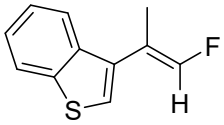


3j, General procedure A, purified by silica gel chromatography (PE : EA = 40:1). Yellow solid, m.p. 55 – 56 °C, 23.5 mg (62% yield, *E/Z* = 67/33); ^{1}H NMR (400 MHz, $CDCl_3$) δ (*E* isomer) 7.59 (d, J = 7.9 Hz, 1H), 7.31 (d, J = 8.3 Hz, 1H), 7.26 – 7.21 (m, 1H), 7.14 – 7.10 (m, 1H), 6.80 (dq, J = 84.8, 1.6 Hz, 1H), 6.40 (s, 1H), 3.70 (s, 3H), 2.06 (dd, J = 3.6, 1.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (*E* isomer) 148.2 (d, J = 265.2 Hz), 138.4, 137.5 (d, J = 12.2 Hz), 127.7, 121.9, 120.6, 119.9, 112.5 (d, J = 12.4 Hz), 109.4, 101.7 (d, J = 2.9 Hz), 30.9, 14.1 (d, J = 3.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ (*E* isomer) -123.62 (dq, J = 84.8, 3.6 Hz). HRMS (ESI, m/z): calcd for $C_{12}H_{13}NF^+$ $[M + H]^+$: 190.1027, found 190.1032.

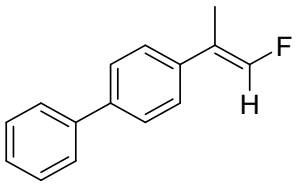


3k[5], General procedure A, purified by silica gel chromatography (PE). Colorless oil, 11.3 mg (32% yield, *E/Z* = 67/33); ^{1}H NMR (400 MHz, $CDCl_3$) δ (*E* isomer) 7.55 – 7.34 (m, 3H), 7.26 – 7.19 (m,

2H), 6.60 (s, 1H), 2.03 (dd, J = 3.6, 1.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (*E* isomer) 154.6, 154.2 (d, J = 8.8 Hz), 148.4 (d, J = 261.6 Hz), 128.7, 124.6, 122.9, 120.6, 111.4 (d, J = 15.2 Hz), 110.9, 103.1 (d, J = 10.1 Hz), 9.7 (d, J = 5.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ (*E* isomer) -132.54 (dq, J = 82.8, 3.6 Hz). HRMS (ESI, m/z): calcd for $C_{11}H_{10}OF^+$ $[M + H]^+$: 177.0710, found 177.0725.



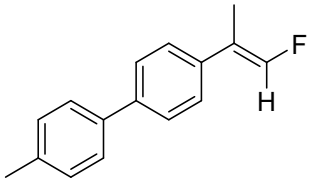
3l[5], General procedure A, purified by silica gel chromatography (PE). White solid, m.p. 71 – 72 °C, 20.8 mg (54% yield, *E/Z* = 66/34); ^{1}H NMR (400 MHz, $CDCl_3$) δ (*E* isomer) 7.76 – 7.68 (m, 2H), 7.35 – 7.08 (m, 3H), 7.20 (s, 1H), 2.14 (dd, J = 3.6, 1.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (*E* isomer) 147.1 (d, J = 262.9 Hz), 140.3 (d, J = 8.6 Hz), 139.9, 138.3, 124.7, 124.6, 123.3, 122.2, 120.8 (d, J = 8.0 Hz), 115.9 (d, J = 13.8 Hz), 12.1 (d, J = 5.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ (*E* isomer) -129.18 (dq, J = 83.6, 3.6 Hz). HRMS (ESI, m/z): calcd for $C_{11}H_{10}FS^+$ $[M + H]^+$: 193.0482, found 193.0483.



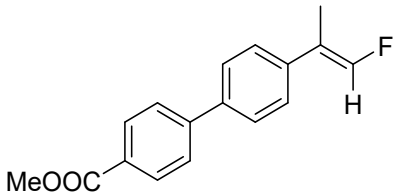
3m[5], General procedure A, (from trifluoromethyl alkene), purified by silica gel chromatography (PE). White solid, 35.2 mg (83% yield, *E/Z* = 85/15); ^{1}H NMR (400 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.63 – 7.58 (m, 4H), 7.49 – 7.45 (m, 2H), 7.42 – 7.37 (m, 3H), 7.00 (dq, J = 84.8, 1.6 Hz, 1H), 2.11 (dd, J = 3.8, 1.6 Hz, 3H); (*Z* isomer) 6.72 (dq, J = 84.6, 1.6 Hz, 1H), 1.97 (dd, J = 5.0, 1.6 Hz, 3H). HRMS (ESI, m/z): calcd for $C_{15}H_{13}FNa^+$ $[M + Na]^+$: 235.0893, found 235.0919.

3m, General procedure B, (from *gem*-difluoroalkene), Ph_2SiH_2 (73.7 mg, 0.40 mmol), 100 °C, purified by silica gel chromatography (PE). White solid, m.p. 106 – 107 °C, 28.4 mg (67% yield, *E/Z* = 91/9); ^{1}H NMR (400 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.65 – 7.56 (m, 4H), 7.49 – 7.45 (m, 2H), 7.43 – 7.35 (m, 3H), 7.00 (dq, J = 84.8, 1.6 Hz, 1H), 2.11 (dd, J = 3.8, 1.6 Hz, 3H); (*Z* isomer) 6.72 (dq, J = 84.4, 1.6 Hz, 1H), 1.97 (dd, J = 5.0, 1.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) (mixture of isomers) δ 146.2 (d, J = 258.5 Hz), 140.7, 140.4, 136.7 (d, J = 8.8 Hz), 129.0, 127.5, 127.4, 127.1, 126.4 (d, J = 3.5 Hz), 119.8 (d, J = 9.8 Hz), 12.3 (d, J = 6.3 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -127.99 – -128.26 (m); (*E* isomer) -130.71 – -130.96 (m).

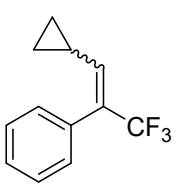
HRMS (ESI, m/z): calcd for $C_{15}H_{14}F^+$ [M + H]$^+$: 213.1074, found 213.1064.



3n, General procedure A, purified by silica gel chromatography (PE). White solid, m.p. 128 – 129 ℃, 43.9 mg (97% yield, *E/Z* = 84/16); ^{1}H NMR (400 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.60 – 7.51 (m, 4H), 7.41 – 7.38 (m, 2H), 7.29 – 7.27 (m, 2H), 6.99 (dq, *J* = 84.8, 1.6 Hz, 1H), 2.43 (s, 3H), 2.11 (dd, *J* = 3.8, 1.6 Hz, 3H); (*Z* isomer) 6.72 (dq, *J* = 84.4, 1.6 Hz, 1H), 1.97 (dd, *J* = 4.8, 1.6 Hz, 3H).^{13}C NMR (101 MHz, $CDCl_3$) (mixture of isomers) δ 146.1 (d, *J* = 258.1 Hz), 140.3, 137.9, 137.3, 136.3 (d, *J* = 8.9 Hz), 129.7, 127.2, 126.9, 126.3 (d, *J* = 3.4 Hz), 119.8 (d, *J* = 10.1 Hz), 21.2, 12.3 (d, *J* = 5.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -128.01 – -128.2 (m); (*E* isomer) -130.92 (dq, *J* = 84.8, 3.8 Hz). HRMS (ESI, m/z): calcd for $C_{16}H_{16}F^+$ [M + H]$^+$: 227.1231, found 227.1254.

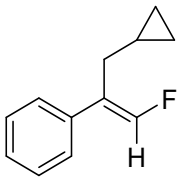


3o, General procedure A, purified by silica gel chromatography (PE). White solid, m.p. 132 – 133 ℃, 29.8 mg (55% yield, *E/Z* = 79/21); ^{1}H NMR (400 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 8.12 – 8.10 (m, 2H), 7.69 – 7.59 (m, 4H), 7.42 – 7.40 (m, 2H), 6.98 (dq, *J* = 84.8, 1.6 Hz, 1H), 3.94 (s, 3H), 2.08 (dd, *J* = 3.8, 1.6 Hz, 3H); (*Z* isomer) 6.71 (dq, *J* = 84.4, 1.6 Hz, 1H), 1.95 (dd, *J* = 4.8, 1.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) (mixture of isomers) δ 167.1, 146.4 (d, *J* = 258.7 Hz), 139.1, 137.6 (d, *J* = 9.3 Hz), 130.3, 127.5, 127.2, 127.1, 127.0, 126.5 (d, *J* = 3.0 Hz), 119.7 (d, *J* = 10.2 Hz), 52.3, 12.3 (d, *J* = 5.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -127.65 (dq, *J* = 84.4, 4.8 Hz); (*E* isomer) -130.04 – -130.29 (m). HRMS (ESI, m/z): calcd for $C_{17}H_{16}FO_2^+$ [M + H]$^+$: 271.1129, found 271.1150.

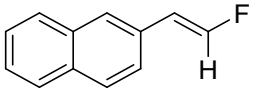


1p, colorless oil, *E/Z* = 74/26; ^{1}H NMR (400 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.42 –

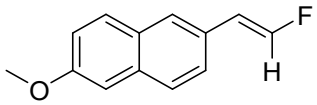
7.37 (m, 5H), 5.75 – 5.72 (m, 1H), 1.44 – 1.35 (m, 1H), 0.85 – 0.82 (m, 2H), 0.61 – 0.59 (m, 2H); (*Z* isomer) 5.29 (d, *J* = 10.9 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) (mixture of isomers) δ 141.3 (q, *J* = 5.8 Hz), 130.2, 128.6, 128.4, 128.4, 128.2, 123.9 (q, *J* = 272.0 Hz), 11.2, 8.3. ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -57.07; (*E* isomer) -64.99.



3p, General procedure A, after adding $Zn(OAc)_2$ (3.7mg, 0.02 mmol) and Xantphos (11.6 mg, 0.02 mmol), add NaOAc (16.4 mg, 0.2 mmol) and use $PhSiH_3$ as silane, purified by silica gel chromatography (PE). Colorless oil, NMR yield 33%, *E/Z* = 77/23. ^{1}H NMR (400 MHz, $CDCl_3$) δ (*Z* isomer) 7.43 – 7.41 (m, 2H), 7.38 – 7.34 (m, 2H), 7.29 – 7.27 (m, 1H), 6.70 (dt, *J* = 84.8, 1.6 Hz, 1H), 2.21 – 2.18 (m, 2H), 0.82 – 0.73 (m, 1H), 0.47 – 0.43 (m, 2H), 0.08 (dt, *J* = 6.0, 4.5 Hz, 2H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ (*Z* isomer) 144.3 (d, *J* = 259.7 Hz), 135.5, 128.1, 128.1, 127.2, 122., 35.5 (d, *J* = 6.3 Hz), 9.4, 4.5. ^{19}F NMR (376 MHz, $CDCl_3$) δ (*Z* isomer) -133.26 (dt, *J* = 84.8, 4.2 Hz). HRMS (ESI, m/z): calcd for $C_{12}H_{17}NF^+$ $[M + NH_4]^+$: 194.1340, found 194.1348.

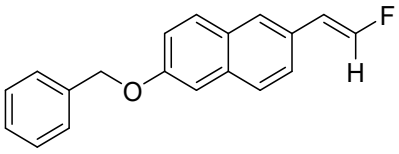


5a[6], General procedure B, purified by silica gel chromatography (PE). White solid, m.p. 67 – 68 °C, 28.9 mg (84% yield, *E/Z* = 95/5); ^{1}H NMR (400 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.82 – 7.77 (m, 3H), 7.65 (s, 1H), 7.49 – 7.20 (m, 4H), 6.56 (dd, *J* = 19.6, 11.2 Hz, 1H); (*Z* isomer) 6.74 (dd, *J* = 82.8, 5.6 Hz, 1H), 5.78 (dd, *J* = 44.8, 5.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) (mixture of isomers) δ 150.6 (d, *J* = 259.3 Hz), 133.7, 132.9, 130.3 (d, *J* = 11.8 Hz), 128.6, 127.9, 126.6, 126.1, 125.9 (d, *J* = 5.0 Hz), 123.5, 114.3 (d, *J* = 16.3 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -121.74 (dd, *J* = 82.8, 44.8 Hz); (*E* isomer) -129.39 (dd, *J* = 83.2, 19.6 Hz). HRMS (ESI, m/z): calcd for $C_{12}H_{10}F^+$ $[M + H]^+$: 173.0761, found 173.0756.

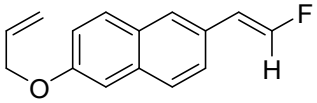


5b, General procedure B, purified by silica gel chromatography (PE : EA = 20:1). White solid, m.p. 77 – 78 °C, 38.4 mg (95% yield, *E/Z* = 94/6); ^{1}H NMR (400 MHz, $CDCl_3$) (mixture of isomers) δ (*E*

isomer) 7.66 – 7.64 (m, 2H), 7.55 (s, 1H), 7.37 – 7.08 (m, 4H), 6.50 (dd, *J* = 19.6, 11.4 Hz, 1H), 3.89 (s, 3H); (*Z* isomer) 6.69 (dd, *J* = 82.8, 5.4 Hz, 1H), 5.71 (dd, *J* = 44.8, 5.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) (mixture of isomers) δ 157.9, 150.1 (d, *J* = 258.0 Hz), 134.1, 129.4, 129.1, 128.0 (d, *J* = 11.7 Hz), 127.4, 125.7 (d, *J* = 4.8 Hz), 124.1, 119.3, 114.2 (d, *J* = 16.5 Hz), 106.0, 55.4. ^{19}F NMR (565 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -122.87 (dd, *J* = 82.8, 44.8 Hz); (*E* isomer) -130.75 (dd, *J* = 83.4, 19.6 Hz). HRMS (ESI, m/z): calcd for $C_{13}H_{12}FO^+$ $[M + H]^+$: 203.0867, found 203.0869

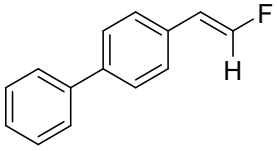


5c, General procedure B, purified by silica gel chromatography (PE). White solid, m.p. 103 – 104 °C, 36.1 mg (65% yield, *E/Z* = 94/6); ^{1}H NMR (600 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.71 – 7.66 (m, 2H), 7.59 (s, 1H), 7.51 – 7.49 (m, 2H), 7.44 – 7.31 (m, 2H), 7.37 – 7.20 (m, 5H), 6.53 (dd, *J* = 19.6, 11.4 Hz, 1H), 5.18 (s, 2H); (*Z* isomer) 6.72 (dd, *J* = 83.1, 5.4 Hz, 1H), 5.74 (dd, *J* = 45.0, 5.4 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) (mixture of isomers) δ 157.1, 150.1 (d, *J* = 257.6 Hz), 136.9, 134.0, 129.4, 129.2, 128.8, 128.2, 128.1 (d, *J* = 11.8 Hz), 127.7, 127.5, 125.7 (d, *J* = 4.7 Hz), 124.1, 119.7, 114.2 (d, *J* = 16.4 Hz), 107.4, 70.2. ^{19}F NMR (565 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -122.77 (dd, *J* = 83.1, 45.0 Hz); (*E* isomer) -130.62 (dd, *J* = 83.4, 19.6 Hz). HRMS (ESI, m/z): calcd for $C_{19}H_{19}FNO^+$ $[M + NH_4]^+$: 296.1445, found 296.1453.

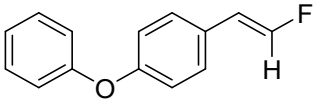


5d, General procedure B, purified by silica gel chromatography (PE : EA = 20:1). White solid, m.p. 60 – 61 °C, 34.7 mg (76% yield, *E/Z* = 95/5); ^{1}H NMR (600 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.70 – 7.65 (m, 2H), 7.57 (s, 1H), 7.37 – 7.17 (m, 3H), 7.12 (s, 1H), 6.52 (dd, *J* = 19.2, 11.4 Hz, 1H), 6.16 – 6.10 (m, 1H), 5.48 (d, *J* = 17.4 Hz, 1H), 5.34 (d, *J* = 10.2 Hz, 1H), 4.65 (d, *J* = 5.4 Hz, 2H); (*Z* isomer) 6.71 (dd, *J* = 82.8, 5.4 Hz, 1H), 5.74 (dd, *J* = 45.0, 5.4 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) (mixture of isomers) δ 156.8, 150.1 (d, *J* = 258.5 Hz), 134.0, 133.2, 129.4, 129.2, 128.1 (d, *J* = 12.1 Hz), 127.5, 125.7 (d, *J* = 5.3 Hz), 124.1, 119.6, 118.0, 114.2 (d, *J* = 16.4 Hz), 107.2, 69.0. ^{19}F NMR (565 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -122.84 (dd, *J* = 82.8, 45.0 Hz); (*E* isomer) -130.70 (dd, *J* = 83.6, 19.2 Hz). HRMS (ESI, m/z): calcd for $C_{15}H_{14}FO^+$ [M +

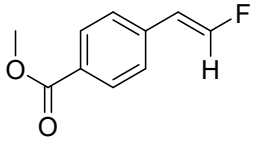
H]$^+$: 229.1023, found 229.1026.



5e[6], General procedure B, purified by silica gel chromatography (PE). White solid, m.p. 100 – 101 °C, 33.7 mg (85% yield, *E/Z* = 95/5); ^{1}H NMR (600 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.61 – 7.56 (m, 4H), 7.47 – 7.45 (m, 2H), 7.38 – 7.16 (m, 4H), 6.45 (dd, *J* = 19.2, 11.4 Hz, 1H); (*Z* isomer) 6.70 (dd, *J* = 82.8, 5.4 Hz, 1H), 5.68 (dd, *J* = 45.0, 5.4 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) (mixture of isomers) δ 150.3 (d, *J* = 259.5 Hz), 140.7, 140.4 (d, *J* = 2.2 Hz), 131.8 (d, *J* = 12.0 Hz), 129.0, 127.6, 127.5, 127.0, 126.7 (d, *J* = 3.2 Hz), 113.7 (d, *J* = 16.1 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -121.68 (dd, *J* = 82.8, 45.0 Hz); (*E* isomer) -129.47 (dd, *J* = 83.2, 19.2 Hz). HRMS (ESI, m/z): calcd for $C_{14}H_{15}FN^+$ $[M + NH_4]^+$: 216.1183, found 216.1178.

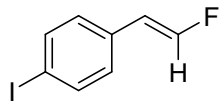


5f, General procedure B, purified by silica gel chromatography (PE). White solid, m.p. 69 – 70 °C, 20.2 mg (47% yield, *E/Z* = 98/2); ^{1}H NMR (600 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.37 – 7.35 (m, 2H), 7.23 – 7.06 (m, 4H), 7.04 – 6.97 (m, 4H), 6.40 (dd, *J* = 19.8, 11.4 Hz, 1H); (*Z* isomer) 6.65 (dd, *J* = 82.8, 5.4 Hz, 1H), 5.60 (dd, *J* = 45.0, 5.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) (mixture of isomers) δ 157.2, 156.9 (d, *J* = 2.2 Hz), 149.8 (d, *J* = 258.0 Hz), 123.0, 127.8, 127.7, 127.6 (d, *J* = 3.0 Hz), 123.6, 119.1 (d, *J* = 16.8 Hz), 113.3 (d, *J* = 16.1 Hz). ^{19}F NMR (565 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -123.86 (dd, *J* = 82.8, 45.0 Hz); (*E* isomer) -130.87 (dd, *J* = 83.5, 19.8 Hz). HRMS (ESI, m/z): calcd for $C_{14}H_{12}FO^+$ $[M + H]^+$: 215.0867, found 215.0888.

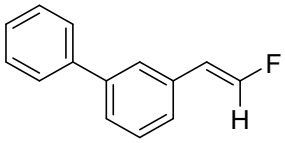


5g, General procedure B, purified by silica gel chromatography (PE : DCM = 4:1). Colorless oil, 25.2 mg (70% yield, *E/Z* = 92/8); ^{1}H NMR (400 MHz, $CDCl_3$) δ (*E* isomer) 7.99 – 7.97 (m, 2H), 7.37 – 7.14 (m, 3H), 6.42 (dd, *J* = 19.2, 11.6 Hz, 1H), 3.91 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ (*E* isomer) 166.9, 151.7 (d, *J* = 263.0 Hz), 137.6 (d, *J* = 12.1 Hz), 130.3, 129.3, 126.1 (d, *J* = 3.3 Hz), 113.6 (d, *J* = 16.5 Hz), 52.3. ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -118.32

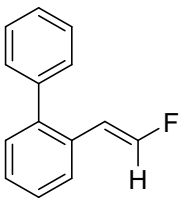
(dd, J = 81.9, 44.3 Hz); (*E* isomer) -125.70 (dd, J = 82.0, 19.2 Hz). HRMS (ESI, m/z): calcd for $C_{10}H_{10}FO_2^+$ [M + H]$^+$: 181.0659, found 181.0669.



5h, General procedure B, Ph_2SiH_2 (73.7 mg, 0.40 mmol), 100 ℃, purified by silica gel chromatography (PE). Yellow oil, 39.7 mg (80% yield, *E/Z* = 96/4); ^{1}H NMR (400 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.64 – 7.61 (m, 2H), 7.17 (dd, J = 82.4, 11.6 Hz, 1H), 7.00 – 6.97 (m, 2H), 6.32 (dd, J = 19.2, 11.6 Hz, 1H); (*Z* isomer) 6.67 (dd, J = 82.4, 5.4 Hz, 1H), 5.55 (dd, J = 44.2, 5.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) (mixture of isomers) δ 150.7 (d, J = 260.9 Hz), 138.0, 132.3 (d, J = 12.3 Hz), 128.0 (d, J = 3.4 Hz), 113.3 (d, J = 16.7 Hz), 92.7. ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -120.33 (dd, J = 82.4, 44.2 Hz); (*E* isomer)-128.04 (dd, J = 82.4, 19.2 Hz). HRMS (ESI, m/z): calcd for $C_8H_6FIK^+$ [M + K]$^+$: 286.9130, found 286.9155.

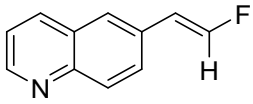


5i, General procedure B, purified by silica gel chromatography (PE). White solid, m.p. 74 – 75 ℃, 39.2 mg (99% yield, *E/Z* = 96/4); ^{1}H NMR (400 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.61 – 7.58 (m, 2H), 7.50 – 7.42 (m, 4H), 7.40 – 7.38 (m, 2H), 7.26 – 7.24 (m, 1H), 7.24 (dd, J = 83.2, 11.6 Hz, 1H), 6.48 (dd, J = 19.2, 11.2 Hz, 1H); (*Z* isomer) 6.71 (dd, J = 82.4, 5.4 Hz, 1H), 5.70 (dd, J = 44.4, 5.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) (mixture of isomers) δ 150.5 (d, J = 259.5 Hz), 142.0, 141.0, 133.3 (d, J = 12.1 Hz), 129.3, 129.0, 127.7, 127.3, 126.5 (d, J = 2.0 Hz), 125.3 (d, J = 3.0 Hz), 125.1 (d, J = 2.9 Hz), 114.0 (d, J = 16.0 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -121.47 (dd, J = 82.4, 44.4 Hz); (*E* isomer) -129.23 (dd, J = 83.2, 19.2 Hz). HRMS (ESI, m/z): calcd for $C_{14}H_{15}FN^+$ [M + NH_4]$^+$: 216.1183, found 216.1193.

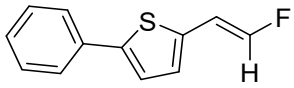


5j, General procedure B, purified by silica gel chromatography (PE). Colorless oil, 36.5 mg (92% yield, *E/Z* = 96/4); ^{1}H NMR (600 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.47 – 7.43 (m, 3H), 7.41 – 7.34 (m, 6H), 7.07 (dd, J = 84.3, 11.4 Hz, 1H), 6.40 (dd, J = 19.8, 11.4 Hz, 1H); (*Z*

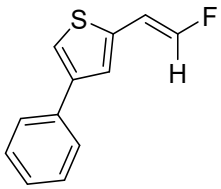
isomer) 6.63 (dd, J = 83.4, 5.4 Hz, 1H), 5.63 (dd, J = 45.0, 5.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) (mixture of isomers) δ 150.2 (d, J = 259.1 Hz), 141.1 (d, J = 4.4 Hz), 140.8, 130.6, 130.5, 129.7, 128.4, 127.8 (d, J = 8.9 Hz), 127.4, 126.2, 113.3 (d, J = 16.7 Hz). ^{19}F NMR (565 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -124.98 (dd, J = 83.4, 45.0 Hz); (*E* isomer) -127.12 (dd, J = 84.3, 19.8 Hz). HRMS (ESI, m/z): calcd for $C_{14}H_{11}FK^+$ $[M + K]^+$: 237.0476, found 237.0445.



5k, General procedure B, purified by silica gel chromatography (PE : EA = 5:1). White solid, m.p. 72 – 73 ℃, 32.9 mg (95% yield, *E/Z* = 95/5); ^{1}H NMR (600 MHz, $CDCl_3$) δ (*E* isomer) 8.86 (s, 1H), 8.09 – 8.02 (m, 2H), 7.63 – 7.23 (m, 4H), 6.55 (dd, J = 19.2, 11.4 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ (*E* isomer) 151.2 (d, J = 252.0 Hz), 150.3, 147.9, 135.9, 131.2 (d, J = 12.1 Hz), 130.1, 128.6, 127.2, 125.4 (d, J = 4.5 Hz), 121.8, 113.7 (d, J = 16.5 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -120.58 (dd, J = 82.6, 43.8 Hz); (*E* isomer) -127.48 (dd, J = 82.8, 18.9 Hz). HRMS (ESI, m/z): calcd for $C_{11}H_9FN^+$ $[M + H]^+$: 174.0714, found 174.0711.

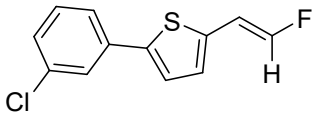


5l, General procedure B, purified by silica gel chromatography (PE). White solid, m.p. 65 – 66 ℃, 40.1 mg (98% yield, *E/Z* = 89/11); ^{1}H NMR (400 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.55 – 7.53 (m, 2H), 7.37 – 7.33 (m, 2H), 7.28 – 6.86 (m, 4H), 6.50 (dd, J = 17.6, 11.2 Hz, 1H); (*Z* isomer) 5.93 (dd, J = 43.2, 5.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) (mixture of isomers) δ 149.8 (d, J = 262.0 Hz), 142.8 (d, J = 3.4 Hz), 134.4 (d, J = 11.6 Hz), 134.1, 129.1 (d, J = 1.8 Hz), 127.8, 127.2 (d, J = 6.6 Hz), 125.8, 123.4, 108.5 (d, J = 20.3 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -120.38 (dd, J = 81.8, 43.2 Hz); (*E* isomer) -129.04 (dd, J = 82.2, 17.6 Hz). HRMS (ESI, m/z): calcd for $C_{12}H_{10}FS^+$ $[M + H]^+$: 205.0482, found 205.0479.

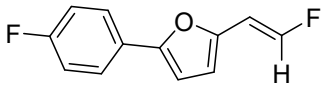


5m, General procedure B, purified by silica gel chromatography (PE). White solid, m.p. 68 – 69 ℃, 40.4 mg (99% yield, *E/Z* = 89/11); ^{1}H NMR (600 MHz, $CDCl_3$) δ (*E* isomer) 7.53 – 7.51 (m, 2H),

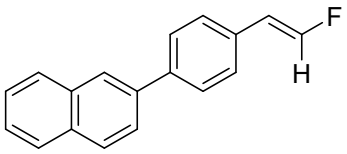
7.38 – 7.35 (m, 2H), 7.28 – 7.26 (m, 1H), 7.23 – 7.07 (m, 3H), 6.53 (dd, J = 17.4, 11.4 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ (*E* isomer) 150.0 (d, J = 262.1 Hz), 142.7, 135.7 (d, J = 12.9 Hz), 135.6, 129.0, 127.5, 126.4, 125.2 (d, J = 6.4 Hz), 118.8 (d, J = 3.3 Hz), 108.3 (d, J = 19.8 Hz). ^{19}F NMR (565 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -120.30 (dd, J = 81.8, 43.0 Hz); (*E* isomer) -128.60 (dd, J = 81.6, 17.4 Hz). HRMS (ESI, m/z): calcd for $C_{12}H_{10}FS^+$ $[M + H]^+$: 205.0482, found 205.0480.



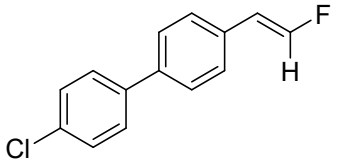
5n, General procedure B, purified by silica gel chromatography (PE). Yellow solid, m.p. 74 – 75 °C, 47.1 mg (99% yield, *E/Z* = 83/17); ^{1}H NMR (400 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.54 – 7.53 (m, 1H), 7.42 – 7.40 (m, 1H), 7.30 – 7.05 (m, 4H), 6.88 – 6.87 (m, 1H), 6.51 (dd, J = 17.4, 11.4 Hz, 1H); (*Z* isomer) 6.68 (dd, J = 81.6, 4.8 Hz, 1H), 5.94 (dd, J = 42.8, 4.8 Hz, 1H). ^{13}C NMR (151 MHz, CD_2Cl_2) (mixture of isomers) δ 150.4 (d, J = 261.9 Hz), 141.2, 136.1, 135.5 (d, J = 12.0 Hz), 135.2, 130.7, 127.9, 127.6 (d, J = 6.6 Hz), 125.8, 124.6, 124.2, 108.6 (d, J = 20.0 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -119.51 (dd, J = 81.6, 42.8 Hz); (*E* isomer) -128.07 (dd, J = 82.1, 17.4 Hz). HRMS (ESI, m/z): calcd for $C_{12}H_9ClFS^+$ $[M + H]^+$: 239.0092, found 239.0093.



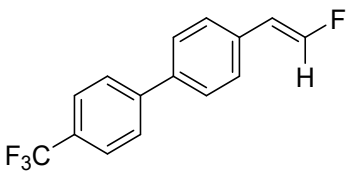
5o, General procedure B, purified by silica gel chromatography (PE). White solid, m.p. 167 – 168 °C, 40.8 mg (99% yield, *E/Z* = 90/10); ^{1}H NMR (600 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.62 – 7.60 (m, 2H), 7.32 (dd, J = 82.8, 11.4 Hz, 1H), 7.09 – 7.06 (m, 2H), 6.56 – 6.55 (m, 1H), 6.27 – 6.23 (m, 2H); (*Z* isomer) 6.64 (dd, J = 80.4, 5.4 Hz, 1H), 5.80 (dd, J = 42.0, 5.4 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) (mixture of isomers) δ 162.4 (d, J = 247.5 Hz), 152.5 (d, J = 3.4 Hz), 150.3 (d, J = 261.4 Hz), 147.4 (d, J = 12.9 Hz), 126.8 (d, J = 3.3 Hz), 125.6 (d, J = 7.8 Hz), 115.9 (d, J = 22.0 Hz), 110.6 (d, J = 8.8 Hz), 106.5, 104.2 (d, J = 20.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -114.03 – -114.08 (m, 1F), -119.72 (dd, J = 80.6 Hz, 42.0 Hz, 1F); (*E* isomer) -113.88 – -113.93 (m, 1F), -130.71 (dd, J = 82.8, 18.1 Hz, 1F). HRMS (ESI, m/z): calcd for $C_{12}H_9F_2O^+$ $[M + H]^+$: 207.0616, found 207.0603.



5p, General procedure B, purified by silica gel chromatography (PE : EA = 20:1). White solid, m.p. 130 – 131 ℃, 45.6 mg (92% yield, *E/Z* = 97/3); ^{1}H NMR (600 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 8.04 (s, 1H), 7.93 – 7.87 (m, 3H), 7.75 – 7.68 (m, 3H), 7.53 – 7.48 (m, 2H), 7.38 – 7.37 (m, 2H), 7.26 (dd, *J* = 82.8, 11.4 Hz, 1H), 6.47 (dd, *J* = 19.2, 11.4 Hz, 1H); (*Z* isomer) 6.71 (dd, *J* = 82.8, 5.4 Hz, 1H), 5.69 (dd, *J* = 45.0, 5.4 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) (mixture of isomers) δ 150.4 (d, *J* = 259.7 Hz), 140.4, 138.0, 133.8, 132.8, 131.9 (d, *J* = 12.1 Hz), 128.7, 128.3, 127.9, 127.8, 126.8 (d, *J* = 3.9 Hz), 126.5, 126.2, 125.7, 125.4, 113.7 (d, *J* = 16.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -121.51 (dd, *J* = 82.8, 45.0 Hz); (*E* isomer) -129.31 (dd, *J* = 82.8, 19.2 Hz). HRMS (ESI, m/z): calcd for $C_{18}H_{14}F^+$ $[M + H]^+$: 249.1074, found 249.1062.

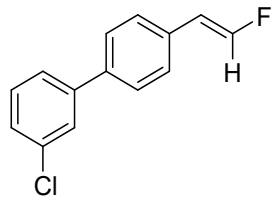


5q, General procedure B, purified by silica gel chromatography (PE). White solid, m.p. 105 – 106 ℃, 45.9 mg (99% yield, *E/Z* = 94/6); ^{1}H NMR (400 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.52 – 7.50 (m, 4H), 7.43 – 7.40 (m, 2H), 7.35 – 7.12 (m, 3H), 6.44 (dd, *J* = 19.2, 11.4 Hz, 1H); (*Z* isomer) 6.71 (dd, *J* = 82.8, 5.4 Hz, 1H), 5.67 (dd, *J* = 44.8, 5.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) (mixture of isomers) δ 150.5 (d, *J* = 259.6 Hz), 139.2 (d, *J* = 2.2 Hz), 139.1, 133.6, 132.2 (d, *J* = 11.9 Hz), 129.1, 128.2, 127.4, 126.8 (d, *J* = 3.0 Hz), 113.6 (d, *J* = 16.1 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -121.26 (dd, *J* = 82.8, 44.8 Hz); (*E* isomer) -128.93 (dd, *J* = 82.5, 19.2 Hz). HRMS (ESI, m/z): calcd for $C_{14}H_{14}ClFN^+$ $[M + NH_4]^+$: 250.0793, found 250.0789.

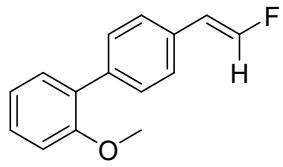


5r, General procedure B, purified by silica gel chromatography (PE). White solid, m.p. 86 – 87 ℃, 33.5 mg (63% yield, *E/Z* = 96/4); ^{1}H NMR (400 MHz, CD_2Cl_2) (mixture of isomers) δ (*E* isomer) 7.75 – 7.69 (m, 4H), 7.61 – 7.59 (m, 2H), 7.40 – 7.17 (m, 3H), 6.46 (dd, *J* = 19.6, 11.6 Hz, 1H); (*Z*

isomer) 6.74 (dd, J = 82.8, 5.2 Hz, 1H), 5.72 (dd, J = 44.8, 5.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) (mixture of isomers) δ 150.7 (d, J = 260.5 Hz), 144.2, 139.0, 132.9 (d, J = 11.9 Hz), 129.6 (d, J = 32.2 Hz), 127.8, 127.3, 126.9 (d, J = 3.0 Hz), 125.9 (q, J = 3.8 Hz), 124.4 (q, J = 271.8 Hz), 113.5 (d, J = 16.2 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -120.87 (dd, J = 82.8 44.8 Hz, 1F); (*E* isomer) -62.42 (s, 3F), -128.45 (dd, J = 82.6, 19.6 Hz, 1F). HRMS (ESI, m/z): calcd for $C_{15}H_{11}F_4^+$ $[M + H]^+$: 267.0791, found 267.0789.

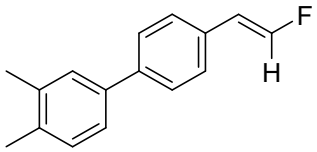


5s, General procedure B, purified by silica gel chromatography (PE). Colorless oil, 45.9 mg (99% yield, *E/Z* = 95/5); ^{1}H NMR (400 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.58 – 5.57 (m, 1H), 7.53 – 7.51 (m, 2H), 7.47 – 7.45 (m, 1H), 7.39 – 7.12 (m, 5H), 6.44 (dd, J = 19.2, 11.4 Hz, 1H); (*Z* isomer) 6.71 (dd, J = 82.8, 5.2 Hz, 1H), 5.67 (dd, J = 44.8, 5.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) (mixture of isomers) δ 150.6 (d, J = 260.1 Hz), 142.5, 139.0 (d, J = 2.7 Hz), 134.9, 132.5 (d, J = 12.2 Hz), 130.2, 127.6, 127.5, 127.2, 126.8 (d, J = 3.1 Hz), 125.2, 113.6 (d, J = 16.3 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -121.09 (dd, J = 82.8, 44.8 Hz); (*E* isomer) -128.76 (dd, J = 83.1, 19.2 Hz). HRMS (ESI, m/z): calcd for $C_{14}H_{11}ClF^+$ $[M + H]^+$: 233.0528, found 233.0551.

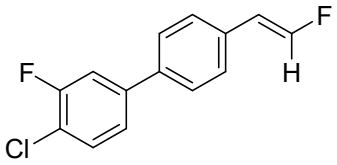


5t, General procedure B, purified by silica gel chromatography (PE : EA = 20:1). Colorless oil, 43.8 mg (96% yield, *E/Z* = 97/3); ^{1}H NMR (400 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.54 – 7.52 (m, 2H), 7.37 – 7.13 (m, 5H), 7.09 – 7.04 (m, 1H), 7.02 (d, J = 8.4 Hz, 1H), 6.47 (dd, J = 19.2, 11.2 Hz, 1H), 3.85 (s, 3H); (*Z* isomer) 6.70 (dd, J = 82.8, 5.2 Hz, 1H), 5.68 (dd, J = 44.8, 5.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) (mixture of isomers) δ 156.6, 150.2 (d, J = 259.0 Hz), 137.9 (d, J = 2.1 Hz), 131.4 (d, J = 11.8 Hz), 130.8, 130.2, 130.0, 128.9, 125.9 (d, J = 2.9 Hz), 121.0, 113.8 (d, J = 15.8 Hz), 111.4, 55.6. ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -122.05 (dd, J = 82.8, 44.8 Hz); (*E* isomer) -129.92 (dd, J = 83.3, 19.2 Hz). HRMS (ESI, m/z): calcd for $C_{15}H_{14}FO^+$

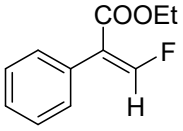
$[M + H]^+$: 229.1023, found 229.1014.



5u, General procedure B, purified by silica gel chromatography (PE). White solid, m.p. 105 – 106 ℃, 38.4 mg (85% yield, *E/Z* = 96/4); ^{1}H NMR (400 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.51 – 7.49 (m, 2H), 7.34 (s, 1H), 7.34 – 7.05 (m, 5H), 6.39 (dd, *J* = 19.2, 11.2 Hz, 1H), 2.29 (d, *J* = 10.2 Hz, 6H); (*Z* isomer) 6.64 (dd, *J* = 82.8, 5.4 Hz, 1H), 5.61 (dd, *J* = 44.8, 5.4 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) (mixture of isomers) δ 150.2 (d, *J* = 259.3 Hz), 140.5 (d, *J* = 1.8 Hz), 138.2, 137.1, 136.0, 131.4 (d, *J* = 11.7 Hz), 130.3, 128.3, 127.4, 126.6 (d, *J* = 3.1 Hz), 124.4, 113.7 (d, *J* = 16.1 Hz), 20.0, 19.6. ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -121.92 (dd, *J* = 82.8, 44.8 Hz); (*E* isomer) -129.79 (dd, *J* = 83.5, 19.2 Hz). HRMS (ESI, m/z): calcd for $C_{16}H_{16}F^+$ $[M + H]^+$: 227.1231, found 227.1224.

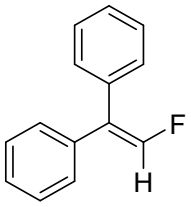


5v, General procedure B, purified by silica gel chromatography (PE). Colorless oil, 49.5 mg (99% yield, *E/Z* = 95/5); ^{1}H NMR (400 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.50 – 7.48 (m, 2H), 7.46 – 7.43 (m, 1H), 7.37 – 7.12 (m, 5H), 6.43 (dd, *J* = 19.2, 11.2 Hz, 1H); (*Z* isomer) 6.71 (dd, *J* = 82.4, 5.4 Hz, 1H), 5.67 (dd, *J* = 44.8, 5.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) (mixture of isomers) δ 159.6, 157.1, 150.6 (d, *J* = 260.7 Hz), 141.1 (d, *J* = 6.9 Hz), 137.9, 132.7 (d, *J* = 12.1 Hz), 130.9, 127.3, 126.7 (d, *J* = 3.0 Hz), 123.1 (d, *J* = 3.5 Hz), 120.0 (d, *J* = 17.6 Hz), 114.1 (dd, *J* = 149.8, 18.9 Hz). ^{19}F NMR (565 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -120.80 (dd, *J* =82.4, 44.8 Hz, 1F); (*E* isomer) -115.05 – -115.09 (m, 1F), -128.37 (dd, *J* = 83.3, 19.2 Hz, 1F). HRMS (ESI, m/z): calcd for $C_{14}H_{10}ClF_2^+$ $[M + H]^+$: 251.0434, found 251.0438.

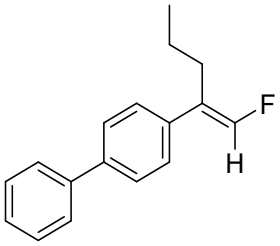


5w, General procedure B, purified by silica gel chromatography (PE : EA = 10:1). Colorless oil, 15.9 mg (41% yield, *E/Z* = 73/27); ^{1}H NMR (400 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.74 (d, *J* = 80.8 Hz, 1H), 7.41 – 7.33 (m, 5H), 4.27 (q, *J* = 7.2 Hz, 2H), 1.31 (t, *J* = 7.2 Hz, 3H); (*Z* isomer)

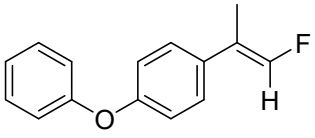
6.99 (d, J = 79.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) (mixture of isomers) δ 166.1 (d, J = 16.4 Hz), 158.0 (d, J = 282.0 Hz), 130.0 (d, J = 2.8 Hz), 128.4, 128.2, 119.8 (d, J = 7.3 Hz), 61.3, 14.3. ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -110.62 (d, J = 79.6 Hz); (*E* isomer) -114.70 (d, J = 80.8 Hz). HRMS (ESI, m/z): calcd for $C_{11}H_{12}FO_2^+$ [M + H]$^+$: 195.0816, found 195.0817.



5x[6], General procedure B, Ph_2SiH_2 (73.7 mg, 0.40 mmol), 100℃, purified by silica gel chromatography (PE). Colorless oil, 39.2 mg (99% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.24 (m, 10H), 6.97 (d, J = 83.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.9 (d, J = 268.7 Hz), 129.9 (d, J = 4.3 Hz), 128.8 (d, J = 3.5 Hz), 128.7, 128.4, 127.9 (d, J = 4.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -128.02 (d, J = 83.2 Hz, 1F). HRMS (ESI, m/z): calcd for $C_{14}H_{12}F^+$ [M + H]$^+$: 199.0918, found 199.0905.

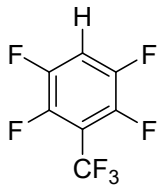


5y, General procedure B, Ph_2SiH_2 (73.7 mg, 0.40 mmol), 100℃, purified by silica gel chromatography (PE). White solid, m.p. 122 – 123 ℃, 21.7 mg (45% yield, *E/Z* = 91/9); ^{1}H NMR (400 MHz, $CDCl_3$) δ (*E* isomer) 7.60 – 7.56 (m, 4H), 7.46 – 7.43 (m, 2H), 7.37 – 7.35 (m, 3H), 6.87 (d, J = 85.6 Hz, 1H), 2.56 (td, J = 7.6, 3.2 Hz, 2H), 1.50 – 1.41 (m, 2H), 0.95 – 0.91 (t, J = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (*E* isomer) 146.1 (d, J = 258.9 Hz), 140.8, 140.4, 135.8 (d, J = 9.3 Hz), 129.0, 127.5, 127.4, 127.3 (d, J = 2.9 Hz), 127.1, 124.7 (d, J = 9.5 Hz), 28.5 (d, J = 4.0 Hz), 21.1, 13.8. ^{19}F NMR (376 MHz, $CDCl_3$) δ (*E* isomer) -131.07 (dt, J = 85.6, 3.2 Hz). HRMS (ESI, m/z): calcd for $C_{17}H_{18}F^+$ [M + H]$^+$: 241.1387, found 241.1373.

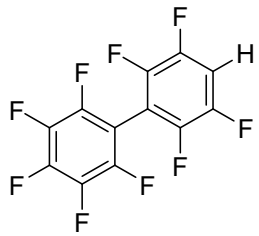


5z, General procedure B, Ph_2SiH_2 (73.7 mg, 0.40 mmol), 100℃, purified by silica gel

chromatography (PE). Colorless oil, 14.6 mg (32% yield, *E/Z* = 89/11); ^{1}H NMR (400 MHz, CD_2Cl_2) (mixture of isomers) δ (*E* isomer) 7.37 – 7.33 (m, 2H), 7.30 – 7.28 (m, 2H), 7.14 – 7.10 (m, 1H), 7.02 – 6.80 (m, 5H), 2.03 (dd, *J* = 3.6, 1.6 Hz, 3H); (*Z* isomer) 6.67 (dq, *J* = 84.8, 1.6 Hz, 1H), 1.90 (dd, *J* = 4.8, 1.6 Hz, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) (mixture of isomers) δ 157.5, 157.2, 146.1 (d, *J* = 256.4 Hz), 132.9 (d, *J* = 8.9 Hz), 130.2, 127.6 (d, *J* = 3.4 Hz), 123.8, 119.3, 119.2, 12.4 (d, *J* = 5.6 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -129.36 (dq, *J* = 84.8, 4.8 Hz); (*E* isomer) -131.74 (dq, *J* = 86.0, 3.6 Hz). HRMS (ESI, m/z): calcd for $C_{15}H_{14}FO^+$ $[M + H]^+$: 229.1023, found 229.1022.



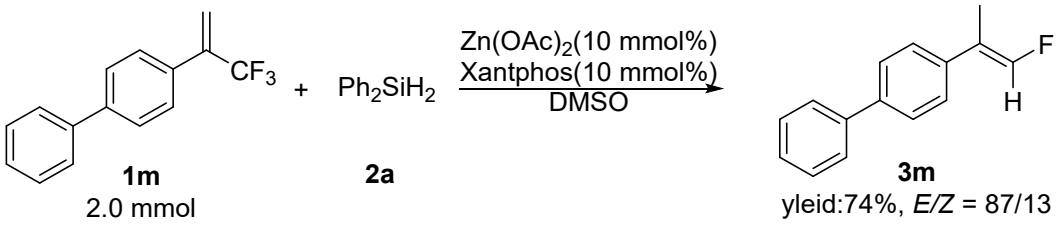
7a[7], General procedure C, when the reaction is completed, trifluoromethylbenzene (0.1 mmol) is added to the sealed tube as the internal standard, resulting in crude ^{19}F NMR yield of 76%. ^{19}F NMR (376 MHz, *d*-DMSO) δ -55.05 – -55.19 (m, 3F), -136.29 – 136.43 (m, 2F), -141.15 – -141.32 (m, 2F). HRMS (ESI, m/z): calcd for $C_7HF_7Na^+$ $[M + Na]^+$: 240.9859, found 240.9870. ^{19}F NMR data is consistent with the reported literature[7].



7b[8], General procedure C, purified by silica gel chromatography (PE). White solid, m.p. 75 – 76 °C, 41.7 mg (66% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.27 (m, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -137.38 – -137.49 (m, 4F), -138.16 – -138.28 (m, 2F), -149.92 – -150.34 (m, 1F), -160.47 – -160.60 (m, 2F). HRMS (ESI, m/z): calcd for $C_{12}HF_9K^+$ $[M + K]^+$: 354.9566, found 354.9571.

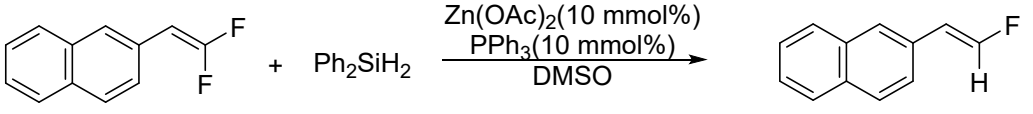
3. Gram-Scale Synthesis and Derivatization Reactions

3.1 Scale-up reaction.



1m 2.0 mmol　　**2a**　　**3m** yleid:74%, *E/Z* = 87/13

$Zn(OAc)_2$ (36.7 mg, 0.2 mmol) and Xantphos (115.7 mg, 0.2 mmol) in DMSO (20.0 mL) were charged into a 100 mL pressure tube under argon. The mixture was stirred for 30 min at room temperature. Then Ph_2SiH_2 (1105.9 mg, 6 mmol) and trifluoromethyl alkene **1m** (496.2 mg, 2 mmol) were added sequentially to the reaction mixture. The reaction tube was then sealed and placed into an oil bath at 120 °C. After stirred for 24 h, the reaction mixture was quenched with H_2O (20 mL) and extracted with dichloromethane. The organic layer was separated dried over Na_2SO_4, concentrated, and purified by silica gel chromatography (PE) to give the monofluoride product **3m** (313.8 mg, yield 74%, *E/Z* = 87/13). ^{1}H NMR (400 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.63 – 7.53 (m, 4H), 7.46 – 7.44 (m, 2H), 7.41 – 7.30 (m, 3H), 6.98 (dq, *J* = 84.9, 1.5 Hz, 1H), 2.09 (dd, *J* = 3.8, 1.5 Hz, 3H); (*Z* isomer) 6.71 (dq, *J* = 84.5, 1.8 Hz, 1H), 1.96 (dd, *J* = 4.9, 1.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) (mixture of isomers) δ 146.2 (d, *J* = 258.6 Hz), 140.8, 140.4, 136.7 (d, *J* = 8.8 Hz), 129.0, 127.5, 127.4, 127.1, 126.4 (d, *J* = 3.0 Hz), 119.8 (d, *J* = 10.1 Hz), 12.3 (d, *J* = 5.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -128.05 – -128.32 (m); (*E* isomer) -130.75 – -131.01 (m).

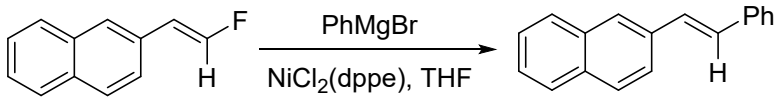


4a 2.0mmol　　**2a**　　**5a** yleid: 90%, *E/Z* = 95/5

$Zn(OAc)_2$ (36.7 mg, 0.2 mmol) and PPh_3 (52.5 mg, 0.2 mmol) in DMSO (20.0 mL) were charged into a 100 mL pressure tube under argon. The mixture was stirred for 30 min at room temperature. Then Ph_2SiH_2 (368.6 mg, 2 mmol) and *gem*-difluoroalkene **4a** (380.1 mg, 2 mmol) were added sequentially to the reaction mixture. The reaction tube was then sealed and placed into an oil bath at 50 °C. After stirred for 24 h, the reaction mixture was quenched with H_2O (20.0 ml) and extracted

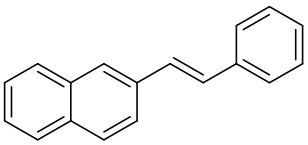
with dichloromethane. The organic layer was separated dried over Na_2SO_4, concentrated, and purified by silica gel chromatography (PE) to give the monofluoride product **5a** (309.5 mg, yield 90%, *E/Z* 19:1). ^{1}H NMR (400 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.84 – 7.75 (m, 3H), 7.65 (s, 1H), 7.53 – 7.16 (m, 4H), 6.56 (dd, *J* = 19.6, 11.2 Hz, 1H); (*Z* isomer) 6.74 (dd, *J* = 82.8, 5.4 Hz, 1H), 5.78 (dd, *J* = 44.8, 5.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) (mixture of isomers) δ 150.6 (d, *J* = 259.3 Hz), 133.7, 132.9, 130.3 (d, *J* = 11.8 Hz), 128.6, 127.9, 126.6, 126.1, 125.9 (d, *J* = 5.0 Hz), 123.5, 114.3 (d, *J* = 16.3 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -121.73 (dd, *J* = 82.8, 44.8 Hz); (*E* isomer) -129.38 (dd, *J* = 83.2, 19.6 Hz).

3.2 Derivatization Reaction.

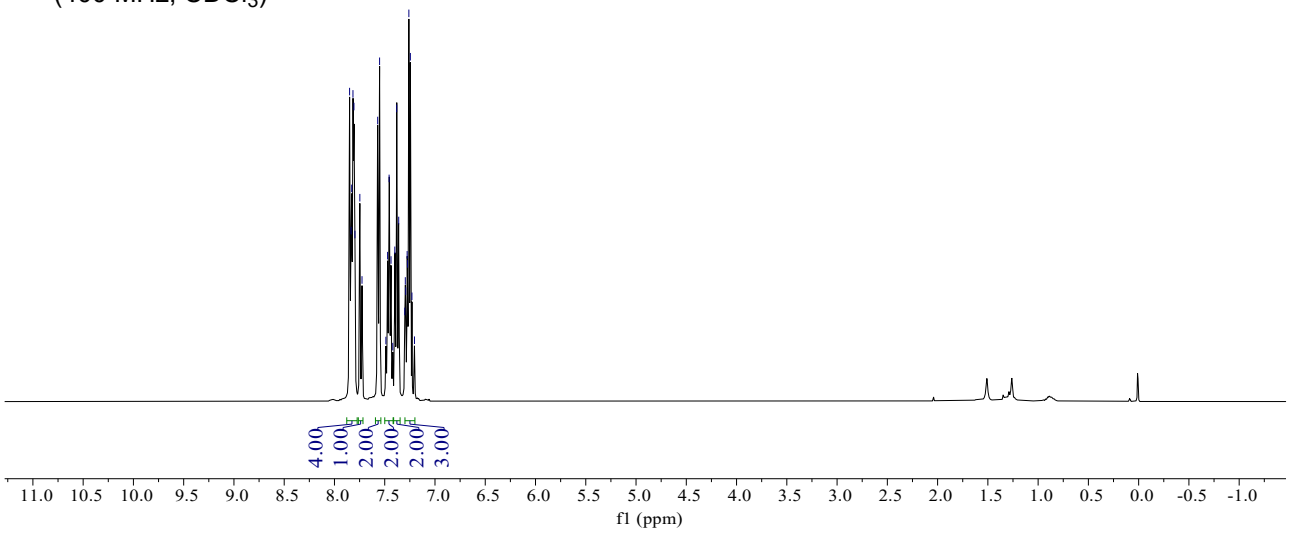


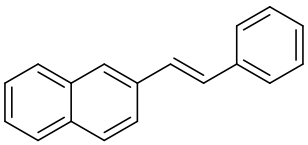
5a **8**, yield:87%

$NiCl_2$(dppe) (4.2 mg, 0.008 mmol) in 0.4 mL dry THF were charged into a 25 mL pressure tube under argon, and then the monofluoride **5a** (34.4mg, 0.2mmol) was added. To this mixture was added dropwise a solution of Grignard reagents in THF (0.8 mmol). After stirred for 2 h at room temperature, the reaction mixture was quenched with saturated aqueous solution of NH_4Cl (2.0 ml) and extracted with ethyl acetate. The organic layer was separated dried over Na_2SO_4, concentrated, and purified by silica gel chromatography (PE) to give the product **8** (40.1 mg, yield 87%)[9]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 – 7.80 (m, 4H), 7.75 – 7.73 (m, 1H), 7.57 – 7.55 (m, 2H), 7.49 – 7.42 (m, 2H), 7.39 – 7.37 (m, 2H), 7.30 – 7.20 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.5, 135.0, 133.9, 133.2, 129.2, 128.9, 128.9, 128. 5, 128.2, 127.8, 127.8, 126.8, 126.7, 126.5, 126.0, 123.7. HRMS (ESI, m/z): calcd for $C_{18}H_{15}^+$ [M + H] $^+$: 231.1168, found 231.1169.

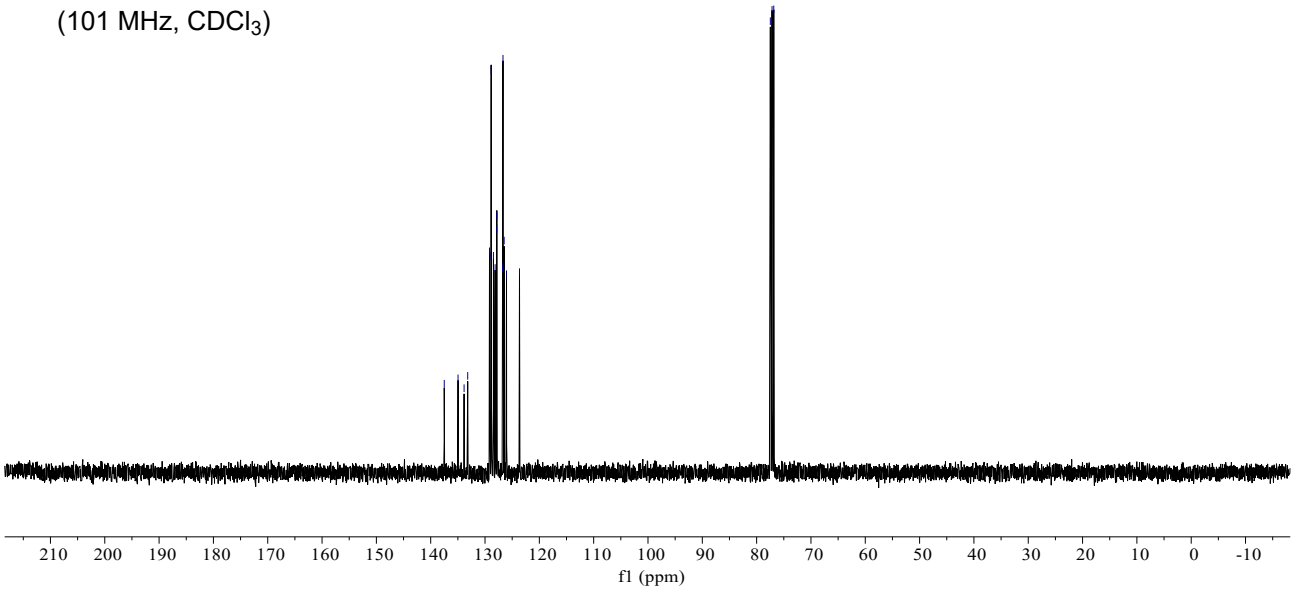


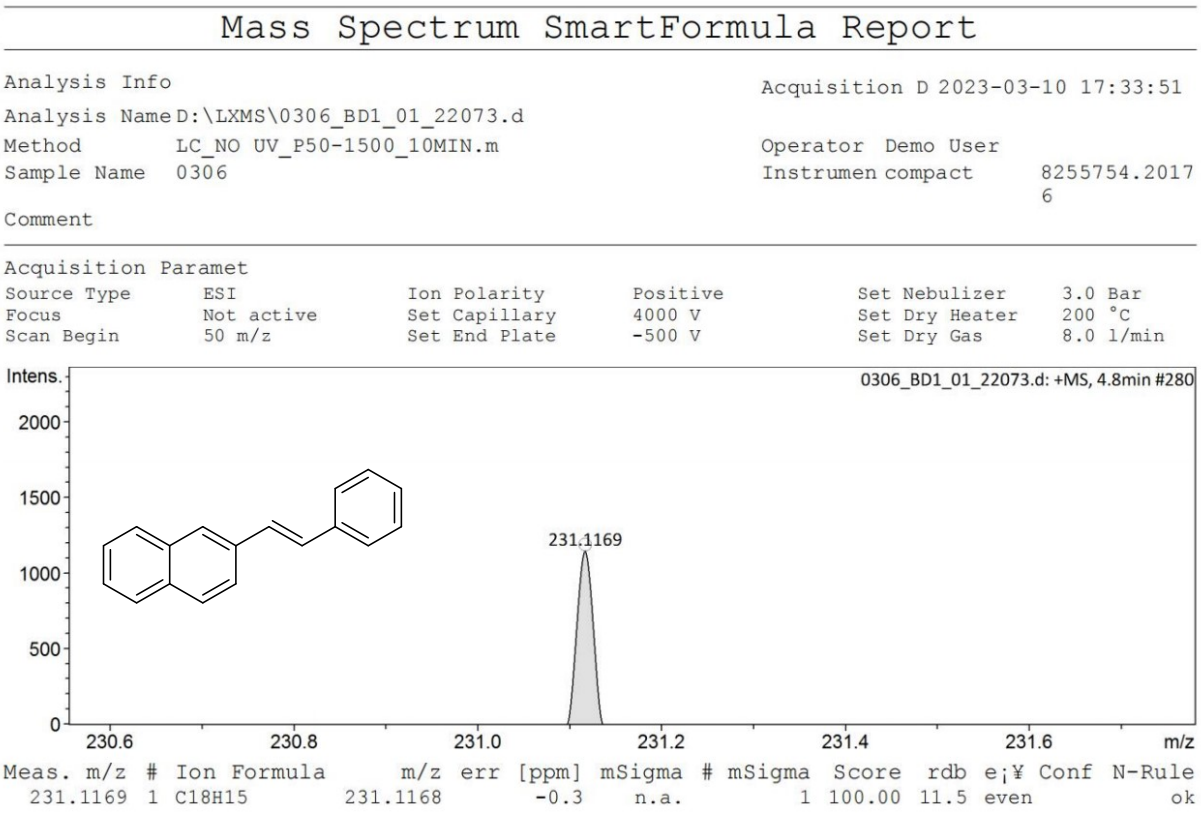
^{1}H NMR
(400 MHz, $CDCl_3$)

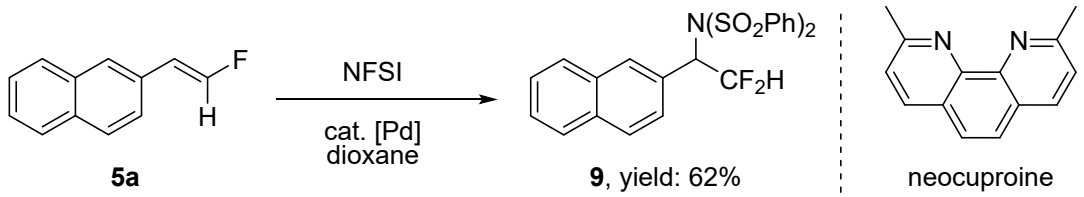




^{13}C NMR
(101 MHz, $CDCl_3$)

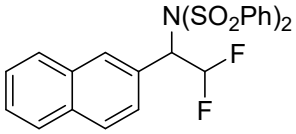




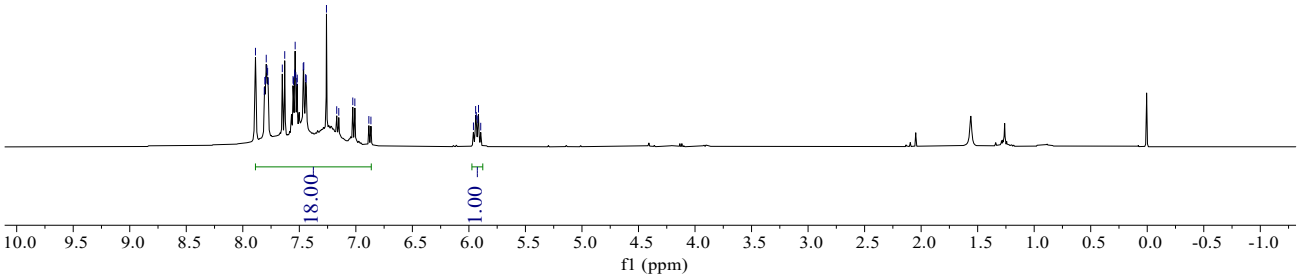


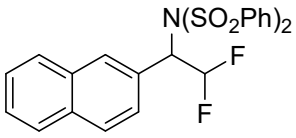
5a **9**, yield: 62% neocuproine

$Pd(OAc)_2$ (2.3 mg, 0.01 mmol), neocuproine (3.1 mg, 0.015 mmol) and N-fluorobenzenesulfonimide (158 mg, 0.5 mmol) in 1,4-dioxane (1.0 mL) were charged into a 25 mL pressure tube under argon, and then the monofluoride **5a** (34.4mg, 0.2mmol) was added. The reaction tube was then sealed and placed in an oil bath at 50 °C. After stirred for 20 h, the reaction mixture was filtered through a pad of celite, eluted with ethyl acetate, concentrated, and purified by silica gel chromatography (PE : EA = 5:1) to give the indicated product **9** (60.4 mg, yield 62%)[10,11]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 – 6.87 (m, 18H), 5.93 (dt, *J* = 10.4, 8.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.6, 133.9, 133.2, 132.8, 128.9, 128.8, 128.6, 128.5, 127.6, 127.3, 126.8, 126.4, 114.5 (dd, *J* = 246.8, 241.8 Hz), 64.0 (dd, *J* = 35.9, 23.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -116.40 (ddd, *J* = 293.0, 57.1, 10.2 Hz, 1F), -124.87 (ddd, *J* = 293.0, 56.4, 8.3 Hz, 1F). HRMS (ESI, m/z): calcd for $C_{24}H_{20}F_2NO_4S_2^+$ $[M + H]^+$: 488.0796, found 488.0773.

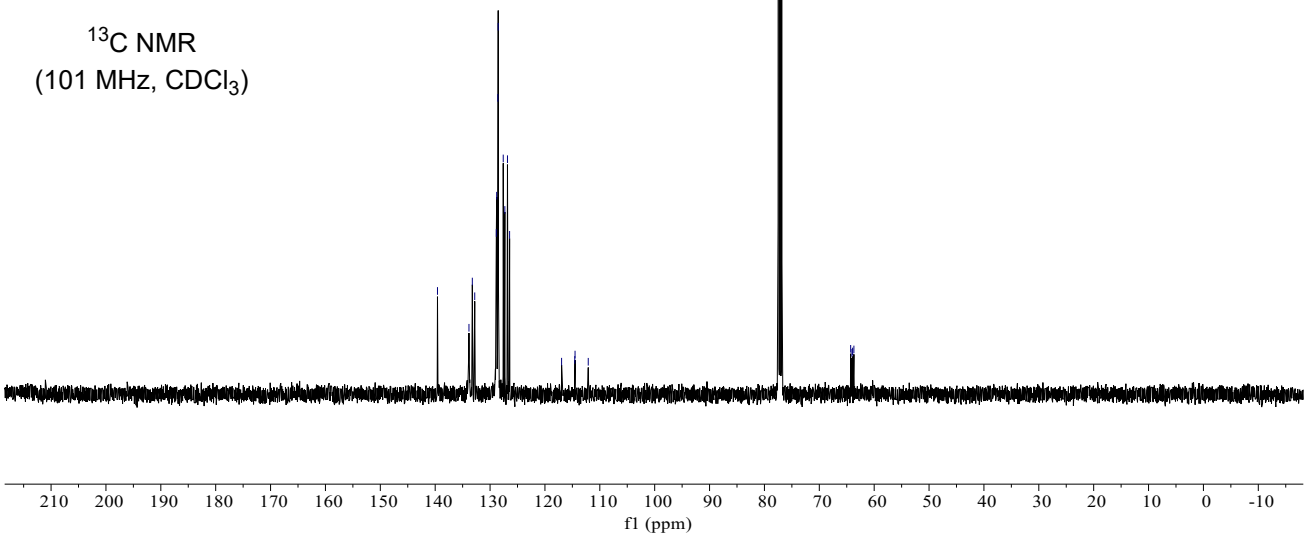


^{1}H NMR
(400 MHz, $CDCl_3$)

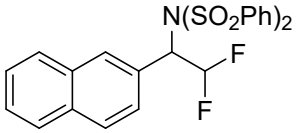




^{13}C NMR
(101 MHz, $CDCl_3$)

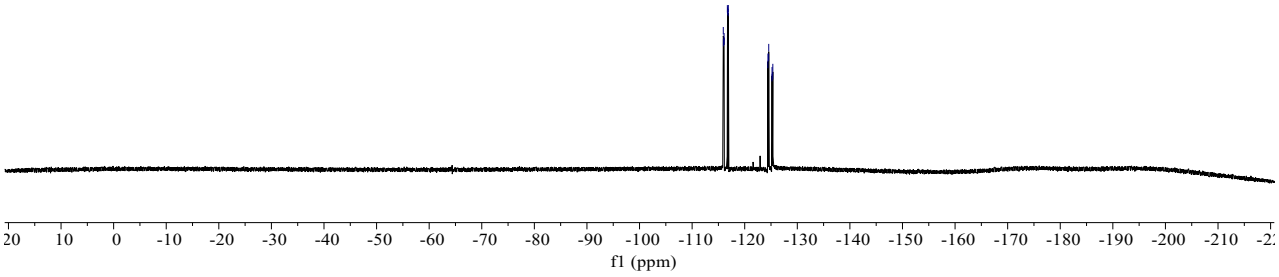


-115.93
-115.95
-116.08
-116.10
-116.70
-116.73
-116.86
-116.88
-124.40
-124.42
-124.55
-124.57
-125.17
-125.20
-125.32
-125.35



^{19}F NMR

(376 MHz, $CDCl_3$)



Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2023-03-10 17:45:57

Analysis Name D:\LXMS\0306_BD2_01_22074.d

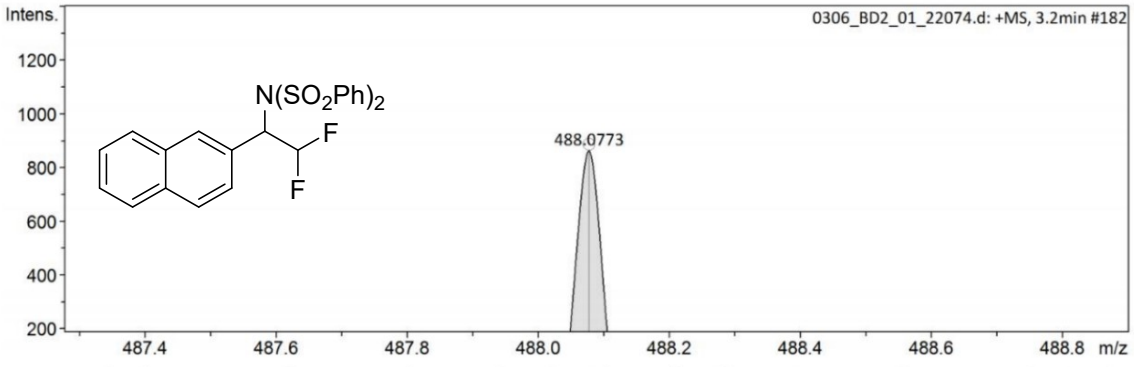
Method LC_NO UV_P50-1500_10MIN.m — Operator Demo User

Sample Name 0306 — Instrumen compact 8255754.2017 6

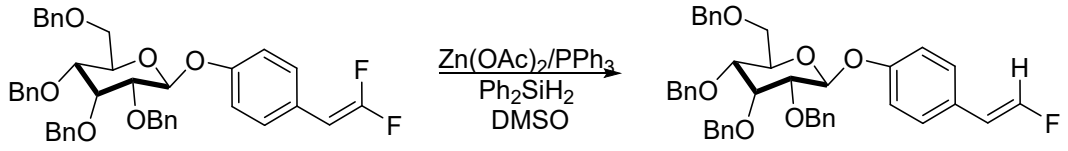
Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥	Conf	N-Rule
488.0773	1	C24H20F2NO4S2	488.0796	4.7	602.7		1	100.00	14.5	even		ok

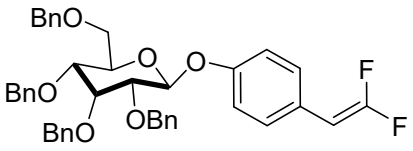


10 **11**, yield: 35%, *E/Z* = 90/10

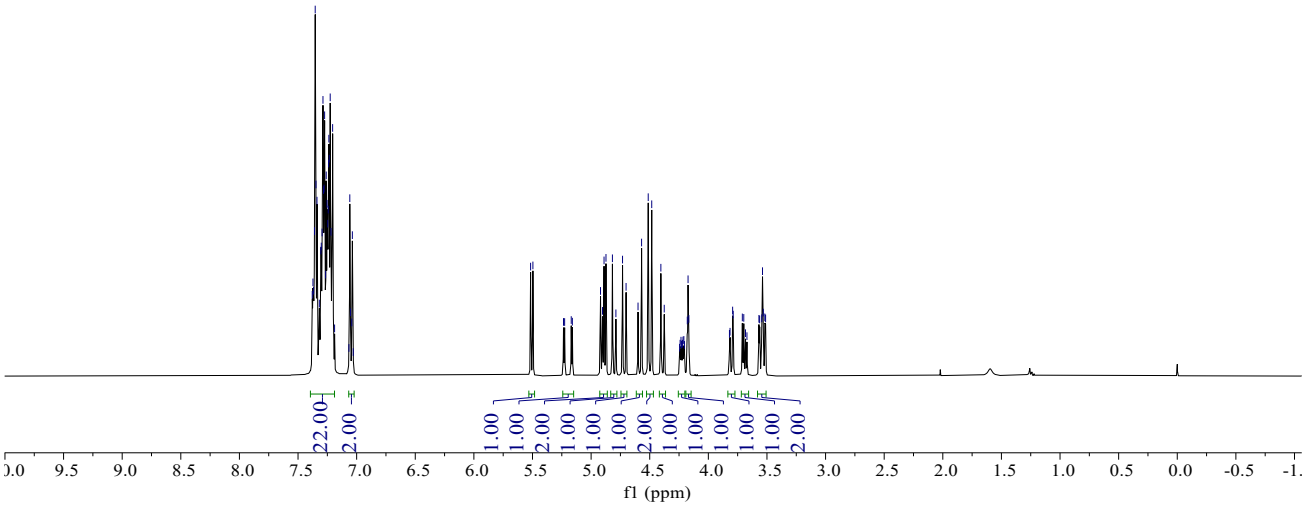
$Zn(OAc)_2$ (3.7 mg, 0.02 mmol) and PPh_3 (5.3 mg, 0.02 mmol) in DMSO (2.0 mL) were charged into a 25 mL pressure tube under argon. The mixture was stirred for 30 min at room temperature. Then Ph_2SiH_2 (73.6 mg, 0.4 mmol) and *gem*-difluoroalkene **10** (135.7mg, 0.2 mmol) were added sequentially to the reaction mixture. The reaction tube was then sealed and placed into an oil bath at 100 °C. After stirred for 24 h, the reaction mixture was quenched with H_2O (2.0 ml) and extracted with dichloromethane. The organic layer was separated dried over Na_2SO_4, concentrated, and purified by silica gel chromatography (PE : EA = 10:1) to give the monofluoride product **11** (46.2 mg, yield 35%, *E/Z* = 90/10).

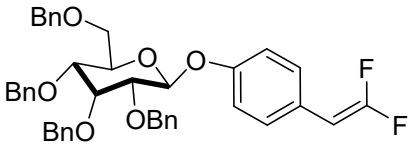
gem-difluoroalkene **10**, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.20 (m, 22H), 7.06 – 7.04 (m, 2H), 5.51 (d, *J* = 7.9 Hz, 1H), 5.20 (dd, *J* = 26.4, 3.8 Hz, 1H), 4.95 – 4.29 (m, 8H), 4.22 (m, 1H), 4.17 (t, *J* = 2.6 Hz, 1H), 3.85 – 3.63 (m, 2H), 3.54 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.6 (t, *J* = 2.3 Hz), 156.0 (dd, *J* = 297.1, 286.9 Hz), 139.0, 138.6, 138.4, 137.9, 128.8 (dd, *J* = 6.2, 3.4 Hz), 128.5, 128.5, 128.4, 128.3, 128.1, 127.9, 127.9, 127.8, 127.8, 127.8, 127.6, 127.6, 124.4 (t, *J* = 6.3 Hz), 117.2, 99.3, 81.7 (dd, *J* = 29.3, 14.2 Hz), 78.8, 75.6, 74.8, 74.7, 73.6, 73.2, 72.9, 71.7, 69.2. ^{19}F NMR (376 MHz, $CDCl_3$) δ -84.07 (dd, *J* = 35.4, 26.2 Hz, 1F), -85.86 (dd, *J* = 36.0, 4.1 Hz, 1F). HRMS (ESI, m/z): calcd for $C_{42}H_{41}F_2O_6^+$ [M + H] $^+$: 679.2866, found 679.2857.

monofluoride product **11**, ^{1}H NMR (400 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.38 – 7.20 (m, 20H), 7.19 – 6.96 (m, 5H), 6.35 (dd, *J* = 19.2, 11.2 Hz, 1H), 5.49 (d, *J* = 7.9 Hz, 1H), 4.94 – 4.36 (m, 8H), 4.22 (m, 1H), 4.18 (t, *J* = 2.6 Hz, 1H), 3.89 – 3.63 (m, 2H), 3.61 – 3.49 (m, 2H); (*Z* isomer) 6.60 (dd, *J* = 82.8, 5.2 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) (mixture of isomers) δ 157.2, 149.4 (d, *J* = 256.8 Hz), 139.0, 138.6, 138.5, 137.9, 128.6, 128.5, 128.4, 128.3, 128.1, 128.0, 127.9, 127.9, 127.8, 127.8, 127.6, 127.6, 127.3 (d, *J* = 3.1 Hz), 126.8 (d, *J* = 12.1 Hz), 117.3, 113.5 (d, *J* = 15.6 Hz), 99.3, 78.8, 75.6, 74.9, 74.7, 73.6, 73.2, 72.9, 71.8, 69.3. ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -124.68 (dd, *J* = 82.8, 45.7 Hz); (*E* isomer) -132.03 (dd, *J* = 84.0, 19.2 Hz). HRMS (ESI, m/z): calcd for $C_{42}H_{42}FO_6^+$ [M + H] $^+$: 661.2960, found 679.2955.

