Catalytic Asymmetric Addition to Cyclic *N*-Acyl-iminium: Access to Sulfone Bearing Contiguous Quaternary Stereocenters

Viraj A. Bhosale,[†] Ivana Císařová,[‡] Martin Kamlar[†] and Jan Veselý*[,†]

[†]*Department of Organic Chemistry, Faculty of Science, Charles University, 128 43 Prague, Czech Republic.*

[†]*Department of Inorganic Chemistry, Faculty of Science, Charles University, 128 43 Prague, Czech Republic.*

Table of Contents

1.1 General Information:

Reaction Setup, Reagents and Solvents: All reactions were carried out under inert argon or nitrogen atmosphere using standard oven dried round bottom flasks, unless otherwise stated. Organocatalytic reactions performed in 4.0 mL vial. All reagents were used as supplied from commercial sources without further purification unless otherwise stated. Tetrahydrofuran, Et_2O, DCM and toluene were purified by distillation on site under inert atmosphere via the following processes: *P*-xylene, toluene, tetrahydrofuran and Et_2O were pre-dried over sodium wire then distilled. DCM were distilled from calcium hydride under inert atmosphere. EtOAc and n-hexanes were distilled.

Heating source: Modular aluminium Heating Blocks for 4 mL vials and oil bath for large scale reaction

Chromatography: Analytical thin-layer chromatography was performed using precoated Merck aluminium silica gel plates (Silica gel 60 F_{254}). Visualization was by ultraviolet fluorescence (λ = 254 and 365 nm) and/or staining with potassium permanganate ($KMnO_4$) or Ceric Ammonium Molybdate (CAM). Flash colomn column chromatography was performed using silica gel (230-400 mesh). All ratios of eluents are quoted as v/v.

Chiral HPLC Analysis: Chiral HPLC was carried out using a LC20AD Shimadzu liquid chromatograph with SPDM20A diode array detector with columns Daicel Chiralpak® IA, Daicel Chiralpak® IB, Daicel Chiralpak® IC, Daicel Chiralpak® AD, Daicel, Daicel Chiralpak® OD-H columns (4.6 x 250 mm, 5.0 μm) in a mixed solvent system of heptane and isopropanol at 25 °C unless otherwise stated.
The racemic compounds were prepared treating with Diphenyl phosphate (0.1 equiv.) in *p*-xylene (0.1 M) at 65-70°C. Samples for measurement of chiral HPLC were prepared by dissolving of corresponding products in *i*-PrOH.

NMR Spectroscopy: ^{1}H NMR spectra were recorded on 400 and 600 MHz Bruker spectrometers. Chemical shifts are reported in parts per million (ppm) and the spectra are calibrated to the resonance resulting from incomplete deuteration of the solvent ($CDCl_3$: 7.26 ppm). ^{13}C NMR spectra were recorded on the same spectrometers with complete proton decoupling using $CDCl_3$ as the internal standard ($^{13}CDCl_3$: 77.16) ^{19}F NMR spectra were recorded on same spectrometer. Data are reported as follows: chemical shift δ, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, bs = broad singlet, m = multiplet or combinations thereof (^{13}C and all other nuclides except ^{1}H are singlets unless otherwise stated. ^{1}H NMR signals are reported in ppm to 2 decimal places and all other nuclide signals to 1 decimal place. Coupling constants are reported in Hz to a maximum of 3 significant figures.

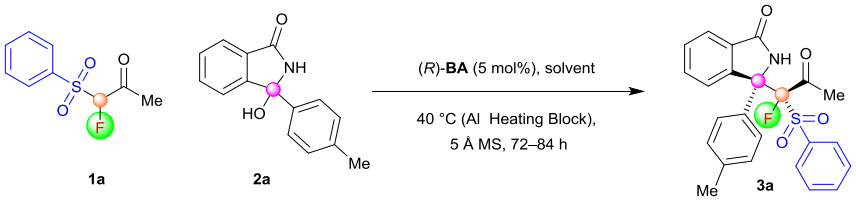
High Resolution Mass Spectrometry (HRMS): High-resolution mass spectra's were recorded with a LCQ Fleet spectrometer and LC-QTOF at the Department of Chemistry at the Charles University. The ionization method is noted—positive/negative electrospray ionization (+/–ESI), Atmospheric pressure chemical ionization (+/–APCI) or Electron Impact Ionization (+/–EI). Samples for measurement of HRMS were prepared by dissolving of the corresponding sample in methanol/CH_3CN. The masses reported as 'Found' and 'calculated for (Calcd for)' are the mass/charge ratios. Measured values are reported to 4 decimal places and are within ± 5 ppm of the calculated value. The calculated values are based on the most abundant isotope unless otherwise stated in the chemical formula.

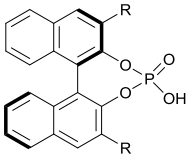
Optical Rotations: Measured in spectrophotometric grade $CHCl_3$ or EtOAc on AU-Tomatica Polarimeter, Autopol III using a sodium lamp (λ = 589 nm, the sodium D line). $[\alpha]_D$ values are reported at the stated temperature, with concentration in g /100 mL.
Names of the compounds: were generated by the computer program Chem Draw.

Single-Crystal X-Ray diffraction: Crystallographic data for were collected on Bruker D8 VENTURE Kappa Duo PHOTONIII by IμS micro-focus sealed tube MoKα (λ= 0.71073) at a temperature of 120(2) K.

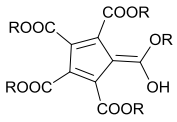
The absolute configuration of the product (**3o, CCDC 2162666**) was confirmed through a single X-ray analysis. The absolute configurations of other products were assigned tentatively by analogy.

2.1. Catalyst and solvent screening[a]





(*R*)-**BA5**: R = -$SiPh_3$
(*R*)-**BA6**: R = 2,4,6-tricyclohexylphenyl



(*R*)-**BA7**: R = (-)-Menthol

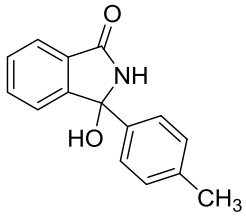
No	(*R*)-BA	solvent	yield (%)[b]	Dr[c]	ee (%)[d]
1	**6**	$PhCH_3$	75	1:1	48
2	**7**	$PhCH_3$	89	10:1	5
3[e]	**5**	$PhCH_3$	79	>4:1	60
4	**5**	$PhCF_3$	70	4:1	70
5	**5**	*p*-xylene	80	>5:1	90
6	**5**	EtOAc	trace	N.D	N.D
7	**5**	$(CH_2Cl_2)_2$	76	7:1	59
8	**5**	CH_2Cl_2	57	4:1	50
9	**5**	PhCl	68	4:1	67
10[f]	**5**	*p*-xylene	73	>8:1	92

[a] General conditions unless otherwise noted: **1a** (0.11 mmol), **2a** (0.10 mmol) and **(*R*)-BA** (0.005 mmol), 100 mg 5Å MS in solvent (1.0 mL) at 40 °C in sealed vial; [b] Isolated yield; [c] Diastereomeric ratio (dr) was determined by crude ^{1}H NMR; [d] Enantiomeric excess (ee) determined by chiral HPLC analysis; [e] 0.03 mmol of BOC_2O % used as an additive; [f] 0.125 mmol (1.25 equiv.) of **1a** in 1.25 mL *p*-xylene.

2.2. Preparation 3-hydroxy isoindolin-1-one (2a-2k)

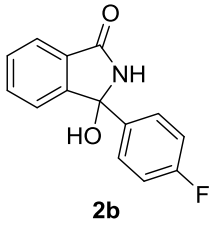
3-Hydroxyisoindolin-1-ones (**2a-2k**) were prepared according to the literature known procedures. [1–3]

3-hydroxy-3-(p-tolyl)isoindolin-1-one (2a)



The obtained data of isoindolin-1-one **2a** is in correspondence with the literature. [1,3]
White solid , Yield: 89%
^{1}H NMR (400 MHz, DMSO): δ 9.19 (s, 1H), 7.63 (d, *J* = 7.0 Hz, 1H), 7.52 (td, *J* = 7.4, 1.3 Hz, 1H), 7.46 (td, *J* = 7.4, 1.1 Hz, 1H), 7.35 (d, *J* = 8.2 Hz, 2H), 7.28 (d, *J* = 7.4 Hz, 1H), 7.14 (d, *J* = 8.0 Hz, 2H), 6.82 (bs, 1H), 2.27 (s, 3H).
^{13}C NMR (101 MHz, DMSO): δ 168.3, 151.0, 139.2, 136.9, 132.3, 130.5, 128.8, 128.7, 125.4, 122.7, 122.5, 87.2, 20.6.
HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{15}H_{13}NNaO_2$ = 262.0838; **Found:** 262.0839

3-(4-fluorophenyl)-3-hydroxyisoindolin-1-one (2b)



2b

The obtained data of isoindolin-1-one **2b** is in correspondence with the literature data.[1,3]

White solid; Yield: 48%

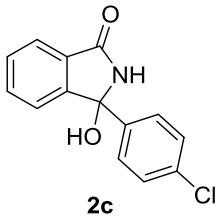
^{1}H NMR (400 MHz, DMSO): δ 9.26 (s, 1H), 7.65 (d, *J* = 7.0 Hz, 1H), 7.55 – 7.45 (m, 4H), 7.31 (d, *J* = 6.4 Hz, 1H), 7.16 (t, *J* = 8.9 Hz, 2H), 6.96 (bs, 1H).

^{13}C NMR (101 MHz, DMSO): δ 168.2, 161.7 (d, *J* = 243.8 Hz), 150.6, 138.4 (d, *J* = 2.9 Hz), 134.3, 132.4, 130.5, 129.0, 127.6 (d, *J* = 8.4 Hz), 122.6 (d, *J* = 12.7 Hz), 114.9 (d, *J* = 21.5 Hz), 86.9.

^{19}F NMR (376 MHz, DMSO): δ -115.0 (tt, *J* = 8.9, 5.5 Hz).

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{14}H_{10}FNNaO_2$ = 266.0588; **Found:** 266.0590

3-(4-chlorophenyl)-3-hydroxyisoindolin-1-one (2c)



2c

The obtained data of **2c** is in correspondence with the literature data.[2]

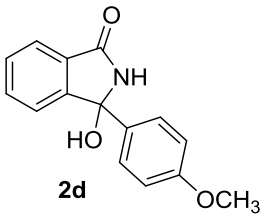
White solid; Yield: 89%

^{1}H NMR (400 MHz, DMSO): δ 9.27 (s, 1H), 7.65 (d, *J* = 7.2 Hz, 1H), 7.54 (td, *J* = 7.4, 1.3 Hz, 1H), 7.51 – 7.45 (m, 3H), 7.44 – 7.37 (m, 2H), 7.30 (d, *J* = 7.4 Hz, 1H), 7.01 (bs, 1H).

^{13}C NMR (101 MHz, DMSO): δ 168.2, 150.4, 141.2, 132.5, 132.4, 130.5, 129.1, 128.2, 127.5, 122.7, 122.6, 86.9

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{14}H_{10}ClNNaO_2$ = 282.0292; **Found:** 282.0294

3-hydroxy-3-(4-methoxyphenyl)isoindolin-1-one (2d)



2d

The obtained data of **2d** is in correspondence with the literature data.[1, 3]

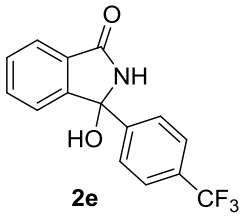
White solid; Yield: 88%

^{1}H NMR (400 MHz, DMSO): δ 9.16 (s, 1H), 7.62 (d, *J* = 7.3 Hz, 1H), 7.52 (t, *J* = 6.7 Hz, 1H), 7.45 (t, *J* = 7.4 Hz, 1H), 7.38 (d, *J* = 8.8 Hz, 2H), 7.28 (d, *J* = 7.4 Hz, 1H), 6.88 (d, *J* = 8.8 Hz, 2H), 6.79 (bs, 1H), 3.72 (s, 3H).

^{13}C NMR (101 MHz, DMSO): δ 168.2, 158.8, 151.1, 134.0, 132.3, 130.5, 128.7, 126.7, 122.6, 122.4, 113.5, 87.1, 55.1

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{15}H_{13}NNaO_3$ = 278.0788; **Found:** 278.0787

3-hydroxy-3-(4-(trifluoromethyl)phenyl)isoindolin-1-one (2e)



2e

The obtained data of isoindolin-1-one **2e** is in correspondence with the literature.[1,3]

White solid, Yield: 81%

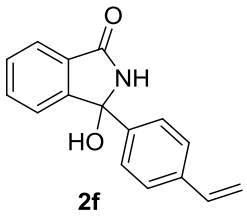
^{1}H NMR (400 MHz, DMSO): δ 9.37 (bs, 1H), 7.78 – 7.65 (m, 5H), 7.55 (td, *J* = 7.4, 1.4 Hz, 1H), 7.50 (td, *J* = 7.4, 1.2 Hz, 1H), 7.32 (d, *J* = 7.1 Hz, 1H), 7.15 (bs, 1H).

^{13}C NMR (101 MHz, DMSO): 168.3, 150.1, 146.8, 132.6, 130.6, 129.30, 128.5, 128.2, 126.5, 125.2 (q, *J* = 3.8 Hz), 122.7 (d, *J* = 6.0 Hz), 86.9

^{19}F NMR (376 MHz, DMSO): δ -60.9.

HRMS (ESI) m/z: $(M+H)^+$ Calcd for $C_{15}H_{10}F_3NNaO_2$ = 316.0556; **Found:** 316.0554

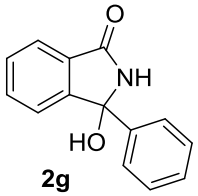
3-hydroxy-3-(4-vinylphenyl)isoindolin-1-one (2f)



2f

The obtained data of isoindolin-1-one **2f** is in correspondence with the literature data.[3]
White solid, Yield: 90%
^{1}H NMR (400 MHz, DMSO): δ 9.24 (s, 1H), 7.65 (d, *J* = 7.1 Hz, 1H), 7.53 (td, *J* = 7.4, 1.3 Hz, 1H), 7.48 (dd, *J* = 7.3, 1.1 Hz, 1H), 7.44 (s, 4H), 7.31 (d, *J* = 7.5 Hz, 1H), 6.91 (s, 1H), 6.71 (dd, *J* = 17.7, 10.9 Hz, 1H), 5.81 (dd, *J* = 17.7, 0.9 Hz, 1H), 5.25 (dd, *J* = 10.9, 0.9 Hz, 1H).
^{13}C NMR (101 MHz, DMSO): δ 168.3, 150.7, 141.7, 136.6, 136.1, 132.3, 130.5, 128.9, 126.0, 125.7, 122.7, 122.5, 114.5, 87.2.
HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{16}H_{13}NNaO_2$ = 274.0838; **Found:** 274.0839

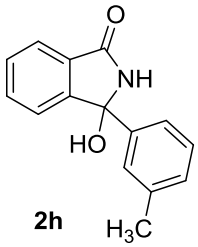
3-hydroxy-3-phenylisoindolin-1-one (2g)



2g

The obtained data of isoindolin-1-one **2g** is in correspondence with the literature.[1,3]
White solid, Yield: 93%
^{1}H NMR (400 MHz, DMSO): δ 9.23 (s, 1H), 7.63 (dt, *J* = 7.2, 1.1 Hz, 1H), 7.52 (td, *J* = 7.4, 1.3 Hz, 1H), 7.49 – 7.44 (m, 3H), 7.37 – 7.25 (m, 4H), 6.89 (bs, 1H).
^{13}C NMR (101 MHz, DMSO): δ 168.3, 150.8, 142.1, 132.3, 130.6, 128.9, 128.2, 127.7, 125.4, 122.7, 122.5, 87.2
HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{14}H_{11}NNaO_2$ = 248.0682; **Found:** 248.0683

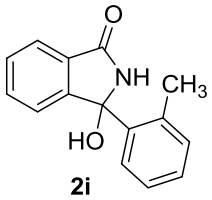
3-hydroxy-3-(m-tolyl)isoindolin-1-one (2h)



2h

The obtained data of isoindolin-1-one **2h** is in correspondence with the literature data.[2]
White solid, Yield: 66%
^{1}H NMR (400 MHz, DMSO): δ 9.20 (s, 1H), 7.63 (d, *J* = 7.3 Hz, 1H), 7.52 (td, *J* = 7.4, 1.3 Hz, 1H), 7.46 (td, *J* = 7.4, 1.1 Hz, 1H), 7.32 – 7.26 (m, 3H), 7.24 (t, *J* = 7.6 Hz, 1H), 7.10 (d, *J* = 7.2 Hz, 1H), 6.85 (bs, 1H), 2.28 (s, 3H).
^{13}C NMR (101 MHz, DMSO): δ 168.3, 150.9, 142.1, 137.2, 132.3, 130.6, 128.87, 128.3, 128.1, 125.9, 122.7, 122.6, 122.5, 87.2, 21.1
HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{15}H_{13}NNaO_2$ = 262.0838; **Found:** 262.0840

3-hydroxy-3-(o-tolyl)isoindolin-1-one (2i)

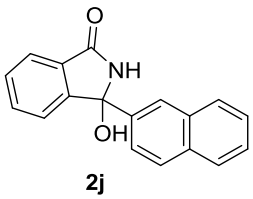


2i

The obtained data of isoindolin-1-one **2i** is in correspondence with the literature data.[2,3]
White solid; Yield: 51%
^{1}H NMR (400 MHz, DMSO): δ 9.08 (s, 1H), 7.90 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.67 (dd, *J* = 6.5, 1.2 Hz, 1H), 7.56 – 7.48 (m, 2H), 7.27 - 7.20 (m, 2H), 7.16 (d, *J* = 6.8 Hz, 1H), 7.07 (d, *J* = 7.1 Hz, 1H), 6.75 (bs, 1H), 1.85 (s, 3H).
^{13}C NMR (101 MHz, DMSO): δ 168.6, 149.9, 138.7, 135.1, 132.4, 131.8, 128.9, 128.0, 127.1, 125.6, 122.5, 122.4, 86.9, 19.9
HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{15}H_{13}NNaO_2$ = 262.0838; **Found:** 262.0838

3-hydroxy-3-(naphthalen-2-yl)isoindolin-1-one (2j)

The obtained data of isoindolin-1-one **2j** is in correspondence with the literature data.[1,3]
White solid, Yield: 68%
^{1}H NMR (400 MHz, DMSO): δ 9.36 (s, 1H), 8.14 (d, *J* = 1.5 Hz, 1H), 7.96 (dd, *J* = 5.5, 4.1



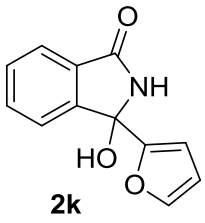
2j

Hz, 1H), 7.87 (dd, *J* = 9.8, 7.1 Hz, 2H), 7.71 – 7.66 (m, 1H), 7.49 – 7.43 (m, 4H), 7.45 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.34 (dt, *J* = 7.7, 0.9 Hz, 1H), 7.07 (bs, 1H).

^{13}C NMR (101 MHz, DMSO): δ 168.4, 150.7, 139.5, 132.6, 132.4, 130.7, 129.0, 128.1, 127.9, 127.4, 126.3, 126.2, 124.0, 123.9, 122.8, 122.6, 87.4

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{18}H_{13}NNaO_2$ = 298.0838; **Found:** 298.0834

3-(furan-2-yl)-3-hydroxyisoindolin-1-one (2k)



2k

The obtained data of isoindolin-1-one **2k** is in correspondence with the literature dat.[1,3]

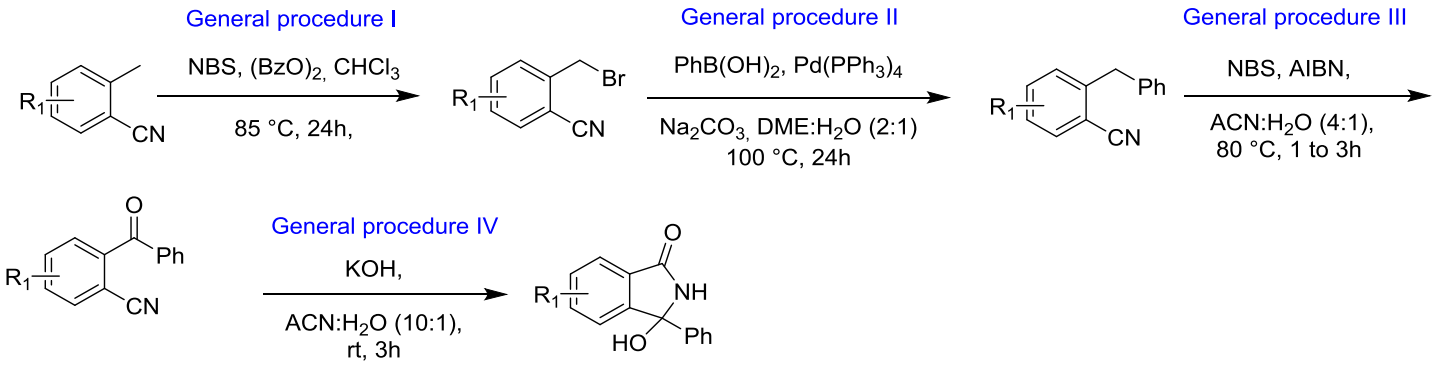
pale yellow solid; Yield: 78%

^{1}H NMR (400 MHz, DMSO): δ 9.33 (s, 1H), 7.67 – 7.57 (m, 2H), 7.58 – 7.46 (m, 2H), 7.03(s, 1H), 6.49 (dd, *J* = 3.3, 0.9 Hz, 1H), 6.41 (dd, *J* = 3.3, 1.8 Hz, 1H).

^{13}C NMR (101 MHz, DMSO): δ 168.0, 153.7, 148.1, 142.9, 132.3, 130.7, 129.4, 122.9, 122.6, 110.3, 106.8, 83.8

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{12}H_9NNaO_3$ = 238.0476; **Found:** 238.0475

2.3 General procedures for synthesis Isoindolinones (2l-2p)[4]



Scheme S1: Synthesis of 3-Hydroxy Isoindolinones 2l-2n

General procedure I

A solution of corresponding 2-methylbenzonitrile (1.00 equiv.) in dry $CHCl_3$ (45 mL) was prepared under argon and *N*-bromosuccinimide (1.15 equiv.) and a catalytic amount of benzoyl peroxide were added. The reaction mixture was stirred for 24 h at 85 °C. After that, the reaction mixture was cooled to ambient temperature and the succinimide was removed by filtration and washed with EtOAc (40 mL). The solvent was evaporated under reduced pressure. Purification by column chromatography on silica (n-hexane/EtOAc = 2:1) afforded compound.

b. General procedure II:

To a solution of corresponding 2-cyanobenzyl bromides (1.00 equiv.) in 1,2-dimethoxy-ethane (1.6 mL) and water (0.8 mL) was added corresponding boronic acid (1.2 equiv.), sodium carbonate (2.1 equiv.) and Tetrakis(triphenyl-phosphine) palladium(0) (0.01 equiv.). The mixture was *vacuum* flushed with nitrogen and then heated to 100 °C overnight. The solvent was removed and the residue was purified by column chromatography (n-hexane/EtOAc; 20:1) afforded compounds.

c. General procedure III

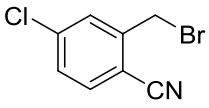
A solution of corresponding 2-benzylbenzonitrile (1.00 equiv.), *N*-Bromosuccinimide (3.5 equiv.) and AIBN (0.1 equiv.) in CH_3CN:H_2O 4:1 (3.5 mL) was heated at 80°C with stirring. After complete consumption of starting material, reaction mixture cooled to room temperature, the solvent was removed under reduced pressure. The

residue obtained dissolved in dichloromethane was washed with water. The organic phase was dried over Na_2SO_4 and concentrated *invacuo*. The crude product was purified by column chromatography (n-hexane/EtOAc; 20:2) afforded compounds.

d. General procedure IV

To a solution of corresponding 2-benzoylbenzonitrile (1.00 equiv.) in acetonitrile: H_2O (10:1), was added KOH (0.3 equiv.) and the mixture was stirred at room temperature until completion of the reaction (1-3h). Then the solution was diluted with dichloromethane and washed with 1N HCl followed by water. Organic layer dried over Na_2SO_4, filtered and concentrated in vacuo. The crude product was purified by flash column chromatography (n-hexane/EtOAc; 3:1 to 2:1) afforded compounds

2-(bromomethyl)-4-chlorobenzonitrile (S1)



S1

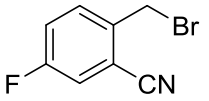
White solid (Yield 57%), The obtained data of isoindolin-1-one is in correspondence with literature data.[4]

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61 (d, *J* = 8.3 Hz, 1H), 7.56 (d, *J* = 2.0 Hz, 1H), 7.42 (s, 1H), 4.58 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 143.0, 139.9, 134.3, 130.9, 129.5, 116.1, 110.9, 28.4.

HRMS (EI) m/z: $(M)^+$ Calcd for C_8H_5BrClN = 228.9294; **Found:** 228,9284

2-(bromomethyl)-5-fluorobenzonitrile (S2)



S2

Brown oil (Yield 61%)

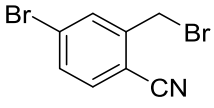
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.55 (dd, *J* = 8.7, 5.2 Hz, 1H), 7.36 (dd, *J* = 7.9, 2.7 Hz, 1H), 7.31 (td, *J* = 8.3, 2.7 Hz, 1H), 4.61 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 161.8 (d, *J* = 252.3 Hz), 137.5 (d, *J* = 3.9 Hz), 132.7 (d, *J* = 8.6 Hz), 121.0 (d, *J* = 21.5 Hz), 120.1 (d, *J* = 25.0 Hz), 115.7 (d, *J* = 2.8 Hz), 114.0 (d, *J* = 9.6 Hz), 28.5.

^{19}F NMR (376 MHz, $CDCl_3$): δ -109.8 (td, *J* = 7.9, 5.1 Hz).

HRMS (EI) m/z: $(M)^+$ Calcd for C_8H_5BrFN = 212.9589; **Found:** 212.9580

4-bromo-2-(bromomethyl)benzonitrile (S3)



S3

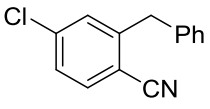
White solid (Yield 64%)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 (s, 1H), 7.57 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.52 (d, *J* = 8.3 Hz, 1H), 4.57 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ. 142.9, 134.3, 133.8, 132.4, 128.2, 116.2, 111.3, 28.3

HRMS (EI) m/z: $(M)^+$ Calcd for $C_8H_5Br_2N$ = 272.8789; **Found:** 272.8780

2-benzyl-4-chlorobenzonitrile (S4)



S4

White solid (Yield 79%). The obtained data of isoindolin-1-one is in correspondence with literature data.[4]

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 (d, *J* = 8.3 Hz, 1H), 7.38 – 7.23 (m, 7H), 4.19 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 147.0, 139.6, 137.9, 134.0, 130.4, 129.1, 129.0, 127.5, 127.1, 117.5, 111.1, 40.1

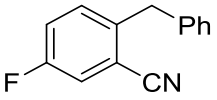
HRMS (APCI) m/z: $(M+H)^+$ Calcd for $C_{14}H_{11}ClN$ = 228.0575; **Found:** 228.0584.

2-benzyl-5-fluorobenzonitrile (S5)

Yellowish oil, Yield 81%

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.33 (d, *J* = 1.8 Hz, 1H), 7.31 (d, *J* = 1.6 Hz, 2H), 7.30 (d, *J* = 1.4 Hz, 1H), 7.27 – 7.17 (m, 5H), 4.17 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 160.6 (d, *J* = 248.5 Hz), 141.2 (d, *J* = 3.7 Hz), 138.6, 132.0 (d, *J* = 8.1 Hz), 129.0, 128.9, 126.9, 120.6 (d, *J* = 21.1 Hz), 119.4 (d, *J* = 24.5 Hz), 117.1 (d, *J* = 2.9 Hz),



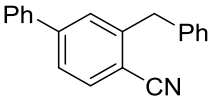
S5

113.7 (d, *J* = 9.2 Hz), 39.55.

^{19}F NMR (376 MHz, $CDCl_3$): δ -114.09 (td, *J* = 7.9, 5.5 Hz).

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{14}H_{10}FNNa$ = 234.0689; **Found:** 234.0691

2-benzyl-4-bromobenzonitrile (S6) {*In this case boronic acid (2.2 equiv.), sodium carbonate (4.2 equiv.) used*}



S6

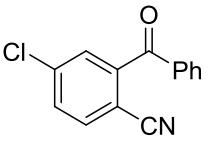
Colorless lequid, (Yield 95%)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, *J* = 8.2 Hz, 1H), 7.62 – 7.52 (m, 4H), 7.50 – 7.39 (m, 3H), 7.38 – 7.29 (m, 4H), 7.28 – 7.23 (m, 1H), 4.28 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 145.9, 145.4, 139.3, 138.8, 133.4, 129.1, 129.0, 128.8, 128.8, 128.6, 127.3, 126.8, 125.6, 118.4, 111.2, 40.4

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{20}H_{15}NNa$ = 292.1097; **Found:** 292.1099

2-benzoyl-4-chlorobenzonitrile (S7)[4]



S7

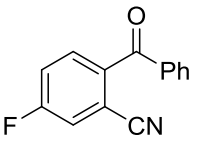
White solid (Yield 83%)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80 (dd, *J* = 8.4, 1.3 Hz, 2H), 7.77 (dd, *J* = 8.1, 0.6 Hz, 1H), 7.70 – 7.65 (m, 1H), 7.65 – 7.60 (m, 2H), 7.56 – 7.50 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 192.4, 143.2, 139.1, 135.4, 135.3, 134.4, 131.6, 130.4, 130.2, 129.0, 116.3, 110.3

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{14}H_8ClNNaO$ = 264.0187; **Found:** 264.0186

2-benzoyl-5-fluorobenzonitrile (S8)



S8

White solid (430 mg; 81%)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.83 – 7.78 (m, 2H), 7.74 – 7.66 (m, 2H), 7.60 – 7.50 (m, 3H), 7.42 (ddd, *J* = 8.6, 7.8, 2.6 Hz, 1H).

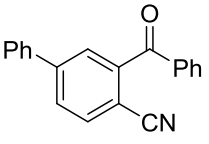
^{13}C NMR (101 MHz, $CDCl_3$): δ 192.7, 163.5 (d, *J* = 256.2 Hz), 137.9, 136.0, 134.1, 132.8 (d, *J* = 8.9 Hz), 130.3, 128.9, 121.6 (d, *J* = 25.0 Hz), 119.6 (d, *J* = 21.3 Hz), 116.0, 114.4 (d, *J* = 9.7 Hz).

^{19}F NMR (376 MHz, $CDCl_3$): δ -105.2

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{14}H_8FNNaO$ = 248.0482; **Found:** 248.0482

3-benzoyl-[1,1'-biphenyl]-4-carbonitrile (S9)

397



S9

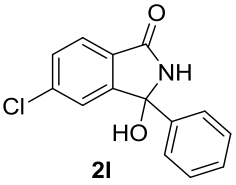
Colorless lequid (220 mg, 93%)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93 – 7.81 (m, 5H), 7.70 – 7.64 (m, 1H), 7.63 – 7.57 (m, 2H), 7.56 – 7.43 (m, 5H)

^{13}C NMR (101 MHz, $CDCl_3$): δ 193.9, 145.3, 142.3, 138.3, 136.1, 134.7, 134.1, 130.5, 129.75, 129.4, 129.2, 128.9, 128.5, 127.4, 117.2, 110.4.

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{20}H_{13}NNaO$ = 306.0889; **Found:** 306.0891

5-chloro-3-hydroxy-3-phenylisoindolin-1-one (2l)[4]



2l

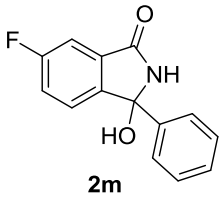
White solid (150 mg; 82%)

^{1}H NMR (400 MHz, DMSO): δ 9.39 (s, 1H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.53 (dd, *J* = 8.0, 1.8 Hz, 1H), 7.52 – 7.47 (m, 2H), 7.42 – 7.27 (m, 4H), 7.06 (s, 1H).

^{13}C NMR (101 MHz, DMSO): δ 167.2, 152.7, 141.3, 137.0, 129.4, 129.3, 128.3, 128.0, 125.50, 124.5, 122.8, 86.9.

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{14}H_{10}ClNNaO_2$ = 282.0292; **Found:** 282.0293

6-fluoro-3-hydroxy-3-phenylisoindolin-1-one (2m)



2m

White solid (300 mg; 79%)

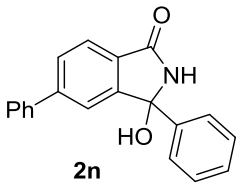
^{1}H NMR (400 MHz, DMSO): δ δ 9.41 (s, 1H), 7.53 – 7.45 (m, 2H), 7.39 – 7.32 (m, 4H), 7.32 – 7.27 (m, 1H), 6.96 (s, 1H).

^{13}C NMR (101 MHz, DMSO): δ 167.0 (d, *J* = 3.2 Hz), 162.6 (d, *J* = 245.4 Hz), 146.7, 141.7, 133.0 (d, *J* = 8.4 Hz), 128.2, 127.8, 125.4, 124.9 (d, *J* = 8.7 Hz), 119.5 (d, *J* = 23.5 Hz), 109.2 (d, *J* = 23.4 Hz) 87.0

^{19}F NMR (376 MHz, DMSO): δ 112.7 (td, *J* = 8.4, 5.4 Hz)

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{14}H_{10}FNNaO_2$ = 266.0588; **Found:** 266.0588

3-hydroxy-3,5-diphenylisoindolin-1-one (2n)



2n

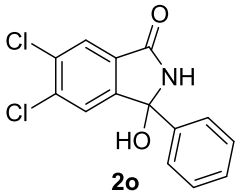
White solid (170 mg; 80%)

^{1}H NMR (400 MHz, DMSO): δ 9.29 (s, 1H), 7.77 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.58 – 7.50 (m, 3H), 7.46 (t, *J* = 7.4 Hz, 2H), 7.40 – 7.33 (m, 3H), 7.29 (t, *J* = 7.2 Hz, 1H), 7.01 (s, 1H).

^{13}C NMR (101 MHz, DMSO): δ 168.0, 151.7, 144.3, 142.0, 139.2, 129.7, 129.0, 128.2, 128.1, 127.81, 127.6, 127.0, 125.5, 123.2, 120.7, 87.3.

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{20}H_{15}NNaO_2$ = 324.0995; **Found:** 324.0995

5,6-dichloro-3-hydroxy-3-phenylisoindolin-1-one (2o)



2o

The obtained data of **2o** is in correspondence with the literature data.[1]

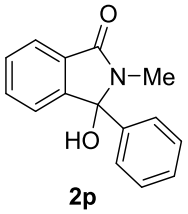
pale yellow solid; Yield: 78%

^{1}H NMR (400 MHz, DMSO): δ 9.55 (s, 1H), 7.87 (s, 1H), 7.57 (s, 1H), 7.50 (d, *J* = 6.8 Hz, 2H), 7.40 – 7.30 (m, 3H), 7.14 (s, 1H).

^{13}C NMR (101 MHz, DMSO): δ 166.0, 150.6, 140.9, 135.1, 132.2, 131.1, 128.4, 128.1, 125.5, 125.03, 124.6, 86.8

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{14}H_9Cl_2NNaO_2$ = 315.9903 ; **Found:** 315.9906

3-hydroxy-2-methyl-3-phenylisoindolin-1-one (2p)



2p

The obtained data of **2p** is in correspondence with literature data.[1]

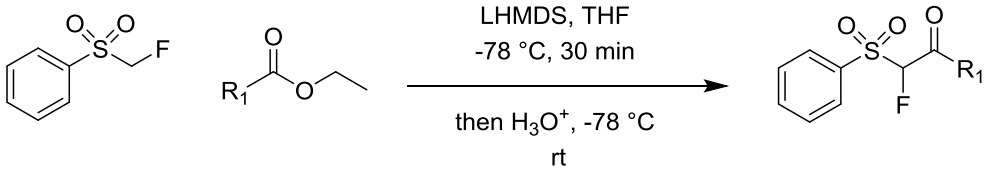
pale yellow solid, Yield 84%

^{1}H NMR (400 MHz, DMSO): δ 7.71 (d, *J* = 6.2 Hz, 1H), 7.58 – 7.46 (m, 2H), 7.43 – 7.24 (m, 6H), 7.01 (bs, 1H), 2.69 (s, 3H).

^{13}C NMR (101 MHz, DMSO): δ 166.8, 149.9, 140.0, 132.7, 130.8, 129.5, 129.0, 128.5, 126.13, 123.1, 122.8, 90.4, 39.9, 24.0

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{15}H_{13}NNaO_2$ = 262.0838; **Found:** 262.0841

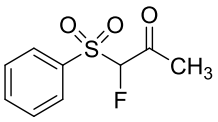
3.1 General Procedure (V) for the Preparation of α-monofluoro-β-ketosulfone[5]



Scheme S2: Synthesis of α-monofluoro-β-ketosulfones (1a, 1i and 1j)

General Procedure (V): A Schlenk tube charged with fluoromethyl phenyl sulfone ($PhSO_2CH_2F$) (1.0 equiv.) and respective ester (1.2 equiv.) in THF (0.2 M) and cooled to –78 ºC, followed by 1.0 M LHMDS in THF (1.2 equiv.) was added dropwise to above mixture at –78 ºC, under the N_2 atmosphere. The reaction mixture was then stirred at –78 ºC for next 30 min, followed by adding saturated HCl water solution (2 mL) at same temperature, and stirred for about 20-30 min at rt. The mixture was extracted with EtOAc (20 Ml × 3), and the combined organic phase was dried over $MgSO_4$. Filtered and concentrated in vacuo. The crude product was purified by flash column chromatography (n-hexanes/EtOAc; 3:1) afforded compounds **1a, 1i and 1j**

1-fluoro-1-(phenylsulfonyl)propan-2-one (1a)[5]



1a

White solid 94%

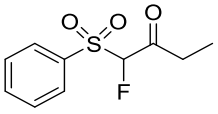
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 – 7.91 (m, 2H), 7.80 – 7.74 (m, 1H), 7.66 – 7.60 (m, 2H), 5.46 (d, *J* = 49.0 Hz, 1H), 2.36 (d, *J* = 3.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 195.6 (d, *J* = 21.8 Hz), 135.5, 135.0, 129.8, 129.7, 101.6 (d, *J* = 234.3 Hz), 27.6

^{19}F NMR (376 MHz, CDCl3): δ = -179.5 (qd, *J* = 48.9 Hz, *J* = 3.8 Hz)

HRMS (ESI) m/z: $(M+NA)^+$ Calcd for $C_9H_9FNO_3S$ = 239.0149; **Found:** 239.0151

1-fluoro-1-(phenylsulfonyl)butan-2-one (1i)[5]



1i

White solid 96%

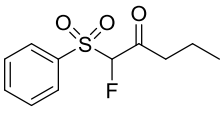
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 (d, *J* = 7.8 Hz, 2H), 7.75 (t, *J* = 7.5 Hz, 1H), 7.68 – 7.56 (m, 2H), 5.49 (dd, *J* = 48.9, 0.8 Hz, 1H), 2.89 – 2.73 (m, 1H), 2.67 – 2.49 (m, 1H), 1.06 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 198.6 (d, *J* = 20.8 Hz), 135.4, 135.1, 129.7, 129.6, δ 101.4 (d, *J* = 234.3 Hz), 33.7, 6.7, 6.7.

^{19}F NMR (376 MHz, $CDCl_3$): δ -181.5 (d, *J* = 48.9 Hz).

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{10}H_{11}FNO_3S$ = 253.0305; **Found:** 253.0303

1-fluoro-1-(phenylsulfonyl)pentan-2-one (1j)



1j

Colorless oil, 93% yield

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 (d, *J* = 7.7 Hz, 2H), 7.75 (t, *J* = 7.5 Hz, 1H), 7.62 (t, *J* = 7.9 Hz, 2H), 5.46 (d, *J* = 48.9 Hz, 1H), 2.84 – 2.66 (m, 1H), 2.57 – 2.49 (m, 1H), 1.66 – 1.57 (m, 2H), 0.91 (t, *J* = 7.4 Hz, 3H).

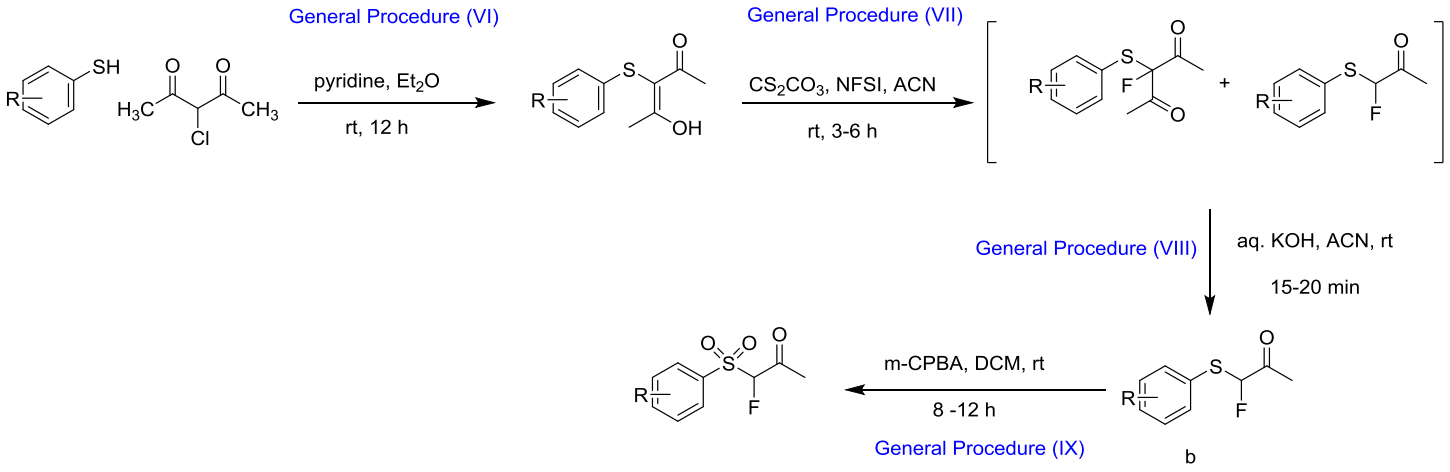
^{13}C NMR (101 MHz, $CDCl_3$): δ 197.9 (d, *J* = 20.6 Hz), 135.4, 135.2, 129.8, 129.6, 101.4 (d, *J* = 234.4 Hz), 42.0, 42.0, 16.1, 16.1, 13.5.

^{19}F NMR (376 MHz, $CDCl_3$): δ -181.30 (d, *J* = 48.9 Hz).

VB-A-847

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{11}H_{13}FNO_3S$ = 267.0462; **Found:** 267.0463

3.2 General modified Procedure for the Preparation of 1-fluoro-1-(phenylsulfonyl)propan-2-one (1b-1h)[6]



Scheme S3: Synthesis of 1-fluoro-1-(phenylsulfonyl)propan-2-one (1b-1h)

General Procedure (VI): (reactions performed on 4.0 mmol scale) To ice cold mixture of respective thiol (1.0 equiv.) and α-chloro acetyl acetone (1.0 equiv.) in diethyl ether (1.0 M) was slowly added pyridine (1.1 equiv.) for a period of 1-3 min. The reaction mixture was vigorously stirred at room temperature for 12 h. Then, additional diethyl ether (15 mL) was added to the reaction mixture, and crude compound was filtered through sintered funnel, and the filtrate containing crude compound was concentrated in vacuo and purified by flash column chromatography (n-hexanes: EtOAc; 100:5) as eluent to obtain the expected α-sulfenyl β-diketone compounds xx-xx.

General Procedure (VII): (reactions performed on 3.0 mmol scale)
To solution of α-sulfenyl β-diketone (1.0 equiv.) in CH_3CN (0.25 M) was added anhydrous Cs_2CO_3 (1.2 equiv). The reaction mixture was stirred at room temperature until it turns into a white turbid heterogeneous reaction mixture (generally 2 h). The round-bottom flask was then placed under the ice bath, and NFSI (1.1 equiv) was added slowly to the above reaction mixture over 10 min. After stirring for extra 5 min the ice bath was removed, and stirring was continued at room temperature for 4 h. Then, the crude product was filtered through sintered funnel, and the residue was washed with EtOAc (5 mL × 2). The filtrate containing crude compound was concentrated in vacuo and purified by flash column chromatography (n-hexanes: EtOAc; 100:5) as eluent to obtain the inseparable mixture of α,α-fluoro sulfenyl β-diketones (major product) along with α-Fluoro β-ketosulfide (minor product), which further used for next step. (Products ratio can be determined from NMR)

Note: *according to previous report [6] we should obtain α-fluoro β-ketosulfides as sole product following reported (above* General Procedure (VII) *protocol, but we observed formation of inseparable mixture of α,α-fluoro sulfenyl β-diketones (major product) along with expected α-Fluoro β-ketosulfide (minor product) (Probably reaction didn't work on large scale experiments as reported) ; so to obtain exclusively only α-Fluoro β-Ketosulfides extra additional step is performed. i.e General Procedure (VIII).*

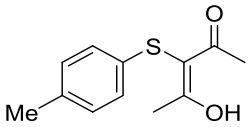
General Procedure (VIII): (reactions performed on 2.0 mmol scale)
To solution of mixture of α,α-fluoro sulfenyl β-diketones and α-Fluoro β- Ketosulfide (1.0 equiv.) in CH_3CN (0.1 M) was added 0.1 N KOH solution (approx. 1 equiv. with respect to α,α-fluoro sulfenyl β-diketone) dropwise over 1 min, The reaction mixture was stirred at room temperature for next 15-20 min (turns dark-red). Quench reaction with 1N HCl (3 ml). The residue was dissolved in EtOAc (25 mL) and washed with 3 ml of H_2O. The organic phase was

separated and dried properly over $MgSO_4$, filtered and later concentrated in vacuo, which is used for next step without further purification.

General Procedure (IX):

To a well-stirred solution of α-Fluoro β- Ketosulfide (1.0 equiv.) in DCM (0.1 M) was added m-CPBA (70%, 4 equiv.) at room temperature, and the reaction mixture was stirred at room temperature for 12 h. Then, the saturated aqueous sodium sulfite solution was added to the reaction mixture, and stirring was continued at room temperature for further 2 h. The crude compound was extracted into DCM (15 mL × 3) and dried over anhydrous Na_2SO_4 and concentrated in vacuo. The crude product was purified by flash column chromatography (n-hexanes/EtOAc; 3:1) afforded sulfone compounds **(S10-S16).**

(E)-4-hydroxy-3-(p-tolylthio)pent-3-en-2-one (S10)[6]

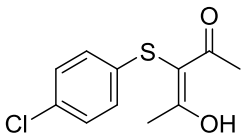


S10

The obtained data of isoindolin-1-one is in correspondence with the literature.[6]
oily solid; yield: 83%.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.09 (d, *J* = 8.0 Hz, 2H), 6.99 (d, *J* = 8.3 Hz, 2H), 2.34 (s, 6H), 2.30 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 198.3, 135.2, 134.3, 130.1, 125.0, 102.2, 24.5, 20.9.
HRMS (ESI) m/z: $(M+H)^+$ Calcd for $C_{12}H_{15}O_2S$ = 223.0787; **Found:** 223.0788

(E)-3-((4-chlorophenyl)thio)-4-hydroxypent-3-en-2-one (S11) [6]

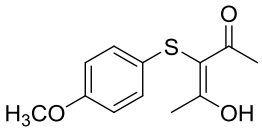
770-798



S11

The obtained data of isoindolin-1-one is in correspondence with the literature. [6]
White solid; yield: 85%
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.33 – 7.23 (m, 2H), 7.08 – 7.01 (m, 2H), 2.35 (s, 6H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 198.4, 136.5, 131.2, 129.4, 126.0, 101.4, 24.5.
HRMS (ESI) m/z: $(M+H)^+$ Calcd for $C_{11}H_{12}ClO_2S$ = 243.0241; **Found:** 243.0239

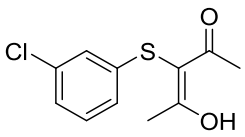
(E)-3-((4-((l1-oxidaneyl)-l5-methyl)phenyl)thio)-4-hydroxypent-3-en-2-one (S12) [6]



S12

The obtained data of isoindolin-1-one is in correspondence with the literature. [6]
White solid 80%
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.04 (d, *J* = 8.8 Hz, 2H), 6.84 (d, *J* = 8.8 Hz, 2H), 3.78 (s, 3H), 2.35 (s, 6H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 198.1, 158.1, 132.8, 128.5, 127.0, 115.0, 103.2, 55.53, 24.6
HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{12}H_{14}NaO_3S$ = 261.0556; **Found:** 261.0559

(E)-3-((3-chlorophenyl)thio)-4-hydroxypent-3-en-2-one (S13)

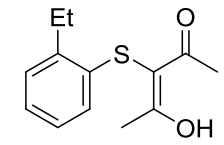


S13

The obtained data of isoindolin-1-one is in correspondence with the literature. [6]
Yellowish oil 79%
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.20 (t, *J* = 7.9 Hz, 1H), 7.11 (ddd, *J* = 7.9, 2.0, 1.0 Hz, 1H), 7.05 (t, *J* = 1.9 Hz, 1H), 6.97 (ddd, *J* = 7.8, 1.8, 1.0 Hz, 1H), 2.33 (s, 6H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 198.55, 140.20, 135.46, 130.39, 125.60, 124.43, 122.83, 100.99, 100.97, 24.52.
HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{11}H_{11}ClNaO_2S$ = 265.0060; **Found:** 265.0060

(E)-3-((2-ethylphenyl)thio)-4-hydroxypent-3-en-2-one (S14)

Yield: 80%
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.18 (dd, *J* = 7.1, 1.9 Hz, 1H), 7.15 – 7.07 (m, 2H), 6.85



S14

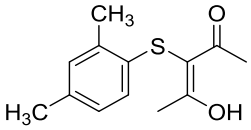
(dd, *J* = 7.5, 1.7 Hz, 1H), 2.77 (q, *J* = 7.5 Hz, 2H), 2.31 (s, 6H), 1.30 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 198.4, 140.4, 136.0, 128.7, 126.8, 125.2, 123.2, 101.0, 101.0, 26.4, 24.4, 14.2

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{13}H_{16}NaO_2S$ = 259.0763; **Found:** 259.0763

(E)-3-((2,4-dimethylphenyl)thio)-4-hydroxypent-3-en-2-one (S15)

Yield : 81%



S15

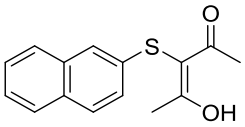
^{1}H NMR (400 MHz, $CDCl_3$): δ 6.99 (s, 1H), 6.94 (d, *J* = 8.7 Hz, 1H), 6.73 (d, *J* = 7.9 Hz, 1H), 2.35 (s, 3H), 2.31 (s, 6H), 2.28 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 198.3, 134.6, 134.3, 133.1, 131.4, 127.5, 123.0, 101.2, 101.2, 24.4, 20.8, 19.6

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{13}H_{16}NaO_2S$ = 259.0763; **Found:** 259.0765

(E)-4-hydroxy-3-(naphthalen-2-ylthio)pent-3-en-2-one (S16) [6]

The obtained data of isoindolin-1-one is in correspondence with the literature. [6]



S16

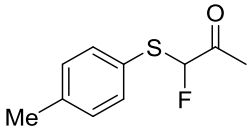
White solid; yield: 77%

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 – 7.75 (m, 2H), 7.71 (d, *J* = 8.3 Hz, 1H), 7.50 – 7.44 (m, 1H), 7.44 – 7.38 (m, 2H), 7.28 – 7.23 (m, 2H), 2.37 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 198.5, 135.4, 134.0, 131.6, 129.0, 127.9, 127.0, 126.9, 125.5, 123.7, 121.9, 101.6, 24.5

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{15}H_{14}NaO_2S$ = 281.0607; **Found:** 281.0606

1-fluoro-1-(p-tolylthio)propan-2-one (S17) [6]



S17

The obtained data of isoindolin-1-one is in correspondence with the literature. [6]

Colorless oil; yield: 73% (2 steps)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.44 (d, *J* = 8.1 Hz, 2H), 7.18 (d, *J* = 8.0 Hz, 2H), 5.97 (d, *J* = 52.3 Hz, 1H), 2.37 (s, 3H), 2.13 (d, *J* = 2.8 Hz, 3H).

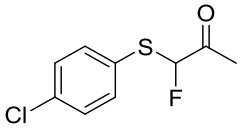
^{13}C NMR (101 MHz, $CDCl_3$): δ 199.7 (d, *J* = 26.9 Hz), 140.0, 134.5 (d, *J* = 1.8 Hz), 130.3, 125.5, 99.8 (d, *J* = 235.6 Hz), 26.3, 21.3

^{19}F NMR (376 MHz, $CDCl_3$): δ -159.1 (dq, *J* = 52.3, 2.8 Hz).

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{10}H_{11}ONaFS$ = 221.0407; **Found:** 221.0408

1-((4-chlorophenyl)thio)-1-fluoropropan-2-one (S18) [6]

The obtained data of isoindolin-1-one is in correspondence with the literature. [6]



S18

Colorless oil; yield: 76% (2 steps)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.47 (d, *J* = 8.7 Hz, 2H), 7.33 (d, *J* = 8.7 Hz, 2H), 5.97 (d, *J* = 52.2 Hz, 1H), 2.14 (d, *J* = 2.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 199.1 (d, *J* = 26.8 Hz), 136.2, 135.5, 135.4, 129.7, 127.74, 127.7, 99.3 (d, *J* = 236.3 Hz). 26.3

^{19}F NMR: (376 MHz, $CDCl_3$): δ -159.2 (dq, *J* = 52.2, 2.9 Hz).

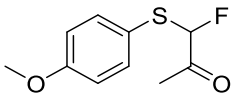
HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_9H_8ClFNaOS$ = 240.9866; **Found:** 240.9838

1-fluoro-1-((4-methoxyphenyl)thio)propan-2-one (S19)

The obtained data of isoindolin-1-one is in correspondence with the literature. [6]

Pale yellow oil; yield: 67% (2 steps)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.48 (d, *J* = 9.0 Hz, 2H), 6.90 (d, *J* = 8.8 Hz, 2H), 5.92 (d, *J* = 52.1 Hz, 1H), 3.83 (s, 3H), 2.10 (d, *J* = 2.9 Hz, 3H).



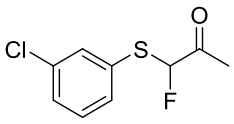
S19

^{13}C NMR (101 MHz, $CDCl_3$): δ 200.0 (d, *J* = 27.4 Hz), 161.1, 136.7 (d, *J* = 1.9 Hz), 119.1, 115.0, 99.7 (d, *J* = 235.2 Hz), 55.4, 26.3

^{19}F NMR: (376 MHz, $CDCl_3$) δ -159.7 (dq, *J* = 52.8, 3.0 Hz).

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{10}H_{11}FNaO_2S$ = 237.0356; **Found:** 237.0357

1-((3-chlorophenyl)thio)-1-fluoropropan-2-one (S20)



S-20

The obtained data of isoindolin-1-one is in correspondence with the literature.[6]

Colorless oil; yield: 71% (2 steps)

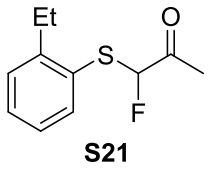
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53 (s, 1H), 7.42 (d, *J* = 7.6 Hz, 1H), 7.36 (d, *J* = 8.1 Hz, 1H), 7.29 (t, *J* = 7.9 Hz, 1H), 6.01 (d, *J* = 52.5 Hz, 1H), 2.18 (d, *J* = 2.8 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 199.0 (d, *J* = 26.5 Hz), 133.4 (d, *J* = 2.0 Hz), 131.8 (d, *J* = 1.9 Hz), 131.4 (d, *J* = 1.9 Hz), 130.5, 129.7, 99.4 (d, *J* = 236.6 Hz), 26.3.

^{19}F NMR (376 MHz, $CDCl_3$): δ -158.7 (dq, *J* = 52.5, 2.7 Hz).

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_9H_8ClFNaOS$ = 240.9861; **Found:** 240.9863

1-((2-ethylphenyl)thio)-1-fluoropropan-2-one (S21)



S21

Colorless oil; yield: 77% (2 steps)

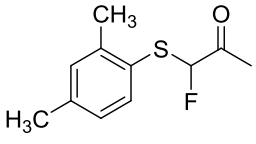
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.57 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.35 – 7.30 (m, 1H), 7.28 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.20 (td, *J* = 7.4, 1.9 Hz, 1H), 5.95 (d, *J* = 53.5 Hz, 1H), 2.91 – 2.83 (m, 2H), 2.13 (d, *J* = 3.0 Hz, 3H), 1.22 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 200.0 (d, *J* = 27.8 Hz), 147.5 (d, *J* = 2.0 Hz), 135.3 (d, *J* = 1.6 Hz), 130.0, 129.4, 128.8 (d, *J* = 1.9 Hz), 127.0, 100.5 (d, *J* = 235.8 Hz), 27.5, 26.2 (d, *J* = 1.8 Hz), 15.4

^{19}F NMR (376 MHz, $CDCl_3$): δ -157.9 (dq, *J* = 53.5, 3.0 Hz).

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{11}H_{13}FNaOS$ = 235.0563; **Found:** 235.0565

1-((2,4-dimethylphenyl)thio)-1-fluoropropan-2-one (S22)



S22

Colorless oil; yield: 78% (2 steps)

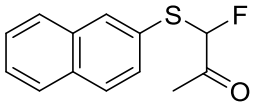
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.43 (d, *J* = 7.8 Hz, 1H), 7.08 (s, 1H), 7.00 (d, *J* = 7.9 Hz, 1H), 5.90 (d, *J* = 53.2 Hz, 1H), 2.44 (s, 3H), 2.31 (s, 3H), 2.10 (d, *J* = 3.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 200.2 (d, *J* = 27.9 Hz), 141.9 (d, *J* = 2.2 Hz), 140.3, 135.91 (d, *J* = 1.6 Hz), 131.8, 127.8, 125.3, 100.4 (d, *J* = 235.6 Hz), 26.2 (d, *J* = 1.5 Hz). 21.2, 21.2

^{19}F NMR (376 MHz, $CDCl_3$): δ -158.72 (dq, *J* = 53.1, 3.0 Hz).

HRMS (ESI) m/z: $(M+ Na)^+$ Calcd for $C_{11}H_{13}FNaOS$ = 235.0563; **Found:** = 235.0563

1-fluoro-1-(naphthalen-2-ylthio)propan-2-one (S23)[6]



S23

The obtained data of isoindolin-1-one is in correspondence with the literature.[6]

Colorless oil; yield: 73% (2 steps)

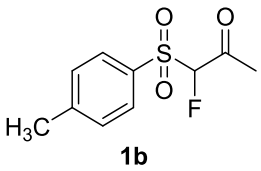
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.06 (d, *J* = 1.6 Hz, 1H), 7.87 – 7.80 (m, 3H), 7.58 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.55 – 7.51 (m, 2H), 6.08 (d, *J* = 52.5 Hz, 1H), 2.15 (d, *J* = 2.8 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 199.5 (d, *J* = 27.0 Hz), 133.8 (d, *J* = 2.2 Hz), 133.6, 133.3, 130.45 (d, *J* = 1.8 Hz), 129.2, 128.0, 127.9, 127.3, 127.0, 126.7 (d, *J* = 1.8 Hz), 99.9 (d, *J* = 235.8 Hz), 26.3

^{19}F NMR (376 MHz, $CDCl_3$): δ -158.50 (dq, *J* = 52.5, 2.8 Hz).

HRMS (ESI) m/z: $(M+ Na)^+$ Calcd for $C_{13}H_{11}FNaOS$ = 257.0407; **Found:** 257.0406

1-fluoro-1-tosylpropan-2-one (1b) [6]



1b

White solid; yield: 90%, The obtained data of isoindolin-1-one is in correspondence with the literature. [6]

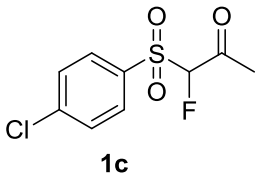
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80 (d, *J* = 8.3 Hz, 2H), 7.41 (d, *J* = 8.0 Hz, 2H), 5.44 (d, *J* = 49.0 Hz, 1H), 2.48 (s, 3H), 2.36 (d, *J* = 3.8 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 195.8 (d, *J* = 21.6 Hz), 147.0, 132.0, 130.3, 129.8, 101.6 (d, *J* = 233.9 Hz). 27.66, 21.99

^{19}F NMR (376 MHz, $CDCl_3$): δ -179.57 (dq, *J* = 49.1, 3.8 Hz).

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{10}H_{11}FNaO_3S$ = 253.0305; **Found:** 253.0308

1-((4-chlorophenyl)sulfonyl)-1-fluoropropan-2-one (1c) [6]



1c

White solid; yield: 92% , The obtained data of isoindolin-1-one is in correspondence with the literature. [6]

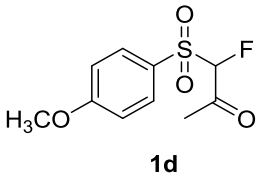
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.86 (d, *J* = 8.3 Hz, 2H), 7.60 (d, *J* = 8.7 Hz, 2H), 5.46 (d, *J* = 48.9 Hz, 1H), 2.39 (d, *J* = 3.8 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 195.4 (d, *J* = 21.6 Hz), 142.7, 133.3, 131.2, 130.1, 101.45 (d, *J* = 234.6 Hz), 27.7

^{19}F NMR (376 MHz, $CDCl_3$): δ -179.4 (dq, *J* = 48.8, 3.7 Hz).

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_9H_8ClFNaO_3S$ = 272.9759; **Found:** 272.9755

1-fluoro-1-((4-methoxyphenyl)sulfonyl)propan-2-one (1d) [6]



1d

White solid; yield: 86%, The obtained data of isoindolin-1-one is in correspondence with the literature. [6]

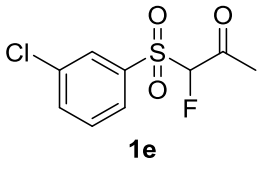
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84 (d, *J* = 8.9 Hz, 2H), 7.05 (d, *J* = 9.0 Hz, 2H), 5.43 (d, *J* = 49.1 Hz, 1H), 3.91 (s, 3H), 2.36 (d, *J* = 3.8 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 195.9 (d, *J* = 21.9 Hz), 165.1, 132.0, 126.0, 114.8, 101.63 (d, *J* = 233.2 Hz), 55.8, 27.5

^{19}F NMR (376 MHz, $CDCl_3$): δ -179.4 (dq, *J* = 49.1, 3.8 Hz).

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{10}H_{11}FNaO_4S$ = 269.0254; **Found:** 269.0257

1-((3-chlorophenyl)sulfonyl)-1-fluoropropan-2-one (1e)



1e

White solid; yield: 89%, The obtained data of isoindolin-1-one is in correspondence with the literature. [6]

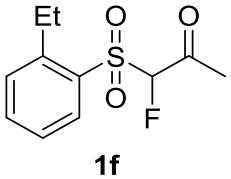
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 (t, *J* = 1.9 Hz, 1H), 7.82 (d, *J* = 7.8 Hz, 1H), 7.73 (ddd, *J* = 8.1, 2.1, 1.1 Hz, 2H), 7.58 (t, *J* = 8.0 Hz, 1H), 5.54 (s, 1H), 5.41 (s, 1H), 2.40 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 195.2 (d, *J* = 21.7 Hz), 136.7, 136.1, 135.7, 130.9, 129.75, 127.9, 101.3 (d, *J* = 235.0 Hz), 27.7.

^{19}F NMR (376 MHz, $CDCl_3$): δ -179.33 (dq, *J* = 48.9, 3.8 Hz).

HRMS (ESI) m/z: $(M+Na)^+$ $C_9H_8ClFNaO_3S$ = 272.9759; **Found:** 272.9756

1-((2-ethylphenyl)sulfonyl)-1-fluoropropan-2-one (1f)



1f

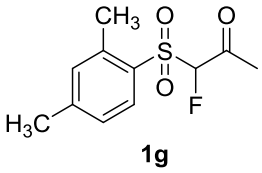
thick oil; yield: 89%

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.65 (td, *J* = 7.6, 1.4 Hz, 1H), 7.46 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.44 – 7.38 (m, 1H), 5.46 (d, *J* = 49.5 Hz, 1H), 3.18 – 2.99 (m, *J* = 7.3 Hz, 2H), 2.39 (d, *J* = 3.9 Hz, 3H), 1.32 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 195.8 (d, *J* = 22.1 Hz), 146.7, 135.5, 133.2, 132.0, 131.73, 126.9, 101.9 (d, *J* = 234.7 Hz), 27.6, 26.6 (d, *J* = 2.1 Hz), 16.4.

^{19}F NMR (376 MHz, $CDCl_3$): δ 179.0 (dq, *J* = 49.6, 3.9 Hz).
HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{11}H_{13}FNaO_3S$ = 267.0462; **Found:** 267.0462

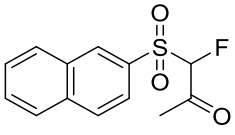
1-((2,4-dimethylphenyl)sulfonyl)-1-fluoropropan-2-one (1g)



1g

White solid; yield: 83%
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.83 (d, *J* = 8.0 Hz, 1H), 7.21 - 7.18 (m, 2H), 5.45 (d, *J* = 49.5 Hz, 1H), 2.66 (s, 3H), 2.41 (s, 3H), 2.39 (d, *J* = 3.8 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 195.9 (d, *J* = 22.1 Hz), 146.7, 140.2, 134.0, 132.1, 130.68, 127.75, 101.96 (d, *J* = 234.0 Hz), 27.63, 21.66, 20.74 (d, *J* = 2.7 Hz).
^{19}F NMR (376 MHz, $CDCl_3$): δ -179.4 (dq, *J* = 49.5, 3.8 Hz).
HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{11}H_{13}FNaO_3S$ = 267.0462; **Found:** 267.0463

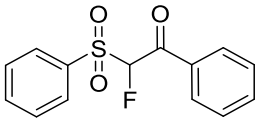
1-fluoro-1-(naphthalen-2-ylsulfonyl)propan-2-one (1h) [6]



1h

White solid; yield: 87%, The obtained data of isoindolin-1-one is in correspondence with the literature. [6]
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.53 (s, 1H), 8.04 (dd, *J* = 8.4, 4.9 Hz, 2H), 7.96 (d, *J* = 7.2 Hz, 1H), 7.87 (dd, *J* = 9.5, 2.0 Hz, 1H), 7.76 – 7.71 (m, 1H), 7.70 – 7.63 (m, 1H), 5.54 (d, *J* = 49.1 Hz, 1H), 2.39 (d, *J* = 3.8 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 195.6 (d, *J* = 22.0 Hz), 136.0, 132.3, 132.0, 131.8, 130.25, 129.89, 129.7, 128.1, 128.1, 123.3, 101.60 (d, *J* = 234.3 Hz), 27.6
^{19}F NMR (376 MHz, $CDCl_3$): δ -179.14 (dq, *J* = 49.6, 3.5 Hz).
HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{13}H_{11}FNaO_3S$ = 289.0305; **Found:** 289.0307

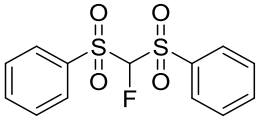
2-fluoro-1-phenyl-2-(phenylsulfonyl)ethan-1-one (1i) [7]



1i

White solid; yield: 83%, The obtained data of isoindolin-1-one is in correspondence with the literature. [7]
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.06 – 7.99 (m, 2H), 7.92 – 7.85 (m, 2H), 7.80 – 7.70 (m, 1H), 7.73 – 7.64 (m, 1H), 7.64 – 7.56 (m, 2H), 7.56 – 7.49 (m, 2H), 6.34 (d, *J* = 48.0 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 186.6 (d, *J* = 17.2 Hz), 135.4, 135.2, 134.8, 134.1, 130.1 (2C), 130.0, 129.9, 129.5 (2C), 129.0 (2C), 100.43 (d, *J* = 232.2 Hz).
^{19}F NMR (376 MHz, $CDCl_3$): δ -179.50 (d, J = 48.0 Hz).
HRMS (ESI) m/z: $(M+NH_4)^+$ Calcd for $C_{14}H_{15}FNO_3S$ = 296.0751; **Found:** 296.0769.

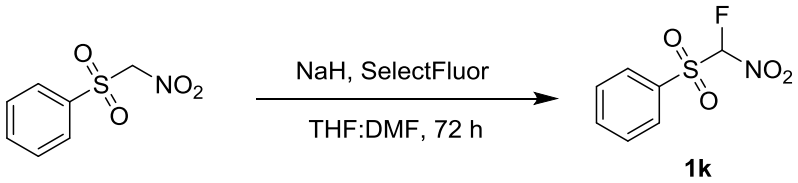
1-fluoro-bis(phenylsulfonyl)methane (1j) [7]



1j

White solid; yield: 80%, The obtained data of isoindolin-1-one is in correspondence with the literature. [7]
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.06 – 7.96 (m, 4H), 7.86 – 7.71 (m, 2H), 7.70 – 7.55 (m, 4H), 5.72 (d, *J* = 45.8 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 135.9 (2C), 135.5 (2C), 130.3 (4C), 129.6 (4C), 107.2, 105.9 (d, *J* = 266.1 Hz).
^{19}F NMR (376 MHz, $CDCl_3$): δ -168.19 (d, *J* = 45.8 Hz).
HRMS (ESI) m/z: $(M+H)^+$ Calcd for $C_{13}H_{12}FO_4S_2$ = 315.0156; **Found:** 315.0150.

3.3 Procedures for (fluoro(nitro)methyl)sulfonyl)benzene (1k)

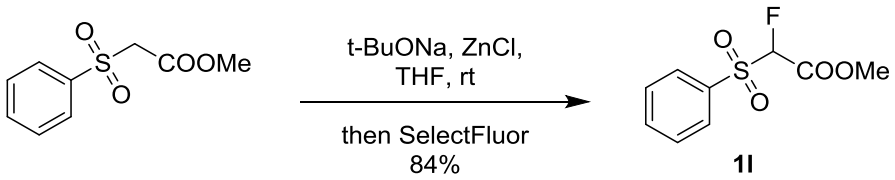


Scheme S4: Synthesis of ((fluoro(nitro)methyl)sulfonyl)benzene (1k)

To a stirring mixture of NaH (1.0 eq.) in dry THF:DMF (10 mL:2 mL) was added nitro(phenylsulfonyl)-methane (1.0 eq.) at 0 °C under argon atmosphere. After stirring for 2 h, SelectFluor (1.0 equiv.) in dry was added portionwise over 5 min at 0 °C. Then reaction mixture was stirred at 25 °C for 3 days, quenched by 2M HCl until it became clear. After extraction with EtOAc, the organic layer was dried over anhydrous Na_2SO_4, filtered and removed under vacuum. The crude product was purified by flash column chromatography on silica gel with EtOAc/hexane to provided (4:1 to 3:1) to give **1k** as white solid in 56 % yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 (d, *J* = 7.1 Hz, 2H), 7.91 – 7.82 (m, 1H), 7.76 – 7.64 (m, 2H), 6.42 (d, *J* = 48.6 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 136.8, 131.5, 130.7, 130.0, δ 111.9 (d, *J* = 283.8 Hz).
^{19}F NMR (376 MHz, $CDCl_3$): δ -141.6
HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_7H_6FNNaO_4S$ = 241.9894; **Found:** 241.9896

3.4 Procedures for Methyl 2-fluoro-2-(phenylsulfonyl)acetate (1l)[7]

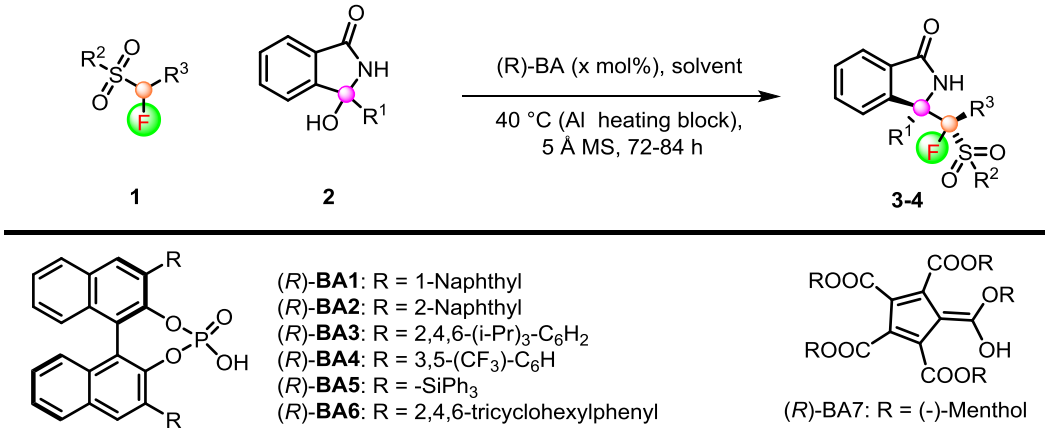


Scheme S5: Synthesis of Methyl 2-fluoro-2-(phenylsulfonyl)acetate (1l)

anhydrous ZnCl2 (2.2 equiv.) and *t*BuONa (2.5 equiv.) were dissolved in 15 mL THF. After 5 minutes, Methyl 2-(phenylsulfonyl)acetate (1.0 equiv.) was added to above mixture under N2 atmosphere. The reaction was stirred for half an hour. Then SelectFluor (2.0 equiv.) was added into the mixture in a flash. The reaction was allowed at room temperature for 2 h and quenched by 2M HCl until it became clear. After extraction with EtOAc, the organic layer was dried over anhydrous Na2SO4, filtered and removed under vacuum. The crude product was purified by flash column chromatography on silica gel with EtOAc/hexane to provide **1l** as colorless liquid in 82% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.94 (d, *J* = 7.3 Hz, 2H), 7.82 – 7.74 (m, 1H), 7.62 (t, *J* = 7.8 Hz, 2H), 5.59 (d, *J* = 47.9 Hz, 1H), 3.85 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 161.61 (d, *J* = 23.8 Hz), 135.5, 134.6, 129.9, 129.6, 97.4 (d, *J* = 232.1 Hz), 53.9
^{19}F NMR (376 MHz, $CDCl_3$): δ -180.5
HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_9H_9FNaO_4S$ = 255.0098; **Found:** 255.0098

4.1 Procedure for organocatalytic reaction:

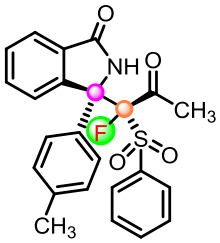


Scheme S6: organocatalytic reaction

An oven-dried 4 mL vial was charged with corresponding 3-hyroxy Isoindolinone (0.1 mmol), respective Fluorosulfones (0.15 mmol), 10 mol % of catalyst (*R*)-TIPSY i.e (*R*)-BA5 and 100 mg 5 Å molecular sieves followed by adition of p-xylene (1.5 mL). Then the reaction was stirred at 40 °C on Modular aluminium Heating Blocks for 72-84 h. Upon completion of the reaction, the resulting mixture was directly subjected to flash column chromatography using (100 DCM to 100:0.5 ml DCM: MeOH) OR (2:1 N-Hexanes: EtOAc) afforded desired products **3a-3o** and **4a-l.**

4.2 Characterization data of products

(R)-3-((*R*)-1-fluoro-2-oxo-1-(phenylsulfonyl)propyl)-3-(p-tolyl)isoindolin-1-one (3a)



3a

Purification by column chromatography (2:1 N-Hexanes: EtOAc) afforded compound **3a** as White foam (yield: 83%)

^{1}H NMR (400 MHz, DMSO): δ 7.87 (dd, *J* = 7.8, 2.4 Hz, 1H), 7.79 (d, *J* = 7.5 Hz, 1H), 7.76 (bs, 1H), 7.61 – 7.41 (m, 7H), 7.36 – 7.27 (m, 2H), 6.95 (d, *J* = 8.2 Hz, 2H), 2.26 (s, 3H), 1.81 (d, *J* = 6.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 196.2 (d, *J* = 27.6 Hz), 168.9, 144.8, 139.0, 135.5, 134.2, 132.6, 132.2 (d, *J* = 2.6 Hz), 130.9, 130.1, 129.9, 129.2, 128.6, 127.0 (d, *J* = 5.3 Hz), 124.7, 124.5 (d, *J* = 2.7 Hz), 109.6 (d, *J* = 245.4 Hz), 66.9 (d, *J* = 21.2 Hz), 28.2, 20.8

^{19}F NMR (376 MHz, $CDCl_3$): δ -149.4

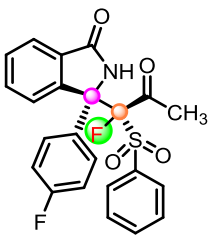
HRMS (ESI) m/z: $(M+H)^+$ Calcd for $C_{24}H_{21}FNO_4S$ = 438.1170; **Found:** 438.1167

$[\alpha]^{20}_D$ = -73.6° (*c* = 0.38, $CHCl_3$).

Diastereomeric excess (*dr*): 20:1

Enantiomeric excess (*ee*): 98%, Determined by HPLC (Chiralpak IH column, *n*-heptane/isopropanol = 90/10, Flow rate 1.0 mL/min, T = 35 °C, λ = 216 nm) retention times: t_{major} = 71.8 min, t_{minor} = 96.8 min.

(*R*)-3-((*R*)-1-fluoro-2-oxo-1-(phenylsulfonyl)propyl)-3-(4-fluorophenyl)isoindolin-1-one (3b)



3b

Purification by column chromatography (2:1 *n*-Hexanes: EtOAc) afforded compound **3b** as White foam solid (yield: 62%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88 – 7.80 (m, 2H), 7.77 (bs, 1H), 7.71 – 7.65 (m, 2H), 7.63 – 7.55 (m, 2H), 7.54 – 7.45 (m, 3H), 7.38 (t, *J* = 7.9 Hz, 2H), 6.86 (t, *J* = 8.6 Hz, 2H), 1.78 (d, *J* = 6.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 196.2 (d, *J* = 27.7 Hz), 169.0, 163.2 (d, *J* = 250.7 Hz), 144.7, 135.5, 134.8, 132.9, 131.3, 131.0, 130.2 (d, *J* = 5.6 Hz), 129.2 (d, *J* = 5.8 Hz), 129.1 (d, *J* = 5.8 Hz), 129.0, 125.0, 124.5 (d, *J* = 2.8 Hz), 115.5 (d, *J* = 21.6 Hz), 109.1 (d, *J* = 248.1 Hz), 66.9 (d, *J* = 21.1 Hz),

28.3

^{19}F NMR (376 MHz, $CDCl_3$): δ -112.6, -149.3

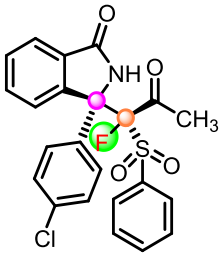
HRMS (ESI) m/z: $(M+H)^+$ Calcd for $C_{23}H_{18}F_2NO_4S$ = 442.0919; **Found:** 442.0916

$[\alpha]^{20}_D$ = -55.8° (*c* = 0.25, $CHCl_3$).

Diastereomeric excess (*dr*): >17:1

Enantiomeric excess (*ee*): 90%, Determined by HPLC (Chiralpak IH column, *n*-heptane/isopropanol = 90/10, Flow rate 1.0 mL/min, T = 35 °C, λ = 225 nm) retention times: t_{major} = 74.3 min, t_{minor} = 85.0 min.

(*R*)-3-(4-chlorophenyl)-3-((*R*)-1-fluoro-2-oxo-1-(phenylsulfonyl)propyl)isoindolin-1-one (3c)



3c

Purification by column chromatography (2:1 N-Hexanes: EtOAc) afforded compound **3c** as white foam solid (yield: 73%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.86 – 7.80 (m, 2H), 7.76 (bs, 1H), 7.66 – 7.55 (m, 4H), 7.55 – 7.44 (m, 3H), 7.41 – 7.33 (m, 2H), 7.12 (d, *J* = 8.9 Hz, 2H), 1.80 (d, *J* = 6.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 196.1 (d, *J* = 28.1 Hz), 169.0, 144.4, 135.6, 135.4, 134.8, 134.0 (d, *J* = 2.8 Hz), 133.0, 131.0, 130.3, 130.2 (d, *J* = 1.5 Hz), 129.0, 128.7, 128.6 (d, *J* = 5.8 Hz), 125.1, 124.4 (d, *J* = 2.9 Hz), 109.3 (d, *J* = 246.6 Hz), δ 66.8 (d, *J* = 20.6 Hz), 28.3

^{19}F NMR (376 MHz, $CDCl_3$): δ -149.4

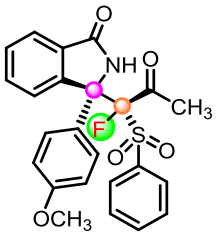
HRMS (ESI) m/z: $(M+H)^+$ Calcd for $C_{23}H_{18}ClFNO_4S$ = 458.0624; **Found:** 458.0620

$[\alpha]^{20}_D$ = -63.9° (*c* = 0.18, $CHCl_3$).

Diastereomeric excess (*dr*): 20:1

Enantiomeric excess (*ee*): 92%, Determined by HPLC (Chiralpak IH column, *n*-heptane/isopropanol = 90/10, Flow rate 1.0 mL/min, T = 35 °C, λ = 228 nm) retention times: t_{major} = 64.6 min, t_{minor} = 77.4 min.

(*R*)-3-((*R*)-1-fluoro-2-oxo-1-(phenylsulfonyl)propyl)-3-(4-methoxyphenyl)isoindolin-1-one (3d)



3d

Purification by column chromatography (2:1 N-Hexanes: EtOAc) afforded compound **3d** as white foam solid (yield: 59%);

^{1}H NMR (400 MHz, $CDCl_3$): 7.85 (dd, *J* = 7.8, 2.5 Hz, 1H), 7.80 (d, *J* = 7.5 Hz, 1H), 7.75 (bs, 1H), 7.61 – 7.46 (m, 7H), 7.39 – 7.30 (m, 2H), 6.84 – 6.77 (m, 1H), 6.68 (d, *J* = 12.2 Hz, 1H), 3.76 (s, 3H), 1.82 (d, *J* = 6.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): 196.4 (d, *J* = 27.1 Hz), 169.1, 160.2, 145.1, 135.7, 134.5, 132.8, 132.2, (d, *J* = 1.6 Hz, 1H), 130.0, 128.8, 128.5 (d, *J* = 5.4 Hz), 124.9, 124.6 (d, *J* = 2.8 Hz), 124.4, 113.9, 109.7 (d, *J* = 249.5 Hz), 66.4 (d, *J* = 20.2 Hz), 55.4, 28.3.

^{19}F NMR (376 MHz, $CDCl_3$): δ -149.2

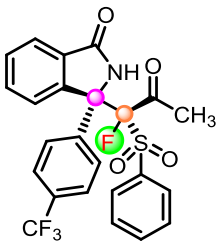
HRMS (ESI) m/z: $(M+H)^+$ Calcd for $C_{24}H_{21}FNO_5S$ = 454.1119; **Found:** 454.1113

$[\alpha]^{20}_D$ = -34.1° (*c* = 0.41, $CHCl_3$).

Diastereomeric excess (*dr*): 8:1

Enantiomeric excess (*ee*): 90%, Determined by HPLC (Chiralpak IH column, *n*-heptane/isopropanol = 90/10, Flow rate 1.0 mL/min, T = 35 °C, λ = 223 nm) retention times: t_{major} = 119.4 min, t_{minor} = 143.8 min.

(*R*)-3-((*R*)-1-fluoro-2-oxo-1-(phenylsulfonyl)propyl)3(4-(trifluoromethyl)phenyl)isoindolin1-one (3e)



3e

Purification by column chromatography (100% DCM to 100:0.5 ml DCM: MeOH) afforded compound **3e** as white foam (66%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.86 – 7.86 (m, 5H), 7.56 -7.52 (m, 3H), 7.47 (d, *J* = 8.3 Hz, 2H), 7.41 (d, *J* = 8.4 Hz, 2H), 7.36 – 7.29 (m, 2H), 1.82 (d, *J* = 6.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 195.9 (d, *J* = 27.7 Hz), 169.0, 144.1, 139.5, 135.2, 135.0, 133.1, 131.2, 131.0, 130.5, 130.1 (d, *J* = 1.7 Hz), 129.0, 127.7 (d, *J* = 6.1 Hz), 125.5 (q, *J* = 4.1 Hz), 125.2, 124.4 (d, *J* = 3.0 Hz), 107.0 (d, *J* = 162.1 Hz), 67.0 (d, *J* = 20.9 Hz), 28.3

^{19}F NMR (376 MHz, $CDCl_3$): δ -62.9, -149.5

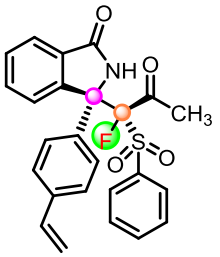
HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{24}H_{17}F_4NaNO_4S$ = 514.0707; **Found:** 514.0711

[α]$^{20}_D$ = -45.1° (*c* = 0.20, $CHCl_3$).

Diastereomeric excess (*dr*): 19:1

Enantiomeric excess (*ee*):>99%, Determined by HPLC (Chiralpak AD column, *n*-heptane/isopropanol = 80/20, Flow rate 1.0 mL/min, T = 25 °C, λ = 223 nm) retention times: t_{major} = 25.3 min, t_{minor} = 80.1 min.

(*R*)-3-((*R*)-1-fluoro-2-oxo-1-(phenylsulfonyl)propyl)-3-(4-vinylphenyl)isoindolin-1-one (3f)



3f

Purification by column chromatography (2:1 N-Hexanes: EtOAc) afforded compound **3f** as white foam solid (yield: 76%);

^{1}H NMR (400 MHz, $CDCl_3$): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (dd, *J* = 7.8, 2.5 Hz, 1H), 7.81 (d, *J* = 7.5 Hz, 1H), 7.76 (bs, 1H), 7.63 – 7.58 (m, 2H), 7.58 – 7.52 (m, 2H), 7.50 (dd, *J* = 7.5, 0.9 Hz, 1H), 7.48 – 7.45 (m, 1H), 7.45 – 7.42 (m, 1H), 7.32 – 7.26 (m, 2H), 7.16 (d, *J* = 8.5 Hz, 2H), 6.62 (dd, *J* = 17.6, 10.9 Hz, 1H), 5.70 (dd, *J* = 17.6, 0.7 Hz, 1H), 5.28 (dd, *J* = 10.9, 0.6 Hz, 1H), 1.84 (d, *J* = 6.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 196.2 (d, *J* = 27.7 Hz), 169.1, 144.7, 138.5, 135.8, 135.5, 134.6, 134.3, 132.8, 131.0, 130.2, 129.0, 128.9, 127.4 (d, *J* = 5.6 Hz).126.3, 124.9, 124.6 (d, *J* = 2.8 Hz), 115.4, 109.6 (d, *J* = 246.3 Hz), 67.0 (d, *J* = 21.2 Hz), 28.4.

^{19}F NMR (376 MHz, $CDCl_3$): δ -149.3.

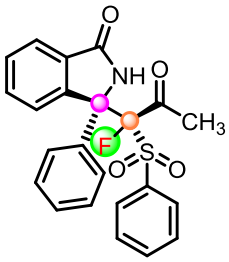
HRMS (ESI) m/z: $(M+H)^+$ Calcd for $C_{25}H_{21}FNO_4S$ = 450.1170; **Found:** 450.1170

[α]$^{20}_D$ = -98.9° (*c* = 0.27, $CHCl_3$).

Diastereomeric excess (*dr*): >20:1

Enantiomeric excess (*ee*): 91%, Determined by HPLC (Chiralpak IH column, *n*-heptane/isopropanol = 90/10, Flow rate 1.0 mL/min, T = 35 °C, λ = 231 nm) retention times: t_{major} = 78.7 min, t_{minor} = 103.2 min.

(*R*)-3-((*R*)-1-fluoro-2-oxo-1-(phenylsulfonyl)propyl)-3-phenylisoindolin-1-one (3g)



3g

Purification by column chromatography (2:1, N-Hexanes: EtOAc) afforded compound **3g** as white foam solid (yield: 70%);

^{1}H NMR (400 MHz, $CDCl_3$): δ ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (dd, *J* = 7.8, 2.4 Hz, 1H), 7.80 (d, *J* = 7.5 Hz, 2H), 7.68 (d, *J* = 7.8 Hz, 2H), 7.58 – 7.53 (m, 2H), 7.53 – 7.44 (m, 3H), 7.31 (t, *J* = 7.9 Hz, 2H), 7.23 (d, *J* = 7.2 Hz, 1H), 7.17 (t, *J* = 7.5 Hz, 2H), 1.81 (d, *J* = 6.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 196.3 (d, *J* = 27.8 Hz), 169.1, 144.8, 135.5, 135.3, 134.6, 132.8, 131.0, 130.2 (d, *J* = 1.7 Hz), 130.1, 129.2, 128.9, 128.6, 127.3 (d, *J* = 5.5 Hz), 124.9, 124.7 (d, *J* = 2.7 Hz), 109.4 (d, *J* = 246.3 Hz), 67.1 (d, *J* = 19.8 Hz), 28.3.

^{19}F NMR (376 MHz, $CDCl_3$): δ -149.2.

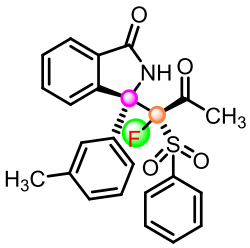
HRMS (ESI) m/z: $(M+H)^+$ Calcd for $C_{23}H_{19}FNO_4S$ = 424.1013; **Found:** 424.1006

[α]$^{20}_D$ = -55.8° (*c* = 0.26, $CHCl_3$).

Diastereomeric excess (*dr*): 18:1

Enantiomeric excess (*ee*): 90%, Determined by HPLC (Chiralpak IH column, *n*-heptane/isopropanol = 90/10, Flow rate 1.0 mL/min, T = 35 °C, λ = 228 nm) retention times: t_{major} = 68.1 min, t_{minor} = 79.9 min.

(*R*)-3-((*R*)-1-fluoro-2-oxo-1-(phenylsulfonyl)propyl)-3-(m-tolyl)isoindolin-1-one (3h)



3h

Purification by column chromatography (2:1, N-Hexanes: EtOAc) afforded compound **3h** as white foam solid (68%).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88 (dd, *J* = 7.5, 2.1 Hz, 1H), 7.82 (d, *J* = 7.1 Hz, 1H), 7.78 (bs, 1H), 7.63 – 7.55 (m, 2H), 7.55 – 7.41 (m, 5H), 7.35 – 7.29 (m, 2H), 7.11– 7.03 (m, 2H), 2.21 (s, 3H), 1.88 (d, *J* = 6.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): 196.2 (d, *J* = 28.0 Hz), 169.1, 144.9, 138.3, 135.6, 135.2 (d, *J* = 2.8 Hz), 134.5, 132.8, 131.0, 130.2 (d, *J* = 1.6 Hz), 130.1, 129.9, 128.7, 128.5, 127.9 (d, *J* = 5.7 Hz), 124.8, 124.7, 124.3 (d, *J* = 5.4 Hz), 109.5 (d, *J* = 245.0 Hz), 67.0 (d, *J* = 21.1 Hz), 28.4, 21.6.

^{19}F NMR (376 MHz, $CDCl_3$): δ -149.1

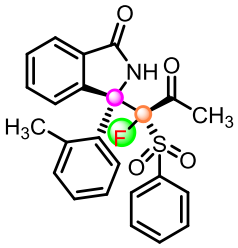
HRMS (ESI) m/z: $(M+H)^+$ Calcd for $C_{24}H_{21}FNO_4S$ = 438.1170; **Found:** 438.1171

$[\alpha]^{20}_D$ = -42.4° (*c* = 0.30, $CHCl_3$).

Diastereomeric excess (*dr*): 14:1

Enantiomeric excess (*ee*):89%, Determined by HPLC (Chiralpak IA column, *n*-heptane/isopropanol = 80/20, Flow rate 1.0 mL/min, T = 25 °C, λ = 199 nm) retention times: t_{major} = 27.8 min, t_{minor} = 26.1 min.

(*R*)-3-((*R*)-1-fluoro-2-oxo-1-(phenylsulfonyl)propyl)-3-(o-tolyl)isoindolin-1-one (3i)



3i

Purification by column chromatography (2:1, N-Hexanes: EtOAc) afforded compound **3h** as white foam solid (53%).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93 – 7.89 (m, 1H), 7.88 – 7.84 (m, 2H), 7.67 (s, 1H), 7.61 – 7.52 (m, 5H), 7.38 (dd, *J* = 8.6, 7.3 Hz, 2H), 7.12 – 7.09 (m, 1H), 6.95 – 6.89 (m, 1H), 2.65 (s, 3H), 1.70 (d, *J* = 6.7 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 196.3 (d, *J* = 29.0 Hz), 168.4, 145.2, 136.7, 135.8, 134.6, 134.4, 132.6, 131.4, 130.0 (d, *J* = 1.5 Hz), 129.9, 129.6 (d, *J* = 13.9 Hz), 128.8, 128.7, 125.9 (d, *J* = 2.0 Hz), 125.4 (d, *J* = 2.1 Hz), 124.5, 123.6, 109.9 (d, *J* = 250.5 Hz), 69.1 (d, *J* = 19.5 Hz), δ 28.2 (d, *J* = 1.5 Hz), 24.8

^{19}F NMR (376 MHz, $CDCl_3$): δ -145.88

HRMS (ESI) m/z: $(M+H)^+$ Calcd for $C_{24}H_{21}FNO_4S$ = 438.1170; **Found:** 438.1172

$[\alpha]^{20}_D$ = -71.3 ° (*c* = 0.3, $CHCl_3$).

Diastereomeric excess (*dr*): 13:1

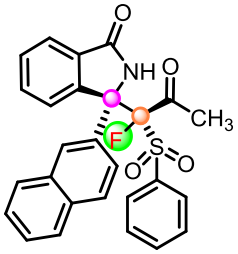
Enantiomeric excess (*ee*): 83%, Determined by HPLC (Chiralpak AD column, *n*-heptane/isopropanol = 80/20, Flow rate 1.0 mL/min, T = 25 °C, λ = 206 nm) retention times: t_{major} = 34.2 min, t_{minor} = 22.3 min.

(*R*)-3-((*R*)-1-fluoro-2-oxo-1-(phenylsulfonyl)propyl)-3-(naphthalen-2-yl)isoindolin-1-one (3J)

Purification by column chromatography (2:1, N-Hexanes: EtOAc) afforded compound **3j** as white foam solid (67%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.16 (bs, 1H), 7.96 (dd, *J* = 7.8, 2.5 Hz, 1H), 7.92 (s, 1H), 7.86 – 7.81 (m, 1H), 7.79 – 7.68 (m, 3H), 7.60 – 7.55(m, 1H), 7.55 – 7.45 (m, 3H), 7.37 – 7.32 (m, 2H), 7.32 – 7.28 (m, 1H), 6.96 (t, *J* = 7.9 Hz, 2H), 1.91 (d, *J* = 6.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 196.2 (d, *J* = 27.5 Hz), 169.2, 144.8, 135.3, 134.4, 133.2, 132.8,



3j

132.8, δ 132.6 (d, *J* = 2.8 Hz), 131.0, 130.2, 130.1 (d, *J* = 1.6 Hz), 129.0, 128.7, 128.49, 128.2, 127.2 (d, *J* = 6.1 Hz), 126.9 (d, *J* = 3.3 Hz), 126.7, 125.0, 124.7 (d, *J* = 2.7 Hz), 124.3 (d, *J* = 8.2 Hz), 109.7 (d, *J* = 246.2 Hz), 67.3 (d, *J* = 21.1 Hz), 28.5.

^{19}F NMR (376 MHz, $CDCl_3$): δ -149.10

HRMS (ESI) m/z: $(M+H)^+$ Calcd for $C_{27}H_{21}FNO_4S$ = 474.1170; **Found:** 474.1173

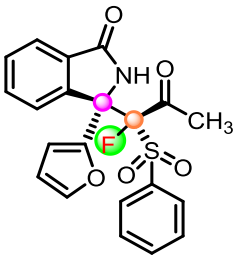
$[\alpha]^{20}_D$ = -48.5° (*c* = 0.65, $CHCl_3$).

Diastereomeric excess (*dr*): 13:1

Enantiomeric excess (*ee*): 89%, Determined by HPLC (Chiralpak IH column, *n*-heptane/isopropanol = 90/10, Flow rate 1.0 mL/min, T = 35 °C, λ = 240 nm) retention times: t_{major} = 83.1 min, t_{minor} = 97.8 min.

(*S*)-3-((*R*)-1-fluoro-2-oxo-1-(phenylsulfonyl)propyl)-3-(furan-2-yl)isoindolin-1-one (3k)

Purification by column chromatography (100% DCM to 100:0.5 ml DCM: MeOH) afforded compound **3k** as white foam (40%);



3k

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 – 7.92(m, 1H), 7.87 – 7.82 (m, 1H), 7.75 – 7.68 (m, 2H), 7.69 – 7.64 (m, 1H), 7.61 (dd, *J* = 7.6, 1.4 Hz, 1H), 7.56 (dd, *J* = 7.4, 1.1 Hz, 1H), 7.54 – 7.47 (m, 2H), 7.43 – 7.39 (m, 1H), 7.24 (dd, *J* = 1.8, 0.9 Hz, 1H), 6.56 (dd, *J* = 3.4, 0.9 Hz, 1H), 6.30 (dd, *J* = 3.4, 1.8 Hz, 1H), 1.71 (d, *J* = 6.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 196.5 (d, *J* = 28.4 Hz), 169.1, 144.2, 142.3, 134.9, 134.6 (d, *J* = 30.8 Hz), 132.8, 130.9, 130.5 (d, *J* = 1.5 Hz), 130.4, 129.2, 125.4 (d, *J* = 4.1 Hz), 124.8, 123.7, 110.7, 110.1, 107.9 (d, *J* = 247.0 Hz), 71.3 (d, *J* = 11.7 Hz), 27.9

^{19}F NMR (376 MHz, $CDCl_3$): δ -150.6

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{21}H_{16}FNaNO_5S$ = 436.0625; **Found:** 436.0625

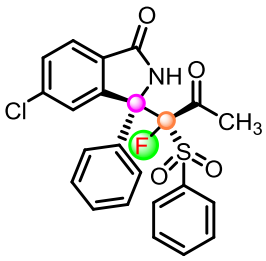
$[\alpha]^{20}_D$ = -26.2° (*c* = 0.31, $CHCl_3$).

Diastereomeric excess (*dr*): 5:1

Enantiomeric excess (*ee*): 93%, Determined by HPLC (Chiralpak IA column, *n*-heptane/isopropanol = 80/20, Flow rate 1.0 mL/min, T = 25 °C, λ = 231 nm) retention times: t_{major} = 26.4 min, t_{minor} = 35.1 min.

(*R*)-5-chloro-3-((*R*)-1-fluoro-2-oxo-1-(phenylsulfonyl)propyl)-3-phenylisoindolin-1-one (3l)

Purification by column chromatography (2:1, N-Hexanes: EtOAc) afforded compound **3h** as white foam (89%);



3l

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 (t, *J* = 2.0 Hz, 1H), 7.78 (bs, 1H), 7.73 (d, *J* = 8.1 Hz, 1H), 7.65 – 7.60 (m, 2H), 7.59 – 7.52 (m, 1H), 7.50 – 7.42 (m, 3H), 7.32 (dd, *J* = 8.5, 7.4 Hz, 2H), 7.26 –7.24 (m, 1H), 7.19 (t, *J* = 8.4, 2H), 1.90 (d, *J* = 6.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 196.3 (d, *J* = 27.5 Hz), 168.0, 146.3, 139.2, 135.4, 134.7, 130.7, 130.2, 130.2, 129.5, 129.4, 128.9, 128.8, 127.2 (d, *J* = 5.6 Hz), 126.0, 125.1 (d, *J* = 3.0 Hz), 109.1 (d, *J* = 246.5 Hz), 67.1 (d, *J* = 19.40 Hz), 28.5

^{19}F NMR (376 MHz, $CDCl_3$): δ -149.2

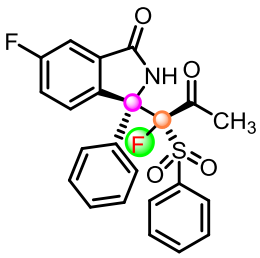
HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{23}H_{17}ClFNaNO_4S$ = 480.0443; **Found:** 480.0436

$[\alpha]^{20}_D$ = +22.7° (*c* = 0.58, EtOAc)

Diastereomeric excess (*dr*): >20:1

Enantiomeric excess (*ee*): 95%, Determined by HPLC (Chiralpak AD column, *n*-heptane/isopropanol = 80/20, Flow rate 1.0 mL/min, T = 25 °C, λ = 233 nm) retention times: t_{major} = 23.0 min, t_{minor} = 33.0 min.

(*R*)-6-fluoro-3-((*R*)-1-fluoro-2-oxo-1-(phenylsulfonyl)propyl)-3-phenylisoindolin-1-one (3m)



3m

Purification by column chromatography (100% DCM to 100:0.5 ml DCM: MeOH) afforded compound **3m** as white foam (73%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.89 - 7.84 (m, 2H), 7.67 – 7.61 (m, 2H), 7.60 – 7.52 (m, 1H), 7.49 – 7.43 (m, 3H), 7.33 (d, *J* = 7.5 Hz, 2H), 7.31 – 7.23 (m, 2H), 7.21 – 7.15 (m, 2H), 1.85 (d, *J* = 6.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ δ196.3 (d, *J* = 27.3 Hz), 167.6, 163.7 (d, *J* = 252.0 Hz), 140.1, 135.3, 134.6, 133.5 (d, *J* = 8.5 Hz), 130.1, 129.2, 129.0, 128.8, 128.6, 127.0 (d, *J* = 5.4 Hz), 126.4, 126.0 (d, *J* = 3.9 Hz), 120.2 (d, *J* = 23.6 Hz), 111.5 (d, *J* = 23.6 Hz), 66.9 (d, *J* = 21.0 Hz), 28.3

^{19}F NMR (376 MHz, $CDCl_3$): δ 109.3 (m), -149.1 (d, *J* = 6.2 Hz).

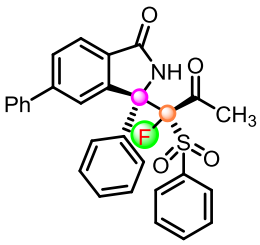
HRMS (ESI) m/z: $(M+H)^+$ Calcd for $C_{23}H_{18}F_2NO_4S$ = 442.0919; **Found:** 442.0917

[α]$^{20}_D$ = -53.3° (*c* = 0.45, $CHCl_3$).

Diastereomeric excess (*dr*): 6:1

Enantiomeric excess (*ee*): 94%, Determined by HPLC (Chiralpak IA column, *n*-heptane/isopropanol = 95/05, Flow rate 1.0 mL/min, T = 35 °C, λ = 229 nm) retention times: t_{major} = 69.2 min, t_{minor} = 62.5 min.

(*R*)-3-((*R*)-1-fluoro-2-oxo-1-(phenylsulfonyl)propyl)-3,5-diphenylisoindolin-1-one (3n)



3n

Purification by column chromatography (100% DCM to 100:0.5 ml DCM: MeOH) afforded compound **3n** as white foam (88%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.06 (bs, 1H), 7.88 (d, *J* = 7.9 Hz, 1H), 7.83 (s, 1H), 7.78 – 7.70 (m, 3H), 7.62 – 7.54 (m, 3H), 7.53 – 7.41 (m, 5H), 7.33 (t, *J* = 7.9 Hz, 2H), 7.28 (d, *J* = 3.8 Hz, 1H), 7.20 (t, *J* = 7.5 Hz, 2H), 1.91 (d, *J* = 6.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 196.3 (d, *J* = 27.7 Hz), 168.9, 146.3, 145.6, 139.9, 135.5, 135.4, 134.6, 130.2 (d, *J* = 1.7 Hz), 129.8, 129.4, 129.2, 129.0, 128.9, 128.7, 128.6, 127.6, 127.3 (d, *J* = 5.4 Hz), 125.1, 123.4, 109.5 (d, *J* = 245.8 Hz), 67.2 (d, *J* = 21.1 Hz), 28.5

^{19}F NMR (376 MHz, $CDCl_3$): δ -149.1

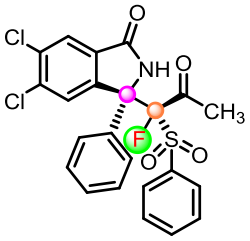
HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{29}H_{22}FNaNO_4S$ = 522.1146; **Found:** 522.1147

[α]$^{20}_D$ = +54.8° (*c* = 0.31, $CHCl_3$).

Diastereomeric excess (*dr*):17:1

Enantiomeric excess (*ee*): 94%, Determined by HPLC (Chiralpak IB column, *n*-heptane/isopropanol = 80/20, Flow rate 1.0 mL/min, T = 25 °C, λ = 242 nm) retention times: t_{major} = 25.5 min, t_{minor} = 18.6 min.

(*R*)-5,6-dichloro-3-((*R*)-1-fluoro-2-oxo-1-(phenylsulfonyl)propyl)-3-phenylisoindolin-1-one (3o)



3o

Purification by column chromatography (2:1, N-Hexanes: EtOAc) afforded compound **3o** as white foam (74%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, *J* = 2.0 Hz, 1H), 7.87 (s, 1H), 7.85 (bs, 1H), 7.62 – 7.54 (m, 3H), 7.45 (d, *J* = 8.5 Hz, 2H), 7.37 – 7.30 (m, 2H), 7.29 – 7.25 (m, 1H), 7.20 (t, *J* = 7.5 Hz, 2H), 1.94 (d, *J* = 6.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 196.5 (d, *J* = 27.9 Hz), 166.8, 143.6, 137.4, 135.4, 135.2, 134.9, 134.5 (d, *J* = 2.7 Hz), 130.9, 130.2, 129.5, 129.0, 128.9, 127.1 (d, *J* = 5.4 Hz), 126.9 (d, *J* = 2.7 Hz), 126.5, 108.9 (d, *J* = 245.7 Hz), 66.9 (d, *J* = 21.1 Hz), 28.7

^{19}F NMR (376 MHz, $CDCl_3$): δ -149.15, -149.17

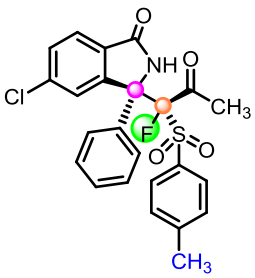
HRMS (ESI) m/z: $(M+H)^+$ Calcd for $C_{23}H_{17}Cl_2FNO_4S$ = 492.0234; **Found:** 492.0234

[α]$^{20}_D$ = +17.2° (*c* = 0.61, $CHCl_3$).

Diastereomeric excess (*dr*): >20:1

Enantiomeric excess (*ee*): 99%, Determined by HPLC (Chiralpak IB column, *n*-heptane/isopropanol = 95/05, Flow rate 1.0 mL/min, T = 25 °C, λ = 223 nm) retention times: t_{major} = 32.9 min, t_{minor} = 41.8 min.

(*R*)-5-chloro-3-((*R*)-1-fluoro-2-oxo-1-tosylpropyl)-3-phenylisoindolin-1-one (4a)



4a

Purification by column chromatography (100% DCM to 100:0.5 ml DCM: MeOH) afforded compound **3m** as white foam (74%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 (t, *J* = 2.0 Hz, 1H), 7.78 (bs, 1H), 7.73 (d, *J* = 8.1 Hz, 1H), 7.68 – 7.61 (m, 2H), 7.47 (dd, *J* = 8.1, 1.7 Hz, 1H), 7.35 –7.28 (m, 3H), 7.21 (dd, *J* = 8.4, 6.7 Hz, 2H), 7.11 (d, *J* = 7.9 Hz, 2H), 2.39 (s, 3H), 1.87 (d, *J* = 6.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 196.4 (d, *J* = 27.9 Hz), 167.8, 146.2, 146.2, 139.0, 134.8 (d, *J* = 2.9 Hz), 132.2, 130.5, 130.1, 130.1, 129.5, 129.1, 128.6, 127.1 (d, *J* = 5.6 Hz), 125.8, 125.0 (d, *J* = 2.9 Hz), 108.8 (d, *J* = 246.1 Hz), 66.9 (d, *J* = 21.2 Hz), 28.4, 21.7.

^{19}F NMR (376 MHz, $CDCl_3$): δ -149.4

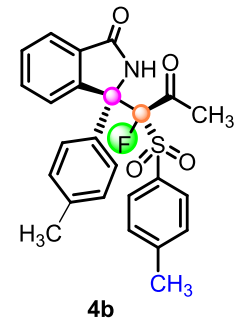
HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{24}H_{19}ClFNNaO_4S$ = 494.0600; **Found:** 494.0594

$[\alpha]^{20}_D$ = +31.3° (*c* = 0.42, EtOAc).

Diastereomeric excess (*dr*): 13:1

Enantiomeric excess (*ee*): 98%, Determined by HPLC (Chiralpak AD column, *n*-heptane/isopropanol = 80/20, Flow rate 1.0 mL/min, T = 25 °C, λ = 199 nm) retention times: t_{major} = 20.5 min, t_{minor} = 22.5 min.

(*R*)-3-((*R*)-1-fluoro-2-oxo-1-tosylpropyl)-3-(p-tolyl)isoindolin-1-one (4b)



4b

Purification by column chromatography (100% DCM to 100:0.5 ml DCM: MeOH) afforded compound **4b** as white foam (69%);

(Major Diastereomer)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87 (dd, *J* = 7.9, 2.3 Hz, 1H), 7.81 – 7.78 (m, 1H), 7.78 – 7.71 (m, 1H), 7.58 – 7.52 (m, 3H), 7.53 – 7.44 (m, 1H), 7.40 – 7.32 (m, 2H), 7.10 (d, *J* = 8.2 Hz, 3H), 6.97 (d, *J* = 8.1 Hz, 1H), 2.40 (s, 3H), 2.28 (s, 3H), 1.79 (d, *J* = 6.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 196.5 (d, *J* = 27.7 Hz), 169.1, 146.0, 145.0, 139.1, 132.7, 132.2, 131.0, 130.2 (d, *J* = 1.5 Hz), 130.0, 129.8, 129.4, 129.2, 127.1 (d, *J* = 5.3 Hz), 124.8, 124.7 (d, *J* = 2.8 Hz), 109.4 (d, *J* = 245.5 Hz), 67.1 (d, *J* = 21.3 Hz), 28.3, 21.8, 21.0

^{13}C NMR (101 MHz, $CDCl_3$): δ ^{19}F NMR (376 MHz, $CDCl_3$) δ -149.6

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{25}H_{22}FNNaO_4S$ = 474.1146; **Found:** 474.1151

$[\alpha]^{20}_D$ = -28.9° (*c* = 0.23, $CHCl_3$).

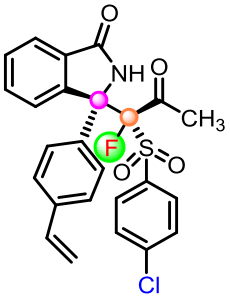
Diastereomeric excess (*dr*): 3:1

Enantiomeric excess (*ee*): 81%, Determined by HPLC (Chiralpak AD column, *n*-heptane/isopropanol = 80/20, Flow rate 1.0 mL/min, T = 25 °C, λ = 213 nm) retention times: t_{major} = 28.9 min, t_{minor} = 38.6 min.

(*R*)-3-((*R*)-1-((4-chlorophenyl)sulfonyl)-1-fluoro-2-oxopropyl)-3-(4-vinylphenyl)isoindolin-1-one (4c)

Purification by column chromatography (2:1, N-Hexanes: EtOAc) afforded compound **4c** as white foam (83%);

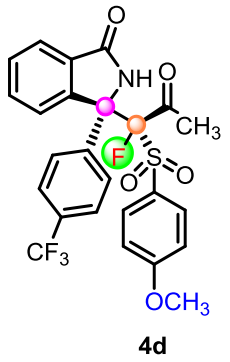
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 – 7.80 (m, 2H), 7.74 (bs, 1H), 7.63 – 7.55 (m, 3H), 7.55 – 7.47 (m, 1H), 7.38 – 7.29 (m, 2H), 7.28 – 7.22 (m, 2H), 7.22 – 7.14 (m, 2H), 6.66 (dd, *J* = 17.6, 11.0, 9.1 Hz, 1H), 5.75 (dd, *J* = 17.6, 8.9, 1H), 5.38 – 5.30 (m, 1H), 1.92 (d, *J* = 6.3 Hz, 3H).



4c

^{13}C NMR (101 MHz, $CDCl_3$): δ 195.91 (d, *J* = 26.6 Hz), 169.07, 144.58, 141.72, 138.86, 135.52, 133.78, 132.99, 131.39 (d, *J* = 1.8 Hz),
130.9, 130.3, 129.3, 129.1, 127.3 (d, *J* = 5.5 Hz), 126.3, 125.0, 124.5, 115.9, 109.7 (d, *J* = 248.3 Hz), 67.0, 28.5.
^{19}F NMR (376 MHz, $CDCl_3$): δ -149.1
HRMS (ESI) m/z: $(M+H)^+$ Calcd for $C_{25}H_{20}ClFNNaO_4S$ = 484.0780; **Found:** 484.0781
[α]$^{20}_D$ = -72.7° (*c* = 0.33, $CHCl_3$).
Diastereomeric excess (*dr*): 5:1
Enantiomeric excess (*ee*): 90%, Determined by HPLC (Chiralpak IA column, *n*-heptane/isopropanol = 90/10, Flow rate 1.0 mL/min, T = 25 °C, λ = 245nm) retention times: t_{major} = 68.7 min, t_{minor} = 43.7 min.

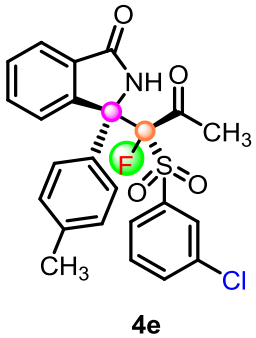
(*R*)-3-((*R*)-1-fluoro-1-((4-methoxyphenyl)sulfonyl)-2-oxopropyl)-3-(4-(trifluoromethyl)-phenyl) isoindolin-1-one (4d)



4d

Purification by column chromatography (100% DCM to 100:0.5 ml DCM: MeOH) afforded compound **4d** as white foam (69%);
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91 – 7.79 (m, 5H), 7.59 (td, *J* = 7.6, 1.3 Hz, 1H), 7.52 (t, *J* = 7.9 Hz, 1H), 7.44 (d, *J* = 8.7 Hz, 2H), 7.38 (d, *J* = 7.5 Hz, 2H), 6.82 – 6.69 (m, 2H), 3.83 (s, 3H), 1.84 (d, *J* = 6.5 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 196.2 (d, *J* = 27.8 Hz), 169.1, 164.9, 144.3, 139.8, 133.0, 132.6, 132.5 (d, *J* = 1.5 Hz), 131.3, 131.0, 130.5, 127.7 (d, *J* = 6.0 Hz), 126.2, 125.4 (q, *J* = 3.8 Hz), 125.1, 124.44 (d, *J* = 2.9 Hz), 114.3, 108.8 (d, *J* = 245.6 Hz), 67.0 (d, *J* = 21.3 Hz), 55.8, 28.4
^{19}F NMR (376 MHz, $CDCl_3$): δ -62.8, -149.7
HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{25}H_{19}F_4NNaO_5S$ = 544.0812; **Found:** 544.0817
[α]$^{20}_D$ = -30.2° (*c* = 0.27, $CHCl_3$).
Diastereomeric excess (*dr*): 20:1
Enantiomeric excess (*ee*): 92%, Determined by HPLC (Chiralpak IA column, *n*-heptane/isopropanol = 90/10, Flow rate 1.0 mL/min, T = 25 °C, λ = 209 nm) retention times: t_{major} = 57.0 min, t_{minor} = 42.3 min.

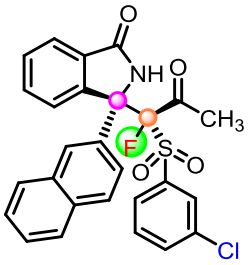
(*R*)-3-((*R*)-1-((3-chlorophenyl)sulfonyl)-1-fluoro-2-oxopropyl)-3-(p-tolyl)isoindolin-1-one (4e)



4e

Purification by column chromatography (100% DCM to 100:0.5 ml DCM: MeOH) afforded compound **3m** as white foam (71%);
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93 – 7.76 (m, 2H), 7.72 (bs, 1H), 7.57 (td, *J* = 7.6, 1.3 Hz, 1H), 7.54 – 7.35 (m, 4H), 7.35 – 7.23 (m, 3H), 7.03 – 6.79 (m, 2H), 2.27 (s, 3H), 1.93 (d, *J* = 6.3 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 195.7 (d, *J* = 28.1 Hz), 144.7, 139.7, 137.2, 135.1, 134.4, 132.9, 131.9, 130.9, 130.2, 129.9, 129.8, 129.3, 128.4 (d, *J* = 3.0 Hz), 127.1 (d, *J* = 5.4 Hz), 124.9, 124.5 (d, *J* = 2.7 Hz), 109.9 (d, *J* = 247.2 Hz), 66.8 (d, *J* = 21.1 Hz), 28.5, 21.1.
^{19}F NMR (376 MHz, $CDCl_3$): δ 18.2, -149.0
HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{24}H_{19}ClFNNaO_4S$ = 494.0600; **Found:** 494.0604
[α]$^{20}_D$ = -29.8° (*c* = 0.28, $CHCl_3$).
Diastereomeric excess (*dr*): 4:1
Enantiomeric excess (*ee*): 85%, Determined by HPLC (Chiralpak AD column, *n*-heptane/isopropanol = 80/20, Flow rate 1.0 mL/min, T = 25 °C, λ = 227 nm) retention times: t_{major} = 32.3 min, t_{minor} = 63.6 min.

(*R*)-3-((*R*)-1-((3-chlorophenyl)sulfonyl)-1-fluoro-2-oxopropyl)-3-(naphthalen-2-yl)isoindolin-1-one (4f)



4f

Purification by column chromatography (100% DCM to 100:0.5 ml DCM: MeOH) afforded compound **4f** as white foam (69%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.16 (bs, 1H), 8.06 – 7.94 (m, 1H), 7.93 – 7.83 (m, 2H), 7.81 – 7.72 (m, 2H), 7.72 – 7.65 (m, 1H), 7.62 (td, *J* = 7.6, 1.3 Hz, 1H), 7.59 – 7.45 (m, 4H), 7.28 – 7.23 (m, 2H), 7.23 – 7.19 (m, 1H), 6.89 (t, *J* = 8.2 Hz, 1H), 2.01 (d, *J* = 6.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 195.6 (d, *J* = 27.4 Hz), 169.0, 144.4, 136.8, 134.9, 134.2, 133.1, 132.8, 132.6, 132.0, 130.8, 130.2, 129.7, 129.4, 128.4, 128.2, 128.0 (d, *J* = 2.3 Hz), 127.3 (d, *J* = 1.6 Hz), 126.8, 126.8, 124.9, 124.5, 123.9 (d, *J* = 7.9 Hz), 109.8 (d, *J* = 245.9 Hz),, 66.9 (d, *J* = 20.9 Hz), 28.5

^{19}F NMR (376 MHz, $CDCl_3$): δ -148.84

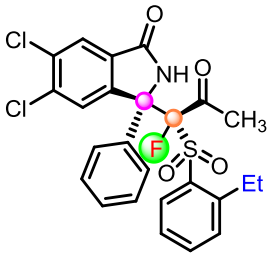
HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{27}H_{19}ClFNNaO_4S$ = 530.0600; **Found:** 530.0603

$[\alpha]^{20}_D$ = -62.8° (*c* = 0.28, $CHCl_3$).

Diastereomeric excess (*dr*): 10:1

Enantiomeric excess (*ee*): 71%, Determined by HPLC (Chiralpak IB column, *n*-heptane/isopropanol = 80/20, Flow rate 0.5 mL/min, T = 25 °C, λ = 206 nm) retention times: t_{major} = 29.7 min, t_{minor} = 43.4 min.

(*R*)-5,6-dichloro-3-((*R*)-1((2-ethylphenyl)sulfonyl)1-fluoro-2-oxopropyl)-3-phenylisoindolin-1one(4g)



4g

Purification by column chromatography (100% DCM to 100:0.5 ml DCM: MeOH) afforded compound **4g** as white foam (74%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99 (d, *J* = 2.2 Hz, 1H), 7.91 (bs, 1H), 7.86 (s, 1H), 7.67 – 7.59 (m, 2H), 7.47 (td, *J* = 7.5, 1.4 Hz, 1H), 7.34 – 7.19 (m, 6H), 7.00 (t, *J* = 8.4 Hz, 1H), 3.17 – 2.86 (m, 2H), 1.87 (d, *J* = 6.2 Hz, 3H), 1.24 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 196.1 (d, *J* = 27.3 Hz), 166.9, 147.5, 143.9, 137.3, 135.4, 135.1, 134.6 (d, *J* = 2.9 Hz), 133.4, 132.3, 131.3, 130.9, 129.5, 128.9, 127.1 (d, *J* = 5.7 Hz), 126.9 (d, *J* = 3.2 Hz), 126.5 (d, *J* = 3.1 Hz), 109.5 (d, *J* = 247.2 Hz), 67.3 (d, *J* = 21.6 Hz), 28.6, (d, *J* = 21.6 Hz), 16.6

^{19}F NMR (376 MHz, $CDCl_3$): δ -149.09

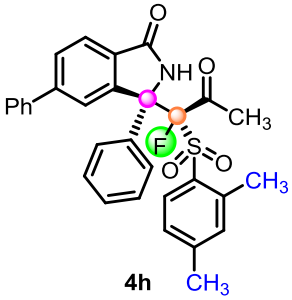
HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{25}H_{20}Cl_2FNNaO_4S$ = 542.0366; **Found:** 542.0370

$[\alpha]^{20}_D$ = -40.8° (*c* = 0.62, $CHCl_3$).

Diastereomeric excess (*dr*): 20:1

Enantiomeric excess (*ee*): 94%, Determined by HPLC (Chiralpak AD column, *n*-heptane/isopropanol = 90/10, Flow rate 1.0 mL/min, T = 25 °C, λ = 227 nm) retention times: t_{major} = 22.9 min, t_{minor} = 28.2 min.

(*R*)-3-((*R*)-1-((2,4-dimethylphenyl)sulfonyl)-1-fluoro-2-oxopropyl)-3,5-diphenylisoindolin-1-one (4h)



4h

Purification by column chromatography (100% DCM to 100:0.5 ml DCM: MeOH) afforded compound **4h** as white foam (82%);

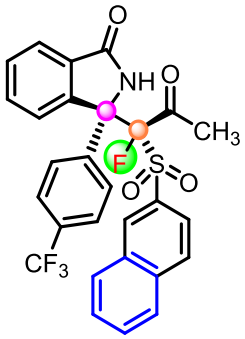
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.06 (s, 1H), 7.89 – 7.83 (m, 2H), 7.83 – 7.74 (m, 2H), 7.69 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.60 – 7.52 (m, 2H), 7.51 – 7.45 (m, 2H), 7.45 – 7.40 (m, 1H), 7.29 – 7.20 (m, 3H), 7.15 (d, *J* = 8.2 Hz, 1H), 7.04 (s, 1H), 6.78 (d, *J* = 8.3 Hz, 1H), 2.62 (s, 3H), 2.32 (s, 3H), 1.82 (d, *J* = 6.2 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 196.2 (d, *J* = 27.5 Hz), 169.0, 146.2, 146.0, 145.8, 140.8, 140.0, 135.6 (d, *J* = 2.9 Hz), 133.4, 132.4, 131.2, 129.8, 129.3, 129.2, 129.0, 128.6, 128.6, 127.6, 127.3, 127.2 (d, *J* = 4.9 Hz), 125.0, 123.5 (d, *J* = 3.2 Hz), 110.2 (d, *J* = 246.2 Hz), 67.6 (d, *J* = 21.7 Hz), 28.3, 21.5, 21.0 (d, *J* = 5.6 Hz).

^{19}F NMR (376 MHz, $CDCl_3$): δ -149.3

HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{31}H_{26}FNNaO_4S$ = 550.1459; **Found:** 550.1463
$[\alpha]^{20}_D$ = +5.5° (*c* = 0.36, $CHCl_3$).
Diastereomeric excess (*dr*): 50:1
Enantiomeric excess (*ee*): 91%, Determined by HPLC (Chiralpak IA column, *n*-heptane/isopropanol = 90/10, Flow rate 1.0 mL/min, T = 25 °C, λ = 212 nm) retention times: t_{major} = 28.9 min, t_{minor} = 41.2 min.

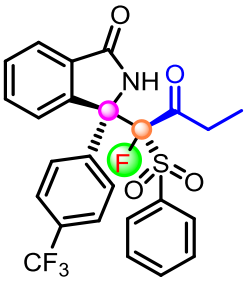
(*R*)-3-((*R*)1-fluoro-1-(naphthalen-2-ylsulfonyl)-2oxopropyl)-3-(4-trifluoromethyl)phenyl) isoindolin-1-one (4i)



4i

Purification by column chromatography (100% DCM to 100:0.5 ml DCM: MeOH) afforded compound **4f** as white foam (65%);
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01 (bs, 1H), 7.89 (s, 1H), 7.87 – 7.79 (m, 5H), 7.79 – 7.73 (m, 2H), 7.70 (t, *J* = 6.9 Hz, 1H), 7.64 – 7.59 (m, 1H), 7.57 (d, *J* = 7.8 Hz, 1H), 7.52 – 7.42 (m, 2H), 7.27 (s, 1H), 1.84 (d, *J* = 6.5 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 196.0 (d, *J* = 27.6 Hz), 169.1, 144.2, 139.5, 135.5, 133.1, 133.0, 132.0, 131.5, 131.0, 130.5 (d, *J* = 6.3 Hz), 129.7, 129.1, 128.2, 127.9, 127.6 (d, *J* = 6.1 Hz), 125.3 (q, *J* = 3.9 Hz), 125.2, 124.8, 124.4 (d, *J* = 2.9 Hz), 124.2, 123.7 (d, *J* = 2.3 Hz), 123.7, 122.1, 109.0 (d, *J* = 246.4 Hz). 67.0 (d, *J* = 21.2 Hz), 28.4.
^{19}F NMR (376 MHz, $CDCl_3$): δ -63.01, -149.3
HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{28}H_{19}F_4NNaO_4S$ = 564.0863; **Found:** 564.0861
$[\alpha]^{20}_D$ = -16.0° (*c* = 0.25, $CHCl_3$).
Diastereomeric excess (*dr*): 17:1
Enantiomeric excess (*ee*): 94%, Determined by HPLC (Chiralpak AD column, *n*-heptane/isopropanol = 80/20, Flow rate 1.0 mL/min, T = 25 °C, λ = 227 nm) retention times: t_{major} = 23.9 min, t_{minor} = 27.8 min.

(*R*)-3-((*R*)-1-fluoro-2-oxo-1-(phenylsulfonyl)butyl)-3-(4-(trifluoromethyl)phenyl)isoindolin-1-one (4j)

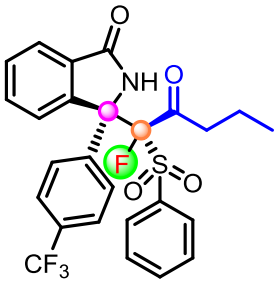


4j

Purification by column chromatography (100% DCM to 100:0.5 ml DCM: MeOH) afforded compound **4f** as white foam (59%);
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91 – 7.79 (m, 5H), 7.63 – 7.54 (m, 2H), 7.53 (d, *J* = 7.5 Hz, 1H), 7.48 (d, *J* = 8.7 Hz, 2H), 7.43 (d, *J* = 8.6 Hz, 2H), 7.33 (t, *J* = 7.9 Hz, 2H), 2.31 – 2.18 (m, 1H), 1.93 – 1.81 (m, 1H), 0.54 (t, *J* = 7.1 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 198.9 (d, *J* = 26.6 Hz), 169.1, 144.1, 139.6, 135.3, 134.9, 133.0, 131.1, 130.5, 130.2 (d, *J* = 1.6 Hz), 129.1, 129.0, 127.7 (d, *J* = 6.1 Hz), 125.5 (d, *J* = 3.6 Hz), 125.1, 124.5 (q, *J* = 2.8 Hz), 109.3 (d, *J* = 247.2 Hz), 67.1 (d, *J* = 20.9 Hz), 34.0, 6.8 (d, *J* = 3.0 Hz).
^{19}F NMR (376 MHz, $CDCl_3$): δ -62.9, -152.6
HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{25}H_{19}F_4NNaO_4S$ = 528.0863; **Found:** 528.0869
$[\alpha]^{20}_D$ = -38.6° (*c* = 0.42, $CHCl_3$).
Diastereomeric excess (*dr*): 9:1
Enantiomeric excess (*ee*): 91%, Determined by HPLC (Chiralpak IA column, *n*-heptane/isopropanol = 80/20, Flow rate 1.0 mL/min, T = 25 °C, λ = 215 nm) retention times: t_{major} = 22.2 min, t_{minor} = 19.1 min.

(*R*)-3-((*R*)-1-fluoro-2-oxo-1-(phenylsulfonyl)pentyl)-3-(4-(trifluoromethyl)phenyl)isoindolin-1one 4k)

Purification by column chromatography (100% DCM to 100:0.5 ml DCM: MeOH) afforded compound **4f** as white foam (63%);
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93 – 7.73 (m, 5H), 7.62 – 7.55 (m, 2H), 7.53 (dd, *J* = 7.5, 0.9



4k

Hz, 1H), 7.49 (d, *J* = 8.3 Hz, 2H), 7.43 (d, *J* = 8.3 Hz, 2H), 7.33 (dd, *J* = 8.4, 7.3 Hz, 2H), 2.24 – 2.15 (m, 1H), 1.87 –1.87 (m, 1H), 1.15 –1.06 (m, 2H), 0.38 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 198.2 (d, *J* = 26.6 Hz), 169.1, 144.2, 139.7, 135.4, 134.9, 133.0, 132.6, 131.2, 130.5, 130.2, 129.1, 129.0, 127.7 (d, *J* = 6.1 Hz), 125.5 (q, *J* = 3.9 Hz), 125.1, 124.5 (d, *J* = 2.7 Hz), 109.1 (d, *J* = 247.4 Hz), 67.1 (d, *J* = 20.4 Hz), 42.2, 15.6 (d, *J* = 2.8 Hz), 12.9

^{19}F NMR (376 MHz, $CDCl_3$): δ -62.94, -152.59

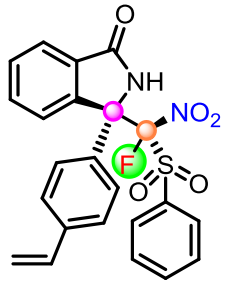
HRMS (ESI) m/z: $(M+Na)^+$ Calcd for $C_{26}H_{21}F_4NNaO_4S$ = 542.1020 =; **Found:** 542.1023

[α]$^{20}_D$ = -33.8° (*c* = 0.40, $CHCl_3$).

Diastereomeric excess (*dr*): 9:1

Enantiomeric excess (*ee*): 93%, Determined by HPLC (Chiralpak IA column, *n*-heptane/isopropanol = 80/20, Flow rate 0.5 mL/min, T = 25 °C, λ = 231 nm) retention times: t_{major} = 37.0 min, t_{minor} = 34.7 min.

(*R*)-3-((*R*)-fluoro(nitro)(phenylsulfonyl)methyl)-3-(4-vinylphenyl)isoindolin-1-one (4l)



4l

Purification by column chromatography (100% DCM to 100:0.5 ml DCM: MeOH) afforded compound **4f** as white foam (80%);

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 – 7.76 (m, 2H), 7.73 – 7.56 (m, 4H), 7.56 – 7.42 (m, 6H), 7.35 (t, *J* = 8.3 Hz, 2H), 6.64 – 6.57 (m, 1H), 5.80 – 5.66 (m, 1H), 5.27 (d, *J* = 10.9 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 169.4, 143.5, 139.0, 136.2, 135.4, 133.2, 133.0, 132.5, 130.95 (d, *J* = 1.5 Hz), 130.6, 130.2, 129.5, 127.6 (d, *J* = 5.0 Hz), 127.3, 125.08 (d, *J* = 4.3 Hz), 124.8, 124.6 (d, *J* = 4.7 Hz), 116.0 (d, *J* = 16.7 Hz), 68.2 (d, *J* = 20.1 Hz).

^{19}F NMR (376 MHz, $CDCl_3$): δ -112.31

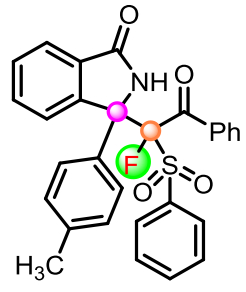
HRMS (ESI) m/z: $(M+ Na)^+$ Calcd for $C_{23}H_{17}FN_2NaO_5S$ = 475.0734 ; **Found:** 475.0738

[α]$^{20}_D$ = +34.6° (*c* = 0.26, $CHCl_3$).

Diastereomeric excess (*dr*): 2:1

Enantiomeric excess (*ee*): 38%, Determined by HPLC (Chiralpak AD column, *n*-heptane/isopropanol = 60/40, Flow rate 1.0 mL/min, T = 25 °C, λ = 227 nm) retention times: t_{major} = 26.3 min, t_{minor} = 18.4 min.

3-(1-fluoro-2-oxo-2-phenyl-1-(phenylsulfonyl)ethyl)-3-(*p*-tolyl)isoindolin-1-one (4m)



4m

Purification by column chromatography (2:1, n-Hexanes: EtOAc) afforded compound **4m** as white foam (50%);

^{1}H NMR (600 MHz, $CDCl_3$): Major diastereoisomer: δ 7.98 (s, 1H), 7.75 – 7.73 (m, 1H), 7.61 – 7.49 (m, 8H), 7.39 – 7.28 (m, 7H), 6.94 (d, *J* = 8.3 Hz, 2H), 2.17 (s, 3H).

^{1}H NMR (400 MHz, $CDCl_3$): Minor diastereoisomer: δ 7.75 – 7.73 (m, 2H), 7.67 – 7.62 (m, 3H), 7.61 – 7.49 (m, 2H), 7.39 – 7.28 (m, 6H), 7.15 (t, *J* = 7.8 Hz, 2H), 7.12 – 7.07 (m, 2H), 7.01 (d, *J* = 8.2 Hz, 2H), 2.28 (s, 3H).

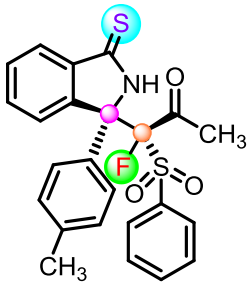
^{13}C NMR (101 MHz, $CDCl_3$): Major diastereoisomer: δ 195.1 (d, *J* = 23.7 Hz), 169.6, 145.2, 138.7, 135.8 (2C), 134.8, 134.0, 132.4 (2C), 131.2, 130.6, 129.7 (4C), 129.3, 128.9 (2C), 128.3 (2C), 127.9, 125.8 (d, J = 4.1 Hz), 125.3 (2C), 124.3, 111.9 (d, J = 252.9 Hz), 69.0 (d, *J* = 23.3 Hz), 20.9.

^{13}C NMR (101 MHz, $CDCl_3$): Minor diastereoisomer: δ 191.2 (d, *J* = 25.5 Hz), 169.4, 145.0, 139.2, 136.3, 134.5 (2C), 134.0, 132.8, 132.6, 131.4, 130.5 (2C), 129.9, 129.8 (2C), 129.4 (2C), 129.0 (2C), 128.8, 128.4, 128.3 (2C), 127.6 (d, *J* = 5.5 Hz), 125.3 (d, *J* = 5.1 Hz), 124.5, 111.5 (d, *J* = 251.4 Hz), 68.3 (d, *J* = 21.2 Hz), 21.0.

^{19}F NMR (376 MHz, $CDCl_3$): δ -146.33 (major), -147.94 (minor).

