Electronic Supplementary Material (ESI) for RSC Advances.

Double Functionalization of 2-Amino-2′-hydroxy-1,1′-biaryls: Synthesis of 4-Nitro-dibenzofurans and Benzofuro-indoles

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Content

Figure S1 ^{1}H NMR spectrum of **substrate for 1i**

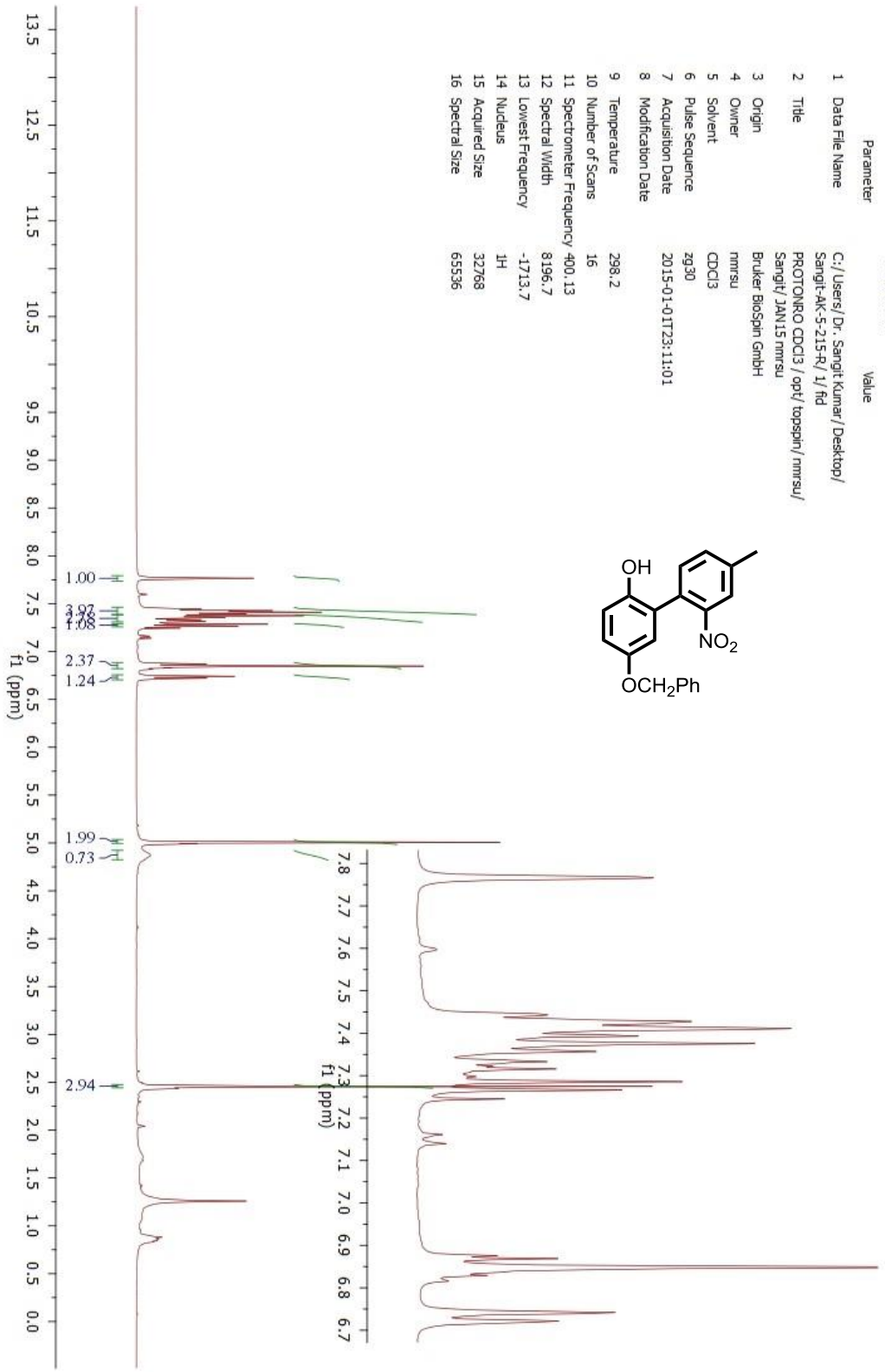

Figure S2 ^{13}C NMR spectrum of **substrate for 1i**

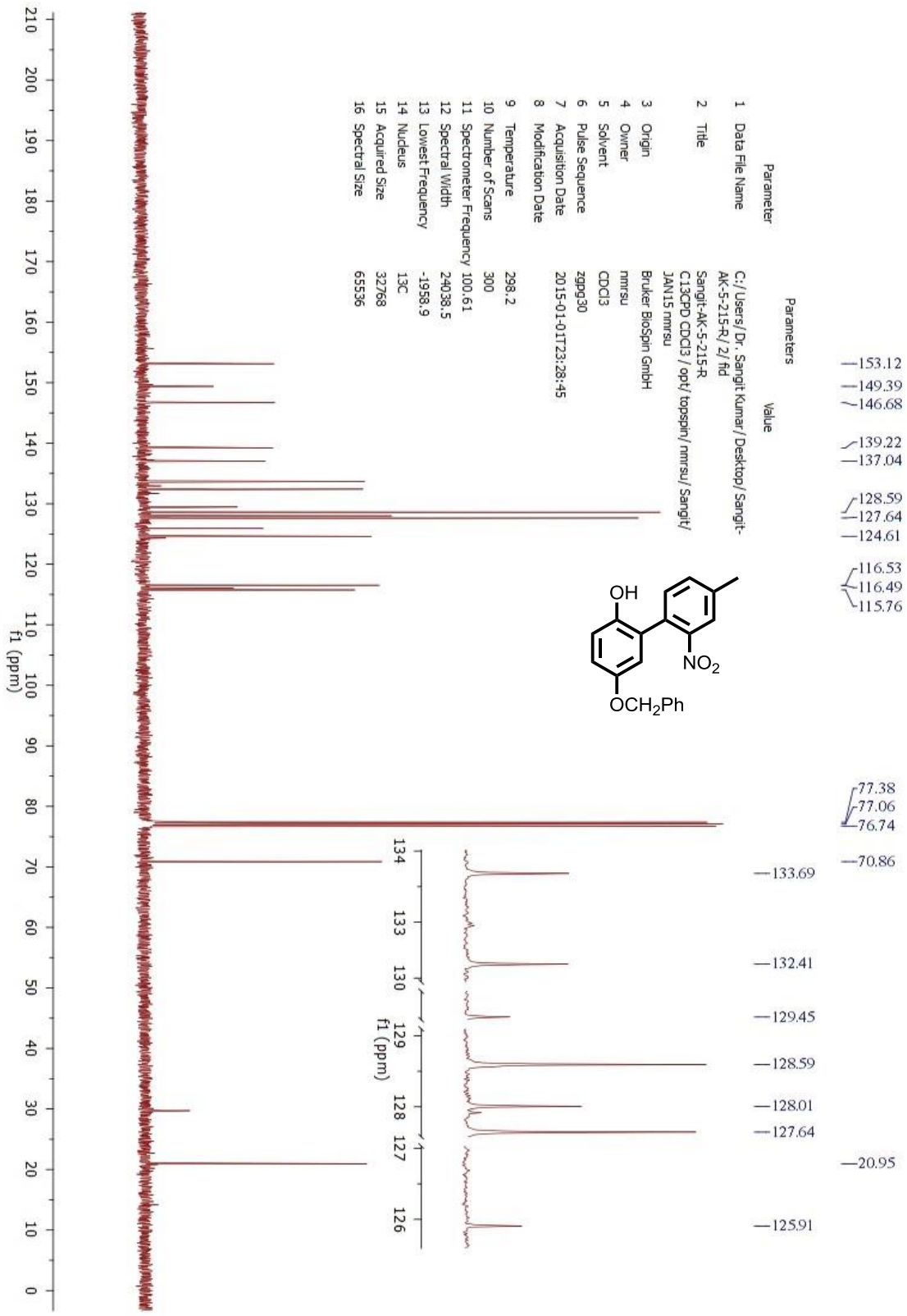

Figure S3 ^{1}H NMR spectrum of 4'-methyl-2'-nitro-5-(trifluoromethoxy)-[1,1'-biphenyl]-2-ol (**substrate for 1j**)

