Supporting Information

Copper-Catalyzed Trifluoromethylation of Alkenes: Synthesis of Trifluoromethylated Benzoxazines

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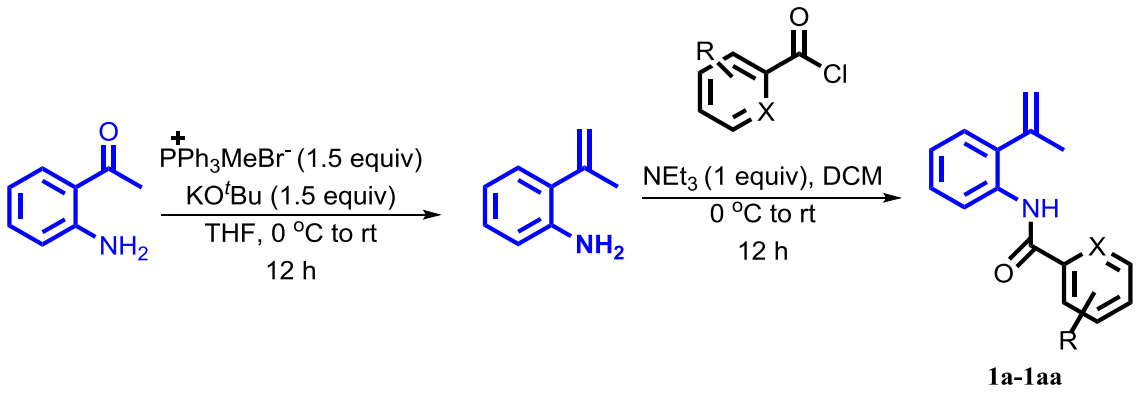
General Experimental Details

All reactions were performed under nitrogen atmosphere in an oven dried glassware containing a magnetic stir bar and sealed with septum. Anhydrous DMSO was purchased from Sigma Aldrich. 2-Aminoacetophenone, substituted benzoic acid and thionyl chloride were purchased from Spectrochem Pvt. Ltd. All fluorinating agents were purchased from Sigma Aldrich Co. India. All reactions were set up using standard Schlenk line techniques. Yields of the reactions were determined chromatographically and spectroscopically for the isolated product and optimized condition, respectively. Reactions were monitored by ^{19}F NMR Spectroscopy and thin-layer Chromatography (TLC). All NMR experiments were carried out on Bruker 400/500 MHz spectrometer in $CDCl_3$ and NMR chemical shifts are reported in ppm referenced to the solvent peaks of $CDCl_3$ (7.24 ppm for 1H and 77±0.07 ppm for ^{13}C), respectively. ^{19}F NMR spectra were recorded on 376.5 MHz Spectrometer and were calibrated using PhF as an external reference (-113.1 ppm). The following abbreviations were used to indicate multiplicity: s (singlet), brs (broad singlet), d (doublet), t (triplet), q (quartet), dd (doublet of doublets) td (triplet of doublet) and m (multiplet). High resolution mass analysis is performed on quadrupole-time-of-flight Bruker MicroTOF-Q II mass spectrometer equipped with an ESI and APCI source; HR-GC mass analysis is performed on Agilent 7200 Accurate mass Q-TOF MS equipped with 7890A GC and LR-GC mass analysis is performed on Agilent Technologies MS-S975C inert XLEI/CIMSD with triple axis detector. Single crystal X-ray data for compounds CCDC No. 1063690 (3f), 1402832 (5e), 1402833 (3z) were collected on a Bruker D8 VENTURE diffractometer equipped with CMOS Photon 100 detector and Mo-Kα (λ = 0.71073 Å) radiation was used. Silica gel (100-200 mesh size) was used for column chromatography purchased from RANKEM Pvt. Ltd. India. TLC analysis of reaction mixtures was performed using Merck silica gel (60 F254) plates.

General Procedure for the synthesis of *N*-(2-(prop-1-en-2-yl)aryl)benzamides 1 (substrates for trifluoromethylated benzoxazines 3)

The substrates **1** for **3** were prepared from 2-aminoacetophenone by following two steps: a) first, conversion of 2-aminoacetophenone into 2-(prop-1-en-2-yl)aniline; b) preparation of *N*-(2-(prop-1-en-2-yl)aryl)benzamides by coupling of aroyl/ acyl chloride with 2-(prop-1-en-2-yl)aniline (**Scheme 1**).

Scheme 1



1a-1aa

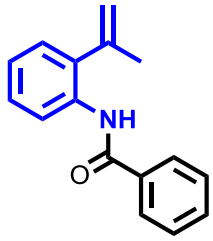
Conversion of 2-Aminoacetophenone into 2-(prop-1-en-2-yl)aniline: A Typical Procedure

To a stirred solution of Ph_3PMeBr (1.5 equiv. 12.2 mmol) in Dry THF (15 mL) was added KO^tBu (1.5 equiv. 12.2 mmol) in portions under nitrogen. After the mixture was stirred at room temperature for 0.5 h, a solution of corresponding benzophenone (1 equiv. 8.14 mmol) in THF (15 mL) was added dropwise. The reaction mixture was then stirred at room temperature under nitrogen overnight. The reaction mixture was quenched with water and extracted with EtOAc (50 mL x 2). The combined organic layers were washed with saturated $NaHCO_3$ (50 mL) and brine (50 mL), dried over anhydrous Na_2SO_4, and concentrated on rotary evaporator under vacuum and the residue was purified by column chromatography on silica gel. A light yellow oil was obtained.[1] yield (0.86 g, 79%), ^{1}H-NMR (400 MHz, $CDCl_3$), δ 7.09-7.04 (m, 2H), 6.75 (td, *J* =

7.4, 1.0 Hz, 1H), 6.7 (d, *J* = 7.8 Hz, 1H), 5.32-5.30 (m, 1H), 5.07 (d, *J* = 1.0 Hz, 1H), 3.84 (s, 2H), 2.09 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 143.5, 142.8, 129.2, 128.2, 127.9, 118.2, 115.5, 115.3, 23.9.

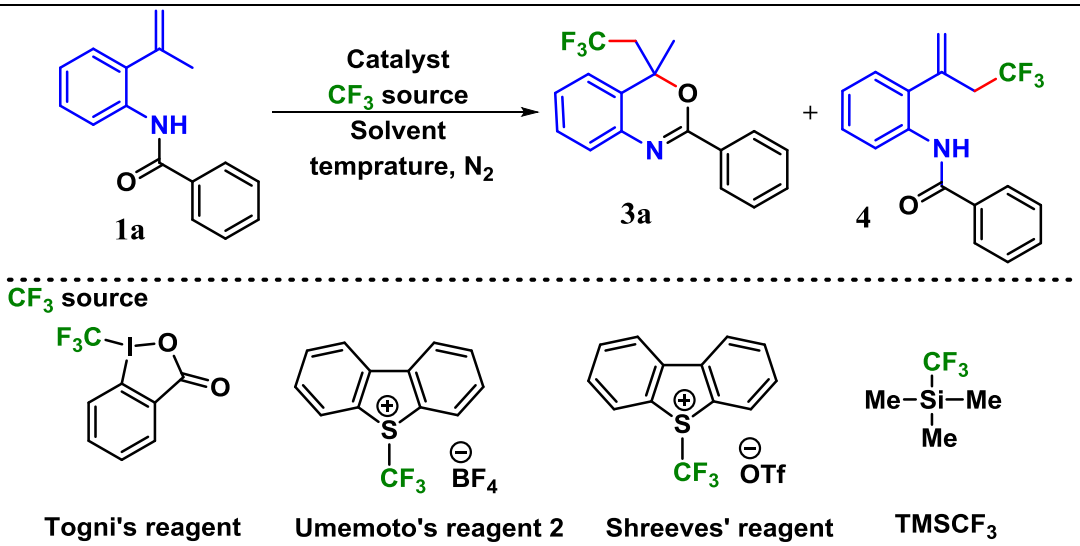
General procedure for the preparation of *N*-(2-(prop-1-en-2-yl)aryl)benzamides

To a stirred solution of benzoyl chloride derivatives (400 mg, 3.3 mmol) in dry CH_2Cl_2 (25 mL), amine (399 mg, 3 mmol), and triethylamine (333 mg, 3.3 mmol) in dry CH_2Cl_2 (20 mL) were added dropwise using a dropping funnel at 0 ^{0}C. The reaction mixture was stirred at room temperature for 12 h. After completion, the reaction was washed by 10 mol % aqueous HCl solution (15 mL), saturated aqueous $NaHCO_3$ solution (15 mL), brine (25 mL) and dried over Na_2SO_4. The organic solvent was removed by rotary evaporator under vacuum and the residue was purified by column chromatography on silica gel using (hexane/ethyl acetate, 9:1). A white solid was obtained.



***N*-(2-(Prop-1-en-2-yl)phenyl)benzamide (1a)**:[2] White solid, yield (0.69 g, 89%). m.p.: 70 – 72 ^{o}C, ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.48 (d, *J* = 8.3 Hz, 1H), 8.45 (bs, 1H), 7.82 (d, *J* = 7.8 Hz, 2H), 7.53 (t, *J* = 7.40Hz, 1H), 7.47 (t, *J* = 7.8 Hz, 2H), 7.31 (td, *J* = 7.8, 1.6 Hz, 1H), 7.18 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.11 (td, *J* = 7.4, 1.0 Hz, 1H), 5.47-5.469 (m, 1H), 5.11-5.10 (m, 1H), 2.11 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 165.1, 143.3, 135.1, 134.0, 133.6, 131.8, 128.8, 128.0, 127.7, 126.9, 123.9, 120.9, 116.8, 24.6.

Table S1. Optimization of reaction conditions[#]



Entry	CF_3 Source	Catalyst (20 mol %)	Base (1.5 equiv)	T (^oC)	Solvent	Yield of 2a (%)[a]
1	Togni's	CuI	—	80	DCE	30[a], 45[b]
2	Shreeve's	CuI	—	80	DCE	37
3	2	CuI	—	80	DCE	52
4	$TMSCF_3$	CuI	—	80	DCE	ND
5	**2**	—	—	80	DCE	ND
6	**2**	CuCl	—	80	DCE	17
7	**2**	CuBr	—	80	DCE	14
8	**2**	CuTc	—	80	DCE	17
9	**2**	$Cu(OTf)_2$	—	80	DCE	6
10	**2**	$[Cu(CH_3CN)_4]BF_4$	—	80	DCE	5
11	**2**	CuCN	—	80	DCE	26
12	**2**	$CuCl_2$	—	80	DCE	9
13	**2**	$Cu(OTf).C_6H_6$	—	80	DCE	8
14	**2**	$[Cu(CH_3CN)_4]PF_6$	—	80	DCE	6
15	**2**	Cu(OAc)	—	80	DCE	27
16	**2**	$Cu(OAc)_2$	—	80	DCE	8
17	**2**	CuI	—	80	DMF	52
18	**2**	CuI	—	80	DMAc	58
19	**2**	CuI	—	80	NMP	39
20	**2**	**CuI**	—	**80**	**DMSO**	**68**
21	**2**	CuI	—	80	1,4-Dioxane	17
22	**2**	CuI	—	80	Toluene	4
23	**2**	CuI	—	80	$CHCl_3$	9
24	**2**	CuI	—	80	CH_3CN	24

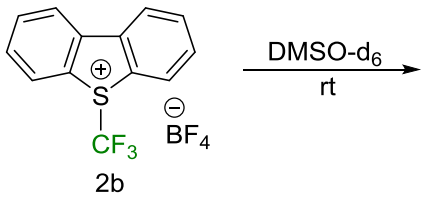
25	**2**	CuI (25 mol %)	—	80	DMSO	66
26	**2**	CuI (50 mol %)	—	80	DMSO	64
27	**2**	CuI	KF	80	DMSO	60
28	**2**	CuI	KF(4 equiv)	80	DMSO	61
29	**2**	CuI	K_3PO_4	80	DMSO	27
30	**2**	CuI	K_2CO_3	80	DMSO	31
31	**2**	CuI	CS_2CO_3	80	DMSO	17
32	**2**	CuI	NaOAc	80	DMSO	18
33	**2**	CuI	CsF	80	DMSO	28
34	**2**	CuI	AgF_2	80	DMSO	9
35	**2**	CuI	—	120	DMSO	52
36	**2**	CuI	—	140	DMSO	12
37	**2**	CuI	—	105	DMSO	52
38	**2**	CuI	—	100	DMSO	49
39	**2**	CuI	—	25	DMSO	3
40	**2**	Cu	—	80	DMSO	18
41	**2**	CuI, 1,10-Phenanthroline	KF	80	DMSO	45
42	**2**	CuI, 2,2'-bipyridine	KF	80	DMSO	33
43	**2**	CuI, $AgNO_3$(0.5)	KF	80	DMSO	55
44	**2**	CuI, Mg power(0.5)	KF	80	DMSO	23
45	**2**	CuI, Ag power (0.5)	KF	80	DMSO	57
46	**2**	CuI, $AgCO_3$(0.5)	KF	80	DMSO	41
47	**2**	CuI, $K_2S_2O_8$(0.5)	KF	80	DMSO	23
48	**2**	CuI, Ag power (0.5)	KF	120	DMSO	16
49	**2**	CuI, Ag power (0.5), 1,10-Phenanthroline	KF	100	DMSO	14

[#] All reactions were carried out at 0.2 mmol of **1a** using 0.35 mmol of **2** in 1 mL of solvent at 80 ^{o}C in a Schlenk tube under nitrogen and the progress of reaction was monitored by TLC upto 35 h. [a] Percentage yield of **3a** determined by ^{19}F-NMR Spectroscopy using fluorobenzene as an internal standard. [b] Yield of **4.** ND = Not detected.

Synthesis of trifluoromethylated benzoxazine (**3a**) from *N*-(2-prop-1-en-2-yl) benzamide (**1a**) was optimized by screening of various trifluromethylating reagents (See Scheme above in the Table S1), Cu salts, bases, oxidants, ligands in various solvents in Schlenk tube at 80 to 120 ^{0}C (Table S1). We began optimization by observing reaction of **1a**, CuI (20 mol%) and Togni's

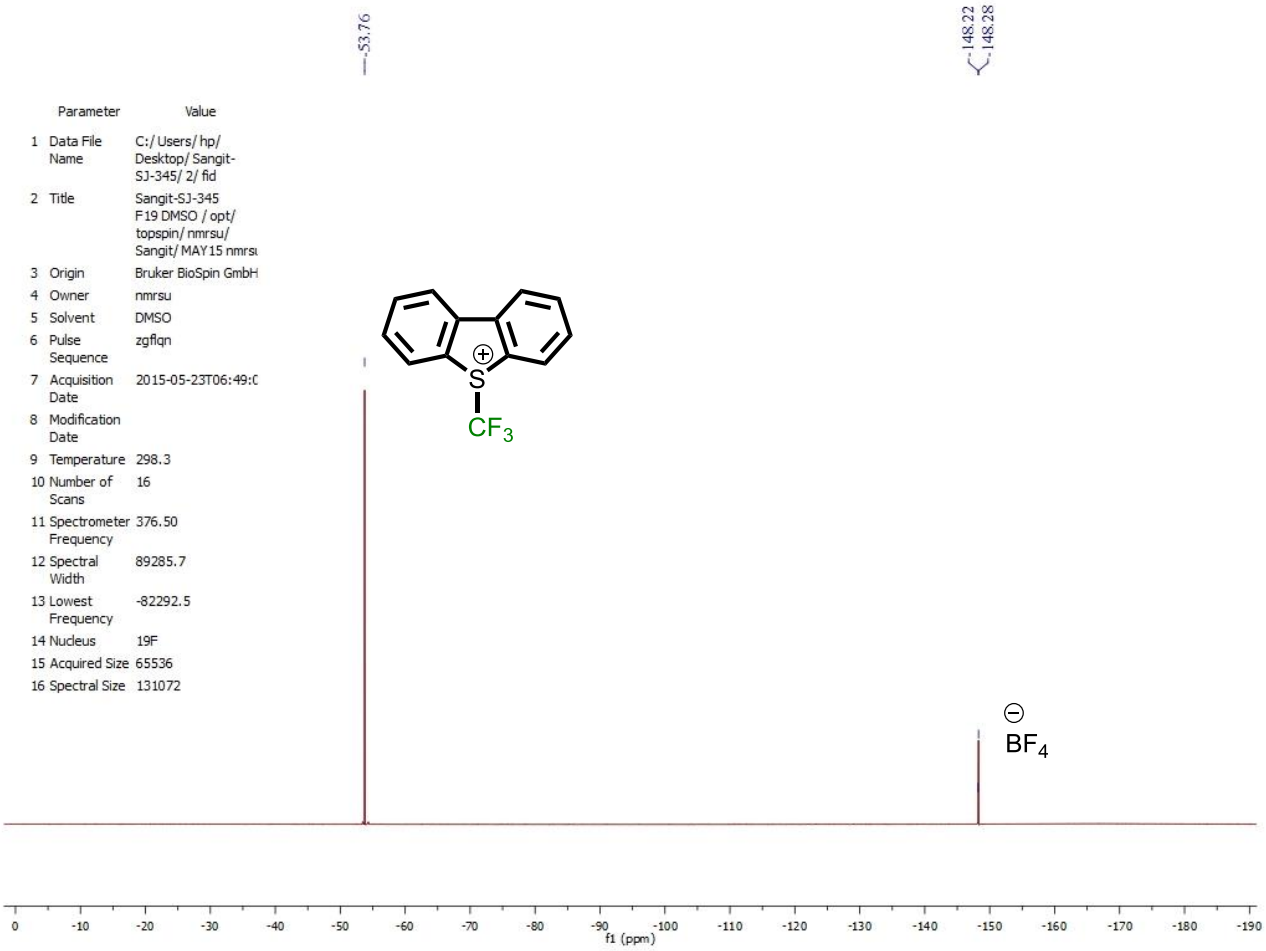
reagent in DCE at 80 ^{0}C under nitrogen atmosphere. Mixture of desired trifluoromethylated benzoxazine **3a** in low yield (30%) along with 45% allylic trifluoromethylated as major product **4a** was observed (entry 1, Table S1). Next, we screened various trifluoromethylating agents such as $TMSCF_3$, Shreeve's, and Umemoto's reagents. No desired product was observed when $TMSCF_3$ was used (entry 2, Table S1). Subsequently, Shreeve's and Umemoto's reagents gave 37% and 52 % desired products **3a**, respectively (entries 2, 3, Table S1). Although, we screened different Cu salts, but no improvement in yield was observed (entries 6-16, Table S1). Nonetheless, CuI was found to be effective for this reaction. We also screen different bases (entries 27-34, Table S1), varying temperatures (entries 35-39, Table S1), addition of different ligands along with additives, and bases (entries 41-49, Table S1). Nonetheless, substantial improved in the yield of **3a** could not be realized. Next, we examined the significance of solvent on reaction outcome (entries 17-24, Table S1), Among a range of solvents tested from DCE to DMAc, DMF, DMSO leads to further improvements in yields and best yield 68% was obtained in DMSO.

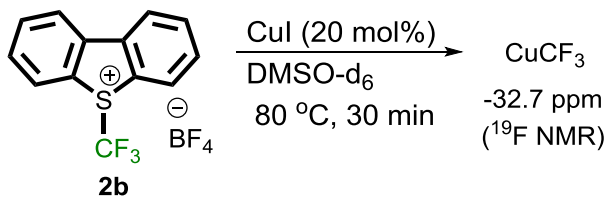
Mechanistic Investigation [3]



2b

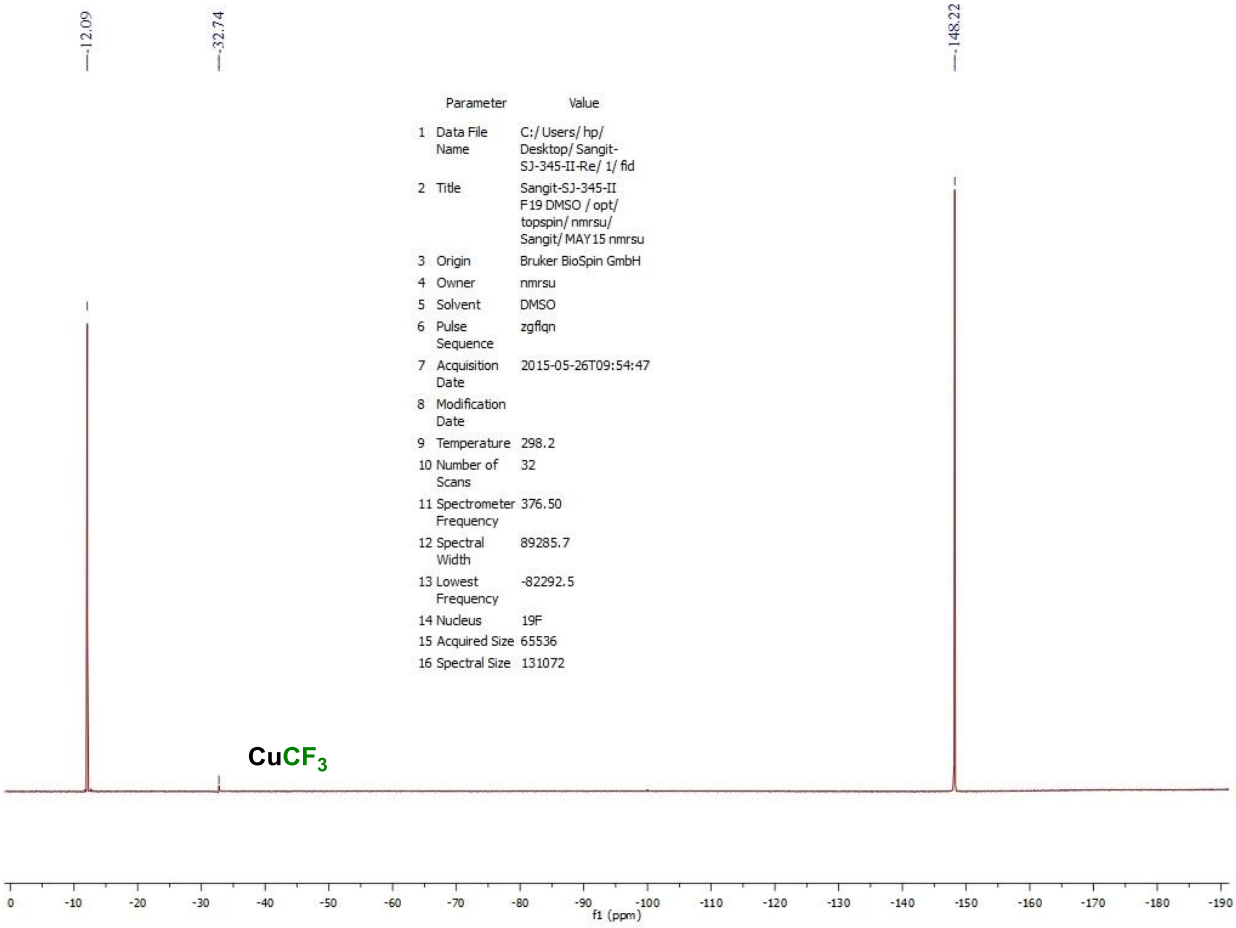
NMR Spectra

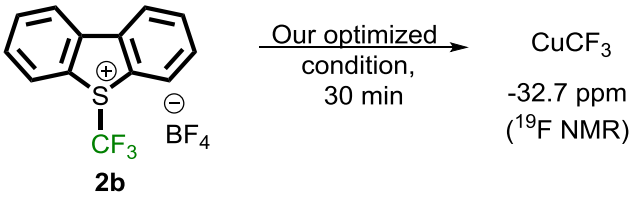




2b

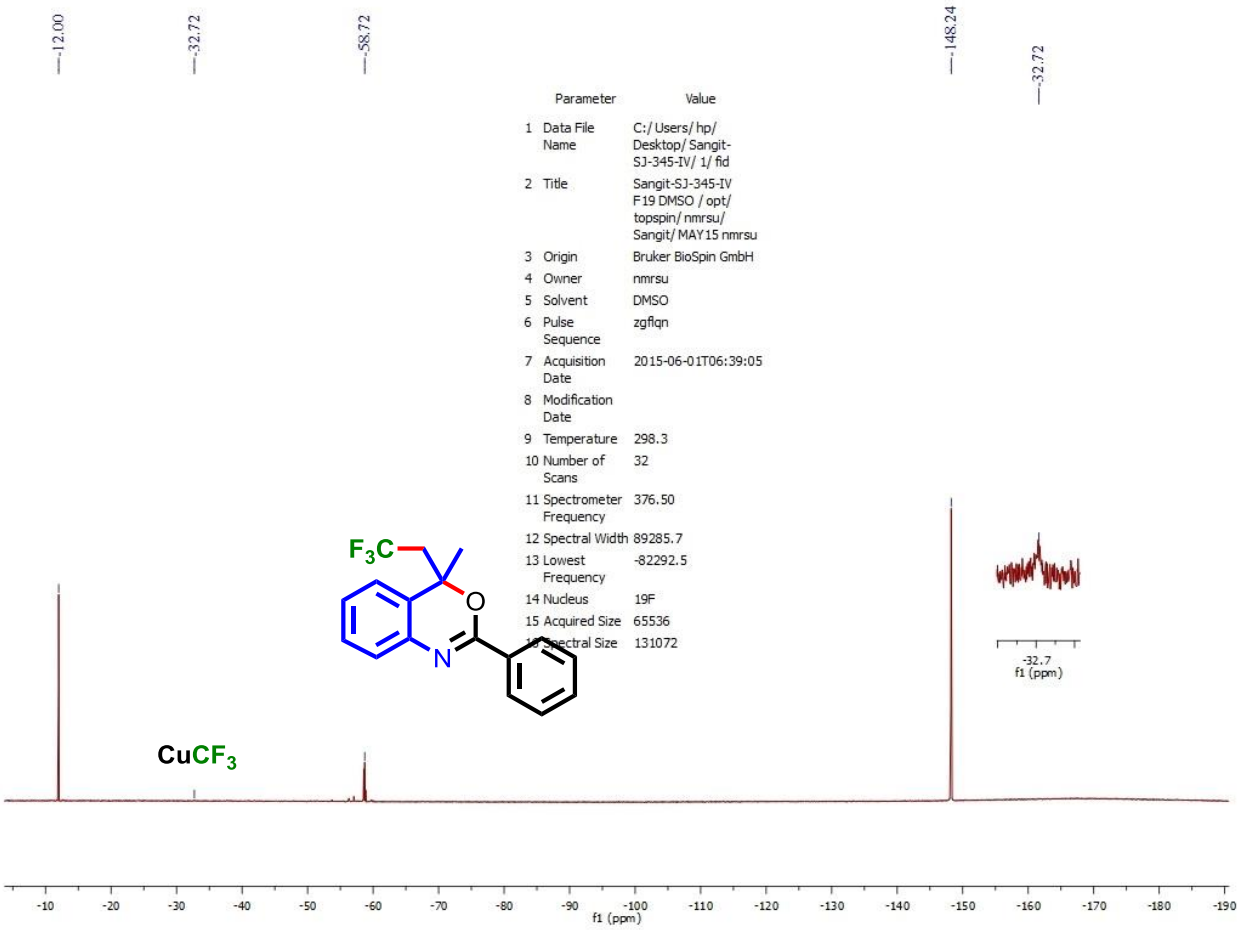
NMR Spectra





2b

NMR Spectra



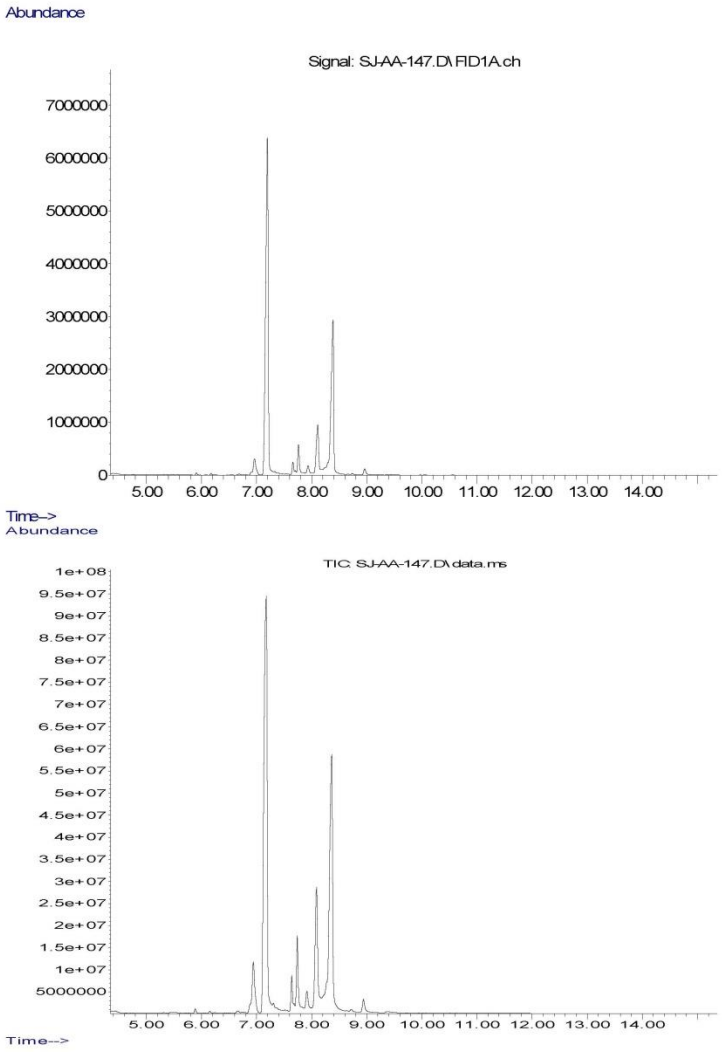
GC-MS Spectra.

Acquisition date: 17/04/15

Sample ID: SJ-345 ***Supervisor***: Dr. Sangit Kumar ***Operator:*** **IISERB-CIF-Mass Facility**

Instrument*: Agilent 7890A GC with 5975C MS system** ***Column*: HP-5** ***Ionization: **EI (70 eV)**

Method: **General_1_HP5_80_DEG.M** ***MSD*: Single Quad**.



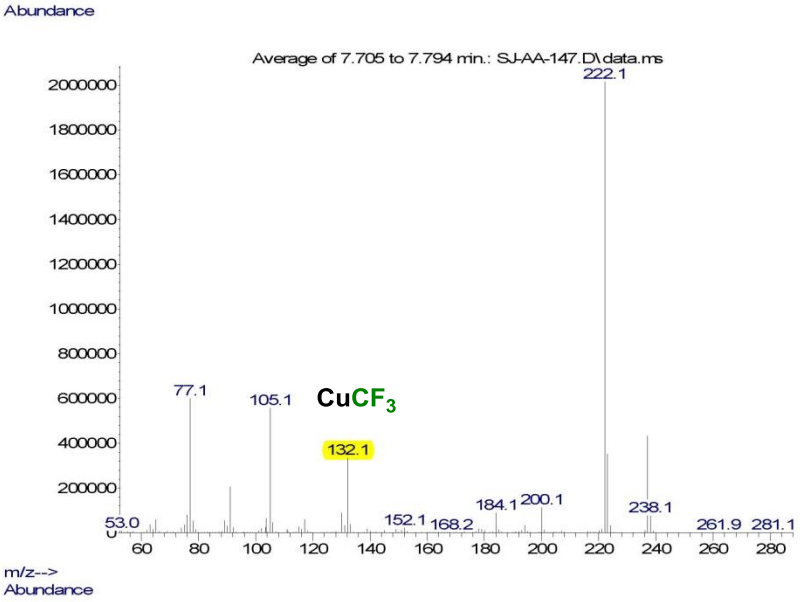
Agilent Technologies

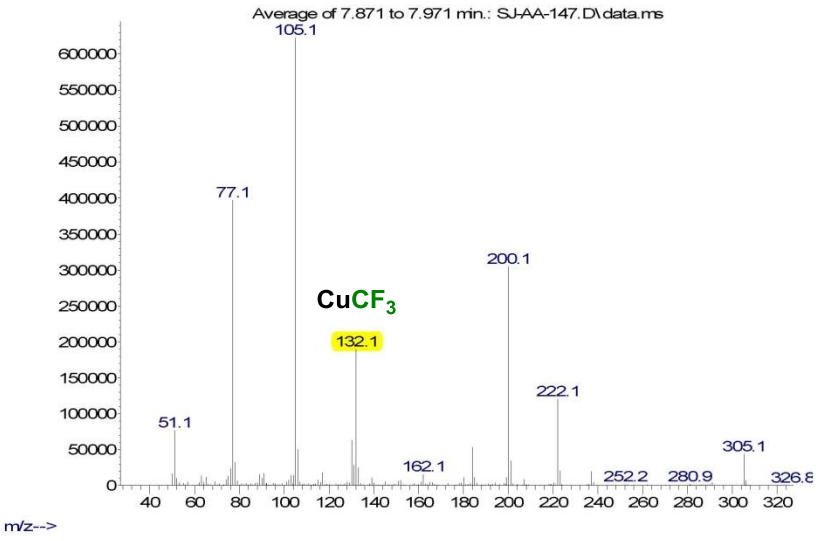
Acquisition date: 17/04/15

Sample ID: SJ-345 | ***Supervisor***: Dr. Sangit Kumar | ***Operator***: **IISERB-CIF-Mass Facility**

Instrument: **Agilent 7890A GC with 5975C MS system** | ***Column***: **HP-5** | ***Ionization***: **EI (70 eV)**

Method: **General_1_HP5_80_DEG.M** | ***MSD***: **Single Quad.**





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Acquisition date: 17/04/15

Sample ID: SJ-345

Supervisor: Dr. Sangit Kumar

Operator: **IISERB-CIF-Mass Facility**

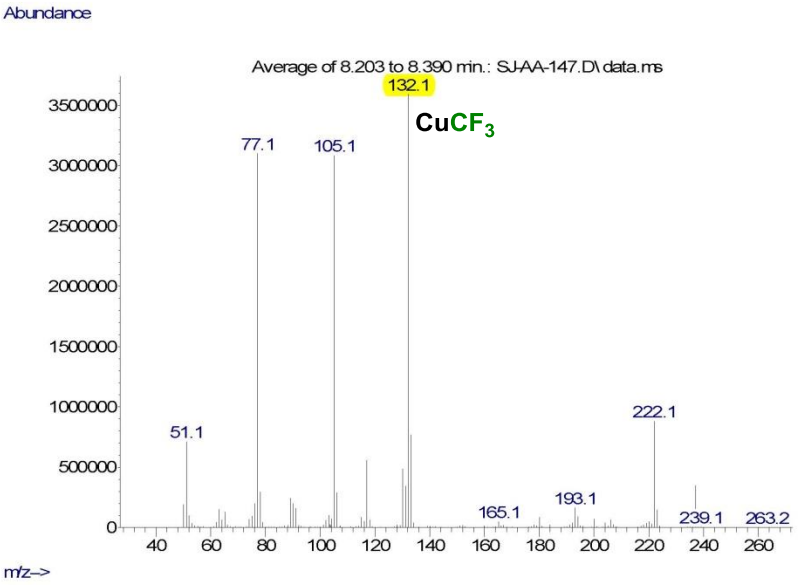
***Instrument*: Agilent 7890A GC with 5975C MS system**

***Column*: HP-5**

Ionization: **EI (70 eV)**

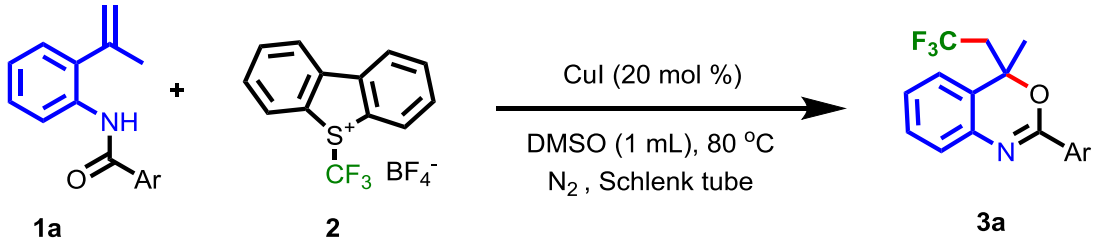
Method: **General_1_HP5_80_DEG.M**

***MSD*: Single Quad.**



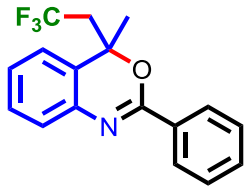
Agilent Technologies

General experimental procedure for trifluoromethylation of *N*-(2-(prop-1-en-2-yl)aryl)benzamides



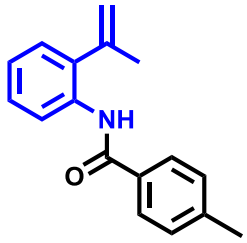
Benzamide 1a (0.047 g, 0.2 mmol, 1.0 equiv), Umemoto's reagent 2 (0.119 g, 0.35 mmol, 1.75 equiv), and CuI (0.008 g, 0.04 mmol, 0.2 equiv) were added to a 25 mL Schlenk tube equipped with magnetic stir bar. The tube was evacuated and backfilled with nitrogen and then DMSO (1 mL) was added to the tube by syringe. The progress of the reaction was monitored by TLC. The reaction mixture was stirred upto 16-35 h at 80 ^{0}C and extracted with ethyl acetate (2 x 15 mL). The combined organic layers were washed with saturated brine (2 x 30 mL), dried over Na_2SO_4, and the organic solvent was removed by rotary evaporator under vacuum and the residue was purified by flash column chromatography on silica gel (petroleum ether: EtOAc = 30: 1) to afford the benzoxazine 3a.

Characterization Data

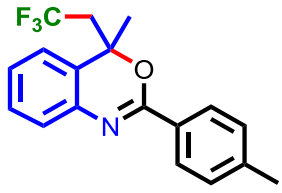


4-Methyl-2-phenyl-4-(2, 2, 2-trifluoromethyl)[*d*][1,3]oxazine (3a):[4] White Solid, yield (0.041 g, 68%), ^{1}H NMR (400 MHz, $CDCl_3$), δ 8.16 (m, 2H), 7.51-7.42 (m, 3H), 7.33-7.31 (m, 2H), 7.23-7.18 (m, 1H), 7.14-7.11 (m, 1H), 2.91-2.79 (m, 1H), 2.67-2.55 (m, 1H), 1.91 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 156.0, 155.7, 138.3, 132.2, 131.5, 129.3, 128.2, 128.1 (q, *J* = 278.0

Hz, CF_3), 128,0 126.9, 125.6, 122.5, 76.6 (q, *J* = 2.2 Hz), 43.1 (q, *J* = 27.1 Hz, CH_2CF_3), 26.6 (d, *J* = 1.5 Hz), ^{19}F NMR (376 MHz, $CDCl_3$), δ -59.89 (t, *J* = 10.5 Hz, 3F), HRMS (ESI), *m/z* calcd for $C_{17}H_{14}F_3NO$ $[M+H]^+$ 306.1100, found 306.1102.

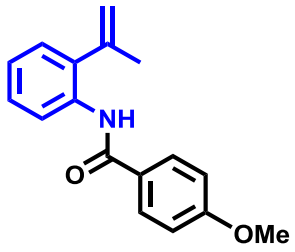


4-Methyl-*N*-(2-(prop-1-en-2-yl)phenyl)benzamide (1b):[5] White solid, yield (0.61 g, 83%). m.p.: 64 – 66 ^{o}C, ^{1}H-NMR (500 MHz, $CDCl_3$), δ 8.47 (d, *J* = 8.5 Hz, 1H), 8.42 (bs, 1H), 7.71 (d, *J* = 8.2 Hz, 2H), 7.31 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.29-7.26 (m, 2H), 7.17 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.09 (td, *J* = 7.8, 1.6 Hz, 1H), 5.46-5.45 (m, 1H), 5.10 (q, *J* = 0.9 Hz, 1H), 2.40 (s, 3H), 2.09 (t, *J* = 1.30 Hz, 3H), ^{13}C NMR (125 MHz, $CDCl_3$), δ 165.0, 143.3, 142.3, 134.1, 133.4, 132.2, 129.5, 128.0, 127.6, 126.9, 123.8, 120.7, 116.8, 24.6, 21.5, HRMS (ESI), *m/z* calcd for $C_{17}H_{17}NO$ $[M+H]^+$ 252.1383, found 252.1400.

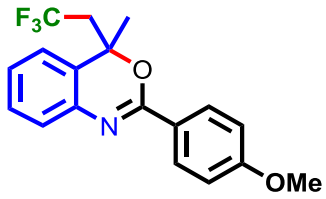


4-Methyl-2-(p-tolyl)-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine (3b): White semi-solid; yield (0.075g, 59%), ^{1}H-NMR (400 MZ, $CDCl_3$), δ 8.05 (d, *J* = 8.1 Hz, 2H), 7.33-7.30 (m, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.21-7.18 (m, 1H), 7.11 (d, *J* = 7.7 Hz, 1H), 2.90-2.78 (m, 1H), 2.65-2.54 (m, 1H), 2.40 (s, 3H), 1.90 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 155.9, 142.0, 138.4, 129.4, 129.3, 129.0, 128.3, 128.0, 126.7, 125.5, 125.1 (q, $J_{C,F}$ = 278.3 Hz, 3F), 122.5, 76.4 (q, *J* = 2.2 Hz), 43.5 (q, *J* = 27.1Hz, CH_2CF_3),

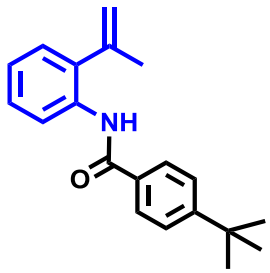
26.1 (d. $J_{C,F}$ = 1.6 Hz), 21.6, ^{19}F NMR (376 MHz, $CDCl_3$), δ -59.8 (t, *J* = 10.5 Hz, 3F), HRMS (ESI), *m/z* calcd for $C_{18}H_{16}F_3NO$ $[M+H]^+$ 320.1257, found 320.1275.



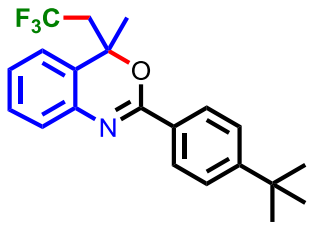
4-Methoxy-N-(2-(prop-1-en-2-yl)phenyl)benzamide (1c):[2] White solid, yield (0.58 g, 82%). m.p.: 102 – 104 ^{o}C, ^{1}H-NMR (500 MHz, $CDCl_3$), δ 8.45 (d, *J* = 8.3 Hz, 1H), 8.37 (bs, 1H), 7.77 (d, *J* = 8.8 Hz, 2H), 7.29 (td, *J* = 7.8, 1.6 Hz, 1H), 7.16 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.08 (td, *J* = 7.5, 1.2 Hz, 1H), 6.96 (d, *J* = 8.9, 2H), 5.46-5.45 (m, 1H), 5.09 (q, *J* = 0.9 Hz, 1H), 3.84 (s, 3H), 2.09 (t, *J* = 1.2 Hz, 3H), ^{13}C NMR (125 MHz, $CDCl_3$), δ 164.6, 162.4, 143.4, 134.2, 133.3, 128.8, 128.0, 127.6, 127.3, 123.6, 120.6, 116.7, 114.0, 55.4, 24.6.



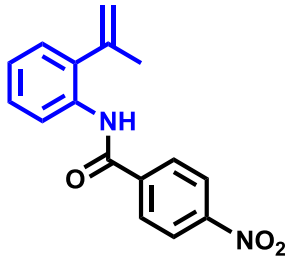
2-(4-Methoxyphenyl)-4-methyl-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine (3c): White semi-solid, yield (0.063 g, 50%), ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.09 (d, *J* = 8.9 Hz, 2H), 7.34-7.27 (m, 2H), 7.18 (td, *J* = 7.7, 1.7 Hz, 1H), 7.10 (d, *J* = 7.6 Hz, 1H), 6.93 (d, *J* = 8.9 Hz, 2H), 3.85 (s, 3H), 2.89-2.77 (m, 1H), 2.64-2.52 (m, 1H), 1.90 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 162.4, 155.7, 138.6, 129.8, 129.2, 128.3, 126.5, 125.6, 125.1 (q, $J_{C,\,F}$ = 279.2 Hz, CF_3), 124.6, 122.4, 113.6, 76.3 (q, $J_{C,\,F}$ = 2.18 Hz), 55.3, 43.5 (q, $J_{C,\,F}$ = 27.1, Hz, CH_2CF_3), ^{19}F NMR (376 MHz, $CDCl_3$), δ -59.8 (t, *J* = 10.5 Hz, 3F), HRMS (ESI), *m/z* calcd for $C_{18}H_{16}F_3NO_2$ $[M+H]^+$ 336.1206, found 336.1210.



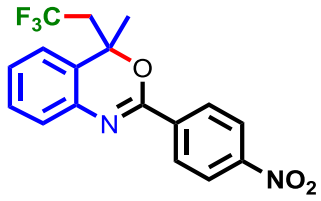
4-(*tert*-Butyl)-N-(2-(prop-1-en-2-yl)phenyl)benzamide (1d):[2] White solid, yield (0.57 g, 86%). m.p.: 108 – 110 ^{o}C, ^{1}H-NMR (500 MHz, $CDCl_3$), δ 8.49 (d, *J* = 8.3 Hz, 1H), 8.45 (bs, 1H), 7.76 (d, *J* = 8.5 Hz, 2H), 7.50 (d, *J* = 8.5 Hz, 2H), 7.31 (td, *J* = 7.8, 1.6 Hz, 1H), 7.17(dd, *J* = 7.7, 1.6Hz, 1H), 7.09 (td, *J* = 7.8, 1.6 Hz, 1H), 5.47-5.46 (m, 1H), 5.10 (q, *J* = 0.9 Hz, 1H), 2.10 (s, 3H), 1.34 (s, 9H), ^{13}C NMR (125 MHz, $CDCl_3$), δ 164.9, 155.3, 143.3, 134.2, 133.4, 132.2, 128.0, 127.6, 126.8, 125.8, 123.7, 120.6, 116.8, 35.0, 31.1, 24.7. HRMS (ESI), *m/z* calcd for $C_{20}H_{23}NO$ $[M+H]^+$ 294.1852, found 294.1856.



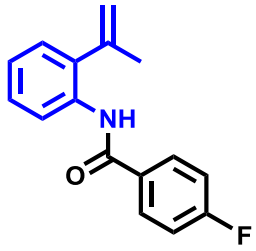
2-(4-(*tert*-Butyl)phenyl)-4-methyl-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine (3d): Pale yellow semi-solid, yield (0.067g, 54%), ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.07 (d, *J* = 7.4 Hz, 2H), 7.45 (d, *J* = 8.5 Hz, 2H), 7.34-7.30 (m, 2H), 7.22-7.18 (m, 1H), 7.11 (d, *J* = 7.7 Hz, 1H), 2.90-2.78 (m, 1H), 2.66-2.55 (m, 1H), 1.90 (s, 3H), 1.34 (s, 9H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 155.8, 155.1, 138.5, 129.4, 129.2, 128.3, 127.8, 126.7, 125.5, 125.2, 125.1 (q, $J_{C,F}$ = 279.2 Hz, CF_3), 122.5, 76.4 (q, $J_{C,F}$ = 2.2 Hz), 43.6 (q, $J_{C,F}$ = 27.1 Hz, CH_2CF_3), 34.9, 31.1, 26.2 (d, $J_{C,F}$ = 1.6 Hz), ^{19}F NMR (376 MHz, $CDCl_3$), δ -59.8 (t, *J* = 10.7 Hz, 3F), HRMS (ESI), *m/z* Calcd for $C_{21}H_{22}F_3NO$ $[M+H]^+$ 362.1726, found 362.1747.



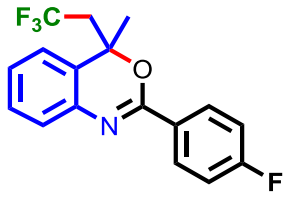
4-Nitro-N-(2-(prop-1-en-2-yl)phenyl)benzamide (1e):[7] Light yellow solid, yield (0.62 g, 92%). m.p.: 130 – 132 ^{o}C, ^{1}H-NMR (500 MHz, $CDCl_3$), δ 8.48 (bs, 1H), 8.43 (d, *J* = 8.0 Hz, 1H), 8.32 (d, *J* = 8.9 Hz, 2H), 7.96 (d, *J* = 8.9 Hz, 2H), 7.33 (td, *J* = 7.8, 1.6 Hz, 1H), 7.20 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.15 (td, *J* = 7.5, 1.1 Hz, 1H), 5.48-5.47(m, 1H), 5.10 (q, *J* = 0.95 Hz, 1H), 2.11 (t, *J* = 1.22 Hz, 3H), ^{13}C NMR (125 MHz, $CDCl_3$), δ 162.9, 149.7, 143.2, 140.6, 133.6, 133.3, 128.2, 128.1, 127.8, 124.6, 124.1, 120.7, 117.0, 24.7, HRMS (ESI), *m/z* calcd for $C_{16}H_{14}N_2O_3$ $[M+H]^+$ 283.1077, found 283.1085.



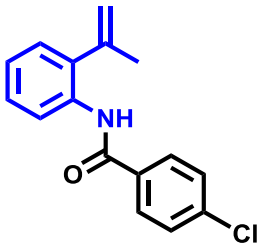
4-Methyl-2-(4-nitrophenyl)-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine (3e): Light yellow-solid, yield (0.114g, 92%). m.p.: 73 – 75 ^{o}C, ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.28 (q, *J* = 8.9 Hz, 4H), 7.38-7.32 (m, 2H), 7.27 (td, *J* = 7.5, 2.14 Hz, 1H), 7.14 (d, *J* = 7.5 Hz, 1H), 2.91-2.79 (m, 1H), 2.68-2.56 (m, 1H), 1.93 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 153.4, 149.5, 138.0, 137.5, 129.6, 128.7, 128.1, 128.0, 126.1, 125.0 (q, $J_{C,F}$ = 278.6, CF_3), 123.4, 122.7, 77.3 (q, $J_{C,F}$ = 2.18), 43.9 (q, $J_{C,F}$ = 27.2 Hz, CH_2CF_3), 26.7 (d, $J_{C,F}$ = 1.6 Hz), ^{19}F NMR (376 MHz, $CDCl_3$), δ -60.0 (t, *J* = 10.5 Hz, 3F),), HRMS (ESI), *m/z* calcd for $C_{17}H_{13}F_3N_2O_3$ $[M+H]^+$ 351.0951, found 351.0978.



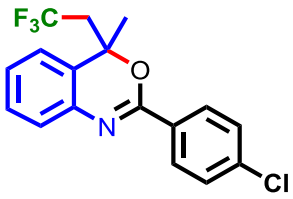
4-Fluoro-N-(2-(prop-1-en-2-yl)phenyl)benzamide (1f): White solid, yield (0.65 g, 89%). m.p.: 100 – 102 ^{o}C, ^{1}H-NMR (500 MHz, $CDCl_3$), δ 8.43 (d, *J* = 8.3 Hz, 1H), 8.37 (bs, 1H), 7.84-7.80 (m, 2H), 7.30 (td, *J* = 7.8 Hz, *J* = 1.6 Hz, 1H), 7.18 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.16-7.09 (m, 3H), 5.47-5.45 (m, 1H), 5.09 (q, *J* = 0.9 Hz, 1H), 2.10 (s, 3H), ^{13}C NMR (125 MHz, $CDCl_3$), δ 165.9, 164.0, 163.9, 143.3, 133.1 (d, $J_{C,F}$ = 39.6 Hz), 131.3 (d, $J_{C,F}$ = 3.2 Hz), 129.3 (d, $J_{C,F}$ = 9.0 Hz), 127.9 (d, $J_{C,F}$ = 49.8 Hz), 124.0, 120.7, 116.8, 116.0, 115.8, 24.6, HRMS (ESI), *m/z* calcd for $C_{16}H_{14}FNO$ $[M+H]^+$ 256.1132, found 256.1121.



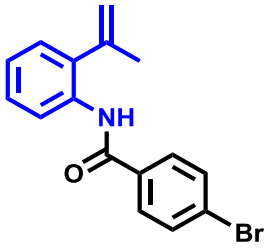
2-(4-Fluorophenyl)-4-methyl-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine (3f): White solid, yield (0.100g, 79%). m.p.: 98 – 100 ^{o}C, ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.15 (dd, *J* = 7.5, 5.6 Hz, 2H), 7.35-7.29 (m, 2H), 7.21 (td, *J* = 7.5, 1.7 Hz, 1H), 7.10 (t, *J* = 7.5 Hz, 3H), 2.90-2.78 (m, 1H), 2.65-2.53 (m, 1H), 1.90 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 166.3, 163.7, 154.8, 138.1, 130.3 (d, $J_{C,F}$ = 8.9 Hz), 129.4, 128.4 (d, *J* = 2.9 Hz), 1.28.1, 127.0, 125.5, 125.0 (q, *J* = 278.4 Hz, CF_3), 122.5, 115.3 ($J_{C,F}$ = 22.0 Hz), 76.7 (q, $J_{C,F}$ = 2.16 Hz), 43.6 (q, *J* = 27.2 Hz, CH_2CF_3), 26.2 (d, *J* = 1.66 Hz), ^{19}F NMR (376 MHz, $CDCl_3$), δ -59.9 (t, *J* = 10.7 Hz, 3F), -108.19 to -108.12 (m, F), HRMS (ESI), *m/z* calcd for $C_{17}H_{13}F_4NO$ $[M+H]^+$ 324.1006, found 324.1021.



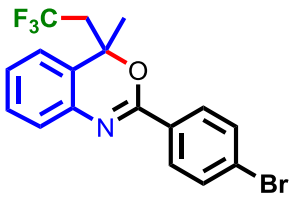
4-Chloro-N-(2-(prop-1-en-2-yl)phenyl)benzamide (1g):[2] White solid, yield (0.58 g, 84%). m.p.: 86 – 88 ^{o}C, ^{1}H-NMR (500 MHz, $CDCl_3$), δ 8.47 (d, *J* = 8.3 Hz, 1H), 8.43 (bs, 1H), 7.79 (d, *J* = 8.6 Hz, 2H), 7.48 (d, *J* = 8.6 Hz, 2H), 7.35 (td, *J* = 7.8, 1.7 Hz, 1H), 7.22 (dd, *J* = 7.8, 1.67 Hz, 1H), 7.16 (td, *J* = 7.5, 1.2 Hz, 1H), 5.51-5.49 (m, 1H), 5.13 (q, *J* = 0.9 Hz, 1H), 2.14 (t, *J* = 1.2 Hz, 3H), ^{13}C NMR (125 MHz, $CDCl_3$), δ 164.0, 143.3, 138.1, 133.7, 133.5, 133.4, 129.1, 128.3, 128.1, 127.7, 124.1, 120.7, 116.8, 24.6.



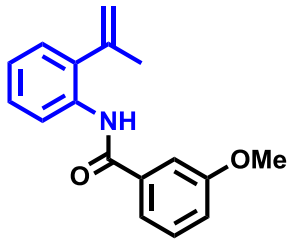
2-(4-Chlorophenyl)-4-methyl-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine (3g): White solid, yield (0.095g, 76%). m.p.: 66 – 68 ^{o}C, ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.08 (d, *J* = 8.6 Hz, 2H), 7.40 (d, *J* = 8.6 Hz, 2H), 7.34-7.29 (m, 2H), 7.22 (dd, *J* = 7.0, 1.6 Hz, 1H), 7.12 (d, *J* = 7.6 Hz, 1H), 2.88-2.79 (m, 1H), 1.9 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 154.7, 138.0, 137.8, 130.7, 129.4, 129.3, 128.5, 128.2, 127.2, 125.7, 125.0 (q, *J* = 278.7 Hz, CF_3), 122.6, 76.7 (q, *J* = 2.1 Hz), 43.7 (q, *J* = 27.3Hz, CH_2CF_3), 26.3 (d, *J* = 1.59 Hz), ^{19}F NMR (376 MHz, $CDCl_3$), δ -59.9 (t, *J* = 10.5 Hz, 3F), HRMS (ESI), *m/z* calcd for $C_{17}H_{13}ClF_3NO$ $[M+H]^+$ 340.0711, found 340.0687.



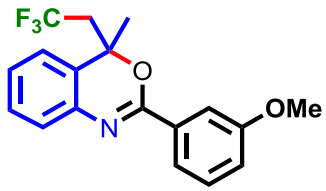
4-Bromo-N-(2-(prop-1-en-2-yl)phenyl)benzamide (1h):[5] White solid, yield (0.59 g, 94%). m.p.: 104 – 108 ^{o}C, ^{1}H-NMR (500MHz, $CDCl_3$), δ 8.42 (d, *J* = 8.3 Hz, 1H), 8.39 (bs, 1H), 7.67 (d, *J* = 8.64Hz, 2H), 7.60 (d, *J* = 8.6 Hz, 2H), 7.30 (td, *J* = 7.8, 1.6 Hz, 1H), 7.17 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.11 (td, *J* = 7.5, 1.2 Hz, 1H), 5.46-5.44 (m, 1H), 5.08 (q, *J* = 1.0 Hz, 1H), 2.09 (t, *J* = 1.2 Hz, 3H), ^{13}C NMR (125 MHz, $CDCl_3$), δ 164.1, 143.3, 133.9, 133.7, 133.5, 132.1, 128.5, 128.1, 127.7, 126.5, 124.1, 120.7, 116.8, 24.6, HRMS (ESI), *m/z* calcd for $C_{16}H_{14}BrNO$ $[M+H]^+$ 316.0332, found 316.0323.



2-(4-Bromophenyl)-4-methyl-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine (3h): Pale yellow semi-solid, yield (0.087g, 74%), ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.01 (d, *J* = 8.5 Hz, 2H), 7.56 (d, *J* = 8.5 Hz, 2H), 7.35-7.29 (m, 2H), 7.22 (t, *J* = 7.2 Hz, 1H), 7.11 (d, *J* = 7.6 Hz, 1H), 2.89-2.77 (m, 1H), 2.64-2.52 (m, 1H), 1.90 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 154.8, 138.0, 131.5, 131.2, 129.5, 129.4, 128.2, 127.2, 126.3, 125.7, 125.1 (q, $J_{C,F}$ = 279 Hz, CF_3), 122.6, 76.8 (q, $J_{C,F}$= 2.2 Hz), 43.7(q, $J_{C,F}$ = 27.2 Hz, CH_2CF_3), 26.3 (d, $J_{C,F}$ = 1.6 Hz), ^{19}F NMR (376 MHz, $CDCl_3$), δ -59.9 (t, *J* = 10.6 Hz, 3F), HRMS (ESI), *m/z* calcd for $C_{17}H_{13}BrF_3NO$ $[M+H]^+$ 384.0224, found 384.0205.

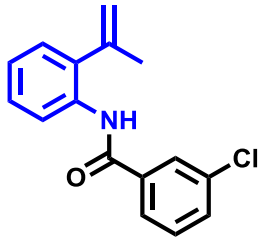


3-Methoxy-N-(2-(prop-1-en-2-yl)phenyl)benzamide (1i): White semi-solid, yield (0.60 g, 85%), ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.47 (d, *J* = 8.2 Hz, 1H), 8.44 (bs, 1H), 7.42 (t, *J* = 2.0 Hz, 1H), 7.36 (t, *J* = 7.9 Hz, 1H), 7.32-7.29 (m, 2H), 7.17 (dd, *J* = 7.7 Hz, *J* = 1.6 Hz, 1H), 7.10 (td, *J* = 7.4, J = 1.2 Hz, 1H), 7.06 (ddd, *J* = 8.2, 2.6, 0.9 Hz, 1H), 5.46-5.46 (m, 1H), 5.10 (q, *J* = 0.1 Hz, 1H), 3.85 (s, 3H), 2.10 (t, *J* = 1.2 Hz, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 164.9, 160.0, 143.3, 136.6, 134.0, 133.5, 129.8, 128.0, 127.6, 123.9, 120.6, 118.4, 118.0, 116.8, 112.4, 55.4, 24.6, HRMS (ESI), *m/z* calcd for $C_{17}H_{17}NO_2$ $[M+H]^+$ 268.1332, found 268.1343.

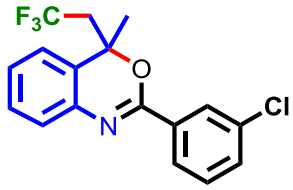


2-(3-Methoxyphenyl)-4-methyl-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine. (3i): White semi-solid, yield (0.058 g, 46%), ^{1}H-NMR (400 MHz, $CDCl_3$), δ 7.74 (d, *J* = 7.6 Hz, 1H), 7.69 (t, *J* = 1.9 Hz, 1H), 7.36-7.32 (m, 3H), 7.23-7.19 (m, 1H), 7.12 (d, *J* = 7.14 Hz, 1H), 7.04 (dd, *J* = 8.0, 2.7, Hz, 1H), 3.87 (s, 3H), 2.90-2.79 (m, 1H), 2.67-2.55 (m, 1H), 1.90 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 159.5, 155.5, 138.2, 133.6, 129.3, 129.2, 127.0, 125.6, 125.0 (q, $J_{C,\,F}$ = 279.0 Hz, CF_3), 122.5, 121.2, 120.5, 118.0, 112.5, 77.2 (q, *J* = 2.12 Hz), 122.5, 121.2, 120.5, 118.0, 112.5, 77.2 (q, *J* = 2.12 Hz), 55.3, 43.6 (q, *J* = 27.2 Hz, CH_2CF_3), 26.7 (d, *J* = 1.61 Hz),

^{19}F NMR (376 MHz, $CDCl_3$), δ -59.8 (t, *J* = 10 0 Hz, 3F), HRMS (ESI), *m/z* calcd for $C_{18}H_{16}F_3NO_2$ $[M+H]^+$ 336.1206, found 336.1222.

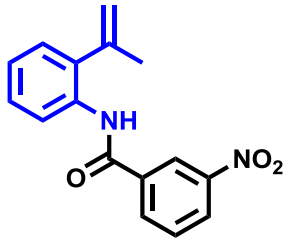


3-Chloro-N-(2-(prop-1-en-2-yl)phenyl)benzamide (1j): White solid, yield (0.55 g, 79%). m.p.: 55 – 57 ^{o}C, ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.41 (d, *J* = 8.2 Hz, 1H), 8.38 (bs, 1H), 7.81 (t, *J* = 1.8 Hz, 1H), 7.6 (dq, *J* = 7.7, 1.5 Hz, 1H), 7.50 (ddd, *J* = 8.0, 2.1, 1.0 Hz, 1H), 7.40 (t, *J* = 7.8 Hz, 1H), 7.30 (td, *J* = 7.8, 1.6 Hz, 1H), 7.18 (dd, *J* = 7.8 Hz, 1.6 Hz, 1H), 7.12 (td, *J* = 7.5 Hz, *J* = 1.2 Hz, 1H), 5.47-5.46 (m, 1H), 5.09 (q, *J* = 0.92 Hz, 1H), 2.10 (t, *J* = 1.2 Hz, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 163.7, 143.2, 136.9, 135.1, 133.6, 131.8, 130.1, 128.1, 127.7, 127.5, 124.7, 124.2, 120.8, 116.9, 24.6, HRMS (ESI), *m/z* calcd for $C_{16}H_{14}ClNO$ $[M+H]^+$ 272.0837, found 272.0839.

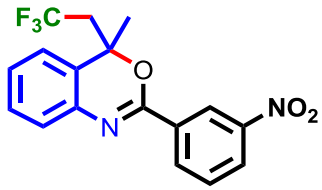


2-(3-Chlorophenyl)-4-methyl-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine (3j): White semi-solid, yield (0.084g, 67%), ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.13 (t, *J* = 1.7 Hz, 1H), 8.02 (d, *J* = 7.76 Hz, 1H), 7.45 (dq, *J* = 8.0, 1.0 Hz, 1H), 7.37 (d, *J* = 8.0 Hz, 1H), 7.32 (td, *J* = 8.0, 1.6 Hz, 2H), 7.23 (td, *J* = 6.2, 1.6 Hz, 1H), 7.12(d, *J* = 7.7 Hz, 1H), 2.87-2.79 (m, 1H), 2.66-2.57 (m, 1H), 1.91(s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 154.3, 137.9, 134.4, 134.0, 131.5, 129.5, 129.4, 128.1, 127.9, 127.3, 126.0, 125.8, 125.0 (q, $J_{C,\ F}$ = 278.2 Hz, CF_3), 122.6, 76.9 (q, $J_{C,\ F}$ =

2.16 Hz), 43.8 (q, $J_{C,\ F}$ = 27.3 Hz, CH_2CF_3), 26.5 (d, $J_{C,\ F}$ = 1.63 Hz), ^{19}F NMR (376 MHz, $CDCl_3$), δ -59.9 (t, *J* = 10.5 Hz, 3F), HRMS (ESI), *m/z* calcd for $C_{17}H_{13}ClF_3NO$ $[M+H]^+$ 340.0711, found 340.0679.

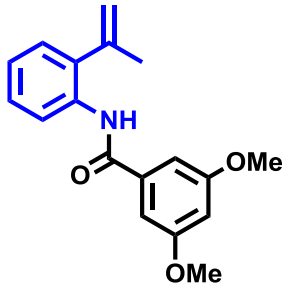


3-Nitro-N-(2-(prop-1-en-2-yl)phenyl)benzamide (1k): White solid, yield (0.50 g, 74%). m.p.: 166 – 168 ^{o}C, ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.64 (t, *J* = 2.0 Hz, 1H), 8.52 (bs, 1H), 8.40-8.36 (m, 2H), 8.14 (dt, *J* = 7.8, 1.3 Hz, 1H), 7.68 (t, *J* = 8.0 Hz, 1H), 7.31 (td, *J* = 7.8, 1.6 Hz, 1H), 7.20 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.14 (td, *J* = 7.8, 1.6 Hz, 1H), 5.51-5.49 (m, 1H), 5.12 (q, *J* = 1.0 Hz, 1H), 2.11 (t, *J* = 1.2 Hz, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 162.6, 148.4, 143.2, 136.7, 133.8, 133.3, 132.8, 130.1, 128.1, 126.8, 126.3, 124.6, 121.9, 120.9, 117.0, 24.6, HRMS (ESI), *m/z* calcd for $C_{16}H_{14}N_2O_3$ $[M+H]^+$ 283.1077, found 283.1097.

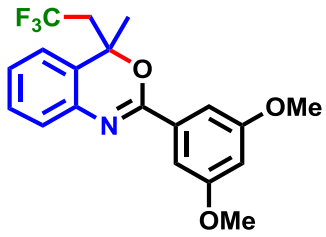


4-Methyl-2-(3-nitrophenyl)-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine (3k): White solid, yield (0.113g, 91%). m.p.: 110 – 112 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$), δ 8.97 (t, *J* = 1.8 Hz, 1H), 8.42 (d, *J* = 7.8 Hz, 1H), 8.33 (dd, *J* = 8.2, 1.3 Hz, 1H), 7.61 (t, *J* = 8.0 Hz, 1H), 7.38-7.33 (m, 2H), 7.28-7.24 (m, 1H), 7.14 (d, *J* = 7.6 Hz, 1H), 2.91-2.79 (m, 1H), 2.69-2.57 (m, 1H), 1.94 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 153.3, 148.3, 137.5, 134.1, 133.5, 129.5, 129.3, 128.0, 127.8, 126.0, 125.8, 124.9 (q, $J_{C,\ F}$ = 278.3Hz, CF_3), 122.9, 122.7, 77.4 (q, $J_{C,\ F}$ = 2.18 Hz),

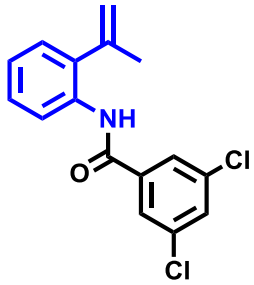
43.9 (q, $J_{C,F}$ = 27.1 Hz, CH_2CF_3), 26.8 (d, $J_{C,F}$ = 1.6 Hz), ^{19}F NMR (376 MHz, $CDCl_3$), δ -60.0 (t, *J* = 10.5 Hz, 3F), HRMS (ESI), *m/z* calcd for $C_{17}H_{13}F_3N_2O_3$ $[M+H]^+$ 351.0951, found 351.0968.



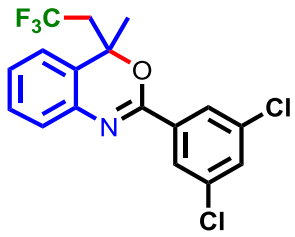
3,5-Dimethoxy-N-(2-(prop-1-en-2-yl)phenyl)benzamide (1l): White solid, yield (0.46 g, 71%). m.p.: 52 – 54 ^{o}C, ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.44 (d, *J* = 8.3 Hz, 1H), 8.38 (bs, 1H), 7.30 (td, *J* = 7.8, 1.6 Hz, 1H), 7.16 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.09 (td, *J* = 7.4, 1.0 Hz, 1H), 6.92 (d, *J* = 2.2 Hz, 2H), 6.59 (t, *J* = 2.2 Hz, 1H), 5.45-5.46 (m, 1H), 5.09-5.08 (m, 1H), 3.82 (s, 6H), 2.09 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 164.8, 161.0, 143.3, 137.3, 133.9, 133.5, 128.0, 127.6, 123.9, 120.6, 116.8, 104.8, 103.7, 55.5, 24.6, HRMS (ESI), *m/z* calcd for $C_{18}H_{19}NO_3$ $[M+H]^+$ 298.1438, found 298.1457.



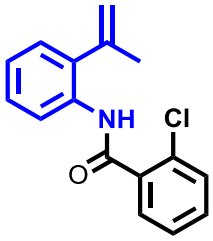
2-(3,5-Dimethoxyphenyl)-4-methyl-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine (3l): Pale yellow semi-solid, trace amount, ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.36 (d, *J* = 8.0 Hz, 1H), 7.52 (d, *J* = 7.3 Hz, 1H), 7.37-7.31 (m, 3H), 7.08 (s, 1H), 6.81-6.80 (m, 1H), 6.65-6.62 (m, 1H), 3.65-3.55 (m, 2H), 2.23 (s, 3H), ^{19}F NMR (376 MHz, $CDCl_3$), δ -59.8 (t, *J* = 10.5 Hz, 3F), HRMS (ESI) *m/z* calcd for $C_{19}H_{18}F_3NO_3$ $[M+ Na]^+$ 388.1131, found 388.1143.



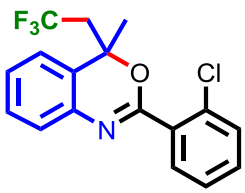
3,5-Dichloro-N-(2-(prop-1-en-2-yl)phenyl)benzamide (1m): White solid, yield (0.49 g, 77%). m.p.: 82 – 84 ^{o}C, ^{1}H-NMR (500 MHz, $CDCl_3$), δ 8.34 (d, *J* = 8.3 Hz, 1H), 8.32 (bs, 1H), 7.64 (d, *J* = 1.8 Hz, 2H), 7.50 (t, *J* = 1.8 Hz, 1H), 7.30 (td, *J* = 7.8, 1.6 Hz, 1H), 7.19 (dd, *J* = 7.8, 1.6, Hz, 1H), 7.13 (td, *J* = 7.5 Hz, 1.13Hz, 1H), 5.48-5.47 (m, 1H), 5.09 (q, *J* = 1.0 Hz, 1H), 2.10 (t, *J* = 1.2 Hz, 3H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.5, 138.0, 135.7, 133.8, 131.3, 131.6, 128.8, 128.8, 128.1, 127.7, 125.6, 124.6, 121.0, 116.9, 24.6, HRMS (ESI), *m/z* calcd for $C_{16}H_{13}Cl_2NO$ $[M+H]^+$ 306.0447, found 306.0452.



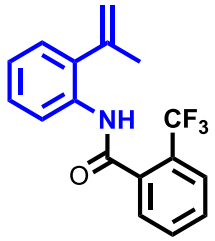
2-(3,5-Dichlorophenyl)-4-methyl-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine (3m): White-solid, yield (0.087g, 74%). m.p.: 66 – 68 ^{o}C, ^{1}H-NMR (400MHz, $CDCl_3$), δ 8.05 (d, *J* = 1.9 Hz, 2H), 7.46 (t, *J* = 1.9 Hz, 1H), 7.34 (td, *J* = 7.4, 1.1 Hz, 1H), 7.30 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.24 (td, *J* = 7.45 Hz, *J* = 1.60 Hz, 1H), 7.12 (d, J = 7.61 Hz, 1H), 2.88-2.76 (m, 1H), 2.67-2.55 (m, 1H), 1.90 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 153.1, 137.5, 135.2, 135.0, 131.2, 129.5, 128.0, 127.7, 126.2, 125.9, 125.1 (q, $J_{C,F}$ = 279.2 Hz, CF_3), 122.7, 77.2 (q, *J* = 27.1 Hz), 43.9 (q, *J* = 27.1Hz, CH_2CF_3), 26.7 (d, *J* = 1.6 Hz), ^{19}F NMR (376 MHz, $CDCl_3$), δ -60.0 (t, *J* = 10.5 Hz, 3F), HRMS (ESI), *m/z* calcd for $C_{17}H_{12}Cl_2F_3NO$ $[M+H]^+$ 374.0321, found 374.0320.



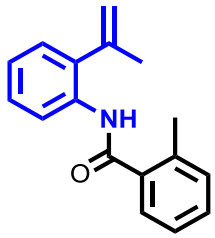
2-Chloro-N-(2-(prop-1-en-2-yl)phenyl)benzamide (1n):[5] White solid, yield (0.52 g, 83%). m.p.: 88 – 90 ^{o}C, ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.46(d, *J* = 8.25Hz, 1H), 8.28 (bs, 1H), 7.72 (dd, *J* = 7.4, 1.6 Hz, 1H), 7.41 (td, *J* = 7.8, 1.6 Hz, 1H), 7.39-7.33 (m, 2H), 7.31 (td, *J* = 7.8, 1.6 Hz, 1H), 7.16 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.11 (td, *J* = 7.5, 1.0 Hz, 1H), 5.34-5.33 (m, 1H), 5.03 (q, *J* = 1.0 Hz, 1H), 2.05 (t, *J* = 1.2 Hz, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 164.4, 142.6, 135.5, 134.0, 133.8, 131.6, 130.5, 130.4, 130.3, 128.0, 127.8, 127.3, 124.3, 121.0, 117.3, 24.7, HRMS (ESI), *m/z* calcd for $C_{16}H_{14}ClNO$ $[M+H]^+$ 272.0837, found 272.0858.



2-(2-Chlorophenyl)-4-methyl-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine (3n): Light brown semi-solid, yield (0.089 g, 71%), ^{1}H-NMR (400 MHz, $CDCl_3$), δ 7.73 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.44 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.39-7.29 (m, 4H), 7.25 (td, *J* = 7.4, 2.0 Hz, 1H), 7.12 (d, *J* = 7.6 Hz, 1H), 2.97-2.74 (m, 2H), 1.90 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 155.8, 137.6, 133.1, 132.3, 131.3, 130.9, 130.6, 129.4, 127.4, 127.0, 126.7, 125.7, 125.0, (q, *J* = 278.1 Hz, CF_3), 123.0, 77.9 (q, *J* = 2.2 Hz), 44.3 (q, *J* = 27.3 Hz, CH_2CF_3), 27.9 (d, *J* = 1.6 Hz), ^{19}F NMR (376 MHz, $CDCl_3$), δ -59.93 (t, *J* = 10.5 Hz, 3F), HRMS (ESI), *m/z* calcd for $C_{17}H_{13}ClF_3NO$ $[M+H]^+$ 340.0711, found 340.0716.

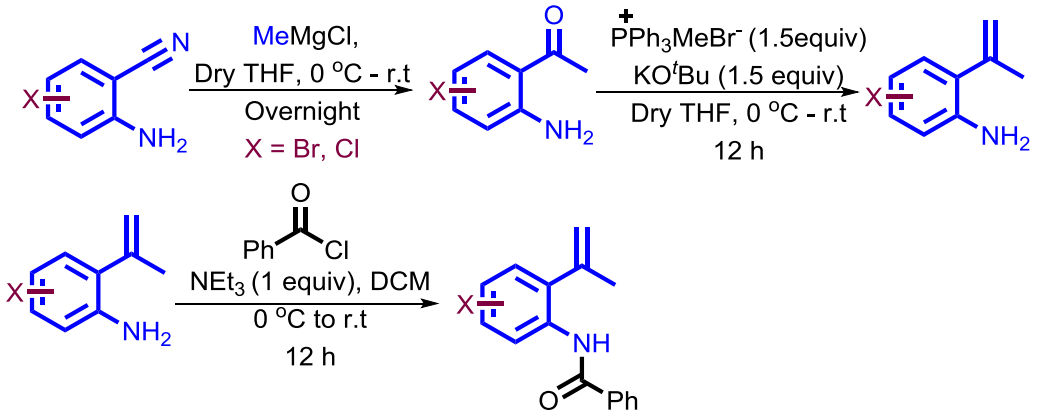


***N*-(2-(Prop-1-en-2-yl)phenyl)-2-(trifluoromethyl)benzamide (1o)**:[8] Yellow solid, yield (0.525 g, 82%). m.p.: 97 – 99 ^{o}C, ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.39 (d, *J* = 8.2 Hz, 1H), 7.84 (bs, 1H), 7.74 (d, *J* = 7.7 Hz, 1H), 7.65-7.55 (m, 3H), 7.32 (td, *J* = 7.7, 2.0 Hz, 1H), 7.18-7.11 (m, 2H), 5.29 (t, *J* = 1.4Hz, 1H), 4.98 (s, 1H), 2.04 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 165.5, 142.6, 136.0 (q, *J* = 2.1 Hz), 134.0, 133.6, 132.2, 130.1, 128.2, 128.0, 127.8, 126.6 (q, *J* = 4.9 Hz, CF_3), 124.9, 124.5, 122.2, 121.2, 116.9, 24.4, HRMS (ESI), *m/z* calcd for $C_{17}H_{14}F_3NO$ $[M+H]^+$ 306.1100, found 306.1107.

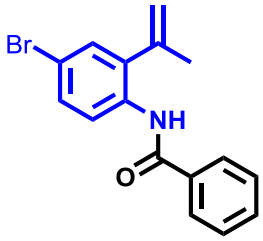


2-Methyl-N-(2-(prop-1-en-2-yl)phenyl)benzamide (1p):[5] White solid, yield (0.628 g, 85%). m.p.: 52 – 54 ^{o}C, ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.45 (d, *J* = 7.5 Hz, 1H), 7.91 (bs, 1H), 7.43 (d, *J* = 7.6 Hz, 1H), 7.38-7.30 (m, 2H), 7.27-7.23 (m, 2H), 7.17 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.12 (td, *J* = 7.6, 1.0 Hz, 1H), 5.34 (t, *J* = 1.6 Hz, 1H), 5.03 (s, 1H), 2.51 (s, 3H), 2.06 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 167.8, 142.9, 136.5, 134.1, 133.8, 131.4, 130.2, 128.0, 127.8, 126.5, 126.0, 124.1, 120.9, 116.9, 24.5, 19.9.

Scheme 2 Synthesis of substituted aniline ring substrates

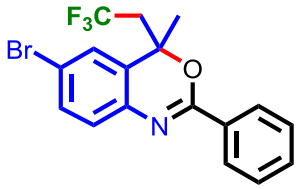


To a stirred solution of Grignard reagent, methylmagnesium chloride (3 equiv, 3.0 M CH_3MgCl) in THF at 0 ^oC was added solid 2-aminobenzonitrile (10 mmol, 1.0 equiv). The reaction mixture was allowed to warm to room temperature and was stirred overnight. Saturated NH_4Cl was then cautiously added dropwise by syringe until gas evolution ceased. The reaction mixture was then diluted with water and dichloromethane. Standard aqueous workup (CH_2Cl_2) followed by flash column chromatography (hexane/ ethyl acetate, 10:1) afforded the desired ketone.[13c] Further, Wittig reaction followed by amide synthesis was done by following previously mentioned method (*vide supra*).

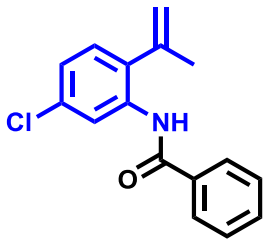


***N*-(4-Bromo-2-(prop-1-en-2-yl)phenyl)benzamide (1q)**: Light yellow solid, yield (0.30 g, 51%). m.p.: 112 – 114 ^oC, ^1H-NMR (400 MHz, $CDCl_3$), δ 12.57 (s, 1H), 8.91 (d, J = 9.0 Hz, 1H), 8.04-8.02 (m, 3H), 7.70 (dd, J = 9.0, 2.3 Hz, 1H), 7.56 (tt, J = 7.2, 2.3 Hz, 1H), 7.51 (tt, J = 7.2, 2.3 Hz, 1H), 4.99-4.95 (m, 1H), 2.70 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 166.1, 140.4,

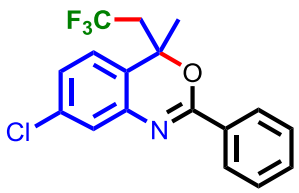
139.3, 138.0, 134.4, 134.2, 132.2, 128.8, 127.5, 123.4, 122.6, 114.7, 114.0, 22.7, HRMS (ESI), *m/z* calcd for $C_{16}H_{14}BrNO$ $[M+Na]^+$ 340.0307, found 339.9959.



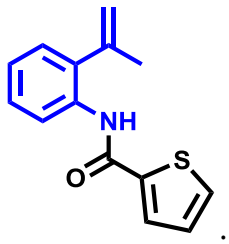
6-Bromo-4-methyl-2-phenyl-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine (3q): Light yellow semi-solid, trace amount. HRMS (ESI), *m/z* calcd for $C_{17}H_{13}BrF_3NO$ $[M+H]^+$ 384.0205, found 384.0219.



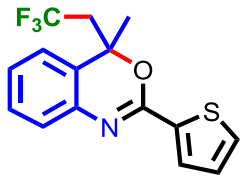
***N*-(5-chloro-2-(prop-1-en-2-yl)phenyl)benzamide (1r)**: White solid, yield (0.25 g, 78%). m.p.: 148 – 150 ^oC, 1H-NMR (500 MHz, $CDCl_3$), 8.65 (d, *J* = 1.8 Hz, 1H), 8.50 (s, 1H), 7.84 (dd, *J* = 8.5 Hz, 2H), 7.59 (tt, *J* = 7.4, 1.2 Hz, 1H), 7.52 (td, *J* = 7.8, 1.5 Hz, 2H), 7.13-7.12 (m, 2H), 5.55-5.53 (m, 1H), 5.15 (q, *J* = 0.9 Hz, 1H), 2.13 (t, *J* = 1.2 Hz, 3H), ^{13}C NMR (125 MHz, $CDCl_3$), δ 165.0, 142.4, 135.1, 134.6, 133.6, 132.0, 131.5, 128.9, 128.5, 126.9, 123.9, 120.5, 117.5, 24.5, HRMS (ESI), *m/z* calcd for $C_{16}H_{14}ClNO$ $[M+H]^+$ 272.0837, found 272.0857.



7-Chloro-4-methyl-2-phenyl-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine (3r): Yellow semi-solid, yield (0.090g, 72%), ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.13 (d, *J* = 7.4 Hz, 2H), 7.51 (t, *J* = 7.2 Hz, 1H), 7.44 (t, *J* = 7.5 Hz, 2H), 7.33 (d, *J* = 1.2 Hz, 1H), 7.18 (dd, *J* = 8.2, 2.0 Hz, 1H), 7.04 (d, *J* = 8.2 Hz, 1H), 2.88-2.78 (m, 1H), 2.66-2.55 (m, 1H), 1.89 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 156.6, 139.8, 134.8, 131.9, 131.8, 128.3, 128.1, 126.7, 126.5, 125.5, 124.9 (q, *J* = 277.5 Hz, CF_3), 123.8, 76.6 (q, *J* = 2.1 Hz), 43.7 (q, *J* = 27.4 Hz, CF_3), 26.5 (d, *J* = 1.5 Hz), ^{19}F NMR (376 MHz, $CDCl_3$), δ -59.9 (t, *J* = 10.6 Hz, 3F), HRMS (ESI), *m/z* calcd for $C_{17}H_{13}ClF_3NO$ $[M+H]^+$ 340.0711, found 340.0726.

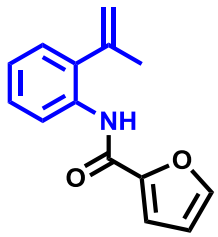


***N*-(2-(prop-1-en-2-yl)phenyl)thiophene-2-carboxamide (1s)**:[2] White solid, yield (0.68 g, 90%). m.p.: 80 – 82 ^{o}C, ^{1}H-NMR (500 MHz, $CDCl_3$), δ 8.40 (d, *J* = 8.3 Hz, 1H), 8.32 (bs, 1H), 7.51-7.49 (m, 2H), 7.29 (td, *J* = 7.8, 1.6 Hz, 1H), 7.17 (dd, *J* = 78, 1.6 Hz, 1H), 7.11-7.10 (m, 1H), 7.08 (dd, *J* = 7.4, 1.2 Hz, 1H), 5.49-5.47 (m, 1H), 5.10 (q, *J* = 1.0 Hz, 1H), 2.10 (t, *J* = 1.2 Hz, 3H), ^{13}C NMR (125 MHz, $CDCl_3$), δ 159.5, 143.2, 139.7, 133.7, 133.2, 130.6, 128.2, 128.1, 127.8, 127.6, 123.9, 120.6, 116.9, 24.6.

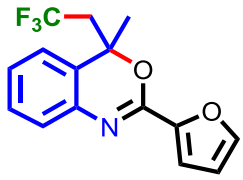


4-Methyl-2-(thiophen-2-yl)-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine (3s): White semi-solid, yield (0.067g, 52%), ^{1}H-NMR (400 MHz, $CDCl_3$), δ 7.72 (dd, *J* = 3.8, 0.1 Hz, 1H),

7.49 (dd, *J* = 5.0 ,1.0 Hz, 1H), 7.32 (td, *J* = 7.0, 1.2 Hz, 1H), 7.28 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.20 (td, *J* = 7.4, 1.6 Hz, 1H), 7.12-7.08 (m, 2H), 2.88-2.79 (m, 1H), 2.61-2.53 (m, 1H), 1.91 (s, 1H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 152.4, 138.2, 136.6, 130.6, 130.3, 129.3, 127.7, 126.7, 125.0 (q, *J* = 279.0 Hz, CF_3), 122.5, 76.9 (q, *J* = 2.15 Hz), 43.4 (q, *J* = 27.3 Hz, CH_2CF_3), 25.9 (d, *J* = 1.60 Hz), ^{19}F NMR (376 MHz, $CDCl_3$), δ -59.8 (t, *J* = 10.5 Hz, 3F), HRMS (ESI), *m/z* Calcd for $C_{15}H_{12}F_3NOS$ $[M+H]^+$ 312.0664, found 312.0680.

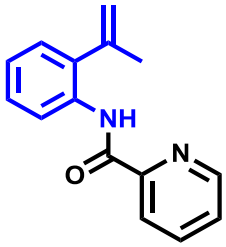


***N*-(2-(Prop-1-en-2-yl)phenyl)furan-2-carboxamide (1t)**:[5] yellow semi-solid, yield (0.69 g, 86%), ^{1}H-NMR (500 MHz, $CDCl_3$), δ 8.63 (bs, 1H), 8.43 (d, *J* = 8.3 Hz, 1H), 7.49-7.48 (m, 1H), 7.28 (td, *J* = 7.8, 1.6, 1H), 7.19 (d, *J* = 3.5 Hz, 1H), 7.16 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.08 (td, *J* = 7.5 Hz, 1.1 Hz, 1H), 6.53-6.52 (m, 1H), 5.46 (t, *J* = 1.6 Hz, 1H), 5.09 (t, *J* = 0.9 Hz, 1H), 2.10(s, 3H), ^{13}C NMR (125 MHz, $CDCl_3$), δ 155.9, 148.1, 144.3, 142.6, 133.6, 133.5, 128.0, 127.7, 123.9, 120.6, 117.1, 115.0, 112.5, 24.5.

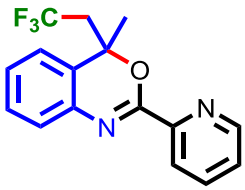


2-(Furan-2-yl)-4-methyl-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine (3t): White solid, yield (0.068, 53%). m.p.:80 – 82 ^{o}C, ^{1}H-NMR (400 MHz, $CDCl_3$), δ 7.39-7.32 (m, 2H), 7.29-7.19 (m, 2H), 7.15-7.07 (m, 2H), 6.90 (dd, *J* = 11.4, 3.5 Hz, 1H), 2.89-2.77 (m, 1H), 2.62-2.50 (m, 1H), 1.91 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 147.5, 137.1, 129.6, 128.2 (d, *J* = 29.0 Hz

), 127.8, 126.1, 125.1 (q, J = 278.8 Hz, CF_3), 124.4, 122.6, 120.5, 117.1, 114.8, 113.1 (q, J = 2.9 Hz), 77.1 (q, J = 2.3 Hz), 43.5 (q, J = 27.1 Hz, CH_2CF_3), 26.1 (d, J = 1.6 Hz), ^{19}F NMR (376 MHz, $CDCl_3$), δ -60.0 (t, J = 10.4 Hz, 3F), HRMS (ESI), *m/z* calcd for $C_{15}H_{12}F_3NO_2$ $[M+H]^+$ 296.0893, found 296.0901.

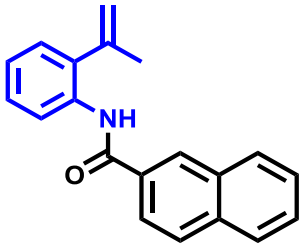


***N*-(2-(Prop-1-en-2-yl)phenyl)picolinamide (1u)**: White semi-solid, yield (0.50 g, 64%), ^{1}H-NMR (500 MHz, $CDCl_3$), δ 10.4 (s, 1H), 8.59-8.57 (m, 2H), 8.27 (dt, J = 7.8, 1.0 Hz, 1H), 7.84 (td, J = 7.7 Hz, 1H), 7.42-7.39 (m, 1H), 7.31 (td, J = 7.8, 1.39 Hz, 1H), 7.19 (dd, J = 1.56 Hz, 1H), 7.09 (td, J = 7.5, 1.2 Hz, 1H), 5.48-5.47 (m, 1H), 5.12 (q, J = 1.0 Hz, 1H), 2.12 (t, J = 1.25 Hz, 3H), ^{13}C NMR (125 MHz, $CDCl_3$), δ 161.9, 150.2, 142.4, 137.5, 134.1, 128.0, 127.9, 126.2, 123.9, 122.3, 120.4, 117.3, 24.3. HRMS (ESI), *m/z* calcd for $C_{15}H_{14}N_2O$ $[M+H]^+$ 239.1179, found 239.1197.

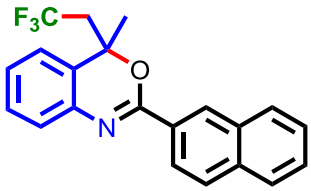


4-Phenyl-2-(pyridin-2-yl)-4-(2,2,2-trifluoroethyl)-4H-benzo[d][1,3]oxazine (3u): Light brown semi-solid, yield (0.063g, 49%), ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.58 (d, J = 5.0 Hz, 1H), 8.51 (d, J = 8.3 Hz, 1H), 8.28 (d, J = 7.8 Hz, 1H), 7.89 (td, J = 7.8, 1.6 Hz, 1H), 7.47-7.44 (m. 1H), 7.37 (td, J = 7.6, 1.6 Hz, 1H), 7.19 (dd, J = 7.6, 1.6 Hz, 1H), 7.14 (td, J = 7.2, 0.9 Hz, 1H), 3.22 (q, J = 10.5 Hz, 2H), 1.57 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 162.0, 149.9, 148.1, 137.6,

134.4, 131.8, 128.7, 128.4, 126.3, 125.5 (q, J = 277.6 Hz, CF_3), 124.1, 123.9, 122.3, 120.9, 77.2, 41.4 (q, J = 29.3 Hz, CH_2CF_3), 22.7 (d, J = 1.6 Hz), ^{19}F NMR (376 MHz, $CDCl_3$), δ -64.5 (t, J = 10.4 Hz, 3F), HRMS (ESI): *m/z* calcd for $C_{16}H_{13}F_3N_2O$ $[M+H]^+$ 307.1053, found 307.1051.

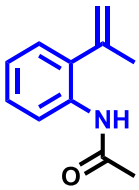


***N*-(2-(Prop-1-en-2-yl)phenyl)-2-naphthamide (1v)**: White solid, yield (0.49 g, 74%). m.p.: 82 – 84 ^{o}C, ^{1}H-NMR (500 MHz, $CDCl_3$), δ 8.59 (bs, 1H), 8.52 (d, J = 8.3 Hz, 1H), 8.34 (d, J = 1.0 Hz, 1H), 7.95-7.92 (m, 2H), 7.89-7.85 (m, 2H), 7.59-7.53 (m, 2H), 7.34 (td, J = 7.8, 1.5 Hz, 1H), 7.12 (td, J = 7.5, 1.2 Hz, 1H), 5.50-5.49 (m, 1H), 5.15 (q, J = 1.0 Hz, 1H), 2.13 (t, J = 1.2 Hz, 3H), ^{13}C NMR (125 MHz, $CDCl_3$), δ 165.2, 143.4, 134.8, 134.1, 133.6, 132.7, 132.3, 129.1, 128.8, 128.1, 127.9, 127.8, 127.7, 127.7, 126.9, 124.0, 123.3, 120.8, 116.8, 24.7, HRMS (ESI), *m/z* calcd for $C_{20}H_{17}NO$ $[M+H]^+$ 288.1383, found 288.1403.

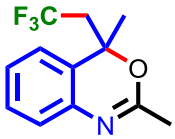


4-Methyl-2-(naphthalen-2-yl)-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine (3v): White semi-solid, yield (0.089 g, 72%), ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.63 (s, 1H), 8.27 (dd, J = 8.7, 1.6 Hz, 1H), 7.96 (d, J = 8.0 Hz, 1H), 7.88 (t, J = 8.6 Hz, 2H), 7.56-7.50 (m, 2H), 7.39-7.35 (m, 2H), 7.26-7.22 (m, 1H), 7.15 (d, J = 7.5 Hz, 1H), 2.95-2.85 (m, 1H), 2.71-2.60 (m, 1H), 1.97 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 155.8, 138.4, 135.0, 132.8, 129.5, 129.3, 129.2, 128.6, 128.3, 127.9, 127.7, 127.5, 127.0, 126.4, 125.7, 125.3 (q, J = 278.3 Hz, CF_3), 124.5, 122.6, 43.7

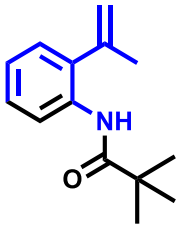
(q, *J* = 27.4 Hz, CH_2CF_3), 26.3, ^{19}F NMR (376 MHz, $CDCl_3$), δ -59.8 (t, *J* = 10.5 Hz, 3F), HRMS (ESI), *m/z* calcd for $C_{21}H_{16}F_3NO$ $[M+H]^+$ 356.1257, found 356.1261.