HRMS (ESI) m/z: (M+ H)$^+$ Calcd for $C_{29}H_{23}FNO_4S$ = 500.1326; **Found:** 500.1326.
Diastereomeric excess (*dr*): 4:3

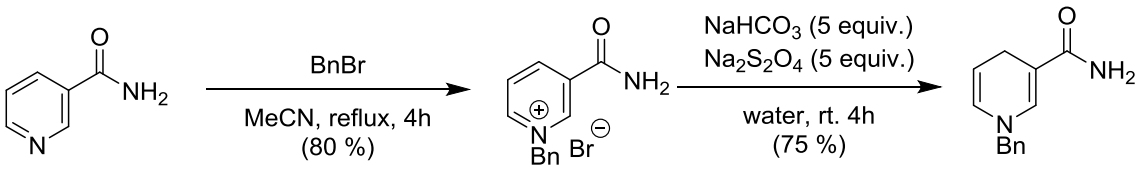
(*R*)-1-fluoro-1-(phenylsulfonyl)-1-((*R*)-3-thioxo-1-(*p*-tolyl)isoindolin-1-yl)propan-2-one (5)



5

Purification by column chromatography (3:1, N-Hexanes: EtOAc) afforded compound **5** as foam (95%);
^{1}H NMR (400 MHz, $CDCl_3$): δ 9.39 (bs, 1H), 8.00 (d, *J* = 7.6 Hz, 1H), 7.87 (dd, *J* = 7.8, 2.4 Hz, 1H), 7.60 (td, *J* = 7.5, 1.3 Hz, 2H), 7.56 – 7.48 (m, 5H), 7.35 (dd, *J* = 8.5, 7.4 Hz, 2H), 6.99 (d, *J* = 8.3 Hz, 2H), 2.29 (s, 3H), 1.86 (d, *J* = 6.2 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 196.1, 195.7, 143.4, 139.4, 137.2, 135.5, 134.6, 132.6, 131.2, 130.31, 130.2, 129.4, 128.8, δ 126.9 (d, *J* = 5.1 Hz), 126.5, 124.0 (d, *J* = 3.2 Hz), 108.7 (d, *J* = 246.6 Hz), 73.4 (d, *J* = 21.2 Hz), 28.2, 21.0
^{19}F NMR (376 MHz, $CDCl_3$): δ -149.8
HRMS (ESI) m/z: (M+ Na)$^+$ Calcd for $C_{24}H_{20}FNNaO_5s$ = 476.0761 ; **Found:** 476.0752
[α]$^{20}_D$ = -80.0° (*c* = 0.25, $CHCl_3$).
Diastereomeric excess (*dr*): 20:1
Enantiomeric excess (*ee*): 93%, Determined by HPLC (Chiralpak IA column, *n*-heptane/isopropanol = 80/20, Flow rate 1.0 mL/min, T = 25 °C, λ = 228 nm) retention times: t_{major} = 8.2 min, t_{minor} = 12.2 min.

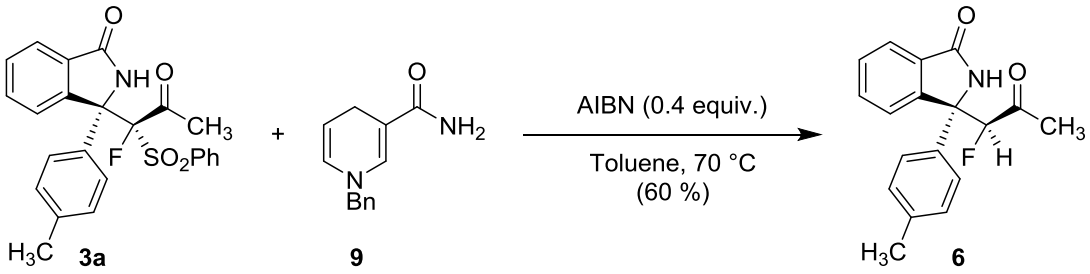
4.3 Preparation of BNAH[8]



8 **9**

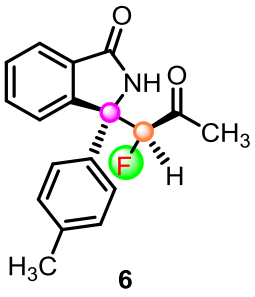
A 100 mL round bottom was filled with nicotinamide (980 mg, 8 mmol), acetonitrile (12 mL) and benzyl bromide (0.95 mL, 8 mmol, 1 equiv.) under Ar. The mixture was stirred under refluxing condition for 4 hours, during which a white precipitate appears. For the workup, the mixture was filtered and the white solid was washed with ether and dried in vaccuo to yield the desired crude product as a white powder (1.88 g, 80%).
A 100 mL flask was filled with the crude nicotinium bromide (1.0 g, 3.4 mmol), water (20 mL) and $NaHCO_3$ (1.43 g, 5 equiv., 17 mmol). Eventually $Na_2S_2O_4$ (2.96 g, 5 equiv., 17 mmol) was added portionwise, during which the mixture turned dark orange. The mixture was stirred for 4h, during which a yellow solid appears. After cooling down under ice bath at 0 °C, the yellow solid was removed by filtration and was washed with cold water to afford the desired product as a pale yellow powder (546 mg, 75%). ^{1}H and ^{13}C NMR correspond to data published in the literature.[9]
^{1}H NMR (400 MHz, CD_3CN): δ 7.41 – 7.24 (m, 5H), 6.98 – 6.94 (m, 1H), 5.84 (dq, *J* = 8.1 Hz, *J´* = 1.7 Hz, 1H), 5.53 (bs, 2H), 4.71 (dt, *J* = 8.0 Hz, *J´* = 3.4 Hz, 1H), 4.30 (s, 2H), 3.05 (dd, *J* = 3.3 Hz, *J´* = 1.5 Hz, 2H).
^{13}C NMR (101 MHz, CD_3CN): δ 170.5, 139.5, 130.3, 129.7 (2C), 128.6 (2C), 128.4 (2C), 103.6, 101.0, 57.5, 23.3.
HRMS (ESI) m/z: (M+H)$^+$ Calcd for $C_{13}H_{15}N_2O$ = 215.1179; **Found:** 215.1189.

4.4 Procedure for desulfonylation reaction:[10]



To the solution of chiral **3a** (23 mg, 0.05 mmol, 1.00 equiv.) in toluene (2 mL), BNAH (32 mg, 0.15 mmol, 3 equiv.) and AIBN (3.3 mg, 0.02 mmol, 0.4 equiv.) was added and heated at 70°C with stirring. After complete consumption of starting material, reaction mixture was cooled to room temperature and loaded directly on silica. Corresponding product was isolated in a mixture of n-hexane/EtOAc; 2:1) as an yellow oil (9 mg, 60%).

(*R*)-1-fluoro-1-(phenylsulfonyl)-1-((*R*)-3-thioxo-1-(*p*-tolyl)isoindolin-1-yl)propan-2-one (6)



Purification by column chromatography (2:1, n-Hexanes: EtOAc) afforded compound **6** as white foam (60%);

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.85 (d, *J* = 7.5 Hz, 1H), 7.66 (d, *J* = 7.7 Hz, 1H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.46 (d, *J* = 8.2 Hz, 2H), 7.30 (s, 1H), 7.15 (d, *J* = 8.1 Hz, 2H), 4.92 (d, *J* = 47.5 Hz, 1H), 2.30 (s, 3H), 2.22 (d, *J* = 5.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 206.9 (d, *J* = 27.5 Hz), 169.7, 147.7, 138.6, 134.6, 132.6, 130.3, 129,9 (2C), 129.3, 125.5 (2C), 124.8 (d, *J* = 3.0 Hz), 124.4, 98.0 (d, *J* = 201.4 Hz), 66.6 (d, *J* = 21.1 Hz), 28.0, 21.1.

^{19}F NMR (376 MHz, $CDCl_3$): δ -184.34 (dd, *J* = 47.5, 4.7 Hz).

HRMS (ESI) m/z: $(M+H)^+$ Calcd for $C_{18}H_{17}FNO_2$ = 298.1238; **Found:** 298.1234.

$[\alpha]^{20}_D$ = -87.0° (*c* = 0.35, $CHCl_3$).

Diastereomeric excess (*dr*): 16:1

Enantiomeric excess (*ee*): 83%, Determined by HPLC (Chiralpak IB column, *n*-heptane/isopropanol = 80/20, Flow rate 1.0 mL/min, T = 25 °C, λ = 200 nm) retention times: t_{major} = 11.6 min, t_{minor} = 8.4 min.

5.1 X-Ray section

Crystallographic data for **3o** were collected on Bruker D8 VENTURE Kappa Duo PHOTONIII by IμS micro-focus sealed tube MoKα (λ= 0.71073) at a temperature of 120(2) K. The structure was solved by direct methods (XT[11a]) and refined by full matrix least squares based on F^2 (SHELXL2018[11b]). The hydrogen atoms on carbon were fixed into idealized positions (riding model) and assigned temperature factors either H_{iso}(H) = 1.2 U_{eq}(pivot atom) or H_{iso}(H) = 1.5 U_{eq} (pivot atom) for methyl moiety. Hydrogen in N-H moiety was found on difference Fourier map and refine in riding model mode with H_{iso}(H) = 1.5 U_{eq}(N). The absolute structure determination was based on anomalous dispersion of S and Cl atoms.

Crystal data for **3o** $C_{23}H_{16}Cl_2FNO_4S$ M_r = 492.33; Orthorhombic, $P\,2_12_12_1$ (No 19), a = 10.4760 (5) Å, b = 14.1768 (7) Å, c = 14.4461 (7) Å , V = 2145.48 (18) Å^3, Z = 4, D_x = 1.524 Mg m^{-3}, colourless prism of dimensions 0.40 × 0.25 × 0.23 mm, multi-scan absorption correction (μ = 0.44 mm^{-1}) T_{min} = 0.87, T_{max} = 0.91; a total of 121548 measured reflections (θ_{max}= 30˚), from which 6247 were unique (R_{int} = 0.025) and 6217 observed according to the $I > 2\sigma(I)$ criterion. The refinement converged (Δ/σ_{max}= 0.001) to R = 0.020 for observed reflections and w$R(F^2)$ = 0.057, GOF = 1.12 for 290 parameters and all 6247 reflections. The final difference map displayed no peaks of chemical significance ($\Delta\rho_{max}$ = 0.32, $\Delta\rho_{min}$ -0.24 e.Å^{-3}). Absolute structure parameter (Flack[12]) 0.004(5)

5.2 Crystallization and X-ray single crystal for compound 3o [CCDC 2162666]

Crystallization:

About 5 mg of **3o** was dissolved in tert-Butyl methyl ether (4.0 ml), DCM (0.5 ml) and MeOH (0.5 ml) and the solvent was evaporated slowly at room atmosphere.

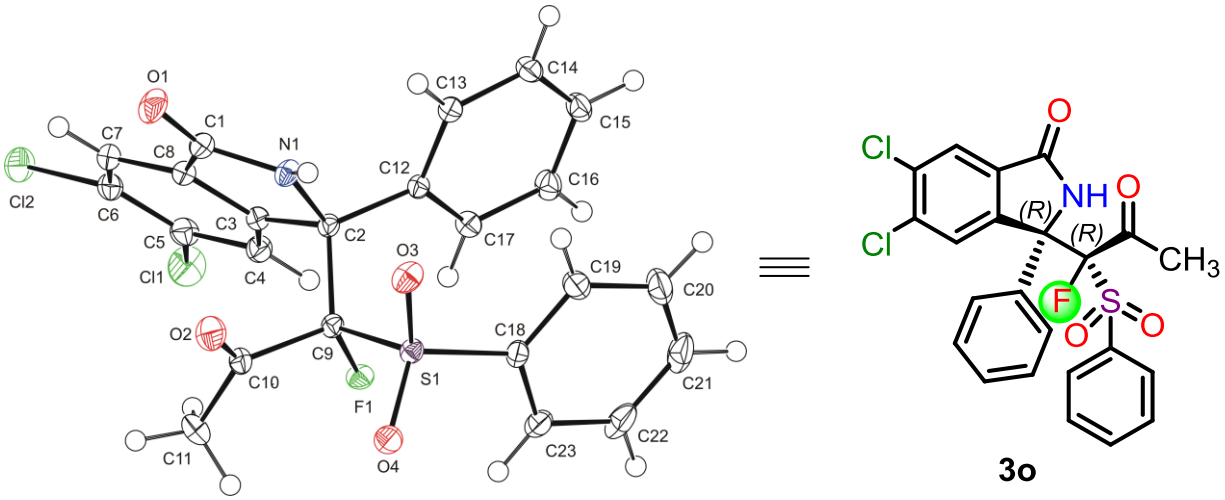


Figure.S1. View on one of symmetrically independent molecule of 3o, the displacement ellipsoids at 50% probability level. (The configuration on C2 and C9 atoms are (*R*, *R*) respectively).

X-ray crystallographic data of **3o** have been deposited with the Cambridge Crystallographic Data Centre (CCDC) under deposition number **2162666** and can be obtained free of charge from the Centre via its website (www.ccdc.cam.ac.uk/getstructures).

5.3. Refinement, Results and discussion

Crystal data, data collection and structure refinement details are summarized in Table 1.

Table 1

Experimental details

Crystal data	
Chemical formula	$C_{23}H_{16}Cl_2FNO_4S$
M_r	492.33
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	120
a, *b*, *c* (Å)	10.4760 (5), 14.1768 (7), 14.4461 (7)
V (Å^3)	2145.48 (18)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.44
Crystal size (mm)	0.40 × 0.25 × 0.23
Data collection	
Diffractometer	Bruker D8 VENTURE Kappa Duo PHOTONIII CMOS
Absorption correction	Multi-scan Krause, L., Herbst-Irmer, R., Sheldrick, G. M., Stalke, D. (2015). "Comparison of silver and molybdenum microfocus X-ray sources for single-crystal structure determination" J. Appl. Cryst. 48, 3-10. doi:10.1107/S1600576714022985
T_{min}, T_{max}	0.87, 0.91
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	121548, 6247, 6217
R_{int}	0.025
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.704
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.020, 0.057, 1.12
No. of reflections	6247

No. of parameters	290
H-atom treatment	H-atom parameters constrained
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.32, -0.24
Absolute structure	Flack x determined using 2724 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	0.004 (5)

Computer programs: Bruker Instrument Service vV6.2.15, *SAINT* V8.40B (Bruker AXS LLC, 2019), SHELXT 2018/2 (Sheldrick, 2018), *SHELXL2018*/3 (Sheldrick, 2018).

Table 2

*Hydrogen-bond geometry (Å, °) for (***3o***)*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O3	0.84	2.35	2.9195 (16)	126

Document origin: *publCIF* [Westrip, S. P. (2010). *J. Apply. Cryst.*, **43**, 920-925].

Computing details

Data collection: Bruker Instrument Service vV6.2.15; cell refinement: *SAINT* V8.40B (Bruker AXS LLC, 2019); data reduction: *SAINT* V8.40B (Bruker AXS LLC, 2019); program(s) used to solve structure: SHELXT 2018/2 (Sheldrick, 2018); program(s) used to refine structure: *SHELXL2018*/3 (Sheldrick, 2018).

Crystal data of (3o)

$C_{23}H_{16}Cl_2FNO_4S$	D_x = 1.524 Mg m^{-3}
M_r = 492.33	Mo $K\alpha$ radiation, λ = 0.71073 Å
Orthorhombic, $P2_12_12_1$	Cell parameters from 9686 reflections
a = 10.4760 (5) Å	θ = 3.7–30.0°
b = 14.1768 (7) Å	μ = 0.44 mm^{-1}
c = 14.4461 (7) Å	T = 120 K
V = 2145.48 (18) Å^3	Prism, colourless
Z = 4	0.40 × 0.25 × 0.23 mm
F(000) = 1008	

Data collection

Bruker D8 VENTURE Kappa Duo PHOTONIII CMOS diffractometer	6247 independent reflections
Radiation source: IμS micro-focus sealed tube	6217 reflections with $I > 2\sigma(I)$
Quazar Mo multilayer optic monochromator	R_{int} = 0.025
ϕ and ω scans	θ_{max} = 30.0°, θ_{min} = 2.0°
Absorption correction: multi-scan Krause, L., Herbst-Irmer, R., Sheldrick, G. M., Stalke, D. (2015). "Comparison of silver and molybdenum microfocus X-ray sources for single-crystal structure determination" J. Appl. Cryst. 48, 3-10. doi:10.1107/S1600576714022985	h = -14→14
T_{min} = 0.87, T_{max} = 0.91	k = -19→19
121548 measured reflections	l = -20→20

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: mixed
$R[F^2 > 2\sigma(F^2)]$ = 0.020	H-atom parameters constrained
$wR(F^2)$ = 0.057	$w = 1/[\sigma^2(F_o^2) + (0.0309P)^2 + 0.4301P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.12	$(\Delta/\sigma)_{max}$ = 0.001
6247 reflections	$\Delta\rangle_{max}$ = 0.32 e Å^{-3}

290 parameters	$\Delta\rangle_{min}$ = -0.24 e Å^{-3}
0 restraints	Absolute structure: Flack x determined using 2724 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Primary atom site location: structure-invariant direct methods	Absolute structure parameter: 0.004 (5)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for (***3o***)*

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.96987 (4)	0.81874 (3)	-0.08227 (3)	0.03066 (9)
Cl2	1.23691 (4)	0.77487 (3)	-0.17331 (3)	0.02969 (9)
S1	0.94357 (3)	0.38427 (2)	0.22249 (2)	0.01355 (6)
F1	0.91120 (8)	0.55744 (6)	0.16907 (6)	0.01570 (15)
O1	1.27798 (10)	0.39176 (8)	-0.05741 (8)	0.0249 (2)
O2	1.21084 (10)	0.45043 (9)	0.17589 (8)	0.0263 (2)
O3	0.98869 (11)	0.29927 (7)	0.17894 (8)	0.0208 (2)
O4	0.98811 (10)	0.41030 (8)	0.31325 (7)	0.0203 (2)
N1	1.08058 (11)	0.39660 (8)	0.01378 (8)	0.0152 (2)
H1	1.085840	0.343290	0.038940	0.023*
C1	1.18221 (13)	0.43390 (10)	-0.03359 (10)	0.0172 (2)
C2	0.98274 (12)	0.46436 (9)	0.04005 (8)	0.0123 (2)
C3	1.03067 (12)	0.55296 (9)	-0.00937 (9)	0.0138 (2)
C4	0.97498 (13)	0.64142 (9)	-0.01762 (9)	0.0168 (2)
H4	0.894989	0.654996	0.010351	0.020*
C5	1.04052 (14)	0.70967 (9)	-0.06839 (10)	0.0189 (3)
C6	1.15918 (15)	0.69007 (10)	-0.10890 (10)	0.0198 (3)
C7	1.21479 (14)	0.60187 (10)	-0.09996 (9)	0.0189 (3)
H7	1.295551	0.588290	-0.126740	0.023*
C8	1.14805 (13)	0.53423 (10)	-0.05045 (9)	0.0157 (2)
C9	0.99205 (12)	0.48363 (9)	0.14681 (9)	0.0128 (2)
C10	1.12953 (13)	0.51041 (11)	0.17757 (10)	0.0180 (2)
C11	1.15062 (16)	0.60939 (12)	0.20973 (12)	0.0275 (3)
H11A	1.118531	0.653452	0.162928	0.041*
H11B	1.242115	0.620085	0.219212	0.041*
H11C	1.105058	0.619527	0.268133	0.041*
C12	0.84952 (12)	0.43451 (9)	0.00683 (8)	0.0129 (2)

C13	0.83545 (13)	0.35090 (10)	-0.04262 (9)	0.0171 (2)
H13	0.907519	0.311382	-0.052076	0.021*
C14	0.71707 (14)	0.32413 (10)	-0.07858 (10)	0.0198 (3)
H14	0.709770	0.267646	-0.113566	0.024*
C15	0.61045 (13)	0.37959 (11)	-0.06341 (10)	0.0198 (3)
H15	0.529583	0.360936	-0.086880	0.024*
C16	0.62293 (13)	0.46330 (10)	-0.01324 (10)	0.0188 (3)
H16	0.550065	0.501655	-0.002481	0.023*
C17	0.74127 (13)	0.49098 (9)	0.02112 (9)	0.0156 (2)
H17	0.748810	0.548470	0.054470	0.019*
C18	0.77623 (12)	0.38467 (10)	0.22219 (9)	0.0151 (2)
C19	0.71328 (14)	0.31211 (11)	0.17619 (10)	0.0207 (3)
H19	0.759434	0.262714	0.146963	0.025*
C20	0.58068 (16)	0.31423 (14)	0.17438 (12)	0.0304 (4)
H20	0.535085	0.264102	0.145898	0.036*
C21	0.51409 (15)	0.38885 (15)	0.21378 (11)	0.0321 (4)
H21	0.423688	0.391047	0.209112	0.038*
C22	0.57871 (15)	0.46020 (14)	0.25989 (11)	0.0273 (3)
H22	0.532268	0.510640	0.287085	0.033*
C23	0.71111 (14)	0.45825 (11)	0.26649 (10)	0.0192 (3)
H23	0.756035	0.505377	0.300014	0.023*

*Atomic displacement parameters (Å^2) for (**3o**)*

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0389 (2)	0.01489 (15)	0.0382 (2)	0.00053 (14)	0.00491 (17)	0.00537 (13)
Cl2	0.0373 (2)	0.02418 (17)	0.02757 (17)	-0.01501 (15)	0.00905 (15)	0.00174 (14)
S1	0.01167 (12)	0.01519 (13)	0.01379 (13)	0.00177 (10)	0.00022 (10)	0.00081 (11)
F1	0.0161 (3)	0.0135 (3)	0.0175 (3)	0.0035 (3)	0.0014 (3)	-0.0029 (3)
O1	0.0164 (5)	0.0264 (5)	0.0319 (5)	0.0045 (4)	0.0077 (4)	-0.0026 (5)
O2	0.0142 (4)	0.0372 (6)	0.0276 (5)	0.0032 (4)	-0.0029 (4)	-0.0021 (5)
O3	0.0225 (5)	0.0154 (4)	0.0244 (5)	0.0050 (4)	0.0055 (4)	0.0011 (4)
O4	0.0156 (4)	0.0302 (5)	0.0152 (4)	0.0008 (4)	-0.0029 (4)	0.0006 (4)
N1	0.0140 (5)	0.0133 (5)	0.0184 (5)	0.0030 (4)	0.0038 (4)	-0.0003 (4)
C1	0.0141 (5)	0.0199 (6)	0.0176 (6)	0.0003 (5)	0.0019 (4)	-0.0032 (5)
C2	0.0111 (5)	0.0116 (5)	0.0141 (5)	0.0004 (4)	0.0016 (4)	-0.0011 (4)
C3	0.0133 (5)	0.0139 (5)	0.0141 (5)	-0.0014 (4)	0.0009 (4)	-0.0013 (4)
C4	0.0176 (5)	0.0145 (5)	0.0182 (5)	-0.0011 (4)	0.0018 (5)	-0.0001 (4)
C5	0.0237 (7)	0.0135 (5)	0.0195 (6)	-0.0028 (5)	0.0006 (5)	0.0002 (4)
C6	0.0235 (7)	0.0190 (6)	0.0168 (6)	-0.0092 (5)	0.0029 (5)	-0.0002 (5)

C7	0.0168 (6)	0.0228 (6)	0.0171 (6)	-0.0057 (5)	0.0031 (5)	-0.0029 (5)
C8	0.0137 (5)	0.0183 (6)	0.0151 (5)	-0.0015 (4)	0.0012 (4)	-0.0023 (4)
C9	0.0104 (5)	0.0130 (5)	0.0150 (5)	0.0015 (4)	0.0008 (4)	-0.0010 (4)
C10	0.0127 (5)	0.0258 (6)	0.0155 (5)	-0.0042 (5)	-0.0002 (4)	-0.0014 (5)
C11	0.0243 (7)	0.0298 (8)	0.0285 (7)	-0.0109 (6)	-0.0009 (6)	-0.0092 (6)
C12	0.0125 (5)	0.0138 (5)	0.0125 (5)	-0.0013 (4)	0.0008 (4)	0.0006 (4)
C13	0.0165 (6)	0.0174 (6)	0.0174 (6)	-0.0027 (5)	0.0032 (5)	-0.0027 (4)
C14	0.0226 (6)	0.0201 (6)	0.0166 (6)	-0.0074 (5)	-0.0001 (5)	-0.0027 (5)
C15	0.0183 (6)	0.0248 (6)	0.0162 (5)	-0.0066 (5)	-0.0039 (5)	0.0016 (5)
C16	0.0145 (6)	0.0222 (6)	0.0198 (6)	0.0003 (5)	-0.0024 (5)	0.0021 (5)
C17	0.0156 (5)	0.0148 (5)	0.0164 (5)	0.0004 (4)	-0.0013 (4)	-0.0001 (4)
C18	0.0120 (5)	0.0191 (6)	0.0142 (5)	-0.0014 (4)	0.0003 (4)	0.0029 (5)
C19	0.0225 (6)	0.0222 (6)	0.0172 (6)	-0.0063 (5)	-0.0019 (5)	0.0013 (5)
C20	0.0231 (7)	0.0450 (10)	0.0230 (7)	-0.0160 (7)	-0.0050 (6)	0.0044 (7)
C21	0.0132 (6)	0.0594 (11)	0.0235 (7)	-0.0044 (7)	-0.0009 (5)	0.0106 (8)
C22	0.0169 (6)	0.0443 (9)	0.0207 (7)	0.0070 (6)	0.0058 (5)	0.0057 (6)
C23	0.0165 (6)	0.0253 (7)	0.0158 (5)	0.0021 (5)	0.0030 (5)	-0.0001 (5)

*Geometric parameters (Å, º) for (**3o**)*

Cl1—C5	1.7260 (15)	C11—H11A	0.9800
Cl2—C6	1.7245 (14)	C11—H11B	0.9800
S1—O3	1.4393 (11)	C11—H11C	0.9800
S1—O4	1.4398 (10)	C12—C13	1.3918 (18)
S1—C18	1.7530 (13)	C12—C17	1.4034 (18)
S1—C9	1.8540 (13)	C13—C14	1.3970 (19)
F1—C9	1.3841 (14)	C13—H13	0.9500
O1—C1	1.2173 (17)	C14—C15	1.383 (2)
O2—C10	1.2038 (19)	C14—H14	0.9500
N1—C1	1.3717 (17)	C15—C16	1.397 (2)
N1—C2	1.4550 (16)	C15—H15	0.9500
N1—H1	0.8405	C16—C17	1.3919 (18)
C1—C8	1.4868 (19)	C16—H16	0.9500
C2—C3	1.5296 (17)	C17—H17	0.9500
C2—C12	1.5353 (18)	C18—C19	1.3909 (19)
C2—C9	1.5693 (18)	C18—C23	1.4011 (19)
C3—C4	1.3882 (18)	C19—C20	1.390 (2)
C3—C8	1.3909 (17)	C19—H19	0.9500
C4—C5	1.3949 (18)	C20—C21	1.389 (3)
C4—H4	0.9500	C20—H20	0.9500
C5—C6	1.402 (2)	C21—C22	1.387 (3)

C6—C7	1.386 (2)	C21—H21	0.9500
C7—C8	1.3855 (19)	C22—C23	1.390 (2)
C7—H7	0.9500	C22—H22	0.9500
C9—C10	1.5544 (18)	C23—H23	0.9500
C10—C11	1.495 (2)		
O3—S1—O4	120.41 (7)	C11—C10—C9	117.08 (12)
O3—S1—C18	109.27 (7)	C10—C11—H11A	109.5
O4—S1—C18	108.99 (6)	C10—C11—H11B	109.5
O3—S1—C9	106.76 (6)	H11A—C11—H11B	109.5
O4—S1—C9	104.68 (6)	C10—C11—H11C	109.5
C18—S1—C9	105.67 (6)	H11A—C11—H11C	109.5
C1—N1—C2	114.98 (11)	H11B—C11—H11C	109.5
C1—N1—H1	120.8	C13—C12—C17	118.41 (12)
C2—N1—H1	121.8	C13—C12—C2	119.43 (11)
O1—C1—N1	126.27 (14)	C17—C12—C2	122.10 (11)
O1—C1—C8	128.43 (13)	C12—C13—C14	121.08 (13)
N1—C1—C8	105.29 (11)	C12—C13—H13	119.5
N1—C2—C3	100.91 (10)	C14—C13—H13	119.5
N1—C2—C12	112.14 (10)	C15—C14—C13	120.23 (13)
C3—C2—C12	112.26 (10)	C15—C14—H14	119.9
N1—C2—C9	109.12 (10)	C13—C14—H14	119.9
C3—C2—C9	107.17 (10)	C14—C15—C16	119.31 (12)
C12—C2—C9	114.31 (10)	C14—C15—H15	120.3
C4—C3—C8	120.49 (12)	C16—C15—H15	120.3
C4—C3—C2	130.08 (12)	C17—C16—C15	120.53 (13)
C8—C3—C2	109.43 (11)	C17—C16—H16	119.7
C3—C4—C5	117.70 (13)	C15—C16—H16	119.7
C3—C4—H4	121.1	C16—C17—C12	120.42 (12)
C5—C4—H4	121.1	C16—C17—H17	119.8
C4—C5—C6	121.23 (13)	C12—C17—H17	119.8
C4—C5—Cl1	118.13 (11)	C19—C18—C23	122.54 (13)
C6—C5—Cl1	120.62 (11)	C19—C18—S1	118.22 (11)
C7—C6—C5	120.85 (12)	C23—C18—S1	119.23 (10)
C7—C6—Cl2	118.74 (11)	C20—C19—C18	117.84 (16)
C5—C6—Cl2	120.38 (11)	C20—C19—H19	121.1
C6—C7—C8	117.42 (13)	C18—C19—H19	121.1
C6—C7—H7	121.3	C21—C20—C19	120.71 (16)
C8—C7—H7	121.3	C21—C20—H20	119.6
C7—C8—C3	122.29 (13)	C19—C20—H20	119.6

C7—C8—C1	128.69 (13)	C22—C21—C20	120.46 (14)
C3—C8—C1	109.00 (11)	C22—C21—H21	119.8
F1—C9—C10	108.42 (10)	C20—C21—H21	119.8
F1—C9—C2	108.78 (10)	C21—C22—C23	120.34 (16)
C10—C9—C2	112.40 (10)	C21—C22—H22	119.8
F1—C9—S1	105.65 (8)	C23—C22—H22	119.8
C10—C9—S1	105.71 (9)	C22—C23—C18	117.98 (15)
C2—C9—S1	115.48 (9)	C22—C23—H23	121.0
O2—C10—C11	124.39 (13)	C18—C23—H23	121.0
O2—C10—C9	118.51 (13)		

*Hydrogen-bond geometry (Å, °) for (**3o**)*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O3	0.84	2.35	2.9195 (16)	126

Document origin: *publCIF* [Westrip, S. P. (2010). *J. Apply. Cryst.*, **43**, 920-925].

6.1 References:

(1) Suneja, R. A. Unhale and V. K. Singh, *Org. Lett.*, 2017, **19**, 476–479;

(2) J. Q. Zhou, W. J. Sheng, J. H. Jia, Q. Ye, J. R. Gao and Y. X. Jia, *Tetrahedron Lett.*, 2013, **54**, 3082–3084.

(3) J. Suć, I. Dokli and M. Gredičak, *Chem. Commun.*, 2016, **52**, 2071–2074.

(4) A. Di Mola, A. Macchia, C. Tedesco, G. Pierri, L. Palombi, R. Filosa and A. Massa, *ChemistrySelect*, 2019, **4**, 4820–4826.

(5) C. Ni, L. Zhang and J. Hu, *J. Org. Chem.*, 2009, **74**, 3767–3771.

(6) B. V. Varun and K. R. Prabhu, *J. Org. Chem.*, 2017, **82**, 9525–9536.

(7) F. Jiang, Y. Zhao and J. Hu, *Org. Chem. Front.*, 2014, **1**, 625–629.

(8) M. Soetens, F. Drouet and O. Riant, *ChemCatChem*., 2017,**9**, 929–933.

(9) G.-B. Shen, K. Xia, X.-T. Li, J.-L. Li, Y.-H. Fu, L. Yuan and X.-Q. Zhu, *J. Phys. Chem. A*, 2016, **120**, 1779−1799.

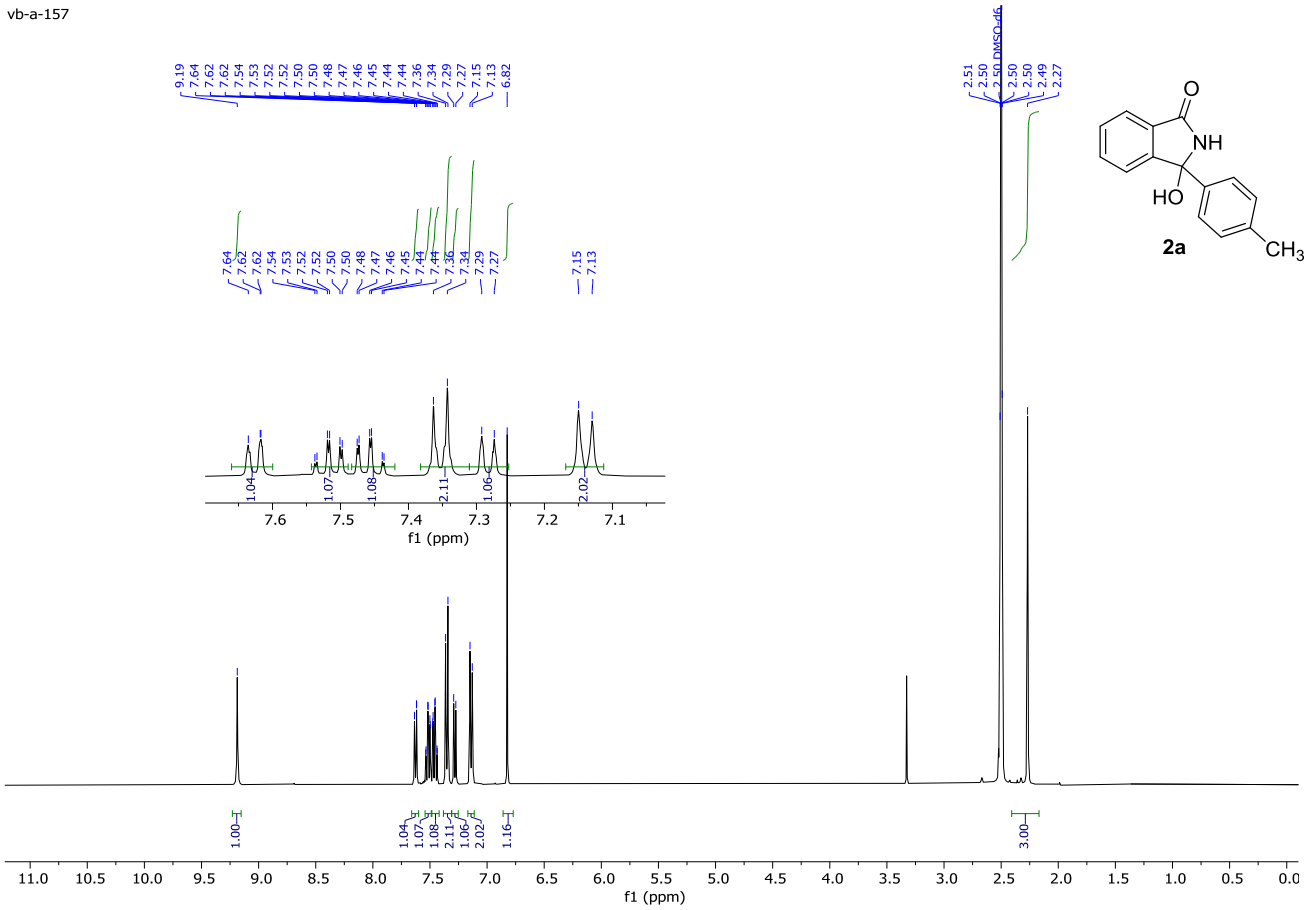
(10) Y. Seo, H. Kim, D. W. Chae and Y. G. Kim, *Tetrahedron: Asymmetry*, 2014, **25**, 625-631.

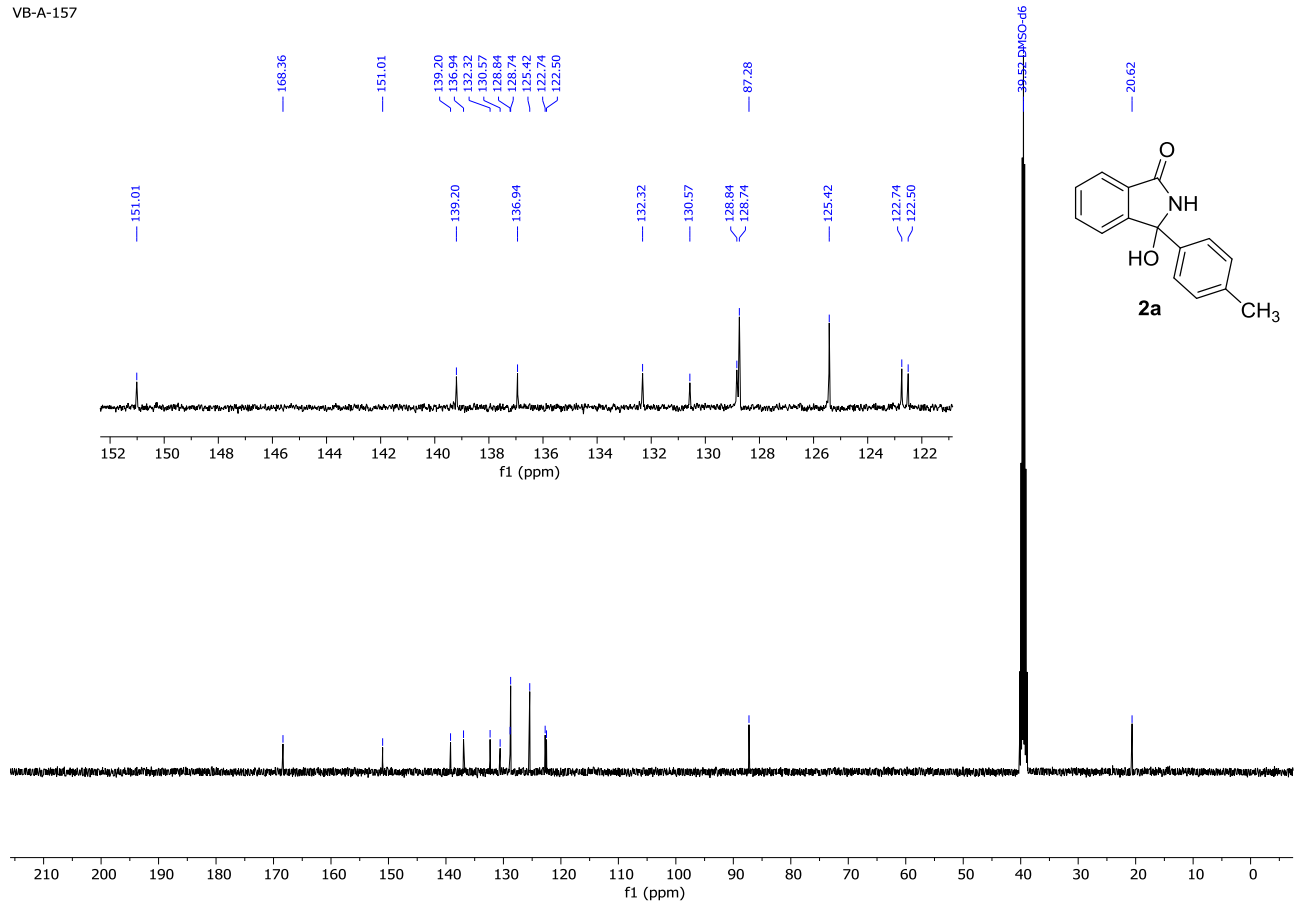
(11a) SHELXT: Sheldrick, G.M. (2015). *Acta Cryst*. **A71**, 3-8.

(11b) SHELXL: Sheldrick, G.M. (2015). *Acta Cryst.* **C71**, 3-8.

(12) Parsons,S., Flack, H.D. and Wagner, T. (2013) *Acta Cryst*. **B69**, 249-259.

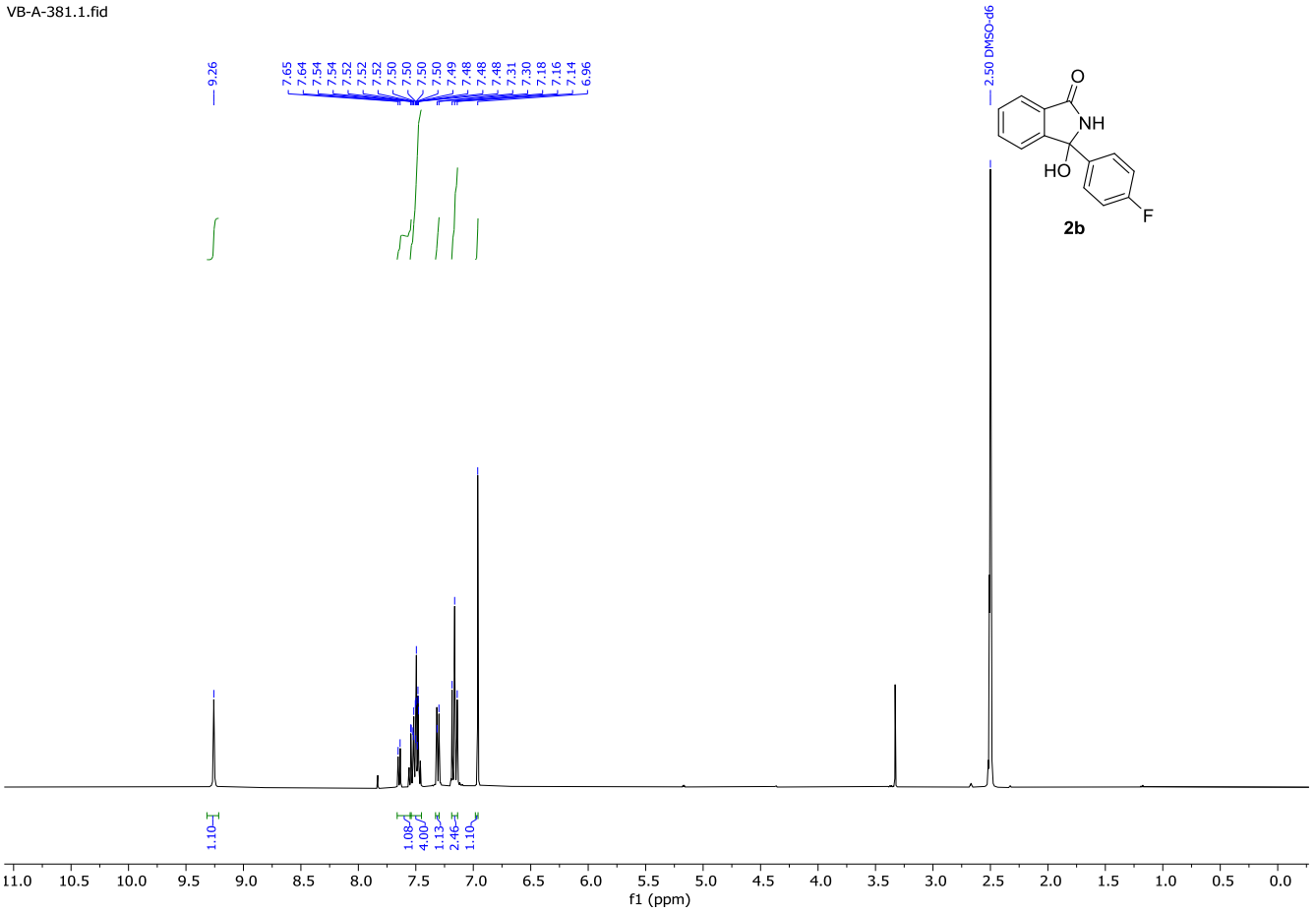
^{1}H NMR (400 MHz, DMSO)

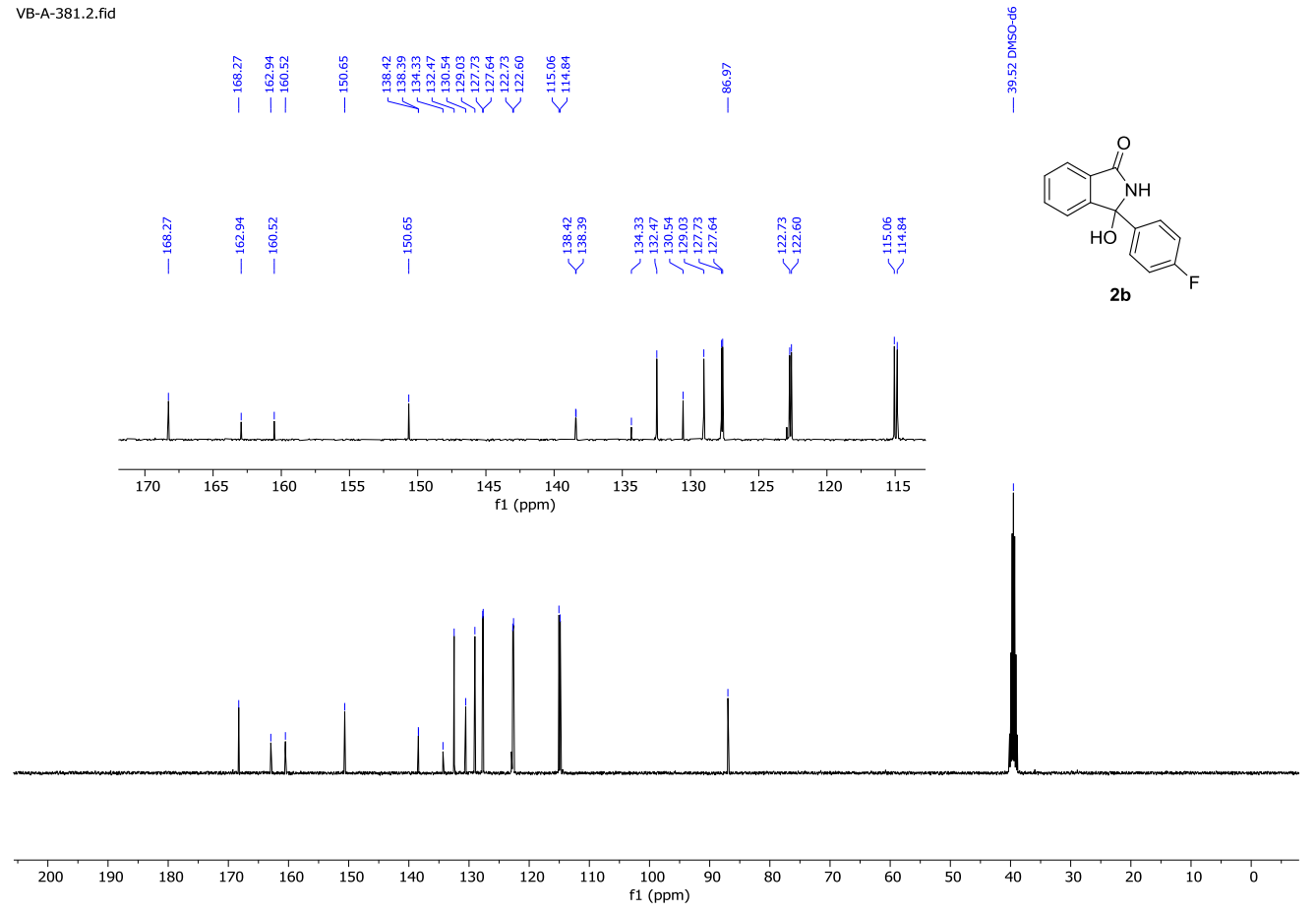




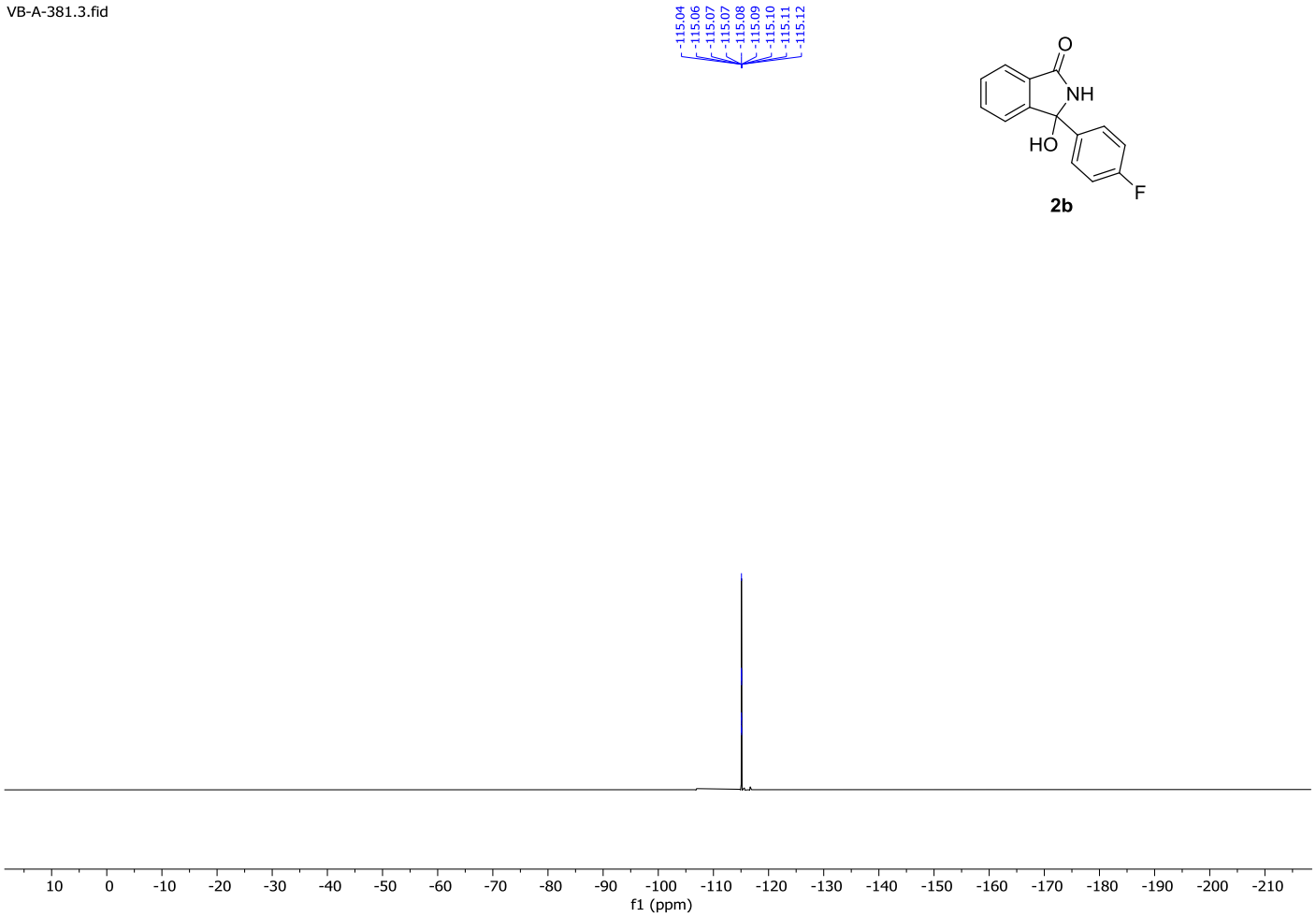
^{13}C NMR (101 MHz, DMSO)

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



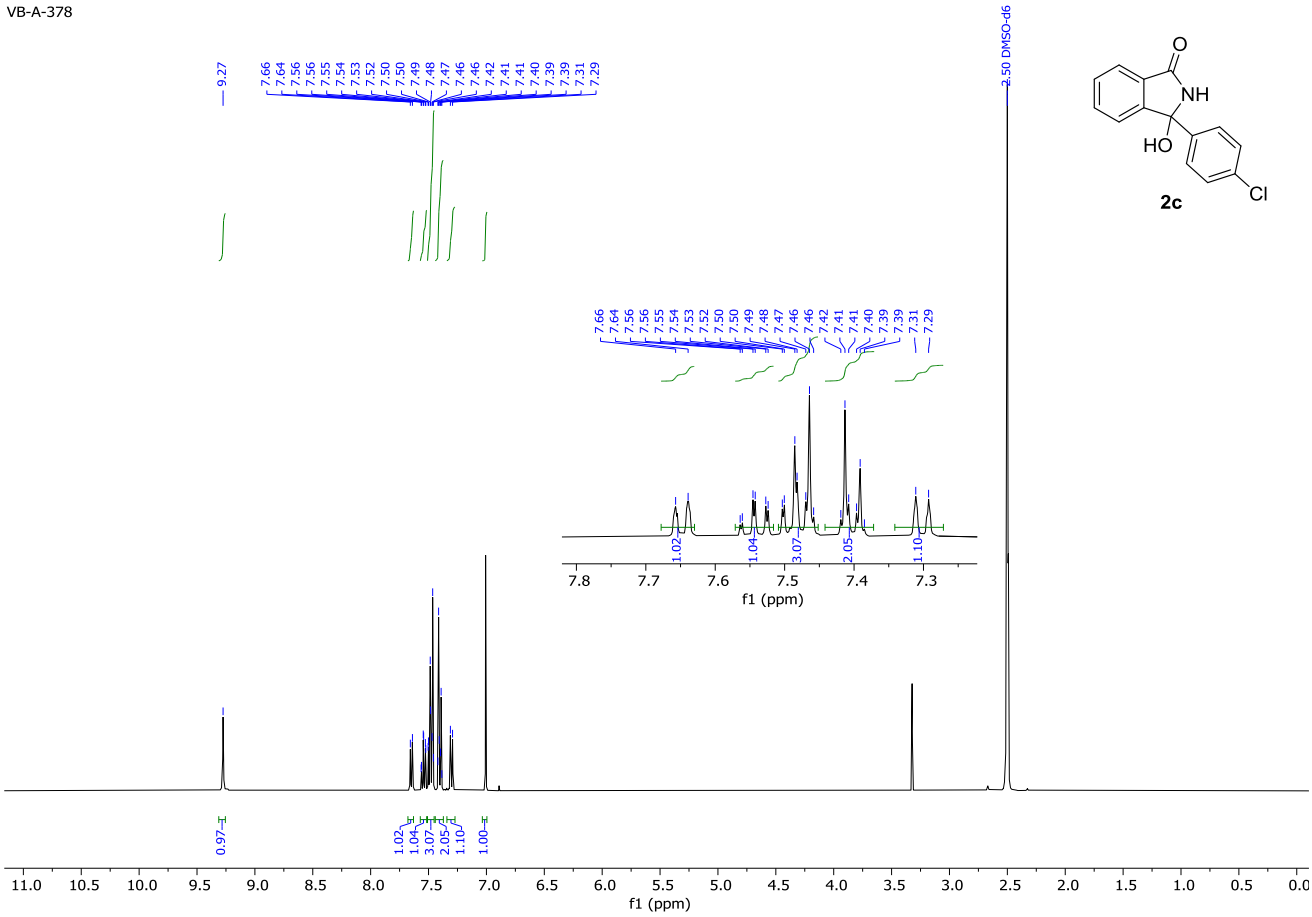


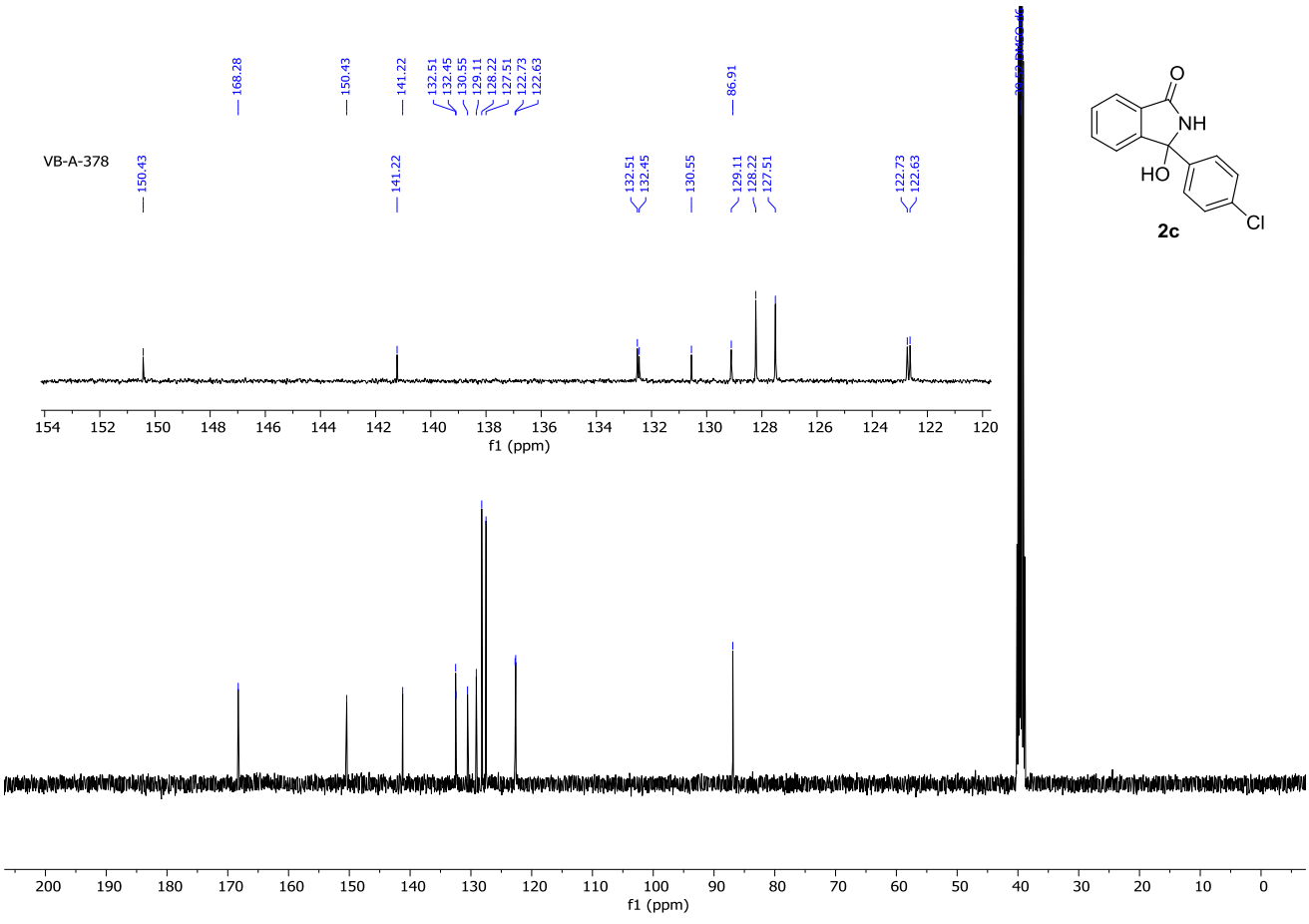
^{13}C NMR (101 MHz, DMSO)



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

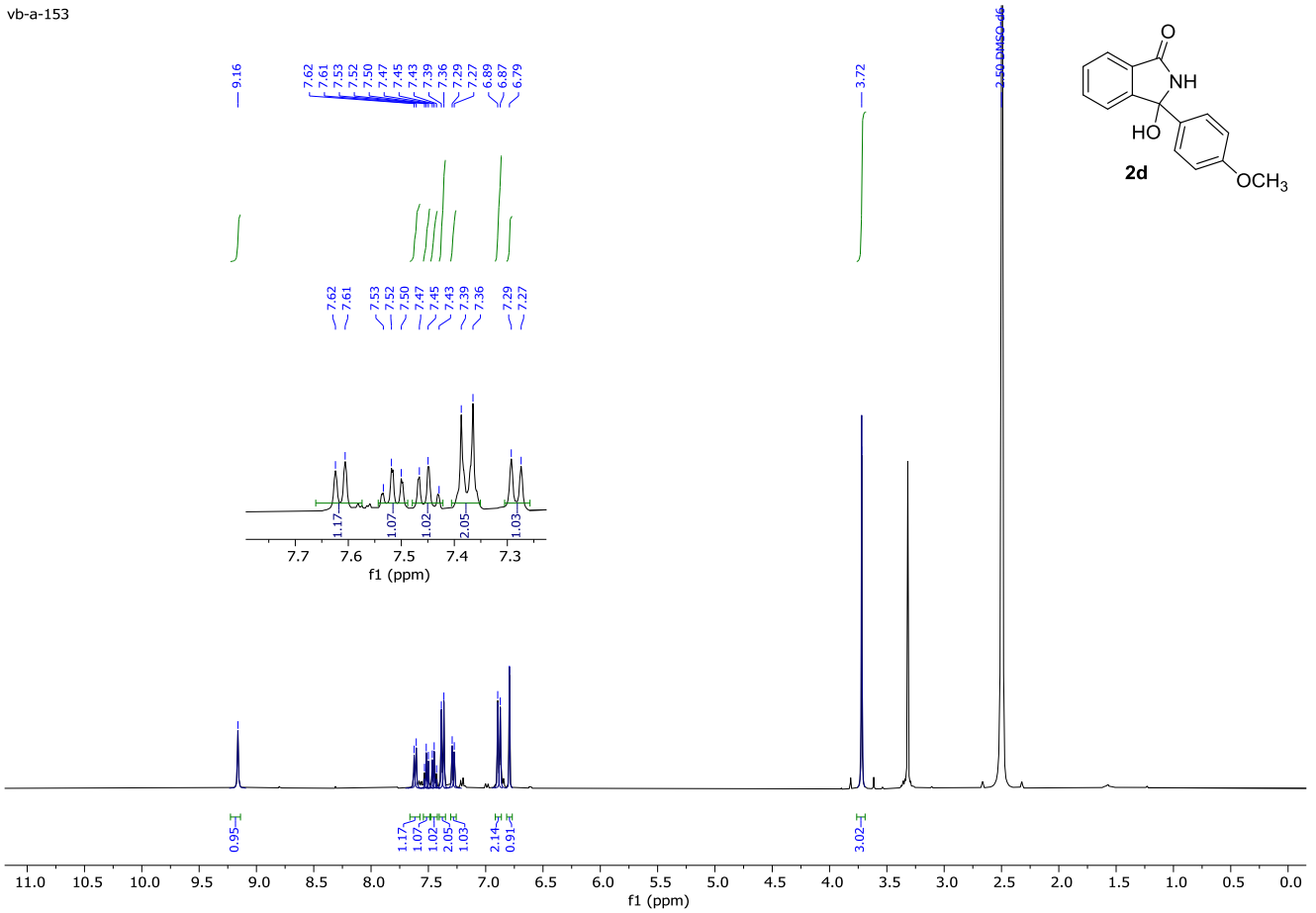
^{1}H NMR (400 MHz, DMSO)

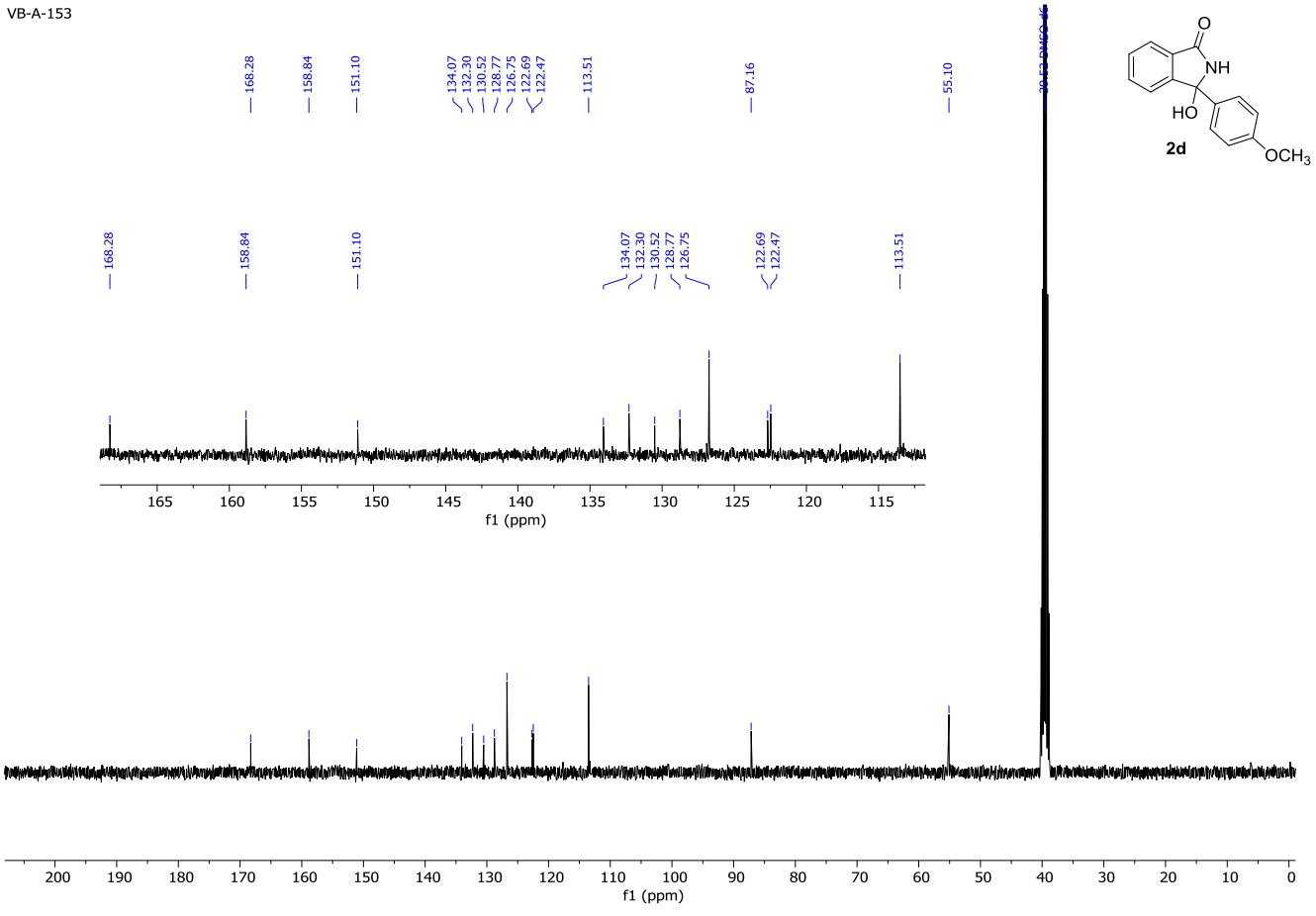




^{13}C NMR (101 MHz, DMSO)

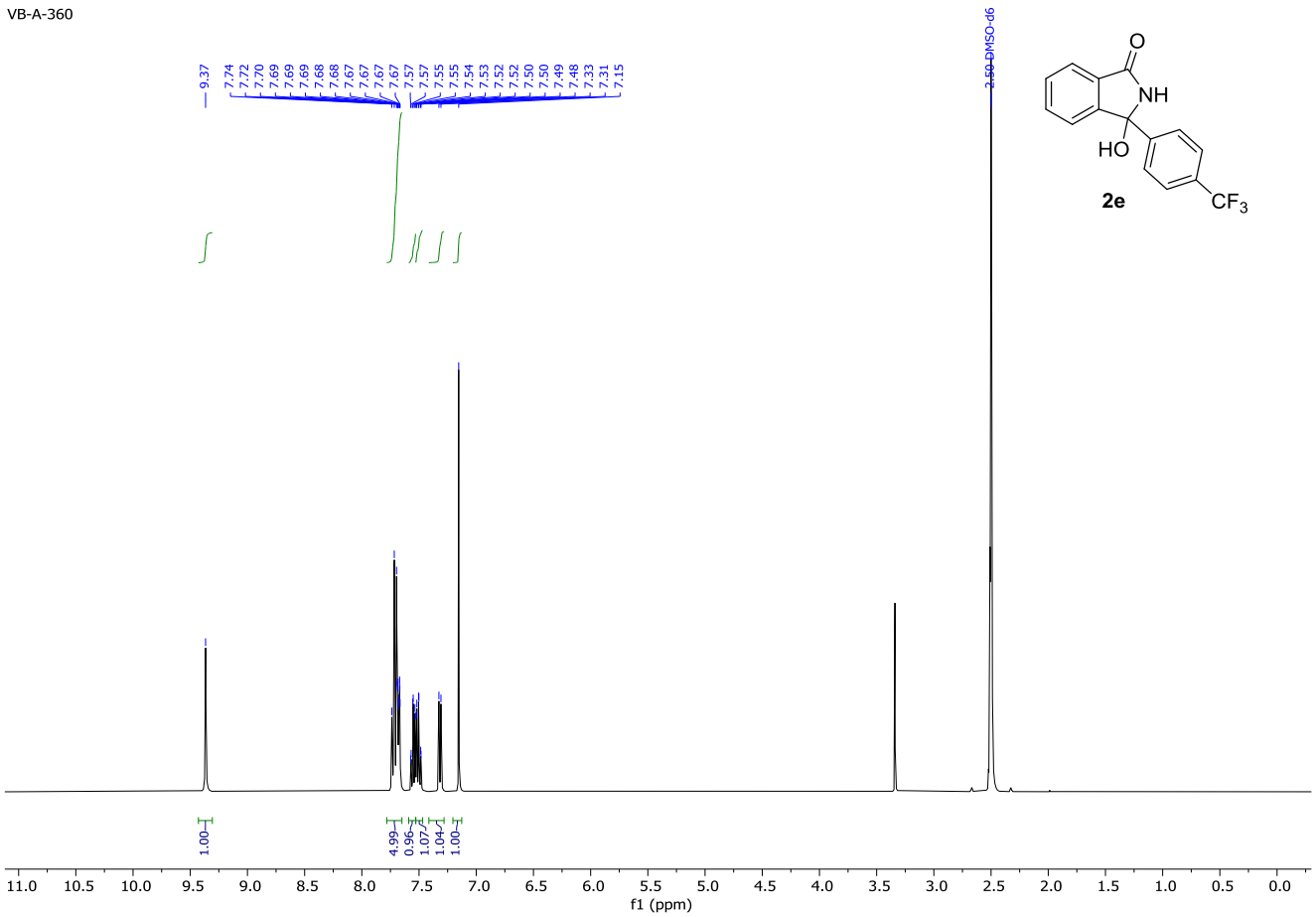
^{1}H NMR (400 MHz, DMSO)

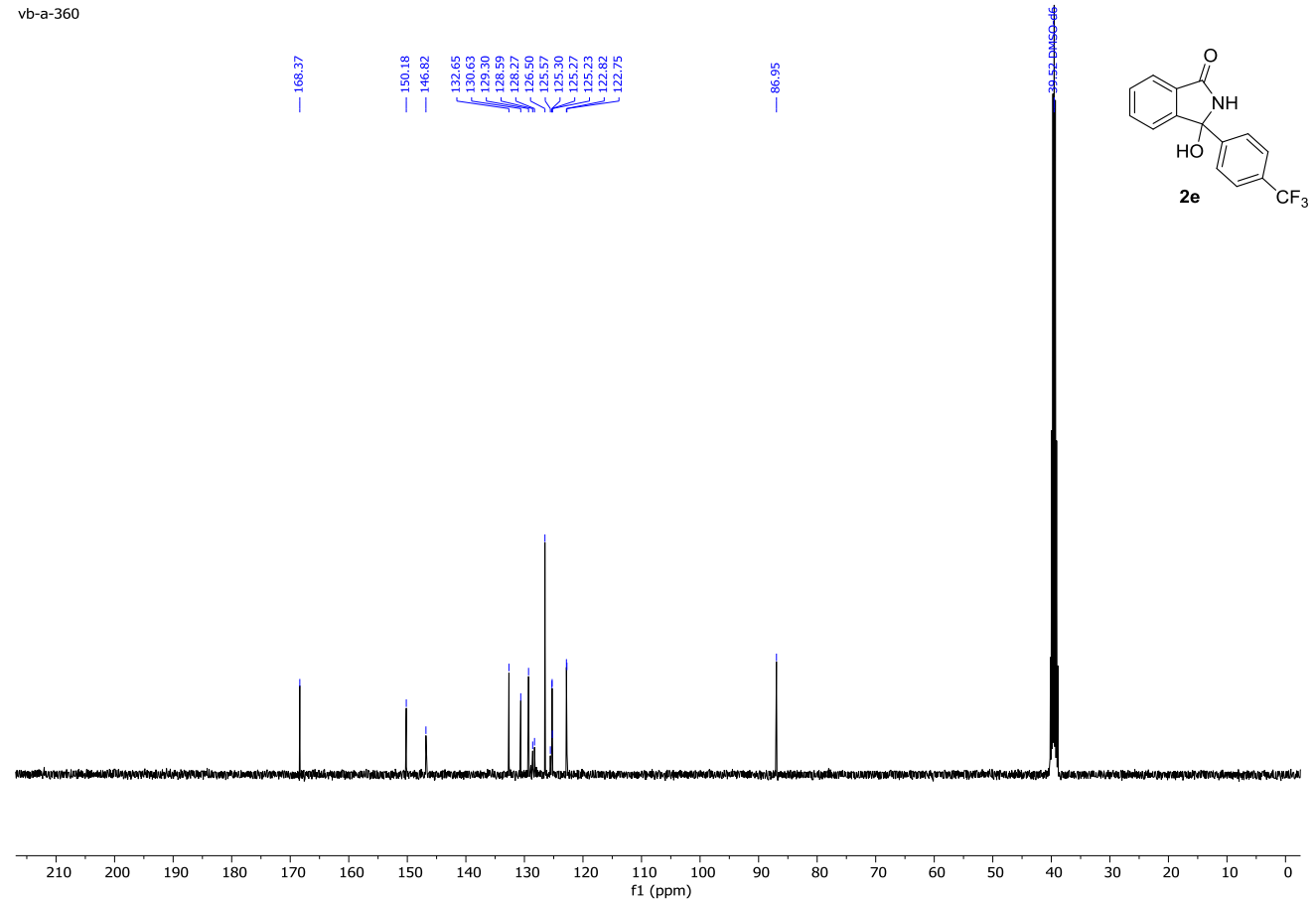




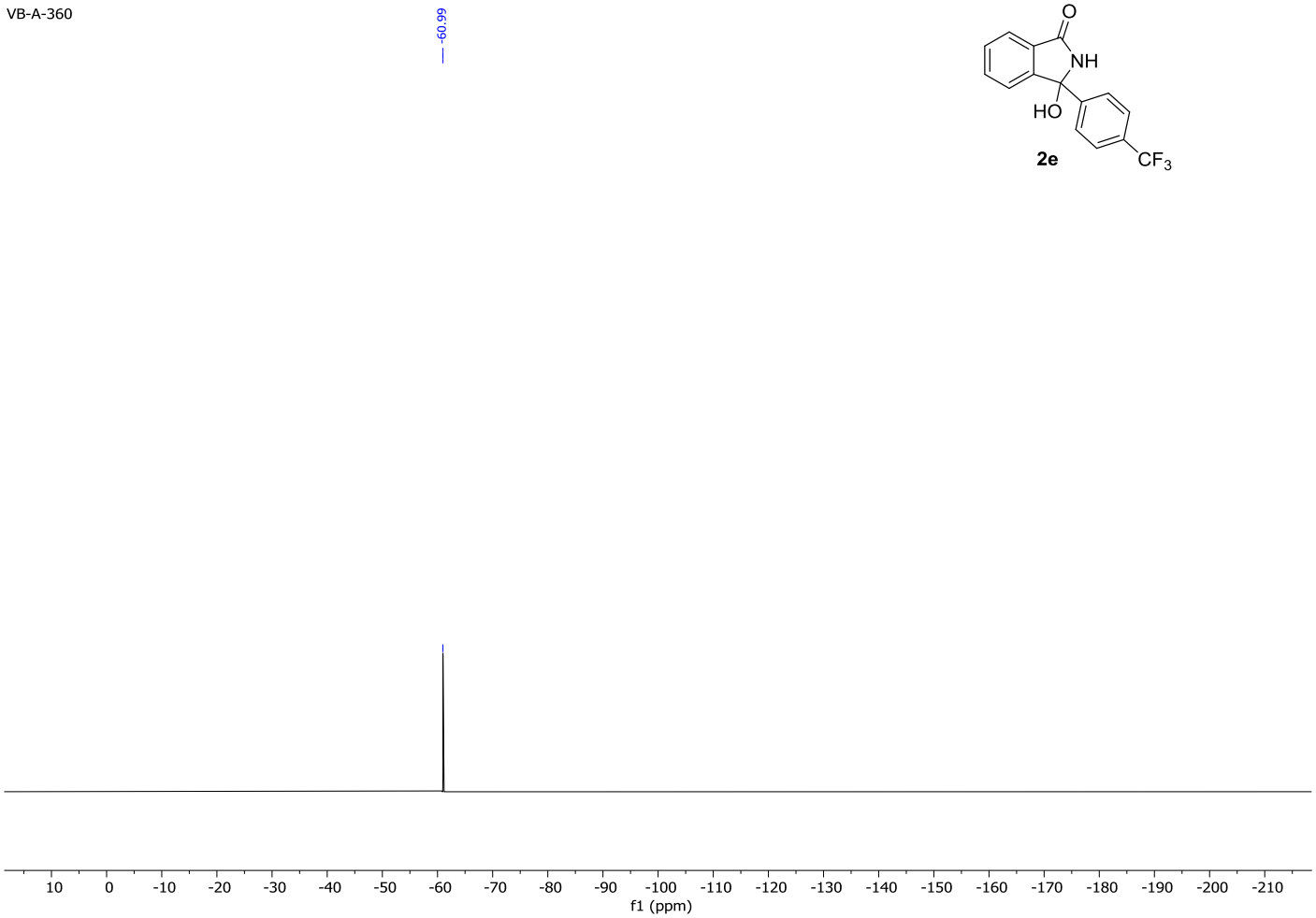
^{13}C NMR (101 MHz, DMSO)

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



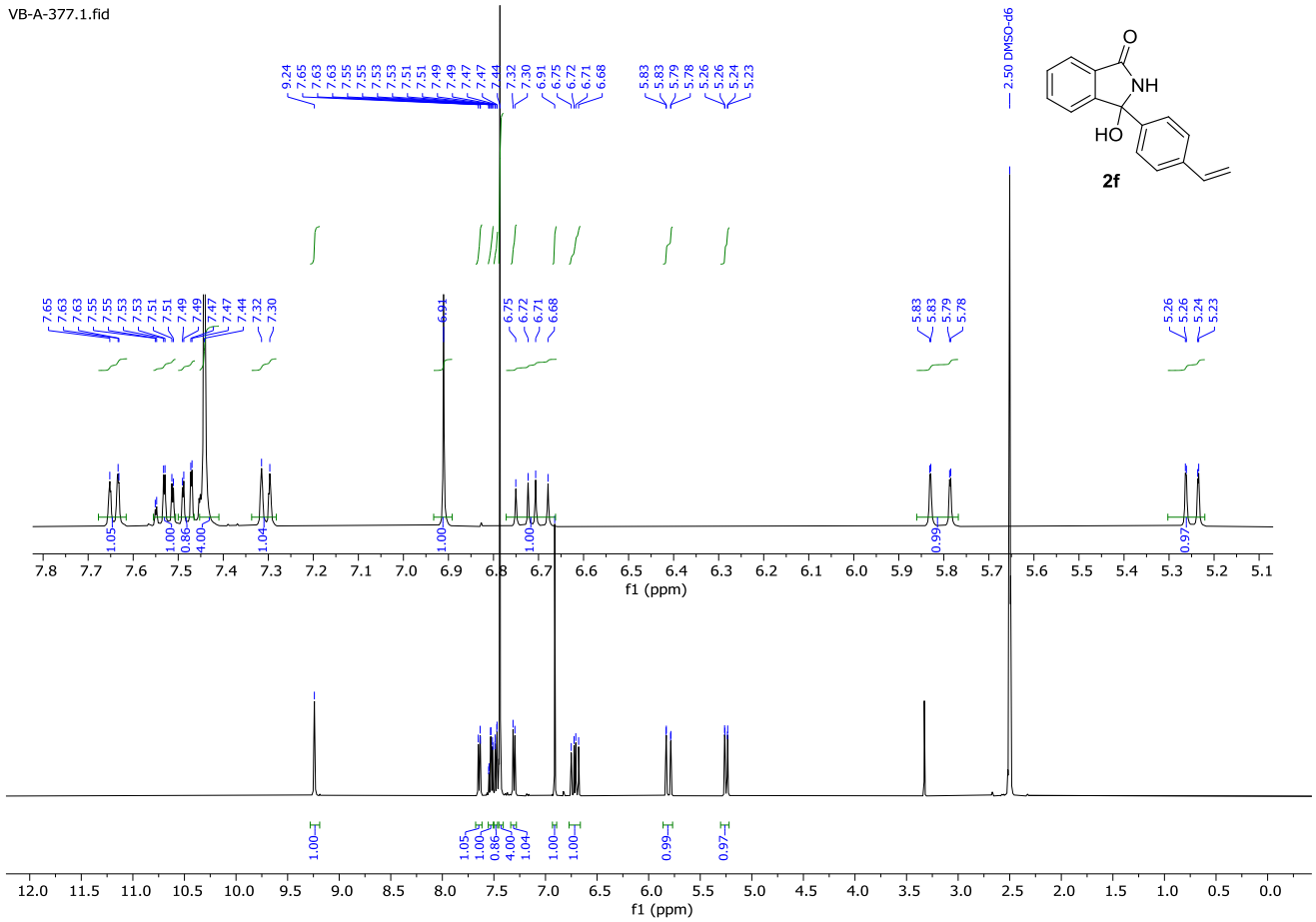


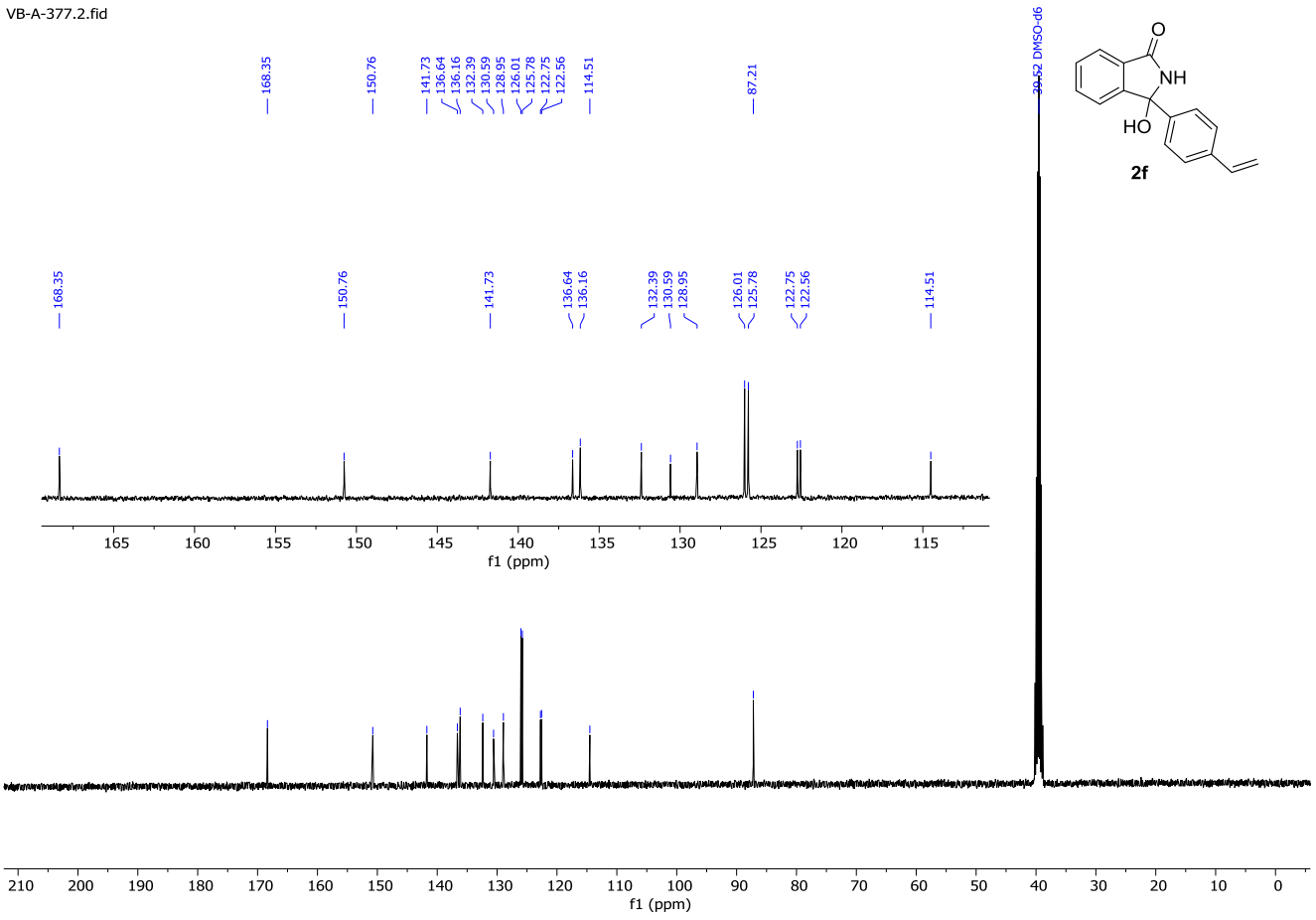
^{13}C NMR (101 MHz, DMSO)



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

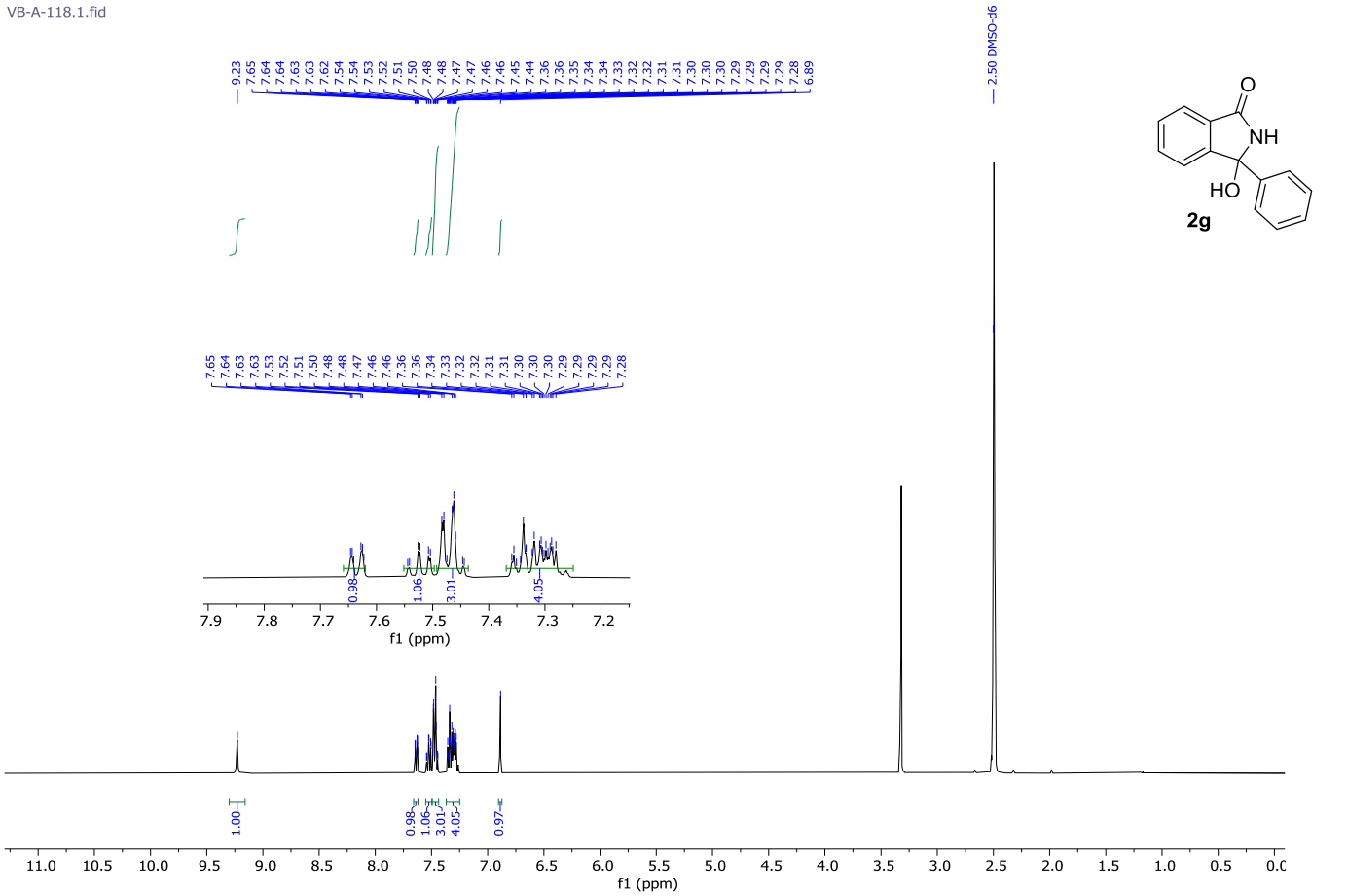
^{1}H NMR (400 MHz, DMSO)

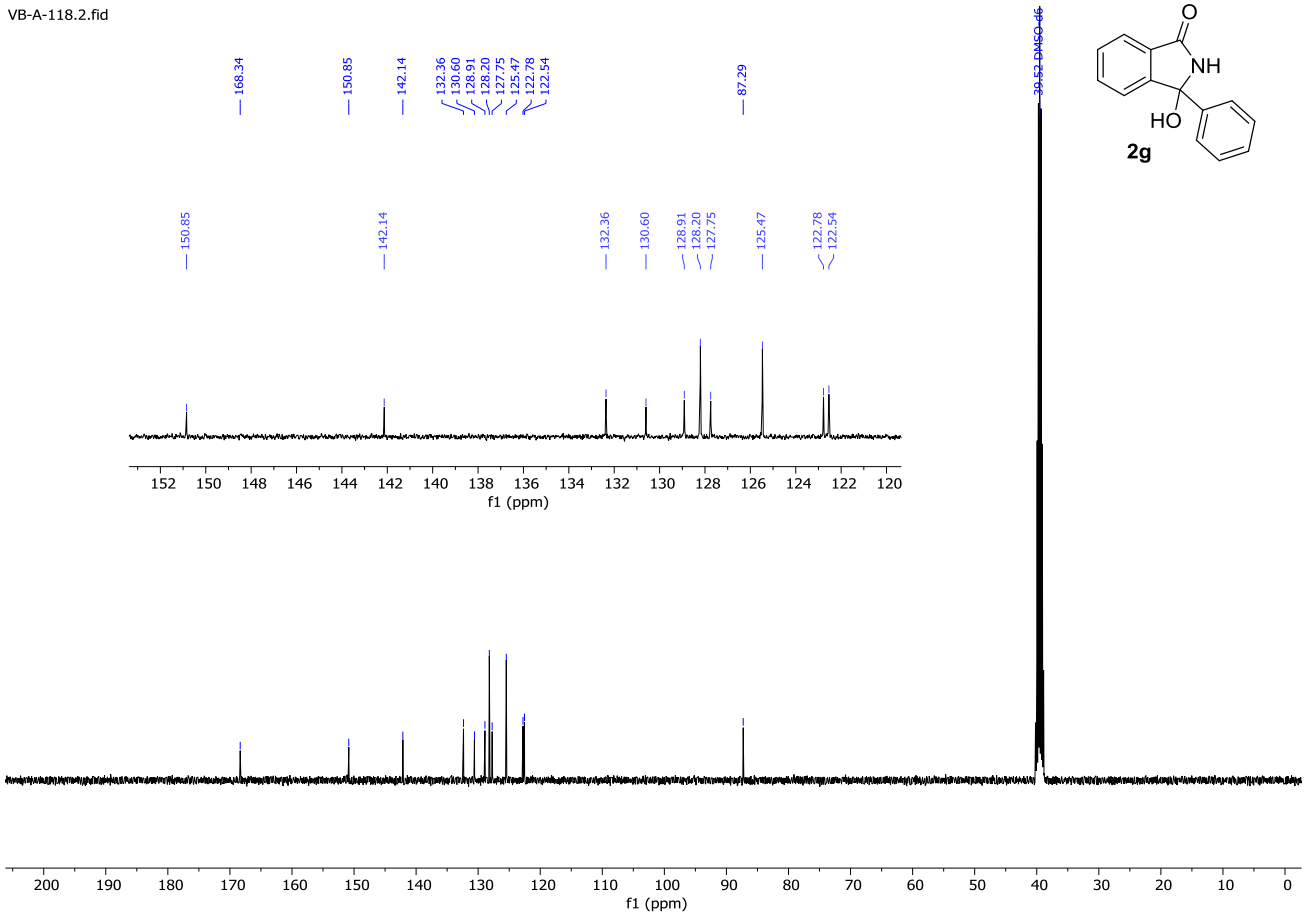




^{13}C NMR (101 MHz, DMSO)

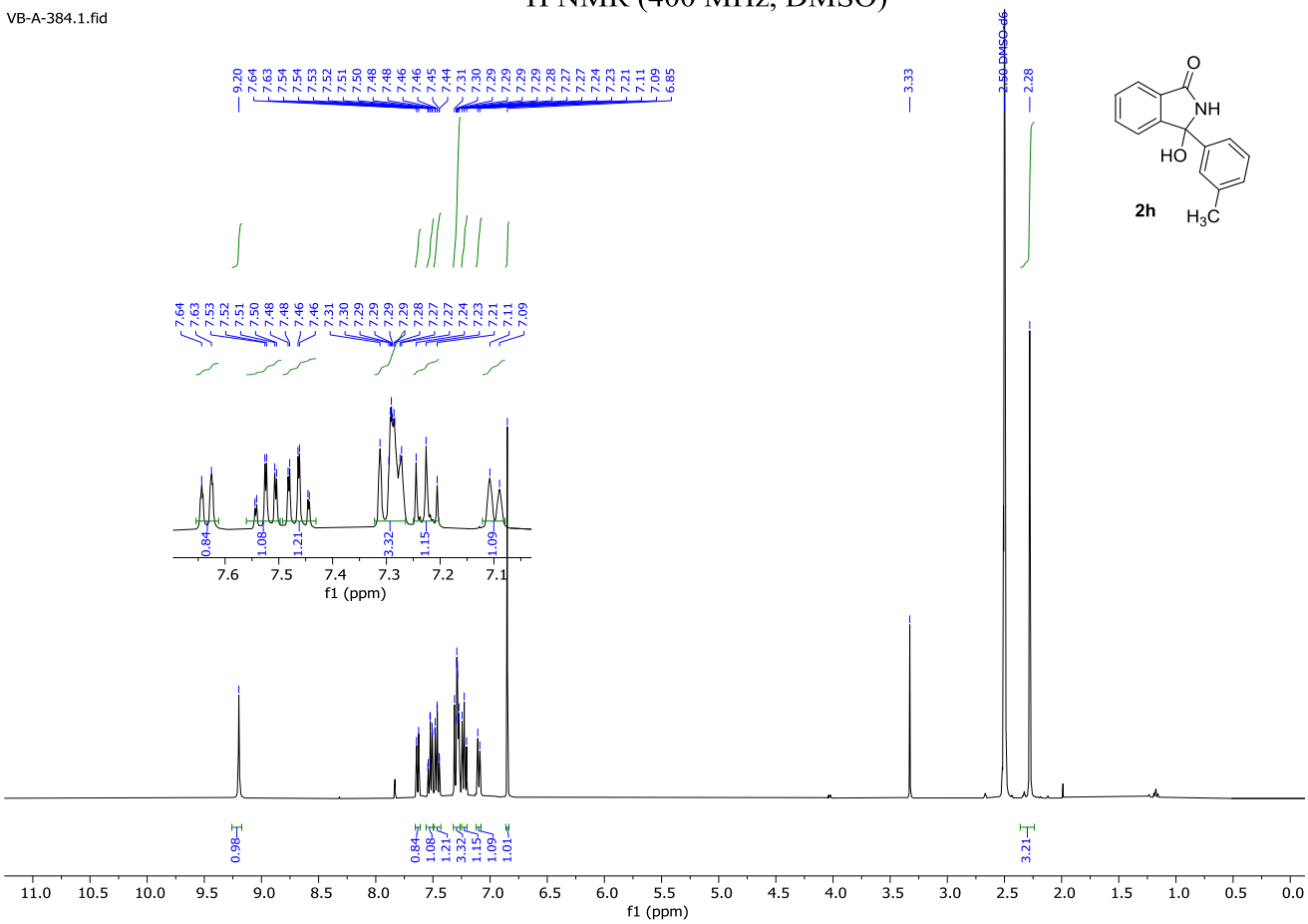
^{1}H NMR (400 MHz, DMSO)

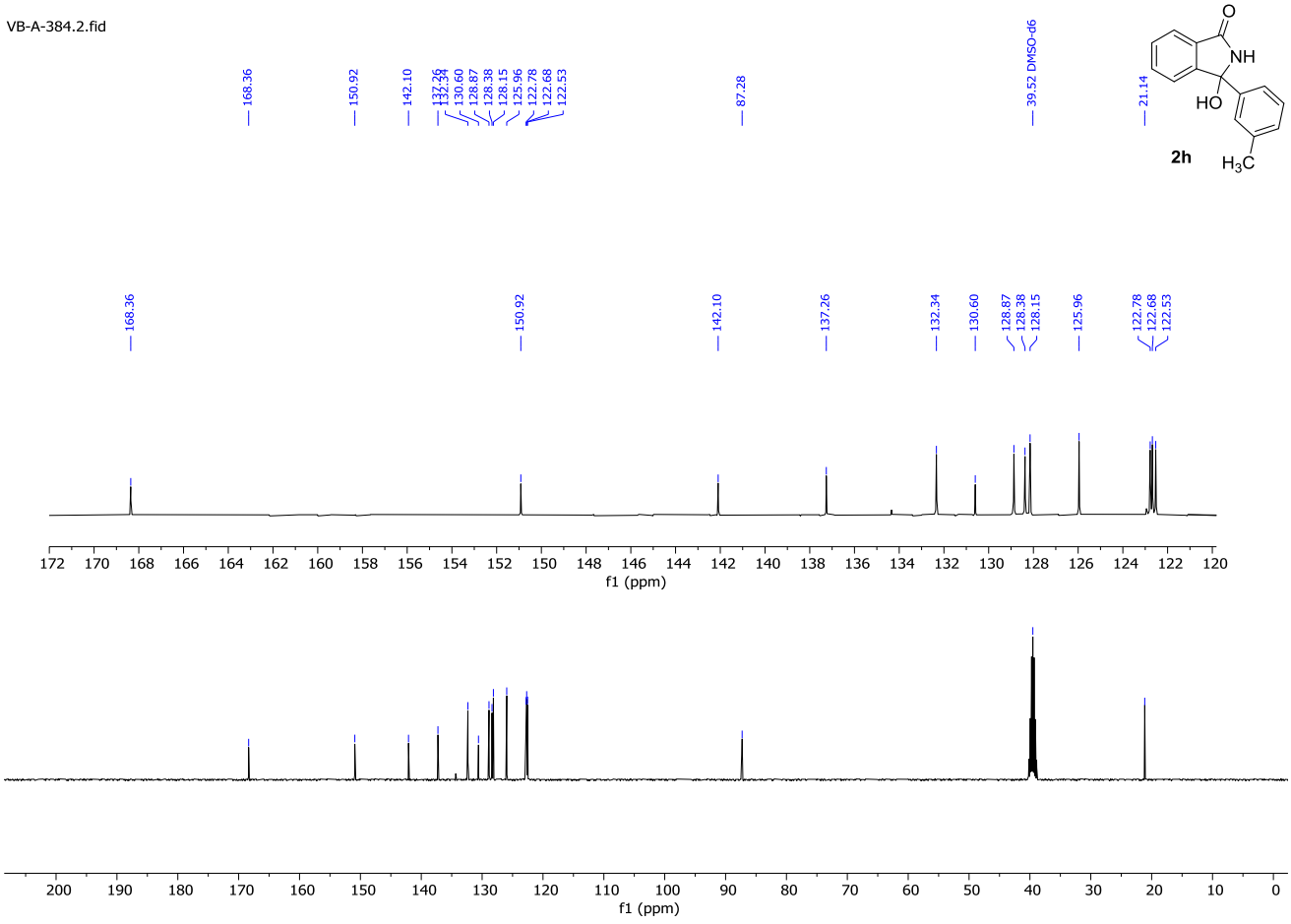




^{13}C NMR (101 MHz, DMSO)

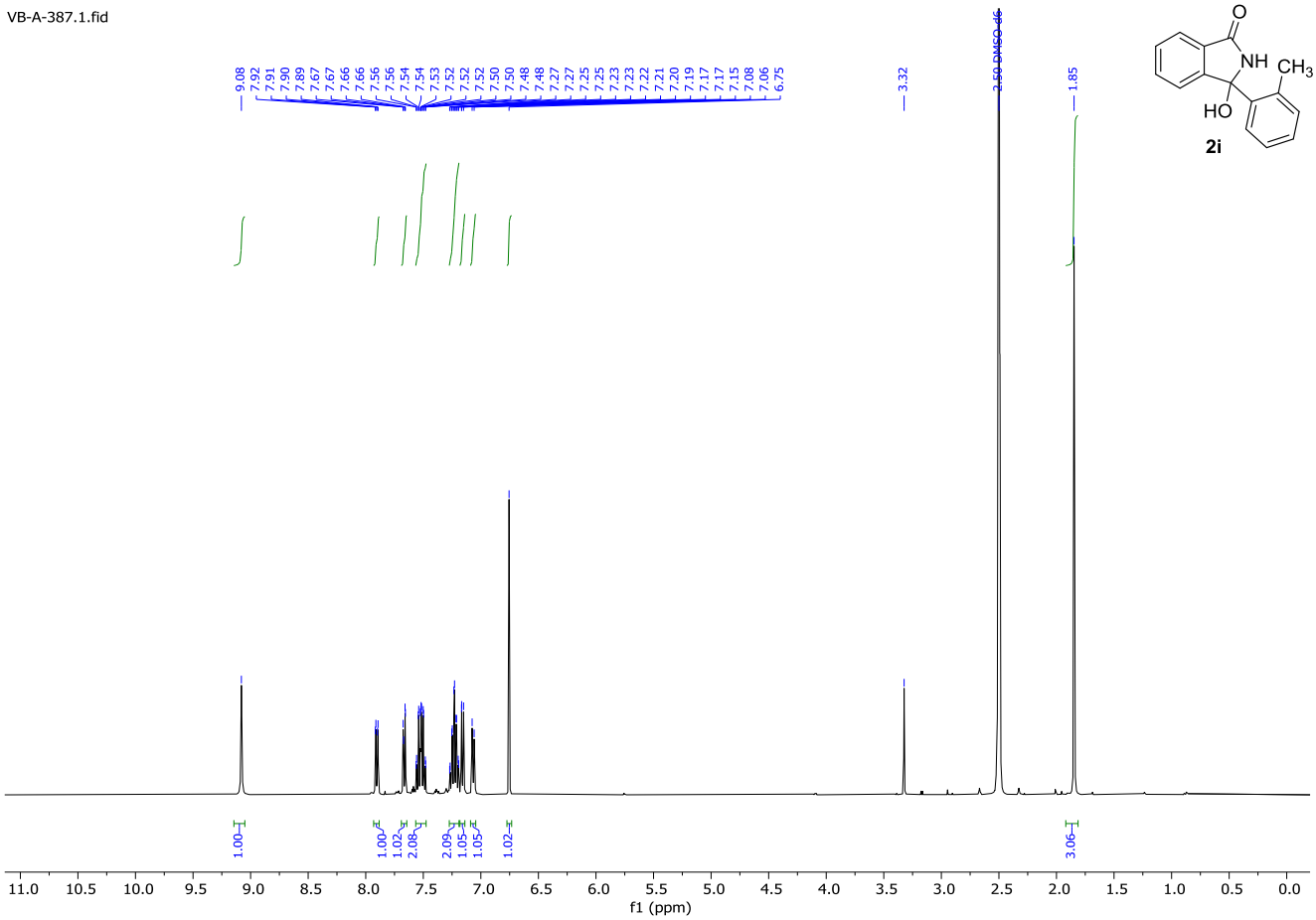
^{1}H NMR (400 MHz, DMSO)

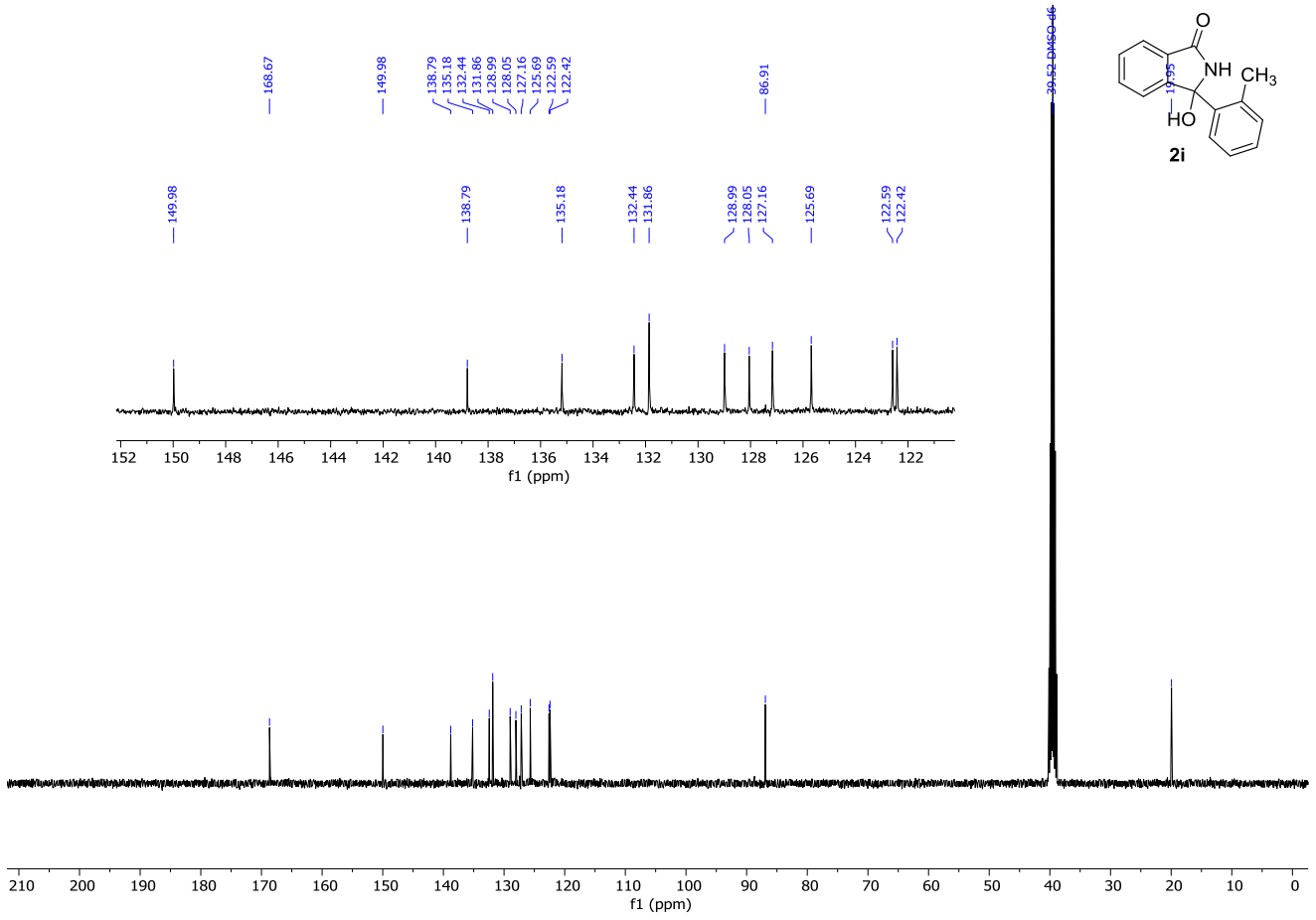




^{13}C NMR (101 MHz, DMSO)

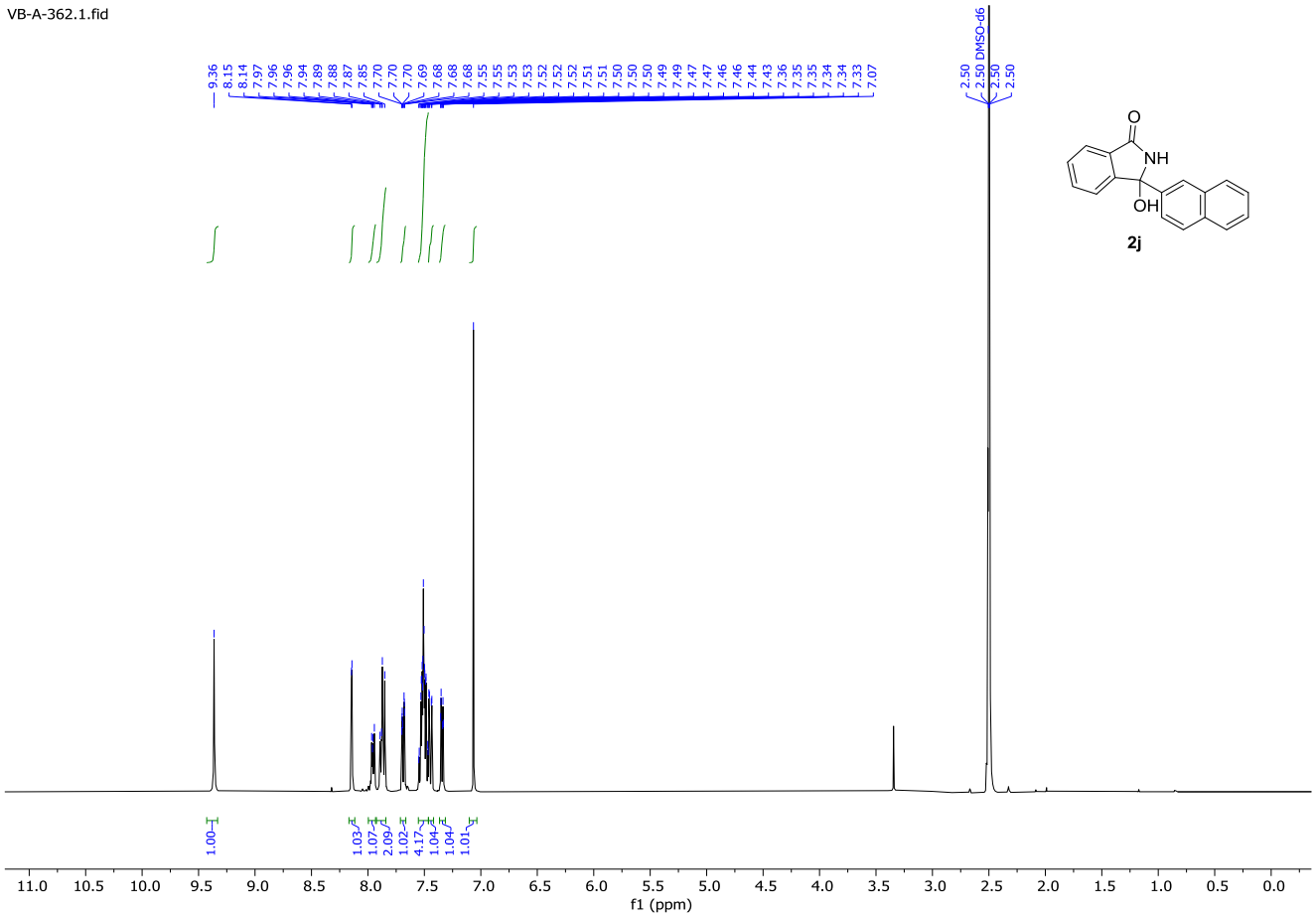
^{1}H NMR (400 MHz, DMSO)

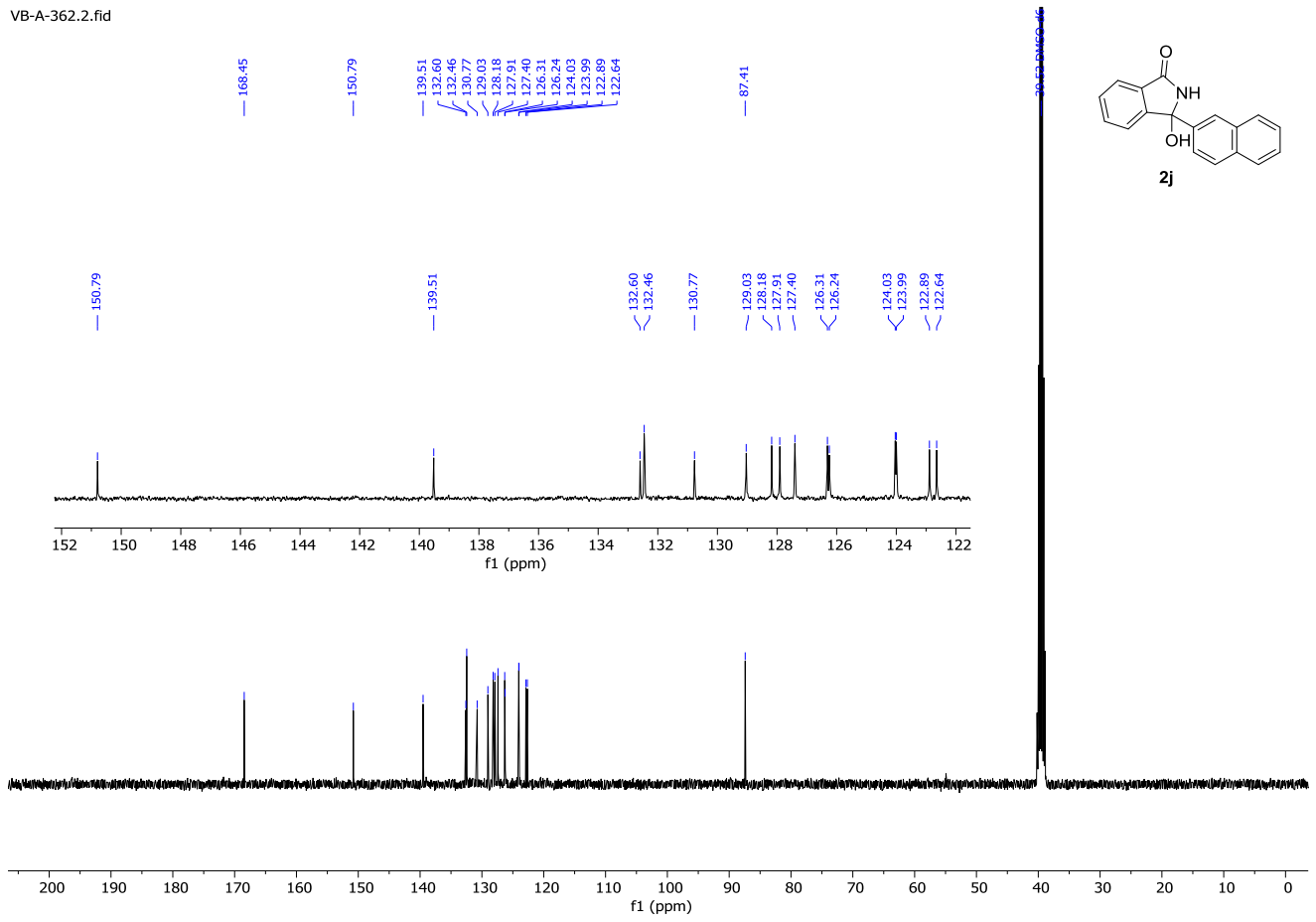




^{13}C NMR (101 MHz, DMSO)

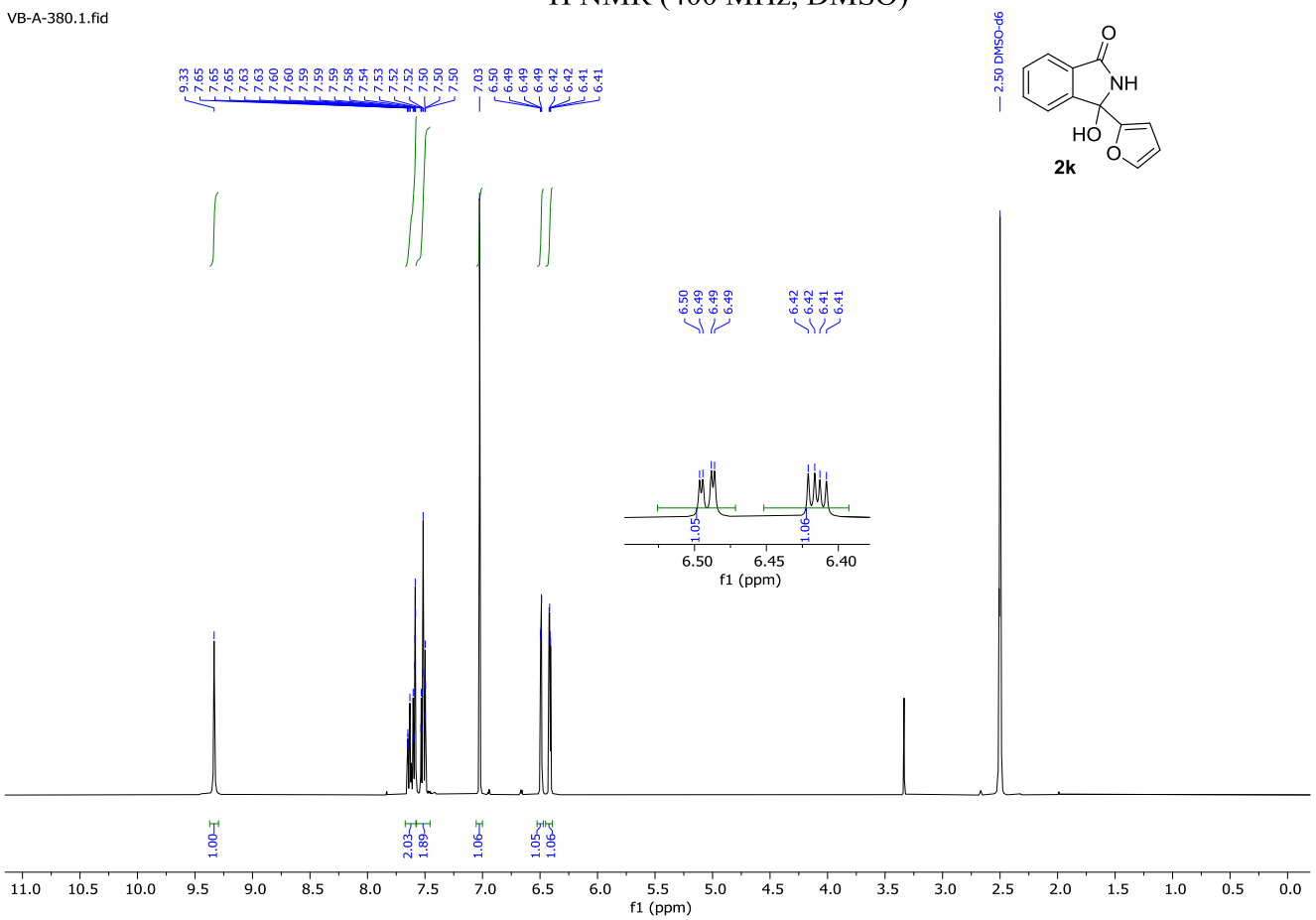
^{1}H NMR (400 MHz, DMSO)

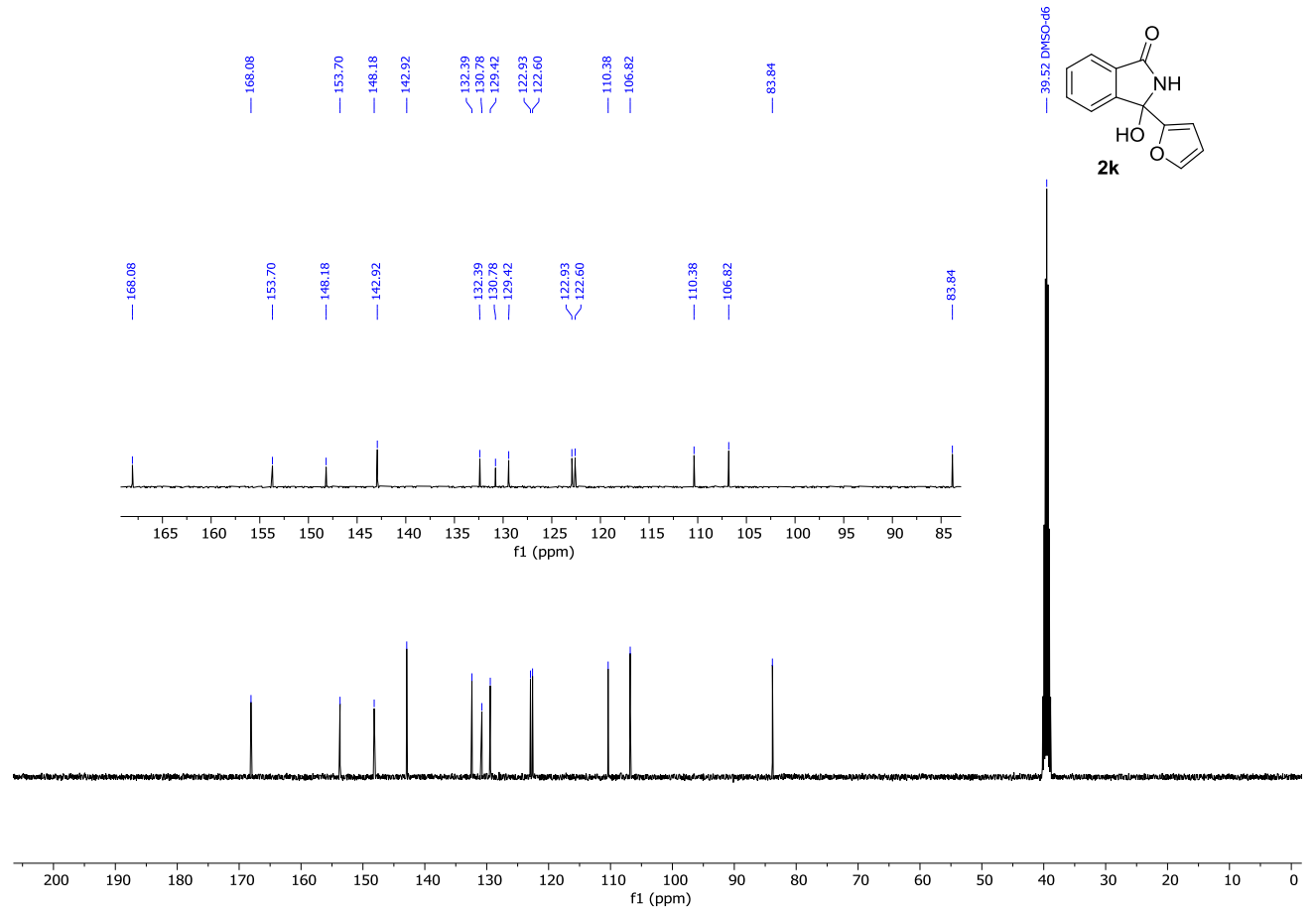




^{13}C NMR (101 MHz, DMSO)

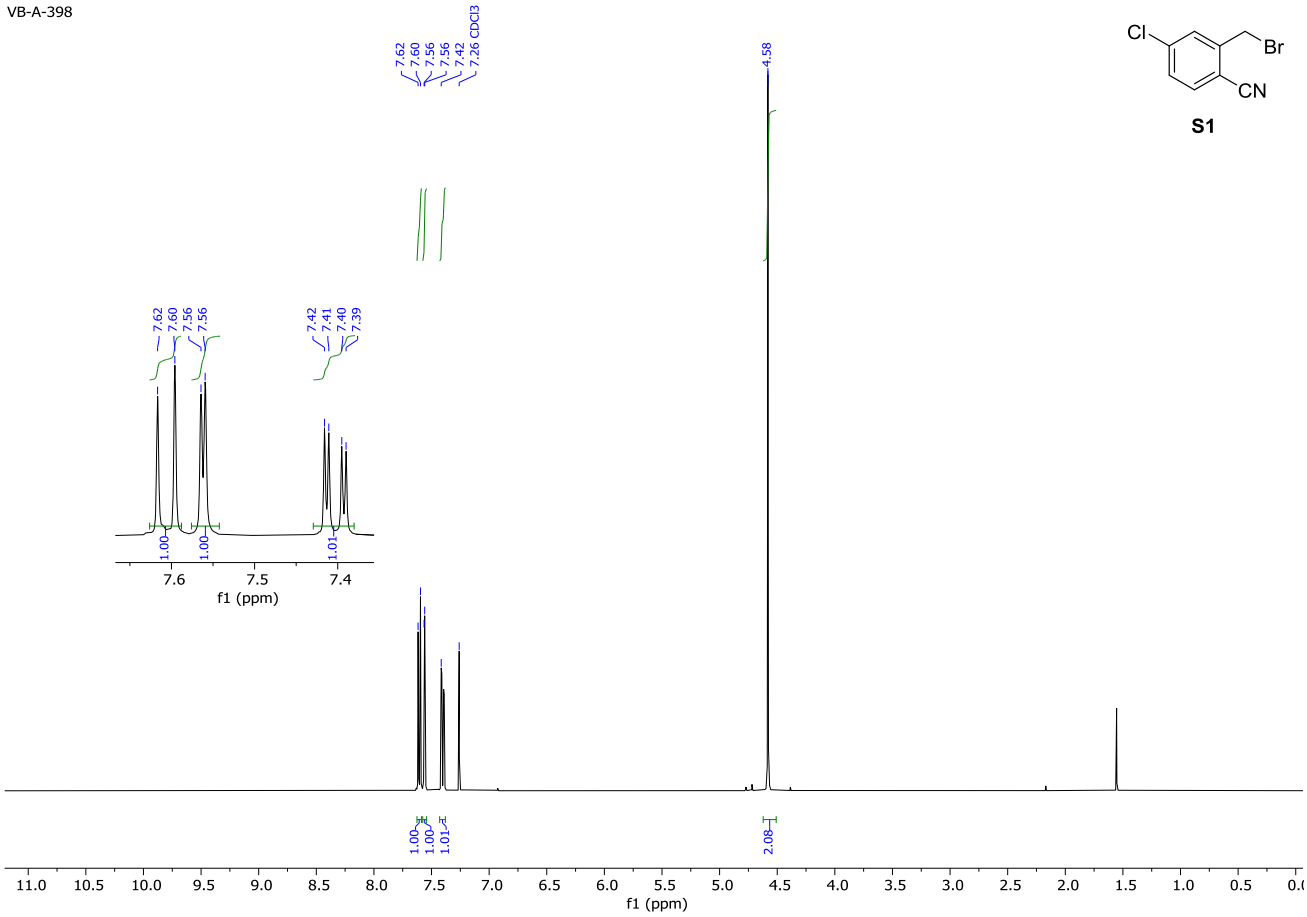
^{1}H NMR (400 MHz, DMSO)

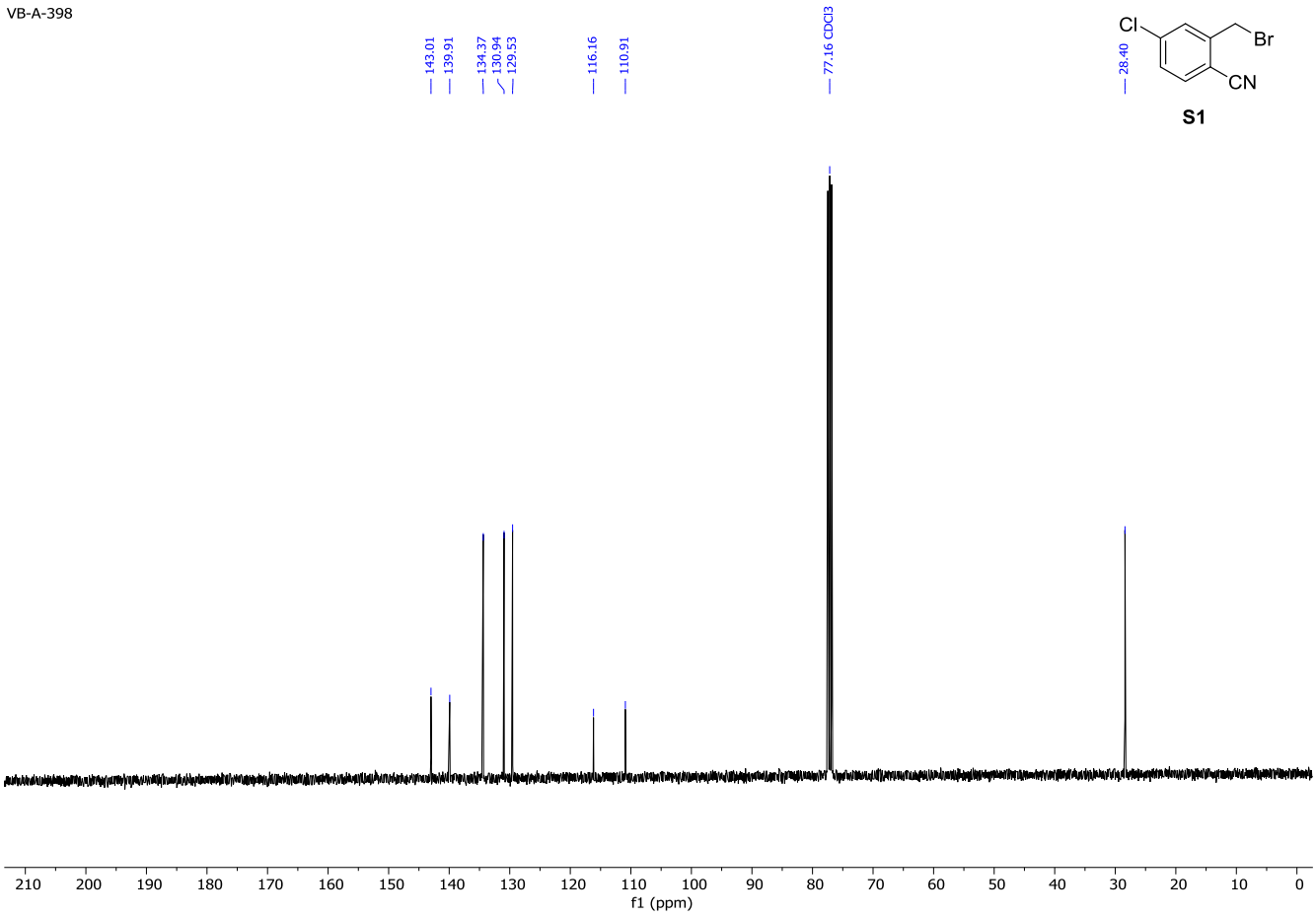




^{13}C NMR (101 MHz, DMSO)

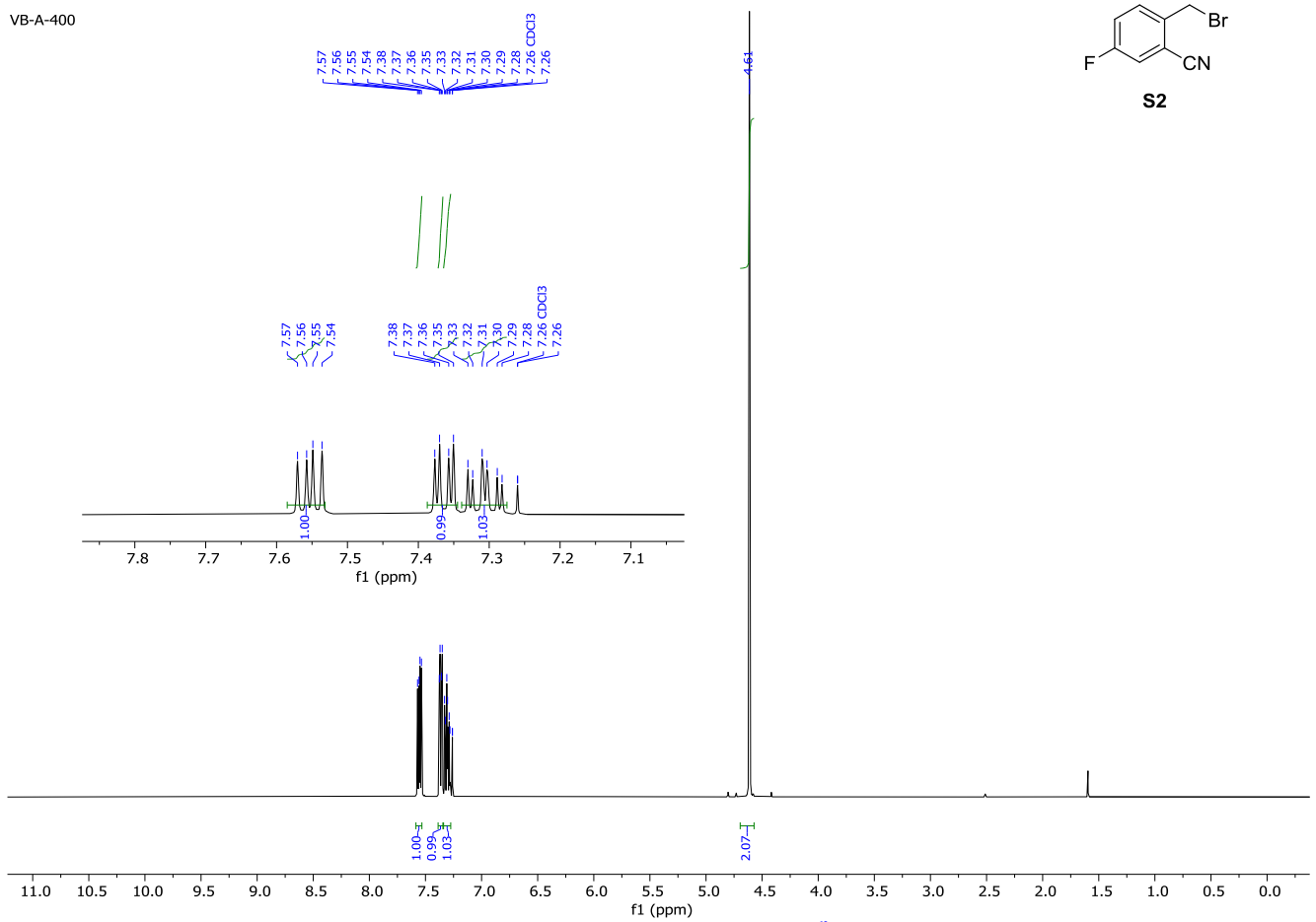
^{1}H NMR (400 MHz, $CDCl_3$)

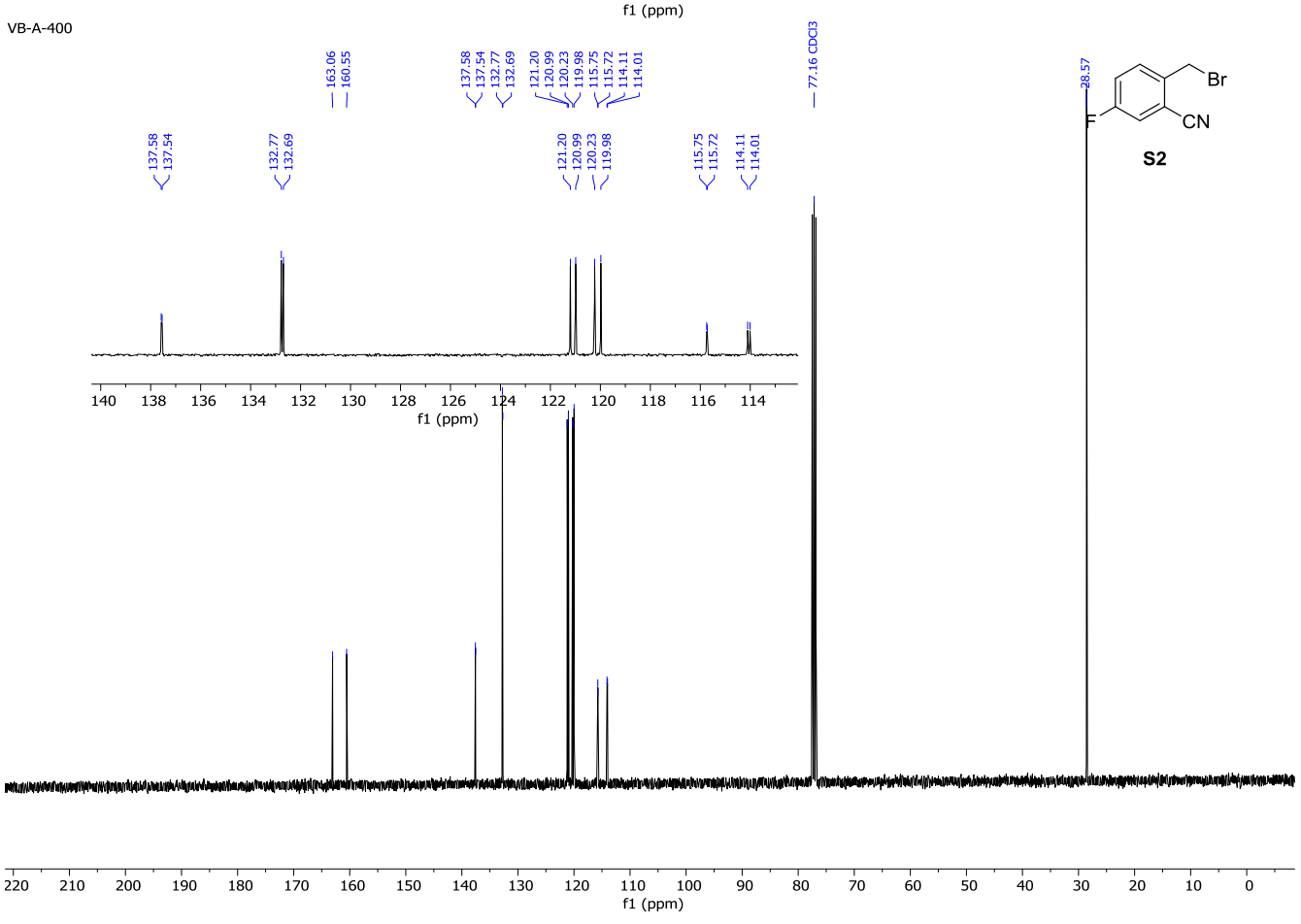




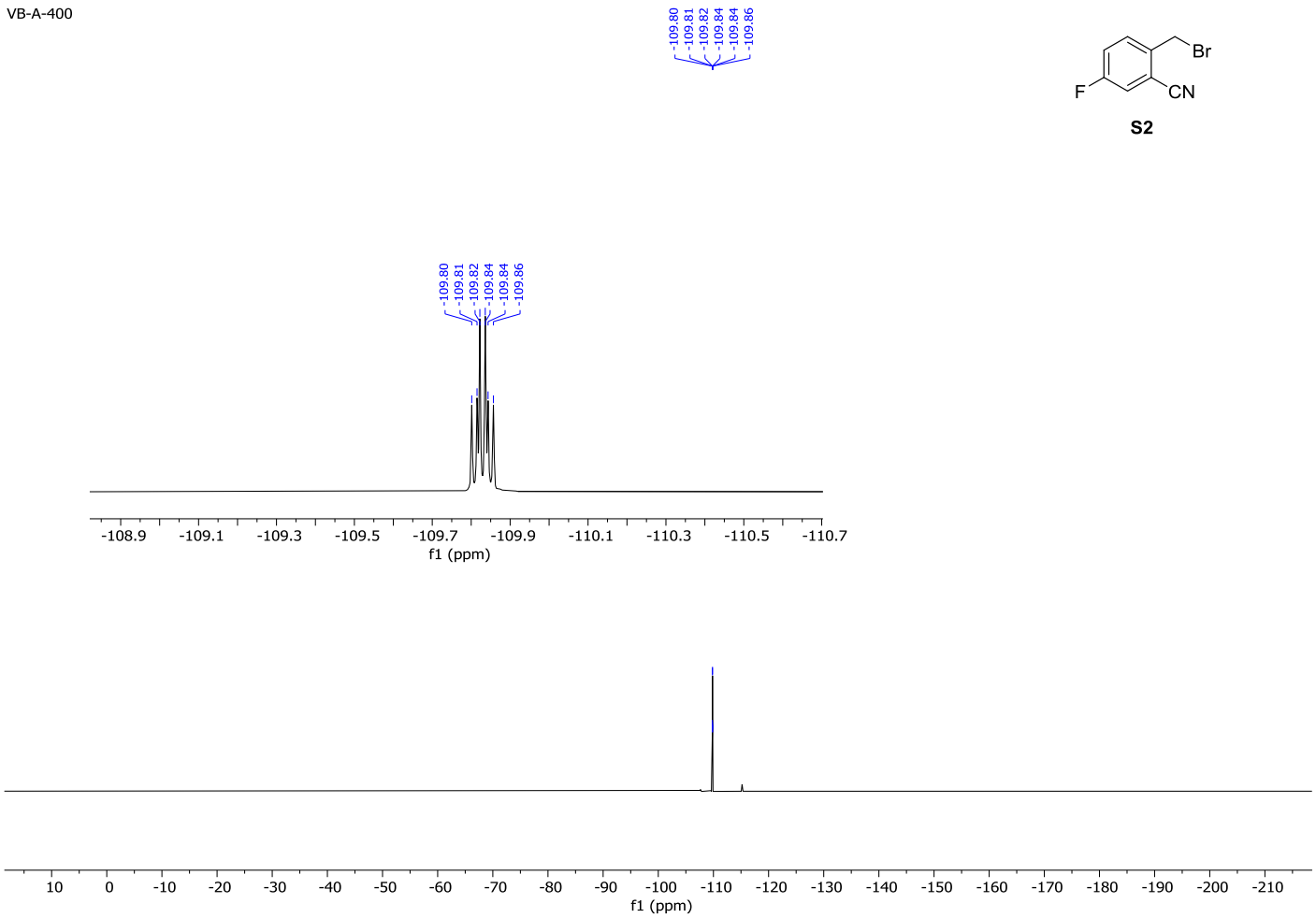
^{13}C NMR (101 MHz, $CDCl_3$)