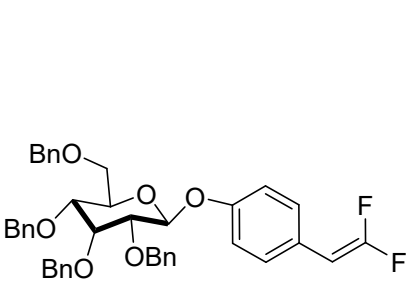


^{1}H NMR
(400 MHz, $CDCl_3$)





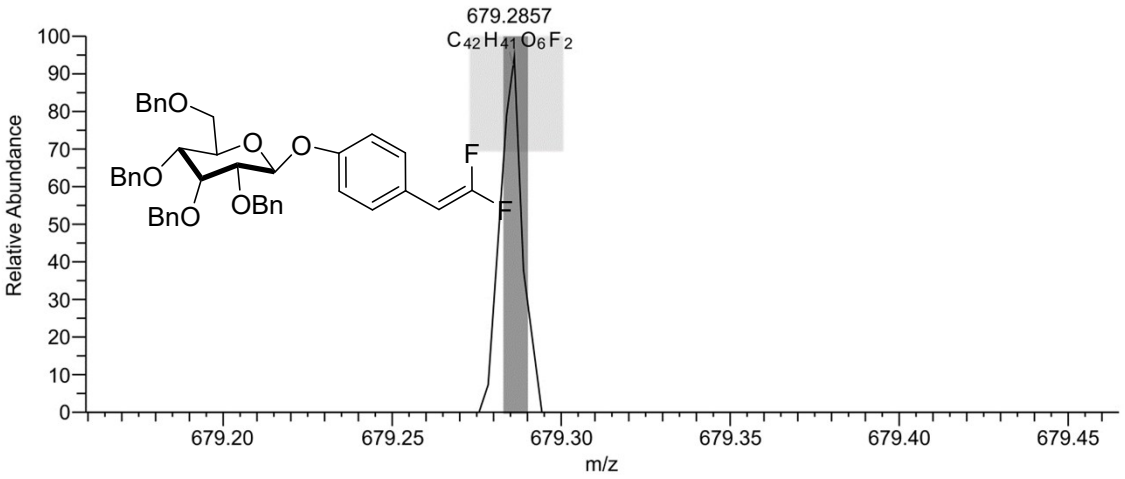
^{13}C NMR
(101 MHz, $CDCl_3$)



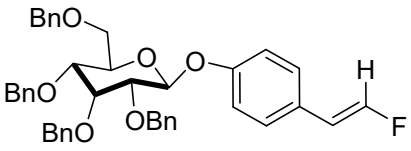
^{19}F NMR

(376 MHz, $CDCl_3$)

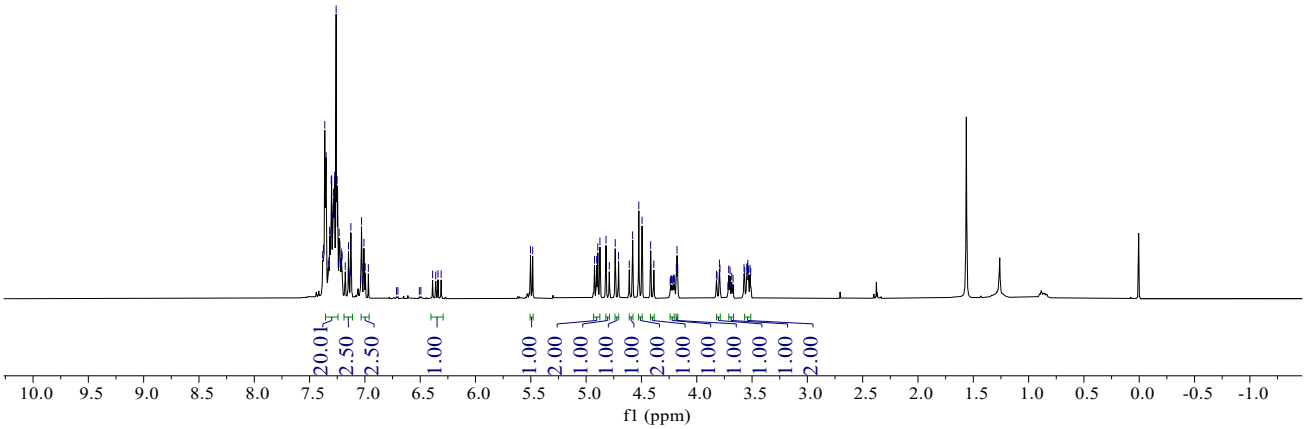
lx-94 #95 RT: 0.71 AV: 1 NL: 2.53E5
T: FTMS + p ESI Full ms [100.0000-1500.0000]

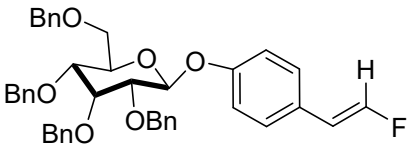


Peak M...	Display...	S Fit	RDB	Delta [p...	Theo....	Rank	Combin...	# Matc...	# Misse...	MS Cov...	Pattern...	MSMS...
679.2857	$C_{42}H_{41}O_6F_2$	28.14857322080024	21.50	-1.28	679.28657	1	96.22	1	1	100	68.76	(Collection)

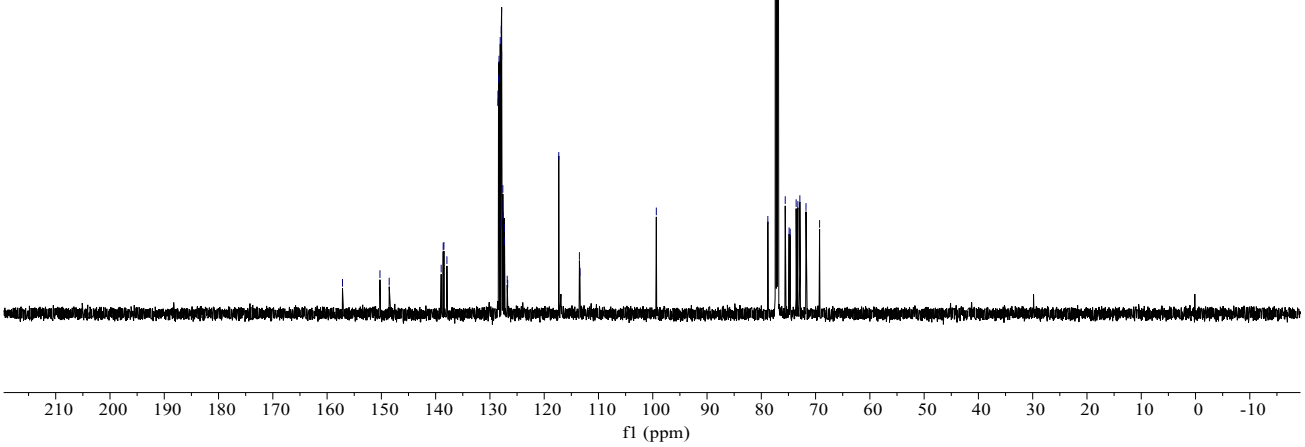


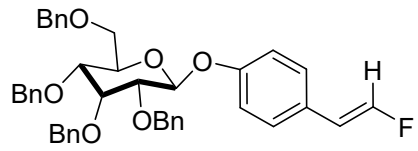
^{1}H NMR
(400 MHz, $CDCl_3$)



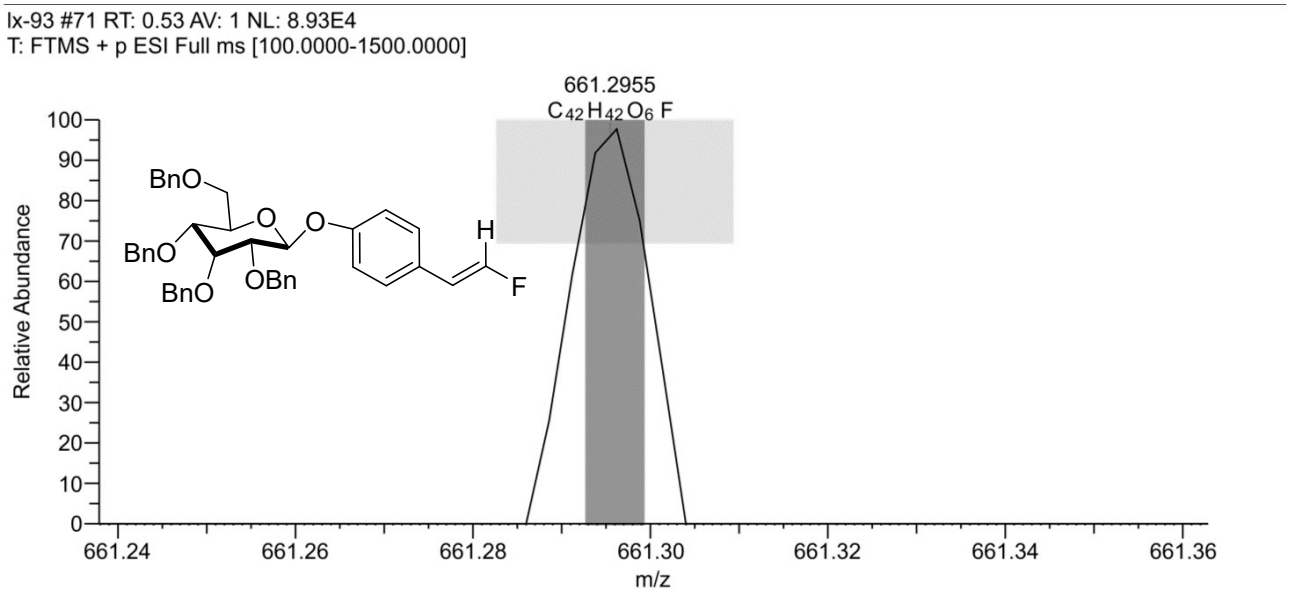


^{13}C NMR
(151 MHz, $CDCl_3$)





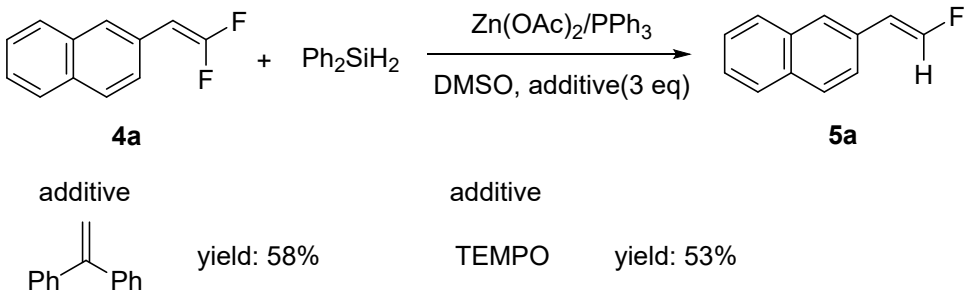
^{19}F NMR
(376 MHz, $CDCl_3$)



Peak M...	Display...	S Fit	RDB	Delta [p...	Theo....	Rank	Combin...	# Matc...	# Misse...	MS Cov...	Pattern...	MSMS...
661.2955	$C_{42}H_{42}O_6F$	28.94587630561 76	21.50	-0.70	661.29599	1	96.26	1	1	100	68.77	(Collection)

4. Mechanism Studies

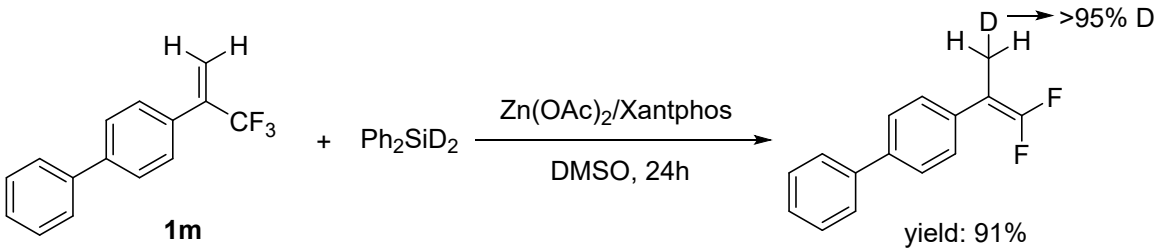
4.1 Radical-probe experiments.



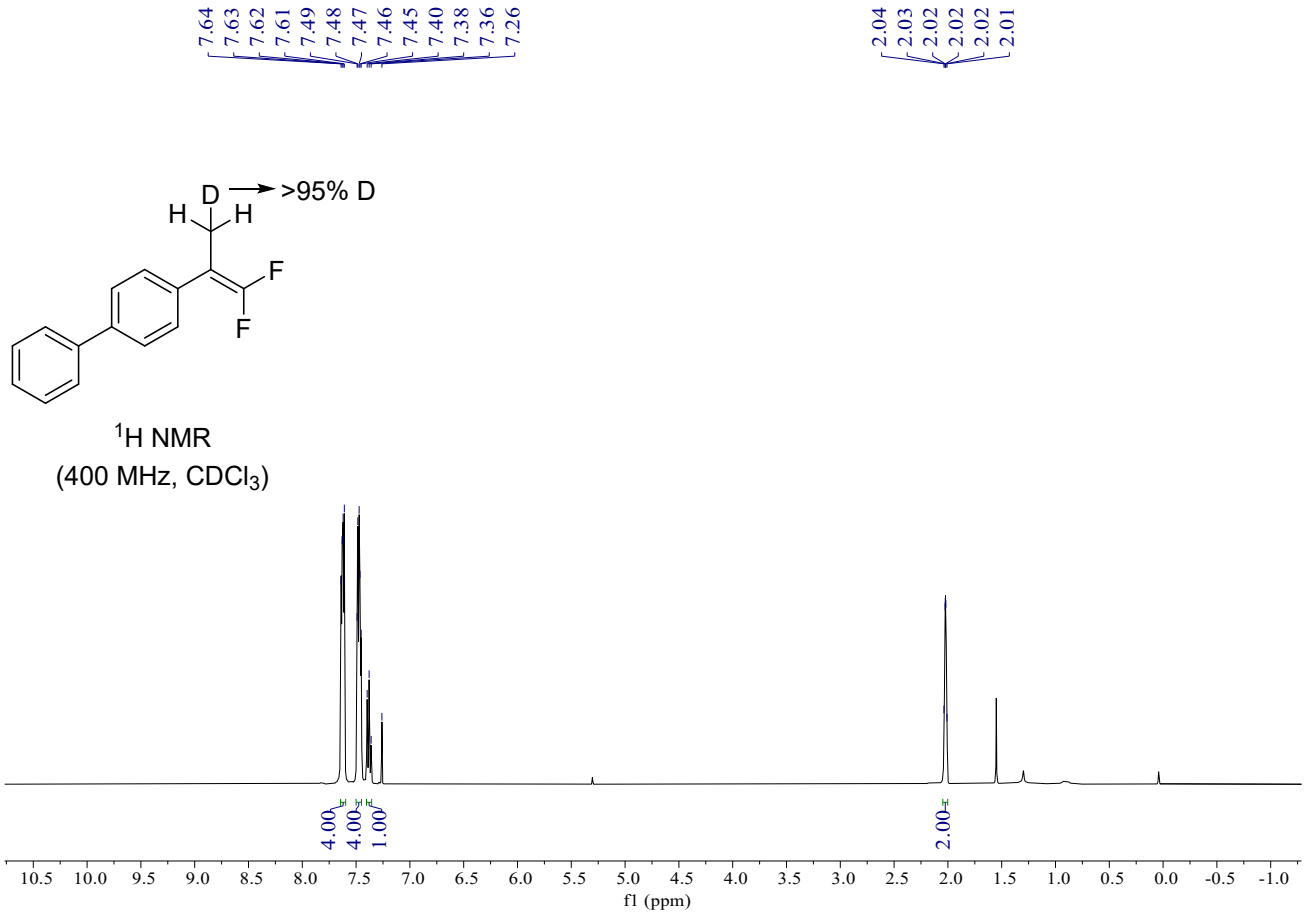
$Zn(OAc)_2$ (3.7 mg, 0.02 mmol) and PPh_3 (5.3 mg, 0.02 mmol) in DMSO (2.0 mL) were charged into a 25 mL pressure tube under argon. The mixture was stirred for 30 min at room temperature. Then Ph_2SiH_2 (36.8 mg, 0.2 mmol), *gem*-difluoroalkene **4a** (38.0 mg, 0.2 mmol) and 1,1-Diphenylethylene (108.2 mg, 0.6 mmol) were added sequentially to the reaction mixture. The reaction tube was then sealed and placed into an oil bath at 50 °C. After stirred for 24 h, the reaction mixture was quenched with H_2O (2.0 ml) and extracted with dichloromethane. The organic layer was separated dried over Na_2SO_4, concentrated, and purified by silica gel chromatography (PE) to give the monofluoride product **5a** (20.0 mg, yield 58%).

$Zn(OAc)_2$ (3.7 mg, 0.02 mmol) and PPh_3 (5.3 mg, 0.02 mmol) in DMSO (2.0 mL) were charged into a 25 mL pressure tube under argon. The mixture was stirred for 30 min at room temperature. Then Ph_2SiH_2 (36.8 mg, 0.2 mmol), *gem*-difluoroalkene **4a** (38.0 mg, 0.2 mmol) and TEMPO (93.8 mg, 0.6 mmol) were added sequentially to the reaction mixture. The reaction tube was then sealed and placed into an oil bath at 50 °C. After stirred for 24 h, the reaction mixture was quenched with H_2O (2.0 ml) and extracted with dichloromethane. The organic layer was separated dried over Na_2SO_4, concentrated, and purified by silica gel chromatography (PE) to give the monofluoride product **5a** (18.3 mg, yield 53%).

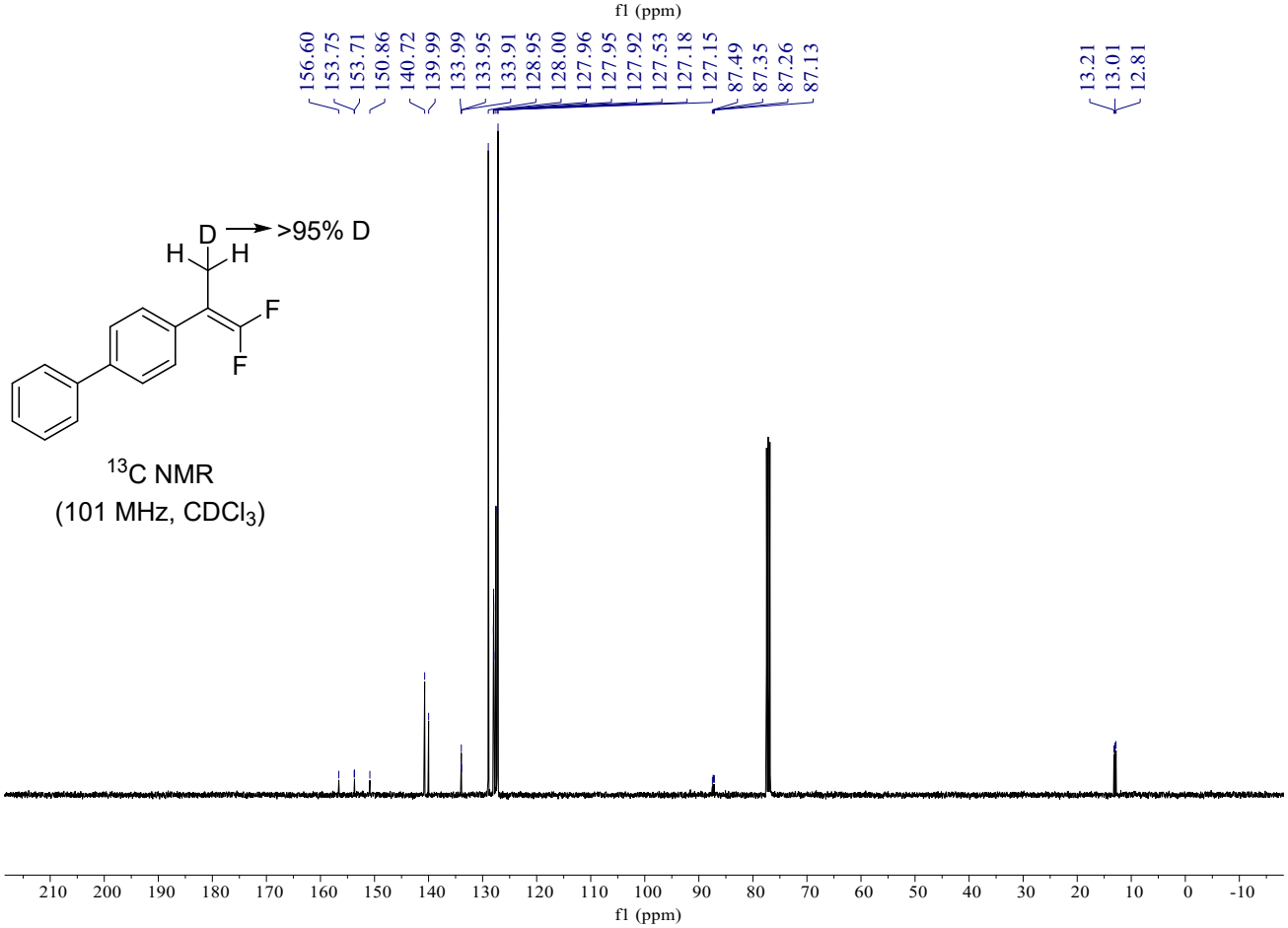
4.2 Deuterium labeling experiments.



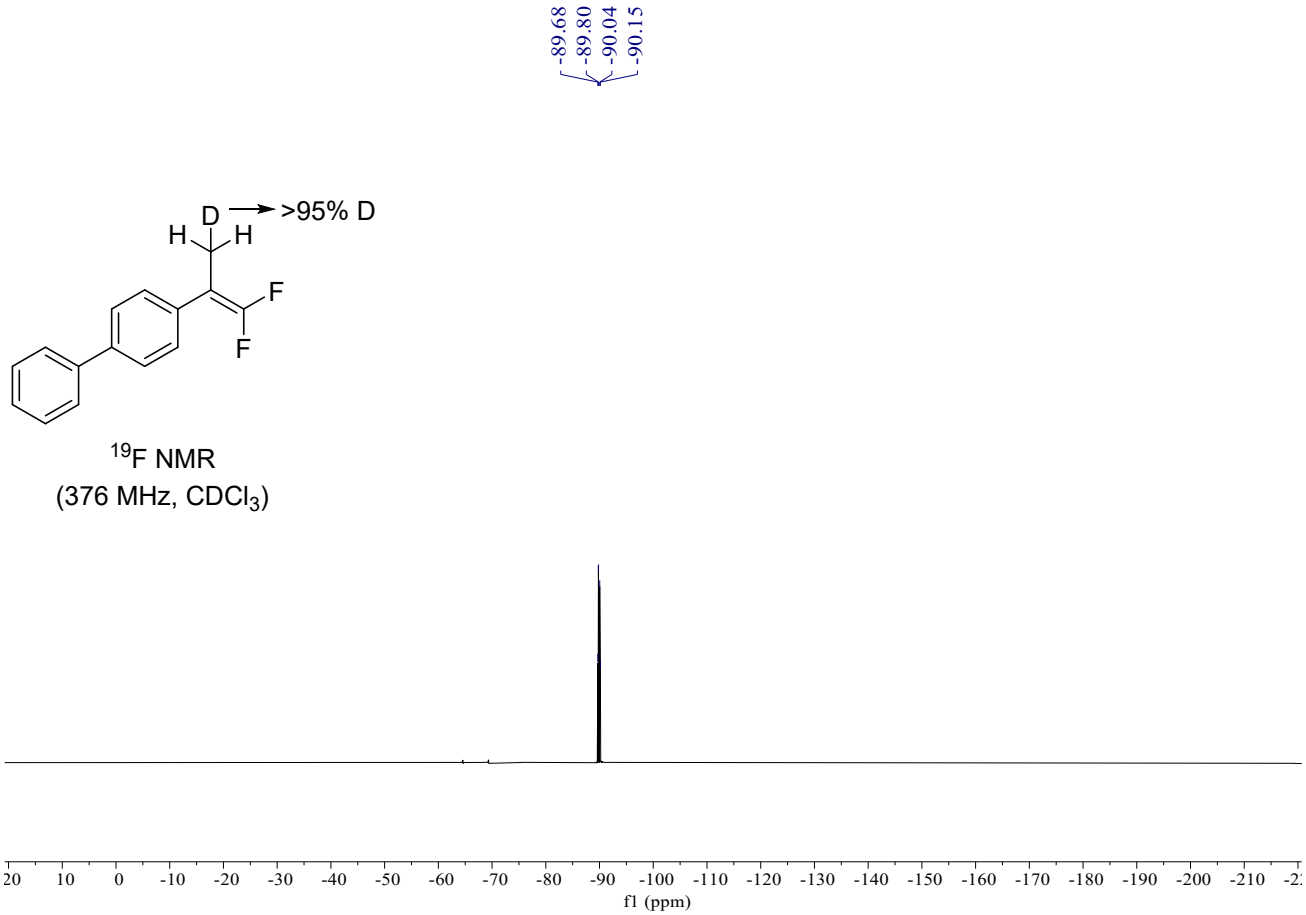
$Zn(OAc)_2$ (3.7 mg, 0.02 mmol) and Xantphos (11.6 mg, 0.02 mmol) in DMSO (2.0 mL) were charged into a 25 mL pressure tube under argon. The mixture was stirred for 30 min at room temperature. Then Ph_2SiD_2 (111.8 mg, 0.6 mmol) and trifluoromethyl alkene **1m** (0.2 mmol, 49.6 mg) were added sequentially to the reaction mixture. The reaction tube was then sealed and placed into an oil bath at 120 °C. After stirred for 24 h, the reaction mixture was quenched with H_2O (2.0 mL) and extracted with dichloromethane. The organic layer was separated dried over Na_2SO_4, concentrated, and purified by silica gel chromatography (PE) to give the monofluoride product (42.1mg, 91% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 – 7.61 (m, 4H), 7.49 – 7.45 (m, 4H), 7.39 – 7.37 (m, 1H), 2.04 – 2.01 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.73 (dd, J = 290.4, 286.6 Hz), 140.72, 139.99, 133.95 (t, J = 4.1 Hz), 128.95, 127.96 (dd, J = 4.9, 3.4 Hz), 127.53, 127.16 (d, J = 3.1 Hz), 87.31 (dd, J = 22.6, 13.9 Hz), 13.21 – 12.81 (m). ^{19}F NMR (376 MHz, $CDCl_3$) δ -89.68 – -90.15 (m).

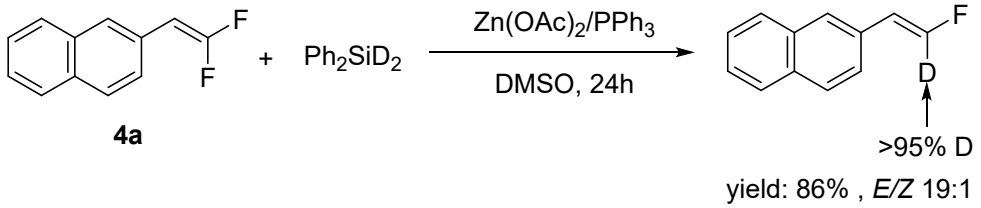


^{1}H NMR
(400 MHz, $CDCl_3$)



^{13}C NMR
(101 MHz, $CDCl_3$)

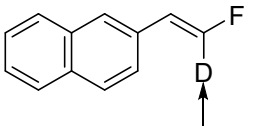




yield: 86% , *E/Z* 19:1

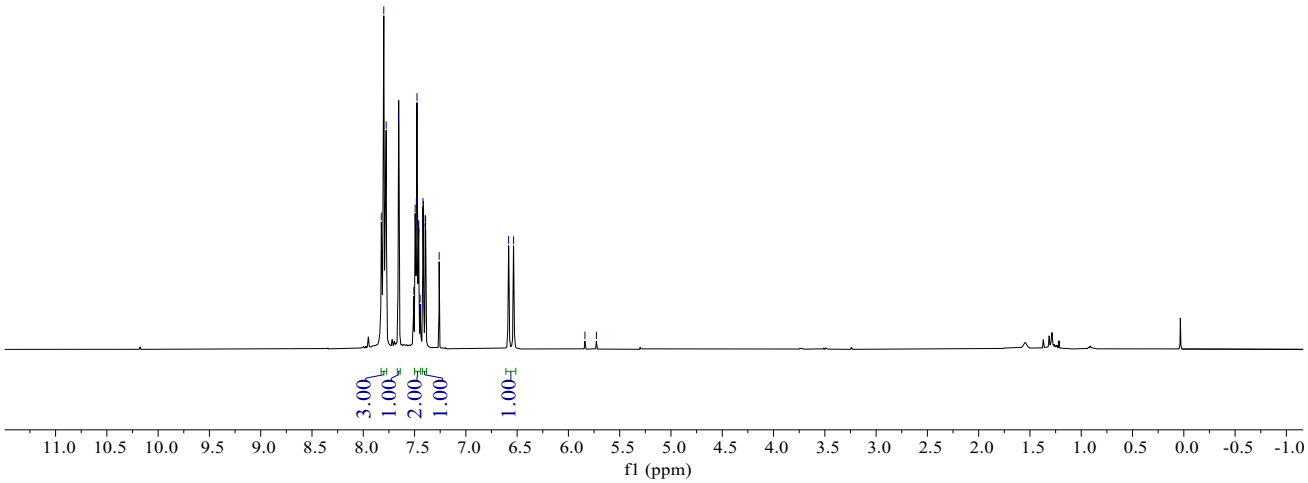
$Zn(OAc)_2$ (3.7 mg, 0.02 mmol) and PPh_3 (5.3 mg, 0.02 mmol) in DMSO (2.0 mL) were charged into a 25 mL pressure tube under argon. The mixture was stirred for 30 min at room temperature. Then Ph_2SiD_2 (37.2 mg, 0.2 mmol) and *gem*-difluoroalkene **4a** (38.0 mg, 0.2 mmol) were added sequentially to the reaction mixture. The reaction tube was then sealed and placed into an oil bath at 50 °C. After stirred for 24 h, the reaction mixture was quenched with H_2O (2.0 mL) and extracted with dichloromethane. The organic layer was separated dried over Na_2SO_4, concentrated, and purified by silica gel chromatography (PE) to give the monofluoride product (29.8mg, 86% yield, *E/Z* 19:1). ^1H NMR (400 MHz, $CDCl_3$) (mixture of isomers) δ (*E* isomer) 7.82 – 7.78 (m, 3H), 7.66 (s, 1H), 7.51 – 7.44 (m, 2H), 7.40 (dd, *J* = 8.4, 1.6 Hz, 1H), 6.56 (d, *J* = 19.6 Hz, 1H); (*Z* isomer) 5.78 (d, *J* = 44.7 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) (mixture of isomers) δ 133.7, 132.9, 130.3 (d,

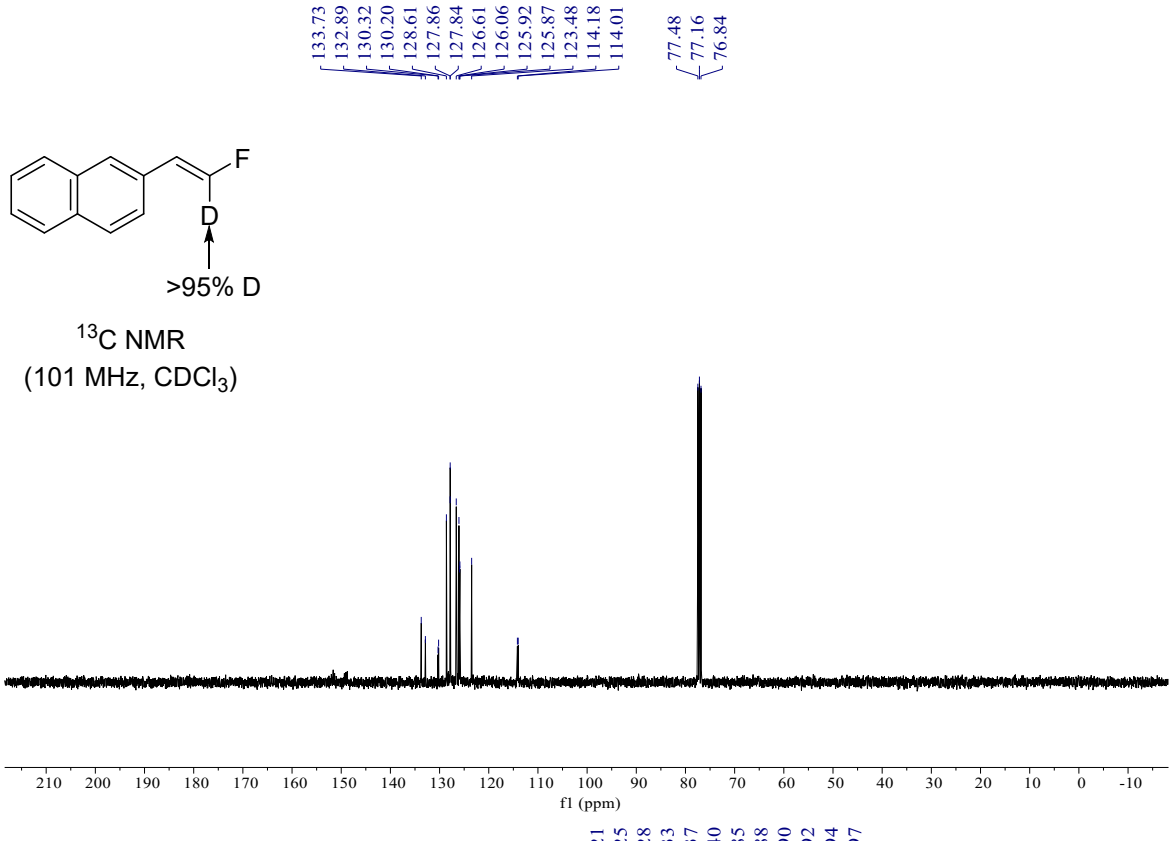
J = 11.7 Hz), 128.6, 127.9 (d, *J* = 1.9 Hz), 126.6, 126.1, 125.9 (d, *J* = 5.0 Hz), 123.5, 114.1 (d, *J* = 16.5 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) (mixture of isomers) δ (*Z* isomer) -122.31 (dt, *J* = 44.5, 12.6 Hz); (*E* isomer) -129.85 – -129.97 (m).

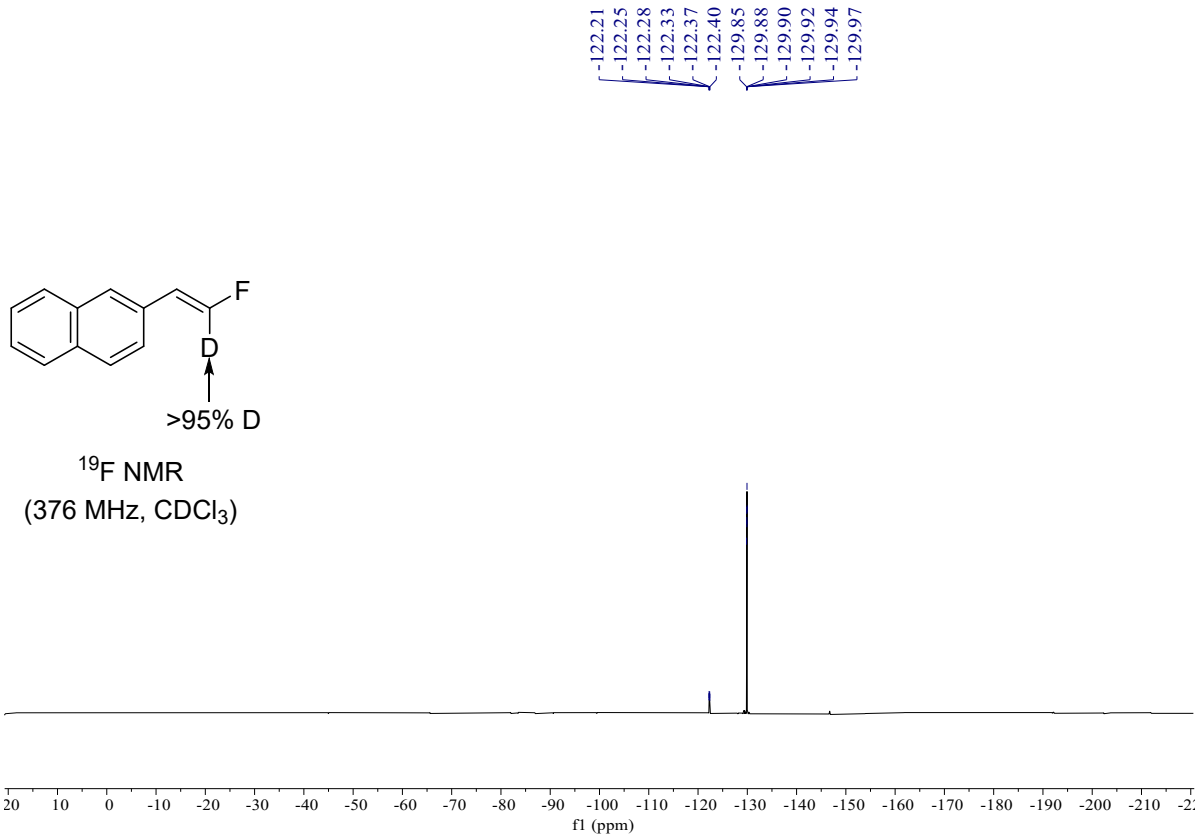


>95% D

^{1}H NMR
(400 MHz, $CDCl_3$)




133.73
132.89
130.32
130.20
128.61
127.86
127.84
126.61
126.06
125.92
125.87
123.48
114.18
114.01
77.48
77.16
76.84
F
D
>95% D
^{13}C NMR
(101 MHz, $CDCl_3$)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-122.21
-122.25
-122.28
-122.33
-122.37
-122.40
-129.85
-129.88
-129.90
-129.92
-129.94
-129.97
F
D
>95% D
^{19}F NMR
(376 MHz, $CDCl_3$)
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

5. Supplementary References

(1) Liu, H. D.; Ge, L.; Wang, D. X.; Chen, N.; Feng, C. Photoredox-Coupled F-Nucleophilic Addition: Allylation of gem-Difluoroalkenes. *Angew. Chem. Int. Ed.* **2019**, *58*, *3918-3922.*

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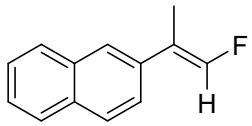
(11) Wu, F.; Li, X.; Chang, J. B.; Bai, D. C. Palladium-catalyzed multi components oxy-aminofluorination and aminofluorination of gem-difluoroalkenes. *Chin. Chem. Lett.* DOI:

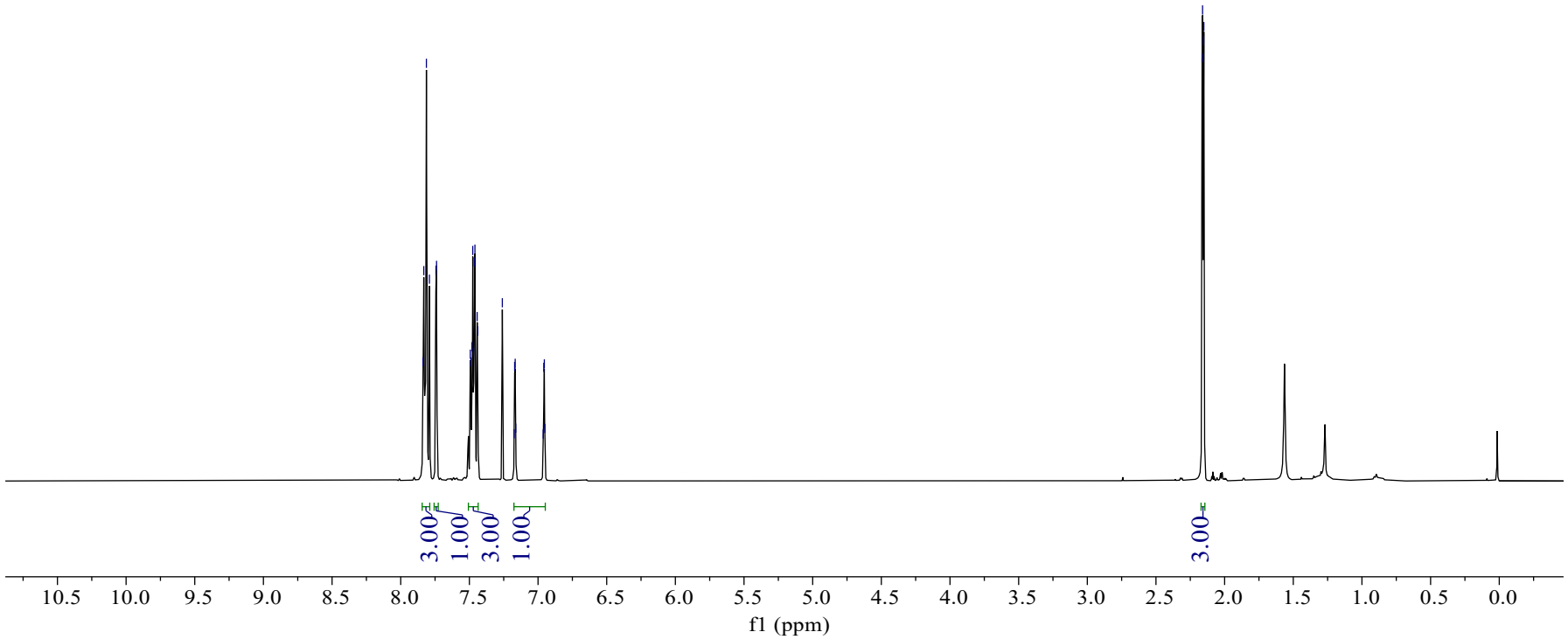
10.1016/j.cclet.2023.109155.

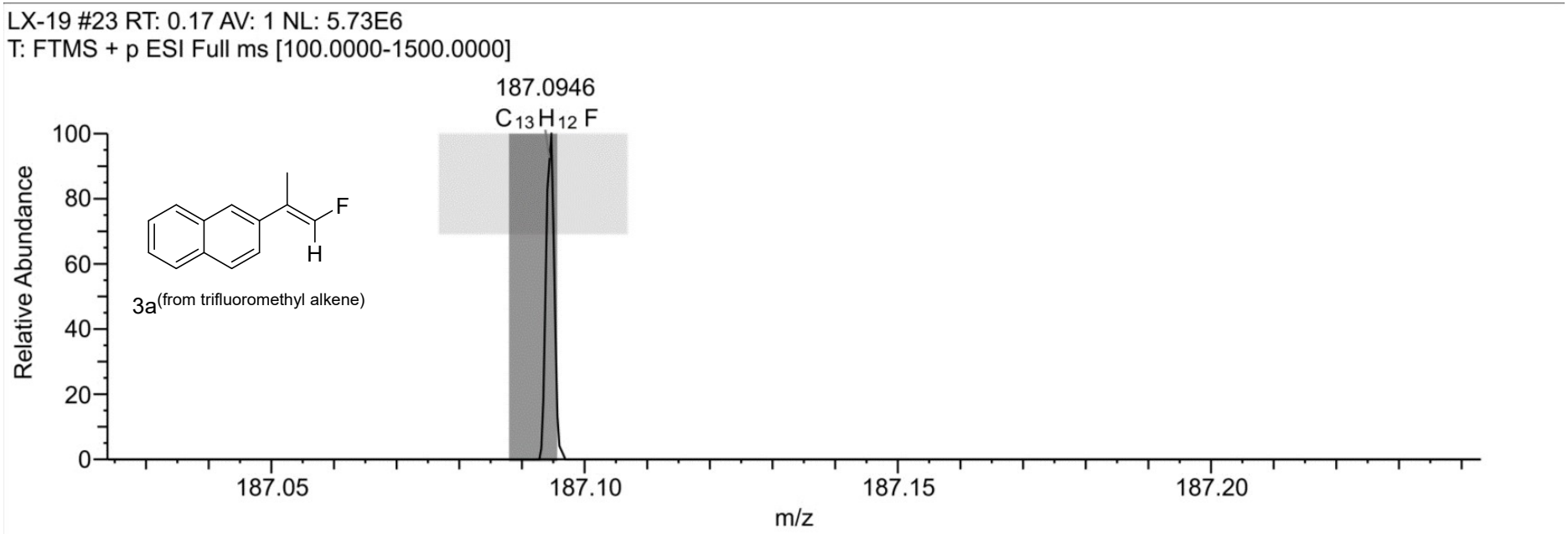
6. NMR Spectra and HRMS Report



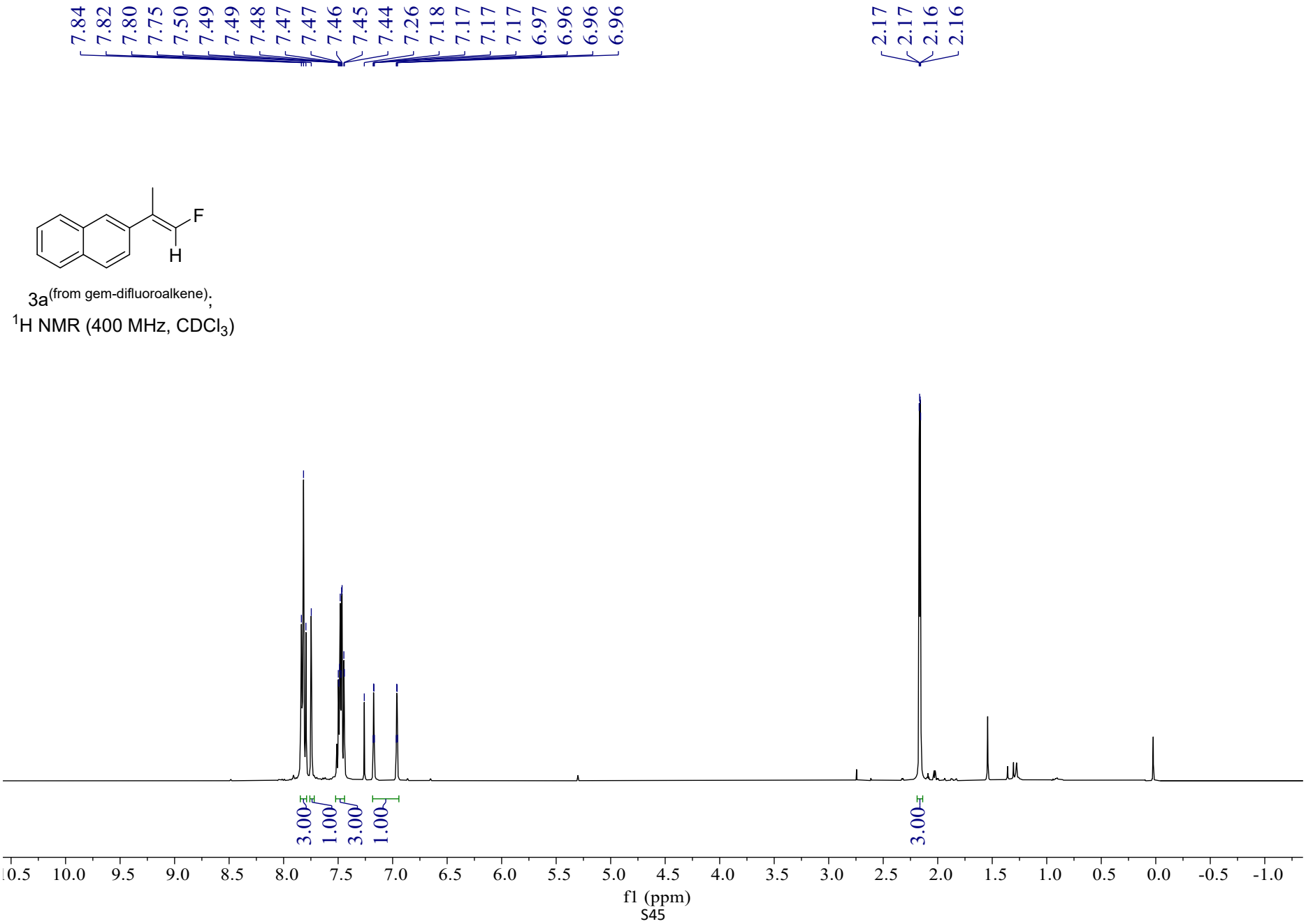
3a(from trifluoromethyl alkene);

^{1}H NMR (400 MHz, $CDCl_3$)

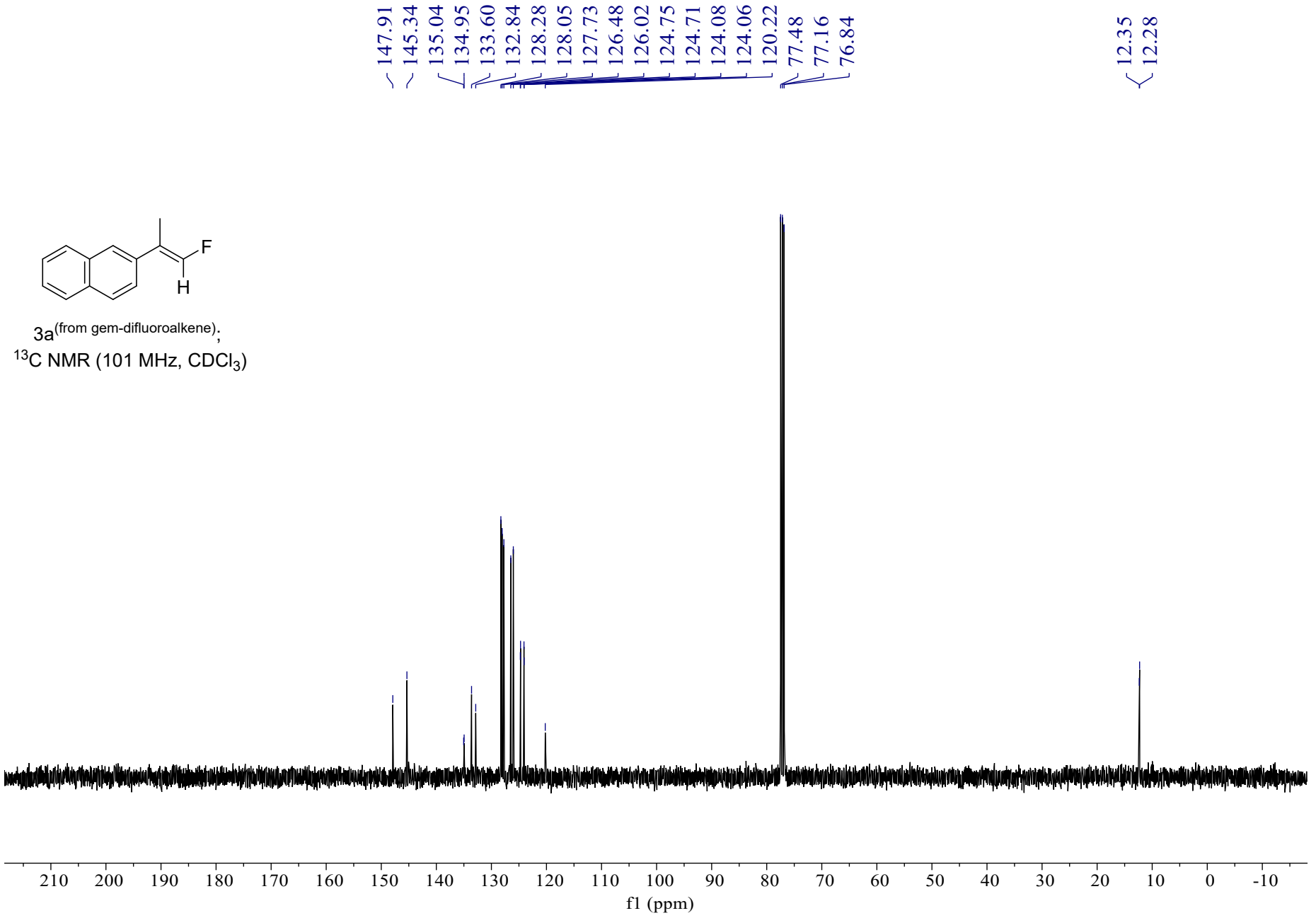




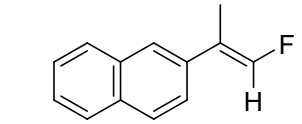
Peak M...	Display...	S Fit	RDB	Delta [p...	Theo....	Rank	Combin...	# Matc...	# Misse...	MS Cov...	Pattern...	MSMS...
187.0946	$C_{13}H_{12}F$	19.5935525710216	7.50	15.31	187.09176	1	95.77	1	1	100	87.68	(Collection)



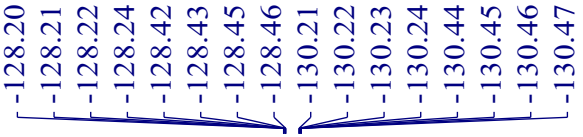
3a(from gem-difluoroalkene);
^{1}H NMR (400 MHz, $CDCl_3$)

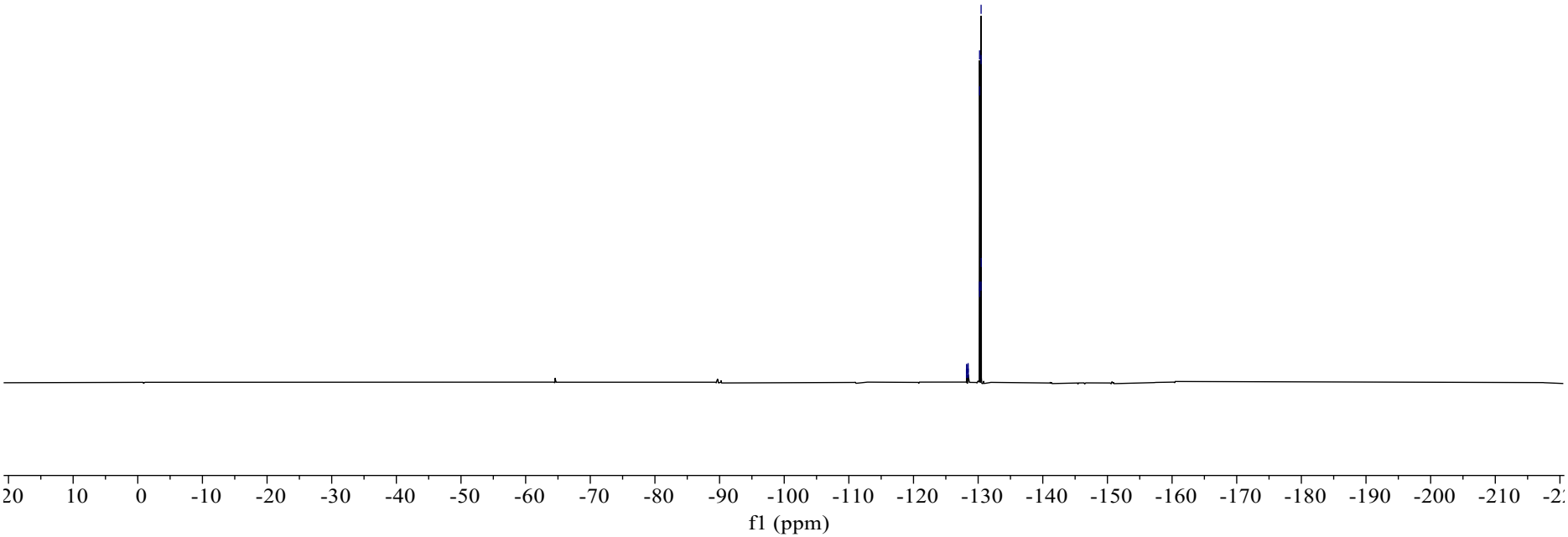


3a(from gem-difluoroalkene);
^{13}C NMR (101 MHz, $CDCl_3$)



3a(from gem-difluoroalkene);
^{19}F NMR (376 MHz, $CDCl_3$)





Mass Spectrum SmartFormula Report

Analysis Info

Acquisition D 2023-01-09 11:26:06

Analysis Name D:\LXMS\0106_RC8_01_20525.d

Method LC_NO UV_P50-1500_6MIN.m

Operator Demo User

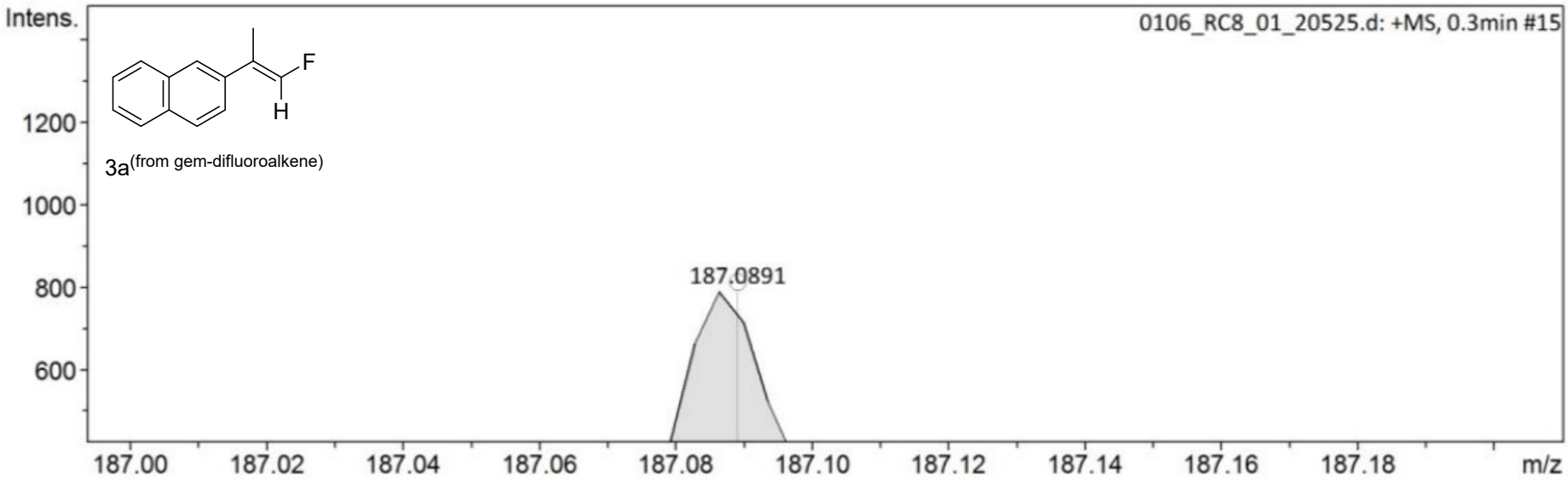
Sample Name 0106

Instrumen compact 8255754.2017 6

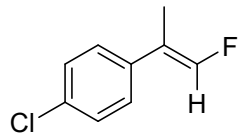
Comment

Acquisition Paramet

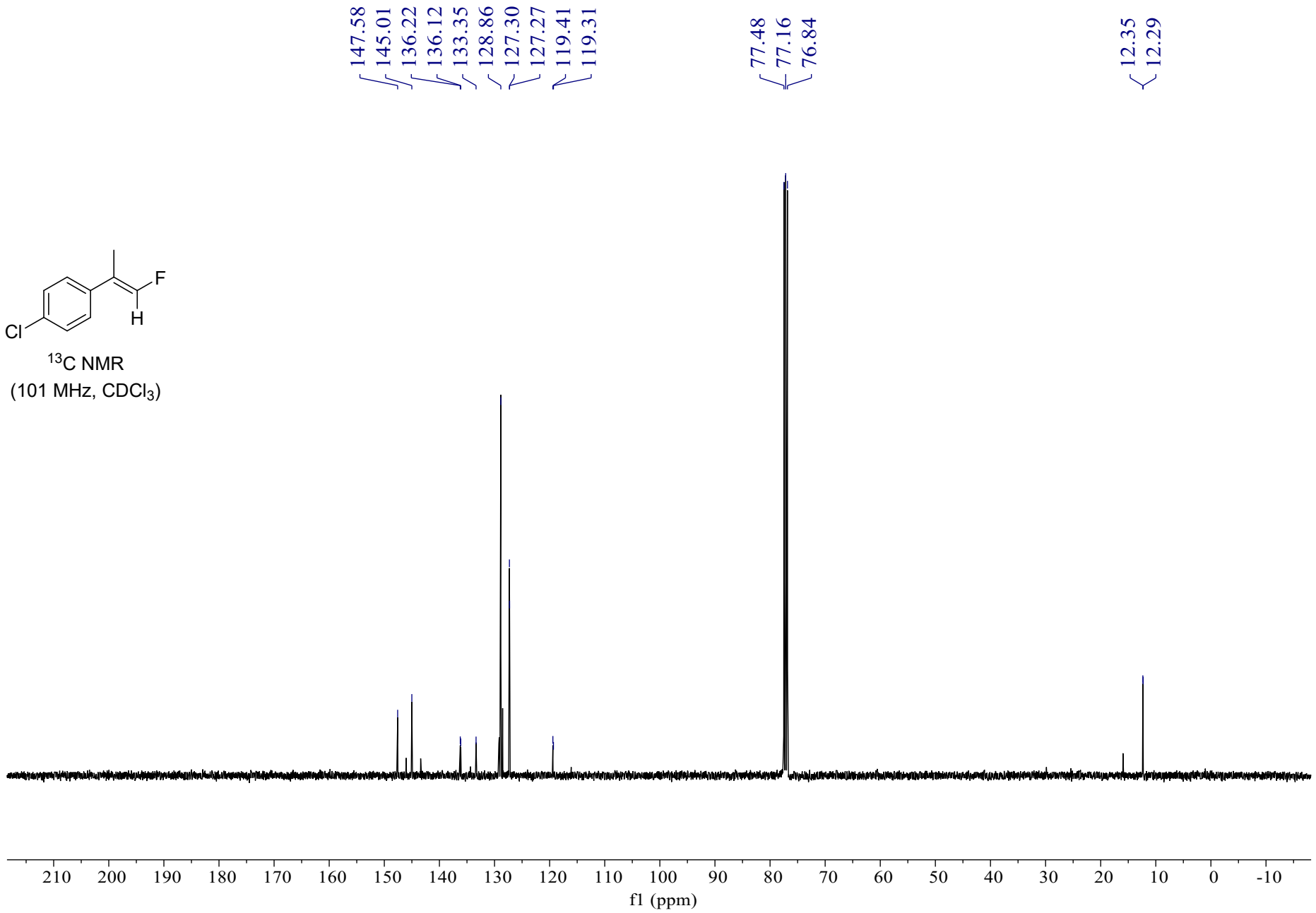
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min



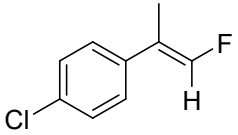
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
187.0891	1	C13H12F	187.0918	14.3	n.a.	1	100.00	7.5	even	ok



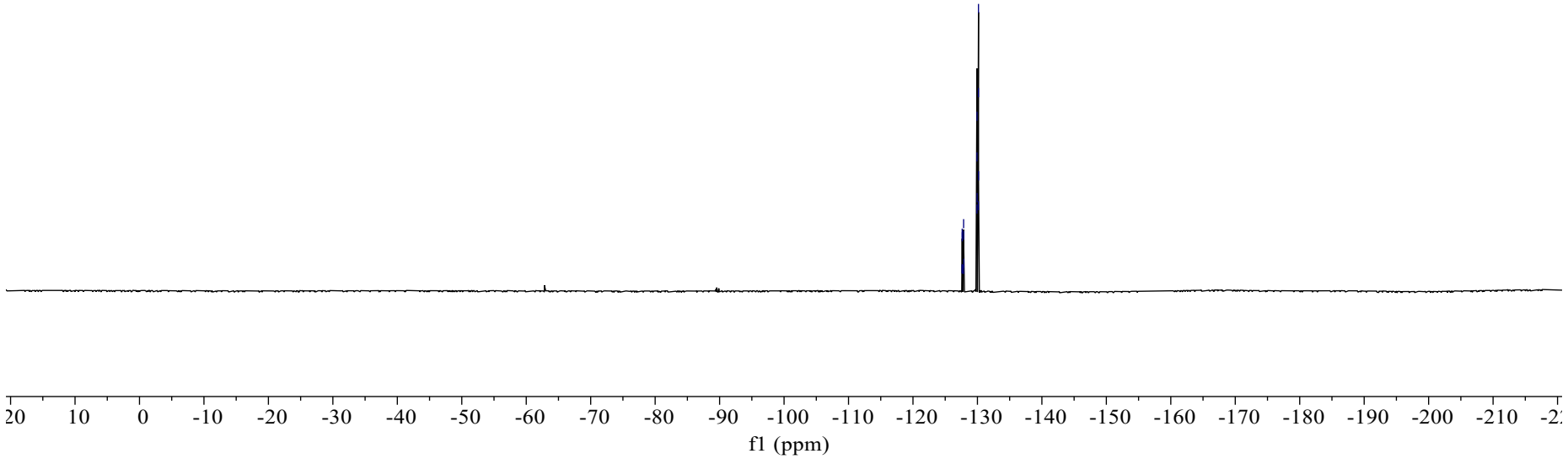
^{1}H NMR
(400 MHz, $CDCl_3$)


147.58
145.01
136.22
136.12
133.35
128.86
127.30
127.27
119.41
119.31
77.48
77.16
76.84
12.35
12.29
F
H
Cl
13C NMR
(101 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

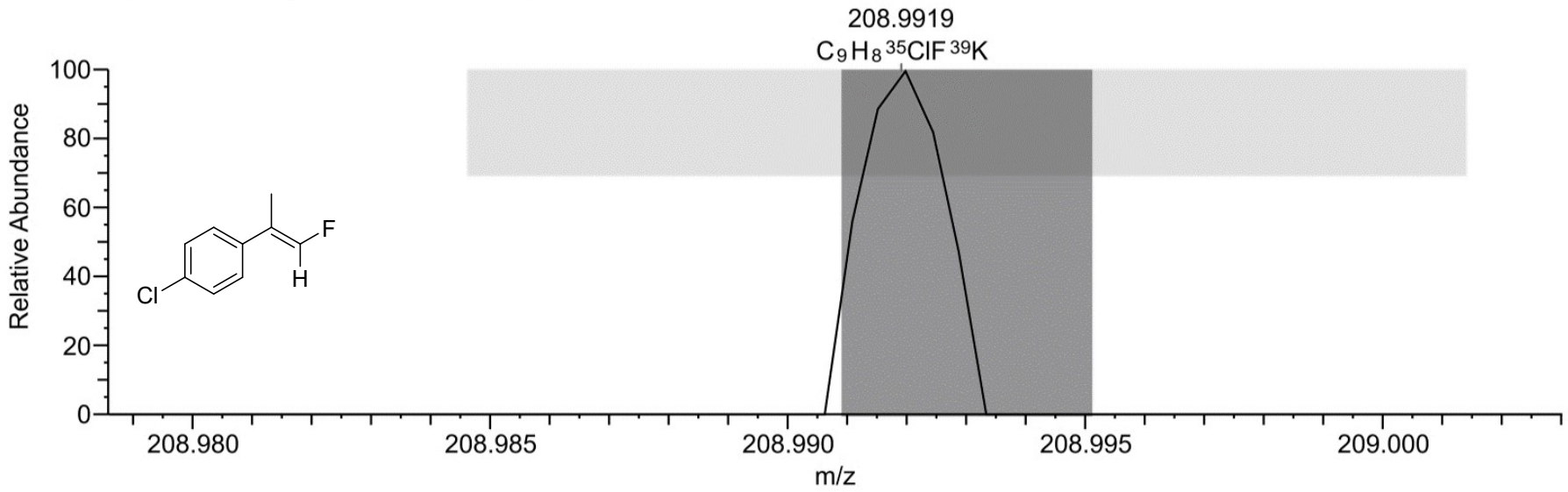
-127.62
-127.63
-127.65
-127.66
-127.84
-127.86
-127.87
-127.88
-129.92
-129.93
-129.94
-129.95
-130.14
-130.15
-130.16
-130.17



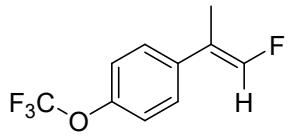
^{19}F NMR
(376 MHz, $CDCl_3$)



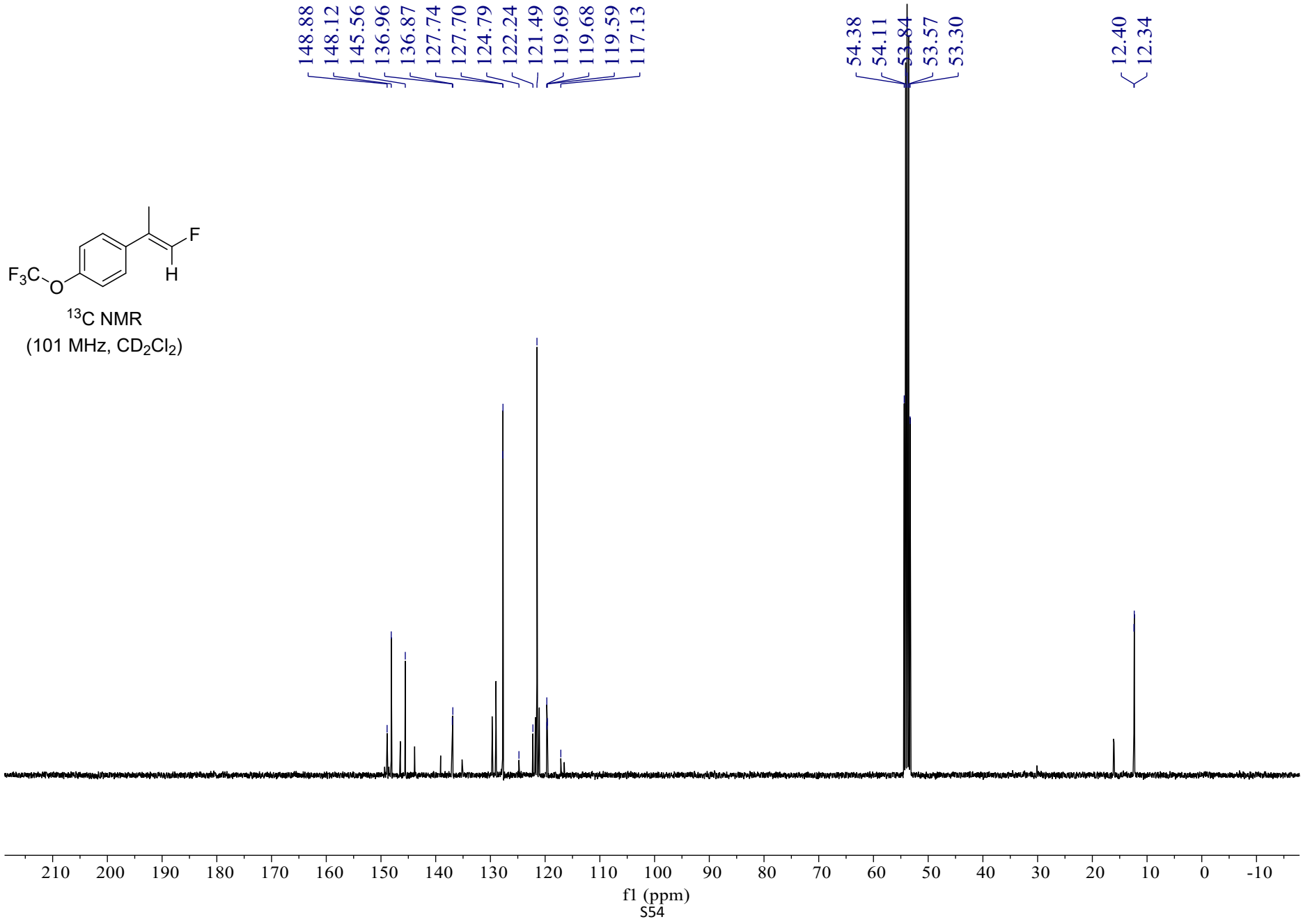
LX-21 #49 RT: 0.37 AV: 1 NL: 1.95E5
T: FTMS + p ESI Full ms [100.0000-1500.0000]

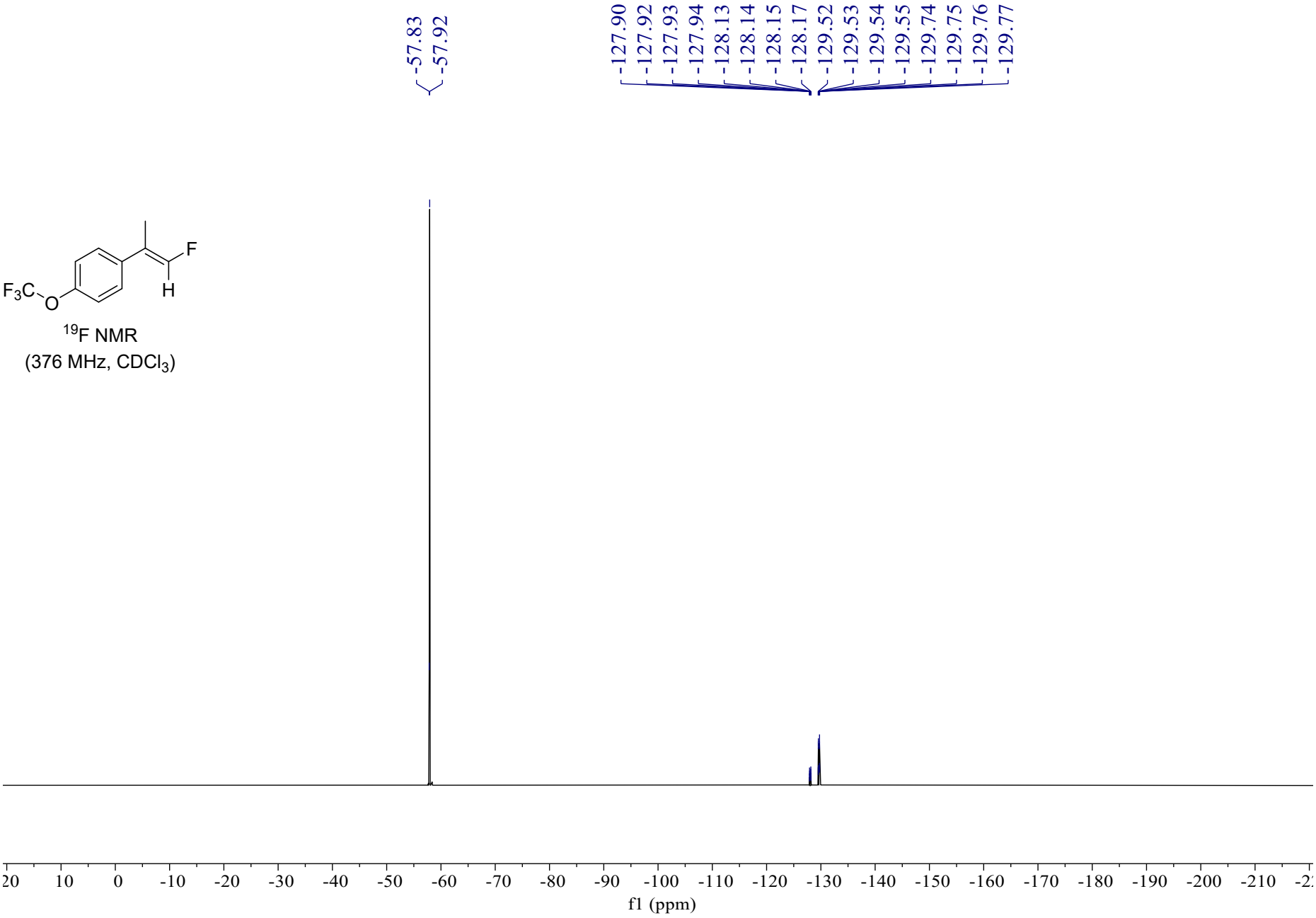


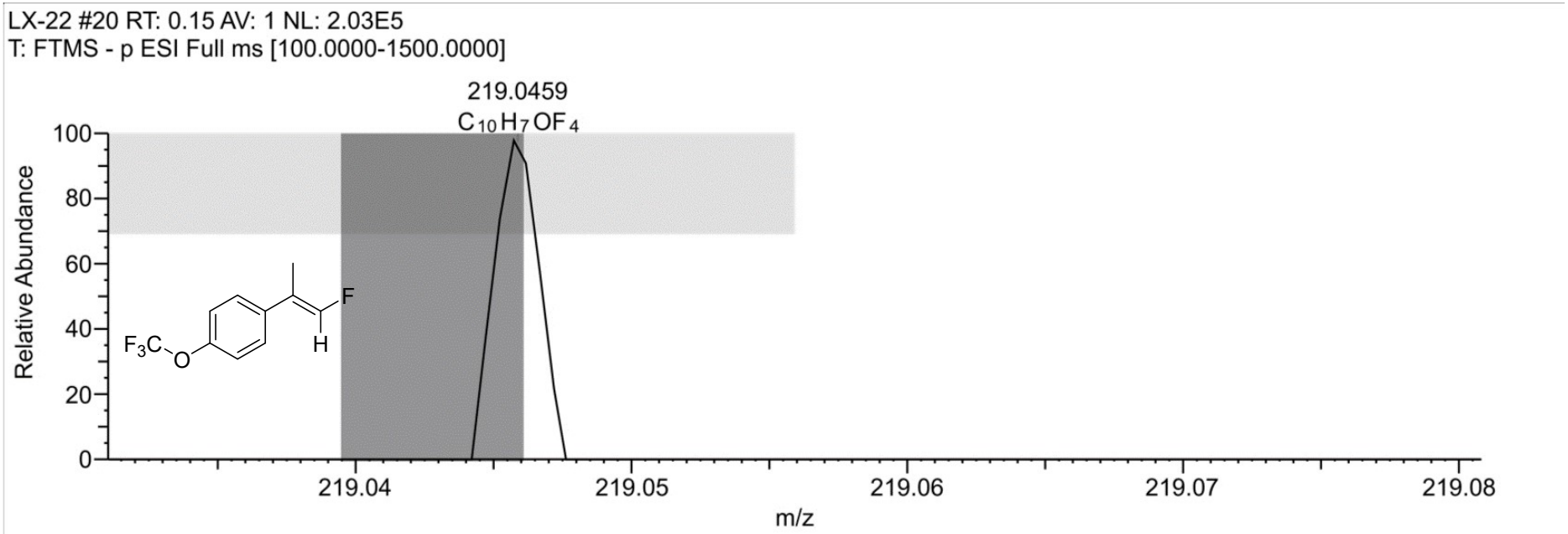
Peak M...	Display...	S Fit	RDB	Delta [p...	Theo....	Rank	Combin...	# Matc...	# Misse...	MS Cov...	Pattern...	MSMS...
208.9919	$C_9H_8{}^{35}ClF^{39}K$	63.2380350586169	4.50	-5.20	208.99301	1	98.07	1	0	100	100	(Collection)



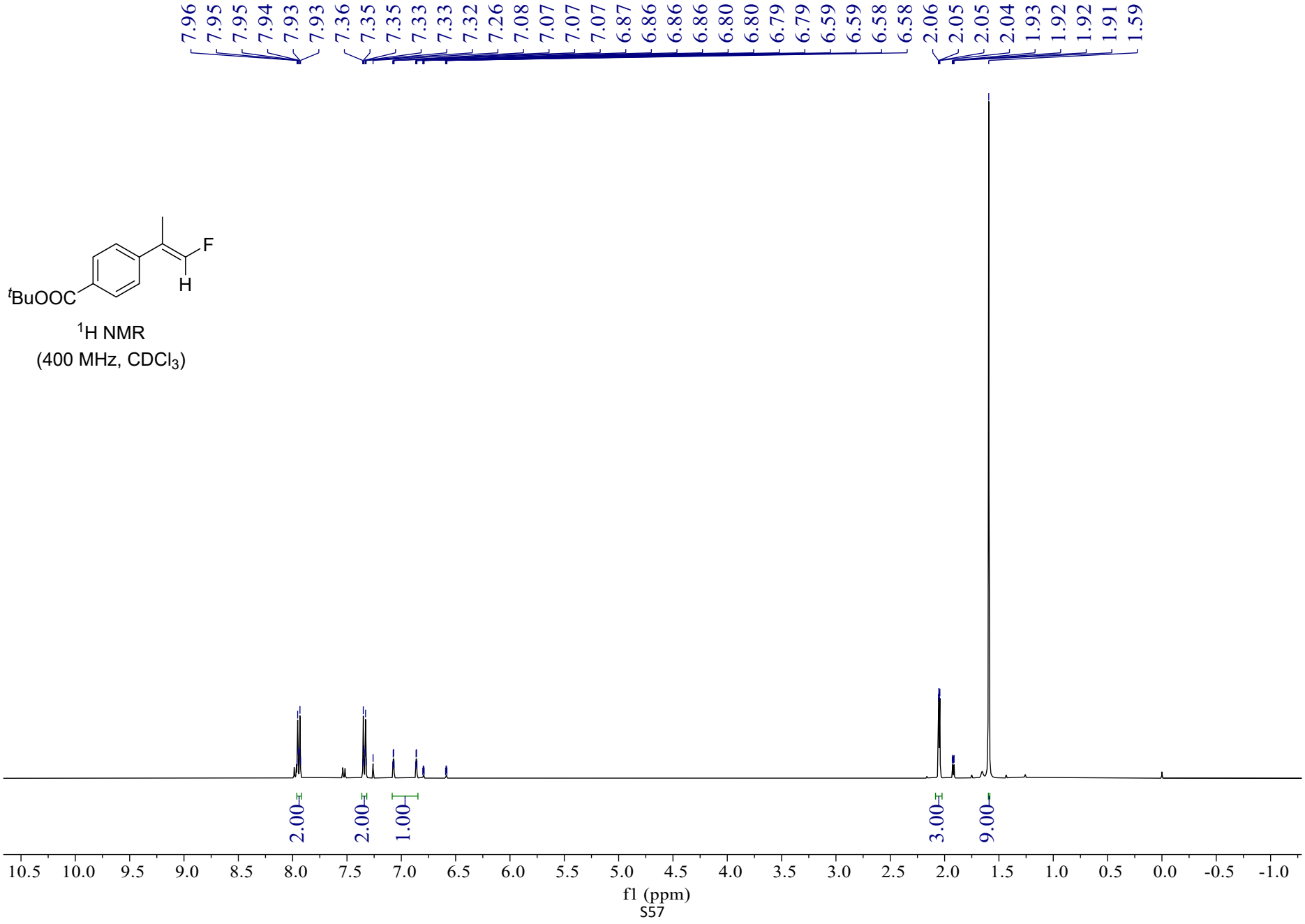
^{1}H NMR
(400 MHz, $CDCl_3$)

