Supplementary Material

Facile conversion of 1,2-dicyanobenzene into chiral bisamidines

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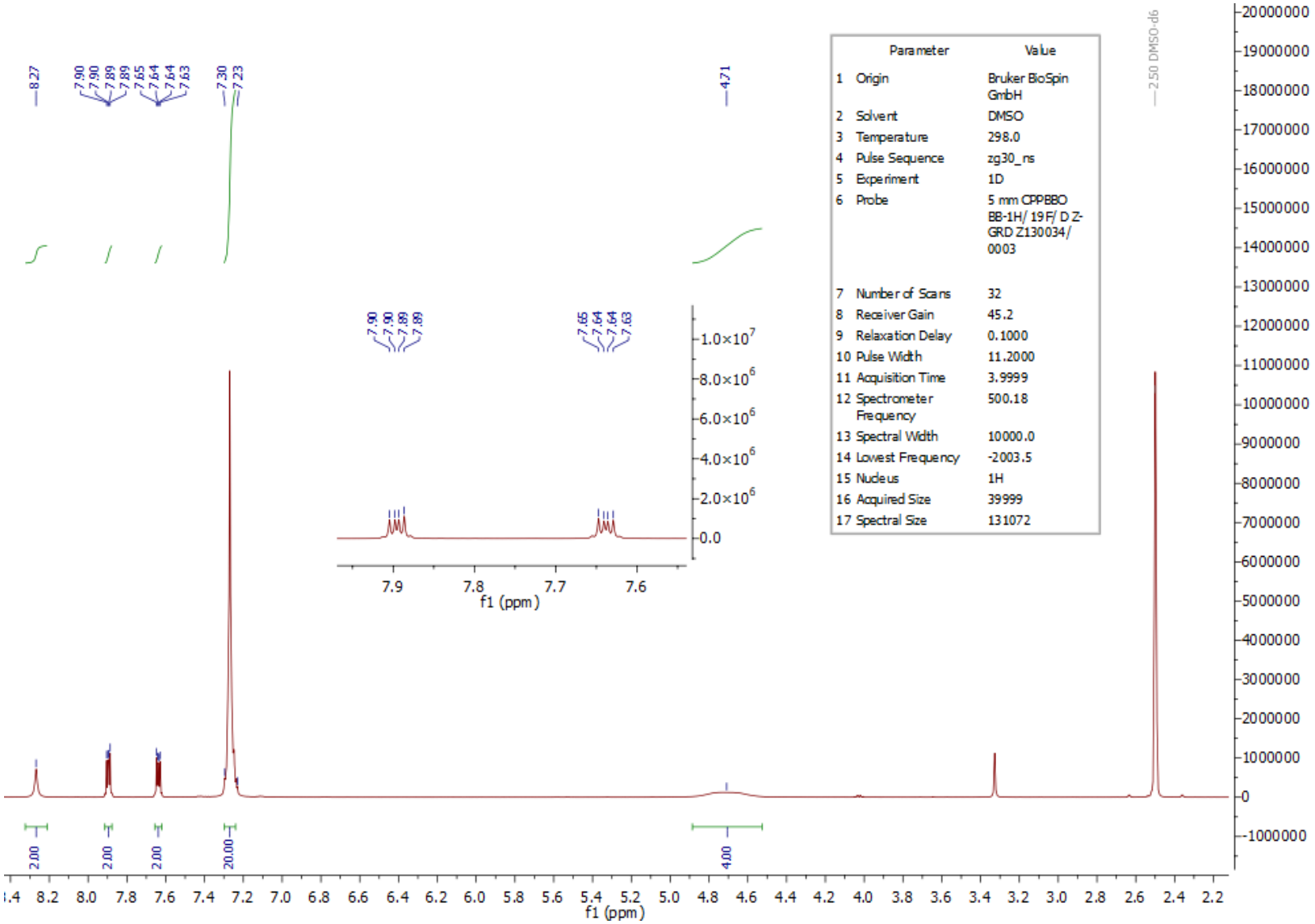
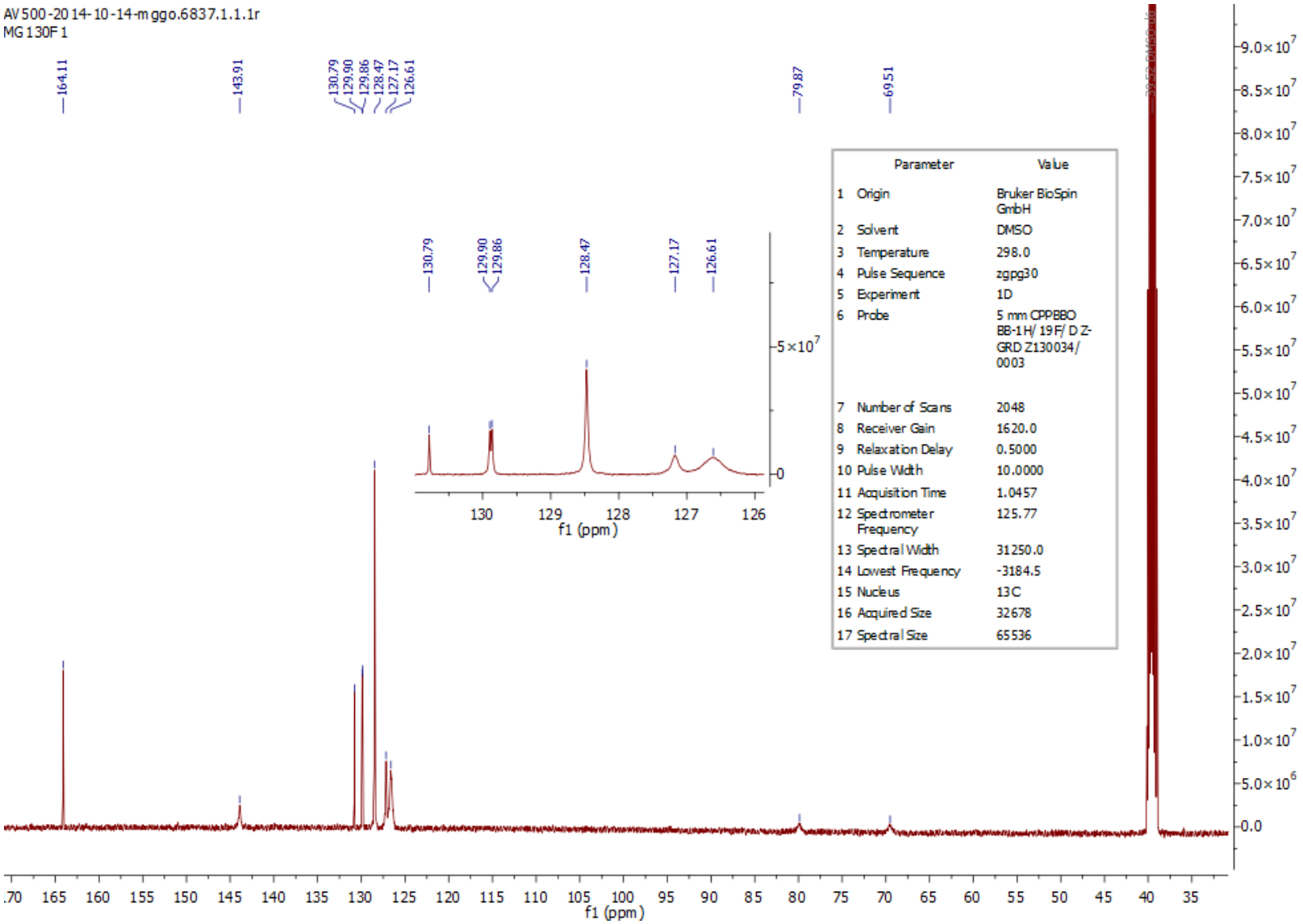
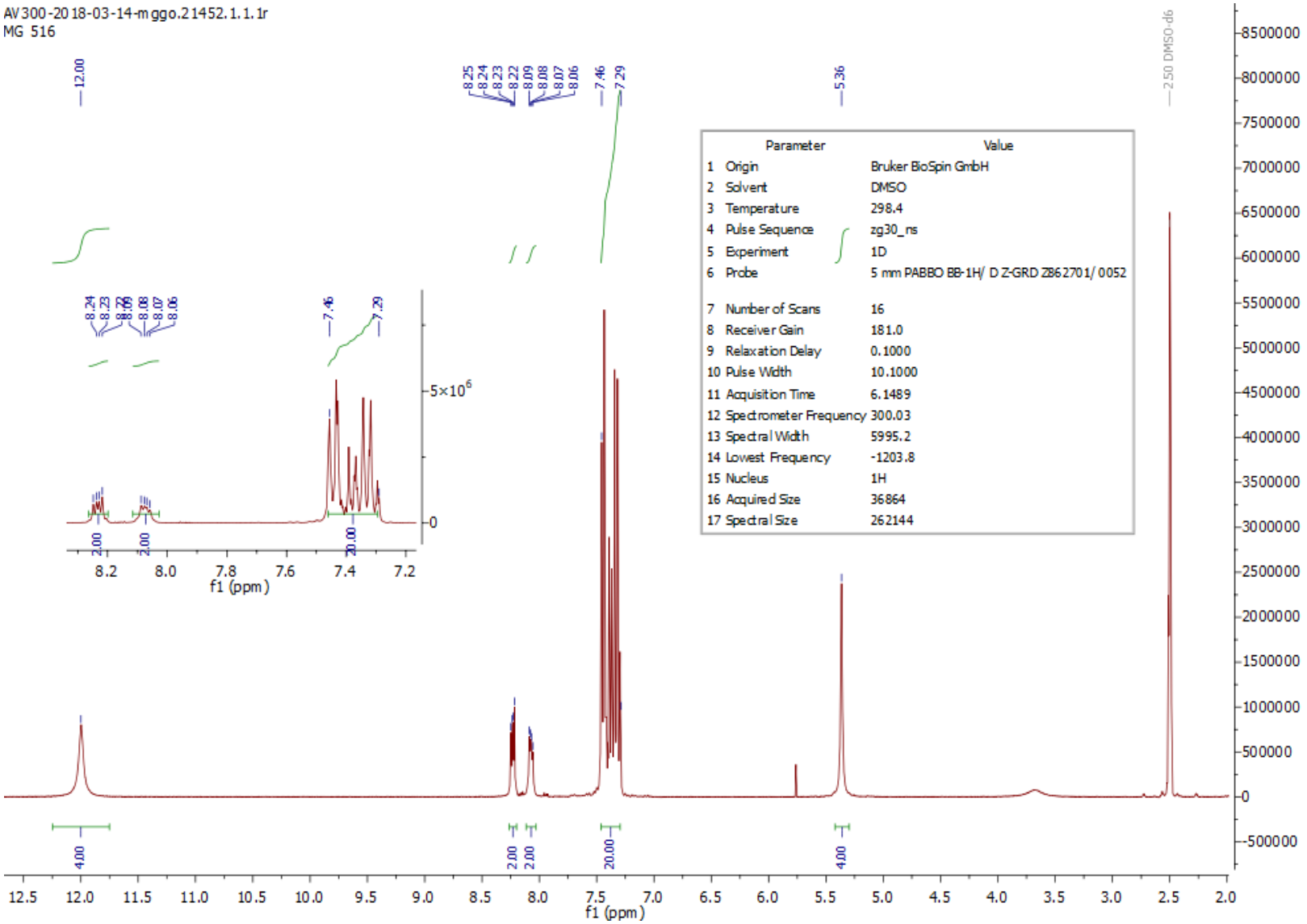
Table of Contents



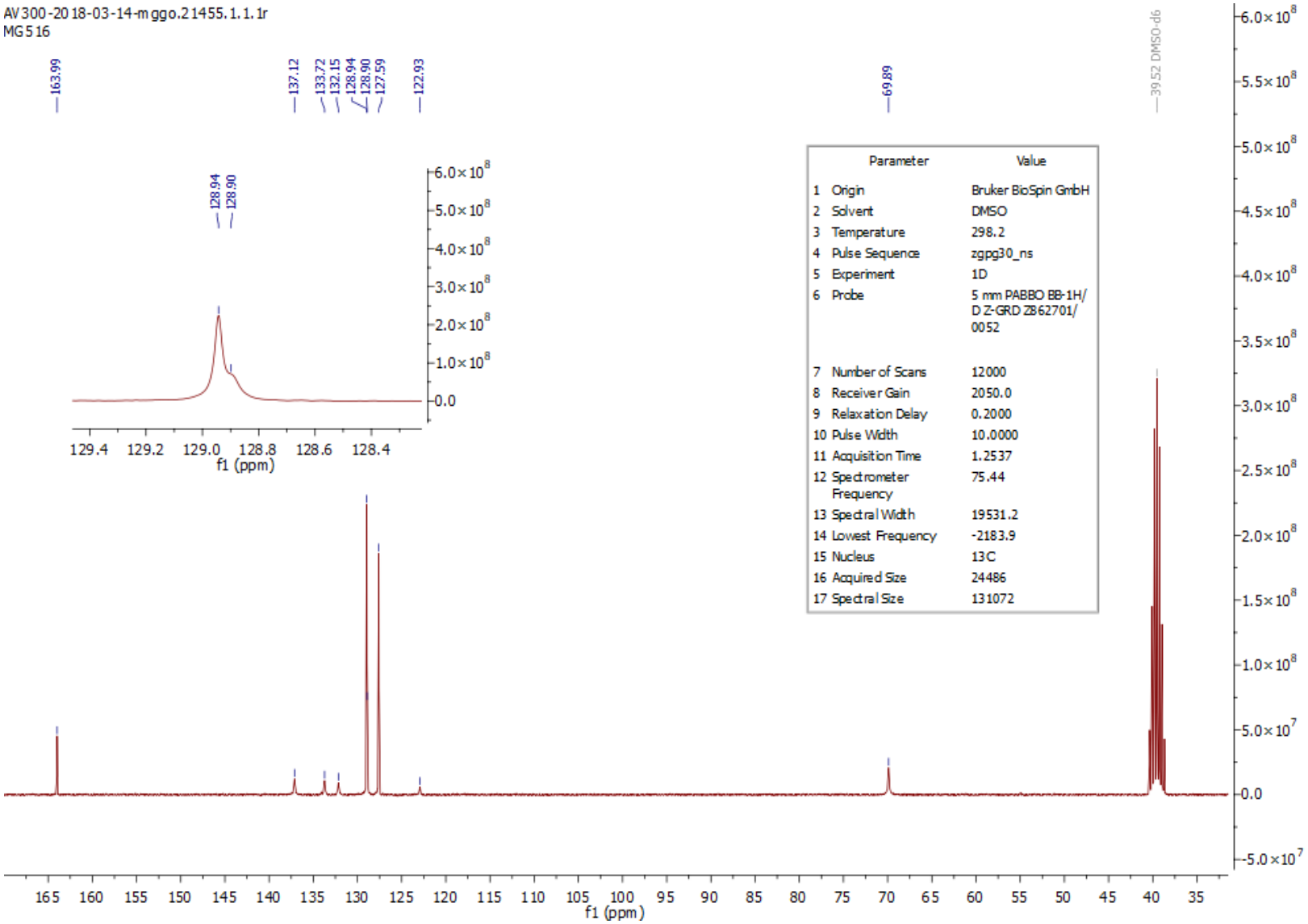
^{1}H NMR spectrum of **6a** (500 MHz, DMSO-d_6)



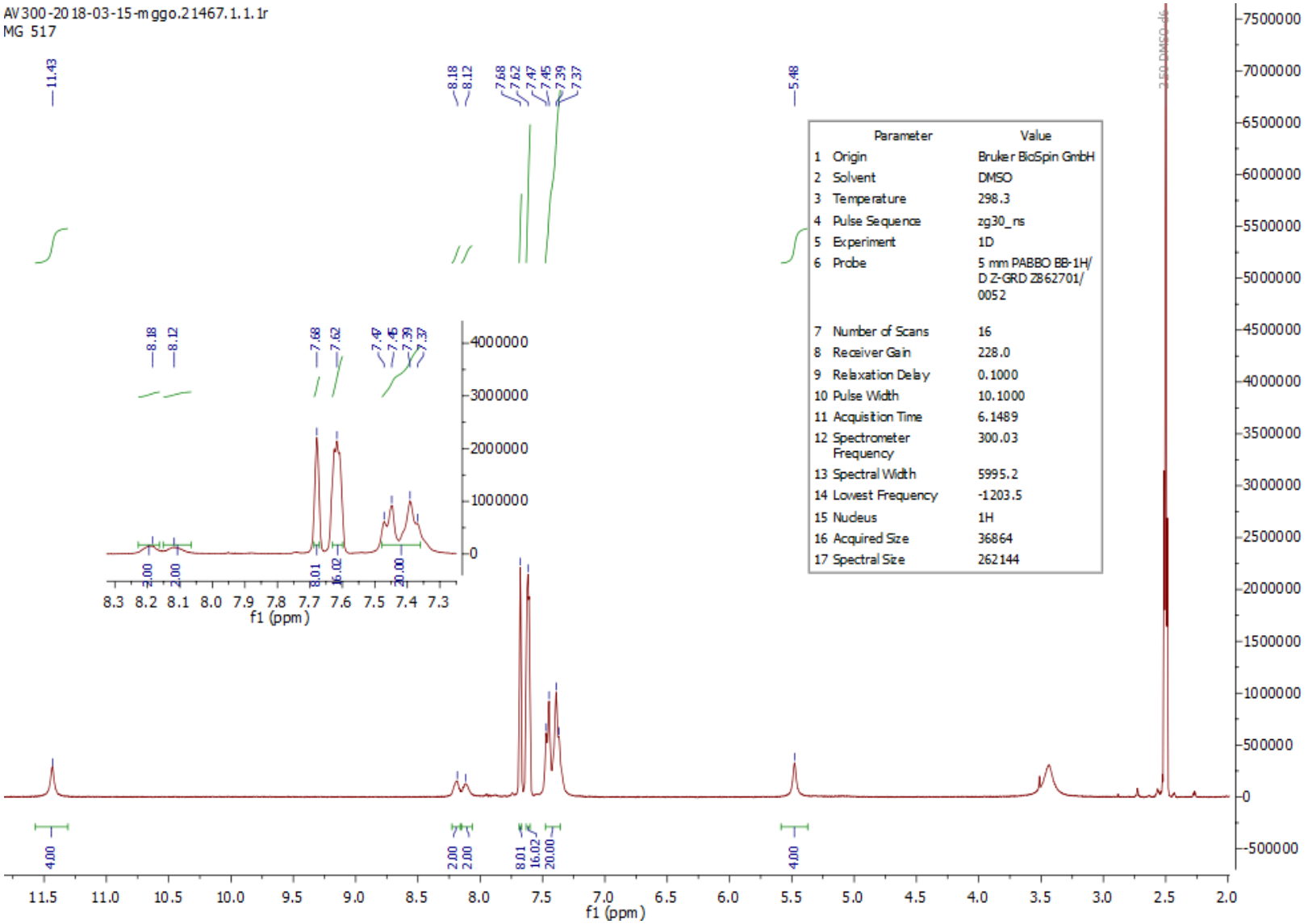
^{13}C NMR spectrum of **6a** (126 MHz, DMSO-d_6)