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



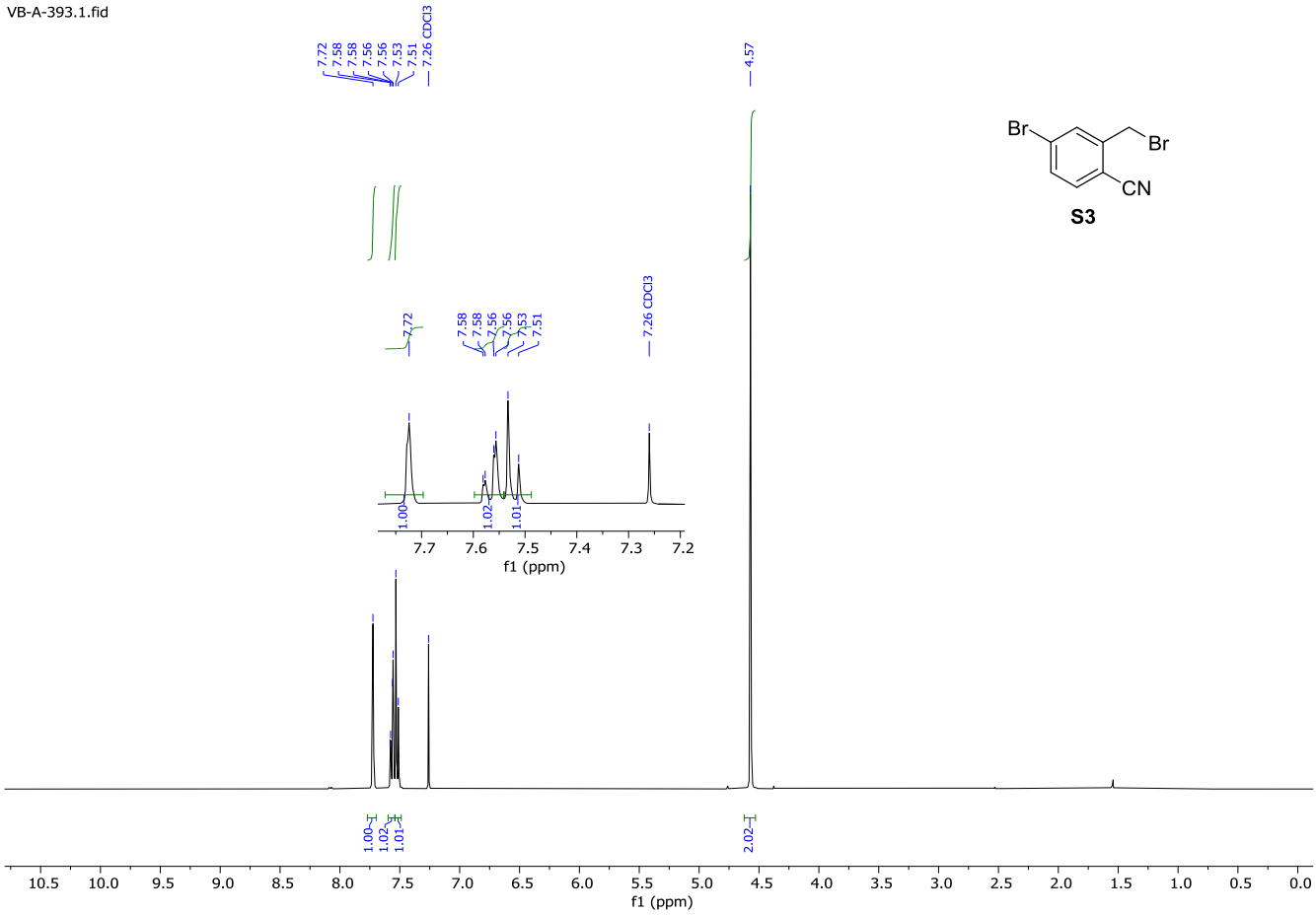


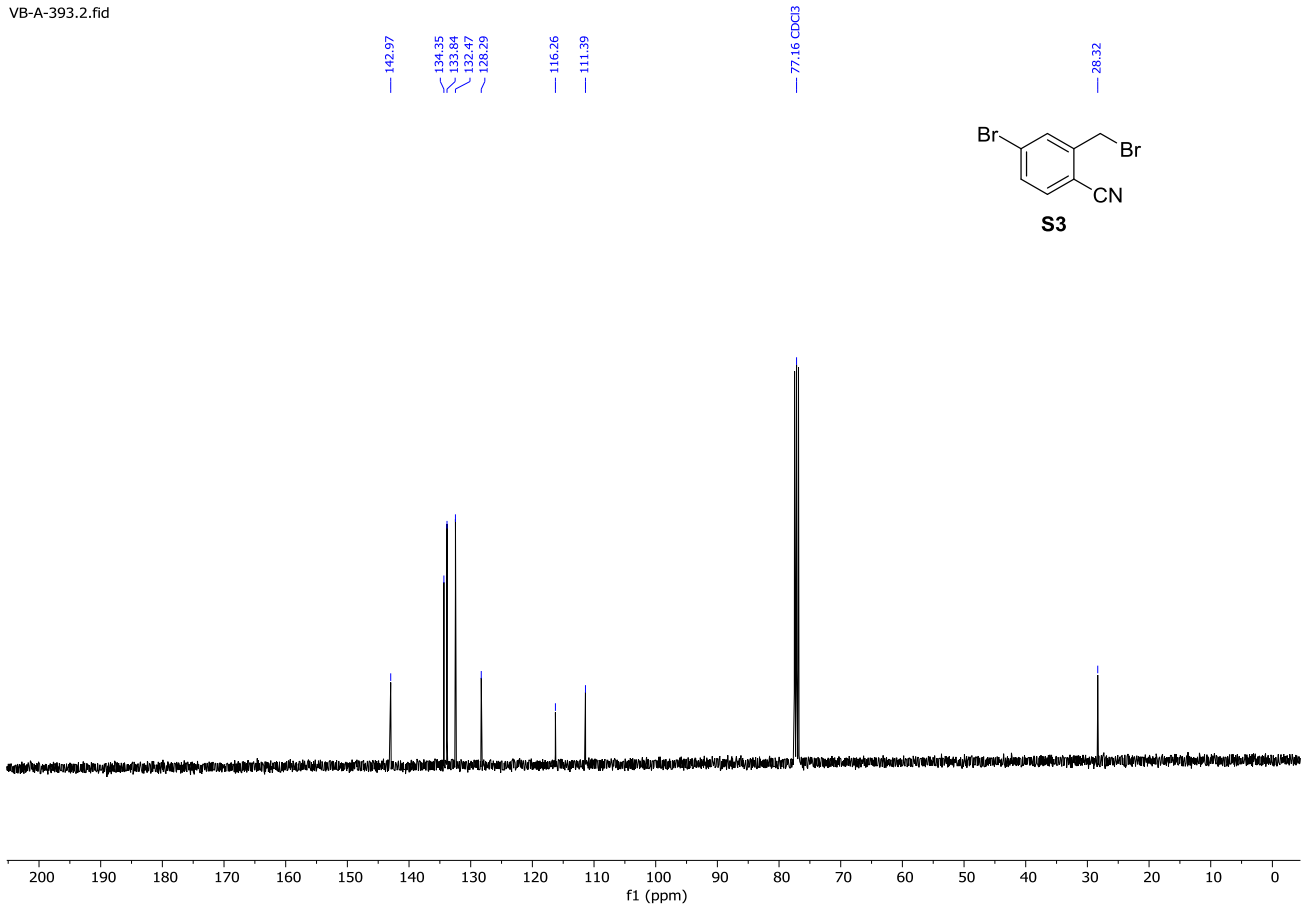
^{13}C NMR (101 MHz, $CDCl_3$)



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

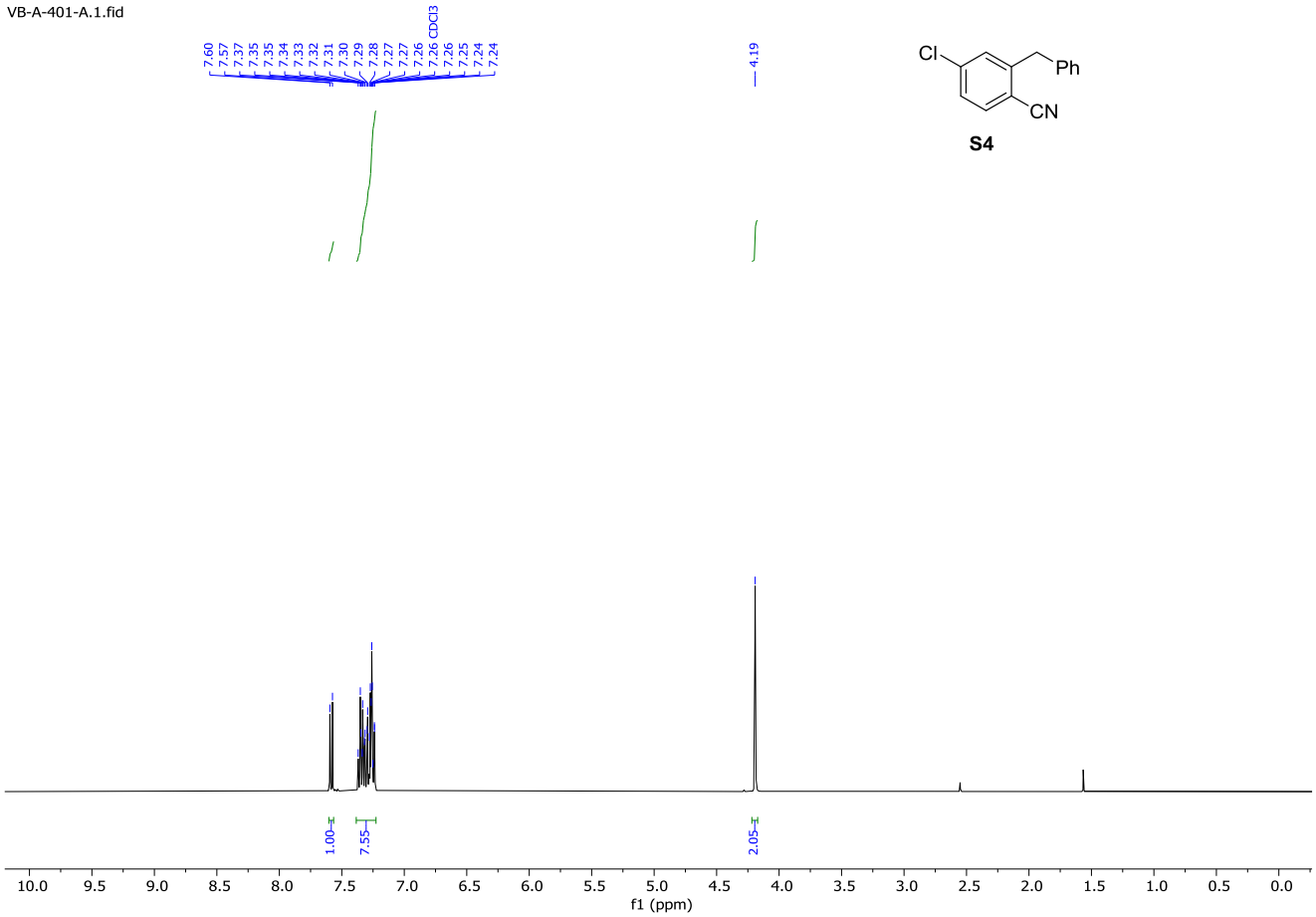
^{1}H NMR (400 MHz, $CDCl_3$)

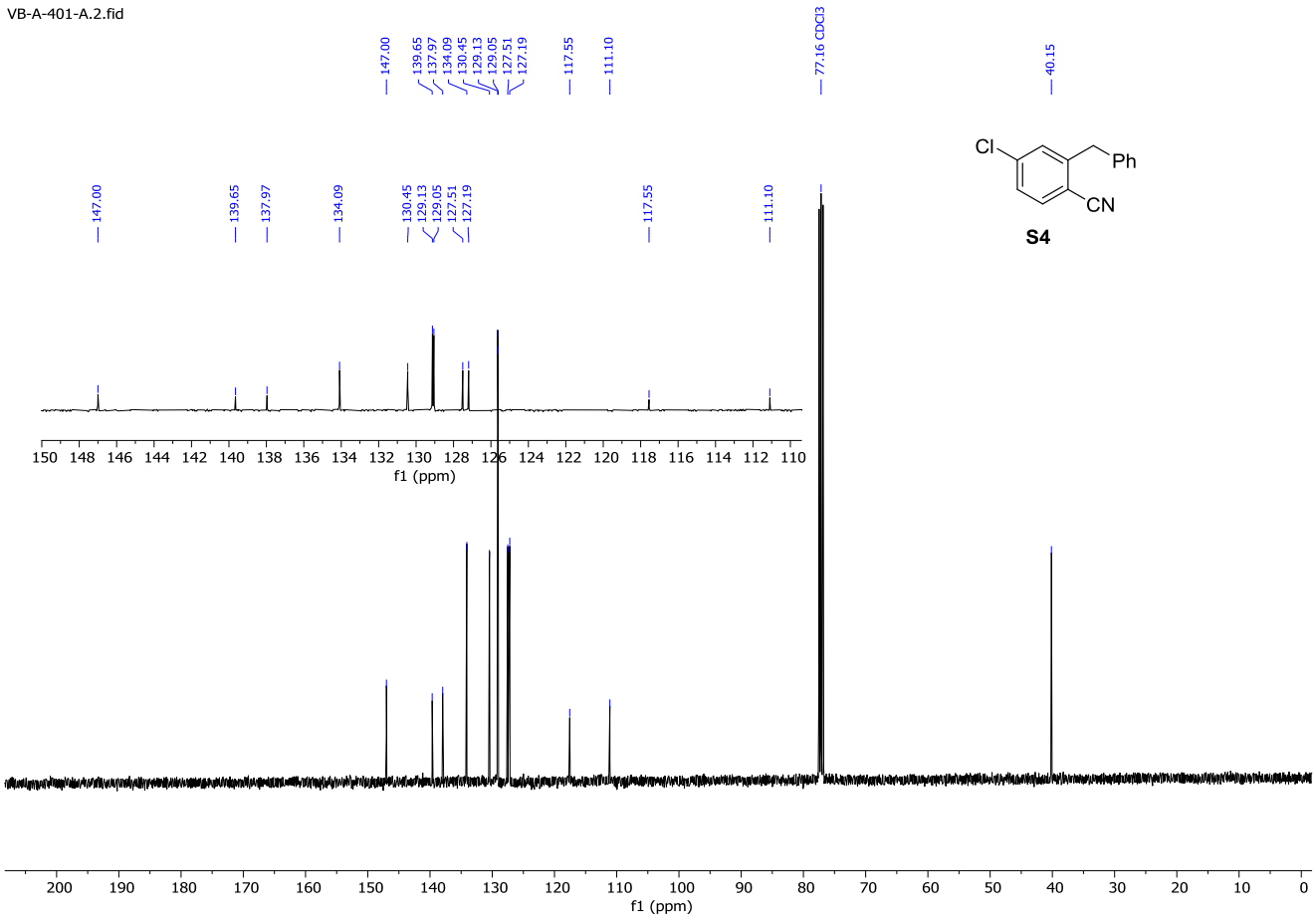




^{13}C NMR (101 MHz, $CDCl_3$)

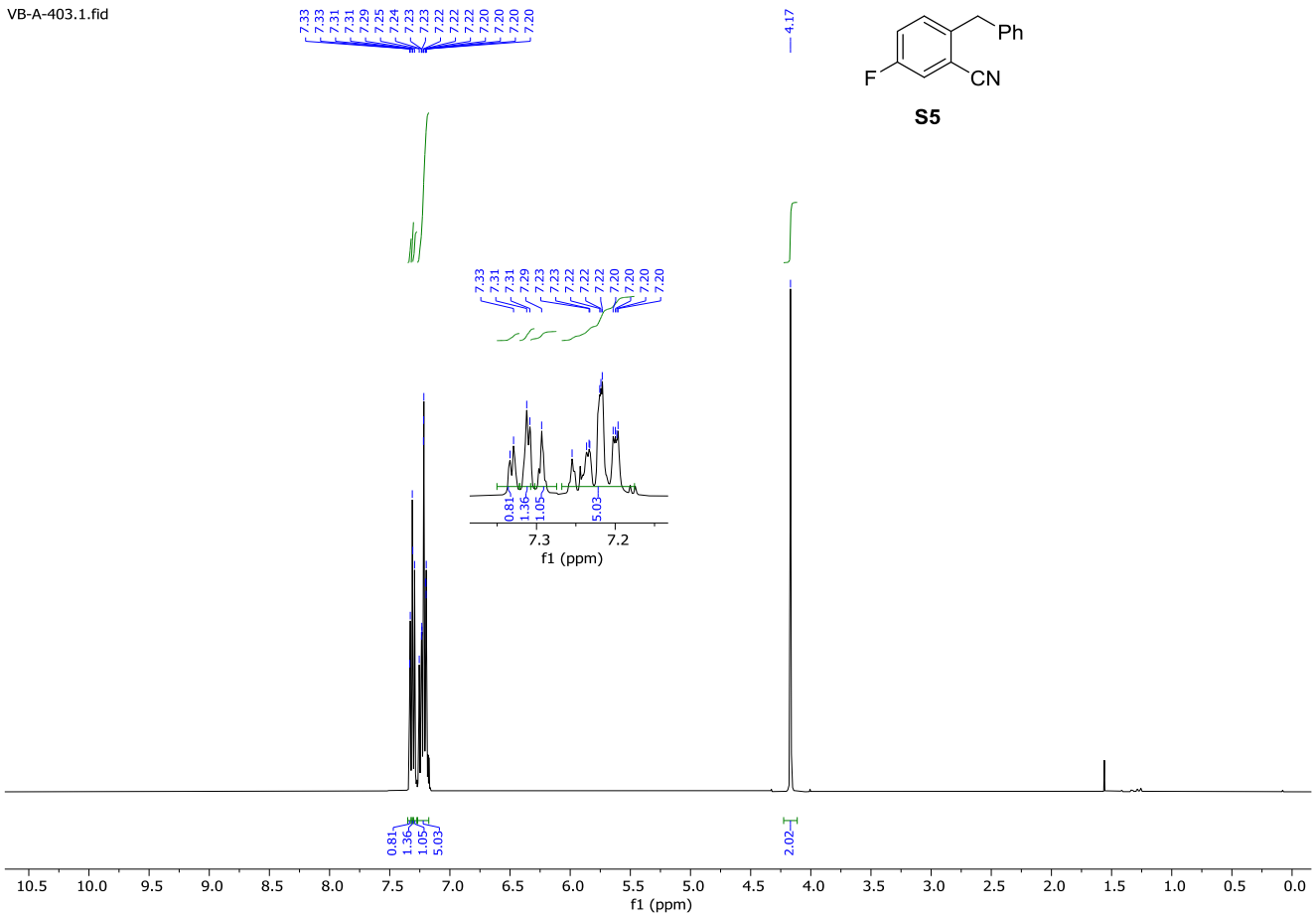
^{1}H NMR (400 MHz, $CDCl_3$)

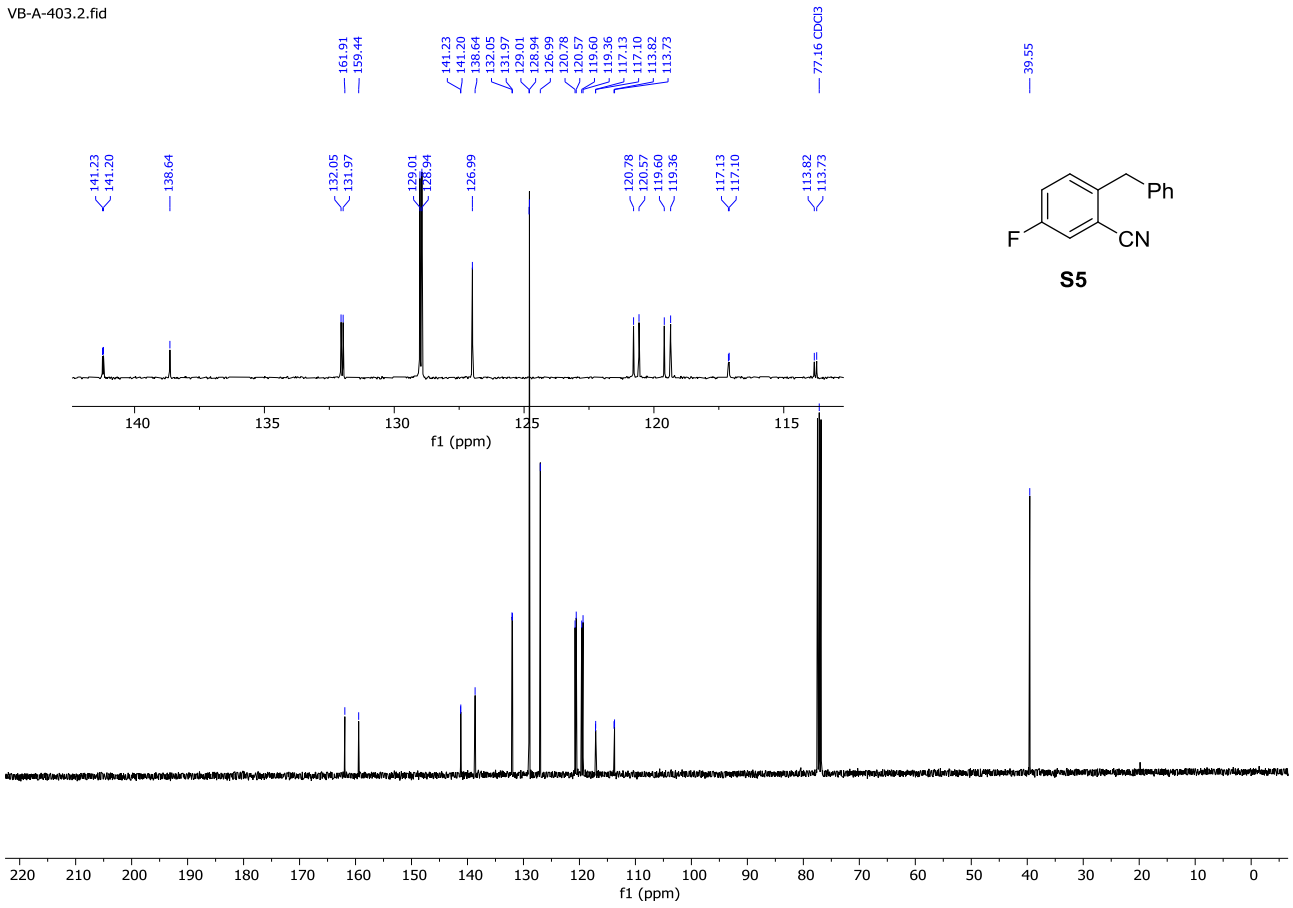




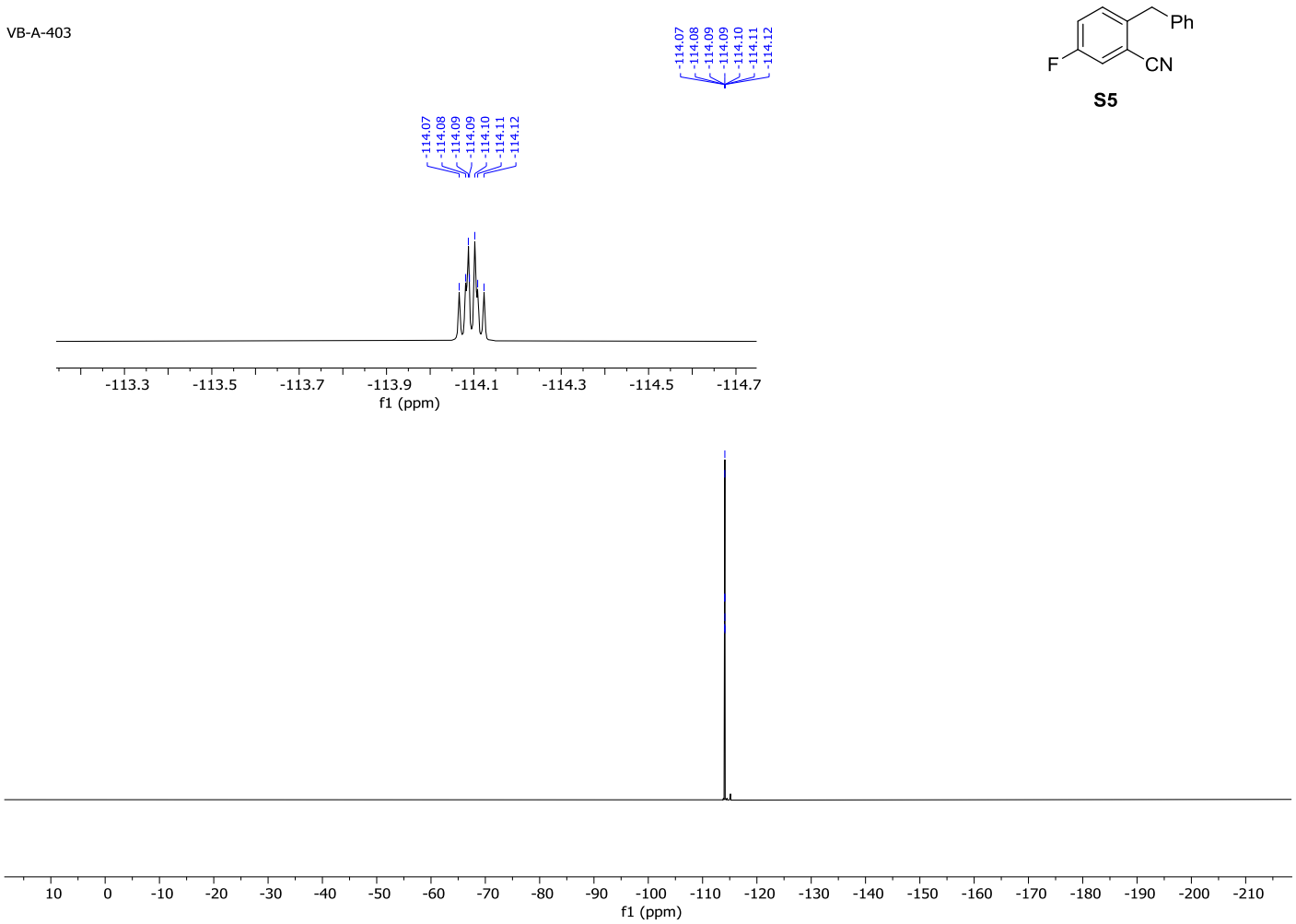
^{13}C NMR (101 MHz, $CDCl_3$)

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



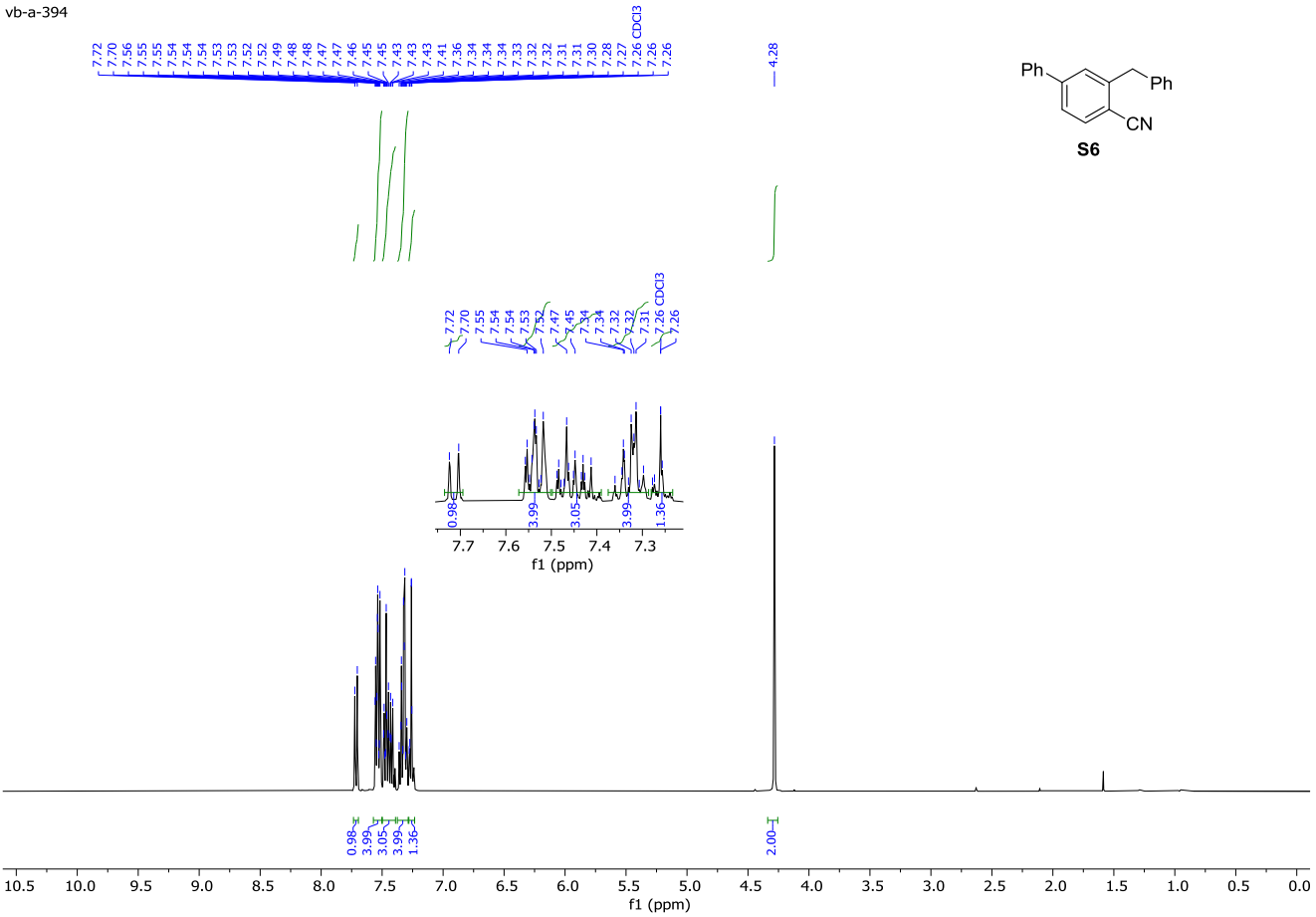


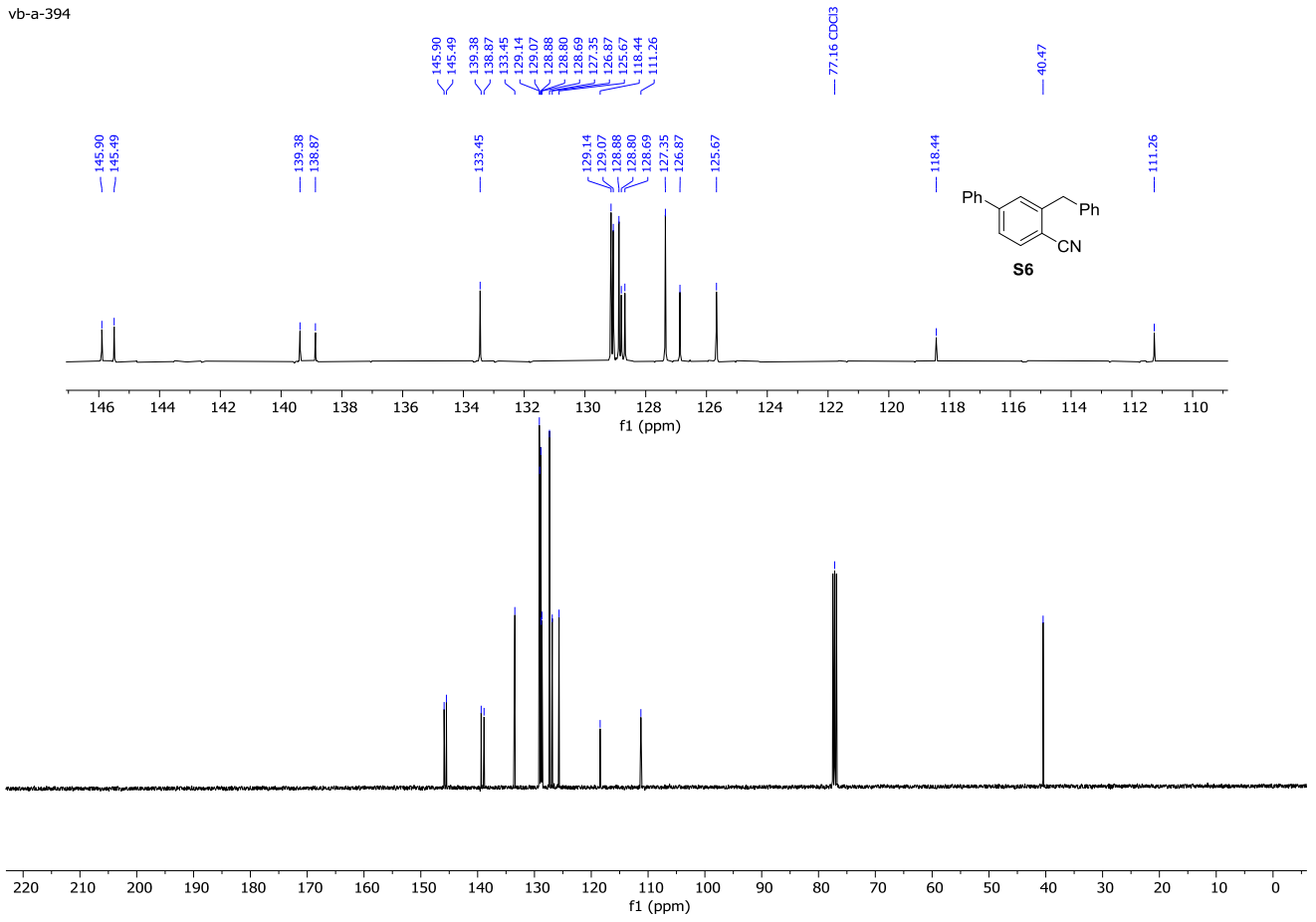
^{13}C NMR (101 MHz, $CDCl_3$)



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

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

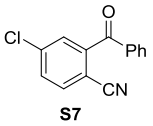




^{13}C NMR (101 MHz, $CDCl_3$)

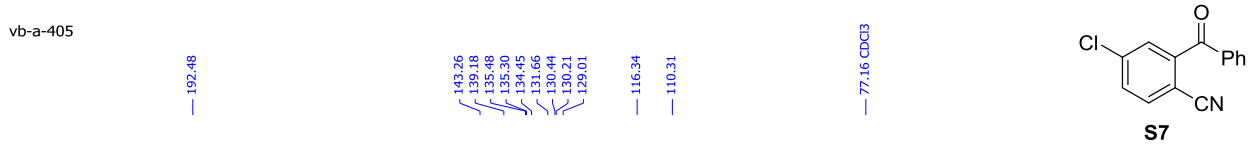
VB-A-405.1.fid

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

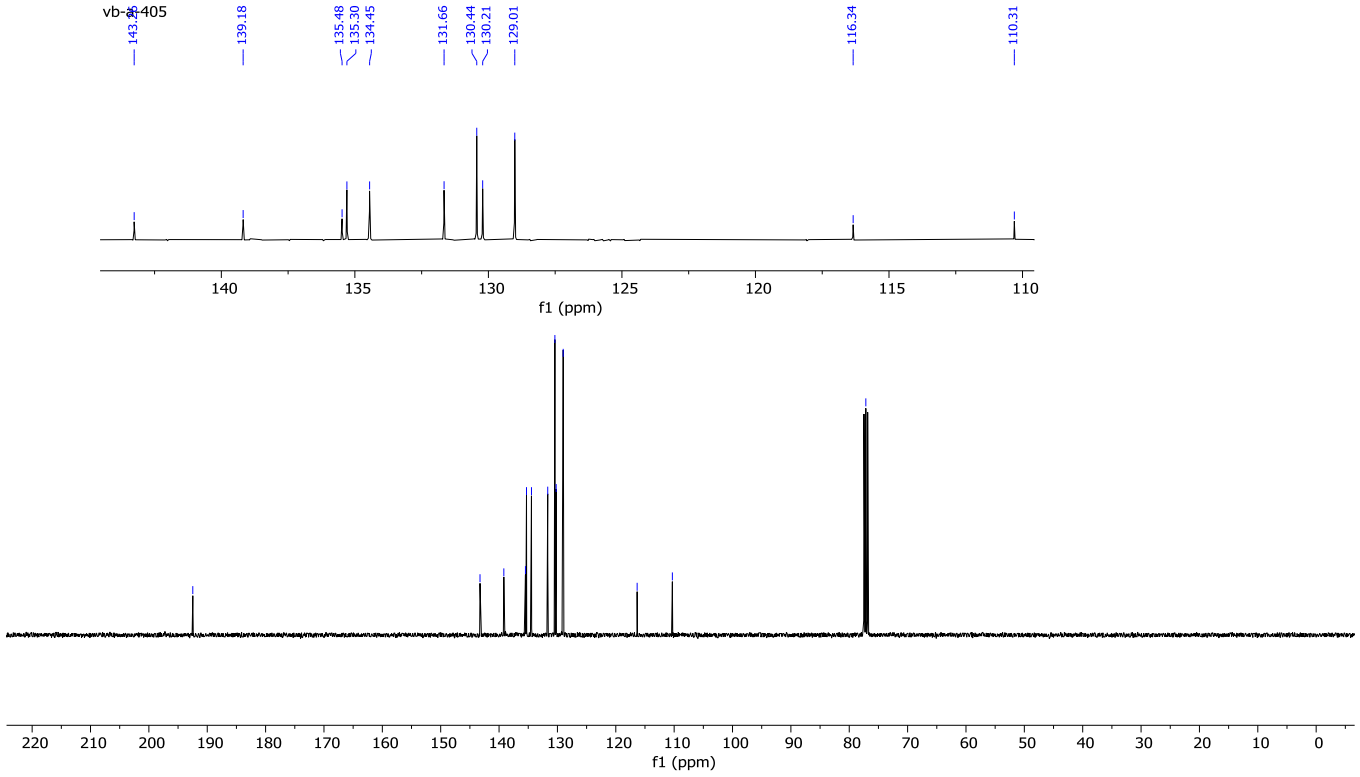


S7

vb-a-405



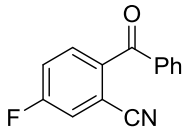
S7



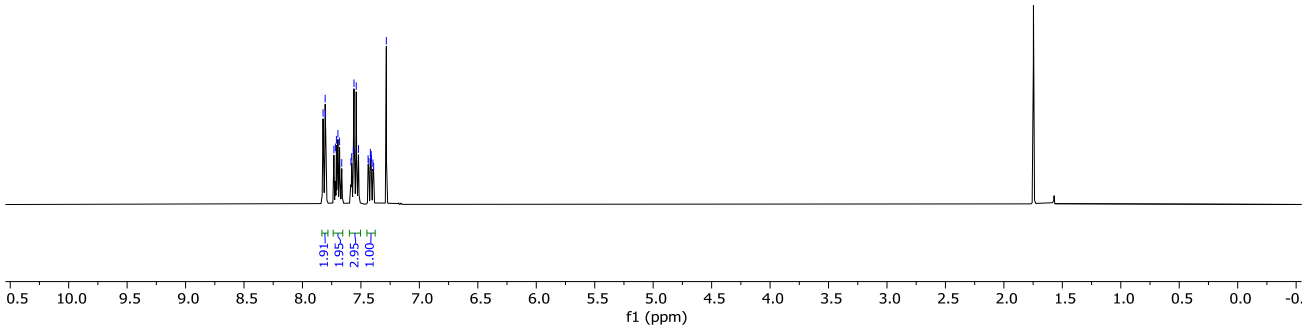
^{13}C NMR (101 MHz, $CDCl_3$)

VB-A-410

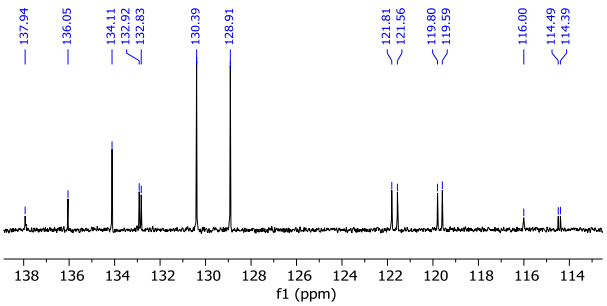
^{1}H NMR (400 MHz, $CDCl_3$)

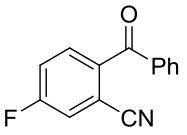


S8

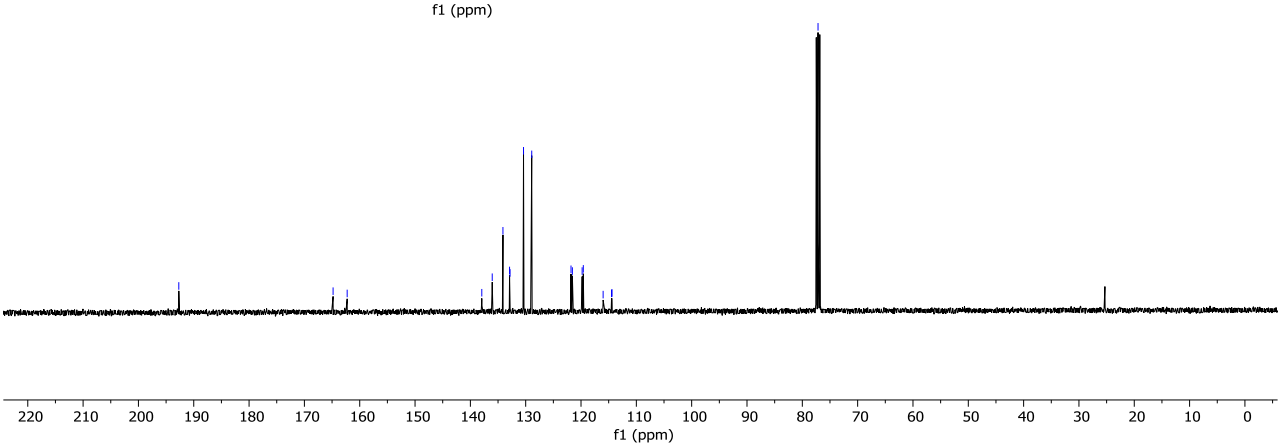


VB-A-410

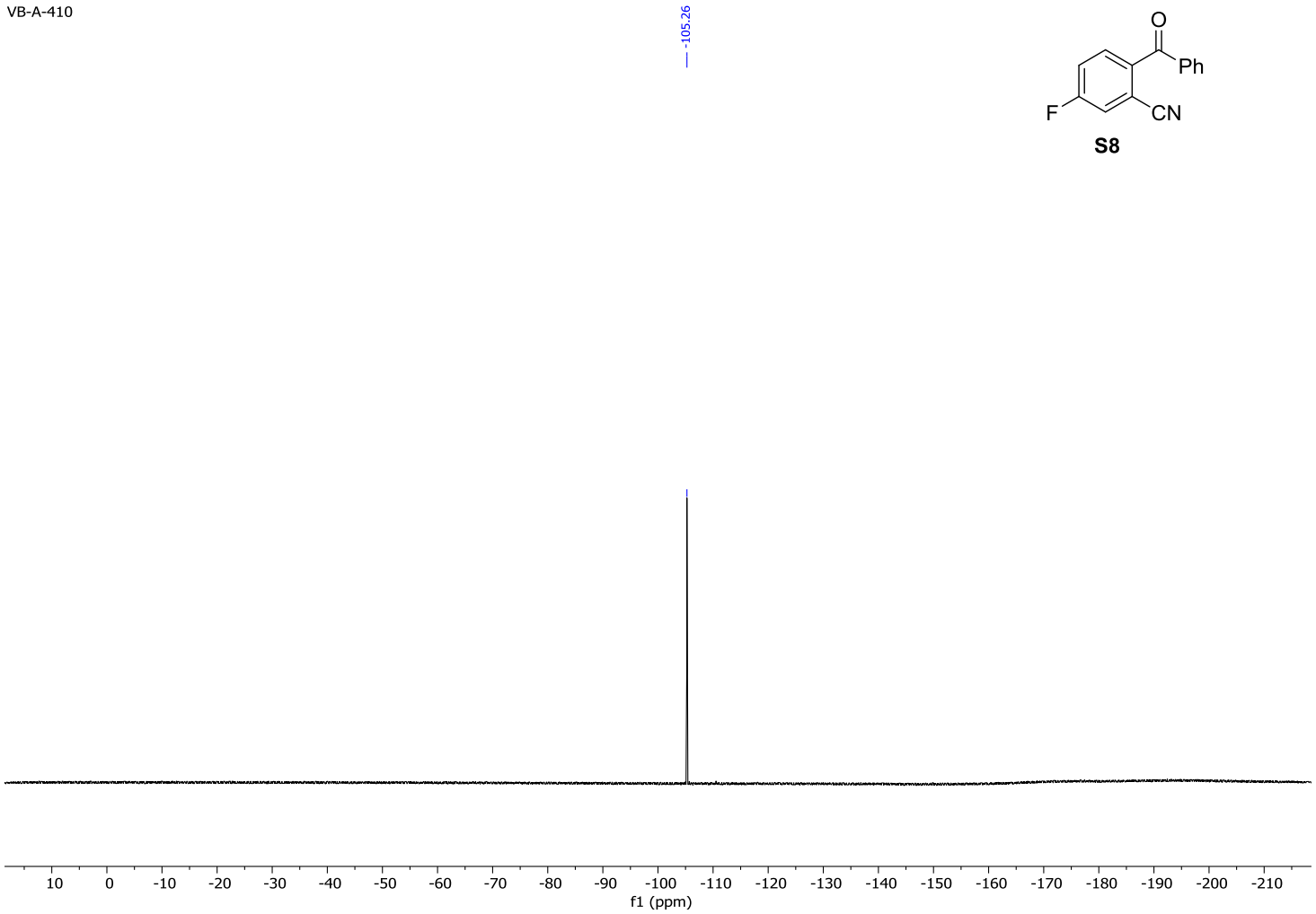




S8

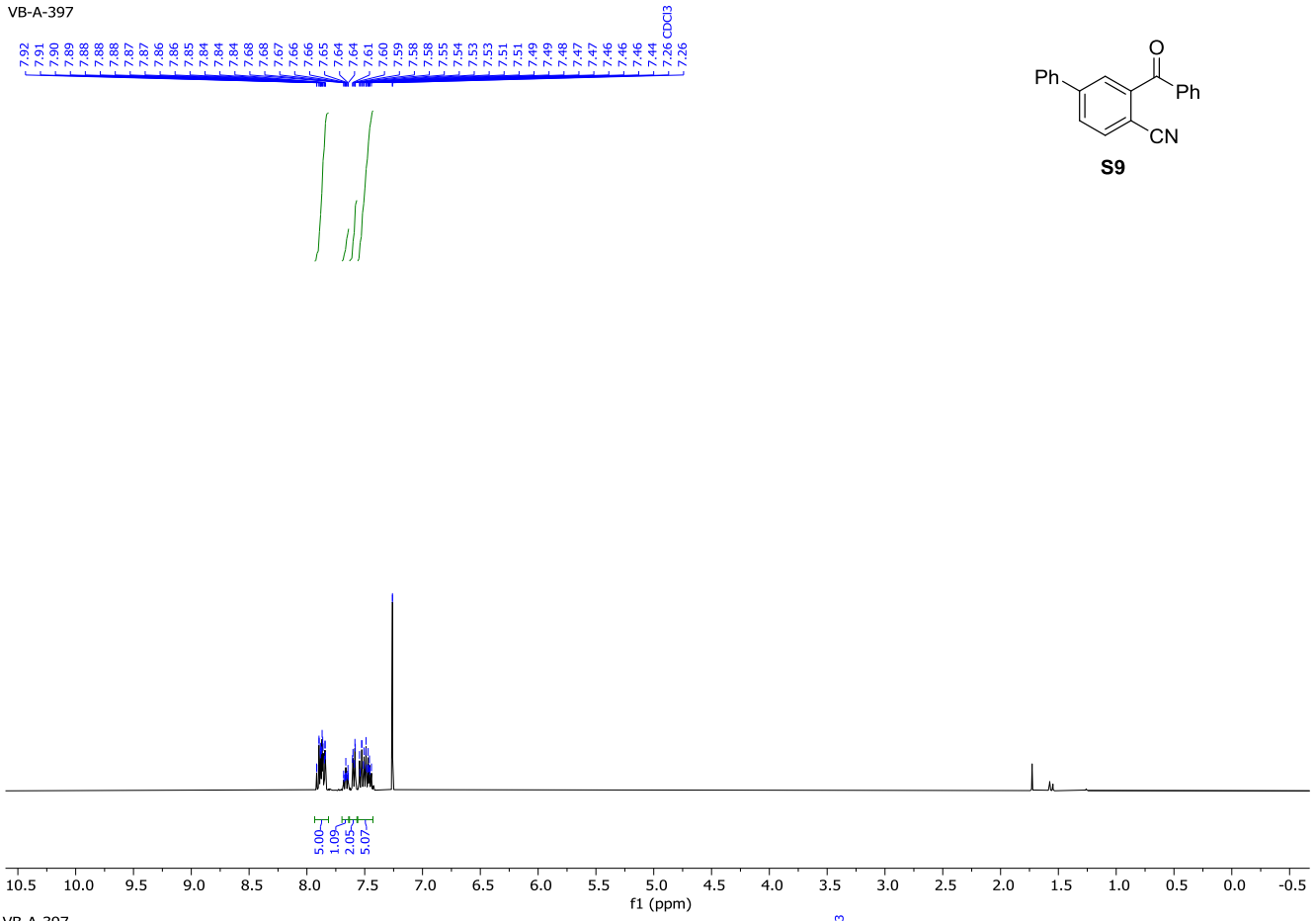


^{13}C NMR (101 MHz, $CDCl_3$)

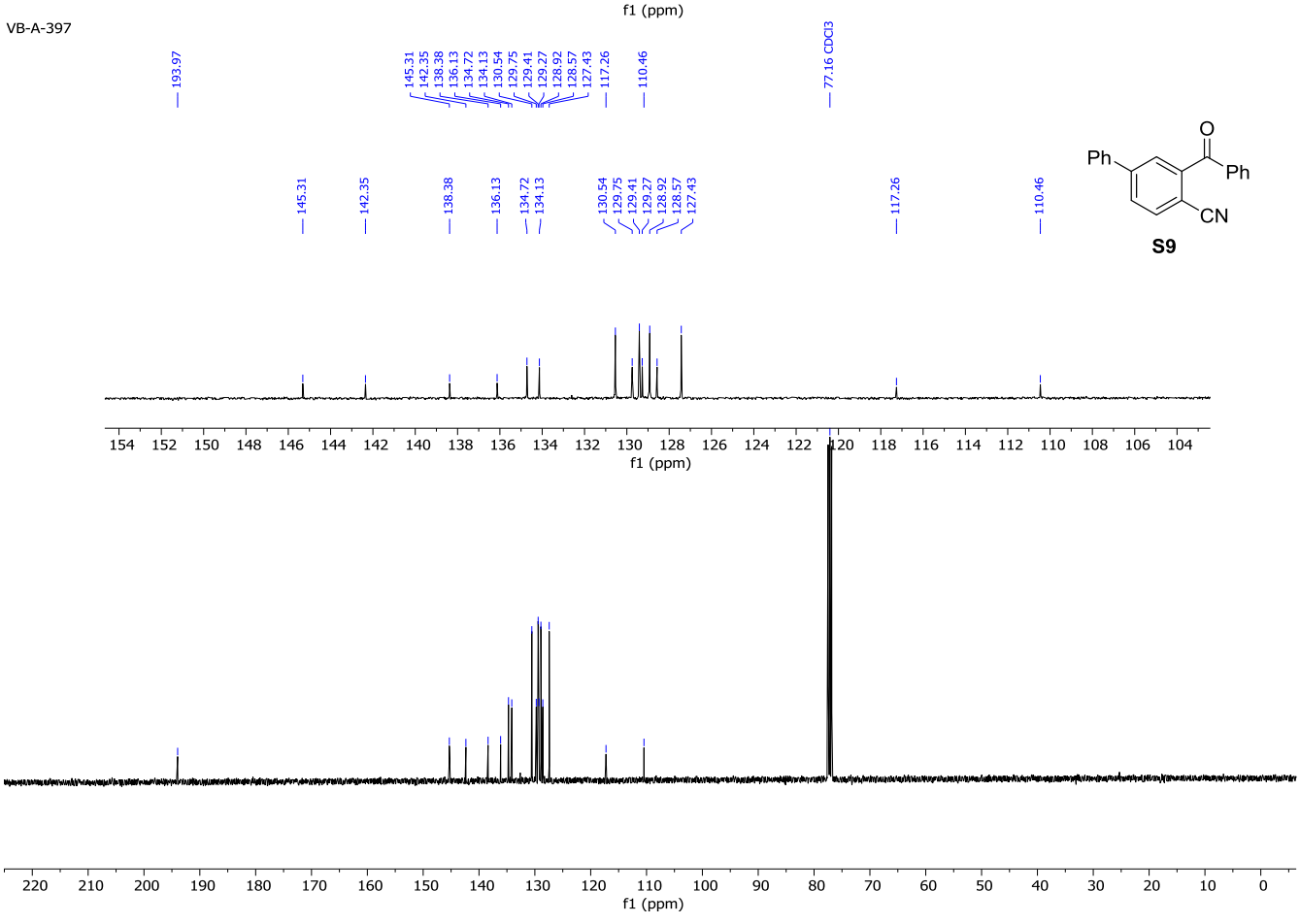


^{19}F NMR (376 MHz, $CDCl_3$)

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



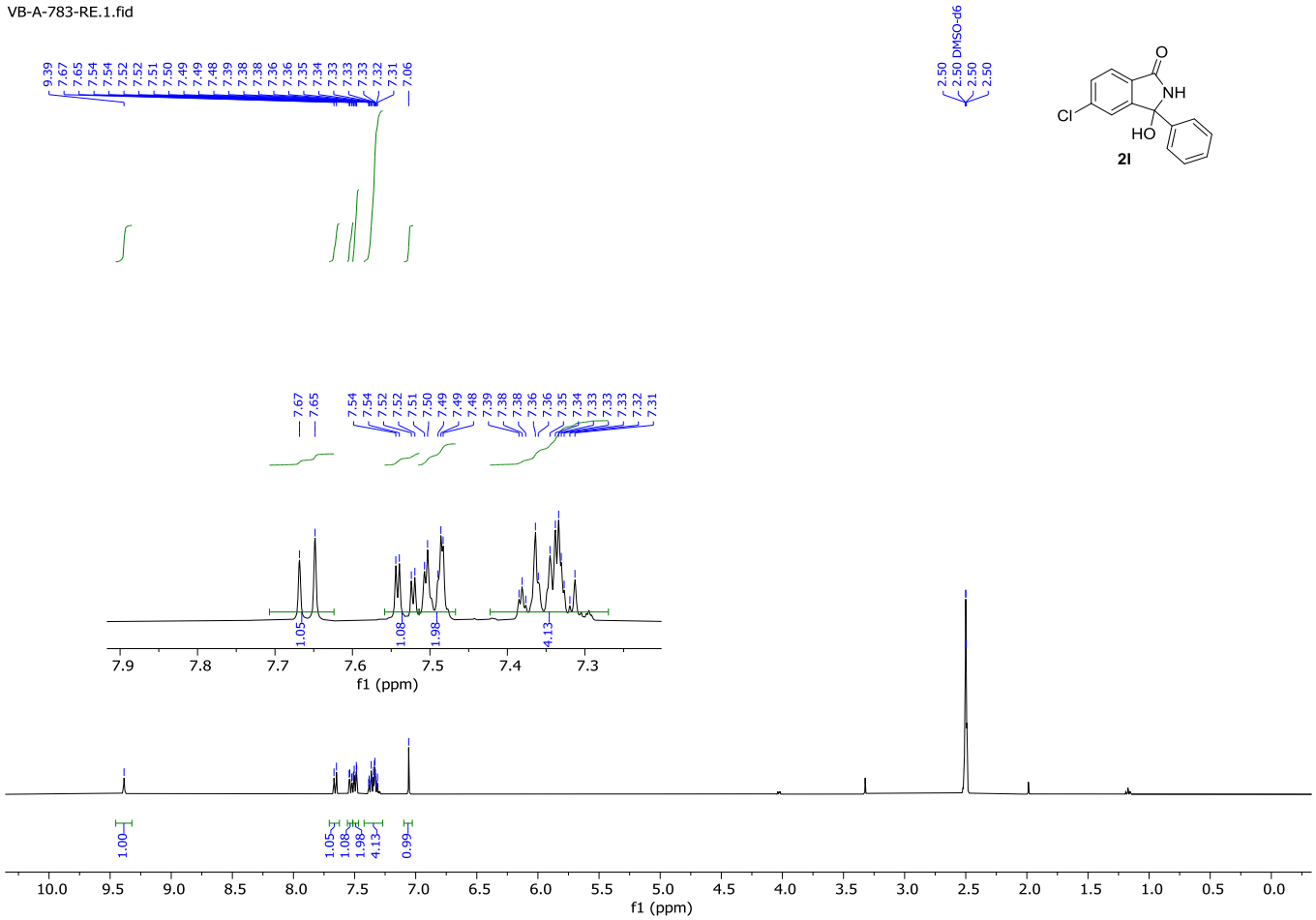
S9

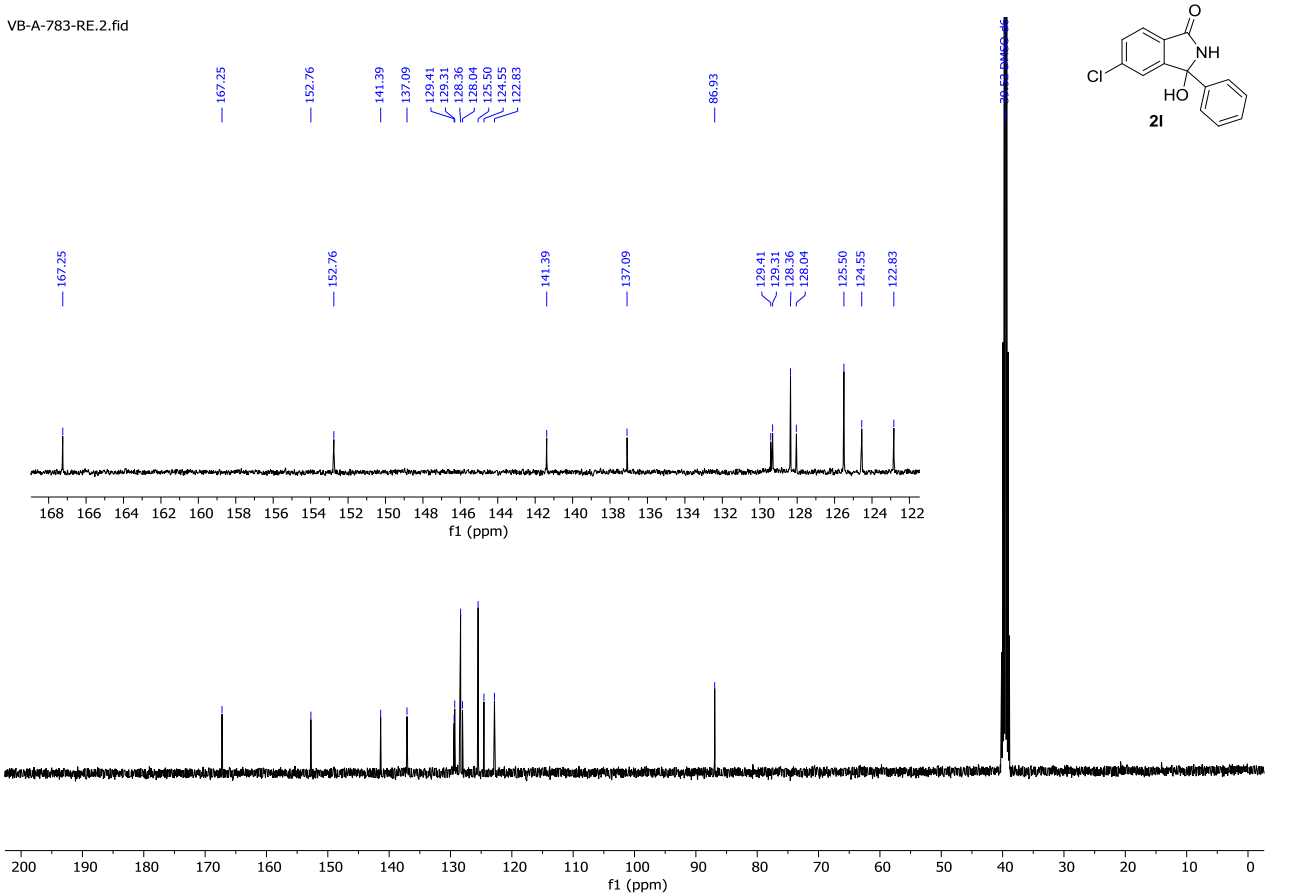


S9

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

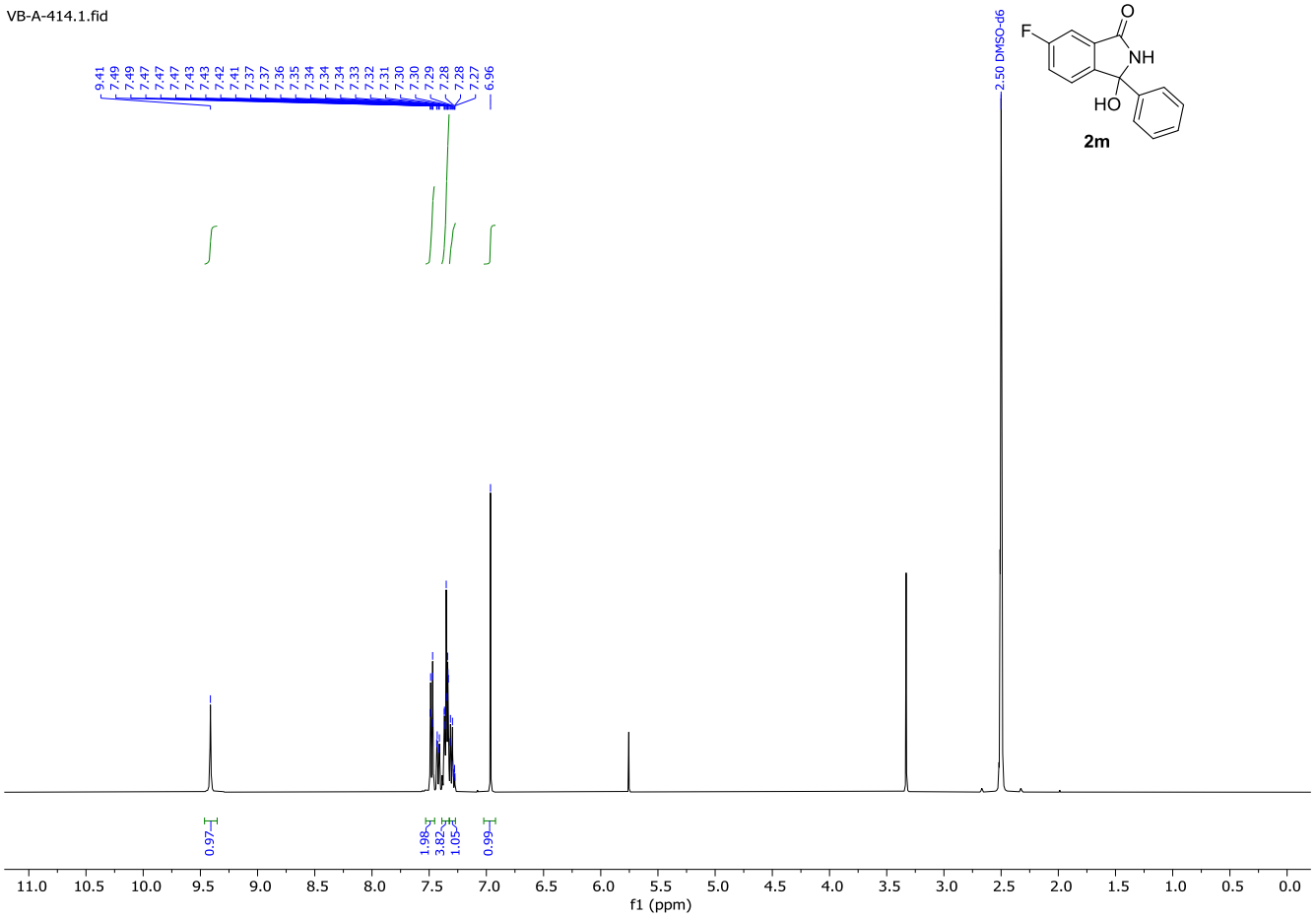
^{1}H NMR (400 MHz, DMSO)

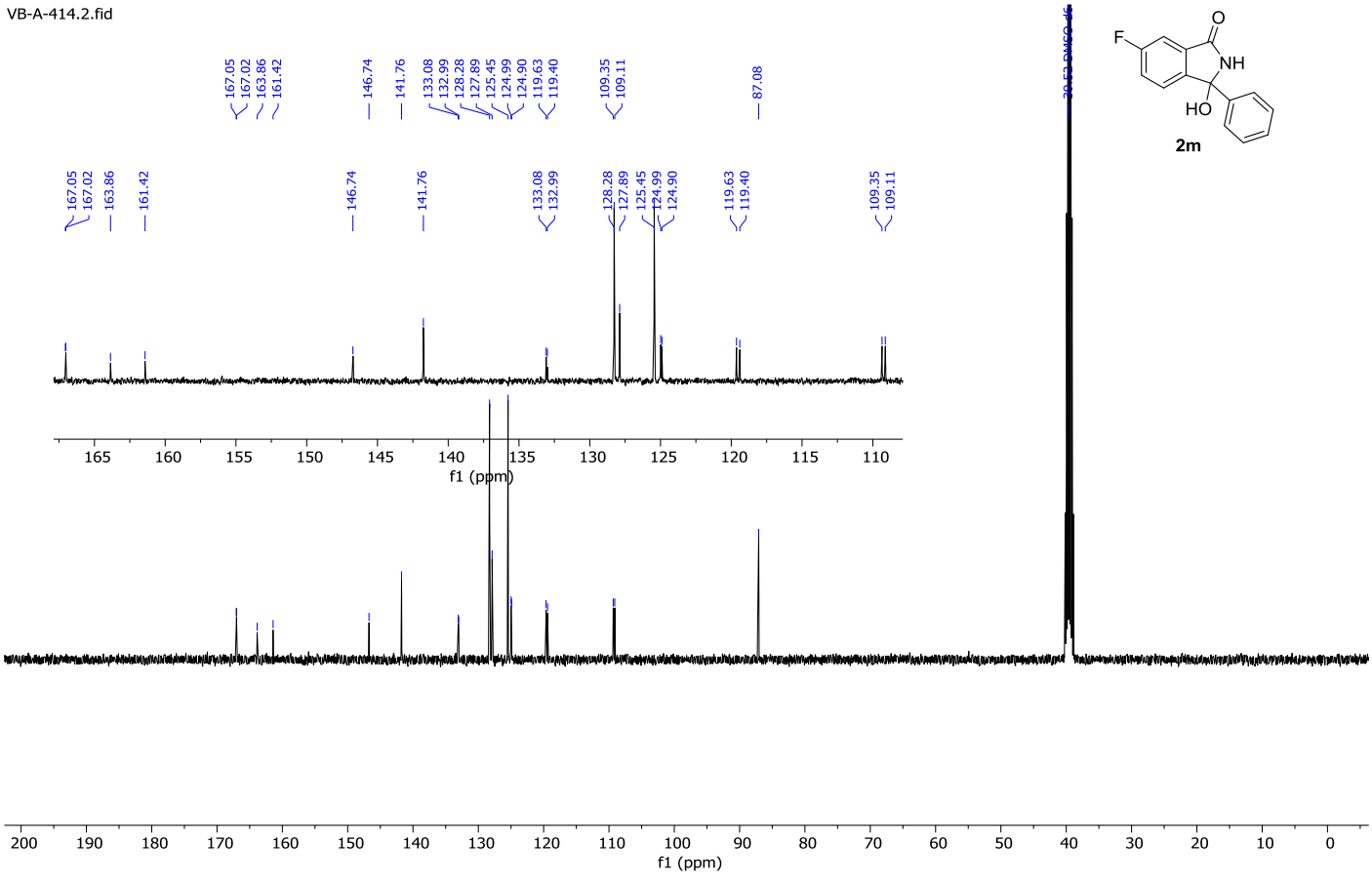




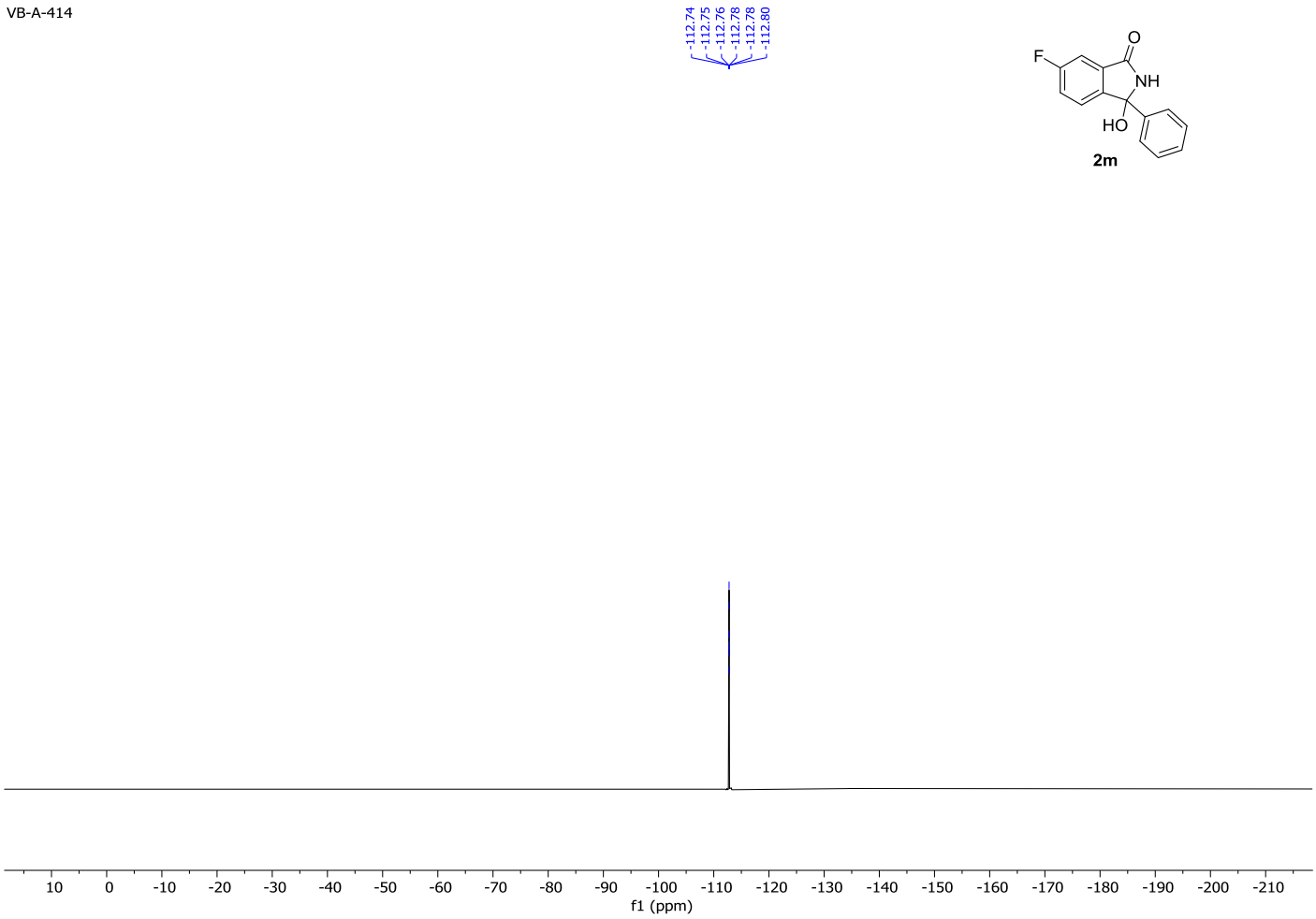
^{13}C NMR (101 MHz, DMSO)

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



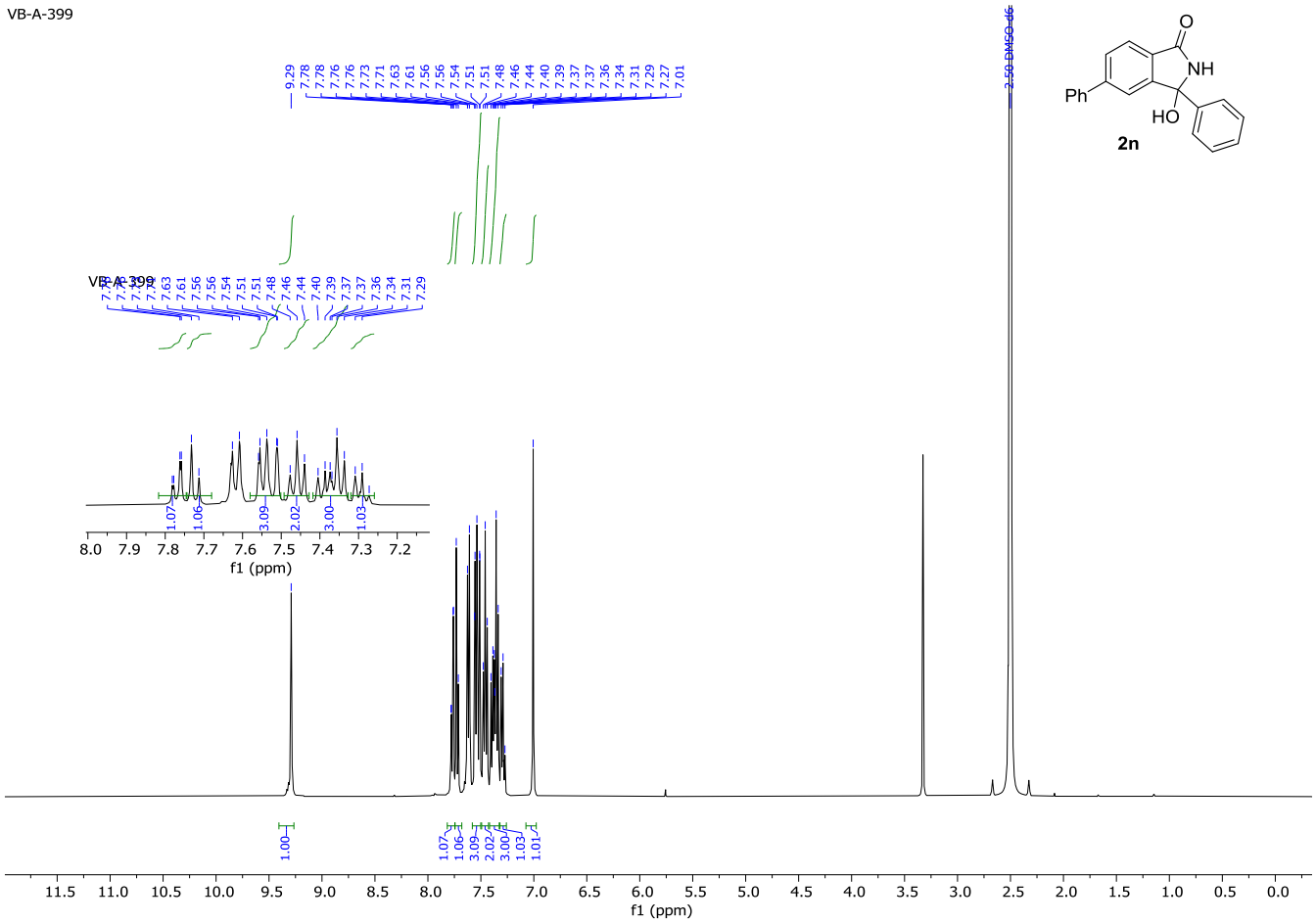


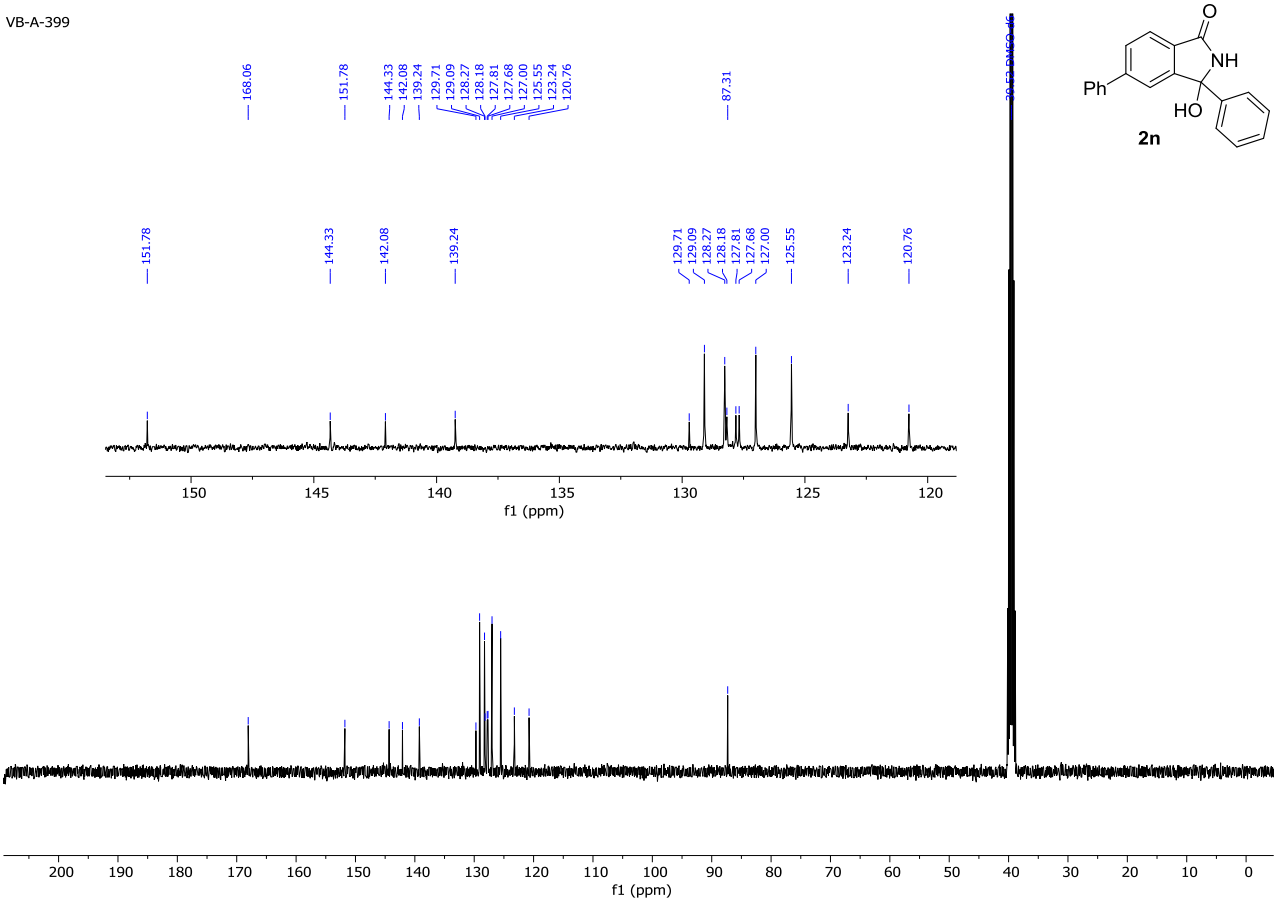
^{13}C NMR (101 MHz, DMSO)



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

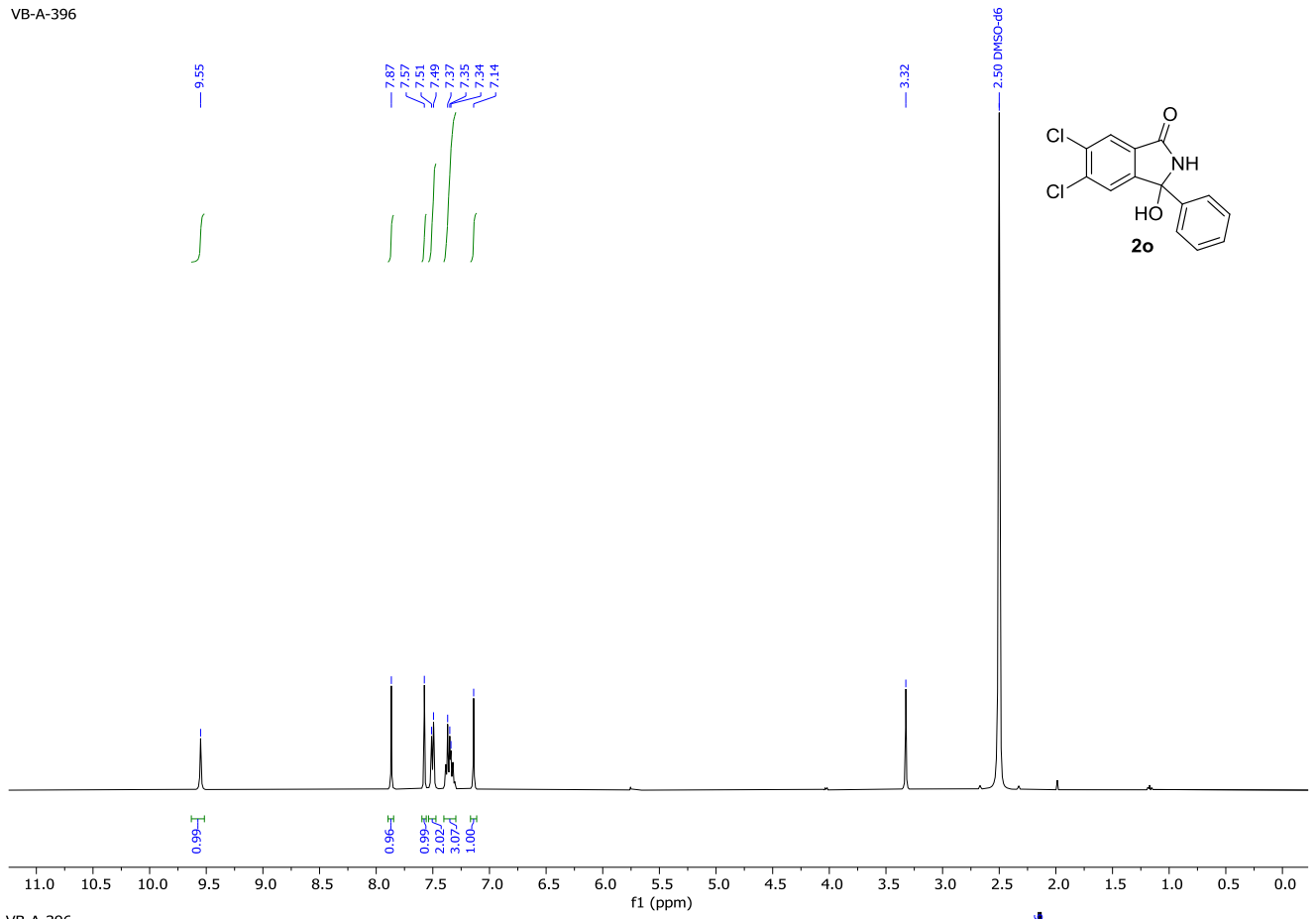
^{1}H NMR (400 MHz, DMSO)

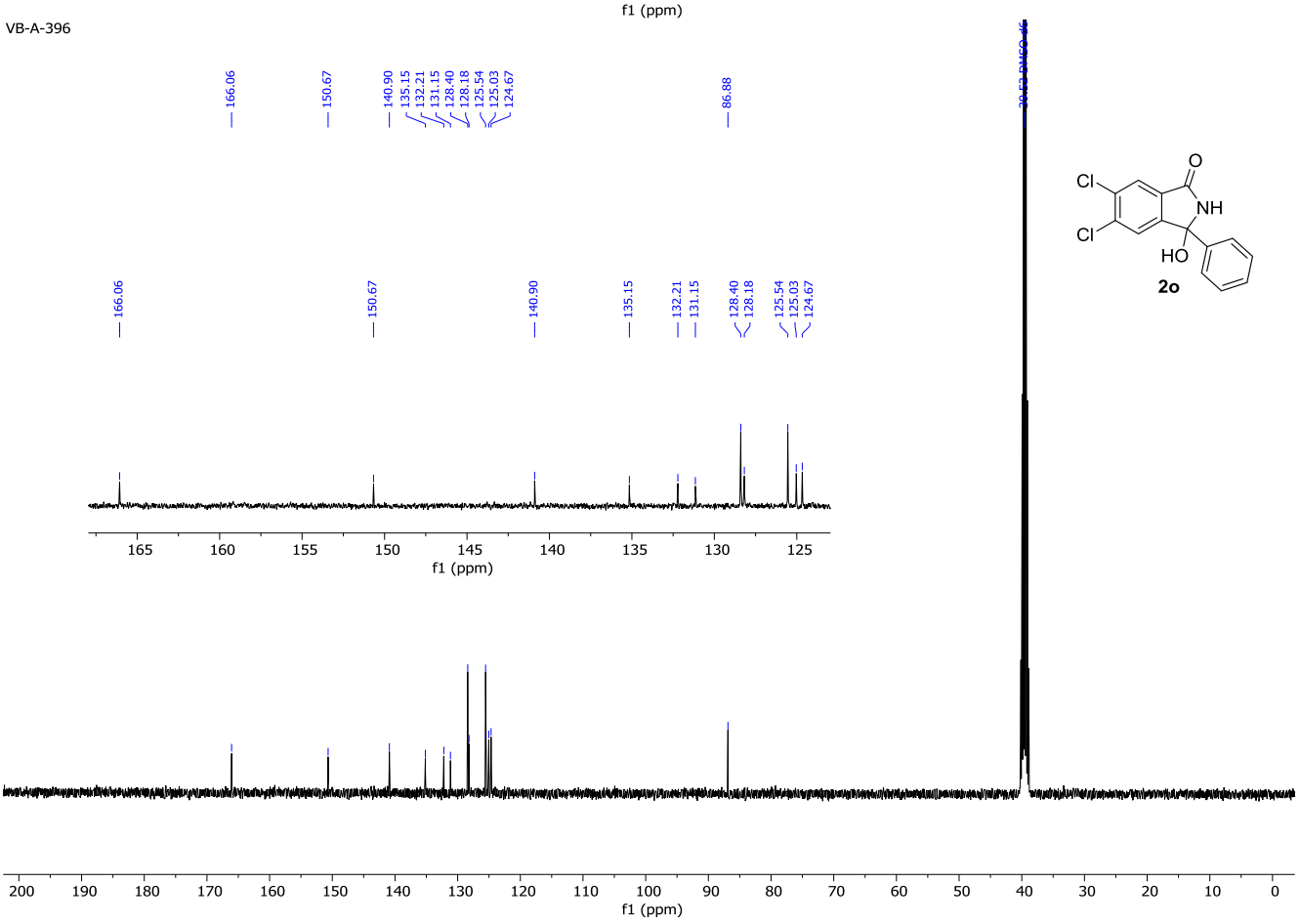




^{13}C NMR (101 MHz, DMSO)

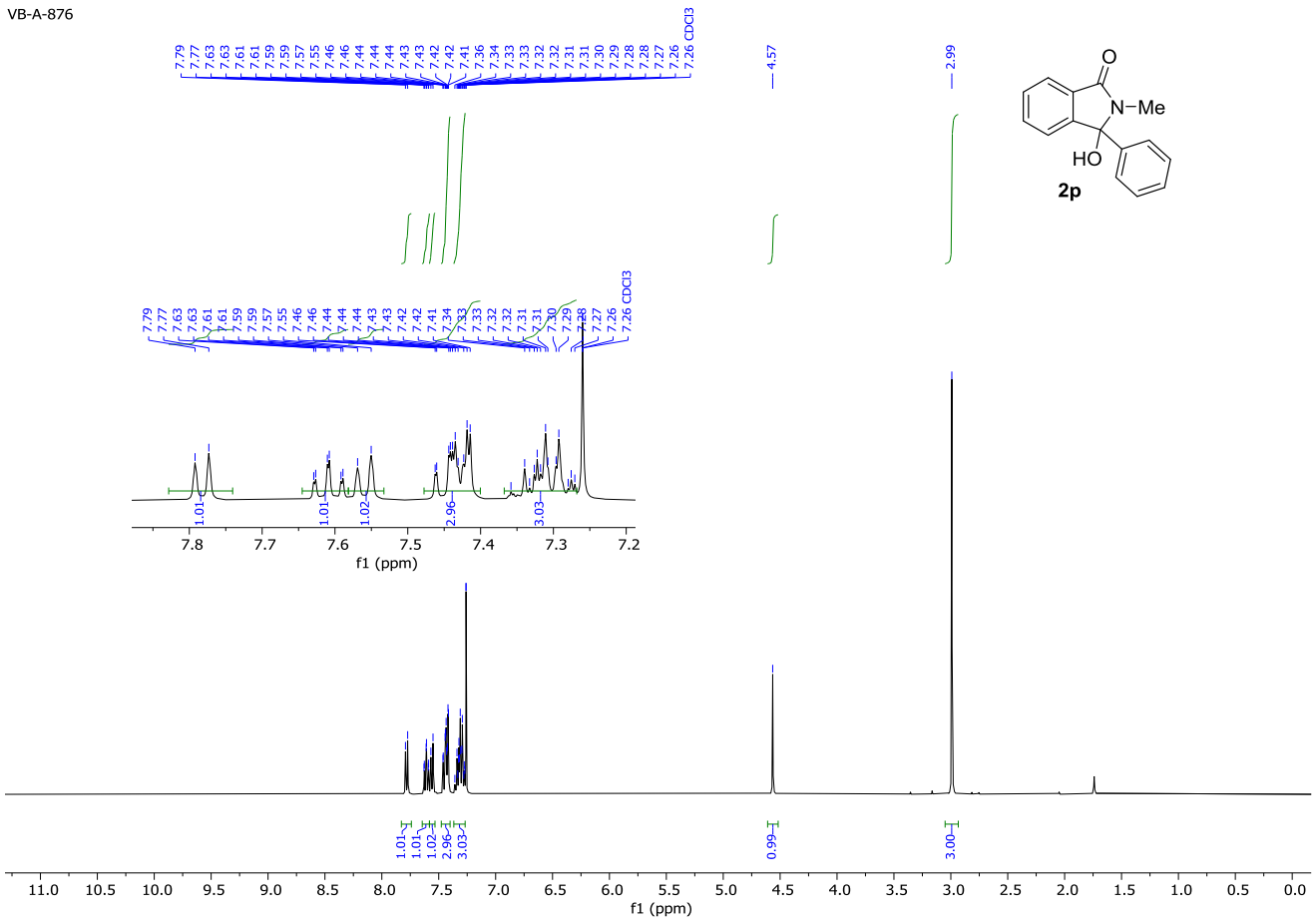
^{1}H NMR (400 MHz, DMSO)

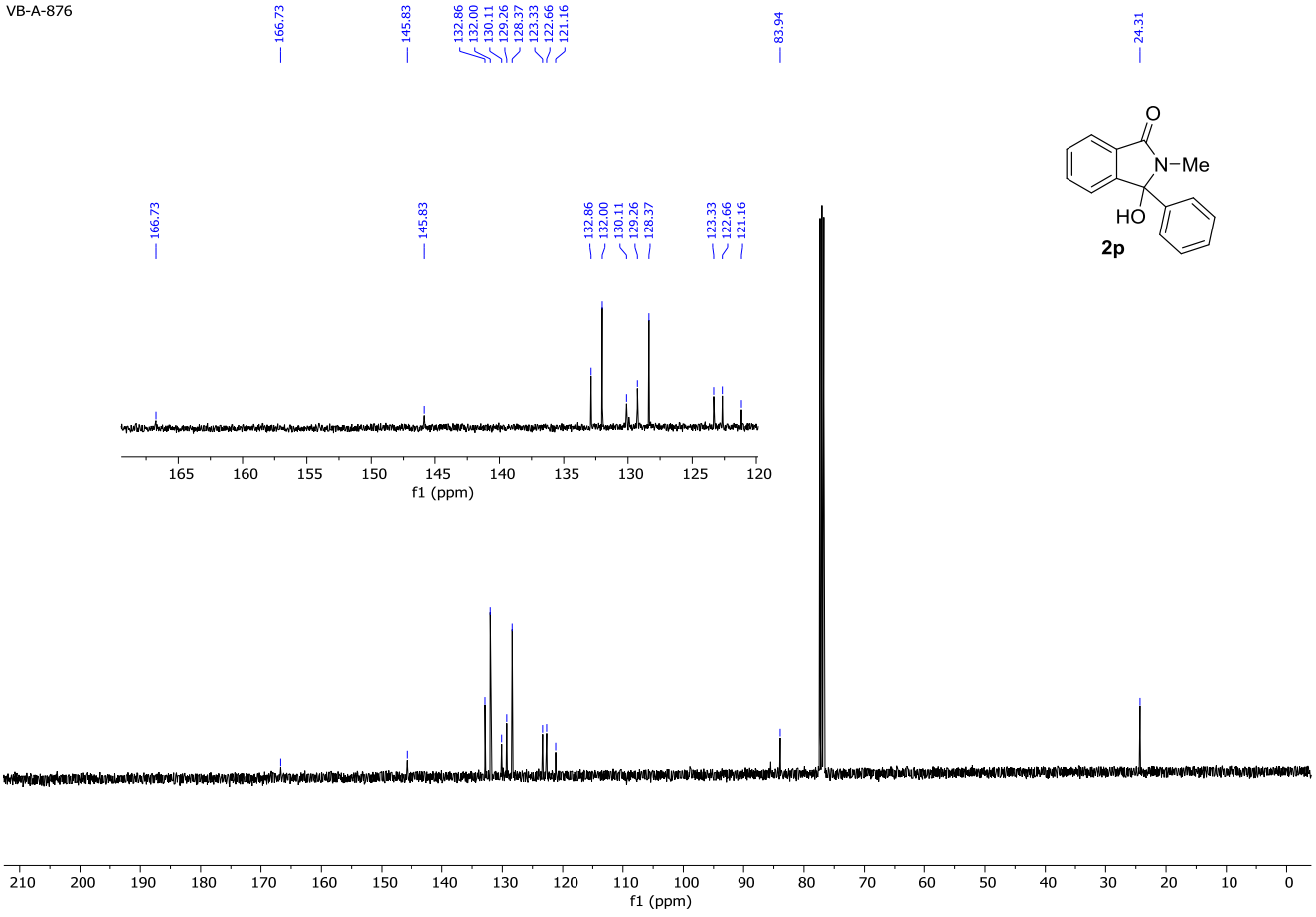




^{13}C NMR (101 MHz, DMSO)

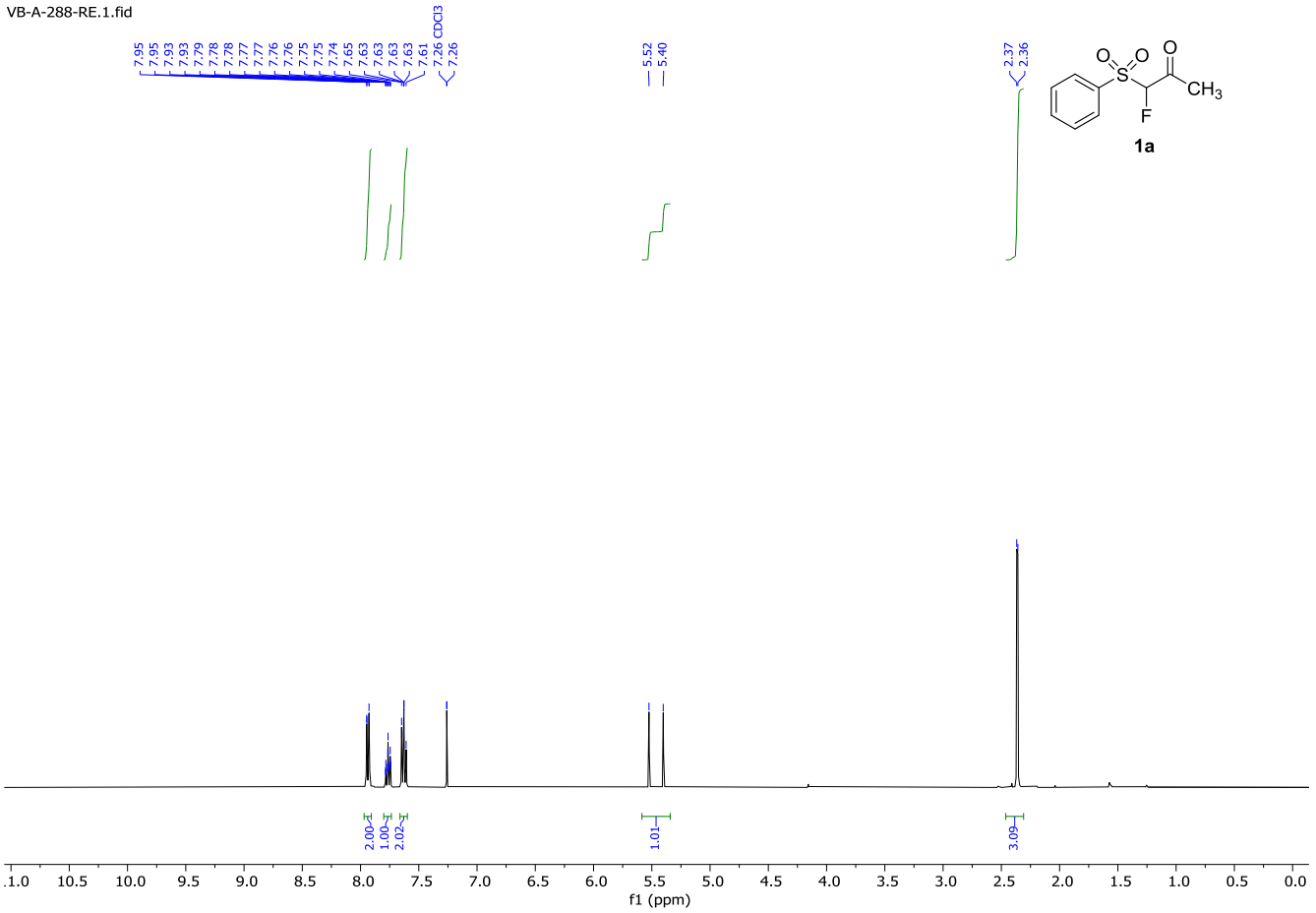
^{1}H NMR (400 MHz, DMSO)

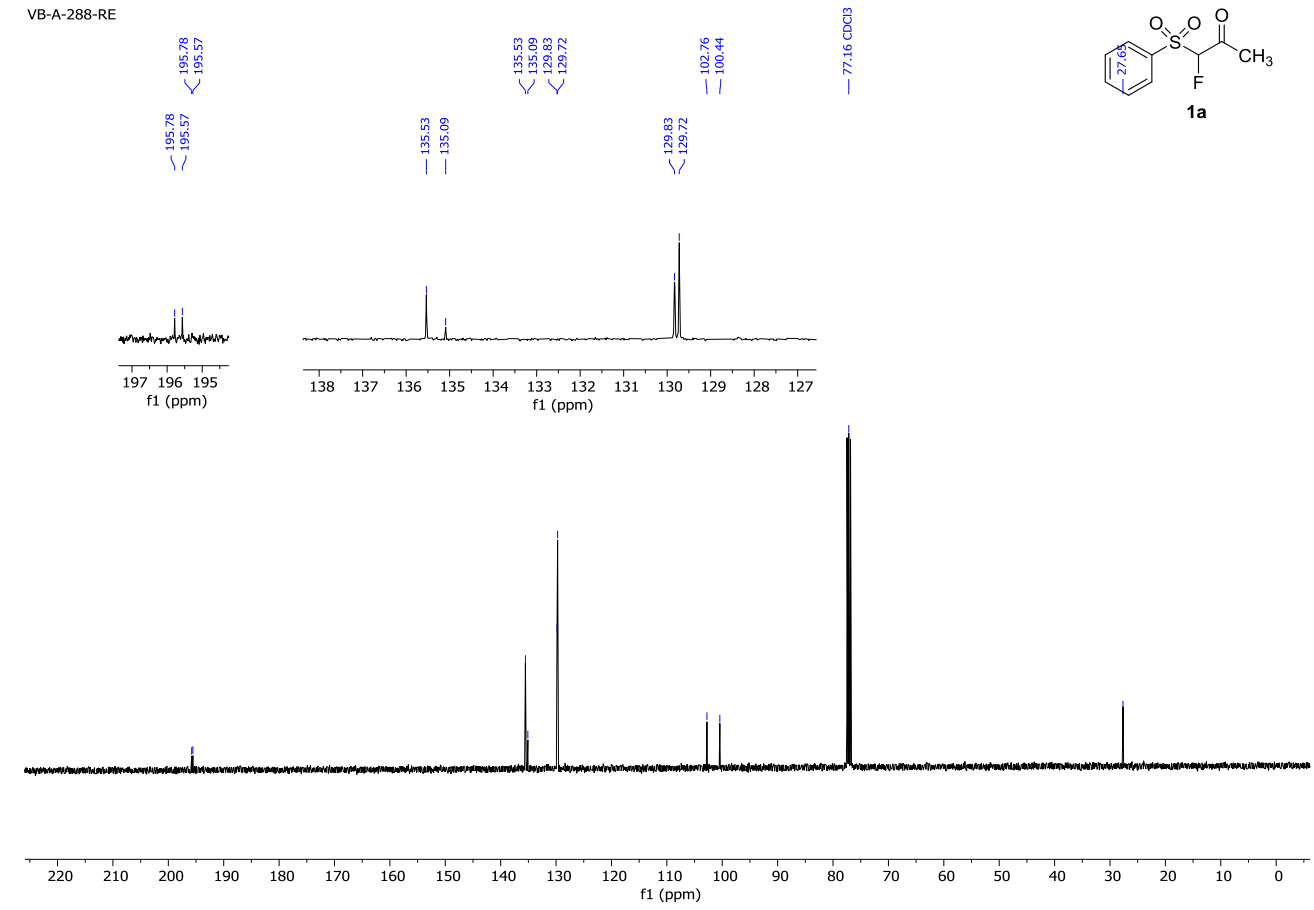




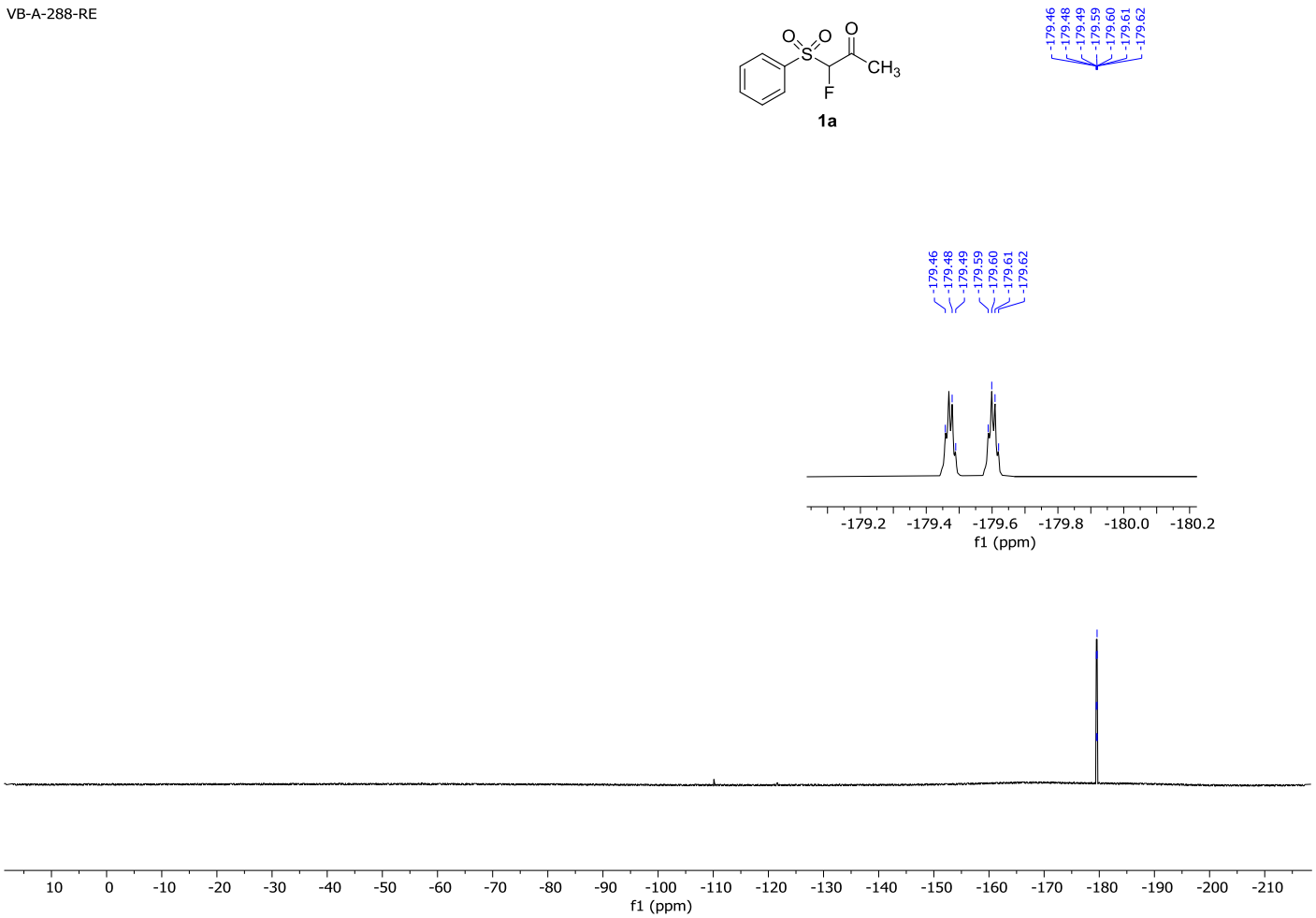
^{13}C NMR (101 MHz, DMSO)

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



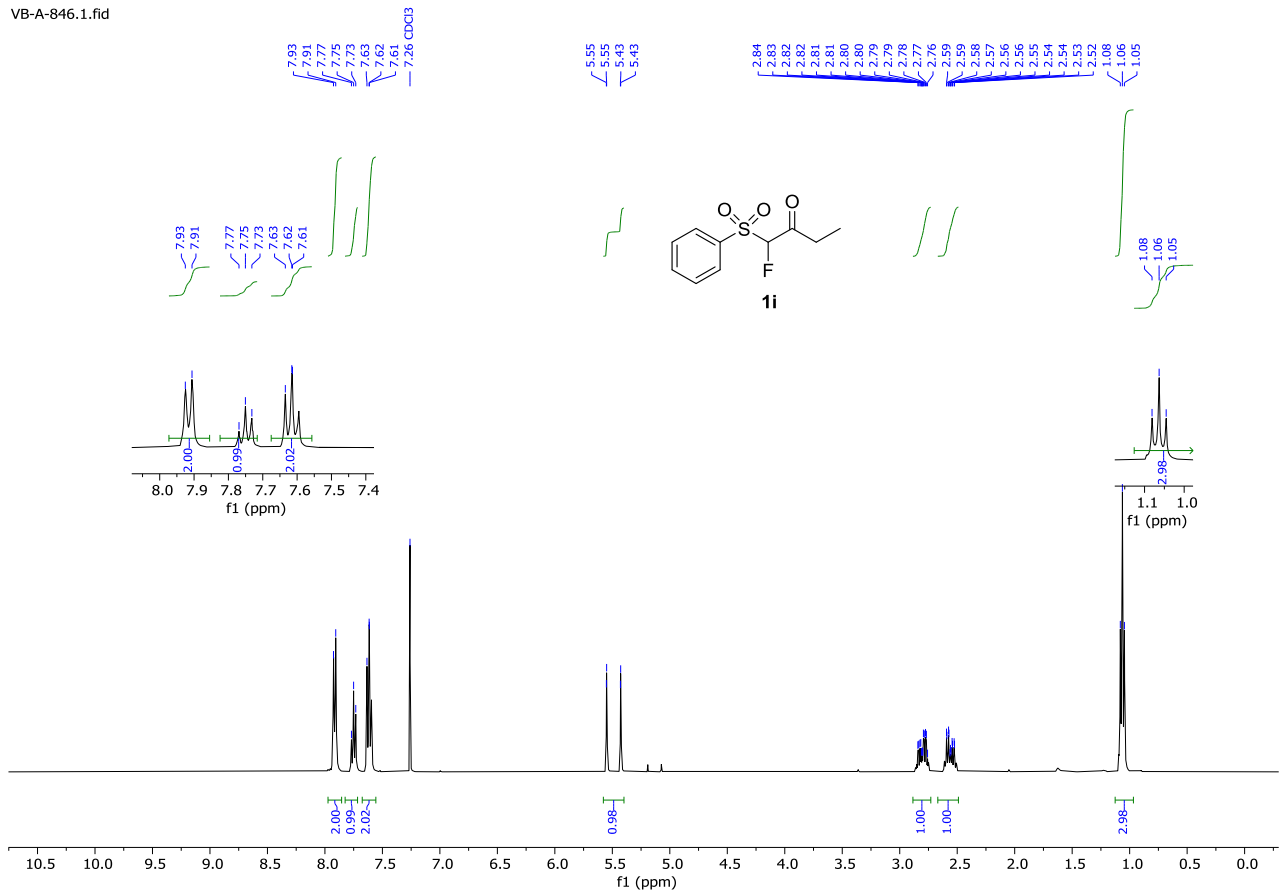


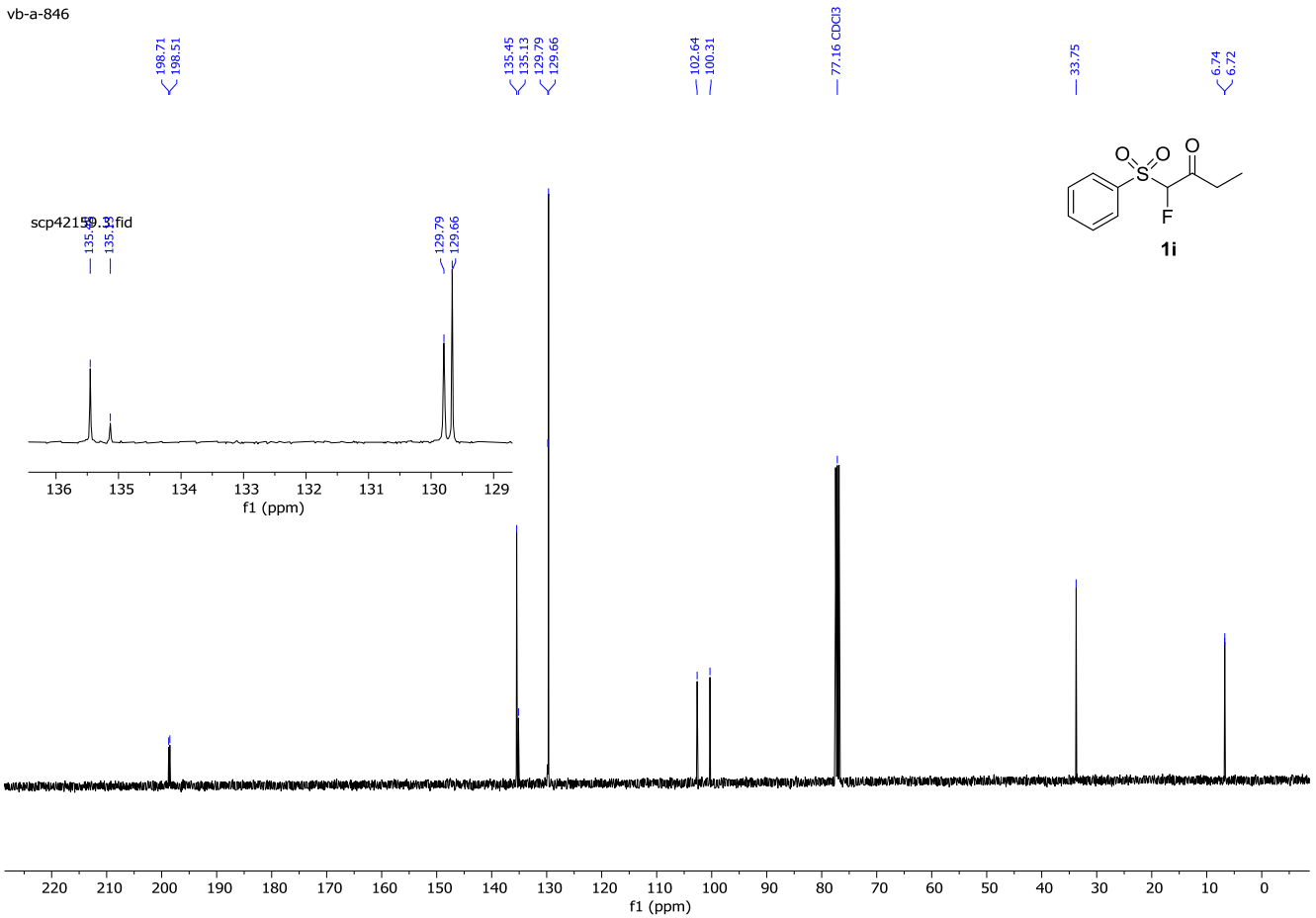
^{13}C NMR (101 MHz, $CDCl_3$)



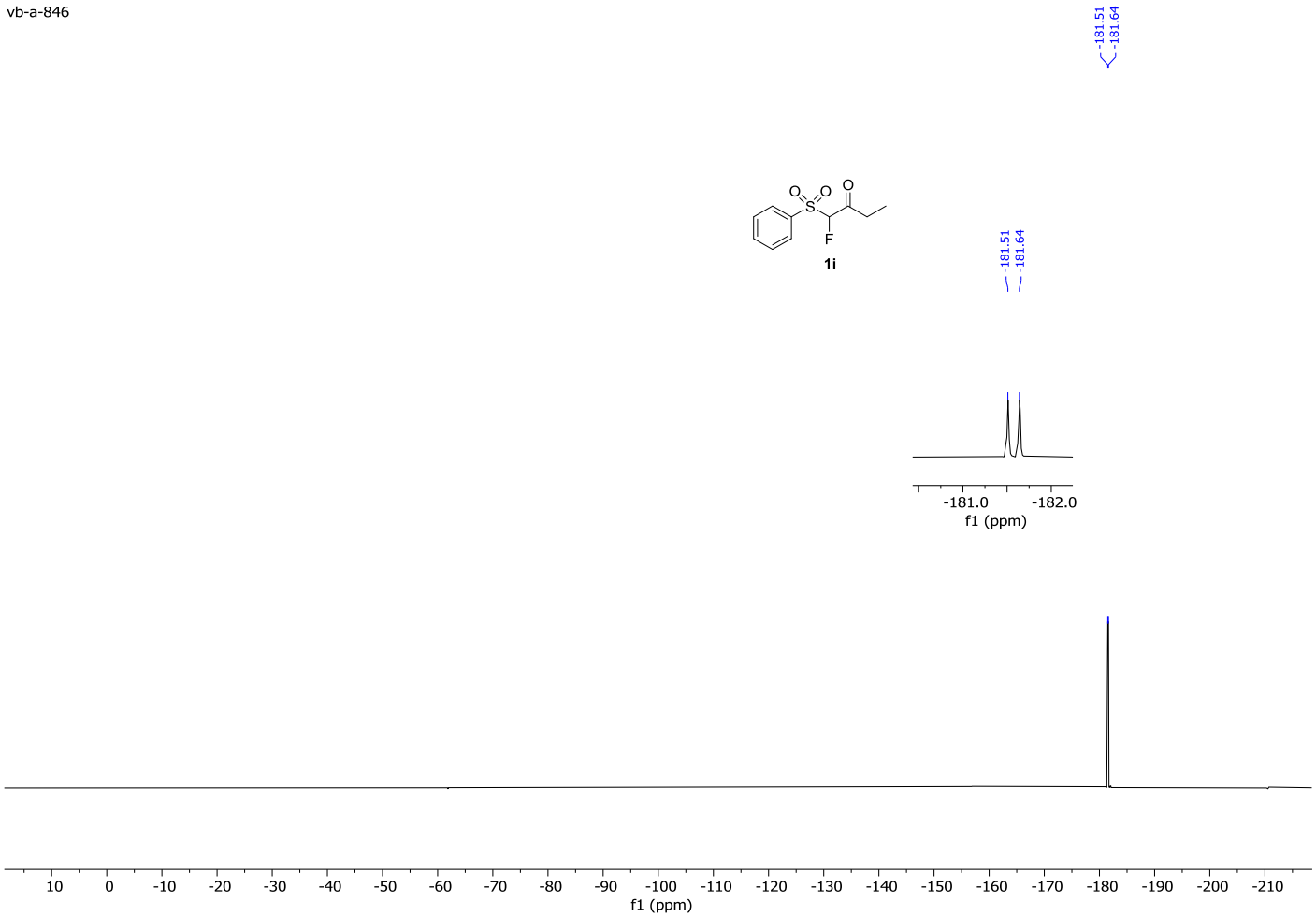
^{19}F NMR (376 MHz, $CDCl_3$)

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



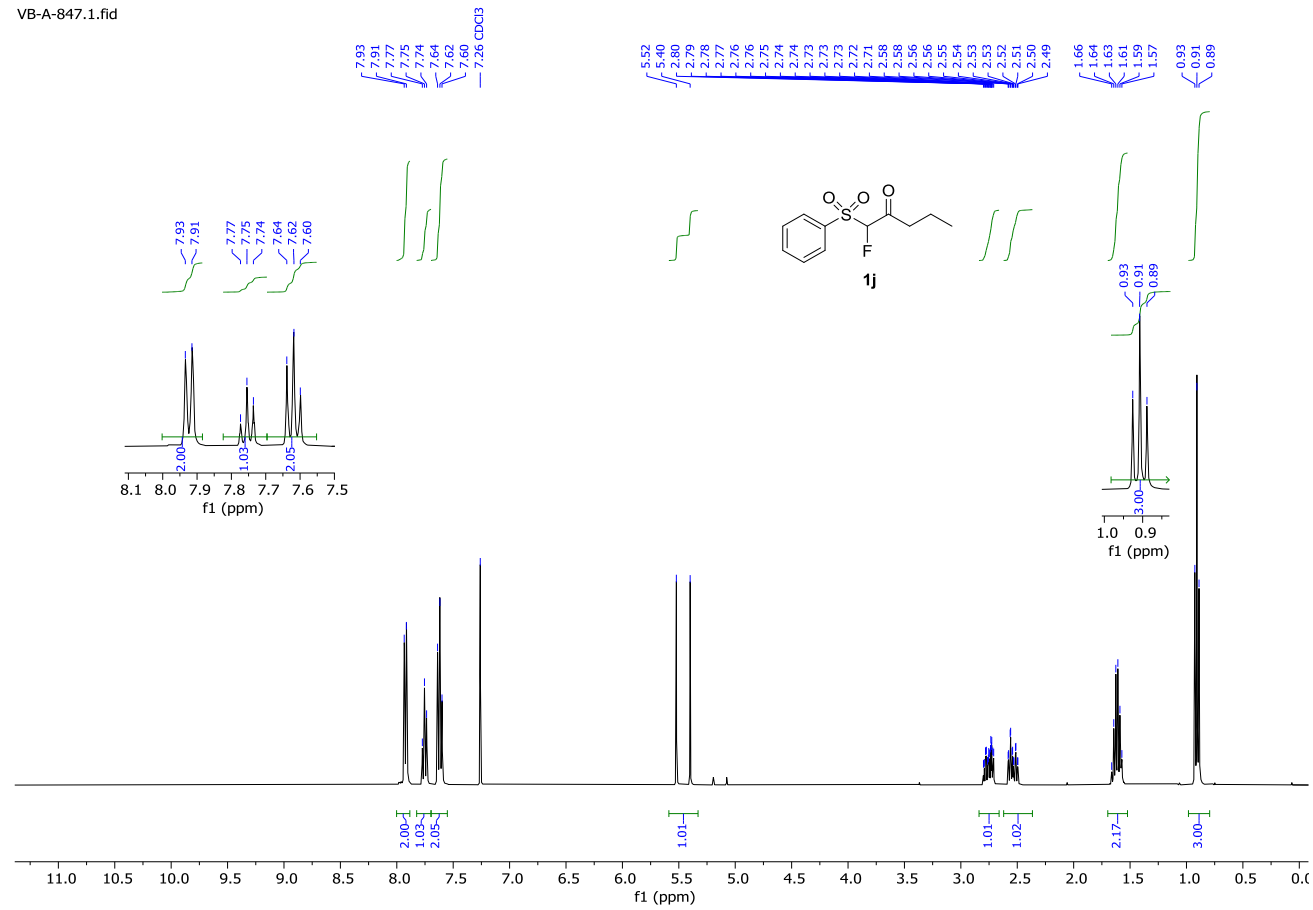


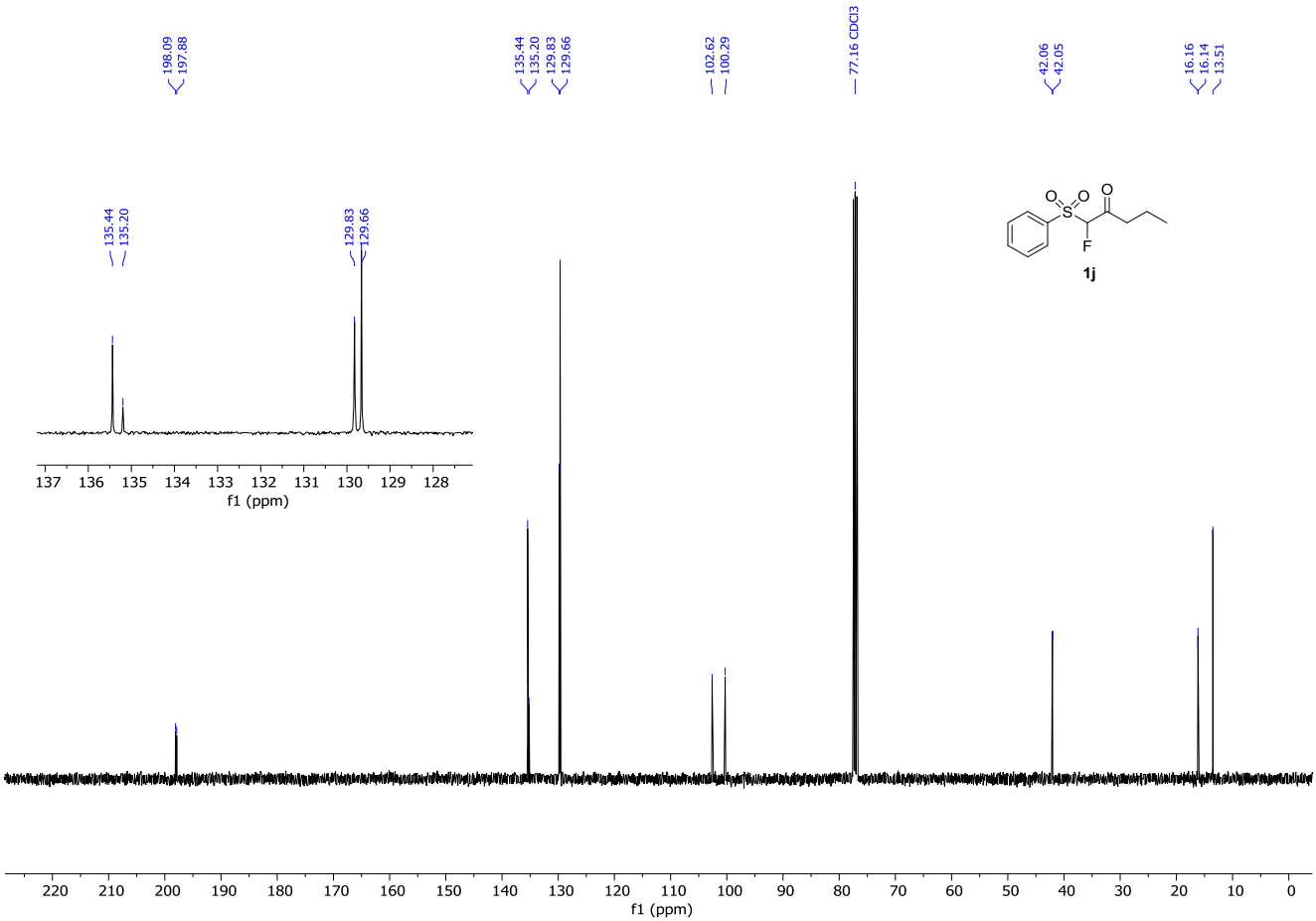
^{13}C NMR (101 MHz, $CDCl_3$)



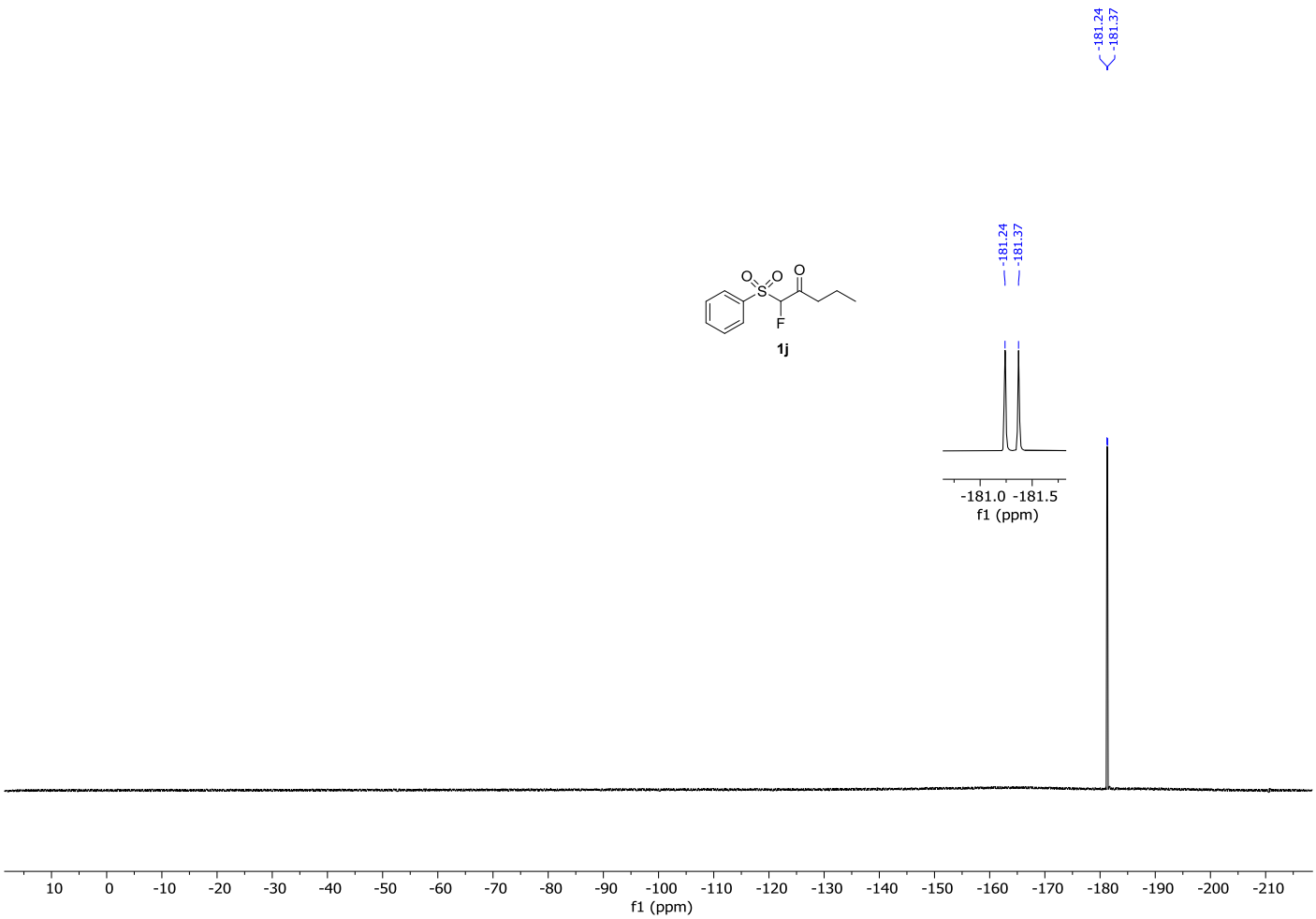
^{19}F NMR (376 MHz, $CDCl_3$)

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





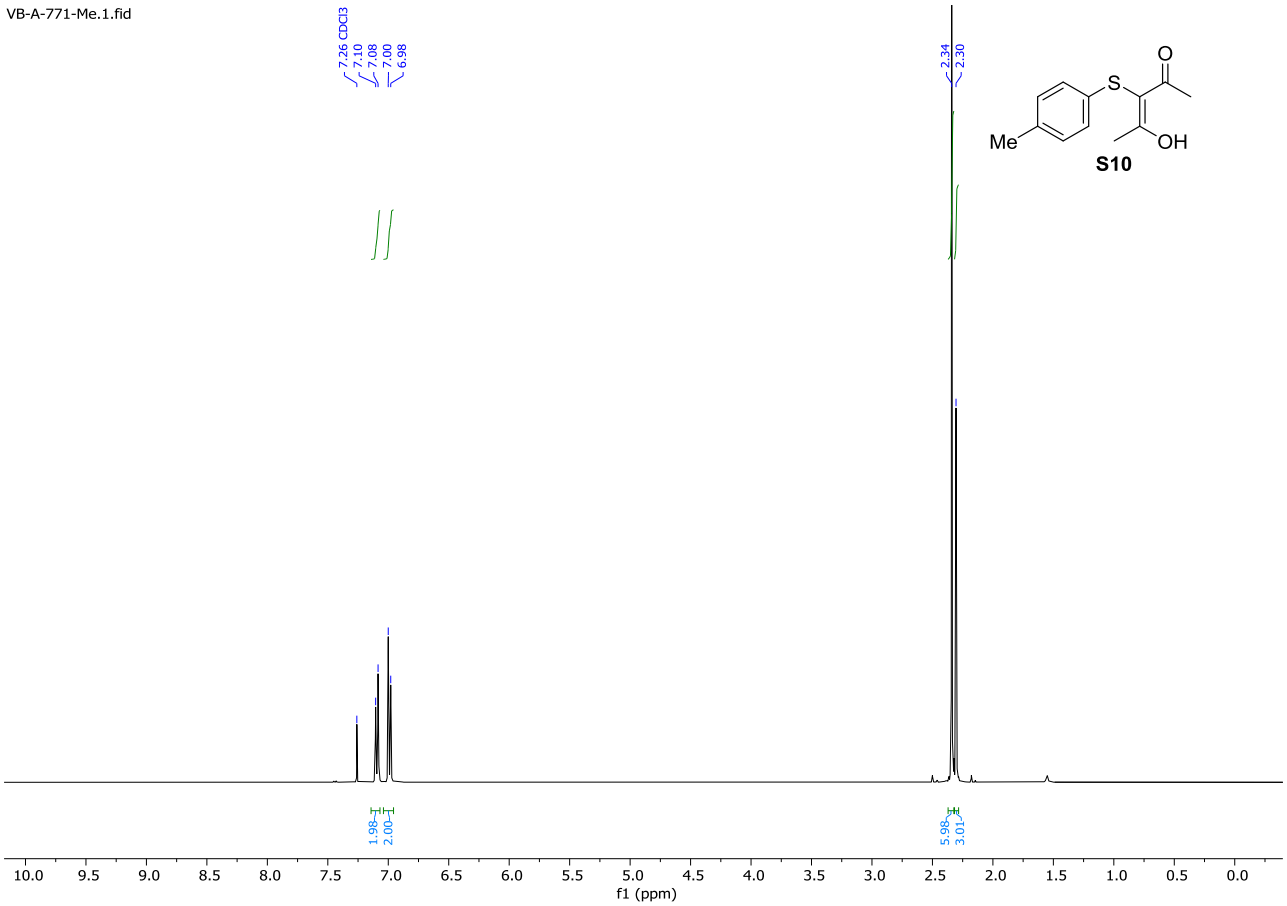
^{13}C NMR (101 MHz, $CDCl_3$)