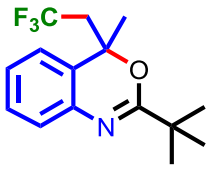
***N*-(2-(Prop-1-en-2-yl)phenyl)acetamide (1w)**:[9] White solid, yield (0.42 g, 76%). m.p.: 50 – 52 ^oC, ^1H-NMR (500 MHz, $CDCl_3$), δ 8.20 (d, *J* = 8.2, Hz, 1H), 7.51 (bs, 1H), 7.23 (td, *J* = 7.8, 1.4 Hz, 1H), 7.11 (d, *J* = 7.4 Hz, 1H), 7.04 (t, *J* = 7.4 Hz, 1H), 5.35 (s, 1H), 4.99 (s, 1H), 2.12 (s, 3H), 2.04 (s, 3H), ^{13}C NMR (125 MHz, $CDCl_3$), δ 168.1, 143.0, 133.9, 133.4, 127.8, 127.6, 123.8, 121.1, 116.7, 24.7, 24.4, HRMS (ESI), *m/z* calcd for $C_{11}H_{13}NO$ $[M+H]^+$ 176.1070, found 176.1088.



2,4-Dimethyl-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine (3w): Pale yellow semi-solid, yield (0.101g, 73%), ^1H-NMR (400 MHz, $CDCl_3$), δ 7.26 (td, *J* = 7.6, 1.4 Hz, 1H), 7.17-7.11 (m, 2H), 7.03 (dd, *J* = 7.5, 0.9 Hz, 1H), 2.77-2.65 (m, 1H), 2.52-2.40 (m, 1H), 2.10 (s, 3H), 1.79 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 159.3, 137.6, 129.2, 127.3, 126.6, 125.01 (q, *J* = 278.1 Hz, CF_3), 124.6, 122.6, 76.1 (q, *J* = 2.19 Hz), 44.1 (q, *J* = 27.1 Hz, CH_2CF_3), 26.9 (d, *J* = 1.64 Hz), 21.5, ^{19}F NMR (376 MHz, CDCl3), δ -60.4 (t, *J* = 10.5Hz, 3F), HRMS (ESI), *m/z* calcd for $C_{12}H_{12}F_3NO$ $[M+H]^+$ 244.0944, found 244.0954.

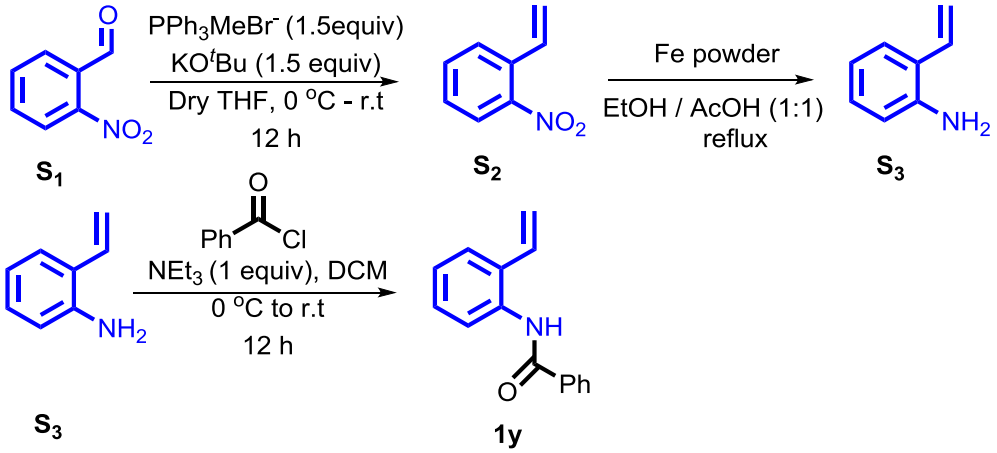


***N*-(2-(Prop-1-en-2-yl)phenyl)pivalamide (1x)**:[2] White solid, yield (0.63 g, 87%). m.p.: 55 – 57 ^{o}C, ^{1}H-NMR (500 MHz, $CDCl_3$), δ 8.36 (d, *J* = 8.25 Hz, 1H), 7.98 (bs, 1H), 7.28 (td, *J* = 7.69, 1.59 Hz, 1H), 7.15 (dd, *J* = 7.69, 1.59Hz, 1H), 7.08 (td, *J* = 7.69, 1.59 Hz, 1H), 5.46-5.44 (m, 1H), 5.06-5.05 (m, 1H), 2.10 (s, 3H), 1.30 (s, 9H), ^{13}C NMR (125 MHz, $CDCl_3$), δ 176.3, 143.3, 134.2, 133.2, 127.9, 127.5, 123.4, 120.4, 116.6, 39.9, 27.5, 24.5.

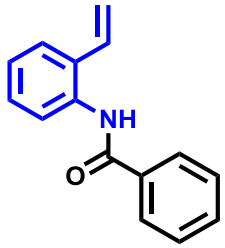


2-(*tert*-Butyl)-4-methyl-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine (3x): Yellow semi-solid, yield (0.091g, 74%), ^{1}H-NMR (400 MHz, $CDCl_3$), δ 7.26 (td, *J* = 7.5, 1.2 Hz, 1H), 7.02 (d, *J* = 7.5 Hz, 1H), 2.80-2.62 (m, 2H), 1.70 (s, 3H), 1.25(s, 9H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 166.6, 138.0, 129.0, 127.4, 126.4, 125.3, 125.1 (q, *J* = 278.8 Hz, CF_3), 122.5, 75.9 (q, *J* = 2.2 Hz), 43.7(q, *J* = 27.1 Hz, CH_2CF_3), 37.1, 27.3, 27.2 (d, J = 1.6 Hz), ^{19}F NMR (376 MHz, $CDCl_3$), δ -59.7 (t, *J* = 10.5 Hz, 3F), HRMS (ESI), *m/z* calcd for $C_{15}H_{18}F_3NO$ $[M+H]^+$ 286.1413, found 286.1426.

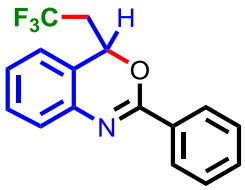
Scheme 3 Synthesis of 2-vinylaniline



2-Vinylaniline was synthesized according to a known procedure.[6] Amide synthesis was done by previously mentioned method (*vide supra*).



***N*-(2-Vinylphenyl)benzamide (1y):**[6] White solid, yield (0.49 g, 77%). m.p.: 152 – 154 ^{o}C, ^{1}H-NMR (500 MHz, $CDCl_3$), δ 7.96 (d, *J* = 7.8 Hz, 1H), 7.93 (bs, 1H), 7.86 (d, *J* = 7.4 Hz, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 7.8 Hz, 2H), 7.43(d, *J* = 7.8 Hz, 1H), 7.31(t, *J* = 7.8 Hz, 1H), 7.17(t, *J* = 7.4 Hz, 1H), 6.84 (dd, *J* = 18.0, 11.0 Hz, 1H), 5.69 (dd, *J* = 18.0, 1.0 Hz, 1H), 5.43 (dd, *J* = 11.0 Hz, 1.0 Hz, 1H), ^{13}C NMR (125 MHz, $CDCl_3$), δ 165.7, 134.7, 134.4, 132.3, 131.9, 130.6, 128.8, 128.6, 127.1, 125.4, 123.6, 118.5, HRMS (ESI), *m/z* calcd for $C_{15}H_{13}NO$ $[M+H]^+$ 224.1070, found 224.1093.

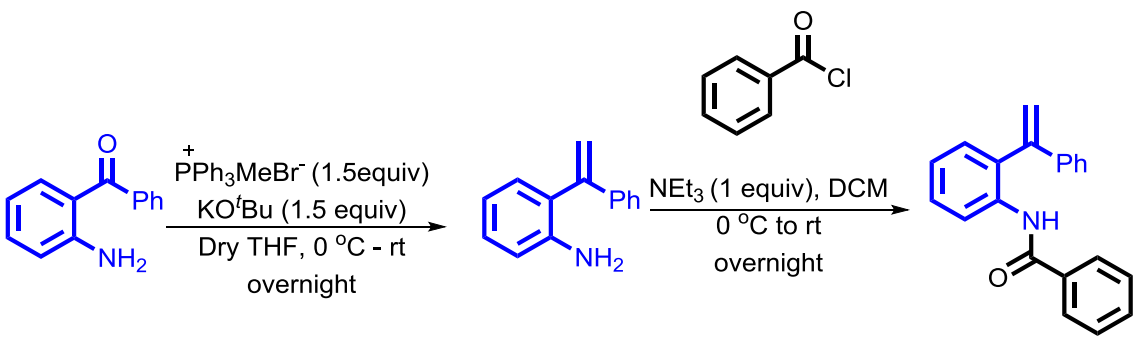


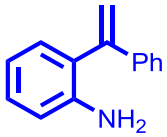
2-Phenyl-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine (3y): Pale yellow semi-solid; yield (0.117g, 90%), ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.17 (d, *J* = 7.9 Hz, 2H), 7.51 (t, *J* = 7.3 Hz, 1H), 7.44 (t, *J* = 7.9 Hz, 2H), 7.39-7.32 (m, 2H), 7.25-7.20 (m, 1H), 7.03 (d, *J*.= 7.5 Hz, 1H), 5.82 (dd, *J* = 10.0, 2.4 Hz, 1H), 2.89-2.77 (m, 1H), 2.55-2.43 (m, 1H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 155.7, 138.9, 131.9, 131.7, 129.7, 128.1, 126.9, 125.4, 125.2 (q, *J* = 278.0 Hz, CF_3), 123.5, 123.3, 70.4, (q, *J* = 3.34 Hz, CH_2CF_3), ^{19}F NMR (376 MHz, $CDCl_3$), δ -63.2 (t, *J* = 10.5Hz, 3F), HRMS (ESI), *m/z* calcd for $C_{16}H_{12}F_3NO$ $[M+H]^+$ 292.0944, found 292.0970.

General procedure for the synthesis of *N*-(2-(1-phenylvinyl)phenyl)benzamide 1z (substrate for trifluoromethylated benzoxazine 3z)

The substrate **1z** for **3z** was prepared from 2-aminobenzophenone by following two steps: a) conversion of 2-aminobenzophenone into 2-(1-phenylvinyl)aniline; b) preparation of *N*-(2-(1-phenylvinyl)phenyl)benzamide by coupling of 2-(1-phenylvinyl)aniline. with benzoyl chloride as mentioned earlier.

Scheme 4

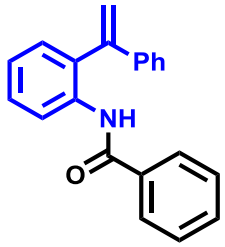




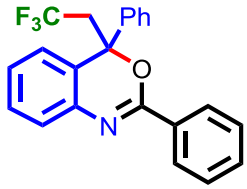
(a) Typical procedure for conversion of 2-aminobenzophenone into 2-(1-phenylvinyl)aniline

To a stirred solution of Ph_3PMeBr (8.37 mmol, 1.5 equiv) in Dry THF (15 mL) was added KO^tBu (8.37 mmol, 1.5 equiv) in portions under nitrogen. After the mixture was stirred at room temperature for 0.5 h, a solution of 2-aminobenzophenone (5.58 mmol, 1 equiv) in THF (15 mL) was added dropwise. The reaction mixture was then stirred at room temperature under nitrogen overnight. The reaction mixture was quenched with water and extracted with EtOAc (50 mL x 2). The combined organic layers were washed with saturated $NaHCO_3$ (50 mL) and brine (50 mL), dried over anhydrous Na_2SO_4, and concentrated on a rotary evaporator under vacuum and the residue was purified by column chromatography on silica gel. A light yellow oil was obtained.[1] yield (1.0 g, 93%), ^{1}H-NMR (400 MHz, $CDCl_3$), δ 7.40 (dd, *J* = 8.0, 1.6 Hz, 2H), 7.35-7.29 (m, 3H), 7.17 (td, *J* = 7.6, 1.5 Hz, 1H), 7.12 (dd, *J* = 7.6, 1.5 Hz, 1H), 6.80 (td, *J* = 7.5 1.0 Hz, 1H), 6.7 (d, *J* = 8.0 Hz, 1H), 5.80 (d, *J* = 1.4 Hz, 1H), 5.36 (d, *J* = 1.47 Hz, 1H), 3.55 (s, 2H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 147.2, 143.3, 139.6, 130.8, 128.8, 128.6, 128.1, 127.3, 126.6, 118.3, 116.1, 115.6.

General Method for the Conversion of 2-(1-Phenylvinyl)aniline into *N*-(2-(1-Phenylvinyl)phenyl)benzamides 1: 2-(1-Phenylvinyl)aniline was converted into *N*-(2-(1-Phenylvinyl)phenyl)benzamides **1** by following synthetic protocol as mentioned above (Scheme 1).

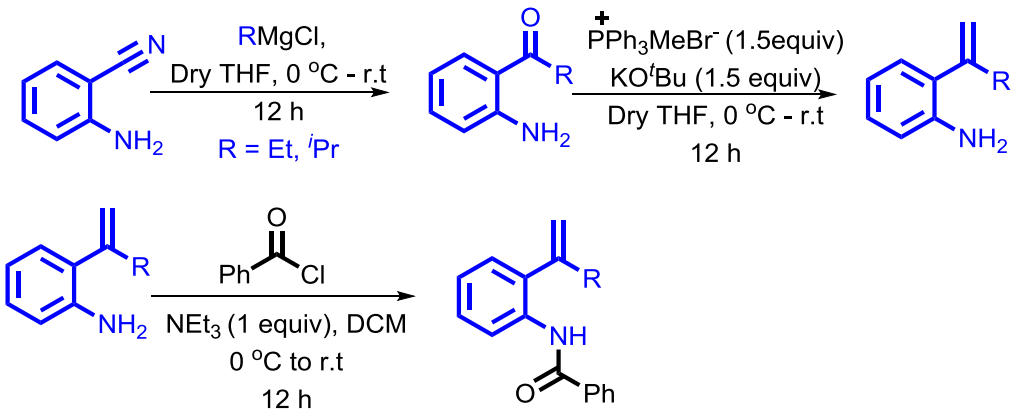


***N*-(2-(1-phenylvinyl)phenyl)benzamide (1z)**:[2] White solid, yield (0.68 g, 79%). m.p.: 79 – 81 ^{o}C, ^{1}H-NMR (500 MHz, $CDCl_3$), δ 8.49 (d, *J* = 8.2 Hz, 1H), 7.79 (s, 1H), 7.45-7.34 (m, 8H), 7.32-7.30 (m, 1H), 7.29-7.27 (m, 3H), 7.19 (td, *J* = 7.5 Hz, 1H), 5.90 (d, *J* = 1.0 Hz, 1H), 5.42 (s, *J* = 1.0 Hz, 1H), ^{13}C NMR (125 MHz, $CDCl_3$), δ 165.0, 146.3, 138.9, 135.4, 134.8, 131.6, 131.5, 130.6, 129.1, 129.0, 128.8, 128.5, 126.8, 126.7, 124.3, 121.0, 117.8.

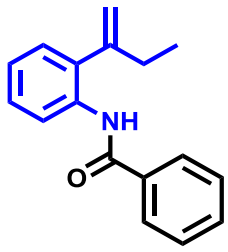


2,4-Diphenyl-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine (3z):[4] White solid, yield (0.116 g, 94%), ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.26 (d, *J* = 8.5 Hz, 2H), 7.54-7.45 (m, 3H), 7.38-7.34 (m, 4H), 7.31-7.20 (m, 5H), 3.28 (q, *J* = 10.0 Hz, 2H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 155.4, 141.7, 138.7, 132.0, 131.6, 129.4, 128.5, 128.4, 128.3, 127.9, 126.5, 126.3, 125.9, 125.4, 125.0 (q, *J* = 279.1 Hz, CF_3), 124.2, 80.0 (q, *J* = 2.2 Hz), 43.4 (q, *J* = 27.1 Hz, CH_2CF_3), ^{19}F NMR (376 MHz, $CDCl_3$), δ -58.5 (t, *J* = 10.0 Hz, 3F), HRMS (ESI), *m/z* calcd for $C_{22}H_{16}F_3NO$ $[M+H]^+$ 368.1257, found 368.1273.

Scheme 5. Synthesis of alkene substituted substrates (1aa-1bb)

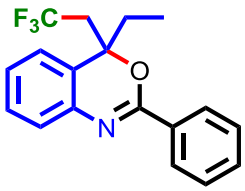


To a stirred solution of Grignard reagent (3 equiv, 3.0 M EtMgBr, 2.0 M ^{i}PrMgCl) in THF at 0 ^{o}C was added solid 2-aminobenzonitrile (1.0 equiv, 10 mmol). The reaction mixture was allowed to warm to room temperature and was stirred overnight. Saturated NH_4Cl was then cautiously added dropwise by syringe until gas evolution ceased. The reaction mixture was then diluted with water and dichloromethane. Standard aqueous workup (CH_2Cl_2) followed by flash column chromatography (hexane/ ethyl acetate, 10:1) afforded the desired ketone.[2] Further, Wittig reaction followed by amide synthesis was carried out as mentioned earlier.

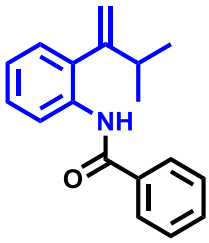


***N*-(2-(But-1-en-2-yl)phenyl)benzamide (1aa):**[2] White solid, yield (0.40 g, 55%). m.p.: 48 – 50 ^{o}C, ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.50 (d, *J* = 8.0 Hz, 1H), 8.41 (s, 1H), 7.80 (d, *J* = 7.3 Hz, 2H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.48 (t, *J* = 2.0 Hz, 2H), 7.32 (td, *J* = 7.6 Hz, 1.8 Hz, 1H), 7.15-7.10 (m, 2H), 5.45 (s, 1H), 5.11 (s, 1H), 2.40 (q, *J* = 7.4 Hz, 2H), 1.06 (t, *J* = 7.4 Hz, 3H), ^{13}C

NMR (125 MHz, $CDCl_3$), δ 164.9, 149.2, 135.1, 134.5, 133.0, 131.7, 128.8, 128.0, 127.9, 126.8, 123.7, 120.4, 114.9, 31.1, 12.5.

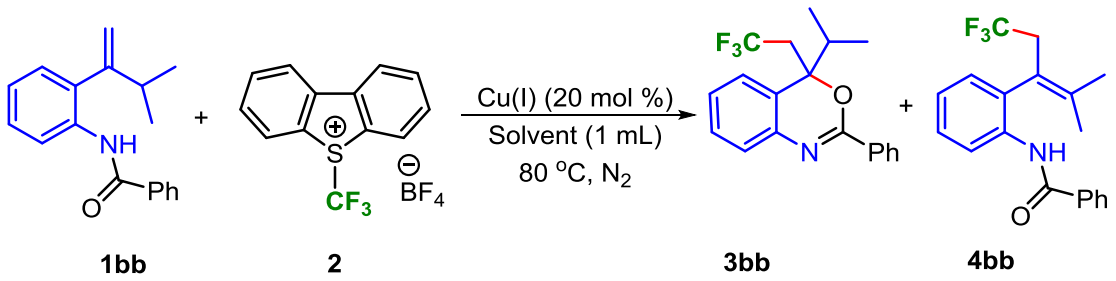


4-Ethyl-2-phenyl-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine (3aa): Light yellow semi-solid, yield (0.094g, 74%), ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.14 (d, *J* = 7.2 Hz, 2H), 7.50-7.42 (m, 3H), 7.31 (d, *J* = 4.0 Hz, 2H), 7.22-7.18 (m, 1H), 7.04 (d, *J* = 7.6 Hz, 1H), 2.89-2.66 (m, 2H), 2.27-2.17 (m, 1H), 2.16-2.08 (m, 1H), 0.91 (t, *J* = 7.3 Hz, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 155.6, 139.1, 132.3, 131.4, 129.1, 128.2, 127.8, 126.6, 125.8, 125.1, 125.0 (q, *J* = 278.8 Hz, CF_3), 123.3, 79.9 (q, *J* = 2.21 Hz), 43.9 (q, *J* = 26.8 Hz, CH_2CF_3), 33.9 (d, *J* = 1.0 Hz), 7.7, ^{19}F NMR (376 MHz, $CDCl_3$), δ -59.5 (t, *J* = 10.5 Hz, 3F), HRMS (ESI), *m/z* calcd for $C_{18}H_{16}F_3NO$ $[M+H]^+$ 320.1257, found 320.1280.



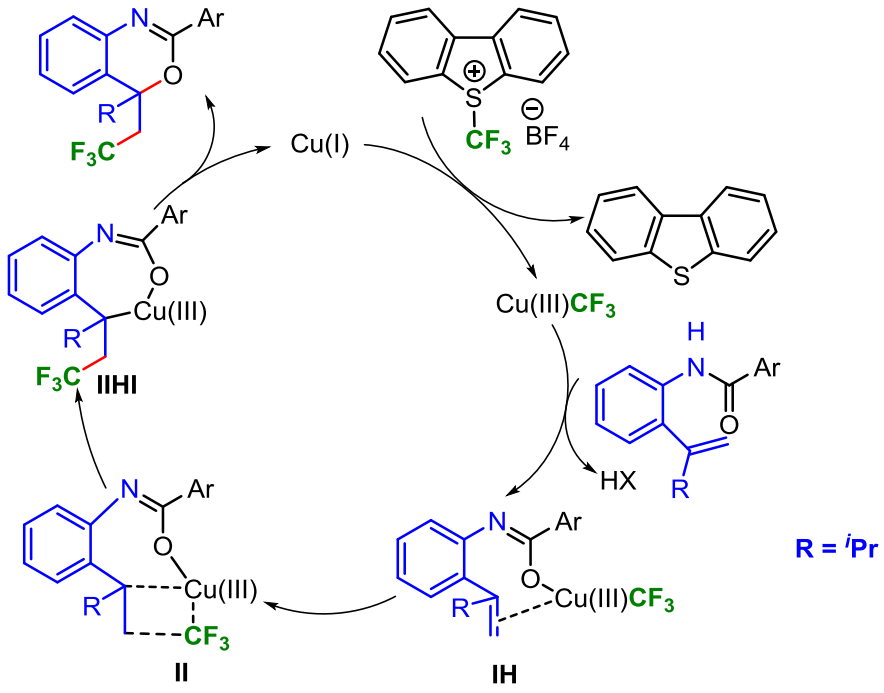
***N*-(2-(3-Methylbut-1-en-2-yl)phenyl)benzamide (1bb):**[2] Yellow solid, yield (0.46 g, 69%). m.p.: 60 – 62 ^{o}C, ^{1}H-NMR (400MHz, $CDCl_3$), δ 8.56 (d, *J* = 8.3 Hz, 1H), 8.42 (s, 1H), 7.85-7.83 (m, 2H), 7.58 (tt, *J* = 7.3, 1.3 Hz, 1H), 7.52 (tt, *J* = 7.3, 1.3 Hz, 2H), 7.39-7.35 (m, 1H), 7.16-7.13 (m, 1H), 5.48 (t, *J* = 1.5 Hz, 1H), 5.14-5.13 (m, 1H), 2.68-2.61 (m, 1H), 1.13 (d, *J* = 6.8 Hz, 6H), ^{13}C NMR (125 MHz, $CDCl_3$), δ 164.8, 153.7, 135.0, 134.8, 133.1, 131.7, 128.8, 128.2, 127.9, 126.8, 123.5, 120.3, 113.7, 35.4, 21.4.

Formation of Benzoxazine (3bb) and Allylic Trifluoromethylation (4bb)

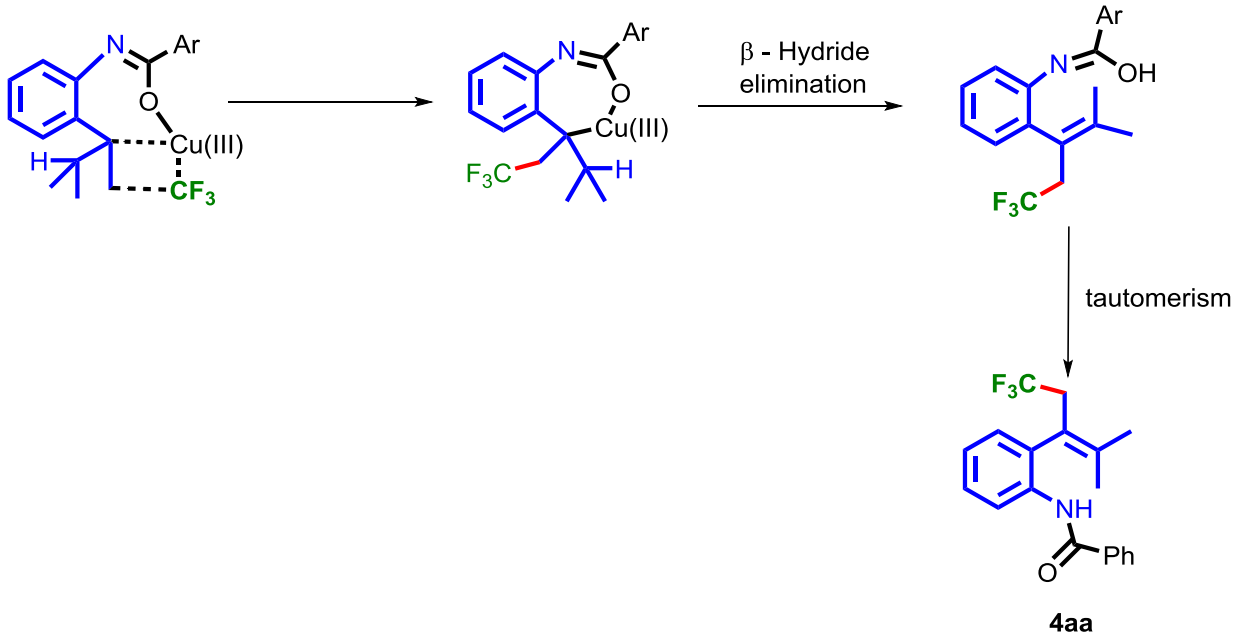


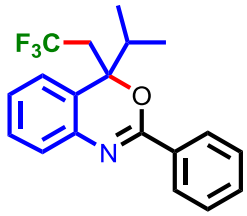
1bb 2 3bb 4bb

Proposed Mechanism for 3bb

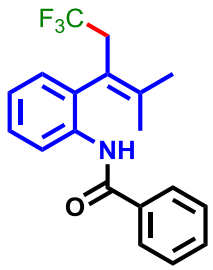


Proposed Mechanism for 4bb

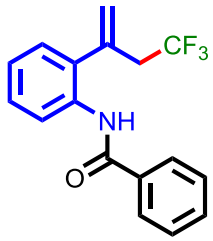




4-Isopropyl-2-phenyl-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine (3bb): Pale yellow semi-solid, yield (0.044g, 35%), ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.12 (d, *J* = 7.5 Hz, 2H), 7.48-7.42 (m, 3H), 7.29 (d, *J* = 3.4 Hz, 2H), 7.19-7.15 (m, 1H), 7.02 (d, *J* = 7.6 Hz, 1H), 3.01-2.94 (m, 1H), 2.82-2.75 (m, 1H), 2.27-2.20 (m, 1H), 1.09 (d, *J* = 6.7 Hz, 3H), 0.89 (d, *J* = 6.72 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$), δ 155.2, 139.1, 132.4, 131.3, 128.9, 128.2, 127.6, 126.2, 125.8, 125.4 (q, *J* = 277.6 Hz, CF_3), 124.2, 123.9, 81.8 (q, *J* = 2.2 Hz), 41.9 (q, *J* = 26.4 Hz, CH_2CF_3), 39.7, 16.8, 15.9, ^{19}F NMR (376 MHz, $CDCl_3$), δ -59.3 (t, *J* = 10.3 Hz, 3F), HRMS (ESI), *m/z* calcd for $C_{19}H_{18}F_3NO$ $[M+H]^+$ 334.1413, found 334.1430.



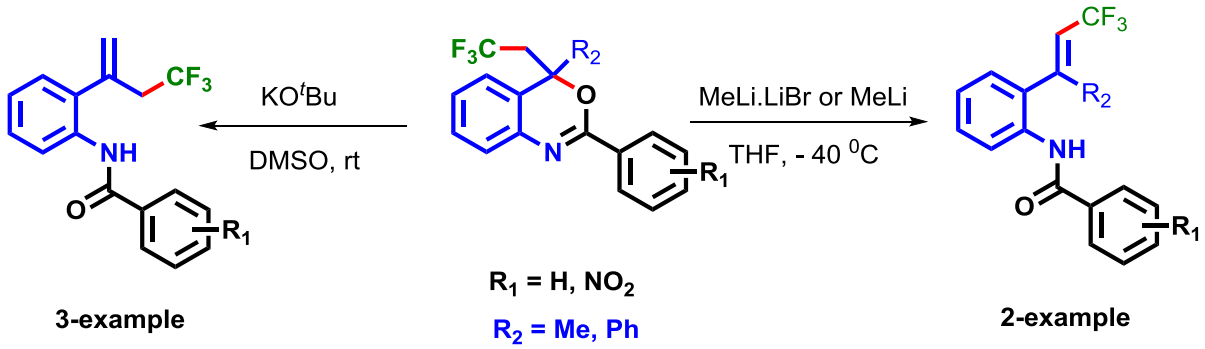
***N*-(2-(5,5,5-Trifluoro-2-methylpent-2-en-3-yl)phenyl)benzamide** (**4bb**): White semi-solid, yield (0.057g), 45%, ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.46 (d, *J* = 8.3 Hz, 1H), 8.04 (s, 1H), 7.77 (*J* = 7.1, 1.5 Hz, 2H), 7.53 (t, *J* = 7.1 Hz, 1H), 7.47 (t, *J* = 7.1 Hz, 2H), 7.33 (td, *J* = 7.8, 1.4 Hz, 1H), 7.13 (td, *J* = 7.4 Hz, 1H), 7.08-7.05 (m, 1H), 3.47-3.36 (m, 1H), 3.1-3.0 (m, 1H), 1.96 (s, 3H), 1.55 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 164.8, 140.8, 135.4, 134.9, 131.8, 128.8, 128.5, 128.2, 126.7, 126.6, 126.4 (q, *J* = 278.5 Hz, CF_3), 124.3, 122.6, 120.7, 119.8 (q, *J* = 2.5 Hz), 38.6 (q, *J* = 28.5 Hz, CH_2CF_3), 22.2, 20.7, ^{19}F NMR (376 MHz, $CDCl_3$), δ -57.7 (dd, *J* = 8.12, 1.9 Hz), -64.0 (t, *J* = 10.5 Hz, 3F), HRMS (ESI), *m/z* calcd for $C_{19}H_{18}F_3NO$ $[M+H]^+$ 334.1413, found 334.1442.



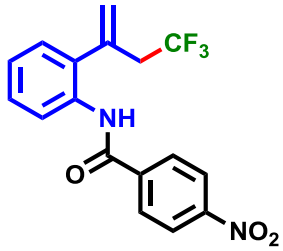
***N*-(2-(4,4,4-Trifluorobut-1-en-2-yl)phenyl)benzamide (4a)**: White solid, yield (0.027g). m.p.: 94 – 96 ^{o}C, 45%. ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.43 (d, *J* = 8.3 Hz, 1H), 8.20 (s, 1H), 7.81 (d, *J* = 7.1, 1.5 Hz, 2H), 7.54 (tt, *J* = 7.3, 1.2 Hz), 7.48 (t, *J* = 7.3 Hz, 2H), 7.38-7.34 (m, 1H), 7.17-7.14 (m, 1H), 5.74 (s, 1H), 5.45 (s, 1H), 3.21 (q, *J* = 10.4 Hz, 2H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 165.2, 136.1 (q, *J* = 3.0 Hz), 134.7, 134.5, 131.9, 131.3, 128.9 (d, *J* = 5.17 Hz), 127.8, 126.8, 125.5 (q, *J* = 278.1 Hz, CF_3), 124.2, 123.7, 121.7, 77.2, 42.0 (q, *J* = 29.1 Hz), ^{19}F NMR (376

MHz, $CDCl_3$), δ -64.5 (t, *J* = 10.5 Hz, 3F), HRMS (ESI), *m/z* calcd for $C_{17}H_{14}F_3NO$ $[M+H]^+$ 306.1100, found 306.1104.

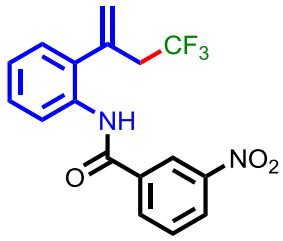
Scheme 6 Further Modification of Trifluoromethylated Benzoxazines



General procedure for ring opening reaction by using KO^{t}Bu (conversion of substituted 4-methyl-2-phenyl-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine to substituted *N*-(2-(4,4,4-trifluorobut-1-en-2-yl)phenyl)benzamide): To a single neck flask, KO^{t}Bu (0.010 g, 0.090 mmol) was added in one portion to the solution of the respective benzoxazine (0.025 g, 0.068 mmol) in DMSO (1 mL) at room temperature. The resulted reaction mixture was stirred at room temperature for 6 h. Next, saturated aqueous $NaHCO_3$ solution (10 mL) was added and the resulting mixture was extracted with ethyl acetate (10 mL × 3). The organic layers were combined, dried over anhydrous Na_2SO_4, filtered and concentrated *in vacuo*. The crude product was purified by column chromatography using (hexane/ethyl acetate, 80:20) to get desired product.

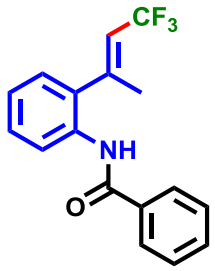


4-Nitro-*N*-(2-(4,4,4-trifluorobut-1-en-2-yl)phenyl)benzamide (5a): White semi-solid, yield (0.012g, 50%), ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.41 (d, *J* = 8.2 Hz, 1H), 8.34 (dd, *J* = 8.7, 3.4 Hz, 2H), 8.23 (bs, 1H), 7.96 (d, *J* = 8.7 Hz, 2H), 7.40-7.37 (m, 1H), 7.19 (dd, *J* = 5.3, 2.0 Hz, 2H), 5.76 (s, 1H), 3.23 (q, *J* = 10.5 Hz, 2H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 163.1, 149.8, 140.8, 136.0, 133.8, 131.8, 131.4, 129.0, 129.0, 127.8, 125.6, 125.1 (q, *J* = 276.8 Hz, CF_3), 124.9, 124.1, 121.6, 77.2, 42.2 (q, *J* = 29.7 Hz, CH_2CF_3), ^{19}F NMR (376 MHz, $CDCl_3$), δ -64.4 (t, *J* = 10.5 Hz, 3F), HRMS (ESI), *m/z* calcd for $C_{17}H_{13}F_3N_2O_3$ $[M-H]^-$ 349.0795, found 349.0821.

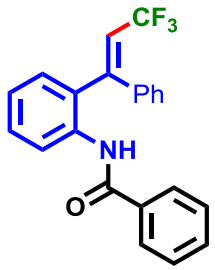


3-Nitro-*N*-(2-(4,4,4-trifluorobut-1-en-2-yl)phenyl)benzamide (5b): White semi-solid, yield (0.018g, 75%), ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.66-8.65 (m, 1H), 8.42-8.37 (m, 2H), 8.27 (s, 1H), 8.13 (t, *J* = 7.76 Hz, 1H), 7.69 (td, *J* = 8.0, 3.3 Hz, 1H), 7.40-7.37 (m, 1H), 7.20-7.18 (m, 1H), 5.79 (s, 1H), 5.47 (s, 1H), 3.24 (q, *J* = 10.5 Hz, 2H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 162.7, 148.5, 136.4, 133.8, 132.6, 131.6, 130.1, 128.9, 127.9, 126.4, 125.6, 125.2 (q, *J* = 277.6 Hz, CF_3), 124.0, 123.1, 121.9, 77.2, 42.2 (q, *J* = 29.1 Hz), ^{19}F NMR (376 MHz, $CDCl_3$), -64.5 (t, *J* = 10.4 Hz, 3F), HRMS (ESI), *m/z* calcd for $C_{17}H_{13}F_3N_2O_3$ $[M-H]^-$ 349.0795, found 349.0825.

General procedure for ring opening reaction by using organolithium reagents (conversion of 4-Methyl-2-phenyl-4-(2,2,2-trifluoroethyl)-4H-benzo[*d*][1,3]oxazine to (*E*)-*N*-(2-(4,4,4-Trifluorobut-2-en-2-yl)phenyl)benzamide): To a solution of trifluoromethylated benzoxazine (40 mg, 0.131 mmol) in THF (2 mL) was added MeLi or MeLi.LiBr (1.5M, 1.5 equiv) at -40 ^{0}C. The reaction mixture was allowed to warm gradually to 0 ^{0}C and stirred for 3 h. The reaction mixture was quenched with water (2 mL) and extracted with CH_2Cl_2 (5 mL x 3). The combined organic layer was dried over Na_2SO_4 and concentrated under vacuum. The residue was purified by silica gel column chromatography (hexane /ethyl acetate, 10:1) to get desired product.

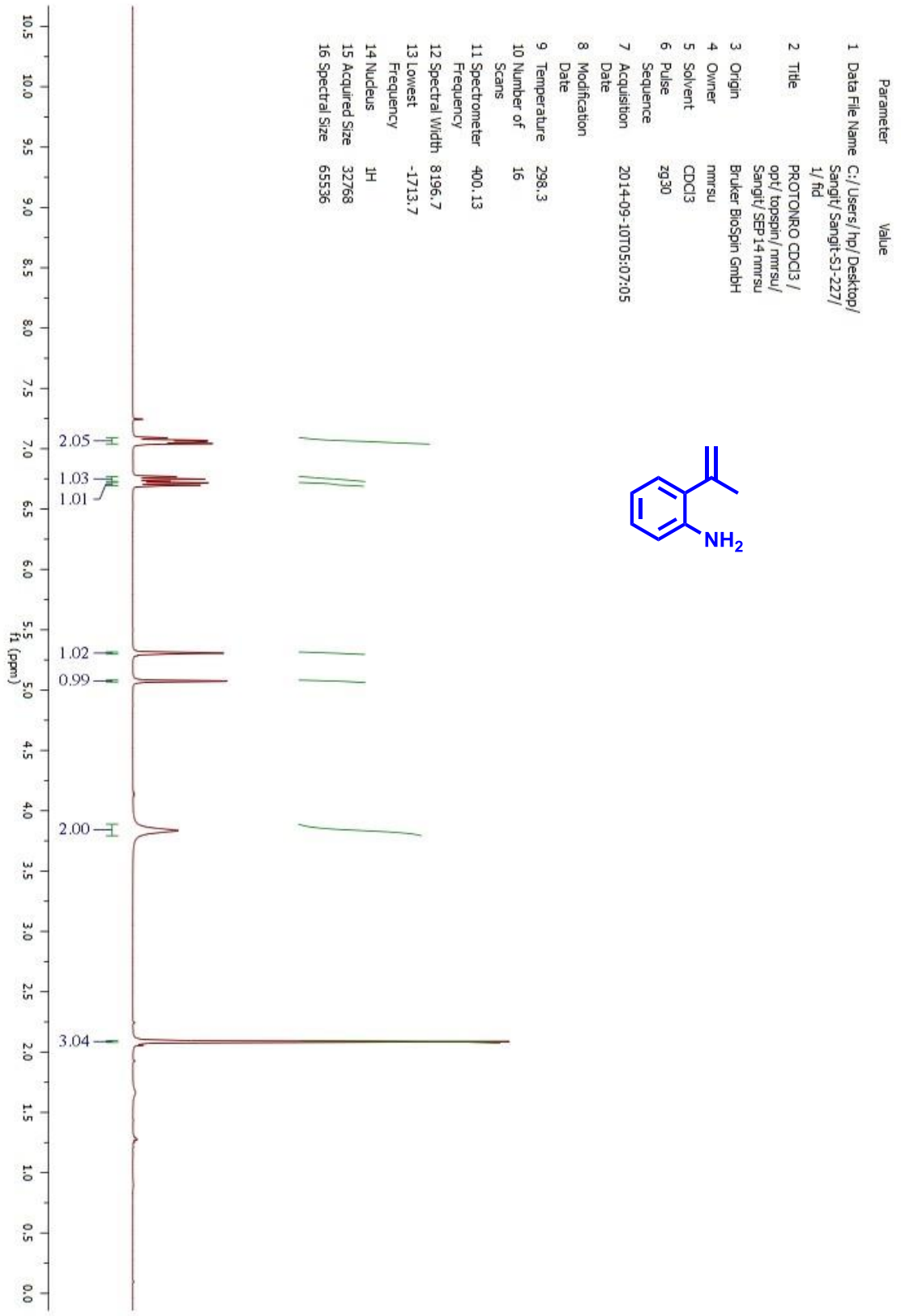


***N*-(2-(4,4,4-Trifluorobut-2-en-2-yl)phenyl)benzamide (5c)**: Pale yellow semi-solid, yield, 0.021 g, 52%, ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.26 (d, *J* = 8.4 Hz, 1H), 7.93 (bs, 1H), 7.81 (d, *J* = 7.3 Hz, 2H), 7.56 (t, *J* = 7.3 Hz, 1H), 7.49 (t, *J* = 7.3 Hz, 2H), 7.40-7.36 (m, 1H), 7.19-7.17 (m, 2H), 5.49 (qd, *J* =8.1, 1.3 Hz, 1H), 2.25 (t, *J* = 1.8 Hz, 3H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 165.2, 148.2 (d. *J* = 5.5 Hz), 134.4, 133.5, 132.1, 129.2, 129.0, 128.2, 127.4, 126.8, 124.9, 122.8 (q, *J* = 271.2 Hz, CF_3), 122.6, 120 (q, *J* = 33.9 Hz), 19.8 (d, *J* = 33.9 Hz), ^{19}F NMR (376 MHz, $CDCl_3$), δ -57.9 (s, 3F), HRMS (ESI), *m/z* calcd for $C_{17}H_{14}F_3NO$ $[M+H]^+$ 306.1100, found 306.1116.

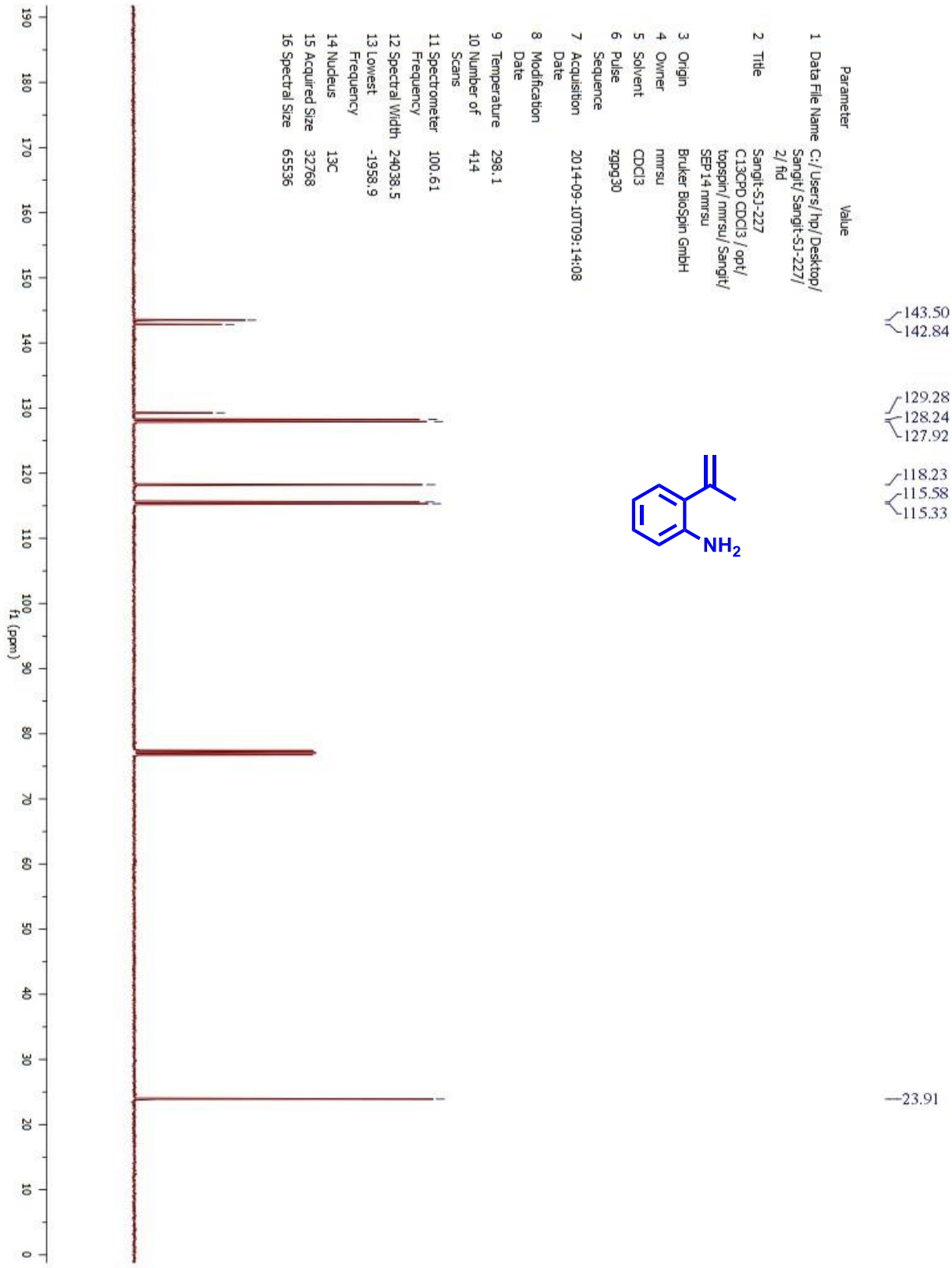


***N*-(2-(3,3,3-Trifluoro-1-phenylprop-1-en-1-yl)phenyl)benzamide (5d)**: White solid, yield (0.018.g, 45%). m.p.: 94 – 96 ^{o}C, ^{1}H-NMR (400 MHz, $CDCl_3$), δ 8.41 (d, *J* = 8.3 Hz, 1H), 7.52-7.33 (m, 12H), 7.28-7.25 (m, 2H), 6.43 (q, *J* = 7.8 Hz, 1H), ^{13}C NMR (100 MHz, $CDCl_3$), δ 165.2, 148.6 (q, *J* = 5.5 Hz), 137.1, 135.0, 134.7, 131.8, 130.5, 129.9, 129.2, 128.7, 127.2, 127.1, 126.7, 124.2, 122.8 (q, *J* = 271.0 Hz, CF_3), 121.9, 118.0 (q, *J* = 33.8 Hz), ^{19}F NMR (376 MHz, $CDCl_3$), δ -56.9 (d *J* = 7.6 Hz, 3F), HRMS (ESI), *m/z* calcd for $C_{22}H_{16}F_3NO$ $[M-H]^-$ 366.1100, found 366.1127.

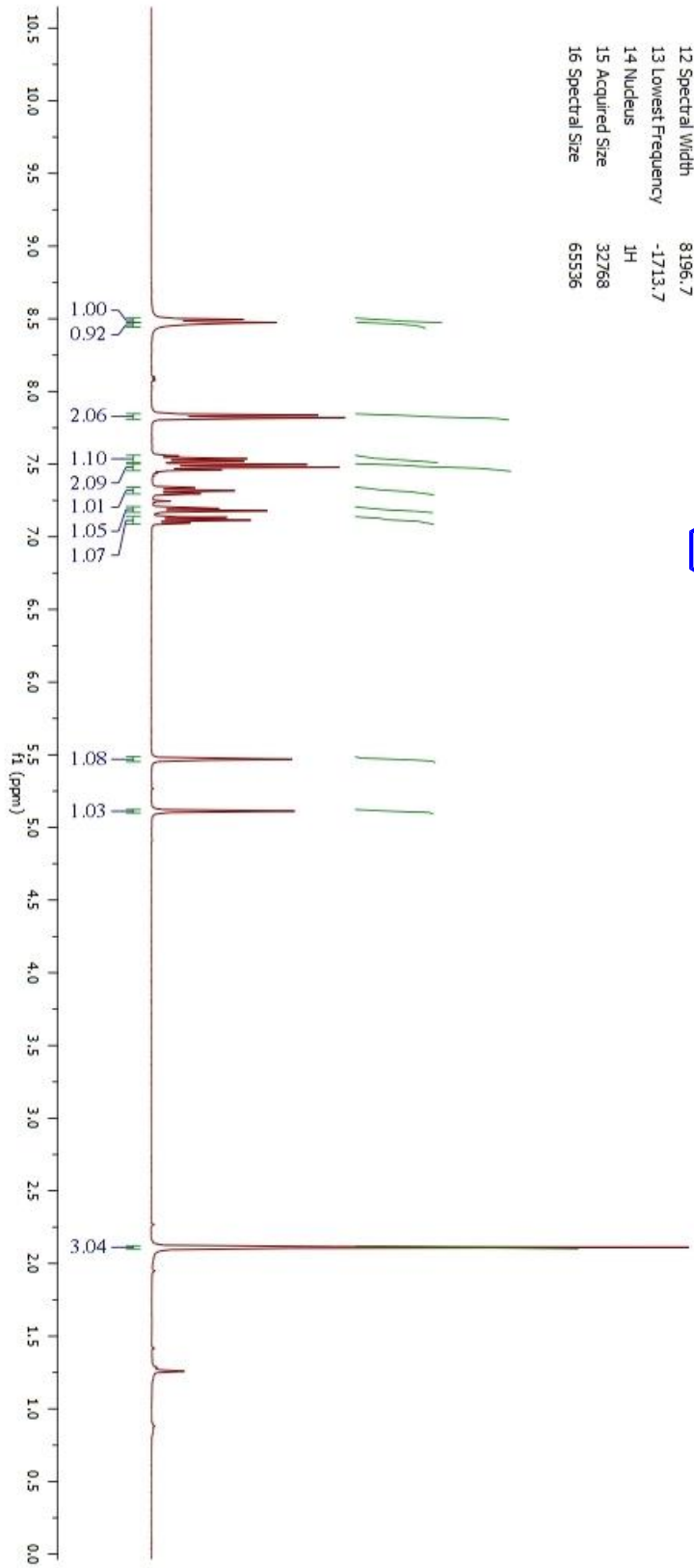
S1 ^{1}H NMR of **2-(prop-1-en-2-yl)aniline**



S2 ^{13}C NMR of **2-(prop-1-en-2-yl)aniline**



S3 ^{1}H NMR of **1a**



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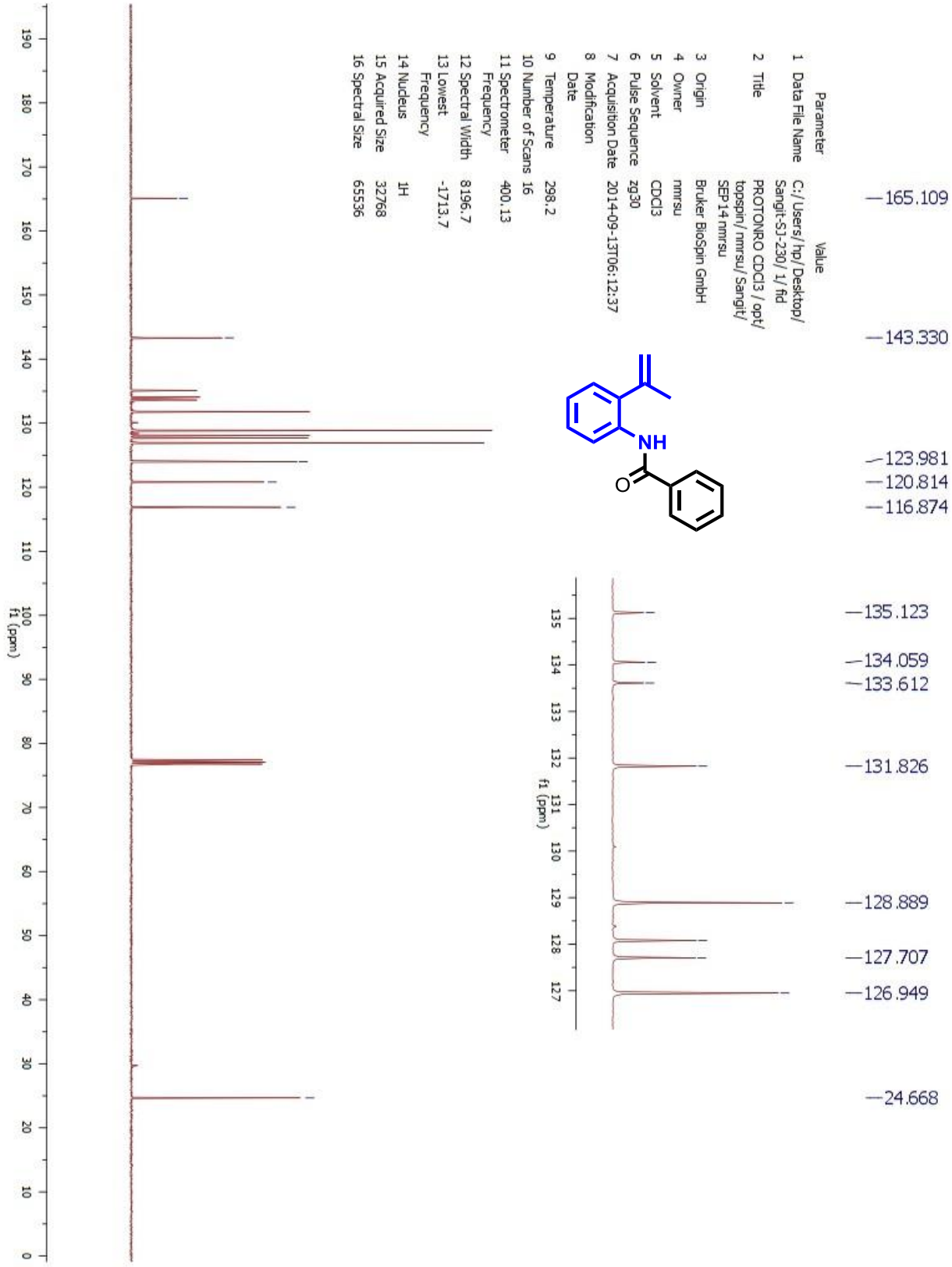
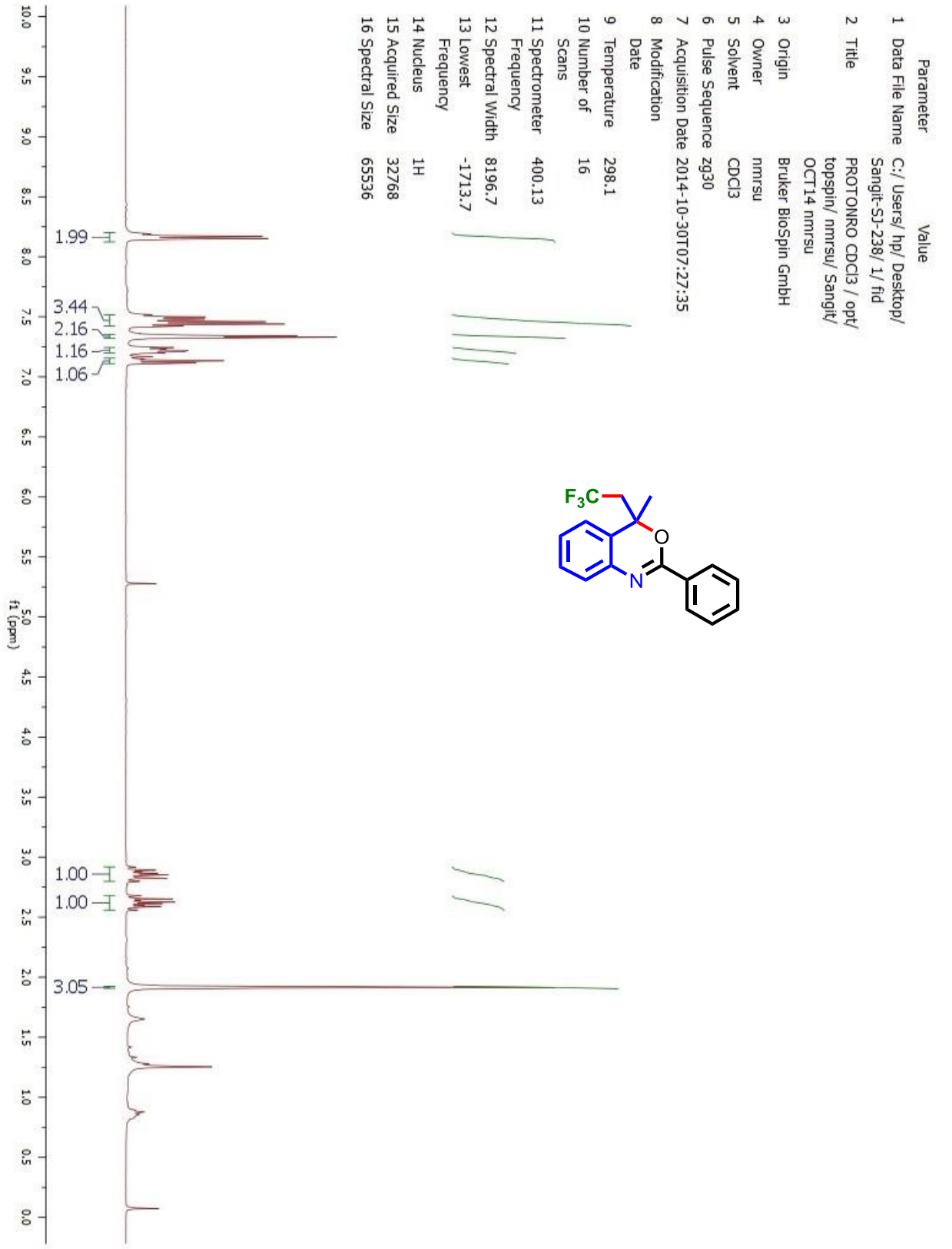
14	Nucleus	1H
15	Acquired Size	32768
16	Spectral Size	65536

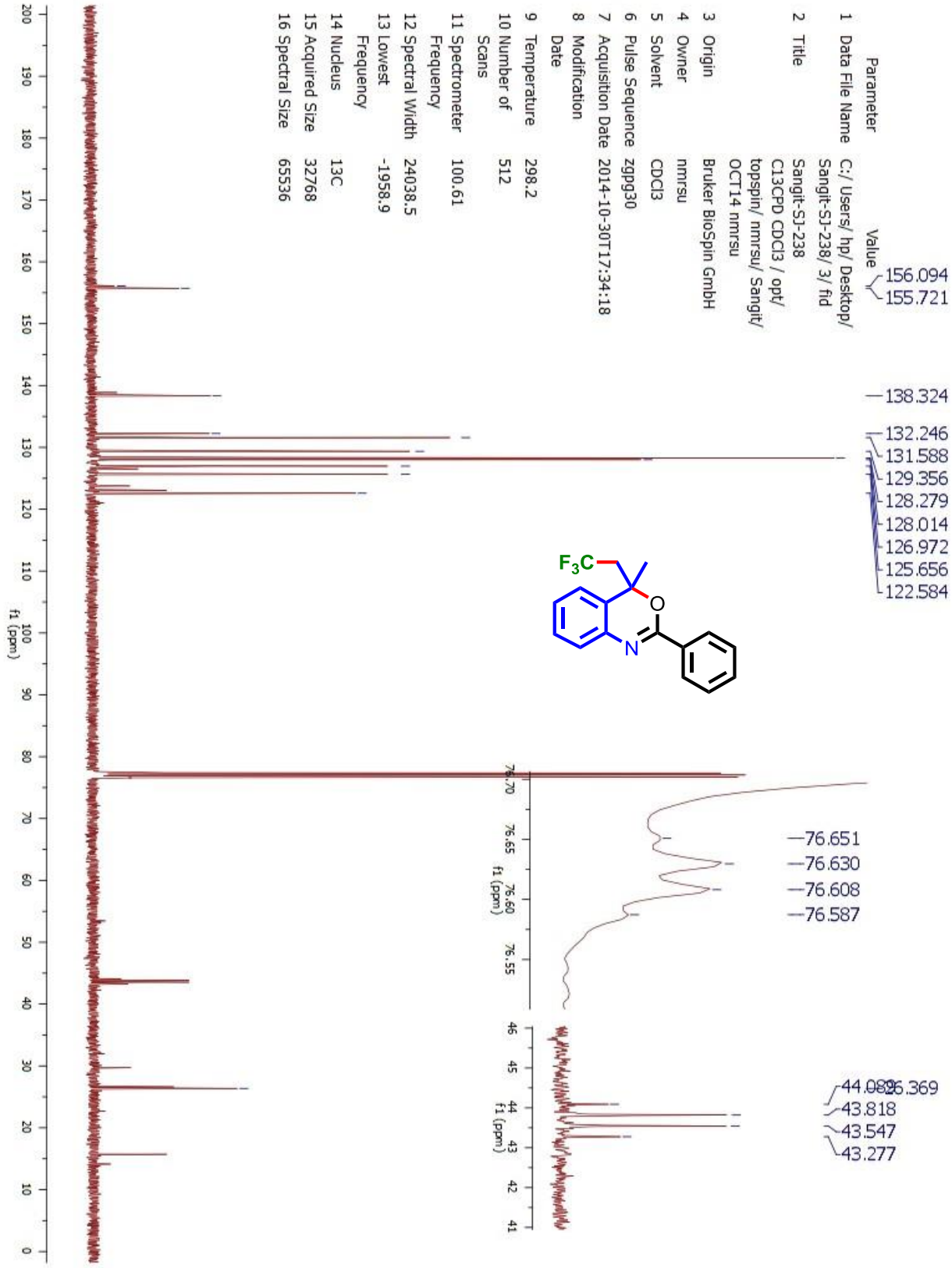
S4 ^{13}C NMR of **1a**



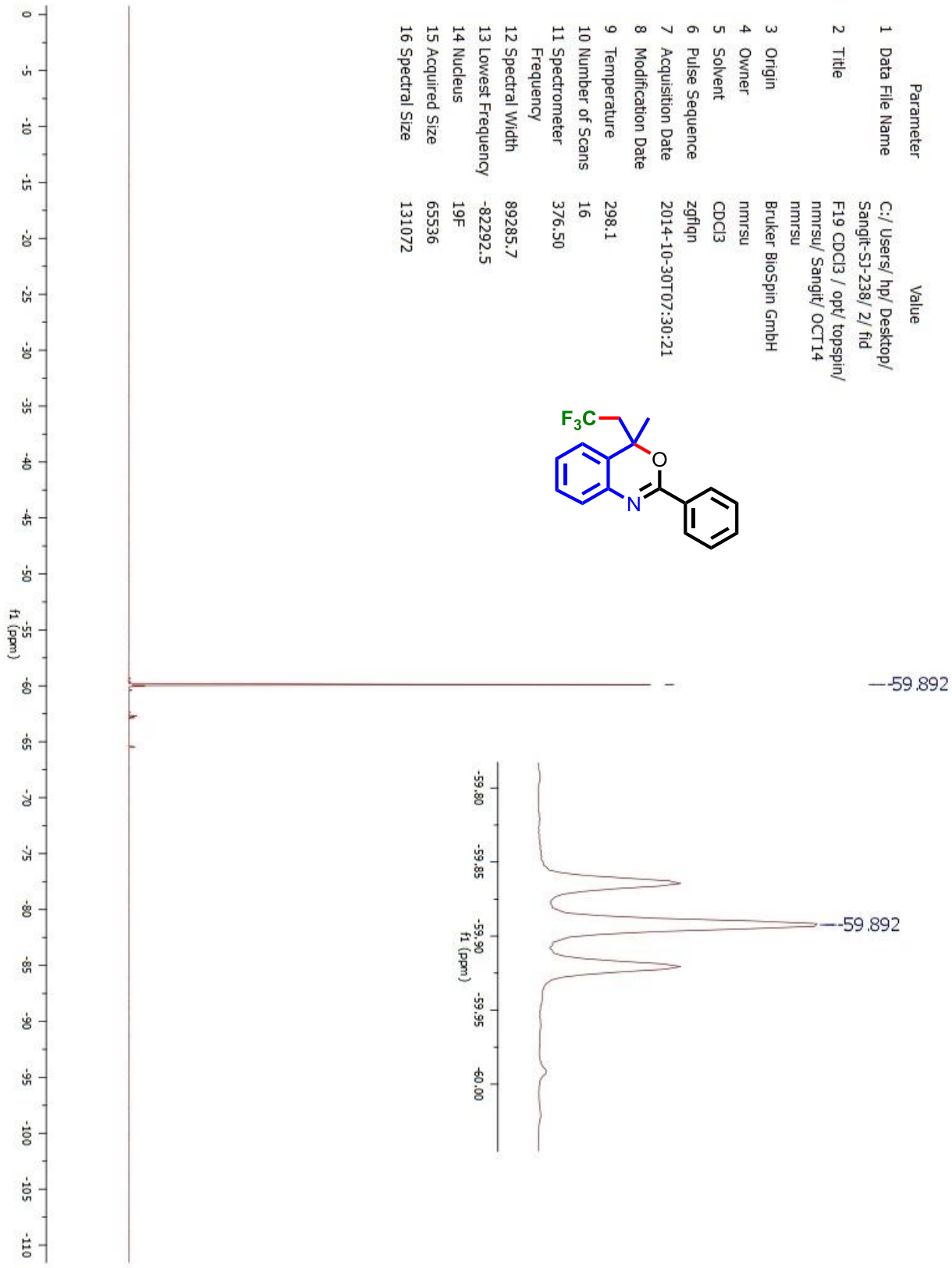
S5 ^{1}H NMR of **3a**



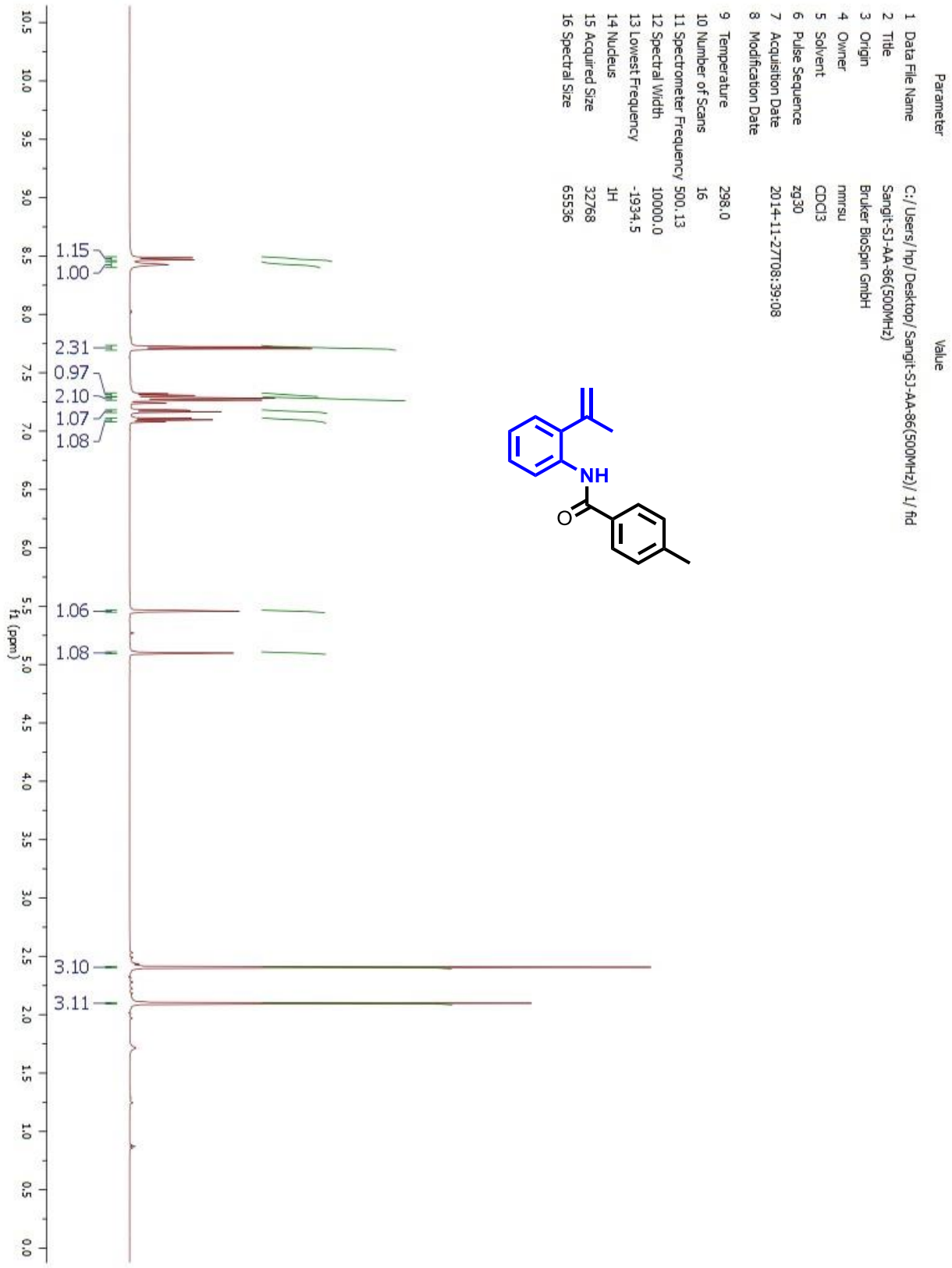
S6 ^{13}C NMR of **3a**



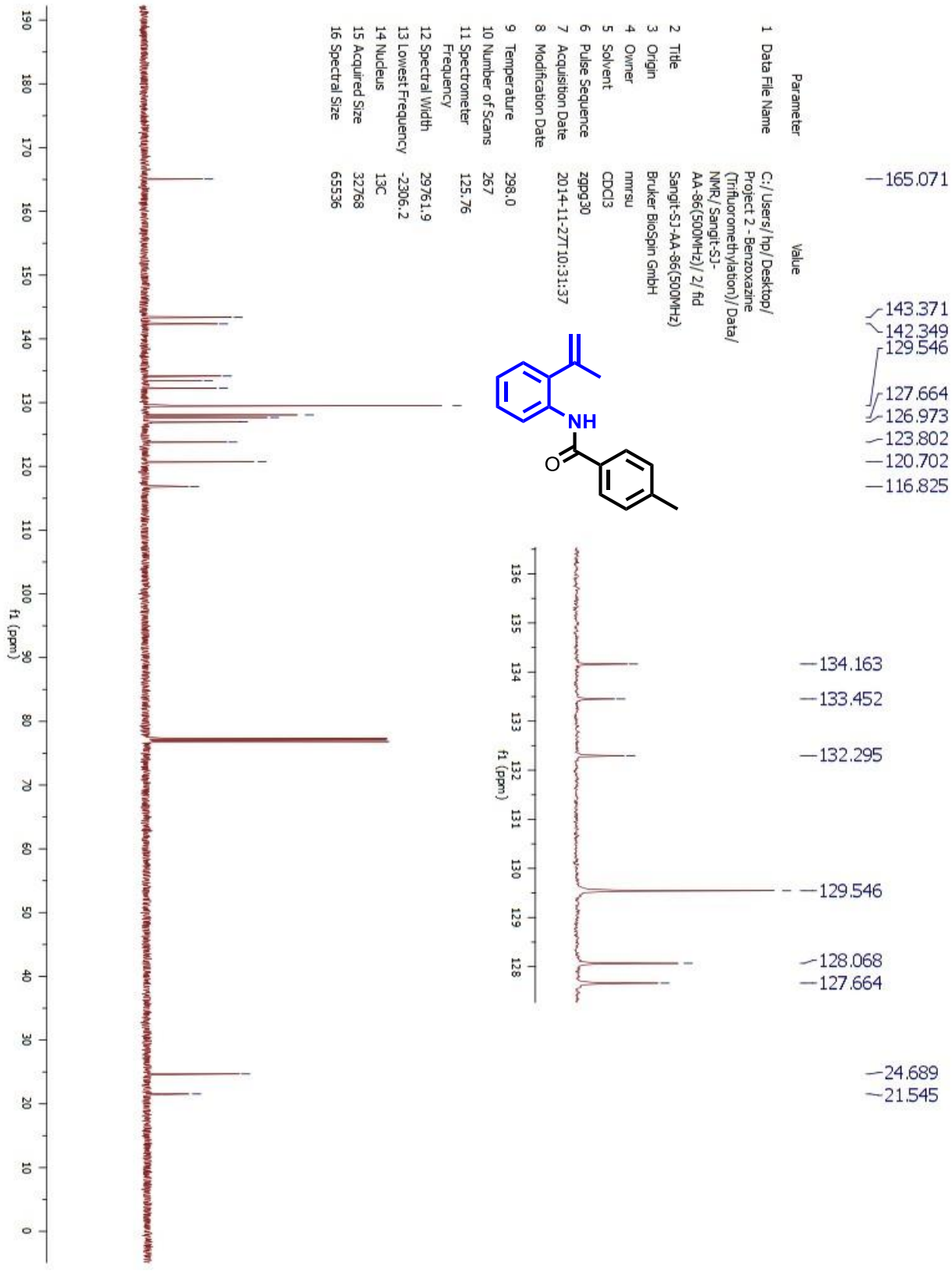
S7 ^{19}F NMR of **3a**



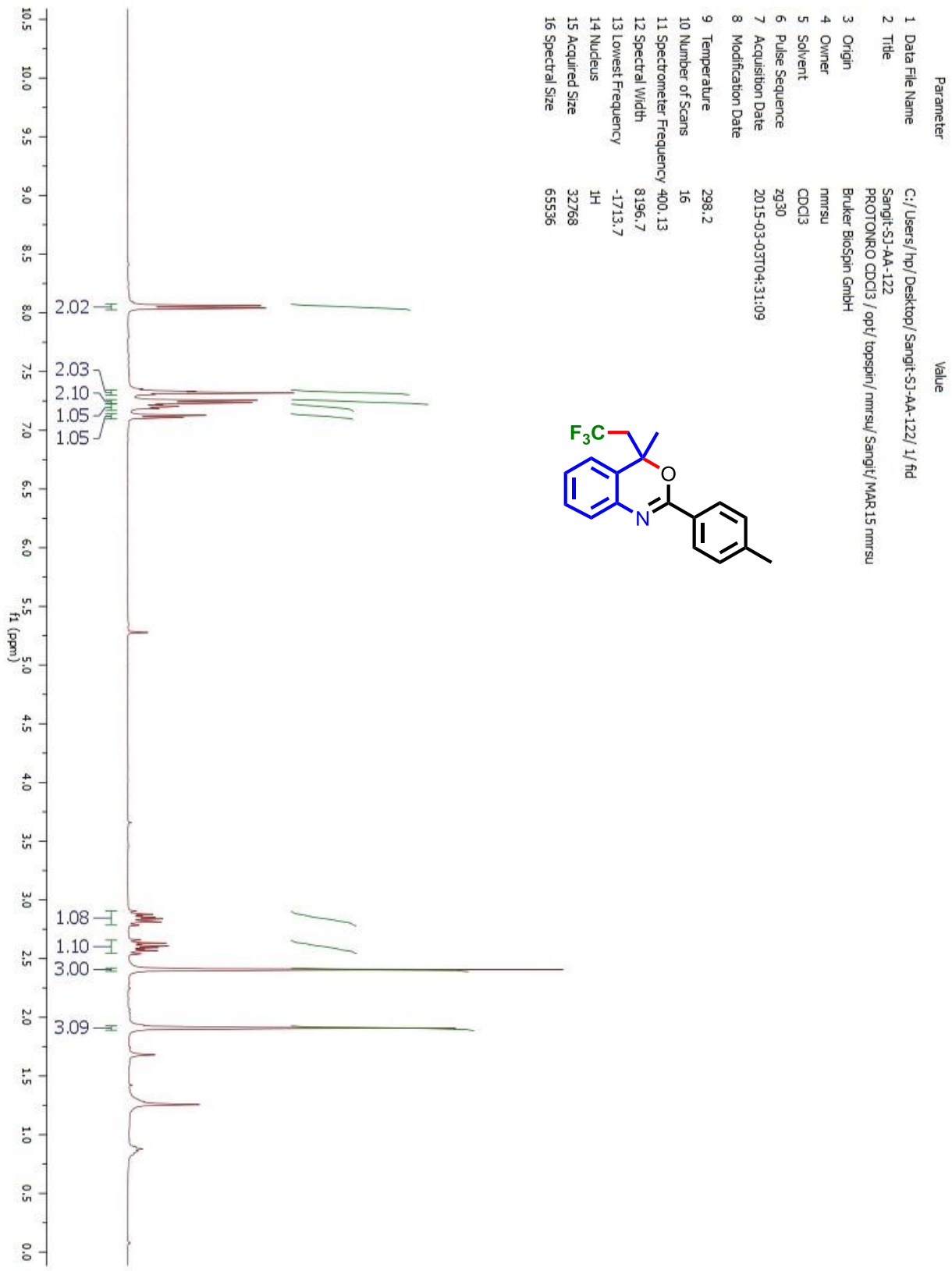
S8 ^{1}H NMR of **1b**



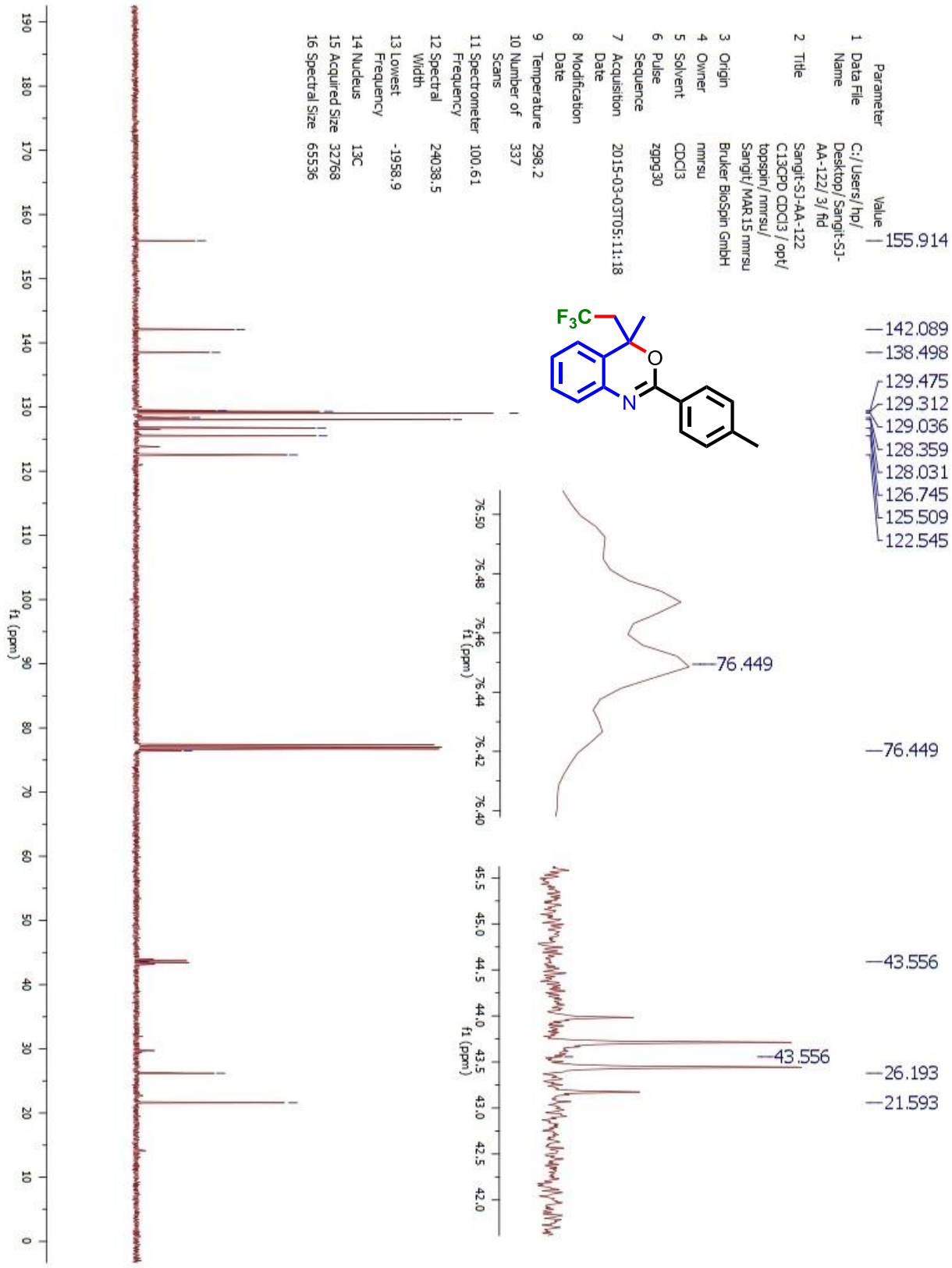
S9 ^{13}C NMR of **1b**



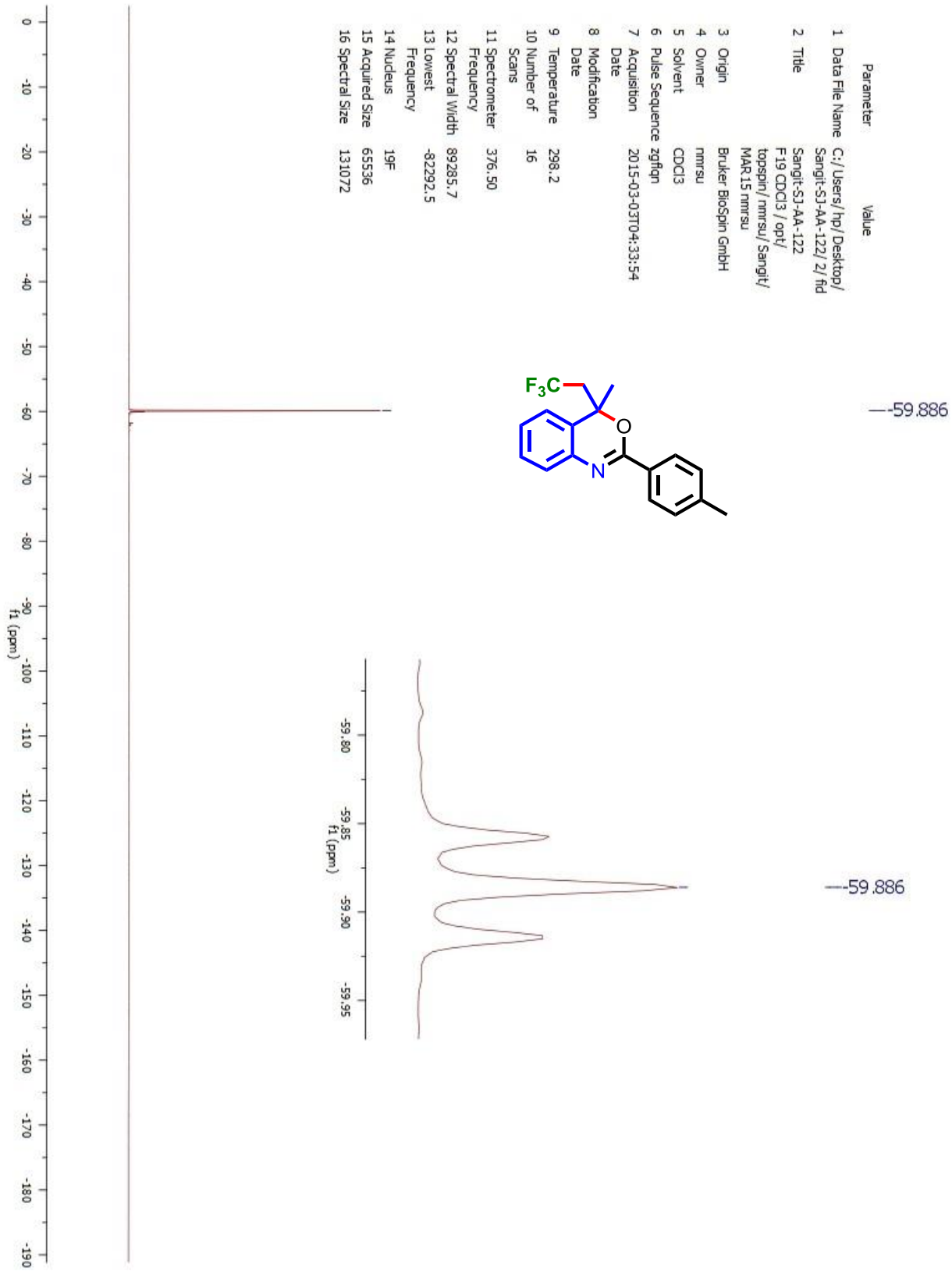
S10 ^{1}H NMR of **3b**



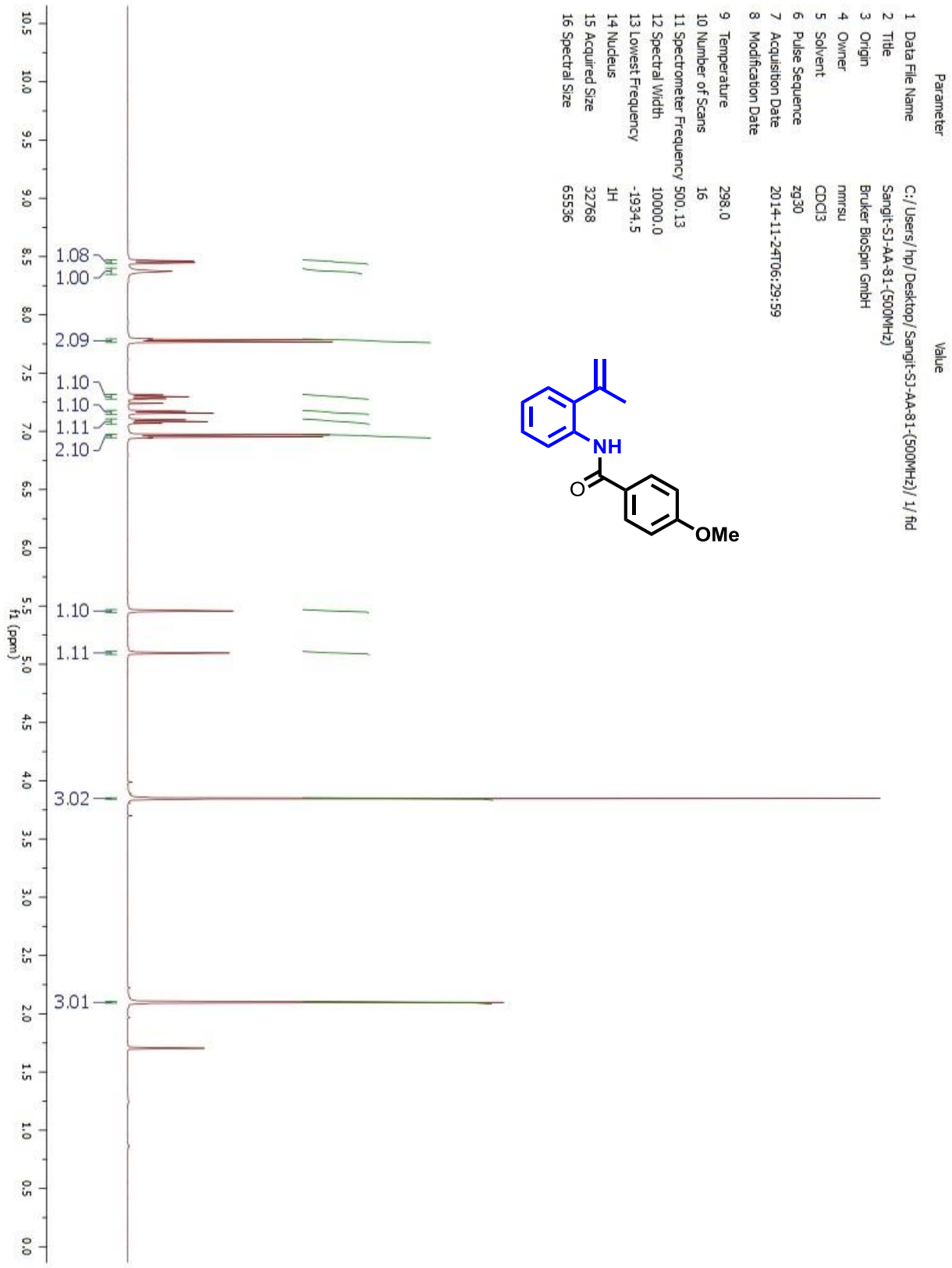
S11 ^{13}C NMR of **3b**



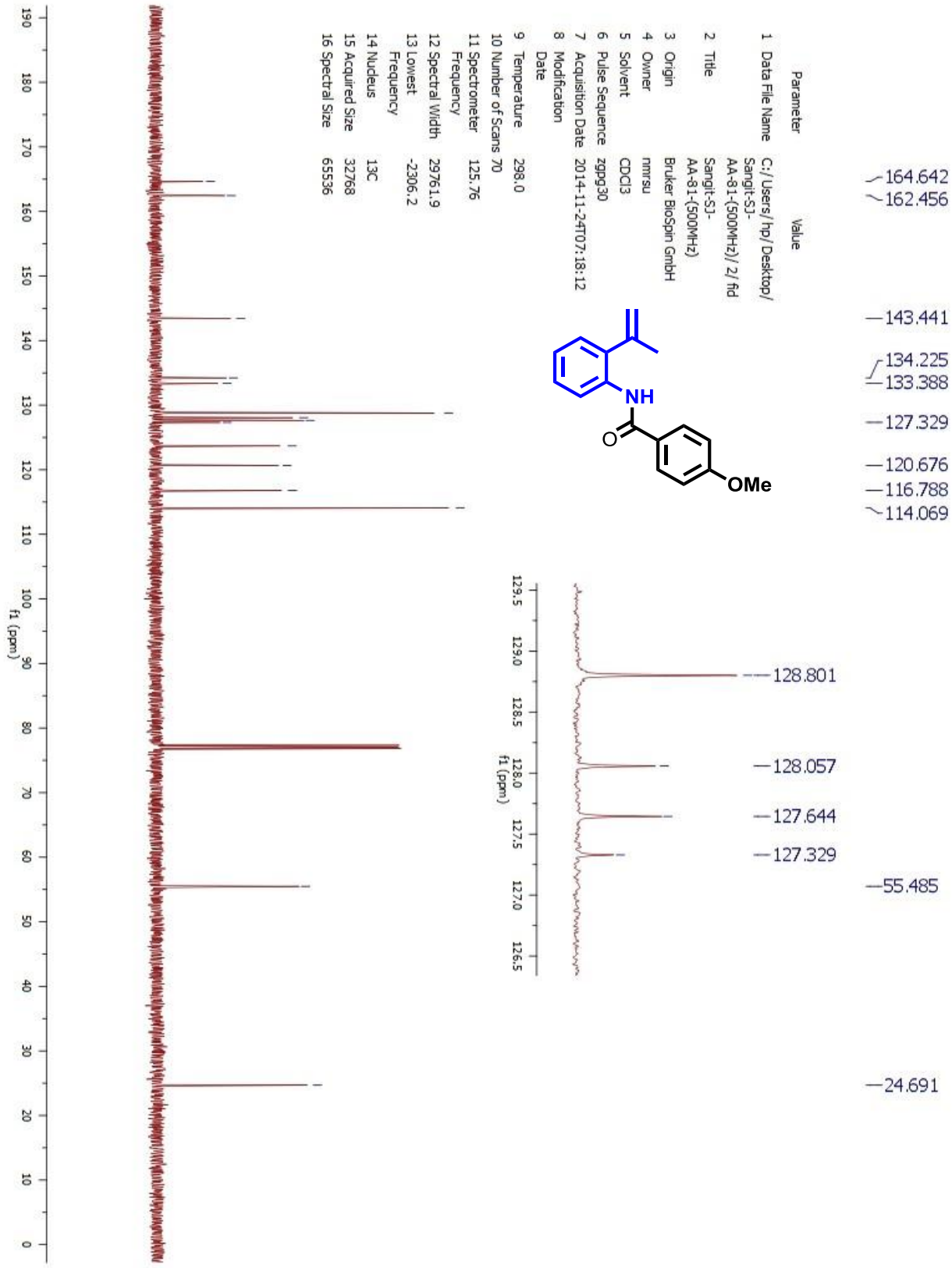
S12 ^{19}F NMR of **3b**



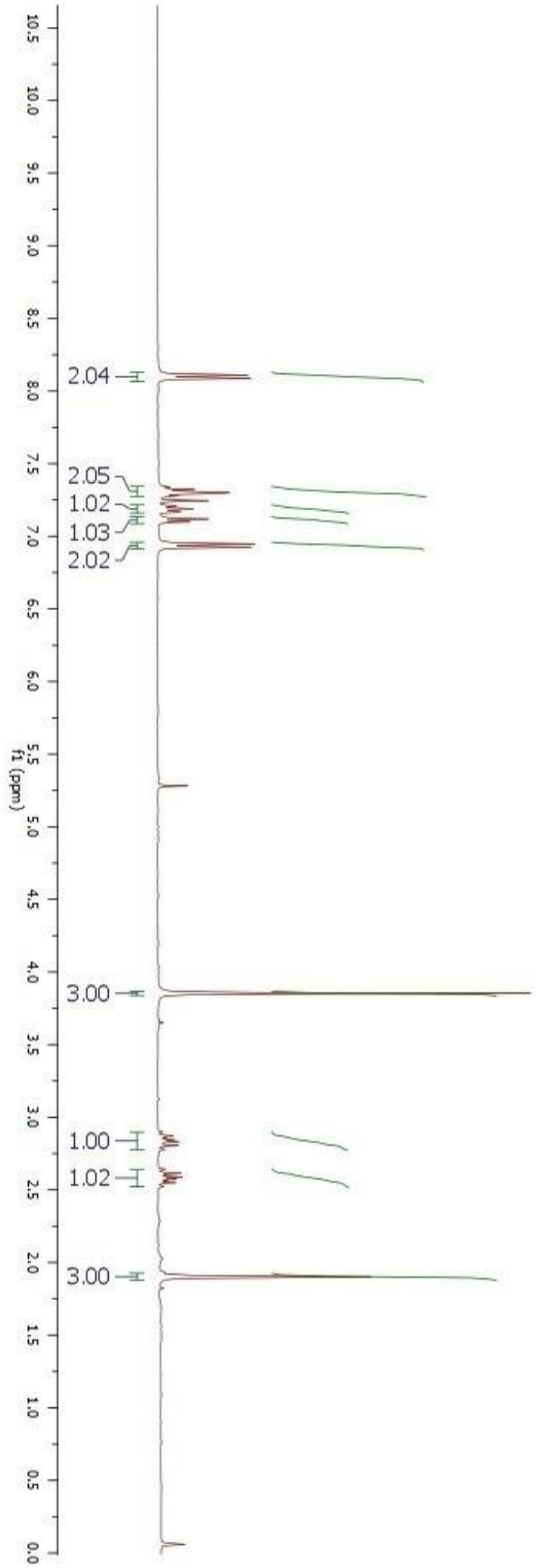
S13 ^{1}H NMR of **1c**



S14 ^{13}C NMR of **1c**



S15 ^{1}H NMR of **3c**



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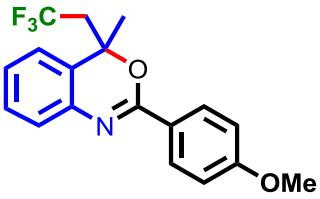
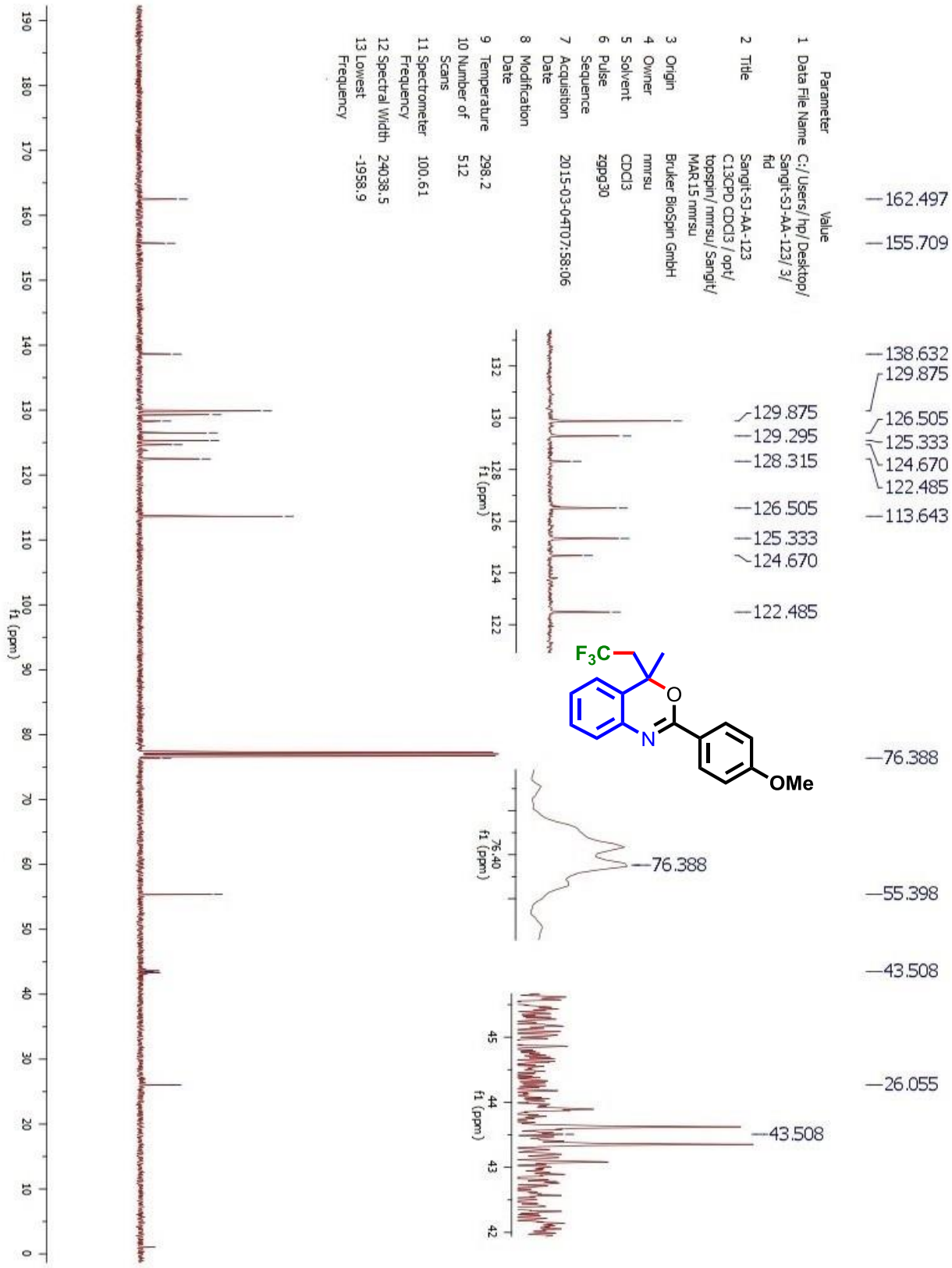
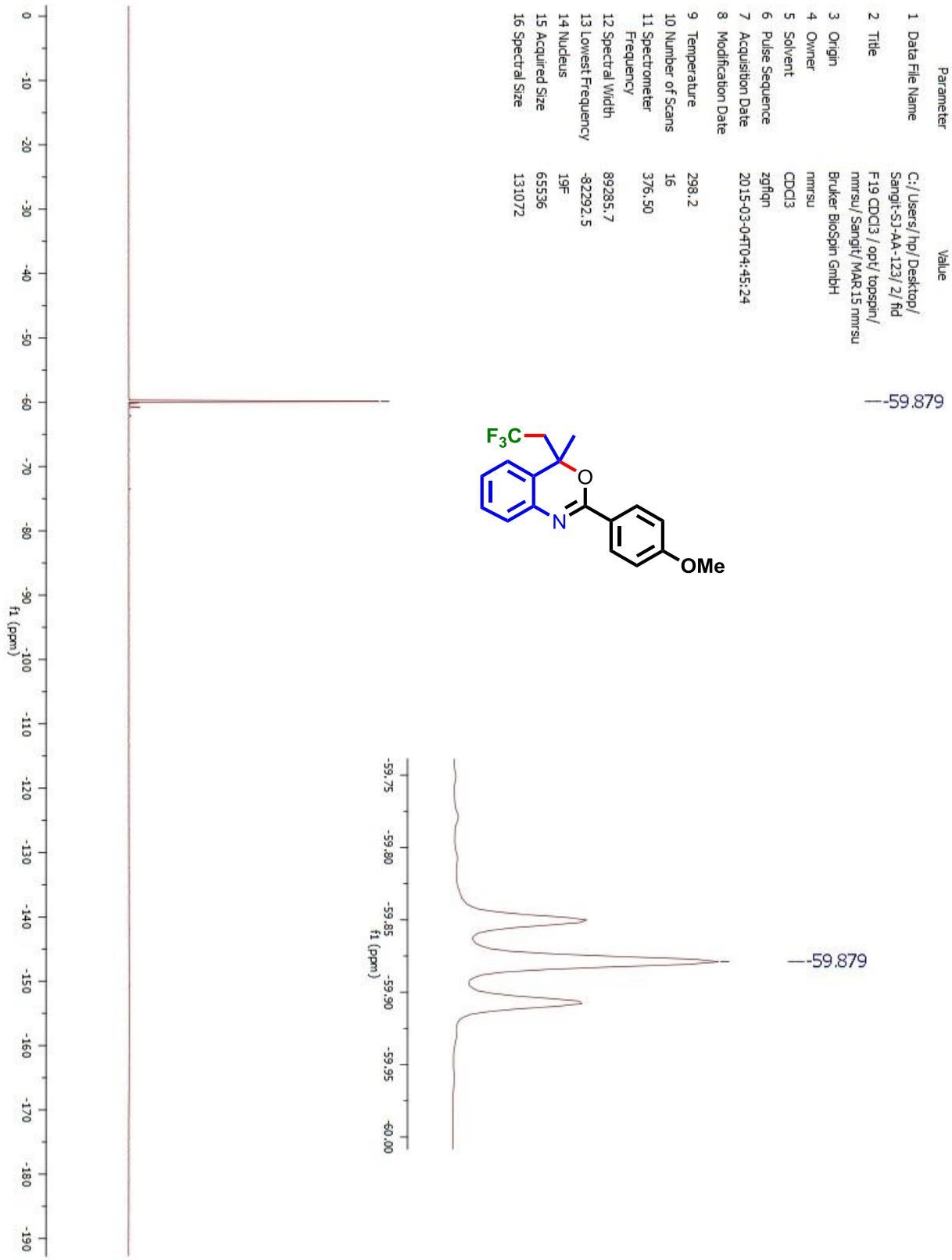
13	Lowest Frequency	-1713.7
14	Nucleus	1H
15	Acquired Size	32768
16	Spectral Size	65536