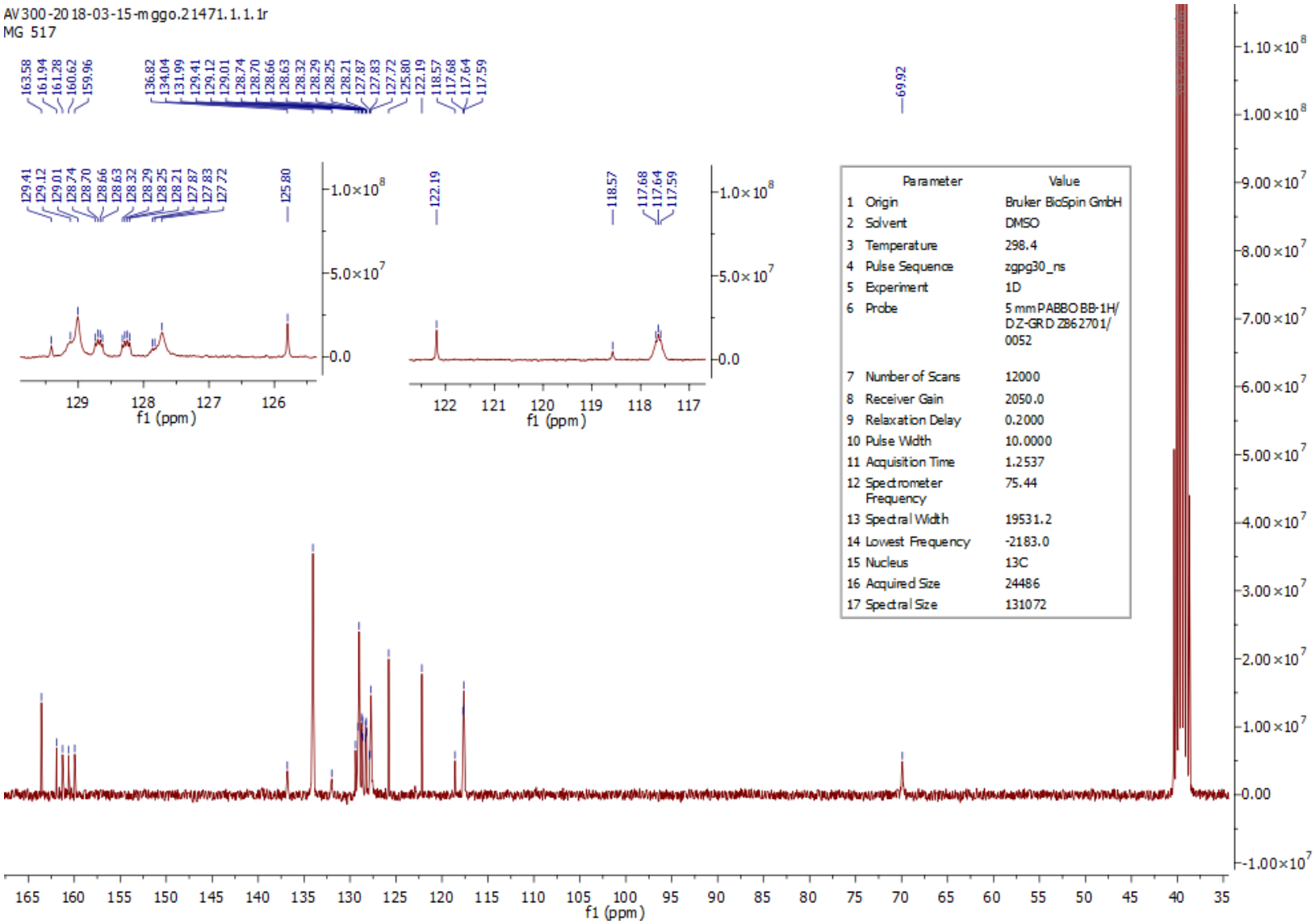
^{1}H NMR spectrum of **7a** (300 MHz, DMSO-d_6)



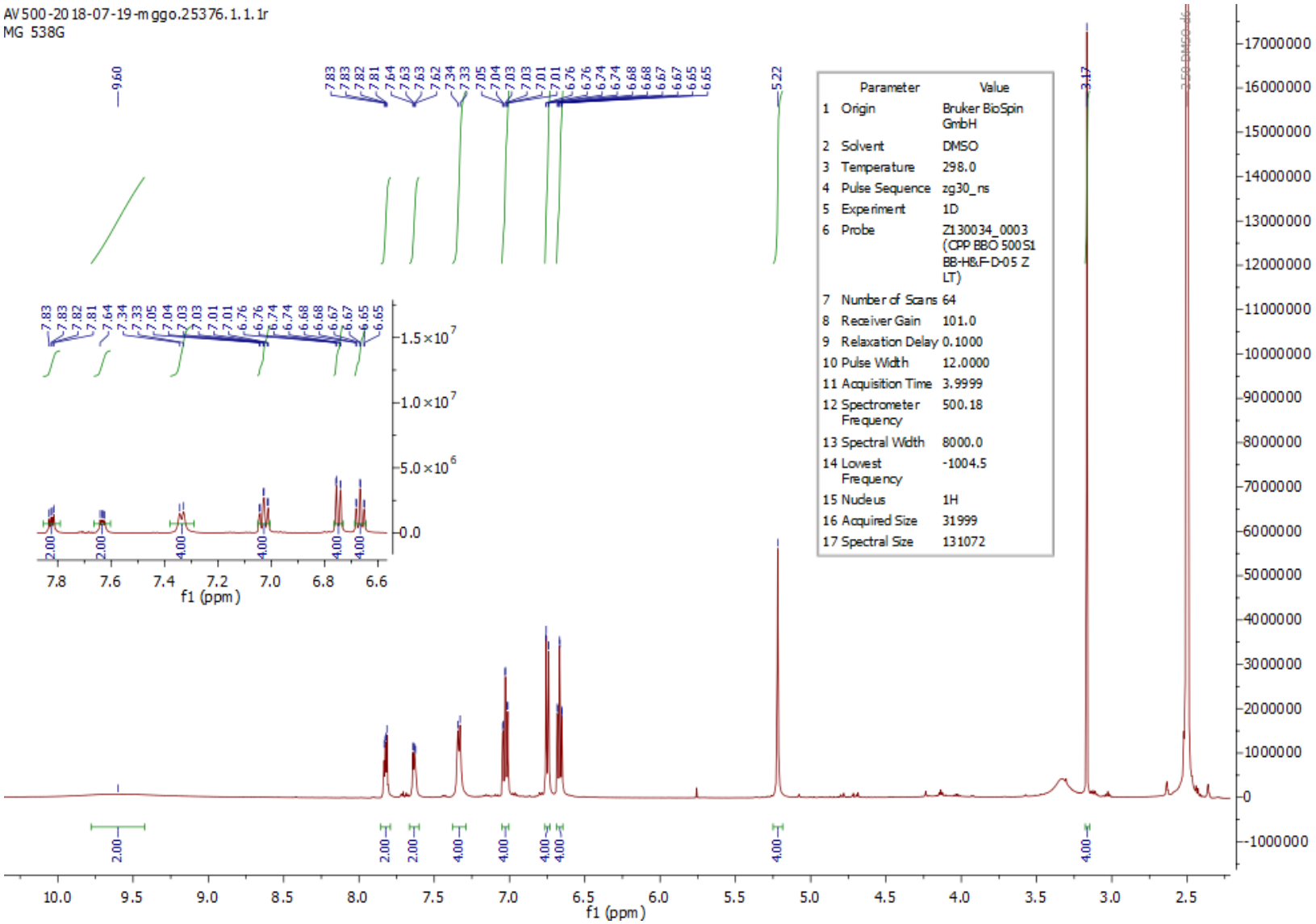
^{13}C NMR spectrum of **7a** (75 MHz, DMSO-d_6)



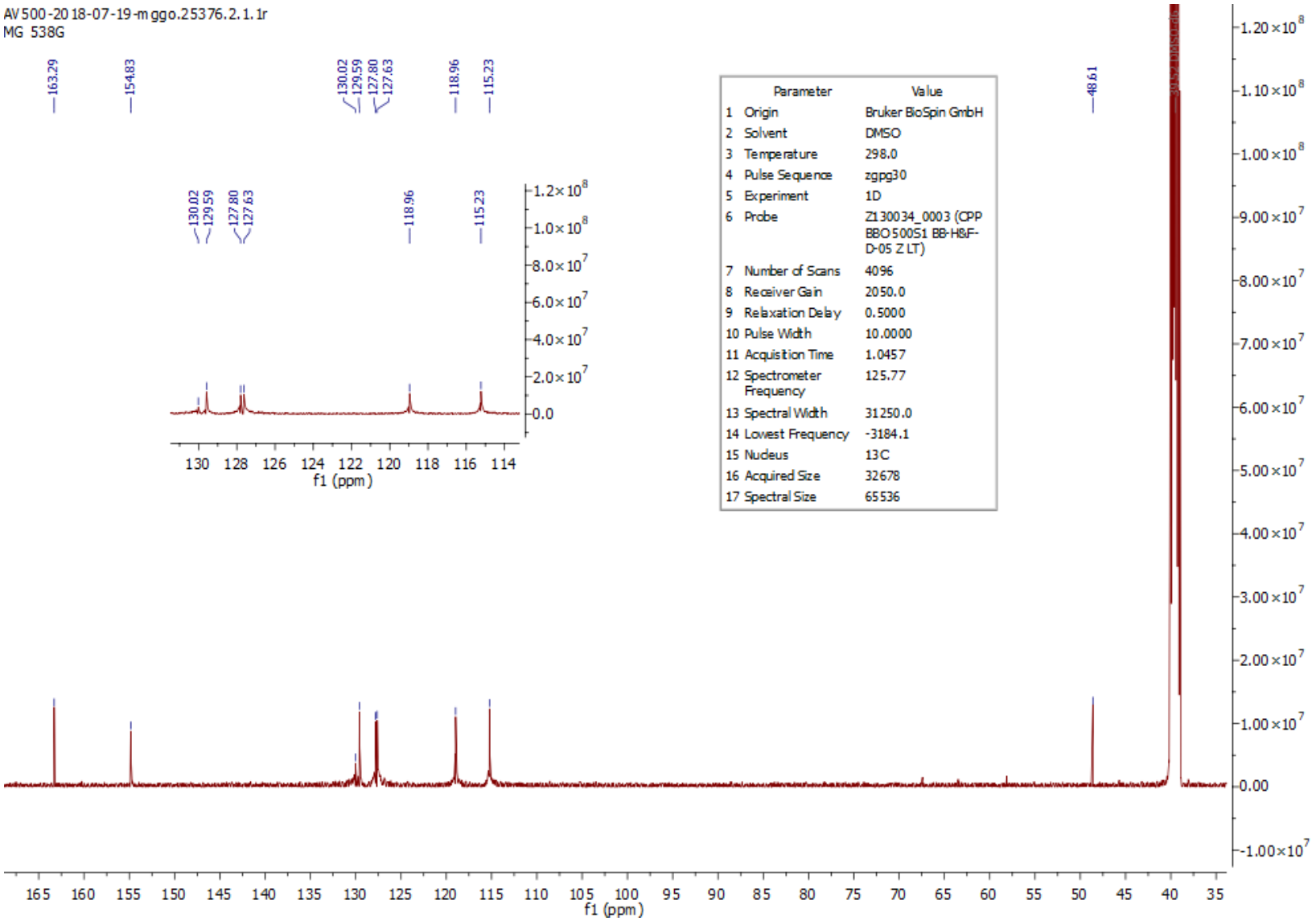
^{1}H NMR spectrum of **8a** (300 MHz, DMSO-d_6)



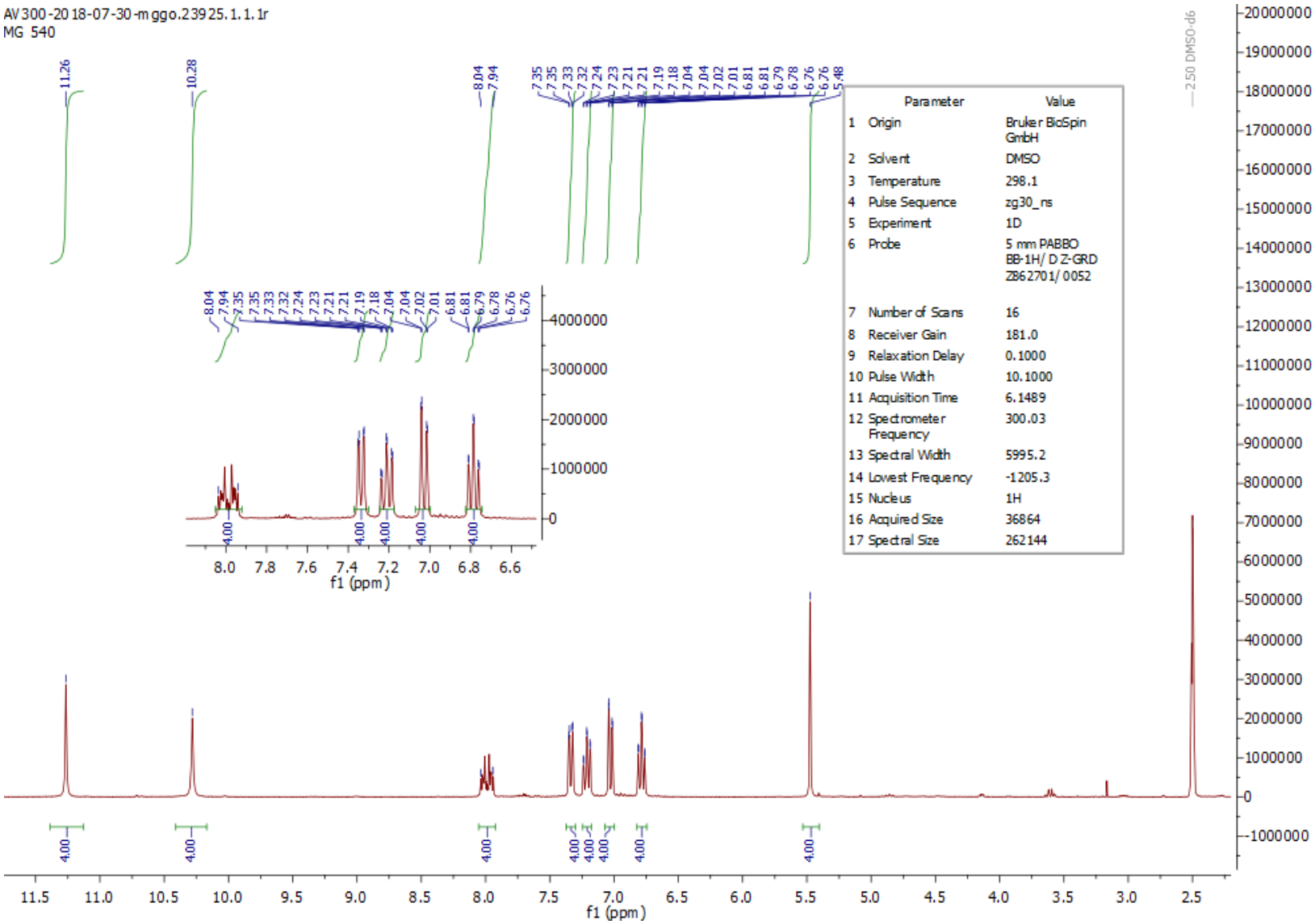
^{13}C NMR spectrum of **8a** (75 MHz, DMSO-d_6)



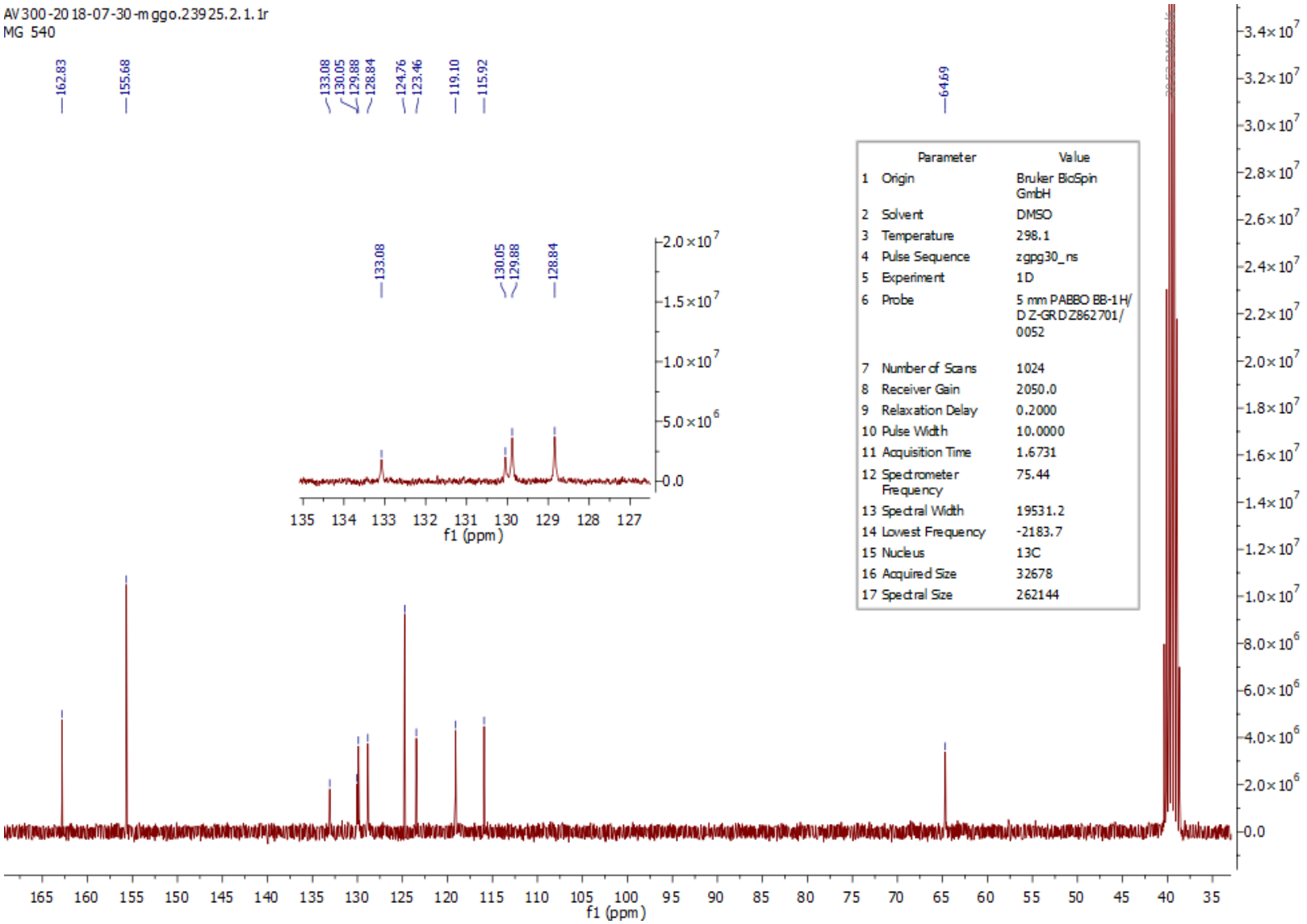
^{1}H NMR spectrum of **6b** (500 MHz, DMSO-d_6)



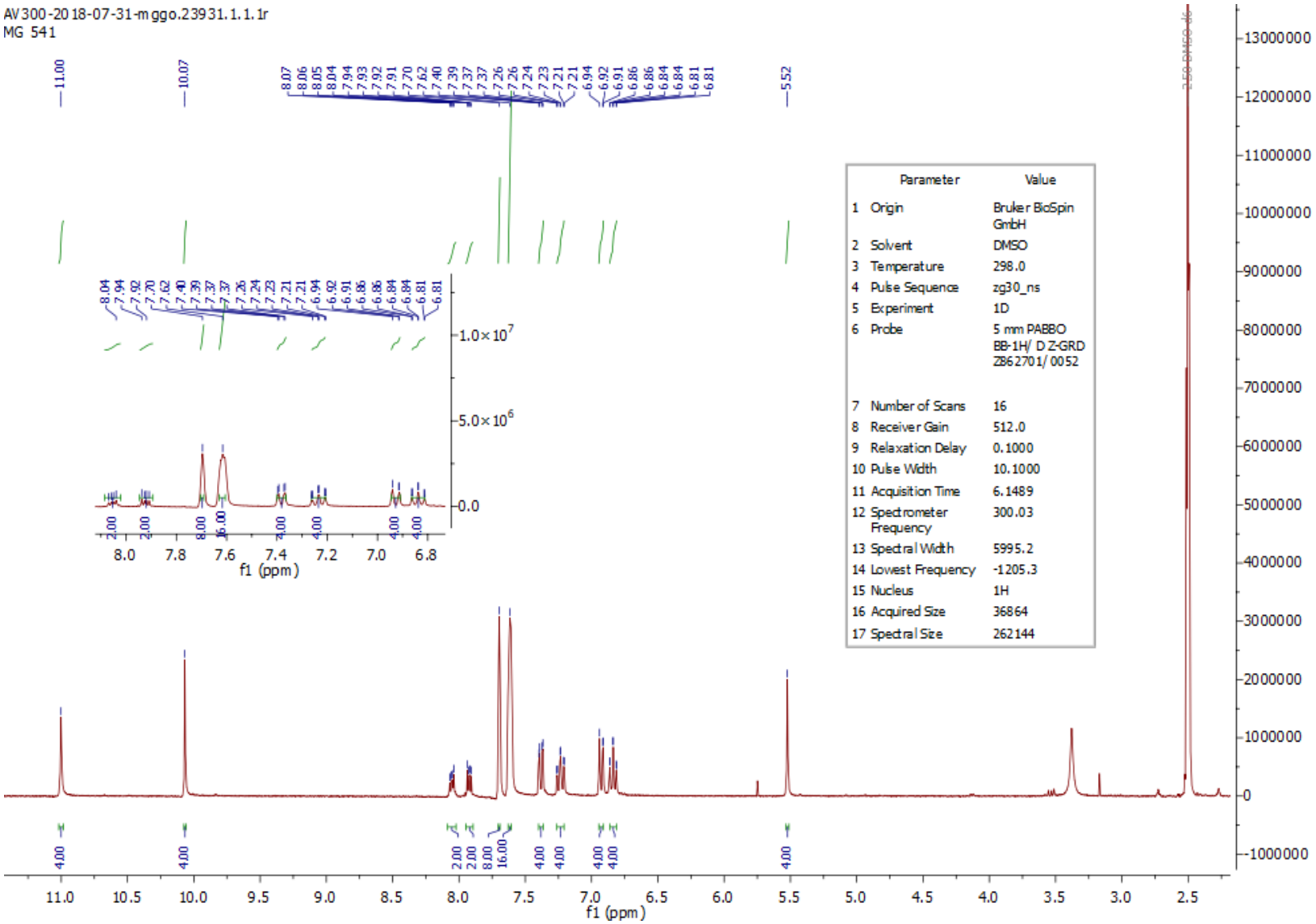
^{13}C NMR spectrum of **6b** (126 MHz, DMSO-d_6)



