Electronic Supplementary Material (ESI) for Chemical Communications.

Electronic Supplementary Information

Rhodium(III)–Catalyzed C–H Activation at the C4-Position of Indole: Switchable Hydroarylation and Oxidative Heck-Type Reaction of Maleimides

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Contents

General Experimental

NMR spectra were recorded on a 400MHz spectrometer in $CDCl_3$, DMSO-d_6, Tetramethylsilane (TMS; δ = 0.00 ppm) served as an internal standard for ^1H NMR. The corresponding residual non-deuterated solvent signal ($CDCl_3$; δ = 77.00 ppm) was used as internal standard for ^{13}C NMR. IR spectra were measured using a FT-IR spectrometer. Mass spectra were obtained with a Q-TOF Mass Spectrometer (ESI-HRMS). Flash column chromatography was carried out by packing glass columns with commercial silica gel 100 - 200 mesh (commercial suppliers) and thin-layer chromatography was carried out using silica gel GF-254. All catalysts, reagents and reactants were procured from commercial suppliers. Dichloroethane solvent was distilled over calcium hydride and stored over molecular sieves and used for all procedures. Other solvents, used for work up and chromatographic procedures were purchased from commercial suppliers and used without any further purification.

Experimental

Typical experimental procedure for Michael addition reaction:

To a pre-dried 8 mL screw cap vial was added Indole derivative (0.2 mmol, 1equiv), $[RhCp^*Cl_2]_2$ (6 mg, 5 mol %), $AgSbF_6$ (14 mg, 20 mol %), maleimide derivative (2 equiv, 0.4mmol), AcOH (36 mg, 3equiv) and AgOAc (100 mg, 3 equiv.) To this mixture DCE (2 mL) was added. The vial was tightly capped and placed in a pre-heated (120 ^oC) metal block. After 12 h or indole derivative consumed (as shown by TLC) the reaction mixture was cooled to room temperature, and diluted with diethyl ether and passed through a short silica gel (100-200 mesh size) bed, and repeatedly washed with diethyl ether (60 mL x 3 times). The combined organic layers were concentrated under reduced pressure and the crude product was purified on a silica gel column using DCM/hexane mixture.

Typical experimental procedure for Heck type reaction:

To a pre-dried 8 mL screw cap vial was added Indole derivative (0.2 mmol, 1 equiv), $[RhCp^*Cl_2]_2$ (9 mg, 7.5 mol %), $AgSbF_6$ (21 mg, 30 mol %), maleimide derivative (2 equiv, 0.4mmol) and Ag_2CO_3 (110 mg, 2 equiv) To this mixture DCE (2 mL) was added. The vial was tightly capped and placed in a pre-heated (120 ^oC) metal block. After 3 h or indole derivative consumed (as shown by TLC) the reaction mixture was cooled to room temperature, and diluted with DCM and passed through a short silica gel (100-200 mesh size) bed, and repeatedly washed with DCM (60 mL x 3 times). The combined organic layers were

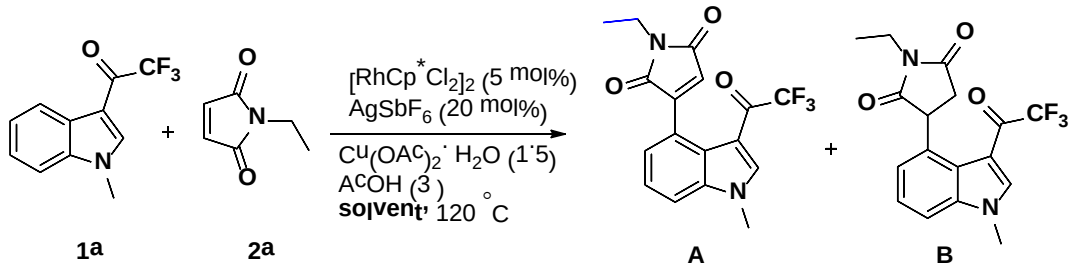
concentrated under reduced pressure and the crude product was purified on a silica gel column using DCM/hexane mixture.

Optimization Reactions

All reactions were carried out on a 0.2mmol scale. Yields are based on ^{1}H NMR using trimethoxybenzene as an internal standard

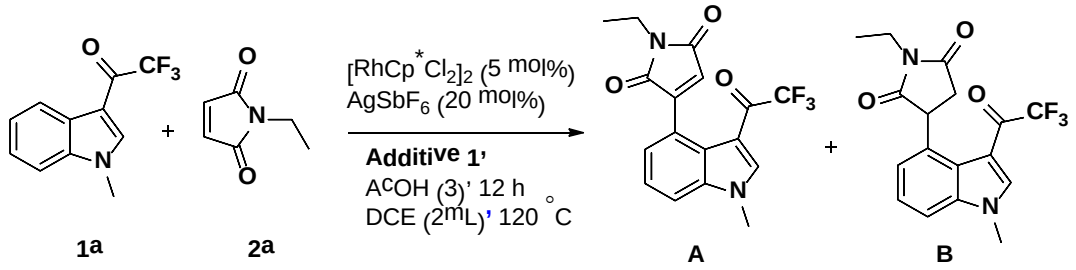
Optimization for 1,4-addtion product:

Table S1: Screening: Solvent



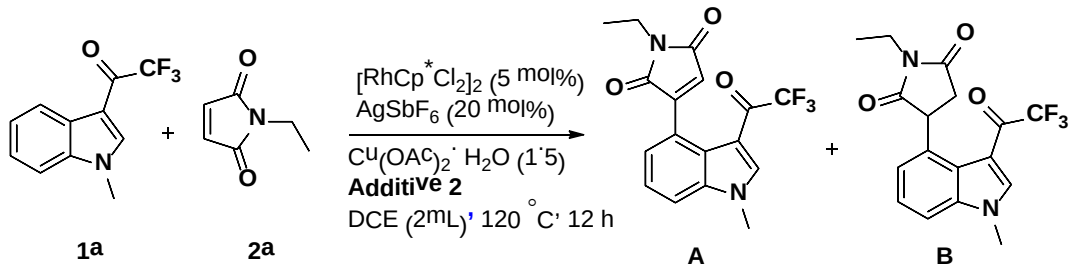
Entry	Solvent (2 mL)	NMR Yield (%)		
		A	**B**	**1a**
1	THF	4	30	56
2	CH_3CN	nd	nd	intatct
3	TFE	25	45	00
4	DCE	6	60	18

Table S2: Screening: Additive 1



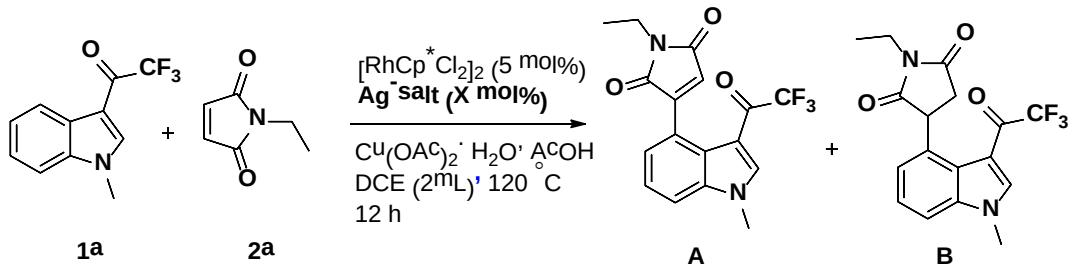
Entry	Additive 1 (equiv)	NMR Yield (%)		
		A	**B**	**1a**
1	$Cu(OAc)_2. H_2O$ (1.5)	6	60	18
2	$Cu(OAc)_2. H_2O$ (2)	6	60	10
3	$Cu(OAc)_2. H_2O$ (0.5)	8	55	23
4	NaOAc (3)	nd	nd	intact
5	KOAc (3)	nd	nd	intact
6	AgOAc (3)	7	70	00
7	AgOAc (1.5)	6	65	03
8	$Cu(OTf)_2$	nd	nd	intact

Table S3: Screening: Additive 2



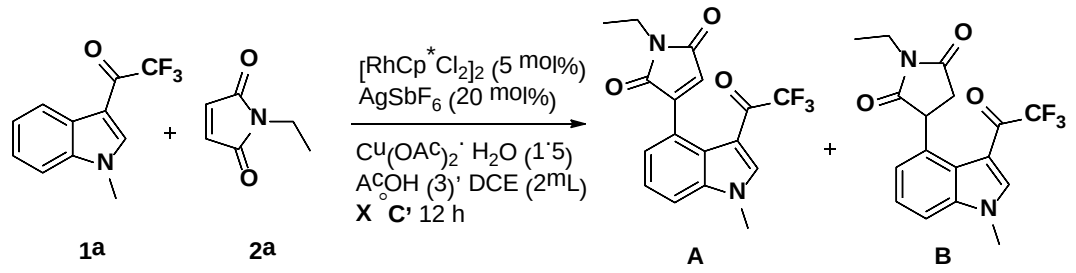
Entry	Rh (mol%)	Silver salt (mol%)	Additive 1 (1.5 equiv)	Additive 2 (equiv)	NMR Yield (%)		
					A	**B**	**1a**
1	5	20	$Cu(OAc)_2$. H_2O	CCl_3COOH (3.5)	nd	nd	nd
2	5	20	AgOAc (3)	AdCOOH(3)	18	46	15
3	5	20	AgOAc (3)	Pivalic Acid(3)	25	50	10
4	5	20	$Cu(OAc)_2$. H_2O	None	25	40	00
5	5	20	$Cu(OAc)_2$. H_2O	AcOH (3)	6	60	18
6	5	20	AgOAc (3)	AcOH (3)	7	70	00
7	5	20	AgOAc (1.5)	AcOH (3)	6	65	00
8	5	20	$Cu(OTf)_2$. (1.5)	AcOH (3)	nd	nd	intact
9	5	20	$Cu(OAc)_2$. H_2O	Triflic Acid(3)	7	18	72
10	5	20	$Cu(OAc)_2$. H_2O	TFAA(3)	nd	nd	intact
11	5	20	none	AcOH (5)	nd	nd	nd
12	7.5	30	$Cu(OAc)_2$. H_2O	AcOH (3)	4	35	50
13	5	20	$Cu(OAc)_2$. H_2O	AcOH (10)	nd	20	56
14	5	20	$Cu(OAc)_2$. H_2O	AcOH (1)	13	50	6

Table S4: Screening: Silver salt



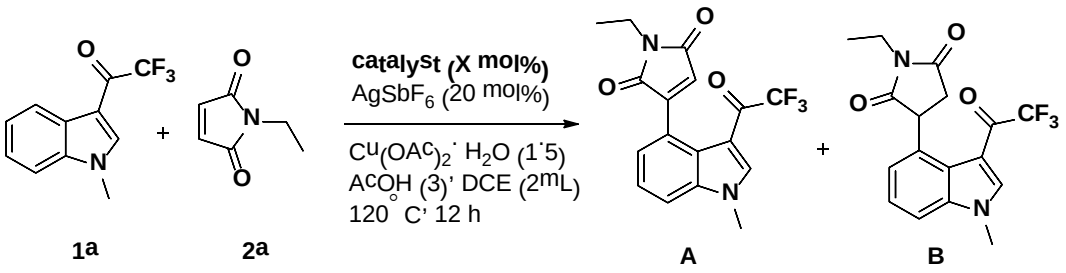
Entry	Rh (mol%)	Silver salt (mol%)	Additive 1 $Cu(OAc)_2$. H_2O (equiv)	Additive 2 (AcOH) (equiv)	NMR Yield (%)		
					A	**B**	**1a**
1	5	$AgSbF_6$(20)	1	3	3	43	45
2	7.5	$AgSbF_6$(30)	1	5	nd	40	36
3	5	$AgBF_4$(20)	1.5	3	3	18	72
4	5	$AgPF_6$(20)	1.5	3	nd	nd	intact
5	5	$AgNTf_2$(20)	1.5	3	10	62	15

Table S5: Screening: Temp



Entry	Temp (°C)	NMR Yield (%)		
		A	**B**	**1a**
1	120	6	60	18
2	140	15	53	9
3	100	3	25	60

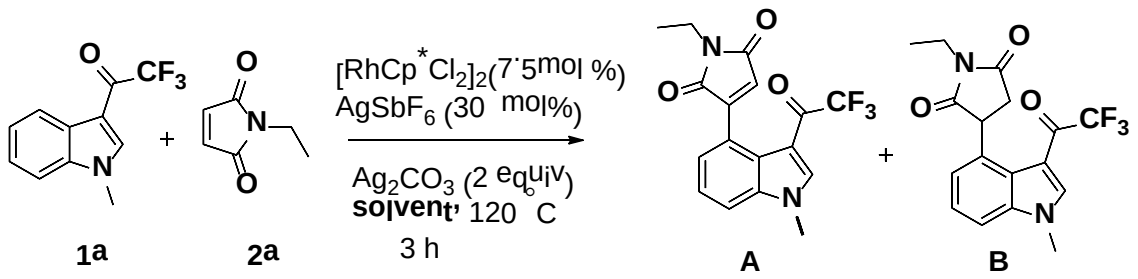
Table S6: Screening: catalyst



Entry	Catalyst (5 mol%)	NMR Yield (%)		
		A	**B**	**1a**
1	$RuCl_2$(p-cymene)	nd	nd	intact
2	(CoCp*(CO)I_2)	nd	nd	intact

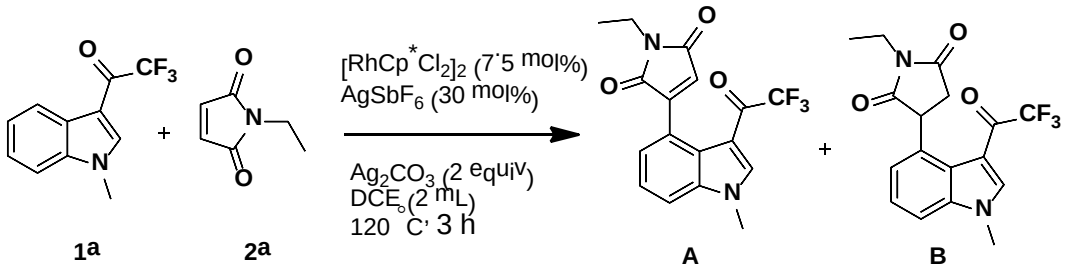
Optimization Table for the Oxidative Heck-Type Product:

Table S7: Solvent Screening



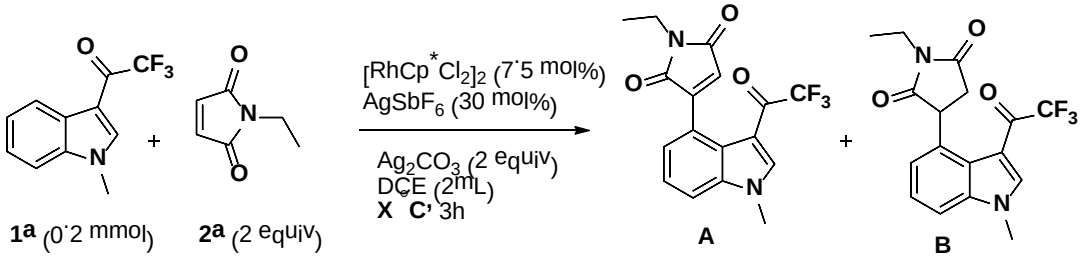
Entry	Solvent (2 mL)	NMR Yield (%)(A+B+1a)		
		A	**B**	**1a**
1	THF	nd	nd	intact
2	CH_3CN	nd	nd	intact
3	Toluene	nd	nd	intact
4	DCE	75	4	nd

Table S8: Screening the amount of maleimide



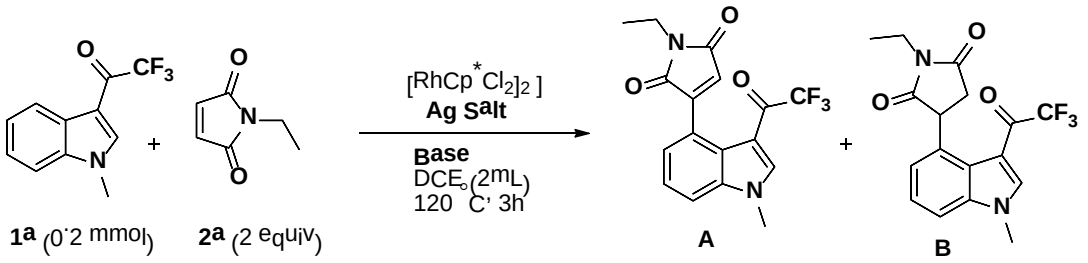
Entry	Maleimide 2a (equiv)	NMR Yield (%)		
		A	**B**	**1a**
1	2	75	4	nd
2	3	52	nd	5
3	1	48	nd	nd

Table S9: Screening: Temp



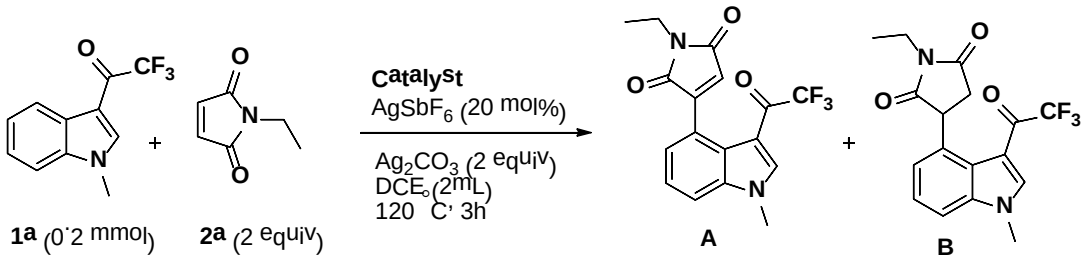
Entry	Temp (^{0}C)	NMR Yield (%) (**A**+**B**+**1a**)		
		A	**B**	**1a**
1	100	48	nd	32
2	120	75	4	nd
3	140	64	4	11

Table S10: Screening: additives



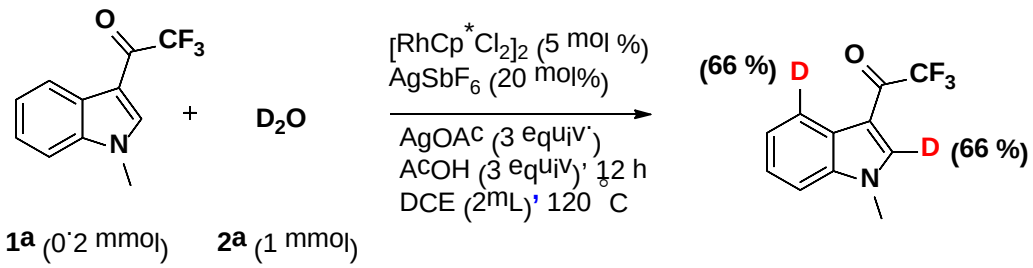
Entry	$(RhCp^*Cl_2)_2$ mol %	Silver Salt (mol %)	Base (equiv)	NMR Yield (%)		
				A	**B**	**1a**
1	5	$AgSbF_6$ (20)	Ag_2CO_3 (2.5)	70	5	18
2	5	$AgSbF_6$ (20)	Ag_2CO_3 (3)	70	nd	17
3	10	$AgSbF_6$(40)	Ag_2CO_3 (2)	60	nd	nd
4	7.5	$AgSbF_6$ (30)	Ag_2CO_3 (3)	56	nd	nd
5	7.5	$AgSbF_6$ (30)	Ag_2CO_3 (2)	75	4	nd
6	7.5	$AgSbF_6$ (30)	Ag_2CO_3 (2.5)	70	5	nd
7	7.5	$AgSbF_6$ (30)	Li_2CO_3 (2)	18	nd	77
8	7.5	$AgSbF_6$ (30)	K_2CO_3(2)	nd	nd	intact
9	7.5	$AgSbF_6$ (30)	Na_2CO_3(2)	11	nd	80
10	7.5	$AgSbF_6$ (30)	Cs_2CO_3(2)	nd	nd	intact
11	7.5	$AgSbF_6$ (30)	DBU(2)	nd	nd	intact
12	7.5	$AgSbF_6$ (30)	NEt_3(2)	nd	nd	intact
13	7.5	$AgSbF_6$ (30)	$AgNO_3$(2)	nd	nd	intact
14	7.5	$AgSbF_6$ (30)	AgOAc(2)	20	nd	18
15	7.5	$AgSbF_6$ (30)	Ag_2O(2)	34	nd	11
16	7.5	$AgSbF_6$ (30)	KOAc(2)	nd	nd	nd
17	7.5	$AgSbF_6$ (30)	NaOAc(2)	nd	nd	nd
18	7.5	AgBF4	Ag_2CO_3 (2)	48	nd	7
19	7.5	AgNTf2	Ag_2CO_3 (2)	30	nd	35

Table S11: Screening catalysts



Entry	Catalyst (5 mol%)	NMR Yield (%)		
		A	**B**	**1a**
1	$RuCl_2$(p-cymene)	nd	nd	88
2	$(IrCp^*Cl2)_2$	nd	nd	intact
3	$(CoCp^*(CO)I_2)$	nd	nd	intact

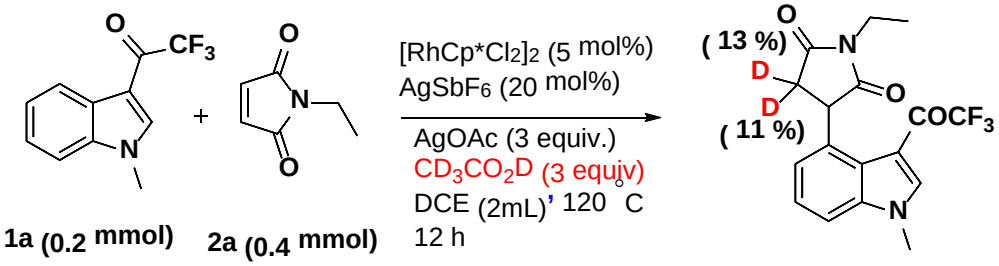
Mechanistic studies (H/D exchange reaction):



1a (0.2 mmol) **2a** (1 mmol)

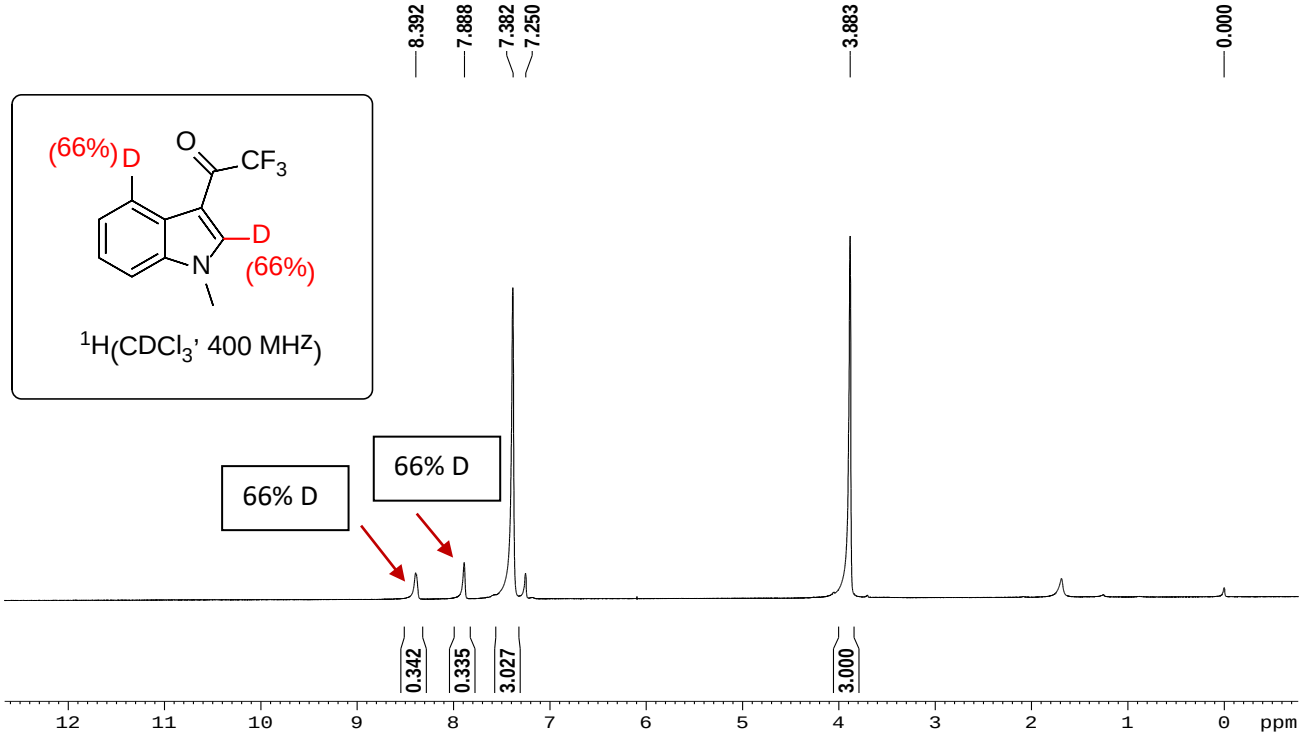
To a pre-dried 8 mL screw cap vial was added Indole derivative (0.2 mmol, 1equiv), $[RhCp^*Cl_2]_2$ (6 mg, 5 mol %), $AgSbF_6$ (14 mg, 20 mol %), D_2O (10 equiv, 1 mmol), AcOH (36 mg, 3equiv) and AgOAc (100 mg, 3 equiv.) To this mixture DCE (2 mL) was added. The vial was tightly capped and placed in a pre-heated (120 °C) metal block. After 12 h, the reaction mixture was cooled to room temperature, and diluted with diethyl ether and passed through a short silica gel (100-200 mesh size) bed, and repeatedly washed with diethyl ether (60 mL x 3 times). The combined organic layers were concentrated under reduced pressure and the crude product was purified on a silica gel column using DCM/hexane mixture.

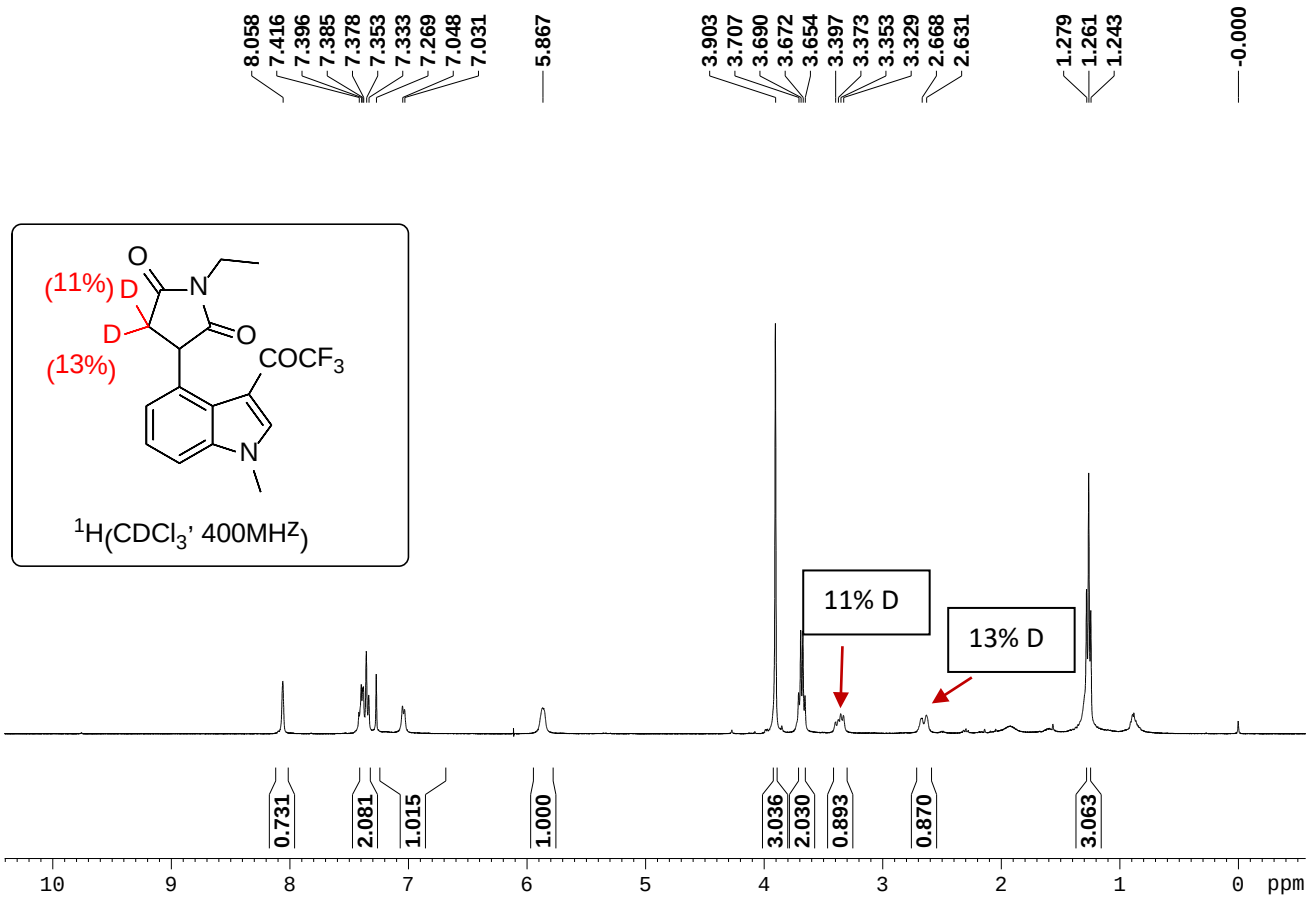
Deuterium incorporation reaction



1a (0.2 mmol) **2a (0.4 mmol)**

To a pre-dried 8 mL screw cap vial was added Indole derivative (0.2 mmol, 1equiv), $[RhCp^*Cl_2]_2$ (6 mg, 5 mol %), $AgSbF_6$ (14 mg, 20 mol %), maleimide derivative (2 equiv, 0.4 mmol), CD_3COOD (38.4 mg, 3equiv) and AgOAc (100 mg, 3 equiv.) To this mixture DCE (2 mL) was added. The vial was tightly capped and placed in a pre-heated (120 °C) metal block. After 12 h, the reaction mixture was cooled to room temperature, and diluted with diethyl ether and passed through a short silica gel (100-200 mesh size) bed, and repeatedly washed with diethyl ether (60 mL x 3 times). The combined organic layers were concentrated under reduced pressure and the crude product was purified on a silica gel column using DCM/hexane mixture.


8.392
7.888
7.382
7.250
3.883
0.000
(66%) D
O
CF3
D
(66%)
N
1H(CDCl3, 400 MHZ)
66% D
66% D
0.342
0.335
3.027
3.000
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm


8.058
7.416
7.396
7.385
7.378
7.353
7.333
7.269
7.048
7.031
5.867
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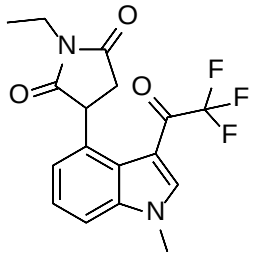
3.690
3.672
3.654
3.397
3.373
3.353
3.329
2.668
2.631
1.279
1.261
1.243
-0.000
(11%) D
O
N
D
(13%)
O
COCF3
N
1H(CDCl3, 400MHZ)
11% D
13% D
0.731
2.081
1.015
1.000
3.036
2.030
0.893
0.870
3.063
10
9
8
7
6
5
4
3
2
1
0
ppm

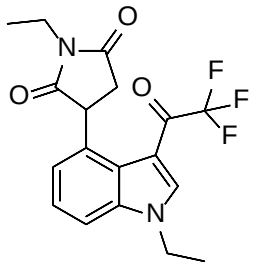
Characterization data for all isolated products:

1. **1-Ethyl-3-(1-methyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)pyrrolidine-2,5-dione (3aa)**



Yield - 47 mg (67%), as a light yellow solid; **mp** – 129 – 131 °C;**R_f**- (70% DCM/Hexane) 0.3;**^{1}H NMR** (400 MHz, $CDCl_3$) δ8.06 (s., 1 H), 7.43 - 7.34 (m, 2 H), 7.04 (d, *J* = 6.8 Hz, 1 H), 5.86 (br. s., 1 H), 3.92 (s, 3 H), 3.68 (q, *J* = 6.9 Hz, 2 H), 3.37 (dd, *J* = 9.3, 18.2 Hz, 1 H), 2.65 (d, *J* = 18.2 Hz, 1 H), 1.25 (t,*J* = 7.2 Hz 3 H); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ178.8, 176.4, 174.3, (q, *J* = 33 Hz) 141.2, 138.6, 133.7, 125.8, 125.5, 122.1, 117.5, (q, *J* = 290 Hz) 109.8, 44.7, 39.3, 34.3, 33.9, 13.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -69.737 ; **HRMS (ESI-TOF)** *(m/z)***–**Calculated for $C_{17}H_{15}F_3N_2O_3$ $(M+Na)^+$.: 375.0932, found $(M+Na)^+$: 375.0928; **IR** (Neat, cm^{-1}): 1701, 1674.

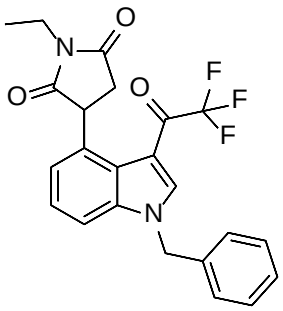
2. **1-Ethyl-3-(1-ethyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)pyrrolidine-2,5-dione (3ba)**



Yield - 50 mg (68%), as a light brown solid; **mp** – 142 – 144 °C; **R_f**- (70% DCM/Hexane) 0.3;**^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.11 (s., 1 H), 7.41 - 7.27 (m, 2 H), 7.03 (br. s., 1 H), 5.87 (br. s., 1 H), 4.28 (q, *J* = 7.3 Hz, 2 H), 3.68 (q, *J* = 7.1 Hz, 2 H), 3.37 (dd, *J* = 9.5, 18.1 Hz, 1 H), 2.68 - 2.64 (m, 1 H), 1.57 (t, *J* = 7.3 Hz, 3 H), 1.26 (t, *J* = 7.2 Hz, 3 H); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ178.8, 176.4, 174.2(q, *J* = 33.9 Hz), 139.7, 137.7, 133.8, 126.0, 125.3, 122.1, 117.5, (q, *J* = 290 Hz) 109.98, 109.92, 44.7, 42.5, 39.3, 33.8, 14.7, 13.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -69.657 ;

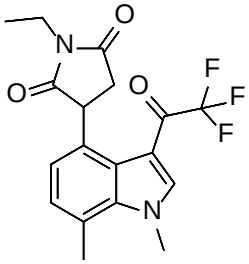
HRMS (ESI-TOF) *(m/z)***–**Calculated for $C_{18}H_{17}F_3N_2O_3$ $(M+Na)^+$: 389.1089, found $(M+Na)^+$: 389.1088; **IR** (Neat, cm^{-1}): 1700, 1673.

3. **3-(1-Benzyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)-1-ethylpyrrolidine-2,5-dione 3ca)**



Yield - 63 mg (74%), as a brown solid; **mp** – 154 – 156 °C;**R_f**- (70% DCM/Hexane) 0.3;**^{1}H NMR** (400 MHz, $CDCl_3$) δ8.13 (s., 1 H), 7.39 - 7.26 (m, 5 H), 7.17 (d, *J* = 7.3 Hz, 2 H), 7.01 (d, *J* = 6.3 Hz, 1 H), 5.86 (br. s., 1 H), 5.41 (s, 2 H), 3.68 (q, *J* = 7.1 Hz, 2 H), 3.38 (dd, *J* = 9.5, 18.1 Hz, 1 H), 2.66 (dd, *J* = 3.9, 18.1 Hz, 1 H), 1.26 (t, *J* = 7.2 Hz, 3 H); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ178.8, 176.4, 174.5(q, *J* = 33.9 Hz), 140.6, 138.1, 134.1, 133.8, 129.2, 128.7, 126.9, 126.1, 125.6, 122.3, 117.4, (q, *J* = 290 Hz) 110.5, 110.3, 51.5, 44.7, 39.4, 33.9, 13.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -69.782 ; **HRMS (ESI-TOF)** *(m/z)***–**Calculated for $C_{23}H_{19}F_3N_2O_3$ $(M+Na)^+$: 451.1245, found $(M+Na)^+$: 451.1248; **IR** (Neat, cm^{-1}): 1698, 1675.

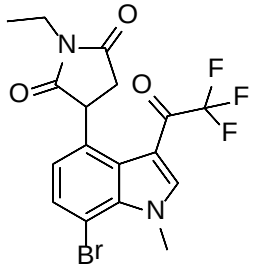
4. **3-(1,7-Dimethyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)-1-ethylpyrrolidine-2,5-dione(3da)**



Yield - 55 mg (75%), as a yellow solid; **mp** – 168 – 170 °C;**R_f**- (70% DCM/Hexane) 0.3;**^{1}H NMR** (400 MHz, $CDCl_3$) δ7.94 (s, 1 H), 7.07 (d, *J* = 7.6 Hz, 1 H), 6.87 (d, *J* = 7.6 Hz, 1 H), 5.76 (dd, *J* = 4.8, 8.8 Hz, 1 H), 4.14 (s, 3 H), 3.66 (q, *J* = 7.1 Hz, 2 H), 3.34 (dd, *J* = 9.6, 18.4 Hz, 1 H), 2.74 (s, 3 H), 2.61 (dd, *J* = 4.3, 18.4 Hz, 1 H), 1.25 (t, *J* = 7.3Hz , 3 H); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ179.0, 176.5, 174.2(d, *J* = 33.7 Hz), 143.05, (d, *J* = 5 Hz), 137.3, 131.6, 128.5, 127.0, 122.2, 121.9, 117.6 (q, *J* = 291 Hz), 109.3, 44.4, 39.3, 38.9, 33.9, 19.6, 13.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -69.537

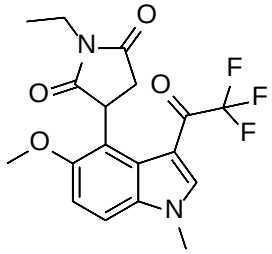
; **HRMS (ESI-TOF)** *(m/z)***–**Calculated for $C_{18}H_{17}F_3N_2O_3$ $(M+Na)^+$: 389.1089, found $(M+Na)^+$: 389.1085; **IR** (Neat, cm^{-1}): 1699, 1674.

5. **3-(7-Bromo-1-methyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)-1-ethylpyrrolidine-2,5-dione (3ea)**



Yield - 47 mg (55%), as a brown solid; **mp** – 154 – 156 °C;**R_f**- (70% DCM/Hexane) 0.3;**^{1}H NMR** (400 MHz, $CDCl_3$) δ8.02 (s., 1 H), 7.53 (d, *J* = 8.1 Hz, 1 H), 6.85 (d, *J* = 7.8 Hz, 1 H), 5.71 (br, s, 1 H), 4.30 (s, 3 H), 3.66 (q, *J* = 7.0 Hz, 2 H), 3.36 (dd, *J* = 9.3, 18.2 Hz, 1 H), 2.62 (dd, *J* = 3.9, 18.1 Hz, 1 H), 1.25 (t, *J* = 7.1 Hz, 3 H); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ178.3, 176.0, 174.2(q, *J* = 34 Hz), 143.92(d, *J* = 4.8 Hz), 135.2, 133.1, 130.7, 128.8, 123.1, 117.3(q, *J* = 290 Hz), 109.3, 104.3, 44.3, 39.4, 38.9, 34.0, 13.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -69.837 ; **HRMS (ESI-TOF)** *(m/z)***–** Calculated for $C_{17}H_{14}BrF_3N_2O_3$ $(M+Na)^+$: 453.0038, found $(M+Na)^+$: 453.0040; **IR** (Neat, cm^{-1}): 1700, 1682.

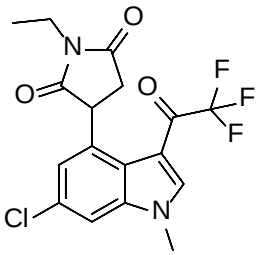
6. **1-Ethyl-3-(5-methoxy-1-methyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)pyrrolidine-2,5-dione (3fa)**



Yield - 42 mg (54%), as a white solid; **mp** – 234 – 236 °C;**R_f**- (70% DCM/Hexane) 0.1;**^{1}H NMR** (400 MHz, $CDCl_3$) δ8.00 (s, 1 H), 7.32 - 7.27 (m, 1 H), 7.05 (d, *J* = 8.8 Hz, 1 H), 5.76 (dd, *J* = 5.7, 9.5 Hz, 1 H), 3.85 (s, 3 H), 3.78 (s, 3 H), 3.66 (q, *J* = 7.1 Hz, 2 H), 3.27 (dd, *J* = 9.6, 17.9 Hz, 1 H), 2.76 (dd, *J* = 5.6, 17.9 Hz, 1 H), 1.26 (t,*J* = 7.3 Hz, 3 H); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ179.8, 176.9, 174.0(q, *J* = 34 Hz), 154.6, 142.02(q, *J* = 5.3 Hz), 133.5, 128.0, 120.2, 117.6(q, *J* = 290 Hz), 110.4, 110.0, 109.3, 56.1, 41.9, 37.1, 34.2, 33.5, 13.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -69.556 ;

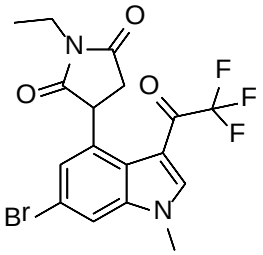
HRMS (ESI-TOF) *(m/z)***–**Calculated for $C_{18}H_{17}F_3N_2O_4$ $(M+Na)^+$: 405.1038, found $(M+Na)^+$: 405.1040; **IR** (Neat, cm^{-1}): 1701, 1666.

7. **3-(6-Chloro-1-methyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)-1-ethylpyrrolidine-2,5-dione (3ga)**



Yield - 43 mg (55%), as a yellow solid; **mp** – 128 – 130 °C ;**R_f-** (70% DCM/Hexane) 0.4;**^{1}H NMR** (400 MHz, $CDCl_3$) δ8.06 (br. s., 1 H), 7.33 (s, 1 H), 6.99 (s., 1 H), 5.83 (br. s., 1 H), 3.88 (s, 3 H), 3.69 (q, *J* = 7.2 Hz, 2 H), 3.34 (dd, *J* = 9.6, 18.4 Hz, 1 H), 2.62 (d, *J* = 17.9 Hz, 1 H), 1.25 (t,*J* = 7.2 Hz , 3 H); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ178.0, 175.8, 174.28 (q, *J* = 34 Hz), 141.8, 139.0, 134.8, 131.2, 124.3, 122.6 , 117.3(q, *J* = 290 Hz), 110.0, 109.8, 44.4, 38.9, 34.3, 34.0, 13.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -69.967 ; **HRMS (ESI-TOF)** *(m/z)***–**Calculated for $C_{17}H_{14}ClF_3N_2O_3$ $(M+Na)^+$: 409.0543, found $(M+Na)^+$: 409.0543; **IR** (Neat, cm^{-1}): 1696, 1681.

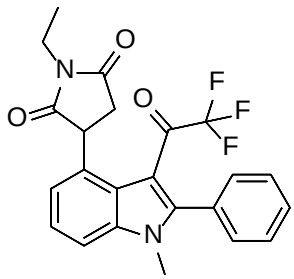
8. **3-(6-Bromo-1-methyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)-1-ethylpyrrolidine-2,5-dione (3ha)**



Yield - 55 mg (63%), as a light brown solid; **mp** – 144 – 146 °C;**R_f-** (70% DCM/Hexane) 0.2;**^{1}H NMR** (400 MHz, $CDCl_3$) δ8.04 (d,*J* = 1.2 Hz, 1 H), 7.50 (d,*J* = 1.2 Hz, 1 H), 7.12 (s, 1 H), 5.82 (dd, *J* = 5.1, 9.1 Hz, 1 H), 3.89 (s, 3 H), 3.69 (q, *J* = 7.1 Hz, 2 H), 3.34 (dd, *J* = 9.6, 18.4 Hz, 1 H), 2.63 (dd, *J* = 4.5, 18.2 Hz, 1 H), 1.26 (t, *J* = 7.2Hz, 3 H); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ178.0, 175.8, 174.3(q, *J* = 35 Hz), 141.6, 139.3, 135.1, 125.2, 124.7, 117.3(q, *J* = 290 Hz), 109.9, 44.4, 38.9, 34.3,

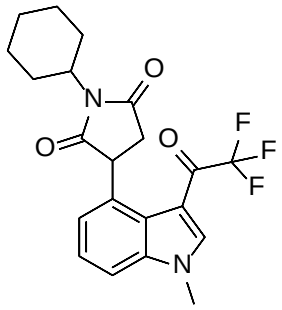
34.0, 13.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -69.971; **HRMS (ESI-TOF)** *(m/z)*– Calculated for $C_{17}H_{14}BrF_3N_2O_3$ $(M+Na)^+$: 453.0038, found $(M+Na)^+$: 453.0038; **IR** (Neat, cm^{-1}): 1694, 1680.

9. **1-Ethyl-3-(1-methyl-2-phenyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)pyrrolidine-2,5-dione (3ia)**



Yield - 51 mg (59%), as a black solid; **mp** – 203 – 205 °C;**R_f**- (70% DCM/Hexane) 0.3;**^{1}H NMR** (400 MHz, $CDCl_3$) δ7.58 - 7.51 (m, 3 H), 7.41 - 7.39 (m, 4 H), 7.07 (dd, *J* = 2.5, 6.1 Hz, 1 H), 4.99 (dd, *J* = 4.5, 9.1 Hz, 1 H), 3.67 - 3.61 (m, 2 H), 3.60 (s, 3 H), 3.26 (dd, *J* = 9.5, 18.3 Hz, 1 H), 2.79 (dd, *J* = 4.7, 18.3 Hz, 1 H), 1.22 (t, *J* = 7.2 Hz, 3 H); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ182.1(q, *J* = 36 Hz), 178.2, 176.3 ,147.5, 138.0, 131.3, 130.7, 130.2, 129.4, 128.4, 125.0, 124.4, 121.0, 115.9(q, *J* = 290 Hz), 110.6, 110.1, 42.7, 36.9, 33.9, 31.3, 13.0; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -71.019; **HRMS (ESI-TOF)** *(m/z)*–Calculated for $C_{23}H_{19}F_3N_2O_3(M+Na)^+$: 451.1245, found $(M+Na)^+$: 451.1247; **IR** (Neat, cm^{-1}): 1702, 1664.

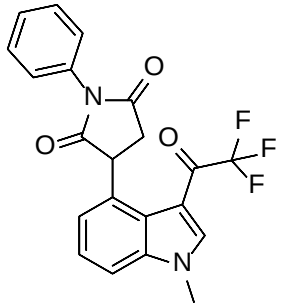
10. **1-Cyclohexyl-3-(1-methyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)pyrrolidine-2,5-dione (3ab)**



Yield - 65 mg (80%), as a light yellow solid; **mp** – 167 – 169 °C;**R_f**- (70% DCM/Hexane) 0.4;**^{1}H NMR** (400 MHz, $CDCl_3$) δ8.06 (s., 1 H), 7.42 - 7.33 (m, 2 H), 7.03 (d, *J* = 6.8 Hz, 1 H), 5.80 - 5.77 (m, 1 H), 4.12 - 4.05 (m, 1 H), 3.92 (s, 3 H), 3.32

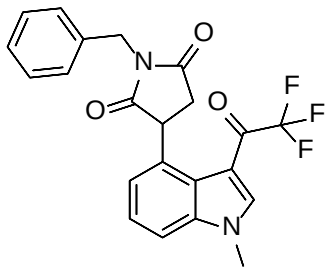
(dd, *J* = 9.7, 18.1 Hz, 1 H), 2.60 (dd, *J* = 3.7, 18.1 Hz, 1 H), 2.31 - 2.21 (m, 2 H), 1.68 (br. s., 4 H), 1.39 - 1.28 (m, 4 H); **$^{13}C\{^{1}H\}$ NMR** (100 MHz, $CDCl_3$) δ179.0, 176.6, 174.2(q, *J* = 34 Hz), 141.2, 138.6, 134.1, 125.7, 125.4, 121.9, 117.5(q, *J* = 290 Hz), 109.79, 109.76, 51.8, 44.3, 39.1, 34.2, 28.7, 25.8, 25.0; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -69.739; **HRMS (ESI-TOF)** *(m/z)***–**Calculated for $C_{21}H_{21}F_3N_2O_3$ $(M+Na)^+$: 429.1402, found $(M+Na)^+$: 429.1406; **IR** (Neat, cm^{-1}): 1699, 1675.