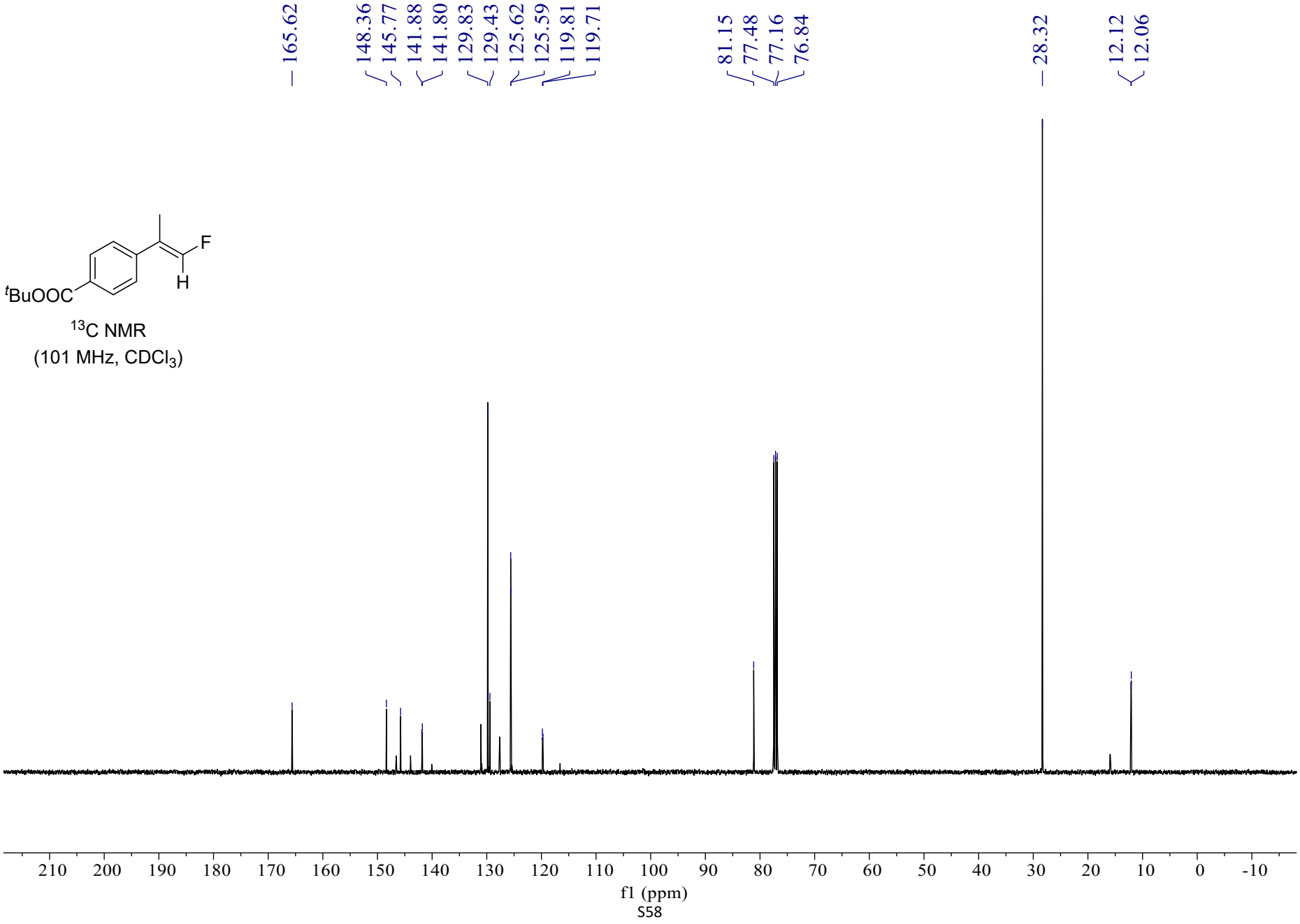

148.88
148.12
145.56
136.96
136.87
127.74
127.70
124.79
122.24
121.49
119.69
119.68
119.59
117.13
54.38
54.11
53.84
53.57
53.30
12.40
12.34
F
F3C
O
H
13C NMR
(101 MHz, CD2Cl2)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-57.83
-57.92
-127.90
-127.92
-127.93
-127.94
-128.13
-128.14
-128.15
-128.17
-129.52
-129.53
-129.54
-129.55
-129.74
-129.75
-129.76
-129.77
F
F3C
O
H
19F NMR
(376 MHz, CDCl3)
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)



Peak M...	Display...	S Fit	RDB	Delta [p...	Theo....	Rank	Combin...	# Matc...	# Misse...	MS Cov...	Pattern...	MSMS...
219.0459	$C_{10}H_7OF_4$	32.661091617313 4	5.50	14.28	219.04275	1	96.46	1	0	100	100	(Collection)


7.96
7.95
7.95
7.94
7.93
7.93
7.36
7.35
7.35
7.33
7.33
7.32
7.26
7.08
7.07
7.07
7.07
6.87
6.86
6.86
6.86
6.80
6.80
6.79
6.79
6.59
6.59
6.58
6.58
2.06
2.05
2.05
2.04
1.93
1.92
1.92
1.91
1.59
F
H
tBuOOC
1H NMR
(400 MHz, CDCl3)
2.00
2.00
1.00
3.00
9.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


165.62
148.36
145.77
141.88
141.80
129.83
129.43
125.62
125.59
119.81
119.71
81.15
77.48
77.16
76.84
28.32
12.12
12.06
F
H
tBuOOC
13C NMR
(101 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

-126.17
-126.18
-126.19
-126.21
-126.39
-126.40
-126.42
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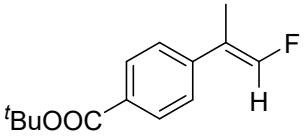
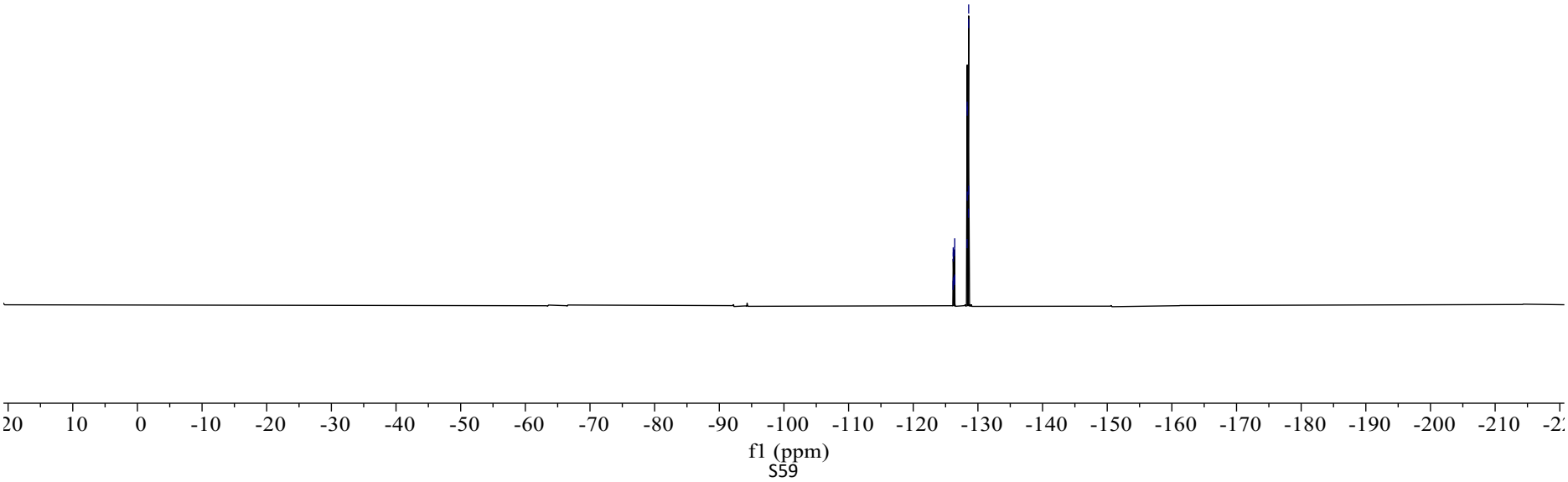
-128.35
-128.55
-128.56
-128.57
-128.58



^{19}F NMR
(376 MHz, $CDCl_3$)



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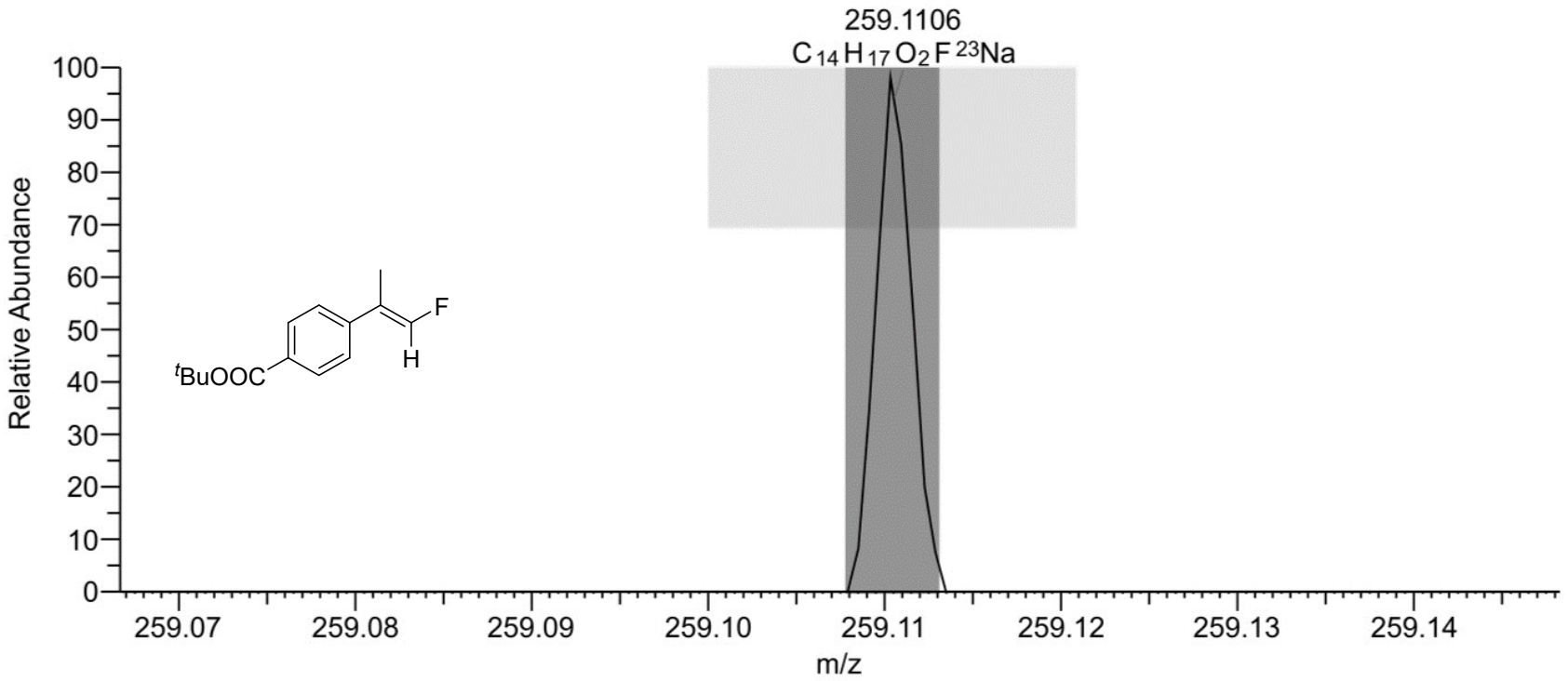
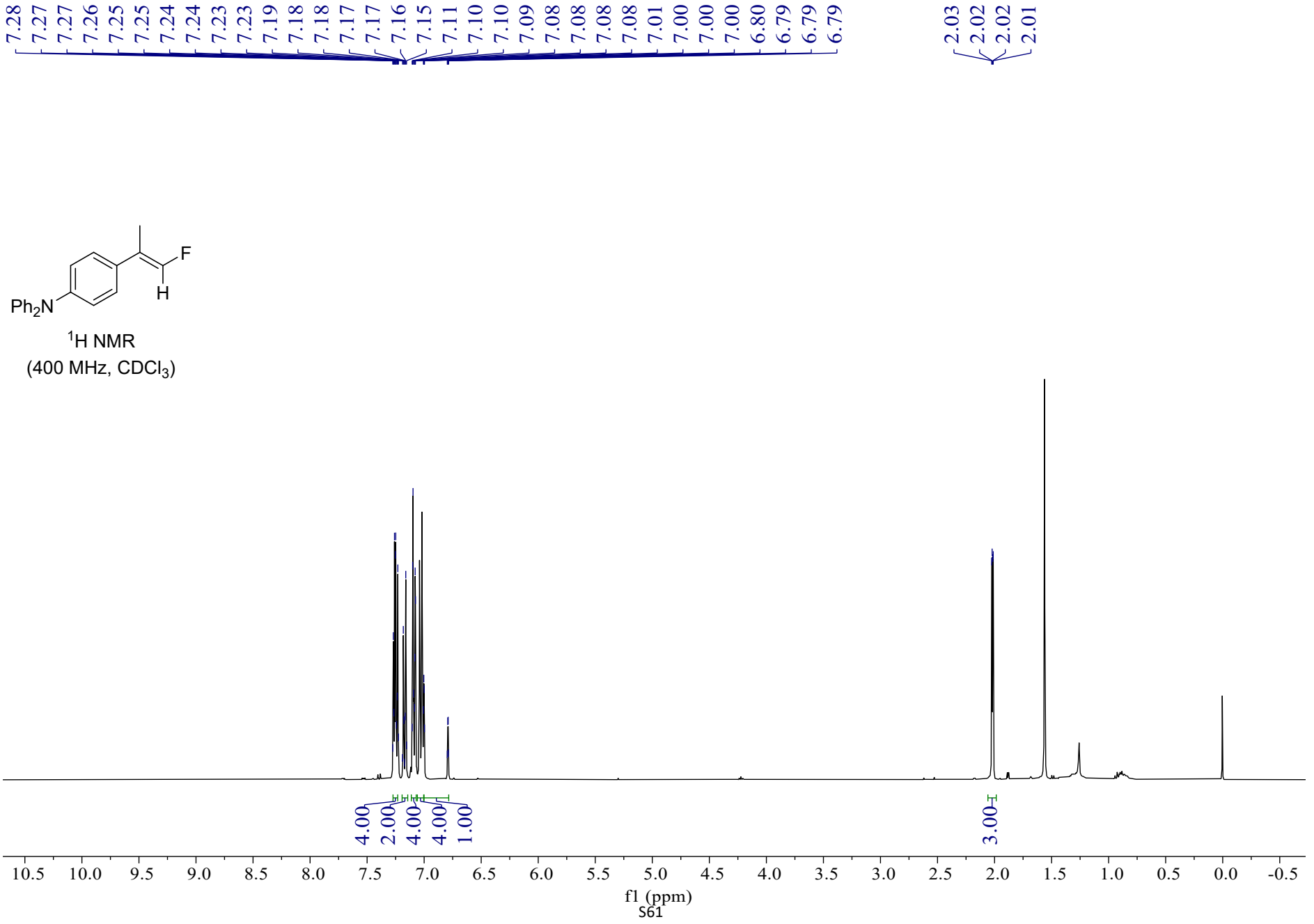
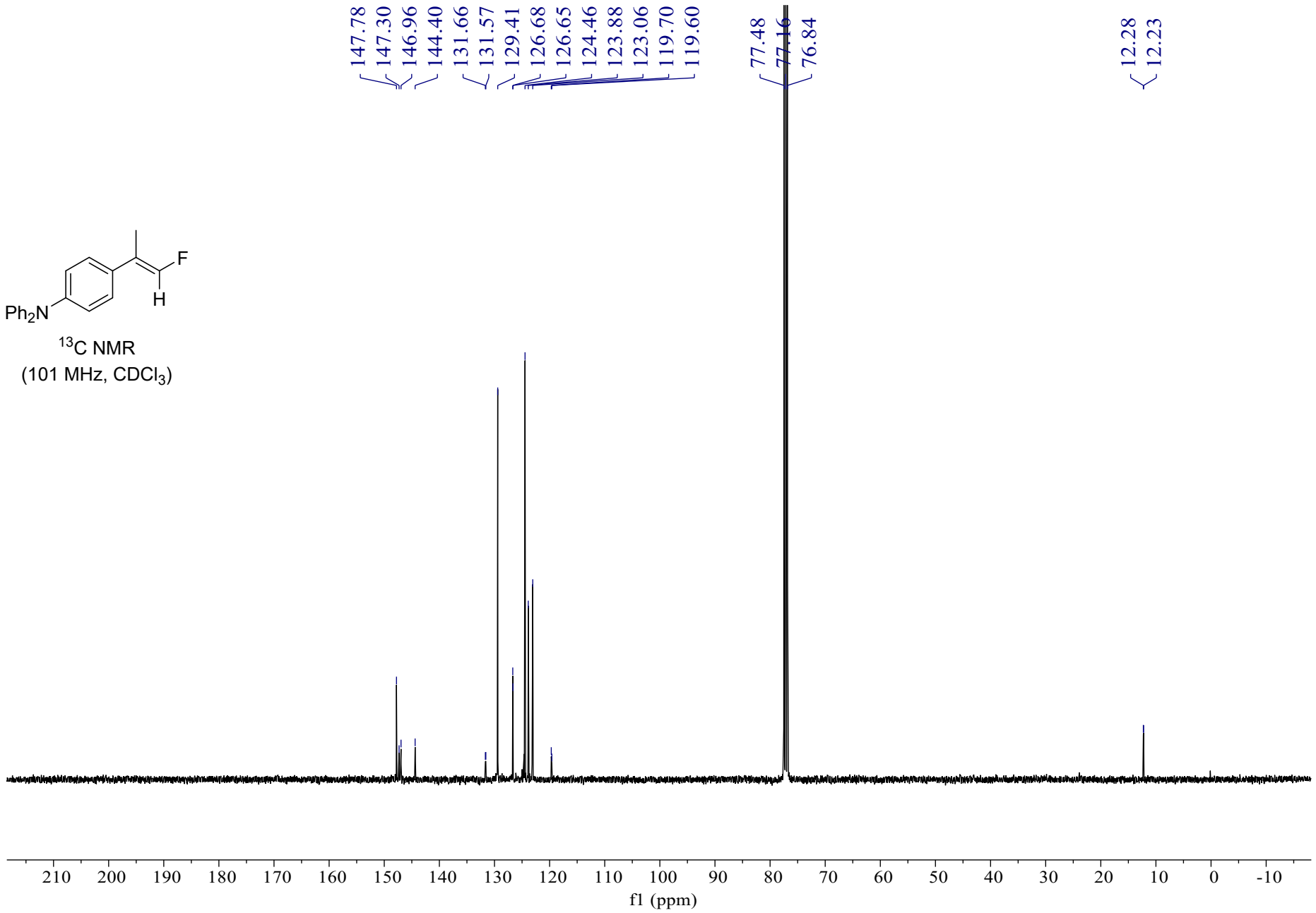
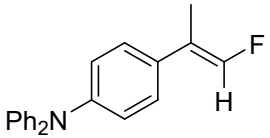


Peak M...	Display...	S Fit	RDB	Delta [p...	Theo....	Rank	Combin...	# Matc...	# Misse...	MS Cov...	Pattern...	MSMS...
259.1106	$C_{14}H_{17}O_2F^{23}Na$	29.269861775712	5.50	0.33	259.11048	1	65.28	1	1	67.28	86.85	(Collection)

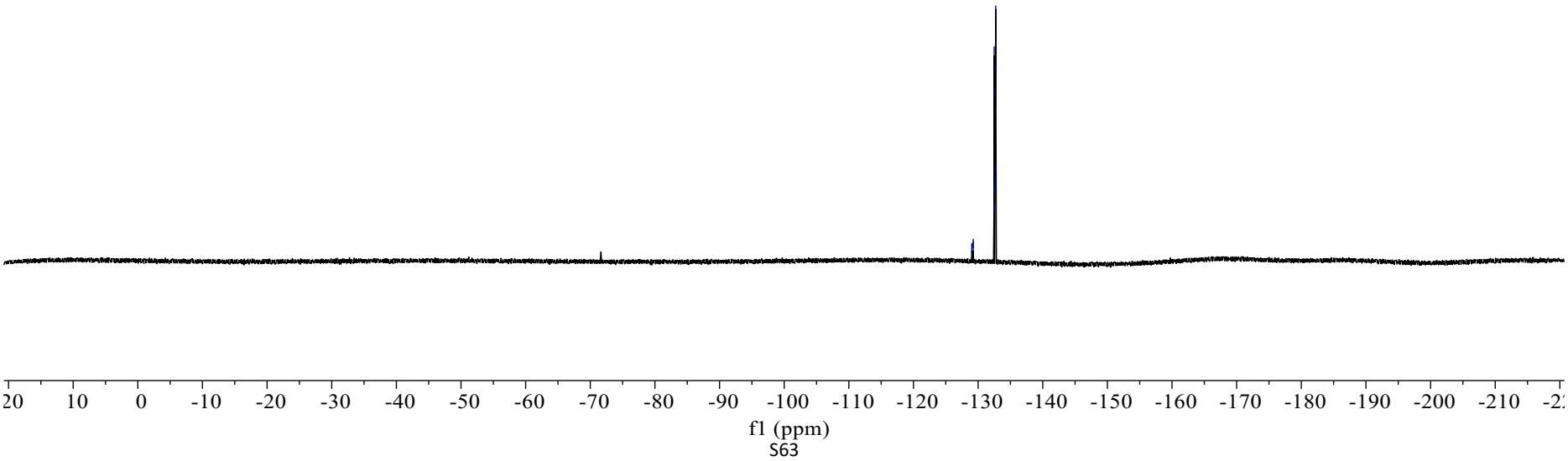

7.28
7.27
7.27
7.26
7.25
7.25
7.24
7.24
7.23
7.23
7.19
7.18
7.18
7.17
7.17
7.16
7.15
7.11
7.10
7.10
7.09
7.08
7.08
7.08
7.08
7.01
7.00
7.00
7.00
6.80
6.79
6.79
6.79
2.03
2.02
2.02
2.01
F
H
Ph2N
1H NMR
(400 MHz, CDCl3)
4.00
2.00
4.00
4.00
1.00
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


147.78
147.30
146.96
144.40
131.66
131.57
129.41
126.68
126.65
124.46
123.88
123.06
119.70
119.60
77.48
77.16
76.84
12.28
12.23
F
H
Ph2N
13C NMR
(101 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

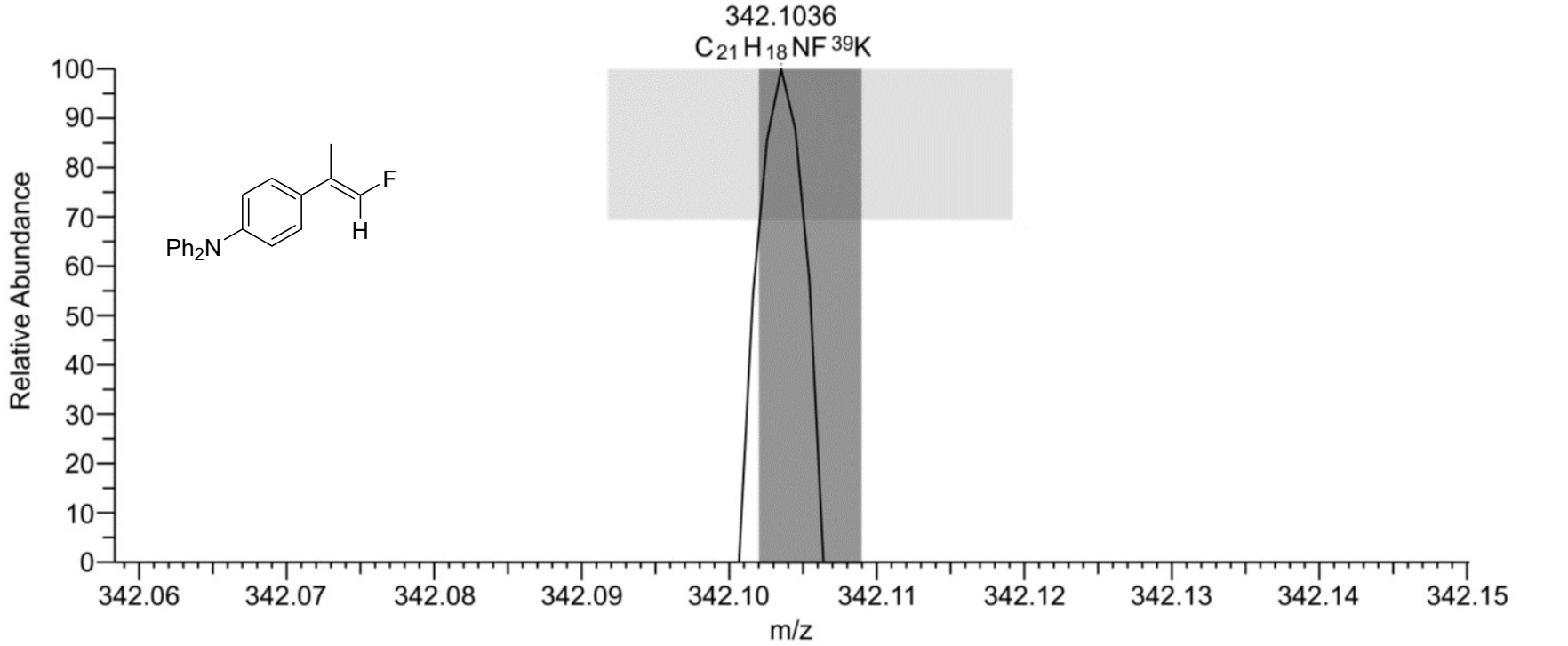
-129.02
-129.24
-129.25
-132.47
-132.48
-132.50
-132.51
-132.70
-132.71
-132.72
-132.73



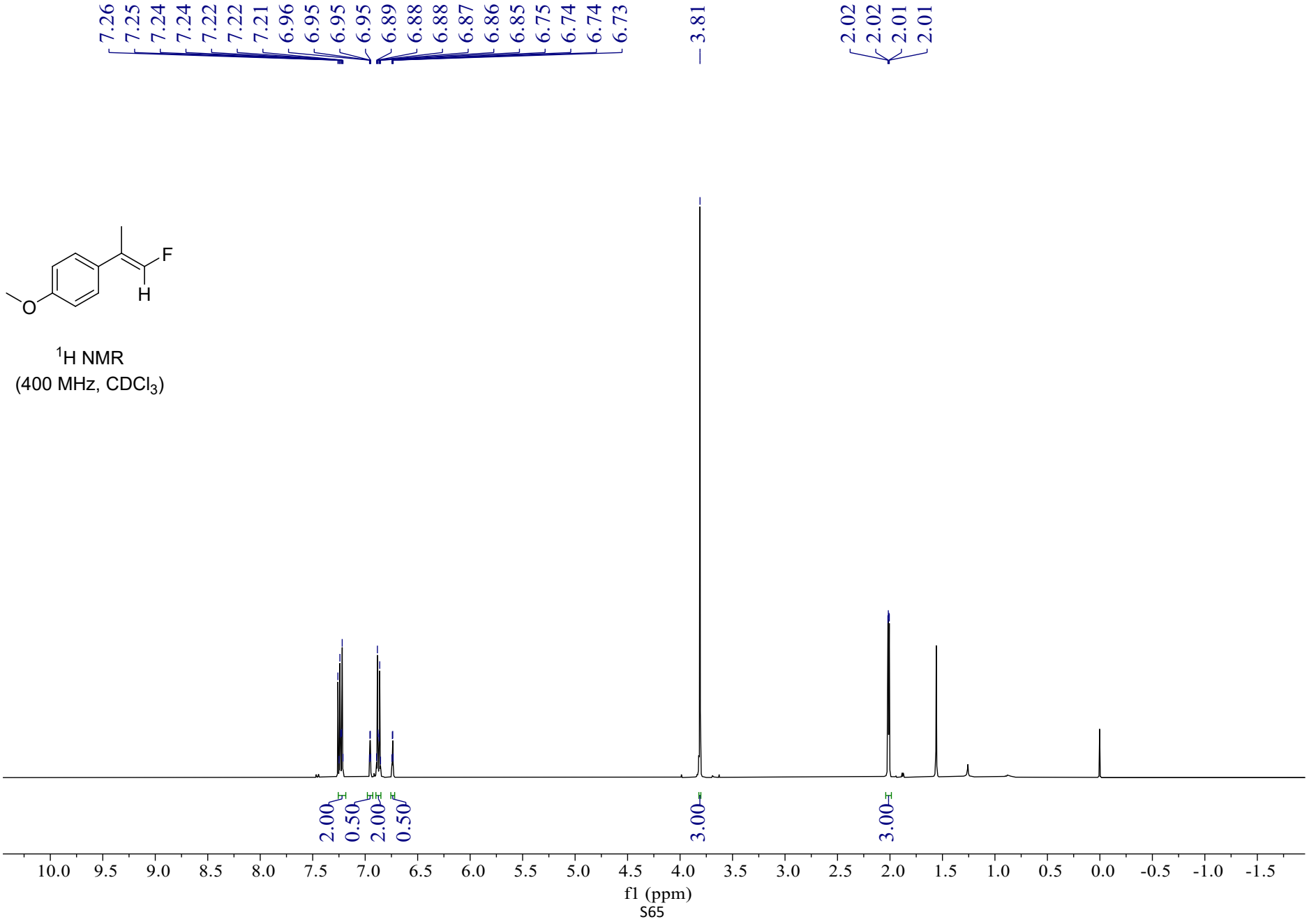
^{19}F NMR
(376 MHz, $CDCl_3$)

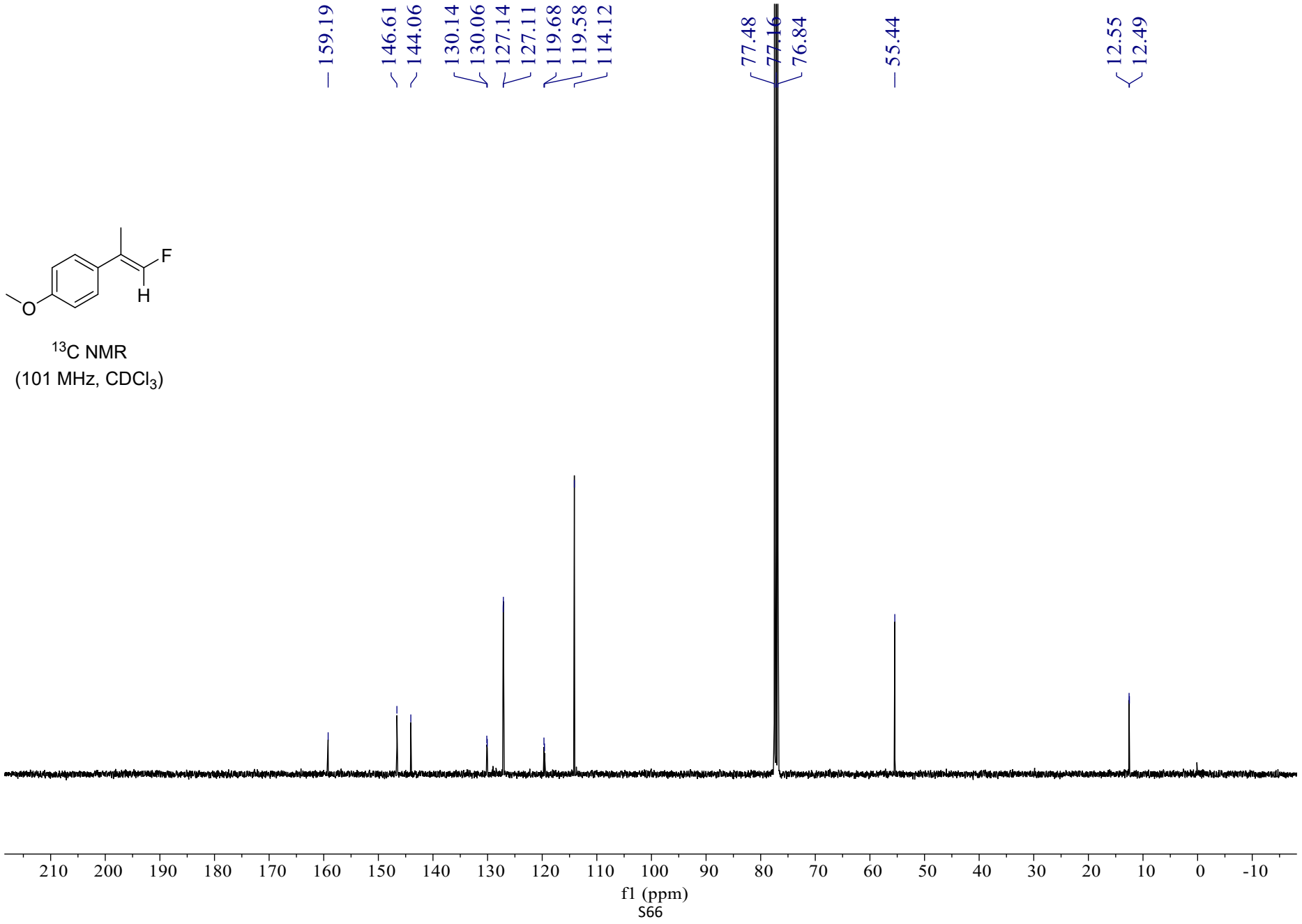


LX-6 #101 RT: 0.76 AV: 1 NL: 2.35E4
T: FTMS + p ESI Full ms [100.0000-1500.0000]

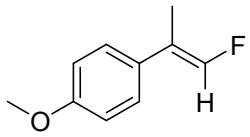


Peak M...	Display...	S Fit	RDB	Delta [p...	Theo....	Rank	Combin...	# Matc...	# Misse...	MS Cov...	Pattern...	MSMS...
342.1036	$C_{21}H_{18}NF^{39}K$	61.1611 703506 556	12.50	-5.49	342.10549	1	97.96	1	0	100	100	(Collection)


7.26
7.25
7.24
7.24
7.22
7.22
7.21
6.96
6.95
6.95
6.95
6.89
6.88
6.88
6.87
6.86
6.85
6.75
6.74
6.74
6.73
3.81
2.02
2.02
2.01
2.01
F
H
O
1H NMR
(400 MHz, CDCl3)
2.00
0.50
2.00
0.50
3.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

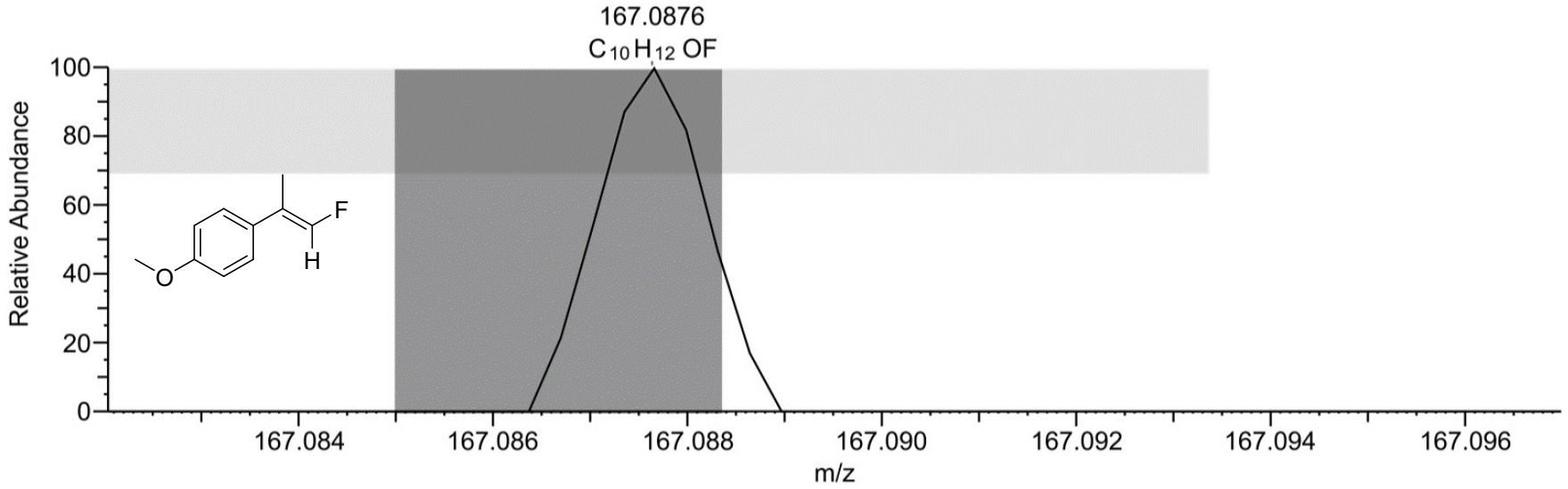


^{13}C NMR
(101 MHz, $CDCl_3$)

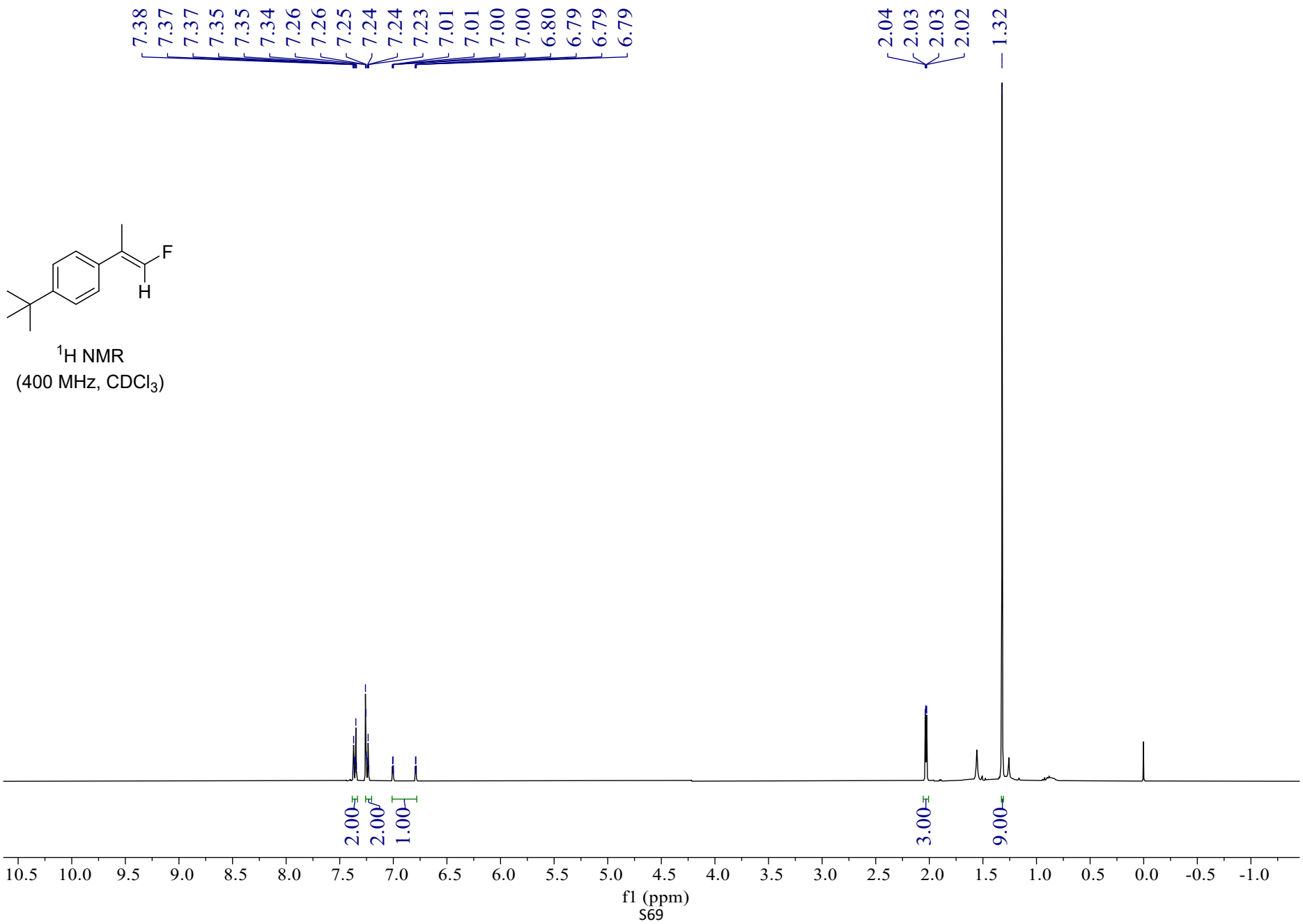


^{19}F NMR
(376 MHz, $CDCl_3$)

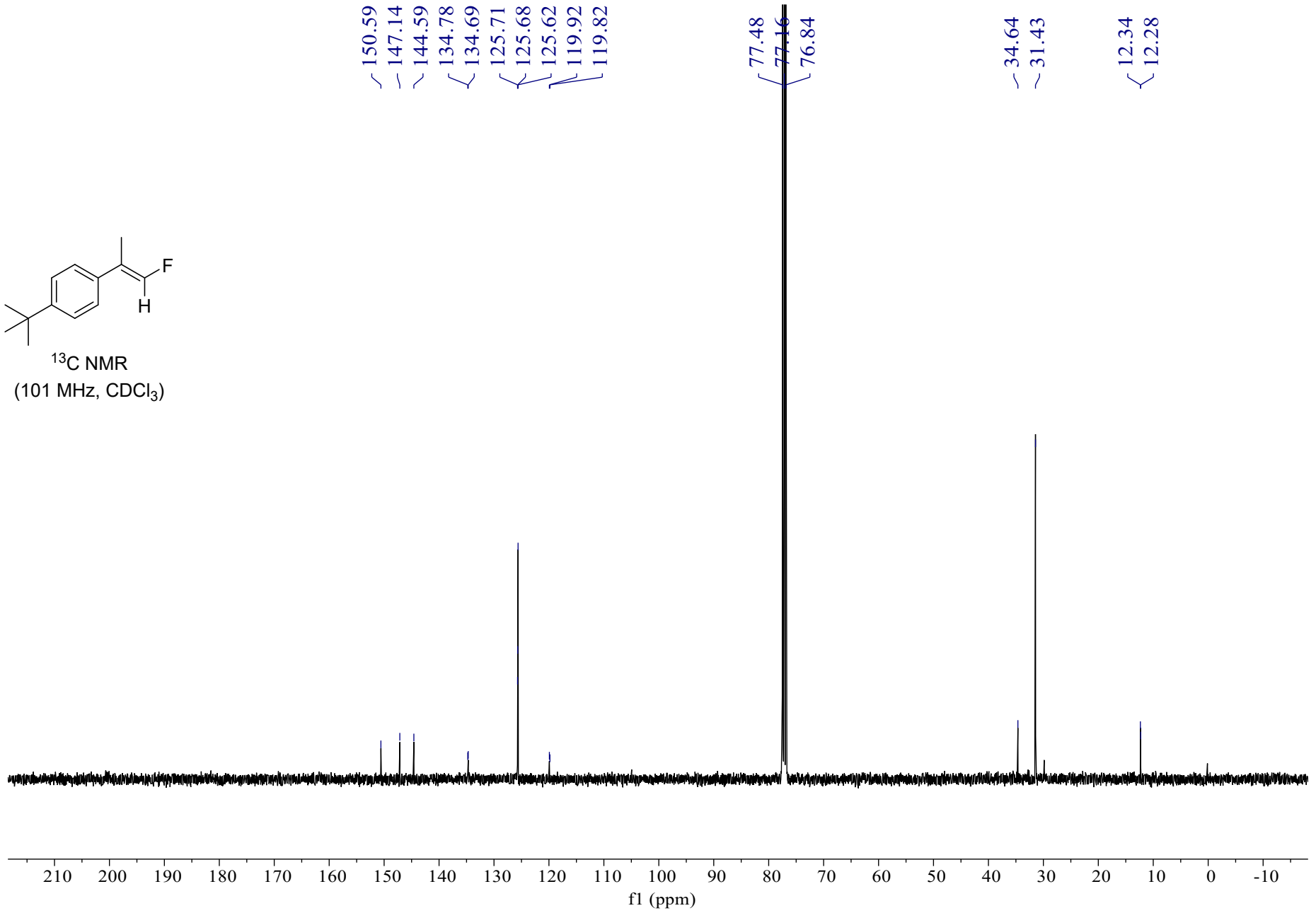
LX-18 #29 RT: 0.21 AV: 1 NL: 3.73E4
T: FTMS + p ESI Full ms [100.0000-1500.0000]



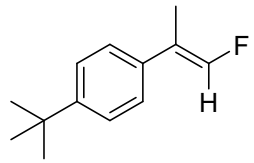
Peak M...	Display...	S Fit	RDB	Delta [p...	Theo....	Rank	Combin...	# Matc...	# Misse...	MS Cov...	Pattern...	MSMS...
167.0876	$C_{10}H_{12}OF$	58.665258578661	4.50	5.85	167.08667	1	97.82	1	0	100	100	(Collection)



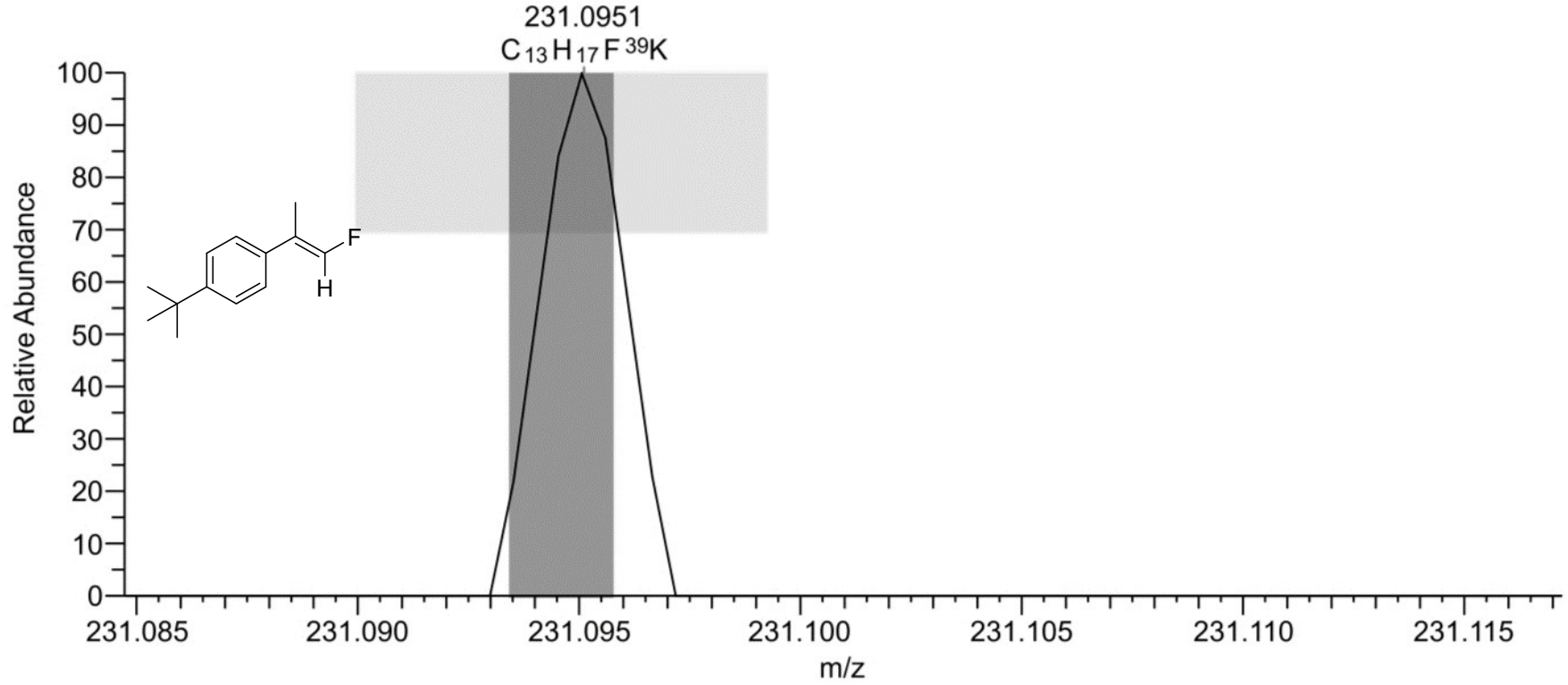
^{1}H NMR
(400 MHz, $CDCl_3$)



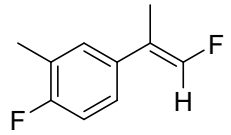
^{13}C NMR
(101 MHz, $CDCl_3$)



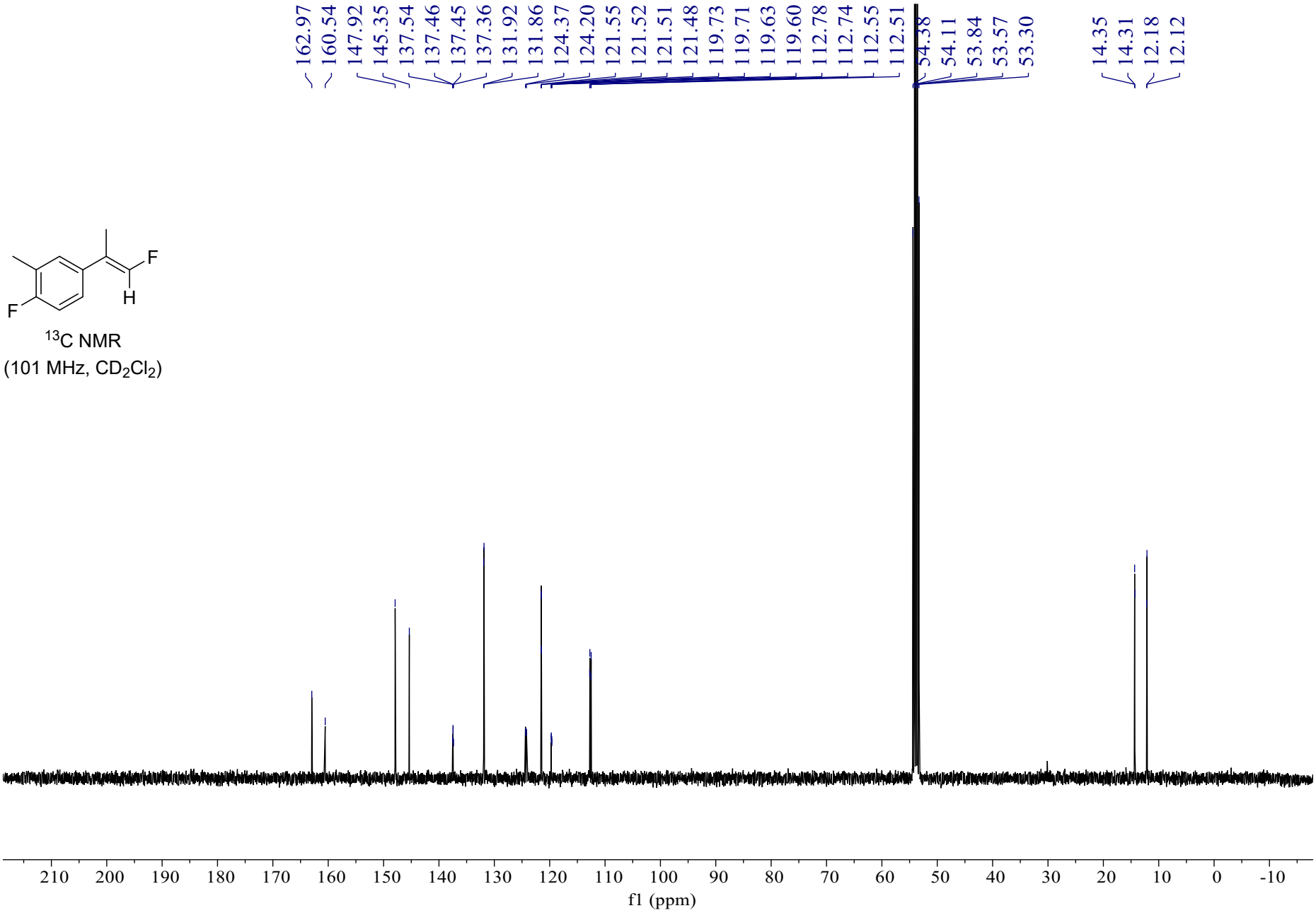
^{19}F NMR
(376 MHz, $CDCl_3$)



Peak M...	Display...	S Fit	RDB	Delta [p...	Theo....	Rank	Combin...	# Matc...	# Misse...	MS Cov...	Pattern...	MSMS...
231.0951	$C_{13}H_{17}F^{39}K$	66.26003929388	4.50	2.39	231.09459	1	98.22	1	0	100	100	(Collection)

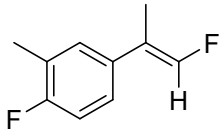


^{1}H NMR
(400 MHz, CD_2Cl_2)

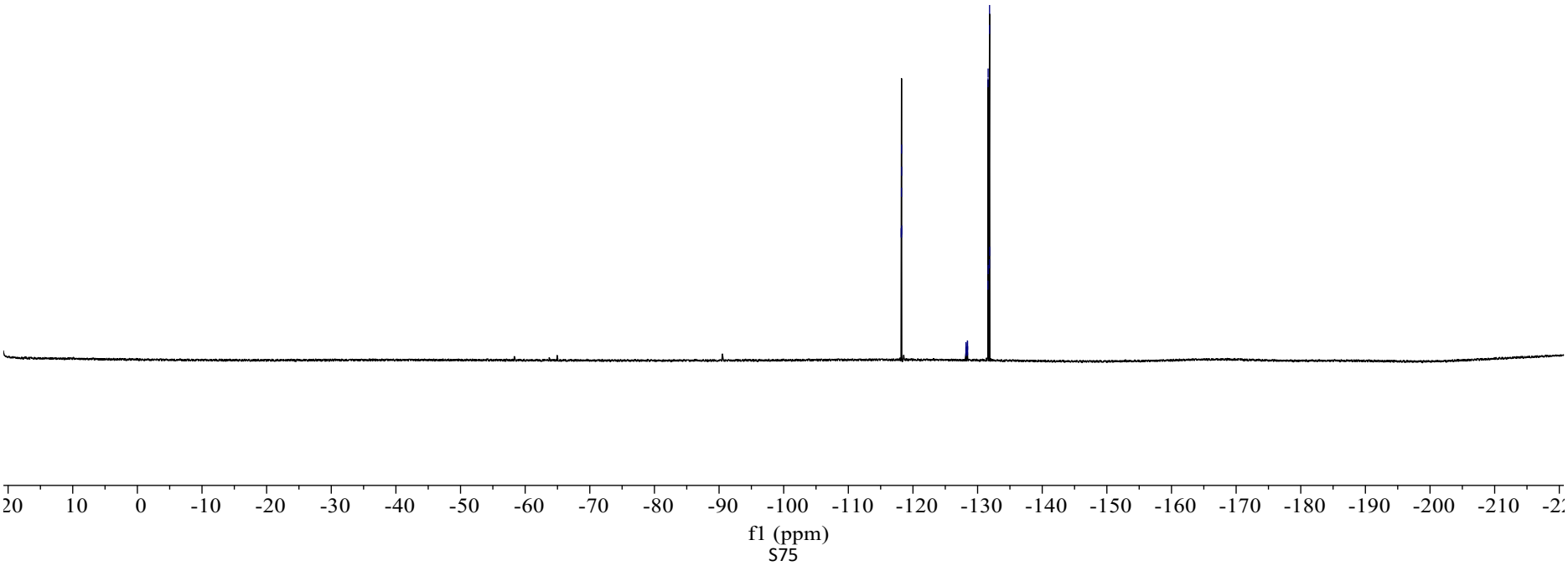


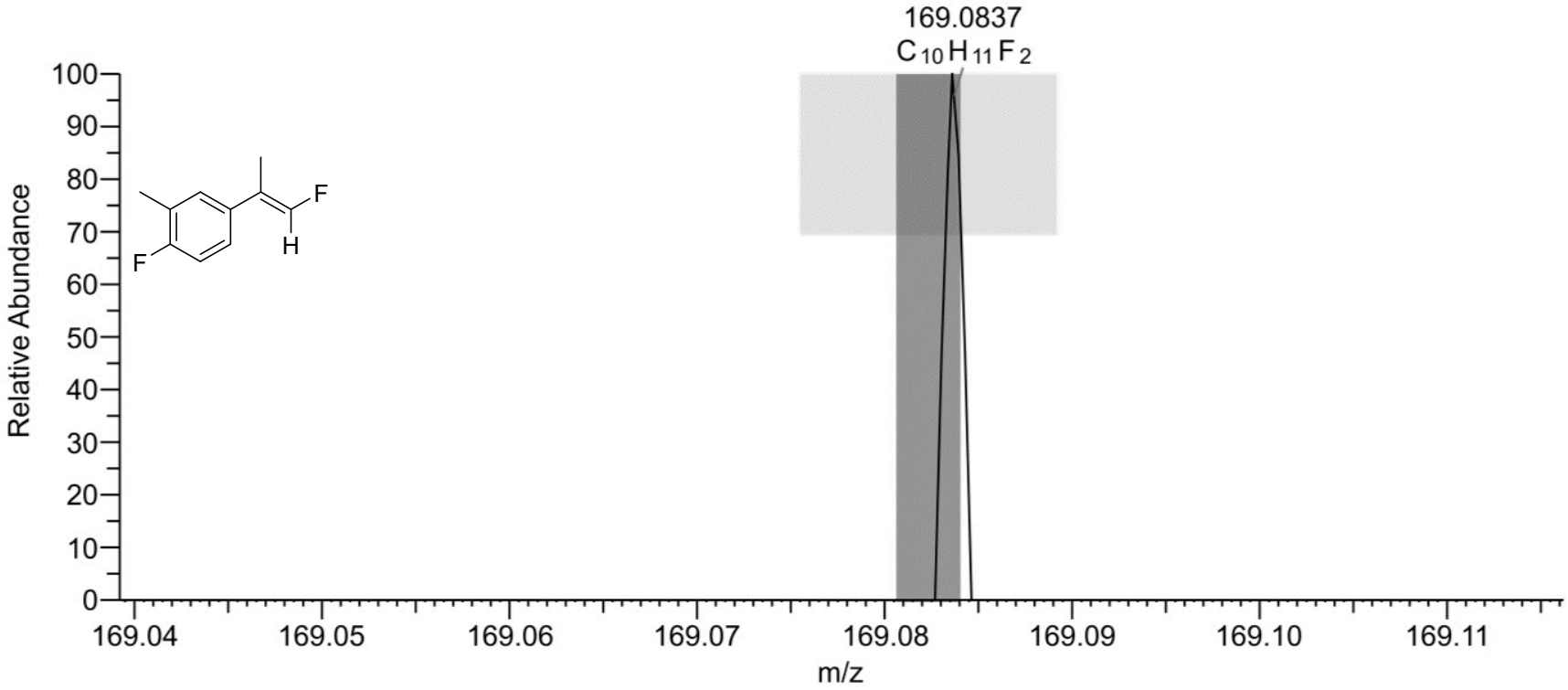
^{13}C NMR
(101 MHz, CD_2Cl_2)

-118.19
-118.20
-118.22
-118.23
-118.25
-118.26
-128.19
-128.20
-128.21
-128.23
-128.41
-128.43
-128.44
-128.45
-131.61
-131.62
-131.63
-131.64
-131.83
-131.84
-131.85
-131.86

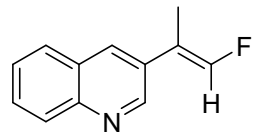


^{19}F NMR
(376 MHz, CD_2Cl_2)

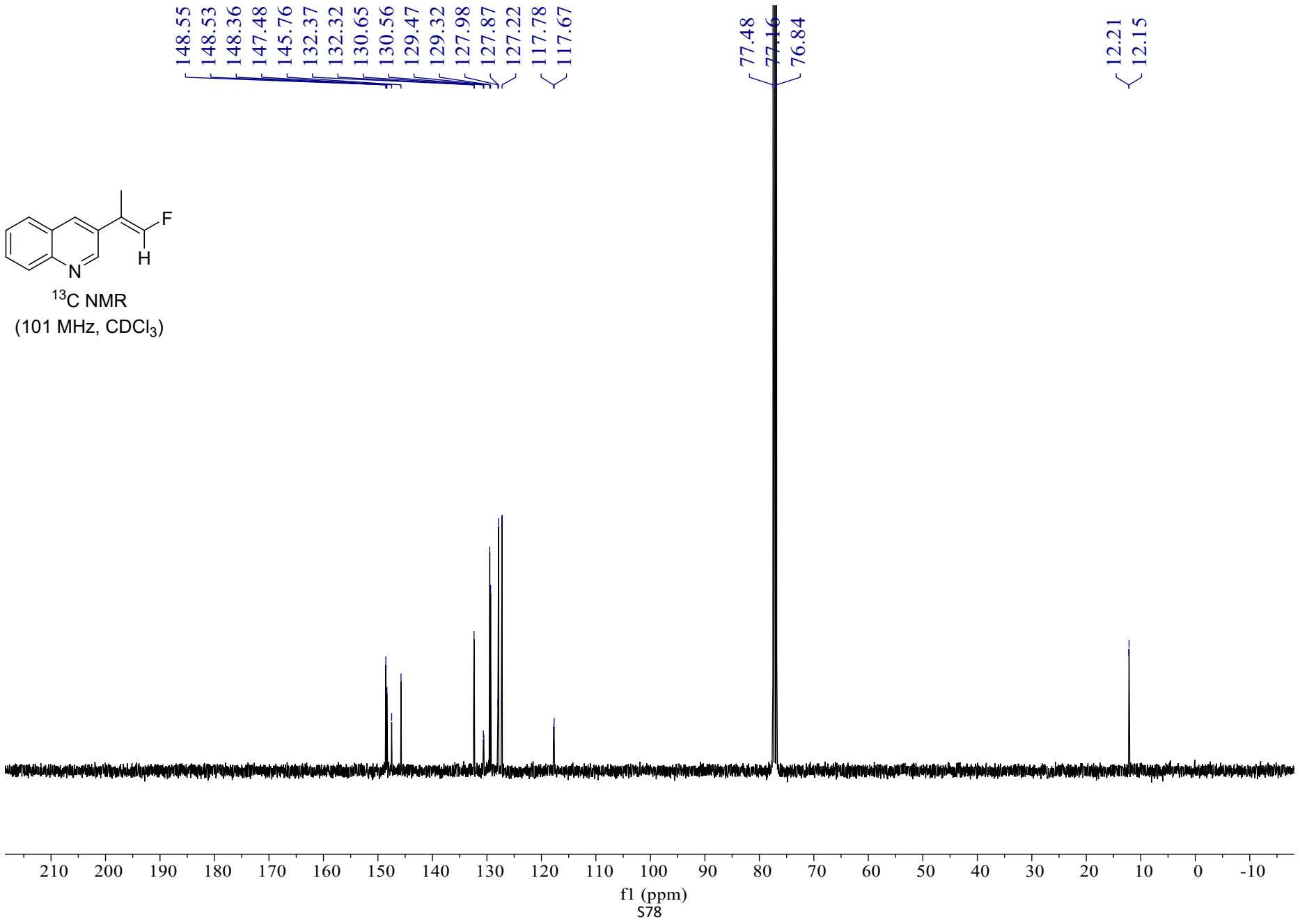




Peak M...	Display...	S Fit	RDB	Delta [p...	Theo....	Rank	Combin...	# Matc...	# Misse...	MS Cov...	Pattern...	MSMS...
169.0837	$C_{10}H_{11}F_2$	41.80101424931117	4.50	8.23	169.08233	1	96.94	1	0	100	100	(Collection)

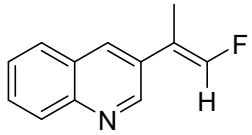


^{1}H NMR
(400 MHz, $CDCl_3$)

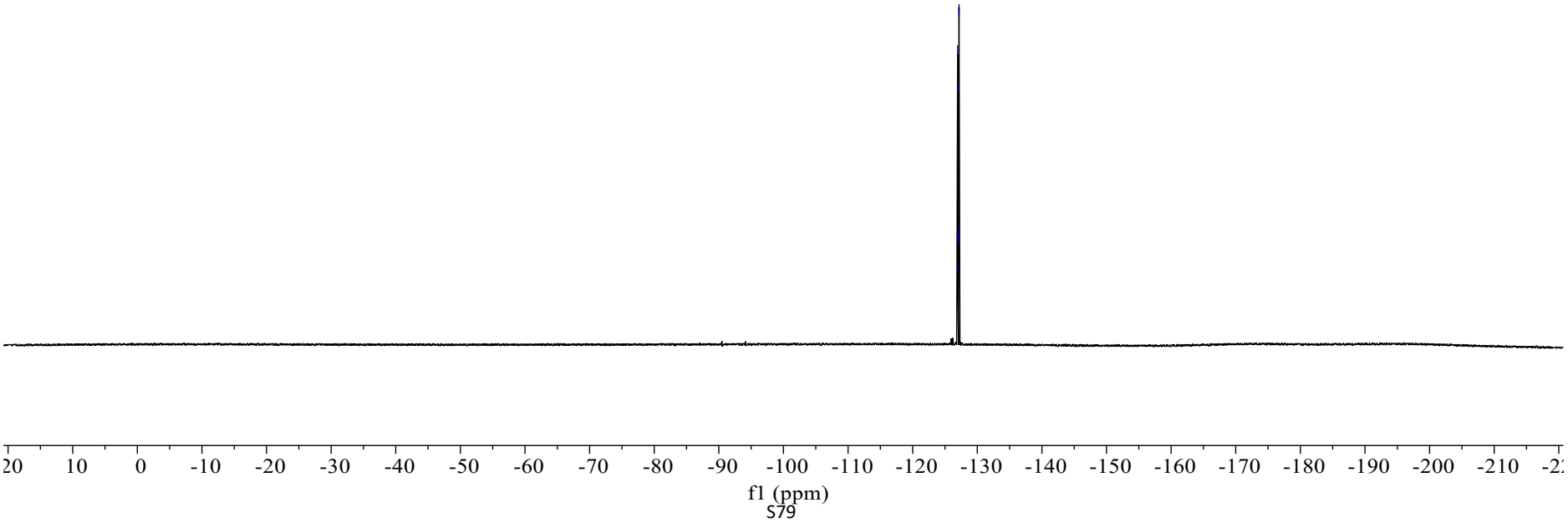


^{13}C NMR
(101 MHz, $CDCl_3$)

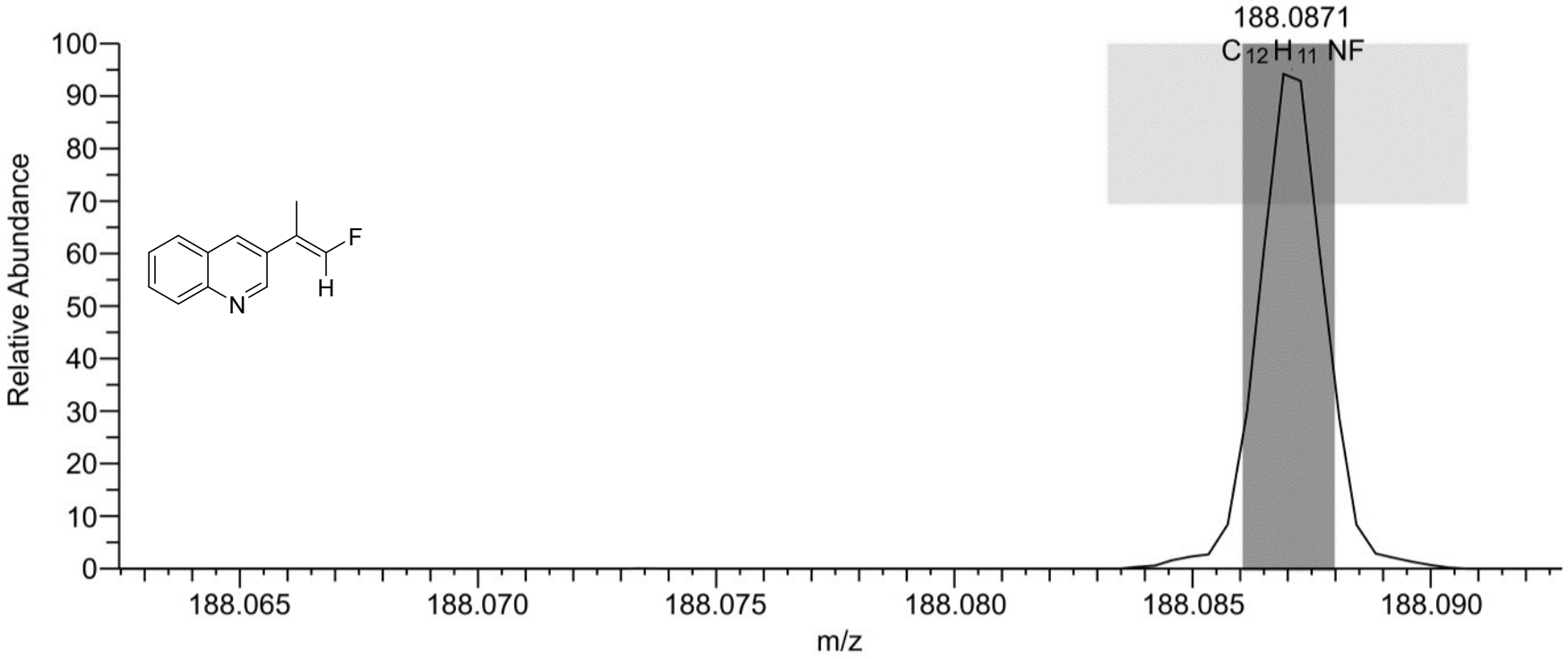
-126.94
-126.95
-126.97
-126.98
-127.17
-127.18
-127.19
-127.20



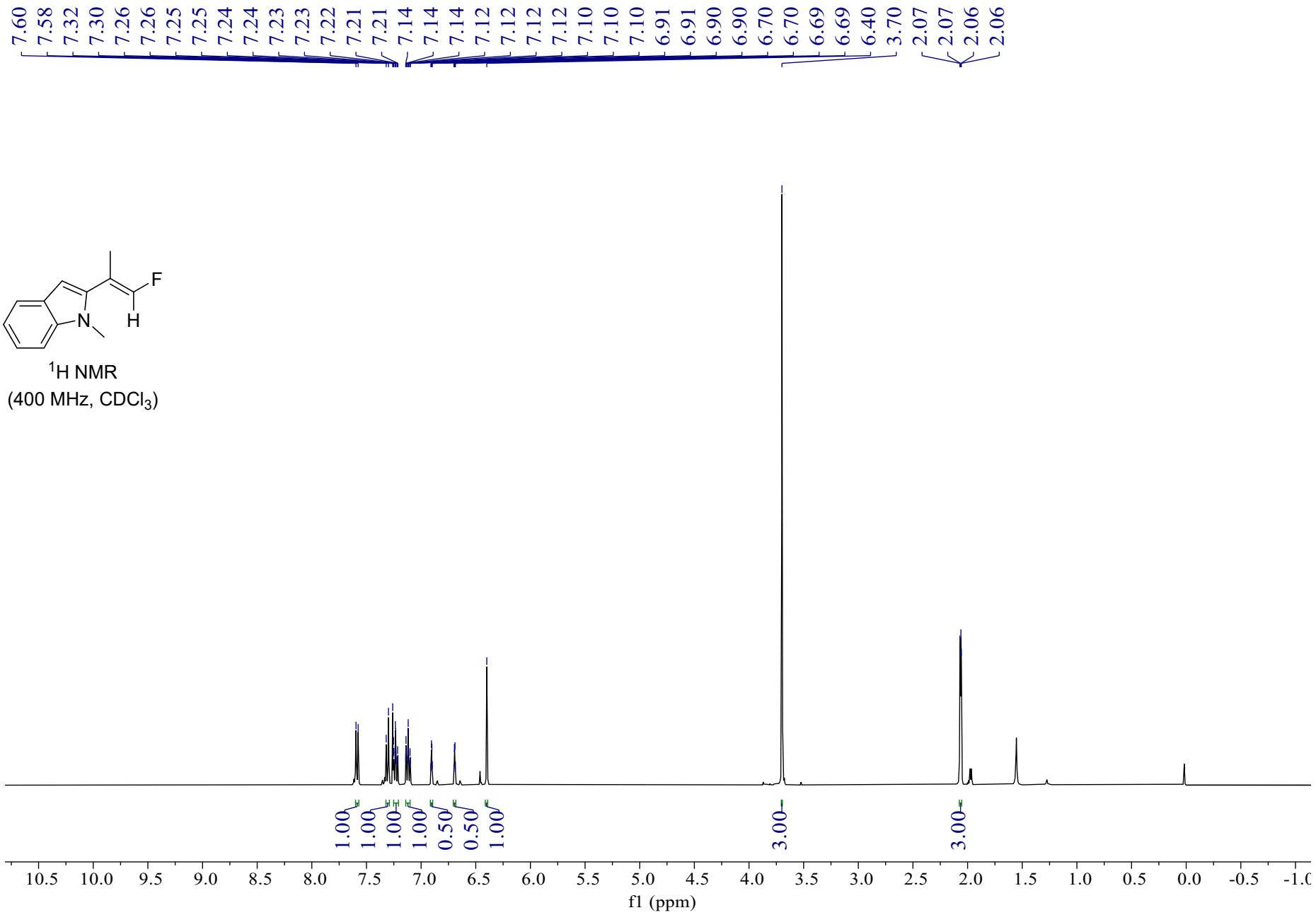
^{19}F NMR
(376 MHz, $CDCl_3$)

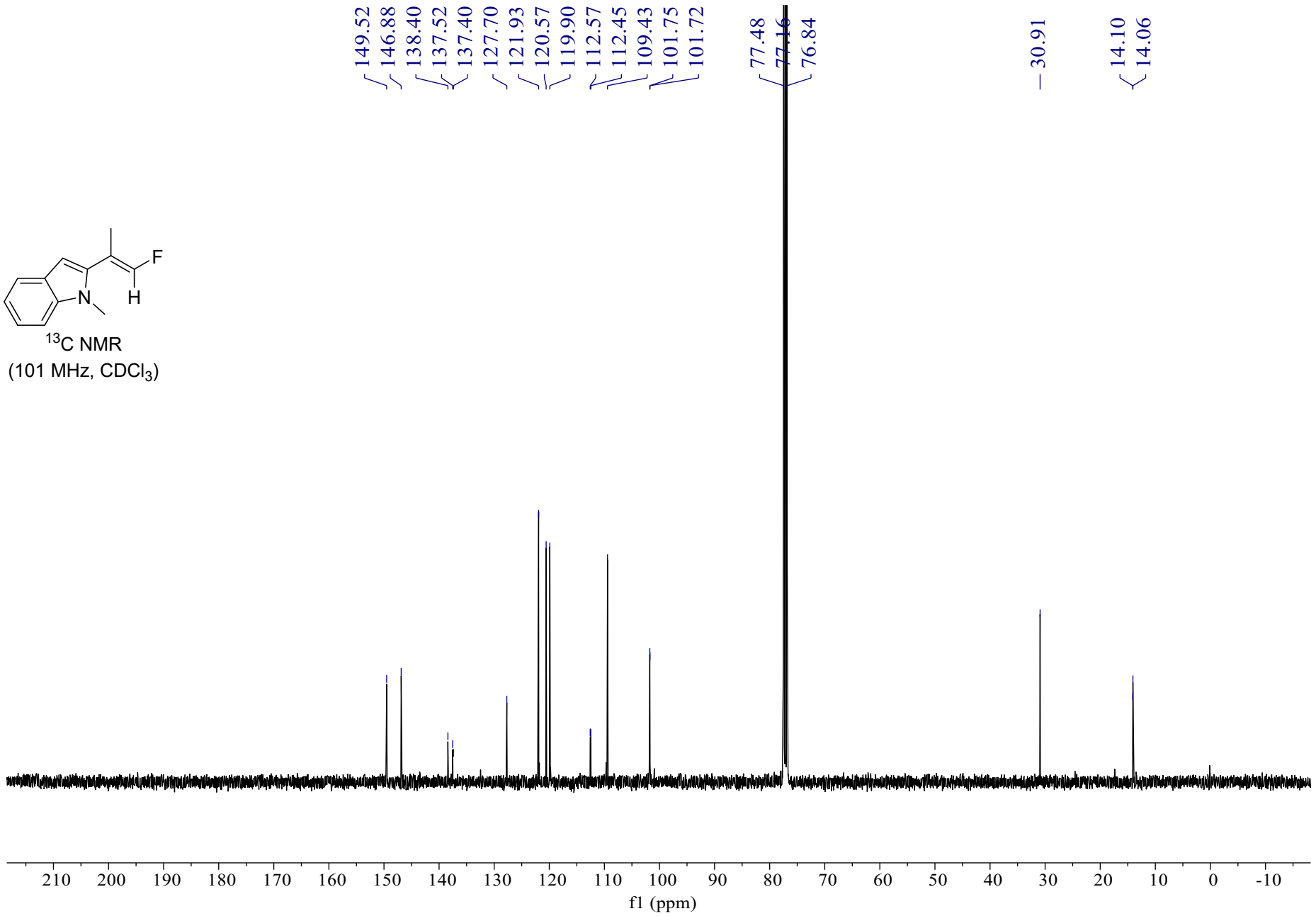


LX-9 #15 RT: 0.11 AV: 1 NL: 2.64E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



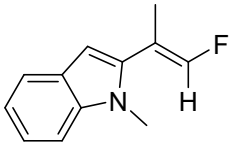
Peak M...	Display...	S Fit	RDB	Delta [p...	Theo....	Rank	Combin...	# Matc...	# Misse...	MS Cov...	Pattern...	MSMS...
188.0871	$C_{12}H_{11}NF$	35.323507192183 7	7.50	0.49	188.08700	1	96.02	4	1	99.39	99.57	(Collection)


7.60
7.58
7.32
7.30
7.26
7.26
7.25
7.25
7.24
7.24
7.23
7.23
7.22
7.21
7.21
7.14
7.14
7.14
7.12
7.12
7.12
7.12
7.10
7.10
7.10
6.91
6.91
6.90
6.90
6.70
6.70
6.69
6.69
6.40
3.70
2.07
2.07
2.06
2.06
F
H
N
^{1}H NMR
(400 MHz, $CDCl_3$)
1.00
1.00
1.00
1.00
0.50
0.50
1.00
3.00
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