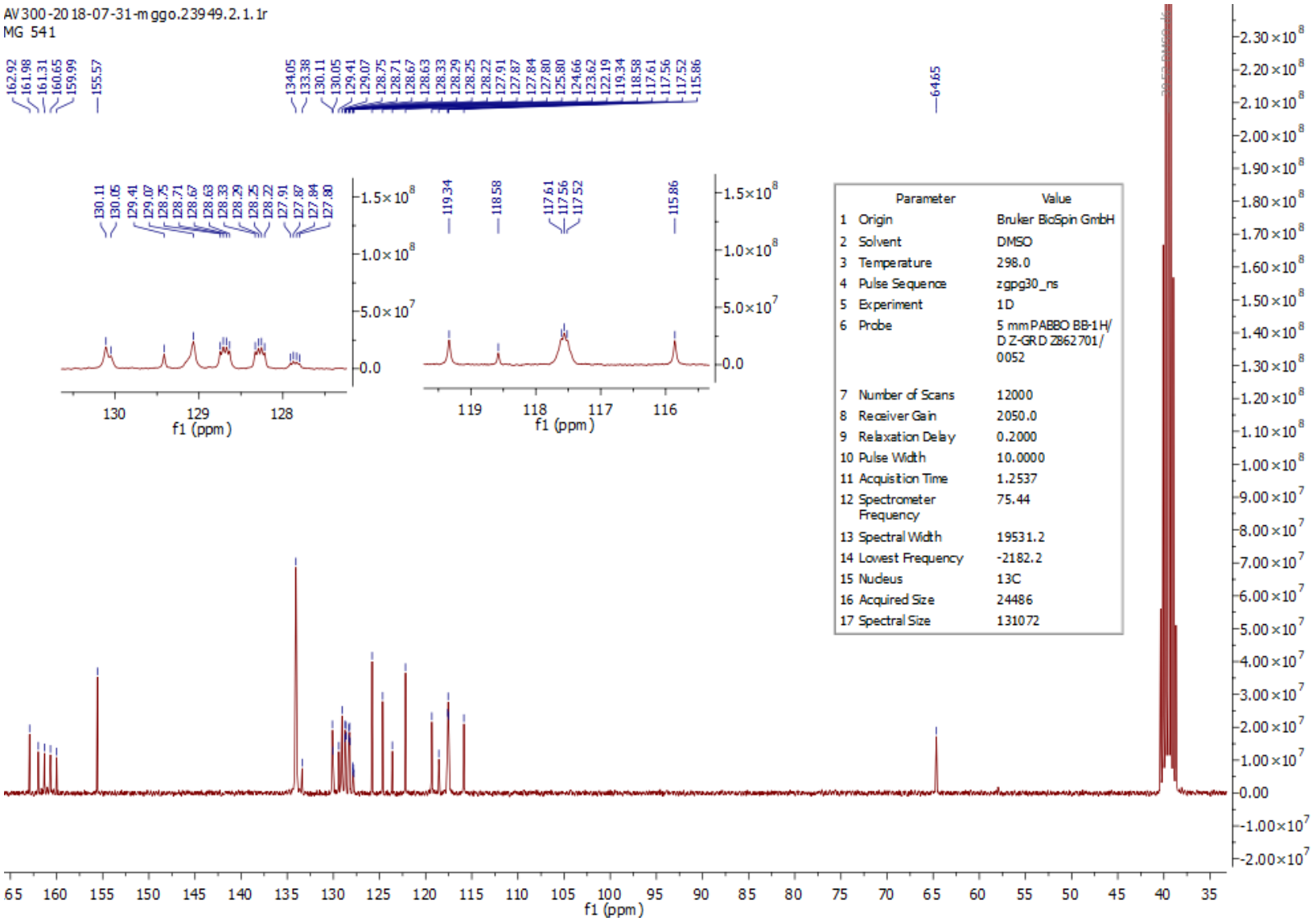
^{1}H NMR spectrum of **7b** (300 MHz, DMSO-d_6)



^{13}C NMR spectrum of **7b** (75 MHz, DMSO-d_6)



^{1}H NMR spectrum of **8b** (300 MHz, DMSO-d_6)



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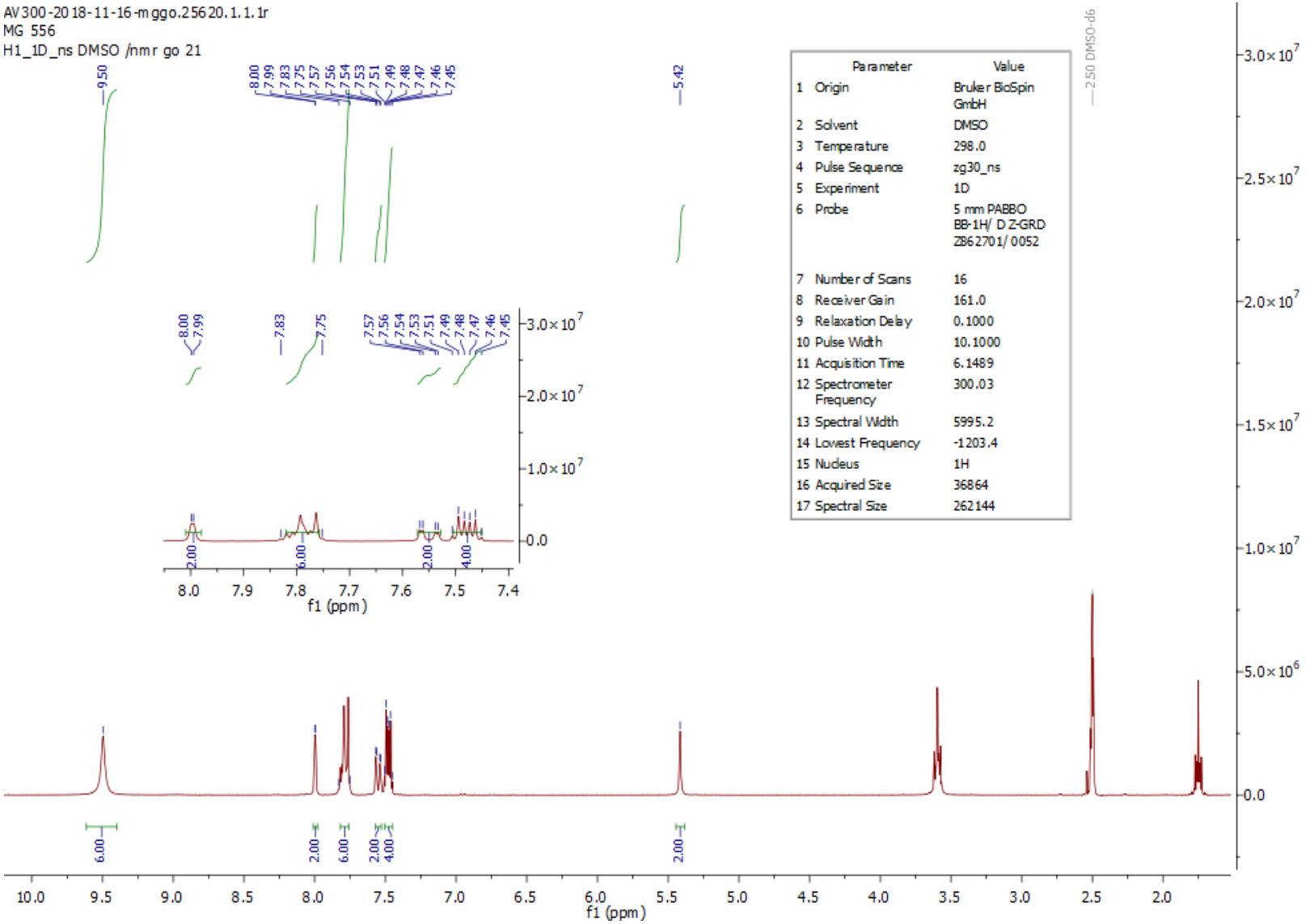
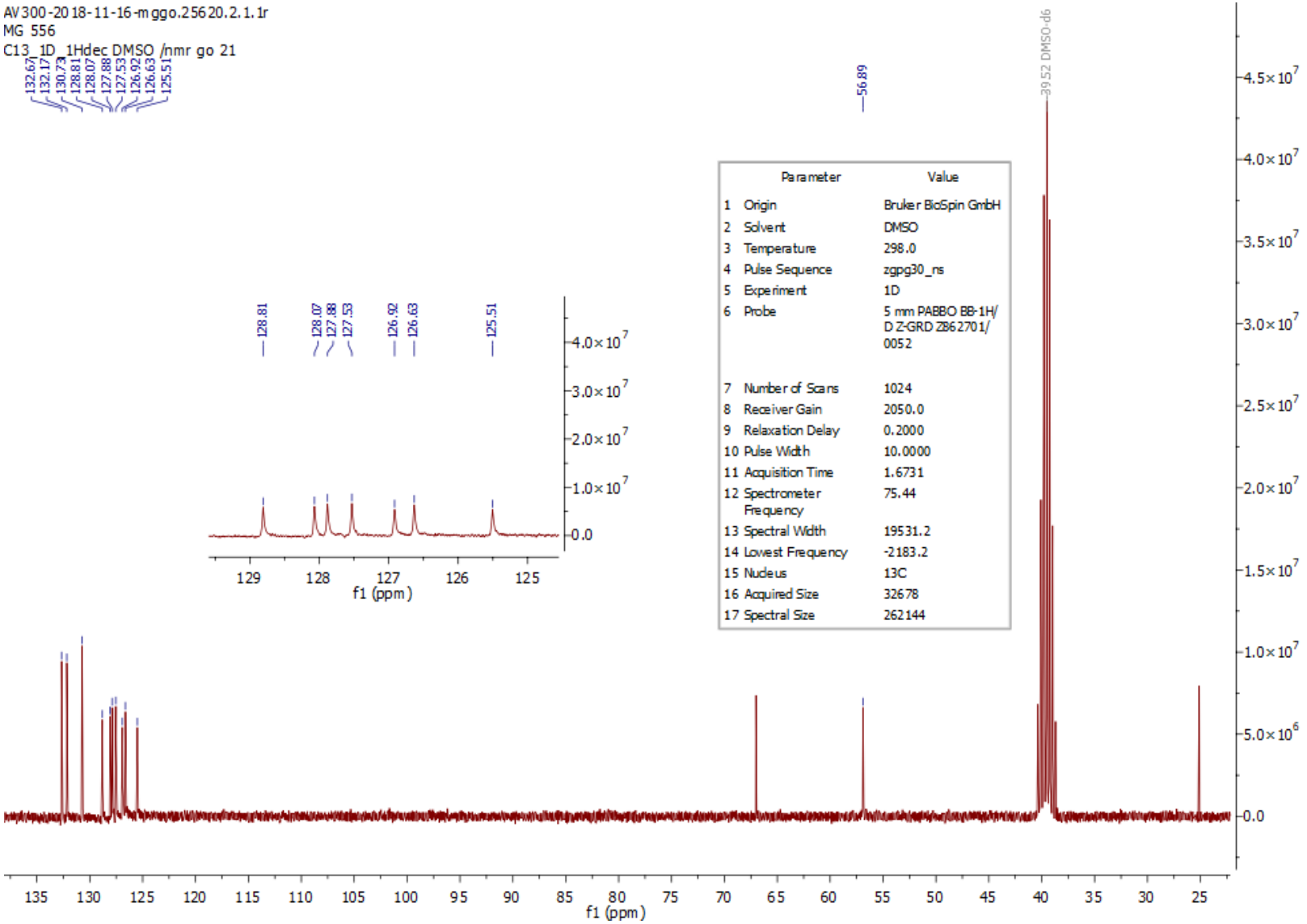
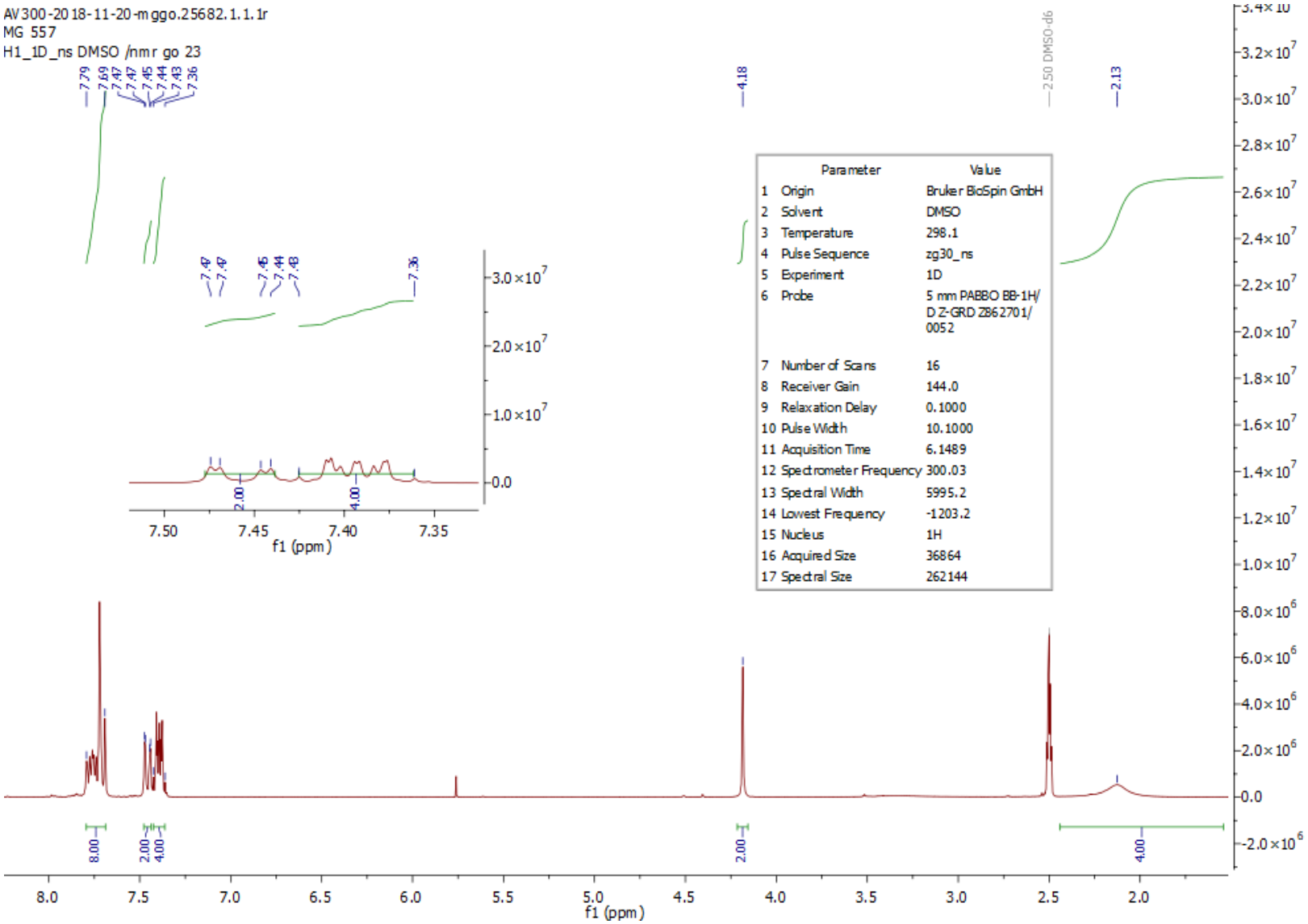


^{1}H NMR spectrum of **5c**·2HCl (300 MHz, DMSO-d_6)



^{13}C NMR spectrum of **5c**·2HCl (75 MHz, DMSO-d_6)



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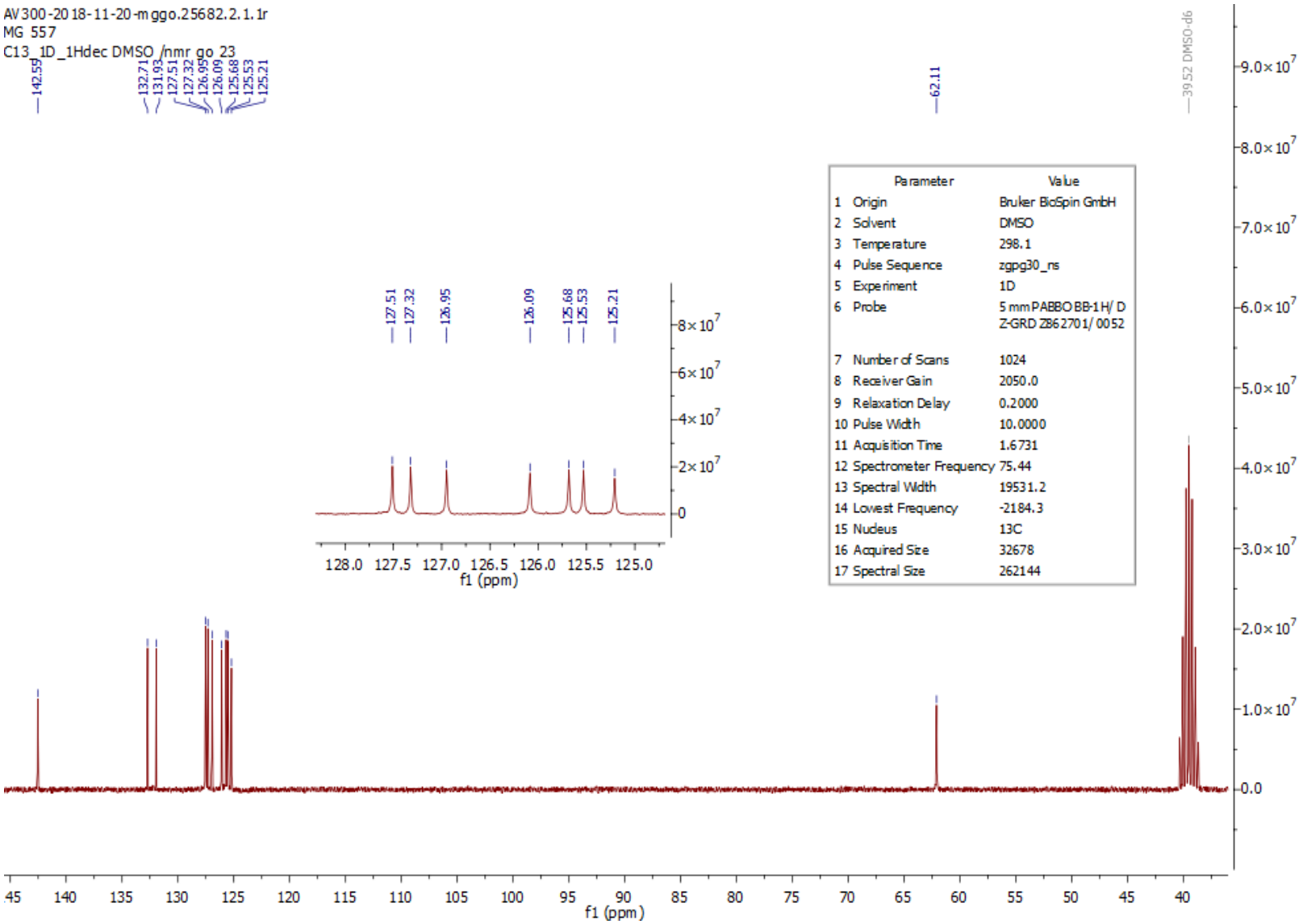

