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Supplementary Information

for

TMSOTf-catalyzed Synthesis of Trisubstituted Imidazoles Using Hexamethyldisilazane as a Nitrogen Source under Neat and Microwave Irradiation Conditions

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Crystal data and structure refinement for compound **3n**

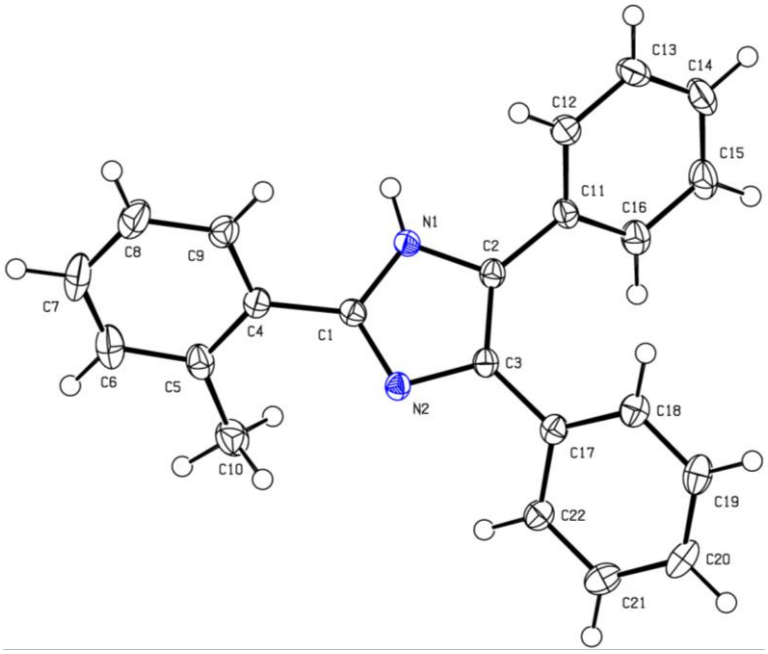


Figure S1. Single X-ray crystal structure of imidazole **3n** (the thermal ellipsoid was drawn at the 50% probability level)

Table S1. Crystal data and structure refinement for i18082

CCDC	2082023	
Identification code	i18082	
Empirical formula	C22 H18 N2	
Formula weight	310.38	
Temperature	100.0(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C c	
Unit cell dimensions	a = 10.7445(3) Å	α= 90°.
	b = 19.4078(5) Å	β= 112.9490(10)°.
	c = 8.7809(2) Å	γ = 90°.
Volume	1686.13(8) $Å^3$	
Z	4	
Density (calculated)	1.223 Mg/m^3	
Absorption coefficient	0.072 mm^{-1}	
F(000)	656	
Crystal size	0.245 x 0.099 x 0.084 mm^3	
Theta range for data collection	2.764 to 27.494°.	
Index ranges	-13<=h<=13, -25<=k<=25, -11<=l<=11	

Reflections collected	24629
Independent reflections	3652 [R(int) = 0.0527]
Completeness to theta = 25.242°	99.6 %
Absorption correction	Numerical
Max. and min. transmission	0.9987 and 0.9811
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3652 / 2 / 223
Goodness-of-fit on F^2	1.064
Final R indices [I>2sigma(I)]	R1 = 0.0334, wR2 = 0.0757
R indices (all data)	R1 = 0.0419, wR2 = 0.0808
Absolute structure parameter	2(3)
Extinction coefficient	n/a
Largest diff. peak and hole	0.155 and -0.164 e.$Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for i18082. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	5306(2)	4864(1)	3924(2)	17(1)
N(2)	4925(2)	4338(1)	5938(2)	17(1)
C(1)	4583(2)	4864(1)	4888(2)	17(1)
C(2)	6145(2)	4296(1)	4339(2)	18(1)
C(3)	5908(2)	3975(1)	5608(2)	17(1)
C(4)	3619(2)	5418(1)	4802(2)	20(1)
C(5)	2378(2)	5284(1)	4920(3)	24(1)
C(6)	1545(3)	5847(1)	4837(3)	34(1)
C(7)	1920(3)	6513(1)	4652(4)	39(1)
C(8)	3140(3)	6637(1)	4526(3)	33(1)
C(9)	3989(2)	6090(1)	4594(3)	24(1)
C(10)	1907(2)	4567(1)	5083(3)	31(1)
C(11)	6982(2)	4130(1)	3409(2)	19(1)
C(12)	7640(2)	4650(1)	2914(3)	23(1)
C(13)	8376(2)	4492(1)	1960(3)	29(1)
C(14)	8456(2)	3818(1)	1493(3)	32(1)
C(15)	7823(2)	3299(1)	1991(3)	30(1)
C(16)	7084(2)	3450(1)	2938(3)	24(1)
C(17)	6548(2)	3368(1)	6608(3)	19(1)

C(18)	7901(2)	3196(1)	6971(3)	23(1)
C(19)	8469(2)	2616(1)	7905(3)	27(1)
C(20)	7716(2)	2200(1)	8511(3)	28(1)
C(21)	6388(2)	2372(1)	8189(3)	26(1)
C(22)	5810(2)	2951(1)	7257(3)	22(1)

Table S3. Bond lengths [Å] and angles [°] for i18082.

N(1)-C(1)	1.354(3)
N(1)-C(2)	1.381(3)
N(1)-H(1)	0.90(3)
N(2)-C(1)	1.327(3)
N(2)-C(3)	1.390(3)
C(1)-C(4)	1.473(3)
C(2)-C(3)	1.383(3)
C(2)-C(11)	1.467(3)
C(3)-C(17)	1.470(3)
C(4)-C(9)	1.397(3)
C(4)-C(5)	1.402(3)
C(5)-C(6)	1.396(3)
C(5)-C(10)	1.507(3)
C(6)-C(7)	1.381(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.380(4)
C(7)-H(7)	0.9500
C(8)-C(9)	1.385(3)
C(8)-H(8)	0.9500
C(9)-H(9)	0.9500
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-C(12)	1.394(3)
C(11)-C(16)	1.400(3)
C(12)-C(13)	1.391(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.385(4)
C(13)-H(13)	0.9500

C(14)-C(15)	1.378(4)
C(14)-H(14)	0.9500
C(15)-C(16)	1.387(3)
C(15)-H(15)	0.9500
C(16)-H(16)	0.9500
C(17)-C(22)	1.400(3)
C(17)-C(18)	1.402(3)
C(18)-C(19)	1.386(3)
C(18)-H(18)	0.9500
C(19)-C(20)	1.388(3)
C(19)-H(19)	0.9500
C(20)-C(21)	1.383(3)
C(20)-H(20)	0.9500
C(21)-C(22)	1.386(3)
C(21)-H(21)	0.9500
C(22)-H(22)	0.9500

C(1)-N(1)-C(2)	108.00(17)
C(1)-N(1)-H(1)	125.8(17)
C(2)-N(1)-H(1)	126.0(17)
C(1)-N(2)-C(3)	105.82(16)
N(2)-C(1)-N(1)	111.27(17)
N(2)-C(1)-C(4)	126.55(18)
N(1)-C(1)-C(4)	122.06(18)
N(1)-C(2)-C(3)	105.40(17)
N(1)-C(2)-C(11)	120.41(18)
C(3)-C(2)-C(11)	134.09(19)
C(2)-C(3)-N(2)	109.48(17)
C(2)-C(3)-C(17)	130.60(18)
N(2)-C(3)-C(17)	119.88(17)
C(9)-C(4)-C(5)	120.6(2)
C(9)-C(4)-C(1)	117.27(19)
C(5)-C(4)-C(1)	122.09(19)
C(6)-C(5)-C(4)	117.4(2)
C(6)-C(5)-C(10)	119.8(2)
C(4)-C(5)-C(10)	122.8(2)
C(7)-C(6)-C(5)	121.9(2)
C(7)-C(6)-H(6)	119.1

C(5)-C(6)-H(6)	119.1
C(8)-C(7)-C(6)	120.2(2)
C(8)-C(7)-H(7)	119.9
C(6)-C(7)-H(7)	119.9
C(7)-C(8)-C(9)	119.5(2)
C(7)-C(8)-H(8)	120.2
C(9)-C(8)-H(8)	120.2
C(8)-C(9)-C(4)	120.4(2)
C(8)-C(9)-H(9)	119.8
C(4)-C(9)-H(9)	119.8
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(12)-C(11)-C(16)	118.79(19)
C(12)-C(11)-C(2)	120.75(19)
C(16)-C(11)-C(2)	120.40(19)
C(13)-C(12)-C(11)	120.4(2)
C(13)-C(12)-H(12)	119.8
C(11)-C(12)-H(12)	119.8
C(14)-C(13)-C(12)	120.1(2)
C(14)-C(13)-H(13)	120.0
C(12)-C(13)-H(13)	120.0
C(15)-C(14)-C(13)	120.1(2)
C(15)-C(14)-H(14)	119.9
C(13)-C(14)-H(14)	119.9
C(14)-C(15)-C(16)	120.3(2)
C(14)-C(15)-H(15)	119.9
C(16)-C(15)-H(15)	119.9
C(15)-C(16)-C(11)	120.4(2)
C(15)-C(16)-H(16)	119.8
C(11)-C(16)-H(16)	119.8
C(22)-C(17)-C(18)	118.12(19)
C(22)-C(17)-C(3)	119.93(18)
C(18)-C(17)-C(3)	121.93(19)
C(19)-C(18)-C(17)	120.4(2)

C(19)-C(18)-H(18)	119.8
C(17)-C(18)-H(18)	119.8
C(18)-C(19)-C(20)	120.7(2)
C(18)-C(19)-H(19)	119.6
C(20)-C(19)-H(19)	119.6
C(21)-C(20)-C(19)	119.4(2)
C(21)-C(20)-H(20)	120.3
C(19)-C(20)-H(20)	120.3
C(20)-C(21)-C(22)	120.3(2)
C(20)-C(21)-H(21)	119.8
C(22)-C(21)-H(21)	119.8
C(21)-C(22)-C(17)	121.0(2)
C(21)-C(22)-H(22)	119.5
C(17)-C(22)-H(22)	119.5

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2$x 10^3)for i18082. 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}
N(1)	19(1)	19(1)	15(1)	1(1)	7(1)	2(1)
N(2)	18(1)	18(1)	16(1)	-1(1)	6(1)	2(1)
C(1)	19(1)	18(1)	14(1)	-2(1)	7(1)	0(1)
C(2)	19(1)	18(1)	17(1)	-2(1)	6(1)	2(1)
C(3)	16(1)	17(1)	17(1)	-2(1)	6(1)	1(1)
C(4)	23(1)	21(1)	13(1)	-1(1)	5(1)	5(1)
C(5)	23(1)	30(1)	20(1)	-3(1)	7(1)	5(1)
C(6)	26(1)	39(1)	36(1)	-4(1)	11(1)	11(1)
C(7)	38(1)	33(1)	42(2)	-2(1)	12(1)	19(1)
C(8)	41(2)	22(1)	34(1)	1(1)	13(1)	9(1)
C(9)	30(1)	22(1)	22(1)	0(1)	10(1)	5(1)
C(10)	22(1)	36(1)	34(1)	1(1)	12(1)	1(1)
C(11)	16(1)	25(1)	16(1)	0(1)	6(1)	4(1)
C(12)	21(1)	30(1)	19(1)	3(1)	7(1)	4(1)
C(13)	22(1)	44(1)	24(1)	11(1)	12(1)	5(1)
C(14)	27(1)	51(2)	24(1)	4(1)	15(1)	14(1)

C(15)	32(1)	35(1)	24(1)	-5(1)	12(1)	11(1)
C(16)	24(1)	26(1)	24(1)	-3(1)	9(1)	3(1)
C(17)	22(1)	17(1)	16(1)	-4(1)	6(1)	1(1)
C(18)	20(1)	22(1)	24(1)	-1(1)	5(1)	0(1)
C(19)	20(1)	25(1)	29(1)	-3(1)	2(1)	4(1)
C(20)	29(1)	17(1)	27(1)	2(1)	0(1)	4(1)
C(21)	30(1)	22(1)	24(1)	1(1)	6(1)	-4(1)
C(22)	20(1)	21(1)	21(1)	1(1)	5(1)	0(1)

Crystal data and structure refinement for compound **3q**

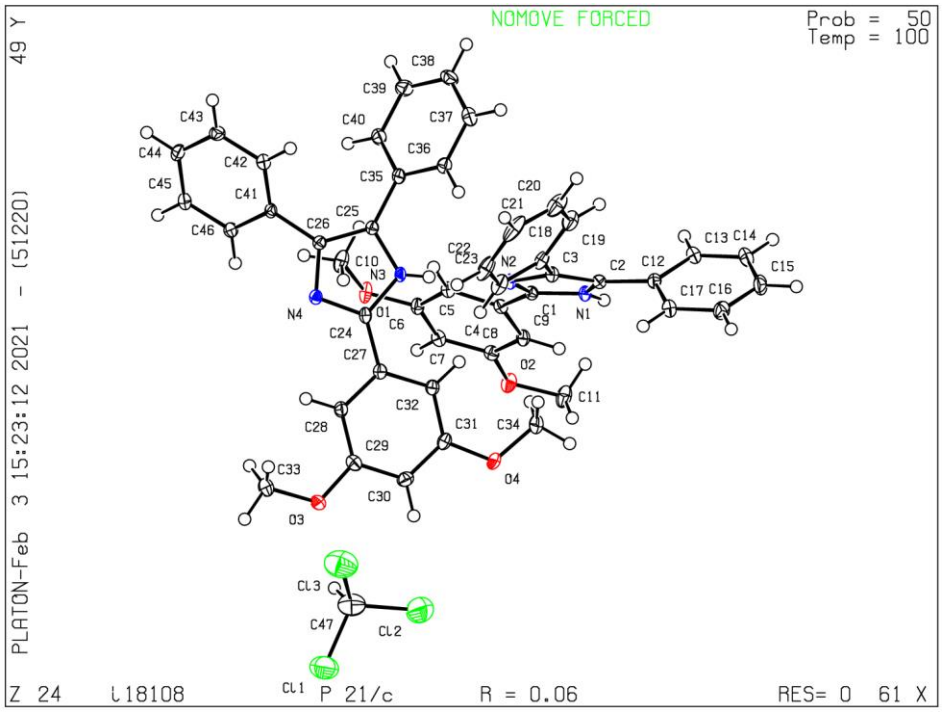


Figure S2. Single X-ray crystal structure of imidazole **3q** (the thermal ellipsoid was drawn at the 50% probability level)

Table S5. Crystal data and structure refinement for i18108.

CCDC	2082029
Identification code	i18108
Empirical formula	C47 H41 Cl3 N4 O4
Formula weight	832.19
Temperature	100.0(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 21/c

Unit cell dimensions	a = 10.2370(4) Å	α= 90°.
	b = 18.3683(6) Å	β= 95.8070(10)°.
	c = 22.3540(8) Å	γ = 90°.
Volume	4181.8(3) $Å^3$	
Z	4	
Density (calculated)	1.322 Mg/m^3	
Absorption coefficient	0.269 mm^{-1}	
F(000)	1736	
Crystal size	0.216 x 0.155 x 0.040 mm^3	
Theta range for data collection	2.141 to 27.103°.	
Index ranges	-13<=h<=13, -23<=k<=23, -28<=l<=28	
Reflections collected	167934	
Independent reflections	9215 [R(int) = 0.1039]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Numerical	
Max. and min. transmission	0.9971 and 0.9646	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9215 / 0 / 535	
Goodness-of-fit on F^2	1.054	
Final R indices [I>2sigma(I)]	R1 = 0.0627, wR2 = 0.1759	
R indices (all data)	R1 = 0.0857, wR2 = 0.1928	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.274 and -1.052 $e.Å^{-3}$	

Table S6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for i18108. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	7496(1)	3601(1)	4147(1)	50(1)
Cl(2)	8235(1)	4966(1)	4716(1)	55(1)
Cl(3)	8207(1)	3665(1)	5431(1)	57(1)
O(1)	1293(2)	7033(1)	7240(1)	18(1)
O(2)	2411(2)	8961(1)	6056(1)	18(1)
O(3)	5272(2)	4495(1)	5660(1)	26(1)
O(4)	6993(2)	6815(1)	6028(1)	20(1)
N(1)	6568(2)	8639(1)	7664(1)	12(1)
N(2)	6260(2)	7497(1)	7927(1)	12(1)
N(3)	5151(2)	6080(1)	8071(1)	12(1)
N(4)	4032(2)	5081(1)	7809(1)	12(1)
C(1)	5714(2)	8073(1)	7643(1)	12(1)
C(2)	7732(2)	8418(1)	7980(1)	12(1)
C(3)	7524(2)	7706(1)	8139(1)	12(1)
C(4)	4389(2)	8074(1)	7320(1)	12(1)
C(5)	3481(2)	7557(1)	7475(1)	13(1)
C(6)	2261(2)	7515(1)	7134(1)	14(1)
C(7)	1945(2)	7981(1)	6656(1)	14(1)
C(8)	2835(2)	8514(1)	6522(1)	14(1)
C(9)	4072(2)	8563(1)	6846(1)	14(1)
C(10)	1587(3)	6516(2)	7714(1)	22(1)
C(11)	3269(3)	9543(2)	5923(1)	23(1)
C(12)	8893(2)	8891(1)	8068(1)	13(1)
C(13)	8789(3)	9616(1)	8251(1)	16(1)
C(14)	9883(3)	10067(2)	8300(1)	21(1)
C(15)	11089(3)	9806(2)	8167(1)	22(1)
C(16)	11204(3)	9085(2)	7988(1)	20(1)
C(17)	10119(3)	8633(1)	7938(1)	16(1)
C(18)	8394(2)	7187(1)	8487(1)	16(1)
C(19)	9151(3)	7394(2)	9012(1)	21(1)
C(20)	9883(3)	6879(2)	9357(1)	28(1)
C(21)	9860(3)	6151(2)	9184(2)	29(1)
C(22)	9122(3)	5942(2)	8661(2)	25(1)

C(23)	8397(3)	6456(1)	8309(1)	19(1)
C(24)	4850(2)	5583(1)	7628(1)	12(1)
C(25)	4475(2)	5902(1)	8554(1)	11(1)
C(26)	3787(2)	5275(1)	8383(1)	12(1)
C(27)	5319(2)	5609(1)	7031(1)	13(1)
C(28)	5094(3)	5012(1)	6647(1)	15(1)
C(29)	5477(3)	5046(1)	6069(1)	18(1)
C(30)	6100(3)	5659(1)	5871(1)	17(1)
C(31)	6350(3)	6244(1)	6258(1)	15(1)
C(32)	5957(2)	6231(1)	6838(1)	14(1)
C(33)	4762(4)	3823(2)	5868(2)	38(1)
C(34)	7363(4)	7409(2)	6419(1)	32(1)
C(35)	4565(3)	6351(1)	9102(1)	13(1)
C(36)	5761(3)	6651(1)	9333(1)	15(1)
C(37)	5850(3)	7072(1)	9852(1)	19(1)
C(38)	4745(3)	7198(2)	10146(1)	20(1)
C(39)	3547(3)	6908(2)	9918(1)	20(1)
C(40)	3451(3)	6485(1)	9399(1)	17(1)
C(41)	2829(2)	4853(1)	8695(1)	12(1)
C(42)	3011(3)	4687(1)	9308(1)	15(1)
C(43)	2046(3)	4304(1)	9573(1)	16(1)
C(44)	902(3)	4086(1)	9237(1)	16(1)
C(45)	726(3)	4241(1)	8625(1)	16(1)
C(46)	1679(2)	4624(1)	8358(1)	14(1)
C(47)	7452(4)	4125(2)	4798(2)	40(1)

Table S7. Bond lengths [Å] and angles [°] for i18108.

Cl(1)-C(47)	1.750(4)
Cl(2)-C(47)	1.759(4)
Cl(3)-C(47)	1.758(4)
O(1)-C(6)	1.367(3)
O(1)-C(10)	1.433(3)
O(2)-C(8)	1.363(3)
O(2)-C(11)	1.433(3)
O(3)-C(29)	1.365(3)
O(3)-C(33)	1.434(4)
O(4)-C(31)	1.366(3)
O(4)-C(34)	1.426(3)
N(1)-C(1)	1.355(3)
N(1)-C(2)	1.383(3)
N(1)-H(1)	0.79(3)
N(2)-C(1)	1.328(3)
N(2)-C(3)	1.387(3)
N(3)-C(24)	1.359(3)
N(3)-C(25)	1.379(3)
N(3)-H(3)	0.74(4)
N(4)-C(24)	1.335(3)
N(4)-C(26)	1.380(3)
C(1)-C(4)	1.471(3)
C(2)-C(3)	1.378(3)
C(2)-C(12)	1.469(3)
C(3)-C(18)	1.471(3)
C(4)-C(5)	1.398(3)
C(4)-C(9)	1.403(3)
C(5)-C(6)	1.398(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.381(4)
C(7)-C(8)	1.390(4)
C(7)-H(7)	0.9500
C(8)-C(9)	1.397(4)
C(9)-H(9)	0.9500
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800

C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-C(17)	1.398(4)
C(12)-C(13)	1.401(4)
C(13)-C(14)	1.388(4)
C(13)-H(13)	0.9500
C(14)-C(15)	1.384(4)
C(14)-H(14)	0.9500
C(15)-C(16)	1.392(4)
C(15)-H(15)	0.9500
C(16)-C(17)	1.382(4)
C(16)-H(16)	0.9500
C(17)-H(17)	0.9500
C(18)-C(19)	1.393(4)
C(18)-C(23)	1.401(4)
C(19)-C(20)	1.391(4)
C(19)-H(19)	0.9500
C(20)-C(21)	1.391(5)
C(20)-H(20)	0.9500
C(21)-C(22)	1.380(5)
C(21)-H(21)	0.9500
C(22)-C(23)	1.394(4)
C(22)-H(22)	0.9500
C(23)-H(23)	0.9500
C(24)-C(27)	1.465(3)
C(25)-C(26)	1.383(3)
C(25)-C(35)	1.471(3)
C(26)-C(41)	1.478(3)
C(27)-C(28)	1.398(3)
C(27)-C(32)	1.405(3)
C(28)-C(29)	1.390(4)
C(28)-H(28)	0.9500
C(29)-C(30)	1.388(4)
C(30)-C(31)	1.389(4)
C(30)-H(30)	0.9500
C(31)-C(32)	1.395(4)

C(32)-H(32)	0.9500
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-C(36)	1.394(4)
C(35)-C(40)	1.399(4)
C(36)-C(37)	1.390(4)
C(36)-H(36)	0.9500
C(37)-C(38)	1.384(4)
C(37)-H(37)	0.9500
C(38)-C(39)	1.386(4)
C(38)-H(38)	0.9500
C(39)-C(40)	1.391(4)
C(39)-H(39)	0.9500
C(40)-H(40)	0.9500
C(41)-C(46)	1.397(4)
C(41)-C(42)	1.398(4)
C(42)-C(43)	1.394(4)
C(42)-H(42)	0.9500
C(43)-C(44)	1.386(4)
C(43)-H(43)	0.9500
C(44)-C(45)	1.390(4)
C(44)-H(44)	0.9500
C(45)-C(46)	1.387(4)
C(45)-H(45)	0.9500
C(46)-H(46)	0.9500
C(47)-H(47)	1.0000

C(6)-O(1)-C(10)	117.2(2)
C(8)-O(2)-C(11)	117.0(2)
C(29)-O(3)-C(33)	117.3(2)
C(31)-O(4)-C(34)	117.7(2)
C(1)-N(1)-C(2)	108.2(2)
C(1)-N(1)-H(1)	125(2)
C(2)-N(1)-H(1)	127(2)

C(1)-N(2)-C(3)	106.0(2)
C(24)-N(3)-C(25)	108.5(2)
C(24)-N(3)-H(3)	125(3)
C(25)-N(3)-H(3)	125(3)
C(24)-N(4)-C(26)	106.3(2)
N(2)-C(1)-N(1)	110.9(2)
N(2)-C(1)-C(4)	123.9(2)
N(1)-C(1)-C(4)	125.1(2)
C(3)-C(2)-N(1)	105.2(2)
C(3)-C(2)-C(12)	132.1(2)
N(1)-C(2)-C(12)	122.6(2)
C(2)-C(3)-N(2)	109.7(2)
C(2)-C(3)-C(18)	130.5(2)
N(2)-C(3)-C(18)	119.8(2)
C(5)-C(4)-C(9)	120.9(2)
C(5)-C(4)-C(1)	118.8(2)
C(9)-C(4)-C(1)	120.2(2)
C(4)-C(5)-C(6)	118.8(2)
C(4)-C(5)-H(5)	120.6
C(6)-C(5)-H(5)	120.6
O(1)-C(6)-C(7)	114.7(2)
O(1)-C(6)-C(5)	124.3(2)
C(7)-C(6)-C(5)	121.0(2)
C(6)-C(7)-C(8)	119.7(2)
C(6)-C(7)-H(7)	120.1
C(8)-C(7)-H(7)	120.1
O(2)-C(8)-C(7)	115.1(2)
O(2)-C(8)-C(9)	124.0(2)
C(7)-C(8)-C(9)	120.9(2)
C(8)-C(9)-C(4)	118.7(2)
C(8)-C(9)-H(9)	120.7
C(4)-C(9)-H(9)	120.7
O(1)-C(10)-H(10A)	109.5
O(1)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
O(1)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5

O(2)-C(11)-H(11A)	109.5
O(2)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
O(2)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(17)-C(12)-C(13)	118.6(2)
C(17)-C(12)-C(2)	120.2(2)
C(13)-C(12)-C(2)	121.1(2)
C(14)-C(13)-C(12)	120.4(2)
C(14)-C(13)-H(13)	119.8
C(12)-C(13)-H(13)	119.8
C(15)-C(14)-C(13)	120.4(3)
C(15)-C(14)-H(14)	119.8
C(13)-C(14)-H(14)	119.8
C(14)-C(15)-C(16)	119.7(3)
C(14)-C(15)-H(15)	120.2
C(16)-C(15)-H(15)	120.2
C(17)-C(16)-C(15)	120.2(3)
C(17)-C(16)-H(16)	119.9
C(15)-C(16)-H(16)	119.9
C(16)-C(17)-C(12)	120.7(2)
C(16)-C(17)-H(17)	119.6
C(12)-C(17)-H(17)	119.6
C(19)-C(18)-C(23)	119.0(2)
C(19)-C(18)-C(3)	121.6(2)
C(23)-C(18)-C(3)	119.3(2)
C(20)-C(19)-C(18)	120.3(3)
C(20)-C(19)-H(19)	119.9
C(18)-C(19)-H(19)	119.9
C(21)-C(20)-C(19)	120.4(3)
C(21)-C(20)-H(20)	119.8
C(19)-C(20)-H(20)	119.8
C(22)-C(21)-C(20)	119.7(3)
C(22)-C(21)-H(21)	120.1
C(20)-C(21)-H(21)	120.1
C(21)-C(22)-C(23)	120.3(3)
C(21)-C(22)-H(22)	119.8

C(23)-C(22)-H(22)	119.8
C(22)-C(23)-C(18)	120.3(3)
C(22)-C(23)-H(23)	119.9
C(18)-C(23)-H(23)	119.9
N(4)-C(24)-N(3)	110.3(2)
N(4)-C(24)-C(27)	124.9(2)
N(3)-C(24)-C(27)	124.8(2)
N(3)-C(25)-C(26)	105.2(2)
N(3)-C(25)-C(35)	121.7(2)
C(26)-C(25)-C(35)	133.1(2)
N(4)-C(26)-C(25)	109.7(2)
N(4)-C(26)-C(41)	119.6(2)
C(25)-C(26)-C(41)	130.5(2)
C(28)-C(27)-C(32)	120.1(2)
C(28)-C(27)-C(24)	119.0(2)
C(32)-C(27)-C(24)	120.9(2)
C(29)-C(28)-C(27)	119.4(2)
C(29)-C(28)-H(28)	120.3
C(27)-C(28)-H(28)	120.3
O(3)-C(29)-C(30)	115.6(2)
O(3)-C(29)-C(28)	123.3(2)
C(30)-C(29)-C(28)	121.0(2)
C(29)-C(30)-C(31)	119.4(2)
C(29)-C(30)-H(30)	120.3
C(31)-C(30)-H(30)	120.3
O(4)-C(31)-C(30)	115.1(2)
O(4)-C(31)-C(32)	124.0(2)
C(30)-C(31)-C(32)	120.9(2)
C(31)-C(32)-C(27)	119.1(2)
C(31)-C(32)-H(32)	120.5
C(27)-C(32)-H(32)	120.5
O(3)-C(33)-H(33A)	109.5
O(3)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
O(3)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
O(4)-C(34)-H(34A)	109.5

O(4)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
O(4)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(36)-C(35)-C(40)	118.7(2)
C(36)-C(35)-C(25)	120.6(2)
C(40)-C(35)-C(25)	120.6(2)
C(37)-C(36)-C(35)	120.8(2)
C(37)-C(36)-H(36)	119.6
C(35)-C(36)-H(36)	119.6
C(38)-C(37)-C(36)	120.1(3)
C(38)-C(37)-H(37)	120.0
C(36)-C(37)-H(37)	120.0
C(37)-C(38)-C(39)	119.8(2)
C(37)-C(38)-H(38)	120.1
C(39)-C(38)-H(38)	120.1
C(38)-C(39)-C(40)	120.5(3)
C(38)-C(39)-H(39)	119.8
C(40)-C(39)-H(39)	119.8
C(39)-C(40)-C(35)	120.2(3)
C(39)-C(40)-H(40)	119.9
C(35)-C(40)-H(40)	119.9
C(46)-C(41)-C(42)	118.9(2)
C(46)-C(41)-C(26)	117.8(2)
C(42)-C(41)-C(26)	123.2(2)
C(43)-C(42)-C(41)	119.9(2)
C(43)-C(42)-H(42)	120.1
C(41)-C(42)-H(42)	120.1
C(44)-C(43)-C(42)	120.8(2)
C(44)-C(43)-H(43)	119.6
C(42)-C(43)-H(43)	119.6
C(43)-C(44)-C(45)	119.5(2)
C(43)-C(44)-H(44)	120.2
C(45)-C(44)-H(44)	120.2
C(46)-C(45)-C(44)	120.1(2)
C(46)-C(45)-H(45)	120.0
C(44)-C(45)-H(45)	120.0

C(45)-C(46)-C(41)	120.8(2)
C(45)-C(46)-H(46)	119.6
C(41)-C(46)-H(46)	119.6
Cl(1)-C(47)-Cl(3)	111.0(2)
Cl(1)-C(47)-Cl(2)	110.3(2)
Cl(3)-C(47)-Cl(2)	109.8(2)
Cl(1)-C(47)-H(47)	108.6
Cl(3)-C(47)-H(47)	108.6
Cl(2)-C(47)-H(47)	108.6

Symmetry transformations used to generate equivalent atoms:

Table S8. Anisotropic displacement parameters ($Å^2$x 10^3)for i18108. 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)	52(1)	60(1)	38(1)	-9(1)	8(1)	-2(1)
Cl(2)	69(1)	47(1)	51(1)	-3(1)	21(1)	-5(1)
Cl(3)	67(1)	60(1)	41(1)	6(1)	-6(1)	14(1)
O(1)	13(1)	14(1)	28(1)	6(1)	0(1)	-3(1)
O(2)	15(1)	19(1)	20(1)	8(1)	-3(1)	-2(1)
O(3)	44(1)	18(1)	19(1)	-8(1)	13(1)	-12(1)
O(4)	28(1)	14(1)	19(1)	2(1)	8(1)	-7(1)
N(1)	12(1)	7(1)	15(1)	1(1)	1(1)	1(1)
N(2)	11(1)	8(1)	16(1)	0(1)	1(1)	0(1)
N(3)	13(1)	7(1)	15(1)	0(1)	3(1)	-1(1)
N(4)	12(1)	9(1)	15(1)	0(1)	3(1)	1(1)
C(1)	12(1)	9(1)	14(1)	-1(1)	2(1)	1(1)
C(2)	11(1)	12(1)	13(1)	-1(1)	1(1)	1(1)
C(3)	10(1)	12(1)	15(1)	1(1)	1(1)	0(1)
C(4)	11(1)	10(1)	14(1)	-2(1)	1(1)	3(1)
C(5)	12(1)	11(1)	16(1)	1(1)	0(1)	2(1)
C(6)	12(1)	10(1)	21(1)	-2(1)	4(1)	0(1)
C(7)	11(1)	13(1)	18(1)	-1(1)	-1(1)	1(1)
C(8)	15(1)	10(1)	15(1)	0(1)	1(1)	3(1)
C(9)	13(1)	11(1)	18(1)	1(1)	1(1)	0(1)
C(10)	20(1)	17(1)	30(2)	10(1)	2(1)	-3(1)
C(11)	20(1)	20(1)	27(2)	11(1)	-2(1)	-4(1)
C(12)	14(1)	13(1)	13(1)	2(1)	-1(1)	-1(1)
C(13)	17(1)	14(1)	18(1)	-2(1)	0(1)	-1(1)
C(14)	23(1)	15(1)	23(1)	-3(1)	-1(1)	-4(1)
C(15)	21(1)	21(1)	23(1)	0(1)	-3(1)	-10(1)
C(16)	14(1)	23(1)	22(1)	1(1)	2(1)	-2(1)
C(17)	15(1)	13(1)	20(1)	0(1)	0(1)	-1(1)
C(18)	11(1)	15(1)	21(1)	6(1)	4(1)	1(1)
C(19)	16(1)	23(1)	23(1)	7(1)	-1(1)	-2(1)
C(20)	17(1)	40(2)	27(2)	17(1)	-1(1)	-2(1)
C(21)	14(1)	33(2)	41(2)	26(1)	8(1)	7(1)
C(22)	16(1)	20(1)	42(2)	14(1)	12(1)	5(1)