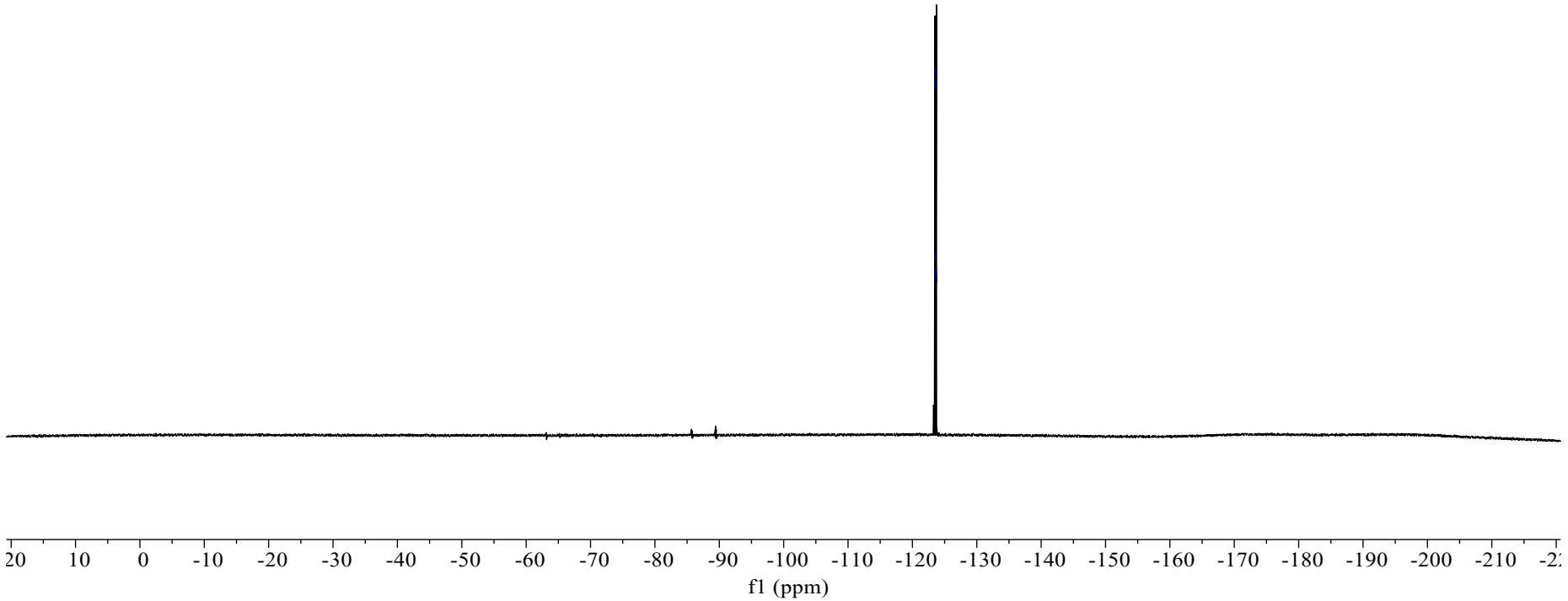


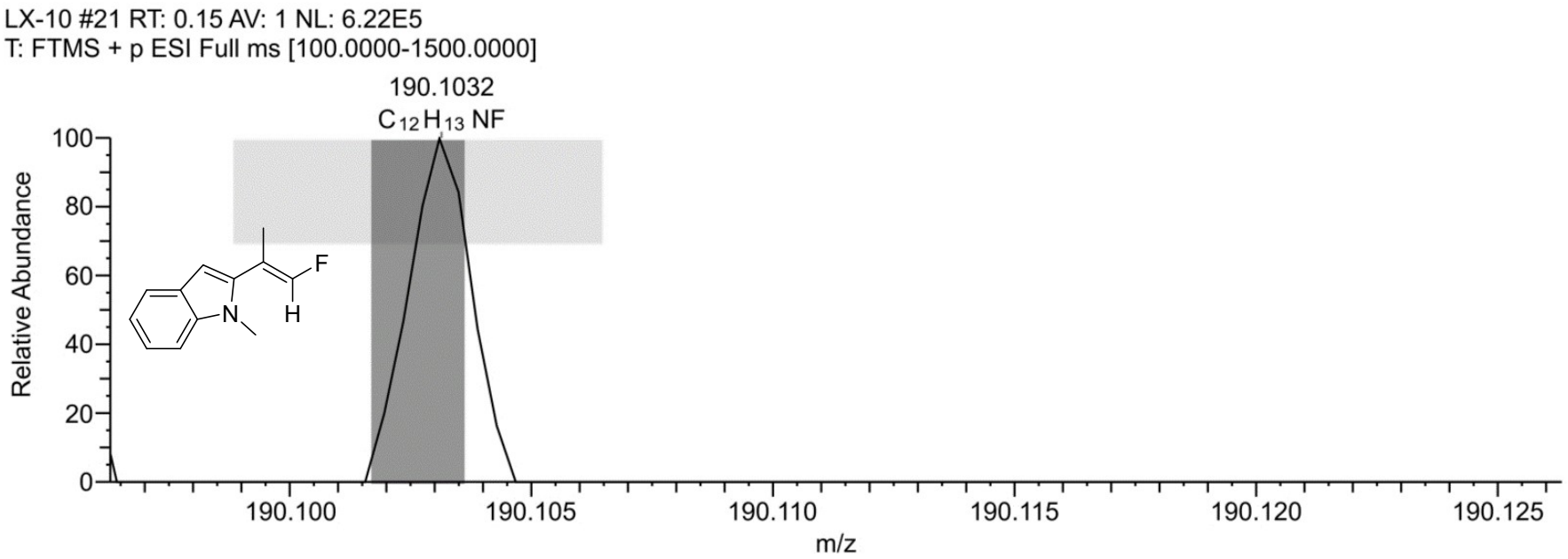
^{13}C NMR
(101 MHz, $CDCl_3$)

-123.50
-123.50
-123.52
-123.53
-123.72
-123.73
-123.74
-123.75

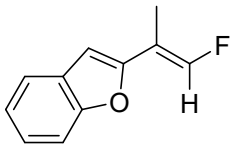


^{19}F NMR
(376 MHz, $CDCl_3$)

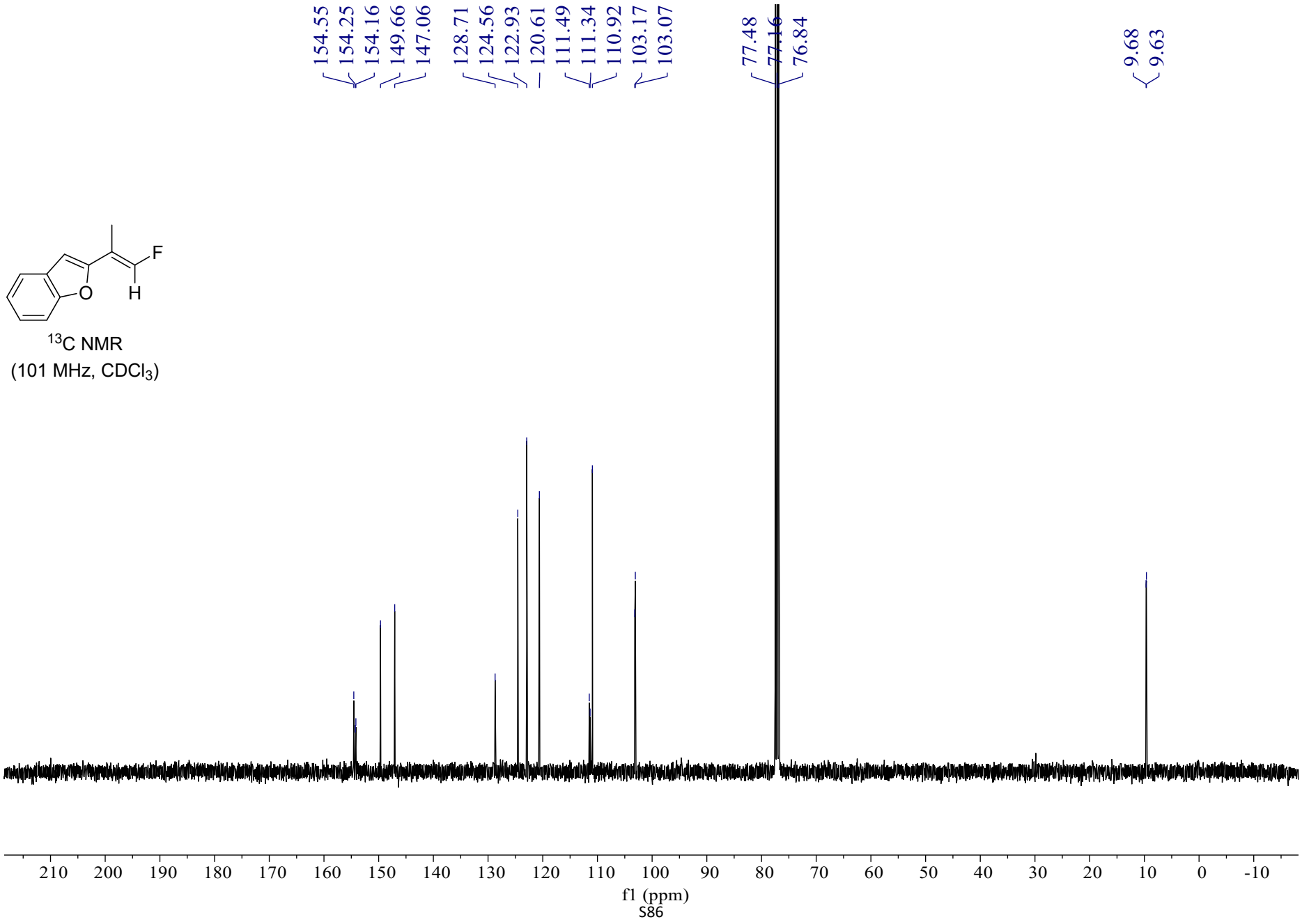


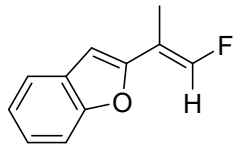


Peak M...	Display...	S Fit	RDB	Delta [p...	Theo....	Rank	Combin...	# Matc...	# Misse...	MS Cov...	Pattern...	MSMS...
190.1032	$C_{12}H_{13}NF$	62.024108758457 9	6.50	2.69	190.10265	1	98	1	0	100	100	(Collection)



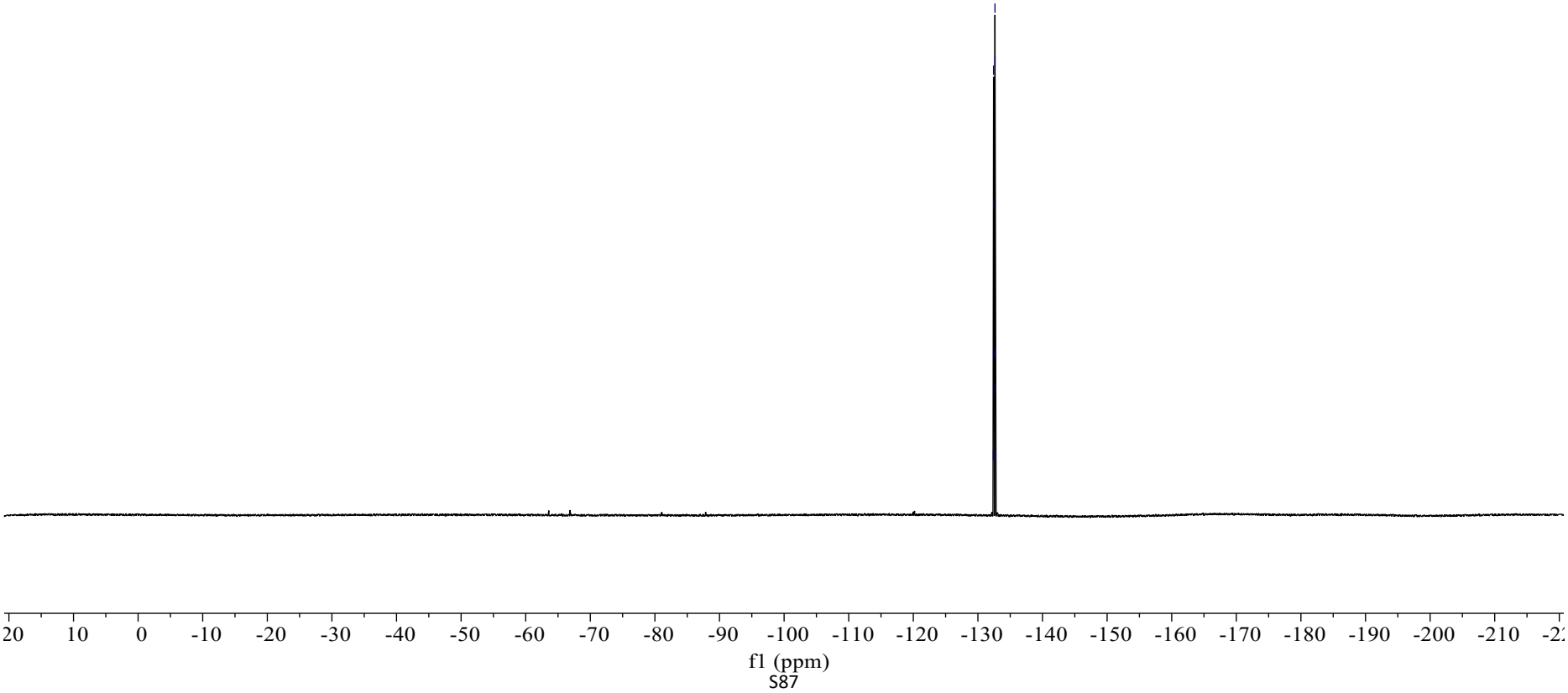
^{1}H NMR
(400 MHz, $CDCl_3$)

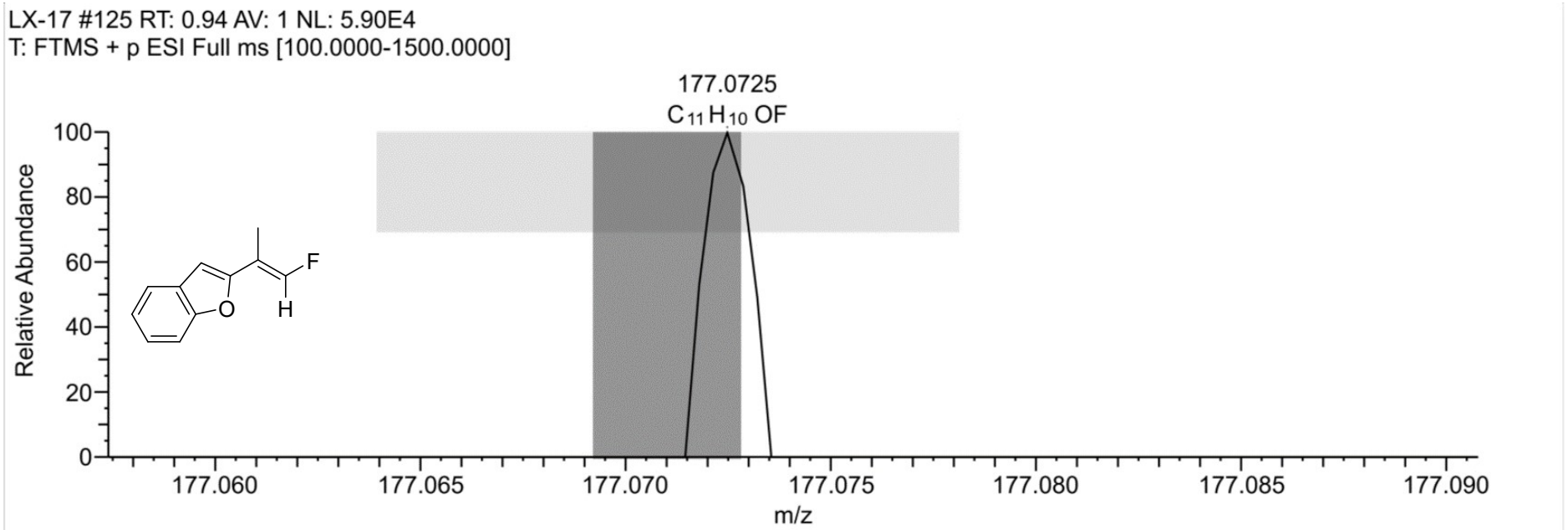

154.55
154.25
154.16
149.66
147.06
128.71
124.56
122.93
120.61
111.49
111.34
110.92
103.17
103.07
77.48
77.16
76.84
9.68
9.63
F
O
H
13C NMR
(101 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



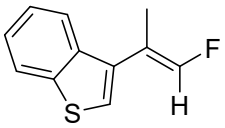
^{19}F NMR

(376 MHz, $CDCl_3$)

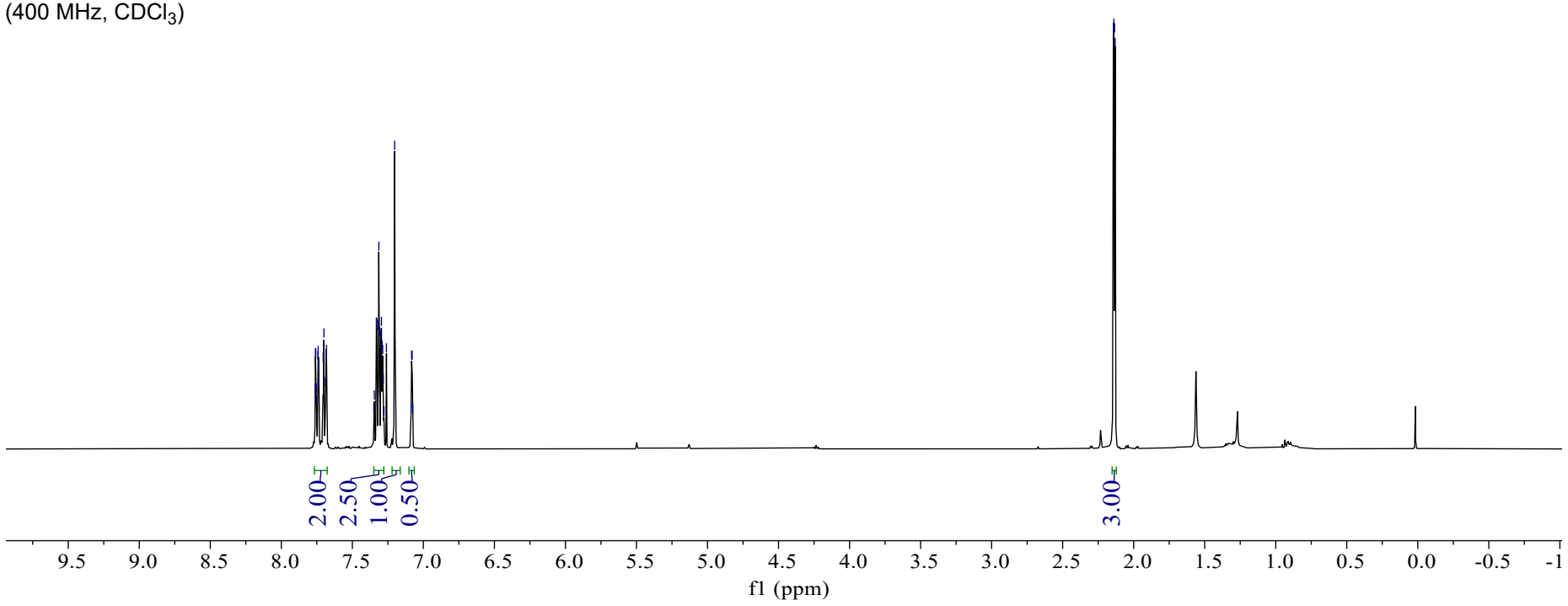


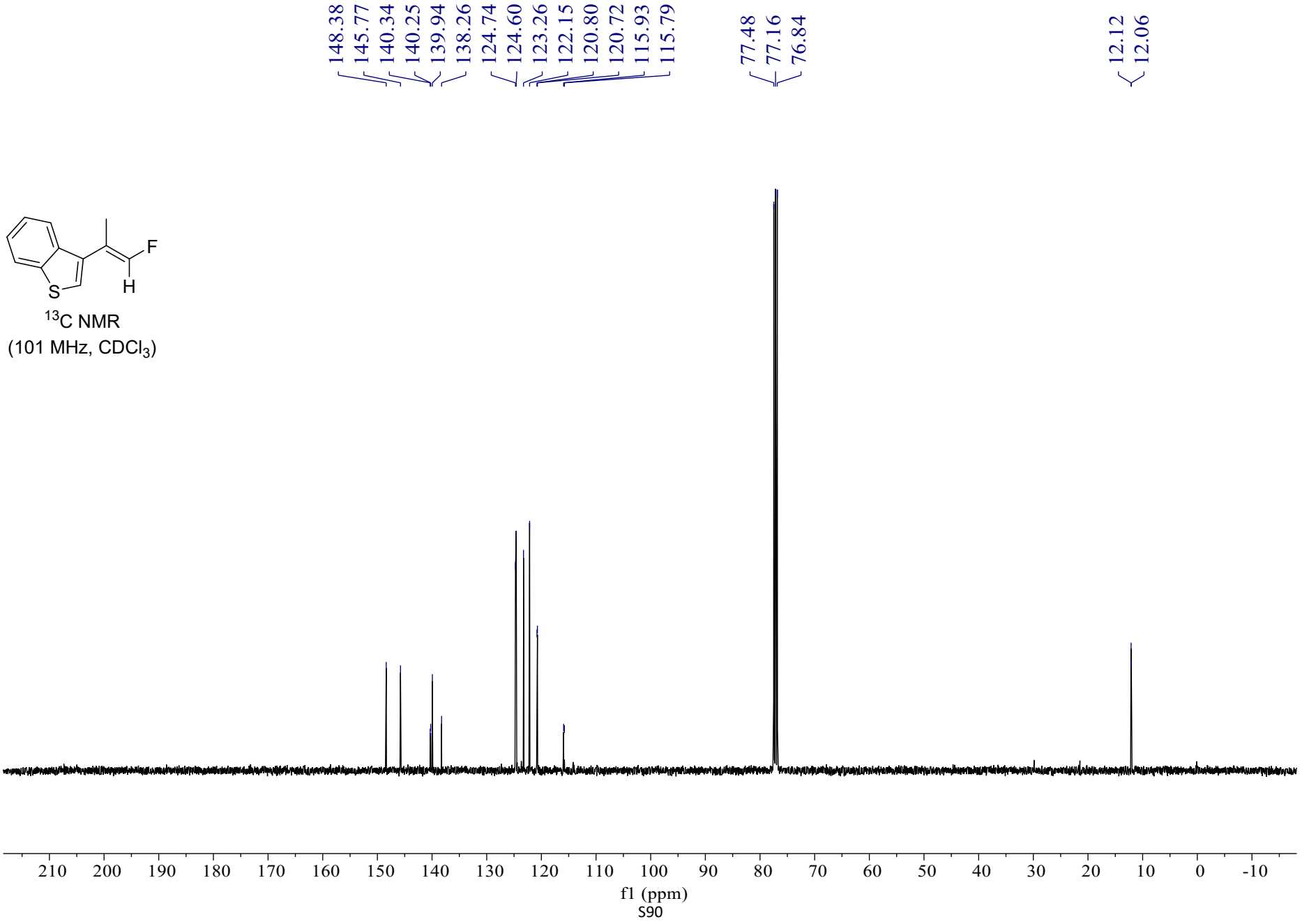


Peak M...	Display...	S Fit	RDB	Delta [p...	Theo....	Rank	Combin...	# Matc...	# Misse...	MS Cov...	Pattern...	MSMS...
177.0725	$C_{11}H_{10}OF$	41.7151195499976	6.50	8.24	177.07102	1	96.93	1	0	100	100	(Collection)

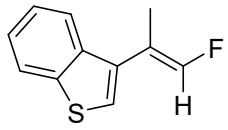


^{1}H NMR
(400 MHz, $CDCl_3$)



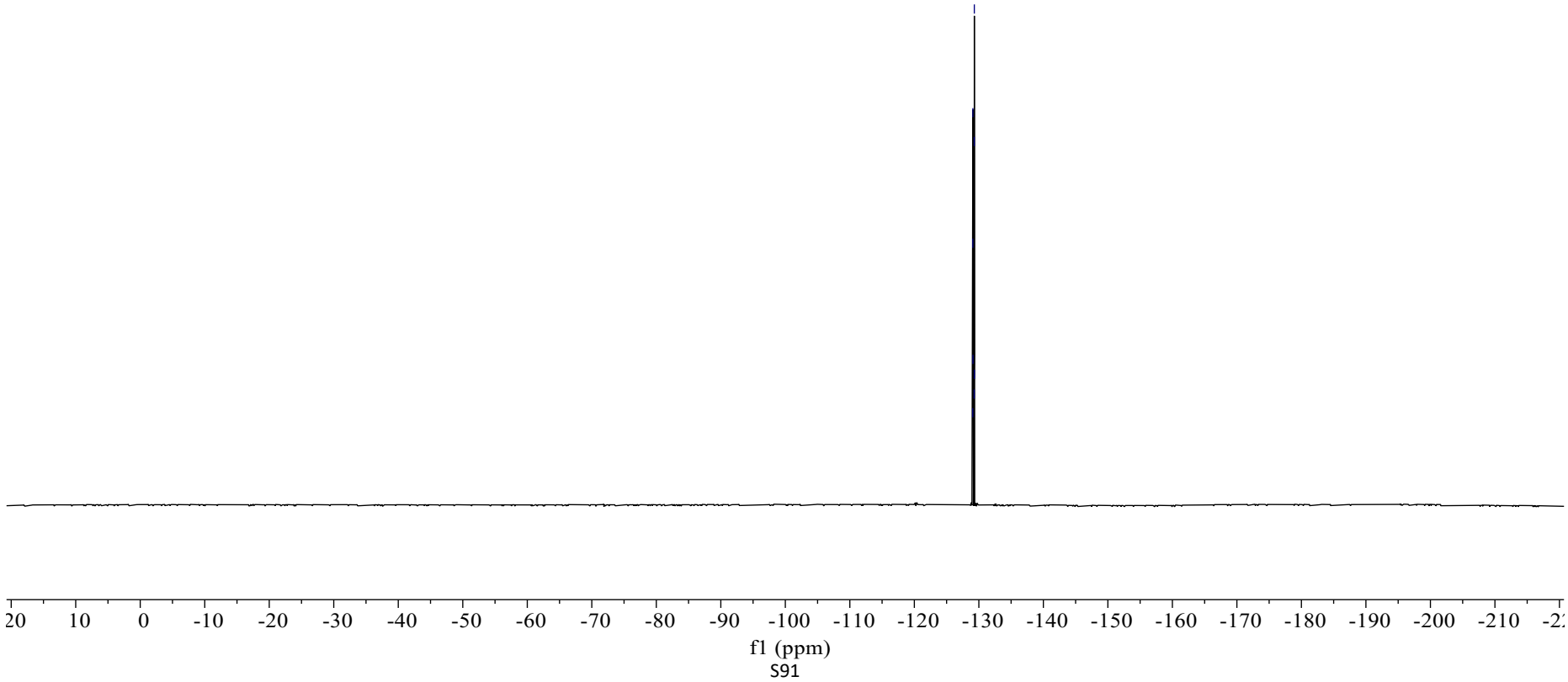

148.38
145.77
140.34
140.25
139.94
138.26
124.74
124.60
123.26
122.15
120.80
120.72
115.93
115.79
77.48
77.16
76.84
12.12
12.06
F
S
H
13C NMR
(101 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

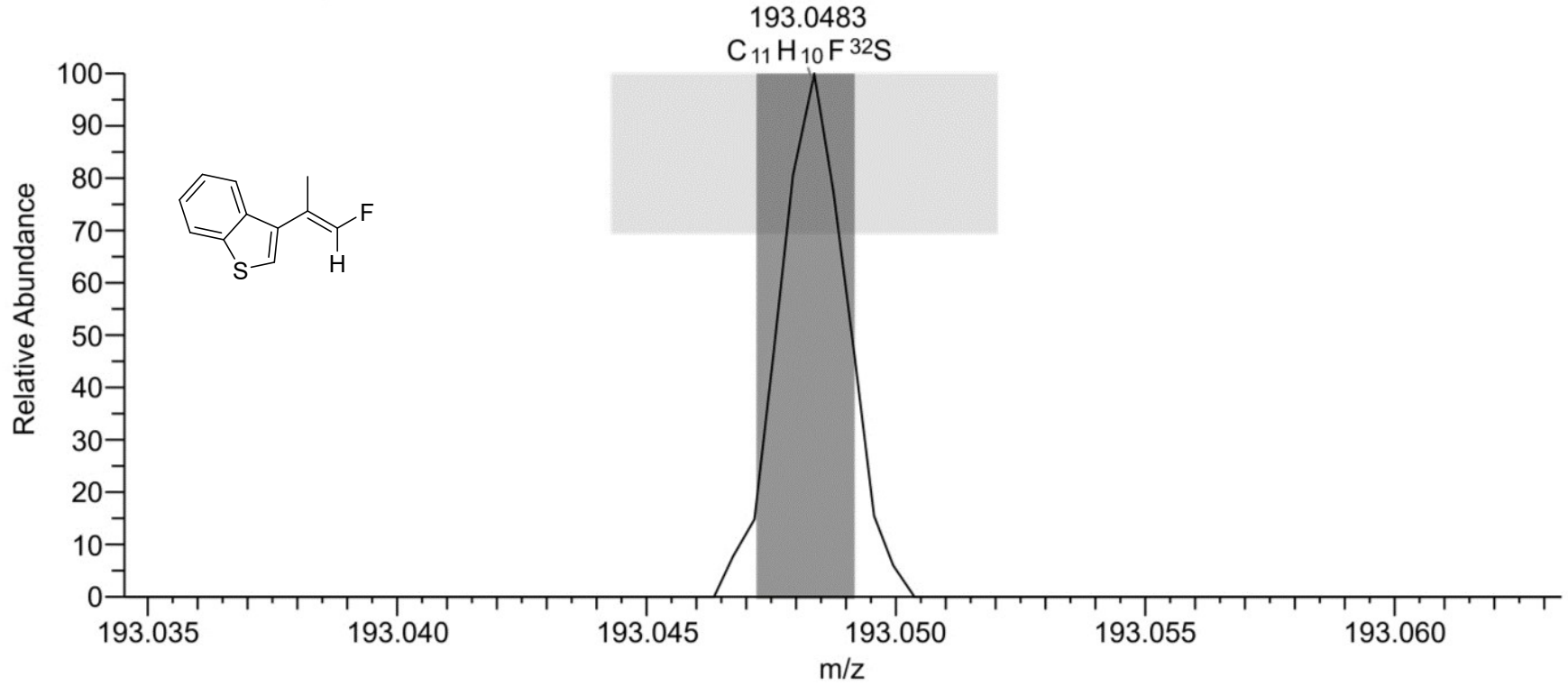
-129.06
-129.07
-129.08
-129.09
-129.28
-129.29
-129.30
-129.31



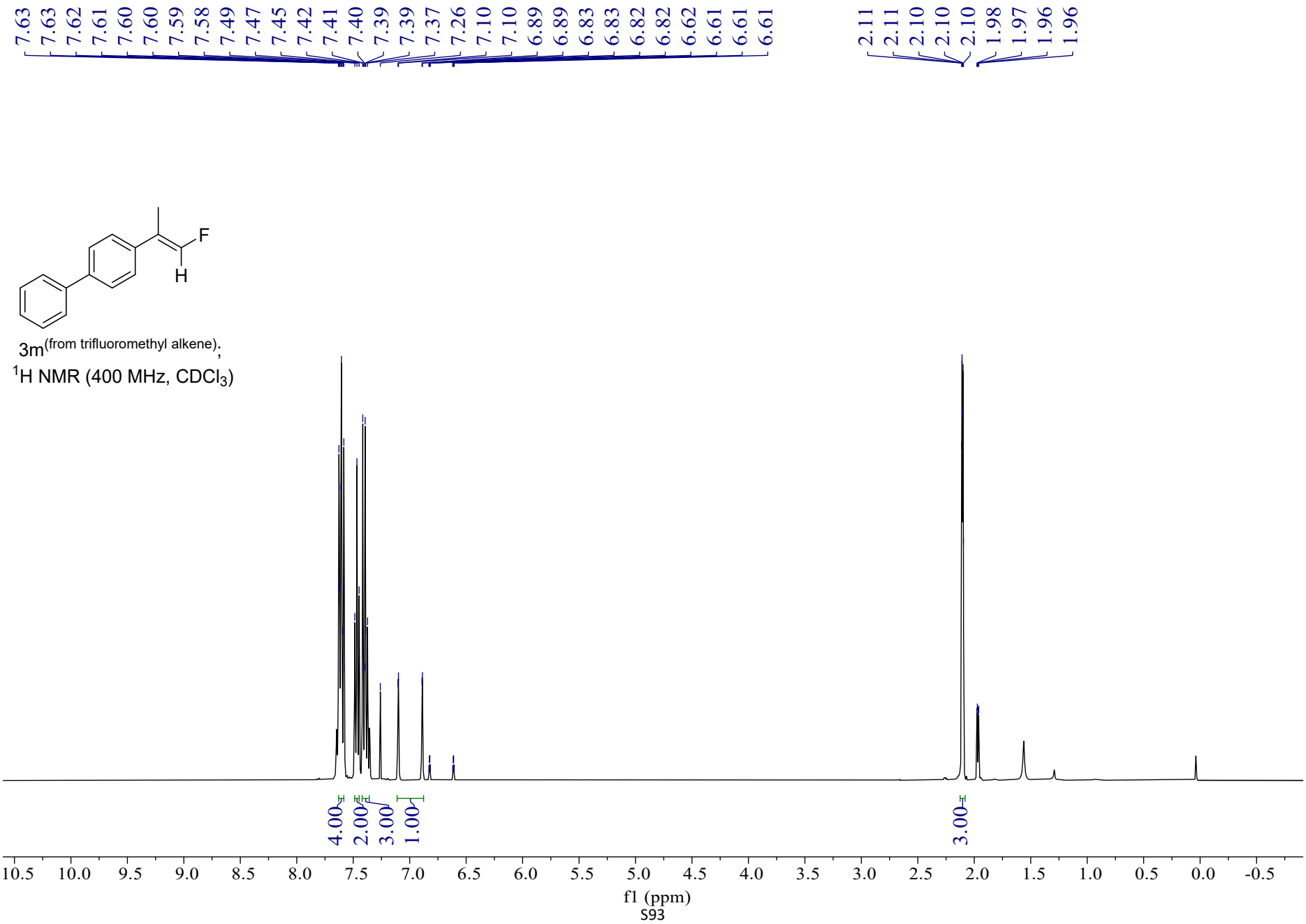
^{19}F NMR

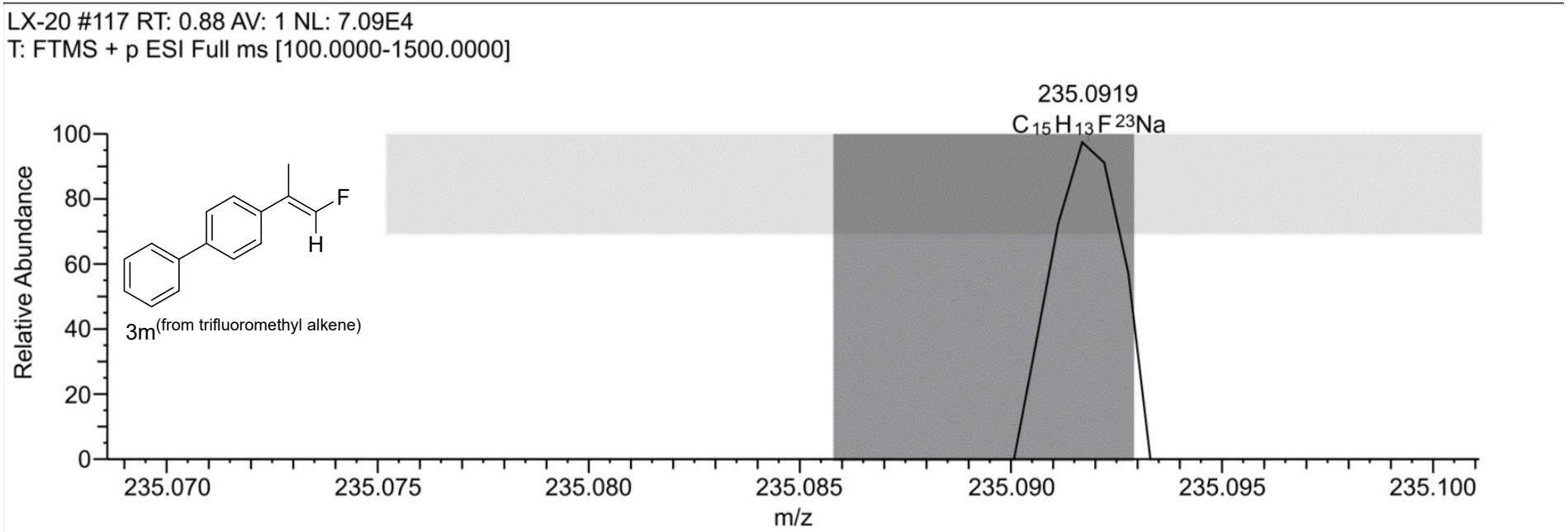
(376 MHz, $CDCl_3$)



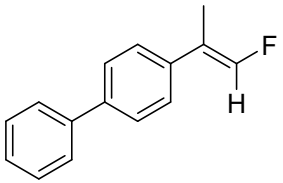


Peak M...	Display...	S Fit	RDB	Delta [p...	Theo....	Rank	Combin...	# Matc...	# Misse...	MS Cov...	Pattern...	MSMS...
193.0483	$C_{11}H_{10}F^{32}S$	87.9826424073948	6.50	0.85	193.04818	1	99.37	1	0	100	100	(Collection)

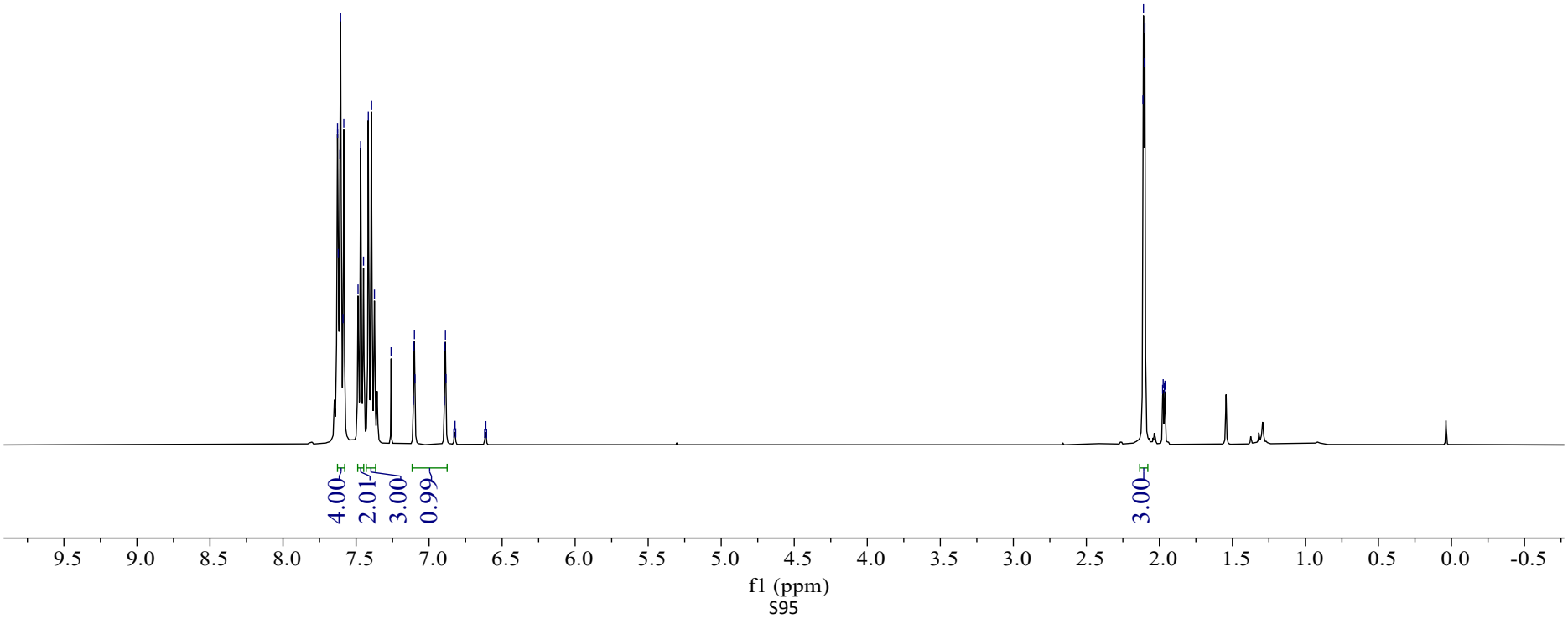

7.63
7.63
7.62
7.61
7.60
7.60
7.59
7.58
7.49
7.47
7.45
7.42
7.41
7.40
7.39
7.39
7.37
7.26
7.10
7.10
6.89
6.89
6.83
6.83
6.82
6.82
6.62
6.61
6.61
6.61
2.11
2.11
2.10
2.10
2.10
1.98
1.97
1.96
1.96
F
H
3m(from trifluoromethyl alkene);
1H NMR (400 MHz, CDCl3)
4.00
2.00
3.00
1.00
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

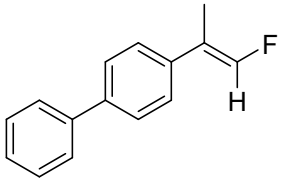


Peak M...	Display...	S Fit	RDB	Delta [p...	Theo....	Rank	Combin...	# Matc...	# Misse...	MS Cov...	Pattern...	MSMS...
235.0919	$C_{15}H_{13}F^{23}Na$	49.4028503376902	8.50	10.73	235.08935	1	97.34	1	0	100	100	(Collection)

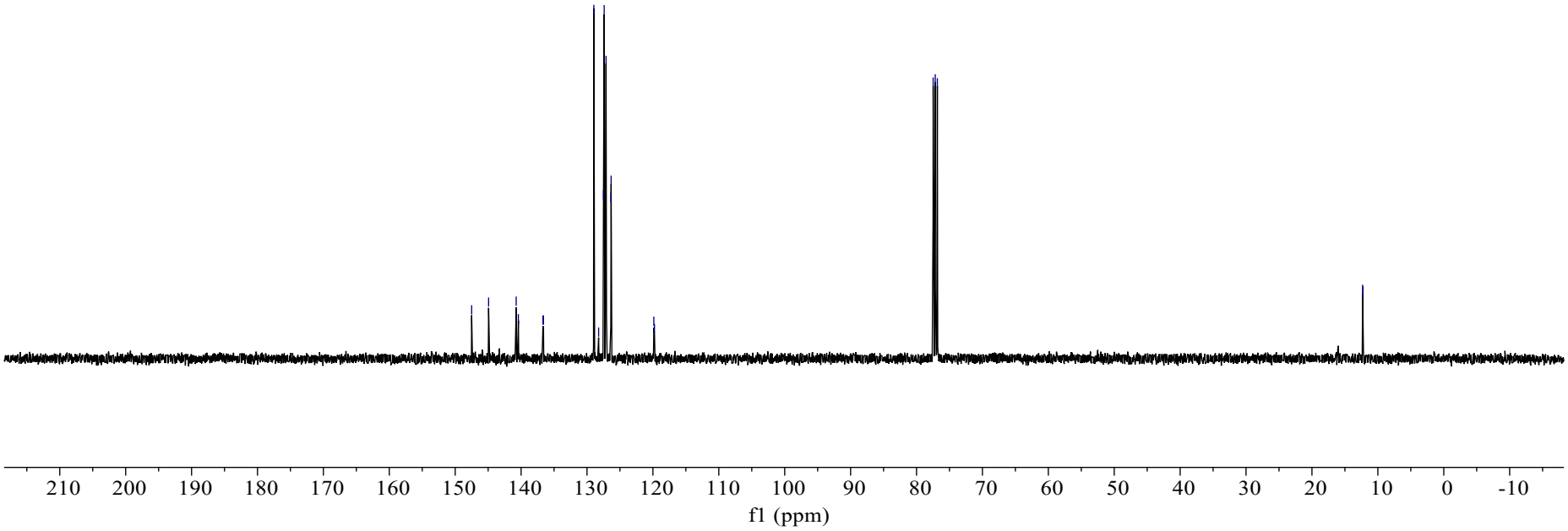


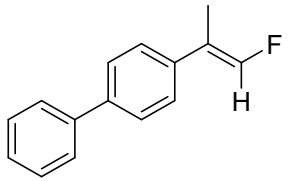
3m(from gem-difluoroalkene);
^{1}H NMR (400 MHz, $CDCl_3$)





3m(from gem-difluoroalkene);
^{13}C NMR (101 MHz, $CDCl_3$)





3m(from gem-difluoroalkene);

^{19}F NMR (376 MHz, $CDCl_3$)

Mass Spectrum SmartFormula Report

Analysis Info

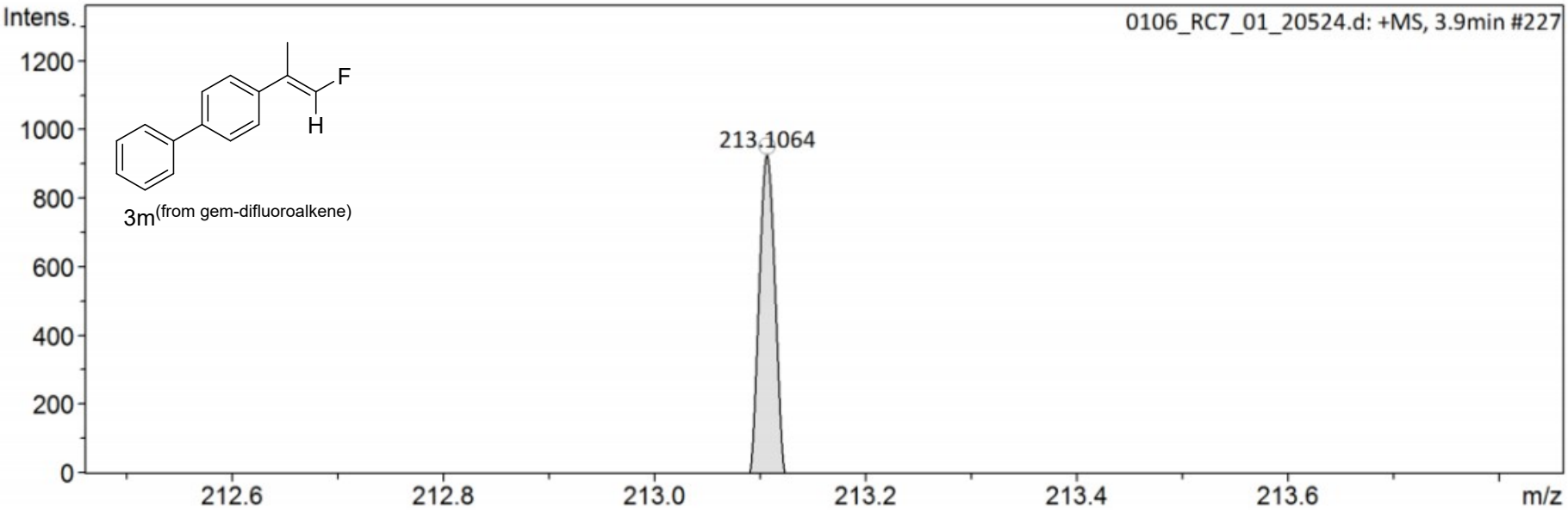
Acquisition D 2023-01-09 11:16:43

Analysis Name D:\LXMS\0106_RC7_01_20524.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0106
Comment

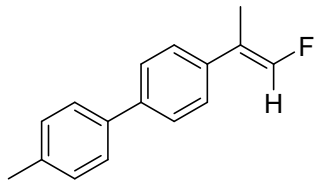
Operator Demo User
Instrumen compact 8255754.2017 6

Acquisition Paramet

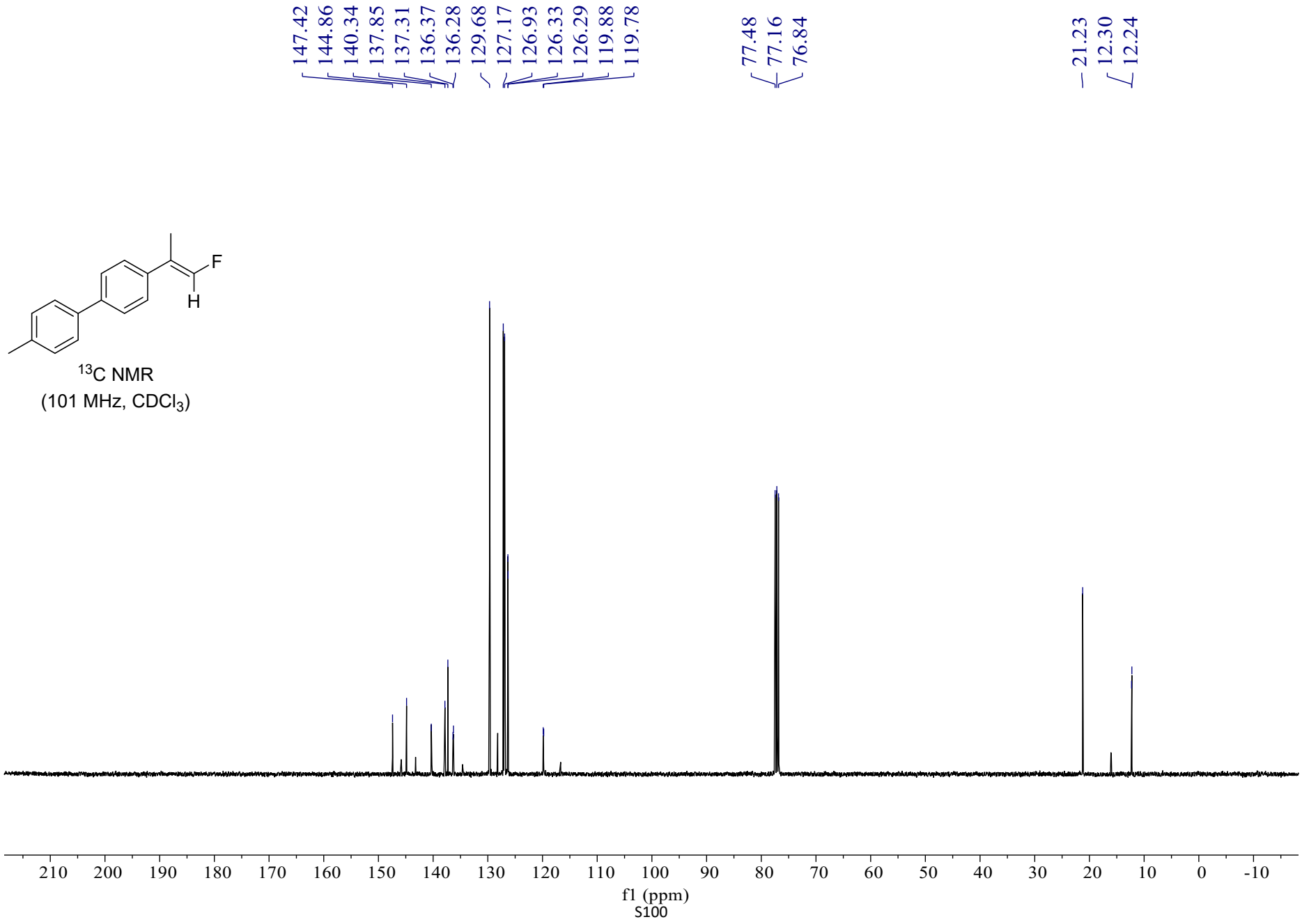
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min



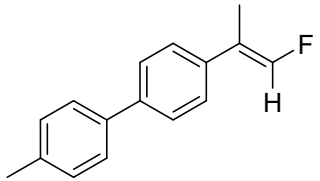
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
213.1064	1	C15H14F	213.1074	4.8	748.6	1	100.00	8.5	even		ok



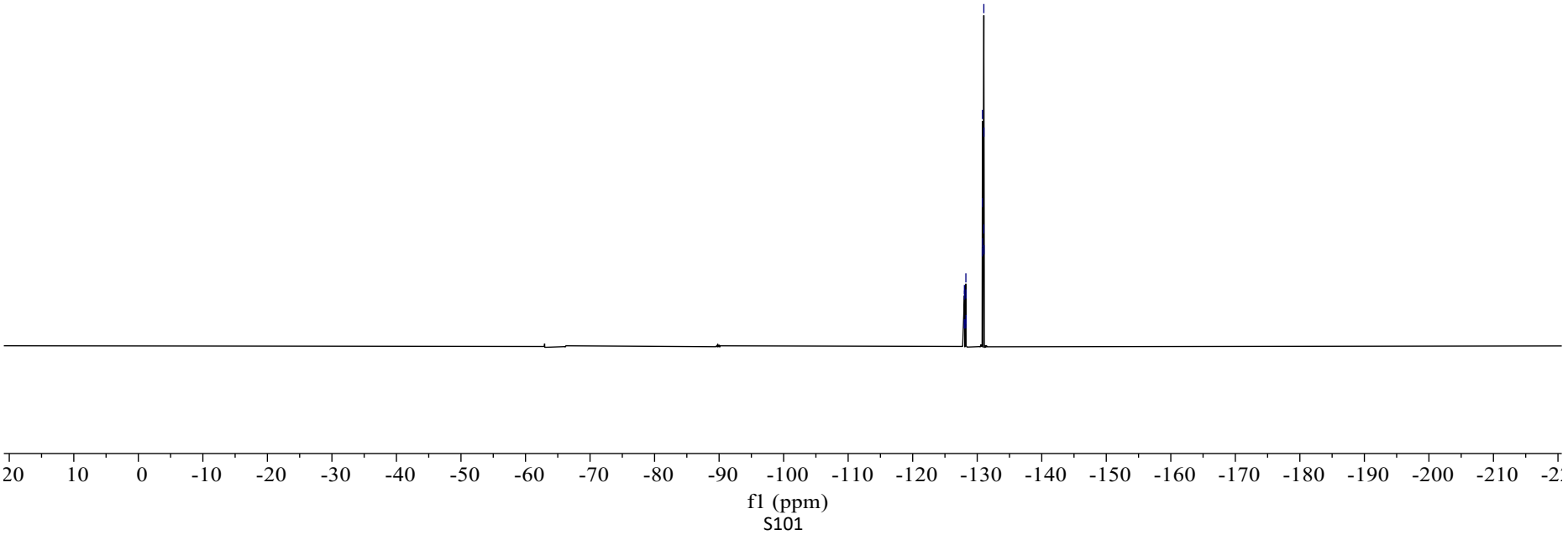
^{1}H NMR
(400 MHz, $CDCl_3$)


147.42
144.86
140.34
137.85
137.31
136.37
136.28
129.68
127.17
126.93
126.33
126.29
119.88
119.78
77.48
77.16
76.84
21.23
12.30
12.24
F
H
13C NMR
(101 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

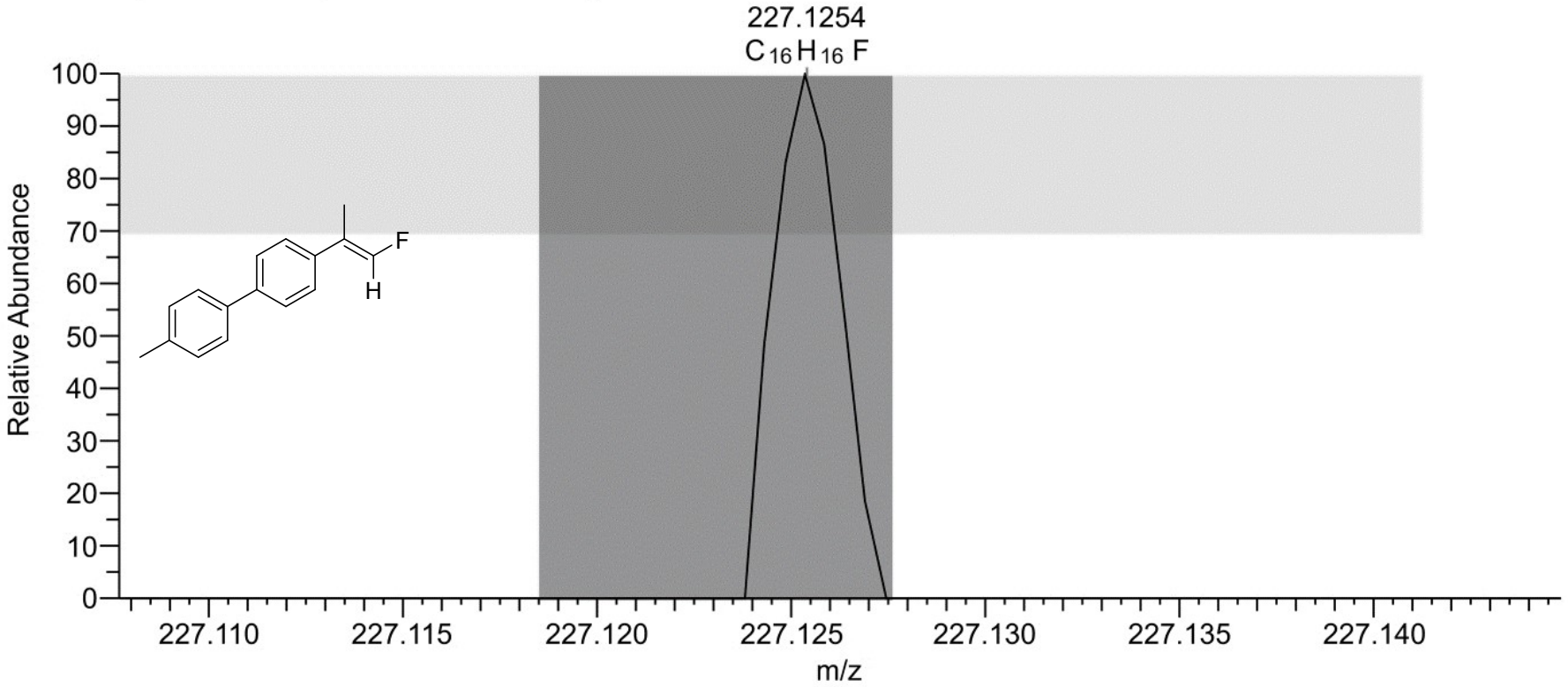
-128.01
-128.02
-128.03
-128.04
-128.23
-128.24
-128.26
-128.27
-130.79
-130.80
-130.81
-130.82
-131.02
-131.03
-131.04
-131.05



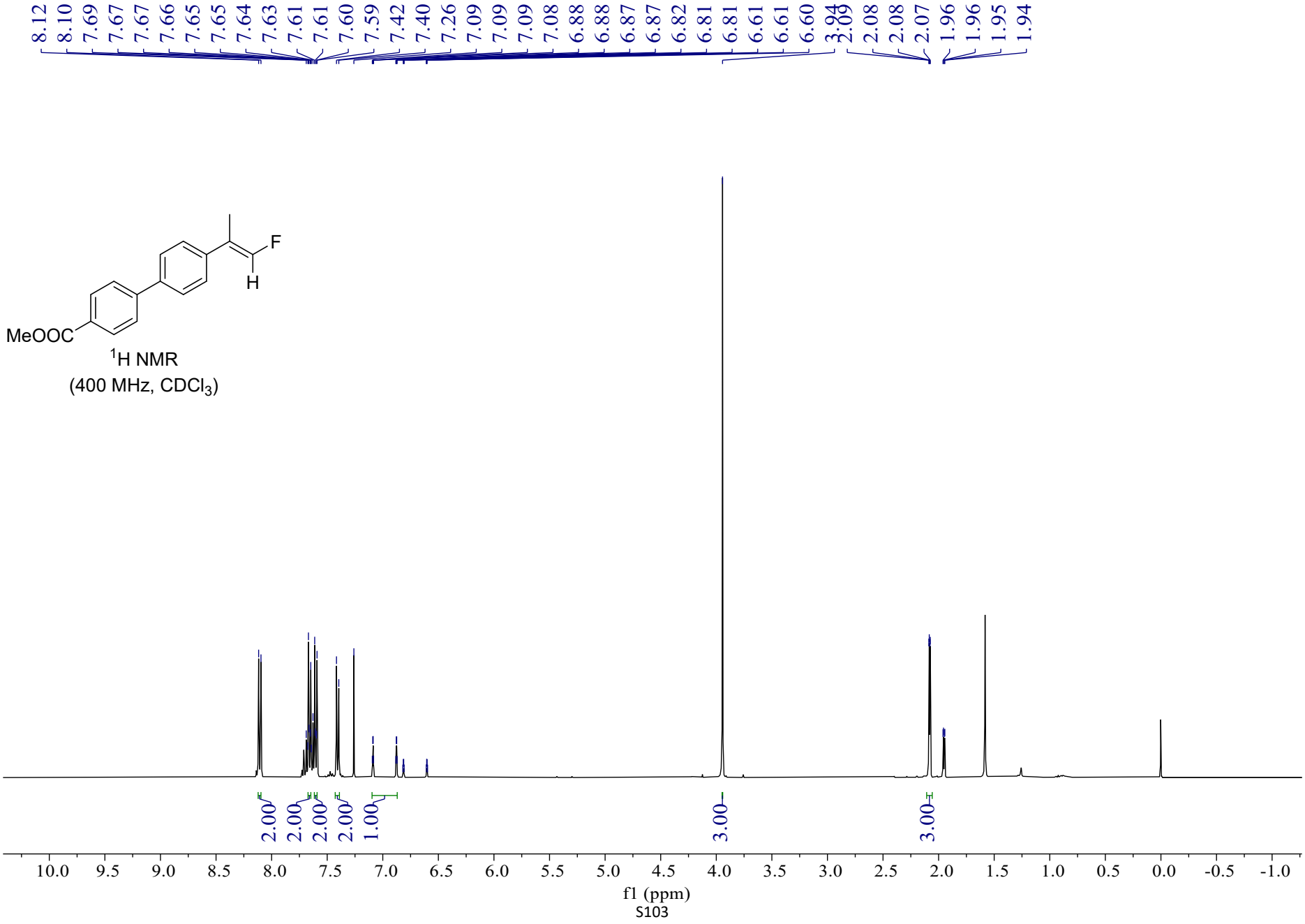
^{19}F NMR
(376 MHz, $CDCl_3$)

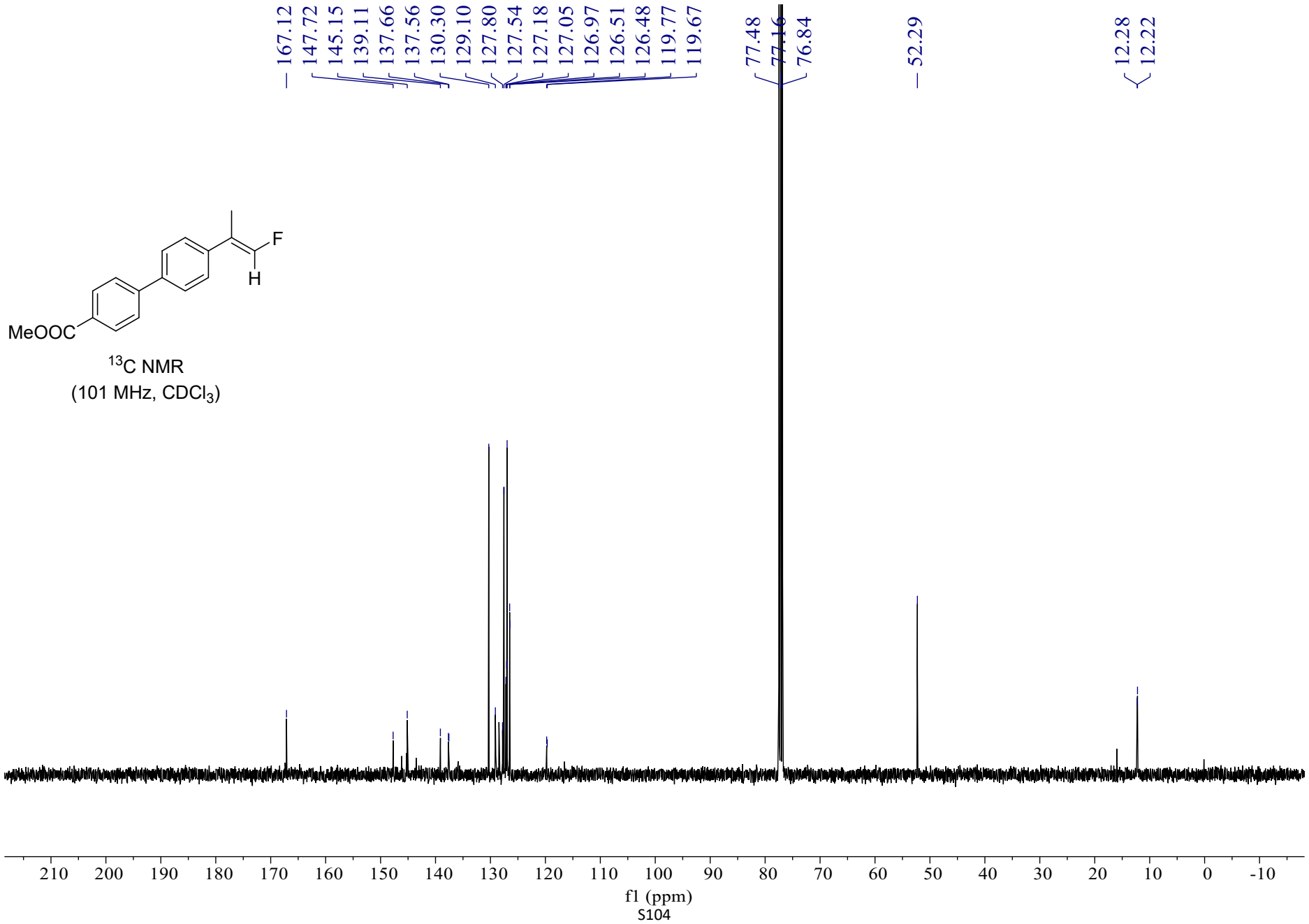


LX-1 #23 RT: 0.17 AV: 1 NL: 3.87E5
T: FTMS + p ESI Full ms [100.0000-1500.0000]

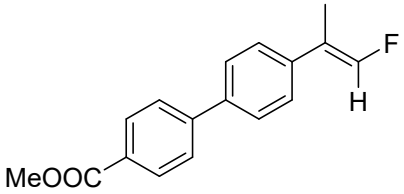


Peak M...	Display...	S Fit	RDB	Delta [p...	Theo....	Rank	Combin...	# Matc...	# Misse...	MS Cov...	Pattern...	MSMS...
227.1254	$C_{16}H_{16}F$	63.07655100152	8.50	10.44	227.12306	1	98.06	1	0	100	100	(Collection)

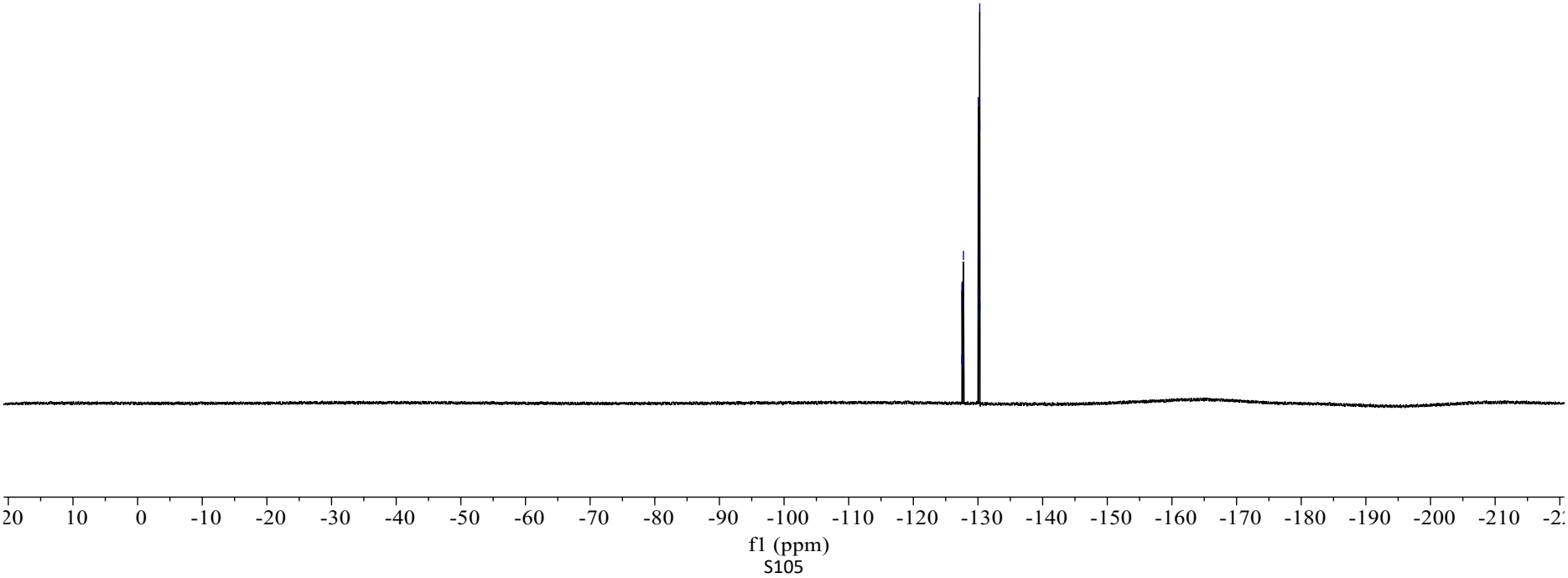

8.12
8.10
7.69
7.67
7.67
7.66
7.65
7.65
7.64
7.63
7.61
7.61
7.60
7.59
7.42
7.40
7.26
7.09
7.09
7.09
7.08
6.88
6.88
6.87
6.87
6.82
6.81
6.81
6.61
6.61
6.60
3.94
2.09
2.08
2.08
2.07
1.96
1.96
1.95
1.94
F
H
MeOOC
1H NMR
(400 MHz, CDCl3)
2.00
2.00
2.00
2.00
1.00
3.00
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


167.12
147.72
145.15
139.11
137.66
137.56
130.30
129.10
127.80
127.54
127.18
127.05
126.97
126.51
126.48
119.77
119.67
77.48
77.16
76.84
52.29
12.28
12.22
F
H
MeOOC
13C NMR
(101 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

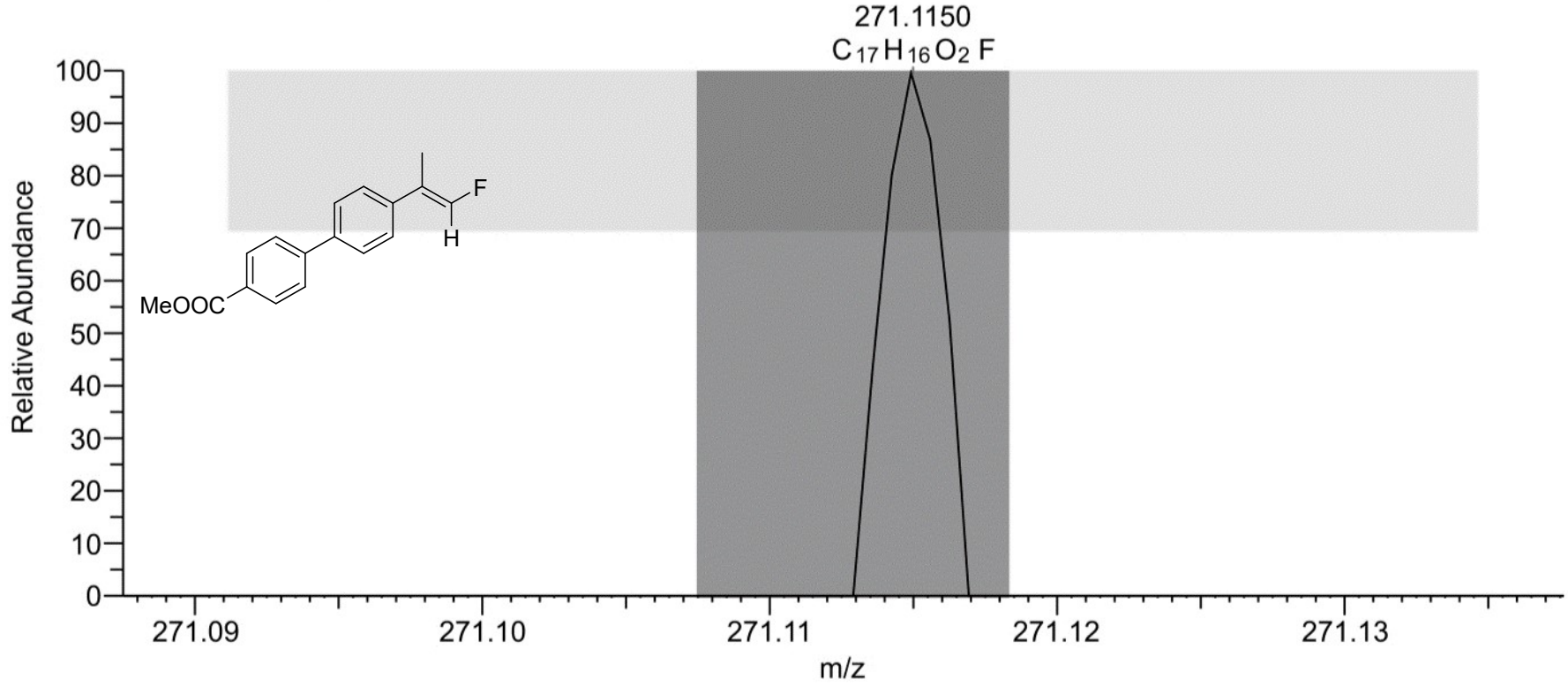
-127.52
-127.53
-127.54
-127.56
-127.74
-127.75
-127.77
-127.78
-130.04
-130.05
-130.06
-130.07
-130.26
-130.27
-130.28
-130.29



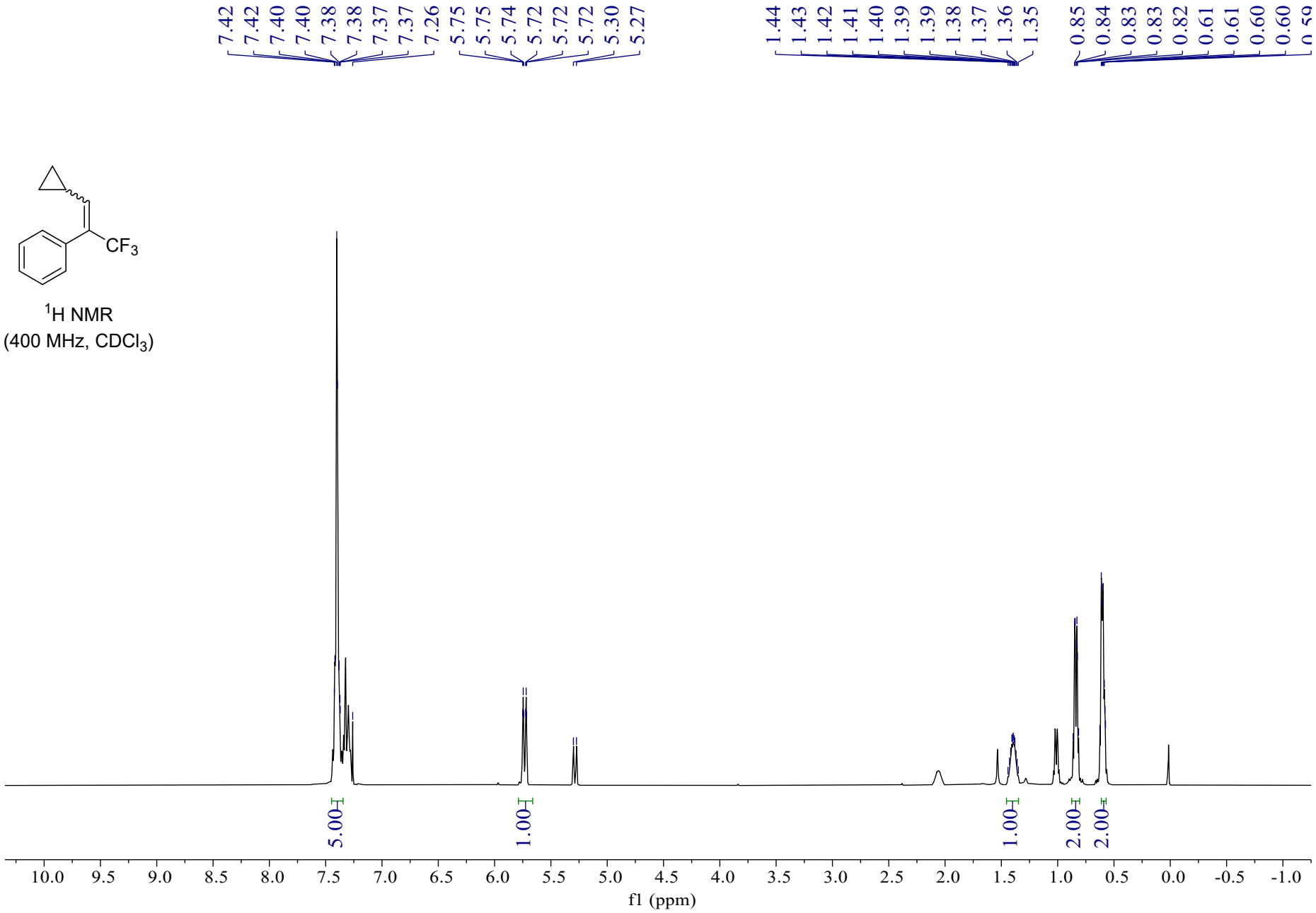
^{19}F NMR
(376 MHz, $CDCl_3$)

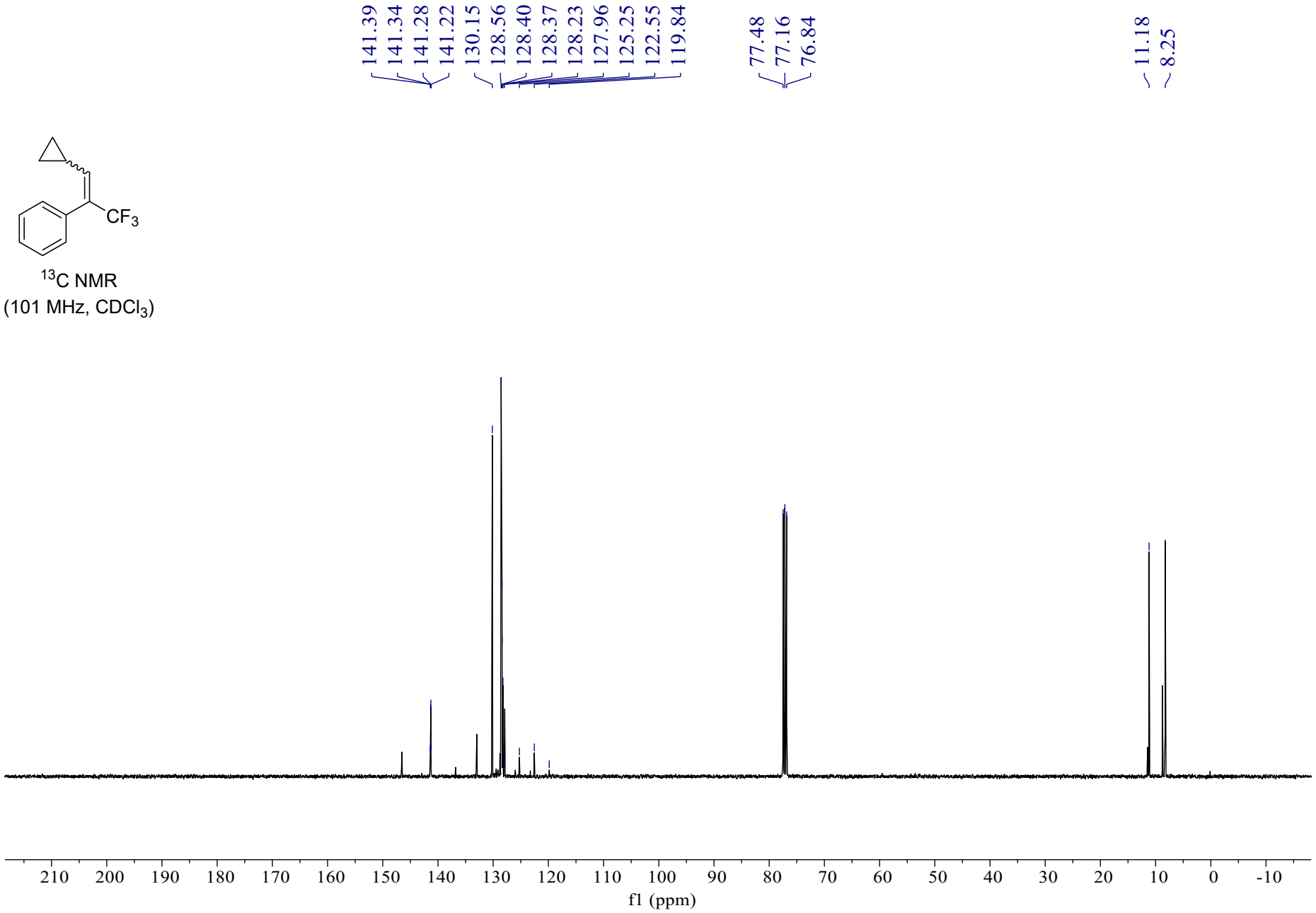


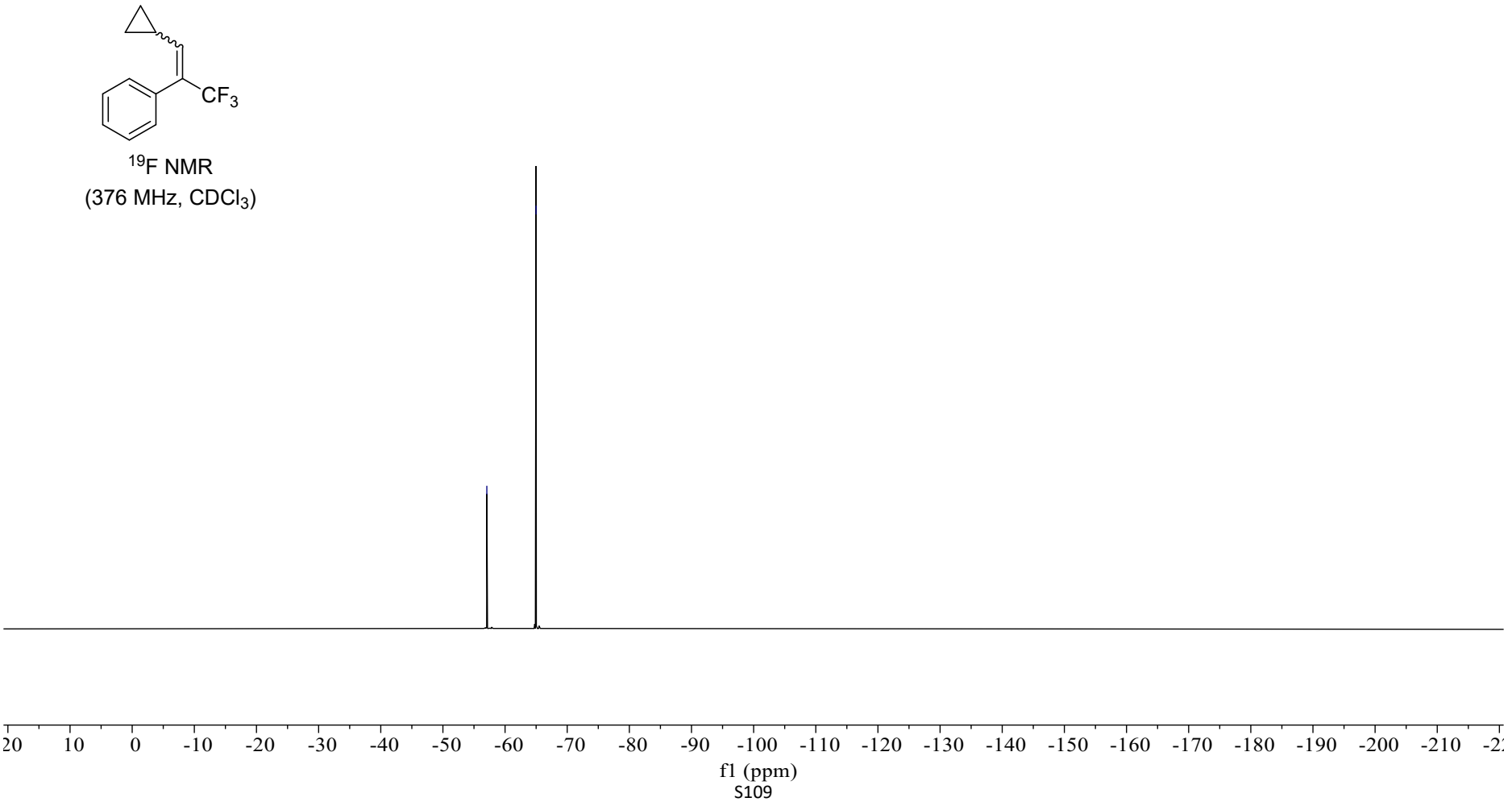
LX-2 #125 RT: 0.94 AV: 1 NL: 2.15E4
T: FTMS + p ESI Full ms [100.0000-1500.0000]