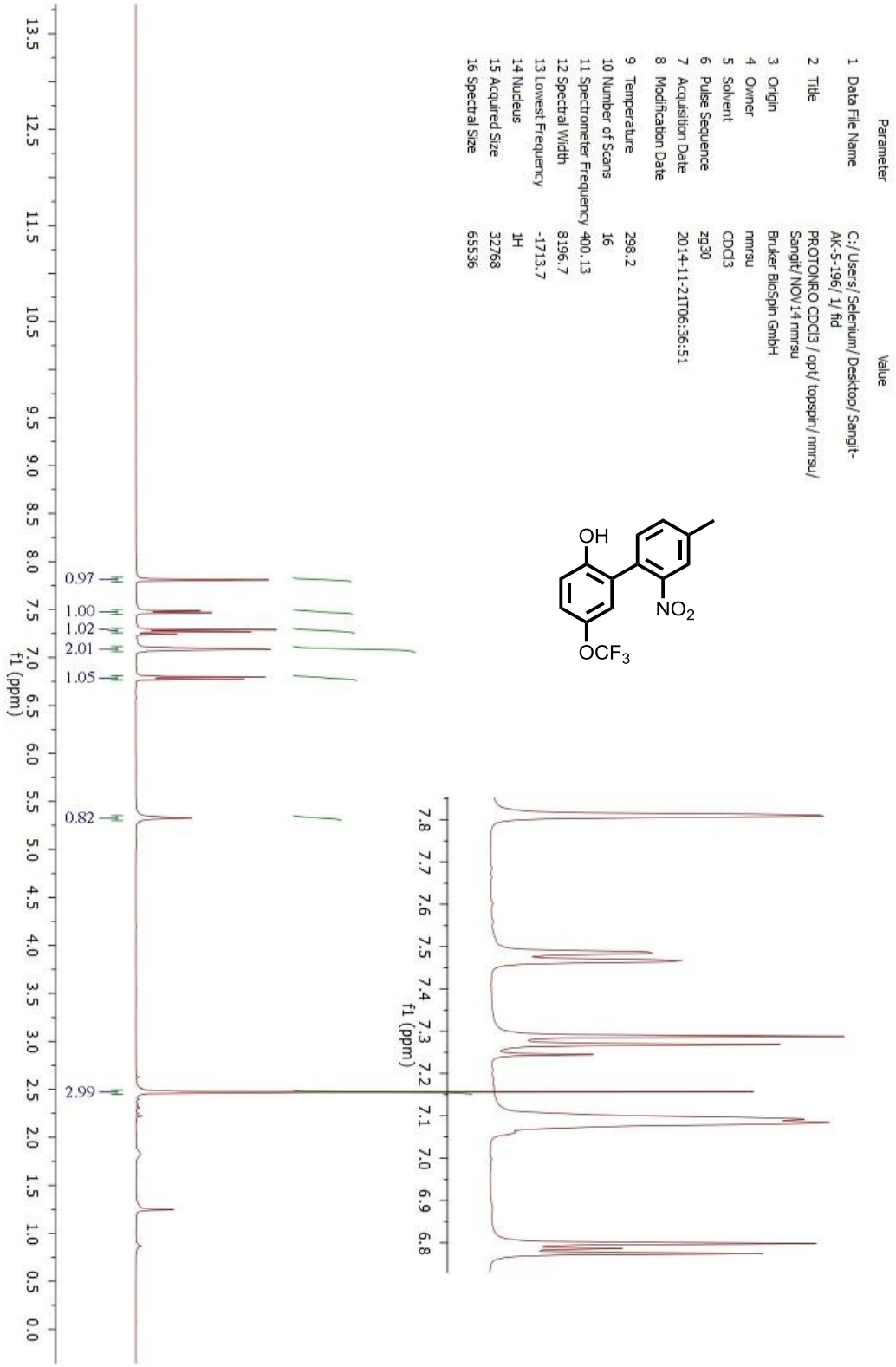

Figure S4 ^{13}C NMR spectrum of **substrate for 1j**

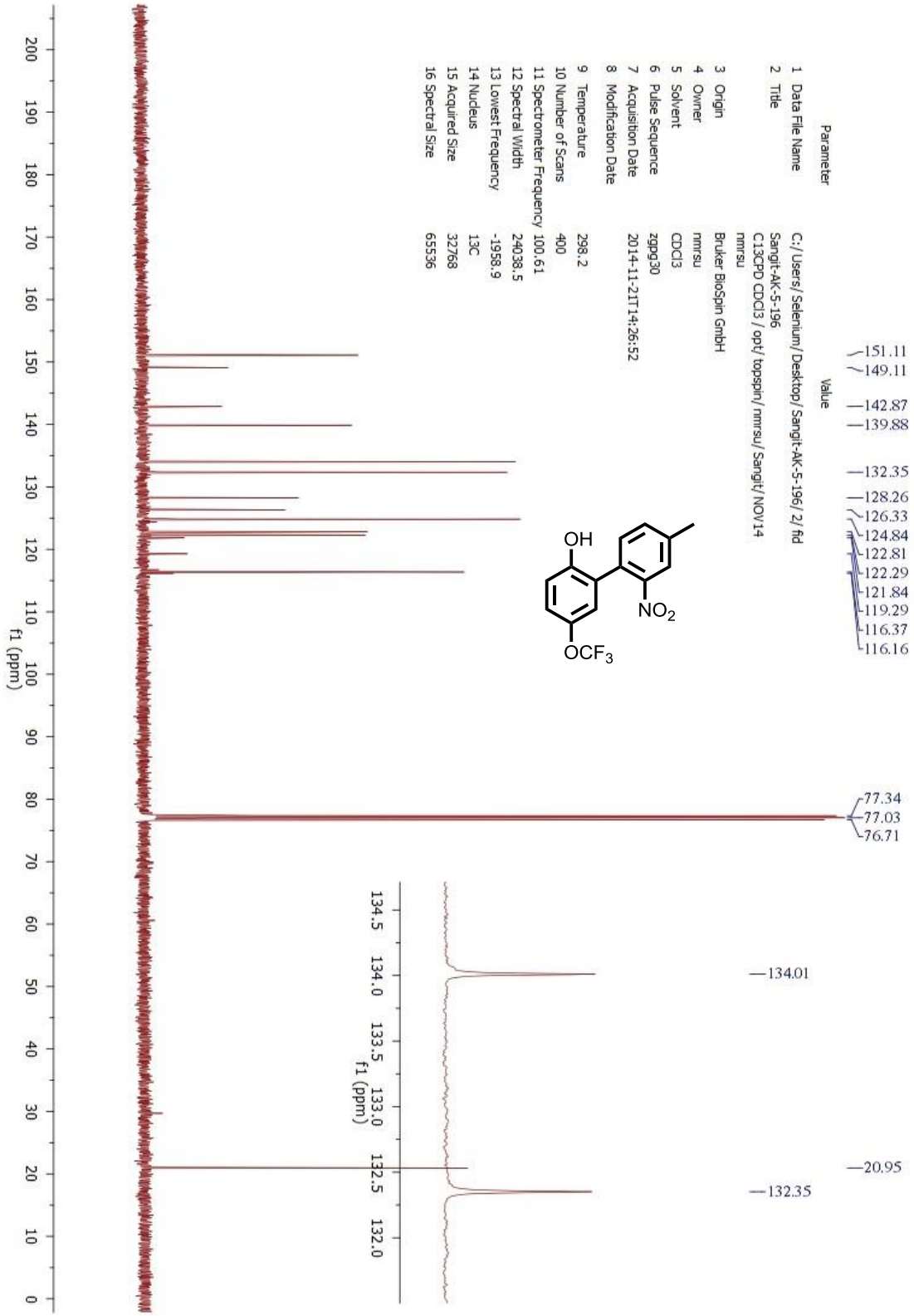

Figure S5 ^{1}H NMR spectrum of **substrate for 1l**

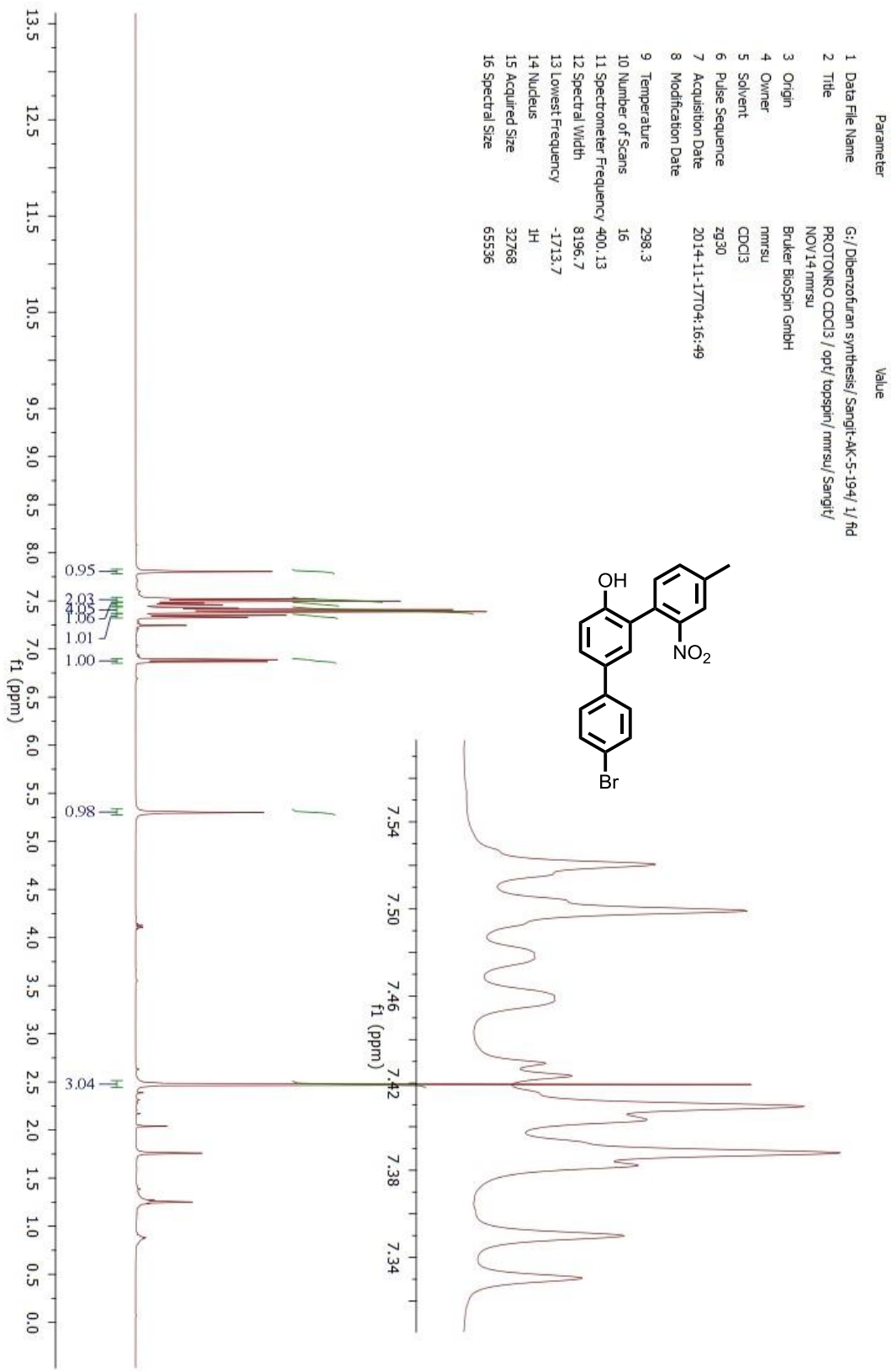

Figure S6 ^{13}C NMR spectrum of **substrate for 1l**

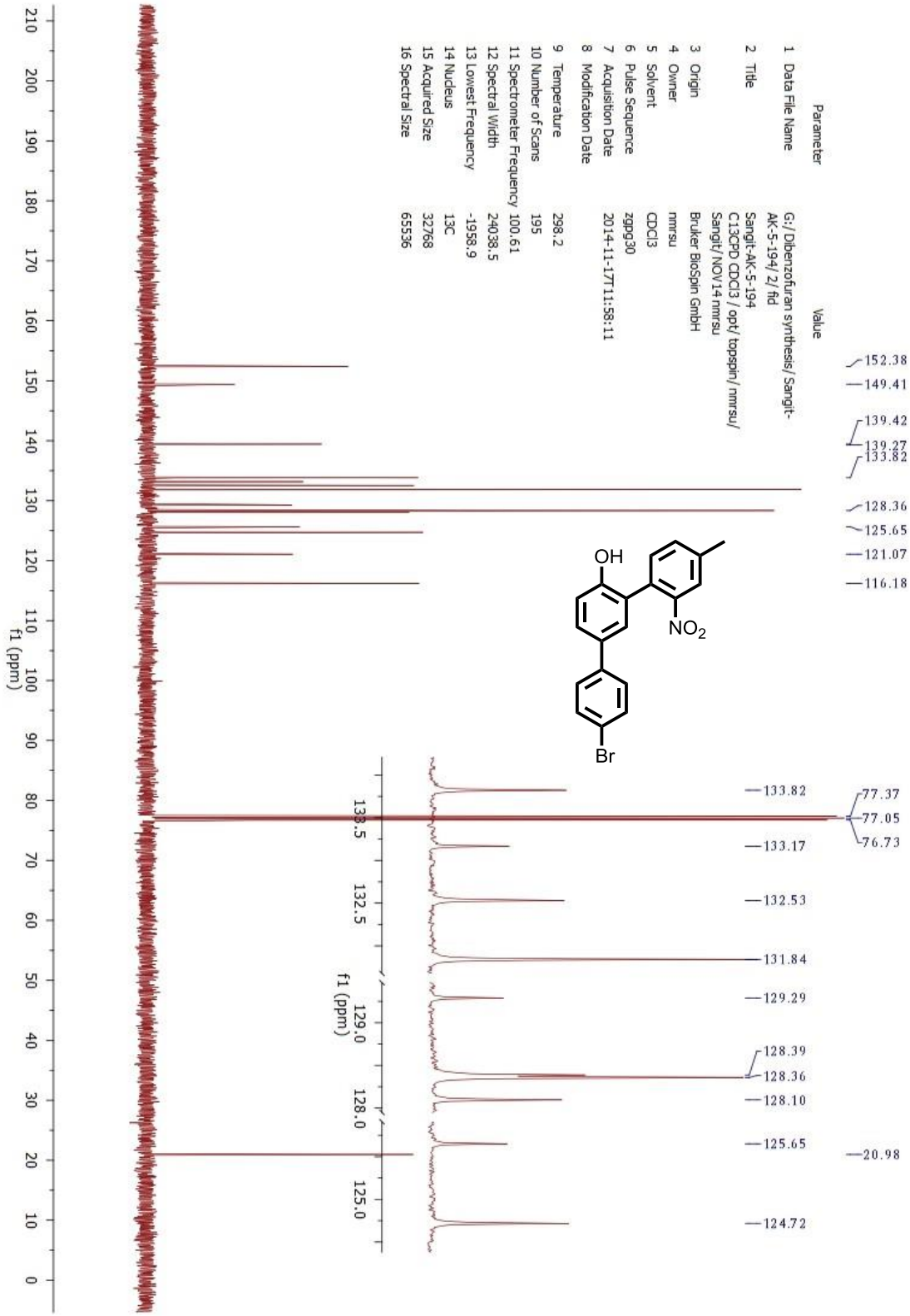

Figure S7 ^{1}H NMR spectrum of **substrate for 1o**

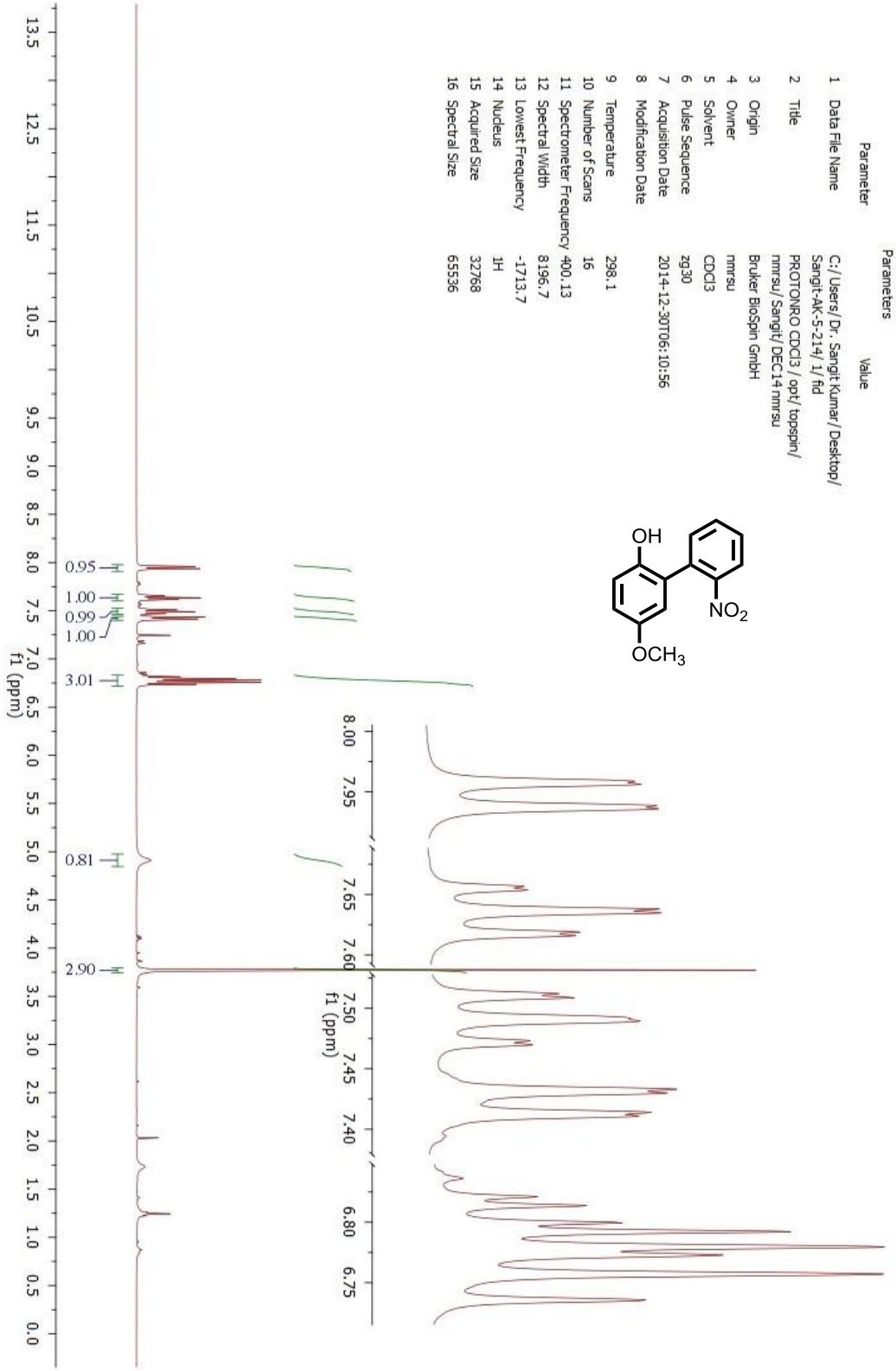

Figure S8 ^{13}C NMR spectrum of **substrate for 1o**

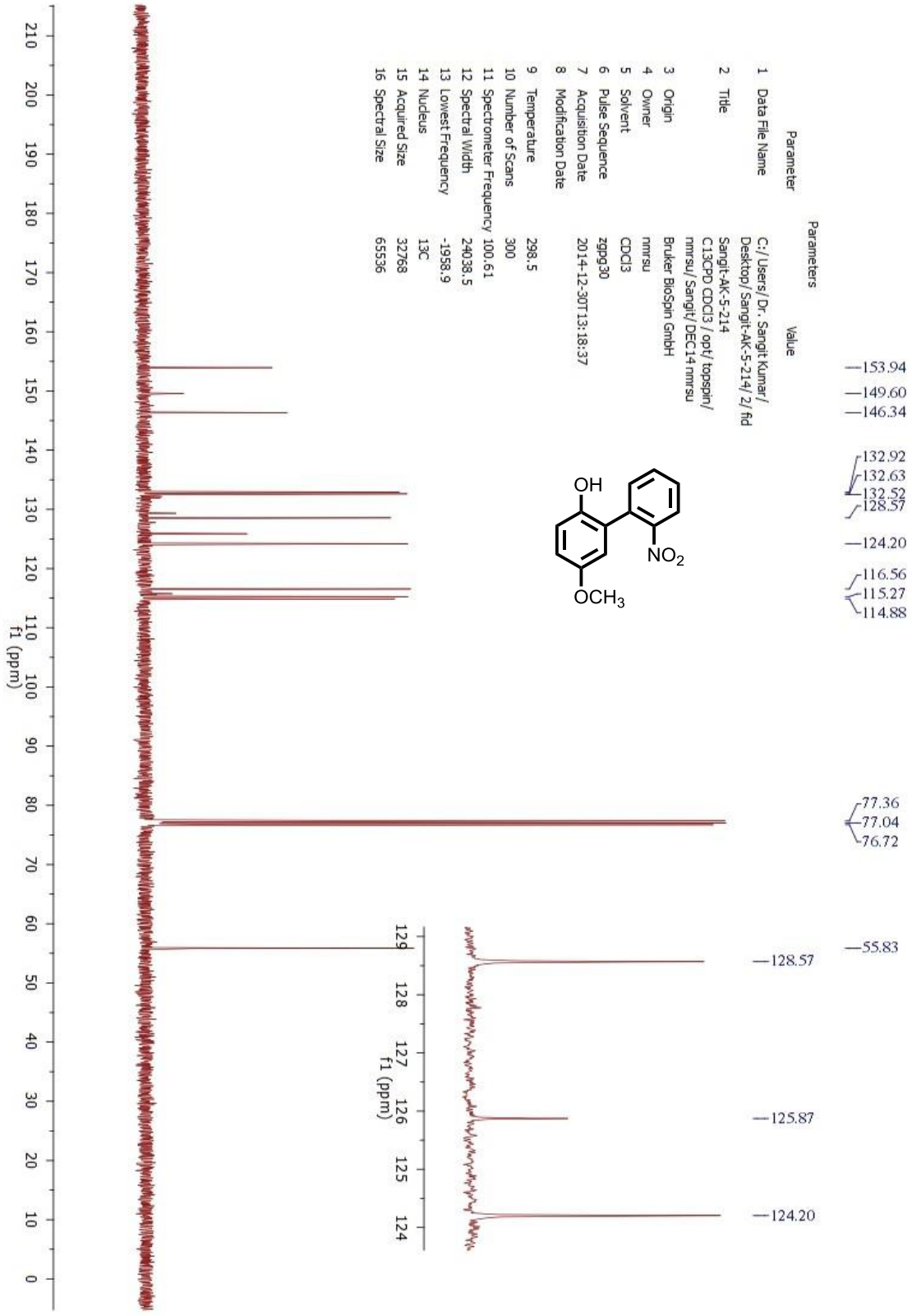

Figure S9 ^{1}H NMR spectrum of **substrate for 1q**

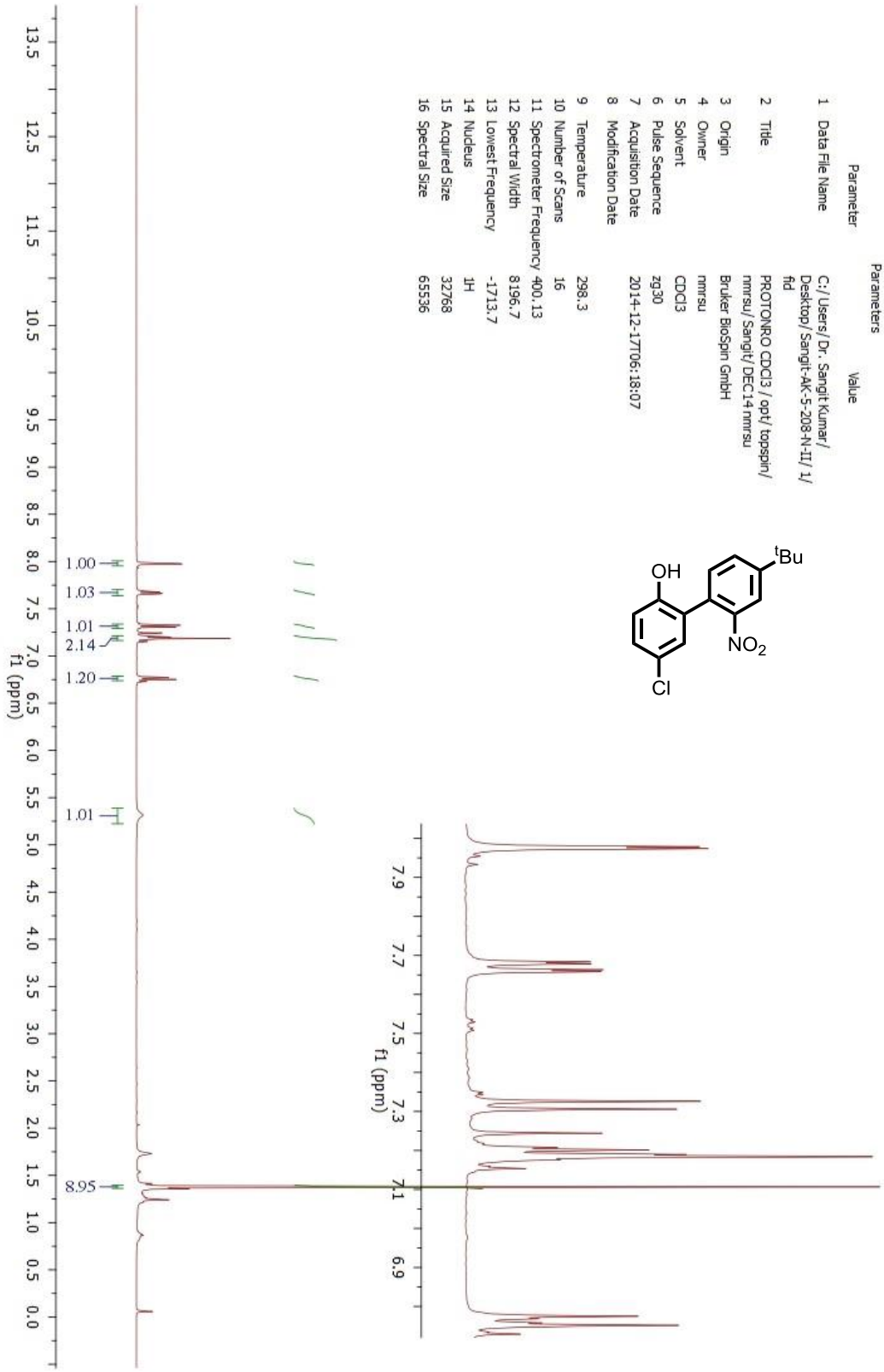

Figure S10 ^{13}C NMR spectrum of **substrate for 1q**

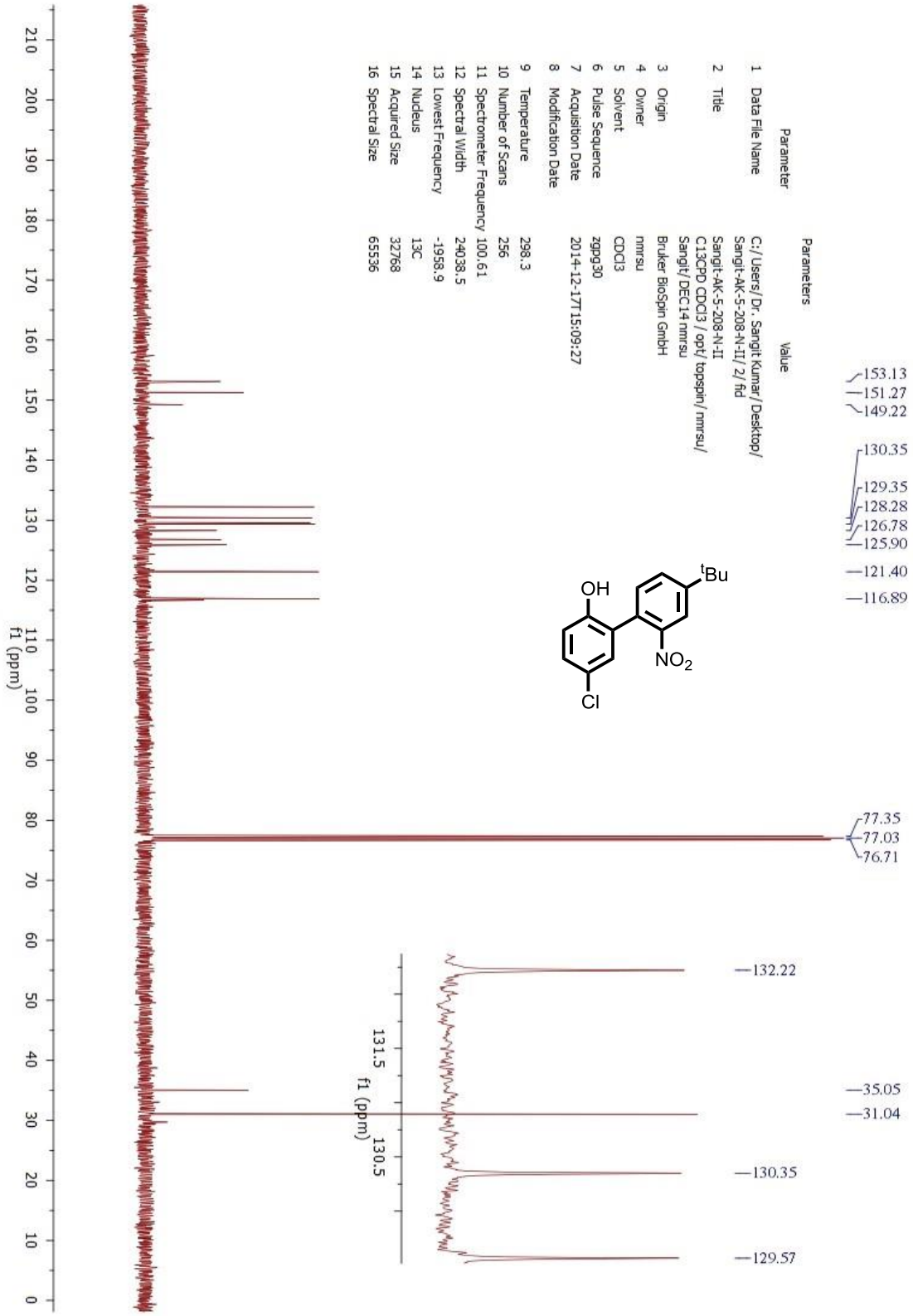

Figure S11 ^{1}H NMR spectrum of **substrate for 1r**

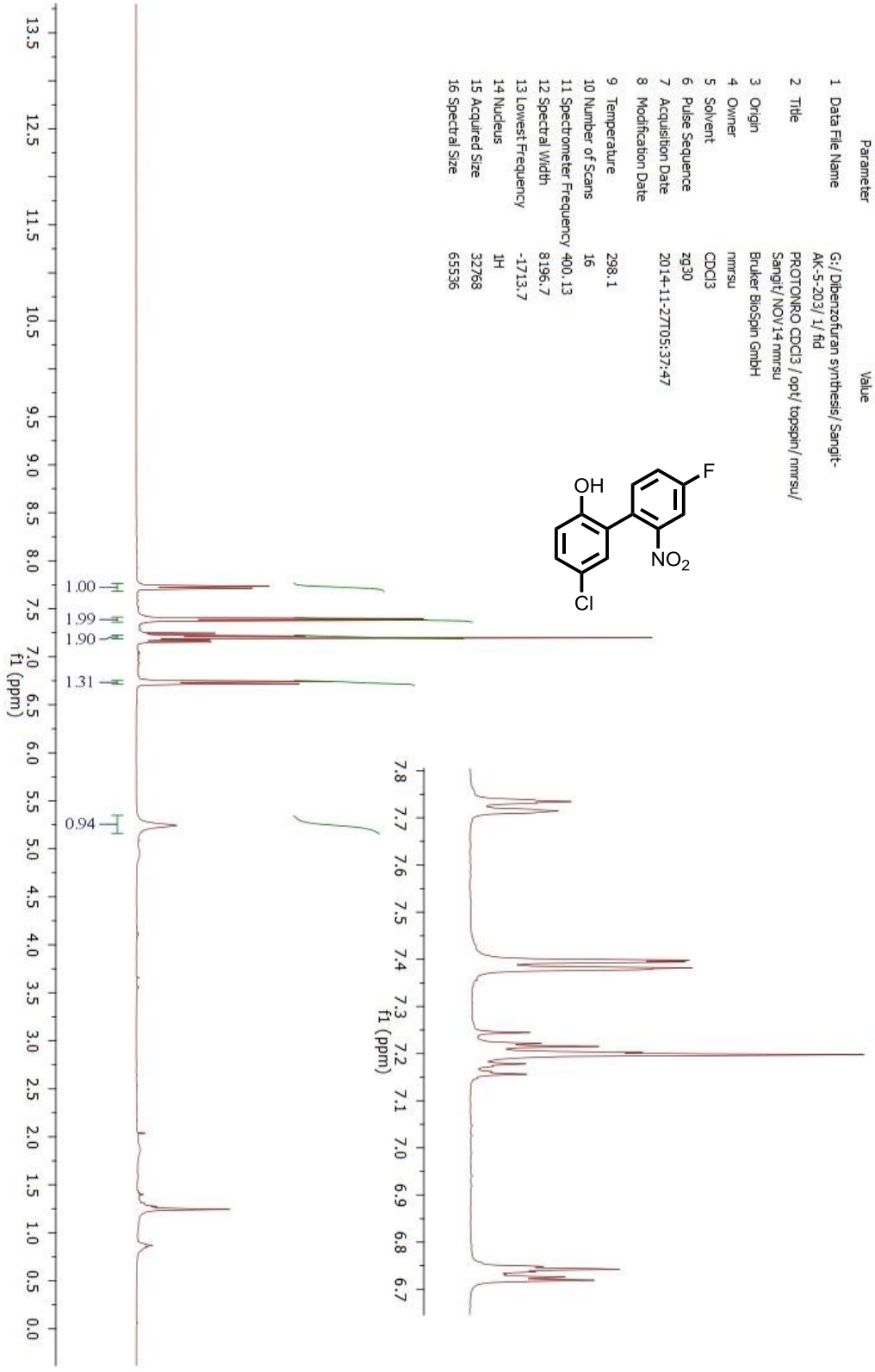

Figure S12 ^{13}C NMR spectrum of **substrate for 1r**

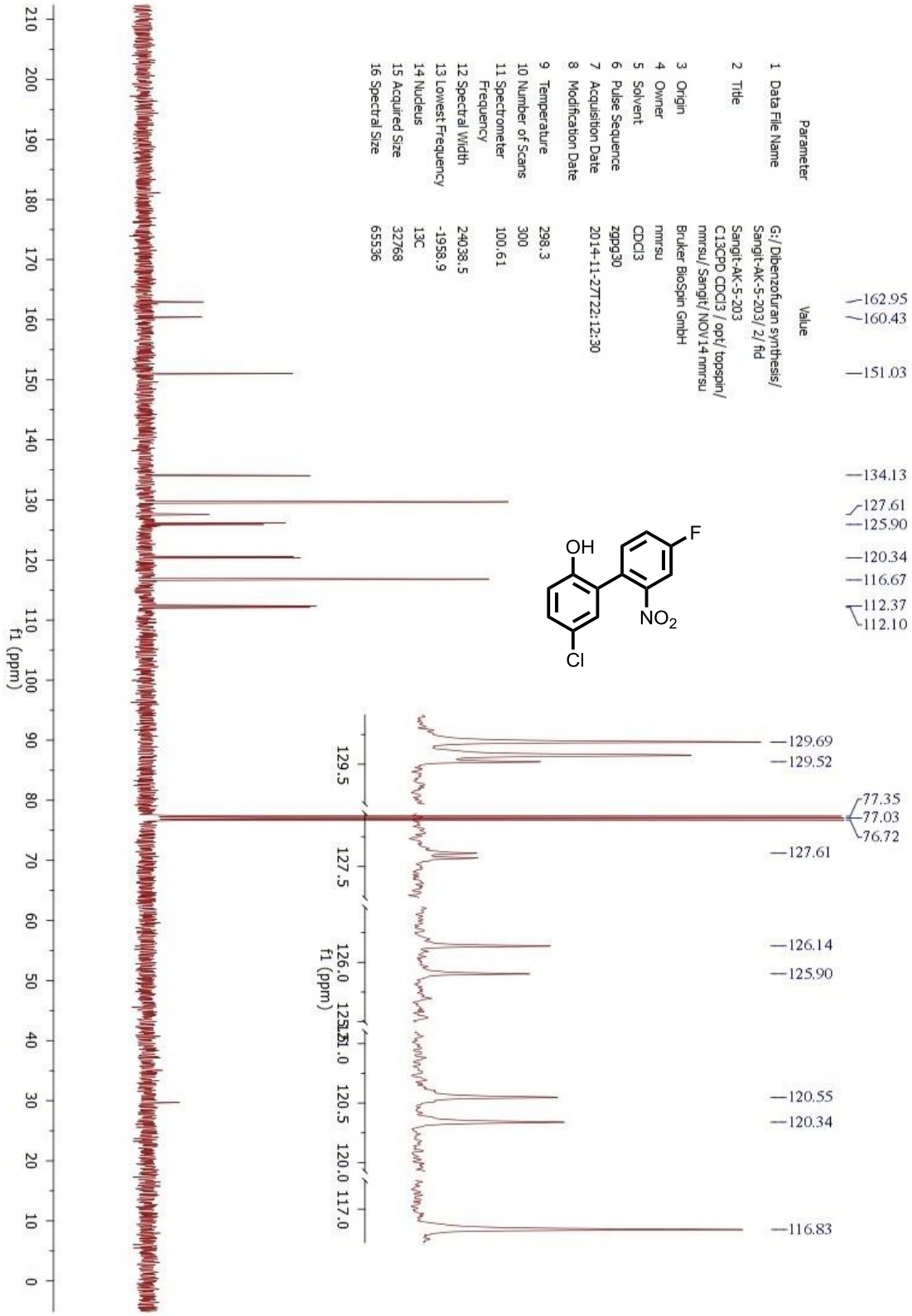

Figure S13 ^{1}H NMR spectrum of **1a**

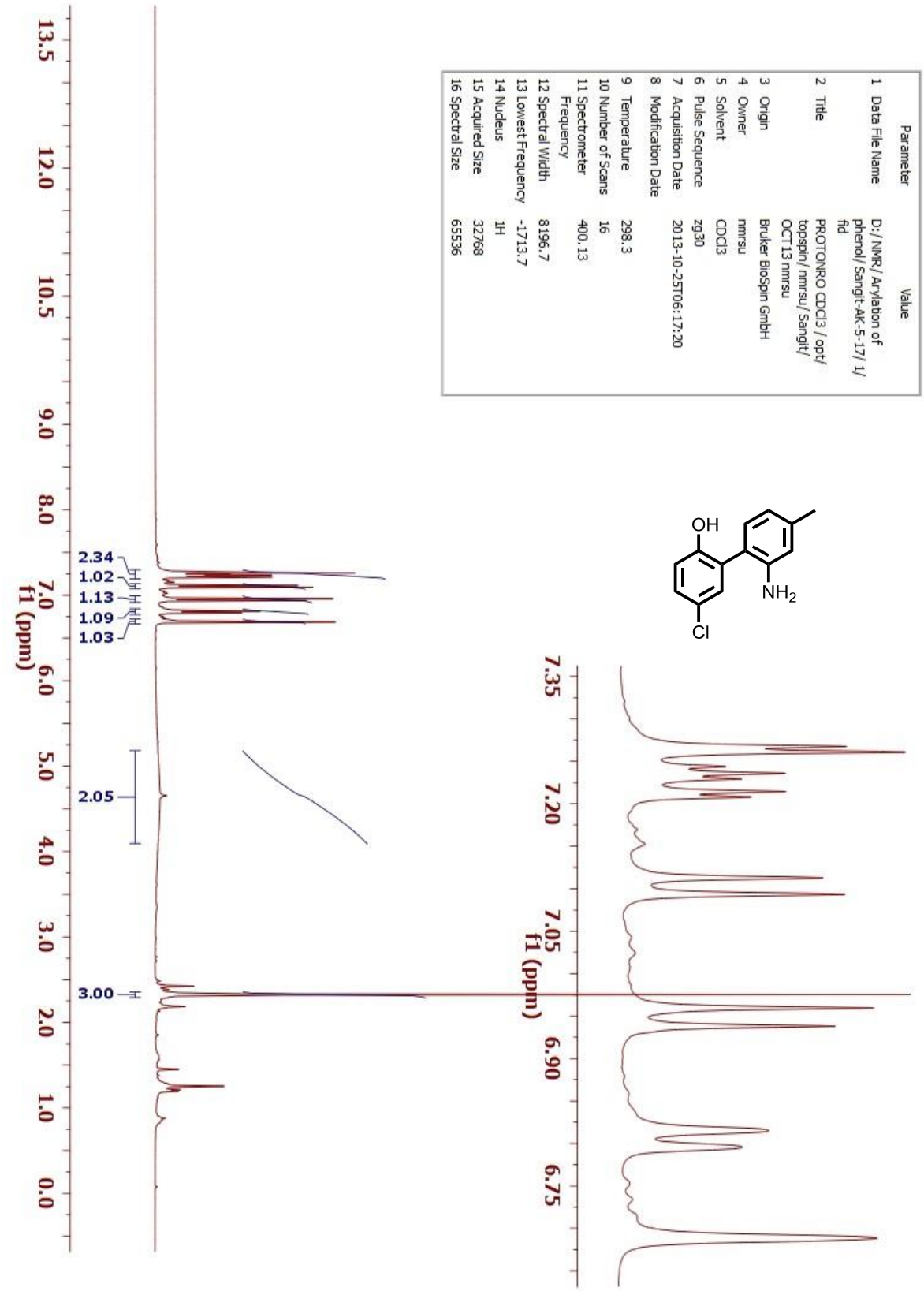

Figure S14 ^{13}C NMR spectrum of **1a**

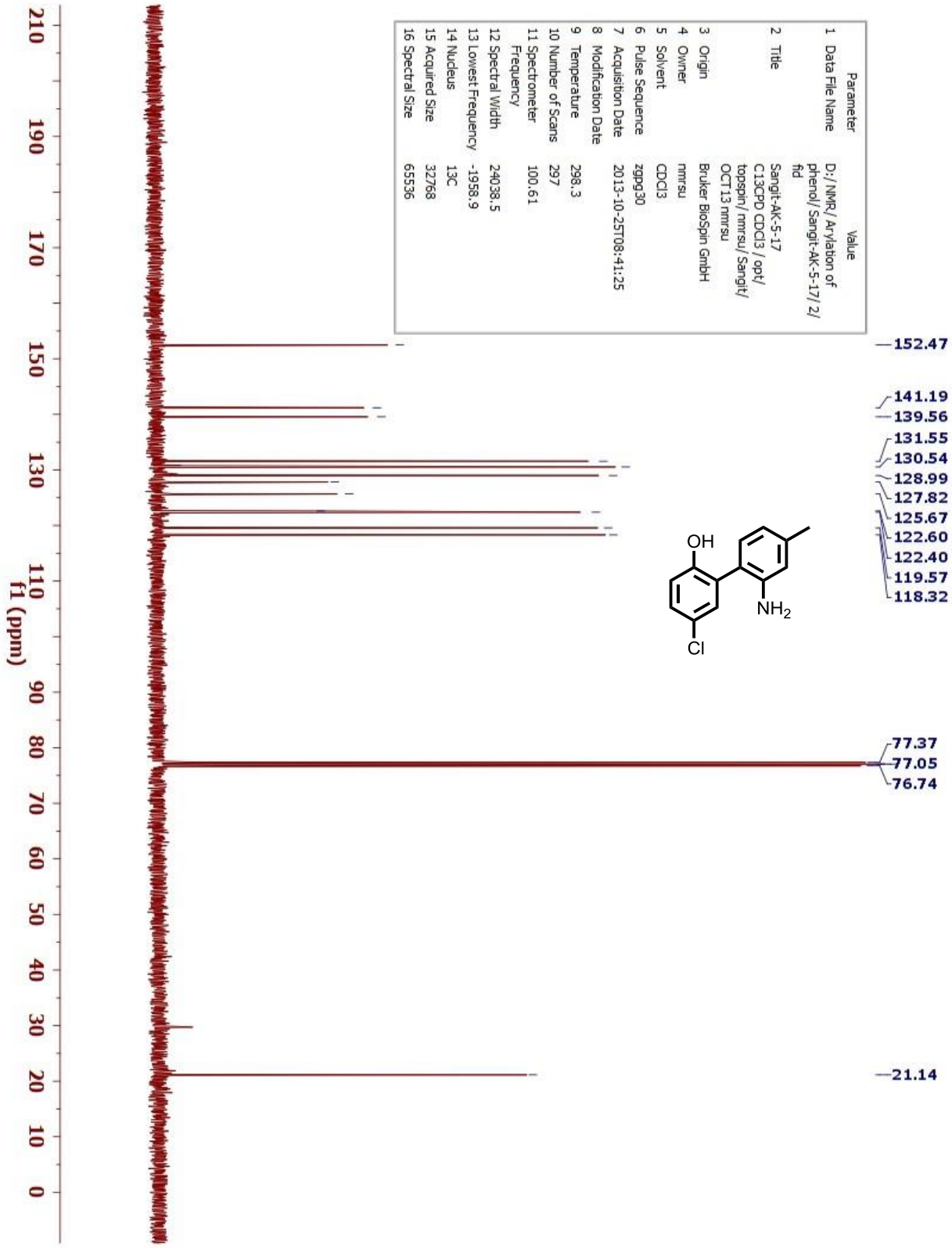

Figure S15 ^{1}H NMR spectrum of **1b**

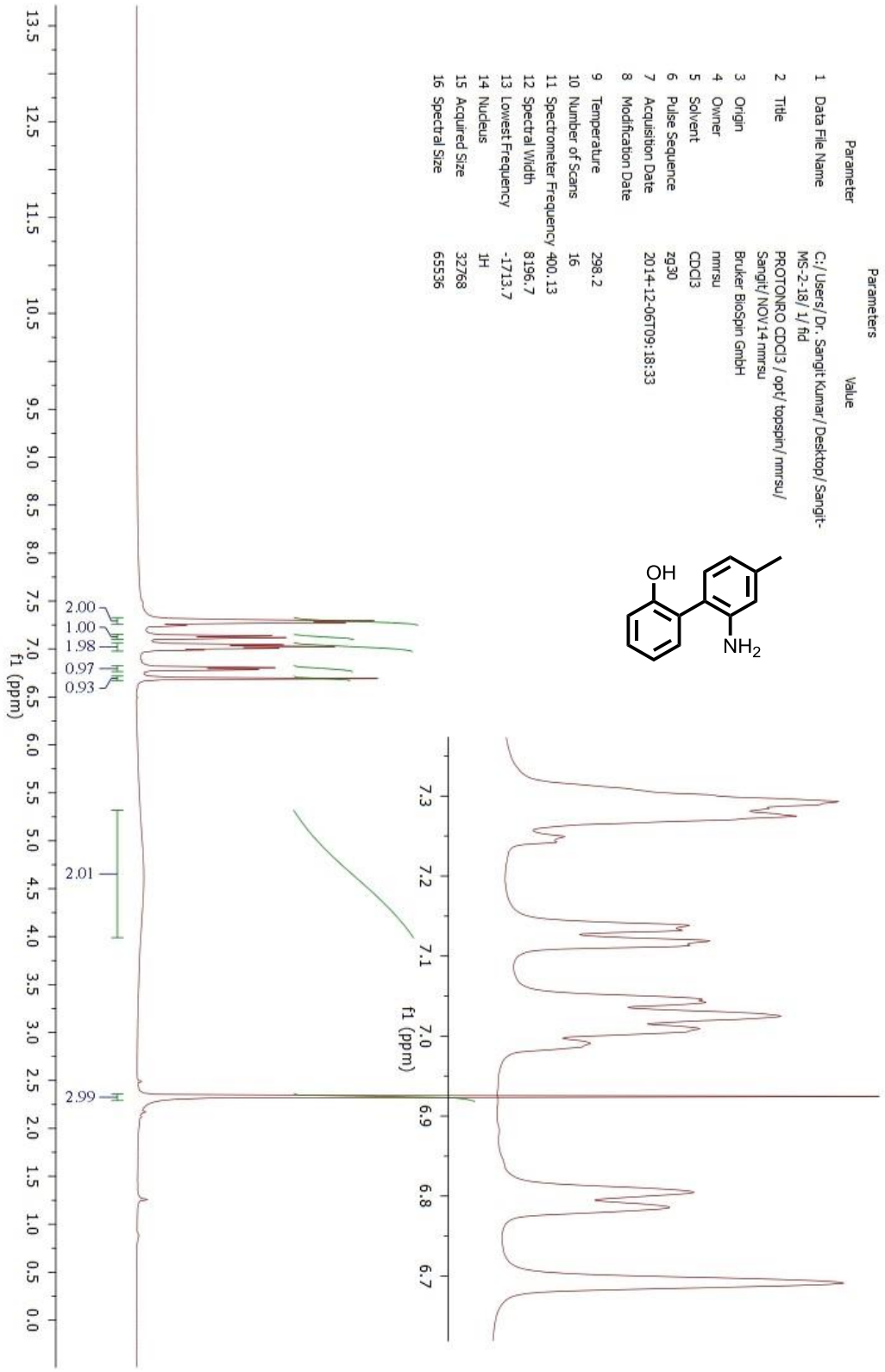

Figure S16 ^{13}C NMR spectrum of **1b**

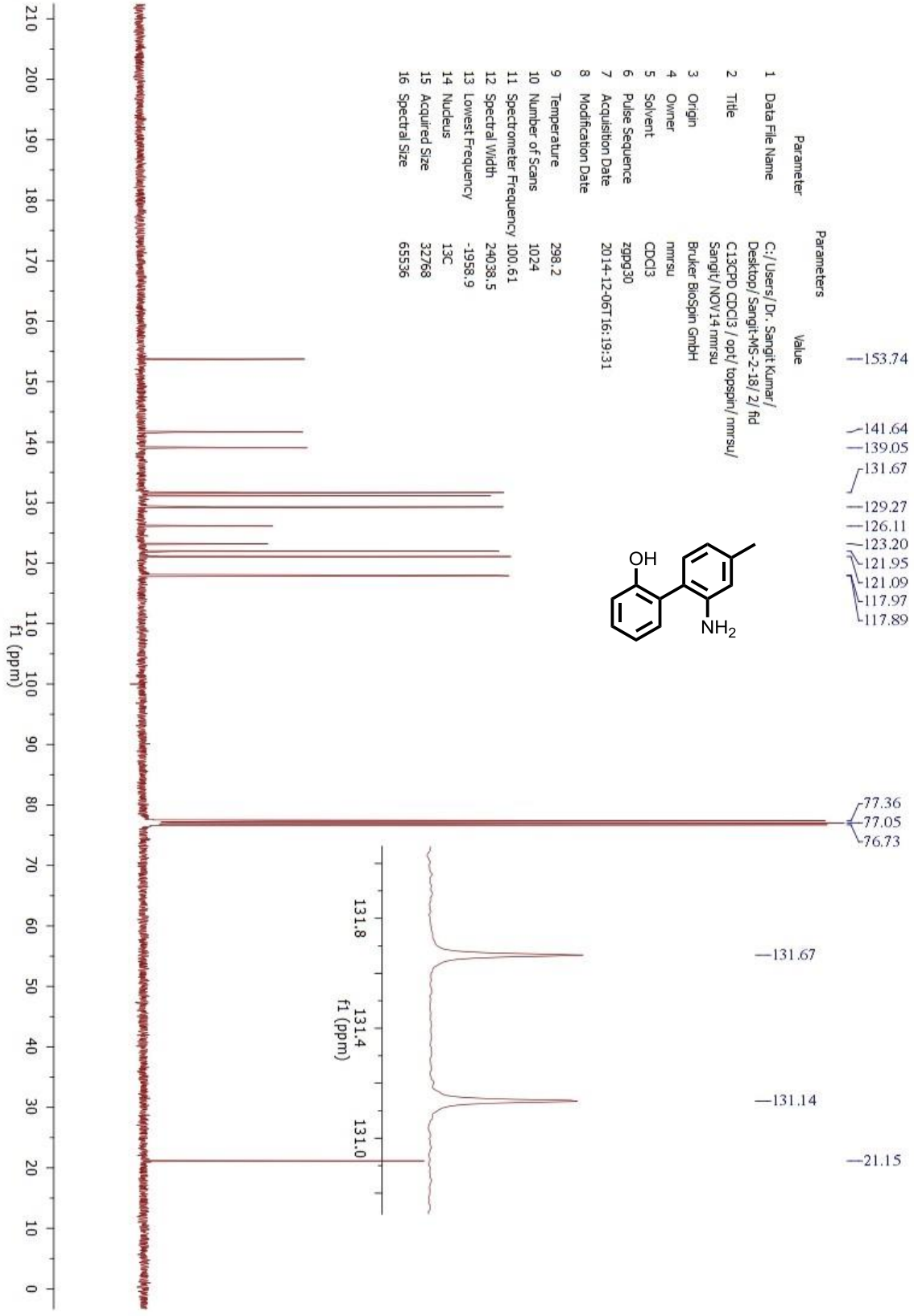

Figure S17 ^{1}H NMR spectrum of **1c**

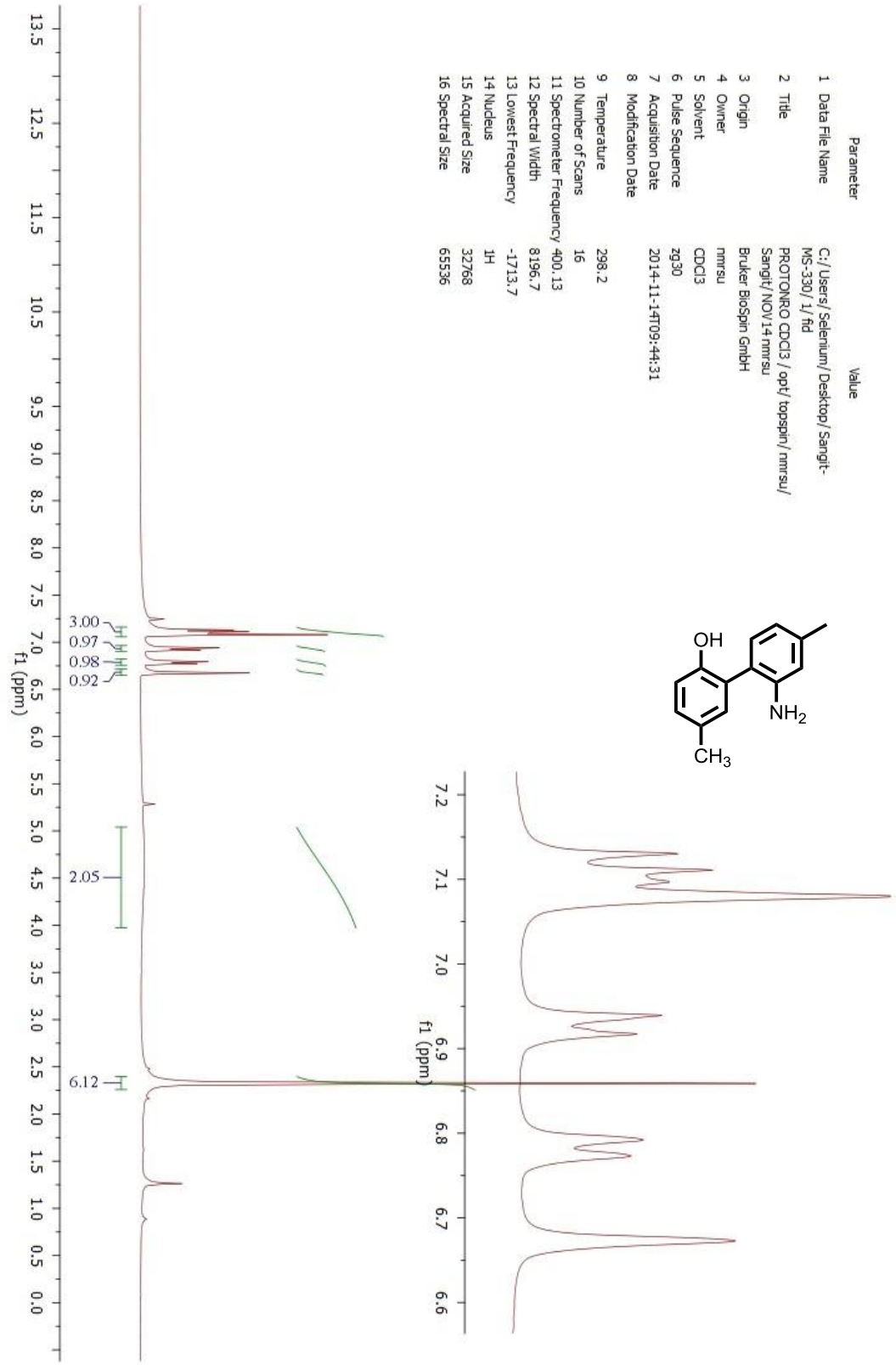

Figure S18 ^{13}C NMR spectrum of **1c**

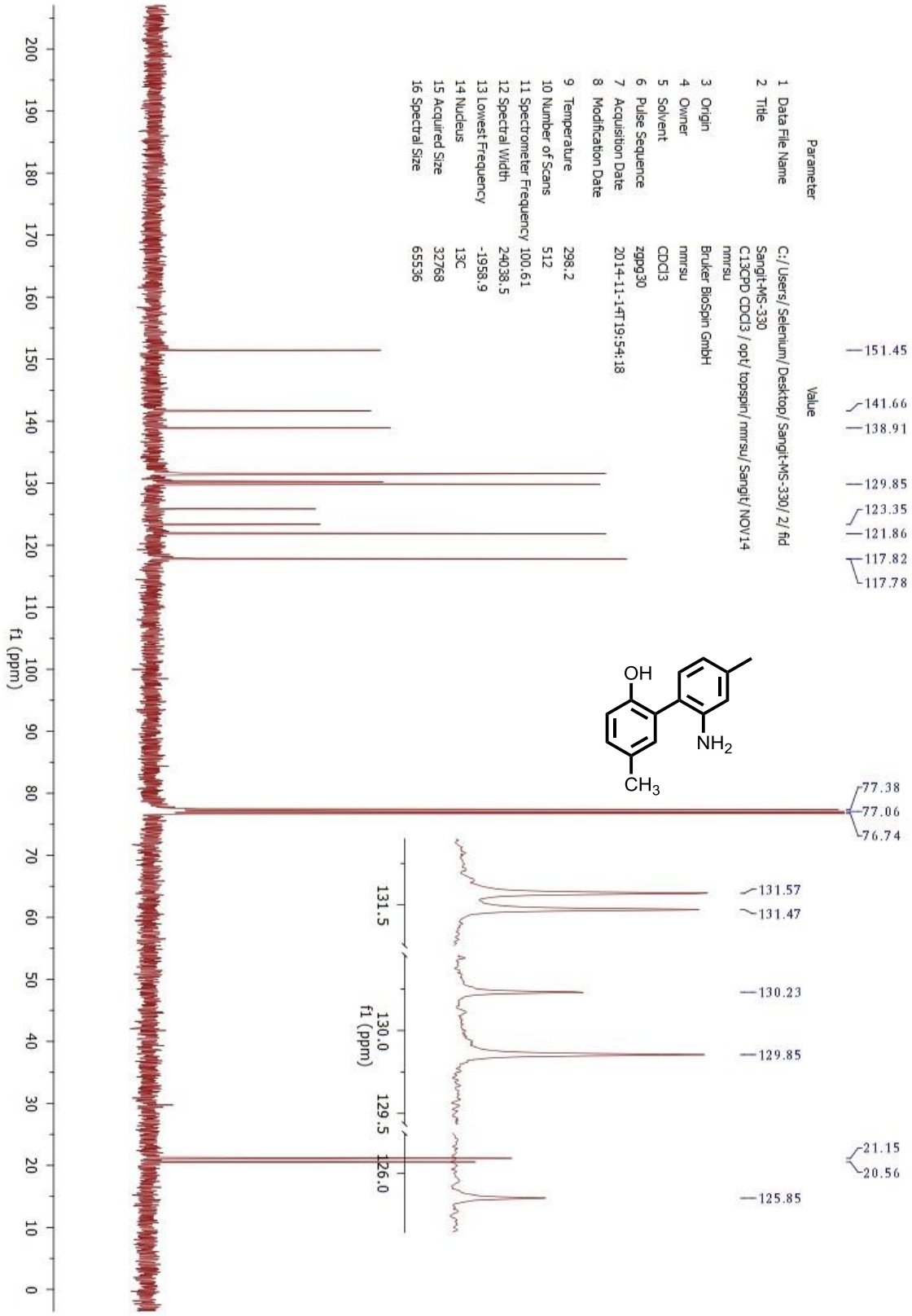

Figure S19 ^{1}H NMR spectrum of **1d**

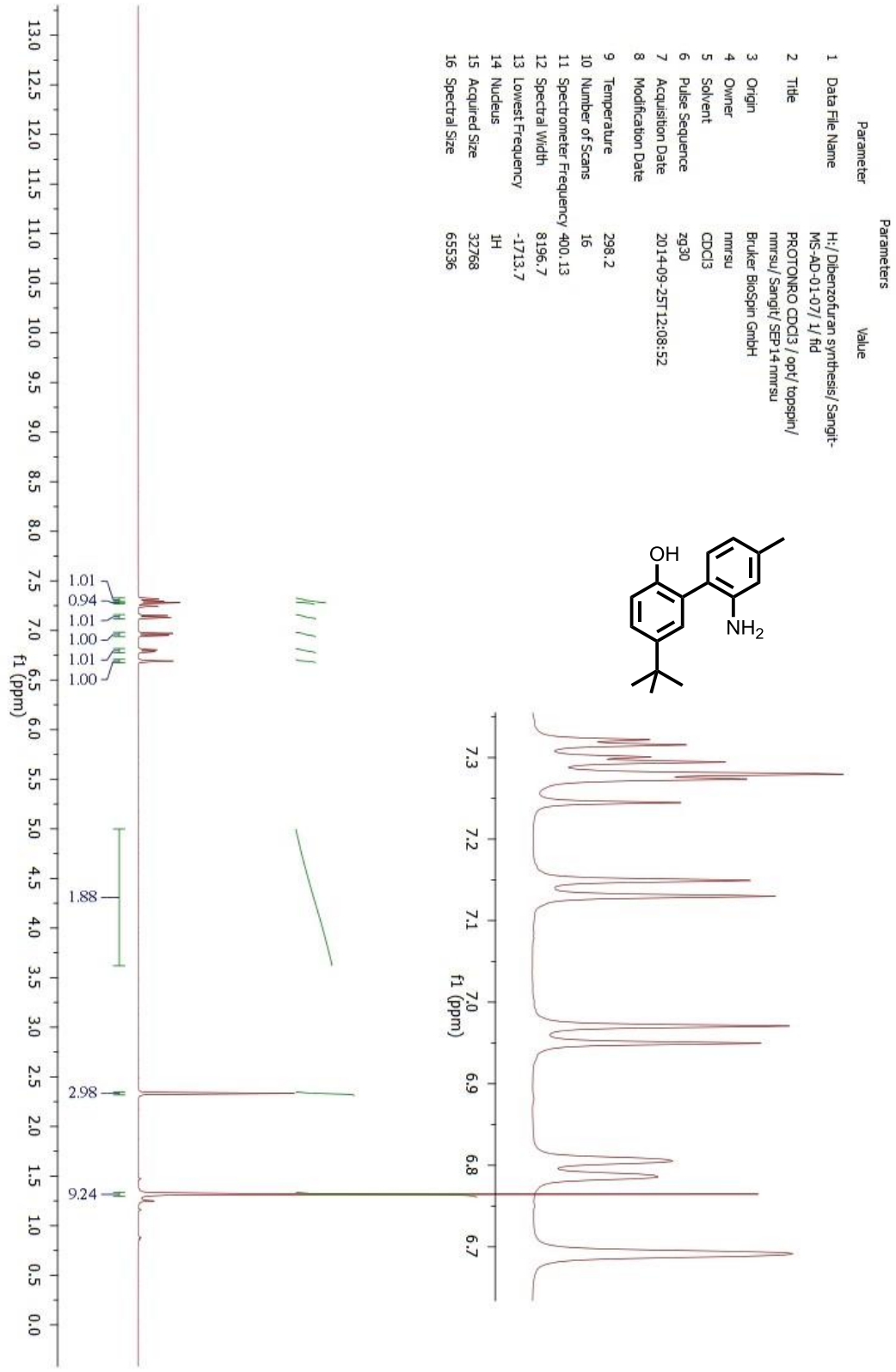

Figure S20 ^{13}C NMR spectrum of **1d**

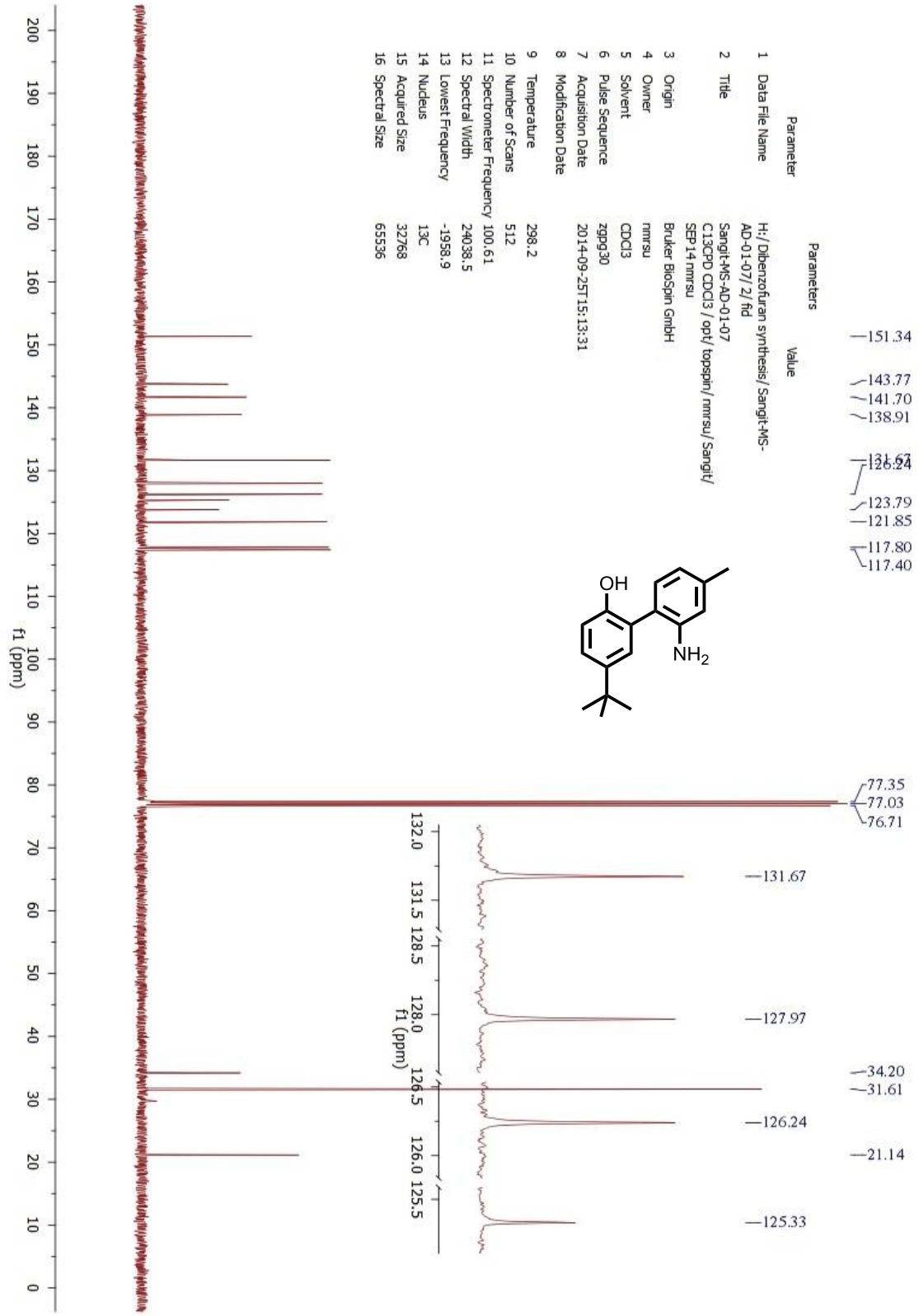

Figure S21 ^{1}H NMR spectrum of **1e**

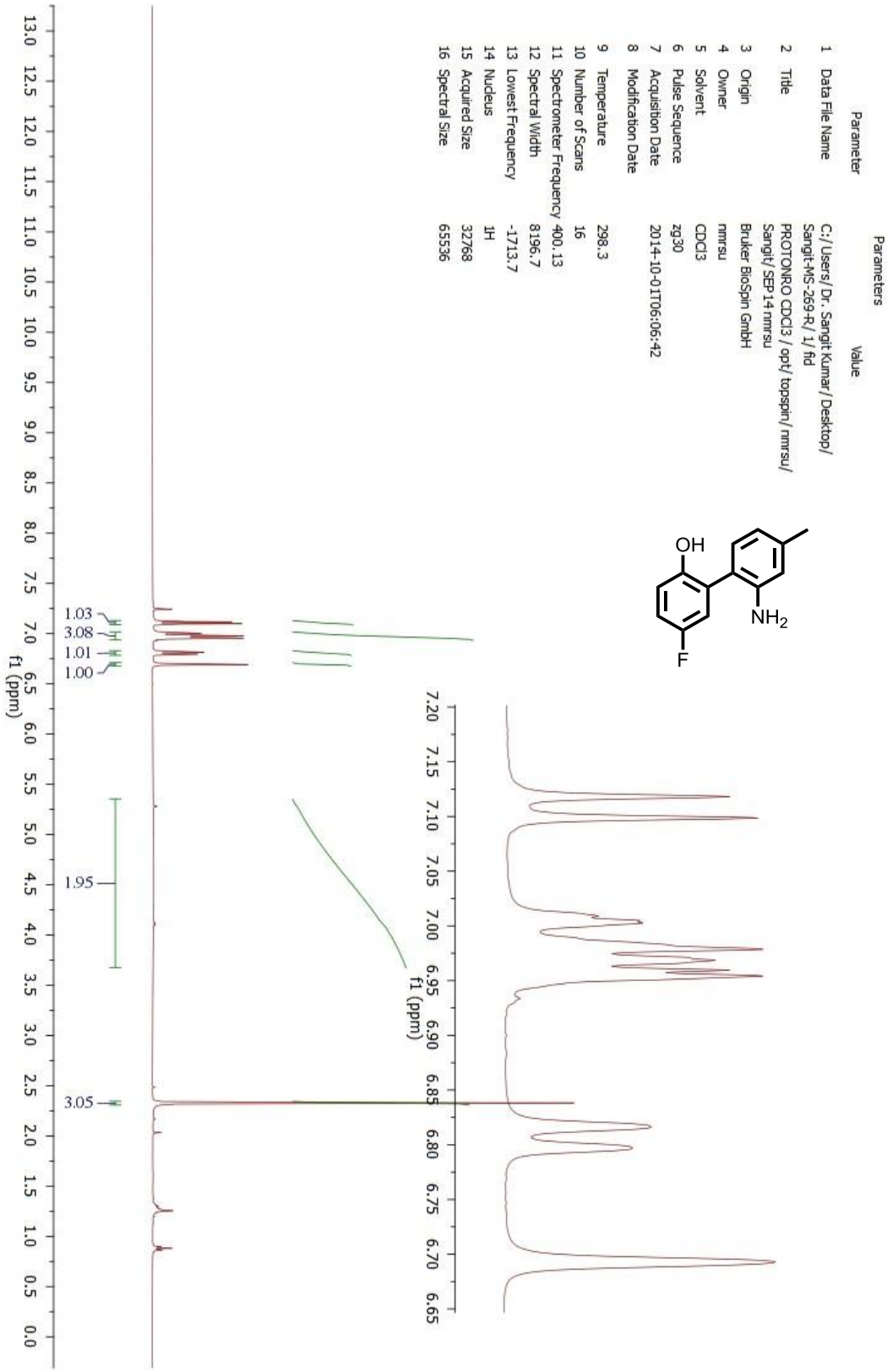

Figure S22 ^{13}C NMR spectrum of **1e**

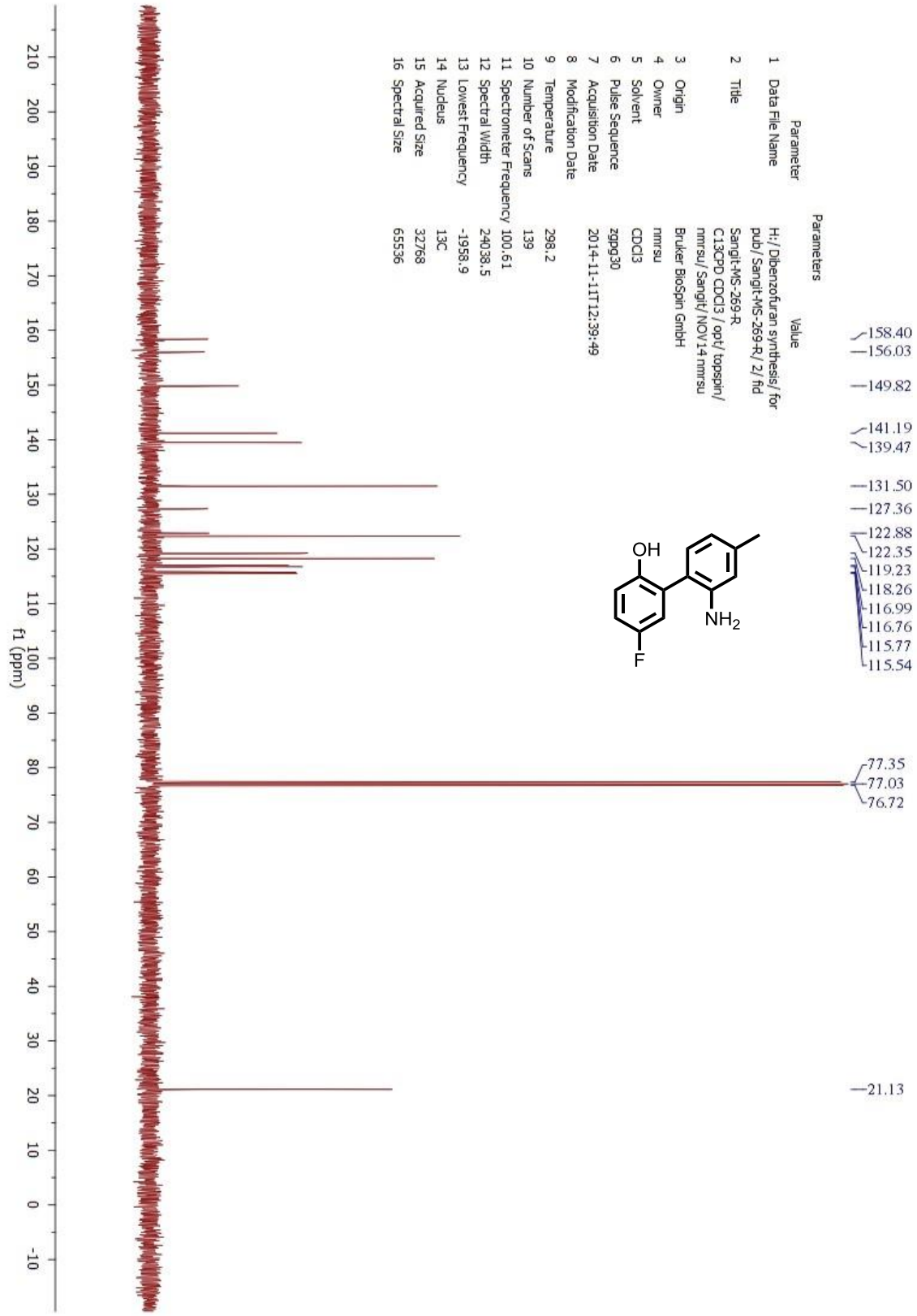

Figure S23 ^{1}H NMR spectrum of **1f**

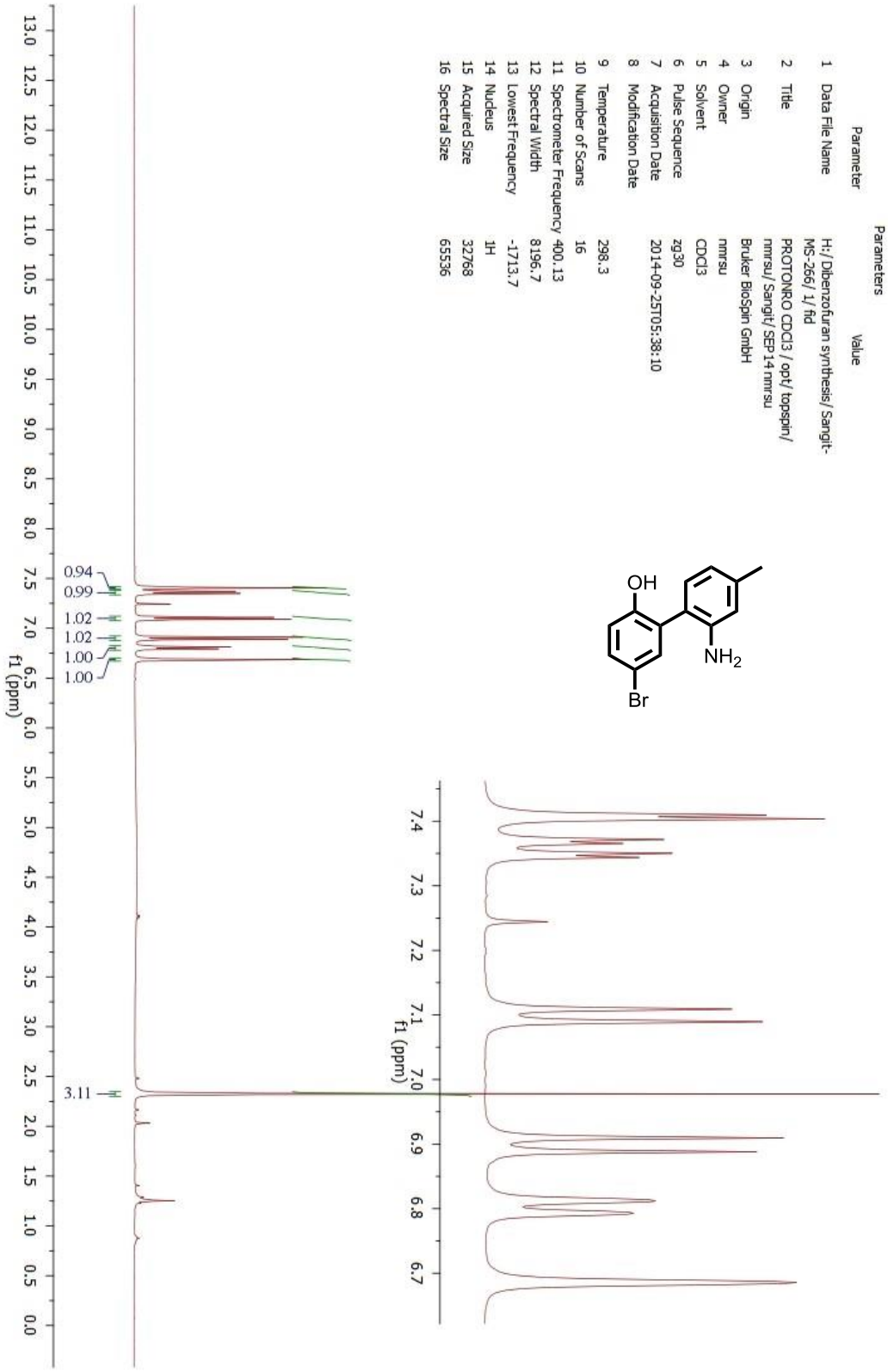

Figure S24 ^{13}C NMR spectrum of **1f**

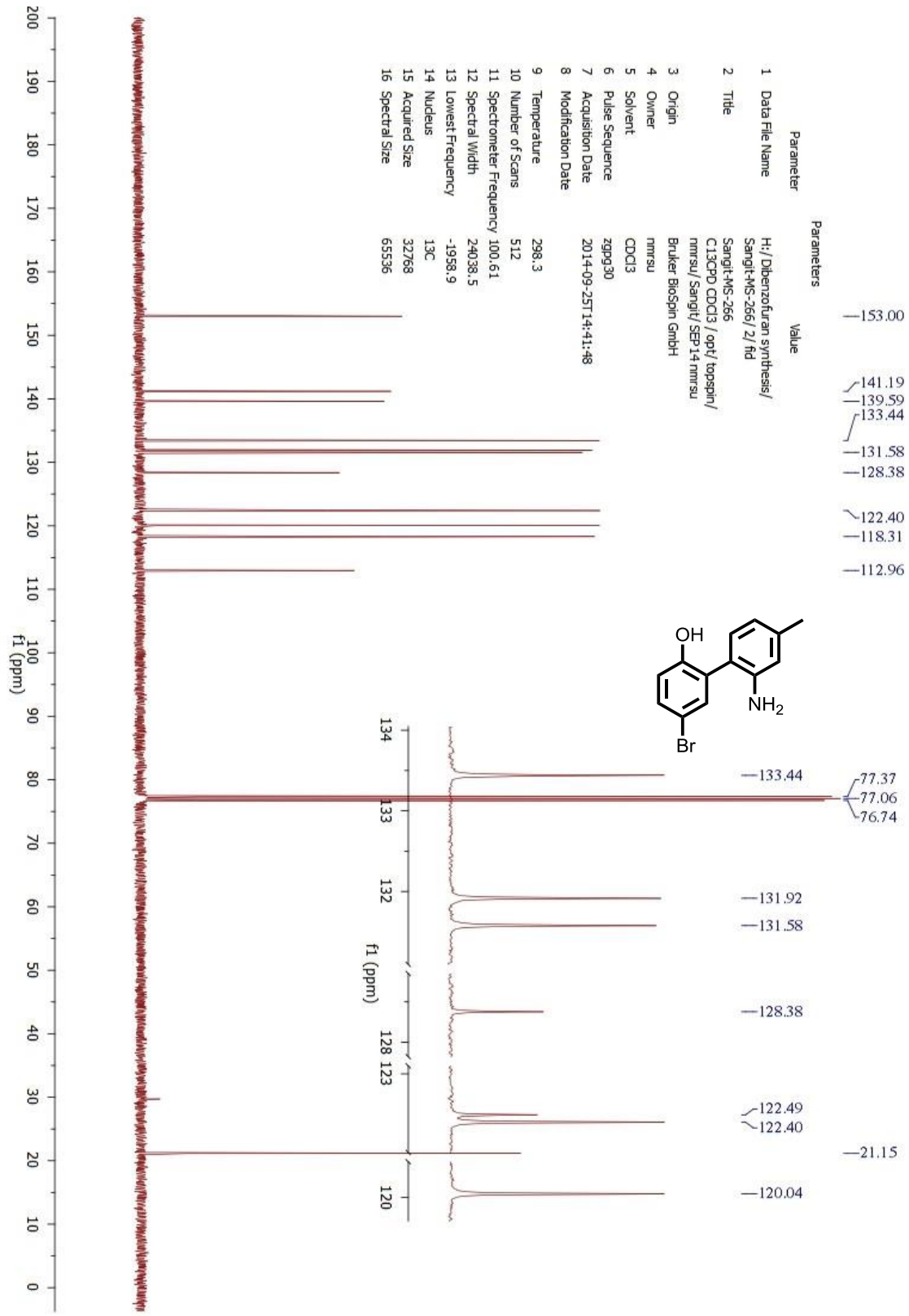

Figure S25 ^{1}H NMR spectrum of **1g**

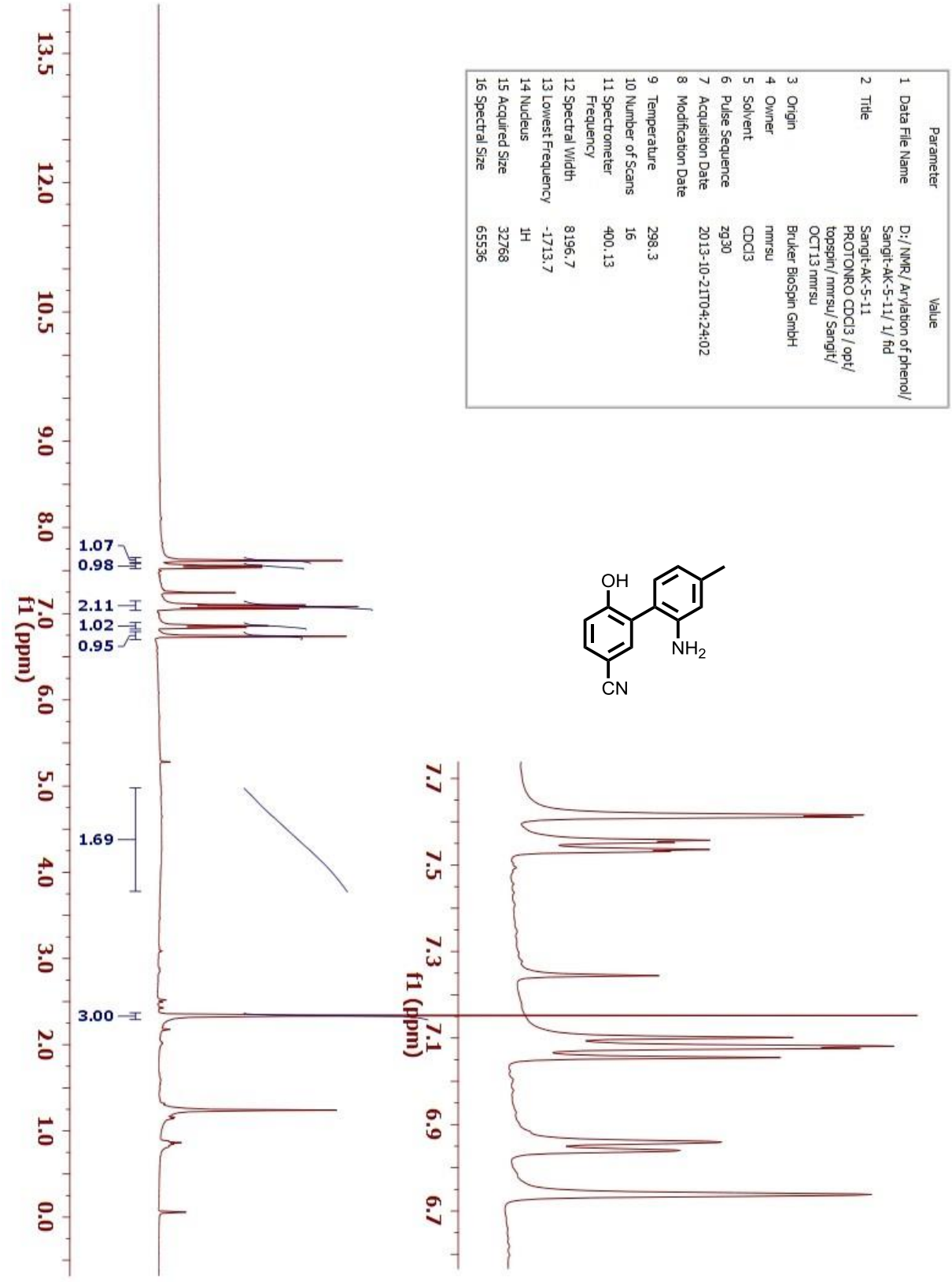

Figure S26 ^{13}C NMR spectrum of **1g**

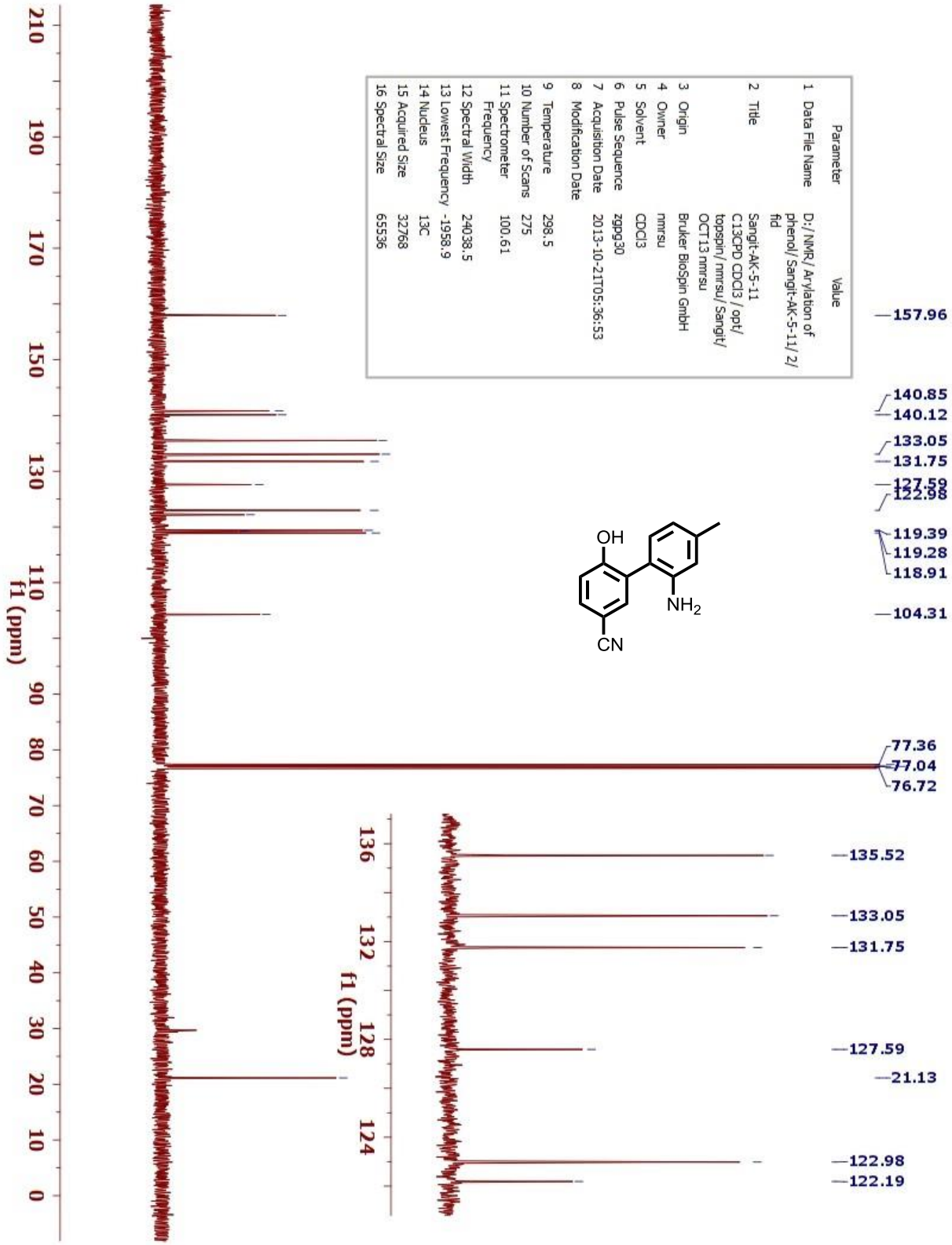

Figure S27 ^{1}H NMR spectrum of **1h**

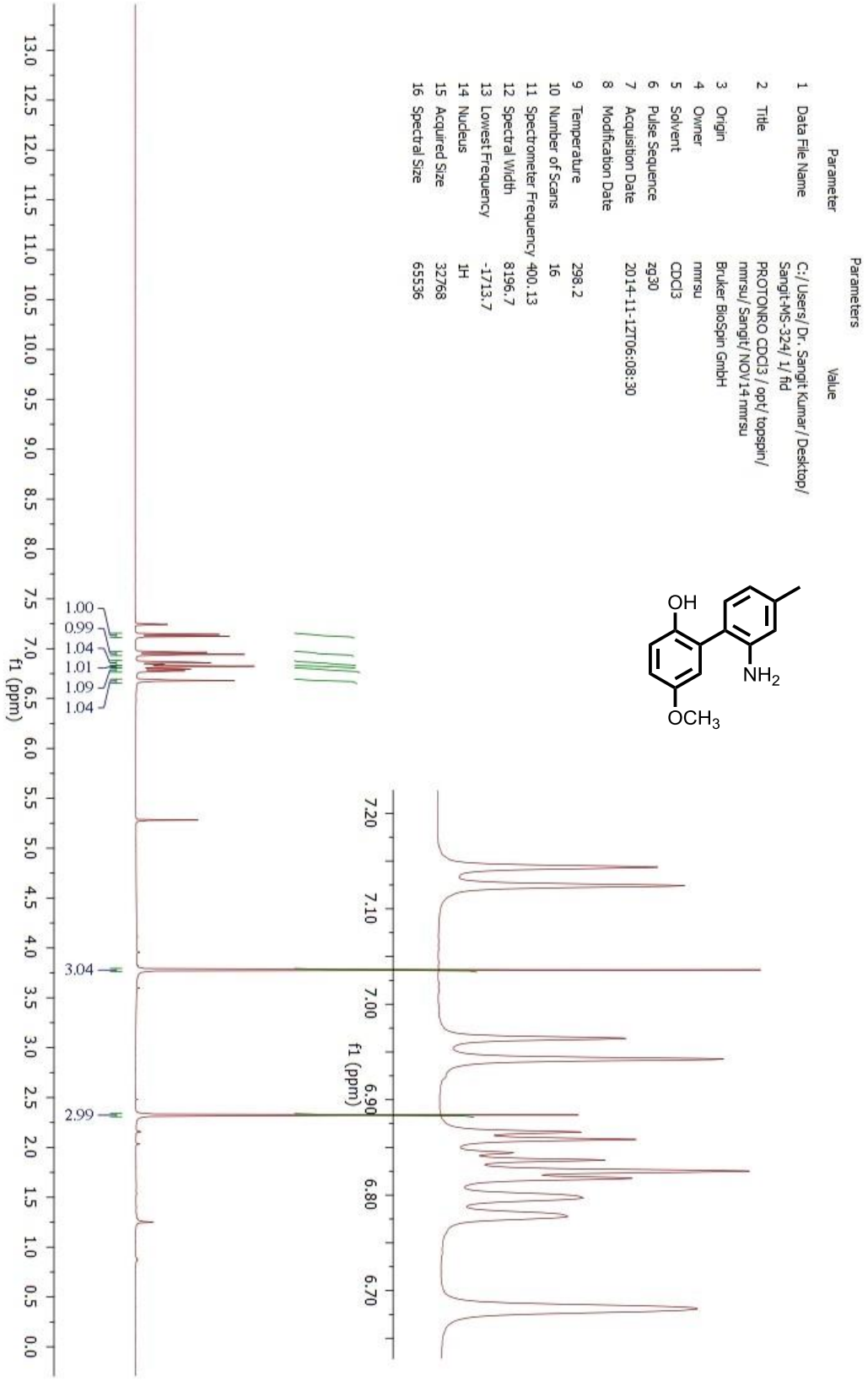

Figure S28 ^{13}C NMR spectrum of **1h**

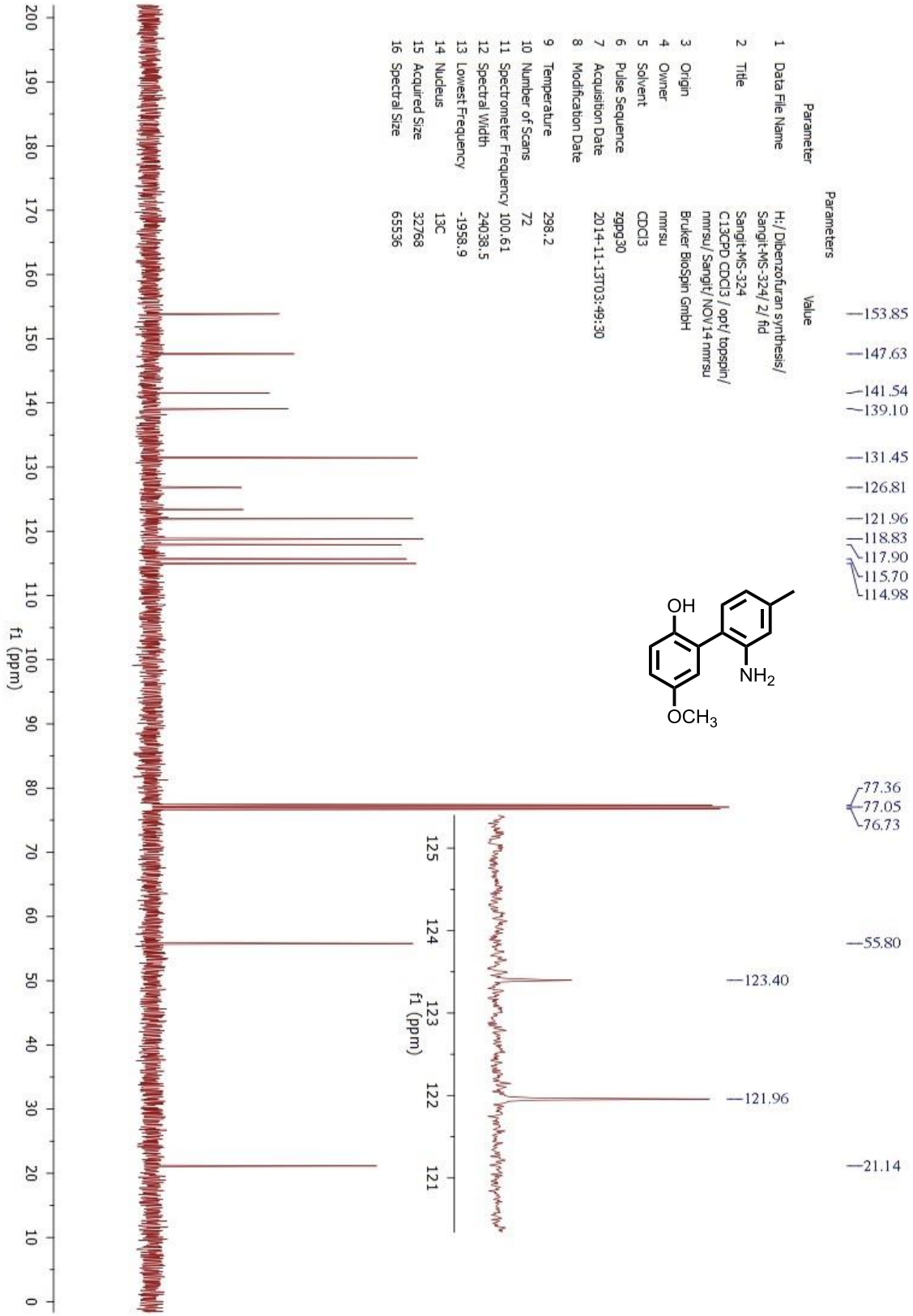

Figure S29 ^{1}H NMR spectrum of **1i**

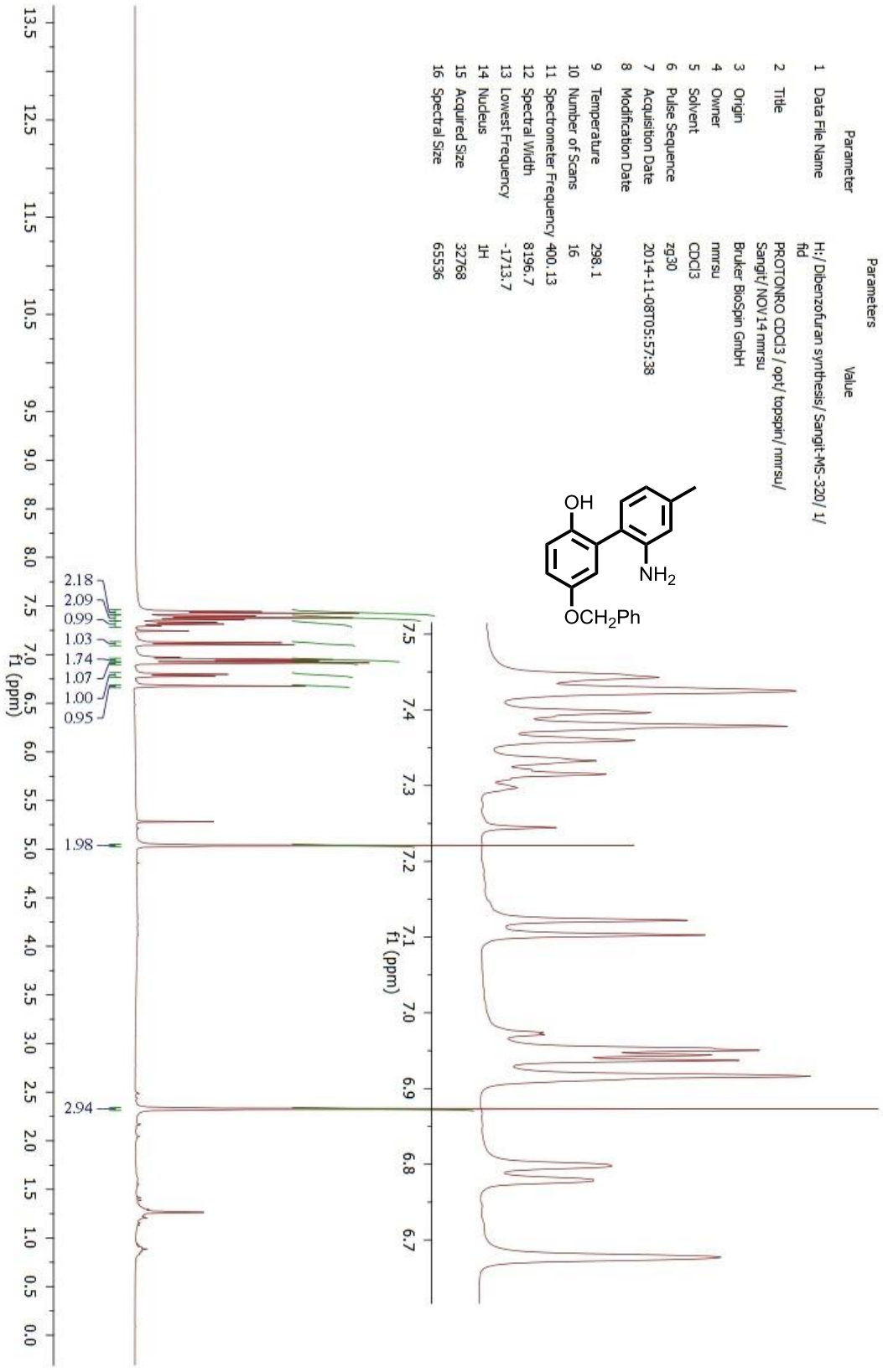

Figure S30 ^{13}C NMR spectrum of **1i**