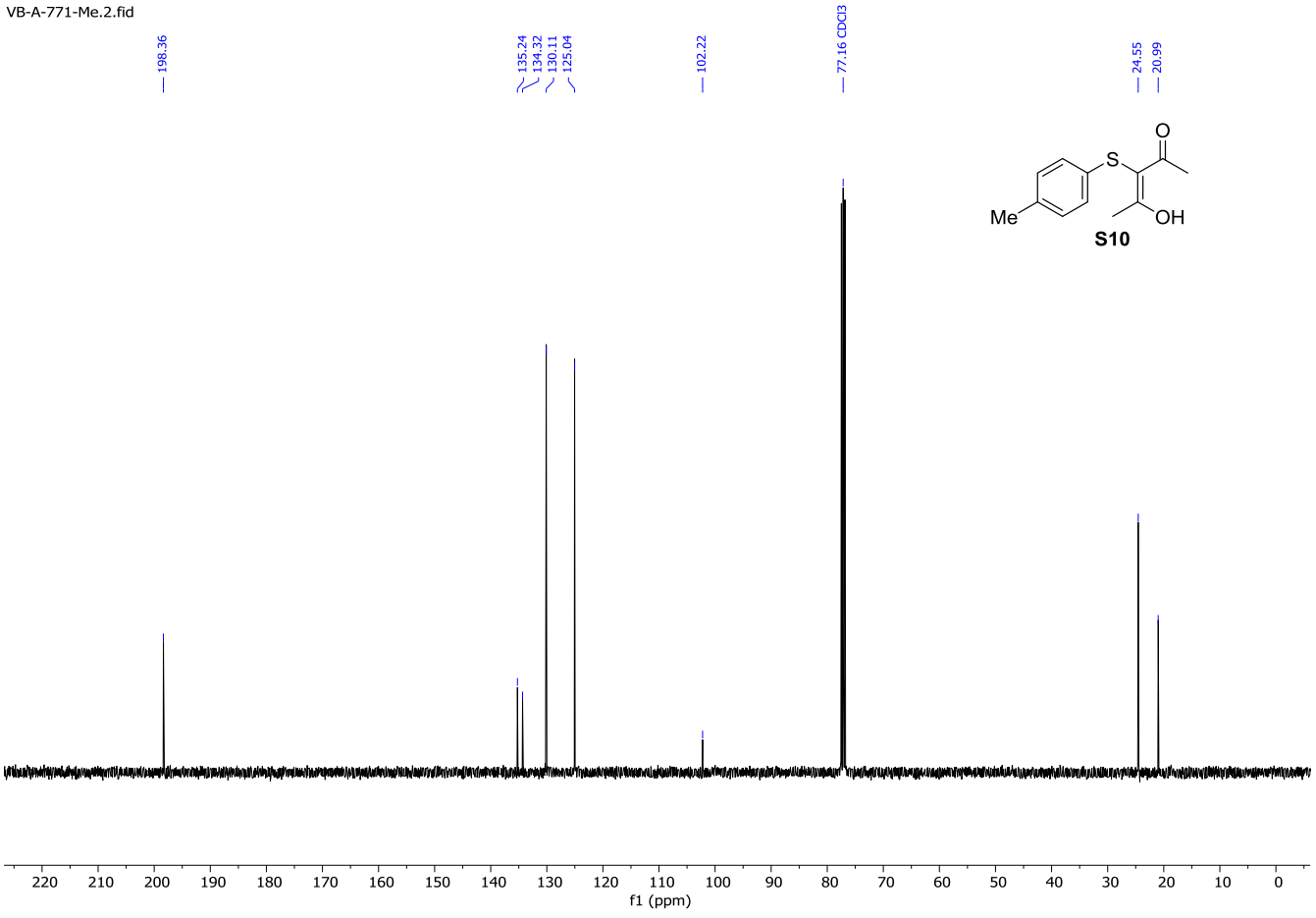


1j

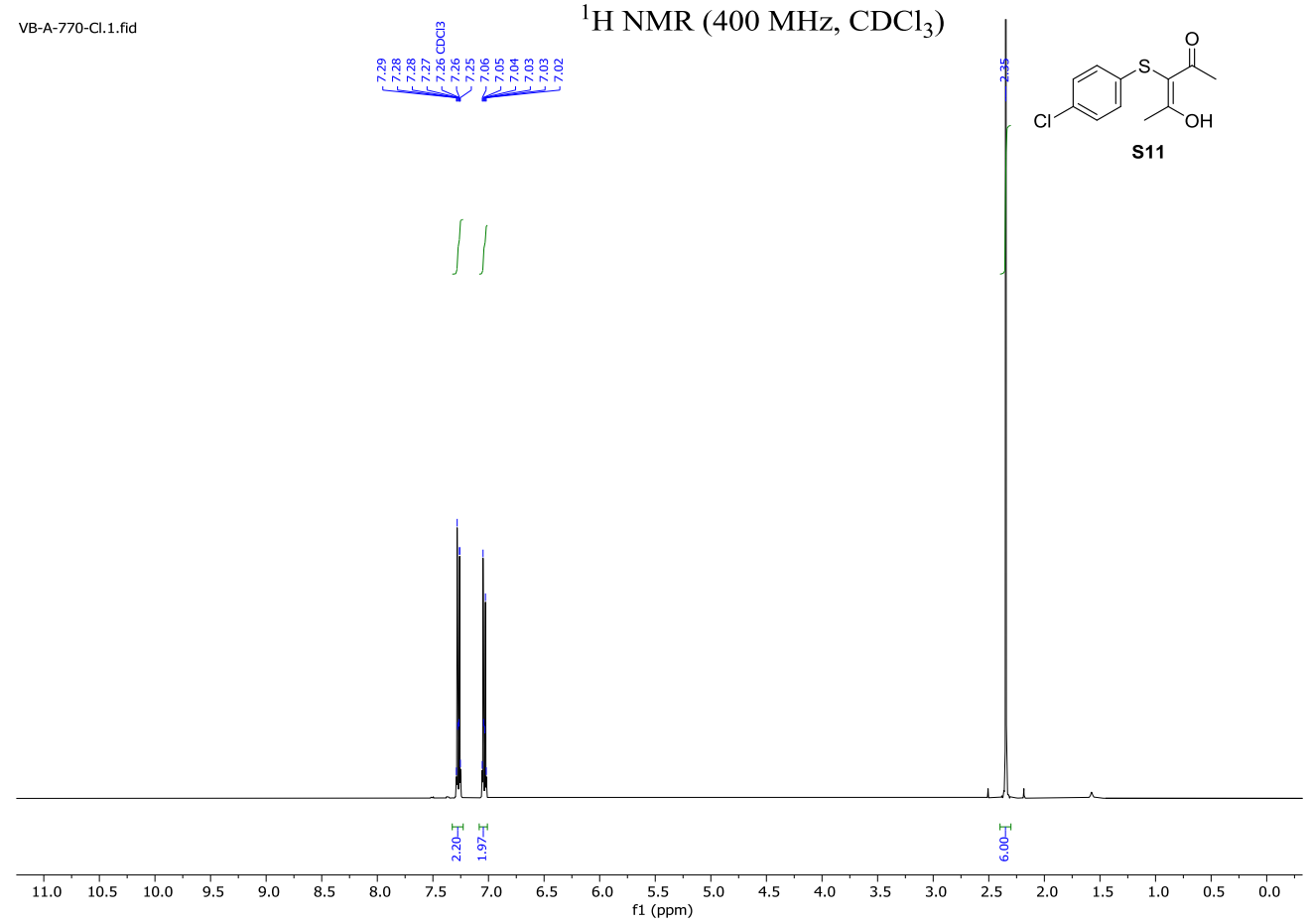
^{19}F NMR (376 MHz, $CDCl_3$)

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

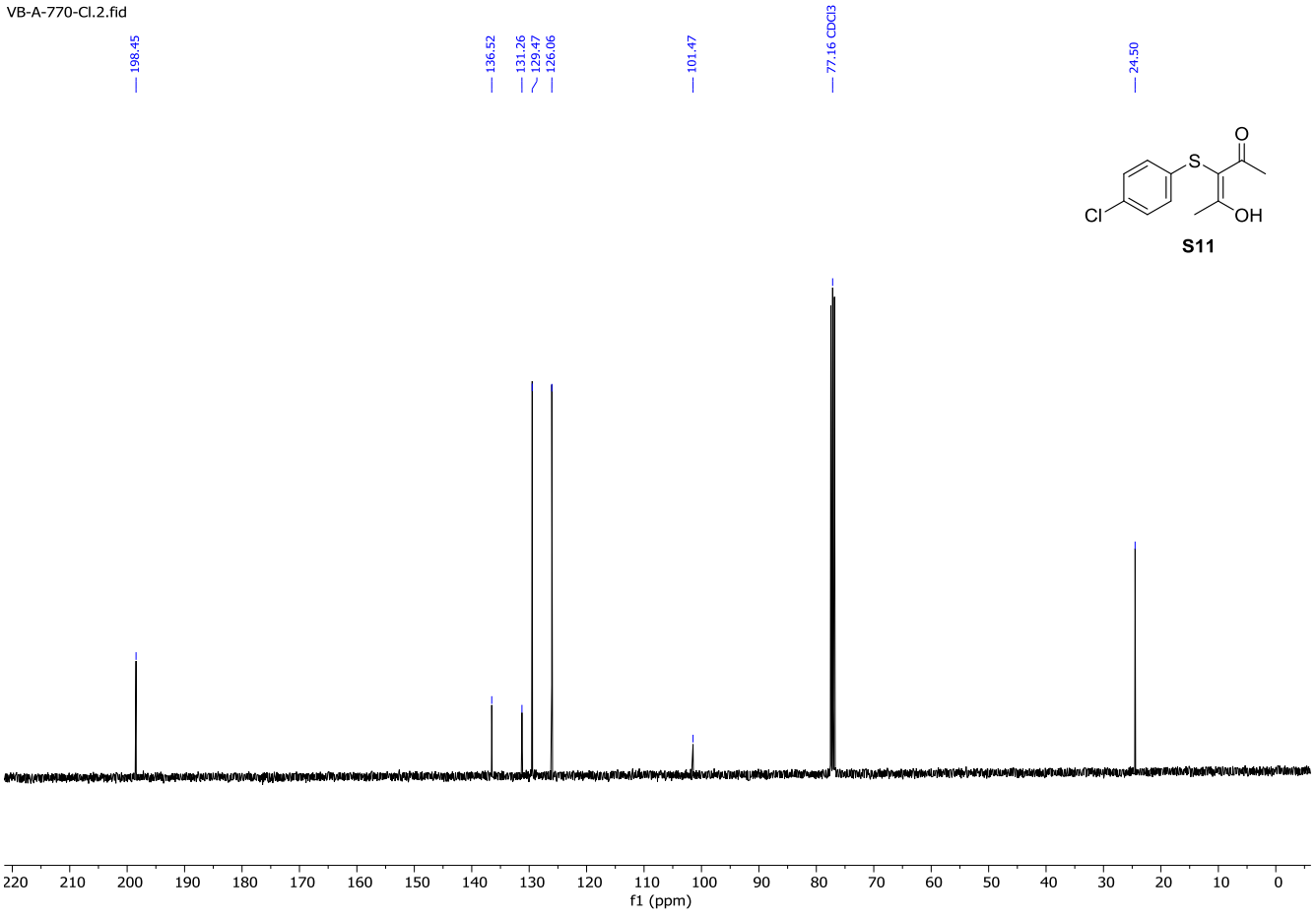




^{1}H NMR (400 MHz, $CDCl_3$)



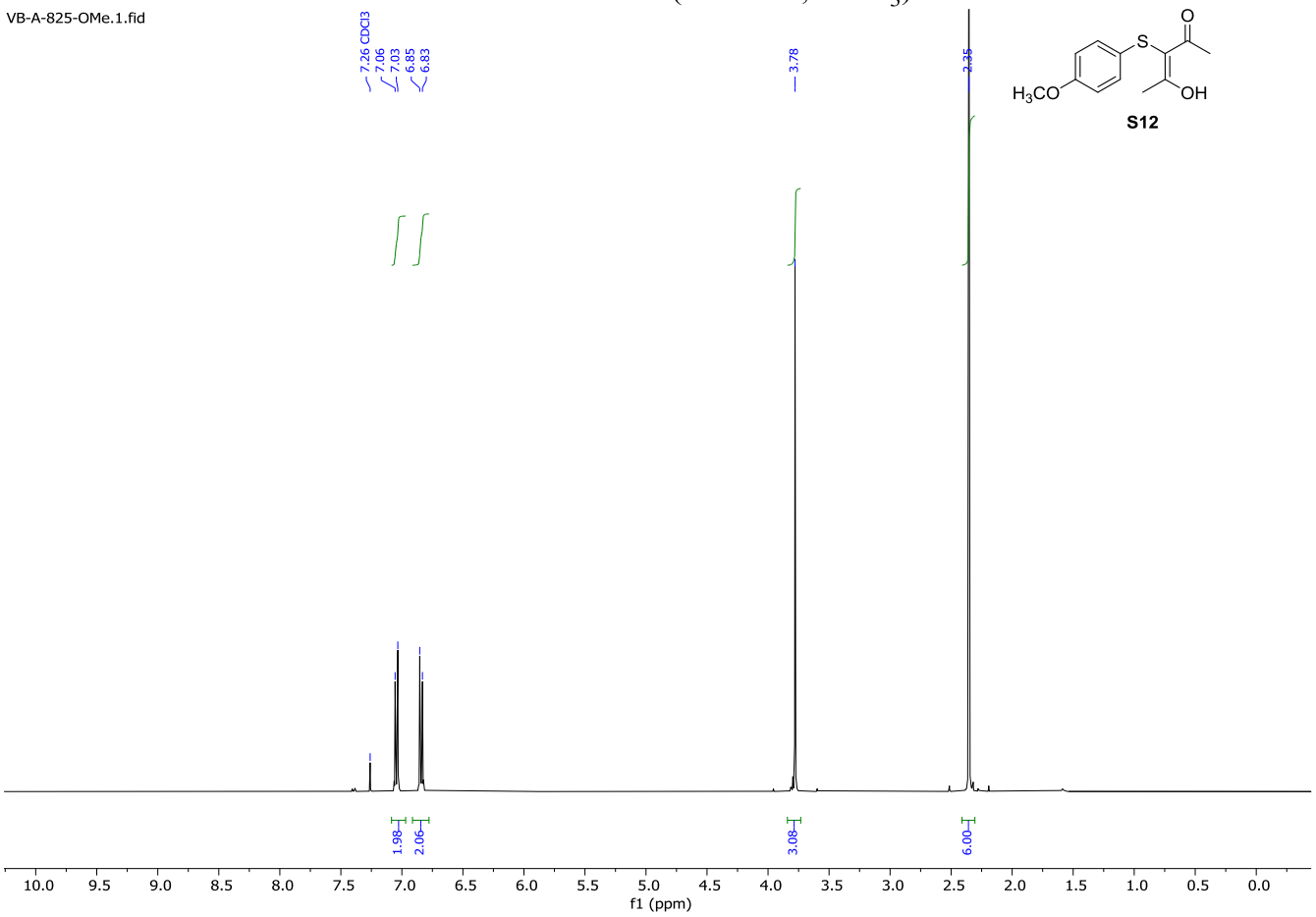
S11

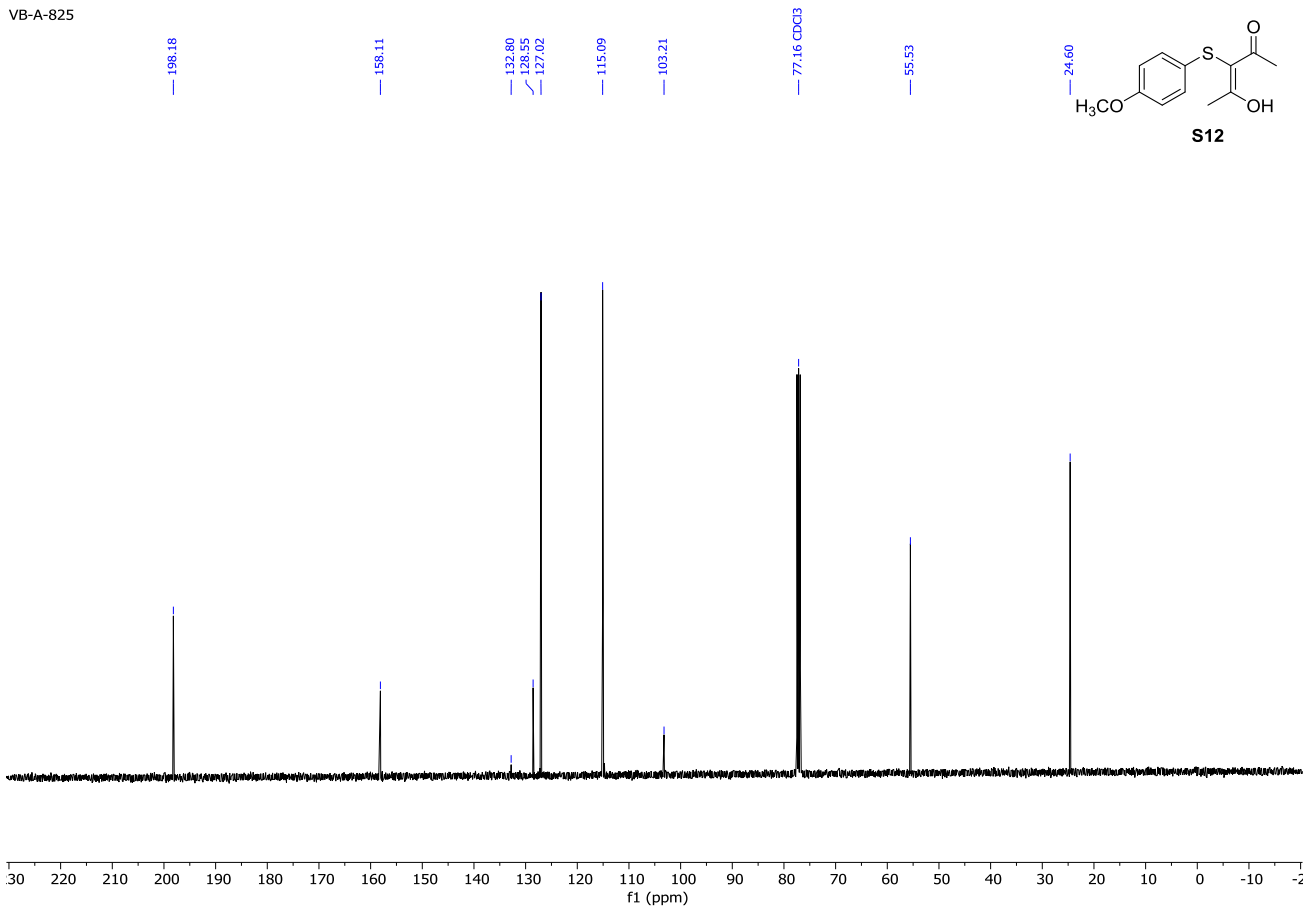


S11

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

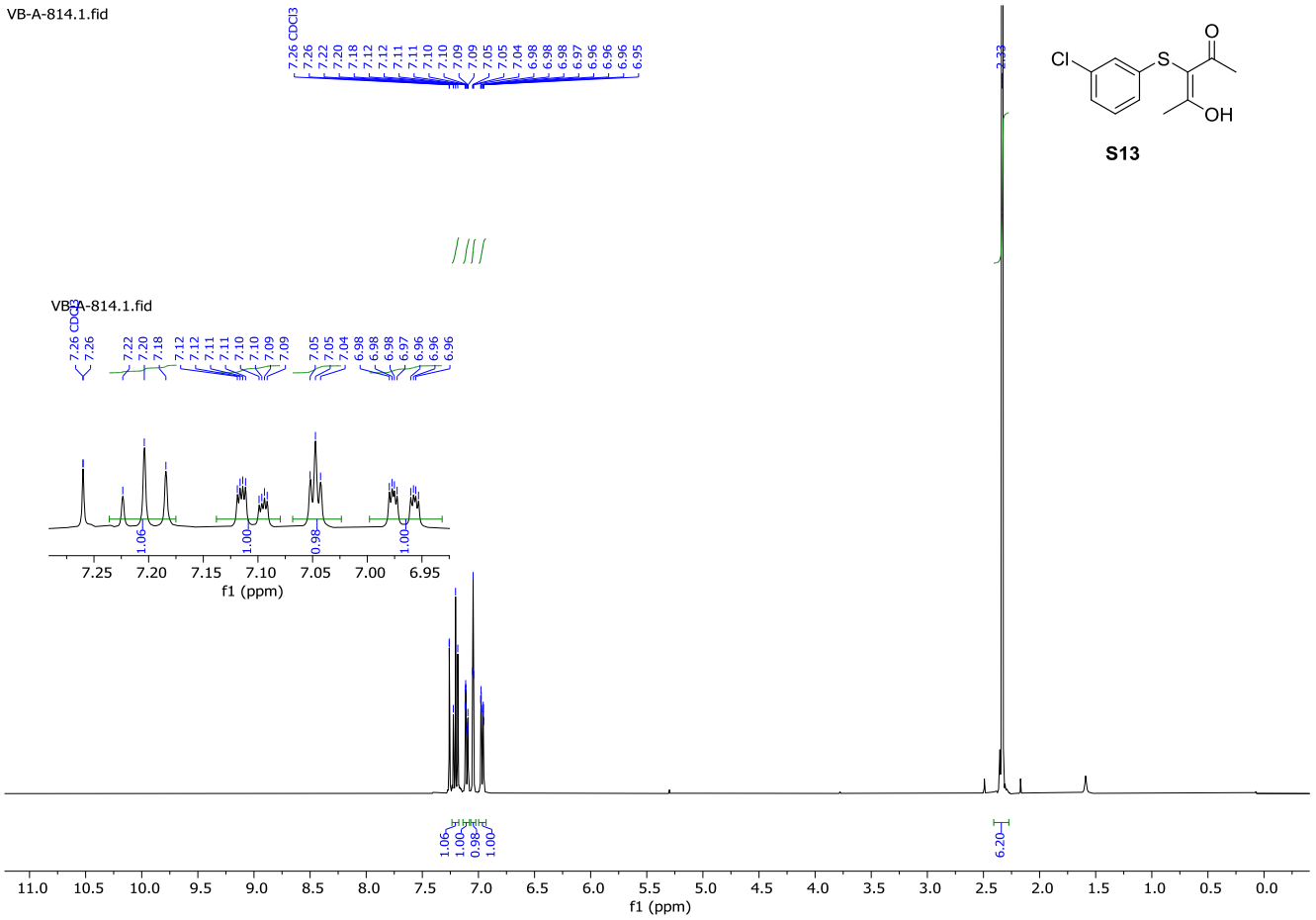
^{1}H NMR (400 MHz, $CDCl_3$)

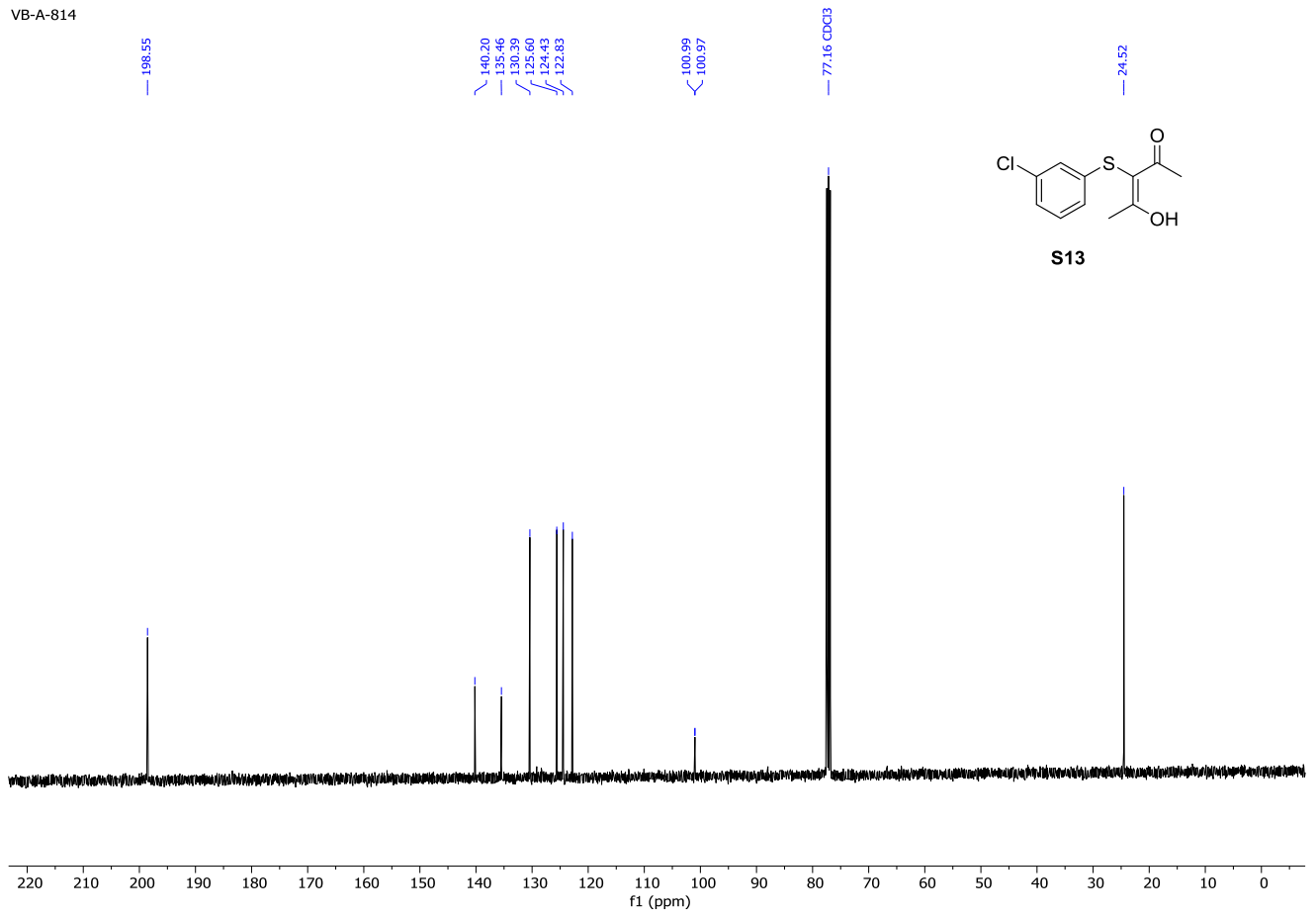




^{13}C NMR (101 MHz, $CDCl_3$)

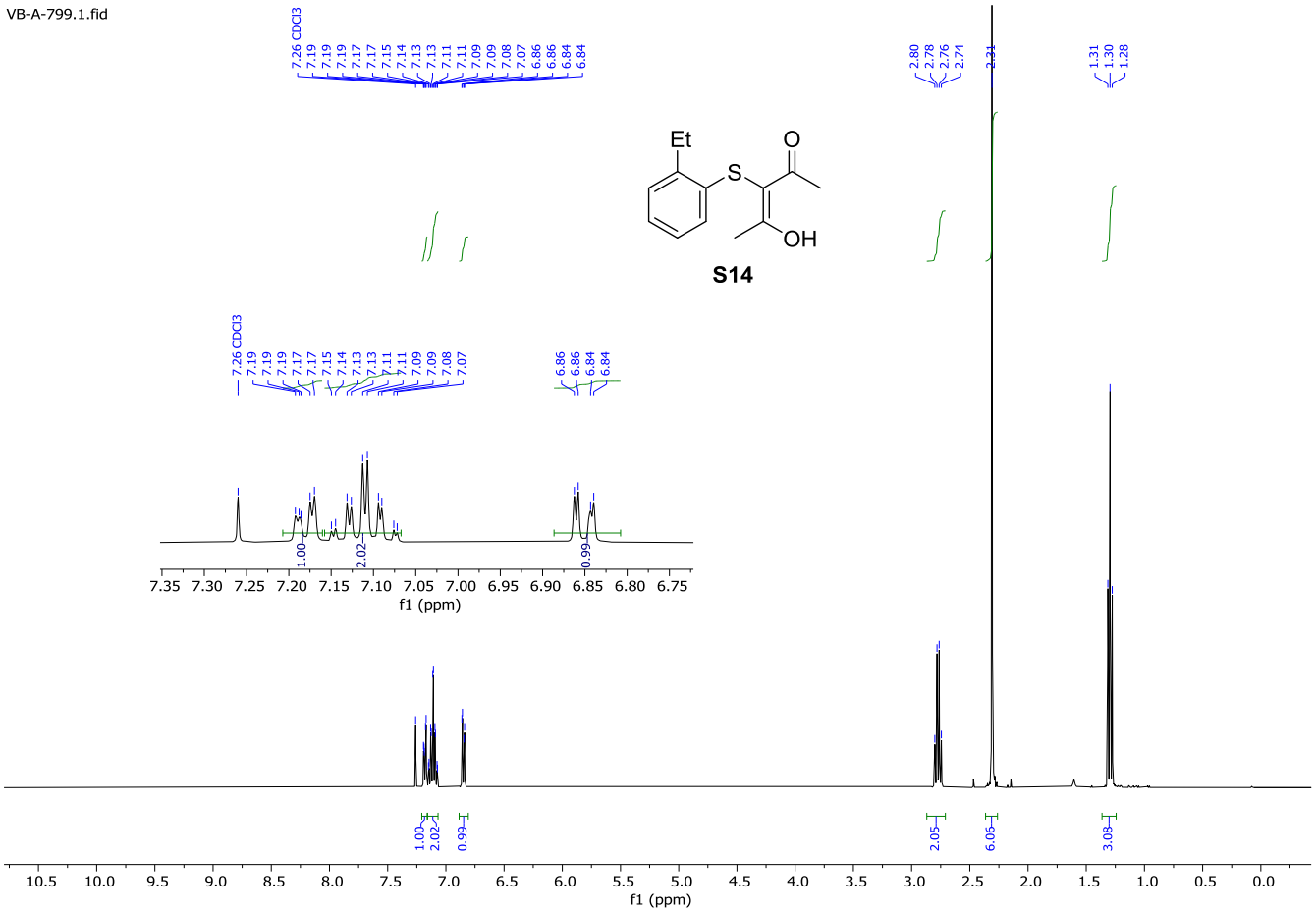
^{1}H NMR (400 MHz, $CDCl_3$)

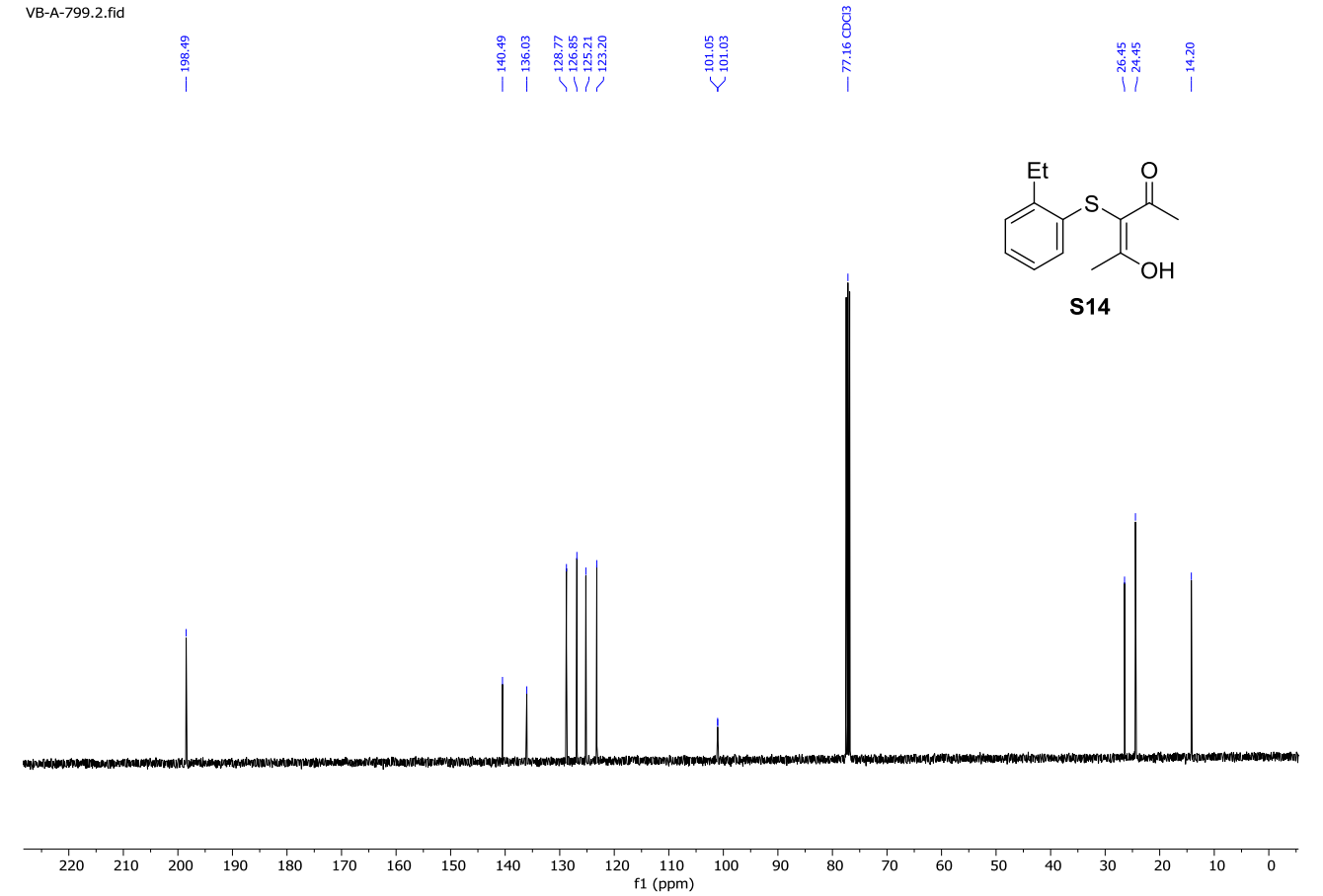




^{13}C NMR (101 MHz, $CDCl_3$)

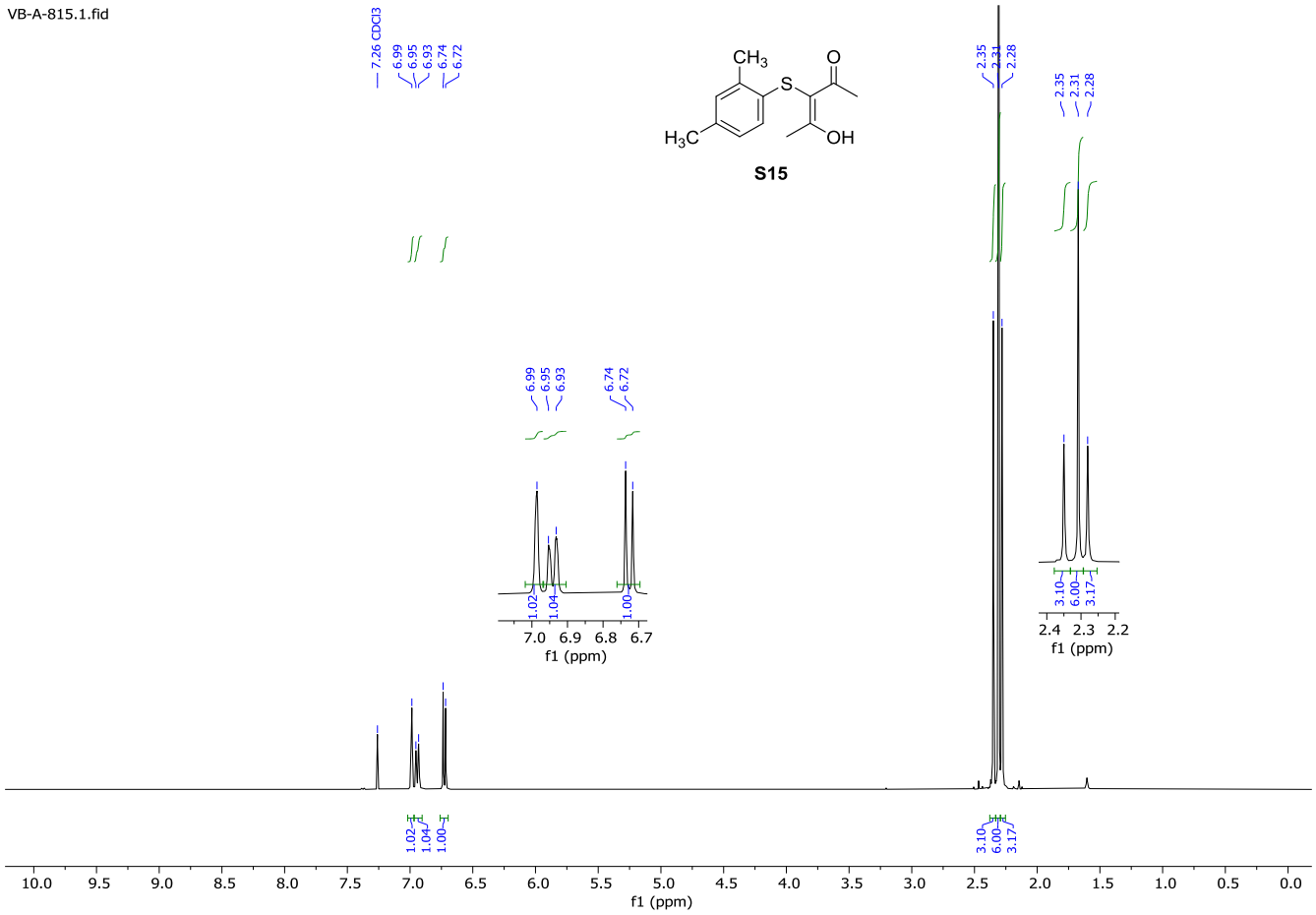
^{1}H NMR (400 MHz, $CDCl_3$)

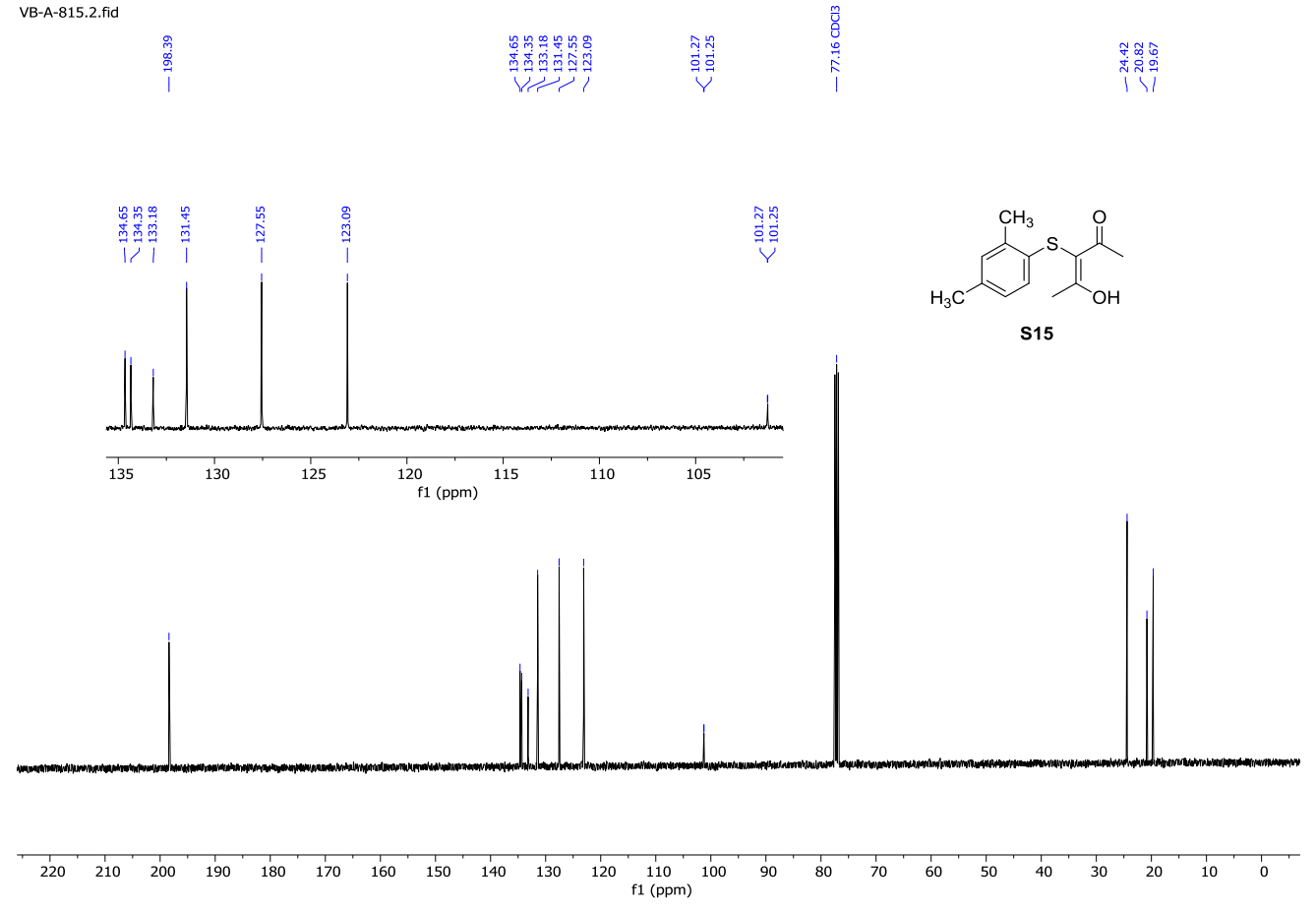




^{13}C NMR (101 MHz, $CDCl_3$)

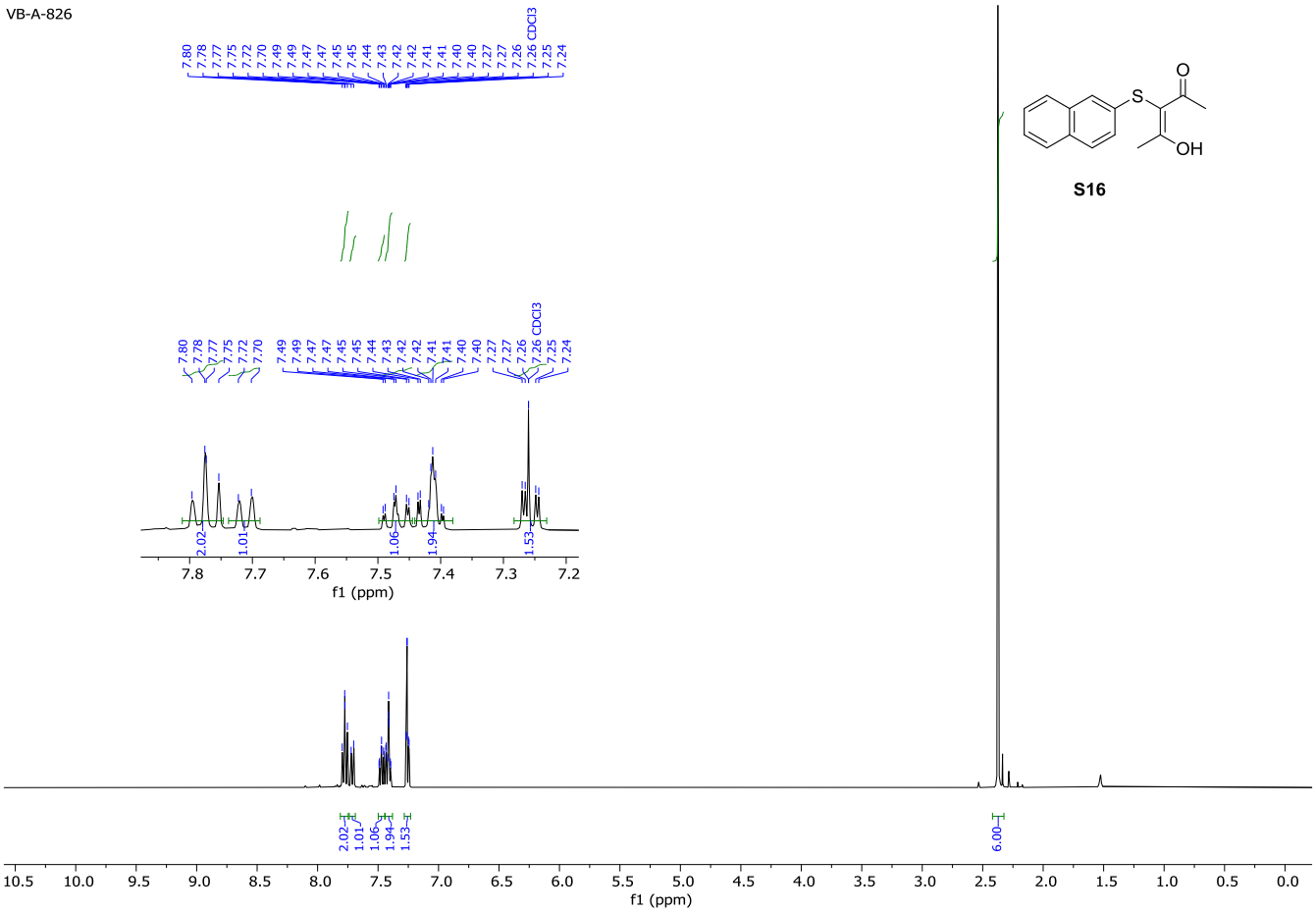
^{1}H NMR (400 MHz, $CDCl_3$)

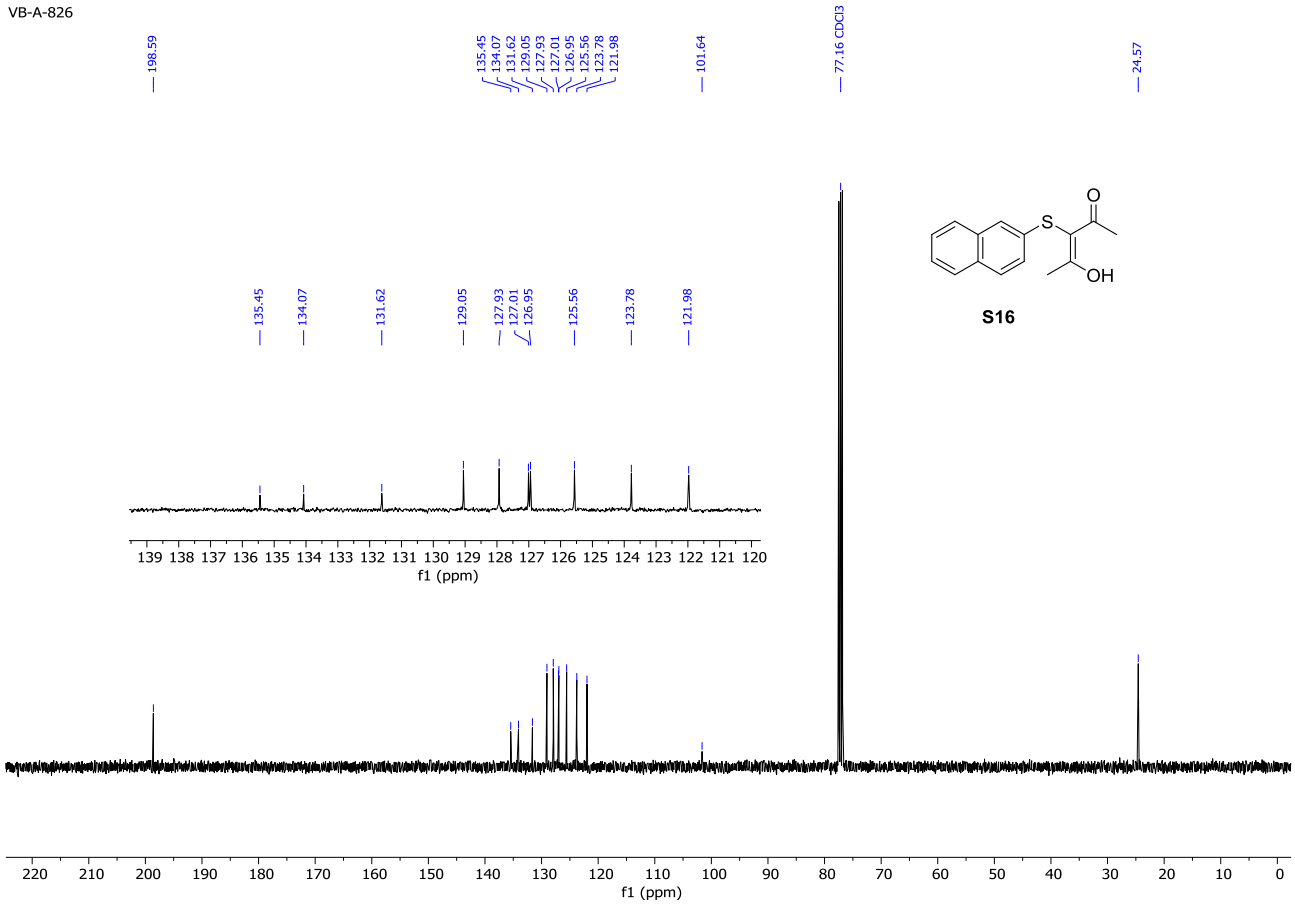




^{13}C NMR (101 MHz, $CDCl_3$)

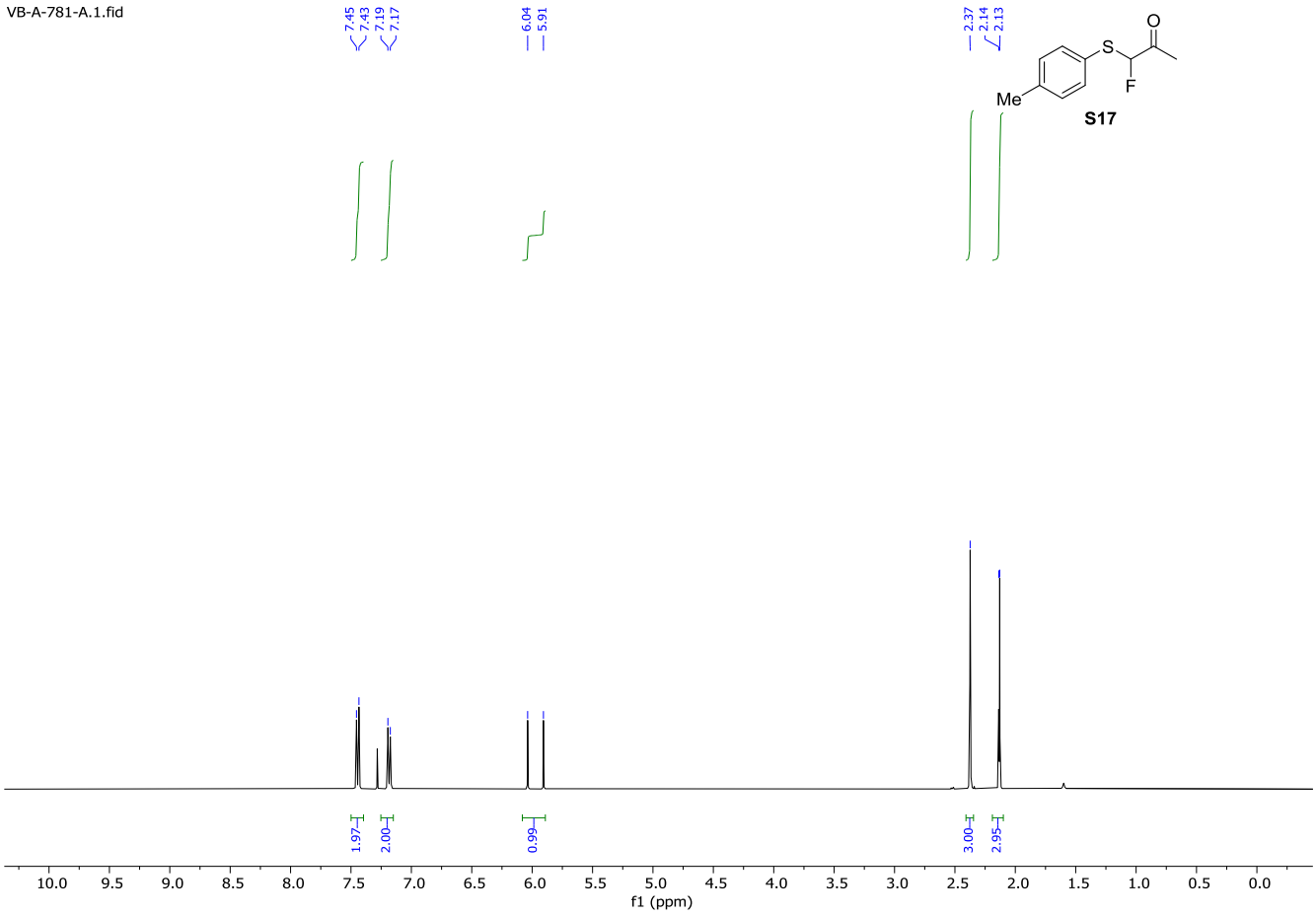
^{1}H NMR (400 MHz, $CDCl_3$)

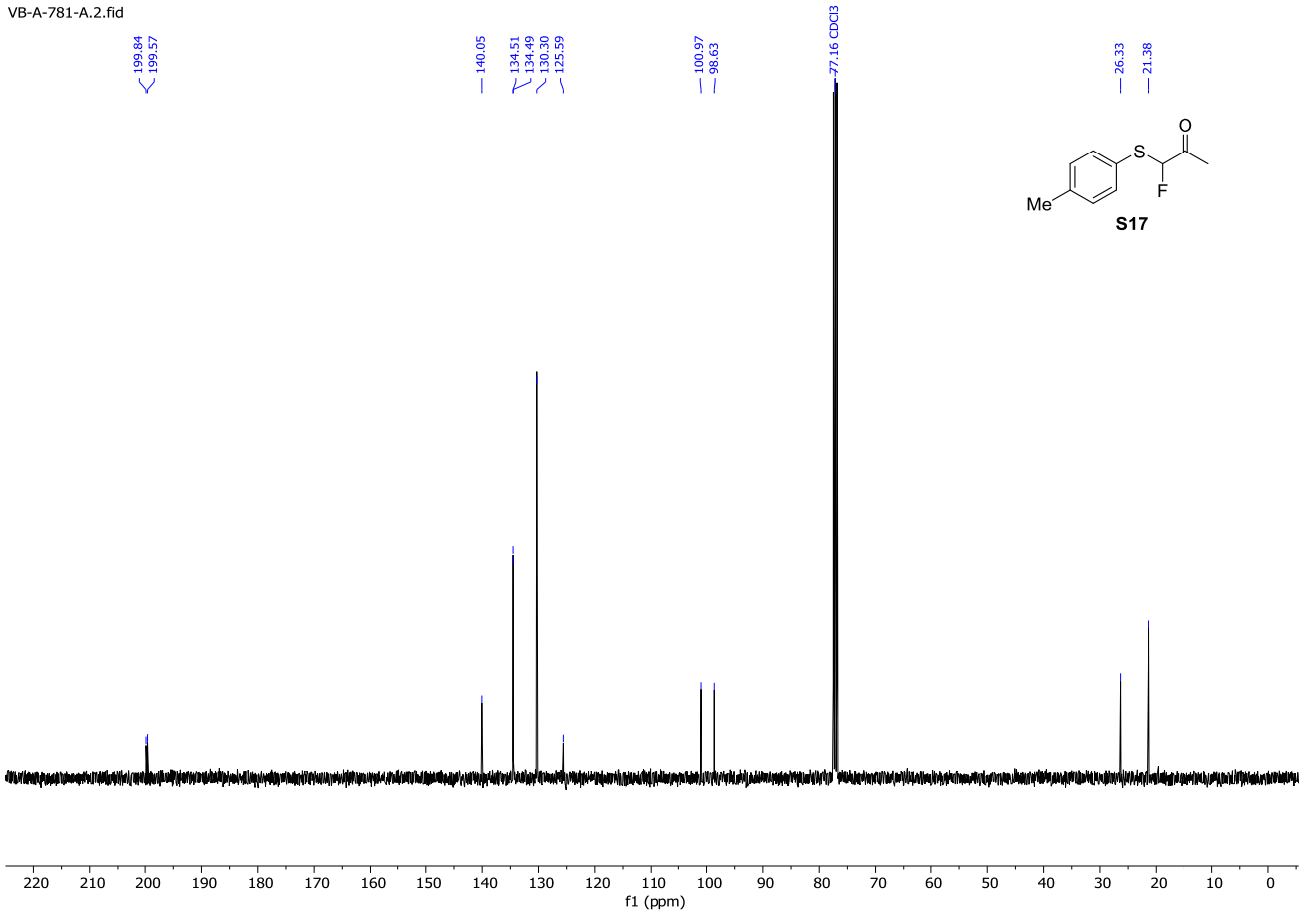




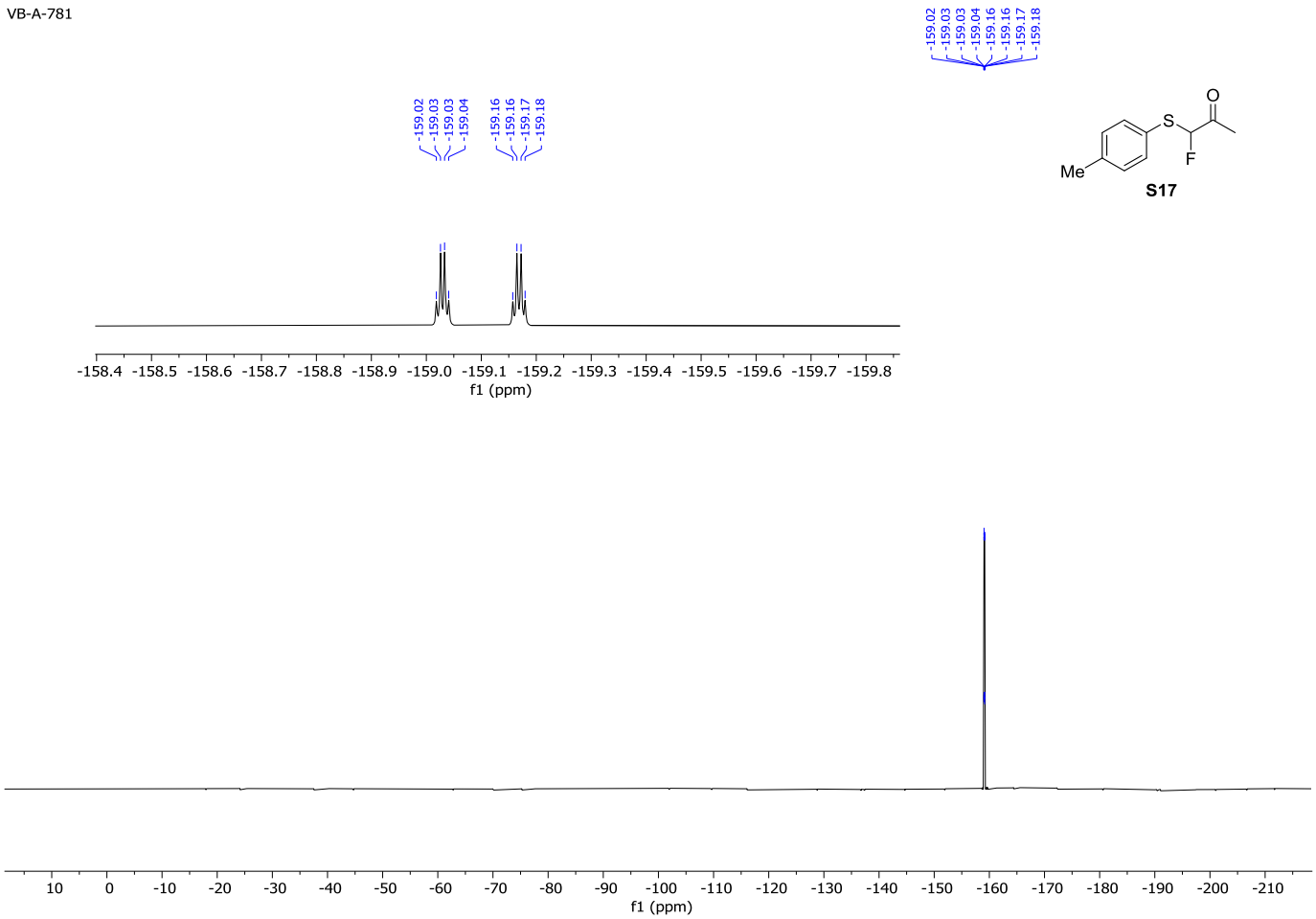
^{13}C NMR (101 MHz, $CDCl_3$)

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



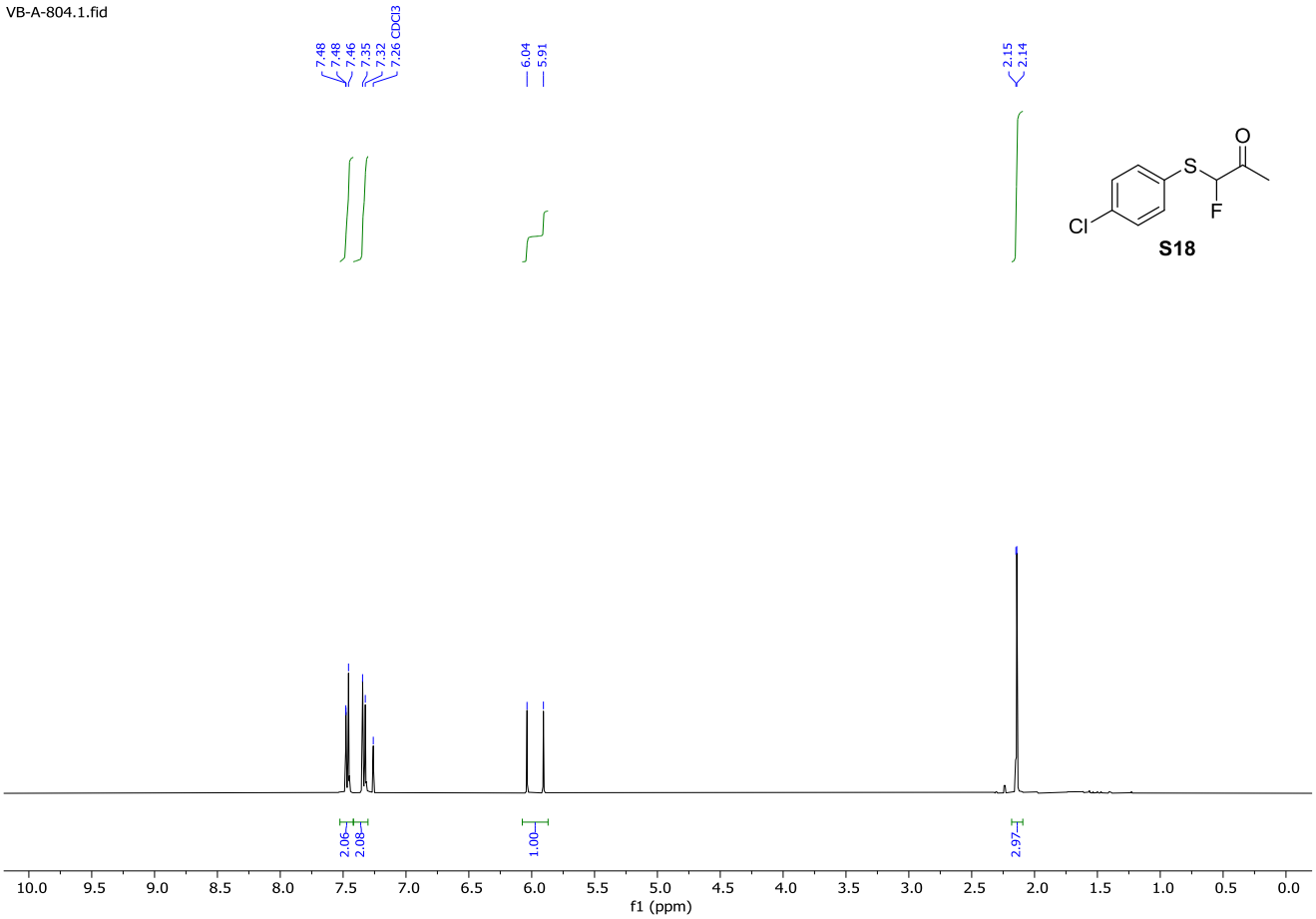


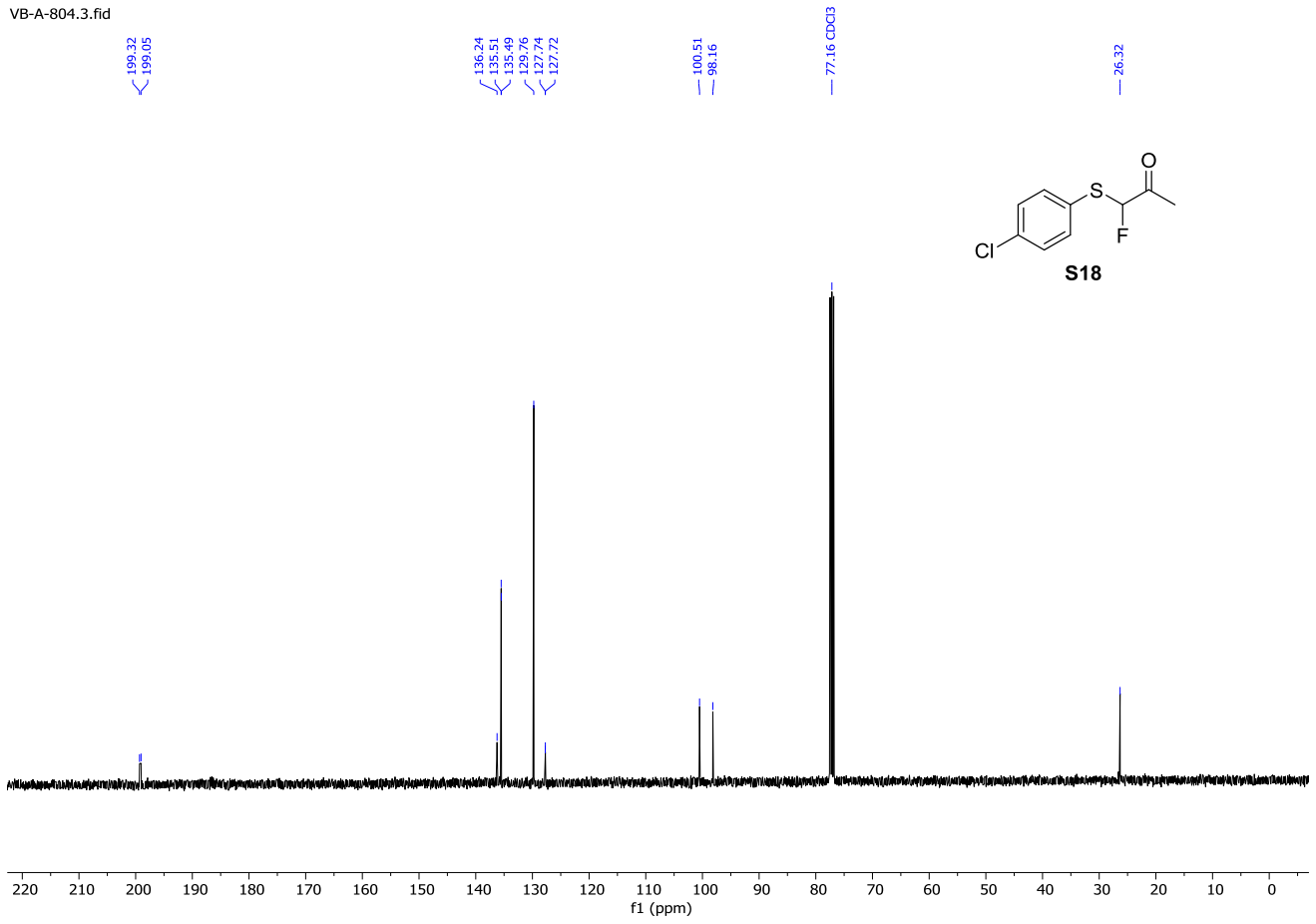
^{13}C NMR (101 MHz, $CDCl_3$)



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

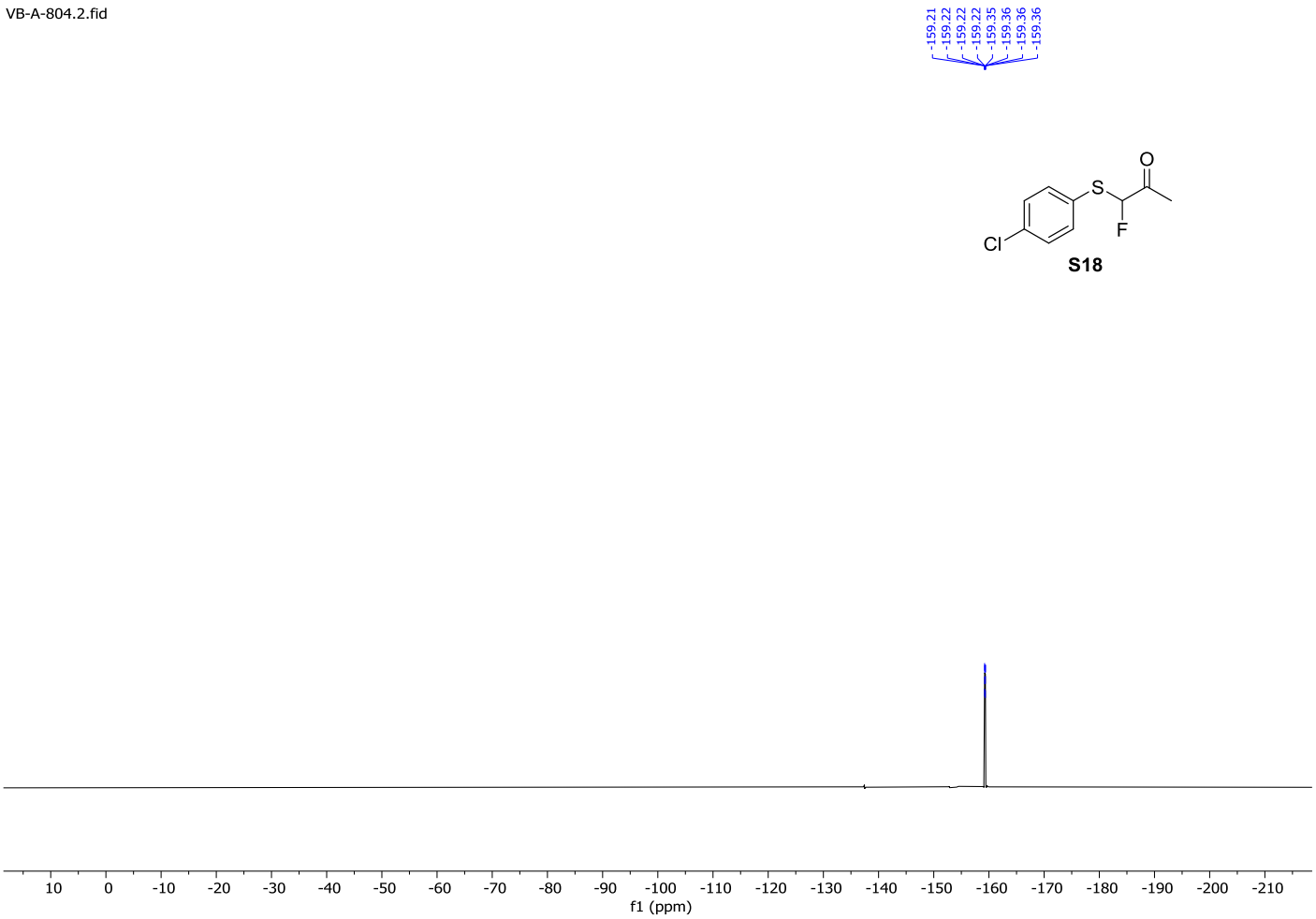
^{1}H NMR (400 MHz, $CDCl_3$)





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

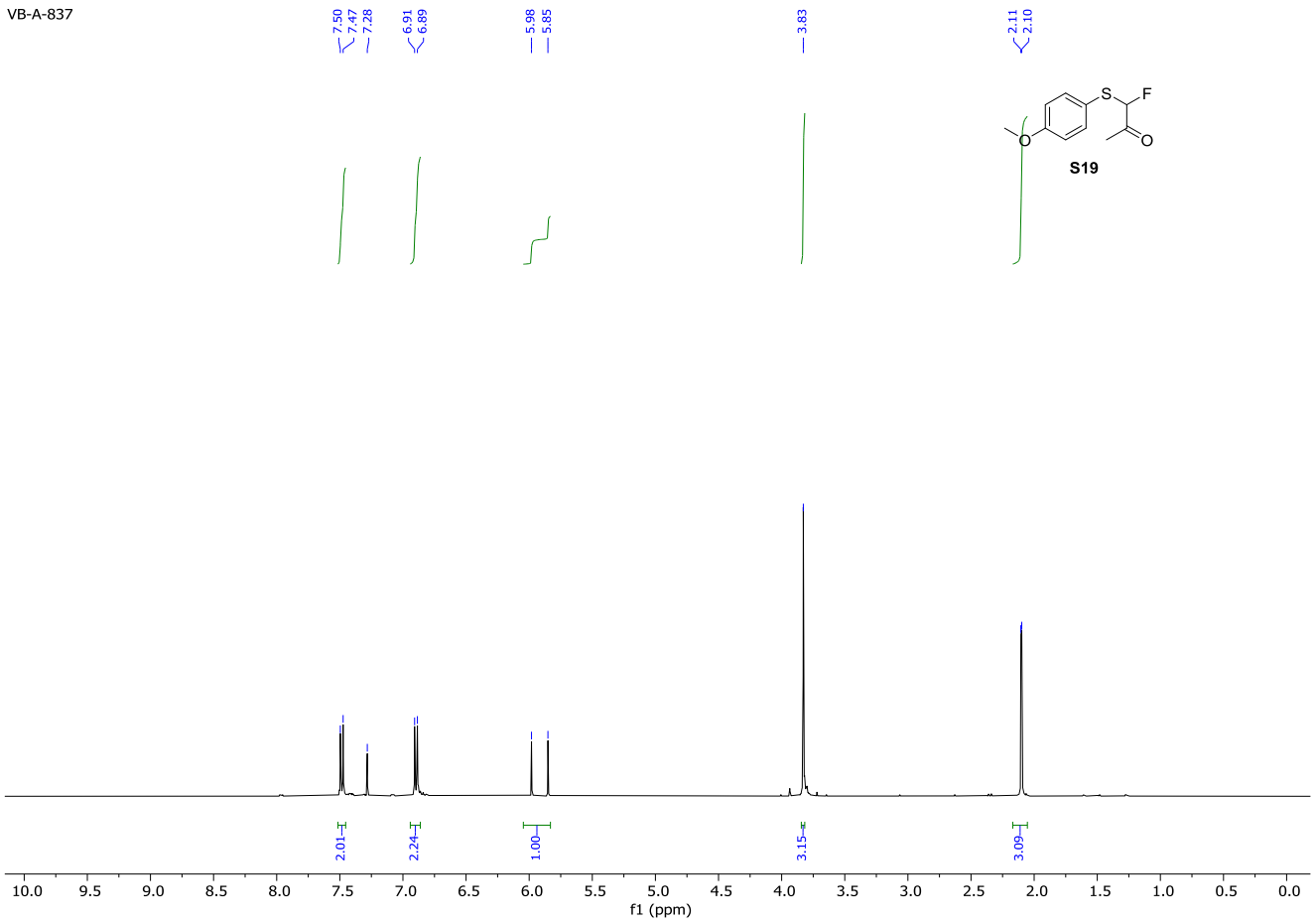
VB-A-804.2.fid

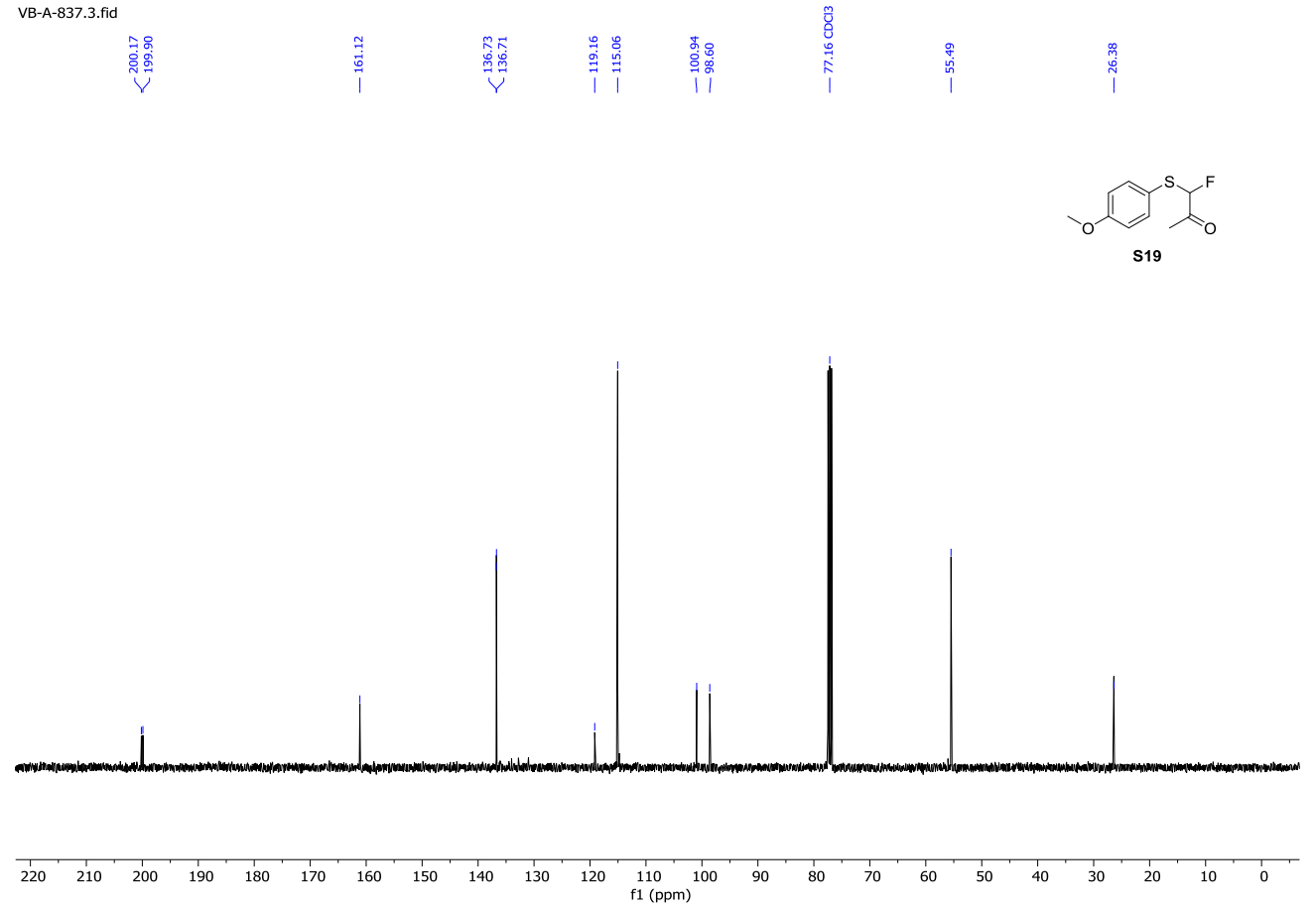


S18

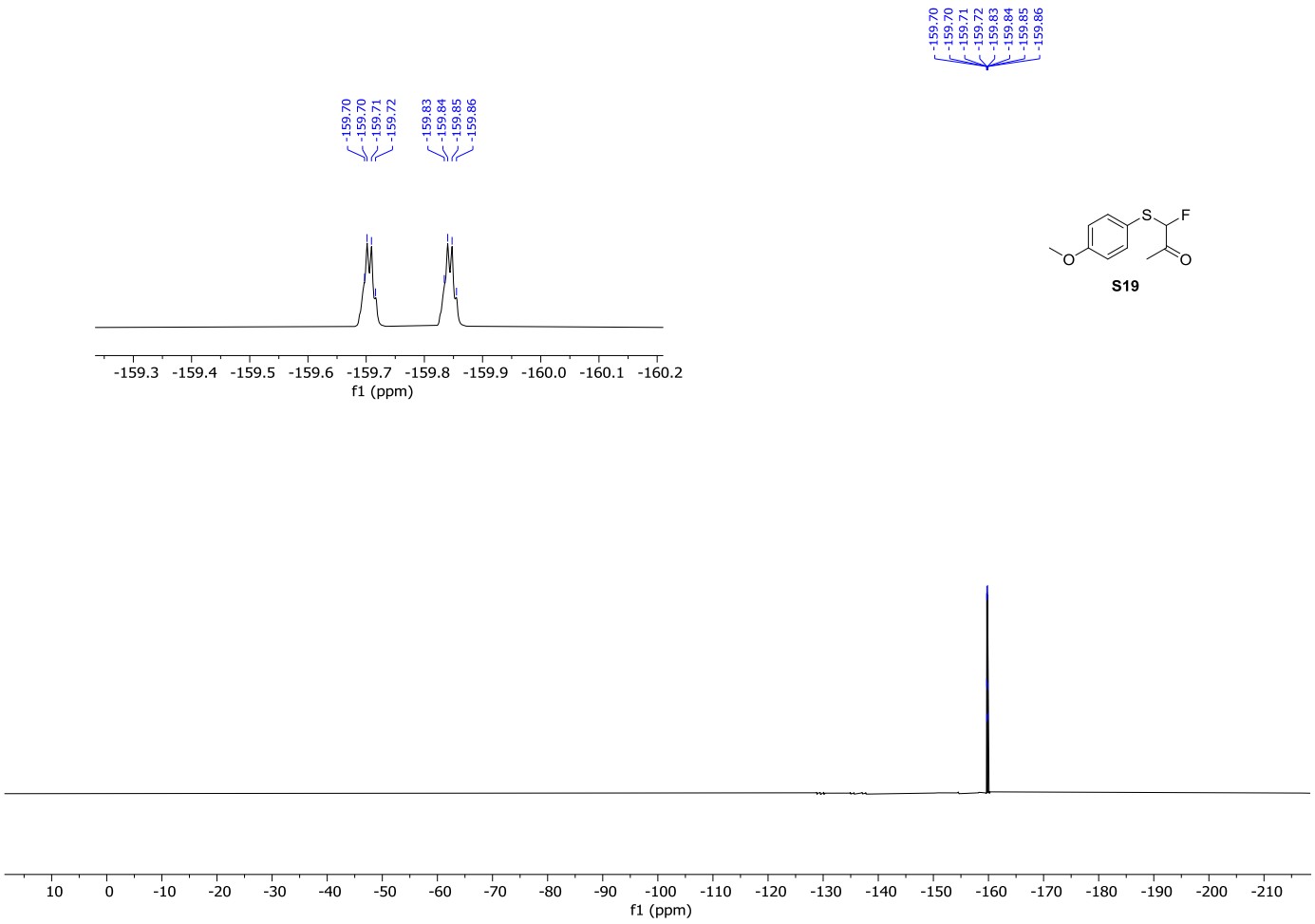
^{19}F NMR (376 MHz, $CDCl_3$)

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





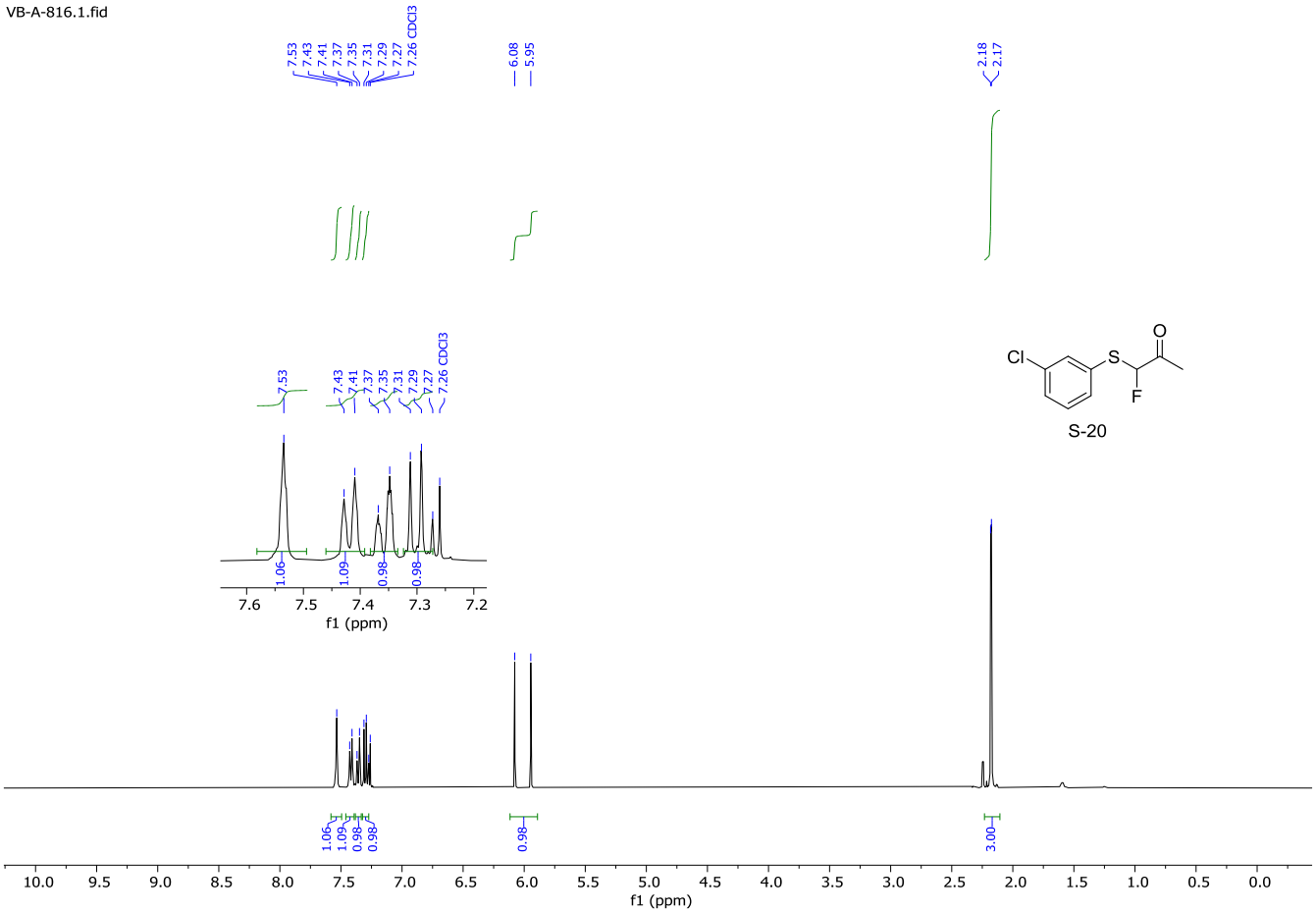
^{13}C NMR (101 MHz, $CDCl_3$)

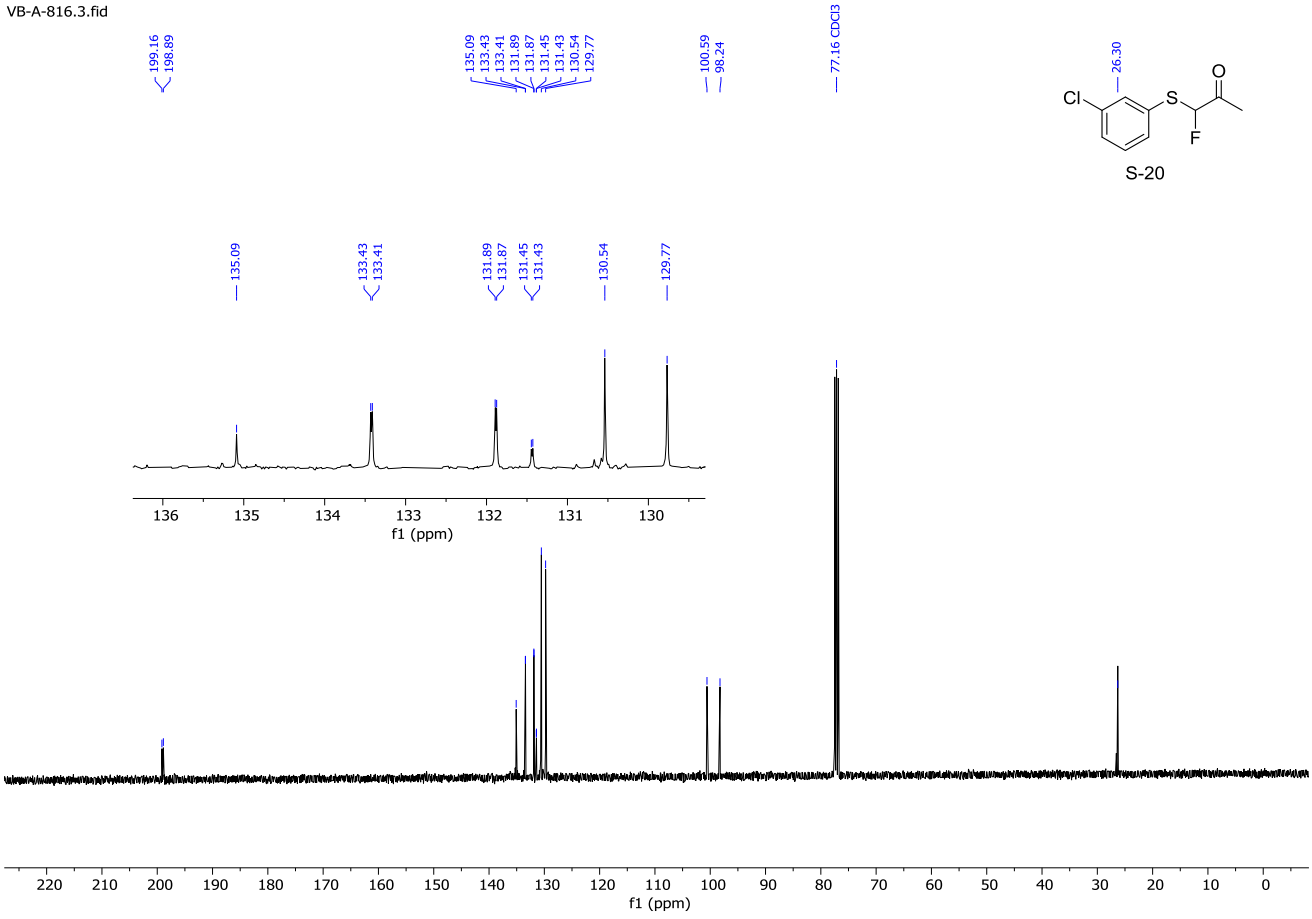


S19

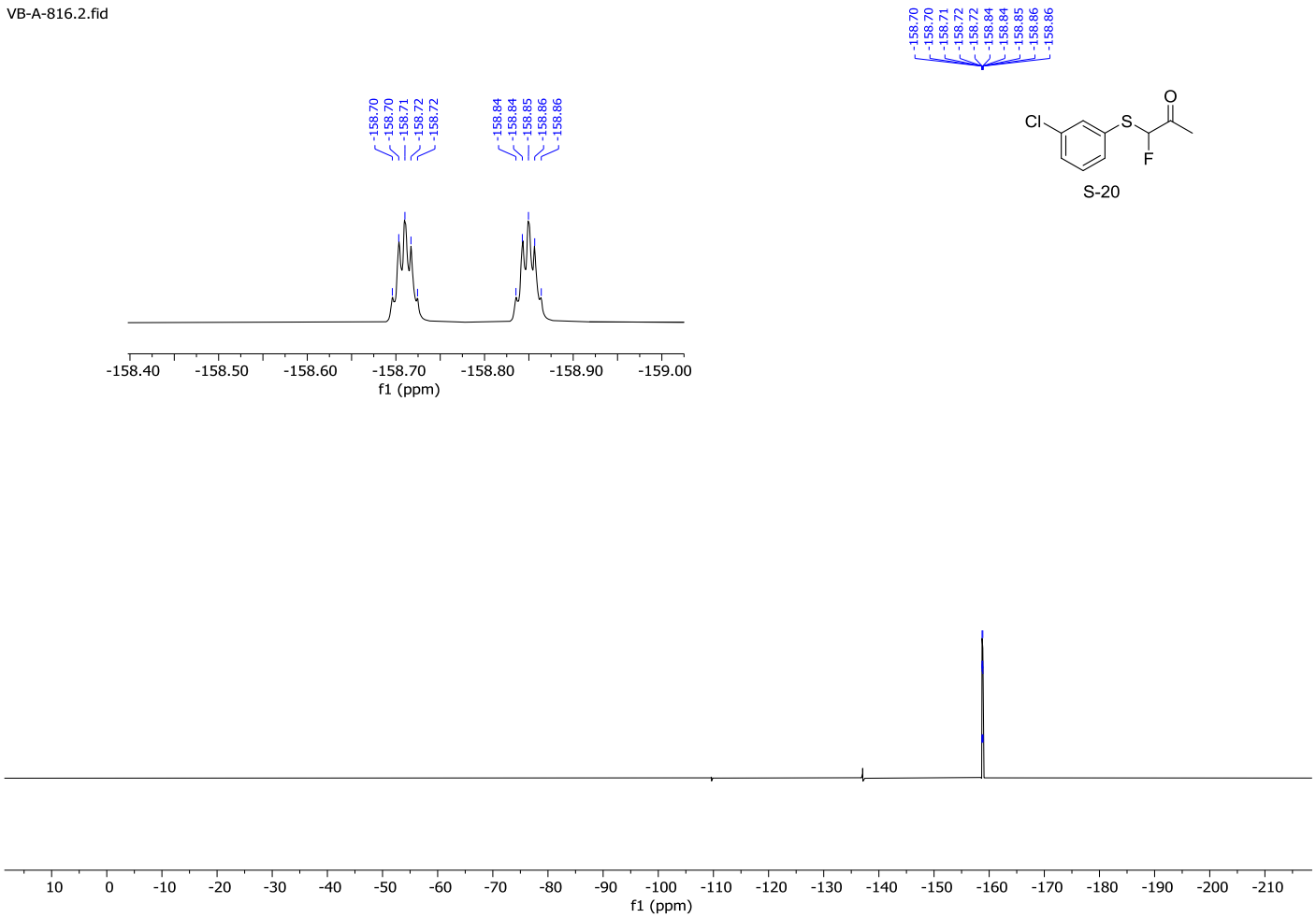
^{19}F NMR (376 MHz, $CDCl_3$)

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



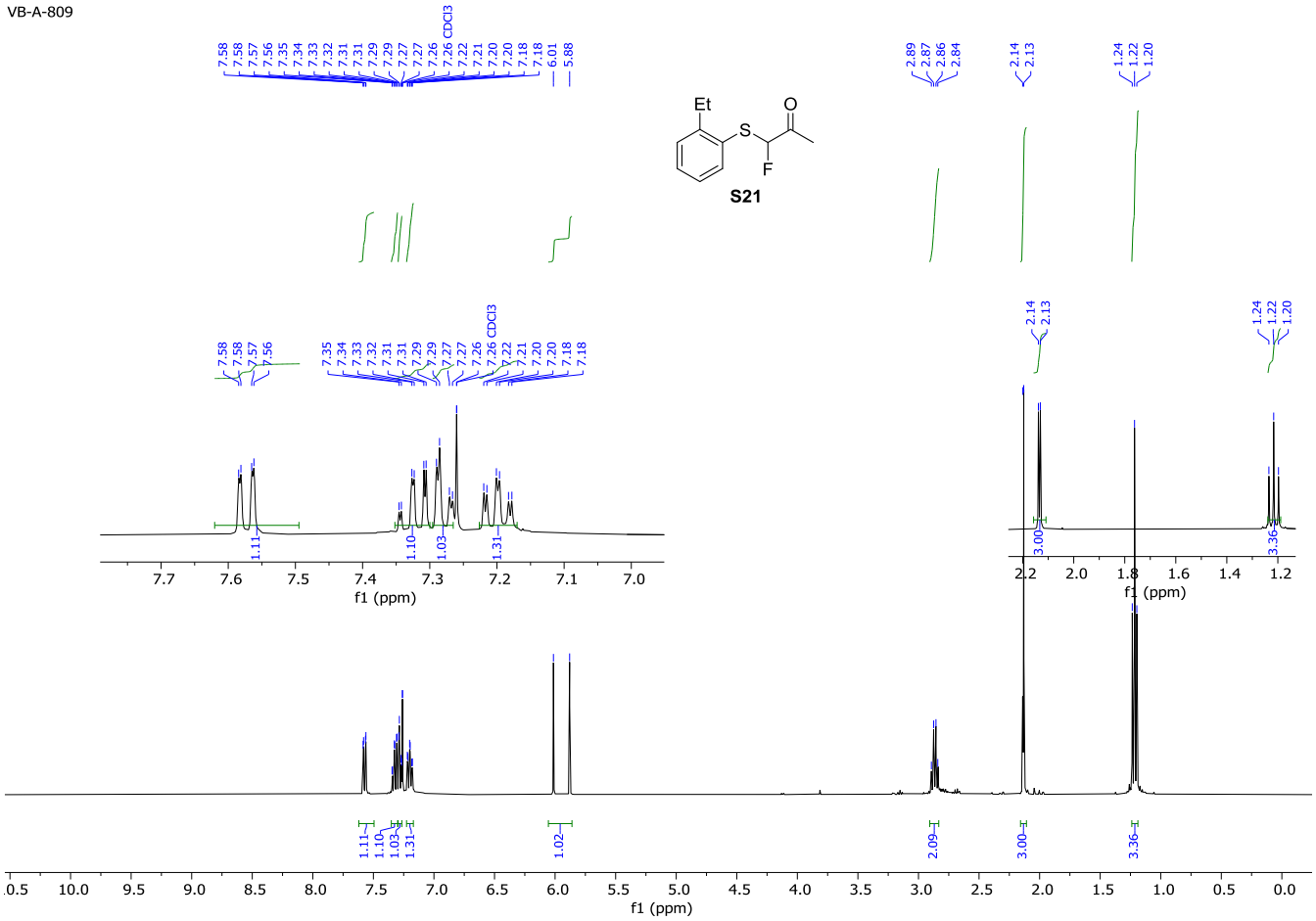


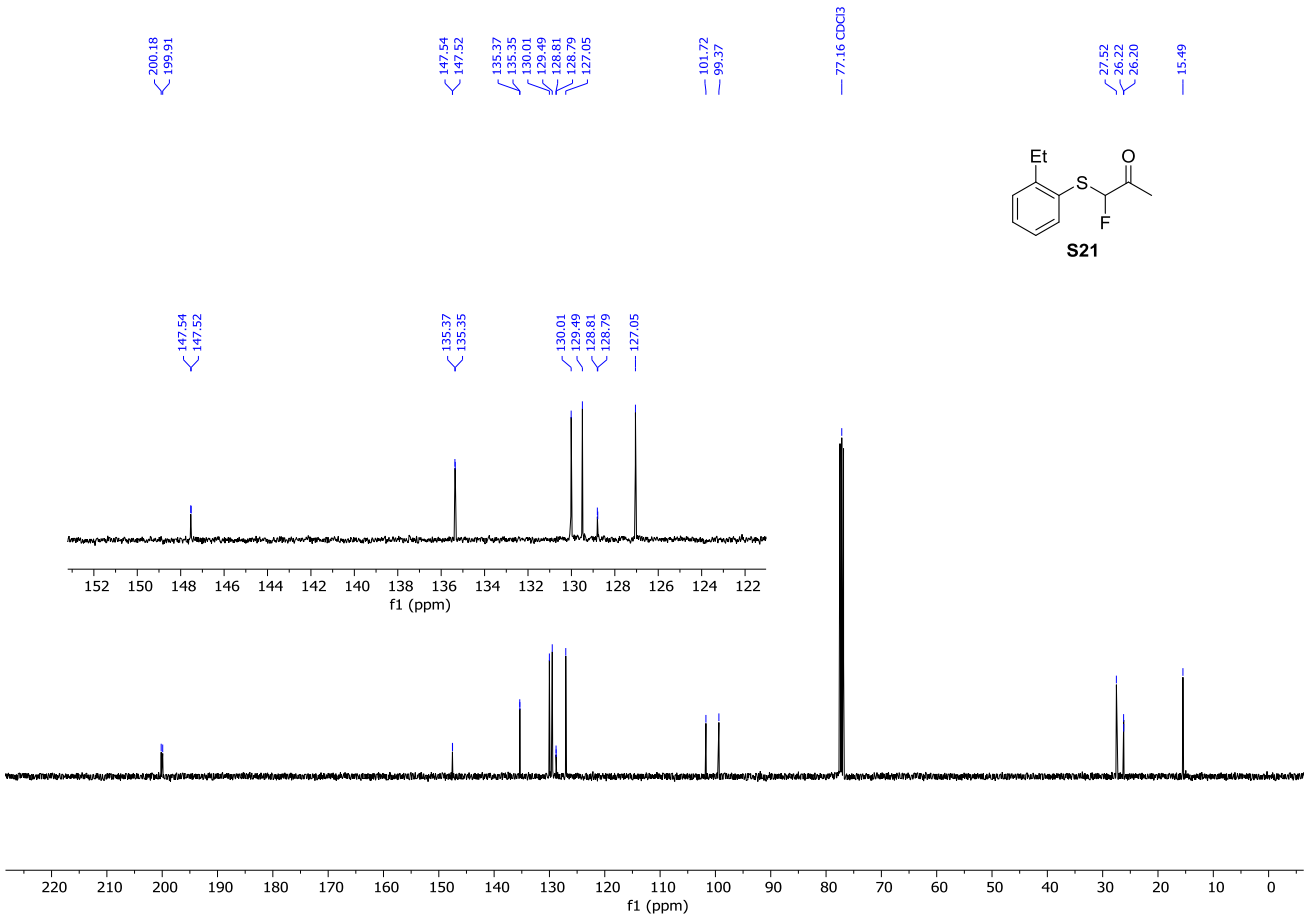
^{13}C NMR (101 MHz, $CDCl_3$)



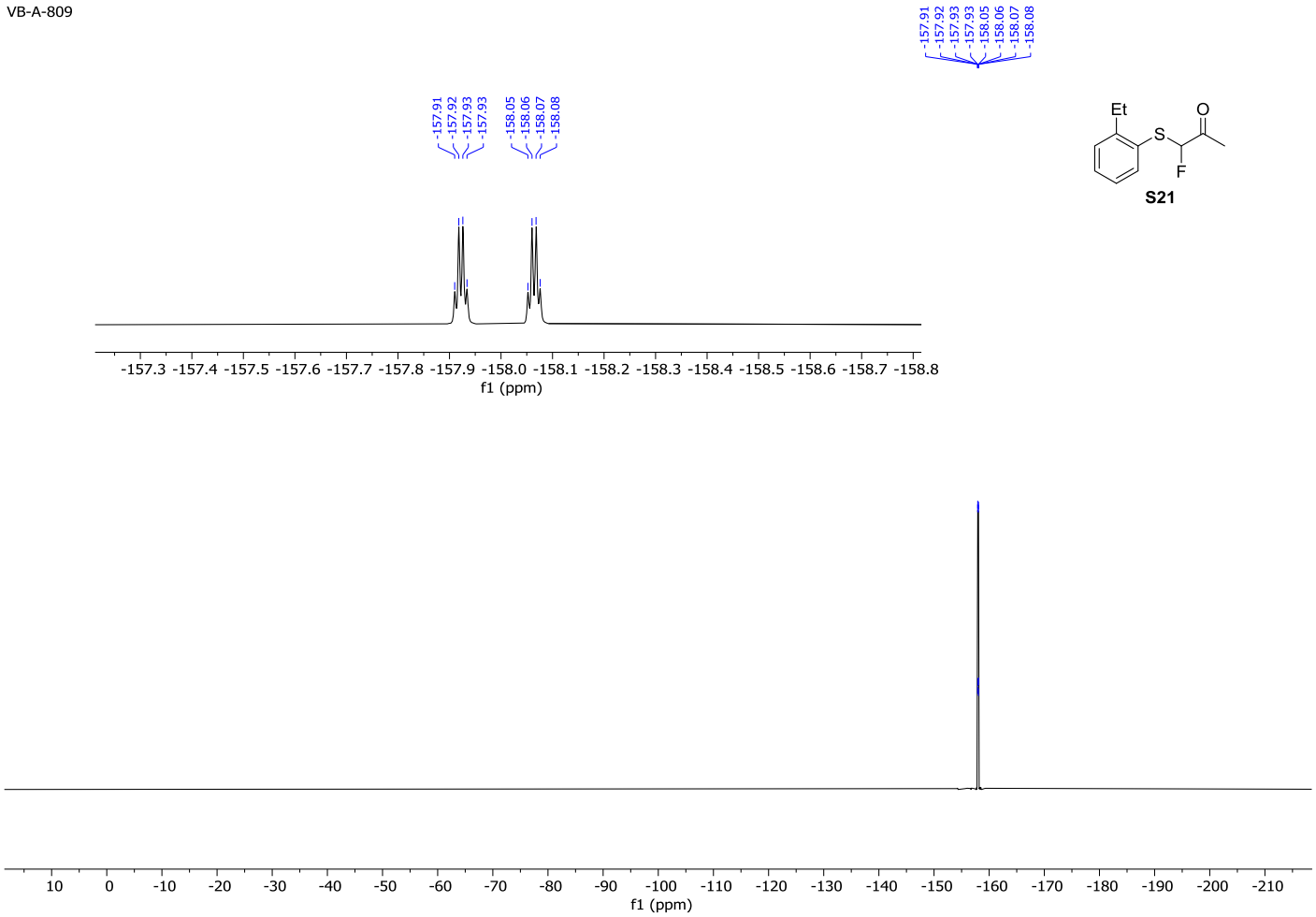
^{19}F NMR (376 MHz, $CDCl_3$)

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



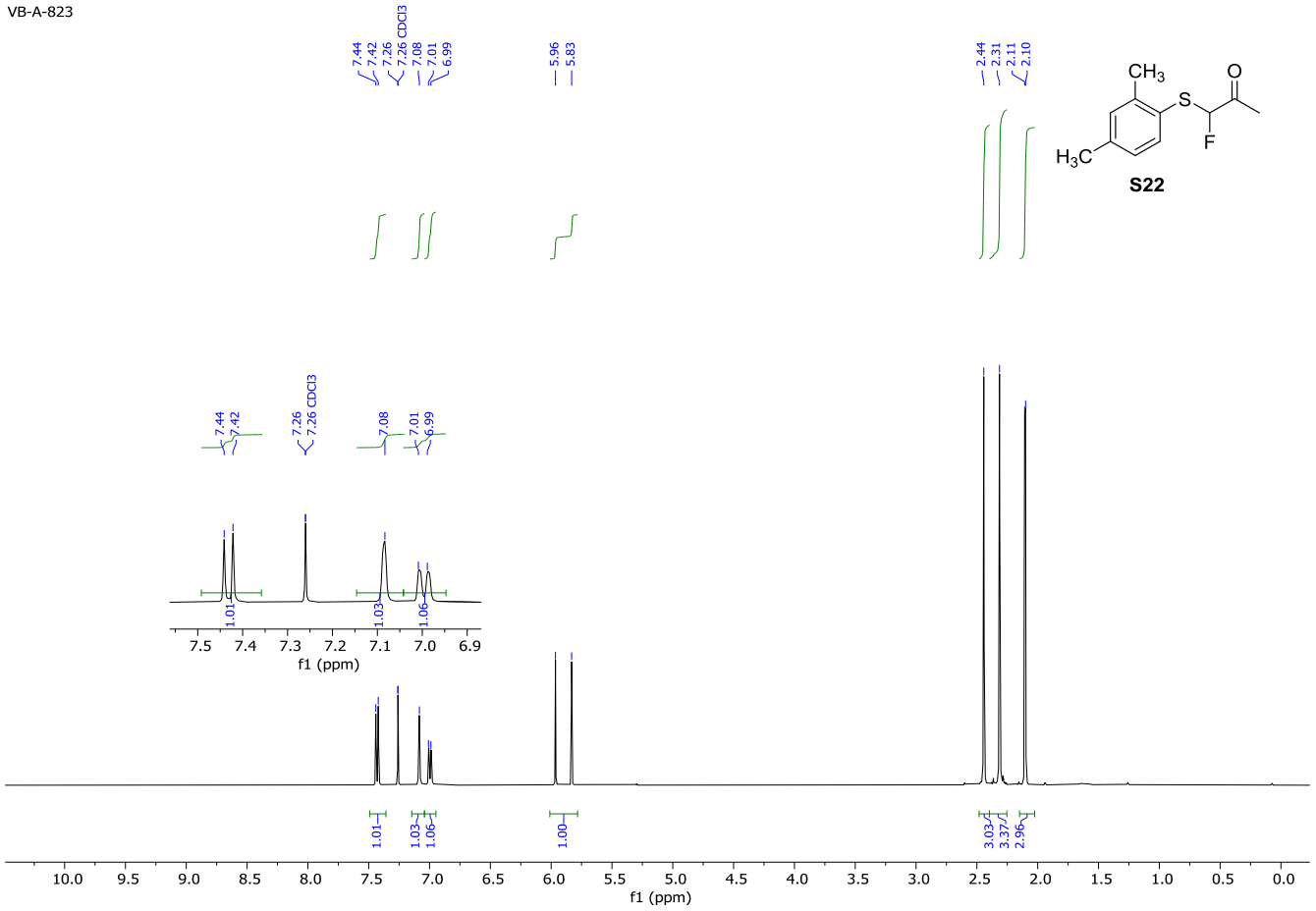


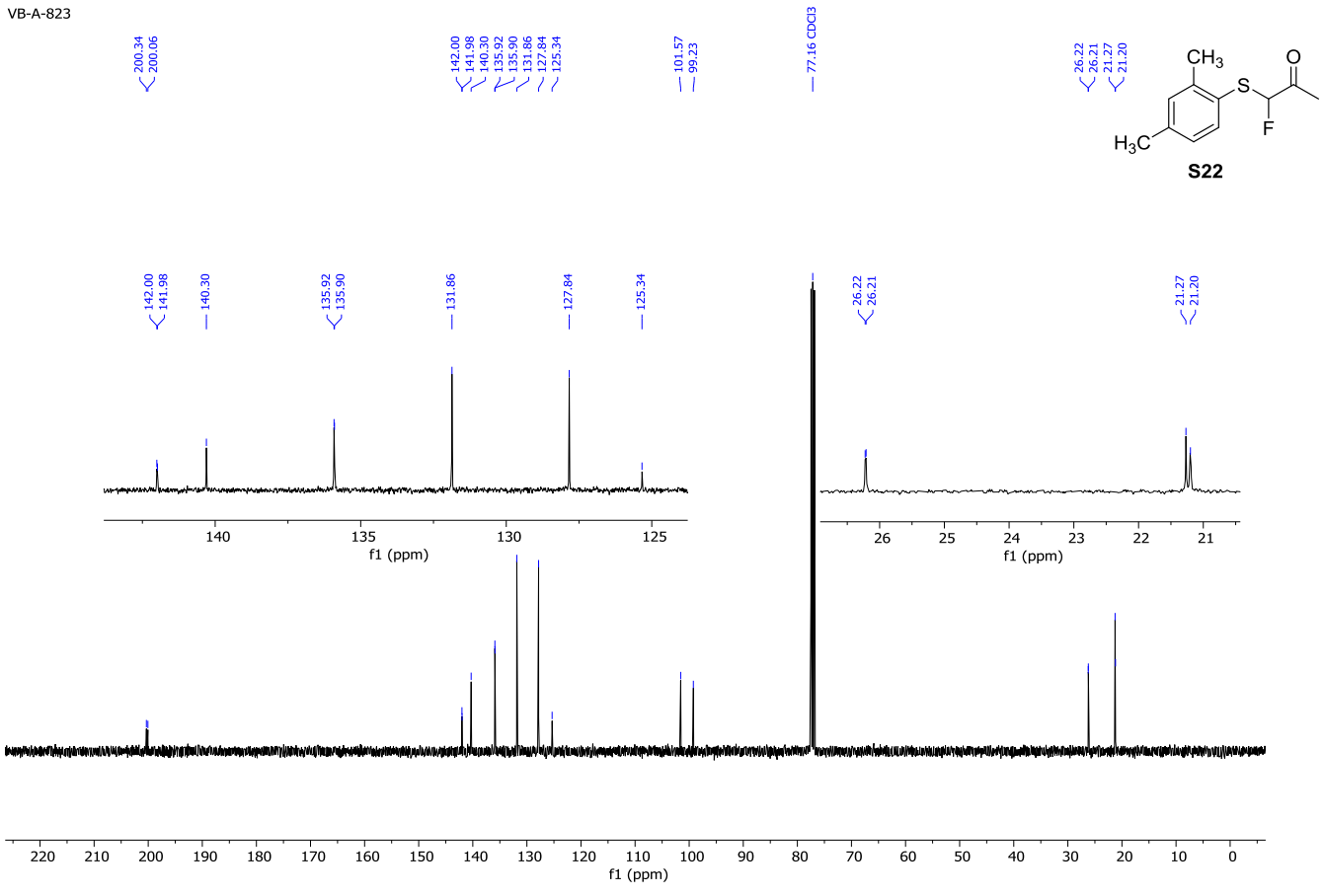
^{13}C NMR (101 MHz, $CDCl_3$)



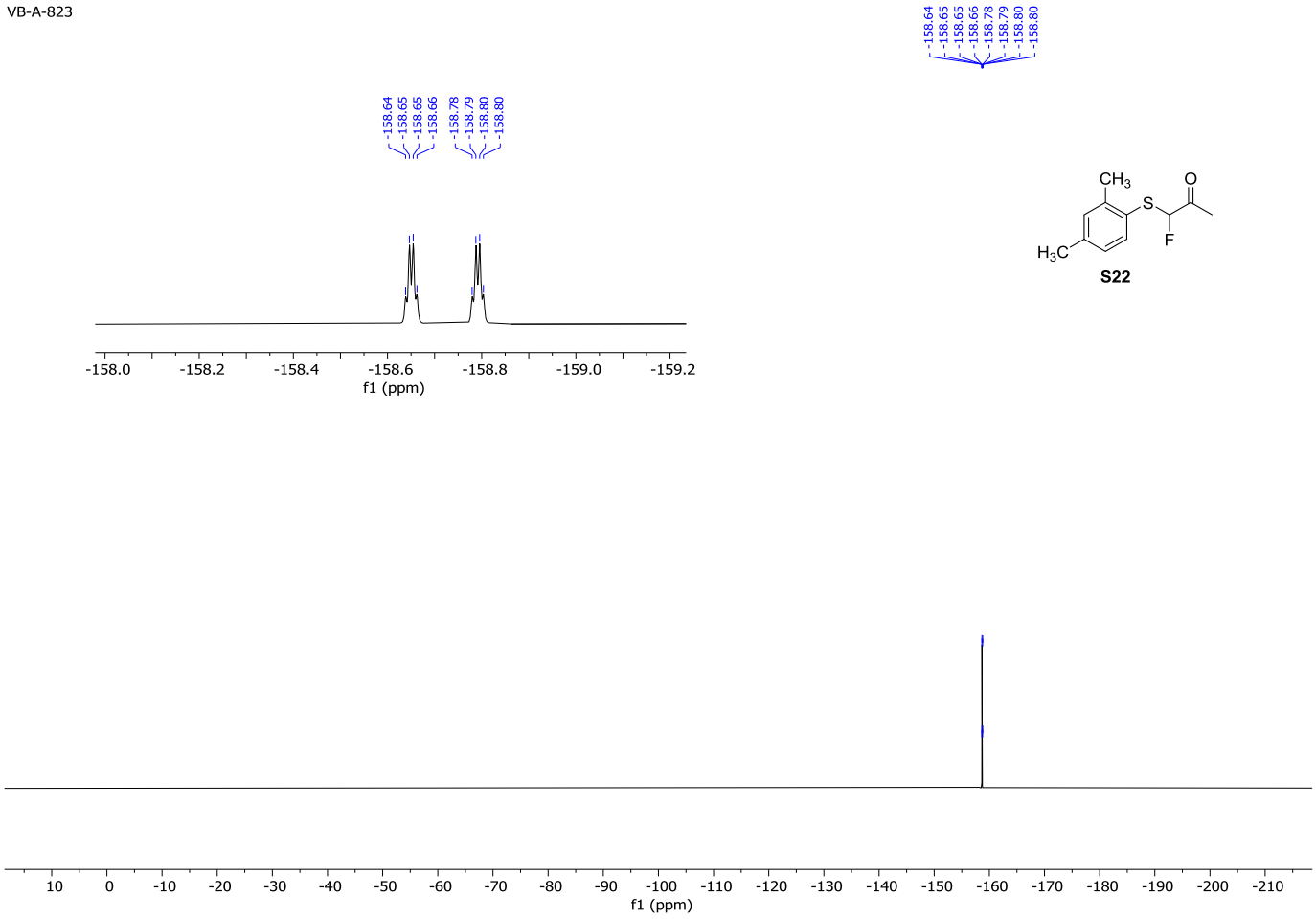
^{19}F NMR (376 MHz, $CDCl_3$)

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



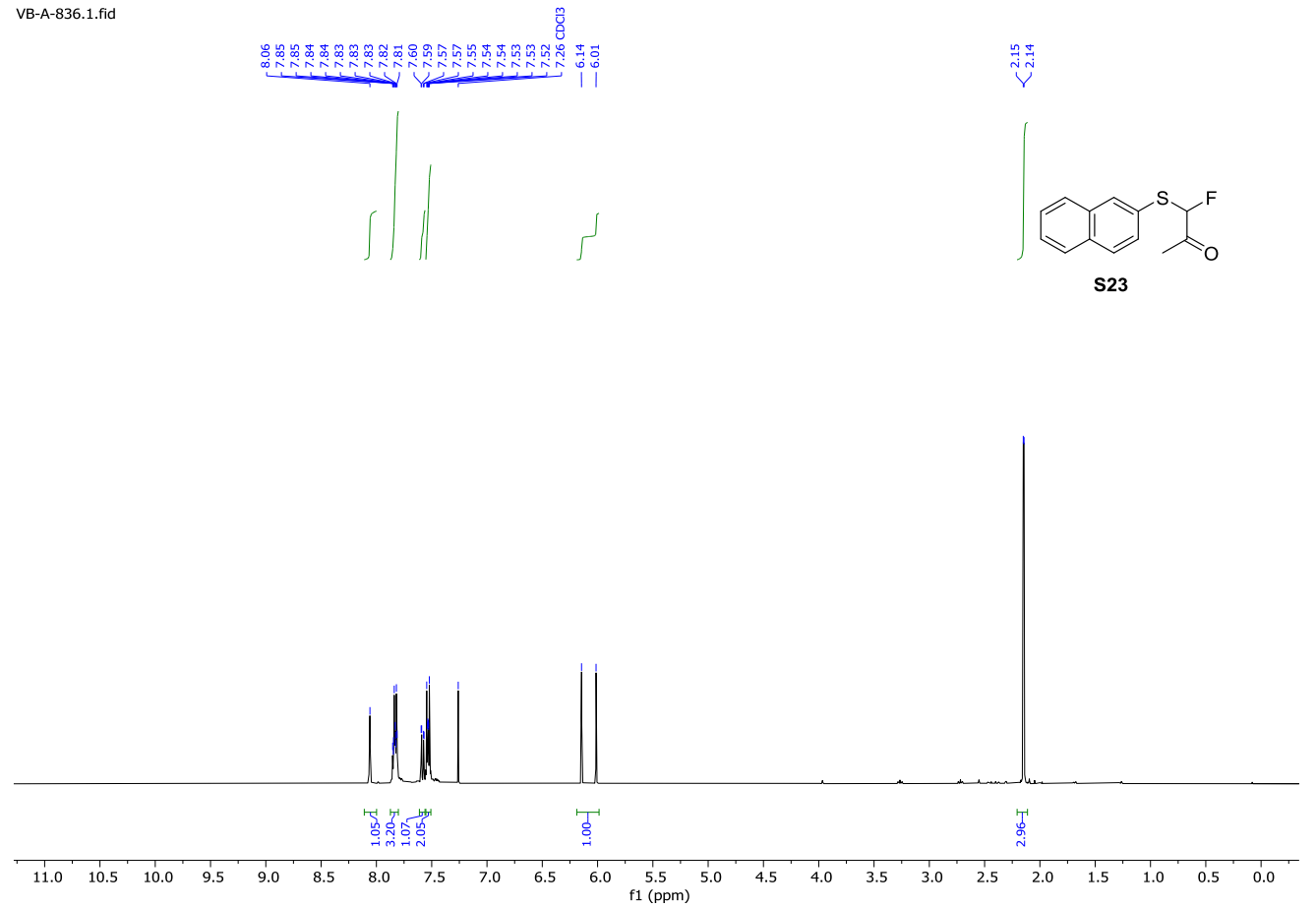


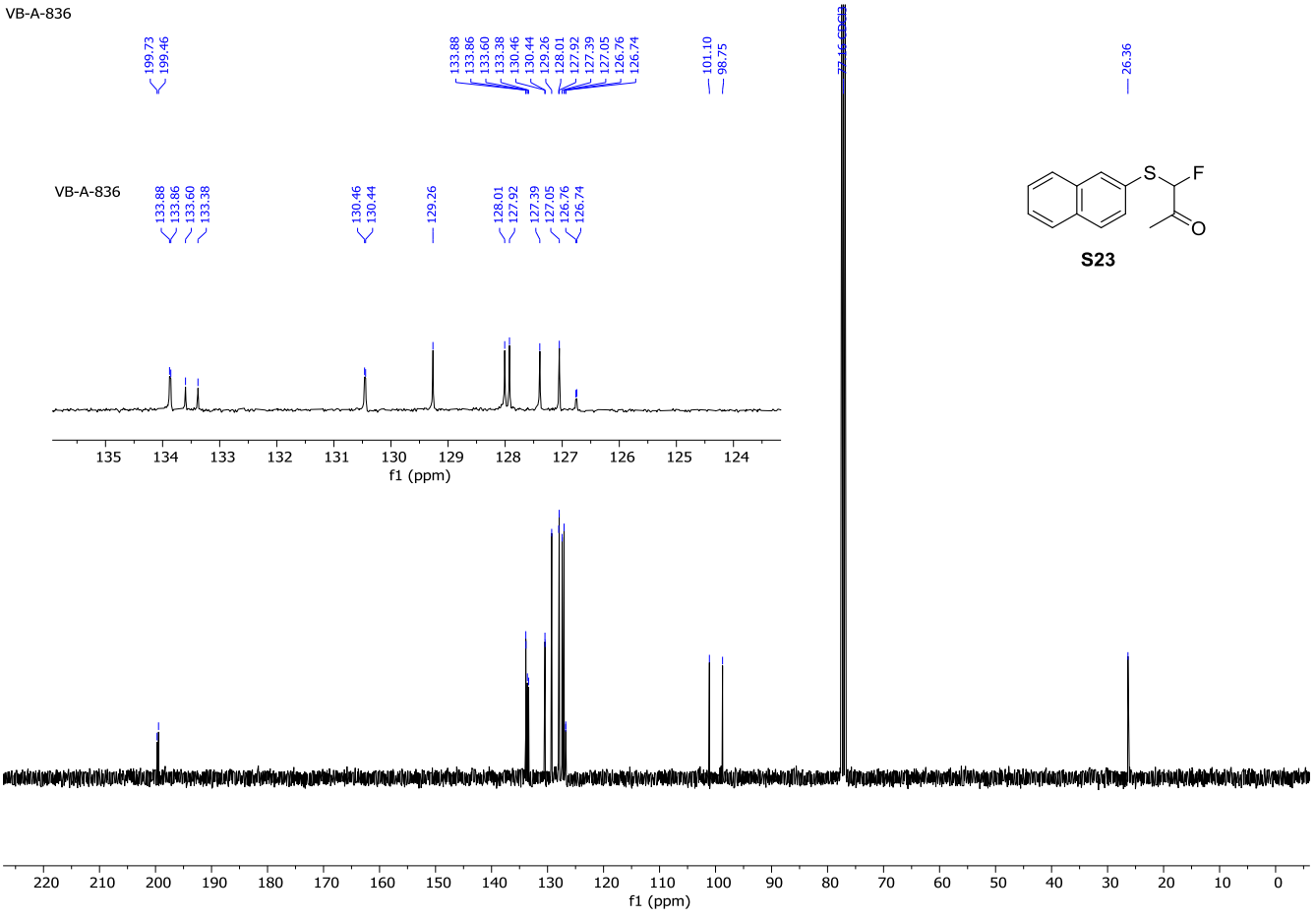
^{13}C NMR (101 MHz, $CDCl_3$)



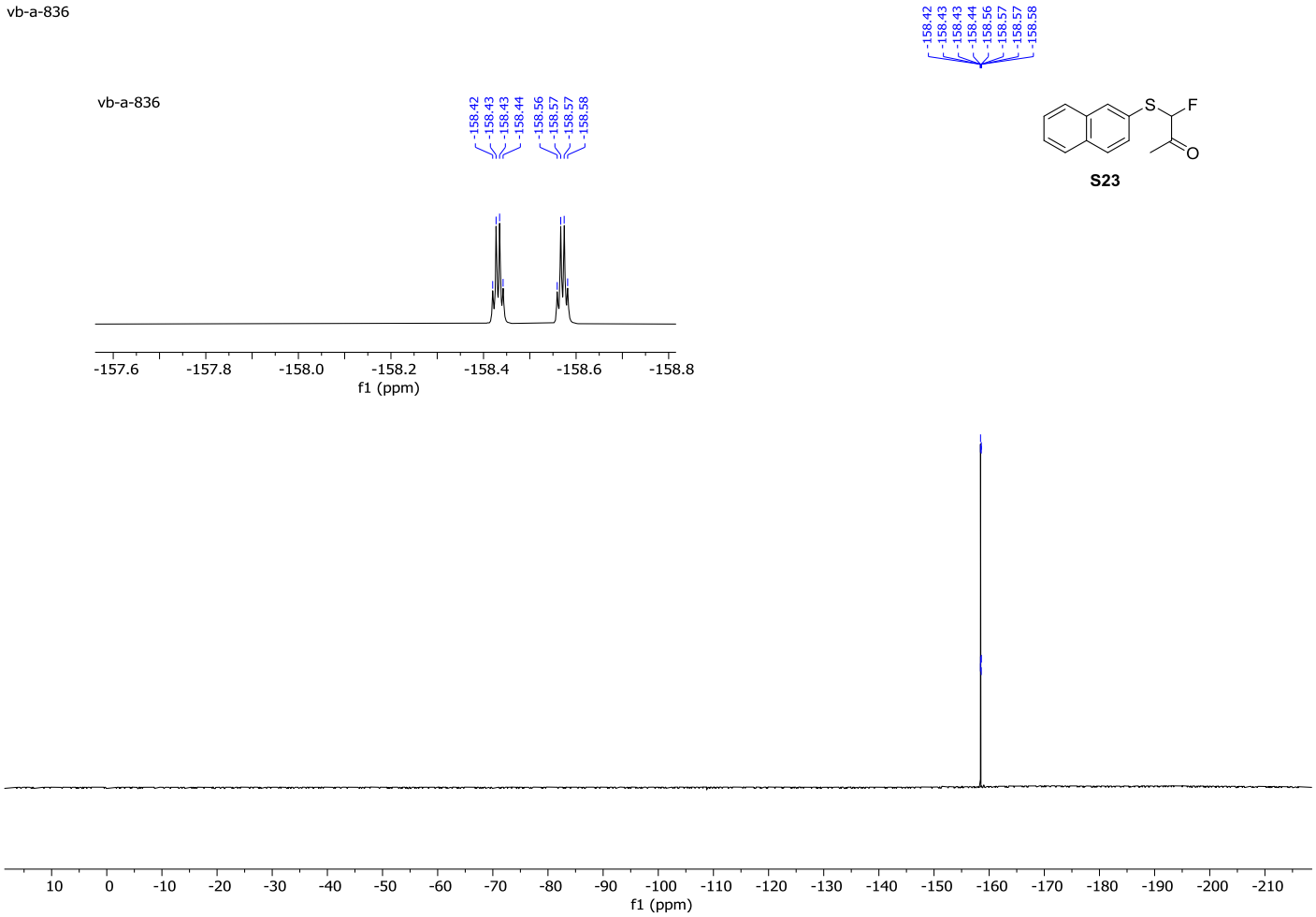
^{19}F NMR (376 MHz, $CDCl_3$)

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



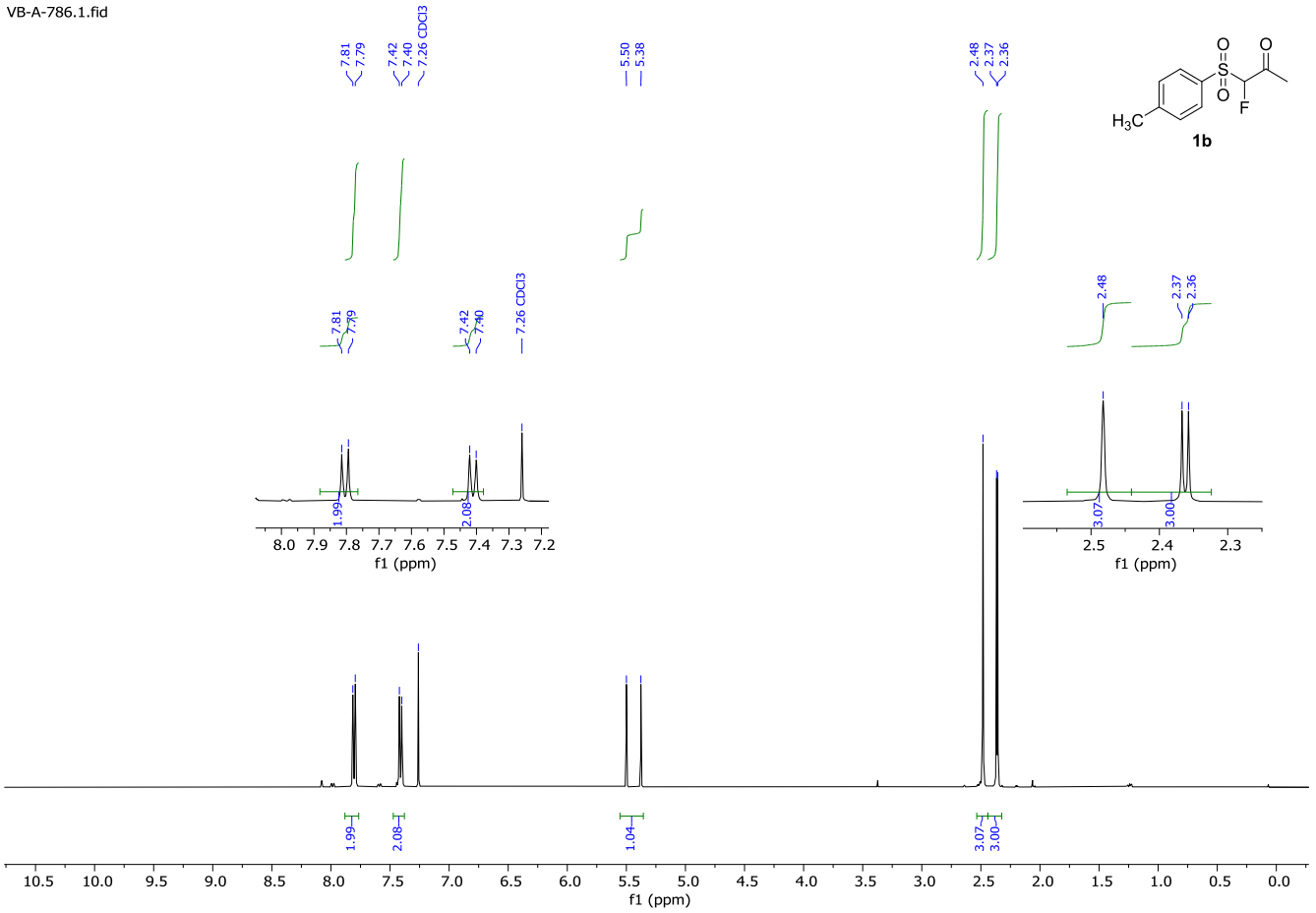


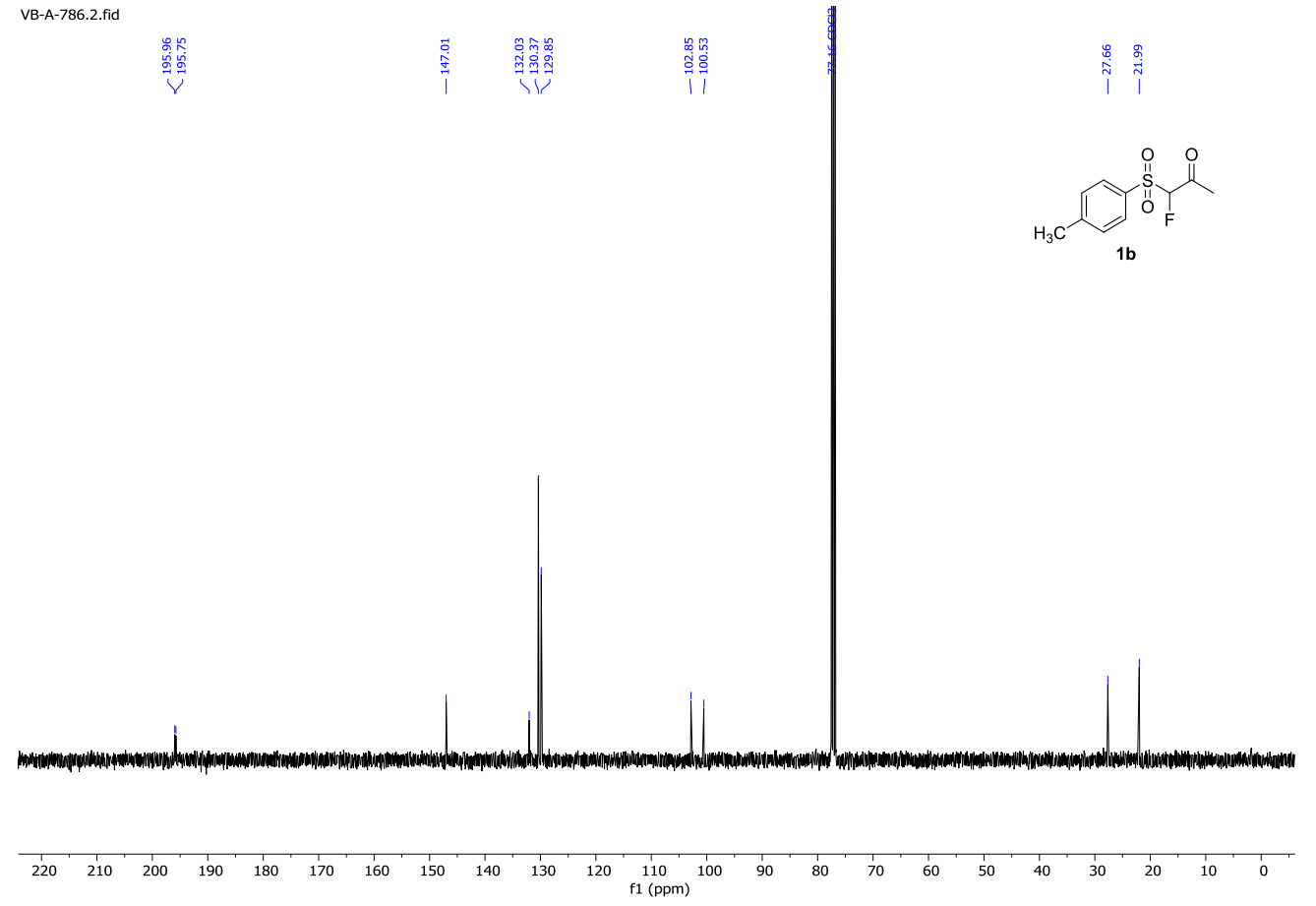
^{13}C NMR (101 MHz, $CDCl_3$)



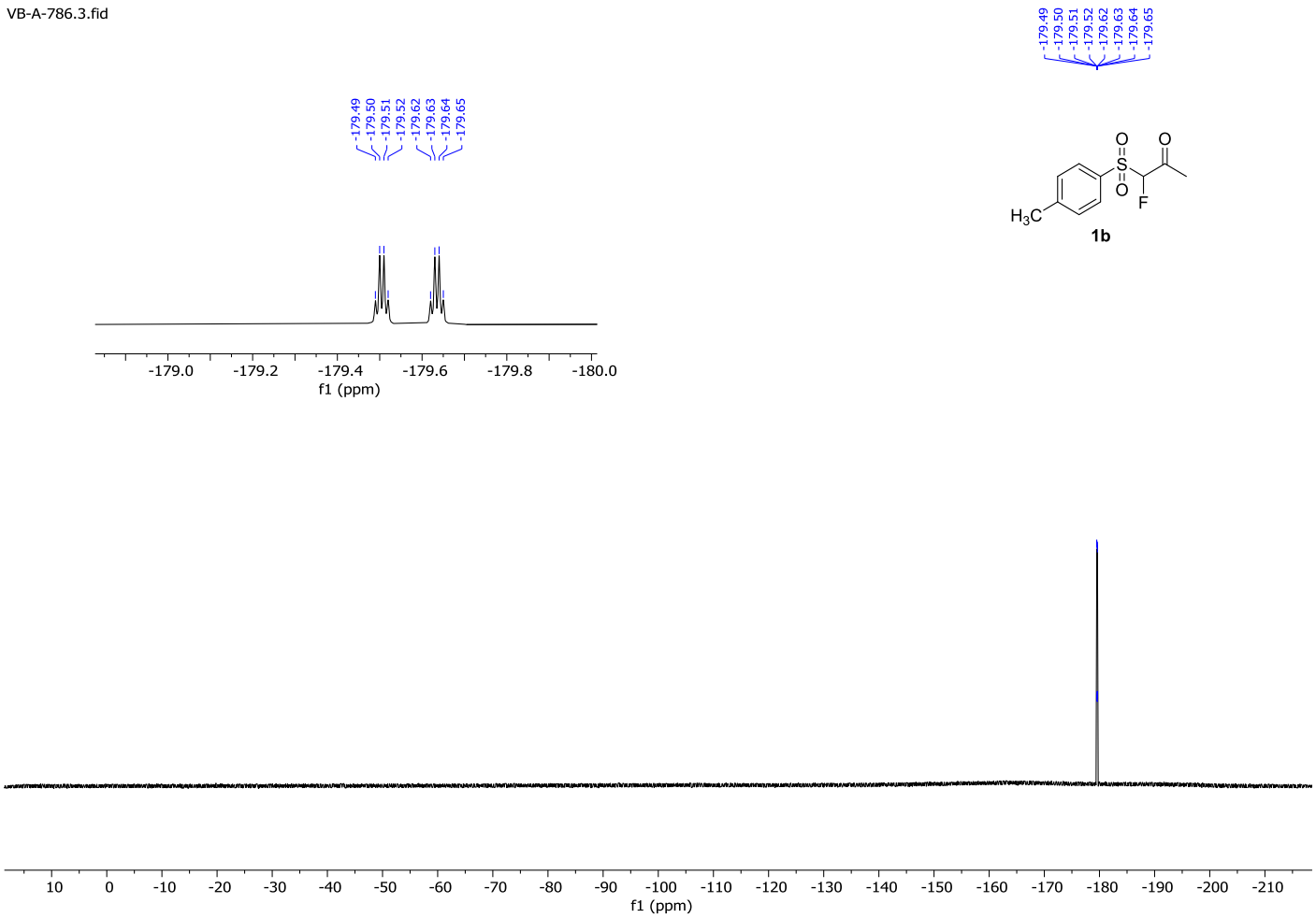
^{19}F NMR (376 MHz, $CDCl_3$)