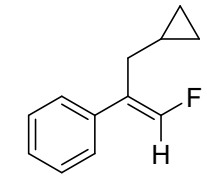


Peak M...	Display...	S Fit	RDB	Delta [p...	Theo....	Rank	Combin...	# Matc...	# Misse...	MS Cov...	Pattern...	MSMS...
271.1150	$C_{17}H_{16}O_2F$	72.5392 394954 232	9.50	7.77	271.11288	1	98.55	1	0	100	100	(Collection)

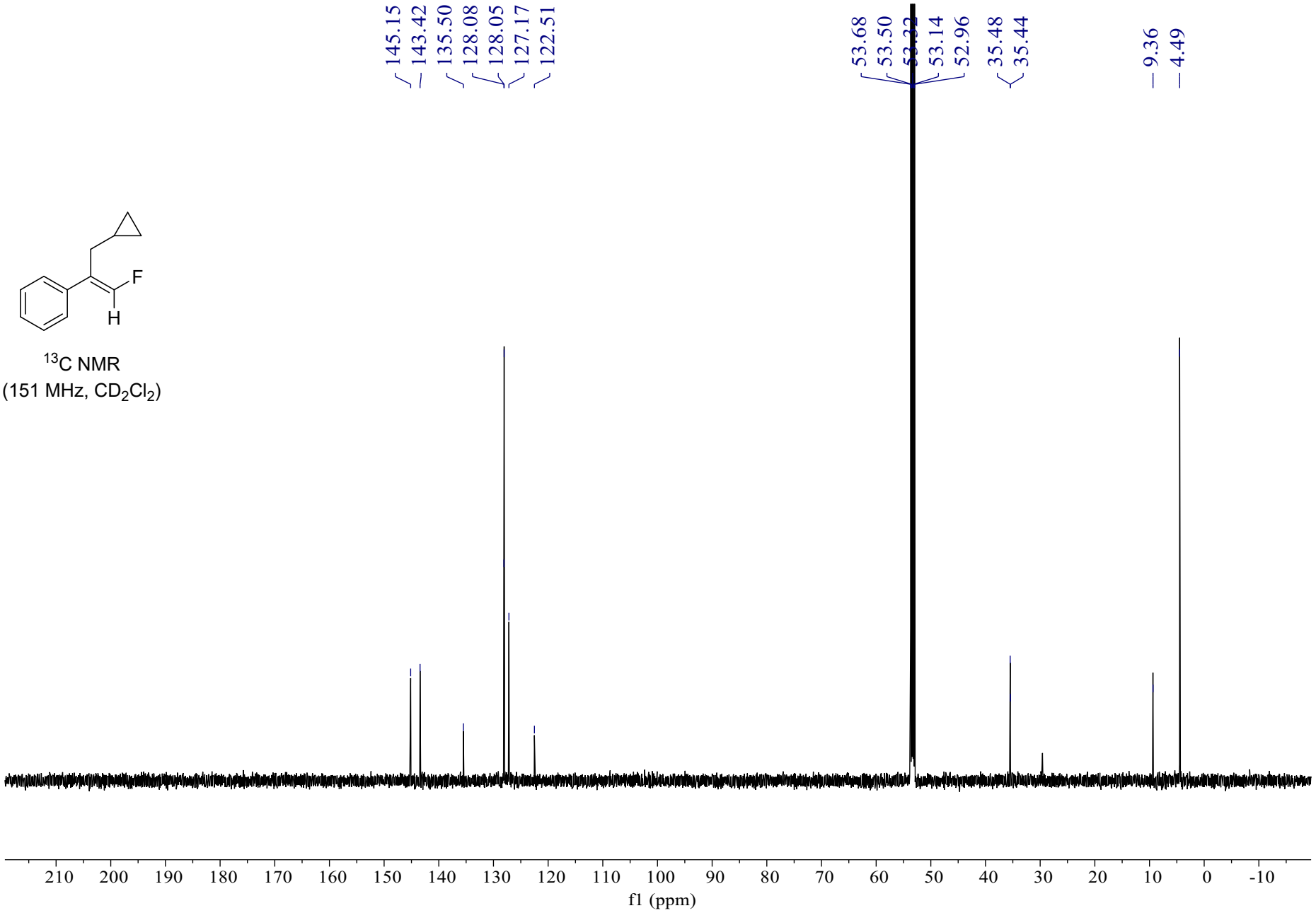

7.42
7.42
7.40
7.40
7.38
7.38
7.37
7.37
7.26
5.75
5.75
5.74
5.72
5.72
5.72
5.30
5.27
1.44
1.43
1.42
1.41
1.40
1.39
1.39
1.38
1.37
1.36
1.35
0.85
0.84
0.83
0.83
0.82
0.61
0.61
0.60
0.60
CF3
1H NMR
(400 MHz, CDCl3)
5.00
1.00
1.00
2.00
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


141.39
141.34
141.28
141.22
130.15
128.56
128.40
128.37
128.23
127.96
125.25
122.55
119.84
77.48
77.16
76.84
11.18
8.25
CF3
13C NMR
(101 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

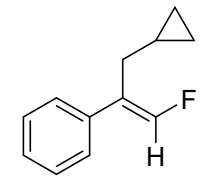

-57.07
-64.99
CF3
19F NMR
(376 MHz, CDCl3)
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)



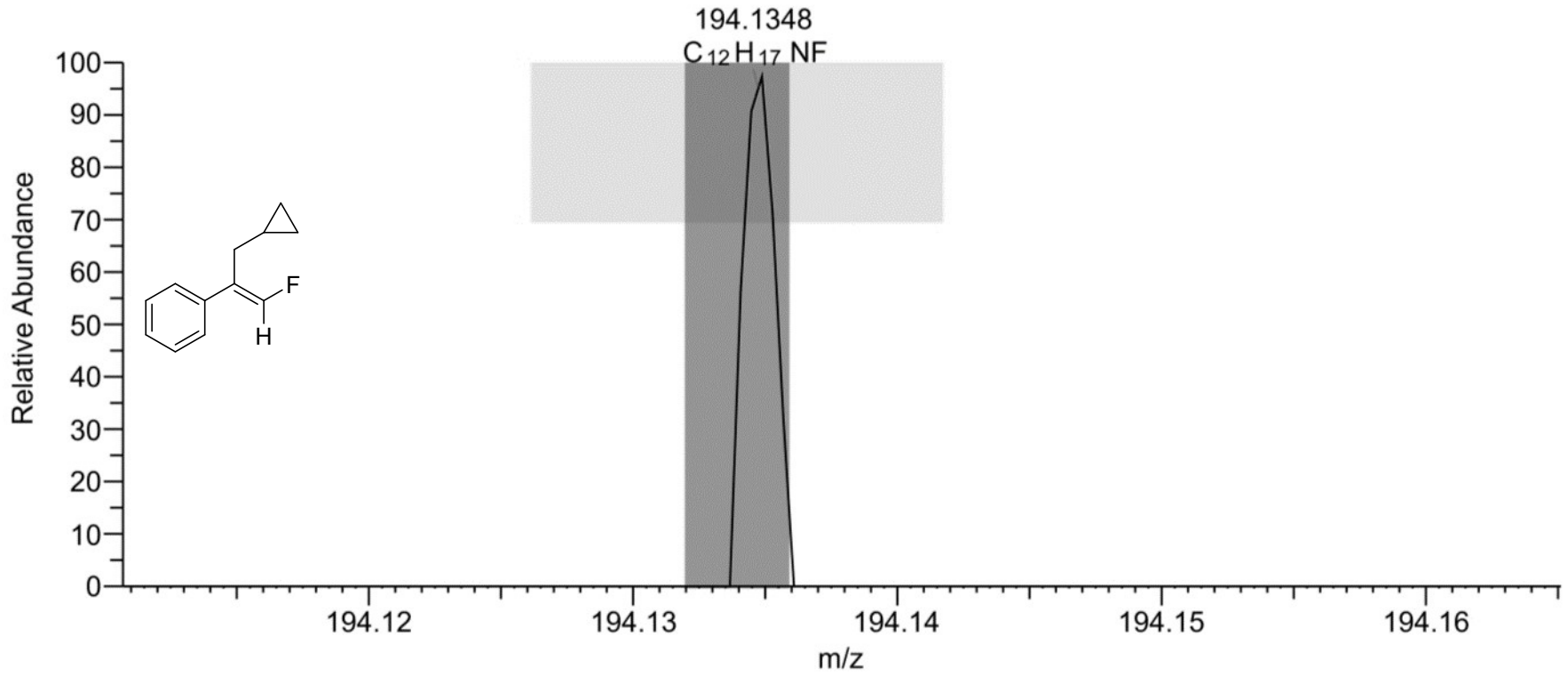
^{1}H NMR
(400 MHz, $CDCl_3$)



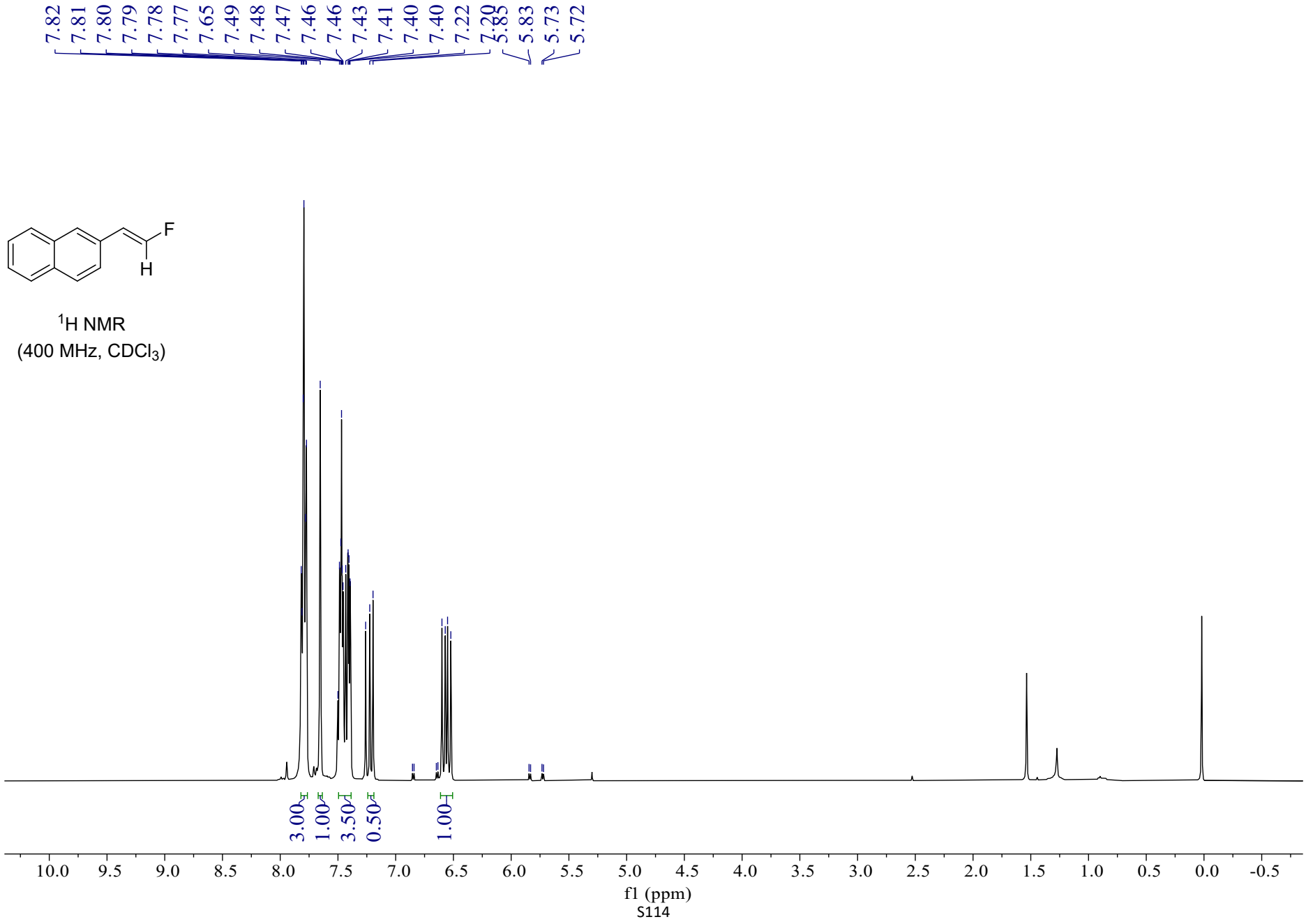
^{13}C NMR
(151 MHz, CD_2Cl_2)

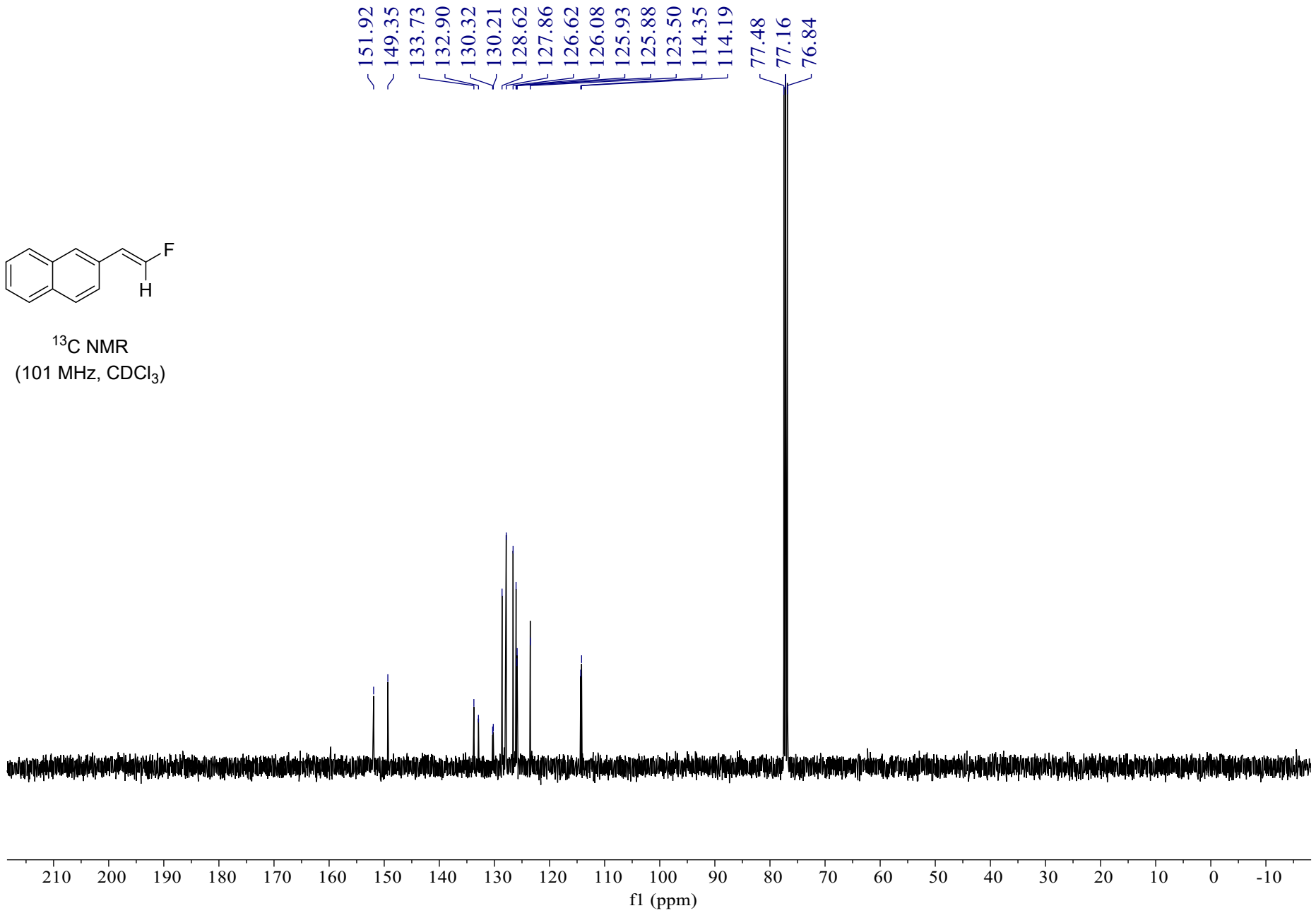


^{19}F NMR
(376 MHz, $CDCl_3$)

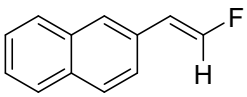


Peak M...	Display...	S Fit	RDB	Delta [p...	Theo....	Rank	Combin...	# Matc...	# Misse...	MS Cov...	Pattern...	MSMS...
194.1348	$C_{12}H_{17}NF$	69.8931630229455	4.50	4.26	194.13395	1	98.42	1	0	100	100	(Collection)


7.82
7.81
7.80
7.79
7.78
7.77
7.65
7.49
7.48
7.47
7.46
7.46
7.43
7.41
7.40
7.40
7.22
7.20
5.85
5.83
5.73
5.72
F
H
1H NMR
(400 MHz, CDCl3)
3.00
1.00
3.50
0.50
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)



^{13}C NMR
(101 MHz, $CDCl_3$)



^{19}F NMR
(376 MHz, $CDCl_3$)

Mass Spectrum SmartFormula Report

Analysis Info

Acquisition D 2023-04-11 15:46:33

Analysis Name D:\LXMS\0411_RA1_01_23192.d

Method LC_NO UV_P50-1500_6MIN.m

Operator Demo User

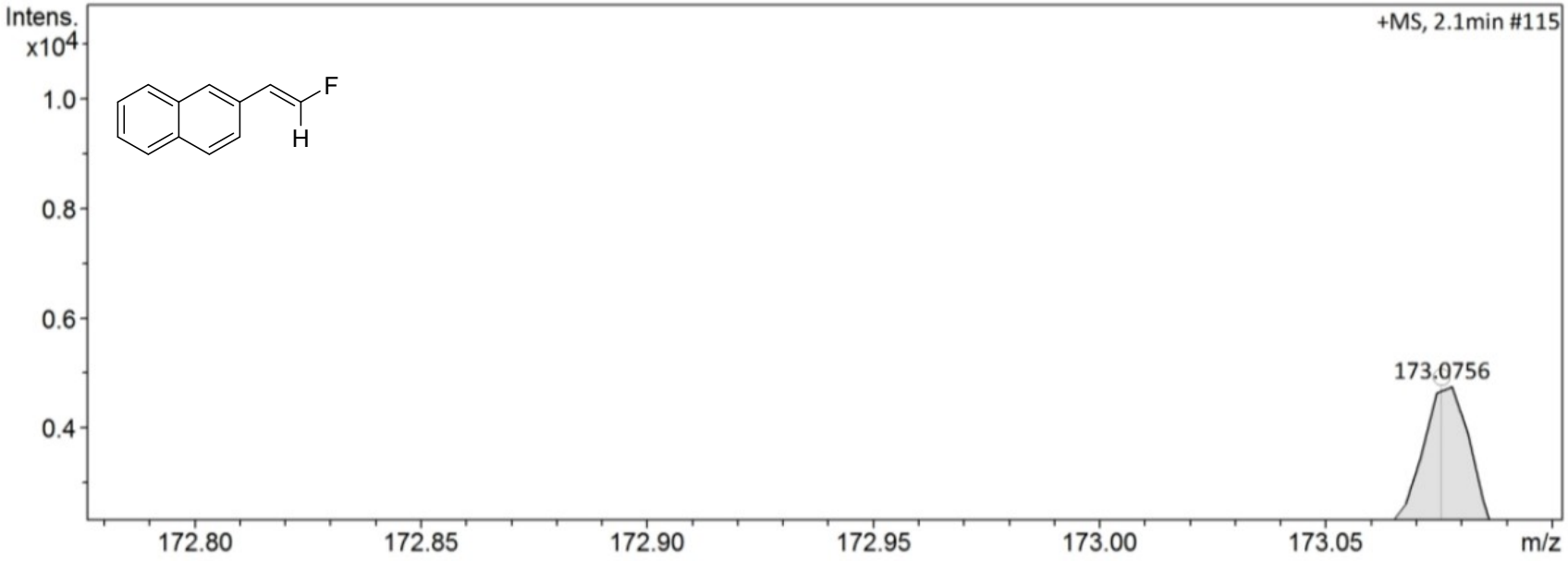
Sample Name 0411

Instrumen compact 8255754.2017 6

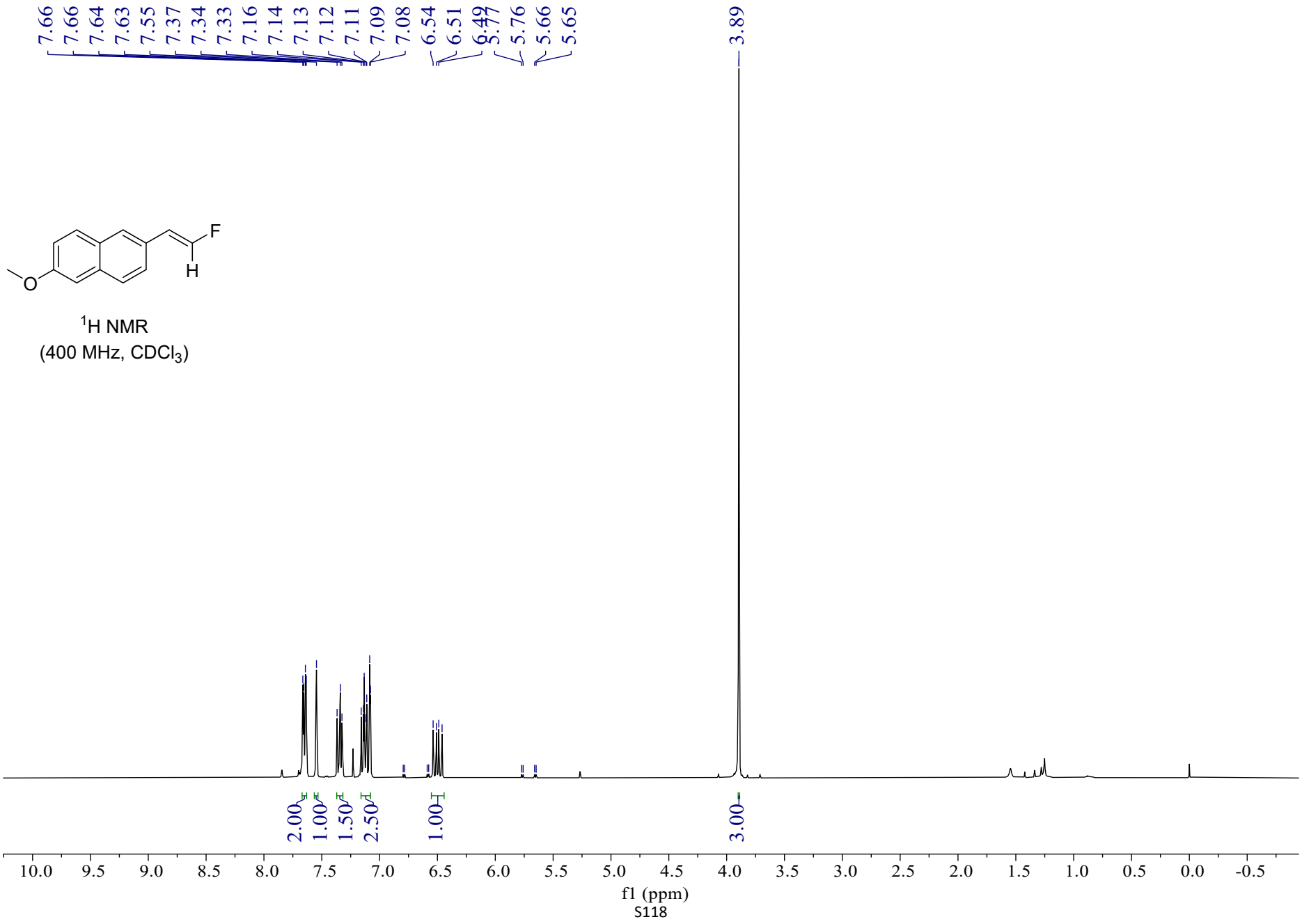
Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min

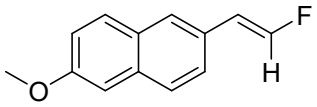


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
173.0756	1	C12H10F	173.0761	2.9	451.8	1	100.00	7.5	even	ok

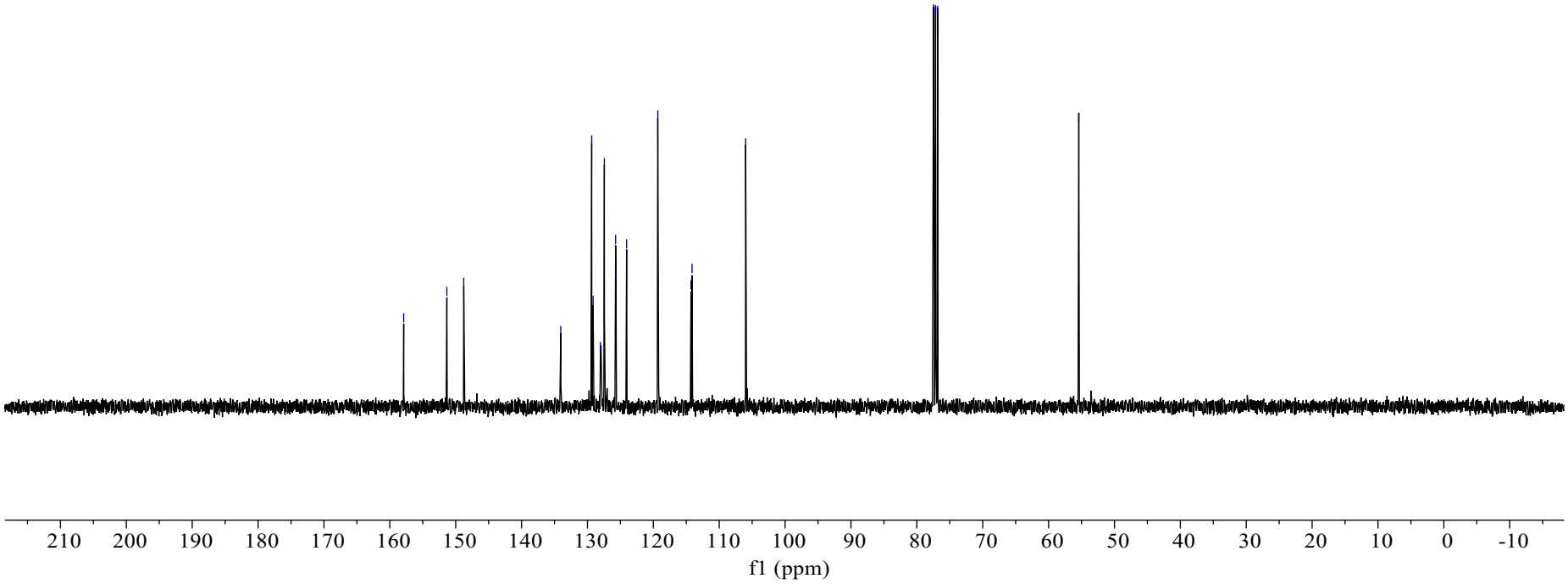


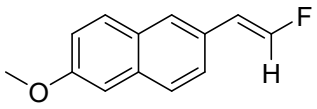
^{1}H NMR
(400 MHz, $CDCl_3$)

157.89
151.34
148.78
134.05
129.36
129.14
128.04
127.92
127.44
125.72
125.68
124.06
119.33
114.29
114.12
105.98
77.48
77.16
76.84
55.42



^{13}C NMR
(101 MHz, $CDCl_3$)





^{19}F NMR
(565 MHz, $CDCl_3$)

Mass Spectrum SmartFormula Report

Analysis Info

Acquisition D 2023-01-09 8:54:17

Analysis Name D:\LXMS\0106_RA4_01_20505.d

Method LC_NO UV_P50-1500_6MIN.m

Operator Demo User

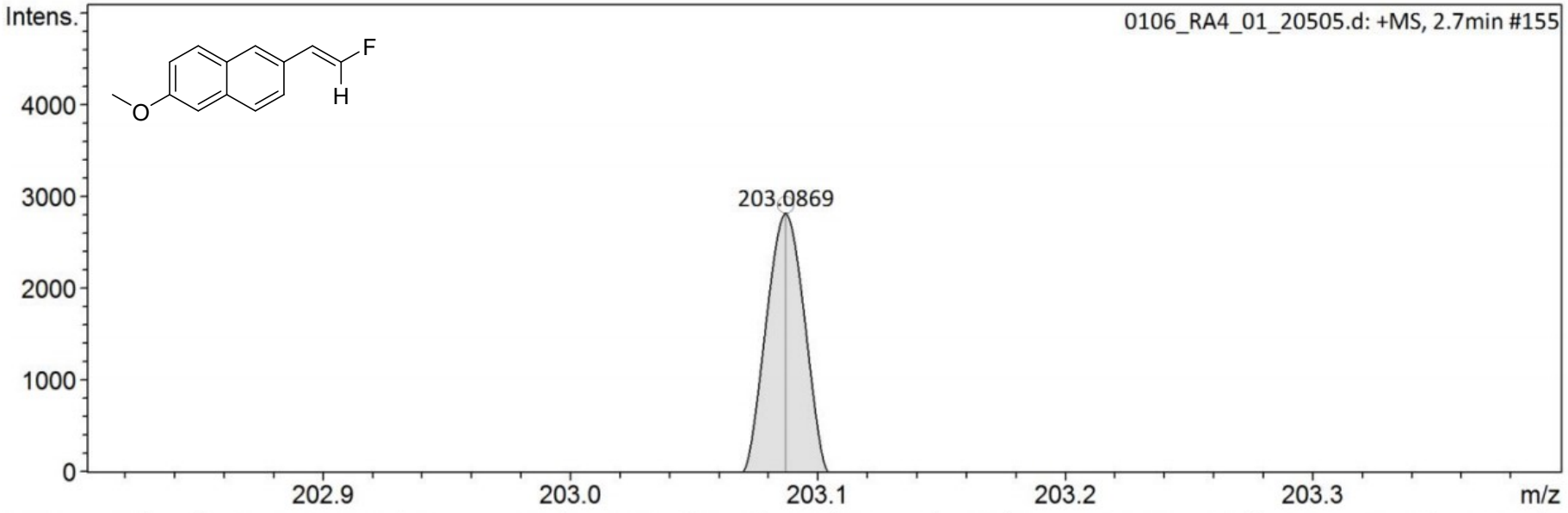
Sample Name 0106

Instrumen compact 8255754.2017 6

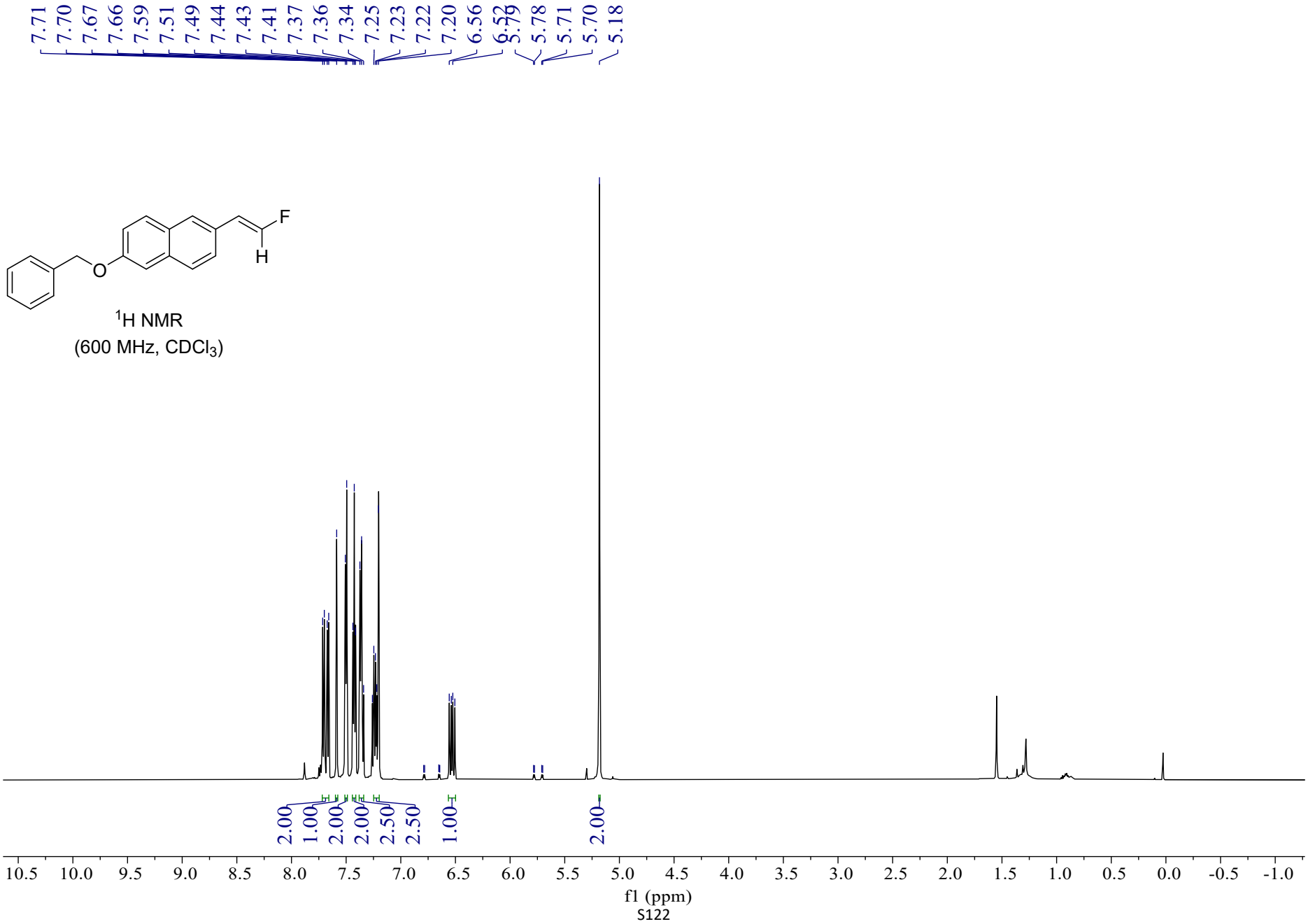
Comment

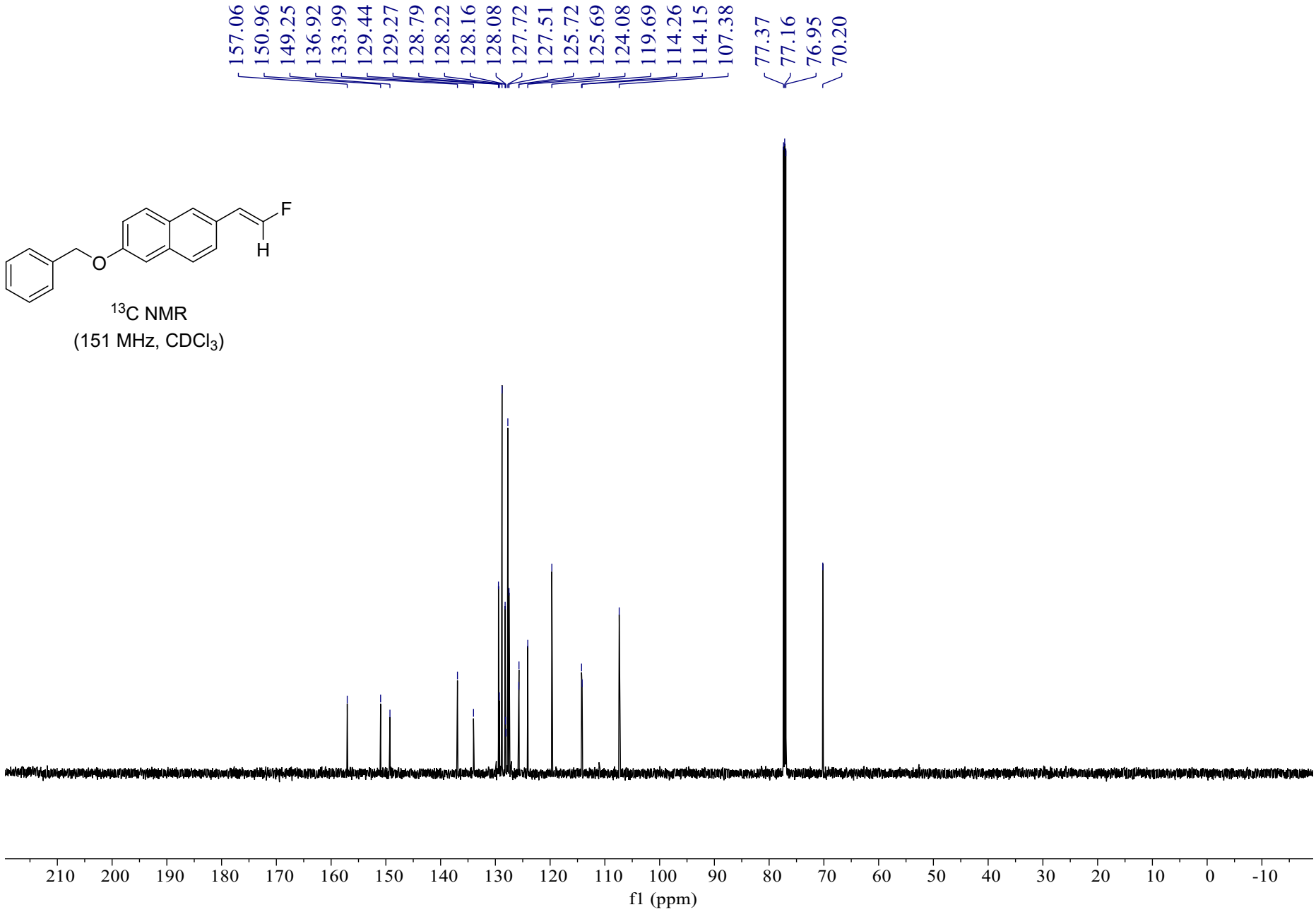
Acquisition Paramet

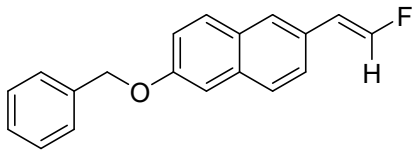
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
203.0869	1	C13H12FO	203.0867	-0.9	102.7	1	100.00	7.5	even		ok


7.71
7.70
7.67
7.66
7.59
7.51
7.49
7.44
7.43
7.41
7.37
7.36
7.34
7.25
7.23
7.22
7.20
6.56
6.52
5.79
5.78
5.71
5.70
5.18
F
H
O
1H NMR
(600 MHz, CDCl3)
2.00
1.00
2.00
2.00
2.50
2.50
1.00
2.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


157.06
150.96
149.25
136.92
133.99
129.44
129.27
128.79
128.22
128.16
128.08
127.72
127.51
125.72
125.69
124.08
119.69
114.26
114.15
107.38
77.37
77.16
76.95
70.20
F
H
O
13C NMR
(151 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



^{19}F NMR

(565 MHz, $CDCl_3$)

Mass Spectrum SmartFormula Report

Analysis Info

Acquisition D 2023-03-10 17:57:12

Analysis Name D:\LXMS\0306_BD3_01_22075.d

Method LC_NO UV_P50-1500_10MIN.m

Operator Demo User

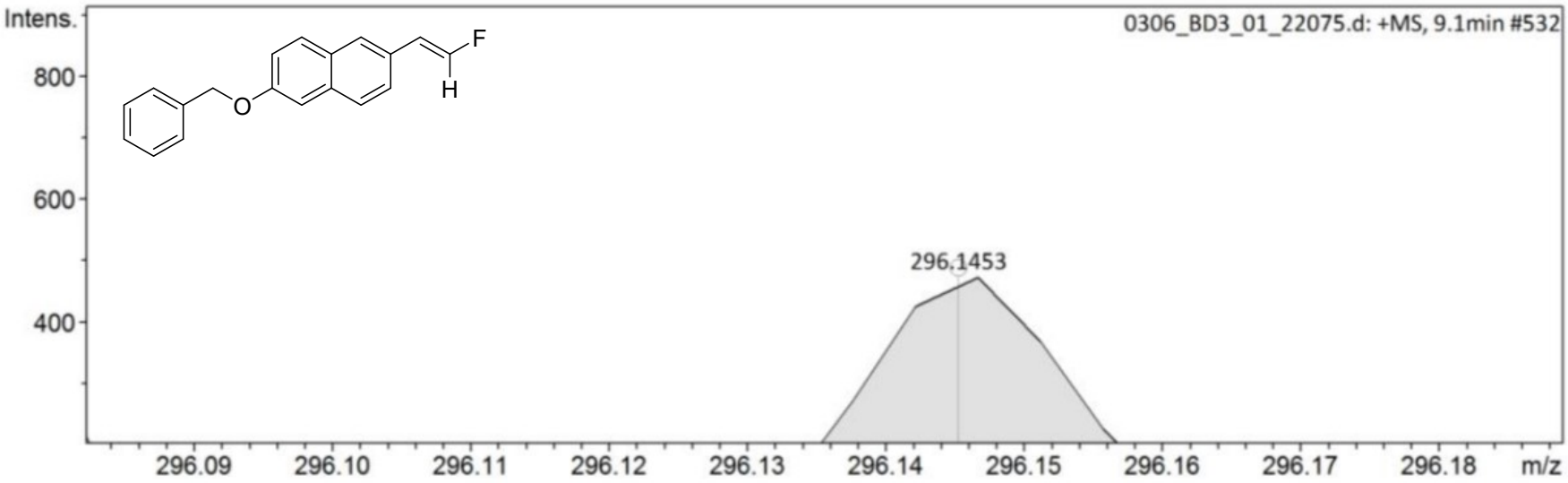
Sample Name 0306

Instrumen compact 8255754.2017 6

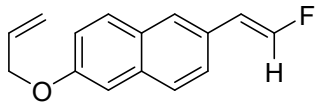
Comment

Acquisition Paramet

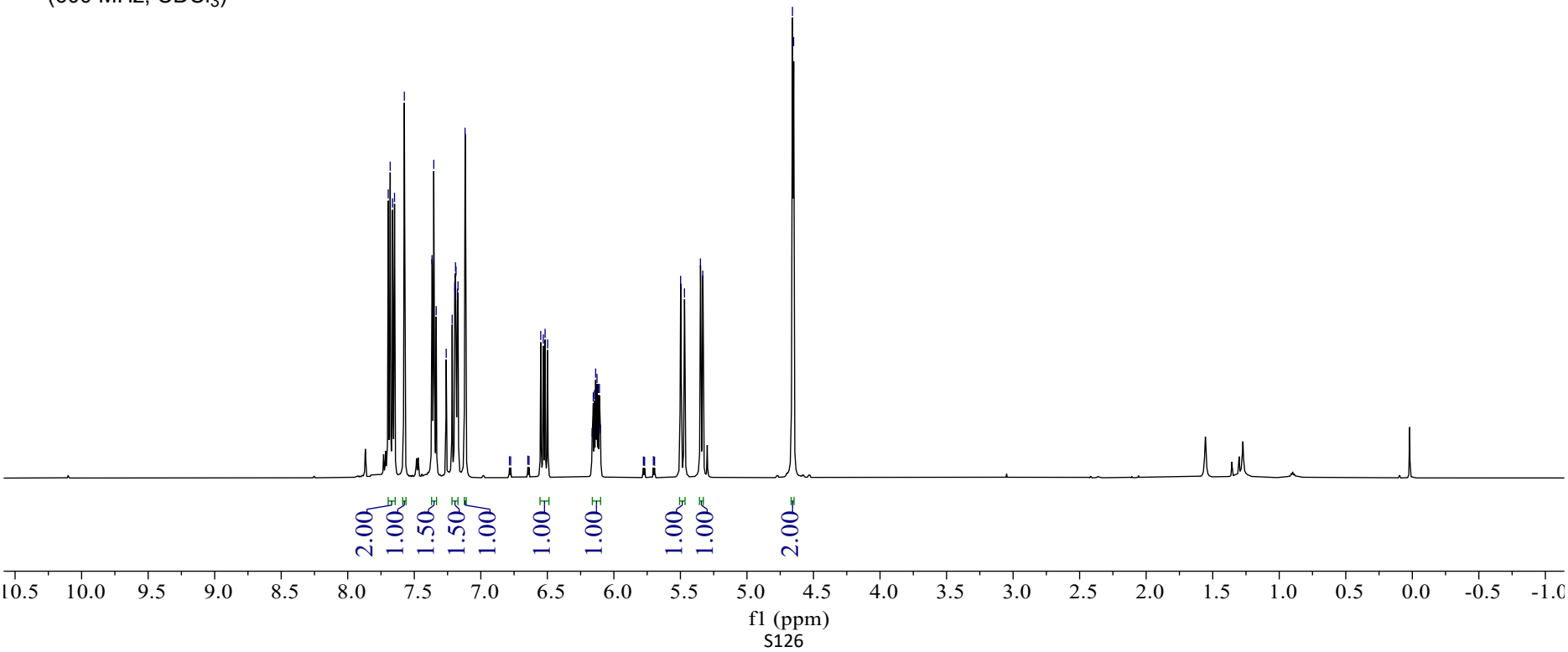
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min

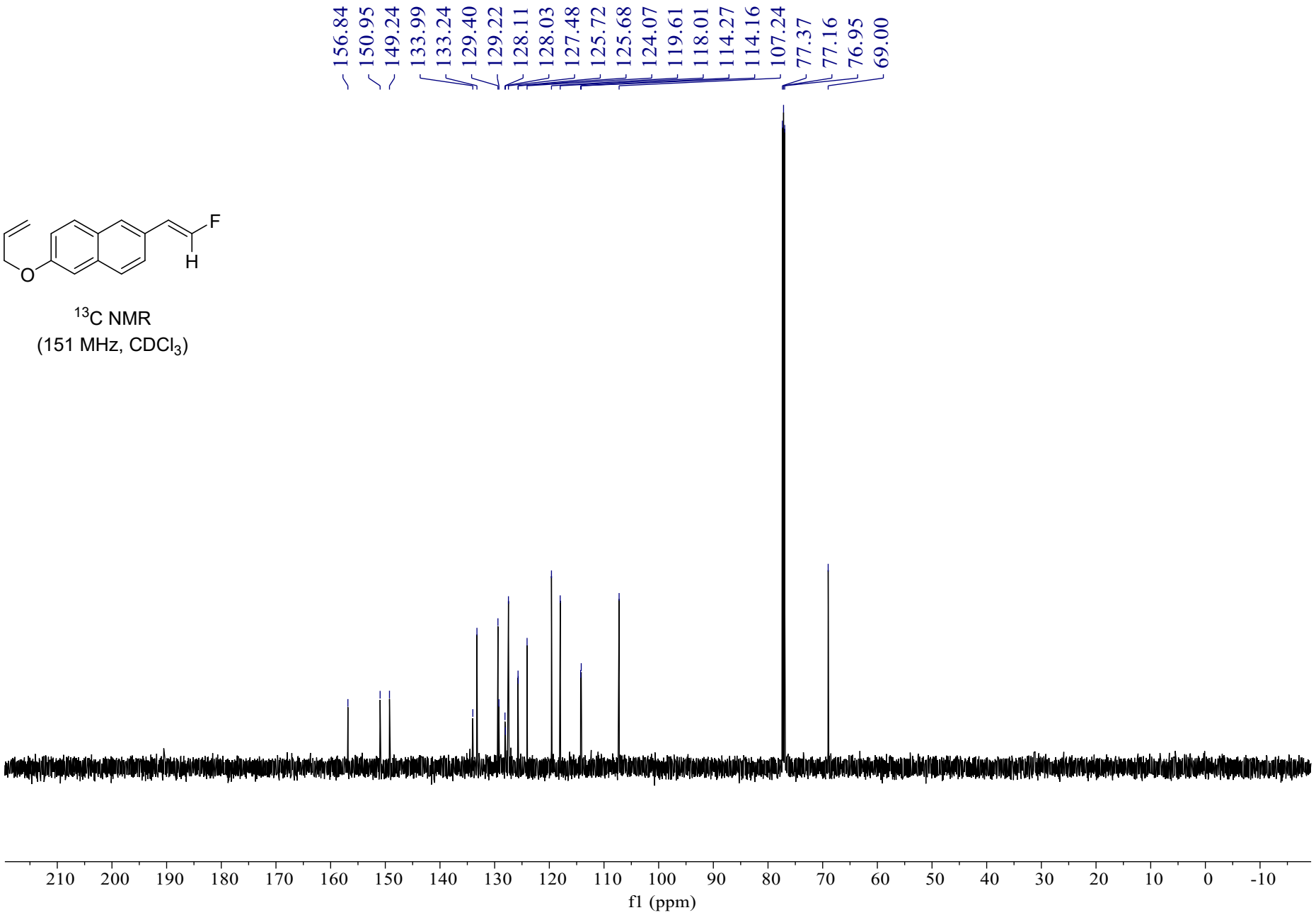


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
296.1453	1	C19H19FNO	296.1445	-2.5	n.a.	1	100.00	10.5	even		ok



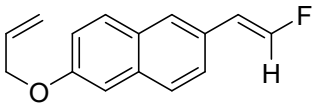
^{1}H NMR
(600 MHz, $CDCl_3$)



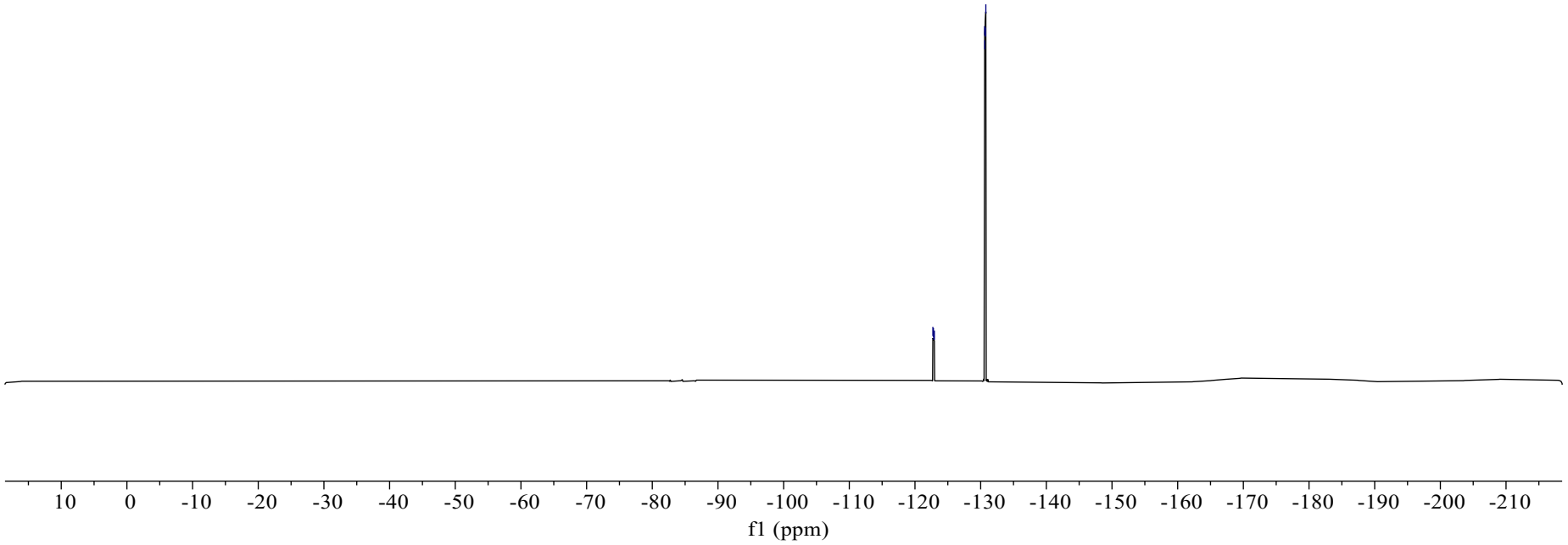


^{13}C NMR
(151 MHz, $CDCl_3$)

-122.72
-122.80
-122.87
-122.95
-130.61
-130.64
-130.76
-130.79



^{19}F NMR
(565 MHz, $CDCl_3$)



Mass Spectrum SmartFormula Report

Analysis Info

Acquisition D 2023-01-09 10:32:19

Analysis Name D:\LXMS\0106_RC1_01_20518.d

Method LC_NO UV_P50-1500_6MIN.m

Operator Demo User

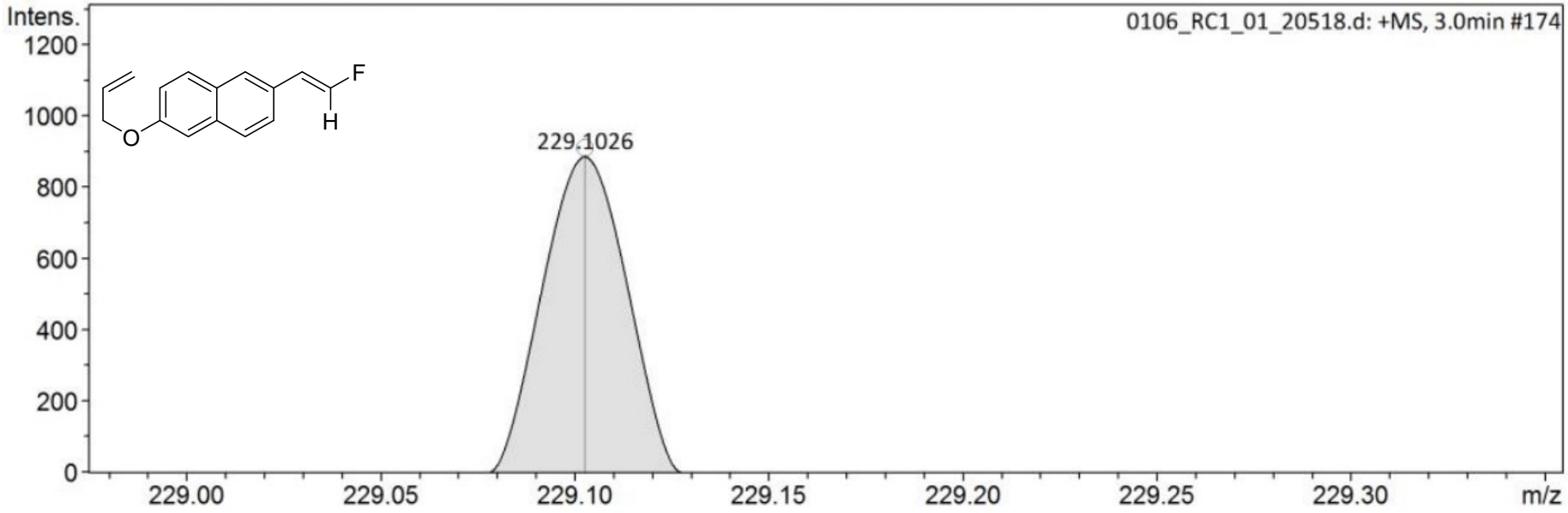
Sample Name 0106

Instrumen compact 8255754.2017 6

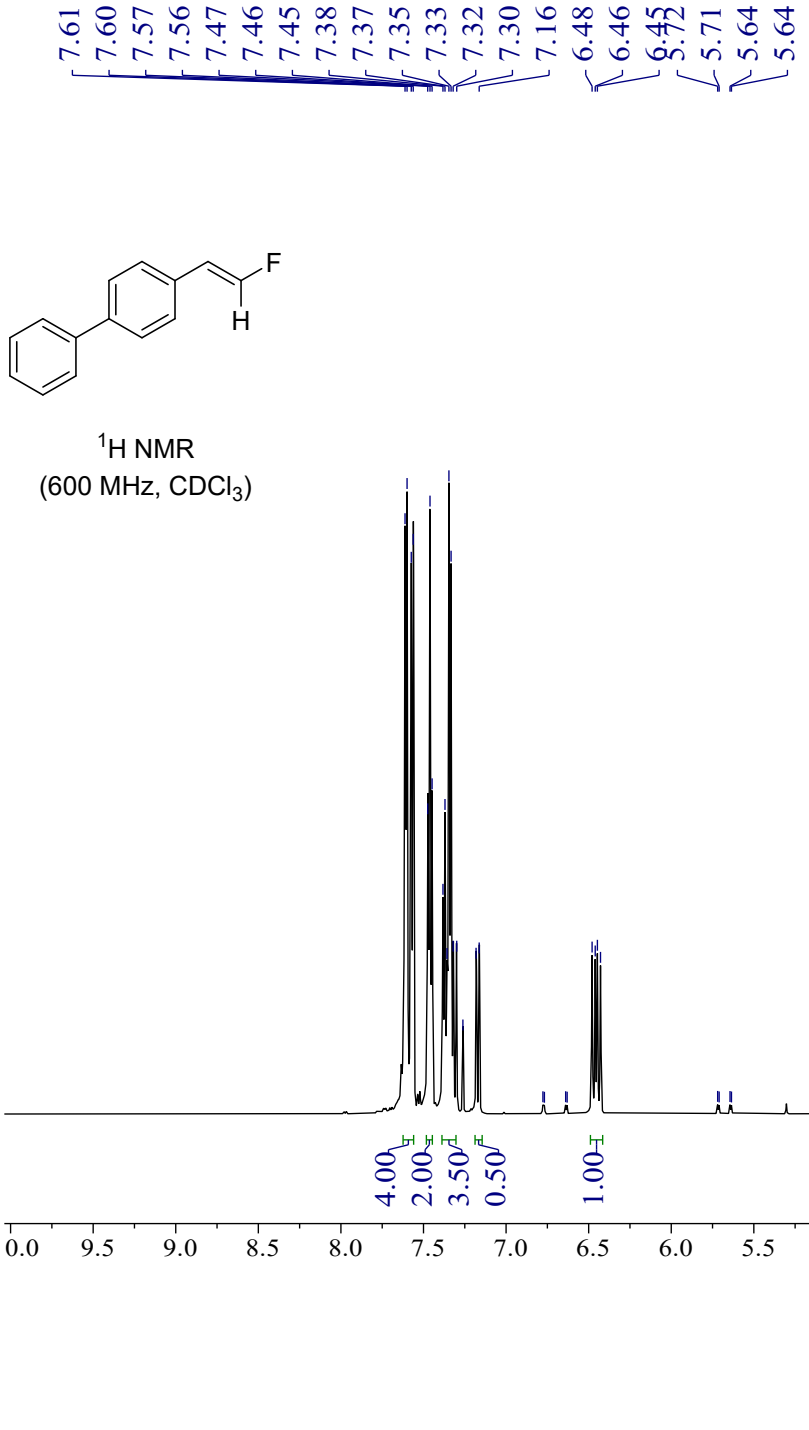
Comment

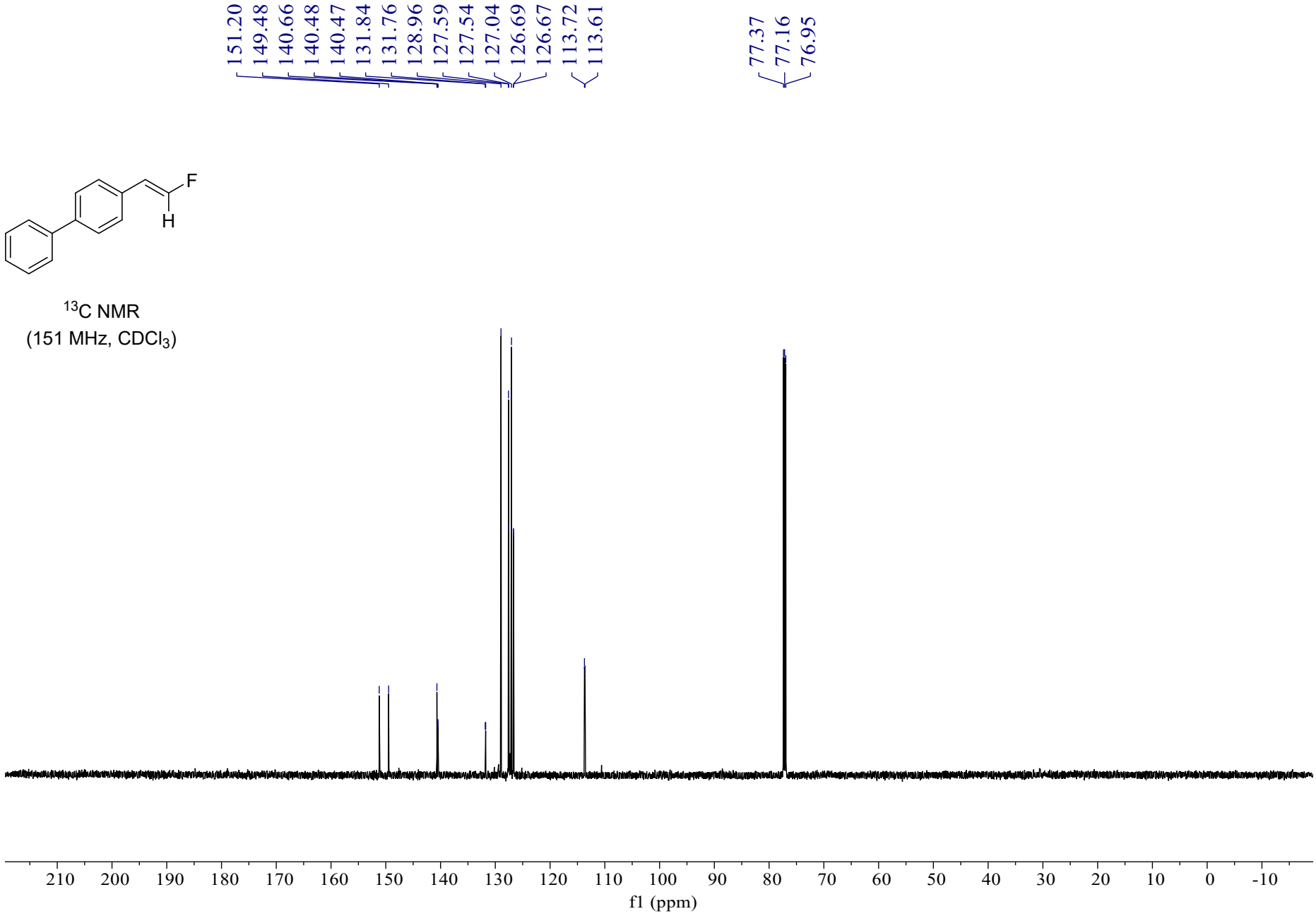
Acquisition Paramet

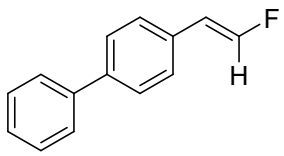
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
229.1026	1	C15H14FO	229.1023	-1.2	n.a.	1	100.00	8.5	even		ok


7.61
7.60
7.57
7.56
7.47
7.46
7.45
7.38
7.37
7.35
7.33
7.32
7.30
7.16
6.48
6.46
6.45
5.72
5.71
5.64
5.64
F
H
1H NMR
(600 MHz, CDCl3)
4.00
2.00
3.50
0.50
1.00
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


151.20
149.48
140.66
140.48
140.47
131.84
131.76
128.96
127.59
127.54
127.04
126.69
126.67
113.72
113.61
77.37
77.16
76.95
F
H
13C NMR
(151 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



^{19}F NMR
(376 MHz, $CDCl_3$)

Mass Spectrum SmartFormula Report

Analysis Info

Acquisition D 2023-01-09 9:01:53

Analysis Name D:\LXMS\0106_RA5_01_20506.d

Method LC_NO UV_P50-1500_6MIN.m

Operator Demo User

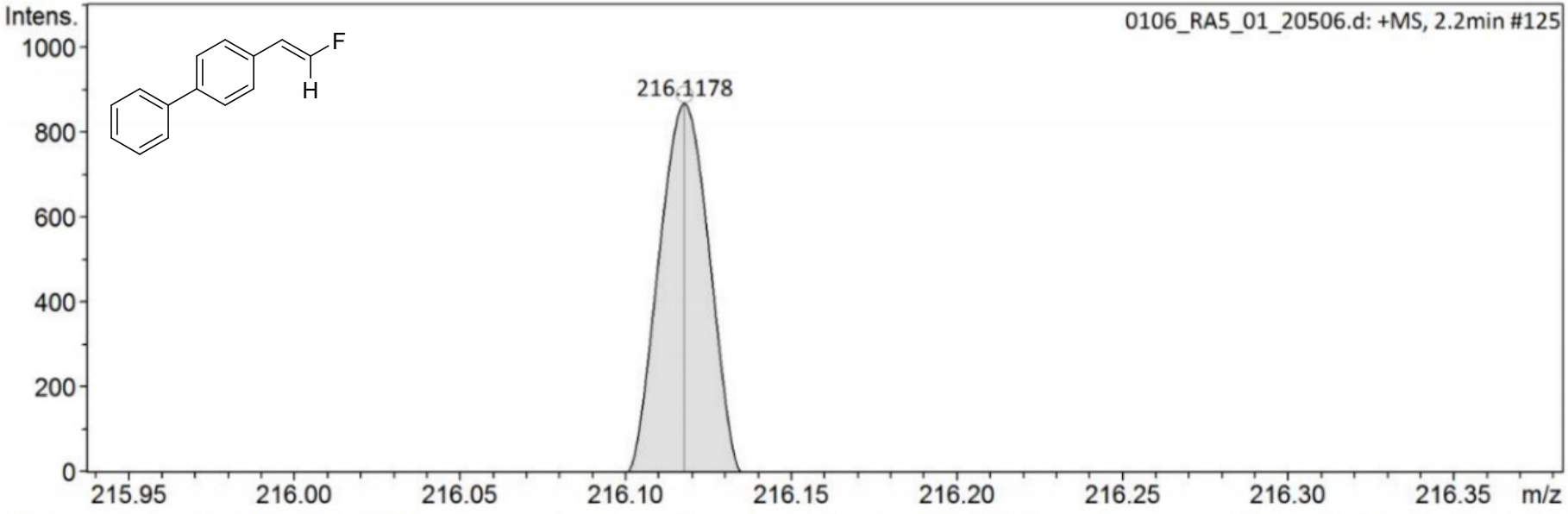
Sample Name 0106

Instrumen compact 8255754.2017 6

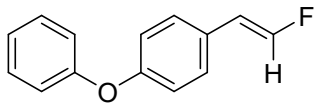
Comment

Acquisition Paramet

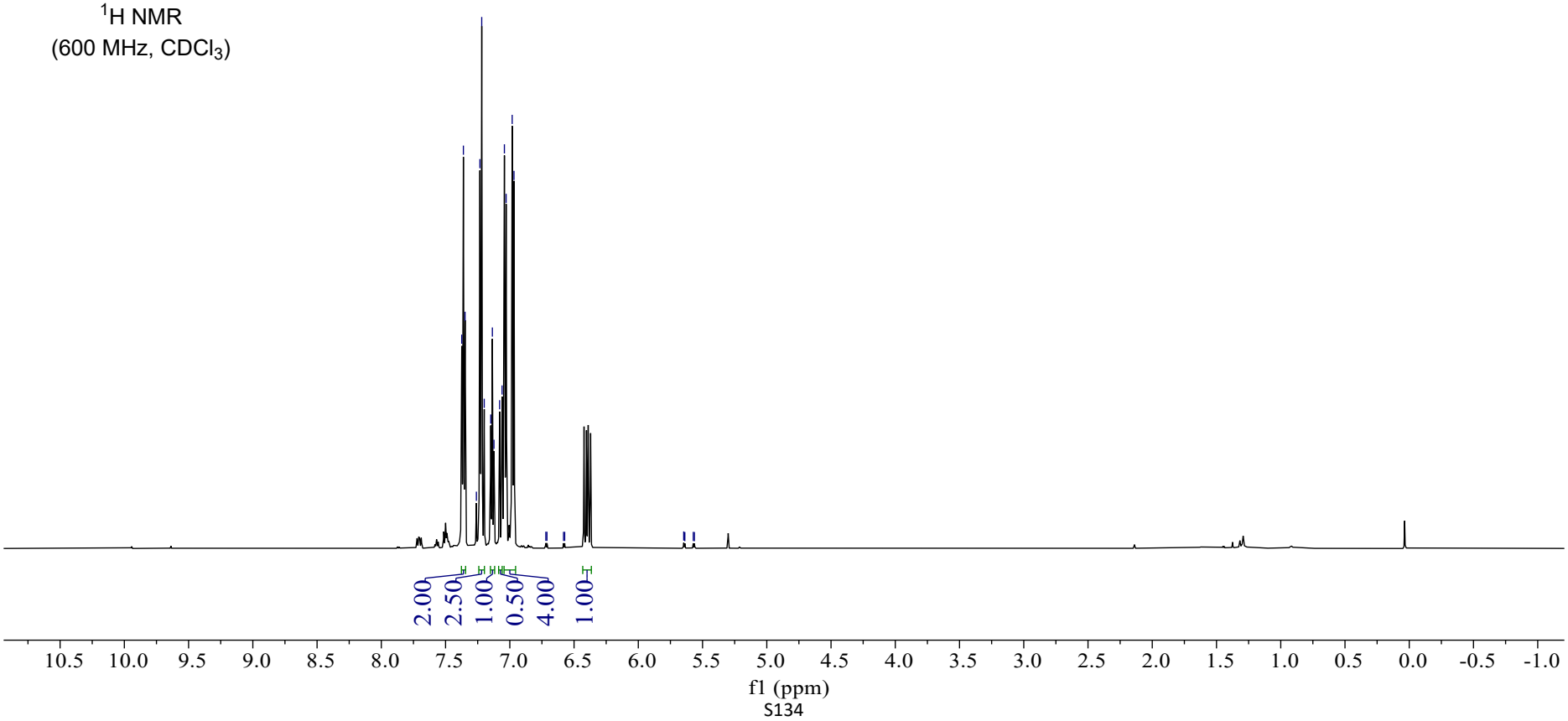
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
216.1178	1	C14H15FN	216.1183	2.4	n.a.	1	100.00	7.5	even		ok

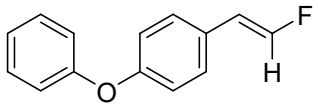


^{1}H NMR
(600 MHz, $CDCl_3$)

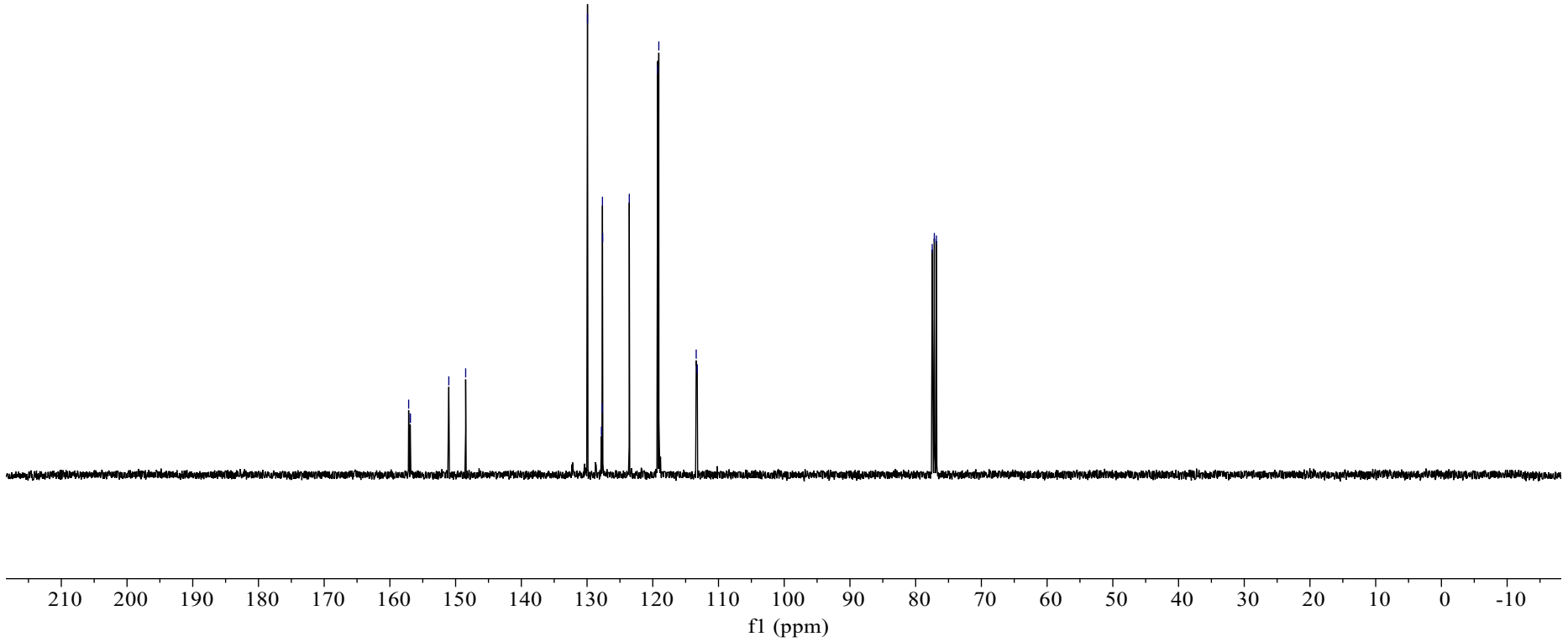


157.15
156.91
156.89
151.04
148.47
129.93
127.82
127.70
127.66
127.63
123.58
119.25
119.08
113.39
113.23

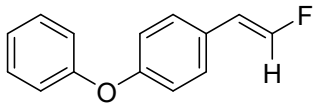
77.48
77.16
76.84



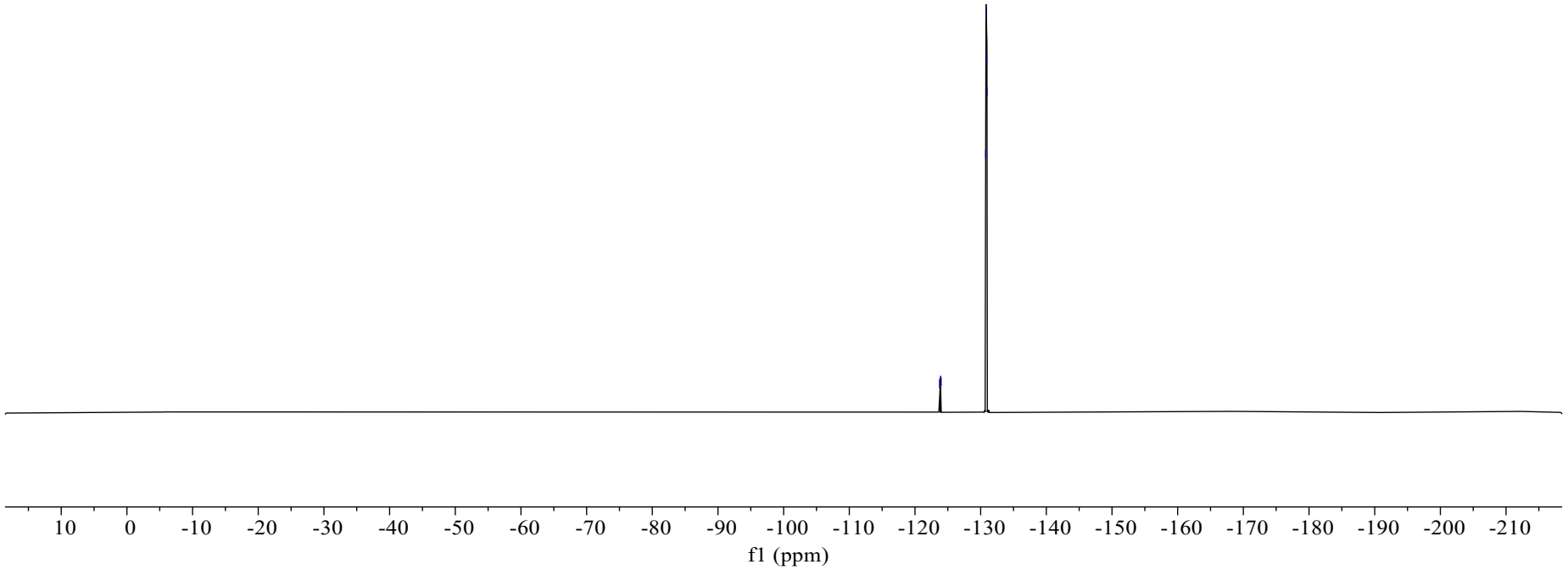
^{13}C NMR
(101 MHz, $CDCl_3$)



-123.75
-123.83
-123.90
-123.98
-130.77
-130.81
-130.92
-130.96



^{19}F NMR
(565 MHz, $CDCl_3$)