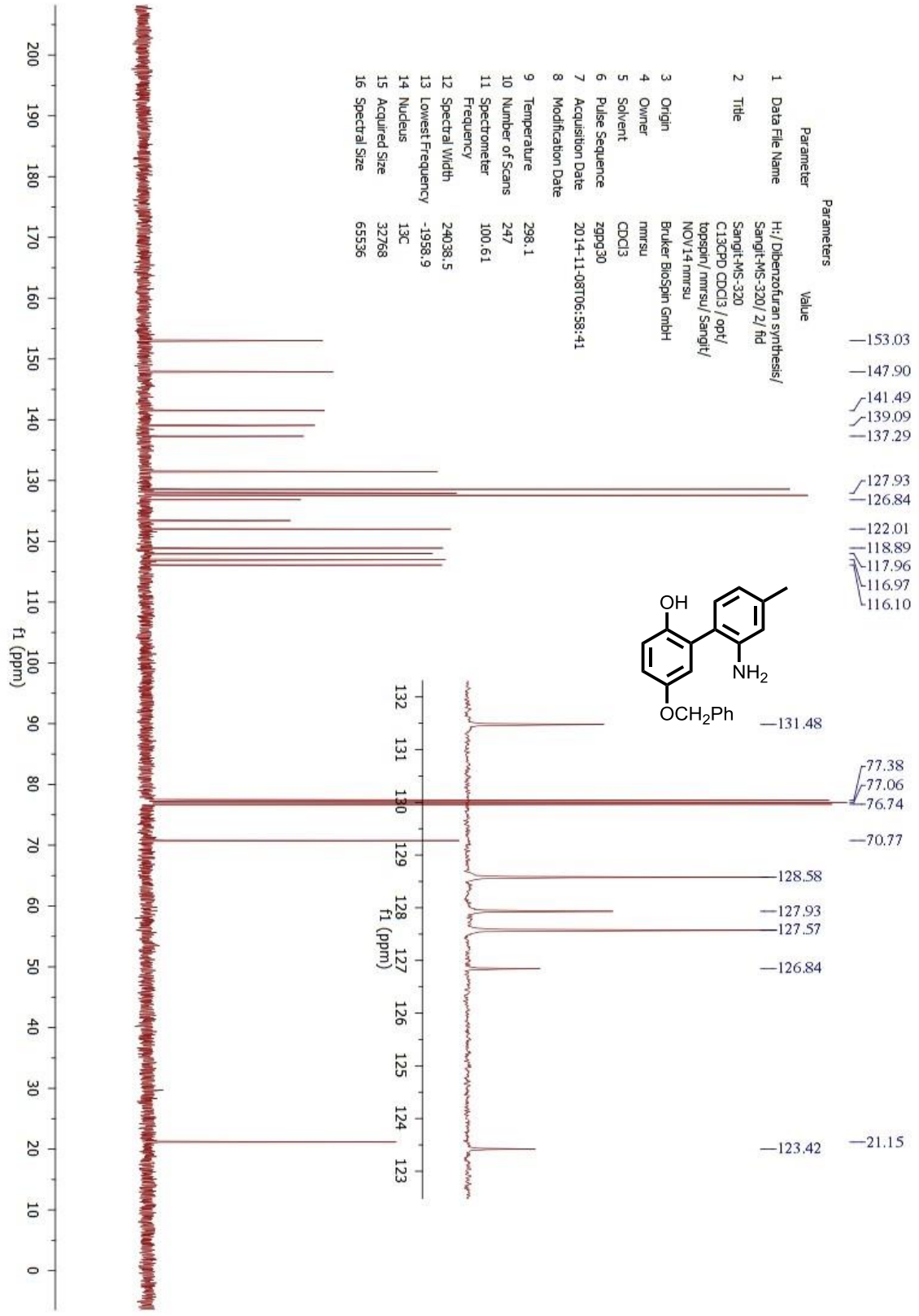

Figure S31 ^{1}H NMR spectrum of **1j**

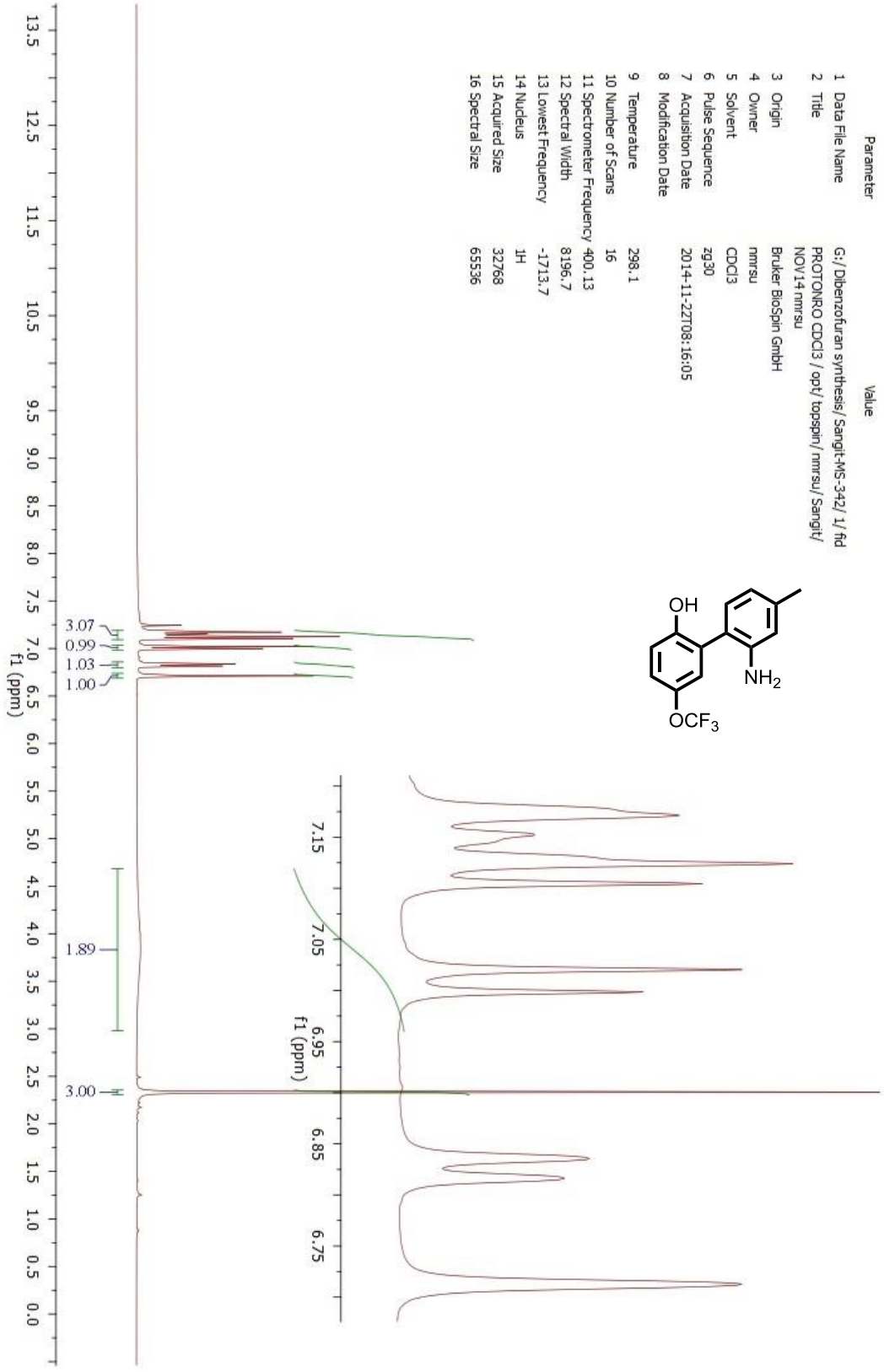

Figure S32 ^{13}C NMR spectrum of **1j**

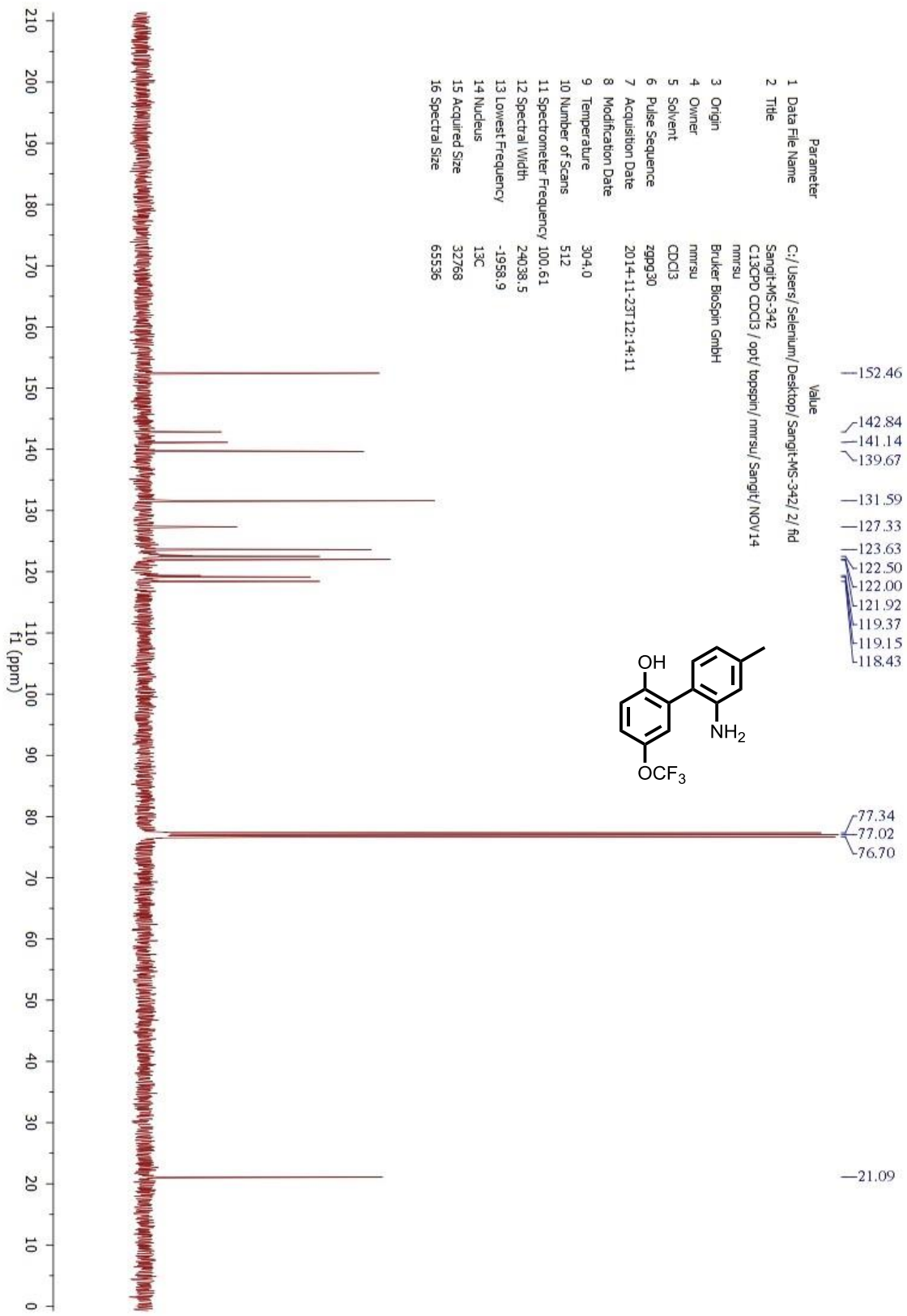

Figure S33 ^{1}H NMR spectrum of **1k**

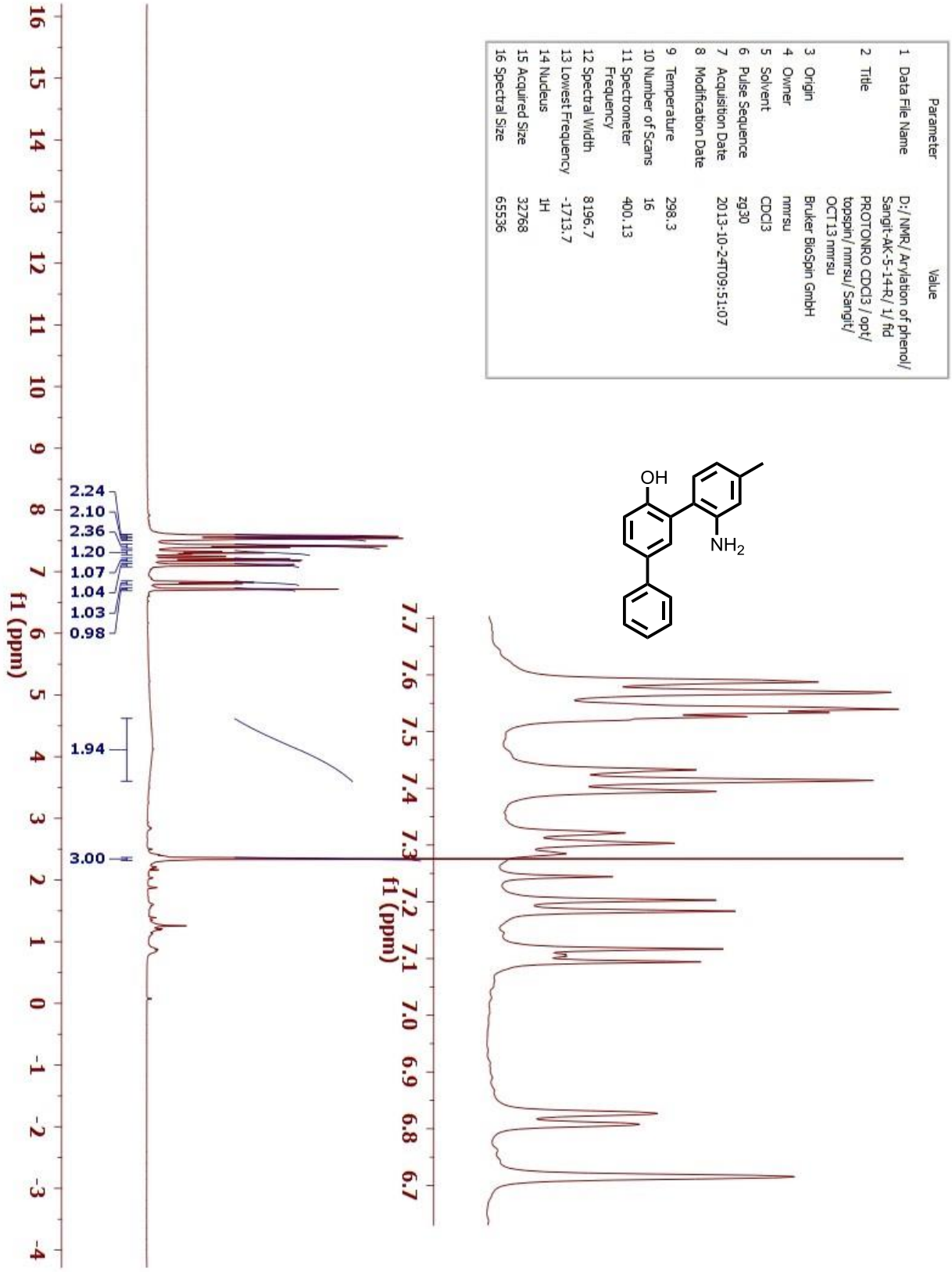

Figure S34 ^{13}C NMR spectrum of **1k**

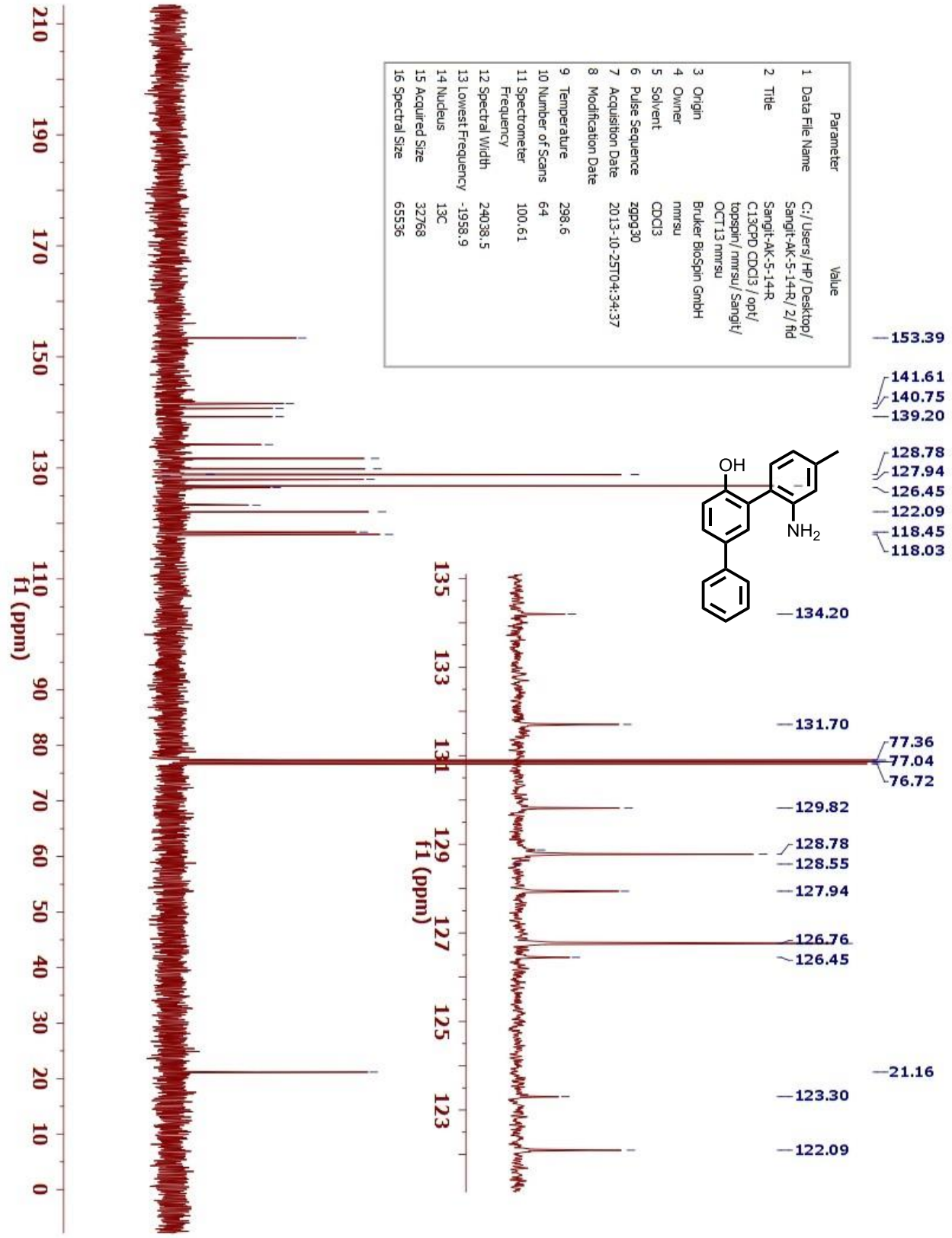

Figure S35 ^{1}H NMR spectrum of **1l**

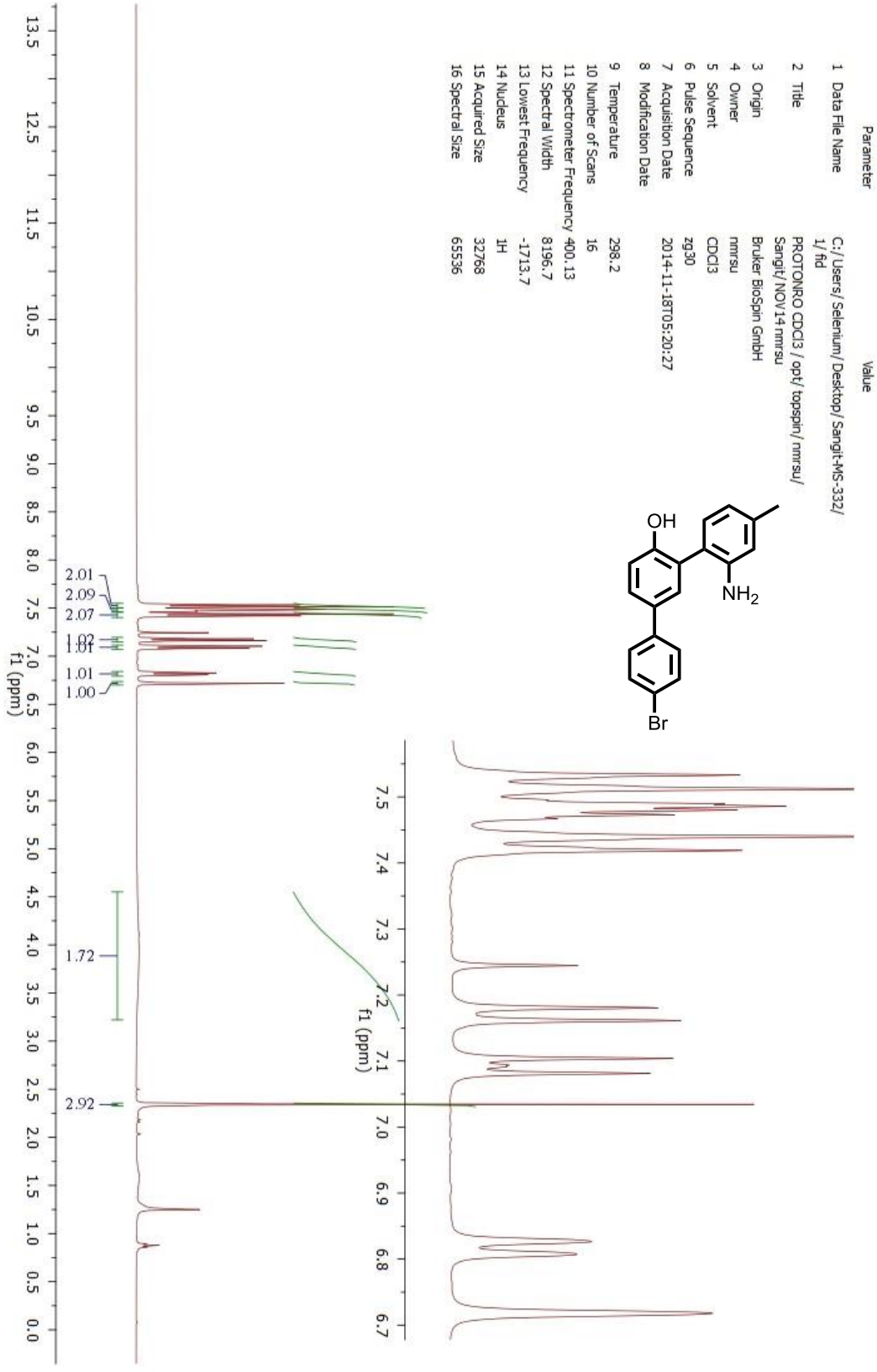

Figure S36 ^{13}C NMR spectrum of **1l**

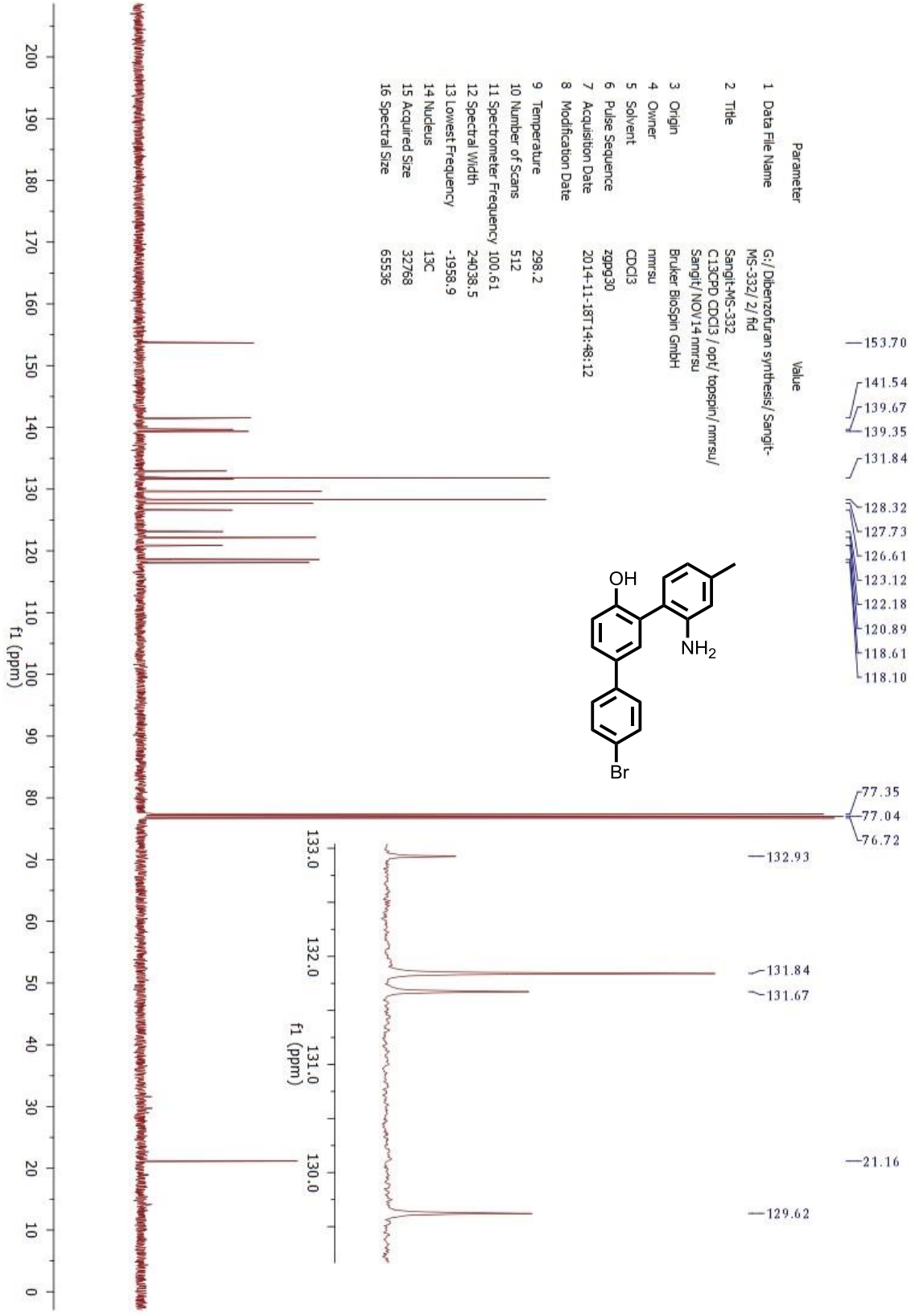

Figure S37 ^{1}H NMR spectrum of **1m**

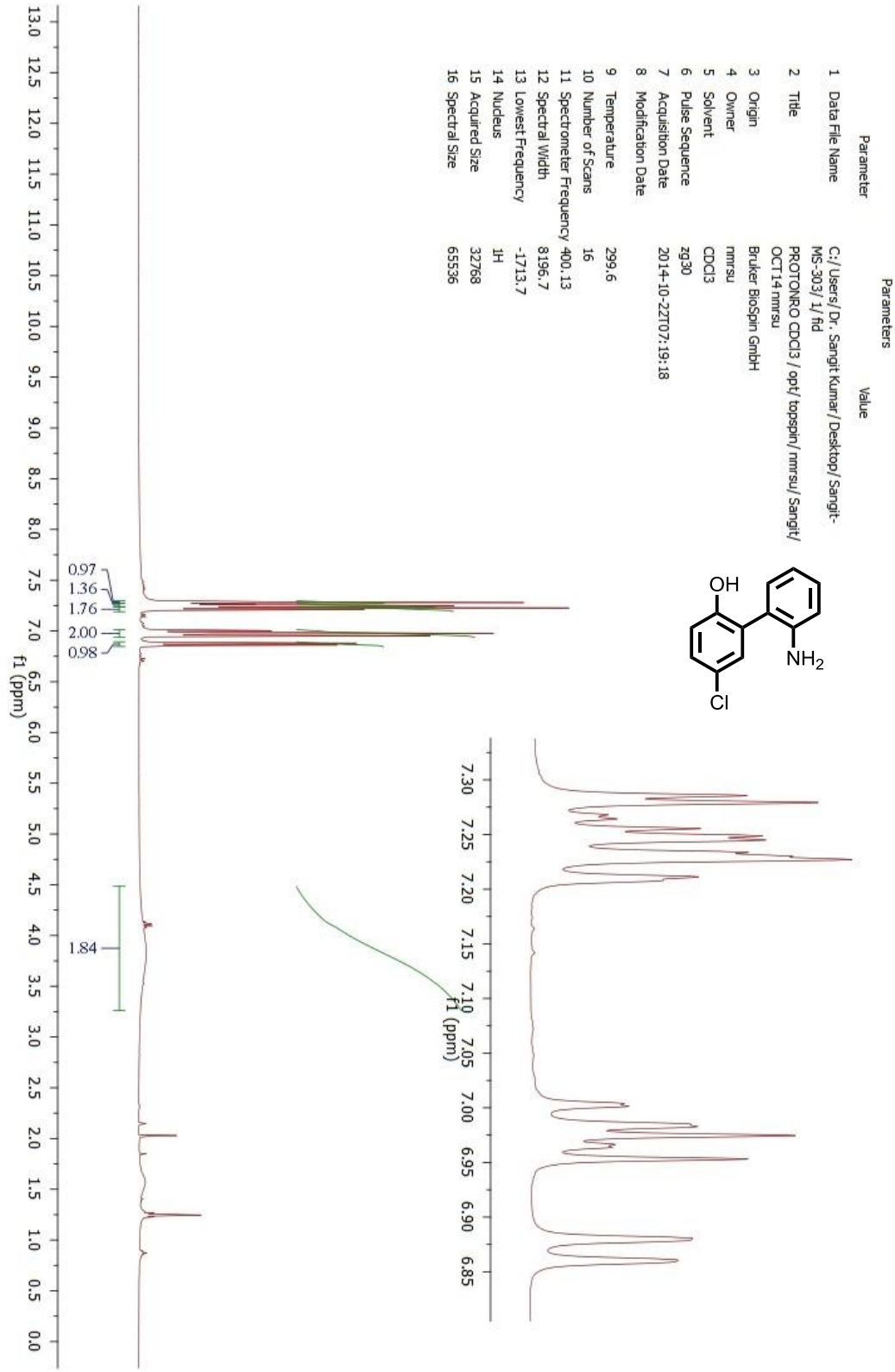

Figure S38 ^{13}C NMR spectrum of **1m**

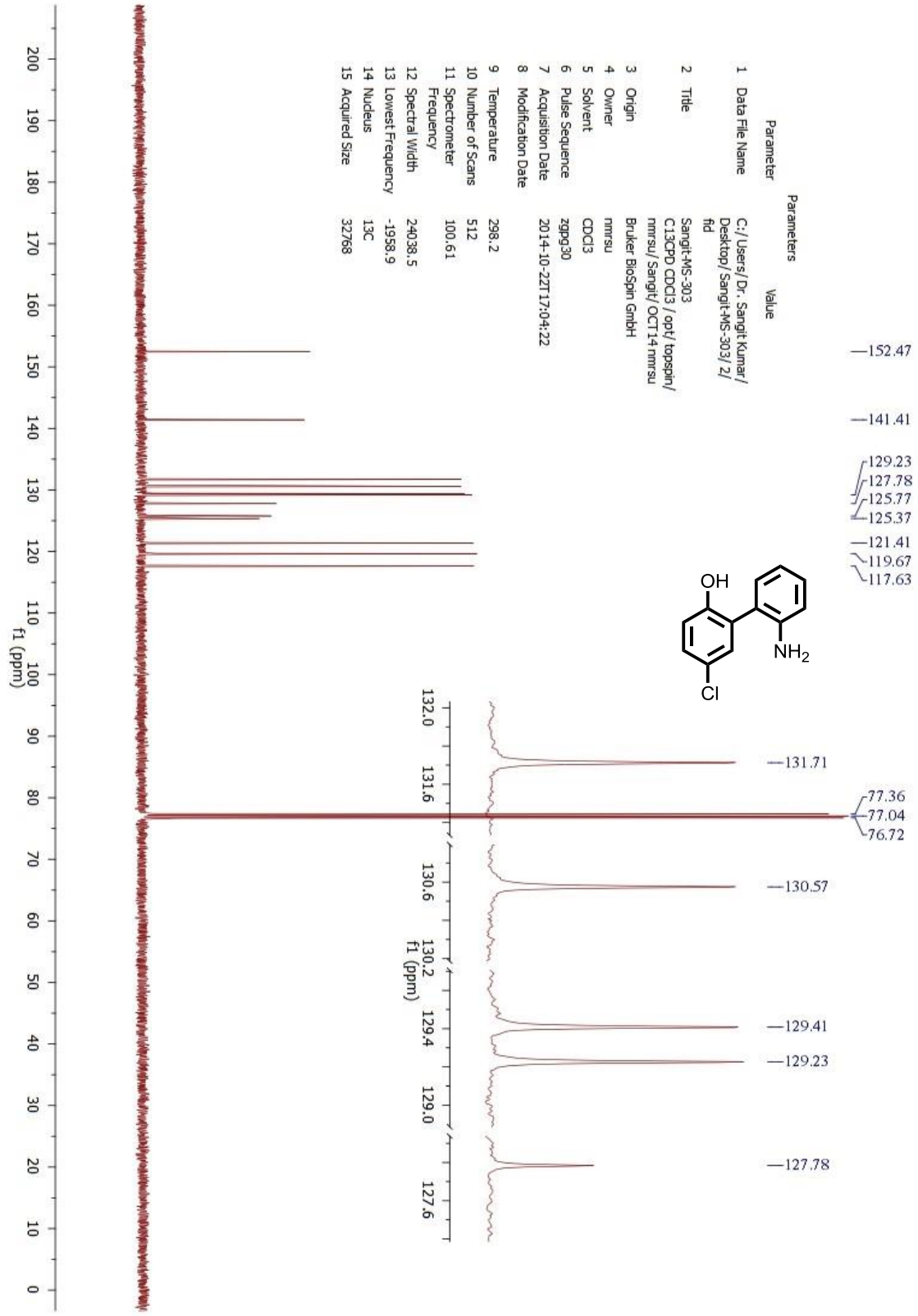

Figure S39 ^{1}H NMR spectrum of **1n**

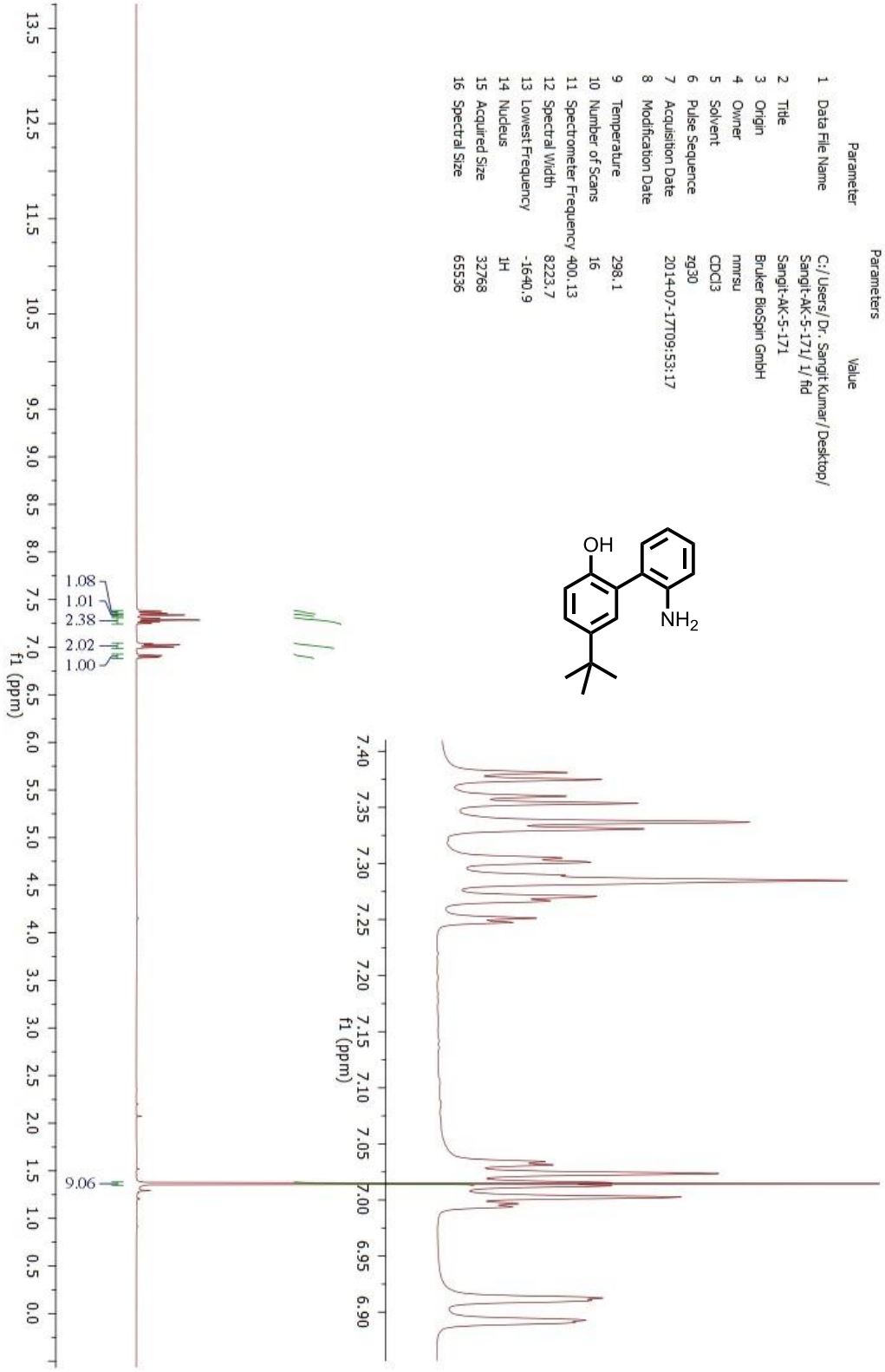

Figure S40 ^{13}C NMR spectrum of **1n**

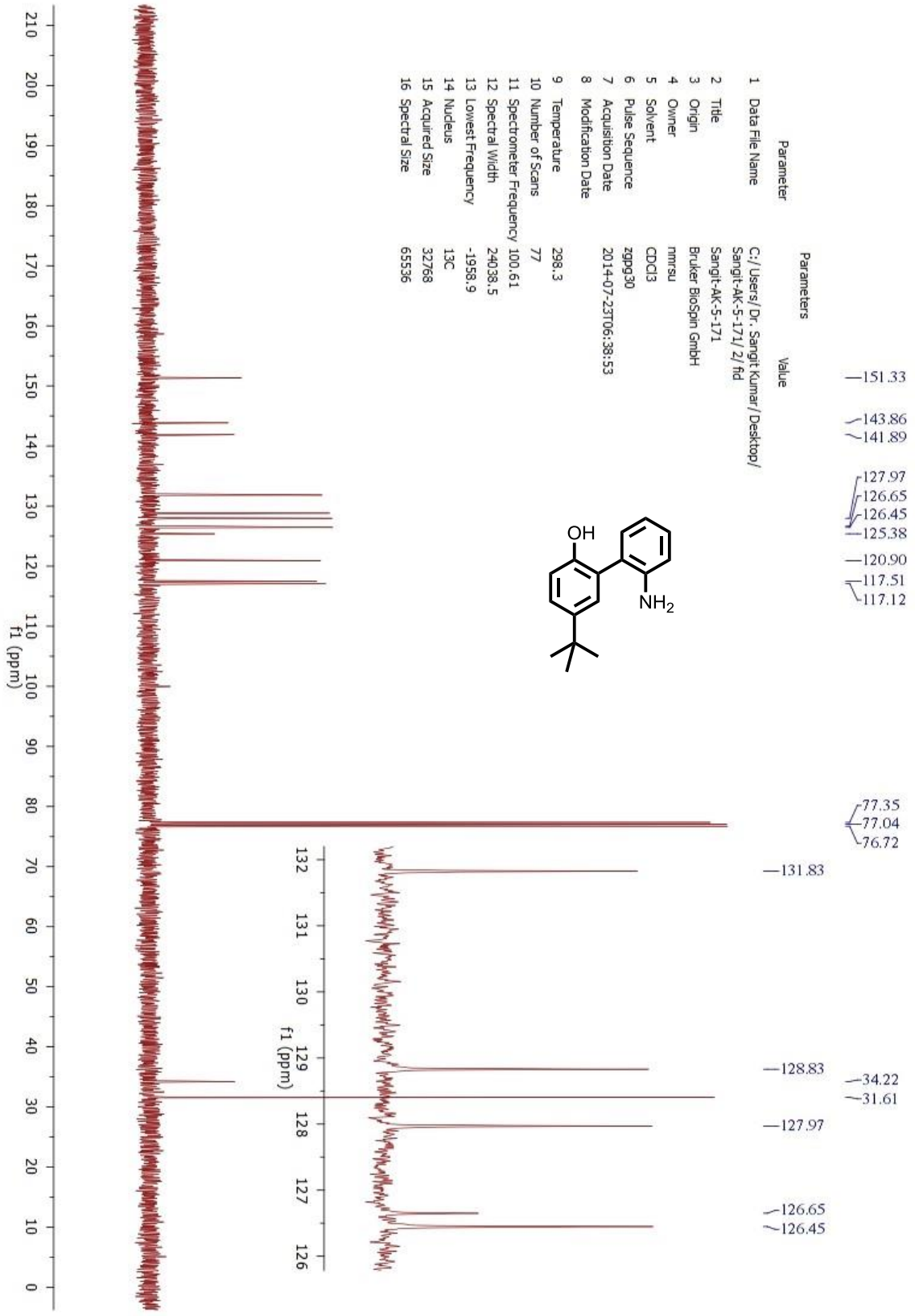

Figure S41 ^{1}H NMR spectrum of **1o**

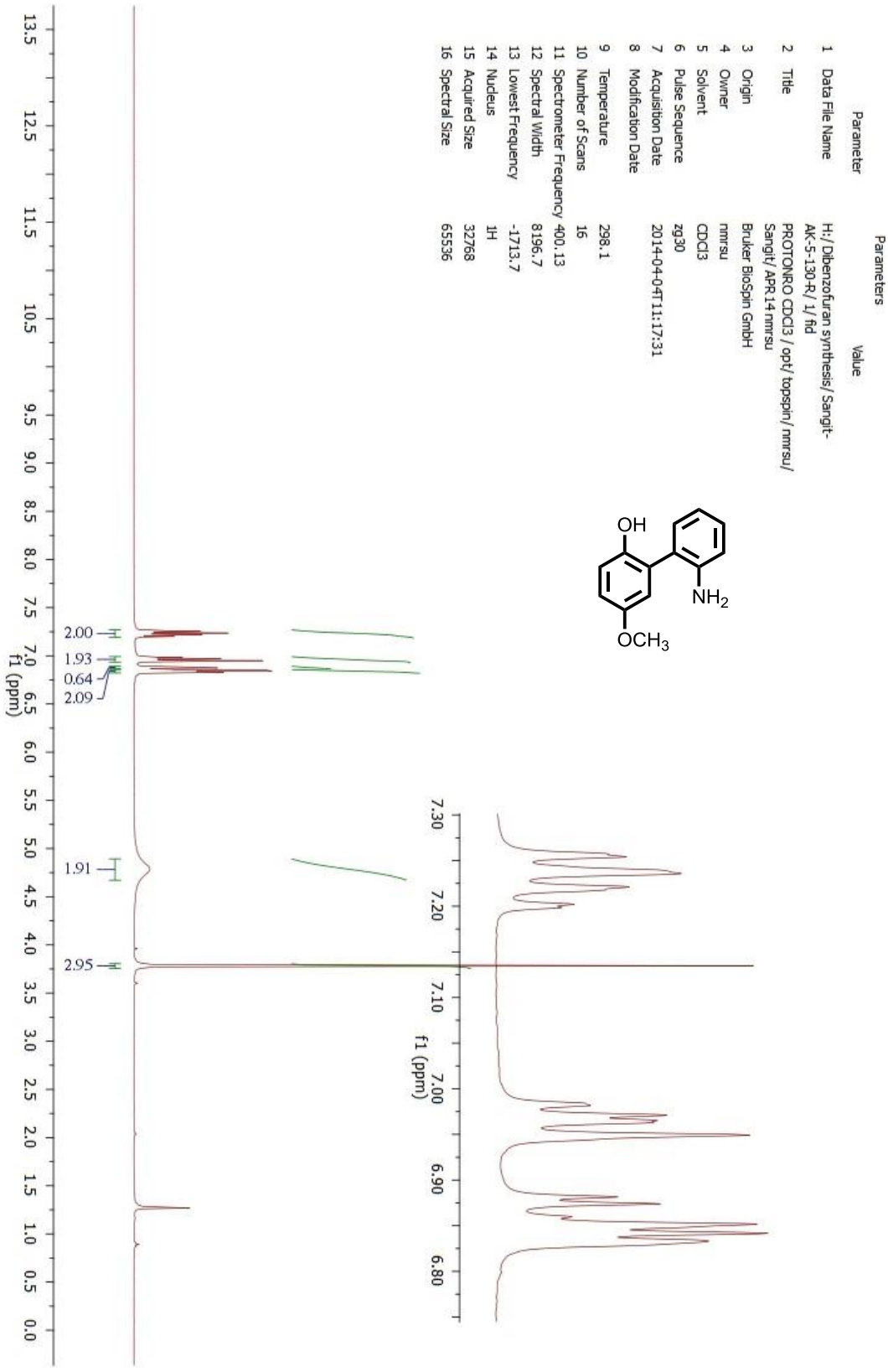

Figure S42 ^{13}C NMR spectrum of **1o**

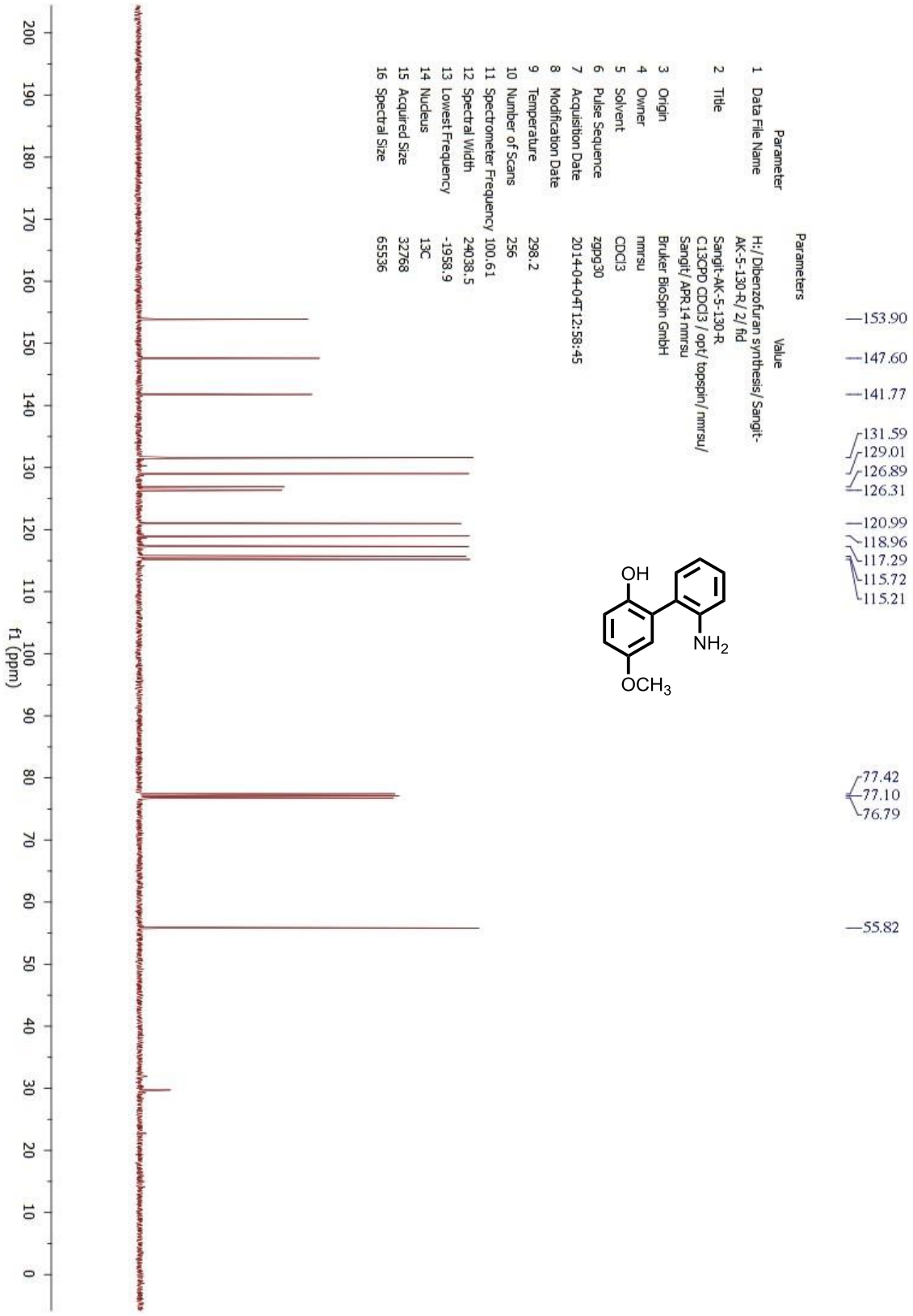

Figure S43 ^{1}H NMR spectrum of **1p**

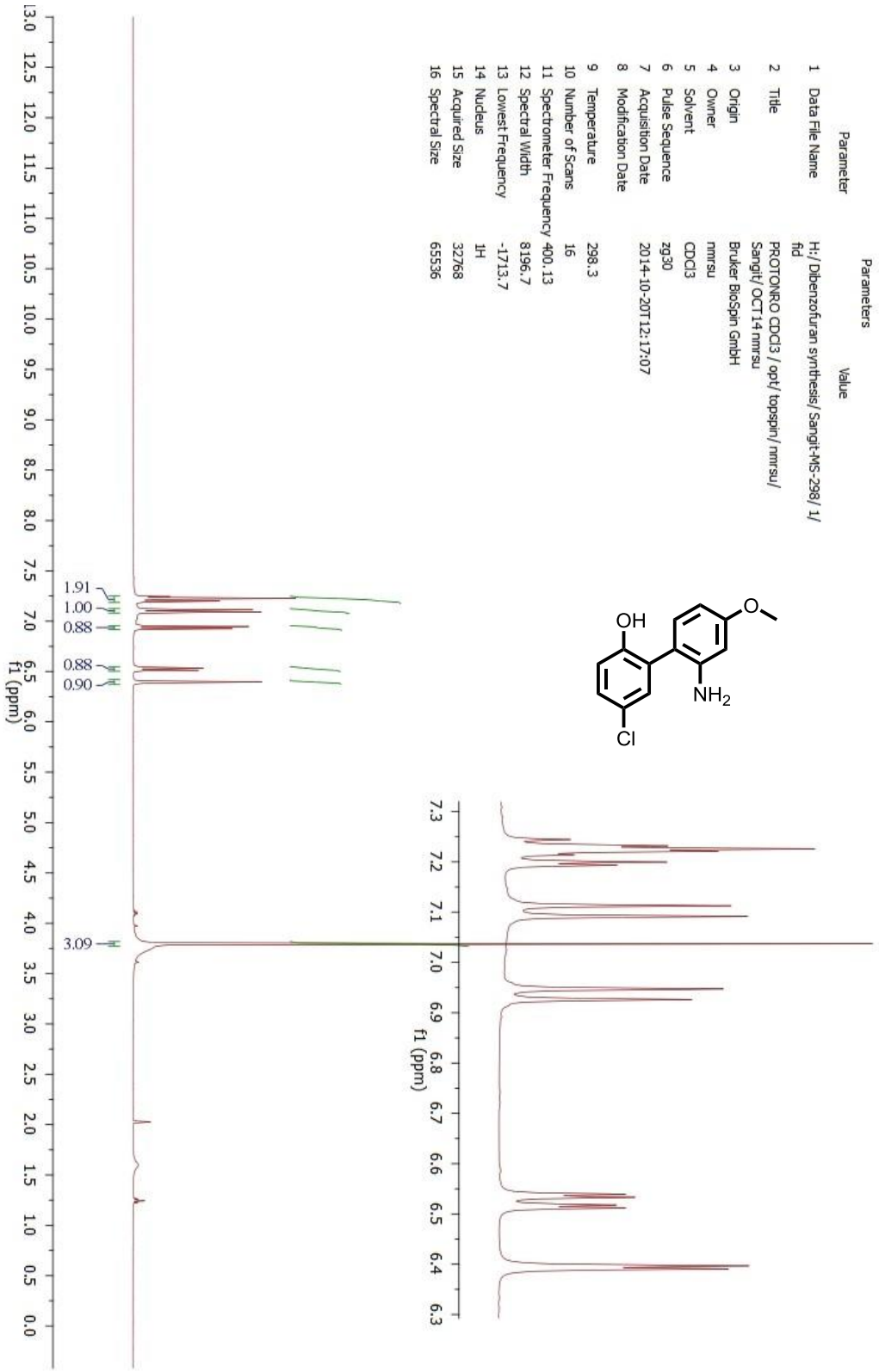

Figure S44 ^{13}C NMR spectrum of **1p**

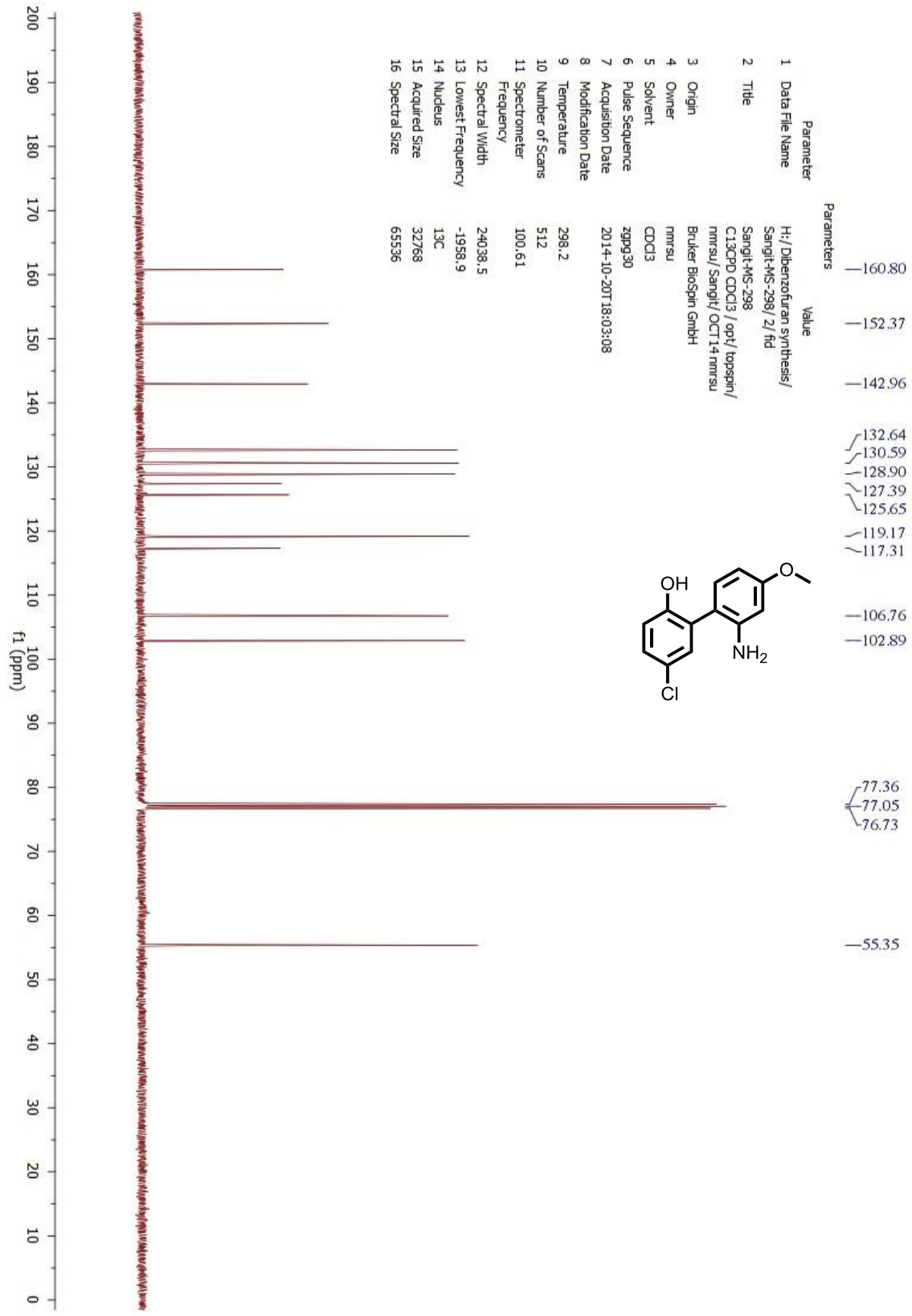

Figure S45 ^{1}H NMR spectrum of **1q**

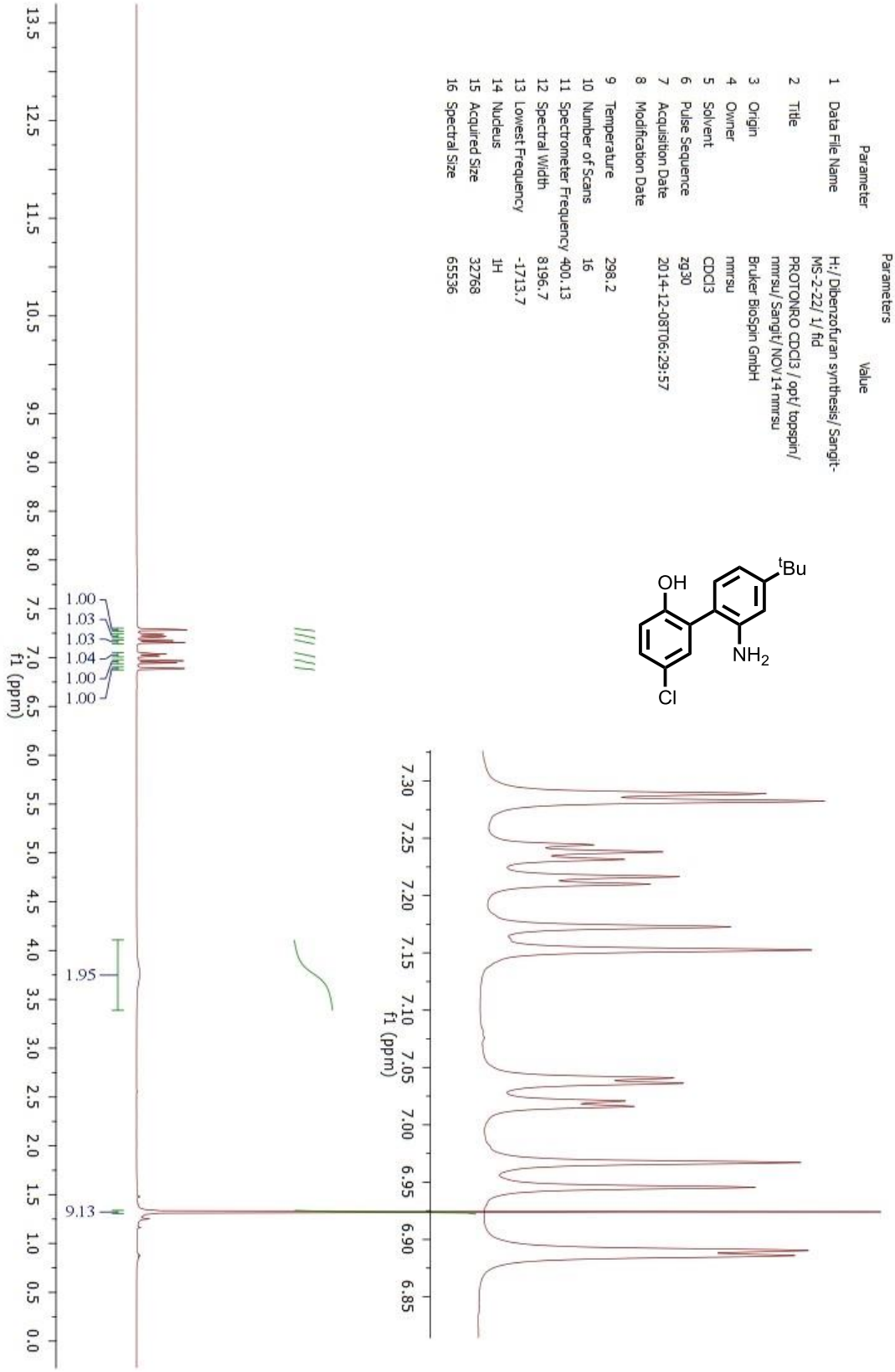

Figure S46 ^{13}C NMR spectrum of **1q**

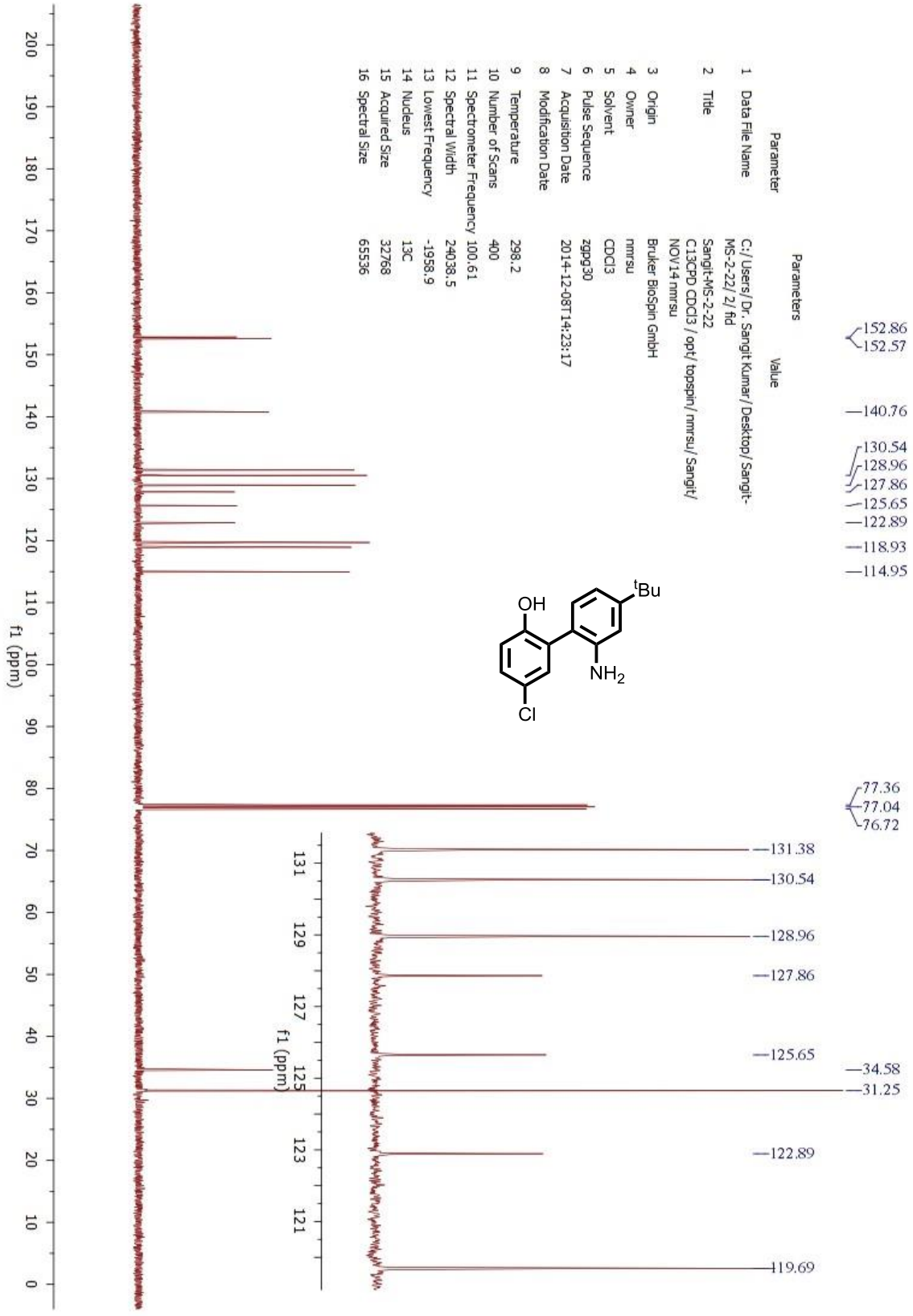

Figure S47 ^{1}H NMR spectrum of **1r**

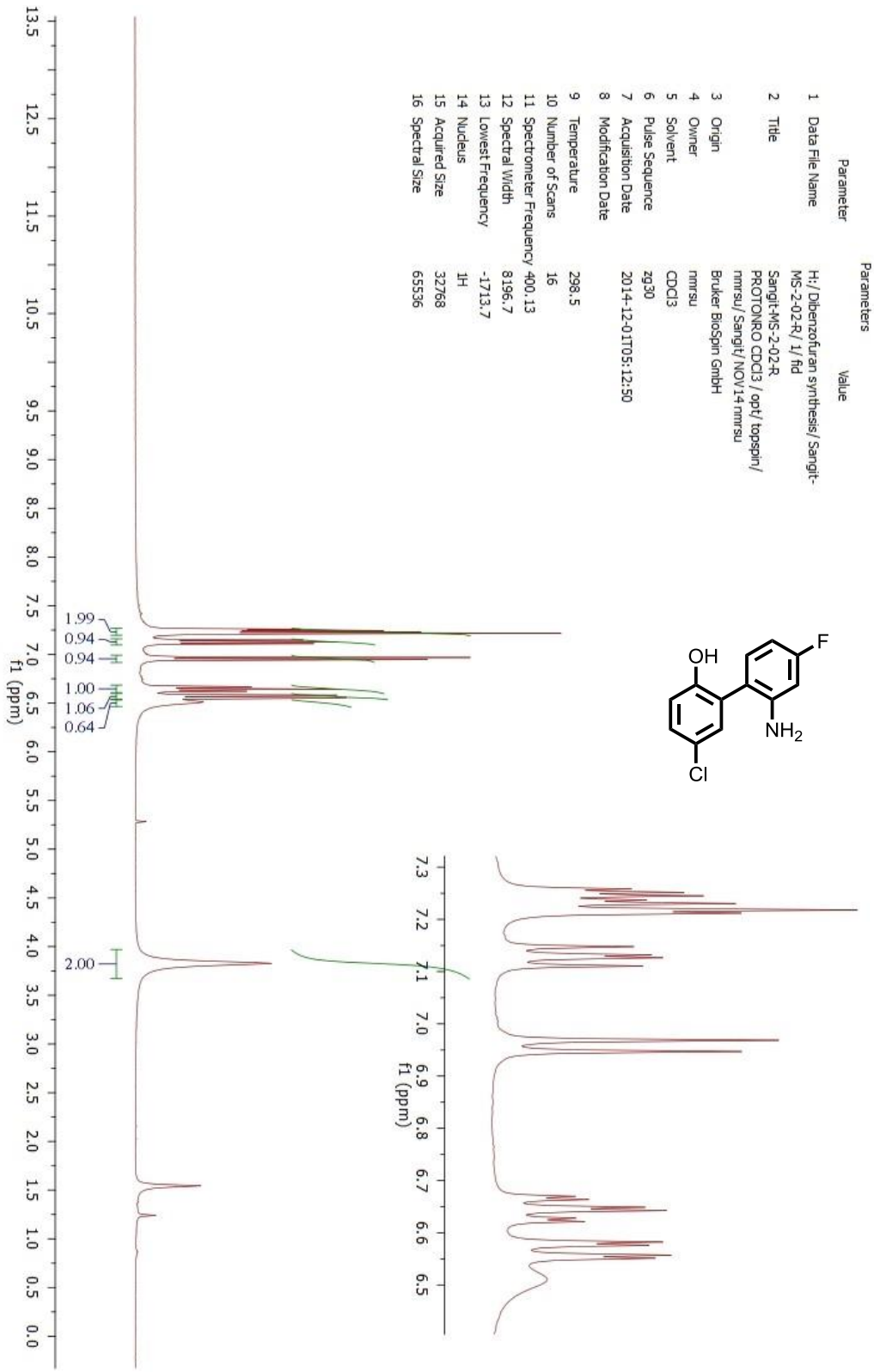

Figure S48 ^{13}C NMR spectrum of **1r**

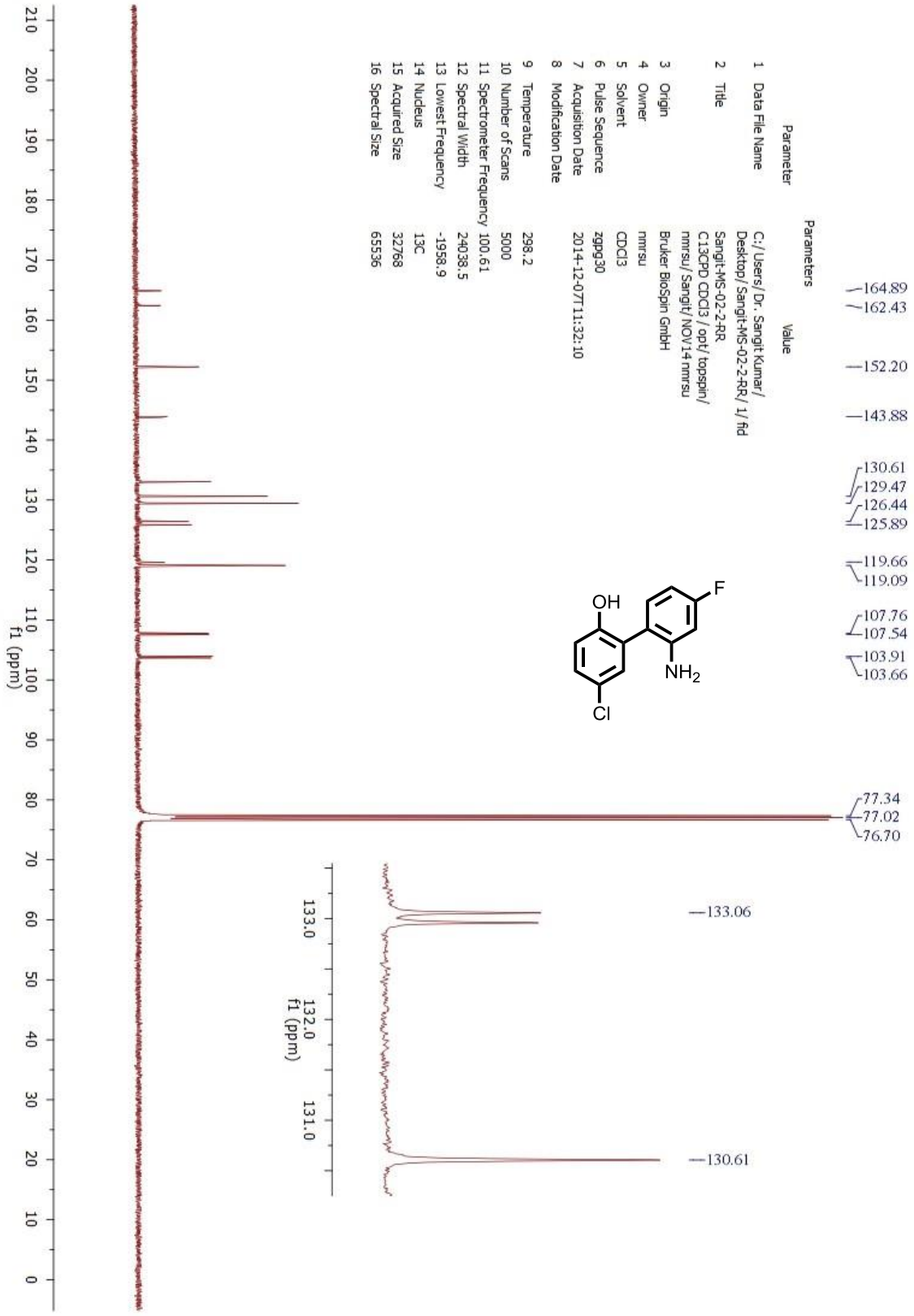

Figure S49 ^{1}H NMR spectrum of **1s**

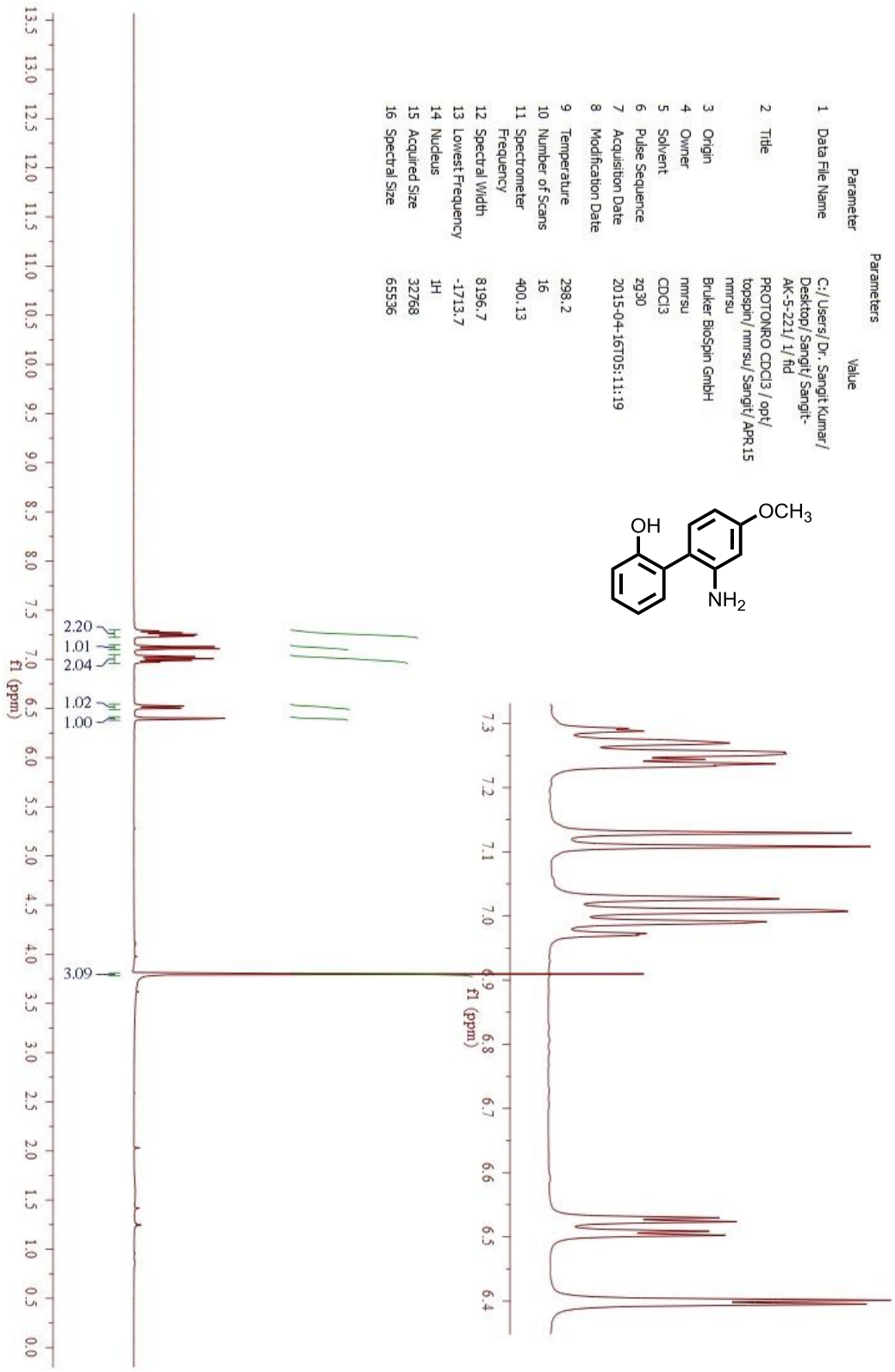

Figure S50 ^{13}C NMR spectrum of **1s**

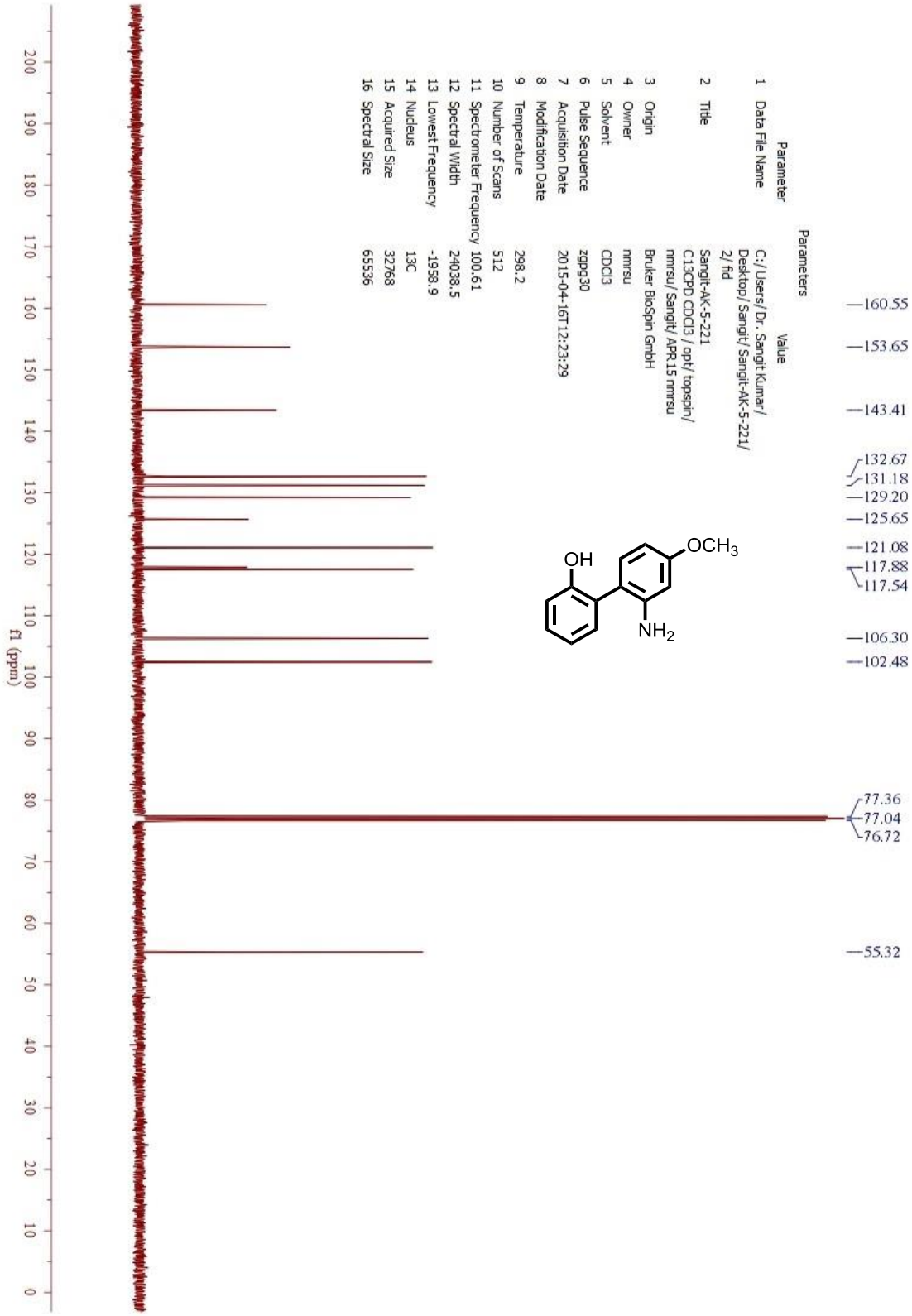

Figure S51 ^{1}H NMR spectrum of **1t**

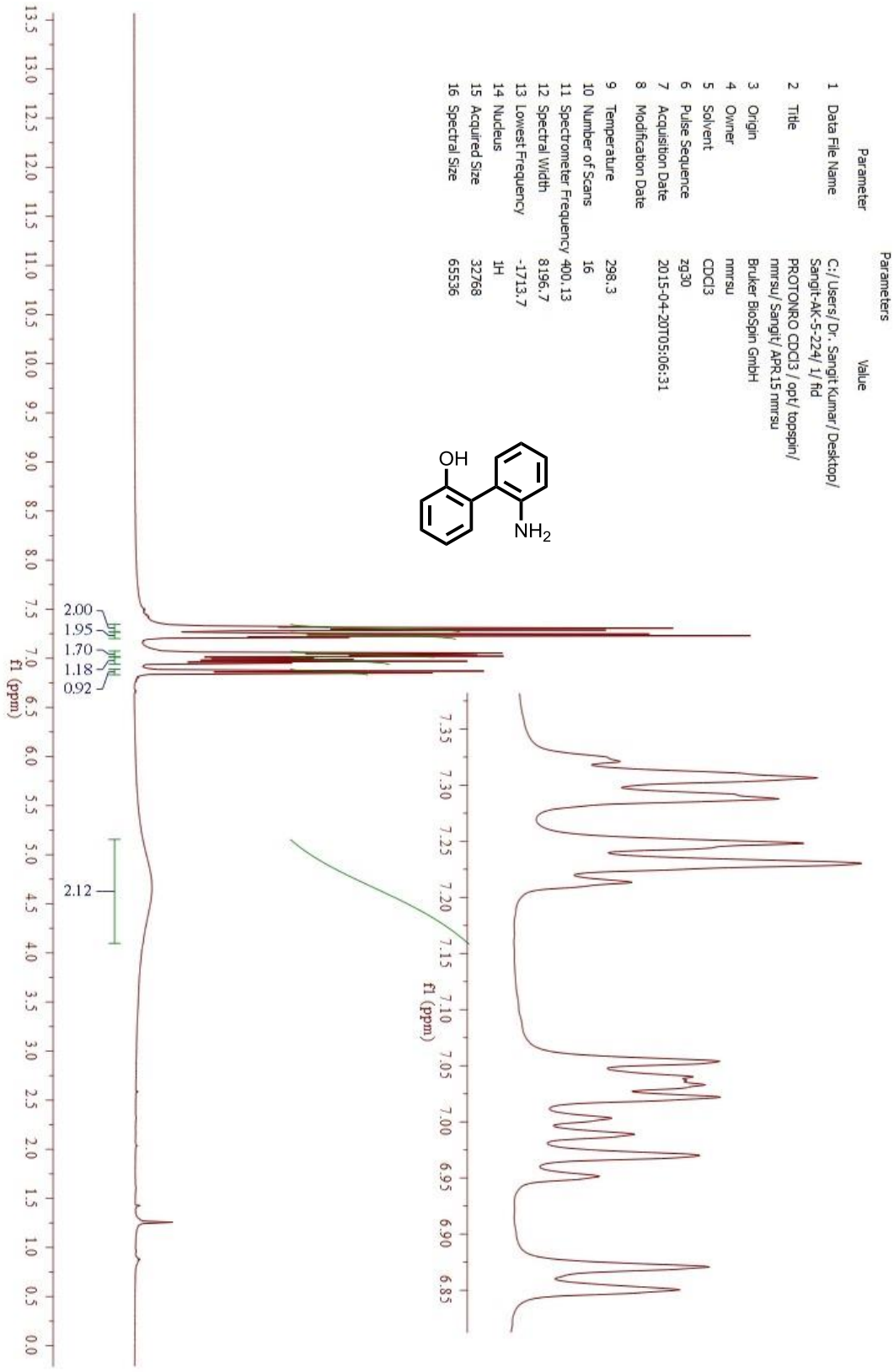

Figure S52 ^{13}C NMR spectrum of **1t**

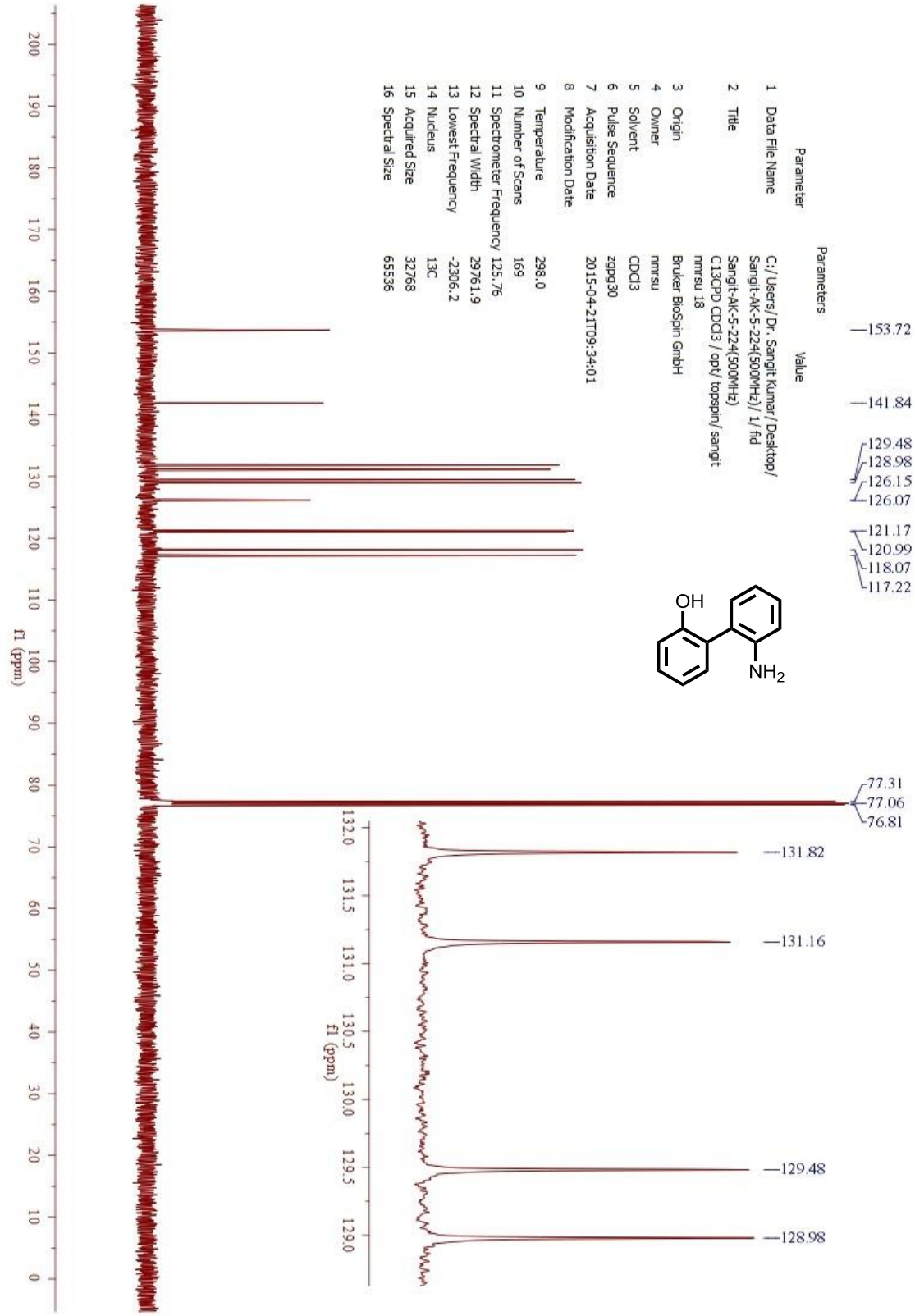

Figure S53 ^{1}H NMR spectrum of **2a**

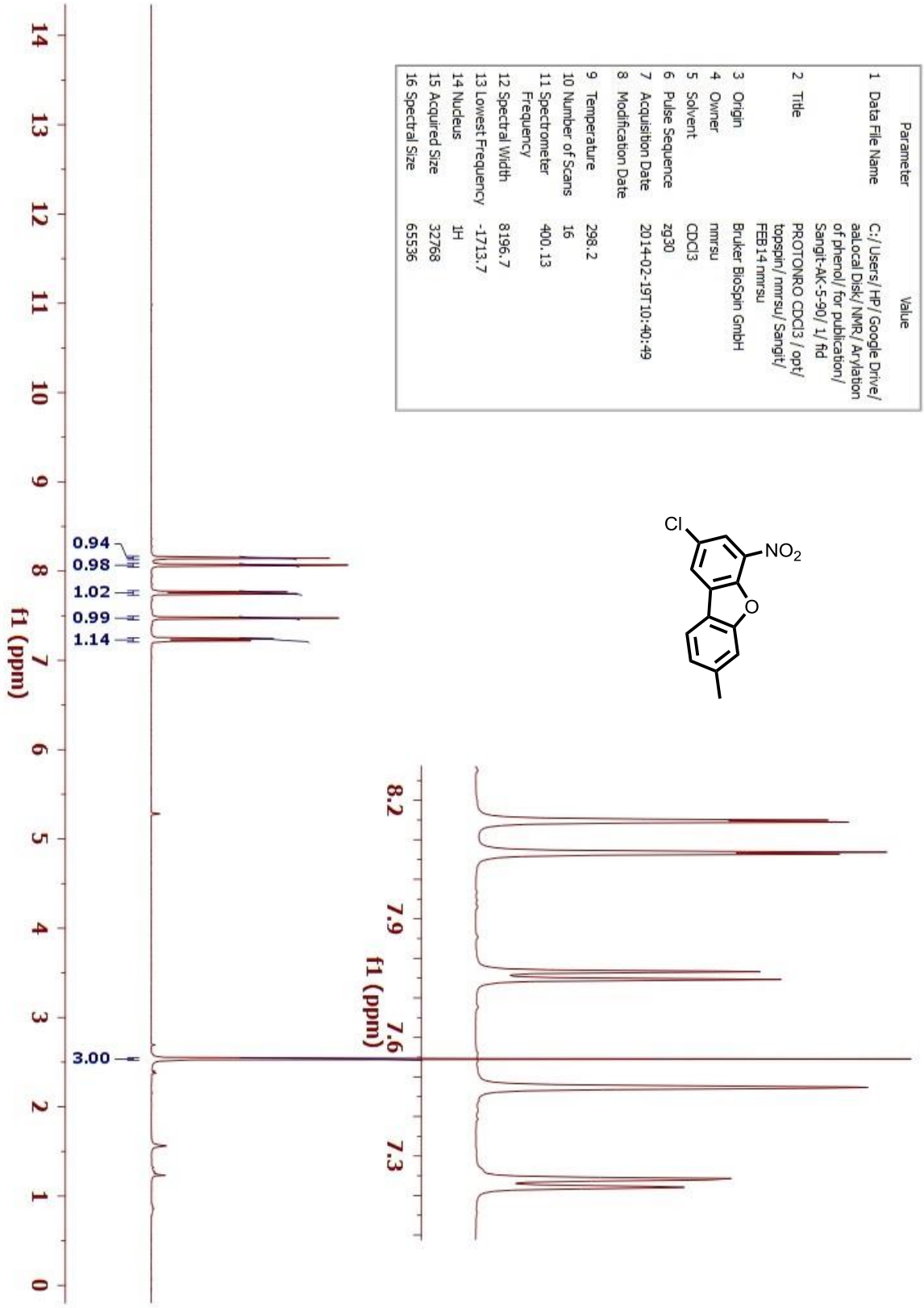

Figure S54 ^{13}C NMR spectrum of **2a**

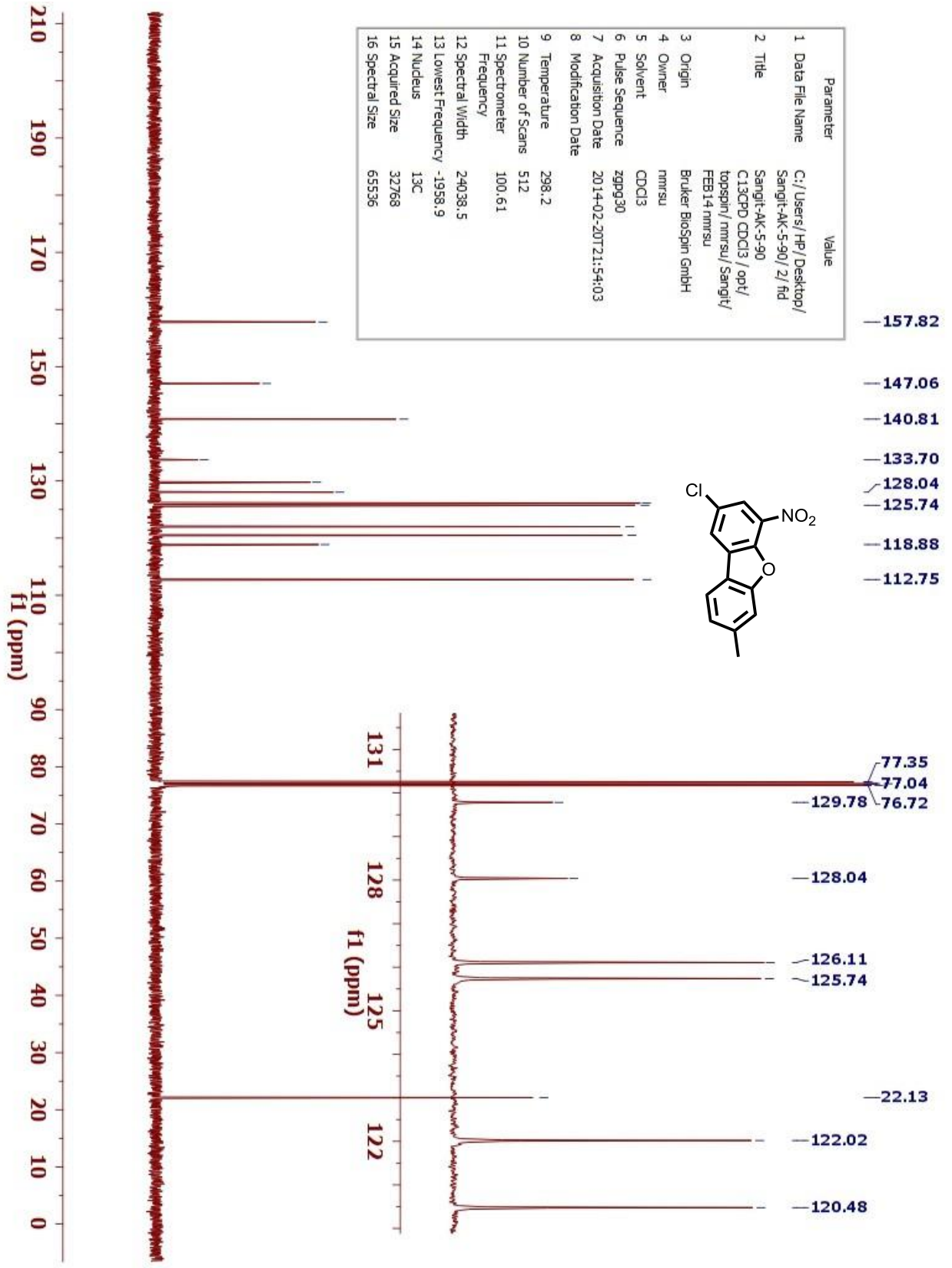

Figure S55 ^{1}H NMR spectrum of **2b**

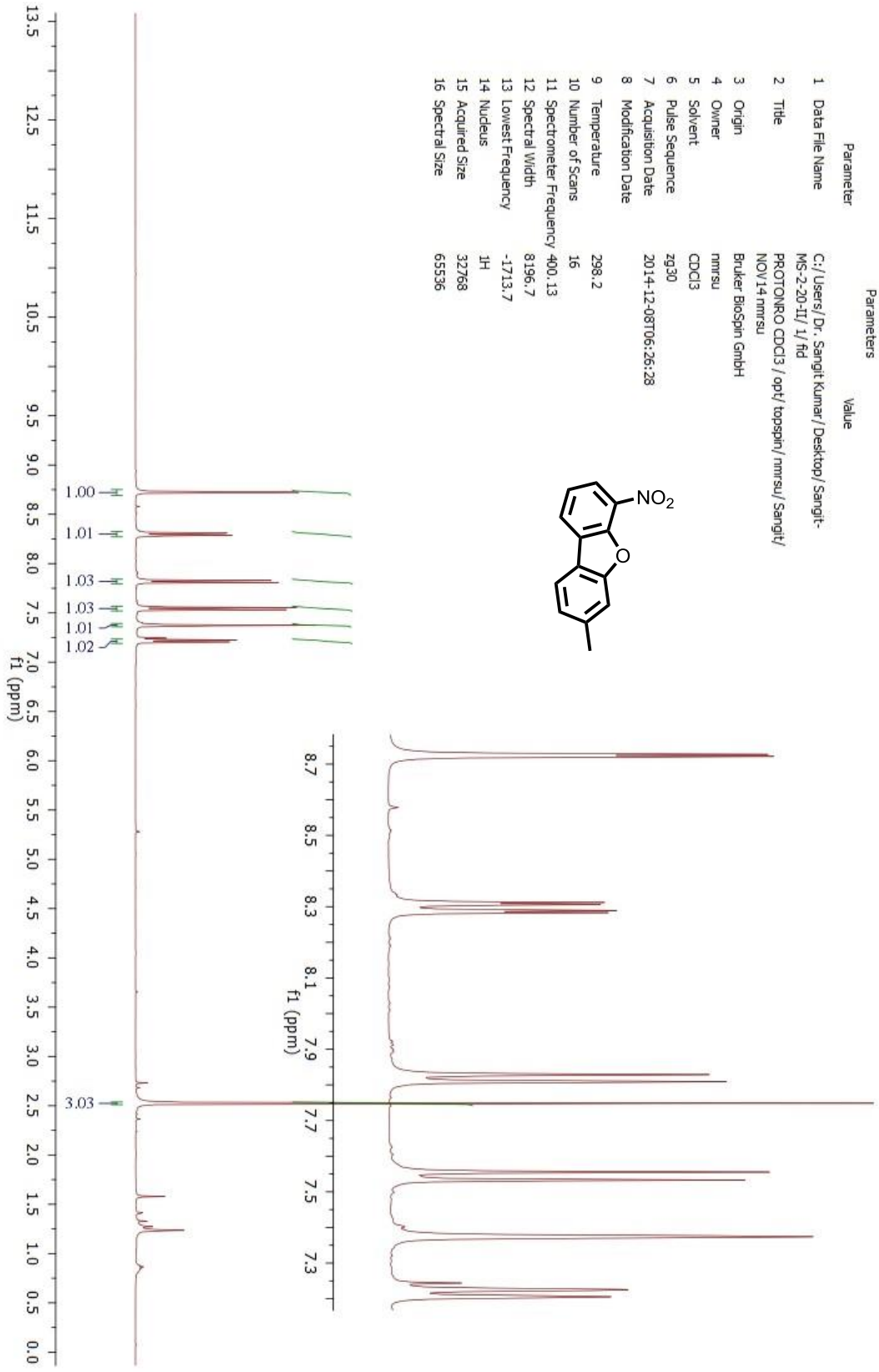

Figure S56 ^{13}C NMR spectrum of **2b**

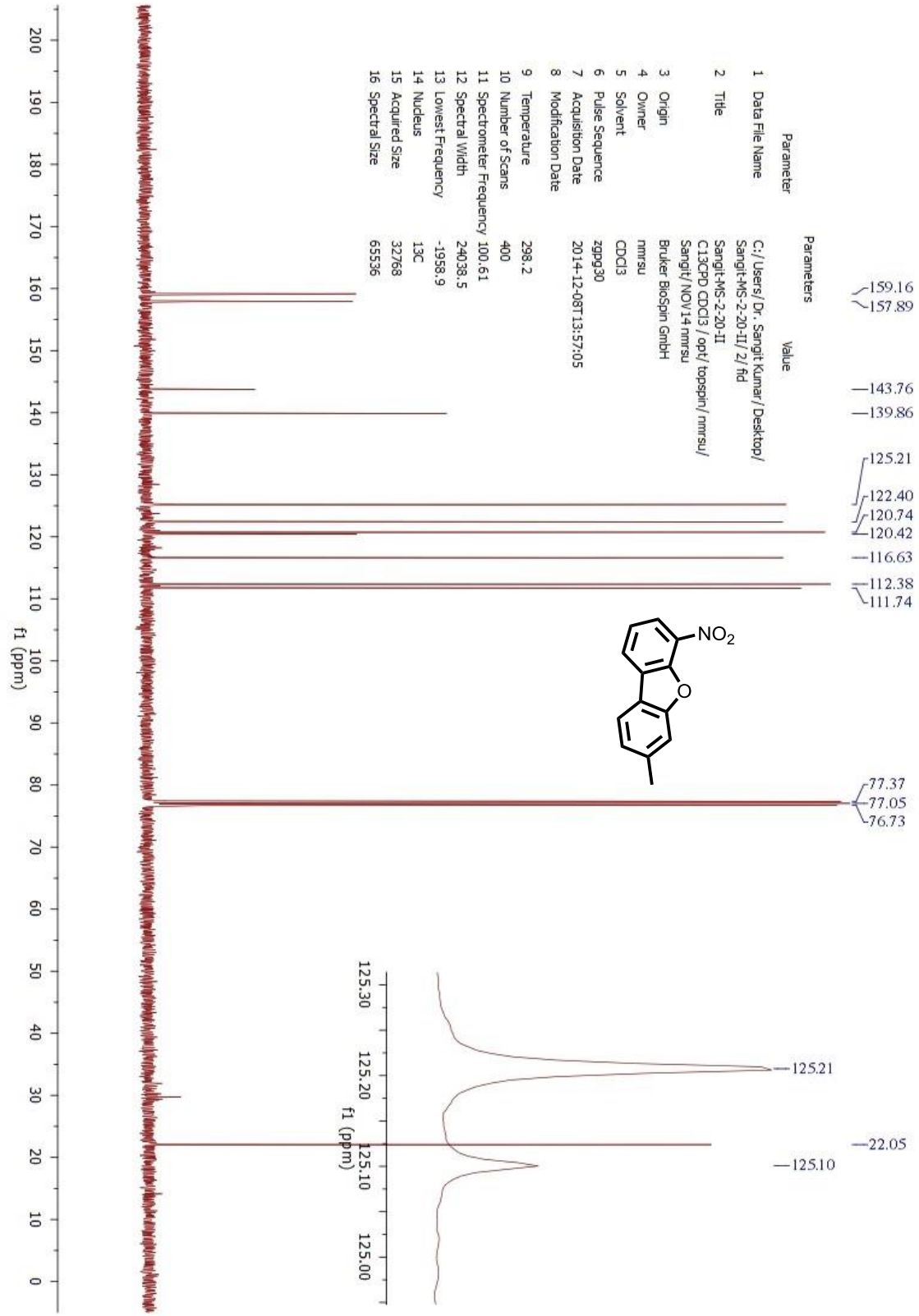

Figure S57 ^{1}H NMR spectrum of **2b'**

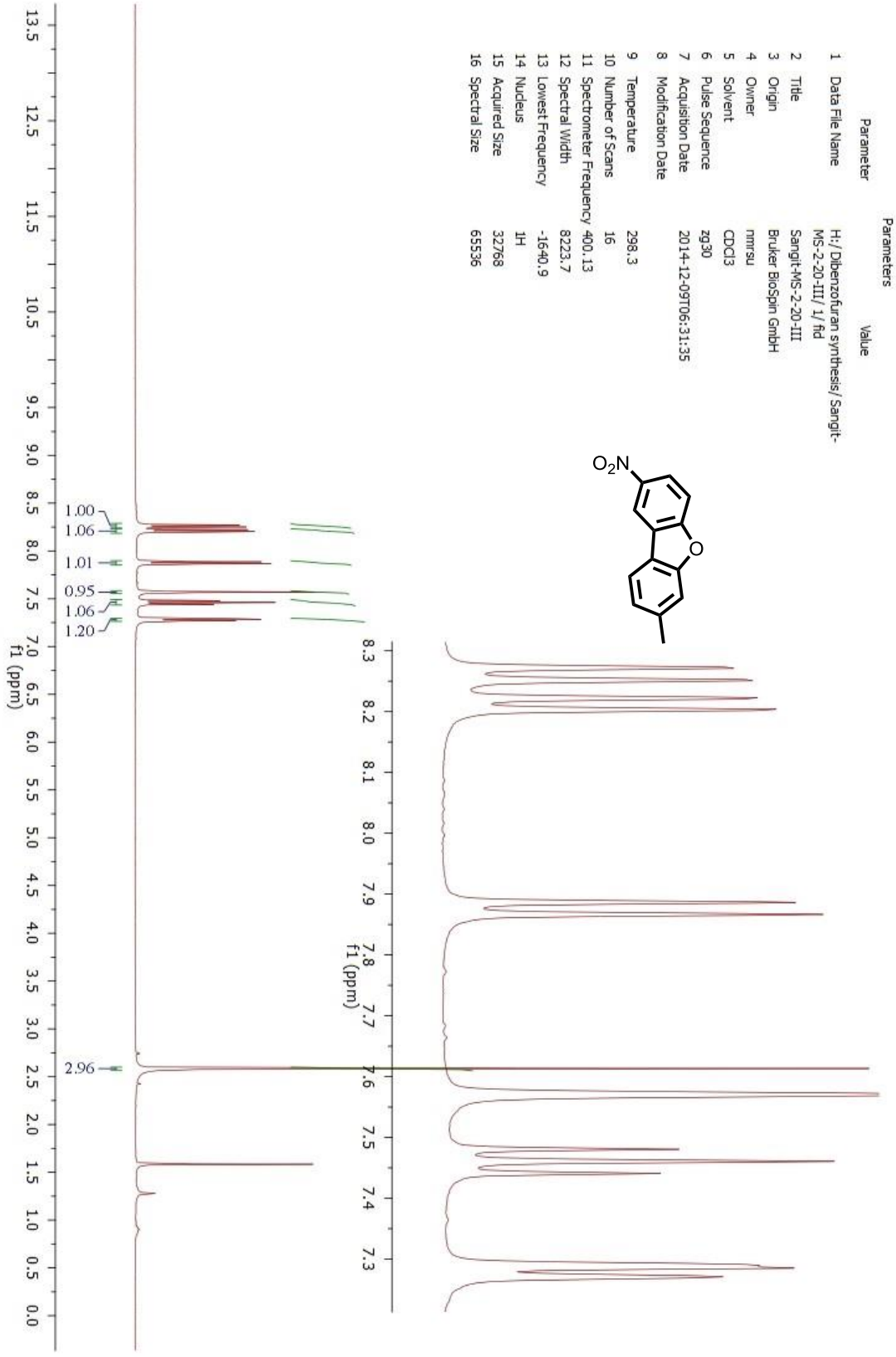

Figure S58 ^{13}C NMR spectrum of **2b'**

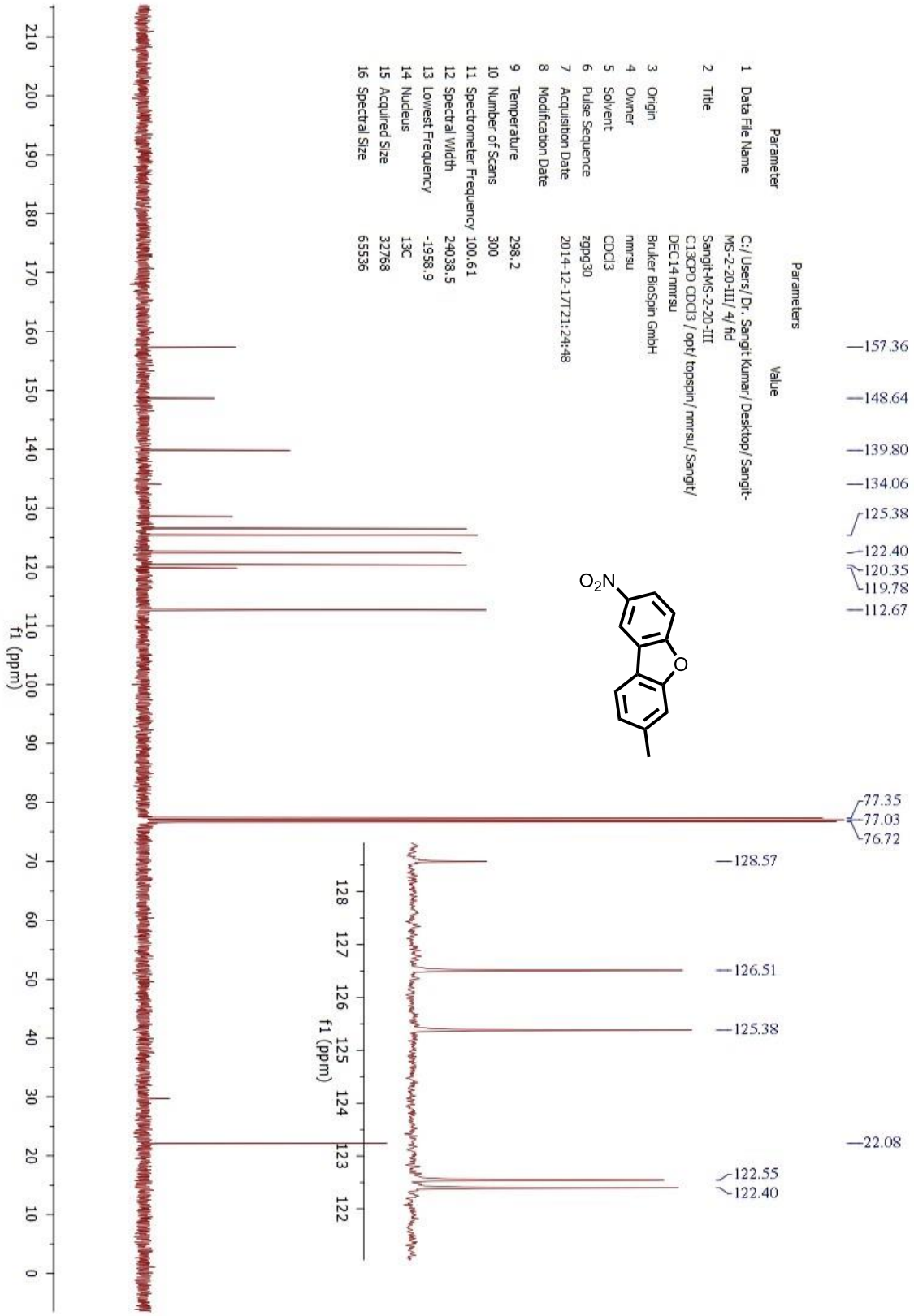