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



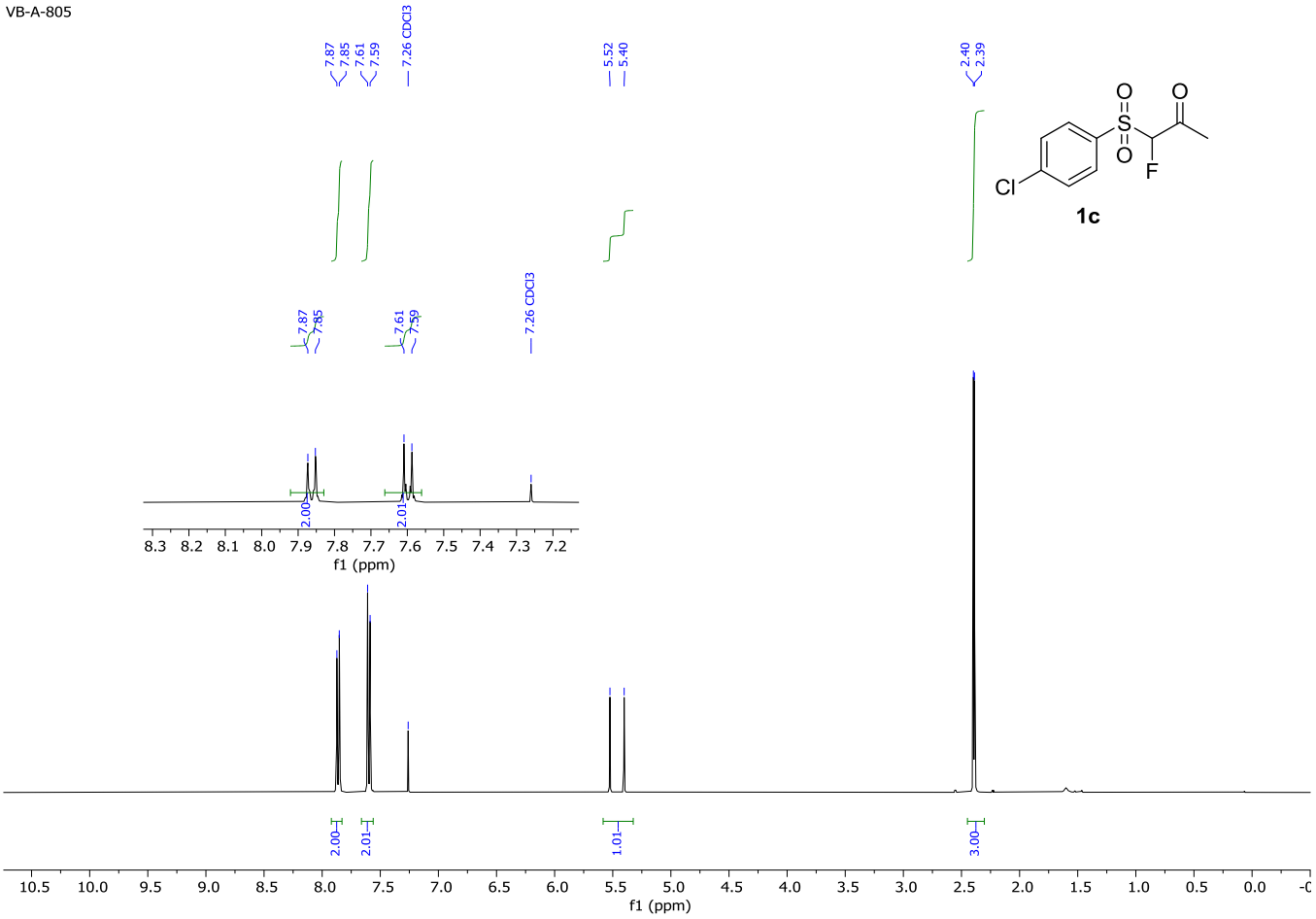


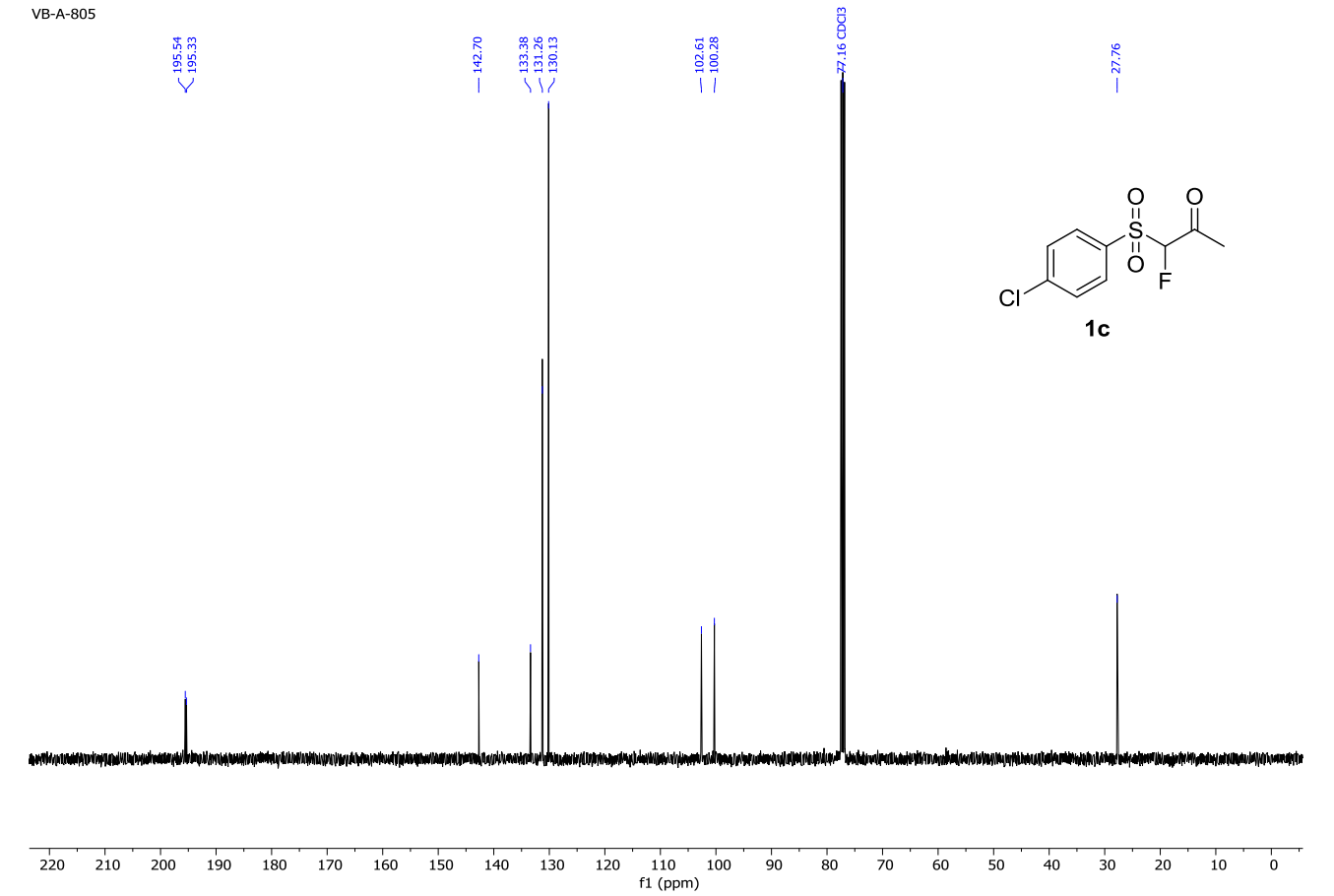
^{13}C NMR (101 MHz, $CDCl_3$)



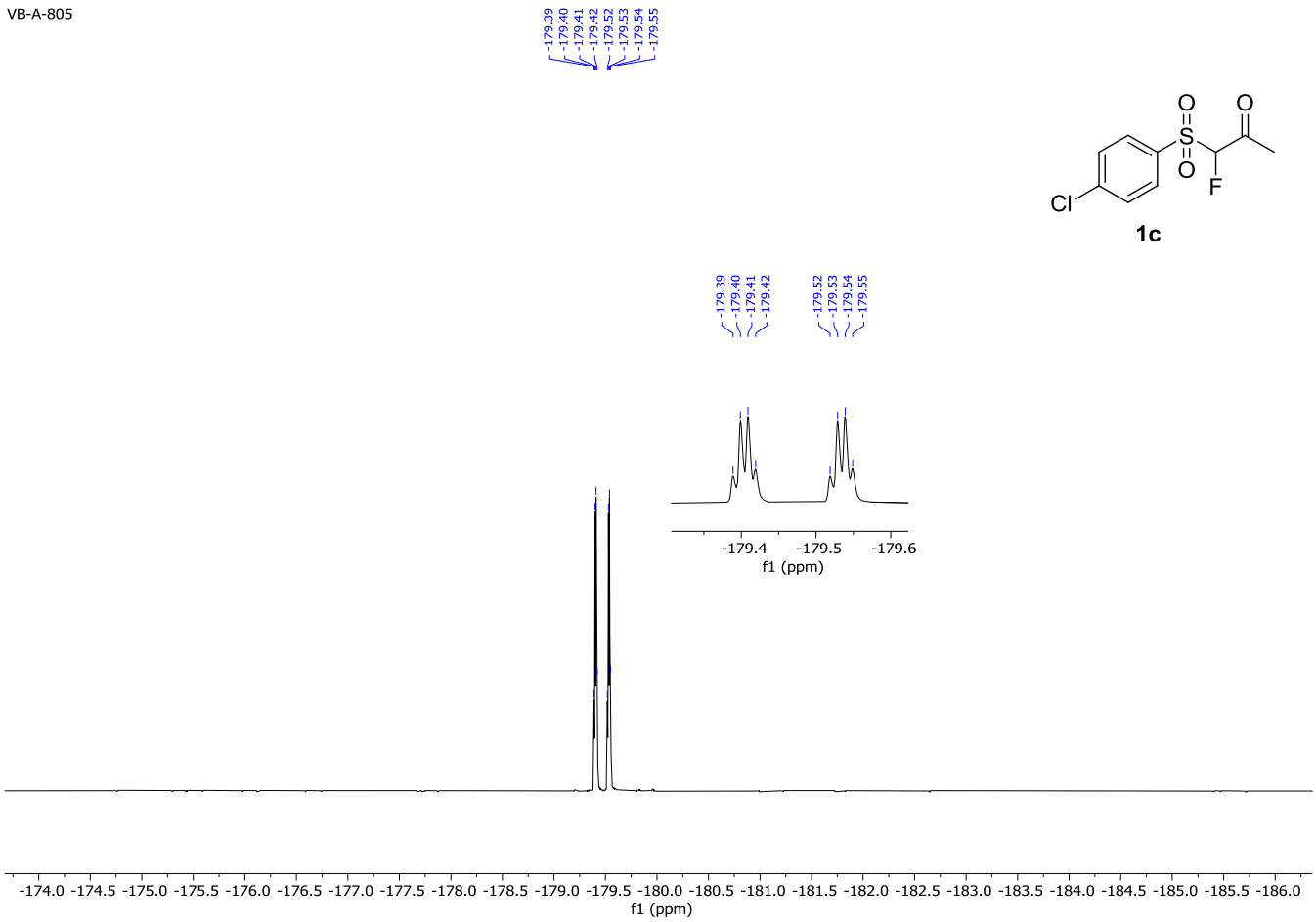
^{19}F NMR (376 MHz, $CDCl_3$)

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



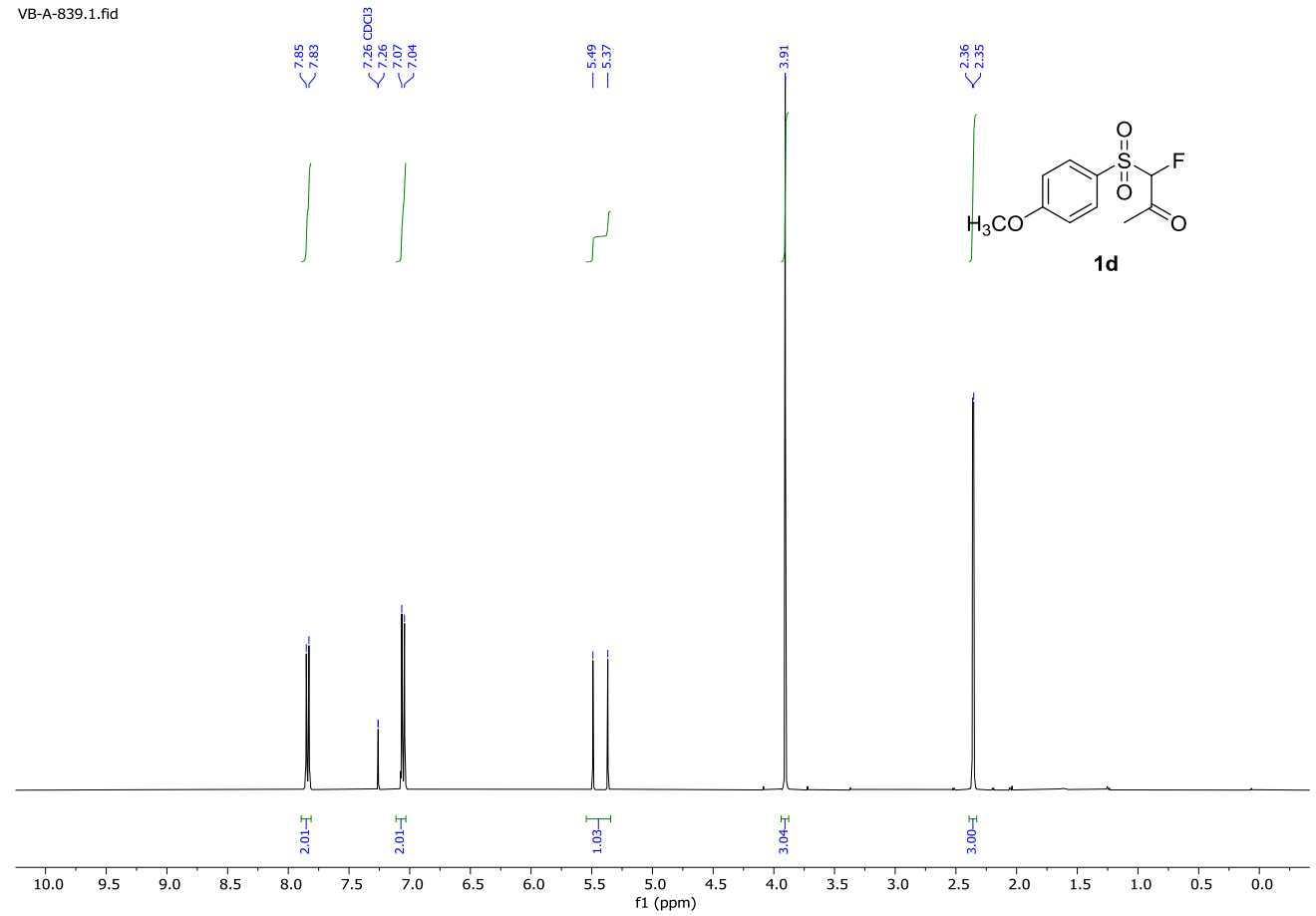


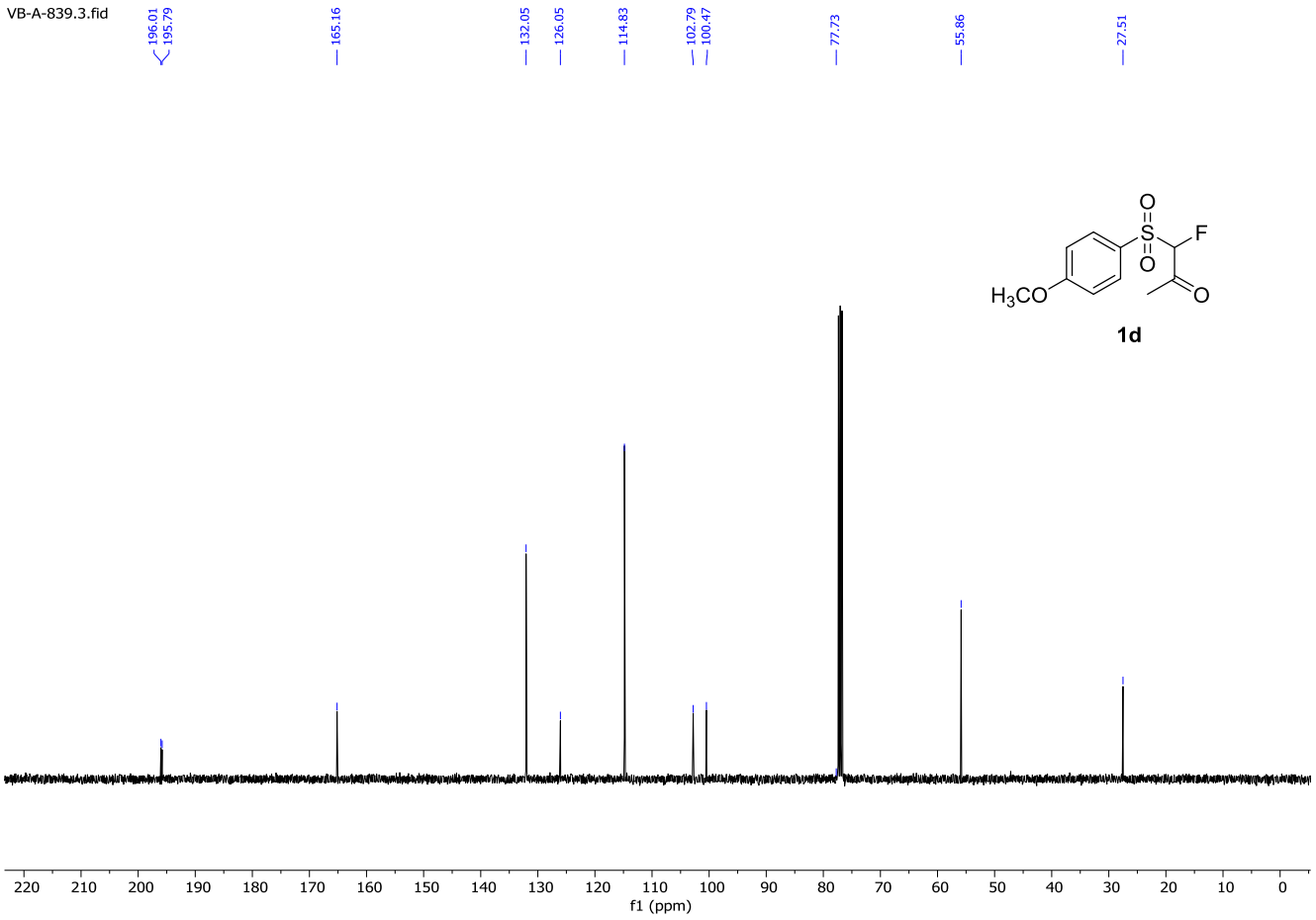
^{13}C NMR (101 MHz, $CDCl_3$)



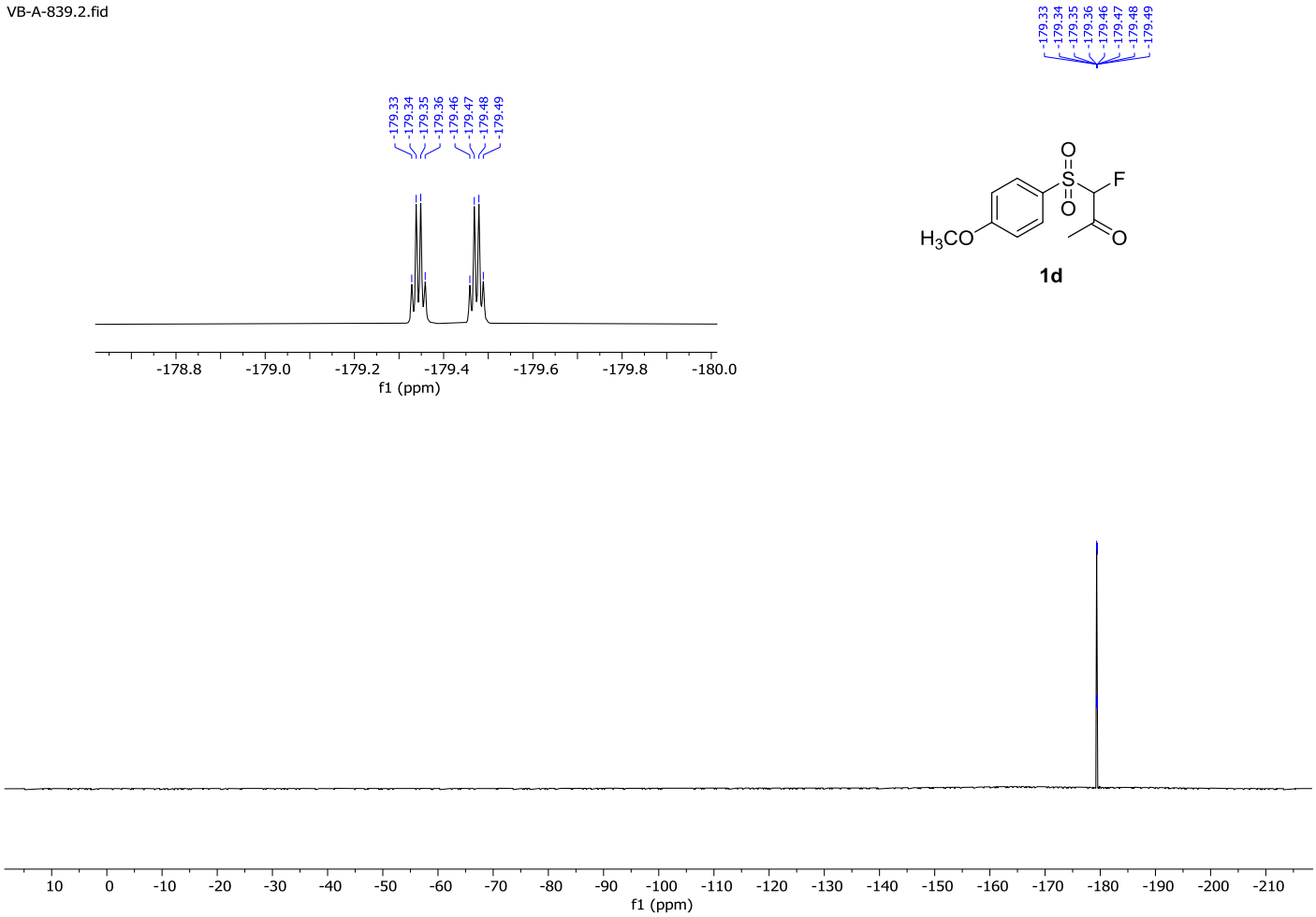
^{19}F NMR (376 MHz, $CDCl_3$)

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



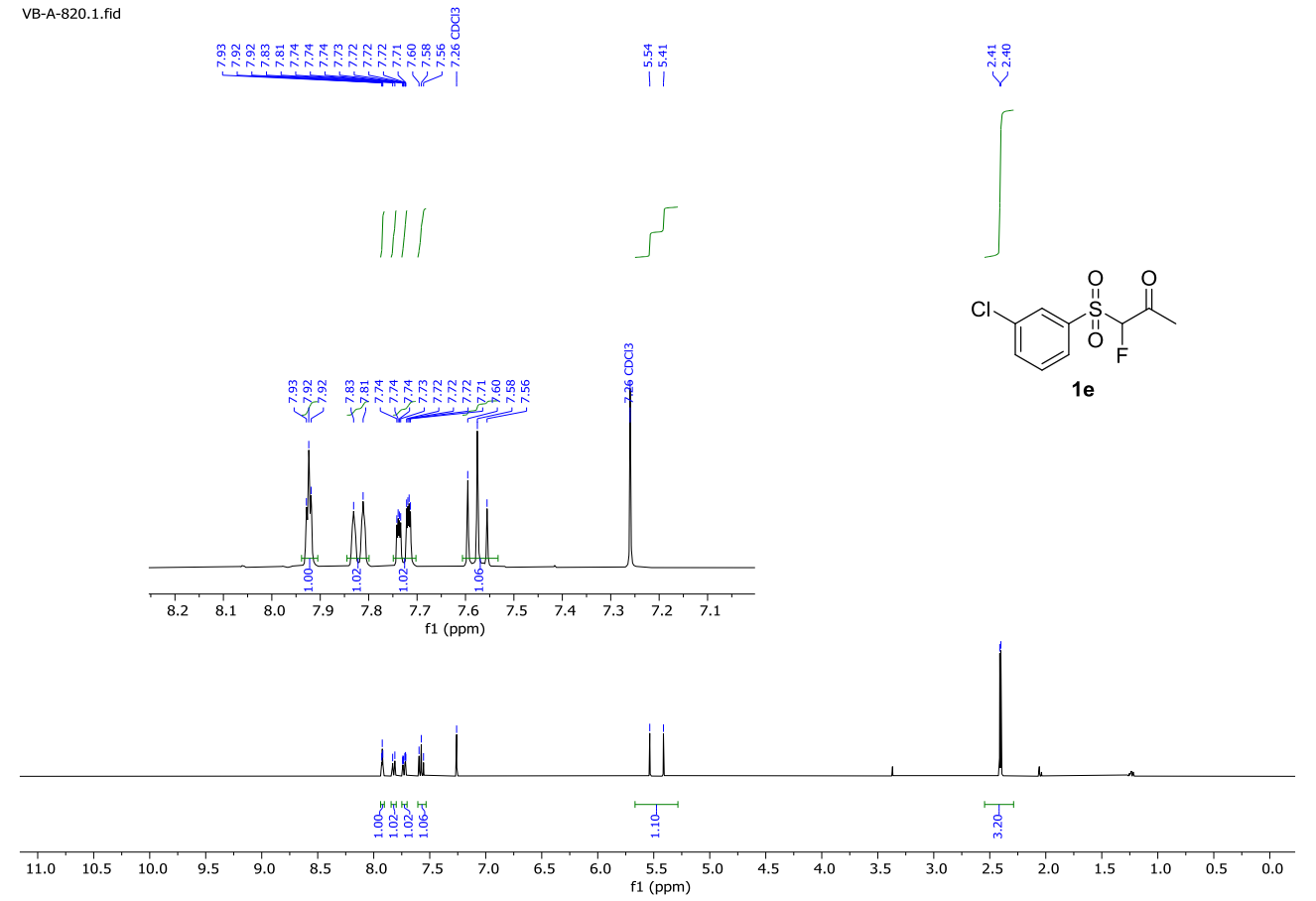


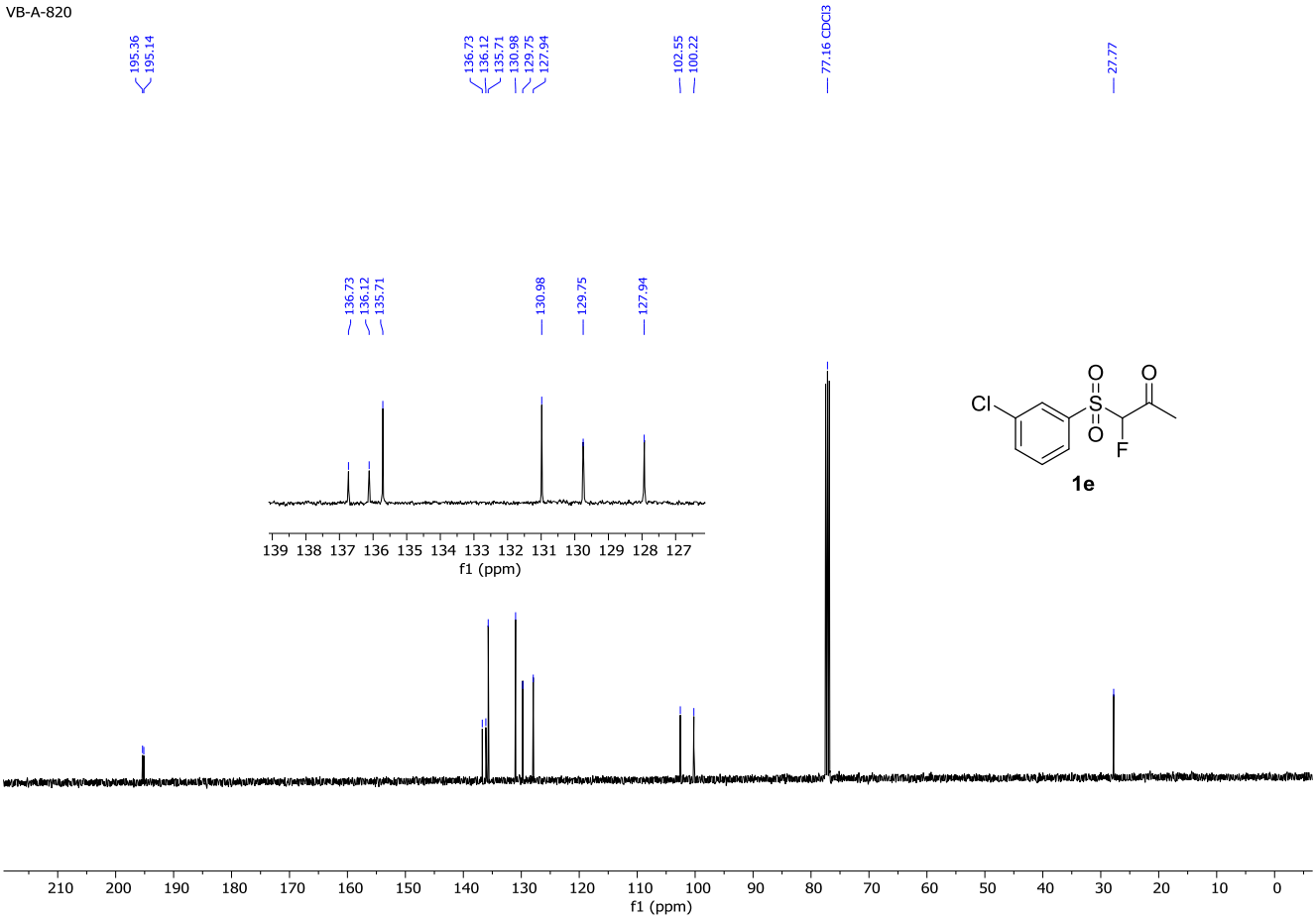
^{13}C NMR (101 MHz, $CDCl_3$)



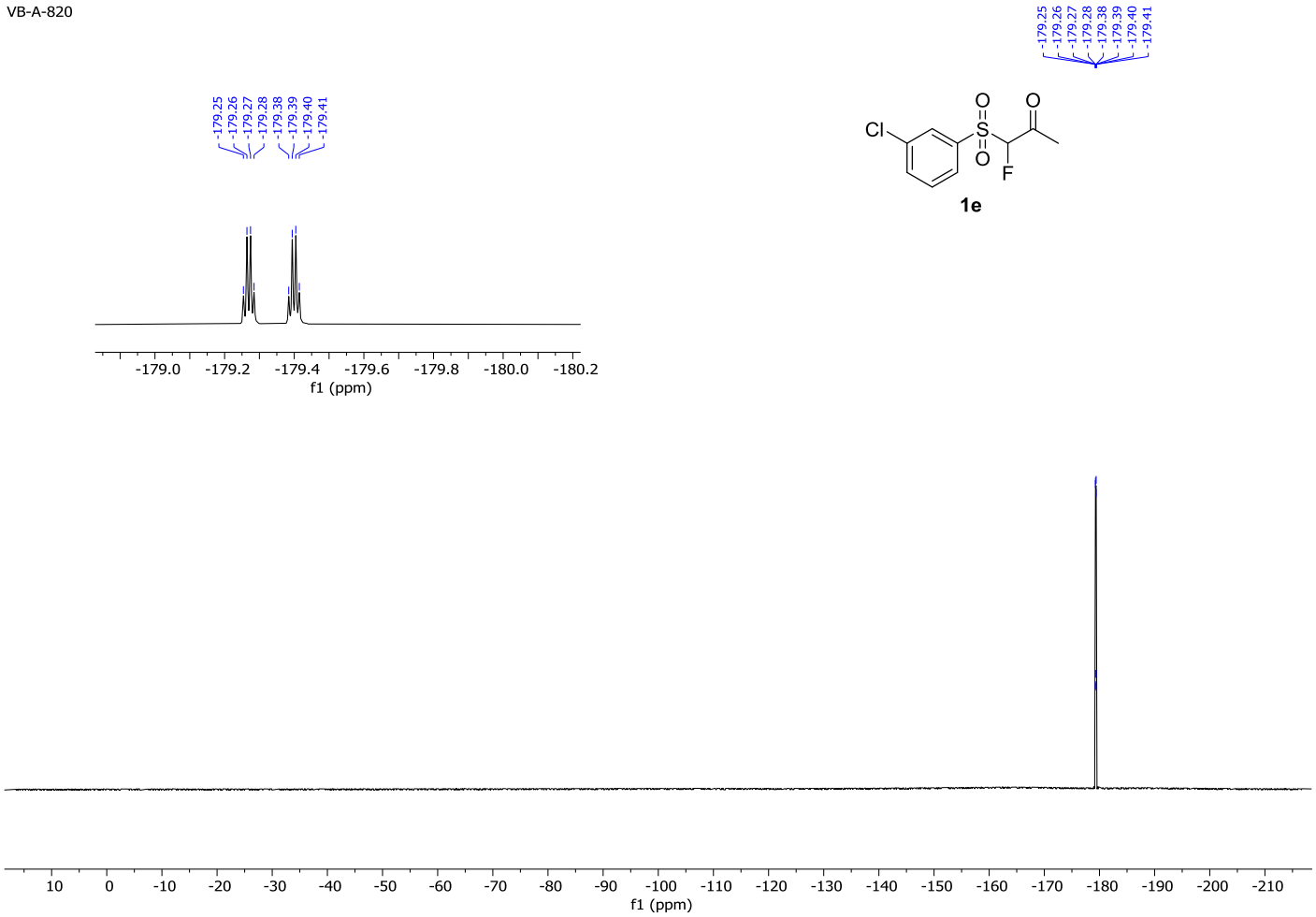
^{19}F NMR (376 MHz, $CDCl_3$)

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



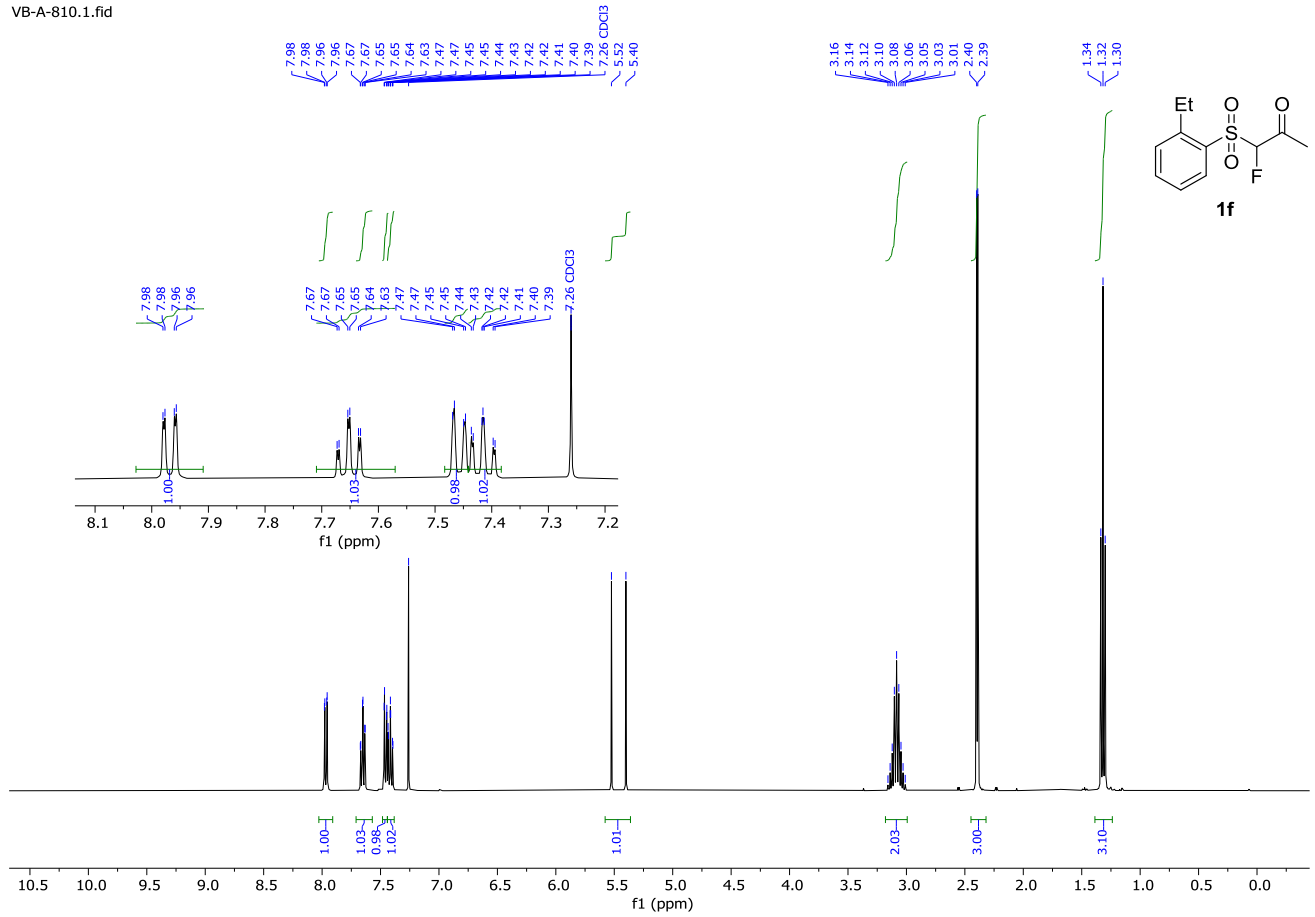


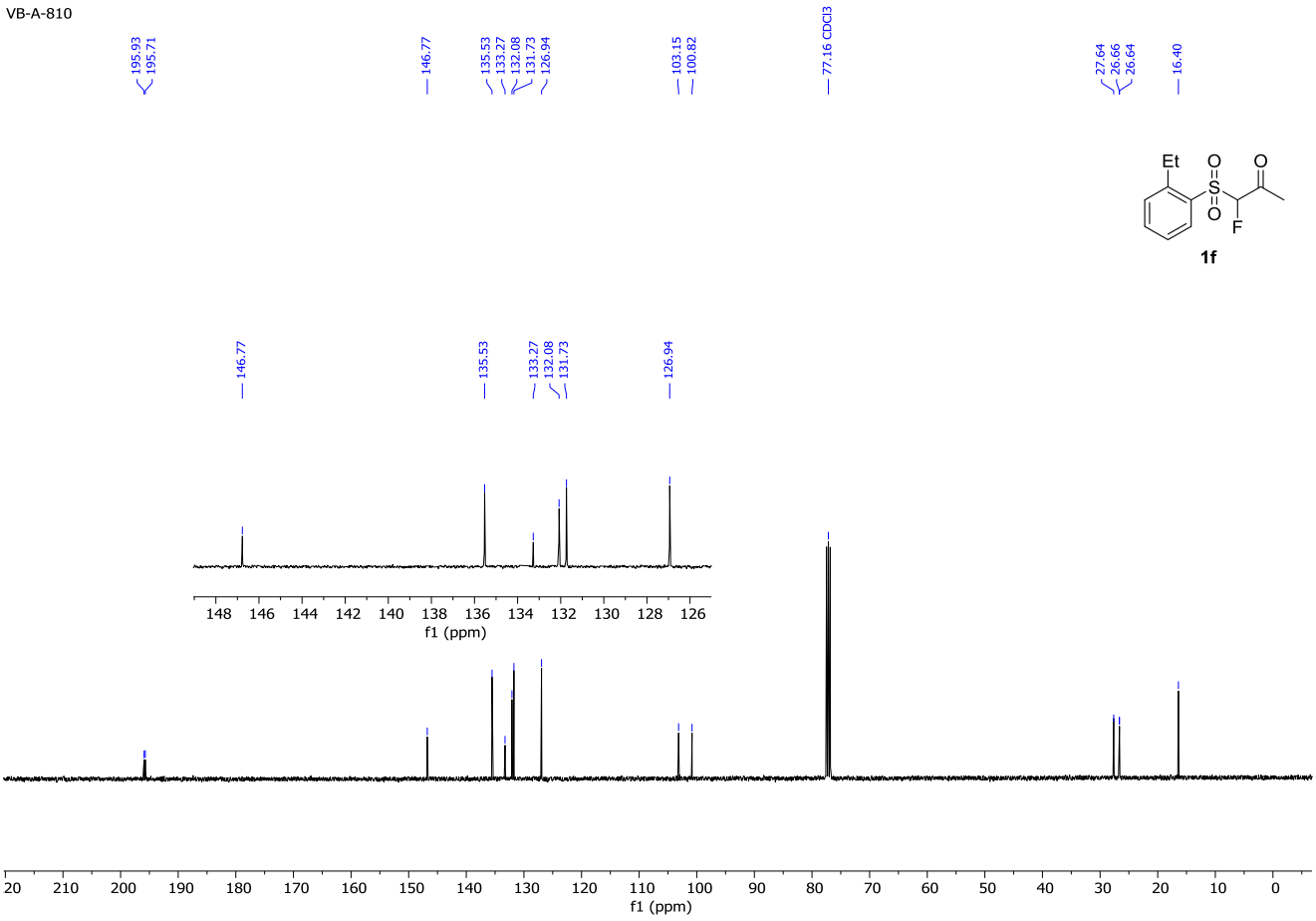
^{13}C NMR (101 MHz, $CDCl_3$)



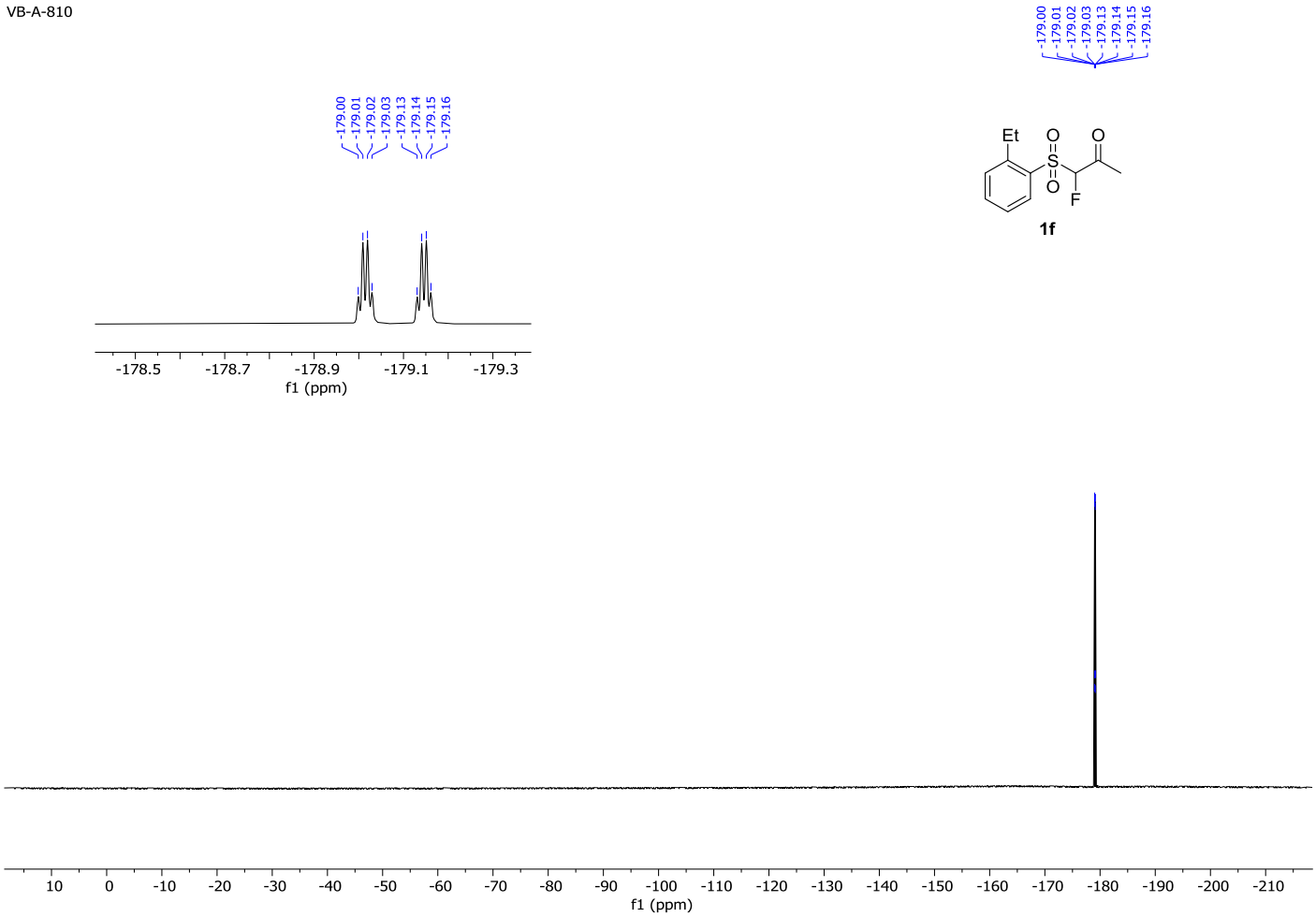
^{19}F NMR (376 MHz, $CDCl_3$)

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



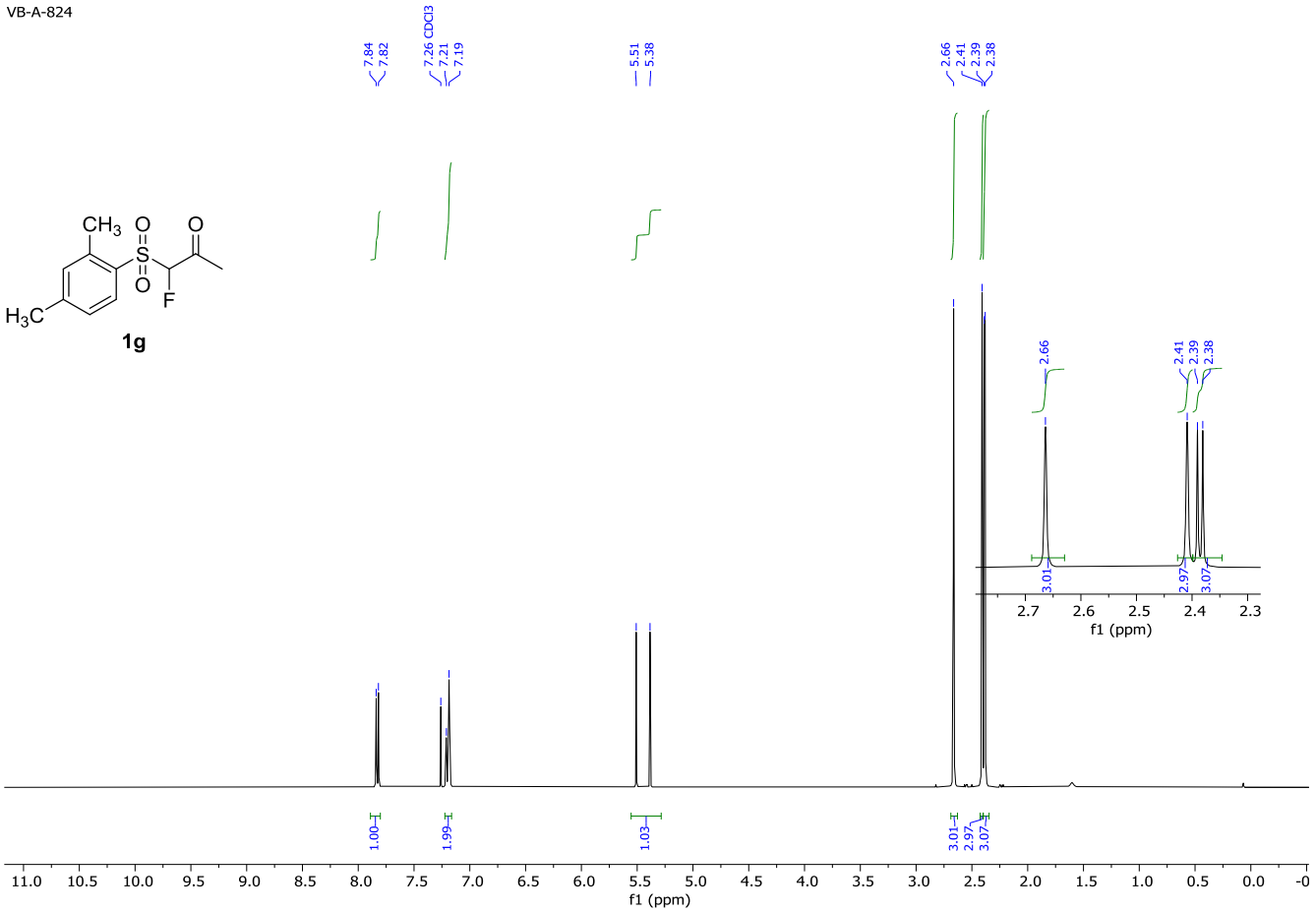


^{13}C NMR (101 MHz, $CDCl_3$)

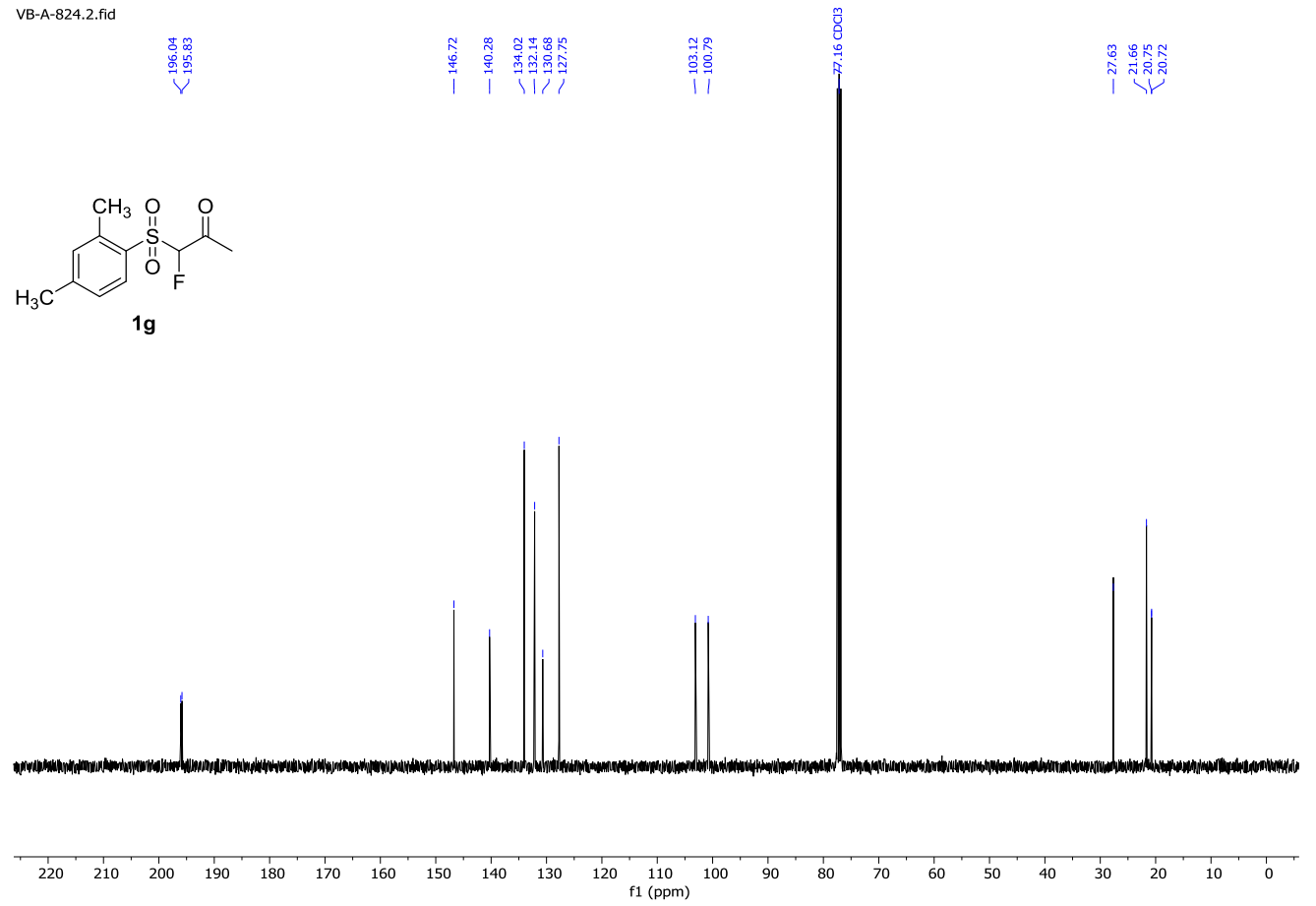


^{19}F NMR (376 MHz, $CDCl_3$)

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

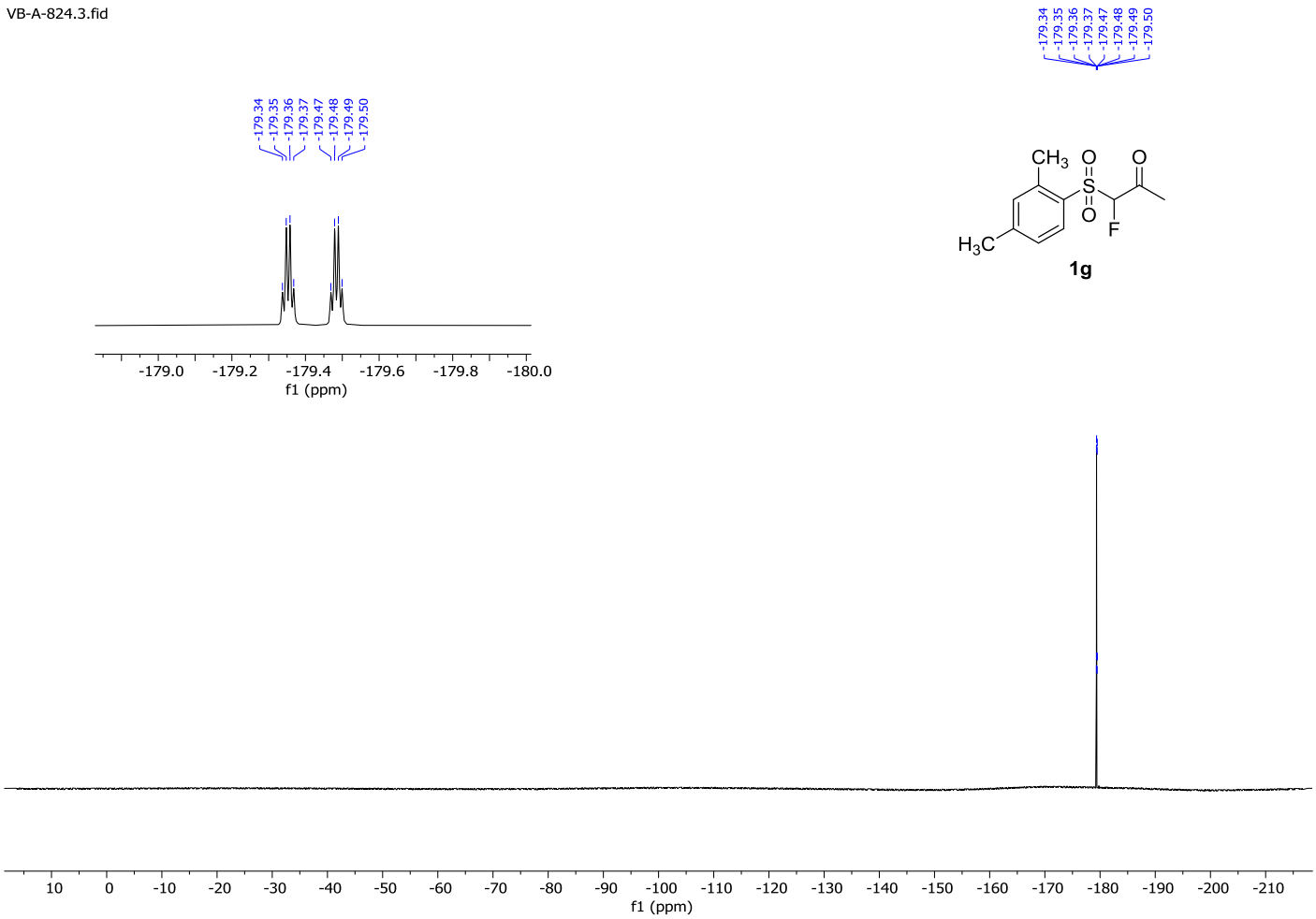


1g



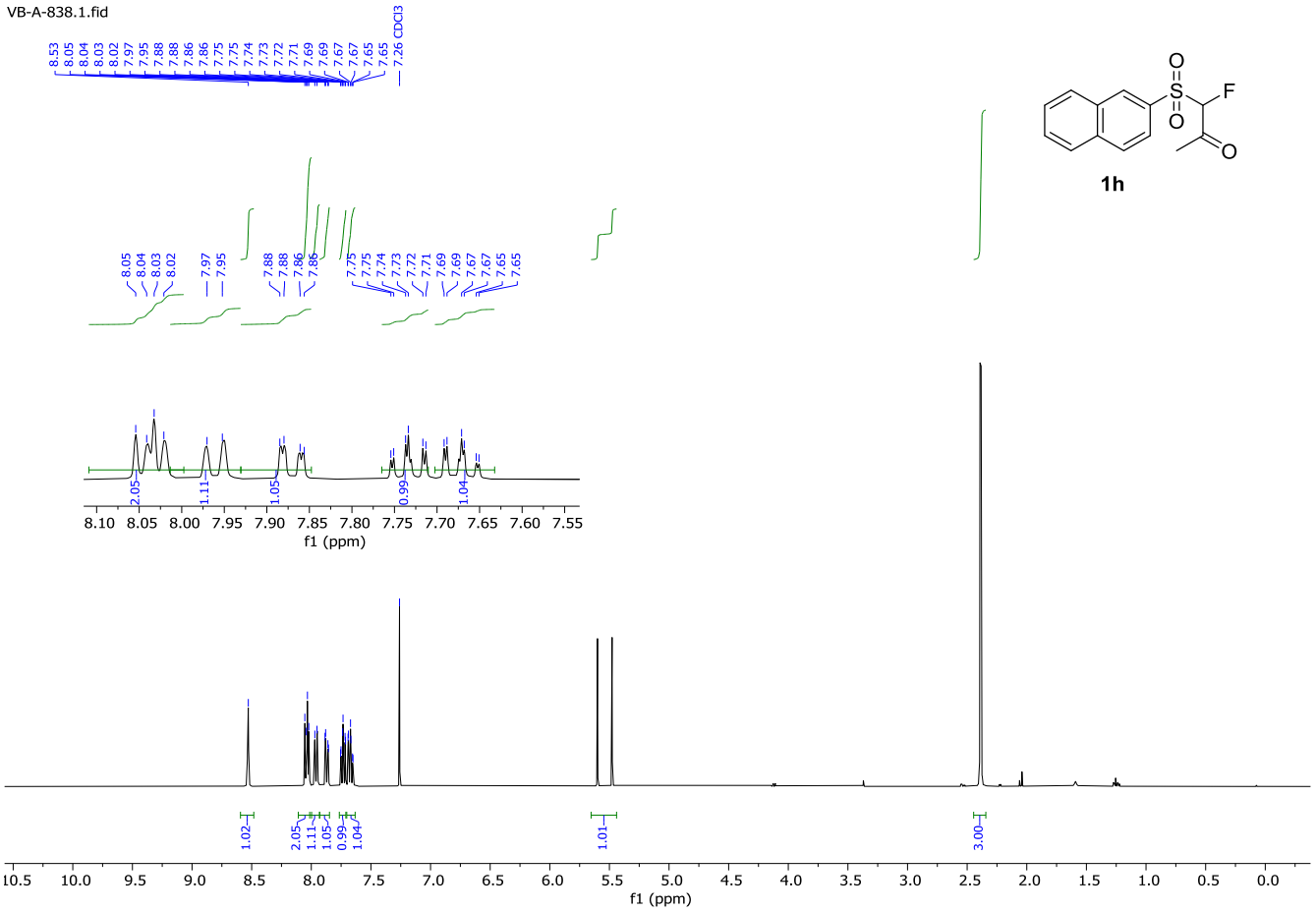
1g

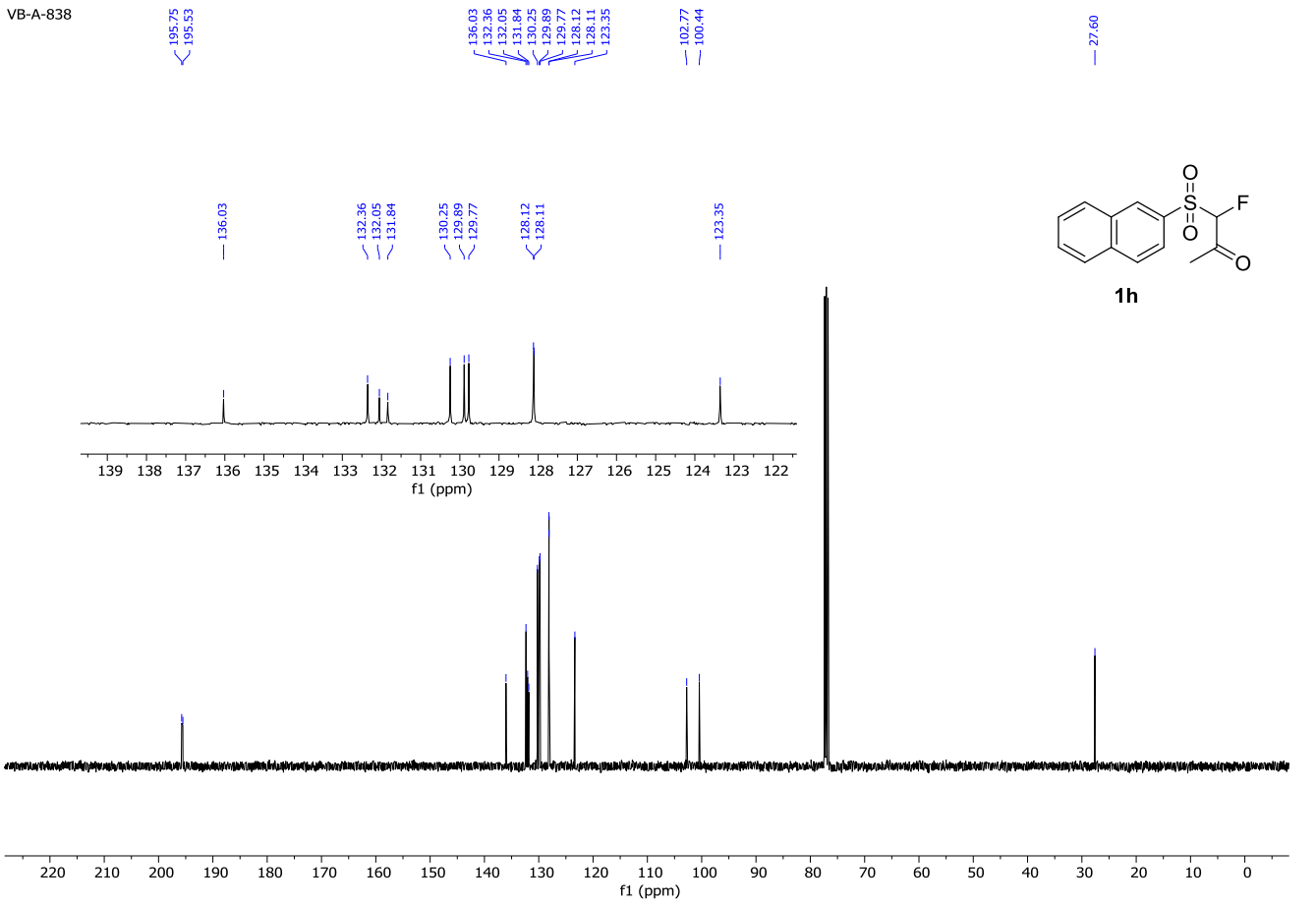
^{13}C NMR (101 MHz, $CDCl_3$)



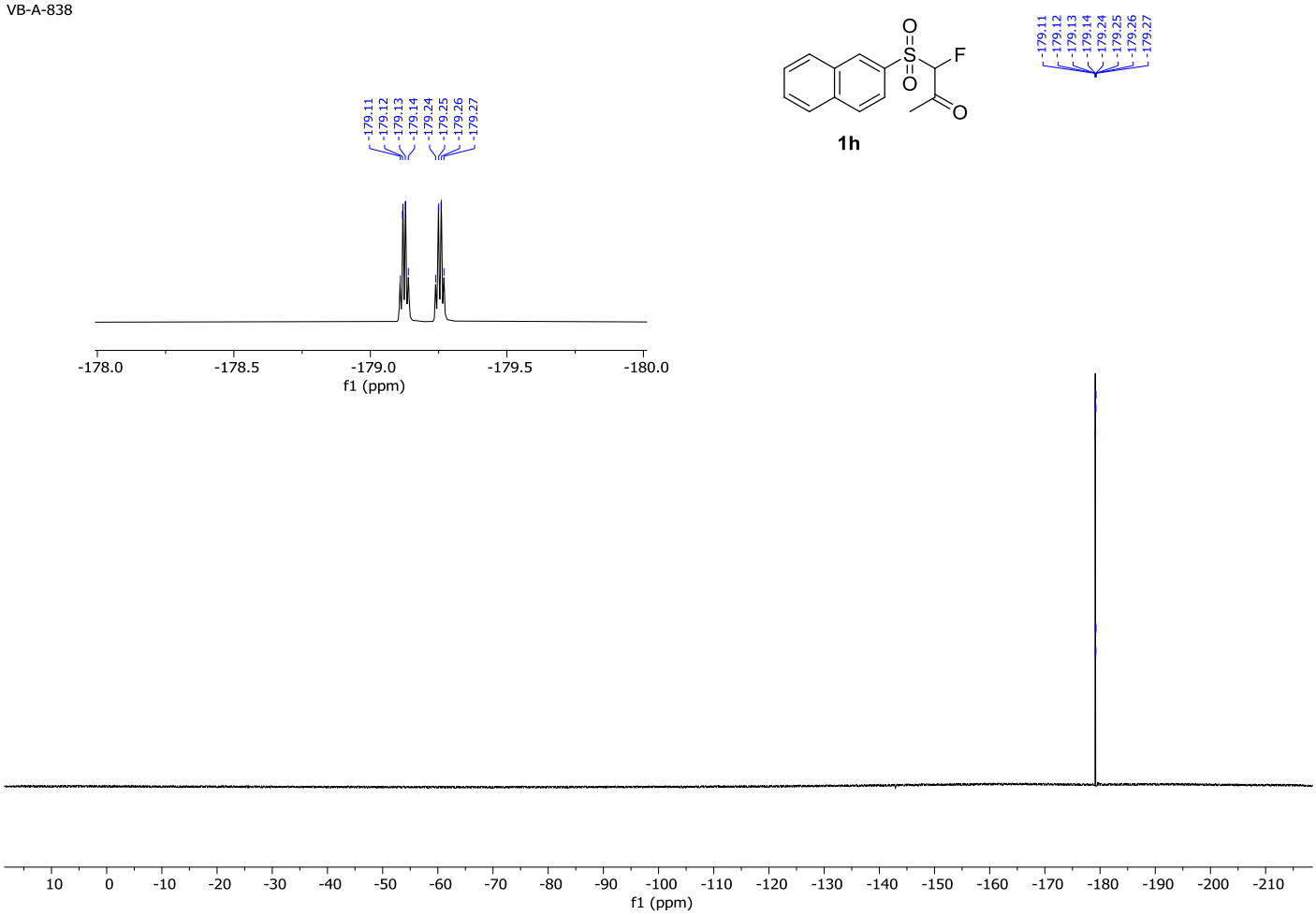
^{19}F NMR (376 MHz, $CDCl_3$)

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



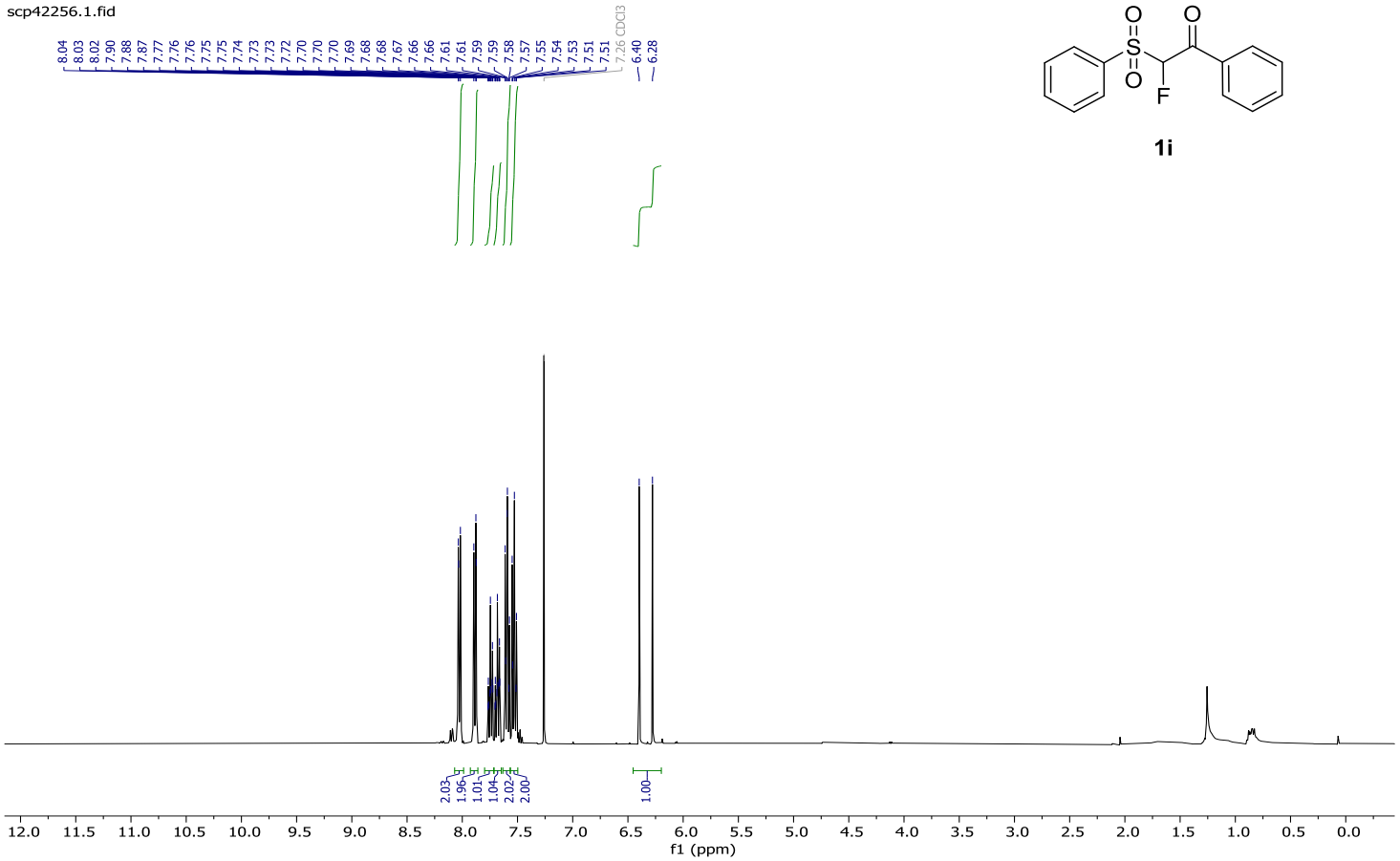


^{13}C NMR (101 MHz, $CDCl_3$)

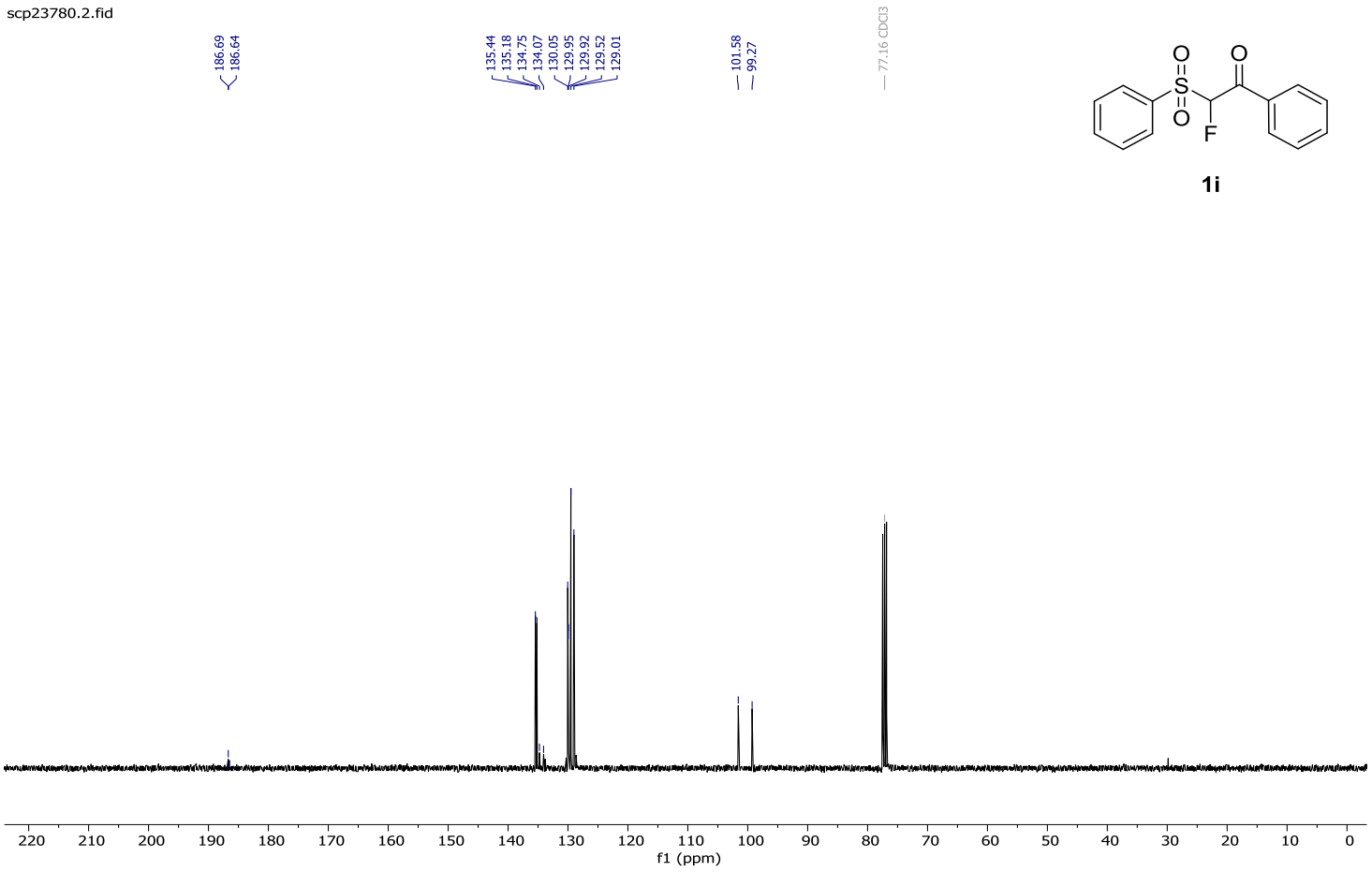


^{19}F NMR (376 MHz, $CDCl_3$)

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

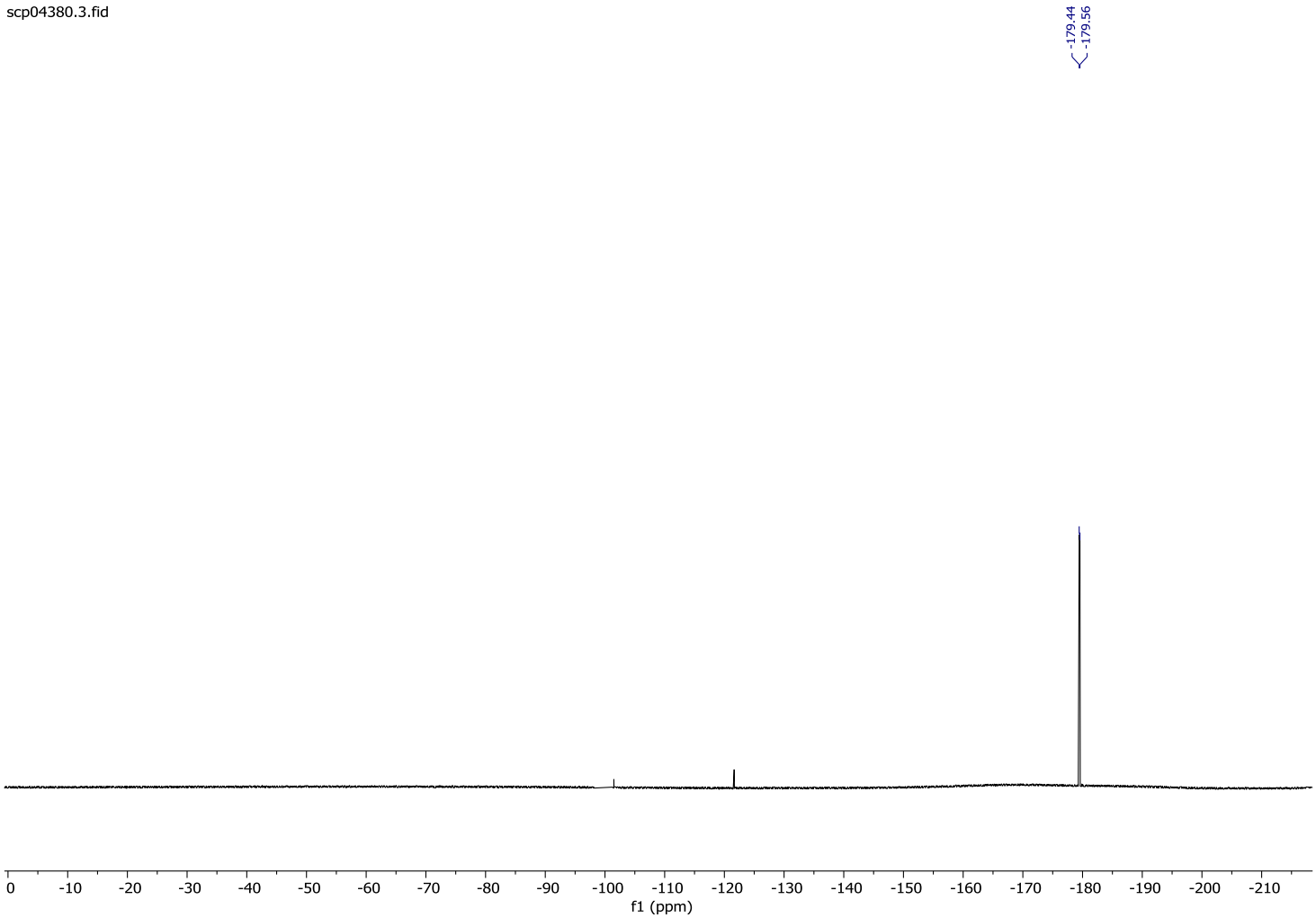


1i



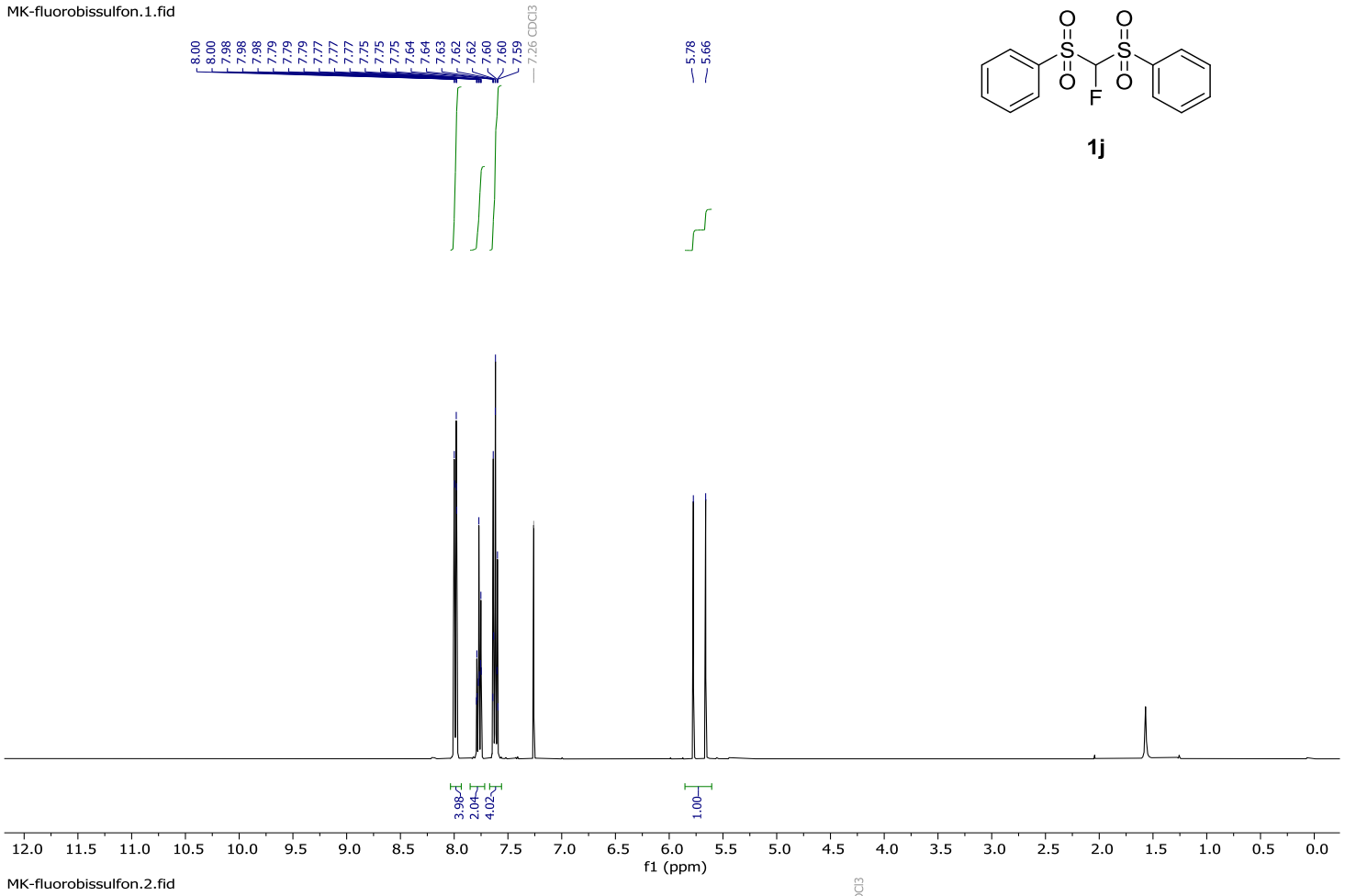
1i

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

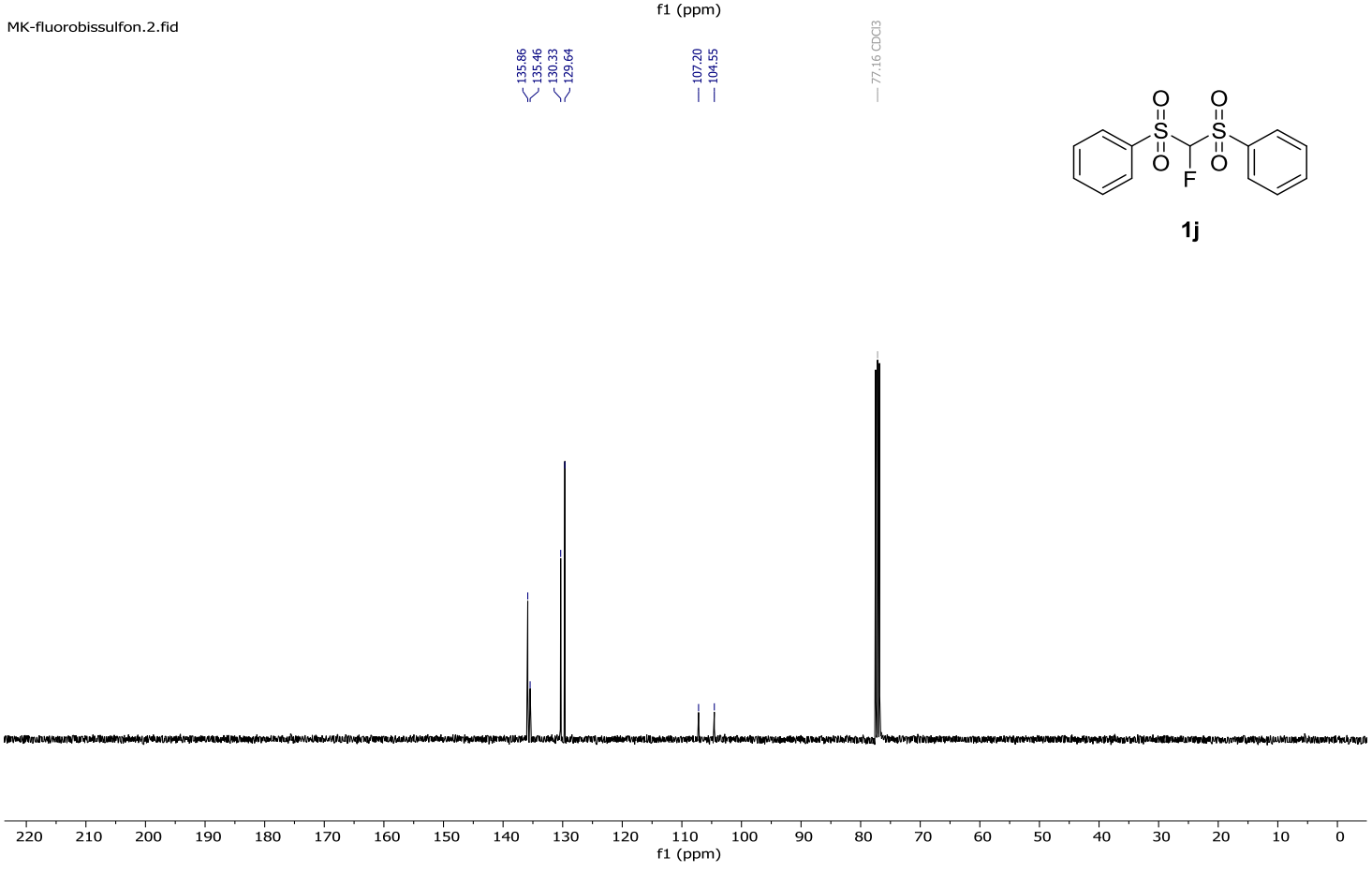


^{19}F NMR (376 MHz, $CDCl_3$)

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

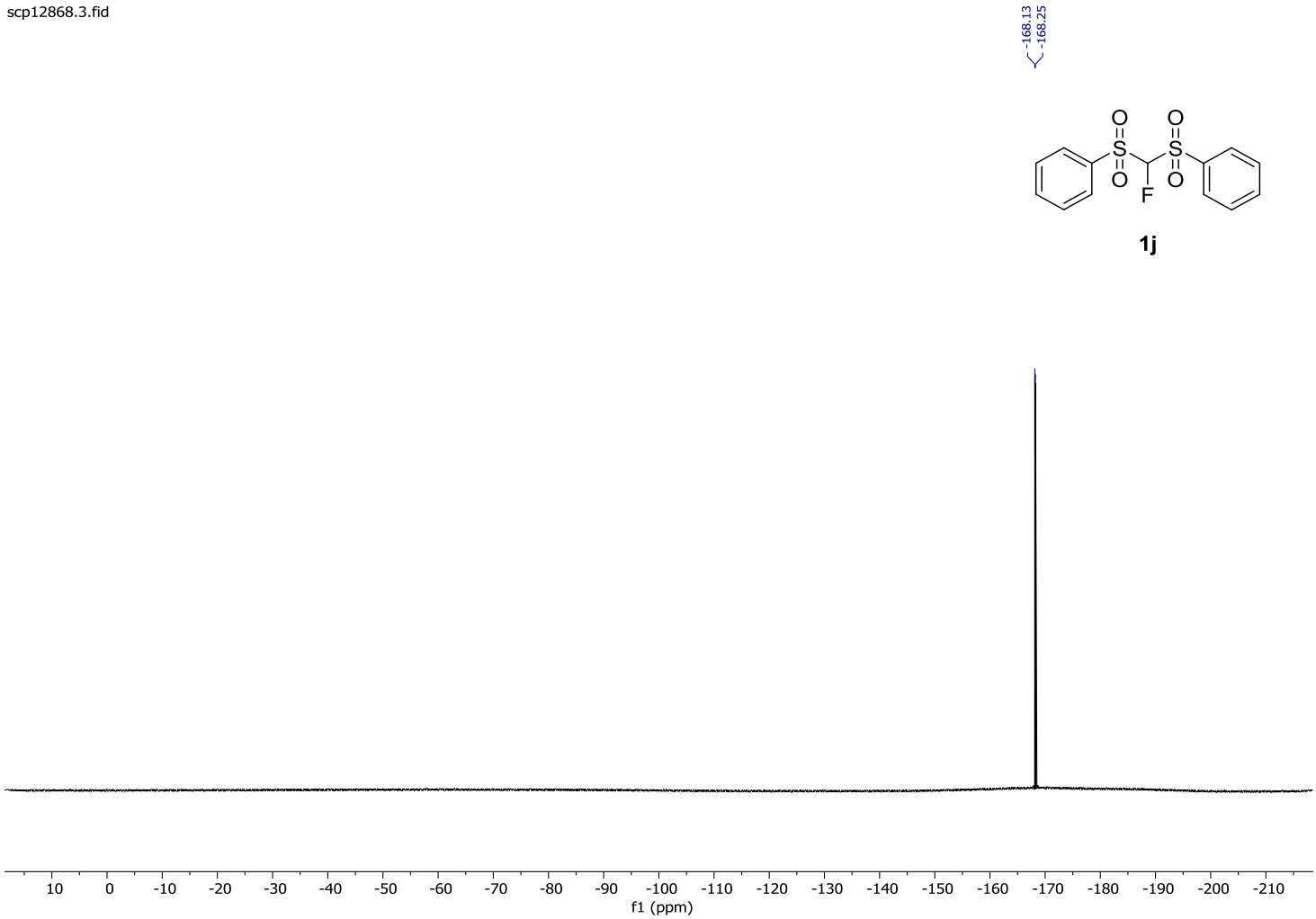


1j



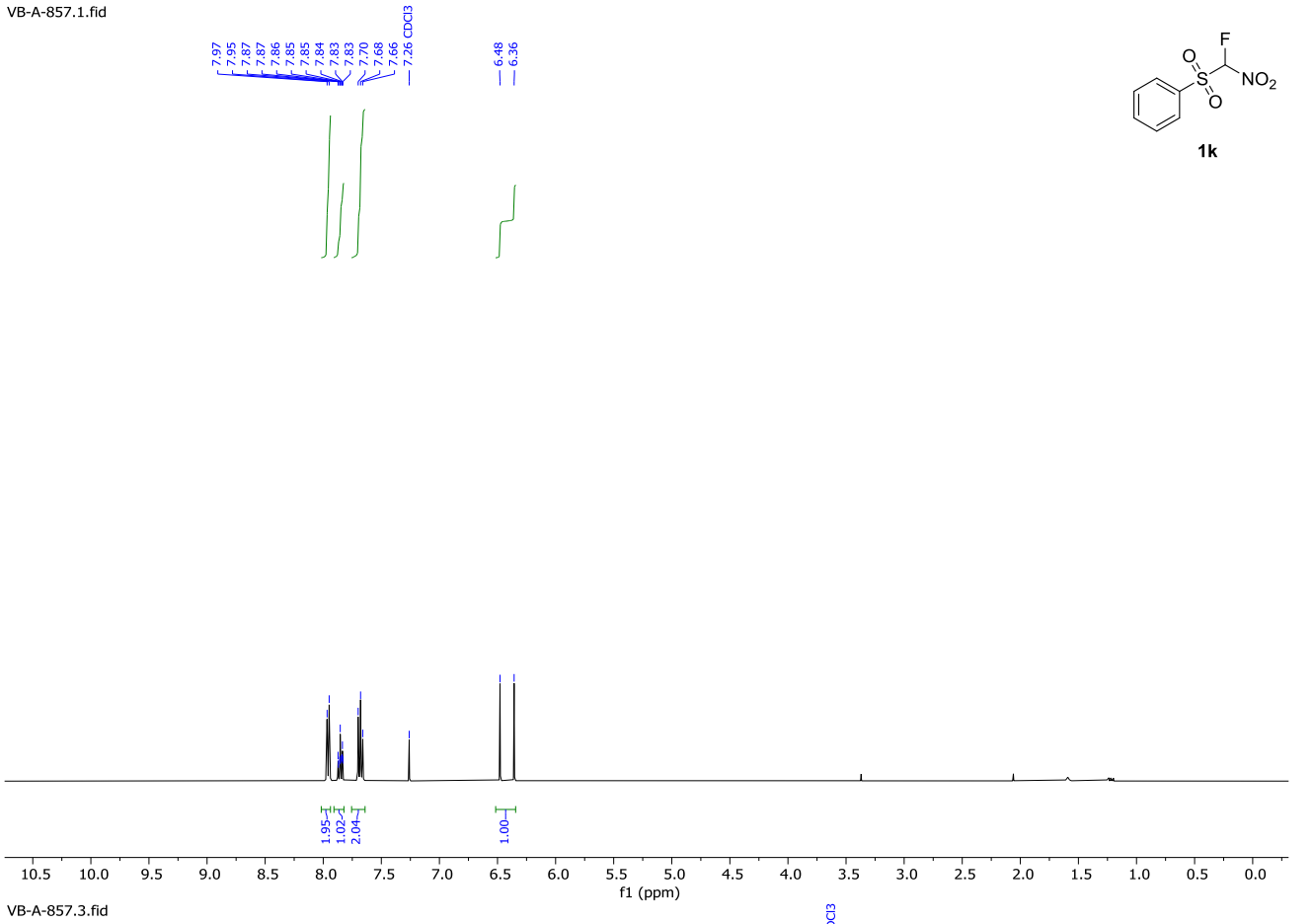
1j

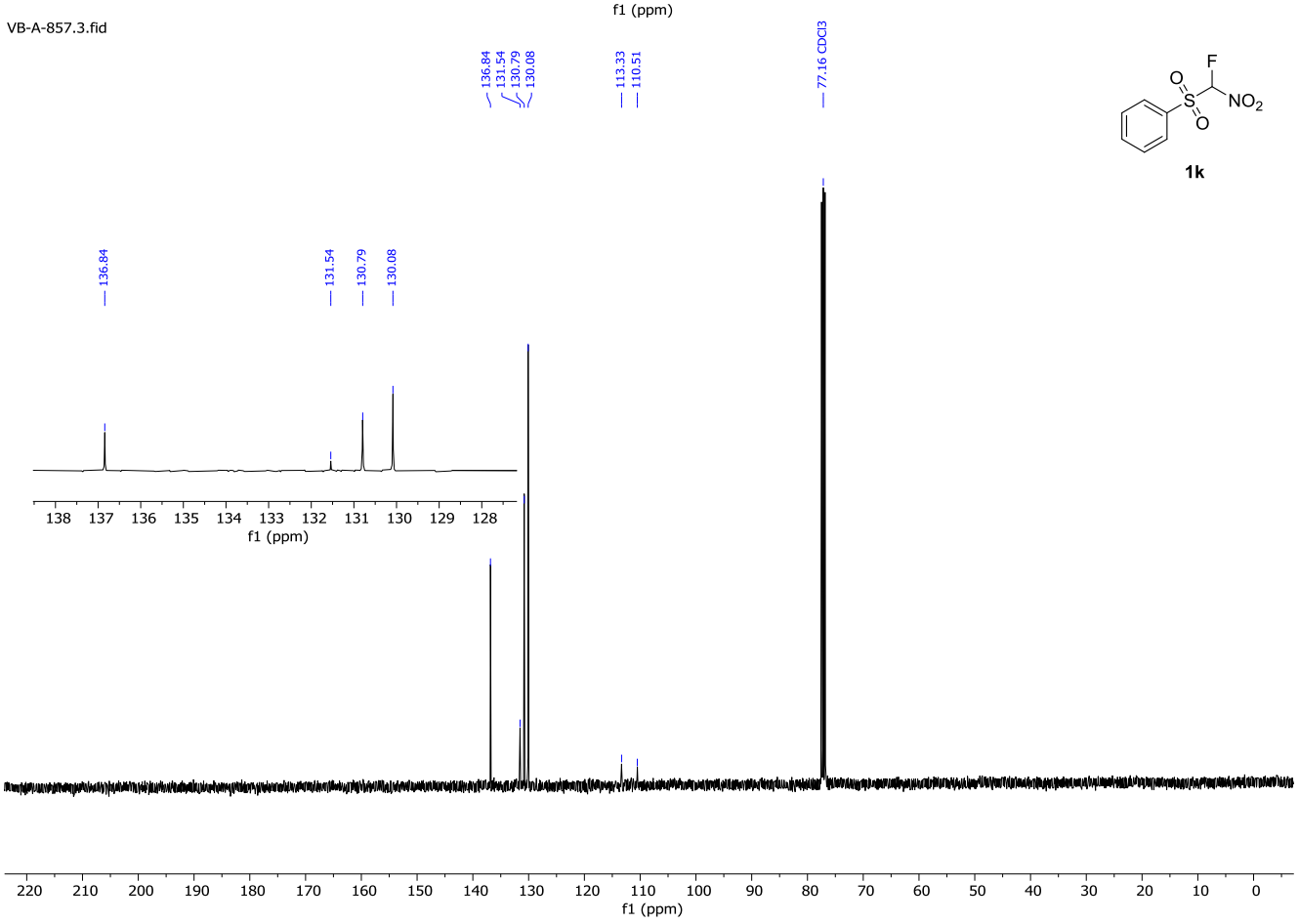
^{13}C NMR (101 MHz, $CDCl_3$)



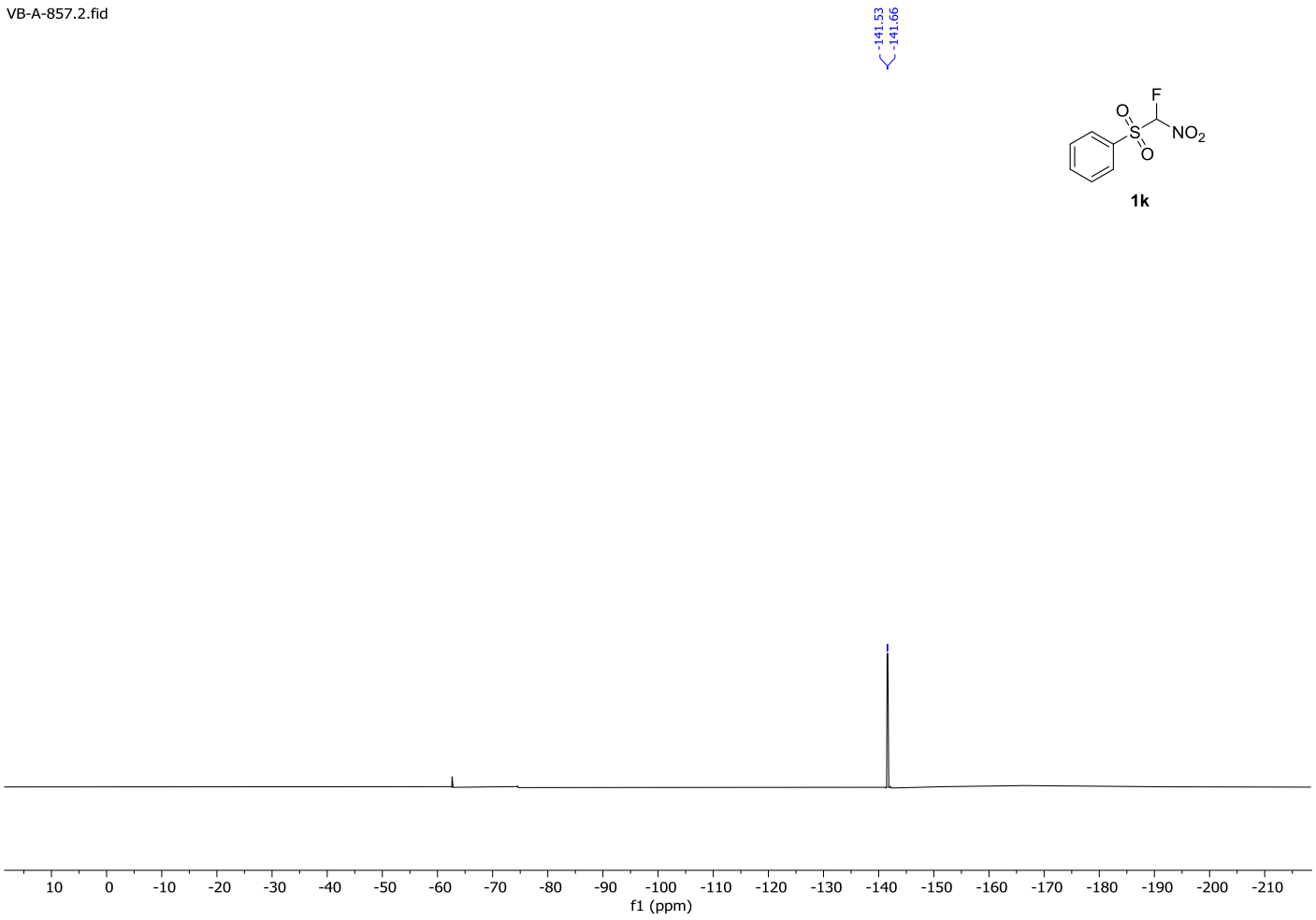
^{19}F NMR (376 MHz, $CDCl_3$)

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



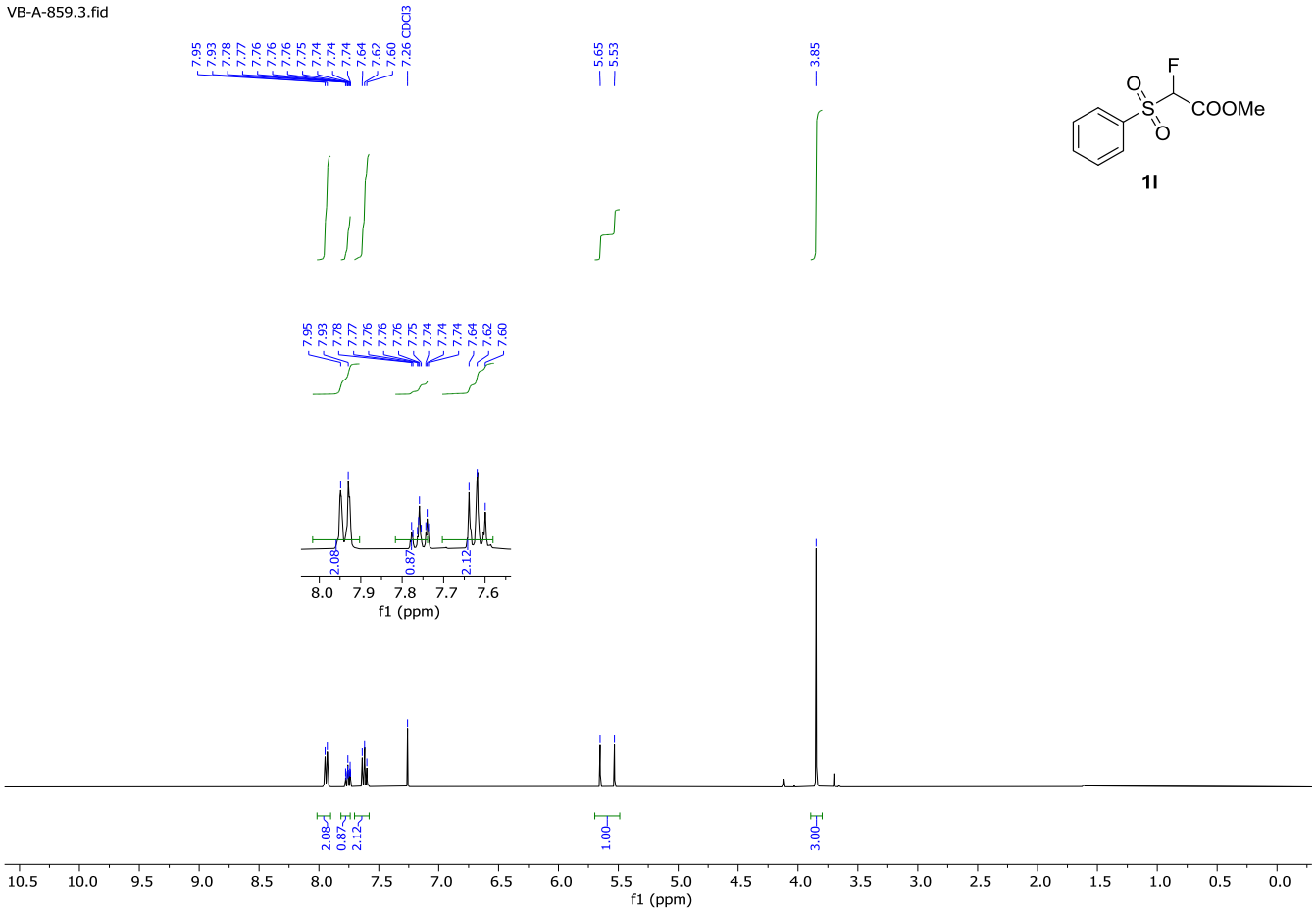


^{13}C NMR (101 MHz, $CDCl_3$)

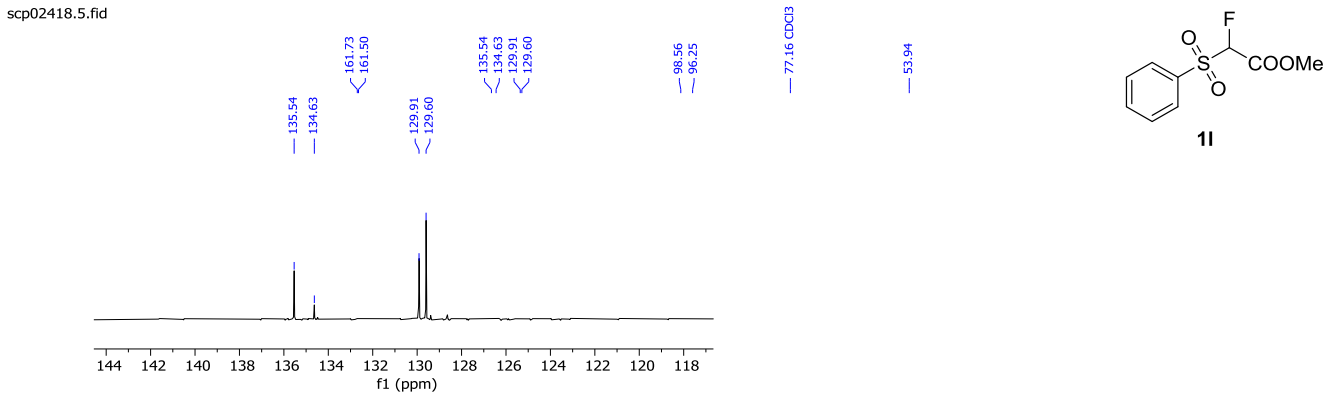


^{19}F NMR (376 MHz, $CDCl_3$)

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

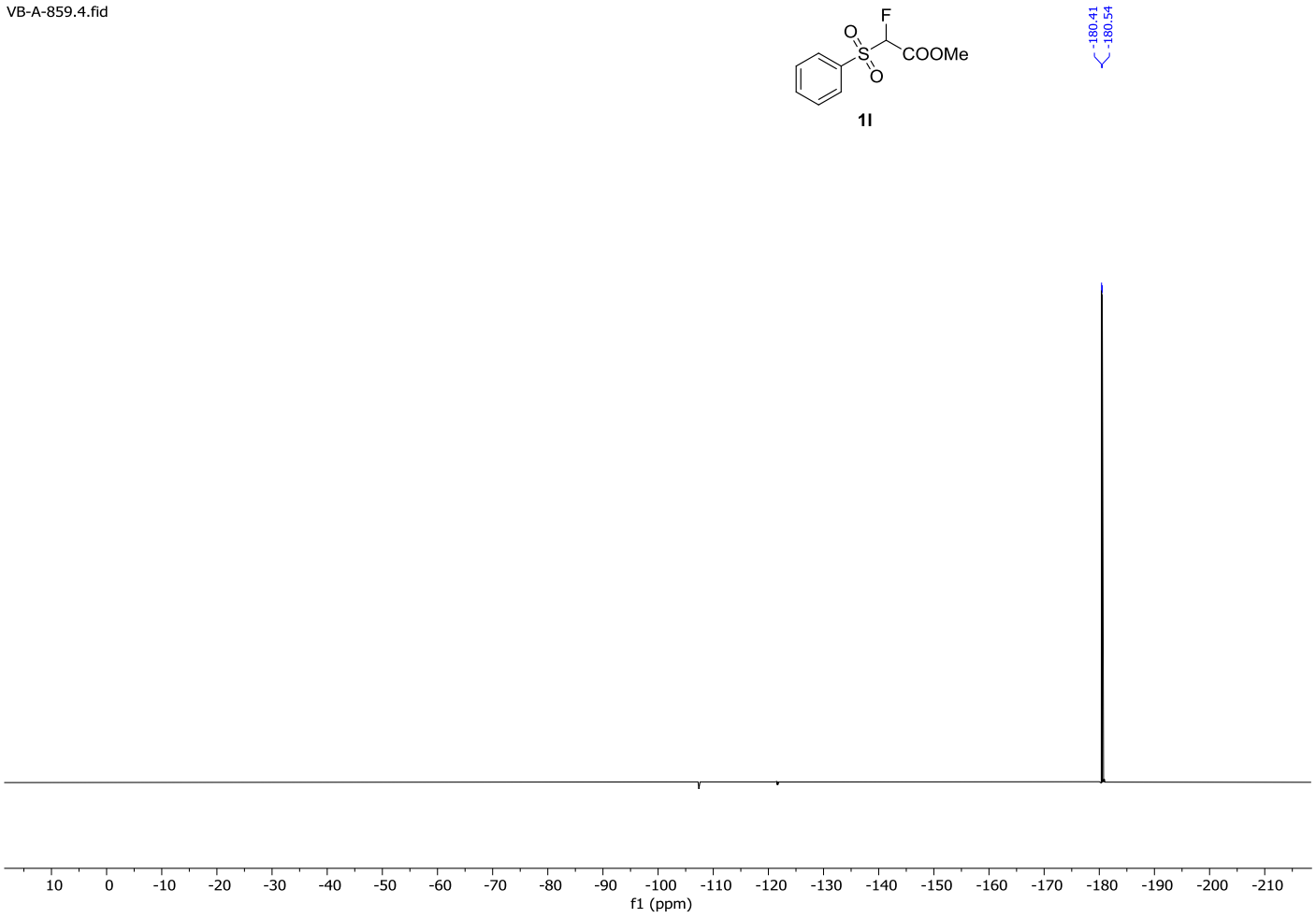


1l



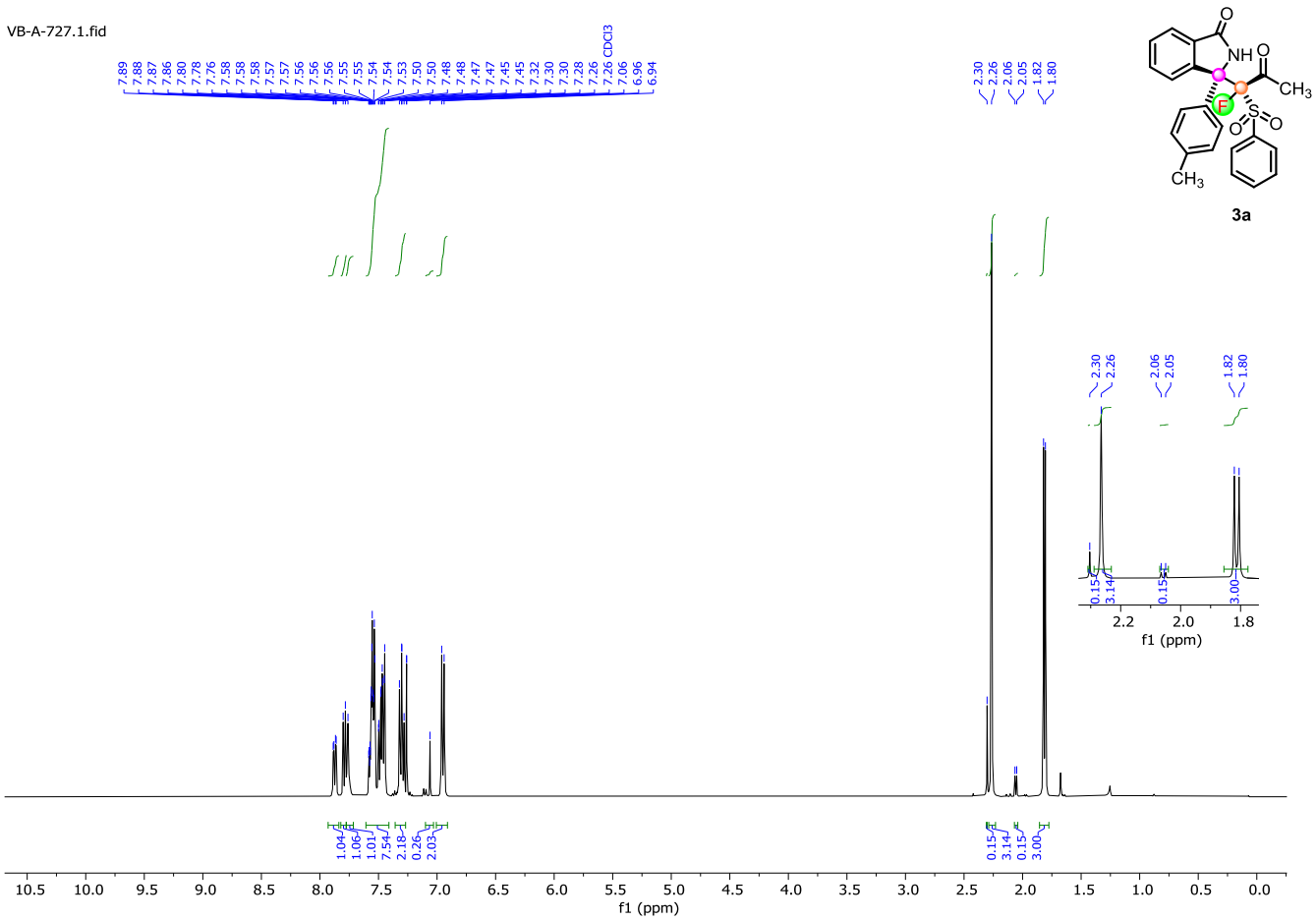
1l

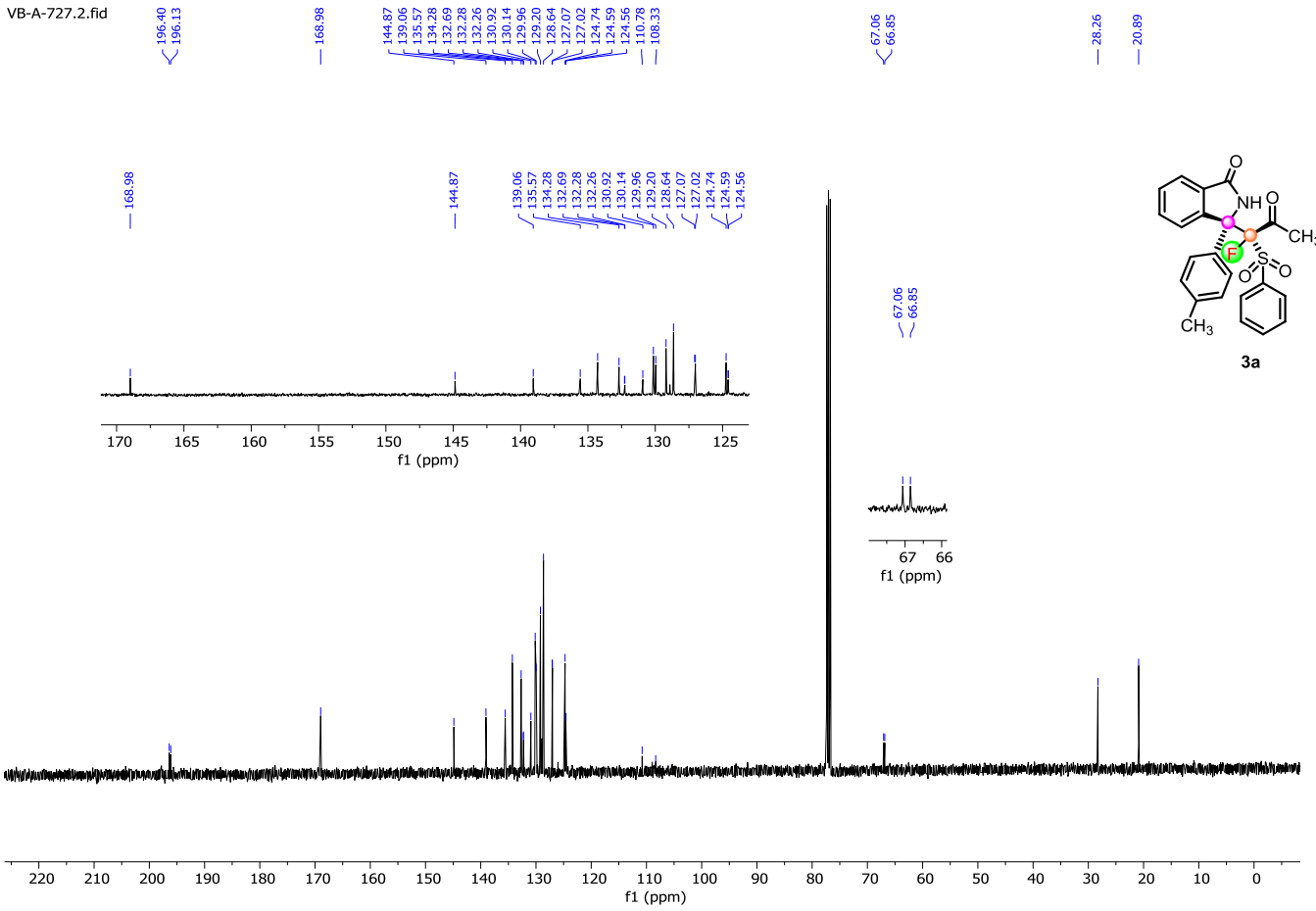
^{13}C NMR (101 MHz, $CDCl_3$)



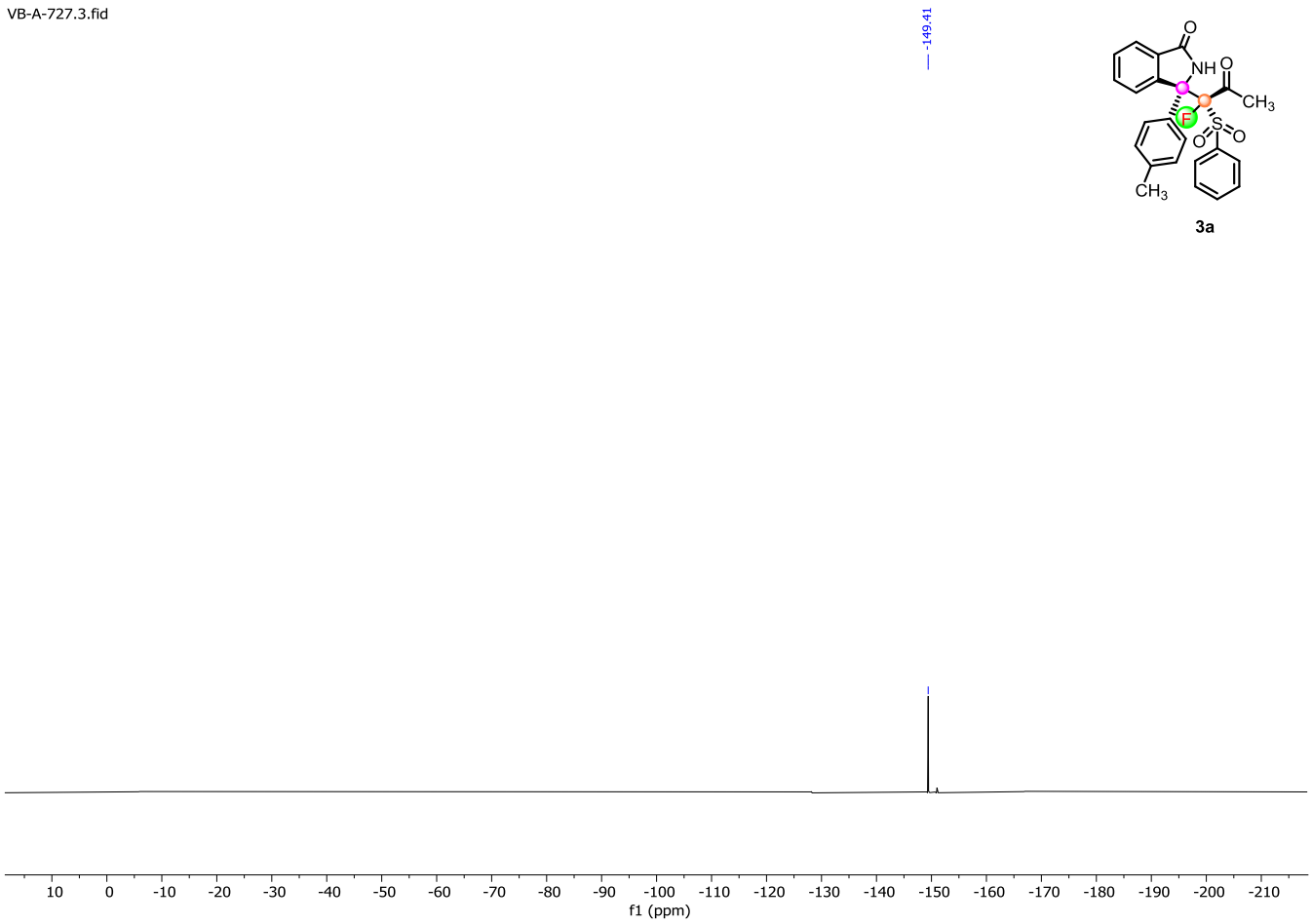
^{19}F NMR (376 MHz, $CDCl_3$)

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

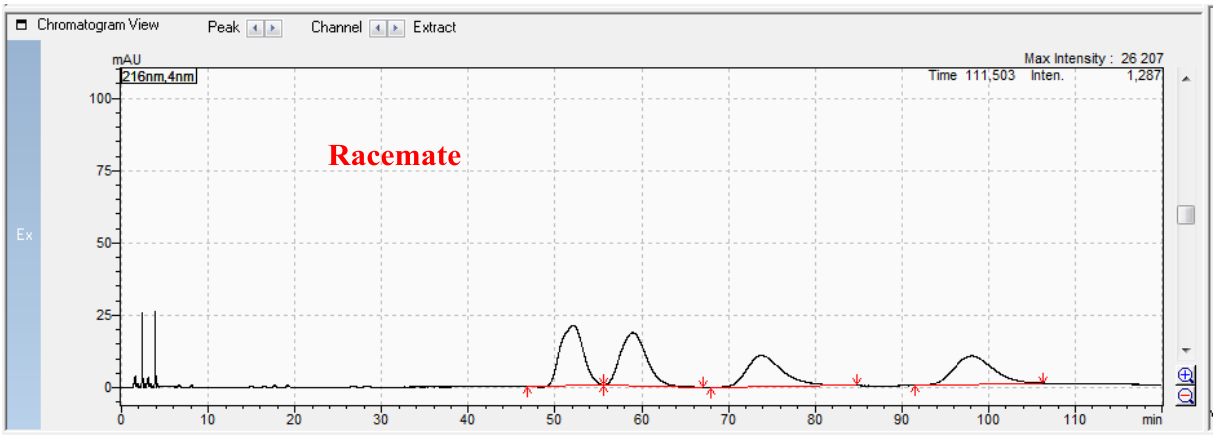




^{13}C NMR (101 MHz, $CDCl_3$)



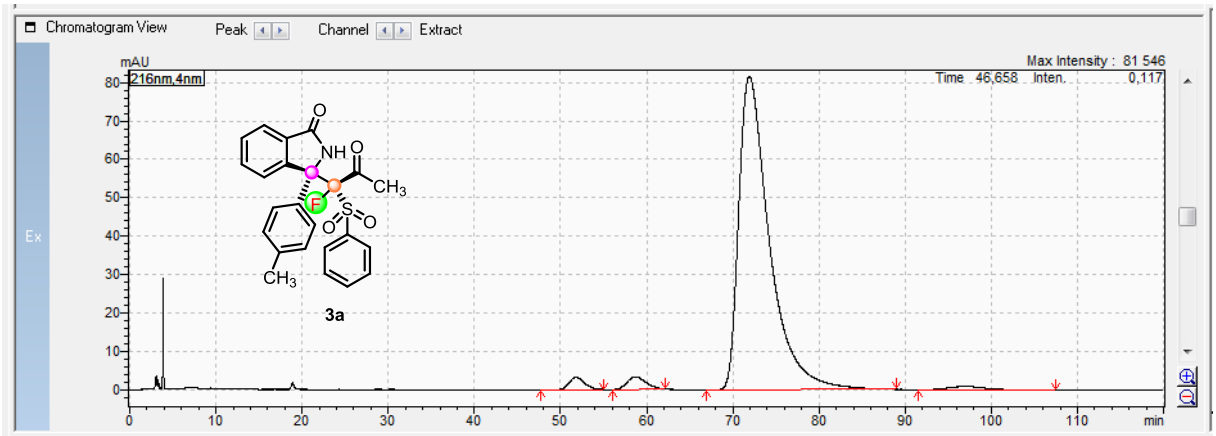
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

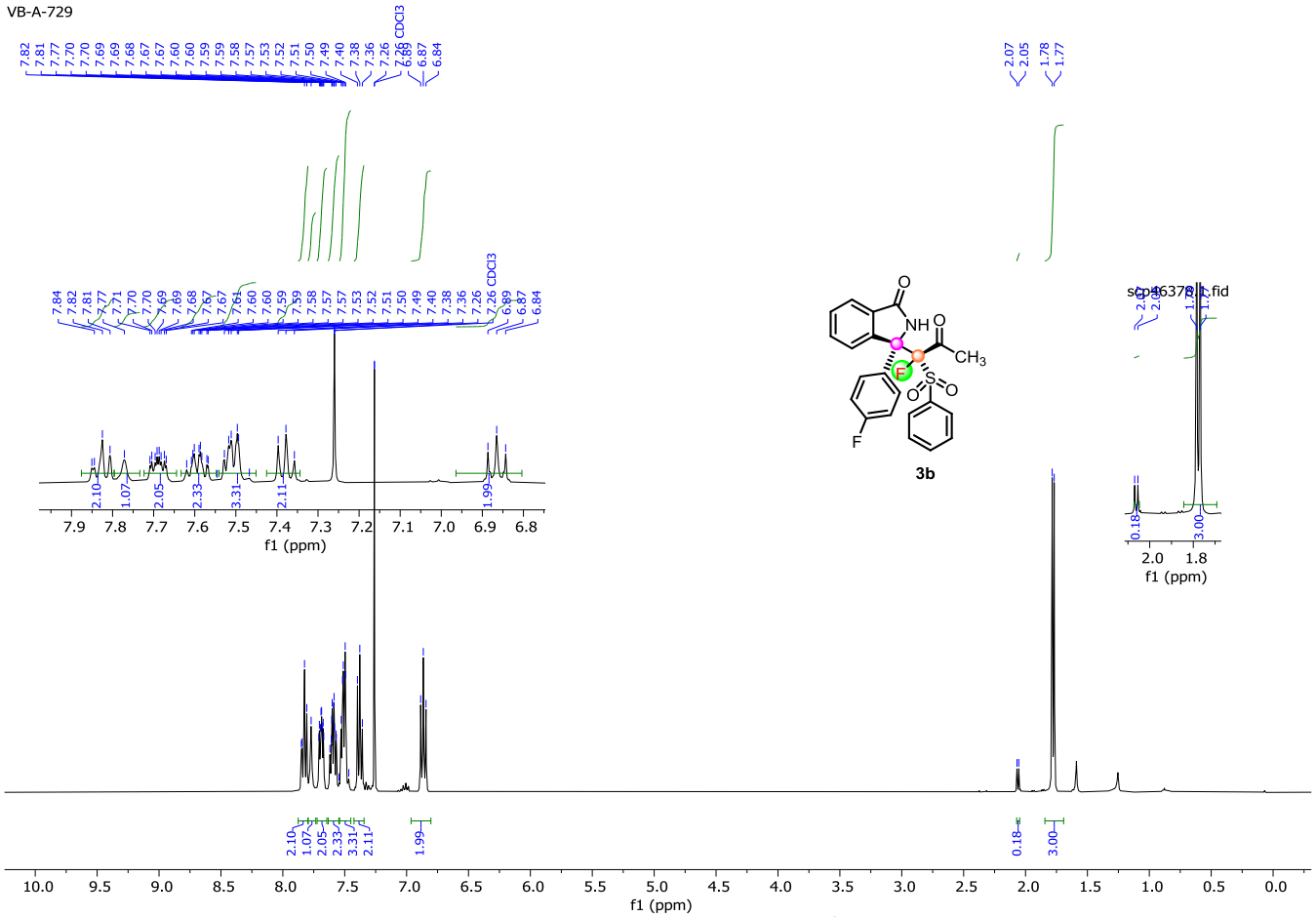
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	52,132	27,260	3740031	20738	0,000000	M	46,805	55,605	27,260
2	59,017	27,471	3769088	18251	0,000000	M	55,605	67,083	27,471
3	73,857	22,720	3117171	10789	0,000000	M	67,979	84,821	22,720
4	97,983	22,549	3093718	9857	0,000000	M	91,531	106,283	22,549
Total		100,000	13720008	59635					100,000

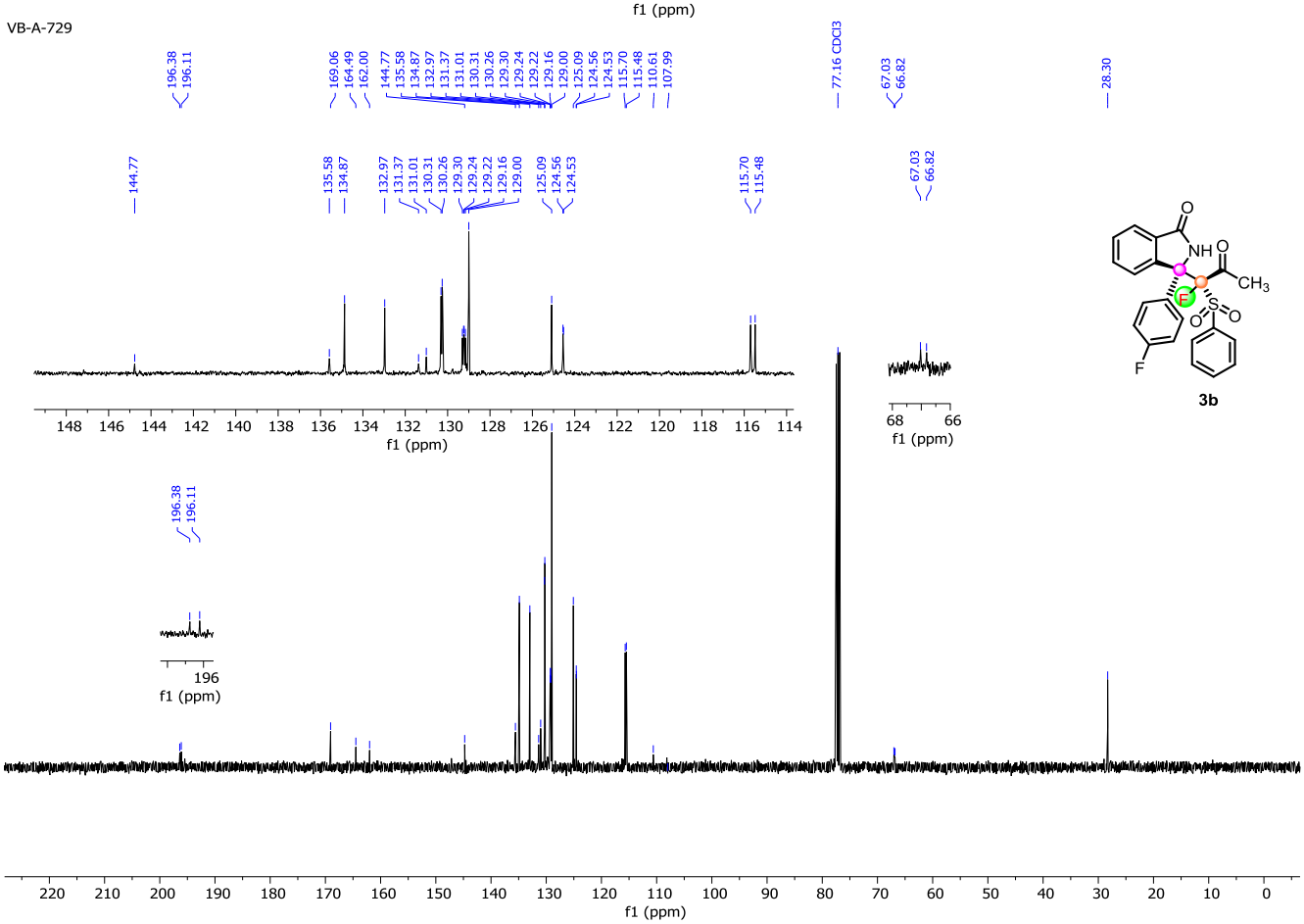


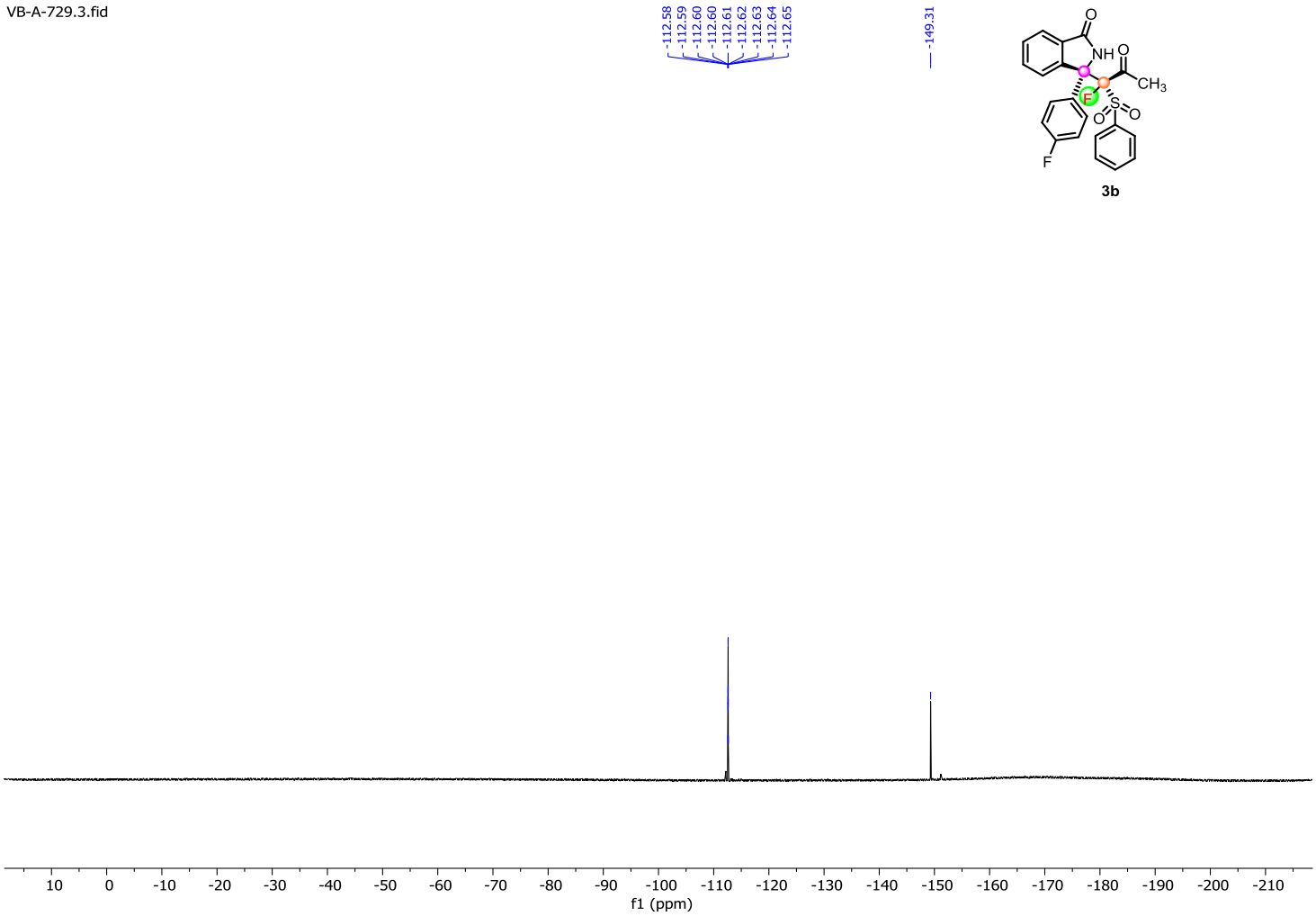
Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