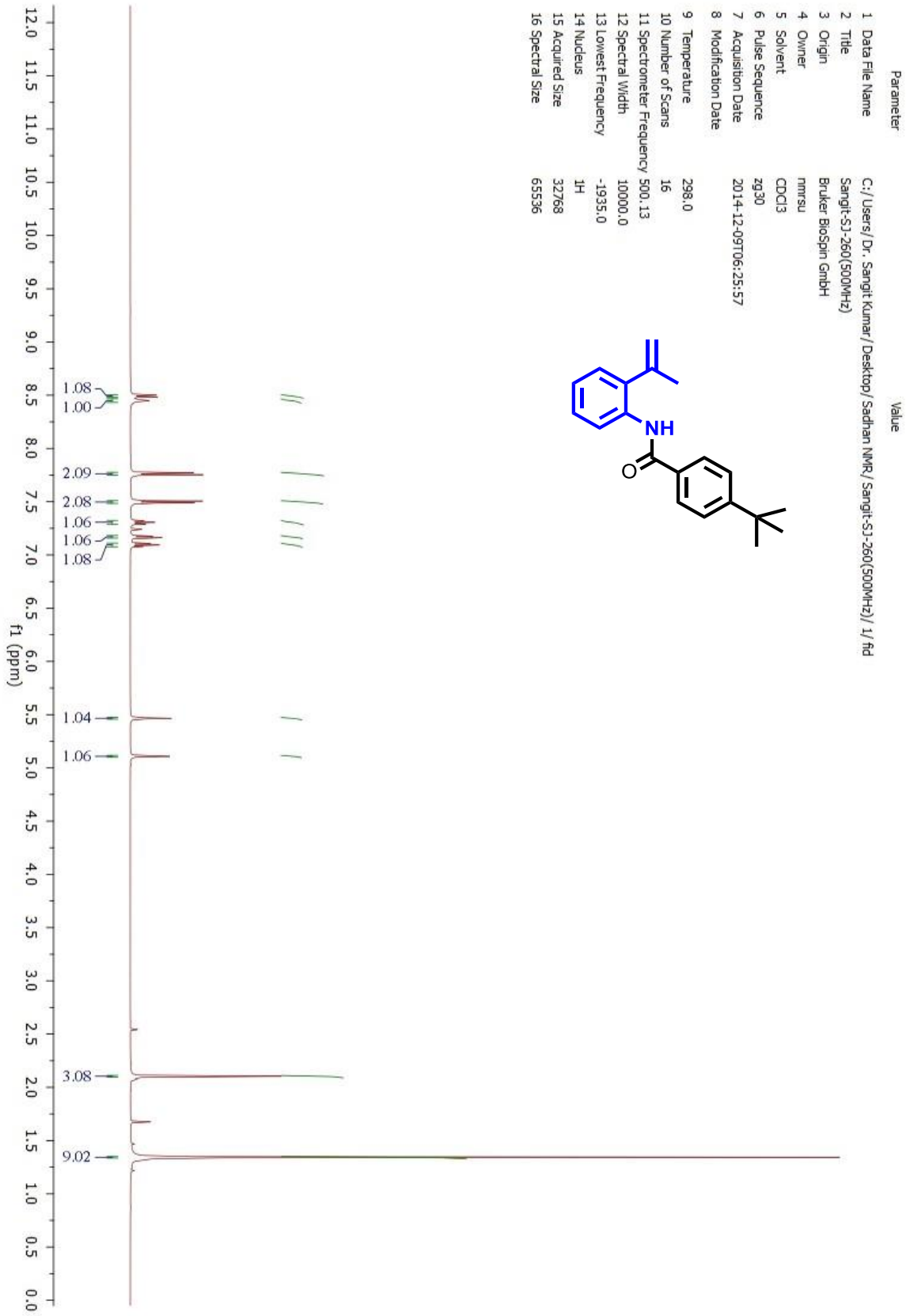
S16 ^{13}C NMR of **3c**



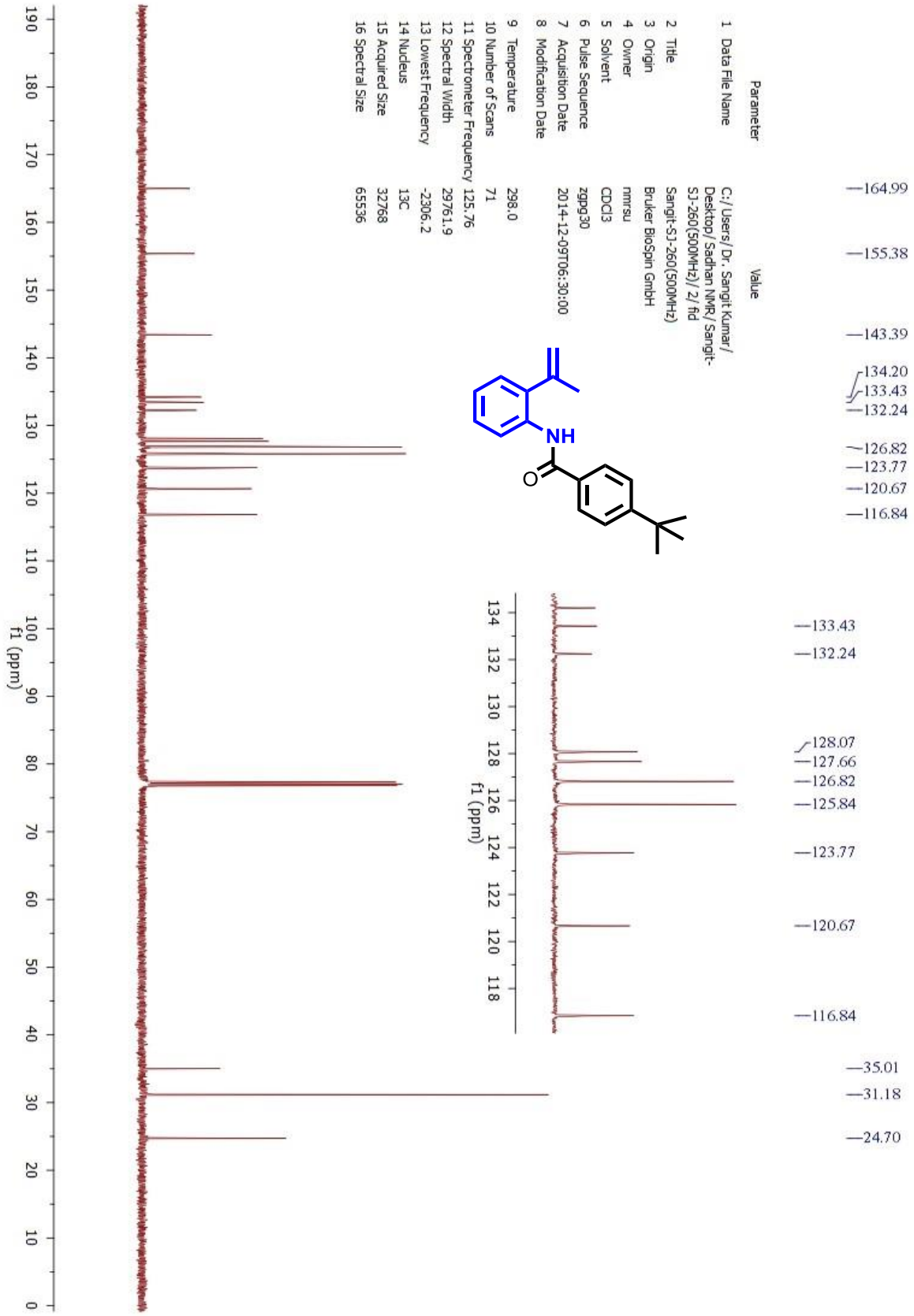
S17 ^{19}F NMR of **3c**



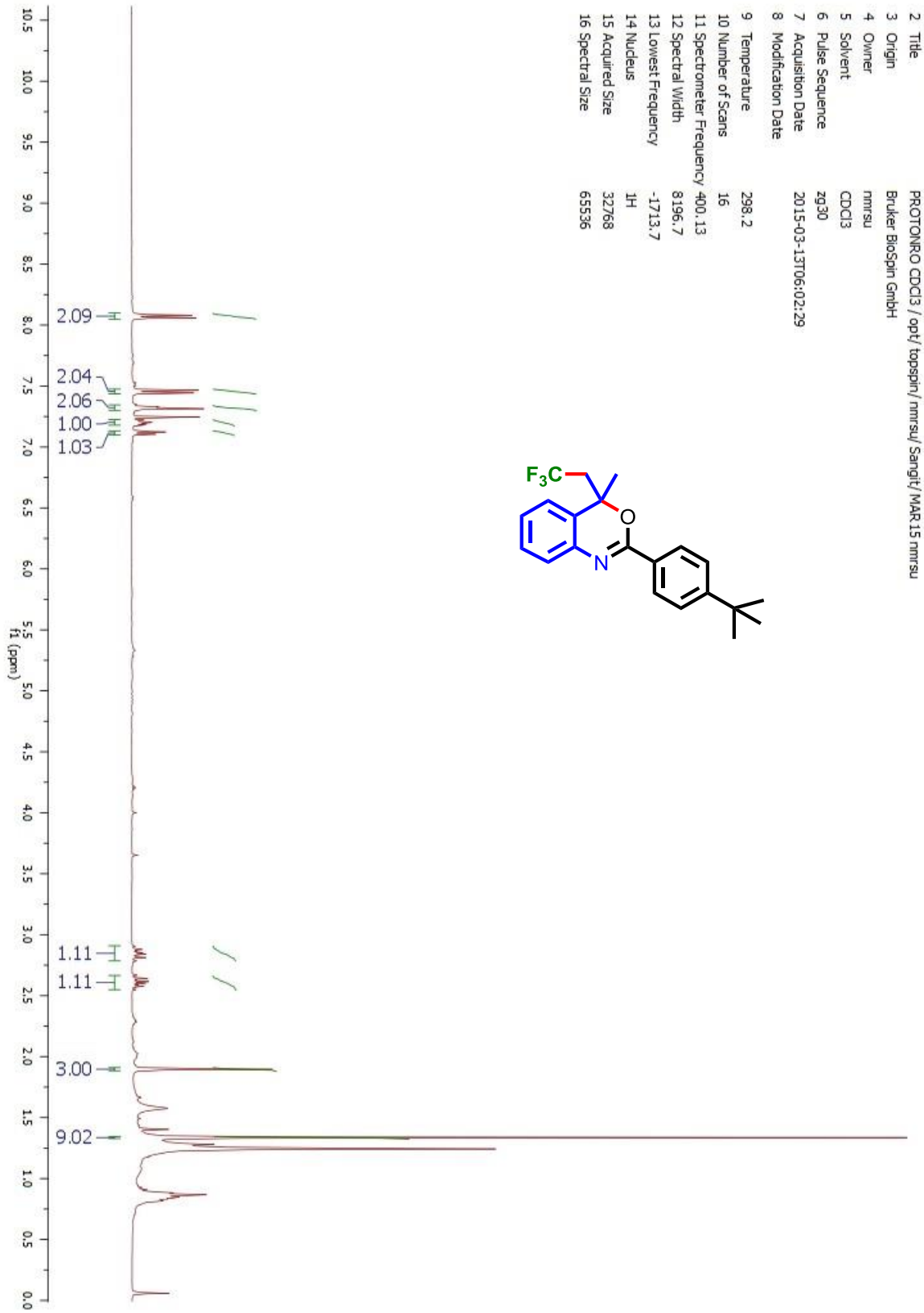
S18 ^{1}H NMR of **1d**



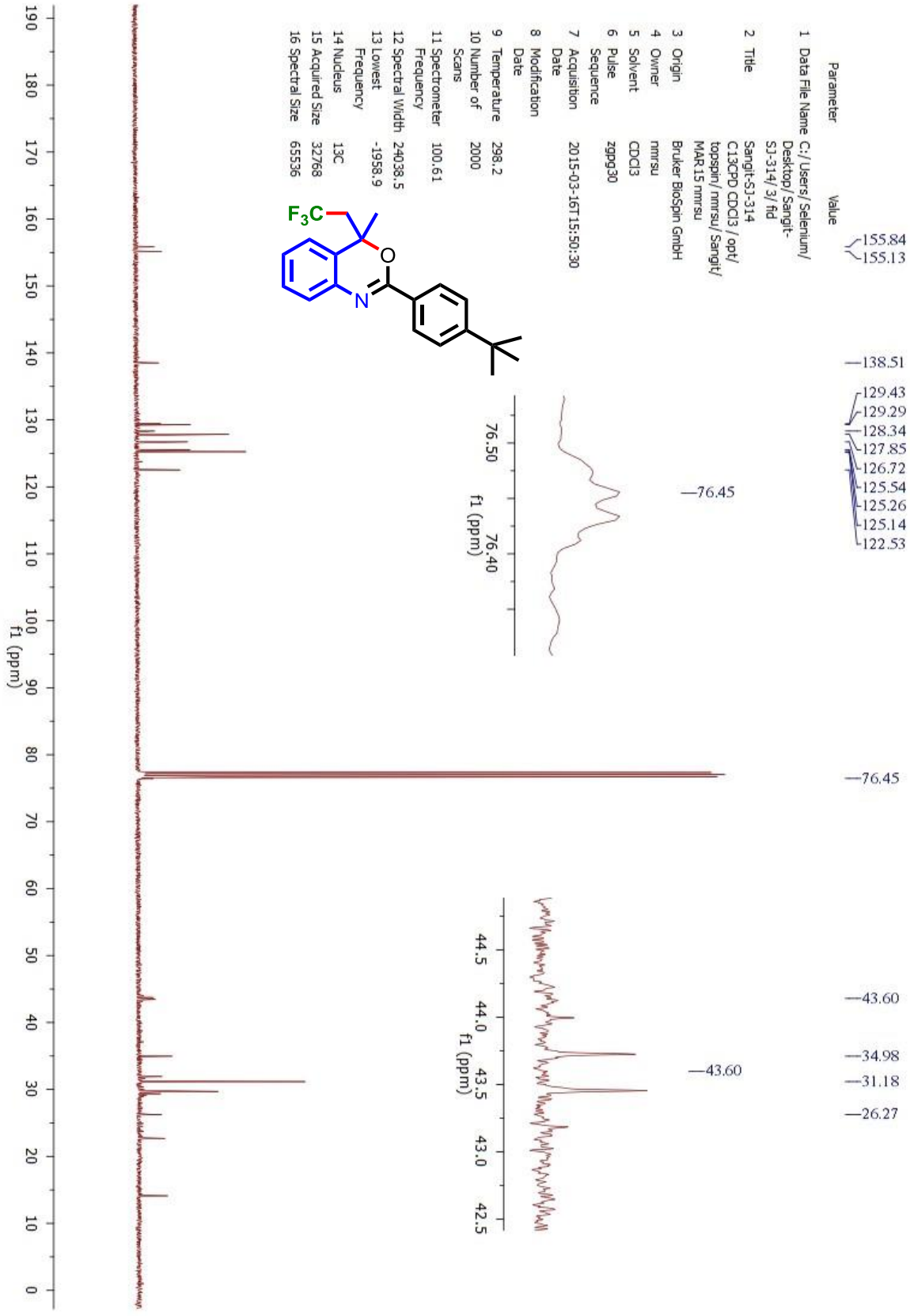
S19 ^{13}C NMR of **1d**



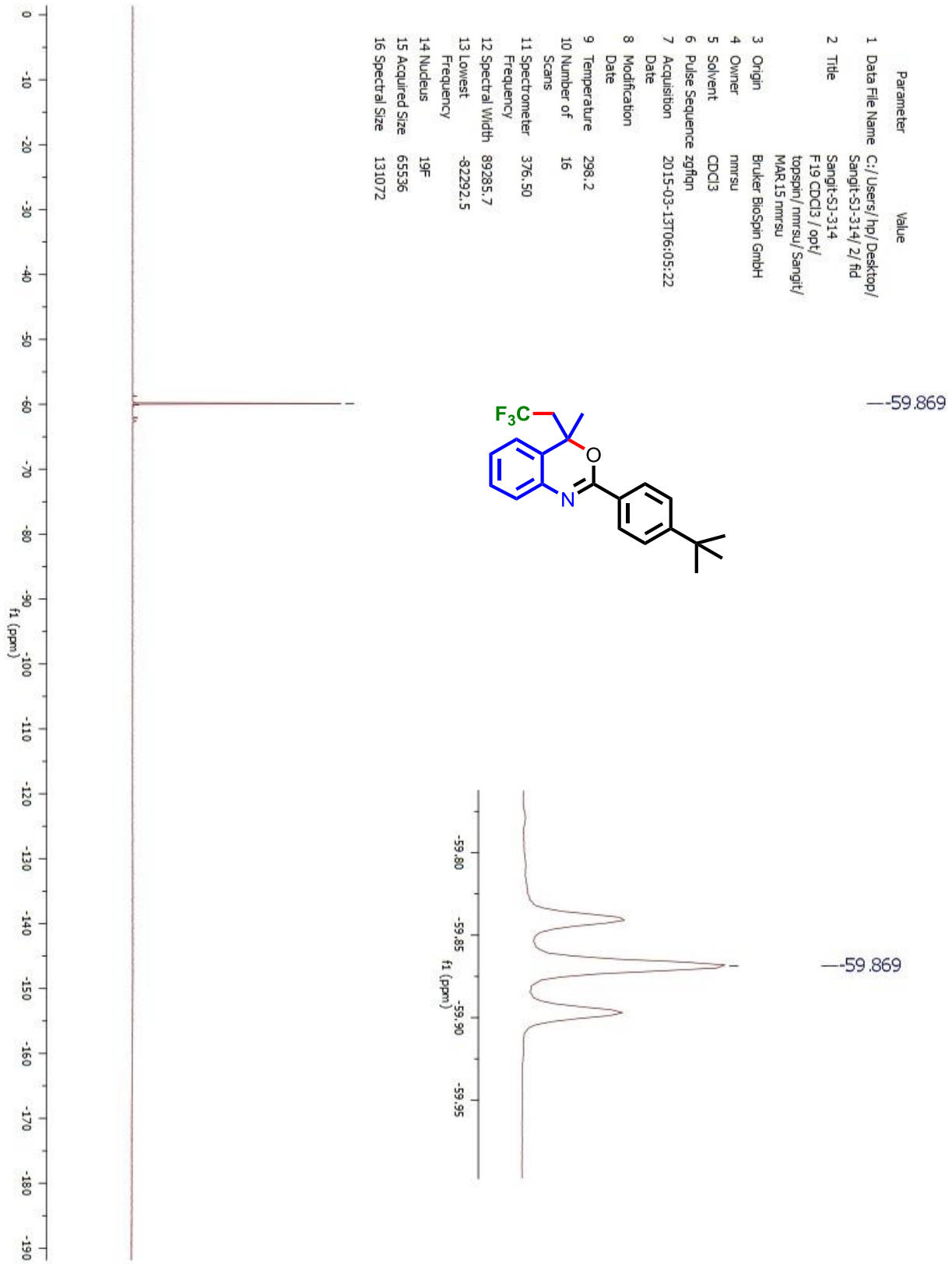
S20 ^{1}H NMR of **3d**



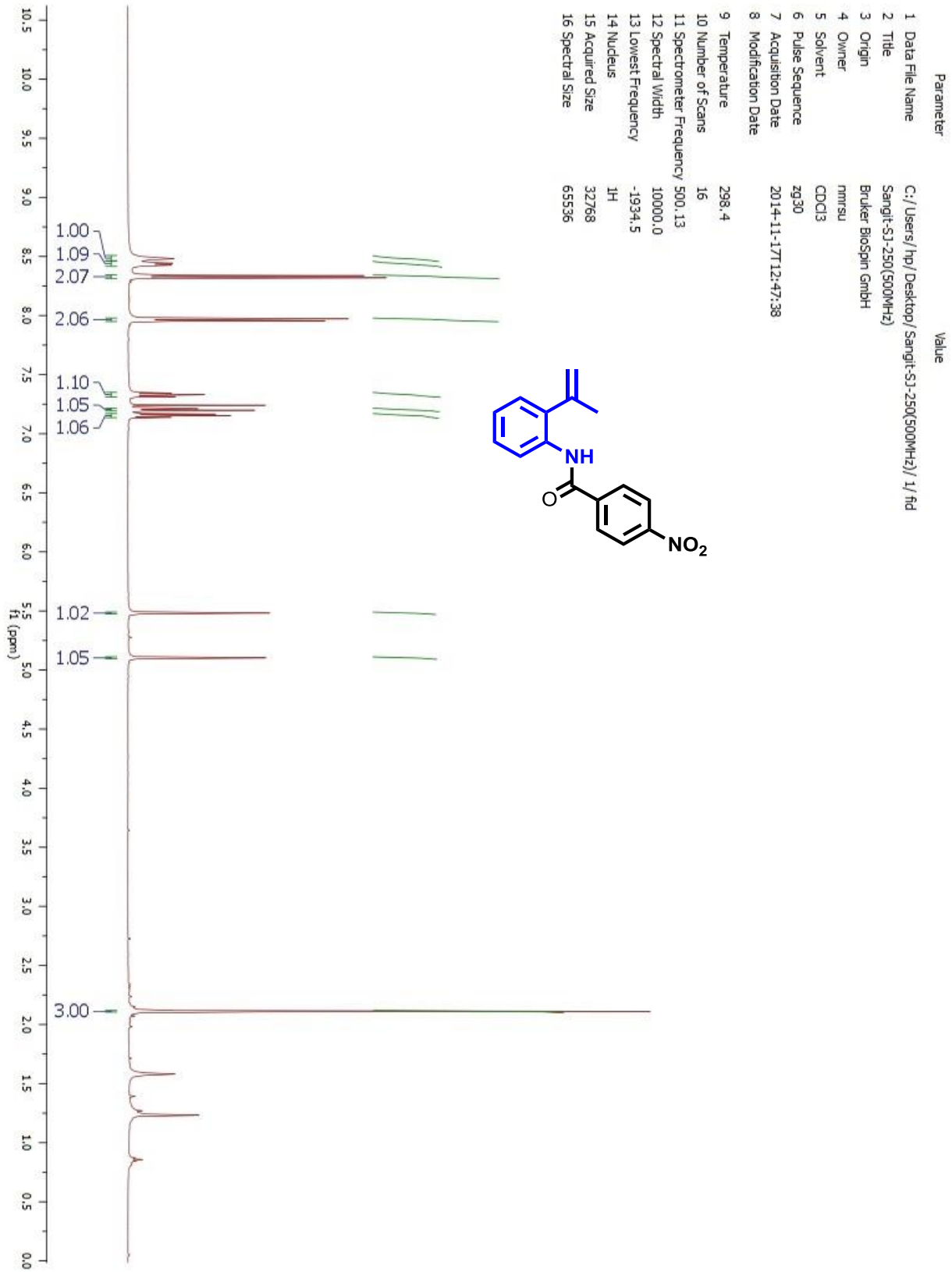
S21 ^{13}C NMR of **3d**



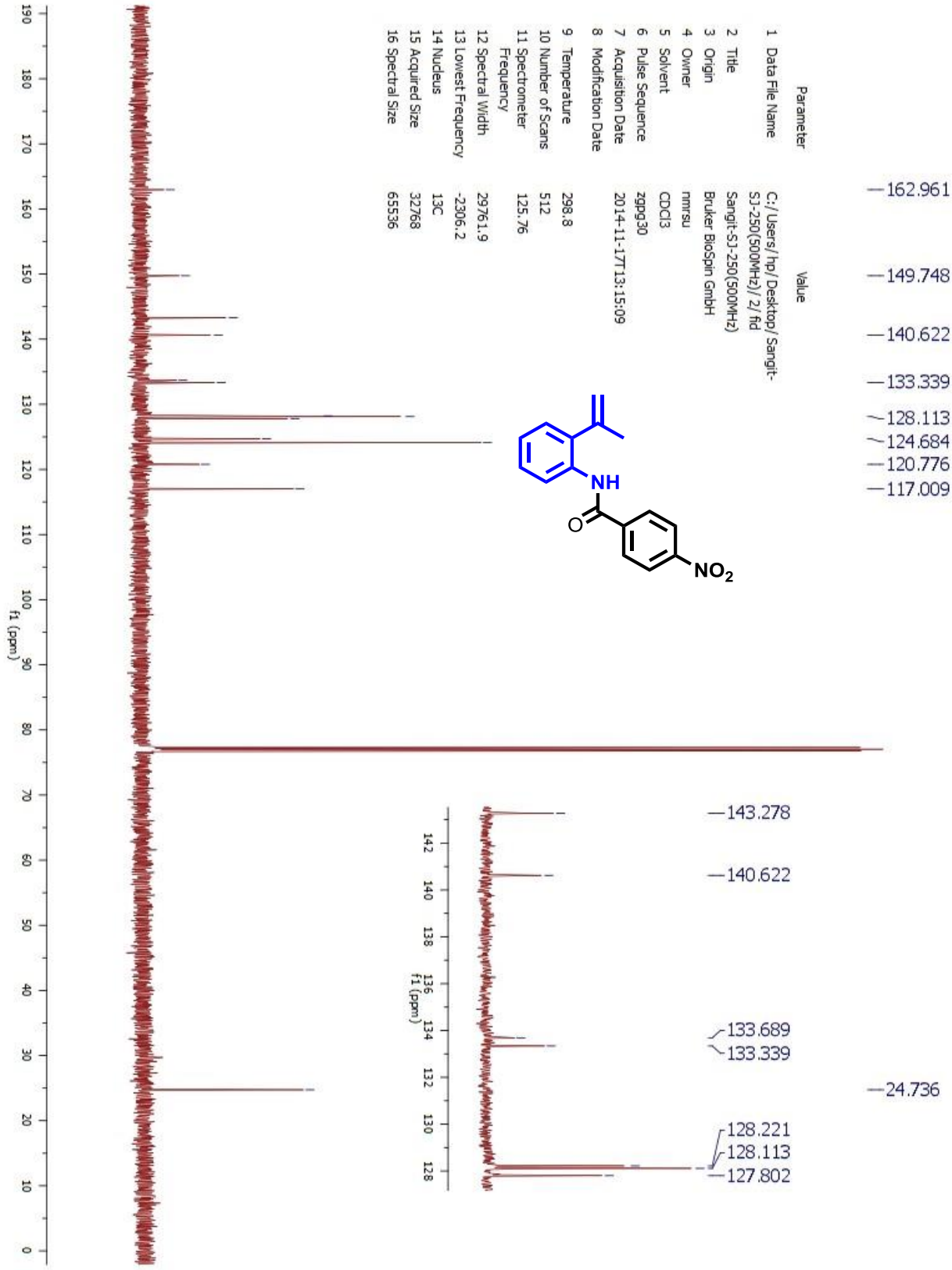
S22 ^{19}F NMR of **3d**



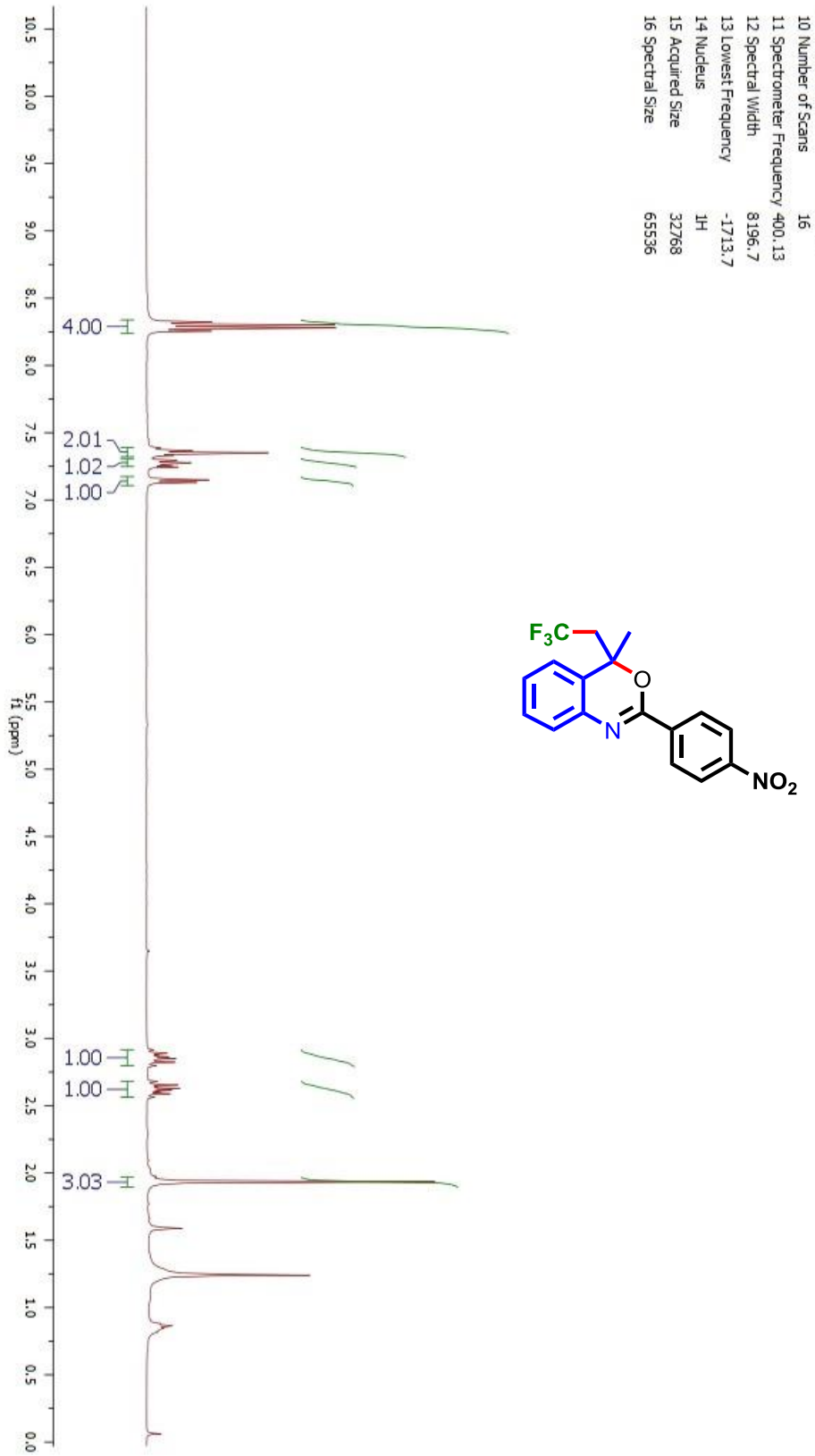
S23 ^{1}H NMR of **1e**



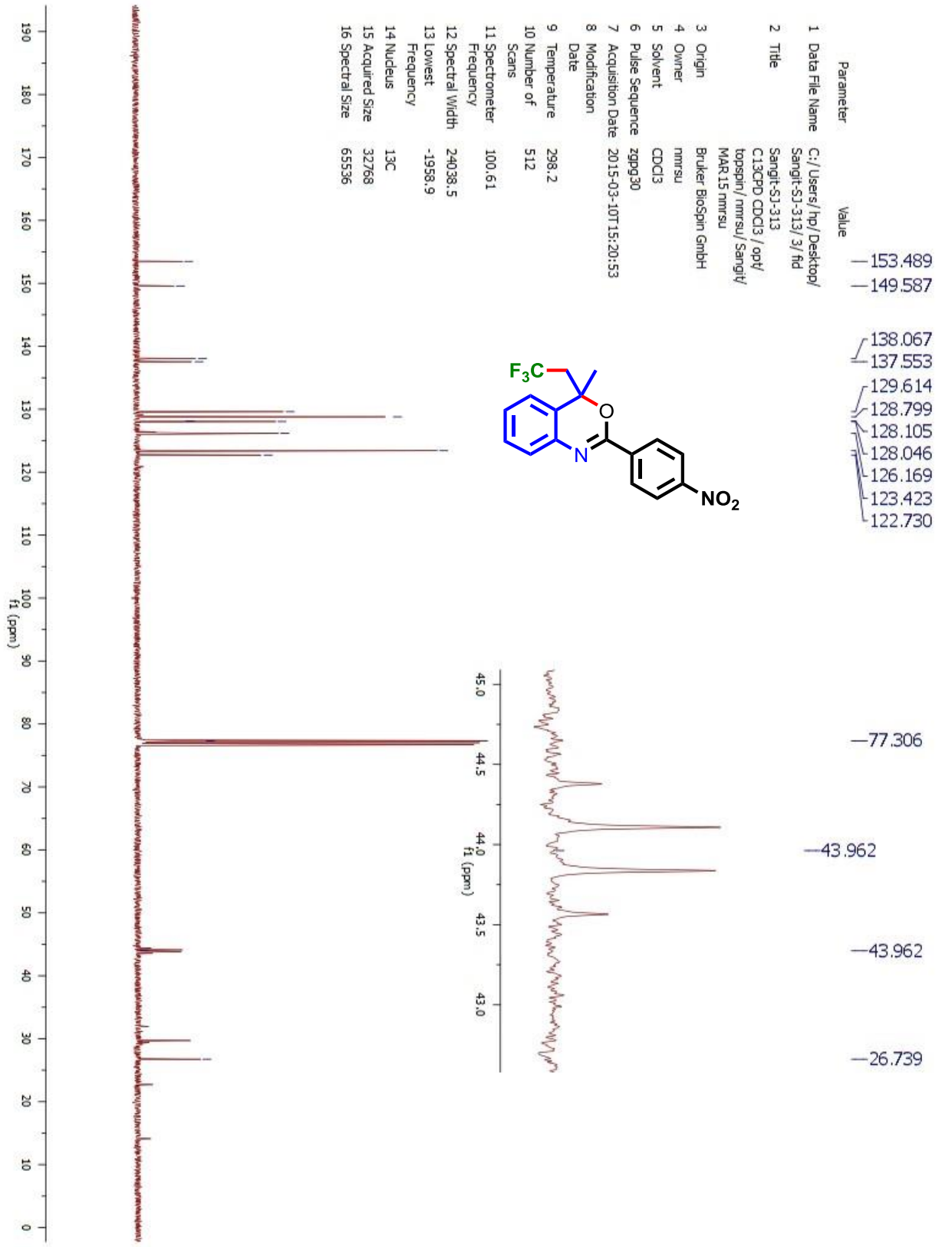
S24 ^{13}C NMR of **1e**



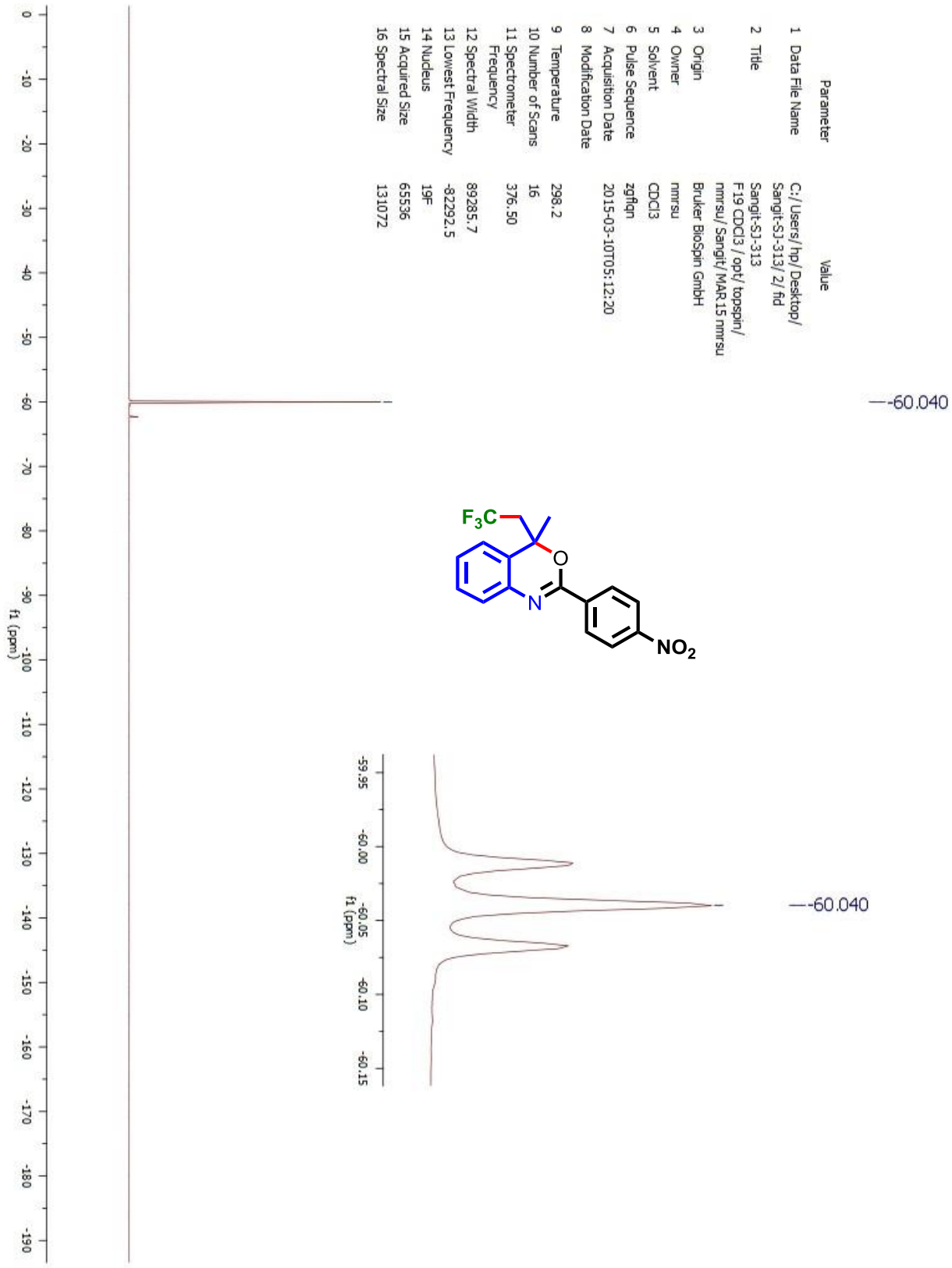
S25 ^{1}H NMR of **3e**



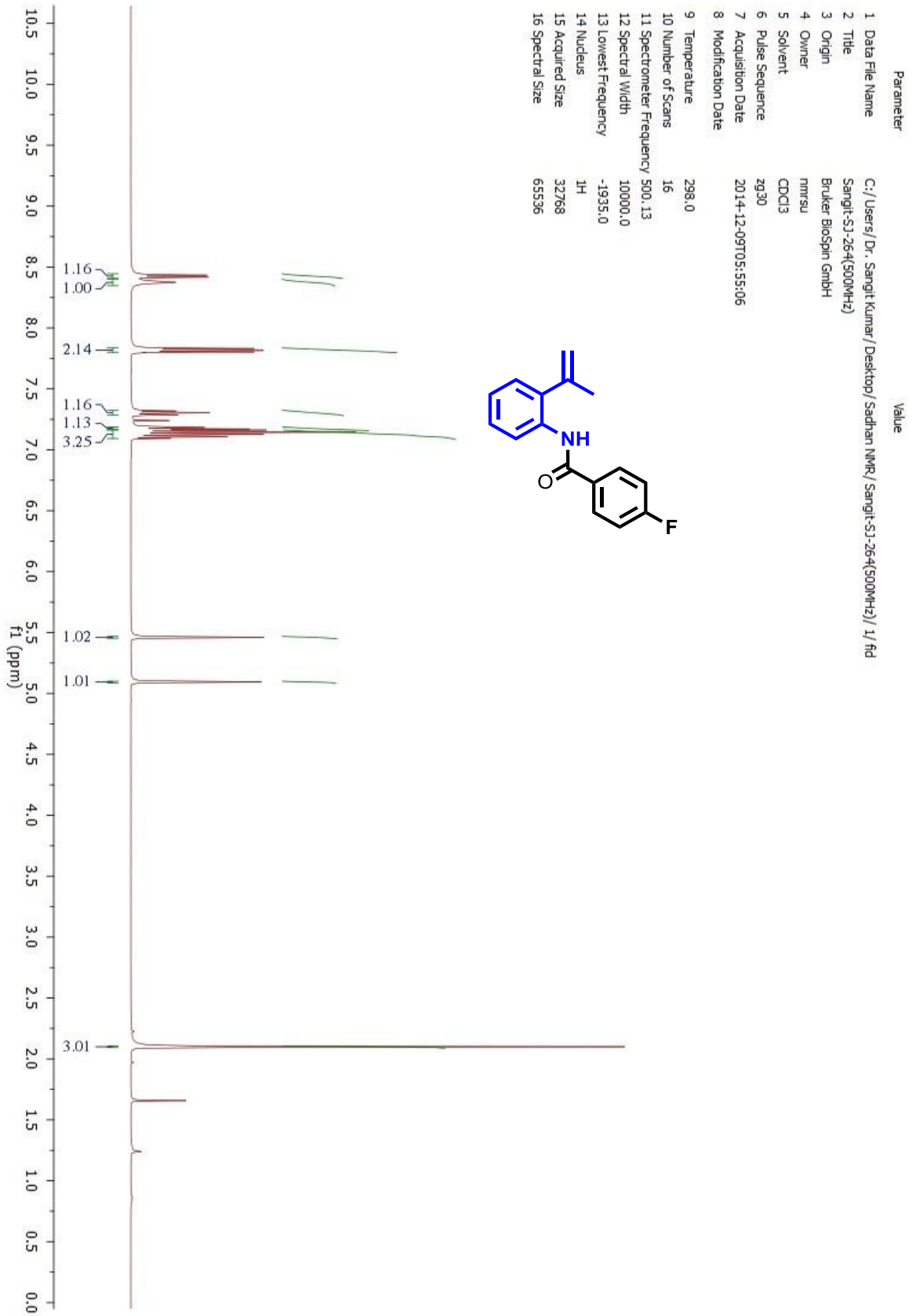
S26 ^{13}C NMR of **3e**



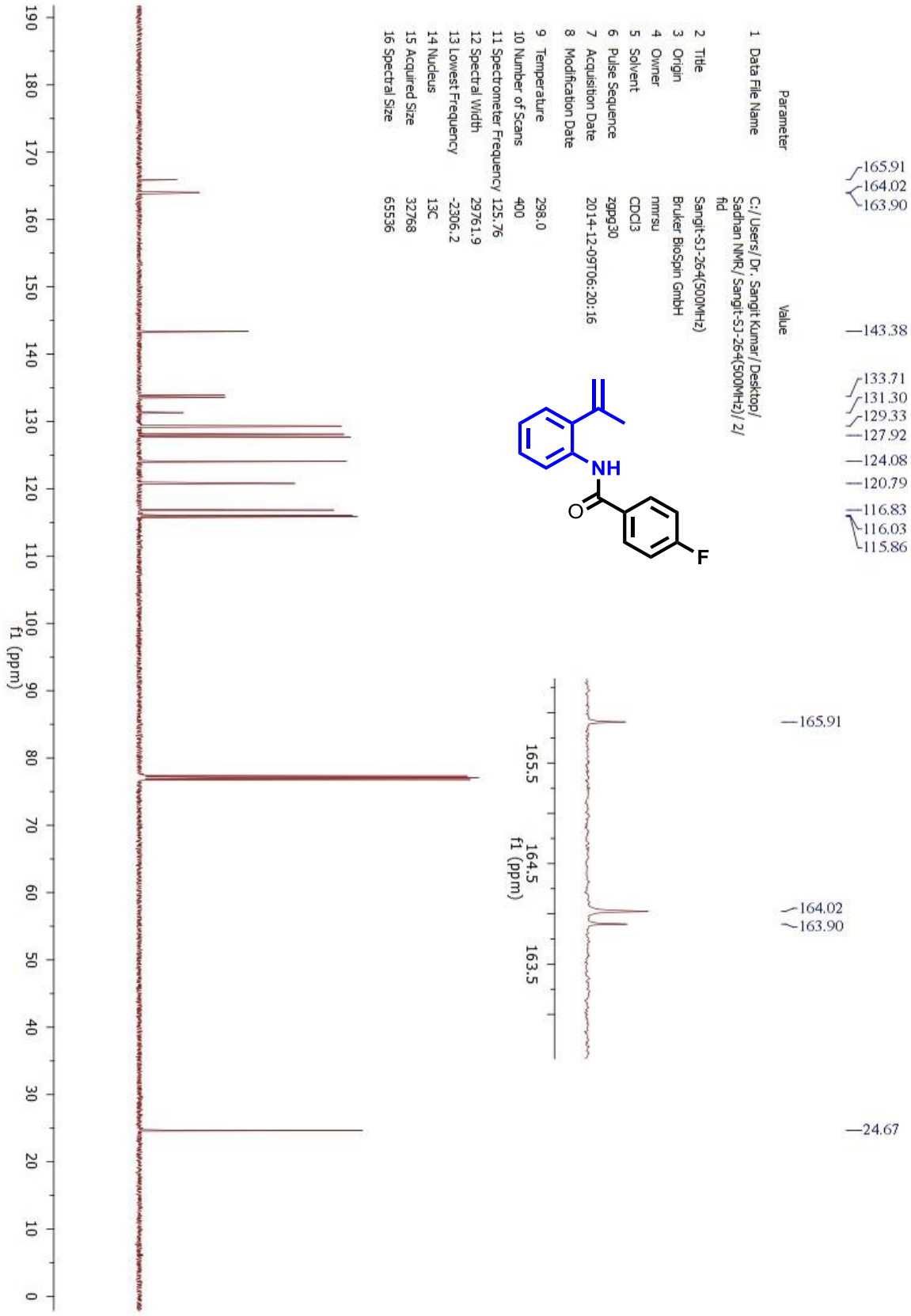
S27 ^{19}F NMR of **3e**



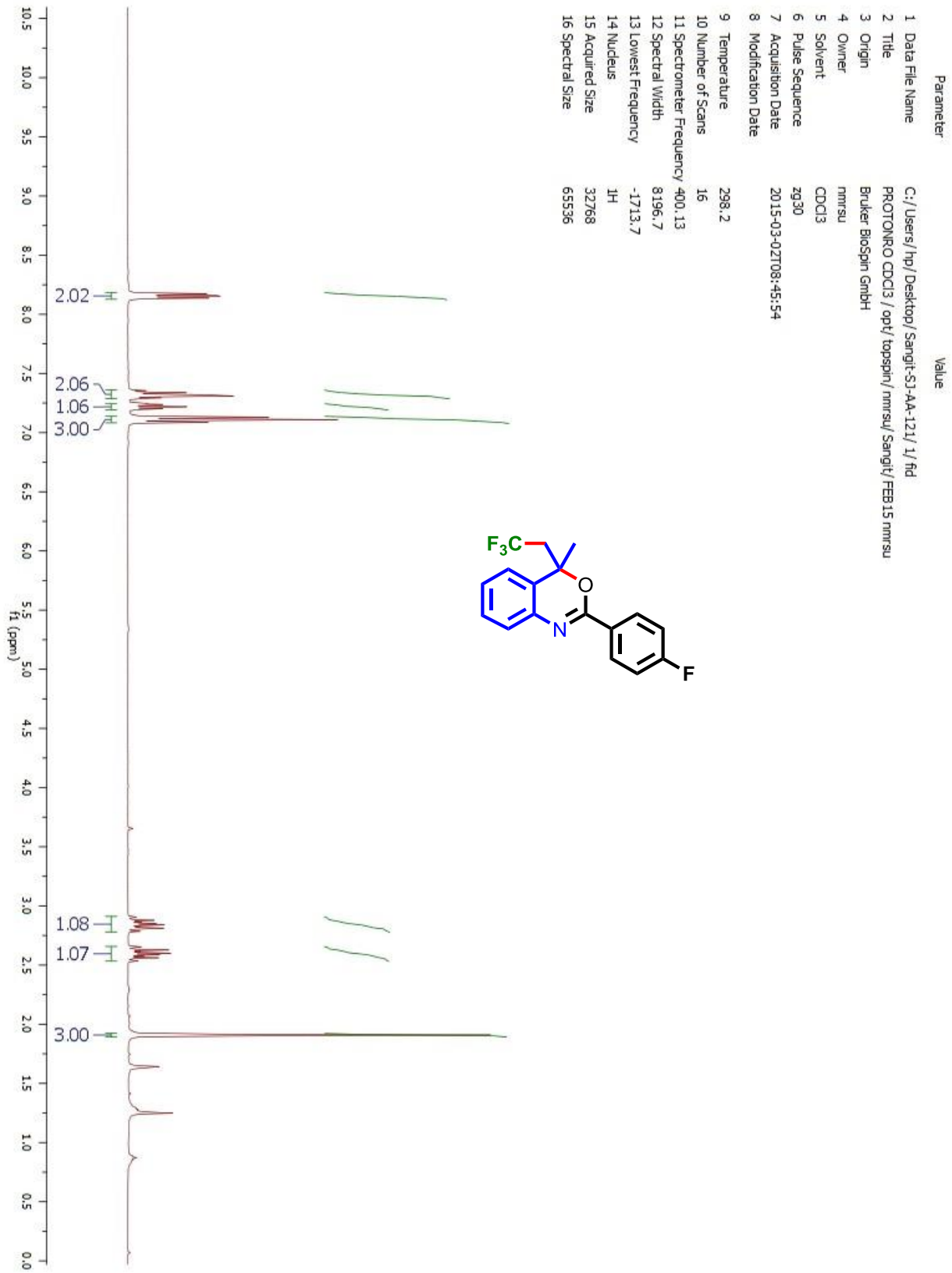
S28 ^{1}H NMR of **1f**



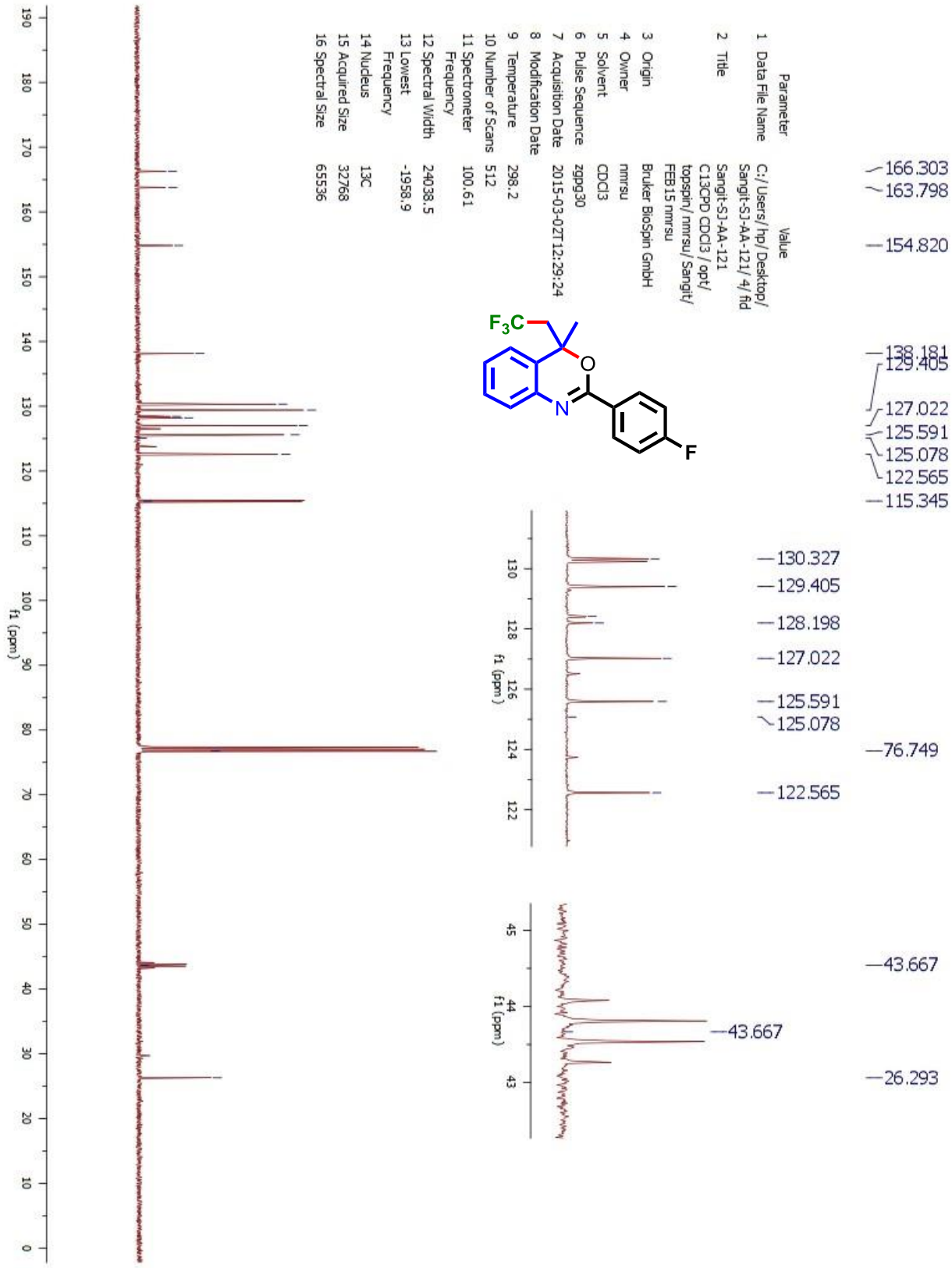
S29 ^{13}C NMR of **1f**



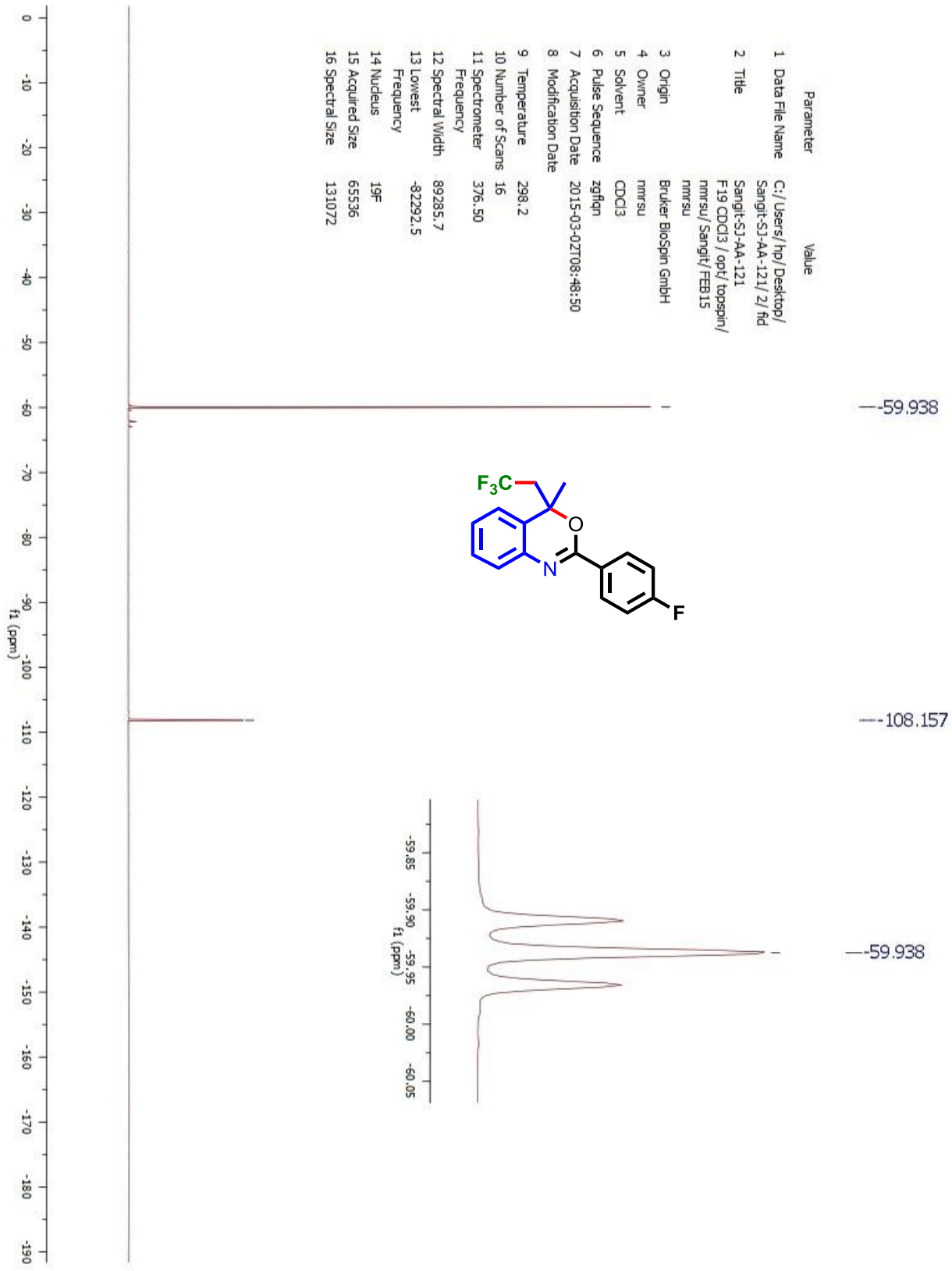
S30 ^{1}H NMR of **3f**



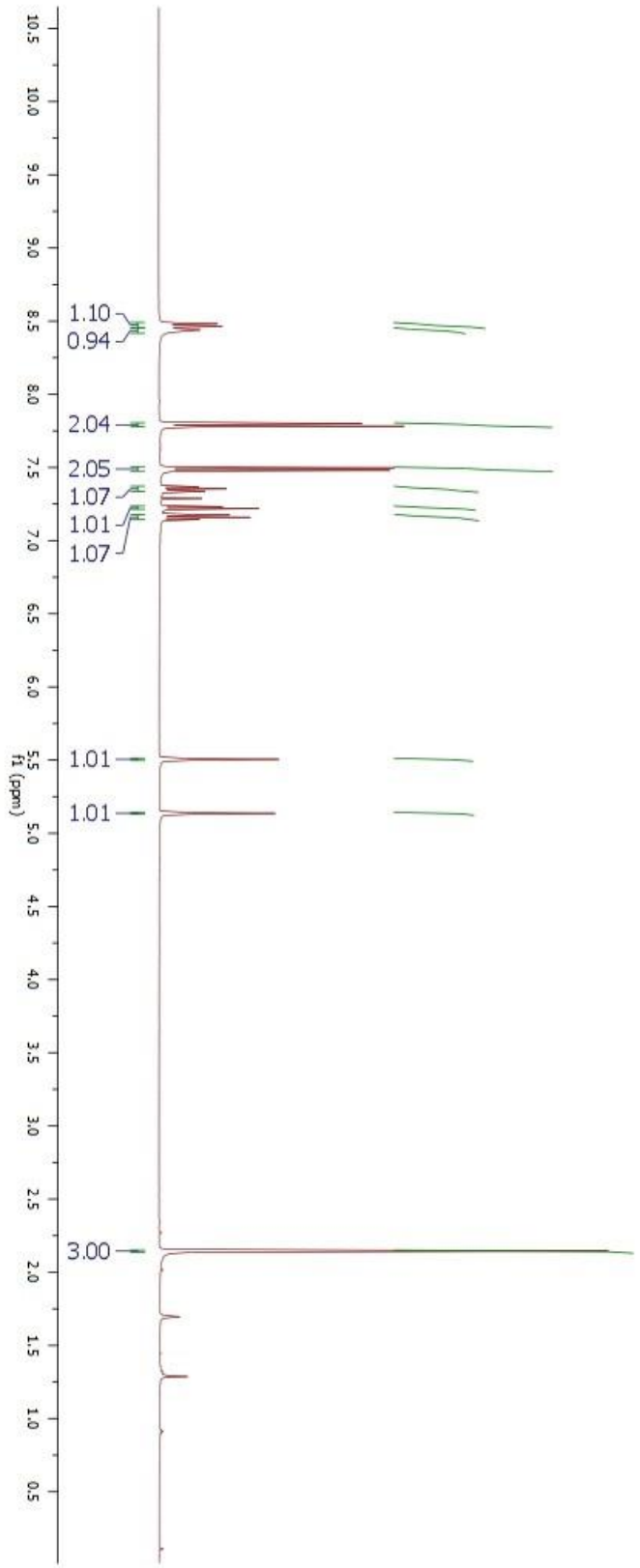
S31 ^{13}C NMR of **3f**



S32 ^{19}F NMR of **3f**



S33 ^{1}H NMR of **1g**



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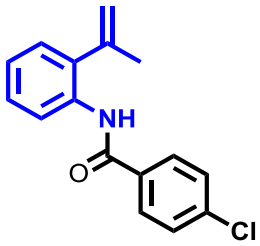
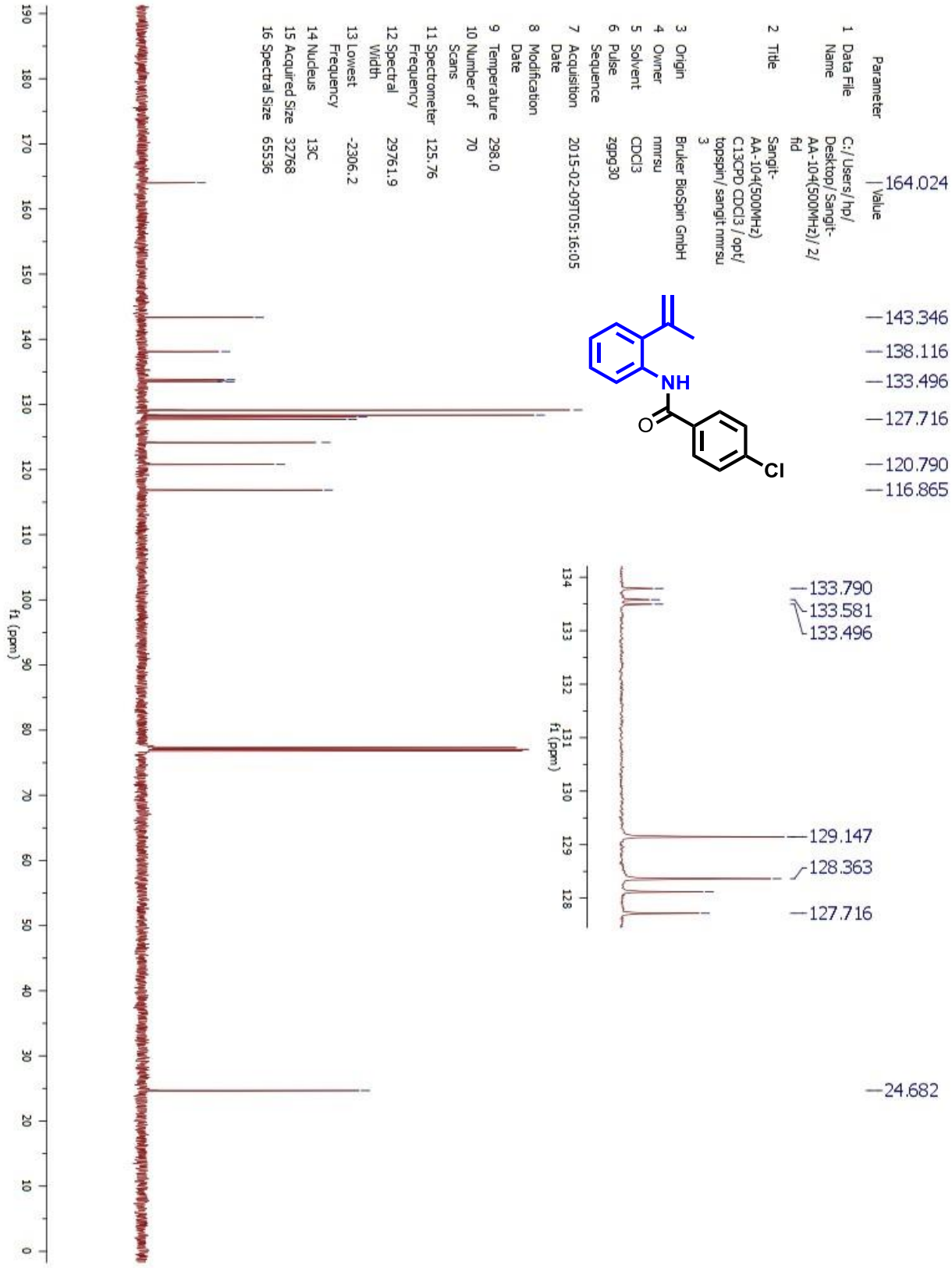
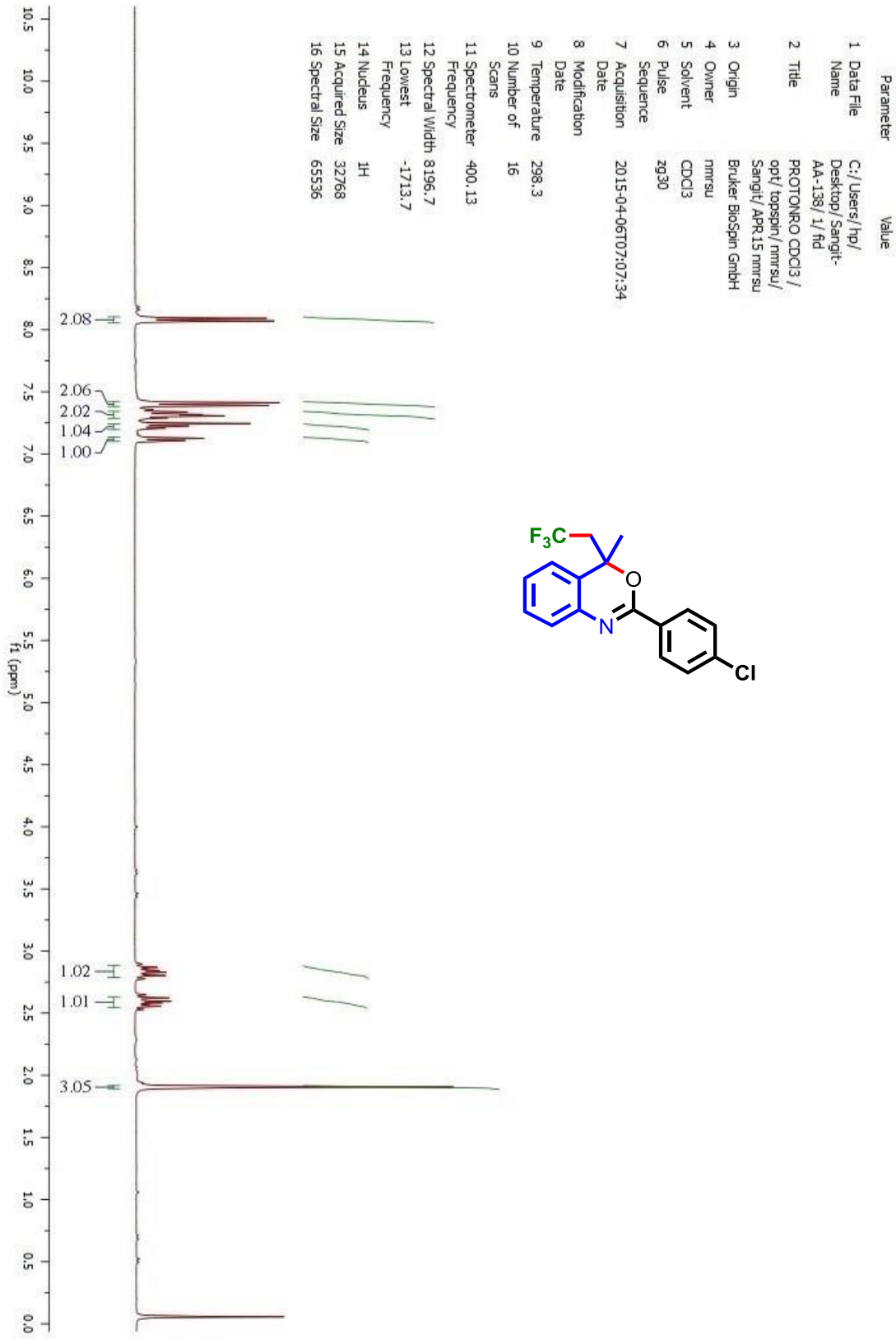


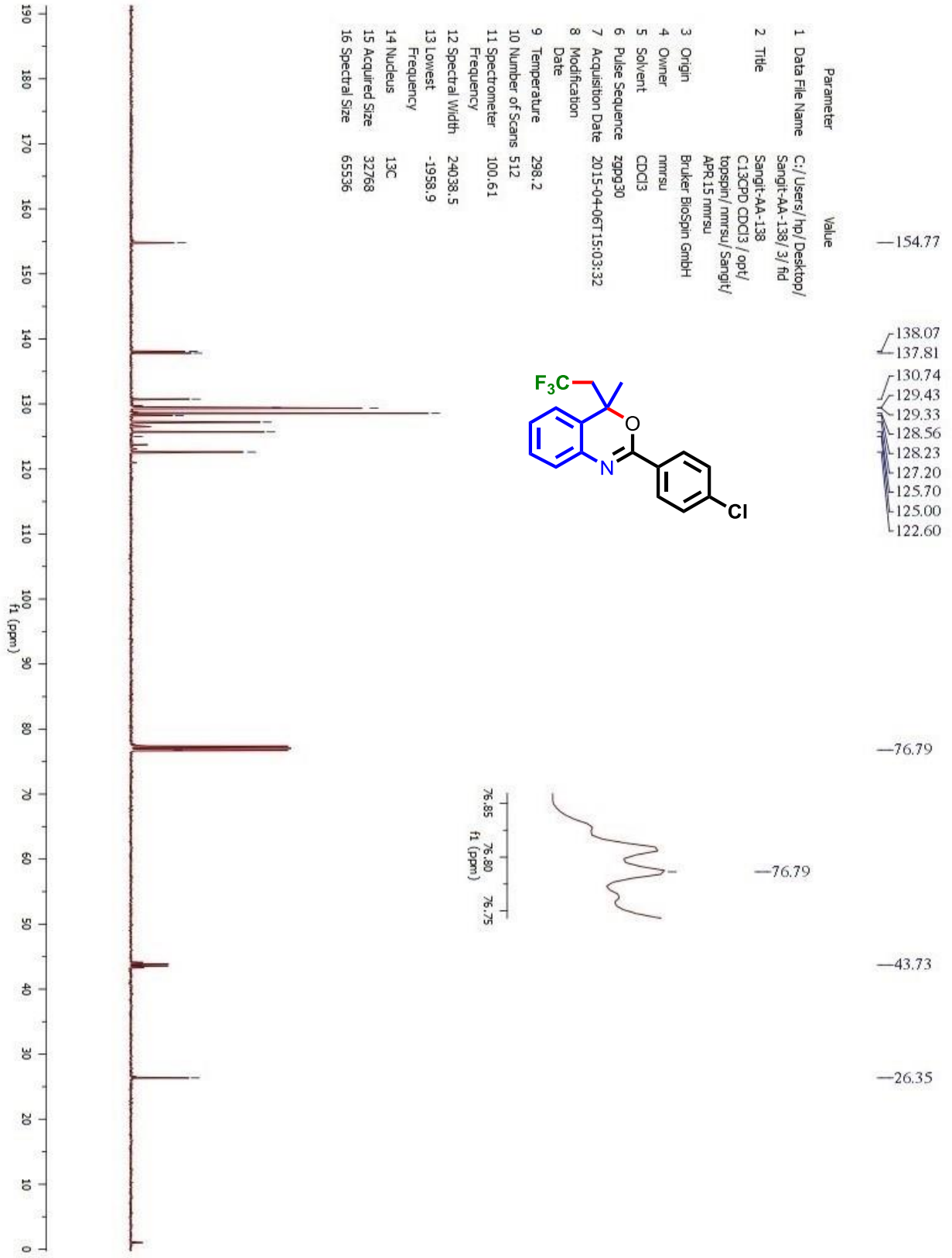
S34 ^{13}C NMR of **1g**



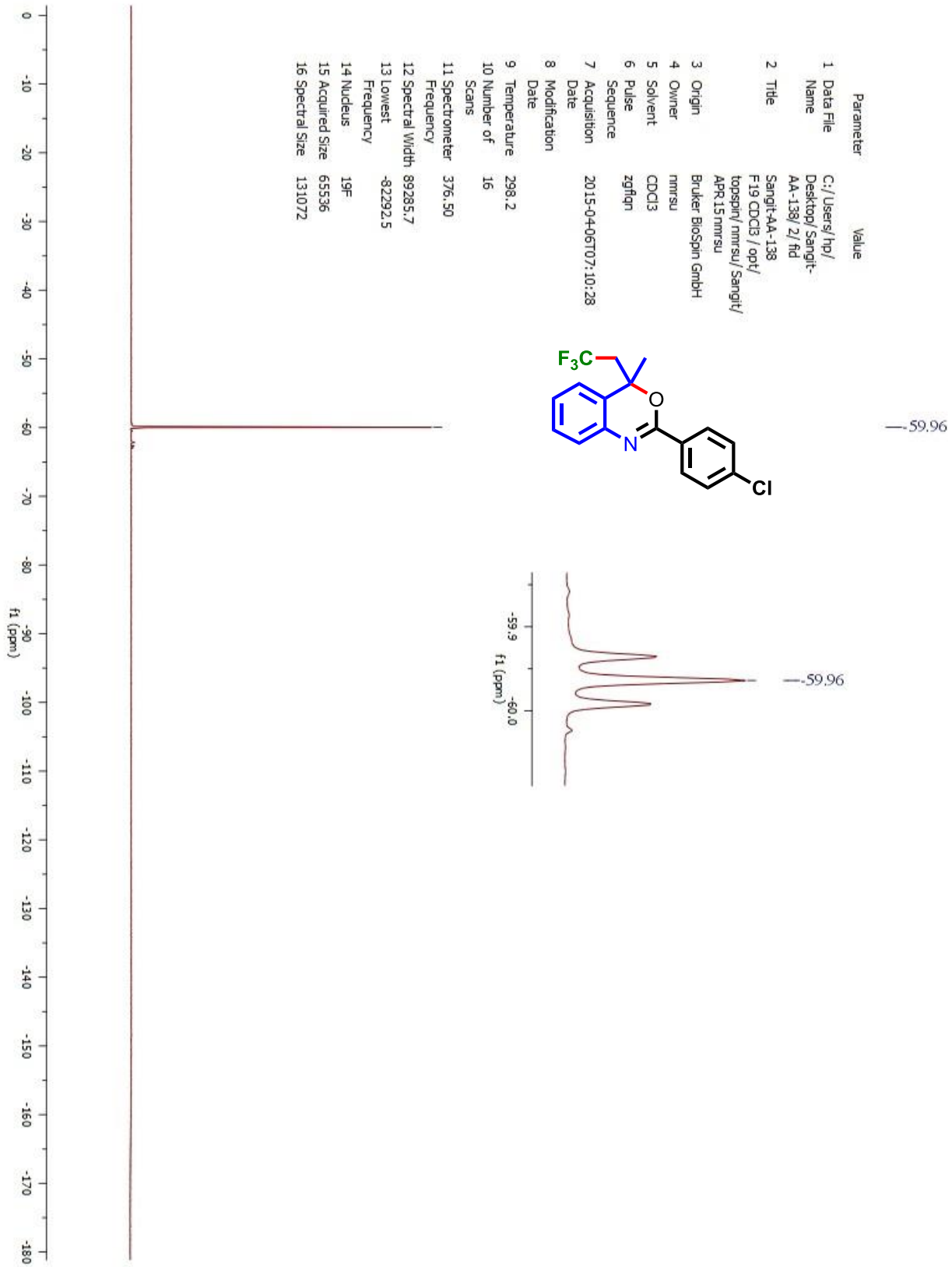
S35 ^{1}H NMR of **3g**



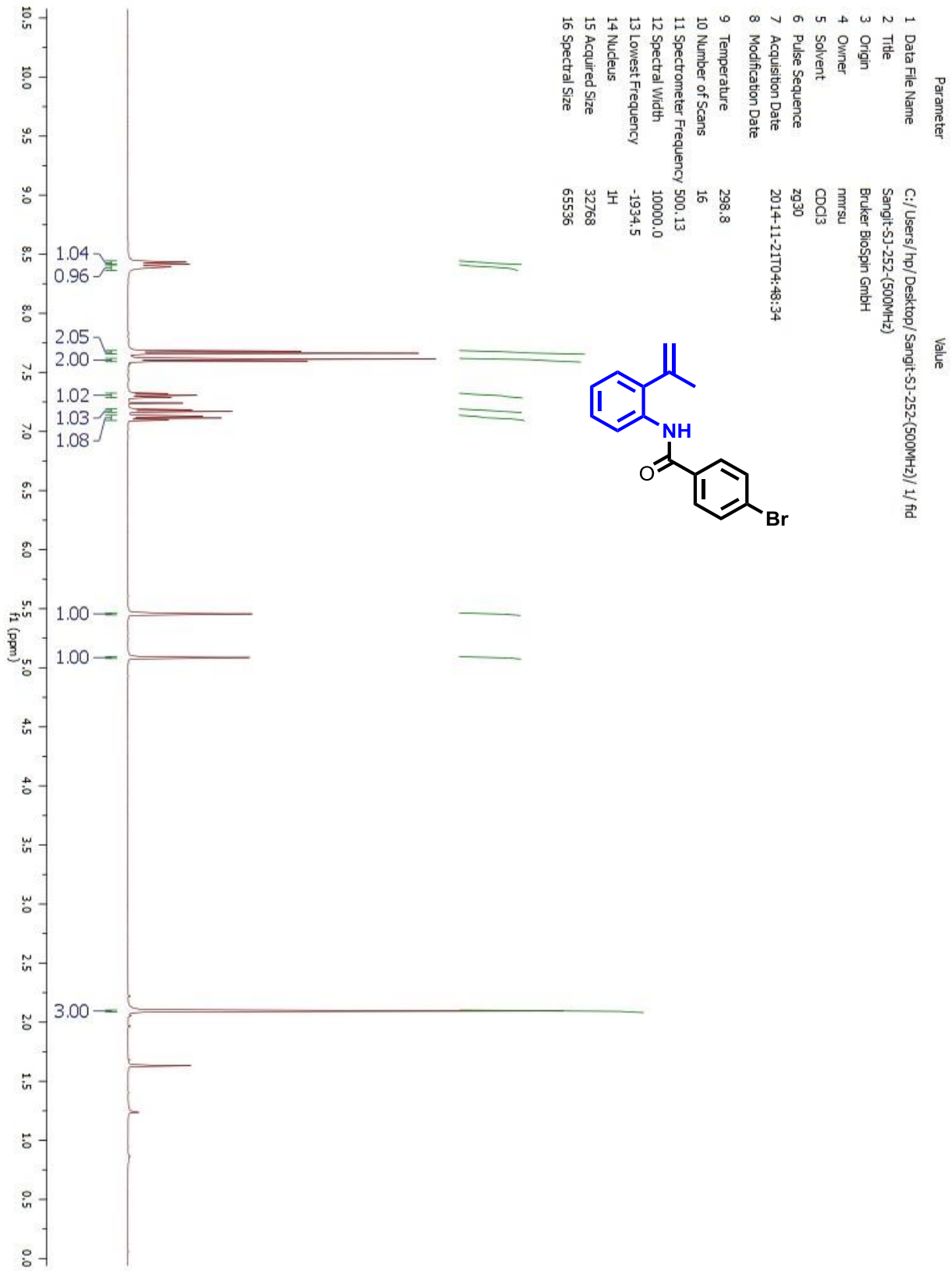
S36 ^{13}C NMR of **3g**



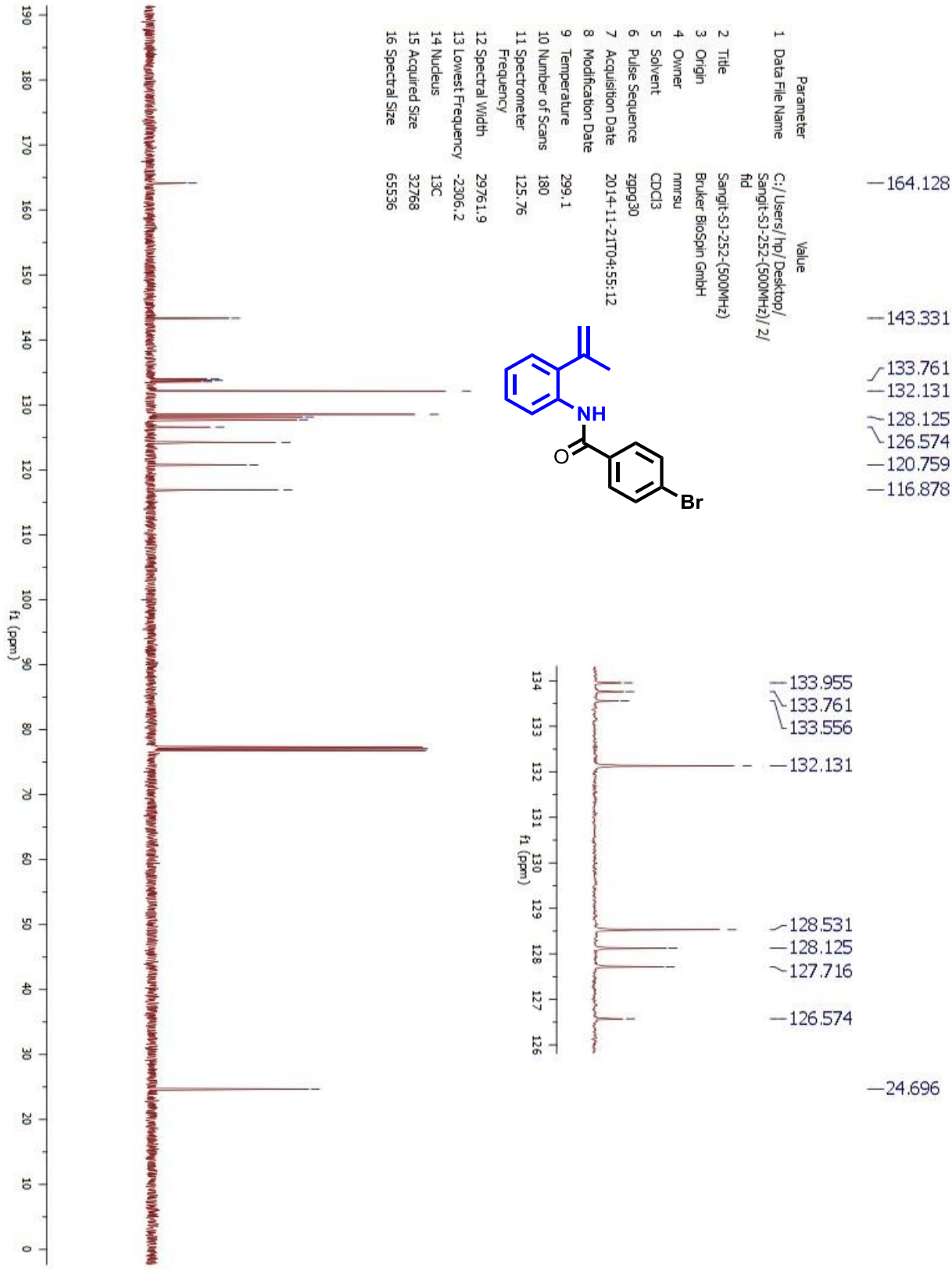
S37 ^{19}F NMR of **3g**



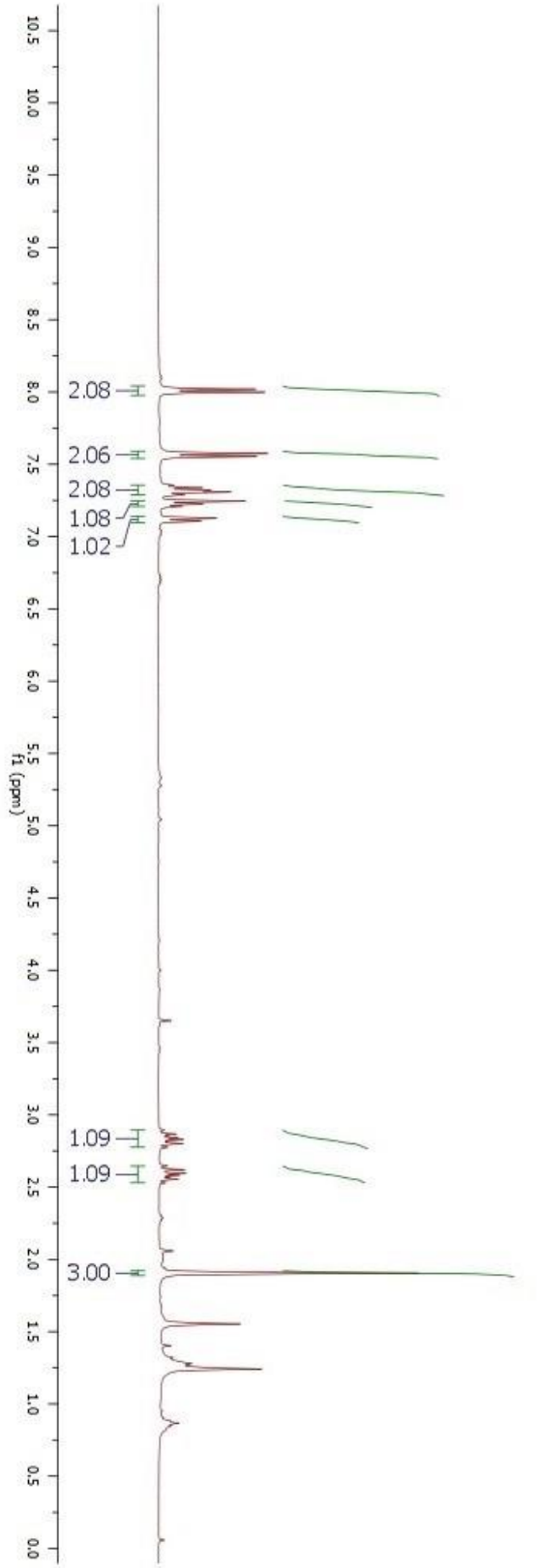
S38 ^{1}H NMR of **1h**



S39 ^{13}C NMR of **1h**



S40 ^{1}H NMR of **3h**



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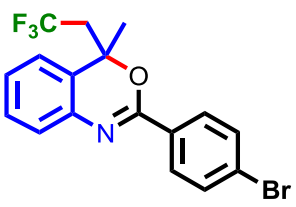
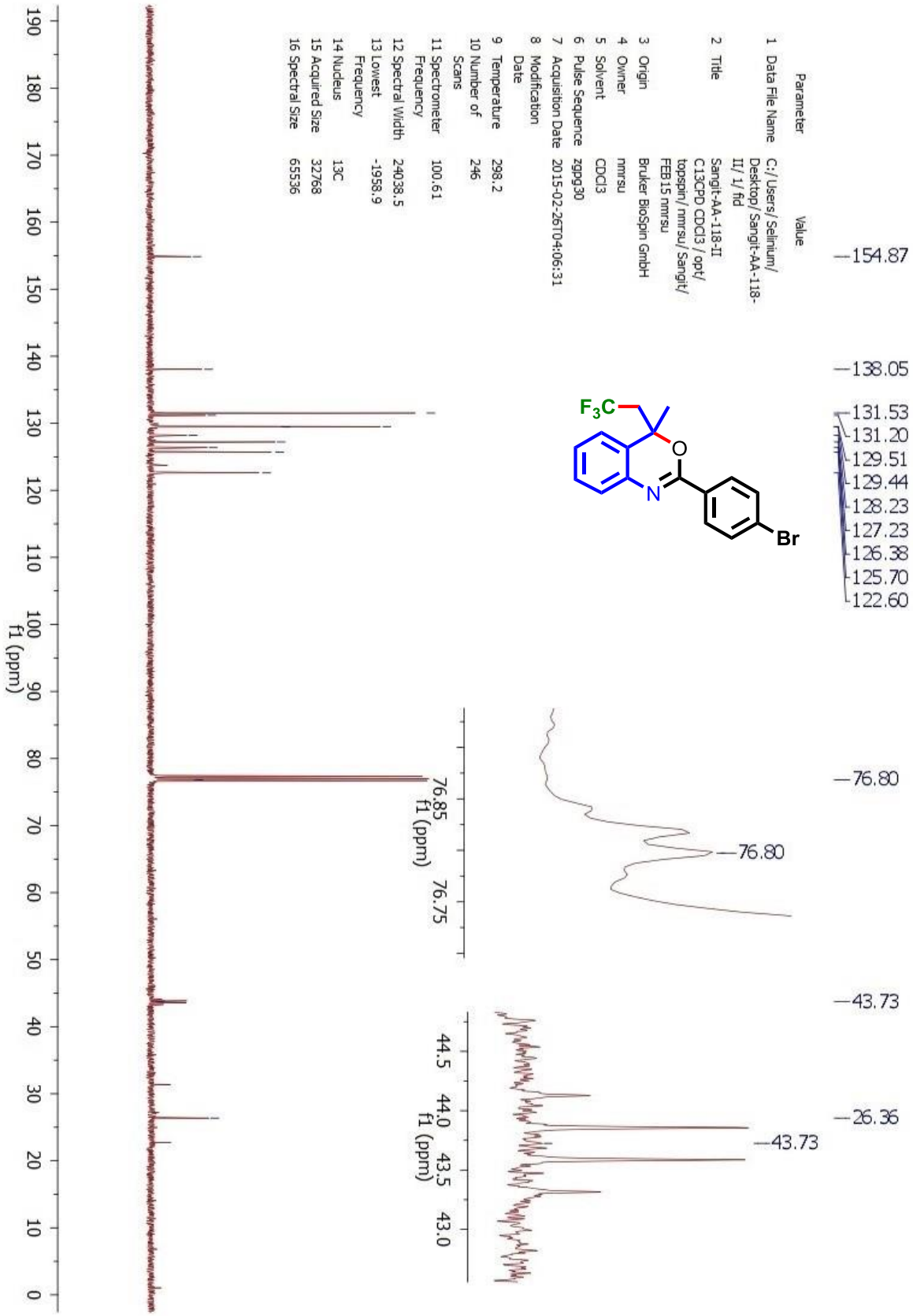
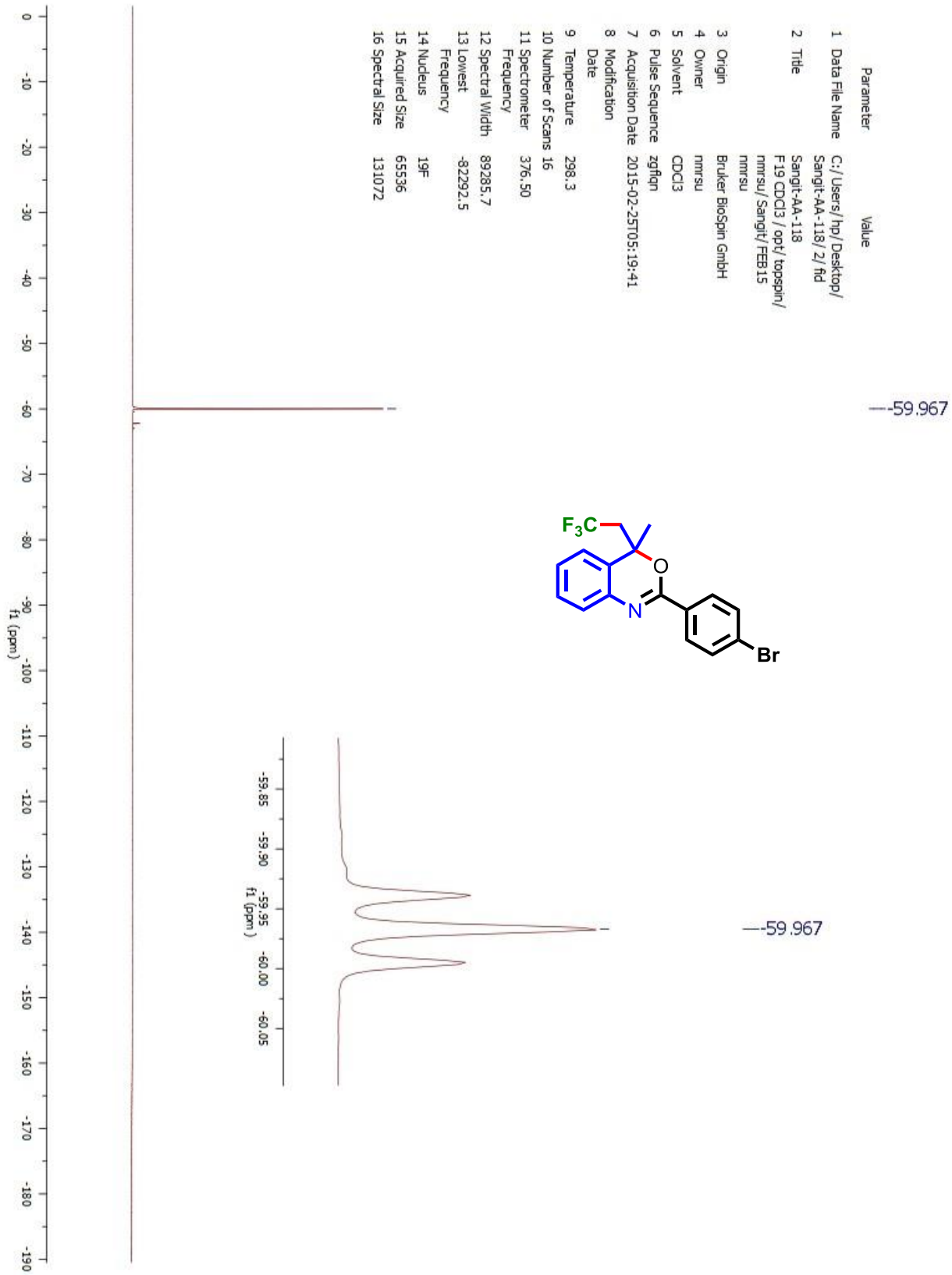
10	Number of Scans	16
11	Spectrometer Frequency	400.13
12	Spectral Width	8196.7
13	Lowest Frequency	-1713.7
14	Nucleus	1H
15	Acquired Size	32768
16	Spectral Size	65536