Figure S59 ^{1}H NMR spectrum of **2c**

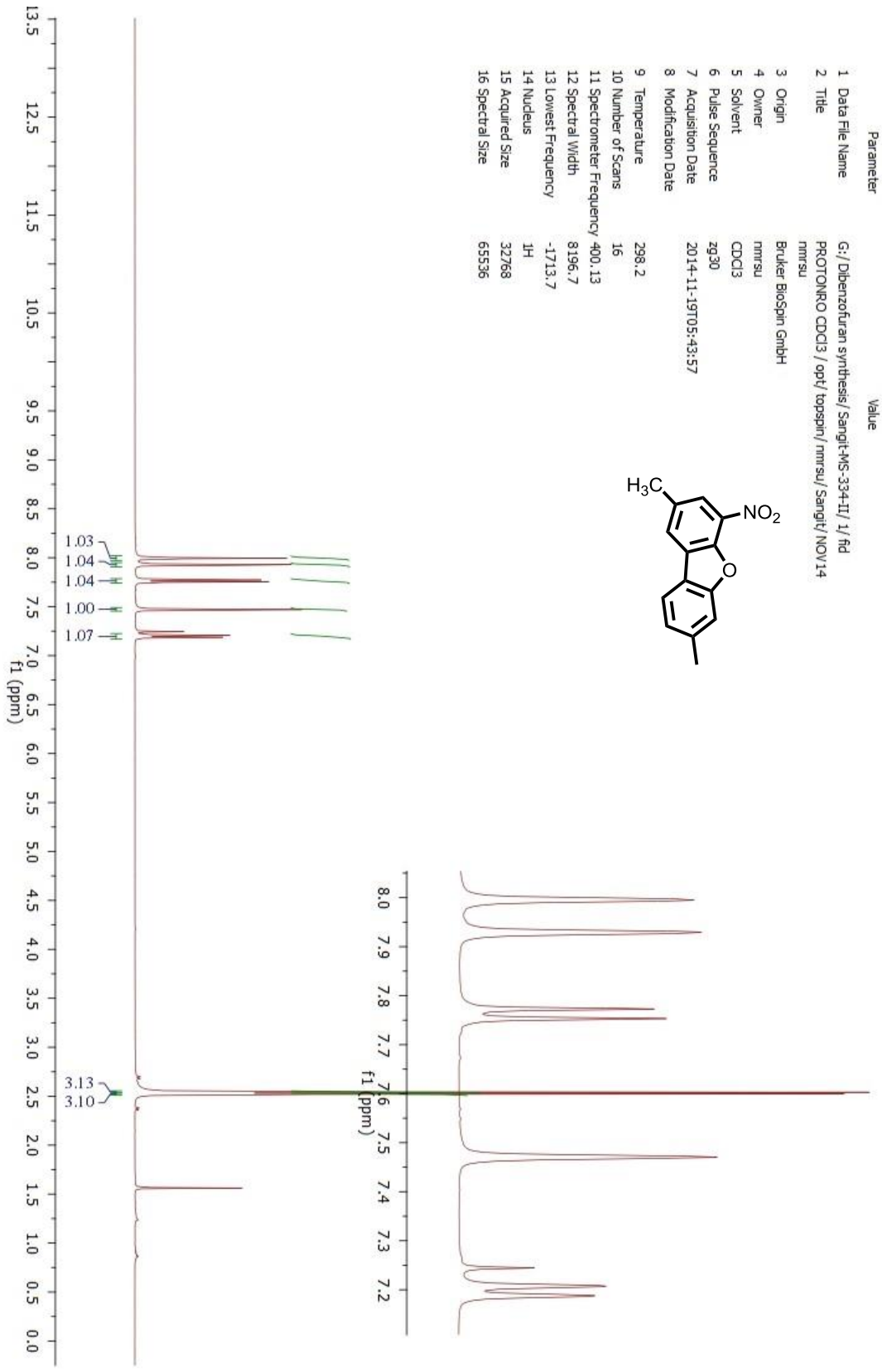

Figure S60 ^{13}C NMR spectrum of **2c**

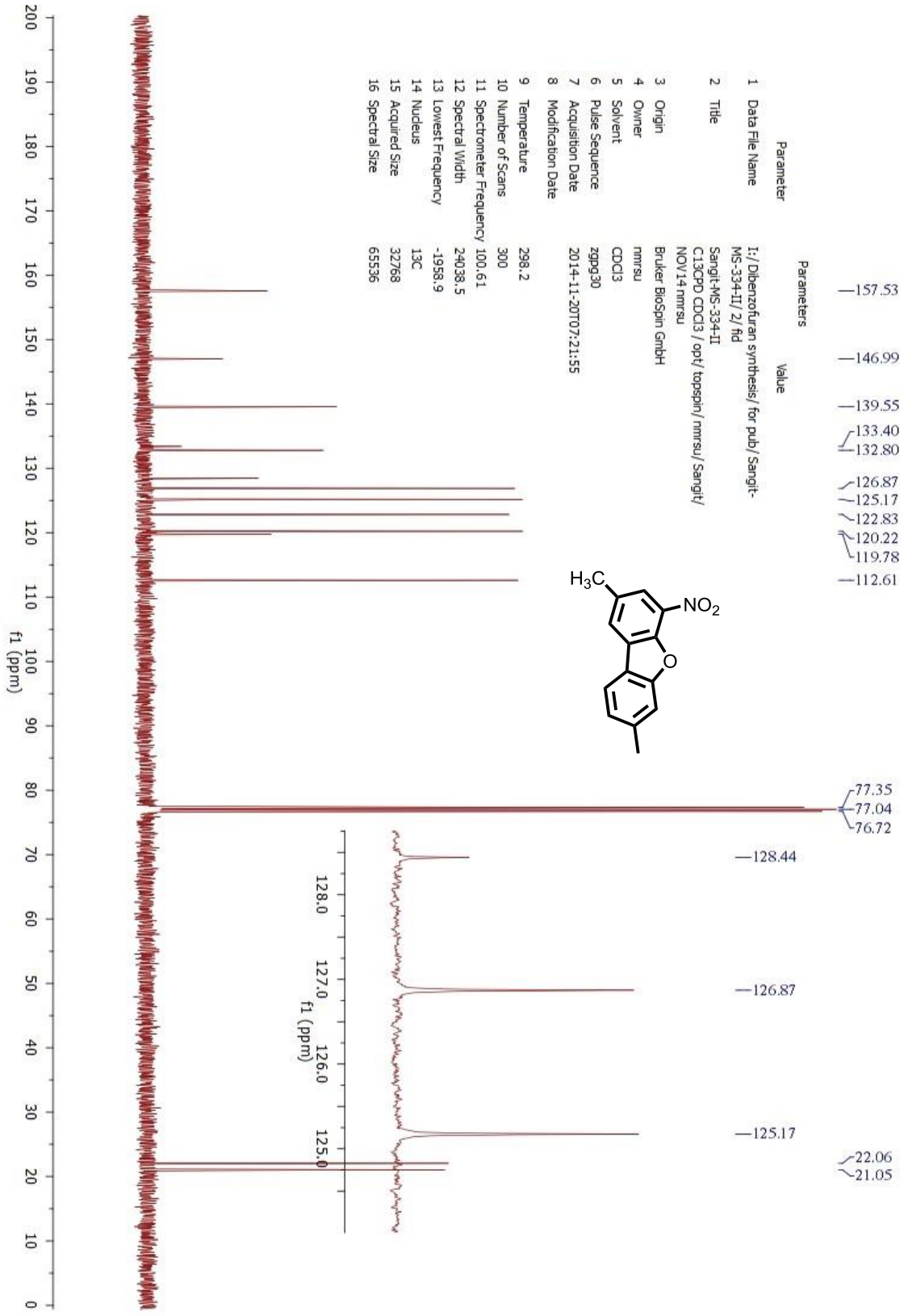

Figure S61 ^{1}H NMR spectrum of **2d**

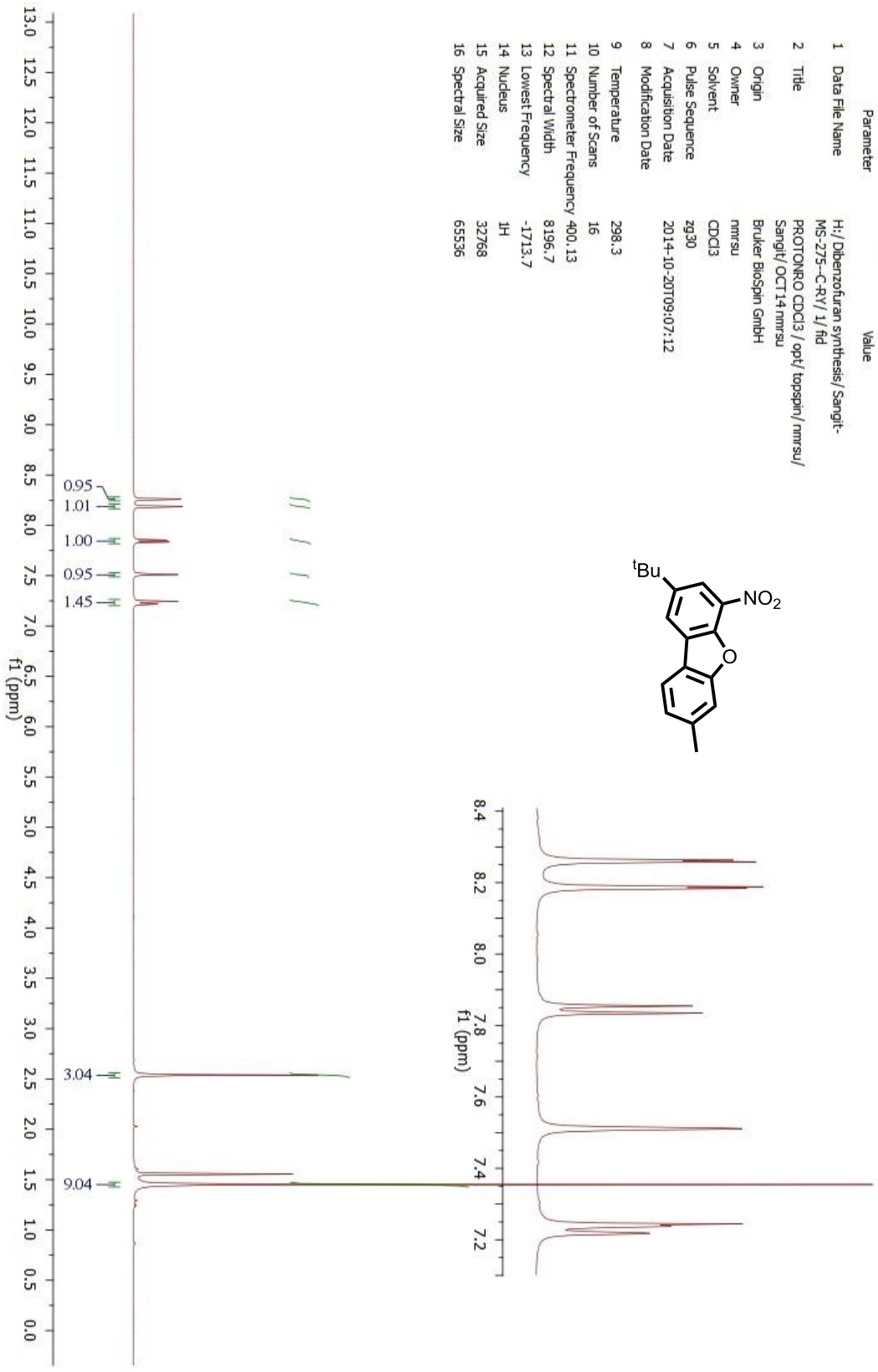

Figure S62 ^{13}C NMR spectrum of **2d**

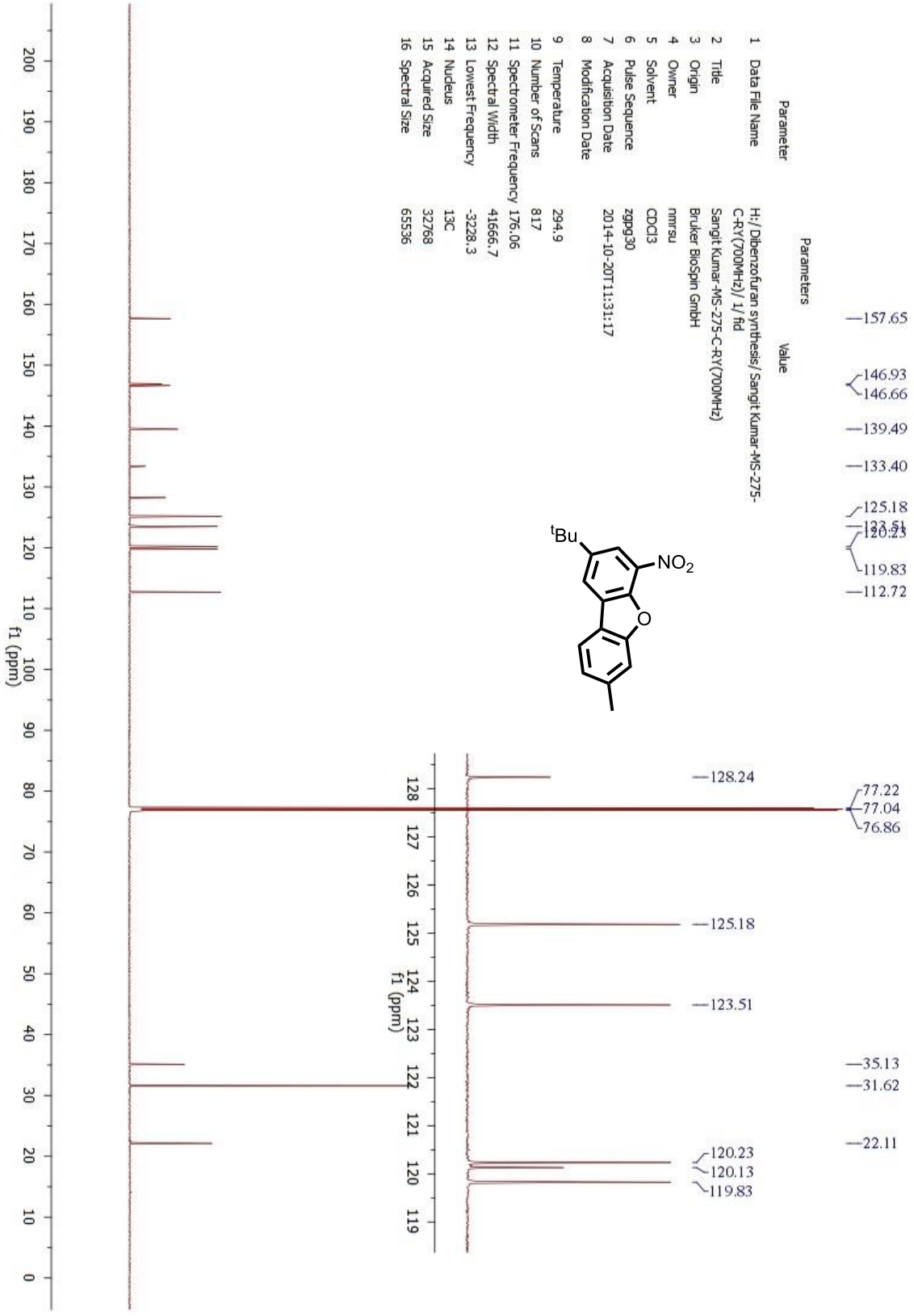

Figure S63 ^{1}H NMR spectrum of **2e**

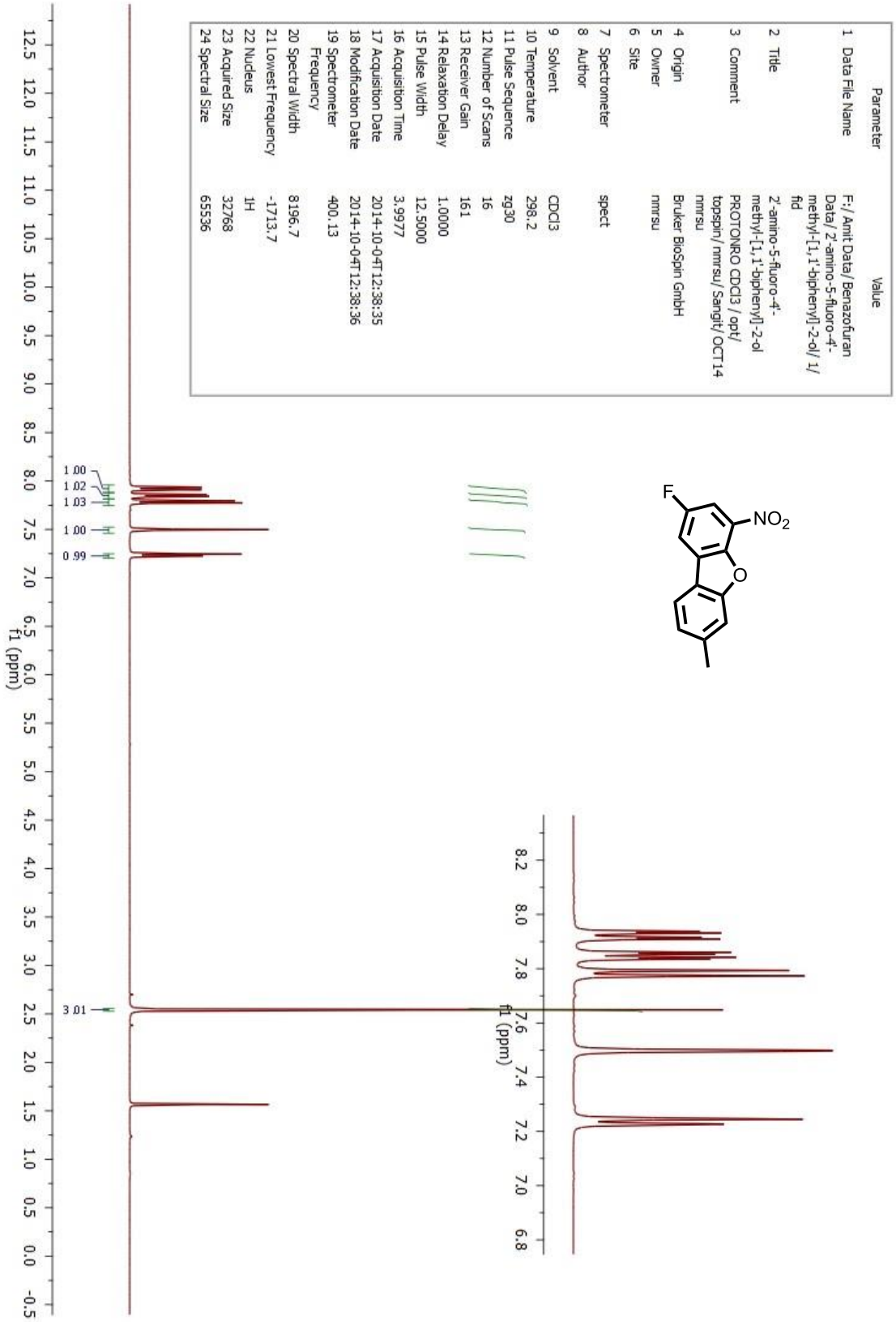

Figure S64 ^{13}C NMR spectrum of **2e**

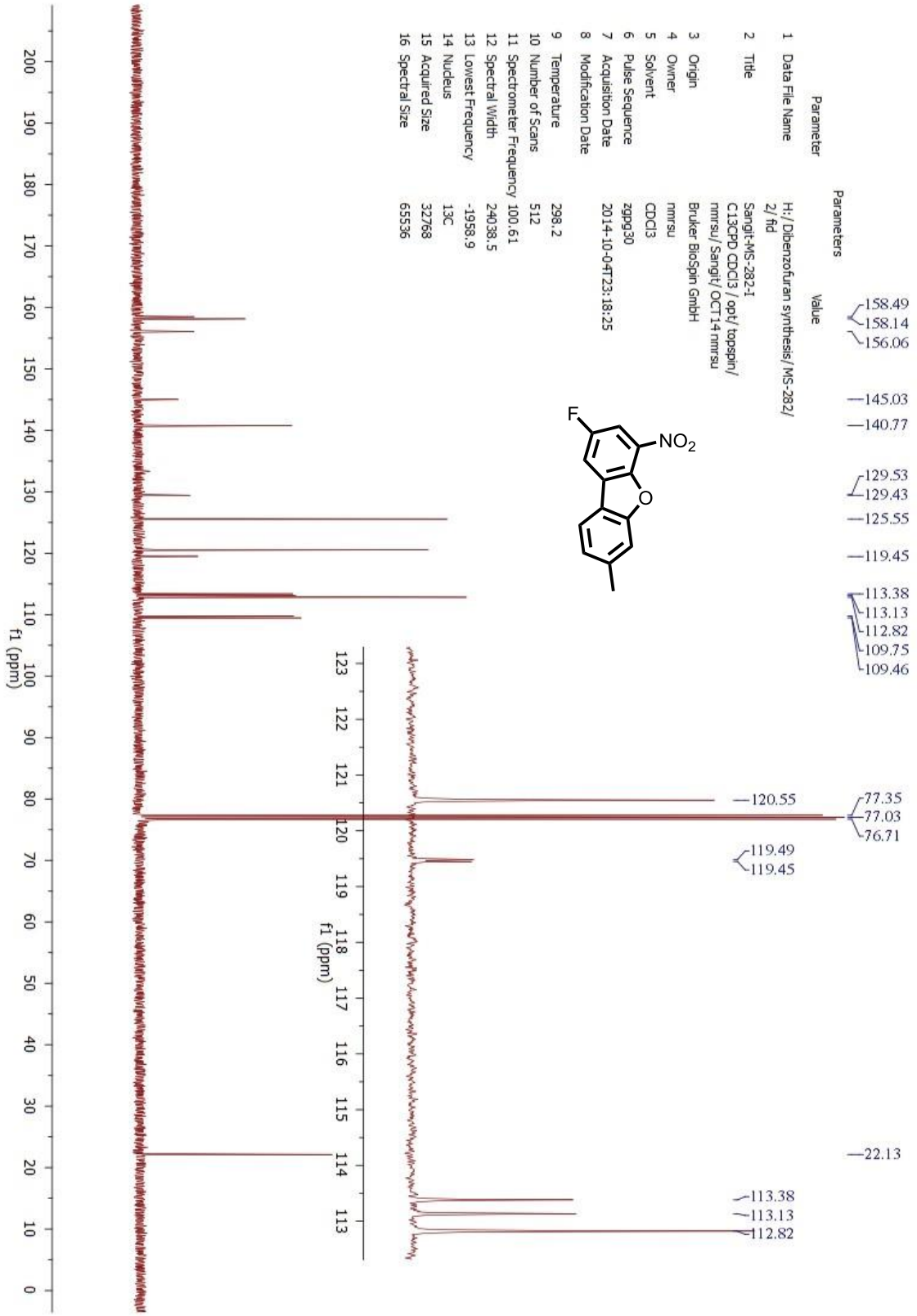

Figure S65 ^{1}H NMR spectrum of **2f**

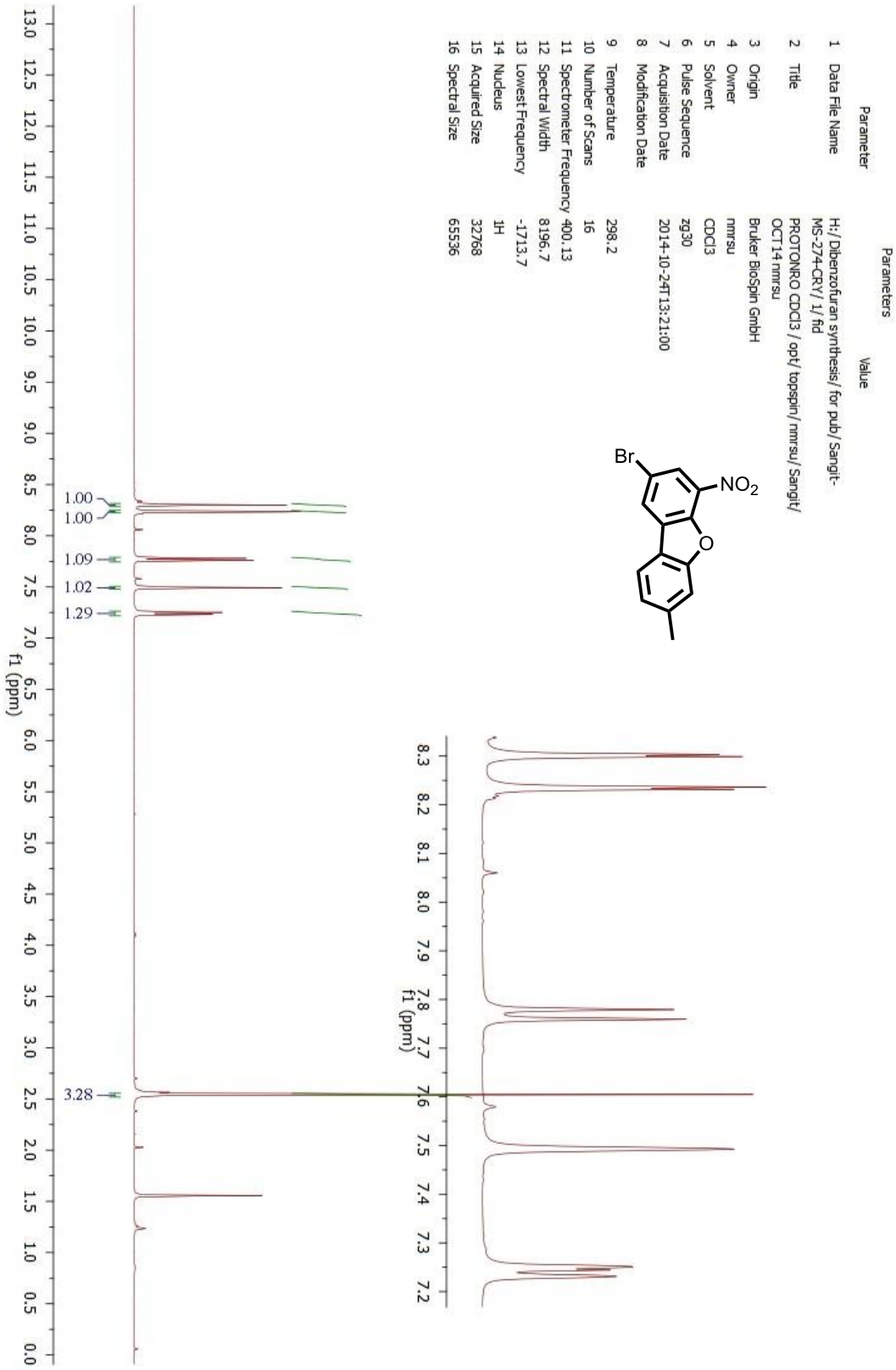

Figure S66 ^{13}C NMR spectrum of **2f**

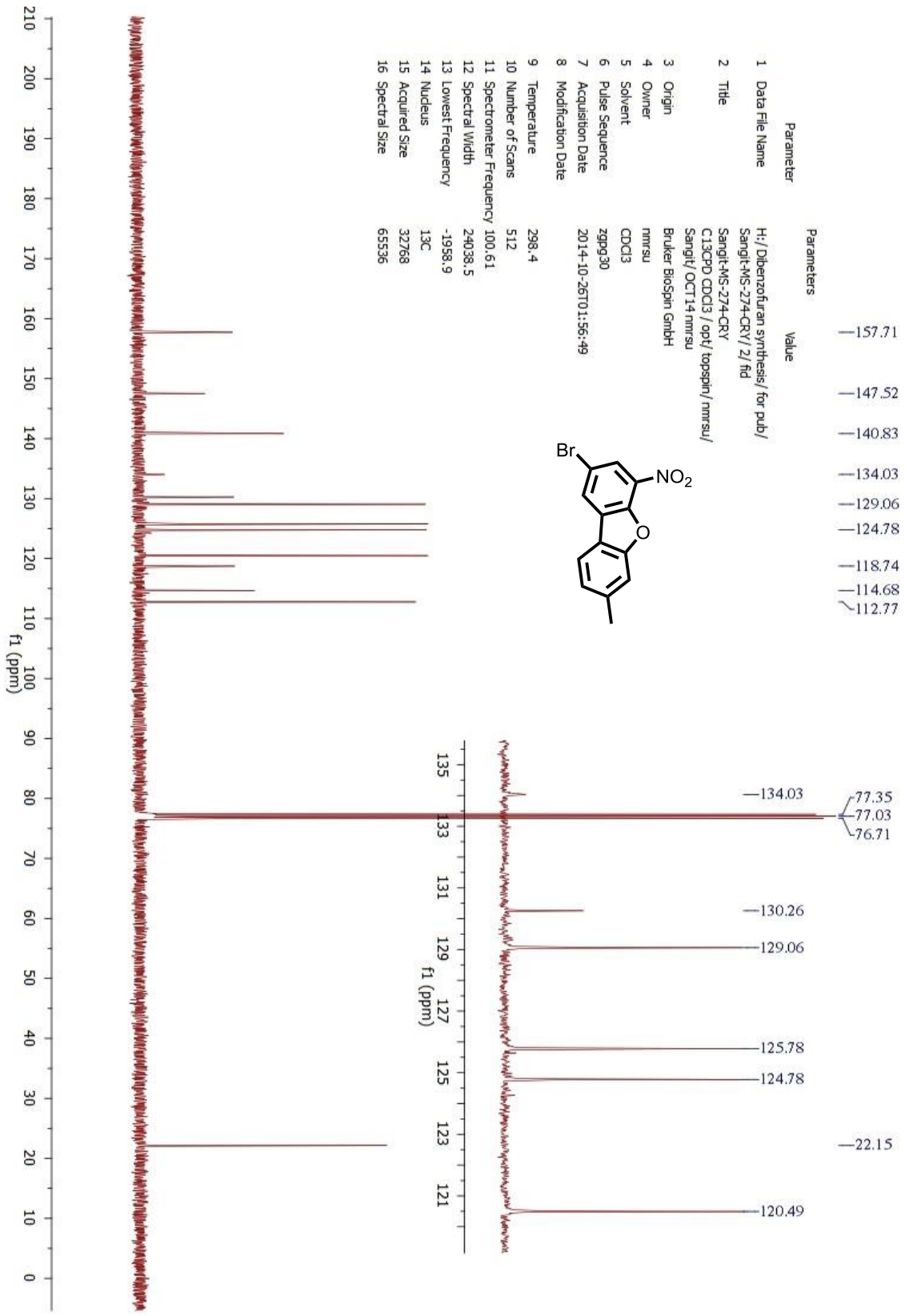

Figure S67 ^{1}H NMR spectrum of **2g**

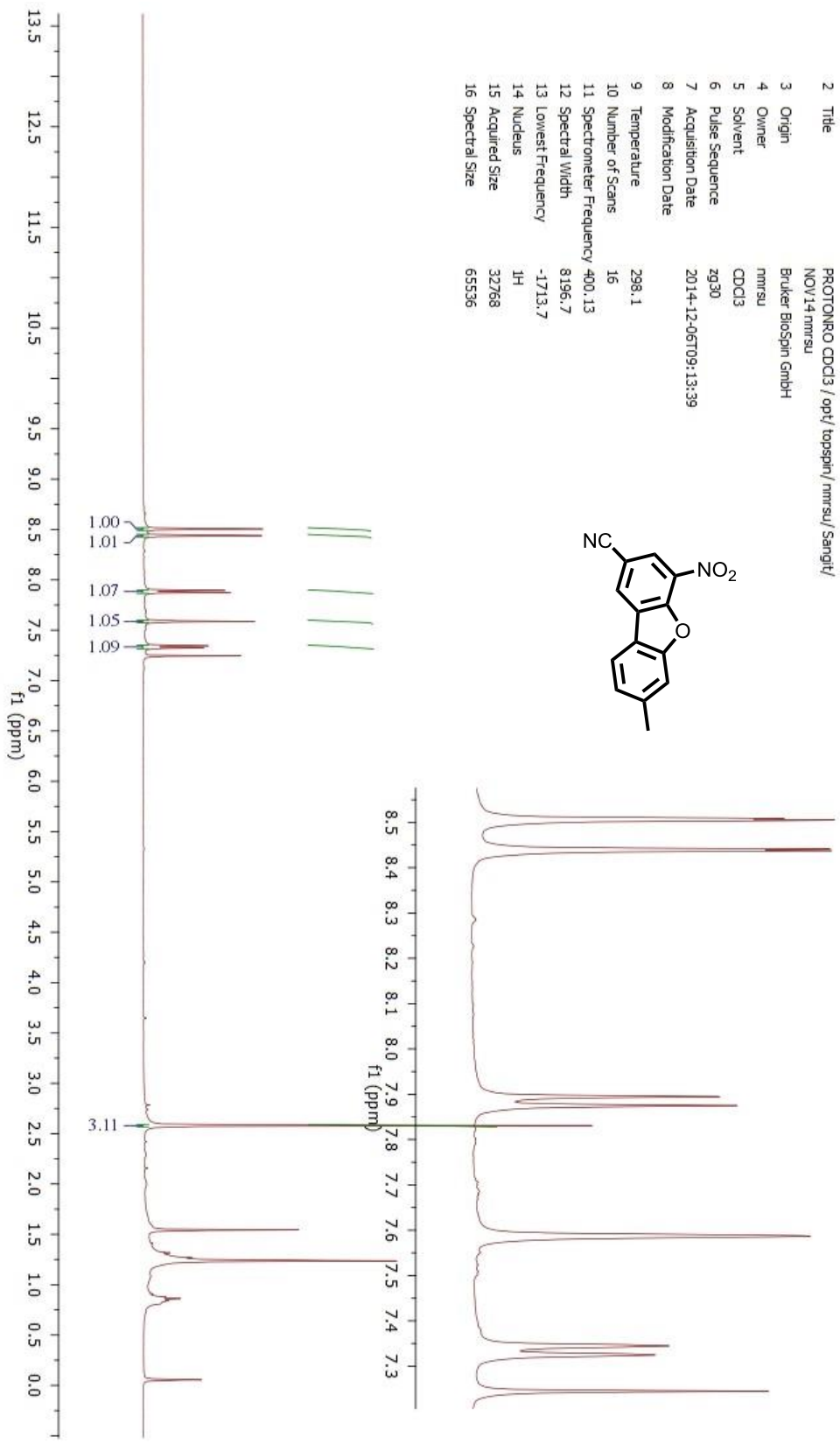

Figure S68 ^{13}C NMR spectrum of **2g**

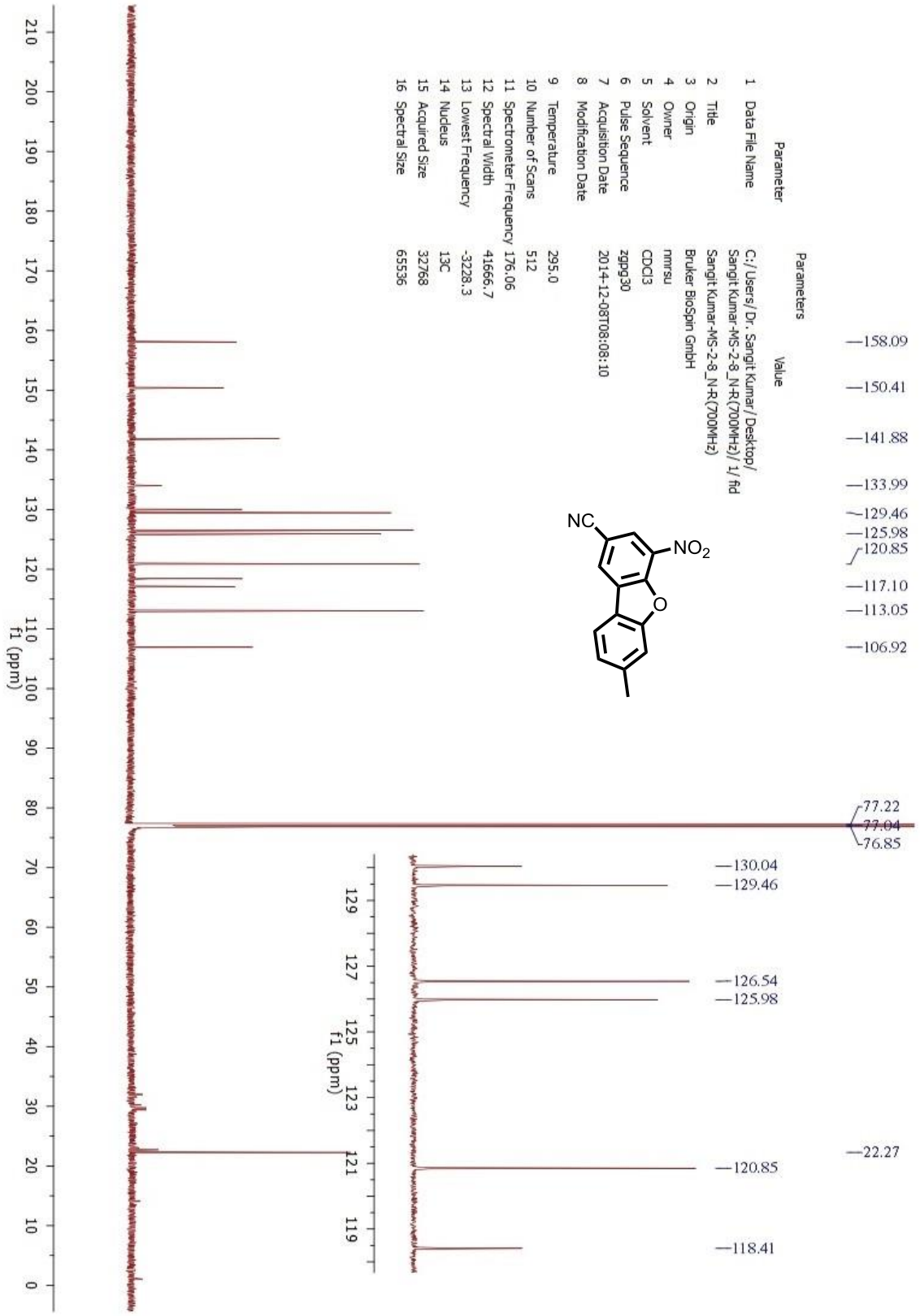

Figure S69 ^{1}H NMR spectrum of **2h**

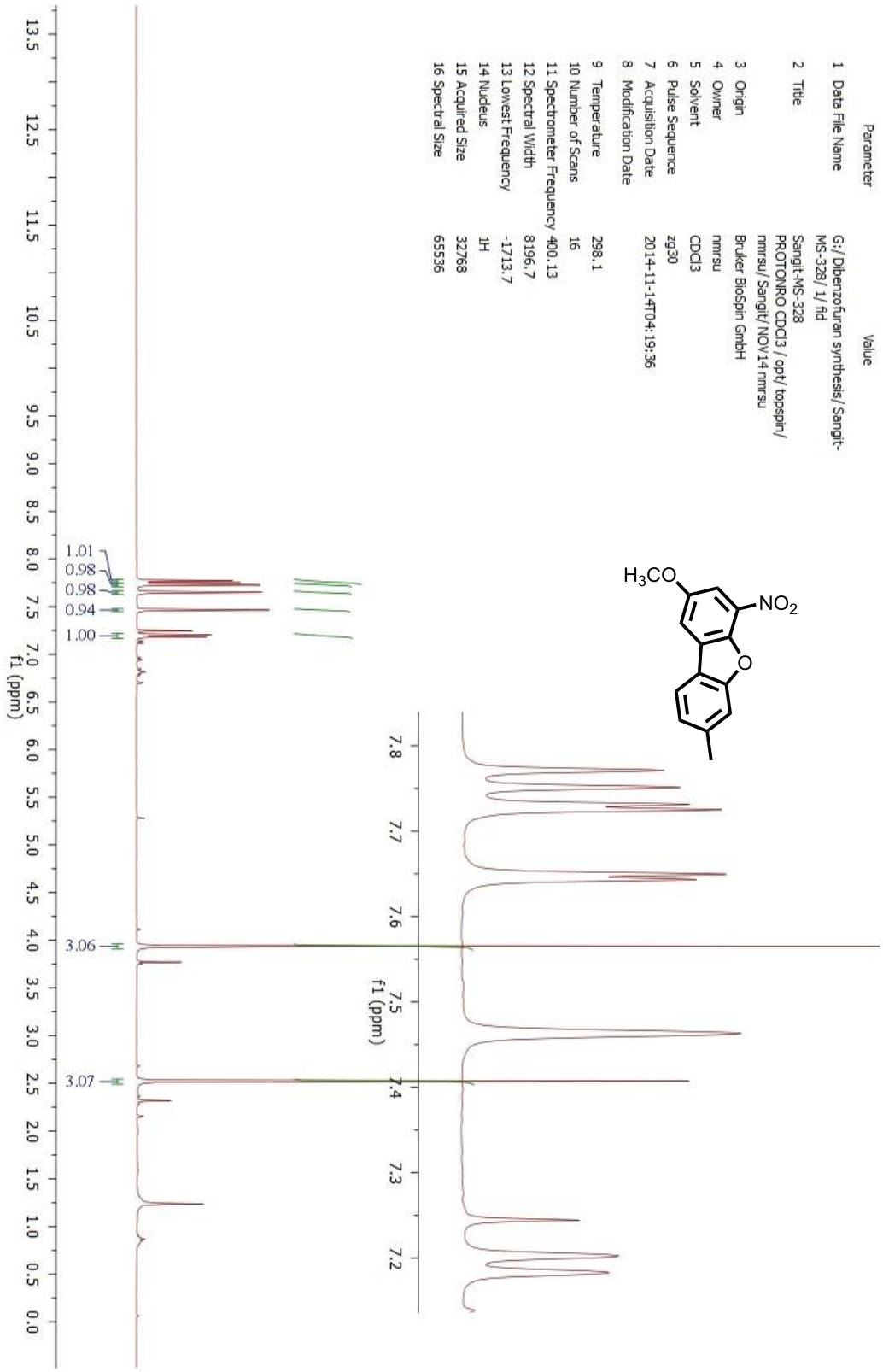

Figure S70 ^{13}C NMR spectrum of **2h**

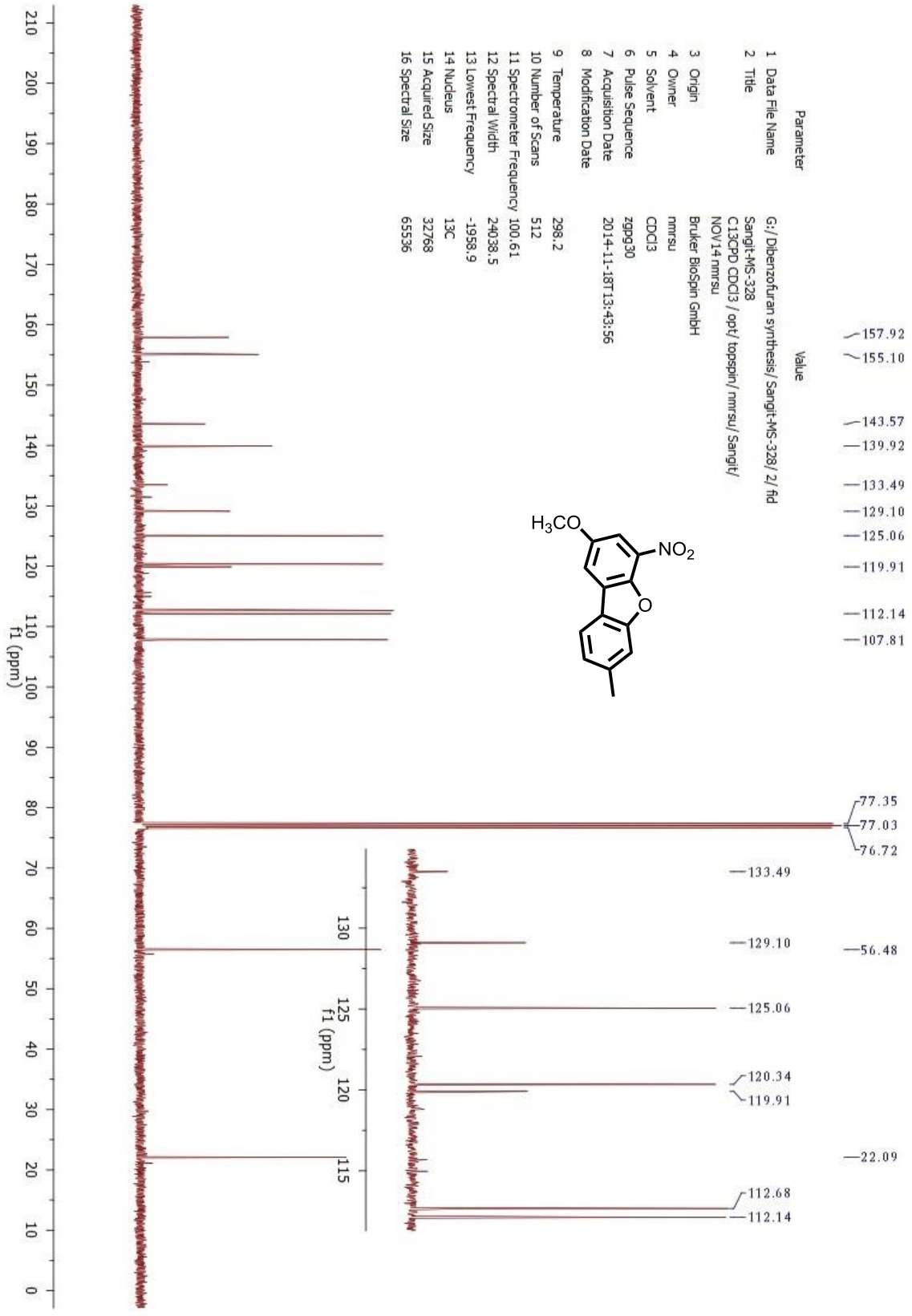

Figure S71 ^{1}H NMR spectrum of **2i**

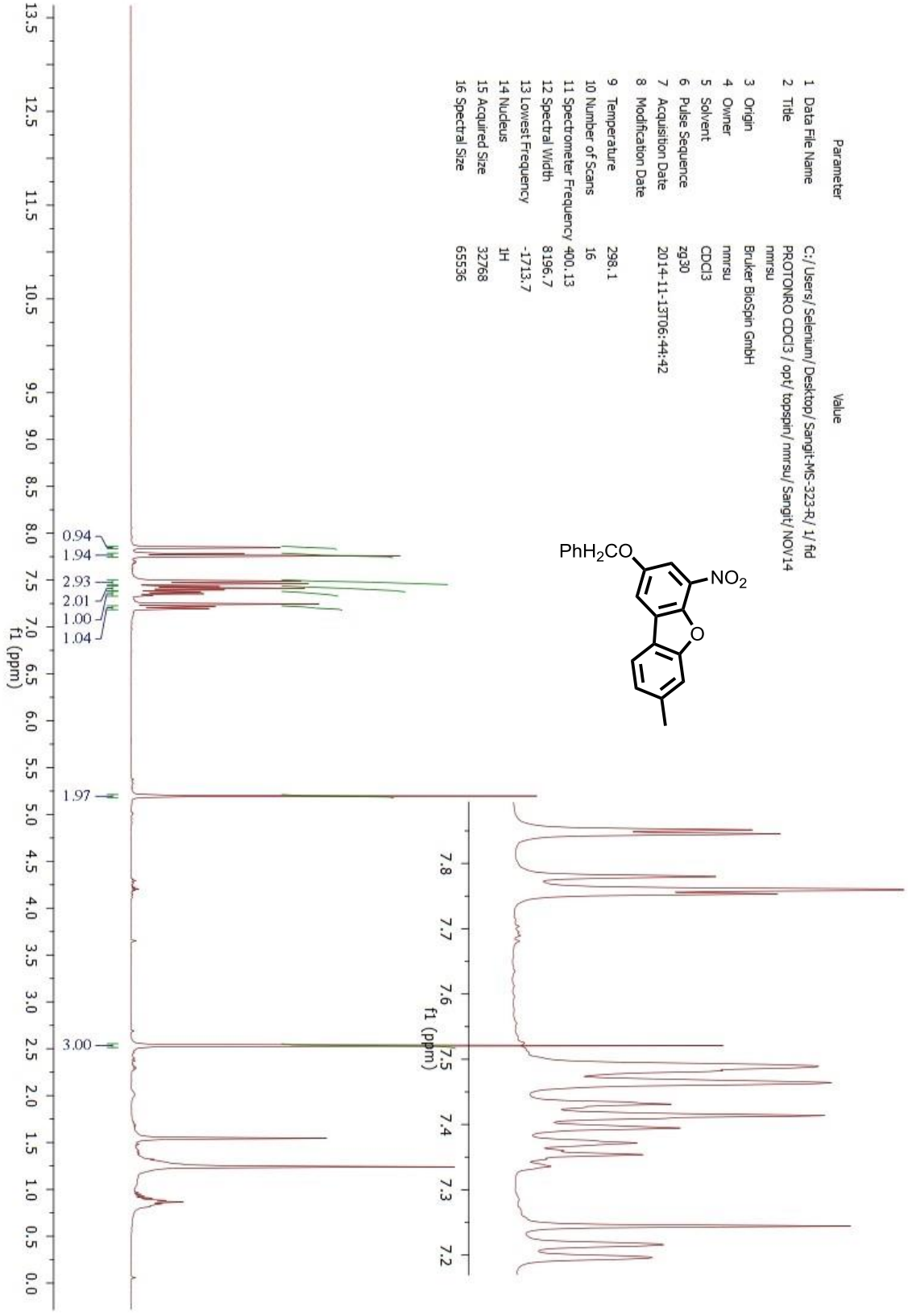

Figure S72 ^{13}C NMR spectrum of **2i**

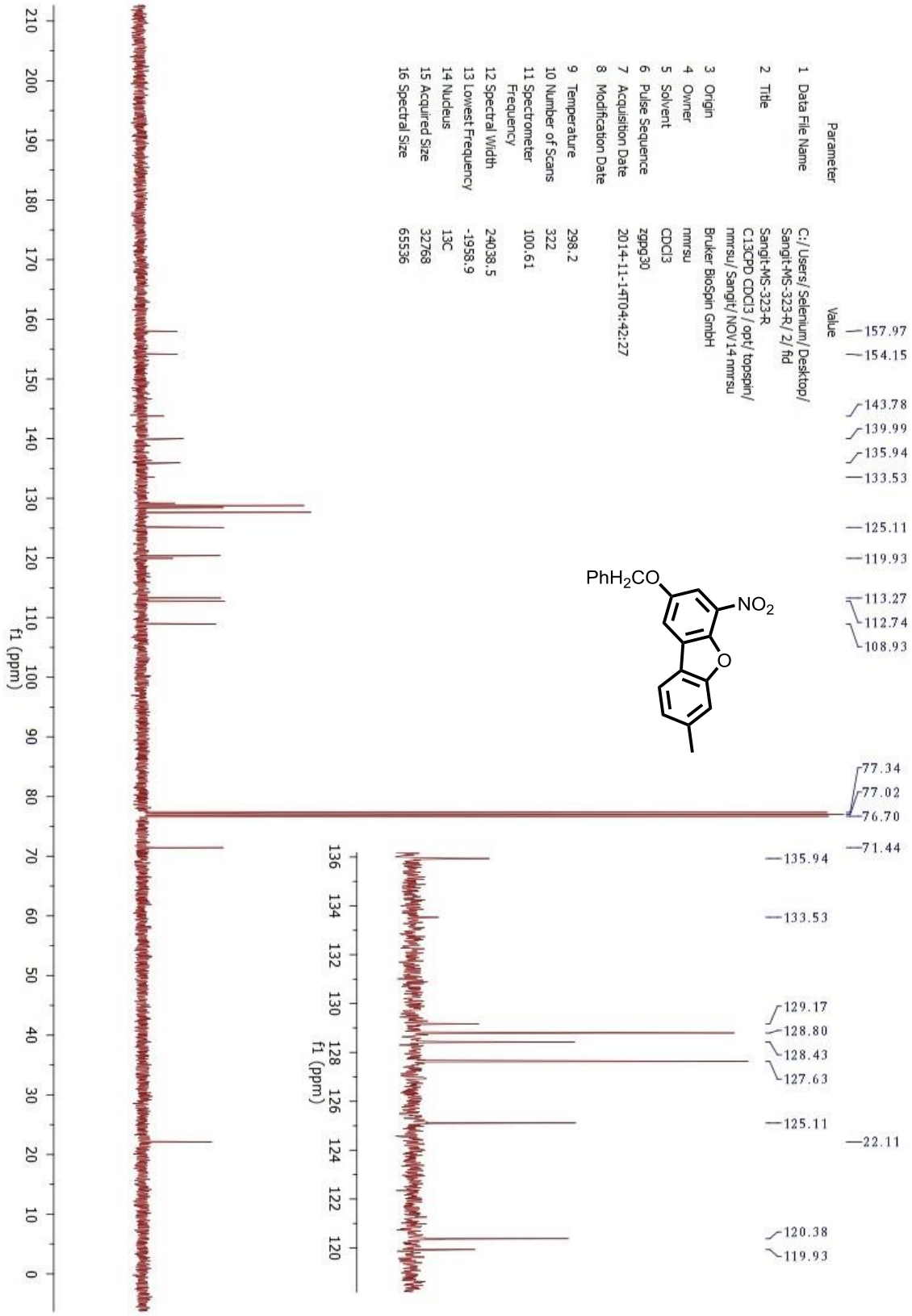

Figure S73 ^{1}H NMR spectrum of **2j**

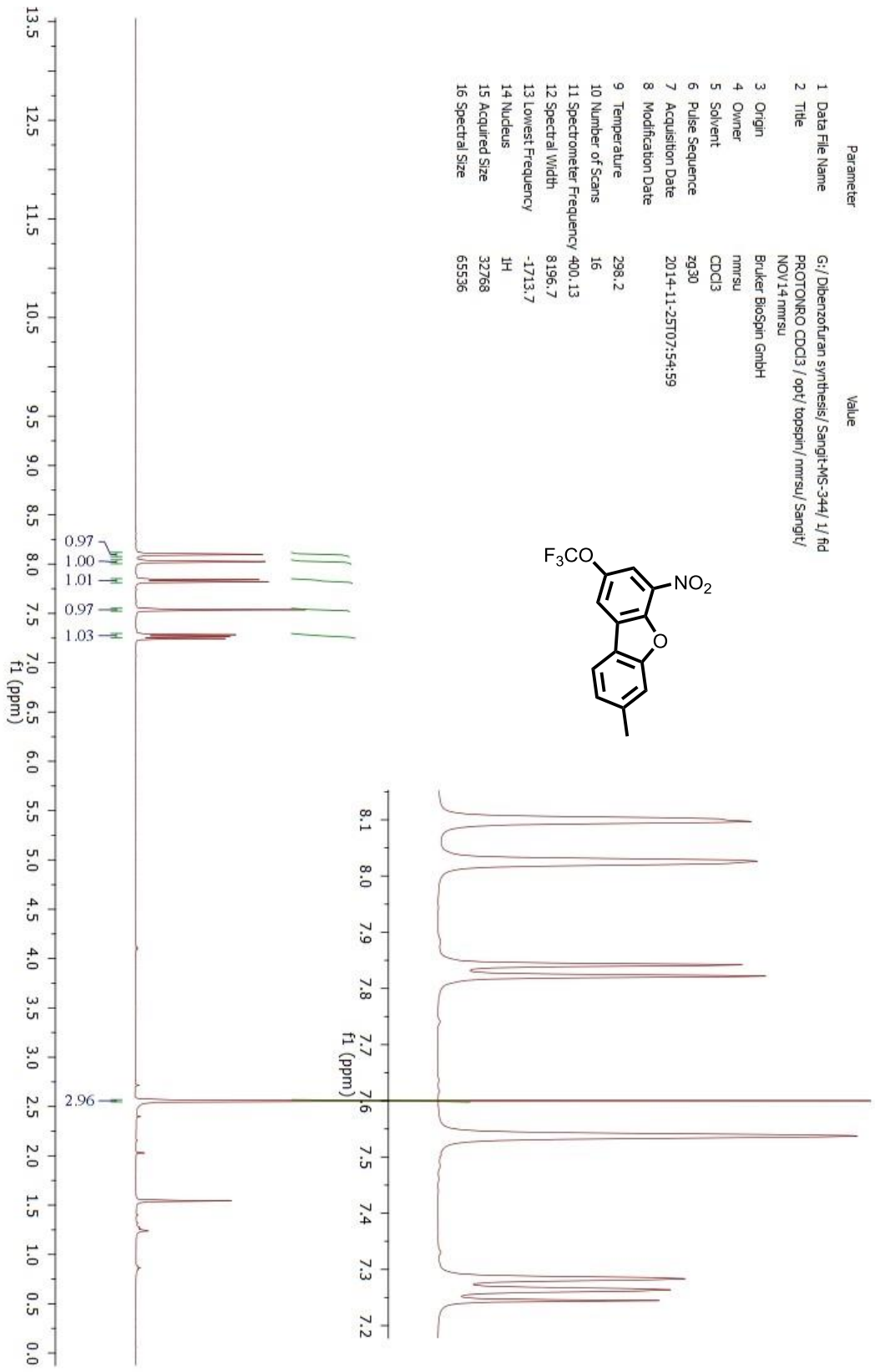

Figure S74 ^{13}C NMR spectrum of **2j**

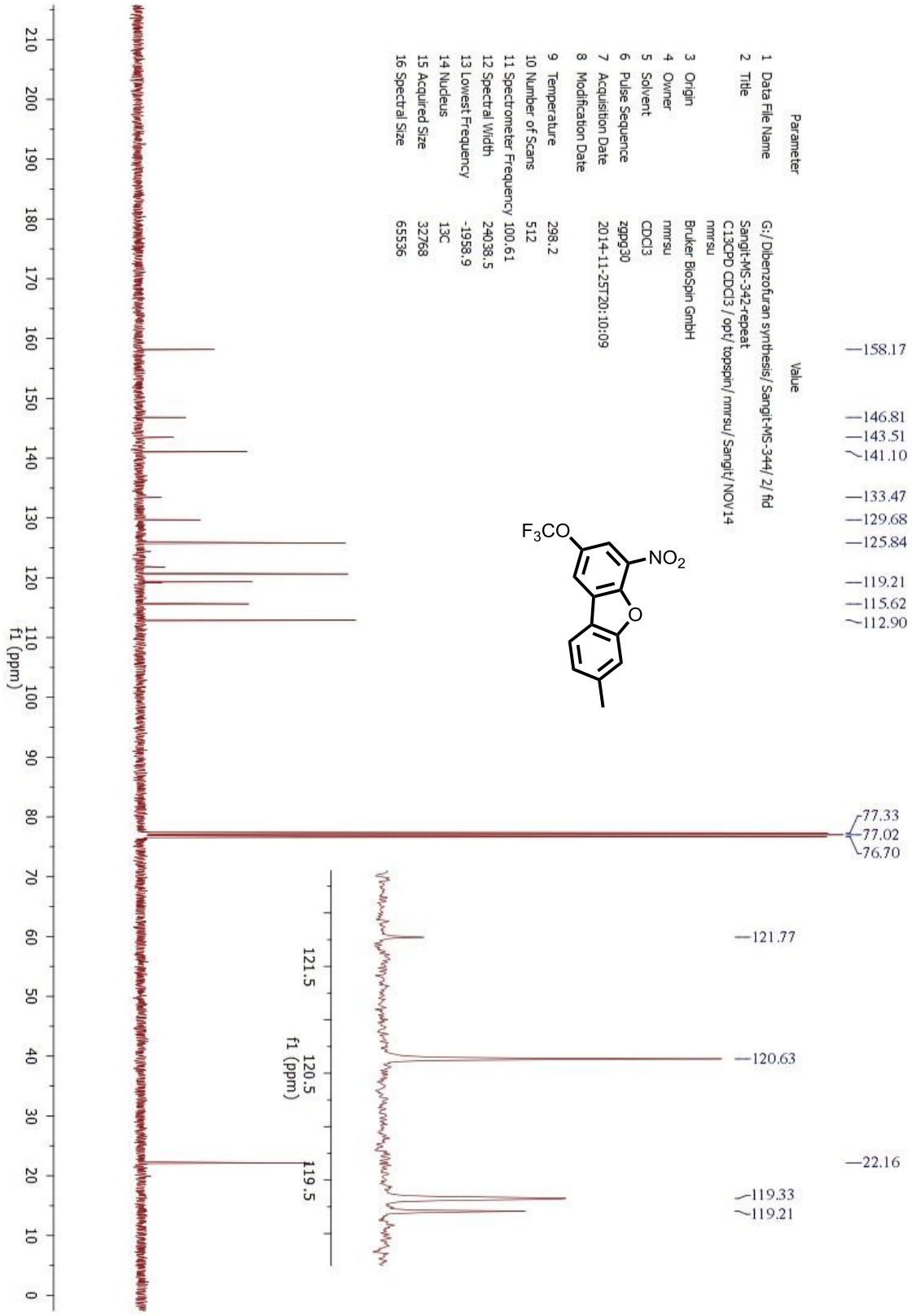

Figure S75 ^{1}H NMR spectrum of **2k**

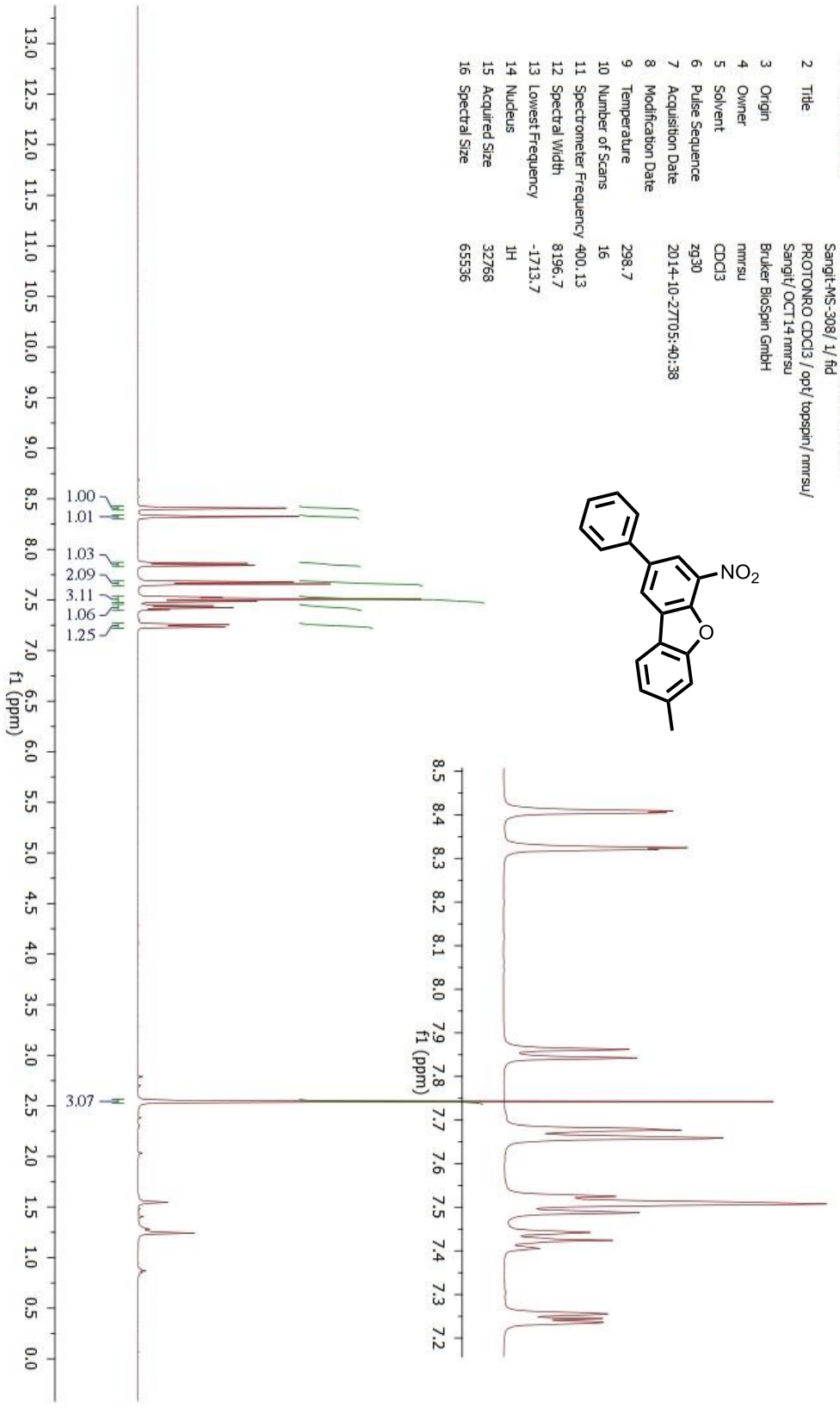

Figure S76 ^{13}C NMR spectrum of **2k**

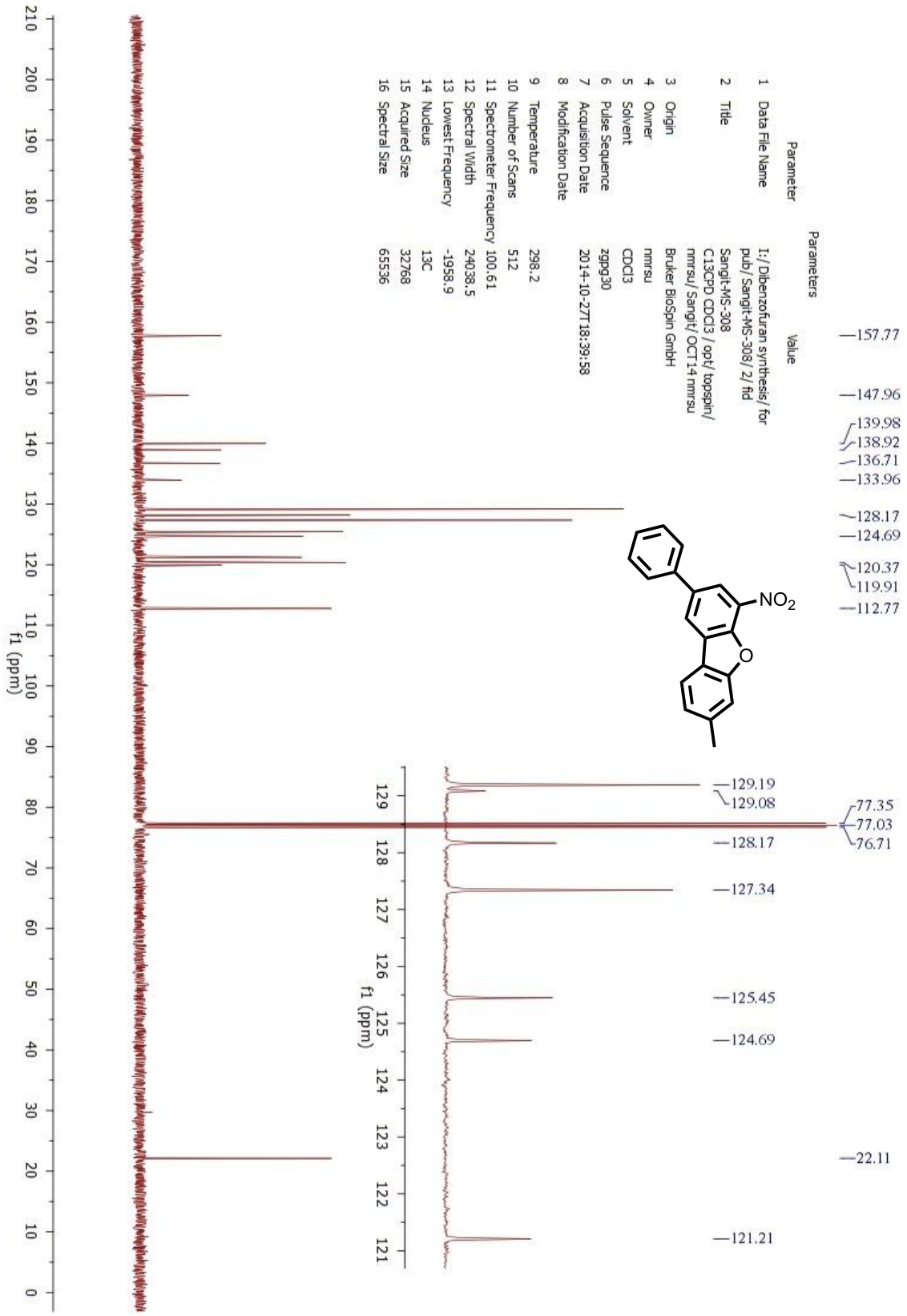

Figure S77 ^{1}H NMR spectrum of **2l**

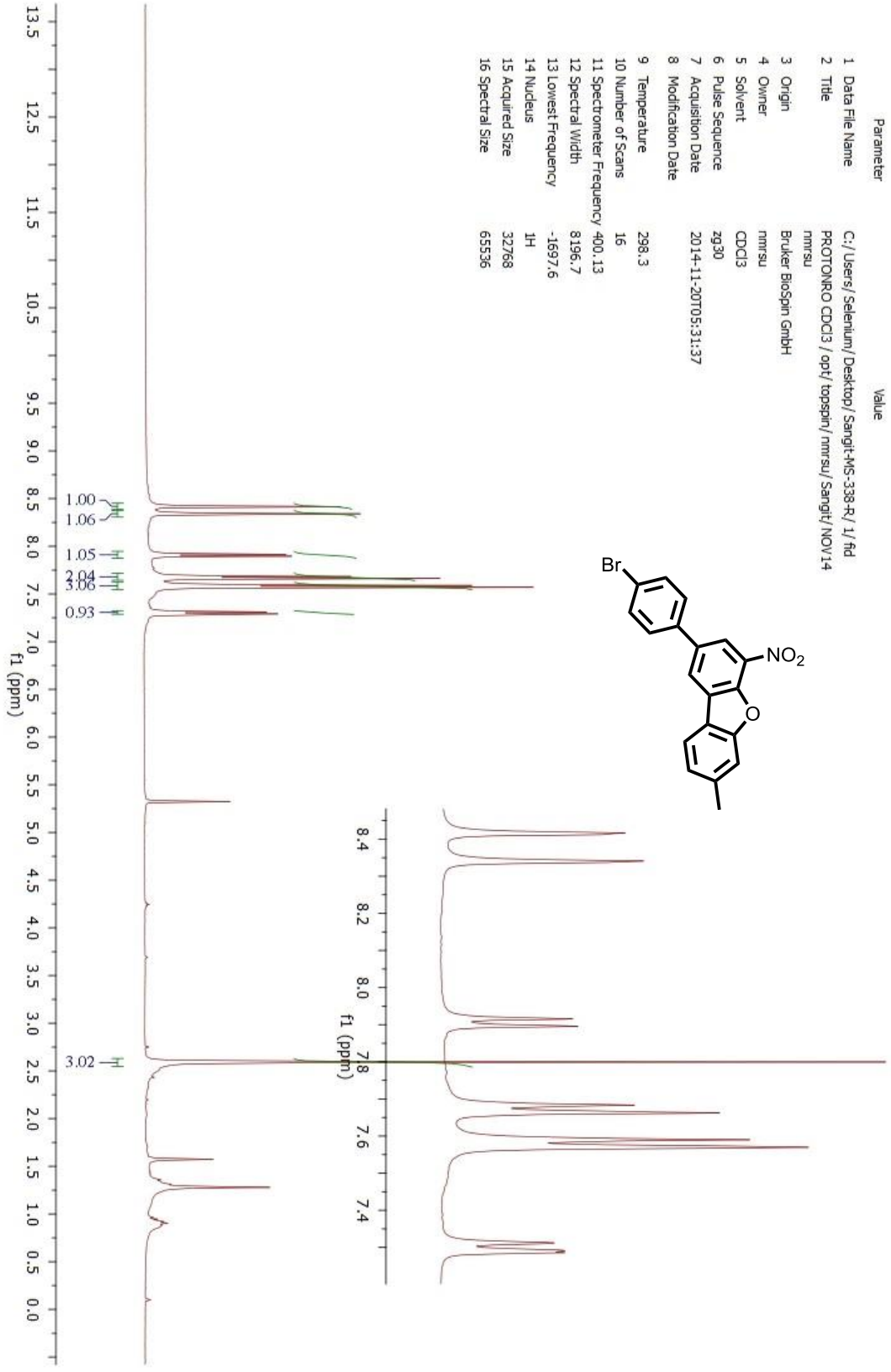

Figure S78 ^{13}C NMR spectrum of **2l**

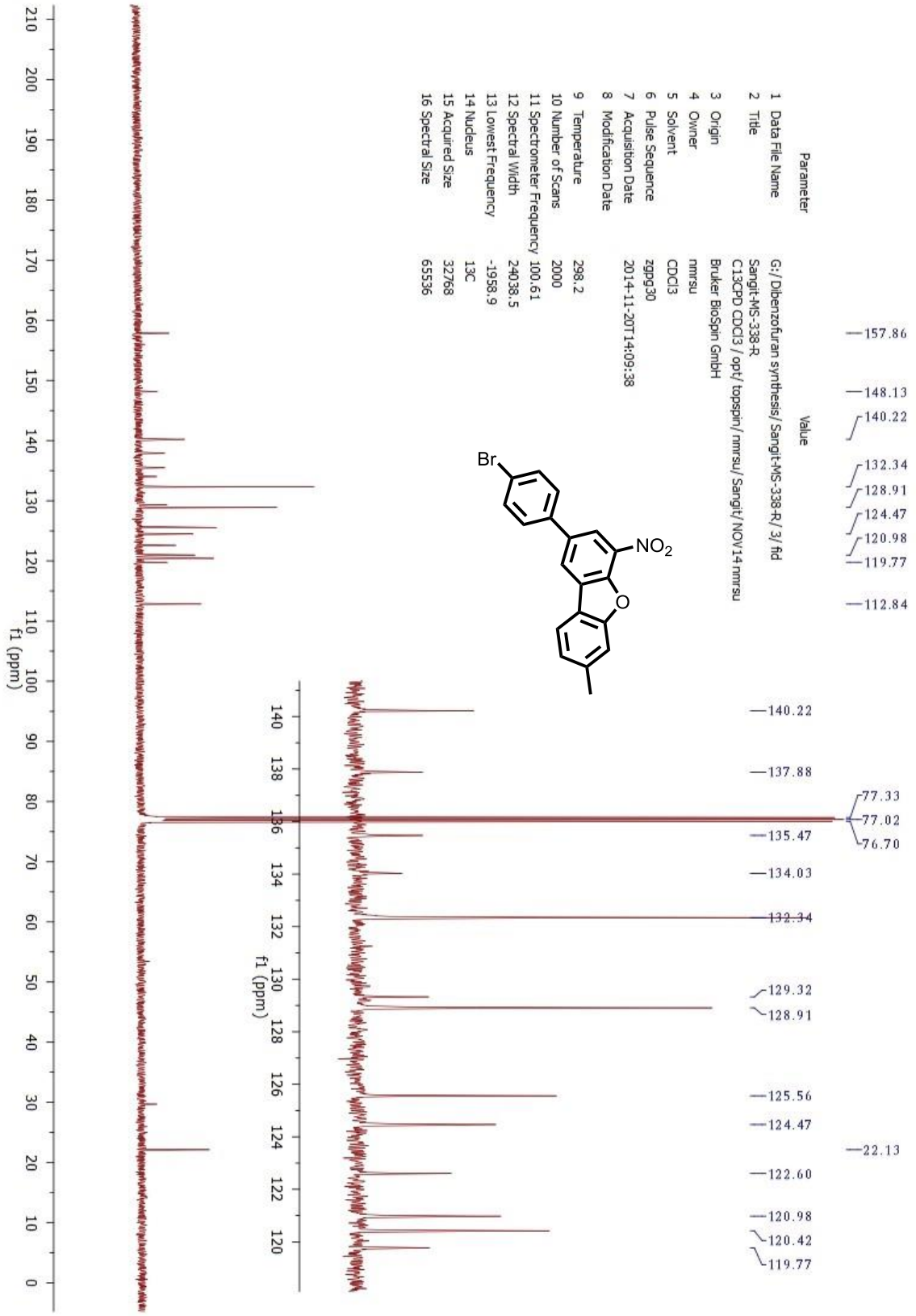

Figure S79 ^{1}H NMR spectrum of **2m**

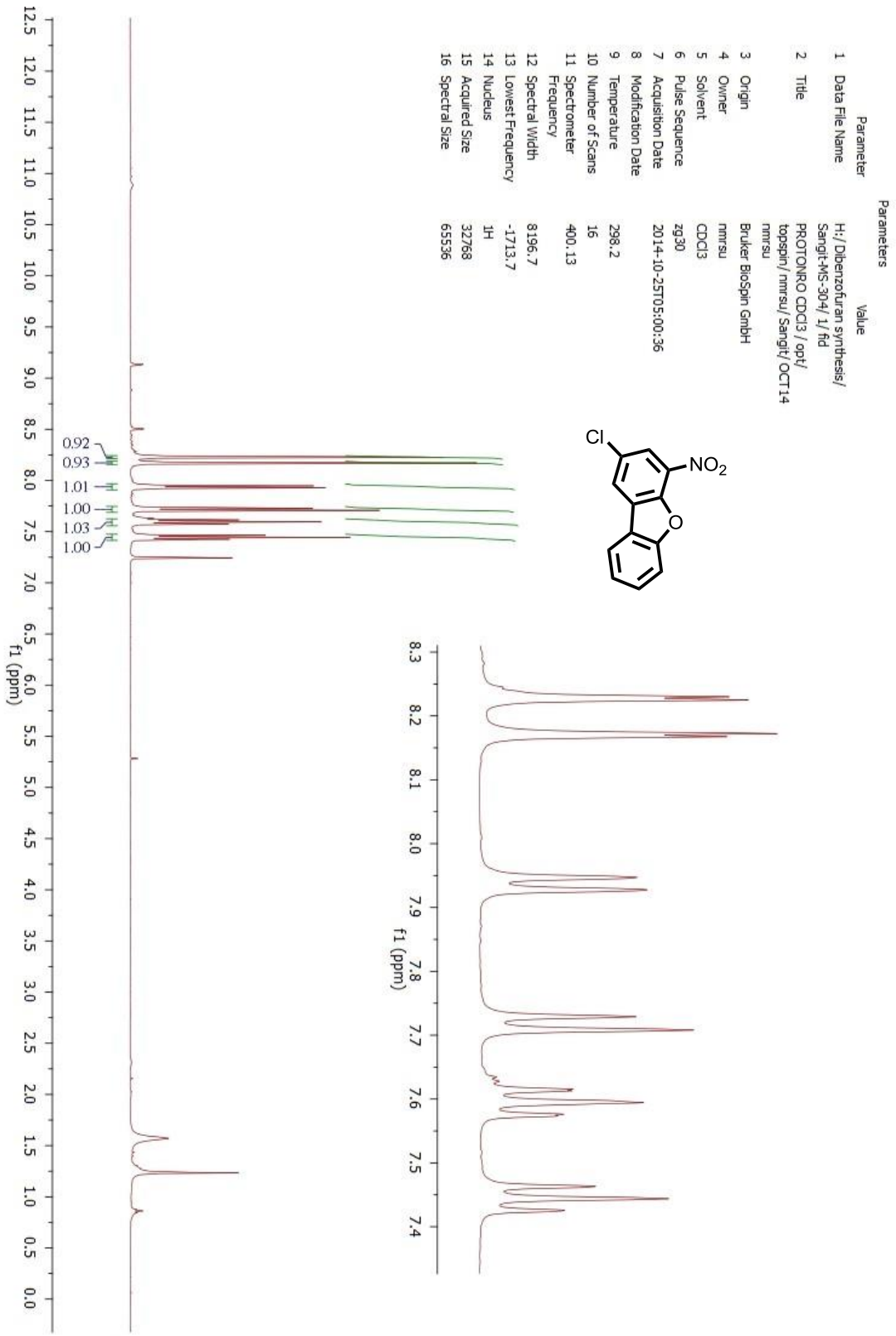

Figure S80 ^{13}C NMR spectrum of **2m**

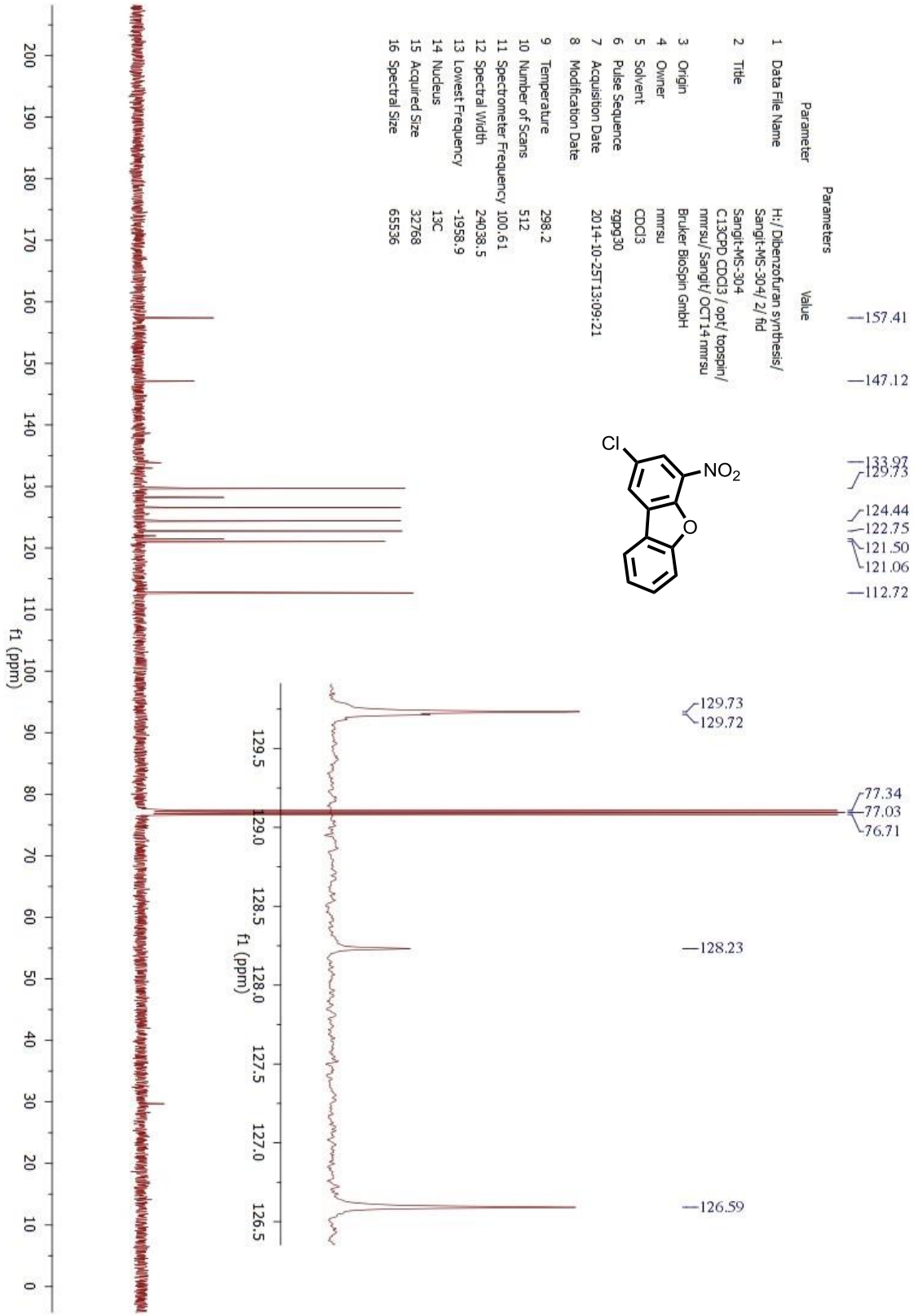

Figure S81 ^{1}H NMR spectrum of **2n**

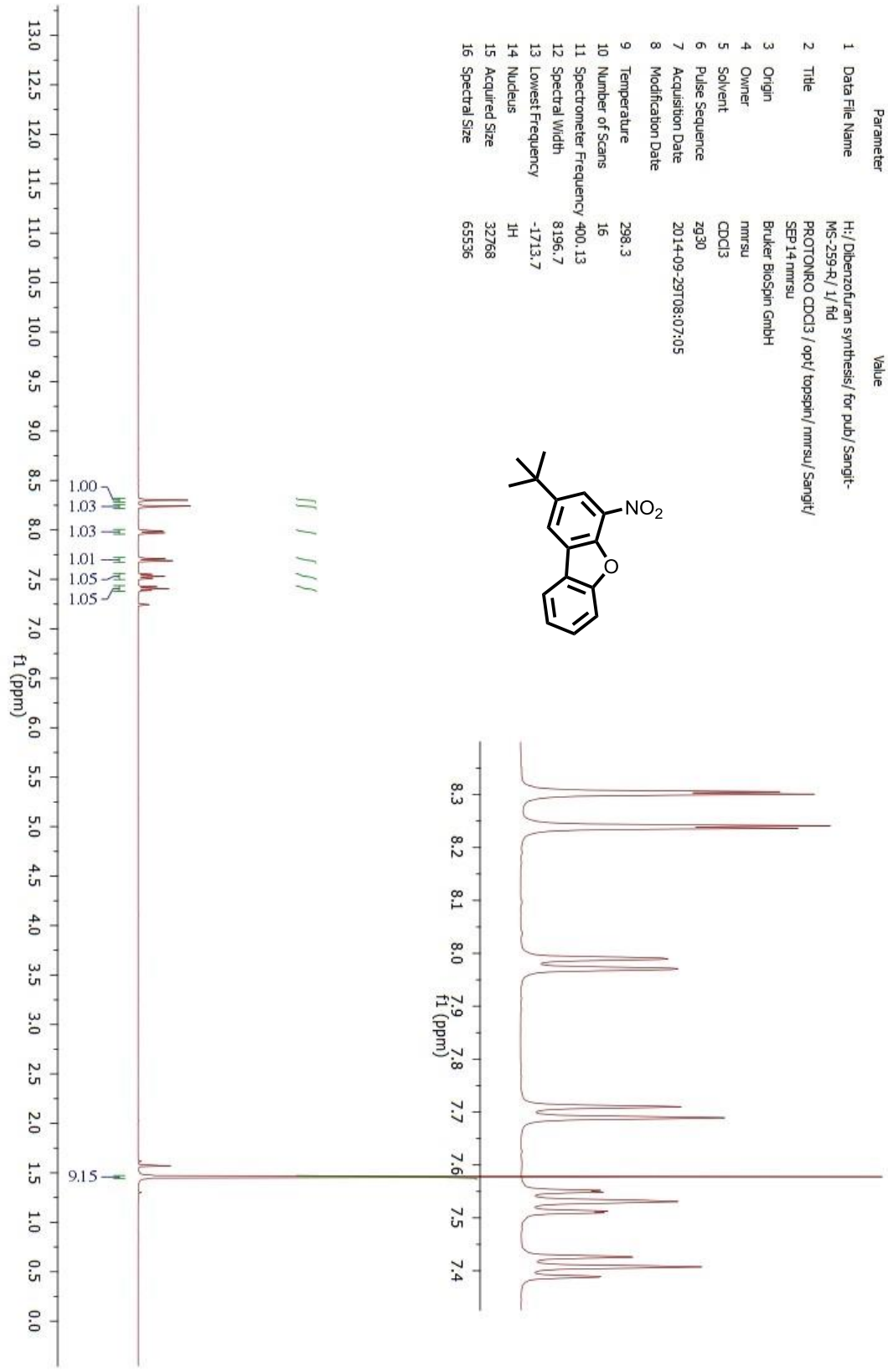

Figure S82 ^{13}C NMR spectrum of **2n**

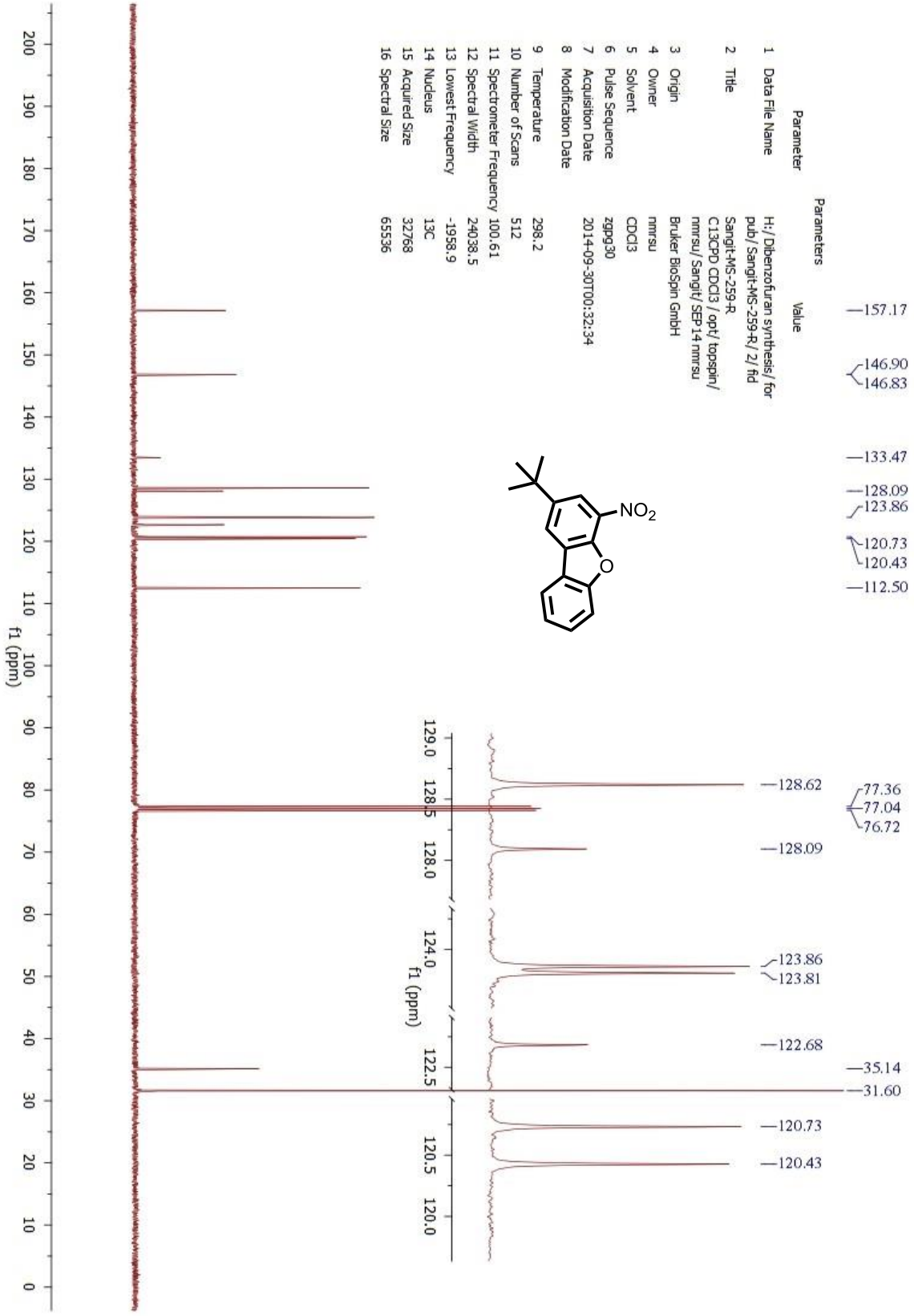

Figure S83 ^{1}H NMR spectrum of **2o**

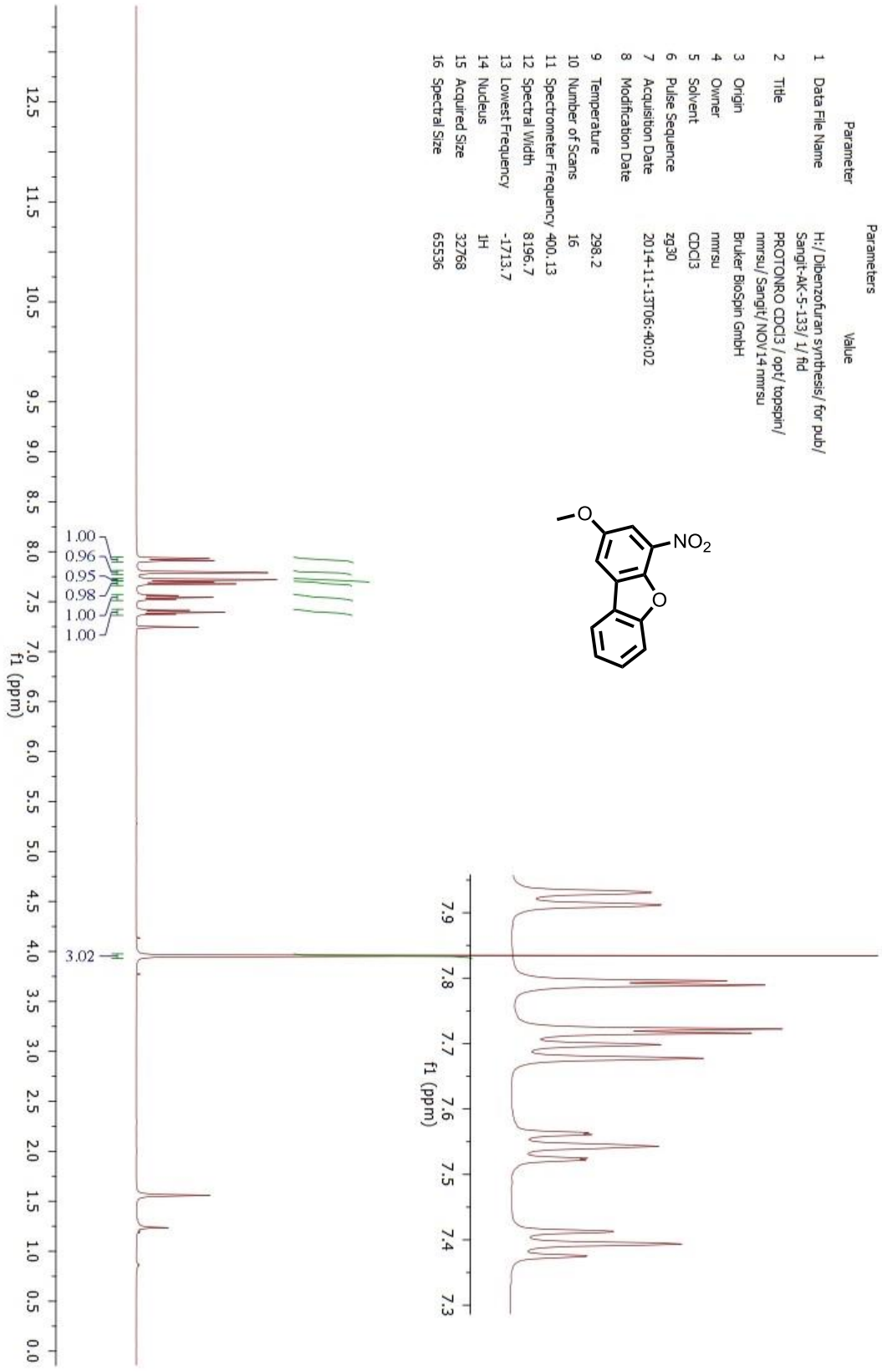

Figure S84 ^{13}C NMR spectrum of **2o**

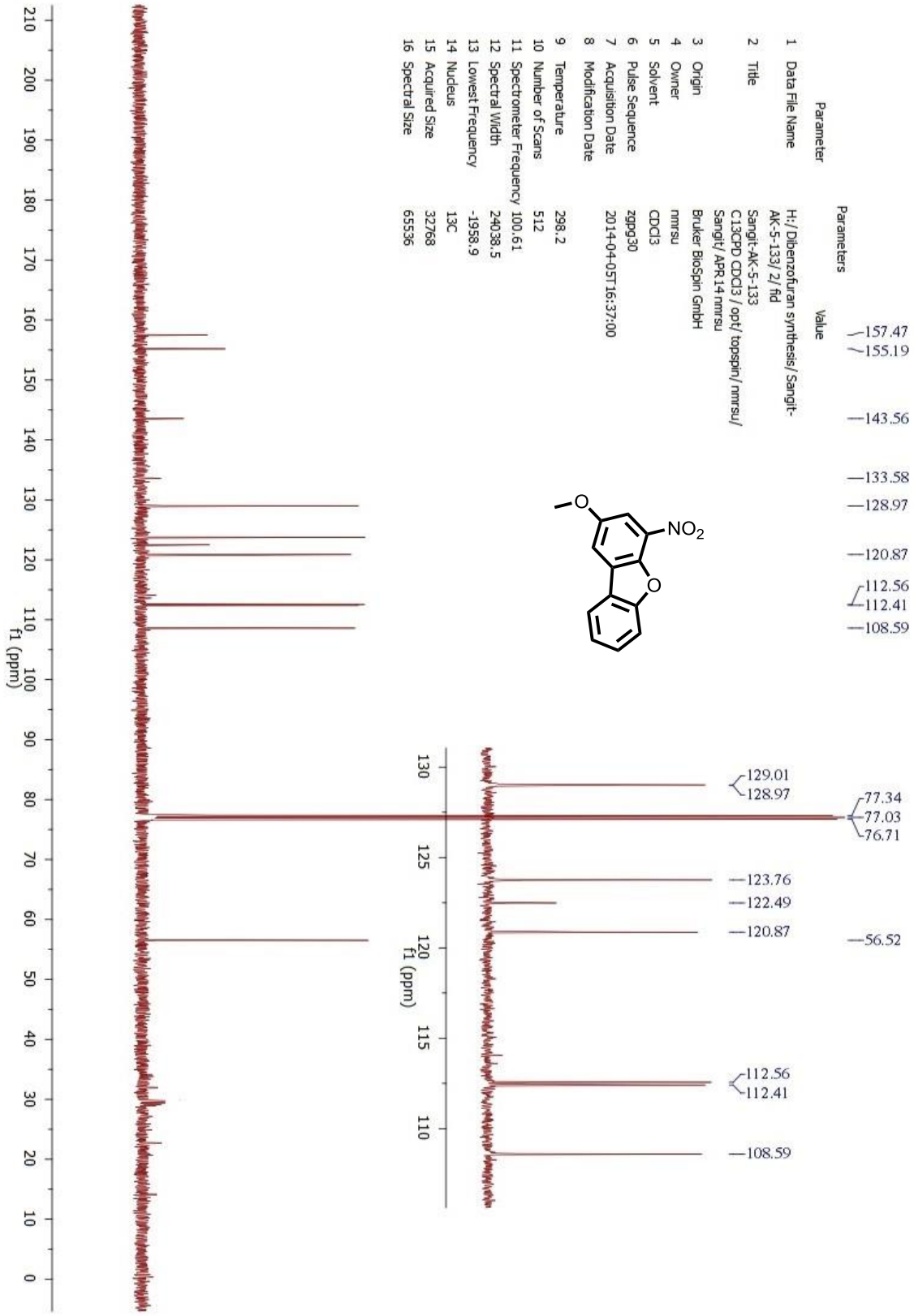

Figure S85 ^{1}H NMR spectrum of **2p**

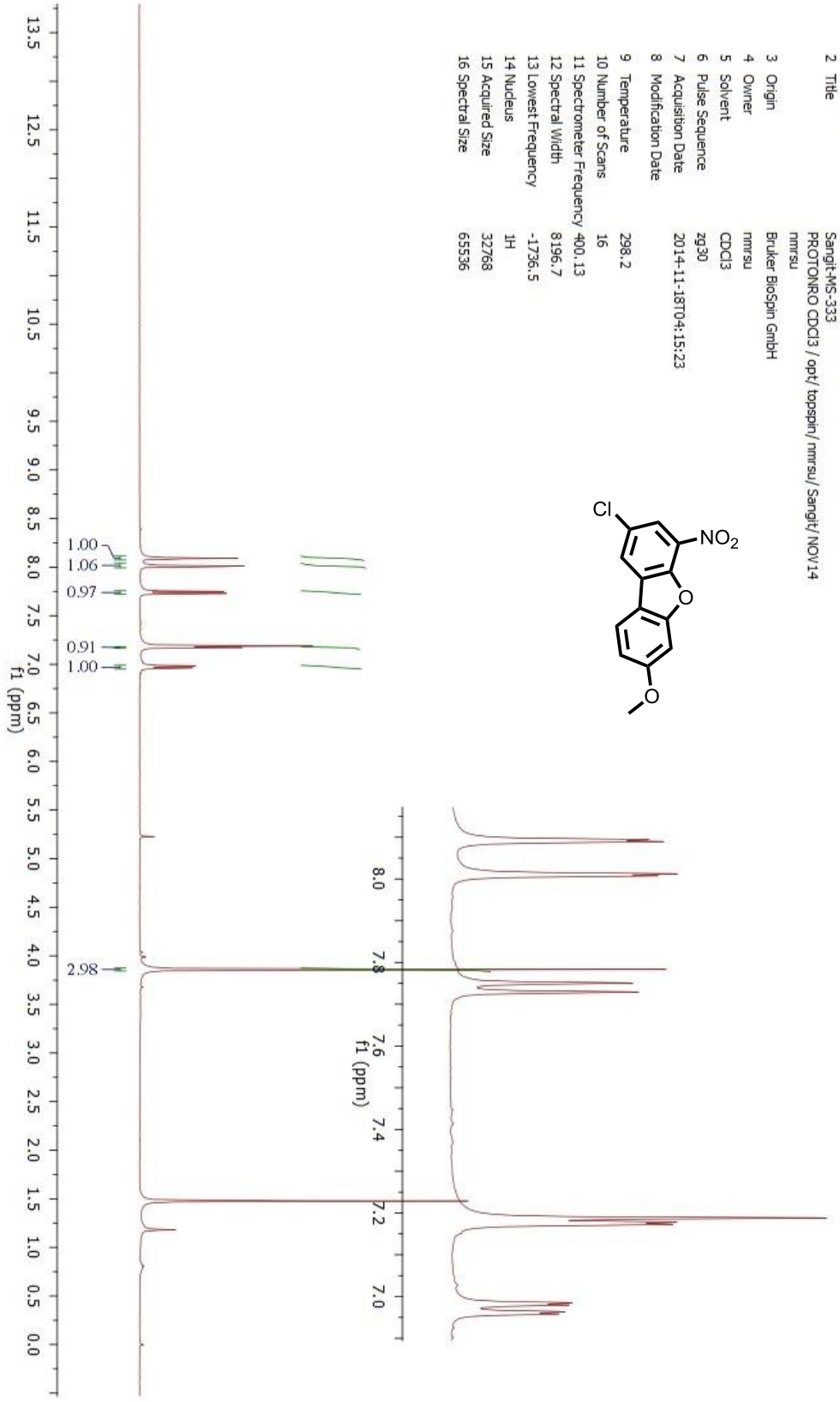

Figure S86 ^{13}C NMR spectrum of **2p**

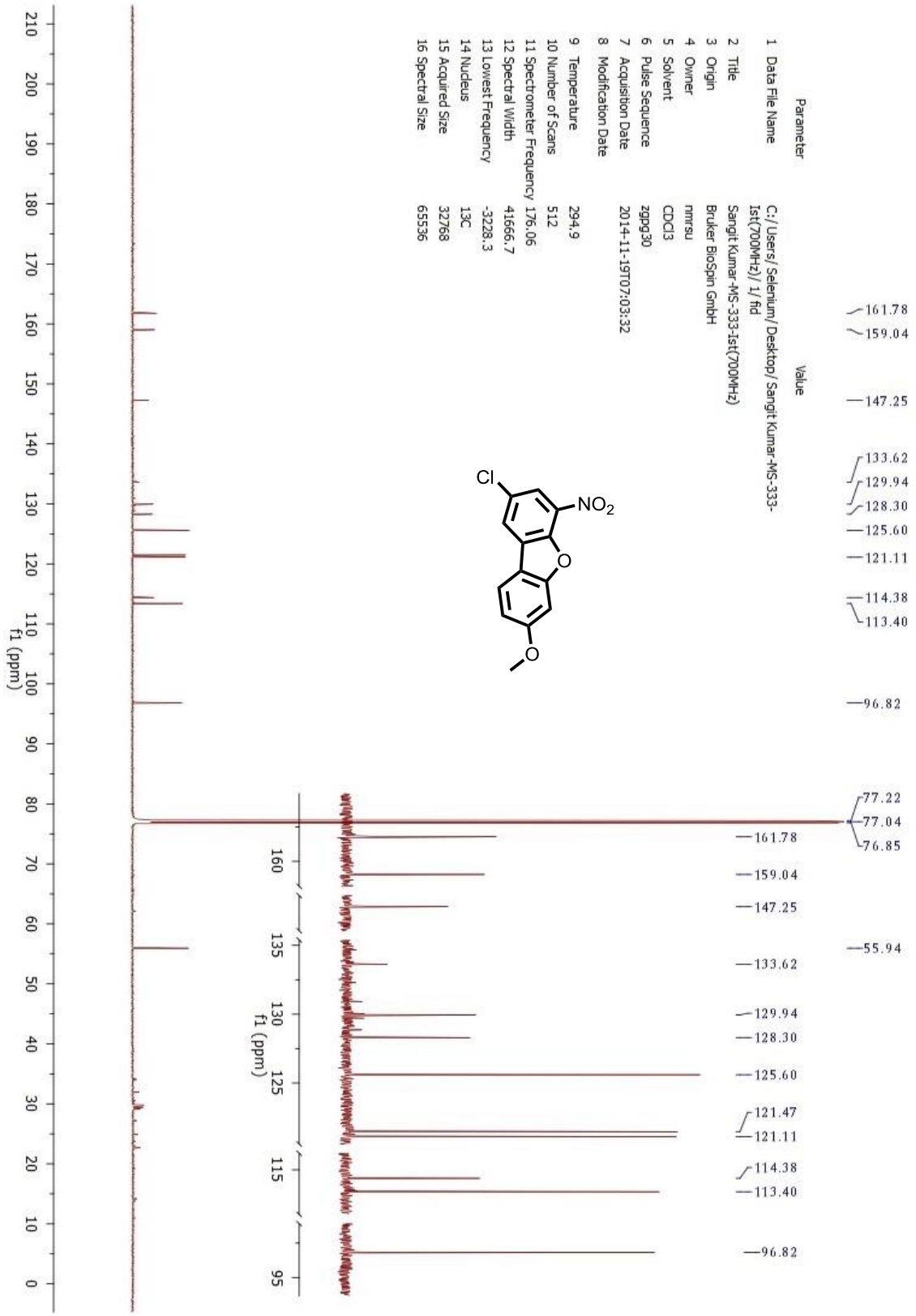

Figure S87 ^{1}H NMR spectrum of **2q**