C(23)	13(1)	16(1)	29(2)	6(1)	6(1)	4(1)
C(24)	11(1)	7(1)	16(1)	1(1)	0(1)	1(1)
C(25)	11(1)	9(1)	14(1)	0(1)	2(1)	1(1)
C(26)	12(1)	11(1)	13(1)	1(1)	1(1)	1(1)
C(27)	12(1)	11(1)	15(1)	1(1)	1(1)	1(1)
C(28)	16(1)	12(1)	18(1)	-2(1)	4(1)	-2(1)
C(29)	20(1)	16(1)	17(1)	-3(1)	2(1)	-1(1)
C(30)	20(1)	18(1)	14(1)	2(1)	4(1)	-1(1)
C(31)	15(1)	13(1)	18(1)	4(1)	2(1)	0(1)
C(32)	15(1)	11(1)	15(1)	1(1)	2(1)	0(1)
C(33)	67(2)	19(2)	32(2)	-12(1)	23(2)	-21(2)
C(34)	49(2)	23(2)	24(2)	-1(1)	9(1)	-20(1)
C(35)	17(1)	7(1)	15(1)	2(1)	1(1)	0(1)
C(36)	15(1)	14(1)	16(1)	1(1)	2(1)	-1(1)
C(37)	20(1)	14(1)	21(1)	0(1)	-3(1)	-2(1)
C(38)	29(2)	14(1)	16(1)	-3(1)	1(1)	1(1)
C(39)	23(1)	18(1)	21(1)	-3(1)	8(1)	2(1)
C(40)	17(1)	15(1)	19(1)	-3(1)	3(1)	-2(1)
C(41)	13(1)	7(1)	16(1)	-1(1)	4(1)	0(1)
C(42)	15(1)	13(1)	16(1)	0(1)	1(1)	-1(1)
C(43)	21(1)	14(1)	14(1)	1(1)	3(1)	1(1)
C(44)	17(1)	13(1)	20(1)	2(1)	7(1)	-1(1)
C(45)	14(1)	13(1)	20(1)	-1(1)	1(1)	-2(1)
C(46)	17(1)	10(1)	15(1)	0(1)	3(1)	1(1)
C(47)	42(2)	45(2)	34(2)	-2(2)	7(2)	7(2)

Crystal data and structure refinement for compound **3s**

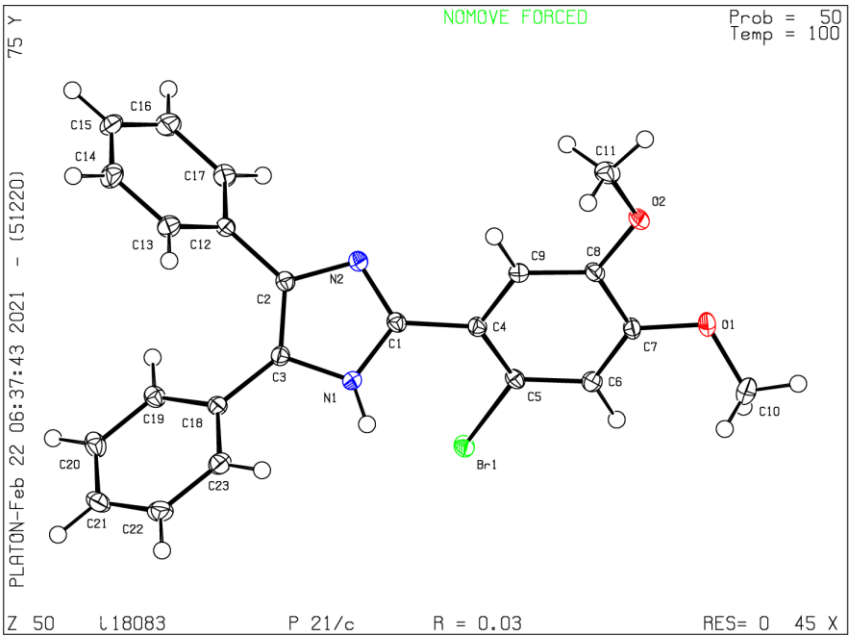


Figure S3. Single X-ray crystal structure of imidazole **3s** (the thermal ellipsoid was drawn at the 50% probability level)

Table S9. Crystal data and structure refinement for i18083.

CCDC	2082025	
Identification code	i18083	
Empirical formula	C23 H19 Br N2 O2	
Formula weight	435.31	
Temperature	100.0(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 9.2089(2) Å	α= 90°.
	b = 19.8306(3) Å	β= 101.4920(10)°.
	c = 10.4519(2) Å	γ = 90°.
Volume	1870.44(6) $Å^3$	
Z	4	
Density (calculated)	1.546 Mg/m^3	
Absorption coefficient	2.220 mm^{-1}	
F(000)	888	
Crystal size	0.201 x 0.185 x 0.095 mm^3	
Theta range for data collection	2.054 to 30.518°.	
Index ranges	-13<=h<=13, -28<=k<=28, -14<=l<=14	

Reflections collected	78302
Independent reflections	5710 [R(int) = 0.0527]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Numerical
Max. and min. transmission	1 and 0.9203
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5710 / 0 / 259
Goodness-of-fit on F^2	1.036
Final R indices [I>2sigma(I)]	R1 = 0.0262, wR2 = 0.0562
R indices (all data)	R1 = 0.0366, wR2 = 0.0603
Extinction coefficient	n/a
Largest diff. peak and hole	0.457 and -0.365 e.$Å^{-3}$

Table S10. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for i18083. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	671(1)	7092(1)	3732(1)	16(1)
O(1)	3529(1)	9029(1)	6611(1)	19(1)
O(2)	4595(1)	8243(1)	8533(1)	17(1)
N(1)	2709(1)	5839(1)	5063(1)	14(1)
N(2)	2329(1)	5853(1)	7092(1)	14(1)
C(1)	2592(2)	6225(1)	6114(1)	13(1)
C(2)	2251(2)	5196(1)	6637(1)	13(1)
C(3)	2482(2)	5177(1)	5370(1)	13(1)
C(4)	2763(2)	6963(1)	6164(1)	13(1)
C(5)	2085(2)	7404(1)	5192(1)	13(1)
C(6)	2344(2)	8097(1)	5282(1)	14(1)
C(7)	3225(2)	8361(1)	6399(1)	14(1)
C(8)	3845(2)	7929(1)	7434(1)	14(1)
C(9)	3647(2)	7240(1)	7296(1)	14(1)
C(10)	3483(2)	9441(1)	5488(2)	30(1)
C(11)	5575(2)	7836(1)	9459(1)	19(1)
C(12)	1942(2)	4633(1)	7460(1)	14(1)
C(13)	2765(2)	4037(1)	7535(1)	18(1)
C(14)	2457(2)	3501(1)	8299(2)	22(1)
C(15)	1339(2)	3558(1)	9008(2)	24(1)
C(16)	531(2)	4153(1)	8953(2)	25(1)
C(17)	819(2)	4685(1)	8178(2)	20(1)
C(18)	2430(2)	4629(1)	4416(1)	13(1)
C(19)	1336(2)	4133(1)	4320(1)	16(1)
C(20)	1237(2)	3621(1)	3395(1)	19(1)
C(21)	2233(2)	3601(1)	2561(1)	22(1)
C(22)	3326(2)	4090(1)	2648(2)	22(1)
C(23)	3432(2)	4604(1)	3570(1)	19(1)

Table S11. Bond lengths [Å] and angles [°] for i18083.

Br(1)-C(5)	1.9022(13)
O(1)-C(7)	1.3634(16)
O(1)-C(10)	1.4237(19)
O(2)-C(8)	1.3675(16)
O(2)-C(11)	1.4328(17)
N(1)-C(1)	1.3611(17)
N(1)-C(3)	1.3780(17)
N(1)-H(1)	0.85(2)
N(2)-C(1)	1.3220(18)
N(2)-C(2)	1.3839(17)
C(1)-C(4)	1.4716(18)
C(2)-C(3)	1.3835(19)
C(2)-C(12)	1.4714(19)
C(3)-C(18)	1.4700(18)
C(4)-C(5)	1.3896(18)
C(4)-C(9)	1.4073(18)
C(5)-C(6)	1.3960(18)
C(6)-C(7)	1.3838(19)
C(6)-H(6)	0.9500
C(7)-C(8)	1.4093(19)
C(8)-C(9)	1.3807(18)
C(9)-H(9)	0.9500
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-C(17)	1.397(2)
C(12)-C(13)	1.397(2)
C(13)-C(14)	1.391(2)
C(13)-H(13)	0.9500
C(14)-C(15)	1.387(2)
C(14)-H(14)	0.9500
C(15)-C(16)	1.391(2)
C(15)-H(15)	0.9500

C(16)-C(17)	1.387(2)
C(16)-H(16)	0.9500
C(17)-H(17)	0.9500
C(18)-C(19)	1.3973(19)
C(18)-C(23)	1.401(2)
C(19)-C(20)	1.3925(19)
C(19)-H(19)	0.9500
C(20)-C(21)	1.387(2)
C(20)-H(20)	0.9500
C(21)-C(22)	1.388(2)
C(21)-H(21)	0.9500
C(22)-C(23)	1.392(2)
C(22)-H(22)	0.9500
C(23)-H(23)	0.9500

C(7)-O(1)-C(10)	116.87(12)
C(8)-O(2)-C(11)	117.14(11)
C(1)-N(1)-C(3)	107.92(12)
C(1)-N(1)-H(1)	125.0(13)
C(3)-N(1)-H(1)	127.0(13)
C(1)-N(2)-C(2)	105.44(11)
N(2)-C(1)-N(1)	111.47(12)
N(2)-C(1)-C(4)	124.27(12)
N(1)-C(1)-C(4)	124.26(12)
C(3)-C(2)-N(2)	110.25(12)
C(3)-C(2)-C(12)	128.64(12)
N(2)-C(2)-C(12)	121.11(12)
N(1)-C(3)-C(2)	104.92(12)
N(1)-C(3)-C(18)	122.22(12)
C(2)-C(3)-C(18)	132.74(12)
C(5)-C(4)-C(9)	117.99(12)
C(5)-C(4)-C(1)	124.72(12)
C(9)-C(4)-C(1)	117.28(12)
C(4)-C(5)-C(6)	121.63(12)
C(4)-C(5)-Br(1)	121.21(10)
C(6)-C(5)-Br(1)	117.05(10)
C(7)-C(6)-C(5)	119.51(12)
C(7)-C(6)-H(6)	120.2

C(5)-C(6)-H(6)	120.2
O(1)-C(7)-C(6)	124.88(13)
O(1)-C(7)-C(8)	115.29(12)
C(6)-C(7)-C(8)	119.80(12)
O(2)-C(8)-C(9)	124.90(12)
O(2)-C(8)-C(7)	115.31(12)
C(9)-C(8)-C(7)	119.78(12)
C(8)-C(9)-C(4)	121.05(12)
C(8)-C(9)-H(9)	119.5
C(4)-C(9)-H(9)	119.5
O(1)-C(10)-H(10A)	109.5
O(1)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
O(1)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
O(2)-C(11)-H(11A)	109.5
O(2)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
O(2)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(17)-C(12)-C(13)	118.92(13)
C(17)-C(12)-C(2)	120.54(13)
C(13)-C(12)-C(2)	120.54(13)
C(14)-C(13)-C(12)	120.48(14)
C(14)-C(13)-H(13)	119.8
C(12)-C(13)-H(13)	119.8
C(15)-C(14)-C(13)	120.17(15)
C(15)-C(14)-H(14)	119.9
C(13)-C(14)-H(14)	119.9
C(14)-C(15)-C(16)	119.62(14)
C(14)-C(15)-H(15)	120.2
C(16)-C(15)-H(15)	120.2
C(17)-C(16)-C(15)	120.43(15)
C(17)-C(16)-H(16)	119.8
C(15)-C(16)-H(16)	119.8
C(16)-C(17)-C(12)	120.37(14)

C(16)-C(17)-H(17)	119.8
C(12)-C(17)-H(17)	119.8
C(19)-C(18)-C(23)	119.10(13)
C(19)-C(18)-C(3)	119.67(13)
C(23)-C(18)-C(3)	121.19(13)
C(20)-C(19)-C(18)	120.64(14)
C(20)-C(19)-H(19)	119.7
C(18)-C(19)-H(19)	119.7
C(21)-C(20)-C(19)	119.81(14)
C(21)-C(20)-H(20)	120.1
C(19)-C(20)-H(20)	120.1
C(20)-C(21)-C(22)	120.09(14)
C(20)-C(21)-H(21)	120.0
C(22)-C(21)-H(21)	120.0
C(21)-C(22)-C(23)	120.43(15)
C(21)-C(22)-H(22)	119.8
C(23)-C(22)-H(22)	119.8
C(22)-C(23)-C(18)	119.93(14)
C(22)-C(23)-H(23)	120.0
C(18)-C(23)-H(23)	120.0

Symmetry transformations used to generate equivalent atoms:

Table S12. Anisotropic displacement parameters ($Å^2$x 10^3)for i18083. 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}
Br(1)	16(1)	15(1)	14(1)	-1(1)	-2(1)	-1(1)
O(1)	27(1)	10(1)	19(1)	-1(1)	2(1)	-2(1)
O(2)	20(1)	16(1)	13(1)	-3(1)	-1(1)	-3(1)
N(1)	17(1)	12(1)	13(1)	1(1)	5(1)	-1(1)
N(2)	14(1)	13(1)	13(1)	-1(1)	2(1)	-1(1)
C(1)	13(1)	13(1)	13(1)	-1(1)	0(1)	0(1)
C(2)	13(1)	13(1)	13(1)	-1(1)	2(1)	0(1)
C(3)	14(1)	12(1)	14(1)	0(1)	2(1)	-1(1)
C(4)	13(1)	12(1)	14(1)	-1(1)	5(1)	0(1)
C(5)	13(1)	14(1)	12(1)	-2(1)	0(1)	-1(1)
C(6)	16(1)	14(1)	14(1)	1(1)	2(1)	2(1)
C(7)	16(1)	10(1)	16(1)	-2(1)	5(1)	-1(1)
C(8)	14(1)	14(1)	12(1)	-3(1)	3(1)	-2(1)
C(9)	15(1)	14(1)	12(1)	0(1)	2(1)	0(1)
C(10)	47(1)	16(1)	25(1)	3(1)	6(1)	-9(1)
C(11)	18(1)	23(1)	15(1)	-1(1)	-1(1)	-2(1)
C(12)	17(1)	14(1)	11(1)	-1(1)	1(1)	-3(1)
C(13)	19(1)	17(1)	16(1)	2(1)	1(1)	1(1)
C(14)	27(1)	17(1)	19(1)	5(1)	-3(1)	0(1)
C(15)	36(1)	21(1)	14(1)	4(1)	1(1)	-11(1)
C(16)	31(1)	26(1)	20(1)	-2(1)	12(1)	-10(1)
C(17)	23(1)	18(1)	19(1)	-2(1)	8(1)	-3(1)
C(18)	16(1)	12(1)	11(1)	1(1)	1(1)	3(1)
C(19)	15(1)	16(1)	15(1)	-1(1)	1(1)	1(1)
C(20)	20(1)	16(1)	19(1)	-2(1)	-4(1)	0(1)
C(21)	35(1)	18(1)	12(1)	-2(1)	0(1)	7(1)
C(22)	33(1)	20(1)	16(1)	1(1)	10(1)	7(1)
C(23)	24(1)	16(1)	18(1)	2(1)	7(1)	2(1)

Crystal data and structure refinement for compound **3w**

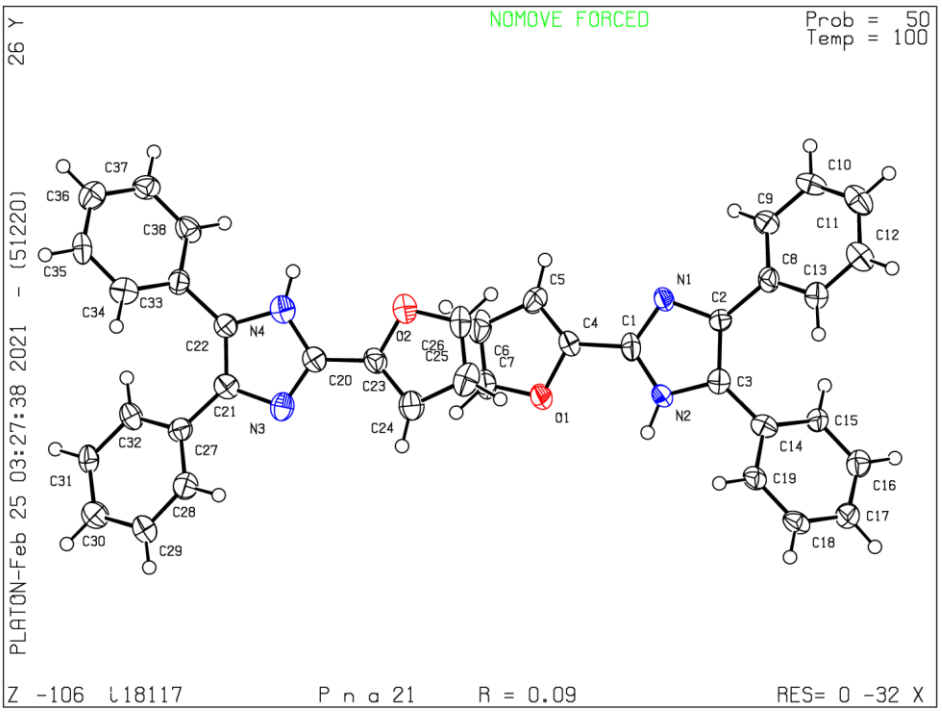


Figure S4. Single X-ray crystal structure of imidazole **3w** (the thermal ellipsoid was drawn at the 50% probability level)

Table S13. Crystal data and structure refinement for i18117.

CCDC	2082032	
Identification code	i18117	
Empirical formula	C38 H28 N4 O2	
Formula weight	572.64	
Temperature	100.0(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P n a 21	
Unit cell dimensions	a = 8.9585(4) Å	α= 90°.
	b = 11.3947(5) Å	β= 90°.
	c = 28.7859(13) Å	γ = 90°.
Volume	2938.4(2) $Å^3$	
Z	4	
Density (calculated)	1.294 Mg/m^3	
Absorption coefficient	0.644 mm^{-1}	
F(000)	1200	
Crystal size	0.320 x 0.090 x 0.060 mm^3	
Theta range for data collection	3.070 to 66.595°.	

Index ranges	-10<=h<=9, -13<=k<=13, -33<=l<=34
Reflections collected	27891
Independent reflections	5125 [R(int) = 0.1401]
Completeness to theta = 66.595°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7528 and 0.6024
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5125 / 1 / 403
Goodness-of-fit on F^2	1.017
Final R indices [I>2sigma(I)]	R1 = 0.0871, wR2 = 0.2137
R indices (all data)	R1 = 0.1249, wR2 = 0.2411
Absolute structure parameter	0.1(4)
Extinction coefficient	n/a
Largest diff. peak and hole	0.550 and -0.323 e.$Å^{-3}$

Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for i18117. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	1603(7)	3907(5)	5150(2)	36(2)
O(2)	5472(7)	6077(5)	4919(2)	40(2)
N(1)	3283(8)	1445(6)	5762(2)	28(2)
N(2)	1123(9)	2322(6)	5888(3)	28(2)
N(3)	3780(9)	8541(7)	4306(2)	34(2)
N(4)	5962(9)	7675(7)	4171(3)	34(2)
C(1)	2351(10)	2299(8)	5627(3)	33(2)
C(2)	2570(9)	889(7)	6133(3)	25(2)
C(3)	1206(10)	1447(8)	6209(3)	28(2)
C(4)	2628(10)	3023(7)	5219(3)	31(2)
C(5)	3612(11)	2976(9)	4877(3)	38(2)
C(6)	3227(12)	3909(10)	4564(4)	46(3)
C(7)	2011(11)	4432(9)	4741(4)	42(2)
C(8)	3310(10)	-78(7)	6384(3)	31(2)
C(9)	4331(10)	-788(8)	6145(3)	34(2)
C(10)	5026(10)	-1699(8)	6372(3)	36(2)
C(11)	4757(11)	-1918(8)	6840(4)	42(2)
C(12)	3749(11)	-1208(8)	7076(4)	40(2)
C(13)	3035(11)	-311(8)	6852(3)	31(2)
C(14)	-41(9)	1206(8)	6522(3)	29(2)
C(15)	-585(10)	58(8)	6587(4)	33(2)
C(16)	-1799(10)	-154(9)	6864(3)	35(2)
C(17)	-2559(11)	768(8)	7068(4)	41(2)
C(18)	-2030(10)	1905(8)	7021(3)	34(2)
C(19)	-789(9)	2123(8)	6744(3)	29(2)
C(20)	4720(10)	7714(7)	4443(3)	29(2)
C(21)	4469(10)	9092(7)	3940(3)	30(2)
C(22)	5837(9)	8569(7)	3850(3)	28(2)
C(23)	4481(10)	6968(8)	4840(3)	33(2)
C(24)	3439(11)	6995(9)	5188(3)	39(2)
C(25)	3831(12)	6079(10)	5505(4)	46(3)
C(26)	5028(12)	5545(8)	5324(3)	39(2)
C(27)	3673(10)	10069(8)	3712(3)	32(2)

C(28)	2642(11)	10714(8)	3959(4)	38(2)
C(29)	1827(11)	11622(8)	3764(3)	41(2)
C(30)	2067(11)	11889(9)	3286(3)	39(2)
C(31)	3109(10)	11268(8)	3036(3)	32(2)
C(32)	3911(11)	10352(8)	3247(3)	32(2)
C(33)	7041(10)	8817(8)	3516(3)	31(2)
C(34)	7492(10)	9985(8)	3427(3)	34(2)
C(35)	8664(11)	10196(9)	3134(3)	36(2)
C(36)	9441(11)	9280(9)	2925(3)	41(2)
C(37)	8983(11)	8128(8)	3011(3)	35(2)
C(38)	7807(10)	7904(8)	3296(3)	35(2)

Table S15. Bond lengths [Å] and angles [°] for i18117.

O(1)-C(7)	1.371(12)
O(1)-C(4)	1.377(10)
O(2)-C(23)	1.368(11)
O(2)-C(26)	1.372(11)
N(1)-C(1)	1.339(11)
N(1)-C(2)	1.398(11)
N(2)-C(1)	1.332(12)
N(2)-C(3)	1.361(12)
N(2)-H(2)	0.91(10)
N(3)-C(20)	1.324(12)
N(3)-C(21)	1.374(11)
N(4)-C(20)	1.362(12)
N(4)-C(22)	1.380(12)
N(4)-H(4)	0.90(11)
C(1)-C(4)	1.458(12)
C(2)-C(3)	1.395(12)
C(2)-C(8)	1.474(12)
C(3)-C(14)	1.461(12)
C(4)-C(5)	1.323(13)
C(5)-C(6)	1.435(15)
C(5)-H(5)	0.9500
C(6)-C(7)	1.341(15)
C(6)-H(6)	0.9500
C(7)-H(7)	0.9500
C(8)-C(13)	1.397(12)
C(8)-C(9)	1.402(13)
C(9)-C(10)	1.375(12)
C(9)-H(9)	0.9500
C(10)-C(11)	1.389(14)
C(10)-H(10)	0.9500
C(11)-C(12)	1.390(14)
C(11)-H(11)	0.9500
C(12)-C(13)	1.367(13)
C(12)-H(12)	0.9500
C(13)-H(13)	0.9500
C(14)-C(19)	1.397(12)

C(14)-C(15)	1.408(12)
C(15)-C(16)	1.369(13)
C(15)-H(15)	0.9500
C(16)-C(17)	1.383(14)
C(16)-H(16)	0.9500
C(17)-C(18)	1.386(13)
C(17)-H(17)	0.9500
C(18)-C(19)	1.390(12)
C(18)-H(18)	0.9500
C(19)-H(19)	0.9500
C(20)-C(23)	1.441(13)
C(21)-C(22)	1.387(12)
C(21)-C(27)	1.476(13)
C(22)-C(33)	1.473(12)
C(23)-C(24)	1.368(14)
C(24)-C(25)	1.431(15)
C(24)-H(24)	0.9500
C(25)-C(26)	1.339(15)
C(25)-H(25)	0.9500
C(26)-H(26)	0.9500
C(27)-C(28)	1.378(13)
C(27)-C(32)	1.392(13)
C(28)-C(29)	1.386(13)
C(28)-H(28)	0.9500
C(29)-C(30)	1.424(14)
C(29)-H(29)	0.9500
C(30)-C(31)	1.376(13)
C(30)-H(30)	0.9500
C(31)-C(32)	1.406(13)
C(31)-H(31)	0.9500
C(32)-H(32)	0.9500
C(33)-C(38)	1.397(12)
C(33)-C(34)	1.414(12)
C(34)-C(35)	1.368(13)
C(34)-H(34)	0.9500
C(35)-C(36)	1.392(14)
C(35)-H(35)	0.9500
C(36)-C(37)	1.397(14)

C(36)-H(36)	0.9500
C(37)-C(38)	1.360(13)
C(37)-H(37)	0.9500
C(38)-H(38)	0.9500

C(7)-O(1)-C(4)	105.4(7)
C(23)-O(2)-C(26)	106.3(7)
C(1)-N(1)-C(2)	105.4(7)
C(1)-N(2)-C(3)	108.8(8)
C(1)-N(2)-H(2)	125(6)
C(3)-N(2)-H(2)	126(6)
C(20)-N(3)-C(21)	105.6(8)
C(20)-N(4)-C(22)	107.2(8)
C(20)-N(4)-H(4)	130(7)
C(22)-N(4)-H(4)	122(7)
N(2)-C(1)-N(1)	111.5(8)
N(2)-C(1)-C(4)	125.7(8)
N(1)-C(1)-C(4)	122.6(8)
C(3)-C(2)-N(1)	108.2(7)
C(3)-C(2)-C(8)	131.2(8)
N(1)-C(2)-C(8)	120.6(7)
N(2)-C(3)-C(2)	106.1(8)
N(2)-C(3)-C(14)	120.9(8)
C(2)-C(3)-C(14)	132.8(8)
C(5)-C(4)-O(1)	111.5(8)
C(5)-C(4)-C(1)	133.7(9)
O(1)-C(4)-C(1)	114.7(8)
C(4)-C(5)-C(6)	106.0(9)
C(4)-C(5)-H(5)	127.0
C(6)-C(5)-H(5)	127.0
C(7)-C(6)-C(5)	106.7(9)
C(7)-C(6)-H(6)	126.7
C(5)-C(6)-H(6)	126.7
C(6)-C(7)-O(1)	110.4(9)
C(6)-C(7)-H(7)	124.8
O(1)-C(7)-H(7)	124.8
C(13)-C(8)-C(9)	118.6(8)
C(13)-C(8)-C(2)	122.4(8)

C(9)-C(8)-C(2)	119.0(8)
C(10)-C(9)-C(8)	119.9(9)
C(10)-C(9)-H(9)	120.0
C(8)-C(9)-H(9)	120.0
C(9)-C(10)-C(11)	121.1(9)
C(9)-C(10)-H(10)	119.5
C(11)-C(10)-H(10)	119.5
C(10)-C(11)-C(12)	118.9(9)
C(10)-C(11)-H(11)	120.6
C(12)-C(11)-H(11)	120.6
C(13)-C(12)-C(11)	120.6(9)
C(13)-C(12)-H(12)	119.7
C(11)-C(12)-H(12)	119.7
C(12)-C(13)-C(8)	121.0(9)
C(12)-C(13)-H(13)	119.5
C(8)-C(13)-H(13)	119.5
C(19)-C(14)-C(15)	117.8(8)
C(19)-C(14)-C(3)	120.6(8)
C(15)-C(14)-C(3)	121.5(8)
C(16)-C(15)-C(14)	121.2(9)
C(16)-C(15)-H(15)	119.4
C(14)-C(15)-H(15)	119.4
C(15)-C(16)-C(17)	120.2(9)
C(15)-C(16)-H(16)	119.9
C(17)-C(16)-H(16)	119.9
C(16)-C(17)-C(18)	120.1(9)
C(16)-C(17)-H(17)	120.0
C(18)-C(17)-H(17)	120.0
C(17)-C(18)-C(19)	119.7(9)
C(17)-C(18)-H(18)	120.1
C(19)-C(18)-H(18)	120.1
C(18)-C(19)-C(14)	120.9(8)
C(18)-C(19)-H(19)	119.6
C(14)-C(19)-H(19)	119.6
N(3)-C(20)-N(4)	111.8(8)
N(3)-C(20)-C(23)	124.2(8)
N(4)-C(20)-C(23)	124.0(8)
N(3)-C(21)-C(22)	110.1(8)

N(3)-C(21)-C(27)	118.0(8)
C(22)-C(21)-C(27)	131.9(8)
N(4)-C(22)-C(21)	105.3(8)
N(4)-C(22)-C(33)	121.3(8)
C(21)-C(22)-C(33)	133.4(8)
O(2)-C(23)-C(24)	109.8(8)
O(2)-C(23)-C(20)	118.2(8)
C(24)-C(23)-C(20)	131.9(9)
C(23)-C(24)-C(25)	106.5(9)
C(23)-C(24)-H(24)	126.8
C(25)-C(24)-H(24)	126.8
C(26)-C(25)-C(24)	106.1(9)
C(26)-C(25)-H(25)	126.9
C(24)-C(25)-H(25)	126.9
C(25)-C(26)-O(2)	111.3(9)
C(25)-C(26)-H(26)	124.3
O(2)-C(26)-H(26)	124.3
C(28)-C(27)-C(32)	118.4(9)
C(28)-C(27)-C(21)	119.7(8)
C(32)-C(27)-C(21)	121.9(8)
C(27)-C(28)-C(29)	122.8(9)
C(27)-C(28)-H(28)	118.6
C(29)-C(28)-H(28)	118.6
C(28)-C(29)-C(30)	118.1(9)
C(28)-C(29)-H(29)	121.0
C(30)-C(29)-H(29)	121.0
C(31)-C(30)-C(29)	119.9(9)
C(31)-C(30)-H(30)	120.0
C(29)-C(30)-H(30)	120.0
C(30)-C(31)-C(32)	120.1(8)
C(30)-C(31)-H(31)	120.0
C(32)-C(31)-H(31)	120.0
C(27)-C(32)-C(31)	120.7(9)
C(27)-C(32)-H(32)	119.7
C(31)-C(32)-H(32)	119.7
C(38)-C(33)-C(34)	118.6(8)
C(38)-C(33)-C(22)	120.8(8)
C(34)-C(33)-C(22)	120.5(8)

C(35)-C(34)-C(33)	119.8(9)
C(35)-C(34)-H(34)	120.1
C(33)-C(34)-H(34)	120.1
C(34)-C(35)-C(36)	121.2(9)
C(34)-C(35)-H(35)	119.4
C(36)-C(35)-H(35)	119.4
C(35)-C(36)-C(37)	118.7(9)
C(35)-C(36)-H(36)	120.6
C(37)-C(36)-H(36)	120.6
C(38)-C(37)-C(36)	120.8(9)
C(38)-C(37)-H(37)	119.6
C(36)-C(37)-H(37)	119.6
C(37)-C(38)-C(33)	120.8(8)
C(37)-C(38)-H(38)	119.6
C(33)-C(38)-H(38)	119.6

Symmetry transformations used to generate equivalent atoms:

Table S16. Anisotropic displacement parameters ($Å^2$x 10^3)for i18117. 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)	33(3)	34(3)	41(4)	13(3)	-2(3)	2(3)
O(2)	46(4)	36(4)	40(4)	7(3)	0(3)	-2(3)
N(1)	30(4)	25(4)	29(4)	7(3)	-2(3)	1(3)
N(2)	30(4)	22(4)	31(4)	4(3)	-1(3)	3(3)
N(3)	38(5)	33(4)	32(4)	0(3)	-1(3)	-8(3)
N(4)	42(5)	29(4)	31(4)	-4(3)	-3(4)	-3(3)
C(1)	37(5)	27(5)	34(5)	9(4)	-3(4)	-7(4)
C(2)	18(4)	29(4)	29(5)	2(4)	-5(3)	-4(3)
C(3)	35(5)	27(4)	24(4)	-3(4)	0(4)	-3(4)
C(4)	36(5)	26(5)	31(5)	6(4)	-2(4)	2(4)
C(5)	41(5)	41(6)	32(5)	3(4)	11(4)	0(4)
C(6)	47(6)	53(6)	37(5)	17(5)	-6(5)	-10(5)
C(7)	40(6)	39(6)	48(6)	21(5)	-2(5)	-4(4)
C(8)	29(5)	23(5)	41(5)	5(4)	-1(4)	-7(3)
C(9)	36(5)	28(5)	38(5)	-2(4)	3(4)	3(4)
C(10)	33(5)	31(5)	45(6)	-9(4)	-7(4)	10(4)
C(11)	41(5)	31(5)	55(6)	2(5)	-21(5)	-2(4)
C(12)	47(6)	32(5)	41(5)	-1(4)	-11(4)	2(4)
C(13)	39(5)	30(5)	26(5)	-2(4)	0(4)	-4(4)
C(14)	25(4)	31(5)	30(5)	-5(4)	-11(4)	1(4)
C(15)	34(5)	25(5)	40(5)	4(4)	10(4)	1(4)
C(16)	32(5)	37(5)	35(5)	5(4)	-5(4)	-6(4)
C(17)	31(5)	42(6)	50(6)	14(5)	3(4)	1(4)
C(18)	36(5)	36(5)	29(5)	0(4)	-6(4)	12(4)
C(19)	26(4)	33(5)	29(5)	5(4)	-8(4)	2(3)
C(20)	33(5)	25(4)	30(5)	-4(4)	-4(4)	-3(4)
C(21)	37(5)	28(5)	25(4)	-6(4)	-3(4)	1(4)
C(22)	31(5)	24(4)	30(5)	-4(4)	0(4)	-2(3)
C(23)	34(5)	33(5)	31(5)	6(4)	-5(4)	2(4)
C(24)	45(6)	40(5)	32(5)	3(5)	-3(4)	-2(4)
C(25)	49(6)	53(6)	36(5)	4(5)	0(5)	-14(5)
C(26)	48(6)	36(5)	34(5)	10(4)	-2(5)	-9(5)
C(27)	30(5)	25(5)	40(5)	-4(4)	5(4)	-4(4)

C(28)	39(6)	38(5)	37(5)	3(4)	3(4)	-2(4)
C(29)	44(6)	36(5)	43(6)	10(4)	-1(5)	5(4)
C(30)	40(5)	39(5)	39(5)	1(4)	-4(4)	2(4)
C(31)	44(5)	29(5)	24(4)	5(4)	1(4)	-3(4)
C(32)	41(5)	22(4)	34(5)	-1(4)	-5(4)	-2(4)
C(33)	34(5)	30(5)	29(5)	4(4)	3(4)	-2(4)
C(34)	34(5)	38(5)	30(5)	-8(4)	-9(4)	-2(4)
C(35)	45(6)	31(5)	33(5)	11(4)	-6(4)	-11(4)
C(36)	39(6)	49(6)	35(5)	1(5)	1(4)	-5(4)
C(37)	38(5)	38(5)	30(5)	-5(4)	2(4)	7(4)
C(38)	47(6)	28(5)	31(5)	-3(4)	-1(4)	6(4)

Crystal data and structure refinement for compound **4h**

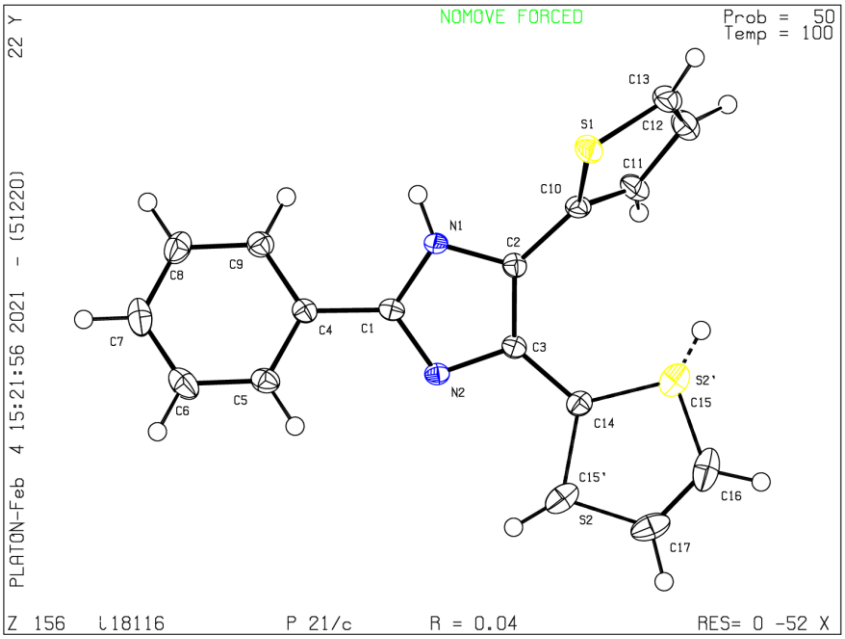


Figure S5. Single X-ray crystal structure of imidazole **4h** (the thermal ellipsoid was drawn at the 50% probability level)

Table S17. Crystal data and structure refinement for i18116.

CCDC	2082036
Identification code	i18116
Empirical formula	C17 H12 N2 S2
Formula weight	308.41
Temperature	100.0(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic

Space group	P 21/c	
Unit cell dimensions	a = 11.1404(4) Å	α= 90°.
	b = 14.6012(6) Å	β= 104.4970(10)°.
	c = 9.2447(3) Å	γ = 90°.
Volume	1455.89(9) $Å^3$	
Z	4	
Density (calculated)	1.407 Mg/m^3	
Absorption coefficient	0.359 mm^{-1}	
F(000)	640	
Crystal size	0.210 x 0.160 x 0.058 mm^3	
Theta range for data collection	2.669 to 27.102°.	
Index ranges	-13<=h<=14, -18<=k<=18, -11<=l<=11	
Reflections collected	42960	
Independent reflections	3206 [R(int) = 0.0754]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Numerical	
Max. and min. transmission	1 and 0.9613	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3206 / 0 / 191	
Goodness-of-fit on F^2	1.049	
Final R indices [I>2sigma(I)]	R1 = 0.0427, wR2 = 0.0999	
R indices (all data)	R1 = 0.0566, wR2 = 0.1065	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.593 and -0.453 $e.Å^{-3}$	

Table S18. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for i18116. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	3650(1)	3829(1)	9063(1)	24(1)
S(2)	4148(1)	4670(1)	2772(1)	29(1)
C(15)	2296(1)	4673(1)	4269(1)	34(1)
S(2')	2296(1)	4673(1)	4269(1)	34(1)
C(15')	4148(1)	4670(1)	2772(1)	29(1)
N(1)	5217(2)	2647(1)	6984(2)	16(1)
N(2)	5418(1)	3202(1)	4828(2)	15(1)
C(1)	5913(2)	2659(1)	5978(2)	15(1)
C(2)	4213(2)	3213(1)	6462(2)	16(1)
C(3)	4354(2)	3557(1)	5123(2)	16(1)
C(4)	7067(2)	2138(1)	6133(2)	16(1)
C(5)	7933(2)	2442(2)	5378(2)	21(1)
C(6)	9021(2)	1964(2)	5494(2)	28(1)
C(7)	9280(2)	1193(2)	6387(3)	30(1)
C(8)	8436(2)	886(2)	7146(2)	26(1)
C(9)	7320(2)	1351(1)	7011(2)	20(1)
C(10)	3274(2)	3351(1)	7298(2)	18(1)
C(11)	2032(2)	3115(2)	6872(2)	24(1)
C(12)	1413(2)	3327(2)	8010(3)	27(1)
C(13)	2166(2)	3705(2)	9238(2)	25(1)
C(14)	3623(2)	4231(1)	4113(2)	18(1)
C(16)	2118(2)	5342(2)	2856(3)	34(1)
C(17)	3036(2)	5339(2)	2142(2)	29(1)

Table S19. Bond lengths [Å] and angles [°] for i18116.

S(1)-C(13)	1.710(2)
S(1)-C(10)	1.7265(19)
S(2)-C(17)	1.571(3)
S(2)-C(14)	1.629(2)
C(15)-C(16)	1.603(3)
C(15)-C(14)	1.653(2)
C(15)-H(15)	0.9500
S(2')-C(16)	1.603(3)
S(2')-C(14)	1.653(2)
C(15')-C(17)	1.571(3)
C(15')-C(14)	1.629(2)
C(15')-H(15')	0.9500
N(1)-C(1)	1.351(2)
N(1)-C(2)	1.378(2)
N(1)-H(1)	0.8800
N(2)-C(1)	1.330(2)
N(2)-C(3)	1.381(2)
C(1)-C(4)	1.470(3)
C(2)-C(3)	1.381(3)
C(2)-C(10)	1.462(3)
C(3)-C(14)	1.458(3)
C(4)-C(9)	1.394(3)
C(4)-C(5)	1.398(3)
C(5)-C(6)	1.379(3)
C(5)-H(5)	0.9500
C(6)-C(7)	1.383(3)
C(6)-H(6)	0.9500
C(7)-C(8)	1.381(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.394(3)
C(8)-H(8)	0.9500
C(9)-H(9)	0.9500
C(10)-C(11)	1.384(3)
C(11)-C(12)	1.428(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.349(3)

C(12)-H(12)	0.9500
C(13)-H(13)	0.9500
C(16)-C(17)	1.349(4)
C(16)-H(16)	0.9500
C(17)-H(17)	0.9500

C(13)-S(1)-C(10)	92.01(10)
C(17)-S(2)-C(14)	97.24(12)
C(16)-C(15)-C(14)	95.60(12)
C(16)-C(15)-H(15)	132.2
C(14)-C(15)-H(15)	132.2
C(16)-S(2')-C(14)	95.60(12)
C(17)-C(15')-C(14)	97.24(12)
C(17)-C(15')-H(15')	131.4
C(14)-C(15')-H(15')	131.4
C(1)-N(1)-C(2)	107.87(15)
C(1)-N(1)-H(1)	126.1
C(2)-N(1)-H(1)	126.1
C(1)-N(2)-C(3)	105.66(15)
N(2)-C(1)-N(1)	111.30(17)
N(2)-C(1)-C(4)	124.35(17)
N(1)-C(1)-C(4)	124.35(17)
N(1)-C(2)-C(3)	105.46(16)
N(1)-C(2)-C(10)	121.57(17)
C(3)-C(2)-C(10)	132.98(18)
C(2)-C(3)-N(2)	109.71(17)
C(2)-C(3)-C(14)	130.45(18)
N(2)-C(3)-C(14)	119.73(16)
C(9)-C(4)-C(5)	119.24(18)
C(9)-C(4)-C(1)	121.90(18)
C(5)-C(4)-C(1)	118.87(18)
C(6)-C(5)-C(4)	120.2(2)
C(6)-C(5)-H(5)	119.9
C(4)-C(5)-H(5)	119.9
C(5)-C(6)-C(7)	120.5(2)
C(5)-C(6)-H(6)	119.8
C(7)-C(6)-H(6)	119.8
C(8)-C(7)-C(6)	120.0(2)

C(8)-C(7)-H(7)	120.0
C(6)-C(7)-H(7)	120.0
C(7)-C(8)-C(9)	120.1(2)
C(7)-C(8)-H(8)	119.9
C(9)-C(8)-H(8)	119.9
C(4)-C(9)-C(8)	120.0(2)
C(4)-C(9)-H(9)	120.0
C(8)-C(9)-H(9)	120.0
C(11)-C(10)-C(2)	127.68(18)
C(11)-C(10)-S(1)	111.02(15)
C(2)-C(10)-S(1)	121.27(15)
C(10)-C(11)-C(12)	111.62(19)
C(10)-C(11)-H(11)	124.2
C(12)-C(11)-H(11)	124.2
C(13)-C(12)-C(11)	113.3(2)
C(13)-C(12)-H(12)	123.4
C(11)-C(12)-H(12)	123.4
C(12)-C(13)-S(1)	112.07(16)
C(12)-C(13)-H(13)	124.0
S(1)-C(13)-H(13)	124.0
C(3)-C(14)-S(2)	120.27(15)
C(3)-C(14)-C(15')	120.27(15)
C(3)-C(14)-C(15)	125.21(15)
S(2)-C(14)-C(15)	114.37(12)
C(3)-C(14)-S(2')	125.21(15)
C(15')-C(14)-S(2')	114.37(12)
C(17)-C(16)-C(15)	116.25(19)
C(17)-C(16)-S(2')	116.25(19)
C(17)-C(16)-H(16)	121.9
C(15)-C(16)-H(16)	121.9
C(16)-C(17)-S(2)	116.47(18)
C(16)-C(17)-C(15')	116.47(18)
C(16)-C(17)-H(17)	121.8
S(2)-C(17)-H(17)	121.8

Symmetry transformations used to generate equivalent atoms:

Table S20. Anisotropic displacement parameters ($Å^2$x 10^3)for i18116. 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}
S(1)	26(1)	29(1)	19(1)	-3(1)	8(1)	4(1)
S(2)	36(1)	23(1)	23(1)	4(1)	-1(1)	2(1)
C(15)	32(1)	36(1)	32(1)	8(1)	4(1)	8(1)
S(2')	32(1)	36(1)	32(1)	8(1)	4(1)	8(1)
C(15')	36(1)	23(1)	23(1)	4(1)	-1(1)	2(1)
N(1)	18(1)	18(1)	12(1)	1(1)	5(1)	1(1)
N(2)	18(1)	16(1)	12(1)	-1(1)	3(1)	-1(1)
C(1)	17(1)	16(1)	12(1)	-2(1)	4(1)	-4(1)
C(2)	17(1)	18(1)	14(1)	-3(1)	4(1)	0(1)
C(3)	18(1)	17(1)	13(1)	-3(1)	4(1)	-1(1)
C(4)	17(1)	19(1)	12(1)	-4(1)	3(1)	-1(1)
C(5)	21(1)	26(1)	16(1)	-1(1)	5(1)	-2(1)
C(6)	19(1)	40(1)	26(1)	-5(1)	9(1)	-4(1)
C(7)	21(1)	38(1)	30(1)	-9(1)	4(1)	8(1)
C(8)	31(1)	23(1)	23(1)	-1(1)	3(1)	8(1)
C(9)	24(1)	20(1)	18(1)	-1(1)	7(1)	1(1)
C(10)	24(1)	18(1)	14(1)	0(1)	7(1)	2(1)
C(11)	26(1)	27(1)	22(1)	-2(1)	13(1)	0(1)
C(12)	24(1)	28(1)	32(1)	-1(1)	14(1)	-1(1)
C(13)	33(1)	23(1)	25(1)	0(1)	15(1)	4(1)
C(14)	22(1)	18(1)	14(1)	-2(1)	3(1)	1(1)
C(16)	29(1)	31(1)	36(1)	-10(1)	-6(1)	11(1)
C(17)	44(1)	22(1)	18(1)	1(1)	0(1)	-6(1)

Crystal data and structure refinement for compound **3z**

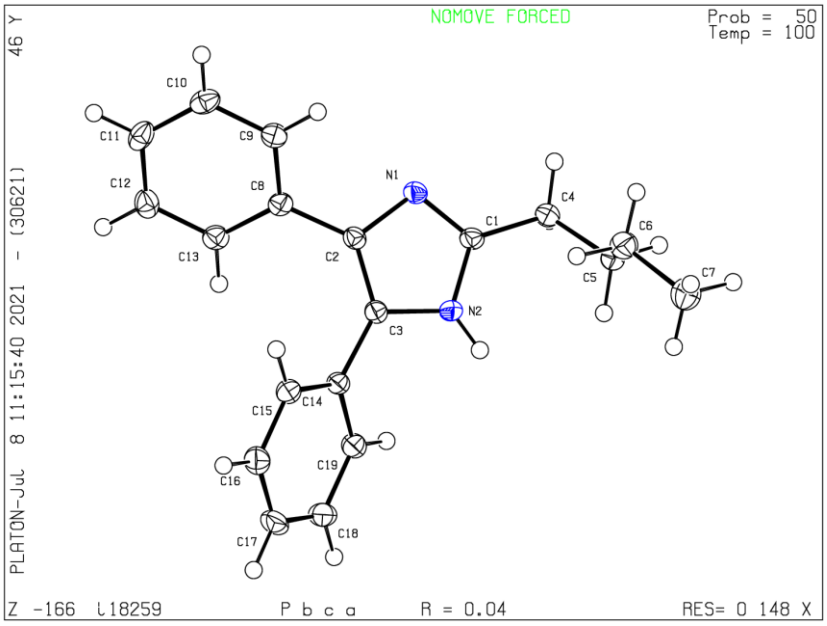


Figure S6. Single X-ray crystal structure of imidazole **3z** (the thermal ellipsoid was drawn at the 50% probability level)

Table S21. Crystal data and structure refinement for i18259.

CCDC	2098033	
Identification code	i18259	
Empirical formula	C19 H20 N2	
Formula weight	276.37	
Temperature	100.0(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P b c a	
Unit cell dimensions	a = 16.5878(5) Å	α= 90°.
	b = 9.2549(3) Å	β= 90°.
	c = 20.0075(6) Å	γ = 90°.
Volume	3071.52(16) $Å^3$	
Z	8	
Density (calculated)	1.195 Mg/m^3	
Absorption coefficient	0.070 mm^{-1}	
F(000)	1184	
Crystal size	0.317 x 0.169 x 0.167 mm^3	
Theta range for data collection	2.036 to 27.101°.	
Index ranges	-21<=h<=21, -11<=k<=11, -25<=l<=25	
Reflections collected	61188	
Independent reflections	3375 [R(int) = 0.0853]	

Completeness to theta = 25.242°	100.0 %
Absorption correction	Numerical
Max. and min. transmission	1 and 0.8011
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3375 / 0 / 191
Goodness-of-fit on F^2	1.056
Final R indices [I>2sigma(I)]	R1 = 0.0398, wR2 = 0.0900
R indices (all data)	R1 = 0.0529, wR2 = 0.0972
Extinction coefficient	n/a
Largest diff. peak and hole	0.240 and -0.210 e.$Å^{-3}$

Table S22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for i18259. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	3099(1)	6079(1)	2710(1)	18(1)
N(2)	2590(1)	3912(1)	2893(1)	18(1)
C(1)	2505(1)	5176(1)	2563(1)	18(1)
C(2)	3585(1)	5355(1)	3165(1)	17(1)
C(3)	3279(1)	3998(1)	3281(1)	17(1)
C(4)	1789(1)	5538(1)	2141(1)	21(1)
C(5)	1495(1)	4318(1)	1688(1)	21(1)
C(6)	2083(1)	3931(2)	1132(1)	27(1)
C(7)	1795(1)	2644(2)	721(1)	34(1)
C(8)	4276(1)	6111(1)	3471(1)	18(1)
C(9)	4732(1)	7083(1)	3093(1)	21(1)
C(10)	5367(1)	7840(1)	3379(1)	24(1)
C(11)	5560(1)	7632(2)	4046(1)	25(1)
C(12)	5109(1)	6679(1)	4428(1)	24(1)
C(13)	4470(1)	5929(1)	4146(1)	21(1)
C(14)	3537(1)	2754(1)	3684(1)	18(1)
C(15)	4348(1)	2343(1)	3715(1)	21(1)
C(16)	4576(1)	1109(2)	4061(1)	26(1)
C(17)	4000(1)	265(2)	4381(1)	28(1)
C(18)	3198(1)	677(2)	4362(1)	25(1)
C(19)	2966(1)	1915(1)	4020(1)	21(1)

Table S23. Bond lengths [Å] and angles [°] for i18259.

N(1)-C(1)	1.3252(17)
N(1)-C(2)	1.3889(16)
N(2)-C(1)	1.3501(16)
N(2)-C(3)	1.3831(16)
N(2)-H(2)	0.8800
C(1)-C(4)	1.4960(18)
C(2)-C(3)	1.3748(17)
C(2)-C(8)	1.4746(18)
C(3)-C(14)	1.4697(17)
C(4)-C(5)	1.5278(18)
C(4)-H(4A)	0.9900
C(4)-H(4AB)	0.9900
C(5)-C(6)	1.521(2)
C(5)-H(5A)	0.9900
C(5)-H(5AB)	0.9900
C(6)-C(7)	1.524(2)
C(6)-H(6A)	0.9900
C(6)-H(6AB)	0.9900
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-C(13)	1.3983(18)
C(8)-C(9)	1.3984(18)
C(9)-C(10)	1.3885(19)
C(9)-H(9)	0.9500
C(10)-C(11)	1.386(2)
C(10)-H(10)	0.9500
C(11)-C(12)	1.386(2)
C(11)-H(11)	0.9500
C(12)-C(13)	1.3874(19)
C(12)-H(12)	0.9500
C(13)-H(13)	0.9500
C(14)-C(19)	1.3983(19)
C(14)-C(15)	1.3998(19)
C(15)-C(16)	1.3876(18)
C(15)-H(15)	0.9500

C(16)-C(17)	1.390(2)
C(16)-H(16)	0.9500
C(17)-C(18)	1.384(2)
C(17)-H(17)	0.9500
C(18)-C(19)	1.3890(18)
C(18)-H(18)	0.9500
C(19)-H(19)	0.9500

C(1)-N(1)-C(2)	105.83(10)
C(1)-N(2)-C(3)	108.05(11)
C(1)-N(2)-H(2)	126.0
C(3)-N(2)-H(2)	126.0
N(1)-C(1)-N(2)	111.16(11)
N(1)-C(1)-C(4)	125.05(11)
N(2)-C(1)-C(4)	123.56(12)
C(3)-C(2)-N(1)	109.61(11)
C(3)-C(2)-C(8)	130.63(11)
N(1)-C(2)-C(8)	119.63(11)
C(2)-C(3)-N(2)	105.34(11)
C(2)-C(3)-C(14)	134.39(12)
N(2)-C(3)-C(14)	120.25(11)
C(1)-C(4)-C(5)	114.98(11)
C(1)-C(4)-H(4A)	108.5
C(5)-C(4)-H(4A)	108.5
C(1)-C(4)-H(4AB)	108.5
C(5)-C(4)-H(4AB)	108.5
H(4A)-C(4)-H(4AB)	107.5
C(6)-C(5)-C(4)	113.79(11)
C(6)-C(5)-H(5A)	108.8
C(4)-C(5)-H(5A)	108.8
C(6)-C(5)-H(5AB)	108.8
C(4)-C(5)-H(5AB)	108.8
H(5A)-C(5)-H(5AB)	107.7
C(5)-C(6)-C(7)	112.17(12)
C(5)-C(6)-H(6A)	109.2
C(7)-C(6)-H(6A)	109.2
C(5)-C(6)-H(6AB)	109.2
C(7)-C(6)-H(6AB)	109.2

H(6A)-C(6)-H(6AB)	107.9
C(6)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(6)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(13)-C(8)-C(9)	118.37(12)
C(13)-C(8)-C(2)	121.48(12)
C(9)-C(8)-C(2)	120.08(11)
C(10)-C(9)-C(8)	120.85(13)
C(10)-C(9)-H(9)	119.6
C(8)-C(9)-H(9)	119.6
C(11)-C(10)-C(9)	120.08(13)
C(11)-C(10)-H(10)	120.0
C(9)-C(10)-H(10)	120.0
C(10)-C(11)-C(12)	119.70(13)
C(10)-C(11)-H(11)	120.2
C(12)-C(11)-H(11)	120.2
C(11)-C(12)-C(13)	120.43(13)
C(11)-C(12)-H(12)	119.8
C(13)-C(12)-H(12)	119.8
C(12)-C(13)-C(8)	120.55(13)
C(12)-C(13)-H(13)	119.7
C(8)-C(13)-H(13)	119.7
C(19)-C(14)-C(15)	118.59(12)
C(19)-C(14)-C(3)	120.12(12)
C(15)-C(14)-C(3)	121.23(12)
C(16)-C(15)-C(14)	120.52(13)
C(16)-C(15)-H(15)	119.7
C(14)-C(15)-H(15)	119.7
C(15)-C(16)-C(17)	120.34(13)
C(15)-C(16)-H(16)	119.8
C(17)-C(16)-H(16)	119.8
C(18)-C(17)-C(16)	119.57(13)
C(18)-C(17)-H(17)	120.2
C(16)-C(17)-H(17)	120.2
C(17)-C(18)-C(19)	120.45(13)

C(17)-C(18)-H(18)	119.8
C(19)-C(18)-H(18)	119.8
C(18)-C(19)-C(14)	120.51(13)
C(18)-C(19)-H(19)	119.7
C(14)-C(19)-H(19)	119.7

Symmetry transformations used to generate equivalent atoms:

Table S24. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for i18259. 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}
N(1)	21(1)	15(1)	19(1)	0(1)	-1(1)	2(1)
N(2)	19(1)	14(1)	21(1)	1(1)	-2(1)	0(1)
C(1)	22(1)	14(1)	19(1)	0(1)	-1(1)	2(1)
C(2)	19(1)	16(1)	16(1)	0(1)	-1(1)	2(1)
C(3)	19(1)	16(1)	17(1)	-1(1)	-1(1)	2(1)
C(4)	22(1)	17(1)	25(1)	2(1)	-4(1)	2(1)
C(5)	22(1)	18(1)	24(1)	3(1)	-4(1)	-1(1)
C(6)	31(1)	25(1)	24(1)	0(1)	-1(1)	-2(1)
C(7)	44(1)	31(1)	28(1)	-5(1)	-4(1)	-1(1)
C(8)	18(1)	14(1)	22(1)	-2(1)	0(1)	3(1)
C(9)	21(1)	19(1)	23(1)	0(1)	0(1)	2(1)
C(10)	21(1)	18(1)	34(1)	-1(1)	3(1)	0(1)
C(11)	21(1)	20(1)	35(1)	-8(1)	-4(1)	1(1)
C(12)	27(1)	23(1)	22(1)	-5(1)	-5(1)	6(1)
C(13)	24(1)	17(1)	22(1)	-2(1)	1(1)	2(1)
C(14)	24(1)	14(1)	16(1)	-2(1)	-2(1)	1(1)
C(15)	25(1)	17(1)	21(1)	-2(1)	-2(1)	1(1)
C(16)	29(1)	20(1)	28(1)	-4(1)	-7(1)	6(1)
C(17)	41(1)	17(1)	25(1)	2(1)	-7(1)	5(1)
C(18)	36(1)	19(1)	22(1)	2(1)	-1(1)	-2(1)
C(19)	23(1)	20(1)	20(1)	0(1)	-1(1)	1(1)

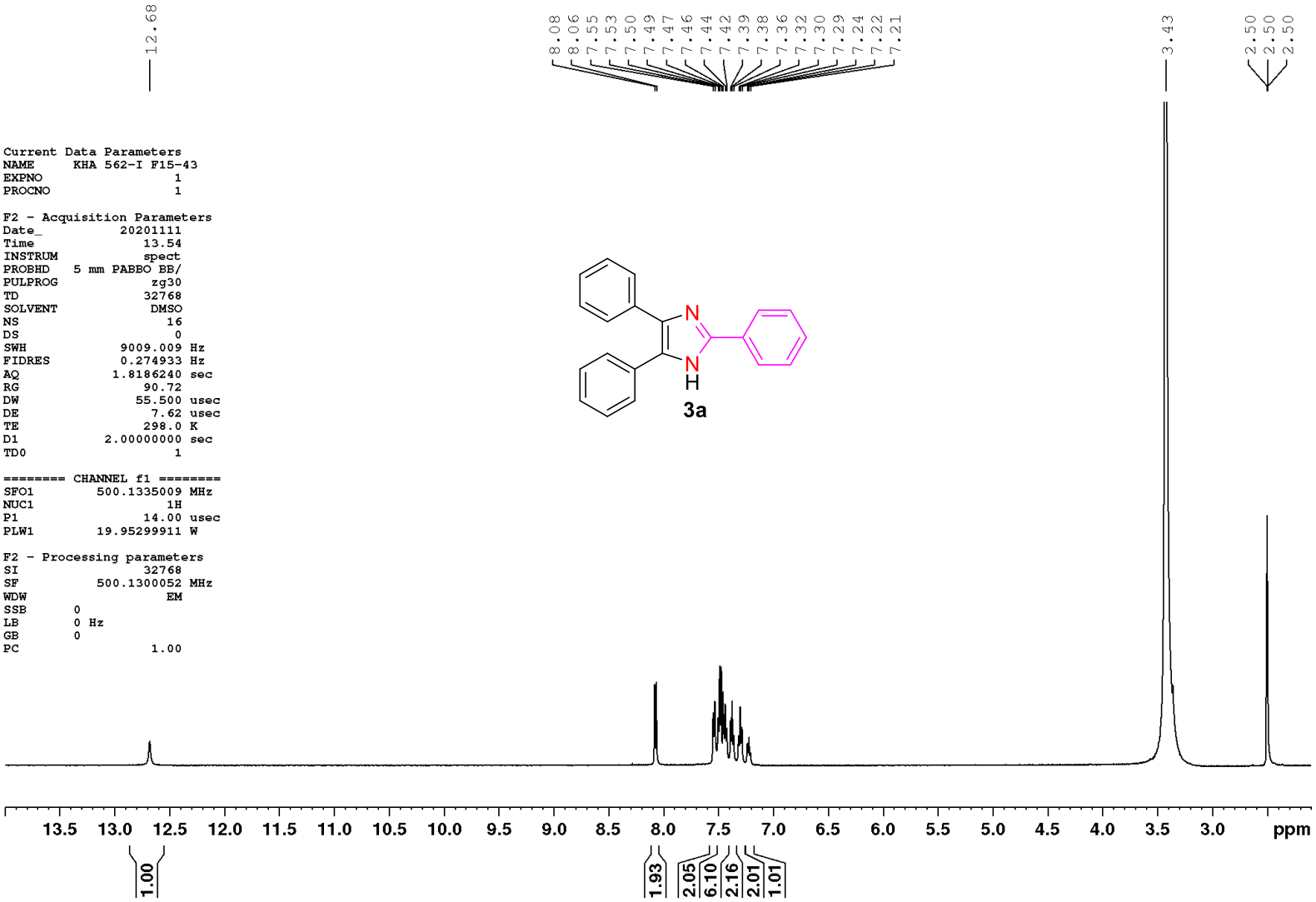


Figure S6. ^{1}H NMR spectrum of compound **3a** (500 MHz, DMSO-d_6, 25 ^{o}C)

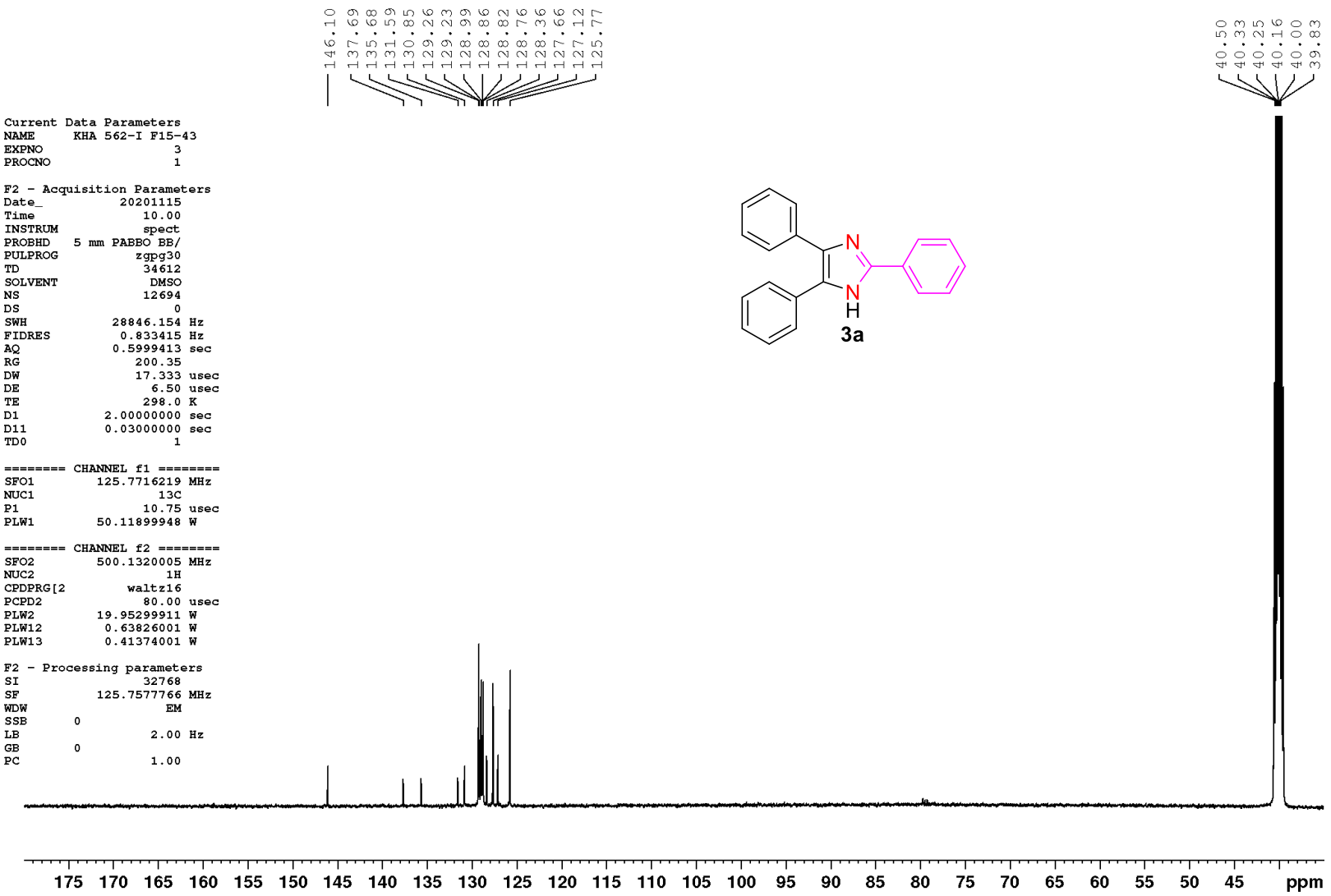


Figure S7. ^{13}C NMR spectrum of compound **3a** (125 MHz, DMSO-d_6, 25 ^{o}C)