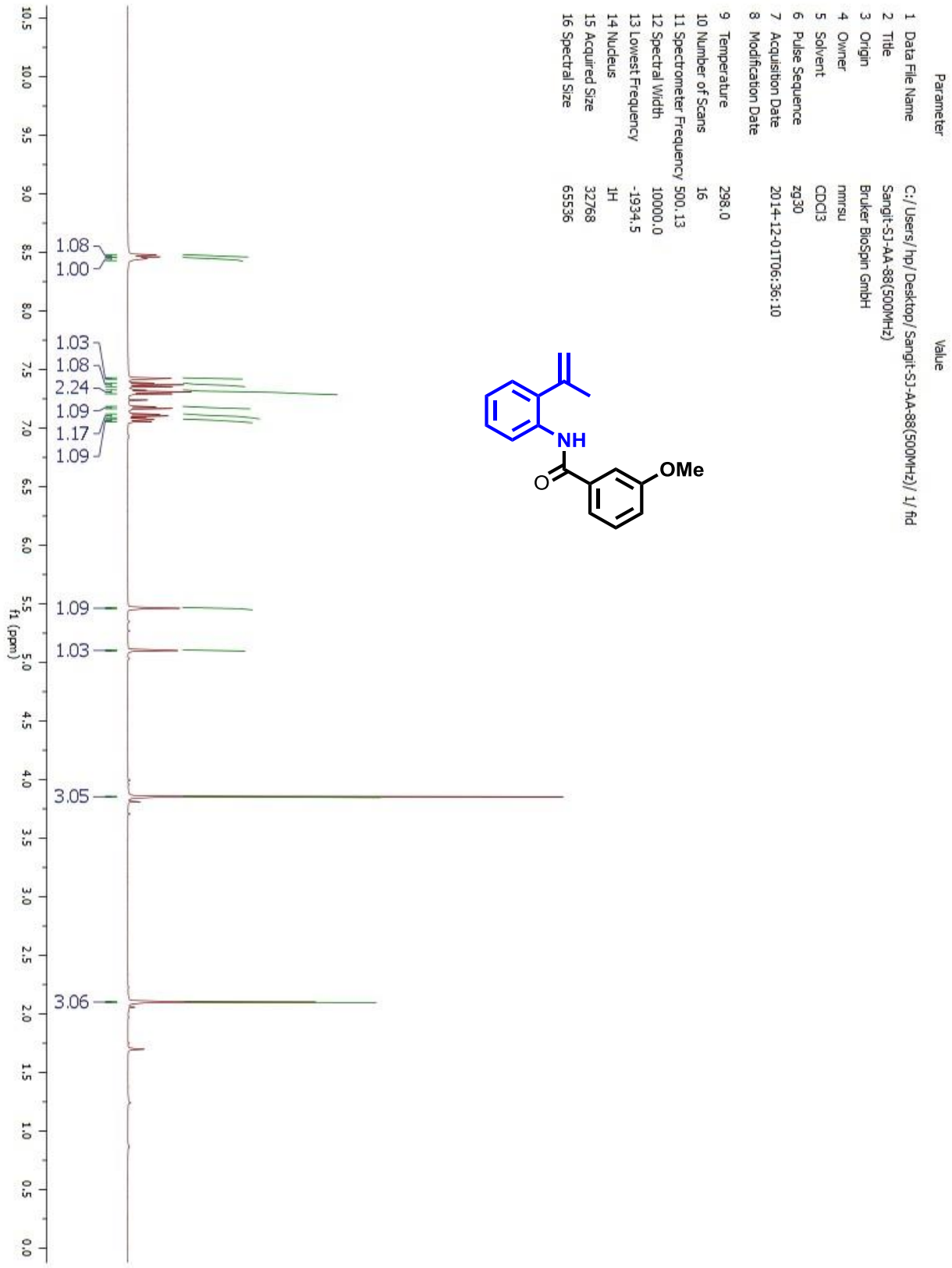
S41 ^{13}C NMR of **3h**



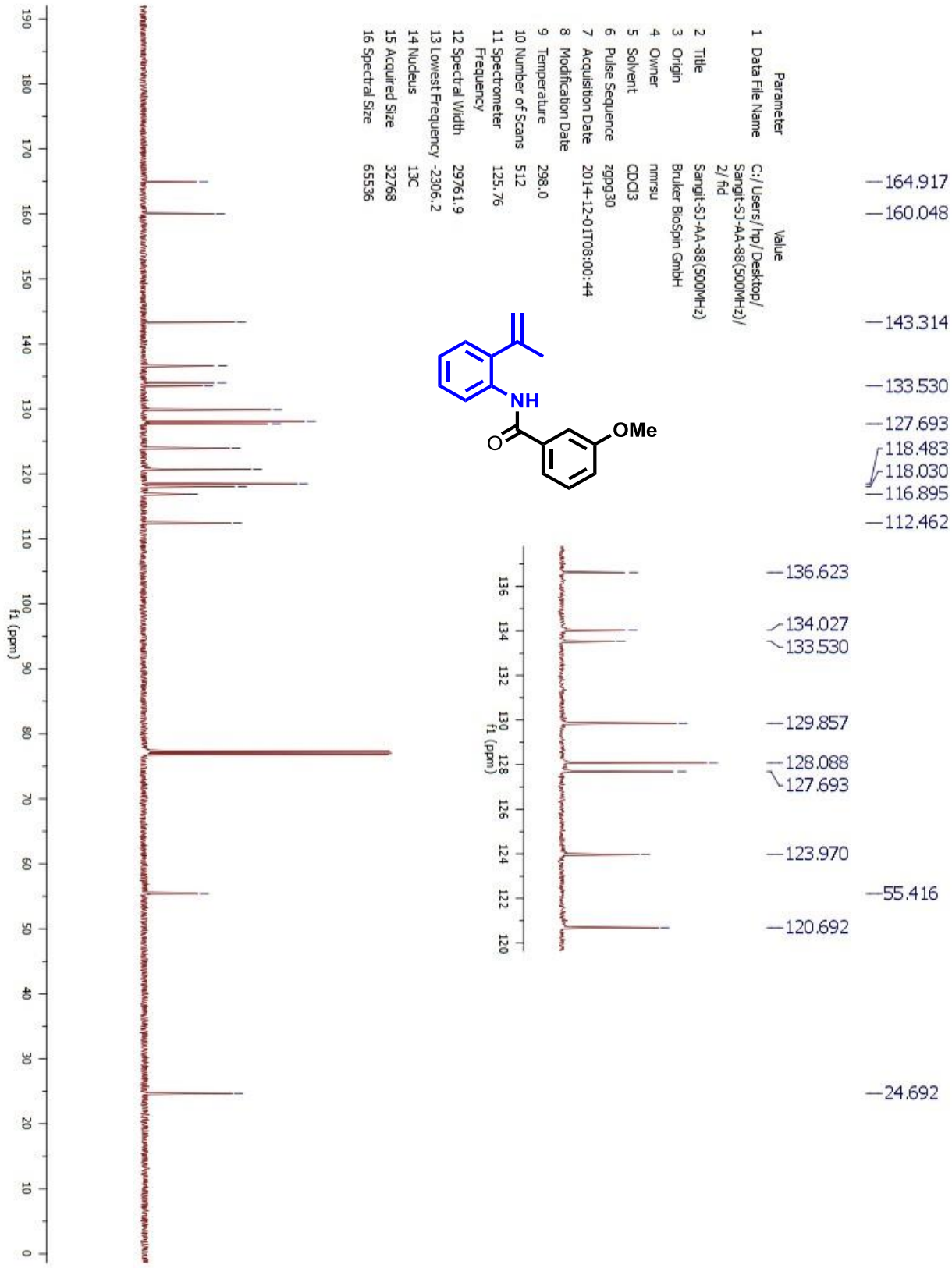
S42 ^{19}F NMR of **3h**



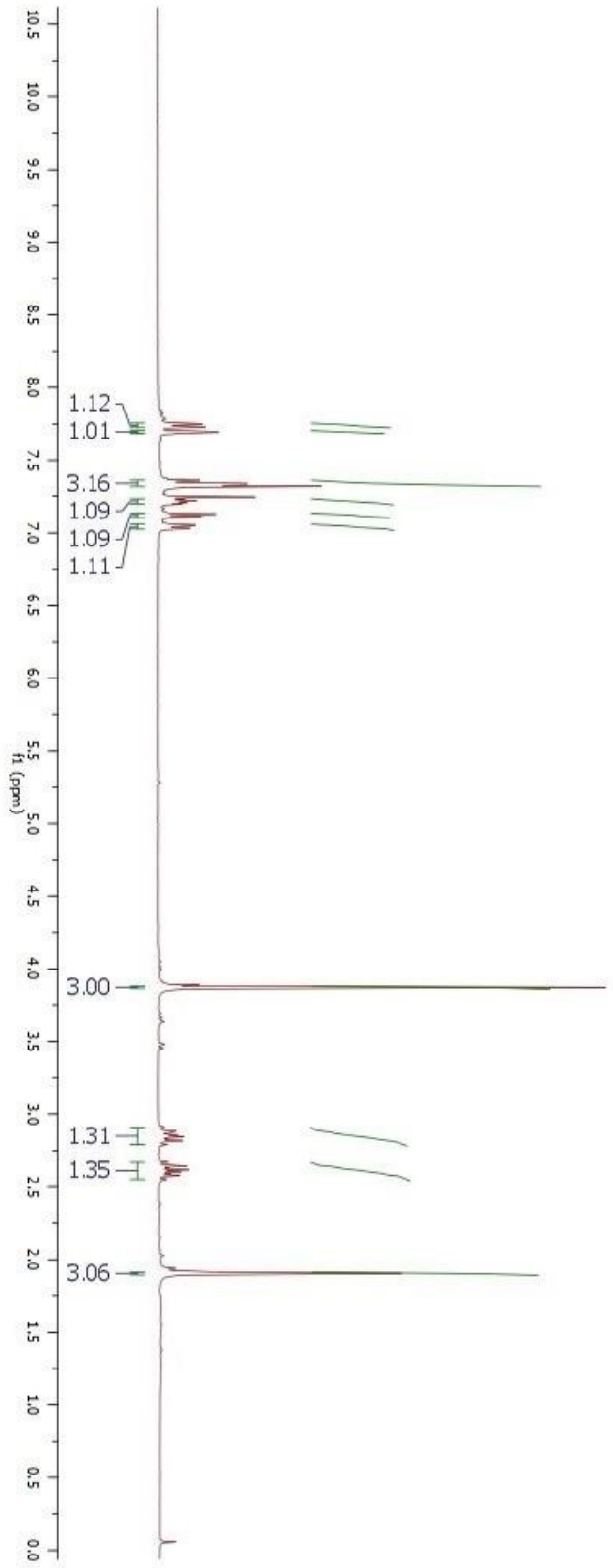
S43 ^{1}H NMR of **1i**



S44 ^{13}C NMR of **1i**



S45 ^{1}H NMR of **3i**



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8 Modification Date	
9 Temperature	298.3
10 Number of Scans	16
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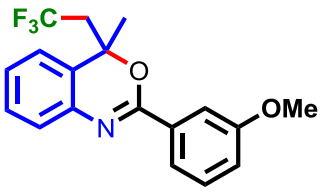
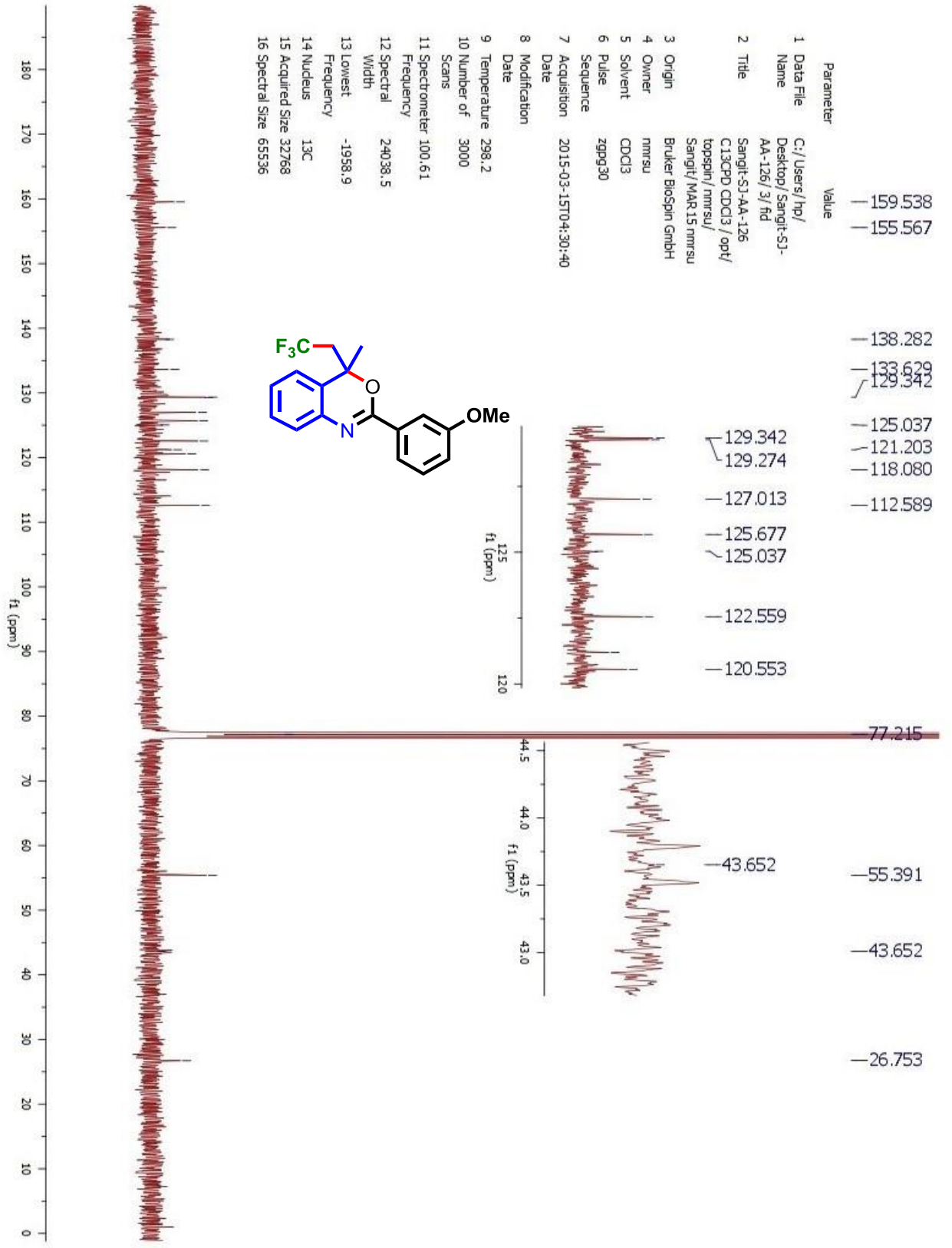
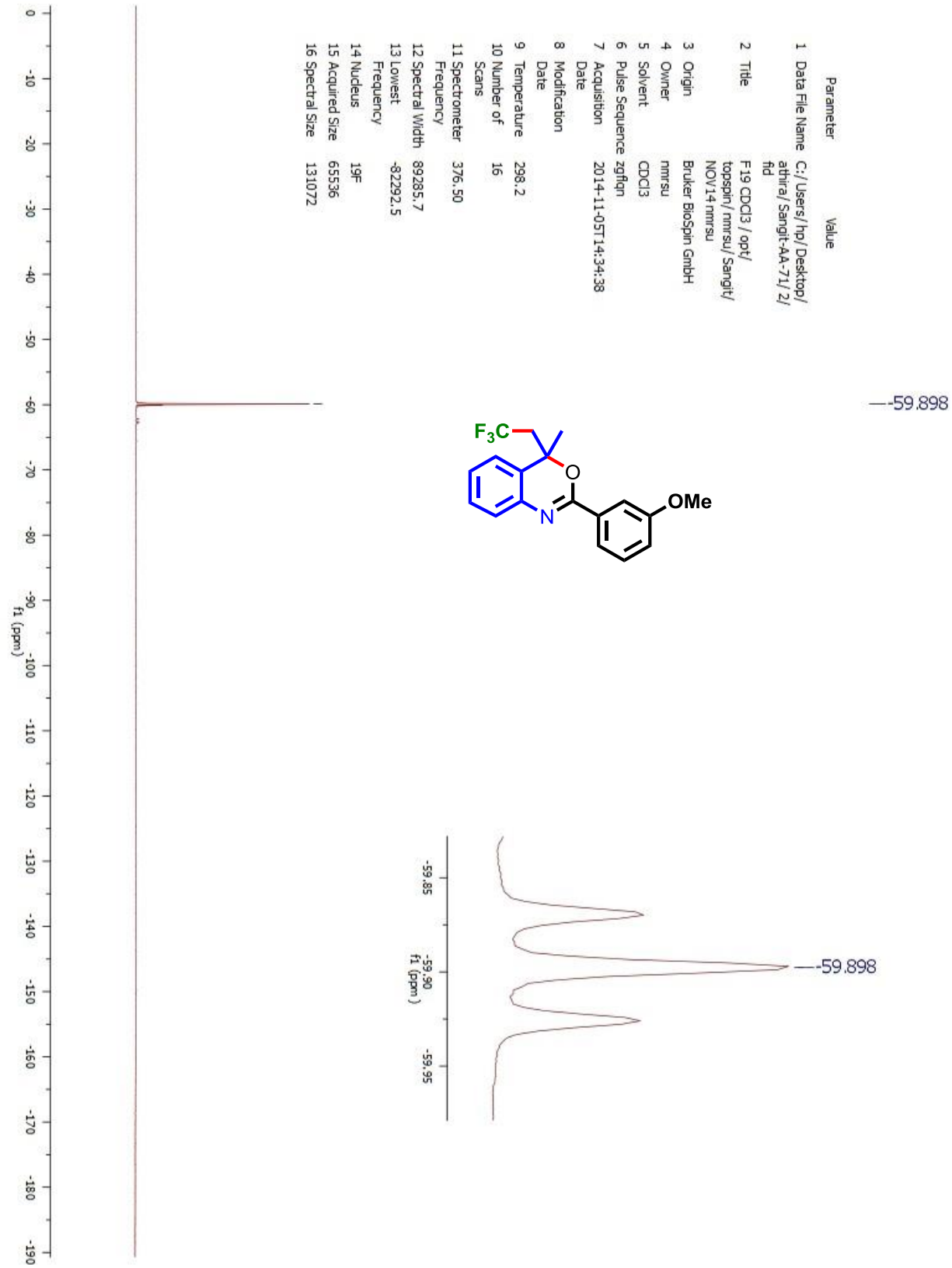
12 Spectral Width	8196.7
13 Lowest Frequency	-1713.7
14 Nucleus	1H
15 Acquired Size	32768
16 Spectral Size	65536



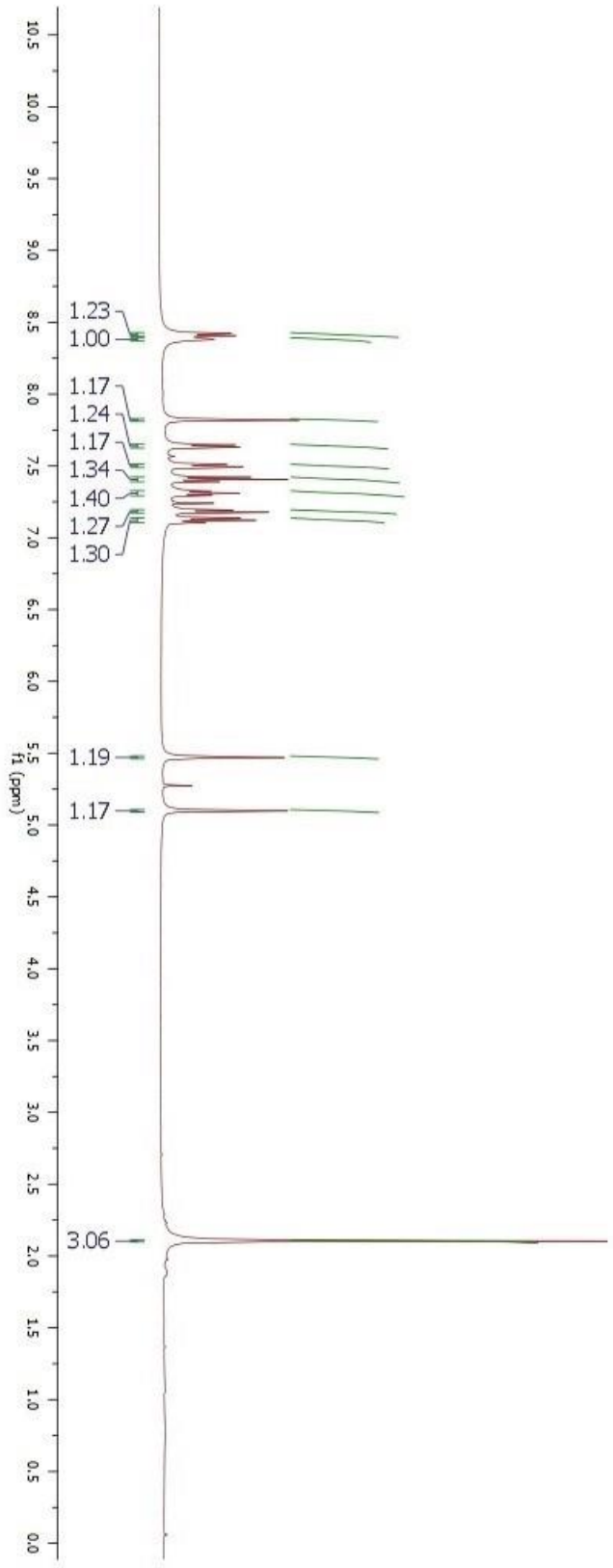
S46 ^{13}C NMR of **3i**



S47 ^{19}F NMR of **3i**



S48 ^{1}H NMR of **1j**



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6	Pulse Sequence	zg30
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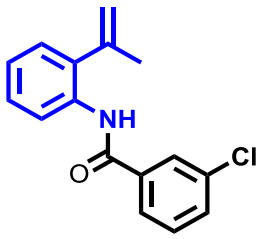
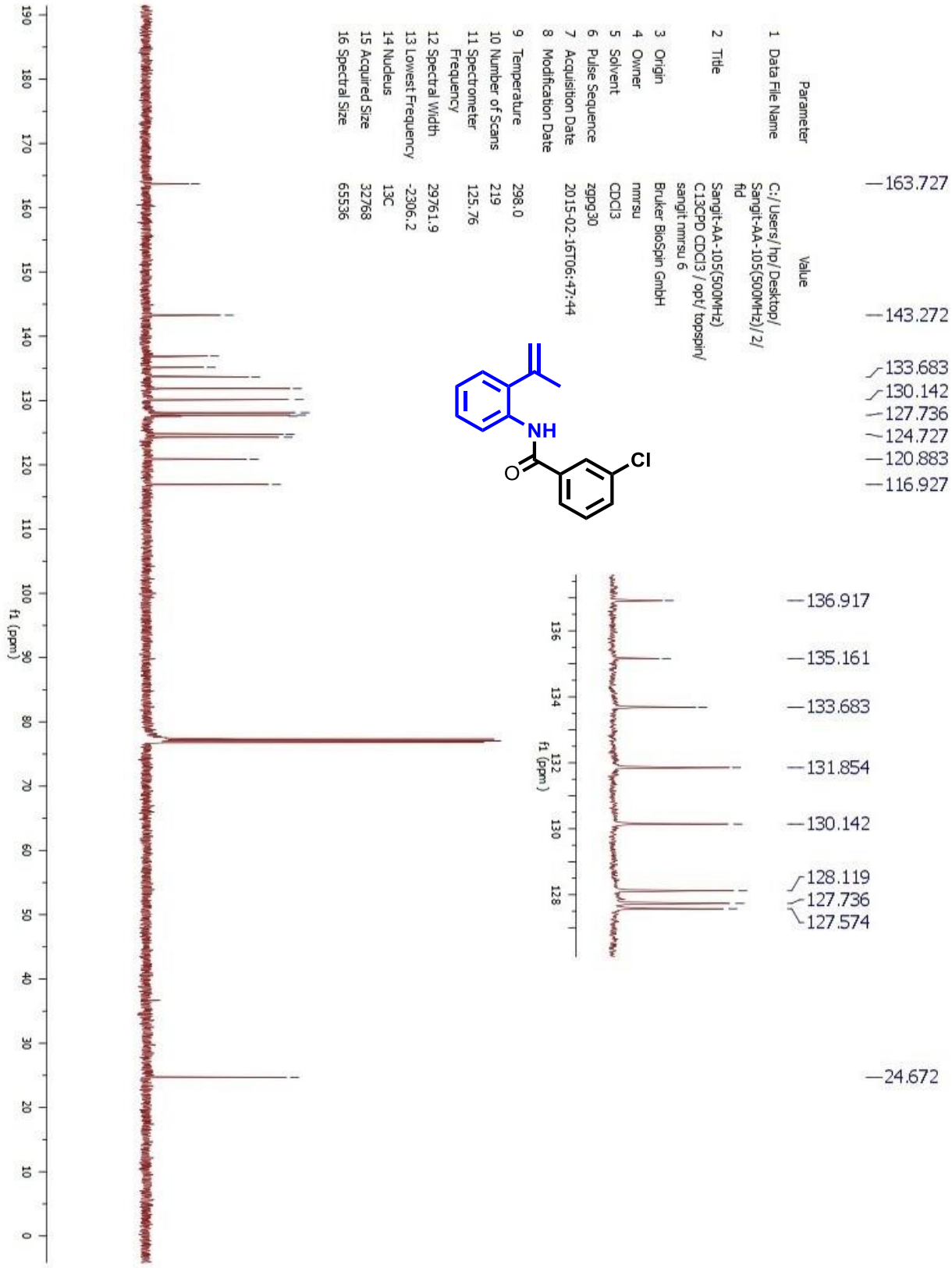
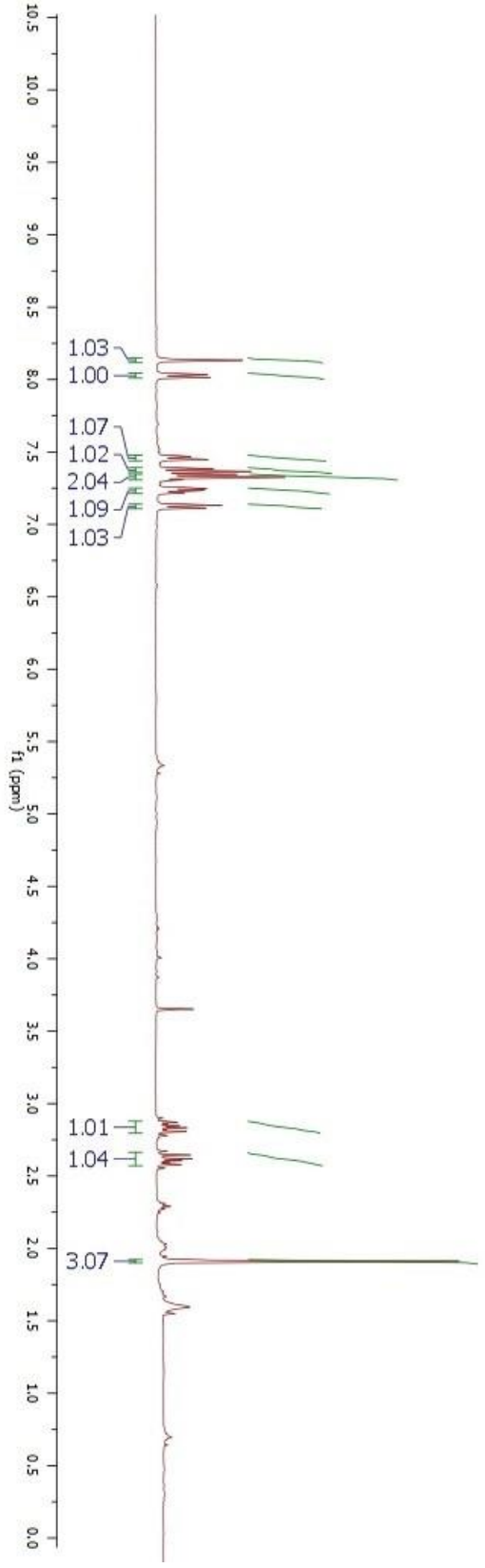
14	Nucleus	1H
15	Acquired Size	32768
16	Spectral Size	65536



S49 ^{13}C NMR of **1j**



S50 ^{1}H NMR of **3j**



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3 Origin	Bruker BioSpin GmbH
4 Owner	nmrsu
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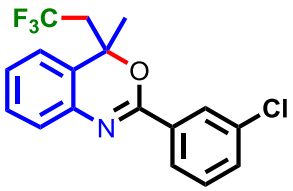
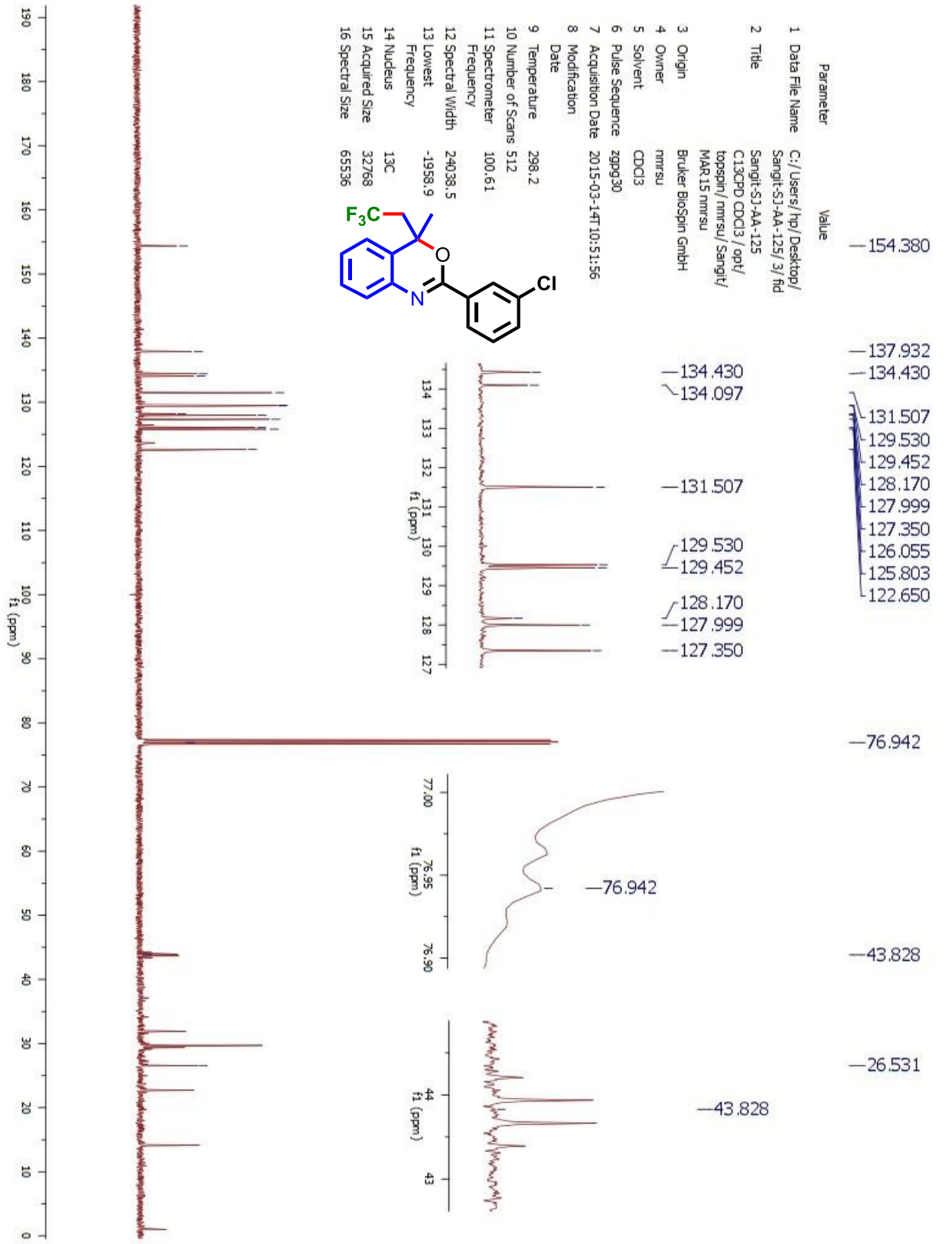
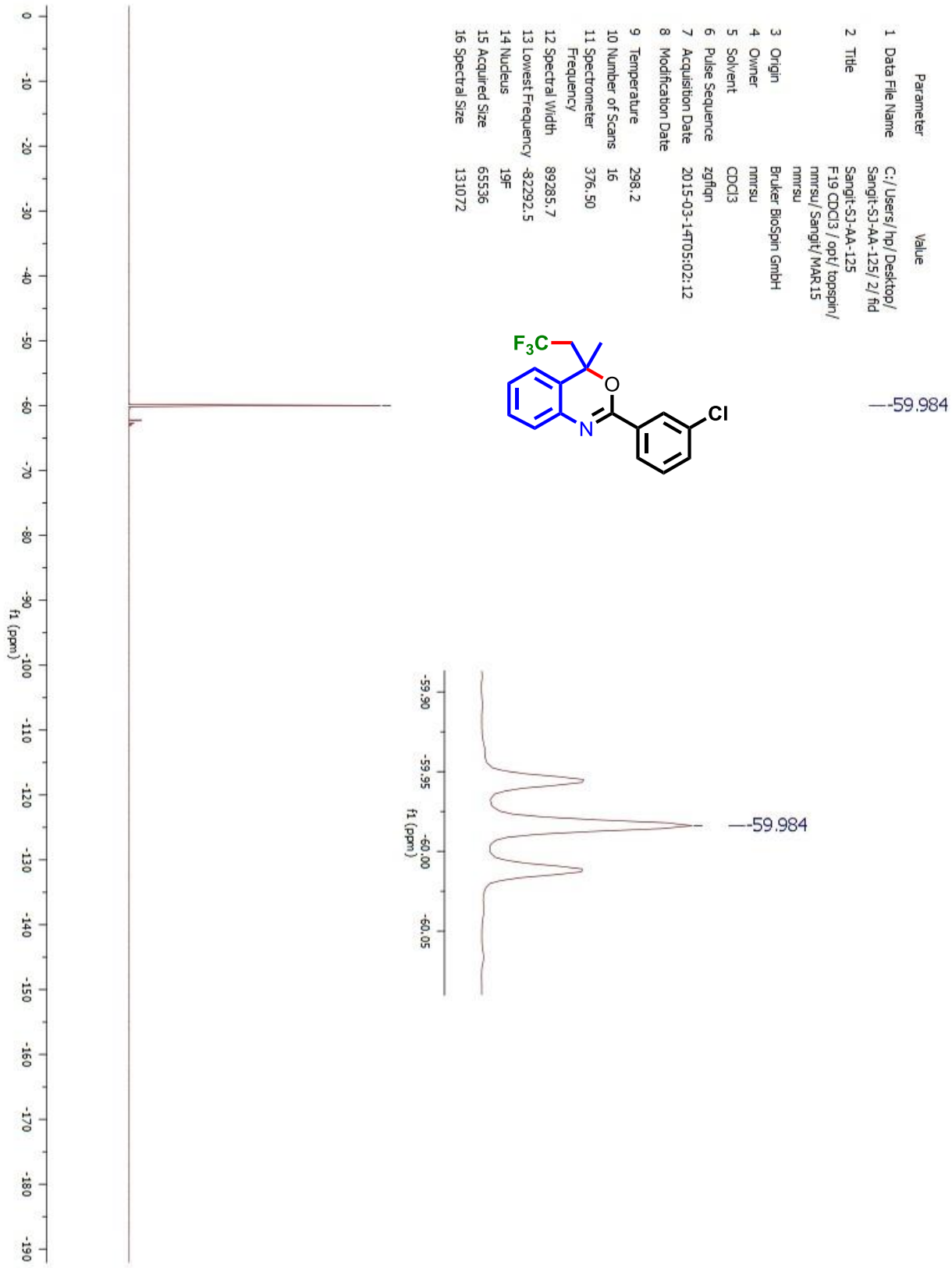
6 Pulse Sequence	zg30
7 Acquisition Date	2015-03-14T04:59:21
8 Modification Date	
9 Temperature	298.2
10 Number of Scans	16
11 Spectrometer Frequency	400.13
12 Spectral Width	8196.7
13 Lowest Frequency	-1713.7
14 Nucleus	1H
15 Acquired Size	32768
16 Spectral Size	65536



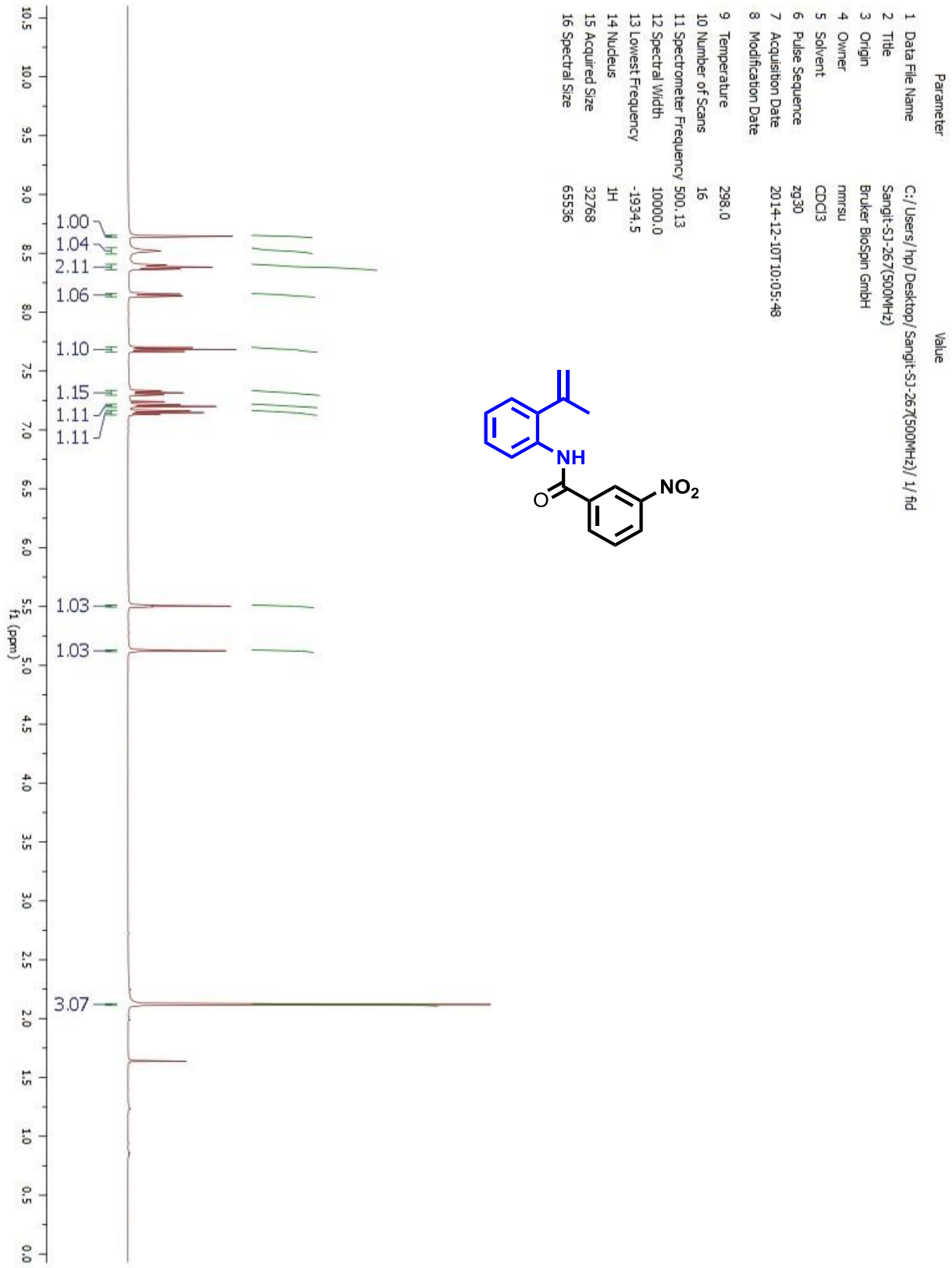
S51 ^{13}C NMR of **3j**



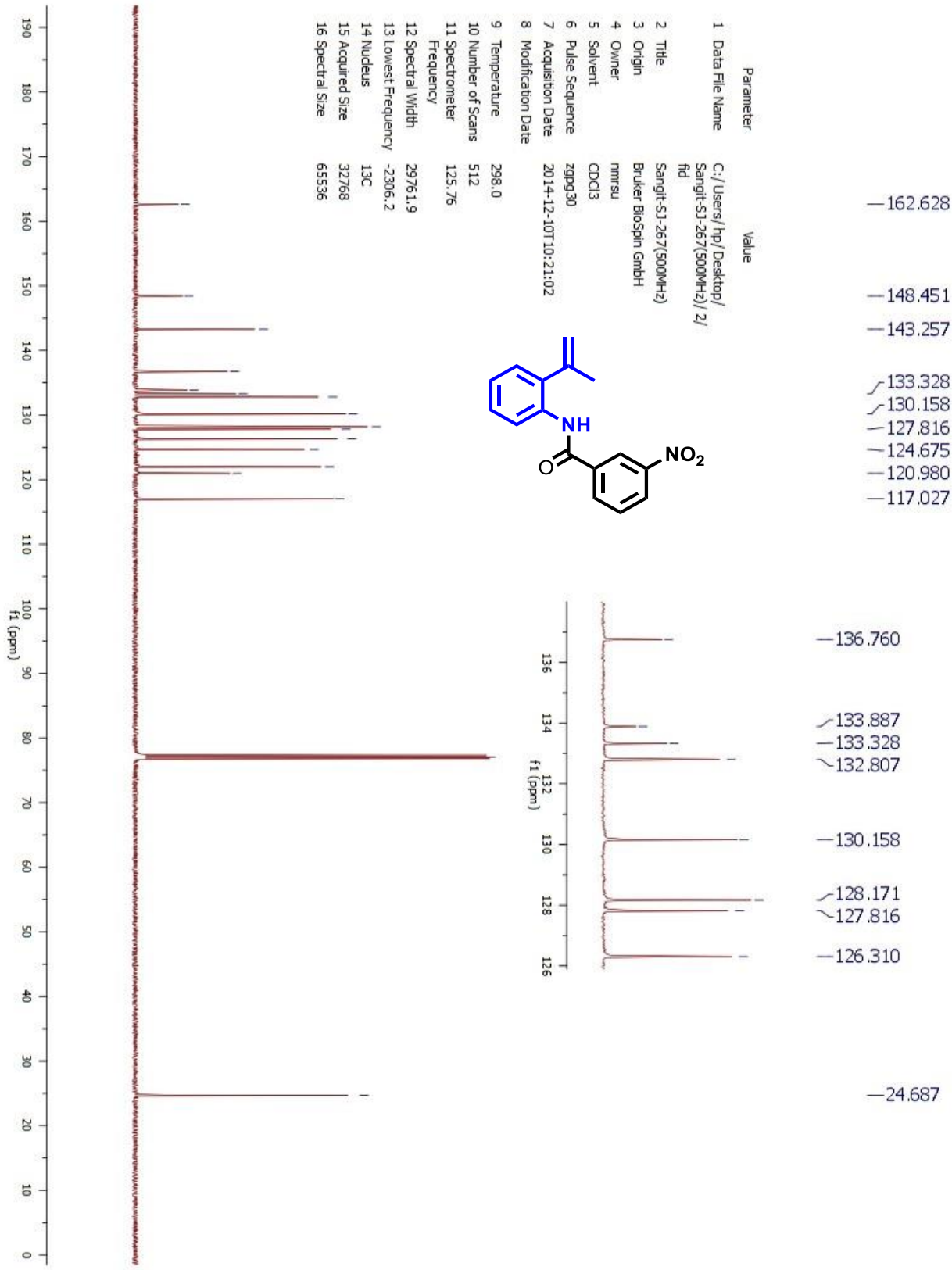
S52 ^{19}F NMR of **3j**



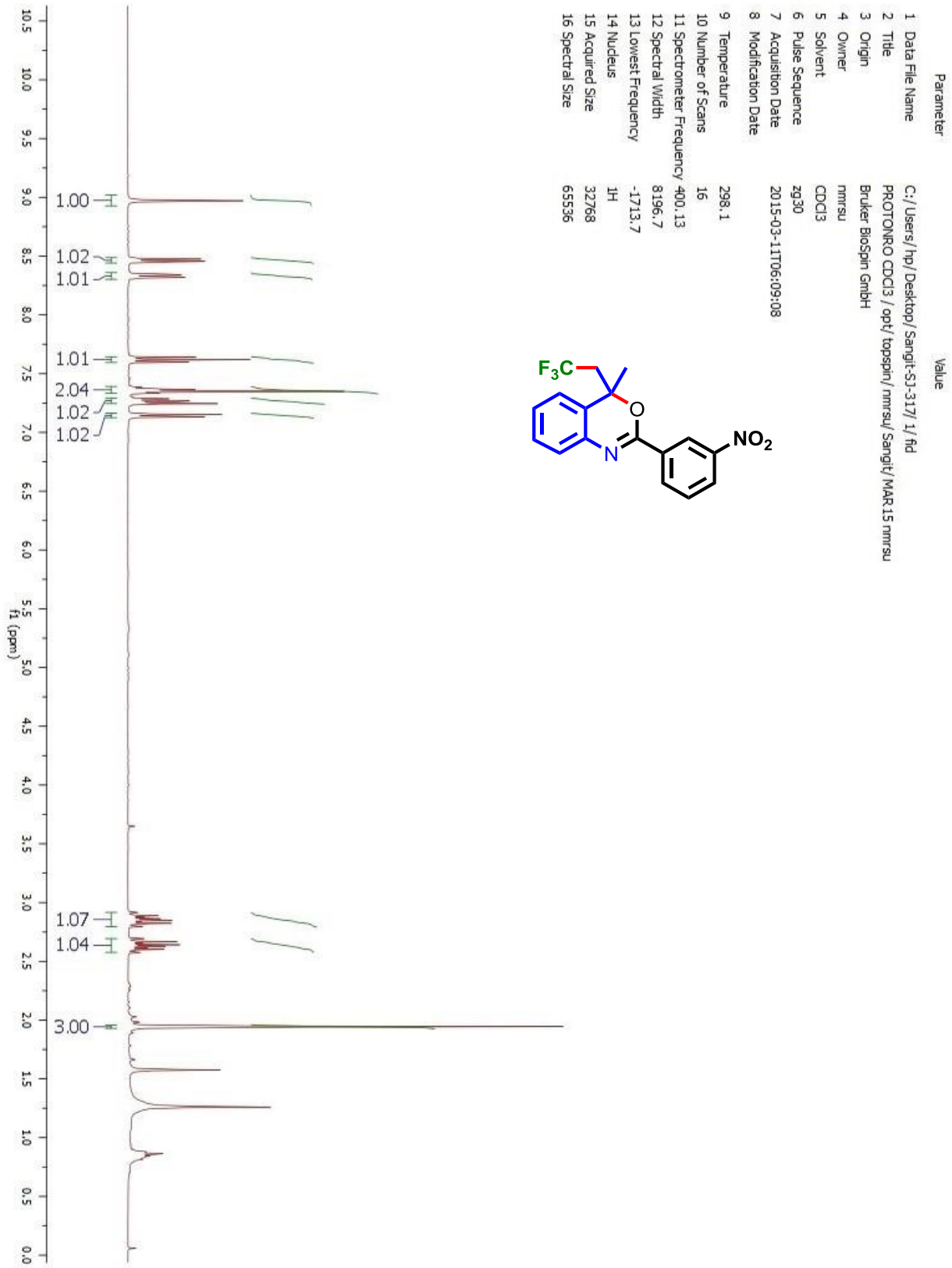
S53 ^{1}H NMR of **1k**



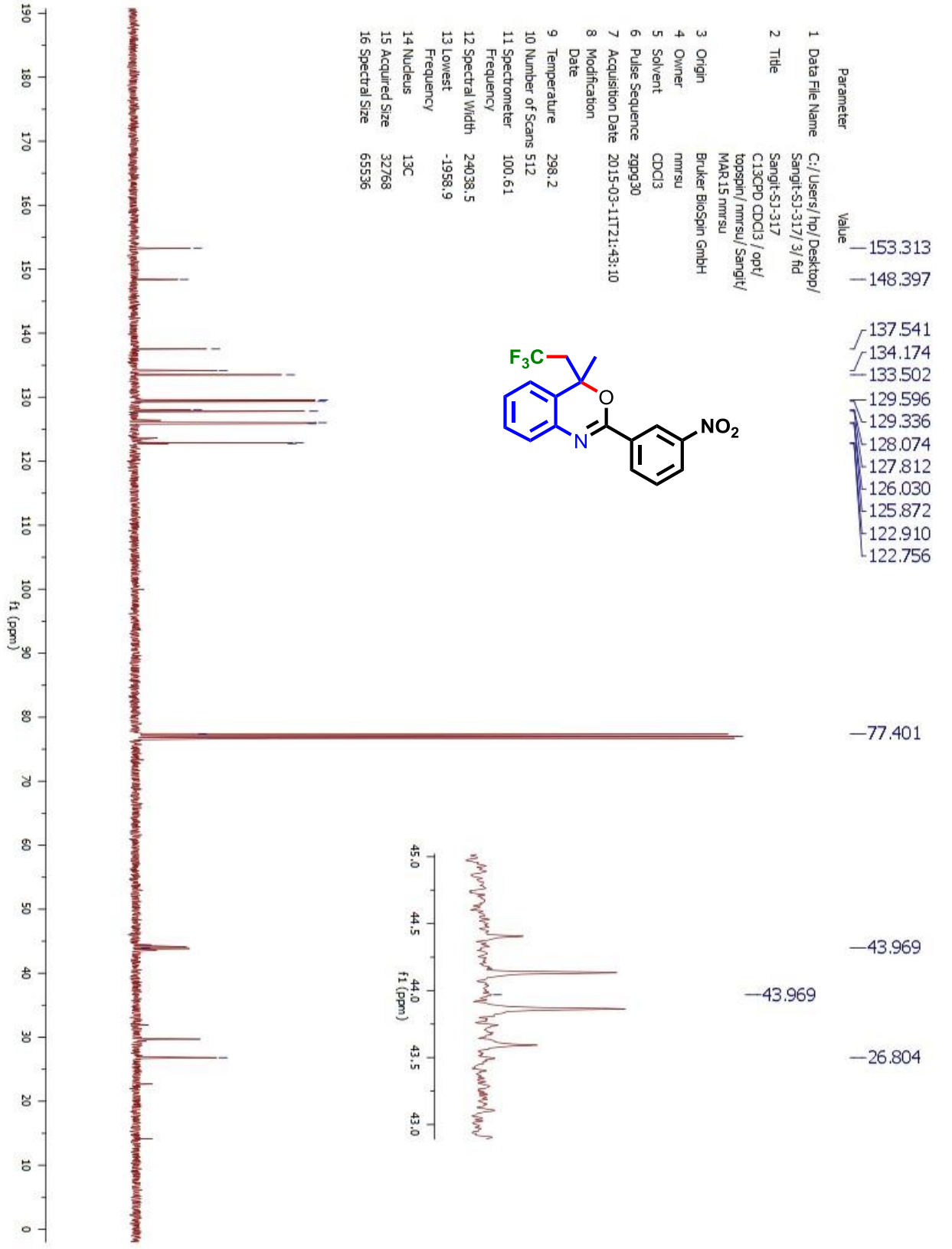
S54 ^{13}C NMR of **1k**



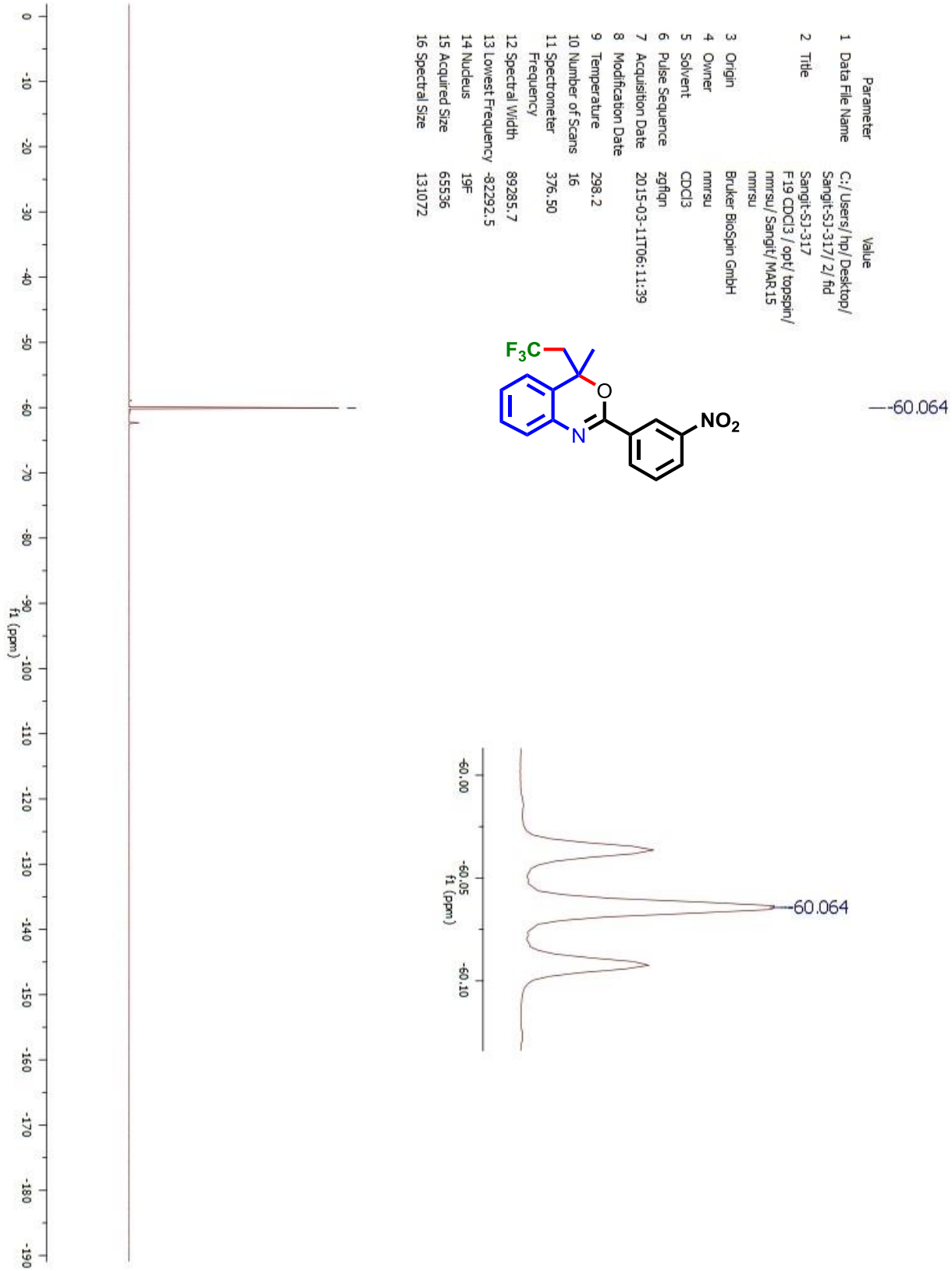
S55 ^{1}H NMR of **3k**



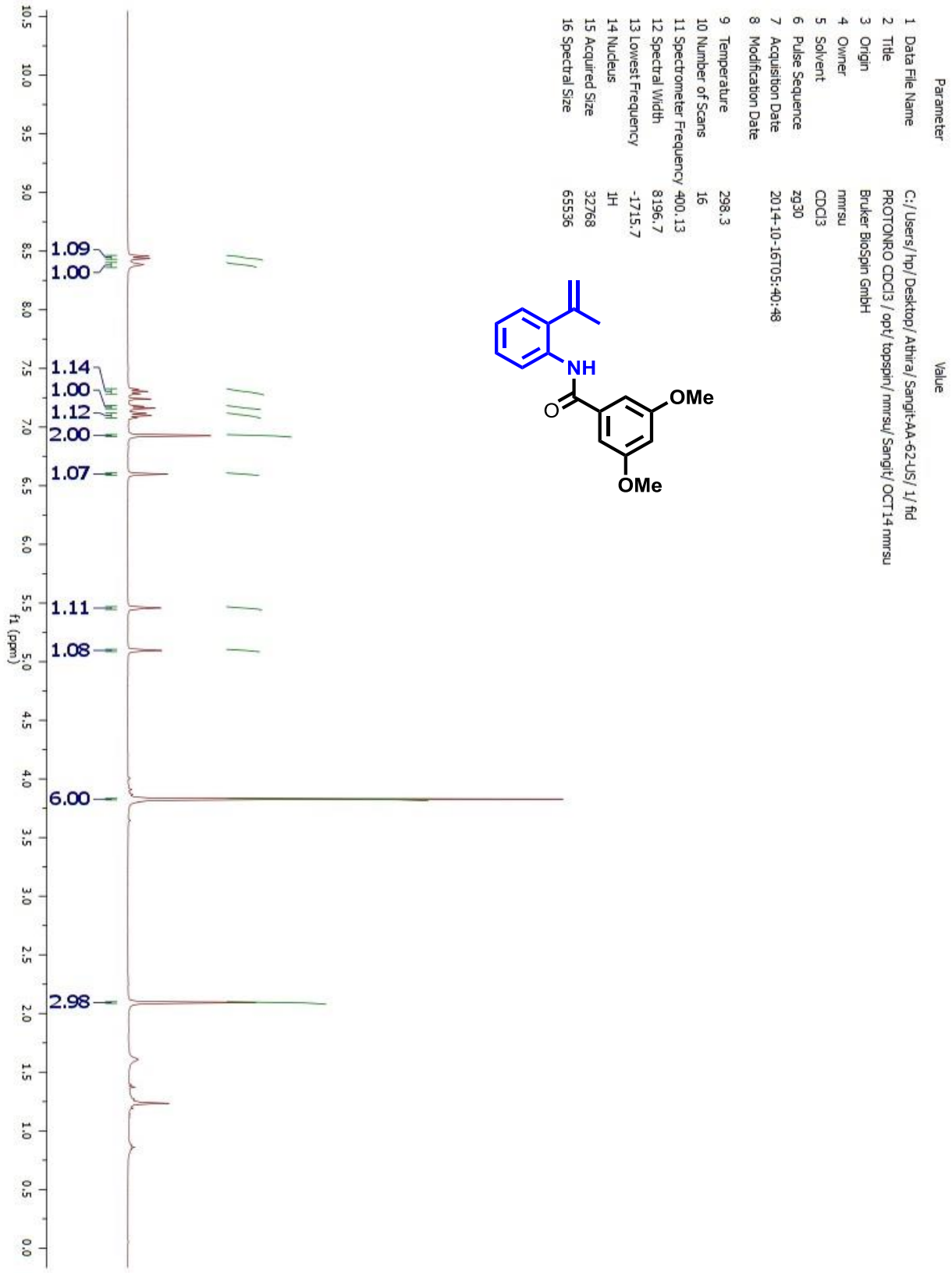
S56 ^{13}C NMR of **3k**



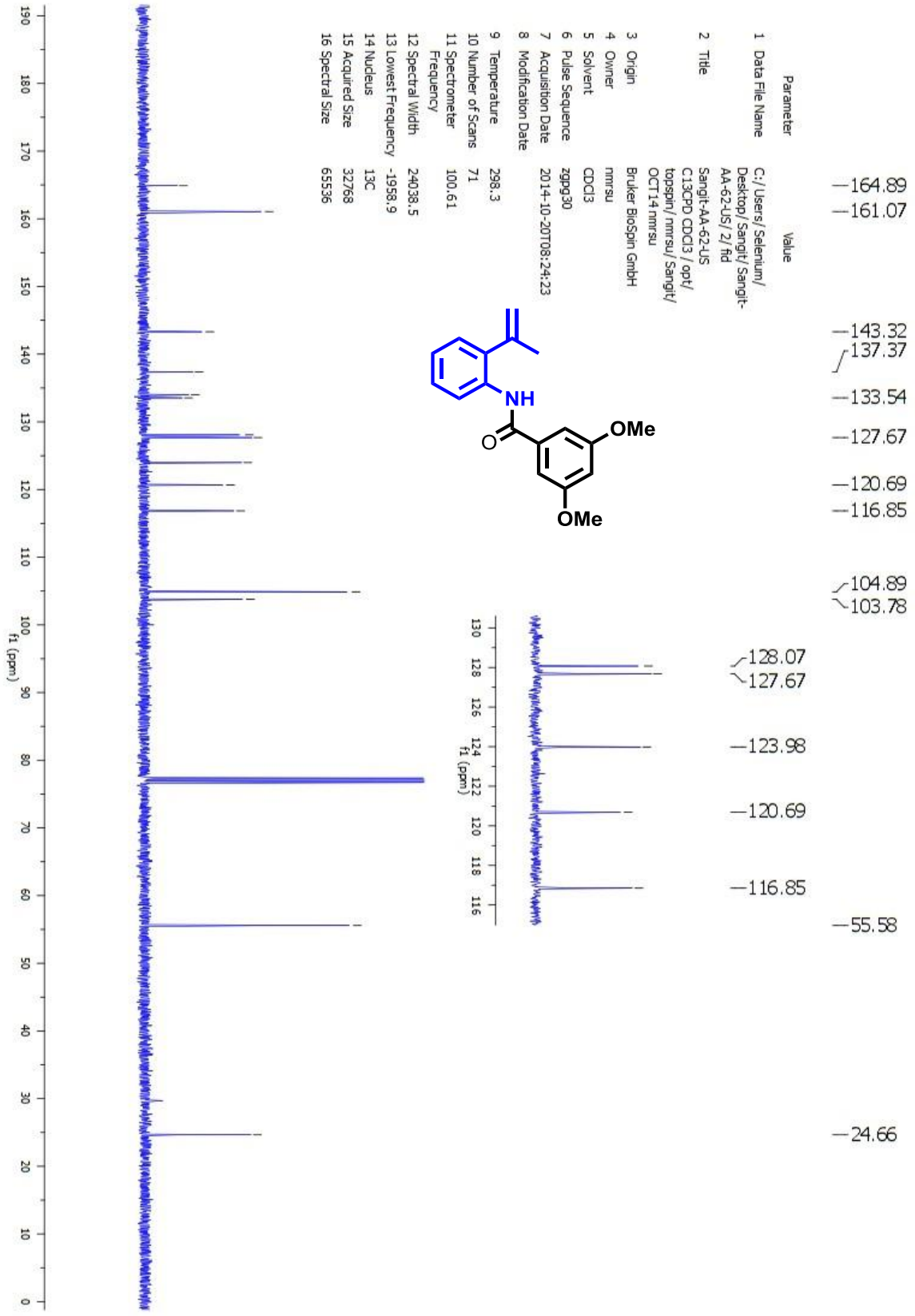
S57 ^{19}F NMR of **3k**



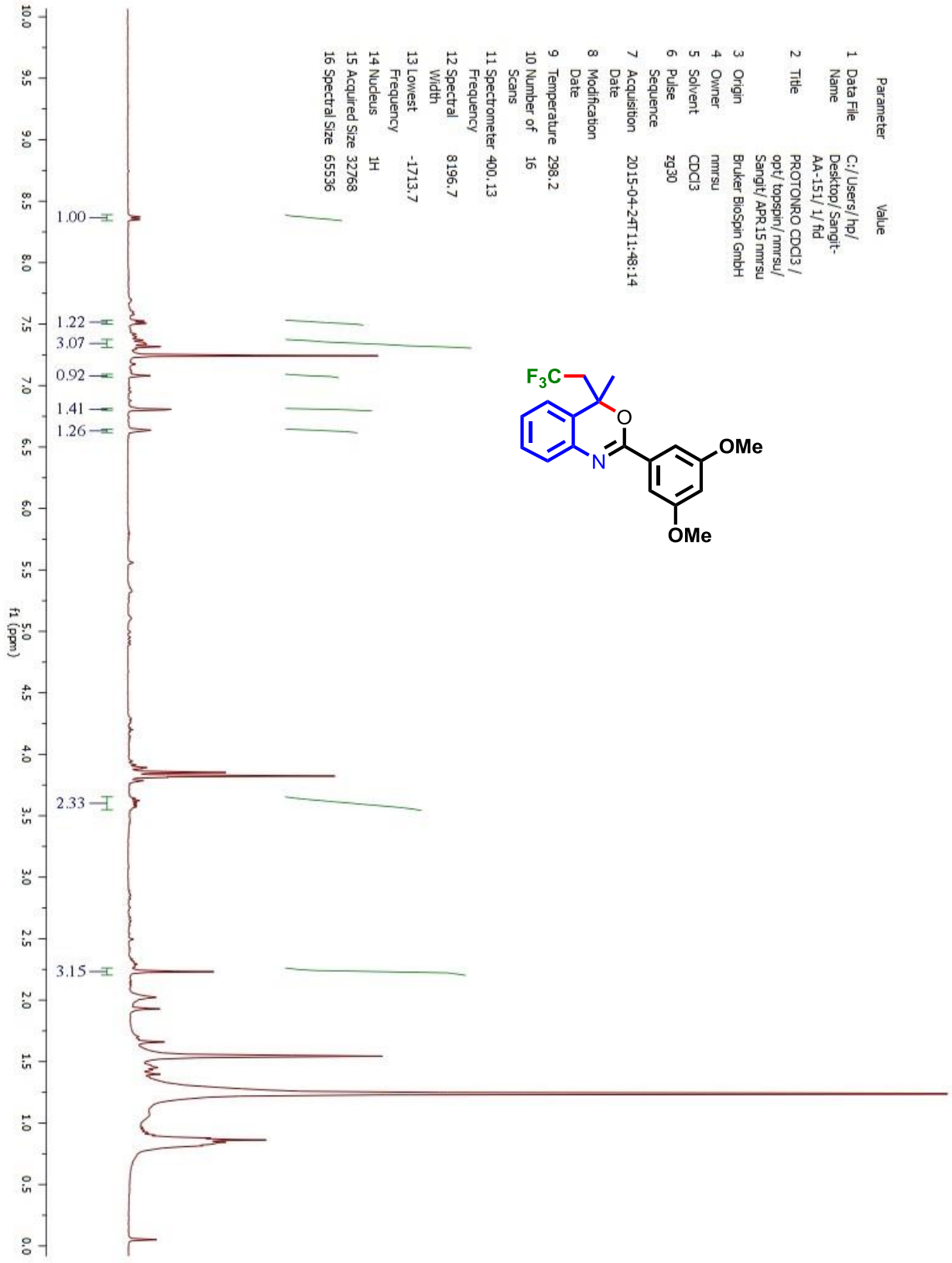
S58 ^{1}H NMR of **1l**



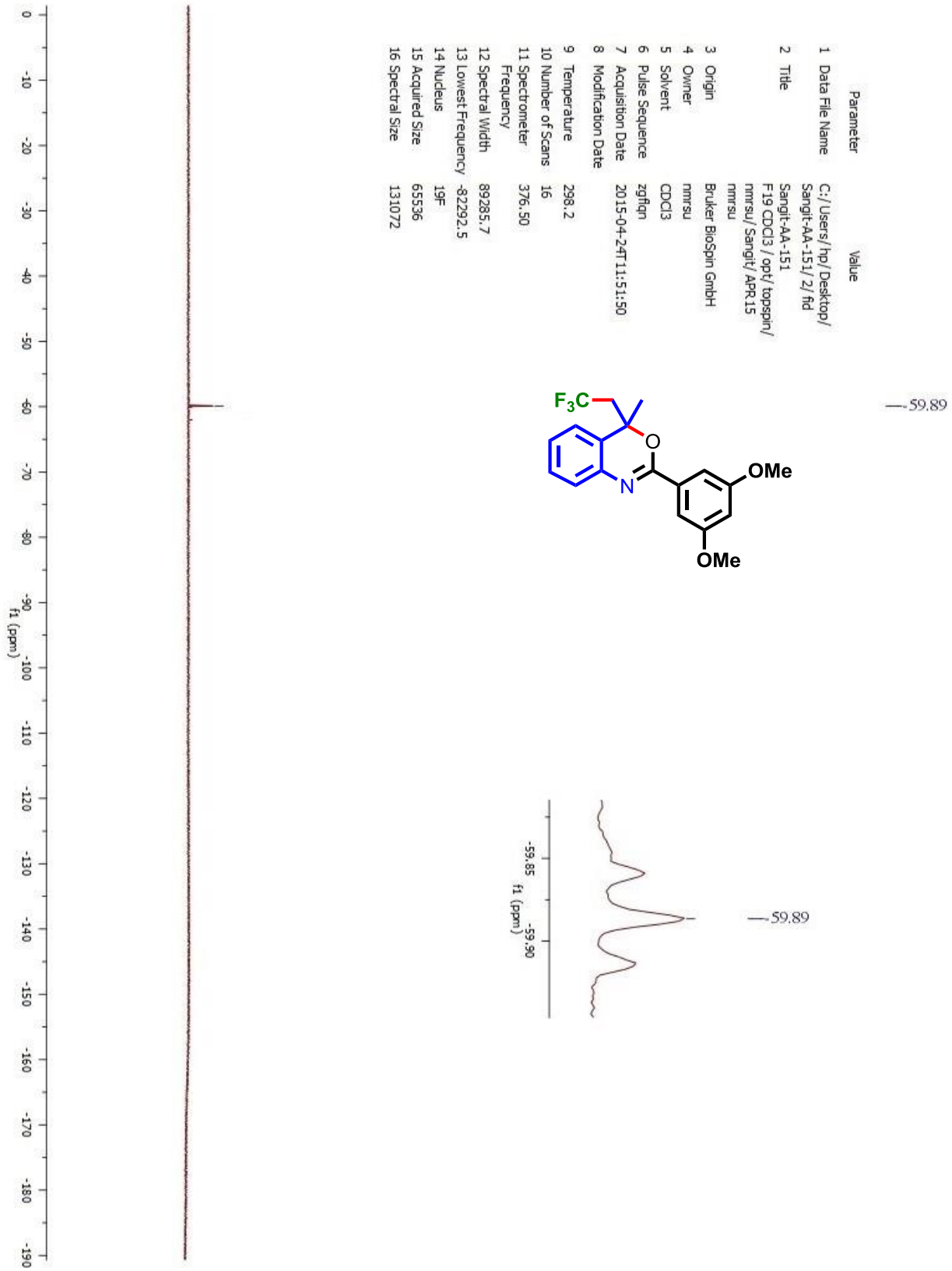
S59 ^{13}C NMR of **1l**



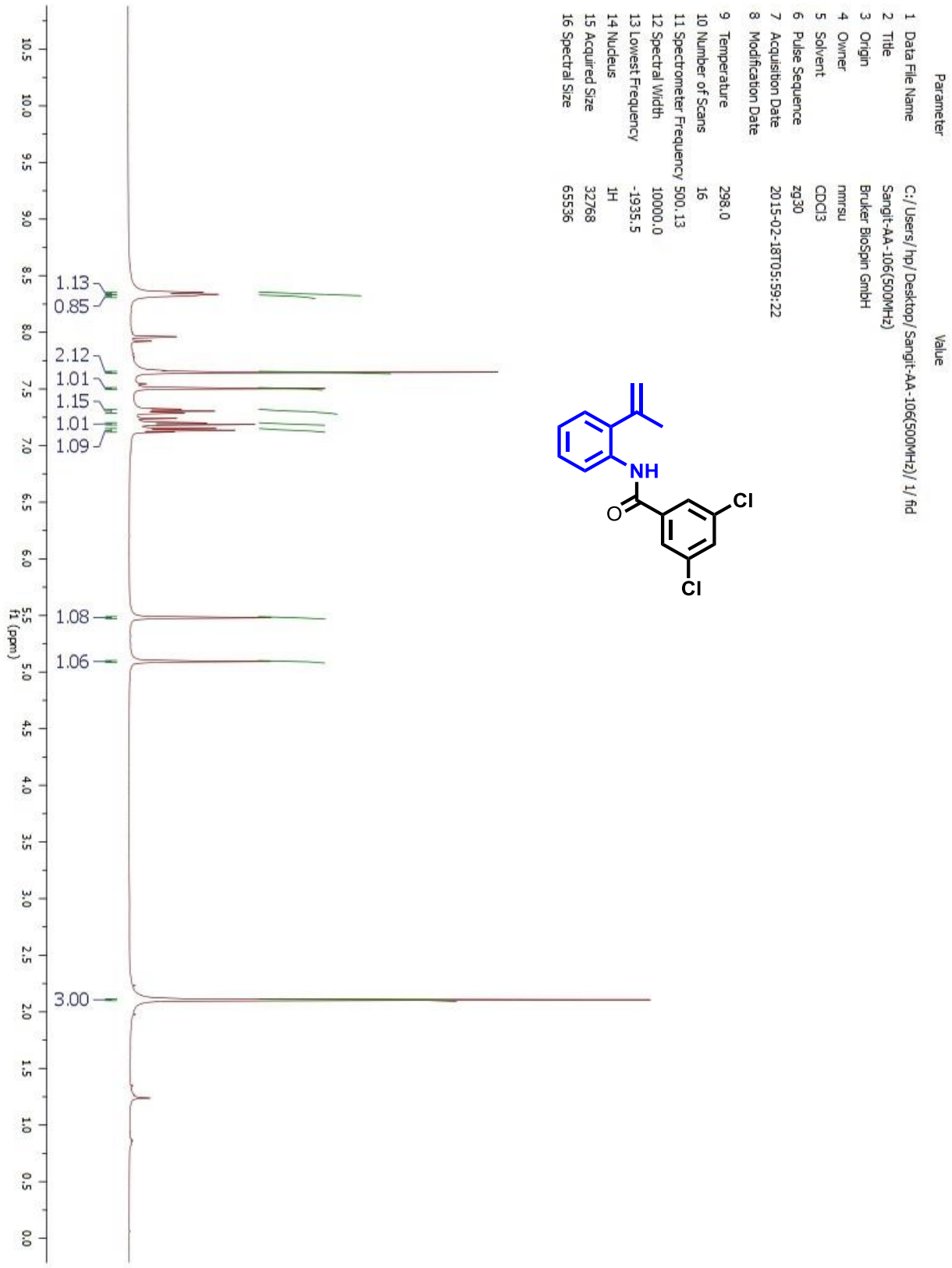
S60 ^{1}H NMR of **3l**



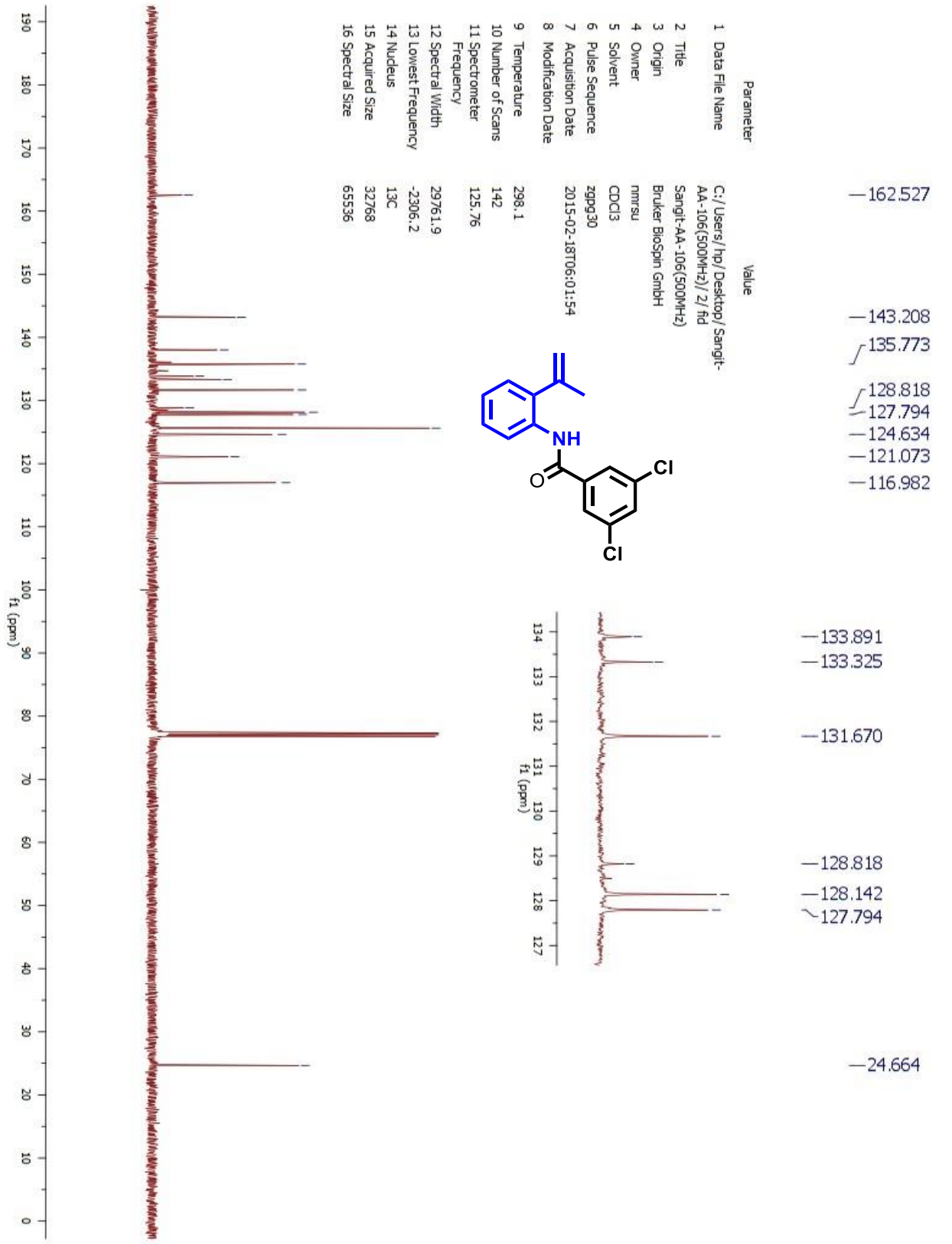
S61 ^{19}F NMR of **3l**



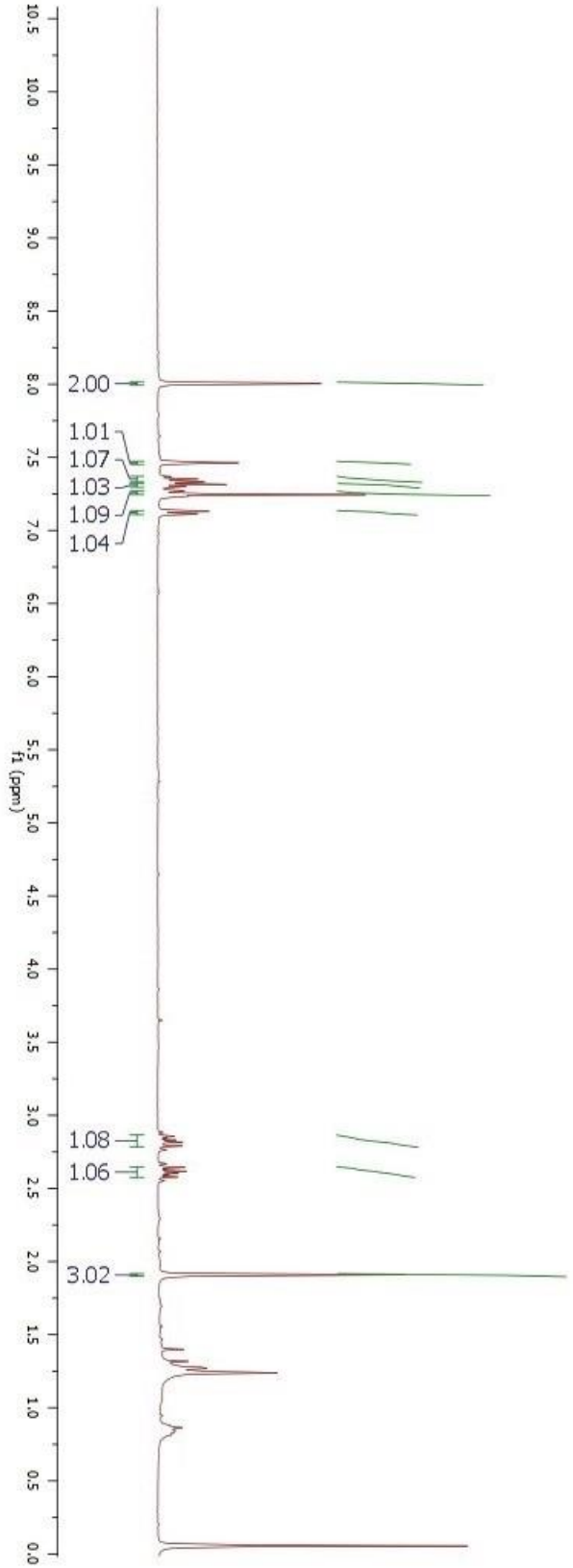
S62 ^{1}H NMR of **1m**



S63 ^{1}H NMR of **1m**



S64 ^{1}H NMR of **3m**



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4 Owner	nmrsu
5 Solvent	CDCl3
6 Pulse Sequence	zg30
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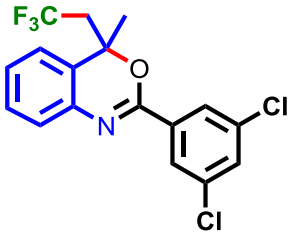
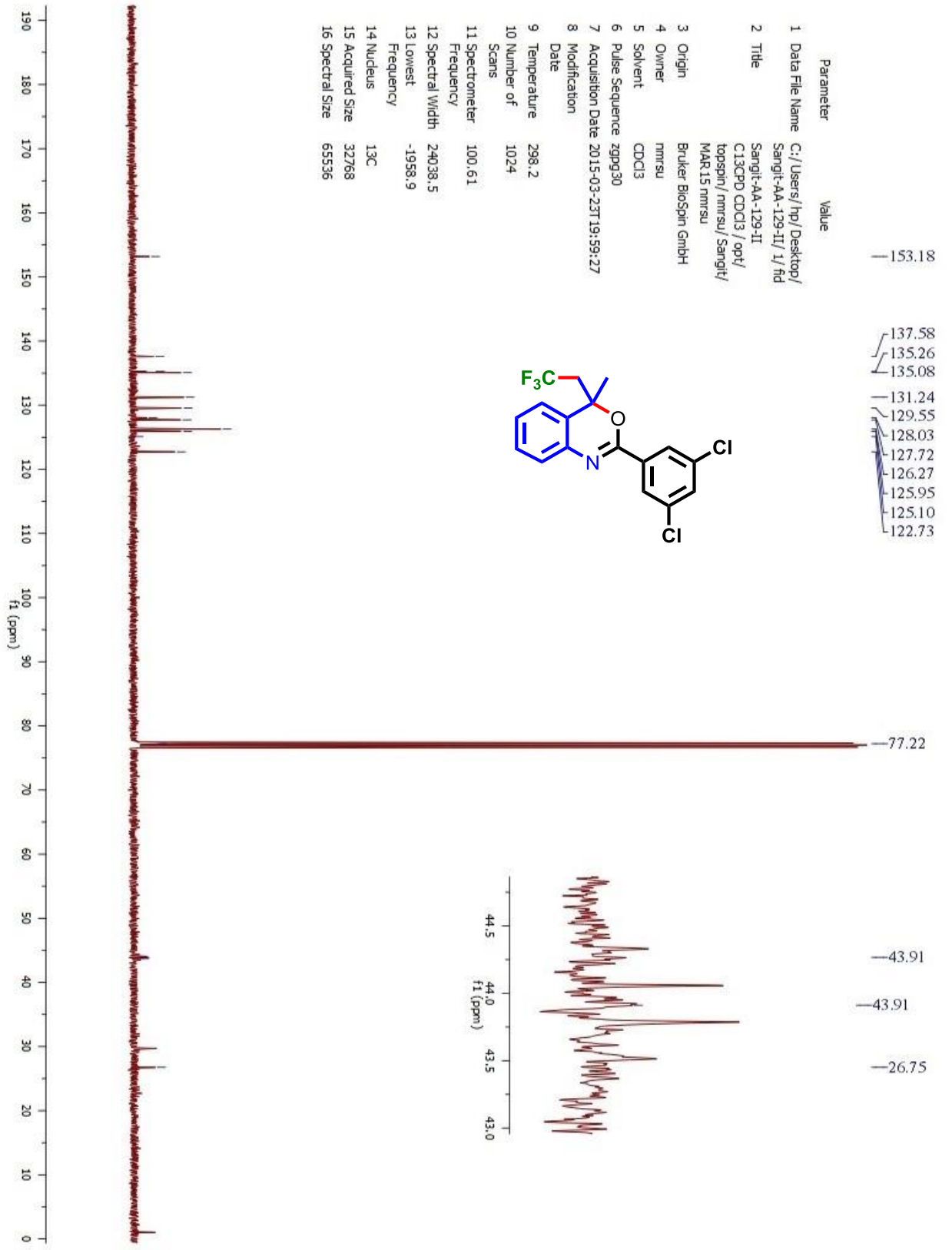
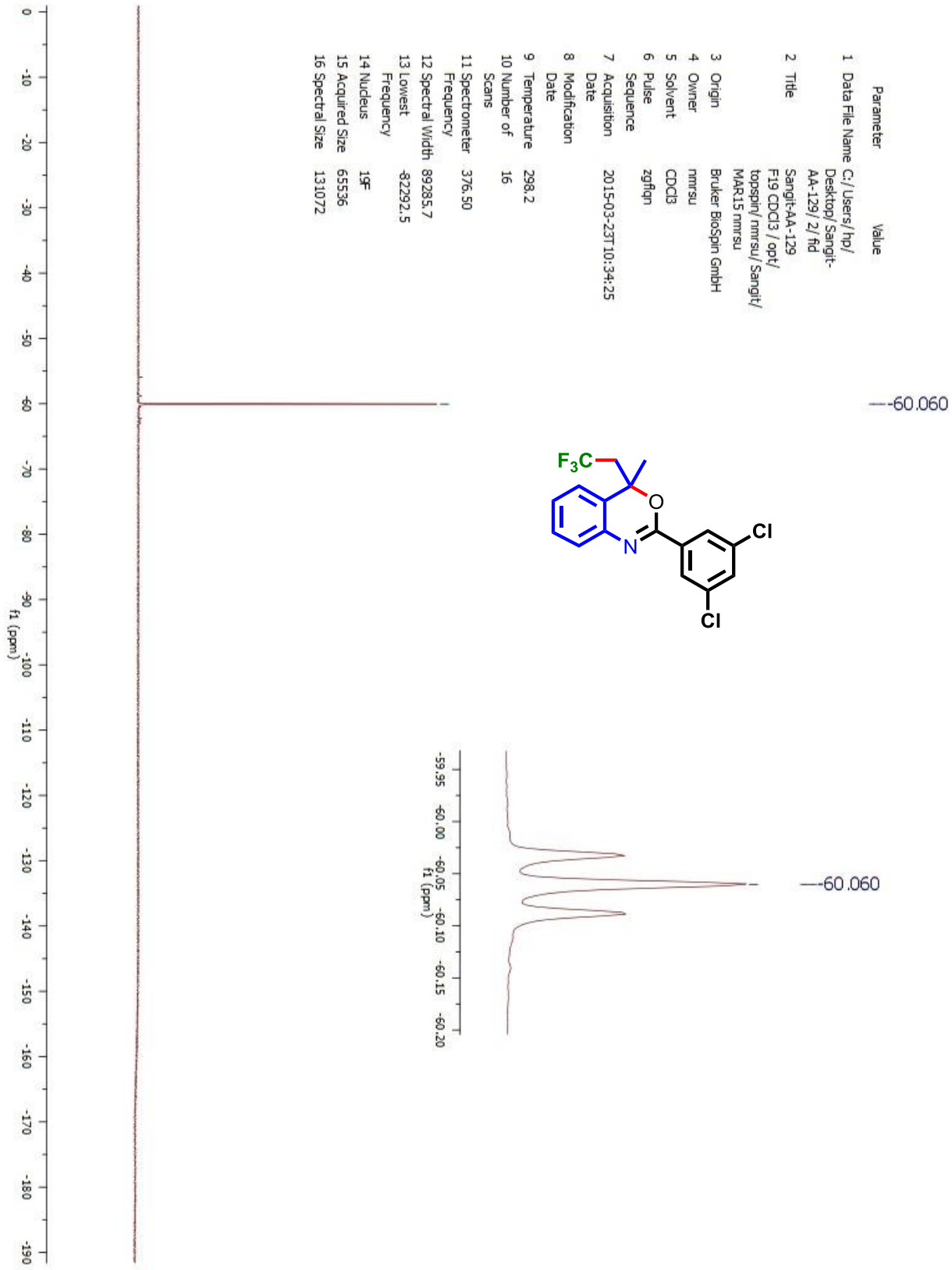
8 Modification Date	
9 Temperature	298.2
10 Number of Scans	16
11 Spectrometer Frequency	400.13
12 Spectral Width	8196.7
13 Lowest Frequency	-1713.7
14 Nucleus	1H
15 Acquired Size	32768
16 Spectral Size	65536