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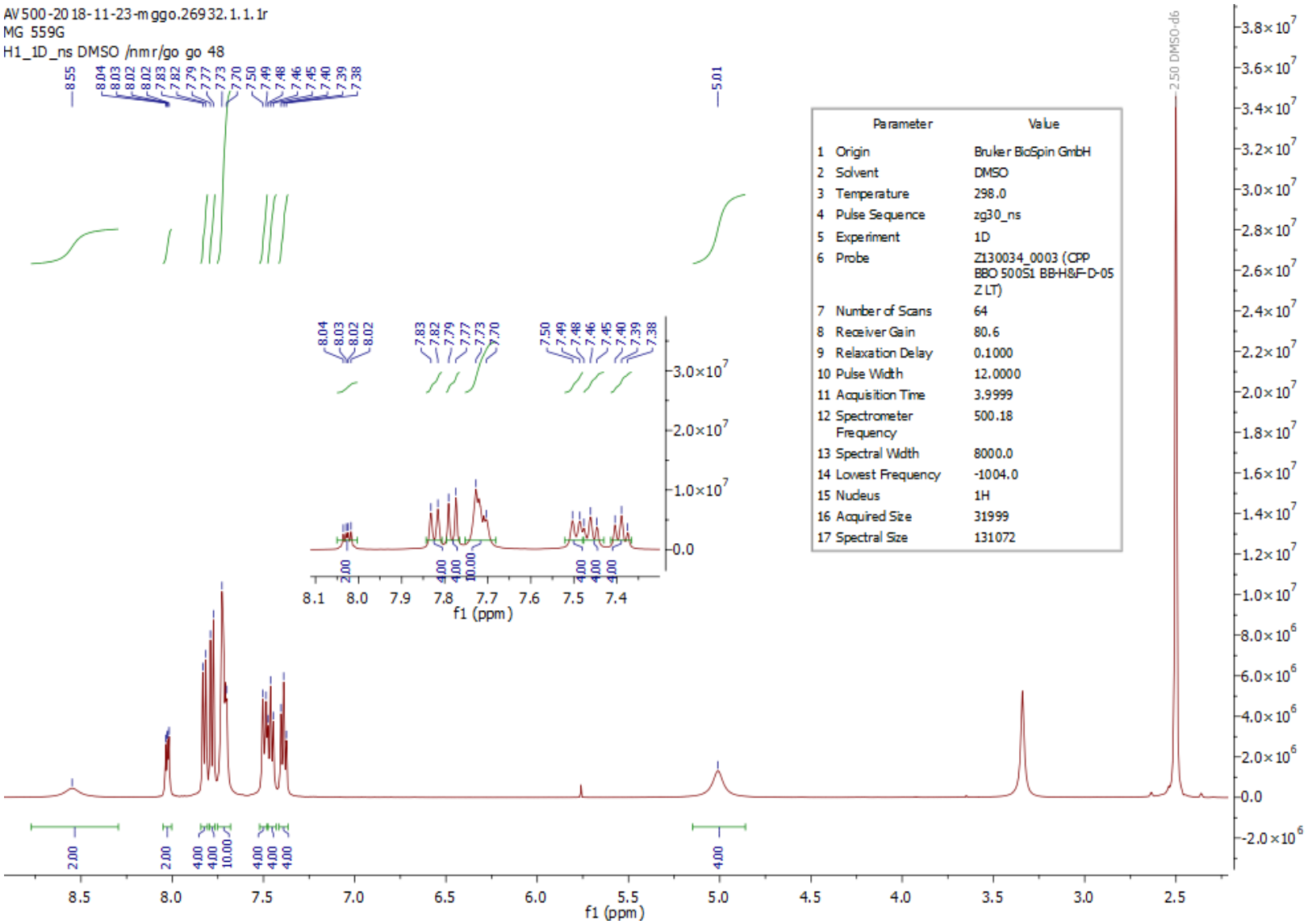
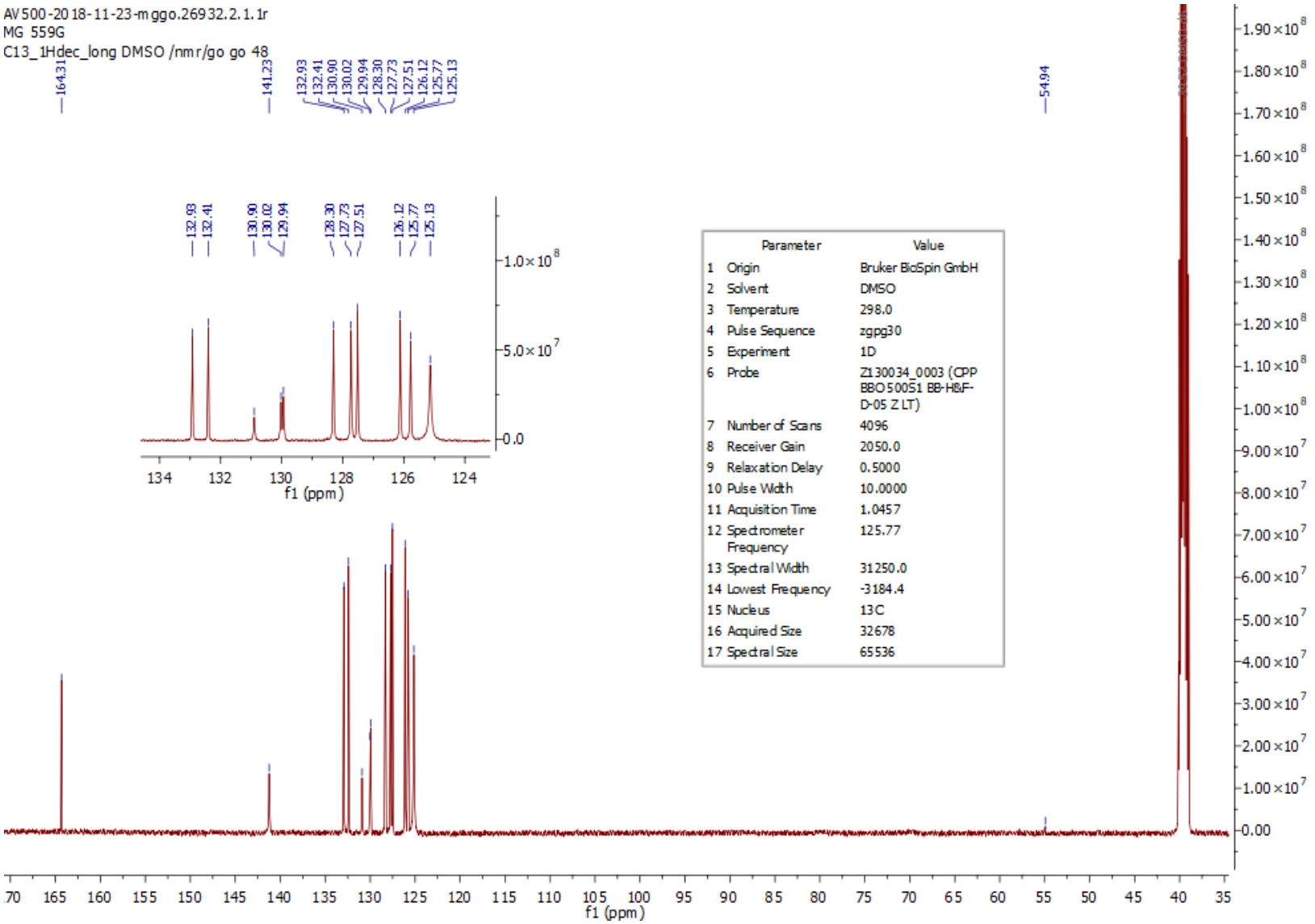
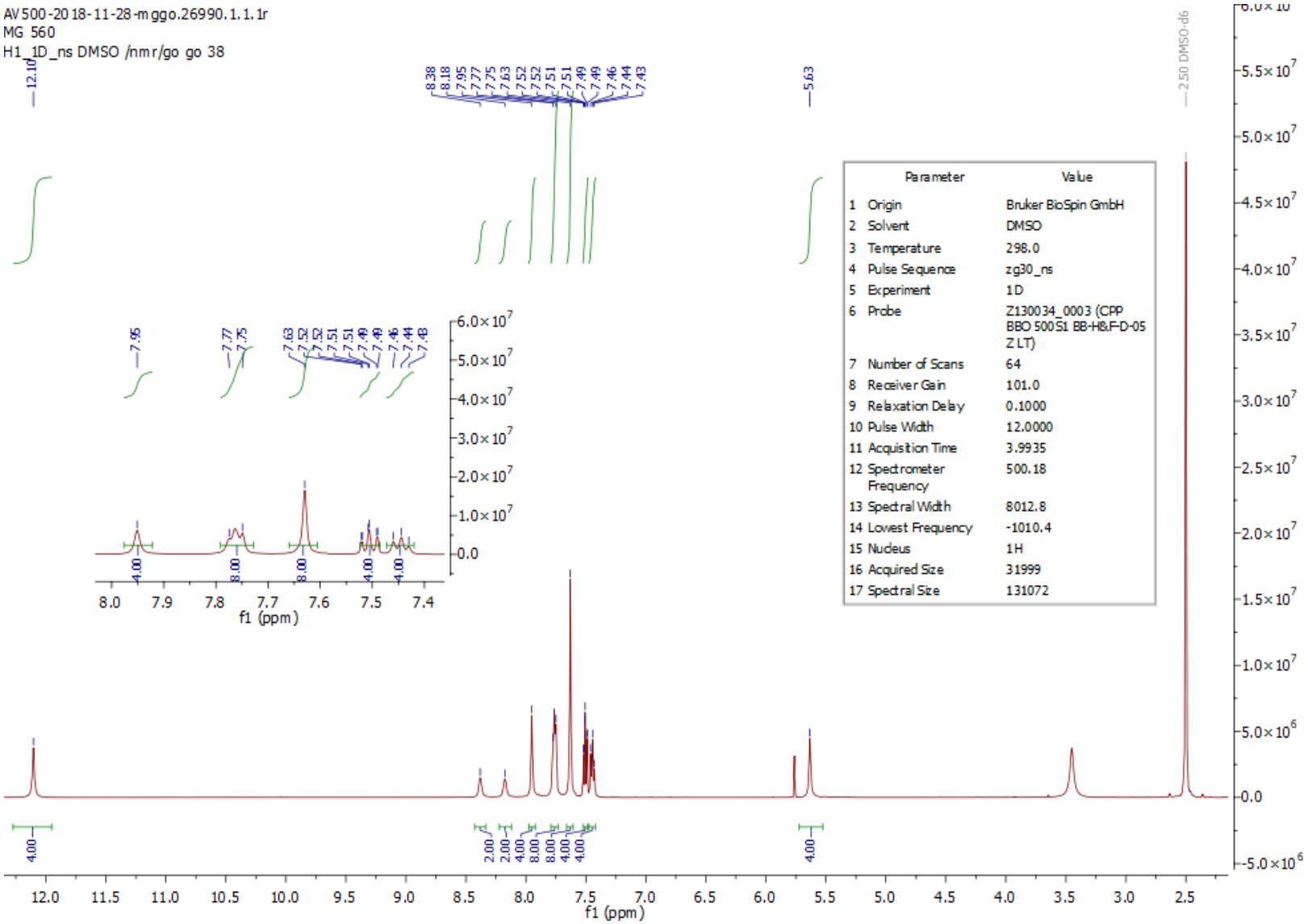


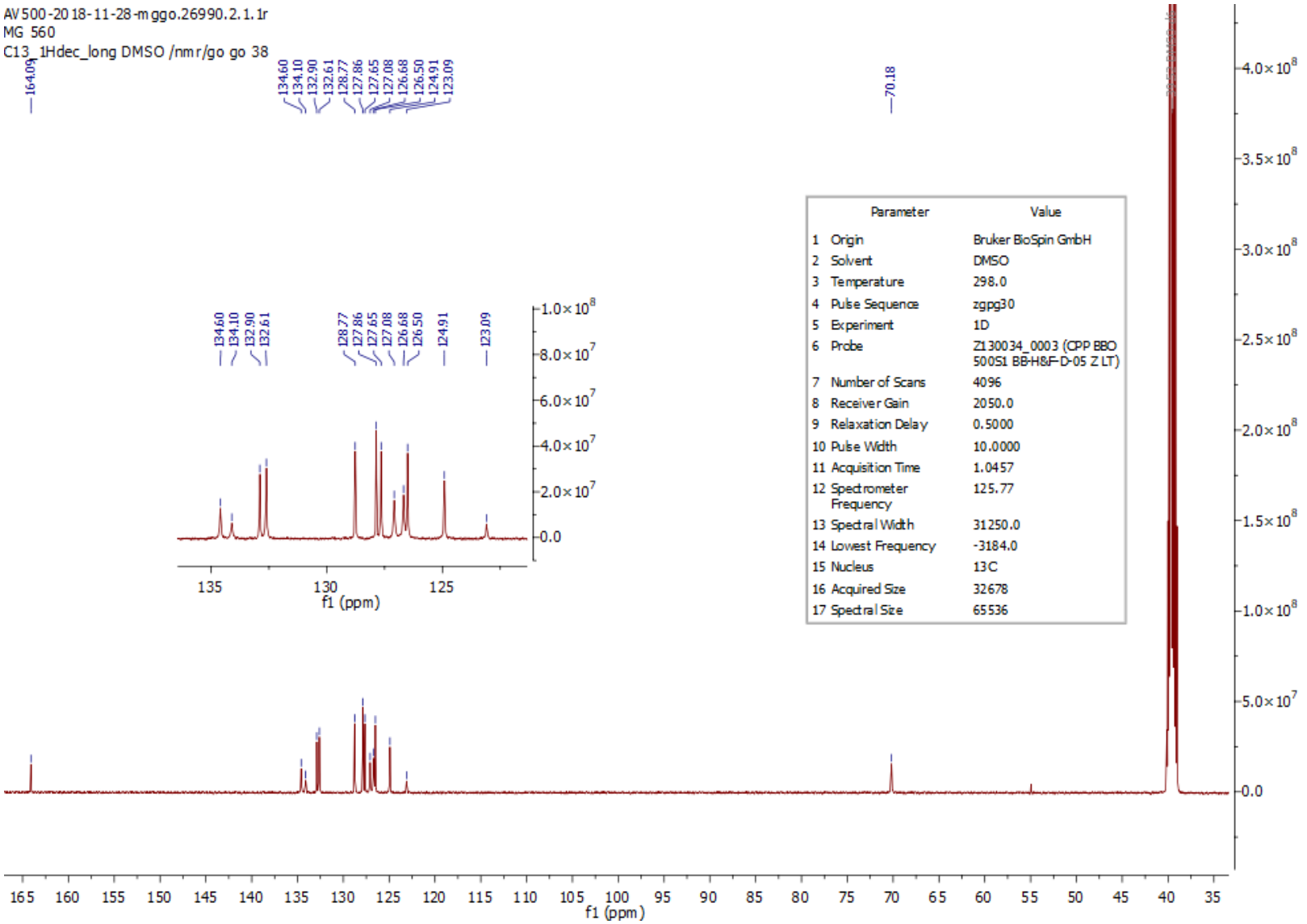
^{1}H NMR spectrum of **6c** (500 MHz, DMSO-d_6)



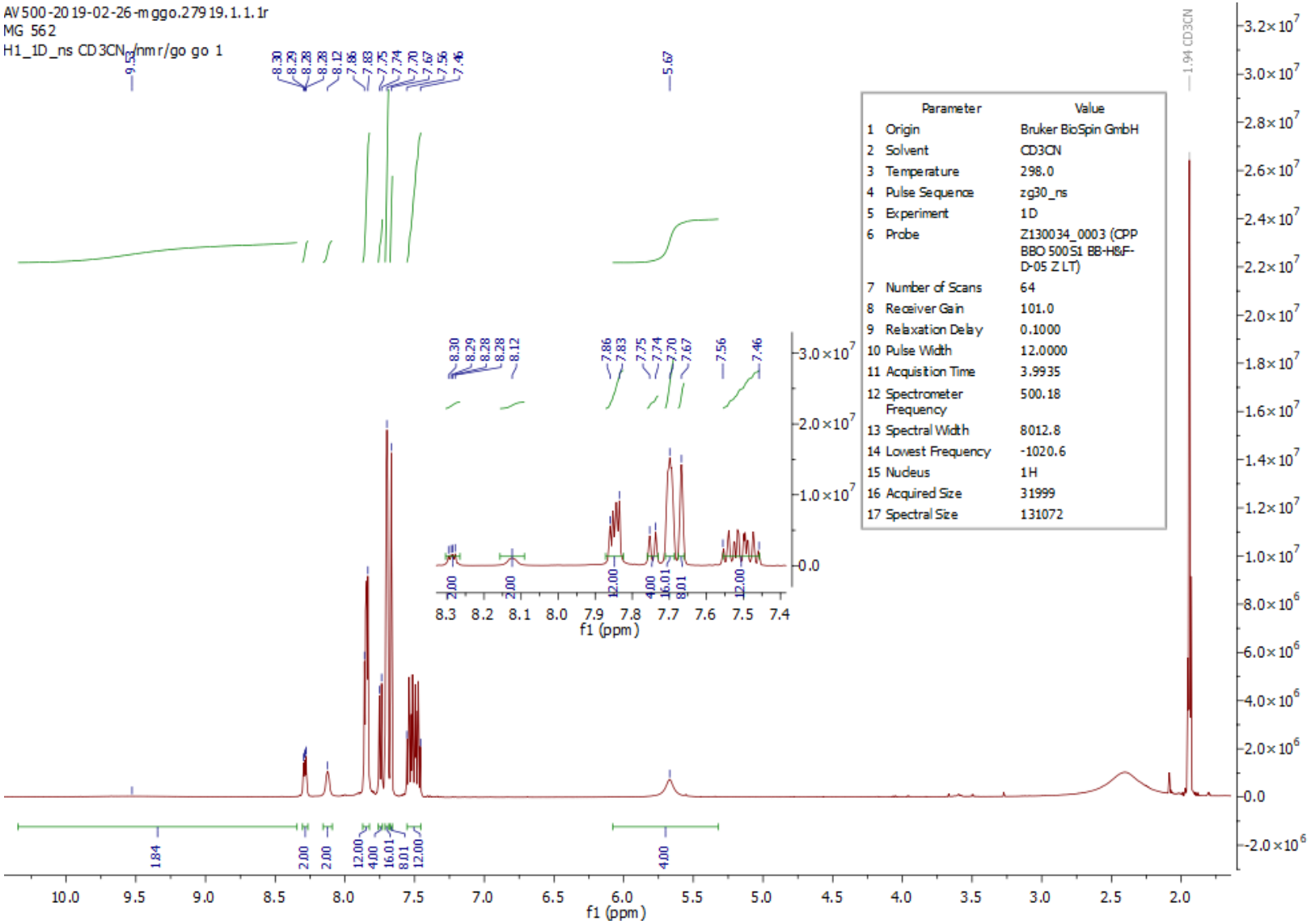
^{13}C NMR spectrum of **6c** (126 MHz, DMSO-d_6)



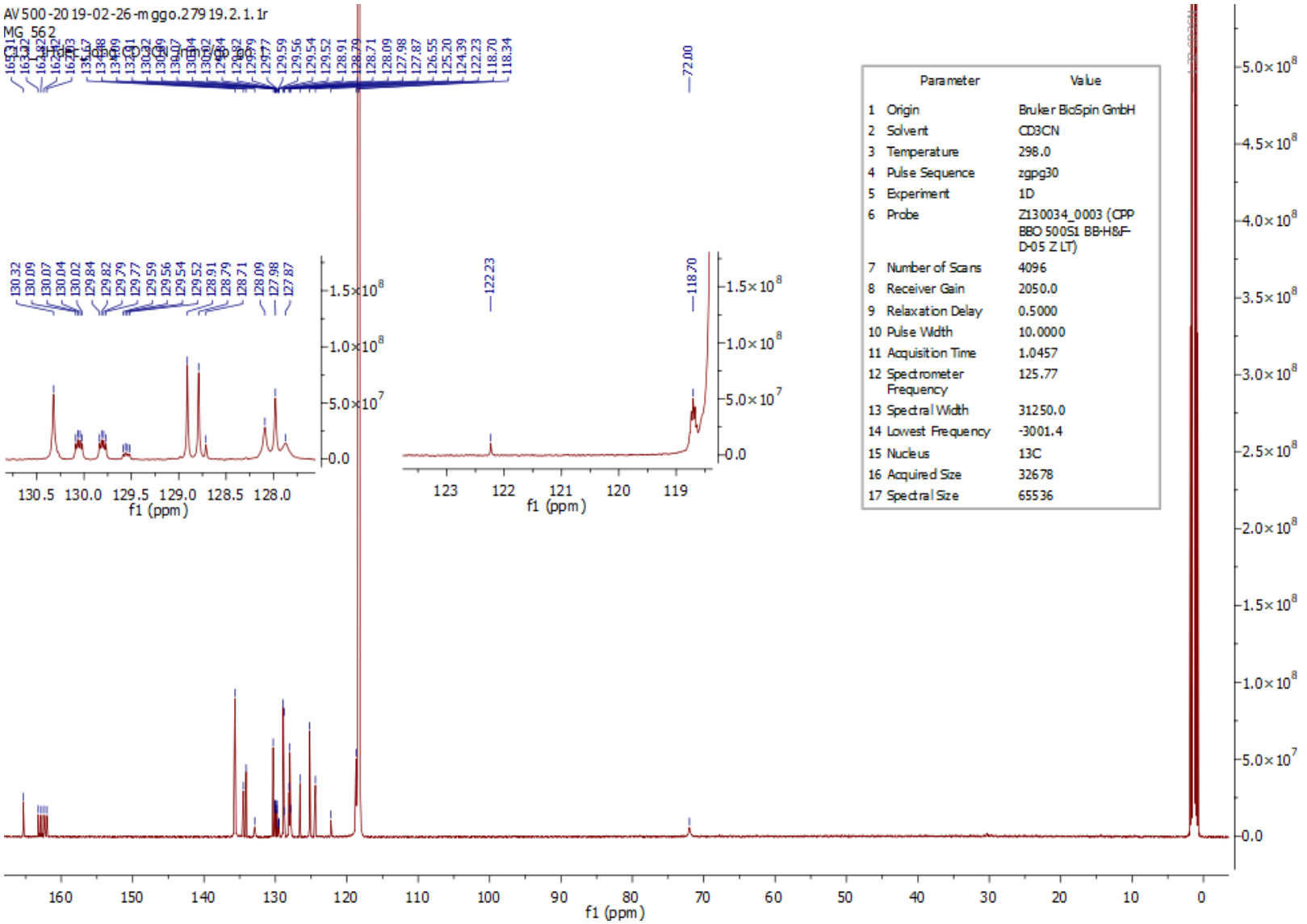
^{1}H NMR spectrum of **7c** (500 MHz, DMSO-d_6)