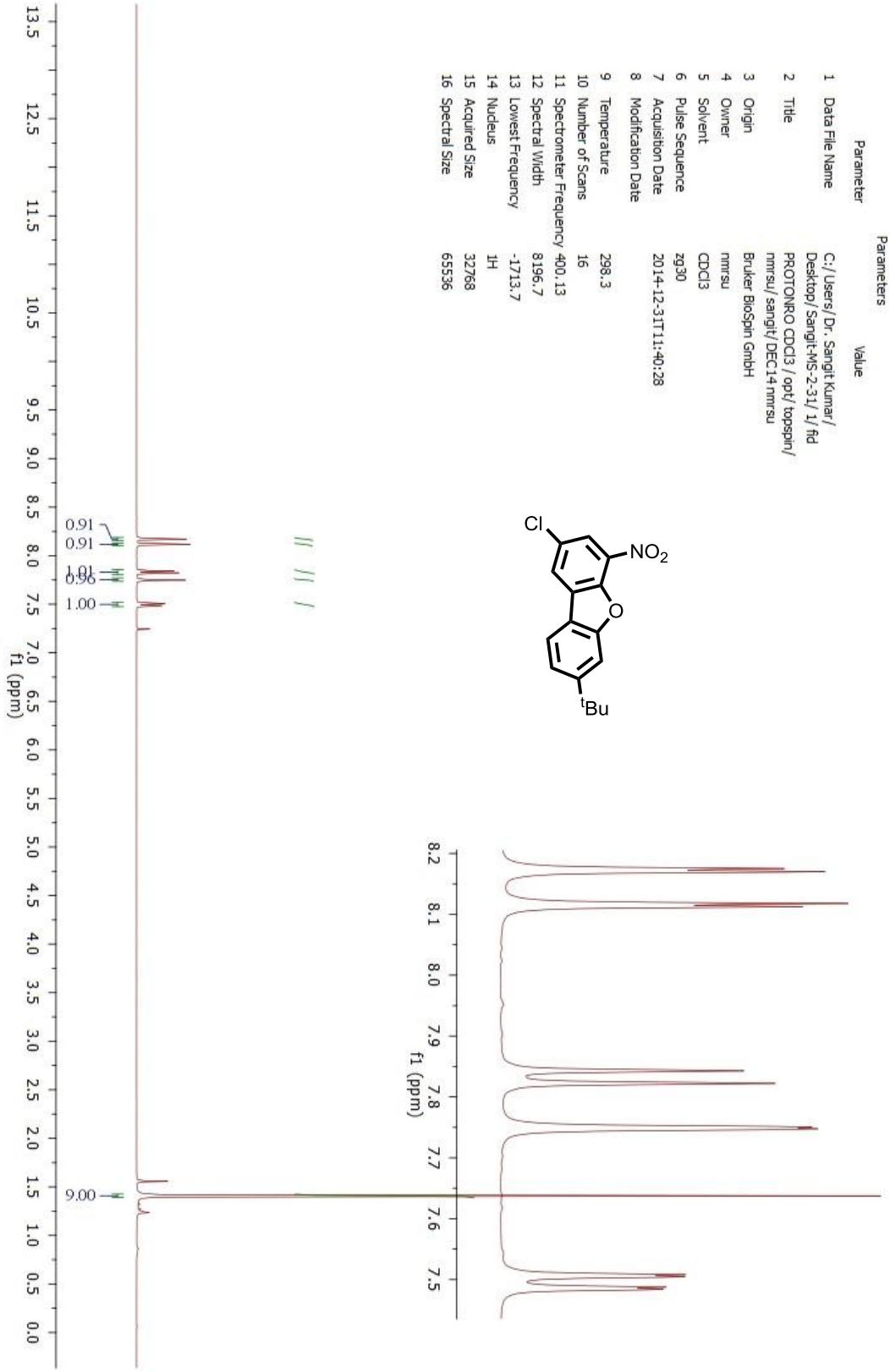

Figure S88 ^{13}C NMR spectrum of **2q**

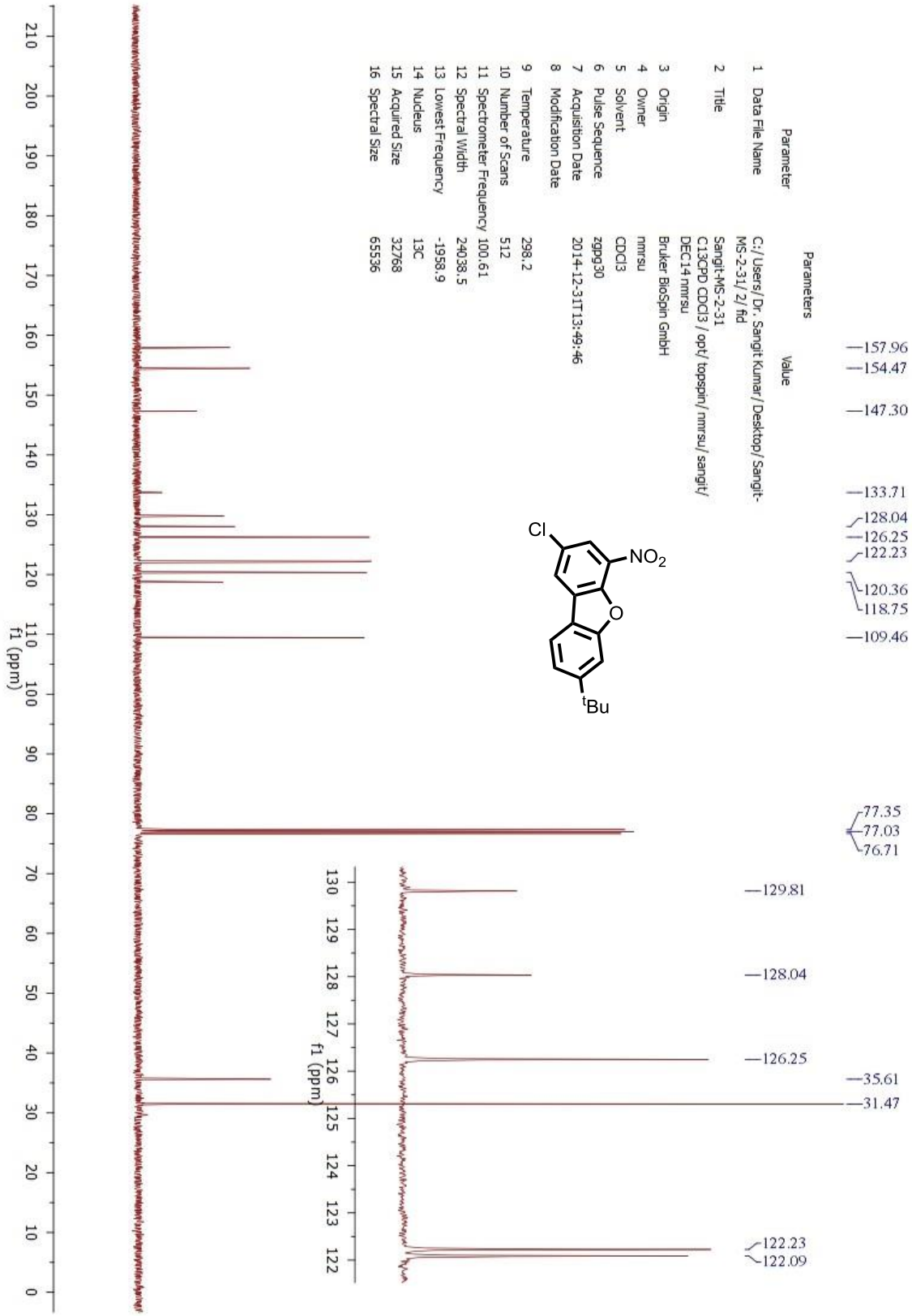

Figure S89 ^{1}H NMR spectrum of **2r**

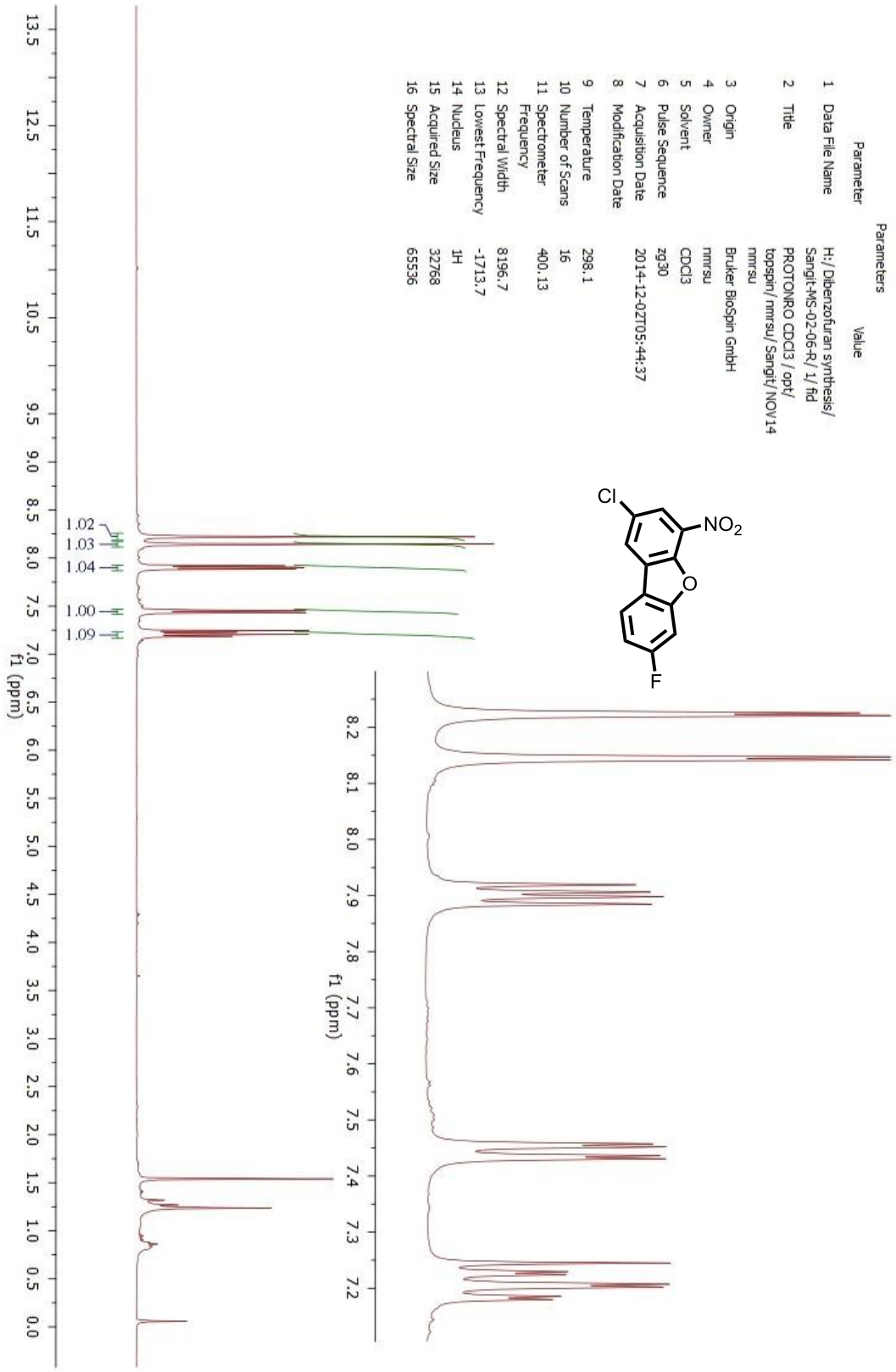

Figure S90 ^{13}C NMR spectrum of **2r**

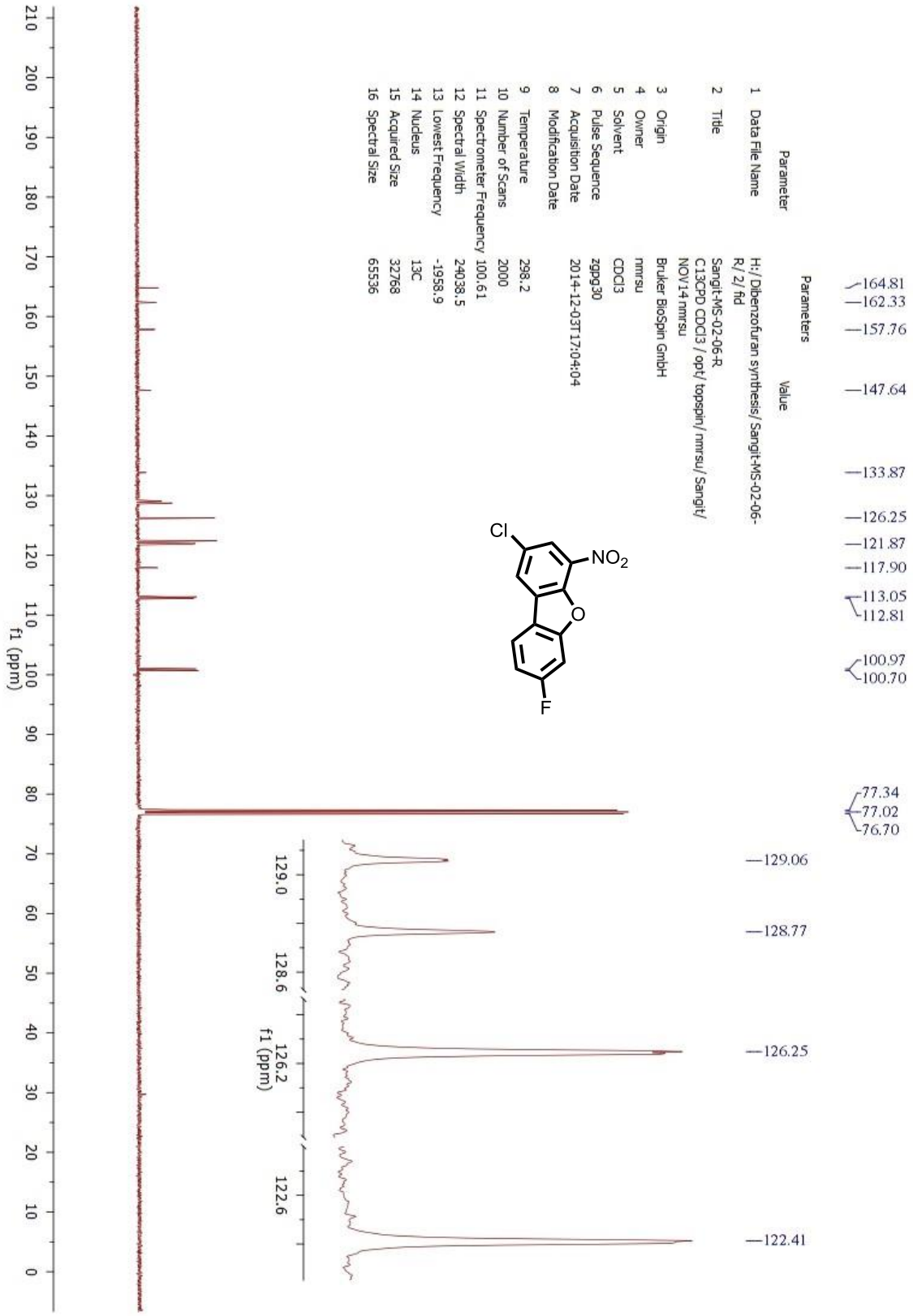

Figure S91 ^{1}H NMR spectrum of **2s**

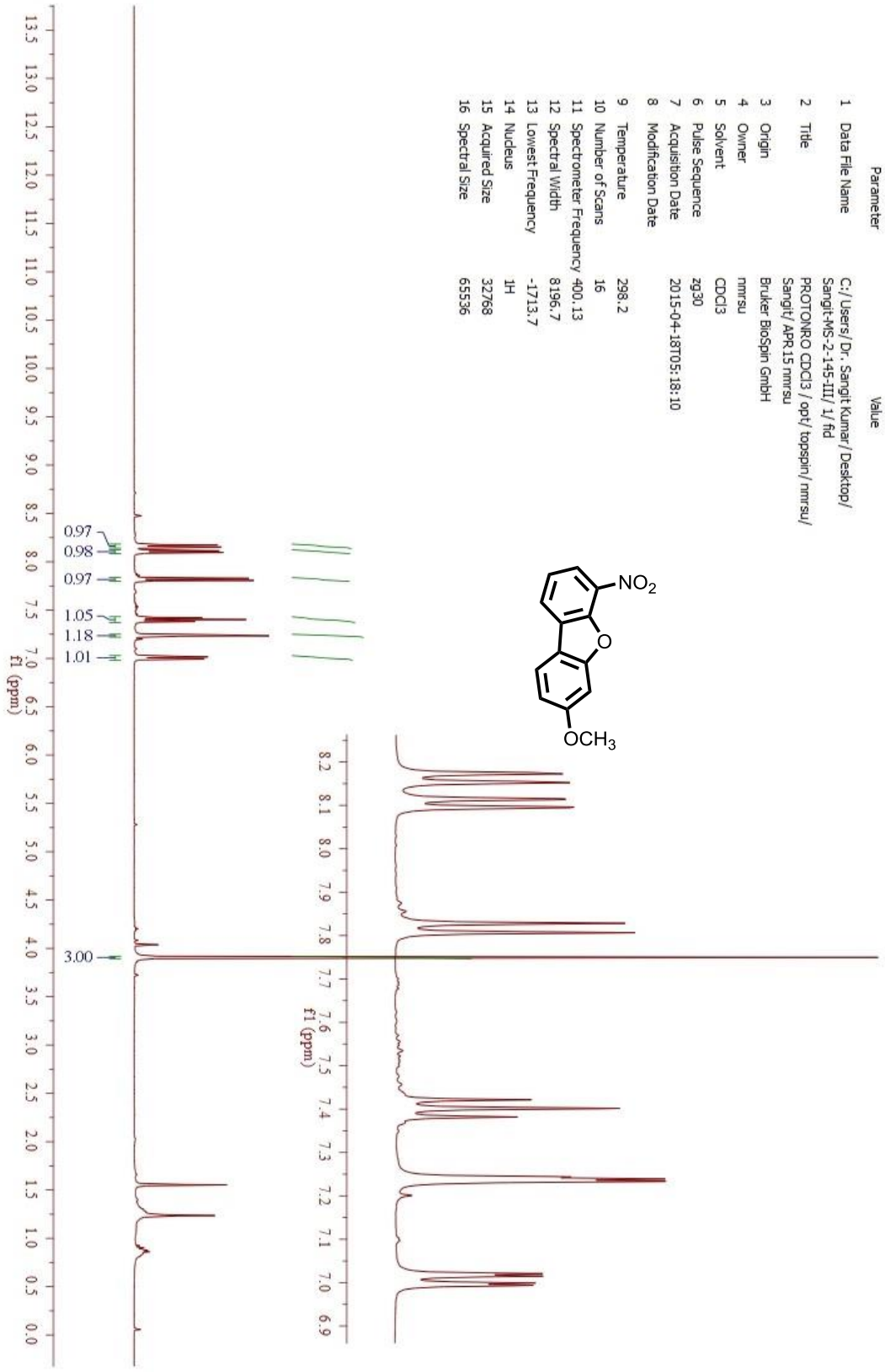

Figure S92 ^{13}C NMR spectrum of **2s**

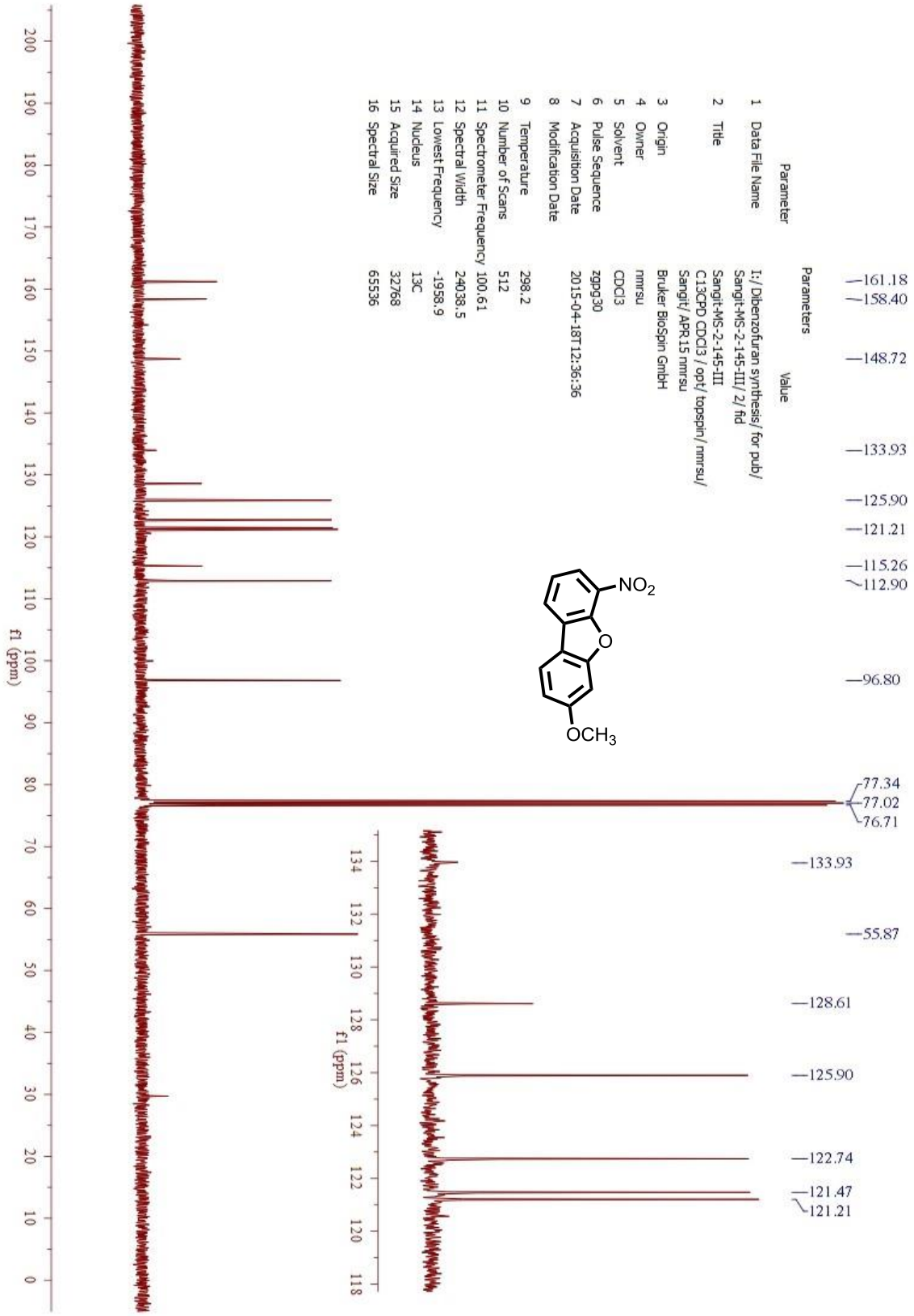

Figure S93 ^{1}H NMR spectrum of **2s'**

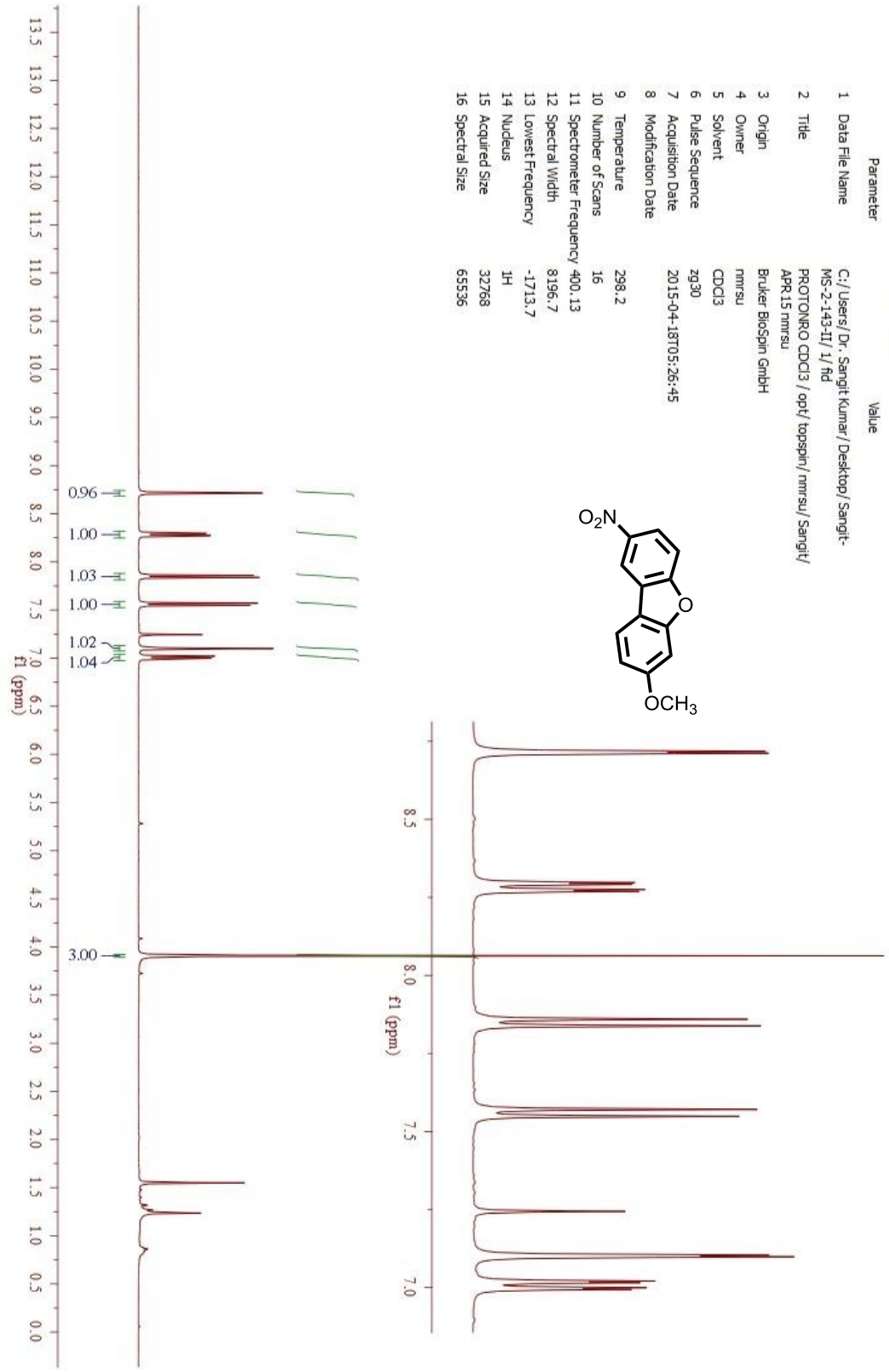

Figure S94 ^{1}C NMR spectrum of **2s'**

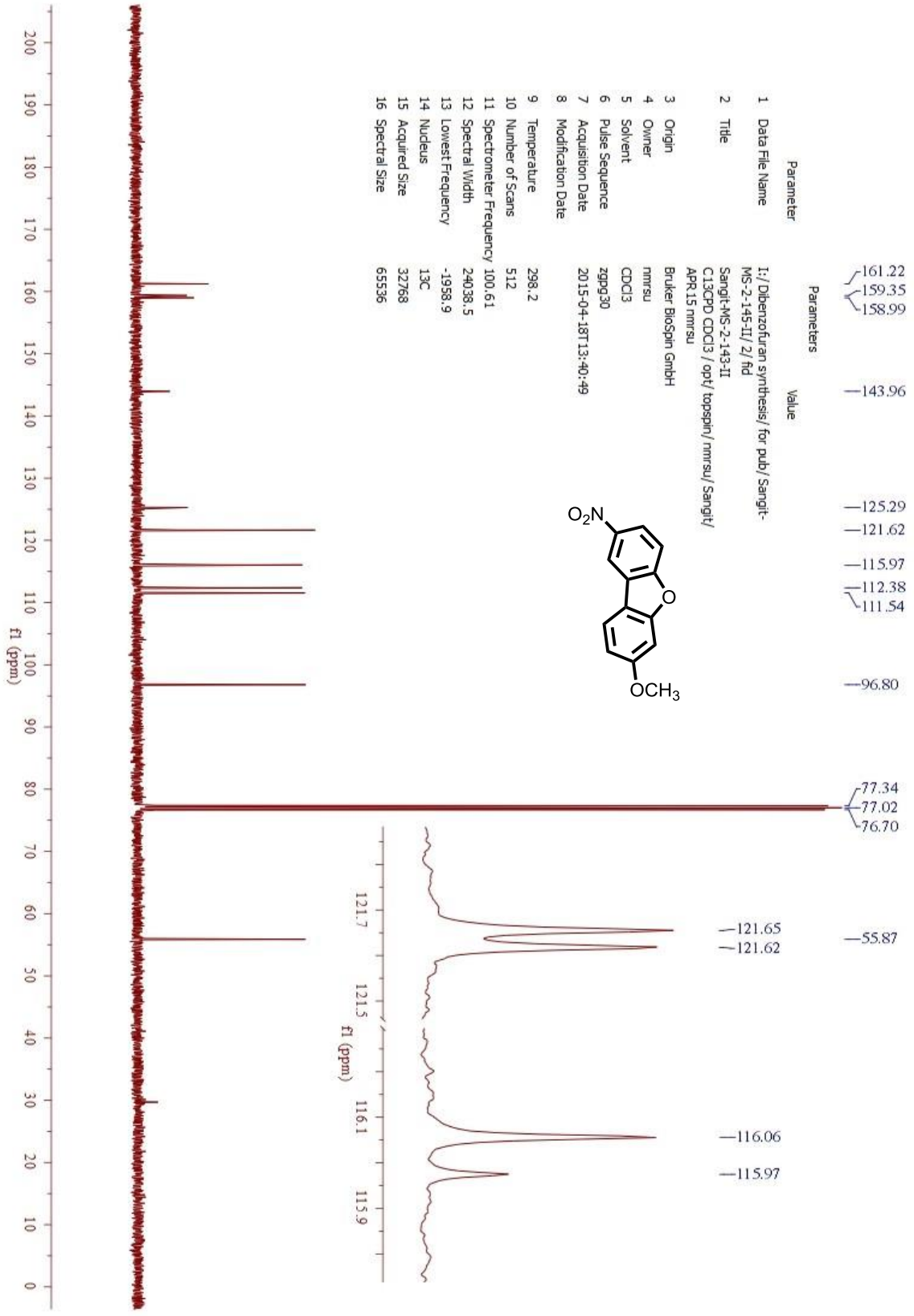

Figure S95 ^{1}H NMR spectrum of **2t**

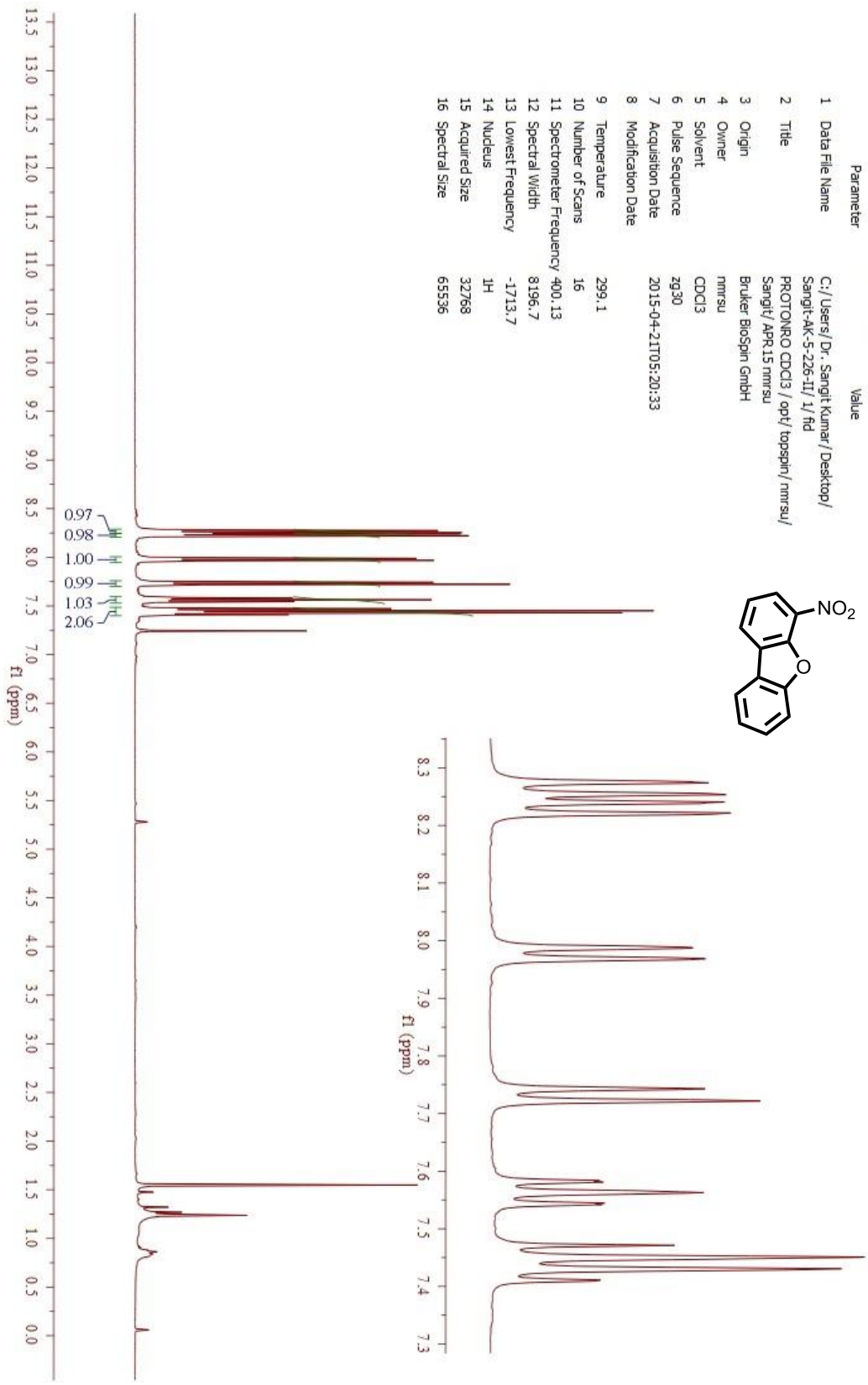

Figure S96 ^{13}C NMR spectrum of **2t**

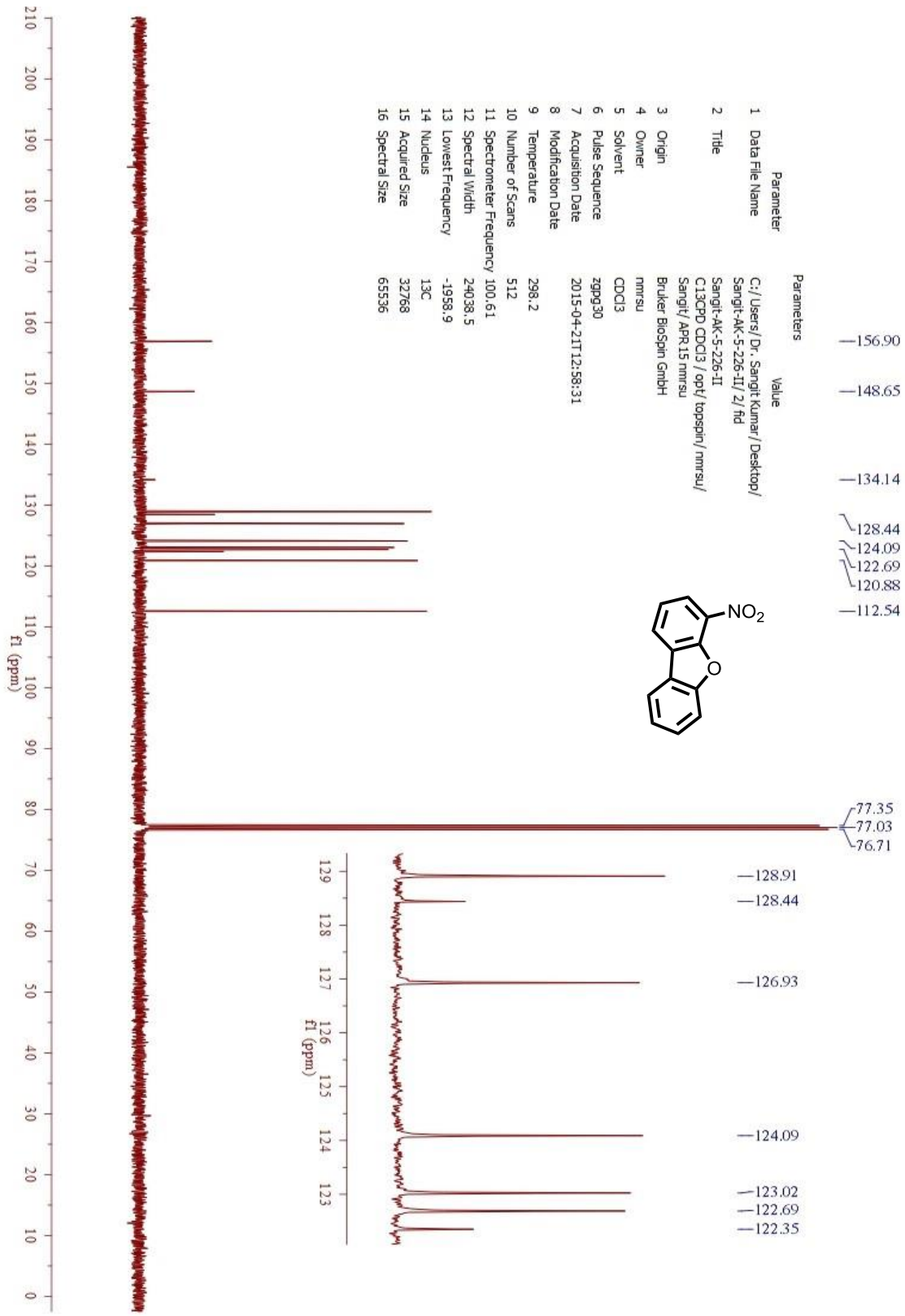

Figure S97 ^{1}H NMR spectrum of **2t'**

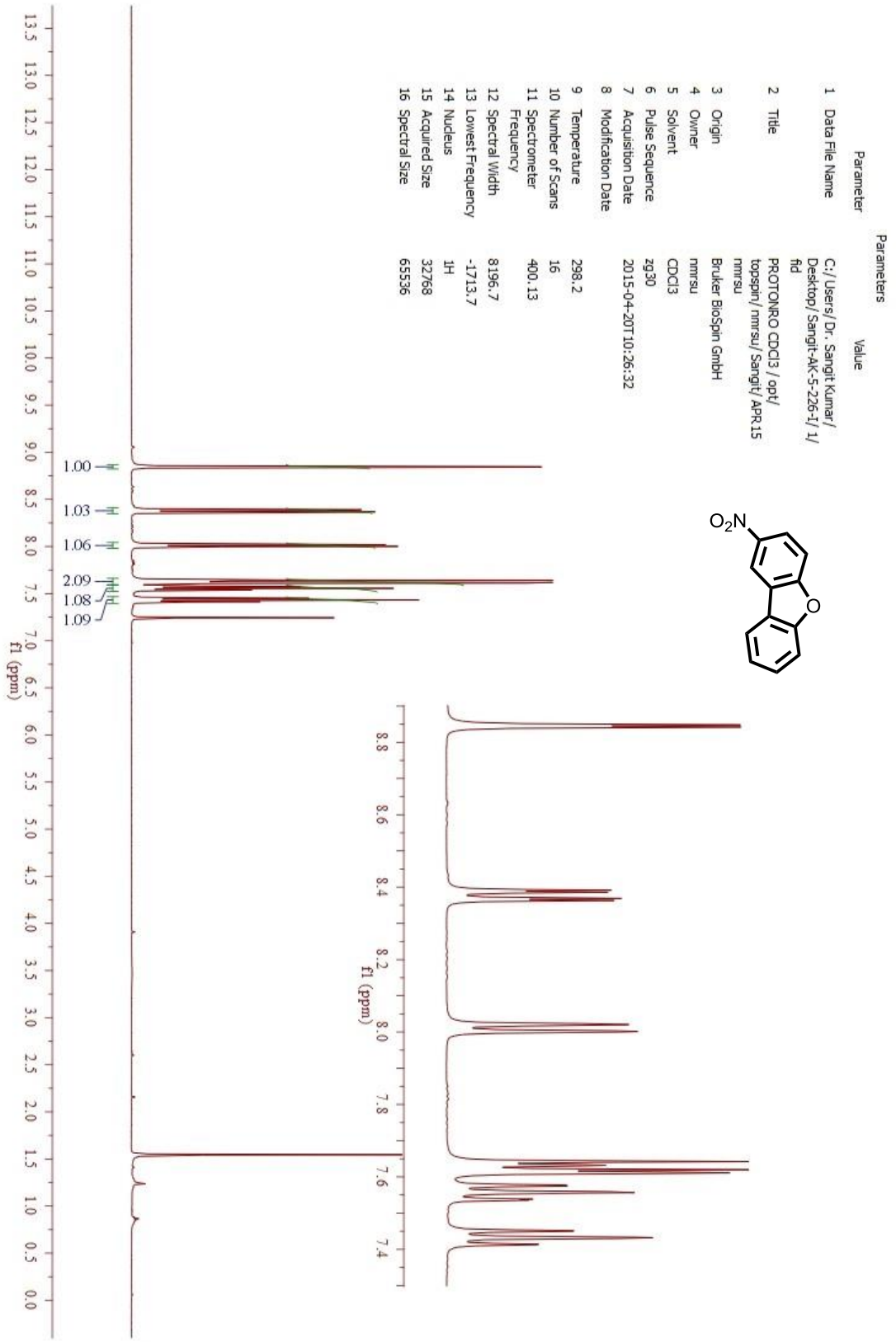

Figure S98 ^{13}C NMR spectrum of **2t'**

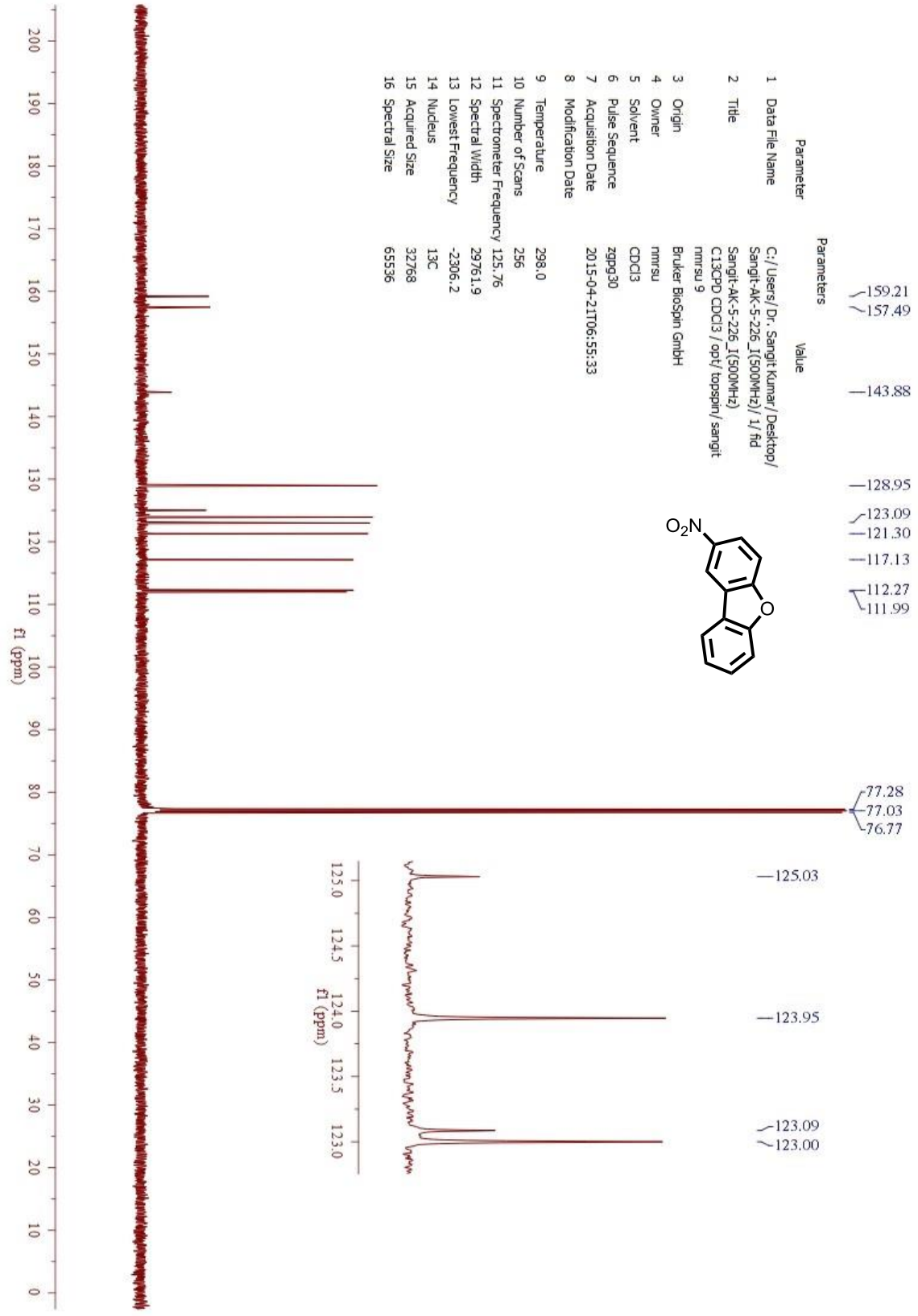

Figure S99 ^{1}H NMR spectrum of **4**

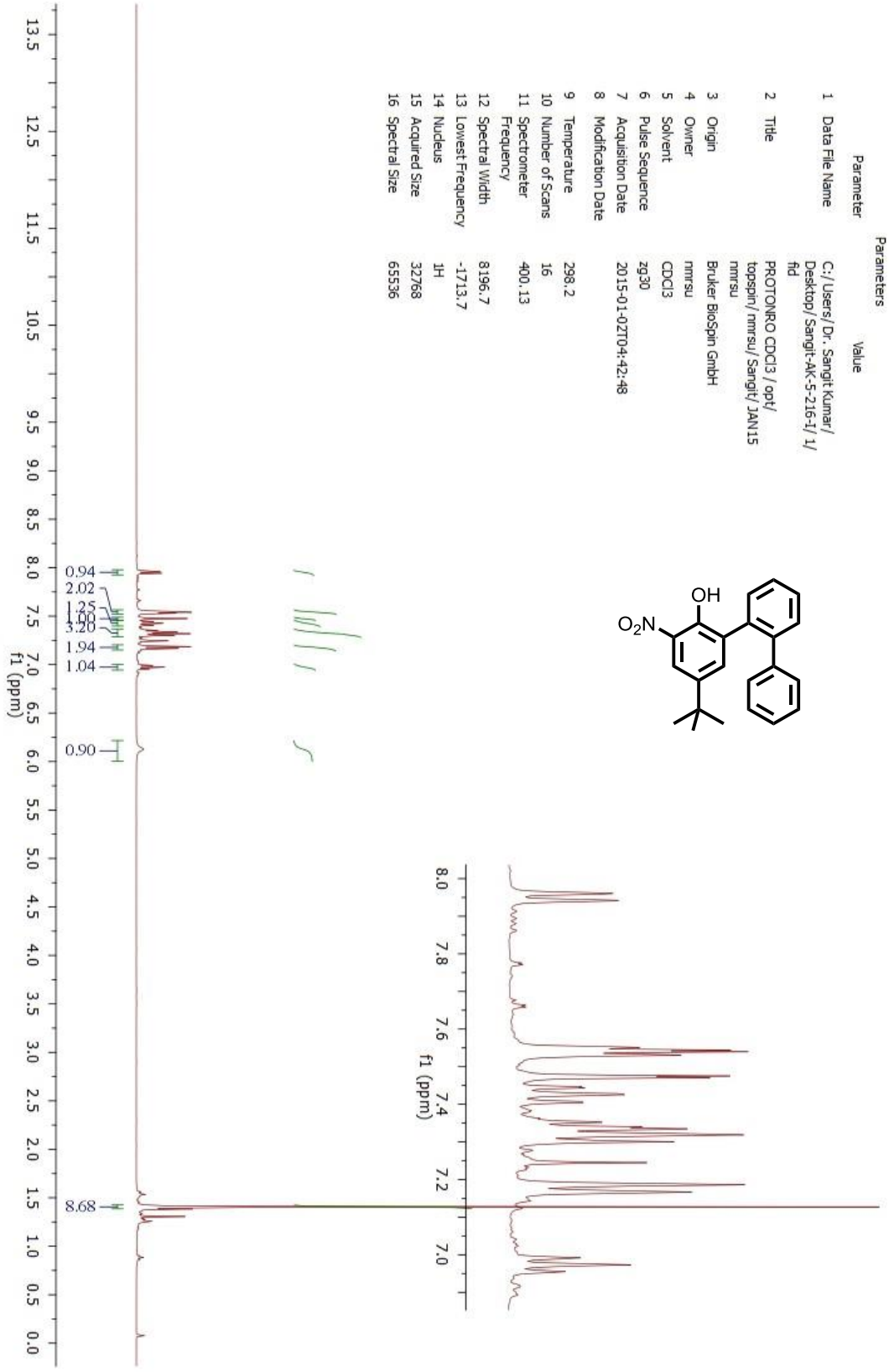

Figure S100 ^{13}C NMR spectrum of **4**

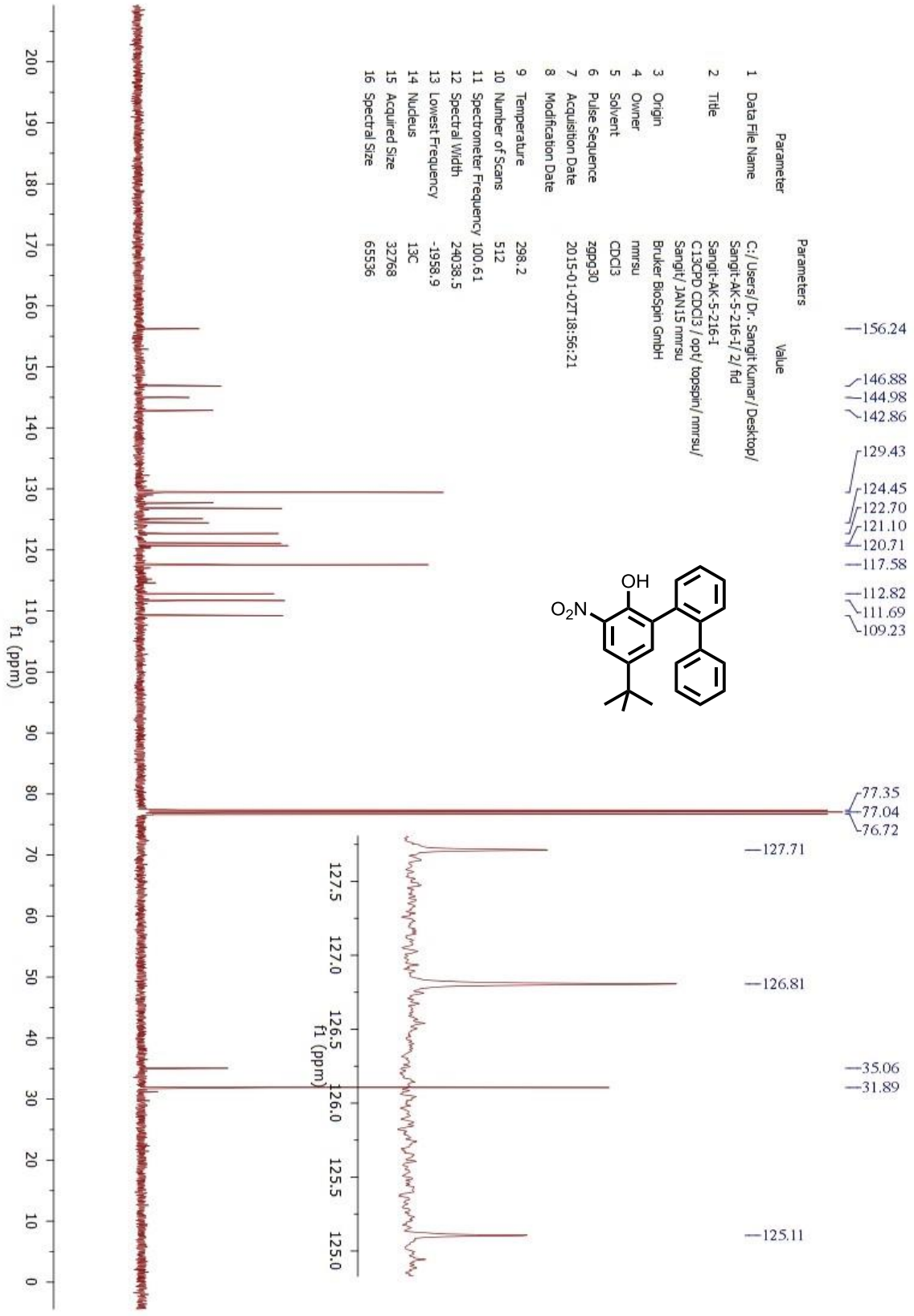

Figure S101 ^{1}H NMR spectrum of **5d**

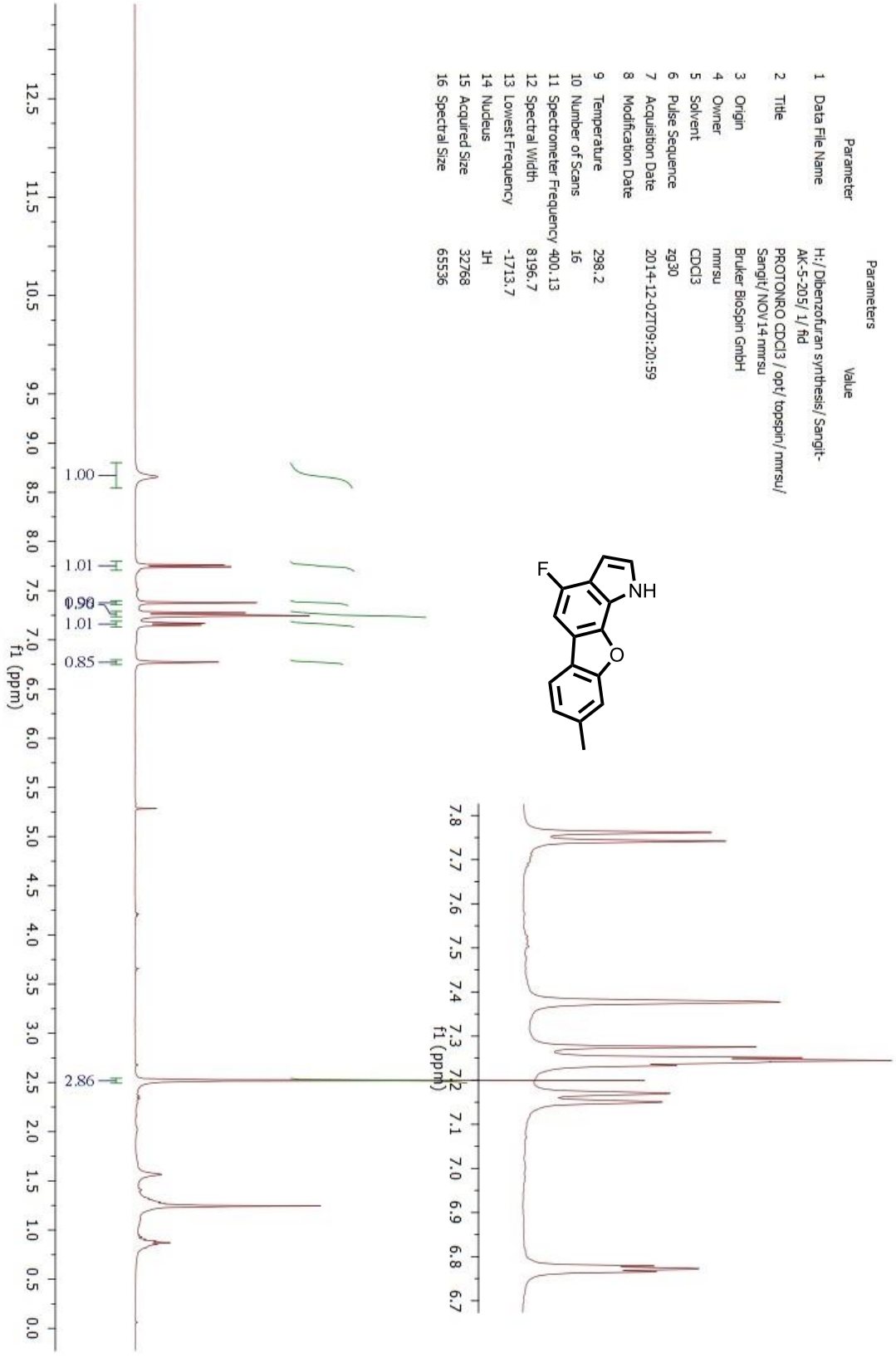

Figure S102 ^{13}C NMR spectrum of **5d**

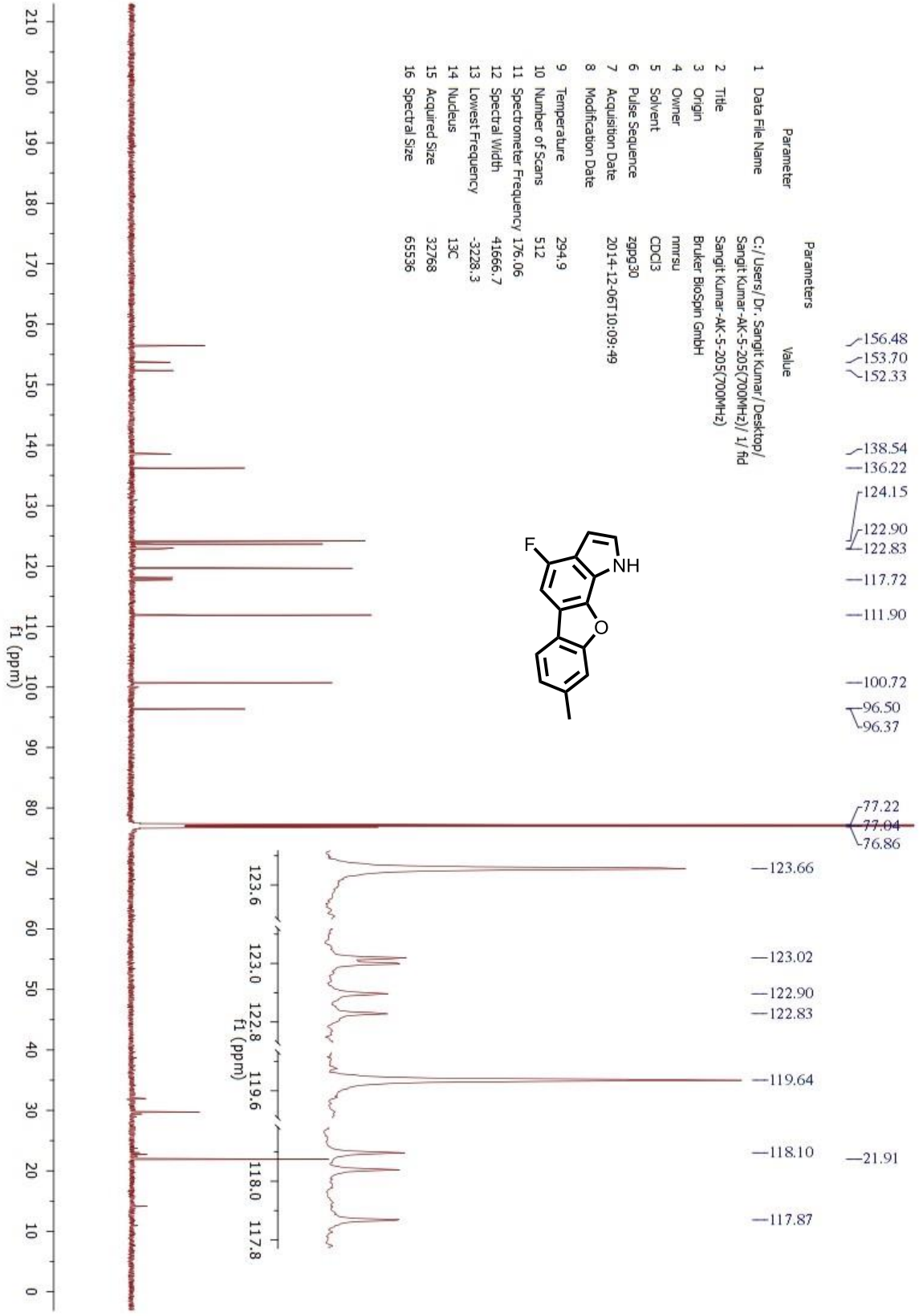

Figure S103 ^{1}H NMR spectrum of **5k**

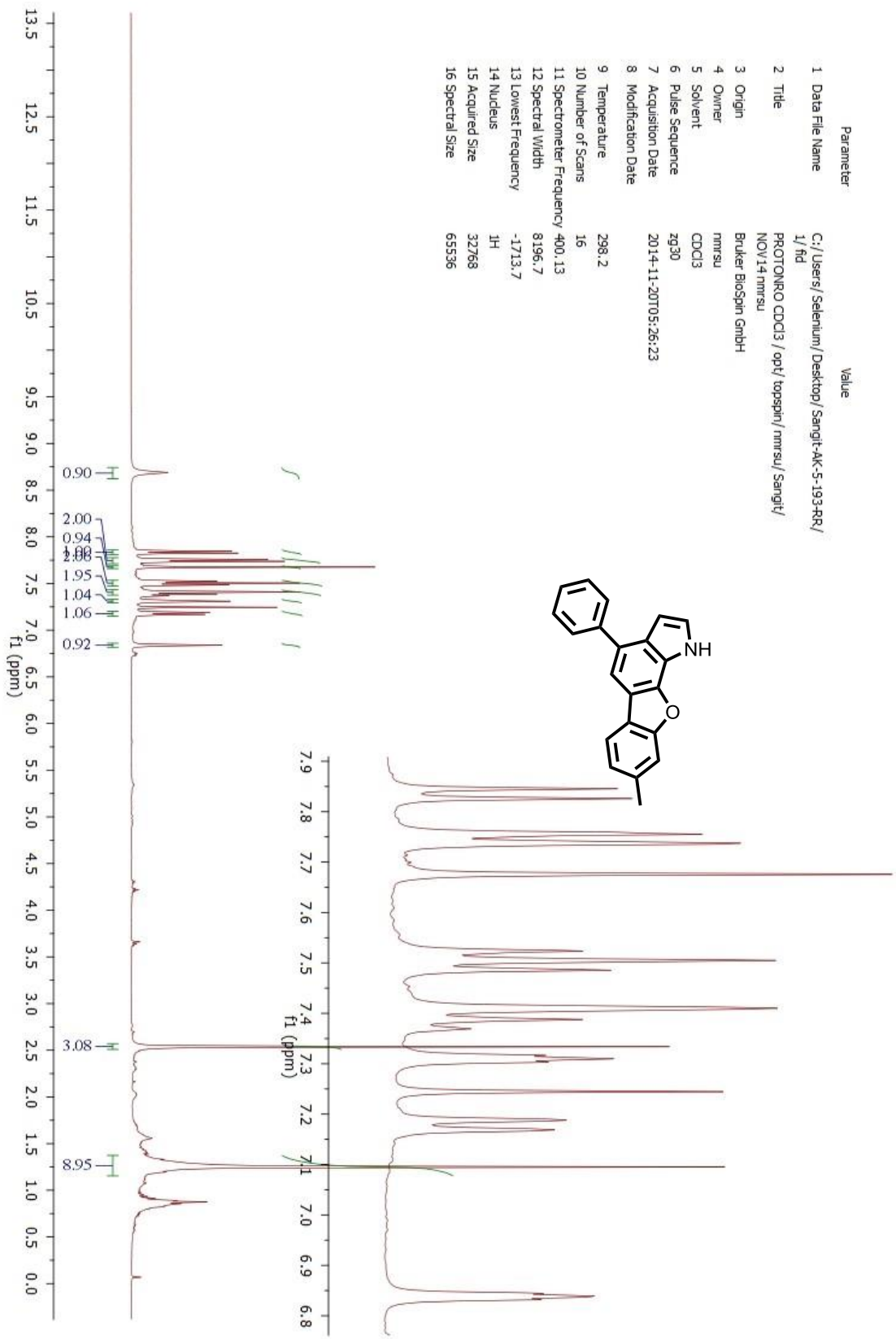

Figure S104 ^{13}C NMR spectrum of **5k**

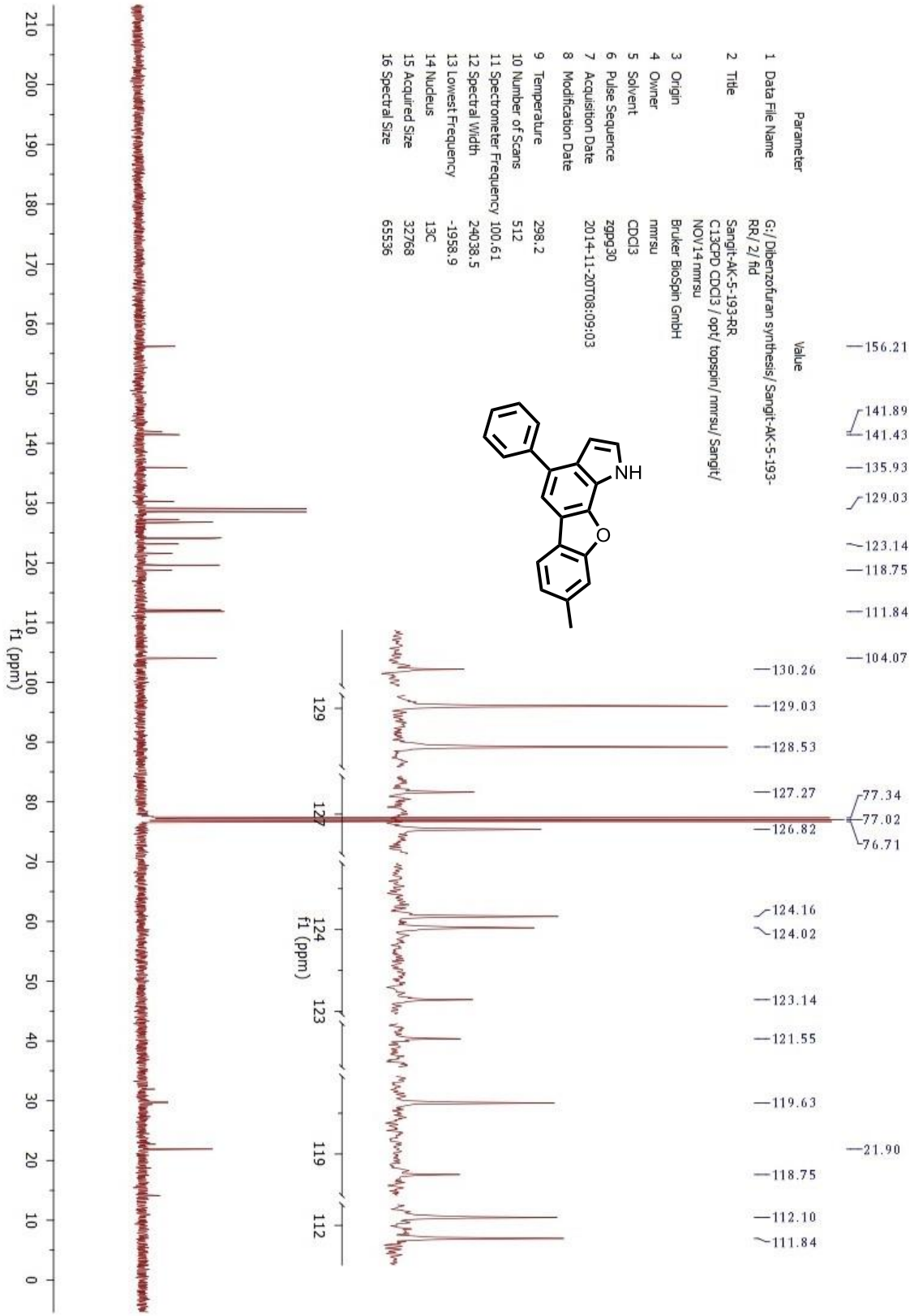

Figure S105 ^{1}H NMR spectrum of **5n**

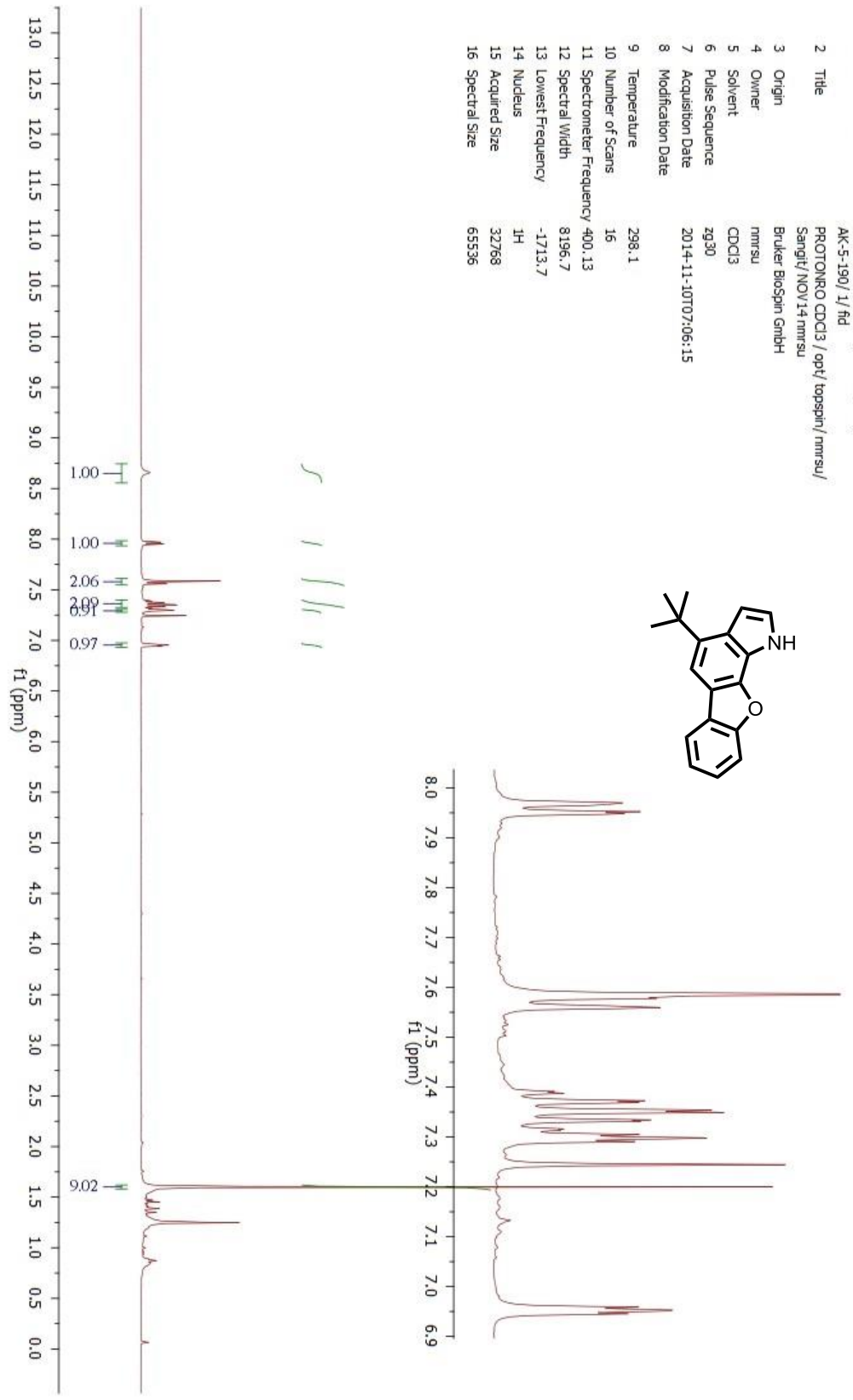

Figure S106 ^{13}C NMR spectrum of **5n**

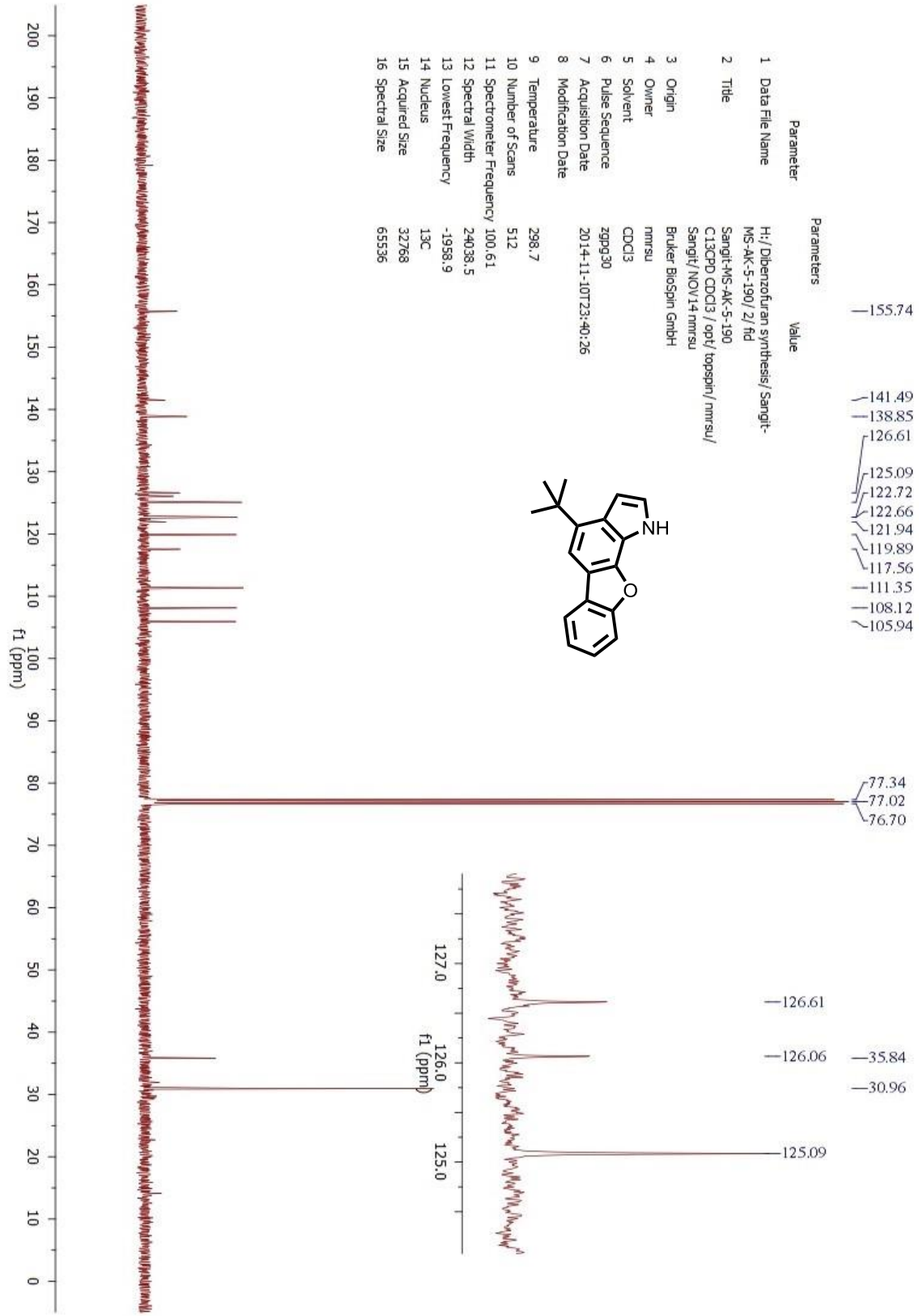

Figure S107 ^{1}H NMR spectrum of **6a**

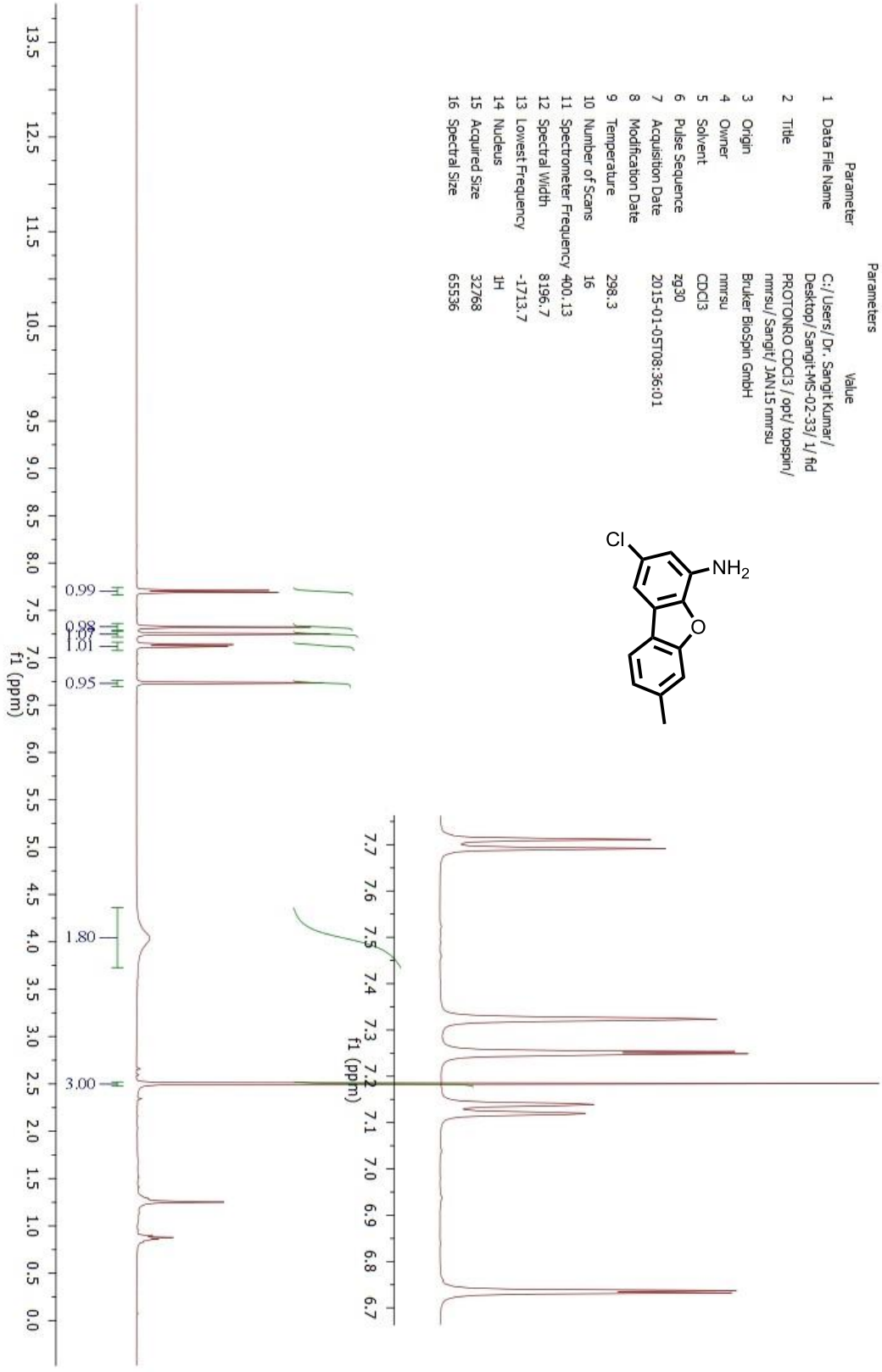

Figure S108 ^{13}C NMR spectrum of **6a**

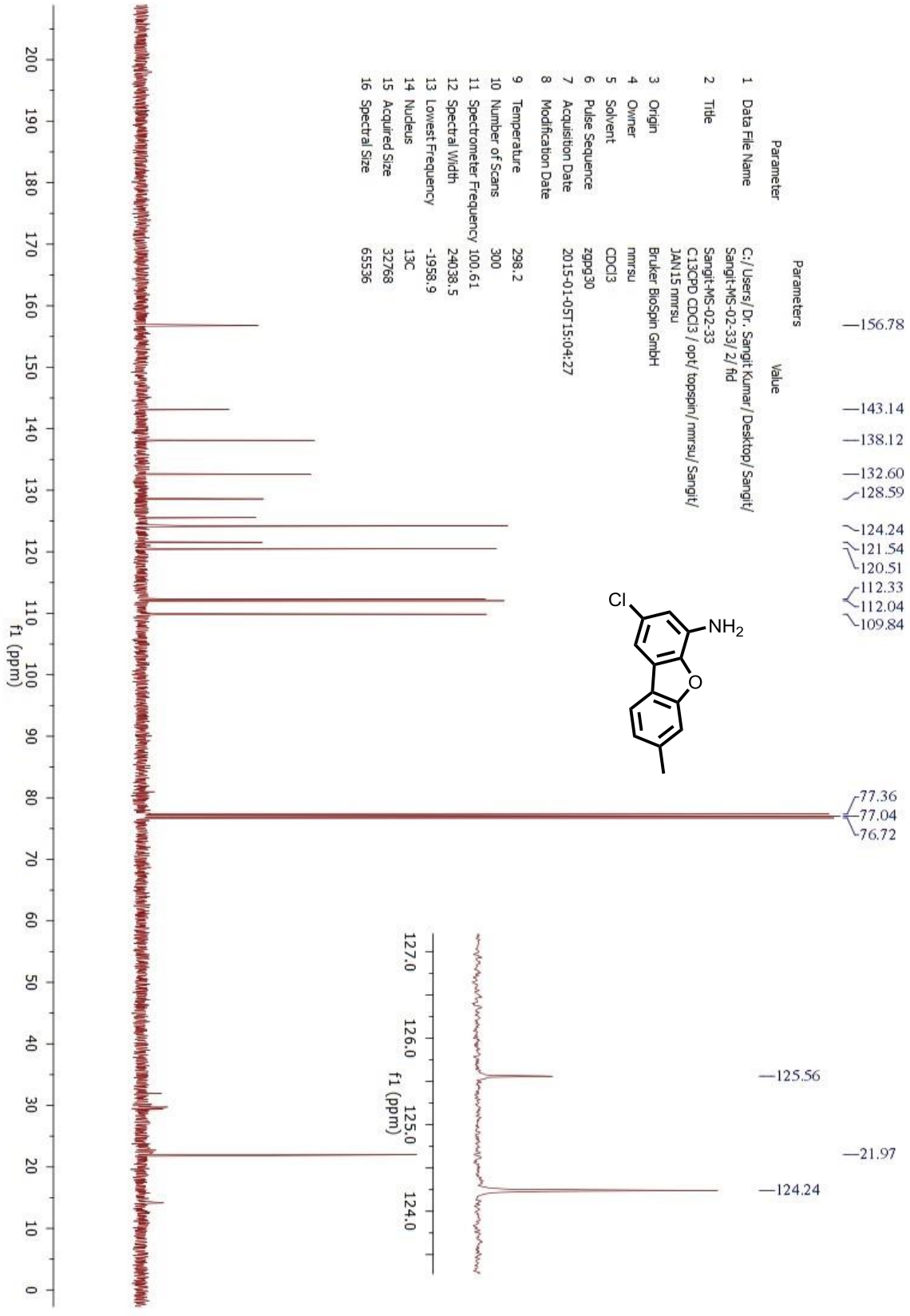

Figure S109 ^{1}H NMR spectrum of **6e**

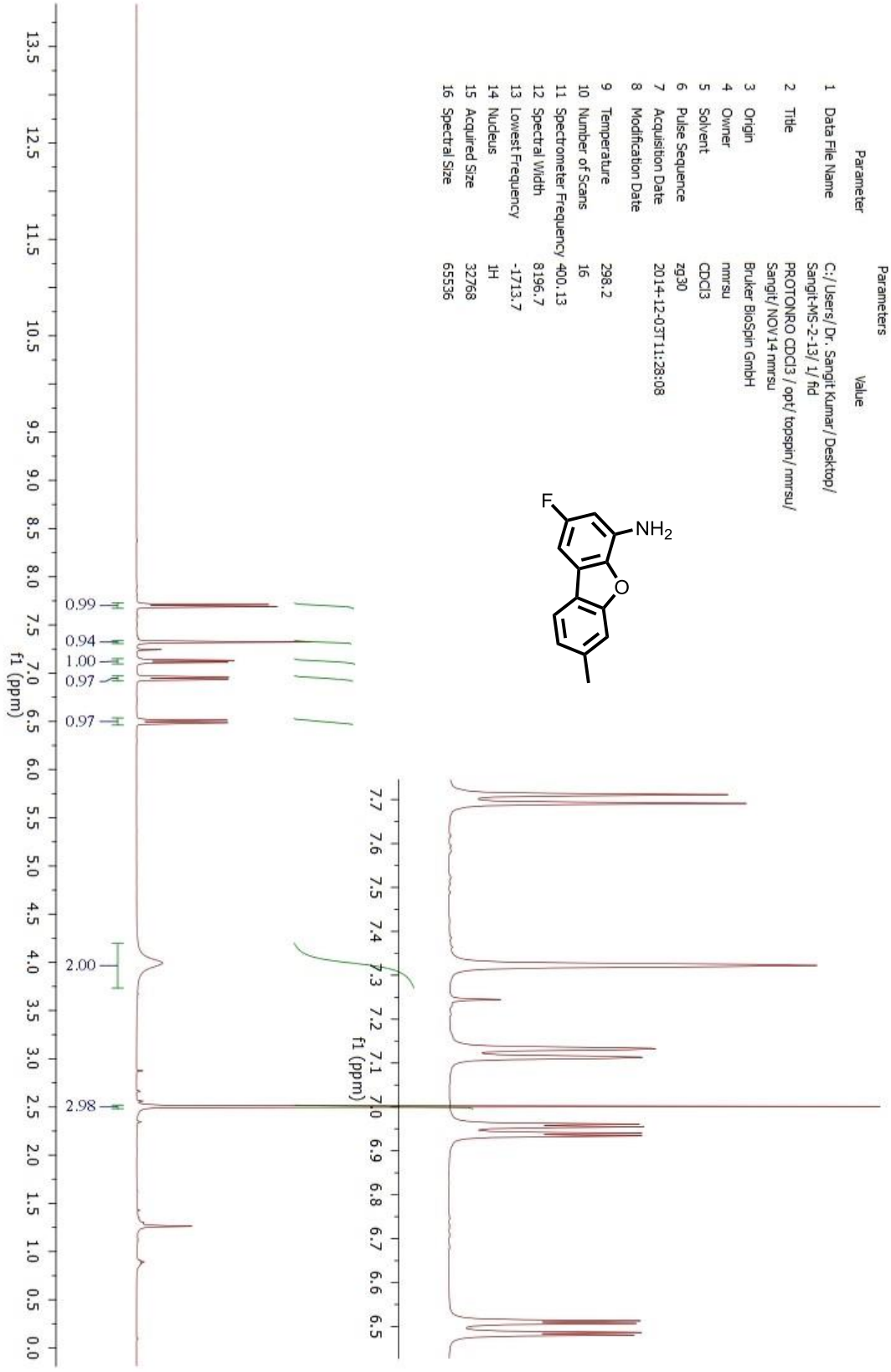

Figure S110 ^{13}C NMR spectrum of **6e**

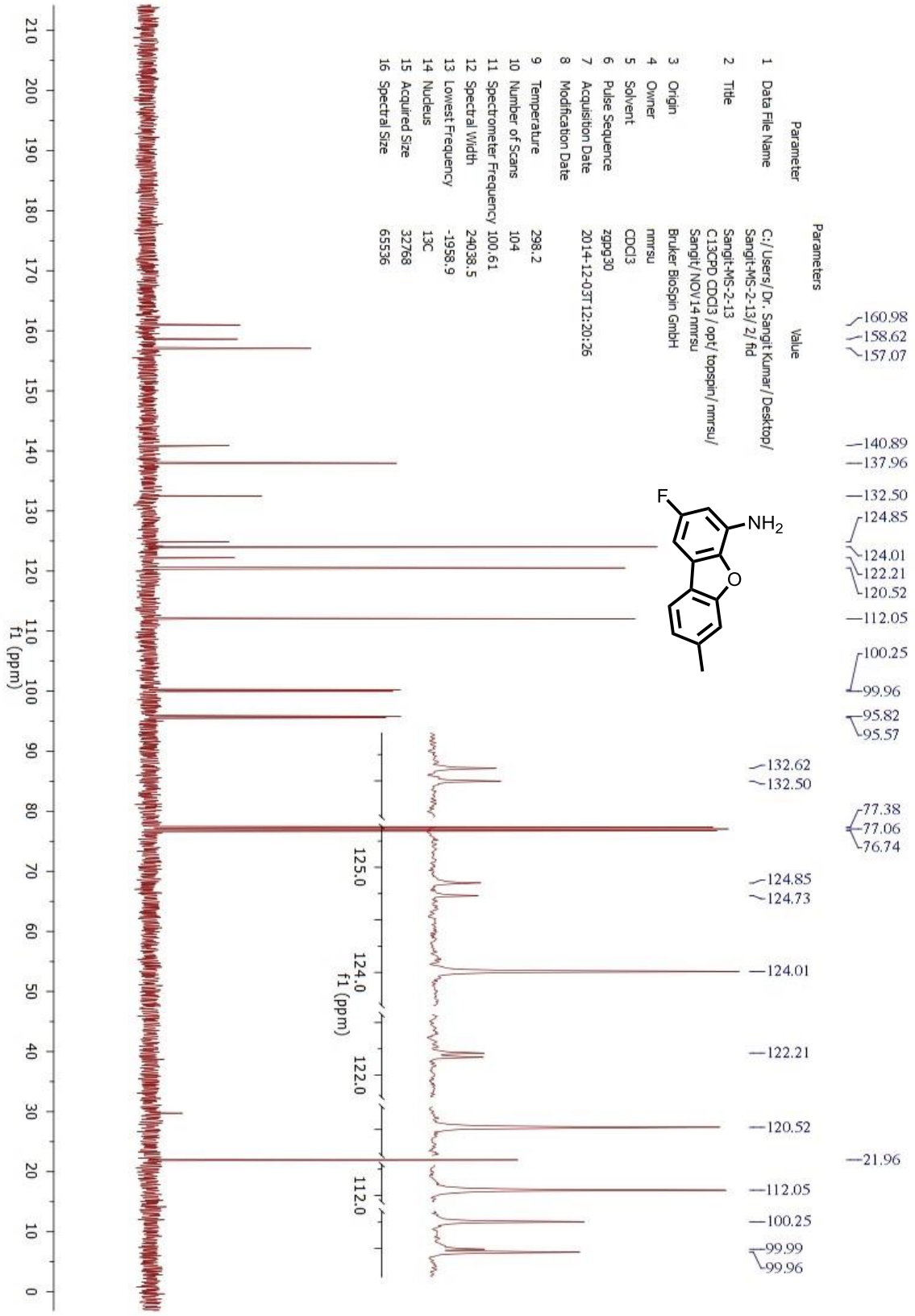

Figure S111^{1}H NMR spectrum of **6l**

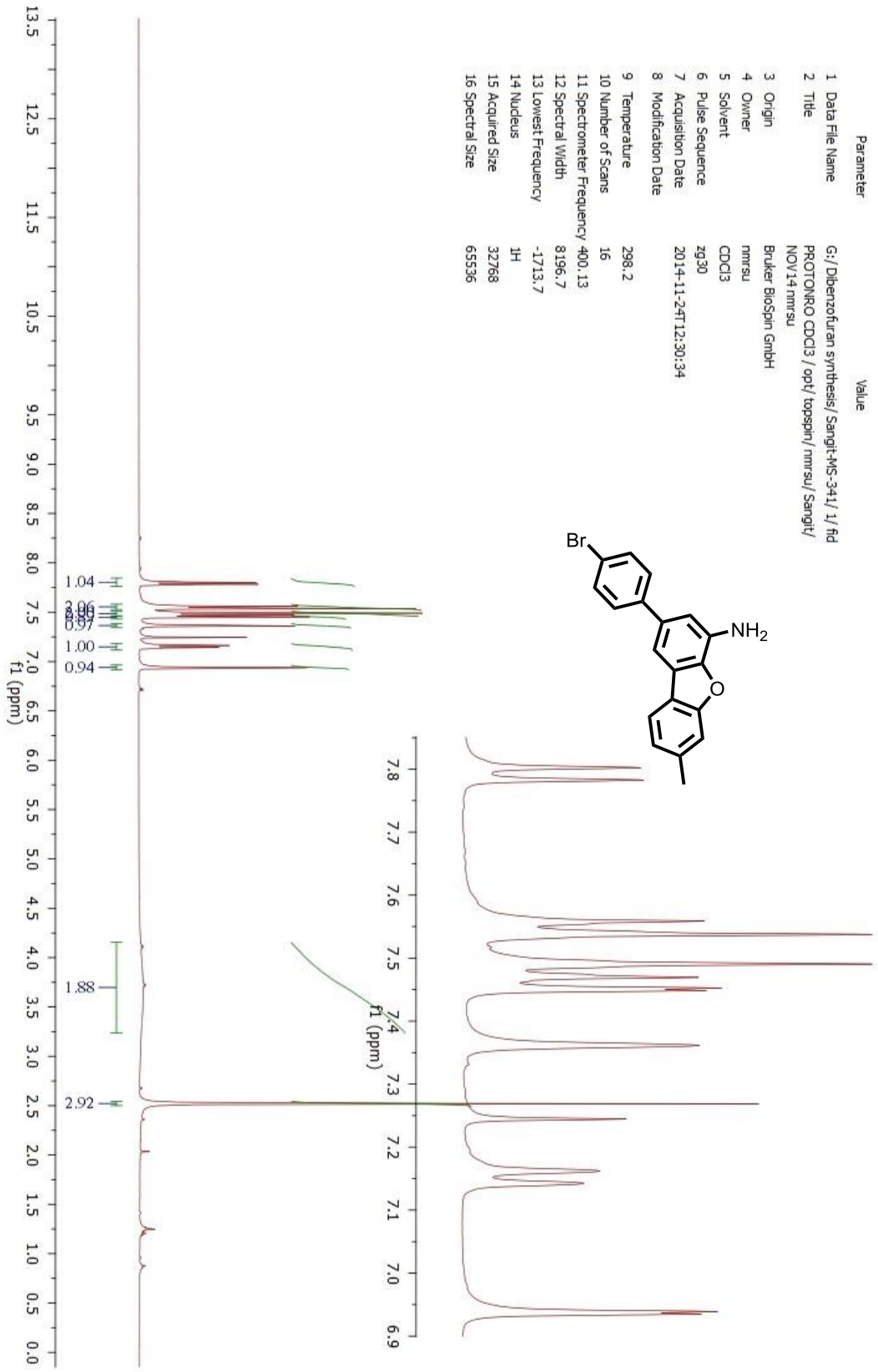

Figure S112 ^{13}C NMR spectrum of **6l**

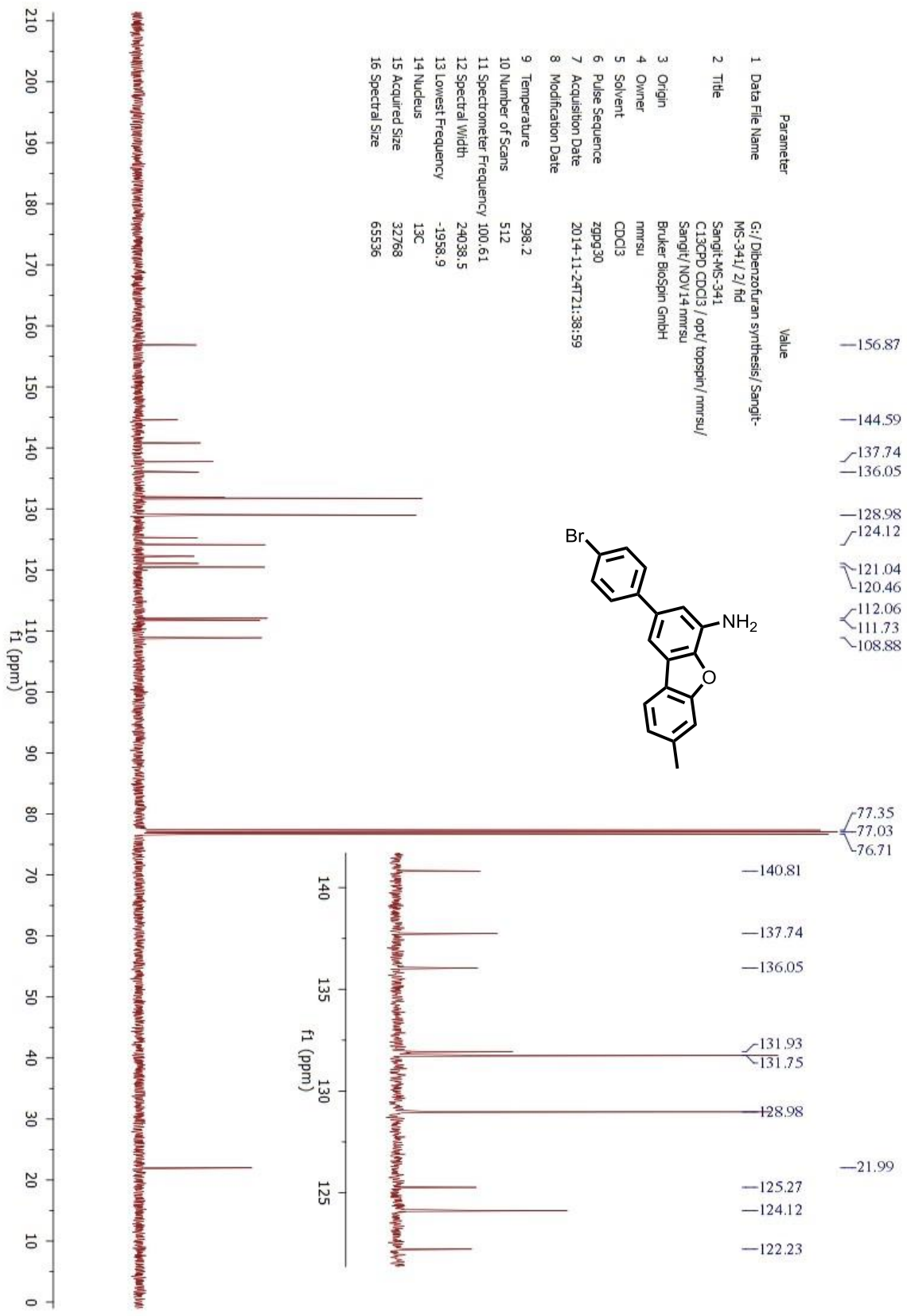

Figure S113 ^{1}H NMR spectrum of **6d**

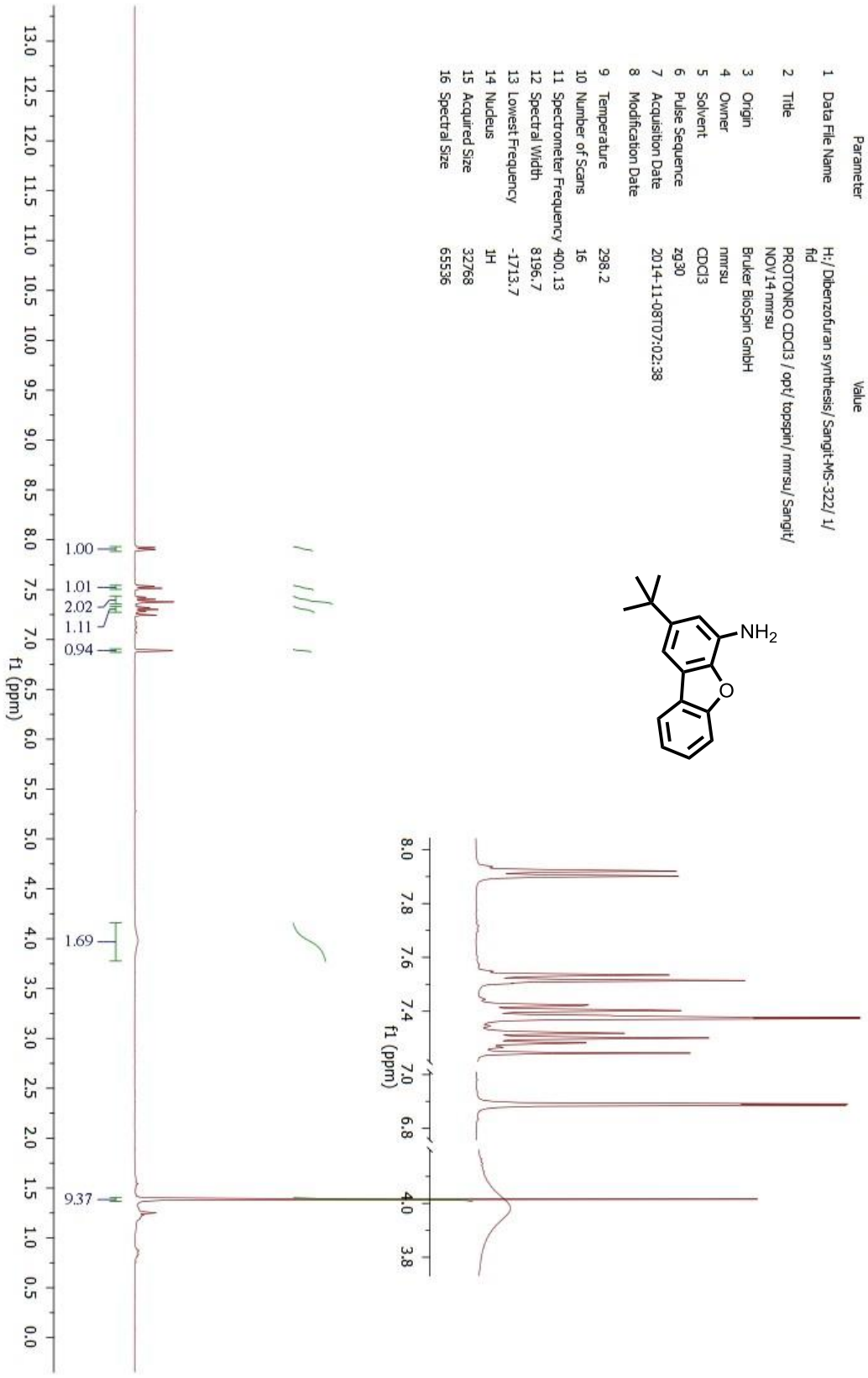

Figure S114[13]C NMR spectrum of **6d**

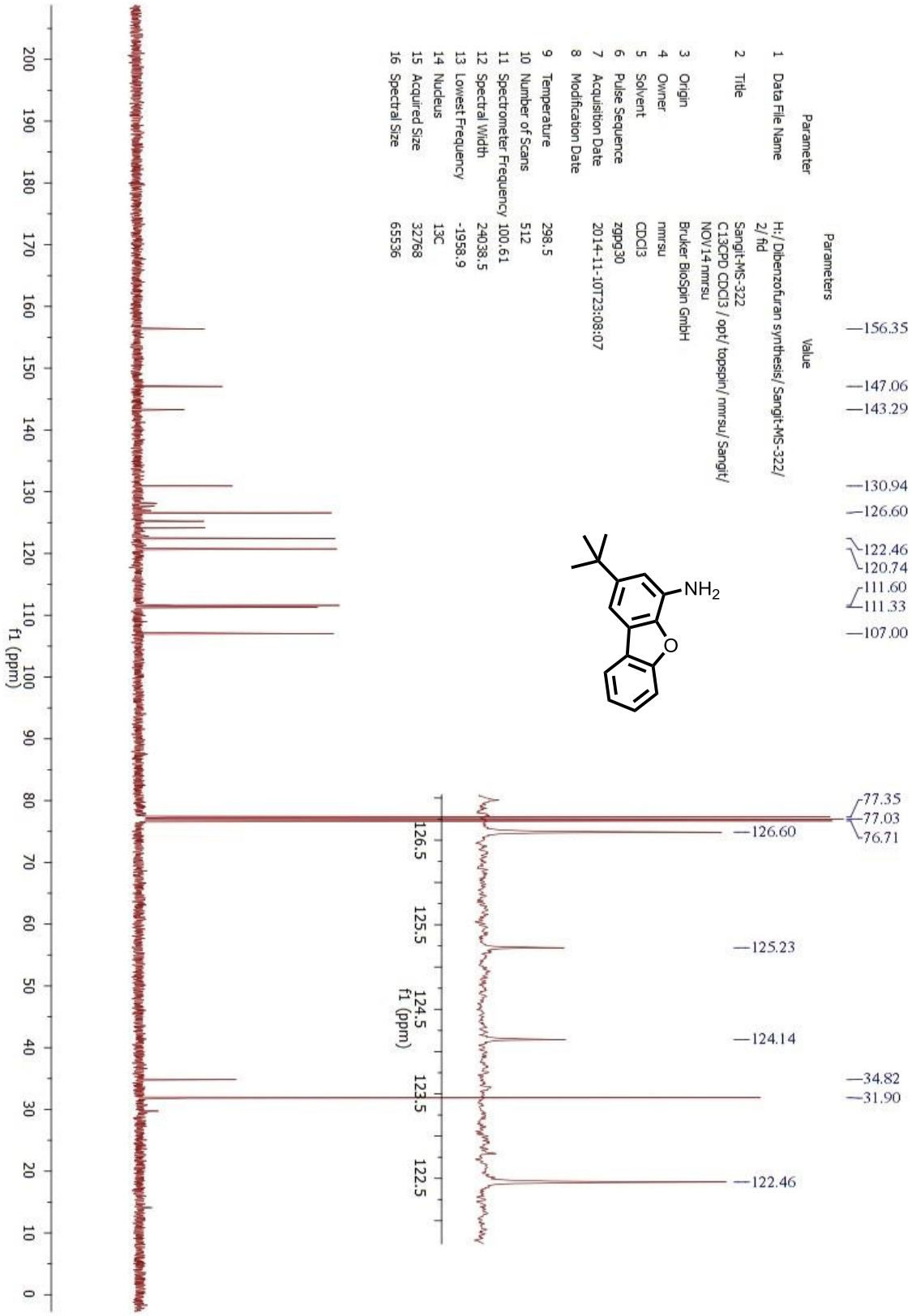

Figure S115 ^{1}H NMR spectrum of **7** and **8**