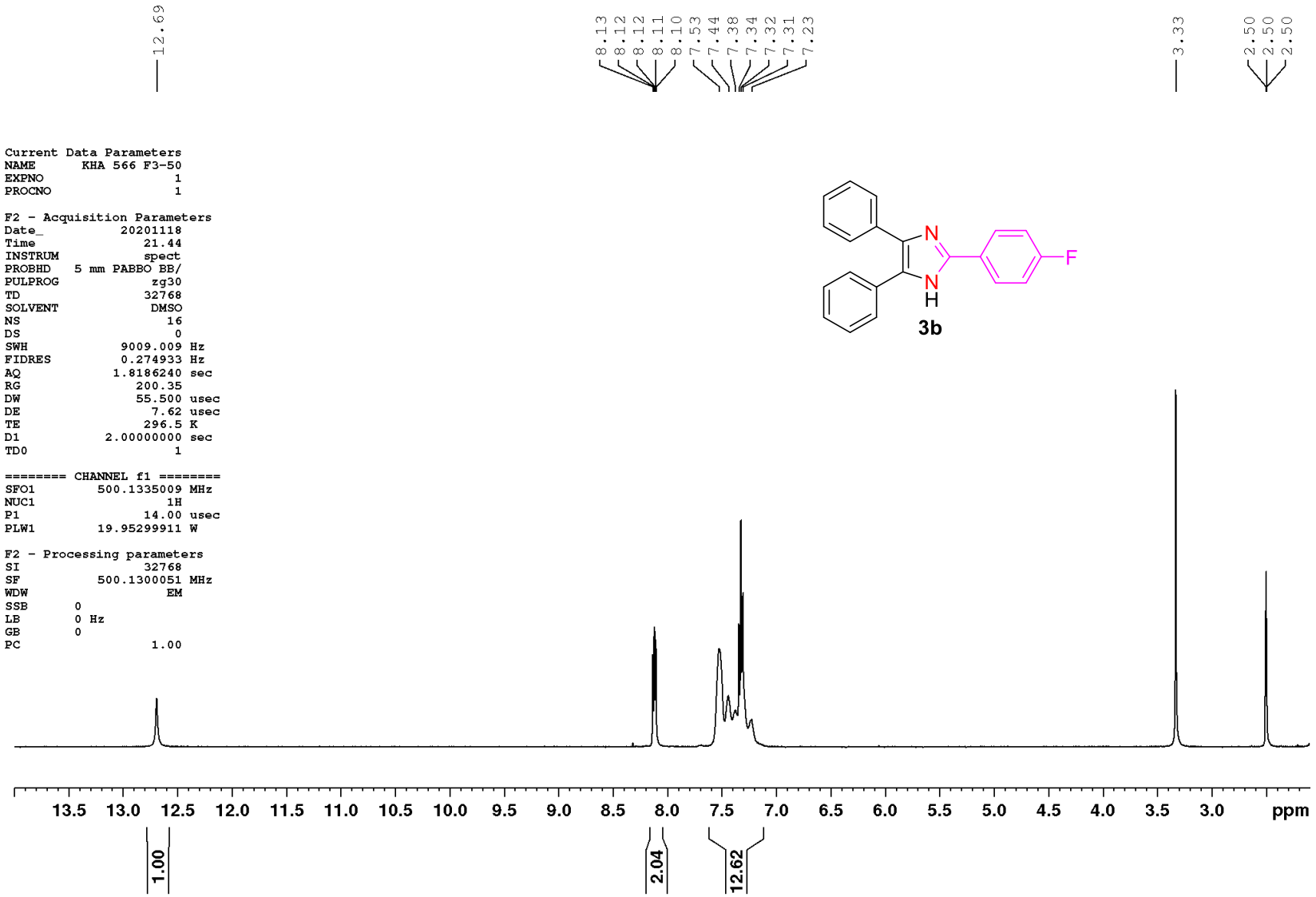


Figure S8. ^{1}H NMR spectrum of compound **3b** (500 MHz, DMSO-d_6, 25 ^{o}C)

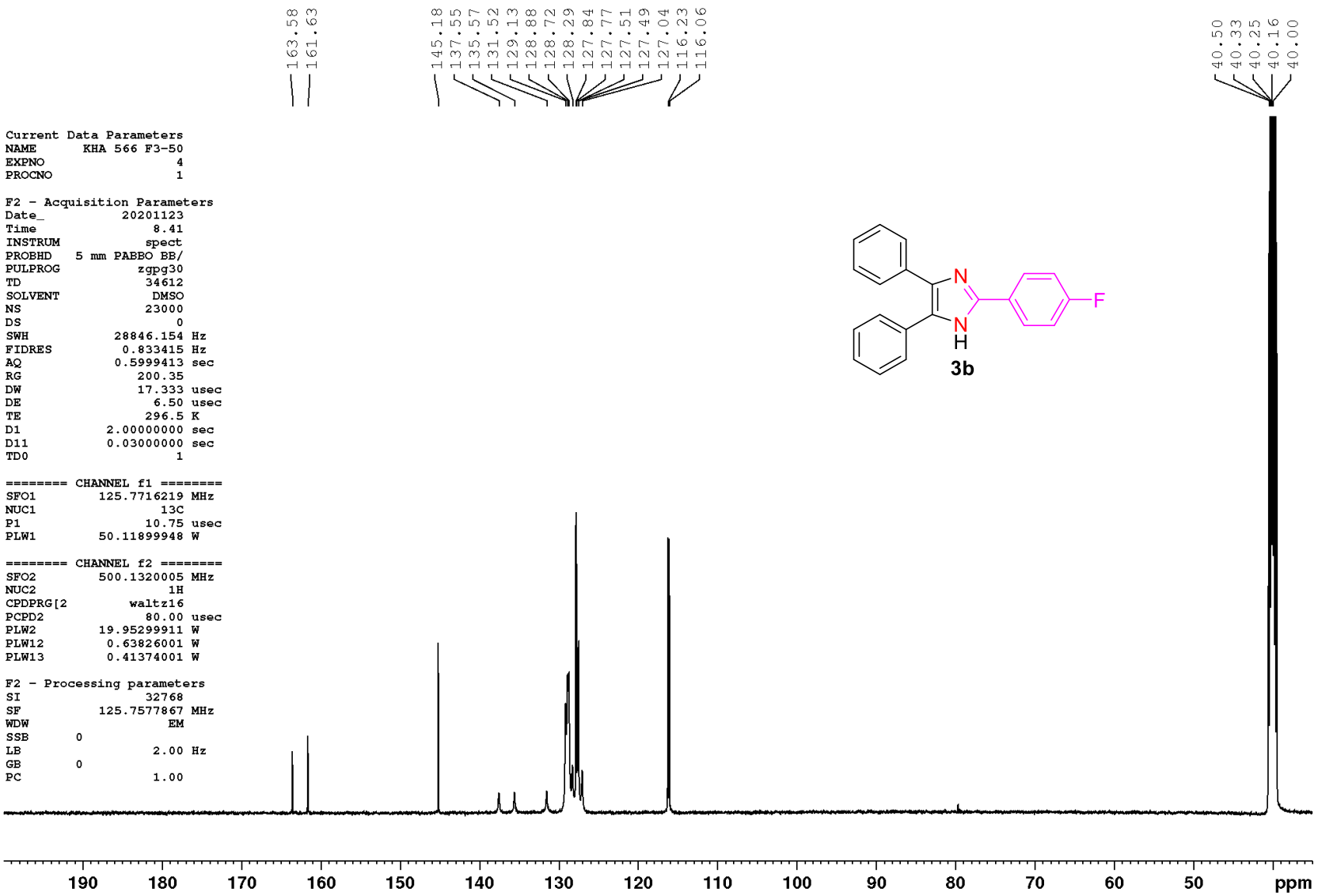


Figure S9. ^{13}C NMR spectrum of compound **3b** (125 MHz, DMSO-d_6, 25 ^{o}C)

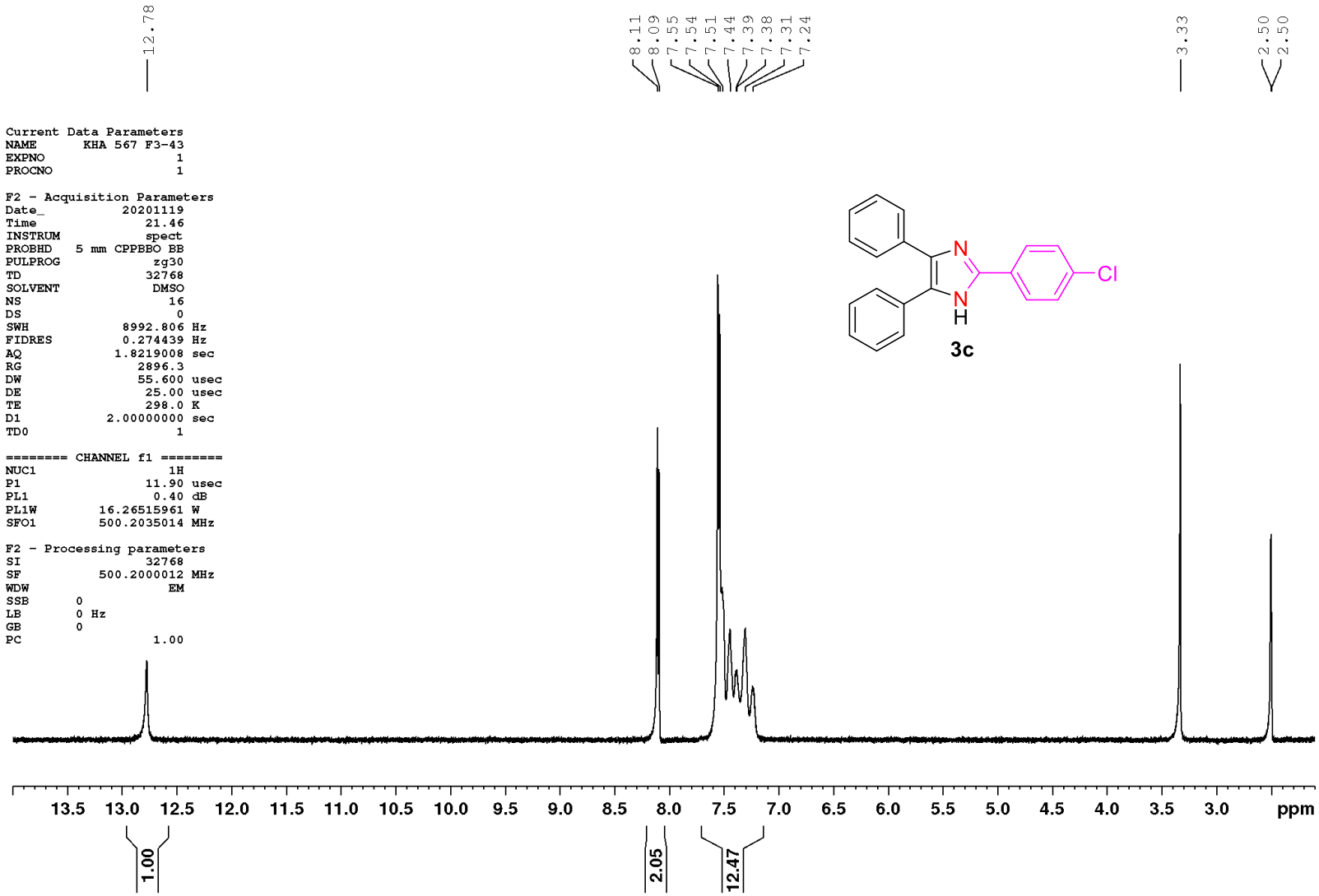


Figure S10. ^{1}H NMR spectrum of compound **3c** (500 MHz, DMSO-d_6, 25 ^{o}C)

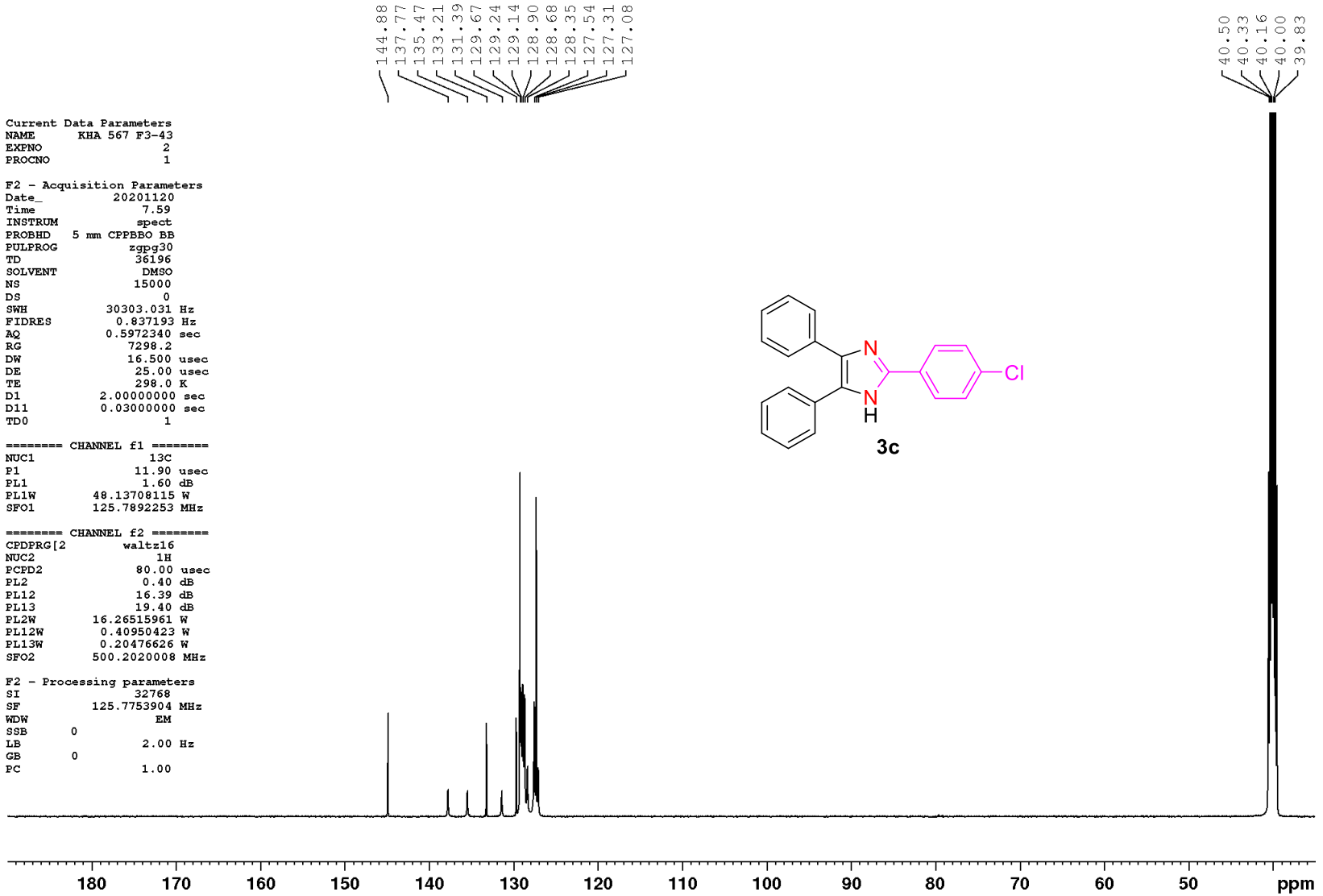


Figure S11. ^{13}C NMR spectrum of compound **3c** (125 MHz, DMSO-d_6, 25 ^{o}C)

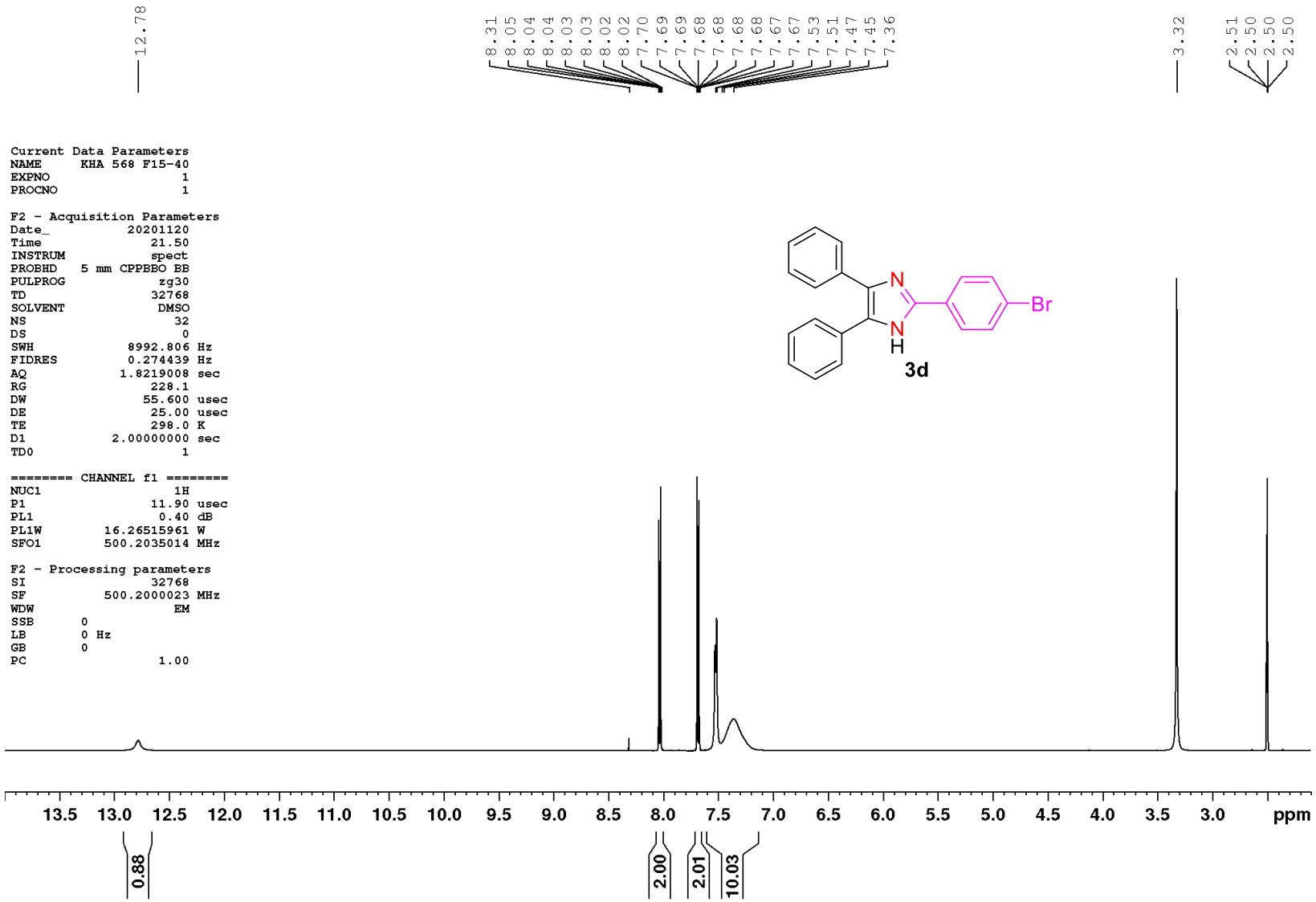


Figure S12. ^{1}H NMR spectrum of compound **3d** (500 MHz, DMSO-d_6, 25 ^{o}C)

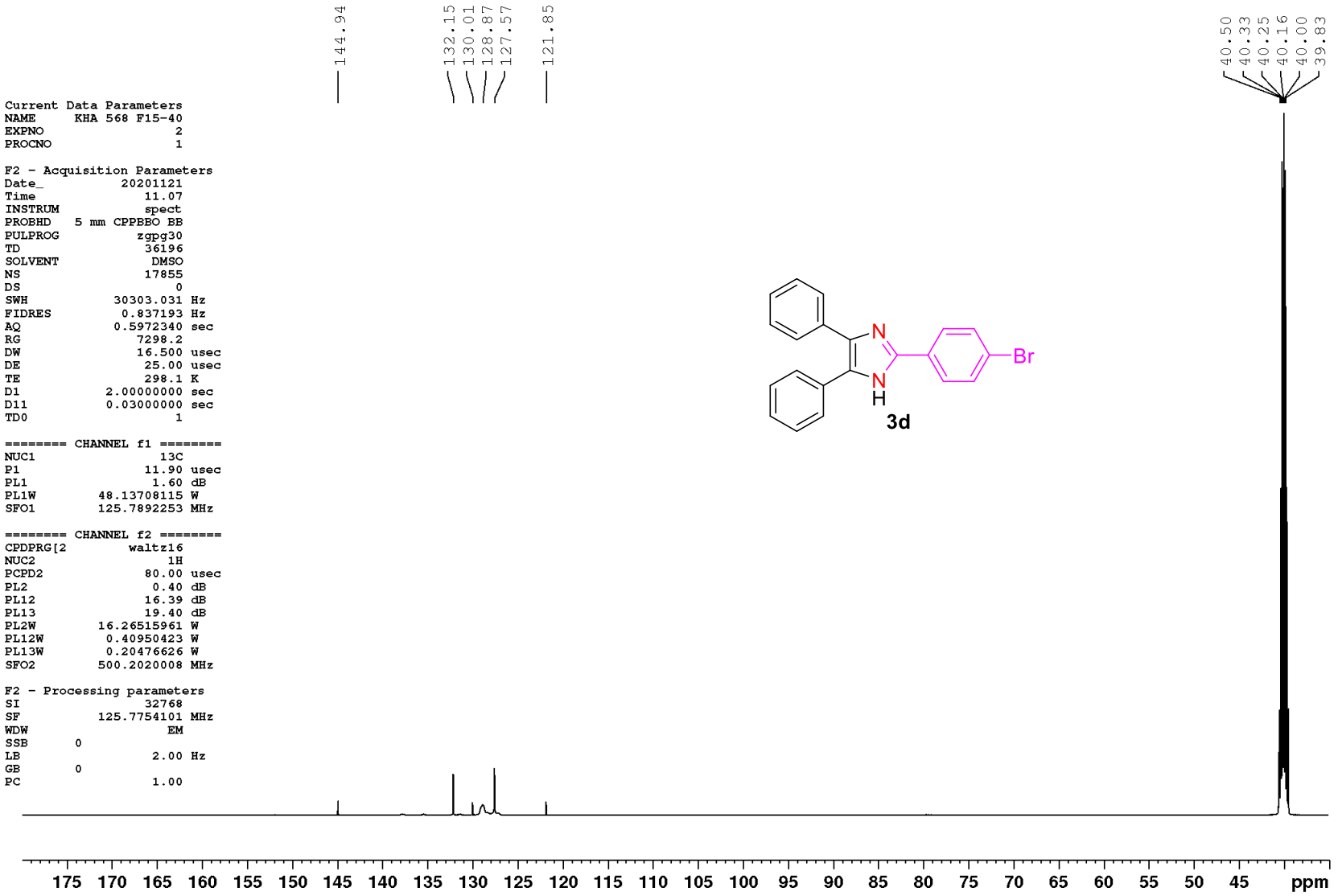


Figure S13. ^{13}C NMR spectrum of compound **3d** (125 MHz, DMSO-d_6, 25 ^{o}C)

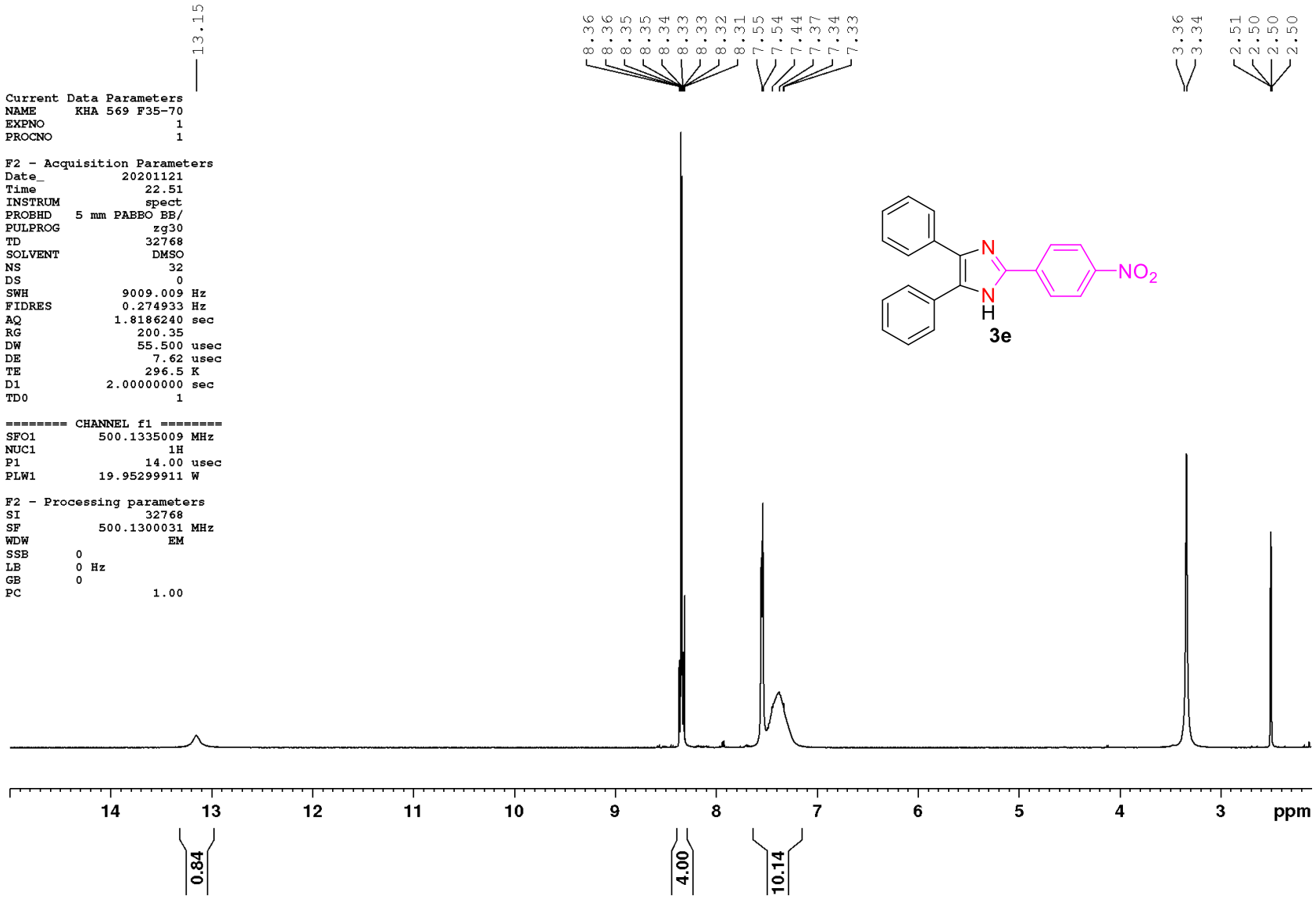


Figure S14. ^{1}H NMR spectrum of compound **3e** (500 MHz, DMSO-d_6, 25 ^{o}C)

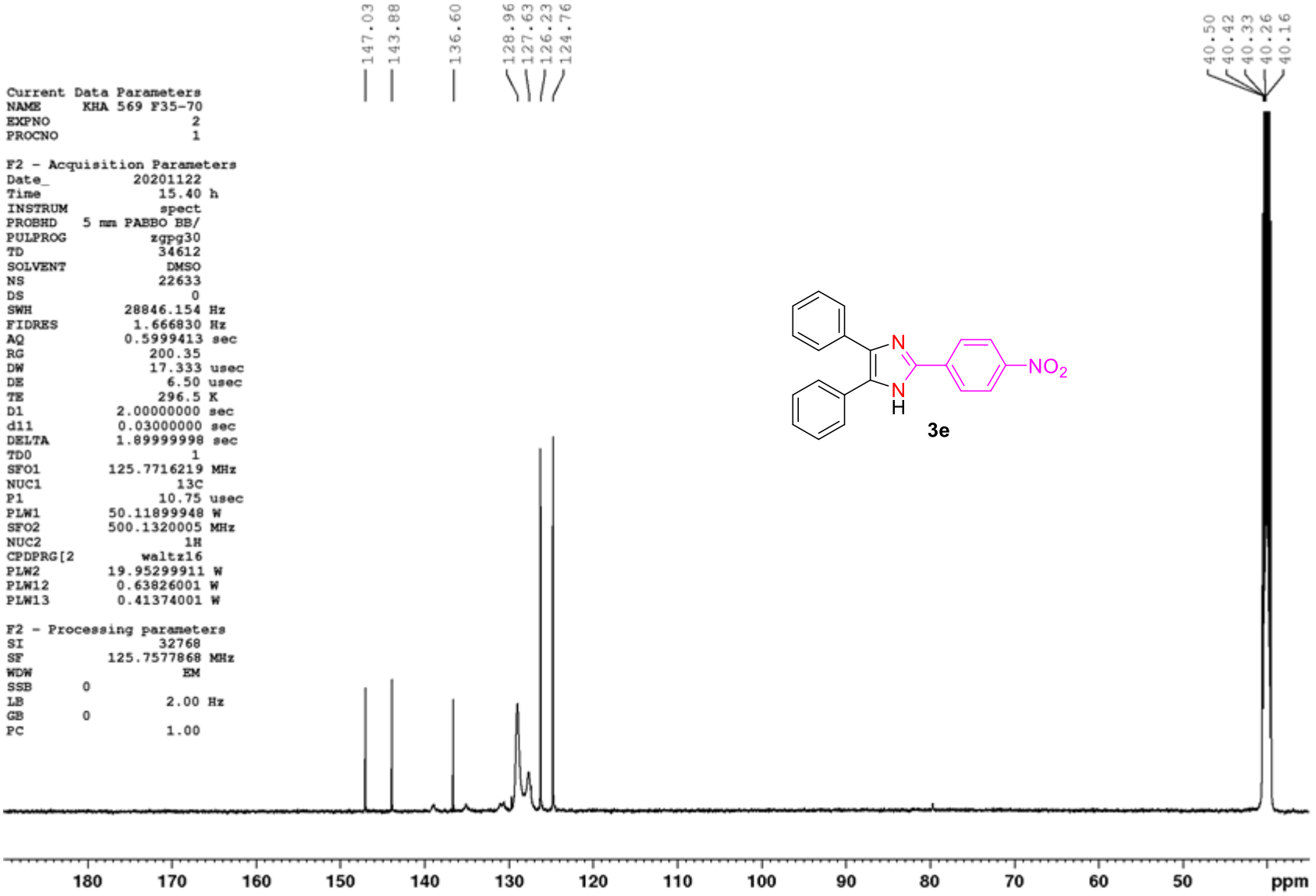


Figure S15. ^{13}C NMR spectrum of compound **3e** (125 MHz, DMSO-d_6, 25 ^{o}C)