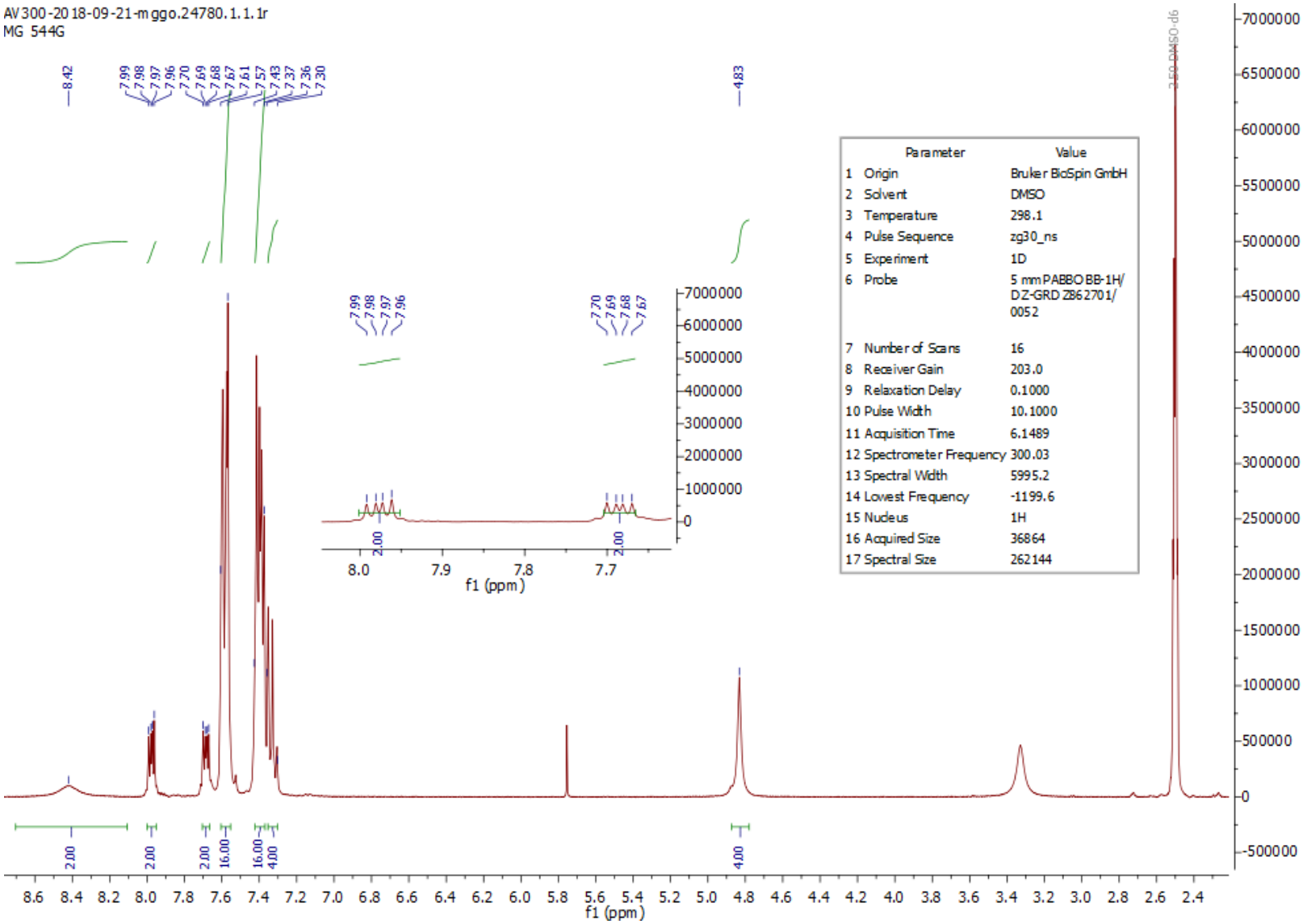
^{13}C NMR spectrum of **7c** (126 MHz, DMSO-d_6)



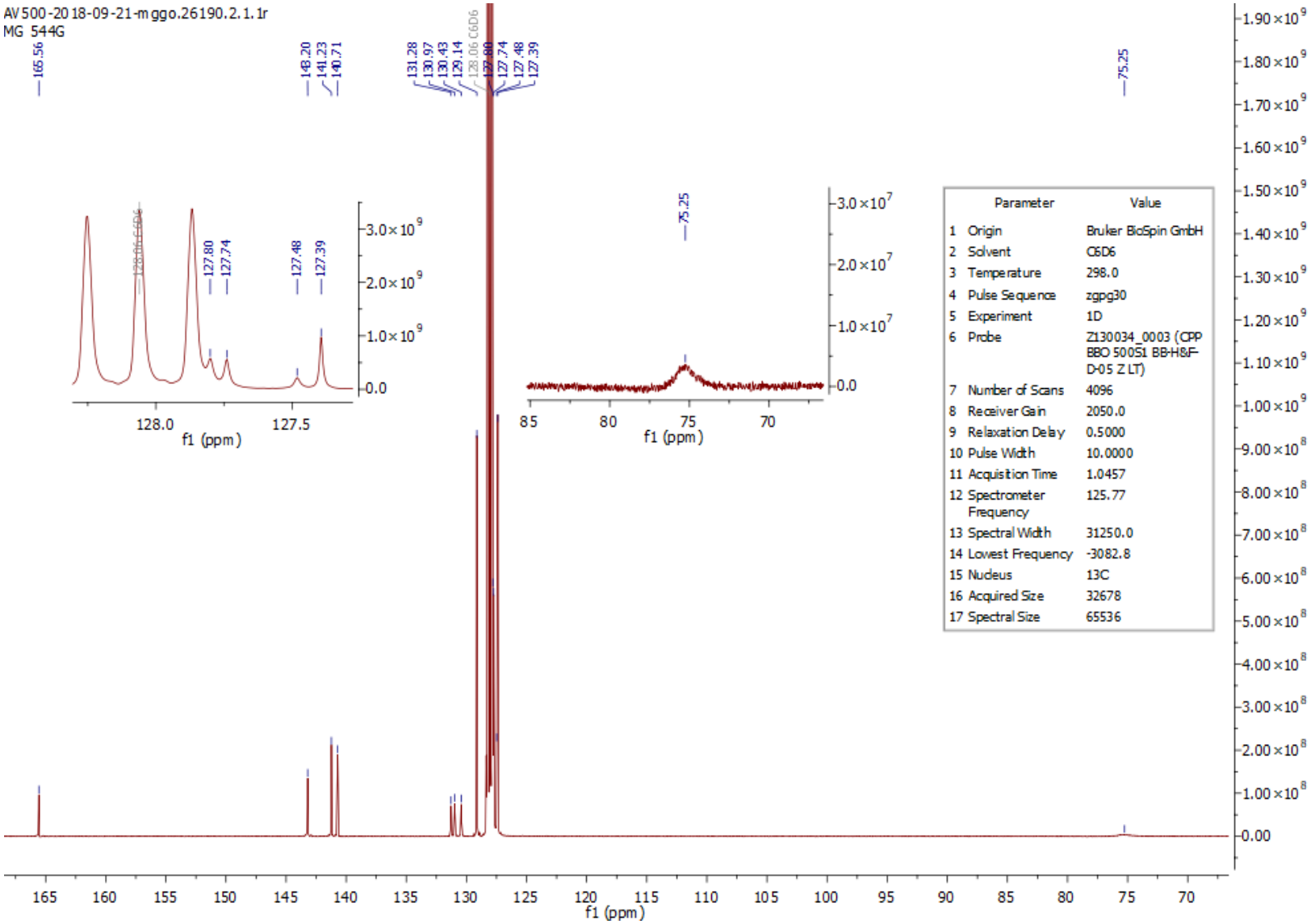
^{1}H NMR spectrum of **8c** (500 MHz, CD_3CN)



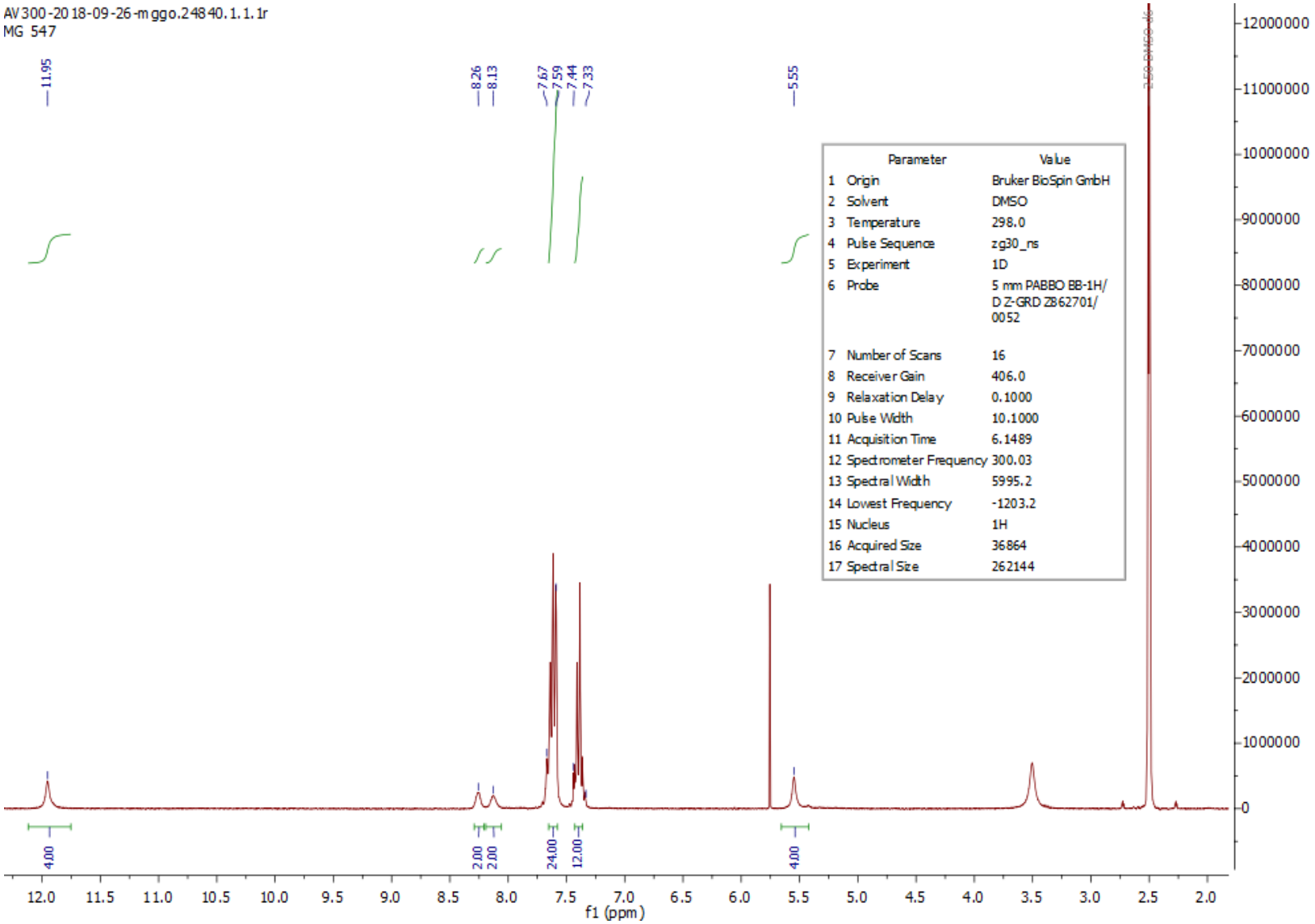
^{13}C NMR spectrum of **8c** (126 MHz, CD_3CN)



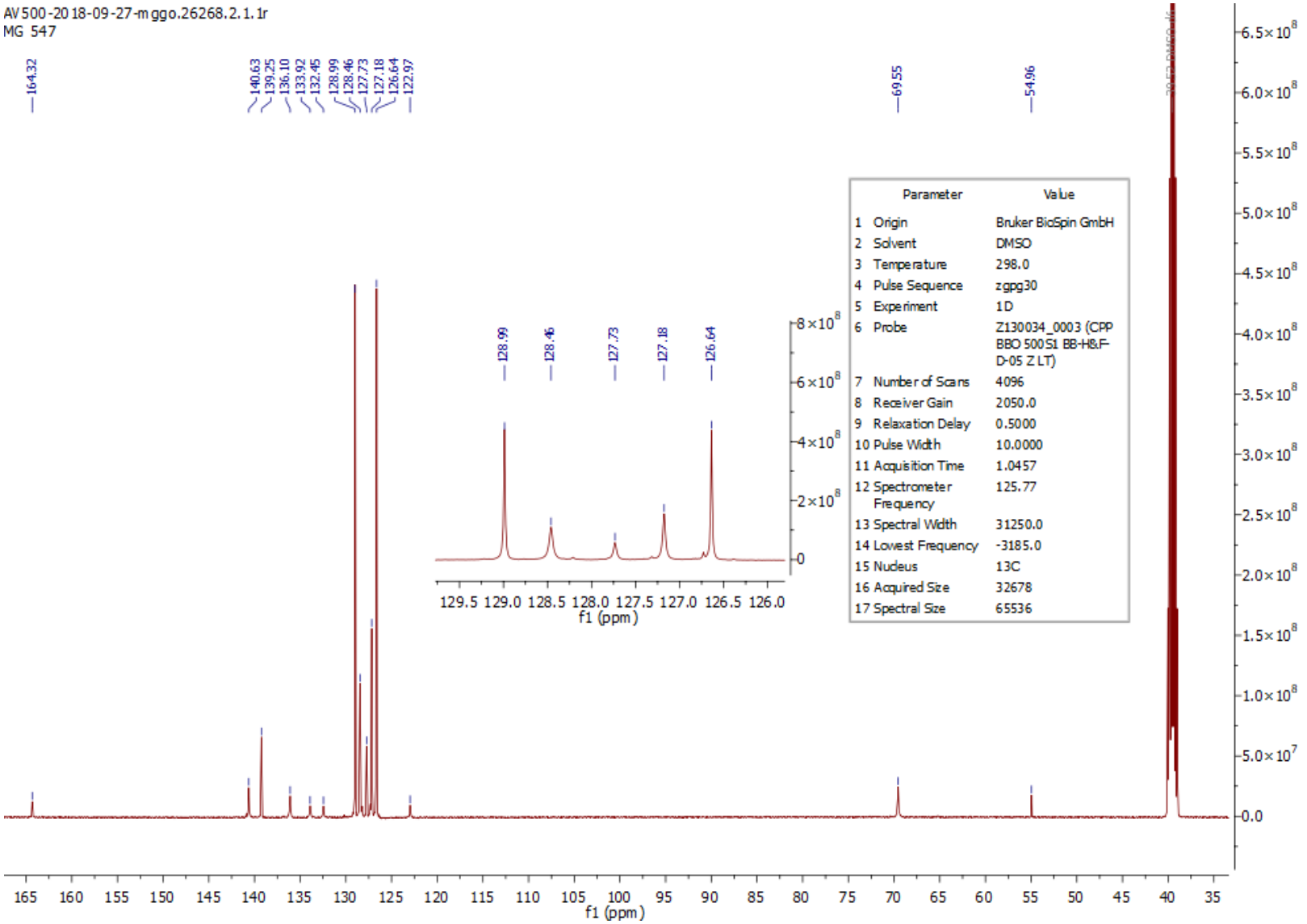
^{1}H NMR spectrum of **6d** (300 MHz, DMSO-d_6)



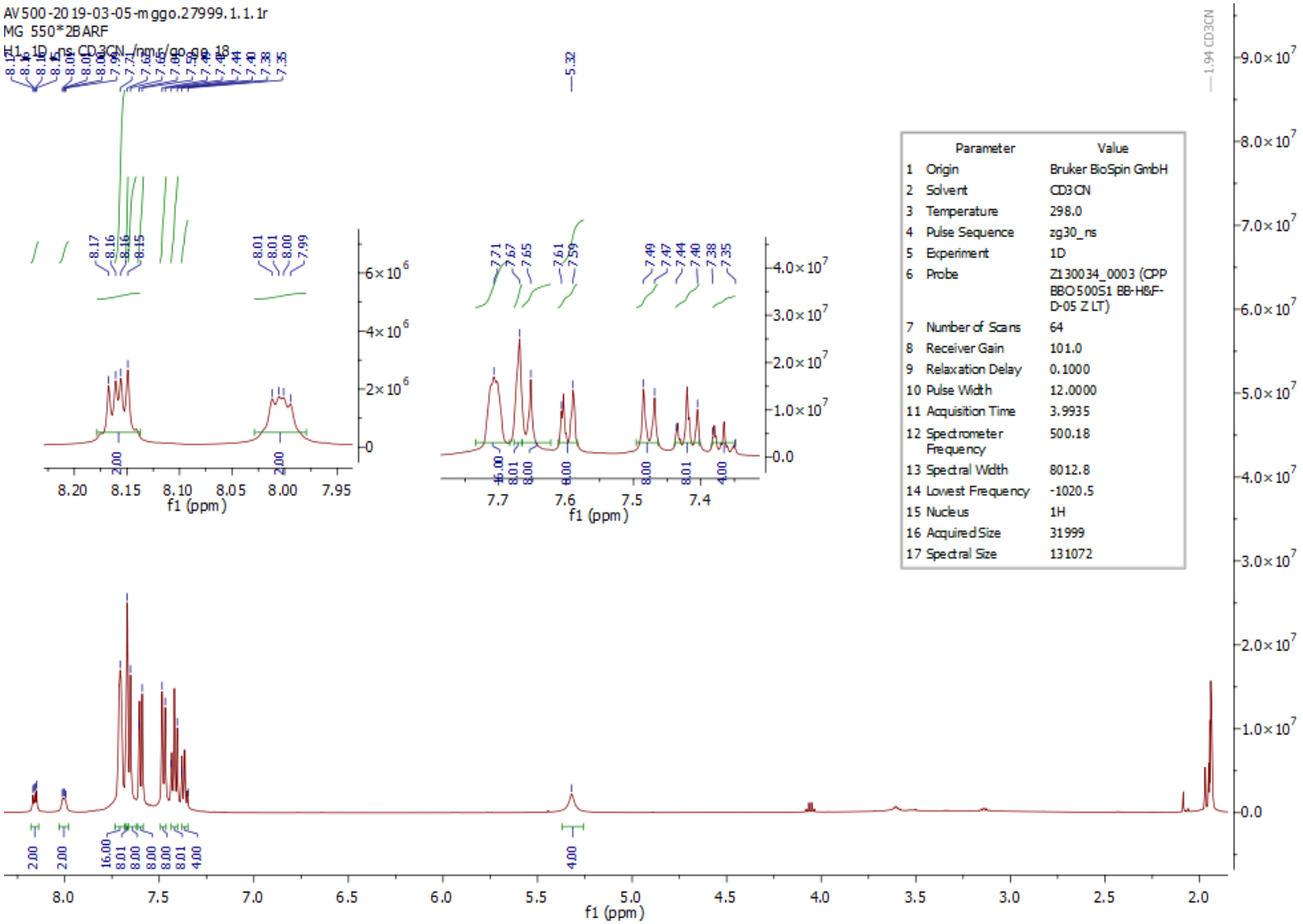
^{13}C NMR spectrum of **6d** (126 MHz, C_6D_6)