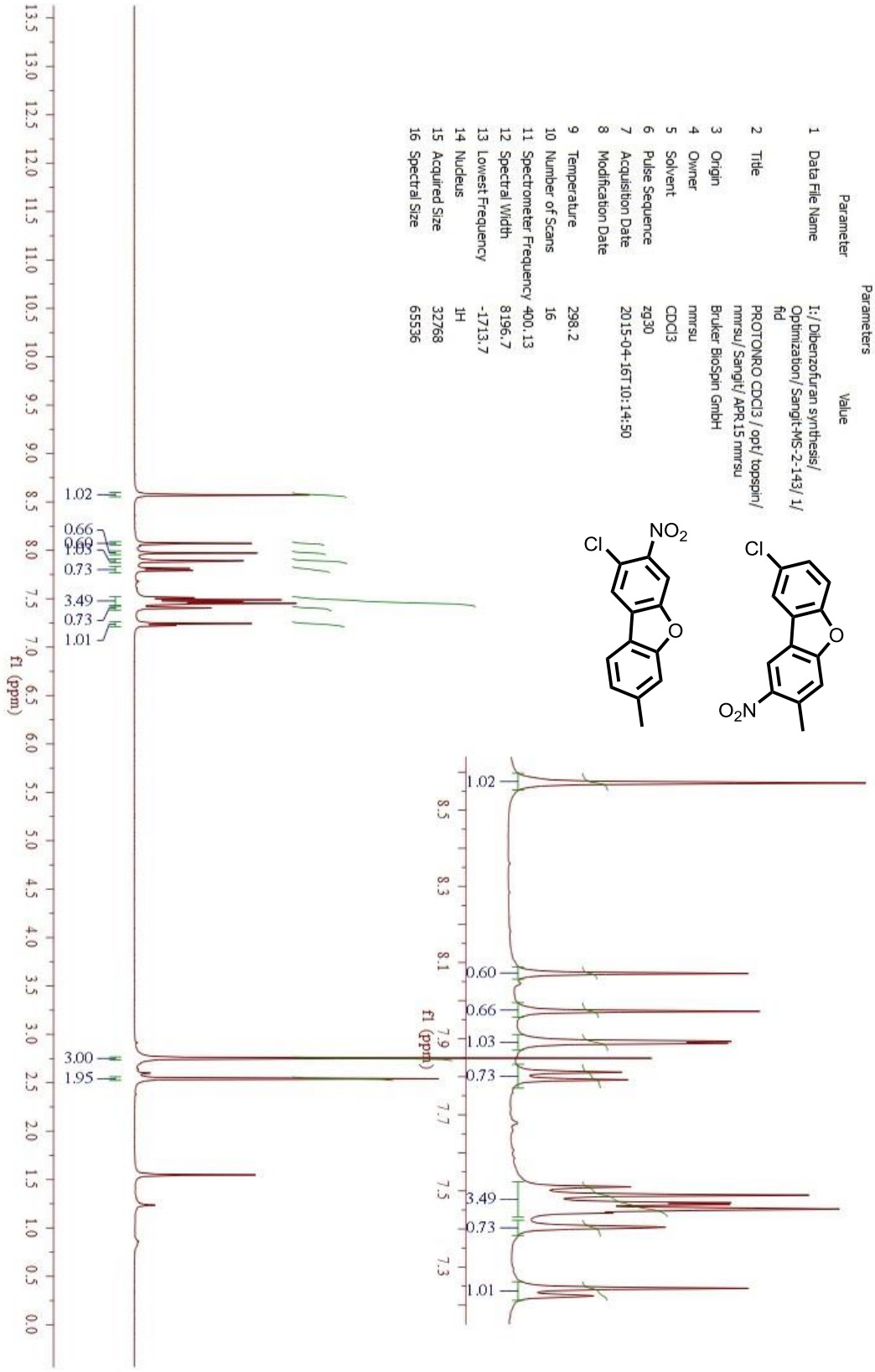

Figure S116^{13}C NMR spectrum of **7** and **8**

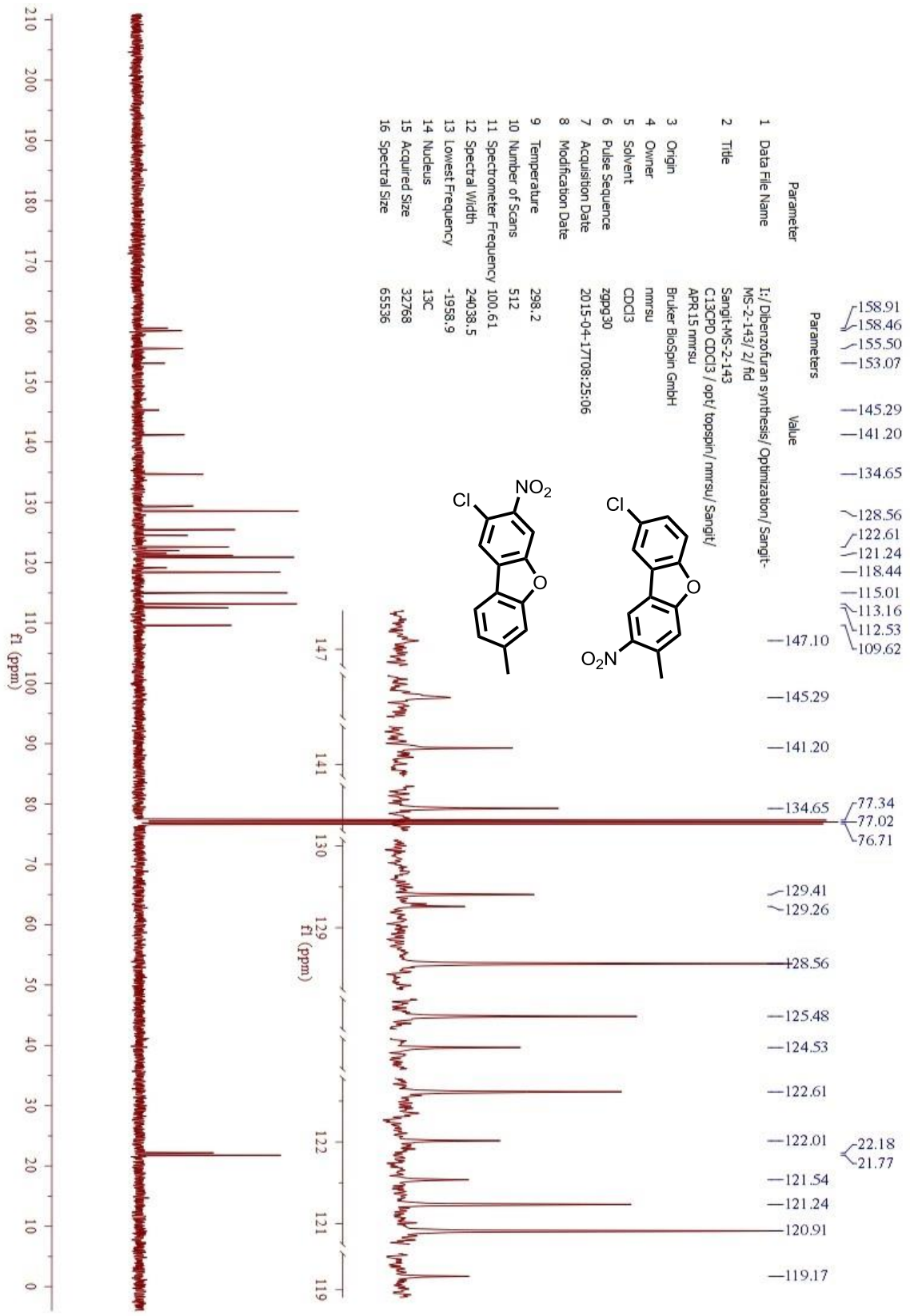

Figure S117. ORTEP views of **1p**

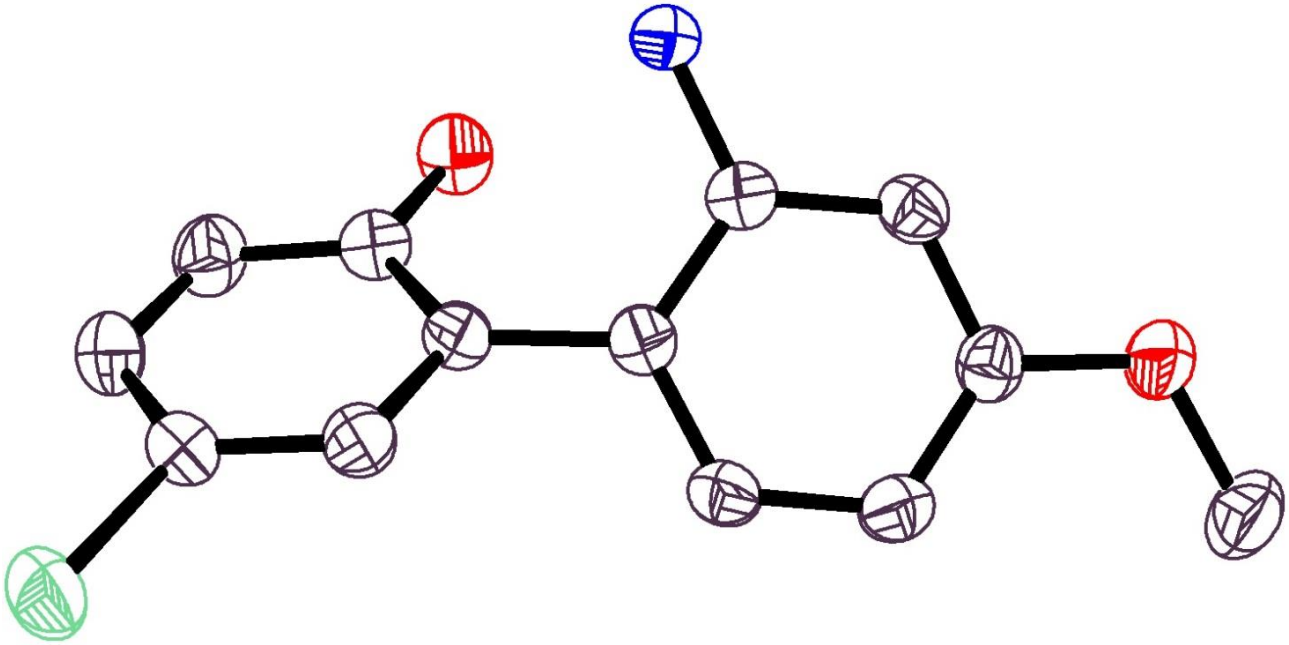

Figure S118 **Packing diagram of 1p**

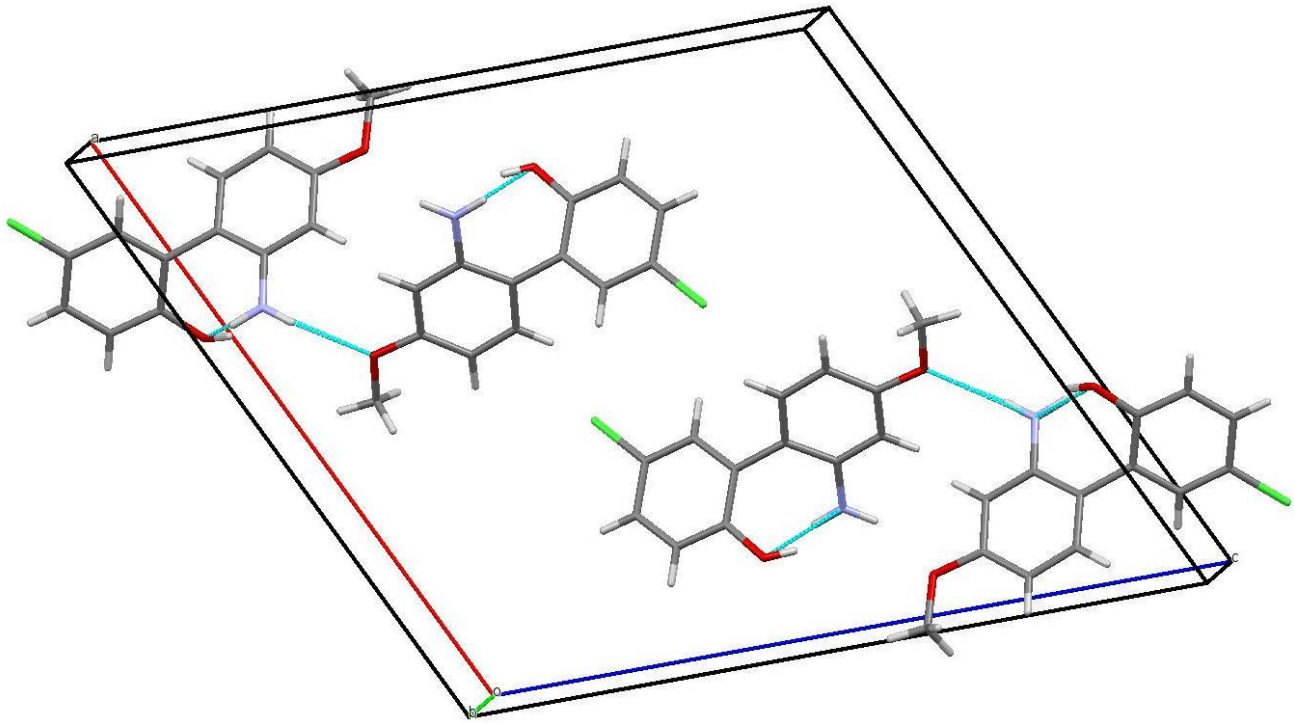

Table S1. Crystal data and structure refinement for 1p.

Identification code	MS-298	
Empirical formula	C_{13} H_{12} Cl N O_2	
Formula weight	249.69	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 17.0453(11) Å	α= 90°.
	b = 4.0783(3) Å	β= 115.131(3)°.
	c = 18.9440(12) Å	γ = 90°.
Volume	1192.25(14) $Å^3$	
Z	4	
Density (calculated)	1.391 Mg/m^3	
Absorption coefficient	0.309 mm^{-1}	
F(000)	520	
Theta range for data collection	1.349 to 25.113°.	
Index ranges	-20<=h<=20, -4<=k<=4, -22<=l<=22	
Reflections collected	14459	
Independent reflections	2115 [R(int) = 0.0351]	
Completeness to theta = 25.242°	98.4 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2115 / 0 / 156	
Goodness-of-fit on F^2	1.072	
Final R indices [I>2sigma(I)]	R1 = 0.0367, wR2 = 0.1046	
R indices (all data)	R1 = 0.0399, wR2 = 0.1082	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.533 and -0.516 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 1p. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	4084(1)	-238(2)	3591(1)	53(1)
O(1)	1540(1)	4729(3)	4663(1)	42(1)
O(2)	4086(1)	4720(3)	8222(1)	46(1)
N(004)	1989(1)	434(4)	5835(1)	36(1)
C(2)	2797(1)	1999(4)	6246(1)	30(1)
C(7)	2984(1)	2603(4)	4988(1)	32(1)
C(1)	3278(1)	3054(4)	5843(1)	31(1)
C(12)	3566(1)	1442(5)	4707(1)	35(1)
C(8)	2153(1)	3505(4)	4440(1)	34(1)
C(3)	3095(1)	2607(4)	7037(1)	33(1)
C(4)	3873(1)	4231(4)	7444(1)	33(1)
C(11)	3333(1)	1236(5)	3917(1)	37(1)
C(6)	4066(1)	4600(4)	6276(1)	35(1)
C(5)	4375(1)	5200(4)	7069(1)	38(1)
C(9)	1934(1)	3293(5)	3648(1)	41(1)
C(10)	2518(1)	2162(5)	3379(1)	42(1)
C(13)	4867(1)	6484(6)	8670(1)	51(1)

Table S3. Selected bond lengths [Å] for 1p.

Cl1—C11	1.7480 (17)	C12—H12	0.93
O1—C8	1.377 (2)	C8—C9	1.386 (2)
O1—H1	0.82	C3—C4	1.387 (2)
O2—C4	1.374 (2)	C3—H3	0.93
O2—C13	1.432 (2)	C4—C5	1.382 (3)

N004—C2	1.414 (2)	C11—C10	1.380 (2)
N004—H00A	0.86	C6—C5	1.386 (2)
N004—H00B	0.86	C6—H6	0.93
C2—C3	1.385 (2)	C5—H5	0.93
C2—C1	1.405 (2)	C9—C10	1.376 (3)
C7—C12	1.393 (2)	C9—H9	0.93
C7—C8	1.404 (2)	C10—H10	0.93
C7—C1	1.489 (2)	C13—H13A	0.96
C1—C6	1.392 (2)	C13—H13B	0.96