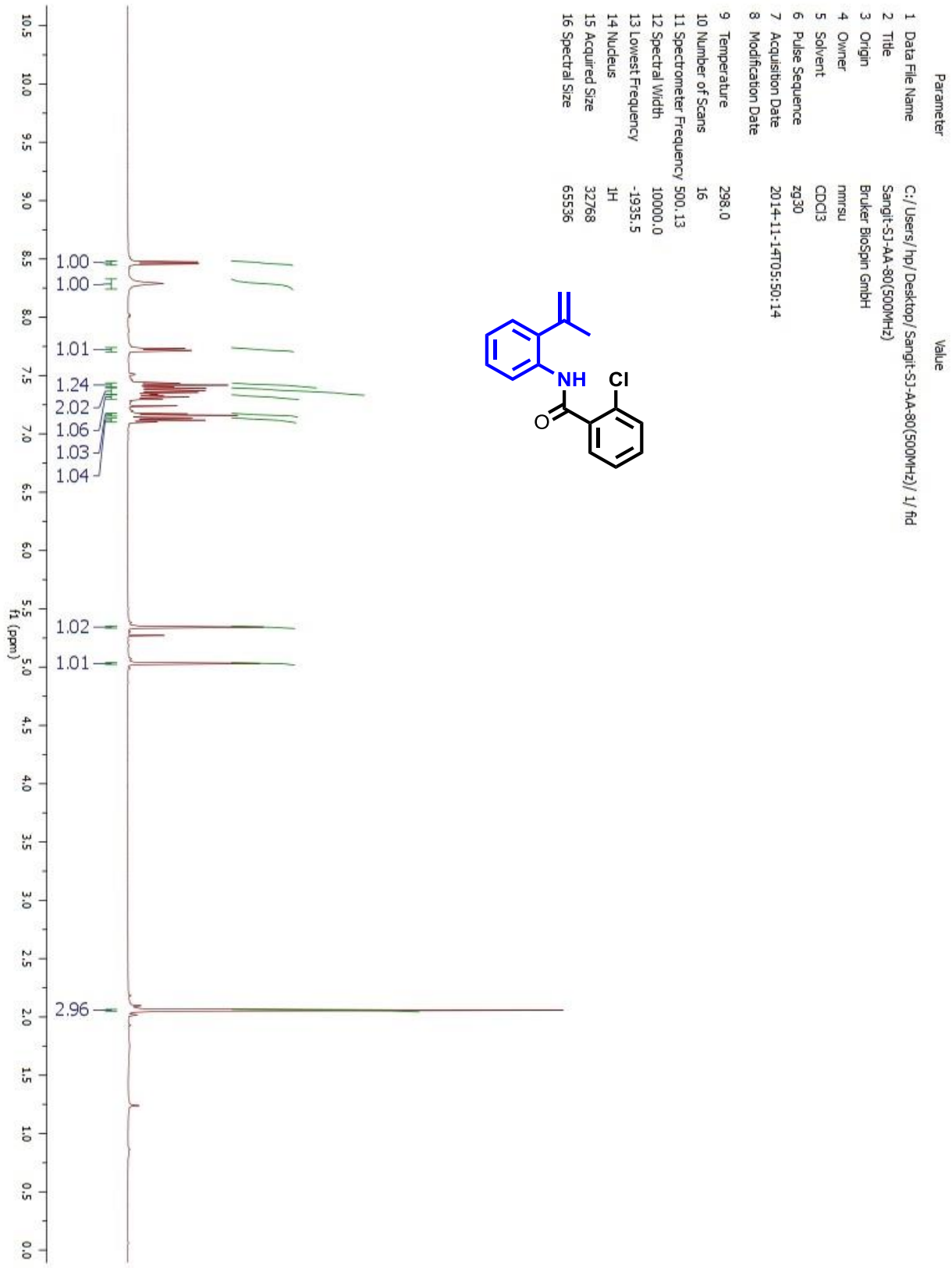
S65 ^{13}C NMR of **3m**



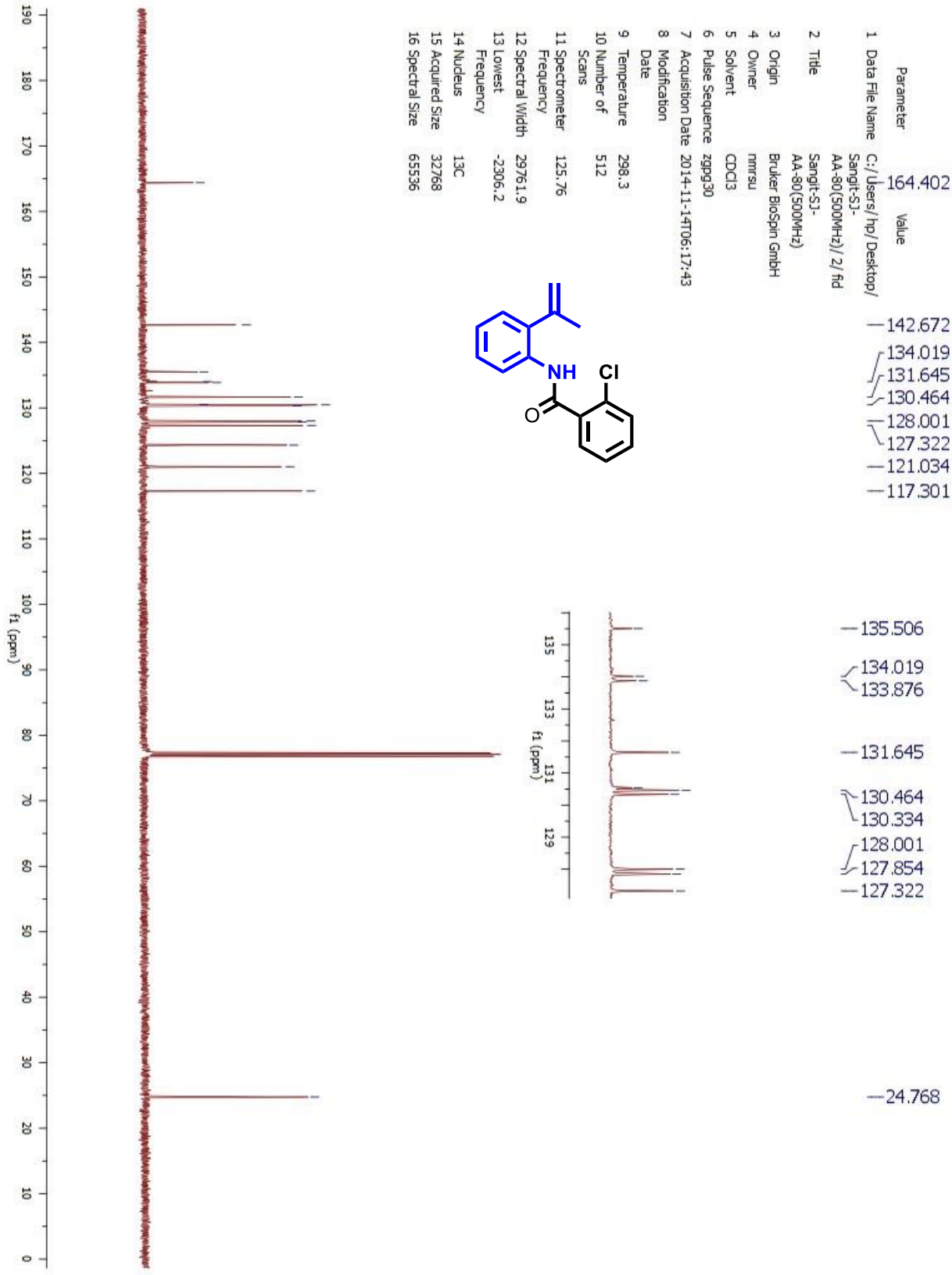
S65 ^{19}F NMR of **3m**



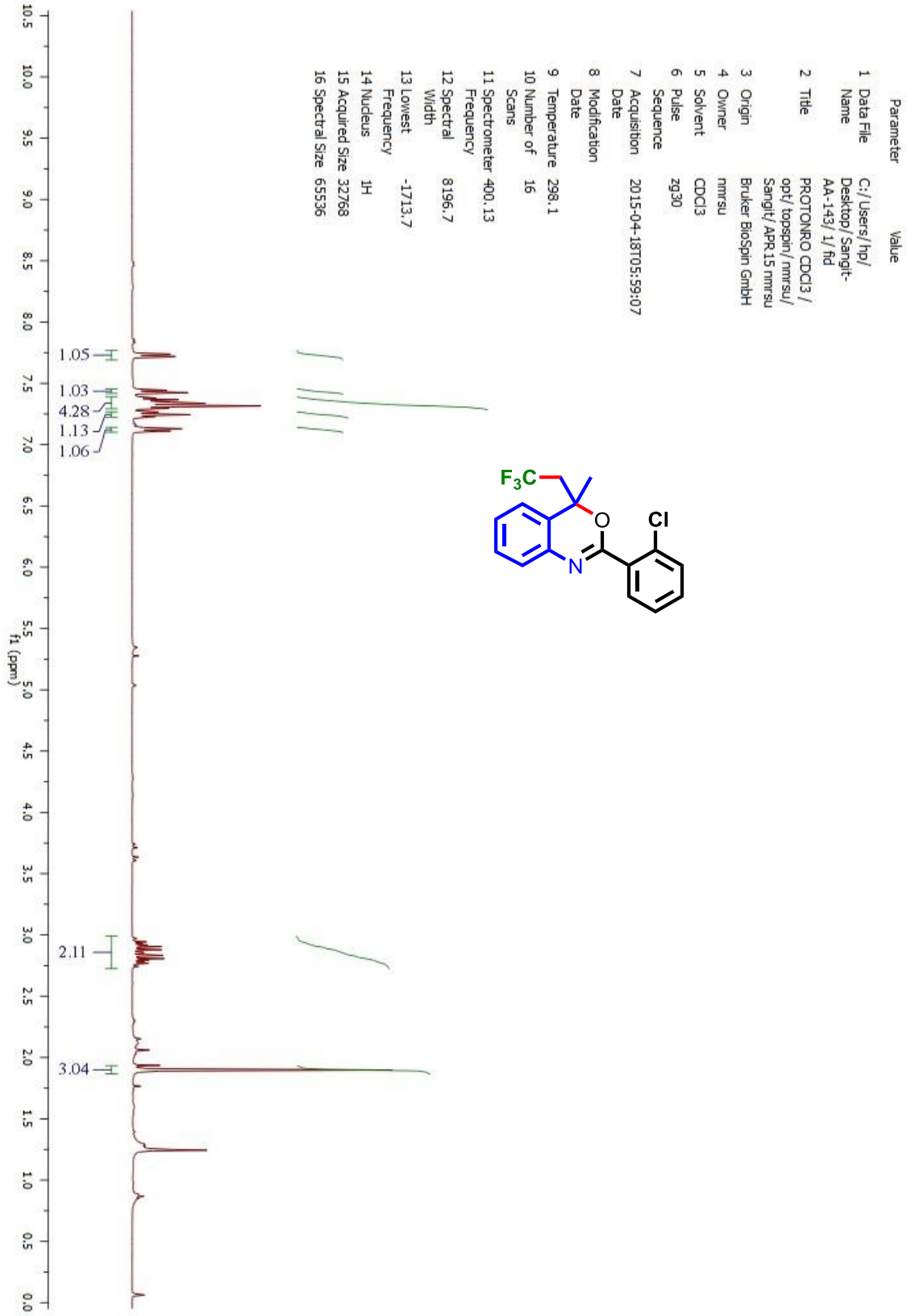
S66 ^{1}H NMR of **1n**



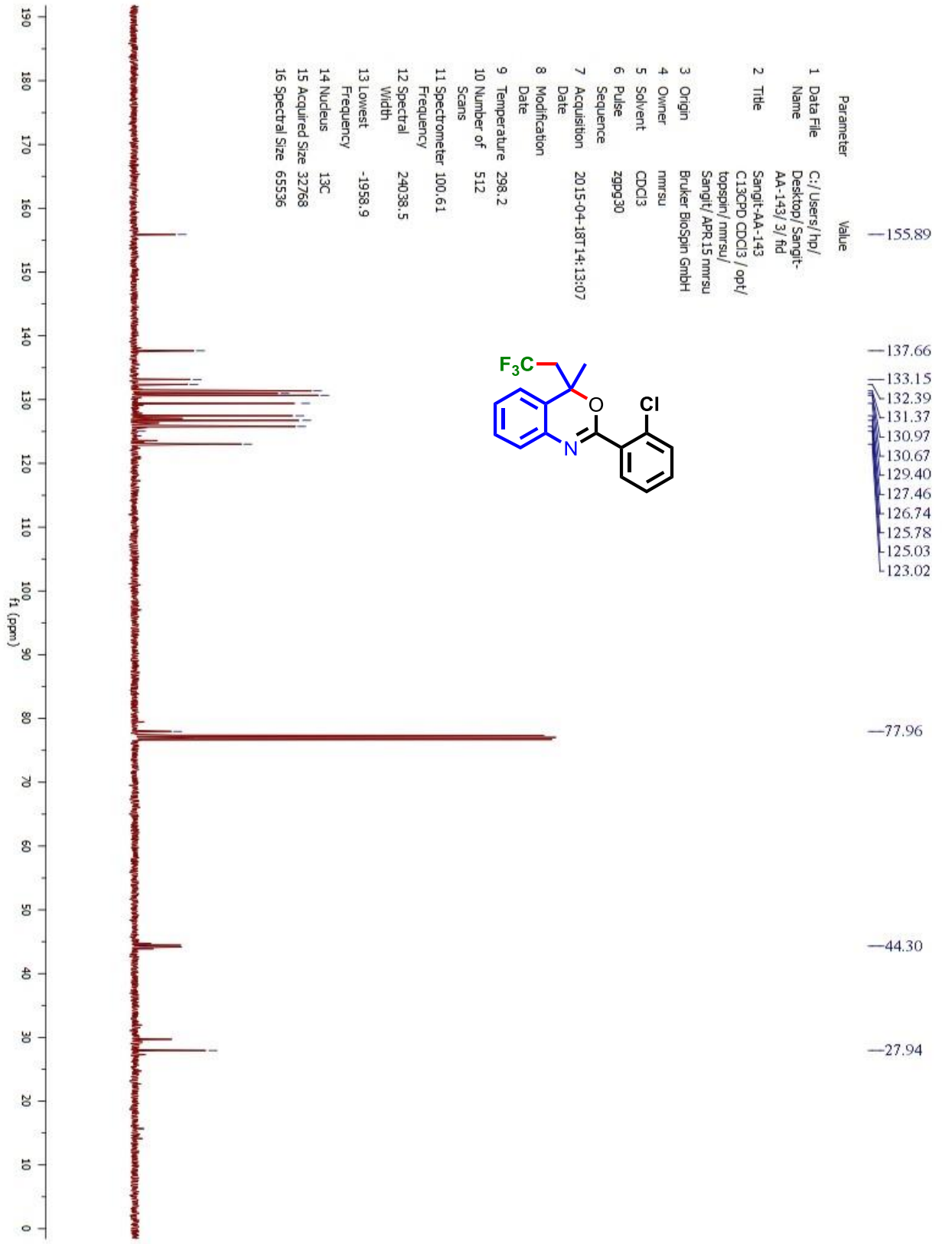
S67 ^{13}C NMR of **1n**



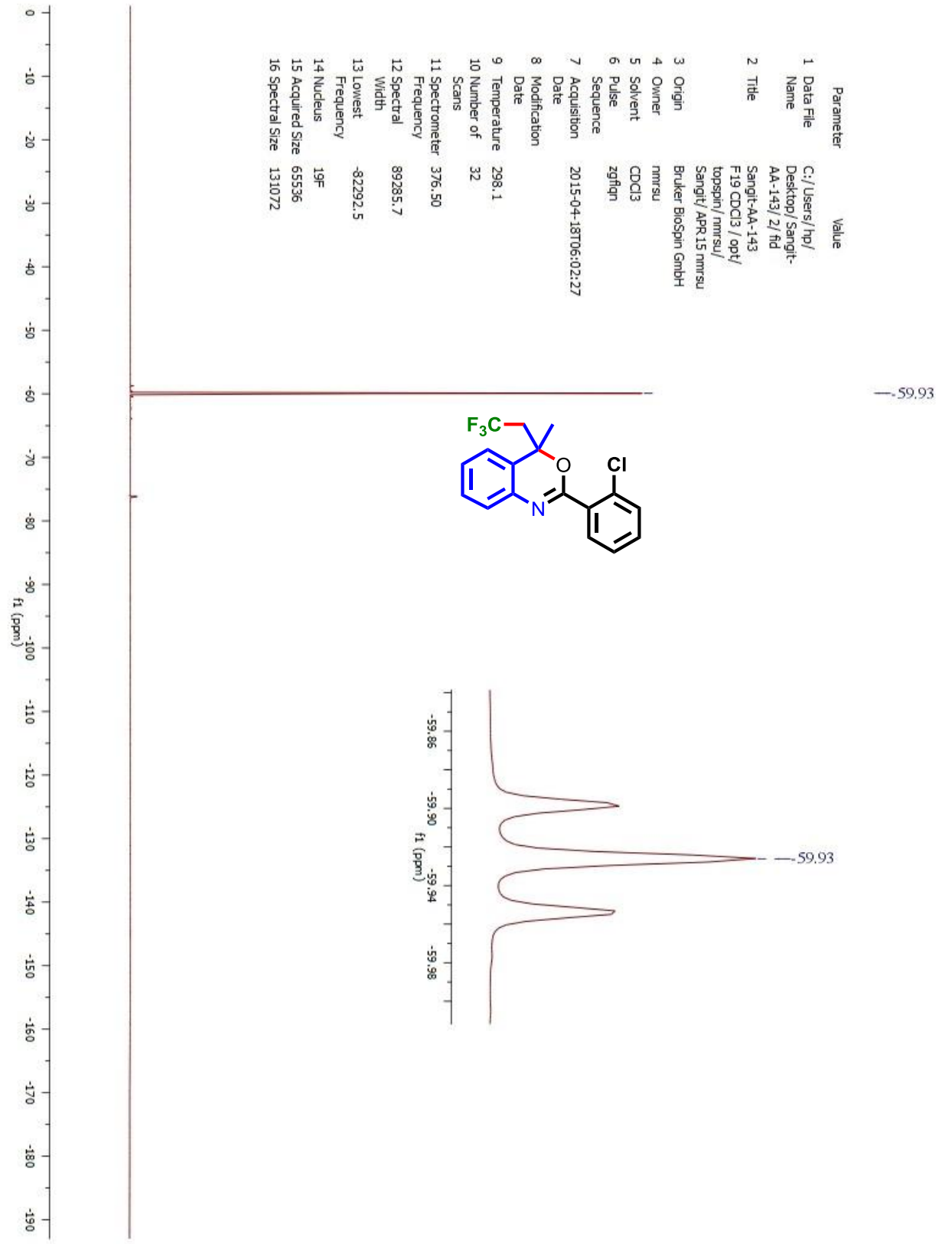
S68 ^{1}H NMR of **3n**



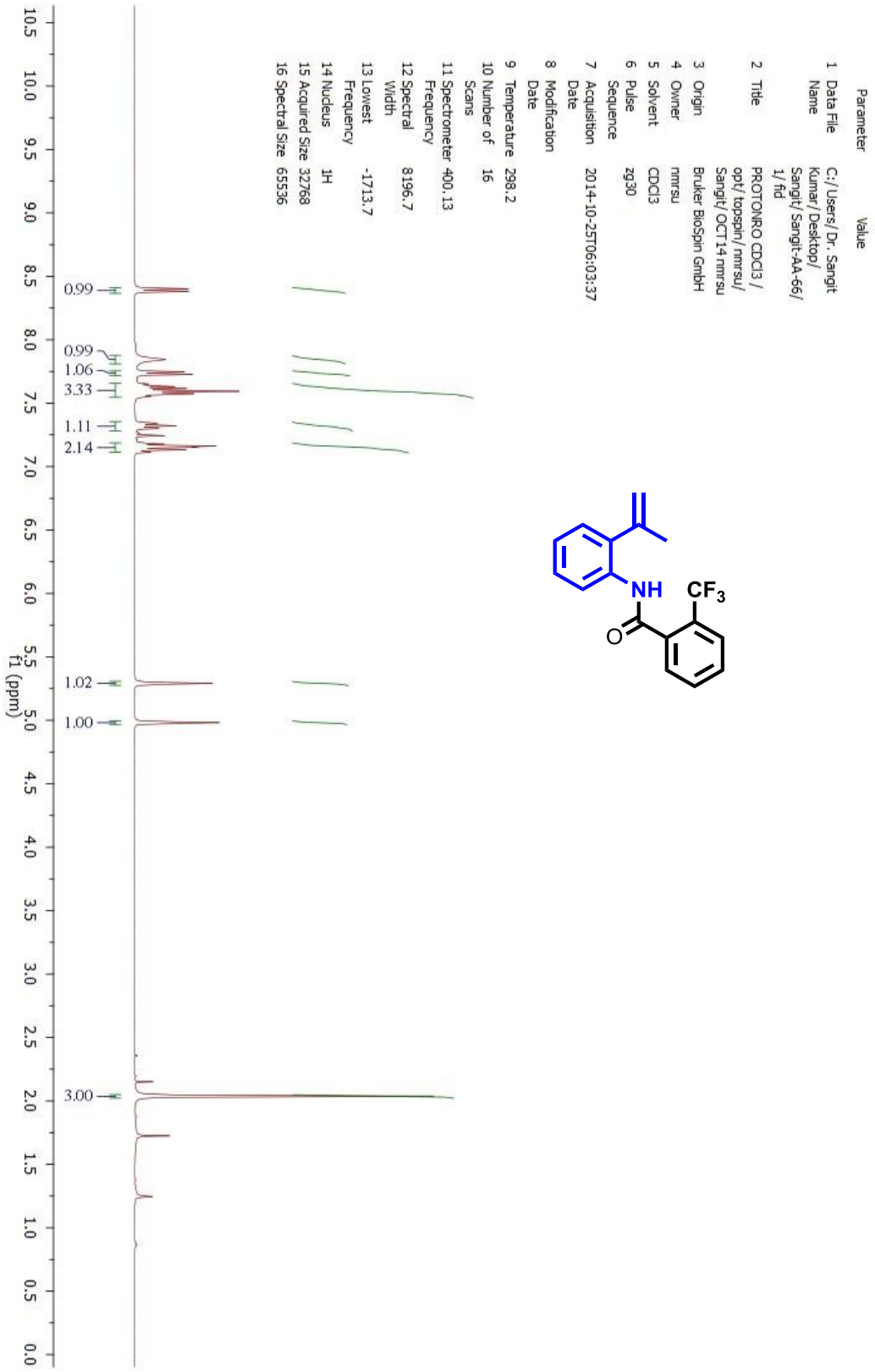
S69 ^{13}C NMR of **3n**



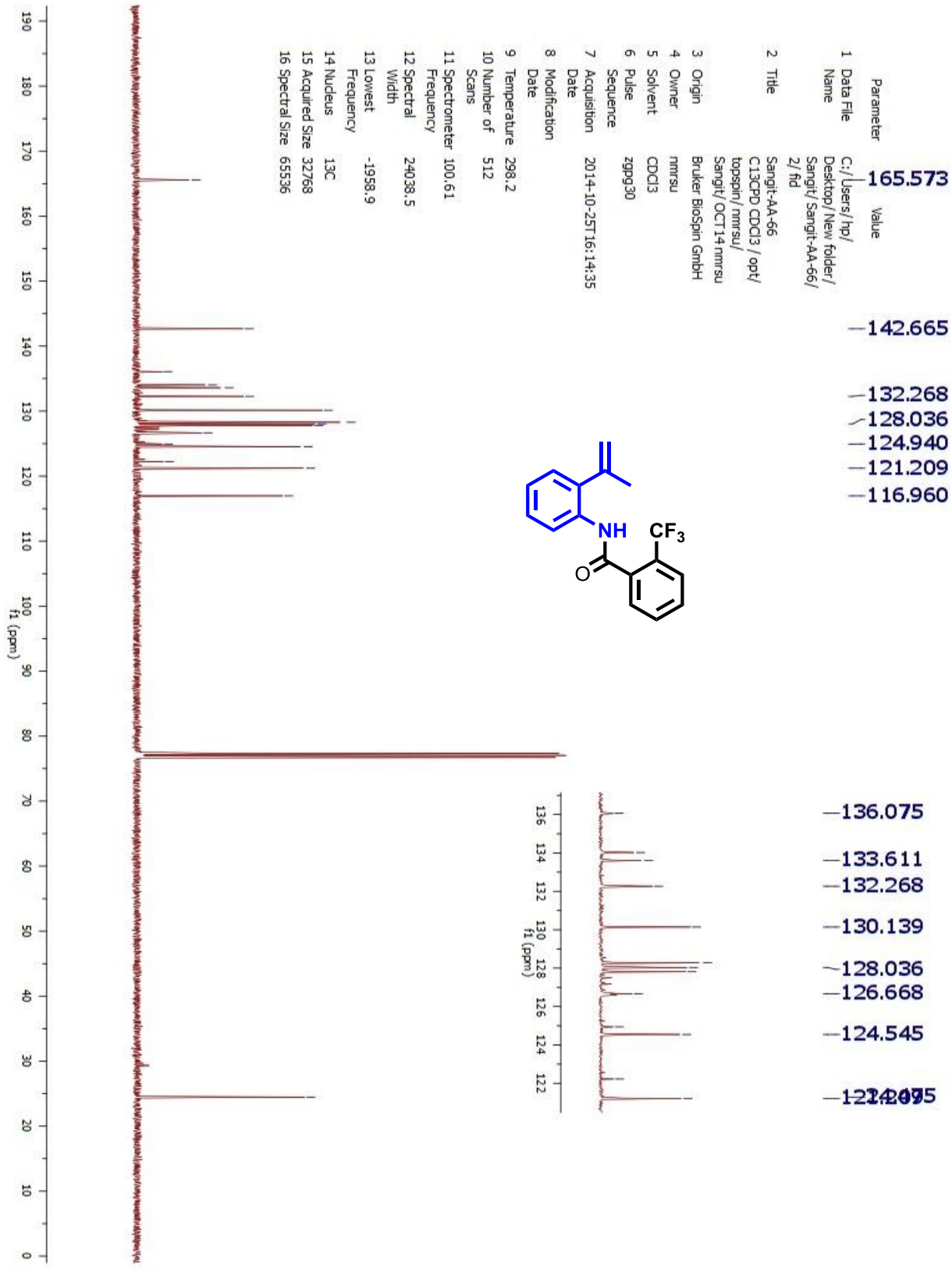
S70 ^{19}F NMR of **3n**



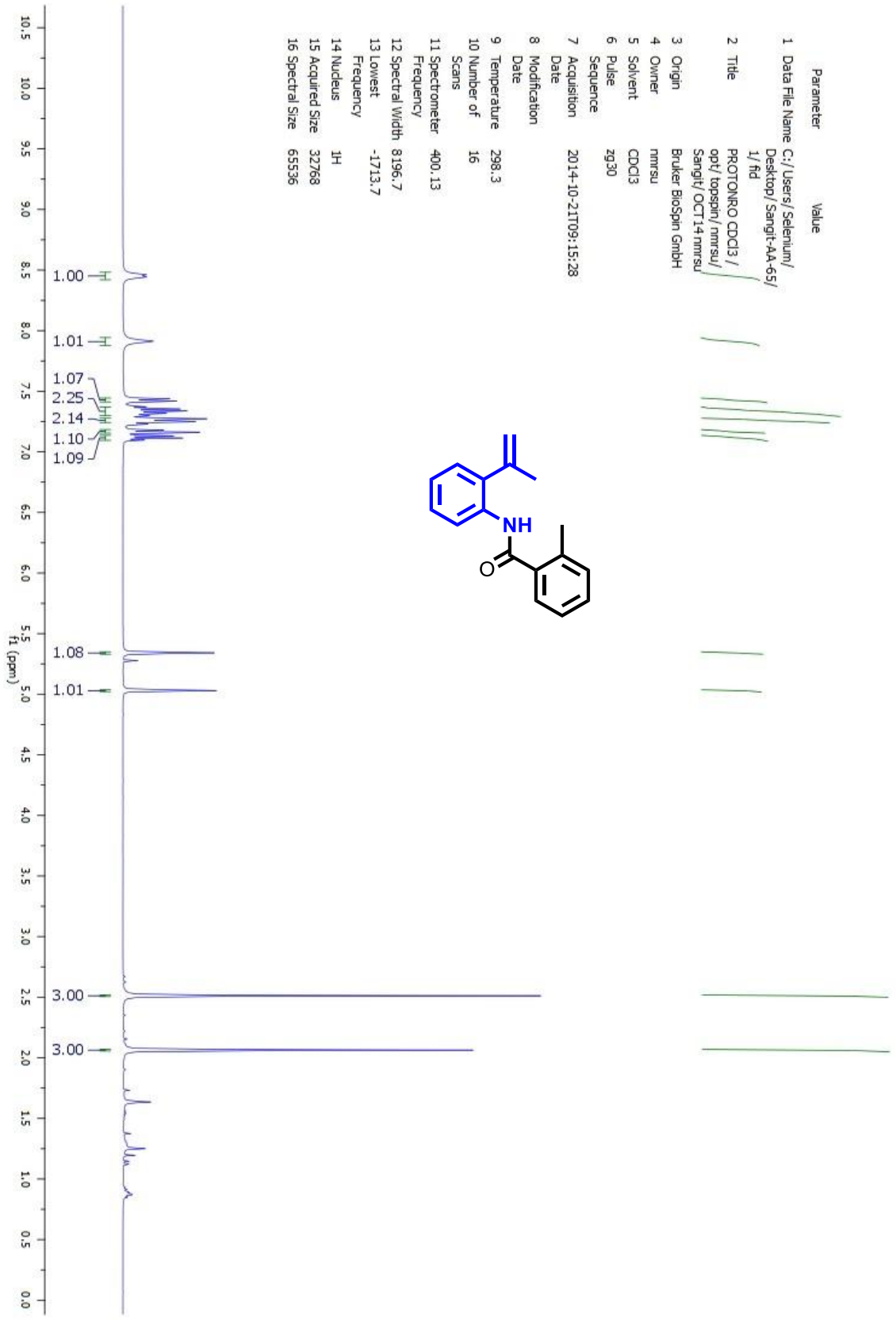
S71 ^{1}H NMR of **1o**



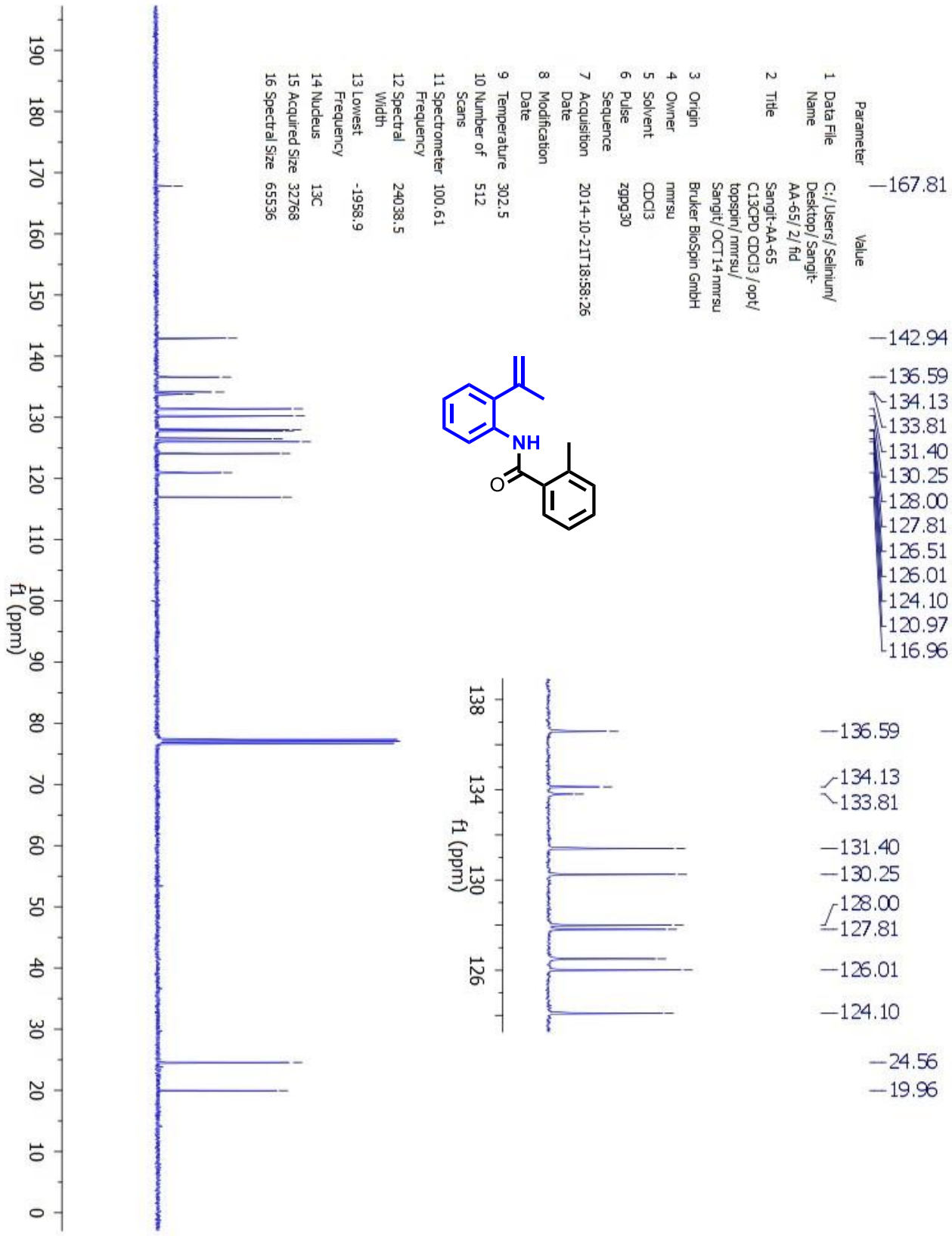
S72 ^{13}C NMR of **1o**



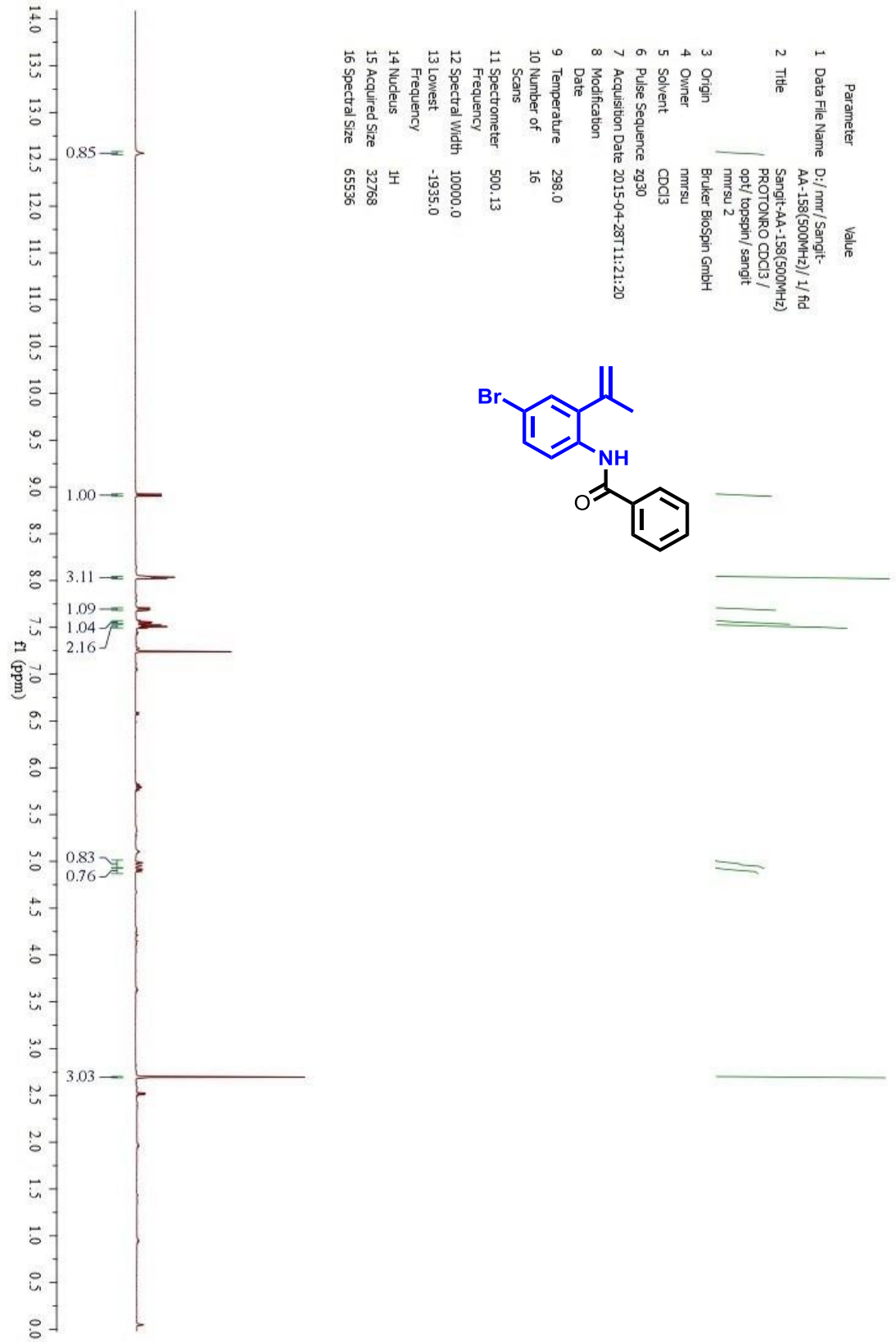
S73 ^{1}H NMR of **1p**



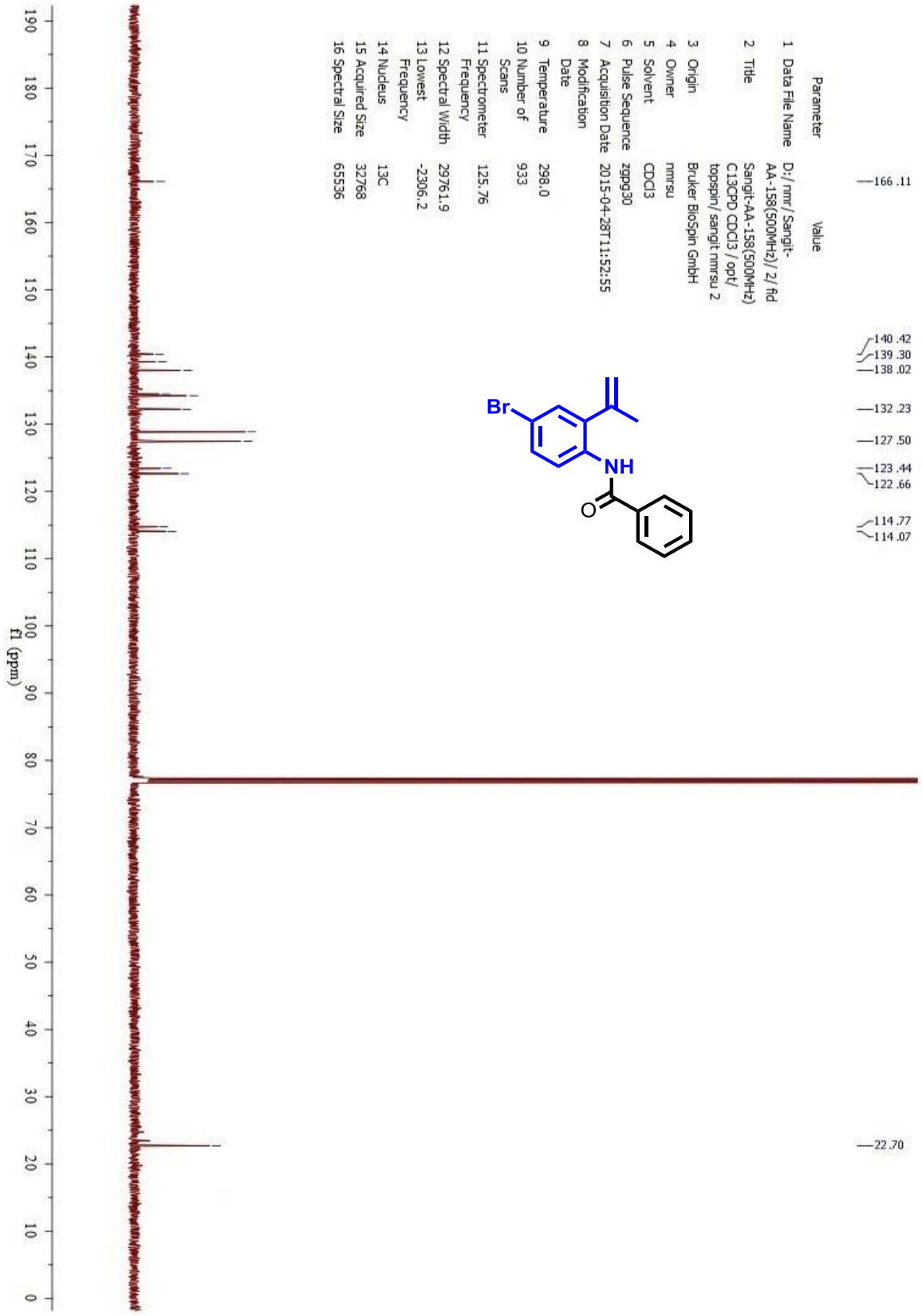
S74 ^{13}C NMR of **1p**



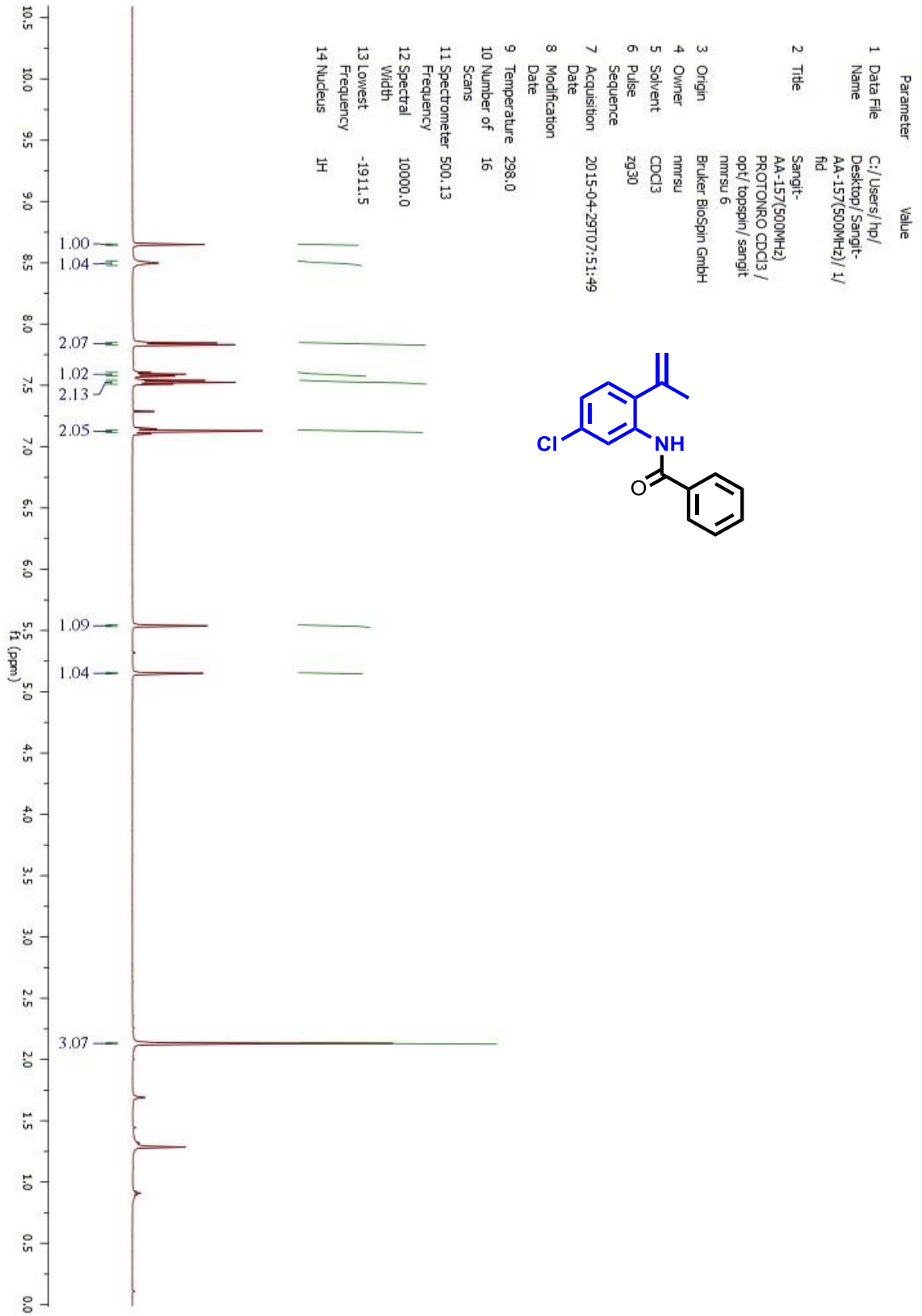
S75 ^{1}H NMR of **1q**



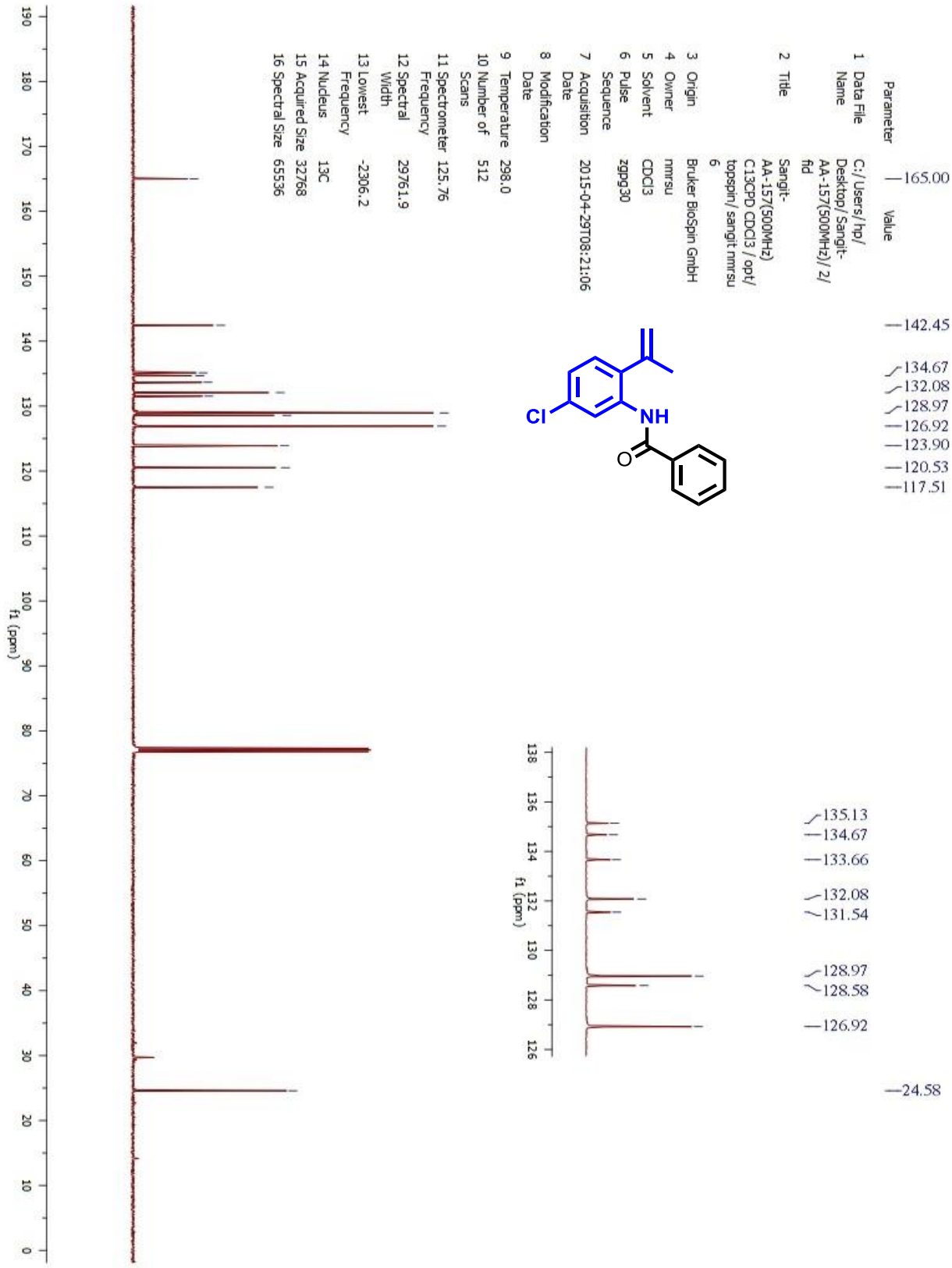
S76 ^{13}C NMR of **1q**



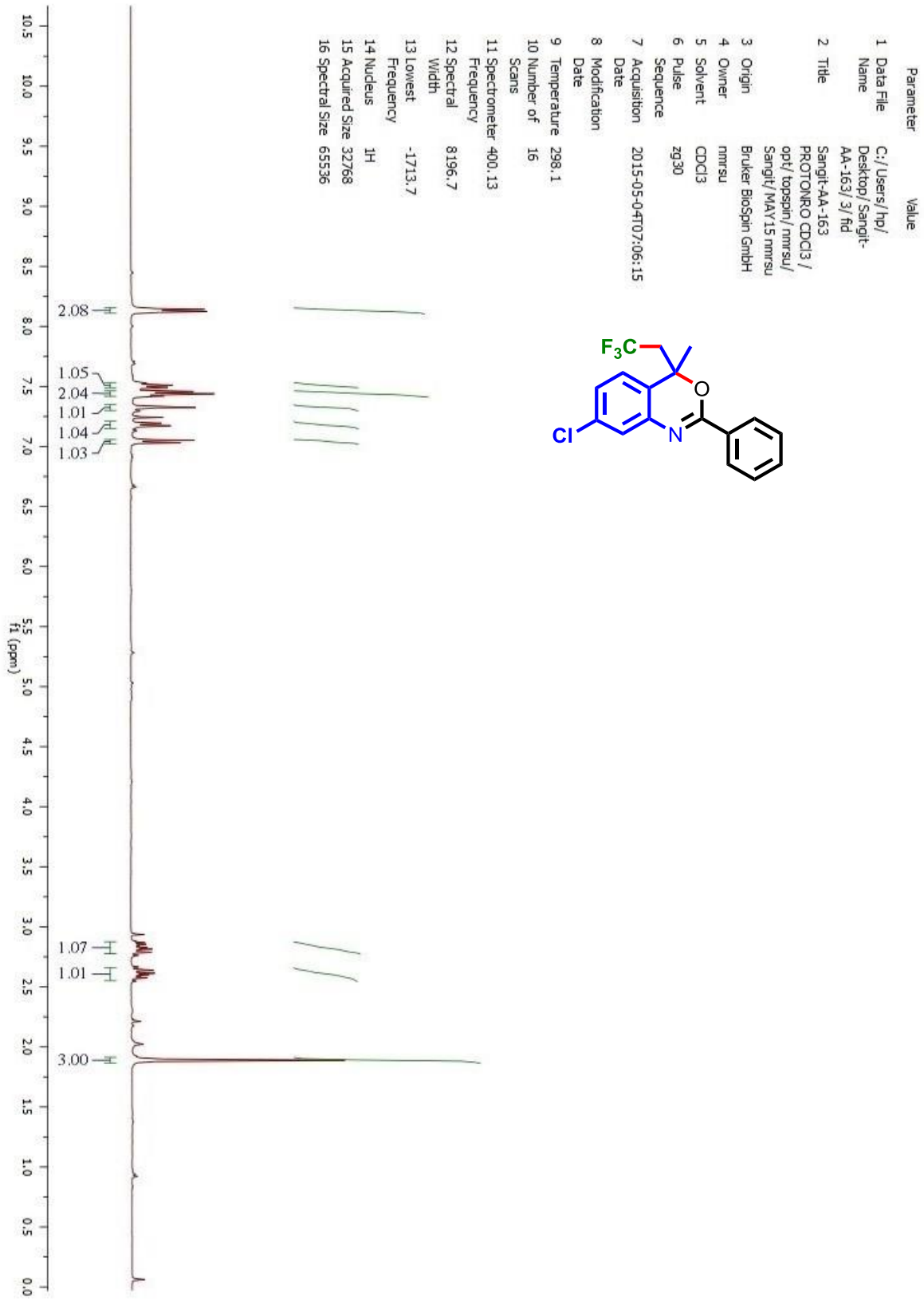
S77 ^{1}H NMR of **1r**



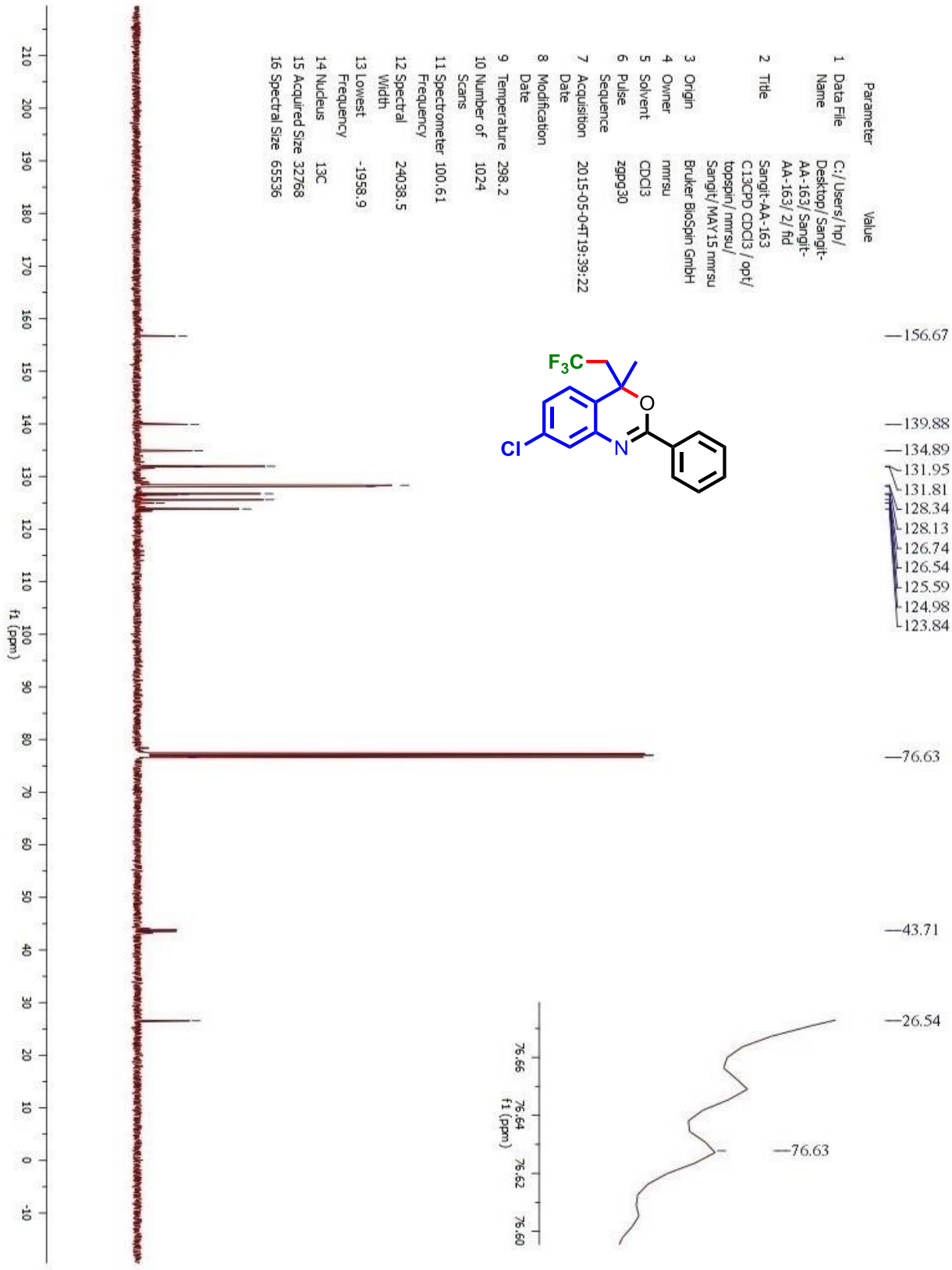
S78 ^{13}C NMR of **1r**



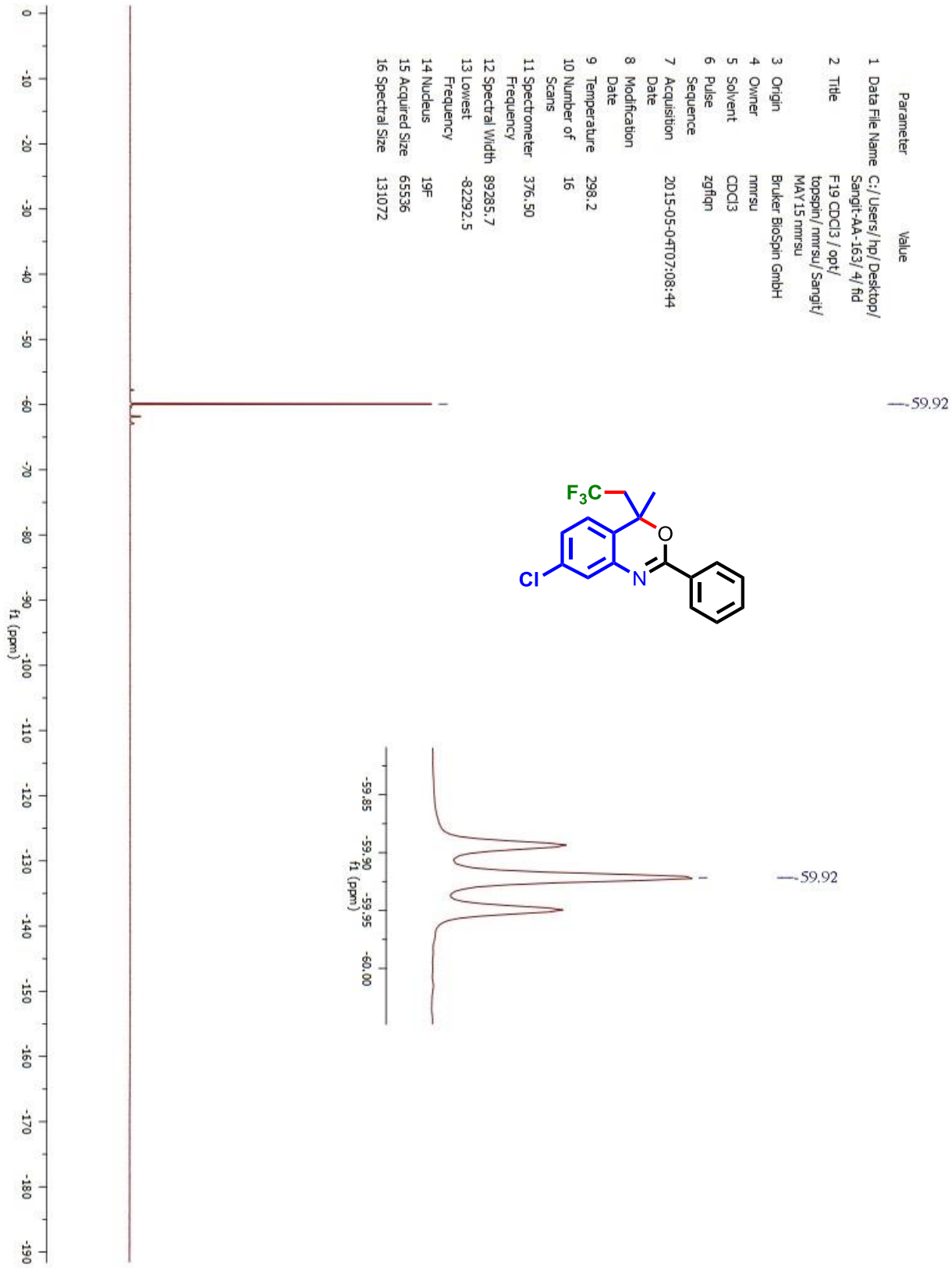
S79 ^{1}H NMR of **3r**



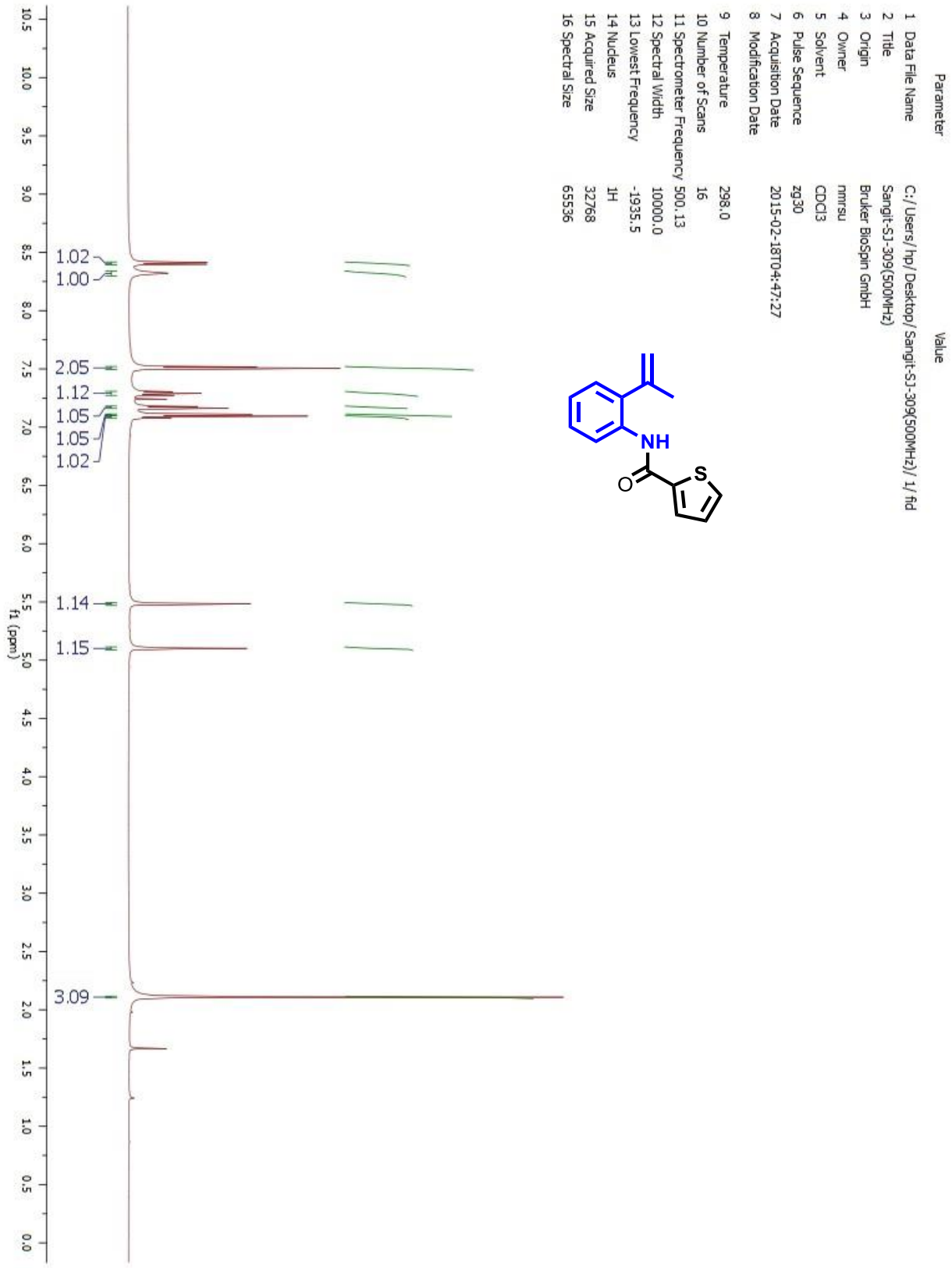
S80 ^{13}C NMR of **3r**



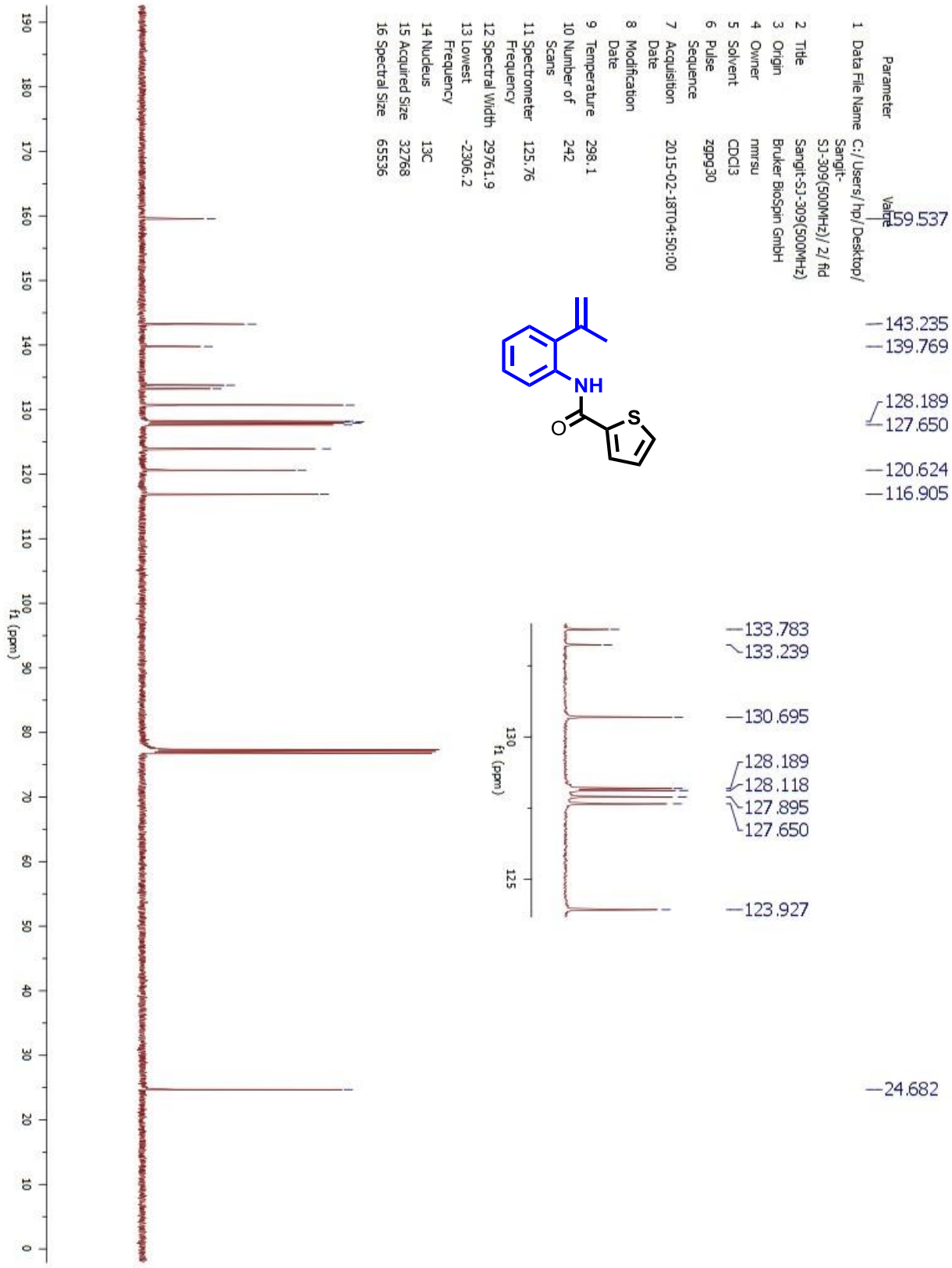
S81 ^{19}F NMR of **3r**



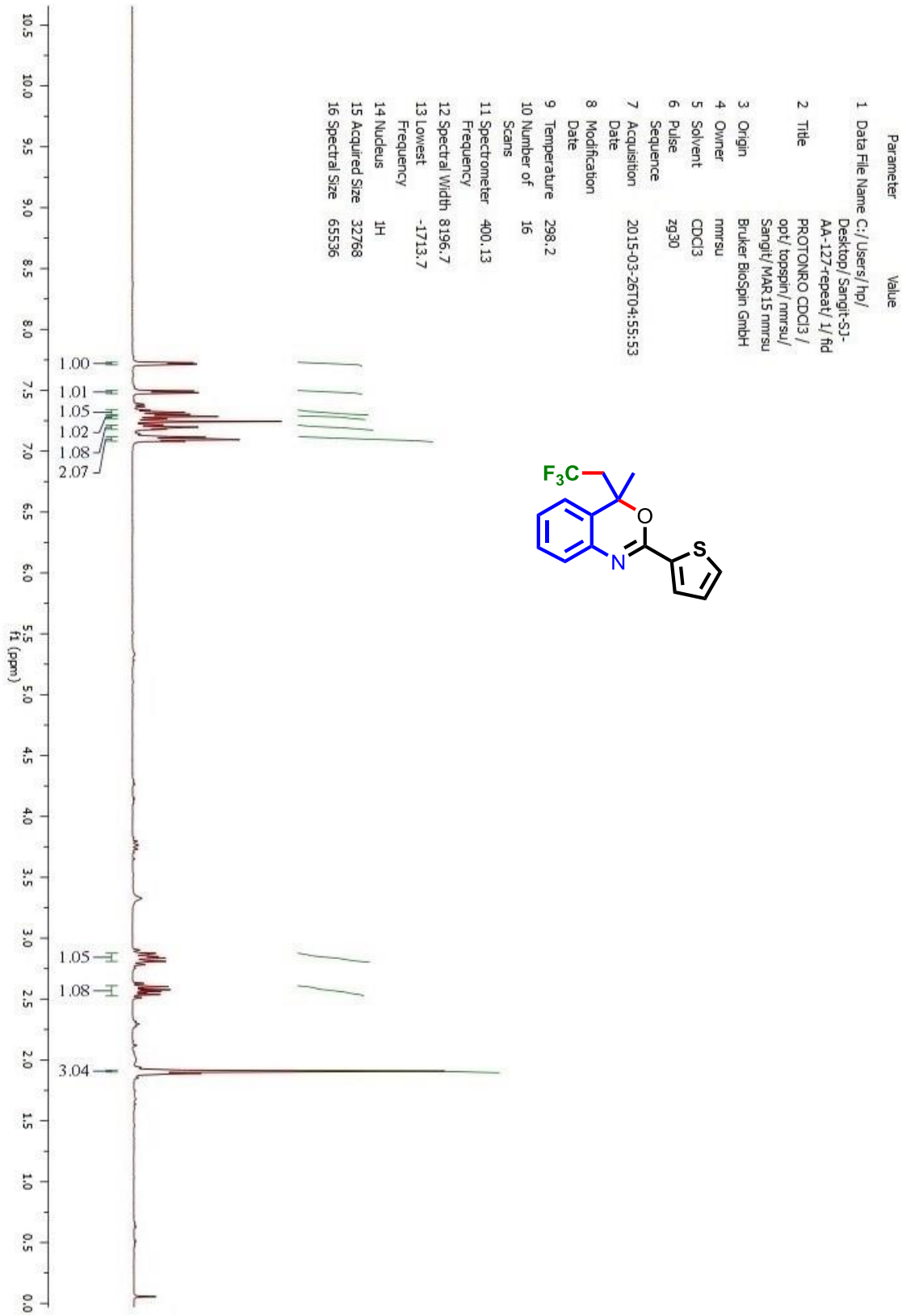
S82 ^{1}H NMR of **1s**



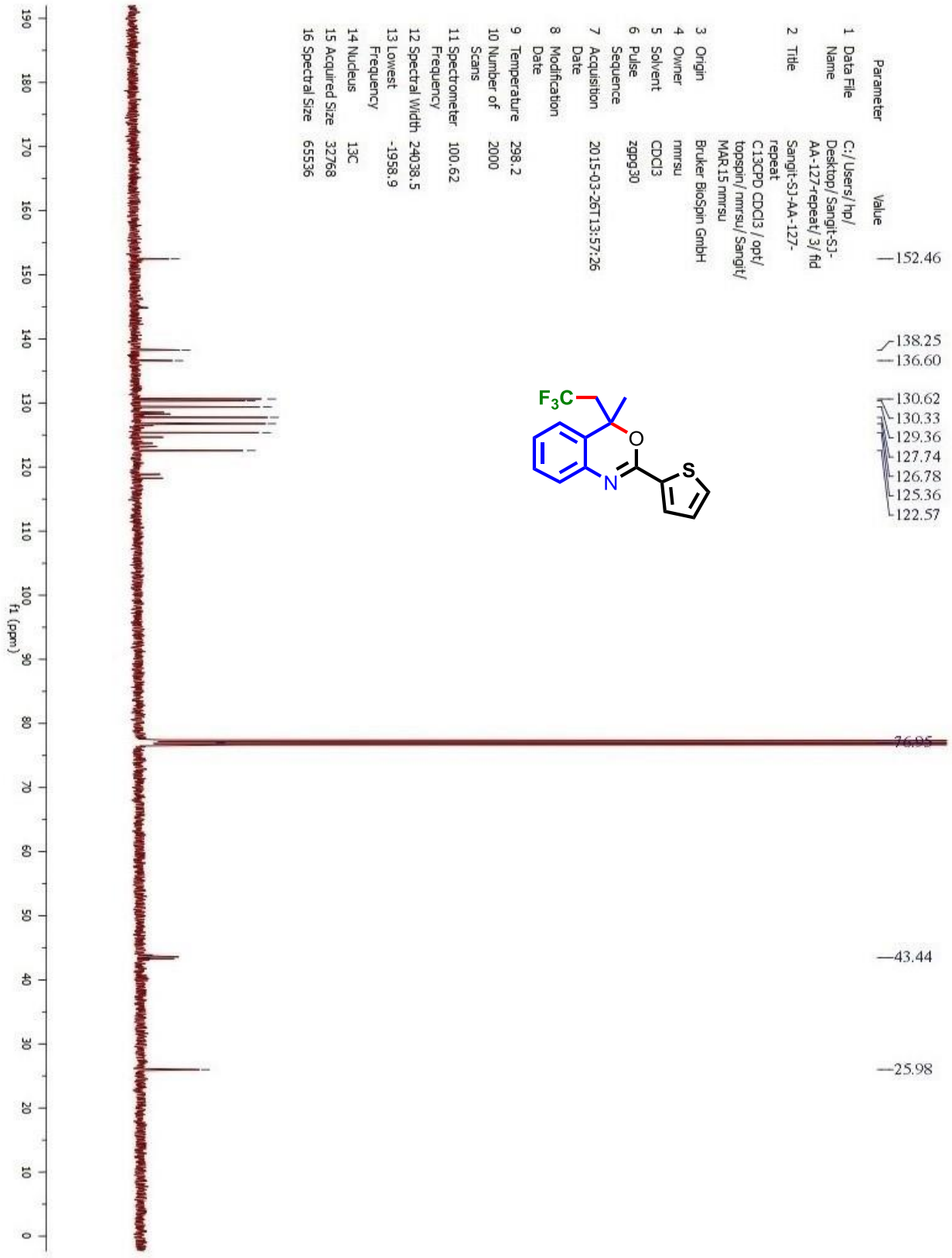
S83 ^{13}C NMR of **1s**



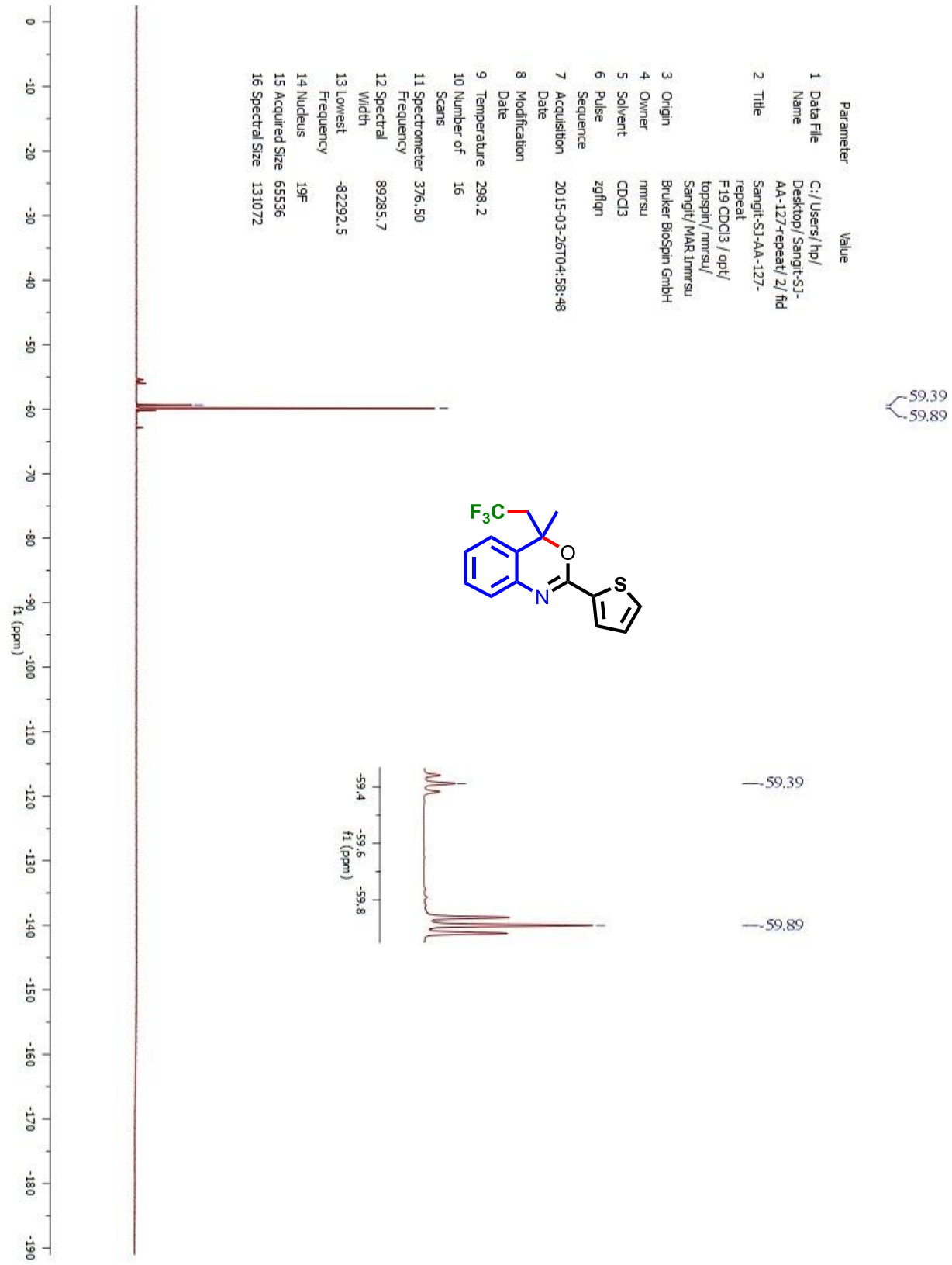
S84 ^{1}H NMR of **3s**



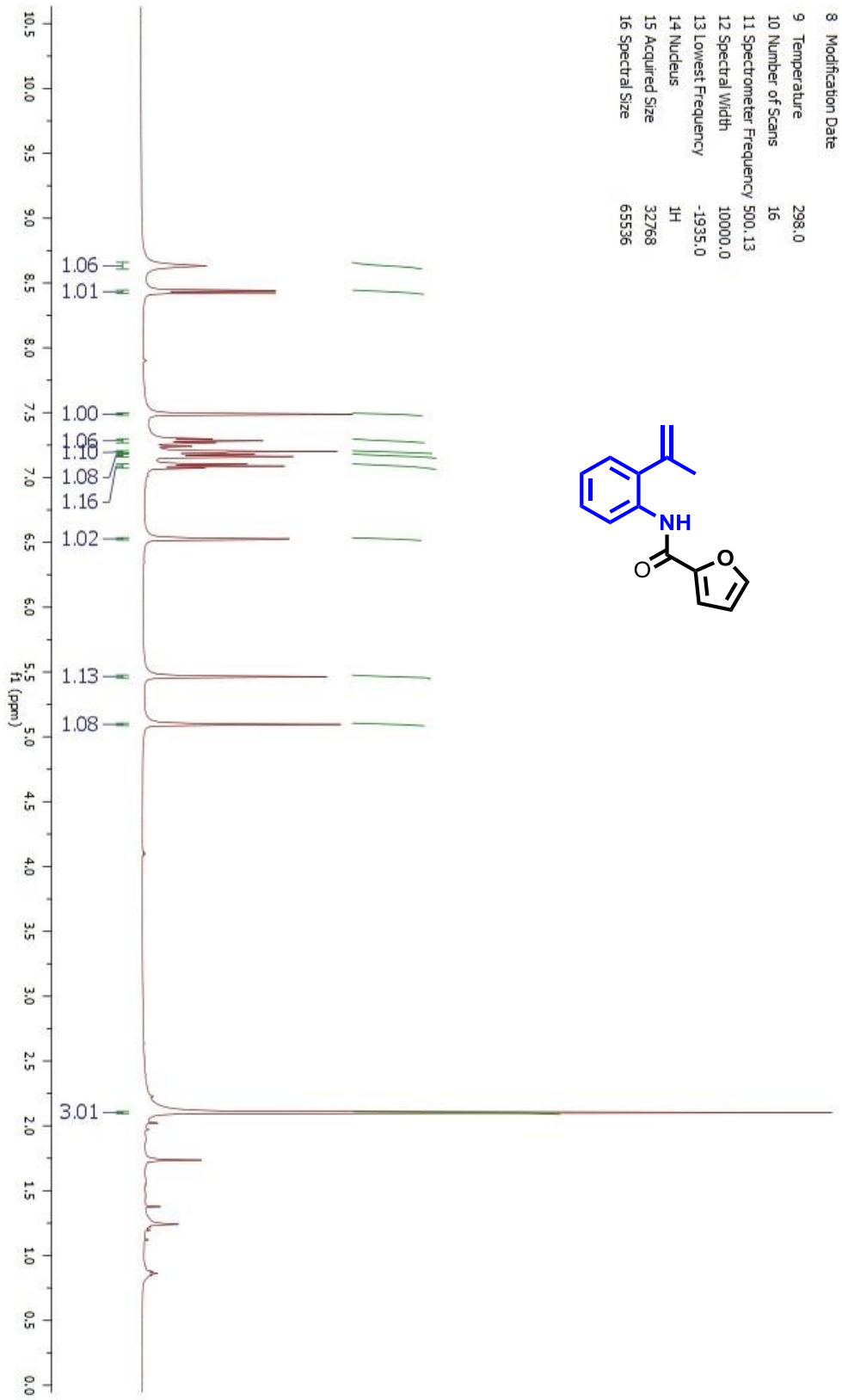
S85 ^{13}C NMR of **3s**



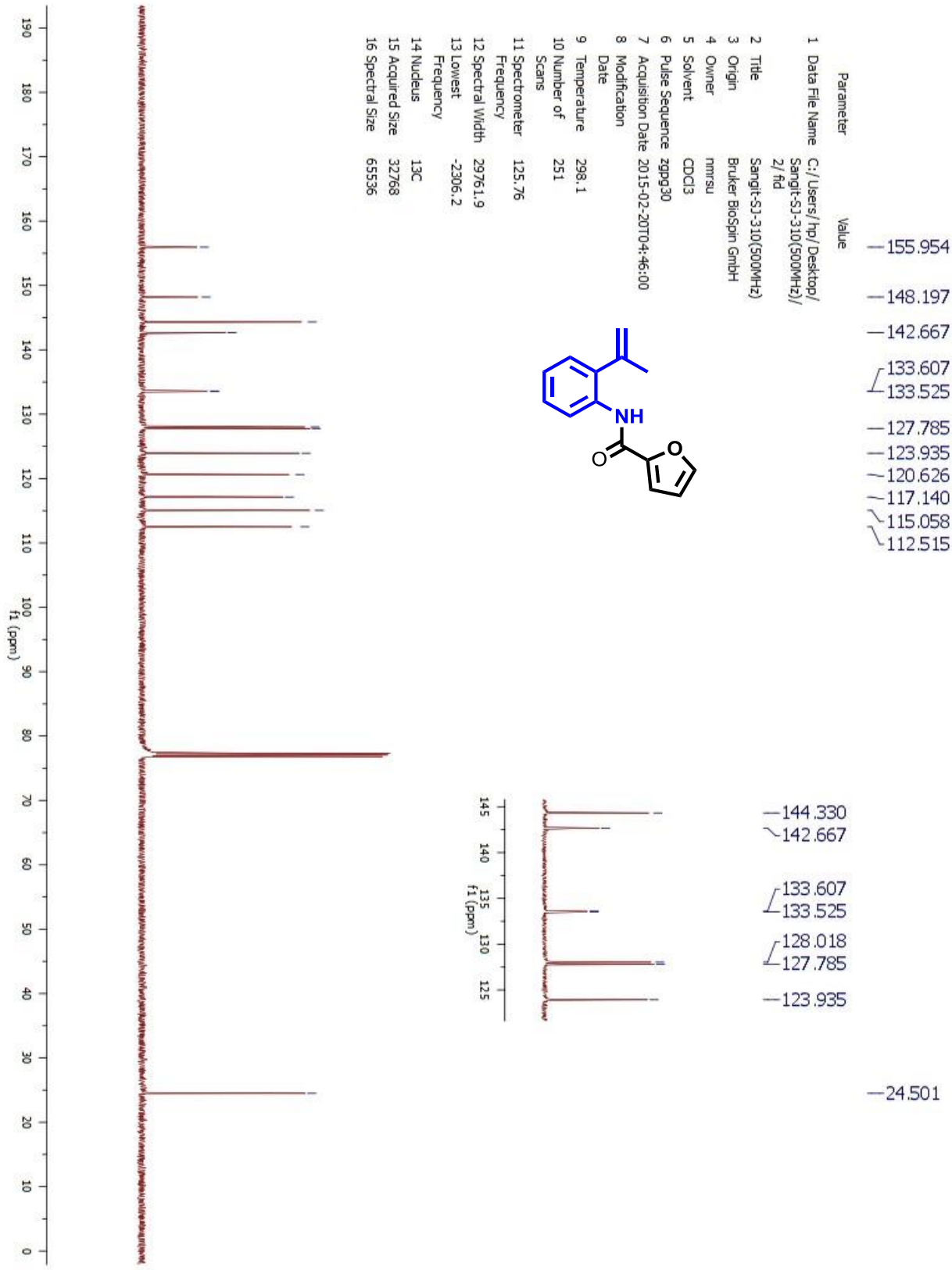
S86 ^{19}F NMR of **3s**



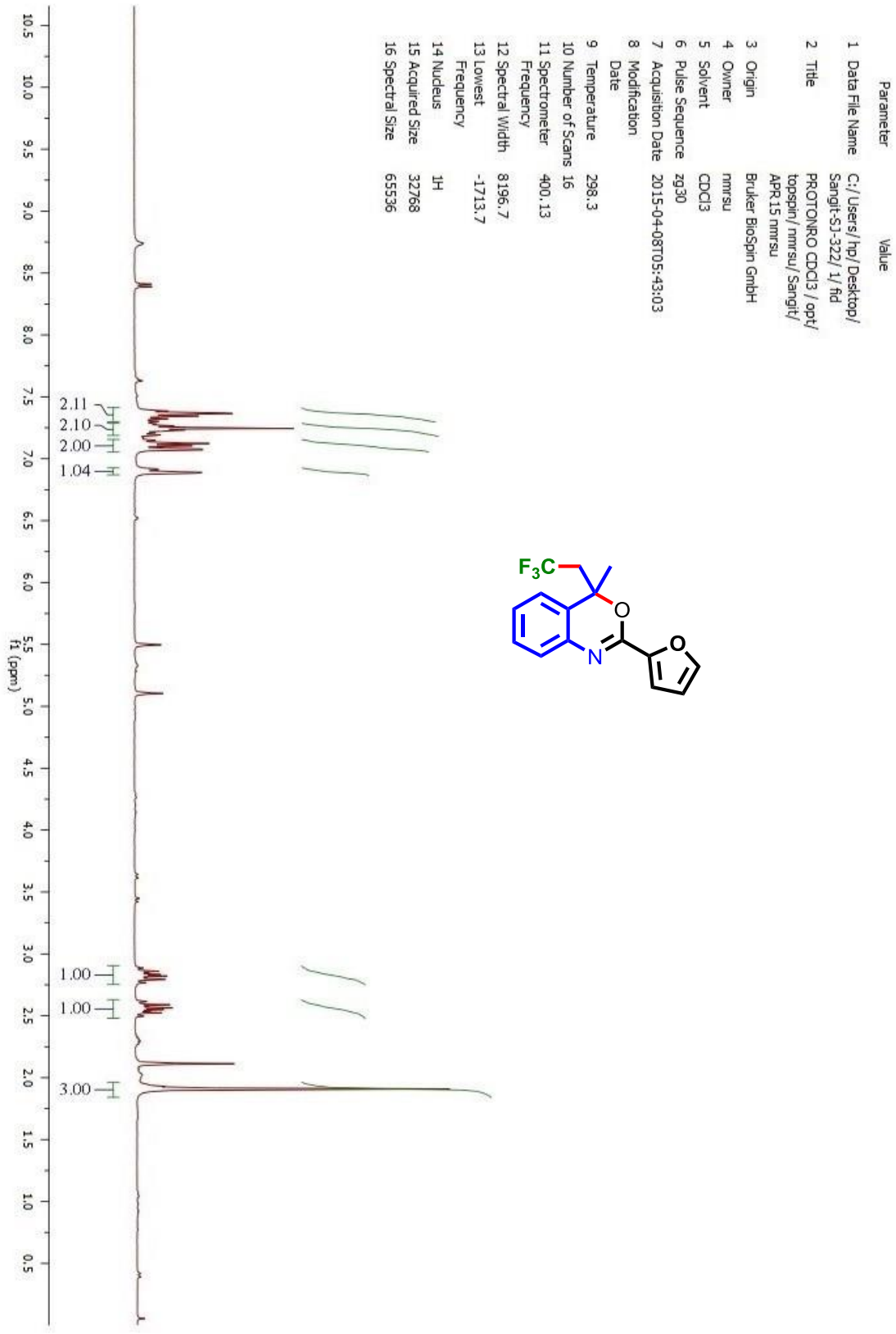
S87 ^{1}H NMR of **1t**



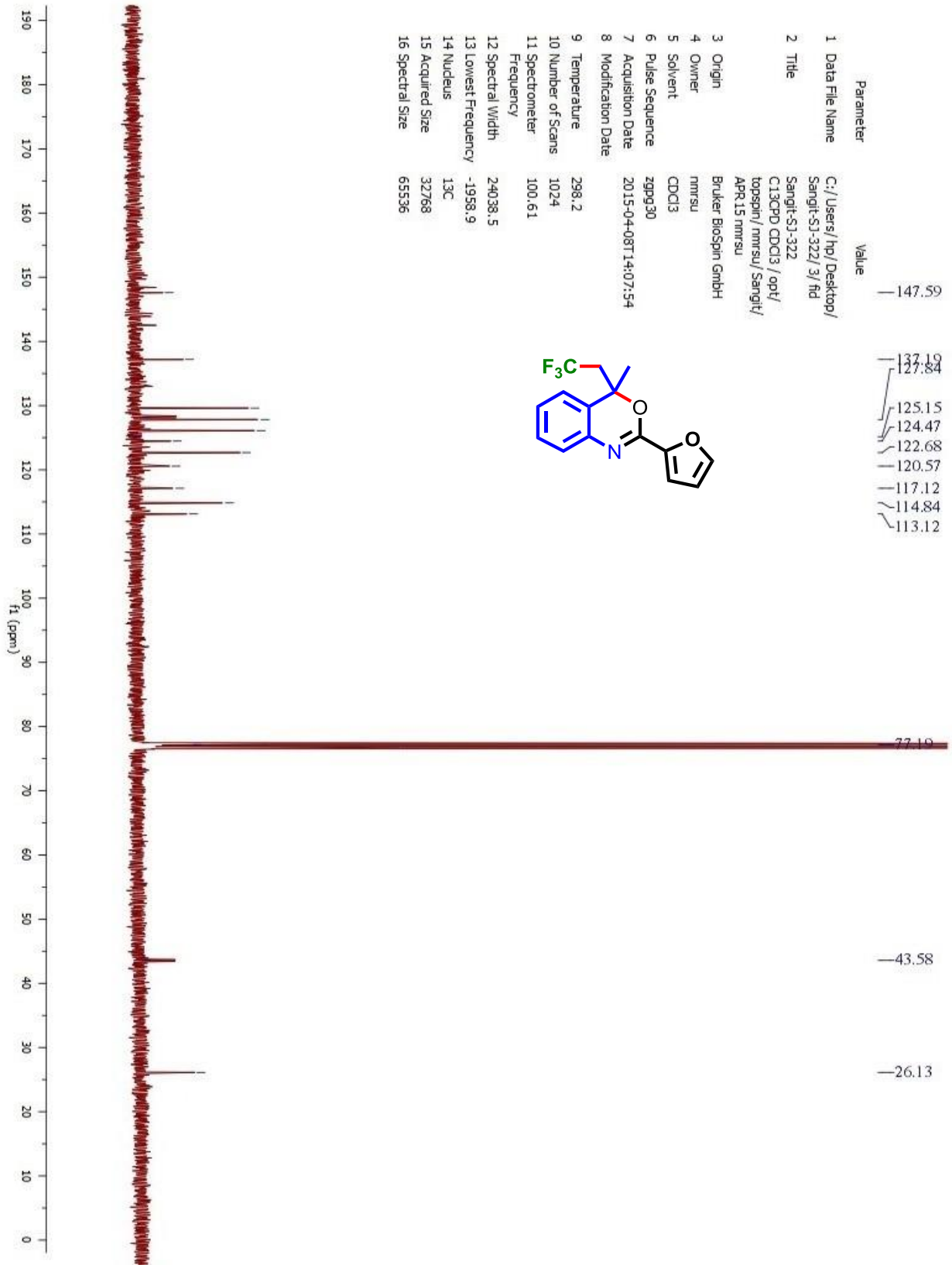
S88 ^{13}C NMR of **1t**



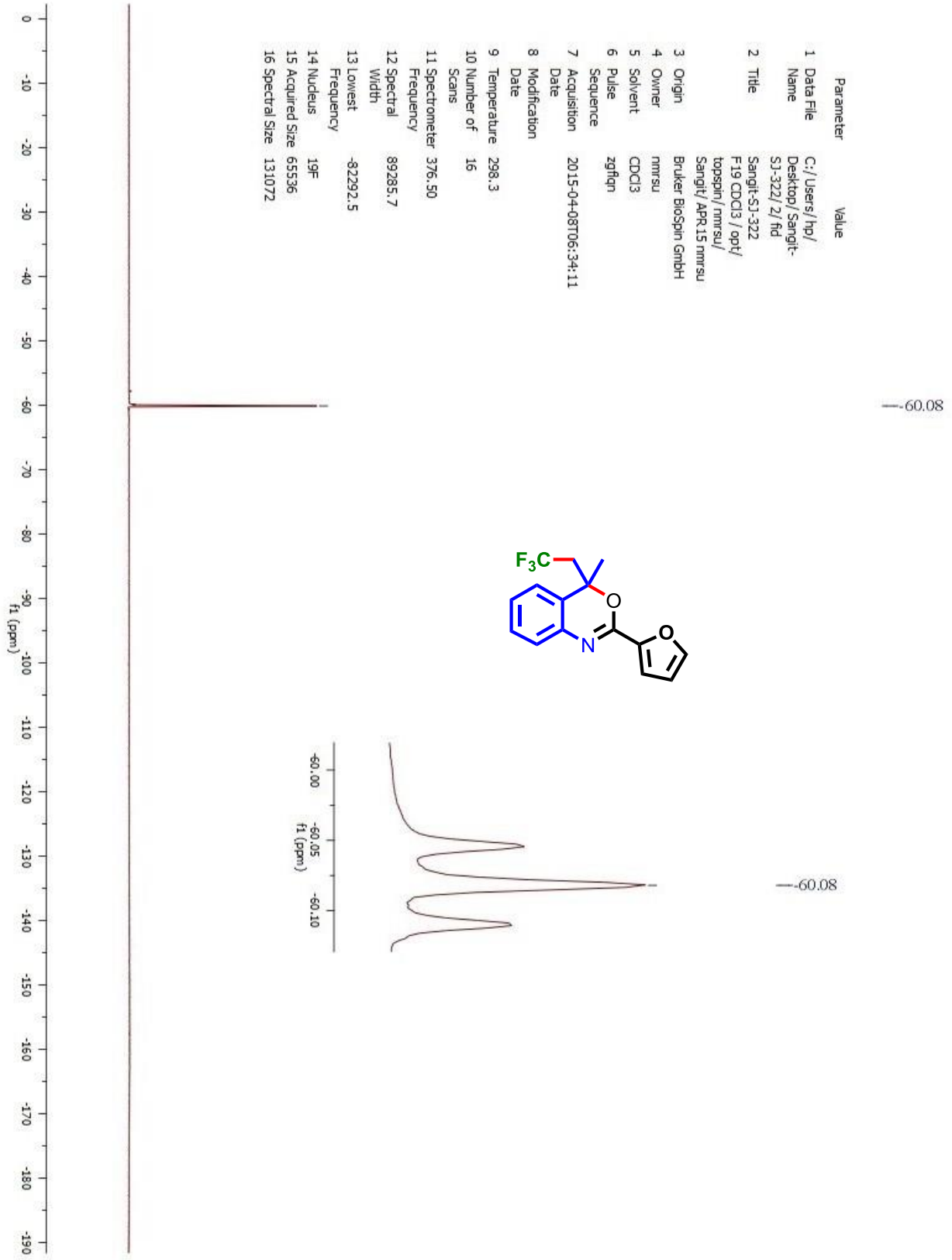
S89 ^{1}H NMR of **3t**



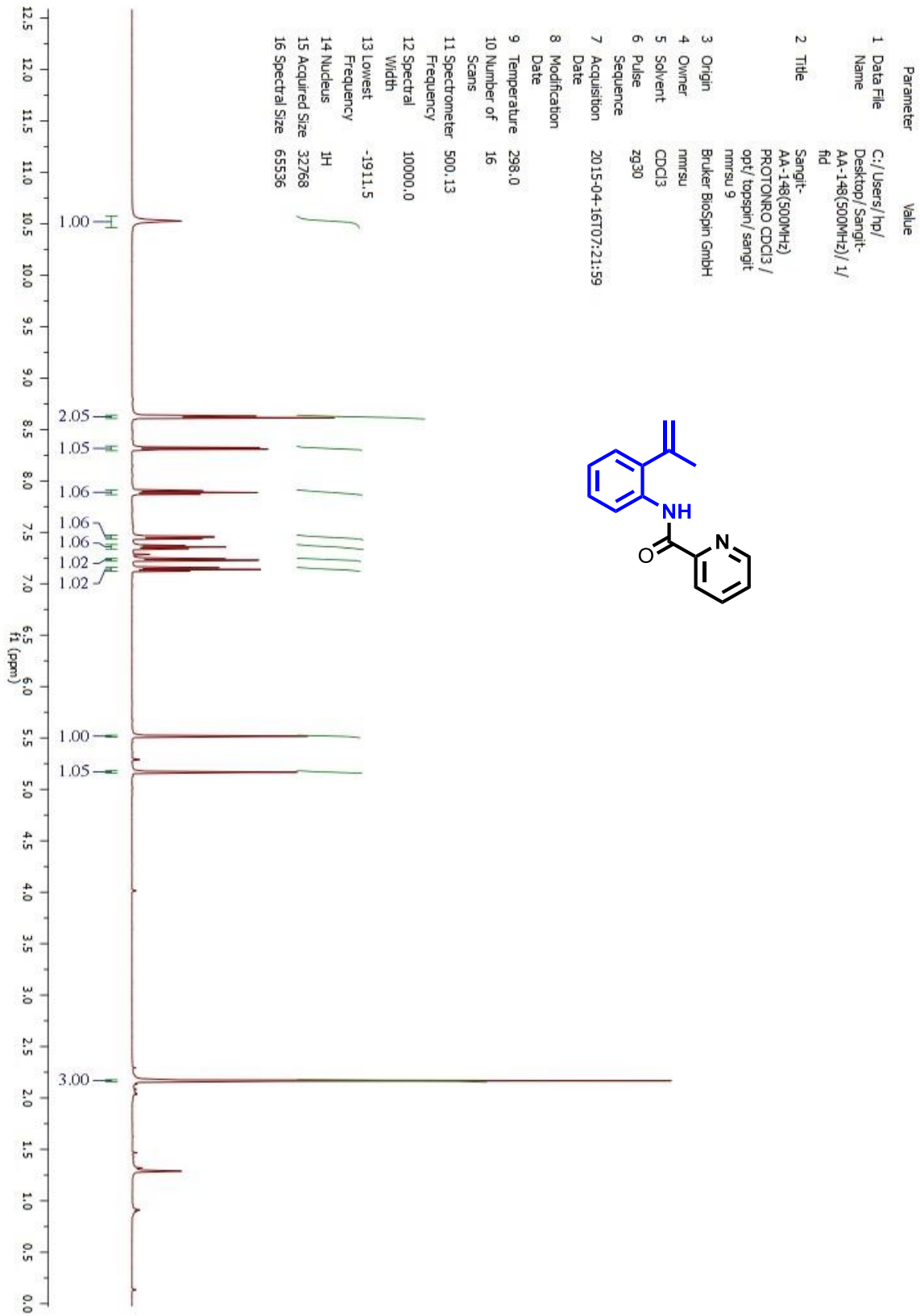
S90 ^{13}C NMR of **3t**



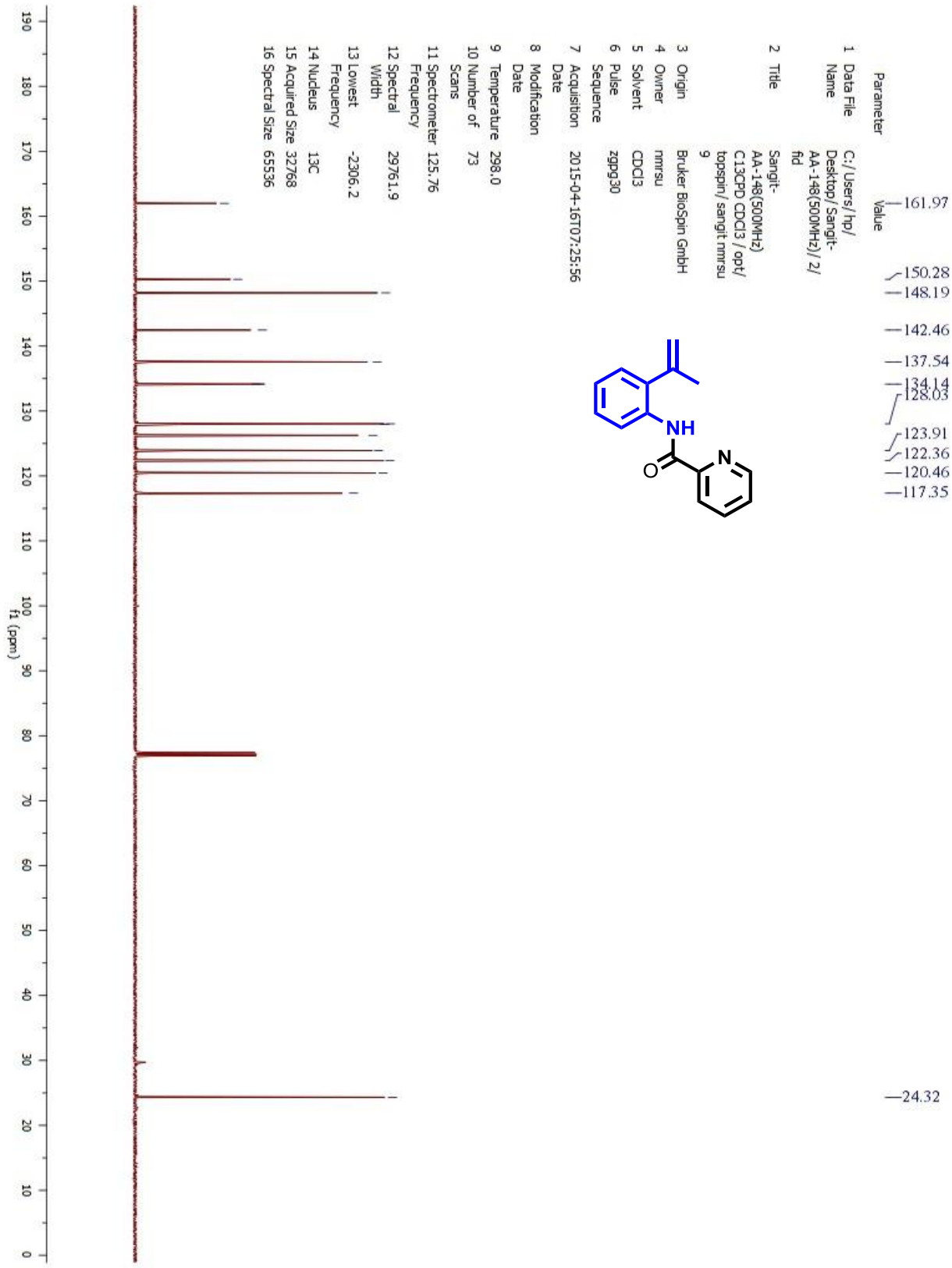
S91 ^{19}F NMR of **3t**