Mass Spectrum SmartFormula Report

Analysis Info

Acquisition D 2023-01-09 9:54:58

Analysis Name D:\LXMS\0106_RB4_01_20513.d

Method LC_NO UV_P50-1500_6MIN.m

Operator Demo User

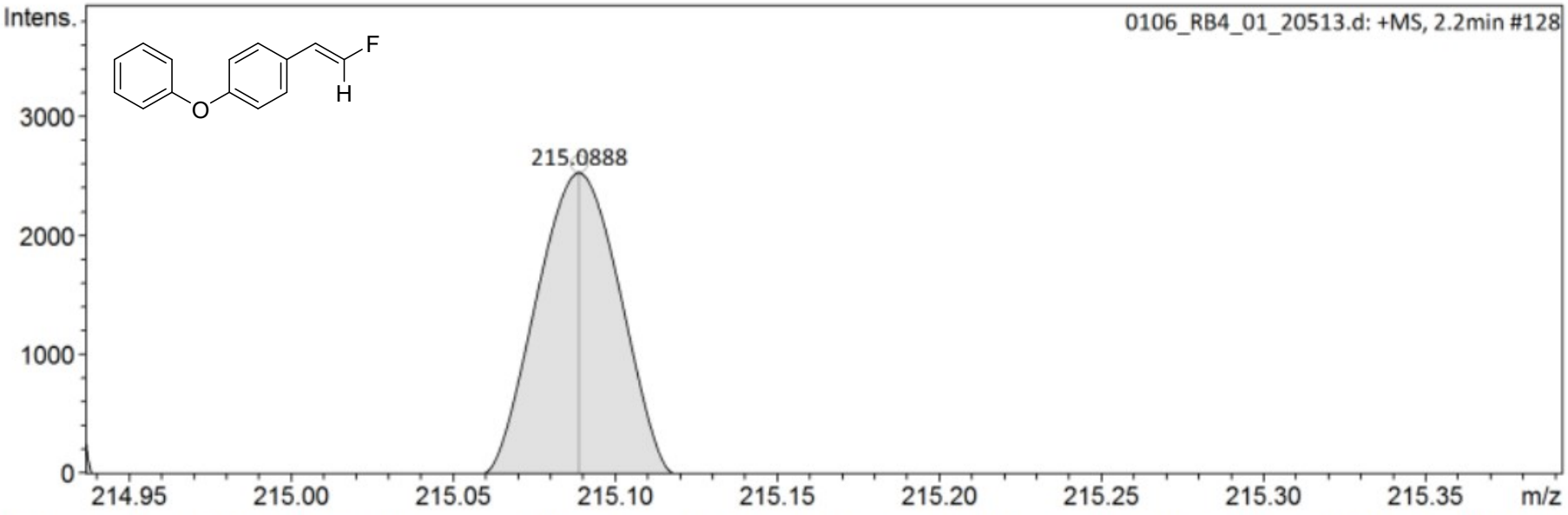
Sample Name 0106

Instrumen compact 8255754.2017 6

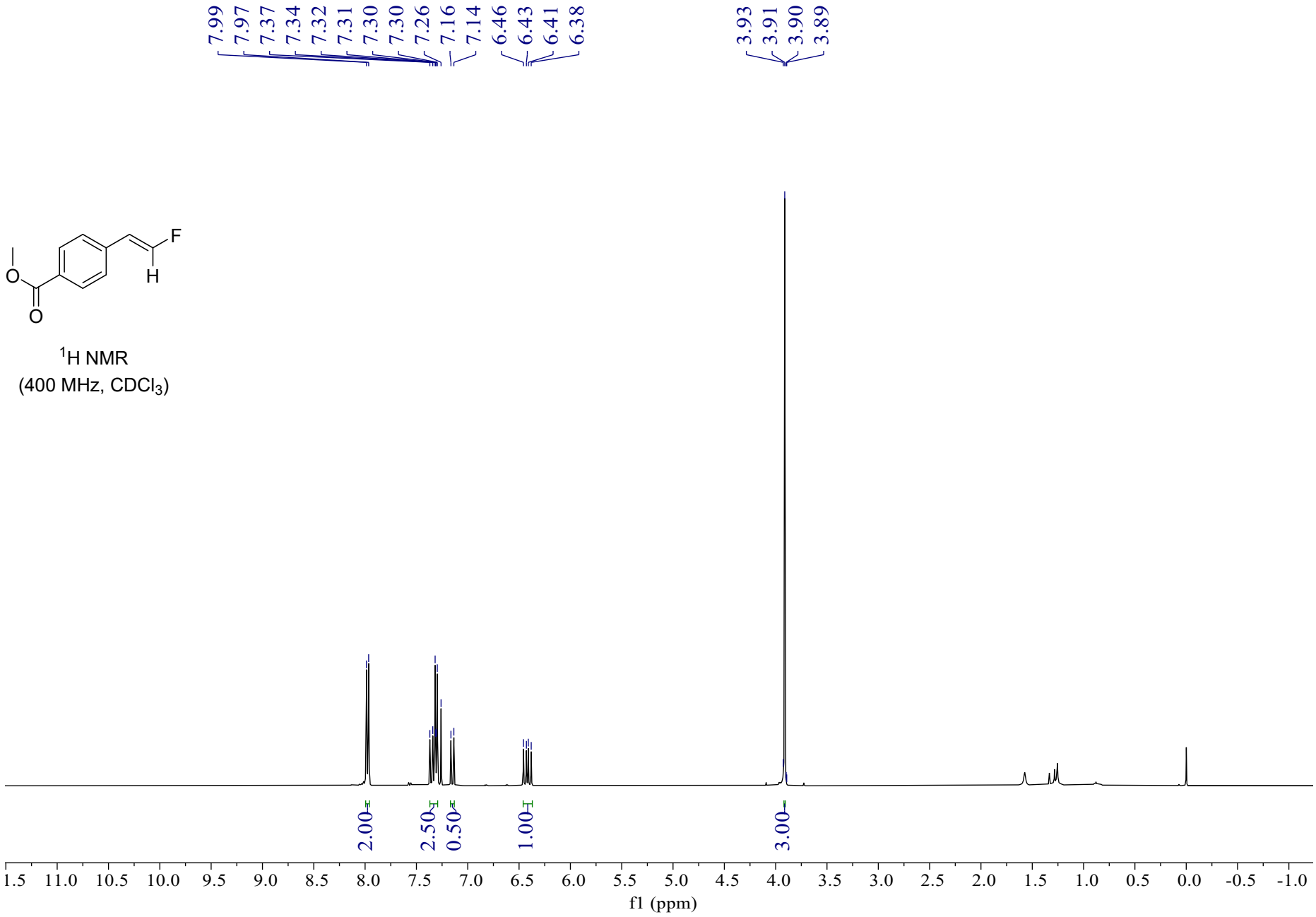
Comment

Acquisition Paramet

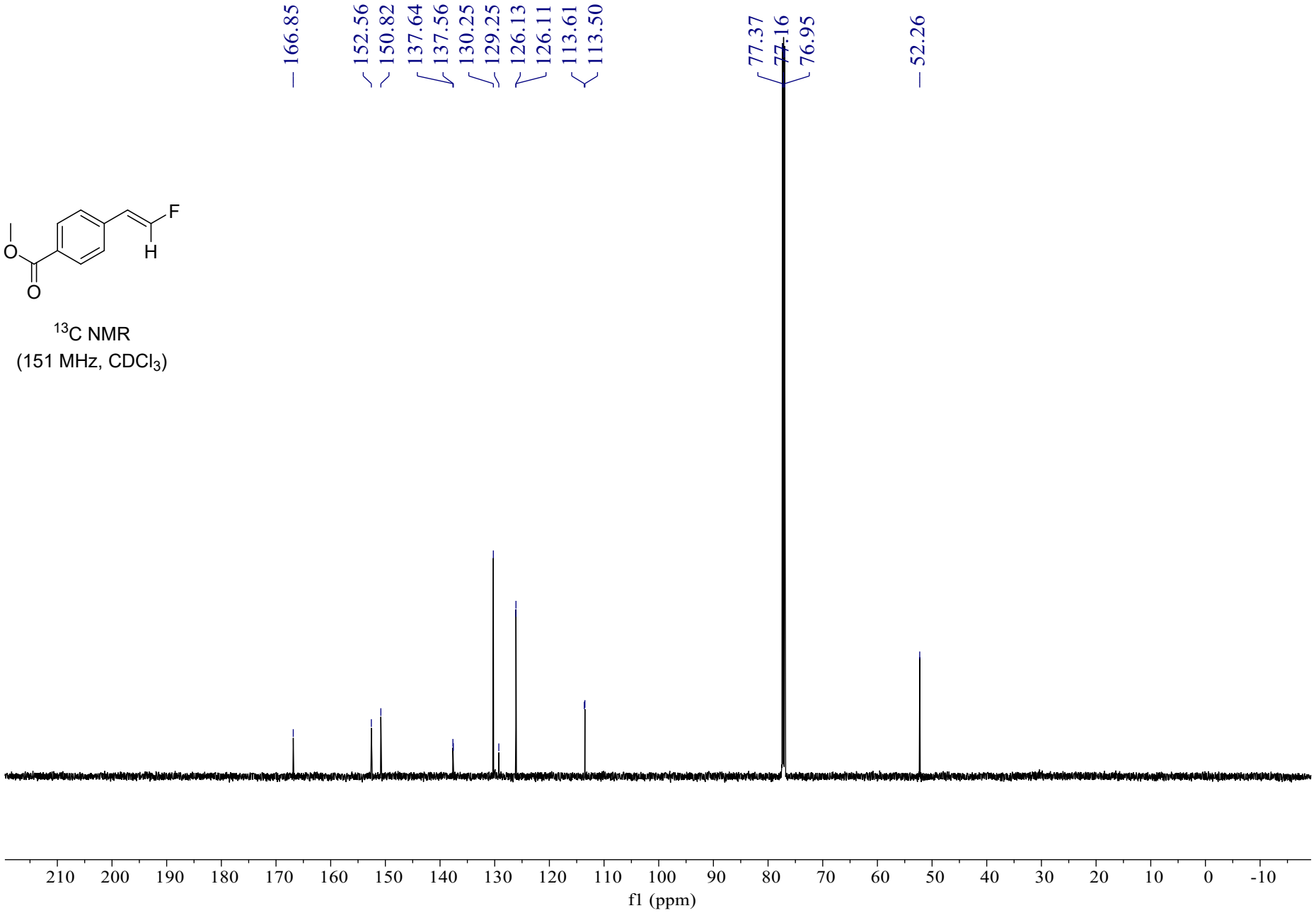
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min

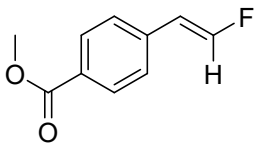


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
215.0888	1	C14H12FO	215.0867	-9.9	n.a.	1	100.00	8.5	even	ok



^{1}H NMR
(400 MHz, $CDCl_3$)


166.85
152.56
150.82
137.64
137.56
130.25
129.25
126.13
126.11
113.61
113.50
77.37
77.16
76.95
52.26
F
H
O
O
13C NMR
(151 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



^{19}F NMR
(376 MHz, $CDCl_3$)

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\LXMS\0106_RC2_01_20519.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0106

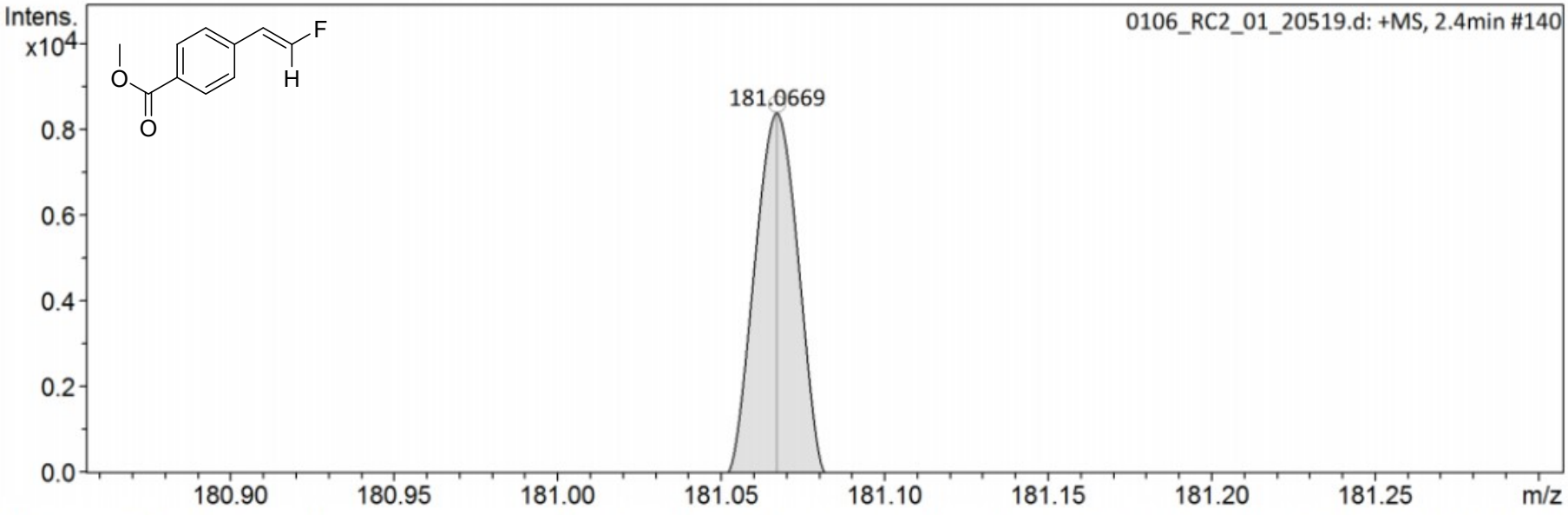
Comment

Acquisition D 2023-01-09 10:39:38

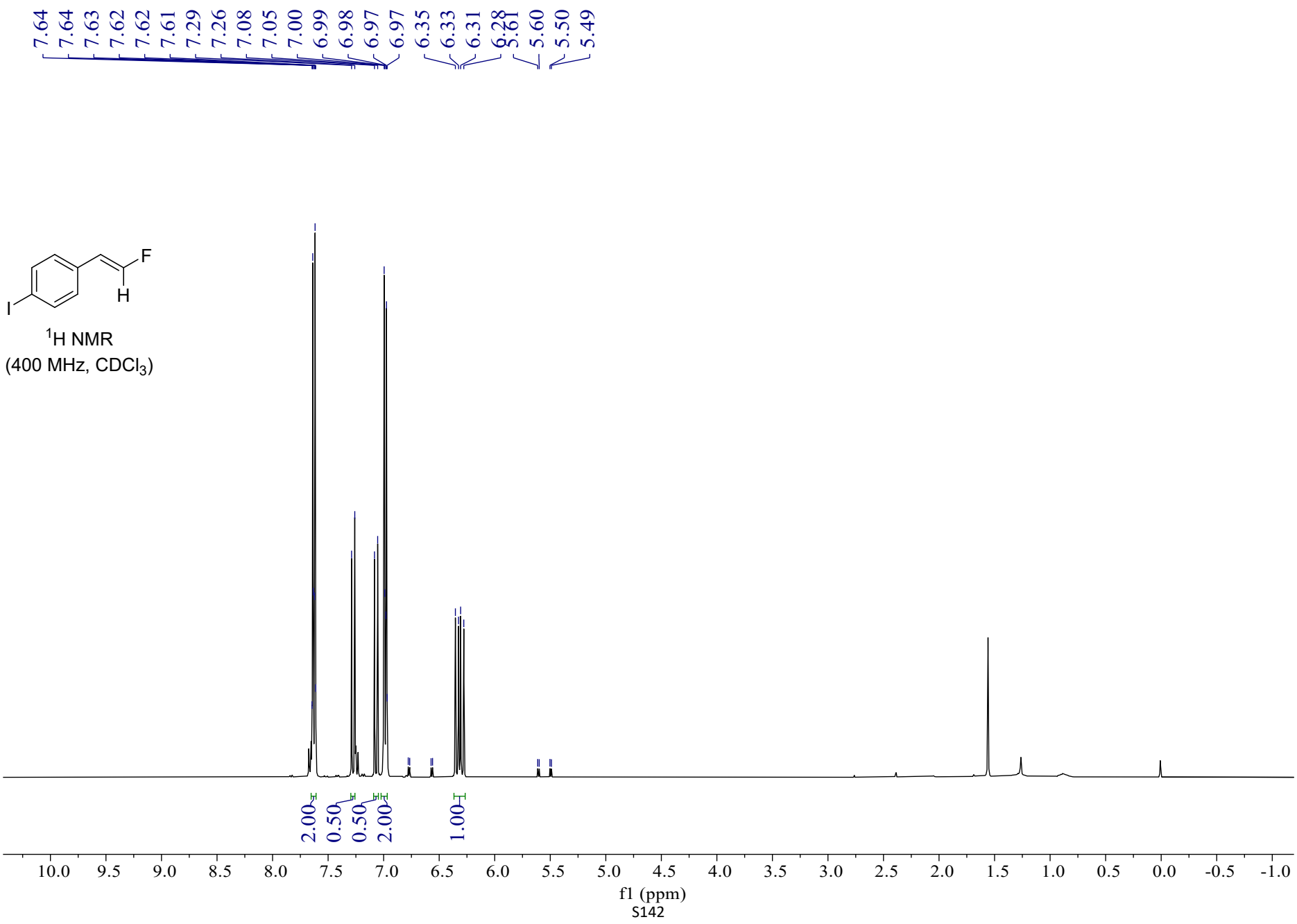
Operator Demo User
Instrumen compact 8255754.2017
6

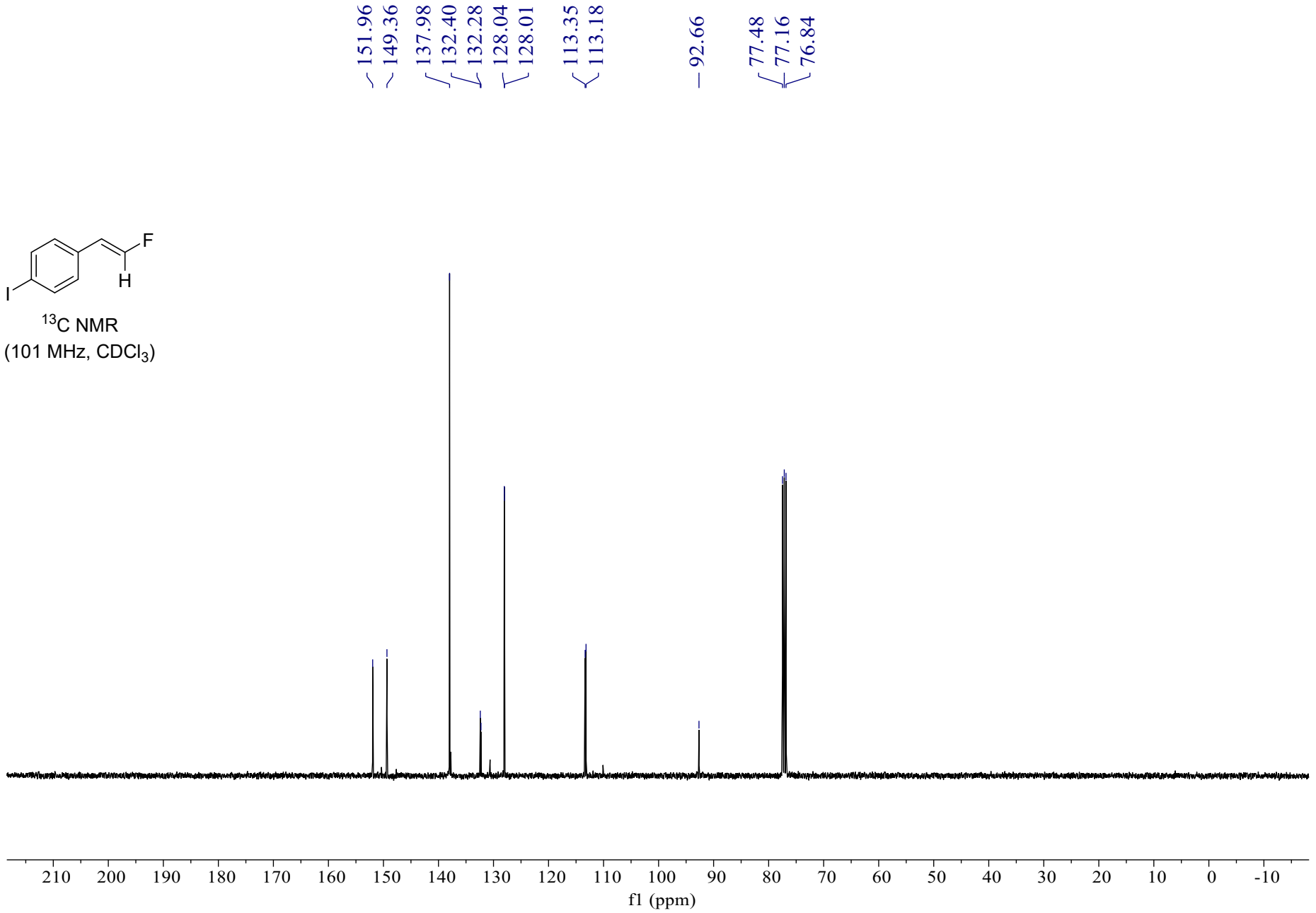
Acquisition Paramet

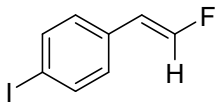
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
181.0669	1	C10H10FO2	181.0659	-5.5	62.2	1	100.00	5.5	even	ok


7.64
7.64
7.63
7.62
7.62
7.61
7.29
7.26
7.08
7.05
7.00
6.99
6.98
6.97
6.97
6.35
6.33
6.31
6.28
6.26
5.61
5.60
5.50
5.49
F
H
I
1H NMR
(400 MHz, CDCl3)
2.00
0.50
0.50
2.00
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

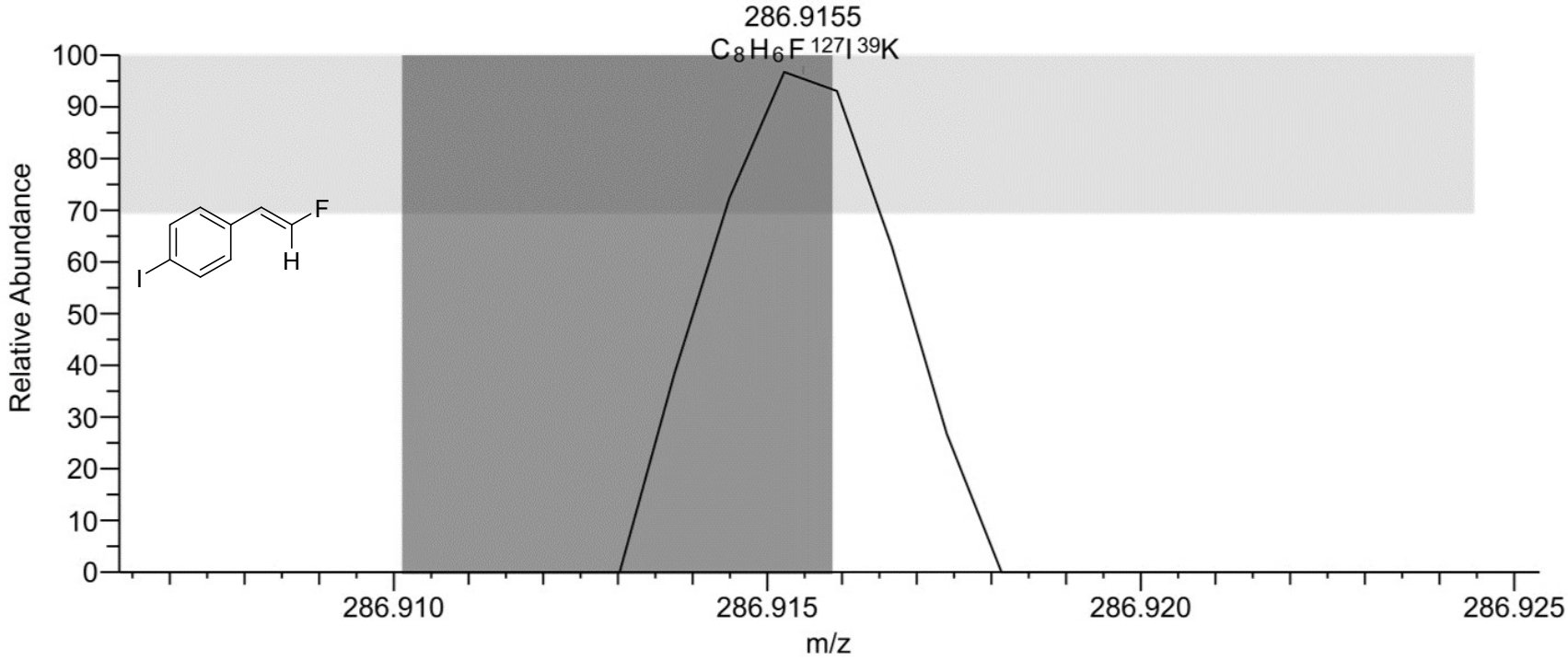

151.96
149.36
137.98
132.40
132.28
128.04
128.01
113.35
113.18
92.66
77.48
77.16
76.84
F
H
I
13C NMR
(101 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



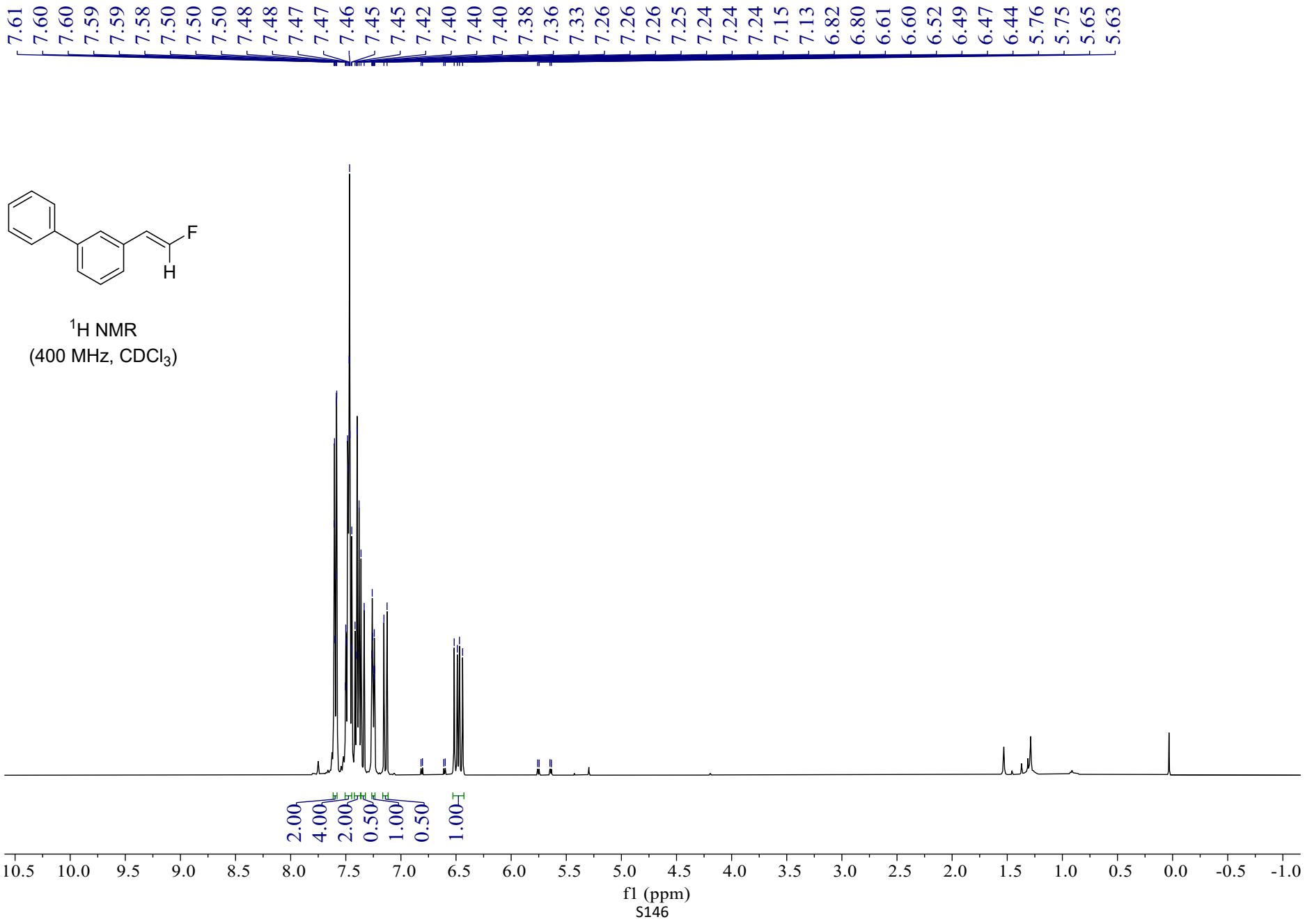
^{19}F NMR

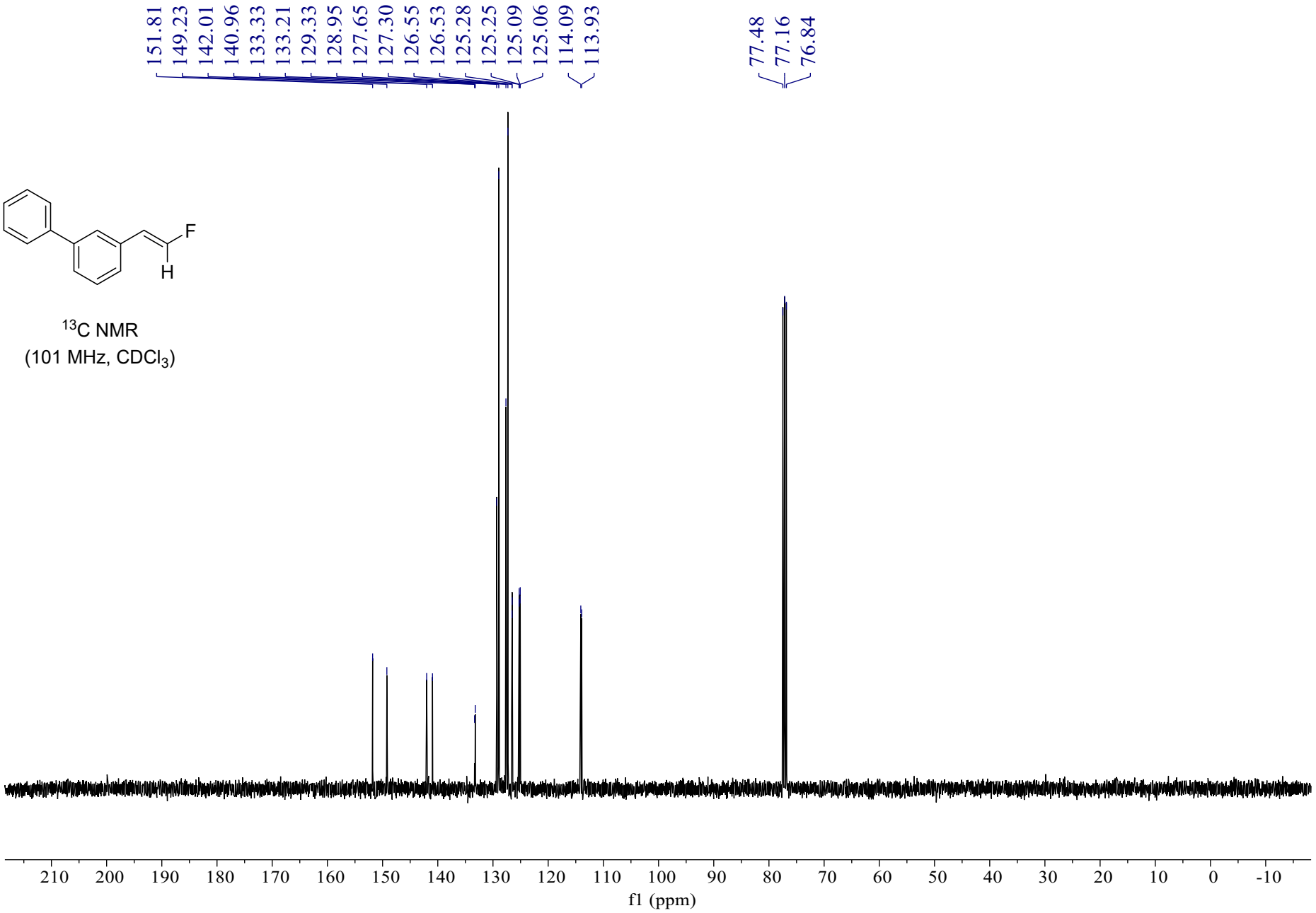
(376 MHz, $CDCl_3$)

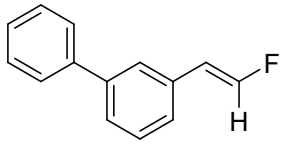
lx-92 #121 RT: 0.91 AV: 1 NL: 2.66E4
T: FTMS + p ESI Full ms [100.0000-1500.0000]



Peak M...	Display...	S Fit	RDB	Delta [p...	Theo....	Rank	Combin...	# Matc...	# Misse...	MS Cov...	Pattern...	MSMS...
286.9155	$C_8H_6F^{127}I^{39}K$	37.9690069517735	4.50	8.77	286.91298	1	96.74	1	0	100	100	(Collection)


7.61 7.60 7.60 7.59 7.59 7.58 7.50 7.50 7.50 7.48 7.48 7.47 7.47 7.46 7.45 7.45 7.42 7.40 7.40 7.40 7.38 7.36 7.33 7.26 7.26 7.26 7.25 7.24 7.24 7.24 7.15 7.13 6.82 6.80 6.61 6.60 6.52 6.49 6.47 6.44 5.76 5.75 5.65 5.63
F
H
1H NMR
(400 MHz, CDCl3)
2.00 4.00 2.00 0.50 1.00 0.50 1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


151.81
149.23
142.01
140.96
133.33
133.21
129.33
128.95
127.65
127.30
126.55
126.53
125.28
125.25
125.09
125.06
114.09
113.93
77.48
77.16
76.84
F
H
^{13}C NMR
(101 MHz, $CDCl_3$)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



^{19}F NMR
(376 MHz, $CDCl_3$)

Mass Spectrum SmartFormula Report

Analysis Info

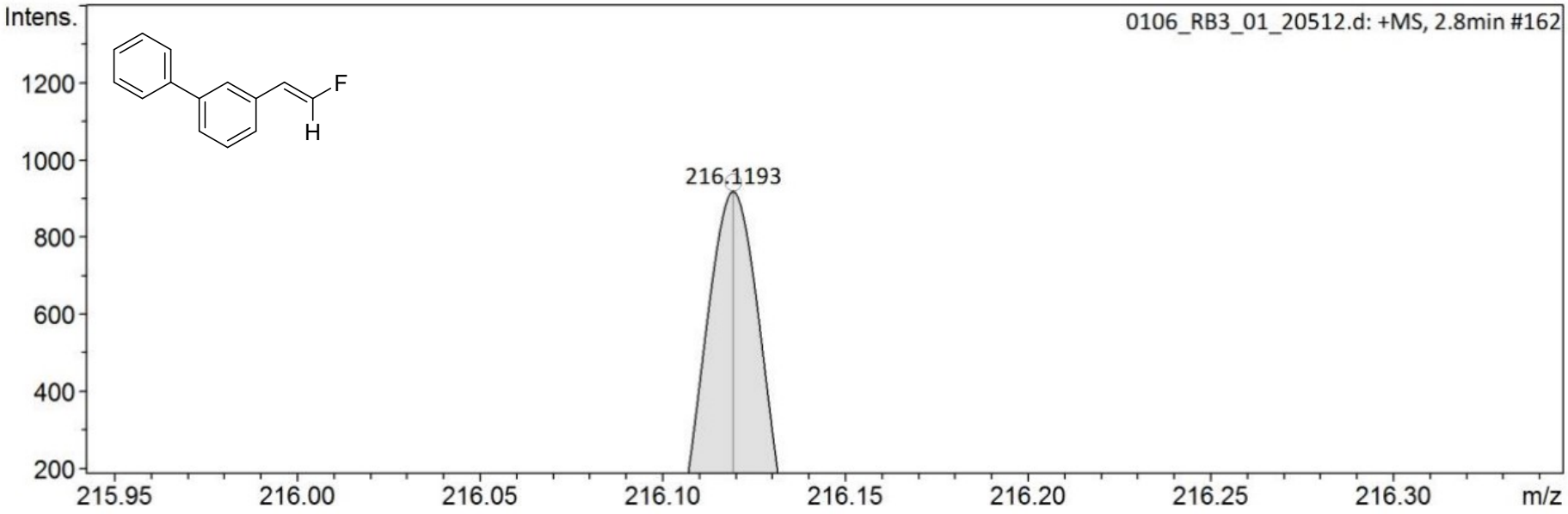
Acquisition D 2023-01-09 9:47:25

Analysis Name D:\LXMS\0106_RB3_01_20512.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0106
Comment

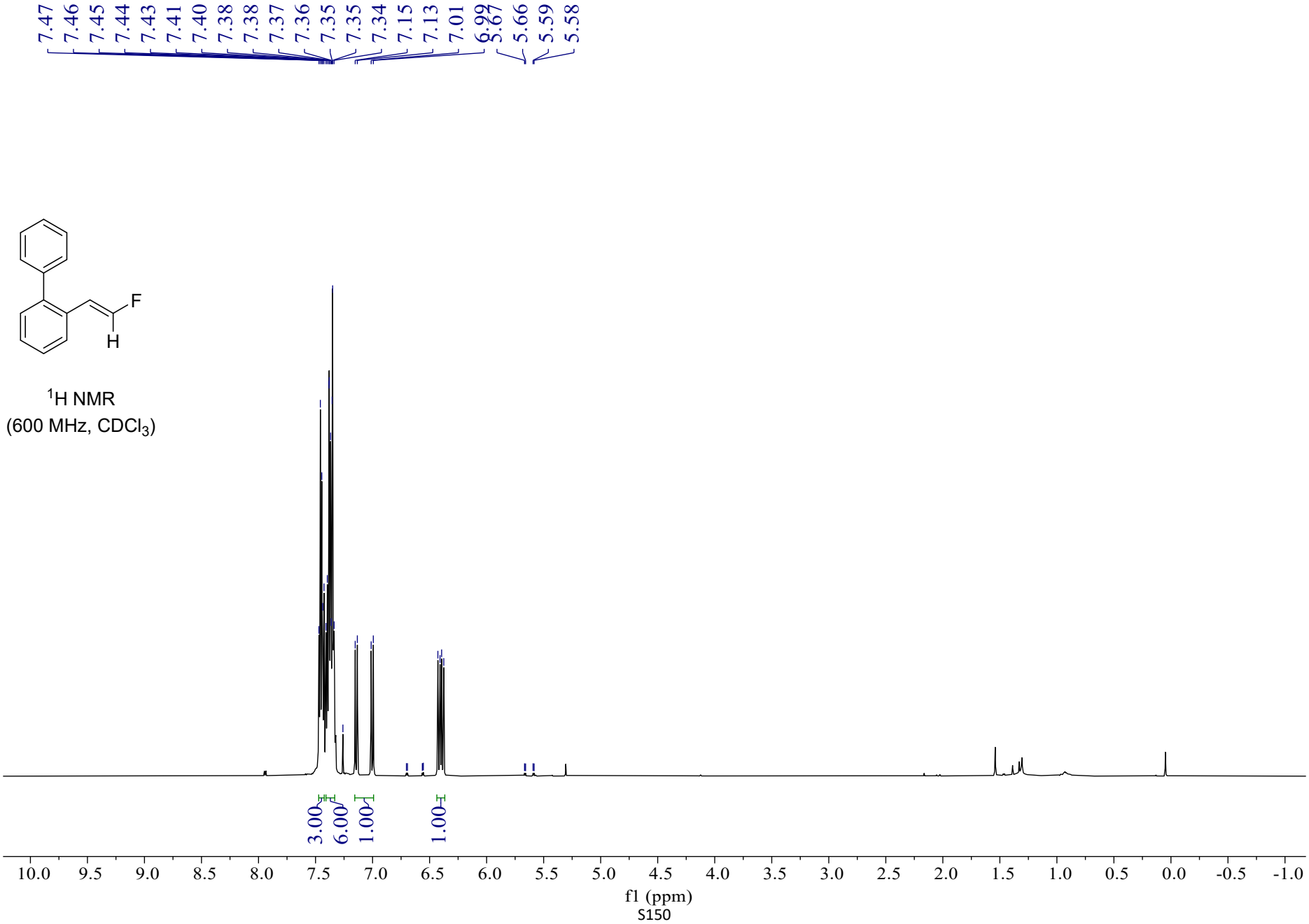
Operator Demo User
Instrumen compact 8255754.20176

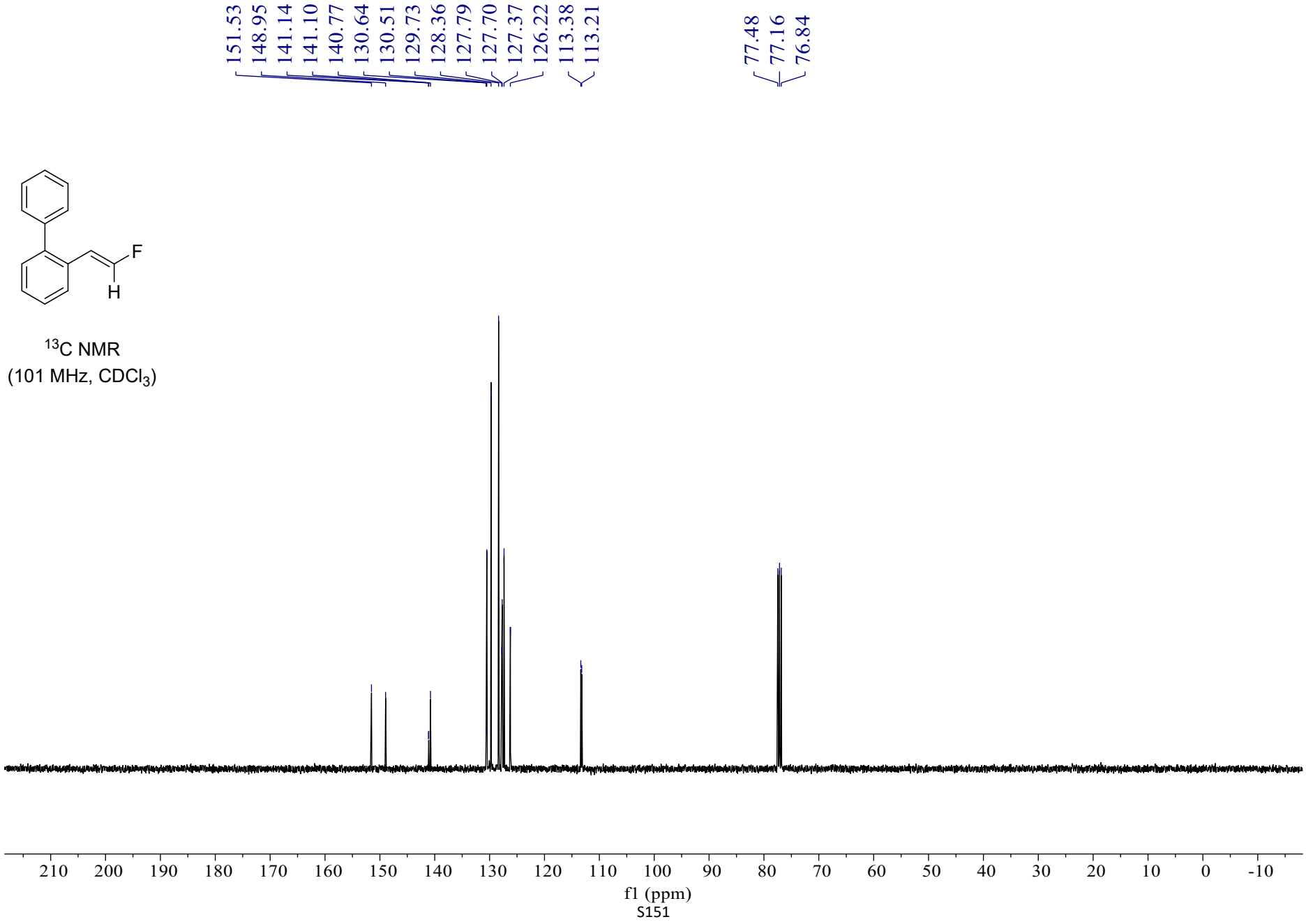
Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min

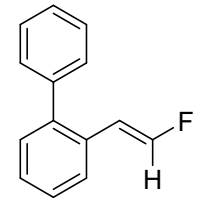


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
216.1193	1	C14H15FN	216.1183	-4.7	n.a.	1	100.00	7.5	even		ok

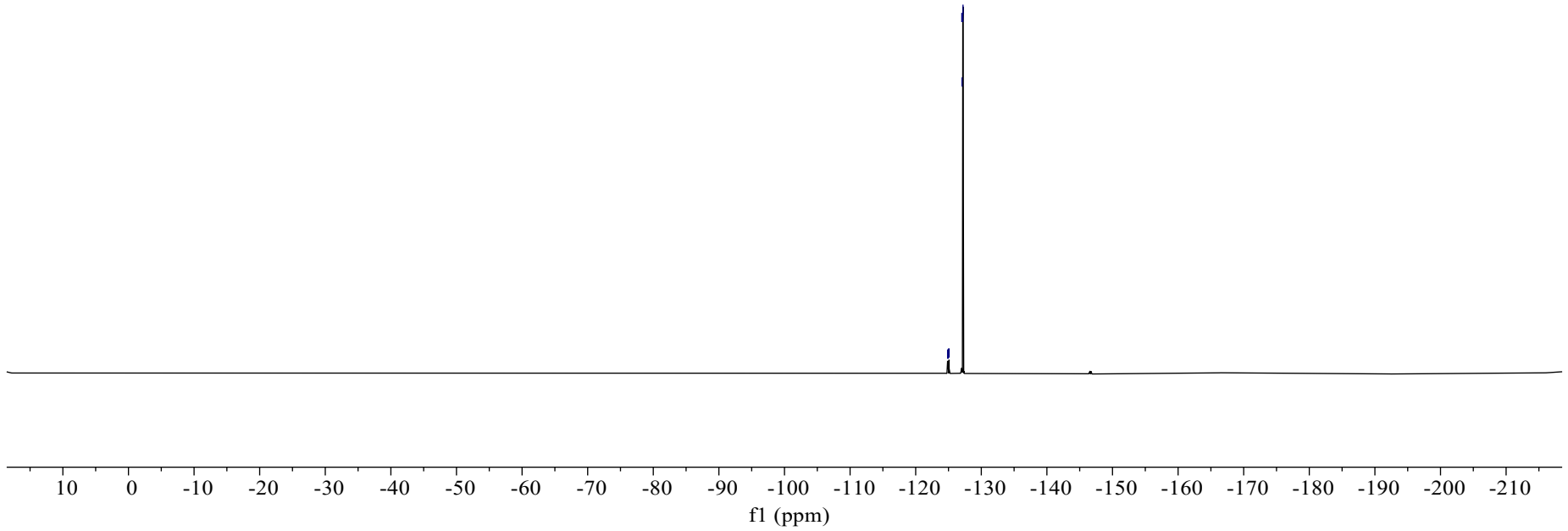

7.47
7.46
7.45
7.44
7.43
7.41
7.40
7.38
7.38
7.37
7.36
7.35
7.35
7.34
7.15
7.13
7.01
6.99
6.97
5.66
5.59
5.58
F
H
1H NMR
(600 MHz, CDCl3)
3.00
6.00
1.00
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


151.53
148.95
141.14
141.10
140.77
130.64
130.51
129.73
128.36
127.79
127.70
127.37
126.22
113.38
113.21
77.48
77.16
76.84
F
H
^{13}C NMR
(101 MHz, $CDCl_3$)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

-124.87
-124.95
-125.01
-125.09
-127.03
-127.06
-127.18
-127.21



^{19}F NMR
(565 MHz, $CDCl_3$)



Mass Spectrum SmartFormula Report

Analysis Info

Acquisition D 2023-03-10 16:35:21

Analysis Name D:\LXMS\0306_BC4_01_22068.d

Method LC_NO UV_P50-1500_10MIN.m

Operator Demo User

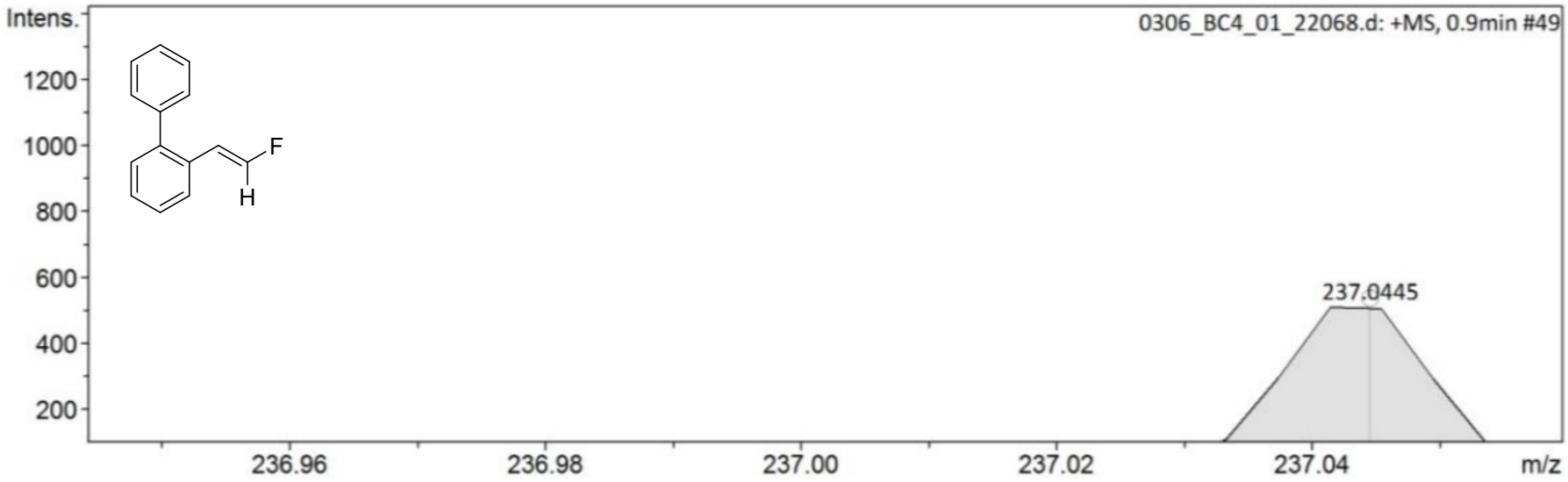
Sample Name 0306

Instrumen compact 8255754.2017 6

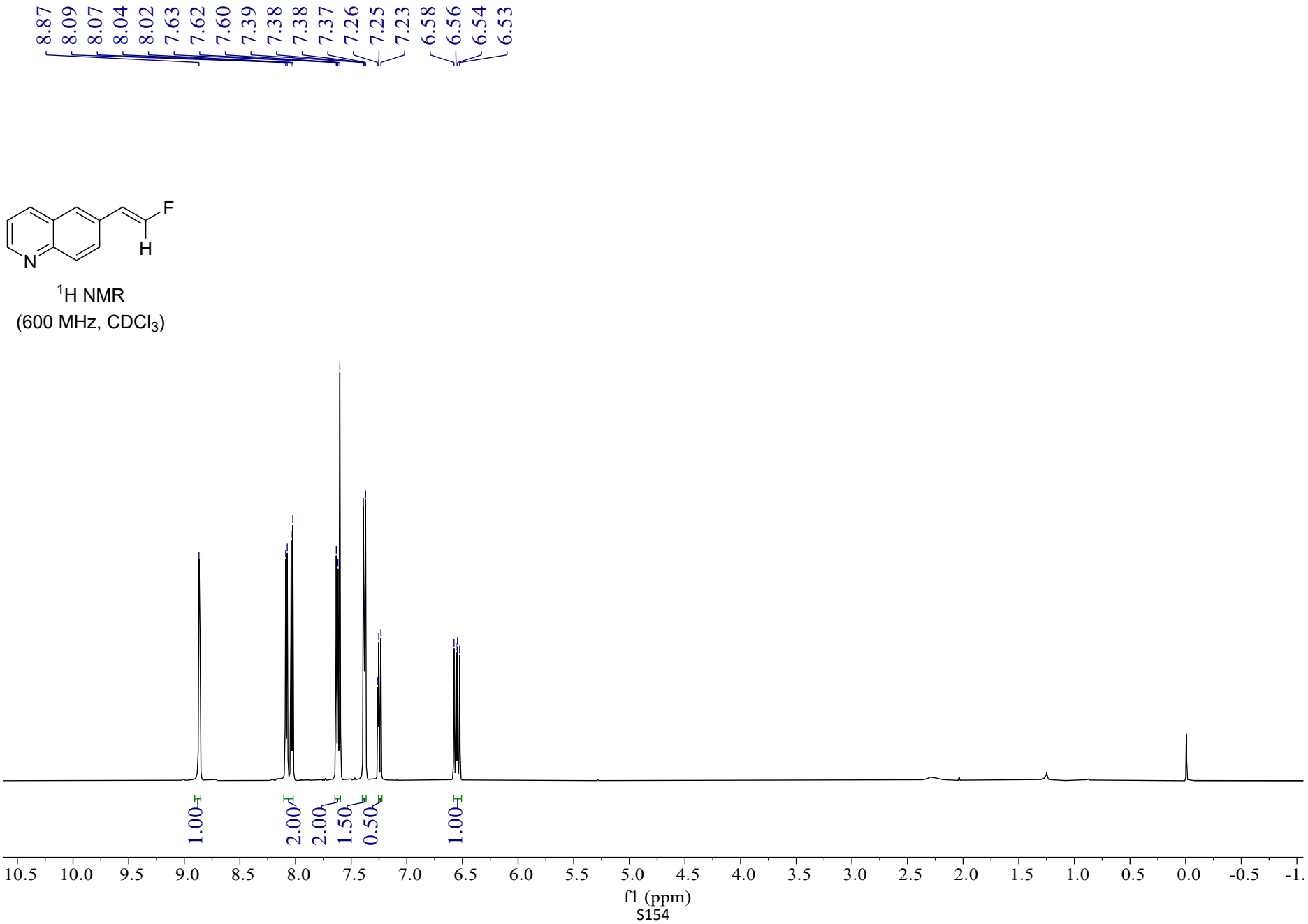
Comment

Acquisition Paramet

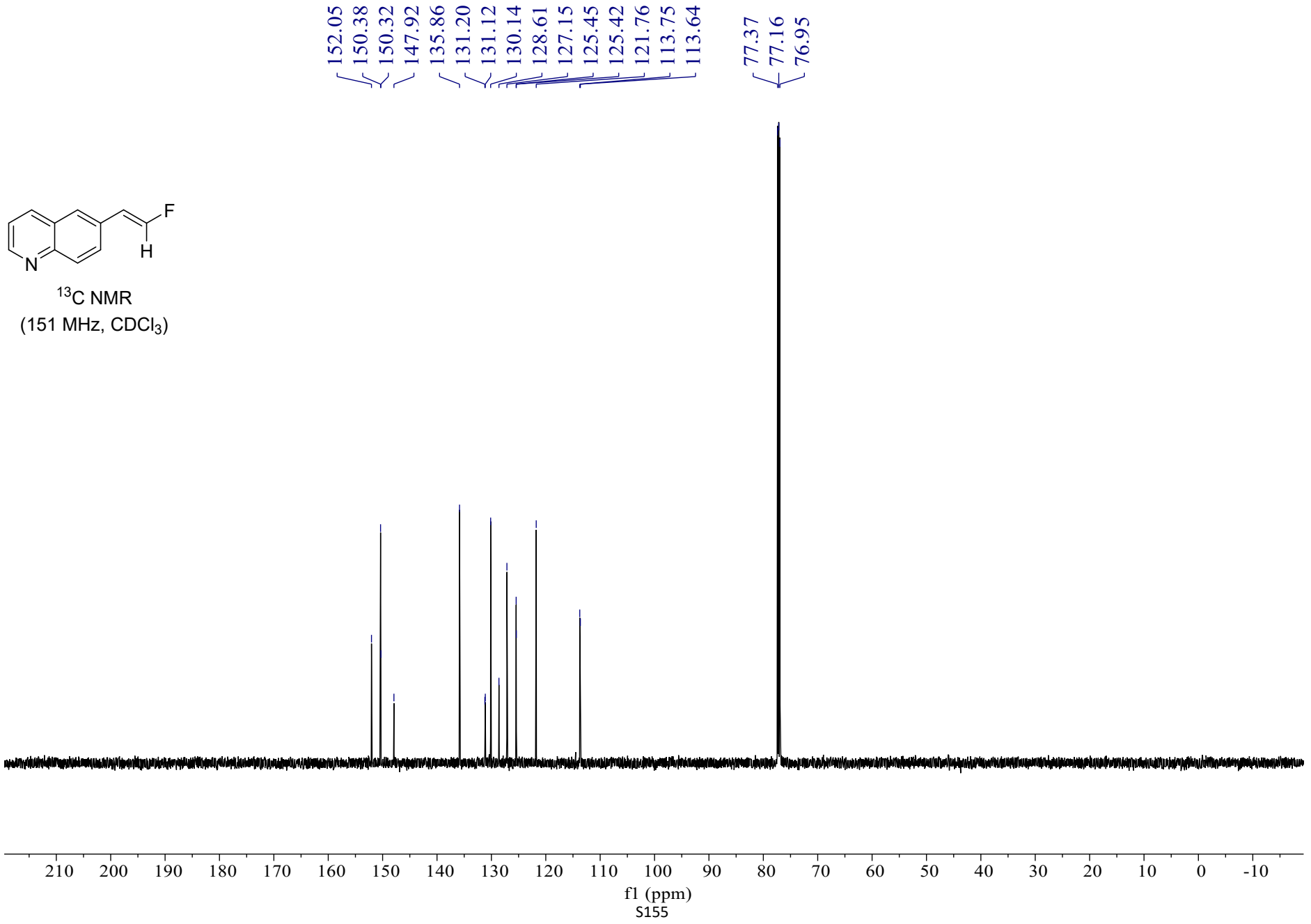
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min



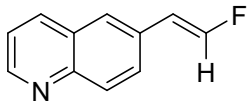
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
237.0445	1	C14H11FK	237.0476	13.1	n.a.	1	100.00	8.5	even		ok



^{1}H NMR
(600 MHz, $CDCl_3$)



^{13}C NMR
(151 MHz, $CDCl_3$)



^{19}F NMR
(376 MHz, $CDCl_3$)

Mass Spectrum SmartFormula Report

Analysis Info

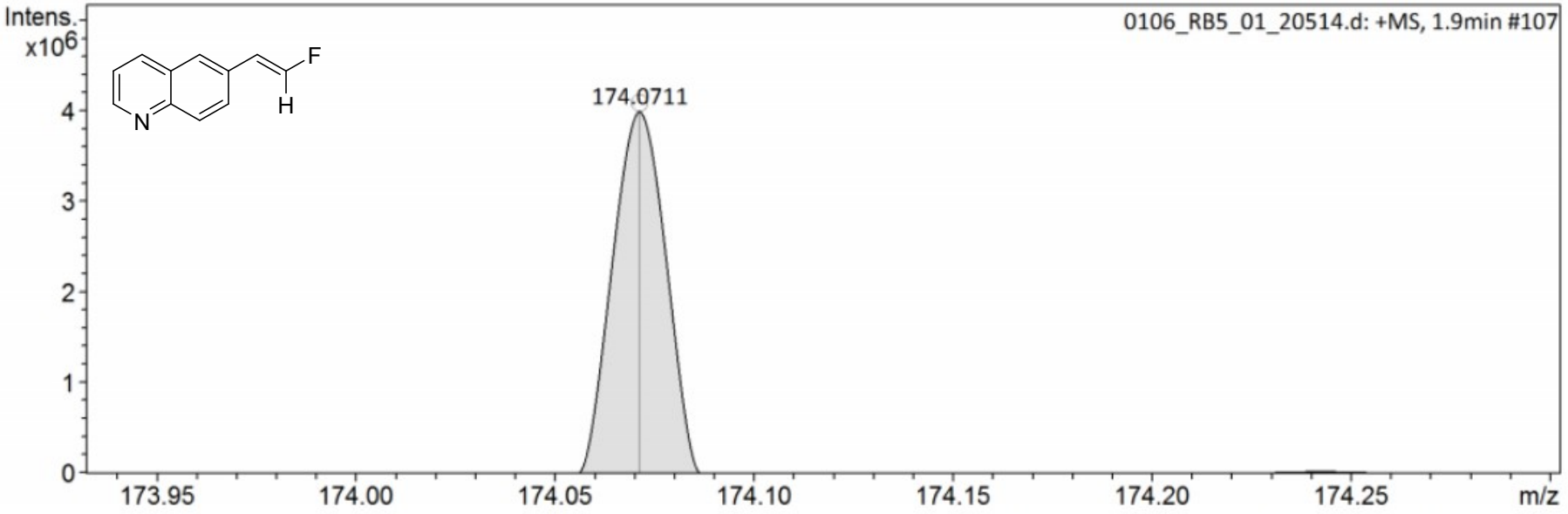
Acquisition D 2023-01-09 10:02:17

Analysis Name D:\LXMS\0106_RB5_01_20514.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0106
Comment

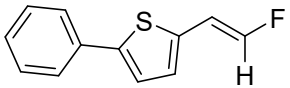
Operator Demo User
Instrumen compact 8255754.2017 6

Acquisition Paramet

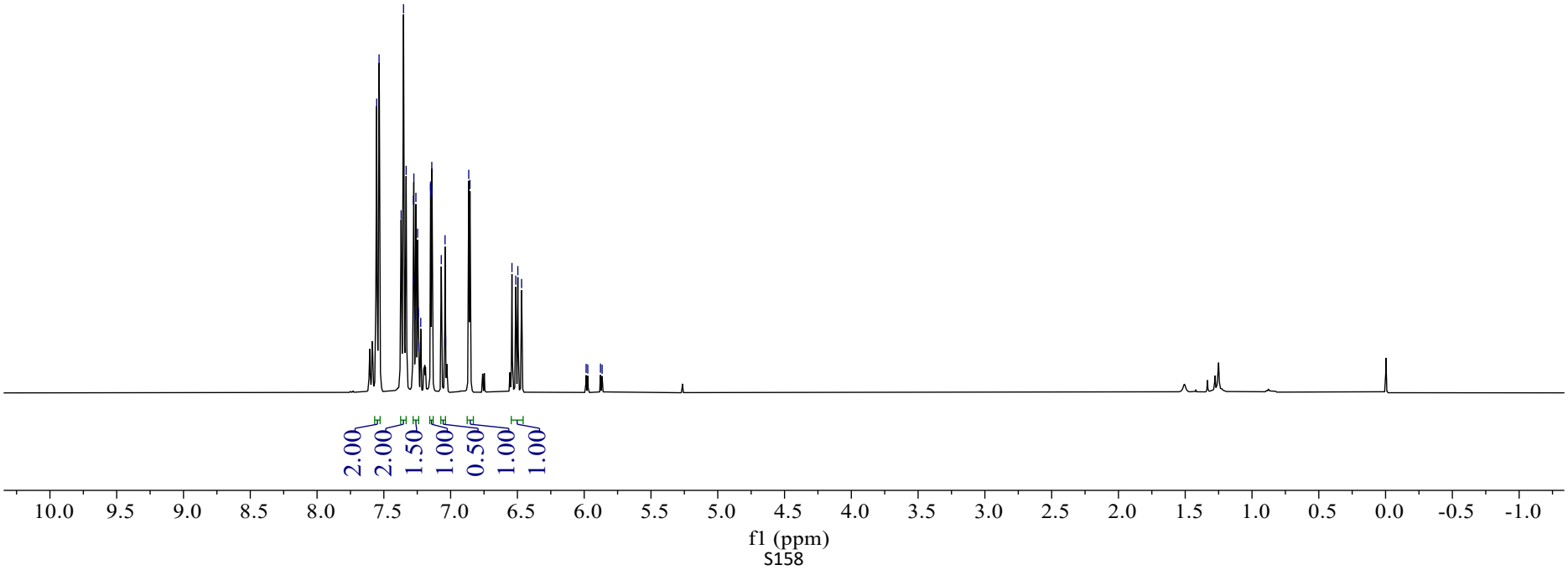
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min

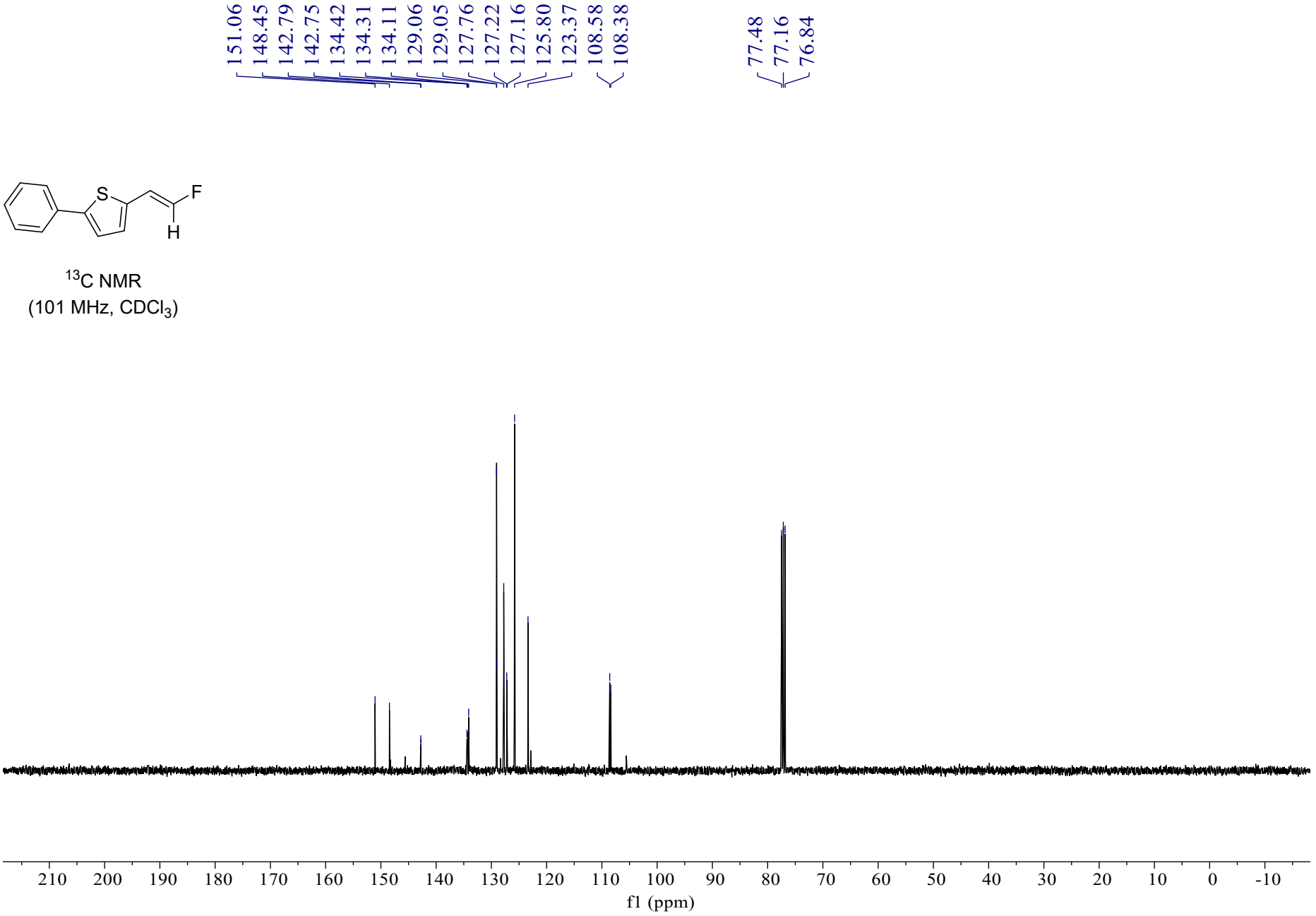


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
174.0711	1	C11H9FN	174.0714	1.3	0.5	1	100.00	7.5	even	ok

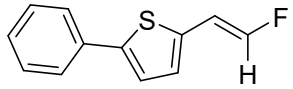


^{1}H NMR
(400 MHz, $CDCl_3$)





^{13}C NMR
(101 MHz, $CDCl_3$)



^{19}F NMR
(376 MHz, $CDCl_3$)

Mass Spectrum SmartFormula Report

Analysis Info

Acquisition D 2023-01-09 10:17:12

Analysis Name D:\LXMS\0106_RB7_01_20516.d

Method LC_NO UV_P50-1500_6MIN.m

Operator Demo User

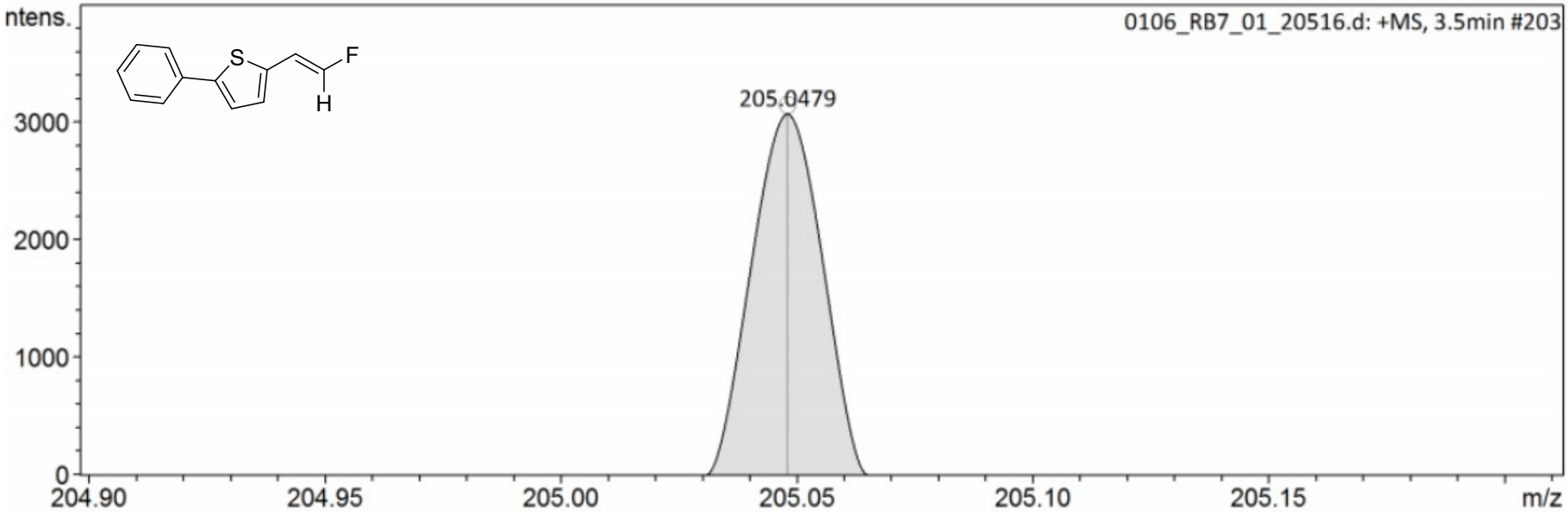
Sample Name 0106

Instrumen compact 8255754.2017 6

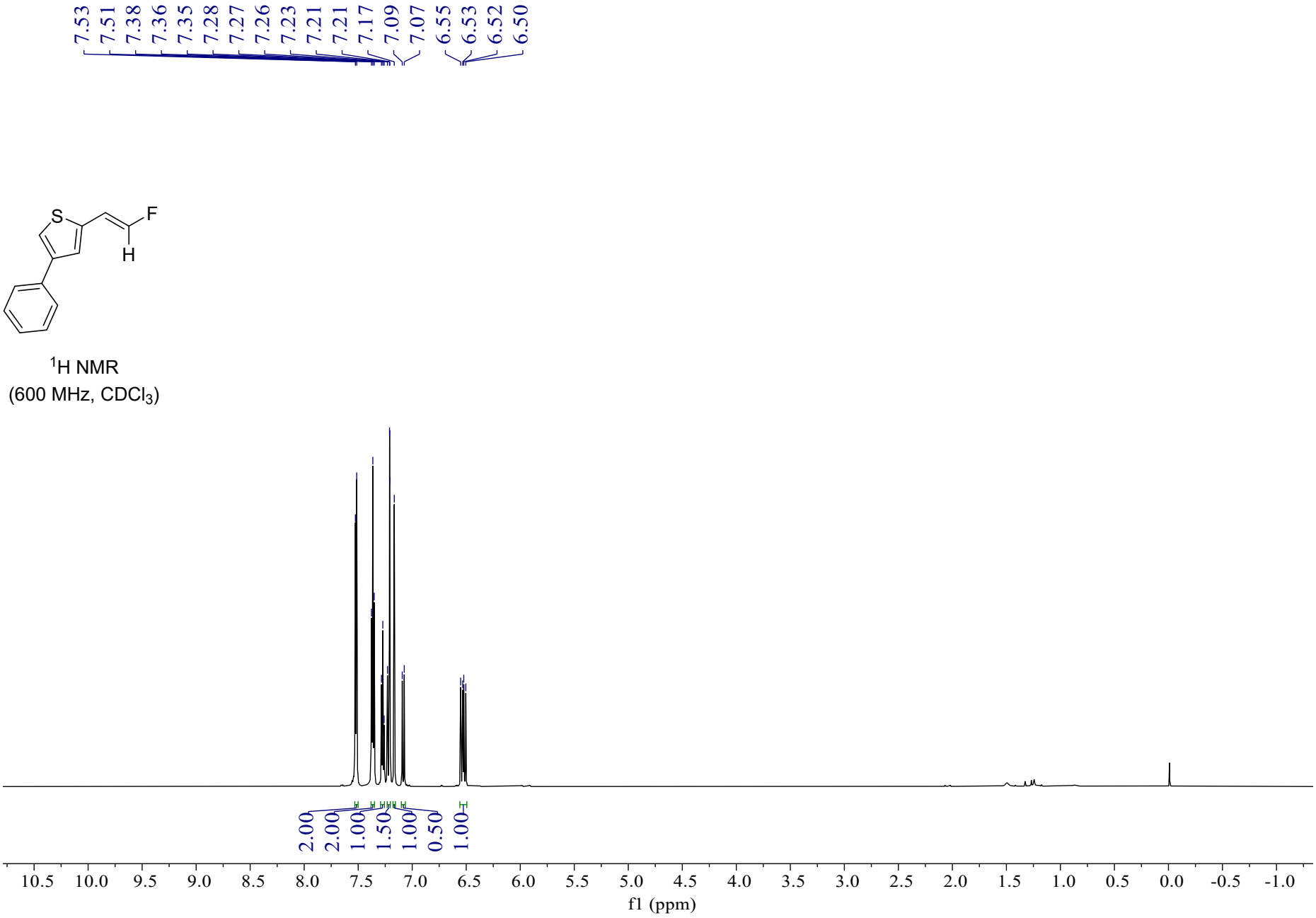
Comment

Acquisition Paramet

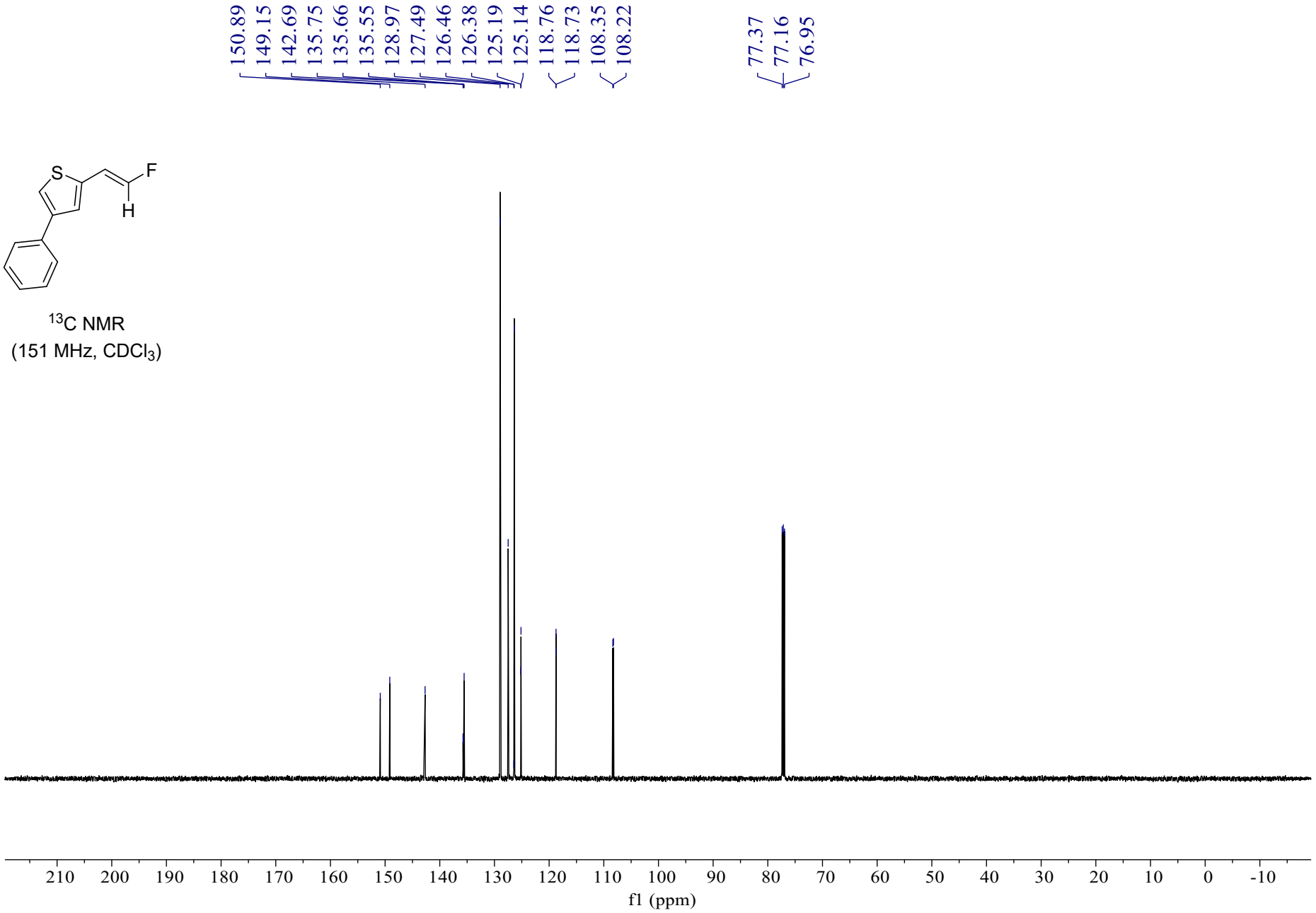
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min



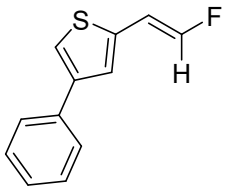
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
205.0479	1	C12H10FS	205.0482	1.3	n.a.	1	100.00	7.5	even	ok



^{1}H NMR
(600 MHz, $CDCl_3$)



^{13}C NMR
(151 MHz, $CDCl_3$)



^{19}F NMR
(565 MHz, $CDCl_3$)

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\LXMS\0106_RD1_01_20526.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0106