11. **3-(1-Methyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)-1-phenylpyrrolidine-2,5-dione (3ac)**



Yield - 50 mg (62%), as a light yellow solid; **mp** – 146 – 148 °C;**R_f**- (70% DCM/Hexane) 0.2;**^{1}H NMR** (400 MHz, $CDCl_3$) δ8.05 (s., 1 H), 7.51 - 7.47 (m, 2 H), 7.43 - 7.33 (m, 5 H), 7.20 (d, *J* = 7.3 Hz, 1 H), 6.12 - 6.08 (m, 1 H), 3.85 (s, 3 H), 3.55 (dd, *J* = 9.9, 18.7 Hz, 1 H), 2.85 (dd, *J* = 4.5, 17.9 Hz, 1 H); **$^{13}C\{^{1}H\}$ NMR** (100 MHz, $CDCl_3$) δ177.9, 175.4, 174.3(q, *J* = 34 Hz), 141.3, 138.6, 133.4, 132.1, 129.1, 128.5, 126.6, 125.8, 125.4, 122.2, 117.5(q, *J* = 290 Hz), 110.0, 109.7, 44.8, 39.3, 34.2; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -69.677; **HRMS (ESI-TOF)** *(m/z)***–**Calculated for $C_{21}H_{15}F_3N_2O_3$ $(M+Na)^+$: 423.0932, found $(M+Na)^+$: 423.0930; **IR** (Neat, cm^{-1}): 1710, 1668.

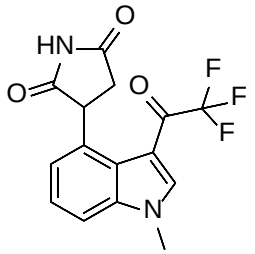
12. **1-Benzyl-3-(1-methyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)pyrrolidine-2,5-dione (3ad)**



Yield - 62 mg (75%), as a light yellow solid; **mp** – 80 – 82 °C;**R_f**- (70% DCM/Hexane) 0.3;**^{1}H NMR** (400 MHz, $CDCl_3$) δ8.04 (d,*J* = 1.2 Hz, 1 H), 7.44 (d, *J*

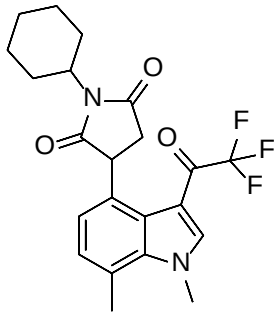
= 6.8 Hz, 2 H), 7.36 - 7.30 (m, 5 H), 6.94 (d, *J* = 4.8 Hz, 1 H), 5.88 (br, s, 1 H), 4.77 (d, *J* = 2.0 Hz, 2 H), 3.88 (s, 3 H), 3.38 (dd, *J* = 9.6, 18.4 Hz, 1 H), 2.67 (dd, *J* = 4.5, 18.7 Hz, 1 H); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ178.6, 176.1, 174.2 (q, *J* = 34 Hz), 141.2, 138.6, 135.9, 133.5, 128.68, 128.64, 127.8, 125.7, 125.4, 122.2, 117.5(q, *J* = 290 Hz), 109.8, 109.7, 44.7, 42.5, 39.3, 34.2; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -69.718 ; **HRMS (ESI-TOF)** *(m/z)***–**Calculated for $C_{22}H_{17}ClF_3N_2O_3$ $(M+Na)^+$: 437.1089, found $(M+Na)^+$: 437.1087; **IR** (Neat, cm^{-1}): 1706, 1672.

13. **3-(1-methyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)pyrrolidine-2,5-dione (3ae)**



Yield - 44 mg (65%), as a yellow solid; **mp-** 202–206 °C;**R_f-** (25% EtOAc/Hexane) 0.1; **^{1}H NMR** (400 MHz, DMSO-d_6) δ11.36 (s, 1H), 8.65 (s, 1H), 7.61(d, *J* = 8.14 Hz, 1H) 7.44 (t, *J* = 7.71 Hz, 1H), 7.20 (d, *J* = 7.28 Hz, 1H), 5.70 (s, 1H), 3.97 (s, 3H), 3.19 (dd, , *J* = 8.67 Hz, 1H), 2.70 (dd, *J* = 5.34 Hz, 1H); **^{13}C{^{1}H} NMR** (100 MHz, DMSO-d_6) δ179.9, 177.6, 172.7 (t, *J* = 33.6 Hz), 143.1, 138.6, 132.9, 125.0, 122.2, 117.4 (q, *J* = 291 Hz), 110.8, 108.3, 45.3, 33.9. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -66.808; **HRMS (ESI-TOF)** *(m/z)***–**Calculated for $C_{15}H_{11}F_3N_2O_3$ $(M+Na)^+$: 325.0800, found $(M+Na)^+$: 325.0799; **IR** (Neat, cm^{-1}): 1710, 1670.

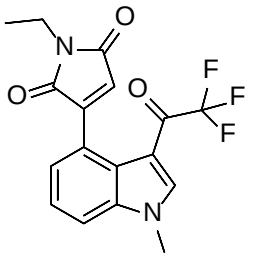
14. **1-Cyclohexyl-3-(1,7-dimethyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)pyrrolidine-2,5-dione (3db)**



Yield - 55 mg (65%), as a light brown solid; **mp** – 173 – 175 °C;**R_f-** (70% DCM/Hexane) 0.3;**^{1}H NMR** (400 MHz, $CDCl_3$) δ7.93 (s, 1 H), 7.07 (d, *J* = 7.6 Hz, 1 H), 6.85 (d, *J* = 7.8 Hz, 1 H), 5.67 (dd, *J* = 4.4, 9.2 Hz, 1 H), 4.16 (s, 3 H), 4.11 - 4.03

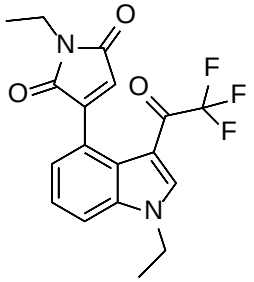
(m, 1 H), 3.29 (dd, *J* = 9.6, 18.4 Hz, 1 H), 2.75 (s, 3 H), 2.56 (dd, *J* = 4.2, 18.3 Hz, 1 H), 2.23 (q, *J* = 12.5 Hz, 2 H), 1.67 (d, *J* = 11.1 Hz, 4 H), 1.41 - 1.17 (m, 4 H); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ179.2, 176.8, 174.1(q, *J* = 34 Hz), 142.95, 142.91, 137.3, 132.0, 128.4, 126.9, 122.0, 121.6, 117.5(d, *J* = 290 Hz), 109.3, 51.8, 44.0 , 39.2, 38.8, 28.7, 25.8, 25.0, 19.5; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -69.541 ; **HRMS (ESI-TOF)** *(m/z)***–**Calculated for $C_{22}H_{23}F_3N_2O_3(M+Na)^+$: 443.1558, found $(M+Na)^+$: 443.1560; **IR** (Neat, cm^{-1}): 1660, 1693.

15. **1-Ethyl-3-(1-methyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)-1H-pyrrole-2,5-dione(4aa)**



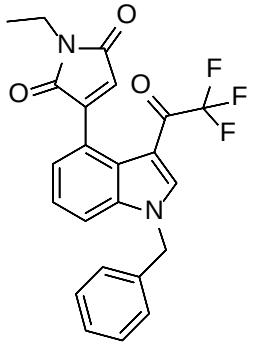
Yield - 53 mg (75%), as a yellow solid; **mp** – 156 – 158 °C;**R_f**- (70% DCM/Hexane) 0.4; **^{1}H NMR** (400 MHz, $CDCl_3$) δ8.00 (d, *J* = 1.8 Hz, 1 H), 7.50 (dd, *J* = 1.0, 8.3 Hz, 1 H), 7.44 (t, *J* = 7.8 Hz, 1 H), 7.28 - 7.26 (q, 1 H), 6.47 (s, 1 H), 3.93 (s, 3 H), 3.64 (q, *J* = 7.3 Hz, 2 H), 1.25 (t,*J* = 7.5 Hz 3 H); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ174.0(q, *J* = 35 Hz), 171.0, 170.7, 149.0, 139.87 (q, *J* = 5.0 Hz), 138.1, 125.7, 124.59, 124.53, 124.1, 123.8, 117.1 (q, *J* = 290 Hz), 112.1, 110.2, 34.2, 32.9, 13.6; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -71.385; **HRMS (ESI-TOF)** *(m/z)***–**Calculated for $C_{17}H_{13}F_3N_2O_3(M+Na)^+$: 373.0776, found $(M+Na)^+$: 373.0778;**IR** (Neat, cm^{-1}): 1705, 1675;

16. **1-Ethyl-3-(1-ethyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)-1H-pyrrole-2,5-dione(4ba)**



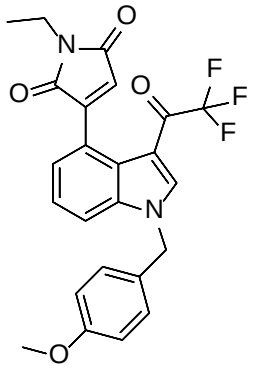
Yield - 50 mg (68%), as a yellow solid; **mp** – 164 – 166 °C; **R_f**- (70% DCM/Hexane) 0.4;**^{1}H NMR** (400 MHz, $CDCl_3$) δ8.04 (s., 1 H), 7.52 (d, *J* = 8.3 Hz, 1 H), 7.42 (t, *J* = 7.8 Hz, 1 H), 7.26 (d, *J* = 1.8 Hz, 1 H), 6.45 (s, 1 H), 4.32 - 4.26 (q, 2 H), 3.66 - 3.61 (m, 2 H), 1.61 - 1.57 (m, 3 H), 1.25 (t, *J* = 7.2 Hz 3 H); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ174.0(q, *J* = 34 Hz), 171.0 ,170.0, 149.1, 138.22(q, *J* = 5.2 Hz), 137.2, 125.6, 124.7, 124.4, 124.2, 123.8, 117.1(q, *J* = 290 Hz), 112.2, 110.2, 42.5, 32.9, 14.8, 13.5; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -71.311; **HRMS (ESI-TOF)** *(m/z)***–** Calculated for $C_{18}H_{15}F_3N_2O_3(M+Na)^+$: 387.0932, found $(M+Na)^+$: 387.0933; **IR** (Neat, cm^{-1}): 1707, 1676.

17. **3-(1-Benzyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)-1-ethyl-1H-pyrrole-2,5-dione(4ca)**



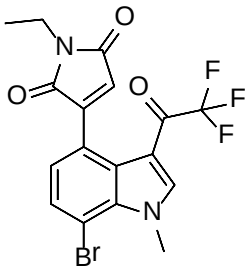
Yield - 50 mg (68%), as a yellow solid; **mp** – 122 – 124 °C; **R_f**- (70% DCM/Hexane) 0.4;**^{1}H NMR** (400 MHz, $CDCl_3$) δ8.05 (s, 1 H), 7.43 (d, *J* = 8.3 Hz, 1 H), 7.38 - 7.34 (q, 4 H), 7.24 (br. s., 1 H), 7.19 (d, *J* = 6.1 Hz, 2 H), 6.46 (s, 1 H), 5.42 (s, 2 H), 3.64 (q, *J* = 7.2 Hz, 2 H), 1.25 (t,*J* = 7.3 Hz 3 H); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ174.2(q, *J* = 34 Hz), 171.0, 170.7, 149.0, 139.22 (q, *J* = 5.3 Hz), 137.6, 134.1, 129.2, 128.6, 126.9, 125.8, 124.7, 124.6, 124.2, 123.9, 117.1 (q, *J* = 290 Hz), 112.8, 110.6, 51.5, 32.9, 13.5; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -71.424; **HRMS (ESI-TOF)** *(m/z)***–** Calculated for $C_{23}H_{17}F_3N_2O_3$ $(M+Na)^+$: 449.1089, found $(M+Na)^+$: 449.1089; **IR** (Neat, cm^{-1}): 1705, 1680.

1-Ethyl-3-(1-(4-methoxybenzyl)-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)-1H-pyrrole-2,5-dione (4da)



Yield - 65 mg (72%), as a yellow solid; **mp** – 130 – 132 °C;**R_f**- (70% DCM/Hexane) 0.3; **^{1}H NMR** (400 MHz, $CDCl_3$) δ8.00 (s, 1 H), 7.45 (d, *J* = 8.26 Hz 1 H), 7.35 (t, *J* = 7.8 Hz, 1 H), 7.24 (d, *J* = 7.3 Hz, 1 H), 7.15 (d , *J* = 8.6 Hz, 2 H), 6.90 (d, *J* = 8.55 Hz, 2 H), 6.45 (s, 1 H), 5.32 (s, 2 H), 3.79 (s, 3 H), 3.63 (q, *J* = 7.1 Hz, 2 H), 1.25 (t, *J* = 7.4 Hz 3 H); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ174.2(q, *J* = 35 Hz), 171.0, 170.7, 159.9, 149.0, 138.96(q, *J* = 5.3 Hz), 137.6, 128.7, 125.9, 125.7, 124.8, 124.5, 124.2, 123.9, 117.0(q, *J* = 290 Hz), 114.6, 112.8, 110.5, 55.3, 51.1, 32.9, 13.5; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -71.492; **HRMS (ESI-TOF)** *(m/z)***–**Calculated for $C_{24}H_{19}F_3N_2O_4$ $(M+Na)^+$: 479.1195, found $(M+Na)^+$: 479.1194; **IR** (Neat, cm^{-1}): 1702, 1671;

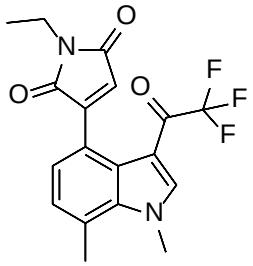
18. **3-(7-Bromo-1-methyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)-1-ethyl-1H-pyrrole-2,5-dione (4ea)**



Yield - 64 mg (75%), as a bright yellow solid; **mp** – 211 – 213 °C;**R_f**- (70% DCM/Hexane) 0.4;**^{1}H NMR** (400 MHz, $CDCl_3$) δ7.95 (s, 1 H), 7.56 (d, *J* = 8.1 Hz, 1 H), 7.06 (d, *J* = 8.1 Hz, 1 H), 6.46 (s, 1 H), 4.30 (s, 3 H), 3.62 (q, *J* = 7.1 Hz, 2 H), 1.24 (t, *J* = 7.2 Hz, 3 H); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ174.1(q, *J* = 35 Hz), 170.8, 170.4, 148.3, 142.42(q, *J* = 5. 2 Hz), 134.8, 129.8, 127.3, 126.6, 123.7, 123.5, 116.9(q, *J* = 290 Hz), 109.7, 107.1, 39.1, 32.9, 13.5; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -

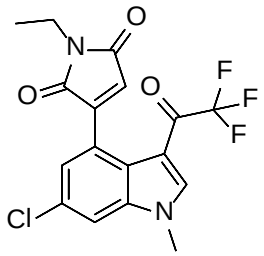
71.570; **HRMS (ESI-TOF)** *(m/z)***–**Calculated for $C_{17}H_{12}BrF_3N_2O_3$ $(M+Na)^+$: 450.9881, found $(M+Na)^+$: 450.9878; **IR** (Neat, cm^{-1}): 1707, 1678.

19. **3-(1,7-Dimethyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)-1-ethyl-1H-pyrrole-2,5-dione (4fa)**



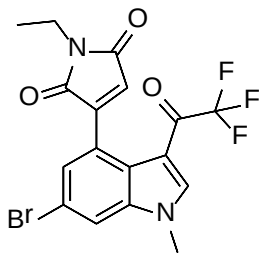
Yield - 48 mg (65%), as a yellow solid; **mp** – 206 – 208 °C;**R_f**- (70% DCM/Hexane) 0.5;**^{1}H NMR** (400 MHz, $CDCl_3$) δ7.88 (s., 1 H), 7.12 (s, 2 H), 6.41 (s, 1 H), 4.18 (s, 3 H), 3.62 (q, *J* = 6.7 Hz, 2 H), 2.81 (s, 3 H), 1.24 (t,*J* = 7.2 Hz 3 H); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ173.7(q, *J* = 30 Hz), 171.2, 170.7, 149.3, 141.42(q, *J* = 5. 2 Hz), 136.9, 127.4, 126.0, 125.5, 124.6, 122.9, 122.1, 117.1(t, *J* = 290 Hz), 109.7, 38.6, 32.8, 19.7, 13.5; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -71.288; **HRMS (ESI-TOF)** *(m/z)***–** Calculated for $C_{18}H_{15}F_3N_2O_3$ $(M+Na)^+$: 387.0932, found $(M+Na)^+$: 387.0935; **IR** (Neat, cm^{-1}): 1709, 1668.

20. **3-(6-Chloro-1-methyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)-1-ethyl-1H-pyrrole-2,5-dione (4ga)**



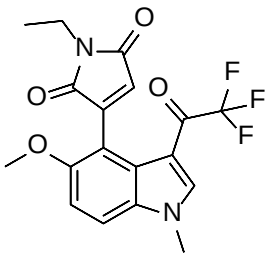
Yield - 43 mg (55%), as a light brown solid; **mp** – 187 – 189 °C;**R_f**- (70% DCM/Hexane) 0.5;**^{1}H NMR** (400 MHz, $CDCl_3$) δ7.99 (s, 1 H), 7.48 (d, *J* = 1.8 Hz, 1 H), 7.27 - 7.25 (d,, *J* = 1.6 Hz 1 H), 6.49 (s, 1 H), 3.90 (s, 3 H), 3.64 (q, *J* = 7.2 Hz, 2 H), 1.25 (t,*J* = 7.2 Hz 3 H); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ174.0 (d, *J* = 34 Hz), 170.5, 170.3, 147.7, 140.26(q, *J* = 5. 2 Hz), 138.7, 130.5, 125.8, 125.2, 124.7, 123.1, 117.0(d, *J* = 290 Hz), 112.0, 110.4, 34.3, 33.0, 13.5; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -71.577; **HRMS (ESI-TOF)** *(m/z)***–**Calculated for $C_{17}H_{12}ClF_3N_2O_3$ $(M+Na)^+$: 407.0386, found $(M+Na)^+$: 407.0388; **IR** (Neat, cm^{-1}): 1705, 1665.

21. **3-(6-bromo-1-methyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)-1-ethyl-1H-pyrrole-2,5-dione (4ha)**



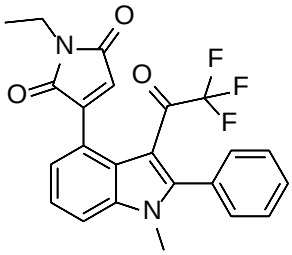
Yield - 47 mg (55%), as a yellow solid; **mp**: 186 – 188 °C;**R_f**- (70% DCM/Hexane) 0.3;**^{1}H NMR** (400 MHz, $CDCl_3$) δ7.97 (s, 1 H), 7.64 (d,*J* = 1.6 Hz 1 H), 7.39 (d,*J* = 1.2 Hz 1 H), 6.48 (s, 1 H), 3.90 (s, 3 H), 3.64 (q, *J* = 7.3 Hz, 2 H), 1.25 (t, *J* = 7.2 Hz, 3 H); **^{13}C{^{1}H} NMR**(100 MHz, $CDCl_3$) δ174.0(q, *J* = 34 Hz), 170.5, 170.3, 147.6 , 140.14(q, *J* = 5. 1 Hz), 138.8, 128.3, 125.4, 124.6, 123.5, 117.7 ,116.9(q, *J* = 290 Hz), 115.0, 110.3, 34.2, 33.0, 13.5; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -71.584; **HRMS (ESI-TOF)** *(m/z)***–**Calculated for $C_{17}H_{12}BrF_3N_2O_3$ $(M+Na)^+$: 450.9881, found $(M+Na)^+$: 449.1087; **IR** (Neat, cm^{-1}): 1704, 1679.

22. **1-Ethyl-3-(5-methoxy-1-methyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)-1H-pyrrole-2,5-dione (4ia)**



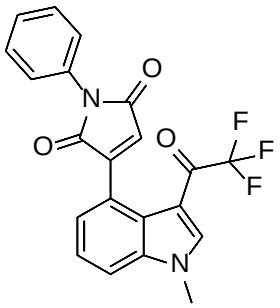
Yield - 38 mg (50%), as a brown solid; **mp** – 156 – 158 °C;**R_f**- (70% DCM/Hexane) 0.2;**^{1}H NMR** (400 MHz, $CDCl_3$) δ7.92 (s, 1 H), 7.39 (d, *J* = 9.1 Hz, 1 H), 7.09 (d, *J* = 8.8 Hz, 1 H), 6.52 (s, 1 H), 3.87 (s, 3 H), 3.84 (s, 3 H), 3.64 (q, *J* = 7.2 Hz, 2 H), 1.26 (s, *J* = 7.2 Hz 3 H); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ173.4(t, *J* = 34 Hz), 171.6, 171.2, 154.9, 142.9, 140.28(q, *J* = 5. 3 Hz), 133.0, 127.4, 126.4 , 118.6(t, *J* = 290 Hz), 112.4, 111.2, 110.0, 109.8, 56.9, 34.1, 32.8, 13.5; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -71.133; **HRMS (ESI-TOF)** *(m/z)***–**Calculated for $C_{18}H_{15}F_3N_2O_4(M+Na)^+$: 403.0882, found $(M+Na)^+$: 403.0883; **IR** (Neat, cm^{-1}): 1702, 1673.

23. **1-Ethyl-3-(1-methyl-2-phenyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)-1H-pyrrole-2,5-dione (4ja)**



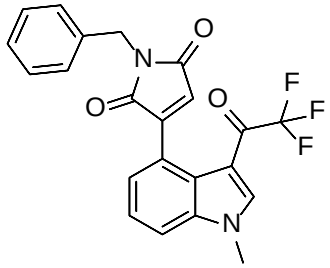
Yield - 43 mg (51%), as a yellow solid; **mp** – 218 – 220 °C; **R_f**- (70% DCM/Hexane) 0.5;**^{1}H NMR** (400 MHz, $CDCl_3$) δ7.55 - 7.50 (m, 4 H), 7.44 - 7.37 (m, 3 H), 7.28 (d, *J* = 7.3 Hz, 1 H), 6.52 (s, 1 H), 3.60 - 3.55 (m, 2 H), 3.55 (s, 3 H), 1.21 (t, *J* = 7.2 Hz, 3 H); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 180.2(q, *J* = 34 Hz), 170.9, 170.5, 148.5, 147.5, 137.6 ,130.6, 130.1, 129.3, 128.2, 125.6, 124.6 ,123.9, 123.6, 118.6(q, *J* = 290 Hz), 112.4, 111.3, 111.1, 32.8, 31.2, 13.5; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -71.809; **HRMS (ESI-TOF)** *(m/z)***–**Calculated for $C_{24}H_{19}F_3N_2O_3$ $(M+Na)^+$: 449.1089, found $(M+Na)^+$: 449.1087; **IR** (Neat, cm^{-1}): 1704, 1669.

24. **3-(1-Methyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)-1-phenyl-1H-pyrrole-2,5-dione (4ab)**



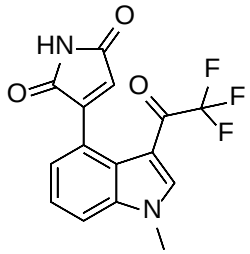
Yield - 50 mg (63%), as a bright yellow solid; **mp** – 177 – 179 °C;**R_f**- (70% DCM/Hexane) 0.3;**^{1}H NMR** (400 MHz, $CDCl_3$) δ8.00 (s, 1 H), 7.50 - 7.42 (m, 6 H), 7.35 (d, *J* = 5.8 Hz, 2 H), 6.62 (s, 1 H), 3.88 (s, 3 H); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ174.0(t, *J* = 34 Hz), 169.9, 169.7, 140.15(q, *J* = 5.3 Hz), 140.0, 138.1, 132.0, 128.9, 127.6, 126.5, 125.8, 124.66, 124.62, 124.0, 123.9, 117.2(q, *J* = 290 Hz), 112.4, 110.1, 34.2; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -71.153; **HRMS (ESI-TOF)** *(m/z)***–**Calculated for $C_{21}H_{13}F_3N_2O_3$ $(M+Na)^+$: 421.0776, found $(M+Na)^+$: 421.0778; **IR** (Neat, cm^{-1}): 1713, 1671.

25. **1-Benzyl-3-(1-methyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)-1H-pyrrole-2,5-dione (4ac)**



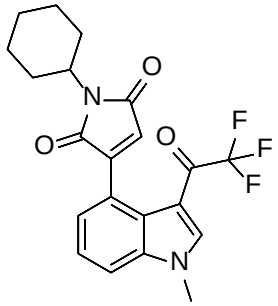
Yield - 49 mg (60%), as a yellow solid; **mp** – 195 – 197 °C;**R_f**- (70% DCM/Hexane) 0.4; **^{1}H NMR** (400 MHz, $CDCl_3$) δ7.99 (s, 1 H), 7.50 - 7.40 (m, 4 H), 7.31 (t, *J* = 7.5 Hz2 H), 7.27 - 7.25 (m, 2 H), 6.49 (s, 1 H), 4.75 (s, 2 H), 3.90 (s, 3 H); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ173.9(q, *J* = 30 Hz), 170.8, 170.5, 149.2, 139.88(d, *J* = 5.2 Hz), 138.1, 136.4, 128.4, 128.2, 127.4, 125.9, 124.6, 124.5, 124.0, 123.7, 117.1(q, *J* = 290 Hz), 112.2, 110.1, 41.6, 34.2; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -71.295; **HRMS (ESI-TOF)** *(m/z)***–**Calculated for $C_{22}H_{15}F_3N_2O_3$ $(M+Na)^+$: 435.0932, found $(M+Na)^+$: 435.0931; **IR** (Neat, cm^{-1}): 1708, 1673.

26. **3-(1-methyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)-1H-pyrrole-2,5-dione (4ad)**



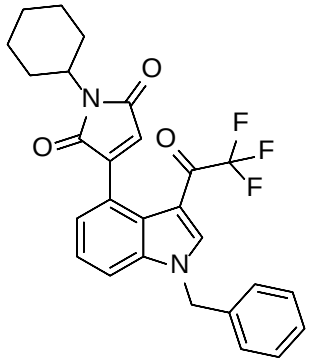
Yield - 50 mg (76%), as a yellow solid; **mp** – (semi solid at RT);**R_f**- (25% EtOAc/Hexane) 0.2;**^{1}H NMR** (400 MHz, DMSO-d_6) δ10.86 (br. s., 1 H), 8.62 (s., 1 H), 7.78 (d, *J* = 8.3 Hz, 1 H), 7.48 (t, *J* = 7.7 Hz, 1 H), 7.32 (d, *J* = 7.3 Hz, 1 H), 6.68 (s, 1 H), 3.99 (s, 3 H); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ173.8 - 172.8 (m), 150.5, 142.89(d, *J* = 2.1 Hz), 138.9, 126.7, 125.6, 125.2, 124.4, 124.0 , 117.8(q, *J* = 166 Hz), 114.1, 109.4, 34.7; **^{19}F NMR** (376 MHz, DMSO-d_6) δ -66.664; **HRMS (ESI-TOF)** *(m/z)***–**Calculated for $C_{15}H_9F_3N_2O_3$ $(M+Na)^+$: 345.0463, found $(M+Na)^+$: 345.0465; **IR** (Neat, cm^{-1}): 3419, 1719, 1647.

27. **1-Cyclohexyl-3-(1-methyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)-1H-pyrrole-2,5-dione(4ae)**



Yield - 60 mg (74%), as a yellow solid; **mp** – 201 – 203 °C;**R_f**- (70% DCM/Hexane) 0.5;**^{1}H NMR** (400 MHz, $CDCl_3$) δ7.98 (s, 1 H), 7.48 (d, *J* = 8.1 Hz, 1 H), 7.43 (t, *J* = 7.8 Hz, 1 H), 7.27 - 7.25 (m, 1 H), 6.41 (s, 1 H), 4.01 - 3.93 (m, 1 H), 3.91 (s, 3 H), 2.15 - 2.03 (m, 2 H), 1.87 - 1.78 (m, 4 H), 1.38 - 1.22 (m, 4 H); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ 173.9(q, *J* = 34 Hz), 171.3, 170.8, 148.5, 139.71(d, *J* = 5.2 Hz), 138.0, 125.6, 124.56, 124.51, 124.2, 123.6, 117.1(q, *J* = 290 Hz), 112.0, 110.2, 50.8, 34.1, 29.7, 26.0 , 25.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -71.411; **HRMS (ESI-TOF)** *(m/z)***–**Calculated for $C_{21}H_{19}F_3N_2O_3$ $(M+Na)^+$: 427.1245, found $(M+Na)^+$: 427.1241; **IR** (Neat, cm^{-1}): 1702, 1676.

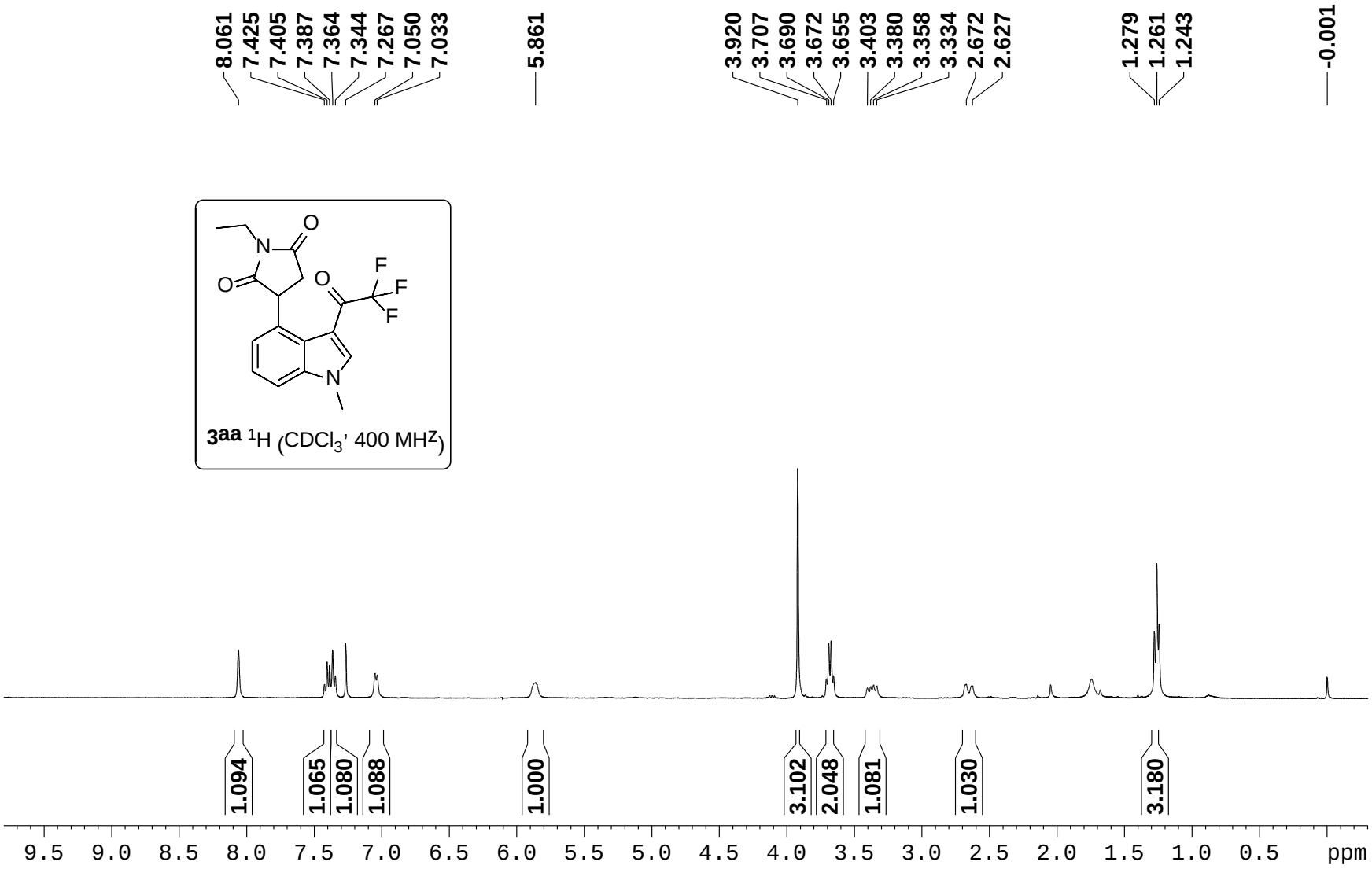
28. **3-(1-Benzyl-3-(2,2,2-trifluoroacetyl)-1H-indol-4-yl)-1-cyclohexyl-1H-pyrrole-2,5-dione (4ce)**

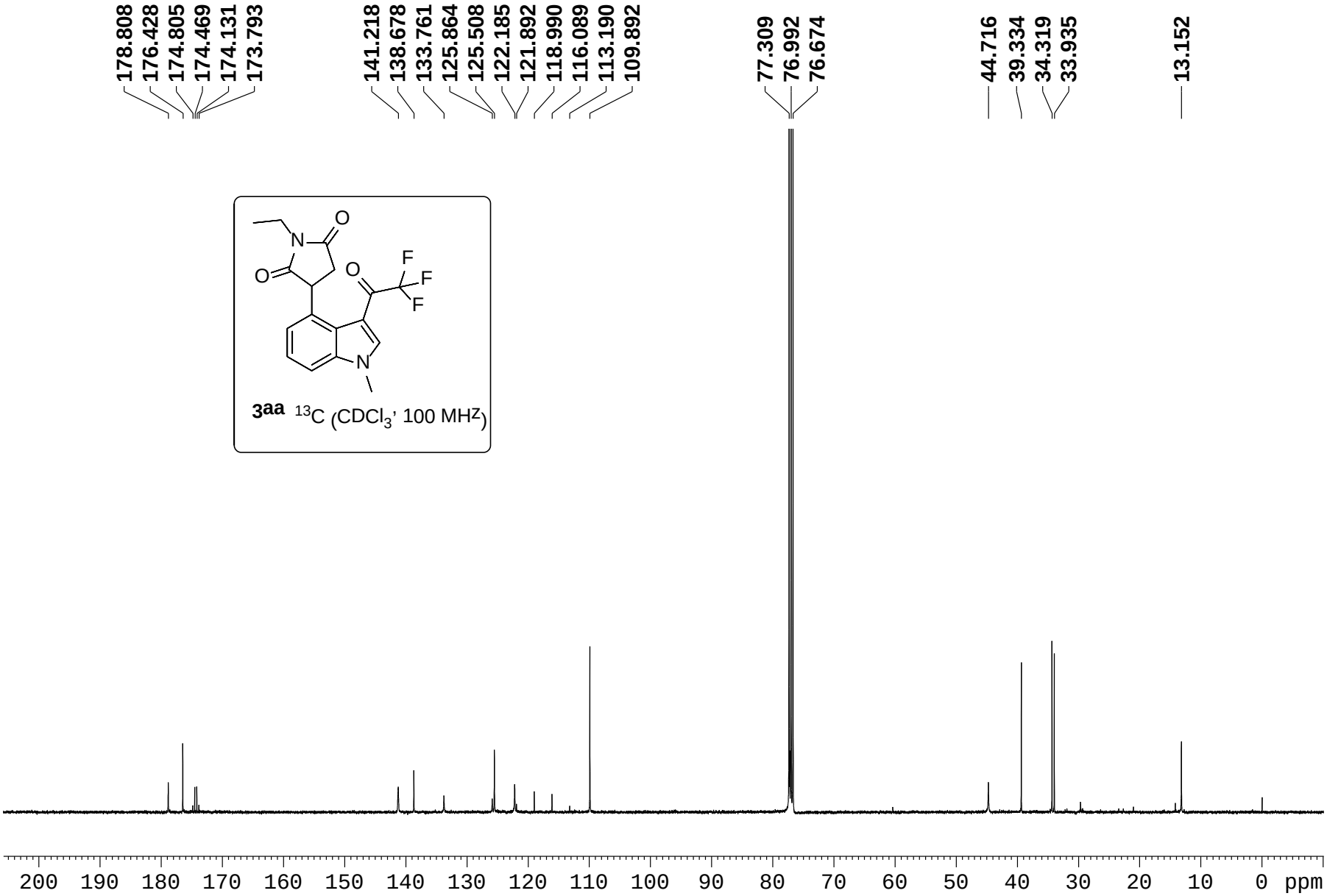


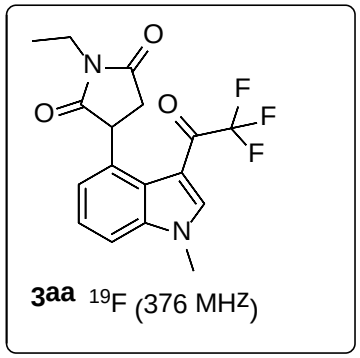
Yield - 55 mg (64 %), as a yellow solid; **mp** – 243 - 245 °C. **R_f**- (70% DCM/Hexane) 0.4;**^{1}H NMR** (400 MHz, $CDCl_3$) δ8.04 (s, 1 H), 7.42 - 7.32 (m, 5 H), 7.24 (d, *J* = 7.3 Hz, 1 H), 7.17 (d, *J* = 6.8 Hz, 2 H), 6.41 (s, 1 H), 5.39 (s, 2 H), 3.98 (q, 1 H), 2.09 (q, *J* = 12.0 Hz, 2 H), 1.81 (br. s., 4 H), 1.37 - 1.19 (m, 4 H); **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$) δ174.2(q, *J* = 30 Hz), 171.2, 170.8, 148.5, 139.11(d, *J* = 5.2 Hz), 137.5, 134.2, 129.2, 128.6, 126.9 ,125.7, 124.8, 124.5, 124.3, 123.7 , 117.0(q, *J* = 290 Hz),

110.6, 51.4, 50.8, 29.7, 26.0, 25.1; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -71.461; **HRMS (ESI-TOF)** *(m/z)*–Calculated for $C_{27}H_{23}F_3N_2O_3$ $(M+Na)^+$: 503.1558, found $(M+Na)^+$: 503.1555; **IR** (Neat, cm^{-1}): 1700, 1676.

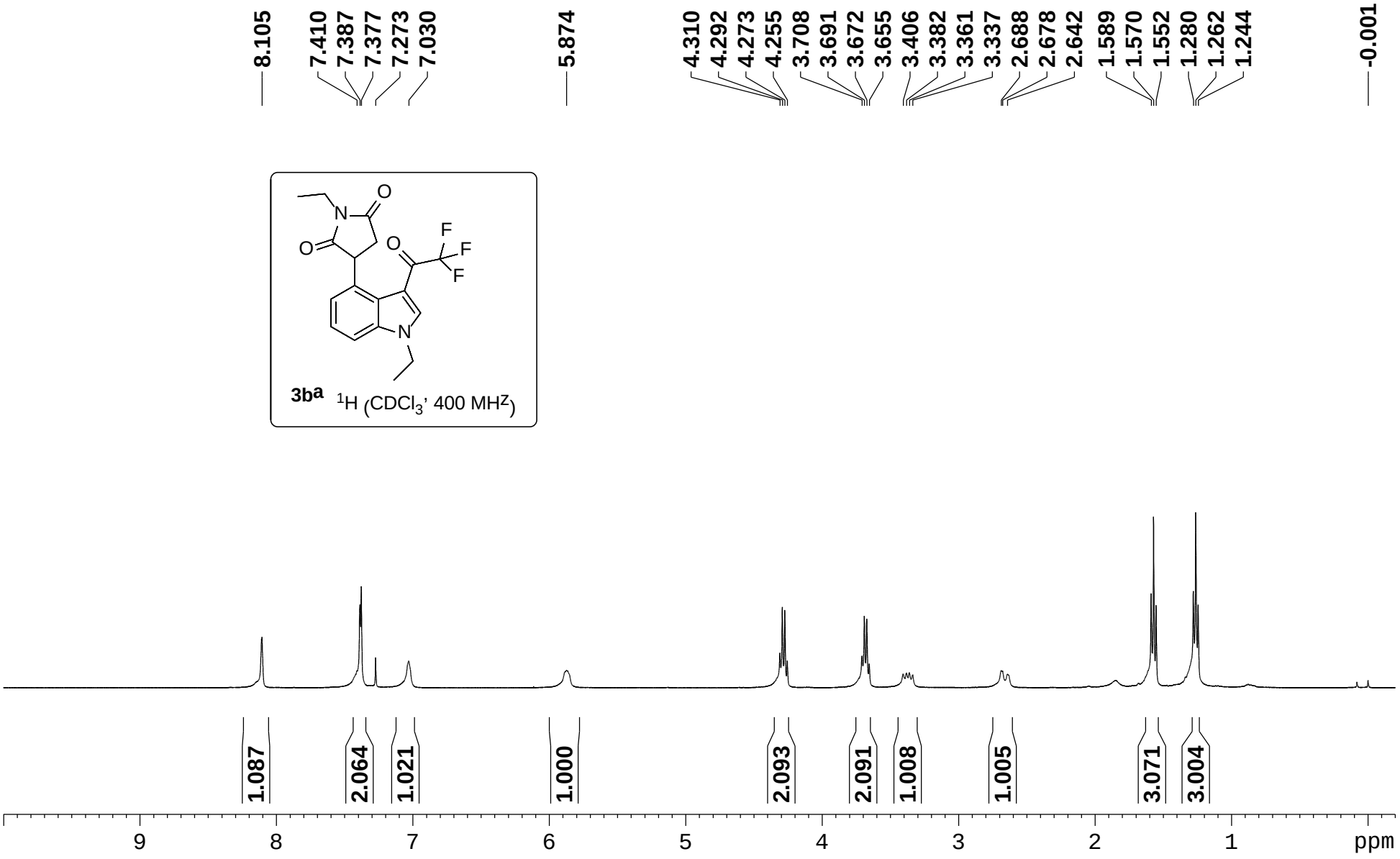
Copies of ^{1}H and ^{13}C NMR



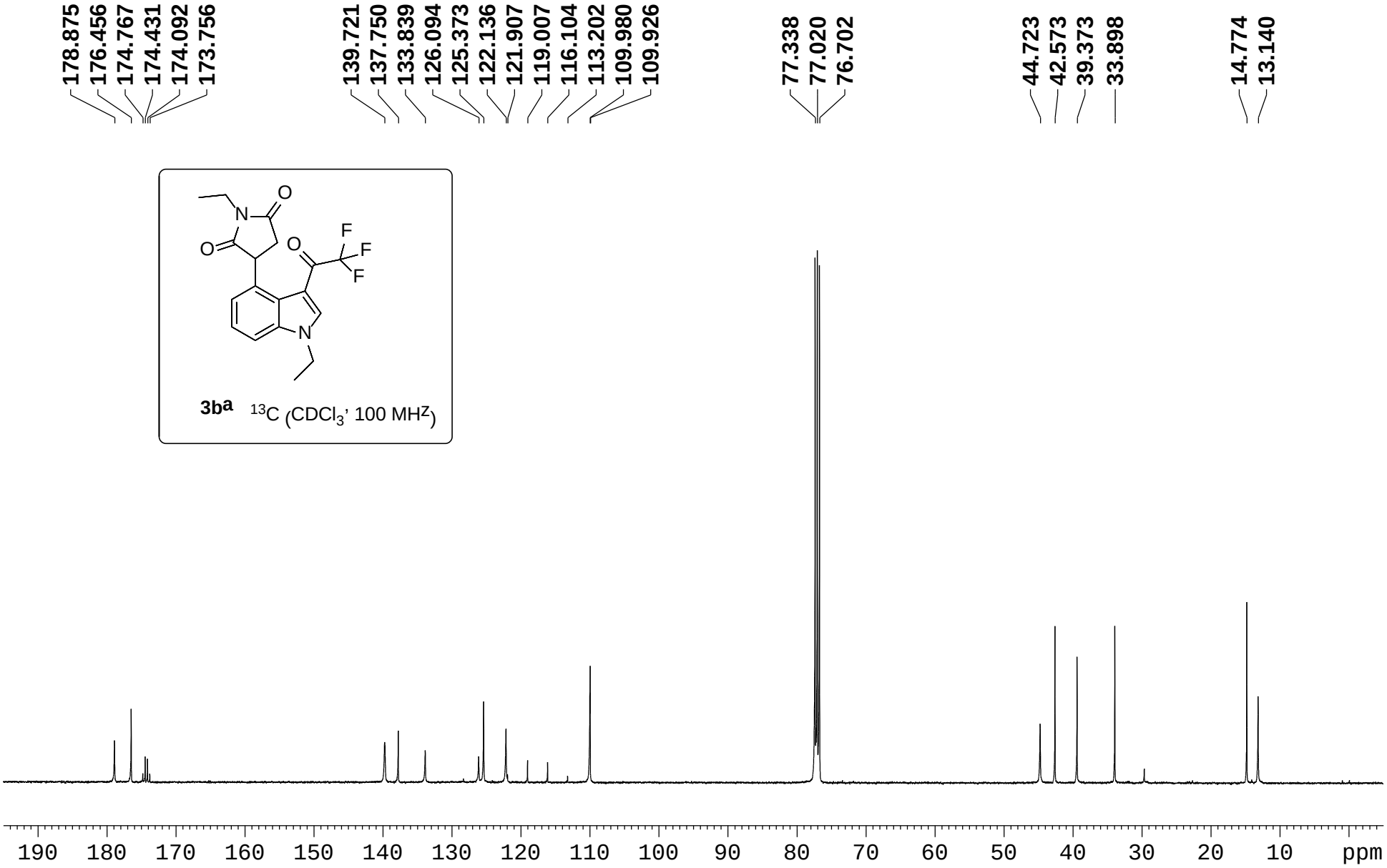

178.808
176.428
174.805
174.469
174.131
173.793
141.218
138.678
133.761
125.864
125.508
122.185
121.892
118.990
116.089
113.190
109.892
77.309
76.992
76.674
44.716
39.334
34.319
33.935
13.152
O
N
O
O
F
F
F
N
3aa 13C (CDCl3, 100 MHz)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

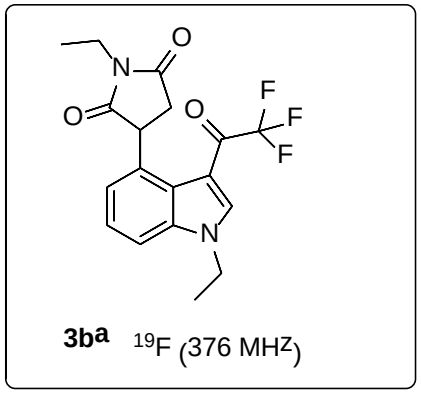


3aa ^{19}F (376 MHz)