C12—C11	1.378 (2)	C13—H13C	0.96

Table S4. Bond angles [°] for 1p.

C8—O1—H1	109.5	O2—C4—C3	114.91 (15)
C4—O2—C13	117.66 (14)	C5—C4—C3	120.27 (15)
C2—N004—H00A	120	C12—C11—C10	121.39 (16)
C2—N004—H00B	120	C12—C11—Cl1	119.18 (13)
H00A—N004—H00B	120	C10—C11—Cl1	119.43 (13)
C3—C2—C1	120.17 (15)	C5—C6—C1	123.09 (15)
C3—C2—N004	120.02 (14)	C5—C6—H6	118.5
C1—C2—N004	119.75 (14)	C1—C6—H6	118.5
C12—C7—C8	117.67 (15)	C4—C5—C6	118.31 (16)
C12—C7—C1	119.47 (14)	C4—C5—H5	120.8

C8—C7—C1	122.73 (15)	C6—C5—H5	120.8
C6—C1—C2	117.28 (15)	C10—C9—C8	121.11 (16)
C6—C1—C7	119.49 (14)	C10—C9—H9	119.4
C2—C1—C7	123.24 (14)	C8—C9—H9	119.4
C11—C12—C7	120.80 (15)	C9—C10—C11	118.51 (16)
C11—C12—H12	119.6	C9—C10—H10	120.7
C7—C12—H12	119.6	C11—C10—H10	120.7
O1—C8—C9	117.71 (15)	O2—C13—H13A	109.5
O1—C8—C7	121.74 (15)	O2—C13—H13B	109.5
C9—C8—C7	120.51 (16)	H13A—C13—H13B	109.5
C2—C3—C4	120.83 (15)	O2—C13—H13C	109.5
C2—C3—H3	119.6	H13A—C13—H13C	109.5
C4—C3—H3	119.6	H13B—C13—H13C	109.5
O2—C4—C5	124.82 (16)		

Table S5. Anisotropic displacement parameters ($Å^2$x 10^3)for 1p. 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}
Cl(1)	44(1)	80(1)	42(1)	-10(1)	25(1)	1(1)
O(1)	36(1)	47(1)	42(1)	2(1)	16(1)	11(1)
O(2)	43(1)	63(1)	32(1)	-11(1)	16(1)	-10(1)
N(004)	34(1)	42(1)	34(1)	-6(1)	17(1)	-10(1)
C(2)	29(1)	27(1)	34(1)	-1(1)	14(1)	2(1)

C(7)	33(1)	31(1)	31(1)	1(1)	14(1)	-1(1)
C(1)	30(1)	31(1)	31(1)	2(1)	13(1)	4(1)
C(12)	30(1)	42(1)	32(1)	1(1)	12(1)	1(1)
C(8)	34(1)	32(1)	37(1)	1(1)	15(1)	2(1)
C(3)	35(1)	33(1)	35(1)	-1(1)	20(1)	0(1)
C(4)	35(1)	35(1)	30(1)	-3(1)	13(1)	3(1)
C(11)	37(1)	42(1)	35(1)	-1(1)	20(1)	-2(1)
C(6)	30(1)	43(1)	36(1)	1(1)	17(1)	-1(1)
C(5)	30(1)	43(1)	38(1)	-4(1)	13(1)	-5(1)
C(9)	38(1)	47(1)	33(1)	5(1)	8(1)	6(1)
C(10)	46(1)	49(1)	29(1)	1(1)	14(1)	-1(1)
C(13)	44(1)	62(1)	37(1)	-13(1)	9(1)	-6(1)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for 1p.

	x	y	z	U(eq)
H(1)	1537	3629	5024	62
H(00A)	1682	-140	6076	43
H(00B)	1804	57	5344	43
H(12)	4118	798	5056	42
H(3)	2769	1918	7298	39
H(6)	4401	5261	6021	42
H(5)	4906	6228	7341	45
H(9)	1383	3927	3292	50
H(10)	2368	2025	2847	50
H(13A)	5354	5295	8672	76
H(13B)	4930	6729	9195	76
H(13C)	4841	8609	8443	76

Figure S119 ORTEP views of **2a**

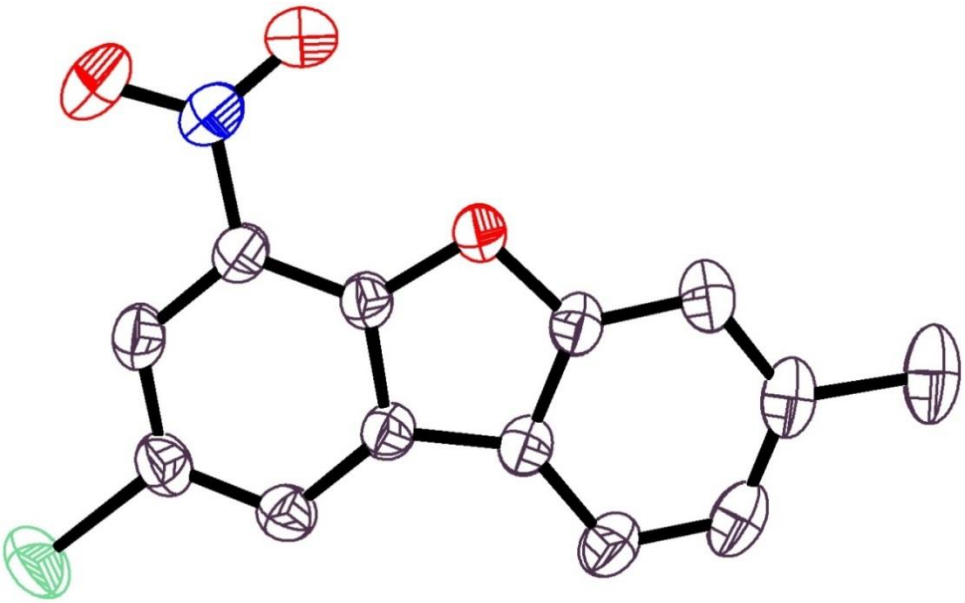

Figure S120 **Packing diagram of 2a.**

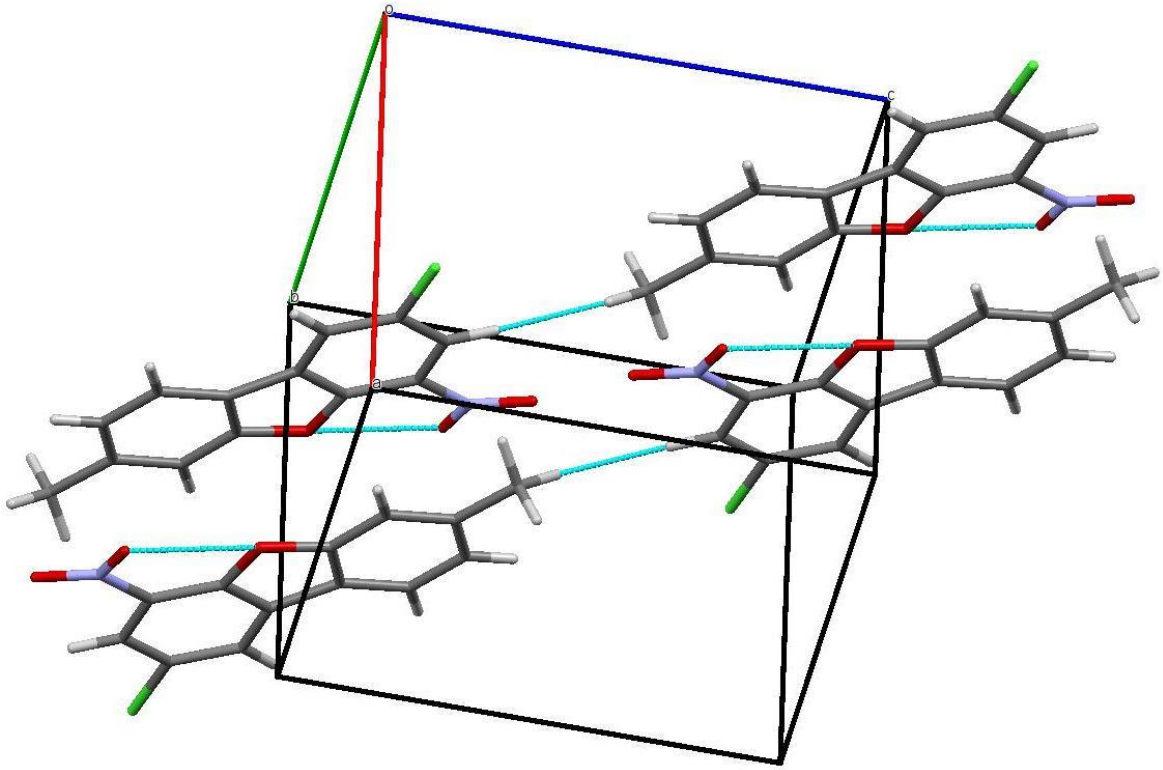

Table S7. Crystal data and structure refinement for 2a.