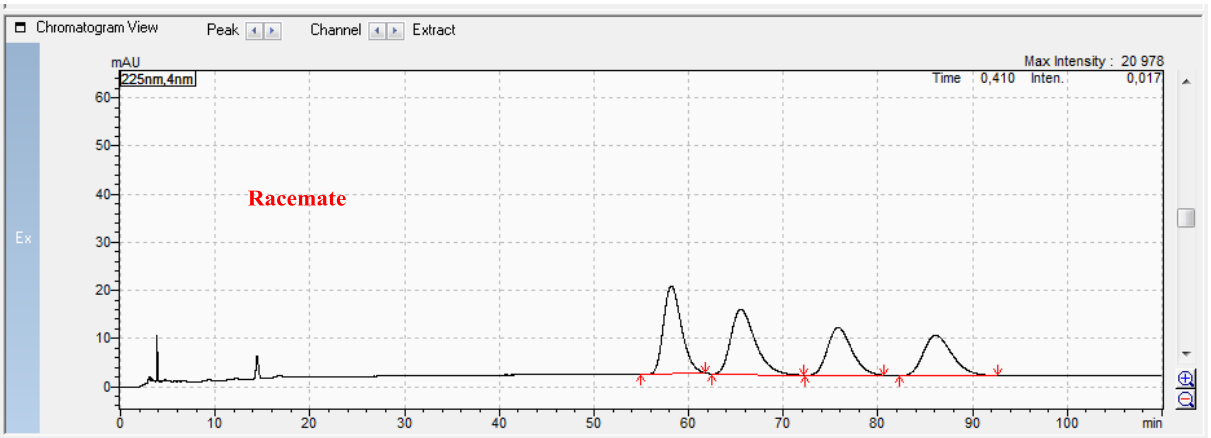
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	51,859	1,859	394828	3230	0,000000	M	47,701	55,008	1,859
2	58,782	2,352	499552	3277	0,000000	M	56,053	62,165	2,352
3	71,892	94,671	20108609	81405	0,000000	M	66,933	88,992	94,671
4	96,847	1,118	237469	889	0,000000	M	91,531	107,477	1,118
Total		100,000	21240458	88801					100,000


VB-A-729
CDCl3
2.10
1.07
2.05
2.33
3.31
2.11
1.99
0.18
3.00
f1 (ppm)
3b
scp46378_1.1.fid


VB-A-729
CDCl3
f1 (ppm)
196
3b



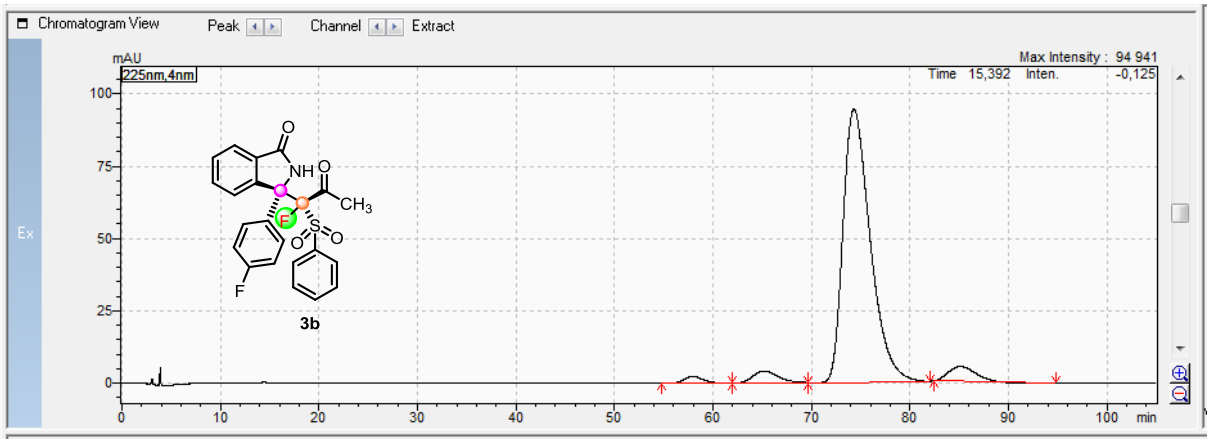
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	58,153	28,774	2411697	18286	0,000000	M	54,933	61,771	28,774
2	65,541	28,718	2407027	13488	0,000000	M	62,453	72,149	28,718
3	75,820	21,113	1769595	9952	0,000000	M	72,288	80,629	21,113
4	86,136	21,395	1793187	8451	0,000000	M	82,261	92,651	21,395
Total		100,000	8381506	50178					100,000

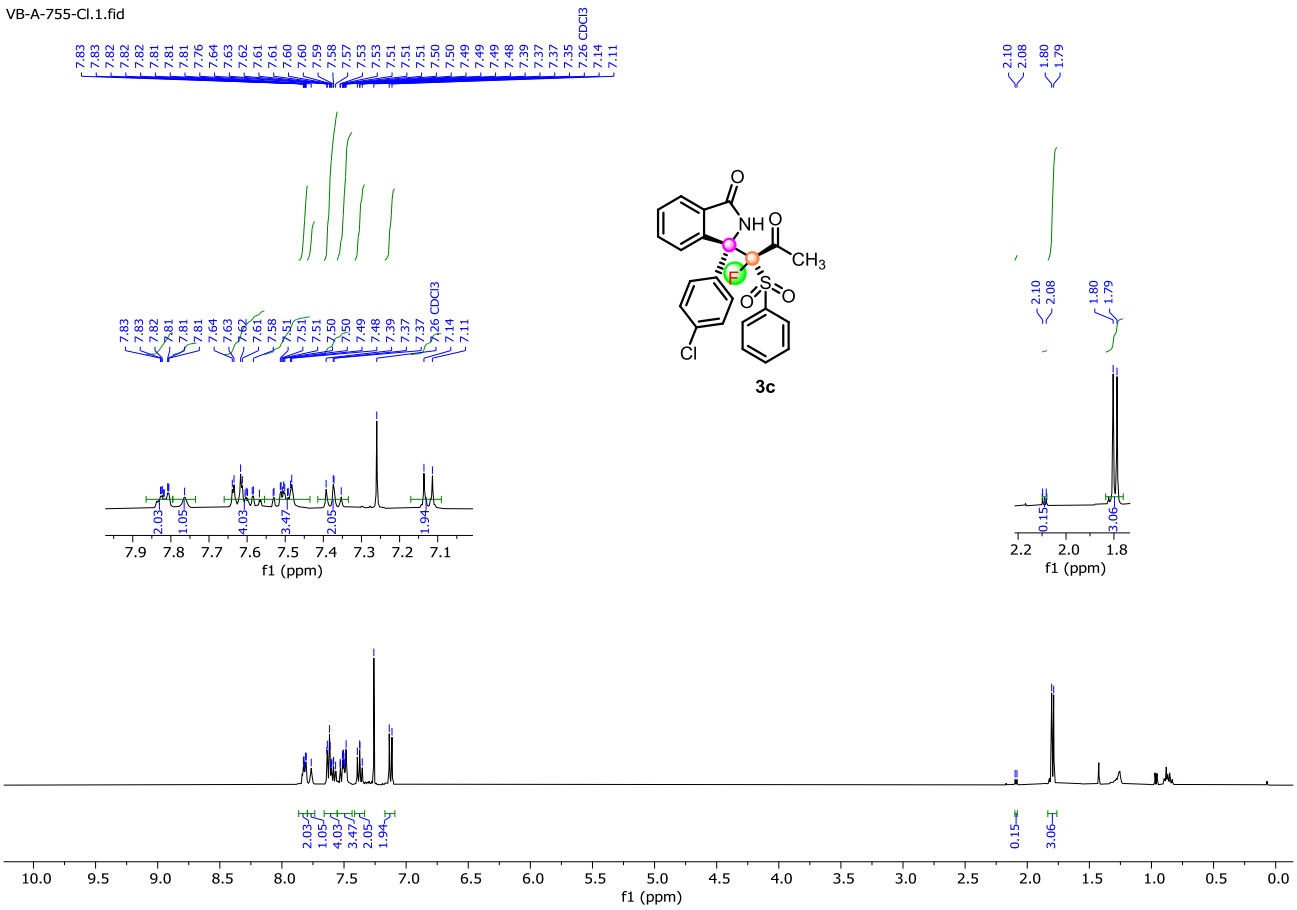


Results View - Peak Table

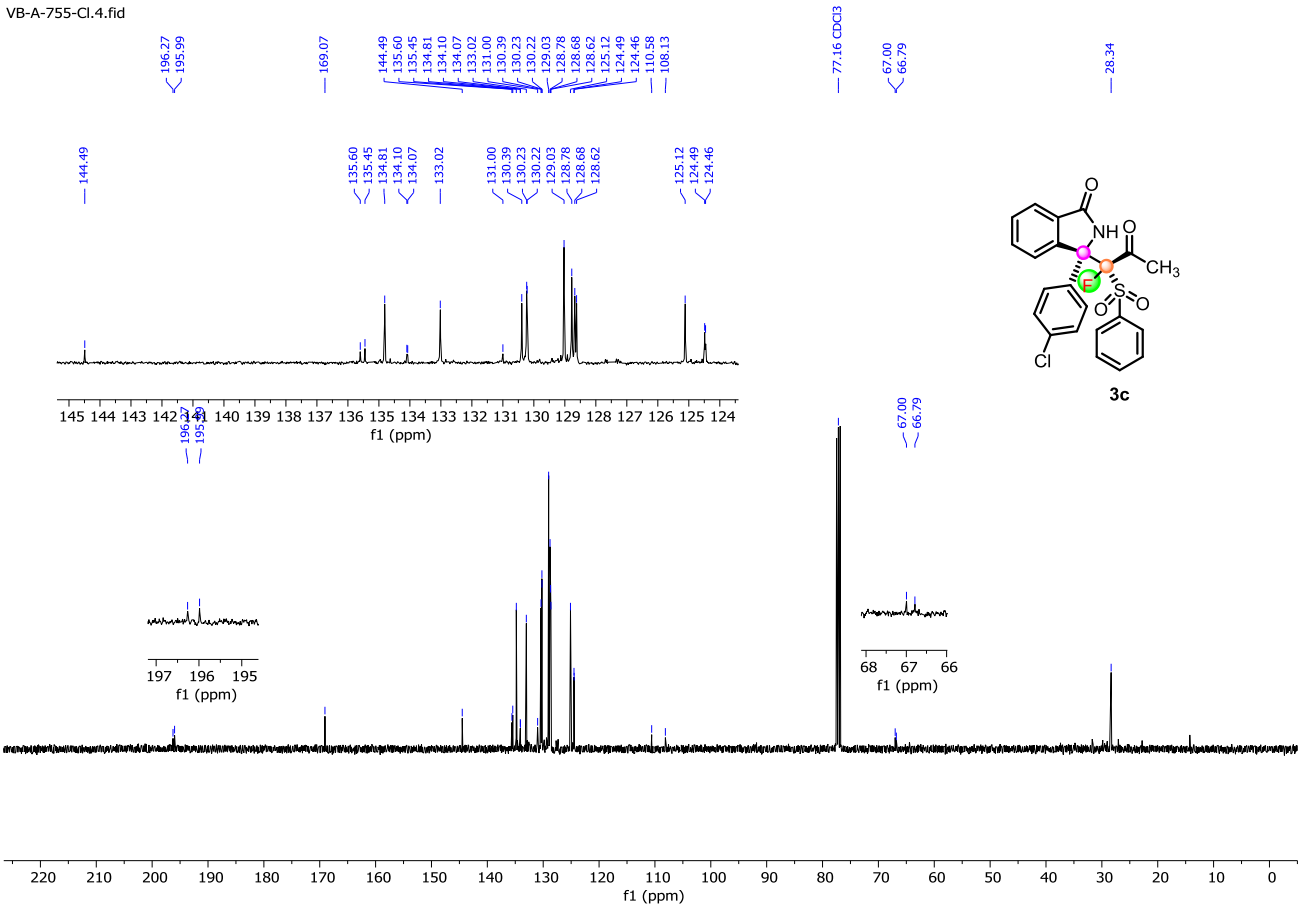
Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	57,931	1,561	313394	2365	0,000000	M	54,784	61,963	1,561
2	65,213	3,591	720876	4149	0,000000	M	61,963	69,653	3,591
3	74,315	90,078	18082506	94585	0,000000	M	69,653	82,048	90,078
4	85,089	4,770	957609	5132	0,000000	M	82,432	94,827	4,770
Total		100,000	20074386	106230					100,000

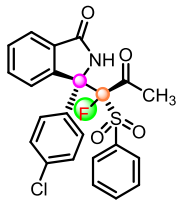
VB-A-755-Cl.1.fid



VB-A-755-Cl.4.fid

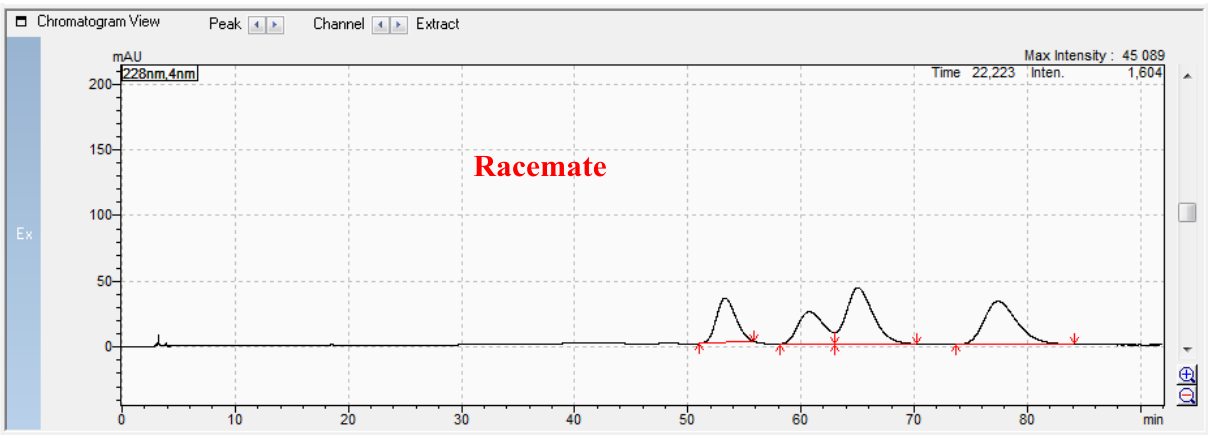


VB-A-755-Cl.3.fid



3c

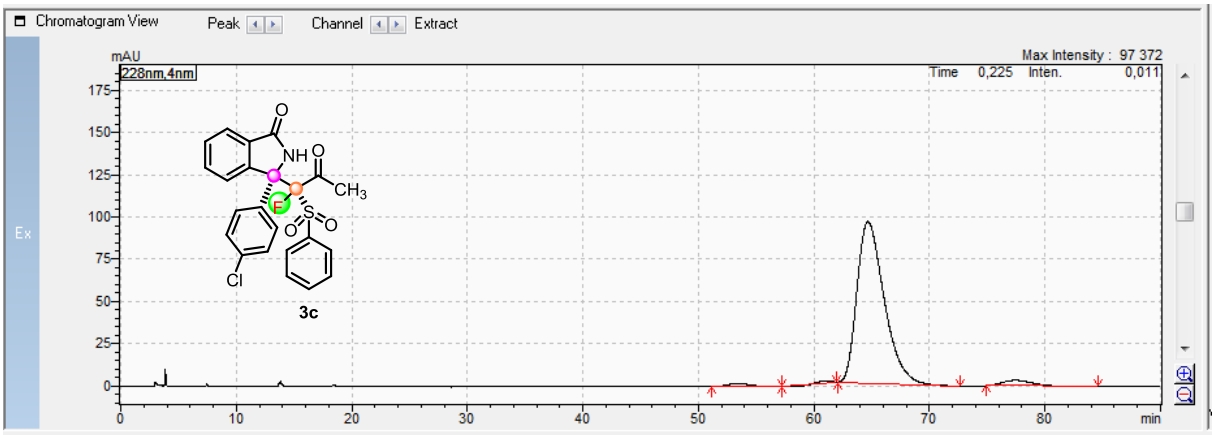
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

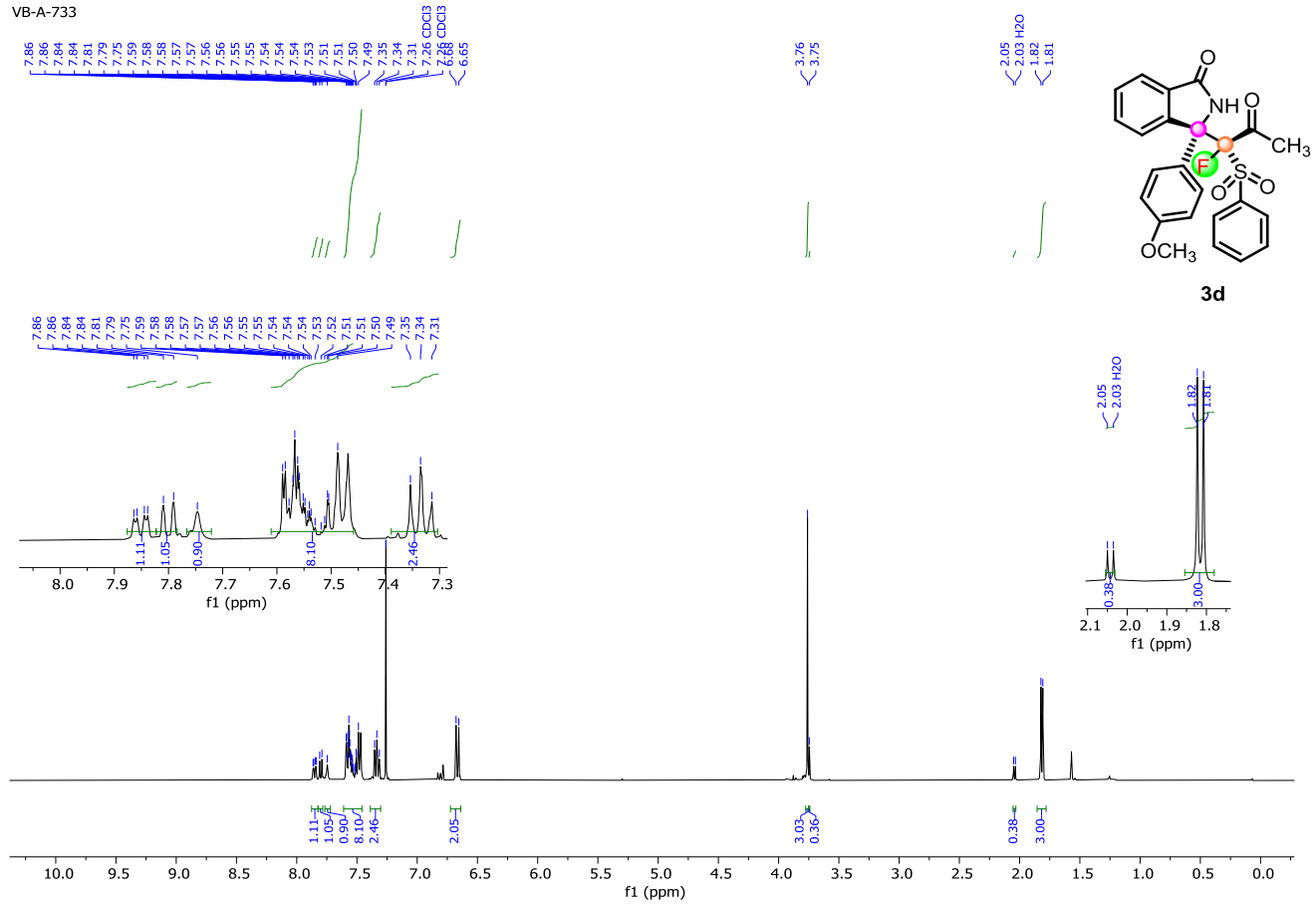
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	53,300	18,486	4012695	33851	0,000000	M	51,008	55,840	18,486
2	60,747	17,862	3877342	24534	0,000000		58,133	62,965	17,862
3	65,026	32,733	7105324	42688	0,000000	V	62,965	70,261	32,733
4	77,411	30,919	6711691	32858	0,000000	M	73,696	84,171	30,919
Total		100,000	21707052	133931					100,000

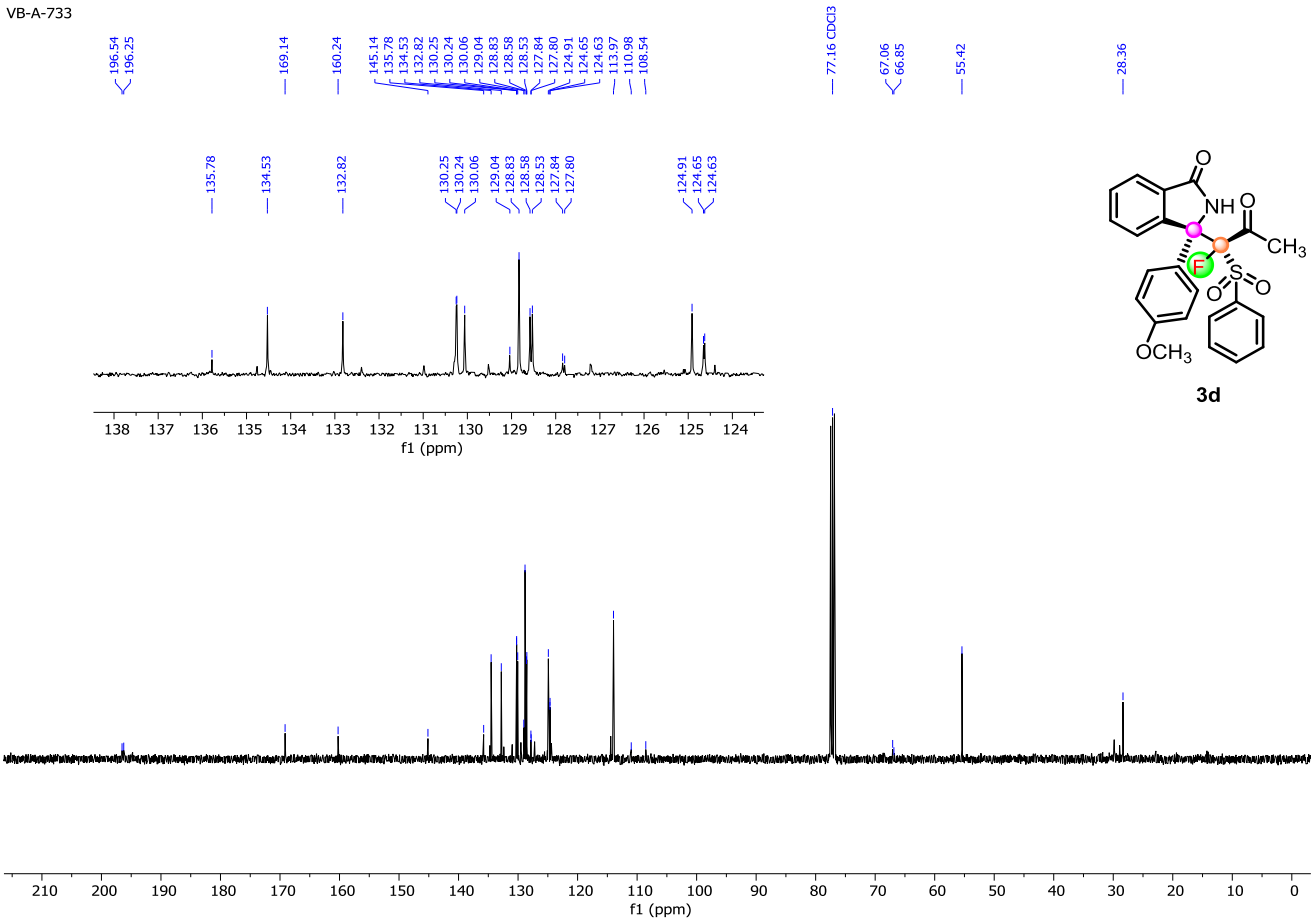


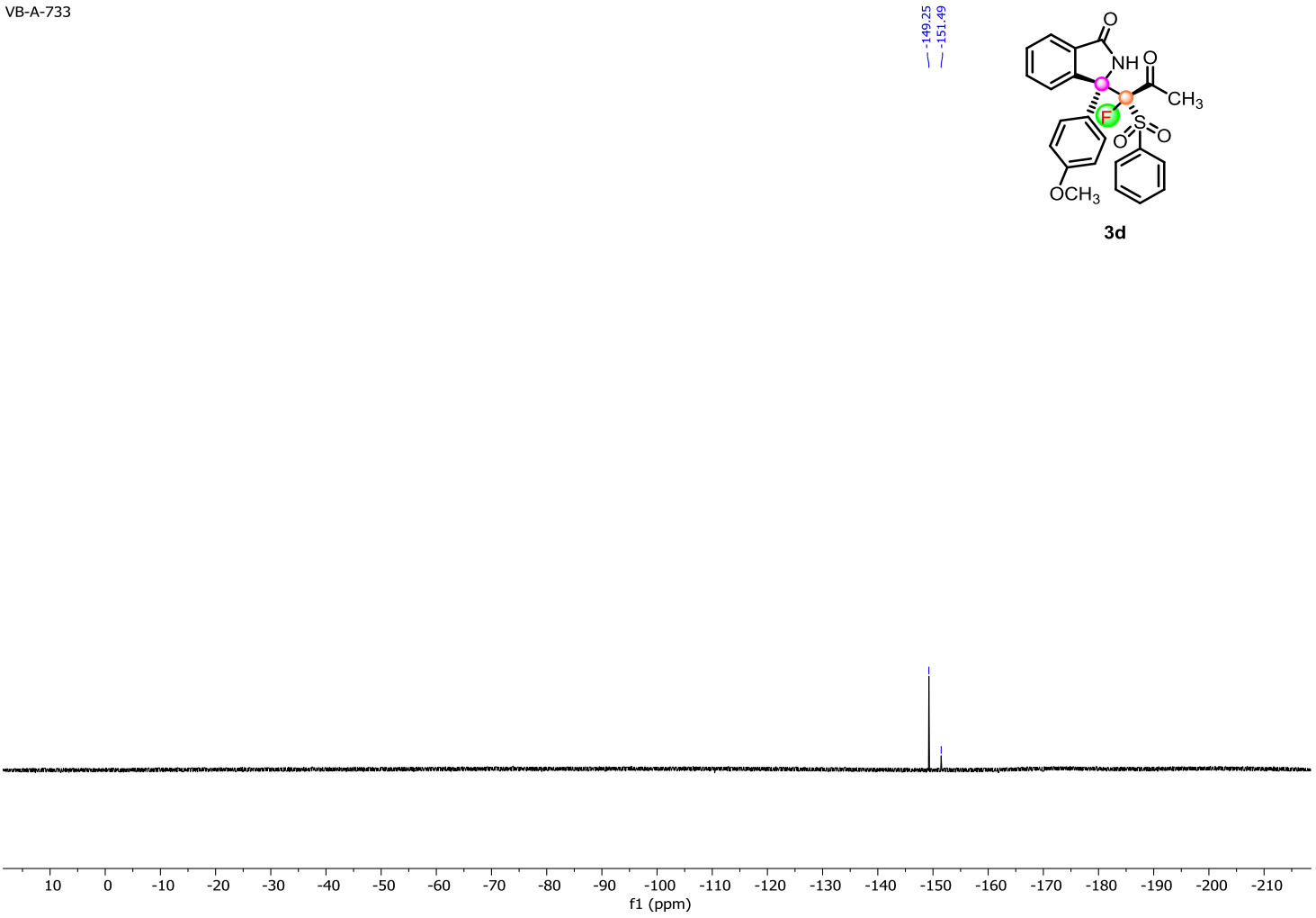
Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

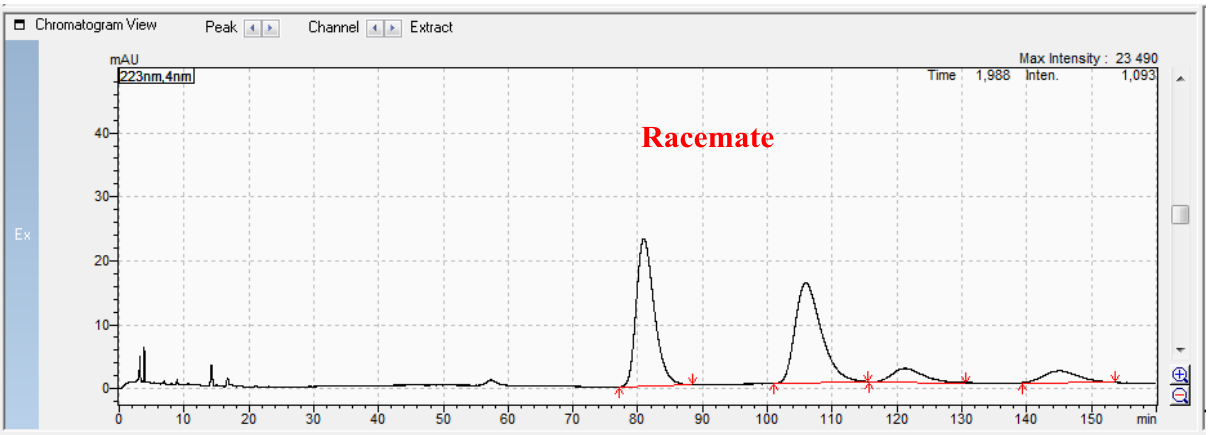
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	53,501	1,337	220788	1819	0,000000	M	51,147	57,227	1,337
2	61,034	0,181	29953	1095	0,000000	M	57,227	61,952	0,181
3	64,660	94,783	15653689	95627	0,000000	M	62,069	72,661	94,783
4	77,422	3,699	610944	3333	0,000000	M	74,912	84,597	3,699
Total		100,000	16515373	101874					100,000


VB-A-733
3d
f1 (ppm)


VB-A-733
3d
f1 (ppm)



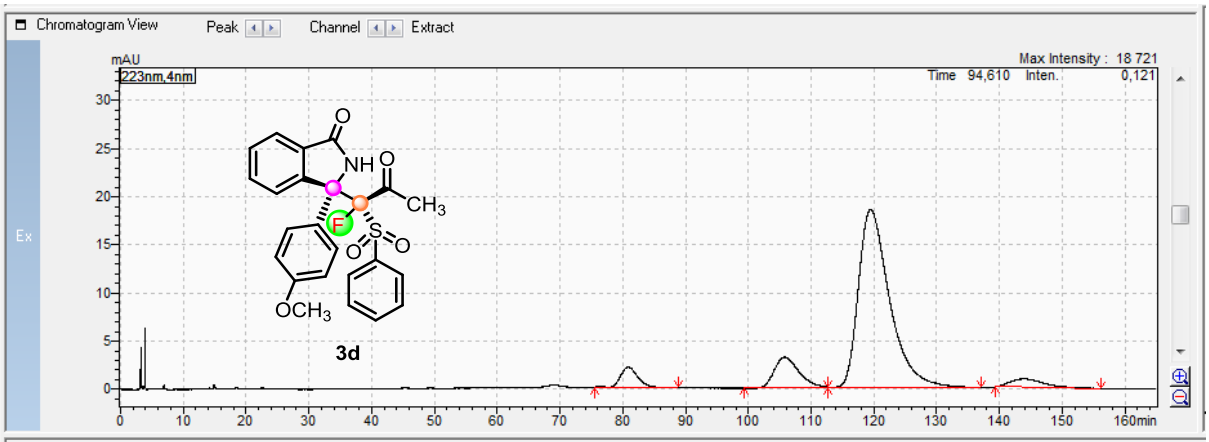
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

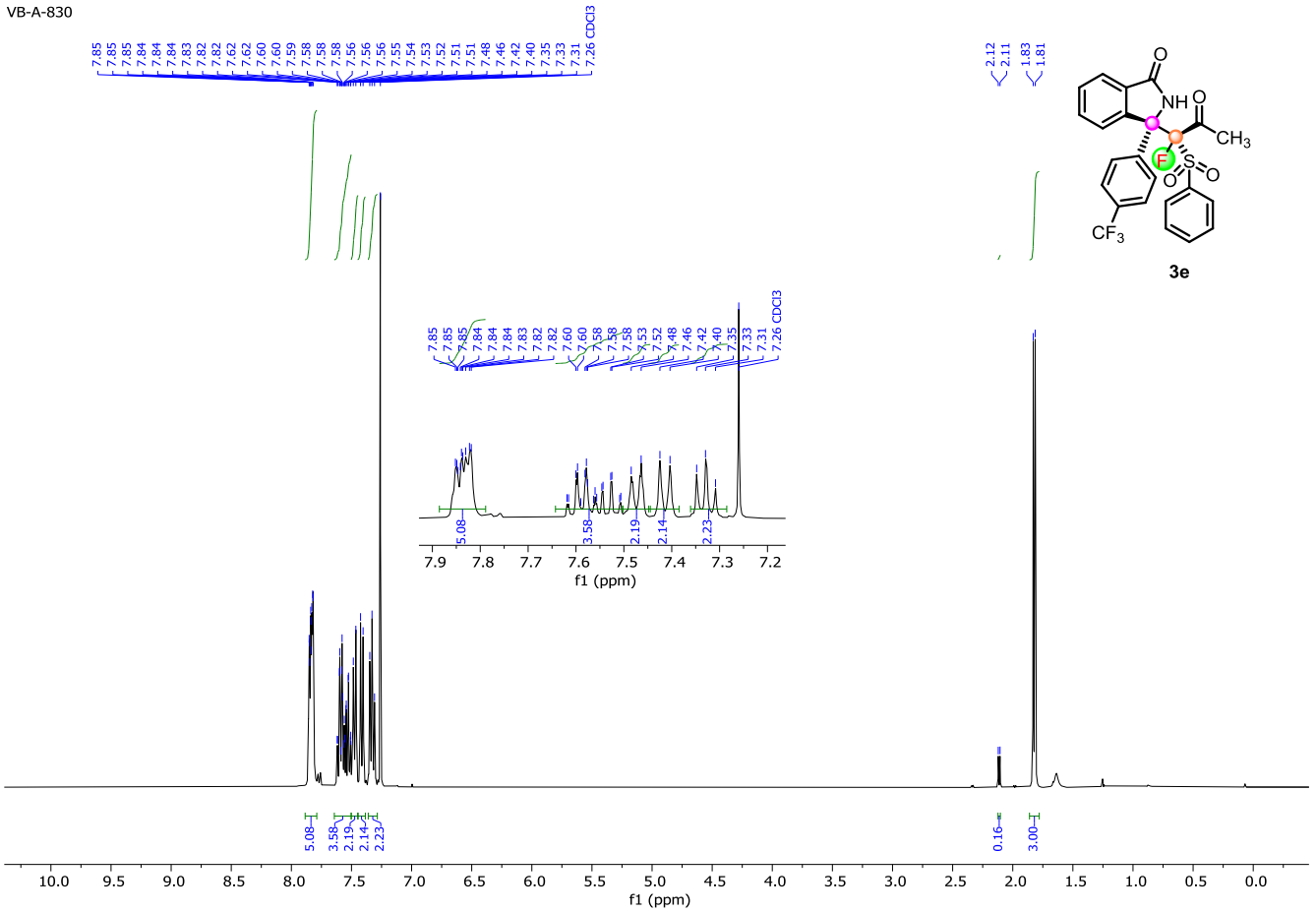
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	80,929	43,444	4447614	23081	0,000000	M	77,120	88,448	43,444
2	105,966	42,958	4397903	15689	0,000000	M	100,971	115,477	42,958
3	121,322	6,811	697242	2145	0,000000	M	115,680	130,581	6,811
4	144,899	6,788	694882	1848	0,000000	M	139,328	153,643	6,788
Total		100,000	10237642	42763					100,000

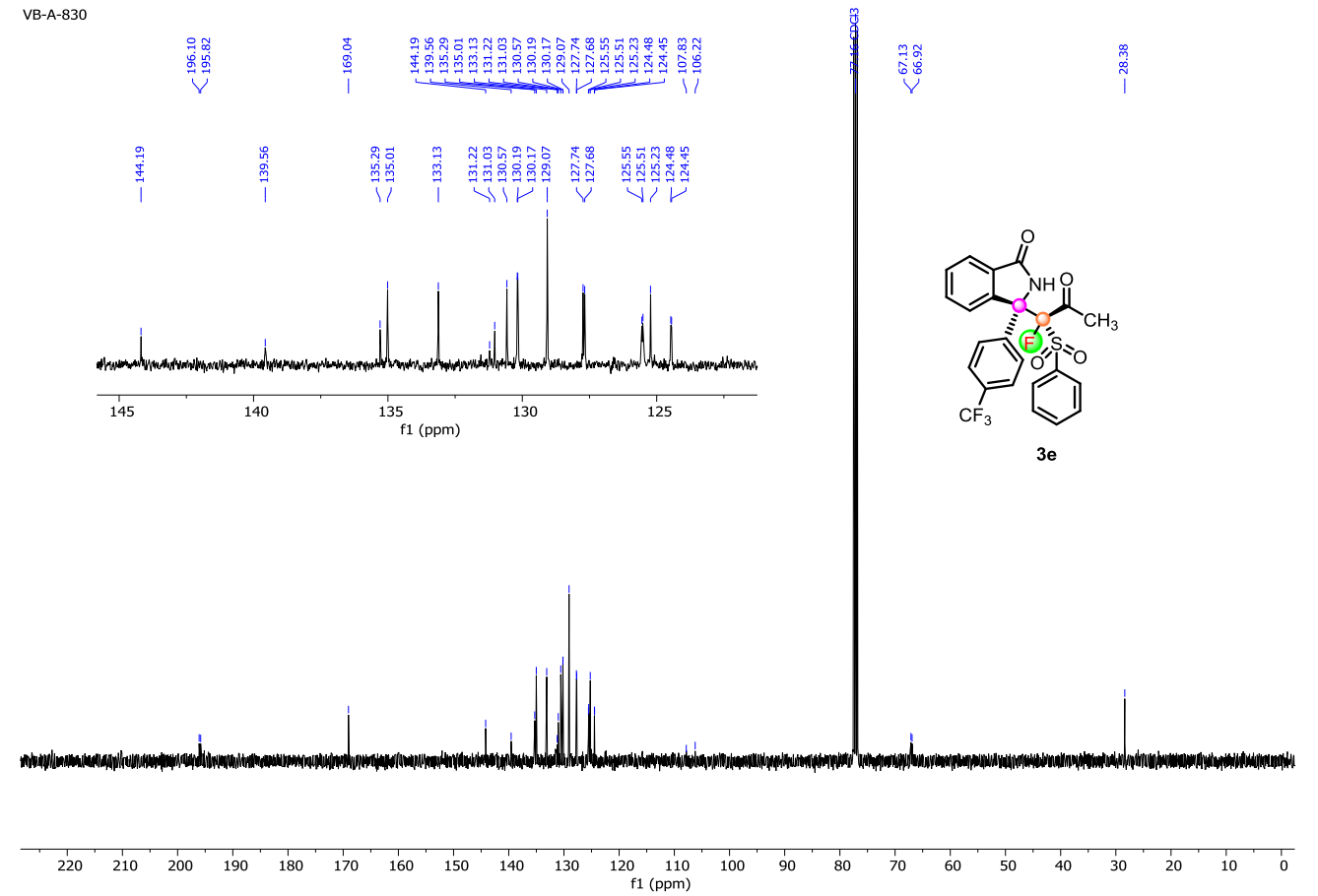


Results View - Peak Table

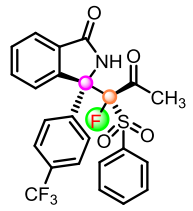
Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	80,866	5,023	399709	2117	0,000000	M	75,520	88,864	5,023
2	105,785	10,677	849666	3163	0,000000	M	99,328	112,672	10,677
3	119,440	80,113	6375153	18507	0,000000	M	112,672	137,088	80,113
4	143,894	4,187	333172	882	0,000000	M	139,349	156,181	4,187
Total		100,000	7957700	24668					100,000


VB-A-830
7.85 7.85 7.85 7.84 7.84 7.84 7.84 7.83 7.82 7.82 7.62 7.62 7.60 7.60 7.59 7.58 7.58 7.58 7.56 7.56 7.56 7.55 7.54 7.53 7.52 7.51 7.51 7.48 7.46 7.42 7.40 7.35 7.33 7.31 7.26 CDCl3
2.12 2.11 1.83 1.81
NH
O
CH3
F
S
CF3
3e
5.08 3.58 2.19 2.14 2.23 0.16 3.00
f1 (ppm)

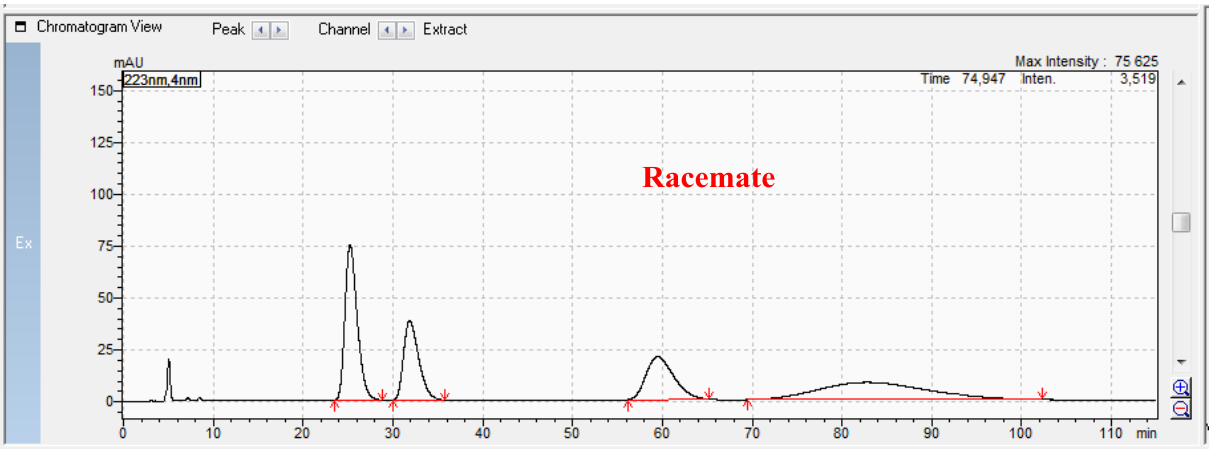

VB-A-830
196.10 195.82 169.04 144.19 139.56 135.29 135.01 133.13 131.22 131.03 130.57 130.19 130.17 129.07 127.74 127.68 125.55 125.51 125.23 124.48 124.45 107.83 106.22 77.16 CDCl3 67.13 66.92 28.38
NH
O
CH3
F
S
CF3
3e
f1 (ppm)

VB-A-830



3e

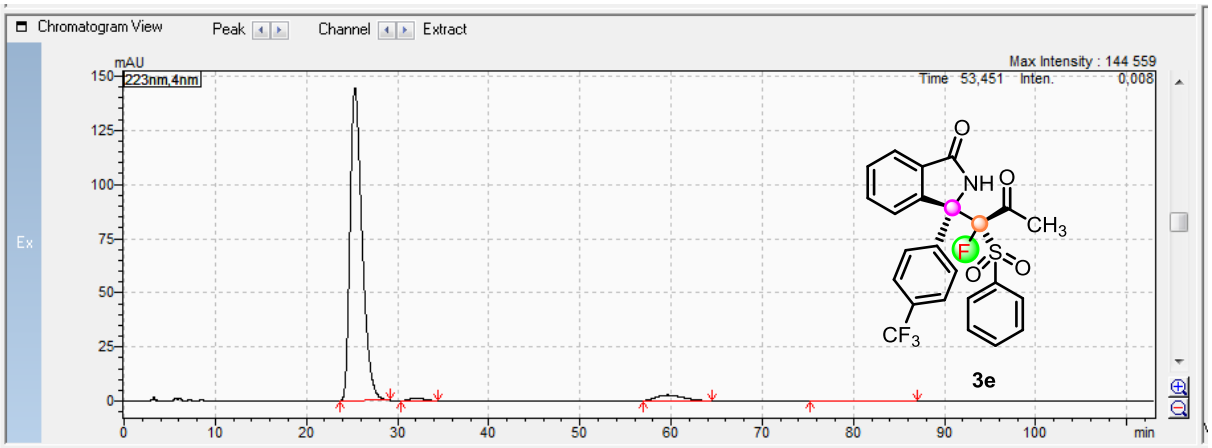
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	25,232	30,801	7133440	74844	0,000000		23,477	28,885	30,801
2	31,872	19,573	4533006	38574	0,000000		29,952	35,765	19,573
3	59,454	19,204	4447606	20659	0,000000		56,171	65,184	19,204
4	82,967	30,421	7045360	8312	0,000000	M	69,483	102,293	30,421
Total		100,000	23159412	142390					100,000

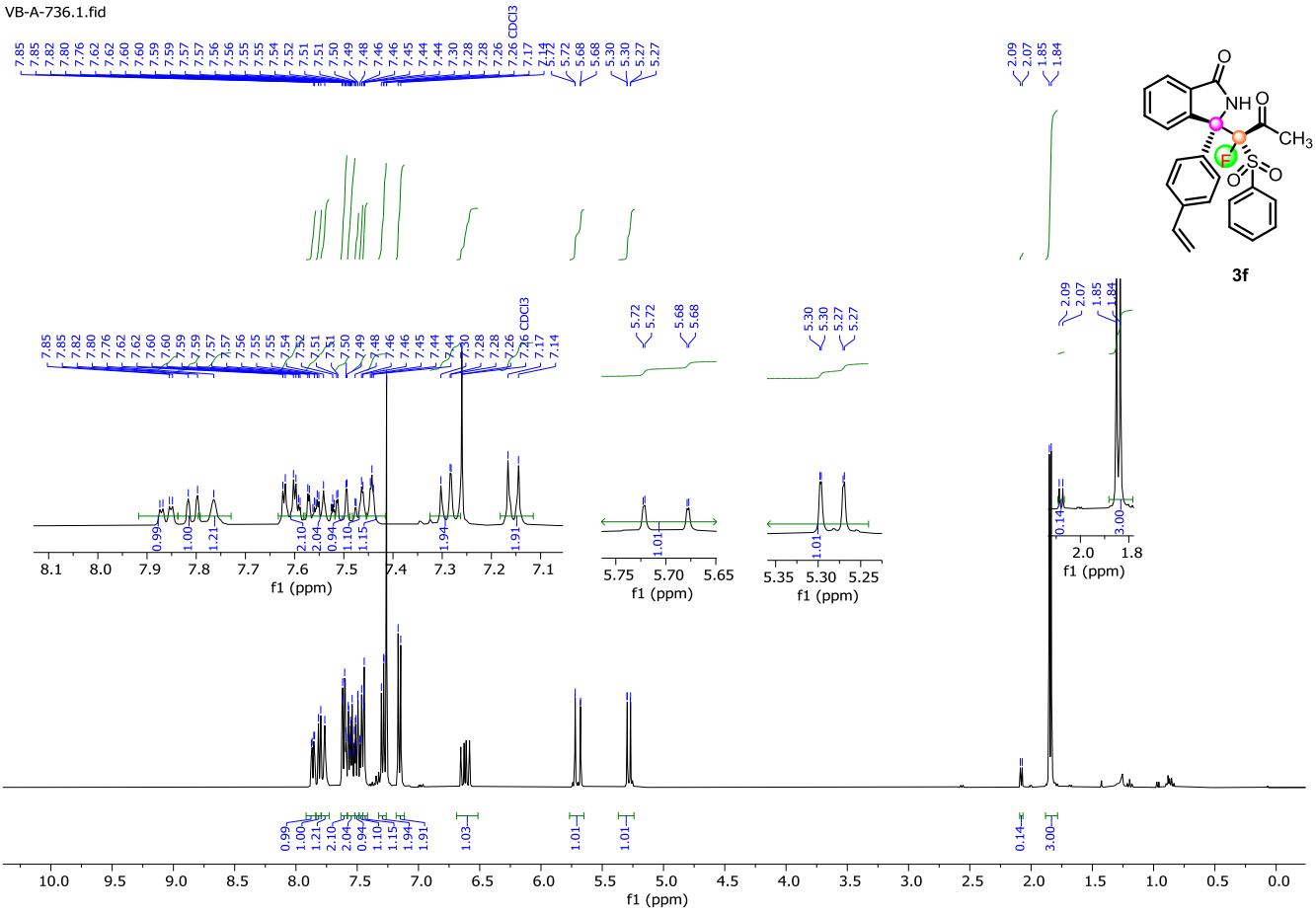


Results View - Peak Table

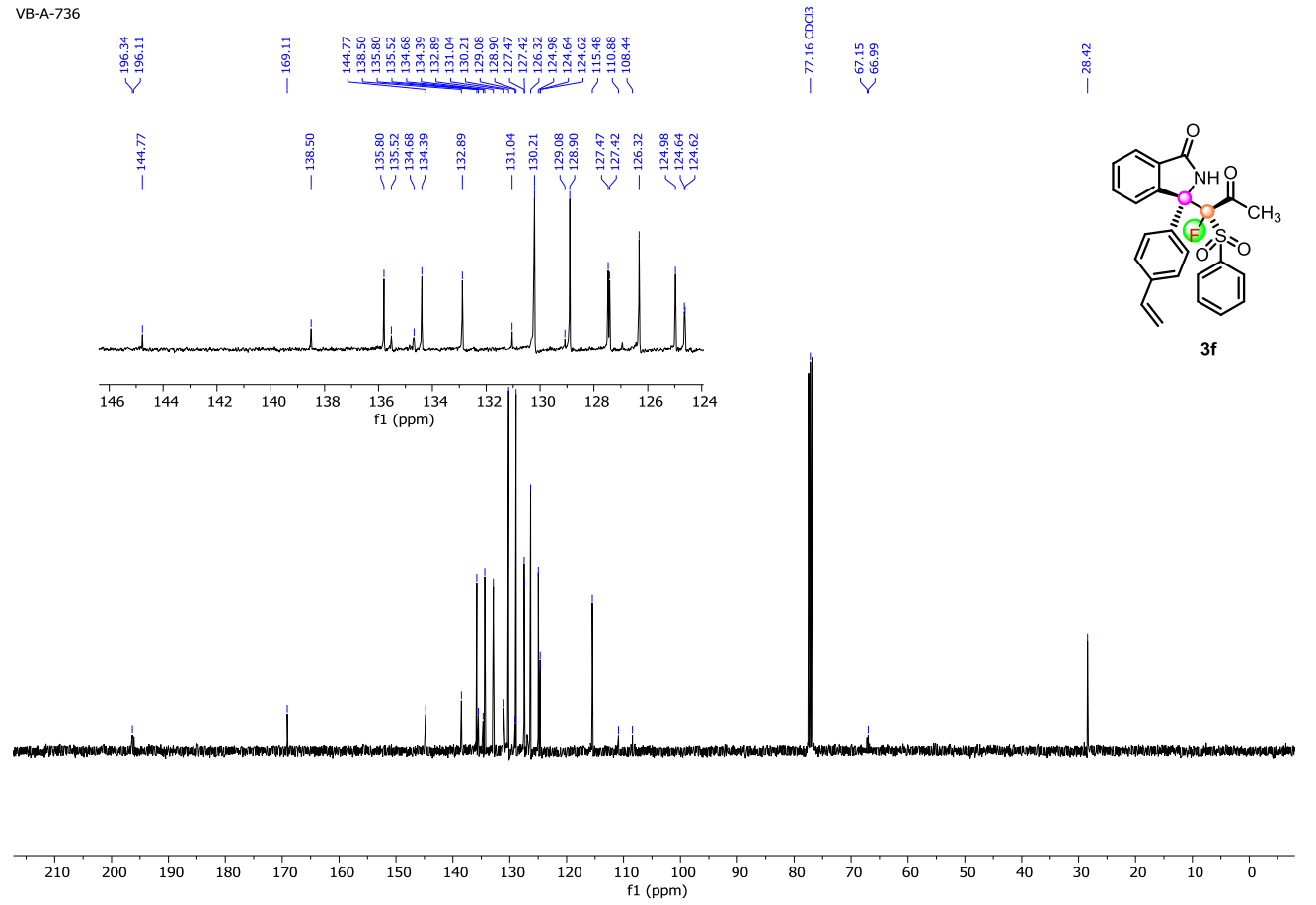
Peak Table | Compound | Group | Calibration Curve

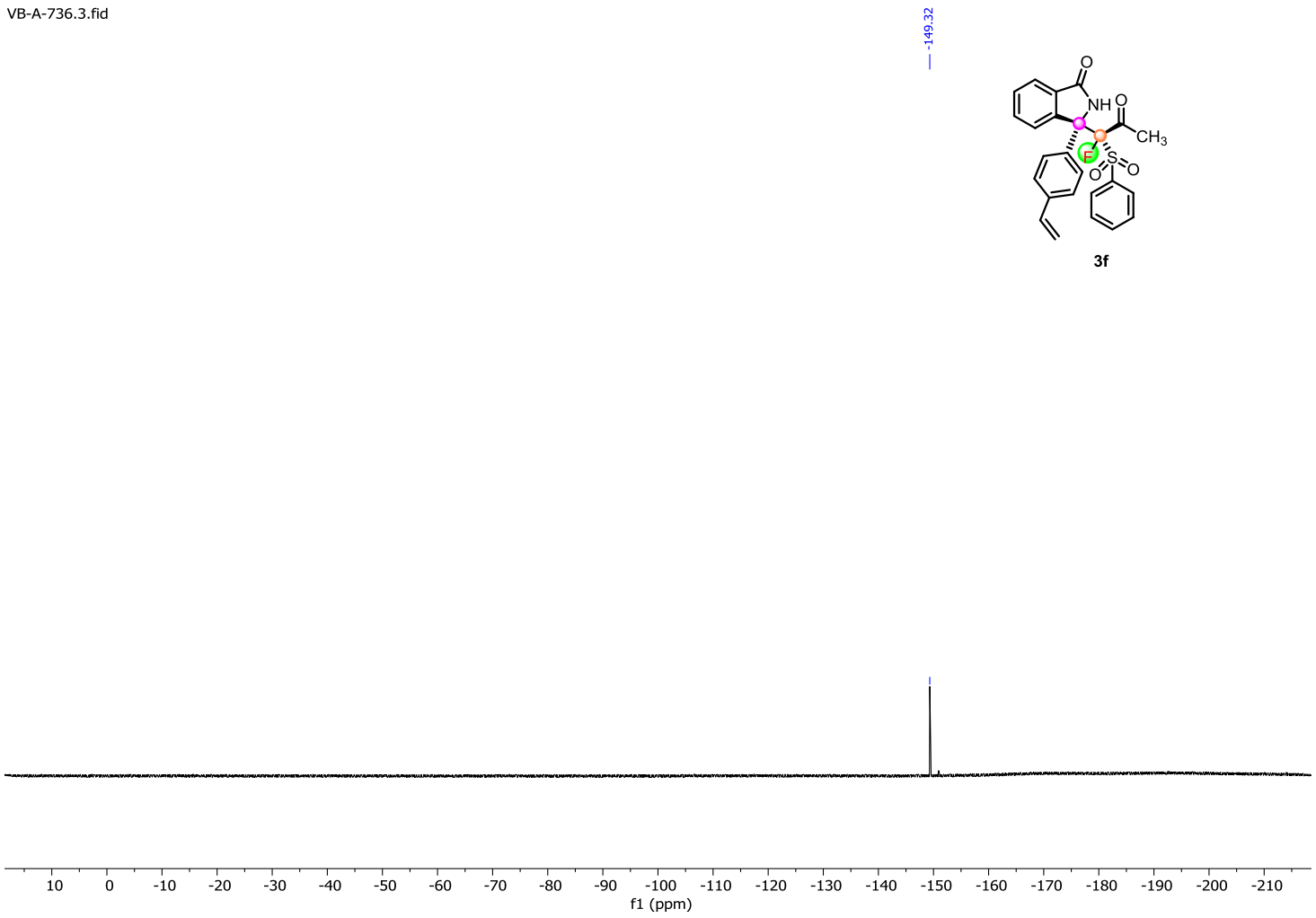
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	25,321	95,079	13297234	144412	0,000000		23,605	29,184	95,079
2	32,010	1,037	144982	1330	0,000000	M	30,357	34,421	1,037
3	59,666	3,875	541995	2649	0,000000	M	56,939	64,491	3,875
4	80,139	0,009	1299	30	0,000000	M	75,243	87,008	0,009
Total		100,000	13985509	148420					100,000

VB-A-736.1.fid

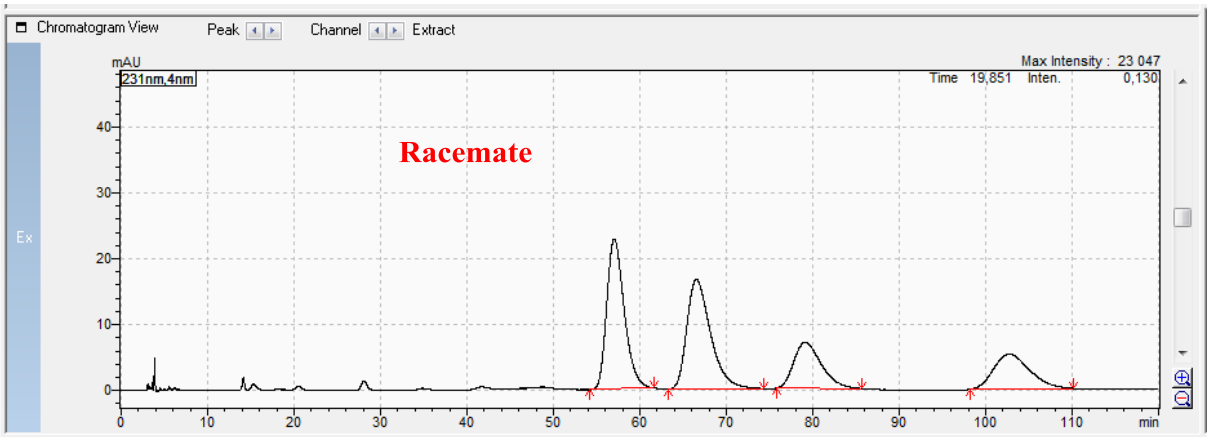


VB-A-736





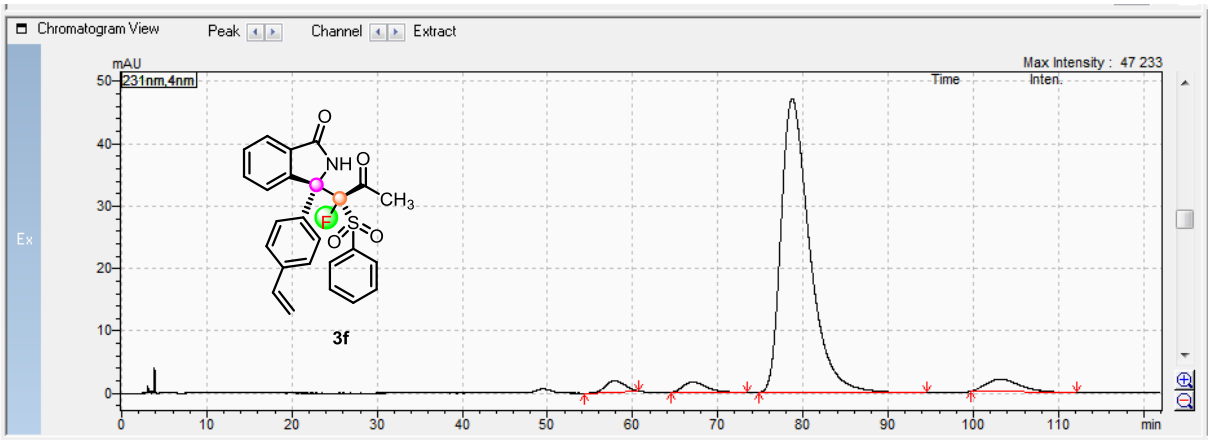
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

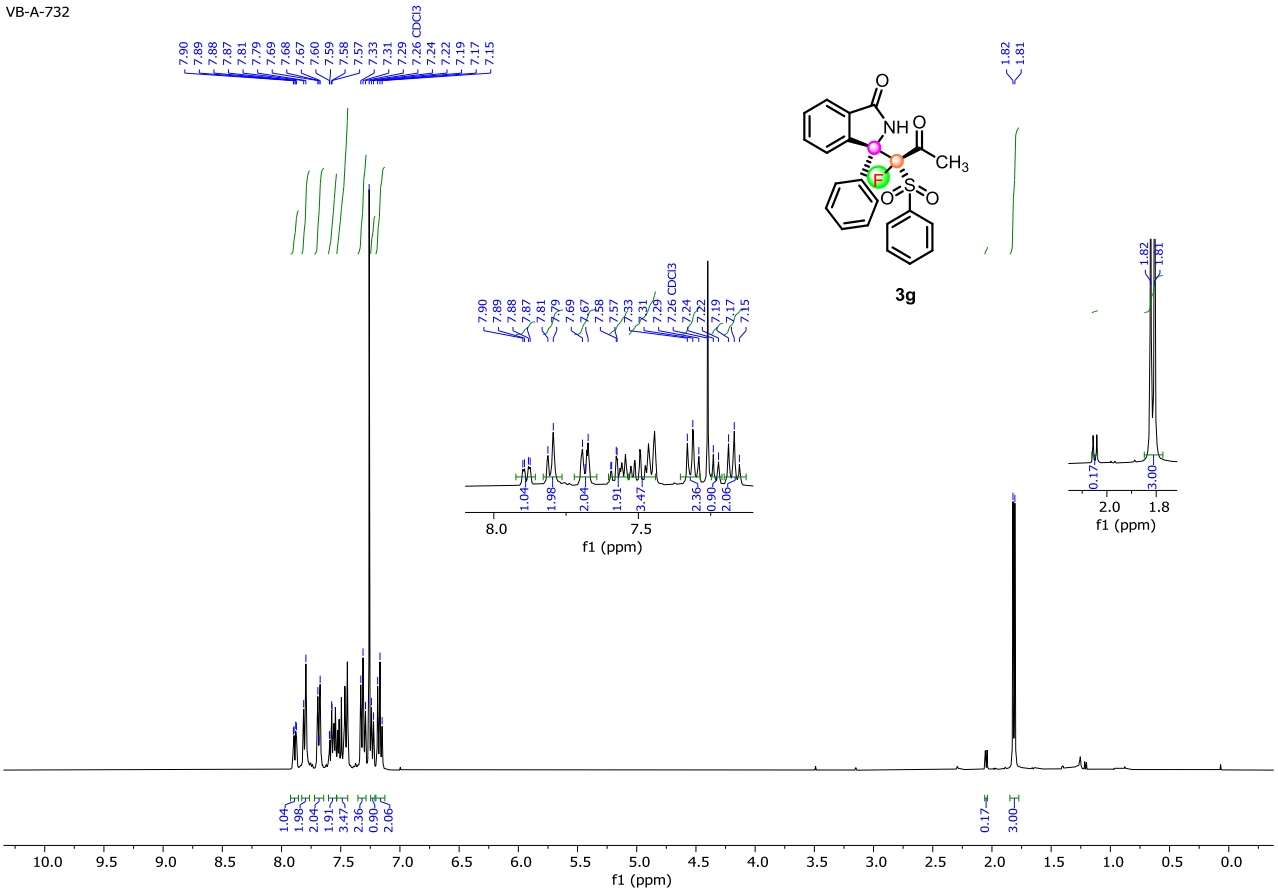
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	57,024	33,934	3210842	22815	0,000000	M	54,176	61,643	33,934
2	66,520	33,400	3160316	16607	0,000000	M	63,285	74,325	33,400
3	79,109	16,371	1549082	7010	0,000000	M	75,819	85,675	16,371
4	102,764	16,295	1541845	5278	0,000000	M	98,208	110,144	16,295
Total		100,000	9462085	51710					100,000

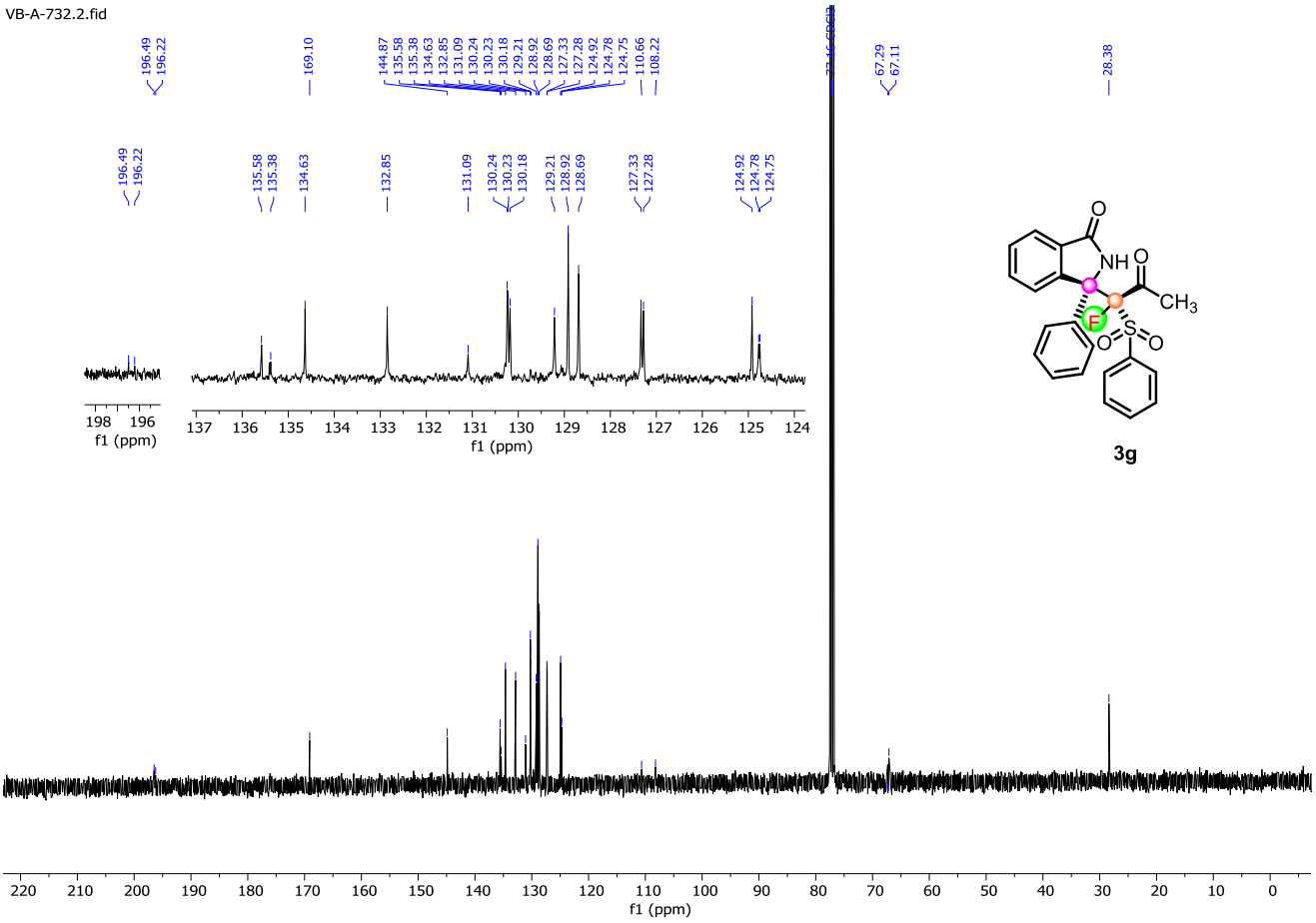


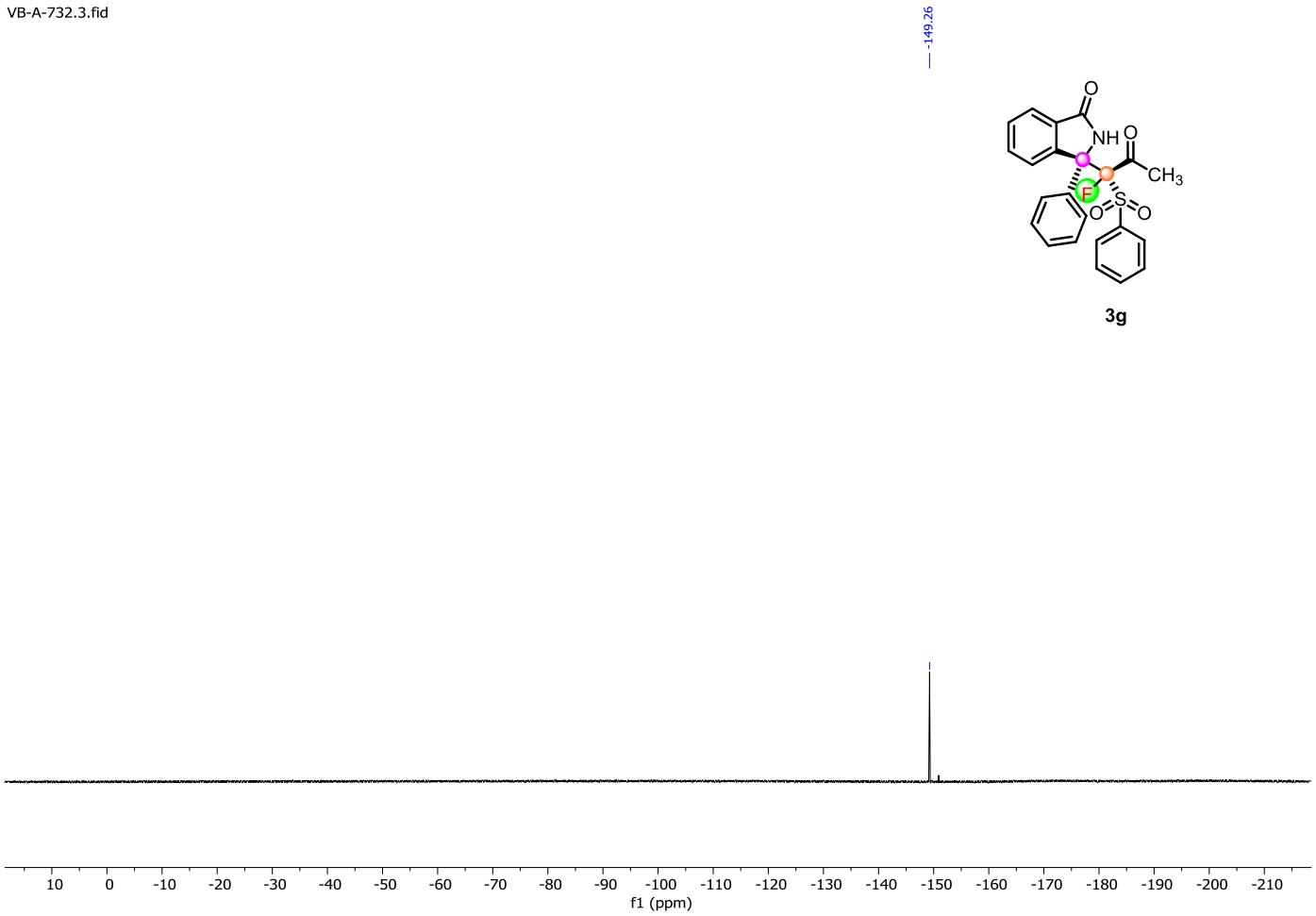
Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

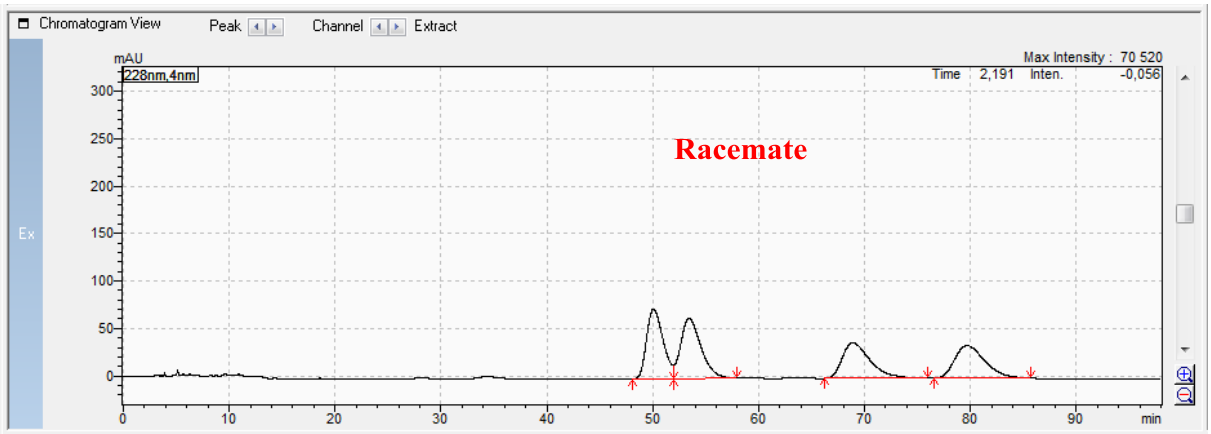
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	58,016	2,288	276432	1735	0,000000	M	54,325	60,704	2,288
2	67,053	2,757	333128	1723	0,000000	M	64,491	73,451	2,757
3	78,736	90,427	10925896	47068	0,000000	M	74,816	94,539	90,427
4	103,201	4,528	547074	1982	0,000000	M	99,701	112,139	4,528
Total		100,000	12082529	52509					100,000


VB-A-732
3g
f1 (ppm)


VB-A-732.2.fid
3g
f1 (ppm)



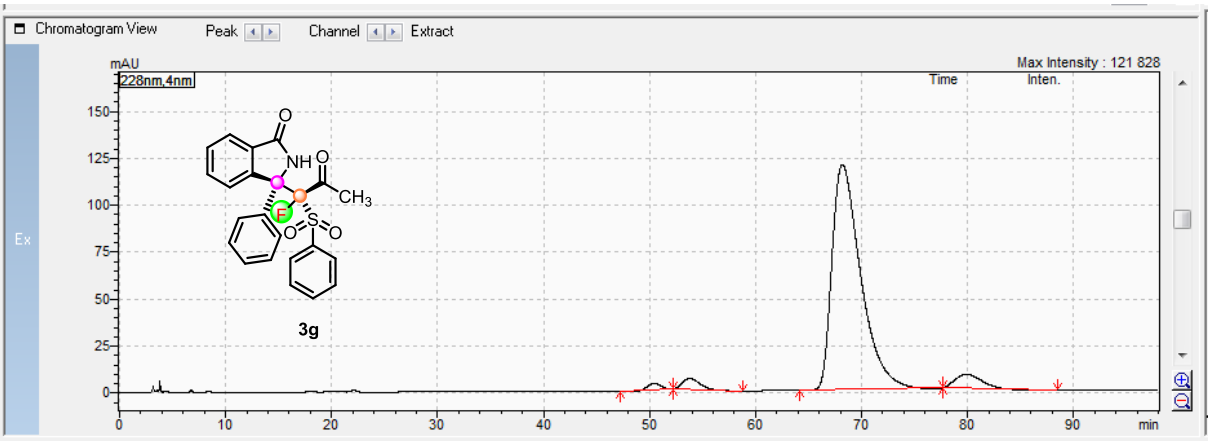
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

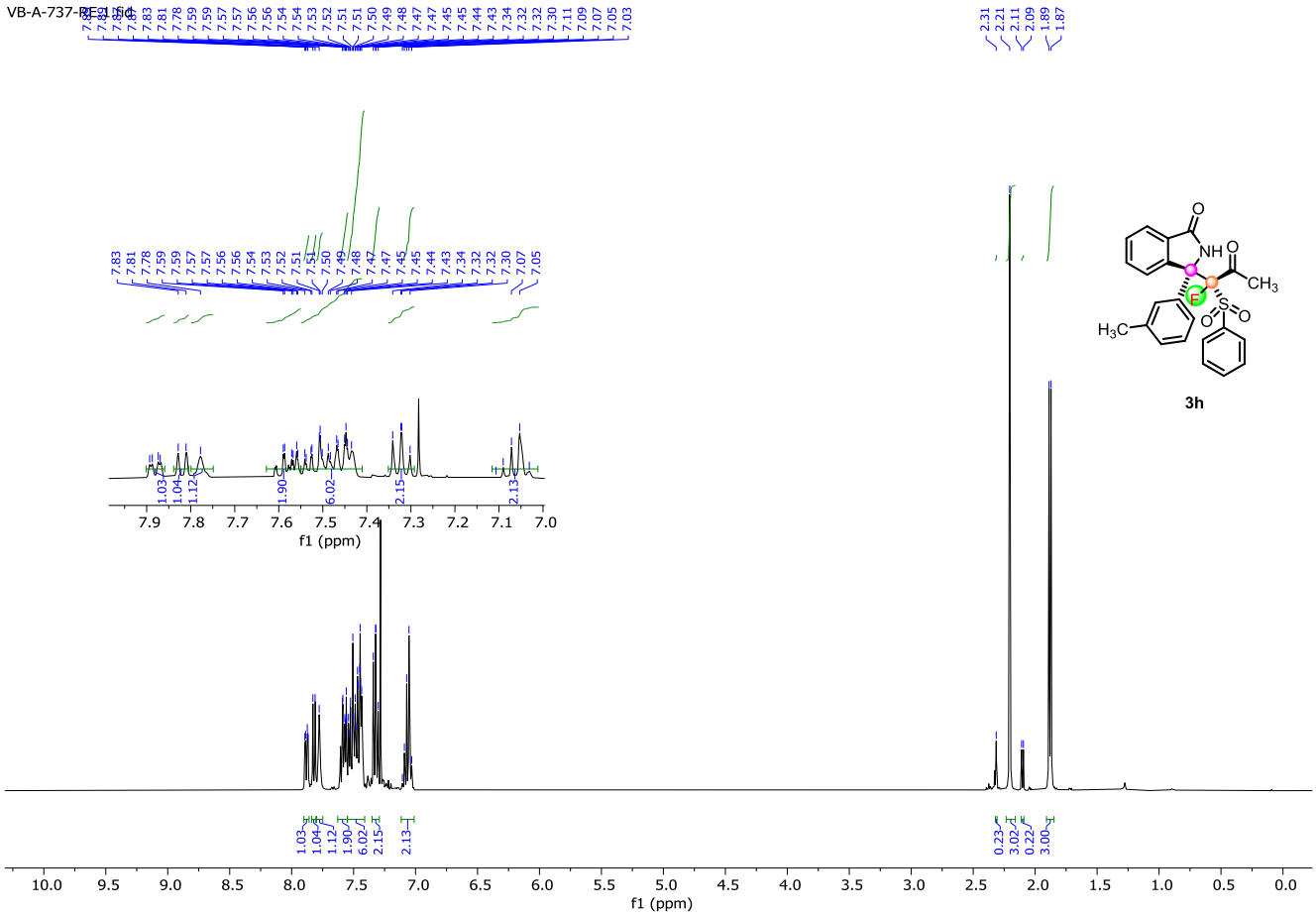
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	50,074	26,495	8015555	73734	0,000000		48,075	51,947	26,495
2	53,435	28,153	8516936	63530	0,000000	V	51,947	57,909	28,153
3	68,926	22,738	6879002	37528	0,000000	M	66,229	75,968	22,738
4	79,694	22,614	6841348	34447	0,000000		76,523	85,664	22,614
Total		100,000	30252840	209239					100,000

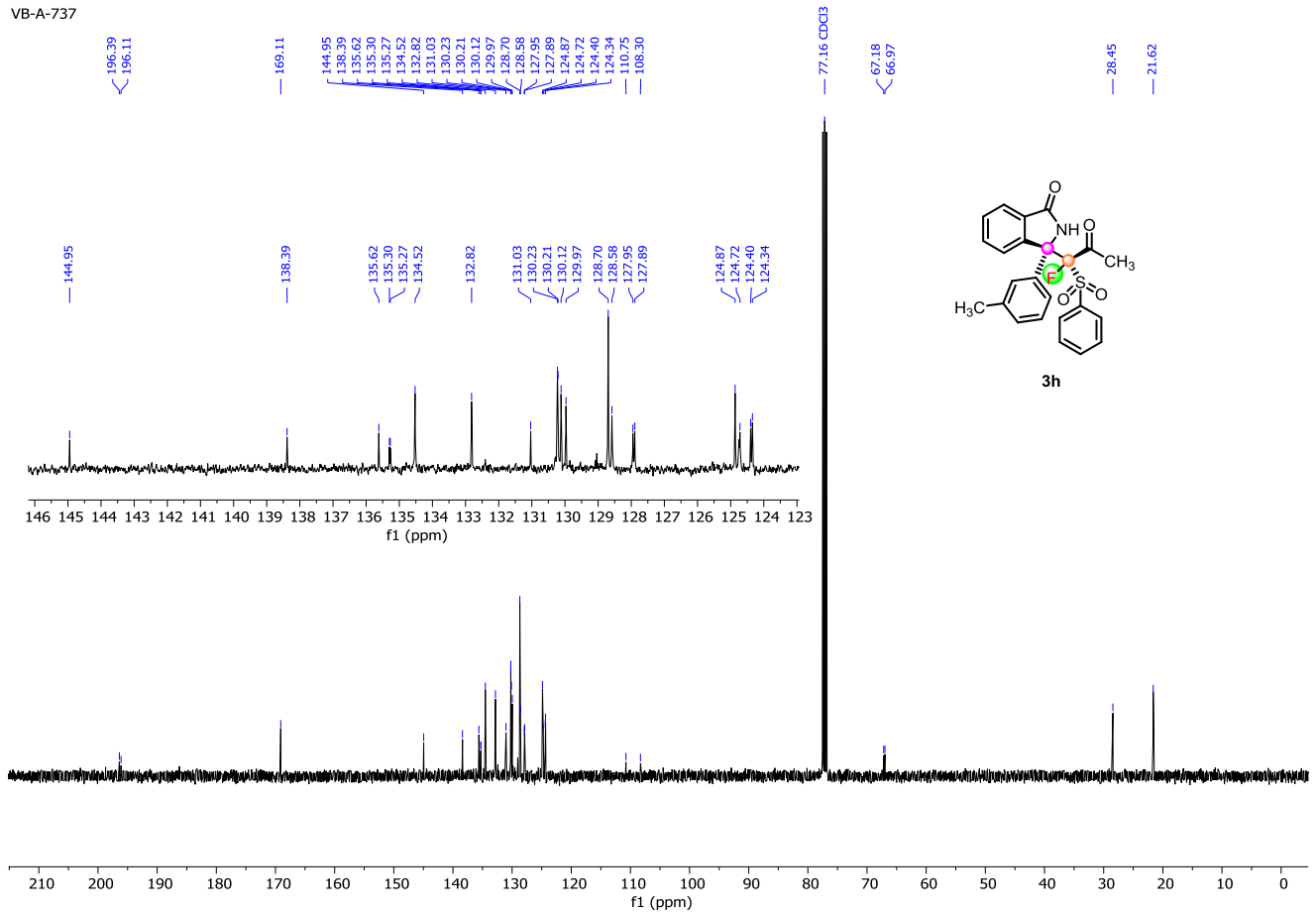


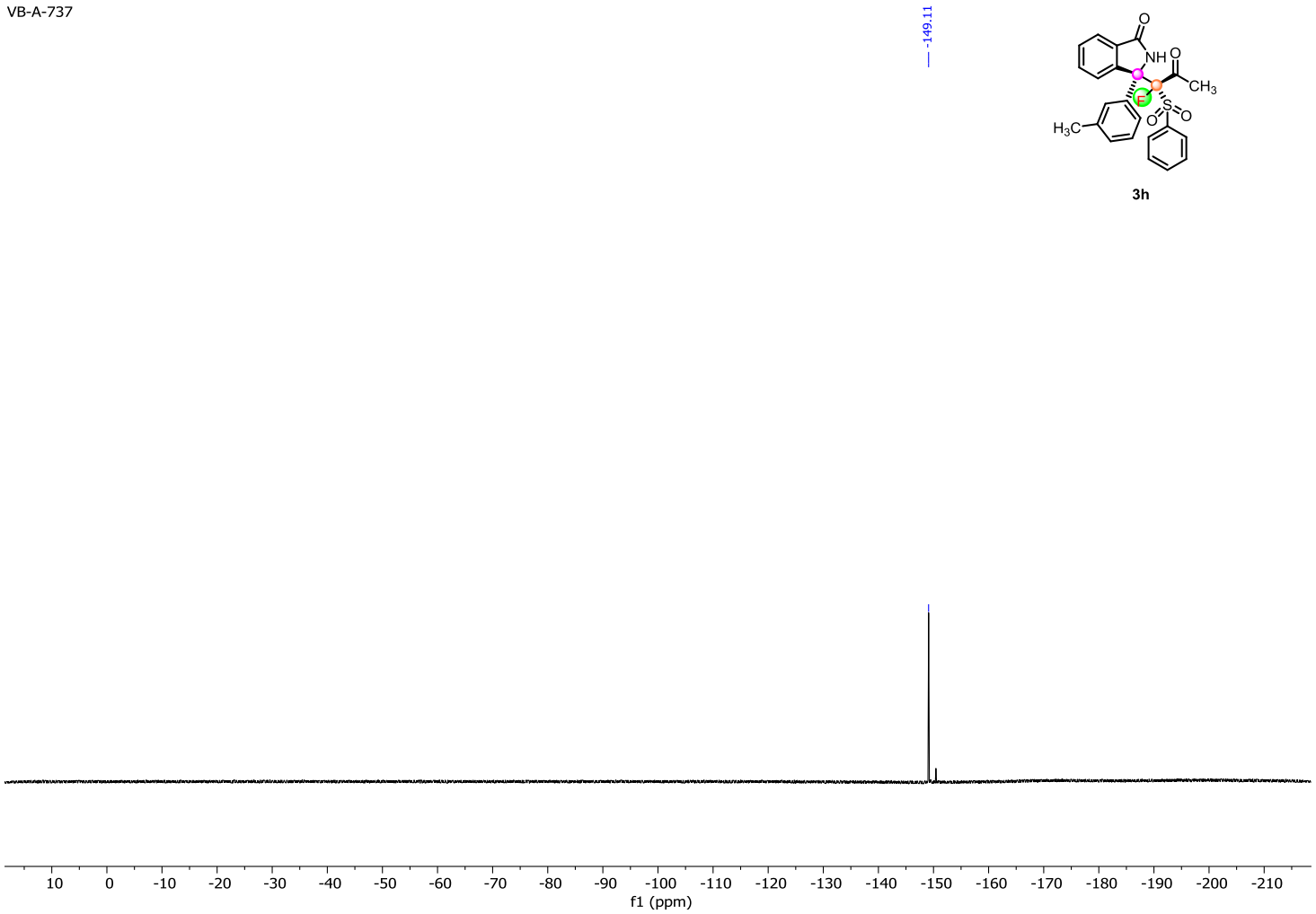
Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

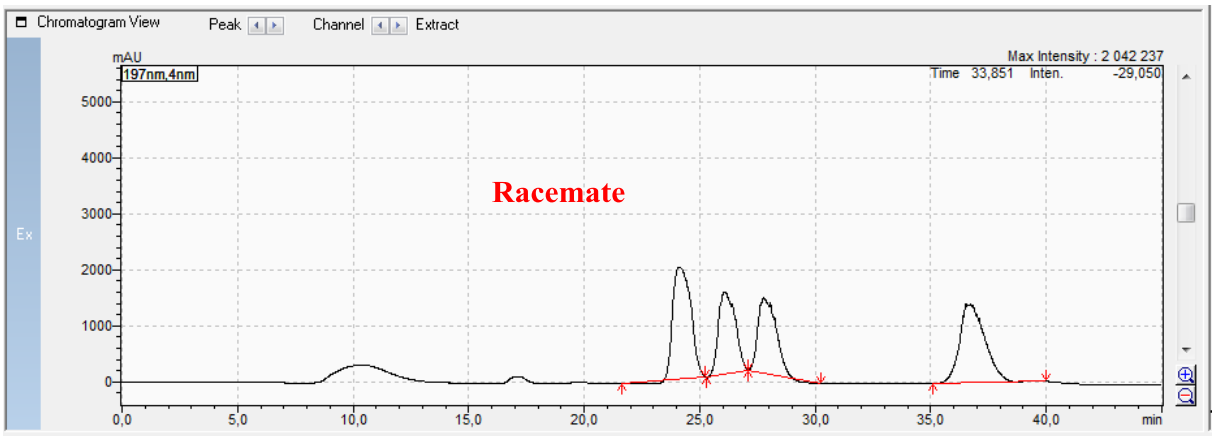
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	50,411	1,152	282658	3373	0,000000	M	47,232	52,224	1,152
2	53,793	2,733	670227	5935	0,000000	M	52,224	58,805	2,733
3	68,194	91,002	22320077	119611	0,000000	M	64,160	77,675	91,002
4	79,922	5,113	1254161	7367	0,000000	M	77,675	88,512	5,113
Total		100,000	24527124	136286					100,000


VB-A-737-RE-1-H
7.83 7.81 7.78 7.59 7.59 7.57 7.56 7.56 7.54 7.53 7.52 7.51 7.50 7.49 7.48 7.47 7.47 7.45 7.44 7.43 7.34 7.32 7.30 7.07 7.05
2.31 2.21 2.11 2.09 1.89 1.87
1.03 1.04 1.12 1.90 6.02 2.15 2.13
0.23 3.02 0.22 3.00
f1 (ppm)
3h


VB-A-737
196.39 196.11 169.11 144.95 138.39 135.62 135.30 135.27 134.52 132.82 131.03 130.23 130.21 130.12 129.97 128.70 128.58 127.95 127.89 124.87 124.72 124.40 124.34 110.75 108.30
77.16 CDCl3
67.18 66.97
28.45 21.62
f1 (ppm)
3h



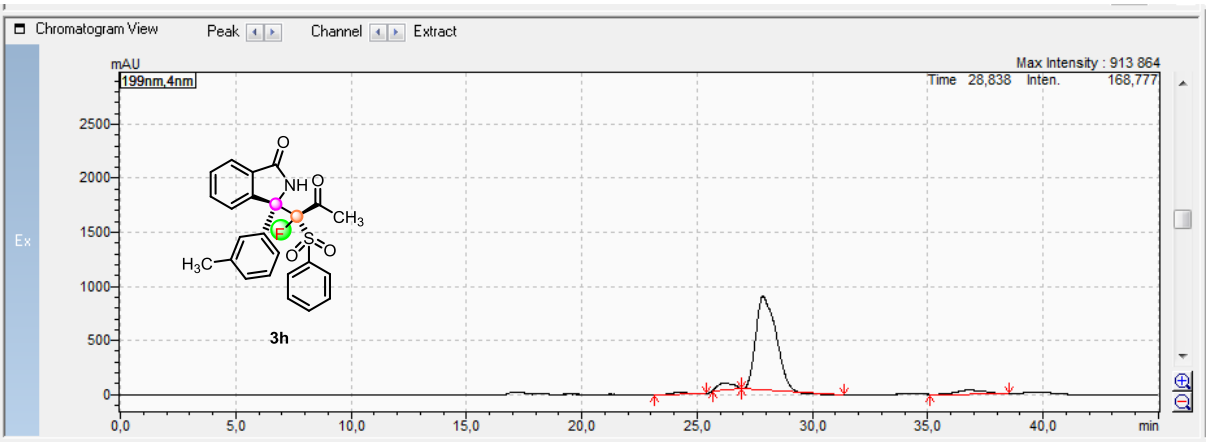
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

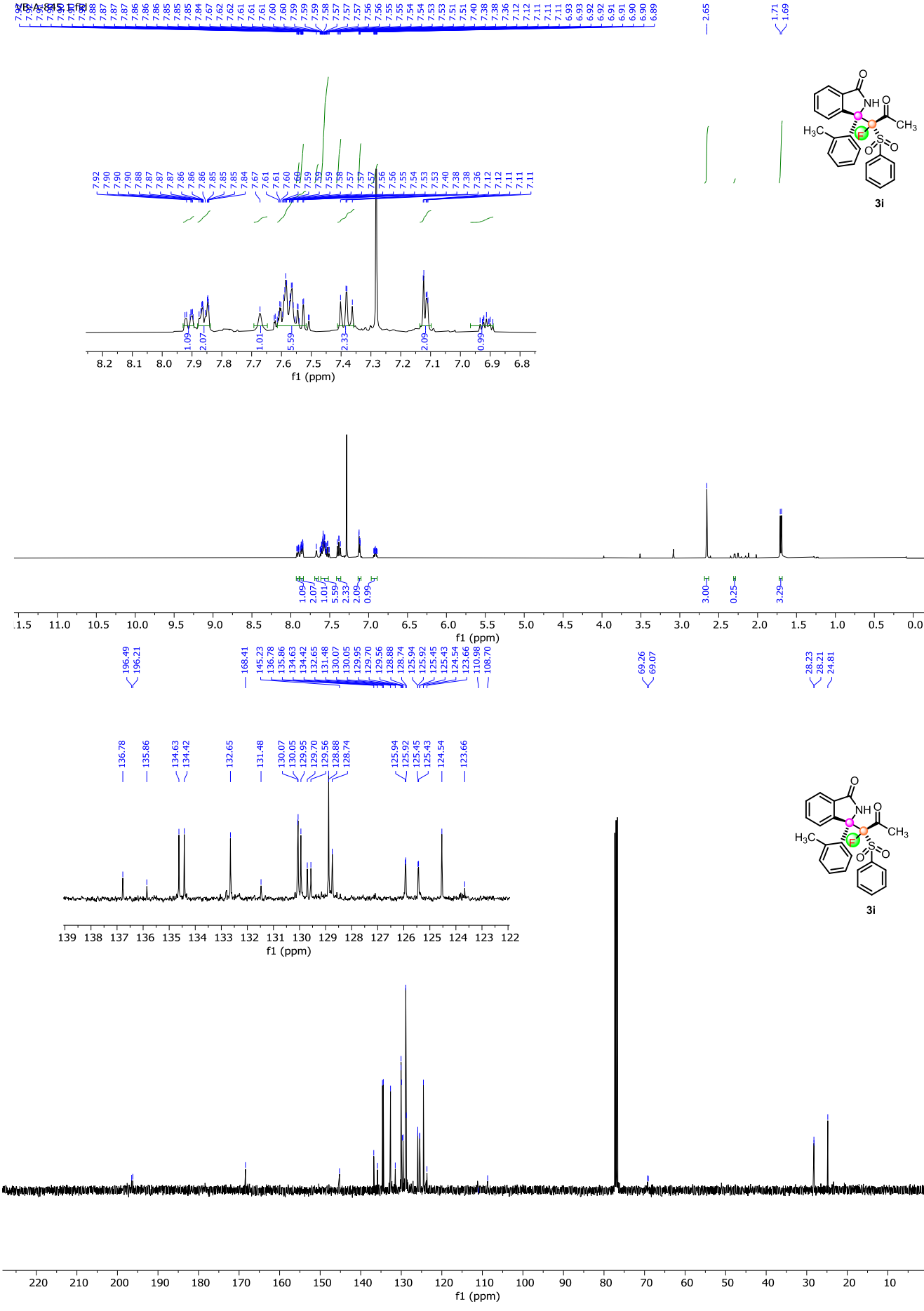
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	24,097	29,364	105535206	1988206	0,000000	M	21,632	25,237	29,364
2	26,078	20,692	74366589	1459641	0,000000	M	25,291	27,093	20,692
3	27,767	19,911	71560250	1339987	0,000000	M	27,093	30,251	19,911
4	36,567	30,033	107938176	1405015	0,000000	M	35,093	39,989	30,033
Total		100,000	359400221	6192849					100,000

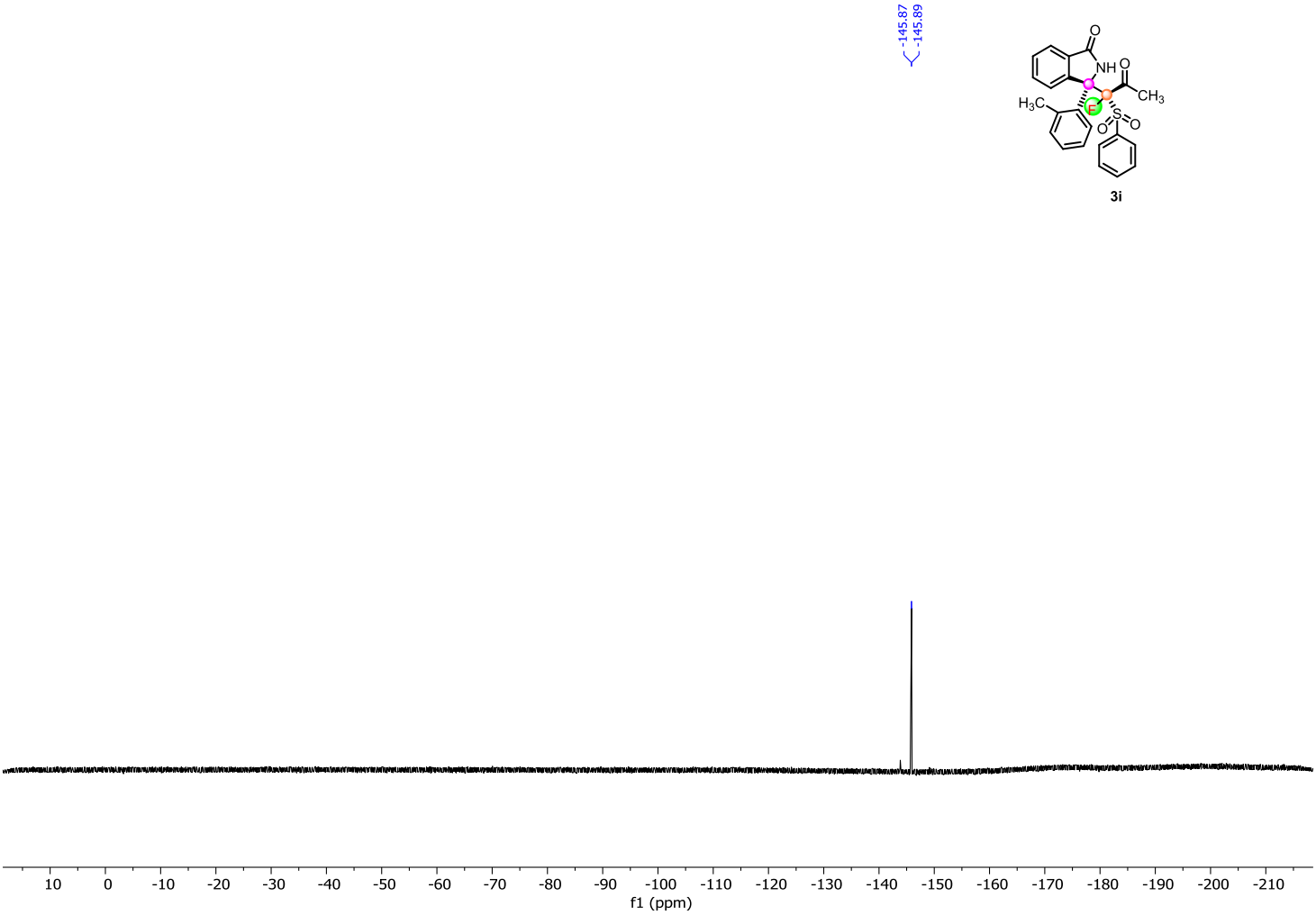


Results View - Peak Table

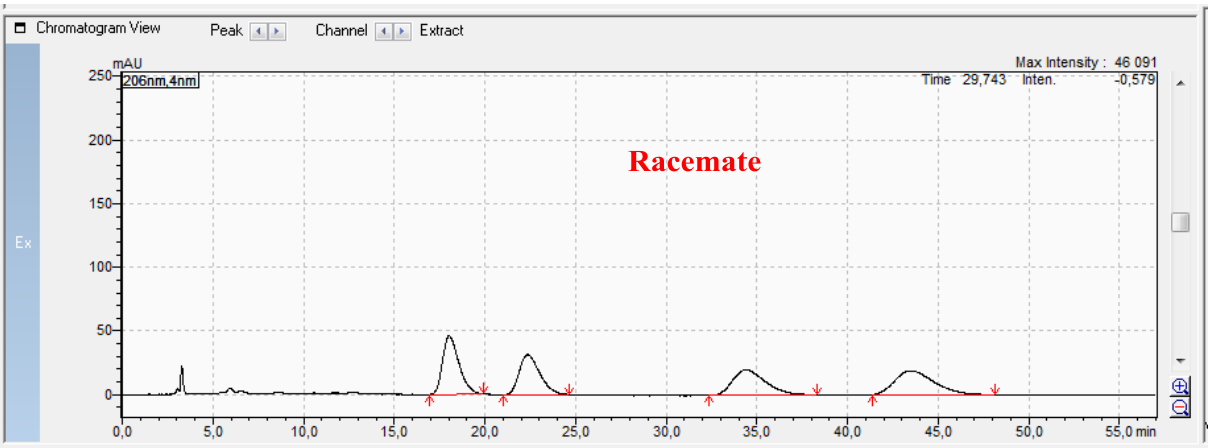
Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	24,186	1,178	694773	13906	0,000000	M	23,147	25,397	1,178
2	26,175	4,861	2866302	60412	0,000000	M	25,685	26,923	4,861
3	27,886	88,361	52103909	871599	0,000000	M	26,923	31,371	88,361
4	36,790	5,600	3302295	38553	0,000000	M	35,093	38,528	5,600
Total		100,000	58967279	984470					100,000


3i
f1 (ppm)
3i
f1 (ppm)
f1 (ppm)



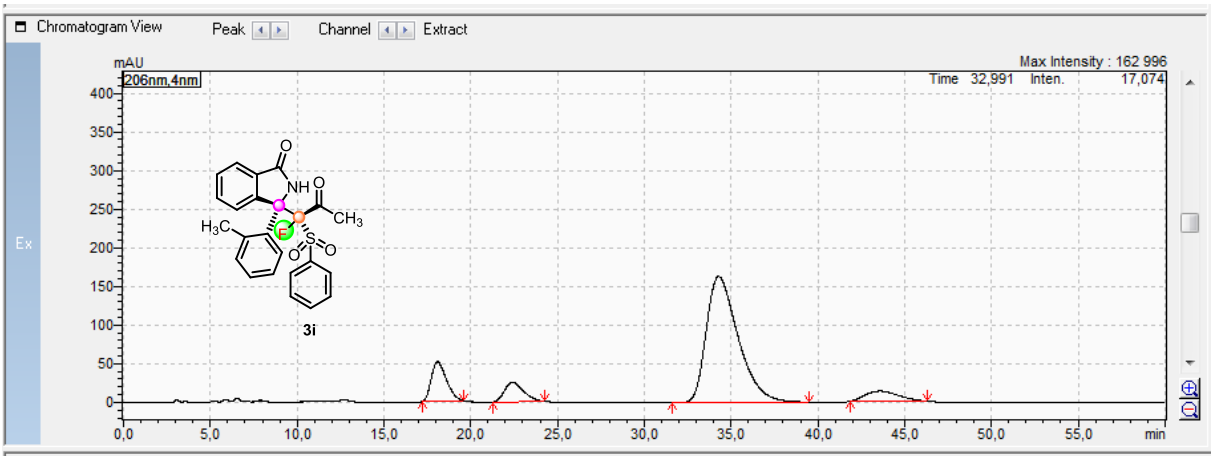
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	18,028	26,574	2857674	45667	0,000000	M	16,949	19,925	26,574
2	22,380	23,074	2481291	31402	0,000000	M	21,013	24,651	23,074
3	34,426	23,642	2542374	19992	0,000000	M	32,363	38,325	23,642
4	43,510	26,710	2872230	18925	0,000000	M	41,376	48,139	26,710
Total		100,000	10753568	115986					100,000

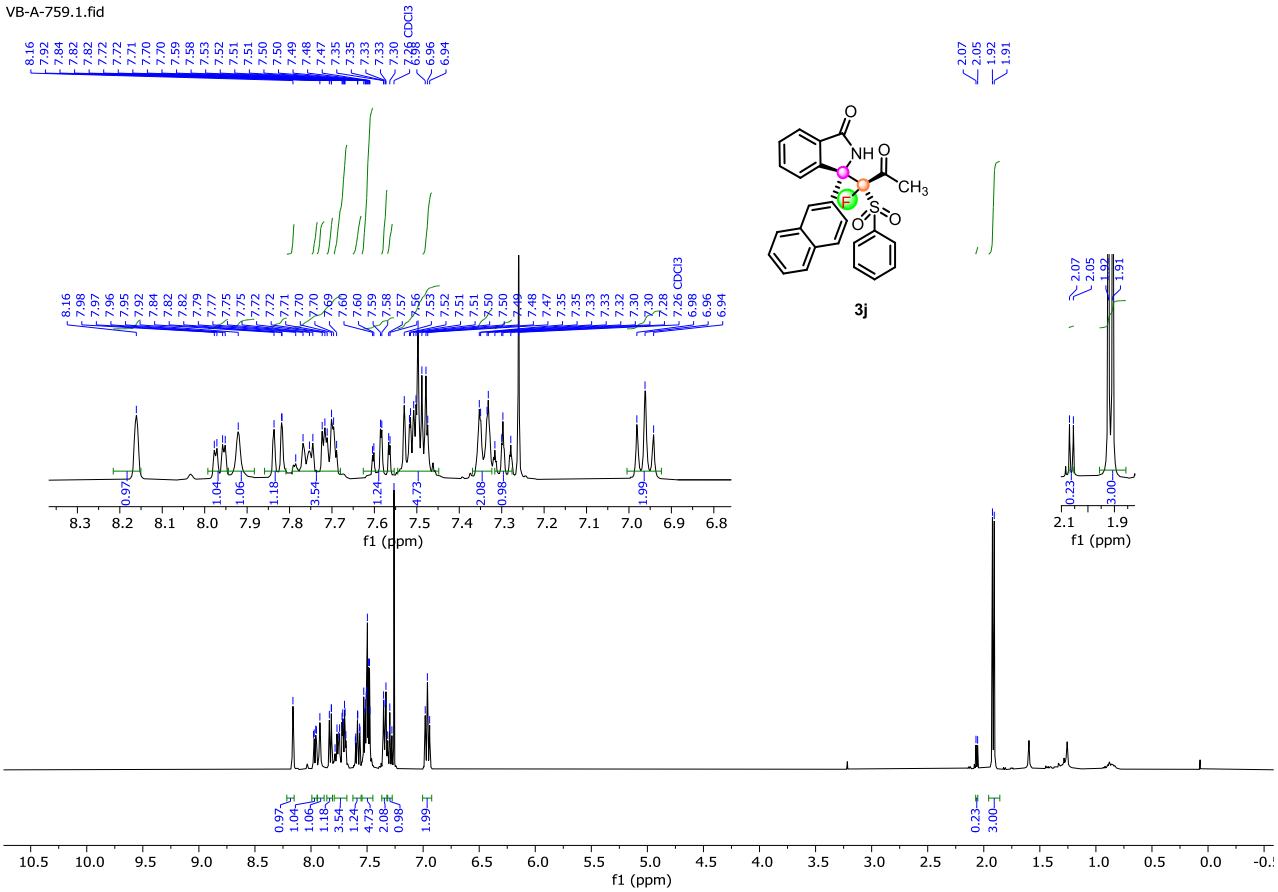


Results View - Peak Table

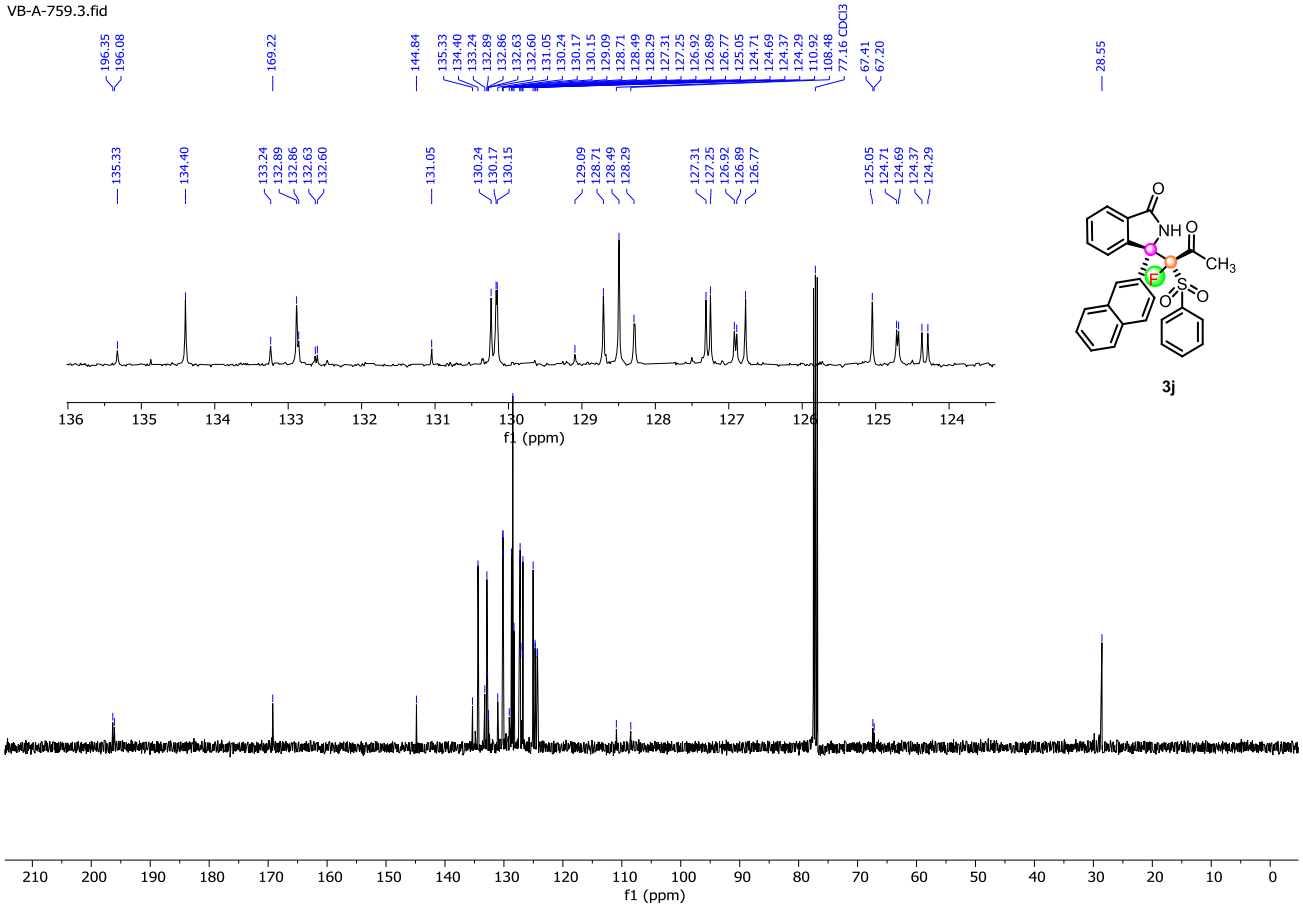
Peak Table | Compound | Group | Calibration Curve

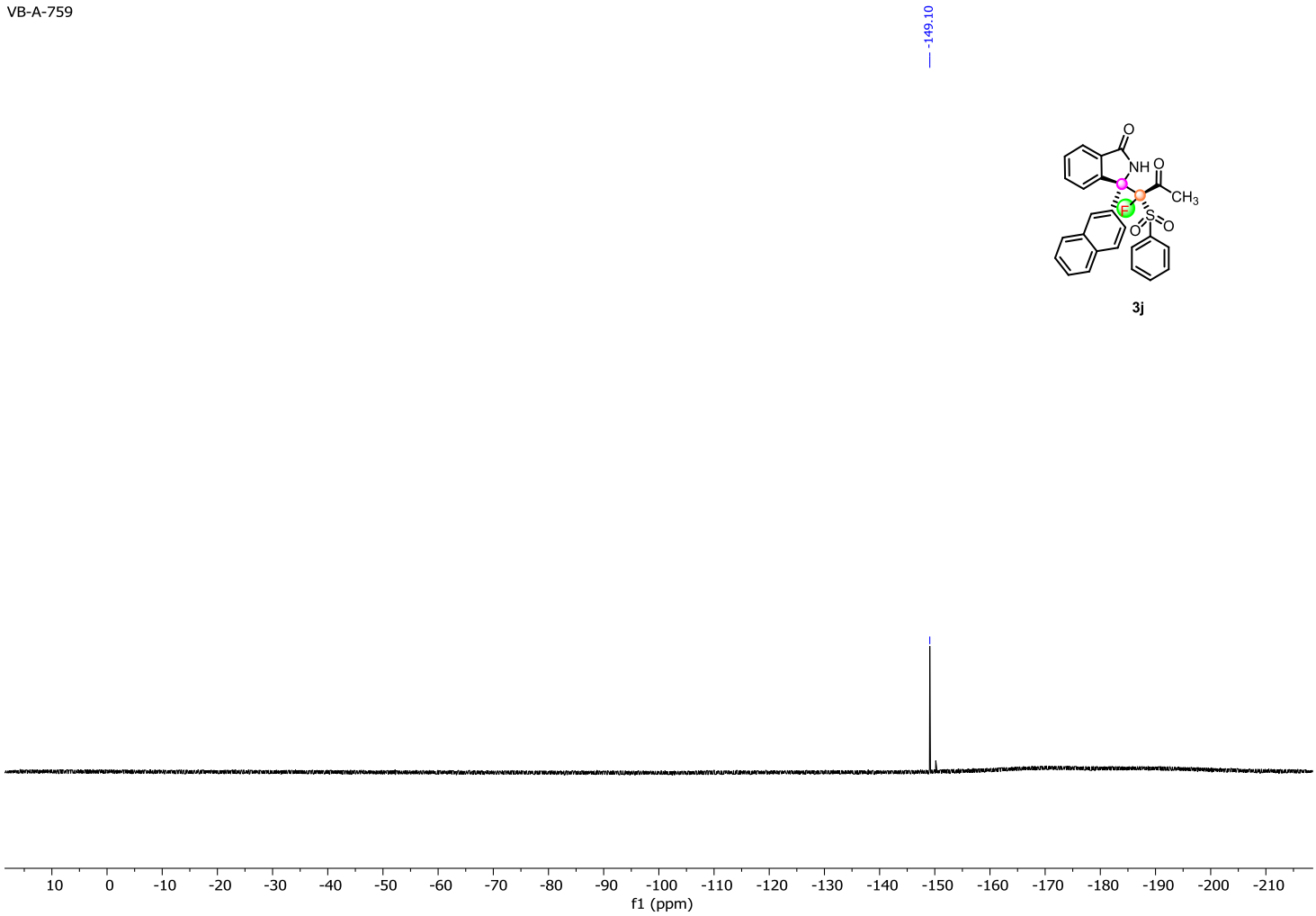
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	18,081	11,185	3080396	50899	0,000000	M	17,227	19,595	11,185
2	22,382	7,025	1934847	25238	0,000000	M	21,280	24,267	7,025
3	34,293	75,441	20777232	162991	0,000000	M	31,616	39,499	75,441
4	43,572	6,349	1748669	13138	0,000000	M	41,867	46,304	6,349
Total		100,000	27541145	252265					100,000

VB-A-759.1.fid

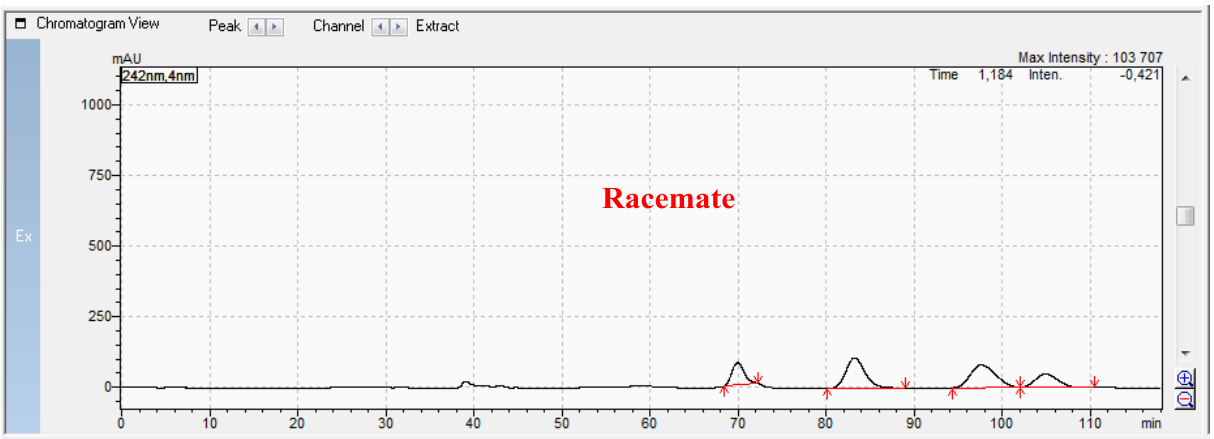


VB-A-759.3.fid





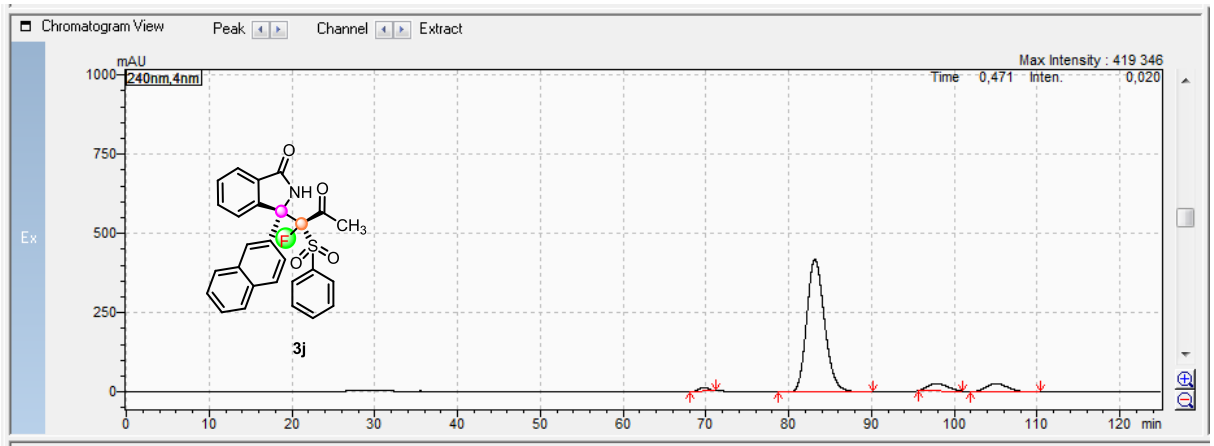
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

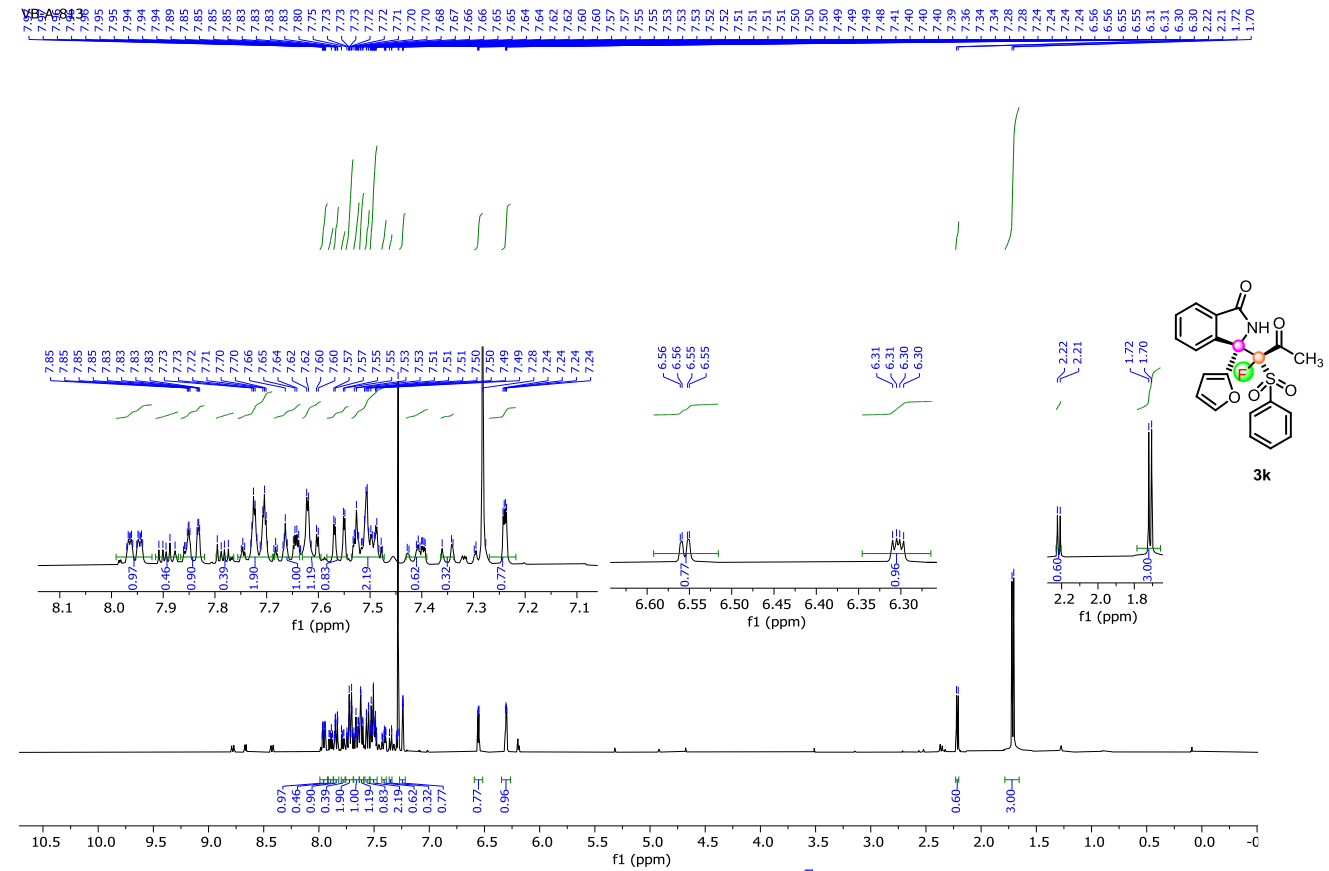
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	69,922	16,387	7842469	79445	0,000000	M	68,405	72,256	16,387
2	83,204	33,678	16117278	106468	0,000000		80,085	89,013	33,678
3	97,613	33,167	15872709	80217	0,000000	M	94,315	102,016	33,167
4	104,914	16,767	8024017	46441	0,000000	M	102,016	110,453	16,767
Total		100,000	47856474	312571					100,000

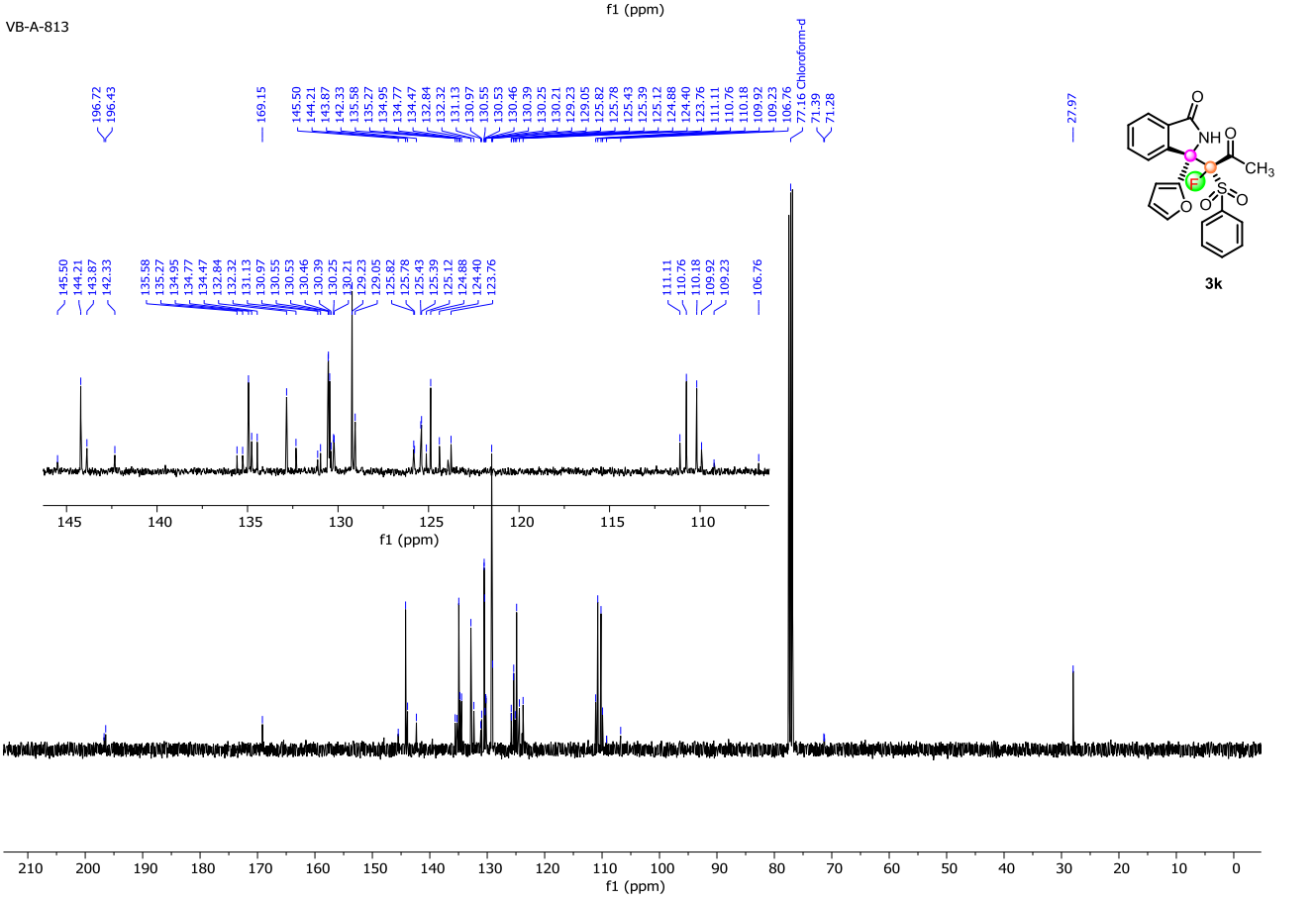


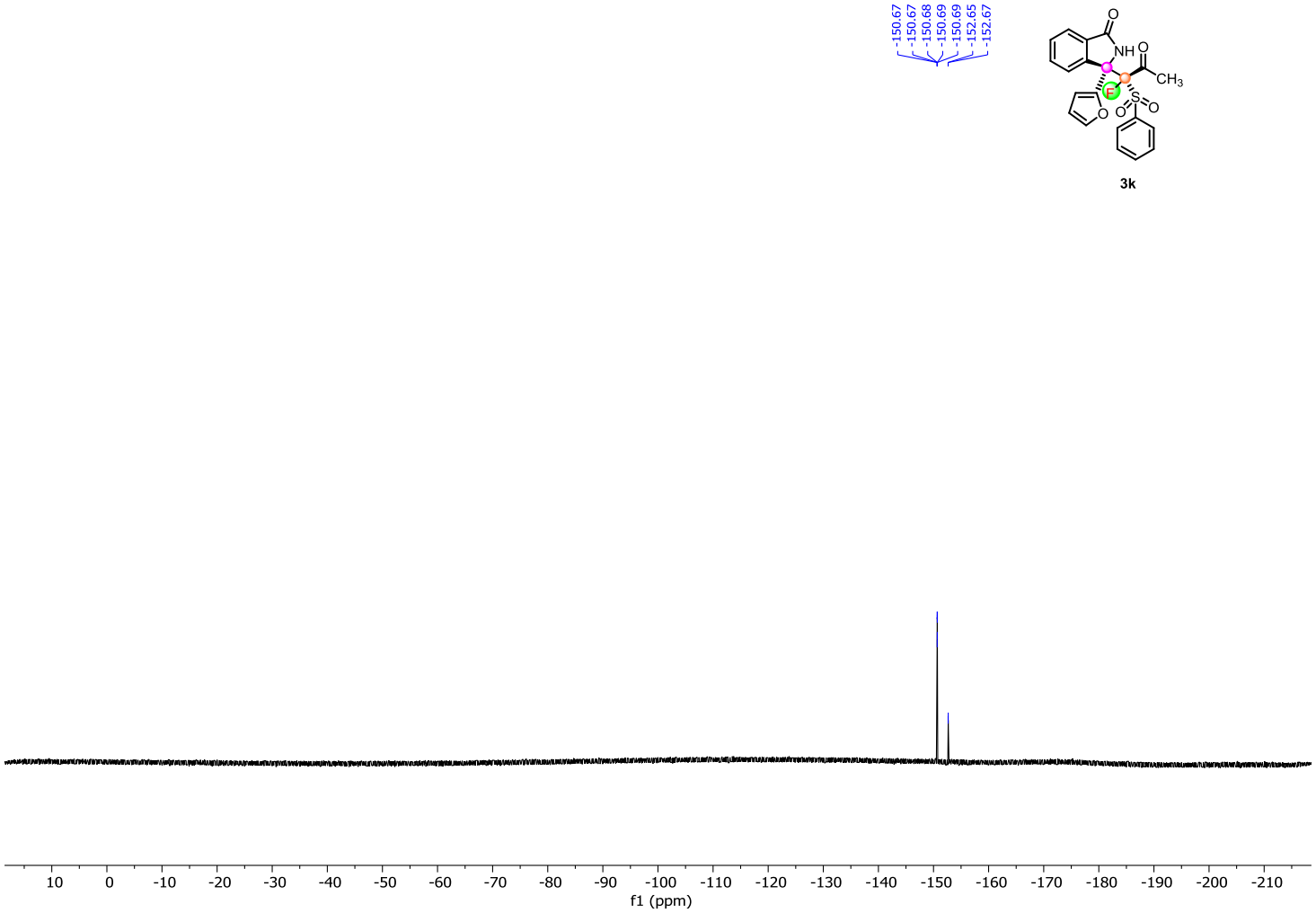
Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

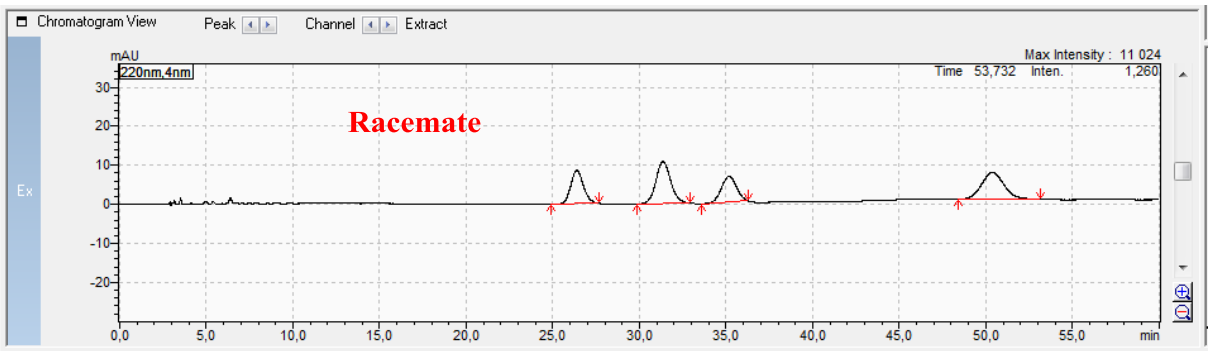
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	69,760	1,354	979194	11269	0,000000	M	68,064	71,211	1,354
2	83,170	86,944	62893401	419763	0,000000	M	78,731	90,187	86,944
3	97,803	5,271	3812772	22513	0,000000	M	95,669	101,003	5,271
4	105,017	6,432	4652651	26238	0,000000	M	101,952	110,421	6,432
Total		100,000	72338019	479783					100,000


VB-A-813
3k
f1 (ppm)


VB-A-813
3k
f1 (ppm)



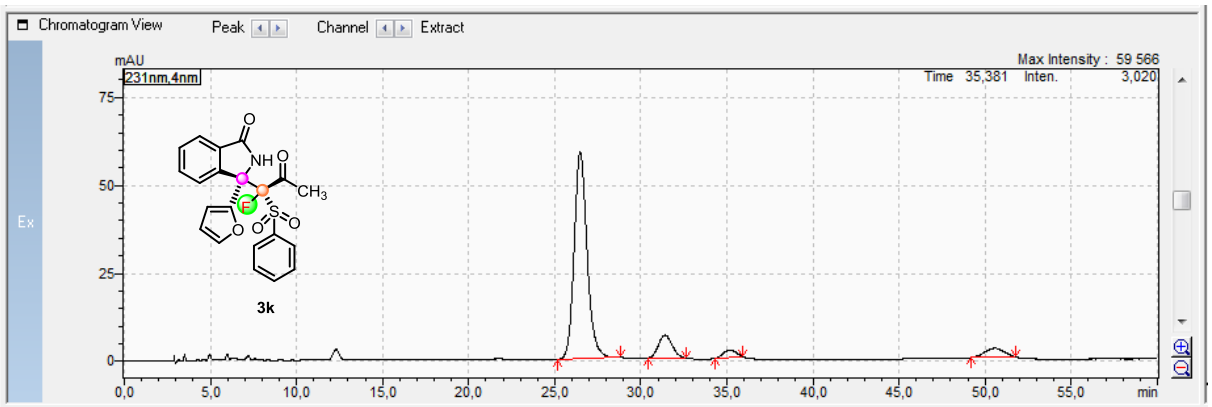
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

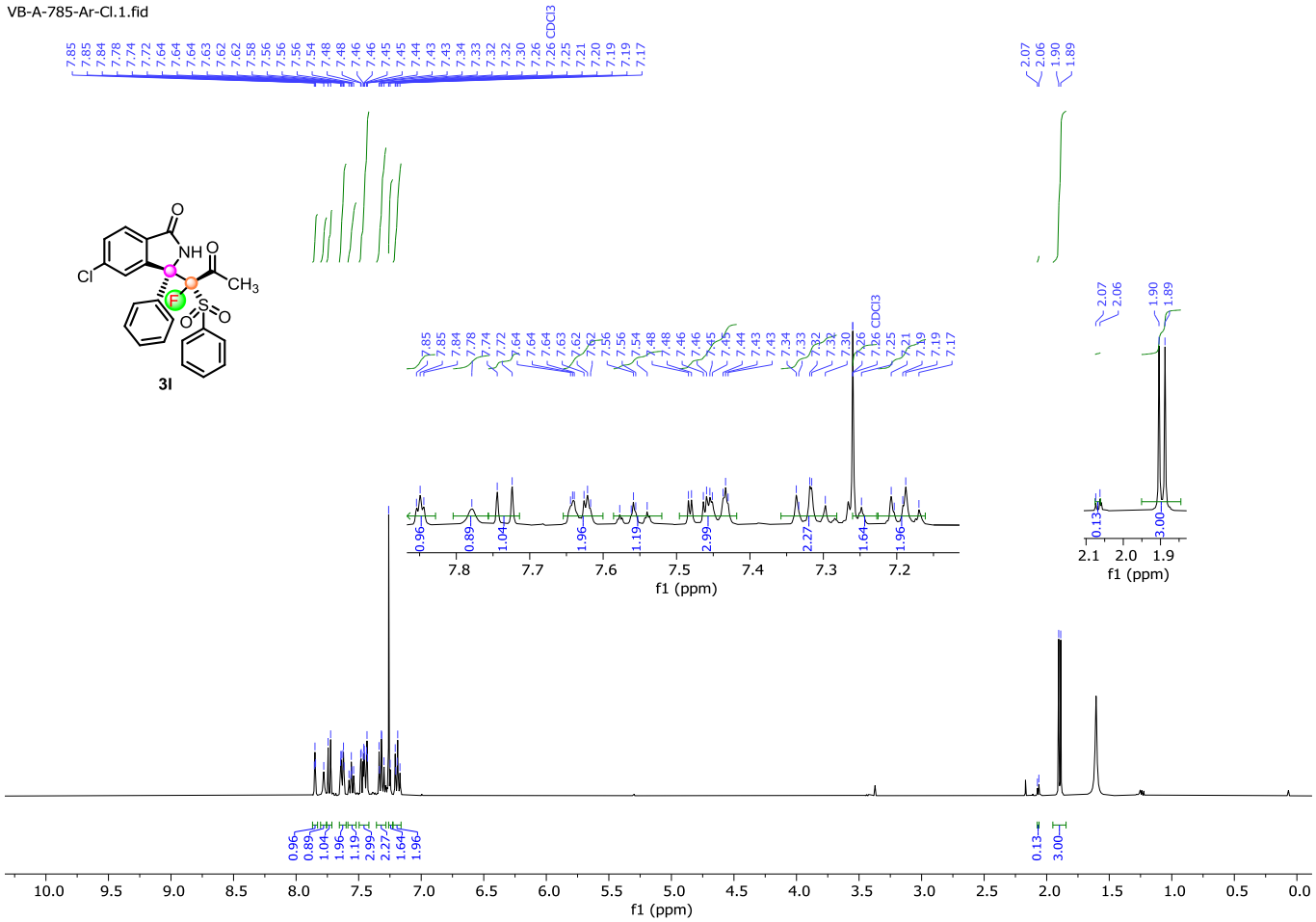
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	26,376	21,037	441818	8613	0,000000	M	24,896	27,669	21,037
2	31,356	30,408	638618	10816	0,000000	M	29,856	32,928	30,408
3	35,178	18,940	397766	6635	0,000000	M	33,579	36,288	18,940
4	50,368	29,615	621956	6847	0,000000	M	48,405	53,152	29,615
Total		100,000	2100159	32911					100,000