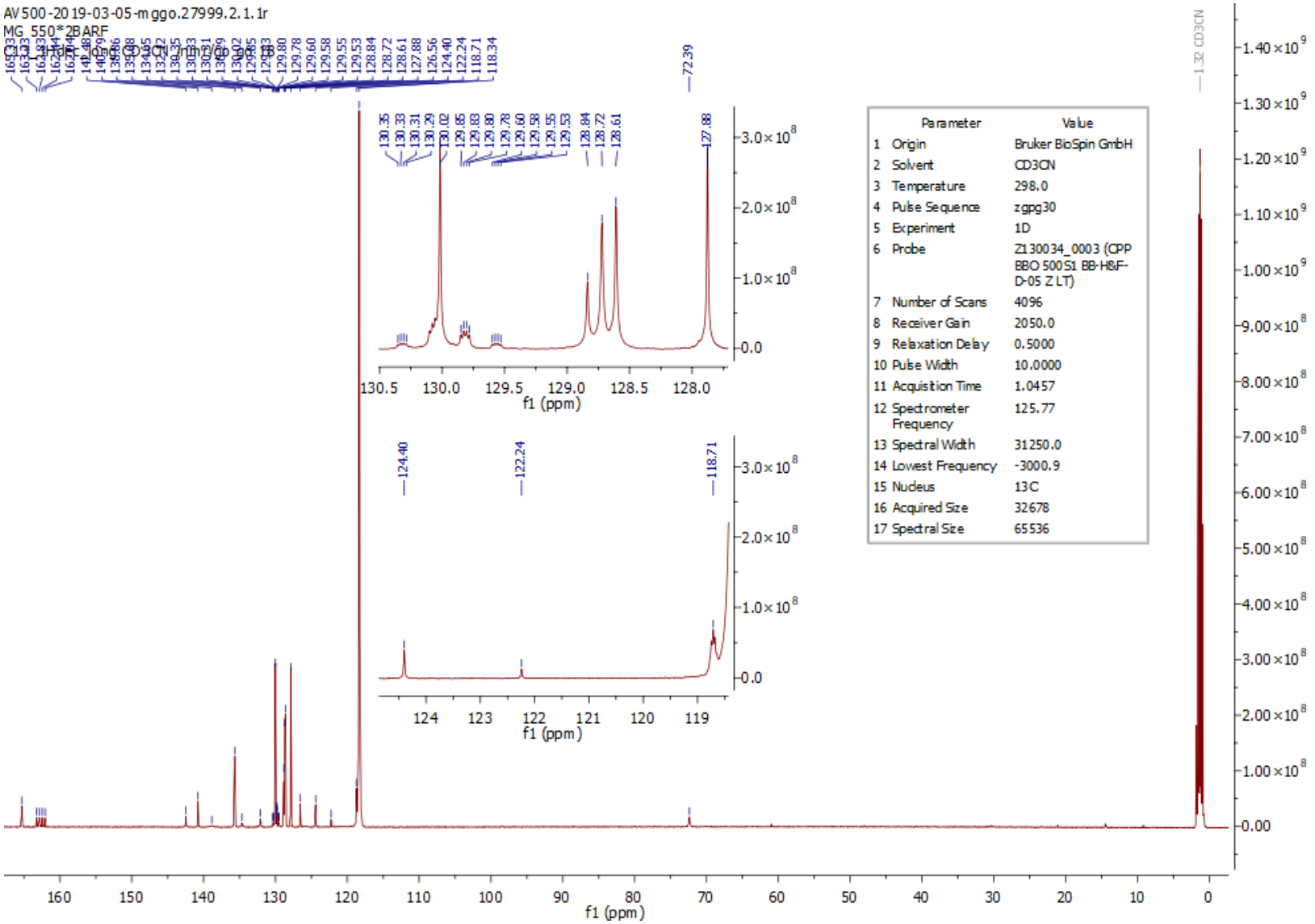
^{1}H NMR spectrum of **7d** (300 MHz, DMSO-d_6)



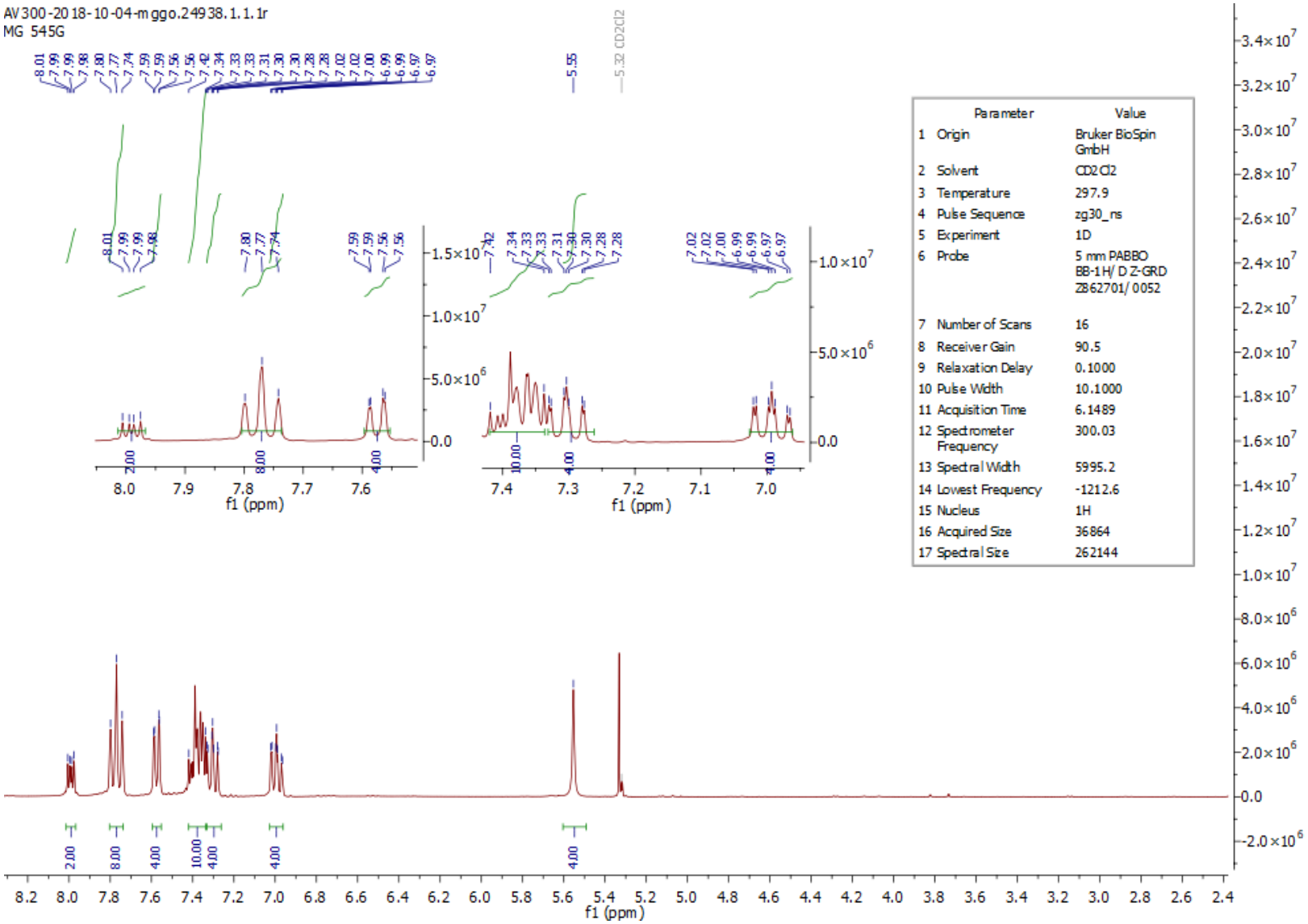
^{13}C NMR spectrum of **7d** (126 MHz, DMSO-d_6)



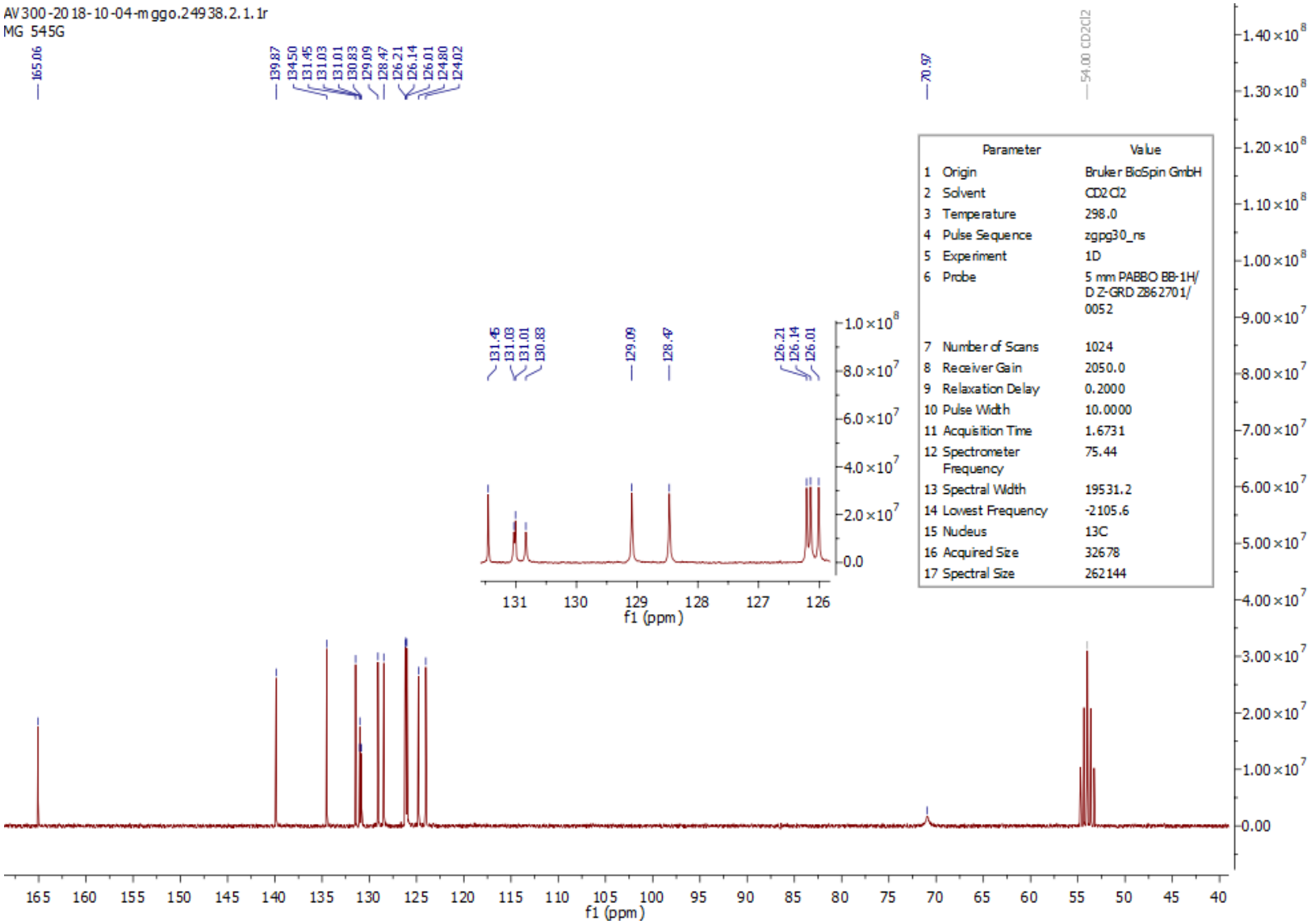
^{1}H NMR spectrum of **8d** (500 MHz, CD_3CN)



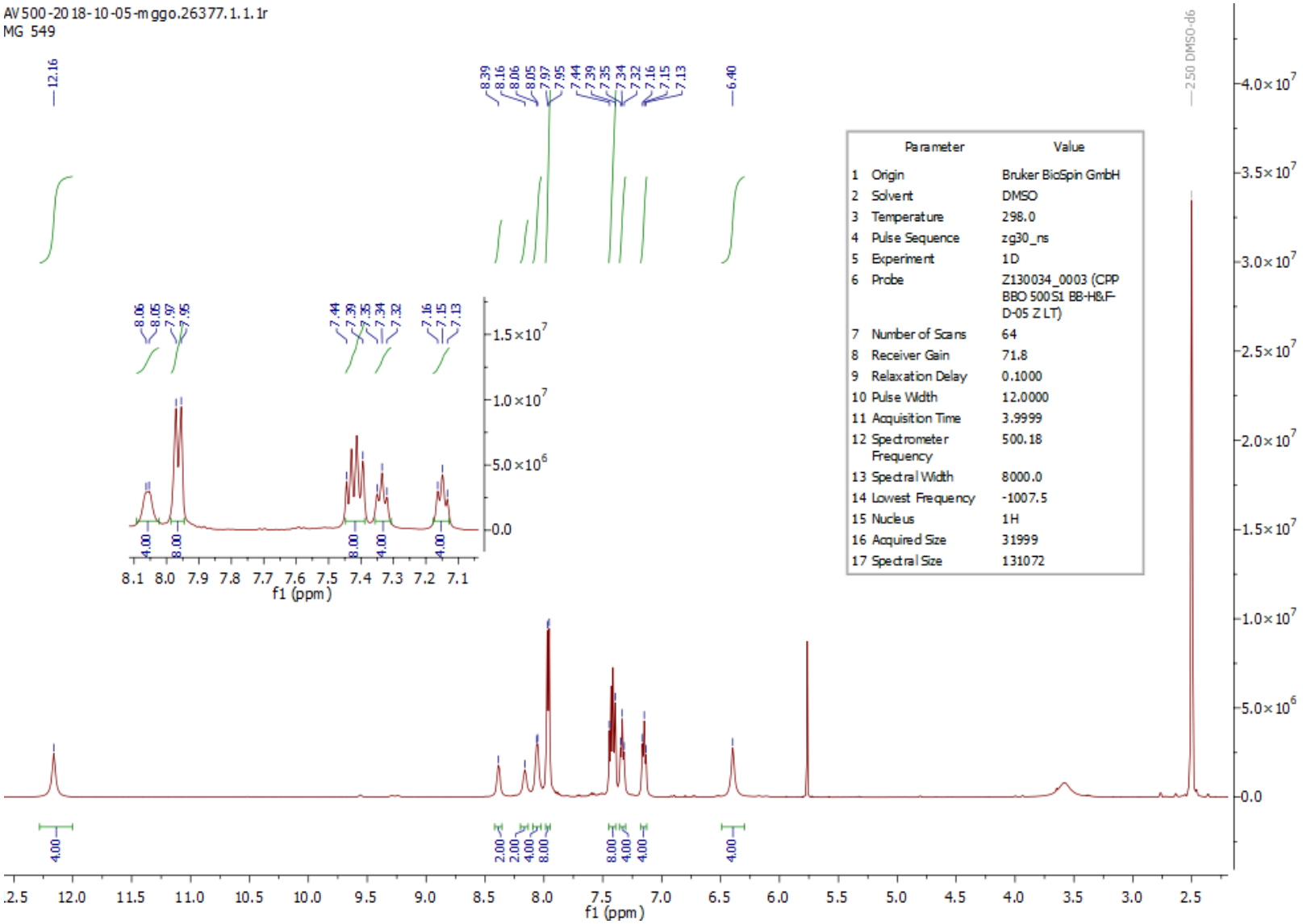
^{13}C NMR spectrum of **8d** (126 MHz, CD_3CN)



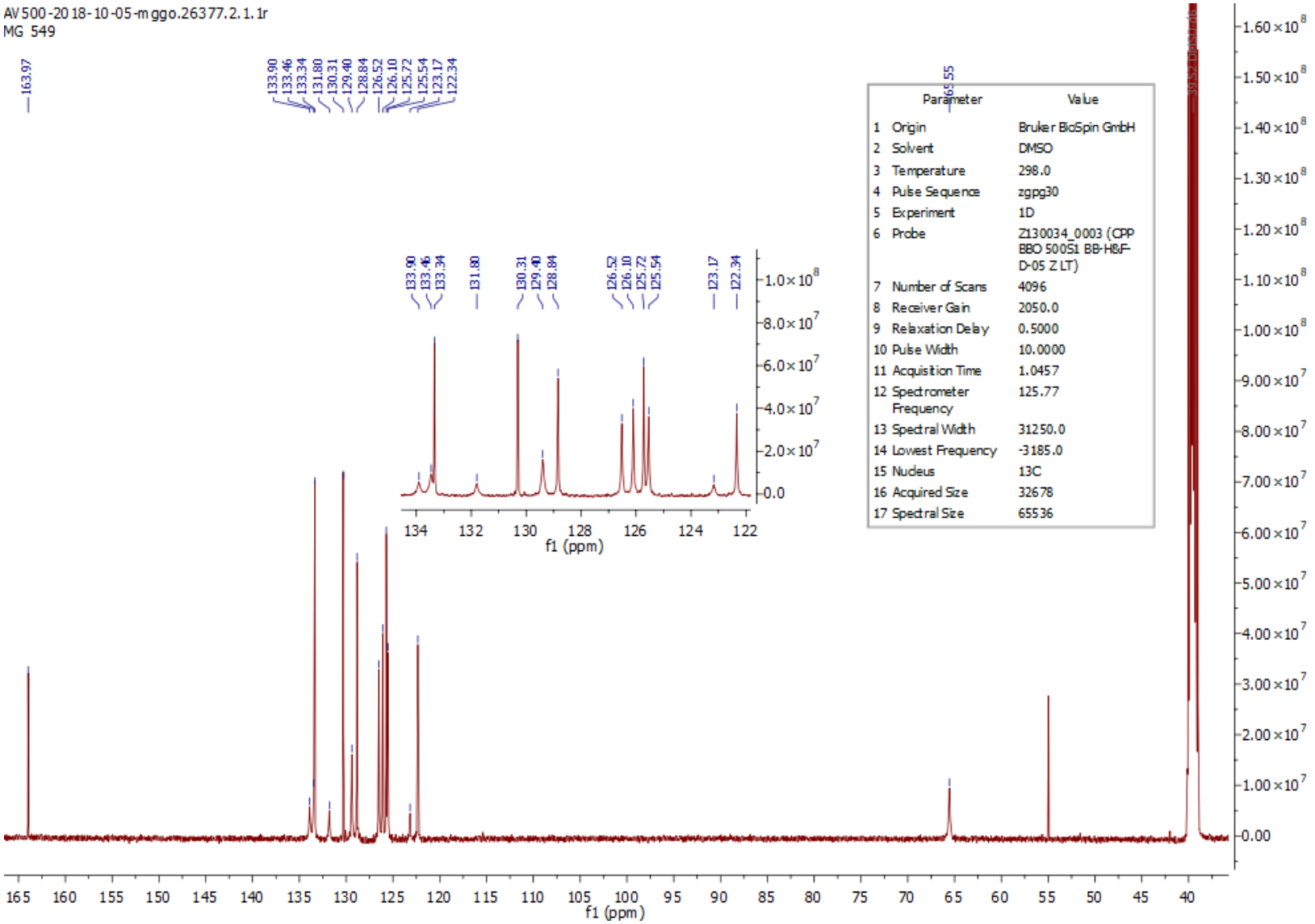
^{1}H NMR spectrum of **6e** (300 MHz, CD_2Cl_2)



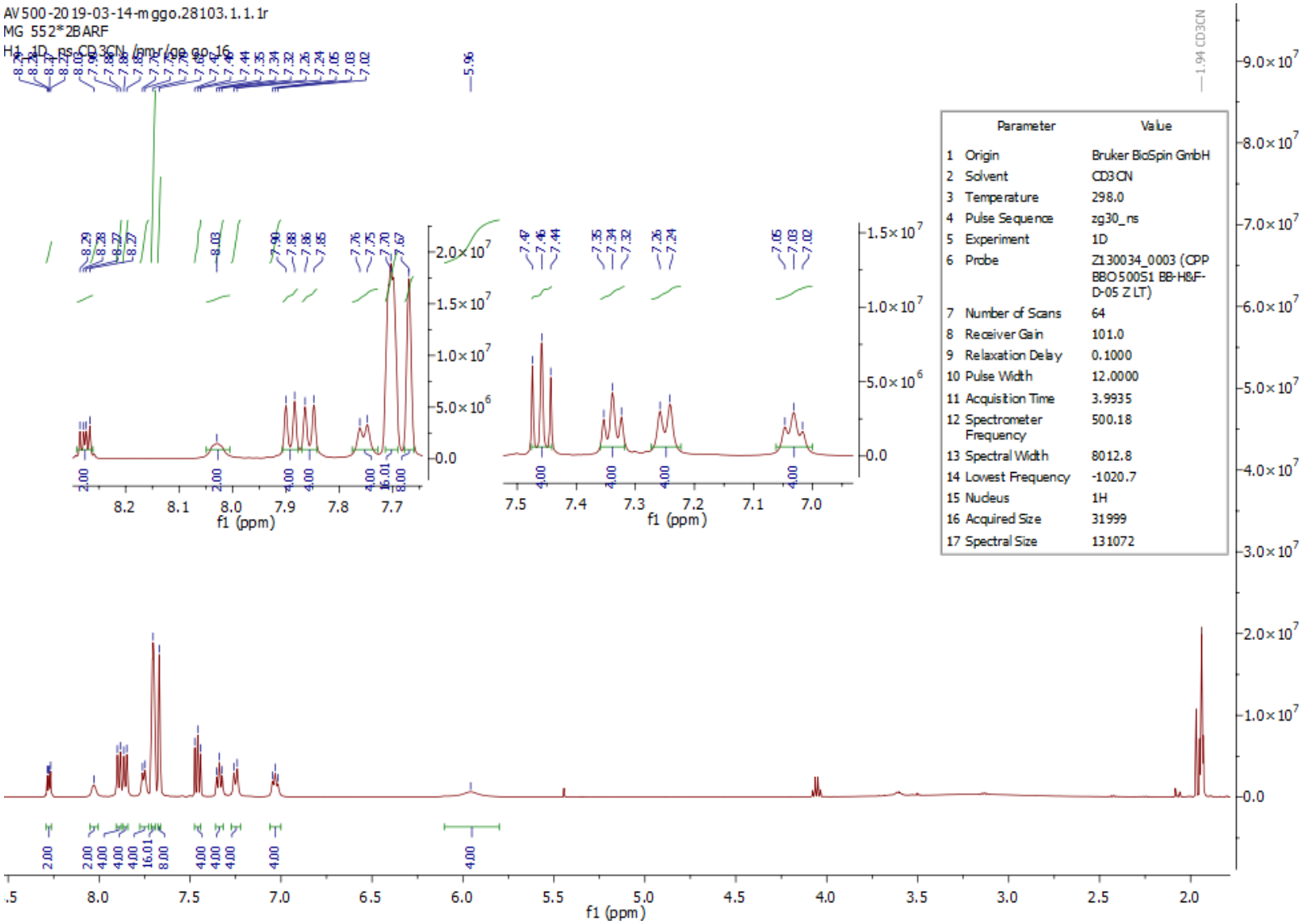
^{13}C NMR spectrum of **6e** (75 MHz, CD_2Cl_2)