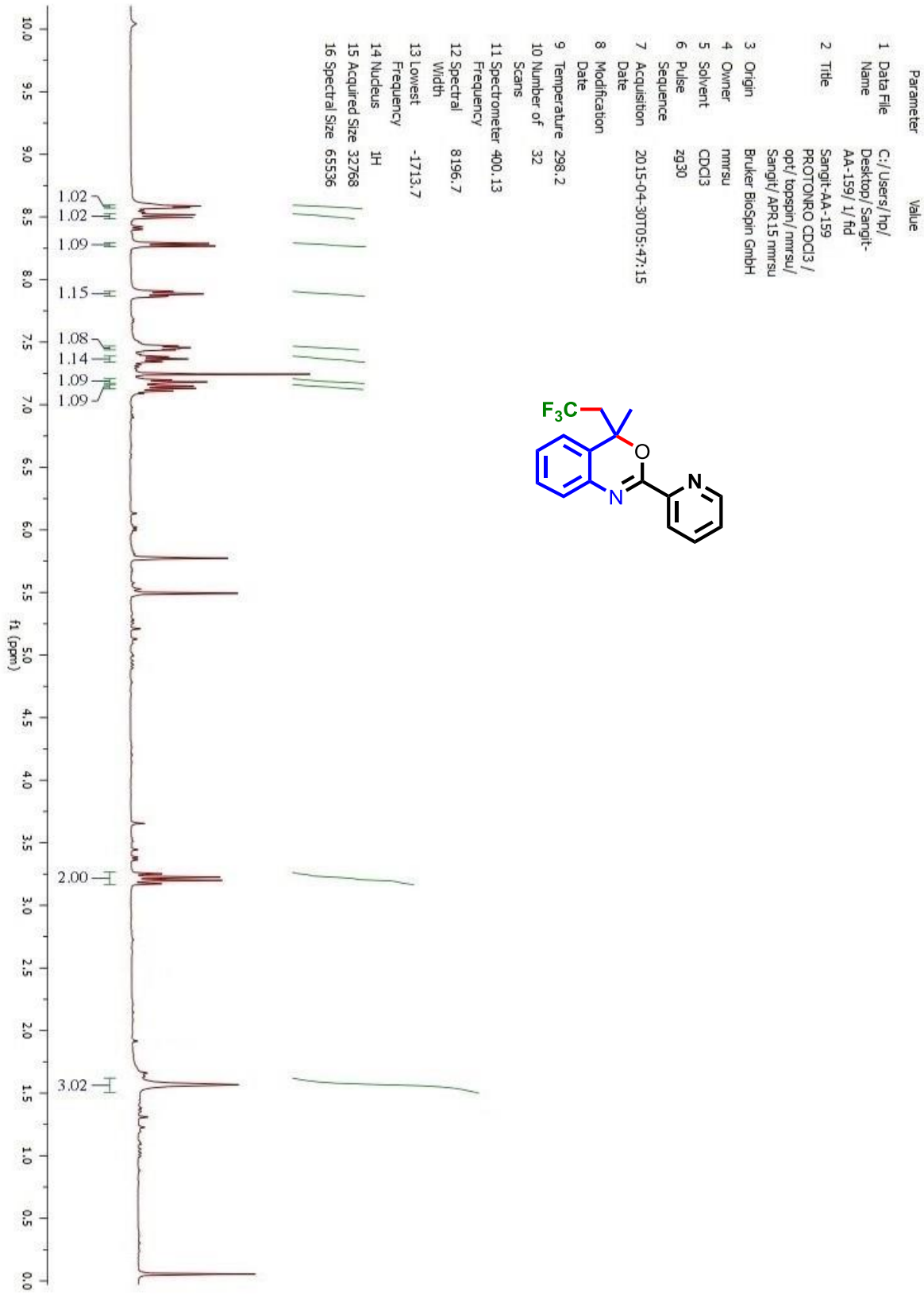
S92 ^{1}H NMR of **1u**



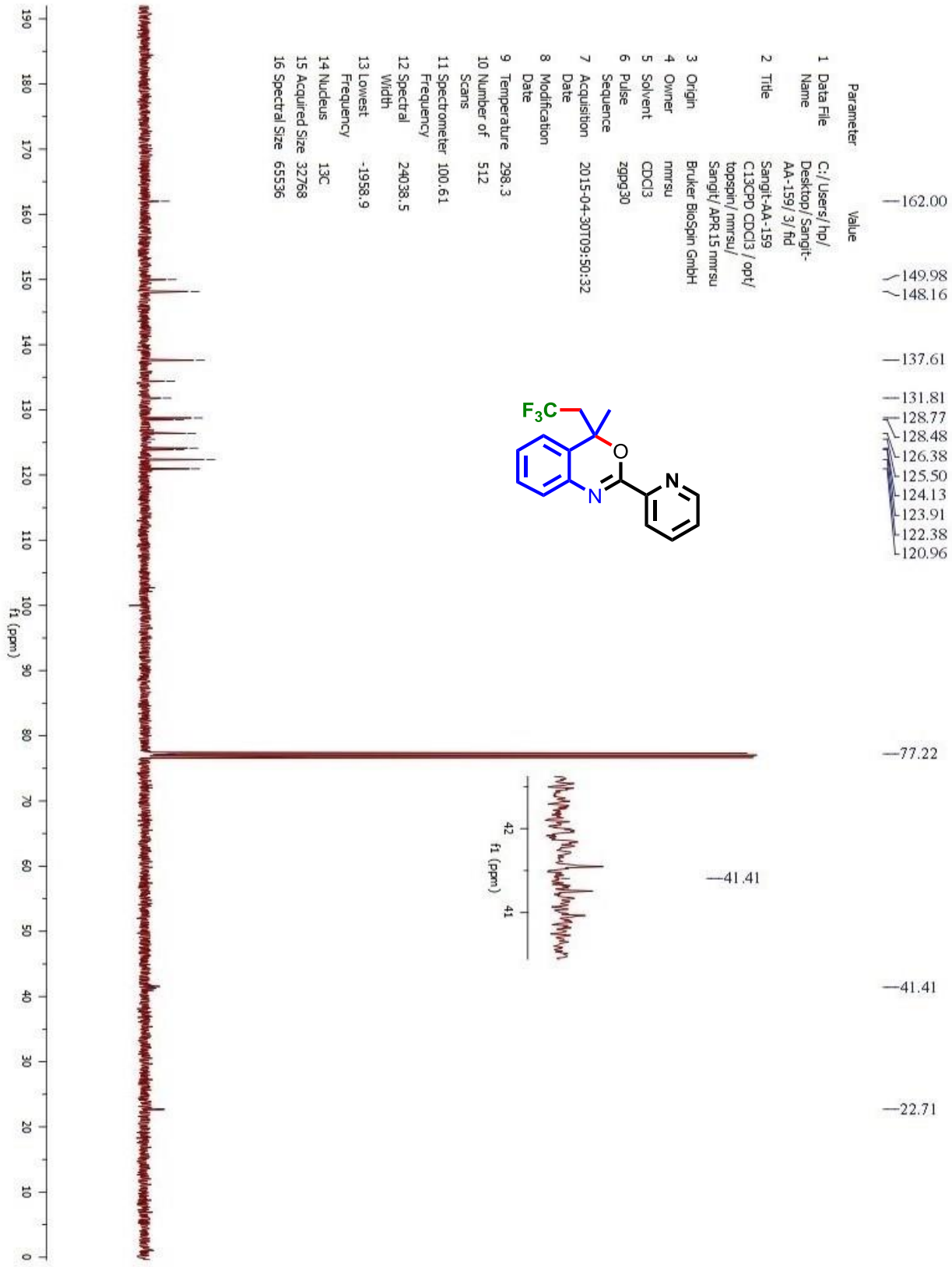
S93 ^{13}C NMR of **1u**



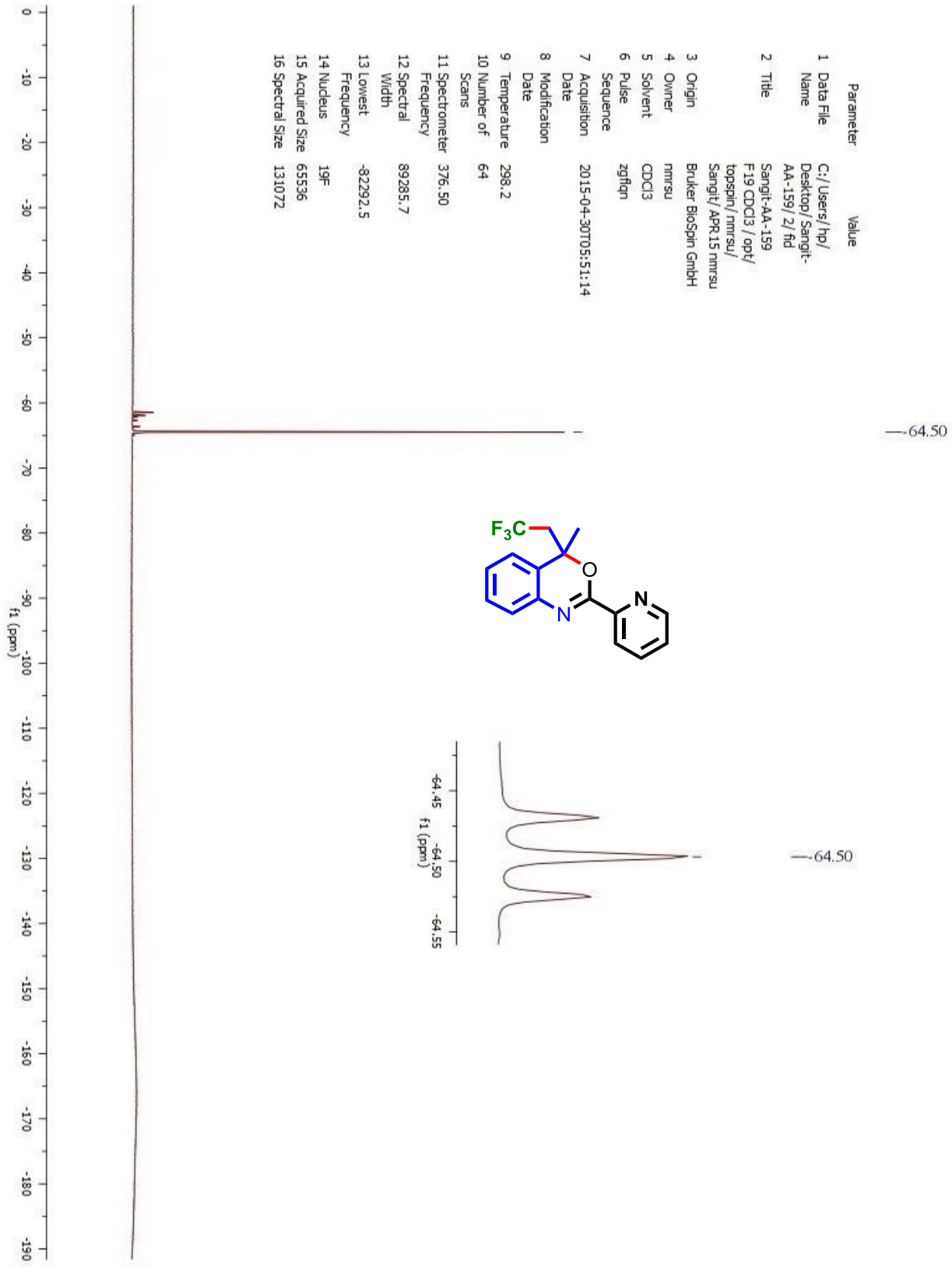
S94 ^{1}H NMR of **3u**



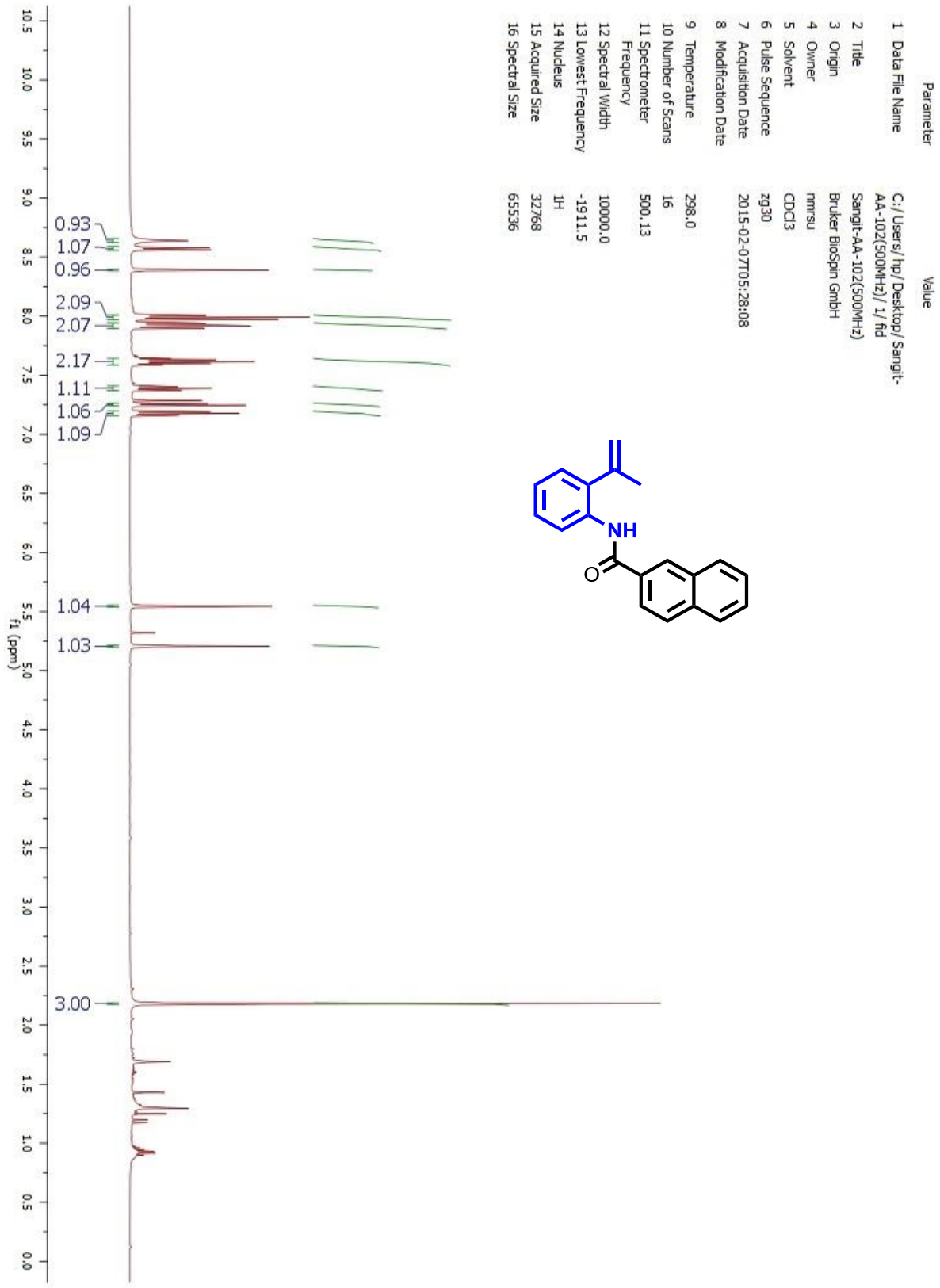
S95 ^{13}C NMR of **3u**



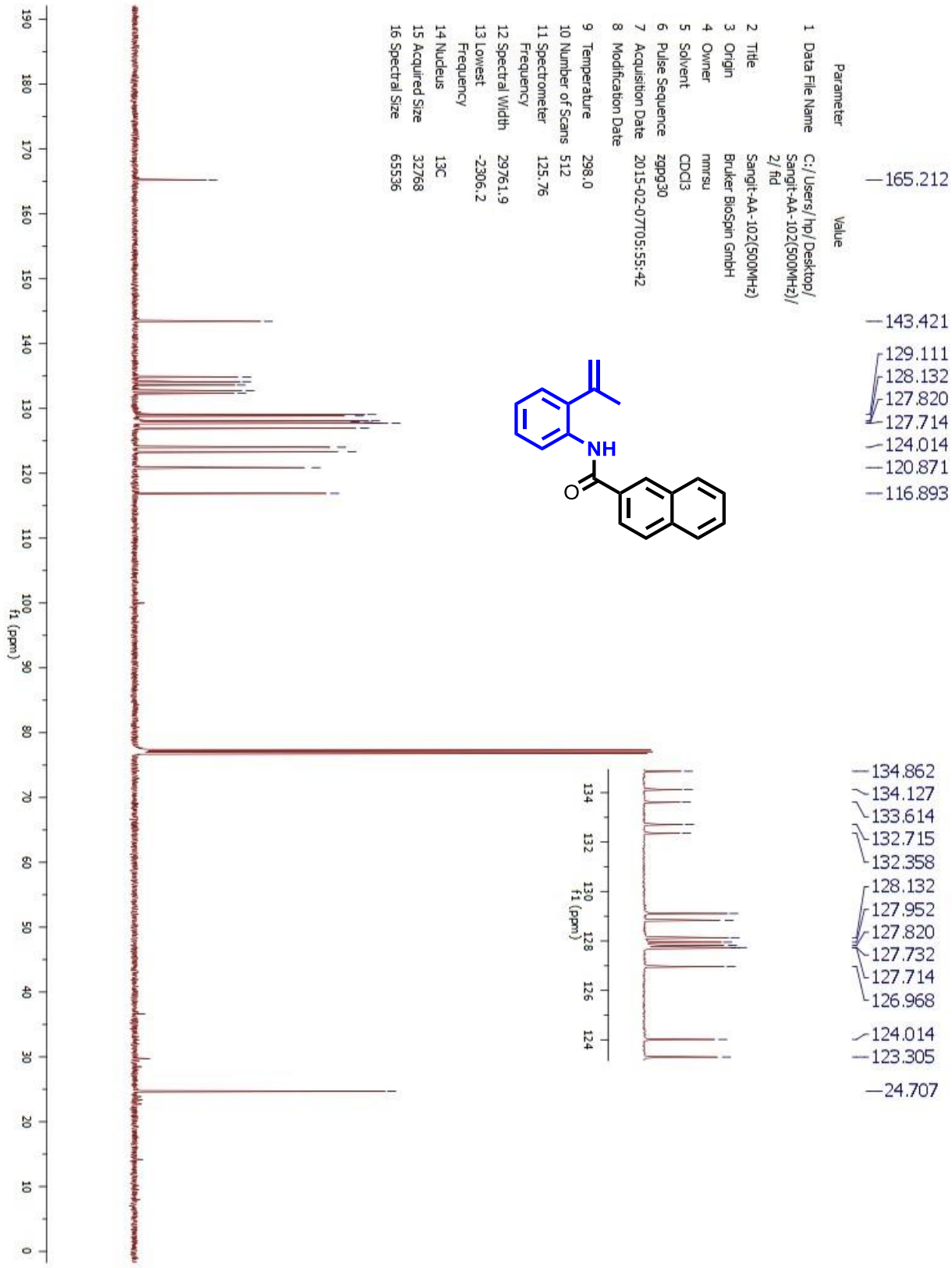
S96 ^{19}F NMR of **3u**



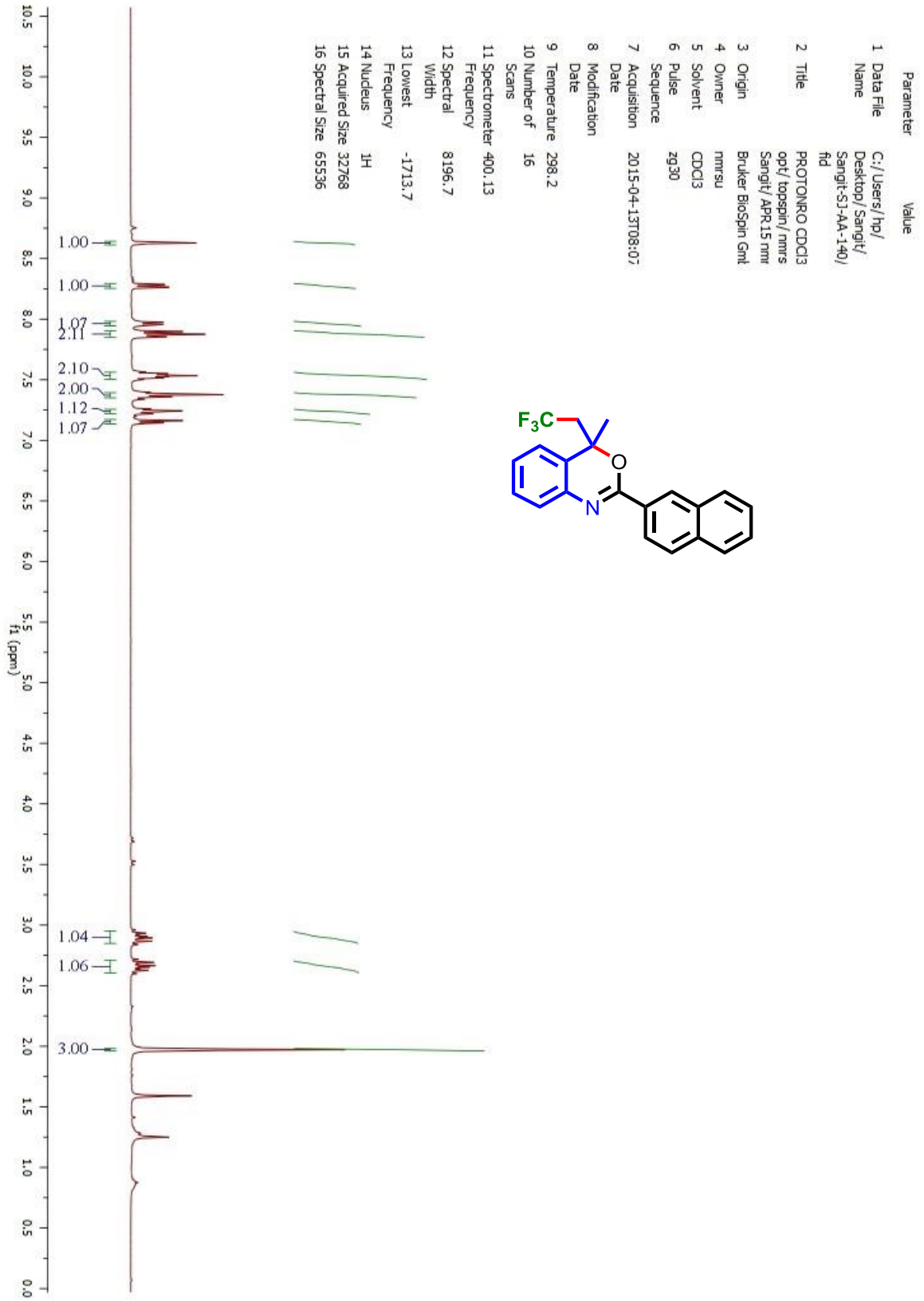
S97 ^{1}H NMR of **1v**



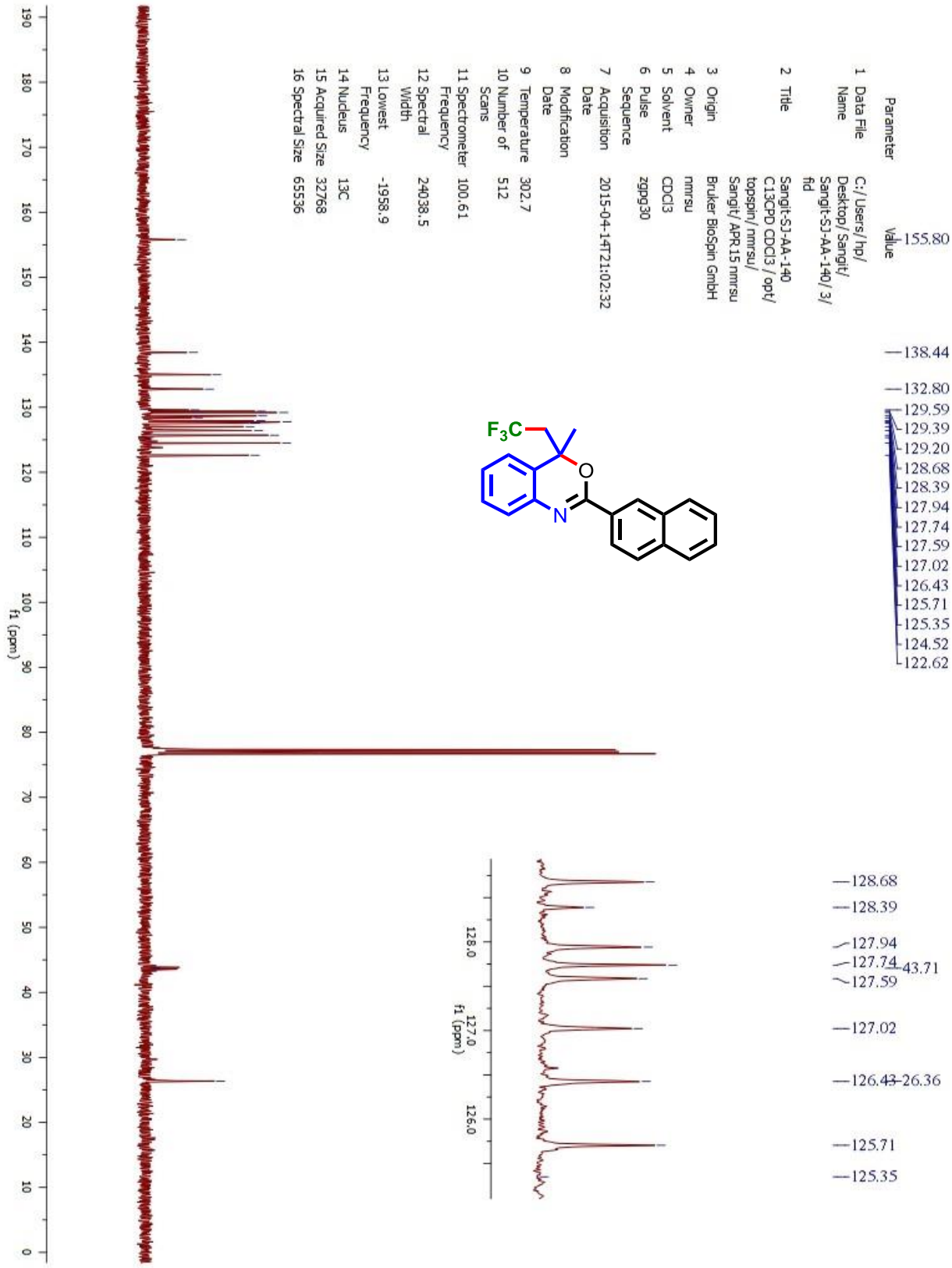
S98 ^{13}C NMR of **1v**



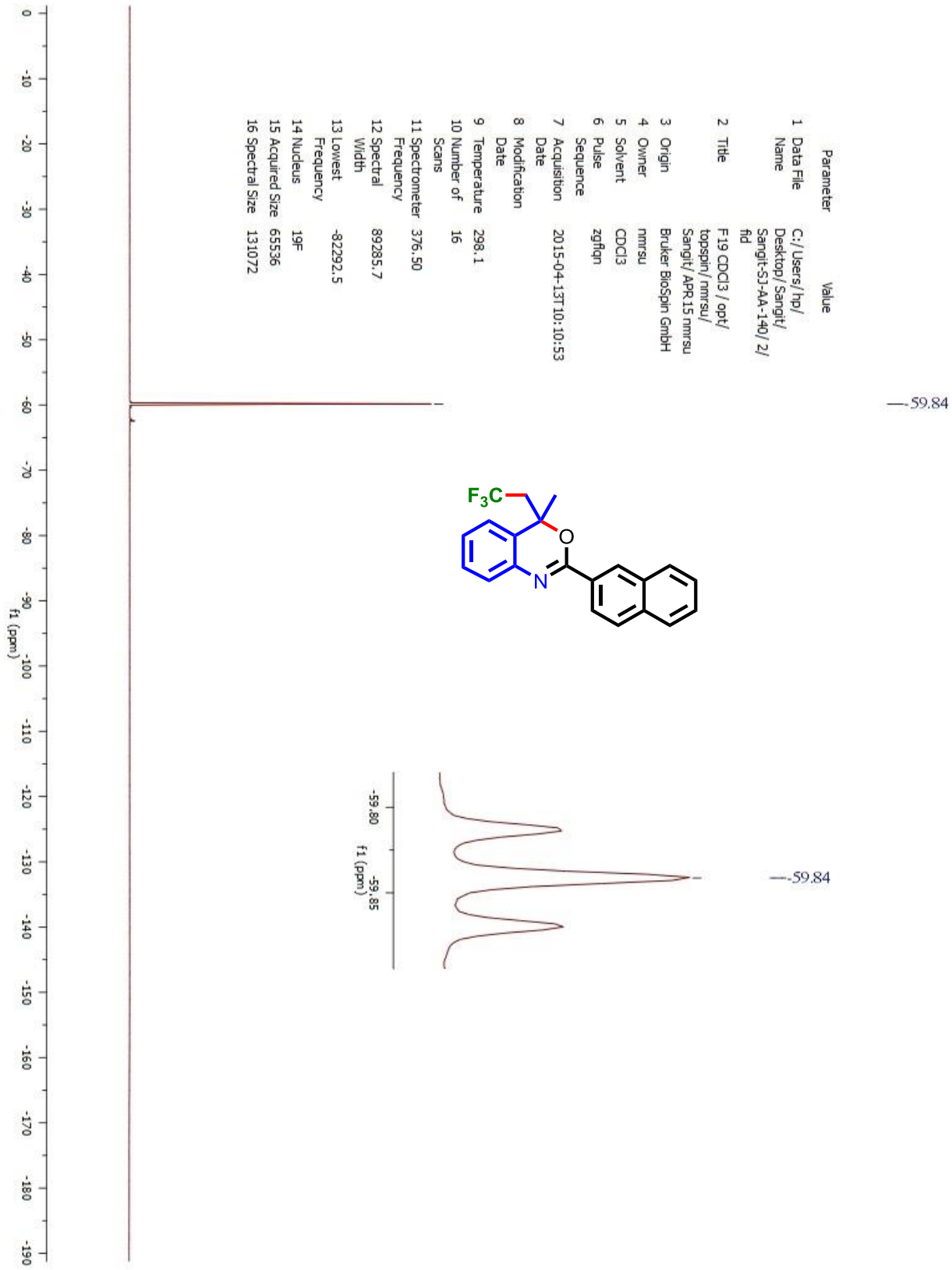
S99 ^{1}H NMR of **3v**



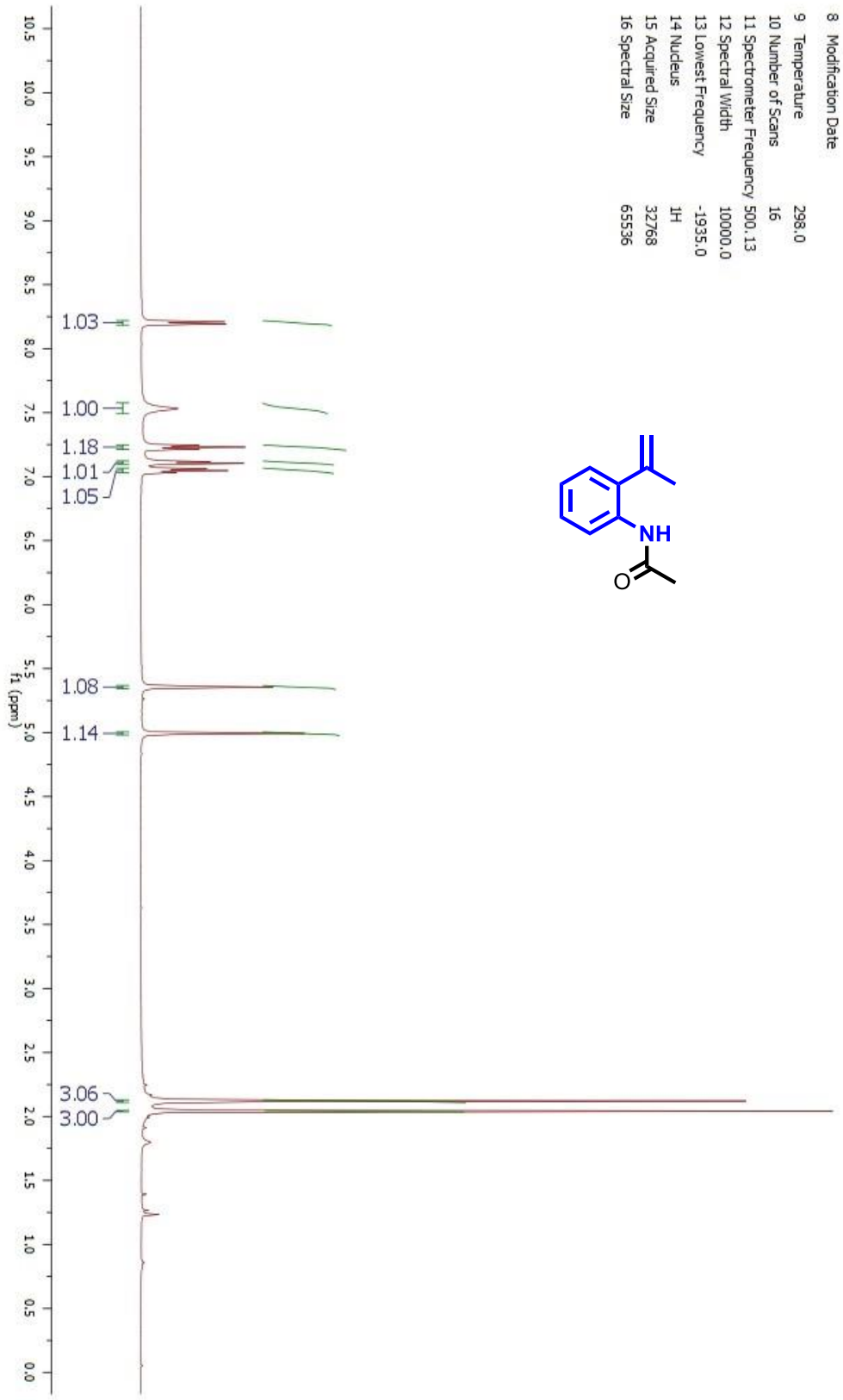
S100 ^{13}C NMR of **3v**



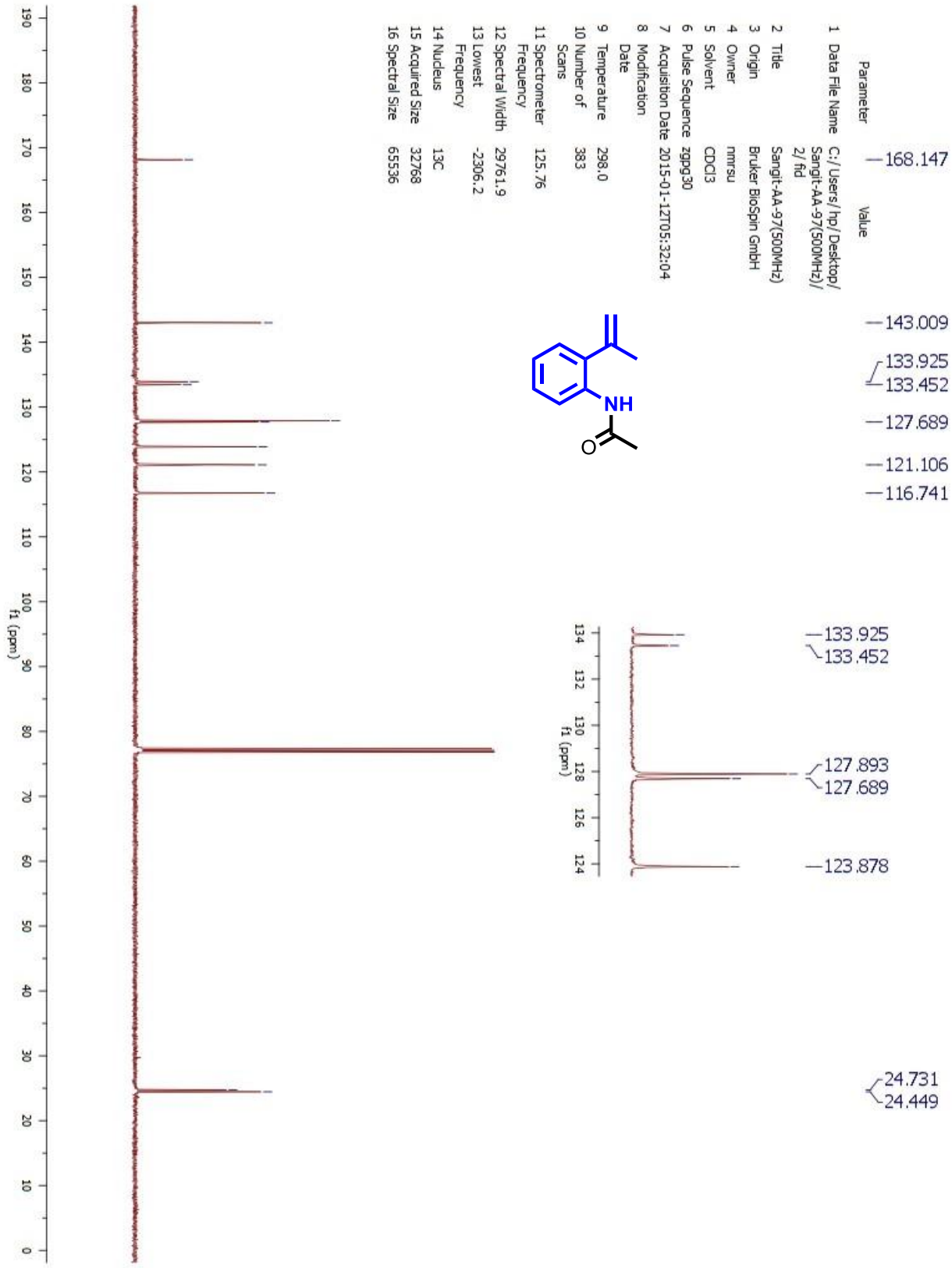
S101 ^{19}F NMR of **3v**



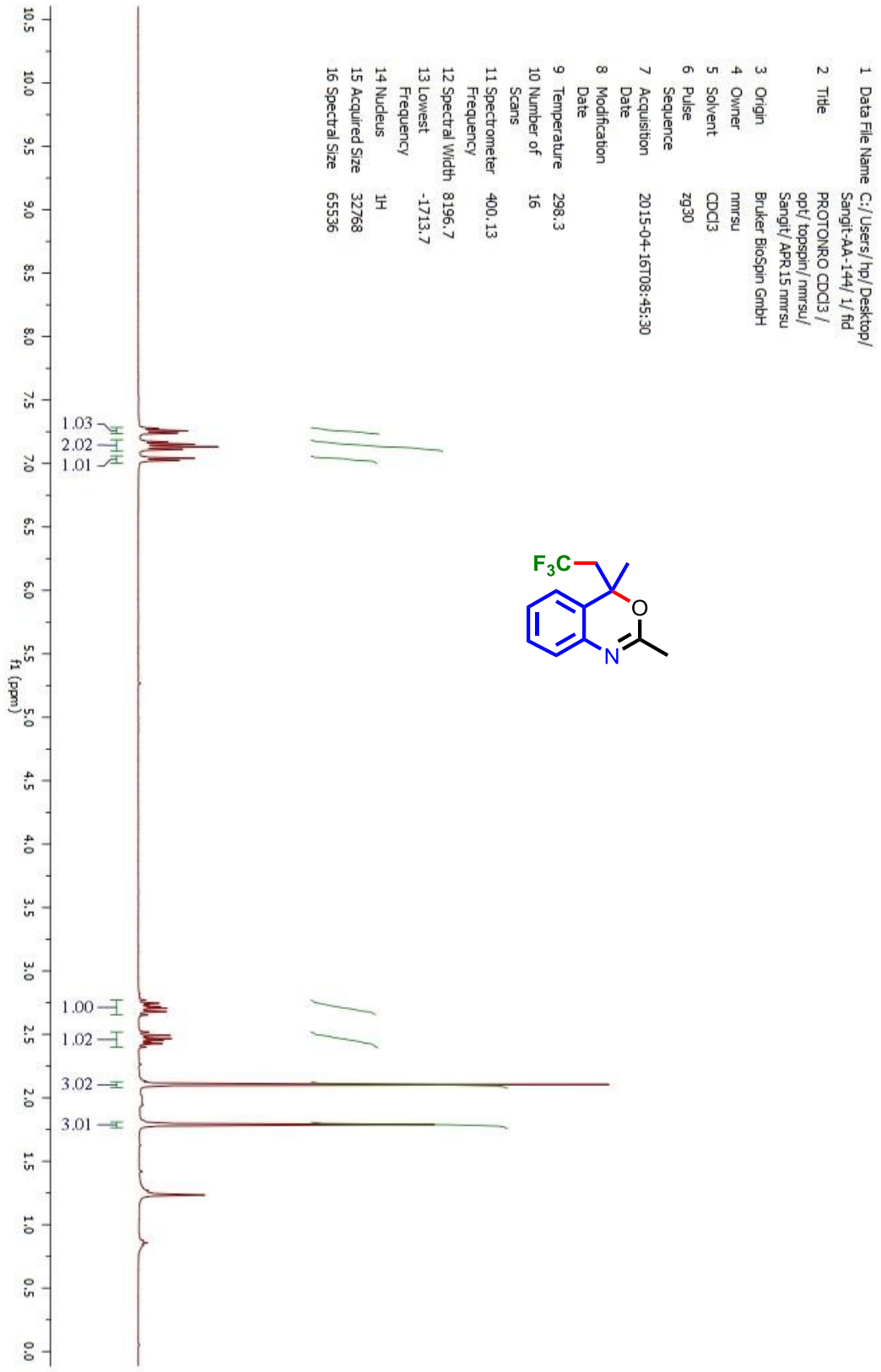
S102 ^{1}H NMR of **1w**



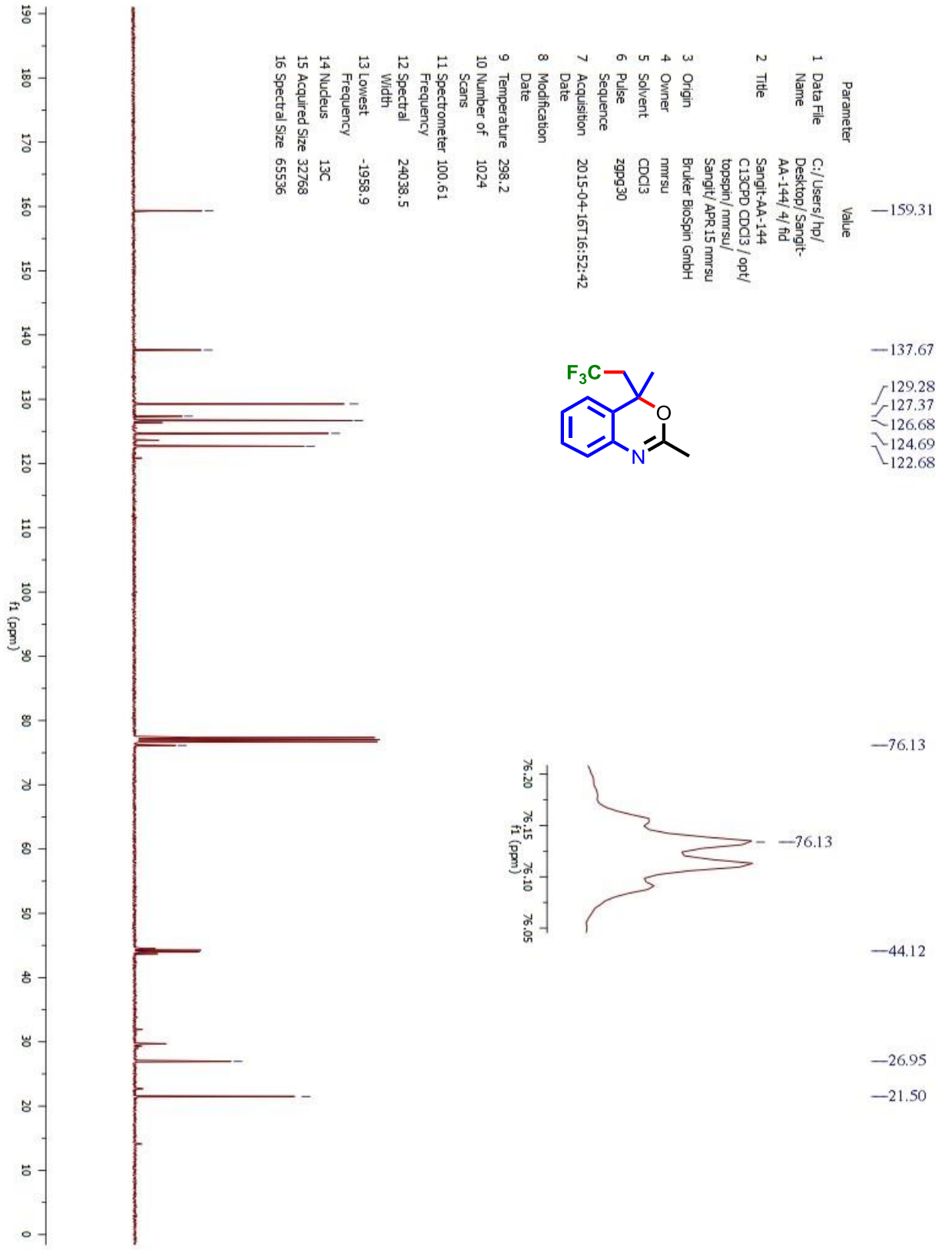
S103 ^{13}C NMR of **1w**



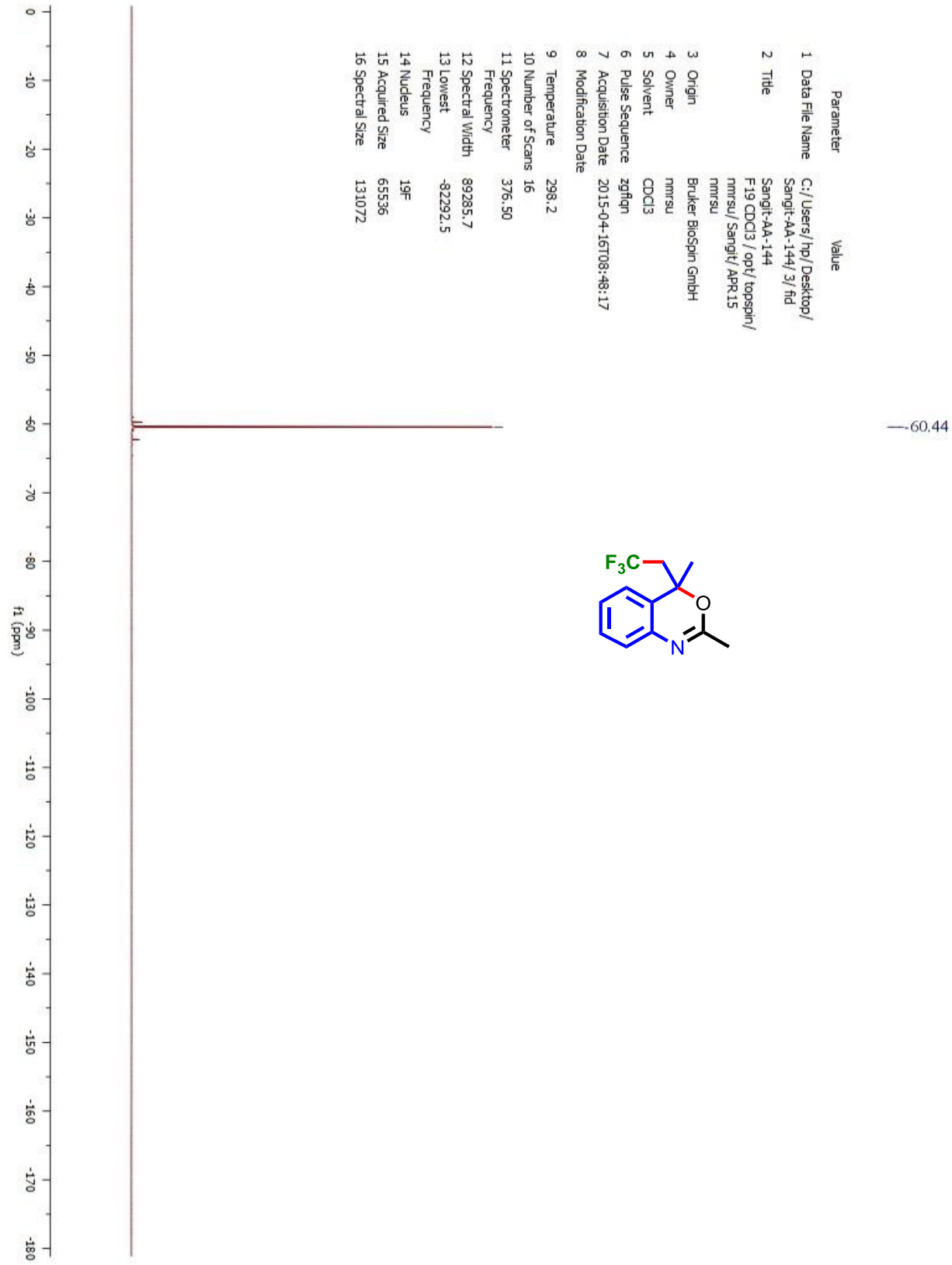
S104 ^{1}H NMR of **3w**



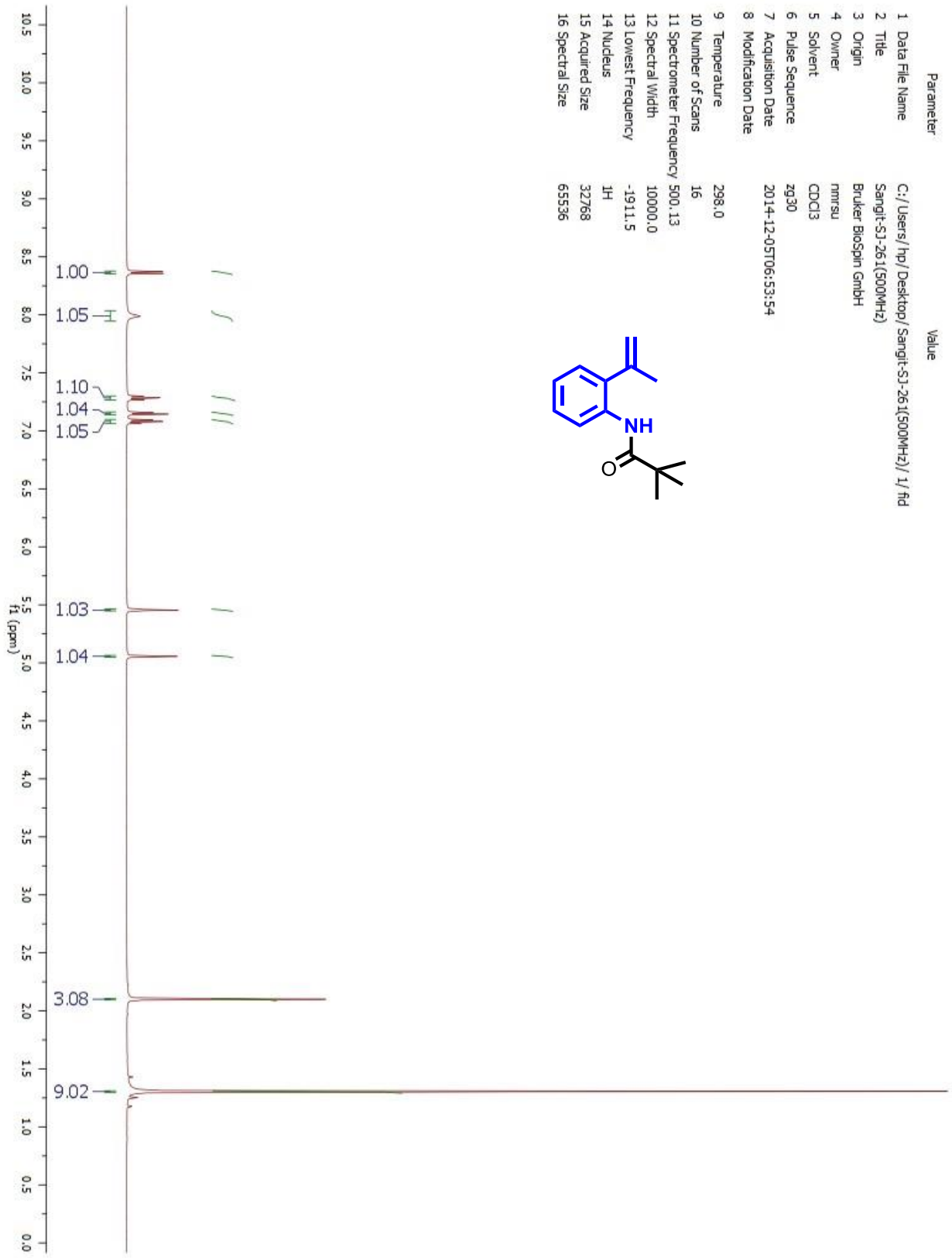
S105 ^{13}C NMR of **3w**



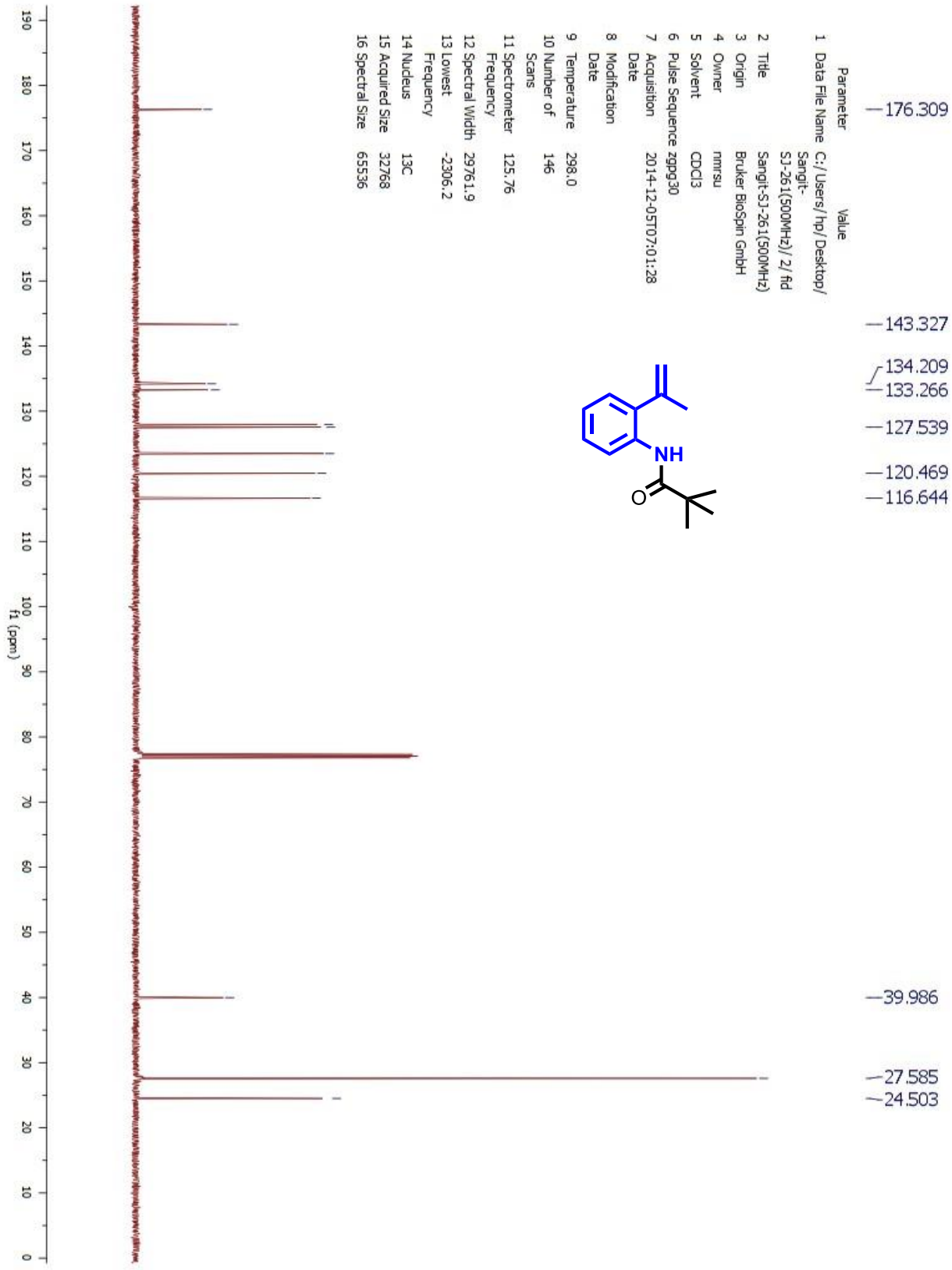
S106 ^{19}F NMR of **3w**



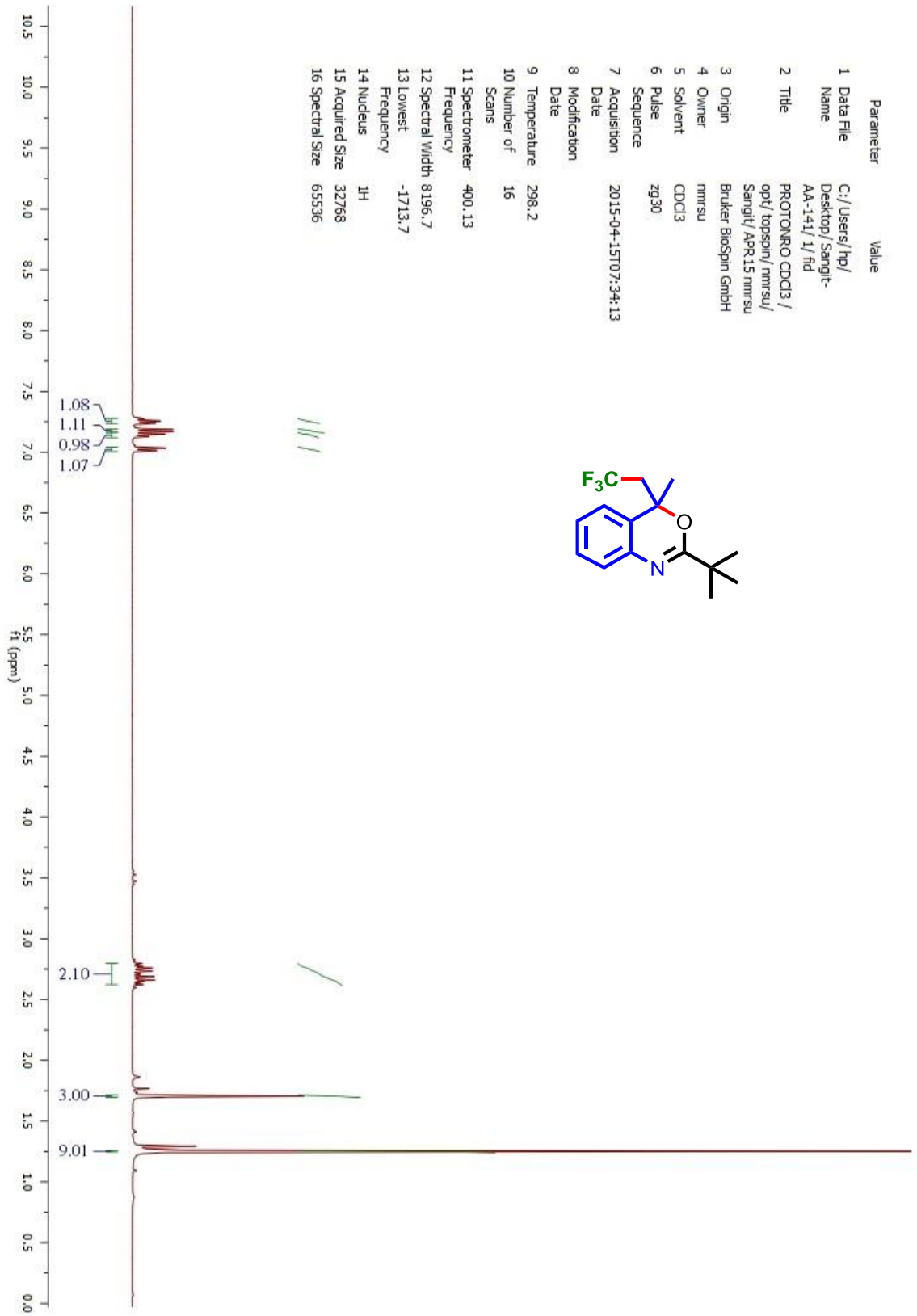
S107 ^{1}H NMR of **1x**



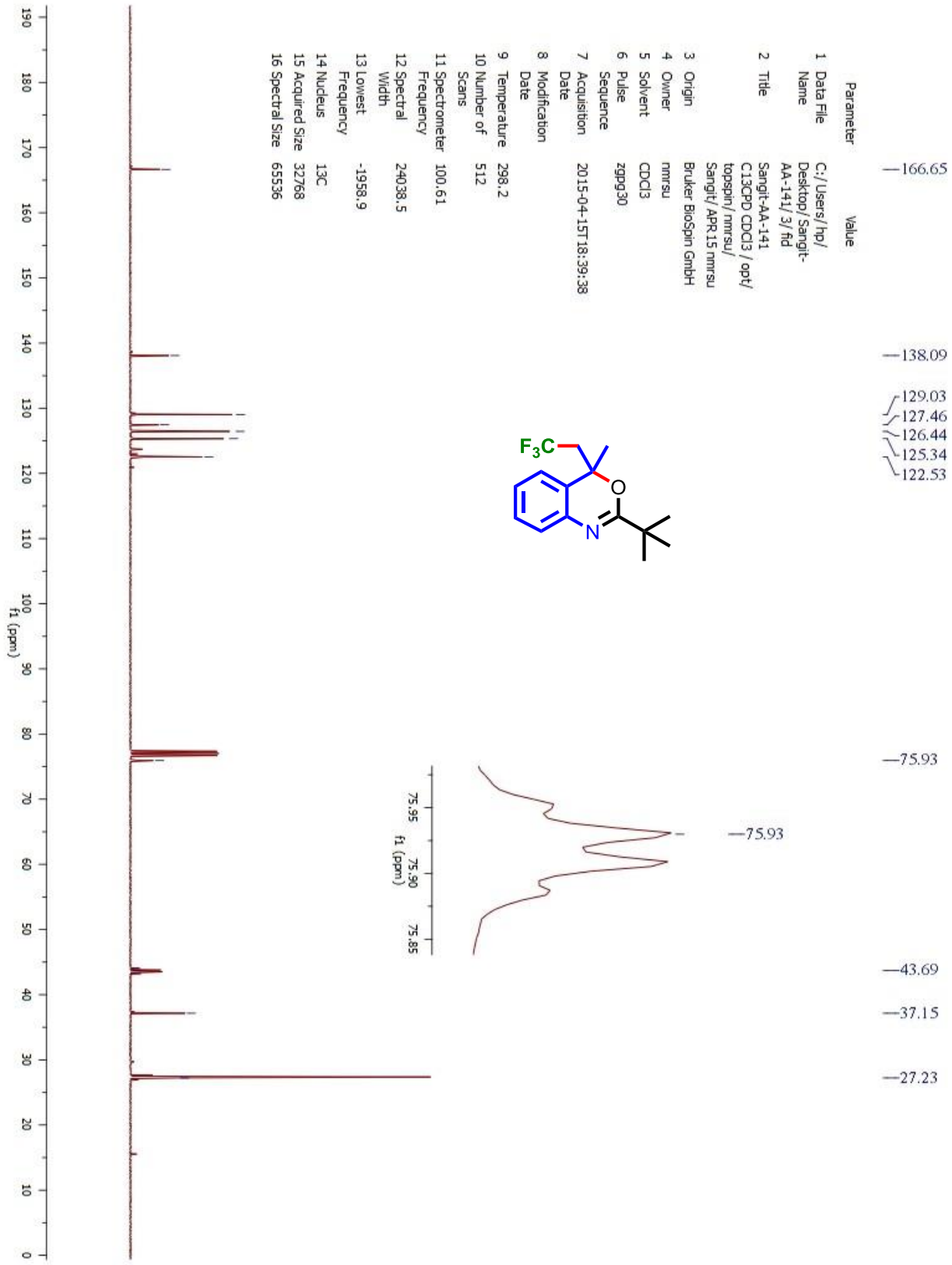
S108 ^{13}C NMR of **1x**



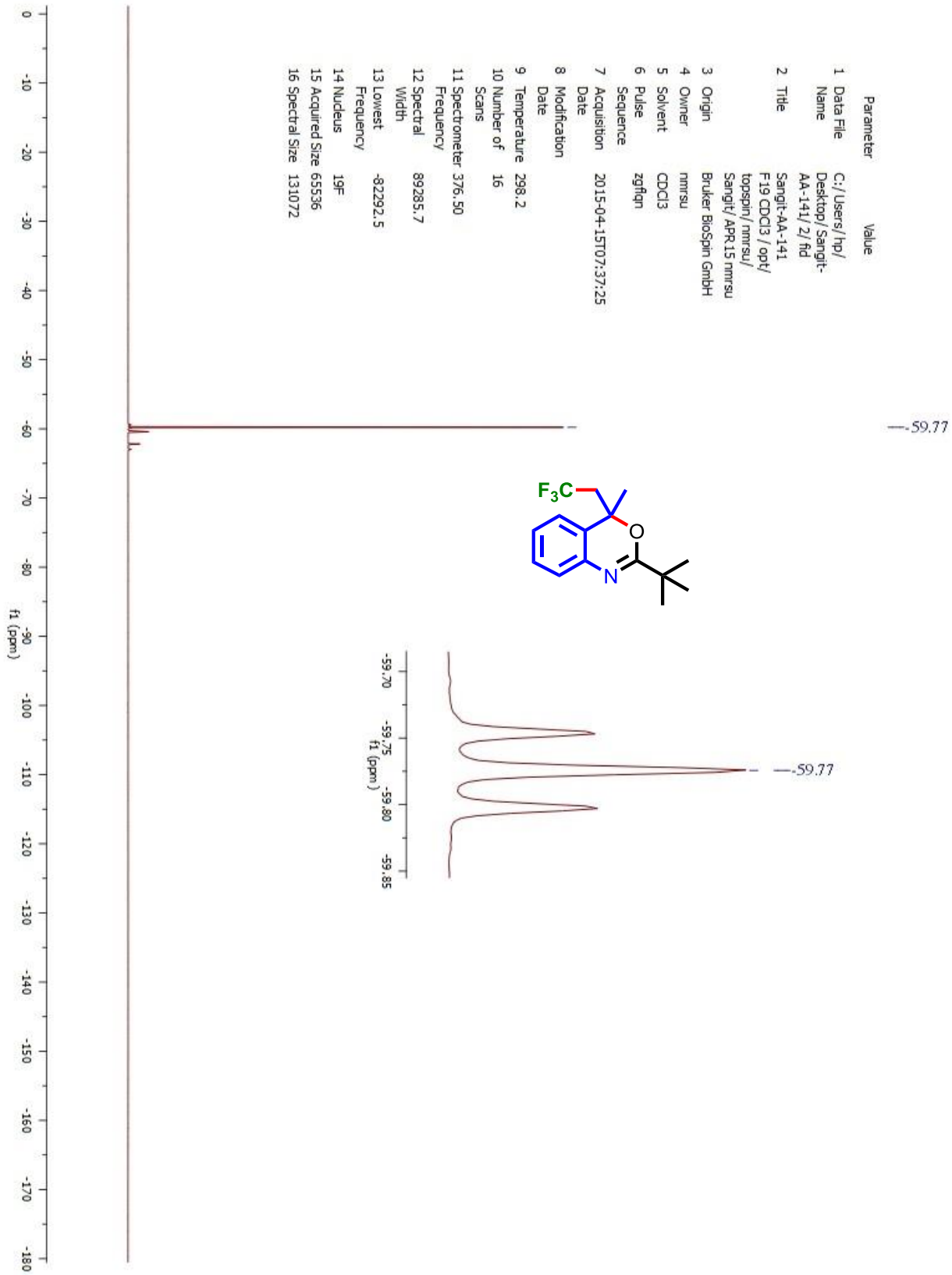
S109 ^{1}H NMR of **3x**



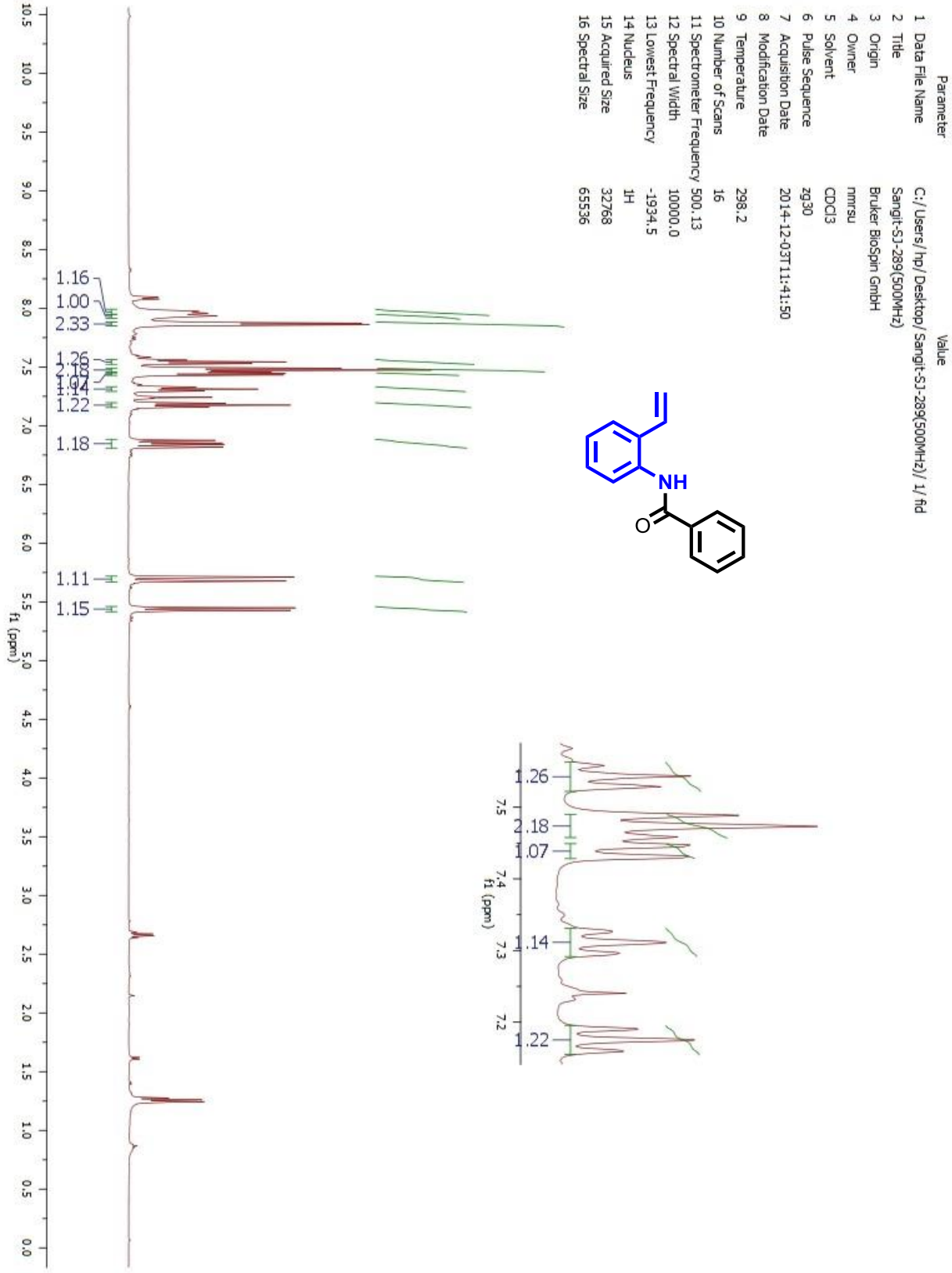
S110 ^{13}C NMR of **3x**



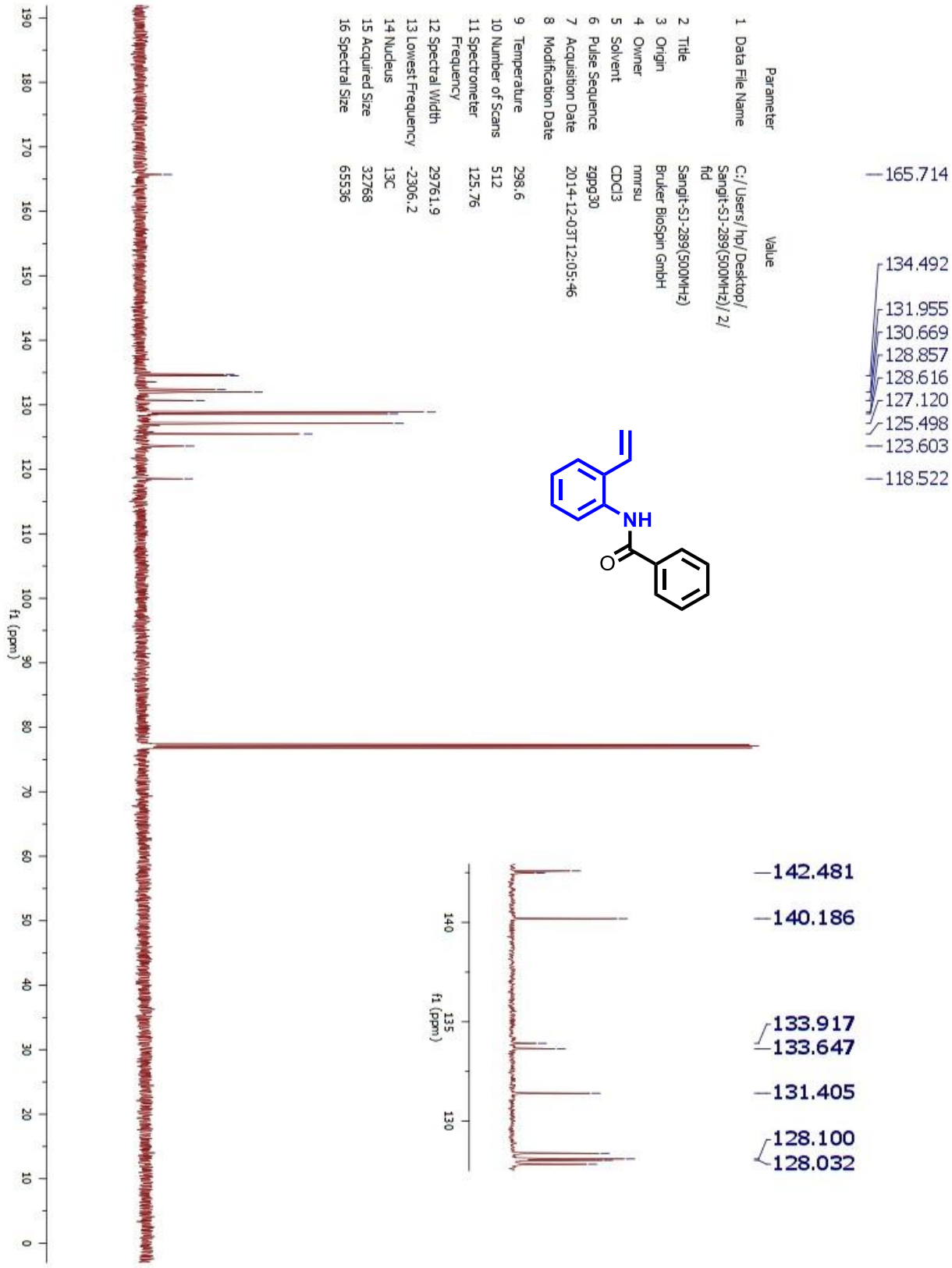
S111 ^{19}F NMR of **3x**



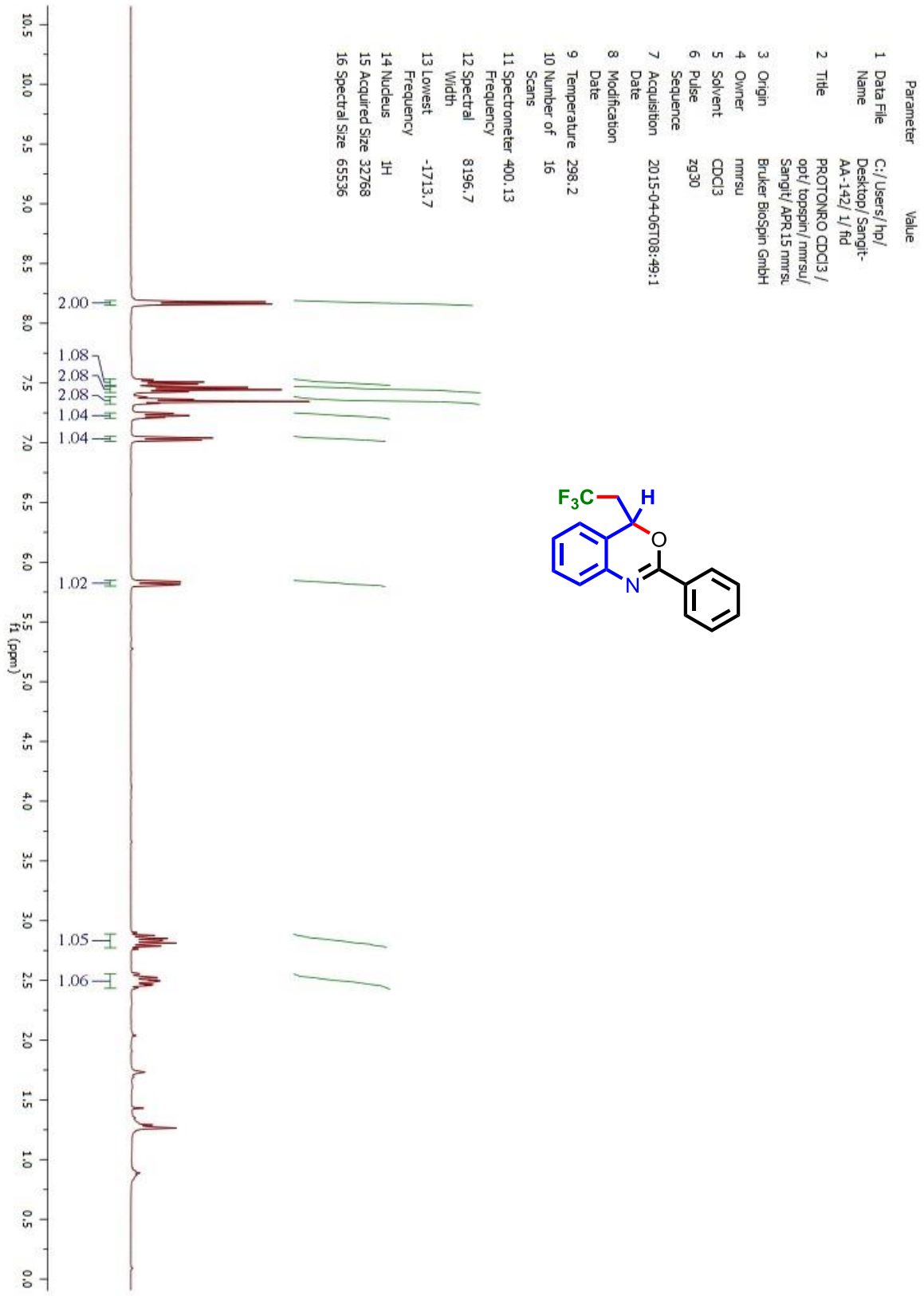
S112 ^{1}H NMR of **1y**



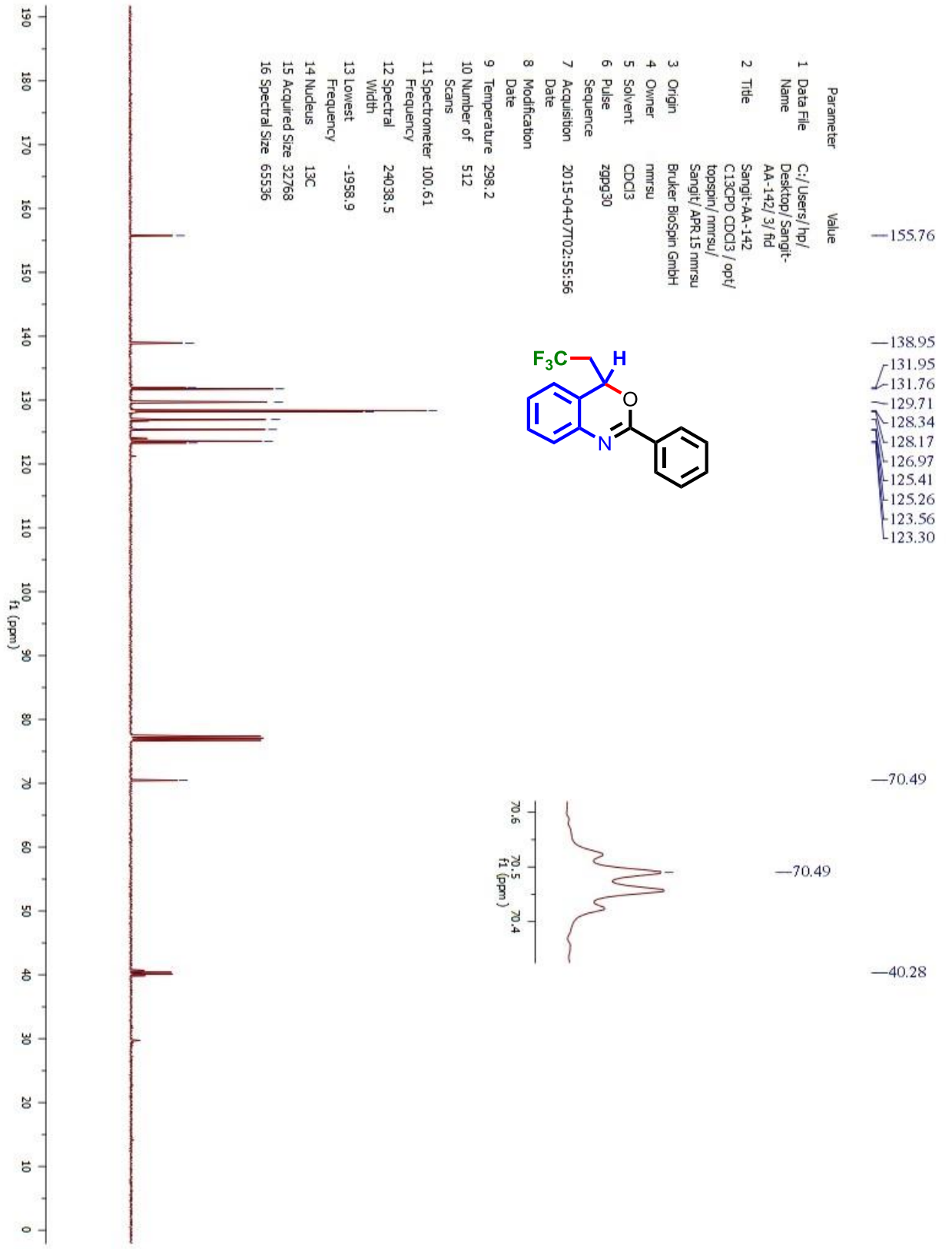
S113 ^{13}C NMR of **1y**



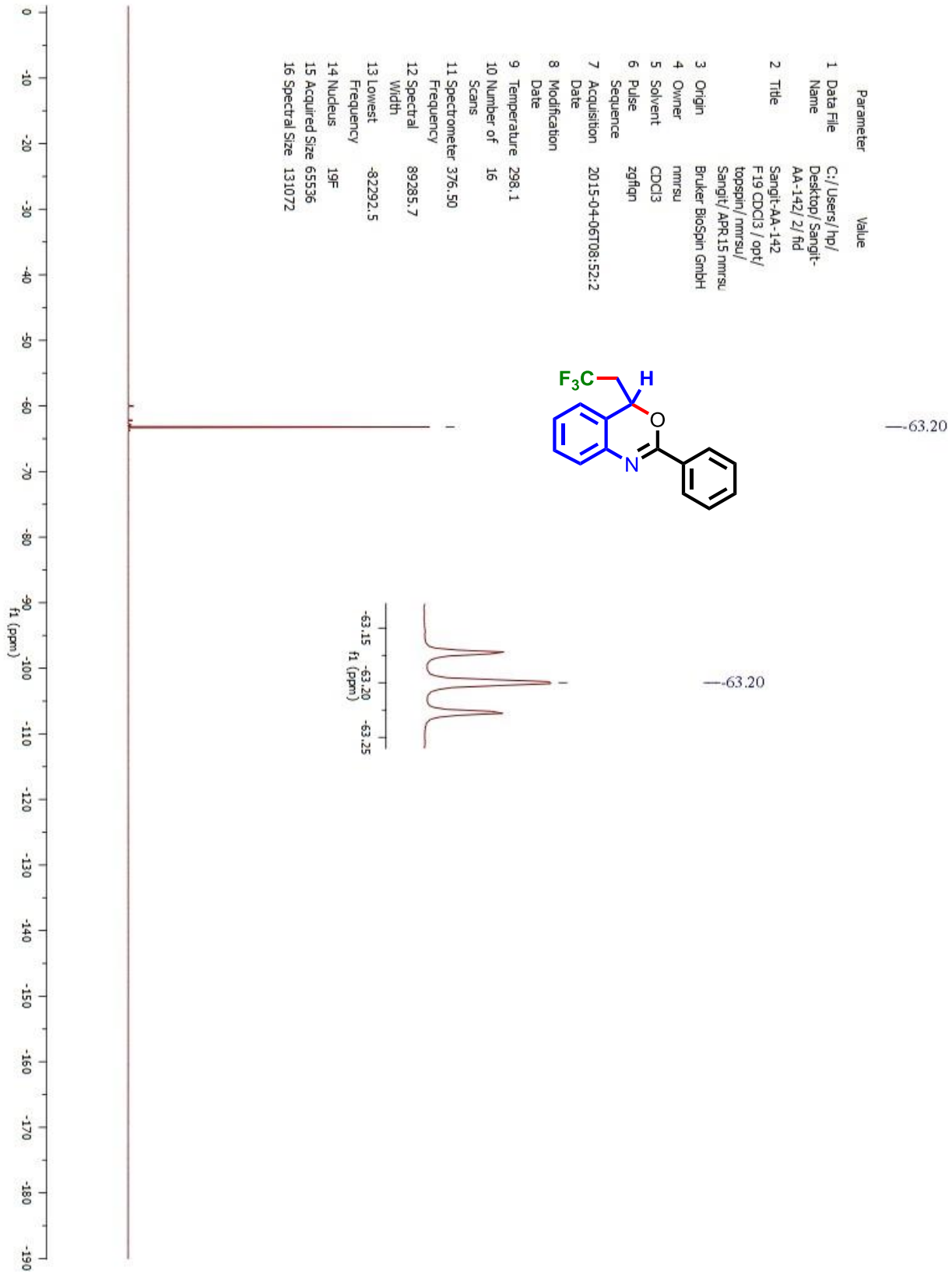
S114 ^{1}H NMR of **3y**



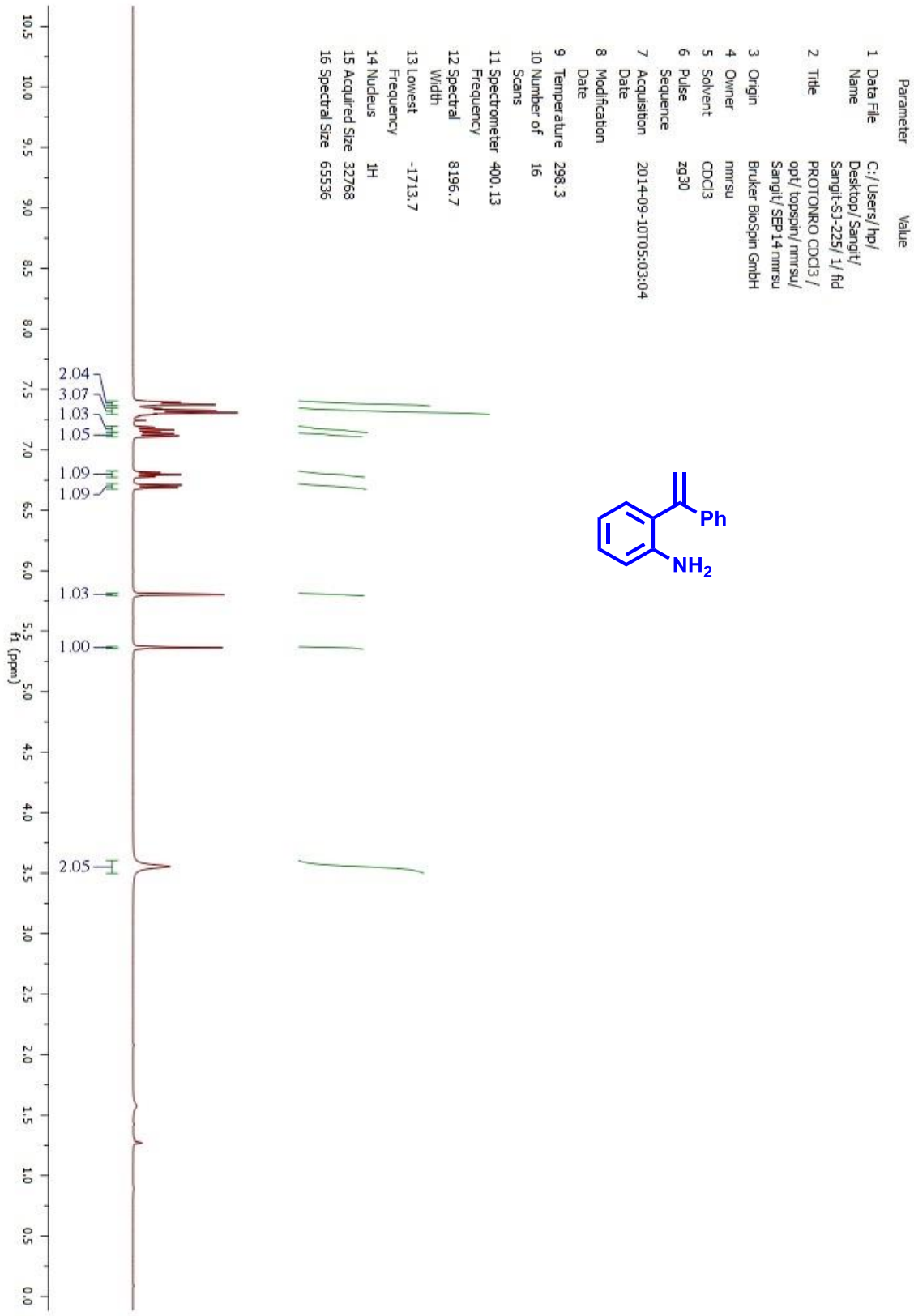
S115 ^{13}C NMR of **3y**



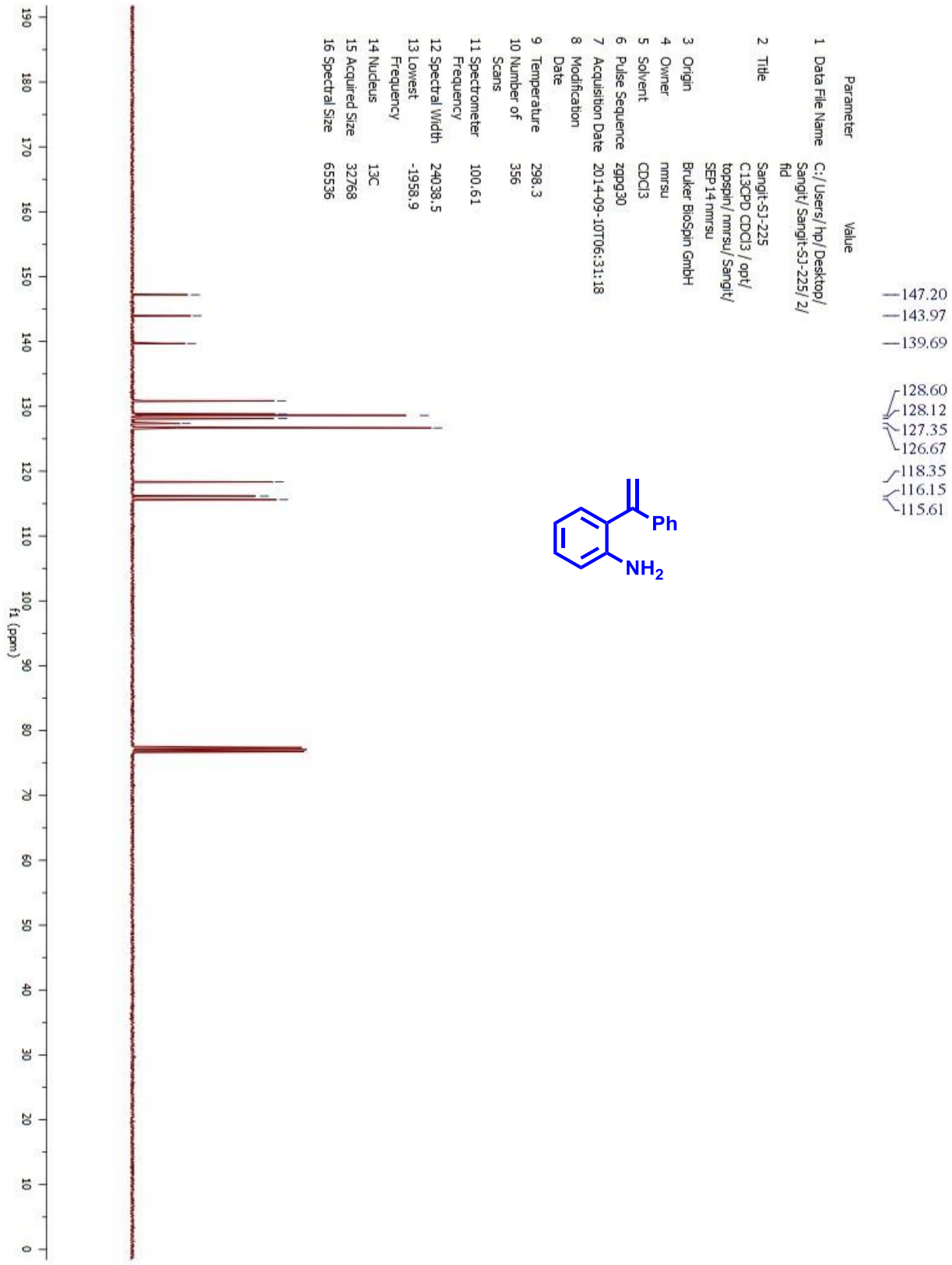
S116 ^{19}F NMR of **3y**



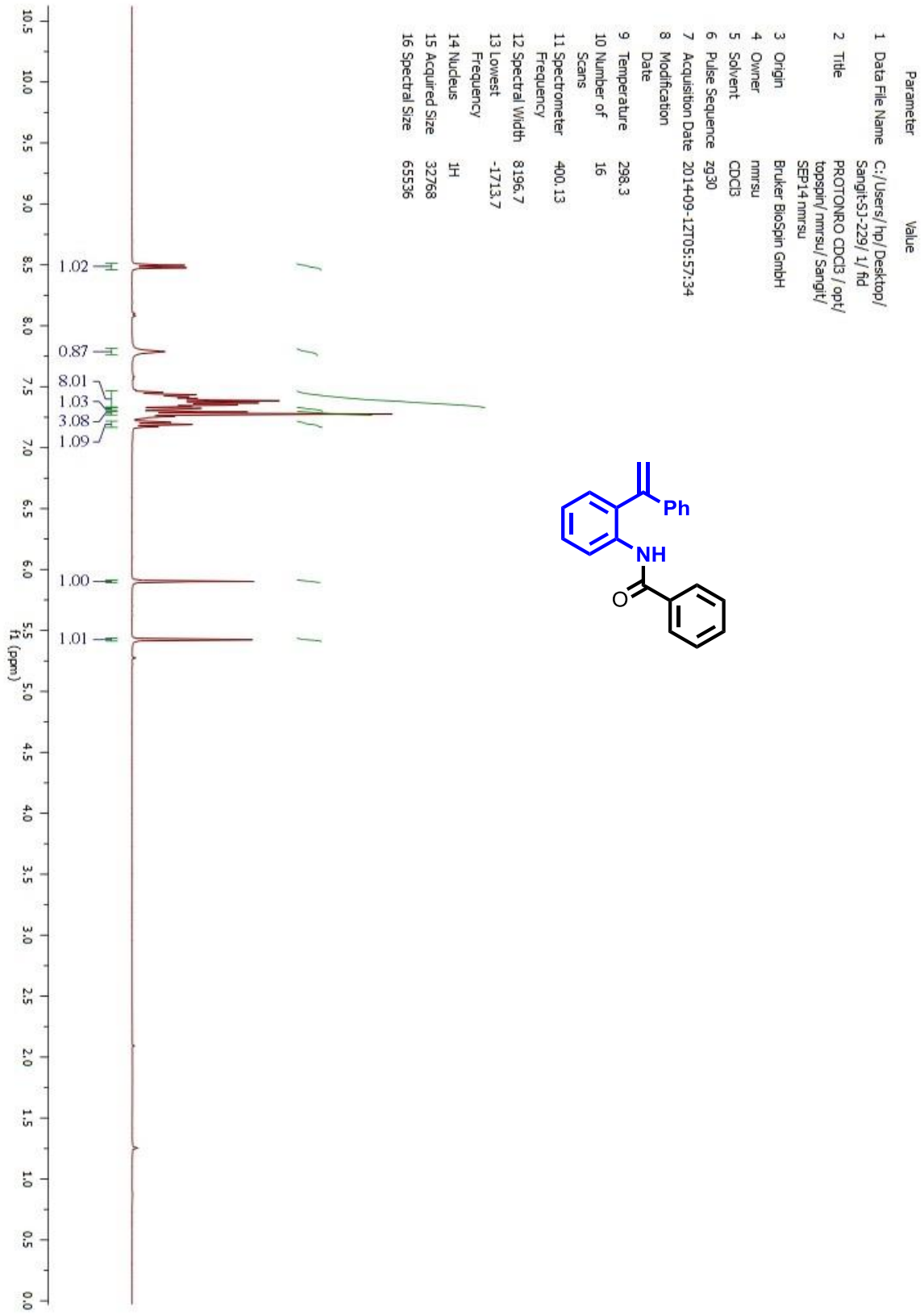
S117 ^{1}H NMR of **2-(1-Phenylvinyl)aniline**



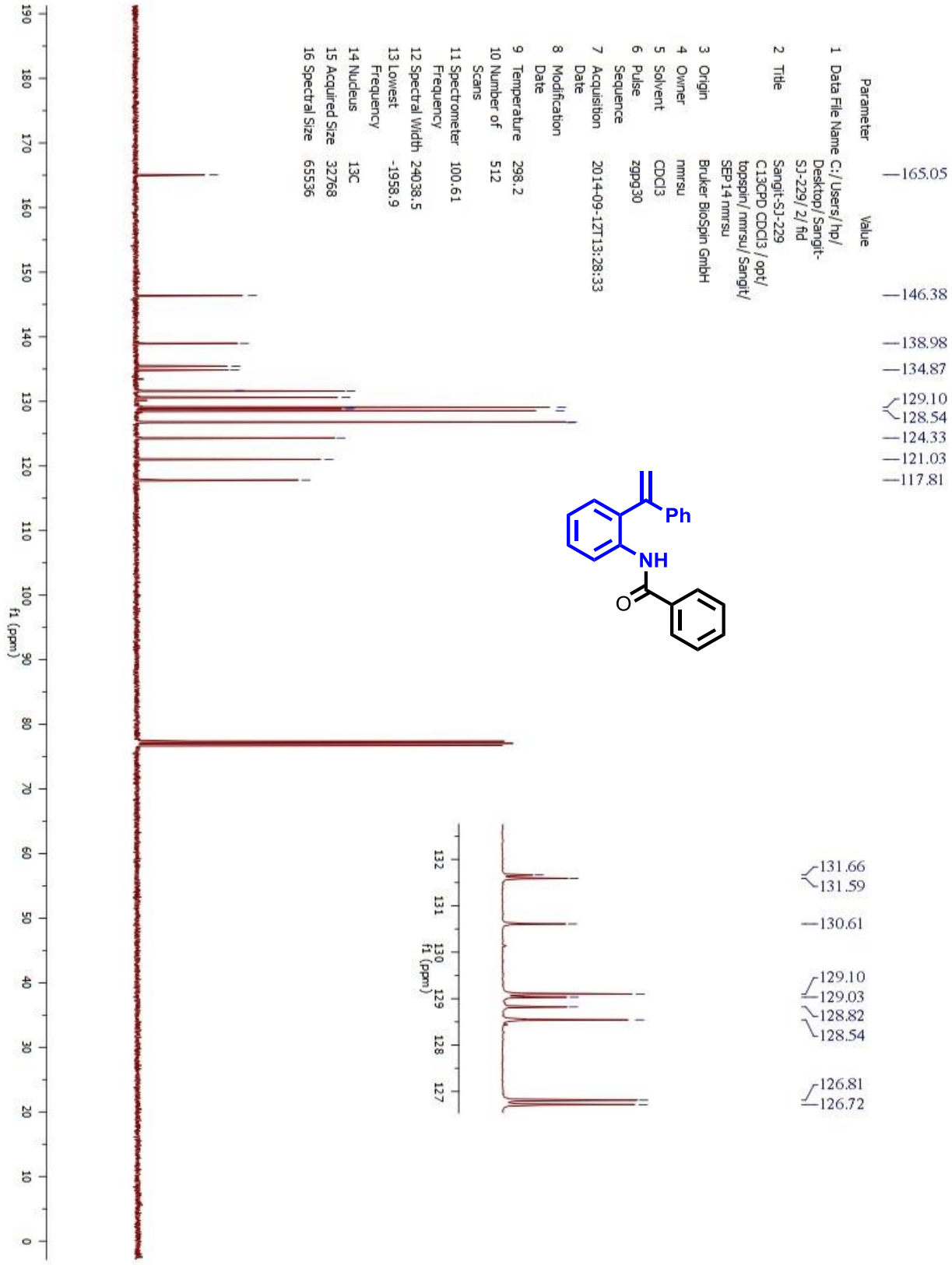
S118 ^{13}C NMR of **2-(1-Phenylvinyl)aniline**