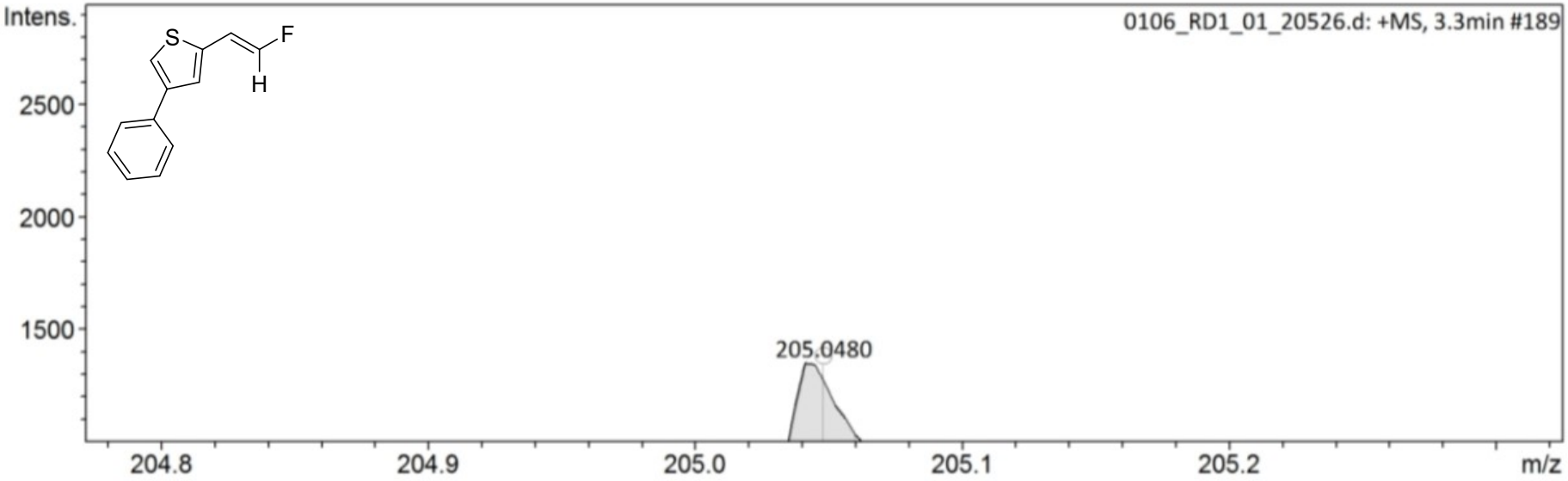
Comment

Acquisition D 2023-01-09 11:33:39

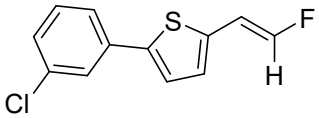
Operator Demo User
Instrumen compact 8255754.2017
6

Acquisition Paramet

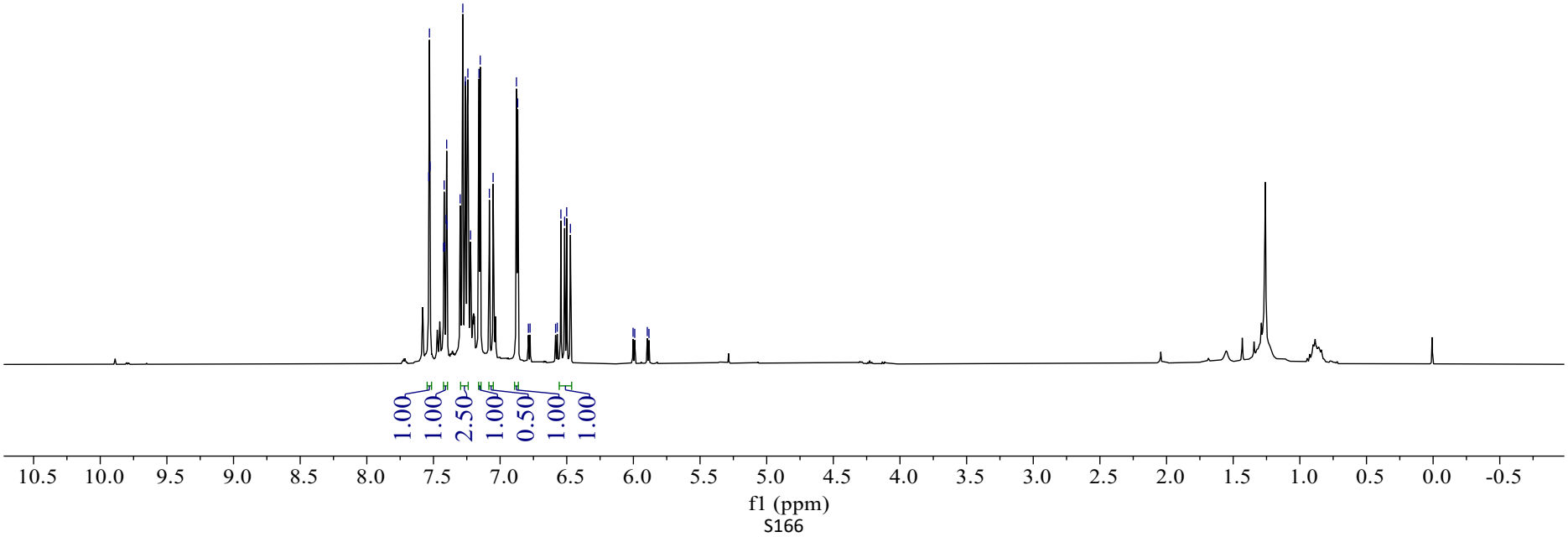
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min

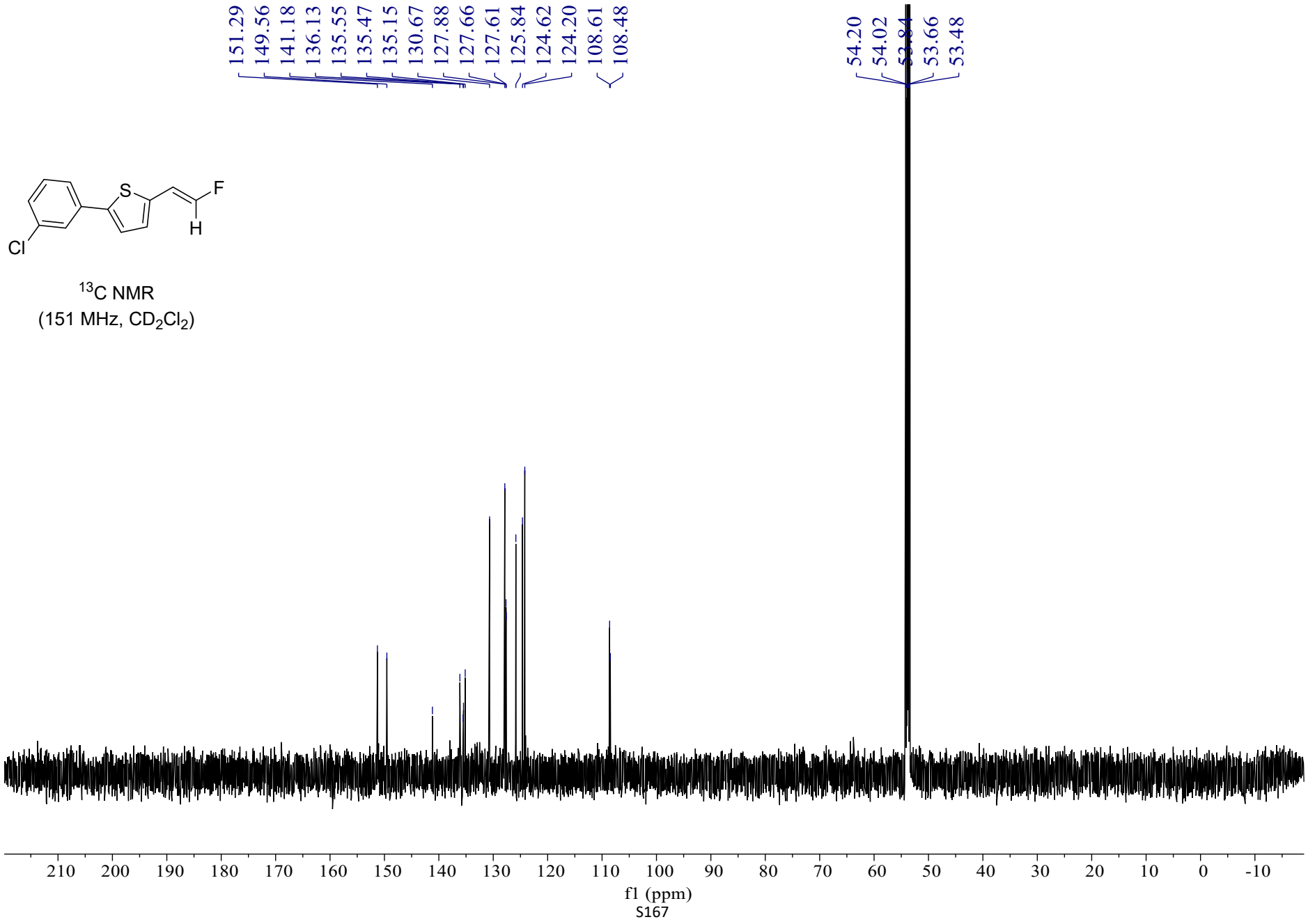


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
205.0480	1	C12H10FS	205.0482	0.9	268.1	1	100.00	7.5	even		ok

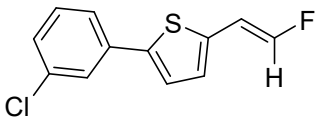


^{1}H NMR
(400 MHz, $CDCl_3$)



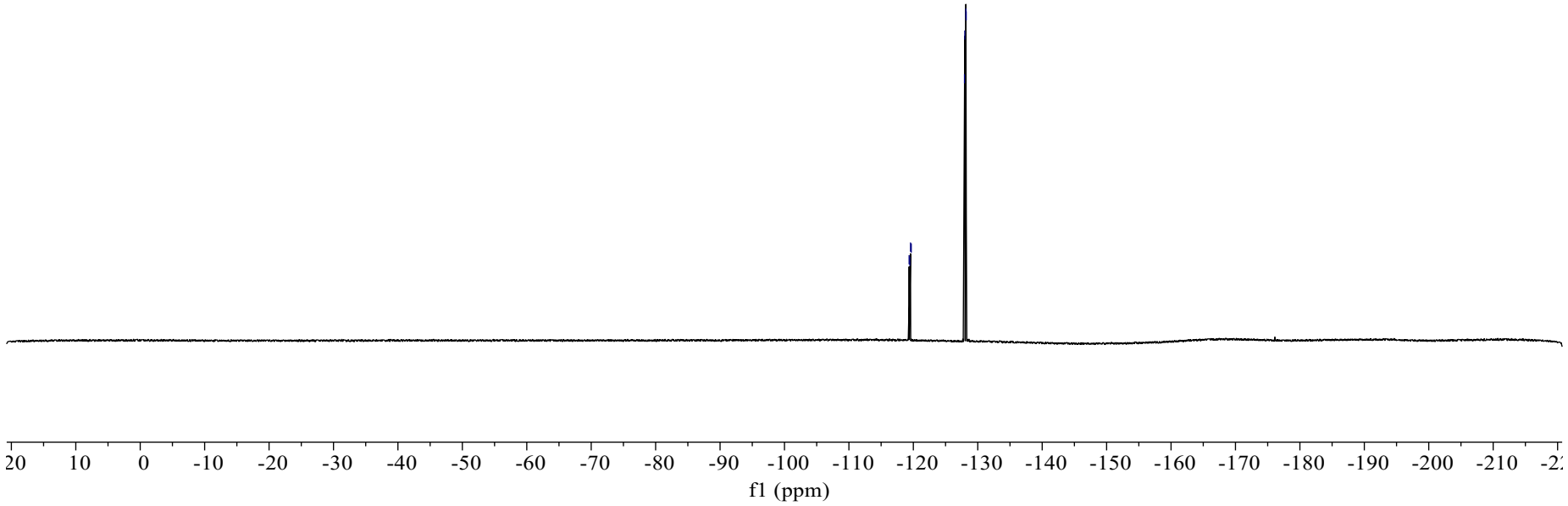


^{13}C NMR
(151 MHz, CD_2Cl_2)



^{19}F NMR
(376 MHz, $CDCl_3$)

-119.35
-119.46
-119.56
-119.68
-127.94
-127.99
-128.16
-128.21



Mass Spectrum SmartFormula Report

Analysis Info

Acquisition D 2023-01-09 10:09:36

Analysis Name D:\LXMS\0106_RB6_01_20515.d

Method LC_NO UV_P50-1500_6MIN.m

Operator Demo User

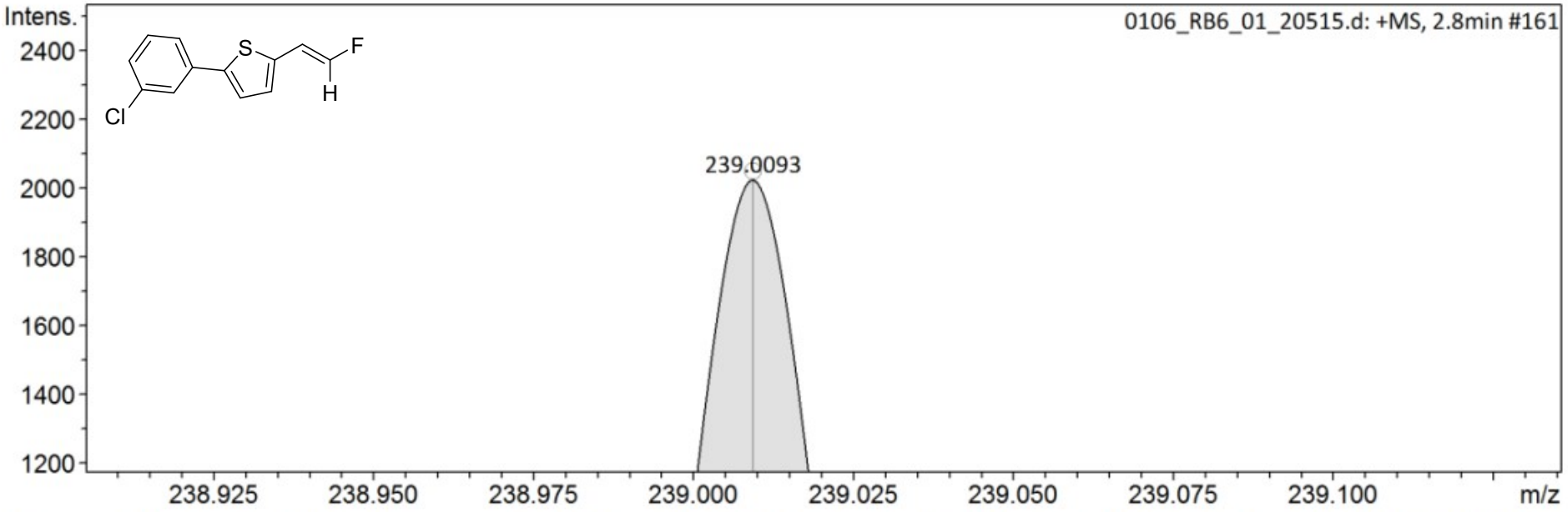
Sample Name 0106

Instrumen compact 8255754.2017 6

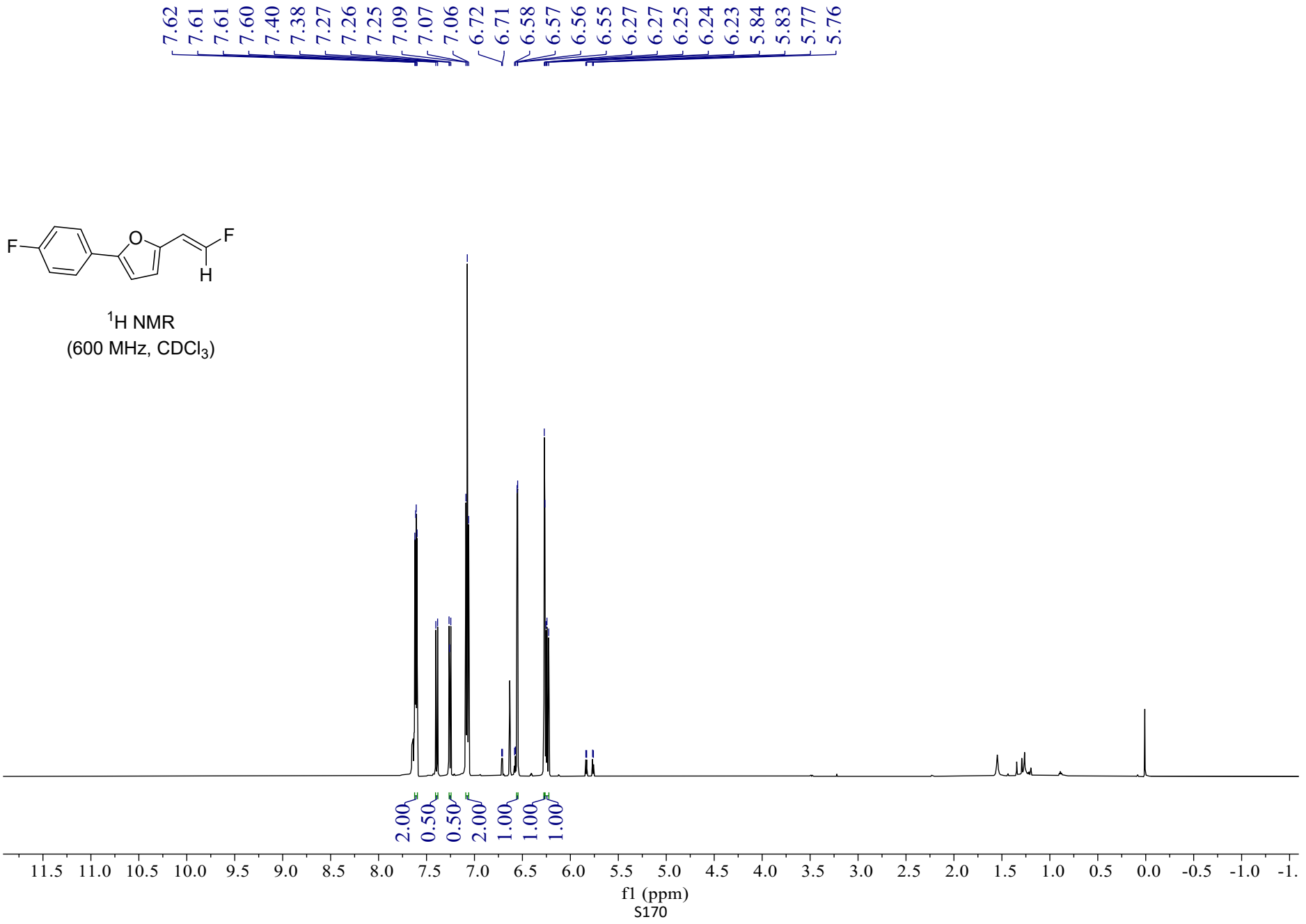
Comment

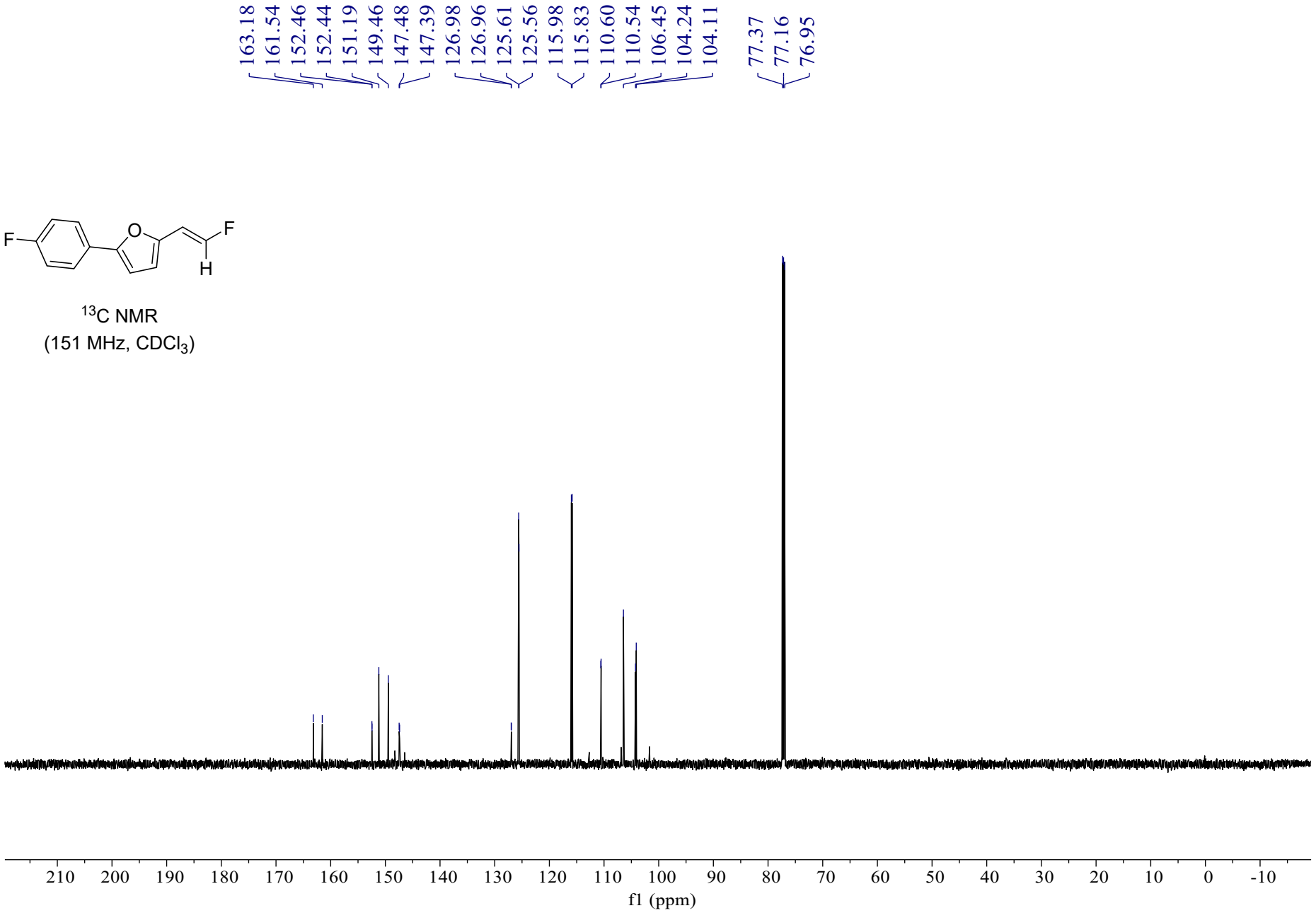
Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min



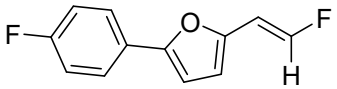
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
239.0093	1	C12H9ClFS	239.0092	-0.5	n.a.	1	100.00	7.5	even	ok


7.62
7.61
7.61
7.60
7.40
7.38
7.27
7.26
7.25
7.09
7.07
7.06
6.72
6.71
6.58
6.57
6.56
6.55
6.27
6.27
6.25
6.24
6.23
5.84
5.83
5.77
5.76
F
O
F
H
1H NMR
(600 MHz, CDCl3)
2.00
0.50
0.50
2.00
1.00
1.00
1.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.
f1 (ppm)

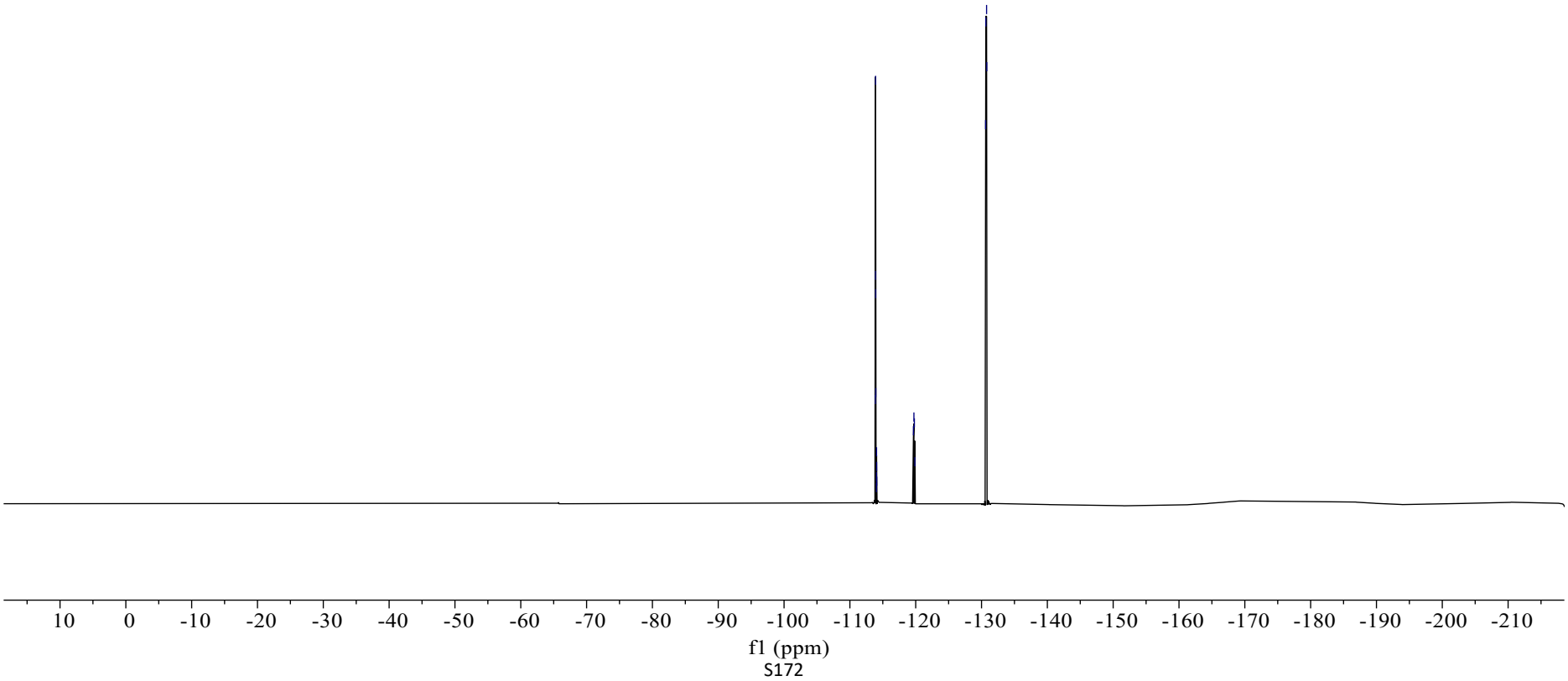


^{13}C NMR
(151 MHz, $CDCl_3$)

-113.88
-113.90
-113.91
-113.92
-113.93
-114.03
-114.04
-114.05
-114.06
-114.08
-119.65
-119.73
-119.80
-119.87
-130.62
-130.65
-130.77
-130.80



^{19}F NMR
(376 MHz, $CDCl_3$)



Mass Spectrum SmartFormula Report

Analysis Info

Acquisition D 2023-01-09 10:25:01

Analysis Name D:\LXMS\0106_RB8_01_20517.d

Method LC_NO UV_P50-1500_6MIN.m

Operator Demo User

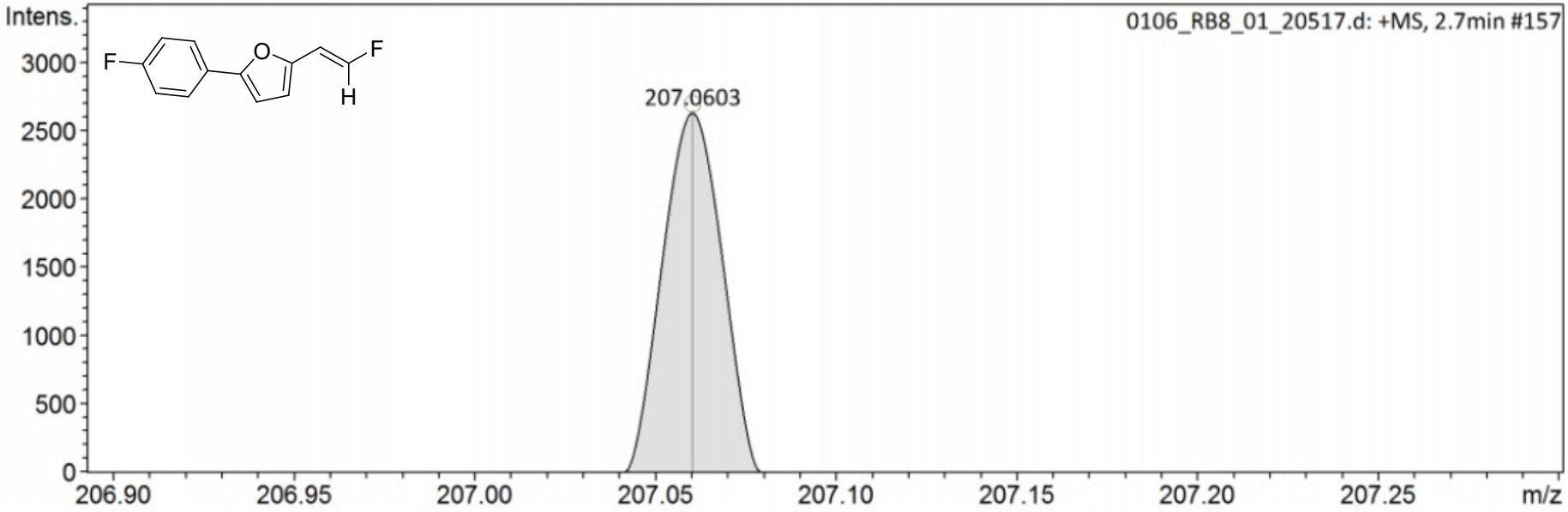
Sample Name 0106

Instrumen compact 8255754.2017 6

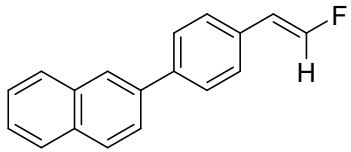
Comment

Acquisition Paramet

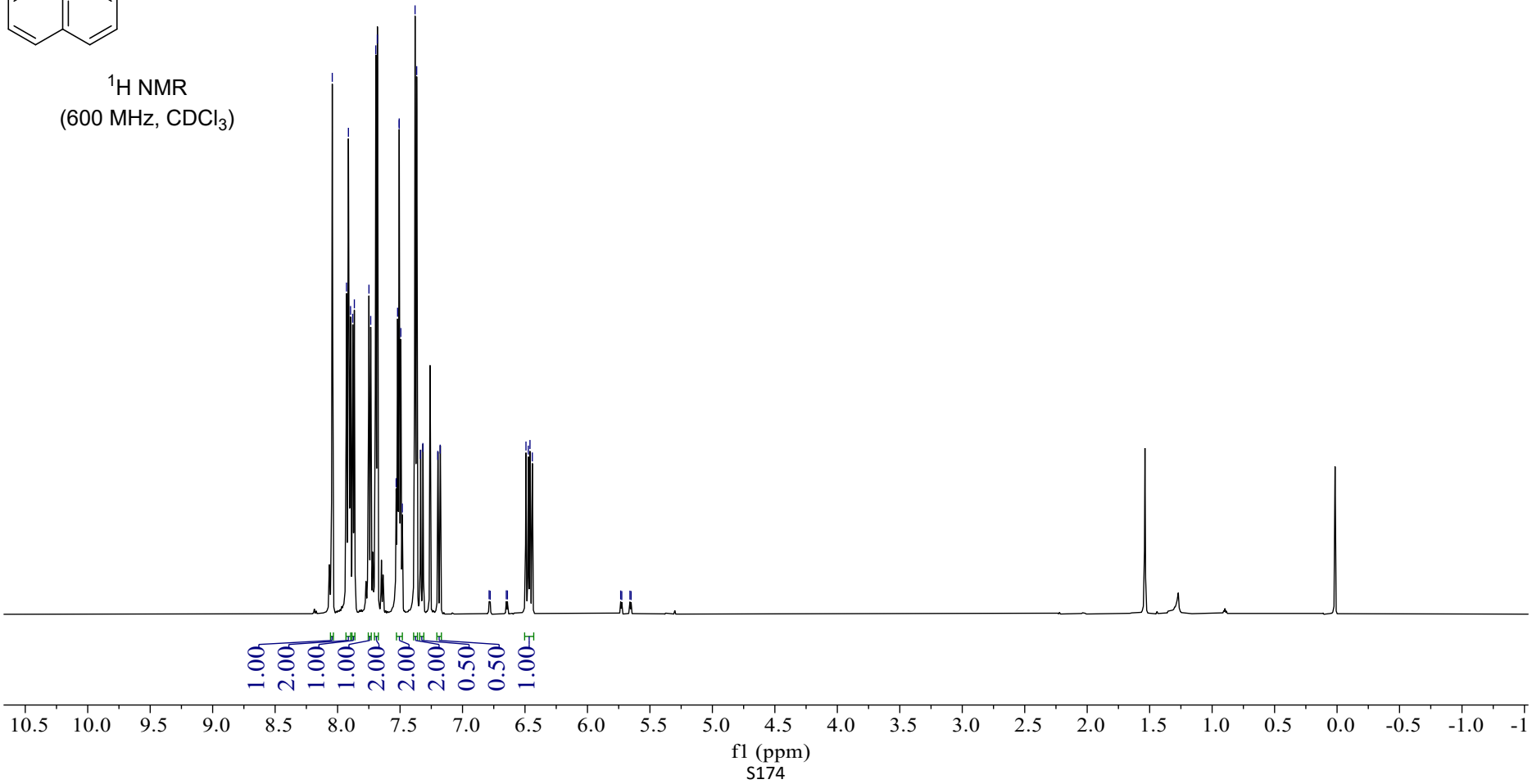
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min

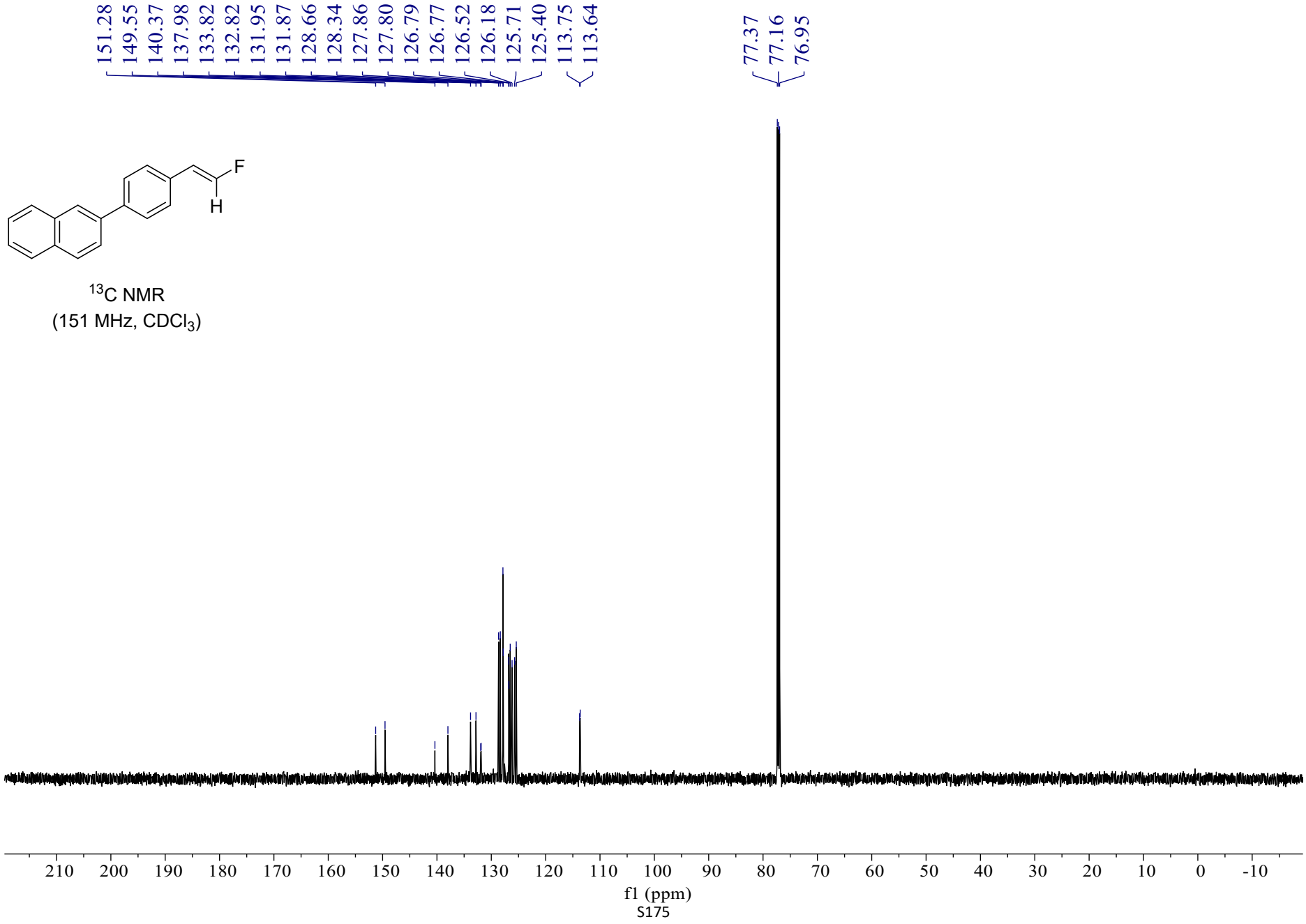


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
207.0603	1	C12H9F2O	207.0616	6.5	208.6	1	100.00	7.5	even	ok

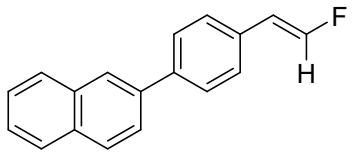


^{1}H NMR
(600 MHz, $CDCl_3$)





^{13}C NMR
(151 MHz, $CDCl_3$)



^{19}F NMR
(376 MHz, $CDCl_3$)

Mass Spectrum SmartFormula Report

Analysis Info

Acquisition D 2023-01-09 9:32:00

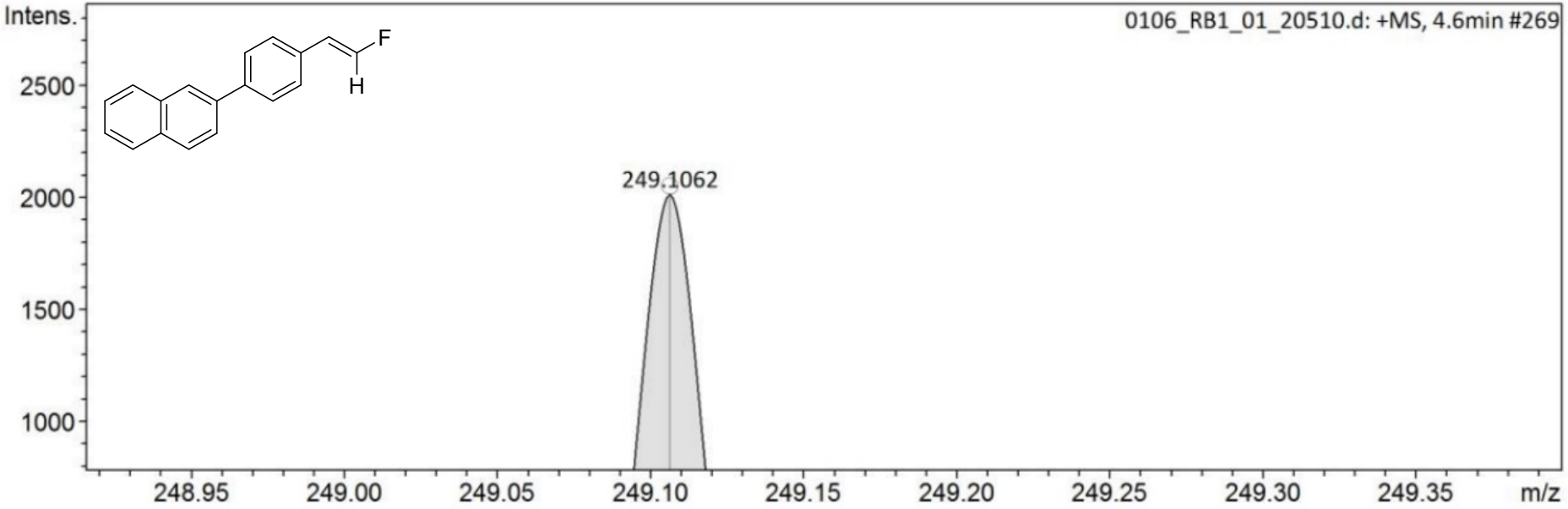
Analysis Name D:\LXMS\0106_RB1_01_20510.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0106

Operator Demo User
Instrumen compact 8255754.2017 6

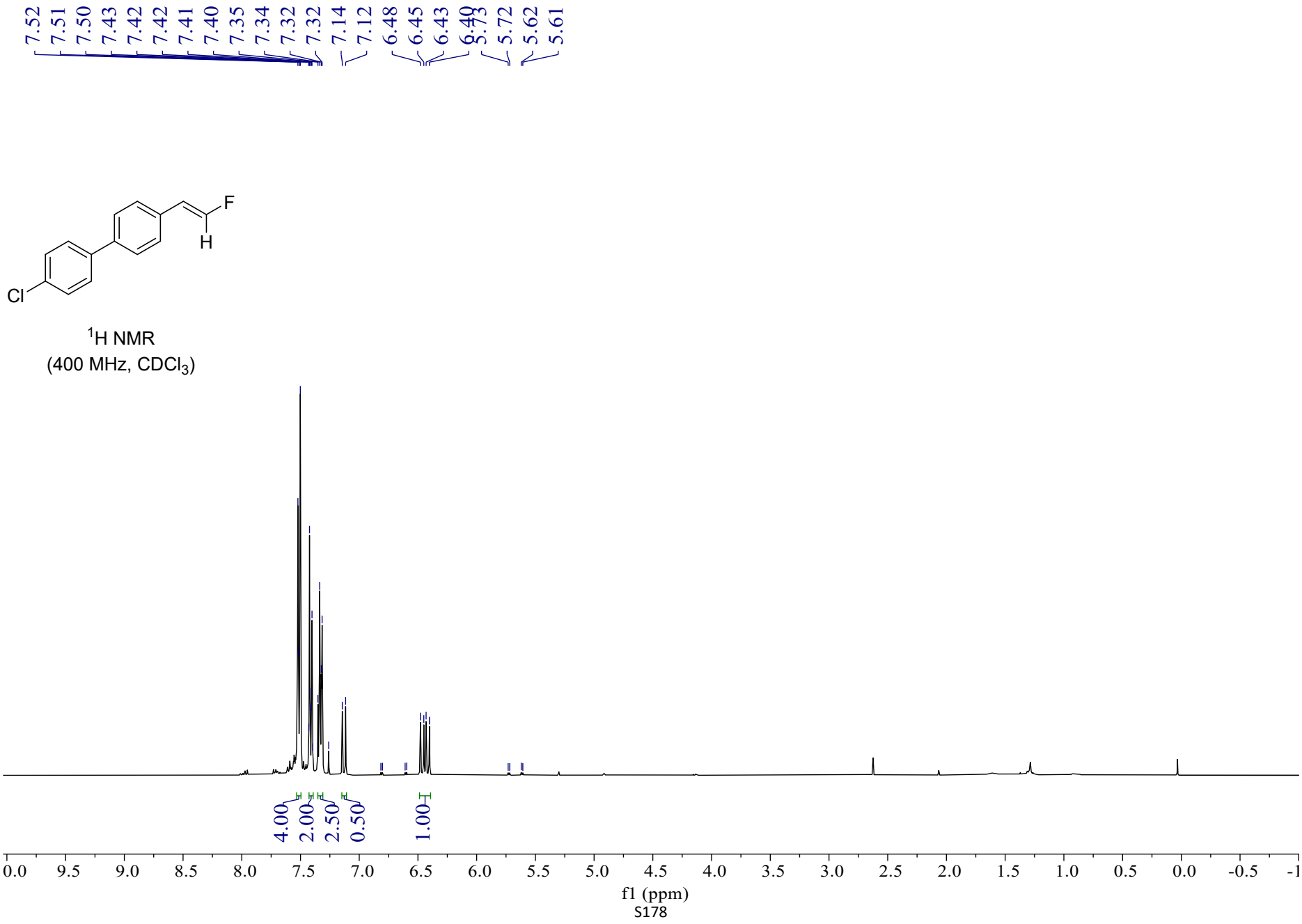
Comment

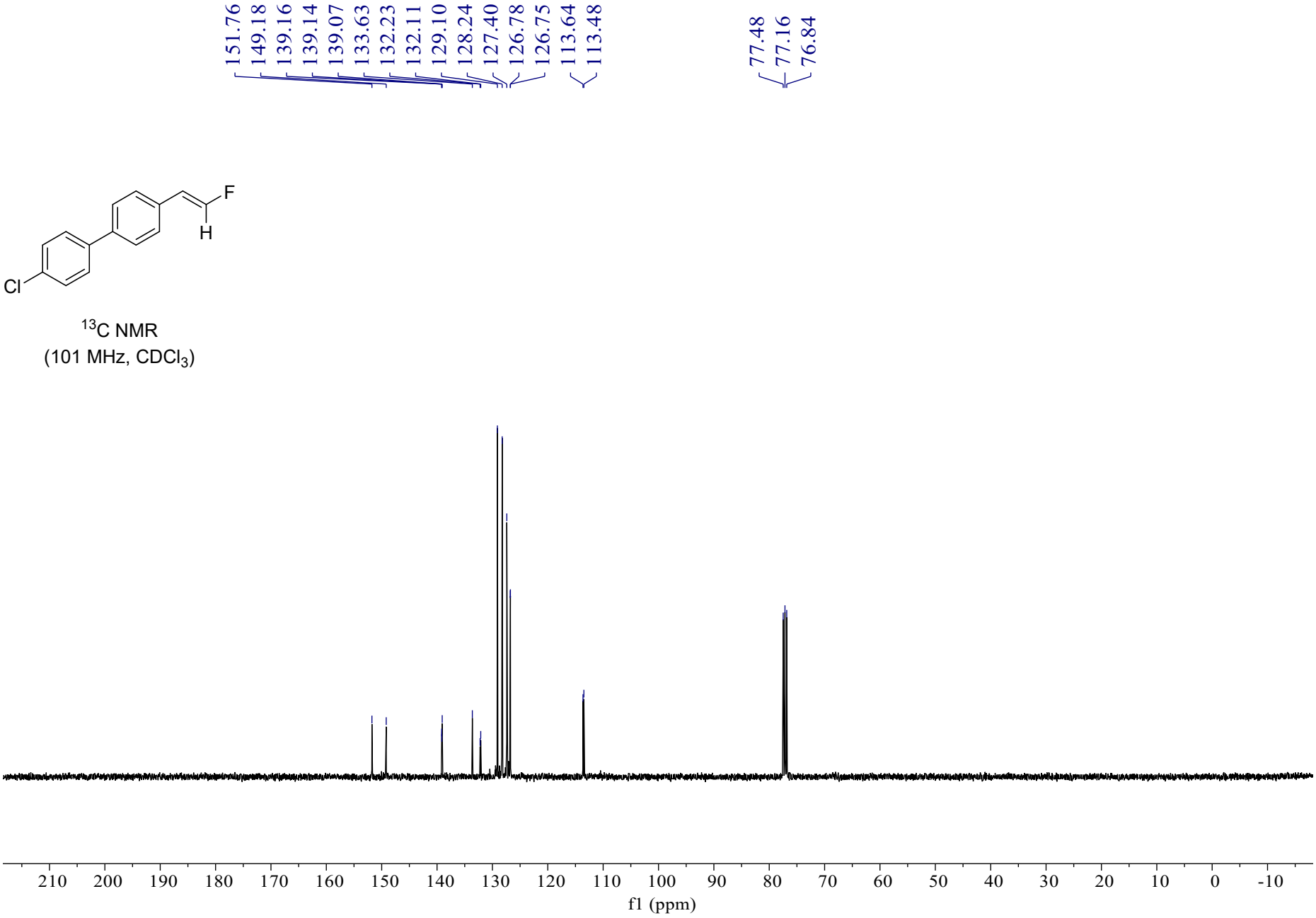
Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min

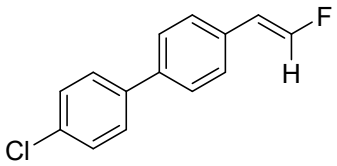


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
249.1062	1	C18H14F	249.1074	4.8	n.a.	1	100.00	11.5	even	ok


7.52
7.51
7.50
7.43
7.42
7.42
7.41
7.40
7.35
7.34
7.32
7.32
7.14
7.12
6.48
6.45
6.43
6.40
5.73
5.72
5.62
5.61
F
H
Cl
1H NMR
(400 MHz, CDCl3)
4.00
2.00
2.50
0.50
1.00
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)



^{13}C NMR
(101 MHz, $CDCl_3$)



^{19}F NMR
(376 MHz, $CDCl_3$)

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\LXMS\0106_RA6_01_20507.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0106

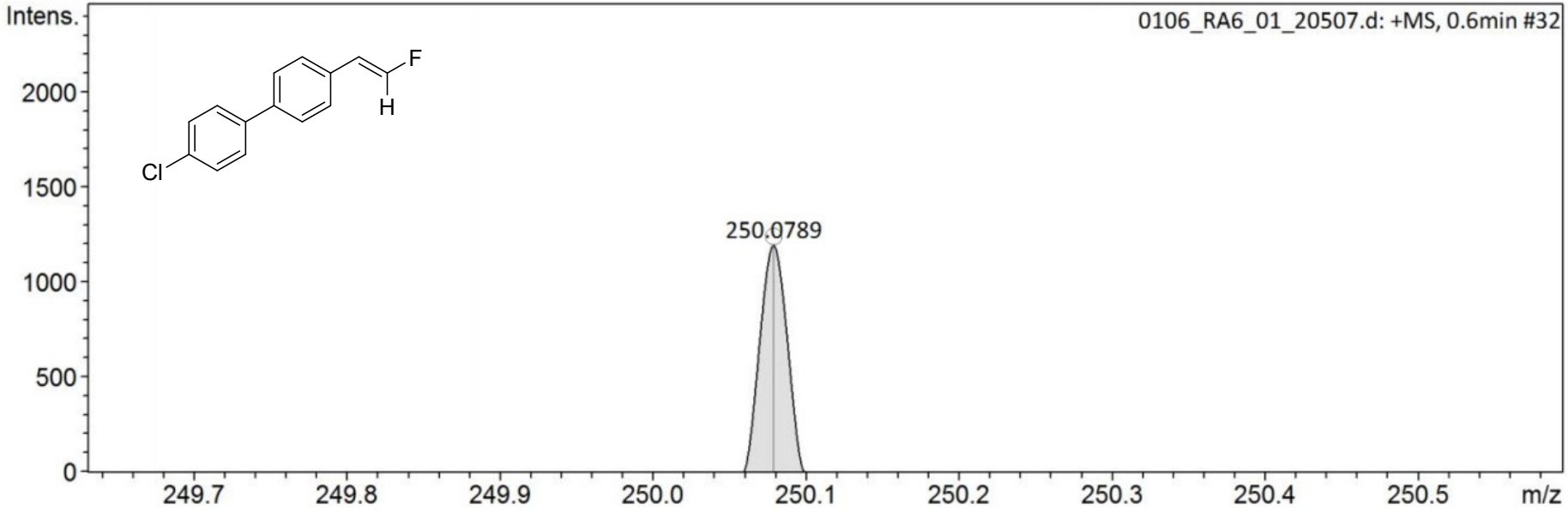
Comment

Acquisition D 2023-01-09 9:09:44

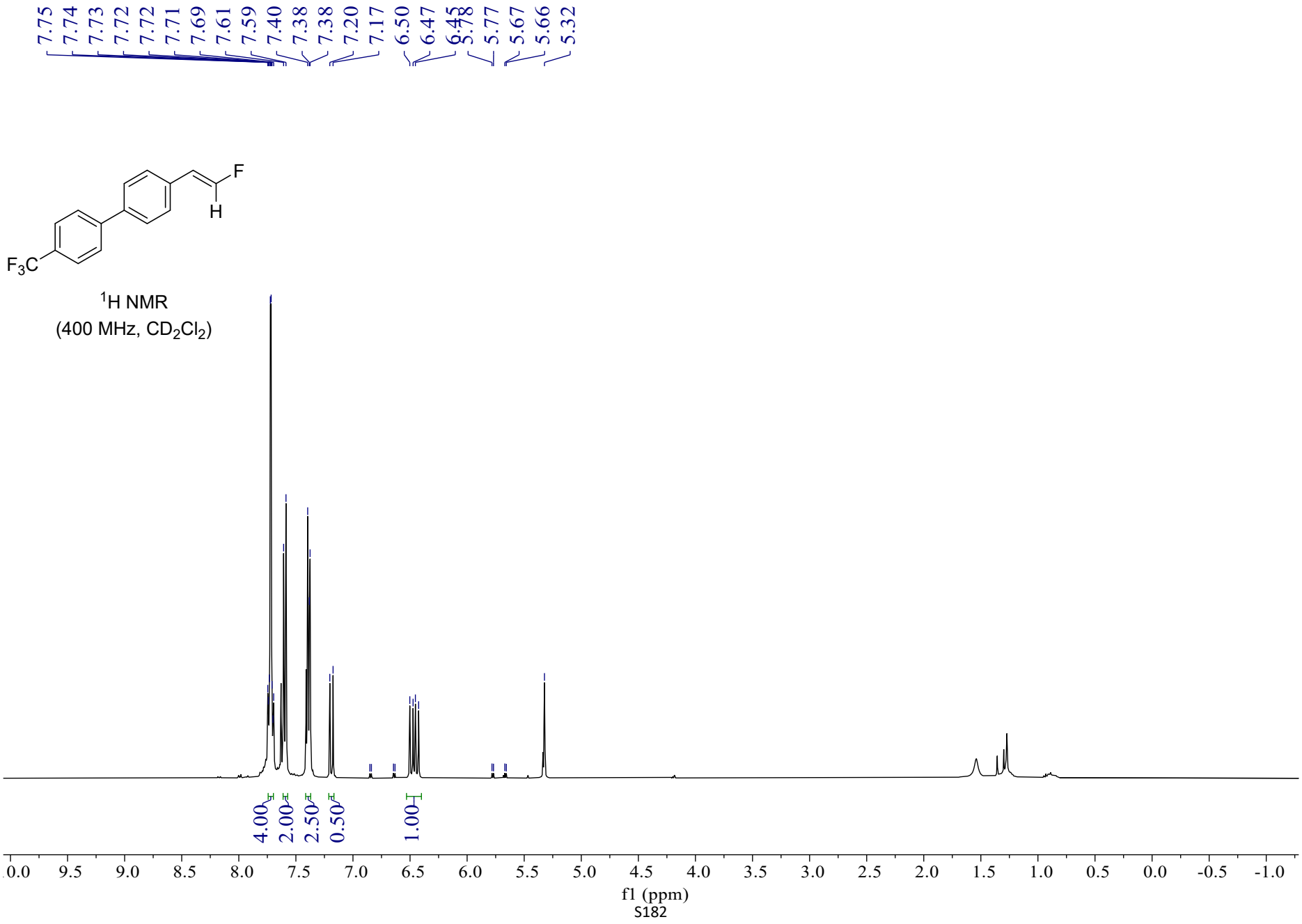
Operator Demo User
Instrumen compact 8255754.2017 6

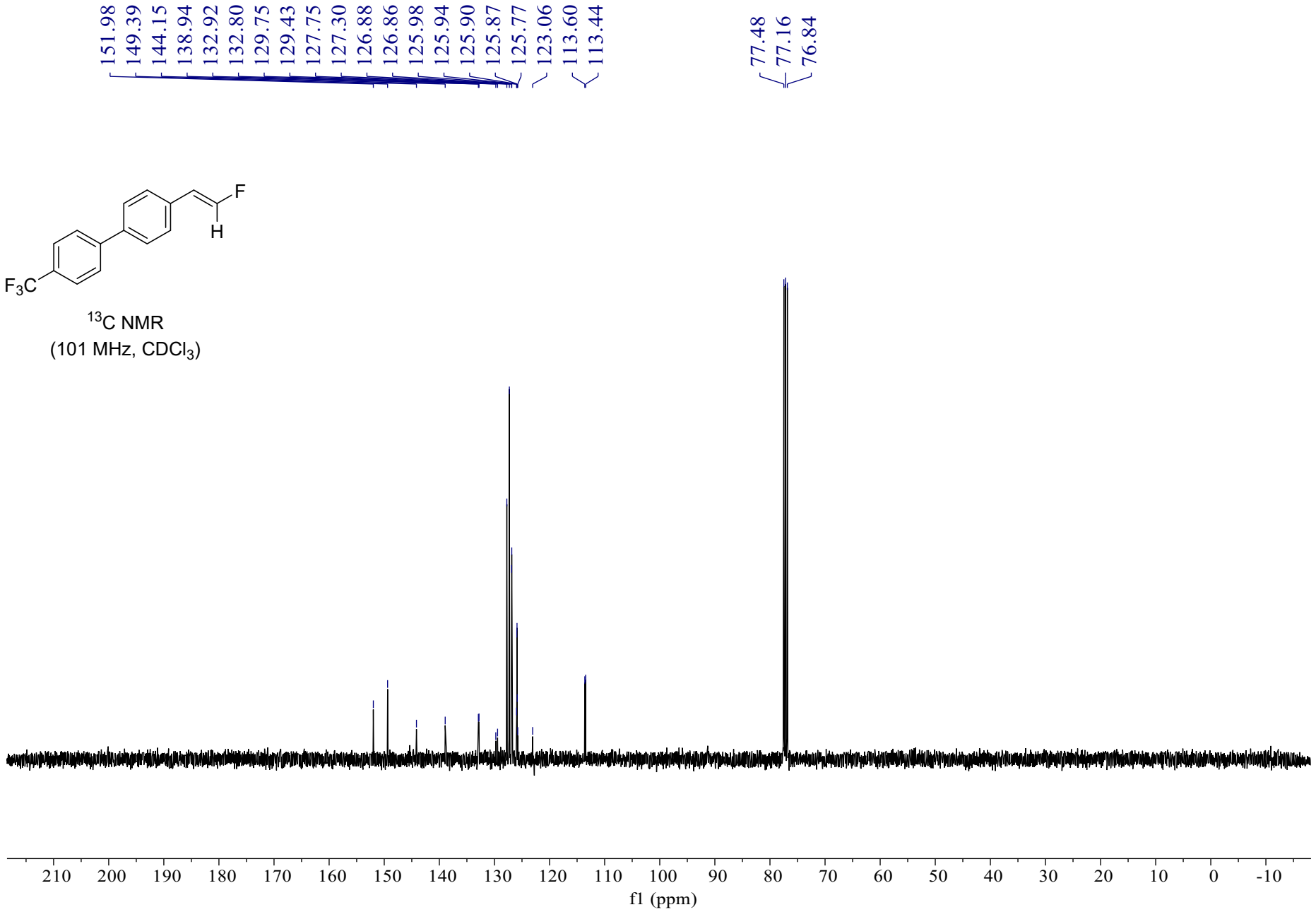
Acquisition Paramet

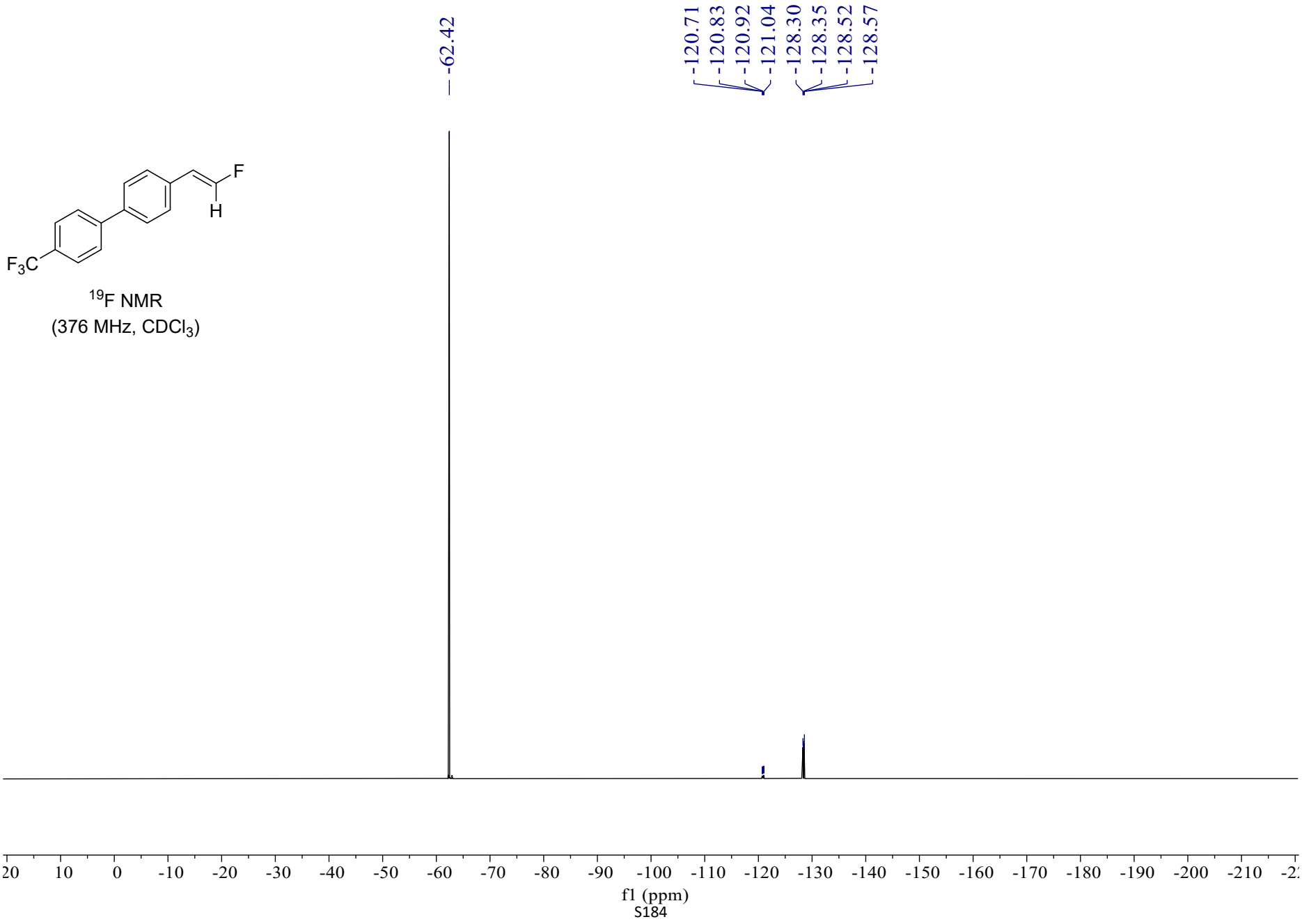
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
250.0789	1	C14H14ClFN	250.0793	1.6	n.a.	1	100.00	7.5	even		ok


7.75
7.74
7.73
7.72
7.72
7.71
7.69
7.61
7.59
7.40
7.38
7.38
7.20
7.17
6.50
6.47
6.45
5.78
5.77
5.67
5.66
5.32
F
H
F3C
1H NMR
(400 MHz, CD2Cl2)
4.00
2.00
2.50
0.50
1.00
f1 (ppm)


151.98
149.39
144.15
138.94
132.92
132.80
129.75
129.43
127.75
127.30
126.88
126.86
125.98
125.94
125.90
125.87
125.77
123.06
113.60
113.44
77.48
77.16
76.84
F
H
F3C
13C NMR
(101 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


-62.42
-120.71
-120.83
-120.92
-121.04
-128.30
-128.35
-128.52
-128.57
F
H
F3C
19F NMR
(376 MHz, CDCl3)
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

Mass Spectrum SmartFormula Report

Analysis Info

Acquisition D 2023-01-09 10:54:33

Analysis Name D:\LXMS\0106_RC4_01_20521.d

Method LC_NO UV_P50-1500_6MIN.m

Operator Demo User

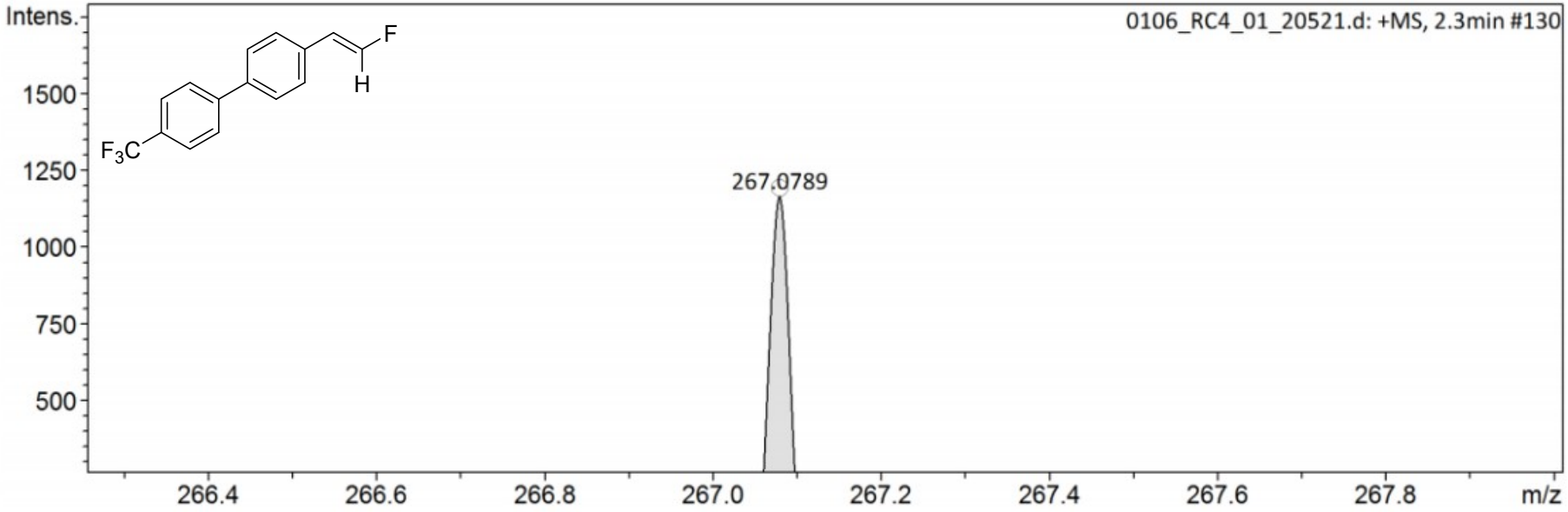
Sample Name 0106

Instrumen compact 8255754.2017 6

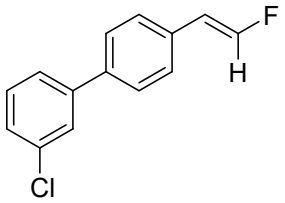
Comment

Acquisition Paramet

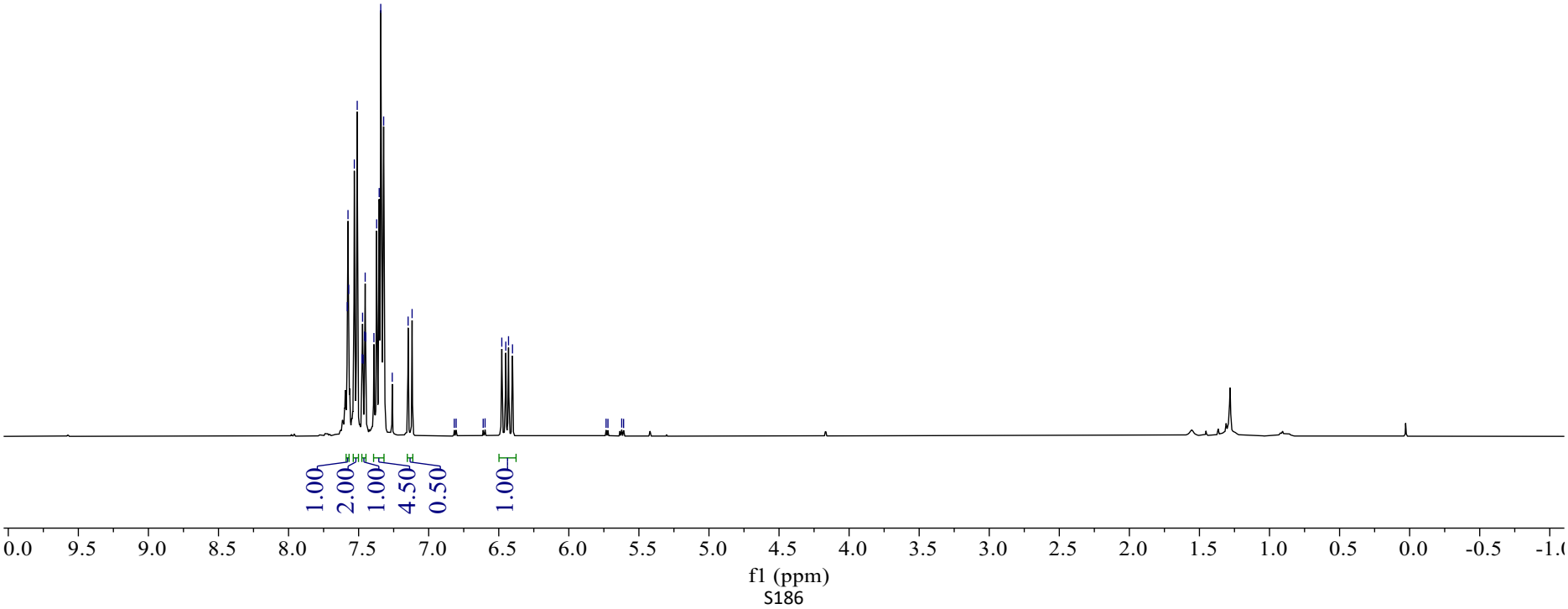
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min

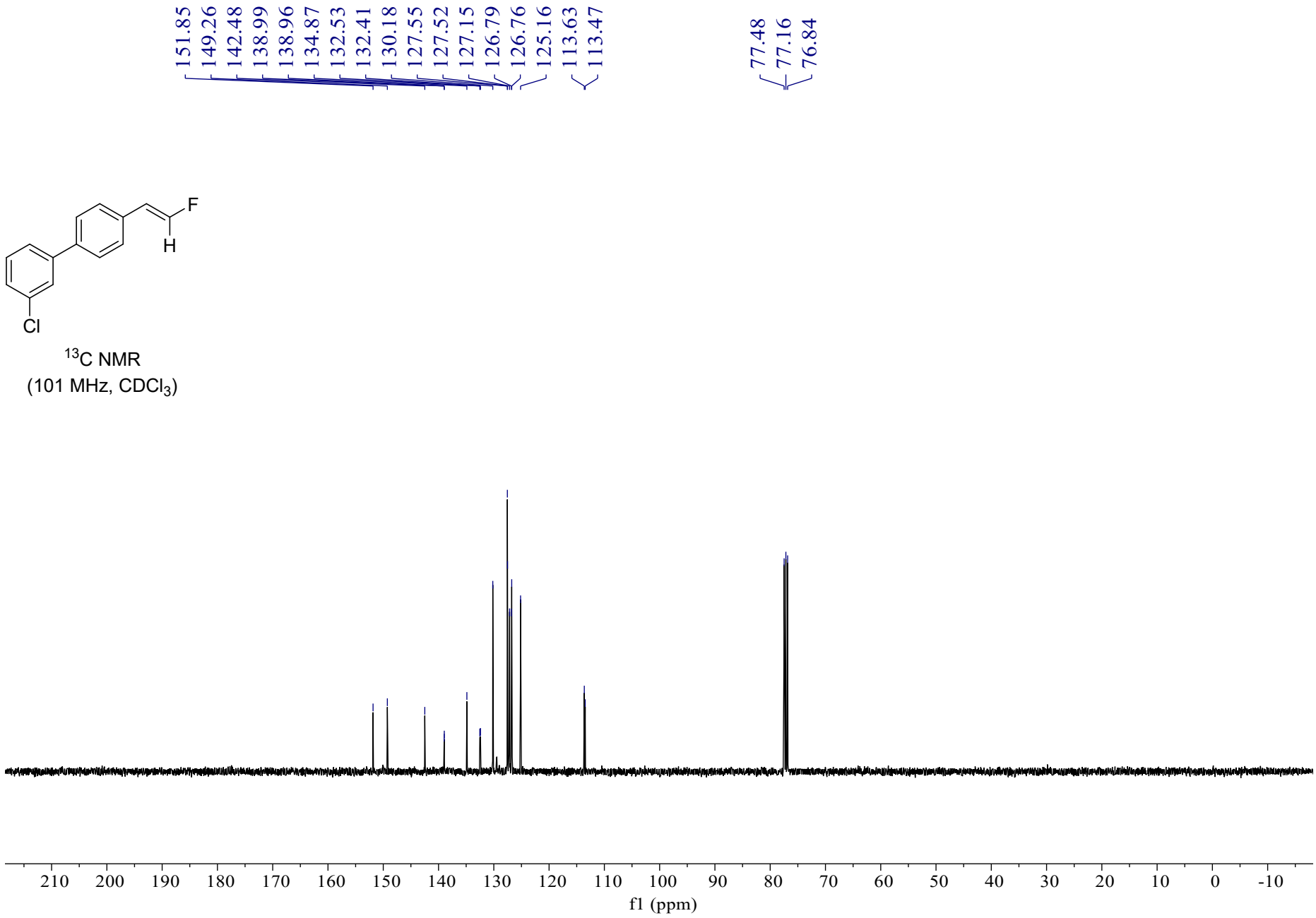


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
267.0789	1	C15H11F4	267.0791	1.1	n.a.	1	100.00	8.5	even		ok

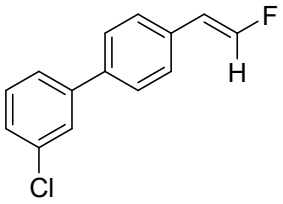


^{1}H NMR
(400 MHz, $CDCl_3$)





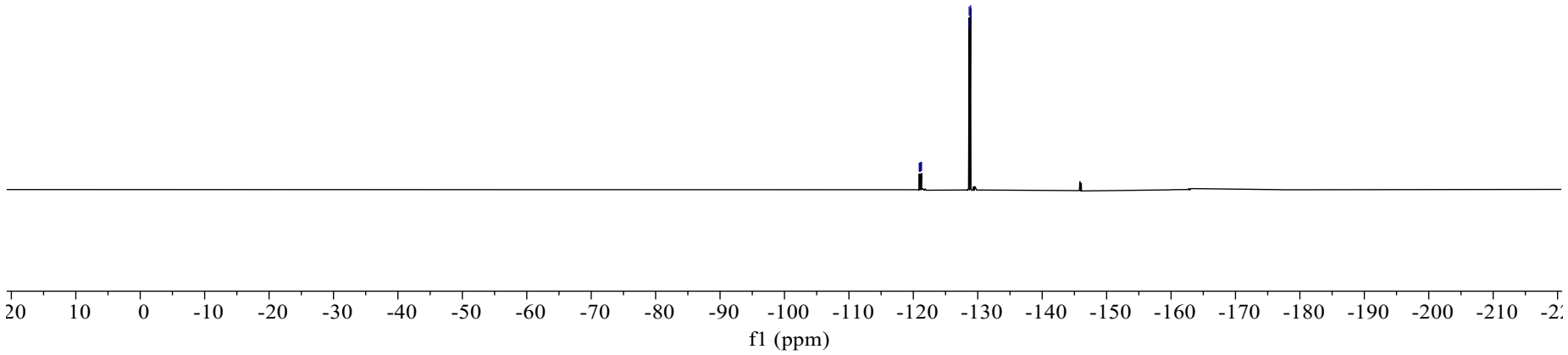
^{13}C NMR
(101 MHz, $CDCl_3$)



^{19}F NMR

(376 MHz, $CDCl_3$)

-120.93
-121.04
-121.15
-121.26
-128.62
-128.67
-128.84
-128.89



Mass Spectrum SmartFormula Report

Analysis Info

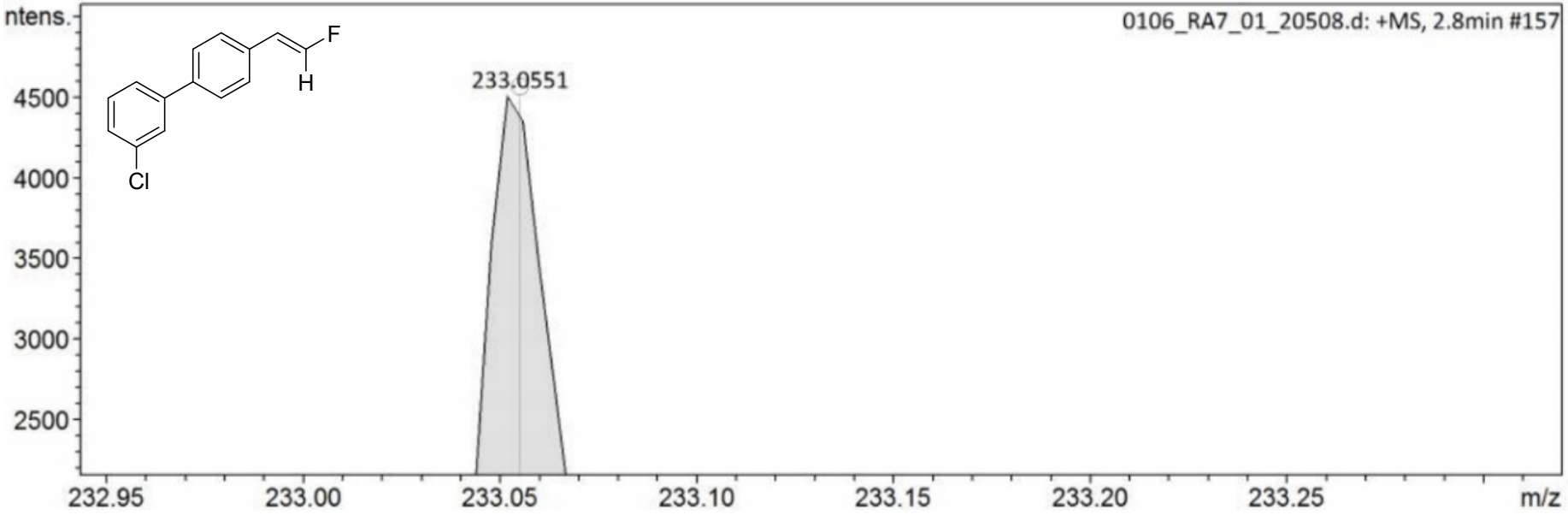
Acquisition D 2023-01-09 9:17:19

Analysis Name D:\LXMS\0106_RA7_01_20508.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0106
Comment

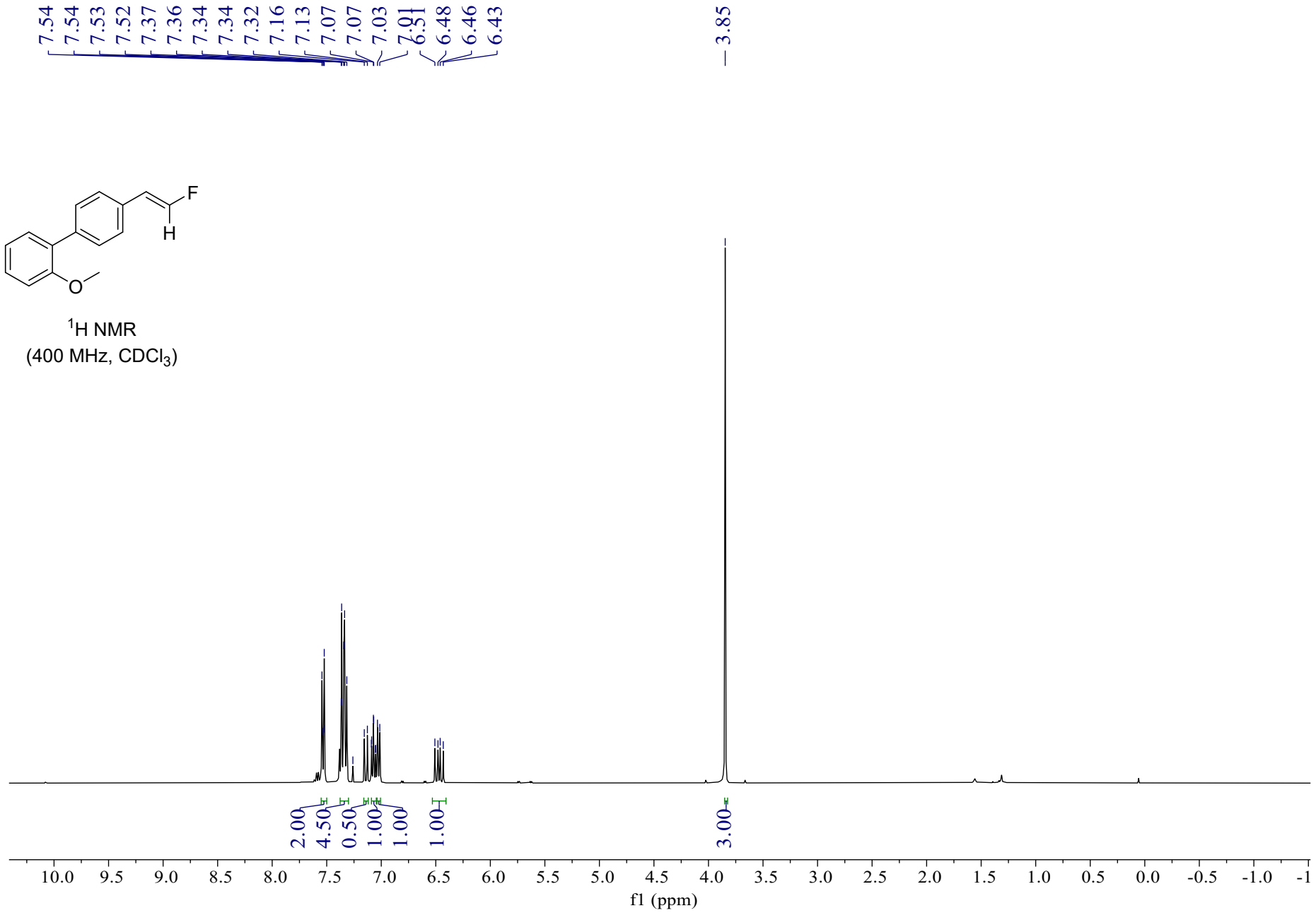
Operator Demo User
Instrumen compact 8255754.2017 6