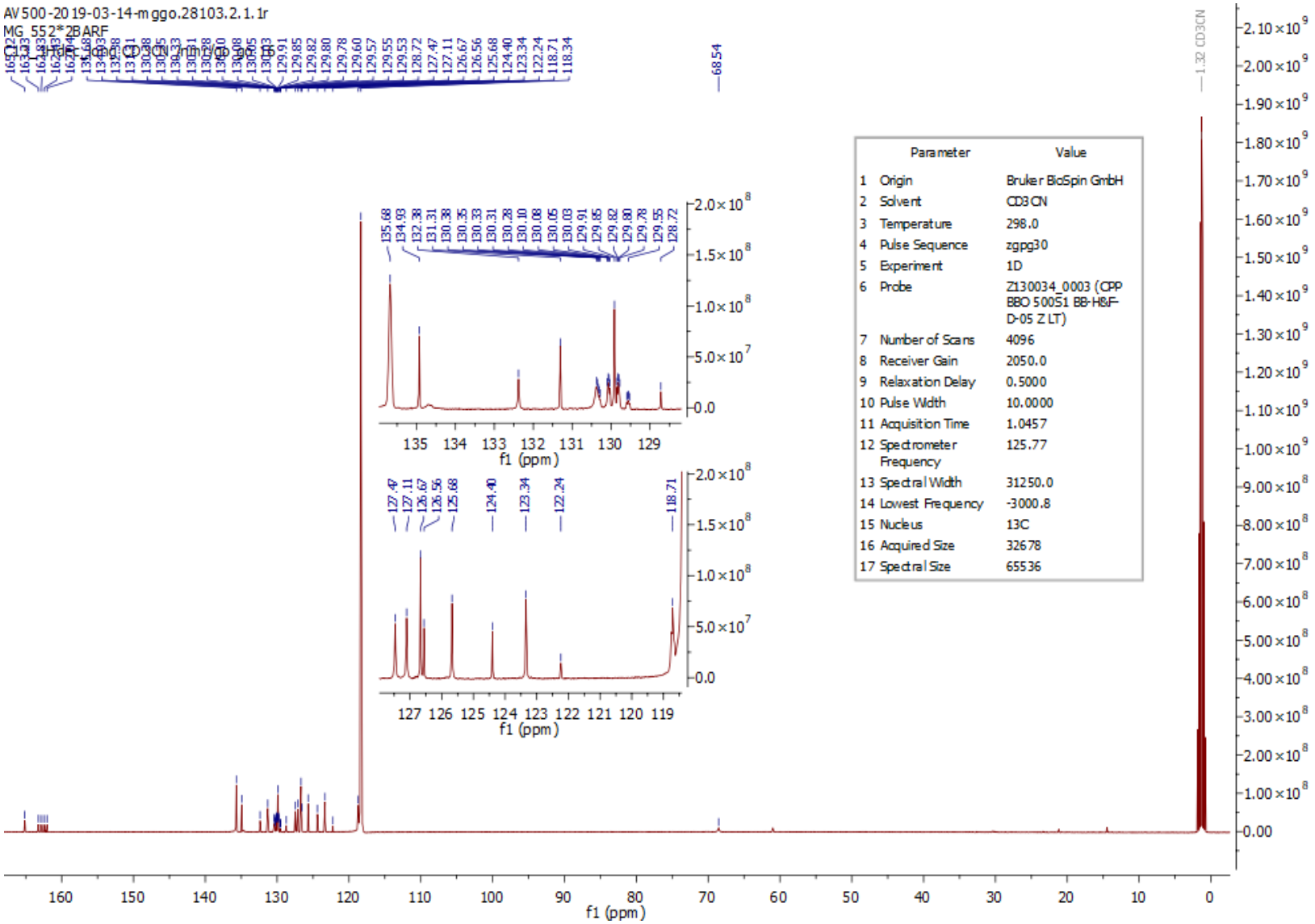
^{1}H NMR spectrum of **7e** (300 MHz, DMSO-d_6)



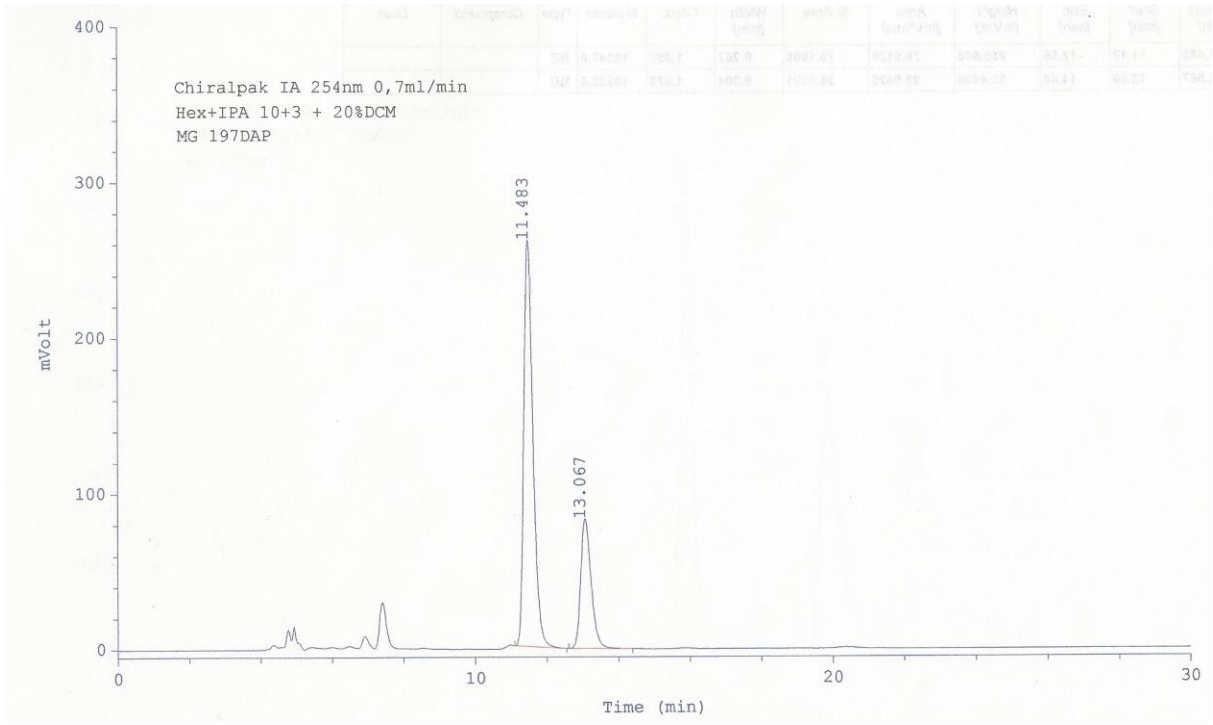
^{13}C NMR spectrum of **7e** (126 MHz, DMSO-d_6)



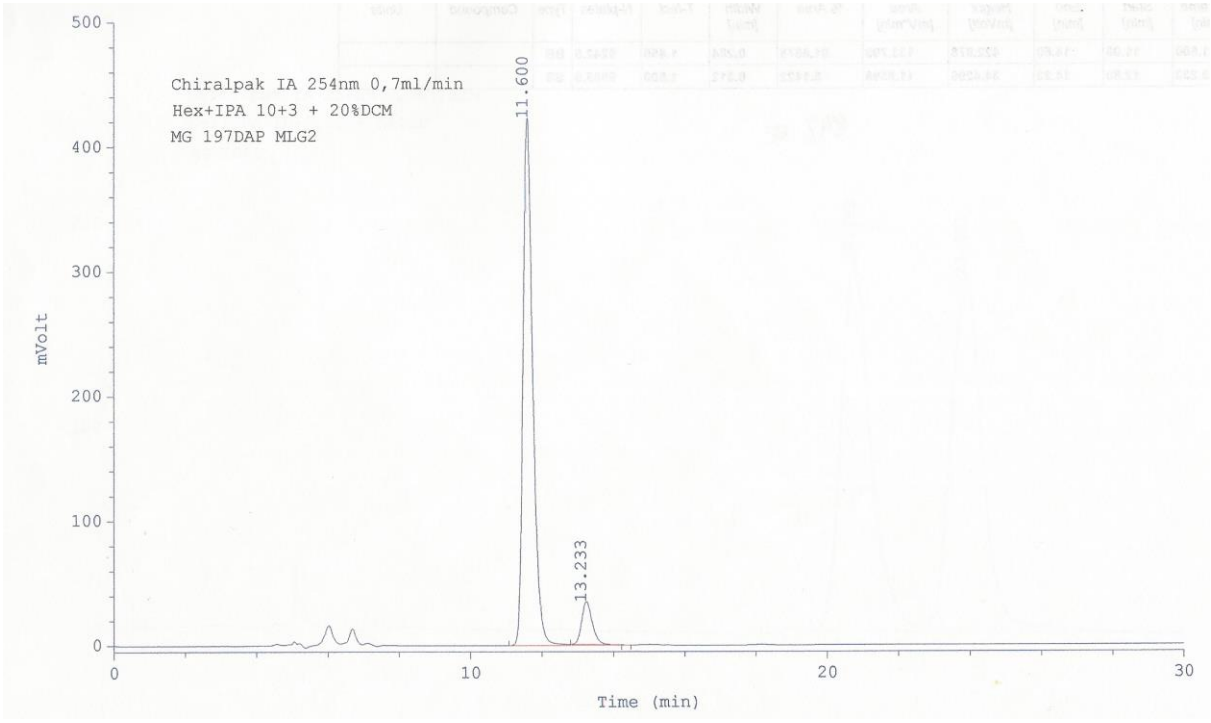
^{1}H NMR spectrum of **8e** (500 MHz, CD_3CN)



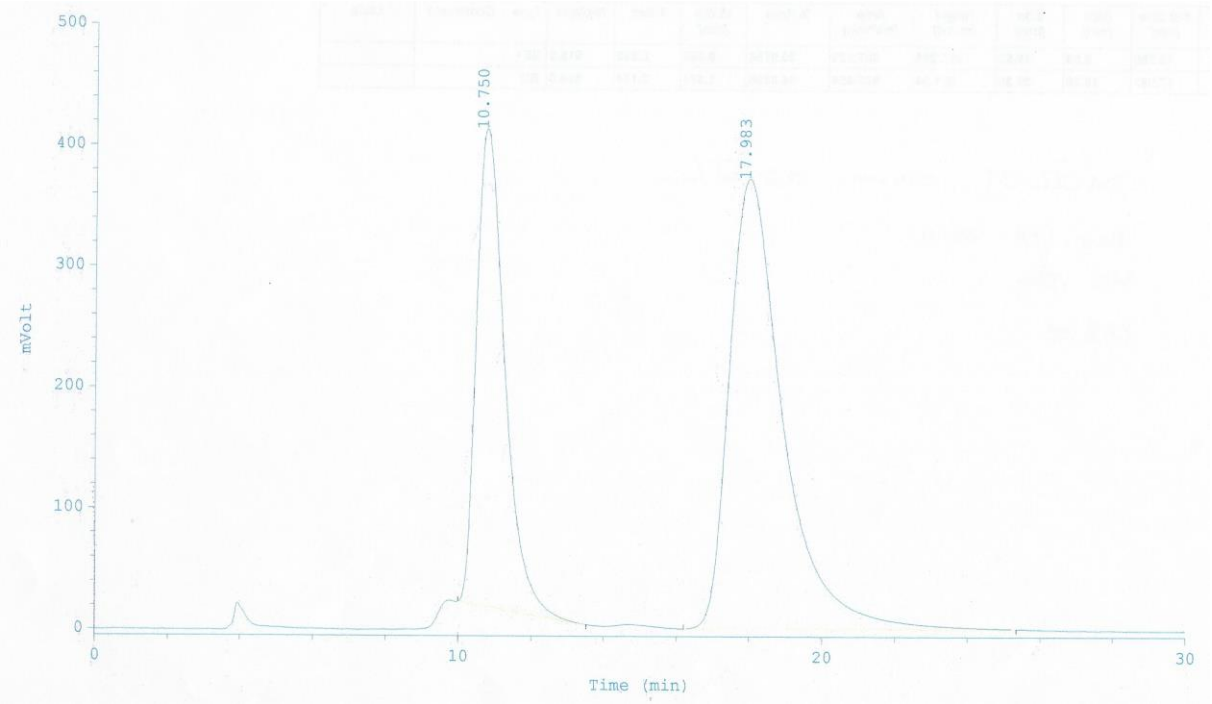
^{13}C NMR spectrum of **8e** (126 MHz, CD_3CN)



Chromatogram of **19** (Chiralpak IA, 254 nm, 0.7 ml/min, *n*-hexane/2-propanol 10:3 + 20 % CH_2Cl_2)



Chromatogram of **19** after recrystallization (Chiralpak IA, 254 nm, 0.7 ml/min, *n*-hexane/2-propanol 10:3 + 20 % CH_2Cl_2)



Chromatogram of **13** (DAICEL OJ, 254 nm, 0.8 ml/min, *n*-hexane/2-propanol 10:4)

Crystal structure determination of bisamidine 6a. Data were collected on a STOE IPDS II two-circle diffractometer with a Genix Microfocus tube with mirror optics using MoK_α radiation (λ = 0.71073 Å). The data were scaled using the frame scaling procedure in the *X-AREA* program system (Stoe & Cie, 2002). The structure was solved by direct methods using the program *SHELXS* (Sheldrick, 2008) and refined against F^2 with full-matrix least-squares techniques using the program *SHELXL* (Sheldrick, 2008).

Due to the absence of anomalous scatterers, the absolute configuration could not be determined. The H atom bonded to N was freely refined. One phenyl ring is disordered over two positions with a site occupation factor of 0.531(15) for the major occupied site. The disordered atoms were isotropically refined and bond lengths and angles in the disordered moieties were restrained to be equal.

Stoe & Cie, *X-AREA*. Diffractometer control program system. Stoe & Cie, Darmstadt, Germany, 2002.

G. M. Sheldrick, *Acta Crystallogr. Sect. A*, 2008, **64**, 112−122.

Table 1. Crystal data and structure refinement for g1.

Identification code	g1	
Empirical formula	$C_{36}H_{30}N_4$	
Formula weight	518.64	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 10.9410(8) Å	α= 90°.
	b = 12.3493(17) Å	β= 90°.
	c = 21.064(2) Å	γ = 90°.
Volume	2846.0(5) $Å^3$	
Z	4	
Density (calculated)	1.210 Mg/m^3	
Absorption coefficient	0.072 mm^{-1}	
F(000)	1096	
Crystal size	0.320 x 0.270 x 0.140 mm^3	
Theta range for data collection	3.338 to 25.584°.	
Index ranges	-13<=h<=12, -11<=k<=14, -21<=l<=25	
Reflections collected	8580	
Independent reflections	5272 [R(int) = 0.0590]	
Completeness to theta = 25.000°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.705	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5272 / 36 / 365	
Goodness-of-fit on F^2	0.938	
Final R indices [I>2sigma(I)]	R1 = 0.0556, wR2 = 0.1188	
R indices (all data)	R1 = 0.0847, wR2 = 0.1292	
Absolute structure parameter	6.8(10)	
Largest diff. peak and hole	0.277 and -0.308 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for g1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	3665(3)	2393(3)	6560(2)	30(1)
N(2)	4714(3)	1947(3)	5673(2)	28(1)
C(1)	3667(3)	1977(3)	5958(2)	28(1)
C(2)	4858(3)	2899(4)	6672(2)	33(1)
C(3)	5636(3)	2325(4)	6145(2)	33(1)
N(3)	-48(3)	3309(3)	5711(2)	29(1)
N(4)	1253(3)	3128(3)	6540(2)	31(1)
C(4)	894(3)	2766(3)	5997(2)	28(1)
C(5)	-198(4)	4345(3)	6039(2)	34(1)
C(6)	493(3)	4094(4)	6678(2)	33(1)
C(11)	2595(3)	1437(3)	5663(2)	28(1)
C(12)	1360(3)	1774(3)	5674(2)	28(1)
C(13)	498(4)	1156(3)	5343(2)	36(1)
C(14)	815(4)	228(4)	5012(2)	40(1)
C(15)	2021(4)	-98(3)	5001(2)	41(1)
C(16)	2892(4)	501(3)	5322(2)	36(1)
C(21)	4872(4)	4127(4)	6606(2)	37(1)
C(22)	5921(4)	4680(5)	6805(2)	50(1)
C(23)	5987(5)	5792(5)	6758(3)	63(2)
C(24)	5014(5)	6378(5)	6506(3)	62(2)
C(25)	3965(4)	5842(4)	6309(2)	49(1)
C(26)	3909(4)	4719(4)	6362(2)	40(1)
C(31)	6350(4)	1350(4)	6382(2)	34(1)
C(32)	7603(4)	1294(5)	6303(3)	52(1)
C(33)	8263(4)	395(5)	6512(3)	66(2)
C(34)	7691(4)	-439(5)	6800(2)	54(1)
C(35)	6435(4)	-416(4)	6881(2)	48(1)
C(36)	5772(4)	474(4)	6672(2)	43(1)
C(51)	326(5)	5294(3)	5673(2)	50(1)
C(52)	128(12)	6391(6)	5772(5)	64(3)
C(53)	682(12)	7188(7)	5401(5)	69(4)
C(54)	1582(12)	6929(8)	4975(5)	74(4)
C(55)	1912(10)	5858(8)	4892(4)	58(3)
C(56)	1338(10)	5060(8)	5244(5)	48(3)
C(52')	-362(11)	6271(7)	5818(5)	51(3)

C(53')	-9(12)	7225(7)	5501(5)	60(4)
C(54')	862(11)	7159(8)	5026(5)	60(4)
C(55')	1410(12)	6210(8)	4864(5)	59(4)
C(56')	1097(11)	5266(8)	5187(5)	47(4)
C(61)	-393(3)	3906(4)	7225(2)	34(1)
C(62)	-888(4)	4784(5)	7546(2)	53(1)
C(63)	-1742(5)	4628(7)	8029(3)	71(2)
C(64)	-2109(5)	3603(7)	8193(3)	77(2)
C(65)	-1645(5)	2739(6)	7875(3)	77(2)
C(66)	-777(5)	2882(4)	7395(2)	53(1)

Table 3. Bond lengths [Å] and angles [°] for g1.