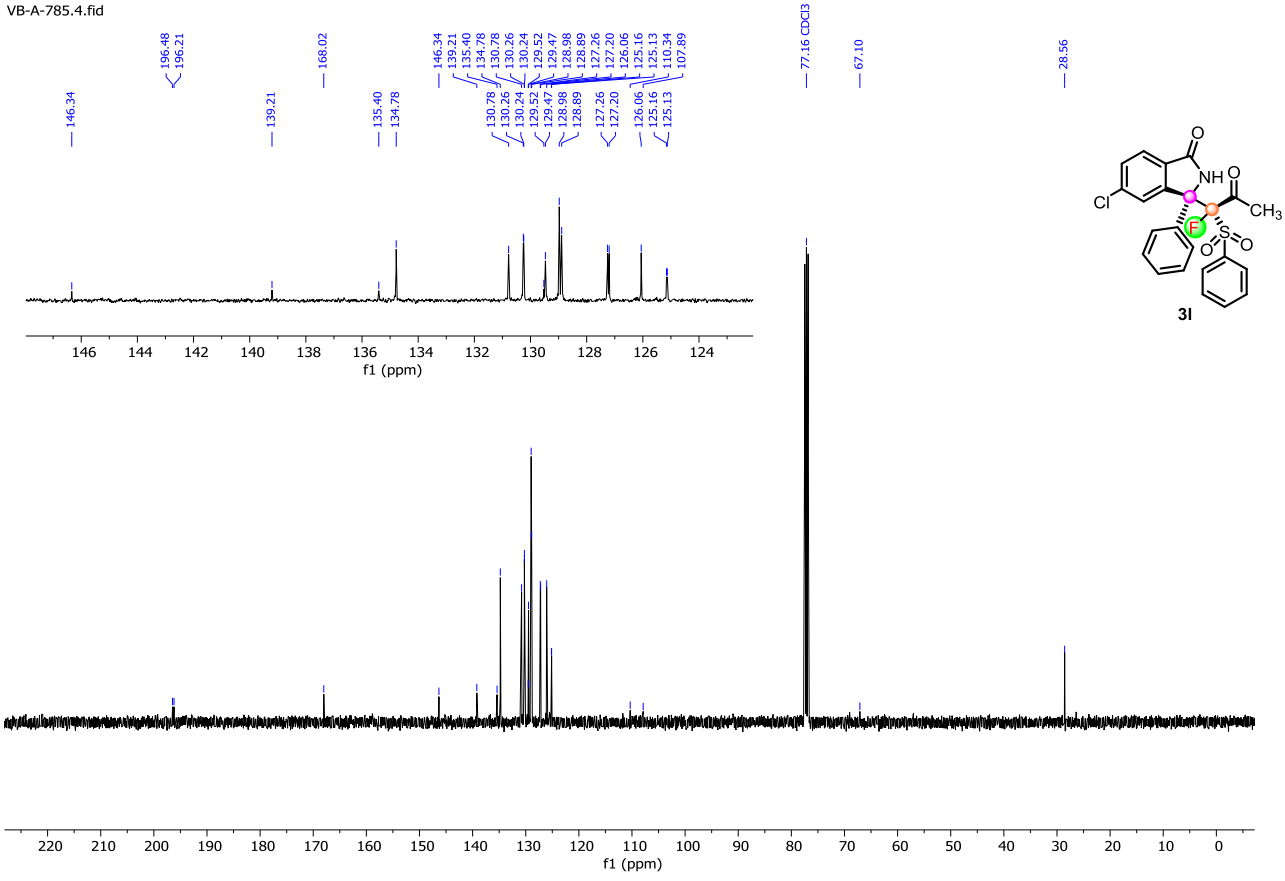


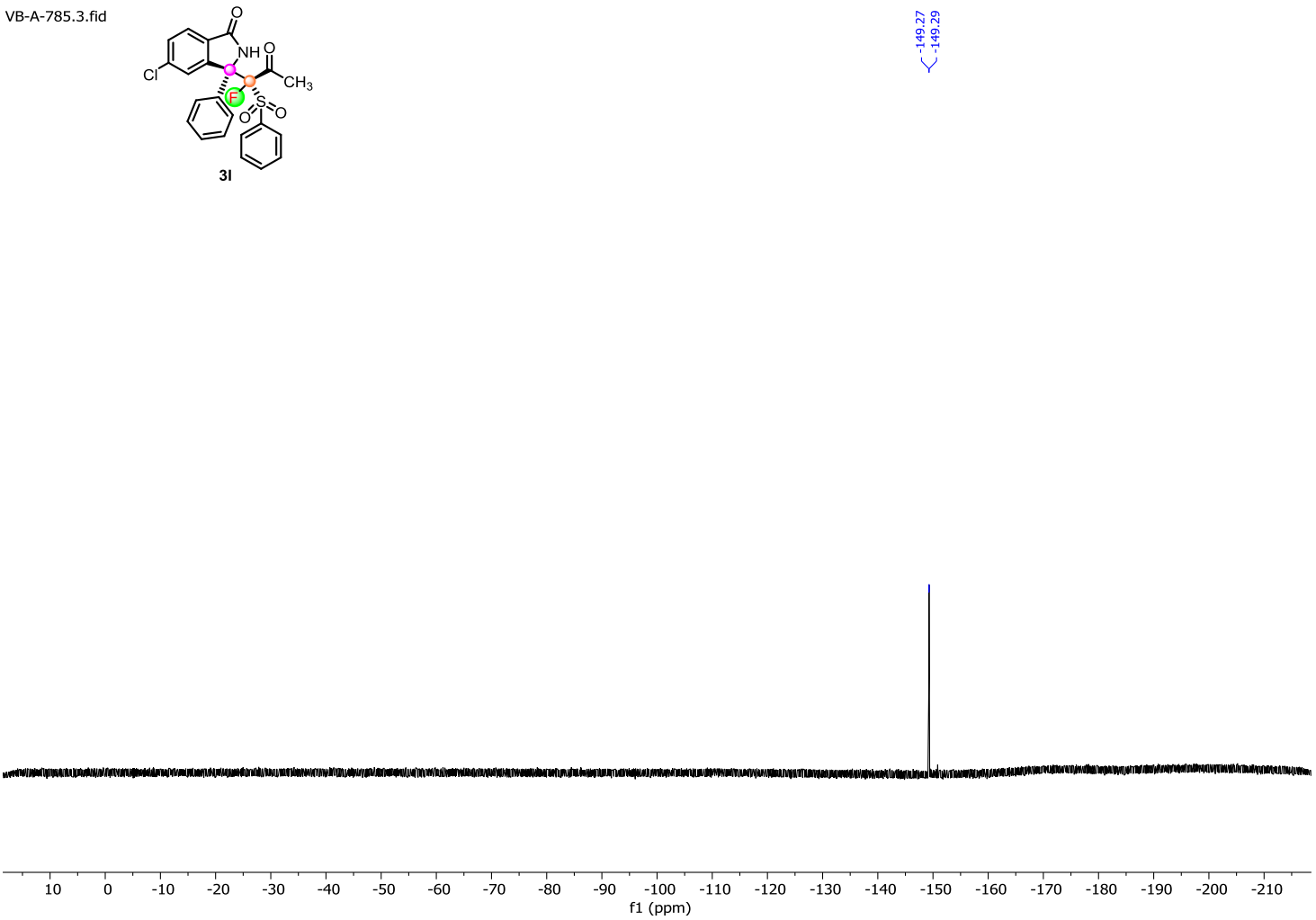
Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

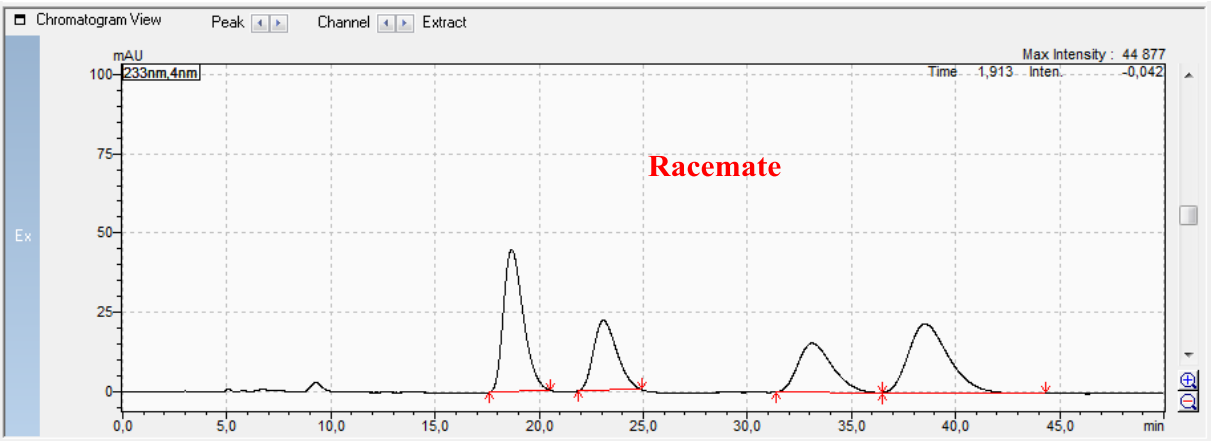
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	26,481	81,950	3062359	58805	0,000000	M	25,163	28,821	81,950
2	31,413	9,718	363143	6509	0,000000	M	30,421	32,640	9,718
3	35,175	2,887	107883	2109	0,000000	M	34,315	35,915	2,887
4	50,569	5,445	203474	2593	0,000000	M	49,184	51,776	5,445
Total		100,000	3736859	70016					100,000


VB-A-785-Ar-Cl.1.fid
3l
f1 (ppm)


VB-A-785.4.fid
3l
f1 (ppm)



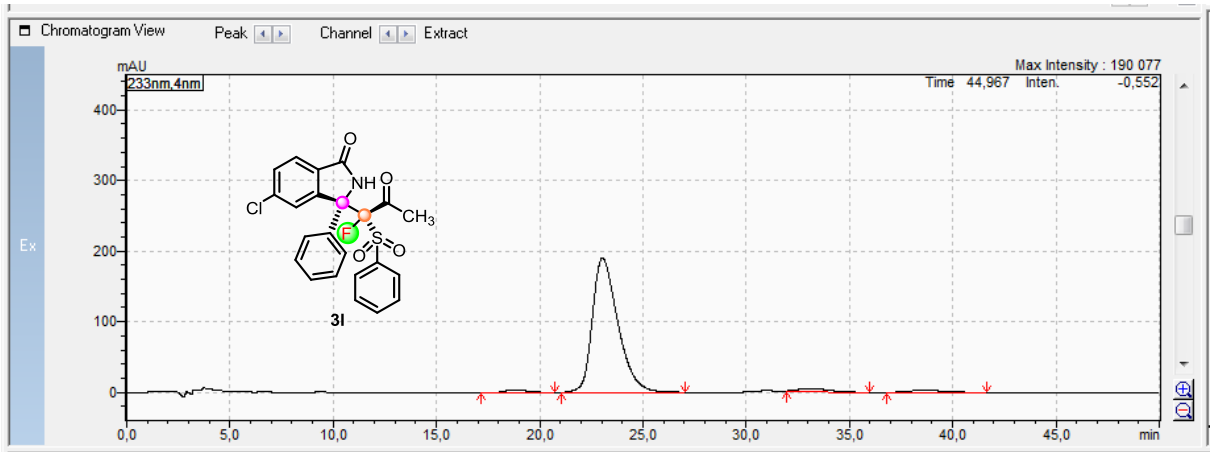
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

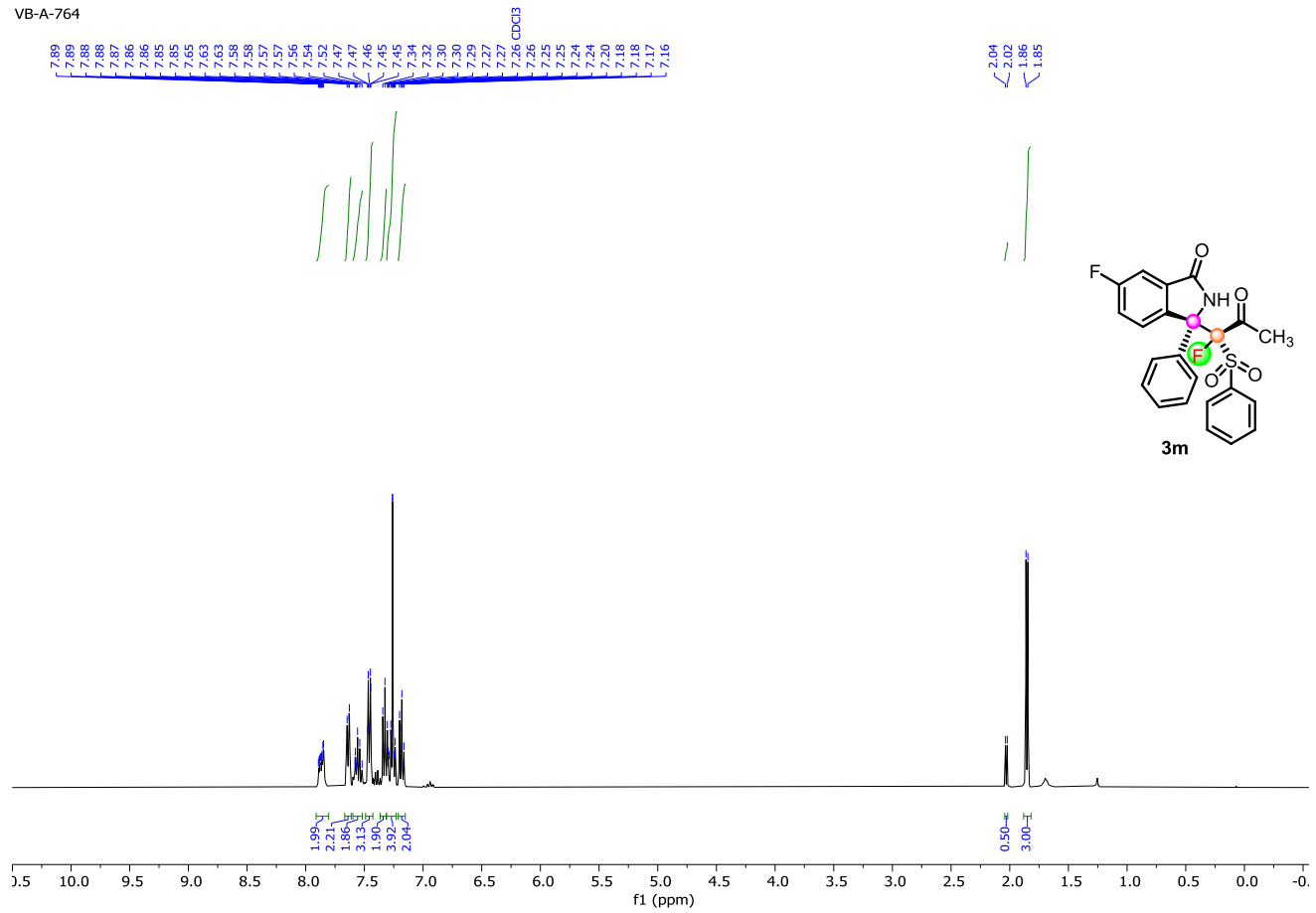
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	18,677	31,477	2932534	44688	0,000000	M	17,600	20,533	31,477
2	23,084	18,463	1720055	21914	0,000000	M	21,877	24,939	18,463
3	33,128	18,875	1758440	15430	0,000000	M	31,381	36,480	18,875
4	38,531	31,186	2905392	21651	0,000000	M	36,480	44,331	31,186
Total		100,000	9316420	103683					100,000



Results View - Peak Table

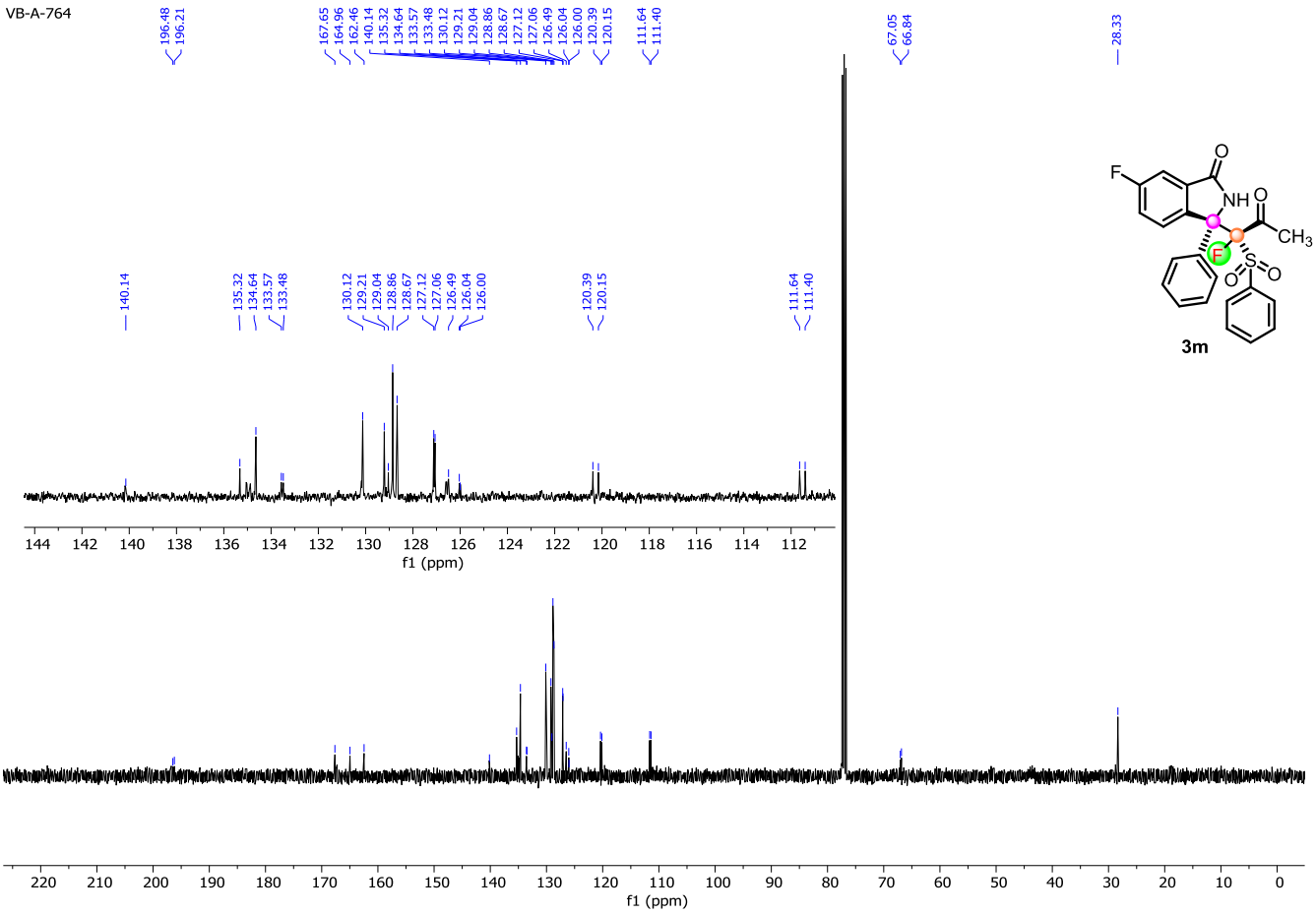
Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	18,777	1,578	274826	4118	0,000000	M	17,152	20,725	1,578
2	23,038	93,928	16362647	190178	0,000000	M	21,045	27,040	93,928
3	33,098	2,235	389416	4062	0,000000	M	31,957	35,968	2,235
4	38,571	2,259	393548	3088	0,000000	M	36,800	41,653	2,259
Total		100,000	17420437	201446					100,000


VB-A-764
CDCl3
f1 (ppm)

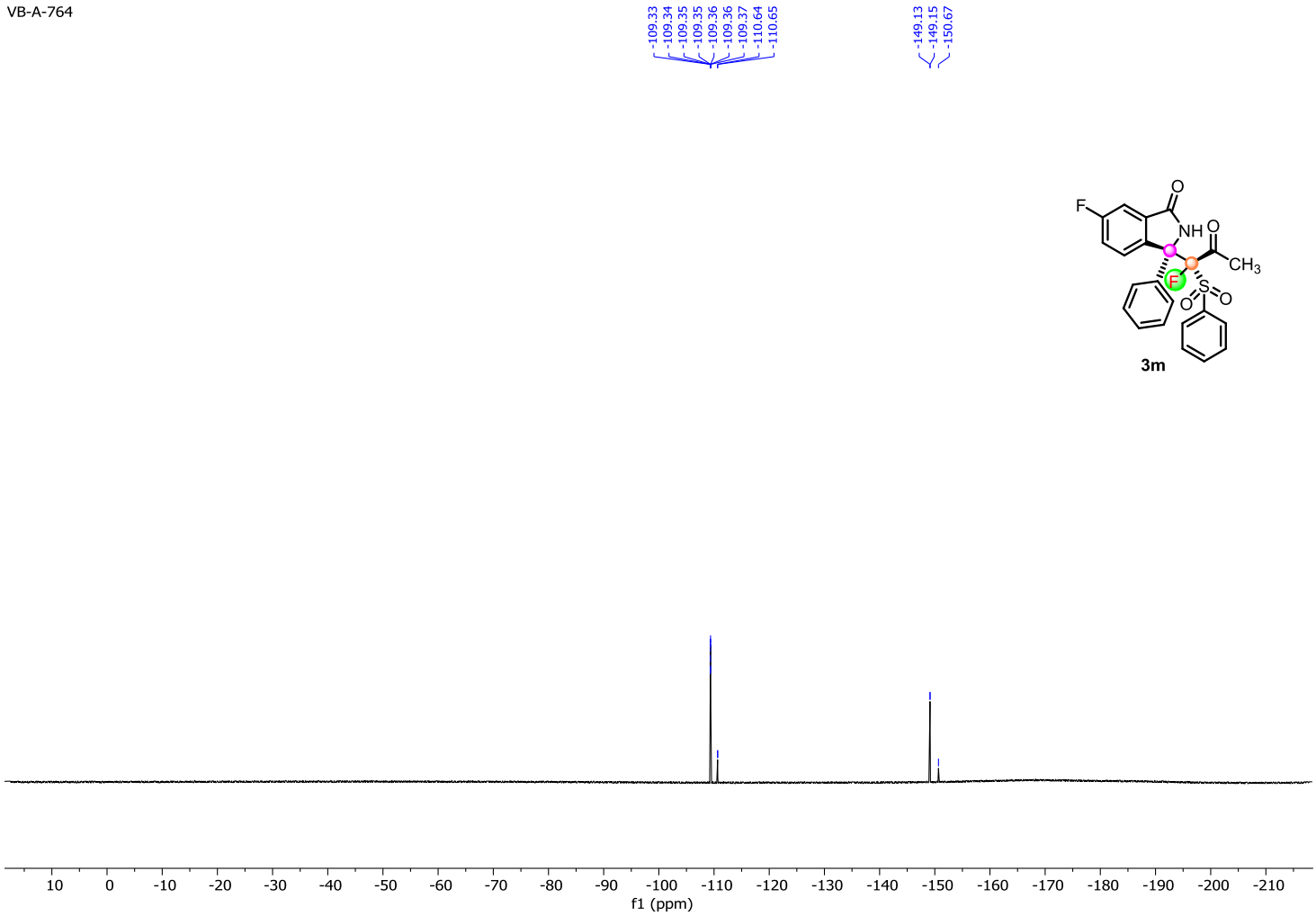
F
O
NH
O
CH3
F
S
O
O

3m

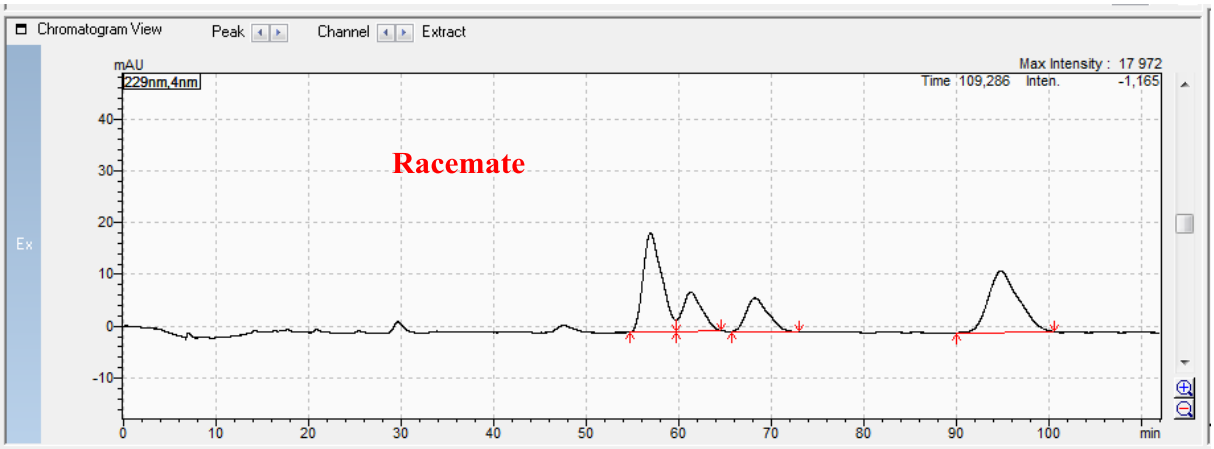

VB-A-764
f1 (ppm)

F
O
NH
O
CH3
F
S
O
O

3m



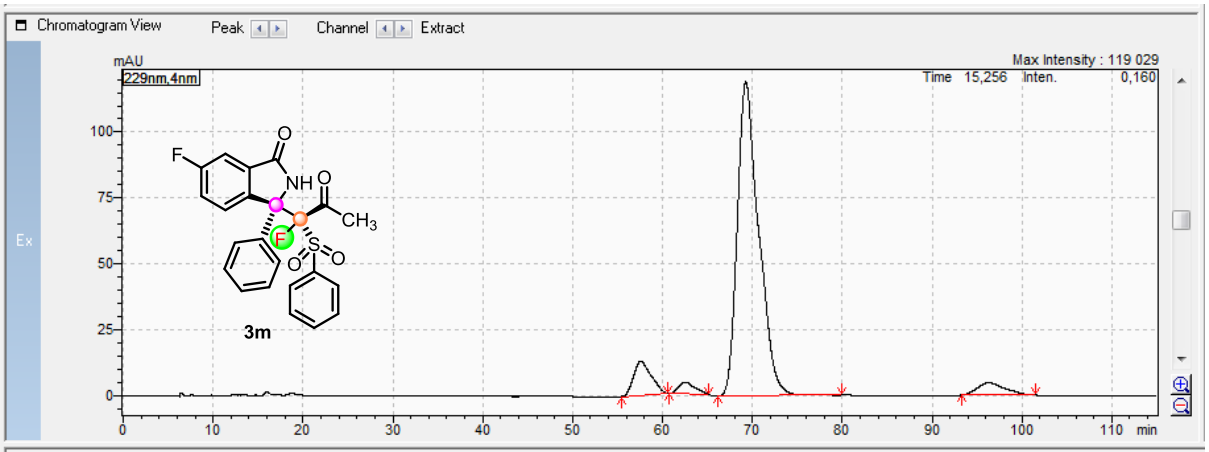
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

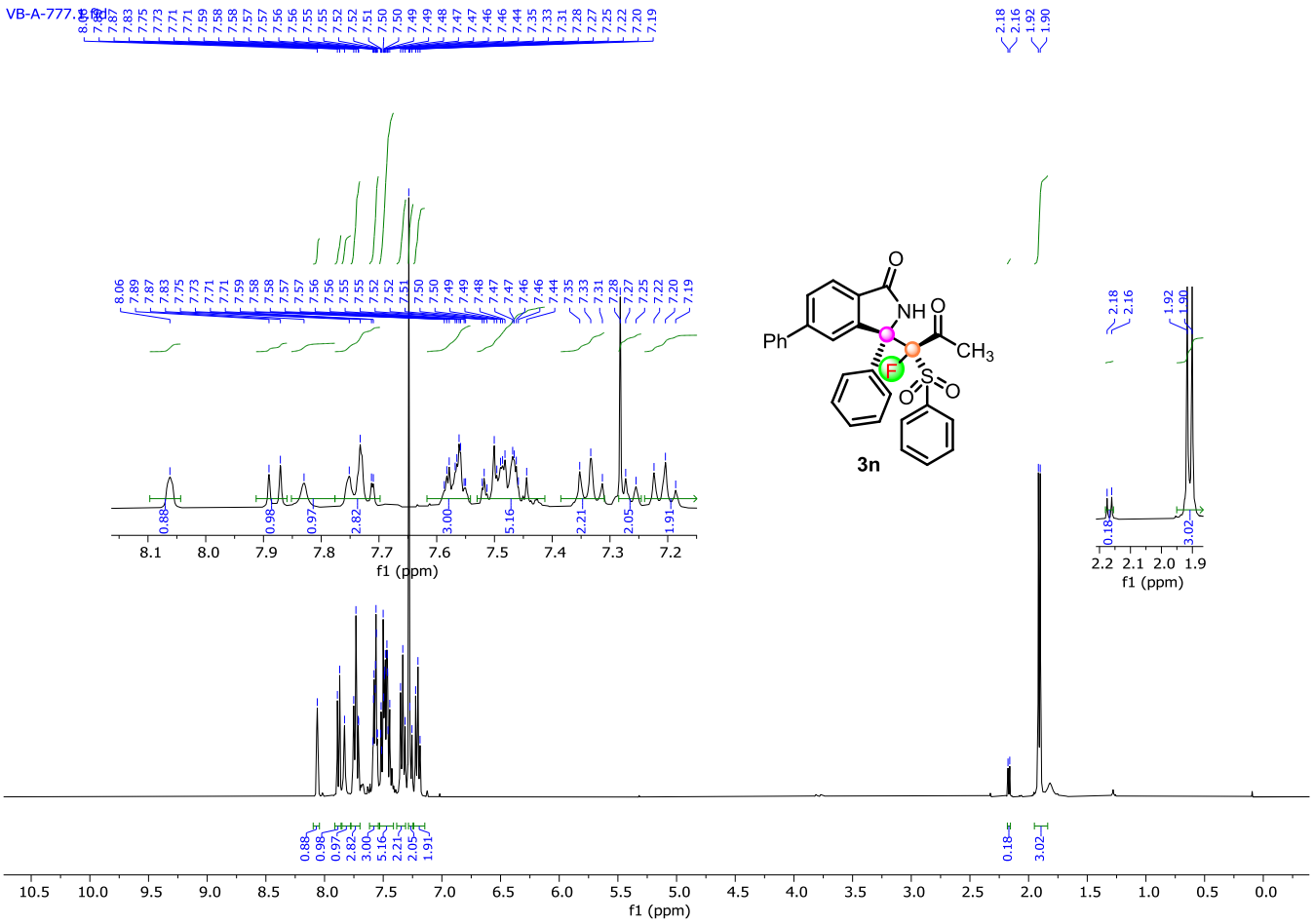
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	56,938	35,341	2653739	19032	0,000000		54,773	59,669	35,341
2	61,274	14,590	1095589	7587	0,000000	V	59,669	64,597	14,590
3	68,233	14,182	1064929	6504	0,000000	M	65,717	73,003	14,182
4	94,793	35,886	2694665	11836	0,000000	M	90,005	100,576	35,886
Total		100,000	7508921	44958					100,000

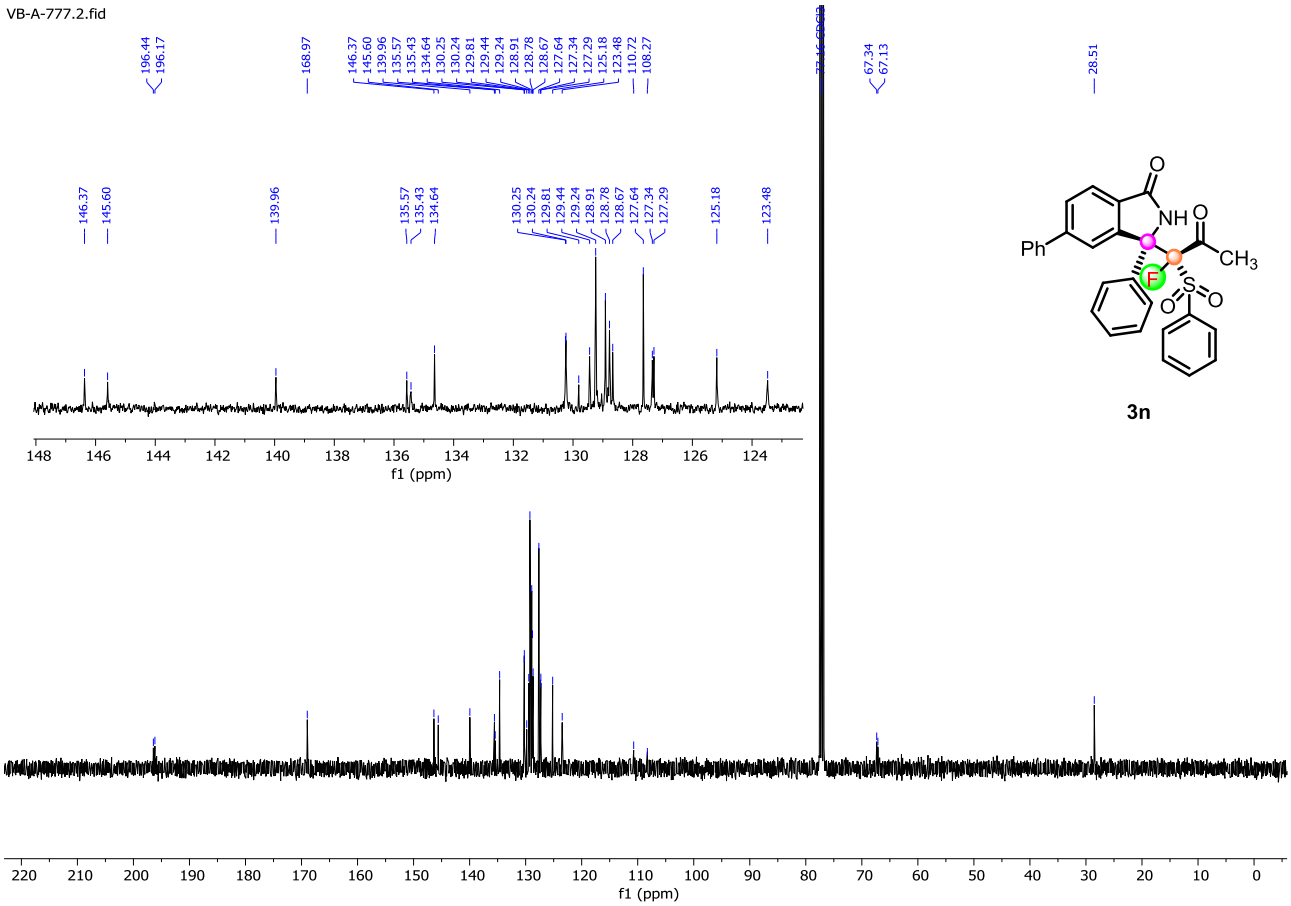


Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

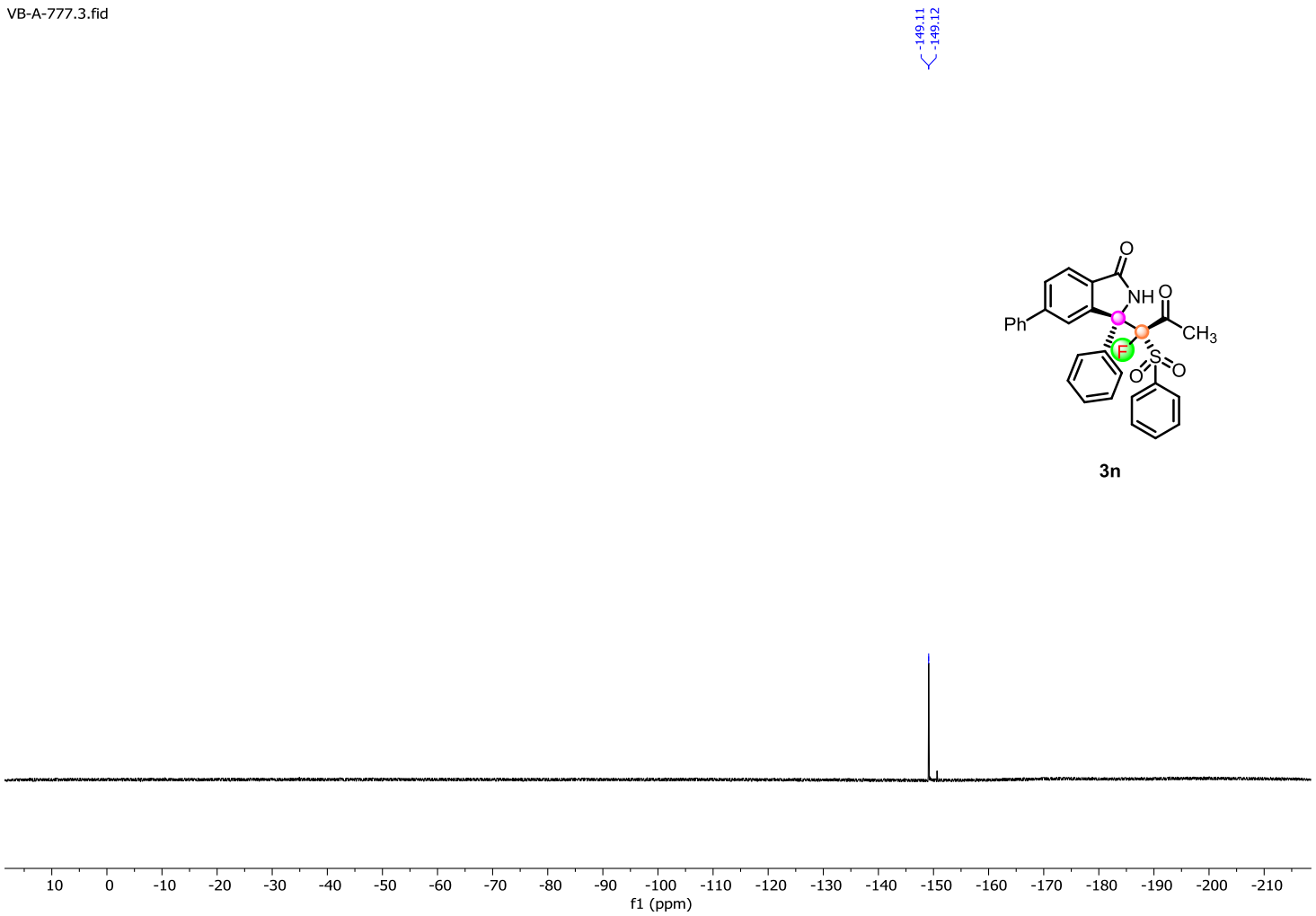
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	57,571	7,621	1752291	12900	0,000000	M	55,445	60,587	7,621
2	62,509	2,530	581761	4559	0,000000	M	60,736	65,131	2,530
3	69,271	85,507	19659487	119036	0,000000	M	66,155	79,947	85,507
4	96,277	4,342	998254	4666	0,000000	M	93,301	101,515	4,342
Total		100,000	22991793	141161					100,000


VB-A-777.1.fid
8.06 7.89 7.87 7.83 7.75 7.73 7.71 7.71 7.59 7.58 7.57 7.57 7.56 7.56 7.55 7.55 7.52 7.52 7.51 7.50 7.50 7.49 7.49 7.48 7.47 7.47 7.46 7.46 7.44 7.35 7.33 7.31 7.28 7.27 7.25 7.22 7.20 7.19
2.18 2.16 1.92 1.90
0.88 0.98 0.97 2.82 3.00 5.16 2.21 2.05 1.91
0.18 3.02
f1 (ppm)
Ph
NH
O
CH3
F
S
O
3n

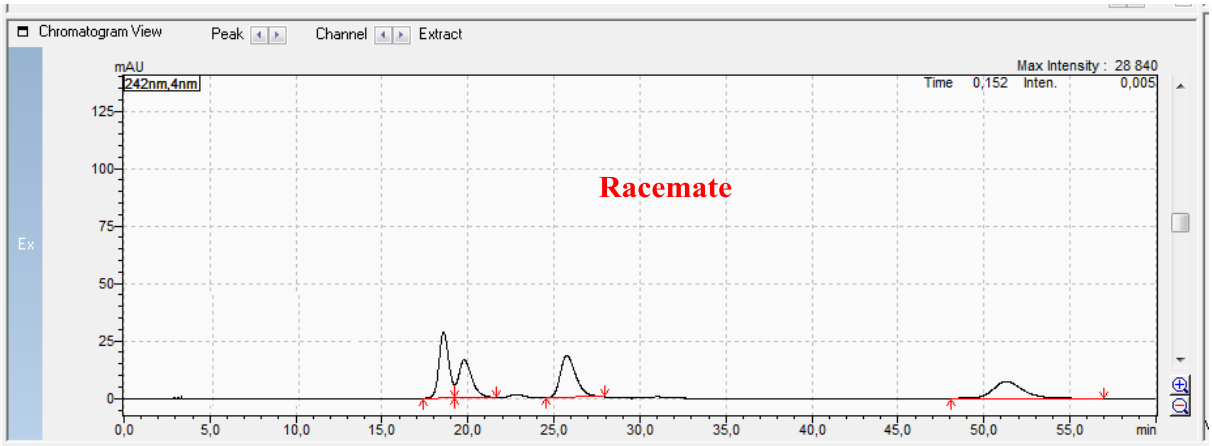

VB-A-777.2.fid
196.44
196.17
168.97
146.37
145.60
139.96
135.57
135.43
134.64
130.25
130.24
129.81
129.44
129.24
128.91
128.78
128.67
127.64
127.34
127.29
125.18
123.48
110.72
108.27
77.16
67.34
67.13
28.51
f1 (ppm)
f1 (ppm)

O
NH
O
Ph
CH3
F
S
O
O

3n



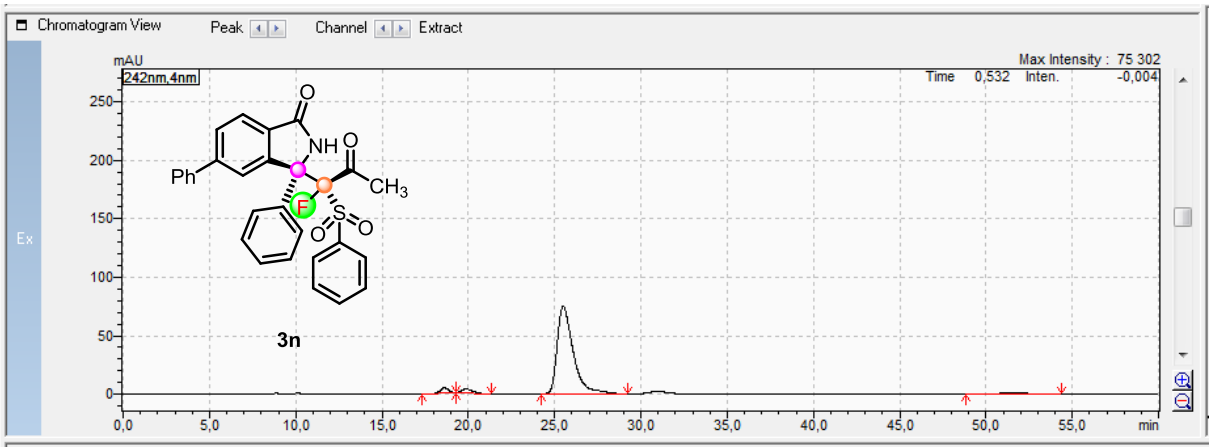
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	18,579	28,356	1158999	28707	0,000000		17,408	19,243	28,356
2	19,783	21,752	889075	16736	0,000000	V	19,243	21,664	21,752
3	25,749	28,397	1160694	18385	0,000000	M	24,533	27,957	28,397
4	51,291	21,495	878583	7337	0,000000	M	48,085	56,971	21,495
Total		100,000	4087351	71165					100,000

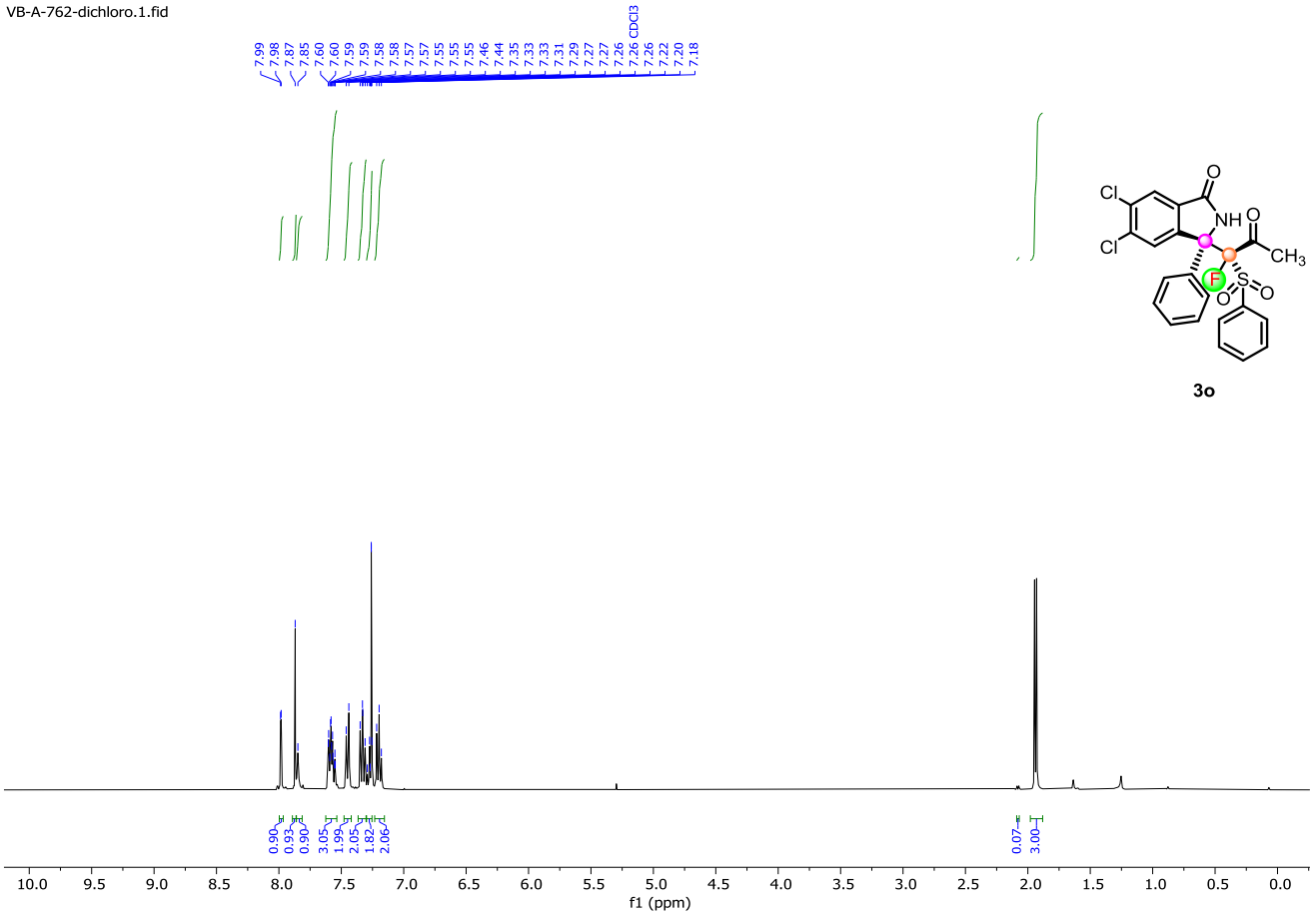


Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

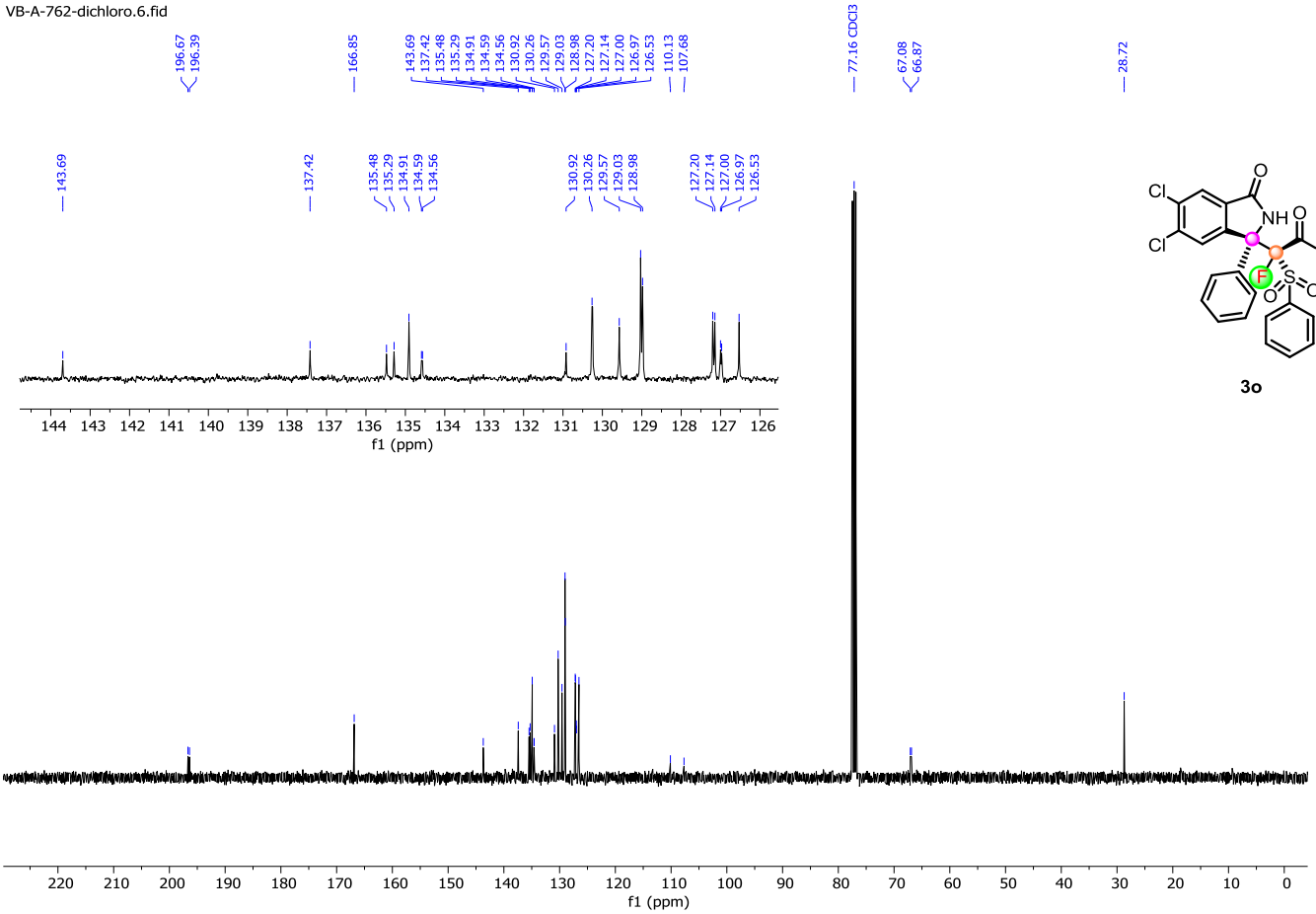
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	18,626	2,887	152965	4597	0,000000	M	17,312	19,296	2,887
2	19,883	2,862	151638	3435	0,000000	M	19,296	21,344	2,862
3	25,502	91,896	4868940	75102	0,000000		24,192	29,227	91,896
4	51,562	2,355	124798	1064	0,000000	M	48,832	54,379	2,355
Total		100,000	5298341	84199					100,000

VB-A-762-dichloro.1.fid

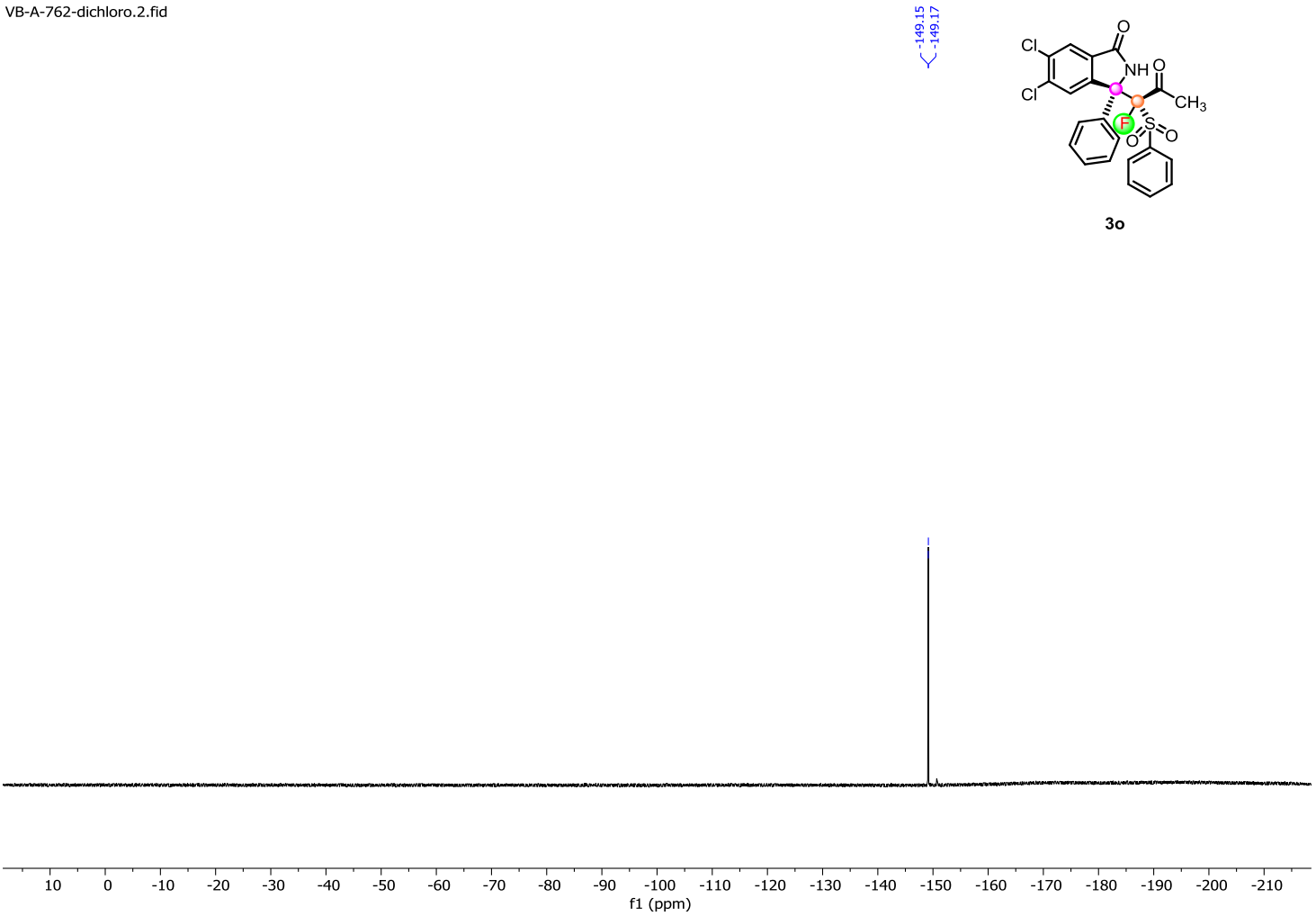


3o

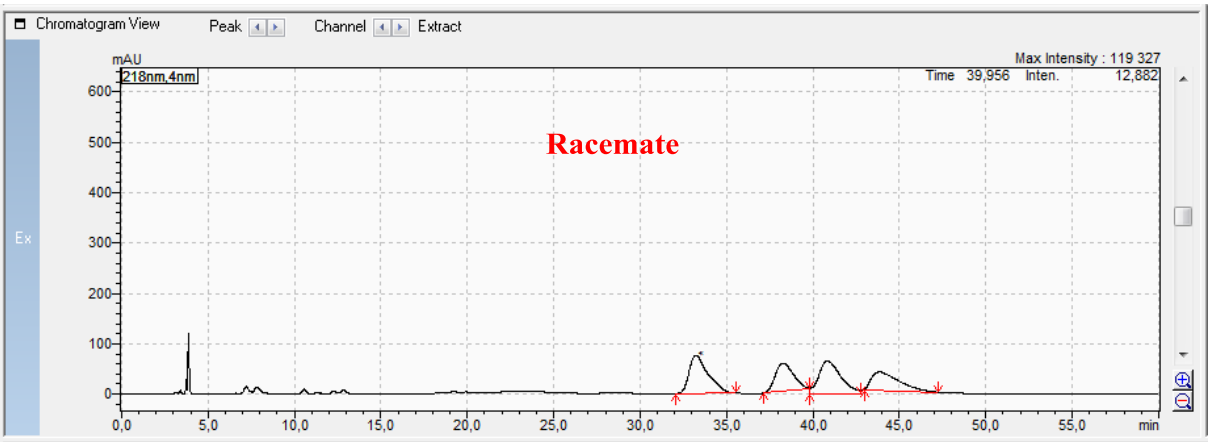
VB-A-762-dichloro.6.fid



3o



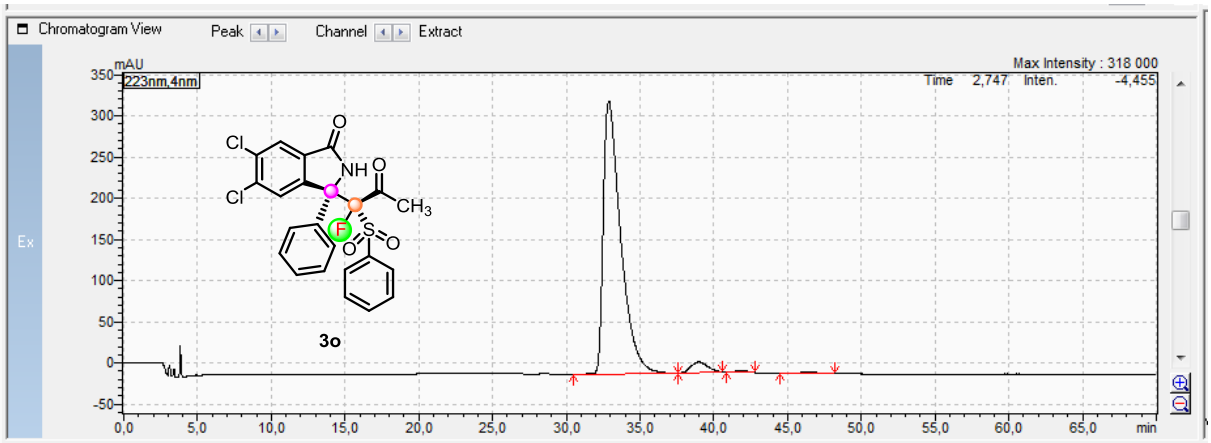
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

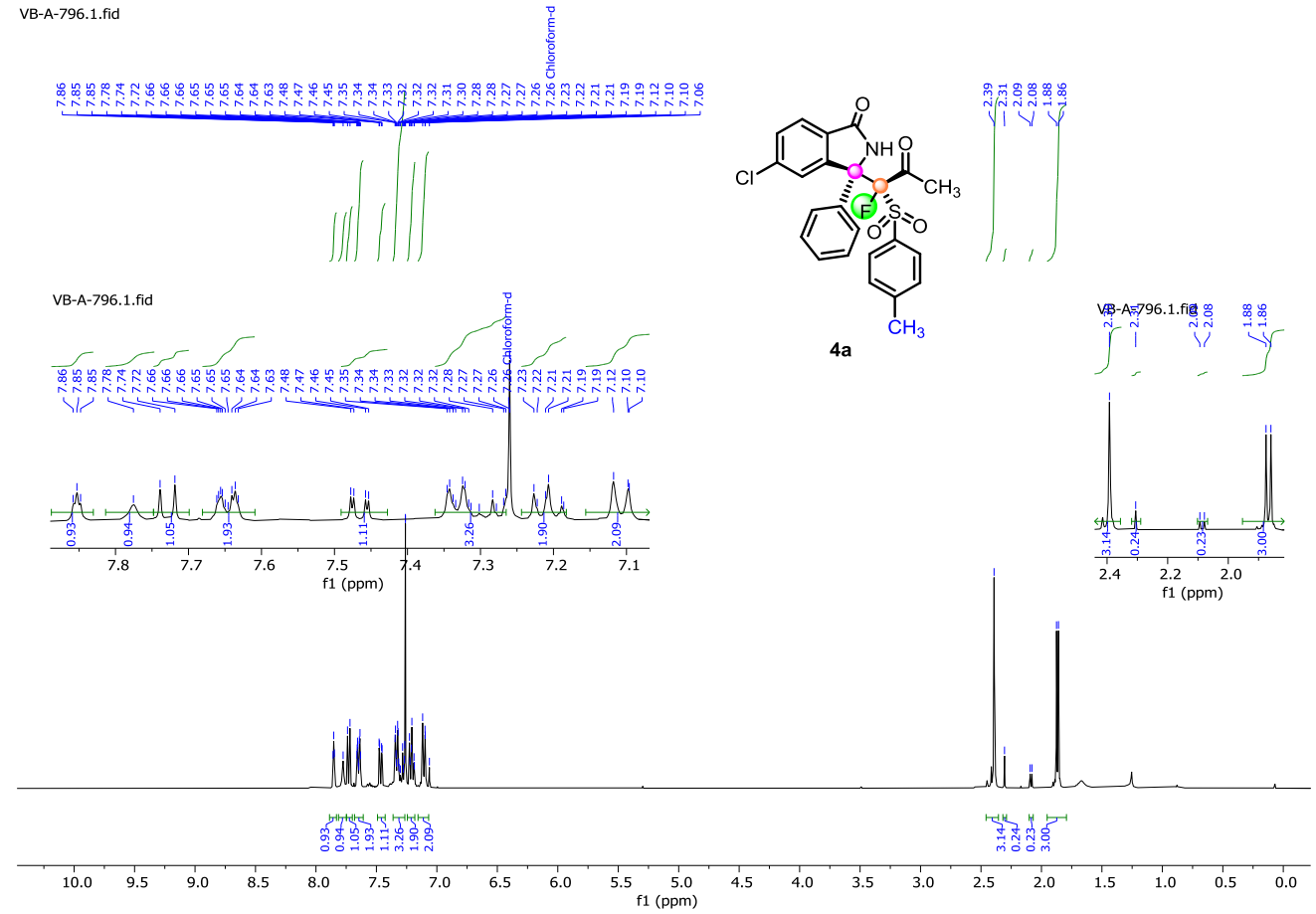
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	33,230	29,718	5815714	75534	0,000000	M	32,053	35,552	29,718
2	38,286	20,583	4028047	55265	0,000000	M	37,141	39,819	20,583
3	40,849	29,598	5792230	65550	0,000000		39,819	42,795	29,598
4	43,862	20,102	3933834	35646	0,000000	M	42,997	47,253	20,102
Total		100,000	19569825	231995					100,000

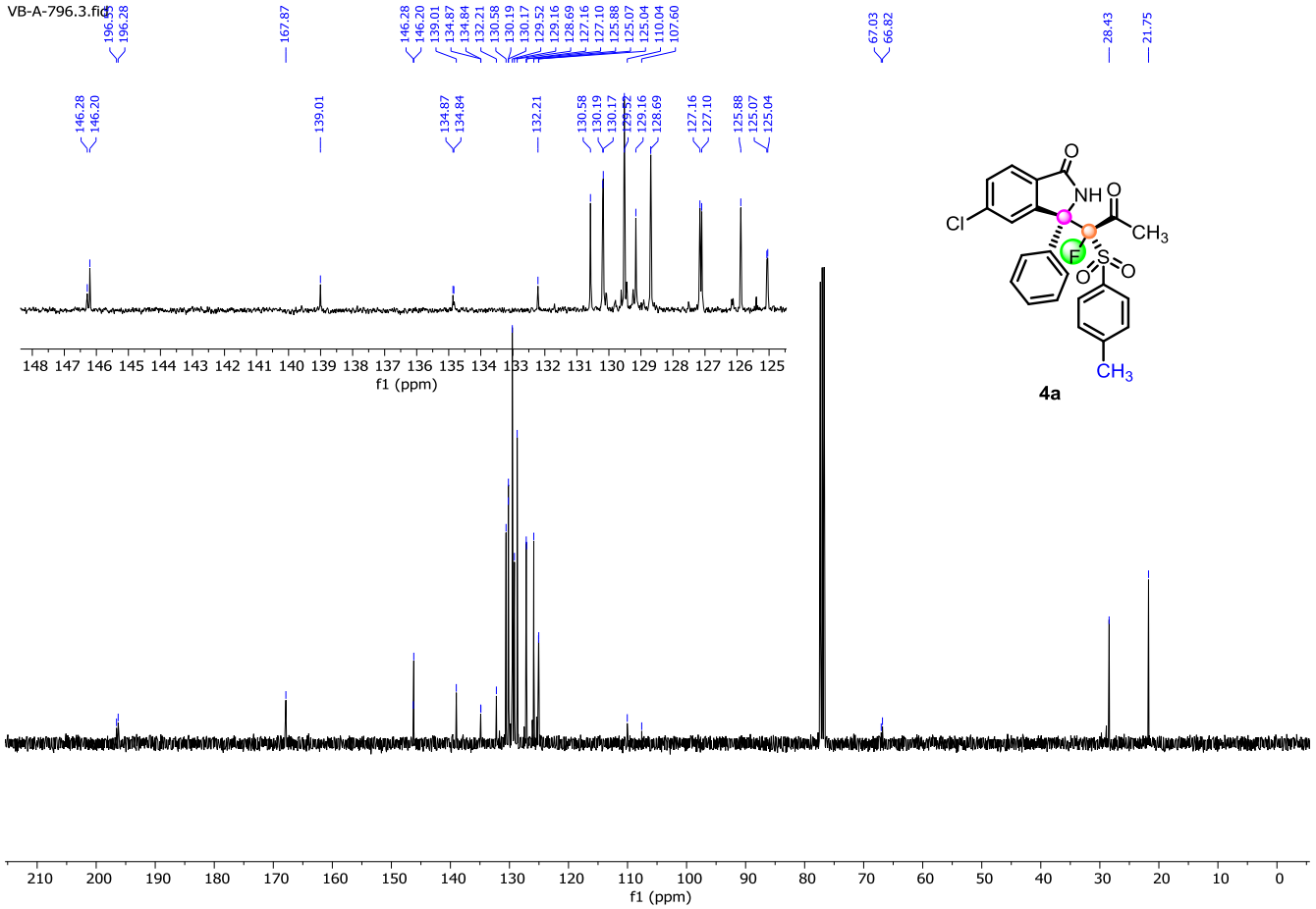


Results View - Peak Table

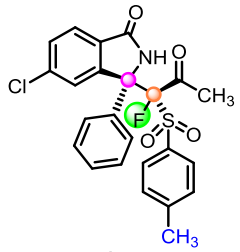
Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	32,890	95,335	27028430	331046	0,000000	M	30,464	37,600	95,335
2	38,993	3,587	1016878	12811	0,000000	M	37,600	40,597	3,587
3	41,826	0,455	129113	2120	0,000000	M	40,853	42,805	0,455
4	46,322	0,623	176542	1783	0,000000	M	44,469	48,203	0,623
Total		100,000	28350962	347760					100,000


VB-A-796.1.fid
Chloroform-d
4a
f1 (ppm)

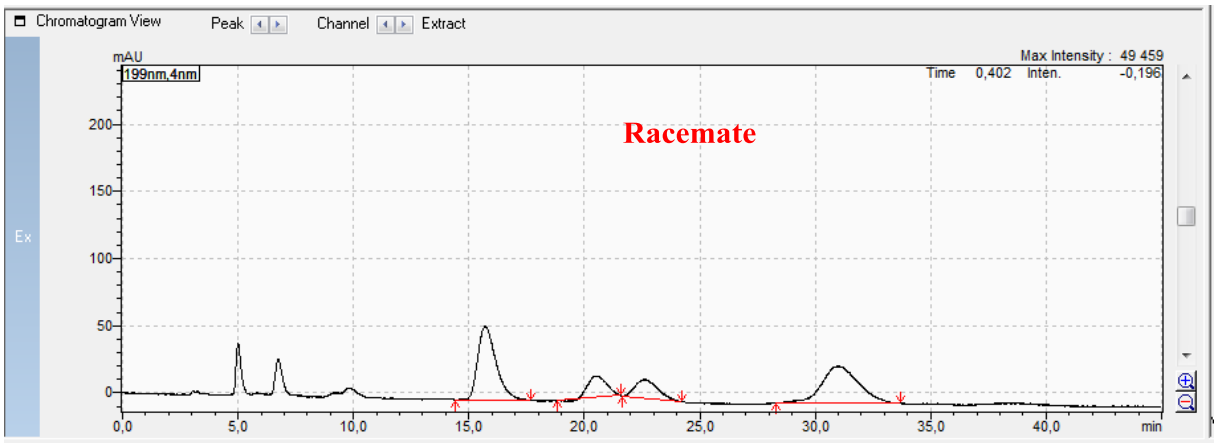

VB-A-796.3.fid
4a
f1 (ppm)

VB-A-796.2.fid



4a

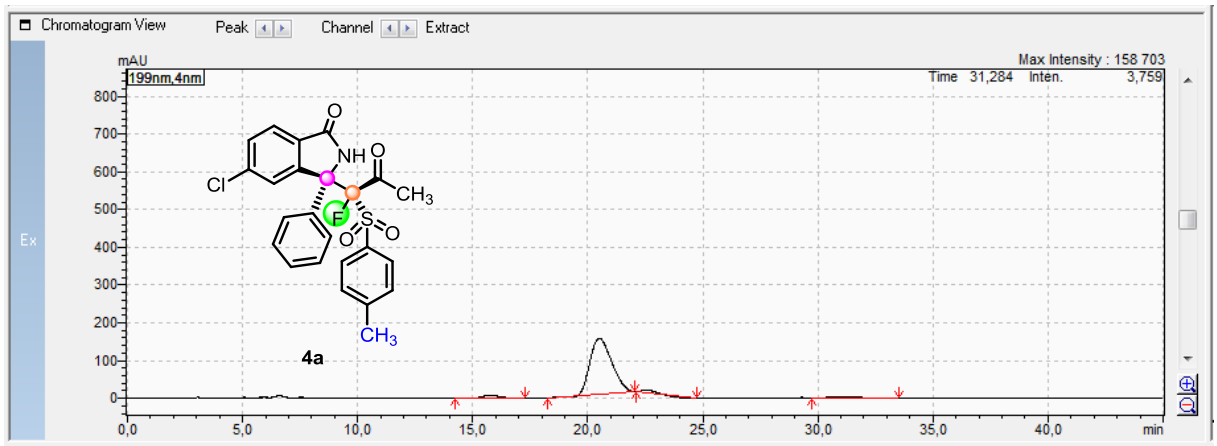
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

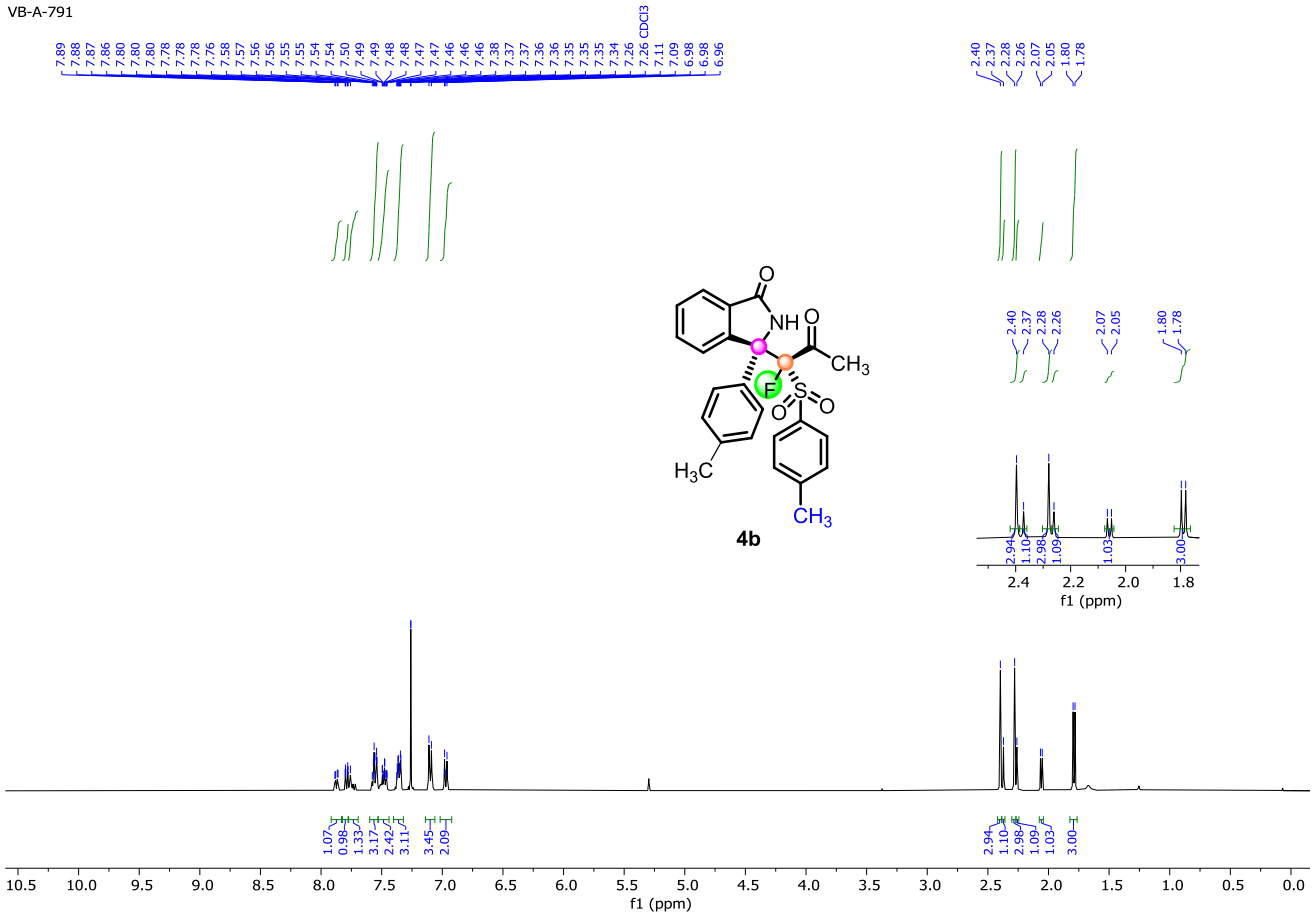
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	15,701	38,017	3003363	54683	0,000000	M	14,411	17,685	38,017
2	20,500	11,146	880497	16009	0,000000	M	18,827	21,579	11,146
3	22,621	11,975	946009	13893	0,000000	M	21,643	24,224	11,975
4	30,989	38,863	3070154	27678	0,000000	M	28,299	33,696	38,863
Total		100,000	7900023	112264					100,000

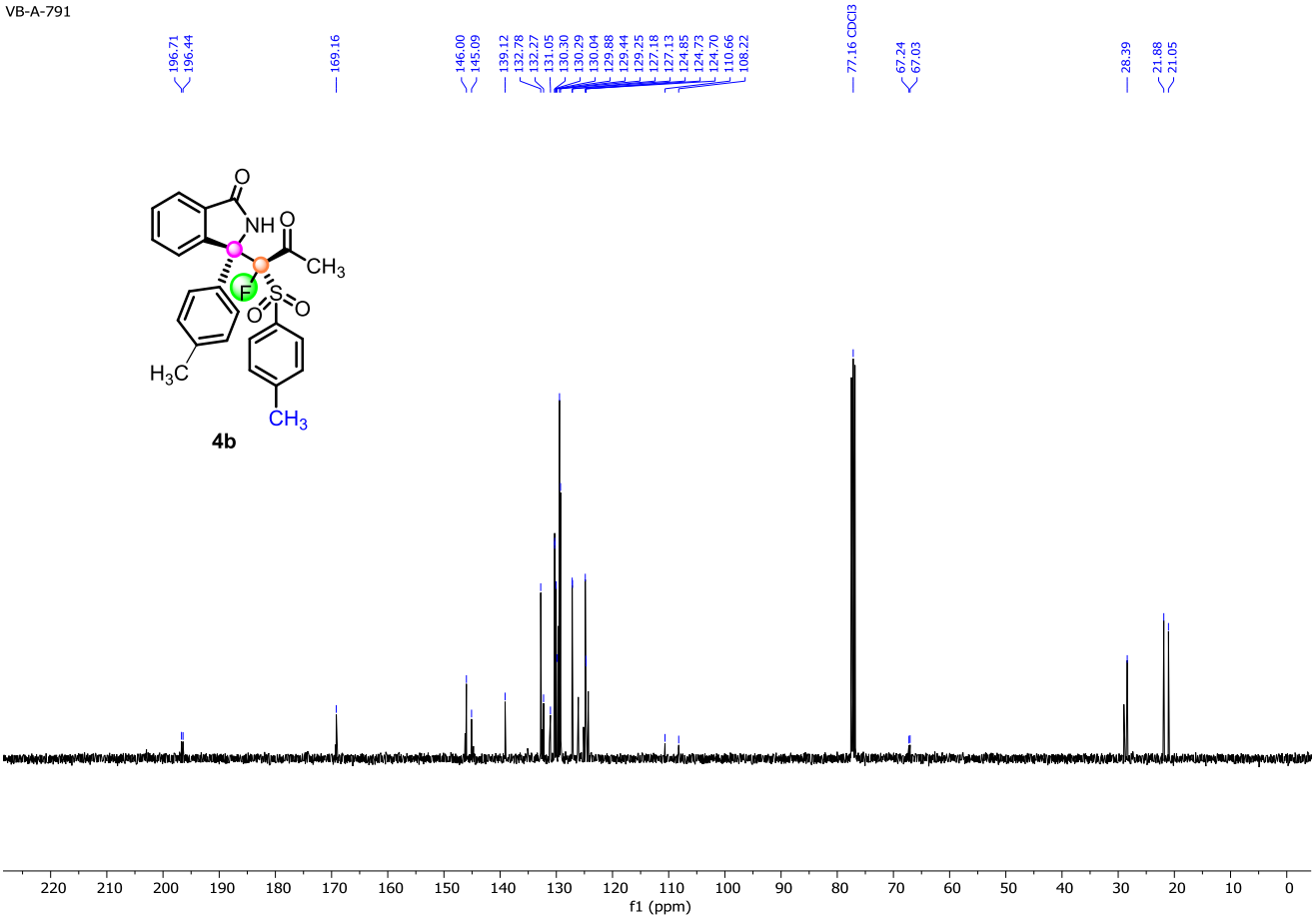


Results View - Peak Table

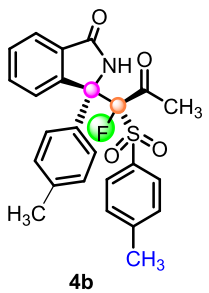
Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	15,768	3,871	414786	8345	0,000000	M	14,240	17,280	3,871
2	20,502	91,653	9821731	147953	0,000000	M	18,251	22,037	91,653
3	22,496	1,034	110775	5848	0,000000	M	22,101	24,736	1,034
4	31,061	3,443	368933	3949	0,000000	M	29,739	33,525	3,443
Total		100,000	10716226	166094					100,000


VB-A-791
4b
f1 (ppm)

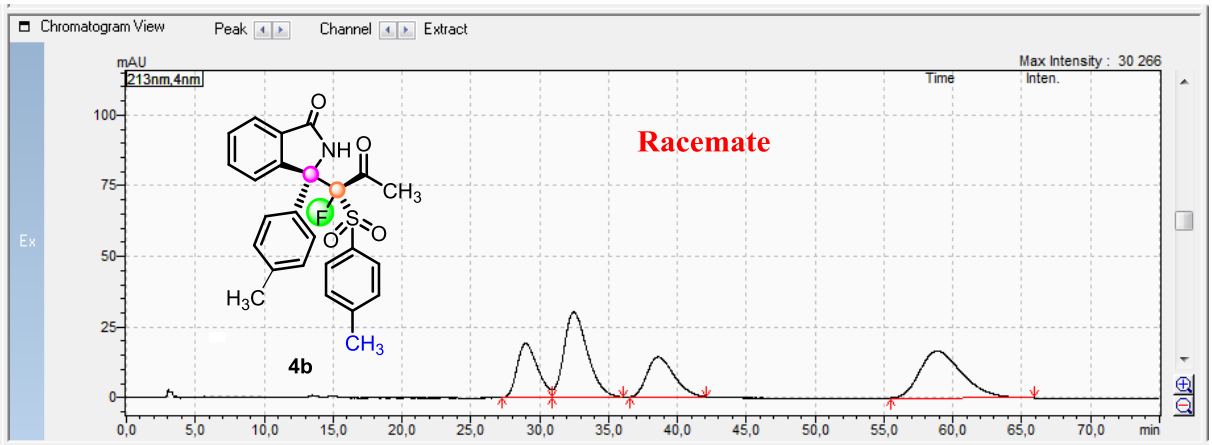

VB-A-791
4b
f1 (ppm)

VB-A-791



4b

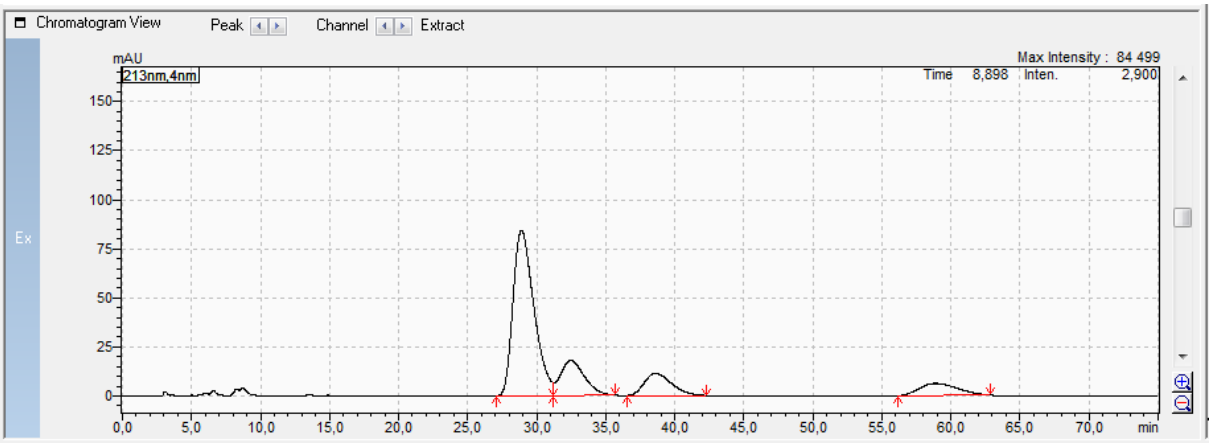
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

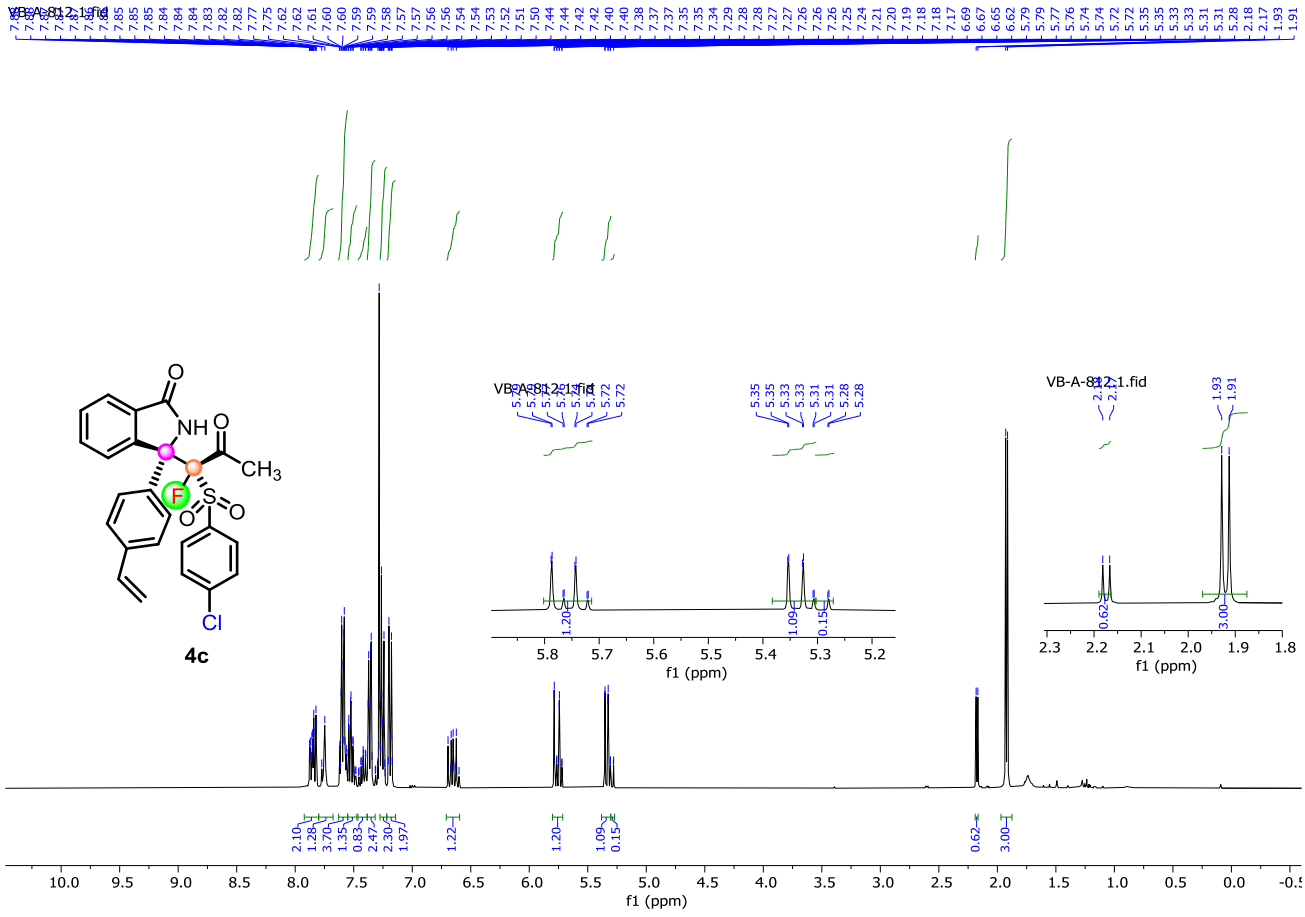
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	28,989	17,967	1980834	19208	0,000000		27,232	30,901	17,967
2	32,476	32,427	3575102	30147	0,000000	SV	30,901	36,053	32,427
3	38,570	17,408	1919207	14140	0,000000		36,565	42,133	17,408
4	58,865	32,198	3549853	16645	0,000000	M	55,488	65,920	32,198
Total		100,000	11024996	80140					100,000

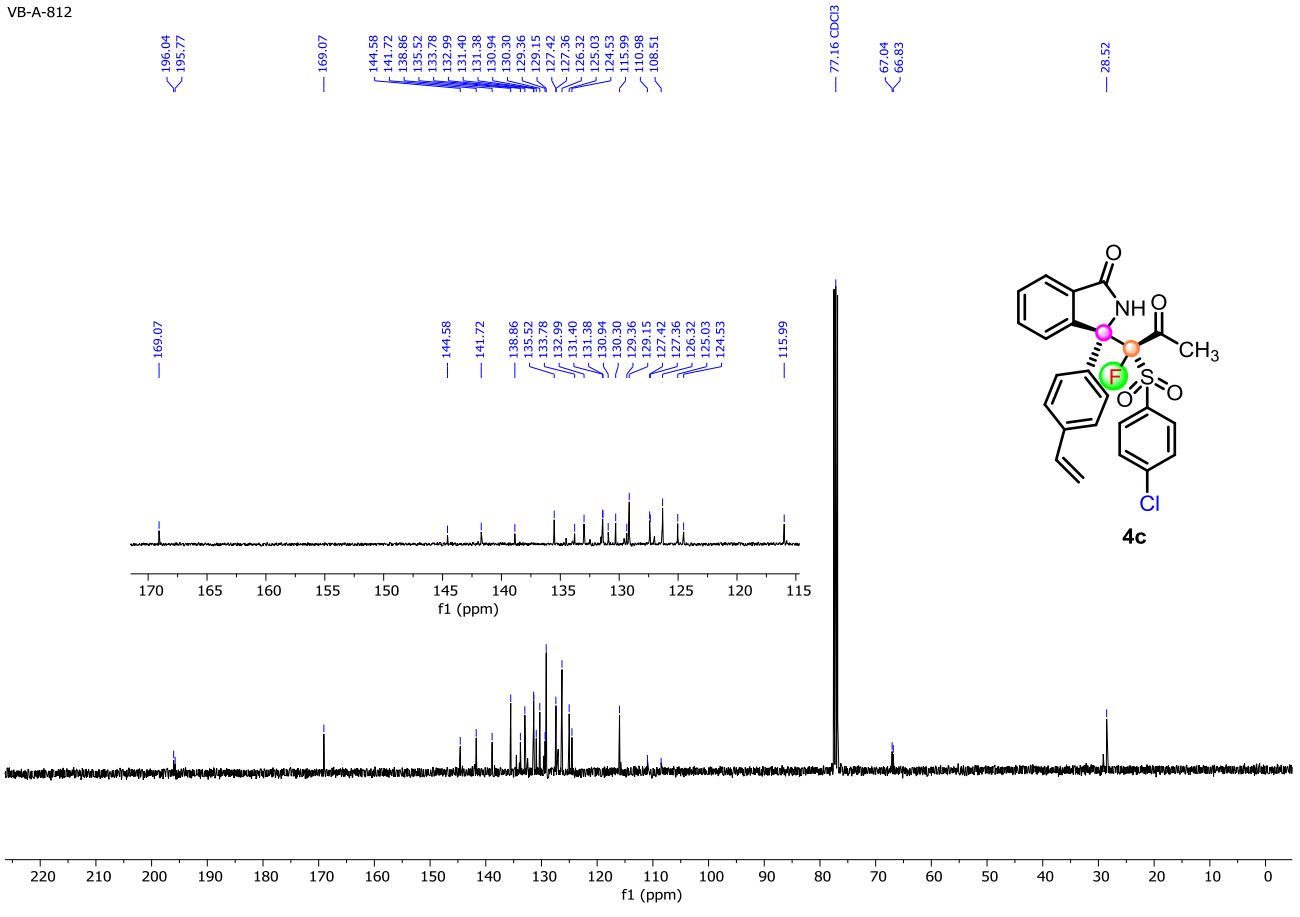


Results View - Peak Table

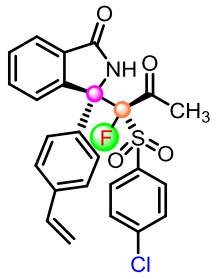
Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	28,902	64,346	8897724	84362	0,000000		27,104	31,221	64,346
2	32,470	15,691	2169680	17964	0,000000	V	31,221	35,691	15,691
3	38,620	11,259	1556887	11336	0,000000	S	36,555	42,272	11,259
4	58,879	8,704	1203612	6206	0,000000		56,117	62,869	8,704
Total		100,000	13827904	119867					100,000

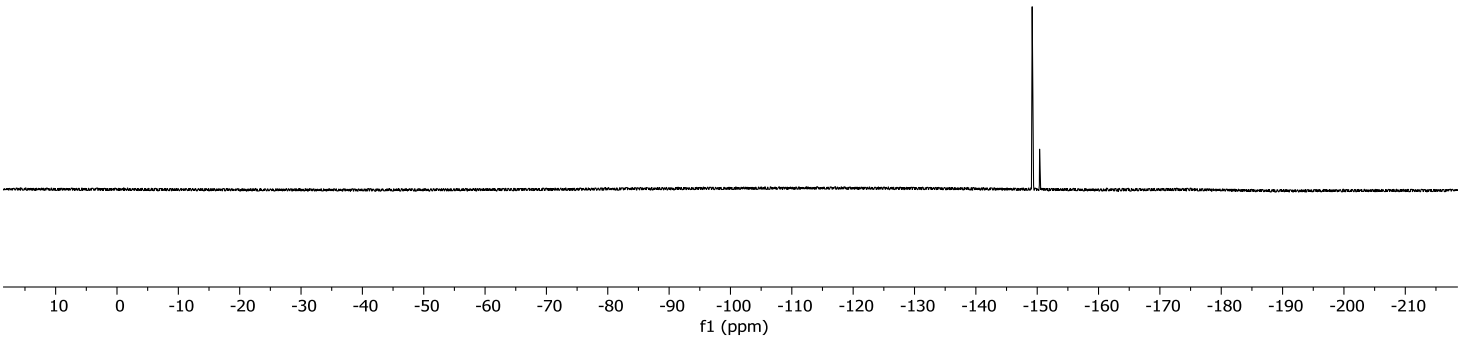

VB-A-812-1.fid
VB-A-812-2.fid
VB-A-812-1.fid
4c
f1 (ppm)


VB-A-812
77.16 CDCl3
4c
f1 (ppm)

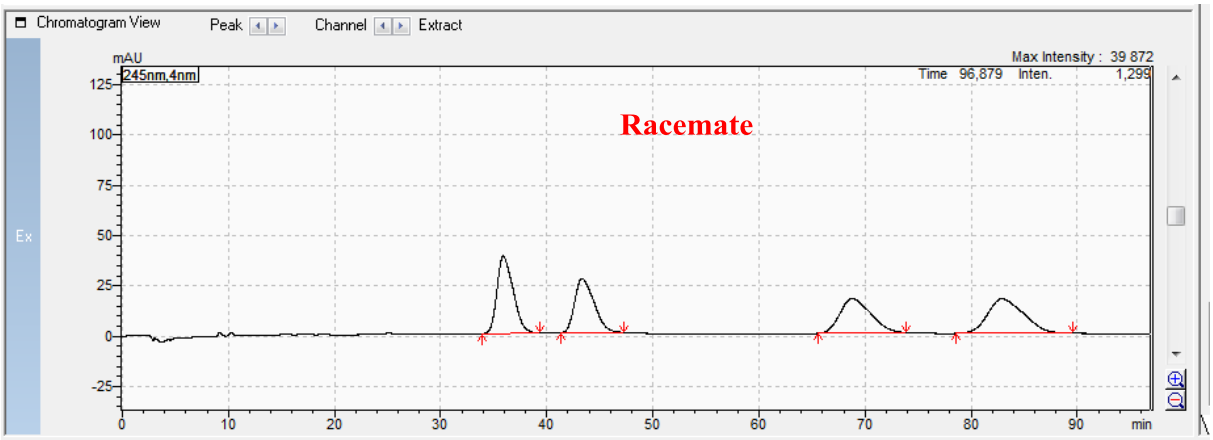
VB-A-812



4c



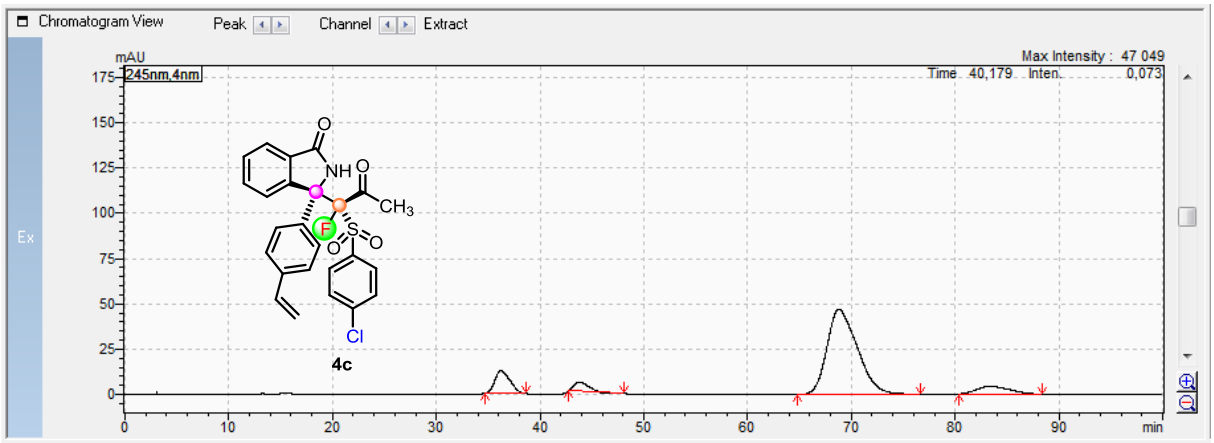
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	35,903	27,141	4075099	38495	0,000000		33,941	39,296	27,141
2	43,331	22,885	3436081	27019	0,000000		41,301	47,317	22,885
3	68,772	22,908	3439448	17141	0,000000	S	65,611	73,824	22,908
4	82,909	27,066	4063714	17252	0,000000	M	78,571	89,579	27,066
Total		100,000	15014342	99906					100,000

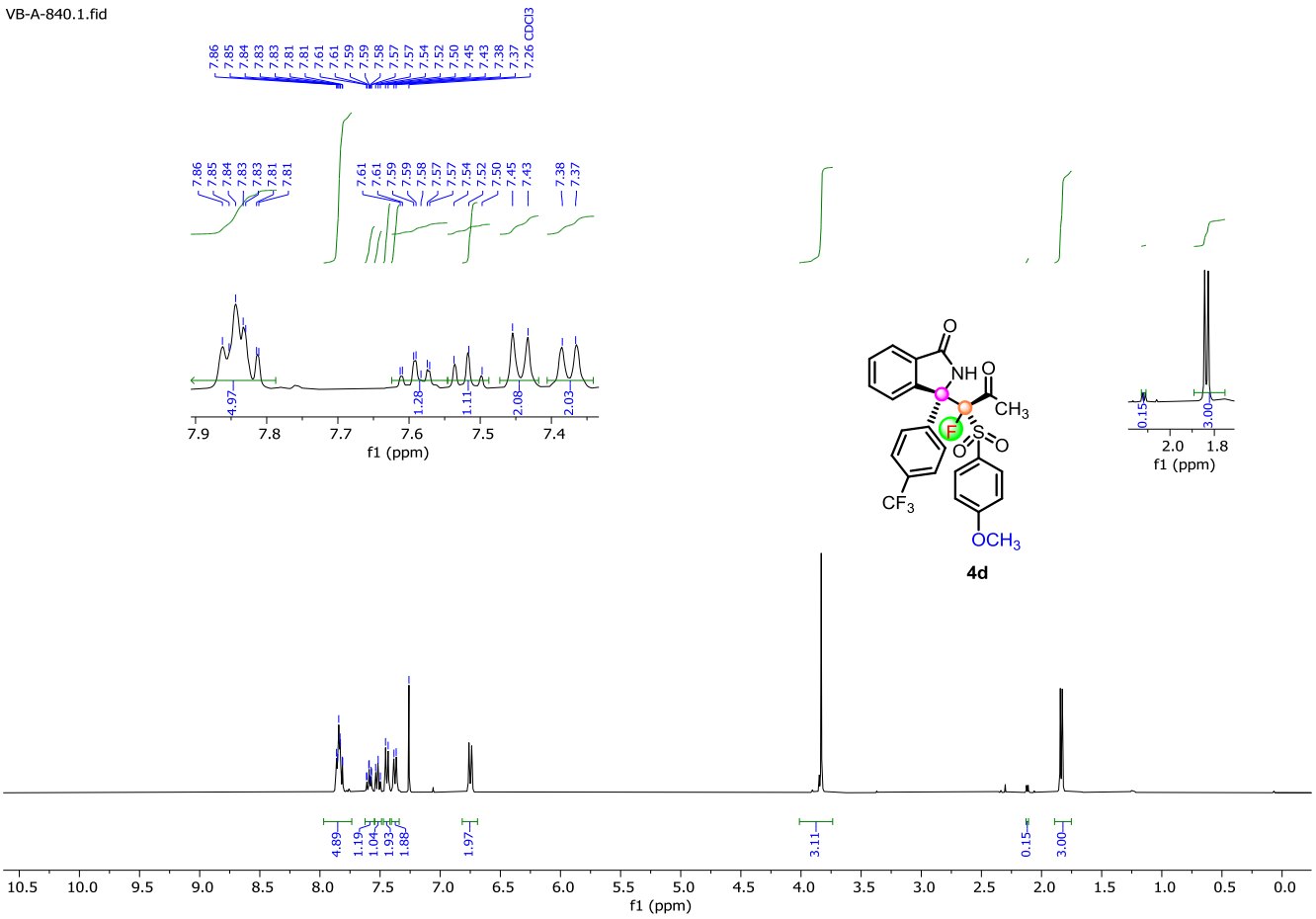


Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

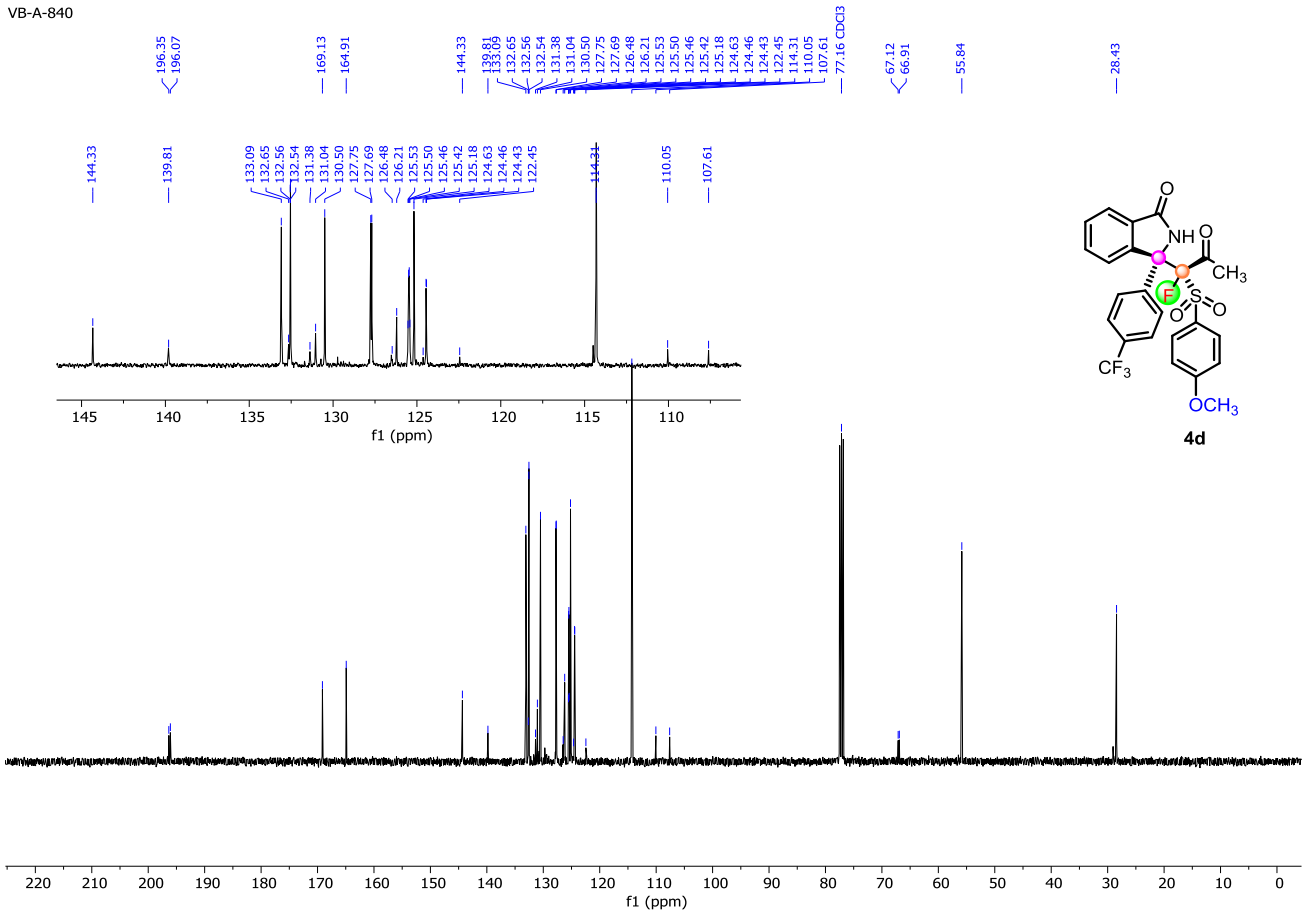
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	36,239	10,372	1270746	12714	0,000000	M	34,699	38,645	10,372
2	43,785	4,109	503444	5057	0,000000	M	42,731	48,085	4,109
3	68,799	77,869	9540414	47022	0,000000	M	64,800	76,661	77,869
4	83,390	7,650	937292	4301	0,000000	M	80,352	88,395	7,650
Total		100,000	12251896	69093					100,000

VB-A-840.1.fid

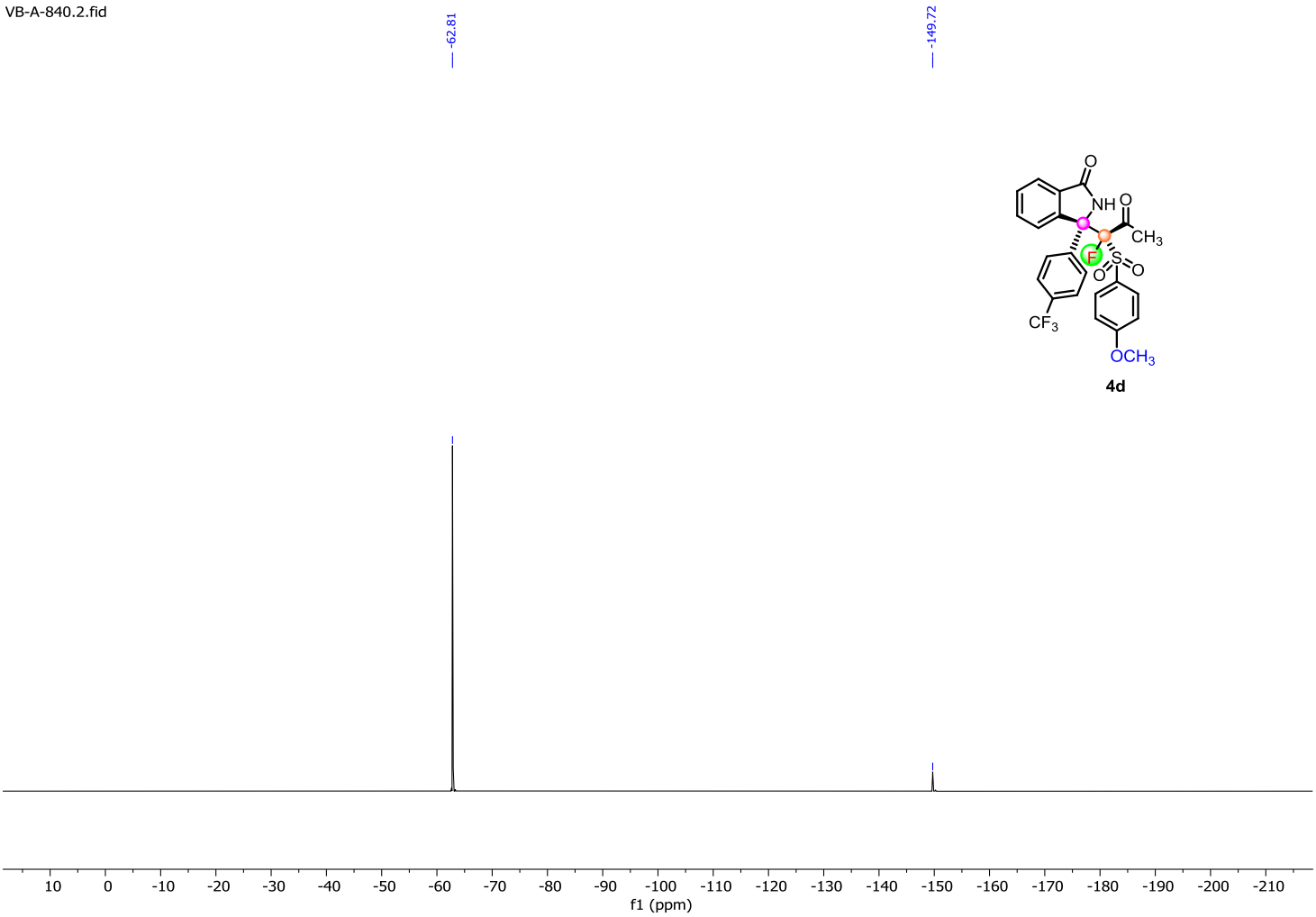


4d

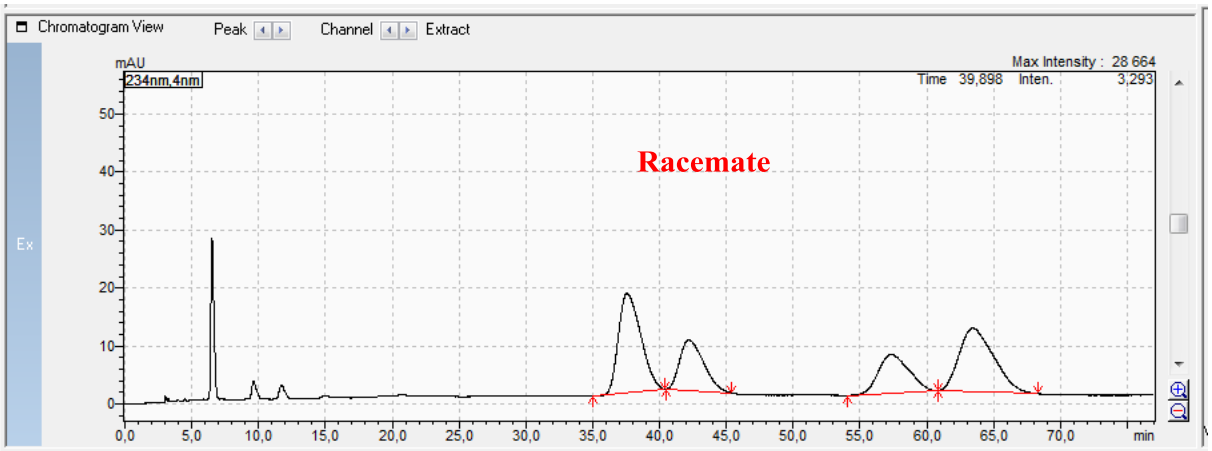
VB-A-840



4d



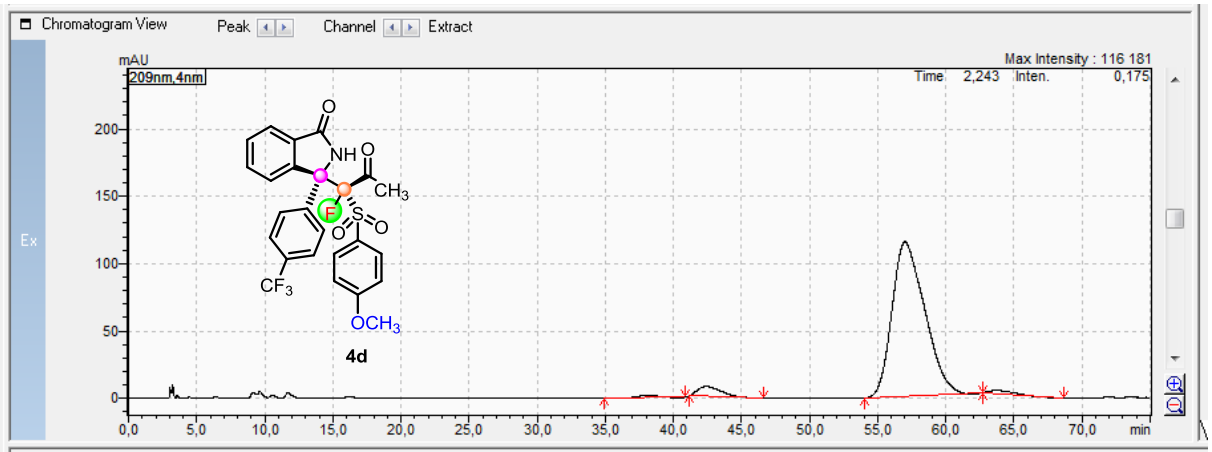
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

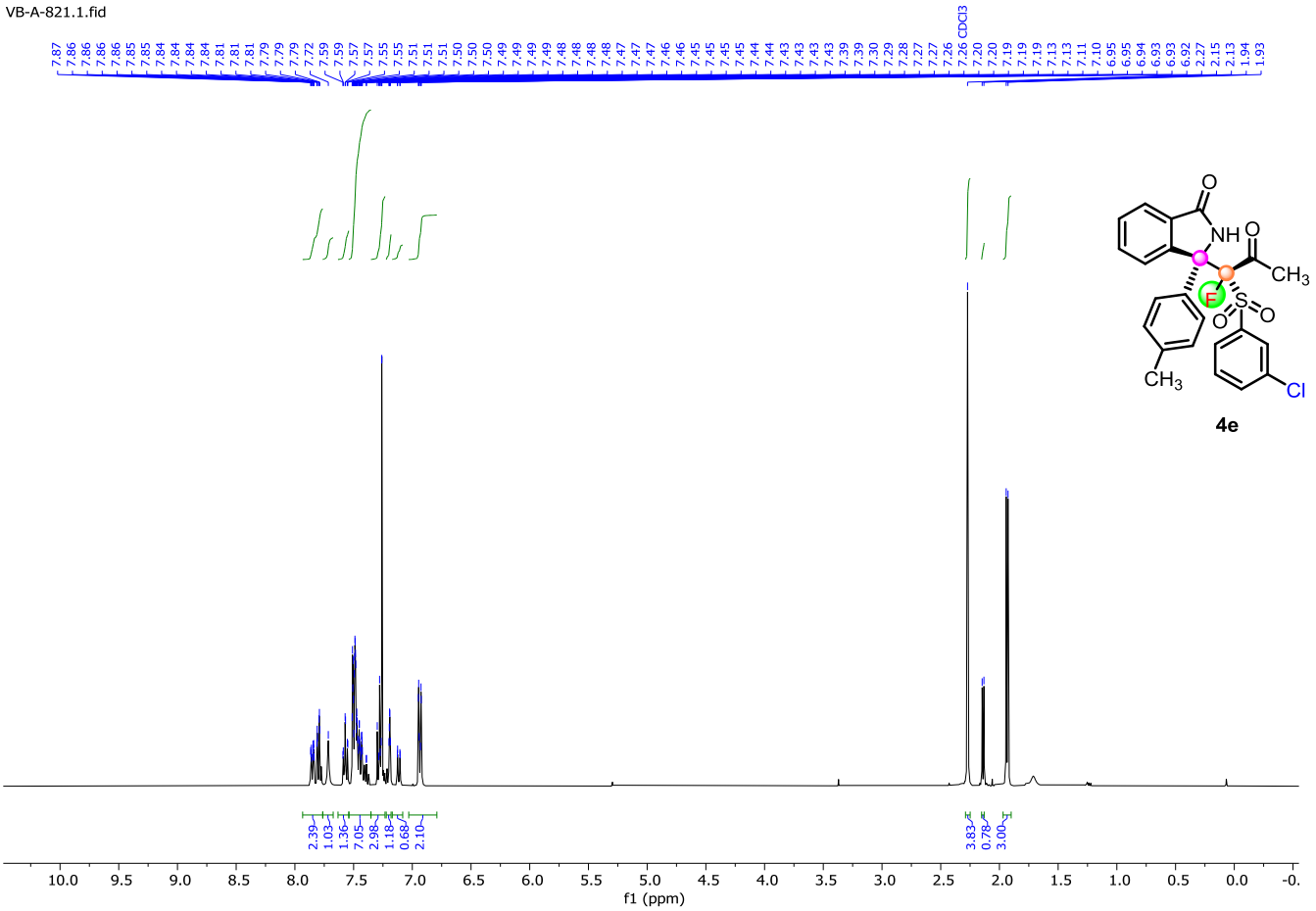
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	37,569	32,456	1985044	17148	0,000000	M	35,008	40,395	32,456
2	42,196	17,887	1093968	8773	0,000000	M	40,501	45,387	17,887
3	57,312	17,198	1051829	6681	0,000000	M	54,059	60,843	17,198
4	63,403	32,459	1985227	10980	0,000000	M	60,843	68,320	32,459
Total		100,000	6116068	43582					100,000



Results View - Peak Table

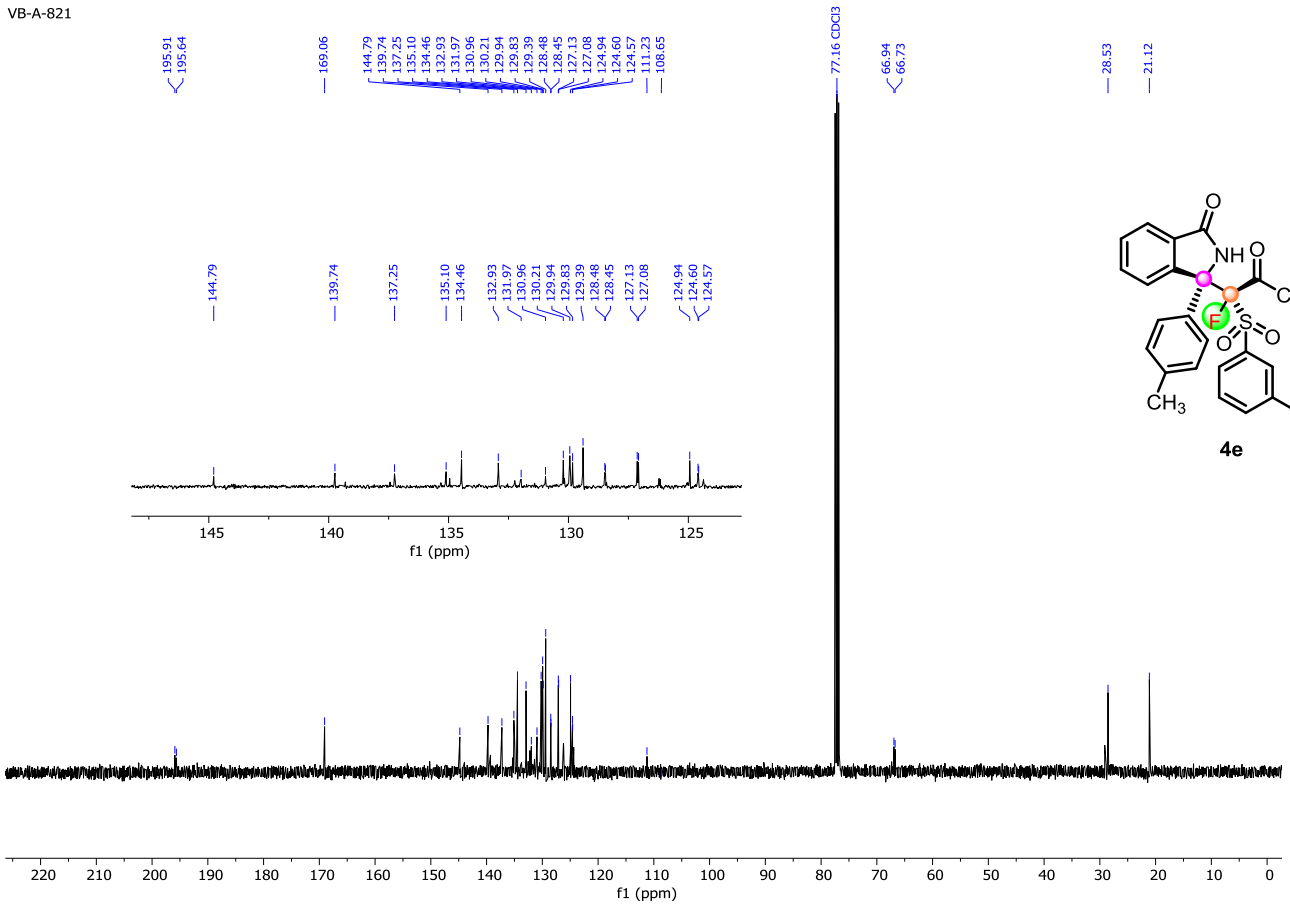
Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	38,145	0,712	143933	1617	0,000000	M	34,923	40,864	0,712
2	42,390	4,173	843075	7273	0,000000	M	41,163	46,624	4,173
3	57,022	94,030	18995759	114554	0,000000	M	54,037	62,720	94,030
4	63,760	1,085	219138	2352	0,000000	M	62,720	68,672	1,085
Total		100,000	20201905	125796					100,000


VB-A-821.1.fid
CDCl3
f1 (ppm)

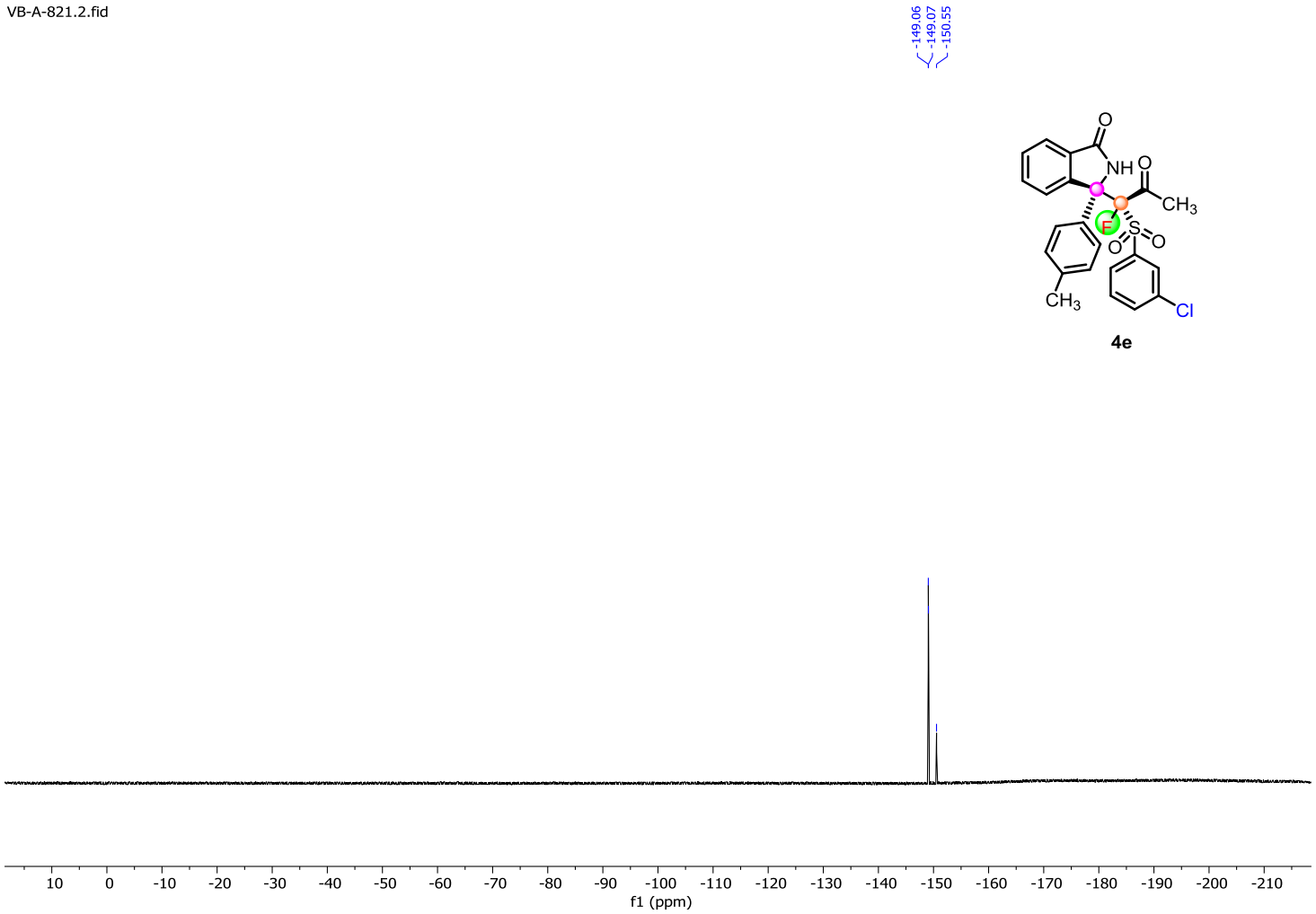
O
NH
O
CH3
F
S
O
O
CH3
Cl

4e

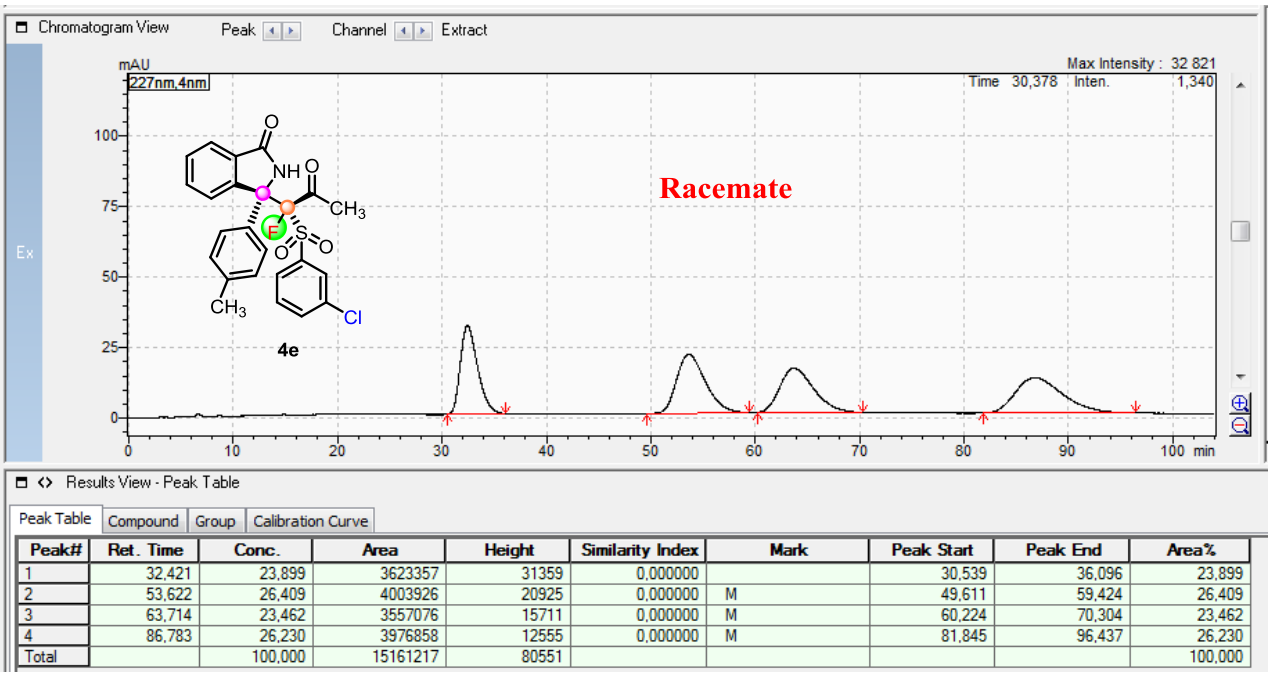

VB-A-821
195.91
195.64
169.06
144.79
139.74
137.25
135.10
134.46
132.93
131.97
130.96
130.21
129.94
129.83
129.39
128.48
128.45
127.13
127.08
124.94
124.60
124.57
111.23
108.65
77.16 CDCl3
66.94
66.73
28.53
21.12
f1 (ppm)

O
NH
O
CH3
F
S
O
O
CH3
Cl

4e



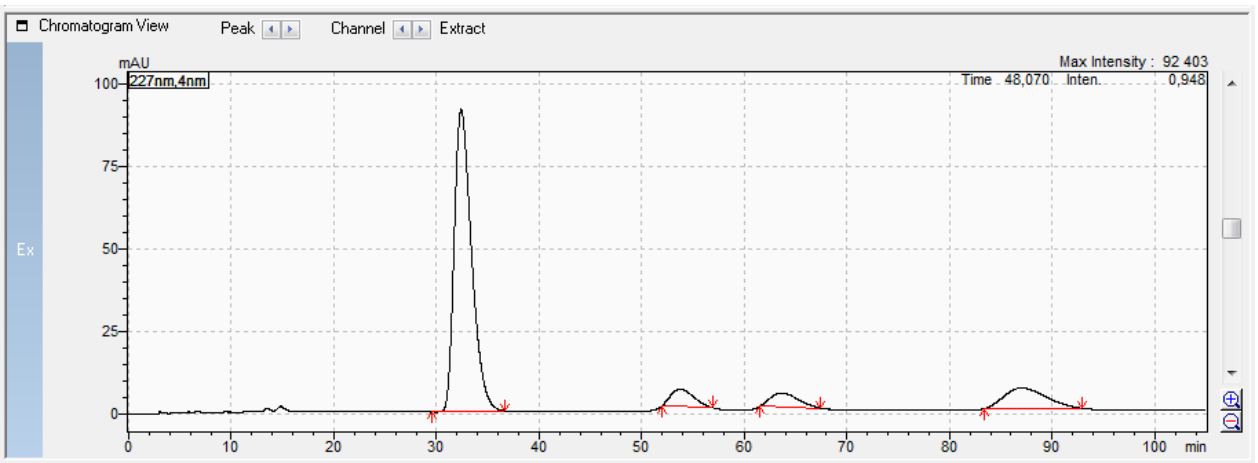
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	32,421	23,899	3623357	31359	0,000000		30,539	36,096	23,899
2	53,622	26,409	4003926	20925	0,000000	M	49,611	59,424	26,409
3	63,714	23,462	3557076	15711	0,000000	M	60,224	70,304	23,462
4	86,783	26,230	3976858	12555	0,000000	M	81,845	96,437	26,230
Total		100,000	15161217	80551					100,000

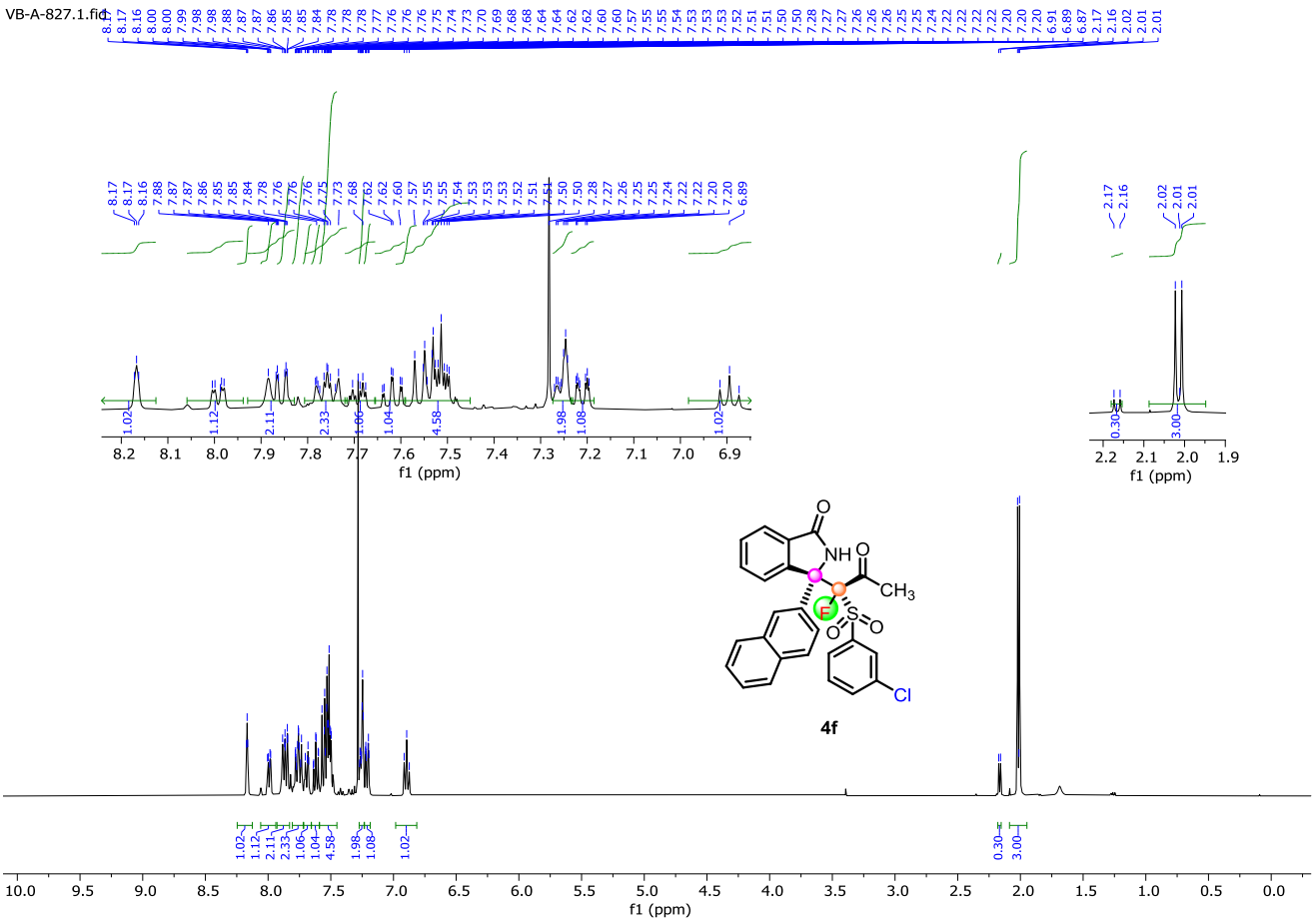


Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

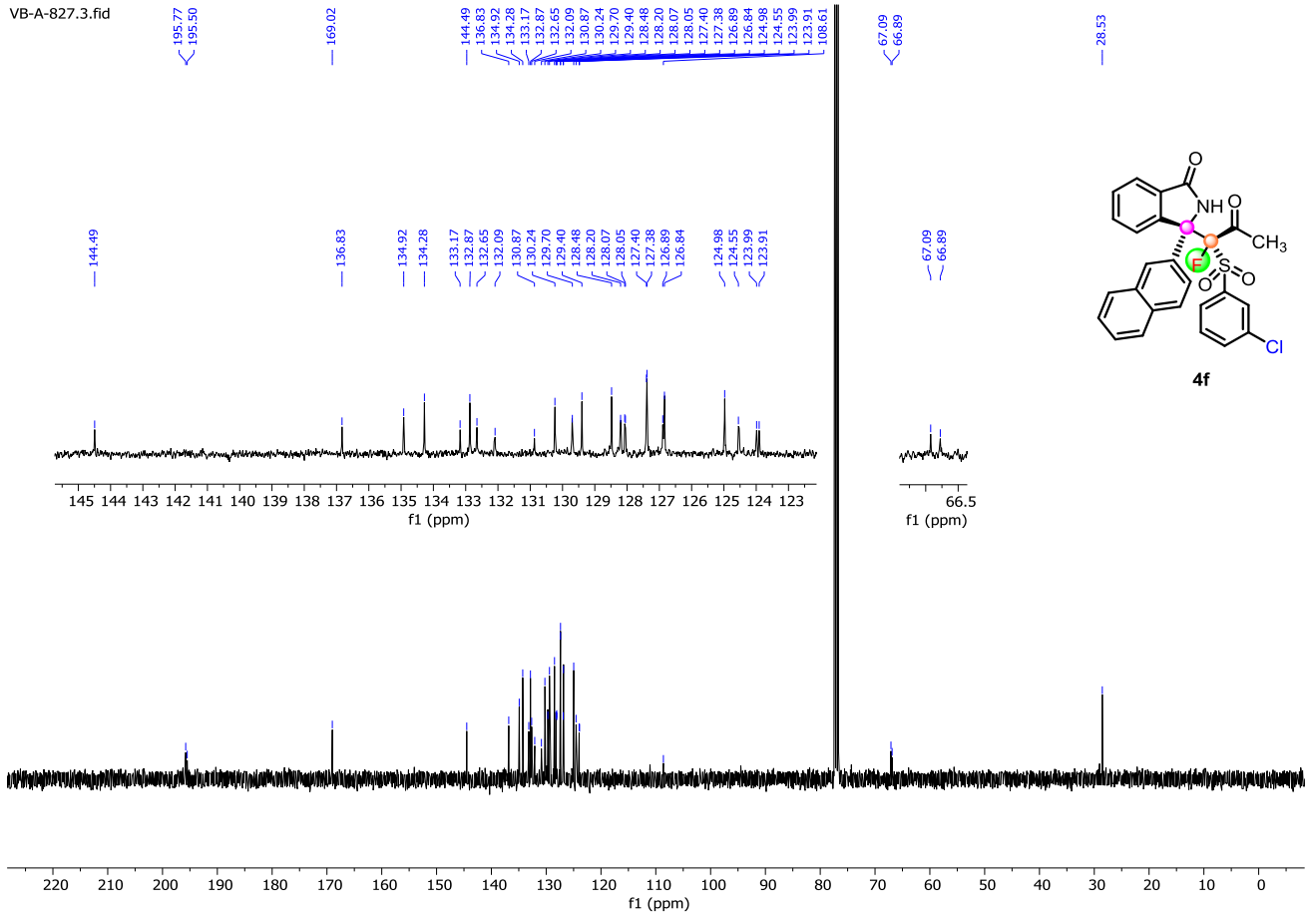
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	32,397	76,054	10742873	91552	0,000000	M	29,536	36,661	76,054
2	53,697	5,785	817171	5214	0,000000	M	51,968	56,928	5,785
3	63,607	5,678	802092	4305	0,000000	M	61,493	67,403	5,678
4	87,058	12,482	1763176	6245	0,000000	M	83,381	92,917	12,482
Total		100,000	14125312	107316					100,000