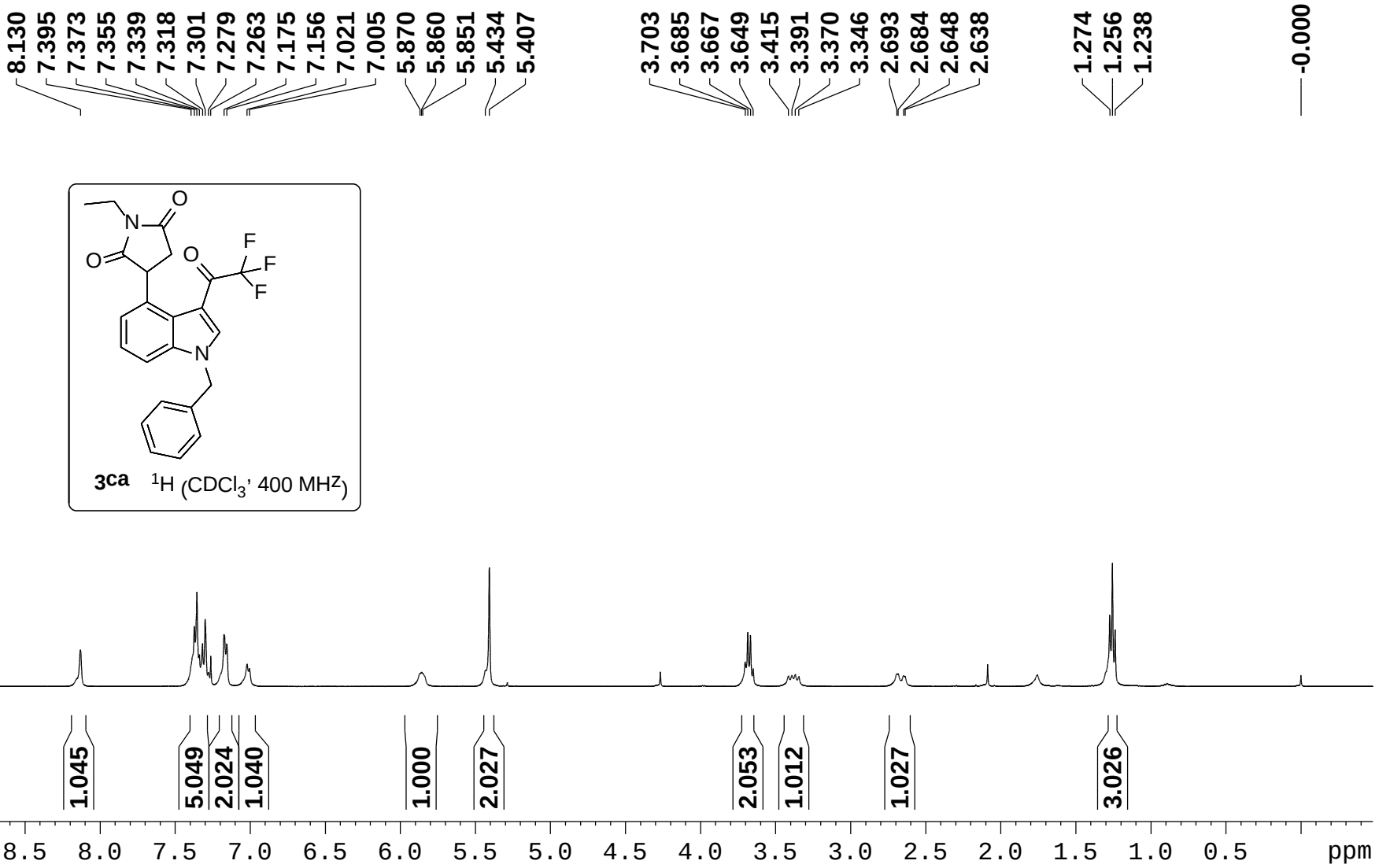


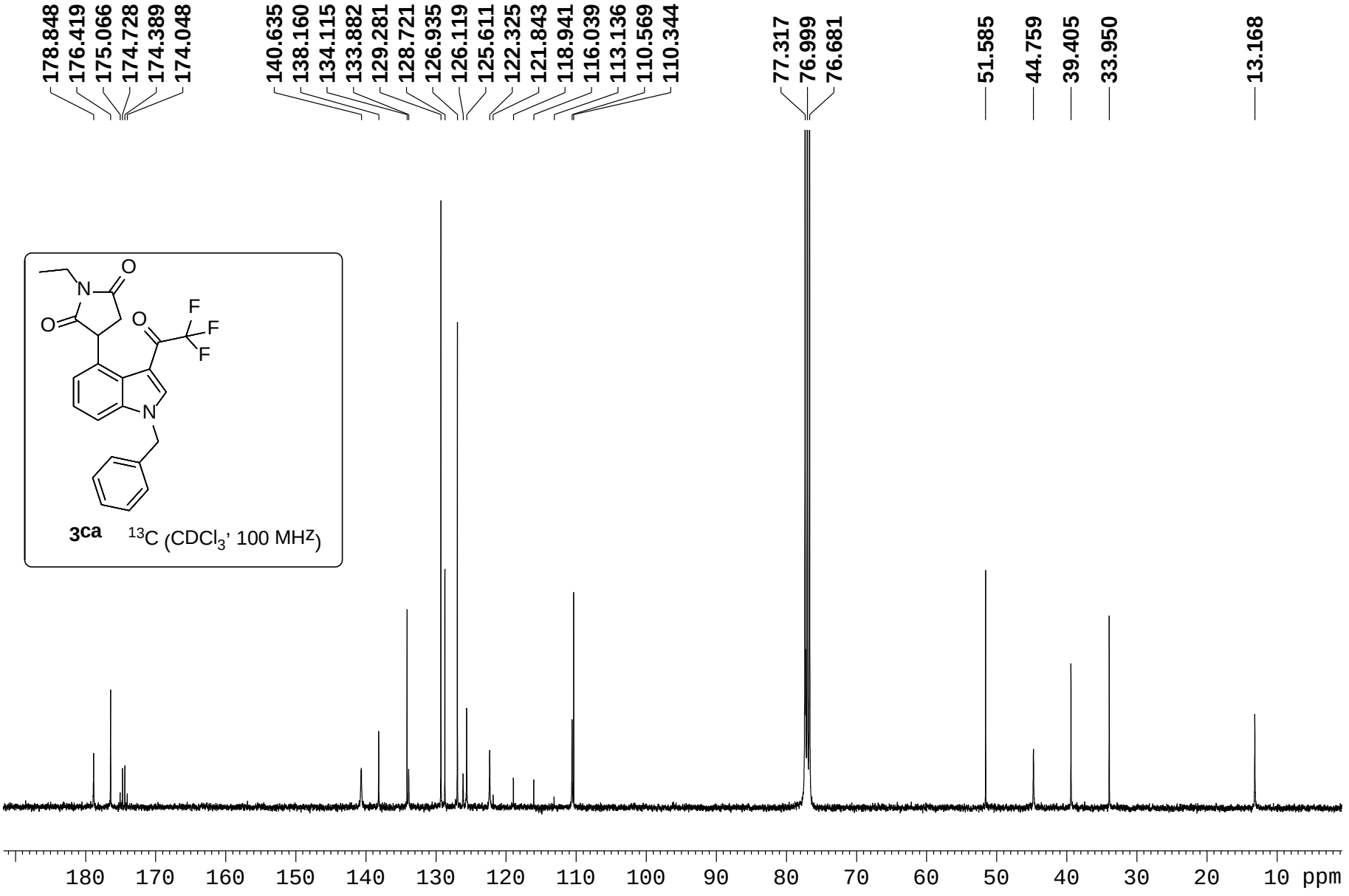
3b[a] ^{1}H ($CDCl_3$, 400 MH^z)

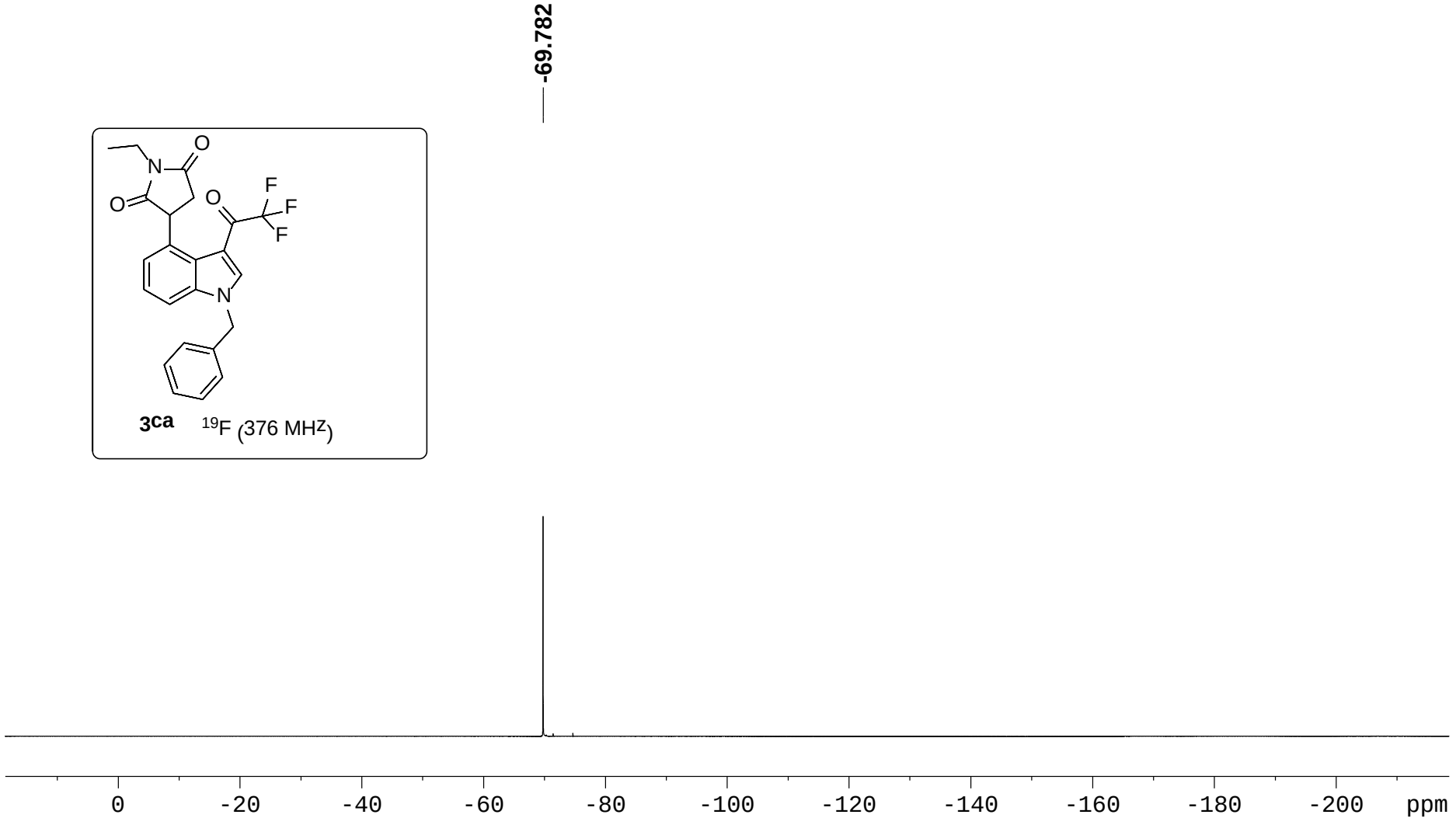

178.875
176.456
174.767
174.431
174.092
173.756
139.721
137.750
133.839
126.094
125.373
122.136
121.907
119.007
116.104
113.202
109.980
109.926
77.338
77.020
76.702
44.723
42.573
39.373
33.898
14.774
13.140
O
N
O
O
F
F
F
N
3ba 13C (CDCl3, 100 MHz)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

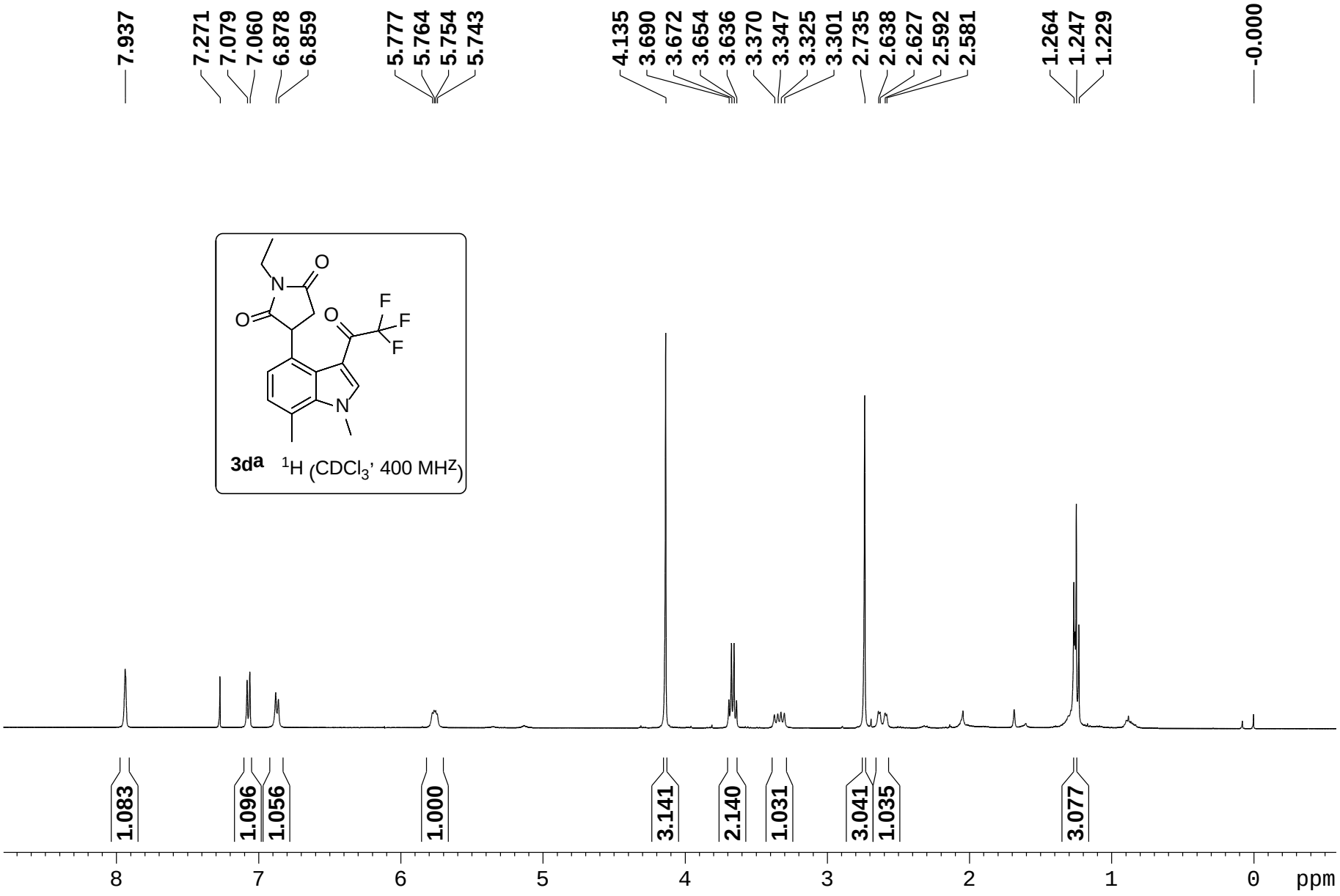


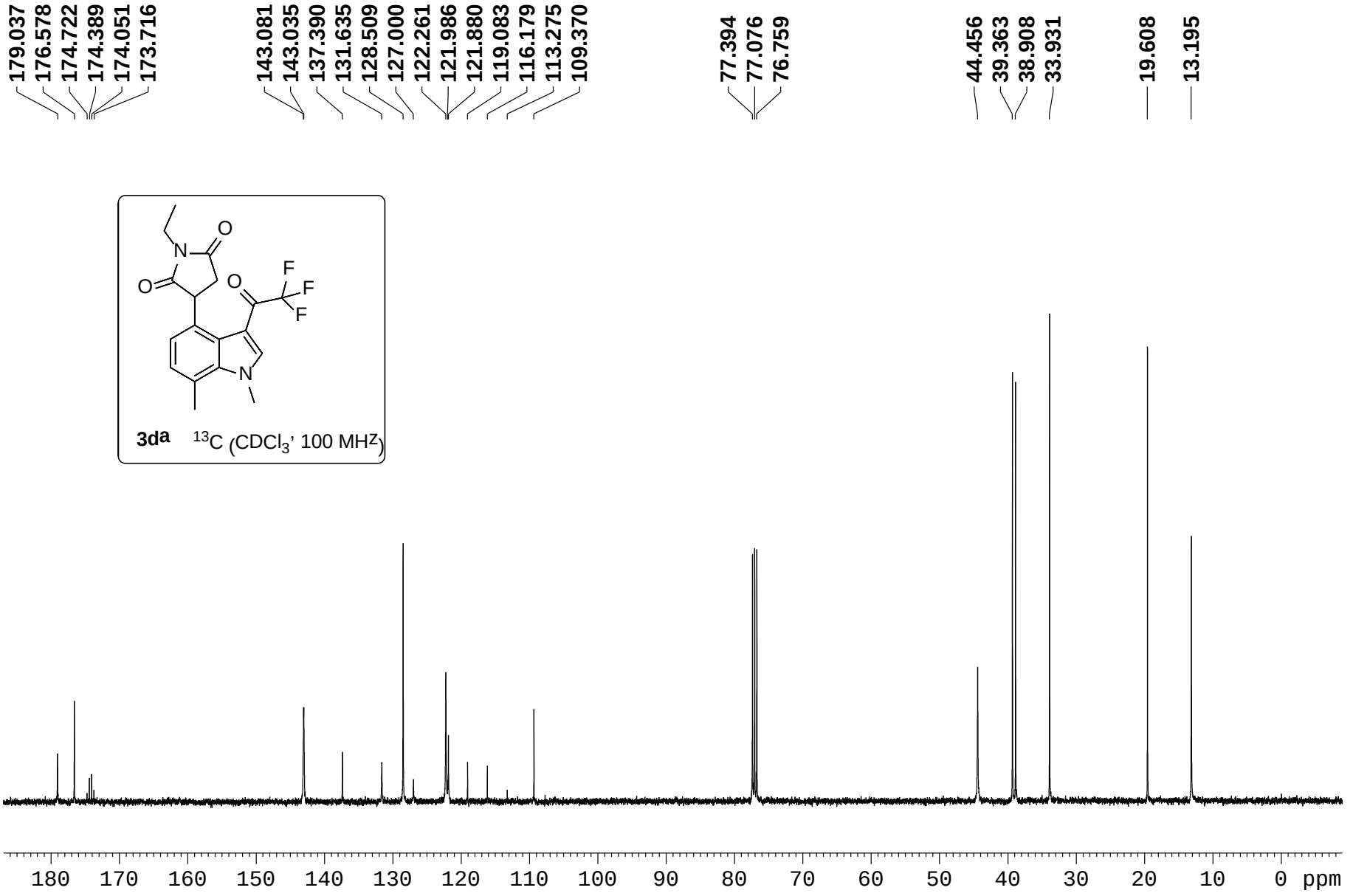
3b[a] ^{19}F (376 MHz)

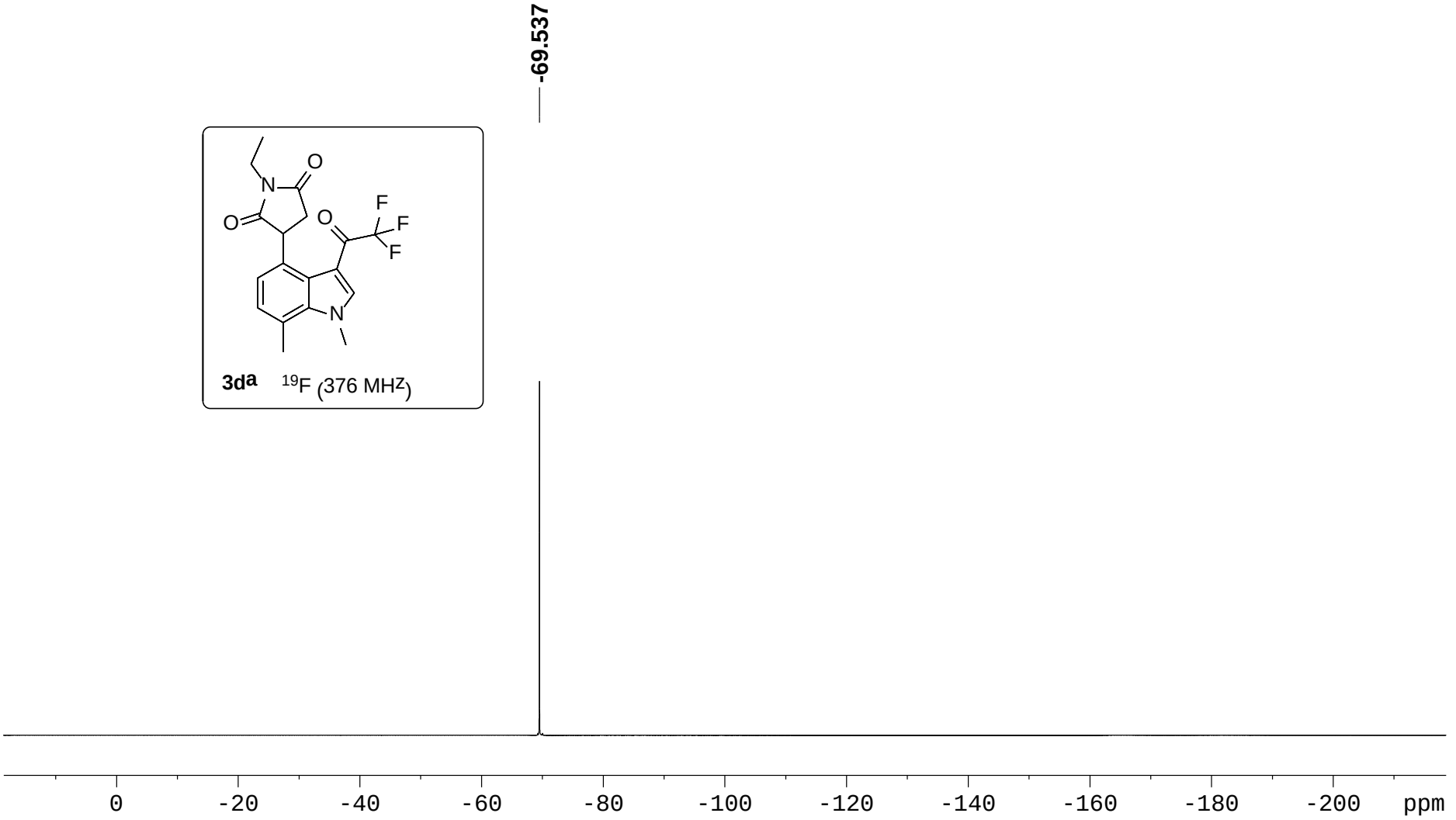

8.130
7.395
7.373
7.355
7.339
7.318
7.301
7.279
7.263
7.175
7.156
7.021
7.005
5.870
5.860
5.851
5.434
5.407
3.703
3.685
3.667
3.649
3.415
3.391
3.370
3.346
2.693
2.684
2.648
2.638
1.274
1.256
1.238
-0.000
O
N
O
O
F
F
F
N
3ca 1H (CDCl3, 400 MHz)
1.045
5.049
2.024
1.040
1.000
2.027
2.053
1.012
1.027
3.026
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
ppm

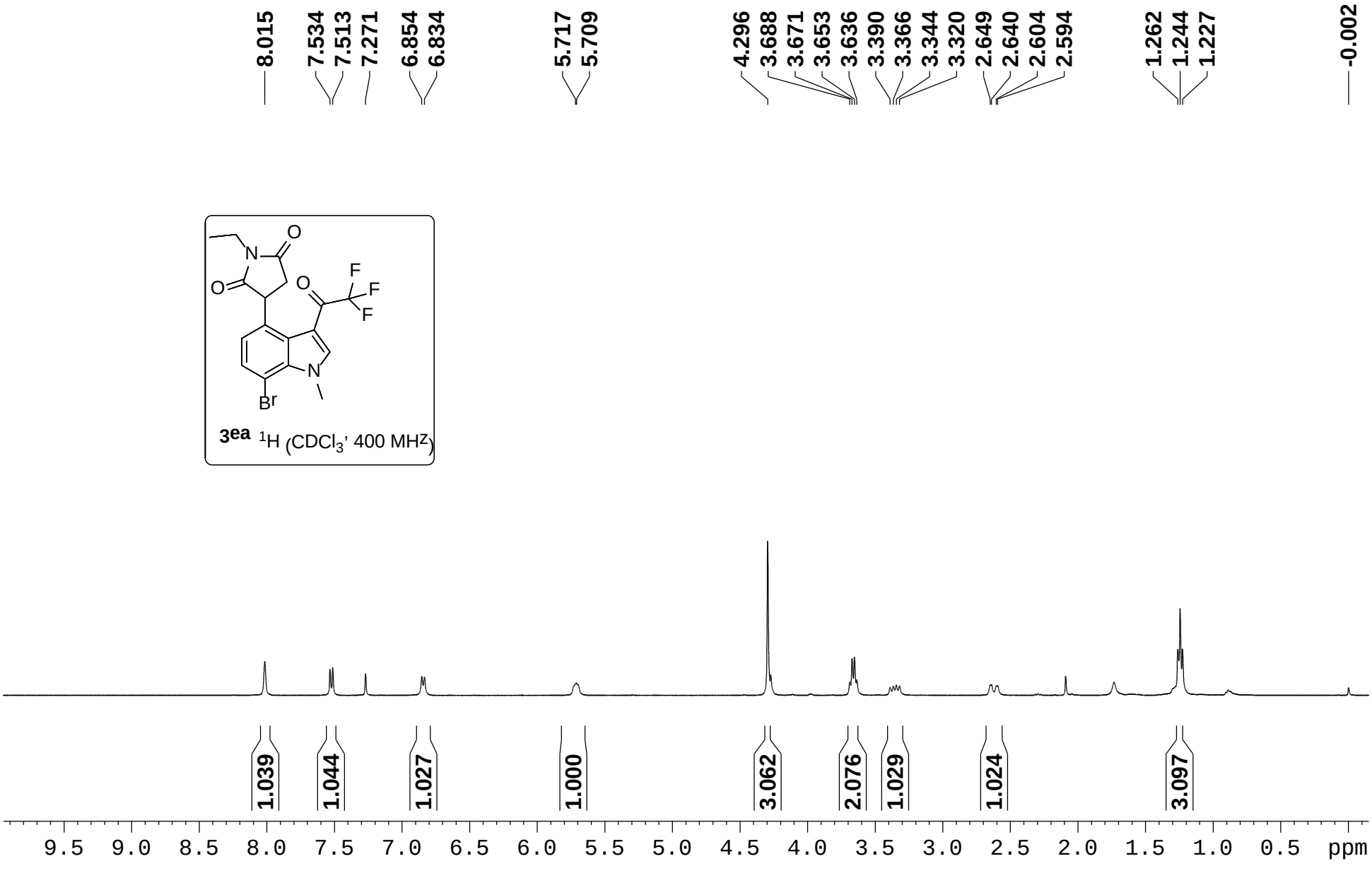

178.848
176.419
175.066
174.728
174.389
174.048
140.635
138.160
134.115
133.882
129.281
128.721
126.935
126.119
125.611
122.325
121.843
118.941
116.039
113.136
110.569
110.344
77.317
76.999
76.681
51.585
44.759
39.405
33.950
13.168
O
N
O
O
F
F
F
N
3ca 13C (CDCl3, 100 MHz)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

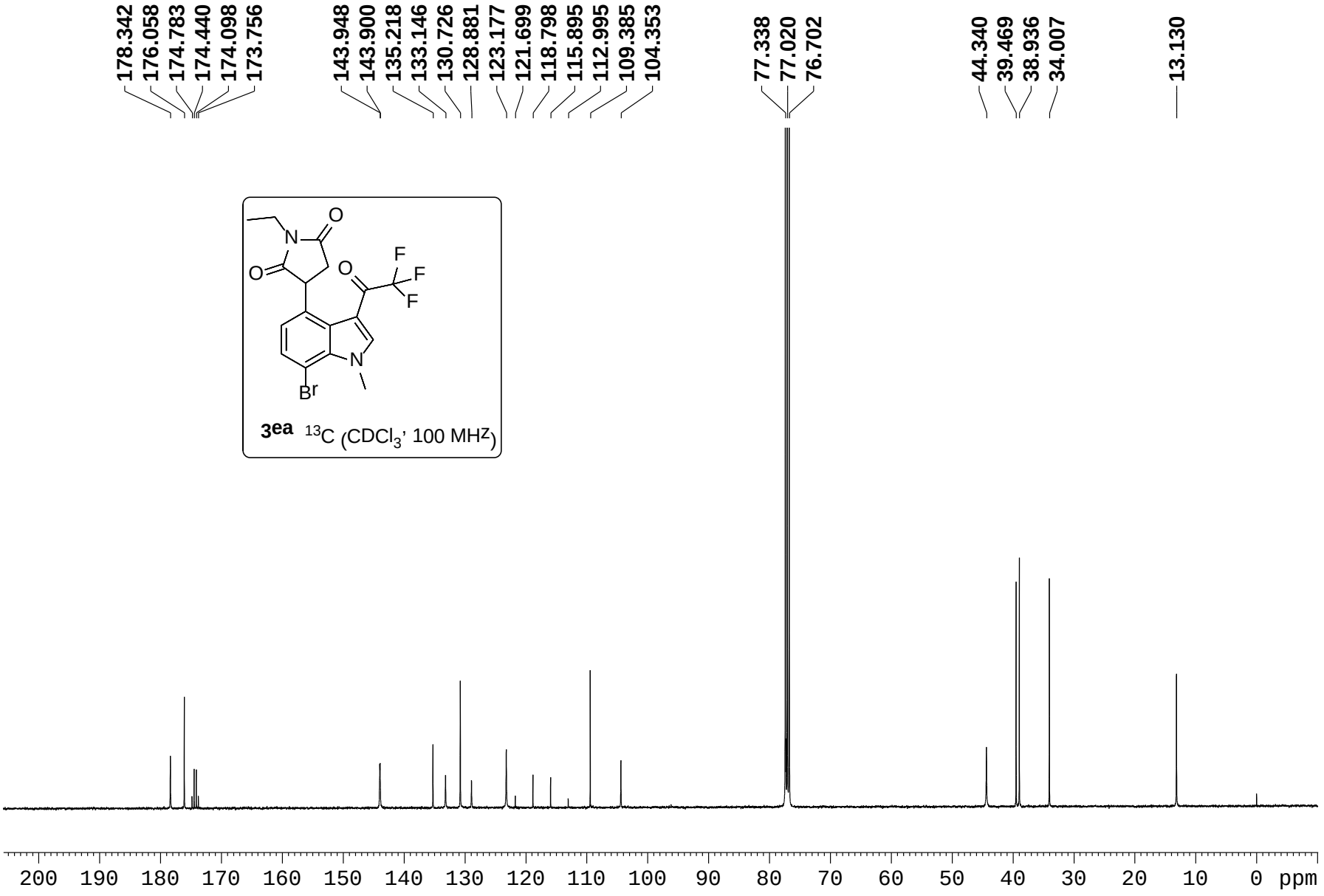

-69.782
O
N
O
O
F
F
F
N
3ca
19F (376 MHZ)
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

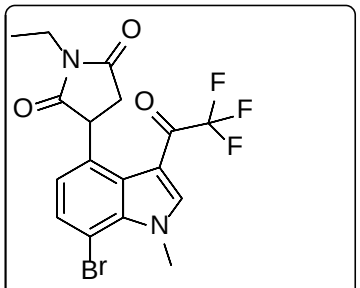

7.937
7.271
7.079
7.060
6.878
6.859
5.777
5.764
5.754
5.743
4.135
3.690
3.672
3.654
3.636
3.370
3.347
3.325
3.301
2.735
2.638
2.627
2.592
2.581
1.264
1.247
1.229
-0.000
O
N
O
O
F
F
F
N
3da 1H (CDCl3, 400 MHz)
1.083
1.096
1.056
1.000
3.141
2.140
1.031
3.041
1.035
3.077
8
7
6
5
4
3
2
1
0
ppm


179.037
176.578
174.722
174.389
174.051
173.716
143.081
143.035
137.390
131.635
128.509
127.000
122.261
121.986
121.880
119.083
116.179
113.275
109.370
77.394
77.076
76.759
44.456
39.363
38.908
33.931
19.608
13.195
O
N
O
O
F
F
F
N
3da 13C (CDCl3, 100 MHz)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

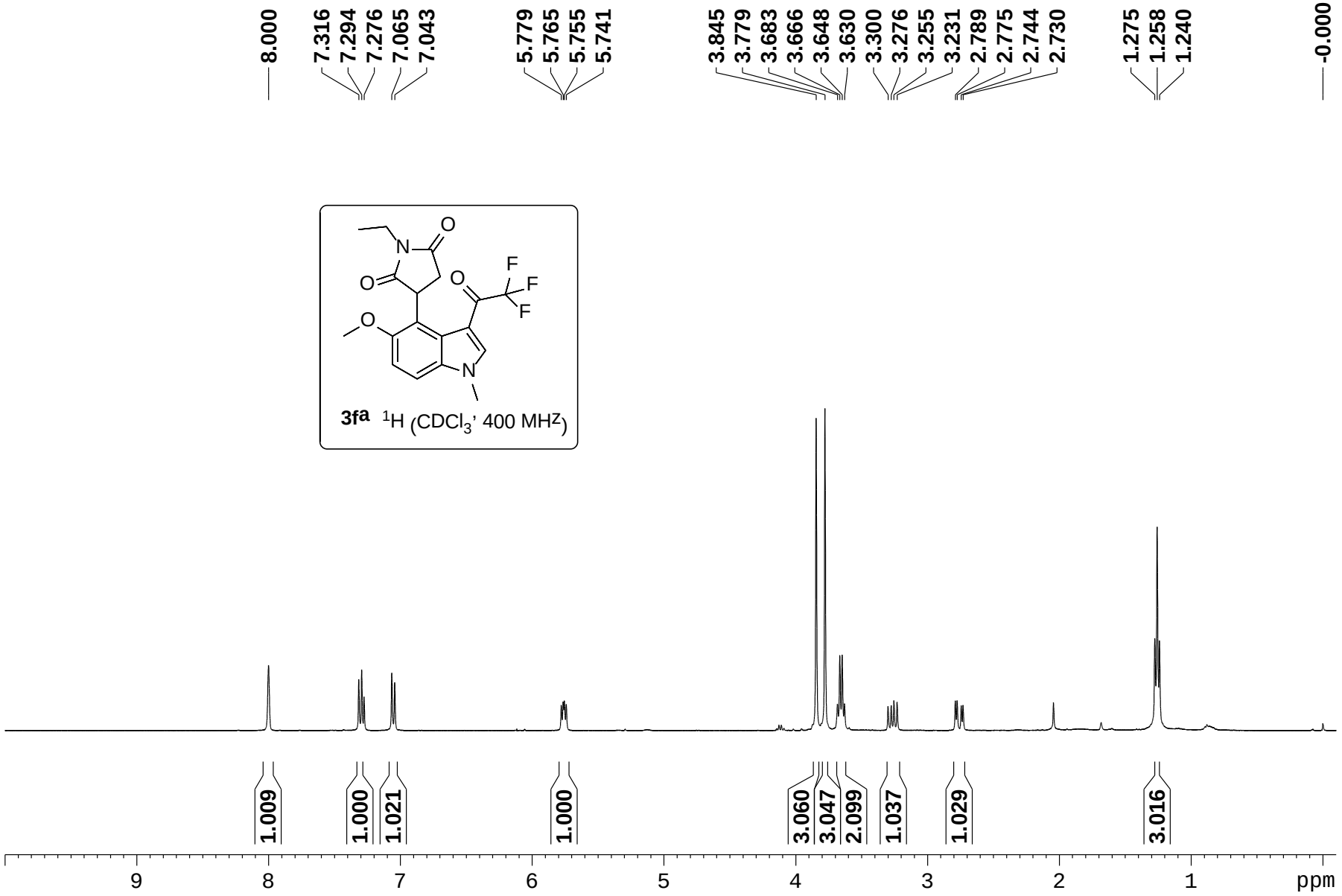

-69.537
O
N
O
O
F
F
F
N
3d[a] ^{19}F (376 MHz)
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

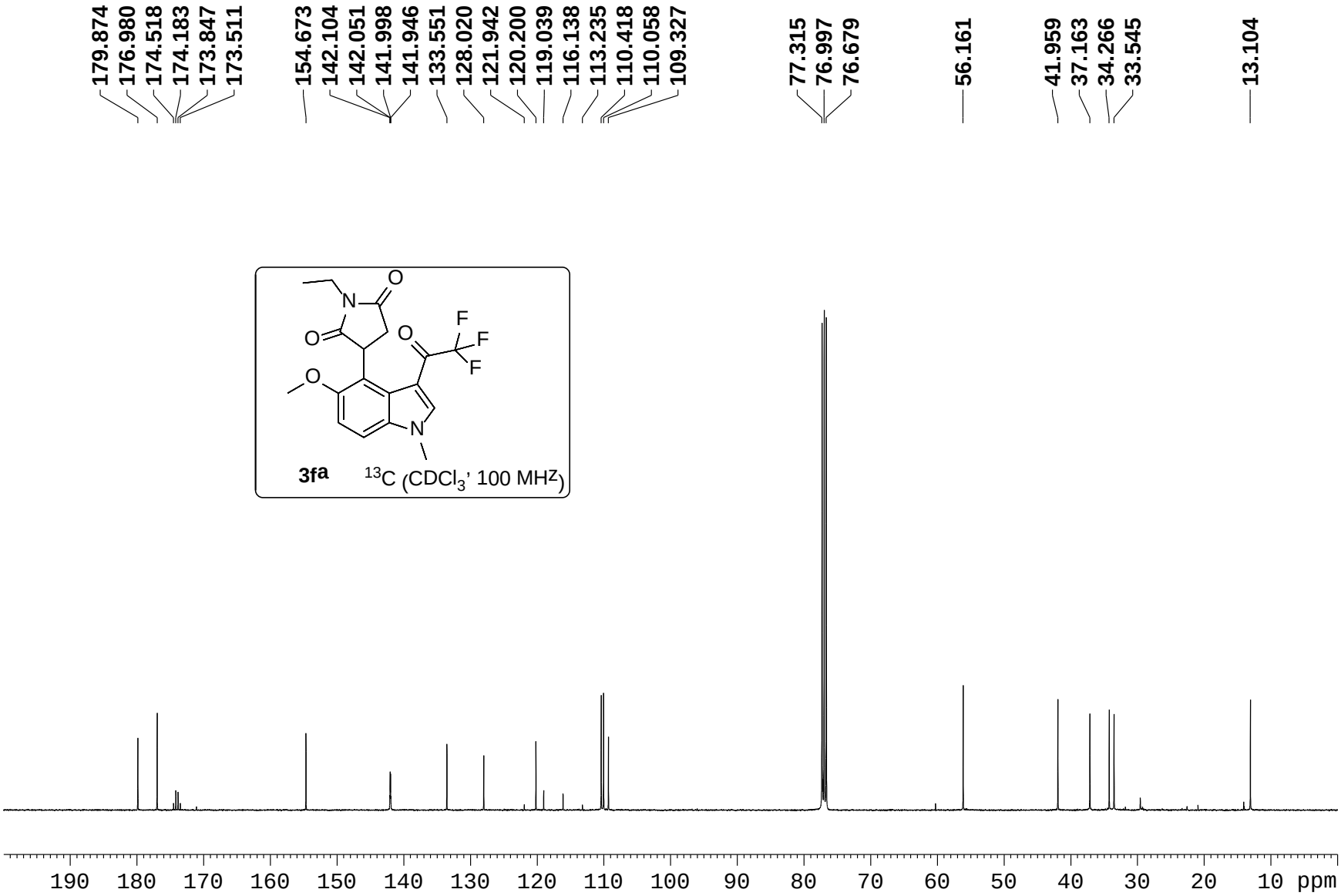

8.015
7.534
7.513
7.271
6.854
6.834
5.717
5.709
4.296
3.688
3.671
3.653
3.636
3.390
3.366
3.344
3.320
2.649
2.640
2.604
2.594
1.262
1.244
1.227
-0.002
O
N
O
O
F
F
F
N
Br
3ea 1H (CDCl3, 400 MHz)
1.039
1.044
1.027
1.000
3.062
2.076
1.029
1.024
3.097
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

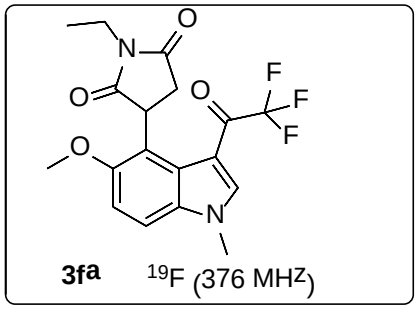

178.342
176.058
174.783
174.440
174.098
173.756
143.948
143.900
135.218
133.146
130.726
128.881
123.177
121.699
118.798
115.895
112.995
109.385
104.353
77.338
77.020
76.702
44.340
39.469
38.936
34.007
13.130
O
N
O
O
F
F
F
N
Br
3ea 13C (CDCl3, 100 MHz)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



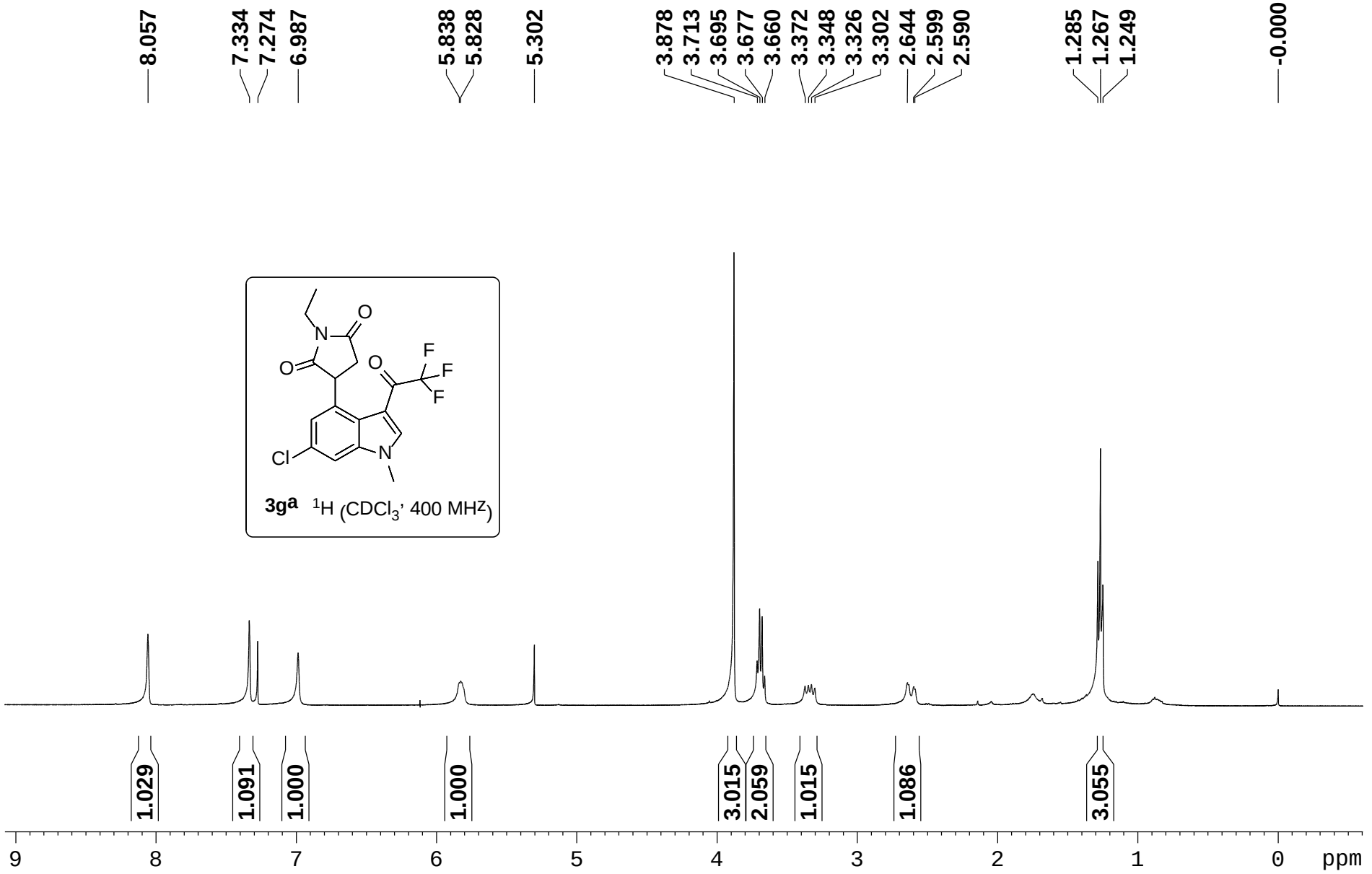
3ea ^{19}F (376 MHz)

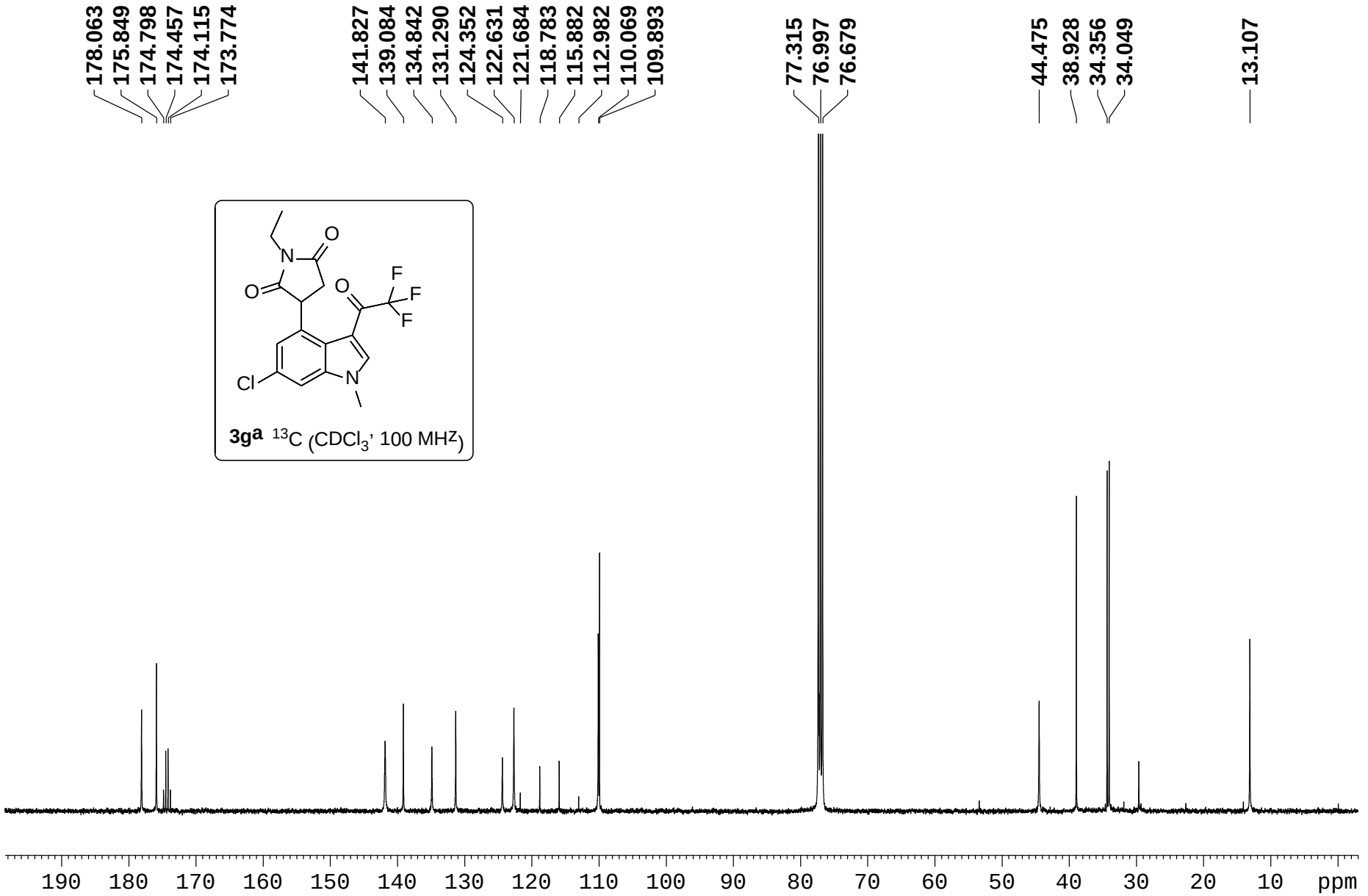

8.000
7.316
7.294
7.276
7.065
7.043
5.779
5.765
5.755
5.741
3.845
3.779
3.683
3.666
3.648
3.630
3.300
3.276
3.255
3.231
2.789
2.775
2.744
2.730
1.275
1.258
1.240
-0.000
O
N
O
O
F
F
F
O
N
3fa 1H (CDCl3, 400 MHz)
1.009
1.000
1.021
1.000
3.060
3.047
2.099
1.037
1.029
3.016
9
8
7
6
5
4
3
2
1
ppm