N(1)-C(1)	1.368(5)
N(1)-C(2)	1.467(5)
N(1)-H(1)	0.83(4)
N(2)-C(1)	1.294(5)
N(2)-C(3)	1.491(5)
C(1)-C(11)	1.486(5)
C(2)-C(21)	1.522(6)
C(2)-C(3)	1.570(6)
C(2)-H(2)	1.0000
C(3)-C(31)	1.519(6)
C(3)-H(3A)	1.0000
N(3)-C(4)	1.369(5)
N(3)-C(5)	1.463(5)
N(3)-H(3)	0.90(4)
N(4)-C(4)	1.290(5)
N(4)-C(6)	1.483(5)
C(4)-C(12)	1.491(5)
C(5)-C(51)	1.516(6)
C(5)-C(6)	1.575(5)
C(5)-H(5)	1.0000
C(6)-C(61)	1.522(6)
C(6)-H(6)	1.0000
C(11)-C(16)	1.399(5)
C(11)-C(12)	1.415(5)
C(12)-C(13)	1.400(5)
C(13)-C(14)	1.385(6)
C(13)-H(13)	0.9500
C(14)-C(15)	1.380(6)
C(14)-H(14)	0.9500
C(15)-C(16)	1.383(6)
C(15)-H(15)	0.9500
C(16)-H(16)	0.9500
C(21)-C(26)	1.382(6)
C(21)-C(22)	1.399(6)
C(22)-C(23)	1.379(8)
C(22)-H(22)	0.9500
C(23)-C(24)	1.392(8)
C(23)-H(23)	0.9500

C(24)-C(25)	1.388(7)
C(24)-H(24)	0.9500
C(25)-C(26)	1.392(7)
C(25)-H(25)	0.9500
C(26)-H(26)	0.9500
C(31)-C(32)	1.383(6)
C(31)-C(36)	1.394(6)
C(32)-C(33)	1.396(7)
C(32)-H(32)	0.9500
C(33)-C(34)	1.350(7)
C(33)-H(33)	0.9500
C(34)-C(35)	1.385(7)
C(34)-H(34)	0.9500
C(35)-C(36)	1.389(7)
C(35)-H(35)	0.9500
C(36)-H(36)	0.9500
C(51)-C(56')	1.327(8)
C(51)-C(52)	1.388(8)
C(51)-C(52')	1.454(8)
C(51)-C(56)	1.457(8)
C(52)-C(53)	1.395(10)
C(52)-H(52)	0.9500
C(53)-C(54)	1.370(11)
C(53)-H(53)	0.9500
C(54)-C(55)	1.382(10)
C(54)-H(54)	0.9500
C(55)-C(56)	1.384(9)
C(55)-H(55)	0.9500
C(56)-H(56)	0.9500
C(52')-C(53')	1.409(10)
C(52')-H(52')	0.9500
C(53')-C(54')	1.385(11)
C(53')-H(53')	0.9500
C(54')-C(55')	1.359(10)
C(54')-H(54')	0.9500
C(55')-C(56')	1.392(10)
C(55')-H(55')	0.9500
C(56')-H(56')	0.9500
C(61)-C(66)	1.379(7)
C(61)-C(62)	1.389(6)

C(62)-C(63)	1.395(8)
C(62)-H(62)	0.9500
C(63)-C(64)	1.372(10)
C(63)-H(63)	0.9500
C(64)-C(65)	1.358(10)
C(64)-H(64)	0.9500
C(65)-C(66)	1.399(7)
C(65)-H(65)	0.9500
C(66)-H(66)	0.9500

C(1)-N(1)-C(2)	107.9(3)
C(1)-N(1)-H(1)	119(3)
C(2)-N(1)-H(1)	122(3)
C(1)-N(2)-C(3)	106.3(3)
N(2)-C(1)-N(1)	116.3(3)
N(2)-C(1)-C(11)	119.4(3)
N(1)-C(1)-C(11)	123.7(3)
N(1)-C(2)-C(21)	114.8(3)
N(1)-C(2)-C(3)	100.2(3)
C(21)-C(2)-C(3)	112.3(3)
N(1)-C(2)-H(2)	109.7
C(21)-C(2)-H(2)	109.7
C(3)-C(2)-H(2)	109.7
N(2)-C(3)-C(31)	108.6(3)
N(2)-C(3)-C(2)	104.2(3)
C(31)-C(3)-C(2)	113.9(3)
N(2)-C(3)-H(3A)	110.0
C(31)-C(3)-H(3A)	110.0
C(2)-C(3)-H(3A)	110.0
C(4)-N(3)-C(5)	107.8(3)
C(4)-N(3)-H(3)	114(3)
C(5)-N(3)-H(3)	124(3)
C(4)-N(4)-C(6)	106.4(3)
N(4)-C(4)-N(3)	116.7(4)
N(4)-C(4)-C(12)	125.9(3)
N(3)-C(4)-C(12)	117.3(3)
N(3)-C(5)-C(51)	113.1(3)
N(3)-C(5)-C(6)	100.2(3)
C(51)-C(5)-C(6)	113.9(3)
N(3)-C(5)-H(5)	109.7

C(51)-C(5)-H(5)	109.7
C(6)-C(5)-H(5)	109.7
N(4)-C(6)-C(61)	112.5(3)
N(4)-C(6)-C(5)	105.1(3)
C(61)-C(6)-C(5)	111.7(3)
N(4)-C(6)-H(6)	109.2
C(61)-C(6)-H(6)	109.2
C(5)-C(6)-H(6)	109.2
C(16)-C(11)-C(12)	118.3(3)
C(16)-C(11)-C(1)	113.7(3)
C(12)-C(11)-C(1)	128.0(4)
C(13)-C(12)-C(11)	118.3(4)
C(13)-C(12)-C(4)	116.5(3)
C(11)-C(12)-C(4)	125.2(3)
C(14)-C(13)-C(12)	122.2(4)
C(14)-C(13)-H(13)	118.9
C(12)-C(13)-H(13)	118.9
C(15)-C(14)-C(13)	119.3(4)
C(15)-C(14)-H(14)	120.4
C(13)-C(14)-H(14)	120.4
C(14)-C(15)-C(16)	119.6(4)
C(14)-C(15)-H(15)	120.2
C(16)-C(15)-H(15)	120.2
C(15)-C(16)-C(11)	122.2(4)
C(15)-C(16)-H(16)	118.9
C(11)-C(16)-H(16)	118.9
C(26)-C(21)-C(22)	118.6(5)
C(26)-C(21)-C(2)	123.6(4)
C(22)-C(21)-C(2)	117.8(4)
C(23)-C(22)-C(21)	120.5(5)
C(23)-C(22)-H(22)	119.7
C(21)-C(22)-H(22)	119.7
C(22)-C(23)-C(24)	120.3(5)
C(22)-C(23)-H(23)	119.9
C(24)-C(23)-H(23)	119.9
C(25)-C(24)-C(23)	119.9(5)
C(25)-C(24)-H(24)	120.1
C(23)-C(24)-H(24)	120.1
C(24)-C(25)-C(26)	119.2(5)
C(24)-C(25)-H(25)	120.4

C(26)-C(25)-H(25)	120.4
C(21)-C(26)-C(25)	121.6(4)
C(21)-C(26)-H(26)	119.2
C(25)-C(26)-H(26)	119.2
C(32)-C(31)-C(36)	117.6(4)
C(32)-C(31)-C(3)	120.6(4)
C(36)-C(31)-C(3)	121.7(3)
C(31)-C(32)-C(33)	121.0(5)
C(31)-C(32)-H(32)	119.5
C(33)-C(32)-H(32)	119.5
C(34)-C(33)-C(32)	120.6(4)
C(34)-C(33)-H(33)	119.7
C(32)-C(33)-H(33)	119.7
C(33)-C(34)-C(35)	120.0(5)
C(33)-C(34)-H(34)	120.0
C(35)-C(34)-H(34)	120.0
C(34)-C(35)-C(36)	119.7(5)
C(34)-C(35)-H(35)	120.2
C(36)-C(35)-H(35)	120.2
C(35)-C(36)-C(31)	121.1(4)
C(35)-C(36)-H(36)	119.4
C(31)-C(36)-H(36)	119.4
C(56')-C(51)-C(52')	120.9(6)
C(52)-C(51)-C(56)	113.9(6)
C(56')-C(51)-C(5)	127.8(5)
C(52)-C(51)-C(5)	128.3(6)
C(52')-C(51)-C(5)	109.8(5)
C(56)-C(51)-C(5)	116.7(5)
C(51)-C(52)-C(53)	122.5(8)
C(51)-C(52)-H(52)	118.8
C(53)-C(52)-H(52)	118.8
C(54)-C(53)-C(52)	121.0(8)
C(54)-C(53)-H(53)	119.5
C(52)-C(53)-H(53)	119.5
C(53)-C(54)-C(55)	119.6(7)
C(53)-C(54)-H(54)	120.2
C(55)-C(54)-H(54)	120.2
C(54)-C(55)-C(56)	119.6(7)
C(54)-C(55)-H(55)	120.2
C(56)-C(55)-H(55)	120.2

C(55)-C(56)-C(51)	122.5(7)
C(55)-C(56)-H(56)	118.8
C(51)-C(56)-H(56)	118.8
C(53')-C(52')-C(51)	116.9(7)
C(53')-C(52')-H(52')	121.6
C(51)-C(52')-H(52')	121.6
C(54')-C(53')-C(52')	118.8(8)
C(54')-C(53')-H(53')	120.6
C(52')-C(53')-H(53')	120.6
C(55')-C(54')-C(53')	122.4(8)
C(55')-C(54')-H(54')	118.8
C(53')-C(54')-H(54')	118.8
C(54')-C(55')-C(56')	119.4(8)
C(54')-C(55')-H(55')	120.3
C(56')-C(55')-H(55')	120.3
C(51)-C(56')-C(55')	120.8(8)
C(51)-C(56')-H(56')	119.6
C(55')-C(56')-H(56')	119.6
C(66)-C(61)-C(62)	118.1(4)
C(66)-C(61)-C(6)	122.1(4)
C(62)-C(61)-C(6)	119.8(4)
C(61)-C(62)-C(63)	120.6(6)
C(61)-C(62)-H(62)	119.7
C(63)-C(62)-H(62)	119.7
C(64)-C(63)-C(62)	120.5(6)
C(64)-C(63)-H(63)	119.8
C(62)-C(63)-H(63)	119.8
C(65)-C(64)-C(63)	119.4(5)
C(65)-C(64)-H(64)	120.3
C(63)-C(64)-H(64)	120.3
C(64)-C(65)-C(66)	120.7(7)
C(64)-C(65)-H(65)	119.6
C(66)-C(65)-H(65)	119.6
C(61)-C(66)-C(65)	120.7(5)
C(61)-C(66)-H(66)	119.7
C(65)-C(66)-H(66)	119.7

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for g1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	24(2)	43(2)	24(2)	-2(2)	2(1)	1(2)
N(2)	26(2)	32(2)	27(2)	4(2)	1(1)	1(1)
C(1)	31(2)	26(2)	26(2)	7(2)	2(2)	2(2)
C(2)	28(2)	43(3)	28(2)	1(2)	-2(2)	0(2)
C(3)	28(2)	40(3)	30(2)	2(2)	0(2)	-2(2)
N(3)	34(2)	28(2)	26(2)	1(2)	-4(2)	-1(1)
N(4)	26(2)	41(2)	27(2)	-2(2)	-1(1)	-1(2)
C(4)	23(2)	34(2)	26(2)	3(2)	1(2)	-6(2)
C(5)	35(2)	32(2)	33(2)	-4(2)	-5(2)	5(2)
C(6)	29(2)	40(3)	30(2)	-6(2)	-3(2)	3(2)
C(11)	33(2)	30(2)	22(2)	8(2)	3(2)	-5(2)
C(12)	31(2)	29(2)	22(2)	6(2)	0(2)	-1(2)
C(13)	37(2)	32(3)	38(2)	6(2)	-6(2)	-6(2)
C(14)	49(2)	30(2)	41(2)	-1(2)	-8(2)	-13(2)
C(15)	50(3)	27(2)	45(2)	-4(2)	3(2)	-5(2)
C(16)	44(2)	27(2)	37(2)	2(2)	8(2)	1(2)
C(21)	35(2)	46(3)	30(2)	-9(2)	5(2)	-2(2)
C(22)	42(2)	61(3)	48(3)	-9(2)	-3(2)	-9(2)
C(23)	56(3)	62(4)	71(4)	-20(3)	-5(3)	-24(3)
C(24)	81(4)	43(3)	62(3)	-15(3)	15(3)	-11(3)
C(25)	48(3)	45(3)	54(3)	-7(2)	14(2)	2(2)
C(26)	41(2)	39(3)	40(2)	-7(2)	3(2)	-5(2)
C(31)	27(2)	48(3)	28(2)	0(2)	-1(2)	0(2)
C(32)	30(2)	62(4)	62(3)	15(3)	1(2)	0(2)
C(33)	33(2)	75(4)	89(4)	28(3)	-5(3)	11(3)
C(34)	50(3)	63(4)	48(3)	12(3)	-4(2)	16(3)
C(35)	56(3)	53(3)	36(2)	12(2)	2(2)	5(3)
C(36)	33(2)	52(3)	45(2)	12(2)	5(2)	4(2)
C(51)	81(3)	29(2)	41(2)	-2(2)	-28(2)	-4(2)
C(61)	27(2)	48(3)	29(2)	-8(2)	-4(2)	4(2)
C(62)	44(2)	62(3)	54(3)	-33(3)	0(2)	-2(2)
C(63)	44(3)	120(6)	50(3)	-47(4)	7(2)	1(3)
C(64)	50(3)	137(7)	45(3)	-4(4)	14(3)	3(4)
C(65)	71(4)	96(5)	64(4)	24(4)	29(3)	7(4)
C(66)	59(3)	50(3)	51(3)	8(2)	14(2)	17(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for g1.

	x	y	z	U(eq)
H(1)	3030(40)	2650(40)	6710(20)	30(11)
H(2)	5169	2689	7101	39
H(3A)	6204	2857	5942	39
H(3)	-60(30)	3230(30)	5290(20)	27(10)
H(5)	-1084	4475	6128	40
H(6)	1039	4717	6785	39
H(13)	-333	1380	5344	43
H(14)	208	-181	4796	48
H(15)	2253	-730	4773	49
H(16)	3719	269	5311	43
H(22)	6592	4286	6974	60
H(23)	6700	6161	6898	76
H(24)	5067	7143	6469	75
H(25)	3294	6236	6140	59
H(26)	3192	4351	6227	48
H(32)	8021	1876	6103	62
H(33)	9123	370	6450	79
H(34)	8149	-1042	6948	64
H(35)	6029	-1006	7080	58
H(36)	4910	486	6727	52
H(52)	-405	6607	6104	77
H(53)	432	7921	5445	83
H(54)	1976	7482	4738	89
H(55)	2530	5670	4595	69
H(56)	1614	4334	5206	58
H(52')	-1018	6266	6114	61
H(53')	-363	7902	5611	72
H(54')	1086	7799	4805	72
H(55')	2001	6191	4534	70
H(56')	1439	4595	5058	57
H(62)	-643	5498	7435	64
H(63)	-2073	5236	8246	85
H(64)	-2681	3499	8527	93
H(65)	-1913	2030	7980	92

H(66)	-449	2268	7184	64

Table 6. Torsion angles [°] for g1.

C(3)-N(2)-C(1)-N(1)	4.3(5)
C(3)-N(2)-C(1)-C(11)	-167.4(3)
C(2)-N(1)-C(1)-N(2)	11.1(5)
C(2)-N(1)-C(1)-C(11)	-177.5(4)
C(1)-N(1)-C(2)-C(21)	100.7(4)
C(1)-N(1)-C(2)-C(3)	-19.8(4)
C(1)-N(2)-C(3)-C(31)	105.0(3)
C(1)-N(2)-C(3)-C(2)	-16.7(4)
N(1)-C(2)-C(3)-N(2)	21.7(4)
C(21)-C(2)-C(3)-N(2)	-100.6(4)
N(1)-C(2)-C(3)-C(31)	-96.4(4)
C(21)-C(2)-C(3)-C(31)	141.3(3)
C(6)-N(4)-C(4)-N(3)	-1.3(4)
C(6)-N(4)-C(4)-C(12)	-177.4(3)
C(5)-N(3)-C(4)-N(4)	14.0(4)
C(5)-N(3)-C(4)-C(12)	-169.5(3)
C(4)-N(3)-C(5)-C(51)	103.1(4)
C(4)-N(3)-C(5)-C(6)	-18.6(4)
C(4)-N(4)-C(6)-C(61)	110.8(4)
C(4)-N(4)-C(6)-C(5)	-10.9(4)
N(3)-C(5)-C(6)-N(4)	17.7(4)
C(51)-C(5)-C(6)-N(4)	-103.4(4)
N(3)-C(5)-C(6)-C(61)	-104.5(4)
C(51)-C(5)-C(6)-C(61)	134.4(4)
N(2)-C(1)-C(11)-C(16)	33.5(5)
N(1)-C(1)-C(11)-C(16)	-137.6(4)
N(2)-C(1)-C(11)-C(12)	-144.6(4)
N(1)-C(1)-C(11)-C(12)	44.3(6)
C(16)-C(11)-C(12)-C(13)	-0.1(5)
C(1)-C(11)-C(12)-C(13)	177.9(4)
C(16)-C(11)-C(12)-C(4)	-178.2(3)
C(1)-C(11)-C(12)-C(4)	-0.2(6)
N(4)-C(4)-C(12)-C(13)	142.5(4)
N(3)-C(4)-C(12)-C(13)	-33.6(5)
N(4)-C(4)-C(12)-C(11)	-39.4(6)
N(3)-C(4)-C(12)-C(11)	144.6(4)
C(11)-C(12)-C(13)-C(14)	0.5(6)
C(4)-C(12)-C(13)-C(14)	178.8(4)

C(12)-C(13)-C(14)-C(15)	-0.7(7)
C(13)-C(14)-C(15)-C(16)	0.5(7)
C(14)-C(15)-C(16)-C(11)	-0.1(7)
C(12)-C(11)-C(16)-C(15)	-0.1(6)
C(1)-C(11)-C(16)-C(15)	-178.4(4)
N(1)-C(2)-C(21)-C(26)	-10.1(5)
C(3)-C(2)-C(21)-C(26)	103.4(4)
N(1)-C(2)-C(21)-C(22)	169.9(4)
C(3)-C(2)-C(21)-C(22)	-76.6(5)
C(26)-C(21)-C(22)-C(23)	0.1(7)
C(2)-C(21)-C(22)-C(23)	-179.9(4)
C(21)-C(22)-C(23)-C(24)	-0.6(8)
C(22)-C(23)-C(24)-C(25)	0.8(8)
C(23)-C(24)-C(25)-C(26)	-0.5(7)
C(22)-C(21)-C(26)-C(25)	0.2(6)
C(2)-C(21)-C(26)-C(25)	-179.8(4)
C(24)-C(25)-C(26)-C(21)	0.0(7)
N(2)-C(3)-C(31)-C(32)	120.4(4)
C(2)-C(3)-C(31)-C(32)	-123.9(5)
N(2)-C(3)-C(31)-C(36)	-58.2(5)
C(2)-C(3)-C(31)-C(36)	57.4(5)
C(36)-C(31)-C(32)-C(33)	-0.5(8)
C(3)-C(31)-C(32)-C(33)	-179.2(5)
C(31)-C(32)-C(33)-C(34)	-0.5(9)
C(32)-C(33)-C(34)-C(35)	1.1(9)
C(33)-C(34)-C(35)-C(36)	-0.8(8)
C(34)-C(35)-C(36)-C(31)	-0.2(7)
C(32)-C(31)-C(36)-C(35)	0.8(7)
C(3)-C(31)-C(36)-C(35)	179.5(4)
N(3)-C(5)-C(51)-C(56')	-15.6(10)
C(6)-C(5)-C(51)-C(56')	98.0(9)
N(3)-C(5)-C(51)-C(52)	165.4(8)
C(6)-C(5)-C(51)-C(52)	-81.0(9)
N(3)-C(5)-C(51)-C(52')	150.1(6)
C(6)-C(5)-C(51)-C(52')	-96.3(6)
N(3)-C(5)-C(51)-C(56)	-27.6(7)
C(6)-C(5)-C(51)-C(56)	86.0(7)
C(56)-C(51)-C(52)-C(53)	12.0(15)
C(5)-C(51)-C(52)-C(53)	179.3(9)
C(51)-C(52)-C(53)-C(54)	-9.0(18)

C(52)-C(53)-C(54)-C(55)	2.6(18)
C(53)-C(54)-C(55)-C(56)	-0.5(18)
C(54)-C(55)-C(56)-C(51)	4.5(17)
C(52)-C(51)-C(56)-C(55)	-9.9(15)
C(5)-C(51)-C(56)-C(55)	-178.7(9)
C(56')-C(51)-C(52')-C(53')	-11.4(15)
C(5)-C(51)-C(52')-C(53')	-178.3(8)
C(51)-C(52')-C(53')-C(54')	7.0(16)
C(52')-C(53')-C(54')-C(55')	-1.5(19)
C(53')-C(54')-C(55')-C(56')	0(2)
C(52')-C(51)-C(56')-C(55')	9.9(17)
C(5)-C(51)-C(56')-C(55')	174.2(9)
C(54')-C(55')-C(56')-C(51)	-4(2)
N(4)-C(6)-C(61)-C(66)	-23.5(5)
C(5)-C(6)-C(61)-C(66)	94.4(5)
N(4)-C(6)-C(61)-C(62)	159.9(4)
C(5)-C(6)-C(61)-C(62)	-82.2(5)
C(66)-C(61)-C(62)-C(63)	0.4(7)
C(6)-C(61)-C(62)-C(63)	177.2(4)
C(61)-C(62)-C(63)-C(64)	-0.2(8)
C(62)-C(63)-C(64)-C(65)	-0.9(9)
C(63)-C(64)-C(65)-C(66)	1.7(10)
C(62)-C(61)-C(66)-C(65)	0.3(7)
C(6)-C(61)-C(66)-C(65)	-176.4(5)
C(64)-C(65)-C(66)-C(61)	-1.4(9)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for g1 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...N(4)	0.83(4)	2.06(4)	2.791(5)	147(4)
N(3)-H(3)...N(2)#1	0.90(4)	2.05(4)	2.944(5)	174(4)

Symmetry transformations used to generate equivalent atoms:

#1 x-1/2,-y+1/2,-z+1