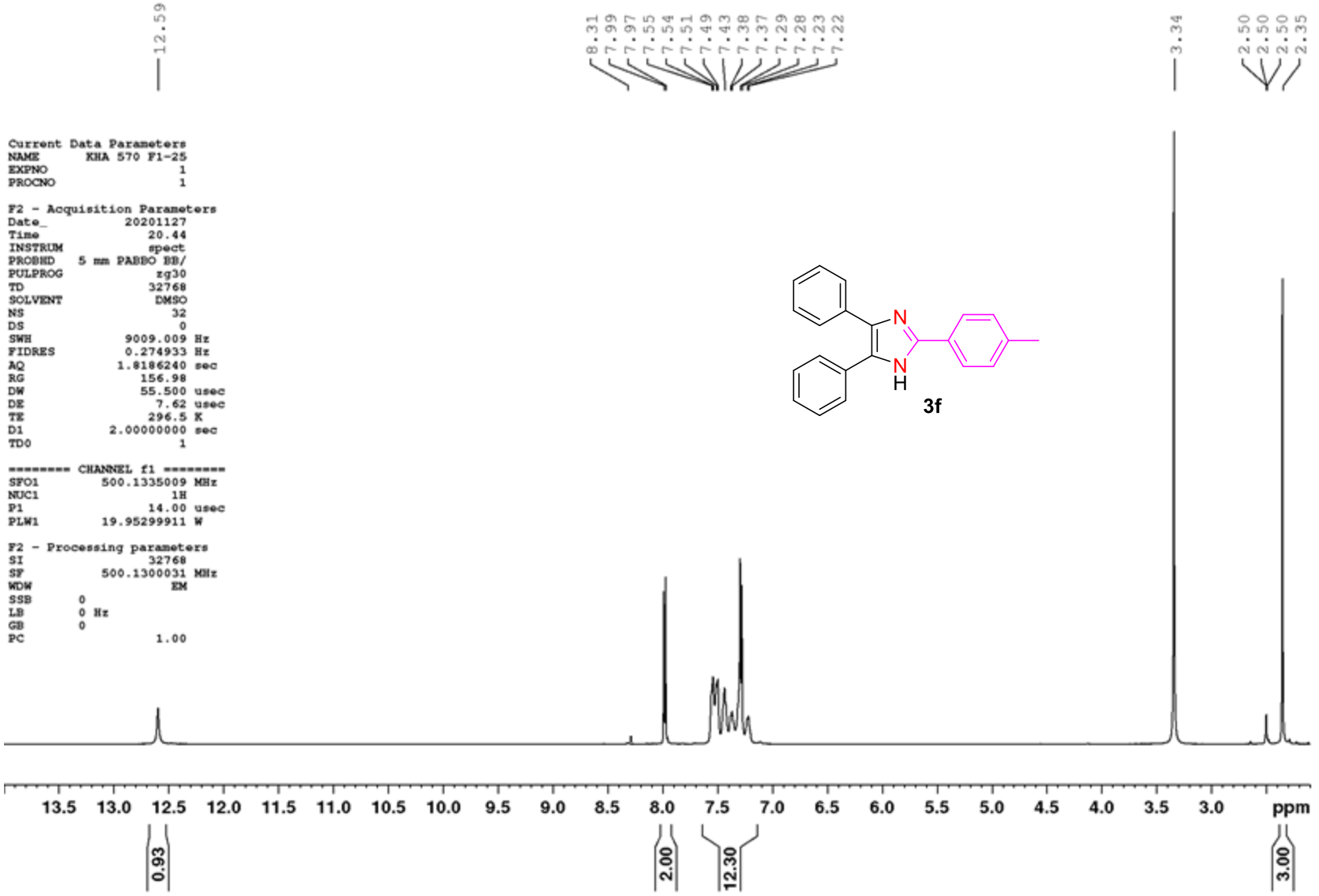
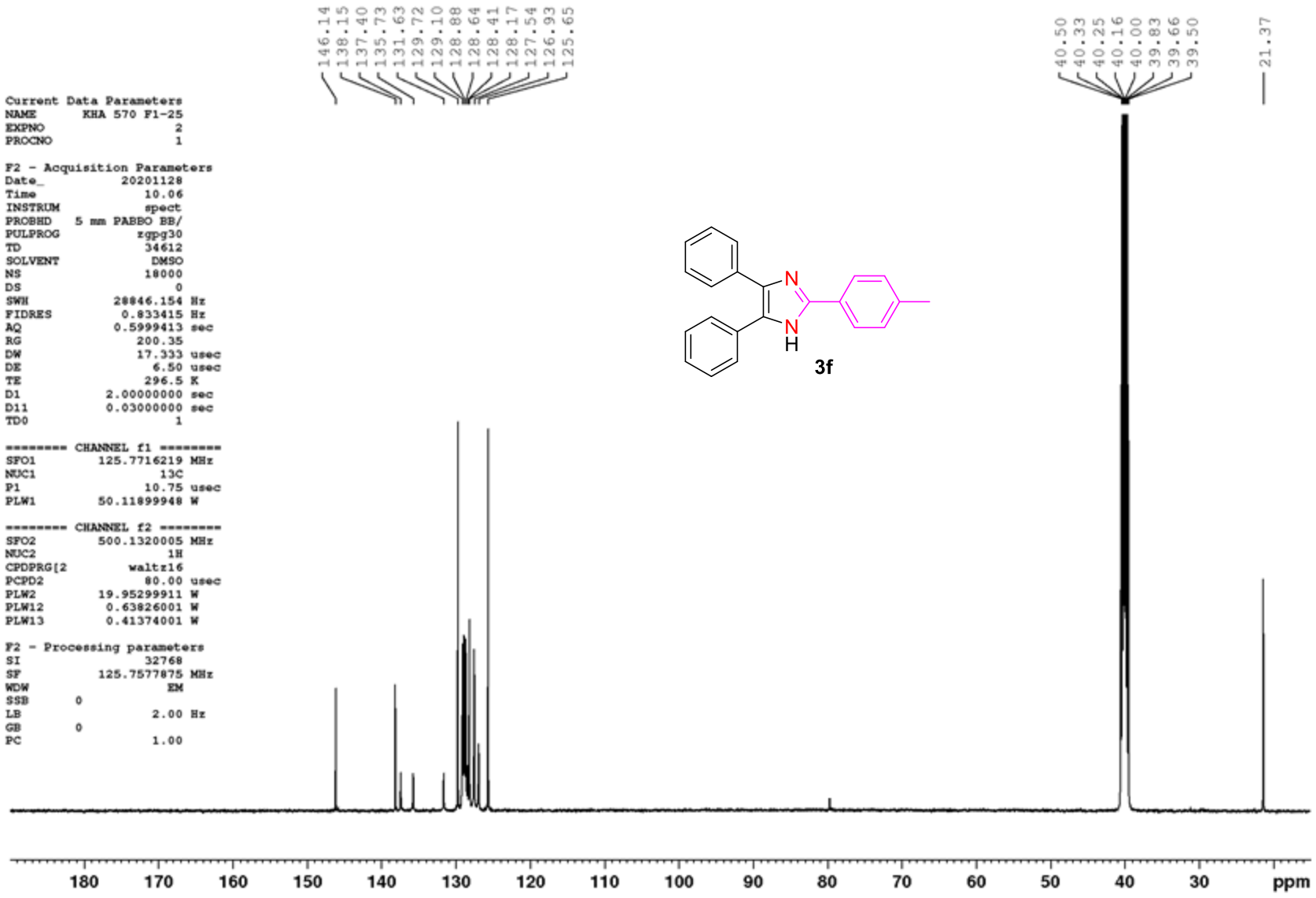


Figure S16. ^{1}H NMR spectrum of compound **3f** (500 MHz, DMSO-d_6, 25 ^{o}C)

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PROCNO                1

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SWH          28846.154 Hz
FIDRES         0.833415 Hz
AQ             0.5999413 sec
RG                200.35
DW               17.333 usec
DE                 6.50 usec
TE                296.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

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NUC1                13C
P1                10.75 usec
PLW1        50.11899948 W

======== CHANNEL f2 ========
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NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        19.95299911 W
PLW12        0.63826001 W
PLW13        0.41374001 W

F2 - Processing parameters
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WDW                 EM
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Figure S17. ^{13}C NMR spectrum of compound **3f** (125 MHz, DMSO-d_6, 25 ^{o}C)

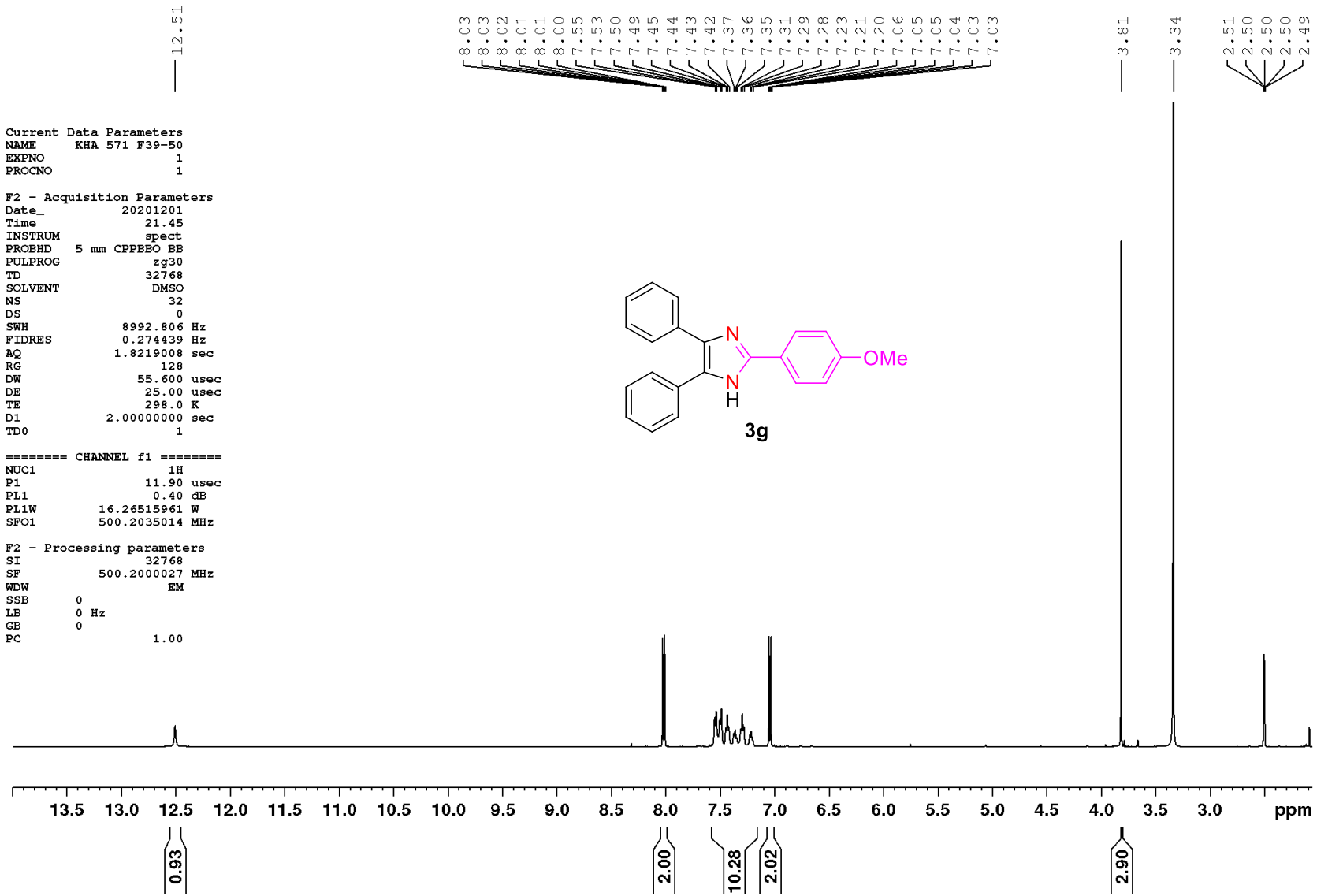


Figure S18. ^{1}H NMR spectrum of compound **3g** (500 MHz, DMSO-d_6, 25 ^{o}C)

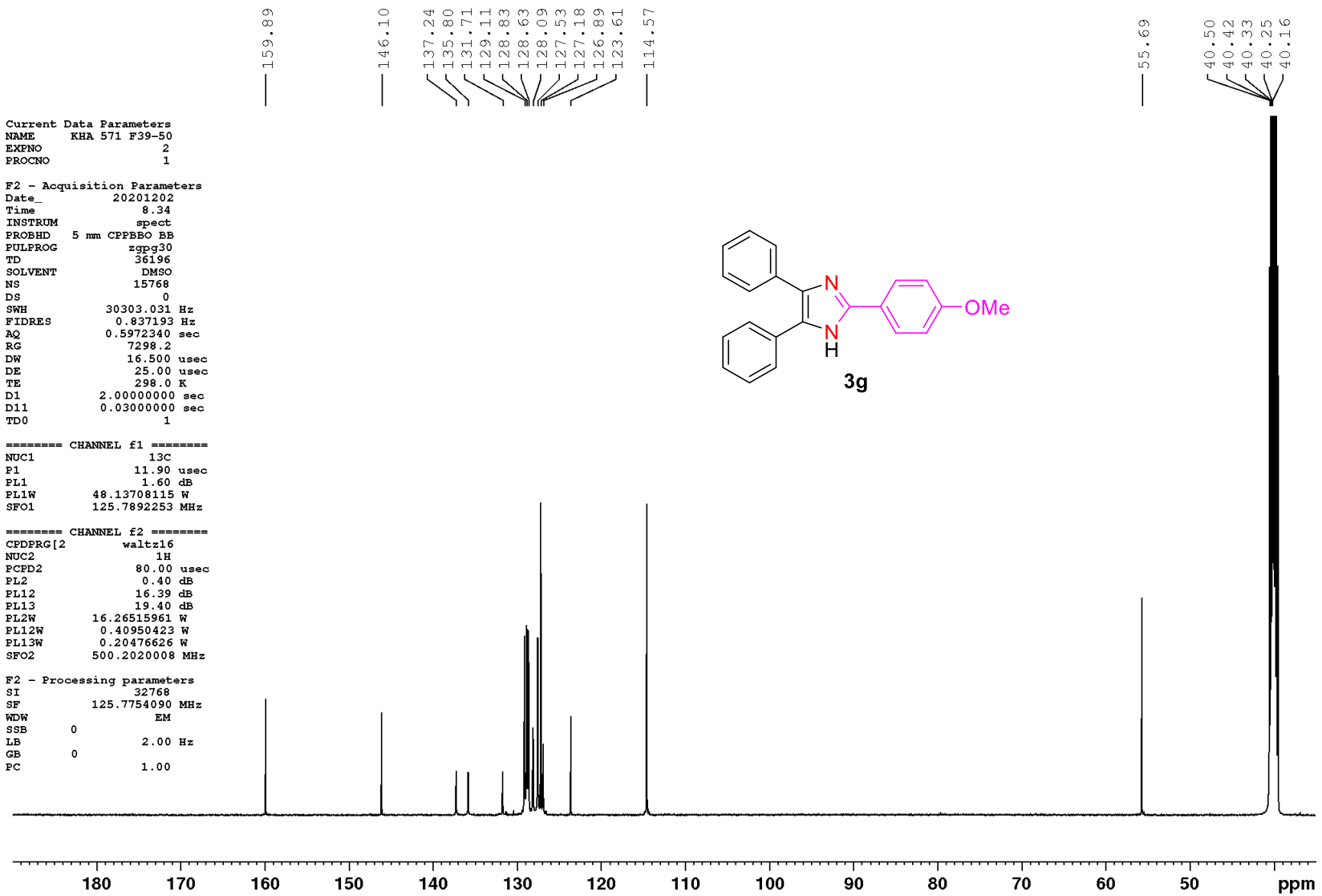


Figure S19. ^{13}C NMR spectrum of compound **3g** (125 MHz, DMSO-d_6, 25 ^{o}C)

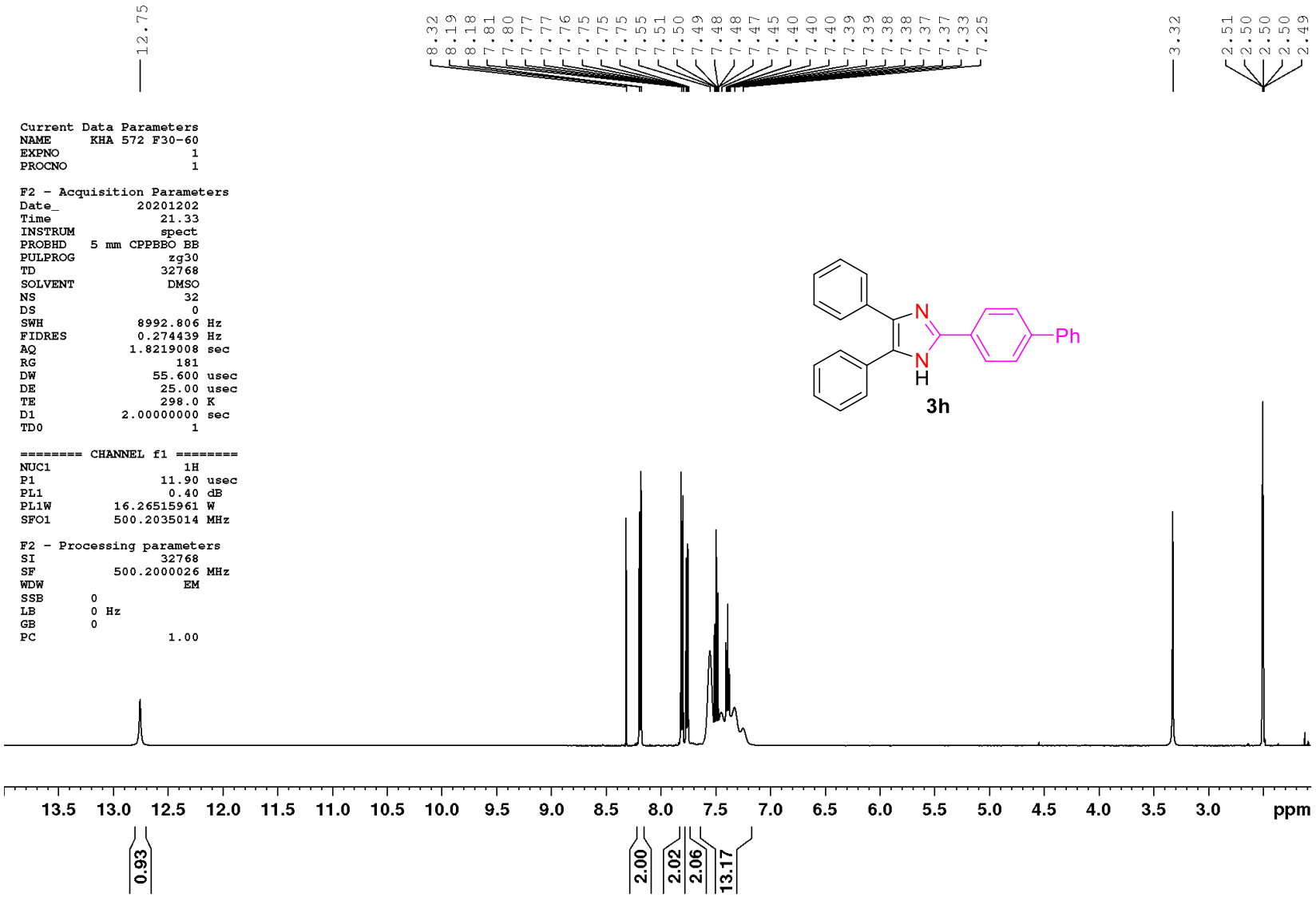


Figure S20. ^{1}H NMR spectrum of compound **3h** (500 MHz, DMSO-d_6, 25 ^{o}C)

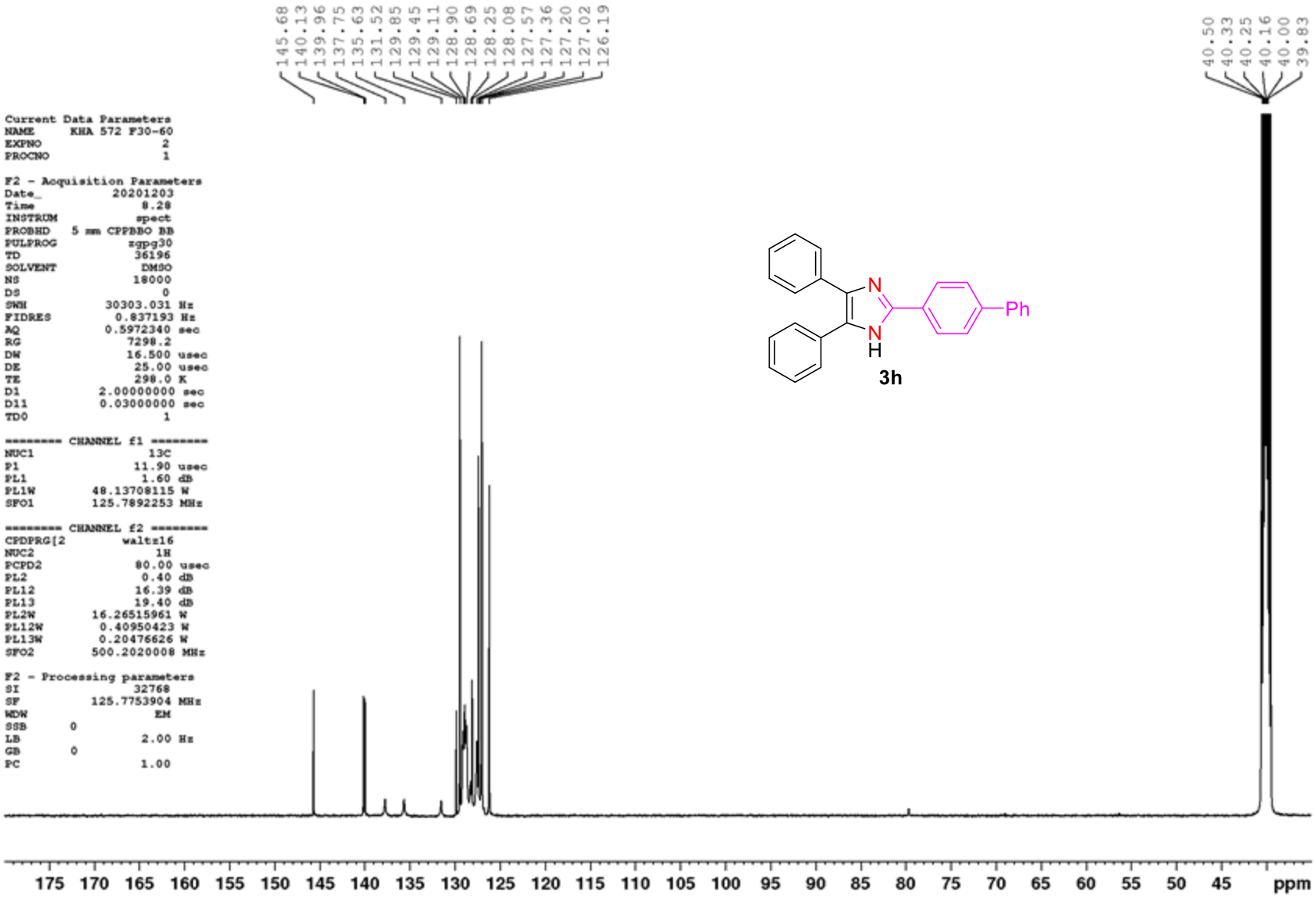


Figure S21. ^{13}C NMR spectrum of compound **3h** (125 MHz, DMSO-d_6, 25 ^{o}C)

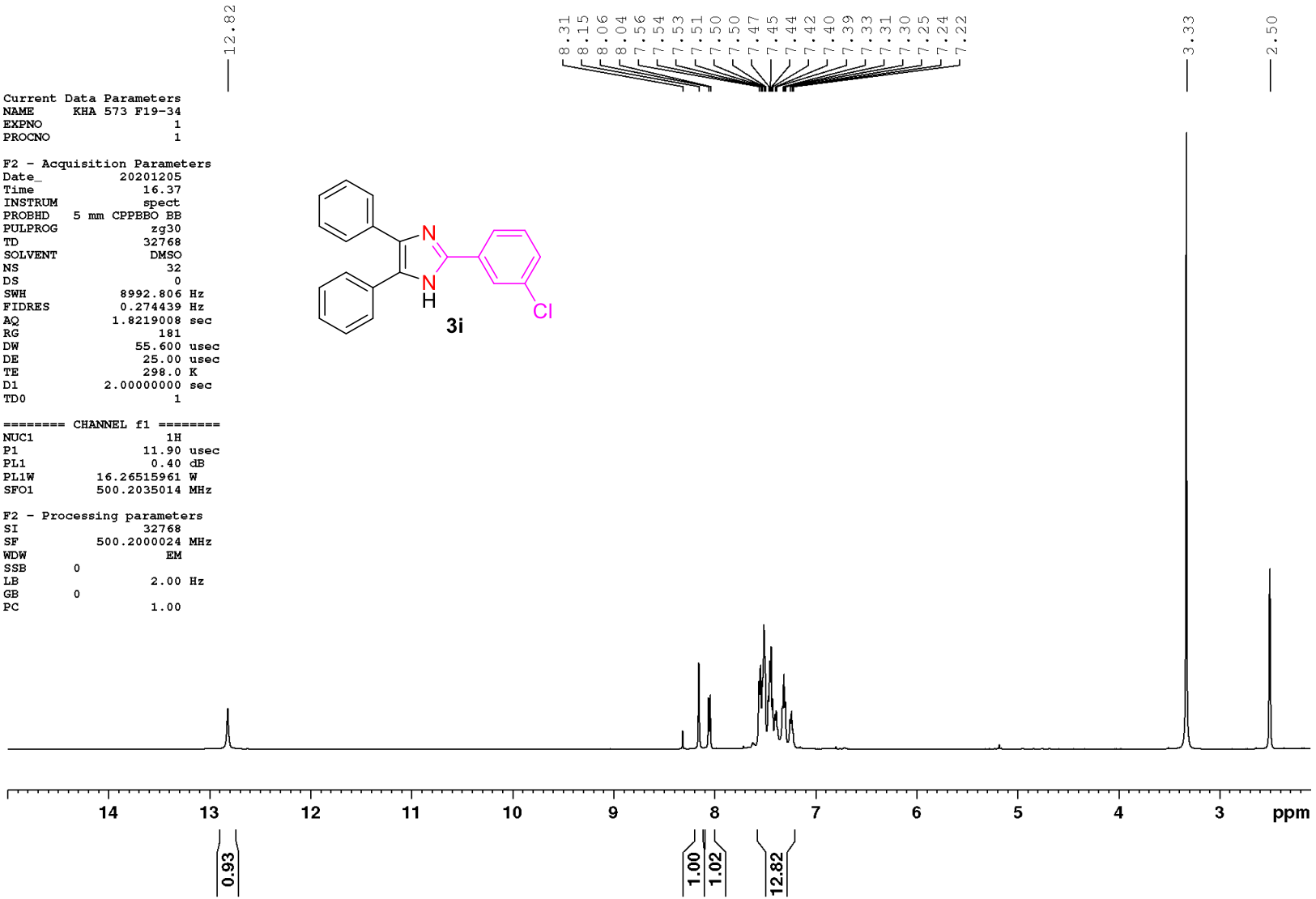


Figure S22. ^{1}H NMR spectrum of compound **3i** (500 MHz, DMSO-d_6, 25 ^{o}C)

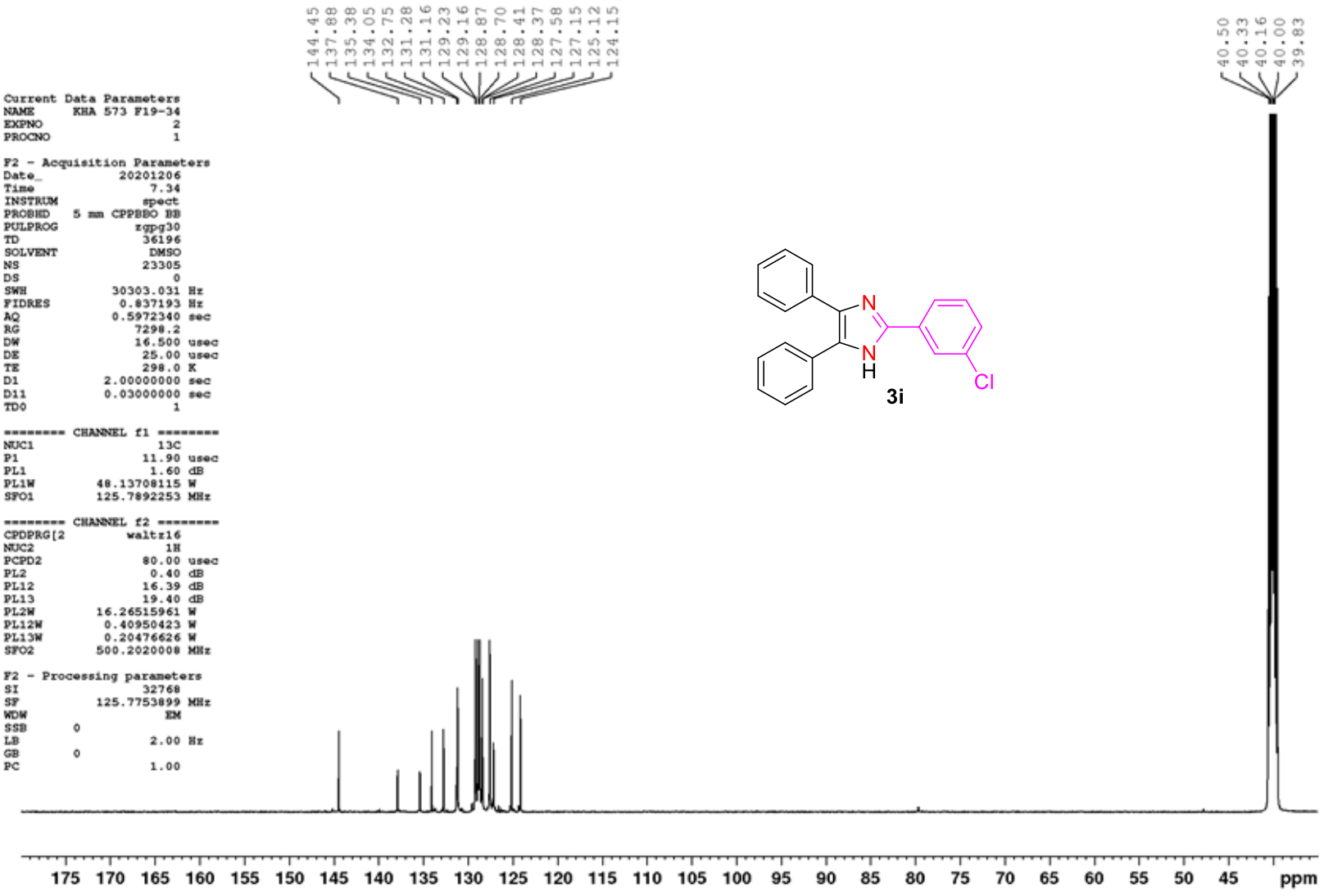


Figure S23. ^{13}C NMR spectrum of compound **3i** (125 MHz, DMSO-d_6, 25 ^{o}C)