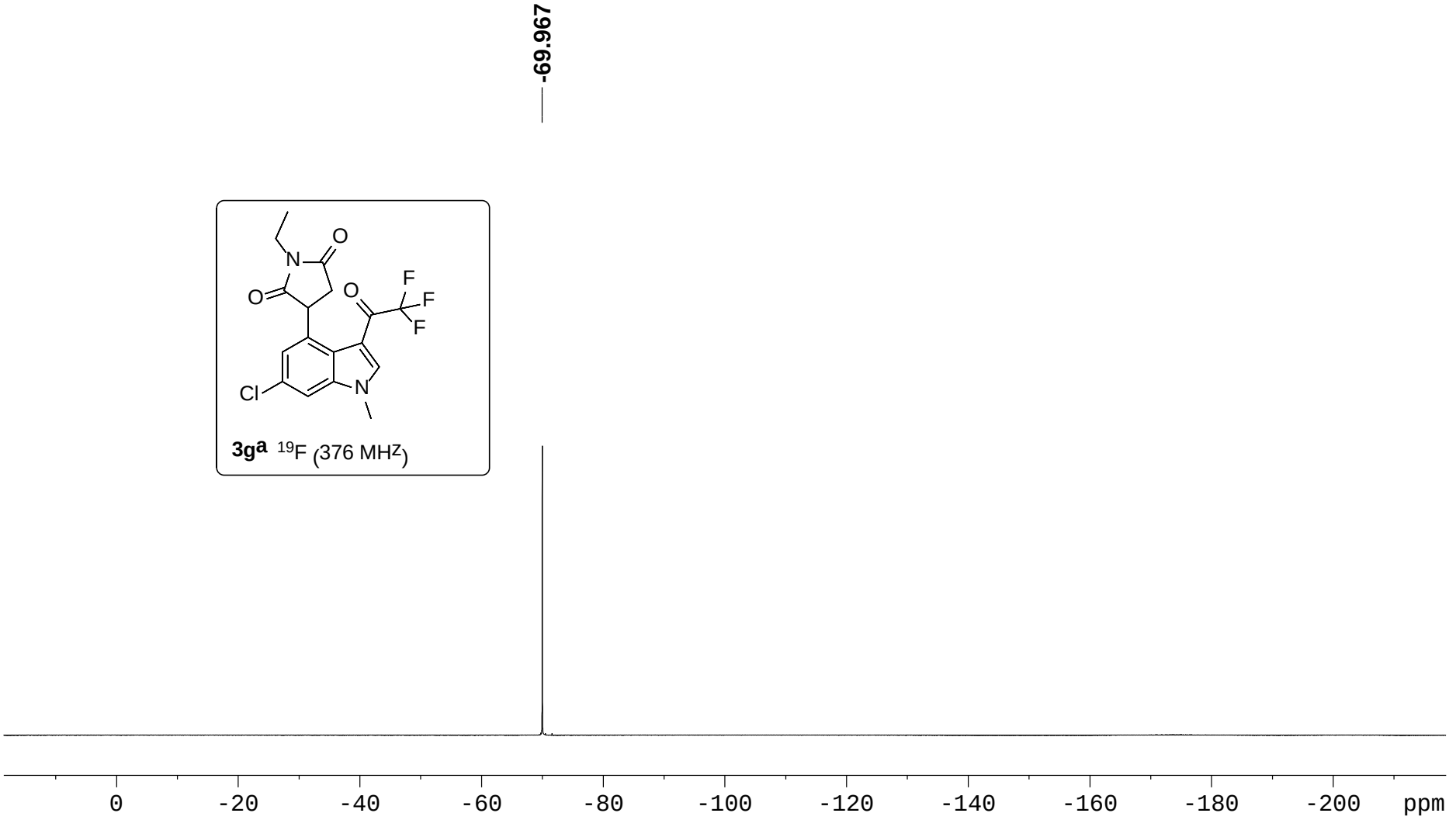

179.874
176.980
174.518
174.183
173.847
173.511
154.673
142.104
142.051
141.998
141.946
133.551
128.020
121.942
120.200
119.039
116.138
113.235
110.418
110.058
109.327
77.315
76.997
76.679
56.161
41.959
37.163
34.266
33.545
13.104
O
N
O
O
F
F
F
O
O
N
3fa
13C (CDCl3, 100 MHz)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

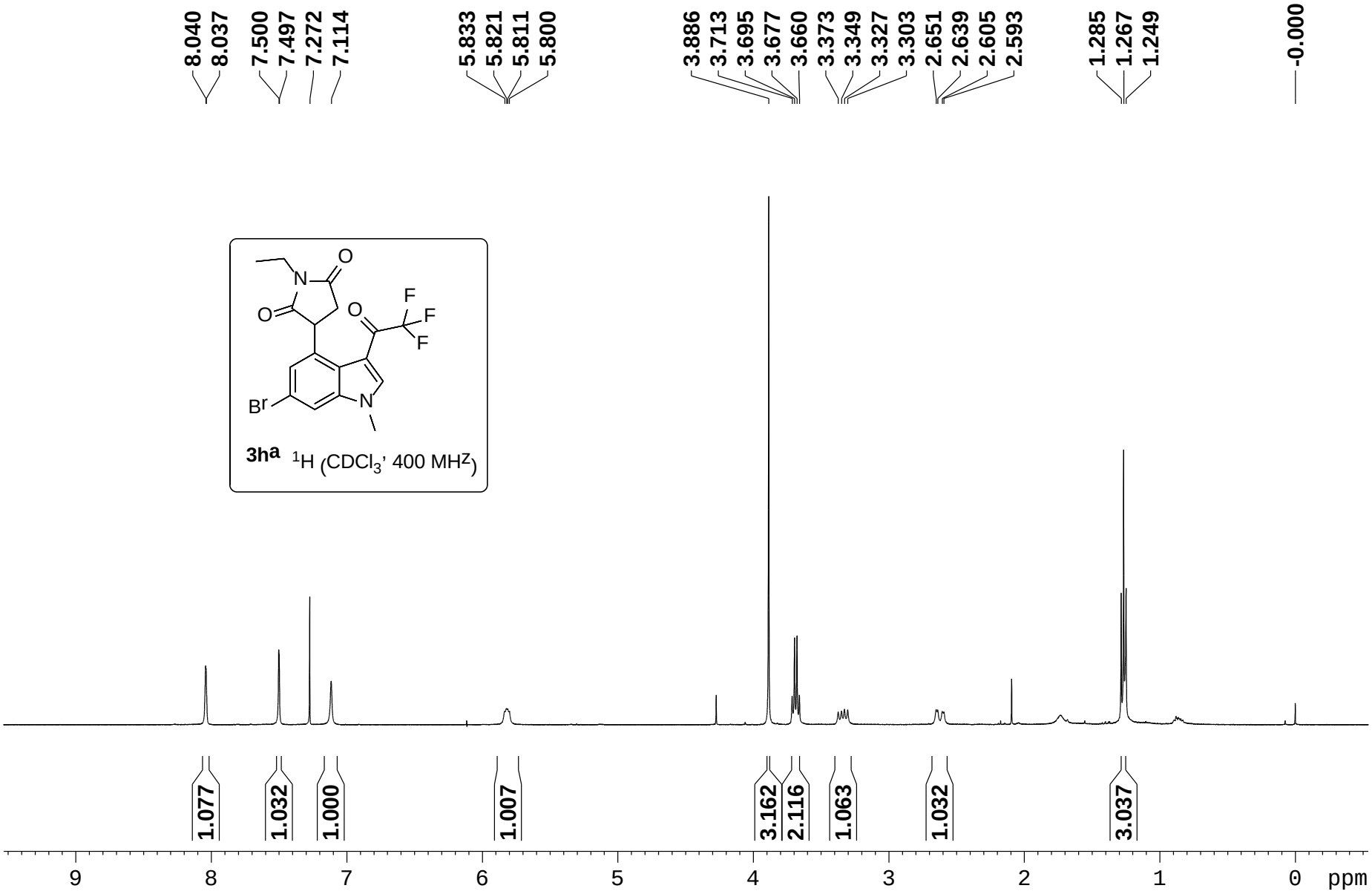


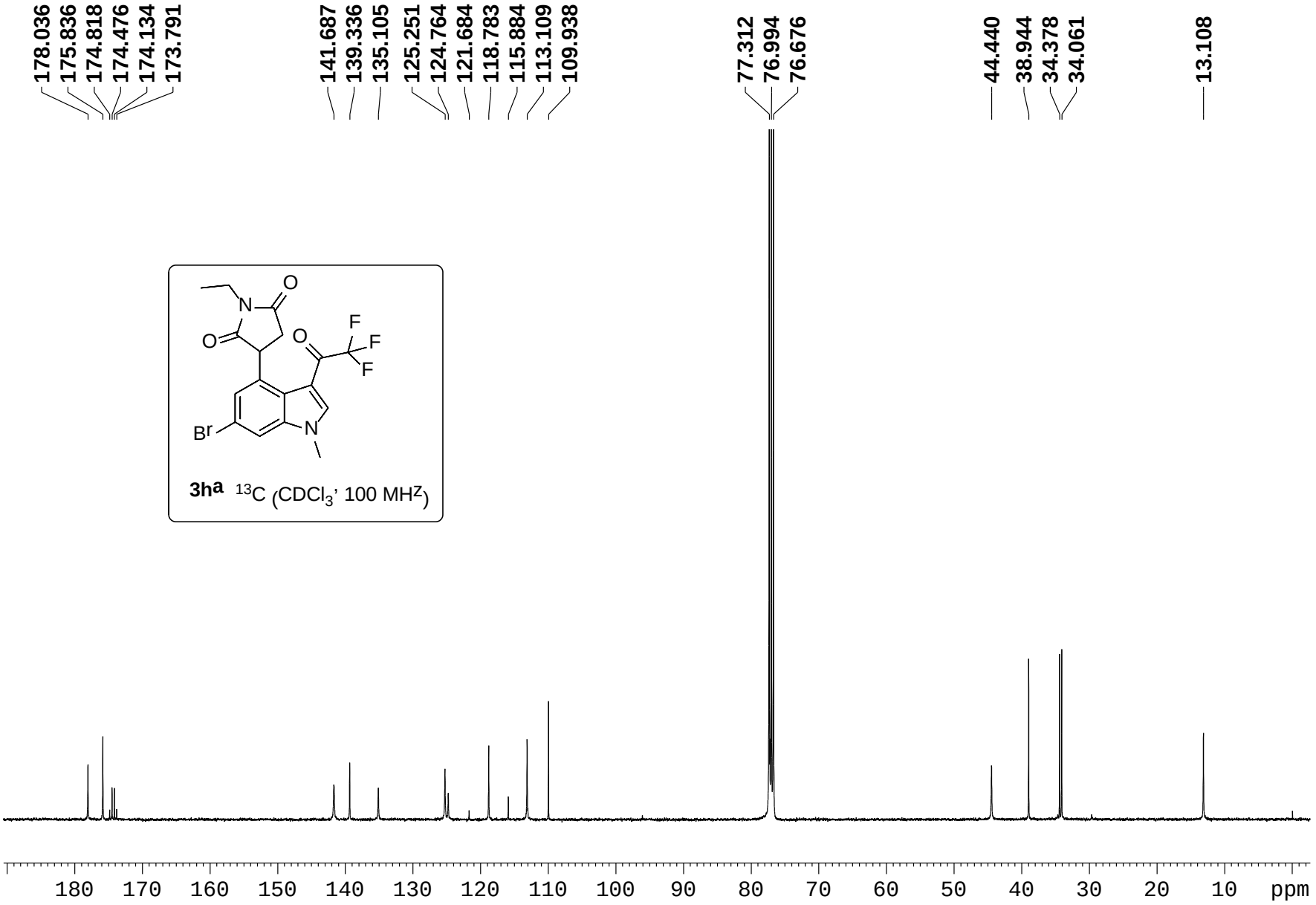
3fa ^{19}F (376 MHz)


8.057
7.334
7.274
6.987
5.838
5.828
5.302
3.878
3.713
3.695
3.677
3.660
3.372
3.348
3.326
3.302
2.644
2.599
2.590
1.285
1.267
1.249
-0.000
3gᵃ ¹H (CDCl₃, 400 MHz)
1.029
1.091
1.000
1.000
3.015
2.059
1.015
1.086
3.055
9
8
7
6
5
4
3
2
1
0
ppm

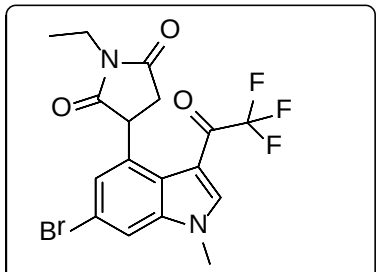

178.063
175.849
174.798
174.457
174.115
173.774
141.827
139.084
134.842
131.290
124.352
122.631
121.684
118.783
115.882
112.982
110.069
109.893
77.315
76.997
76.679
44.475
38.928
34.356
34.049
13.107
O
N
O
O
F
F
F
Cl
N
3g[a] ^{13}C ($CDCl_3$, 100 MHz)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


-69.967
O
N
O
O
F
F
F
Cl
N
3g[a] 19F (376 MHZ)
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

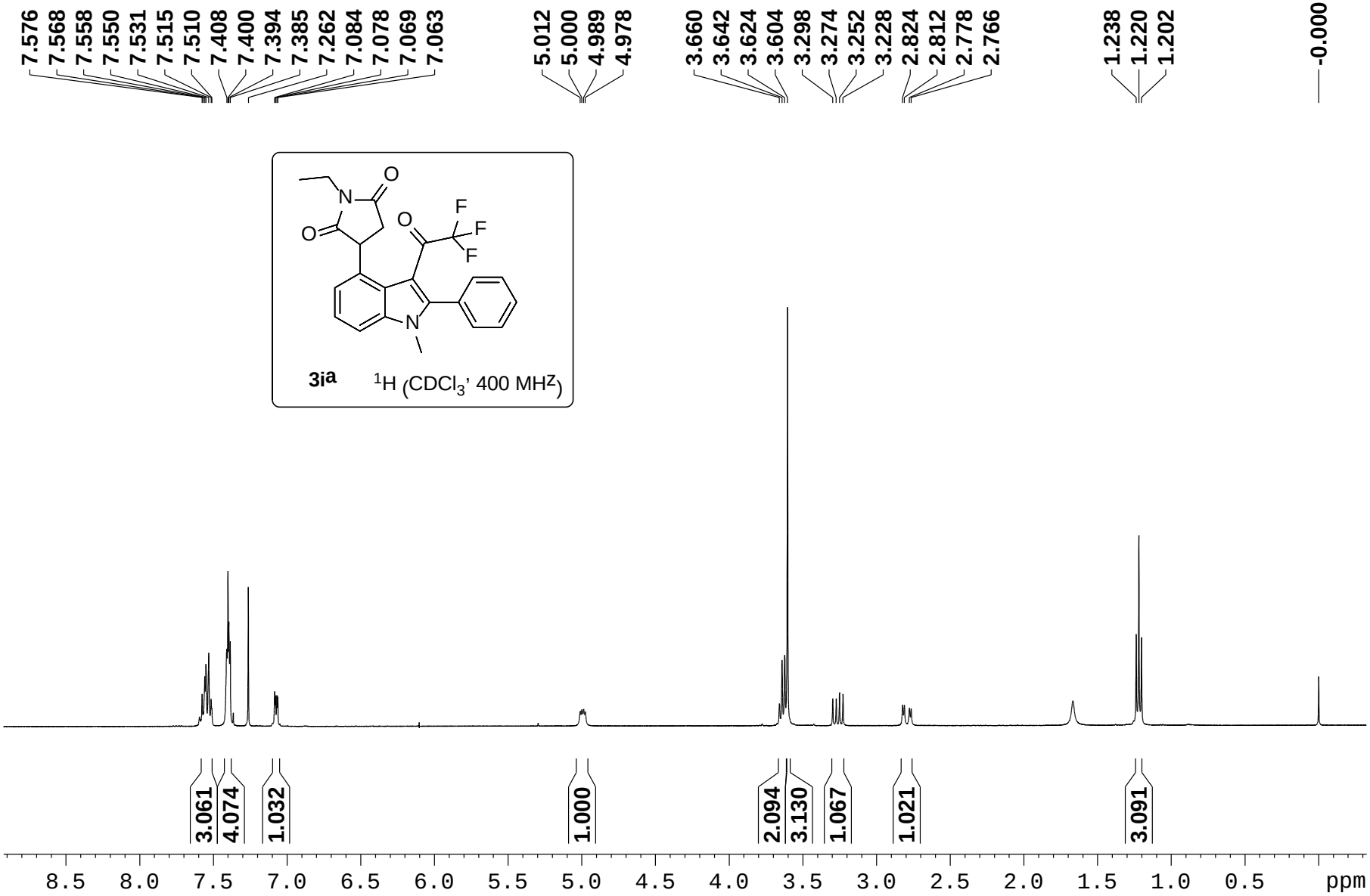

8.040
8.037
7.500
7.497
7.272
7.114
5.833
5.821
5.811
5.800
3.886
3.713
3.695
3.677
3.660
3.373
3.349
3.327
3.303
2.651
2.639
2.605
2.593
1.285
1.267
1.249
-0.000
O
N
O
O
F
F
F
Br
N
3h^a ^1H (CDCl3, 400 MHz)
1.077
1.032
1.000
1.007
3.162
2.116
1.063
1.032
3.037
9
8
7
6
5
4
3
2
1
0
ppm

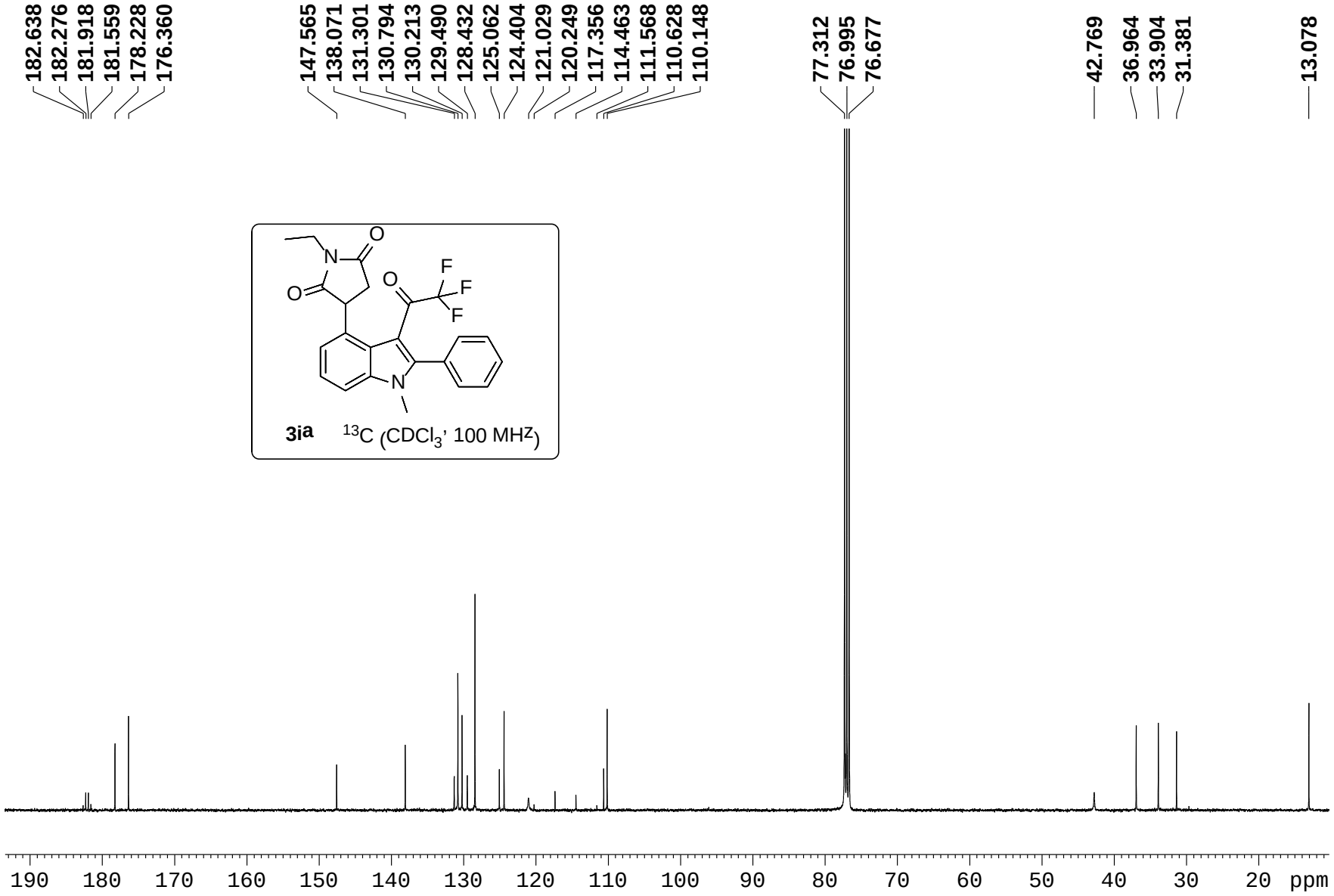


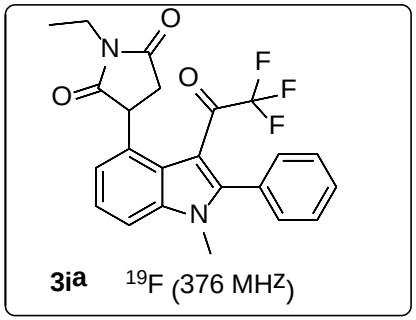
3ha ^{13}C ($CDCl_3$, 100 MHz)



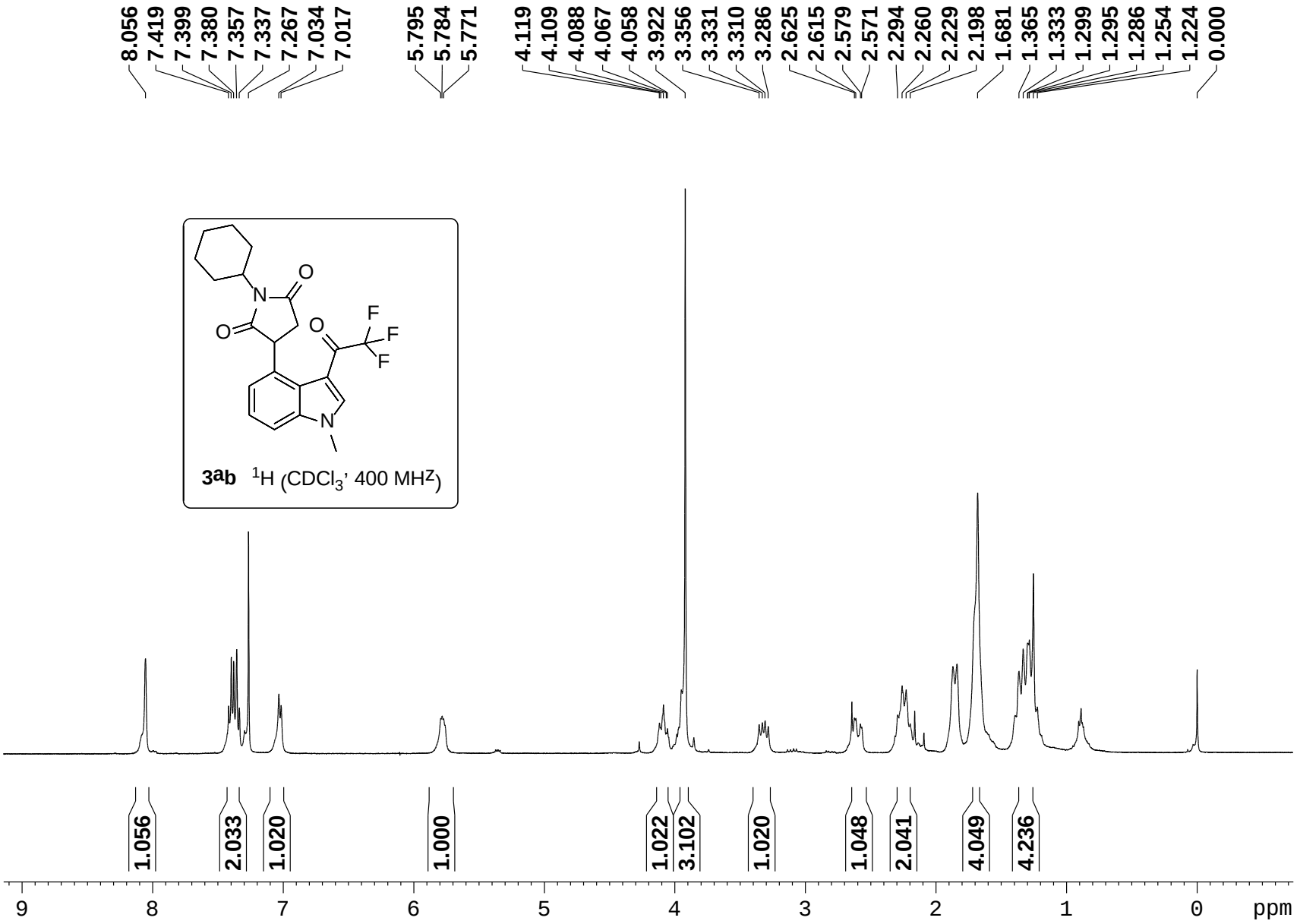
3ha ^{19}F (376 MHz)

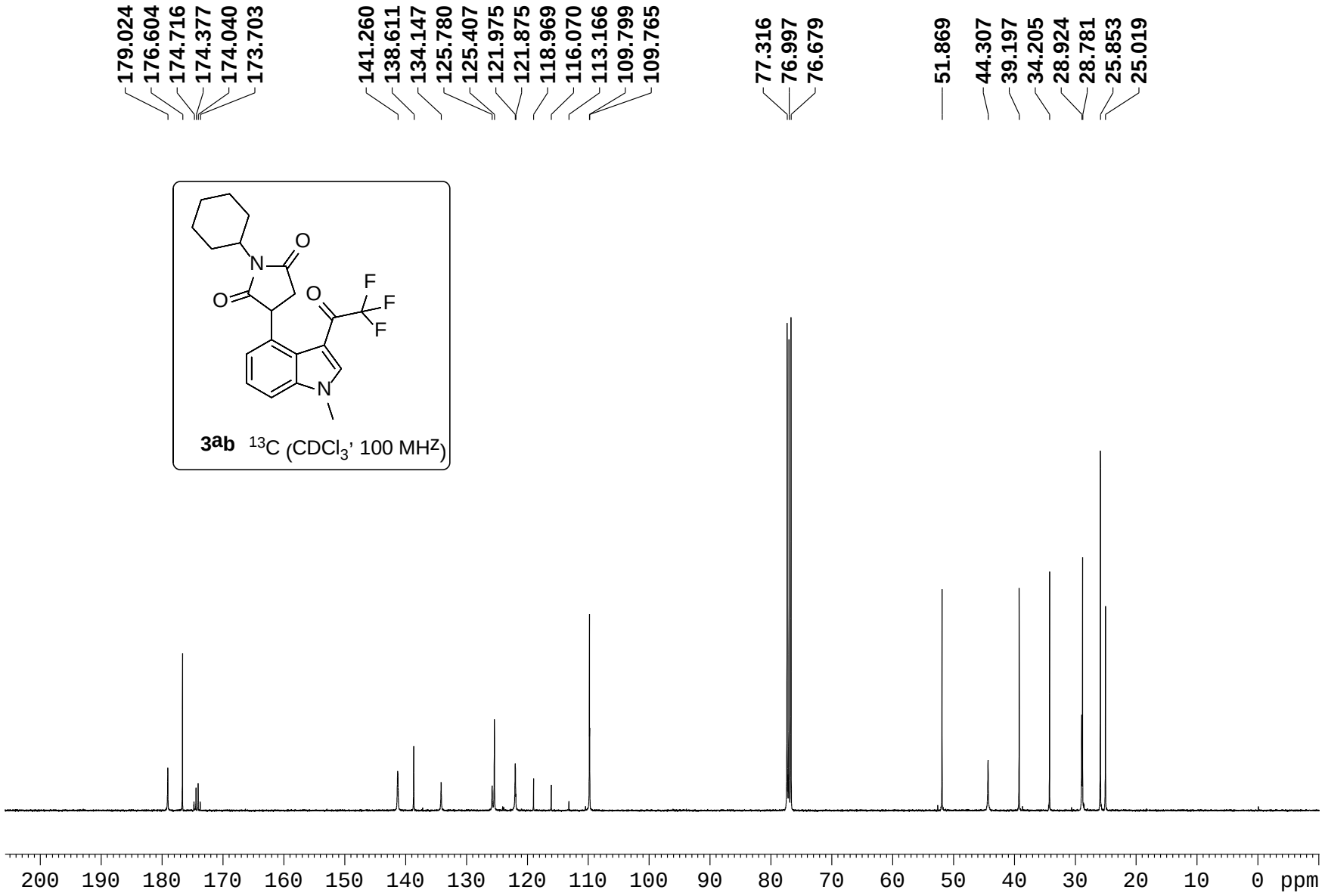

7.576
7.568
7.558
7.550
7.531
7.515
7.510
7.408
7.400
7.394
7.385
7.262
7.084
7.078
7.069
7.063
5.012
5.000
4.989
4.978
3.660
3.642
3.624
3.604
3.298
3.274
3.252
3.228
2.824
2.812
2.778
2.766
1.238
1.220
1.202
-0.000
3i^a
1H (CDCl3, 400 MHz)
3.061
4.074
1.032
1.000
2.094
3.130
1.067
1.021
3.091
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

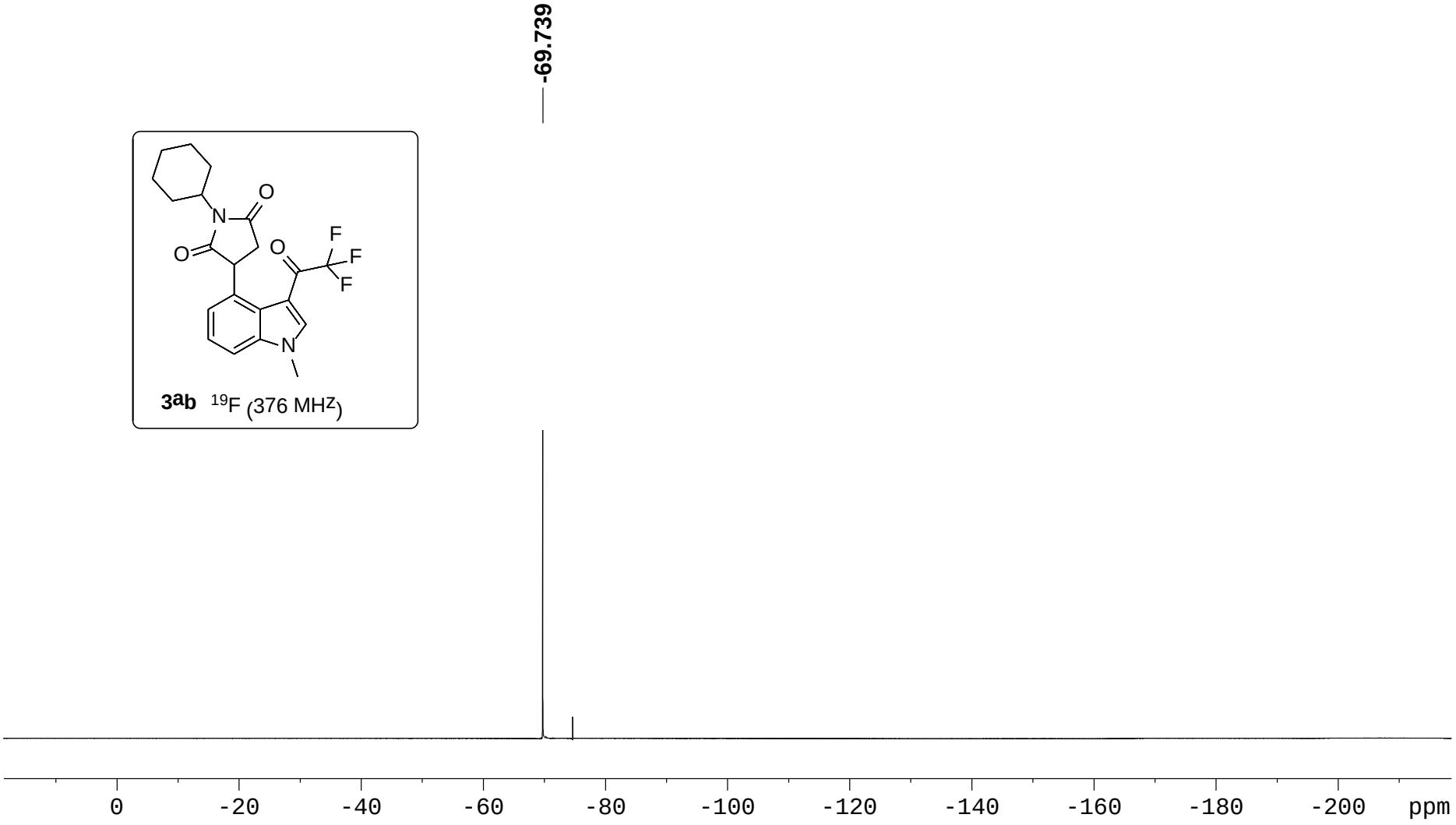

182.638
182.276
181.918
181.559
178.228
176.360
147.565
138.071
131.301
130.794
130.213
129.490
128.432
125.062
124.404
121.029
120.249
117.356
114.463
111.568
110.628
110.148
77.312
76.995
76.677
42.769
36.964
33.904
31.381
13.078
O
N
O
O
F
F
F
N
3ia
13C (CDCl3, 100 MHz)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

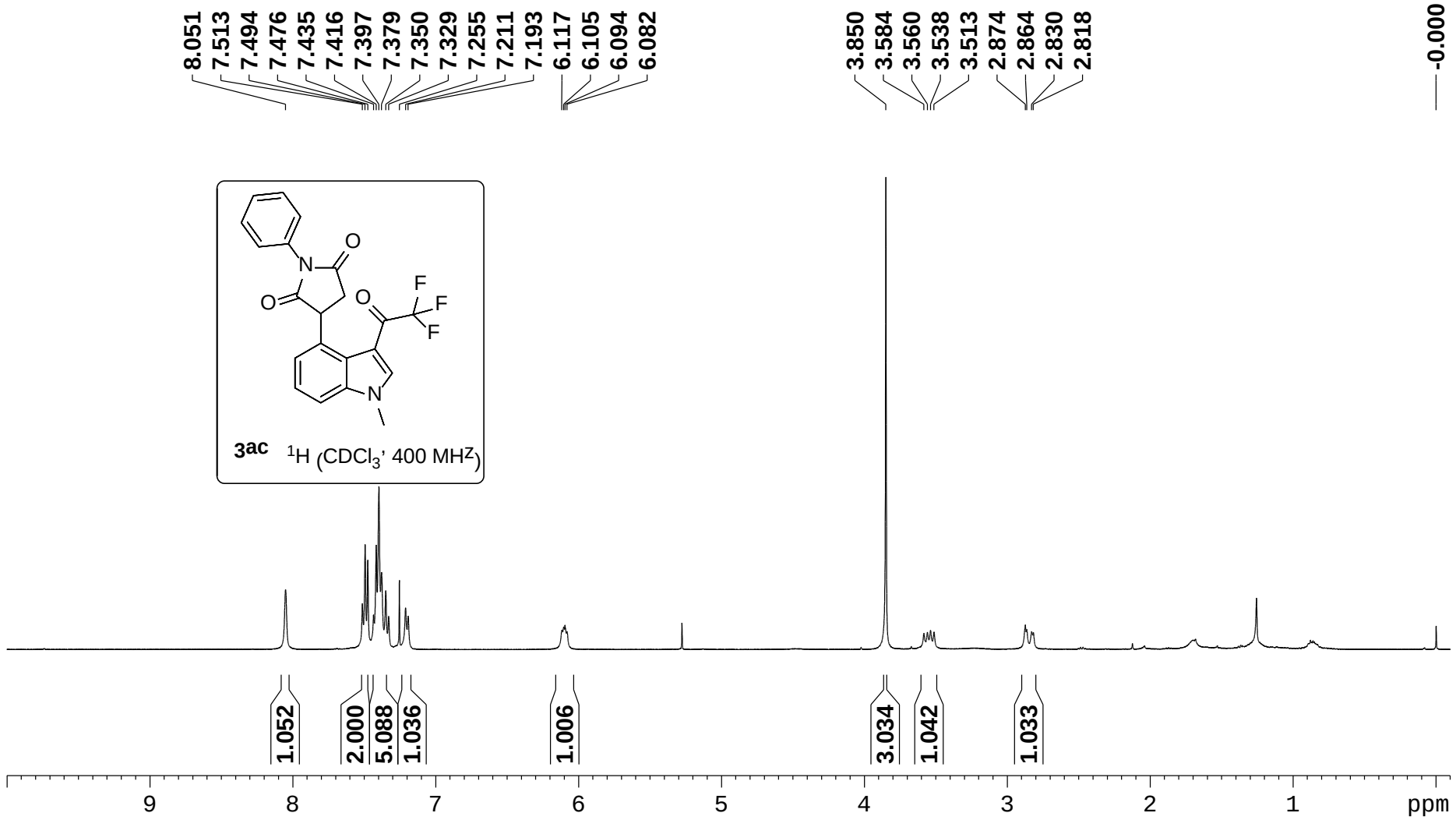

O
N
O
O
F
F
F
N
3ia
19F (376 MHZ)

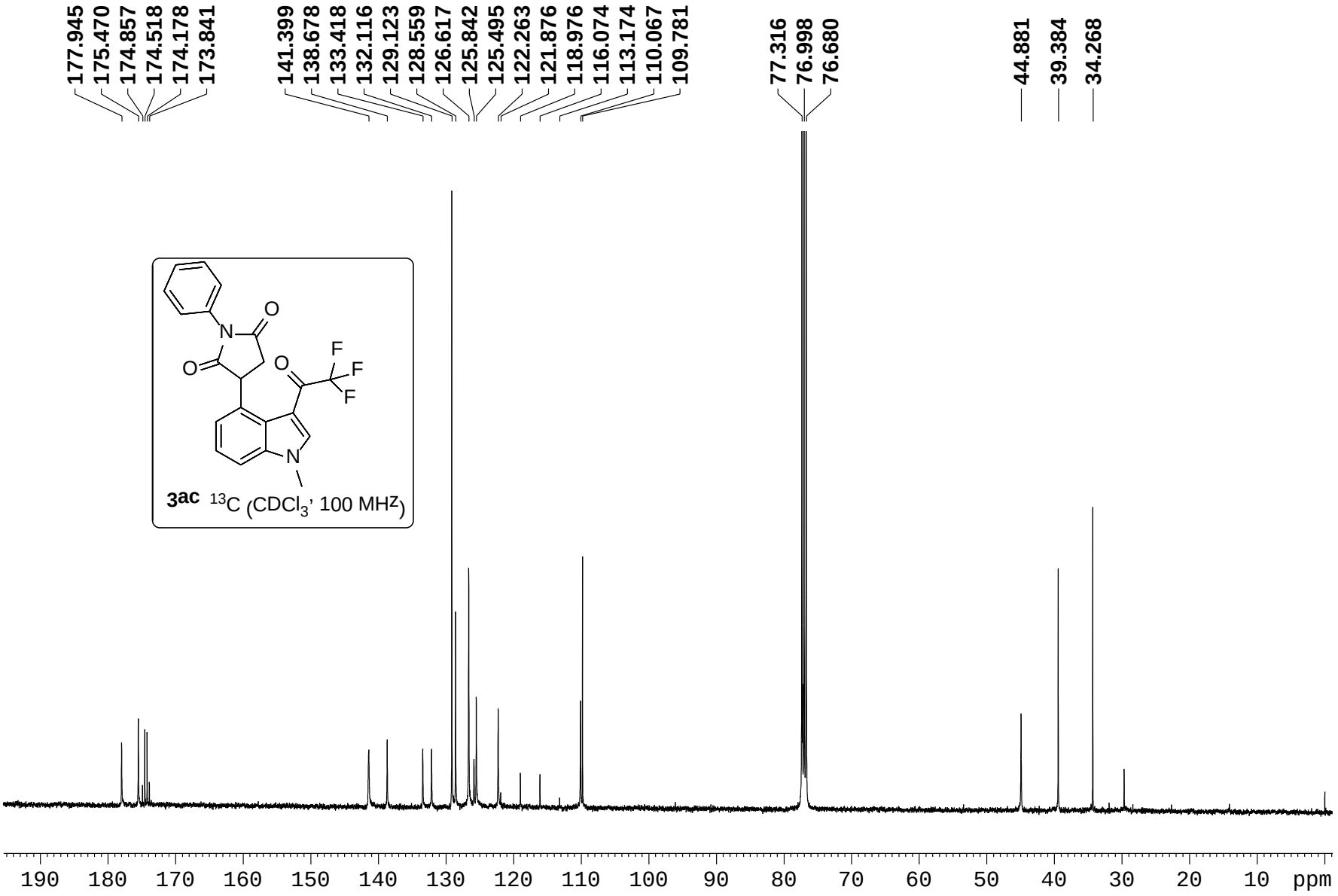
-71.019
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

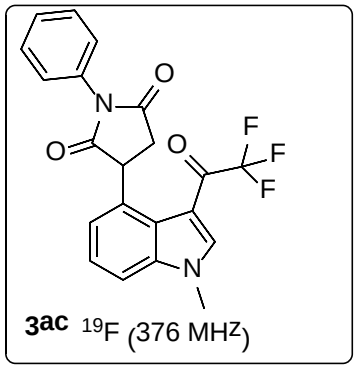

8.056
7.419
7.399
7.380
7.357
7.337
7.267
7.034
7.017
5.795
5.784
5.771
4.119
4.109
4.088
4.067
4.058
3.922
3.356
3.331
3.310
3.286
2.625
2.615
2.579
2.571
2.294
2.260
2.229
2.198
1.681
1.365
1.333
1.299
1.295
1.286
1.254
1.224
0.000
O
N
O
O
F
F
F
N
3ab 1H (CDCl3, 400 MHz)
1.056
2.033
1.020
1.000
1.022
3.102
1.020
1.048
2.041
4.049
4.236
9
8
7
6
5
4
3
2
1
0
ppm


179.024
176.604
174.716
174.377
174.040
173.703
141.260
138.611
134.147
125.780
125.407
121.975
121.875
118.969
116.070
113.166
109.799
109.765
77.316
76.997
76.679
51.869
44.307
39.197
34.205
28.924
28.781
25.853
25.019
O
N
O
O
F
F
F
N
3ab 13C (CDCl3, 100 MHz)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

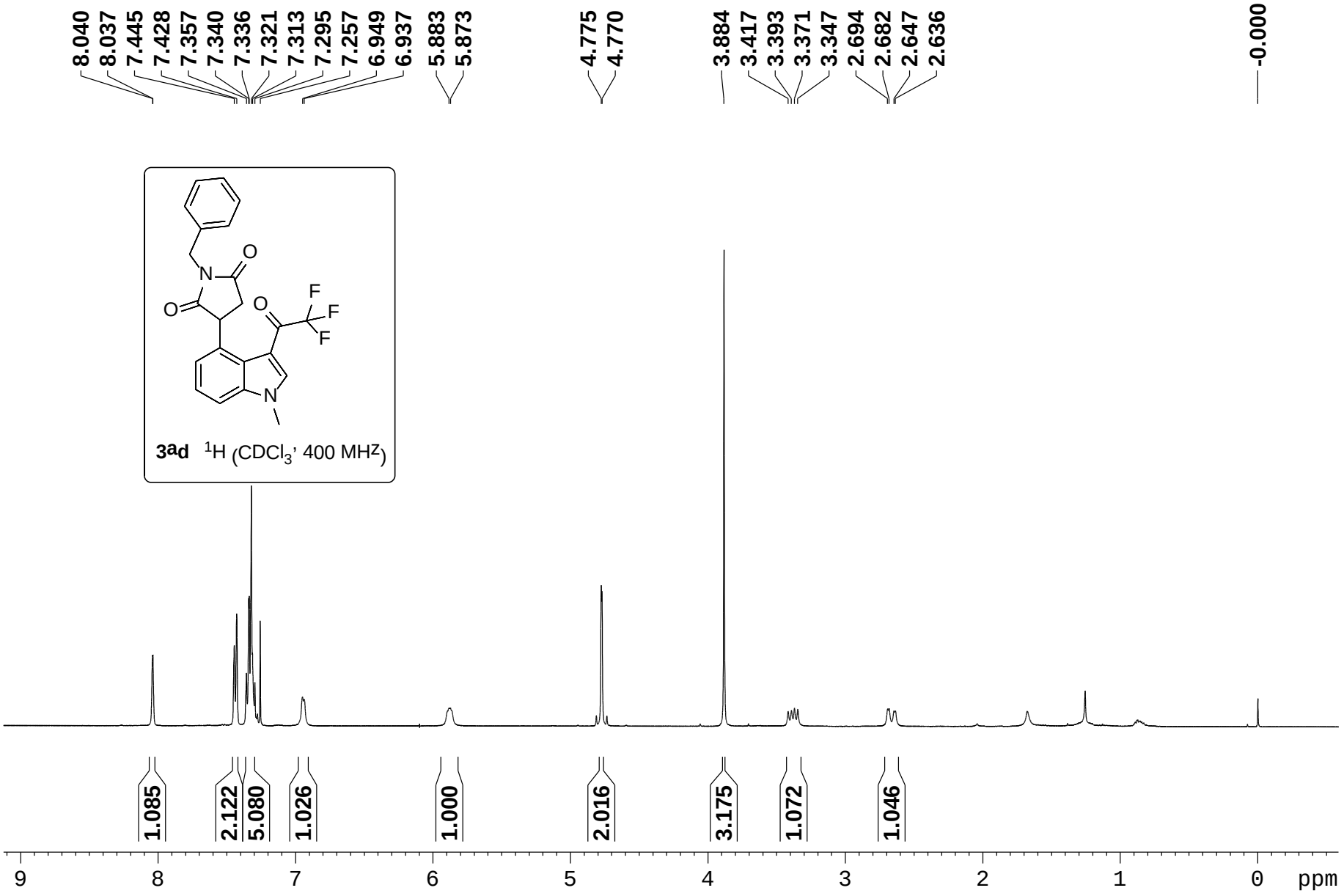

-69.739
O
N
O
O
F
F
F
N
3ab 19F (376 MHz)
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