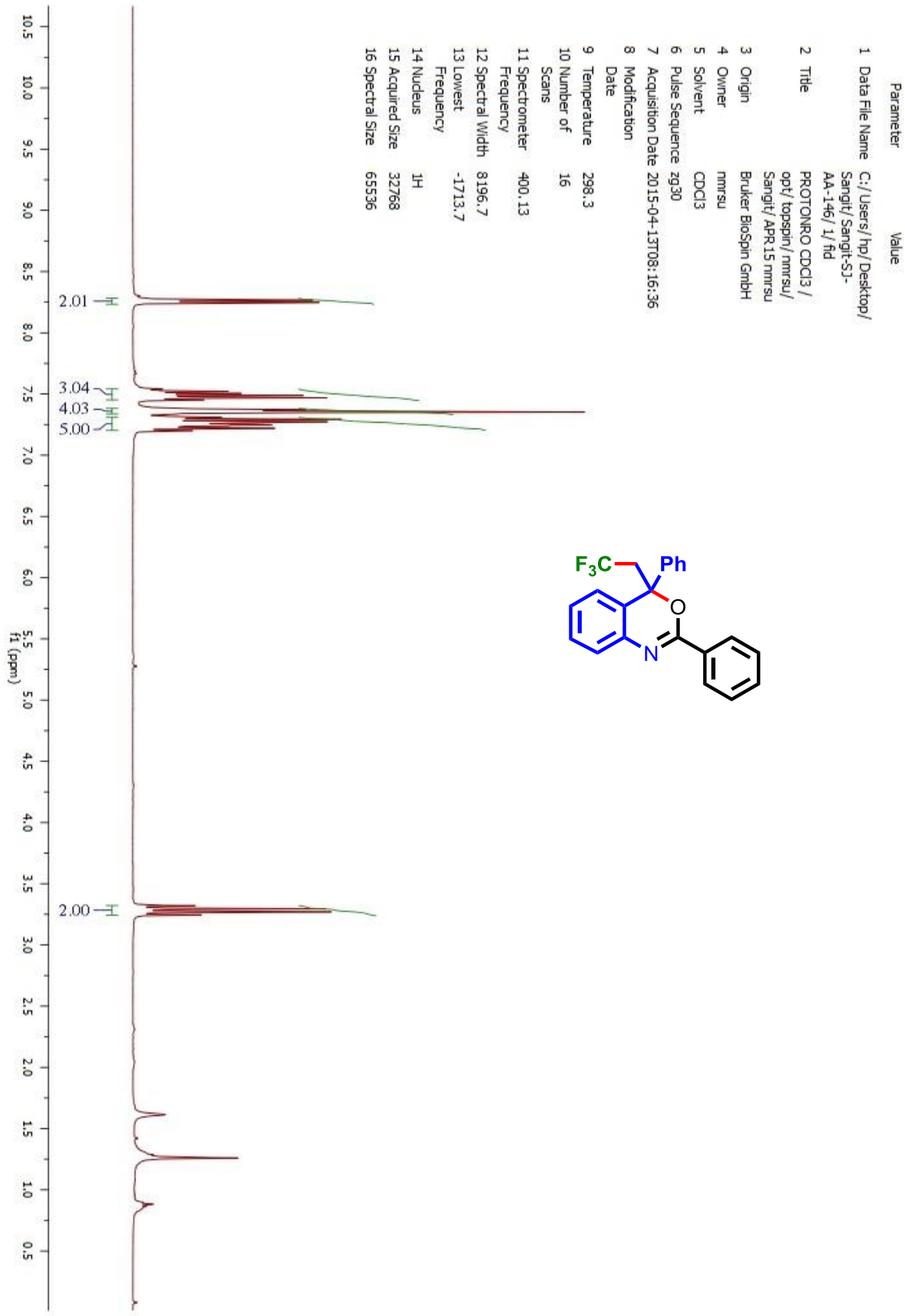
S119 ^{1}H NMR of **1z**



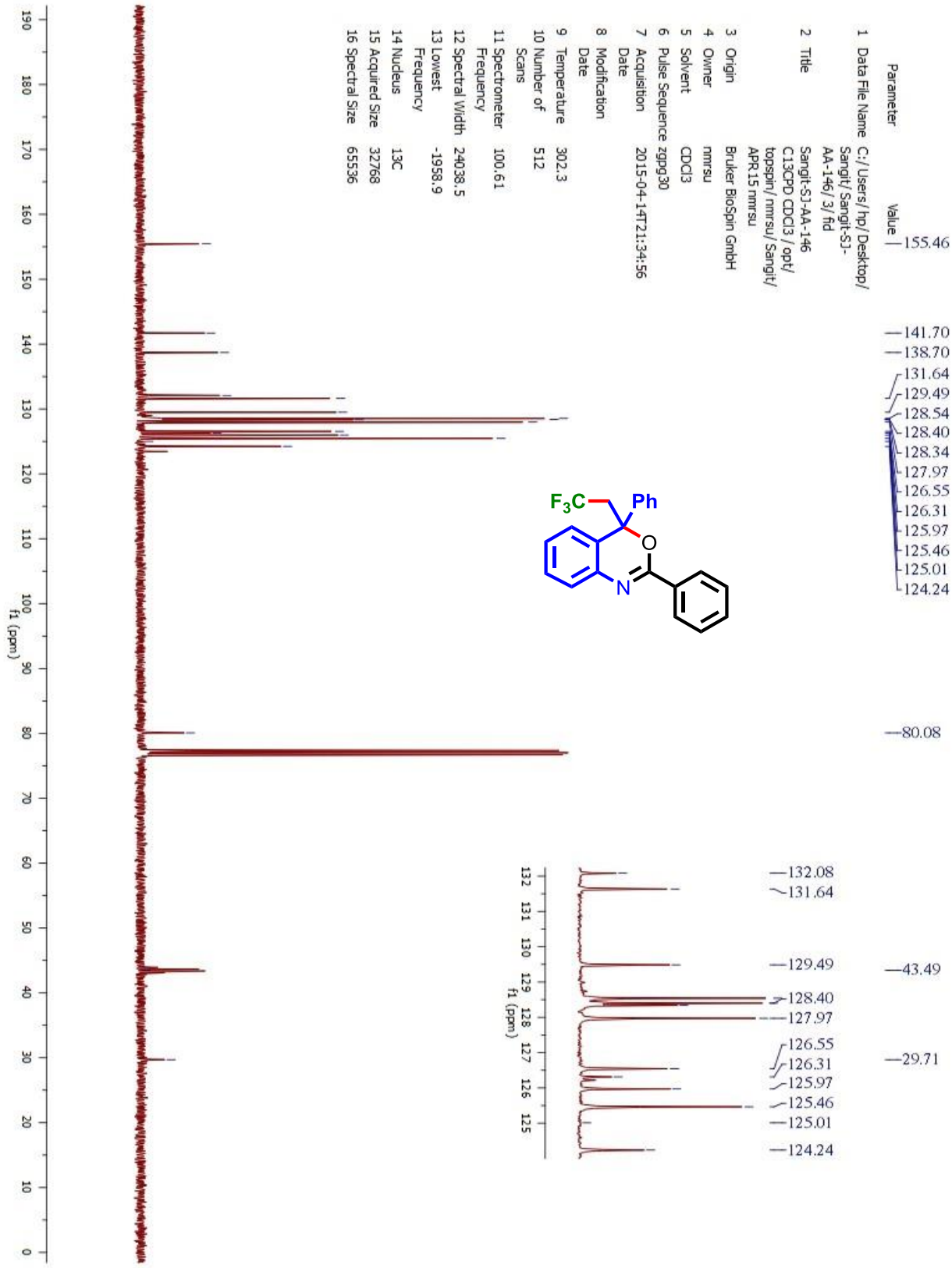
S120 ^{13}C NMR of **1z**



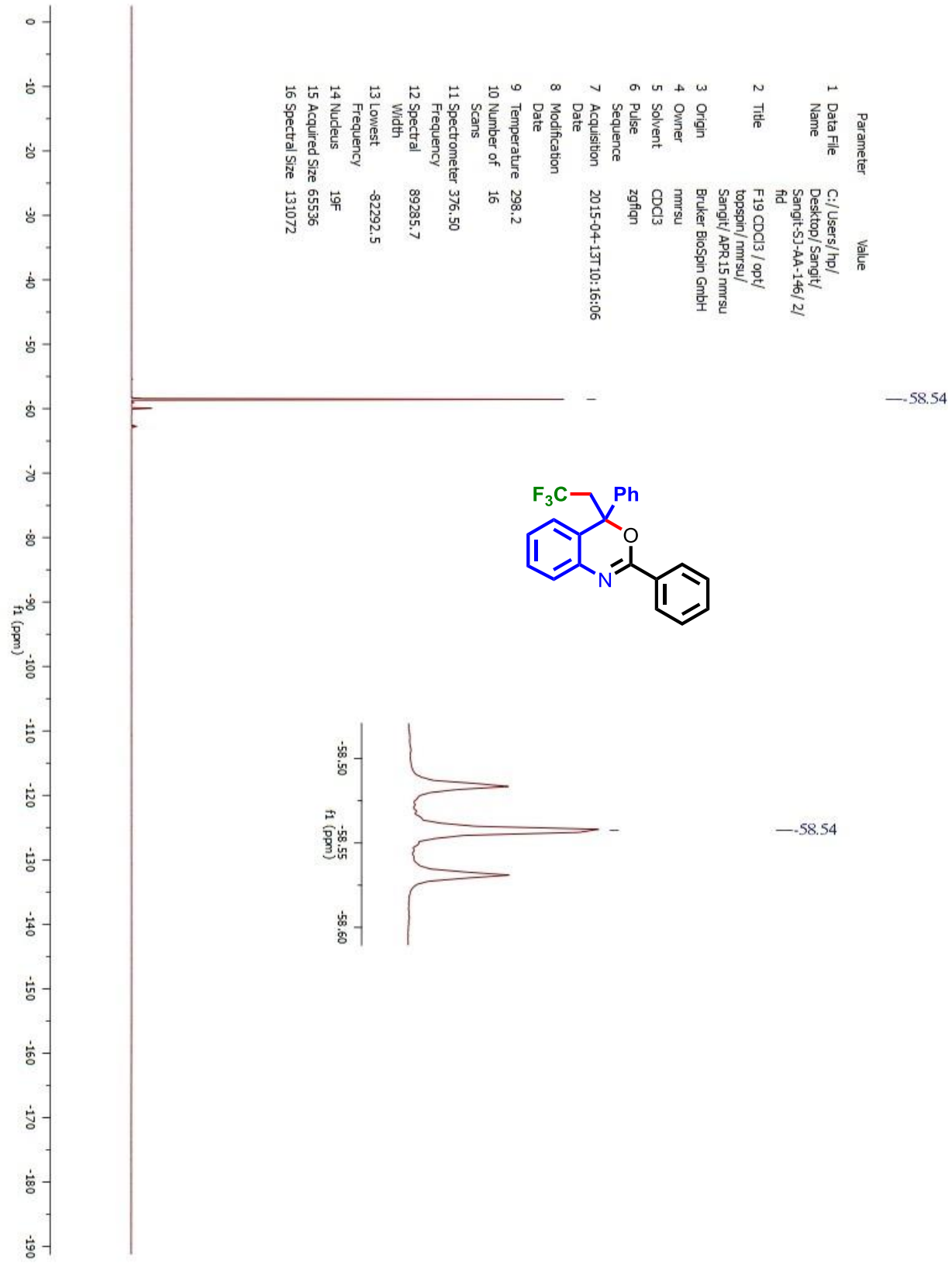
S121 ^{1}H NMR of **3z**



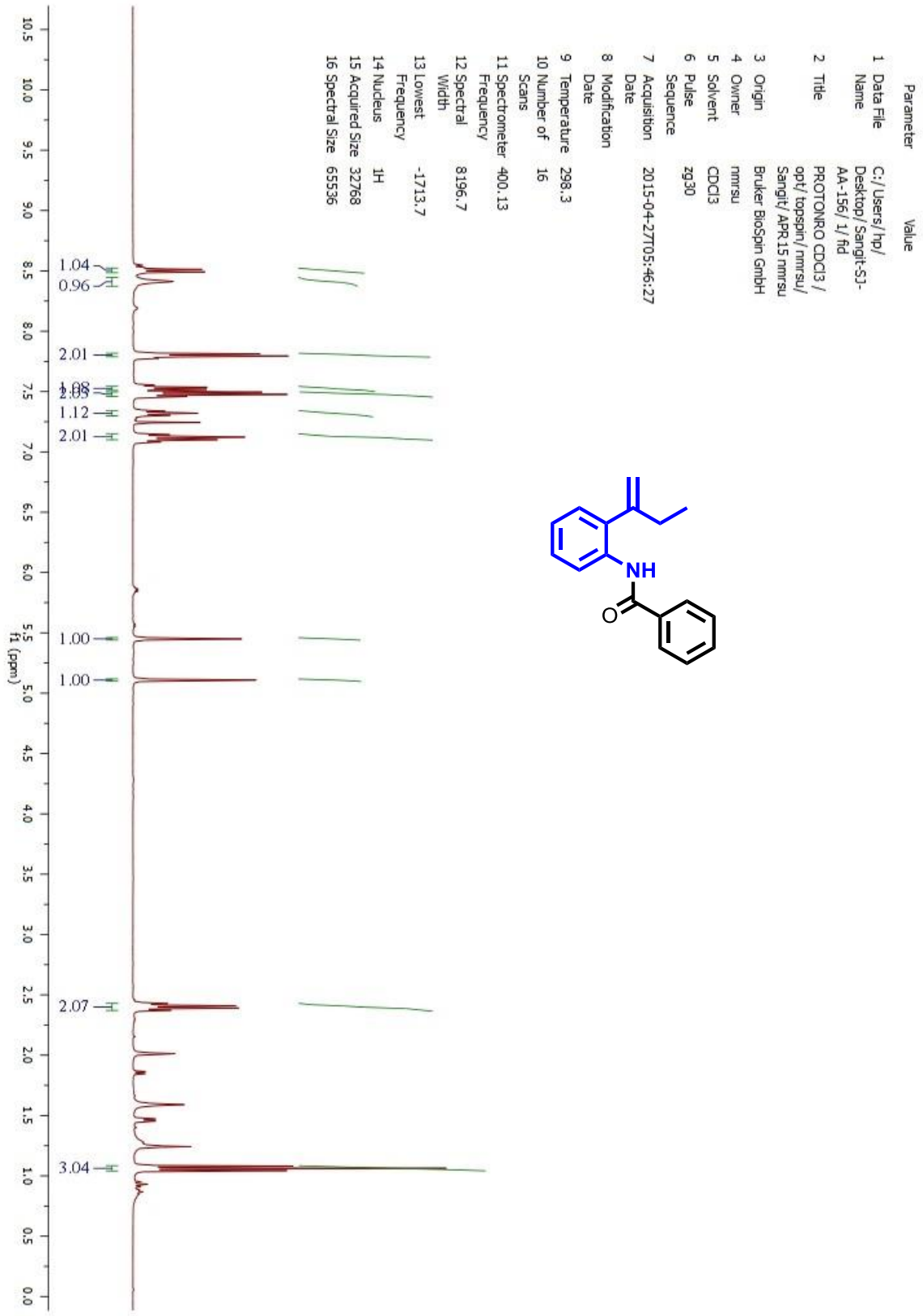
S122 ^{13}C NMR of **3z**



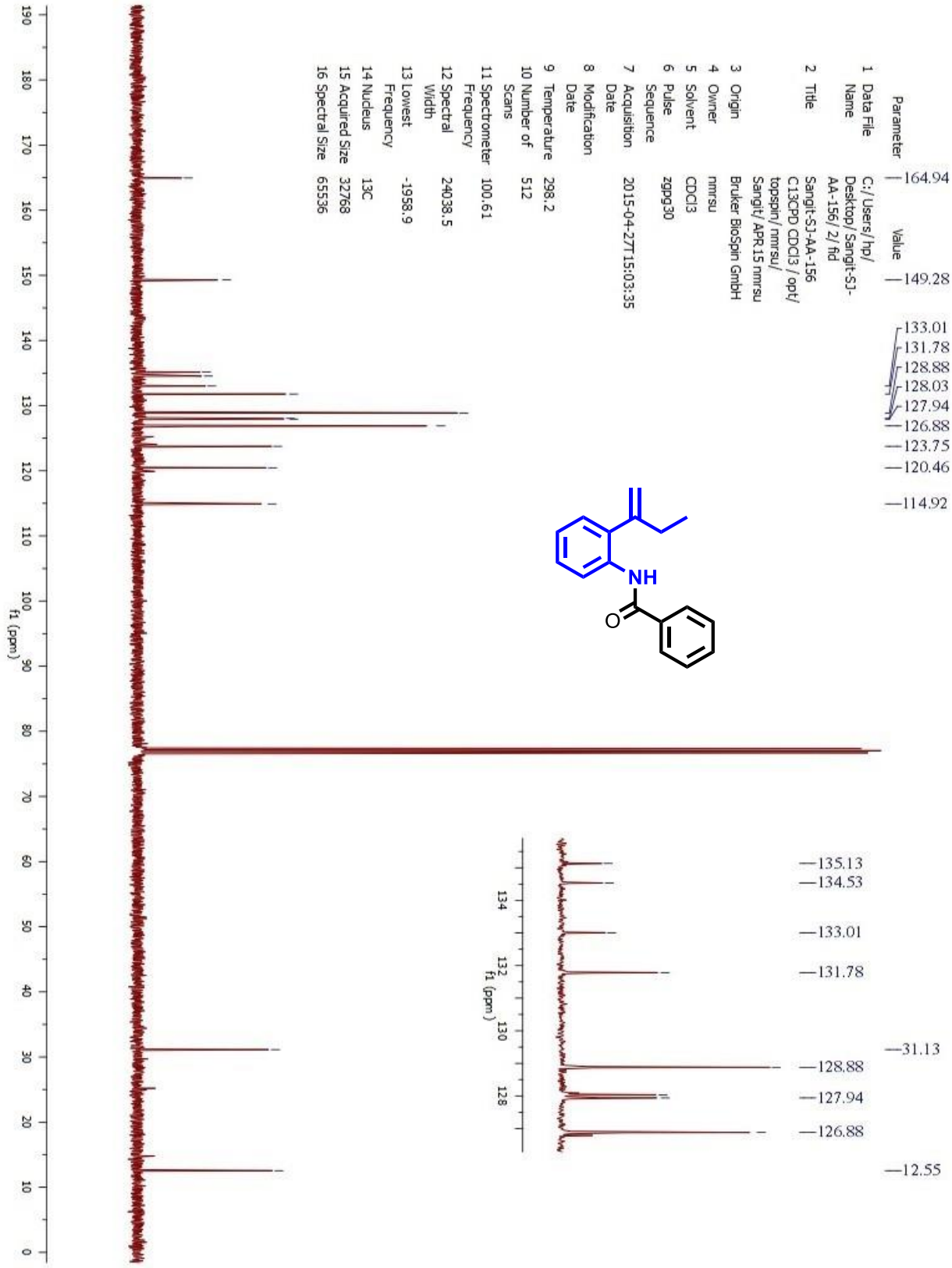
S123 ^{19}F NMR of **3z**



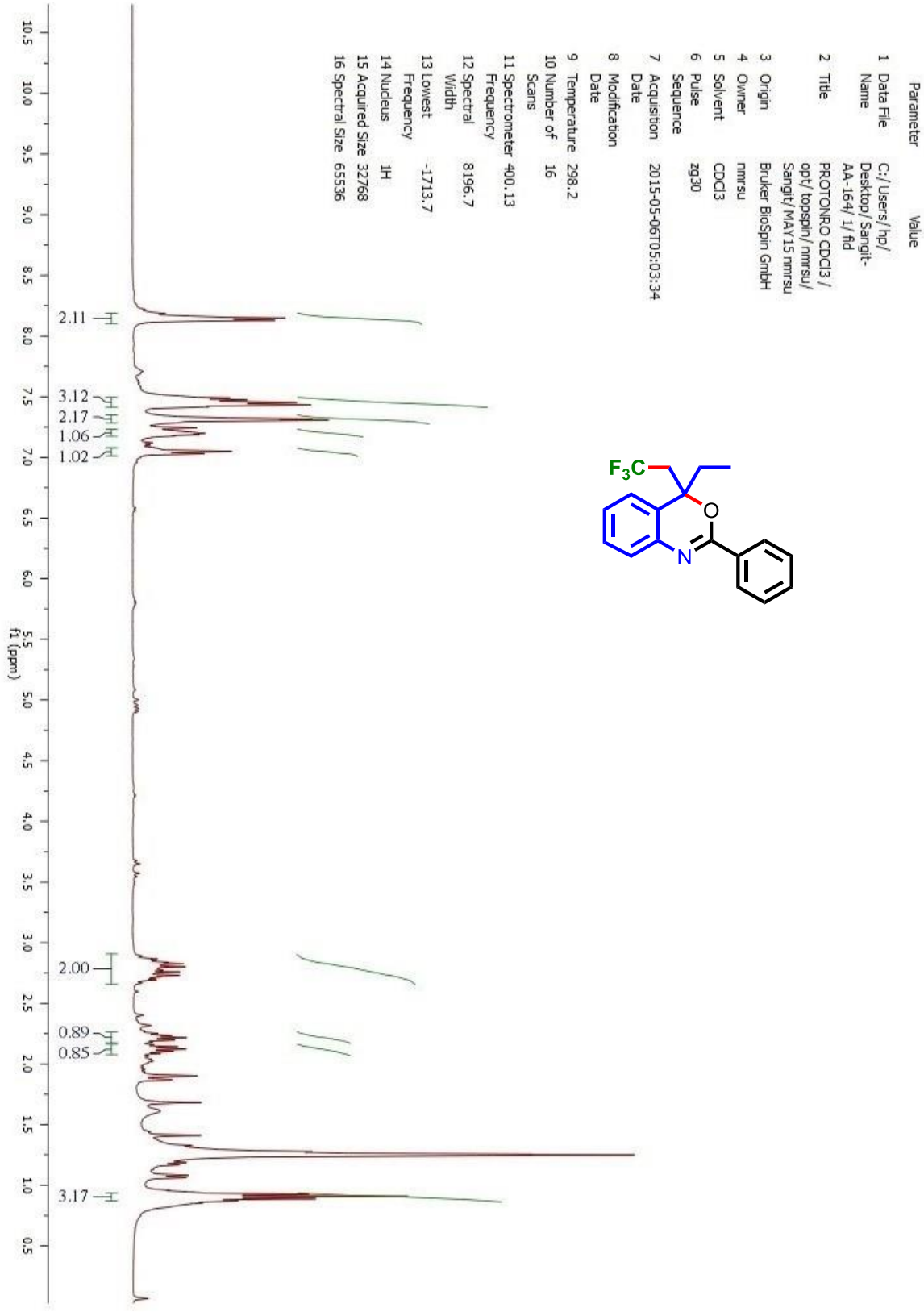
S124 ^{1}H NMR of **1aa**



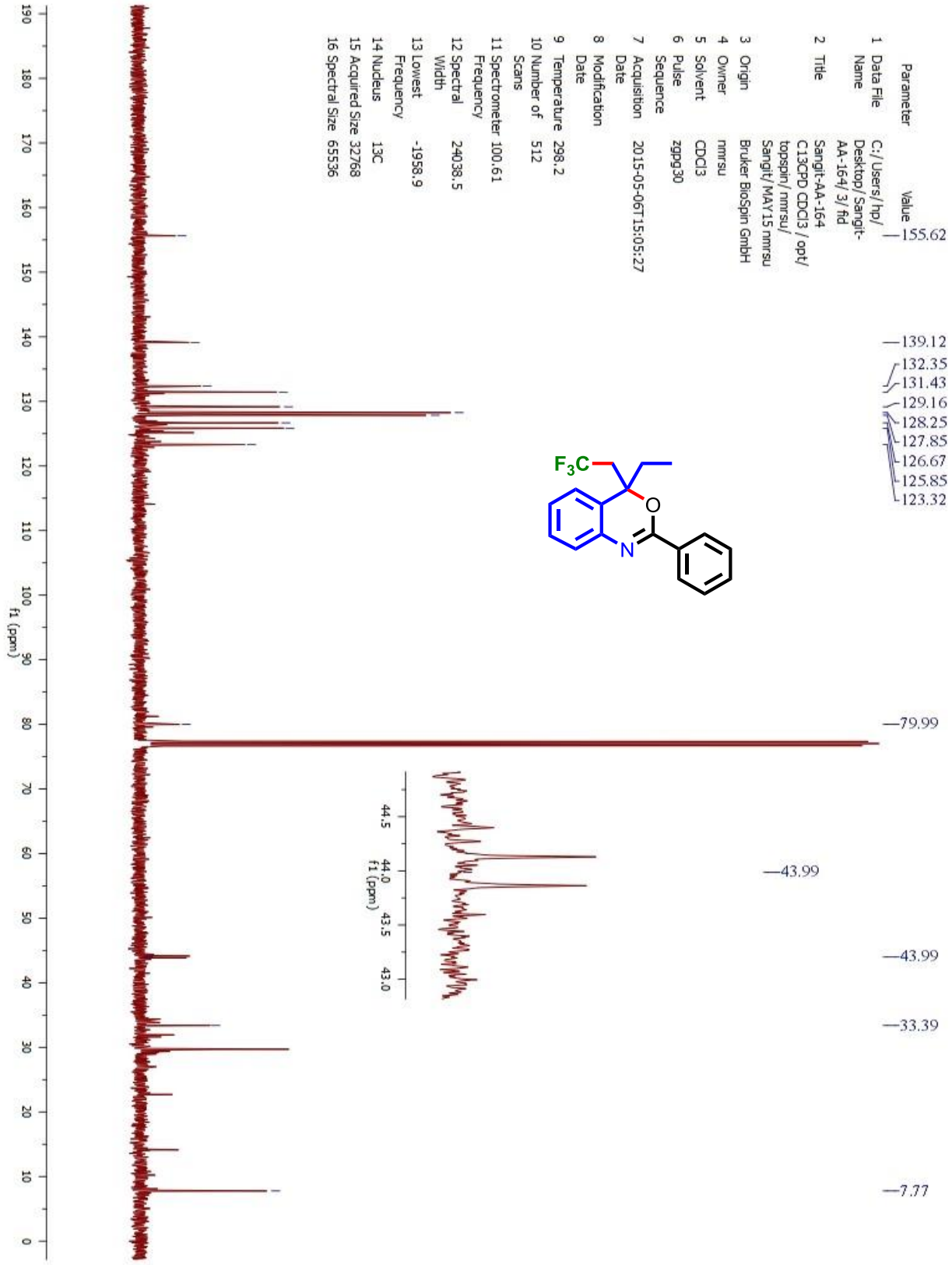
S125 ^{13}C NMR of **1aa**



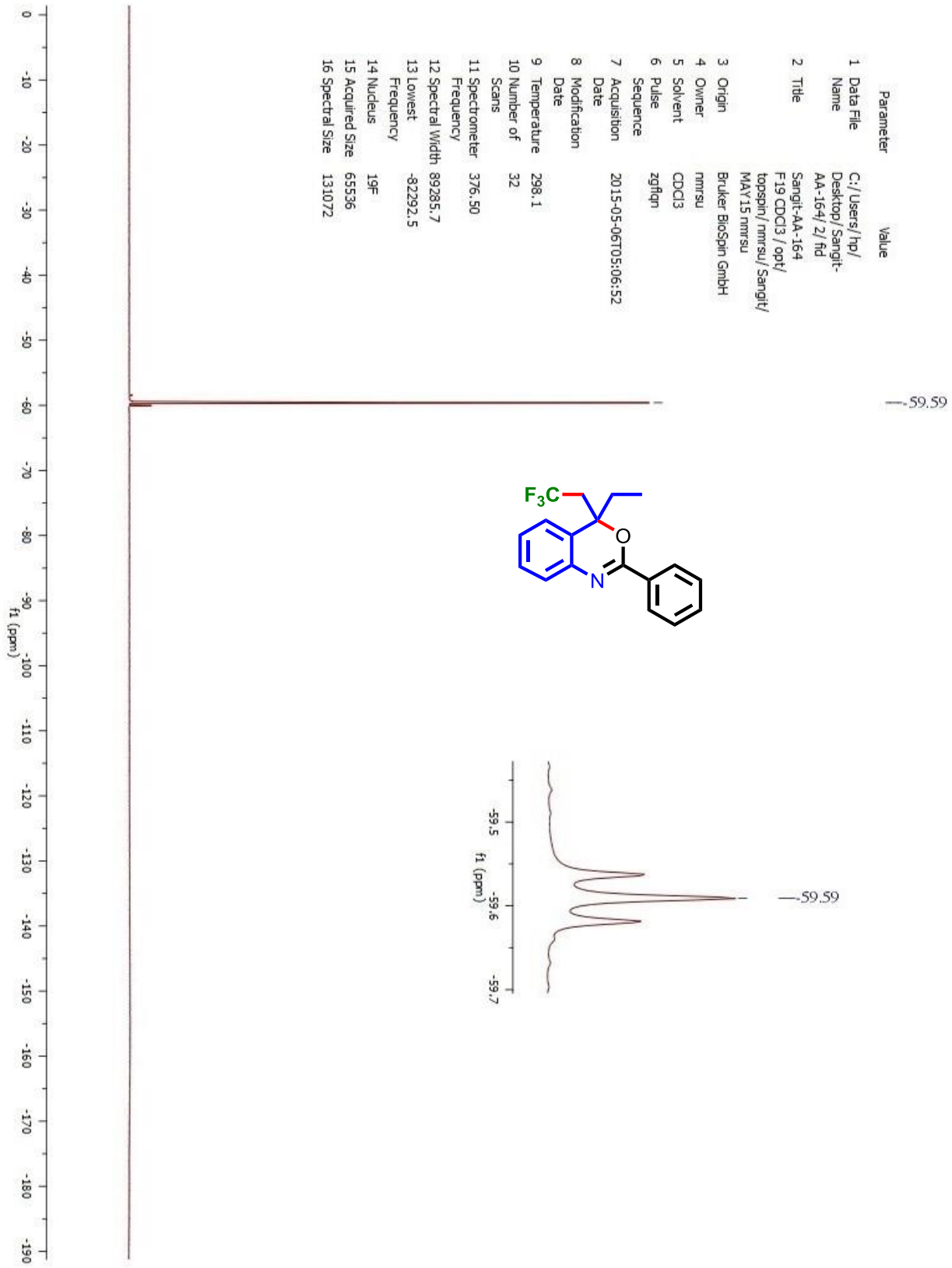
S126 ^{1}H NMR of **3aa**



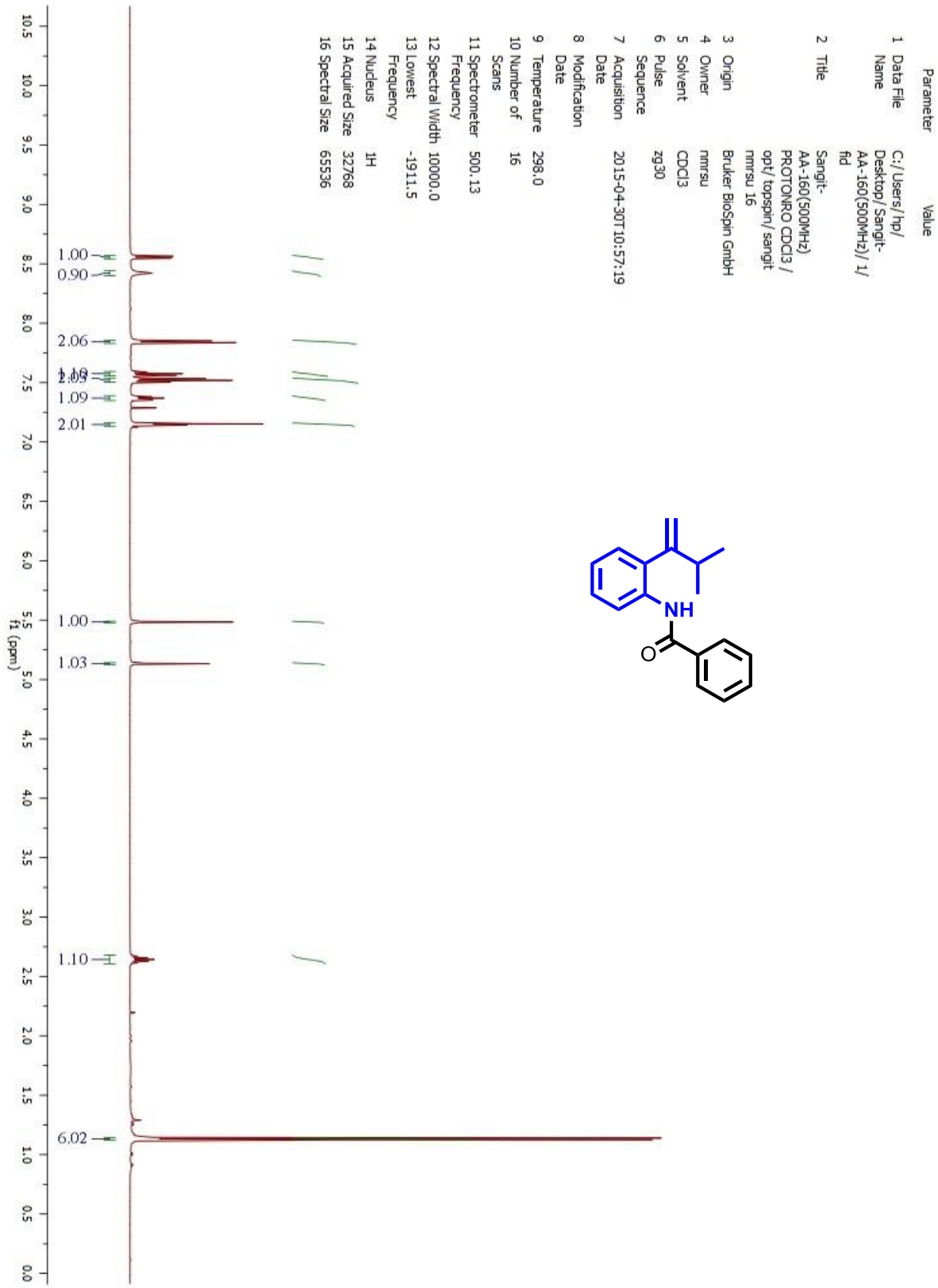
S127 ^{13}C NMR of **3aa**



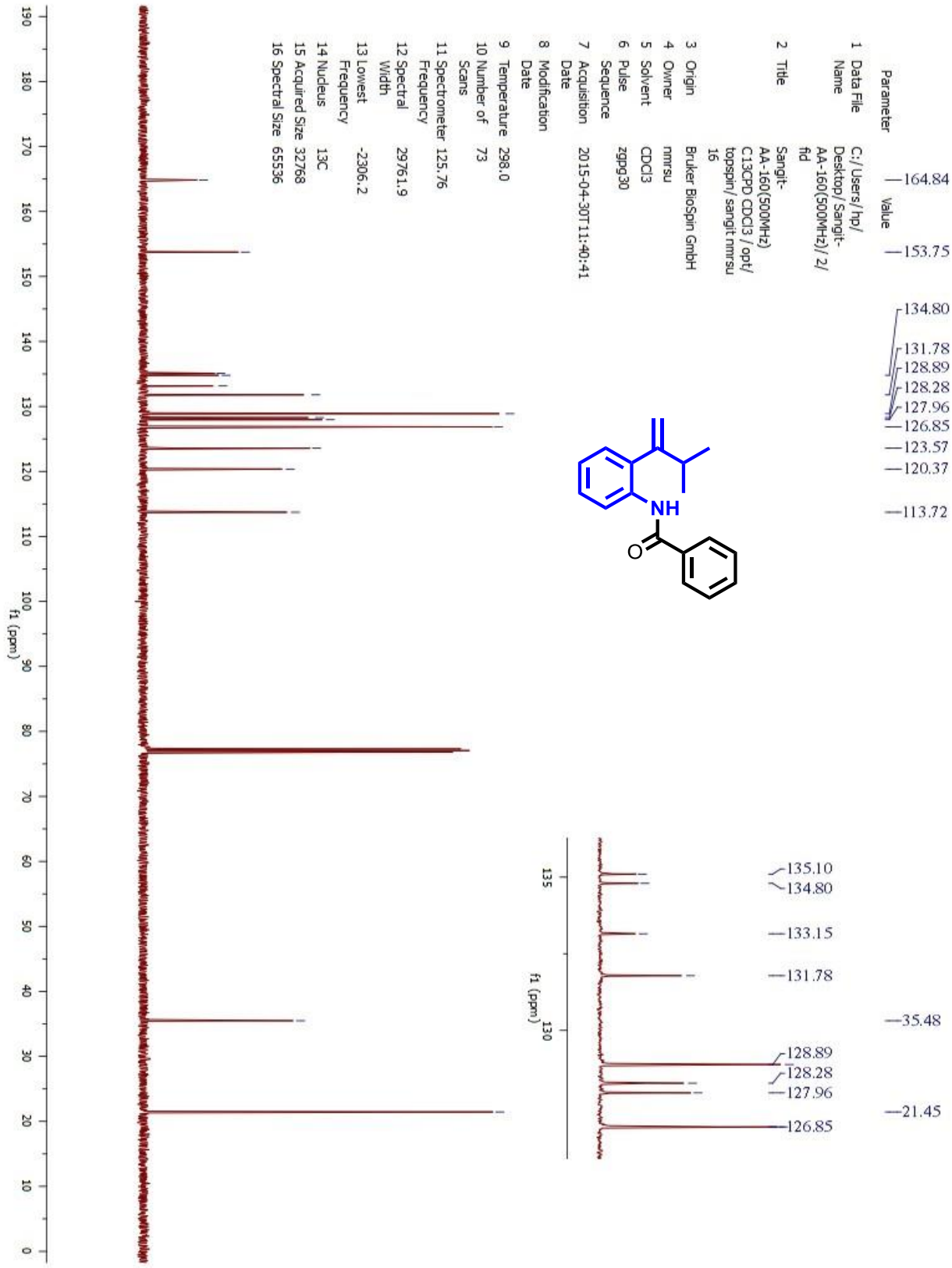
S128 ^{19}F NMR of **3aa**



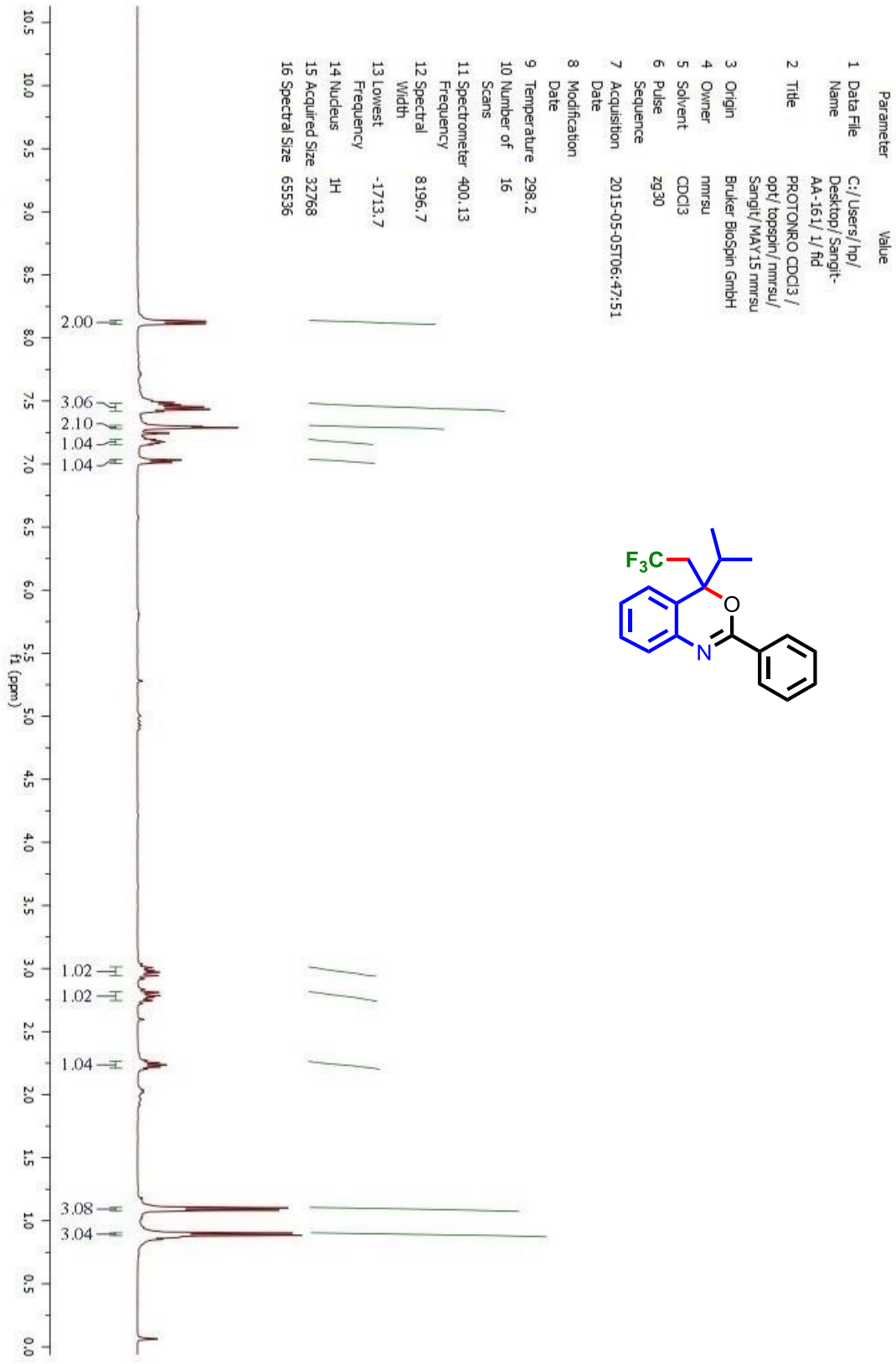
S129 ^{1}H NMR of **1bb**



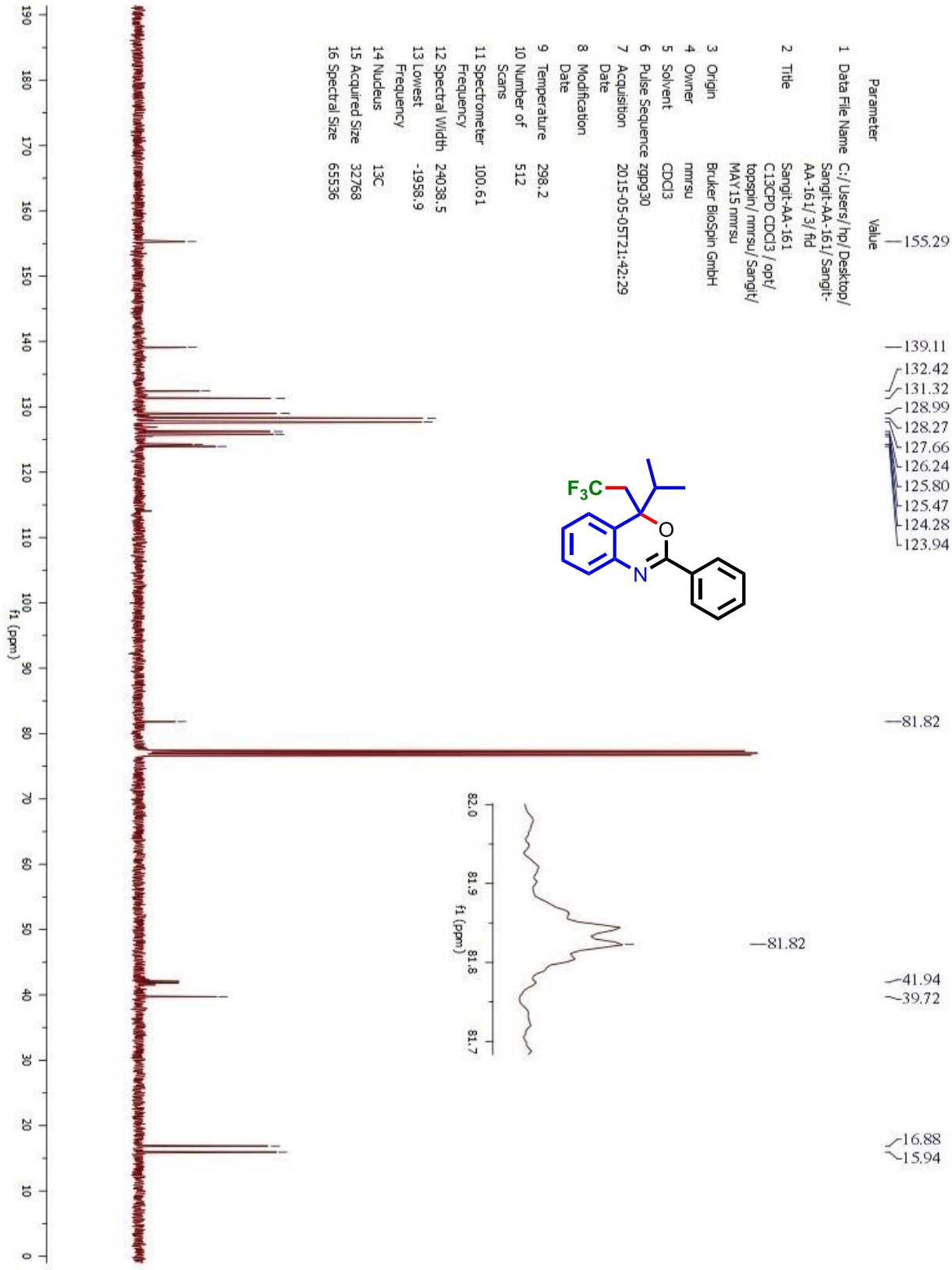
S130 ^{13}C NMR of **1bb**



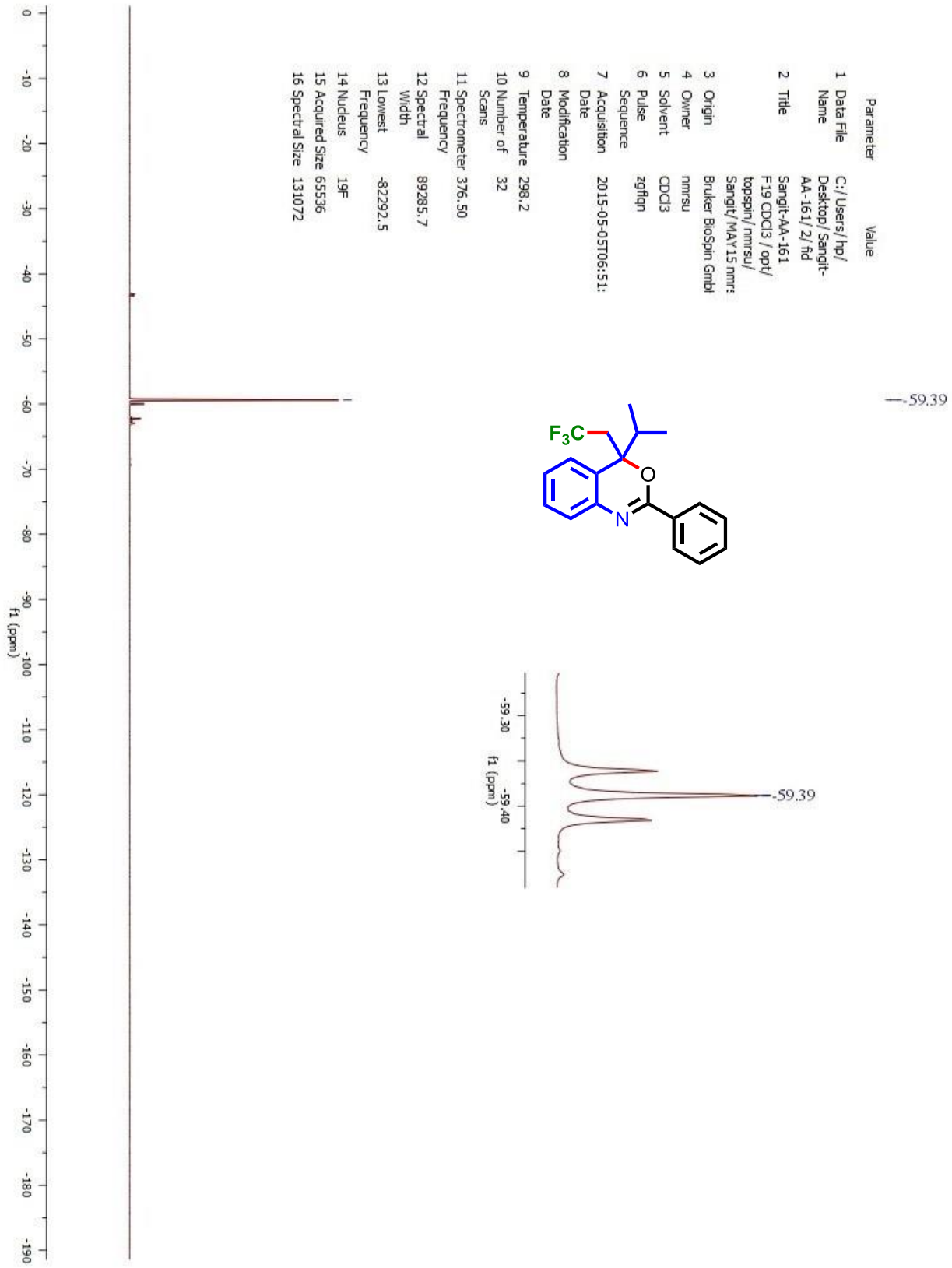
S131 ^{1}H NMR of **3bb**



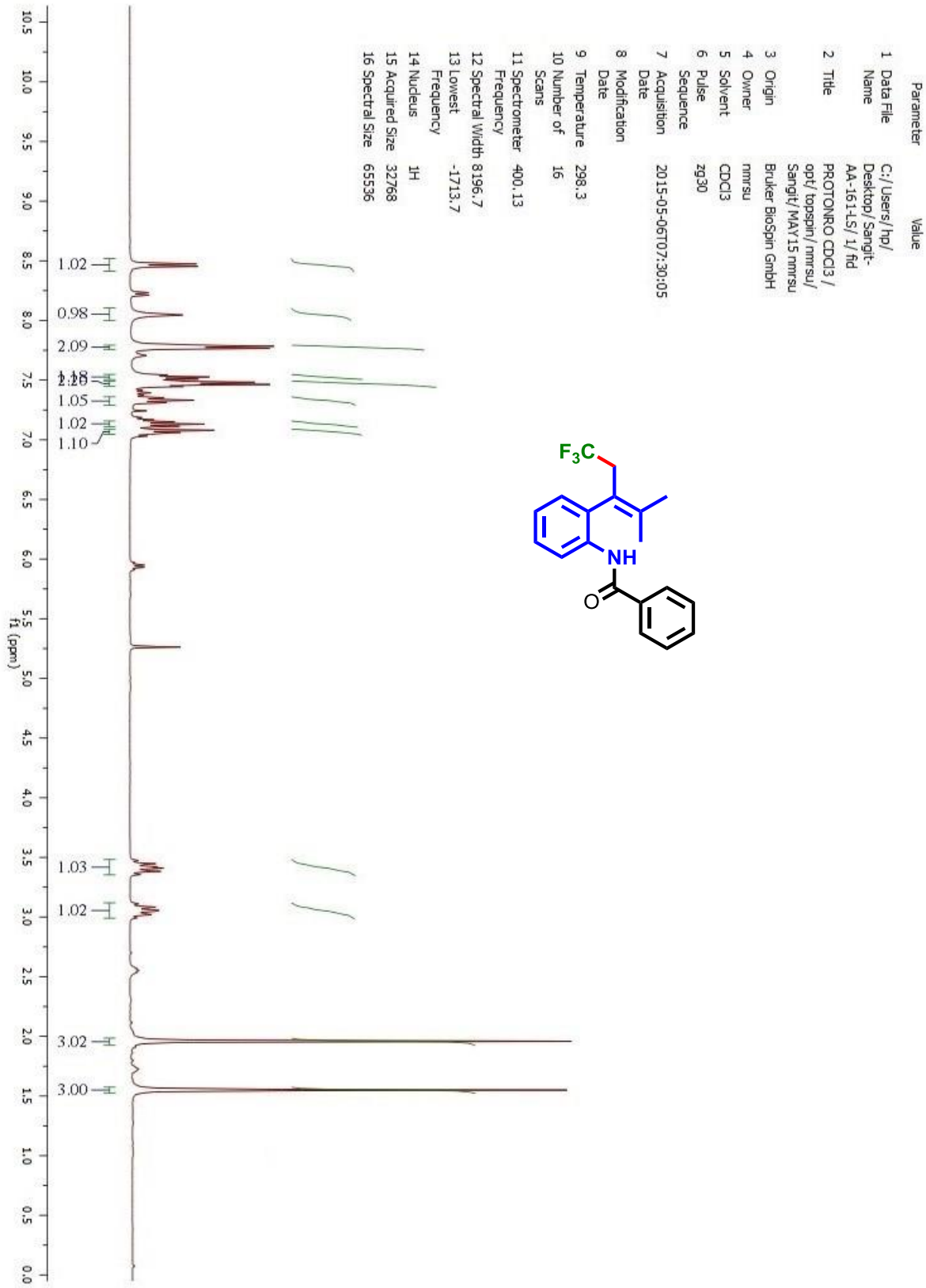
S132 ^{13}C NMR of **3bb**



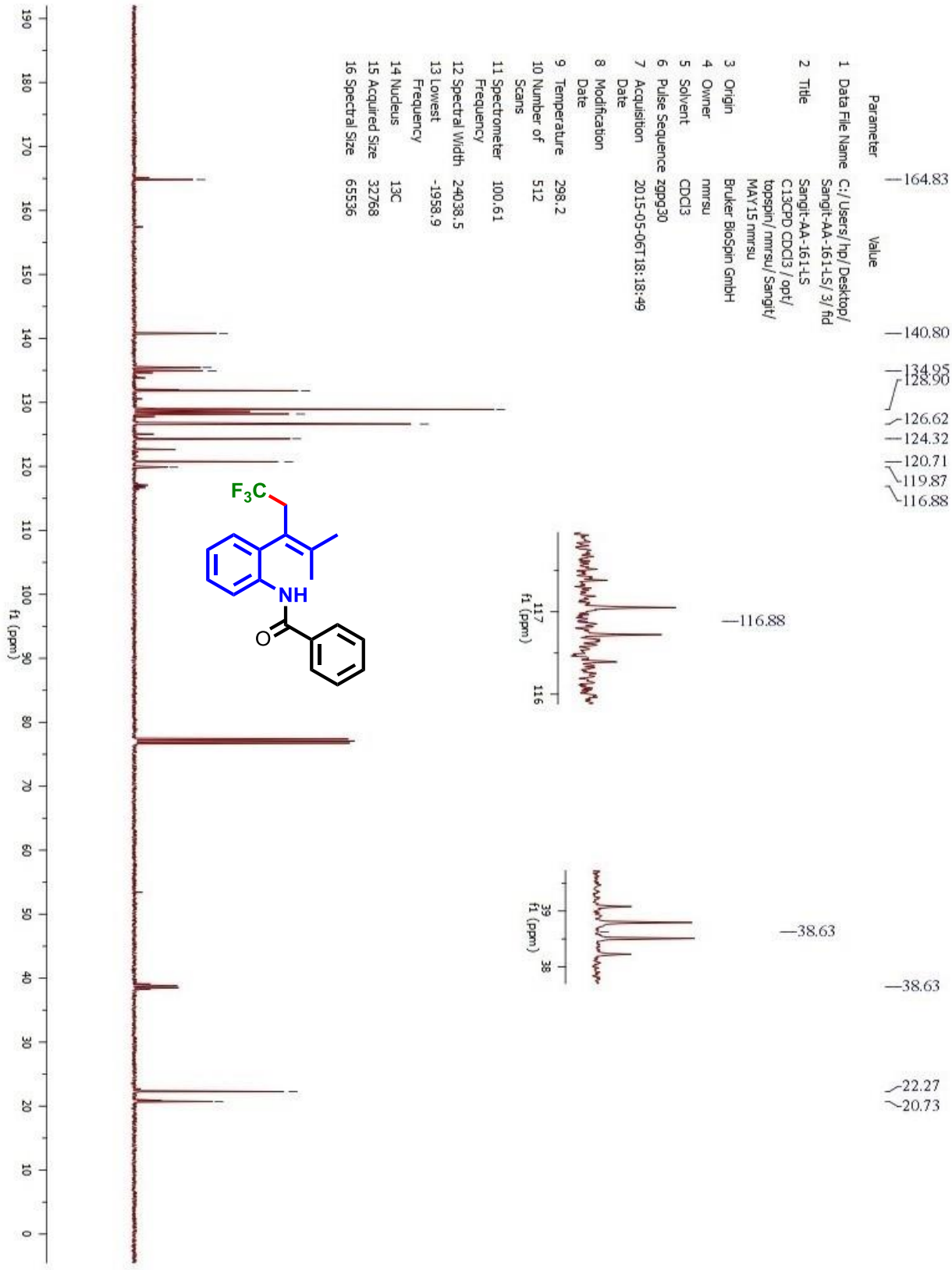
S133 ^{19}F NMR of **3bb**



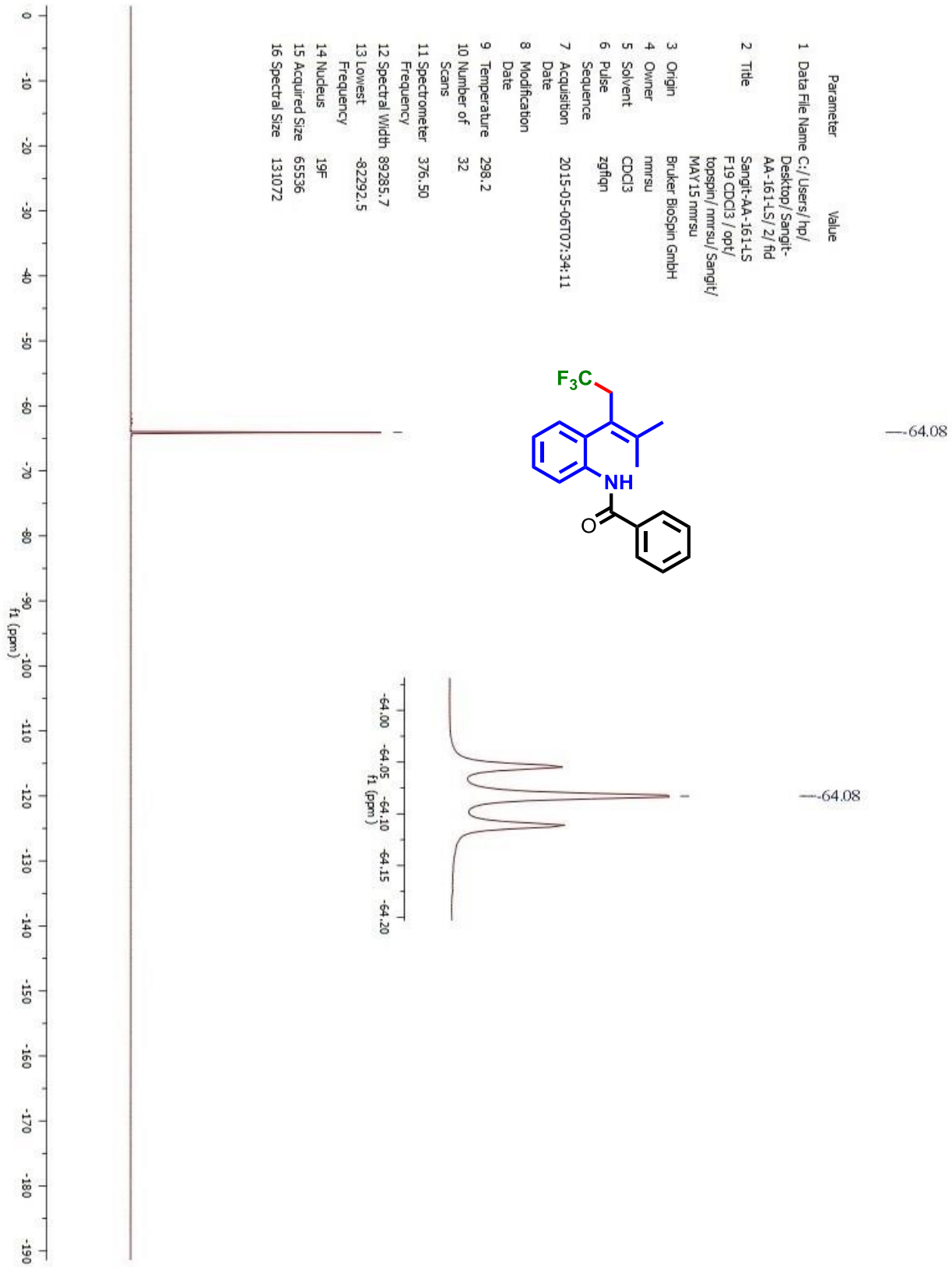
S134 ^{1}H NMR of **4bb**



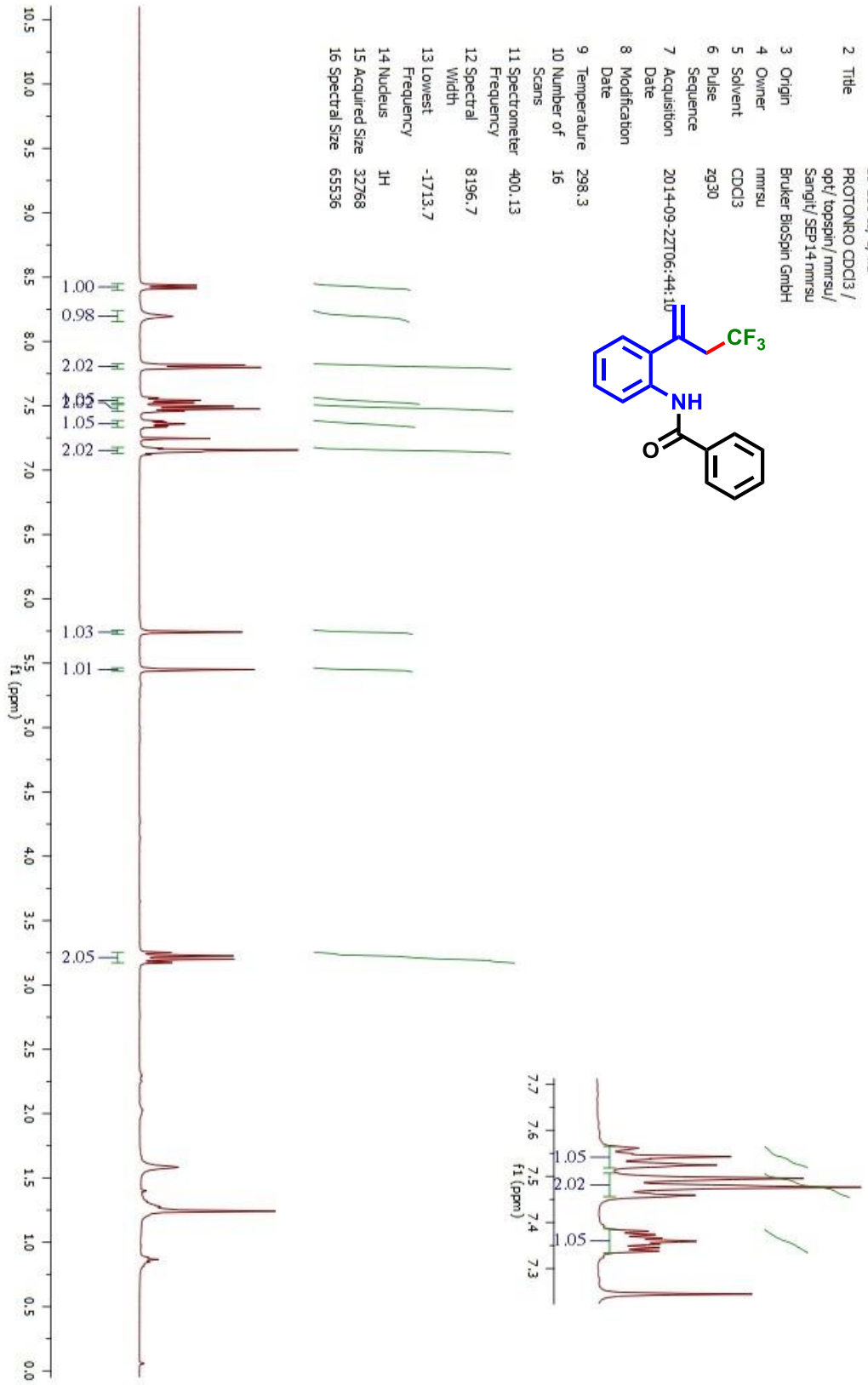
S135 ^{13}C NMR of **4bb**



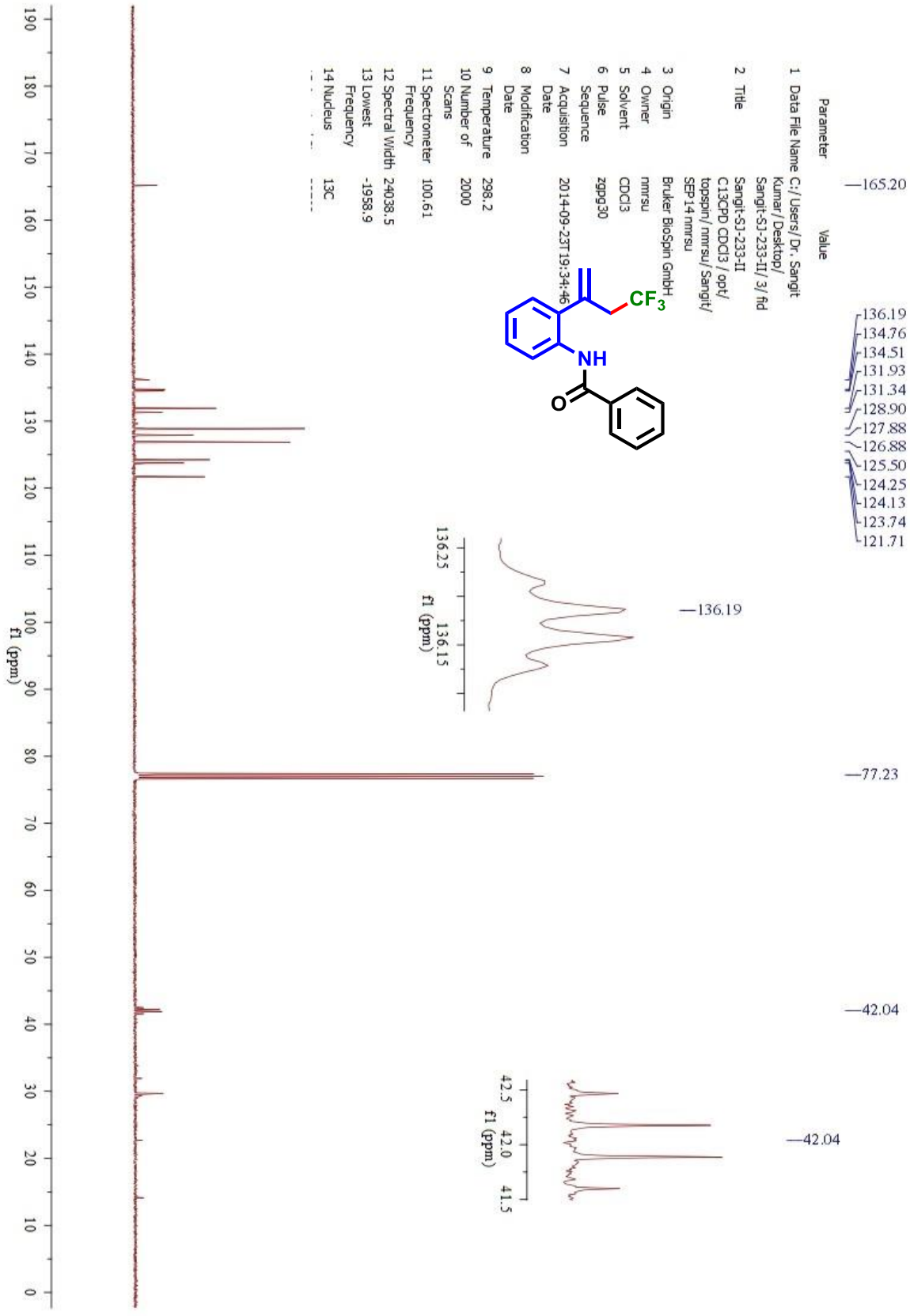
S136 ^{19}F NMR of **4bb**



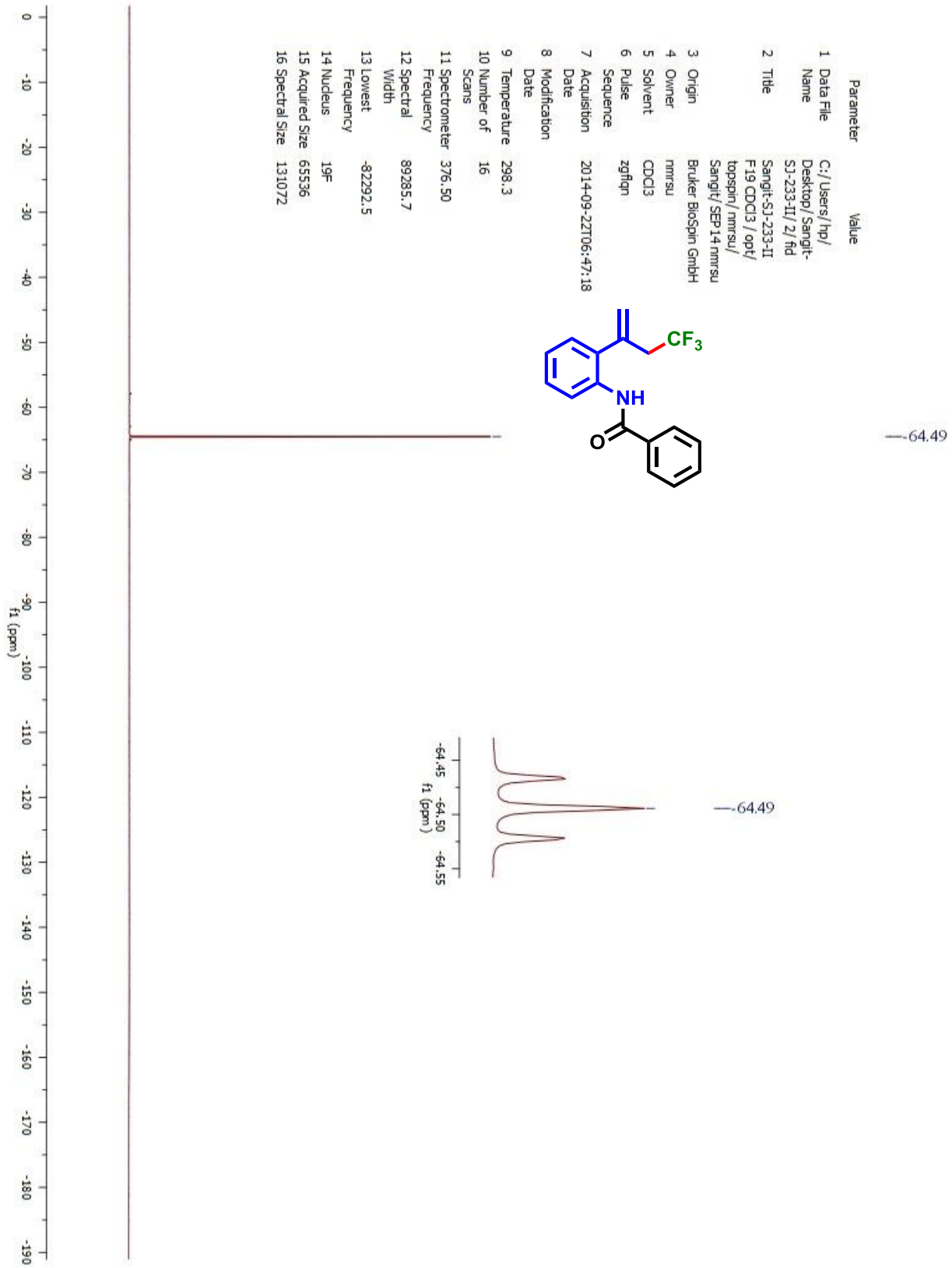
S137 ^{1}H NMR of **4a**



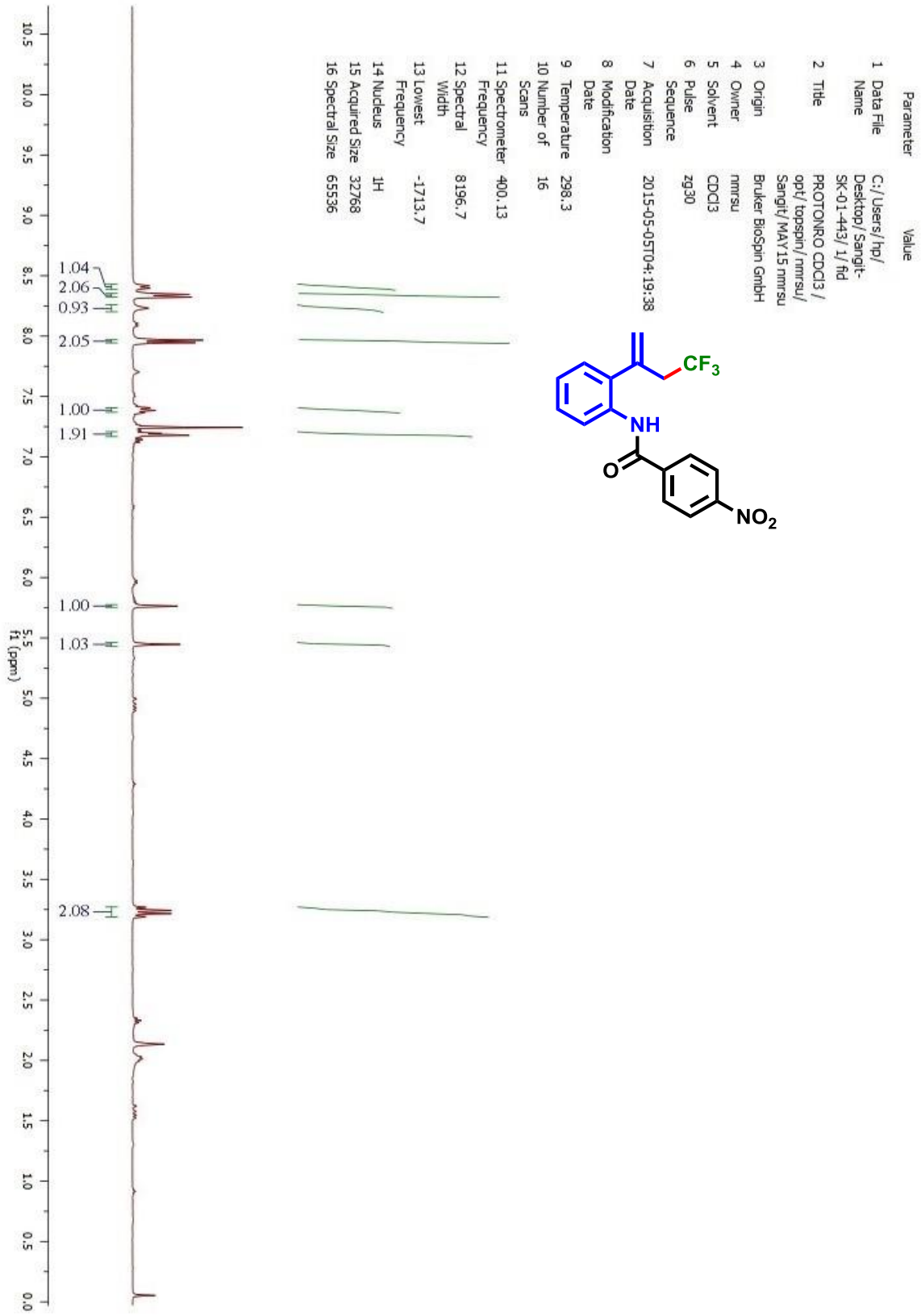
S138 ^{13}C NMR of **4a**



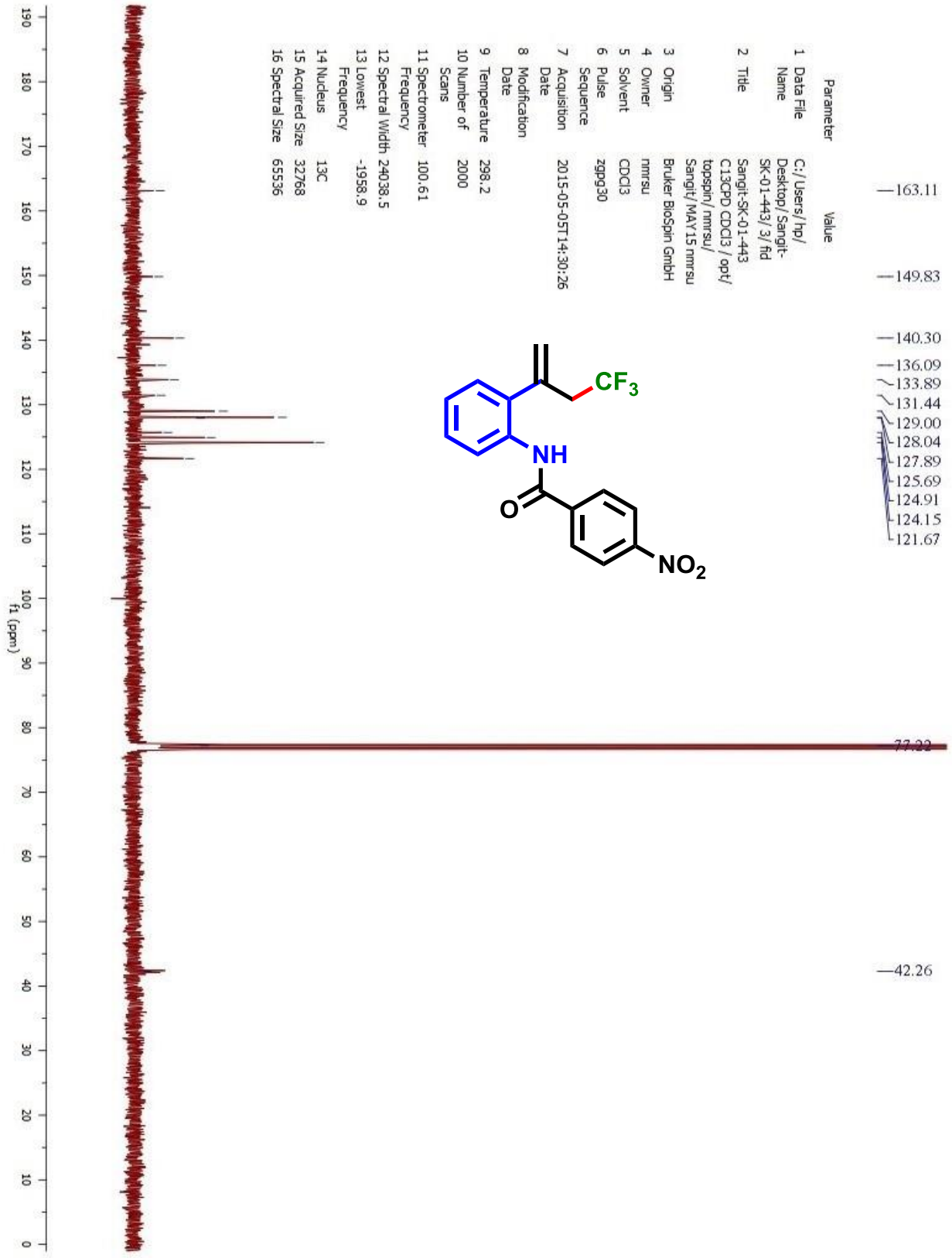
S139 ^{19}F NMR of **4a**



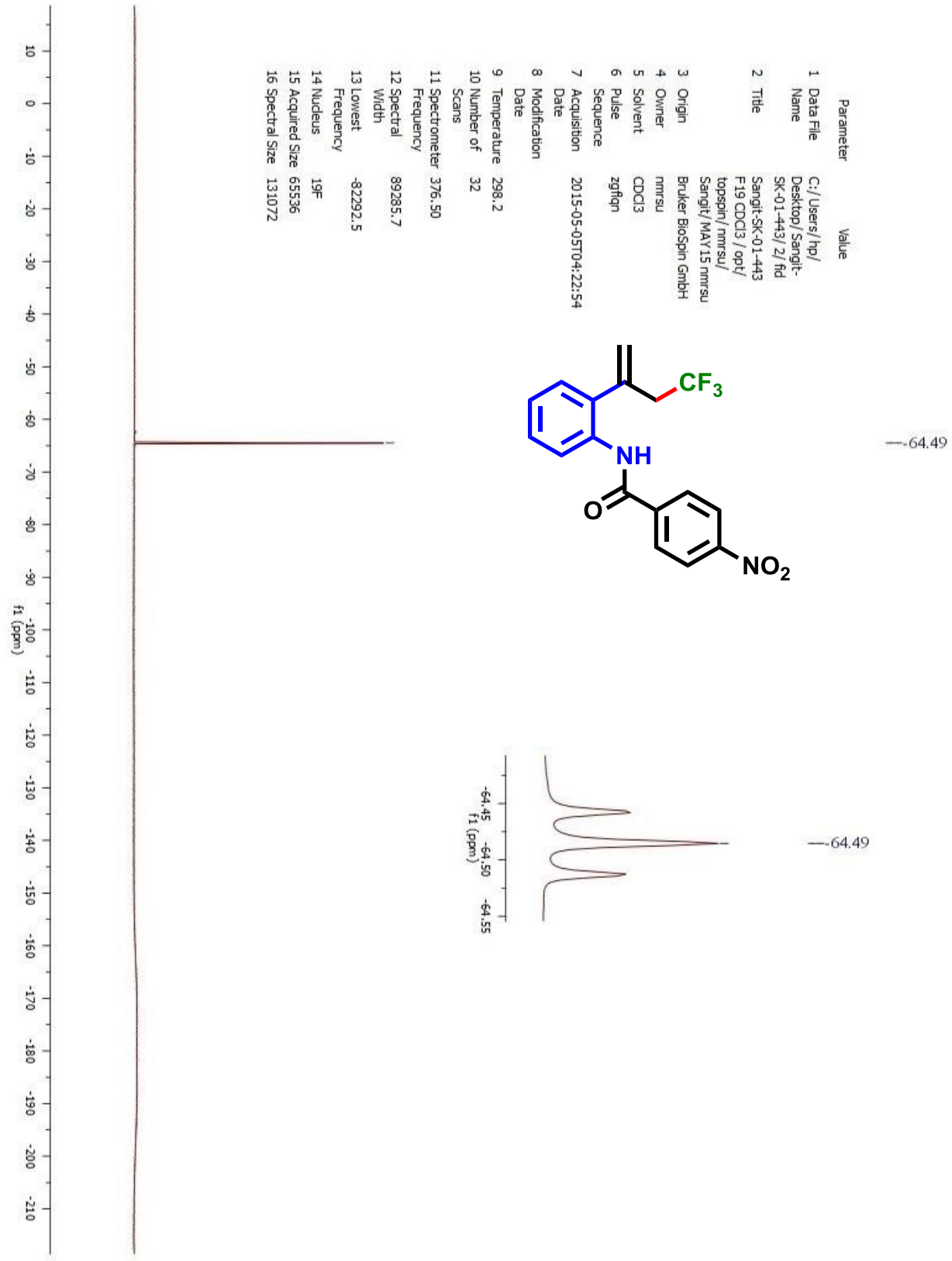
S140 ^{1}H NMR of **5a**



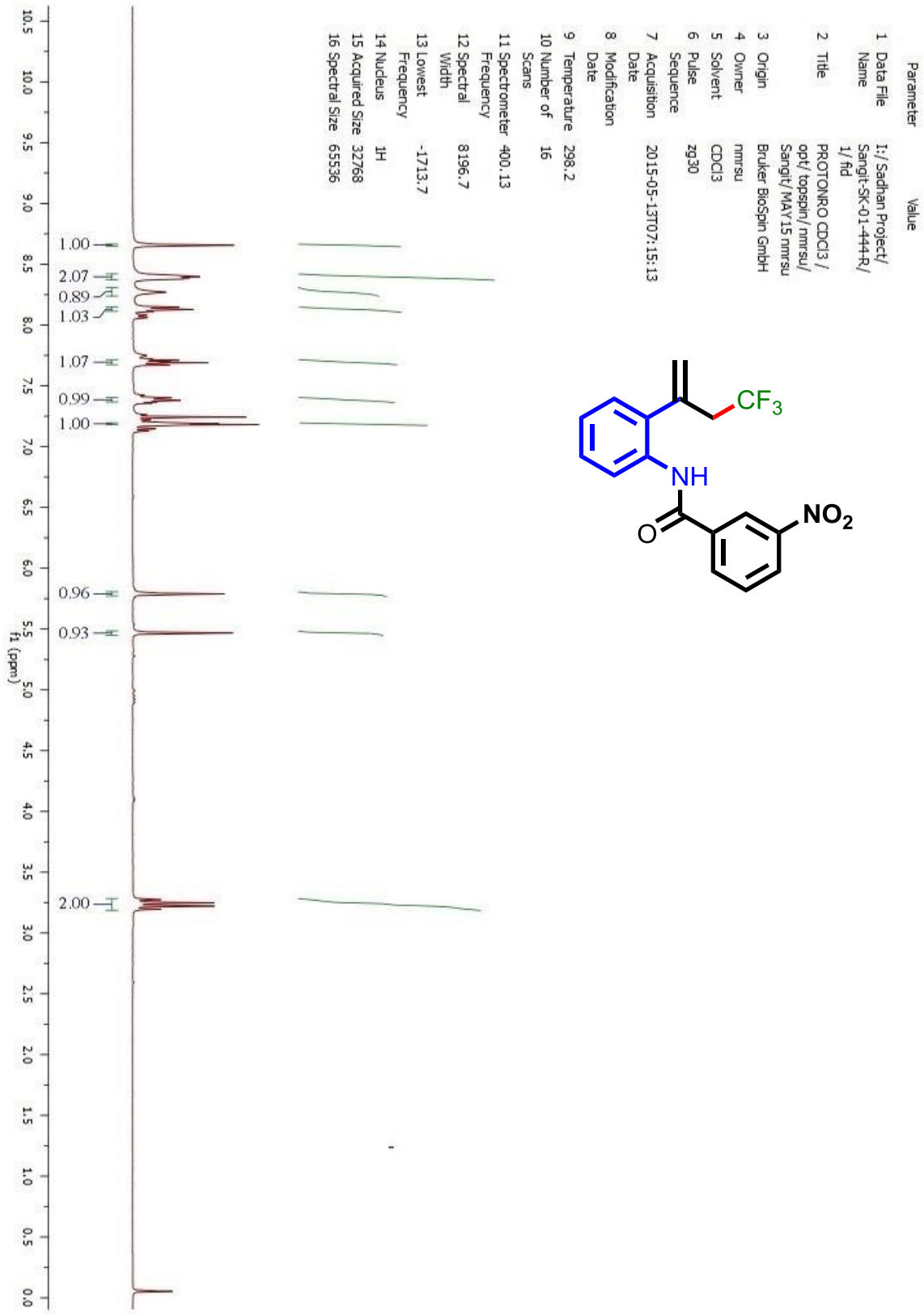
S141 ^{13}C NMR of **5a**



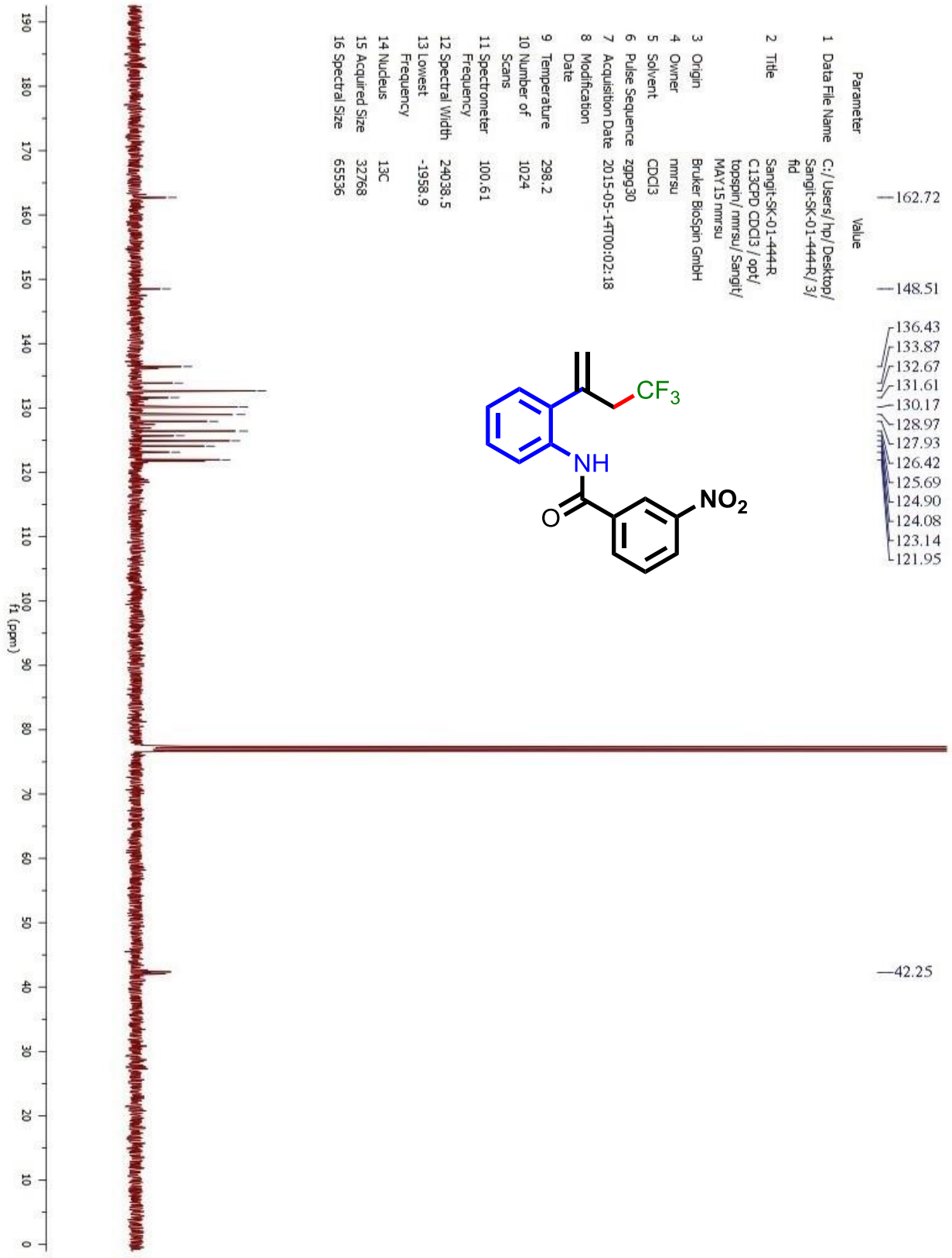
S142 ^{19}F NMR of **5a**



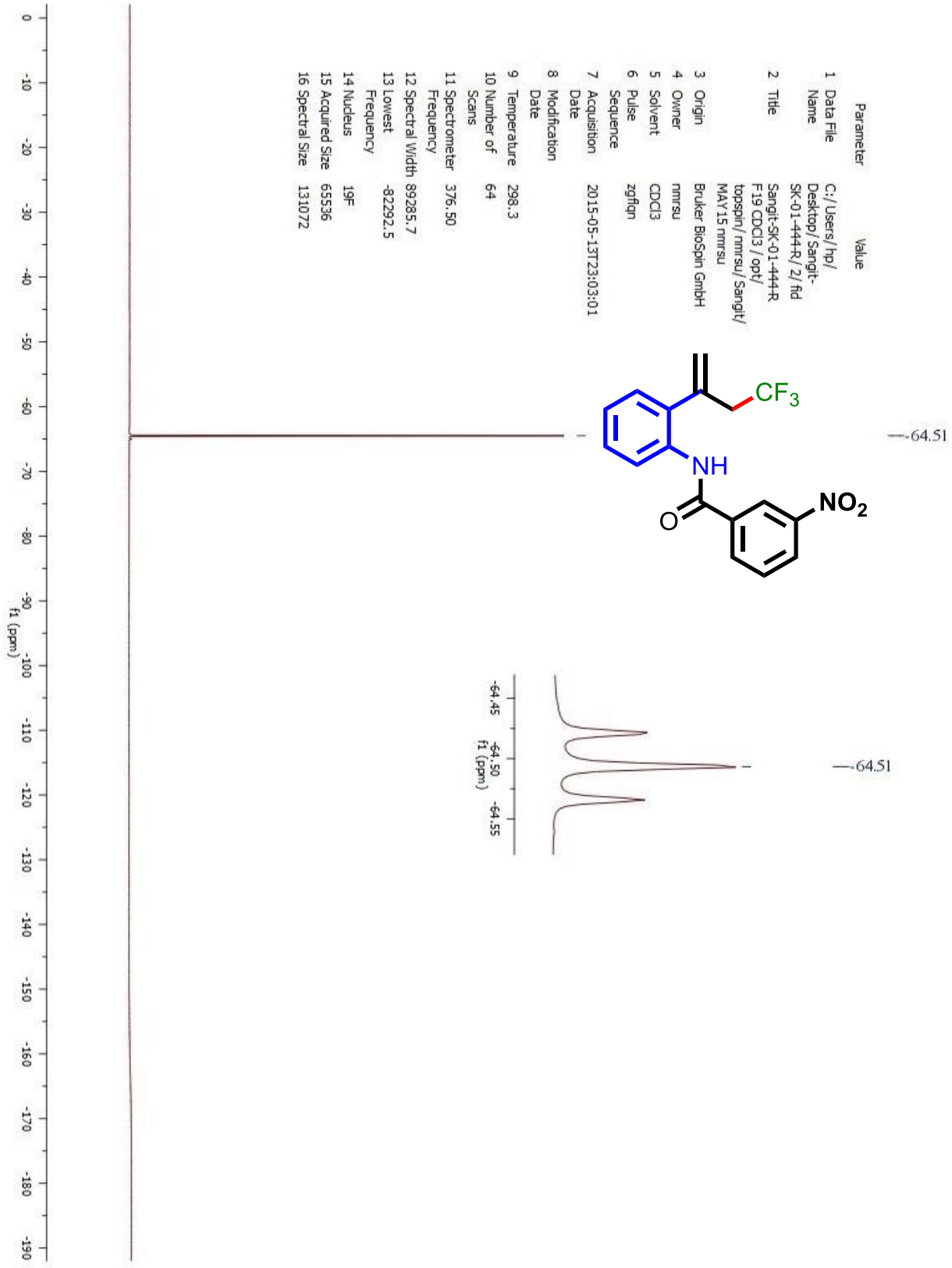
S143 ^{1}H NMR of **5b**



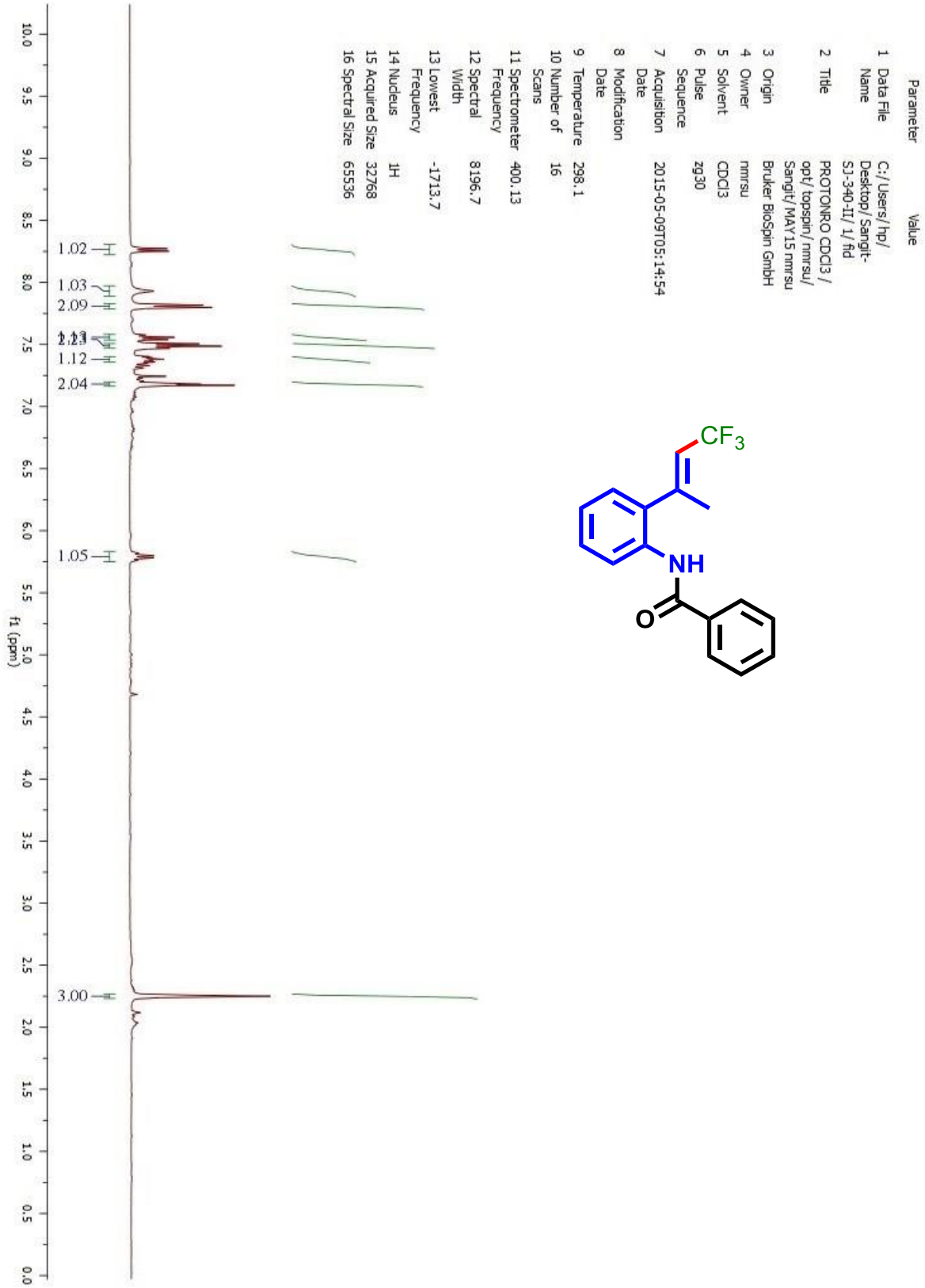
S144 ^{13}C NMR of **5b**



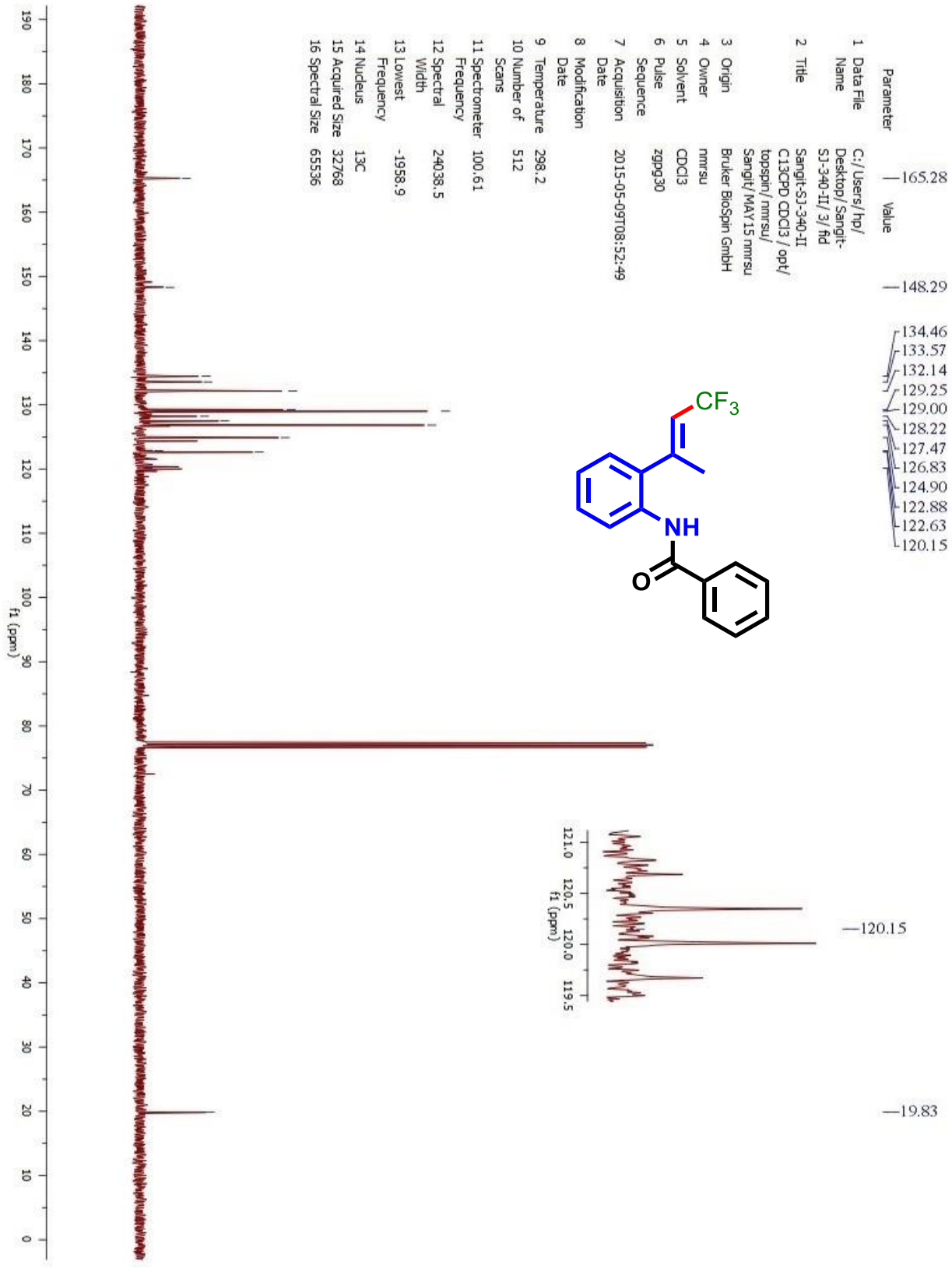
S145 ^{19}F NMR of **5b**



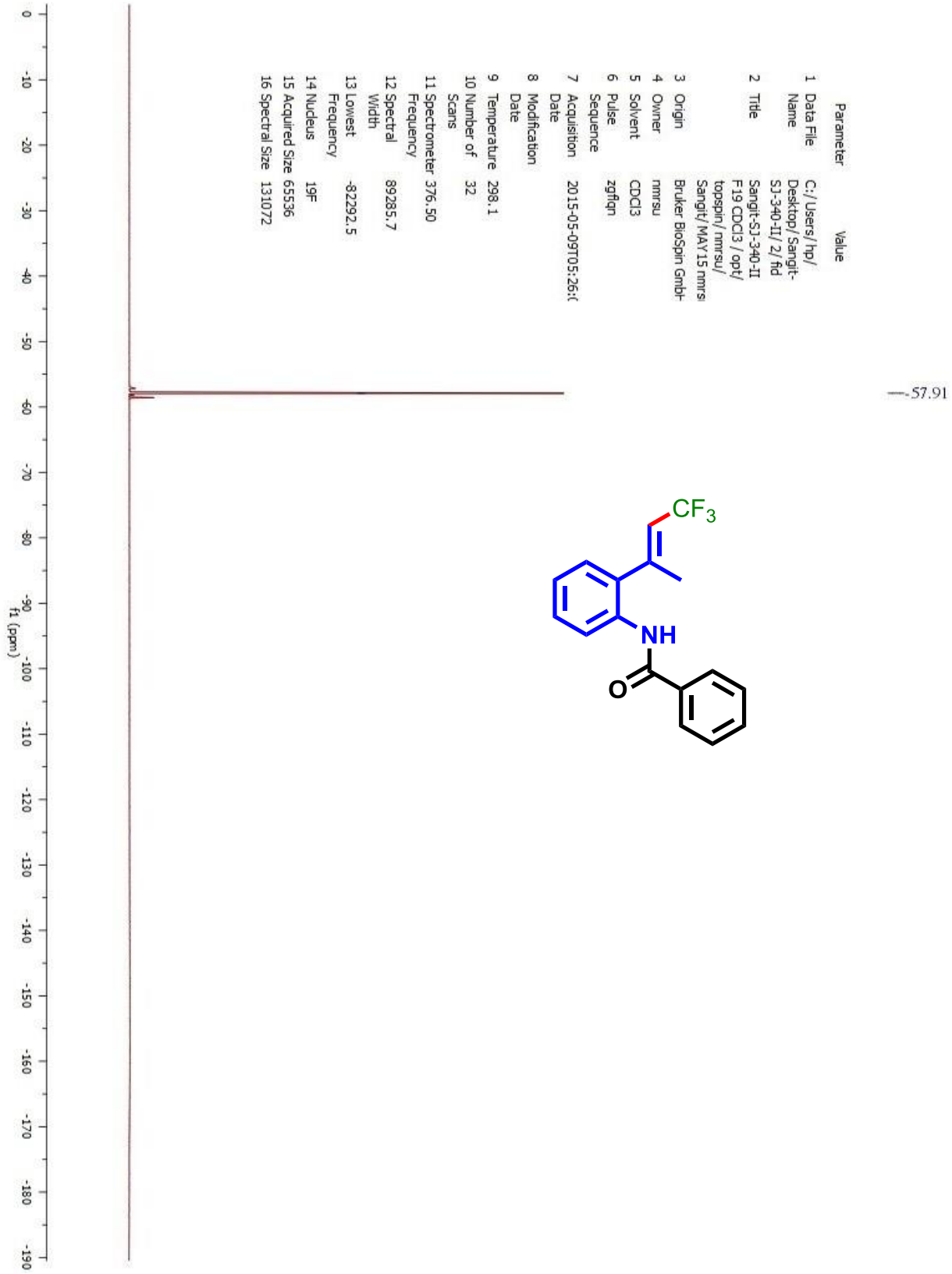
S146 ^{1}H NMR of **5c**



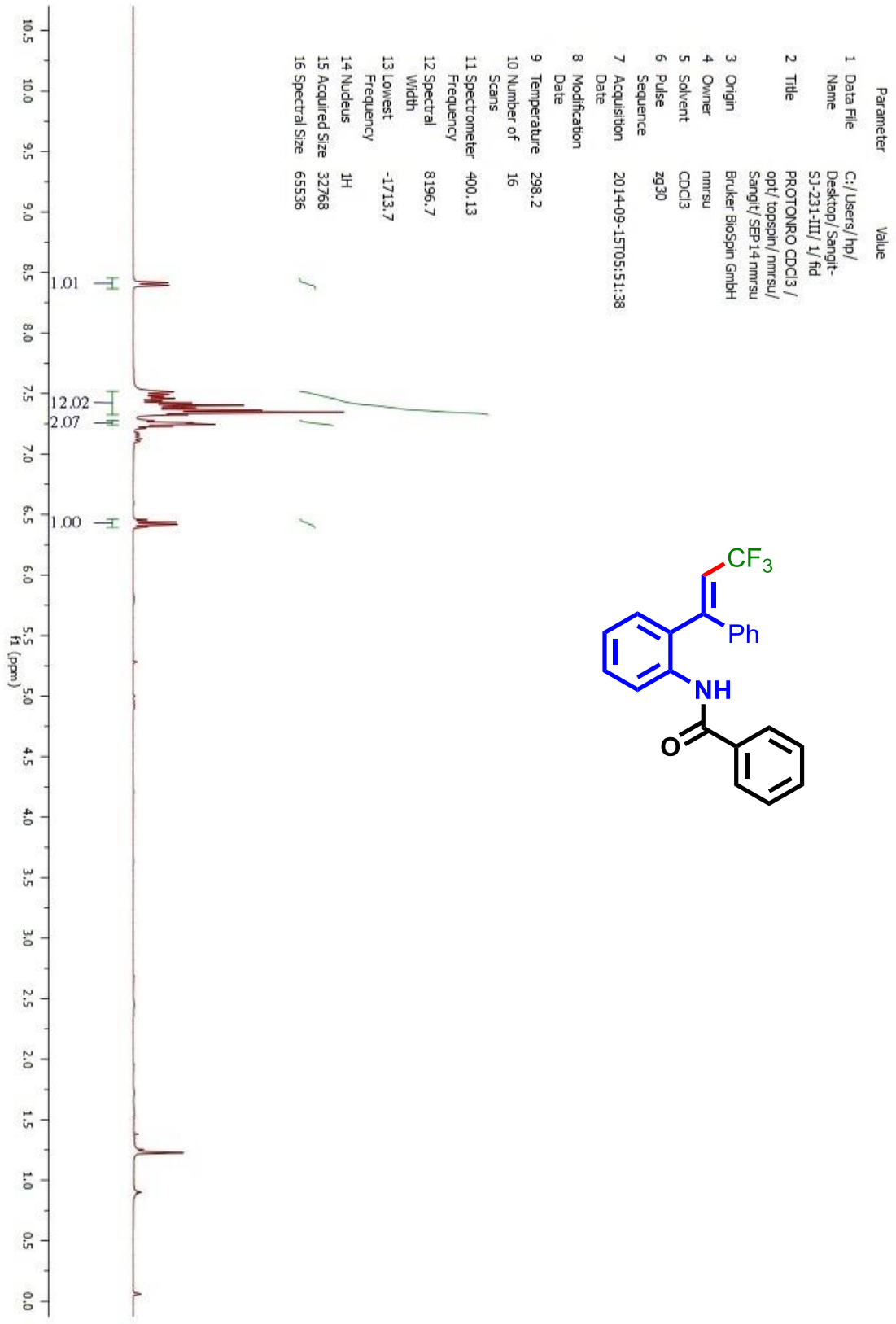
S147 ^{13}C NMR of **5c**



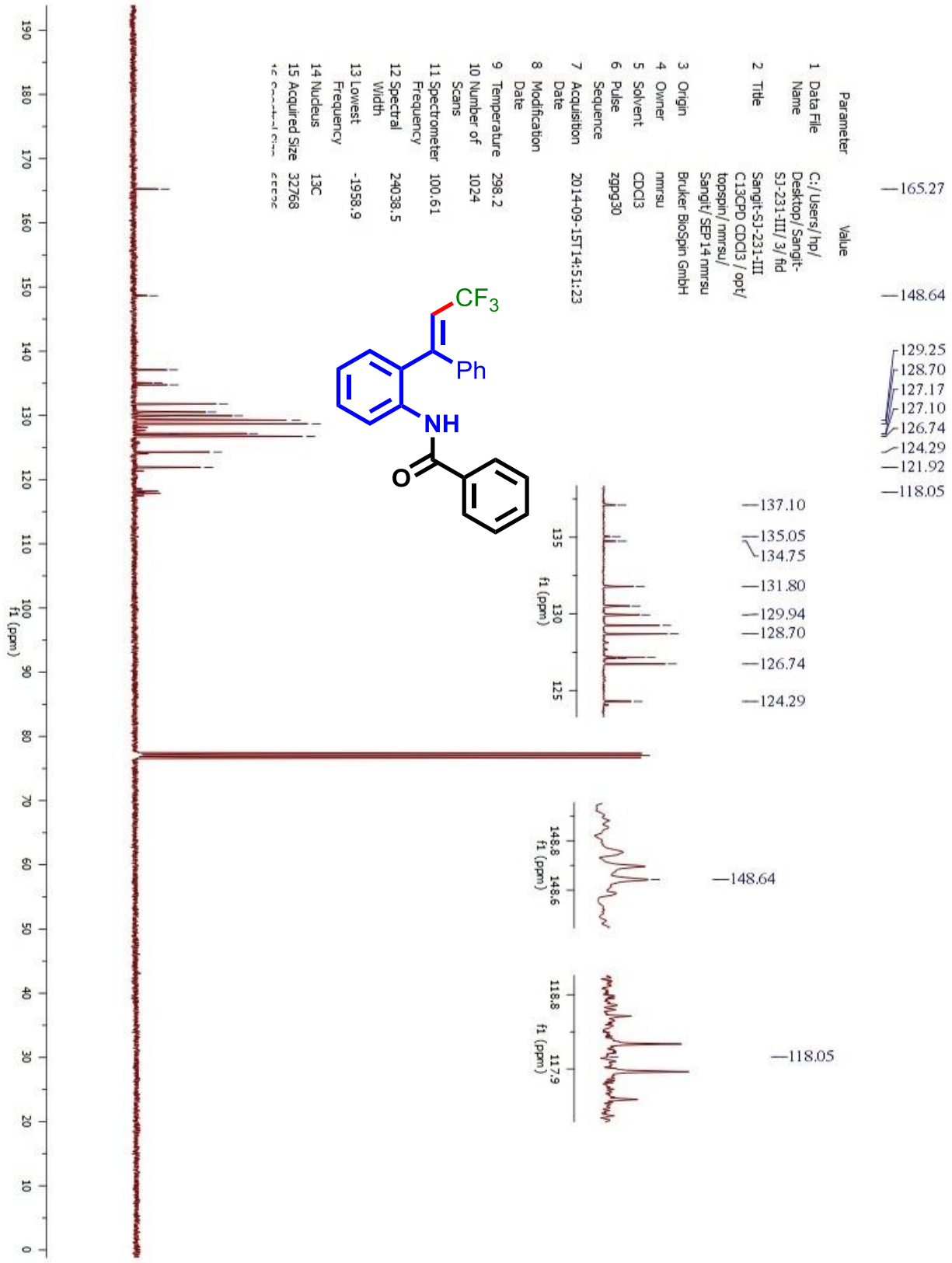
S148 ^{19}F NMR of **5c**



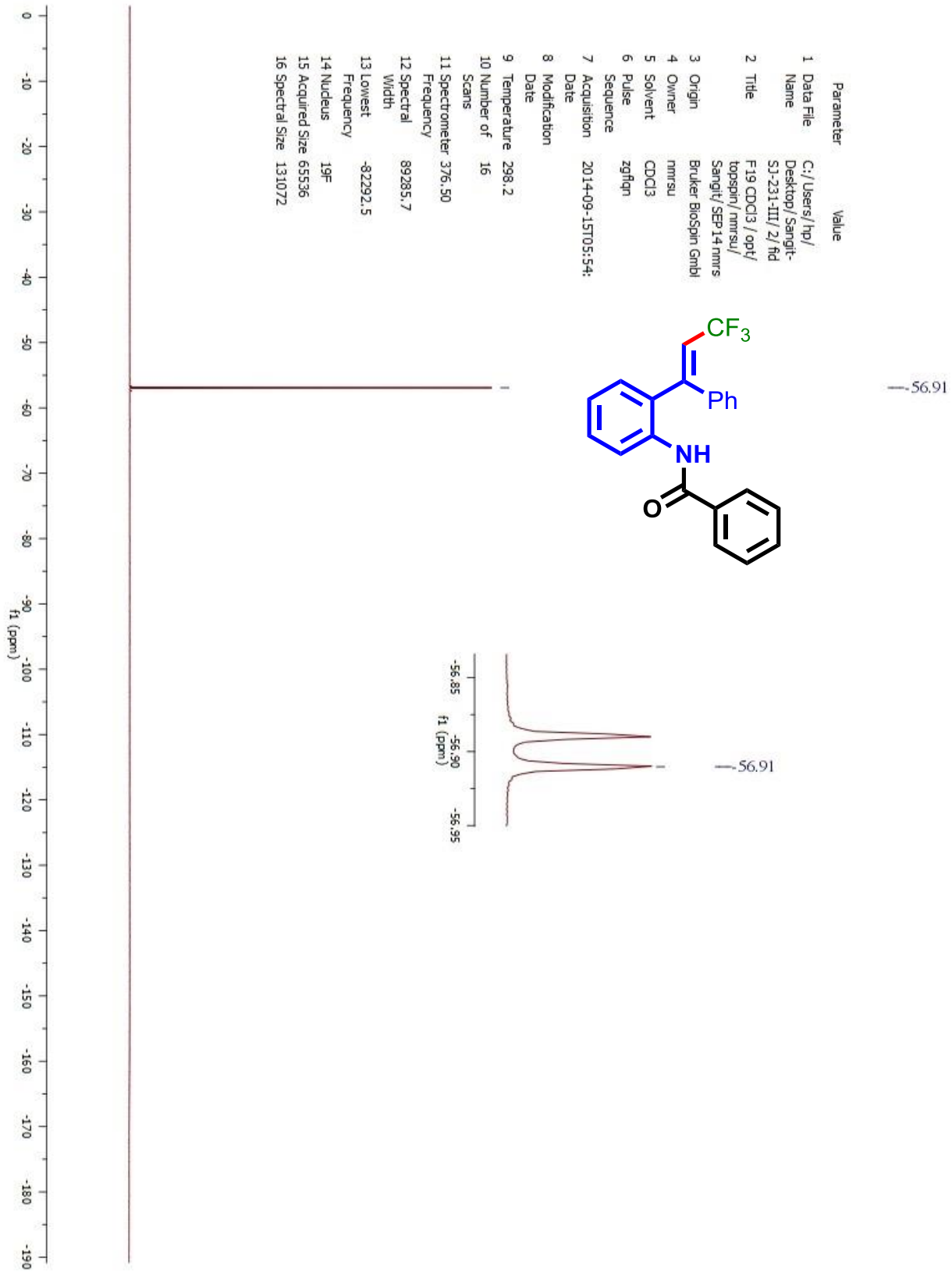
S149 ^{1}H NMR of **5d**



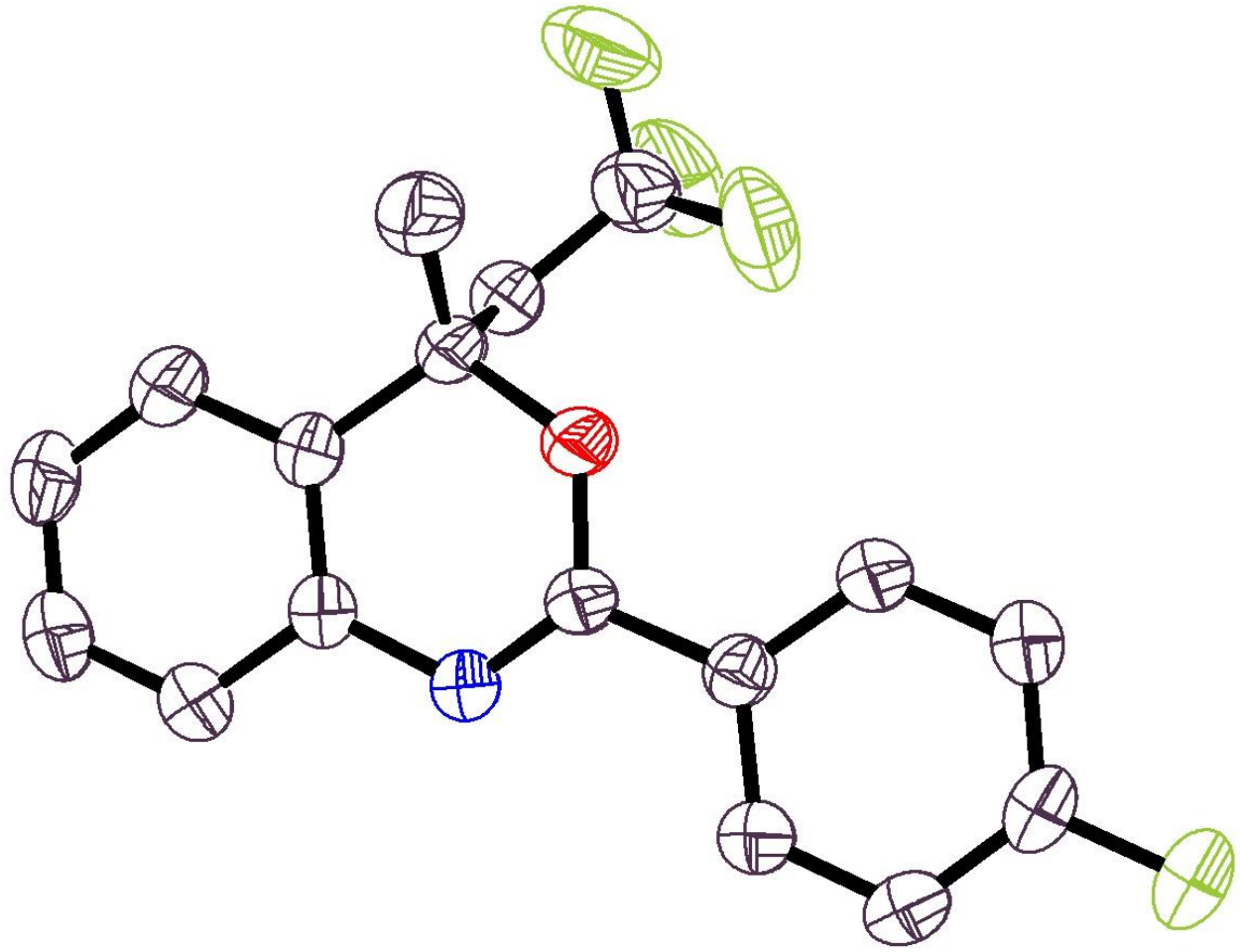
S150 ^{13}C NMR of **5d**



S151 ^{19}F NMR of **5d**



ORTEP View of 3f with 50% ellipsoidal probability



Packing diagram of 3f

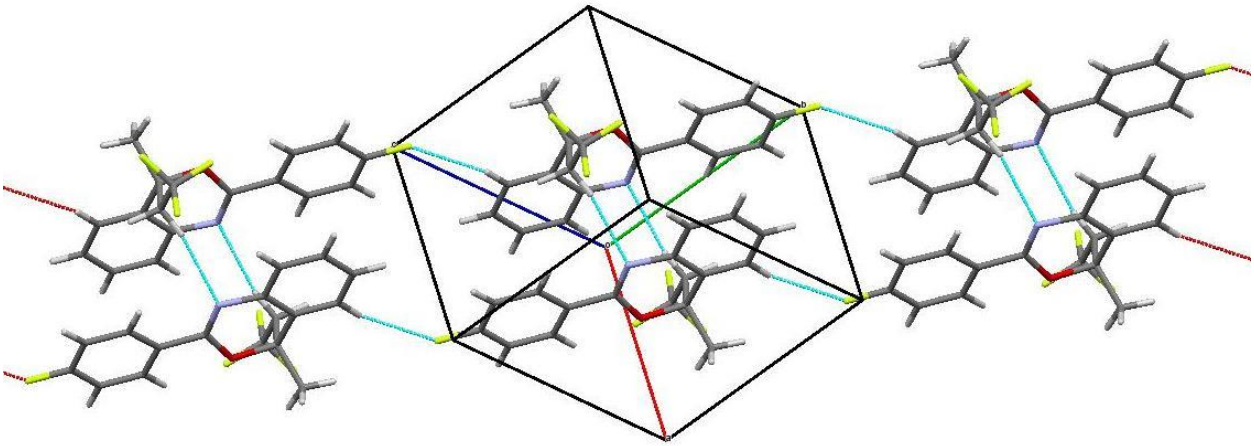


Table 1. Crystal data and structure refinement for 3f

Identification code	**SJ-AA-121 (CCDC No.** 1063690**)**	
Empirical formula	$C_{17}\ H_{13}\ F_4\ N\ O$	
Formula weight	323.28	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 7.3417(10) Å	α= 75.006(4)°.
	b = 10.0649(14) Å	β= 89.015(4)°.
	c = 10.3982(14) Å	γ = 78.726(4)°.
Volume	727.42(17) $Å^3$	
Z	2	
Density (calculated)	1.476 Mg/m^3	
Absorption coefficient	0.127 mm^{-1}	
F(000)	332	
Theta range for data collection	2.029 to 26.435°.	
Index ranges	-9<=h<=9, -12<=k<=12, -13<=l<=13	
Reflections collected	21469	
Independent reflections	2970 [R(int) = 0.0366]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2970 / 0 / 209	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2sigma(I)]	R1 = 0.0481, wR2 = 0.1194	
R indices (all data)	R1 = 0.0819, wR2 = 0.1373	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.213 and -0.202 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 3f U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	8355(2)	3570(1)	4009(1)	53(1)
F(1)	8564(2)	-1374(1)	9075(1)	83(1)
F(4)	7044(2)	3393(2)	551(2)	99(1)
F(2)	6803(3)	2117(1)	2494(2)	108(1)
N(1)	7343(2)	4885(2)	5524(2)	46(1)
F(3)	4390(2)	3263(2)	1318(2)	104(1)
C(1)	7232(2)	6134(2)	4506(2)	40(1)
C(11)	7867(2)	3725(2)	5225(2)	38(1)
C(12)	8065(2)	2367(2)	6235(2)	39(1)
C(7)	7867(3)	4731(2)	2820(2)	43(1)
C(17)	8362(3)	1110(2)	5877(2)	48(1)
C(6)	7491(3)	6123(2)	3184(2)	43(1)
C(8)	6065(3)	4573(2)	2206(2)	50(1)
C(13)	7932(3)	2338(2)	7576(2)	49(1)
C(2)	6838(3)	7405(2)	4846(2)	51(1)
C(3)	6671(3)	8657(2)	3882(2)	55(1)
C(14)	8096(3)	1082(2)	8532(2)	57(1)
C(4)	6905(3)	8648(2)	2570(2)	60(1)

C(10)	9547(3)	4585(2)	1963(2)	58(1)
C(16)	8531(3)	-152(2)	6828(2)	54(1)
C(5)	7319(3)	7390(2)	2224(2)	59(1)
C(15)	8391(3)	-133(2)	8134(2)	53(1)
C(9)	6095(3)	3323(2)	1670(2)	64(1)

Table 3. Selected bond lengths [Å] for 3f

O1—C11	1.348 (2)	C8—C9	1.499 (3)
O1—C7	1.459 (2)	C8—H8A	0.99
F1—C15	1.358 (2)	C8—H8B	0.99
F4—C9	1.338 (3)	C13—C14	1.376 (3)
F2—C9	1.307 (3)	C13—H13	0.95
N1—C11	1.271 (2)	C2—C3	1.377 (3)
N1—C1	1.409 (2)	C2—H2	0.95
F3—C9	1.327 (3)	C3—C4	1.375 (3)
C1—C6	1.387 (3)	C3—H3	0.95
C1—C2	1.390 (3)	C14—C15	1.367 (3)
C11—C12	1.475 (2)	C14—H14	0.95
C12—C17	1.386 (2)	C4—C5	1.380 (3)
C12—C13	1.390 (3)	C4—H4	0.95
C7—C10	1.515 (3)	C10—H10A	0.98

C7—C6	1.517 (2)	C10—H10B	0.98
C7—C8	1.532 (3)	C10—H10C	0.98
C17—C16	1.378 (3)	C16—C15	1.365 (3)
C17—H17	0.95	C16—H16	0.95
C6—C5	1.387 (3)	C5—H5	0.95

Table 4. Selected bond angles [°] for 3f

C11—O1—C7	121.02 (13)	C3—C2—H2	119.6
C11—N1—C1	118.15 (15)	C1—C2—H2	119.6
C6—C1—C2	119.74 (17)	C4—C3—C2	119.64 (18)
C6—C1—N1	121.71 (16)	C4—C3—H3	120.2
C2—C1—N1	118.55 (16)	C2—C3—H3	120.2
N1—C11—O1	125.89 (16)	C15—C14—C13	118.62 (18)
N1—C11—C12	121.77 (16)	C15—C14—H14	120.7
O1—C11—C12	112.30 (14)	C13—C14—H14	120.7
C17—C12—C13	118.78 (17)	C3—C4—C5	120.07 (19)
C17—C12—C11	121.48 (16)	C3—C4—H4	120
C13—C12—C11	119.73 (16)	C5—C4—H4	120
O1—C7—C10	104.03 (14)	C7—C10—H10A	109.5
O1—C7—C6	110.55 (14)	C7—C10—H10B	109.5
C10—C7—C6	112.08 (16)	H10A—C10—H10B	109.5

O1—C7—C8	107.60 (15)	C7—C10—H10C	109.5
C10—C7—C8	114.80 (16)	H10A—C10—H10C	109.5
C6—C7—C8	107.66 (15)	H10B—C10—H10C	109.5
C16—C17—C12	121.01 (18)	C15—C16—C17	118.26 (18)
C16—C17—H17	119.5	C15—C16—H16	120.9
C12—C17—H17	119.5	C17—C16—H16	120.9
C5—C6—C1	118.94 (17)	C4—C5—C6	120.9 (2)
C5—C6—C7	121.75 (17)	C4—C5—H5	119.6
C1—C6—C7	119.26 (16)	C6—C5—H5	119.6
C9—C8—C7	118.47 (17)	F1—C15—C16	118.47 (18)
C9—C8—H8A	107.7	F1—C15—C14	118.80 (18)
C7—C8—H8A	107.7	C16—C15—C14	122.73 (18)
C9—C8—H8B	107.7	F2—C9—F3	107.5 (2)
C7—C8—H8B	107.7	F2—C9—F4	106.5 (2)
H8A—C8—H8B	107.1	F3—C9—F4	104.46 (19)
C14—C13—C12	120.59 (18)	F2—C9—C8	114.70 (18)
C14—C13—H13	119.7	F3—C9—C8	110.58 (19)
C12—C13—H13	119.7	F4—C9—C8	112.4 (2)
C3—C2—C1	120.71 (19)		

Table 5. Anisotropic displacement parameters ($Å^2$x 10^3) for 3f The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	84(1)	36(1)	32(1)	-6(1)	2(1)	2(1)
F(1)	135(1)	47(1)	54(1)	7(1)	6(1)	-16(1)
F(4)	130(1)	106(1)	75(1)	-57(1)	6(1)	-17(1)
F(2)	179(2)	44(1)	99(1)	-17(1)	-48(1)	-14(1)
N(1)	65(1)	36(1)	38(1)	-10(1)	5(1)	-10(1)
F(3)	107(1)	101(1)	123(1)	-50(1)	-22(1)	-36(1)
C(1)	44(1)	35(1)	42(1)	-9(1)	2(1)	-9(1)
C(11)	43(1)	39(1)	32(1)	-9(1)	-1(1)	-7(1)
C(12)	40(1)	38(1)	37(1)	-8(1)	-1(1)	-6(1)
C(7)	59(1)	35(1)	31(1)	-5(1)	2(1)	-5(1)
C(17)	65(1)	41(1)	37(1)	-10(1)	-1(1)	-8(1)
C(6)	51(1)	36(1)	40(1)	-6(1)	2(1)	-8(1)
C(8)	61(1)	43(1)	43(1)	-10(1)	1(1)	-8(1)
C(13)	65(1)	42(1)	39(1)	-11(1)	1(1)	-7(1)
C(2)	64(1)	43(1)	50(1)	-16(1)	5(1)	-13(1)
C(3)	61(1)	36(1)	68(1)	-15(1)	2(1)	-10(1)
C(14)	80(2)	53(1)	34(1)	-7(1)	4(1)	-10(1)
C(4)	74(2)	36(1)	63(1)	-1(1)	1(1)	-12(1)

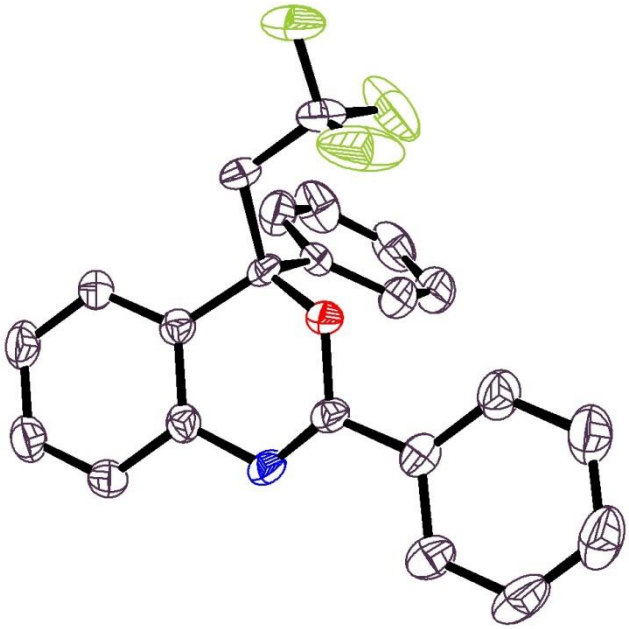
C(10)	65(1)	53(1)	55(1)	-14(1)	15(1)	-8(1)
C(16)	75(1)	36(1)	50(1)	-10(1)	2(1)	-9(1)
C(5)	82(2)	44(1)	44(1)	-3(1)	6(1)	-11(1)
C(15)	68(1)	40(1)	43(1)	3(1)	1(1)	-10(1)
C(9)	80(2)	61(2)	51(1)	-18(1)	-11(1)	-8(1)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 3f

	x	y	z	U(eq)
H(17)	8452	1117	4963	58
H(8A)	5112	4563	2892	59
H(8B)	5642	5425	1471	59
H(13)	7727	3192	7835	59
H(2)	6683	7411	5754	61
H(3)	6396	9521	4123	66
H(14)	8005	1060	9450	69
H(4)	6781	9509	1900	72
H(10A)	10627	4723	2417	87
H(10B)	9299	5291	1106	87
H(10C)	9803	3645	1812	87

H(16)	8738	-1013	6581	65
H(5)	7489	7393	1315	70

ORTEP view of 3z with 50% ellipsoidal probability



Packing diagram of 3z

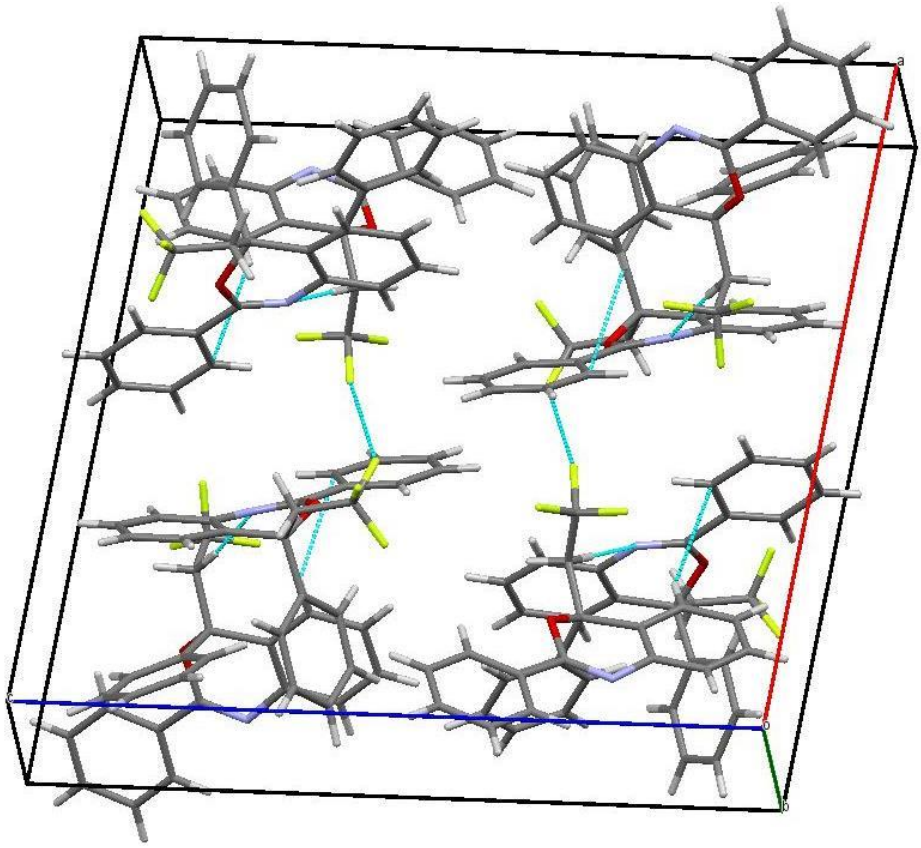


Table 7. Crystal data and structure refinement for 3z

Identification code	**AA-146 (CCDC No.** 1402833**)**	
Empirical formula	C_{22} H_{16} F_3 N O	
Formula weight	367.36	
Temperature	140(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P $2_{1/c}$	
Unit cell dimensions	a = 16.972(3) Å	α= 90°.
	b = 11.3201(16) Å	β= 98.676(5)°.
	c = 18.722(3) Å	γ = 90°.
Volume	3555.7(10) $Å^3$	
Z	8	
Density (calculated)	1.372 Mg/m^3	
Absorption coefficient	0.106 mm^{-1}	
F(000)	1520	
Theta range for data collection	2.109 to 24.432°.	
Index ranges	-19<=h<=19, -13<=k<=13, -21<=l<=21	
Reflections collected	72735	
Independent reflections	5859 [R(int) = 0.1793]	
Completeness to theta = 25.242°	90.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5859 / 0 / 487	
Goodness-of-fit on F^2	1.149	
Final R indices [I>2sigma(I)]	R1 = 0.0842, wR2 = 0.2066	
R indices (all data)	R1 = 0.1296, wR2 = 0.2331	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.742 and -0.503 $e.Å^{-3}$	

Table 8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 3z. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(2)	6302(2)	5272(2)	3309(2)	28(1)
O(1)	2094(2)	4763(3)	3306(2)	32(1)
F(1)	4495(2)	5658(3)	3449(2)	58(1)
F(4)	6467(2)	8720(3)	3978(2)	67(1)
F(5)	7104(2)	7199(4)	4401(2)	84(1)
F(3)	3715(2)	4325(3)	3735(2)	85(1)
F(6)	5860(2)	7120(3)	4065(2)	88(1)
N(1)	1176(2)	4171(3)	2312(2)	29(1)
F(2)	3749(2)	4717(3)	2624(2)	81(1)
N(2)	6262(2)	3786(3)	2437(2)	30(1)
C(1)	1585(2)	4859(4)	1863(2)	25(1)
C(16)	1425(3)	4155(3)	2984(2)	26(1)
C(2)	1430(3)	4682(4)	1124(2)	32(1)
C(28)	6819(2)	5721(4)	2206(2)	27(1)
C(32)	7730(3)	5630(4)	3388(2)	28(1)
C(23)	6533(3)	4620(4)	1960(2)	30(1)
C(31)	6526(3)	7550(4)	3897(3)	39(1)
C(38)	6144(2)	4155(4)	3054(2)	27(1)

C(29)	6887(3)	5961(4)	3009(2)	27(1)
C(17)	1083(3)	3383(4)	3487(2)	28(1)
C(39)	5796(3)	3406(4)	3565(2)	32(1)
C(7)	2280(3)	5867(4)	2966(2)	31(1)
C(30)	6668(3)	7251(4)	3155(2)	34(1)
C(3)	1808(3)	5332(4)	659(2)	38(1)
C(6)	2154(3)	5709(4)	2148(2)	30(1)
C(24)	6475(3)	4327(4)	1232(2)	36(1)
C(8)	3146(3)	6143(4)	3296(3)	34(1)
C(25)	6715(3)	5124(5)	751(3)	42(1)
C(27)	7054(3)	6510(4)	1712(2)	38(1)
C(10)	1748(3)	6861(4)	3196(2)	30(1)
C(20)	401(3)	1912(4)	4411(3)	43(1)
C(44)	5483(3)	2301(4)	3338(3)	41(1)
C(33)	7869(3)	4704(4)	3866(3)	40(1)
C(22)	457(3)	2641(4)	3215(3)	38(1)
C(18)	1373(3)	3372(4)	4224(3)	40(1)
C(26)	7011(3)	6217(5)	990(3)	43(1)
C(40)	5777(3)	3759(5)	4273(3)	42(1)
C(5)	2542(3)	6337(4)	1679(3)	39(1)
C(4)	2368(3)	6171(5)	938(3)	45(1)
C(19)	1024(3)	2643(4)	4683(3)	44(1)

C(21)	112(3)	1915(5)	3674(3)	46(1)
C(34)	8639(3)	4387(5)	4166(3)	49(1)
C(9)	3763(3)	5209(4)	3274(3)	43(1)
C(37)	8387(3)	6251(5)	3229(3)	43(1)
C(15)	1435(4)	6758(5)	3831(3)	53(2)
C(35)	9282(3)	4995(5)	3994(3)	51(2)
C(13)	910(3)	8695(5)	3693(3)	48(1)
C(42)	5160(3)	1944(6)	4531(3)	56(2)
C(41)	5451(3)	3036(5)	4754(3)	54(2)
C(43)	5170(3)	1575(5)	3828(3)	55(2)
C(11)	1626(3)	7880(4)	2818(3)	43(1)
C(36)	9155(3)	5958(6)	3534(3)	55(2)
C(14)	1008(4)	7643(5)	4072(3)	59(2)
C(12)	1207(3)	8802(5)	3067(3)	50(1)

Table 9. Selected bond lengths [Å] for 3z.

O2—C38	1.364 (5)	C25—C26	1.383 (7)
O2—C29	1.442 (5)	C25—H18	0.95
O1—C16	1.385 (5)	C27—C26	1.383 (7)
O1—C7	1.458 (5)	C27—H20	0.95
F1—C9	1.336 (6)	C10—C11	1.354 (7)
F4—C31	1.338 (5)	C10—C15	1.378 (7)
F5—C31	1.316 (6)	C20—C19	1.377 (7)

F3—C9	1.333 (6)	C20—C21	1.392 (7)
F6—C31	1.314 (6)	C20—H14	0.95
N1—C16	1.265 (5)	C44—C43	1.396 (7)
N1—C1	1.404 (5)	C44—H32	0.95
F2—C9	1.334 (6)	C33—C34	1.389 (7)
N2—C38	1.272 (5)	C33—H23	0.95
N2—C23	1.423 (6)	C22—C21	1.382 (7)
C1—C2	1.383 (6)	C22—H16	0.95
C1—C6	1.410 (6)	C18—C19	1.388 (7)
C16—C17	1.467 (6)	C18—H12	0.95
C2—C3	1.370 (7)	C26—H19	0.95
C2—H1	0.95	C40—C41	1.392 (7)
C28—C27	1.387 (6)	C40—H28	0.95
C28—C23	1.391 (6)	C5—C4	1.387 (7)
C28—C29	1.514 (6)	C5—H4	0.95
C32—C33	1.376 (6)	C4—H3	0.95
C32—C37	1.388 (6)	C19—H13	0.95
C32—C29	1.544 (6)	C21—H15	0.95
C23—C24	1.392 (6)	C34—C35	1.369 (8)
C31—C30	1.484 (7)	C34—H24	0.95
C38—C39	1.468 (6)	C37—C36	1.381 (7)
C29—C30	1.541 (6)	C37—H27	0.95
C17—C22	1.390 (6)	C15—C14	1.354 (7)
C17—C18	1.393 (6)	C15—H11	0.95
C39—C40	1.388 (7)	C35—C36	1.386 (8)
C39—C44	1.401 (7)	C35—H25	0.95
C7—C6	1.524 (6)	C13—C12	1.349 (7)
C7—C8	1.537 (6)	C13—C14	1.383 (8)
C7—C10	1.545 (6)	C13—H9	0.95

C30—H22	0.99	C42—C41	1.372 (8)
C30—H21	0.99	C42—C43	1.384 (8)
C3—C4	1.389 (7)	C42—H30	0.95
C3—H2	0.95	C41—H29	0.95
C6—C5	1.372 (6)	C43—H31	0.95
C24—C25	1.379 (7)	C11—C12	1.383 (7)
C24—H17	0.95	C11—H7	0.95
C8—C9	1.493 (7)	C36—H26	0.95