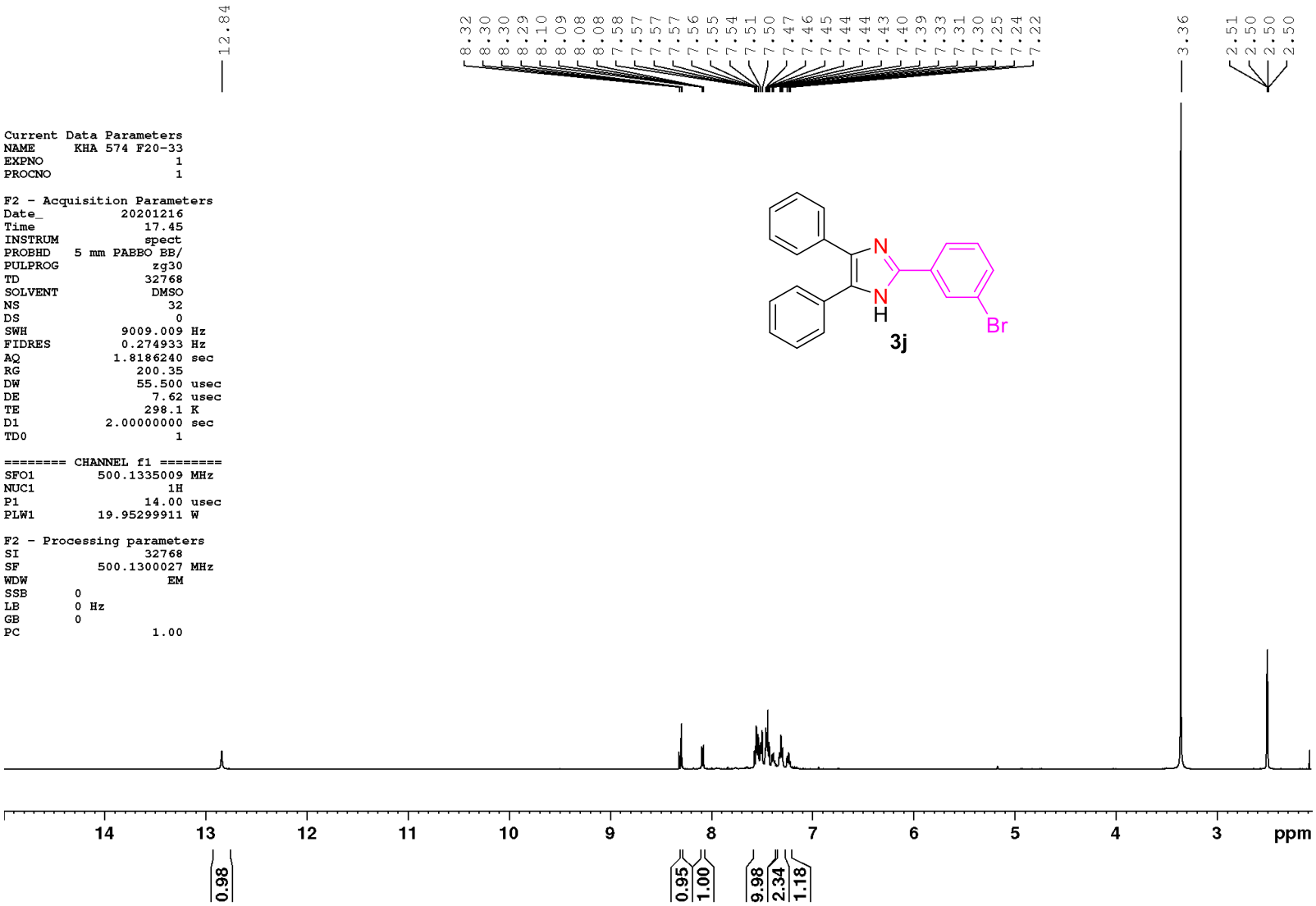


Figure S24. ^{1}H NMR spectrum of compound **3j** (500 MHz, DMSO-d_6, 25 ^{o}C)

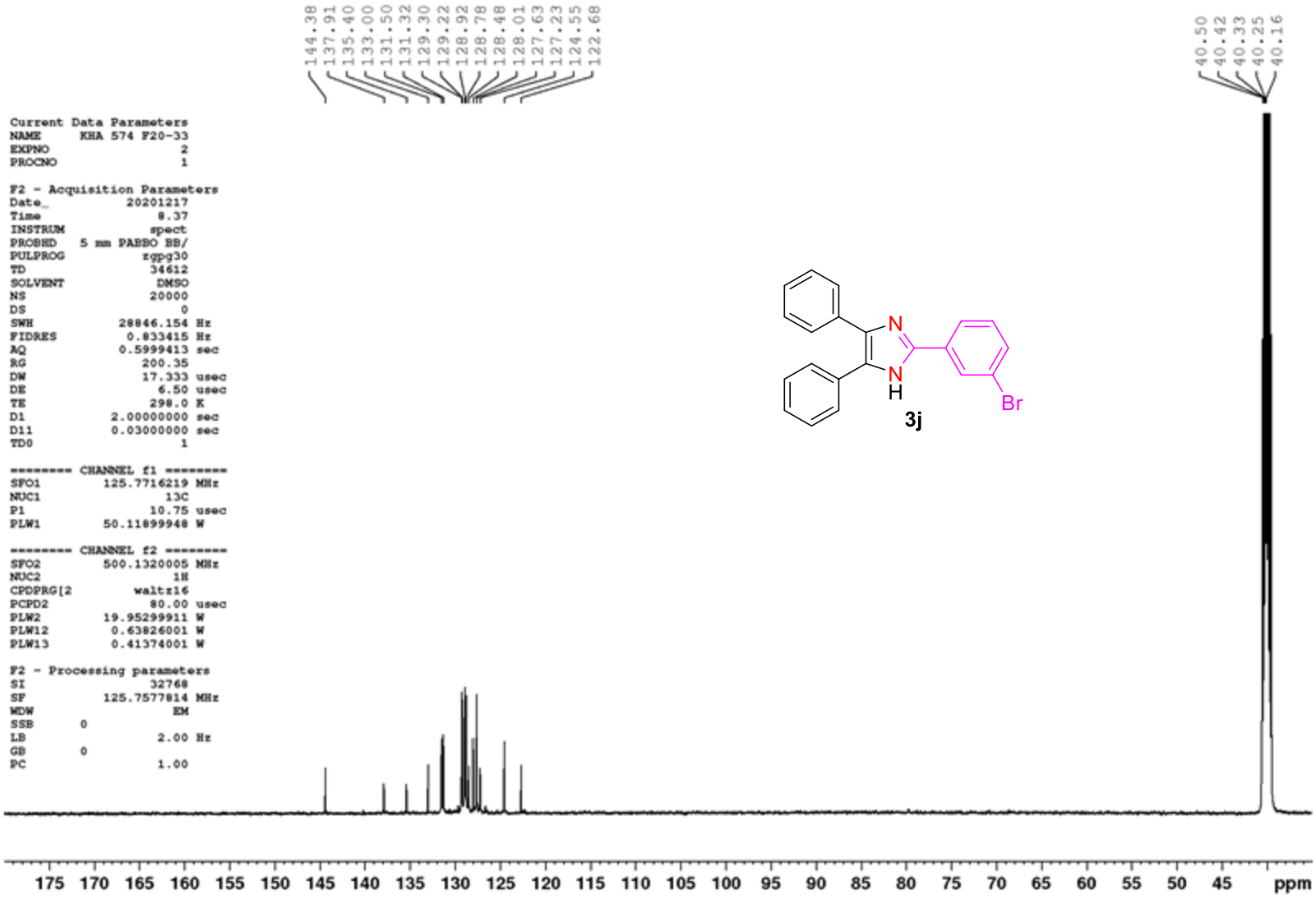


Figure S25. ^{13}C NMR spectrum of compound **3j** (125 MHz, DMSO-d_6, 25 ^{o}C)

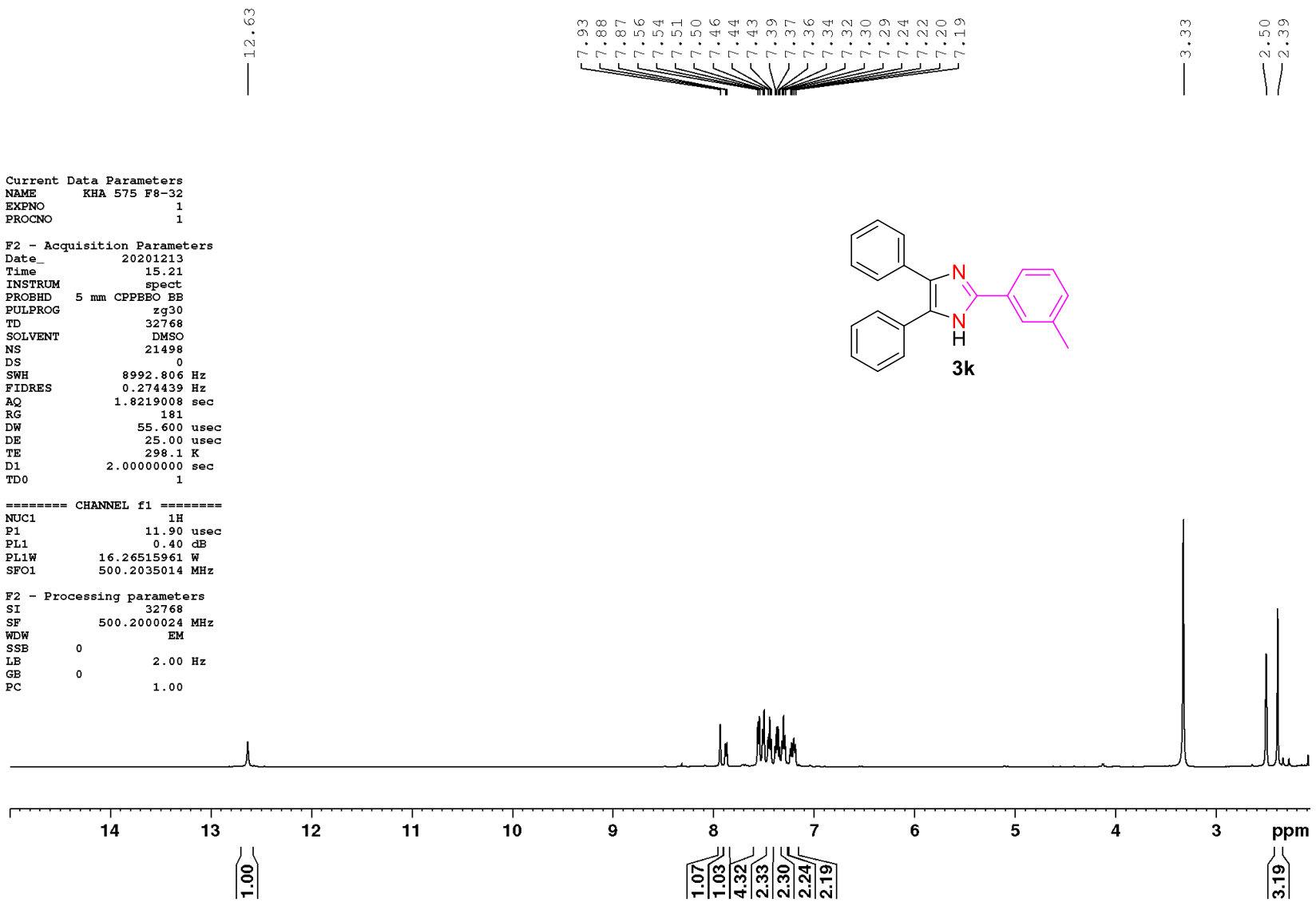


Figure S26. ^{1}H NMR spectrum of compound **3k** (500 MHz, DMSO-d_6, 25 ^{o}C)

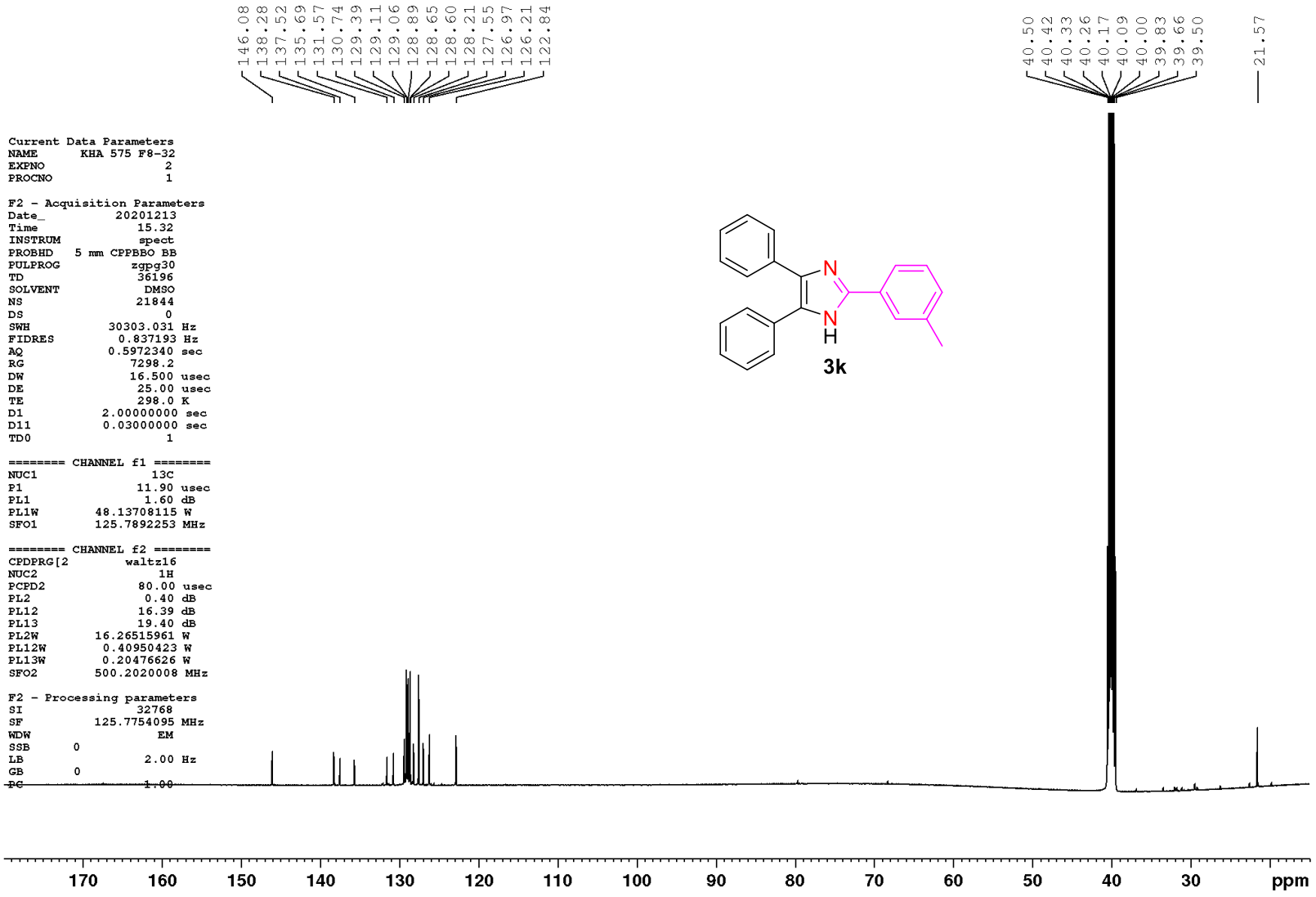


Figure S27. ^{13}C NMR spectrum of compound **3k** (125 MHz, DMSO-d_6, 25 ^{o}C)

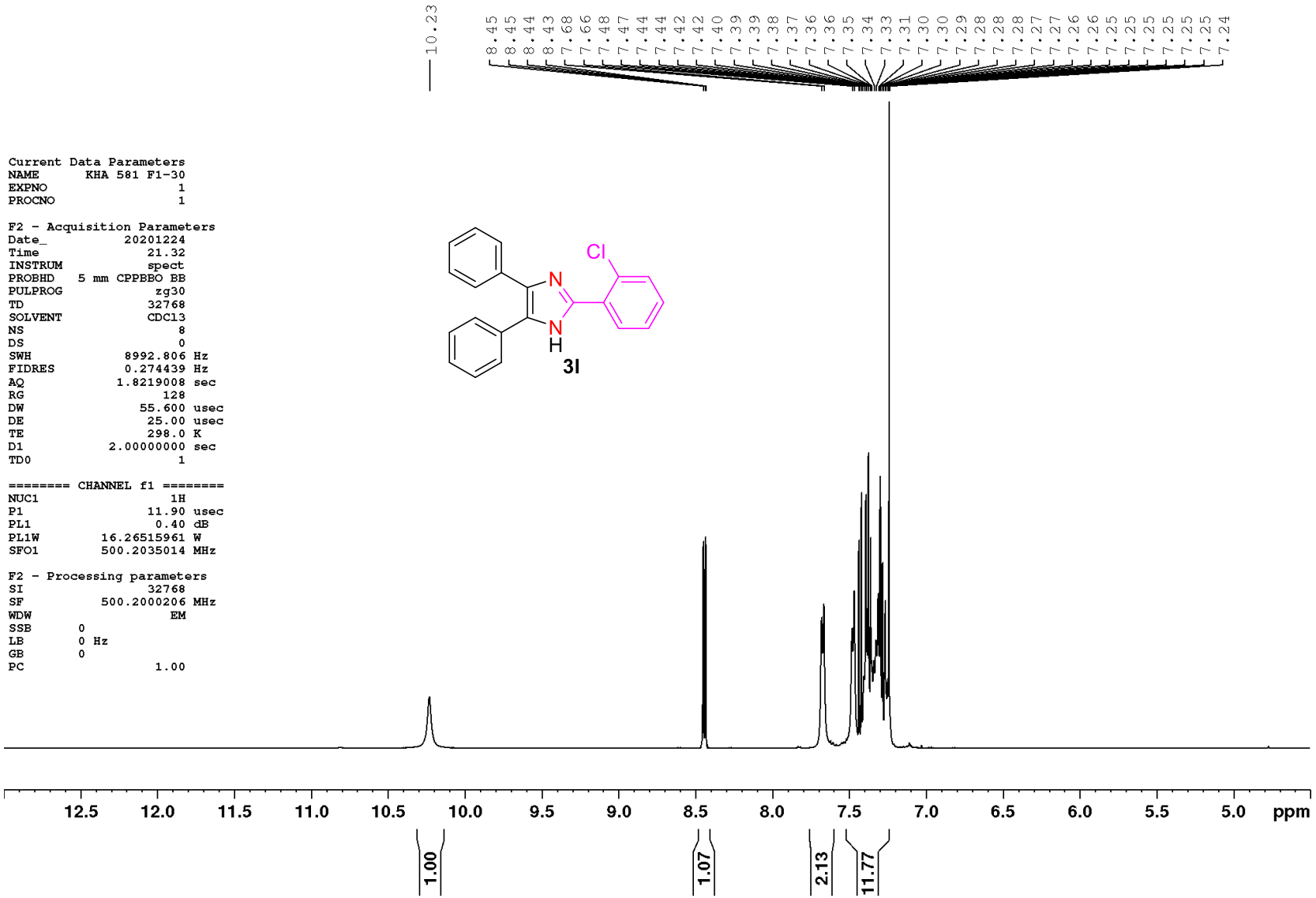


Figure S28. ^{1}H NMR spectrum of compound **3l** (500 MHz, $CDCl_3$, 25 ^{o}C)

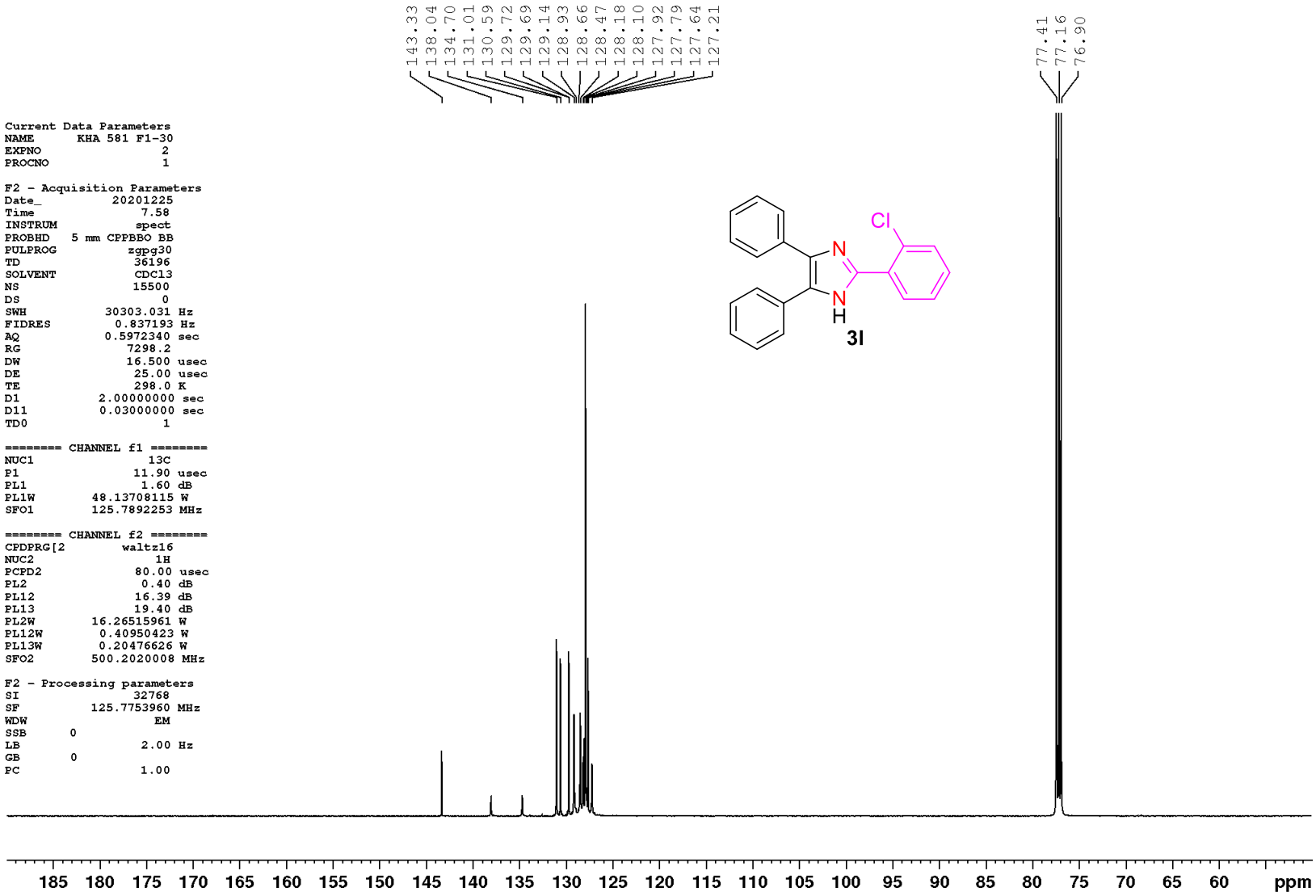


Figure S29. ^{13}C NMR spectrum of compound **3l** (125 MHz, $CDCl_3$, 25 ^oC)

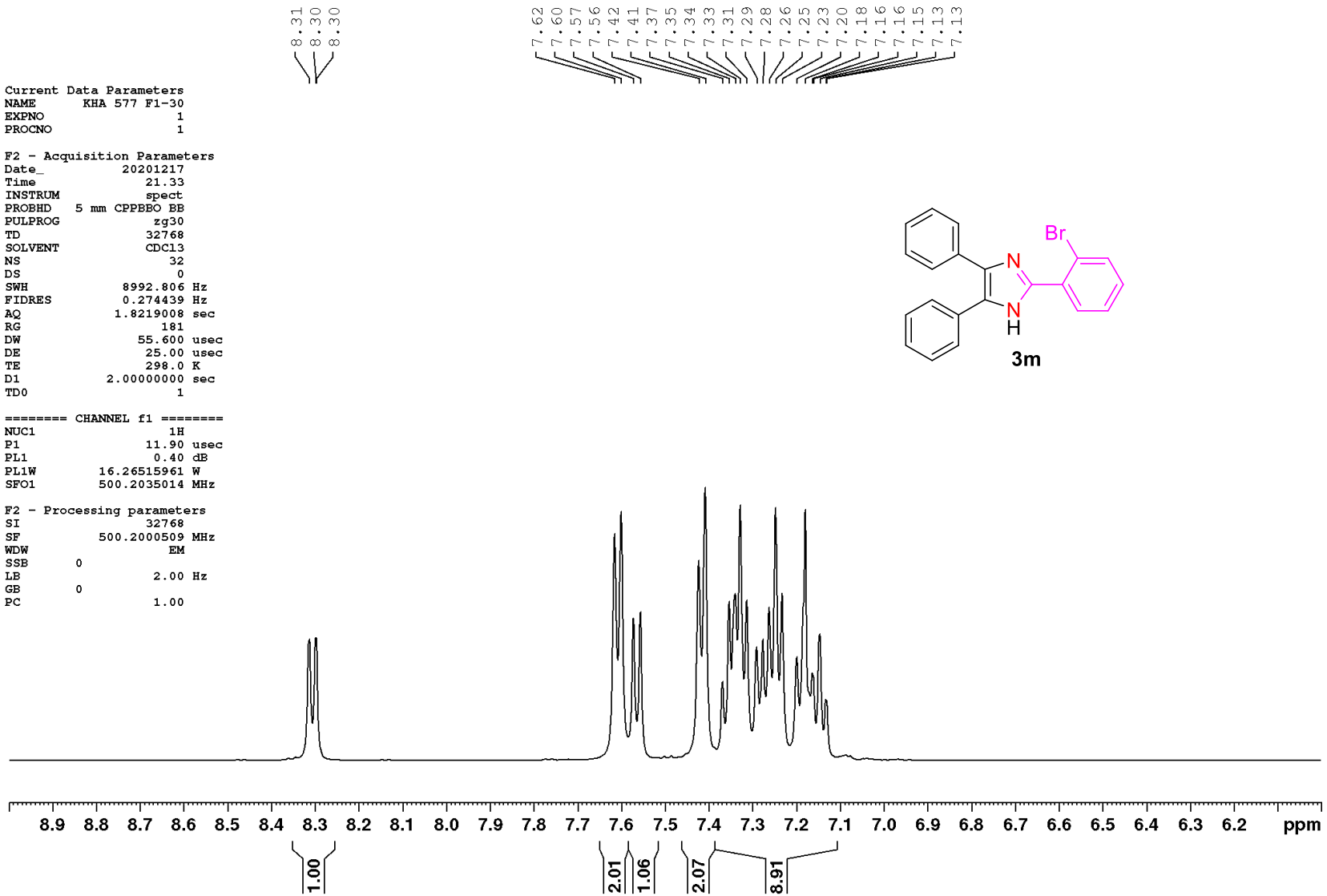


Figure S30. ^{1}H NMR spectrum of compound **3m** (500 MHz, $CDCl_3$, 25 ^{o}C)

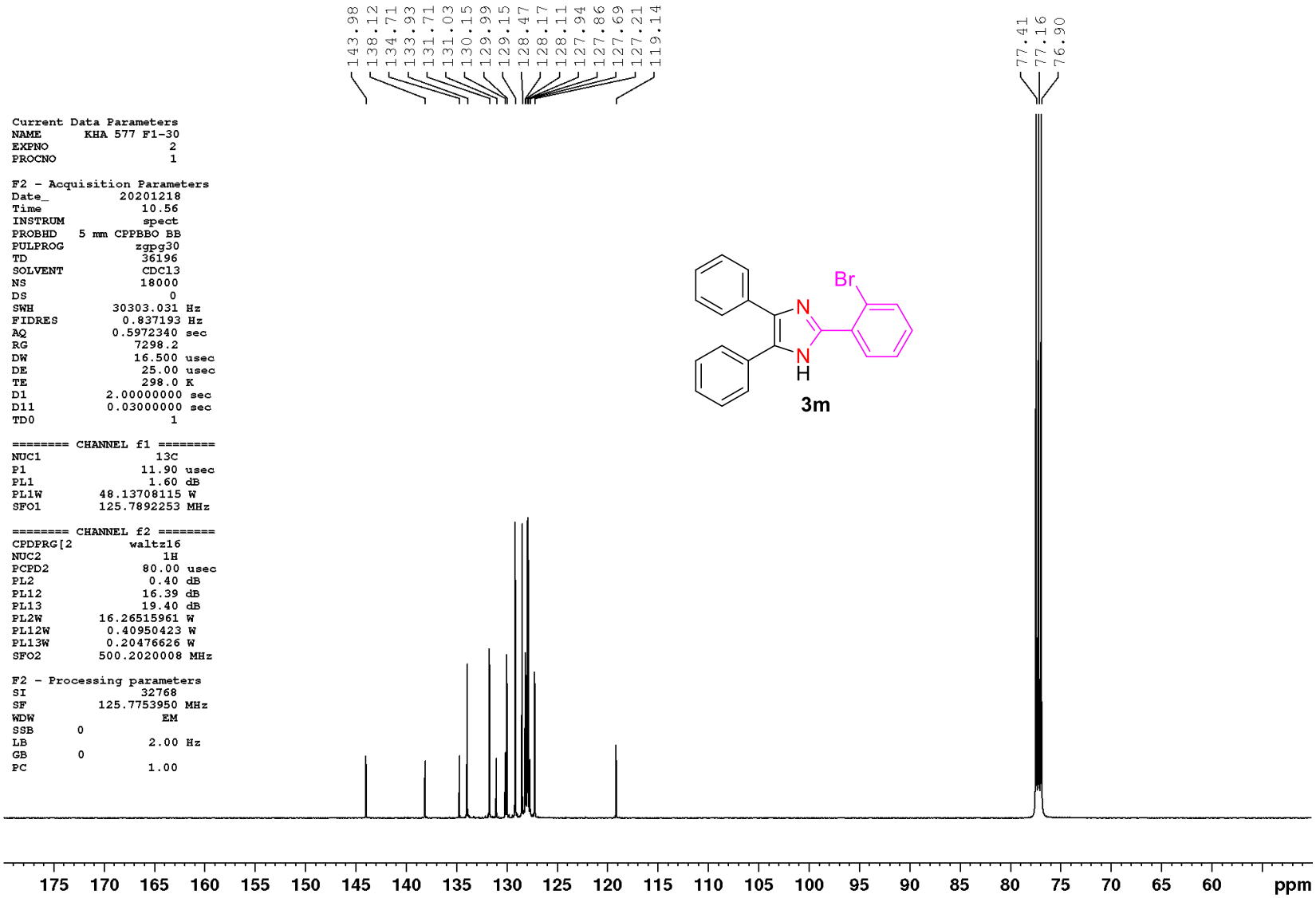


Figure S31. ^{13}C NMR spectrum of compound **3m** (125 MHz, $CDCl_3$, 25 °C)

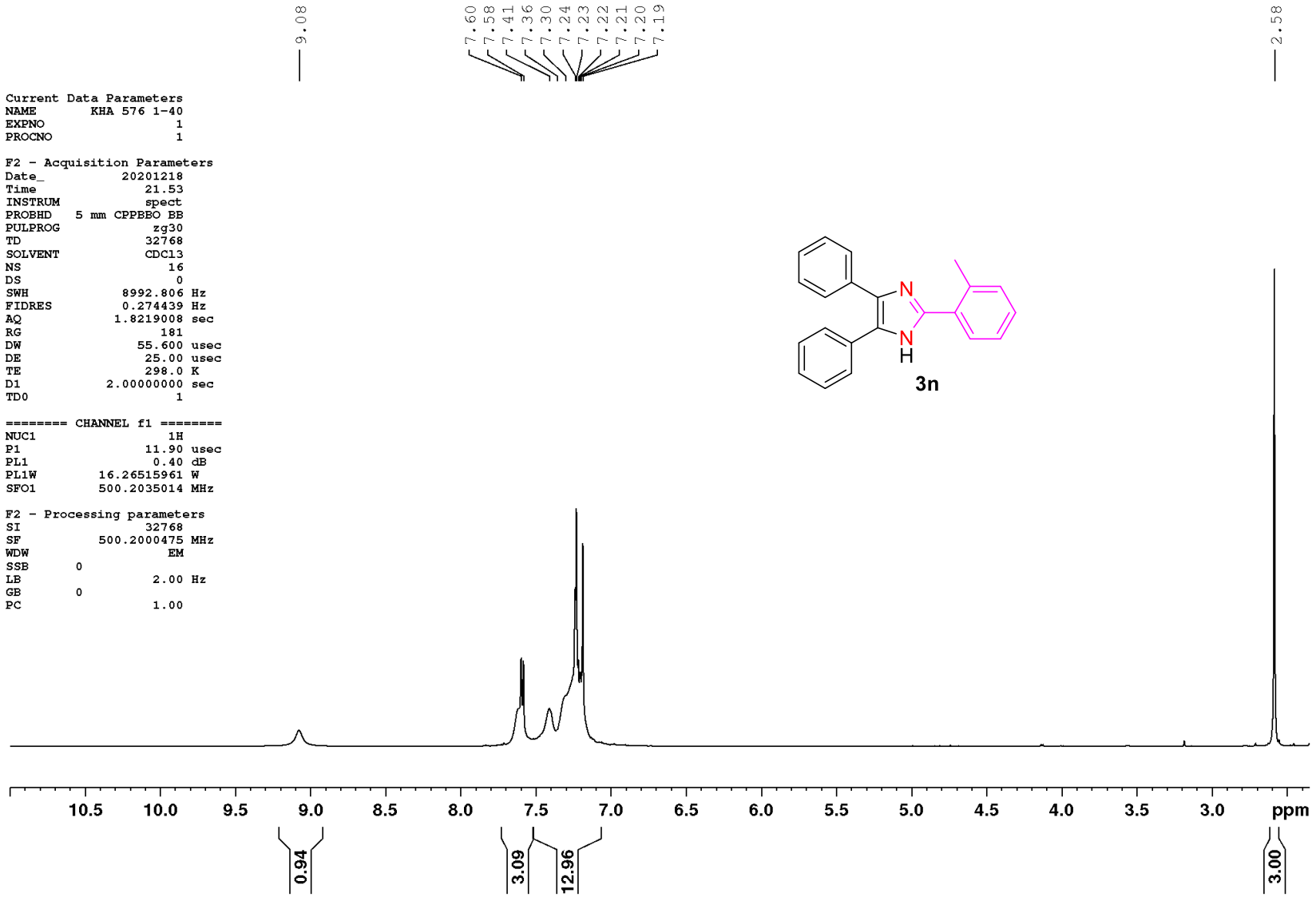


Figure S32. ^{1}H NMR spectrum of compound **3n** (500 MHz, $CDCl_3$, 25 ^{o}C)