Acquisition Paramet

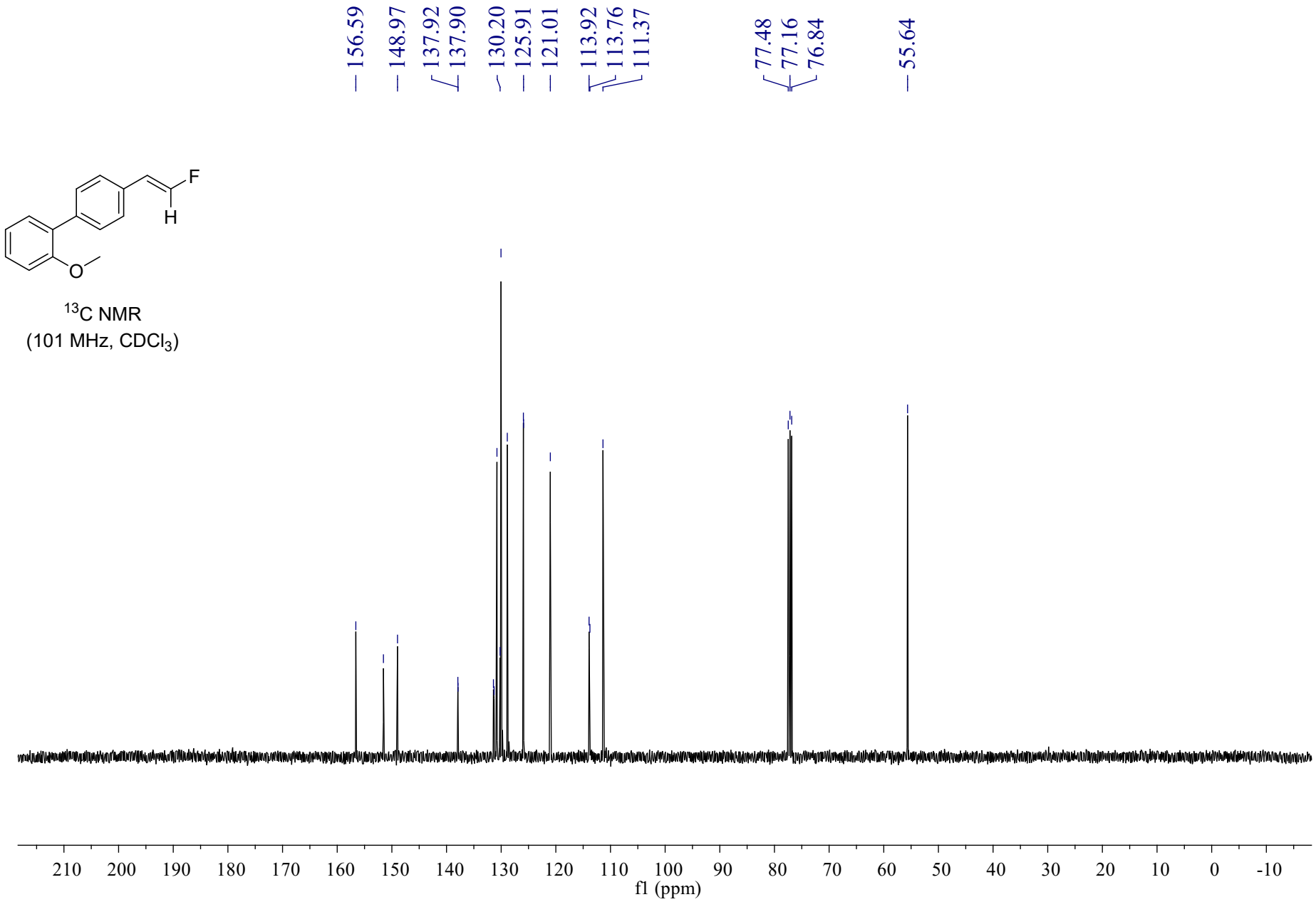
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min

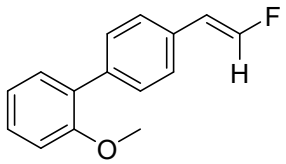


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
233.0551	1	C14H11ClF	233.0528	-9.9	130.5	1	100.00	8.5	even	ok



^{1}H NMR
(400 MHz, $CDCl_3$)


156.59
148.97
137.92
137.90
130.20
125.91
121.01
113.92
113.76
111.37
77.48
77.16
76.84
55.64
F
H
O
^{13}C NMR
(101 MHz, $CDCl_3$)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



^{19}F NMR
(376 MHz, $CDCl_3$)

Mass Spectrum SmartFormula Report

Analysis Info

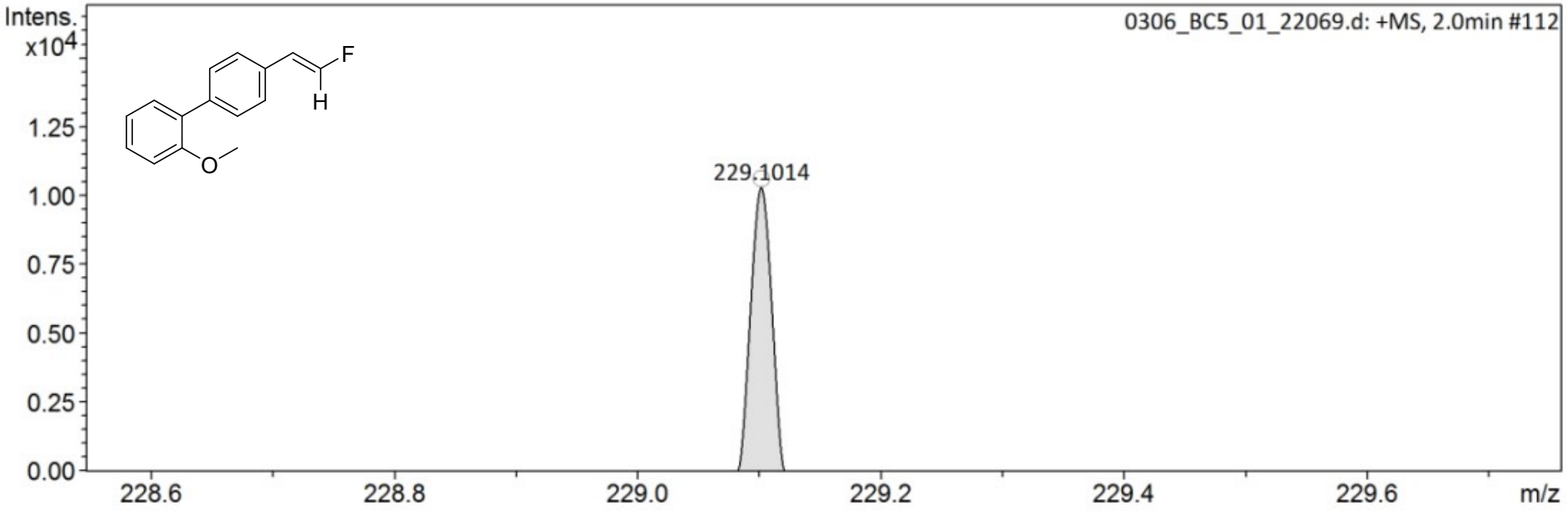
Acquisition D 2023-03-10 16:47:41

Analysis Name D:\LXMS\0306_BC5_01_22069.d
Method LC_NO UV_P50-1500_10MIN.m
Sample Name 0306
Comment

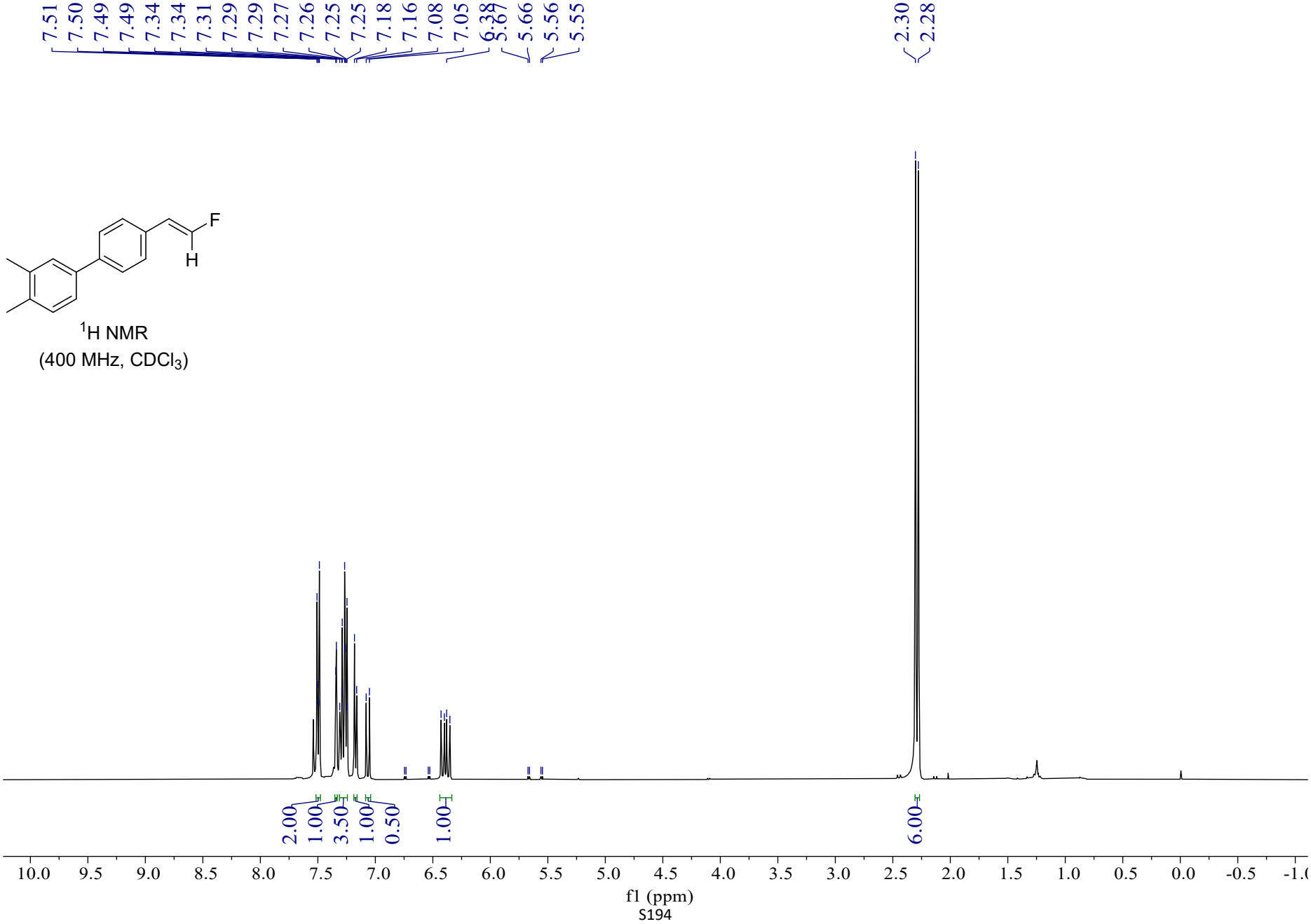
Operator Demo User
Instrumen compact 8255754.2017 6

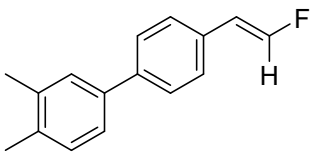
Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min

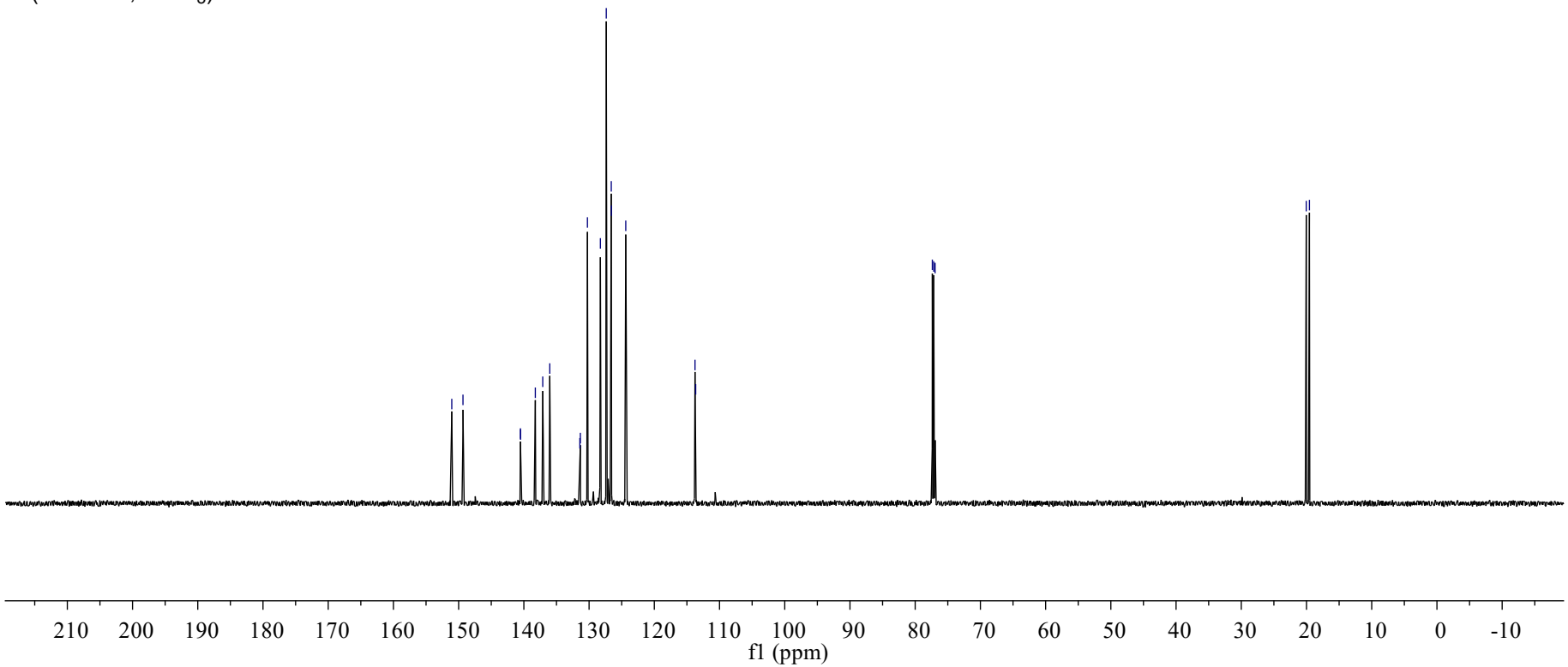


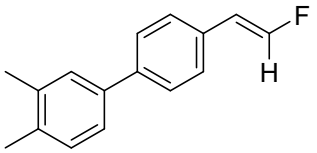
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥	Conf	N-Rule
229.1014	1	C15H14FO	229.1023	3.8	39.0		1	100.00	8.5	even		ok


7.51
7.50
7.49
7.49
7.34
7.34
7.31
7.29
7.29
7.27
7.26
7.25
7.25
7.18
7.16
7.08
7.05
6.38
6.37
5.66
5.56
5.55
2.30
2.28
F
H
1H NMR
(400 MHz, CDCl3)
2.00
1.00
3.50
1.00
0.50
1.00
6.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

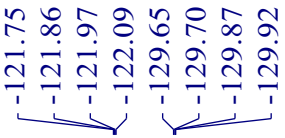


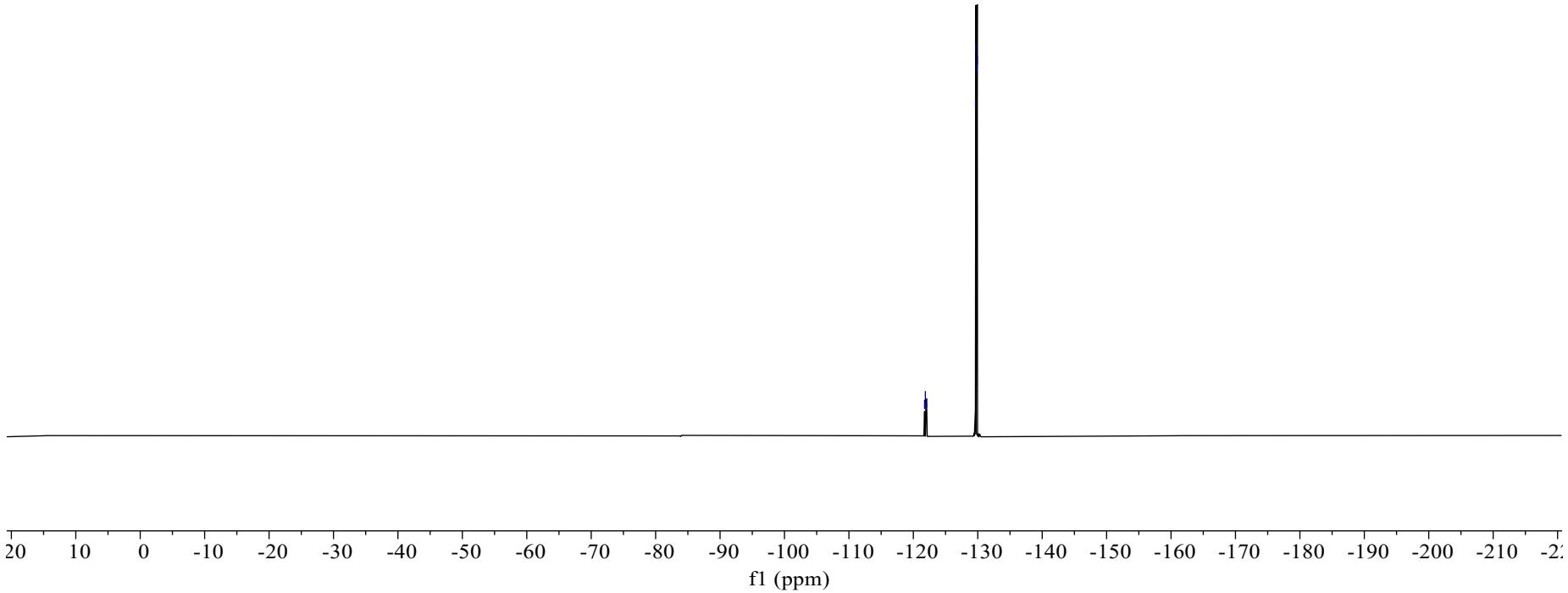
5u; ^{13}C NMR
(151 MHz, $CDCl_3$)





^{19}F NMR
(376 MHz, $CDCl_3$)





Mass Spectrum SmartFormula Report

Analysis Info

Acquisition D 2023-01-09 9:24:39

Analysis Name D:\LXMS\0106_RA8_01_20509.d

Method LC_NO UV_P50-1500_6MIN.m

Operator Demo User

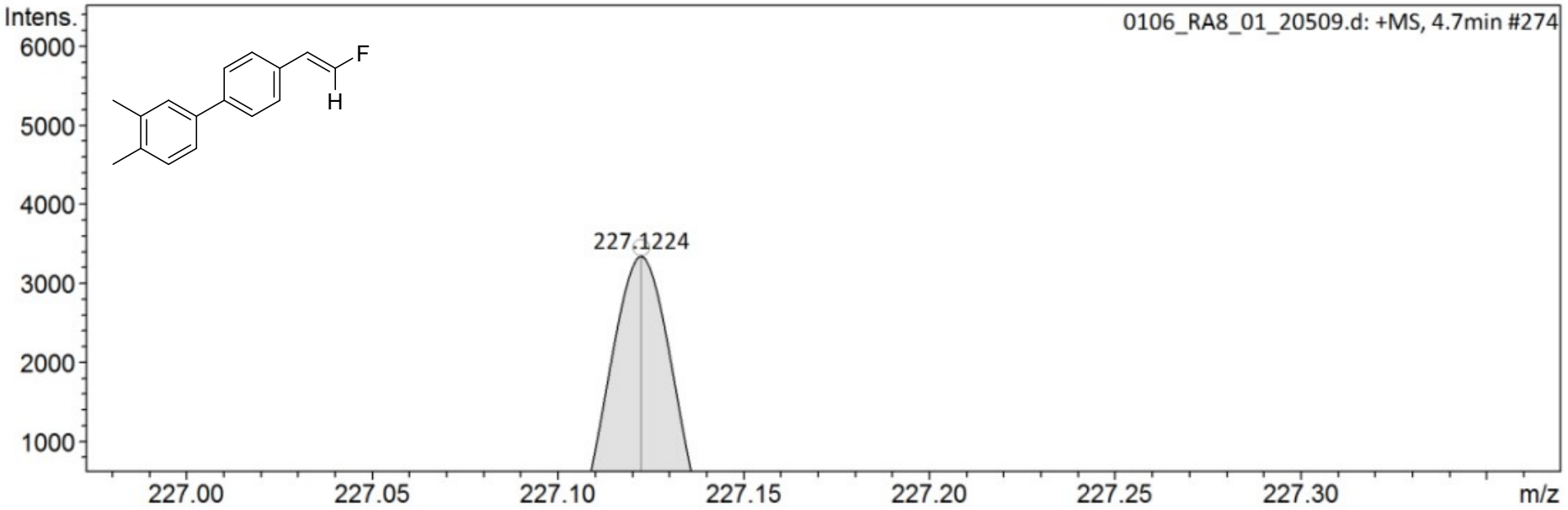
Sample Name 0106

Instrumen compact 8255754.2017 6

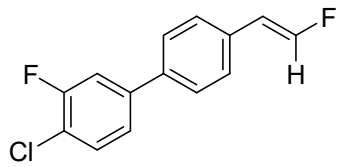
Comment

Acquisition Paramet

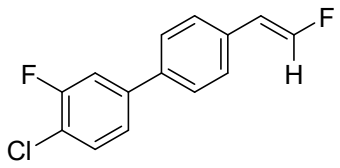
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min



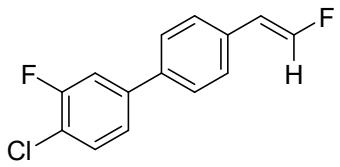
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
227.1224	1	C16H16F	227.1231	3.0	n.a.	1	100.00	8.5	even		ok



^{1}H NMR
(400 MHz, $CDCl_3$)

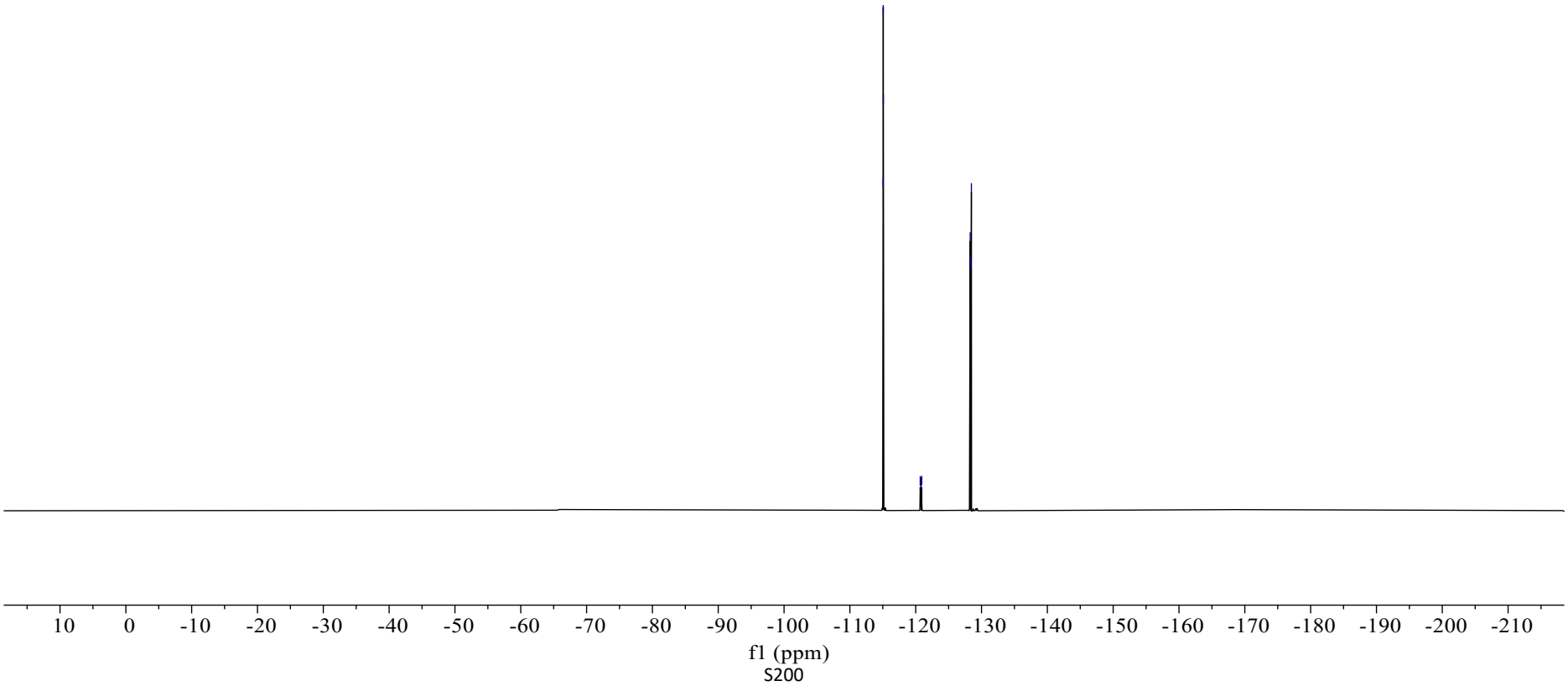


^{13}C NMR
(101 MHz, $CDCl_3$)



^{19}F NMR
(565 MHz, $CDCl_3$)

-115.05
-115.07
-115.09
-120.69
-120.77
-120.83
-120.91
-128.28
-128.31
-128.43
-128.46



Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\LXMS\0106_RB2_01_20511.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0106

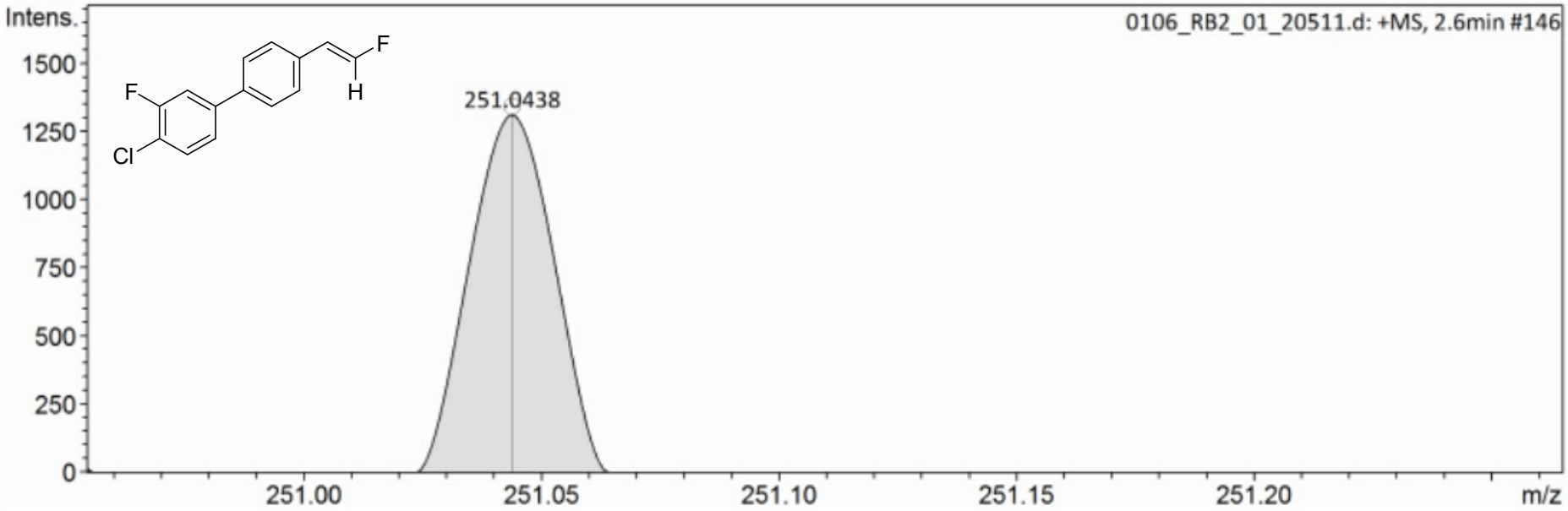
Comment

Acquisition D 2023-01-09 9:39:18

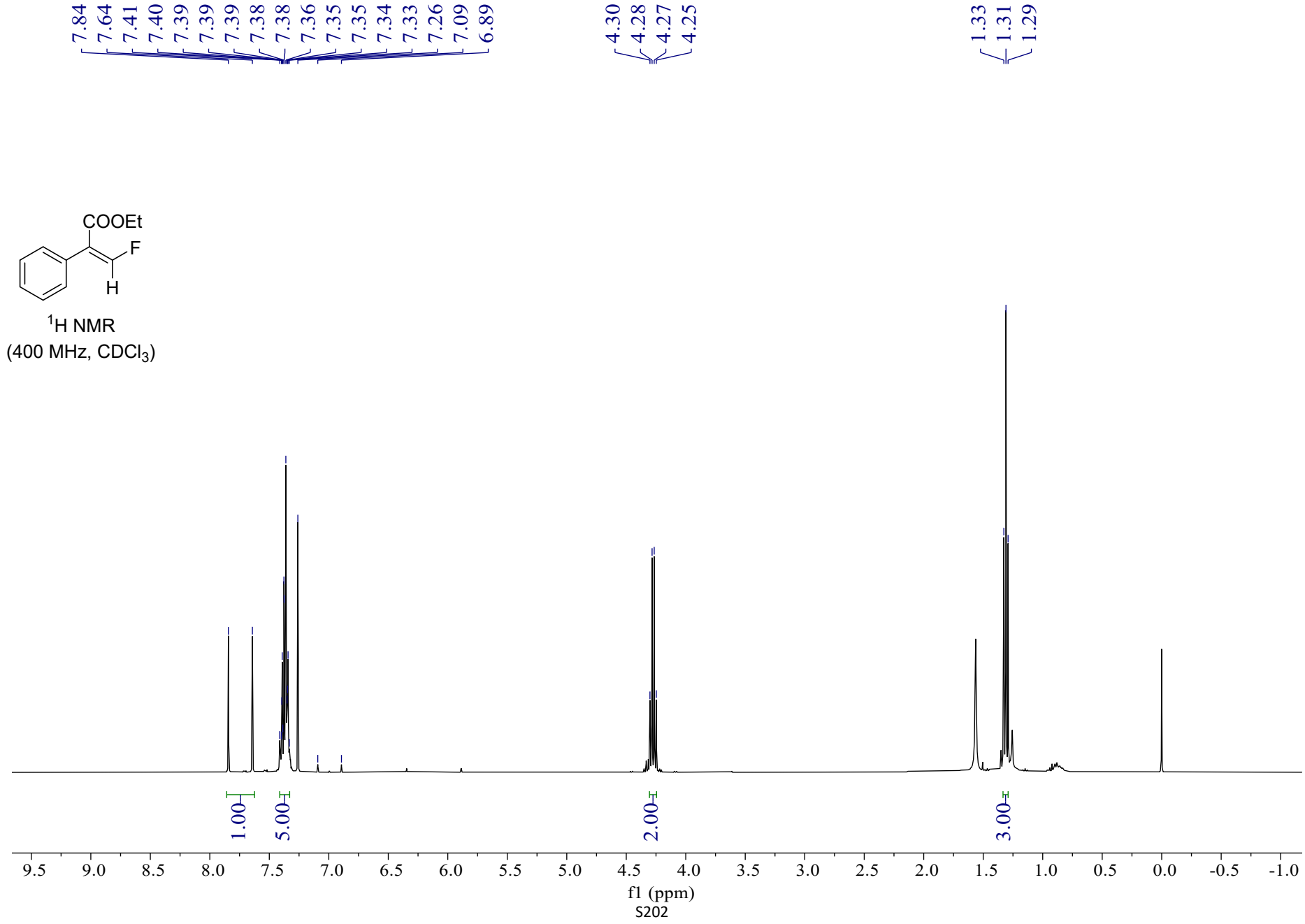
Operator Demo User
Instrumen compact 8255754.2017 6

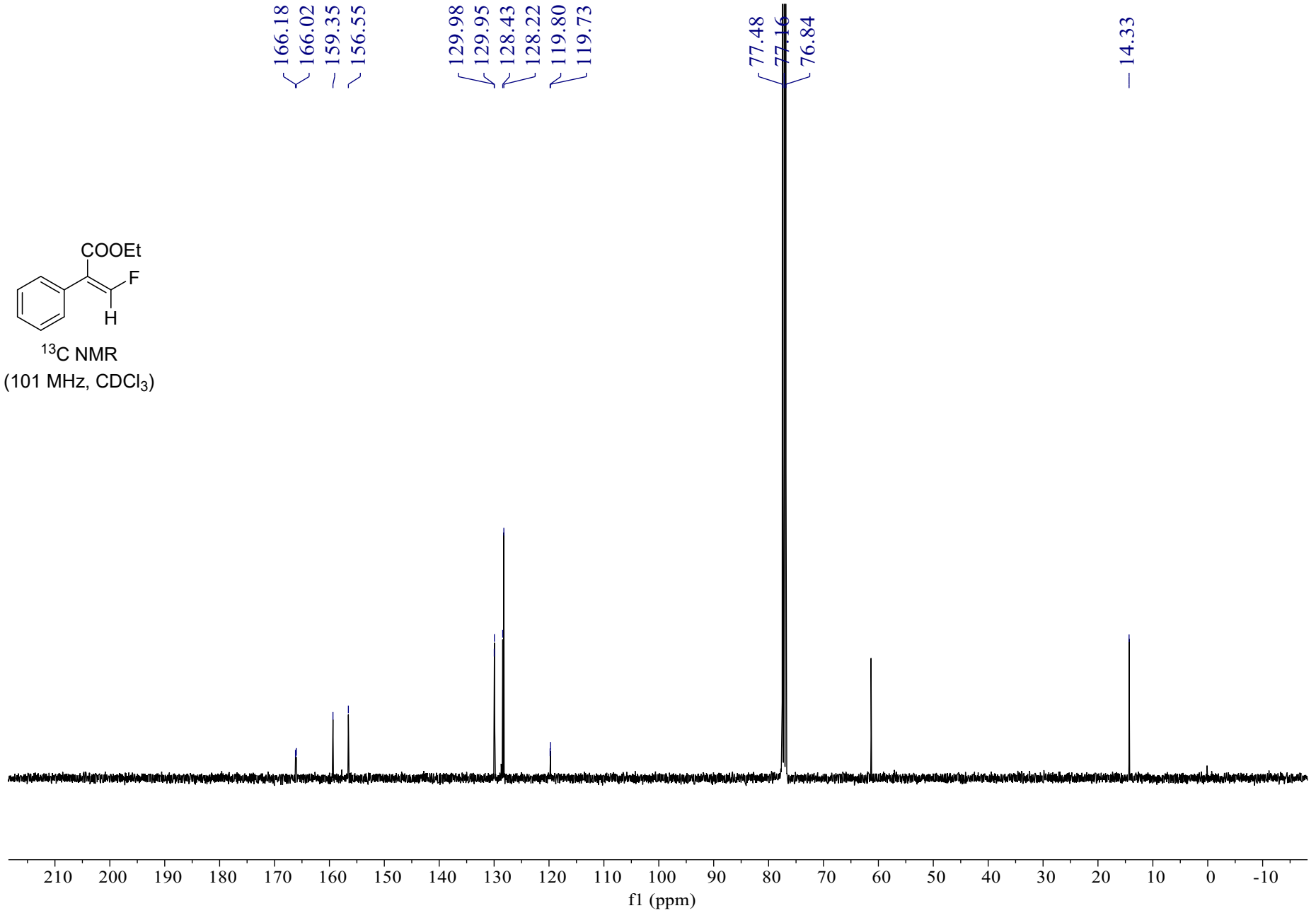
Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min

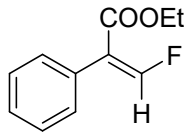


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
251.0438	1	C14H10ClF2	251.0434	-1.9	n.a.	1	100.00	8.5	even	ok


7.84
7.64
7.41
7.40
7.39
7.39
7.39
7.38
7.38
7.36
7.35
7.35
7.34
7.33
7.26
7.09
6.89
4.30
4.28
4.27
4.25
1.33
1.31
1.29
COOEt
F
H
1H NMR
(400 MHz, CDCl3)
1.00
5.00
2.00
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

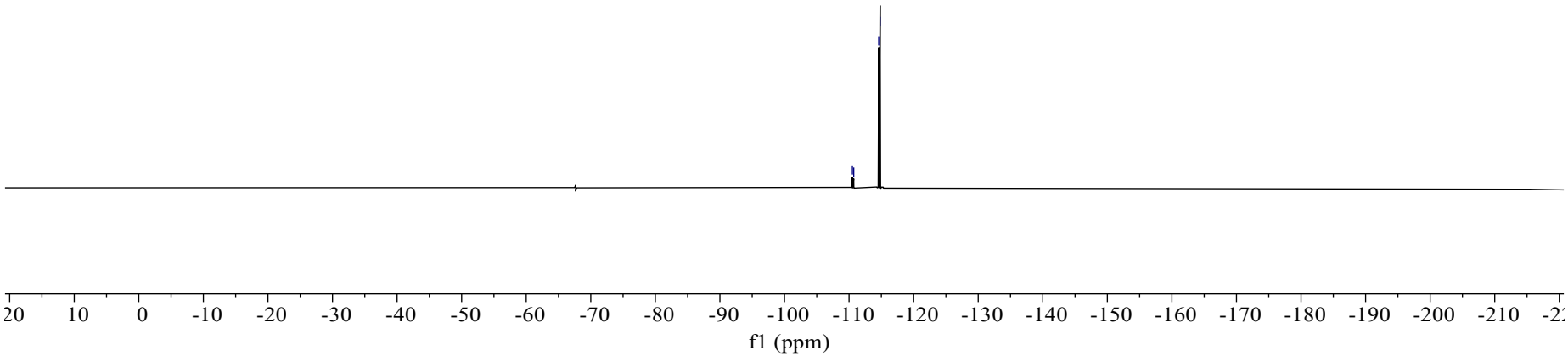

166.18
166.02
159.35
156.55
129.98
129.95
128.43
128.22
119.80
119.73
77.48
77.16
76.84
14.33
COOEt
F
H
13C NMR
(101 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

-110.52
-110.73
-114.59
-114.80

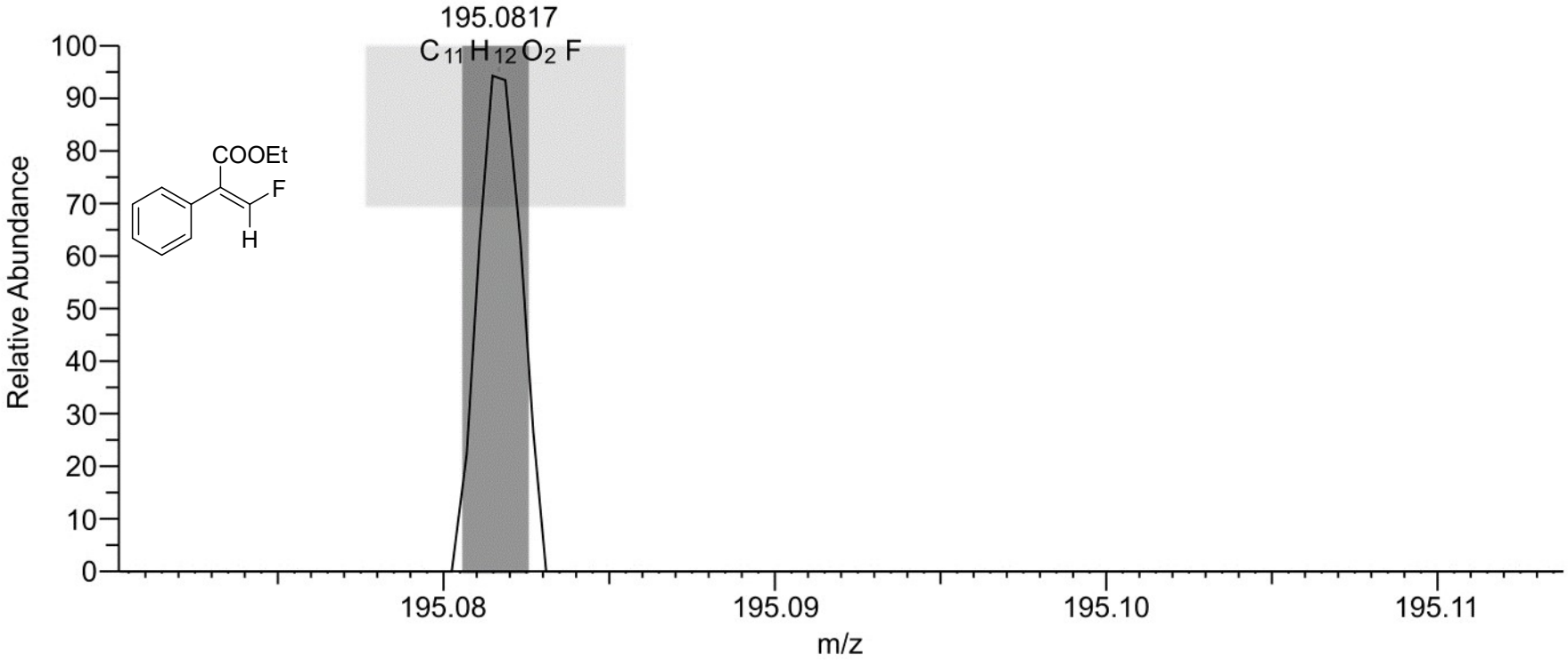


^{19}F NMR

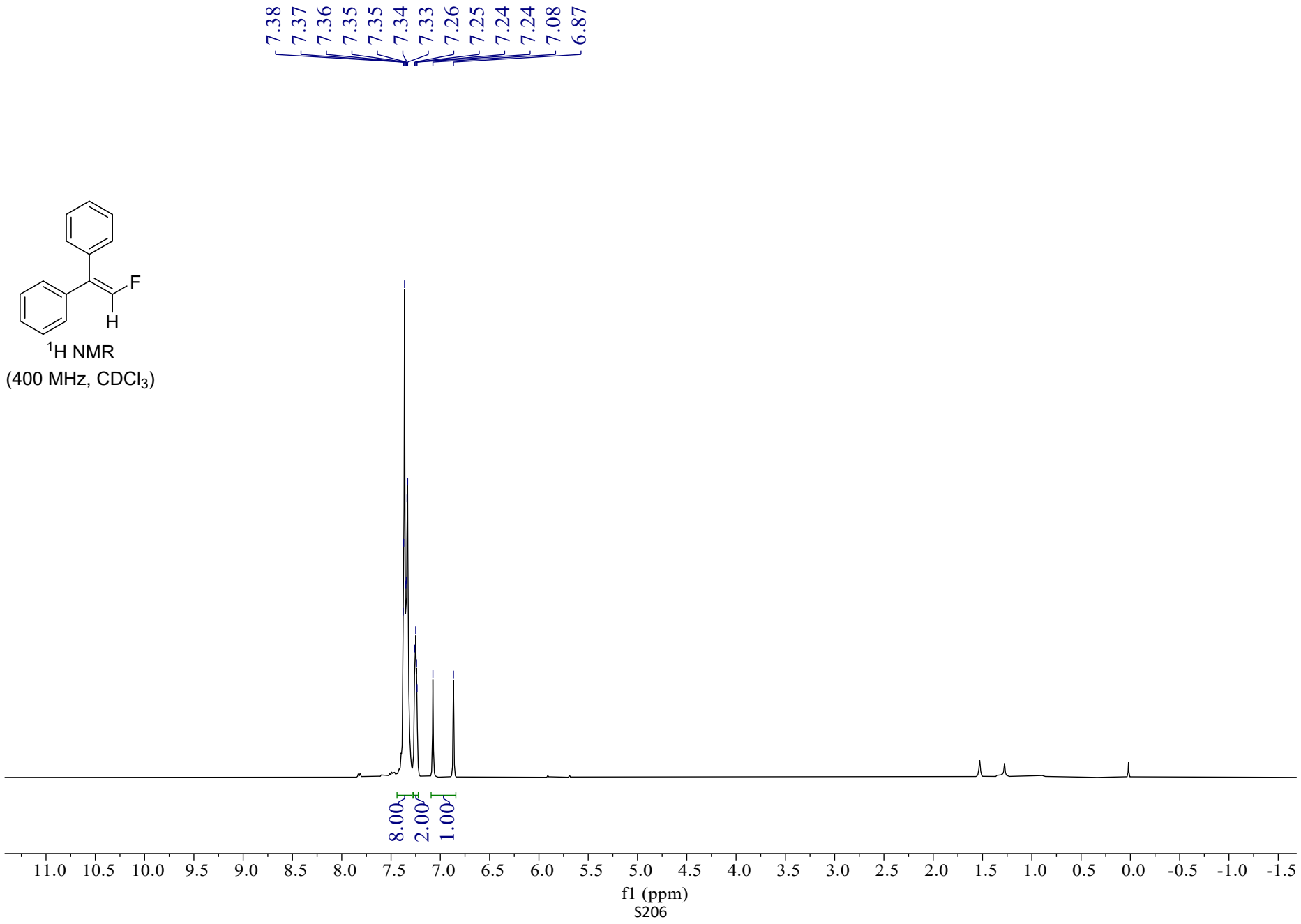
(376 MHz, $CDCl_3$)

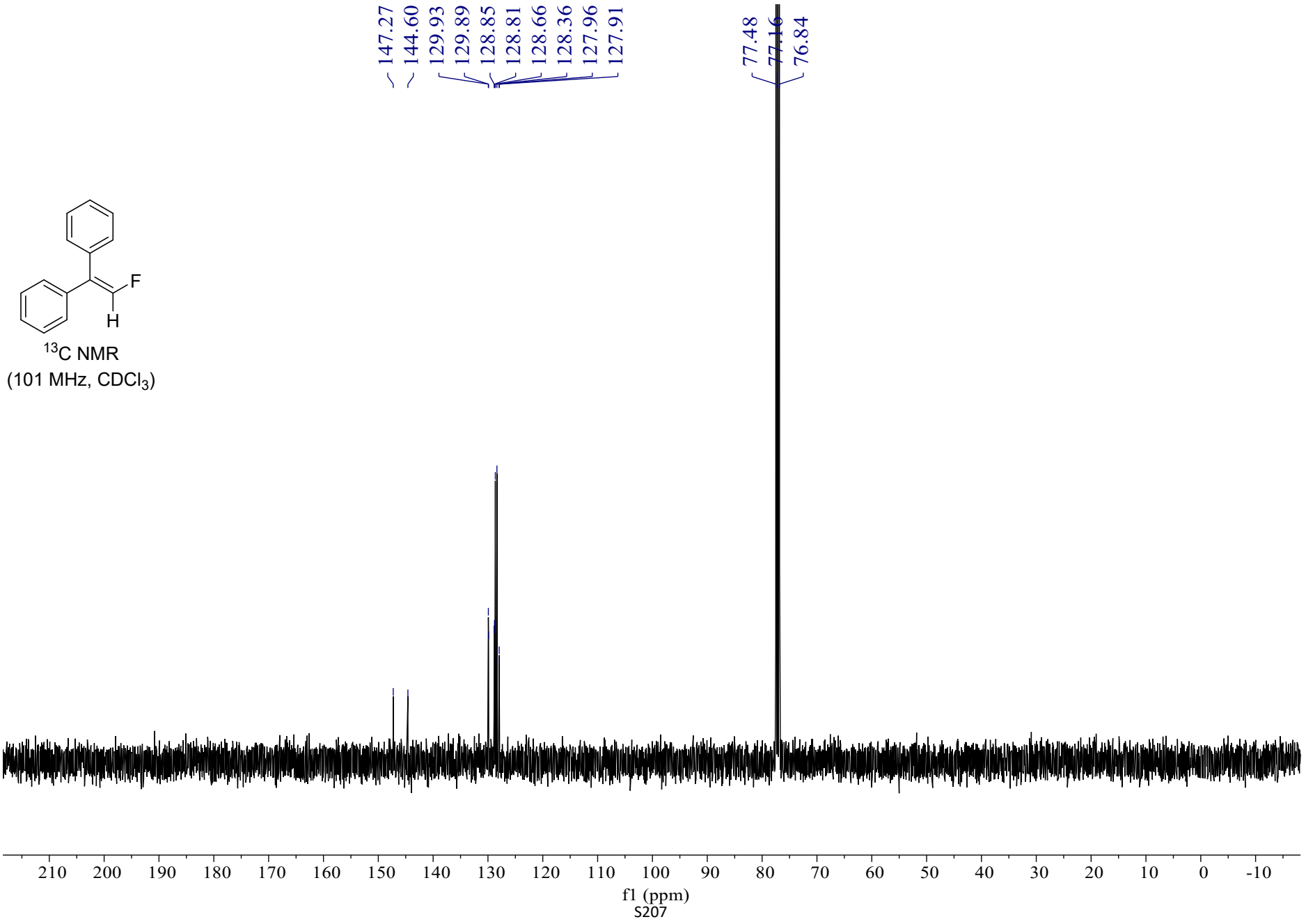


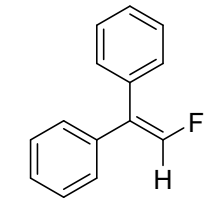
LX-13 #31 RT: 0.23 AV: 1 NL: 6.57E4
T: FTMS + p ESI Full ms [100.0000-1500.0000]



Peak M...	Display...	S Fit	RDB	Delta [p...	Theo....	Rank	Combin...	# Matc...	# Misse...	MS Cov...	Pattern...	MSMS...
195.0817	$C_{11}H_{12}O_2F$	90.83281057123 94	5.50	0.65	195.08158	1	99.52	1	0	100	100	(Collection)


7.38
7.37
7.36
7.35
7.35
7.34
7.33
7.26
7.25
7.24
7.24
7.08
6.87
F
H
^{1}H NMR
(400 MHz, $CDCl_3$)
8.00
2.00
1.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)


147.27
144.60
129.93
129.89
128.85
128.81
128.66
128.36
127.96
127.91
77.48
77.16
76.84
F
H
^{13}C NMR
(101 MHz, $CDCl_3$)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



^{19}F NMR

(376 MHz, $CDCl_3$)

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\LXMS\0306_BC1_01_22065.d
Method LC_NO UV_P50-1500_10MIN.m
Sample Name 0306

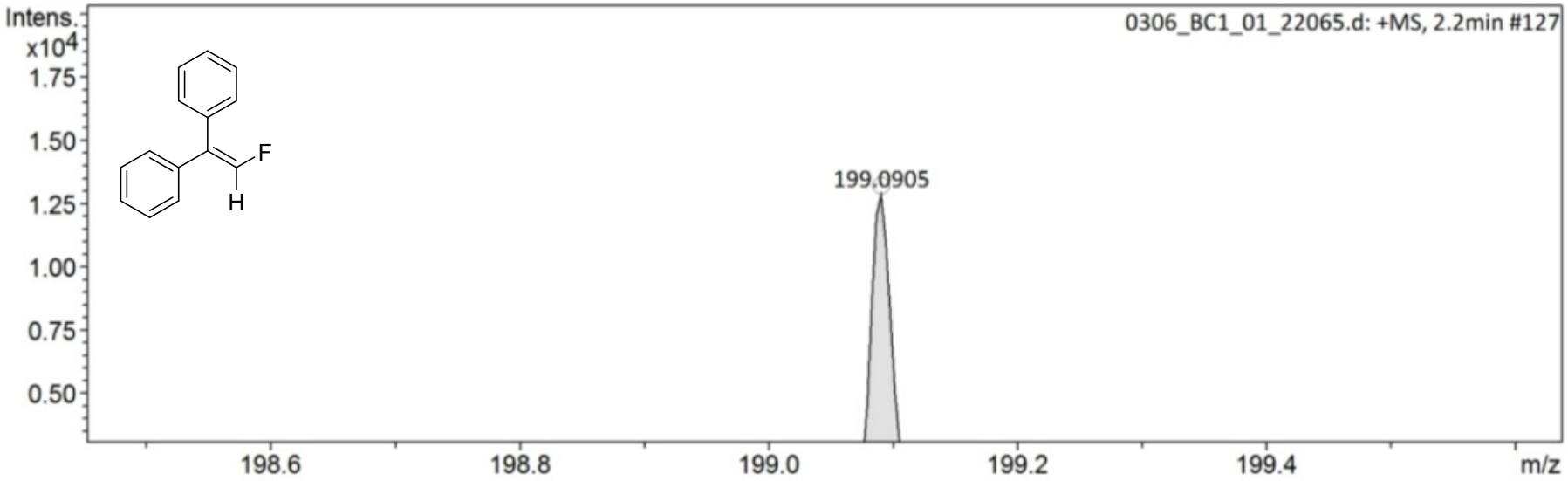
Comment

Acquisition D 2023-03-10 15:59:10

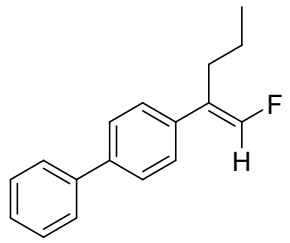
Operator Demo User
Instrumen compact 8255754.2017 6

Acquisition Paramet

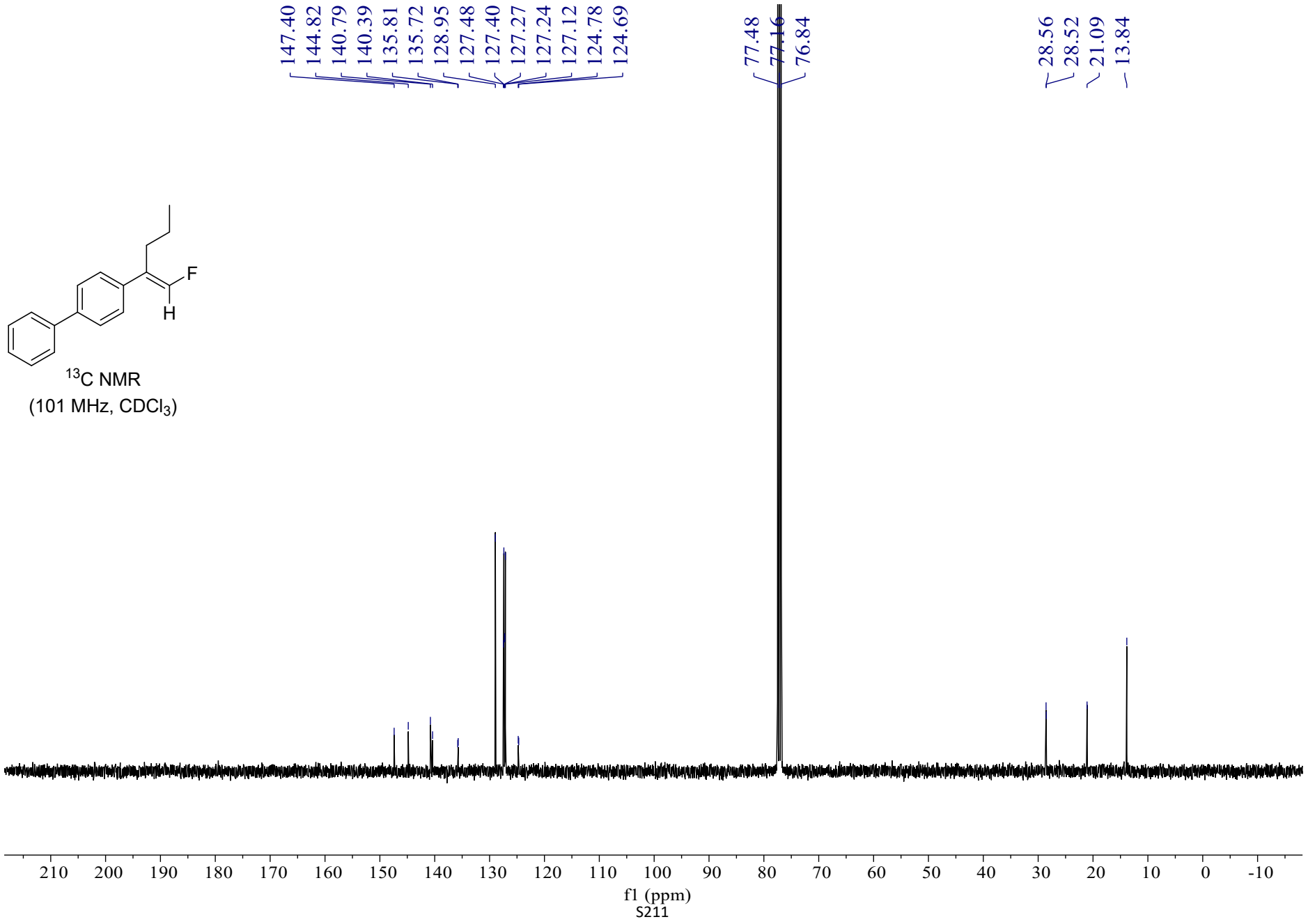
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min

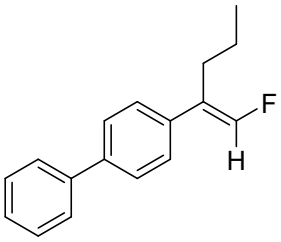


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
199.0905	1	C14H12F	199.0918	6.2	n.a.	1	100.00	8.5	even		ok



^{1}H NMR
(400 MHz, $CDCl_3$)


147.40
144.82
140.79
140.39
135.81
135.72
128.95
127.48
127.40
127.27
127.24
127.12
124.78
124.69
77.48
77.16
76.84
28.56
28.52
21.09
13.84
F
H
^{13}C NMR
(101 MHz, $CDCl_3$)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



^{19}F NMR
(376 MHz, $CDCl_3$)

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\LXMS\0306_BC2_01_22066.d
Method LC_NO UV_P50-1500_10MIN.m
Sample Name 0306

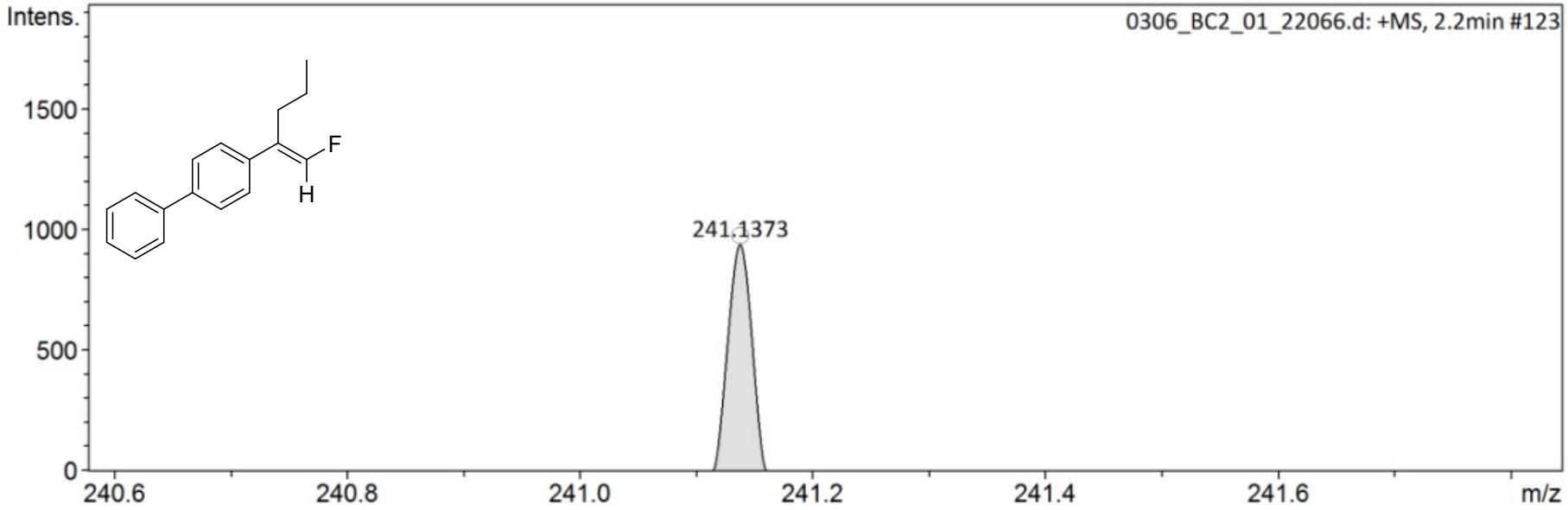
Comment

Acquisition D 2023-03-10 16:11:02

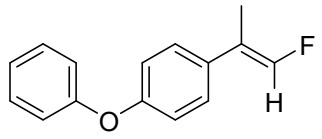
Operator Demo User
Instrumen compact 8255754.2017
6

Acquisition Paramet

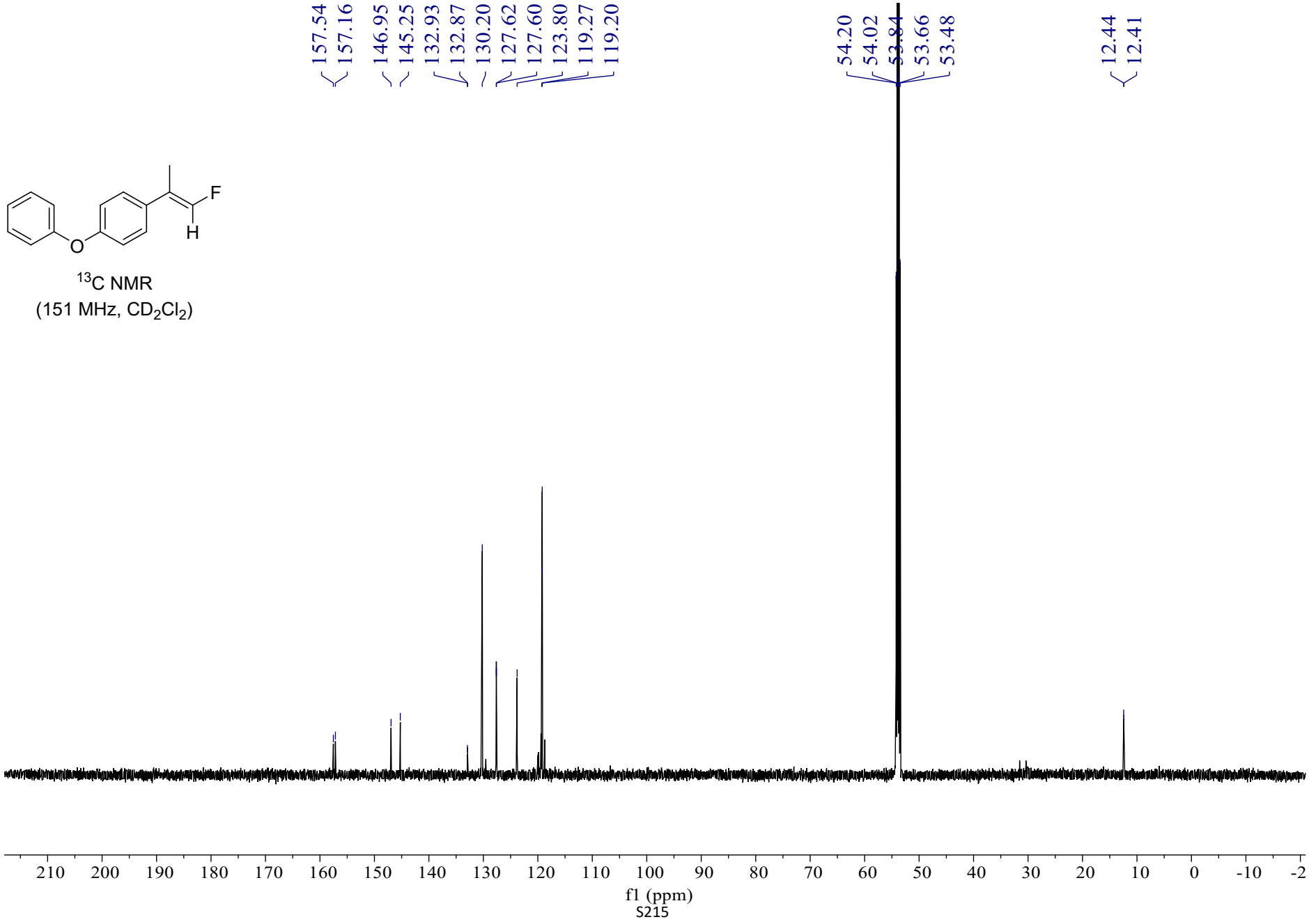
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min

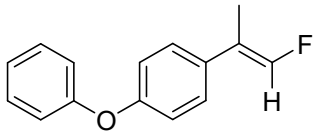


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
241.1373	1	C17H18F	241.1387	5.7	n.a.	1	100.00	8.5	even	ok



^{1}H NMR
(400 MHz, CD_2Cl_2)


157.54
157.16
146.95
145.25
132.93
132.87
130.20
127.62
127.60
123.80
119.27
119.20
54.20
54.02
53.84
53.66
53.48
12.44
12.41
F
H
O
^{13}C NMR
(151 MHz, CD_2Cl_2)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (ppm)



^{19}F NMR

(376 MHz, $CDCl_3$)

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\LXMS\0306_BC3_01_22067.d
Method LC_NO UV_P50-1500_10MIN.m
Sample Name 0306

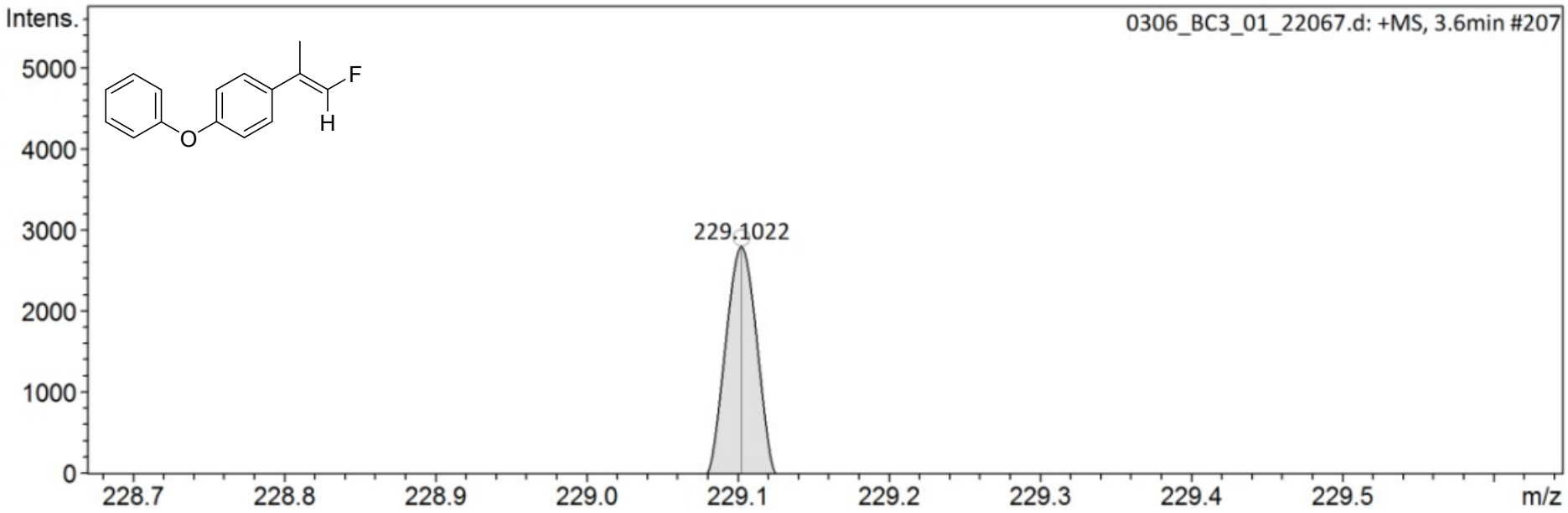
Comment

Acquisition D 2023-03-10 16:23:17

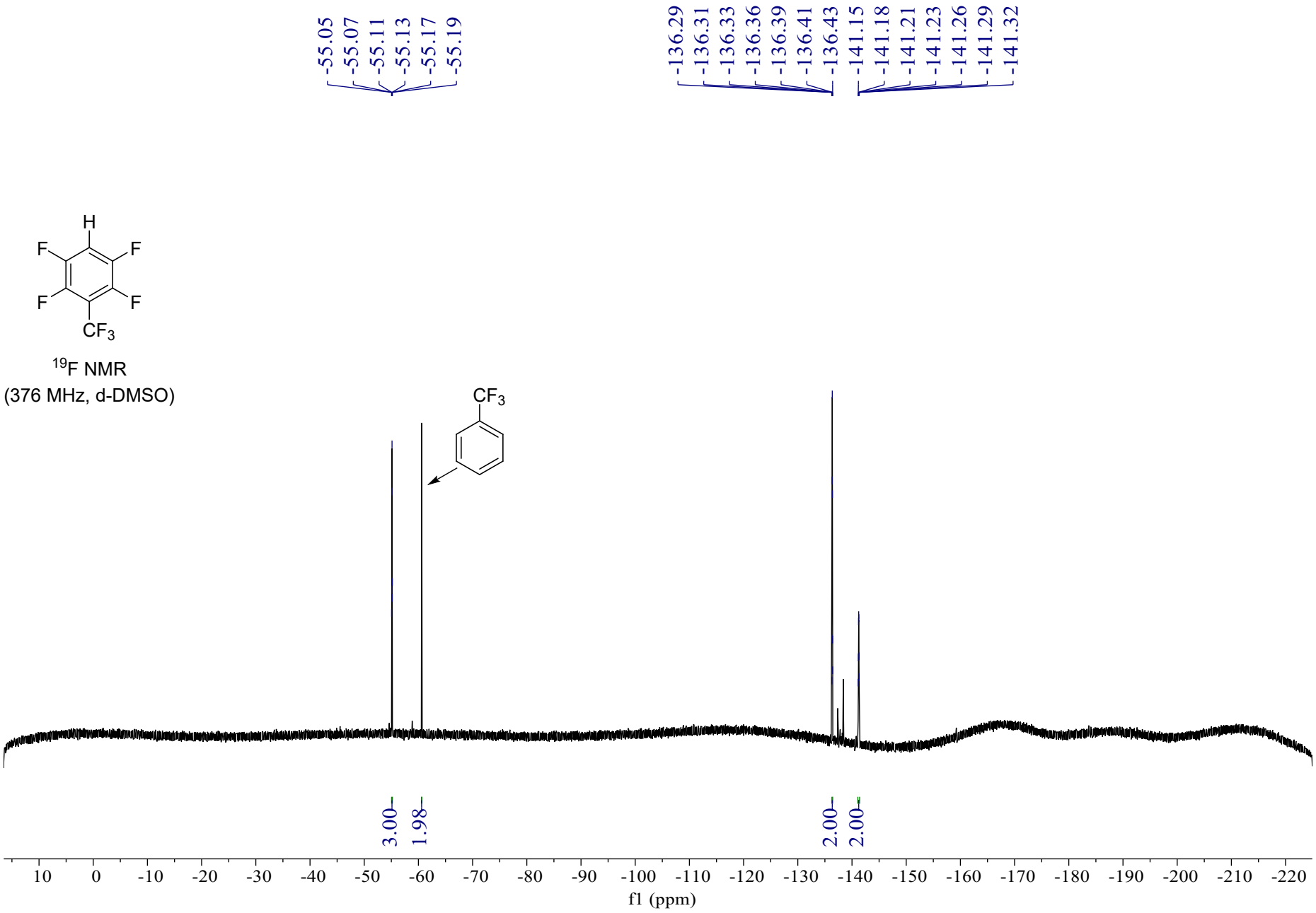
Operator Demo User
Instrumen compact 8255754.2017 6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
229.1022	1	C15H14FO	229.1023	0.6	n.a.	1	100.00	8.5	even	ok


-55.05
-55.07
-55.11
-55.13
-55.17
-55.19
-136.29
-136.31
-136.33
-136.36
-136.39
-136.41
-136.43
-141.15
-141.18
-141.21
-141.23
-141.26
-141.29
-141.32
H
F
F
F
F
CF3
19F NMR
(376 MHz, d-DMSO)
CF3
3.00
1.98
2.00
2.00
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

Mass Spectrum SmartFormula Report

Analysis Info

Acquisition D 2023-03-10 17:22:20

Analysis Name D:\LXMS\0306_BC8_01_22072.d

Method LC_NO UV_P50-1500_10MIN.m

Operator Demo User

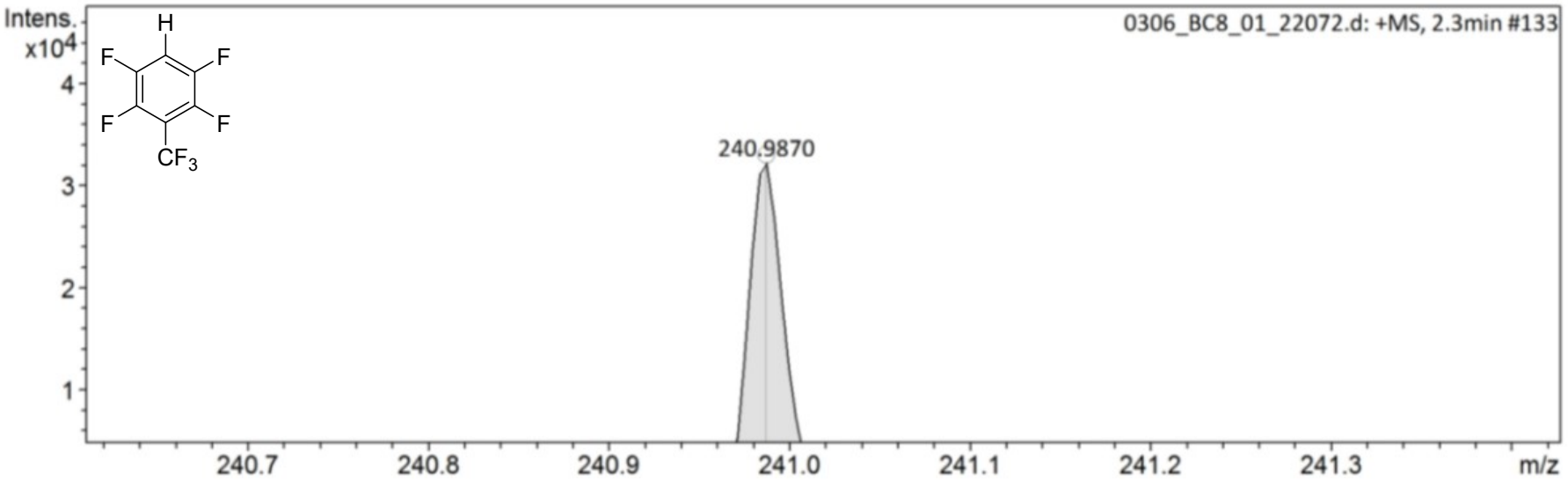
Sample Name 0306

Instrumen compact 8255754.2017 6

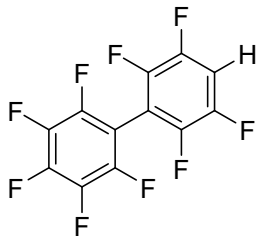
Comment

Acquisition Paramet

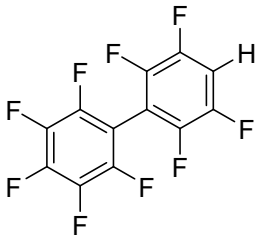
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
240.9870	1	C7HF7Na	240.9859	-4.7	57.7	1	100.00	3.5	even	ok



^{1}H NMR
(400 MHz, $CDCl_3$)



^{19}F NMR
(376 MHz, $CDCl_3$)

Mass Spectrum SmartFormula Report

Analysis Info

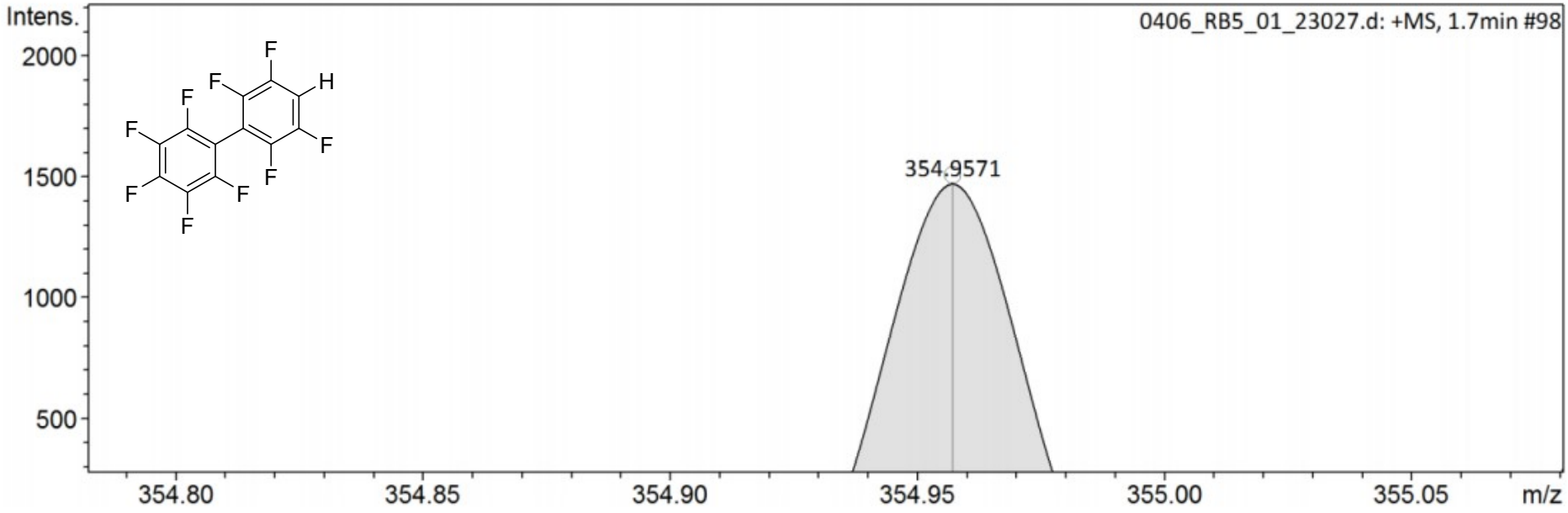
Acquisition D 2023-04-06 14:55:16

Analysis Name D:\LXMS\0406_RB5_01_23027.d
Method LC_NO UV_P50-1500_6MIN.m
Sample Name 0406
Comment

Operator Demo User
Instrumen compact 8255754.2017 6

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
354.9571	1	C12HF9K	354.9566	-1.3	n.a.	1	100.00	7.5	even	ok