C8—H5	0.99	C14—H10	0.95
C8—H6	0.99	C12—H8	0.95

Table 10. Selected bond angles [°] for 3z.

C38—O2—C29	118.3 (3)	C11—C10—C7	121.6 (4)
C16—O1—C7	117.0 (3)	C15—C10—C7	119.9 (4)
C16—N1—C1	118.8 (4)	C19—C20—C21	120.1 (5)
C38—N2—C23	117.5 (4)	C19—C20—H14	120
C2—C1—N1	118.9 (4)	C21—C20—H14	120
C2—C1—C6	119.5 (4)	C43—C44—C39	119.4 (5)
N1—C1—C6	121.6 (4)	C43—C44—H32	120.3
N1—C16—O1	123.7 (4)	C39—C44—H32	120.3
N1—C16—C17	122.8 (4)	C32—C33—C34	121.2 (5)
O1—C16—C17	113.2 (4)	C32—C33—H23	119.4
C3—C2—C1	121.4 (4)	C34—C33—H23	119.4
C3—C2—H1	119.3	C21—C22—C17	120.3 (4)
C1—C2—H1	119.3	C21—C22—H16	119.9
C27—C28—C23	118.5 (4)	C17—C22—H16	119.9
C27—C28—C29	124.1 (4)	C19—C18—C17	119.9 (5)
C23—C28—C29	117.4 (4)	C19—C18—H12	120.1
C33—C32—C37	117.4 (4)	C17—C18—H12	120.1

C33—C32—C29	122.7 (4)	C27—C26—C25	119.6 (5)
C37—C32—C29	119.9 (4)	C27—C26—H19	120.2
C28—C23—C24	120.5 (4)	C25—C26—H19	120.2
C28—C23—N2	121.1 (4)	C39—C40—C41	121.1 (5)
C24—C23—N2	118.3 (4)	C39—C40—H28	119.4
F6—C31—F5	106.9 (5)	C41—C40—H28	119.4
F6—C31—F4	104.9 (4)	C6—C5—C4	121.3 (5)
F5—C31—F4	106.1 (4)	C6—C5—H4	119.3
F6—C31—C30	114.0 (4)	C4—C5—H4	119.3
F5—C31—C30	113.3 (4)	C5—C4—C3	119.9 (5)
F4—C31—C30	111.0 (4)	C5—C4—H3	120.1
N2—C38—O2	125.0 (4)	C3—C4—H3	120.1
N2—C38—C39	122.4 (4)	C20—C19—C18	120.3 (5)
O2—C38—C39	112.6 (4)	C20—C19—H13	119.9
O2—C29—C28	109.7 (3)	C18—C19—H13	119.9
O2—C29—C30	104.1 (3)	C22—C21—C20	119.9 (5)
C28—C29—C30	111.2 (3)	C22—C21—H15	120.1
O2—C29—C32	109.6 (3)	C20—C21—H15	120.1
C28—C29—C32	109.8 (3)	C35—C34—C33	120.6 (5)
C30—C29—C32	112.3 (4)	C35—C34—H24	119.7
C22—C17—C18	119.6 (4)	C33—C34—H24	119.7
C22—C17—C16	118.6 (4)	F3—C9—F2	106.4 (4)
C18—C17—C16	121.8 (4)	F3—C9—F1	105.8 (4)
C40—C39—C44	119.0 (4)	F2—C9—F1	105.7 (4)
C40—C39—C38	121.7 (4)	F3—C9—C8	113.7 (5)
C44—C39—C38	119.3 (4)	F2—C9—C8	113.8 (4)
O1—C7—C6	109.3 (3)	F1—C9—C8	110.7 (4)
O1—C7—C8	104.8 (3)	C36—C37—C32	121.9 (5)
C6—C7—C8	114.1 (4)	C36—C37—H27	119

O1—C7—C10	109.1 (3)	C32—C37—H27	119
C6—C7—C10	111.5 (4)	C14—C15—C10	121.4 (5)
C8—C7—C10	107.7 (3)	C14—C15—H11	119.3
C31—C30—C29	117.4 (4)	C10—C15—H11	119.3
C31—C30—H22	107.9	C34—C35—C36	119.1 (5)
C29—C30—H22	107.9	C34—C35—H25	120.4
C31—C30—H21	107.9	C36—C35—H25	120.4
C29—C30—H21	107.9	C12—C13—C14	119.4 (5)
H22—C30—H21	107.2	C12—C13—H9	120.3
C2—C3—C4	119.2 (4)	C14—C13—H9	120.3
C2—C3—H2	120.4	C41—C42—C43	120.4 (5)
C4—C3—H2	120.4	C41—C42—H30	119.8
C5—C6—C1	118.6 (4)	C43—C42—H30	119.8
C5—C6—C7	125.0 (4)	C42—C41—C40	119.5 (5)
C1—C6—C7	116.4 (4)	C42—C41—H29	120.2
C25—C24—C23	119.9 (5)	C40—C41—H29	120.2
C25—C24—H17	120.1	C42—C43—C44	120.5 (5)
C23—C24—H17	120.1	C42—C43—H31	119.7
C9—C8—C7	118.5 (4)	C44—C43—H31	119.7
C9—C8—H5	107.7	C10—C11—C12	120.9 (5)
C7—C8—H5	107.7	C10—C11—H7	119.6
C9—C8—H6	107.7	C12—C11—H7	119.6
C7—C8—H6	107.7	C37—C36—C35	119.6 (5)
H5—C8—H6	107.1	C37—C36—H26	120.2
C24—C25—C26	120.2 (4)	C35—C36—H26	120.2
C24—C25—H18	119.9	C15—C14—C13	119.6 (5)
C26—C25—H18	119.9	C15—C14—H10	120.2
C26—C27—C28	121.3 (5)	C13—C14—H10	120.2
C26—C27—H20	119.3	C13—C12—C11	120.2 (5)

C28—C27—H20	119.3	C13—C12—H8	119.9
C11—C10—C15	118.3 (5)	C11—C12—H8	119.9

Table 11. Anisotropic displacement parameters ($Å^2$x 10^3) for 3z. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(2)	35(2)	22(2)	26(2)	-3(1)	7(1)	-1(1)
O(1)	37(2)	22(2)	36(2)	2(1)	-3(1)	-7(1)
F(1)	37(2)	45(2)	89(2)	-8(2)	-6(2)	-3(1)
F(4)	101(3)	31(2)	71(2)	-21(2)	19(2)	1(2)
F(5)	104(3)	105(3)	35(2)	-22(2)	-14(2)	51(2)
F(3)	49(2)	47(2)	152(4)	45(2)	-9(2)	5(2)
F(6)	91(3)	74(3)	116(3)	-57(2)	72(3)	-41(2)
N(1)	31(2)	27(2)	27(2)	0(2)	0(2)	-4(2)
F(2)	66(2)	71(2)	98(3)	-44(2)	-14(2)	26(2)
N(2)	38(2)	19(2)	34(2)	2(2)	6(2)	2(2)
C(1)	26(2)	20(2)	28(2)	-2(2)	1(2)	6(2)
C(16)	33(3)	12(2)	31(3)	-5(2)	0(2)	-1(2)
C(2)	33(3)	28(3)	34(3)	-4(2)	0(2)	6(2)
C(28)	26(2)	26(2)	29(2)	2(2)	2(2)	1(2)
C(32)	36(3)	27(2)	21(2)	-3(2)	2(2)	0(2)
C(23)	33(3)	29(3)	26(2)	2(2)	3(2)	7(2)
C(31)	44(3)	24(3)	48(3)	-10(2)	9(3)	-3(2)
C(38)	28(2)	21(2)	32(3)	1(2)	3(2)	2(2)
C(29)	35(3)	16(2)	30(2)	3(2)	6(2)	2(2)
C(17)	35(3)	16(2)	32(3)	-1(2)	6(2)	-1(2)
C(39)	28(3)	31(3)	38(3)	5(2)	9(2)	2(2)
C(7)	46(3)	14(2)	32(3)	2(2)	6(2)	-12(2)
C(30)	47(3)	17(2)	37(3)	-1(2)	3(2)	1(2)
C(3)	47(3)	41(3)	25(2)	-4(2)	3(2)	11(2)

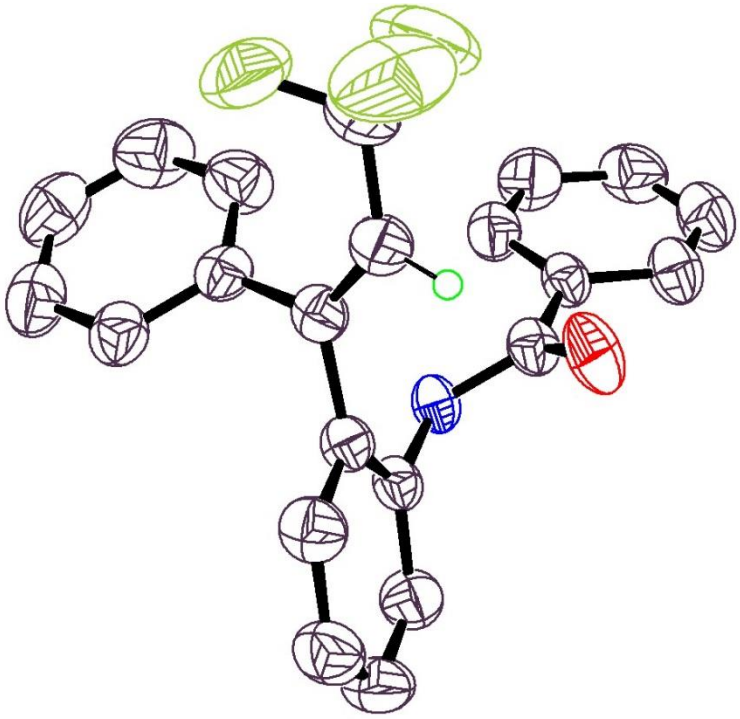
C(6)	37(3)	18(2)	37(3)	-1(2)	8(2)	2(2)
C(24)	49(3)	28(3)	31(3)	-5(2)	7(2)	7(2)
C(8)	34(3)	25(2)	40(3)	-2(2)	-3(2)	-1(2)
C(25)	56(3)	45(3)	27(3)	2(2)	5(2)	10(3)
C(27)	48(3)	34(3)	29(3)	4(2)	-1(2)	-7(2)
C(10)	27(2)	32(3)	28(2)	-2(2)	-4(2)	-10(2)
C(20)	49(3)	34(3)	49(3)	12(2)	17(3)	0(2)
C(44)	35(3)	37(3)	51(3)	2(2)	8(2)	-7(2)
C(33)	47(3)	33(3)	39(3)	5(2)	3(2)	5(2)
C(22)	36(3)	40(3)	36(3)	1(2)	1(2)	-5(2)
C(18)	54(3)	23(3)	41(3)	0(2)	0(2)	-7(2)
C(26)	52(3)	47(3)	31(3)	12(2)	9(2)	-2(3)
C(40)	40(3)	48(3)	40(3)	7(2)	9(2)	-9(2)
C(5)	45(3)	29(3)	42(3)	-4(2)	8(2)	-5(2)
C(4)	62(4)	40(3)	34(3)	6(2)	16(3)	-1(3)
C(19)	63(4)	34(3)	36(3)	6(2)	12(3)	-3(3)
C(21)	42(3)	42(3)	54(3)	8(3)	4(3)	-18(2)
C(34)	57(4)	44(3)	43(3)	7(3)	-6(3)	19(3)
C(9)	42(3)	31(3)	52(3)	-2(3)	-9(2)	-10(2)
C(37)	45(3)	45(3)	39(3)	9(2)	6(2)	-3(2)
C(15)	80(4)	38(3)	43(3)	10(3)	20(3)	12(3)
C(35)	42(3)	71(4)	38(3)	-7(3)	-2(2)	20(3)
C(13)	61(4)	33(3)	51(3)	-7(3)	11(3)	15(3)
C(42)	43(3)	70(4)	54(4)	24(3)	7(3)	-12(3)
C(41)	53(4)	68(4)	41(3)	13(3)	6(3)	-13(3)
C(43)	45(3)	40(3)	78(4)	14(3)	6(3)	-16(3)
C(11)	50(3)	36(3)	45(3)	2(2)	13(2)	9(2)
C(36)	38(3)	82(5)	45(3)	-4(3)	5(3)	-8(3)
C(14)	82(4)	58(4)	43(3)	-1(3)	31(3)	21(3)
C(12)	61(4)	32(3)	56(4)	8(3)	8(3)	12(3)

Table 12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 3z.

	x	y	z	U(eq)
H(1)	1055	4098	934	39
H(22)	7102	7764	3036	41
H(21)	6181	7455	2816	41
H(2)	1688	5210	152	46
H(17)	6269	3579	1066	43
H(5)	3316	6850	3047	41
H(6)	3148	6362	3808	41
H(18)	6678	4923	255	51
H(20)	7248	7266	1872	46
H(14)	169	1405	4726	52
H(32)	5484	2048	2854	49
H(23)	7430	4274	3994	48
H(16)	265	2633	2711	45
H(12)	1810	3863	4412	48
H(19)	7183	6762	660	52
H(28)	5990	4507	4431	51
H(4)	2938	6896	1866	46
H(3)	2632	6631	621	53
H(13)	1214	2647	5187	52
H(15)	-322	1418	3488	55
H(24)	8720	3742	4493	59
H(27)	8307	6895	2901	51
H(11)	1521	6052	4106	63
H(25)	9808	4760	4188	61
H(9)	636	9337	3872	58
H(30)	4951	1439	4862	67
H(29)	5431	3296	5233	65

H(31)	4961	821	3678	66
H(7)	1830	7963	2376	52
H(26)	9593	6415	3430	66
H(10)	776	7543	4500	70
H(8)	1128	9513	2797	60

ORTEP View of 5d with 50% ellipsoidal probability



Packing diagram of 5d

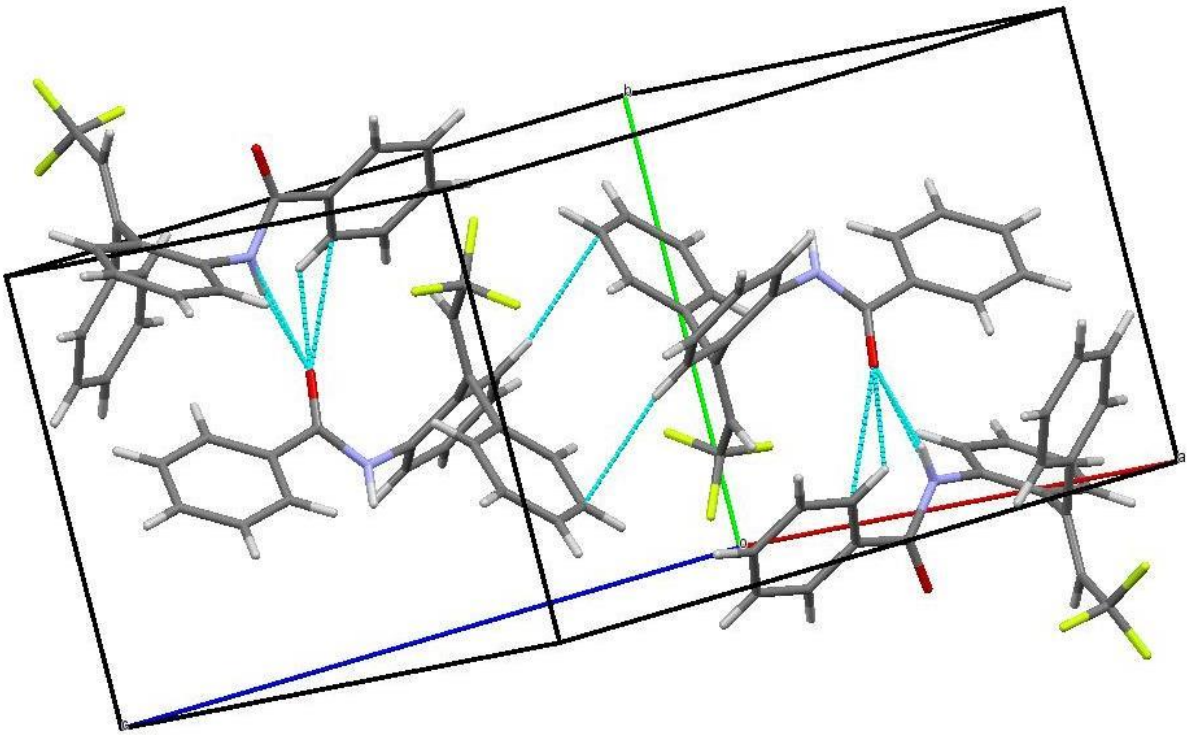


Table 13. Crystal data and structure refinement for 5d.

Identification code	SJ-231 **(CCDC No.** 1402832)	
Empirical formula	C_{22} H_{16} F_3 N O	
Formula weight	367.36	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2_1/n	
Unit cell dimensions	a = 12.8017(8) Å	α= 90°.
	b = 9.6398(6) Å	β= 105.362(4)°.
	c = 15.4464(10) Å	γ = 90°.
Volume	1838.1(2) $Å^3$	
Z	4	
Density (calculated)	1.328 Mg/m^3	
Absorption coefficient	0.102 mm^{-1}	
F(000)	760	
Theta range for data collection	2.406 to 25.394°.	
Index ranges	-15<=h<=15, -11<=k<=11, -18<=l<=18	
Reflections collected	46069	
Independent reflections	3384 [R(int) = 0.1770]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3384 / 0 / 244	
Goodness-of-fit on F^2	1.012	
Final R indices [I>2sigma(I)]	R1 = 0.0563, wR2 = 0.1264	
R indices (all data)	R1 = 0.1246, wR2 = 0.1525	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.300 and -0.241 $e.Å^{-3}$	

Table 14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 5d. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	2120(2)	6369(2)	7261(1)	64(1)
N(1)	2527(2)	4147(2)	7036(1)	40(1)
F(2)	6079(2)	6873(2)	6649(2)	98(1)
F(1)	5383(2)	7688(3)	7622(2)	131(1)
F(3)	5270(2)	8772(2)	6403(2)	126(1)
C(6)	2873(2)	5031(3)	5660(2)	39(1)
C(17)	2678(2)	4936(3)	8552(2)	41(1)
C(1)	2215(2)	4299(3)	6079(2)	39(1)
C(10)	4779(2)	4359(3)	6466(2)	42(1)
C(16)	2424(2)	5218(3)	7574(2)	43(1)
C(7)	3975(2)	5501(3)	6174(2)	41(1)
C(8)	4166(2)	6847(3)	6313(2)	50(1)
C(11)	4901(2)	3378(3)	5839(2)	52(1)
C(22)	2087(3)	5654(3)	9041(2)	55(1)
C(2)	1249(2)	3751(3)	5585(2)	54(1)
C(18)	3453(2)	3998(3)	8993(2)	54(1)
C(5)	2513(2)	5235(3)	4738(2)	53(1)
C(4)	1544(3)	4696(3)	4250(2)	61(1)
C(3)	913(3)	3939(3)	4669(2)	63(1)
C(12)	5629(3)	2297(3)	6092(3)	66(1)
C(9)	5203(3)	7529(4)	6747(3)	68(1)
C(21)	2261(3)	5407(4)	9951(2)	69(1)
C(15)	5388(3)	4207(3)	7344(2)	64(1)
C(20)	3018(3)	4471(4)	10373(2)	70(1)
C(19)	3625(3)	3770(4)	9900(2)	71(1)
C(13)	6235(3)	2175(4)	6958(3)	74(1)
C(14)	6109(3)	3121(4)	7585(3)	81(1)

Table 15. Selected bond lengths [Å] and angles [°] for 5d

O1—C16	1.232 (3)	C22—H16	0.95
N1—C16	1.354 (3)	C2—C3	1.377 (4)
N1—C1	1.433 (3)	C2—H2	0.95
N1—H1	0.88	C18—C19	1.378 (4)
F2—C9	1.331 (4)	C18—H12	0.95
F1—C9	1.318 (4)	C5—C4	1.371 (4)
F3—C9	1.323 (4)	C5—H5	0.95
C6—C1	1.384 (3)	C4—C3	1.371 (4)
C6—C5	1.390 (4)	C4—H4	0.95
C6—C7	1.494 (4)	C3—H3	0.95
C17—C18	1.381 (4)	C12—C13	1.362 (5)
C17—C22	1.388 (4)	C12—H8	0.95
C17—C16	1.483 (4)	C21—C20	1.358 (5)
C1—C2	1.375 (4)	C21—H15	0.95
C10—C15	1.381 (4)	C15—C14	1.380 (5)
C10—C11	1.392 (4)	C15—H11	0.95
C10—C7	1.493 (4)	C20—C19	1.377 (5)
C7—C8	1.327 (4)	C20—H14	0.95
C8—C9	1.473 (4)	C19—H13	0.95

C8—H6	0.95	C13—C14	1.371 (5)
C11—C12	1.384 (4)	C13—H9	0.95
C11—H7	0.95	C14—H10	0.95
C22—C21	1.384 (4)		

Table 16. Selected bond angles [°] for 5d

C16—N1—C1	120.6 (2)	C4—C5—C6	121.0 (3)
C16—N1—H1	119.7	C4—C5—H5	119.5
C1—N1—H1	119.7	C6—C5—H5	119.5
C1—C6—C5	118.2 (3)	C5—C4—C3	120.2 (3)
C1—C6—C7	120.9 (2)	C5—C4—H4	119.9
C5—C6—C7	120.8 (2)	C3—C4—H4	119.9
C18—C17—C22	118.8 (3)	C4—C3—C2	119.5 (3)
C18—C17—C16	123.9 (3)	C4—C3—H3	120.3
C22—C17—C16	117.3 (3)	C2—C3—H3	120.3
C2—C1—C6	120.4 (3)	C13—C12—C11	120.6 (3)
C2—C1—N1	119.8 (2)	C13—C12—H8	119.7
C6—C1—N1	119.8 (2)	C11—C12—H8	119.7
C15—C10—C11	118.2 (3)	F1—C9—F3	107.0 (3)
C15—C10—C7	122.7 (3)	F1—C9—F2	104.3 (3)
C11—C10—C7	119.1 (3)	F3—C9—F2	103.8 (3)
O1—C16—N1	121.2 (3)	F1—C9—C8	114.2 (3)

O1—C16—C17	121.8 (2)	F3—C9—C8	111.6 (3)
N1—C16—C17	117.1 (2)	F2—C9—C8	115.0 (3)
C8—C7—C10	126.1 (3)	C20—C21—C22	120.3 (3)
C8—C7—C6	119.4 (3)	C20—C21—H15	119.8
C10—C7—C6	114.5 (2)	C22—C21—H15	119.8
C7—C8—C9	127.9 (3)	C14—C15—C10	120.6 (3)
C7—C8—H6	116	C14—C15—H11	119.7
C9—C8—H6	116	C10—C15—H11	119.7
C12—C11—C10	120.4 (3)	C21—C20—C19	120.2 (3)
C12—C11—H7	119.8	C21—C20—H14	119.9
C10—C11—H7	119.8	C19—C20—H14	119.9
C21—C22—C17	120.2 (3)	C20—C19—C18	120.0 (3)
C21—C22—H16	119.9	C20—C19—H13	120
C17—C22—H16	119.9	C18—C19—H13	120
C1—C2—C3	120.6 (3)	C12—C13—C14	119.5 (3)
C1—C2—H2	119.7	C12—C13—H9	120.2
C3—C2—H2	119.7	C14—C13—H9	120.2
C19—C18—C17	120.5 (3)	C13—C14—C15	120.7 (3)
C19—C18—H12	119.8	C13—C14—H10	119.7
C17—C18—H12	119.8	C15—C14—H10	119.7

Table 17. Anisotropic displacement parameters ($Å^2$x 10^3) for 5d. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	105(2)	32(1)	61(1)	3(1)	30(1)	12(1)
N(1)	51(1)	28(1)	44(1)	0(1)	17(1)	3(1)
F(2)	52(1)	88(2)	146(2)	-16(2)	14(1)	-16(1)
F(1)	131(2)	166(3)	93(2)	-63(2)	22(2)	-63(2)
F(3)	95(2)	61(1)	201(3)	23(2)	2(2)	-30(1)
C(6)	42(2)	35(2)	41(2)	-1(1)	12(1)	0(1)
C(17)	49(2)	34(2)	46(2)	-5(1)	20(1)	-5(1)
C(1)	45(2)	30(1)	43(2)	-4(1)	13(1)	0(1)
C(10)	39(2)	39(2)	51(2)	4(1)	17(1)	-8(1)
C(16)	49(2)	33(2)	51(2)	-2(1)	20(1)	-4(1)
C(7)	46(2)	44(2)	37(2)	0(1)	17(1)	-6(1)
C(8)	48(2)	45(2)	58(2)	-5(2)	13(2)	-4(2)
C(11)	50(2)	53(2)	59(2)	1(2)	22(2)	-2(2)
C(22)	70(2)	49(2)	56(2)	-1(2)	31(2)	0(2)
C(2)	51(2)	52(2)	61(2)	-5(2)	18(2)	-11(2)
C(18)	55(2)	53(2)	56(2)	-3(2)	16(2)	5(2)
C(5)	58(2)	57(2)	44(2)	4(2)	15(2)	-3(2)
C(4)	66(2)	68(2)	43(2)	-3(2)	5(2)	3(2)

C(3)	52(2)	66(2)	63(2)	-11(2)	2(2)	-11(2)
C(12)	63(2)	53(2)	90(3)	-1(2)	35(2)	4(2)
C(9)	71(3)	47(2)	83(3)	-12(2)	17(2)	-14(2)
C(21)	85(3)	70(2)	62(2)	-11(2)	37(2)	-2(2)
C(15)	68(2)	59(2)	59(2)	0(2)	6(2)	3(2)
C(20)	77(2)	90(3)	43(2)	-4(2)	15(2)	-10(2)
C(19)	70(2)	84(3)	53(2)	4(2)	7(2)	11(2)
C(13)	60(2)	63(2)	100(3)	18(2)	21(2)	12(2)
C(14)	76(3)	77(3)	76(3)	14(2)	-2(2)	8(2)

Table 18. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 5d.

	x	y	z	U(eq)
H(1)	2787	3349	7276	48
H(6)	3560	7444	6109	61
H(7)	4480	3450	5233	63
H(16)	1561	6316	8750	66
H(2)	809	3238	5879	65
H(12)	3869	3506	8668	65
H(5)	2944	5756	4441	63

H(4)	1309	4848	3621	73
H(3)	250	3547	4330	75
H(8)	5708	1635	5658	79
H(15)	1850	5896	10281	83
H(11)	5311	4856	7785	77
H(14)	3128	4298	10997	84
H(13)	4164	3129	10200	85
H(9)	6742	1439	7126	89
H(10)	6521	3027	8191	97

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