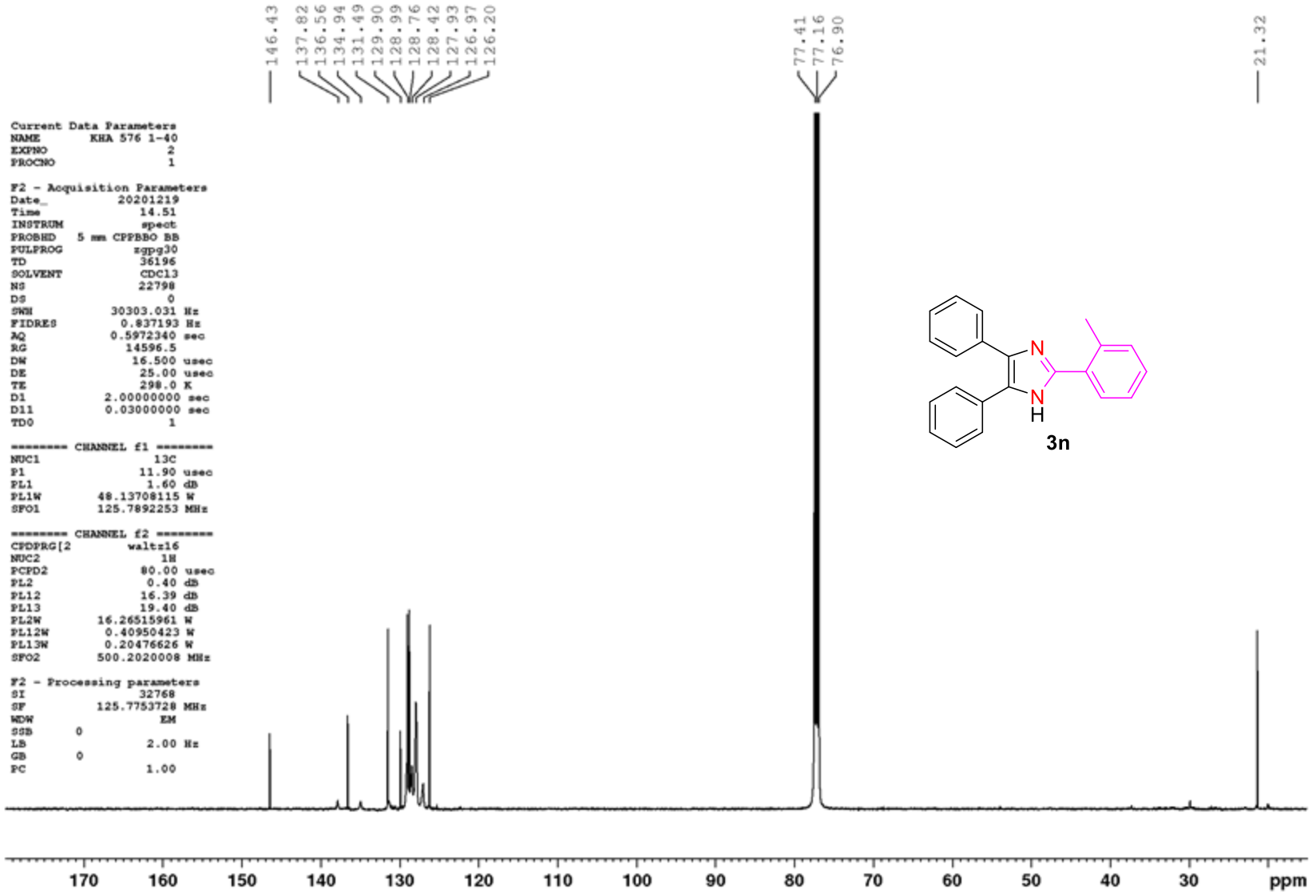


Figure S33. ^{13}C NMR spectrum of compound **3n** (125 MHz, $CDCl_3$, 25 ^{o}C)

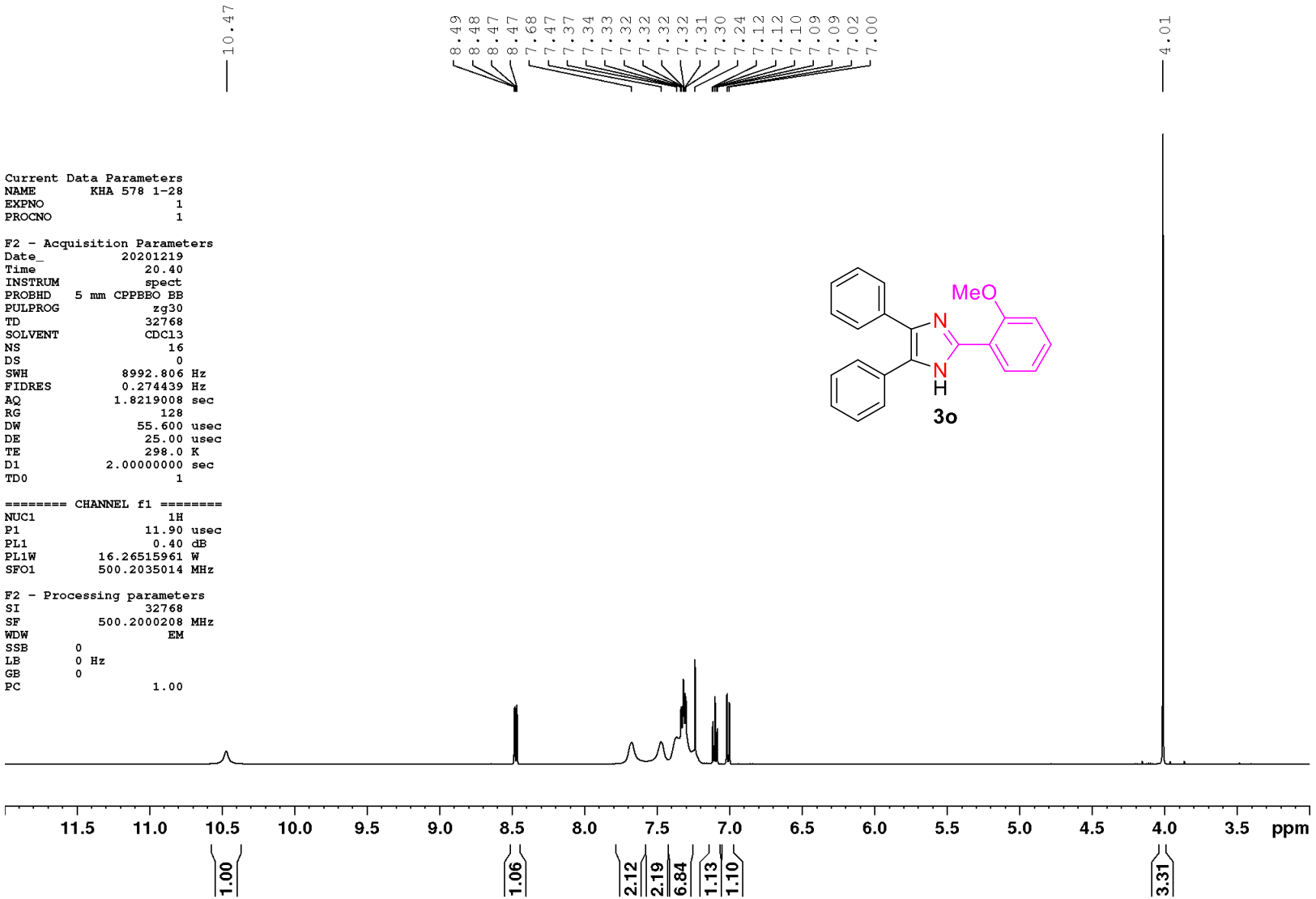


Figure S34. ^{1}H NMR spectrum of compound **3o** (500 MHz, $CDCl_3$, 25 ^{o}C)

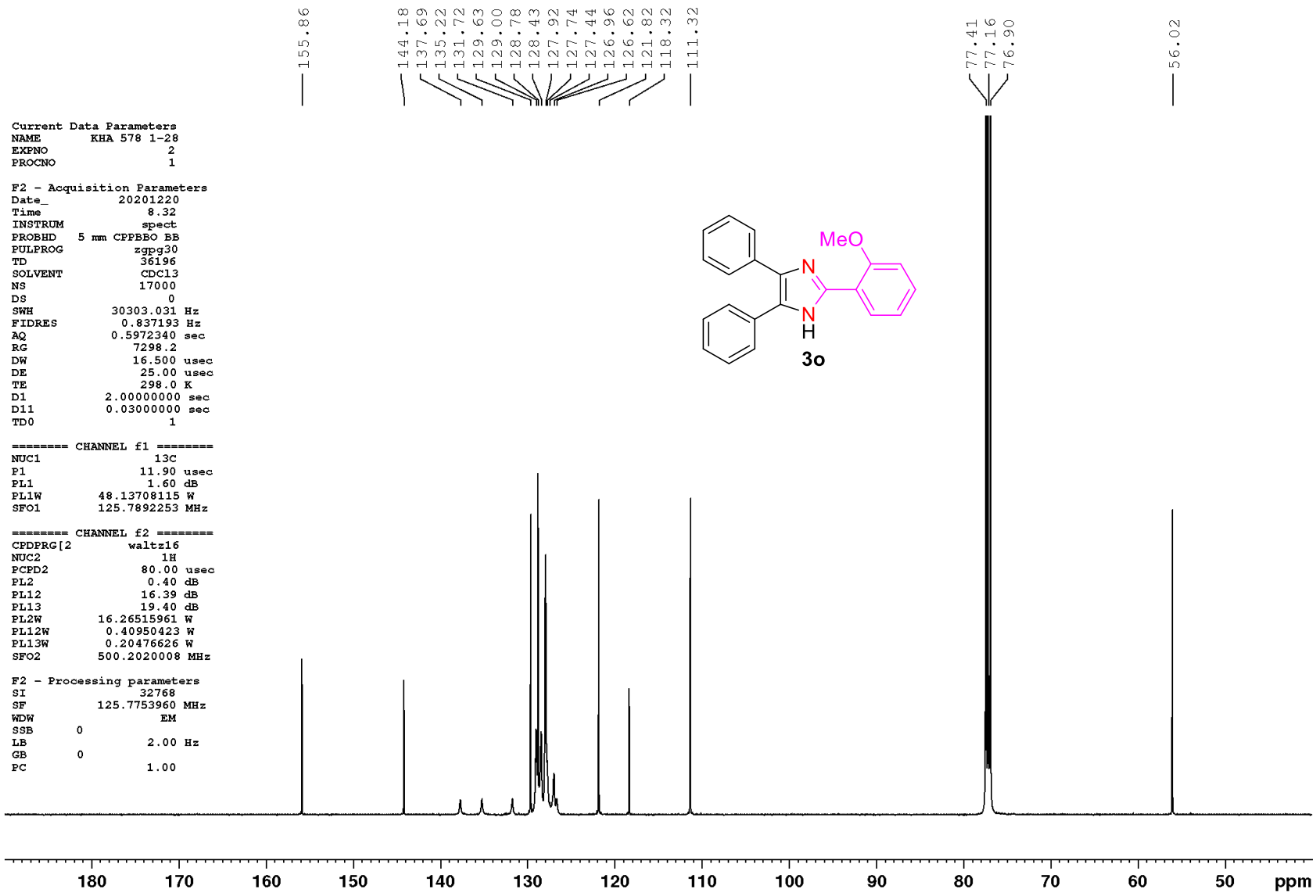


Figure S35. ^{13}C NMR spectrum of compound **3o** (125 MHz, $CDCl_3$, 25 ^{o}C)

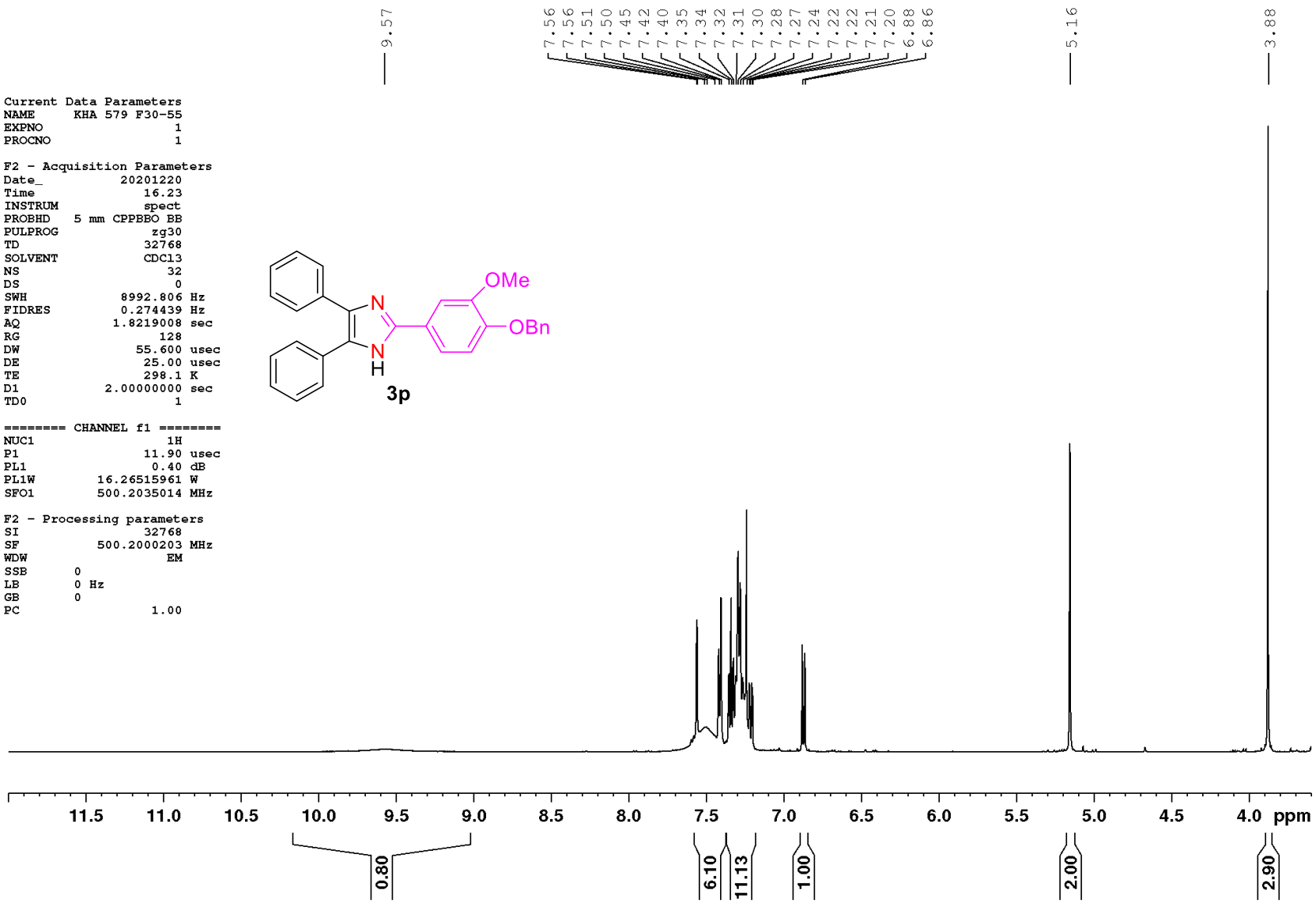


Figure S36. ^{1}H NMR spectrum of compound **3p** (500 MHz, $CDCl_3$, 25 ^{o}C)

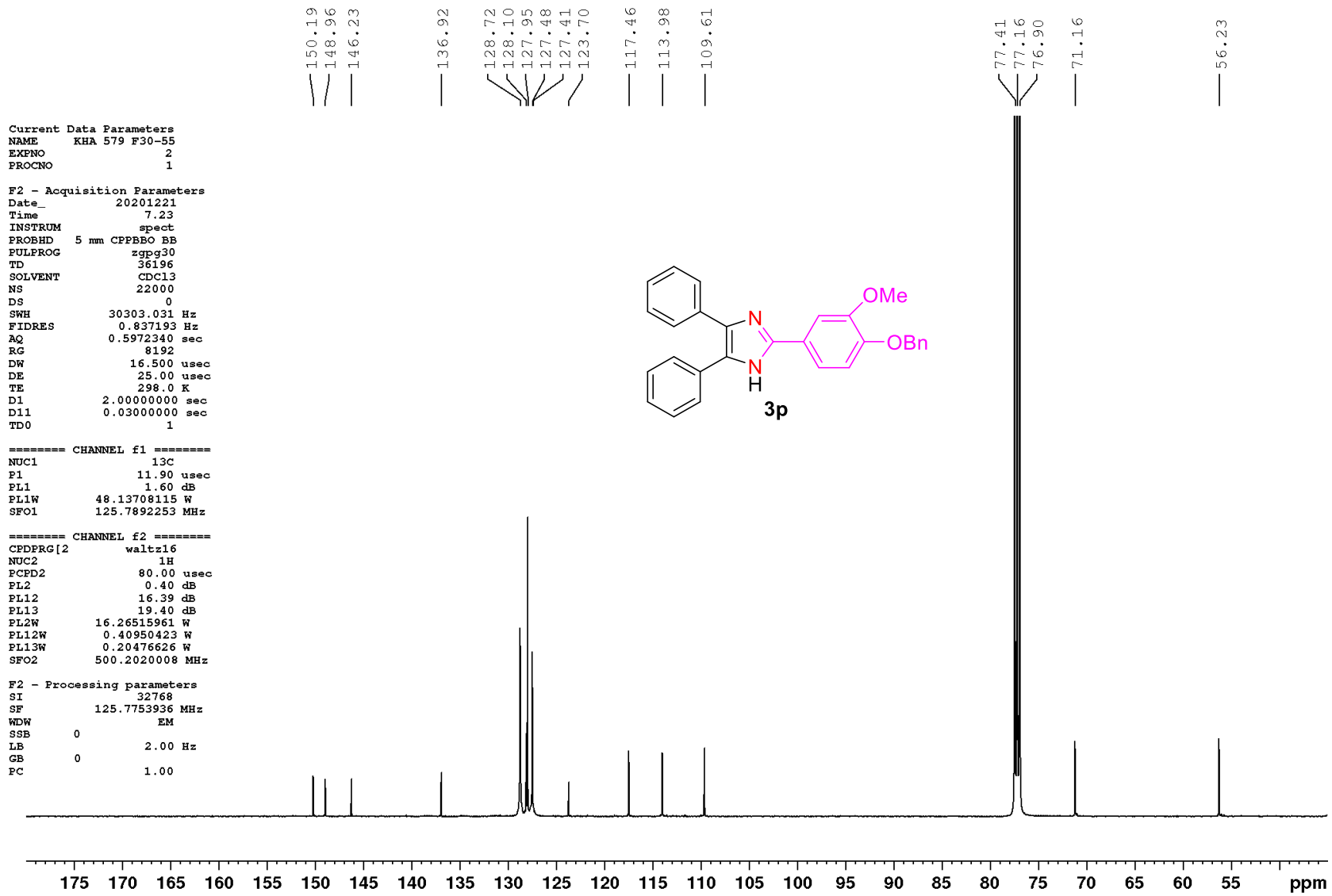


Figure S37. ^{13}C NMR spectrum of compound **3p** (125 MHz, $CDCl_3$, 25 °C)

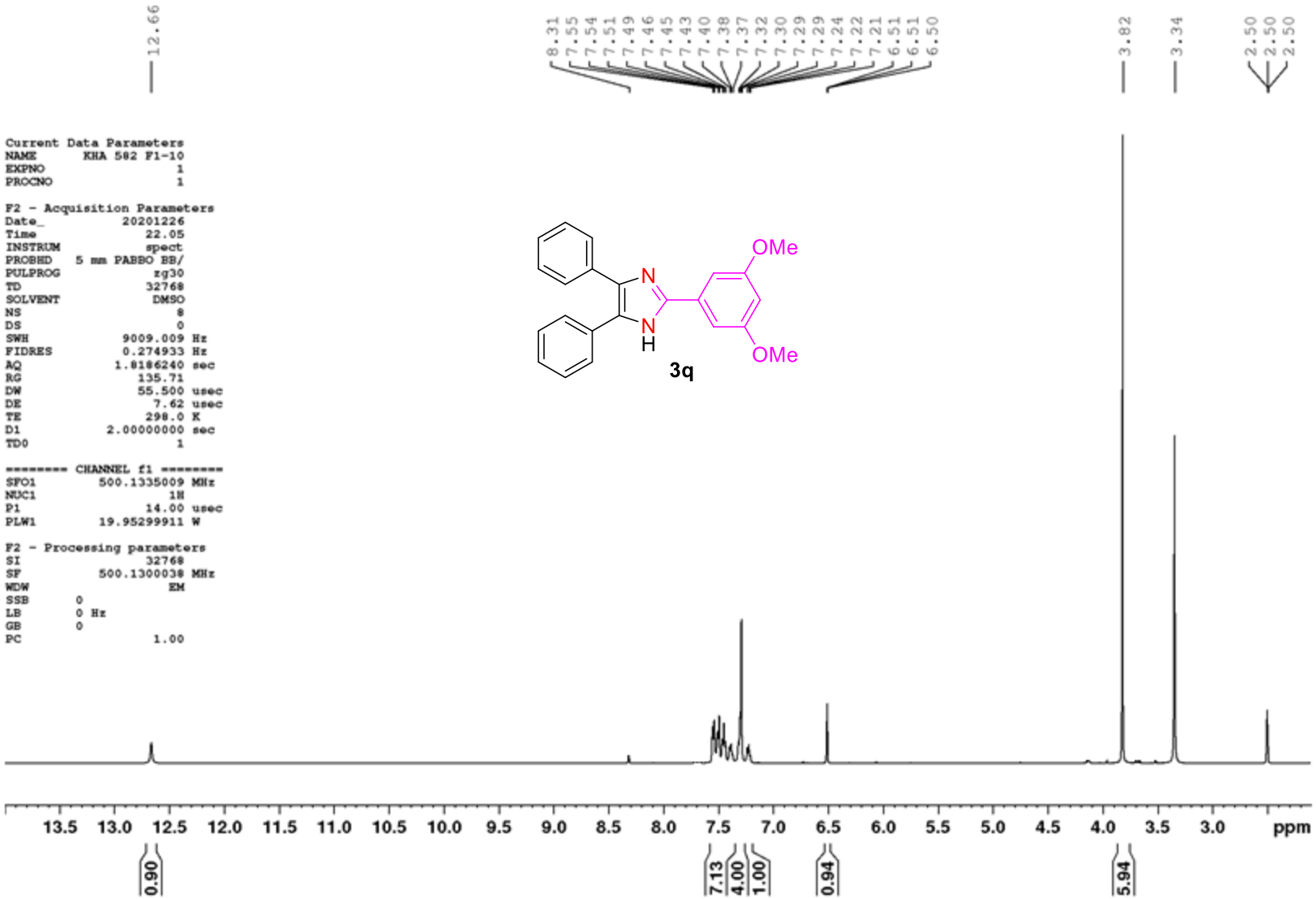


Figure S38. ^{1}H NMR spectrum of compound **3q** (500 MHz, DMSO-d_6, 25 ^{o}C)

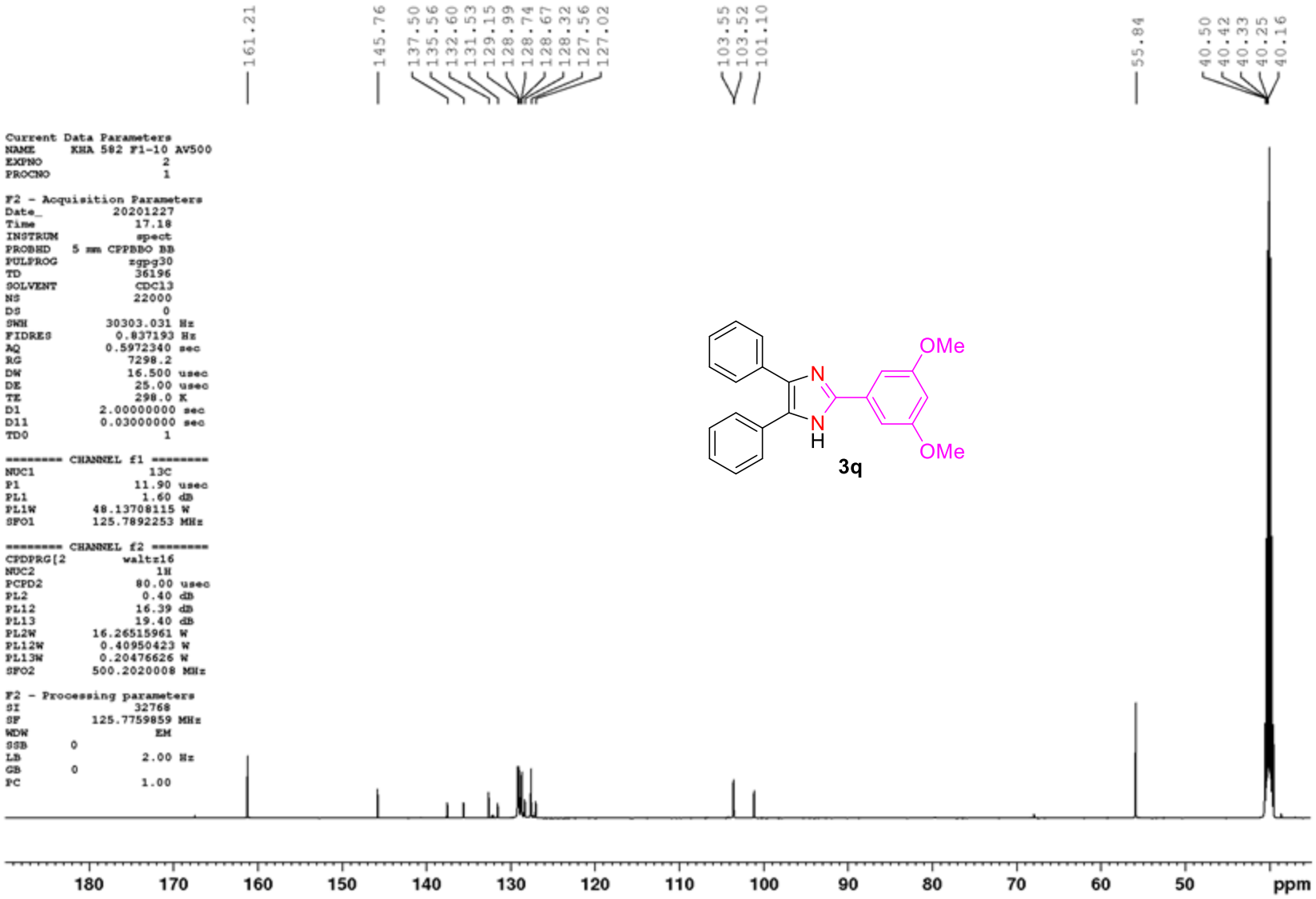


Figure S39. ^{13}C NMR spectrum of compound **3q** (125 MHz, DMSO-d_6, 25 ^{o}C)

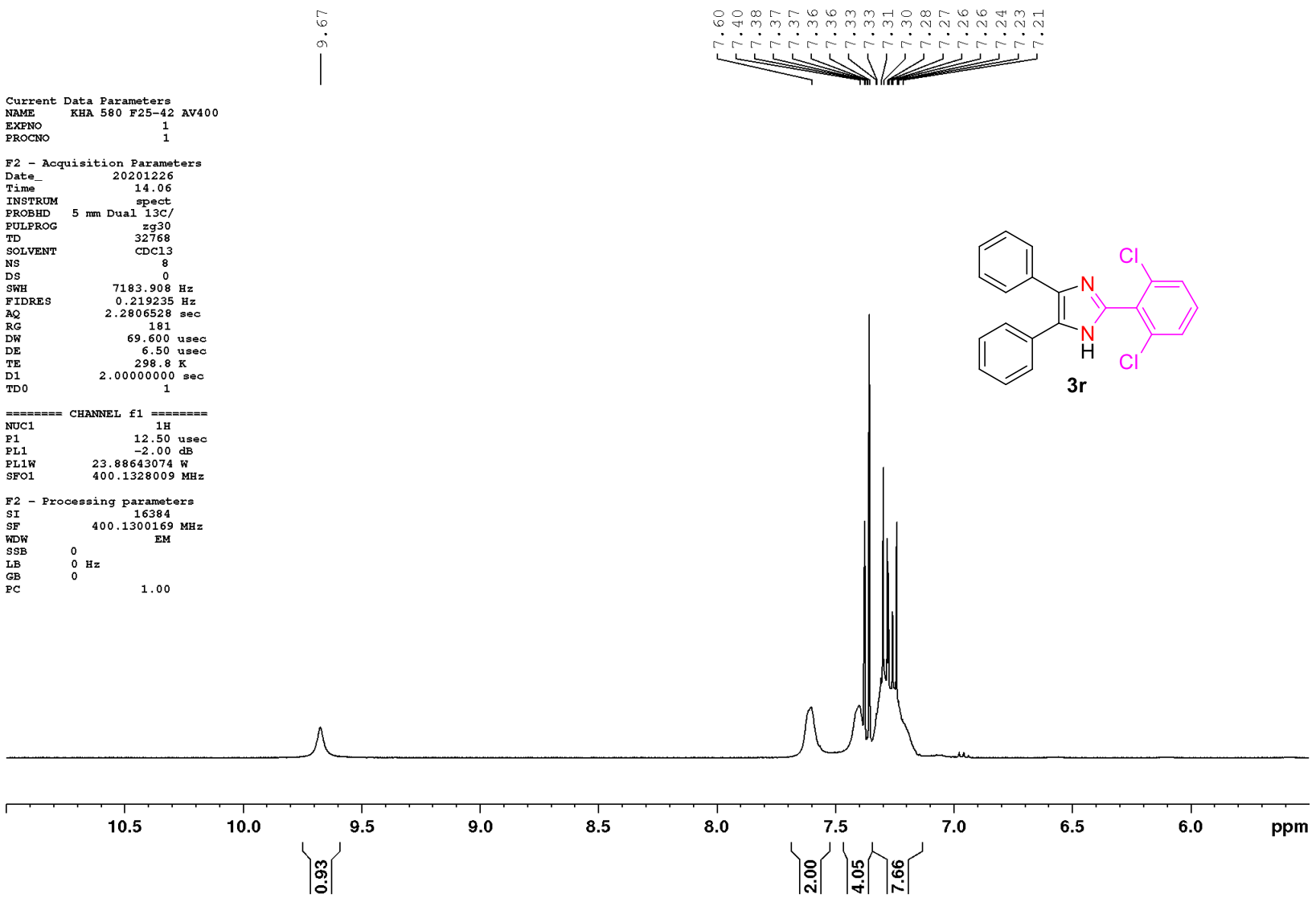


Figure S40. ^{1}H NMR spectrum of compound **3r** (400 MHz, $CDCl_3$, 25 ^{o}C)