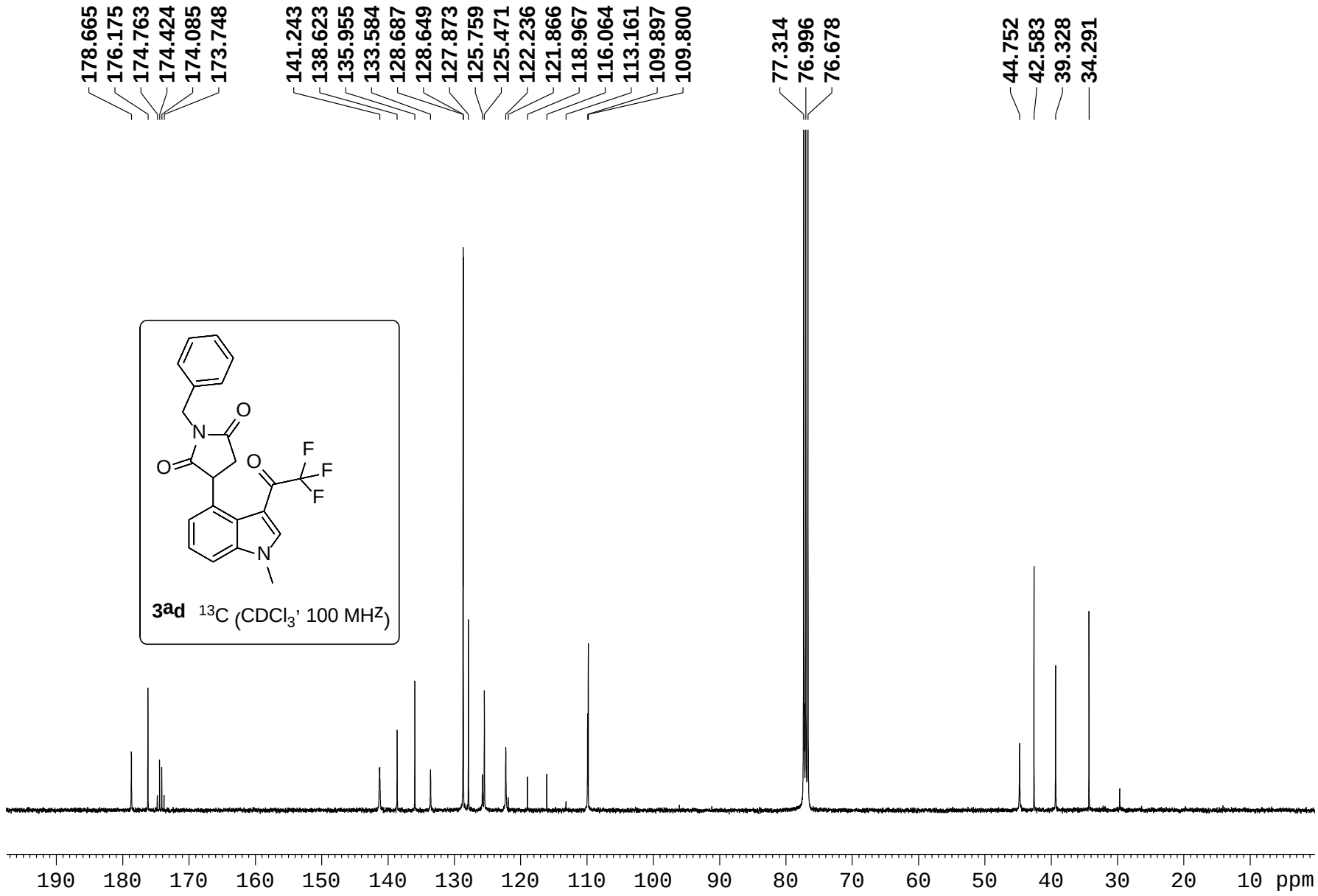

8.051
7.513
7.494
7.476
7.435
7.416
7.397
7.379
7.350
7.329
7.255
7.211
7.193
6.117
6.105
6.094
6.082
3.850
3.584
3.560
3.538
3.513
2.874
2.864
2.830
2.818
-0.000
O
N
O
O
F
F
F
N
3ac
1H (CDCl3, 400 MHz)
1.052
2.000
5.088
1.036
1.006
3.034
1.042
1.033
9
8
7
6
5
4
3
2
1
ppm

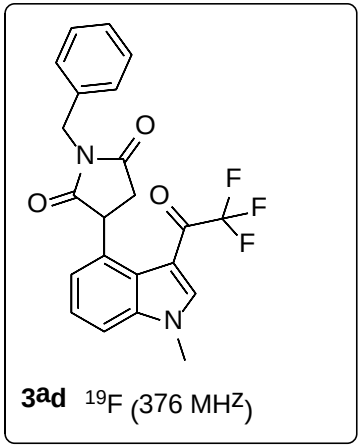

177.945
175.470
174.857
174.518
174.178
173.841
141.399
138.678
133.418
132.116
129.123
128.559
126.617
125.842
125.495
122.263
121.876
118.976
116.074
113.174
110.067
109.781
77.316
76.998
76.680
44.881
39.384
34.268
O
N
O
O
F
F
F
N
3ac 13C (CDCl3, 100 MHz)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



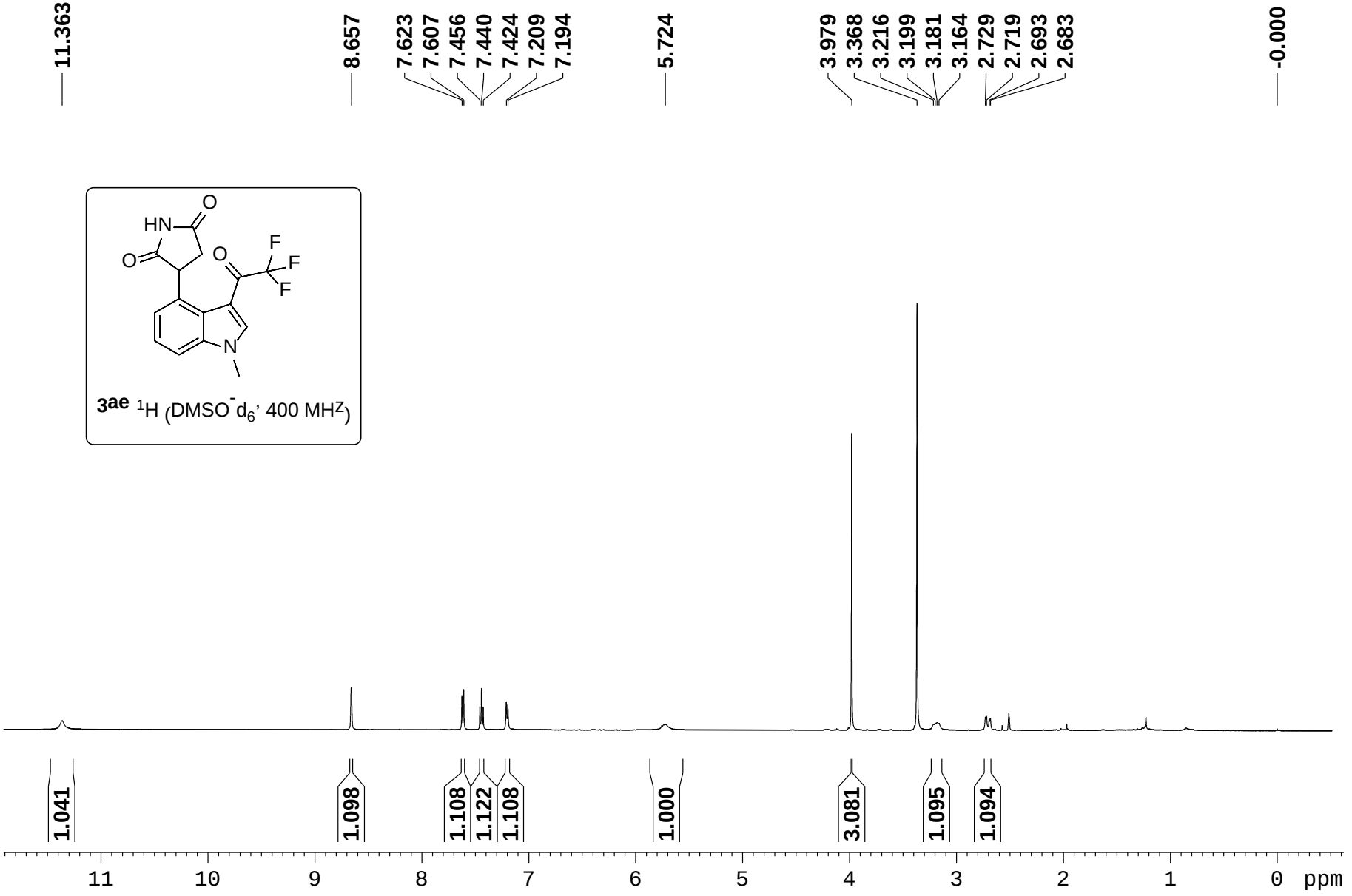
3ac ^{19}F (376 MHz)

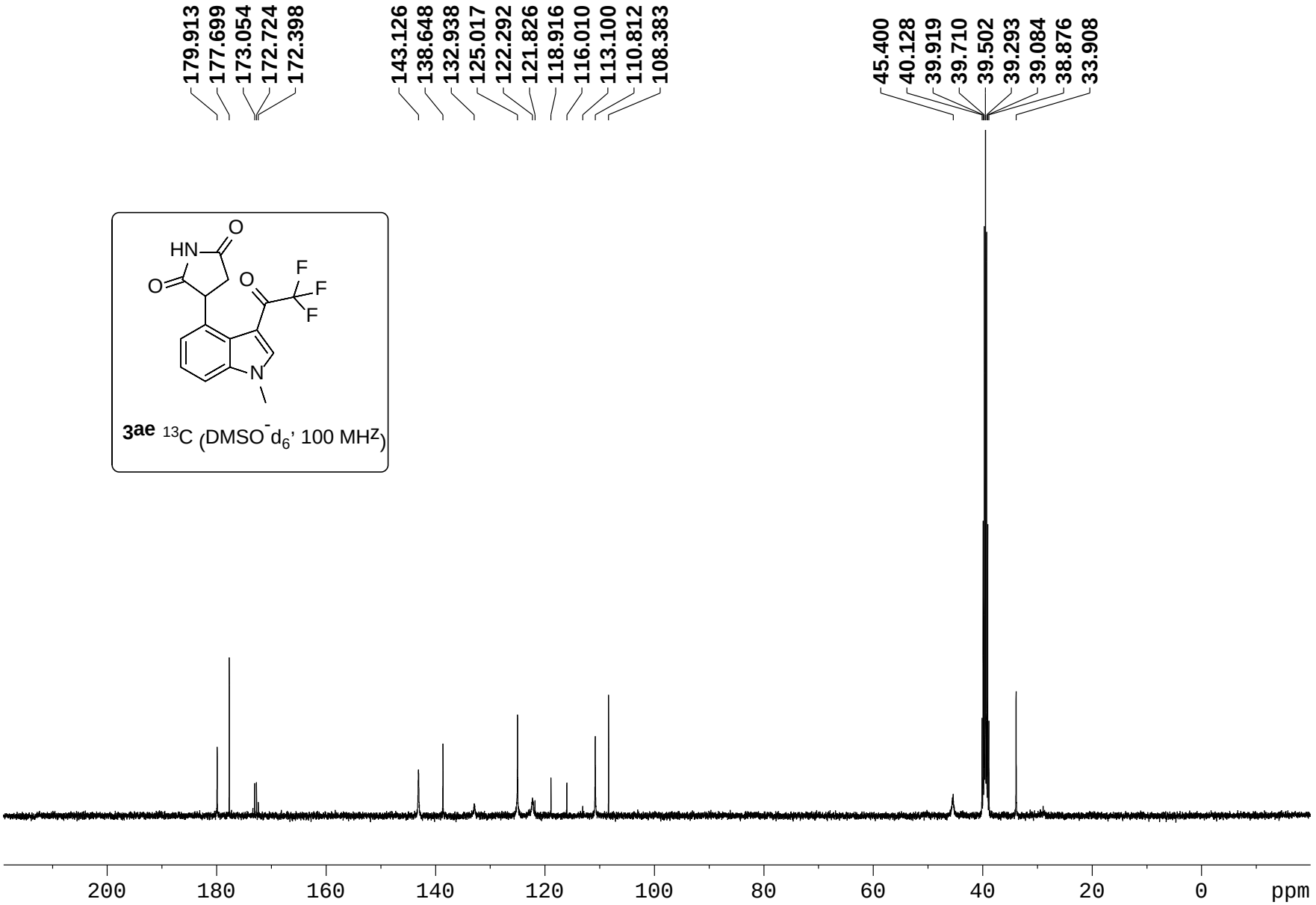

8.040
8.037
7.445
7.428
7.357
7.340
7.336
7.321
7.313
7.295
7.257
6.949
6.937
5.883
5.873
4.775
4.770
3.884
3.417
3.393
3.371
3.347
2.694
2.682
2.647
2.636
-0.000
O
N
O
O
F
F
F
N
3ad 1H (CDCl3, 400 MHz)
1.085
2.122
5.080
1.026
1.000
2.016
3.175
1.072
1.046
9
8
7
6
5
4
3
2
1
0
ppm


178.665
176.175
174.763
174.424
174.085
173.748
141.243
138.623
135.955
133.584
128.687
128.649
127.873
125.759
125.471
122.236
121.866
118.967
116.064
113.161
109.897
109.800
77.314
76.996
76.678
44.752
42.583
39.328
34.291
O
N
O
O
F
F
F
N
3ad 13C (CDCl3, 100 MHz)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

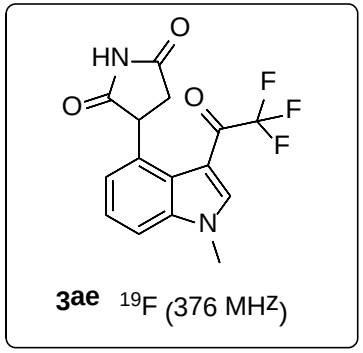


3ad ^{19}F (376 MHz)

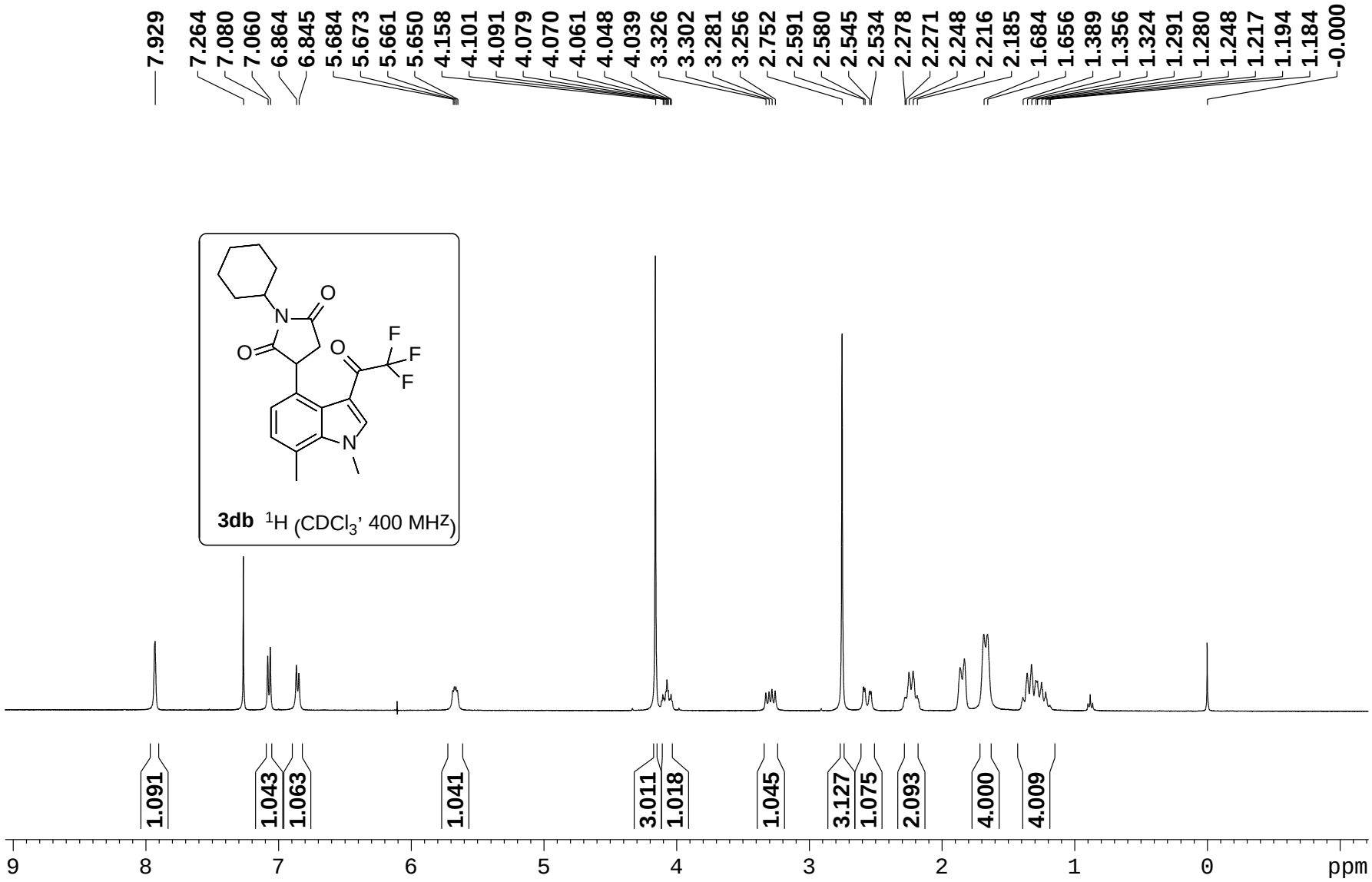

11.363
8.657
7.623
7.607
7.456
7.440
7.424
7.209
7.194
5.724
3.979
3.368
3.216
3.199
3.181
3.164
2.729
2.719
2.693
2.683
-0.000
HN
O
O
O
F
F
F
N
3ae 1H (DMSO-d6, 400 MHz)
1.041
1.098
1.108
1.122
1.108
1.000
3.081
1.095
1.094
11
10
9
8
7
6
5
4
3
2
1
0
ppm

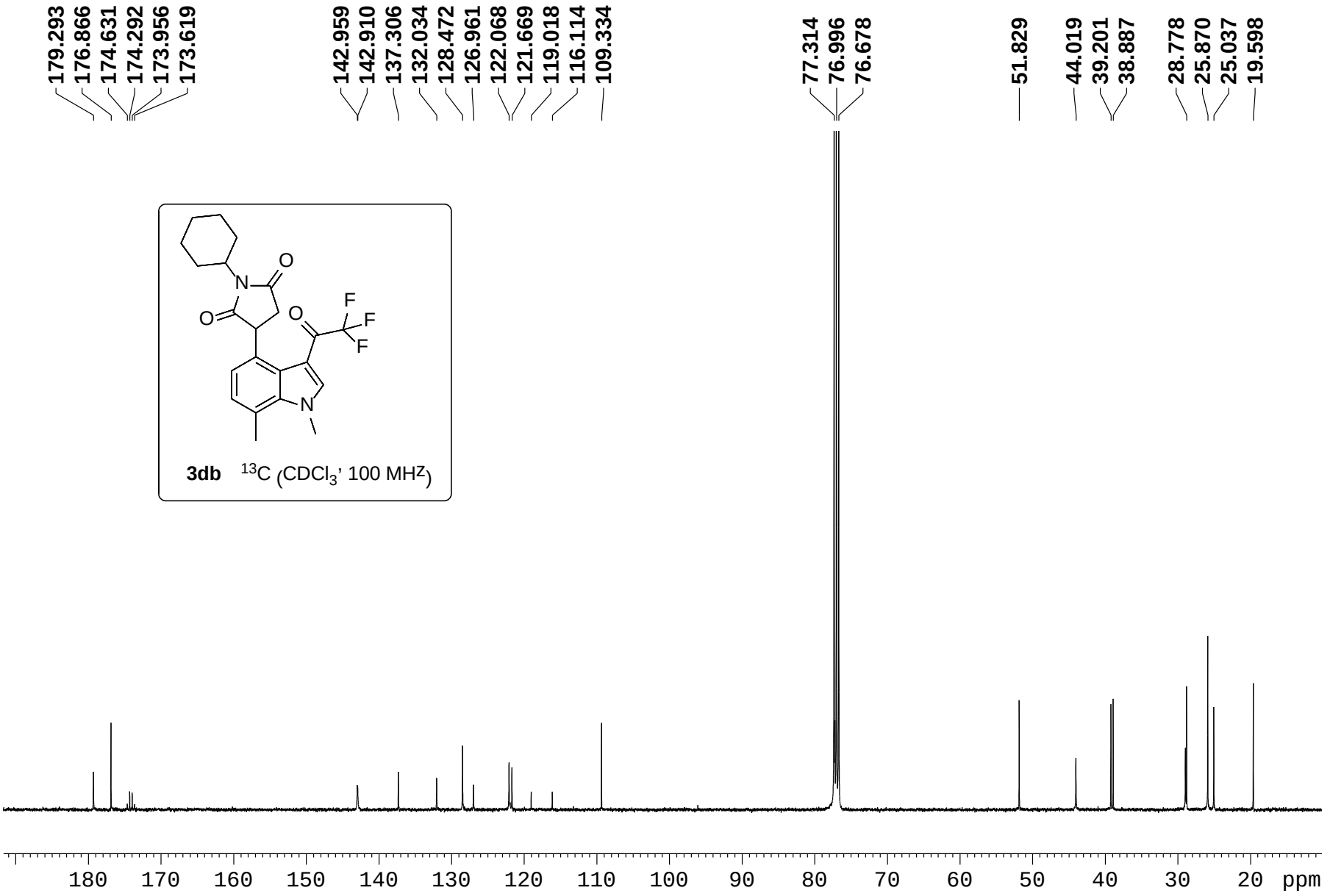


3ae ^{13}C ($DMSO^{-}d_6$, 100 MHz)

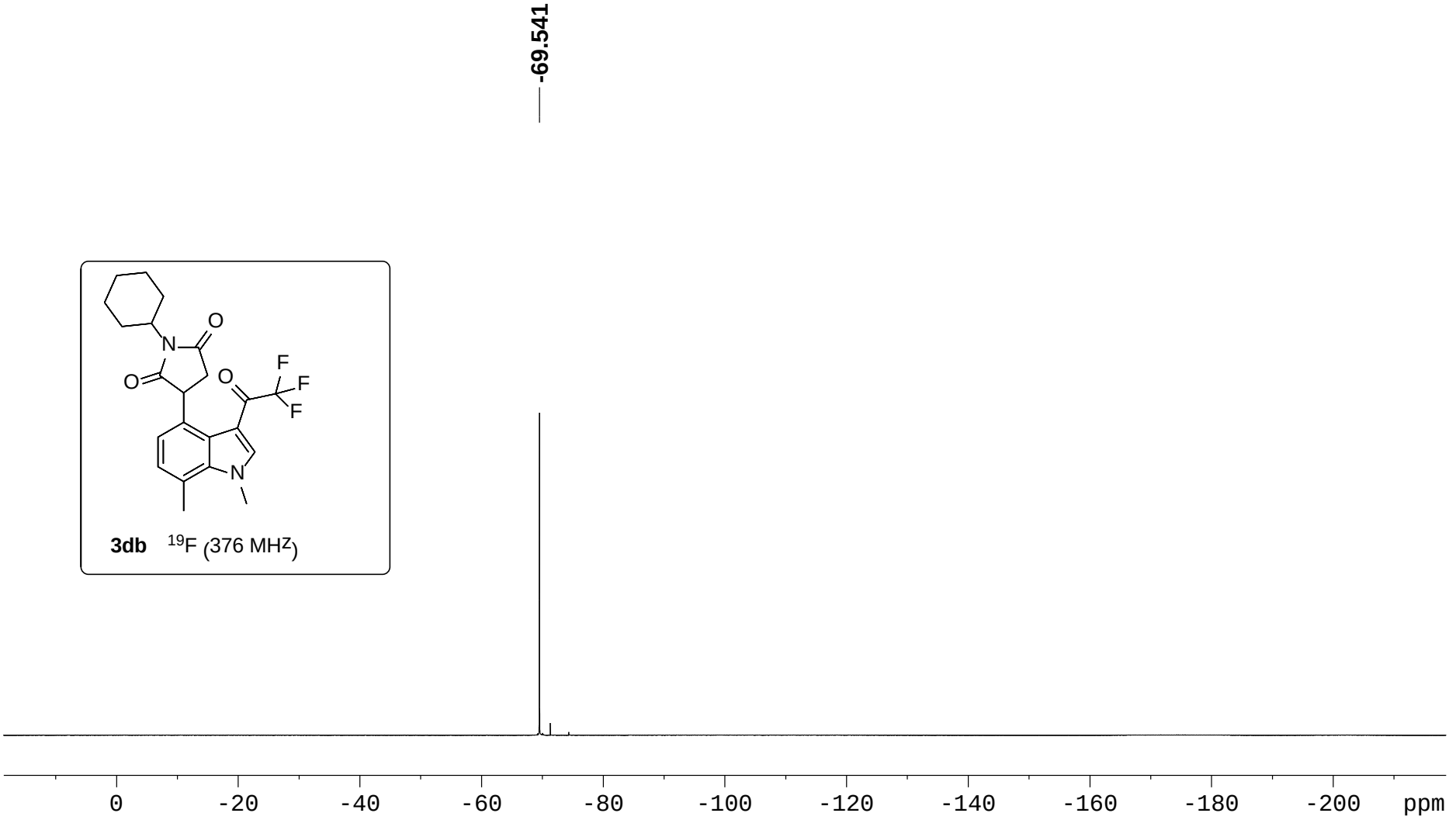


3ae ^{19}F (376 MHz)

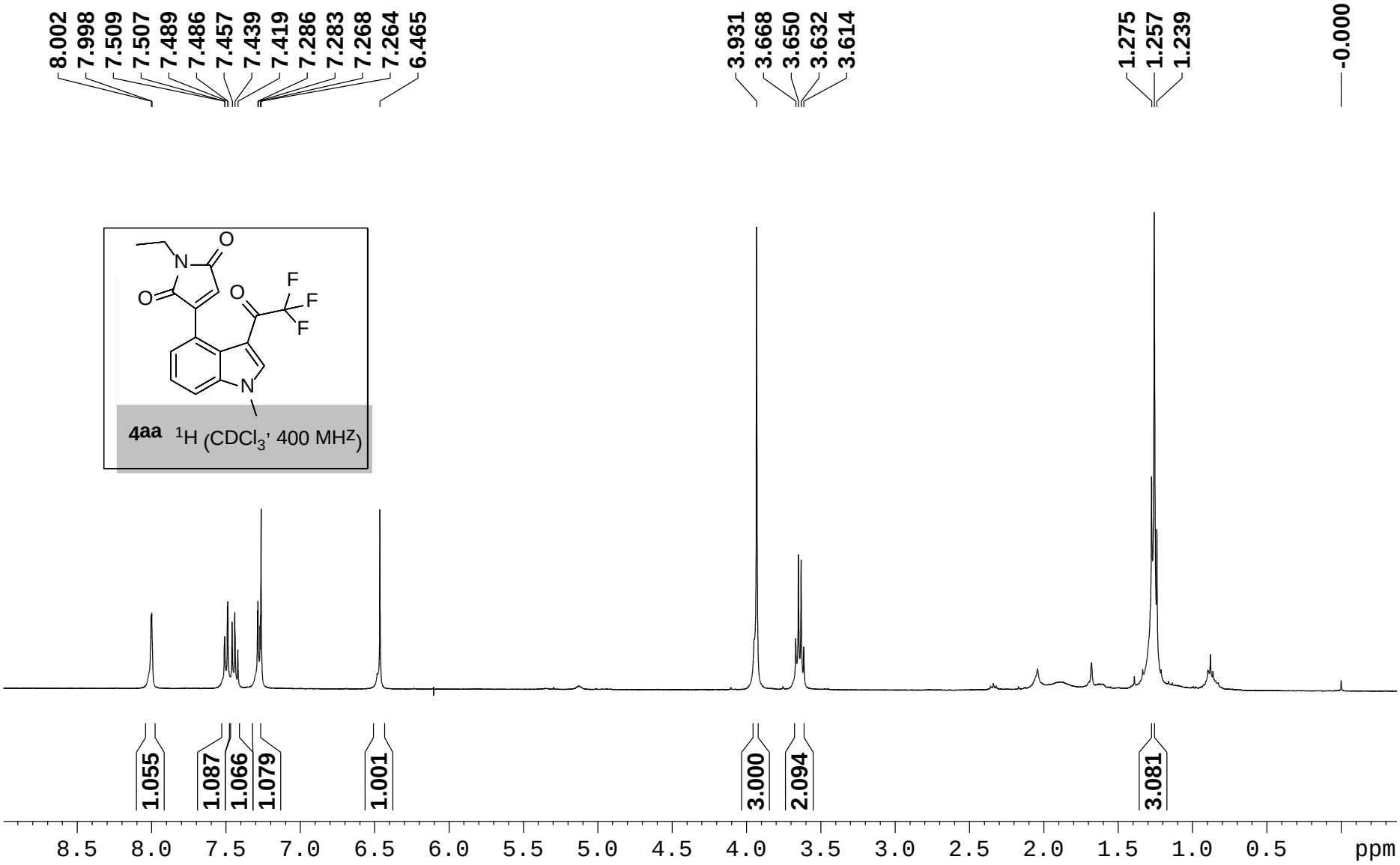

7.929
7.264
7.080
7.060
6.864
6.845
5.684
5.673
5.661
5.650
4.158
4.101
4.091
4.079
4.070
4.061
4.048
4.039
3.326
3.302
3.281
3.256
2.752
2.591
2.580
2.545
2.534
2.278
2.271
2.248
2.216
2.185
1.684
1.656
1.389
1.356
1.324
1.291
1.280
1.248
1.217
1.194
1.184
-0.000
O
N
O
O
F
F
F
N
3db 1H (CDCl3, 400 MHz)
1.091
1.043
1.063
1.041
3.011
1.018
1.045
3.127
1.075
2.093
4.000
4.009
9
8
7
6
5
4
3
2
1
0
ppm

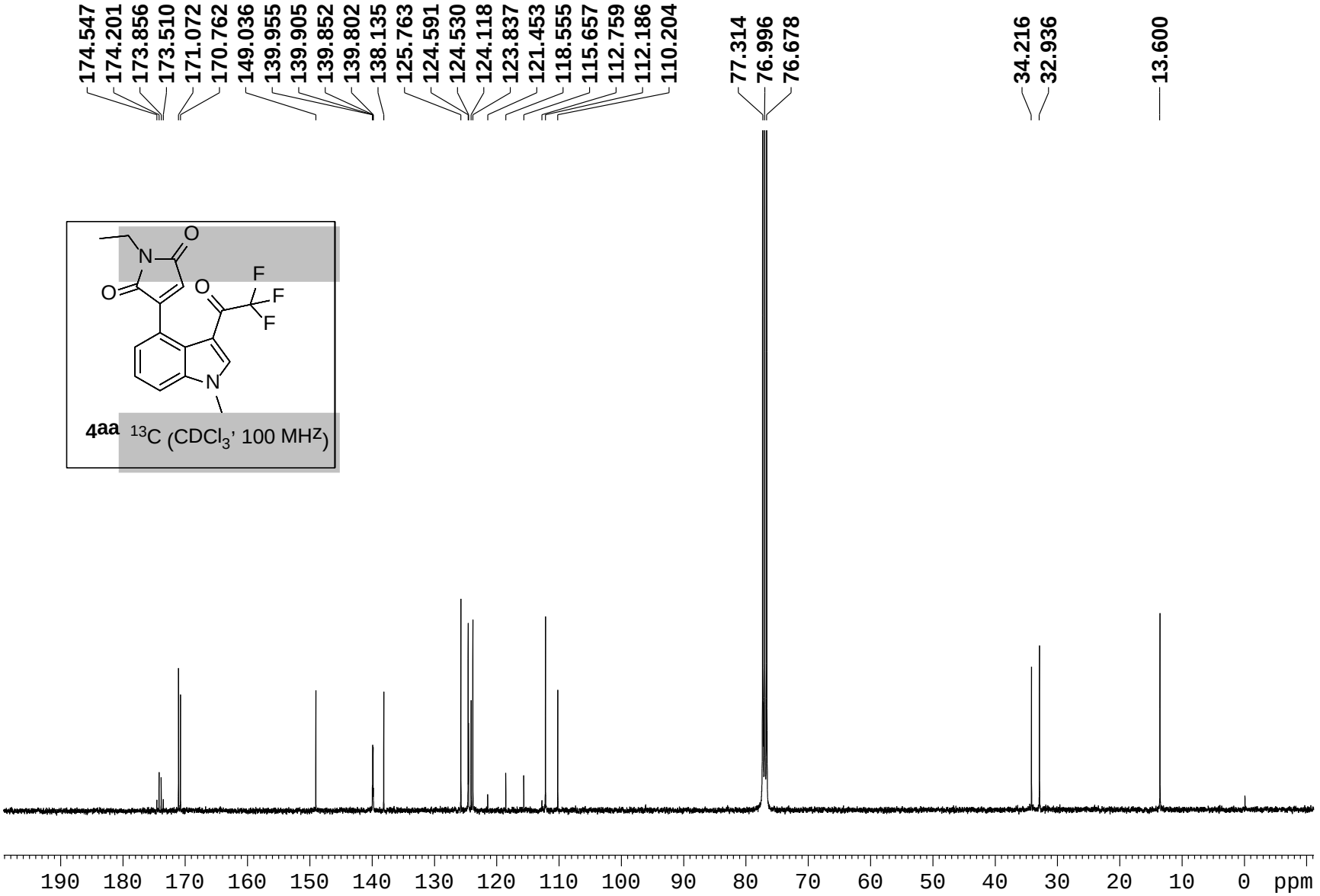


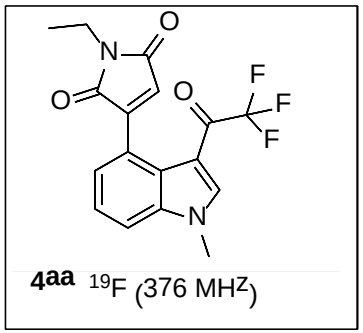
3db ^{13}C ($CDCl_3$, 100 MHz)



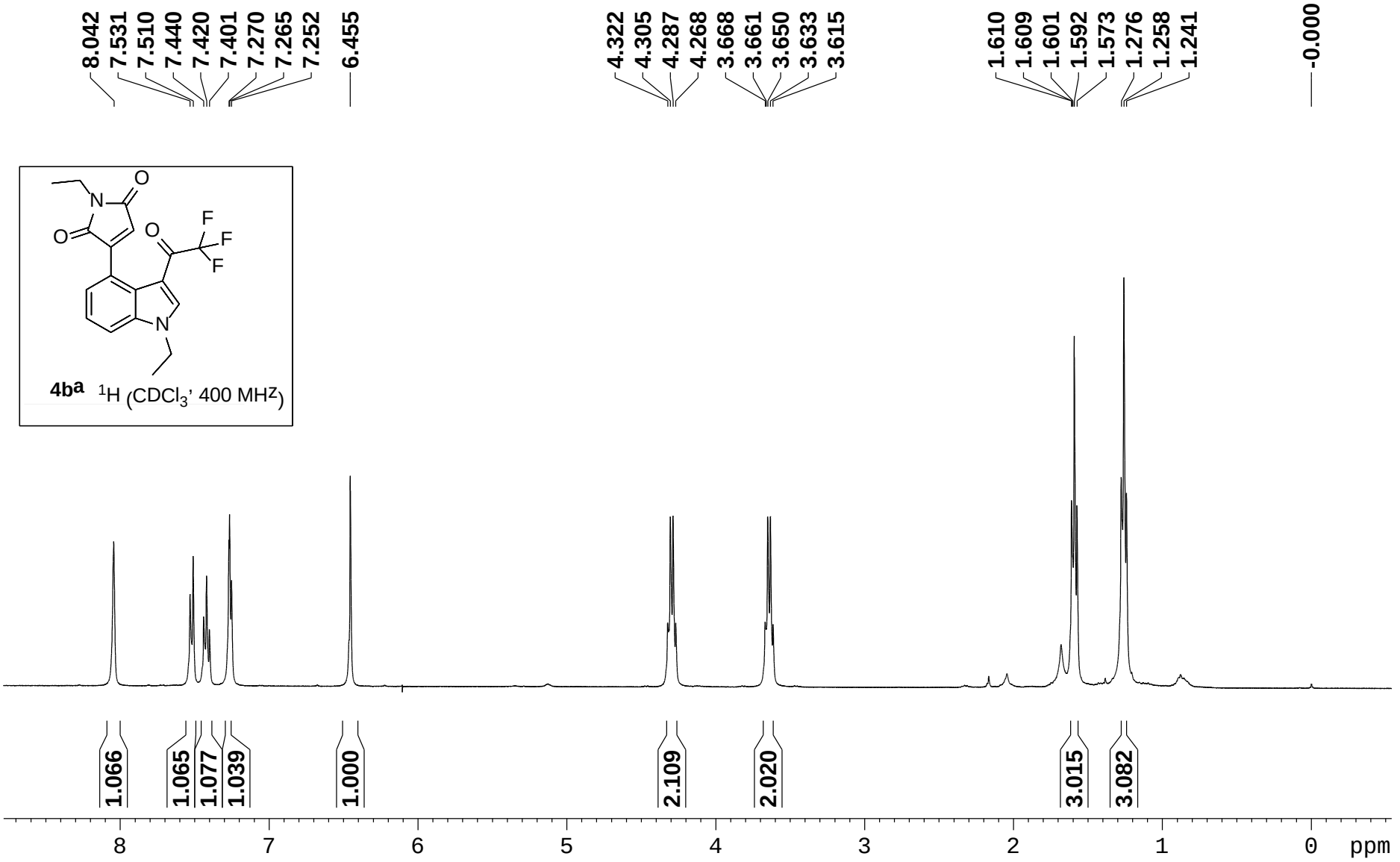
3db ^{19}F (376 MHz)

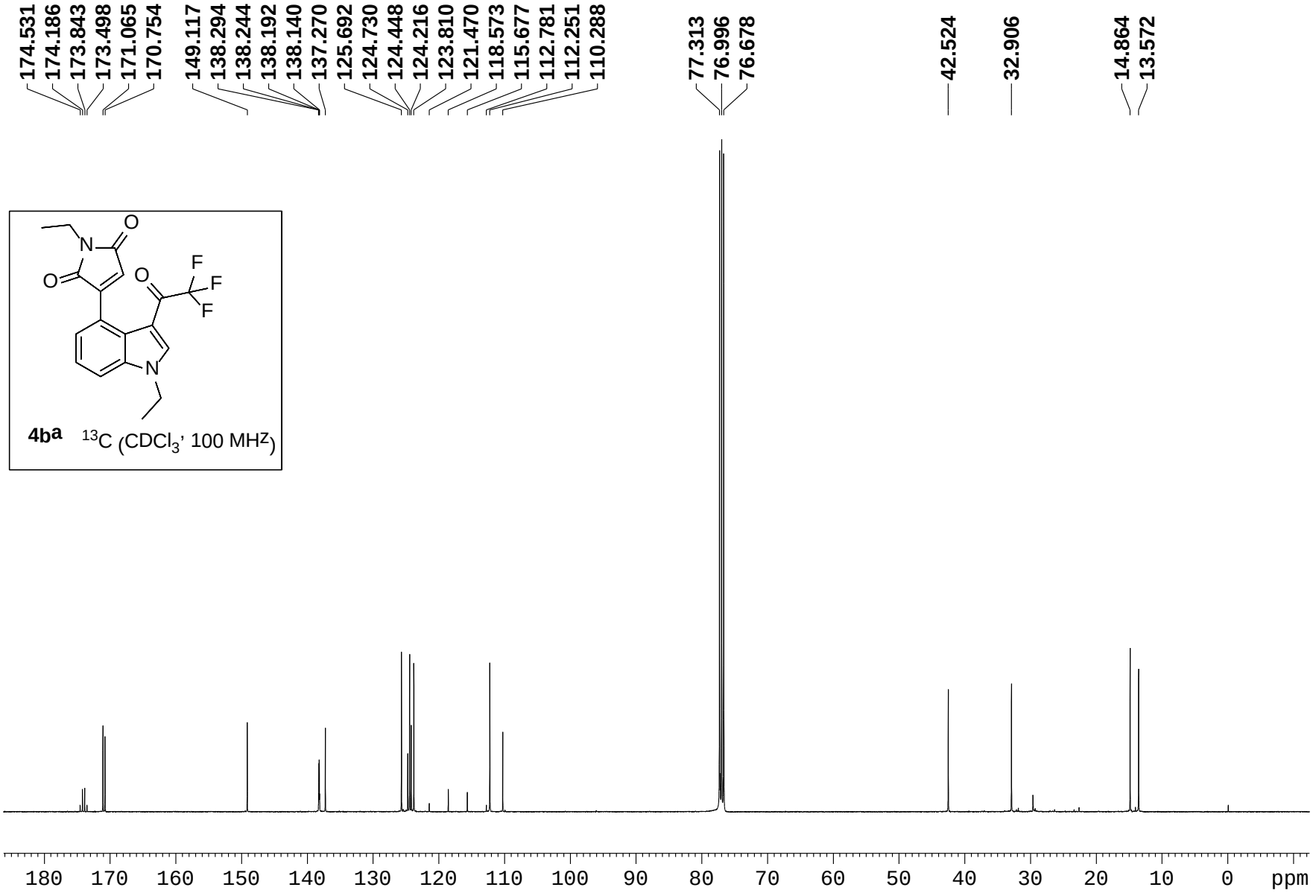

8.002
7.998
7.509
7.507
7.489
7.486
7.457
7.439
7.419
7.286
7.283
7.268
7.264
6.465
3.931
3.668
3.650
3.632
3.614
1.275
1.257
1.239
-0.000
4aa ^{1}H ($CDCl_3$, 400 MHz)
1.055
1.087
1.066
1.079
1.001
3.000
2.094
3.081
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

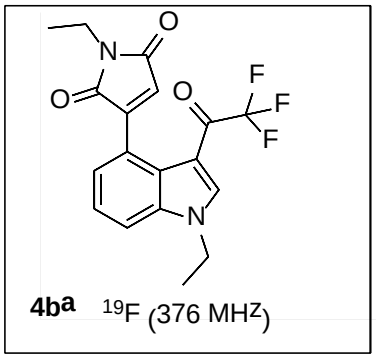

174.547
174.201
173.856
173.510
171.072
170.762
149.036
139.955
139.905
139.852
139.802
138.135
125.763
124.591
124.530
124.118
123.837
121.453
118.555
115.657
112.759
112.186
110.204
77.314
76.996
76.678
34.216
32.936
13.600
O
N
O
O
F
F
F
N
4aa 13C (CDCl3, 100 MHz)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



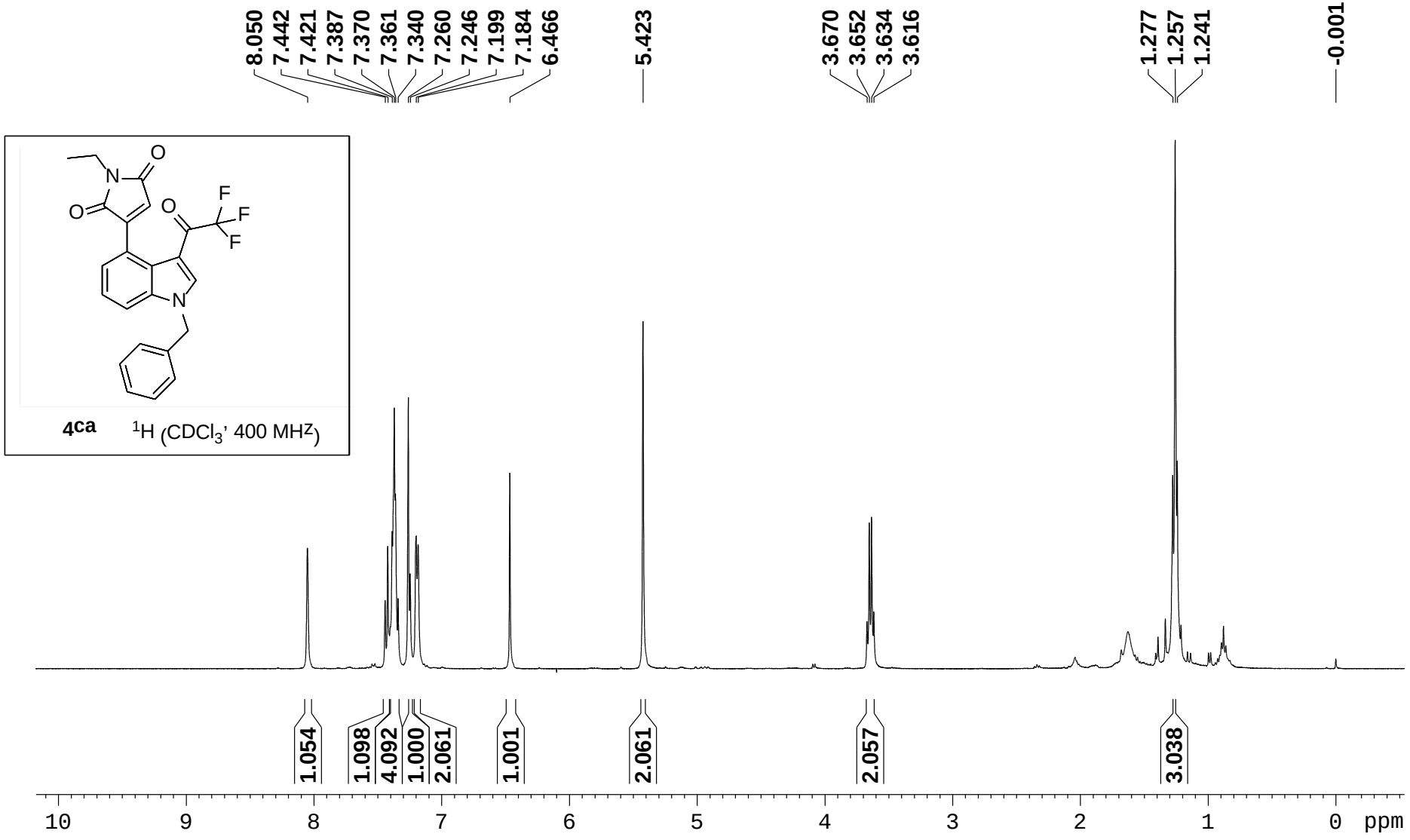
4aa ^{19}F (376 MHz)