Identification code	AK-5-90	
Empirical formula	C_{13} H_8 Cl N O_3	
Formula weight	261.65	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.2089(4) Å	α= 78.365(2)°.
	b = 8.7381(5) Å	β= 88.899(2)°.
	c = 10.2105(6) Å	γ = 67.042(2)°.
Volume	578.80(6) $Å^3$	
Z	2	
Density (calculated)	1.501 Mg/m^3	
Absorption coefficient	0.328 mm^{-1}	
F(000)	268	
Theta range for data collection	2.590 to 27.517°.	
Index ranges	-9<=h<=9, -11<=k<=11, -13<=l<=13	
Reflections collected	20323	
Independent reflections	2667 [R(int) = 0.0283]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2667 / 0 / 165	
Goodness-of-fit on F^2	1.040	
Final R indices [I>2sigma(I)]	R1 = 0.0370, wR2 = 0.1030	
R indices (all data)	R1 = 0.0441, wR2 = 0.1088	
Extinction coefficient	0.043(8)	
Largest diff. peak and hole	0.261 and -0.182 $e.Å^{-3}$	

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 2a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(01)	2996(1)	-5637(1)	11892(1)	64(1)
O(1)	2194(2)	1423(1)	10685(1)	40(1)
C(5)	2825(2)	-2732(2)	10262(1)	41(1)
C(3)	2539(2)	-2738(2)	12628(1)	42(1)
C(1)	2371(2)	-216(2)	11101(1)	35(1)
C(7)	2628(2)	187(2)	8856(1)	37(1)
C(6)	2633(2)	-1052(2)	10032(1)	35(1)
C(2)	2339(2)	-1065(2)	12398(1)	39(1)
C(11)	2245(2)	3152(2)	8486(2)	46(1)
C(4)	2773(2)	-3544(2)	11566(2)	43(1)
C(8)	2798(2)	220(2)	7486(1)	47(1)
O(3)	2467(3)	-1154(2)	14653(1)	88(1)
C(12)	2356(2)	1652(2)	9308(1)	38(1)
O(2)	1608(3)	1269(2)	13320(1)	94(1)
N(1)	2110(2)	-251(2)	13539(1)	55(1)
C(10)	2415(2)	3170(2)	7128(2)	50(1)
C(9)	2681(2)	1711(2)	6652(2)	53(1)
C(13)	2298(3)	4767(3)	6171(2)	72(1)

Table S9. Bond lengths [Å] for 2a.

Cl01—C4	1.7347 (14)	C2—N1	1.4573 (19)
O1—C1	1.3645 (15)	C11—C12	1.3806 (19)
O1—C12	1.3888 (16)	C11—C10	1.388 (2)
C5—C4	1.384 (2)	C11—H009	0.95

C5—C6	1.3903 (18)	C8—C9	1.378 (2)
C5—H003	0.95	C8—H011	0.95
C3—C4	1.382 (2)	O3—N1	1.2141 (19)
C3—C2	1.3824 (19)	O2—N1	1.2058 (19)
C3—H004	0.95	C10—C9	1.397 (3)
C1—C2	1.3864 (18)	C10—C13	1.507 (2)
C1—C6	1.4021 (18)	C9—H017	0.95
C7—C12	1.390 (2)	C13—H1AA	0.98
C7—C8	1.397 (2)	C13—H1AB	0.98
C7—C6	1.4444 (18)	C13—H1AC	0.98

Table S10. Bond angles [°] for 2a.

C1—O1—C12	105.37 (10)	C3—C4—Cl01	118.38 (11)
C4—C5—C6	118.16 (13)	C5—C4—Cl01	119.53 (12)
C4—C5—H003	120.9	C9—C8—C7	118.13 (15)
C6—C5—H003	120.9	C9—C8—H011	120.9
C4—C3—C2	119.74 (13)	C7—C8—H011	120.9
C4—C3—H004	120.1	C11—C12—O1	124.33 (13)
C2—C3—H004	120.1	C11—C12—C7	124.04 (13)
O1—C1—C2	127.61 (12)	O1—C12—C7	111.63 (11)
O1—C1—C6	112.03 (11)	O2—N1—O3	124.05 (15)
C2—C1—C6	120.36 (12)	O2—N1—C2	118.23 (13)

C12—C7—C8	118.48 (13)	O3—N1—C2	117.71 (14)
C12—C7—C6	105.66 (11)	C11—C10—C9	119.87 (14)
C8—C7—C6	135.85 (13)	C11—C10—C13	119.81 (17)
C5—C6—C1	120.22 (12)	C9—C10—C13	120.31 (16)
C5—C6—C7	134.48 (13)	C8—C9—C10	122.53 (14)
C1—C6—C7	105.31 (11)	C8—C9—H017	118.7
C3—C2—C1	119.43 (12)	C10—C9—H017	118.7
C3—C2—N1	118.56 (12)	C10—C13—H1AA	109.5
C1—C2—N1	122.01 (13)	C10—C13—H1AB	109.5
C12—C11—C10	116.95 (15)	H1AA—C13—H1AB	109.5
C12—C11—H009	121.5	C10—C13—H1AC	109.5
C10—C11—H009	121.5	H1AA—C13—H1AC	109.5
C3—C4—C5	122.08 (13)	H1AB—C13—H1AC	109.5

Table S11. Anisotropic displacement parameters ($Å^2$x 10^3) for 2a. 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}
Cl(01)	82(1)	35(1)	77(1)	-8(1)	18(1)	-27(1)
O(1)	56(1)	36(1)	33(1)	-6(1)	3(1)	-23(1)
C(5)	46(1)	39(1)	42(1)	-13(1)	7(1)	-20(1)
C(3)	46(1)	40(1)	37(1)	0(1)	5(1)	-19(1)
C(1)	39(1)	34(1)	33(1)	-5(1)	2(1)	-18(1)
C(7)	39(1)	41(1)	33(1)	-5(1)	2(1)	-19(1)

C(6)	37(1)	38(1)	32(1)	-7(1)	3(1)	-18(1)
C(2)	45(1)	42(1)	31(1)	-7(1)	5(1)	-19(1)
C(11)	50(1)	42(1)	45(1)	2(1)	-2(1)	-23(1)
C(4)	45(1)	34(1)	50(1)	-5(1)	6(1)	-18(1)
C(8)	52(1)	56(1)	34(1)	-9(1)	4(1)	-25(1)
O(3)	156(2)	82(1)	31(1)	-9(1)	7(1)	-53(1)
C(12)	41(1)	41(1)	32(1)	-2(1)	0(1)	-20(1)
O(2)	181(2)	57(1)	51(1)	-24(1)	27(1)	-50(1)
N(1)	81(1)	57(1)	35(1)	-13(1)	12(1)	-34(1)
C(10)	48(1)	55(1)	42(1)	9(1)	-3(1)	-24(1)
C(9)	55(1)	70(1)	31(1)	1(1)	1(1)	-29(1)
C(13)	79(1)	72(1)	56(1)	24(1)	-6(1)	-37(1)

Table S12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 2a.

	x	y	z	U(eq)
H(003)	2989	-3307	9544	49
H(004)	2515	-3331	13513	50
H(009)	2061	4128	8835	55
H(011)	2989	-757	7139	56
H(017)	2786	1749	5719	63
H(1AA)	2919	5364	6611	108
H(1AB)	880	5506	5904	108
H(1AC)	3017	4470	5375	108

Table S13. Torsion angles [°] for 2a.

C12—O1—C1—C2	178.94 (13)	C6—C5—C4—Cl01	179.68 (10)
C12—O1—C1—C6	−0.30 (14)	C12—C7—C8—C9	−0.2 (2)

C4—C5—C6—C1	−0.7 (2)	C6—C7—C8—C9	178.83 (15)
C4—C5—C6—C7	179.46 (14)	C10—C11—C12—O1	−179.32 (13)
O1—C1—C6—C5	−179.53 (11)	C10—C11—C12—C7	0.1 (2)
C2—C1—C6—C5	1.2 (2)	C1—O1—C12—C11	179.58 (13)
O1—C1—C6—C7	0.37 (15)	C1—O1—C12—C7	0.10 (14)
C2—C1—C6—C7	−178.94 (12)	C8—C7—C12—C11	−0.1 (2)
C12—C7—C6—C5	179.59 (14)	C6—C7—C12—C11	−179.36 (13)
C8—C7—C6—C5	0.5 (3)	C8—C7—C12—O1	179.42 (12)
C12—C7—C6—C1	−0.28 (14)	C6—C7—C12—O1	0.12 (15)
C8—C7—C6—C1	−179.40 (15)	C3—C2—N1—O2	−168.02 (17)
C4—C3—C2—C1	0.2 (2)	C1—C2—N1—O2	12.3 (2)
C4—C3—C2—N1	−179.53 (13)	C3—C2—N1—O3	13.0 (2)
O1—C1—C2—C3	179.92 (13)	C1—C2—N1—O3	−166.68 (16)
C6—C1—C2—C3	−0.9 (2)	C12—C11—C10—C9	0.1 (2)
O1—C1—C2—N1	−0.4 (2)	C12—C11—C10—C13	179.71 (14)
C6—C1—C2—N1	178.78 (13)	C7—C8—C9—C10	0.4 (2)
C2—C3—C4—C5	0.3 (2)	C11—C10—C9—C8	−0.4 (2)
C2—C3—C4—Cl01	−179.42 (11)	C13—C10—C9—C8	−179.99 (16)
C6—C5—C4—C3	−0.1 (2)		

Figure S121 ORTEP views of **2d**

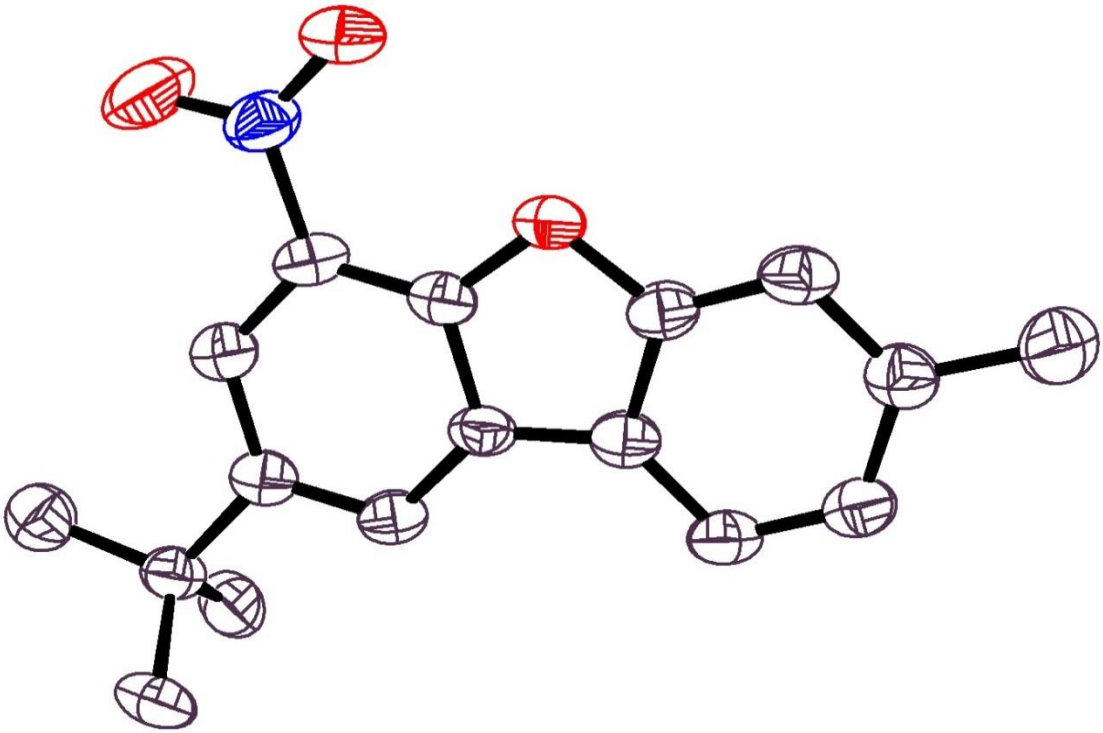

Figure S122 **Packing Diagram of 2d**

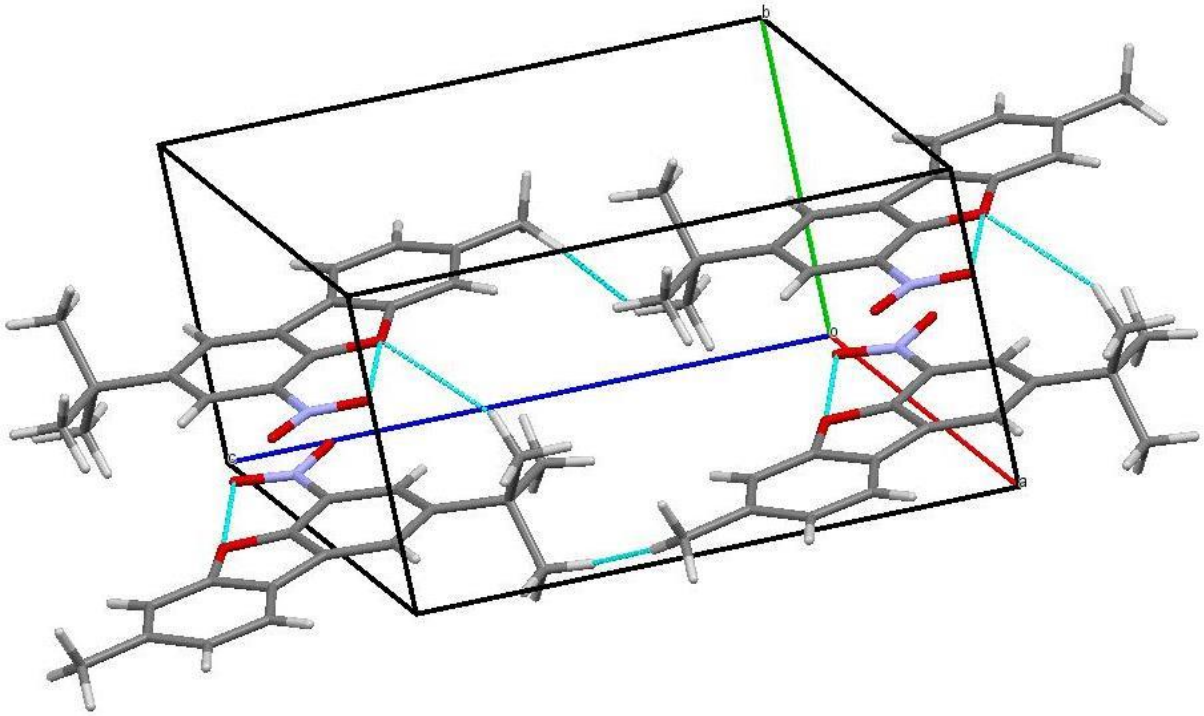

Table S14. Crystal data and structure refinement for 2d

Identification code	**2d**	
Empirical formula	C_{17} H_{17} N O_3	
Formula weight	283.31	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2_1	
Unit cell dimensions	a = 8.8713(5) Å	α= 90°.
	b = 7.0968(4) Å	β= 110.095(3)°.
	c = 12.0516(6) Å	γ = 90°.
Volume	712.55(7) $Å^3$	
Z	2	
Density (calculated)	1.320 Mg/m^3	
Absorption coefficient	0.091 mm^{-1}	
F(000)	300	
Theta range for data collection	1.799 to 26.954°.	
Index ranges	-11<=h<=11, -9<=k<=9, -15<=l<=13	
Reflections collected	7512	
Independent reflections	2880 [R(int) = 0.0325]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2880 / 1 / 195	
Goodness-of-fit on F^2	1.048	
Final R indices [I>2sigma(I)]	R1 = 0.0434, wR2 = 0.1095	
R indices (all data)	R1 = 0.0573, wR2 = 0.1200	
Absolute structure parameter	1.9(10)	
Extinction coefficient	0.049(6)	
Largest diff. peak and hole	0.196 and -0.167 $e.Å^{-3}$	

Table S15. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 2d. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(3)	1110(2)	567(14)	-1410(2)	88(1)
O(2)	2036(2)	556(15)	465(2)	87(1)
O(1)	5219(2)	456(9)	1663(1)	43(1)
N(1)	2216(2)	482(11)	-484(2)	50(1)
C(1)	6809(10)	2234(7)	-2967(6)	56(2)
C(2)	5864(3)	488(12)	-2883(2)	44(1)
C(3)	5596(3)	511(12)	-1690(2)	40(1)
C(4)	6925(3)	486(12)	-646(2)	42(1)
C(5)	6721(2)	469(11)	442(2)	40(1)
C(6)	7805(2)	460(11)	1653(2)	40(1)
C(7)	6838(2)	477(11)	2351(2)	40(1)
C(8)	7421(3)	440(11)	3563(2)	44(1)
C(9)	9077(3)	493(12)	4120(2)	44(1)
C(10)	9798(3)	461(14)	5443(2)	56(1)
C(11)	6826(9)	-1299(7)	-2953(6)	55(2)
C(12)	4074(3)	459(12)	-1595(2)	42(1)
C(13)	3850(2)	492(12)	-510(2)	41(1)
C(14)	5169(2)	461(11)	514(2)	38(1)
C(15)	9459(3)	454(12)	2213(2)	45(1)
C(16)	10060(3)	443(13)	3427(2)	48(1)
C(17)	4291(3)	445(15)	-3922(2)	58(1)

Table S16. Selected bond lengths [Å] for 2d

O3—N1	1.208 (3)	C7—C8	1.372 (3)
O2—N1	1.209 (3)	C8—C9	1.390 (3)

O1—C14	1.370 (2)	C8—H5	0.93
O1—C7	1.390 (2)	C9—C16	1.400 (3)
N1—C13	1.460 (3)	C9—C10	1.501 (3)
C1—C2	1.519 (10)	C10—H2	0.96
C1—H12	0.96	C10—H7	0.96
C1—H11	0.96	C10—H6	0.96
C1—H1	0.96	C11—H17	0.96
C2—C17	1.522 (3)	C11—H3	0.96
C2—C3	1.536 (3)	C11—H16	0.96
C2—C11	1.547 (9)	C12—C13	1.388 (3)
C3—C12	1.395 (3)	C12—H10	0.93
C3—C4	1.398 (3)	C13—C14	1.378 (3)
C4—C5	1.384 (3)	C15—C16	1.375 (3)
C4—H4	0.93	C15—H9	0.93
C5—C14	1.409 (3)	C16—H8	0.93
C5—C6	1.446 (3)	C17—H15	0.96
C6—C15	1.389 (3)	C17—H14	0.96
C6—C7	1.392 (3)	C17—H13	0.96

Table S17. Selected Bond angles [°] for 2d

C14—O1—C7	105.74 (15)	C8—C9—C10	120.4 (2)
O3—N1—O2	122.8 (2)	C16—C9—C10	120.5 (2)
O3—N1—C13	118.6 (2)	C9—C10—H2	109.5

O2—N1—C13	118.3 (2)	C9—C10—H7	109.5
C2—C1—H12	109.5	H2—C10—H7	109.5
C2—C1—H11	109.5	C9—C10—H6	109.5
H12—C1—H11	109.5	H2—C10—H6	109.5
C2—C1—H1	109.5	H7—C10—H6	109.5
H12—C1—H1	109.5	C2—C11—H17	109.5
H11—C1—H1	109.5	C2—C11—H3	109.5
C1—C2—C17	109.4 (6)	H17—C11—H3	109.5
C1—C2—C3	108.7 (5)	C2—C11—H16	109.5
C17—C2—C3	112.16 (18)	H17—C11—H16	109.5
C1—C2—C11	109.75 (18)	H3—C11—H16	109.5
C17—C2—C11	107.8 (6)	C13—C12—C3	122.2 (2)
C3—C2—C11	109.0 (5)	C13—C12—H10	118.9
C12—C3—C4	117.8 (2)	C3—C12—H10	118.9
C12—C3—C2	122.9 (2)	C14—C13—C12	119.37 (18)
C4—C3—C2	119.25 (18)	C14—C13—N1	121.64 (19)
C5—C4—C3	120.58 (19)	C12—C13—N1	118.9 (2)
C5—C4—H4	119.7	O1—C14—C13	128.86 (18)
C3—C4—H4	119.7	O1—C14—C5	111.66 (18)
C4—C5—C14	120.5 (2)	C13—C14—C5	119.5 (2)
C4—C5—C6	134.32 (19)	C16—C15—C6	118.4 (2)

C14—C5—C6	105.23 (18)	C16—C15—H9	120.8
C15—C6—C7	118.3 (2)	C6—C15—H9	120.8
C15—C6—C5	135.6 (2)	C15—C16—C9	122.8 (2)
C7—C6—C5	106.02 (18)	C15—C16—H8	118.6
C8—C7—O1	124.71 (18)	C9—C16—H8	118.6
C8—C7—C6	123.9 (2)	C2—C17—H15	109.5
O1—C7—C6	111.34 (19)	C2—C17—H14	109.5
C7—C8—C9	117.6 (2)	H15—C17—H14	109.5
C7—C8—H5	121.2	C2—C17—H13	109.5
C9—C8—H5	121.2	H15—C17—H13	109.5
C8—C9—C16	118.9 (2)	H14—C17—H13	109.5

Table S18. Anisotropic displacement parameters ($Å^2$x 10^3) for 2d. The anisotropic displacement factor exponent takes the form: $-2\pi^2$[h2a*2U^{11} + ... + 2 h k a* b* U^{12}]

	U11	U22	U33	U23
O(3)	36(1)	159(3)	69(1)	23(4)
O(2)	47(1)	157(3)	69(1)	-19(4)
O(1)	38(1)	51(1)	48(1)	-2(2)
N(1)	37(1)	58(1)	62(1)	-1(3)
C(1)	61(5)	60(3)	53(3)	-10(3)
C(2)	41(1)	48(1)	48(1)	-5(4)
C(3)	42(1)	38(1)	47(1)	2(3)
C(4)	35(1)	48(1)	50(1)	2(4)
C(5)	36(1)	38(1)	50(1)	-7(3)
C(6)	40(1)	39(1)	47(1)	2(3)

C(7)	35(1)	38(1)	51(1)	2(3)
C(8)	45(1)	44(1)	52(1)	11(3)
C(9)	45(1)	38(1)	51(1)	-6(3)
C(10)	54(2)	65(2)	53(2)	19(4)
C(11)	62(4)	52(3)	66(4)	-12(3)
C(12)	38(1)	41(1)	49(1)	0(3)
C(13)	33(1)	40(1)	55(1)	10(3)
C(14)	40(1)	36(1)	47(1)	-4(3)
C(15)	39(1)	51(1)	54(1)	4(4)
C(16)	39(1)	54(1)	54(1)	1(4)
C(17)	55(2)	72(2)	49(1)	1(4)

Table S19. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 2d

	x	y	z	U(eq)
H(12)	6893	2300	-3740	85
H(11)	7864	2170	-2383	85
H(1)	6267	3336	-2834	85
H(4)	7955	482	-682	51
H(5)	6733	381	3996	52
H(2)	9055	-106	5764	85
H(7)	10027	1727	5734	85
H(6)	10774	-258	5678	85
H(17)	6235	-2399	-2881	82
H(3)	7844	-1282	-2322	82
H(16)	6995	-1326	-3698	82
H(10)	3179	401	-2281	50
H(9)	10144	458	1776	55
H(8)	11167	401	3805	58
H(15)	4512	346	-4646	87

H(14)	3702	1583	-3929	87
H(13)	3666	-620	-3846	87

Table S20. Torsion angles [°] for 2d

C1—C2—C3—C12	122.3 (8)	C4—C3—C12—C13	3.7 (12)
C17—C2—C3—C12	1.2 (12)	C2—C3—C12—C13	−179.6 (7)
C11—C2—C3—C12	−118.1 (8)	C3—C12—C13—C14	−4.0 (12)
C1—C2—C3—C4	−61.1 (8)	C3—C12—C13—N1	178.4 (8)
C17—C2—C3—C4	177.9 (7)	O3—N1—C13—C14	177.8 (8)
C11—C2—C3—C4	58.5 (8)	O2—N1—C13—C14	4.2 (13)
C12—C3—C4—C5	−1.9 (12)	O3—N1—C13—C12	−4.6 (13)
C2—C3—C4—C5	−178.7 (7)	O2—N1—C13—C12	−178.3 (8)
C3—C4—C5—C14	0.5 (12)	C7—O1—C14—C13	−178.3 (7)
C3—C4—C5—C6	−179.3 (8)	C7—O1—C14—C5	0.5 (9)
C4—C5—C6—C15	−0.5 (16)	C12—C13—C14—O1	−178.9 (7)
C14—C5—C6—C15	179.7 (10)	N1—C13—C14—O1	−1.4 (13)
C4—C5—C6—C7	178.9 (9)	C12—C13—C14—C5	2.4 (12)
C14—C5—C6—C7	−0.9 (8)	N1—C13—C14—C5	179.9 (8)
C14—O1—C7—C8	−178.6 (7)	C4—C5—C14—O1	−179.6 (7)
C14—O1—C7—C6	−1.1 (8)	C6—C5—C14—O1	0.2 (9)
C15—C6—C7—C8	−1.7 (12)	C4—C5—C14—C13	−0.7 (12)
C5—C6—C7—C8	178.7 (7)	C6—C5—C14—C13	179.1 (7)
C15—C6—C7—O1	−179.2 (7)	C7—C6—C15—C16	0.7 (13)

C5—C6—C7—O1	1.2 (8)	C5—C6—C15—C16	−179.9 (9)
O1—C7—C8—C9	−179.2 (8)	C6—C15—C16—C9	−1.9 (13)
C6—C7—C8—C9	3.6 (11)	C8—C9—C16—C15	3.9 (13)
C7—C8—C9—C16	−4.5 (11)	C10—C9—C16—C15	179.5 (9)
C7—C8—C9—C10	179.9 (7)		

Figure S123 ORTEP views of **2e**

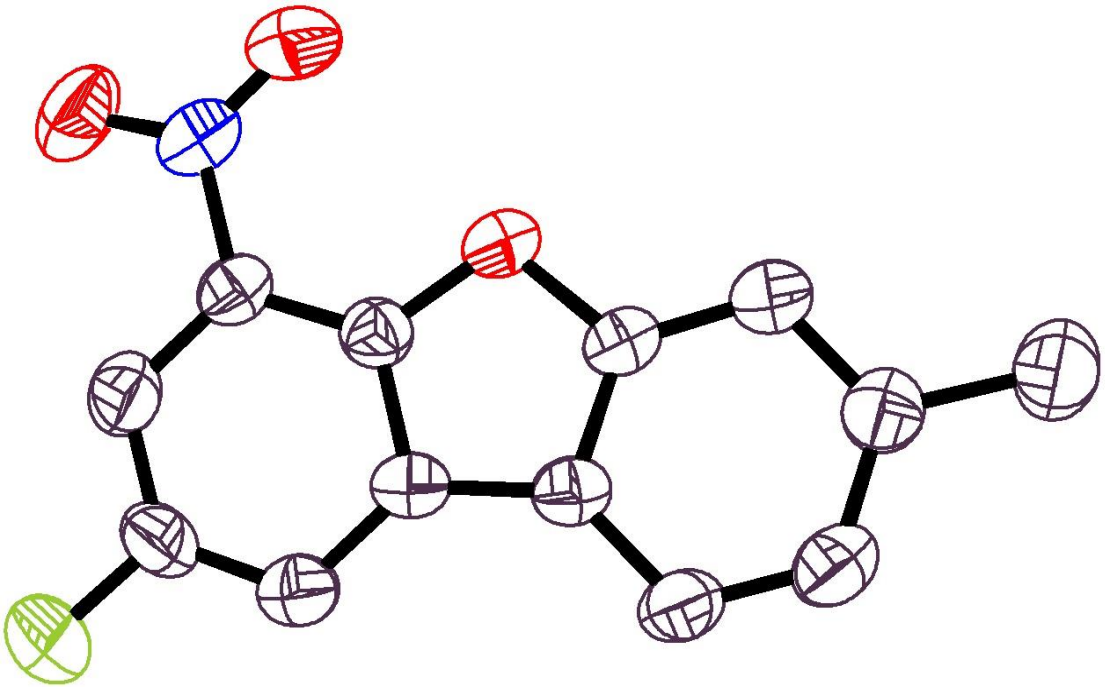

Figure S124 **Packing diagram of 2e.**

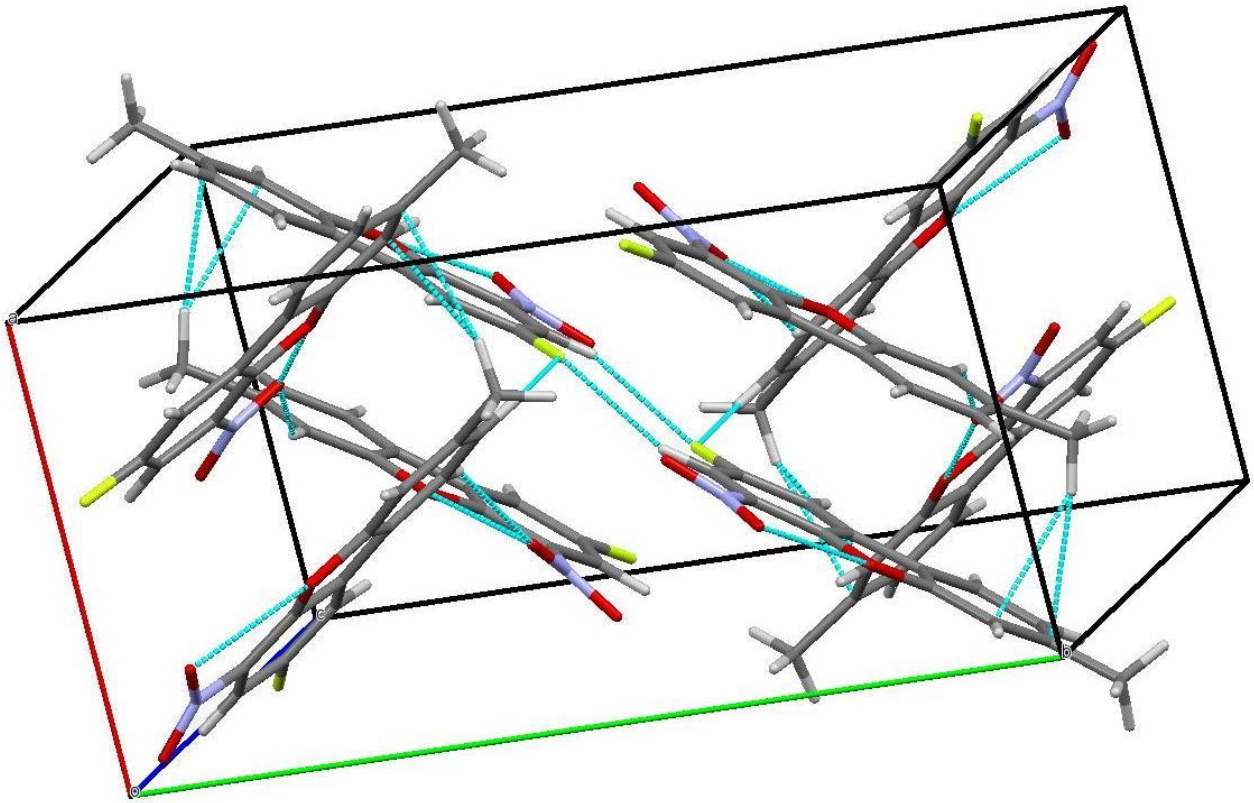

Table S21. Crystal data and structure refinement for 2e.

Identification code	MS_282_I	
Empirical formula	C_{13} H_8 F N O_3	
Formula weight	245.20	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P $2_{1/c}$	
Unit cell dimensions	a = 9.2951(8) Å	α= 90°.
	b = 17.4748(14) Å	β= 100.270(5)°.
	c = 13.7550(11) Å	γ = 90°.
Volume	2198.4(3) $Å^3$	
Z	8	

Density (calculated)	1.482 Mg/m^3
Absorption coefficient	0.118 mm^{-1}
F(000)	1008
Theta range for data collection	2.227 to 25.101°.
Index ranges	-11<=h<=11, -20<=k<=20, -16<=l<=16
Reflections collected	49564
Independent reflections	3911 [R(int) = 0.1670]
Completeness to theta = 25.242°	98.3 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3911 / 0 / 327
Goodness-of-fit on F^2	1.042
Final R indices [I>2sigma(I)]	R1 = 0.0628, wR2 = 0.1153
R indices (all data)	R1 = 0.1498, wR2 = 0.1433
Extinction coefficient	n/a
Largest diff. peak and hole	0.163 and -0.173 $e.Å^{-3}$

Table S22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 2e. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(4)	3698(2)	2627(1)	5248(1)	52(1)
O(1)	1608(2)	7596(1)	2813(1)	50(1)
F(1)	3705(3)	5447(1)	5554(2)	87(1)
F(2)	890(2)	3897(1)	7995(1)	83(1)
N(1)	3623(3)	6393(2)	2281(2)	57(1)
O(3)	4545(3)	5913(2)	2191(2)	77(1)
O(2)	3093(3)	6828(2)	1628(2)	90(1)
N(2)	1821(4)	3995(2)	4689(2)	65(1)

O(5)	2652(3)	3840(2)	4130(2)	106(1)
C(8)	788(3)	8040(2)	3364(2)	43(1)
O(6)	818(4)	4436(2)	4477(2)	97(1)
C(25)	4414(3)	2026(2)	5803(2)	46(1)
C(14)	2964(3)	3014(2)	5879(2)	45(1)
C(1)	2226(3)	7027(2)	3437(2)	43(1)
C(19)	3194(3)	2677(2)	6820(2)	45(1)
C(20)	4157(3)	2041(2)	6770(2)	44(1)
C(7)	893(3)	7753(2)	4318(2)	44(1)
C(6)	1831(3)	7093(2)	4375(2)	44(1)
C(15)	2074(4)	3641(2)	5669(2)	48(1)
C(18)	2491(4)	2980(2)	7546(2)	53(1)
C(16)	1364(4)	3943(2)	6386(2)	55(1)
C(2)	3143(3)	6453(2)	3239(2)	47(1)
C(11)	-686(4)	8765(2)	4615(2)	56(1)
C(9)	2(3)	8667(2)	3013(2)	51(1)
C(24)	5262(4)	1492(2)	5444(2)	52(1)
C(12)	123(4)	8134(2)	4955(2)	53(1)
C(23)	5900(4)	933(2)	6087(3)	55(1)
C(17)	1612(4)	3597(2)	7298(2)	54(1)
C(3)	3647(4)	5921(2)	3961(3)	56(1)
C(5)	2346(4)	6563(2)	5098(2)	55(1)
C(10)	-762(4)	9046(2)	3652(2)	52(1)
C(4)	3218(4)	5993(2)	4862(2)	58(1)
C(21)	4822(4)	1482(2)	7416(3)	56(1)
C(22)	5678(4)	939(2)	7071(3)	61(1)
C(13)	-1640(4)	9750(2)	3320(3)	69(1)
C(26)	6825(4)	315(2)	5741(3)	76(1)

Table S23. Selected bond lengths [Å] for 2e.

O4—C14	1.374 (3)	C18—H18	0.95
O4—C25	1.395 (4)	C16—C17	1.375 (4)
O1—C1	1.371 (3)	C16—H16	0.95
O1—C8	1.402 (3)	C2—C3	1.381 (4)
F1—C4	1.366 (4)	C11—C12	1.369 (4)
F2—C17	1.369 (3)	C11—C10	1.403 (4)
N1—O2	1.213 (4)	C11—H11	0.95
N1—O3	1.221 (3)	C9—C10	1.392 (4)
N1—C2	1.468 (4)	C9—H9	0.95
N2—O6	1.205 (3)	C24—C23	1.379 (4)
N2—O5	1.214 (3)	C24—H24	0.95
N2—C15	1.464 (4)	C12—H12	0.95
C8—C9	1.357 (4)	C23—C22	1.406 (5)
C8—C7	1.391 (4)	C23—C26	1.508 (5)
C25—C24	1.369 (4)	C3—C4	1.374 (4)
C25—C20	1.393 (4)	C3—H3	0.95
C14—C15	1.373 (4)	C5—C4	1.360 (4)
C14—C19	1.403 (4)	C5—H5	0.95
C1—C2	1.375 (4)	C10—C13	1.503 (4)
C1—C6	1.408 (4)	C21—C22	1.376 (4)
C19—C18	1.392 (4)	C21—H21	0.95

C19—C20	1.436 (4)	C22—H22	0.95
C20—C21	1.390 (4)	C13—H13A	0.98
C7—C12	1.395 (4)	C13—H13B	0.98
C7—C6	1.440 (4)	C13—H13C	0.98
C6—C5	1.381 (4)	C26—H26A	0.98
C15—C16	1.384 (4)	C26—H26B	0.98
C18—C17	1.359 (4)	C26—H26C	0.98

Table S24. Bond angles [°] for 2e.

C14—O4—C25	105.5 (2)	C10—C11—H11	118.8
C1—O1—C8	105.7 (2)	C8—C9—C10	117.5 (3)
O2—N1—O3	123.7 (3)	C8—C9—H9	121.3
O2—N1—C2	118.2 (3)	C10—C9—H9	121.3
O3—N1—C2	118.2 (3)	C25—C24—C23	117.5 (3)
O6—N2—O5	122.9 (3)	C25—C24—H24	121.2
O6—N2—C15	118.9 (3)	C23—C24—H24	121.2
O5—N2—C15	118.2 (3)	C11—C12—C7	118.8 (3)
C9—C8—C7	124.8 (3)	C11—C12—H12	120.6
C9—C8—O1	124.4 (3)	C7—C12—H12	120.6
C7—C8—O1	110.9 (3)	C24—C23—C22	119.4 (3)
C24—C25—C20	124.4 (3)	C24—C23—C26	120.6 (3)
C24—C25—O4	124.4 (3)	C22—C23—C26	119.9 (3)

C20—C25—O4	111.2 (3)	C18—C17—F2	118.4 (3)
C15—C14—O4	127.5 (3)	C18—C17—C16	125.0 (3)
C15—C14—C19	121.1 (3)	F2—C17—C16	116.6 (3)
O4—C14—C19	111.4 (3)	C4—C3—C2	118.1 (3)
O1—C1—C2	127.6 (3)	C4—C3—H3	120.9
O1—C1—C6	111.5 (3)	C2—C3—H3	120.9
C2—C1—C6	120.9 (3)	C4—C5—C6	117.6 (3)
C18—C19—C14	119.2 (3)	C4—C5—H5	121.2
C18—C19—C20	134.9 (3)	C6—C5—H5	121.2
C14—C19—C20	105.9 (3)	C9—C10—C11	119.0 (3)
C21—C20—C25	117.7 (3)	C9—C10—C13	120.5 (3)
C21—C20—C19	136.3 (3)	C11—C10—C13	120.5 (3)
C25—C20—C19	106.0 (3)	C5—C4—F1	118.8 (3)
C8—C7—C12	117.5 (3)	C5—C4—C3	124.4 (3)
C8—C7—C6	106.3 (3)	F1—C4—C3	116.8 (3)
C12—C7—C6	136.2 (3)	C22—C21—C20	118.9 (3)
C5—C6—C1	119.5 (3)	C22—C21—H21	120.6
C5—C6—C7	134.8 (3)	C20—C21—H21	120.6
C1—C6—C7	105.7 (3)	C21—C22—C23	122.0 (3)
C14—C15—C16	120.0 (3)	C21—C22—H22	119
C14—C15—N2	121.5 (3)	C23—C22—H22	119

C16—C15—N2	118.4 (3)	C10—C13—H13A	109.5
C17—C18—C19	117.4 (3)	C10—C13—H13B	109.5
C17—C18—H18	121.3	H13A—C13—H13B	109.5
C19—C18—H18	121.3	C10—C13—H13C	109.5
C17—C16—C15	117.3 (3)	H13A—C13—H13C	109.5
C17—C16—H16	121.4	H13B—C13—H13C	109.5
C15—C16—H16	121.4	C23—C26—H26A	109.5
C1—C2—C3	119.5 (3)	C23—C26—H26B	109.5
C1—C2—N1	121.9 (3)	H26A—C26—H26B	109.5
C3—C2—N1	118.6 (3)	C23—C26—H26C	109.5
C12—C11—C10	122.4 (3)	H26A—C26—H26C	109.5
C12—C11—H11	118.8	H26B—C26—H26C	109.5

Table S25. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 2e. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(4)	63(2)	61(2)	35(1)	-3(1)	18(1)	4(1)
O(1)	59(2)	54(1)	39(1)	-4(1)	15(1)	4(1)
F(1)	115(2)	81(2)	60(1)	14(1)	5(1)	31(1)
F(2)	106(2)	94(2)	61(1)	-16(1)	45(1)	14(1)
N(1)	63(2)	61(2)	50(2)	-13(2)	16(2)	-2(2)
O(3)	80(2)	76(2)	84(2)	-16(2)	37(2)	14(2)
O(2)	118(2)	110(2)	46(2)	5(2)	30(2)	36(2)
N(2)	82(2)	71(2)	44(2)	2(2)	14(2)	14(2)

O(5)	135(3)	139(3)	57(2)	35(2)	50(2)	57(2)
C(8)	44(2)	49(2)	39(2)	-6(2)	11(2)	-2(2)
O(6)	121(3)	108(2)	62(2)	16(2)	21(2)	56(2)
C(25)	48(2)	51(2)	40(2)	-3(2)	12(2)	-4(2)
C(14)	48(2)	54(2)	36(2)	-10(2)	16(2)	-5(2)
C(1)	46(2)	44(2)	39(2)	-2(2)	4(2)	-2(2)
C(19)	52(2)	51(2)	33(2)	-4(2)	14(2)	-10(2)
C(20)	47(2)	49(2)	36(2)	-1(2)	11(2)	-7(2)
C(7)	43(2)	51(2)	38(2)	-3(2)	7(2)	-4(2)
C(6)	48(2)	51(2)	35(2)	-2(2)	7(2)	-4(2)
C(15)	55(2)	55(2)	34(2)	-4(2)	12(2)	-3(2)
C(18)	64(2)	65(2)	34(2)	-1(2)	18(2)	-8(2)
C(16)	61(2)	54(2)	51(2)	-10(2)	14(2)	3(2)
C(2)	49(2)	48(2)	42(2)	-9(2)	8(2)	-2(2)
C(11)	53(2)	63(3)	53(2)	-14(2)	13(2)	2(2)
C(9)	56(2)	54(2)	42(2)	-4(2)	8(2)	2(2)
C(24)	57(2)	63(2)	41(2)	-10(2)	21(2)	-6(2)
C(12)	55(2)	65(2)	43(2)	-5(2)	15(2)	3(2)
C(23)	48(2)	51(2)	66(2)	-7(2)	13(2)	-9(2)
C(17)	64(2)	63(2)	41(2)	-15(2)	25(2)	-3(2)
C(3)	55(2)	53(2)	57(2)	-9(2)	2(2)	7(2)
C(5)	60(2)	61(2)	42(2)	-2(2)	10(2)	3(2)
C(10)	48(2)	52(2)	53(2)	-7(2)	4(2)	-1(2)
C(4)	73(3)	55(2)	43(2)	9(2)	-1(2)	7(2)
C(21)	64(2)	62(2)	45(2)	4(2)	18(2)	-7(2)
C(22)	60(2)	62(3)	61(3)	5(2)	11(2)	-3(2)
C(13)	66(3)	65(3)	76(3)	-5(2)	11(2)	12(2)
C(26)	66(3)	66(3)	96(3)	-15(2)	16(2)	4(2)

Table S26. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 2e.

	x	y	z	U(eq)
H(18)	2621	2764	8190	63
H(16)	732	4372	6253	66
H(11)	-1215	9022	5048	67
H(9)	-25	8842	2356	61
H(24)	5406	1507	4778	62
H(12)	159	7958	5613	64
H(3)	4272	5516	3838	67
H(5)	2100	6596	5738	66
H(21)	4687	1475	8085	68
H(22)	6133	556	7512	73
H(13A)	-1187	10195	3686	104
H(13B)	-2638	9687	3445	104
H(13C)	-1667	9828	2611	104
H(26A)	7859	418	5997	114
H(26B)	6660	309	5017	114
H(26C)	6557	-183	5984	114

Figure S125 ORTEP views of **2o**

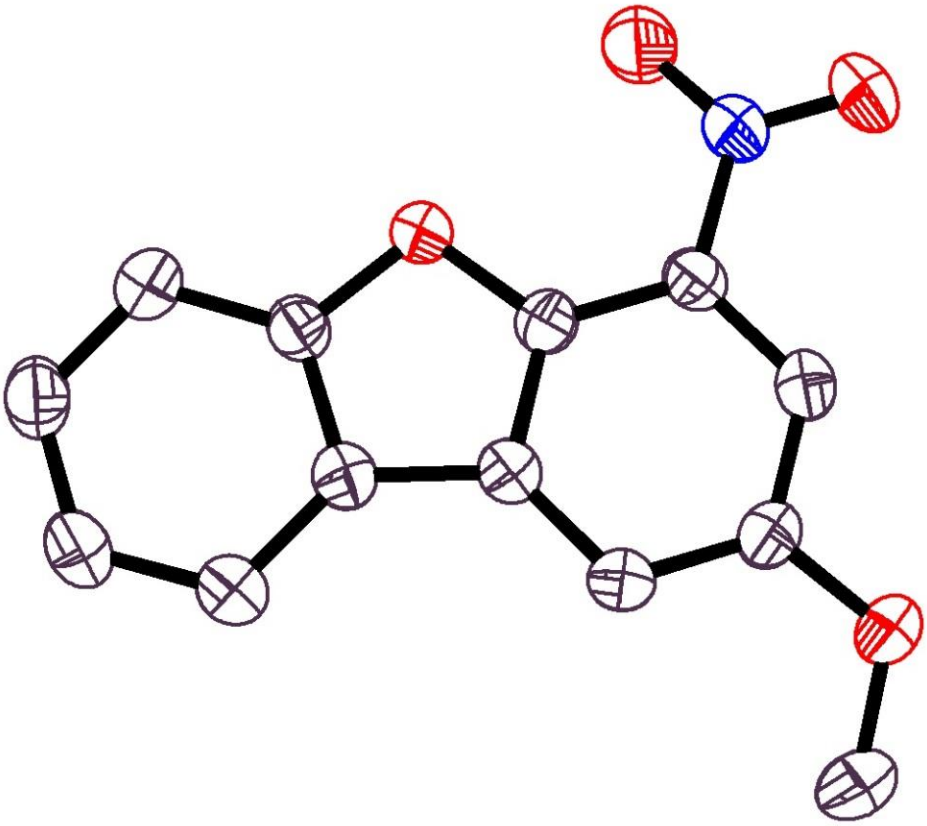

Figure S126 **Packing diagram of 2o**

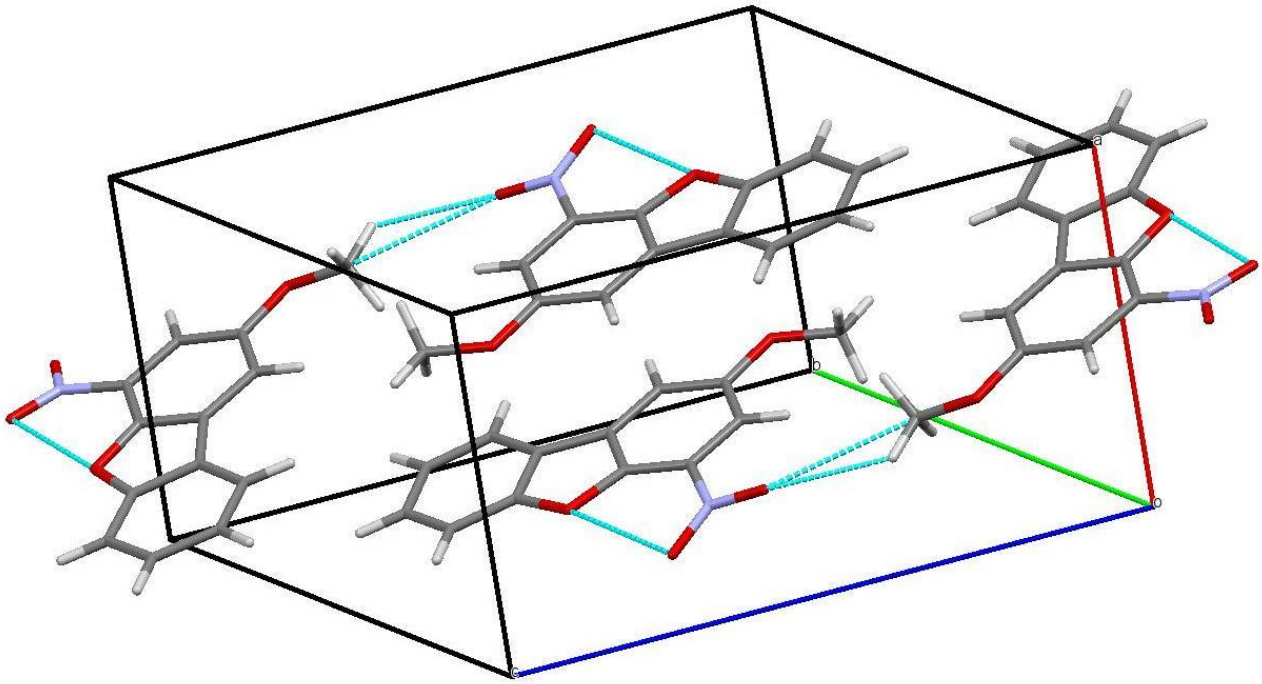

Table S27. Crystal data and structure refinement for 2o

Identification code	**2o**	
Empirical formula	C_{13} H_8 N O_4	
Formula weight	242.20	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 7.3355(3) Å	α= 82.618(2)°.
	b = 10.3916(4) Å	β= 86.176(2)°.
	c = 14.2893(5) Å	γ = 84.050(2)°.
Volume	1072.82(7) $Å^3$	
Z	4	
Density (calculated)	1.500 Mg/m^3	
Absorption coefficient	0.113 mm^{-1}	
F(000)	500	
Theta range for data collection	2.305 to 25.079°.	
Index ranges	-8<=h<=8, -12<=k<=12, -16<=l<=16	
Reflections collected	33794	
Independent reflections	3811 [R(int) = 0.0497]	
Completeness to theta = 25.242°	98.2 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3811 / 0 / 327	
Goodness-of-fit on F^2	1.077	
Final R indices [I>2sigma(I)]	R1 = 0.0380, wR2 = 0.1004	
R indices (all data)	R1 = 0.0561, wR2 = 0.1165	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.197 and -0.168 $e.Å^{-3}$	

Table S28. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 2o. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	8030(2)	9307(1)	-621(1)	37(1)
O(5)	8705(2)	5476(1)	3409(1)	39(1)
O(8)	5846(2)	5037(1)	7072(1)	54(1)
O(4)	4885(2)	8710(1)	2991(1)	56(1)
O(6)	9112(3)	7980(1)	3659(1)	70(1)
O(7)	7520(3)	8837(1)	4774(1)	71(1)
N(1)	7275(2)	6652(2)	313(1)	45(1)
O(2)	7648(3)	6747(2)	-532(1)	74(1)
O(3)	7202(3)	5609(1)	802(1)	74(1)
N(2)	8124(3)	7896(2)	4376(1)	47(1)
C(20)	7661(2)	4297(2)	4777(1)	34(1)
C(25)	8018(2)	5529(2)	4320(1)	35(1)
C(24)	7667(3)	6609(2)	4799(1)	36(1)
C(6)	7460(2)	11221(2)	41(1)	35(1)
C(14)	8819(3)	4171(2)	3275(1)	36(1)
C(11)	6901(3)	7839(2)	758(1)	35(1)
C(10)	6130(3)	7767(2)	1671(1)	39(1)
C(19)	8209(3)	3407(2)	4084(1)	36(1)
C(12)	7273(2)	9045(2)	280(1)	33(1)
C(7)	6885(2)	10164(2)	725(1)	34(1)
C(1)	8129(3)	10645(2)	-753(1)	35(1)
C(22)	6571(3)	5254(2)	6169(1)	39(1)
C(9)	5705(3)	8898(2)	2101(1)	39(1)
C(21)	6944(3)	4154(2)	5701(1)	39(1)
C(23)	6928(3)	6475(2)	5724(1)	39(1)
C(8)	6088(3)	10102(2)	1638(1)	39(1)

C(5)	7460(3)	12563(2)	22(1)	43(1)
C(2)	8791(3)	11325(2)	-1572(1)	43(1)
C(15)	9467(3)	3684(2)	2452(1)	43(1)
C(18)	8279(3)	2061(2)	4074(1)	44(1)
C(3)	8760(3)	12660(2)	-1580(2)	47(1)
C(4)	8108(3)	13264(2)	-793(2)	48(1)
C(16)	9525(3)	2349(2)	2463(2)	49(1)
C(26)	5520(3)	6112(2)	7606(2)	52(1)
C(17)	8945(3)	1553(2)	3261(2)	49(1)
C(13)	4106(4)	9840(2)	3393(2)	69(1)

Table S29. Selected bond lengths [Å] for 2o.

O1—C12	1.373 (2)	C12—C7	1.392 (2)
O1—C1	1.388 (2)	C7—C8	1.389 (2)
O5—C25	1.370 (2)	C1—C2	1.374 (3)
O5—C14	1.387 (2)	C22—C23	1.386 (3)
O8—C22	1.364 (2)	C22—C21	1.391 (3)
O8—C26	1.424 (2)	C9—C8	1.384 (3)
O4—C9	1.369 (2)	C21—H21	0.95
O4—C13	1.423 (3)	C23—H23	0.95
O6—N2	1.214 (2)	C8—H8	0.95
O7—N2	1.222 (2)	C5—C4	1.376 (3)
N1—O2	1.215 (2)	C5—H5	0.95
N1—O3	1.216 (2)	C2—C3	1.384 (3)
N1—C11	1.453 (2)	C2—H2	0.95

N2—C24	1.457 (2)	C15—C16	1.381 (3)
C20—C21	1.384 (3)	C15—H15	0.95
C20—C25	1.402 (2)	C18—C17	1.376 (3)
C20—C19	1.450 (3)	C18—H18	0.95
C25—C24	1.382 (3)	C3—C4	1.391 (3)
C24—C23	1.390 (3)	C3—H3	0.95
C6—C1	1.387 (3)	C4—H4	0.95
C6—C5	1.391 (3)	C16—C17	1.390 (3)
C6—C7	1.451 (2)	C16—H16	0.95
C14—C15	1.376 (3)	C26—H26A	0.98
C14—C19	1.392 (3)	C26—H26B	0.98
C11—C10	1.383 (3)	C26—H26C	0.98
C11—C12	1.391 (2)	C17—H17	0.95
C10—C9	1.393 (3)	C13—H13A	0.98
C10—H10	0.95	C13—H13B	0.98
C19—C18	1.396 (3)	C13—H13C	0.98

Table S30. Selected Bond angles [°] for 2o

C12—O1—C1	105.06 (13)	O4—C9—C10	114.72 (16)
C25—O5—C14	105.58 (13)	C8—C9—C10	120.98 (17)
C22—O8—C26	118.31 (16)	C20—C21—C22	118.90 (17)
C9—O4—C13	117.12 (16)	C20—C21—H21	120.6

O2—N1—O3	122.93 (17)	C22—C21—H21	120.6
O2—N1—C11	118.39 (16)	C22—C23—C24	119.93 (17)
O3—N1—C11	118.67 (16)	C22—C23—H23	120
O6—N2—O7	123.22 (17)	C24—C23—H23	120
O6—N2—C24	118.60 (16)	C9—C8—C7	118.64 (17)
O7—N2—C24	118.16 (17)	C9—C8—H8	120.7
C21—C20—C25	120.67 (17)	C7—C8—H8	120.7
C21—C20—C19	134.37 (17)	C4—C5—C6	118.18 (18)
C25—C20—C19	104.96 (15)	C4—C5—H5	120.9
O5—C25—C24	128.20 (16)	C6—C5—H5	120.9
O5—C25—C20	112.08 (15)	C1—C2—C3	116.24 (18)
C24—C25—C20	119.71 (16)	C1—C2—H2	121.9
C25—C24—C23	119.95 (17)	C3—C2—H2	121.9
C25—C24—N2	121.79 (16)	C14—C15—C16	116.20 (18)
C23—C24—N2	118.22 (16)	C14—C15—H15	121.9
C1—C6—C5	118.95 (17)	C16—C15—H15	121.9
C1—C6—C7	105.61 (15)	C17—C18—C19	118.34 (18)
C5—C6—C7	135.44 (17)	C17—C18—H18	120.8
C15—C14—O5	124.64 (17)	C19—C18—H18	120.8
C15—C14—C19	123.97 (17)	C2—C3—C4	121.22 (19)
O5—C14—C19	111.39 (15)	C2—C3—H3	119.4

C10—C11—C12	119.57 (16)	C4—C3—H3	119.4
C10—C11—N1	119.01 (16)	C5—C4—C3	121.53 (19)
C12—C11—N1	121.41 (16)	C5—C4—H4	119.2
C11—C10—C9	120.02 (17)	C3—C4—H4	119.2
C11—C10—H10	120	C15—C16—C17	121.48 (19)
C9—C10—H10	120	C15—C16—H16	119.3
C14—C19—C18	118.54 (17)	C17—C16—H16	119.3
C14—C19—C20	105.99 (15)	O8—C26—H26A	109.5
C18—C19—C20	135.45 (17)	O8—C26—H26B	109.5
O1—C12—C11	127.84 (16)	H26A—C26—H26B	109.5
O1—C12—C7	112.25 (15)	O8—C26—H26C	109.5
C11—C12—C7	119.91 (16)	H26A—C26—H26C	109.5
C8—C7—C12	120.85 (16)	H26B—C26—H26C	109.5
C8—C7—C6	133.84 (16)	C18—C17—C16	121.45 (19)
C12—C7—C6	105.31 (15)	C18—C17—H17	119.3
C2—C1—C6	123.88 (17)	C16—C17—H17	119.3
C2—C1—O1	124.35 (17)	O4—C13—H13A	109.5
C6—C1—O1	111.77 (15)	O4—C13—H13B	109.5
O8—C22—C23	123.65 (17)	H13A—C13—H13B	109.5
O8—C22—C21	115.52 (17)	O4—C13—H13C	109.5
C23—C22—C21	120.83 (17)	H13A—C13—H13C	109.5

O4—C9—C8	124.30 (17)	H13B—C13—H13C	109.5

Table S31. Anisotropic displacement parameters ($Å^2$x 10^3) for 2o. 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)	47(1)	31(1)	34(1)	-4(1)	5(1)	-4(1)
O(5)	49(1)	33(1)	36(1)	-2(1)	6(1)	-9(1)
O(8)	77(1)	45(1)	39(1)	-4(1)	16(1)	-8(1)
O(4)	80(1)	46(1)	39(1)	-6(1)	18(1)	-11(1)
O(6)	100(1)	42(1)	63(1)	-2(1)	33(1)	-19(1)
O(7)	121(2)	33(1)	58(1)	-10(1)	16(1)	-9(1)
N(1)	57(1)	33(1)	44(1)	-6(1)	3(1)	-7(1)
O(2)	134(2)	44(1)	44(1)	-14(1)	15(1)	-17(1)
O(3)	122(2)	30(1)	65(1)	-1(1)	17(1)	-5(1)
N(2)	65(1)	34(1)	42(1)	-3(1)	2(1)	-8(1)
C(20)	32(1)	32(1)	37(1)	-1(1)	-1(1)	-4(1)
C(25)	34(1)	35(1)	34(1)	-1(1)	0(1)	-5(1)
C(24)	40(1)	31(1)	38(1)	-1(1)	-3(1)	-6(1)
C(6)	35(1)	33(1)	37(1)	-3(1)	-2(1)	-4(1)
C(14)	36(1)	31(1)	40(1)	-3(1)	-1(1)	-5(1)
C(11)	38(1)	29(1)	37(1)	-5(1)	-3(1)	-2(1)
C(10)	45(1)	34(1)	38(1)	1(1)	-1(1)	-5(1)
C(19)	35(1)	35(1)	37(1)	-2(1)	0(1)	-5(1)
C(12)	34(1)	35(1)	31(1)	-3(1)	-2(1)	-4(1)
C(7)	35(1)	31(1)	35(1)	-4(1)	-3(1)	-3(1)
C(1)	36(1)	30(1)	38(1)	-2(1)	-1(1)	-3(1)
C(22)	41(1)	41(1)	33(1)	-1(1)	3(1)	-4(1)
C(9)	44(1)	41(1)	32(1)	-4(1)	3(1)	-6(1)
C(21)	43(1)	34(1)	39(1)	2(1)	1(1)	-6(1)

C(23)	43(1)	36(1)	38(1)	-6(1)	-1(1)	-3(1)
C(8)	46(1)	34(1)	37(1)	-9(1)	1(1)	-5(1)
C(5)	49(1)	35(1)	45(1)	-7(1)	1(1)	-6(1)
C(2)	45(1)	43(1)	38(1)	-3(1)	6(1)	-6(1)
C(15)	45(1)	43(1)	39(1)	-4(1)	6(1)	-6(1)
C(18)	54(1)	33(1)	44(1)	-1(1)	4(1)	-7(1)
C(3)	51(1)	41(1)	48(1)	5(1)	4(1)	-10(1)
C(4)	56(1)	32(1)	55(1)	-1(1)	3(1)	-10(1)
C(16)	53(1)	47(1)	46(1)	-13(1)	7(1)	-2(1)
C(26)	59(1)	60(1)	40(1)	-15(1)	8(1)	-12(1)
C(17)	59(1)	34(1)	55(1)	-9(1)	5(1)	-4(1)
C(13)	91(2)	61(2)	53(1)	-15(1)	30(1)	-7(1)

Table S32. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 2o

	x	y	z	U(eq)
H(10)	5889	6946	2005	47
H(21)	6710	3317	6011	47
H(23)	6667	7219	6050	47
H(8)	5811	10869	1937	47
H(5)	7024	12983	557	52
H(2)	9244	10902	-2104	51
H(15)	9853	4234	1908	52
H(18)	7877	1509	4614	53
H(3)	9192	13173	-2133	57
H(4)	8111	14181	-819	58
H(16)	9972	1967	1913	58
H(26A)	6665	6514	7629	78
H(26B)	5075	5807	8250	78

H(26C)	4597	6756	7307	78
H(17)	9009	638	3245	59
H(13A)	5089	10342	3538	103
H(13B)	3384	9577	3975	103
H(13C)	3308	10380	2942	103