VB-A-827.1.fid



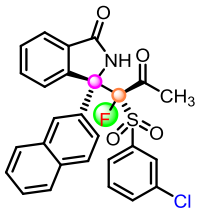
4f

VB-A-827.3.fid



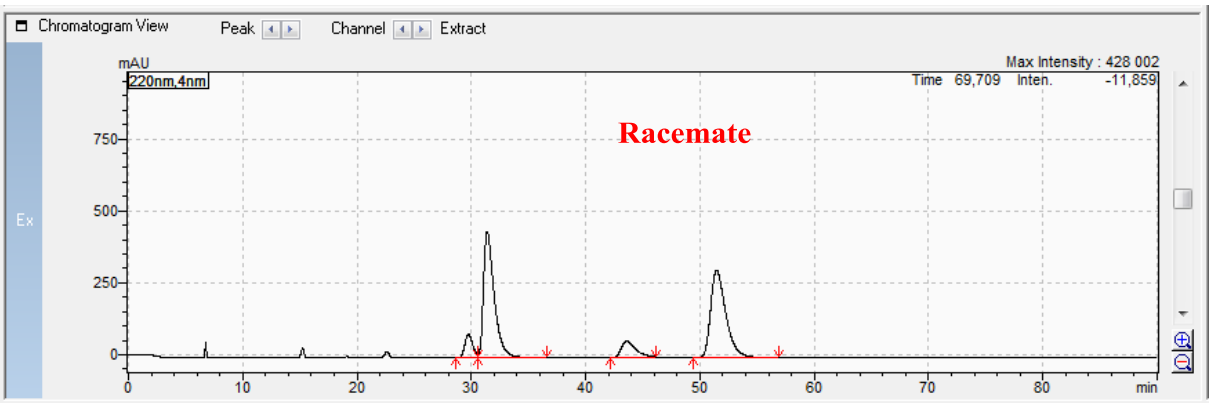
4f

VB-A-827.2.fid



4f

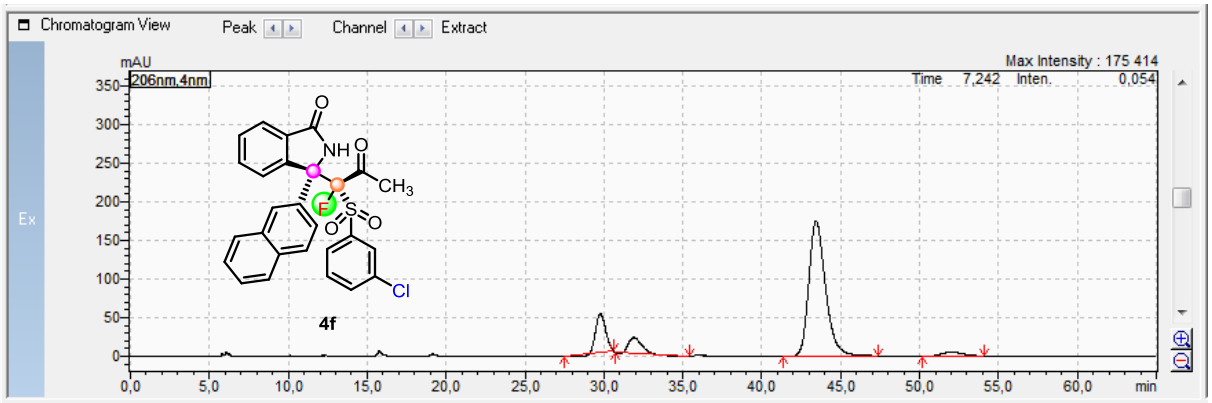
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

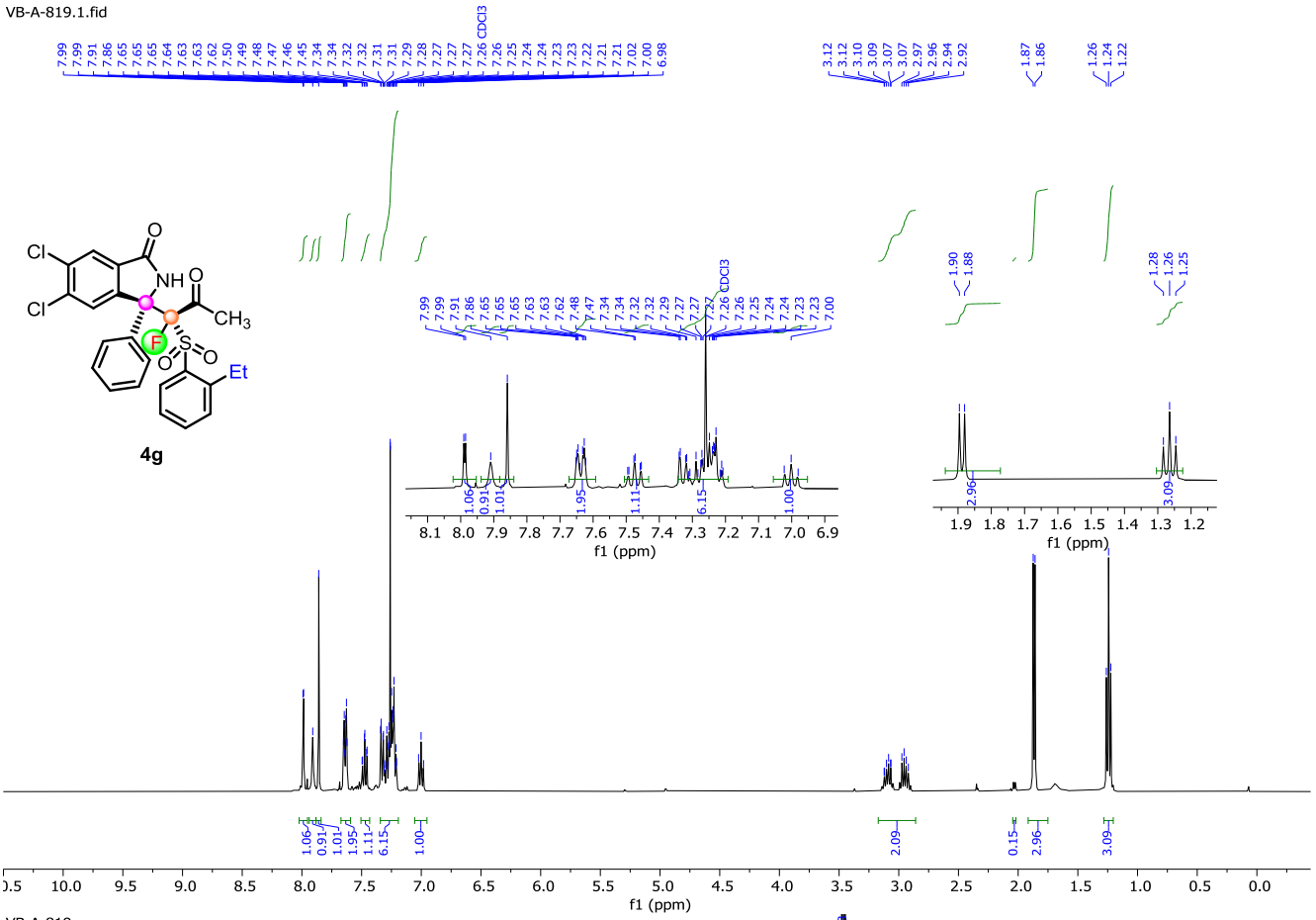
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	29,739	6,028	4004508	82338	0,000000		28,640	30,560	6,028
2	31,389	43,588	28954760	439371	0,000000	SV	30,560	36,629	43,588
3	43,607	7,609	5054449	57736	0,000000	M	42,165	46,155	7,609
4	51,458	42,775	28415103	304687	0,000000	M	49,408	56,907	42,775
Total		100,000	66428819	884131					100,000

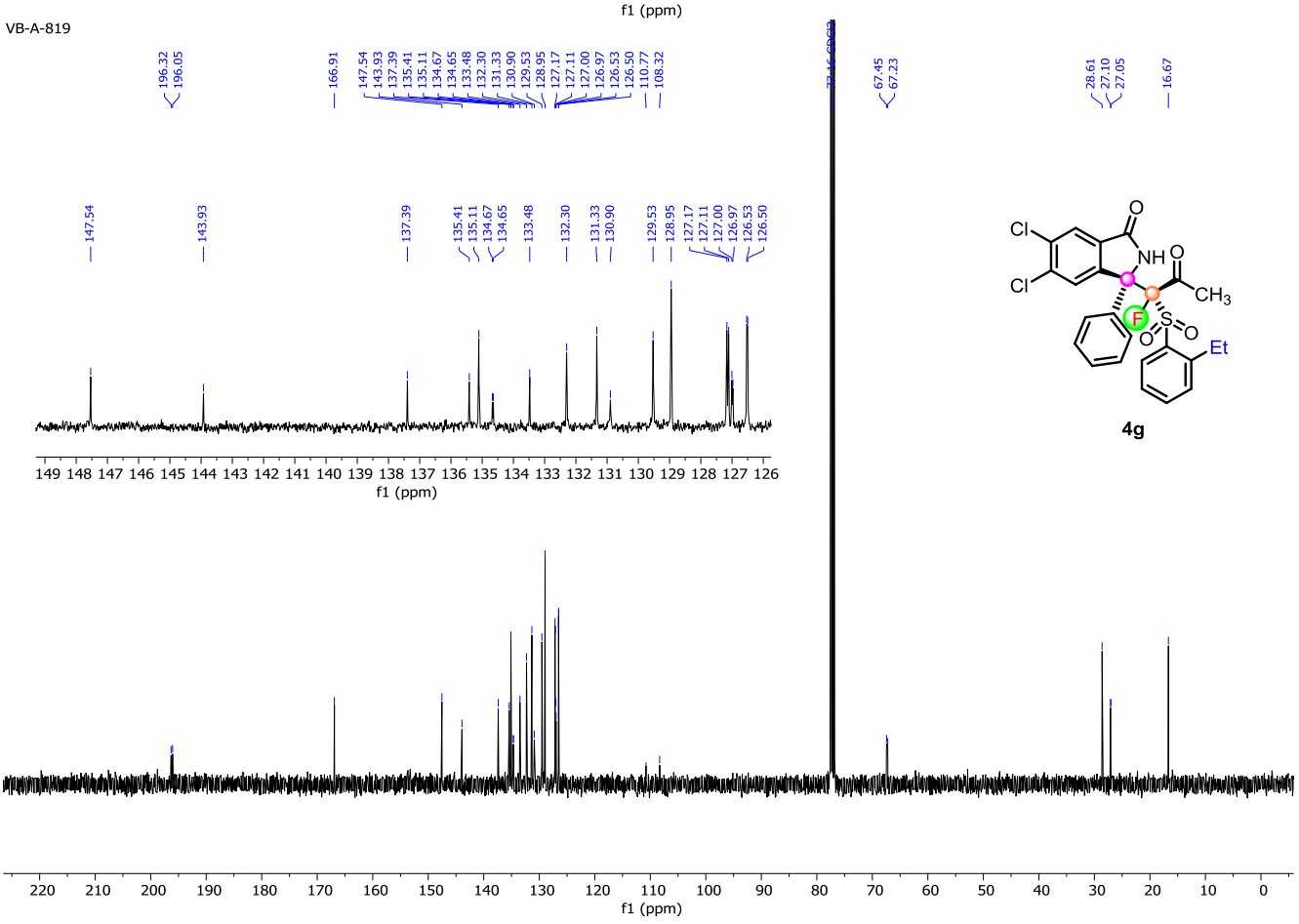


Results View - Peak Table

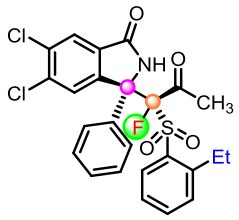
Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	29,772	12,765	2106864	50006	0,000000	M	27,488	30,624	12,765
2	31,890	6,365	1050507	20398	0,000000	M	30,709	35,424	6,365
3	43,438	78,017	12877085	175100	0,000000	M	41,355	47,381	78,017
4	52,045	2,853	470959	5328	0,000000	M	50,165	54,101	2,853
Total		100,000	16505414	250832					100,000


VB-A-819.1.fid
CDCl3
4g
f1 (ppm)

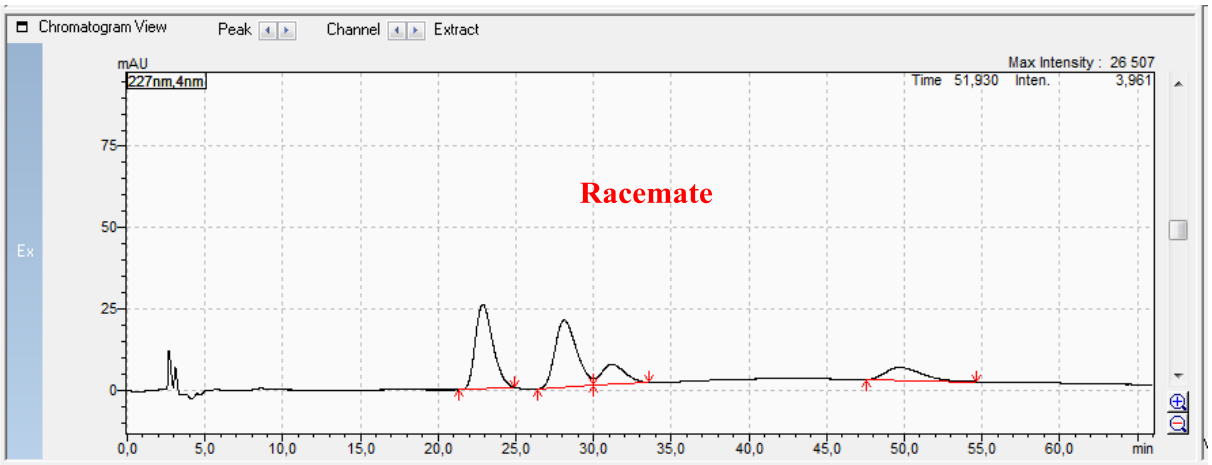

VB-A-819
4g
f1 (ppm)

VB-A-819.2.fid



4g

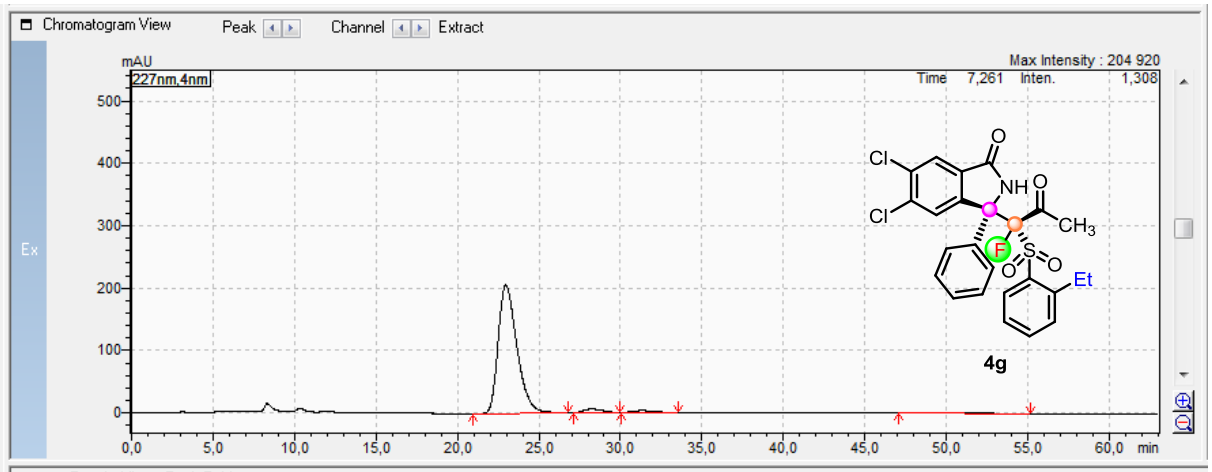
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	22,864	37,970	2030510	25938	0,000000	M	21,333	24,917	37,970
2	28,115	37,375	1998668	20677	0,000000		26,432	30,016	37,375
3	31,210	12,482	667521	6249	0,000000	V	30,016	33,557	12,482
4	49,739	12,173	650971	3985	0,000000	M	47,563	54,635	12,173
Total		100,000	5347671	56848					100,000

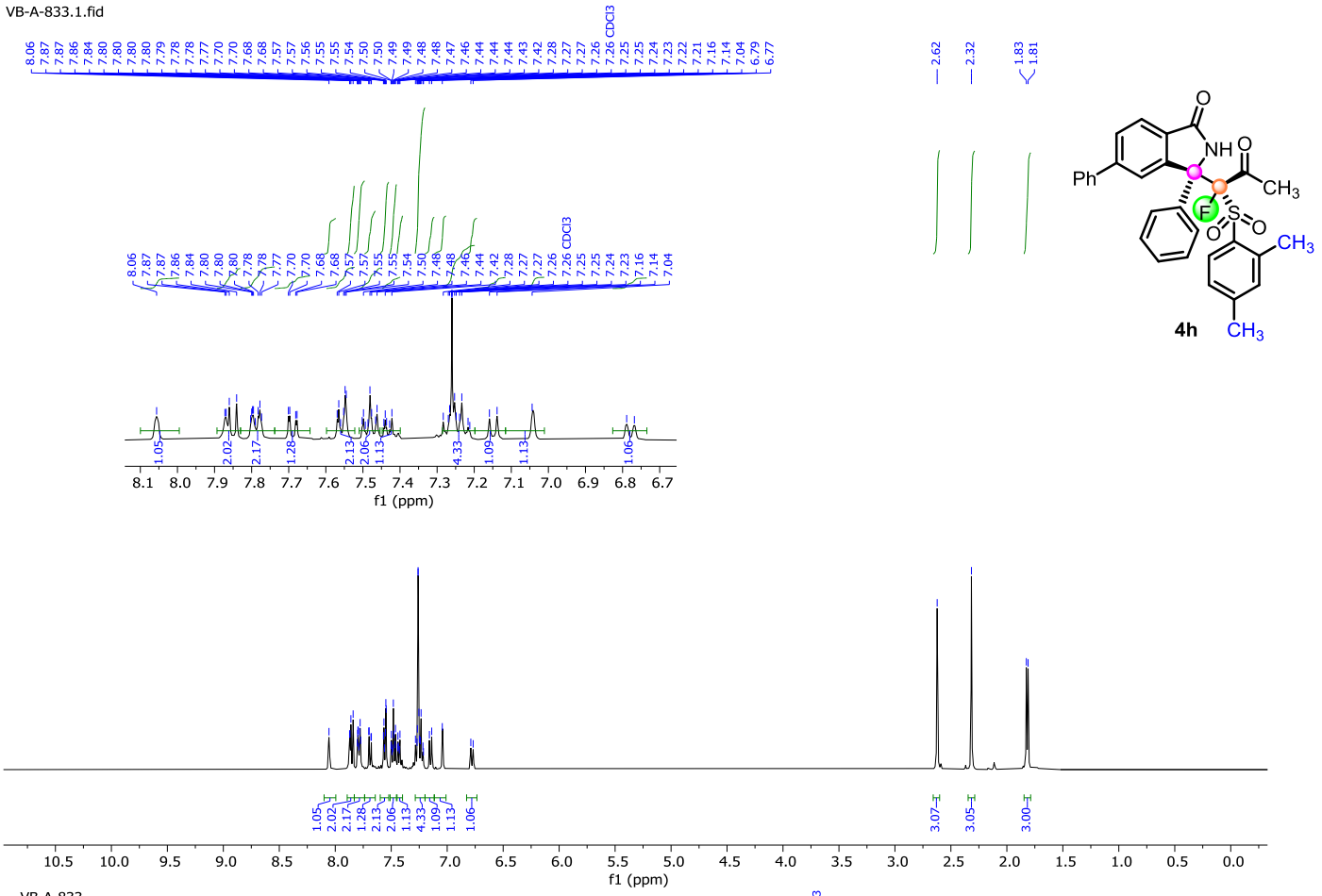


Results View - Peak Table

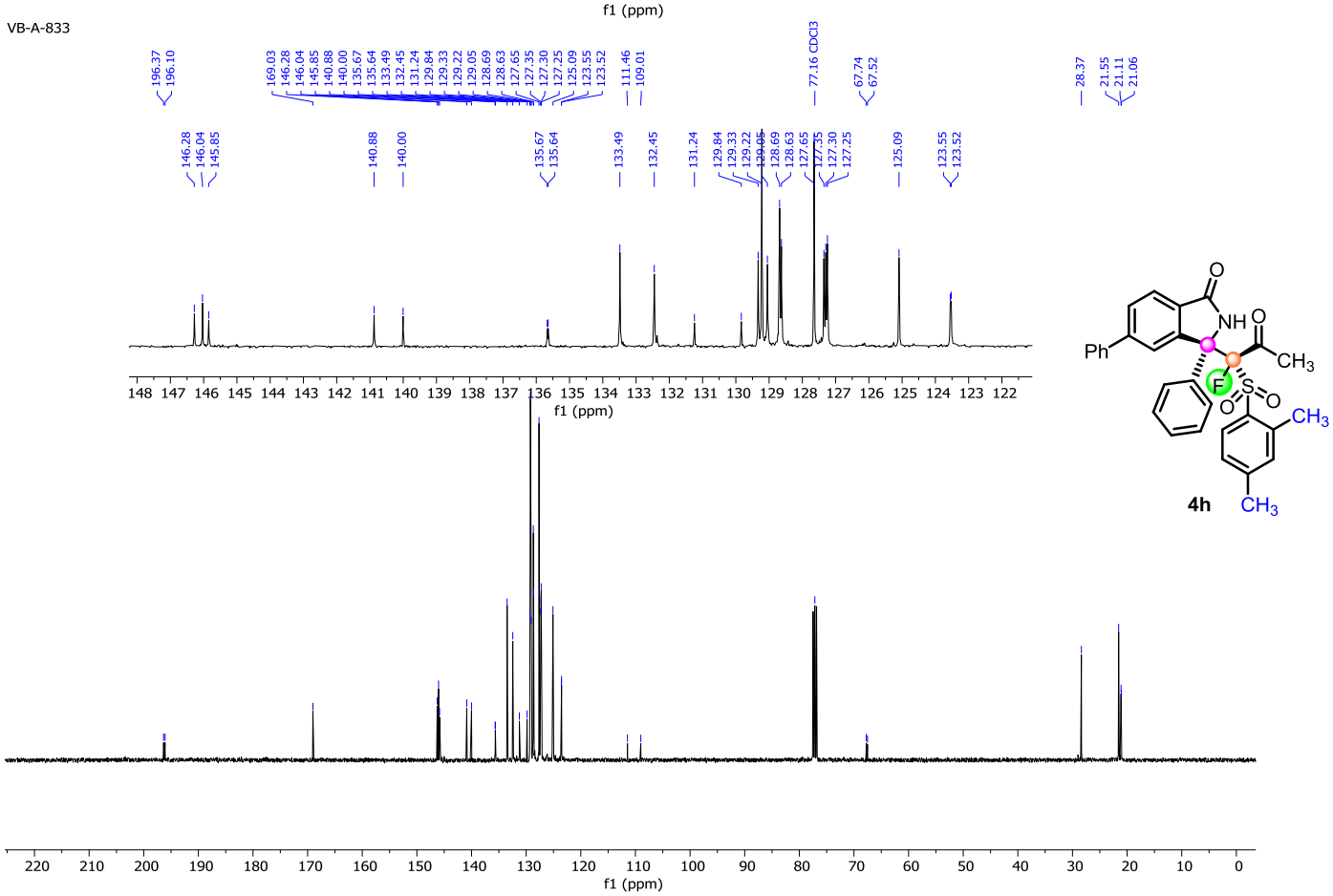
Peak Table | Compound | Group | Calibration Curve

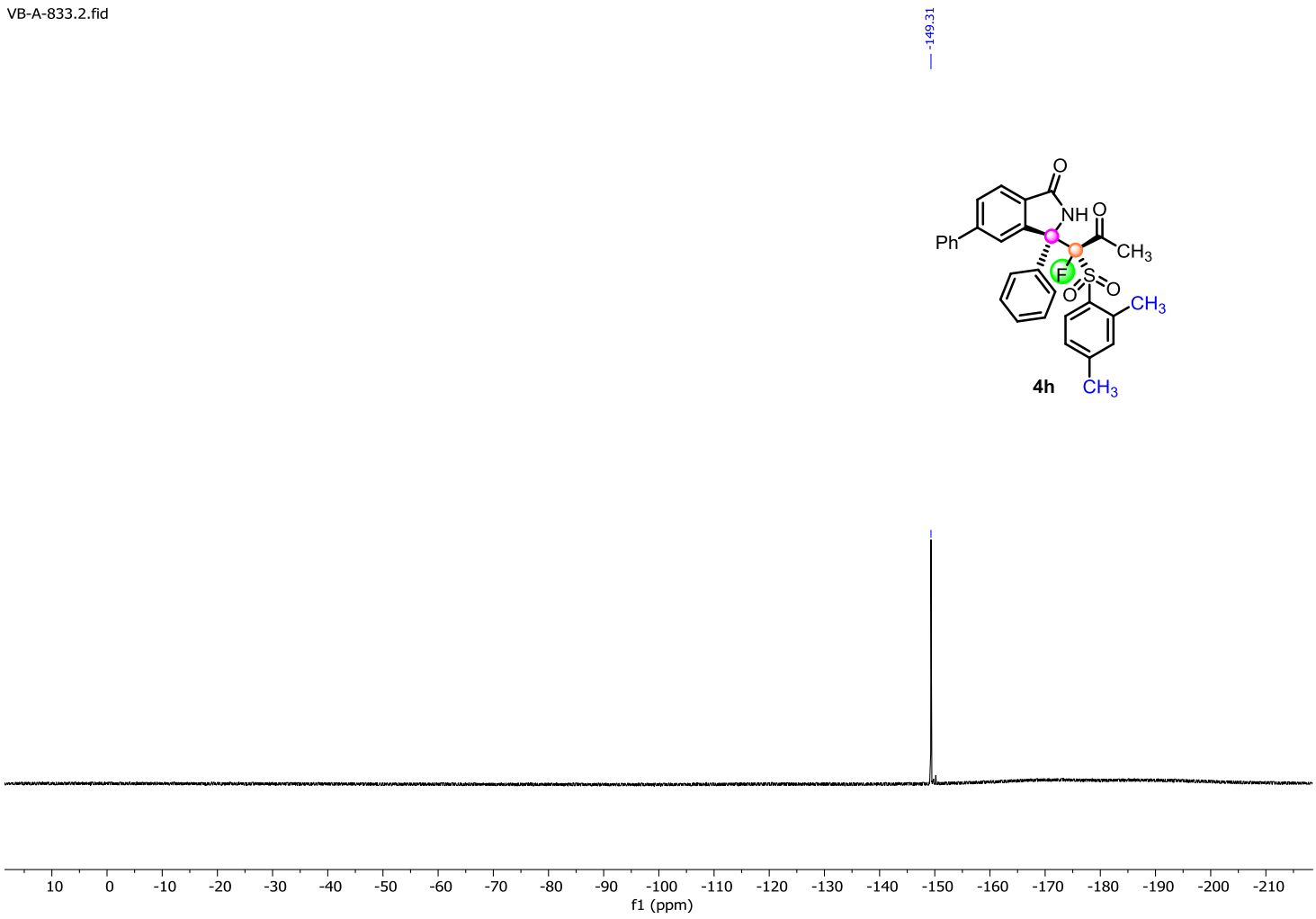
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	22,970	93,564	16478426	205919	0,000000	M	20,949	26,784	93,564
2	28,247	2,848	501614	5978	0,000000	M	27,125	29,963	2,848
3	31,294	2,109	371458	3669	0,000000		30,005	33,536	2,109
4	49,572	1,478	260390	1520	0,000000	M	47,072	55,168	1,478
Total		100,000	17611887	217086					100,000

VB-A-833.1.fid

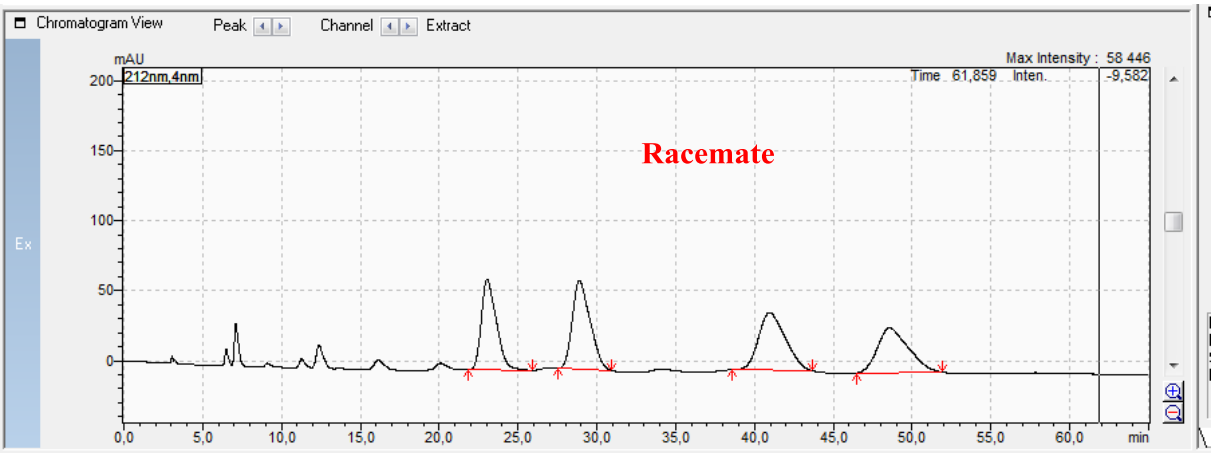


VB-A-833





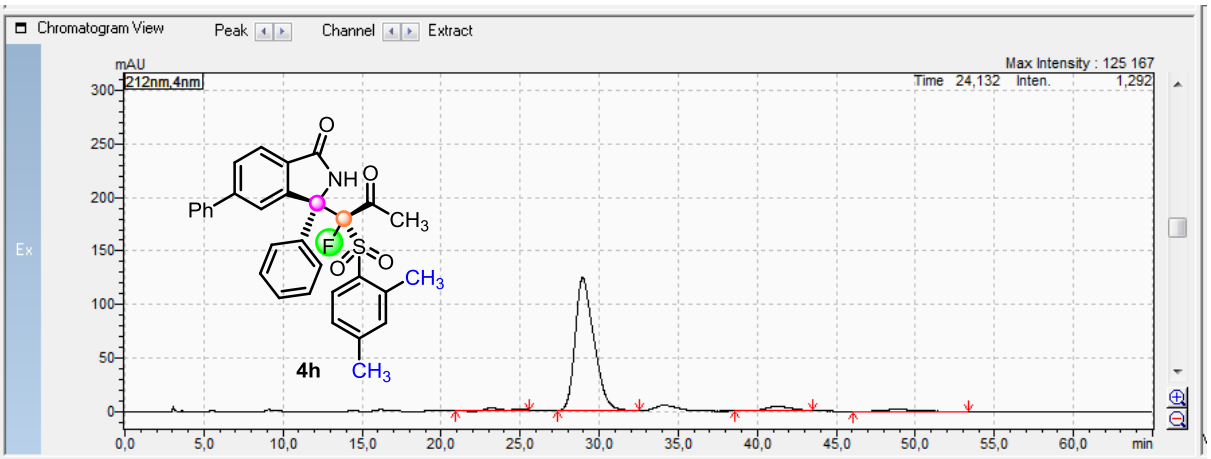
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	23,037	23,221	4307070	65039	0,000000	M	21,835	25,888	23,221
2	28,900	26,978	5003884	63459	0,000000	M	27,531	30,933	26,978
3	40,939	26,314	4880741	41189	0,000000	M	38,581	43,680	26,314
4	48,571	23,488	4356576	31913	0,000000	M	46,475	51,915	23,488
Total		100,000	18548272	201599					100,000

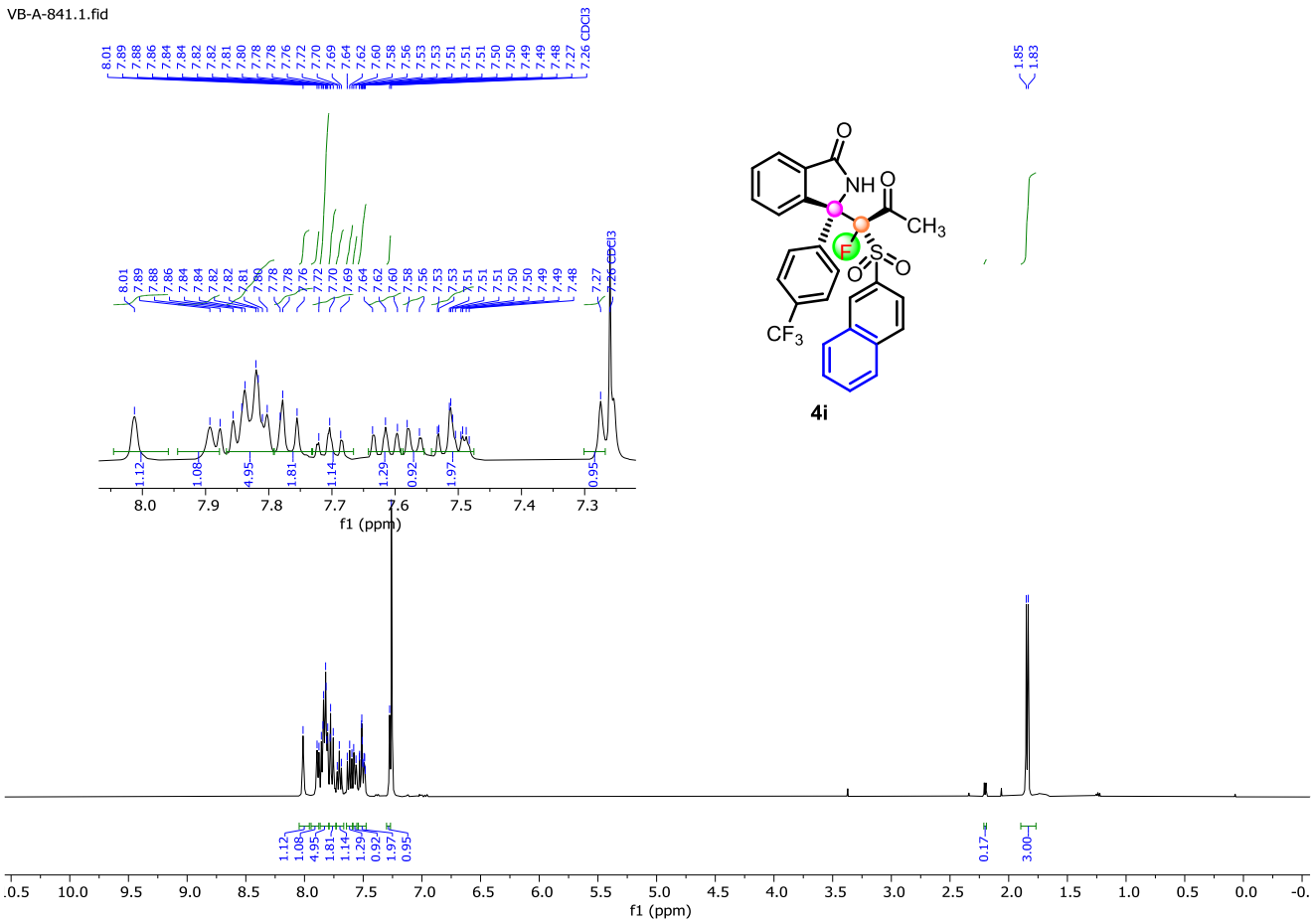


Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

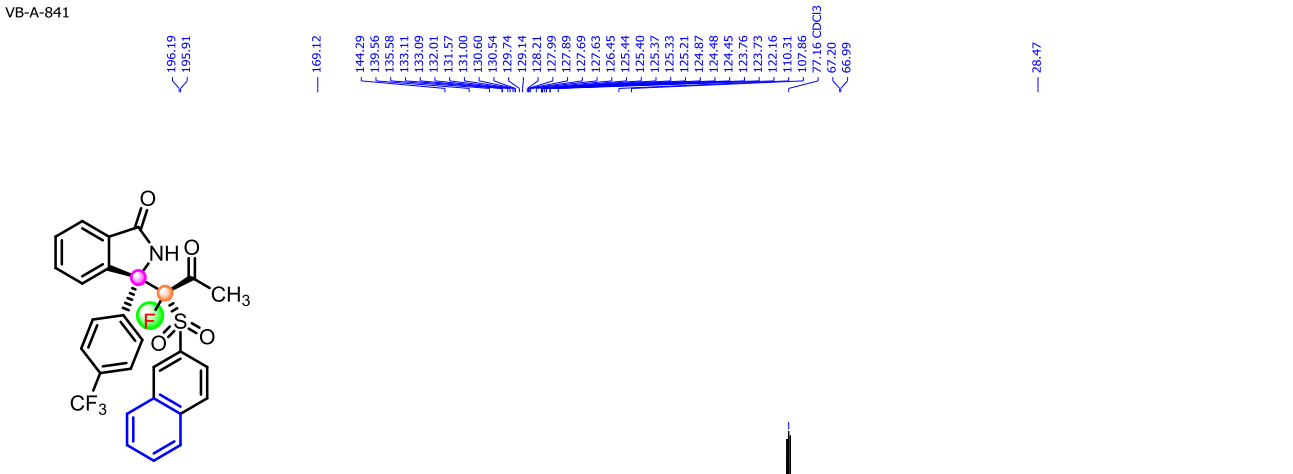
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	23,128	0,859	95262	2212	0,000000	M	20,907	25,579	0,859
2	28,960	92,647	10275700	124316	0,000000	M	27,360	32,544	92,647
3	41,197	4,330	480300	4156	0,000000	M	38,581	43,509	4,330
4	48,865	2,164	239997	1780	0,000000	M	46,059	53,365	2,164
Total		100,000	11091259	132463					100,000

VB-A-841.1.fid

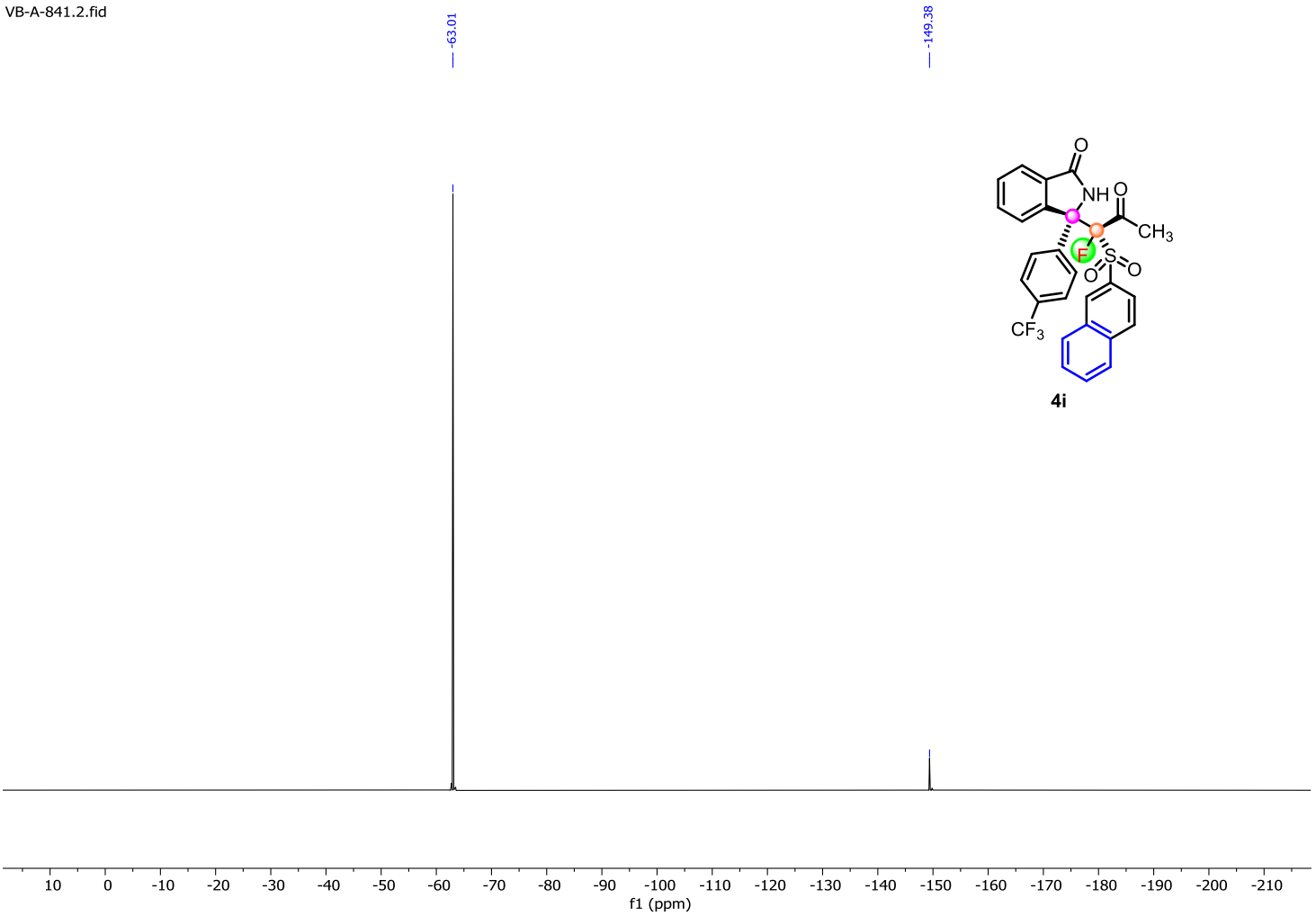


4i

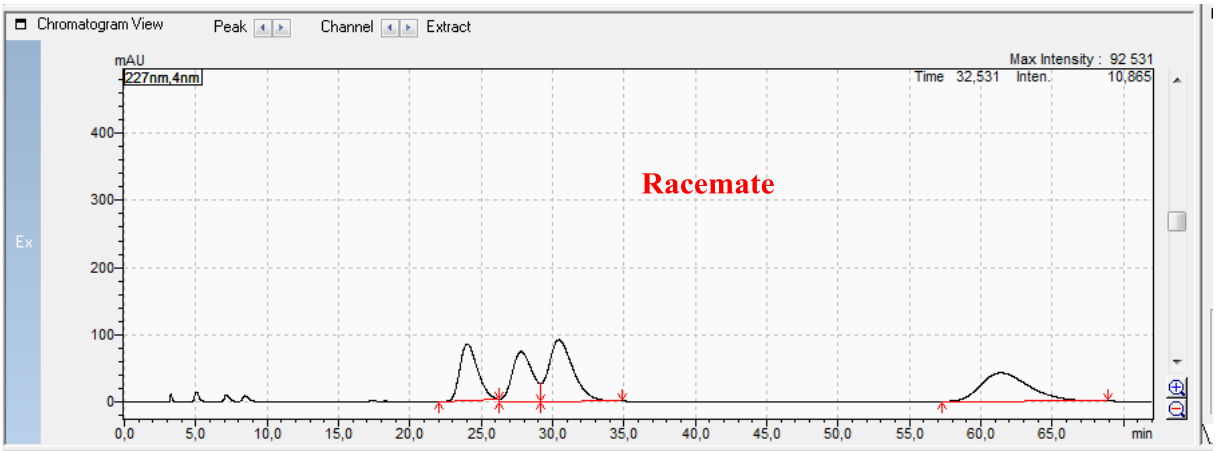
VB-A-841



4i



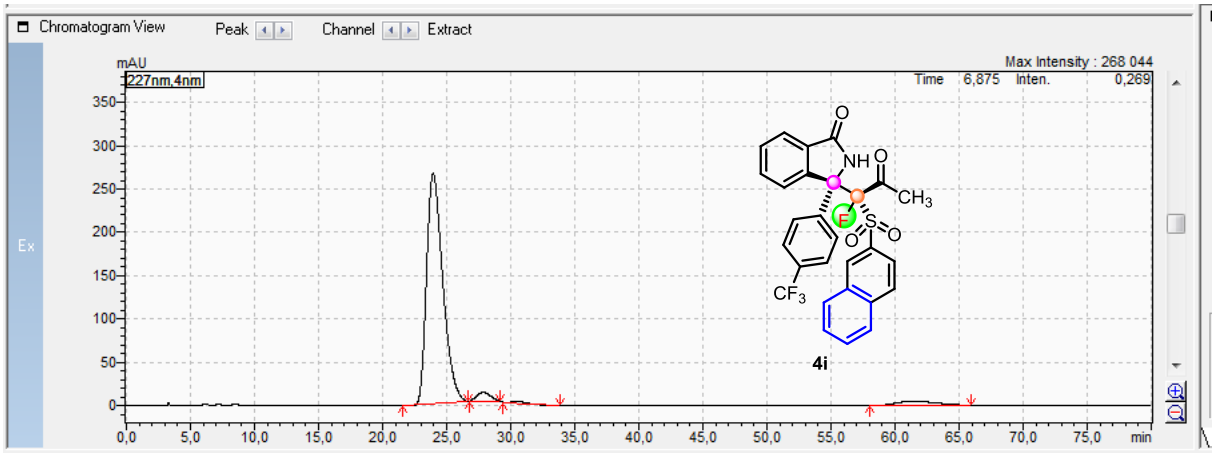
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

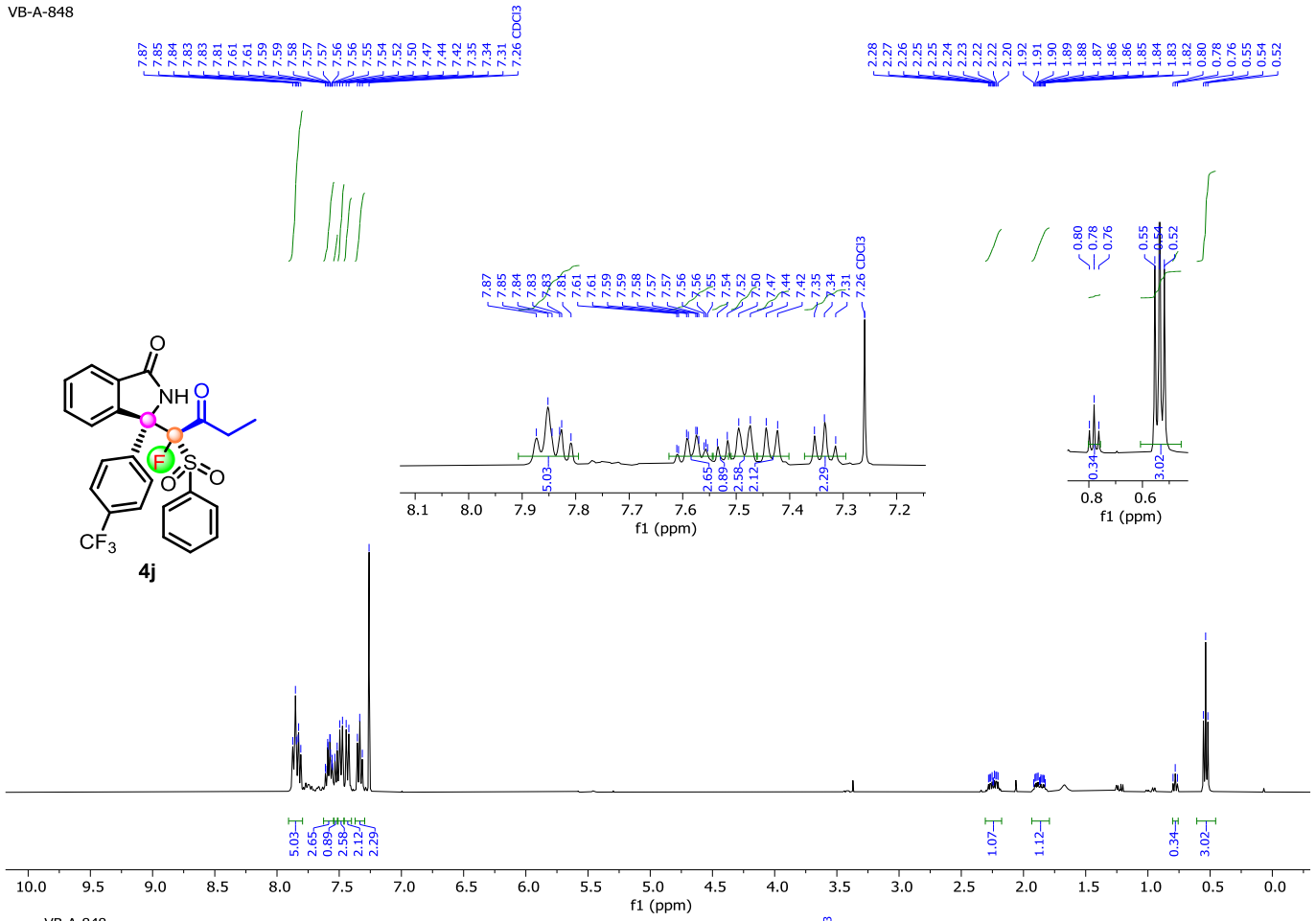
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	24,017	20,343	7204994	84172	0,000000	M	22,027	26,251	20,343
2	27,784	20,503	7261698	74128	0,000000		26,251	29,163	20,503
3	30,440	30,727	10882721	91725	0,000000	V	29,163	34,880	30,727
4	61,403	28,426	10067855	42427	0,000000	M	57,280	68,907	28,426
Total		100,000	35417267	292451					100,000

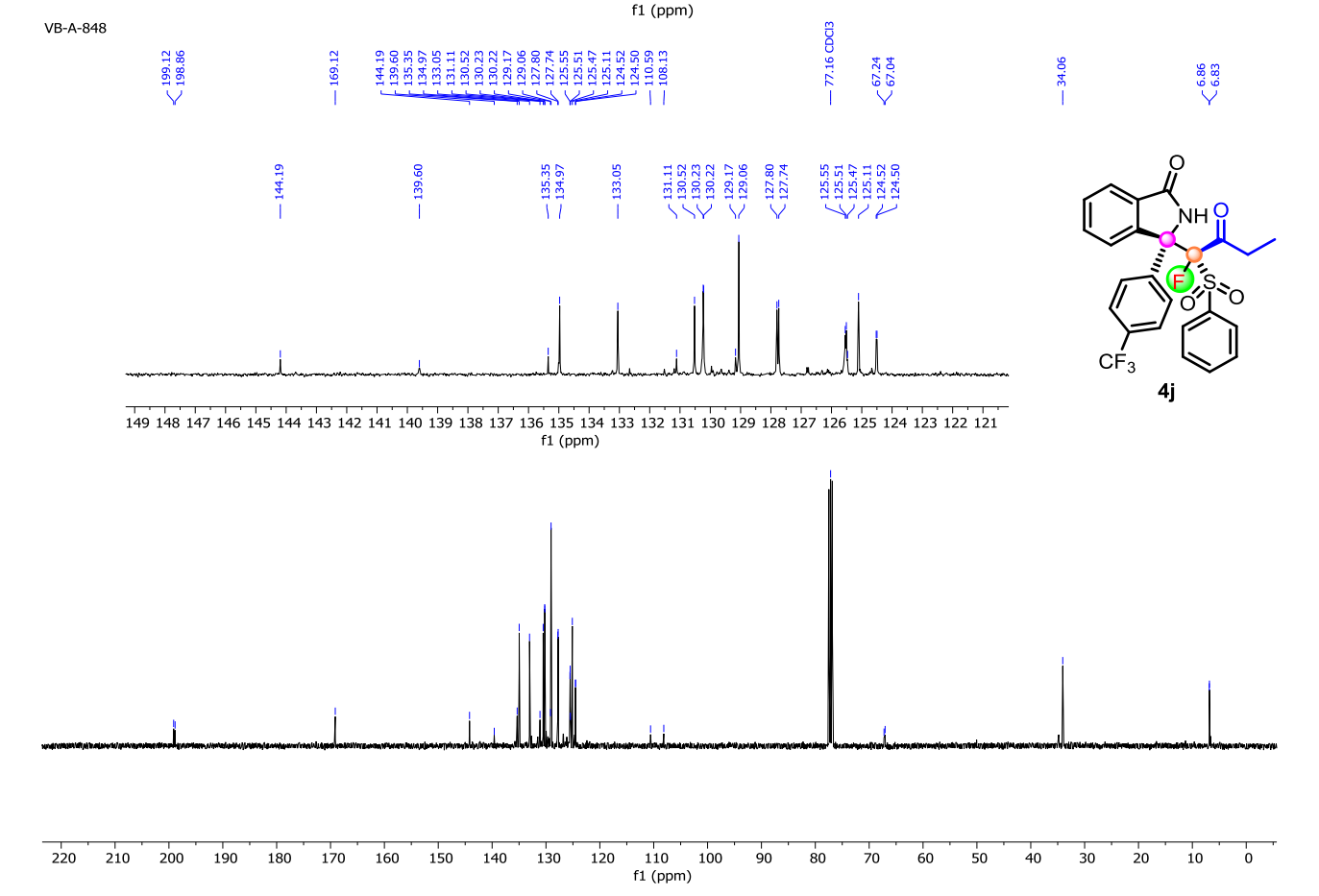


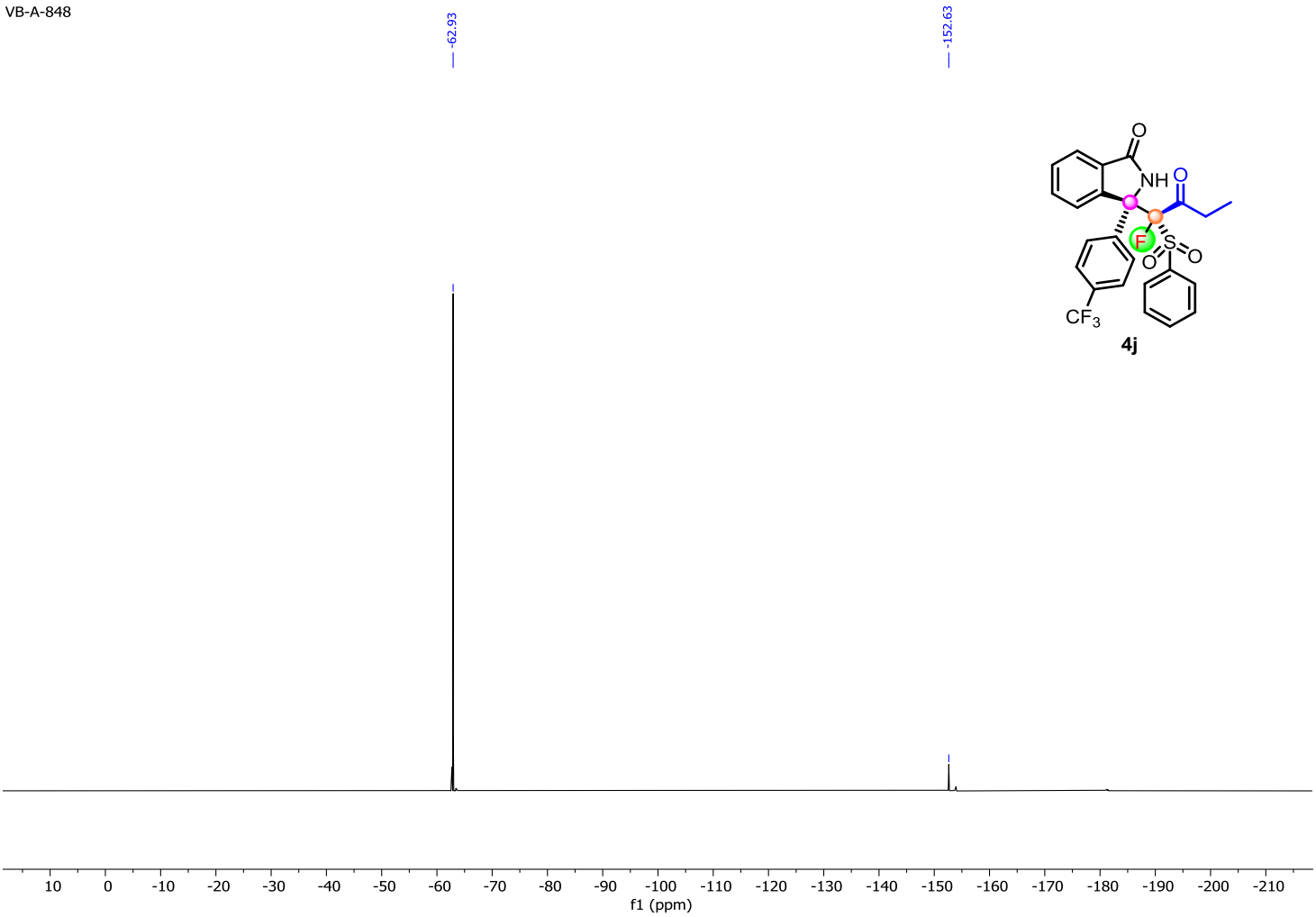
Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

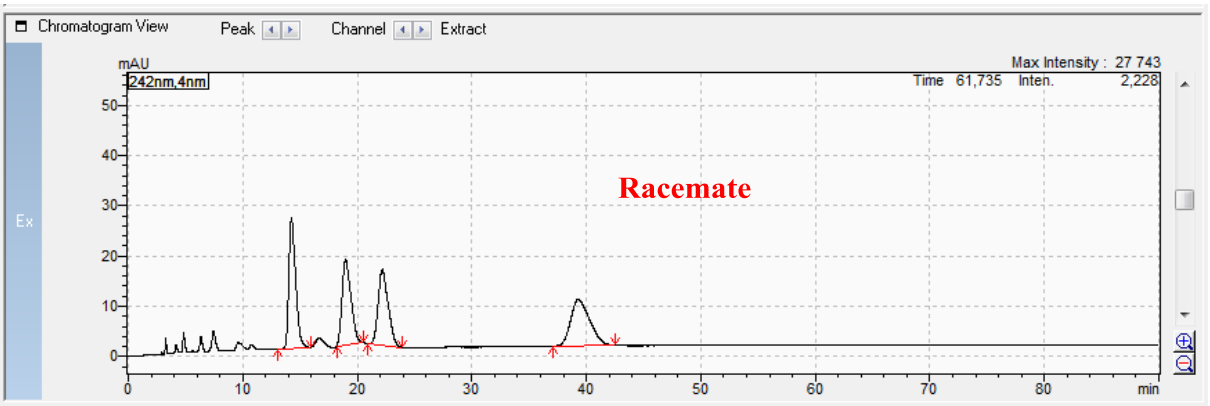
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	23,945	92,453	23313407	265705	0,000000	M	21,568	26,667	92,453
2	27,822	3,120	786770	10163	0,000000	M	26,773	29,163	3,120
3	30,496	0,227	57127	1685	0,000000	M	29,376	33,856	0,227
4	61,514	4,201	1059323	4892	0,000000	M	58,016	65,941	4,201
Total		100,000	25216626	282445					100,000


VB-A-848
7.87 7.85 7.84 7.83 7.83 7.81 7.61 7.61 7.59 7.59 7.58 7.57 7.57 7.56 7.56 7.55 7.54 7.52 7.50 7.47 7.44 7.42 7.35 7.34 7.31 7.26 CDCl3
2.28 2.27 2.26 2.25 2.25 2.24 2.23 2.22 2.22 2.20 1.92 1.91 1.90 1.89 1.88 1.87 1.86 1.86 1.85 1.84 1.83 1.82 0.80 0.78 0.76 0.55 0.54 0.52
NH
F
S
O
CF3
4j
5.03 2.65 0.89 2.58 2.12 2.29
1.07 1.12 0.34 3.02
f1 (ppm)


VB-A-848
199.12 198.86 169.12 144.19 139.60 135.35 134.97 133.05 131.11 130.52 130.23 130.22 129.17 129.06 127.80 127.74 125.55 125.51 125.47 125.11 124.52 124.50 110.59 108.13 77.16 CDCl3 67.24 67.04 34.06 6.86 6.83
144.19 139.60 135.35 134.97 133.05 131.11 130.52 130.23 130.22 129.17 129.06 127.80 127.74 125.55 125.51 125.47 125.11 124.52 124.50
NH
F
S
O
CF3
4j
f1 (ppm)



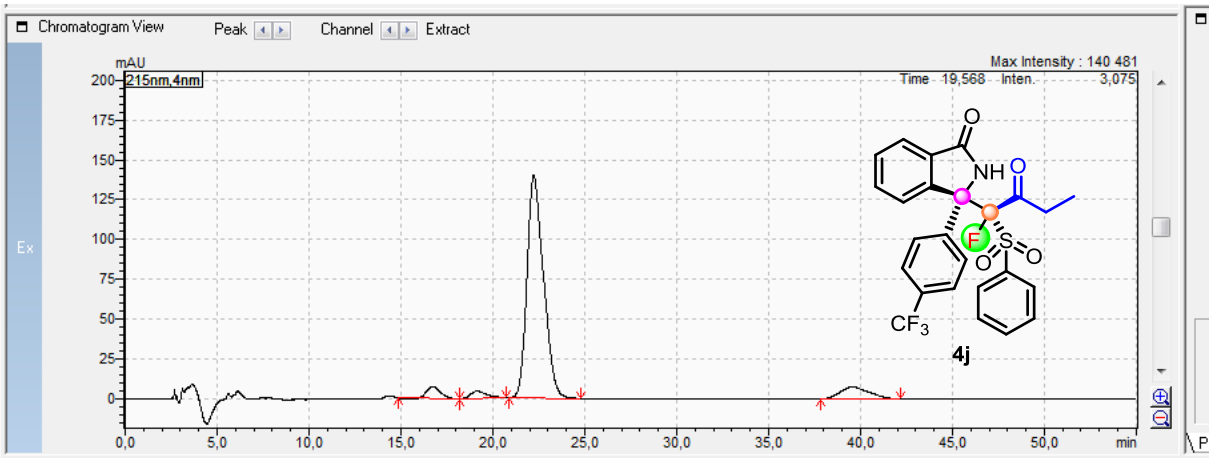
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

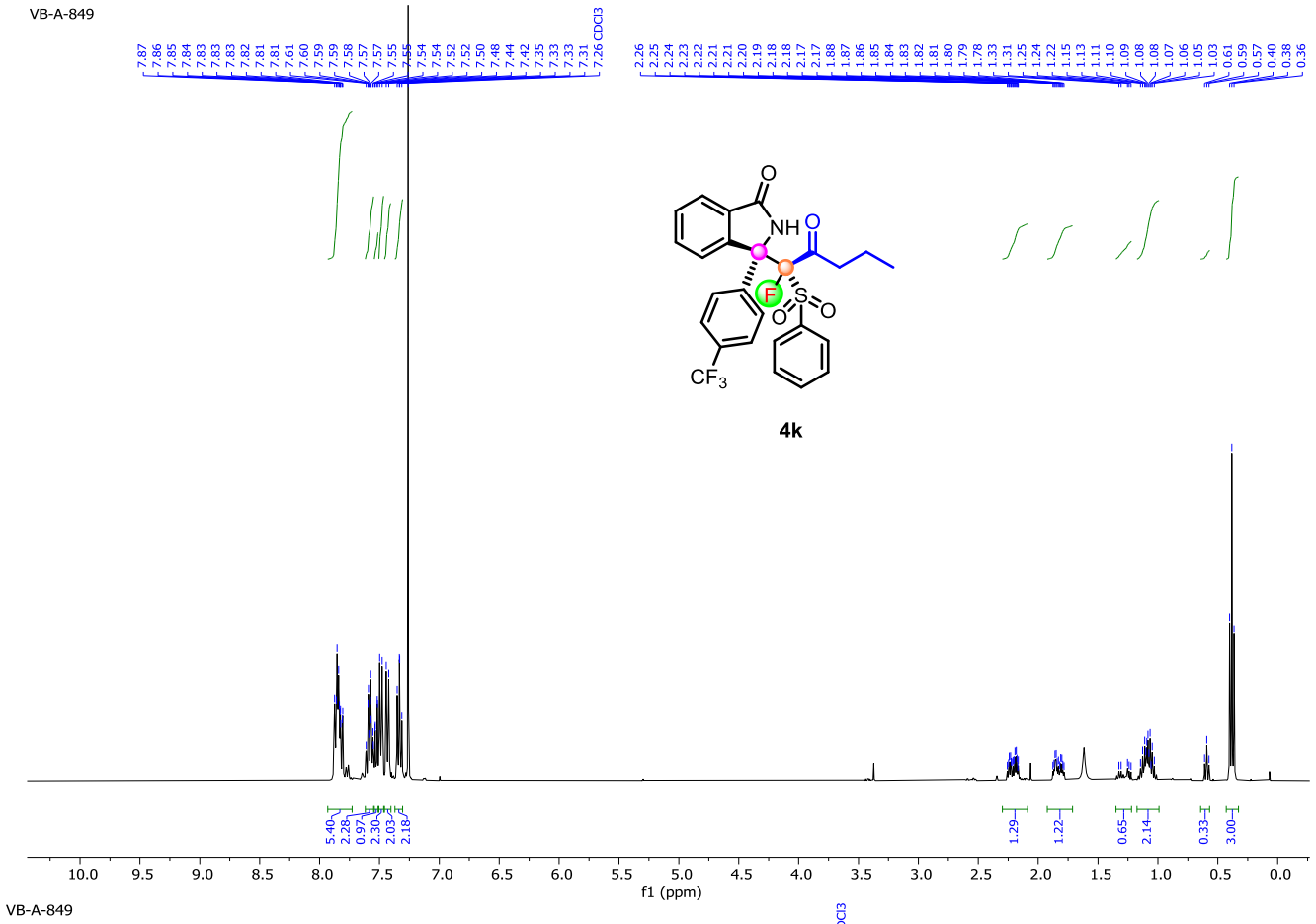
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	14,247	26,862	1066041	26103	0,000000	M	12,992	15,947	26,862
2	18,978	23,166	919383	16934	0,000000	M	18,187	20,555	23,166
3	22,180	22,982	912068	15045	0,000000	M	20,907	23,979	22,982
4	39,307	26,990	1071139	9274	0,000000	M	37,088	42,517	26,990
Total		100,000	3968631	67356					100,000



Results View - Peak Table

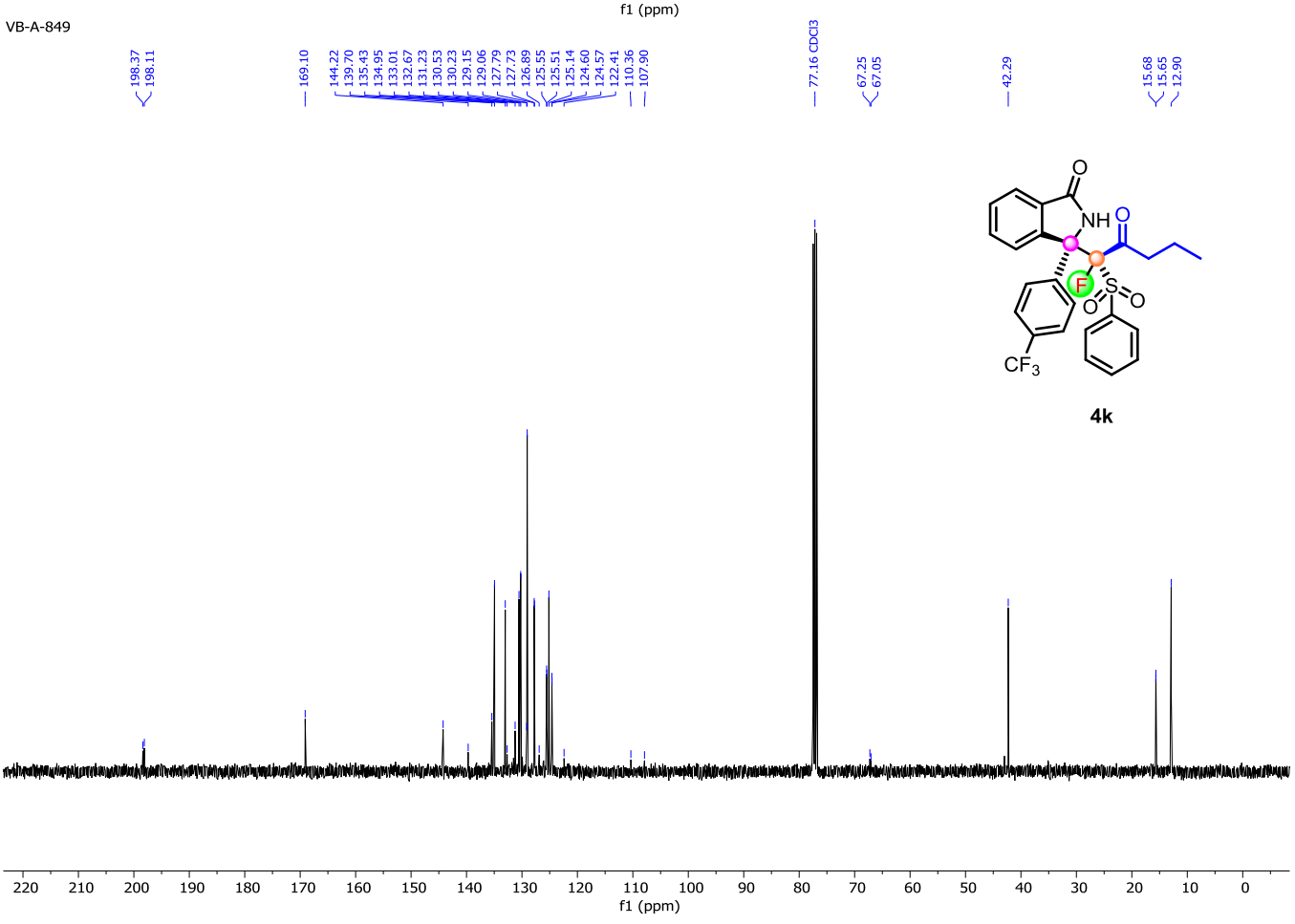
Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	16,722	3,563	363057	7298	0,000000	M	14,859	18,187	3,563
2	19,127	2,624	267345	4381	0,000000		18,197	20,757	2,624
3	22,229	85,663	8729163	140100	0,000000		20,907	24,757	85,663
4	39,563	8,151	830546	7513	0,000000		37,813	42,165	8,151
Total		100,000	10190112	159292					100,000


VB-A-849
CDCl3
f1 (ppm)

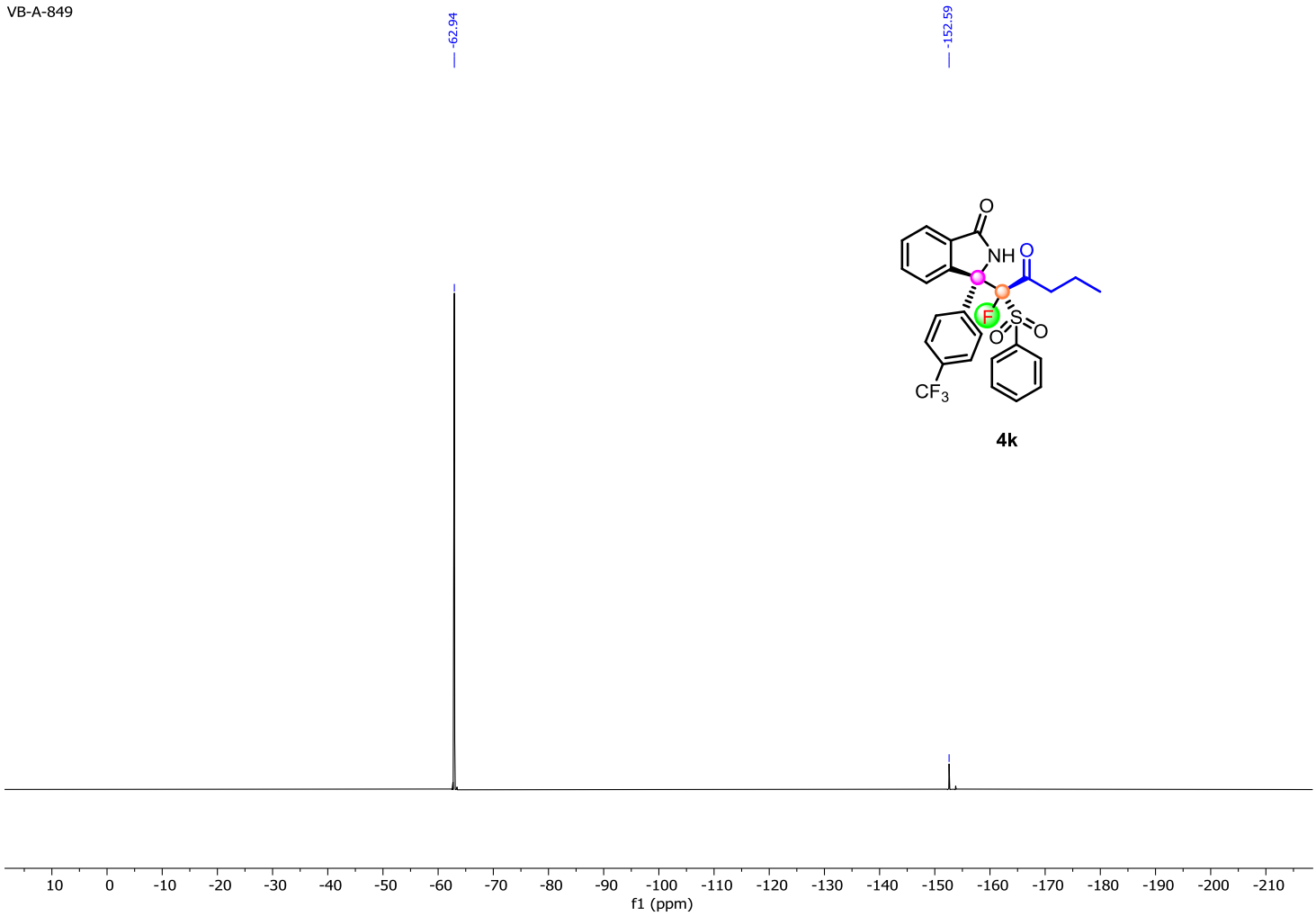
O
NH
O
F
S
O
O
CF3

4k

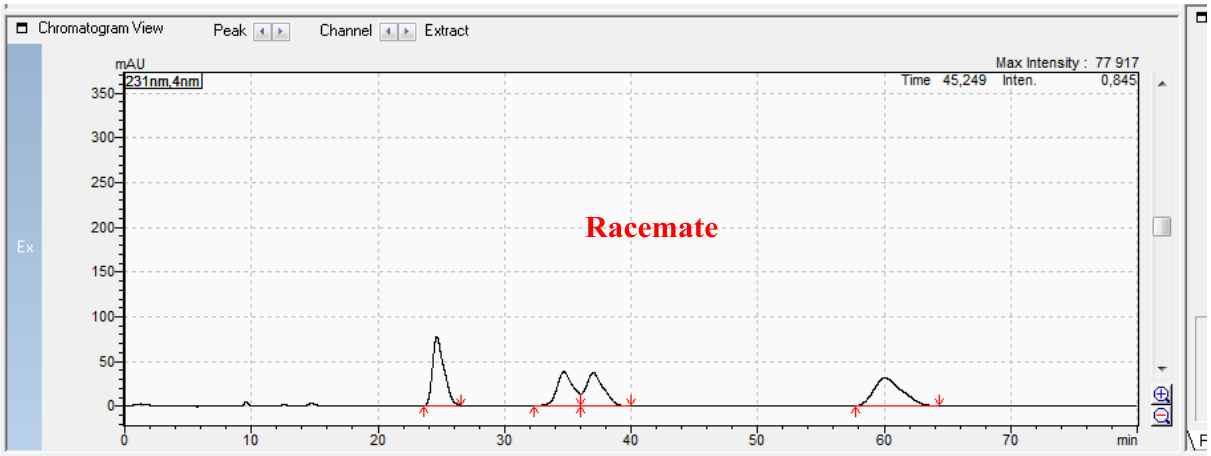

VB-A-849
77.16 CDCl3
f1 (ppm)

O
NH
O
F
S
O
O
CF3

4k



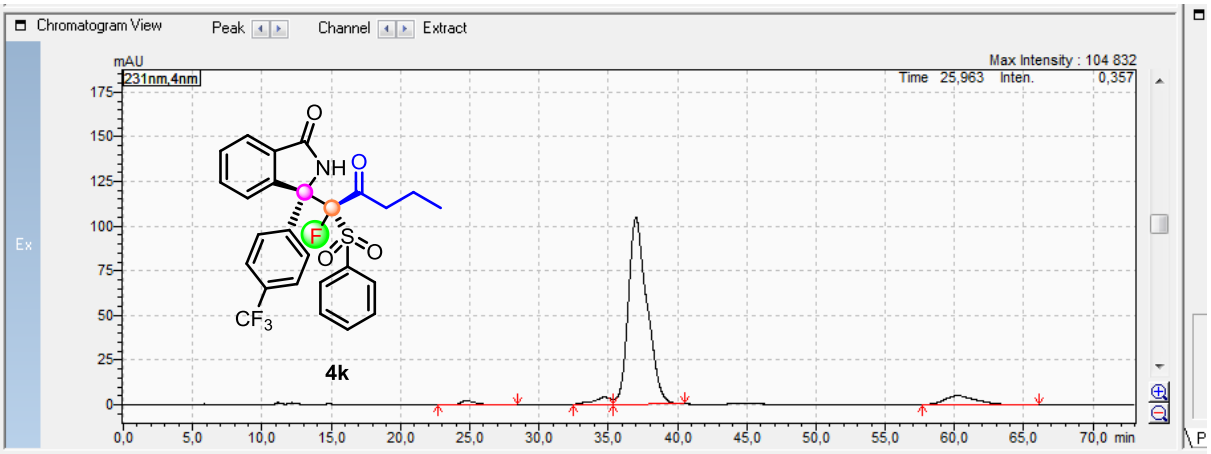
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

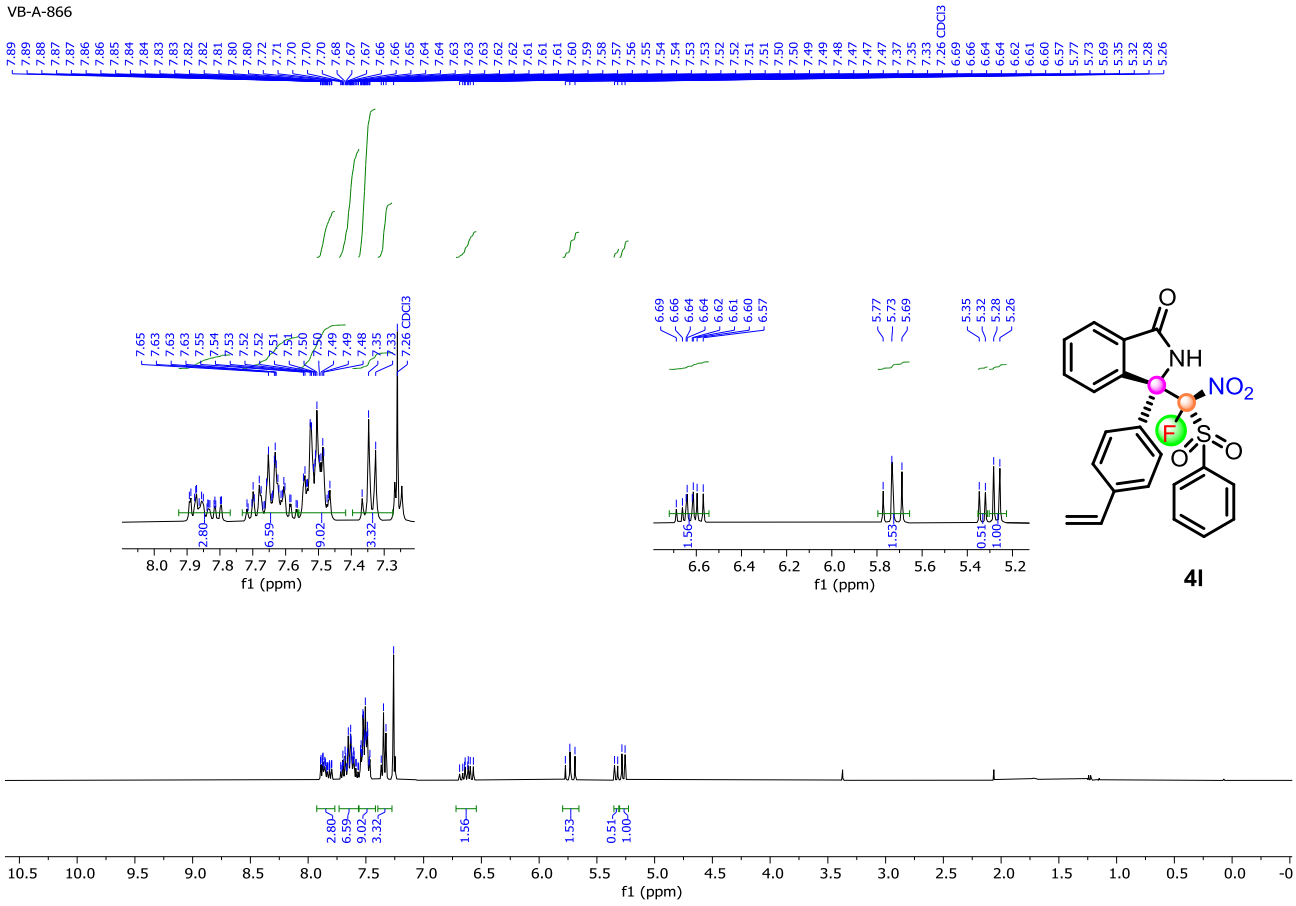
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	24,651	29,051	4882199	77585	0,000000	M	23,627	26,560	29,051
2	34,694	20,787	3493412	38350	0,000000		32,309	36,032	20,787
3	37,019	21,401	3596629	37490	0,000000	V	36,032	39,979	21,401
4	60,066	28,760	4833363	31424	0,000000	M	57,739	64,352	28,760
Total		100,000	16805603	184850					100,000



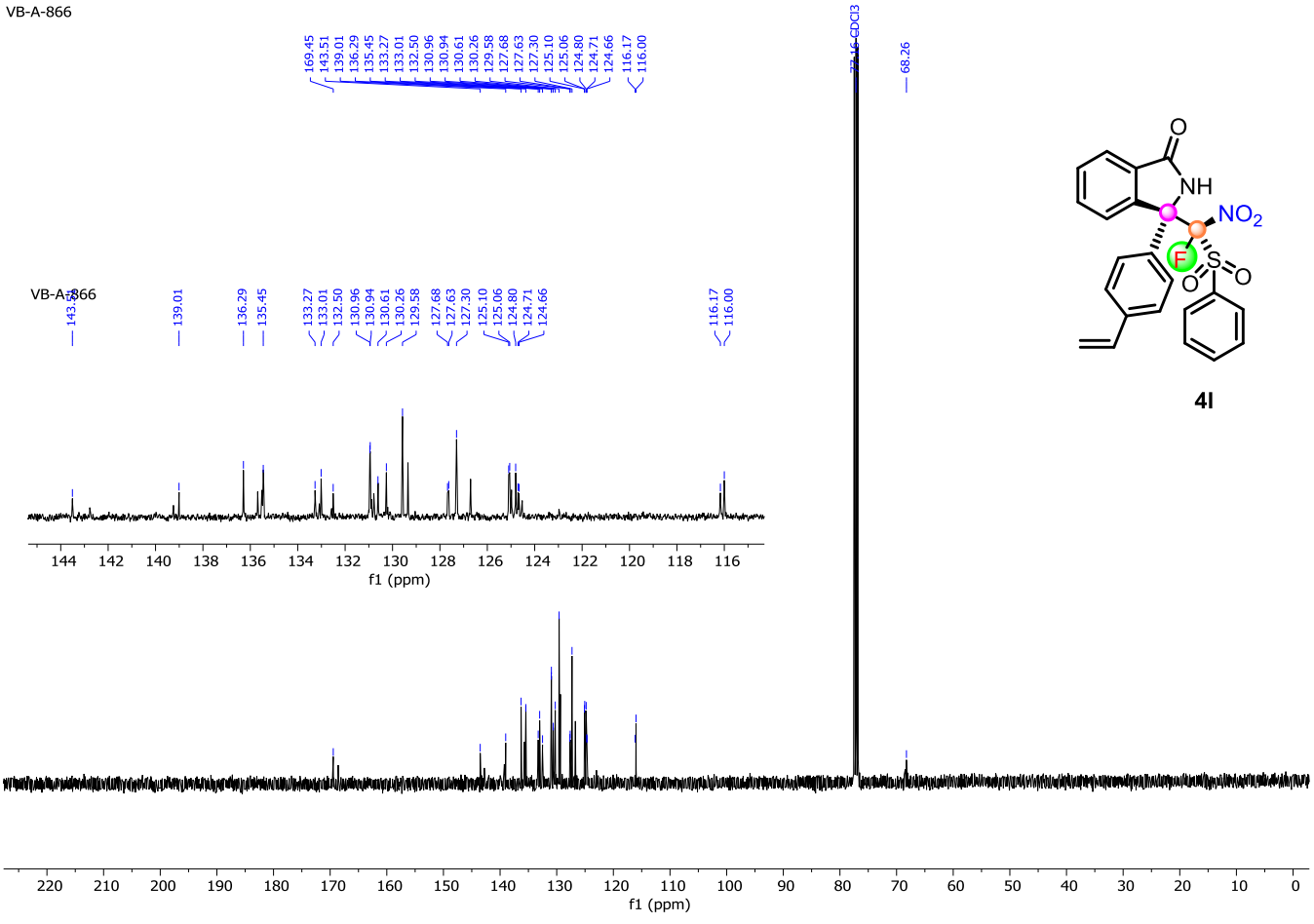
Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

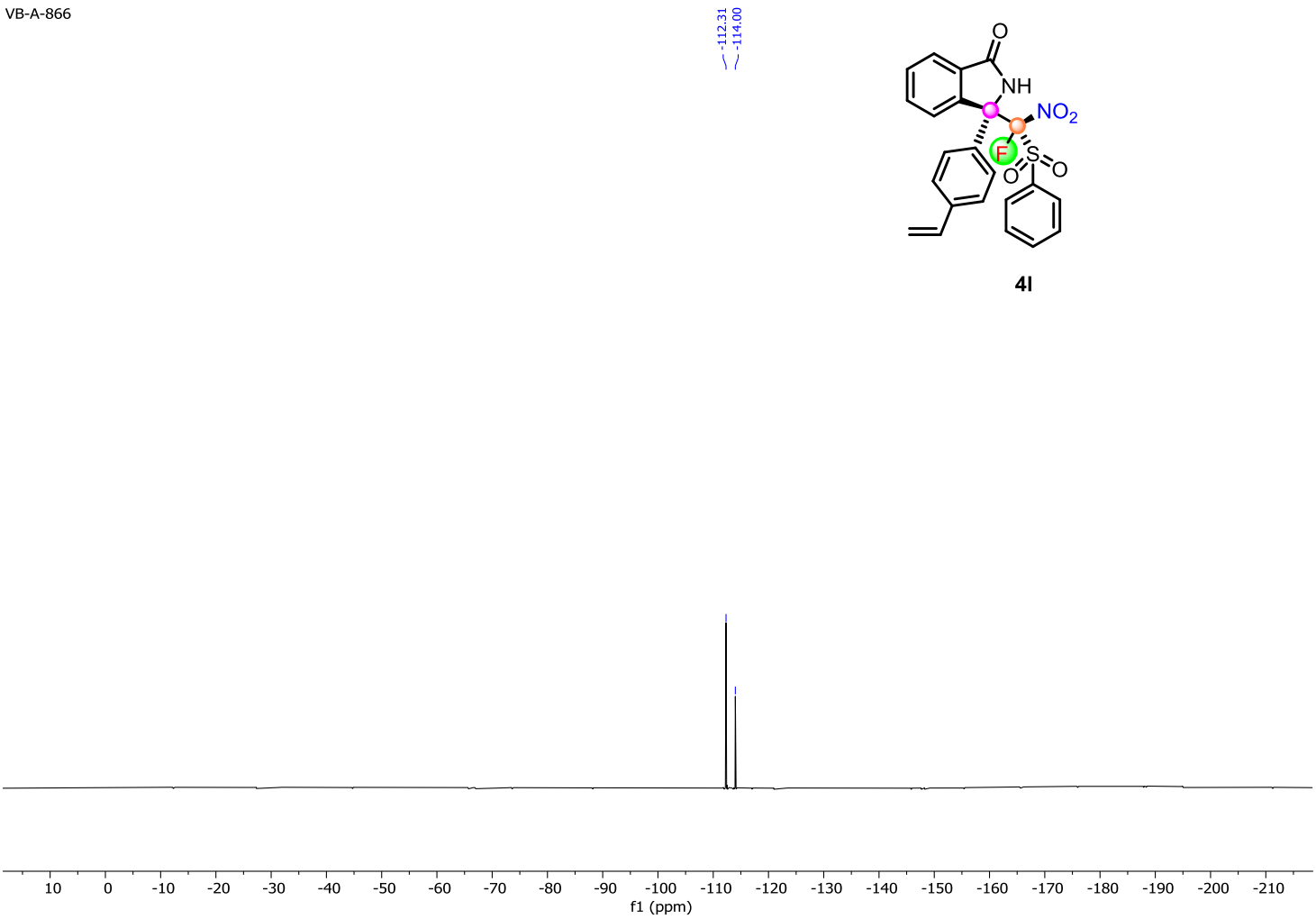
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	24,767	1,075	119336	2134	0,000000	M	22,709	28,459	1,075
2	34,729	3,179	352746	3938	0,000000		32,437	35,392	3,179
3	37,005	88,893	9865142	104495	0,000000	V	35,392	40,480	88,893
4	60,203	6,854	760589	4939	0,000000	M	57,675	66,101	6,854
Total		100,000	11097813	115507					100,000



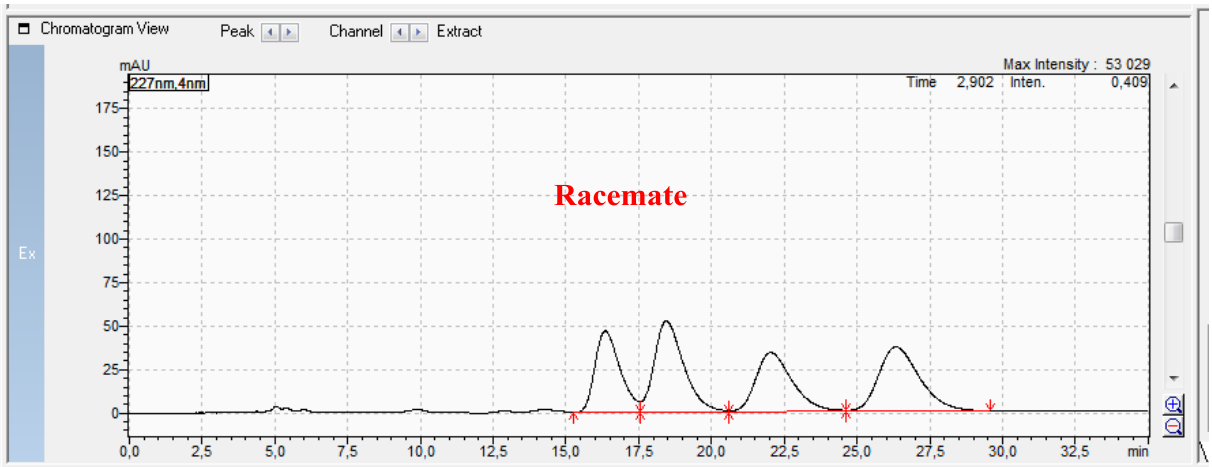
4l



4l



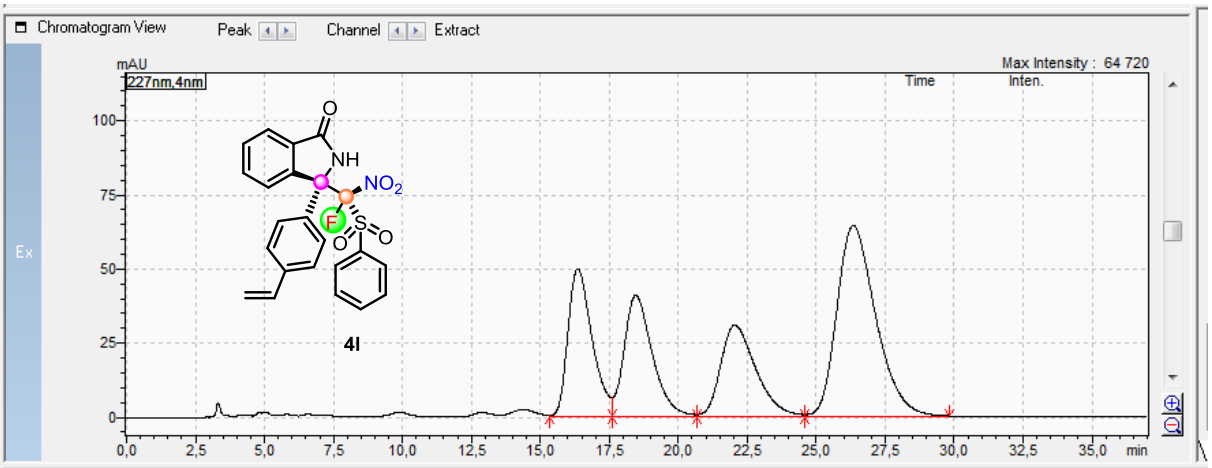
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	16,349	21,488	2824643	46935	0,000000		15,275	17,536	21,488
2	18,446	28,270	3716187	52518	0,000000	V	17,536	20,608	28,270
3	22,034	22,620	2973462	34024	0,000000	V	20,608	24,619	22,620
4	26,336	27,622	3630985	37007	0,000000	V	24,619	29,600	27,622
Total		100,000	13145278	170485					100,000

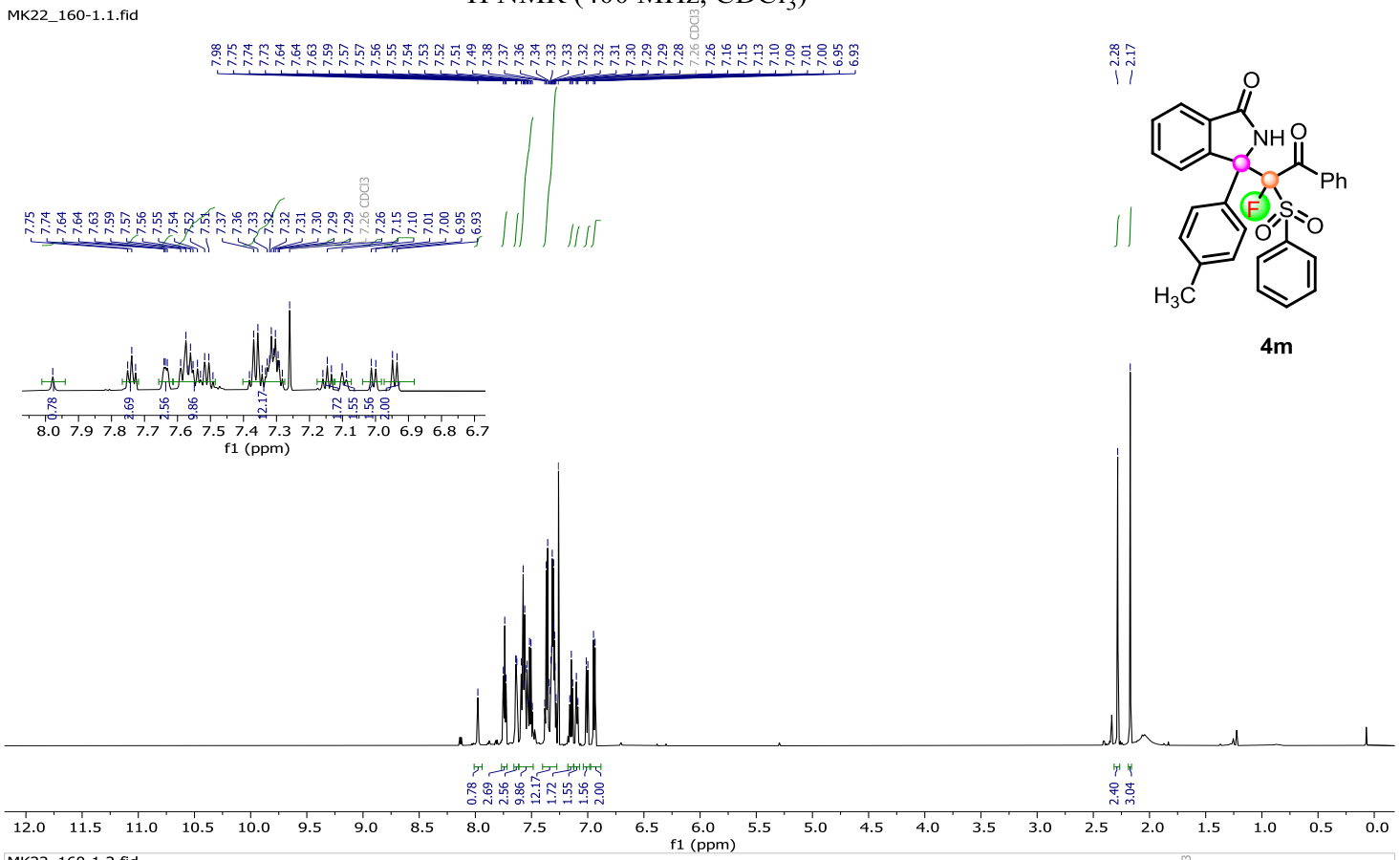


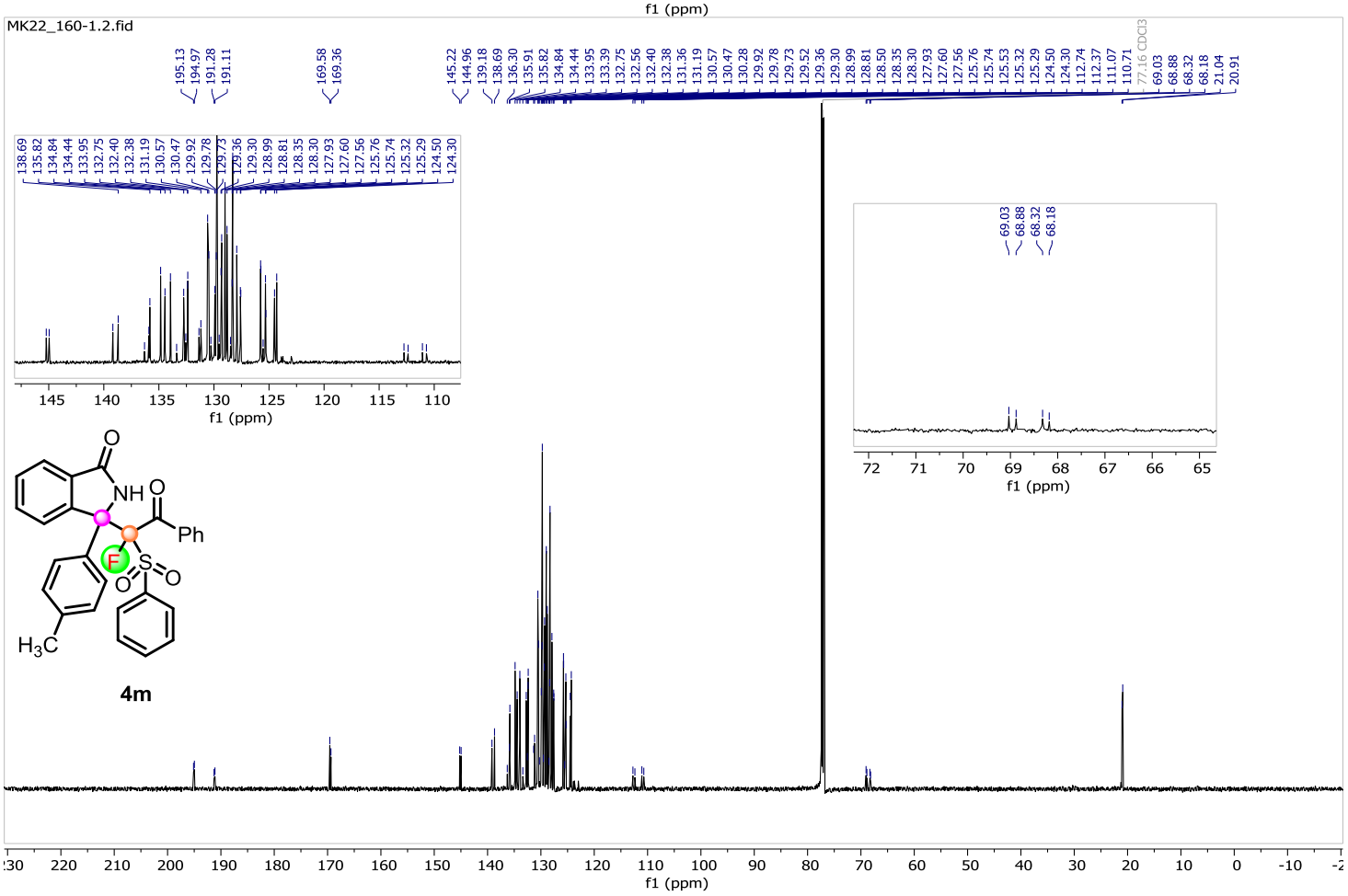
Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

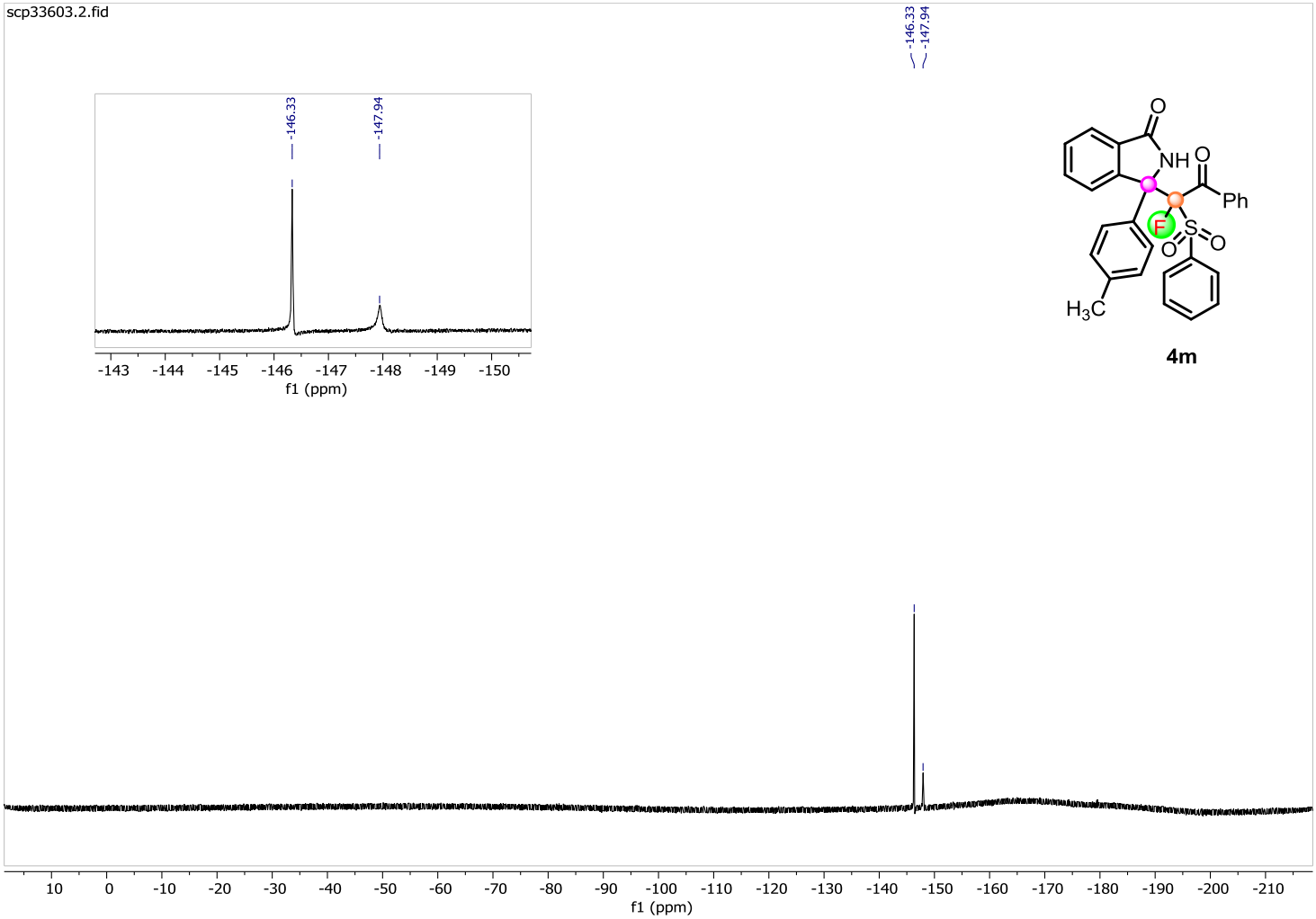
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	16,357	20,245	3023122	49887	0,000000		15,339	17,589	20,245
2	18,457	19,522	2915108	40951	0,000000	V	17,589	20,661	19,522
3	22,057	18,194	2716824	30739	0,000000	V	20,661	24,576	18,194
4	26,347	42,040	6277663	64290	0,000000	V	24,576	29,813	42,040
Total		100,000	14932717	185867					100,000

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



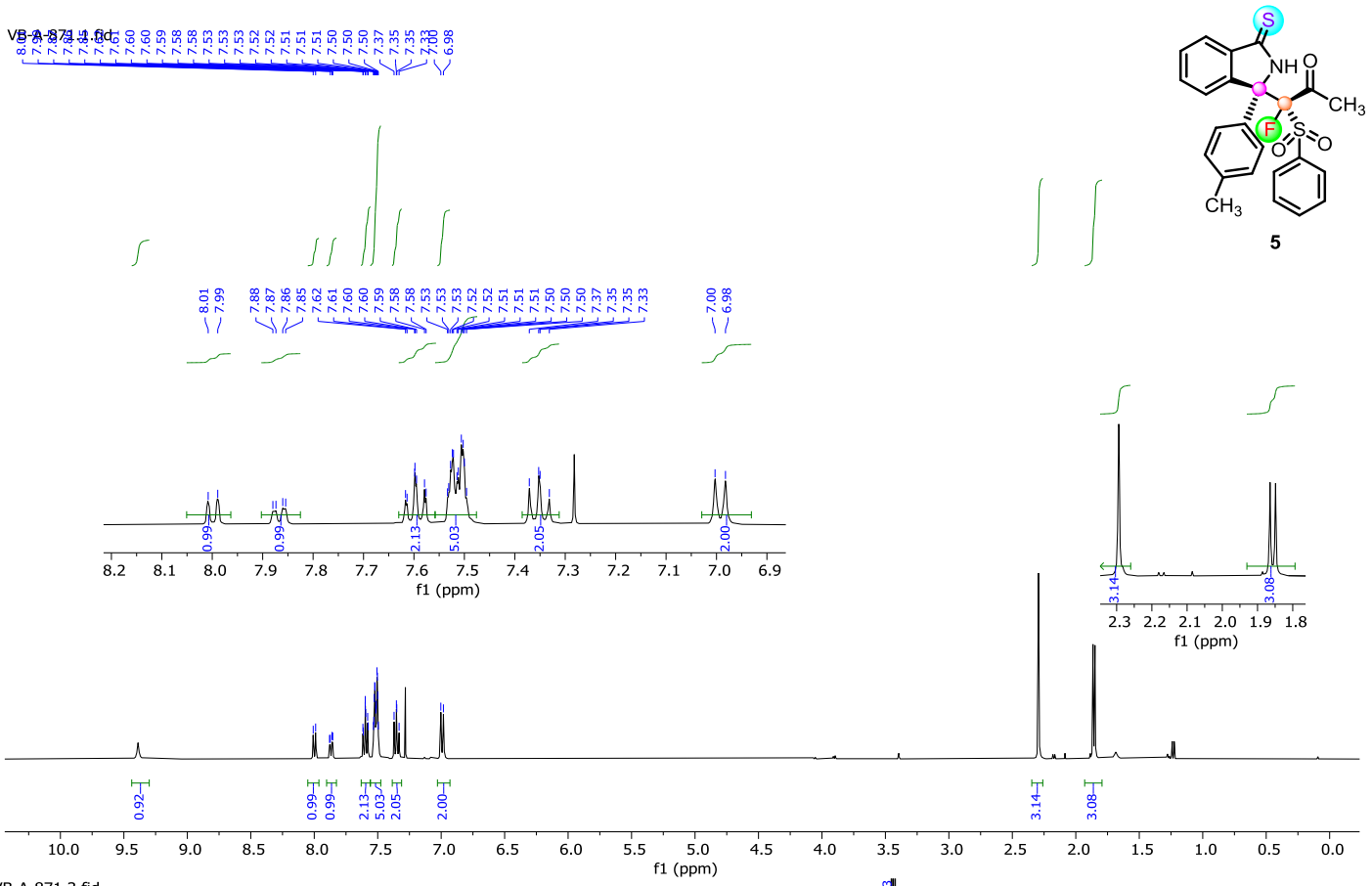


^{13}C NMR (101 MHz, $CDCl_3$)



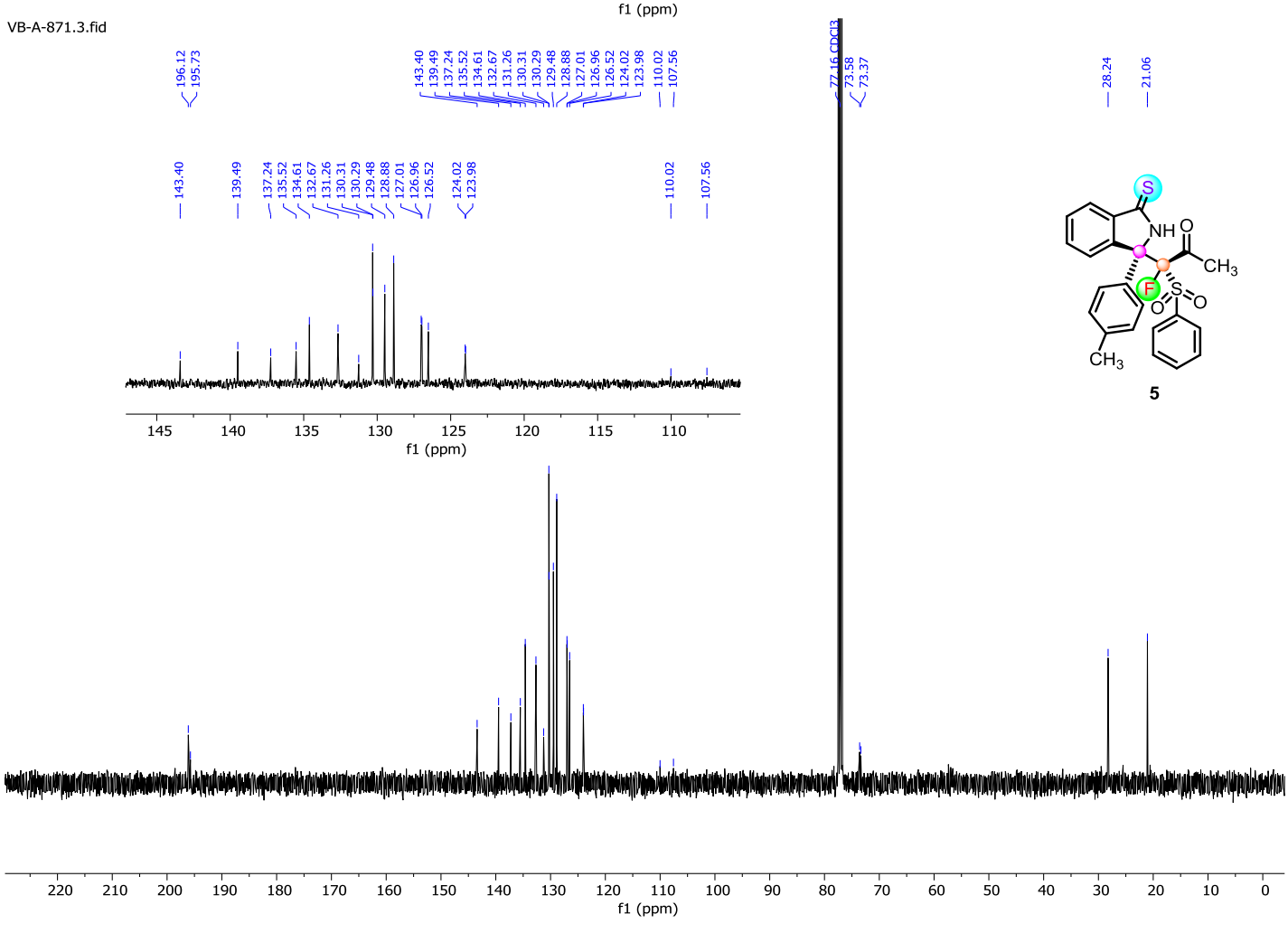
^{19}F NMR (376 MHz, $CDCl_3$)

VB-A-871.1.fid

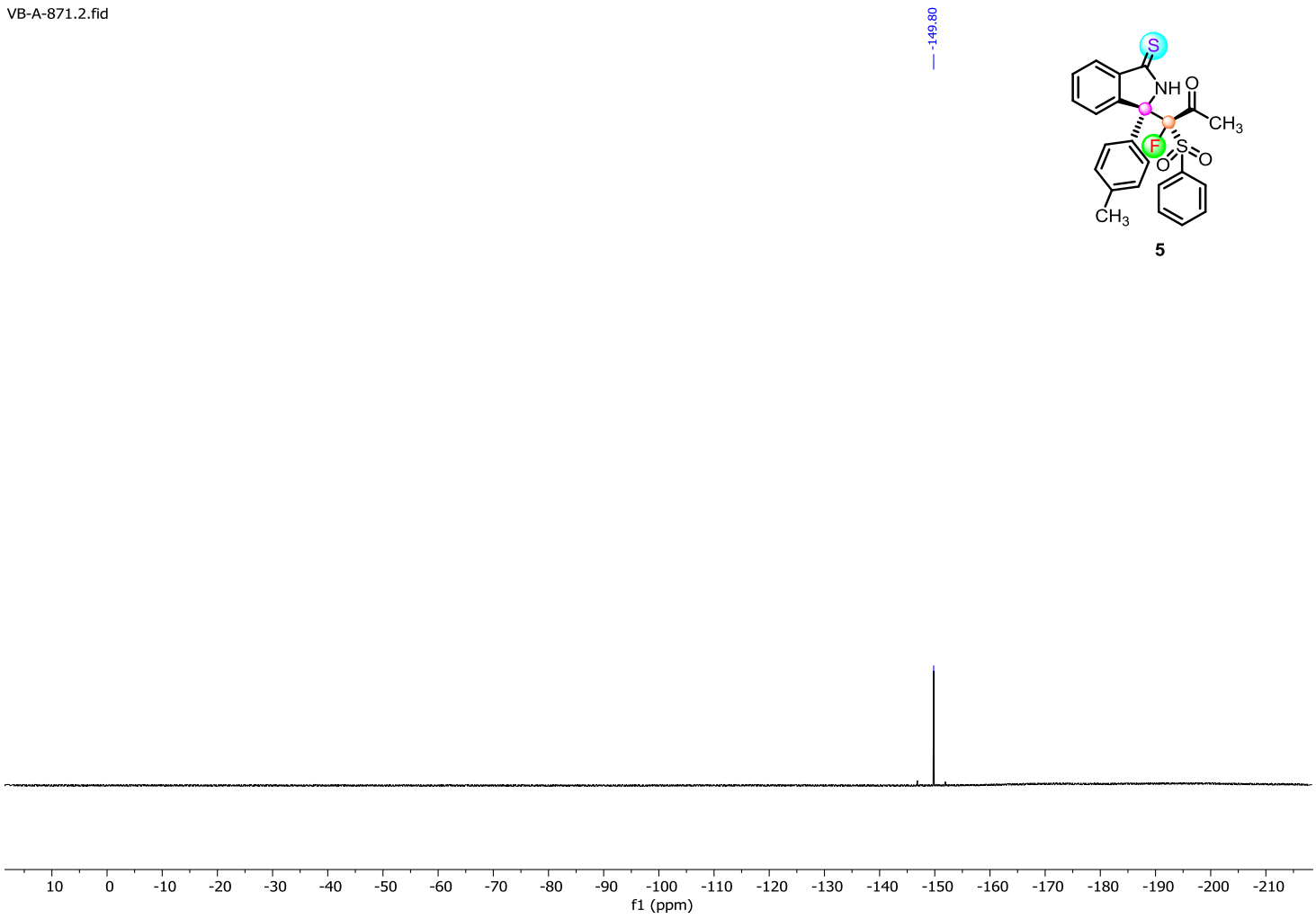


5

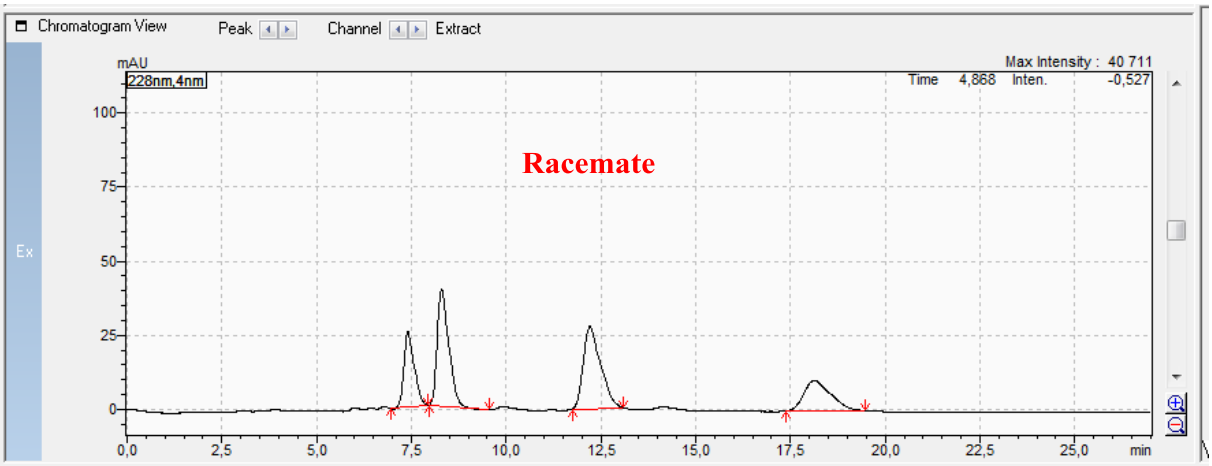
VB-A-871.3.fid



5



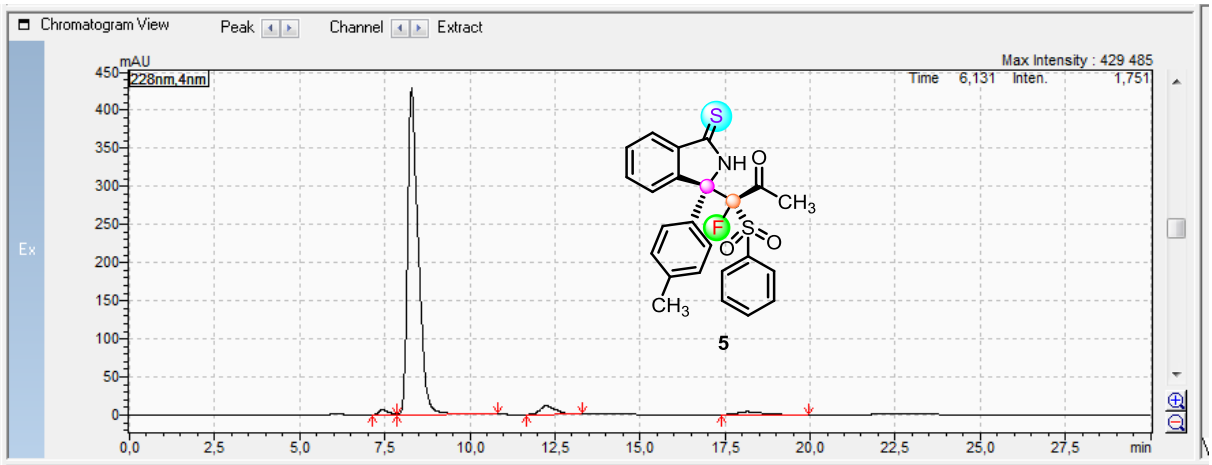
^{19}F NMR (376 MHz, $CDCl_3$)



Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	7,407	17,754	481176	25526	0,000000	M	6,955	7,936	17,754
2	8,295	31,127	843621	39708	0,000000	M	7,968	9,557	31,127
3	12,210	32,248	874016	27618	0,000000	M	11,755	13,088	32,248
4	18,129	18,871	511458	10396	0,000000	M	17,376	19,477	18,871
Total		100,000	2710272	103249					100,000

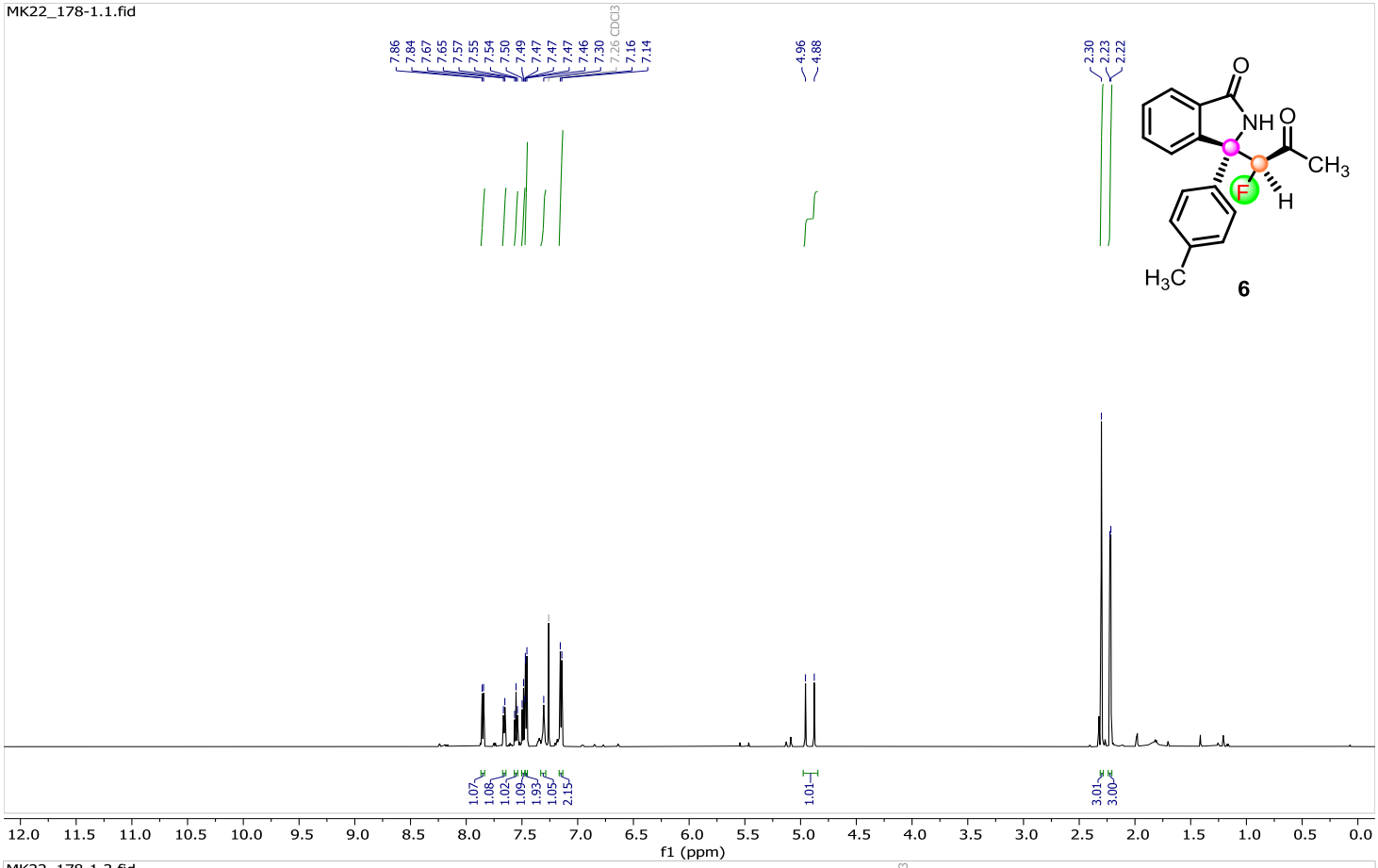


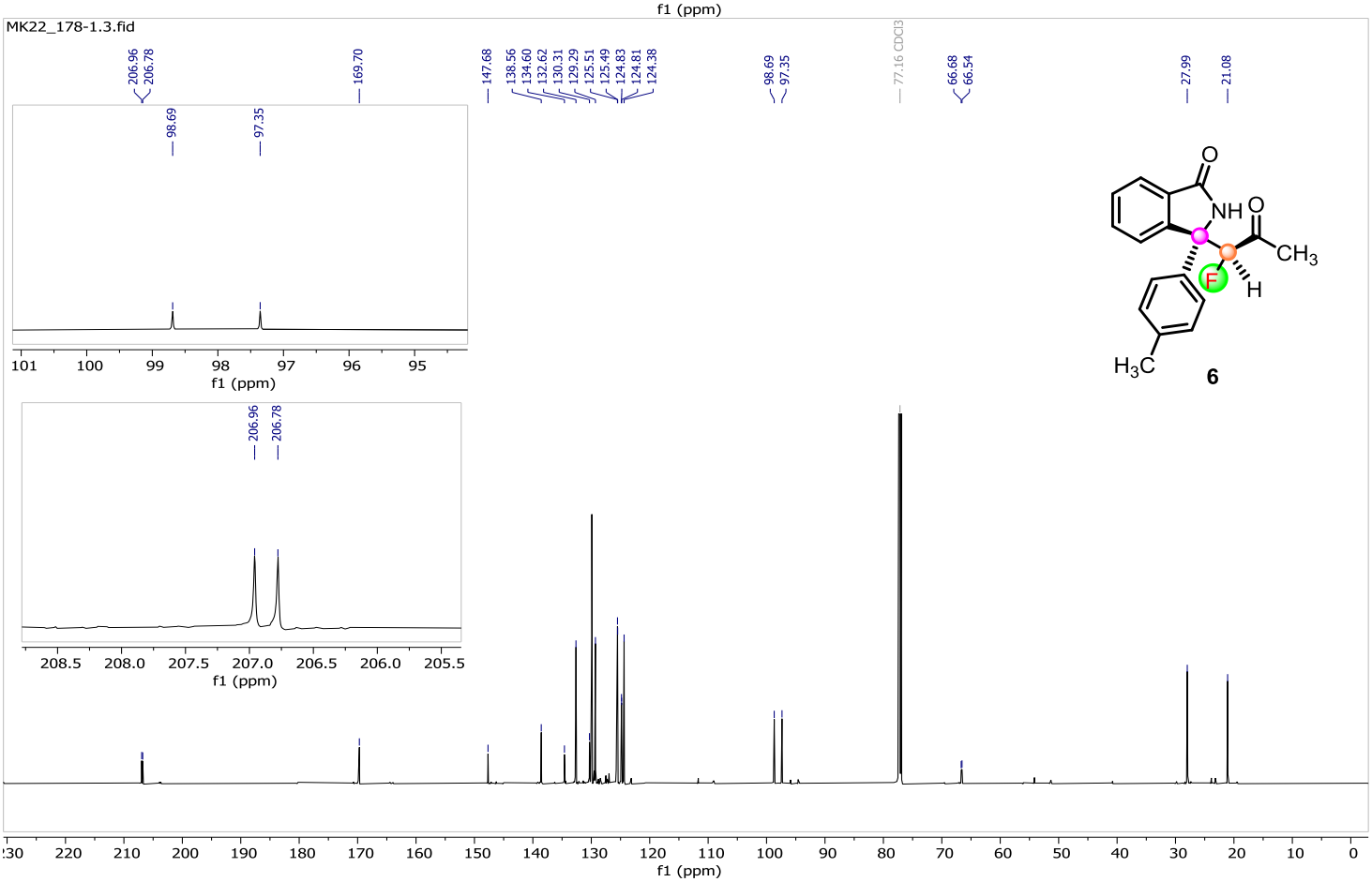
Results View - Peak Table

Peak Table | Compound | Group | Calibration Curve

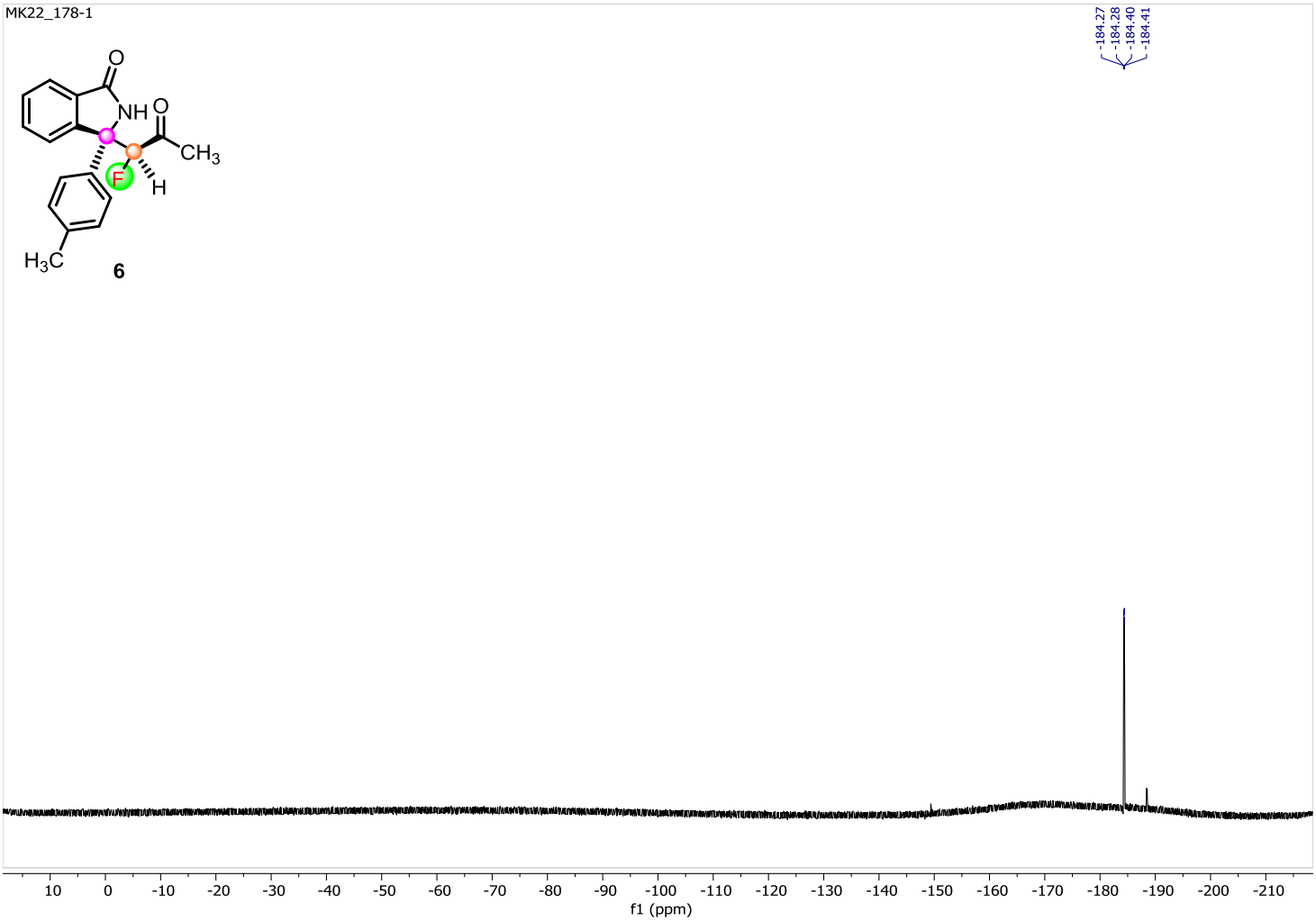
Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	7,431	1,235	123084	6612	0,000000		7,115	7,872	1,235
2	8,289	93,381	9303047	428749	0,000000	V	7,872	10,816	93,381
3	12,239	3,588	357499	11057	0,000000		11,680	13,323	3,588
4	18,144	1,795	178857	3784	0,000000	M	17,397	19,957	1,795
Total		100,000	9962488	450202					100,000

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

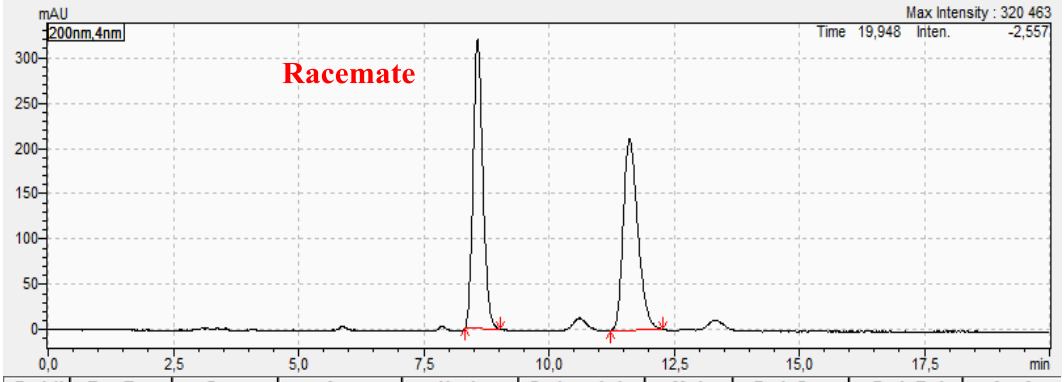




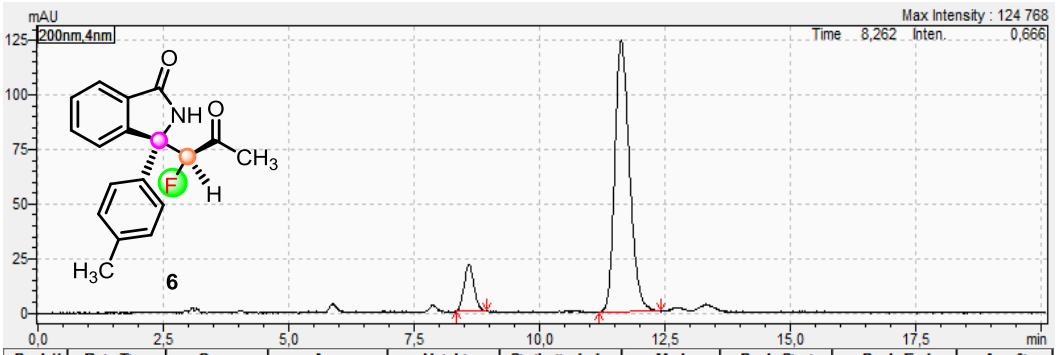
^{13}C NMR (101 MHz, $CDCl_3$)



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



Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	8,577	50,108	4305738	318332	0,000000	M	8,331	9,024	50,108
2	11,611	49,892	4287144	210656	0,000000	M	11,243	12,288	49,892
Total		100,000	8592882	528988					100,000



Peak#	Ret. Time	Conc.	Area	Height	Similarity Index	Mark	Peak Start	Peak End	Area%
1	8,590	8,379	232293	19251	0,000000	M	8,416	8,811	8,379
2	11,632	91,621	2540097	124185	0,000000	M	11,189	12,416	91,621
Total		100,000	2772390	143437					100,000