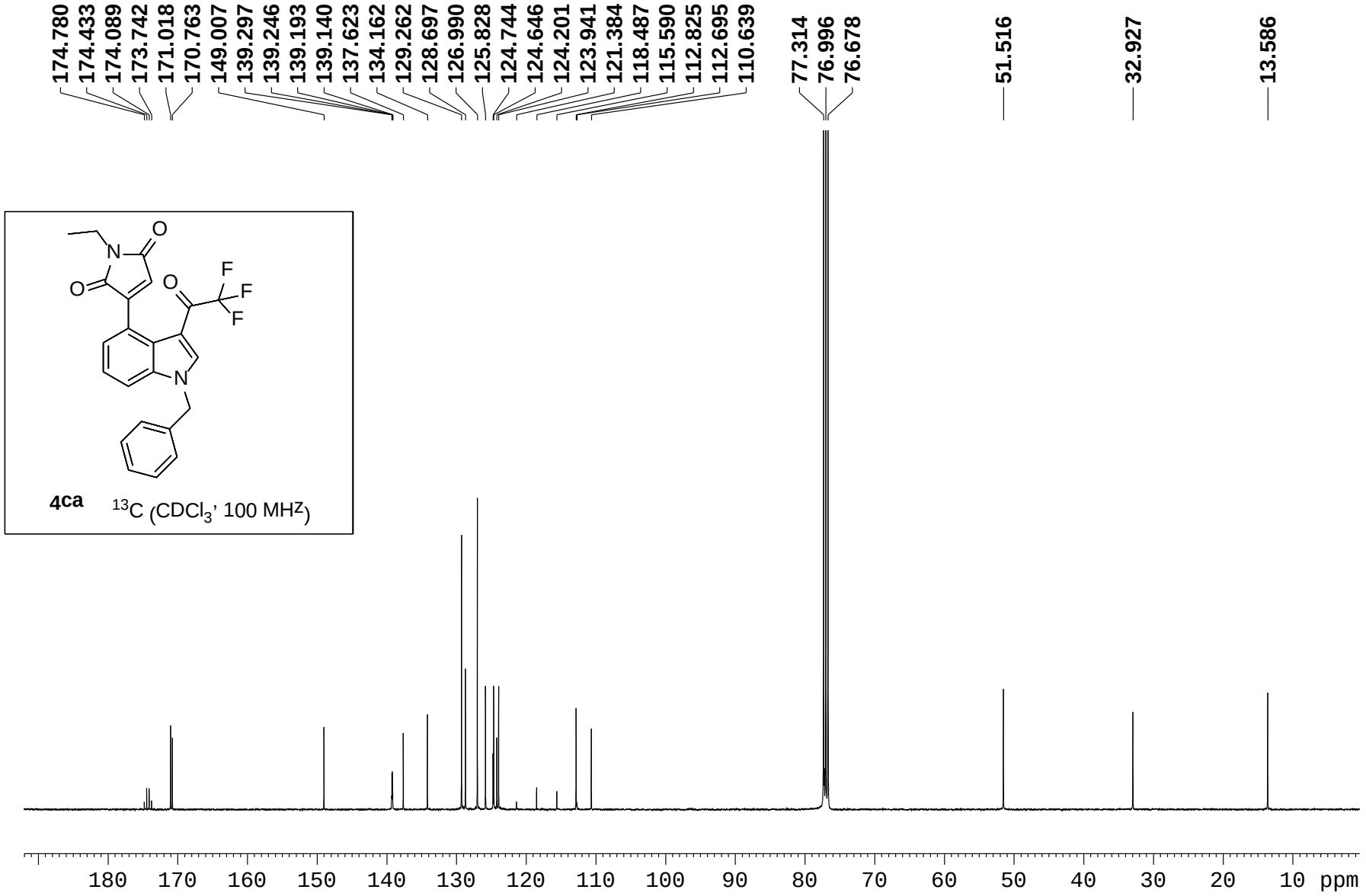

8.042
7.531
7.510
7.440
7.420
7.401
7.270
7.265
7.252
6.455
4.322
4.305
4.287
4.268
3.668
3.661
3.650
3.633
3.615
1.610
1.609
1.601
1.592
1.573
1.276
1.258
1.241
-0.000
4ba 1H (CDCl3, 400 MHz)
1.066
1.065
1.077
1.039
1.000
2.109
2.020
3.015
3.082
8
7
6
5
4
3
2
1
0
ppm

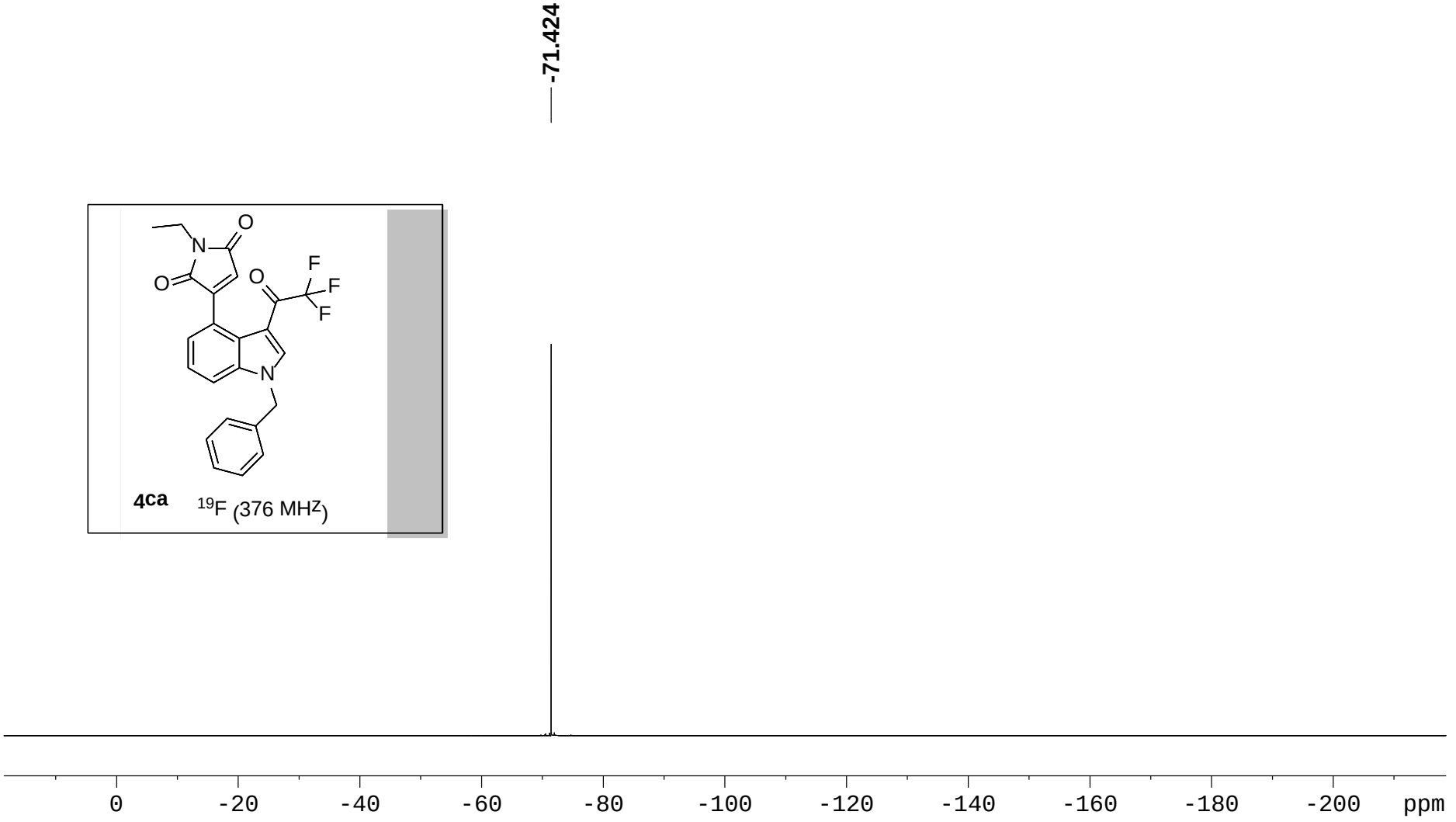

174.531
174.186
173.843
173.498
171.065
170.754
149.117
138.294
138.244
138.192
138.140
137.270
125.692
124.730
124.448
124.216
123.810
121.470
118.573
115.677
112.781
112.251
110.288
77.313
76.996
76.678
42.524
32.906
14.864
13.572
O
N
O
O
F
F
F
N
4b^a ^13C (CDCl3, 100 MHz)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

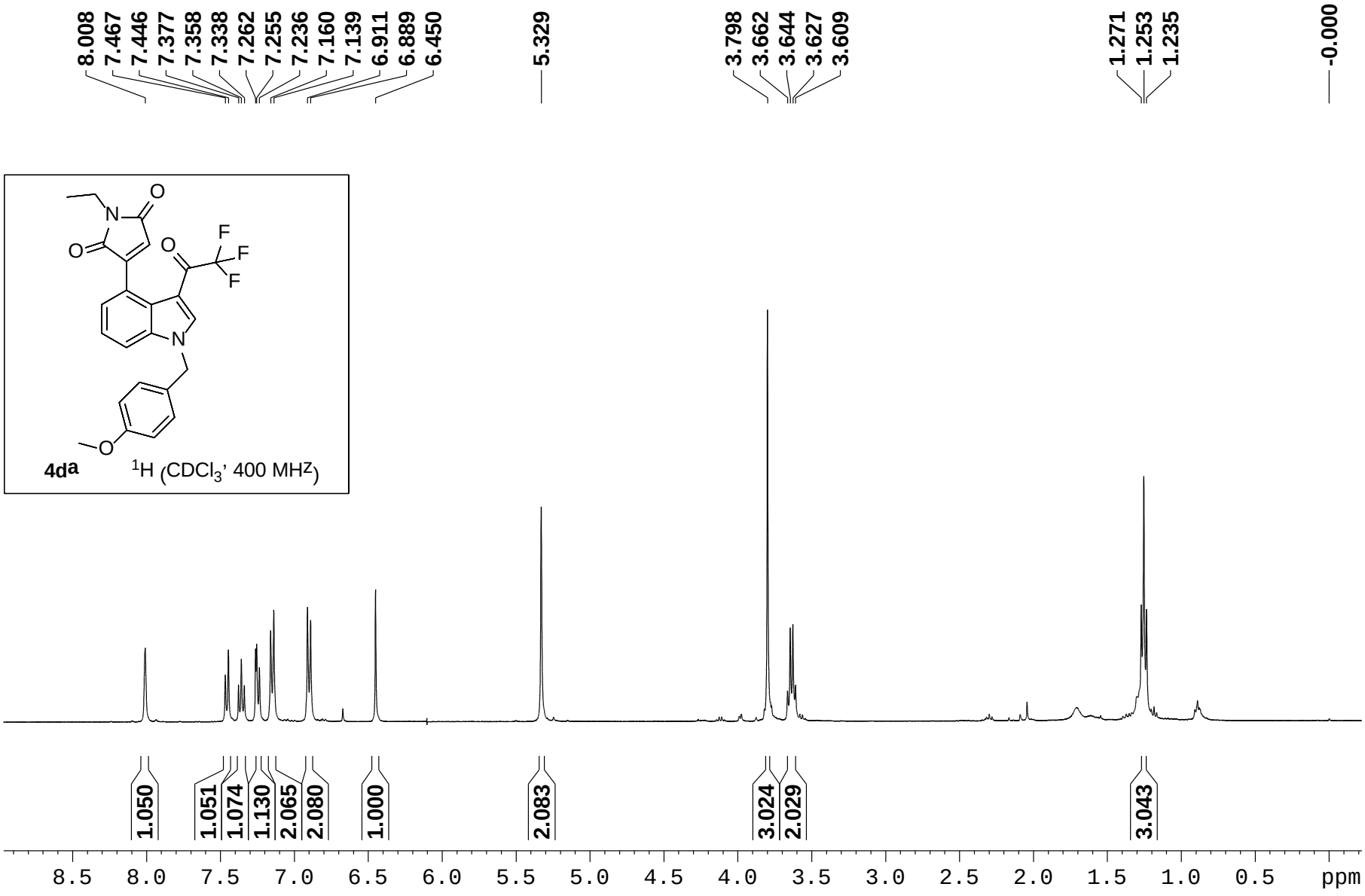


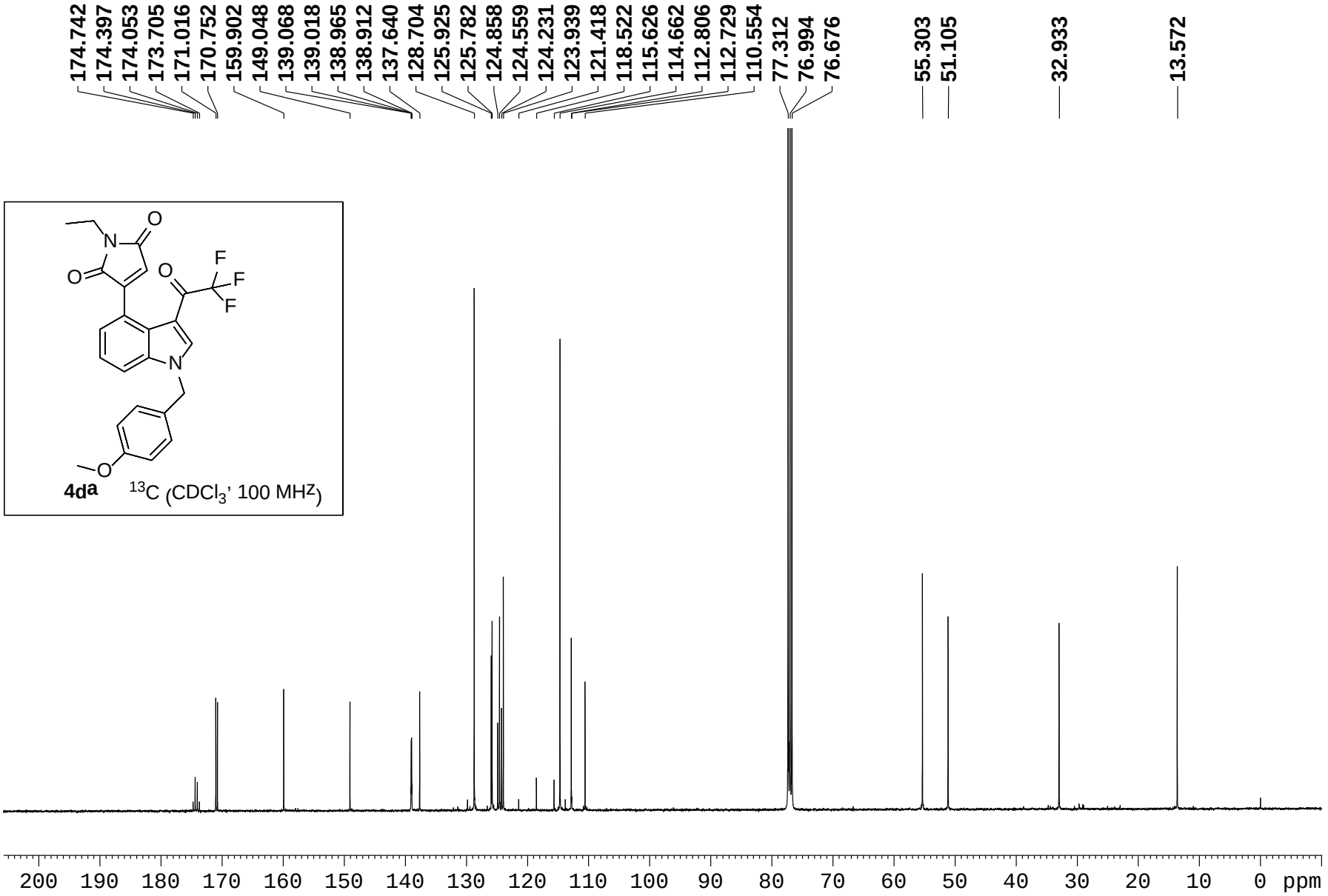
4ba ^{19}F (376 MHz)

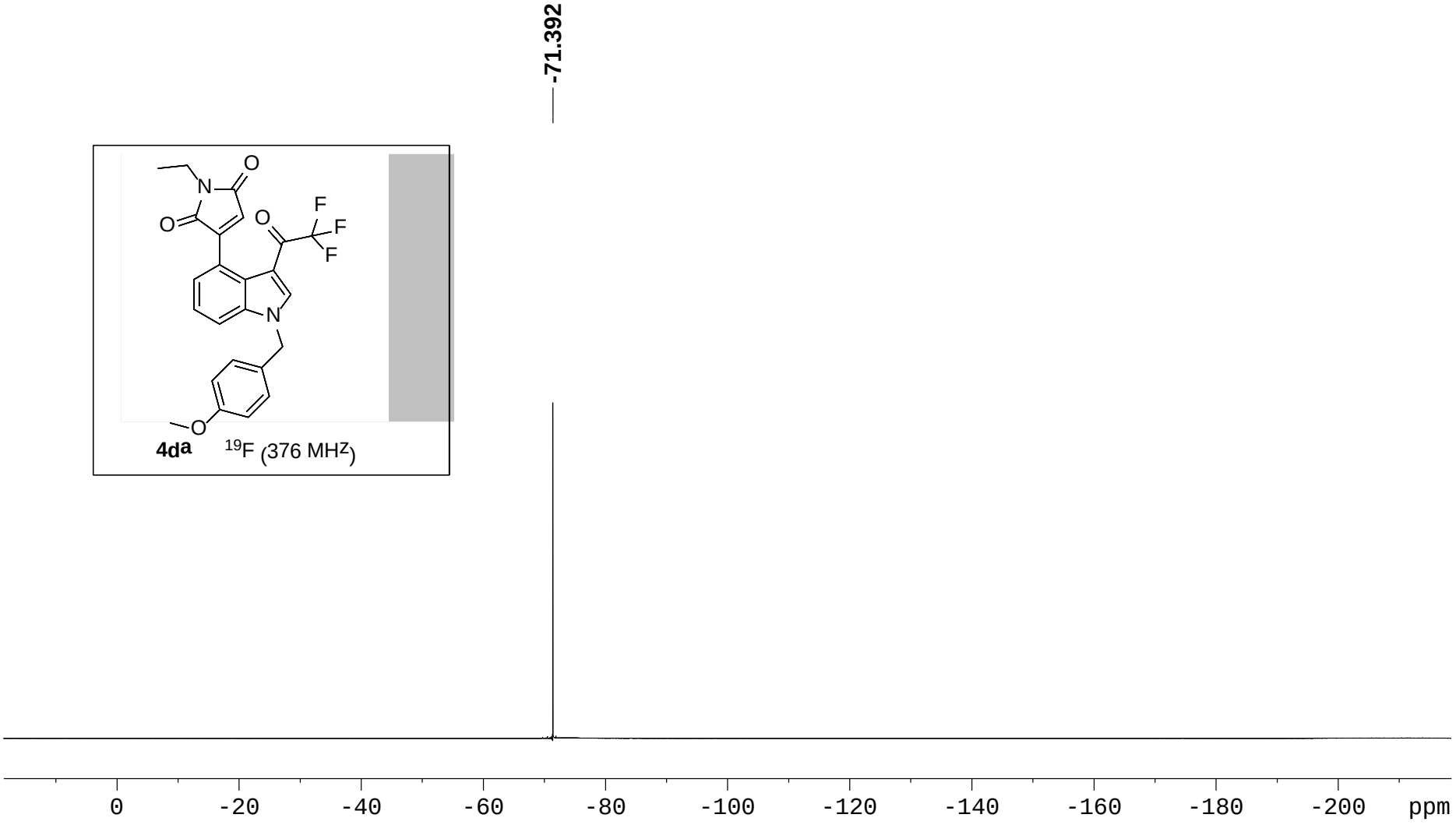

8.050
7.442
7.421
7.387
7.370
7.361
7.340
7.260
7.246
7.199
7.184
6.466
5.423
3.670
3.652
3.634
3.616
1.277
1.257
1.241
-0.001
4ca
1H (CDCl3, 400 MHz)
1.054
1.098
4.092
1.000
2.061
1.001
2.061
2.057
3.038
10
9
8
7
6
5
4
3
2
1
0
ppm

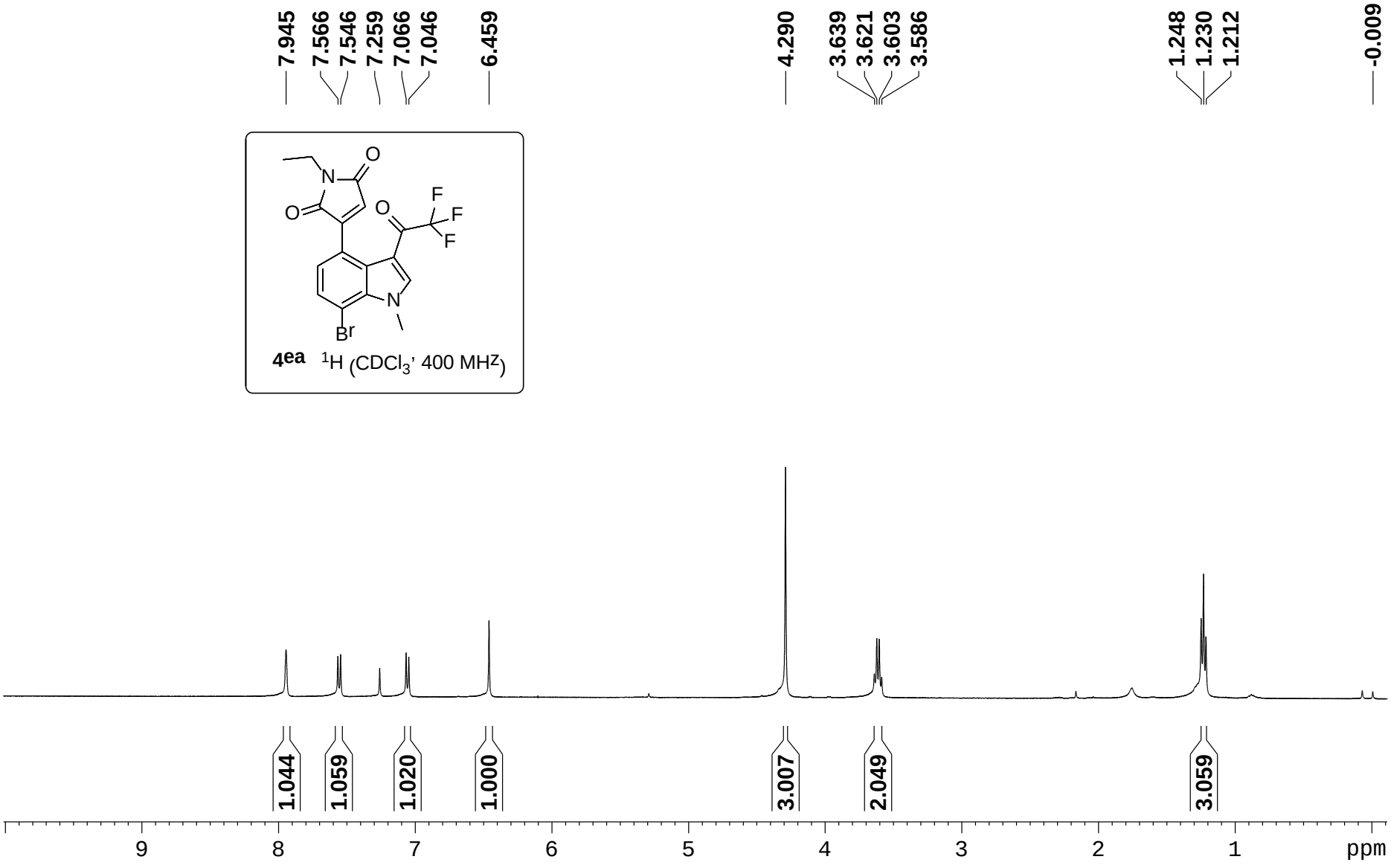

174.780
174.433
174.089
173.742
171.018
170.763
149.007
139.297
139.246
139.193
139.140
137.623
134.162
129.262
128.697
126.990
125.828
124.744
124.646
124.201
123.941
121.384
118.487
115.590
112.825
112.695
110.639
77.314
76.996
76.678
51.516
32.927
13.586
O
N
O
O
F
F
F
N
4ca
13C (CDCl3, 100 MHz)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

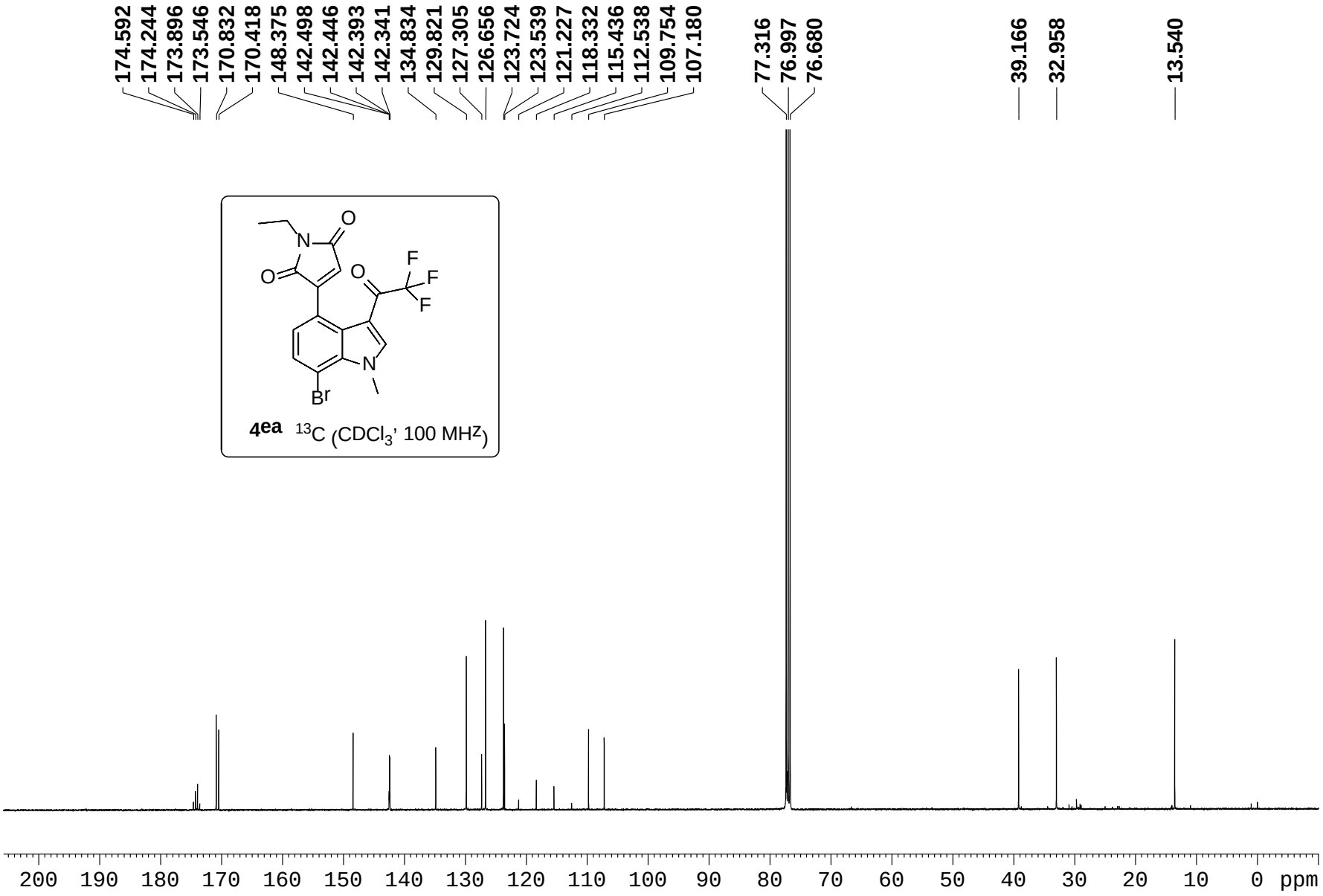

-71.424
4ca
19F (376 MHz)
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

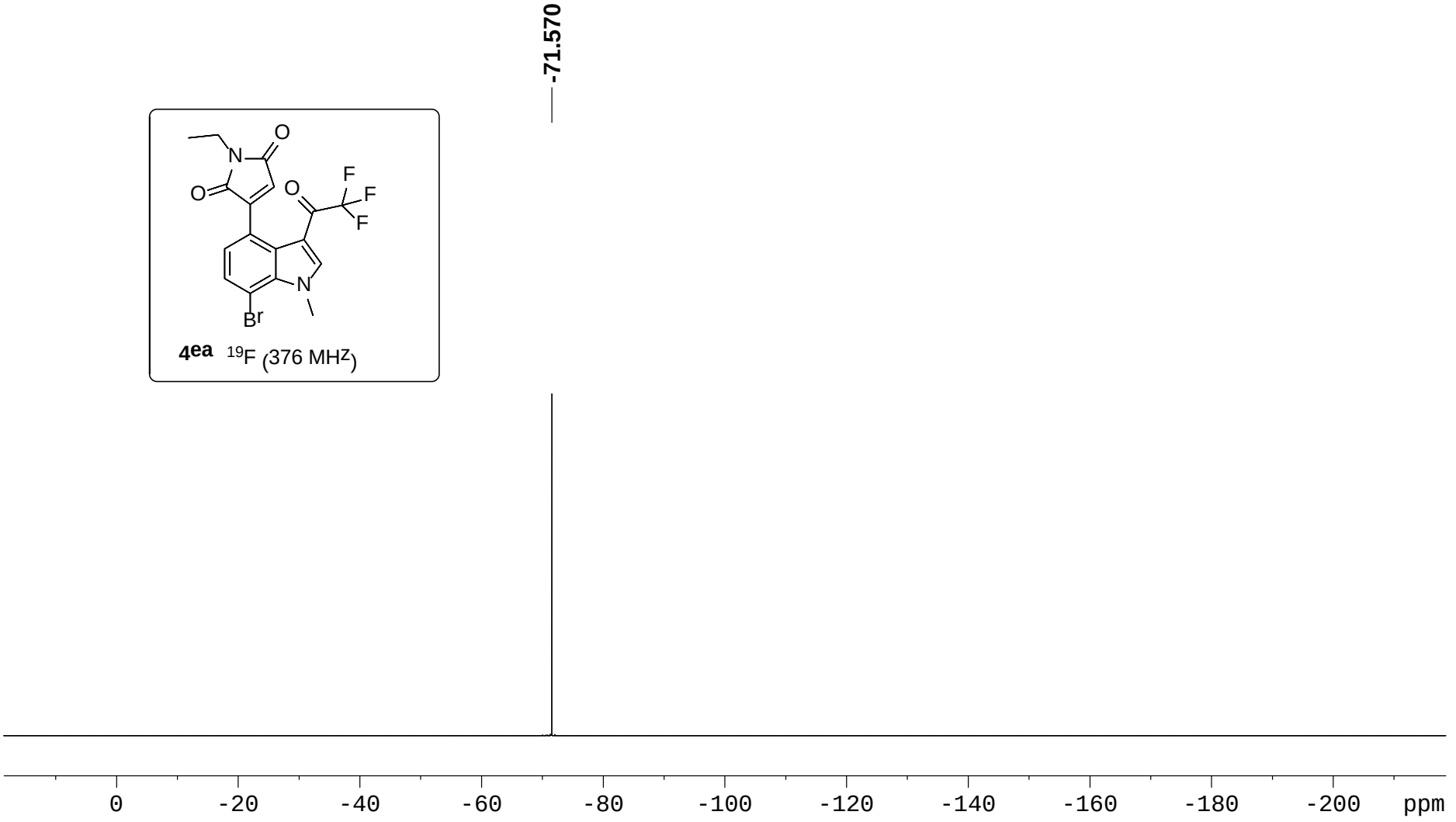

8.008
7.467
7.446
7.377
7.358
7.338
7.262
7.255
7.236
7.160
7.139
6.911
6.889
6.450
5.329
3.798
3.662
3.644
3.627
3.609
1.271
1.253
1.235
-0.000
4d^a
1H (CDCl3, 400 MHz)
1.050
1.051
1.074
1.130
2.065
2.080
1.000
2.083
3.024
2.029
3.043
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

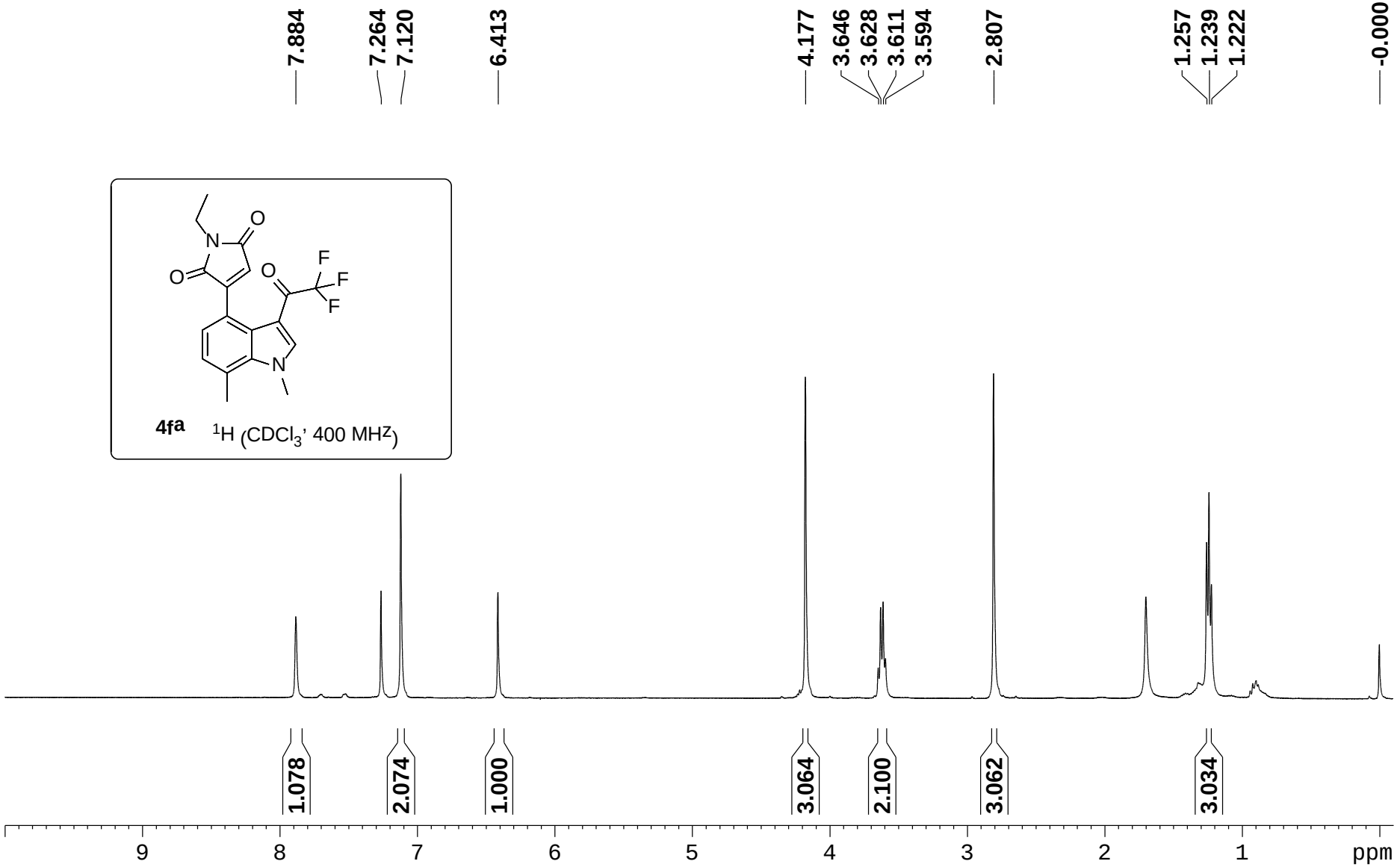

174.742
174.397
174.053
173.705
171.016
170.752
159.902
149.048
139.068
139.018
138.965
138.912
137.640
128.704
125.925
125.782
124.858
124.559
124.231
123.939
121.418
118.522
115.626
114.662
112.806
112.729
110.554
77.312
76.994
76.676
55.303
51.105
32.933
13.572
O
N
O
O
F
F
F
N
O
4d^a
13C (CDCl3, 100 MHz)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

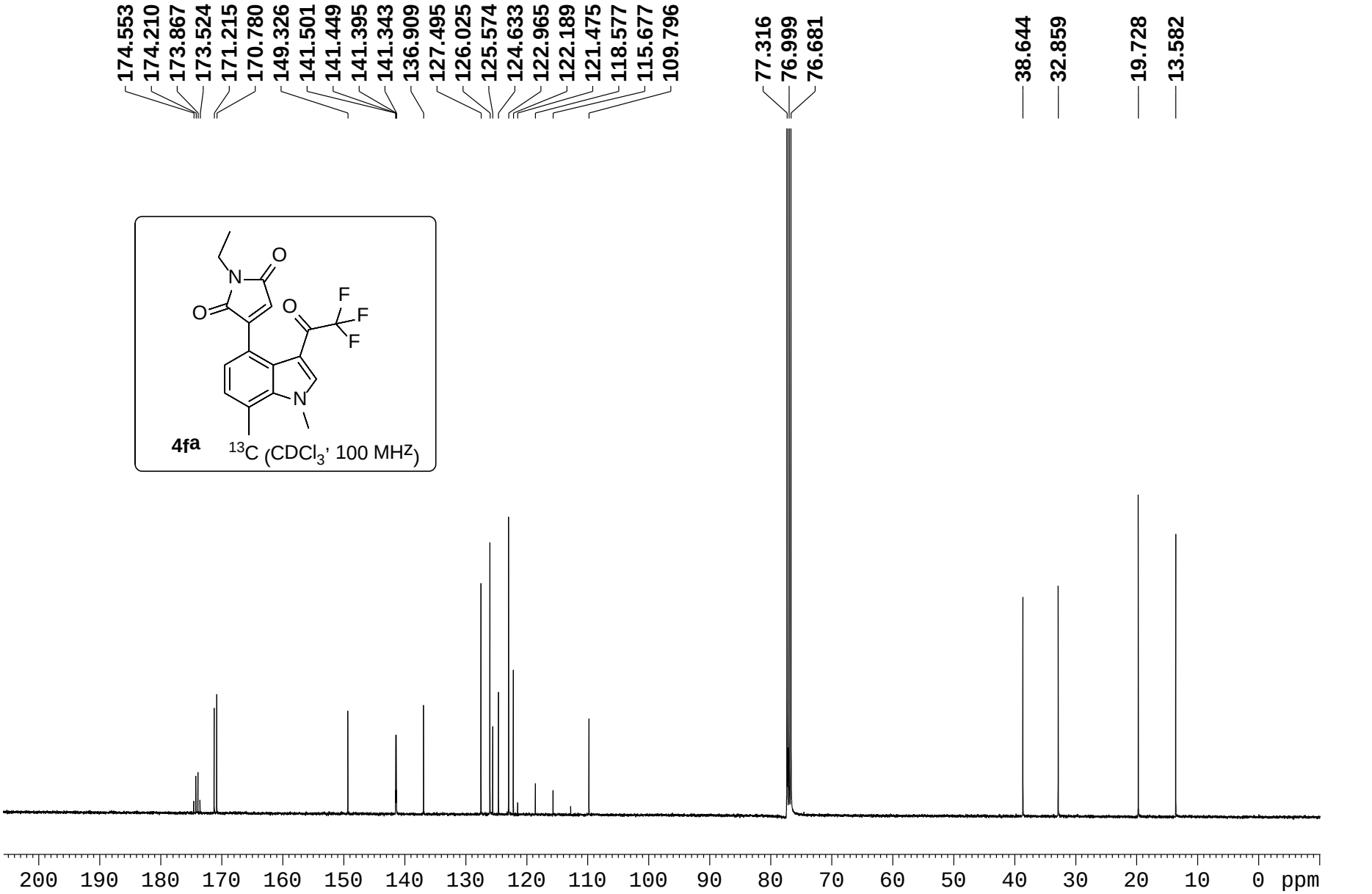

-71.392
4d[a] ^{19}F (376 MHz)
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

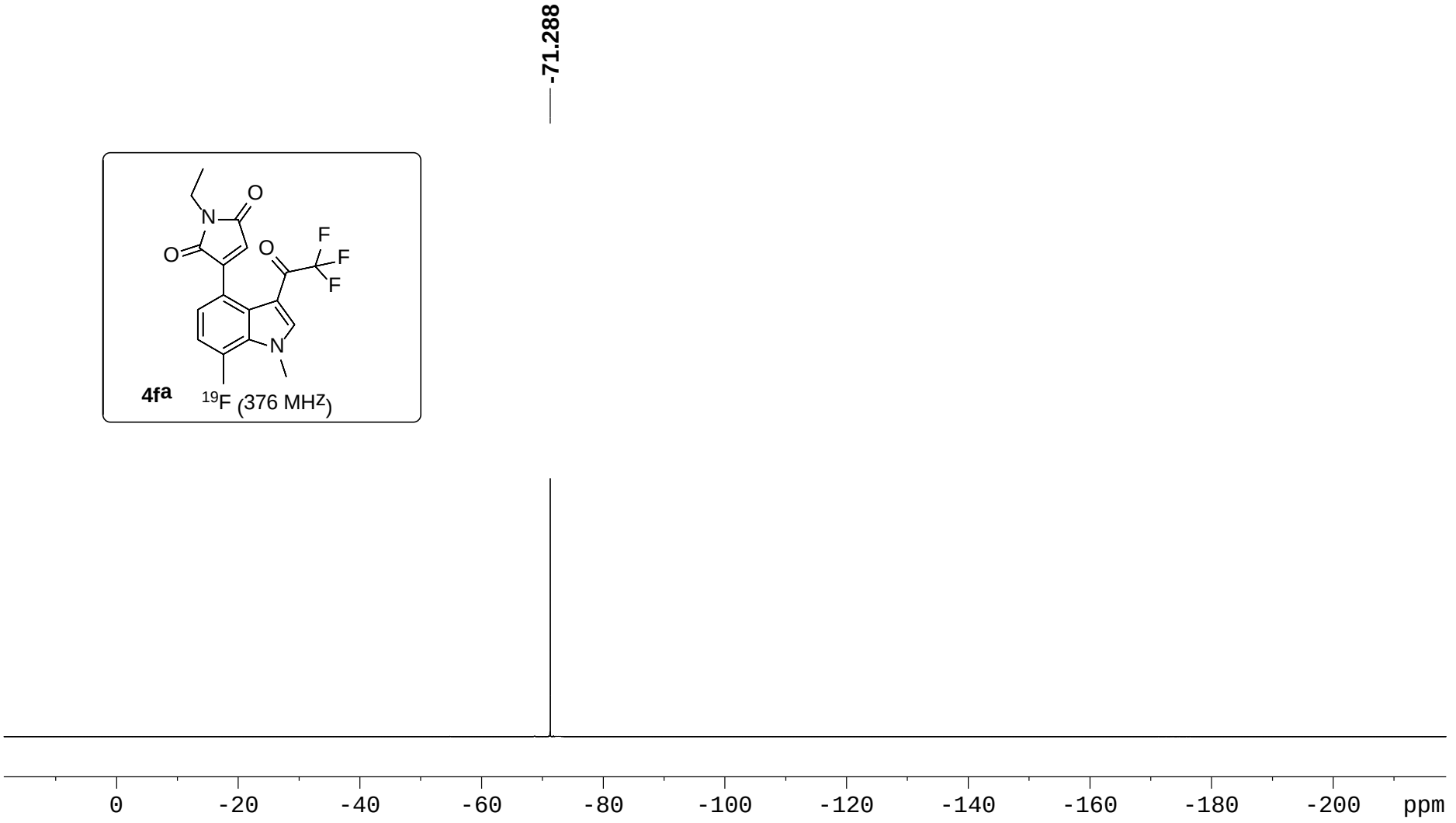

7.945
7.566
7.546
7.259
7.066
7.046
6.459
4.290
3.639
3.621
3.603
3.586
1.248
1.230
1.212
-0.009
O
N
O
O
F
F
F
N
Br
4ea ¹H (CDCl3, 400 MHz)
1.044
1.059
1.020
1.000
3.007
2.049
3.059
9
8
7
6
5
4
3
2
1
ppm

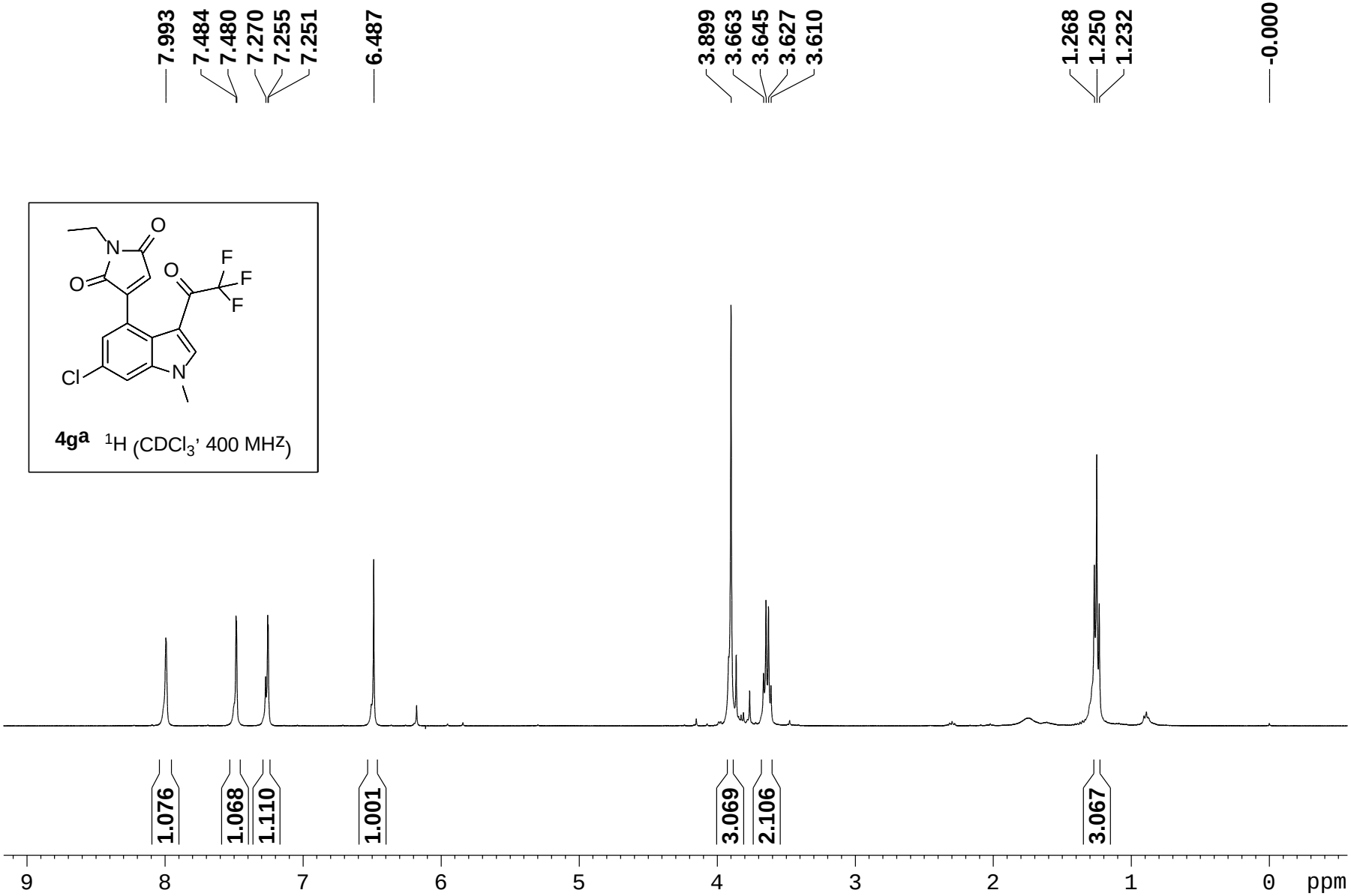

174.592
174.244
173.896
173.546
170.832
170.418
148.375
142.498
142.446
142.393
142.341
134.834
129.821
127.305
126.656
123.724
123.539
121.227
118.332
115.436
112.538
109.754
107.180
77.316
76.997
76.680
39.166
32.958
13.540
O
N
O
O
F
F
F
N
Br
4ea 13C (CDCl3, 100 MHz)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

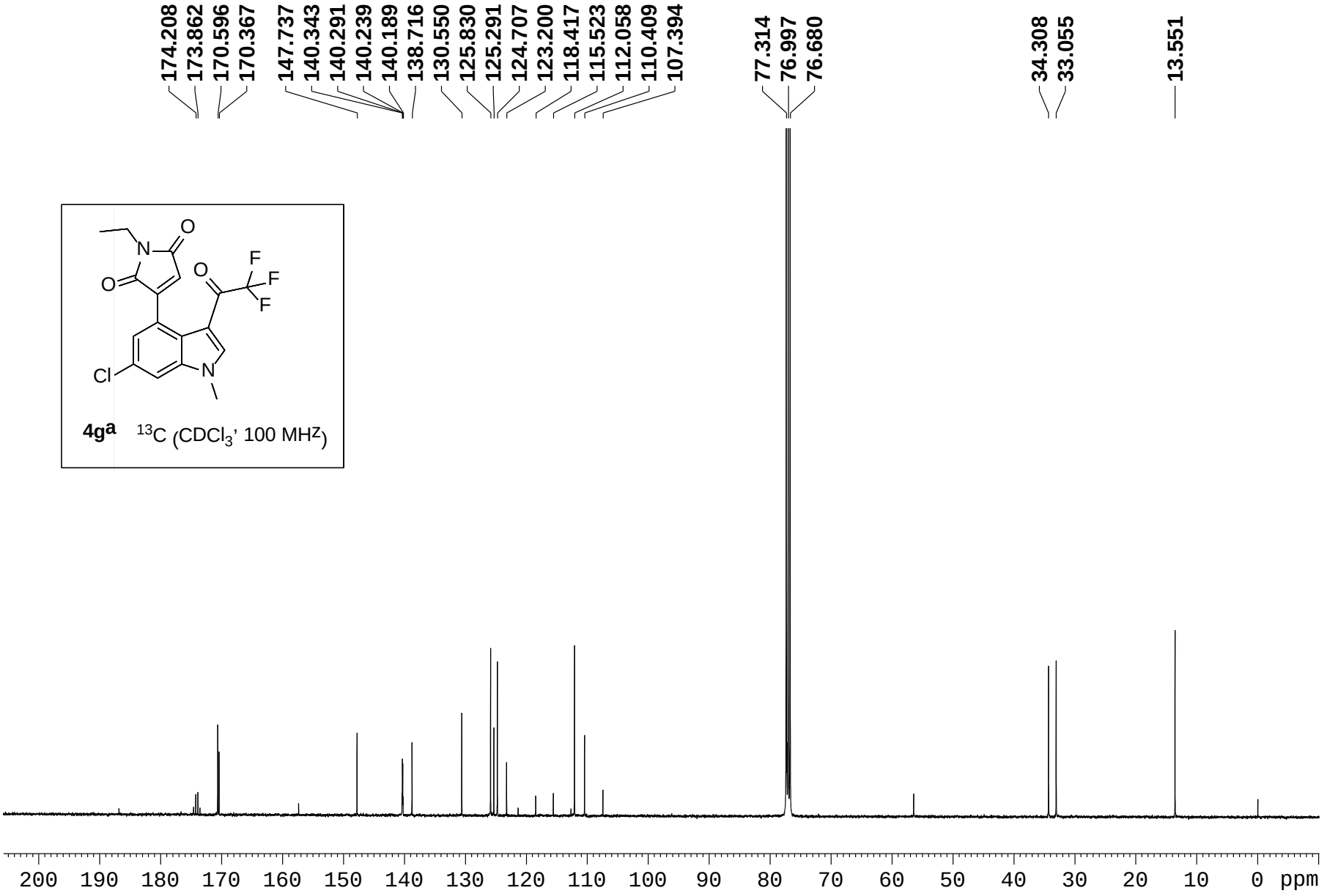

-71.570
O
N
O
O
F
F
F
N
Br
4ea 19F (376 MHz)
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

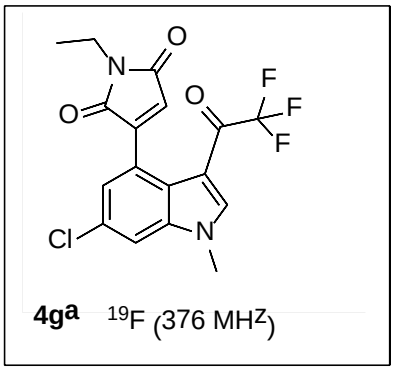

7.884
7.264
7.120
6.413
4.177
3.646
3.628
3.611
3.594
2.807
1.257
1.239
1.222
-0.000
O
N
O
O
F
F
F
N
4fa
1H (CDCl3, 400 MHz)
1.078
2.074
1.000
3.064
2.100
3.062
3.034
9
8
7
6
5
4
3
2
1
ppm


174.553
174.210
173.867
173.524
171.215
170.780
149.326
141.501
141.449
141.395
141.343
136.909
127.495
126.025
125.574
124.633
122.965
122.189
121.475
118.577
115.677
109.796
77.316
76.999
76.681
38.644
32.859
19.728
13.582
O
N
O
O
F
F
F
N
4fa
13C (CDCl3, 100 MHZ)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

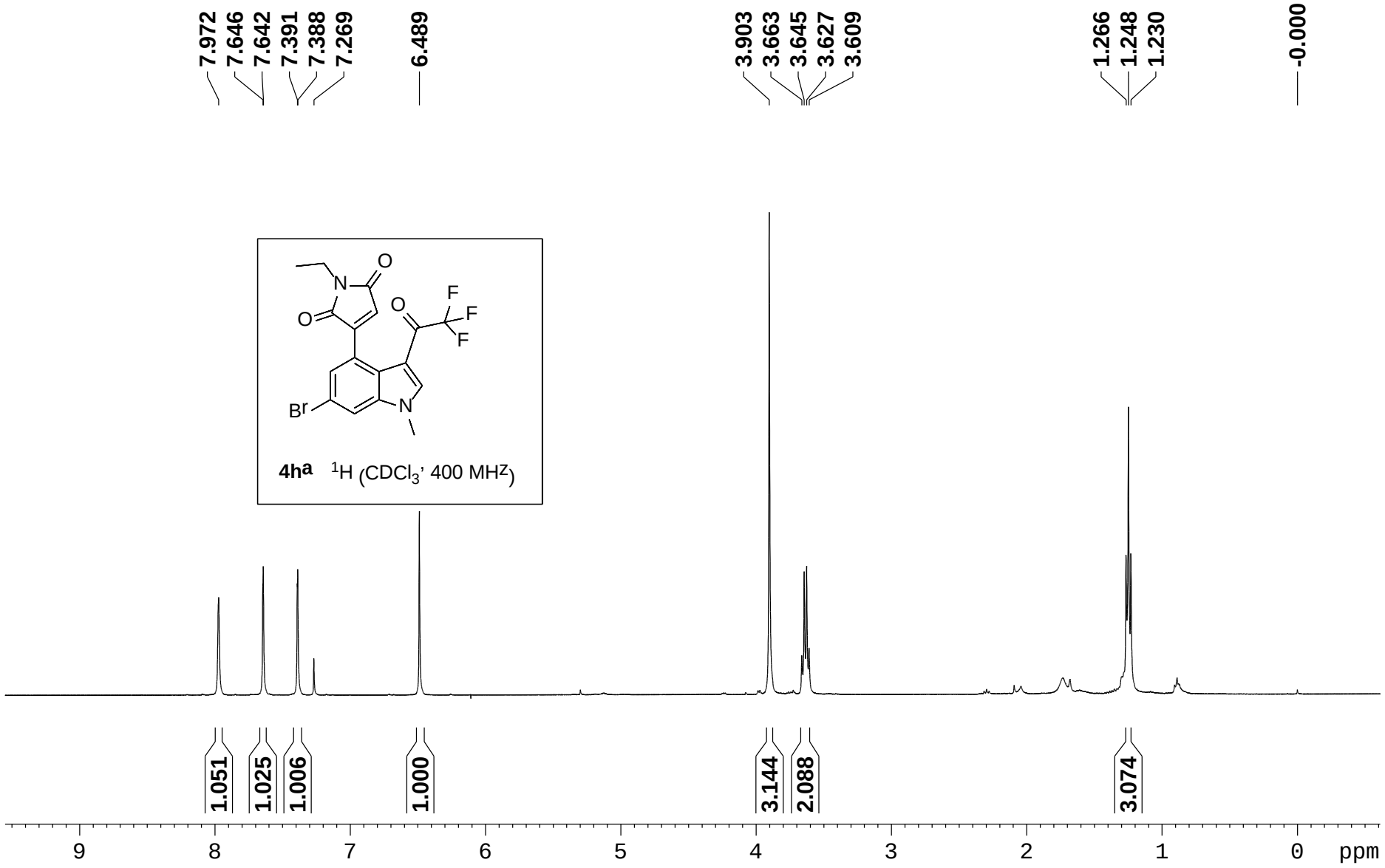

-71.288
4fa
19F (376 MHz)
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

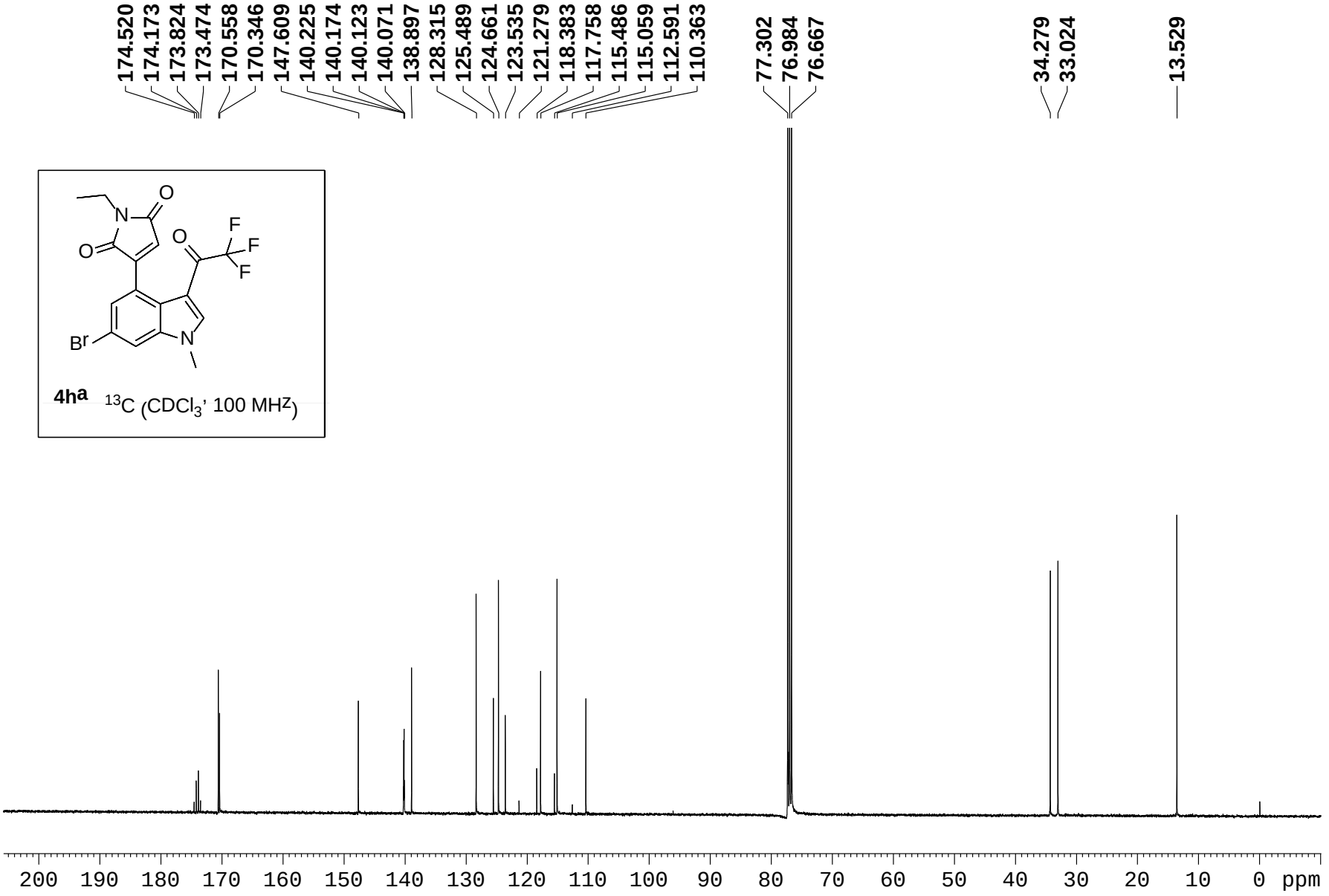

7.993
7.484
7.480
7.270
7.255
7.251
6.487
3.899
3.663
3.645
3.627
3.610
1.268
1.250
1.232
-0.000
O
N
O
O
F
F
F
Cl
N
4ga 1H (CDCl3, 400 MHz)
1.076
1.068
1.110
1.001
3.069
2.106
3.067
9
8
7
6
5
4
3
2
1
0
ppm

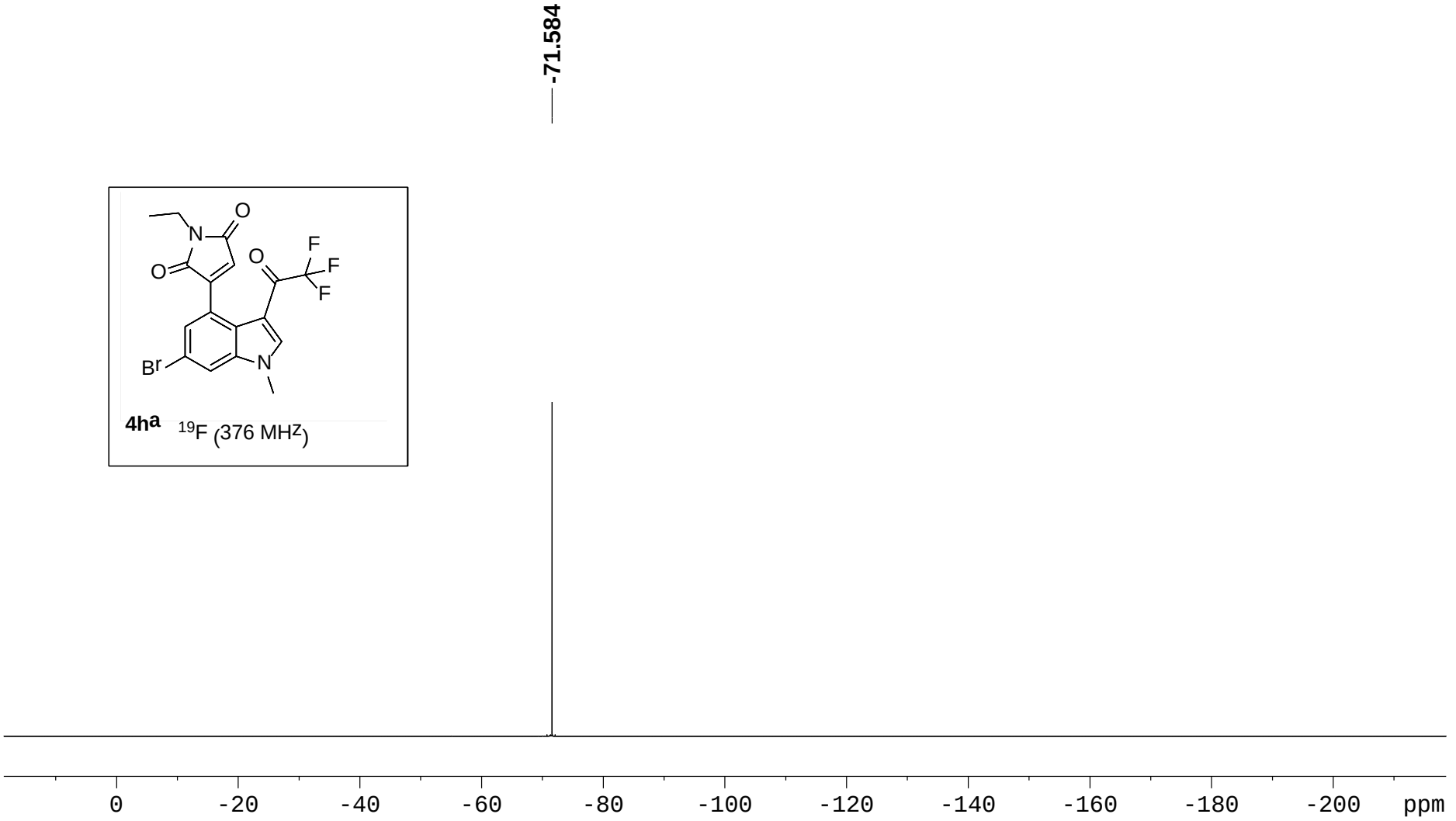

174.208
173.862
170.596
170.367
147.737
140.343
140.291
140.239
140.189
138.716
130.550
125.830
125.291
124.707
123.200
118.417
115.523
112.058
110.409
107.394
77.314
76.997
76.680
34.308
33.055
13.551
O
N
O
O
F
F
F
Cl
N
4g[a] ^{13}C ($CDCl_3$, 100 MHz)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

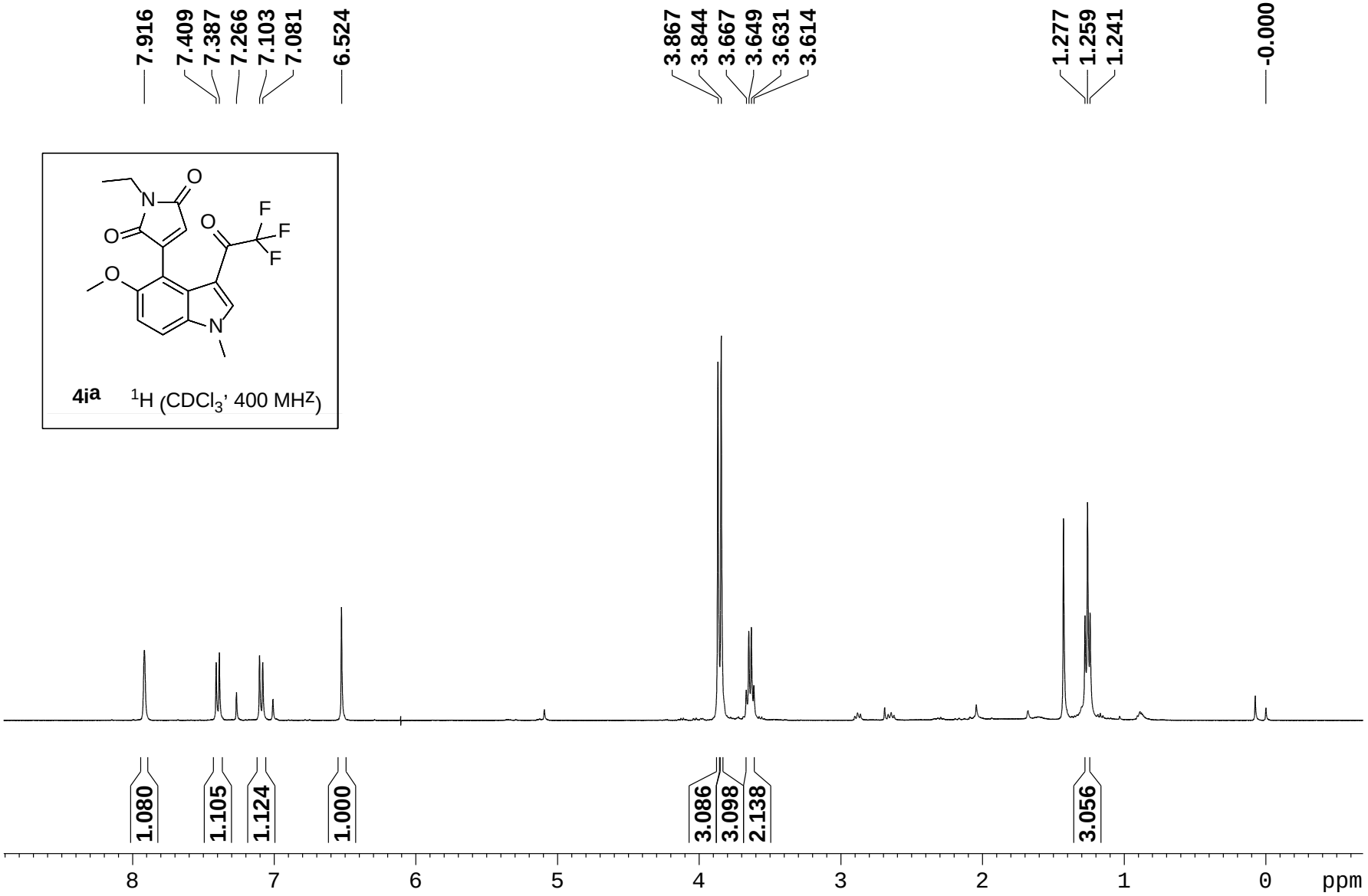


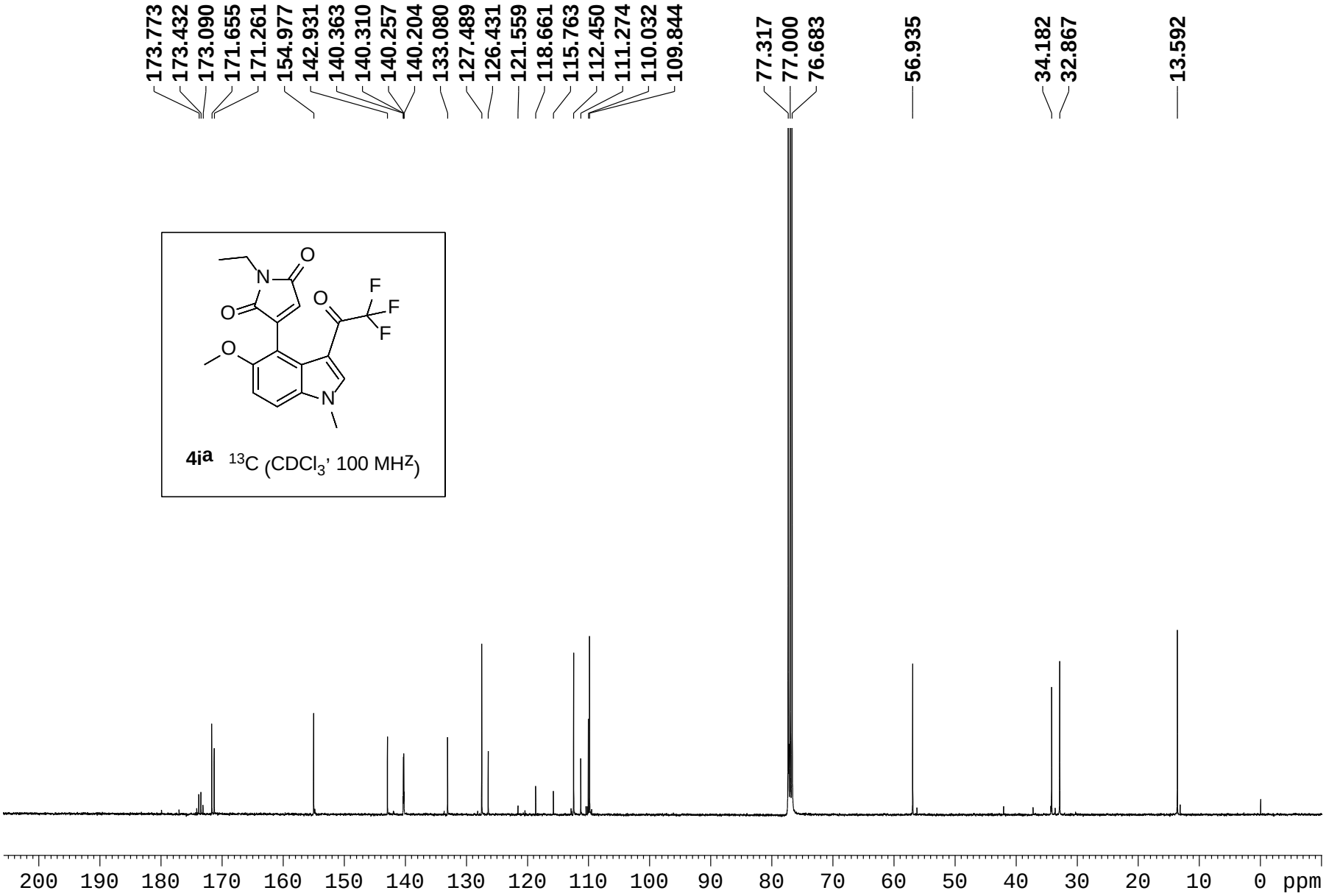
4g[a] ^{19}F (376 MHz)


7.972
7.646
7.642
7.391
7.388
7.269
6.489
3.903
3.663
3.645
3.627
3.609
1.266
1.248
1.230
-0.000
O
N
O
O
F
F
F
Br
N
4ha 1H (CDCl3, 400 MHz)
1.051
1.025
1.006
1.000
3.144
2.088
3.074
9
8
7
6
5
4
3
2
1
0
ppm

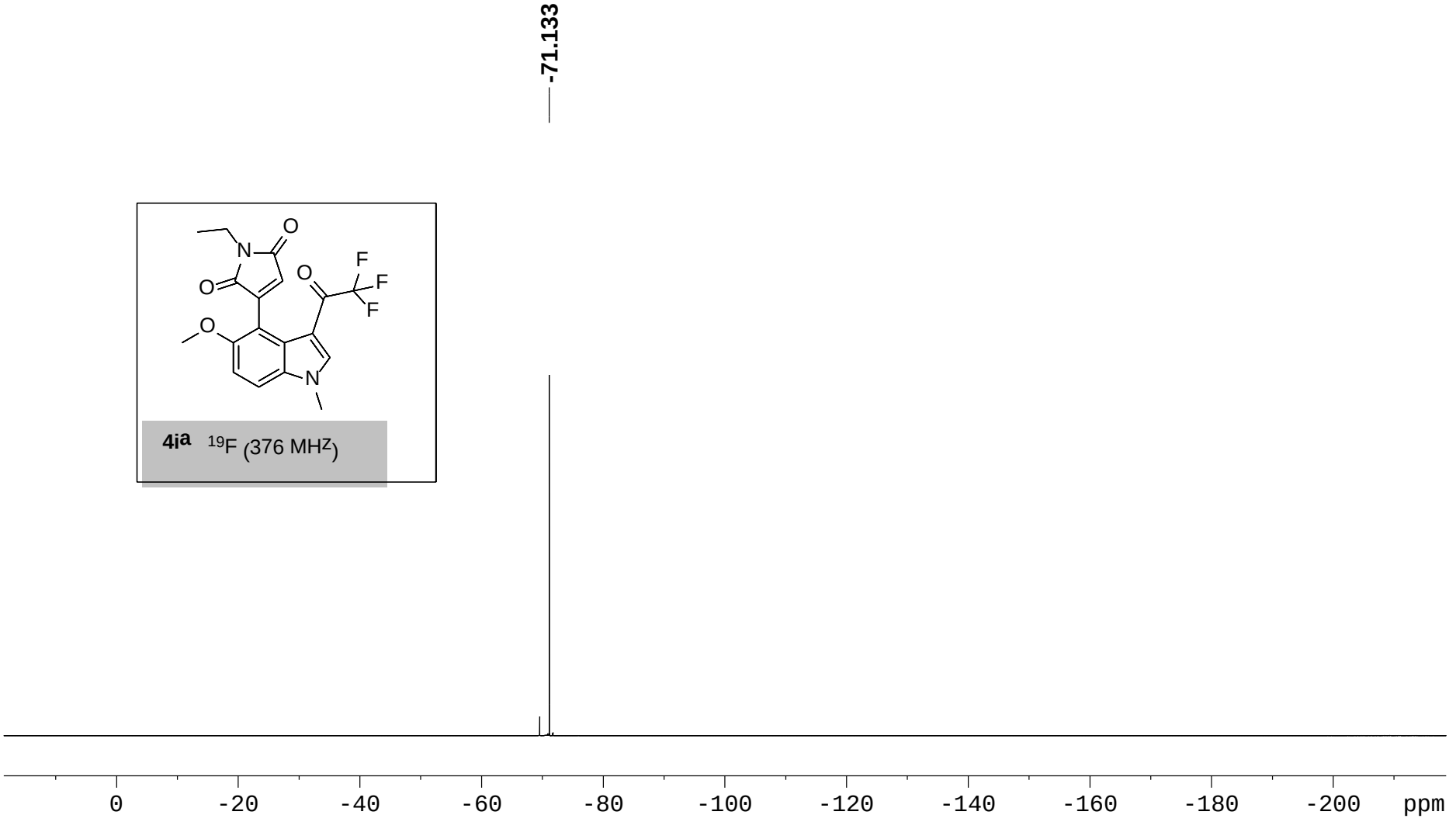

174.520
174.173
173.824
173.474
170.558
170.346
147.609
140.225
140.174
140.123
140.071
138.897
128.315
125.489
124.661
123.535
121.279
118.383
117.758
115.486
115.059
112.591
110.363
77.302
76.984
76.667
34.279
33.024
13.529
O
N
O
O
F
F
F
Br
N
4ha 13C (CDCl3, 100 MHz)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

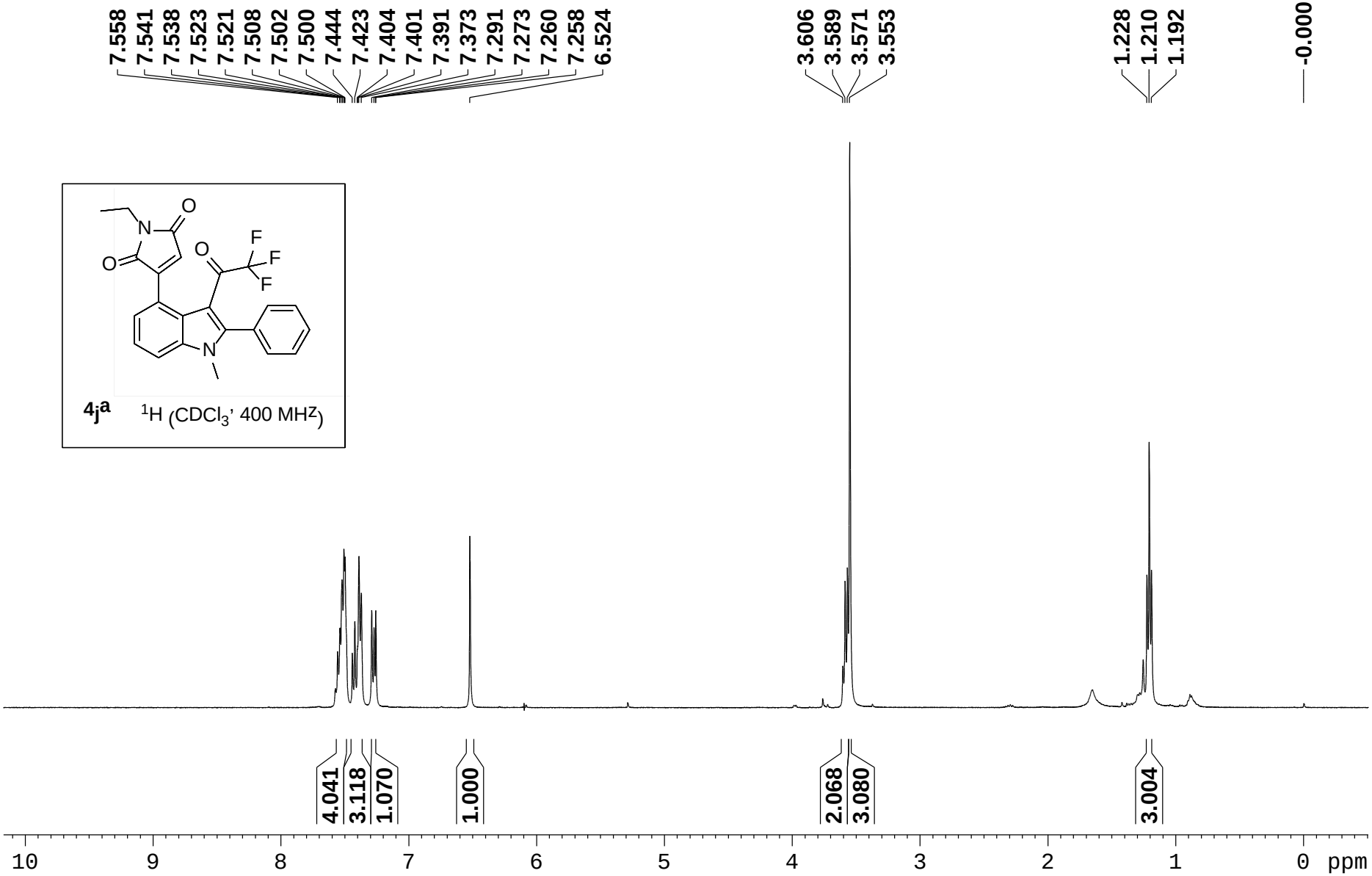

-71.584
O
N
O
O
F
F
F
Br
N
4ha
19F (376 MHz)
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm


7.916
7.409
7.387
7.266
7.103
7.081
6.524
3.867
3.844
3.667
3.649
3.631
3.614
1.277
1.259
1.241
-0.000
O
N
O
O
F
F
F
O
N
4ia
1H (CDCl3, 400 MHz)
1.080
1.105
1.124
1.000
3.086
3.098
2.138
3.056
8
7
6
5
4
3
2
1
0
ppm

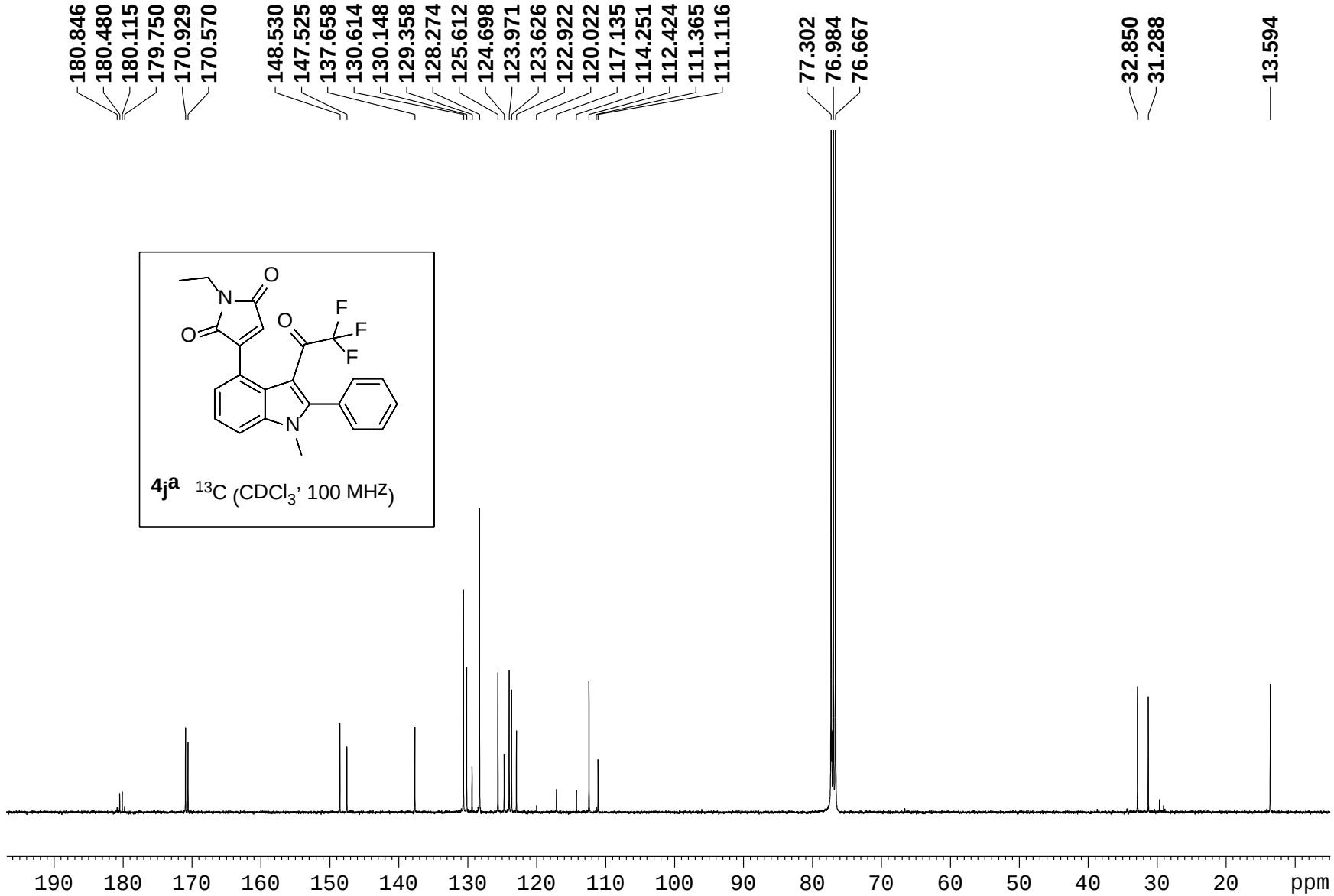


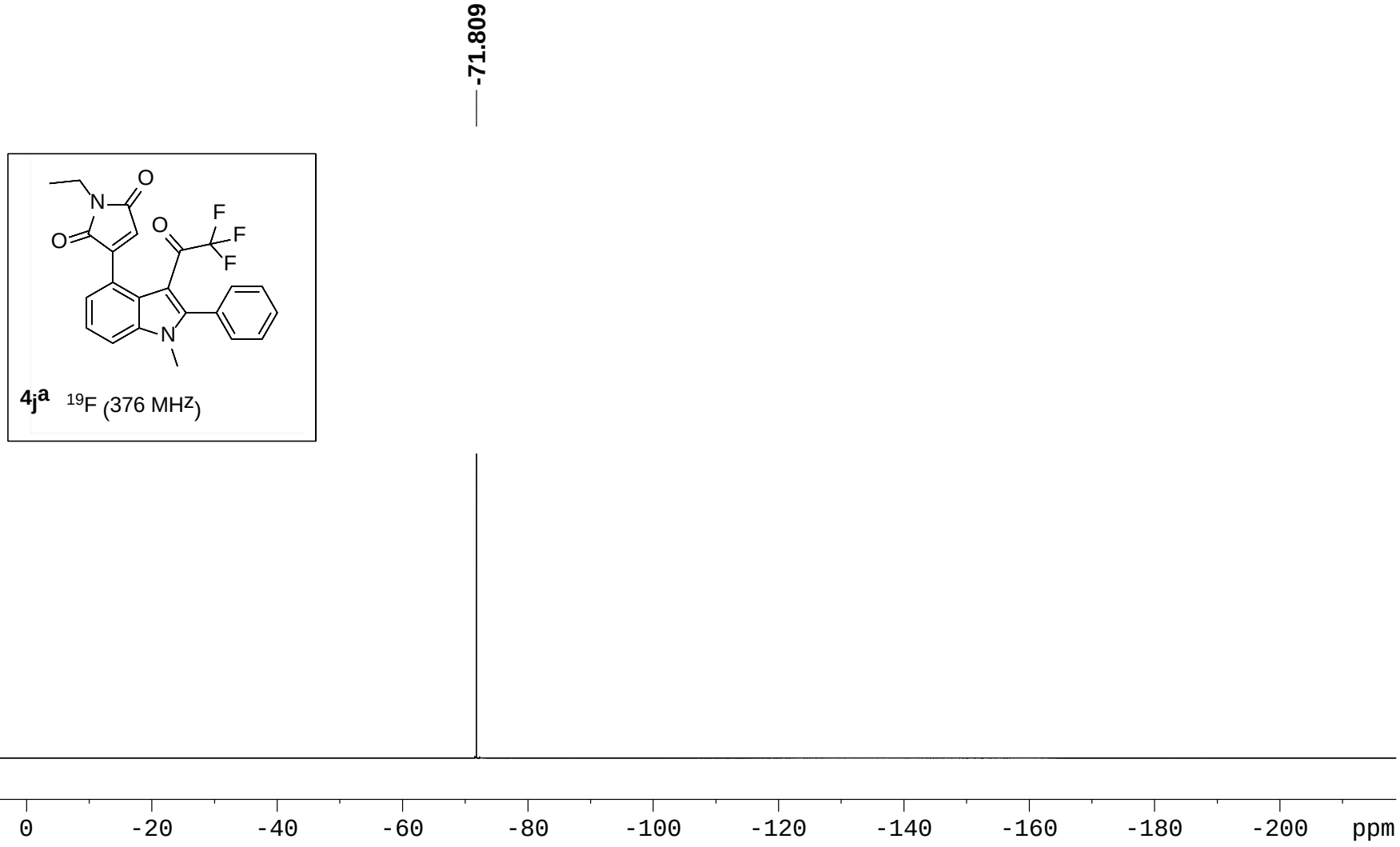
4ia ^{13}C ($CDCl_3$, 100 MH^Z)

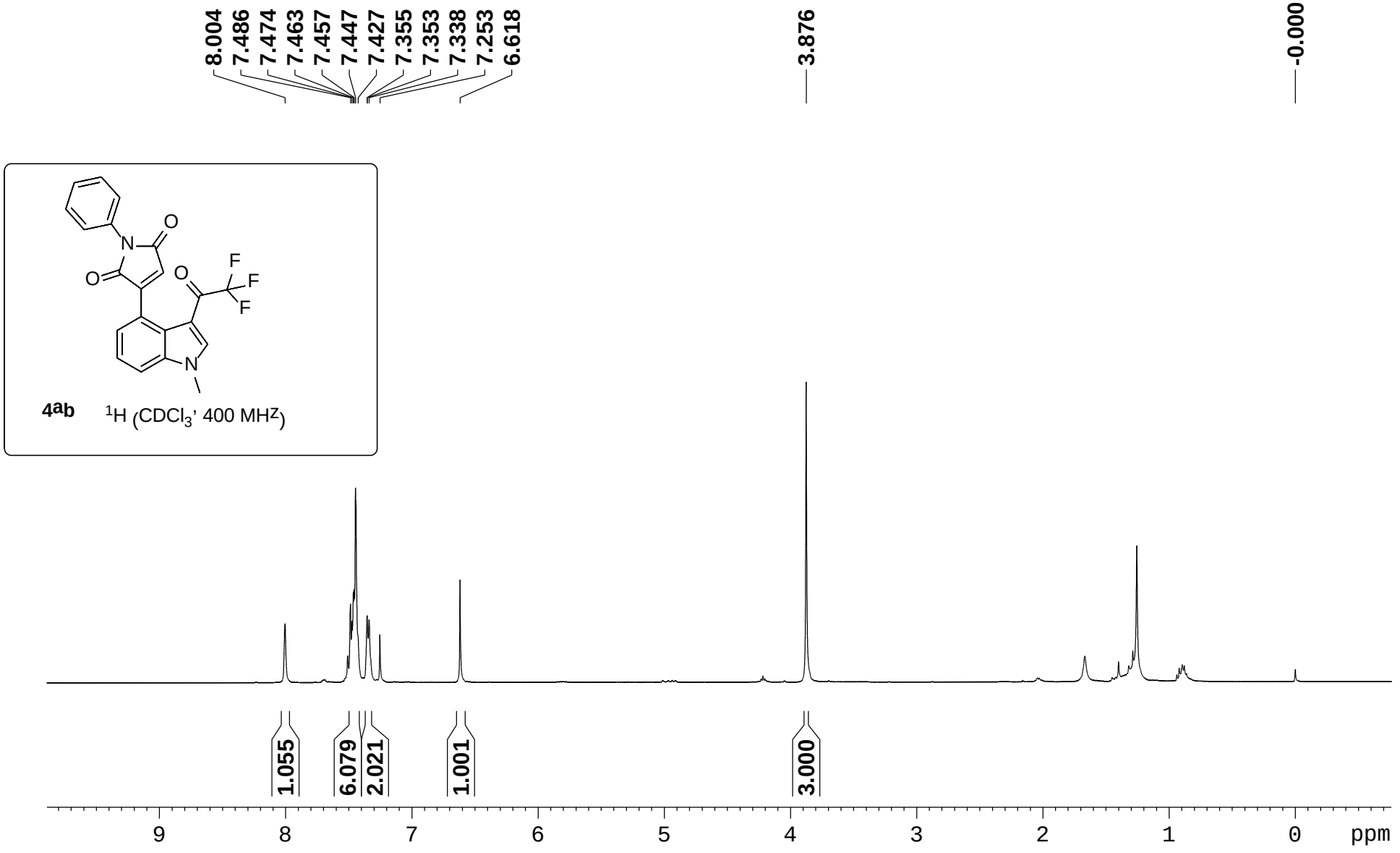

-71.133
O
N
O
O
F
F
F
O
O
N
4ia 19F (376 MHz)
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

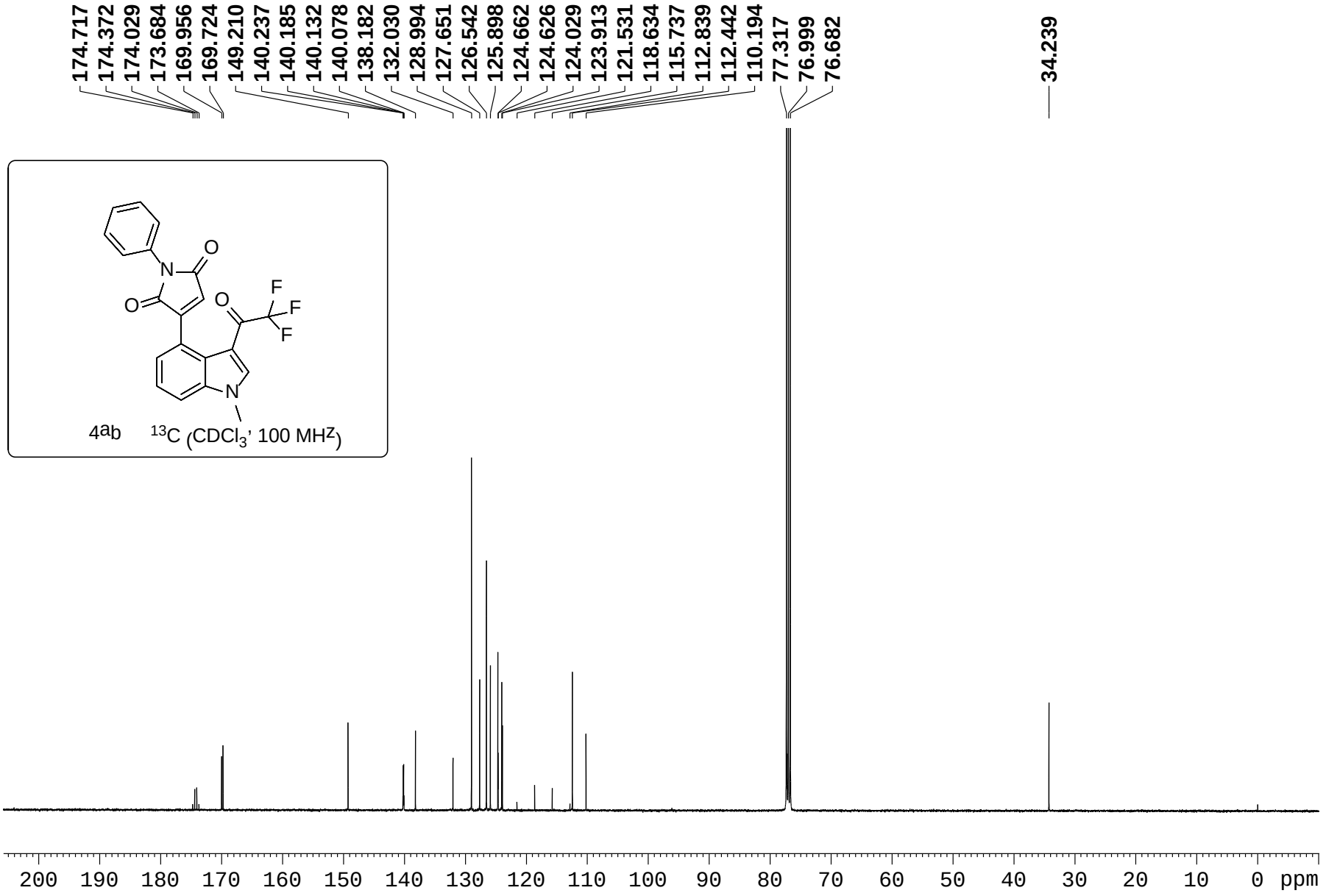


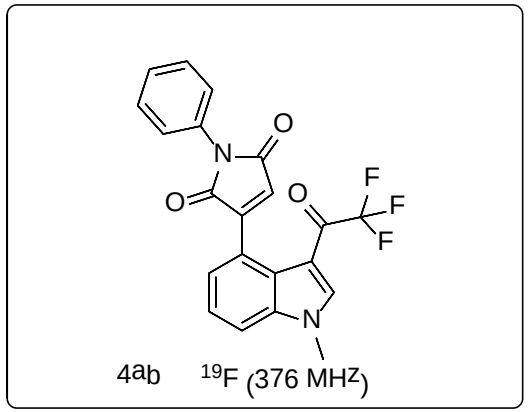
4j[a] ^{1}H ($CDCl_3$, 400 MHz)


180.846
180.480
180.115
179.750
170.929
170.570
148.530
147.525
137.658
130.614
130.148
129.358
128.274
125.612
124.698
123.971
123.626
122.922
120.022
117.135
114.251
112.424
111.365
111.116
77.302
76.984
76.667
32.850
31.288
13.594
O
N
O
O
F
F
F
N
4j[a] 13C (CDCl3, 100 MHz)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

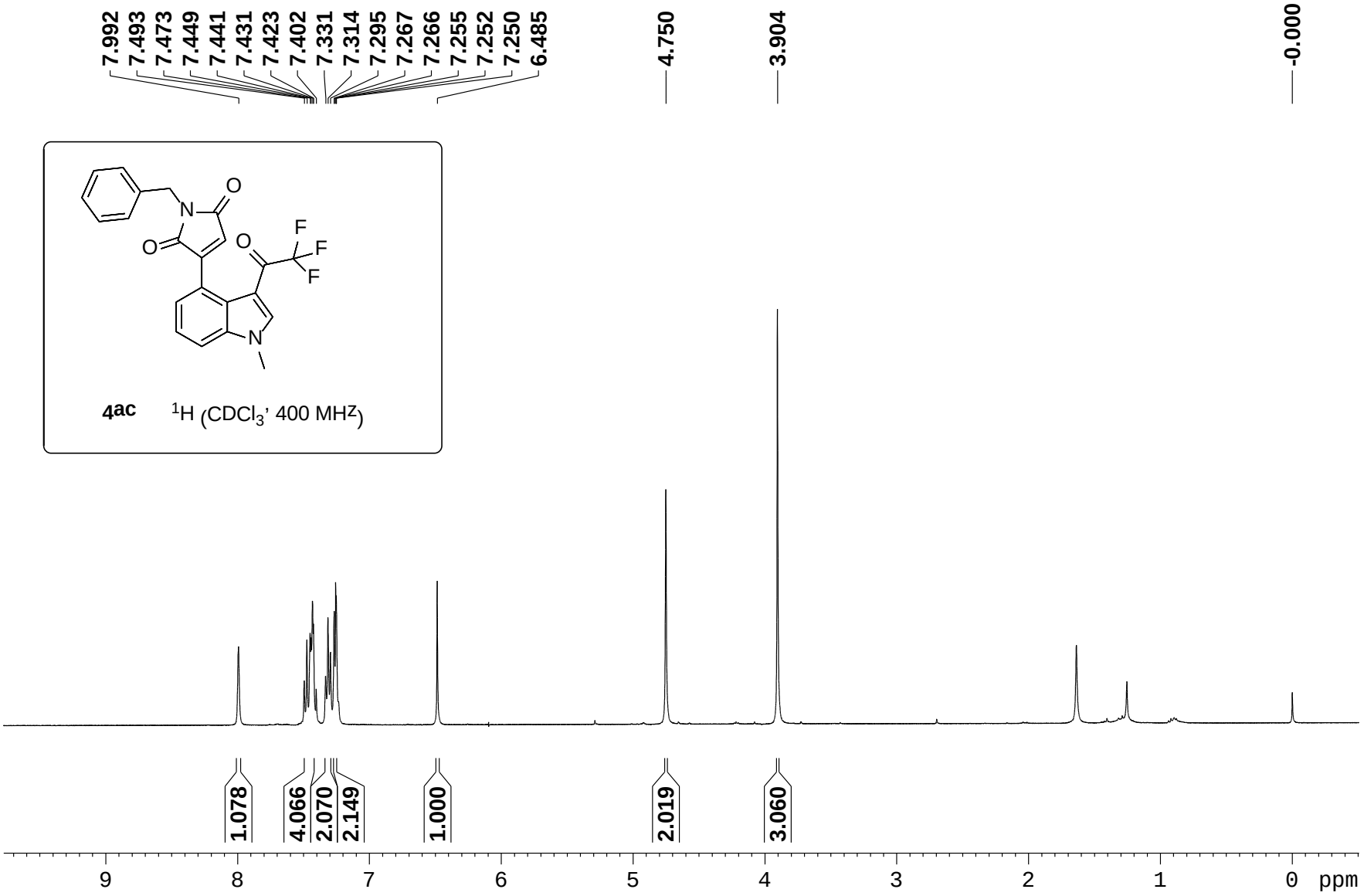

-71.809
O
N
O
O
F
F
F
N
4j^a ^19F (376 MHZ)
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

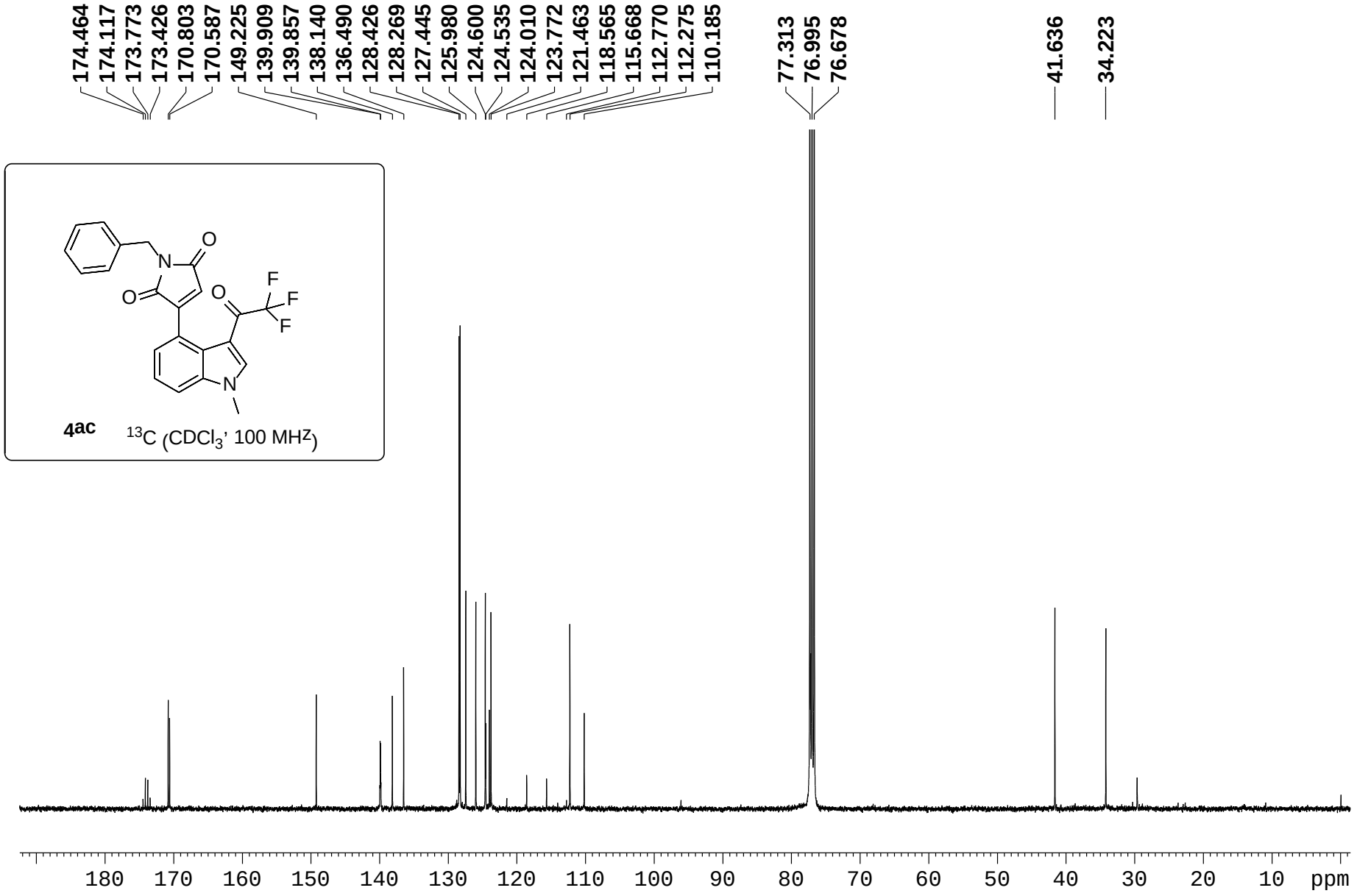

8.004
7.486
7.474
7.463
7.457
7.447
7.427
7.355
7.353
7.338
7.253
6.618
3.876
-0.000
O
N
O
O
F
F
F
N
4ab
1H (CDCl3, 400 MHz)
1.055
6.079
2.021
1.001
3.000
9
8
7
6
5
4
3
2
1
0
ppm

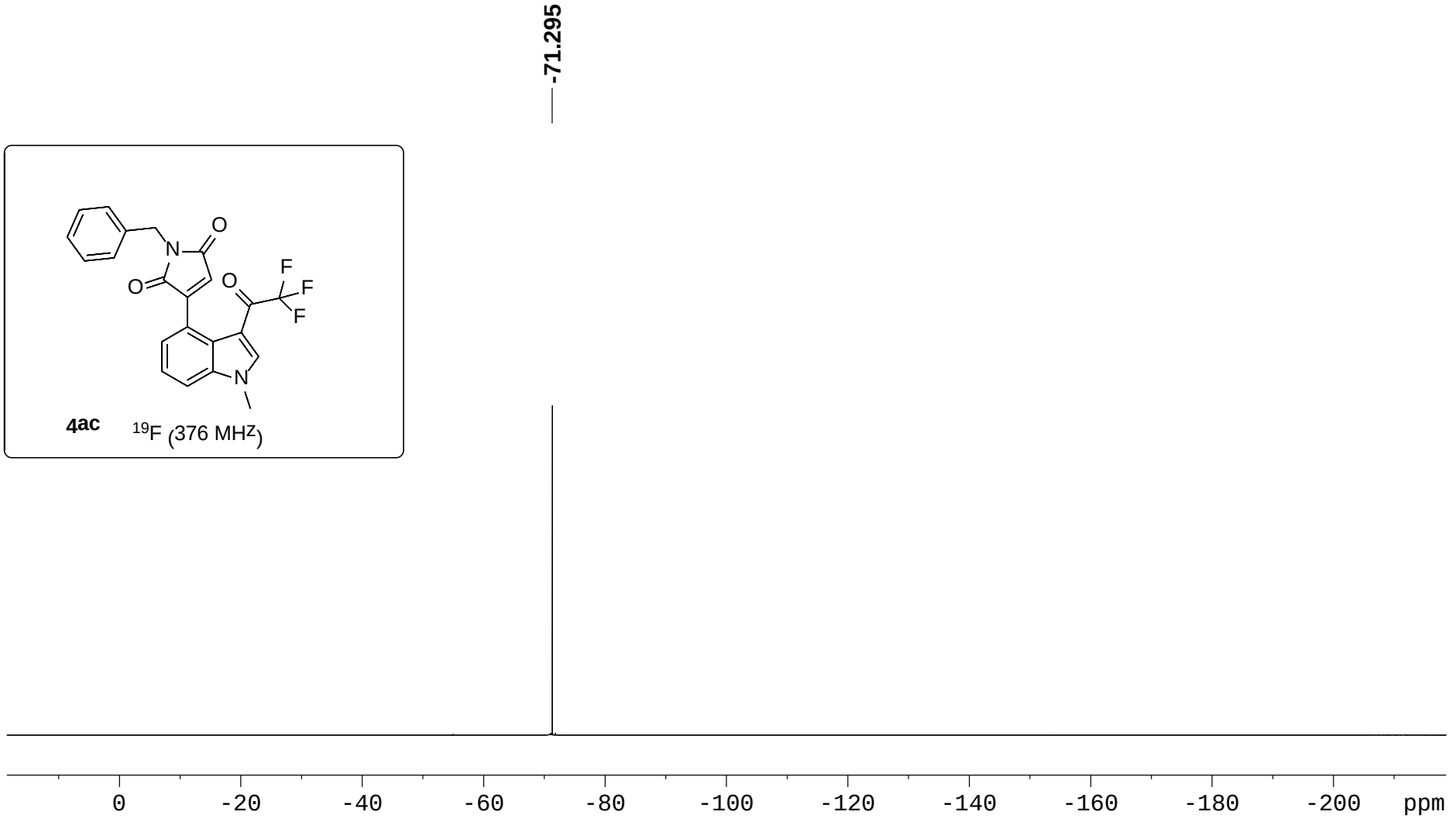

174.717
174.372
174.029
173.684
169.956
169.724
149.210
140.237
140.185
140.132
140.078
138.182
132.030
128.994
127.651
126.542
125.898
124.662
124.626
124.029
123.913
121.531
118.634
115.737
112.839
112.442
110.194
77.317
76.999
76.682
34.239
O
N
O
O
F
F
F
N
4ab
13C (CDCl3, 100 MHz)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

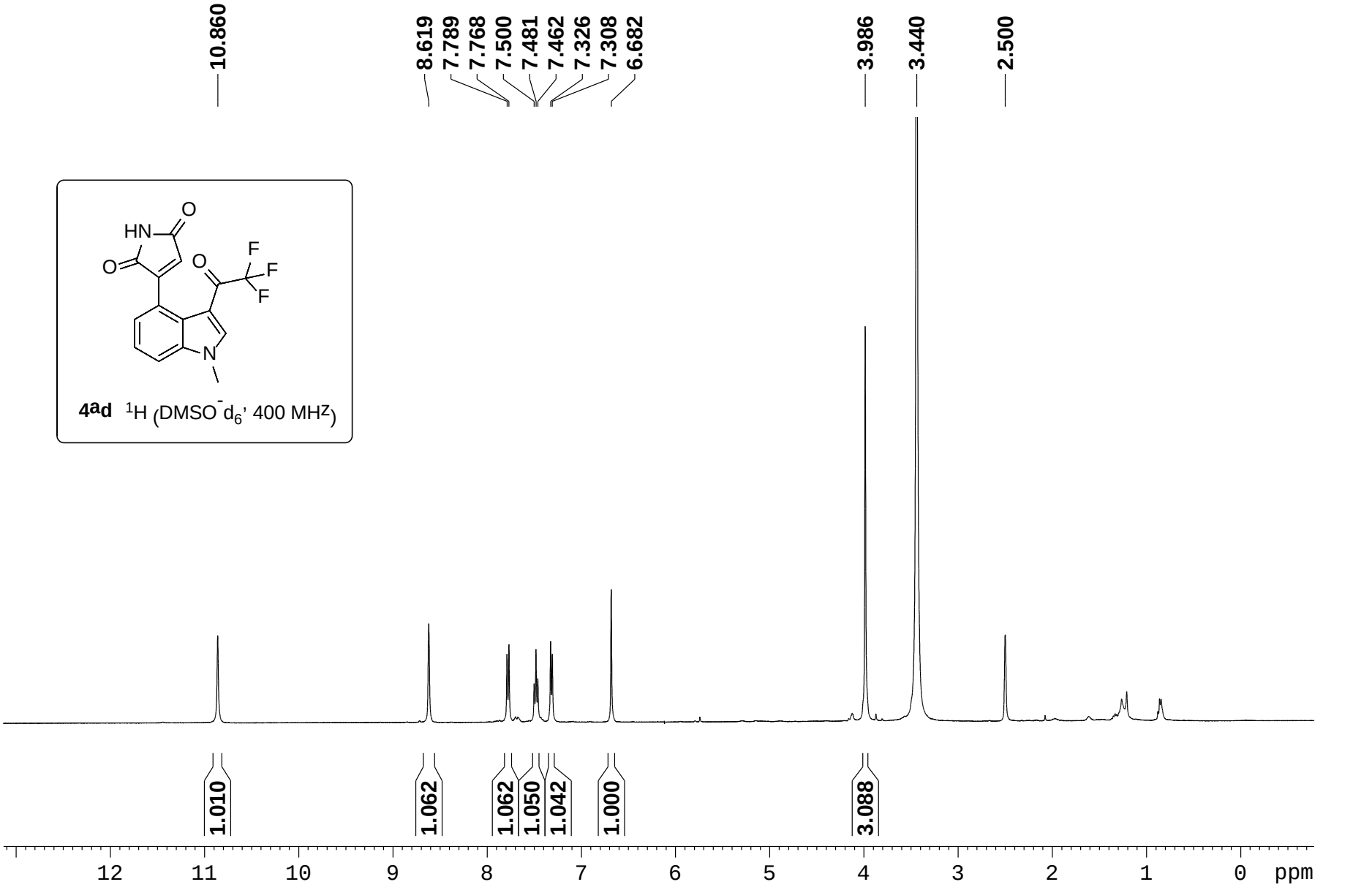


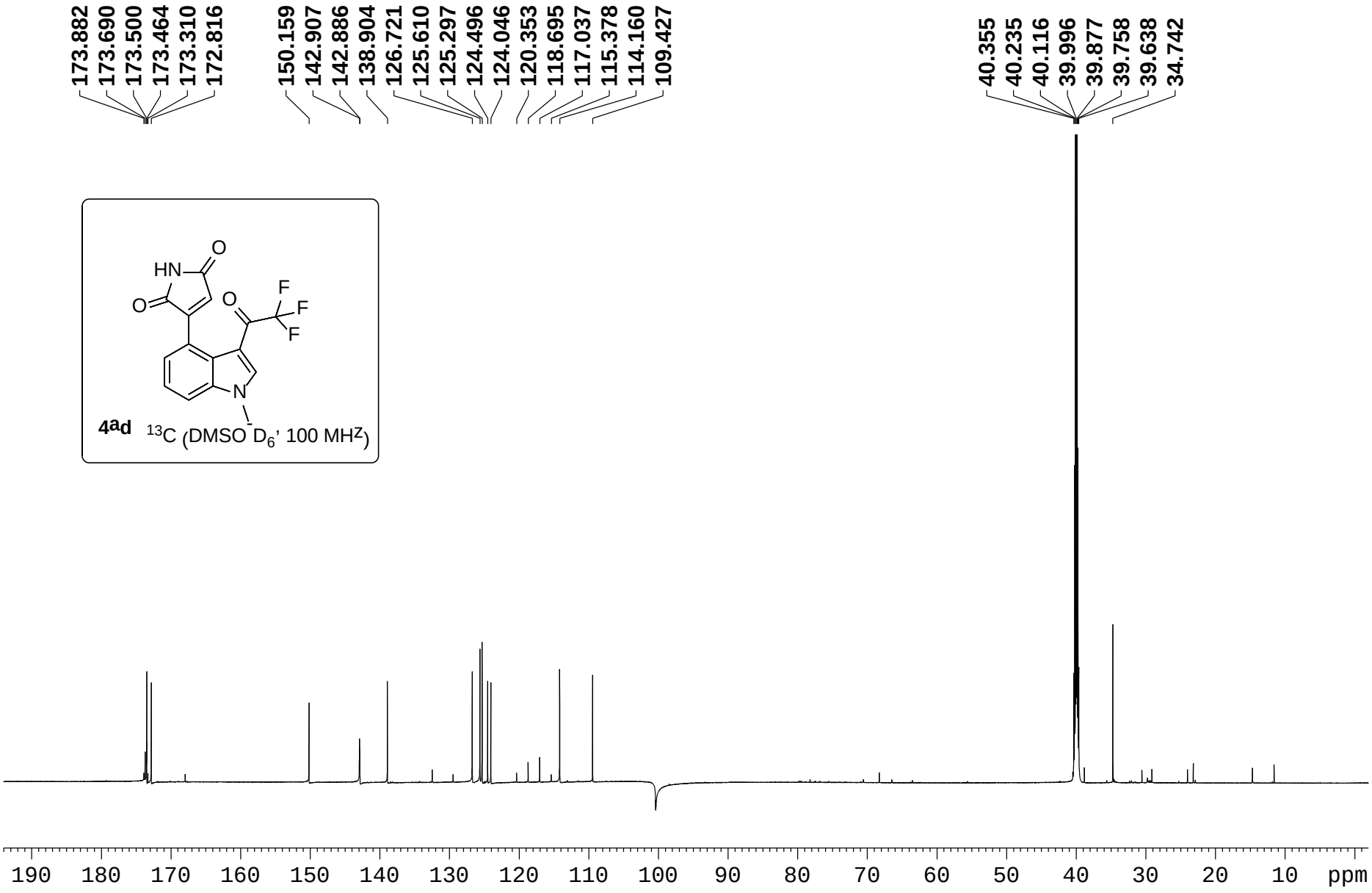
4ab ^{19}F (376 MHz)

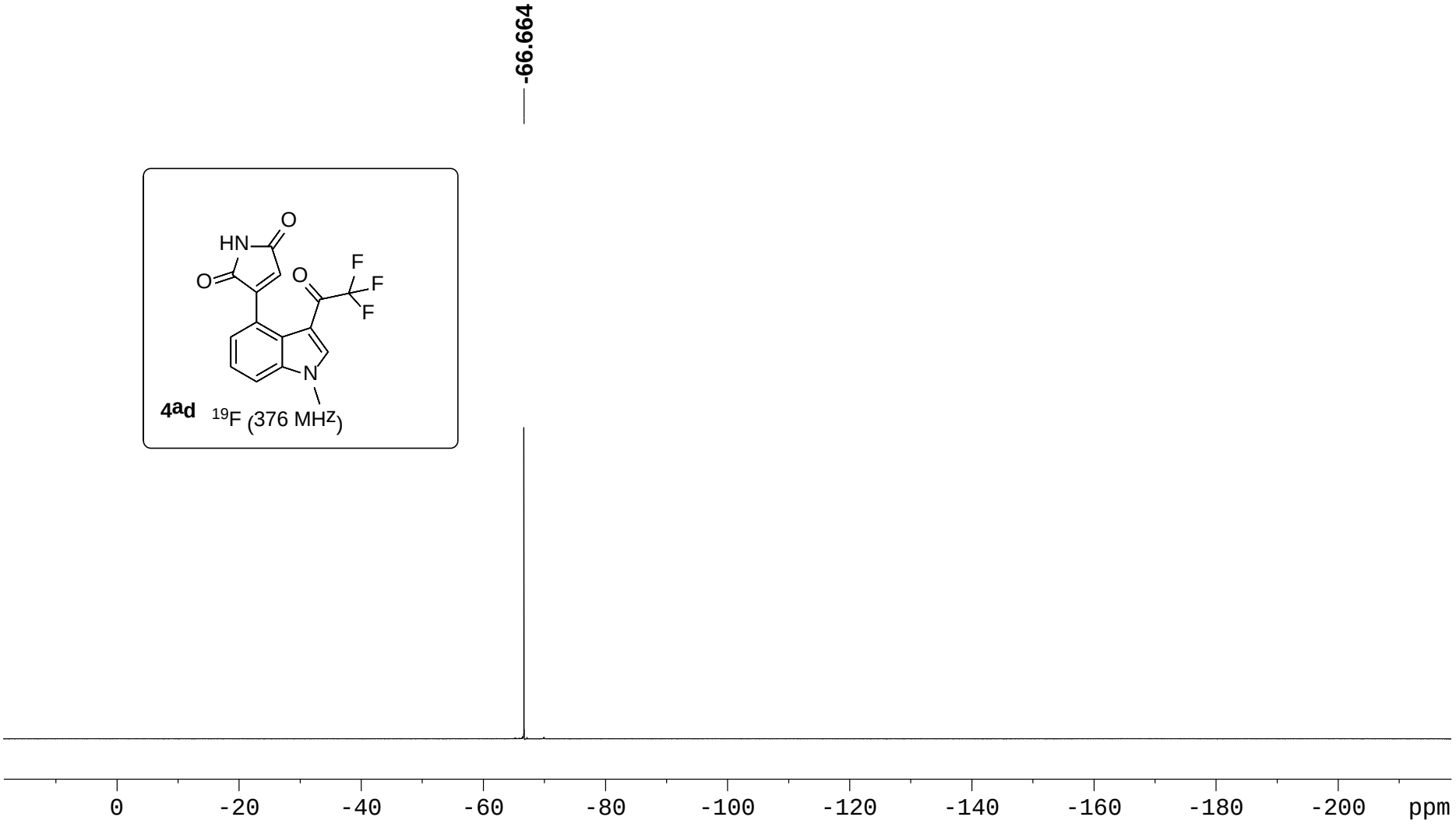

7.992
7.493
7.473
7.449
7.441
7.431
7.423
7.402
7.331
7.314
7.295
7.267
7.266
7.255
7.252
7.250
6.485
4.750
3.904
-0.000
O
N
O
O
F
F
F
N
4ac
1H (CDCl3, 400 MHz)
1.078
4.066
2.070
2.149
1.000
2.019
3.060
9
8
7
6
5
4
3
2
1
0
ppm

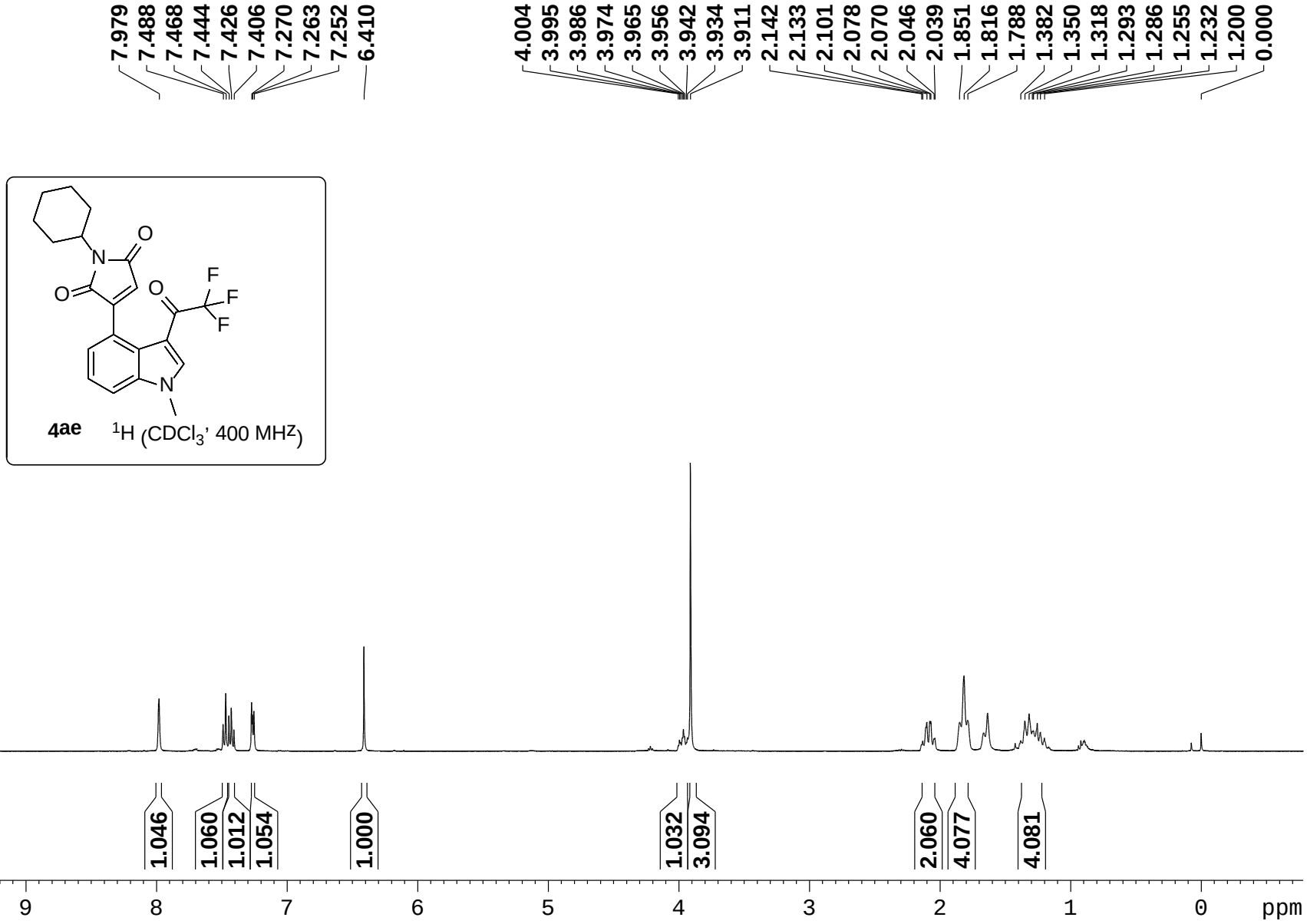

174.464
174.117
173.773
173.426
170.803
170.587
149.225
139.909
139.857
138.140
136.490
128.426
128.269
127.445
125.980
124.600
124.535
124.010
123.772
121.463
118.565
115.668
112.770
112.275
110.185
77.313
76.995
76.678
41.636
34.223
O
N
O
O
F
F
F
N
4ac
13C (CDCl3, 100 MHz)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

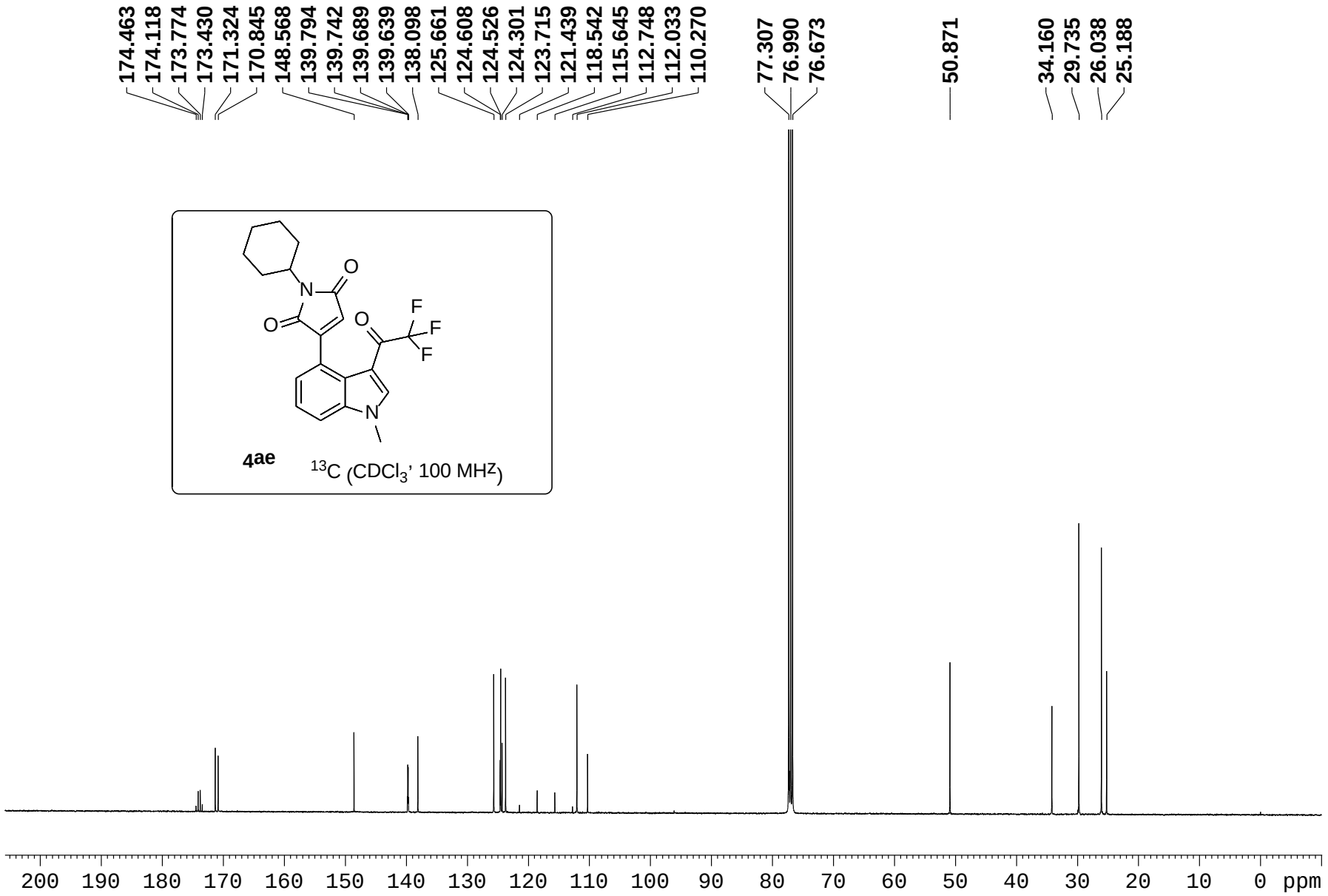

-71.295
O
N
O
O
F
F
F
N
4ac
19F (376 MHz)
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

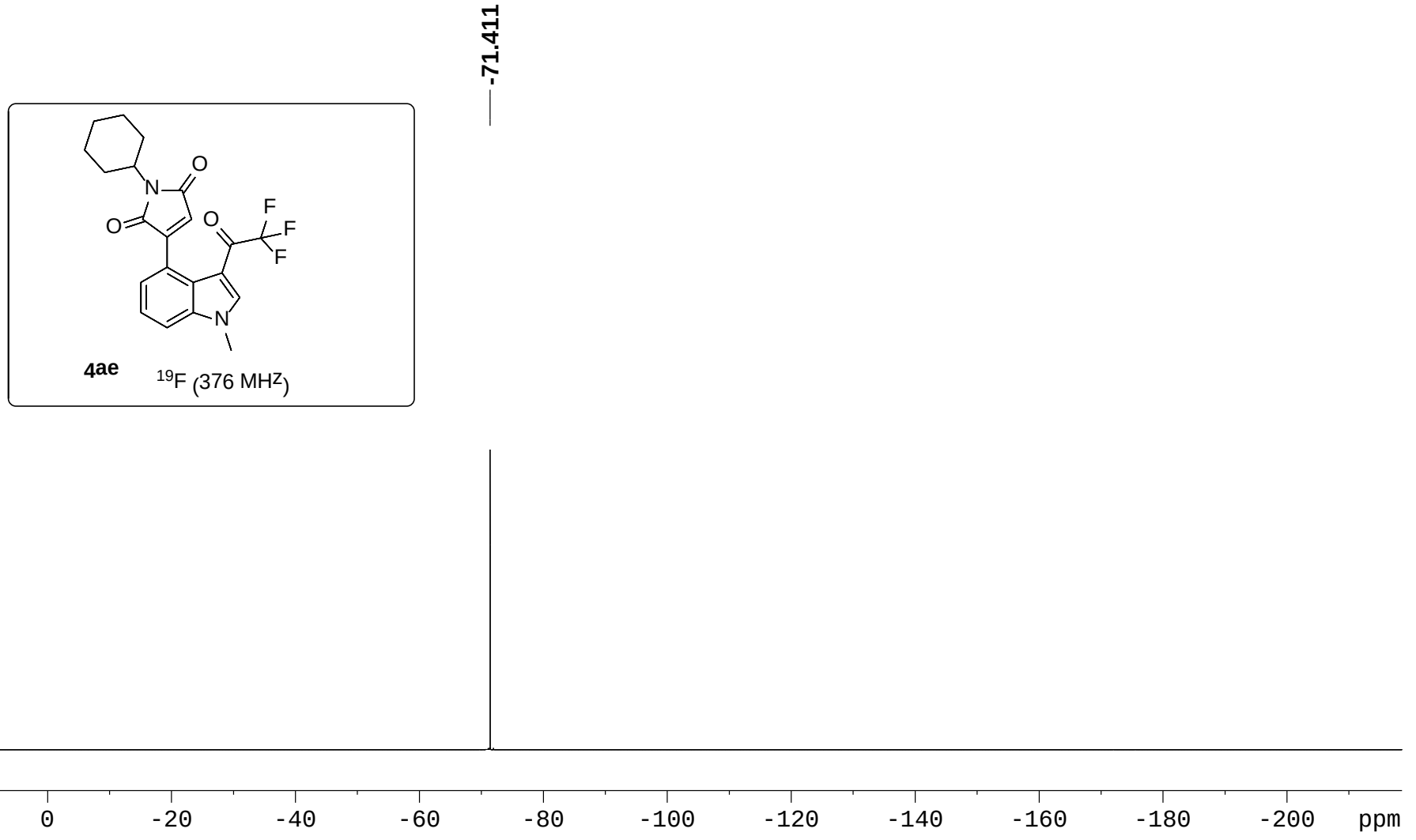

10.860
8.619
7.789
7.768
7.500
7.481
7.462
7.326
7.308
6.682
3.986
3.440
2.500
HN
O
O
O
F
F
F
N
4ad 1H (DMSO-d6, 400 MHz)
1.010
1.062
1.062
1.050
1.042
1.000
3.088
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm

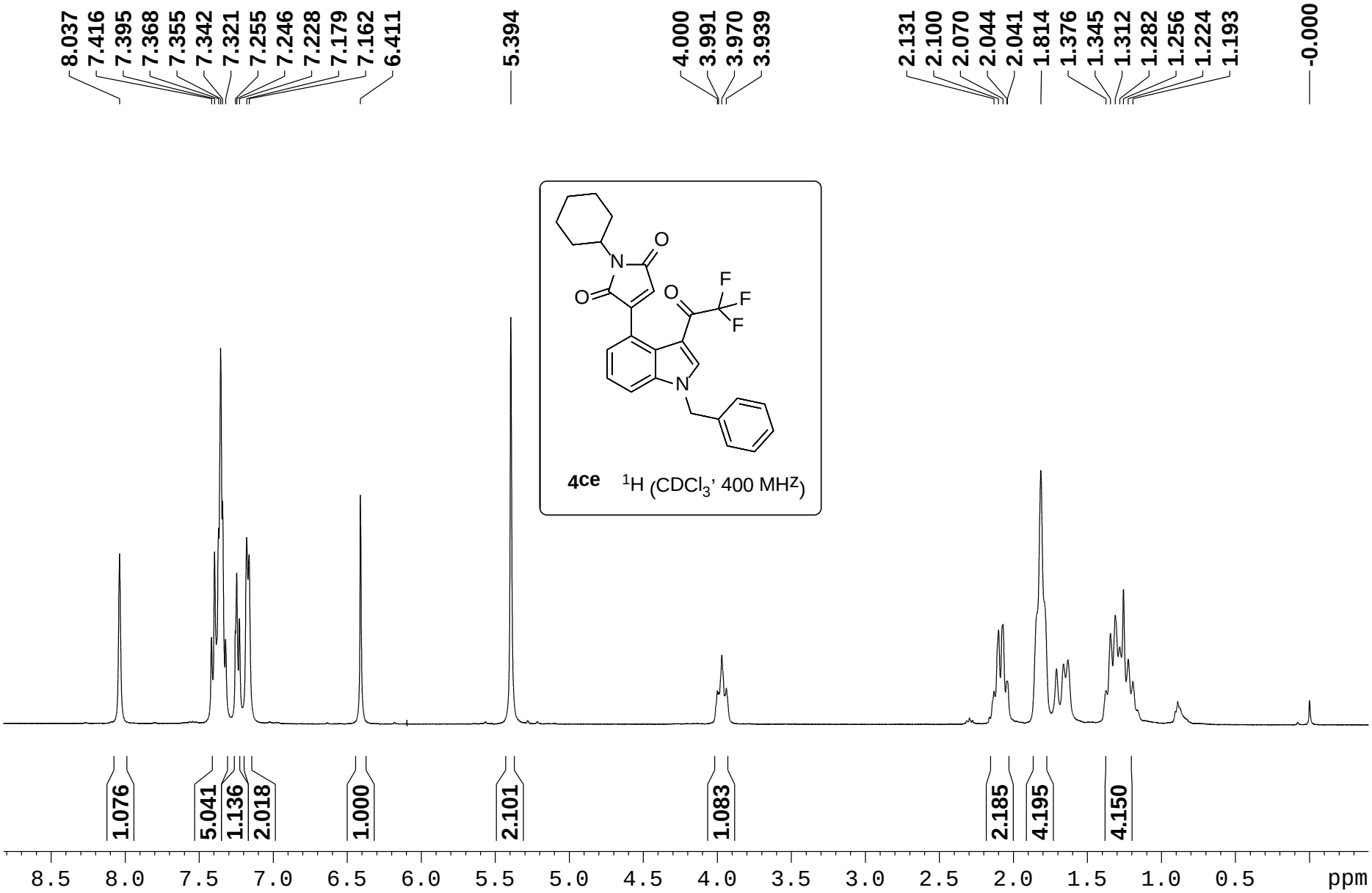

173.882
173.690
173.500
173.464
173.310
172.816
150.159
142.907
142.886
138.904
126.721
125.610
125.297
124.496
124.046
120.353
118.695
117.037
115.378
114.160
109.427
40.355
40.235
40.116
39.996
39.877
39.758
39.638
34.742
HN
O
O
O
F
F
F
N
4ad 13C (DMSO D6, 100 MHz)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

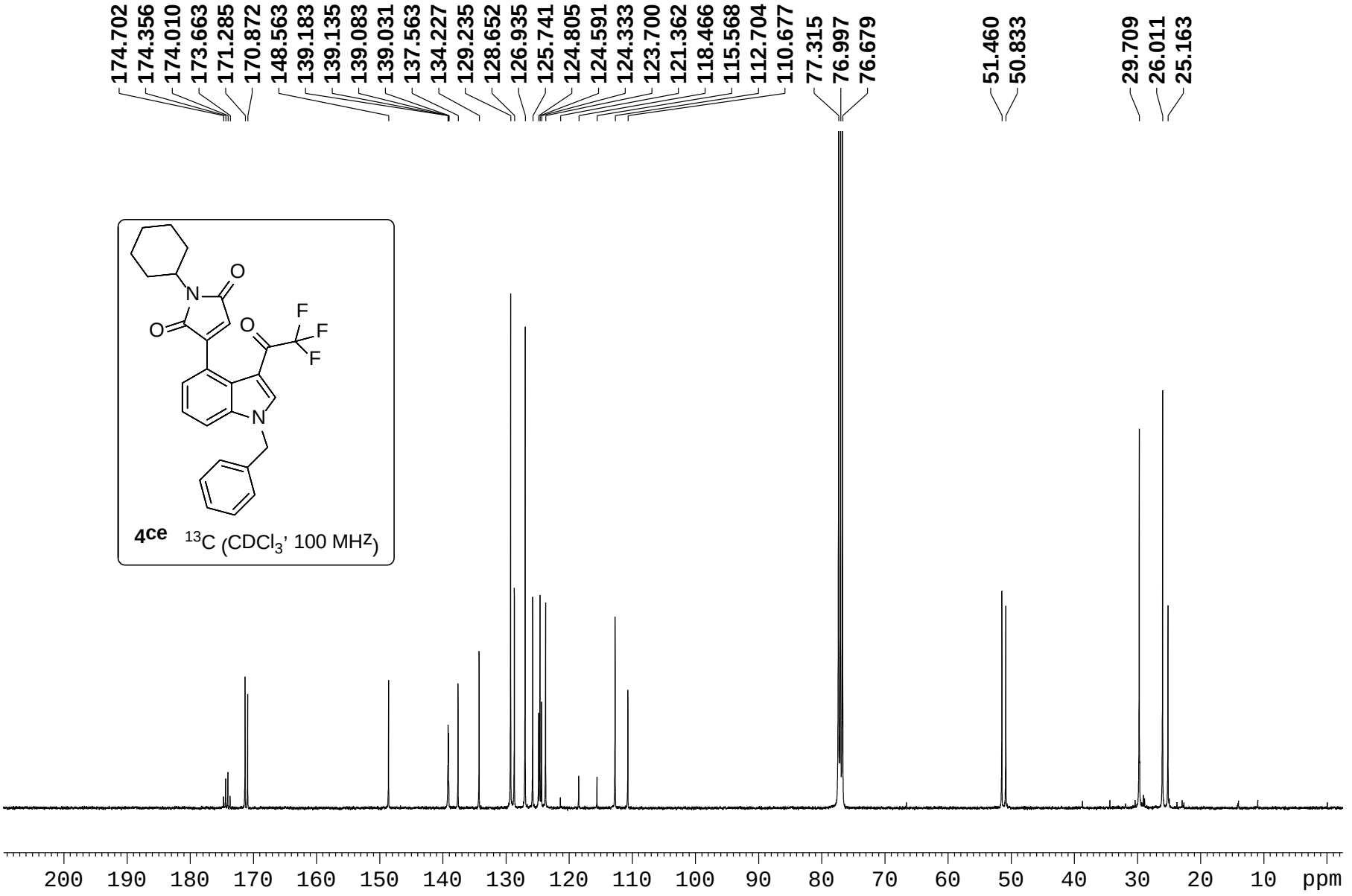

-66.664
HN
O
O
O
F
F
F
N
4ad 19F (376 MHz)
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

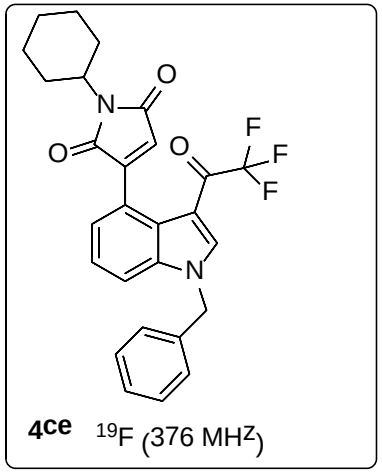

7.979
7.488
7.468
7.444
7.426
7.406
7.270
7.263
7.252
6.410
4.004
3.995
3.986
3.974
3.965
3.956
3.942
3.934
3.911
2.142
2.133
2.101
2.078
2.070
2.046
2.039
1.851
1.816
1.788
1.382
1.350
1.318
1.293
1.286
1.255
1.232
1.200
0.000
O
N
O
O
F
F
F
N
4ae
1H (CDCl3, 400 MHz)
1.046
1.060
1.012
1.054
1.000
1.032
3.094
2.060
4.077
4.081
9
8
7
6
5
4
3
2
1
0
ppm


174.463
174.118
173.774
173.430
171.324
170.845
148.568
139.794
139.742
139.689
139.639
138.098
125.661
124.608
124.526
124.301
123.715
121.439
118.542
115.645
112.748
112.033
110.270
77.307
76.990
76.673
50.871
34.160
29.735
26.038
25.188
O
N
O
O
F
F
F
N
4ae
13C (CDCl3, 100 MHz)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


-71.411
O
N
O
O
F
F
F
N
4ae
19F (376 MHz)
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm


8.037
7.416
7.395
7.368
7.355
7.342
7.321
7.255
7.246
7.228
7.179
7.162
6.411
5.394
4.000
3.991
3.970
3.939
2.131
2.100
2.070
2.044
2.041
1.814
1.376
1.345
1.312
1.282
1.256
1.224
1.193
-0.000
O
N
O
O
F
F
F
N
4ce 1H (CDCl3, 400 MHz)
1.076
5.041
1.136
2.018
1.000
2.101
1.083
2.185
4.195
4.150
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm


174.702
174.356
174.010
173.663
171.285
170.872
148.563
139.183
139.135
139.083
139.031
137.563
134.227
129.235
128.652
126.935
125.741
124.805
124.591
124.333
123.700
121.362
118.466
115.568
112.704
110.677
77.315
76.997
76.679
51.460
50.833
29.709
26.011
25.163
O
N
O
O
F
F
F
N
4ce 13C (CDCl3, 100 MHz)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



4ce ^{19}F (376 MHz)