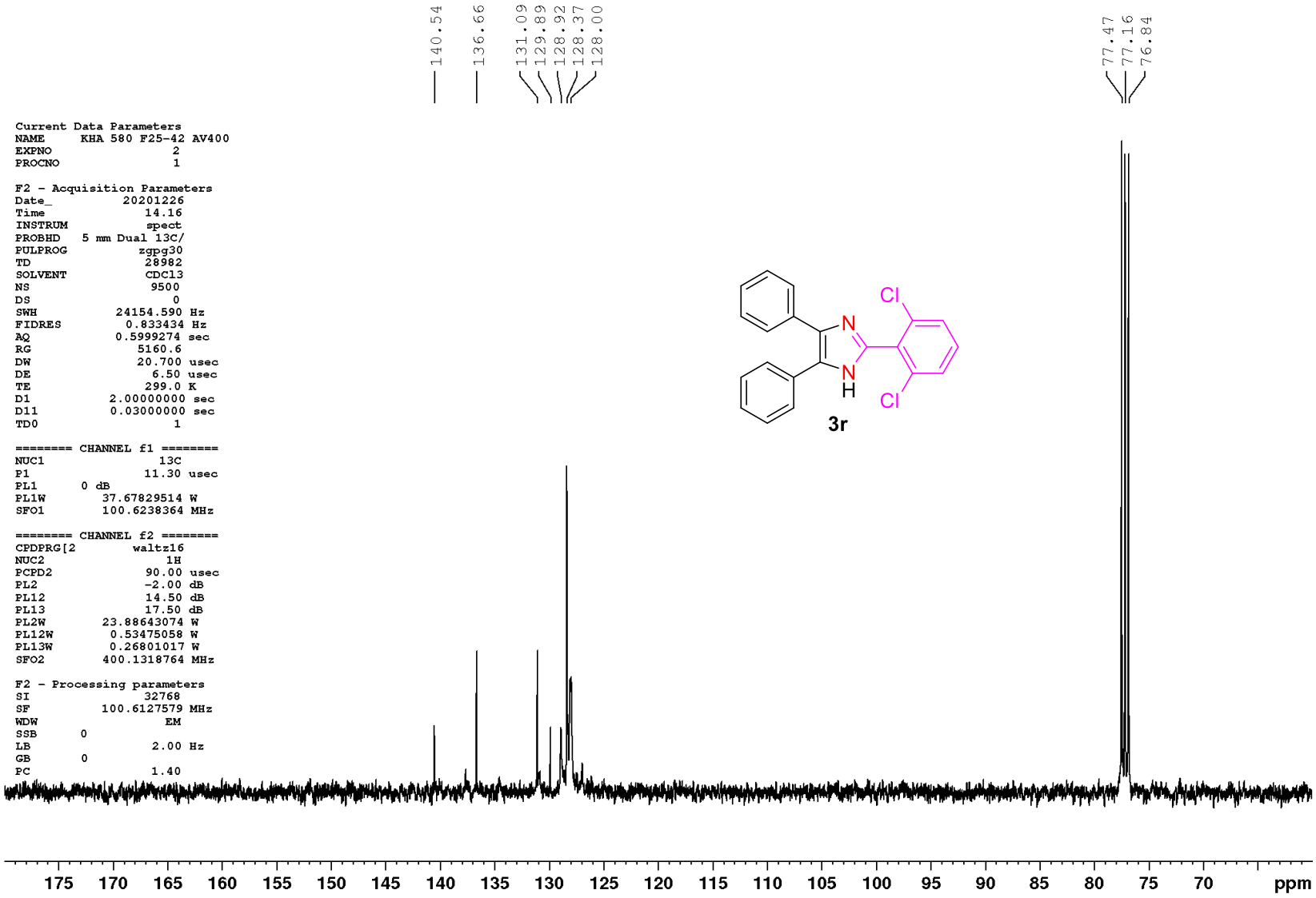


Figure S41. ^{13}C NMR spectrum of compound **3r** (100 MHz, $CDCl_3$, 25 ^oC)

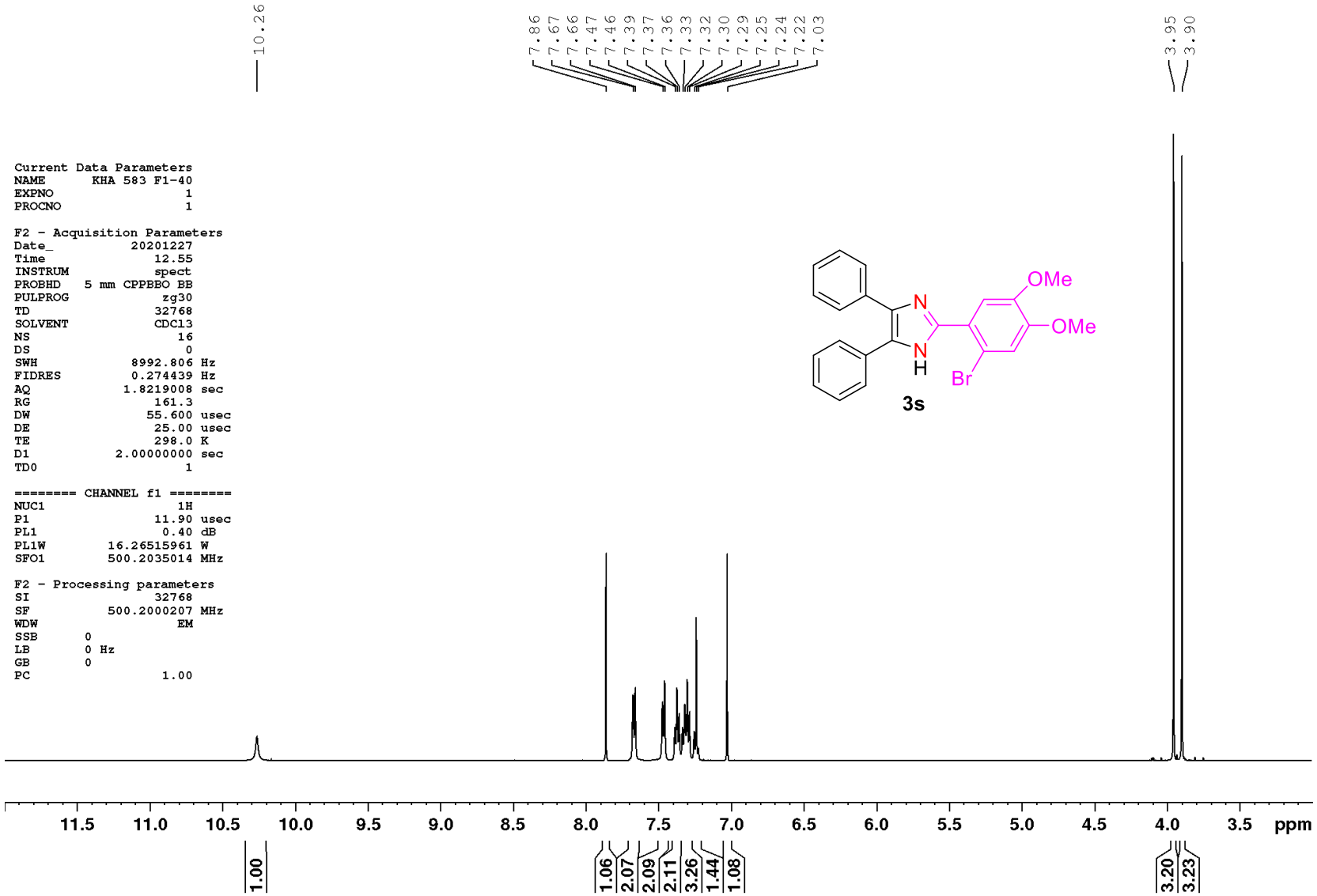


Figure S42. ^{1}H NMR spectrum of compound **3s** (500 MHz, $CDCl_3$, 25 ^{o}C)

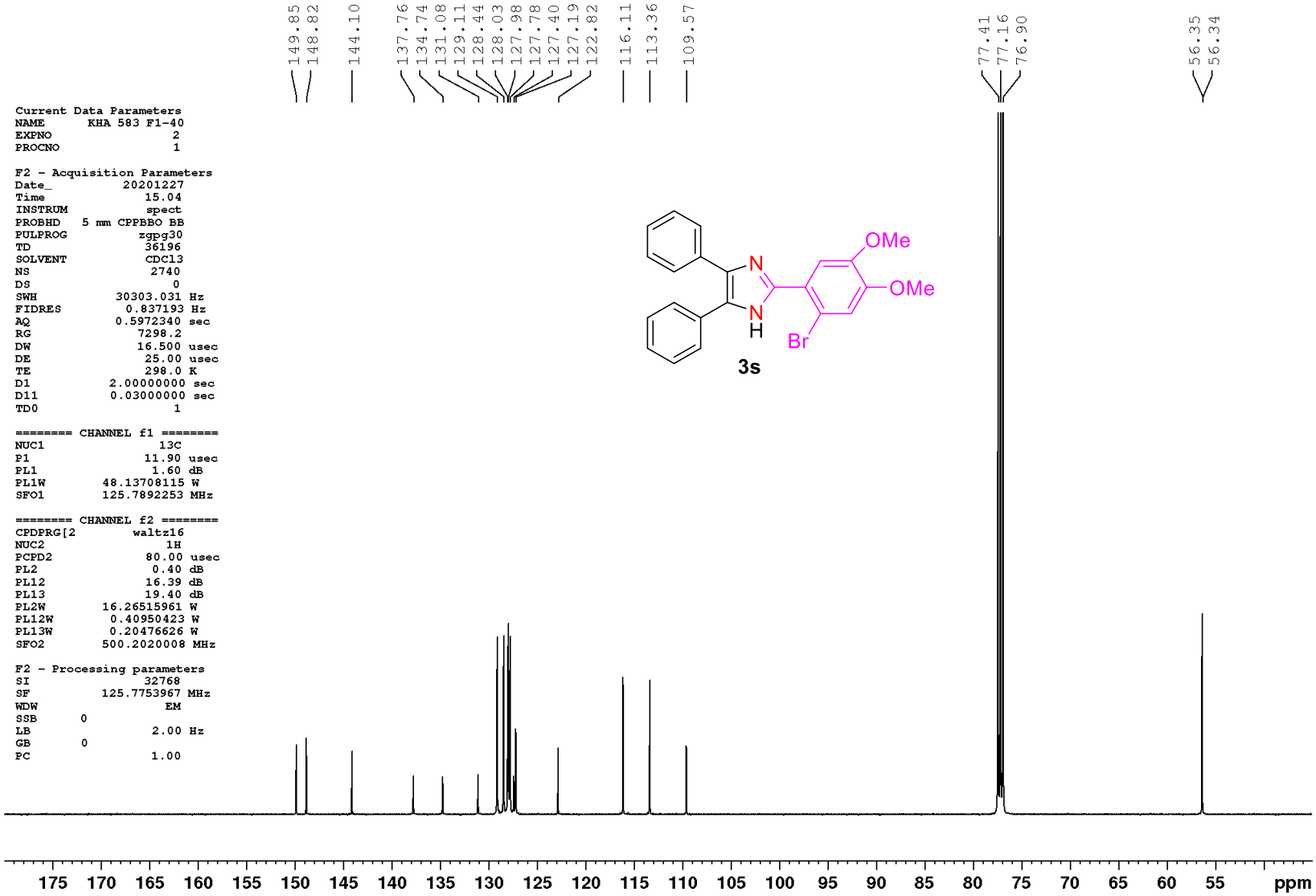


Figure S43. ^{13}C NMR spectrum of compound **3s** (125 MHz, $CDCl_3$, 25 ^oC)

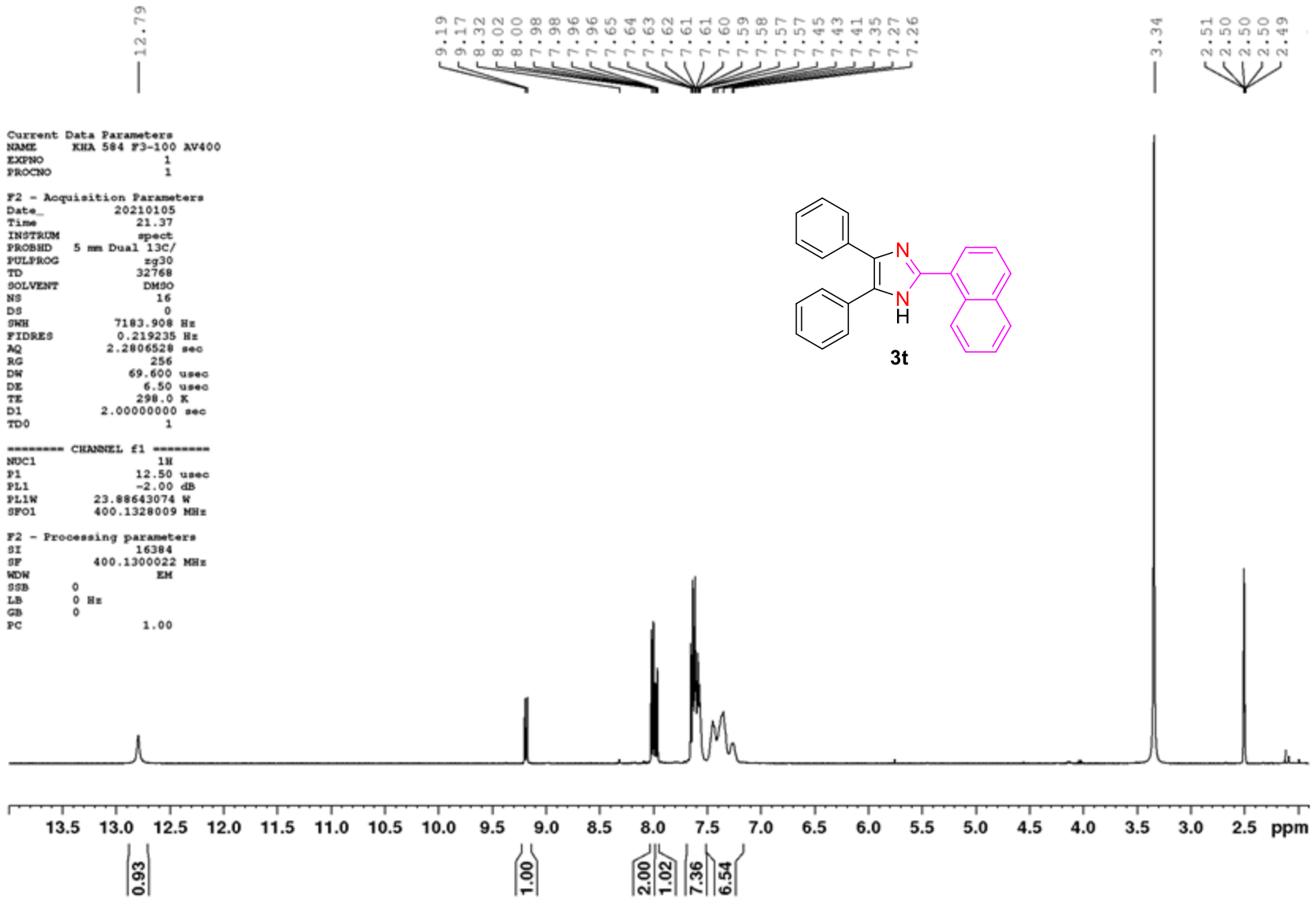


Figure S44. ^{1}H NMR spectrum of compound **3t** (400 MHz, DMSO-d_6, 25 ^{o}C)

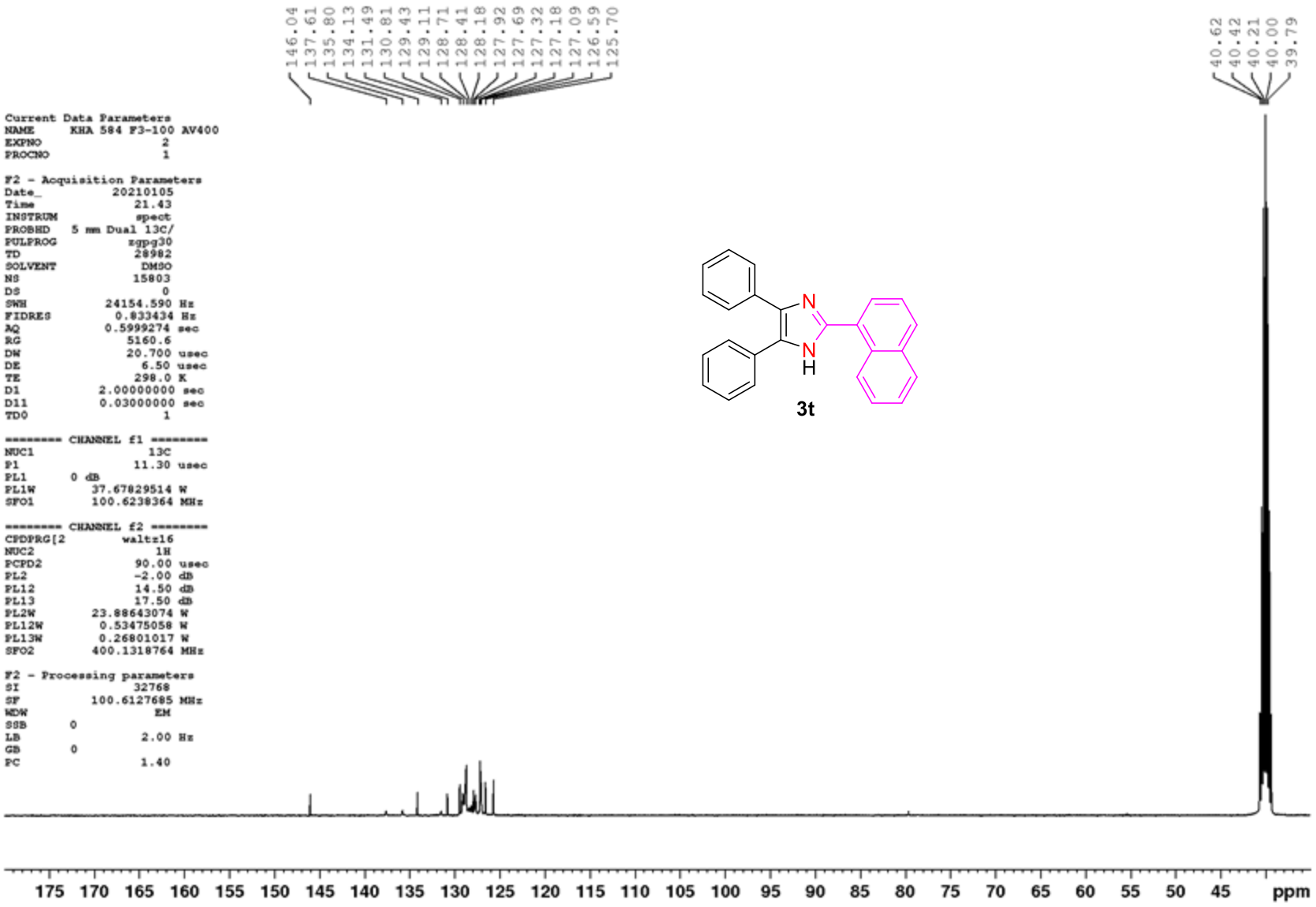


Figure S45. ^{13}C NMR spectrum of compound **3t** (100 MHz, DMSO-d_6, 25 ^{o}C)

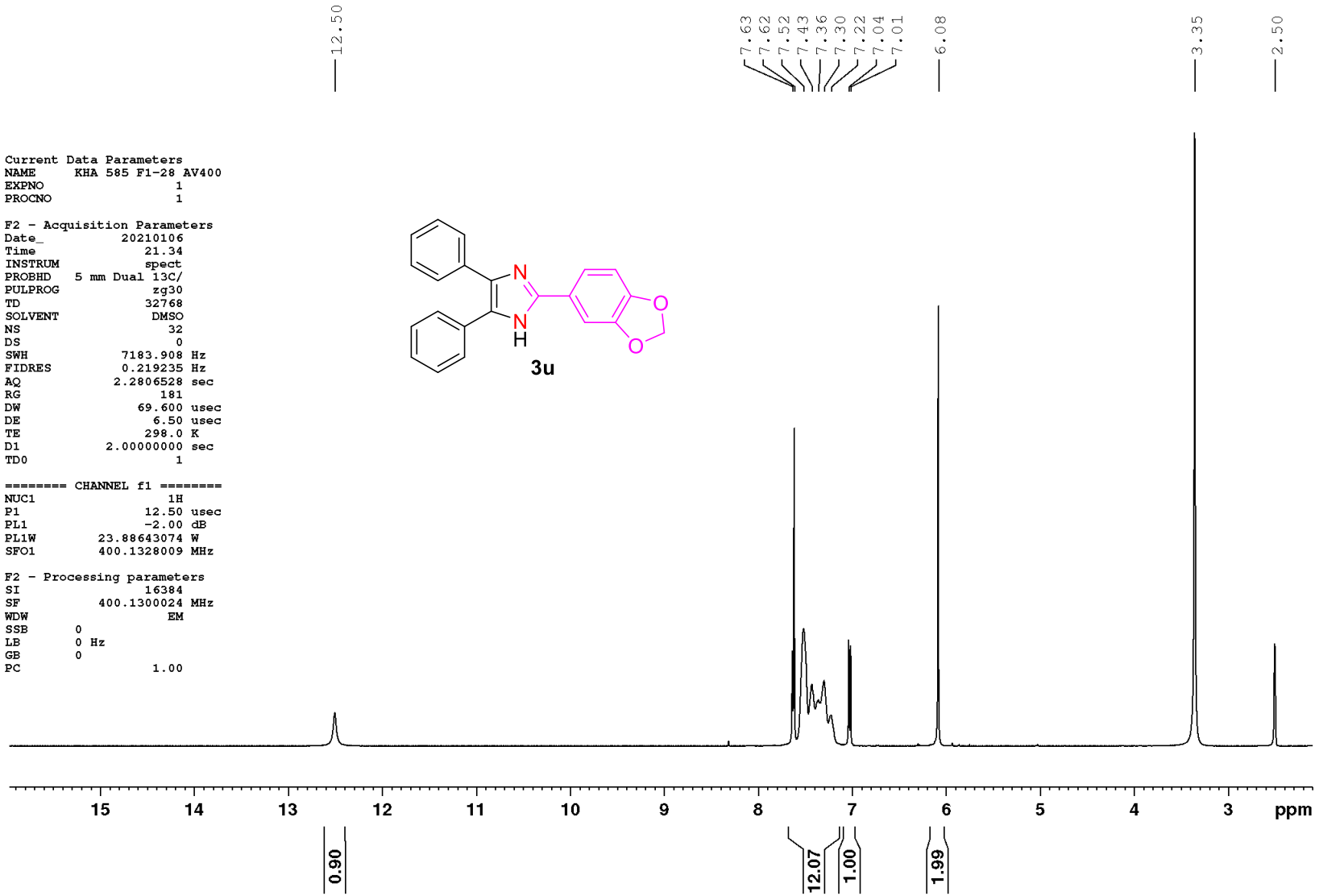


Figure S46. ^{1}H NMR spectrum of compound **3u** (400 MHz, DMSO-d_6, 25 ^{o}C)

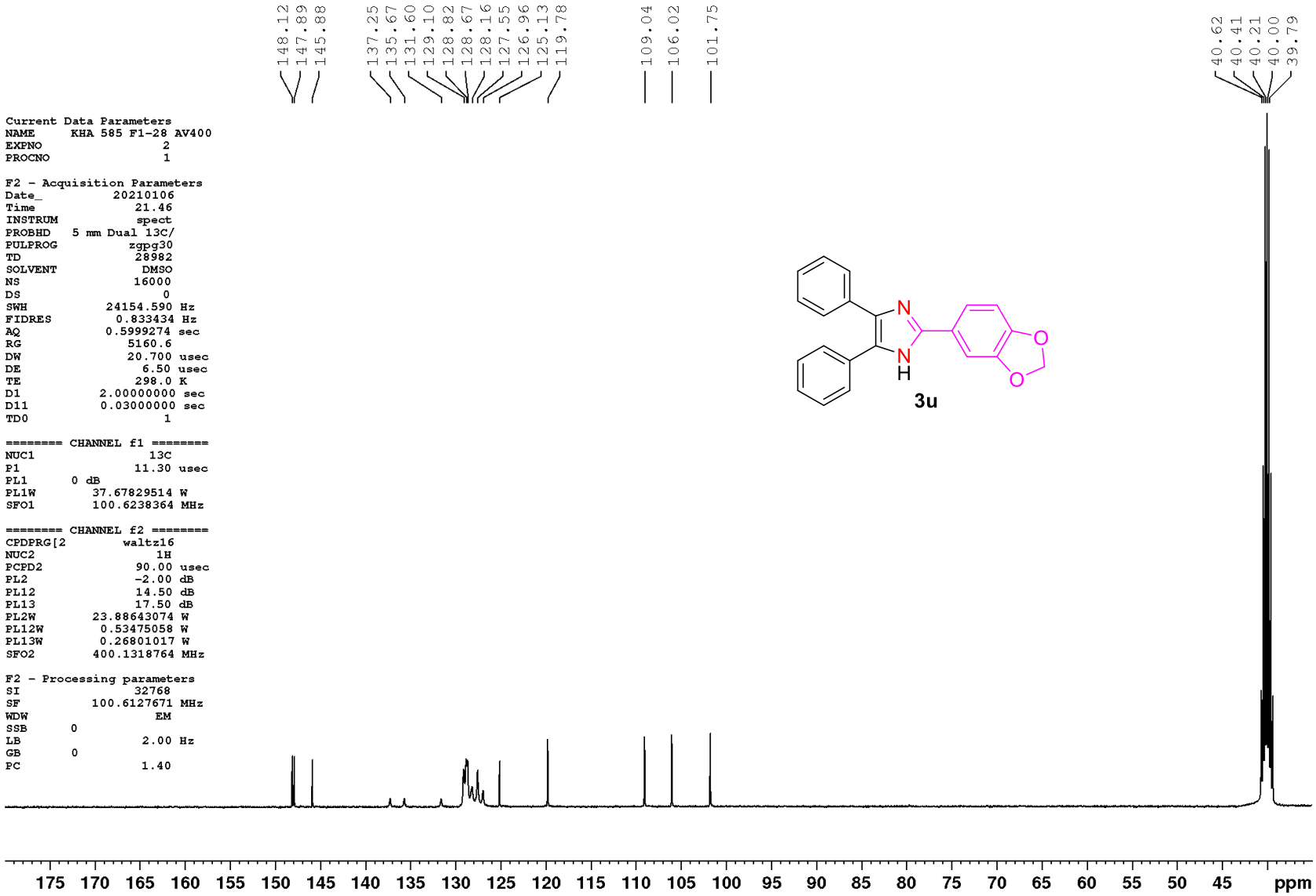


Figure S47. ^{13}C NMR spectrum of compound **3u** (100 MHz, DMSO-d_6, 25 ^{o}C)

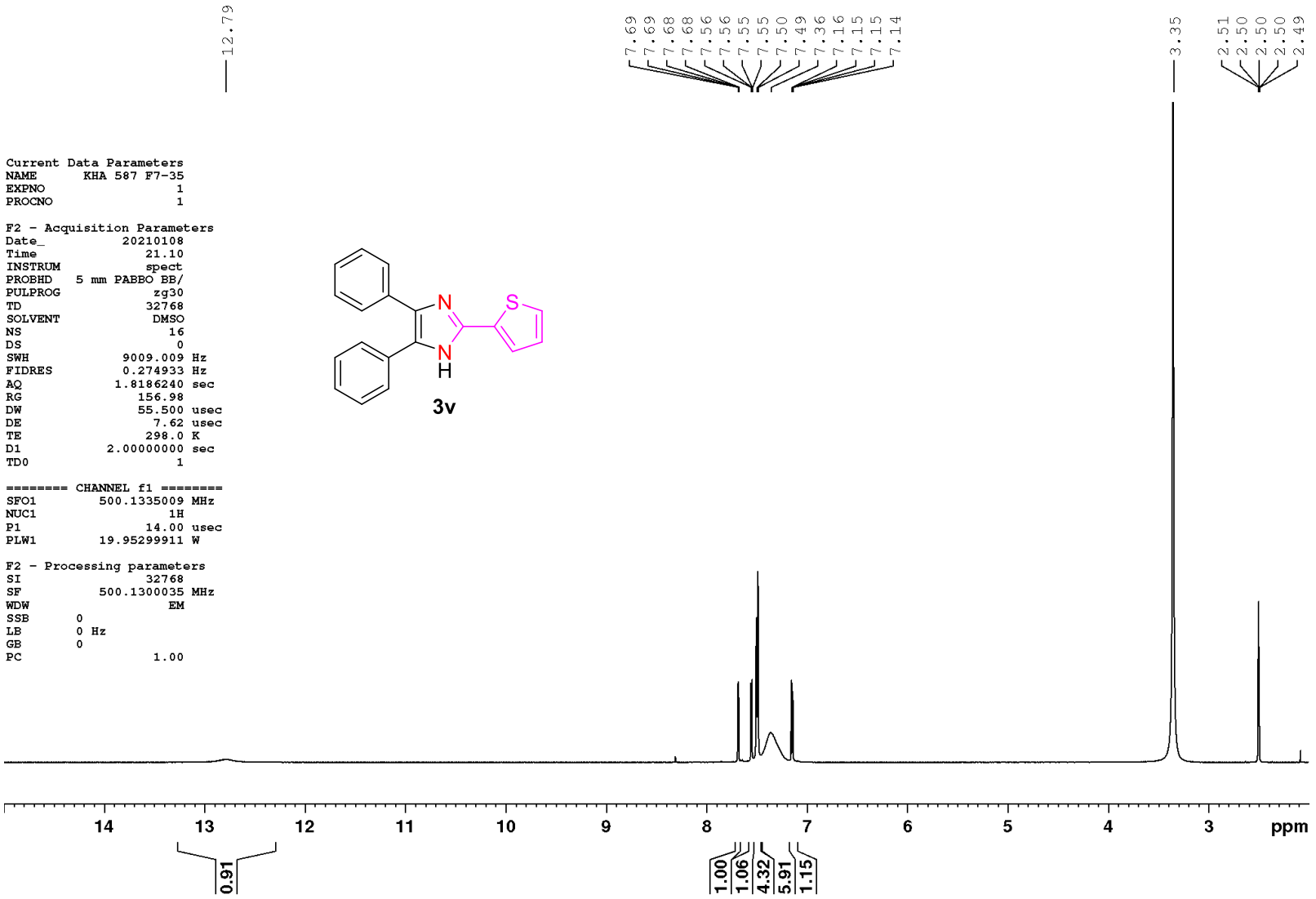


Figure S48. ^{1}H NMR spectrum of compound **3v** (500 MHz, DMSO-d_6, 25 ^{o}C)

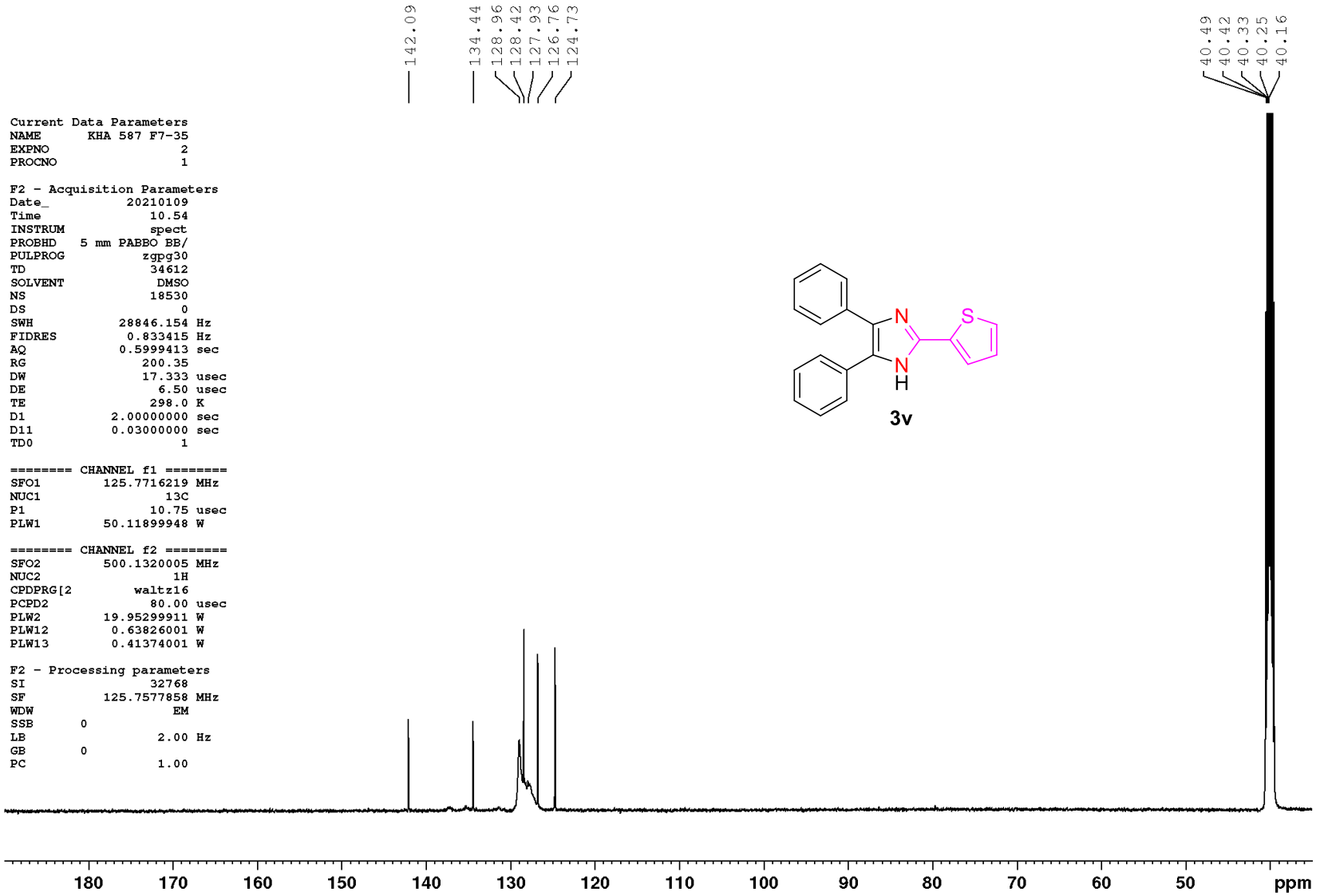


Figure S49. ^{13}C NMR spectrum of compound **3v** (125 MHz, DMSO-d_6, 25 ^{o}C)

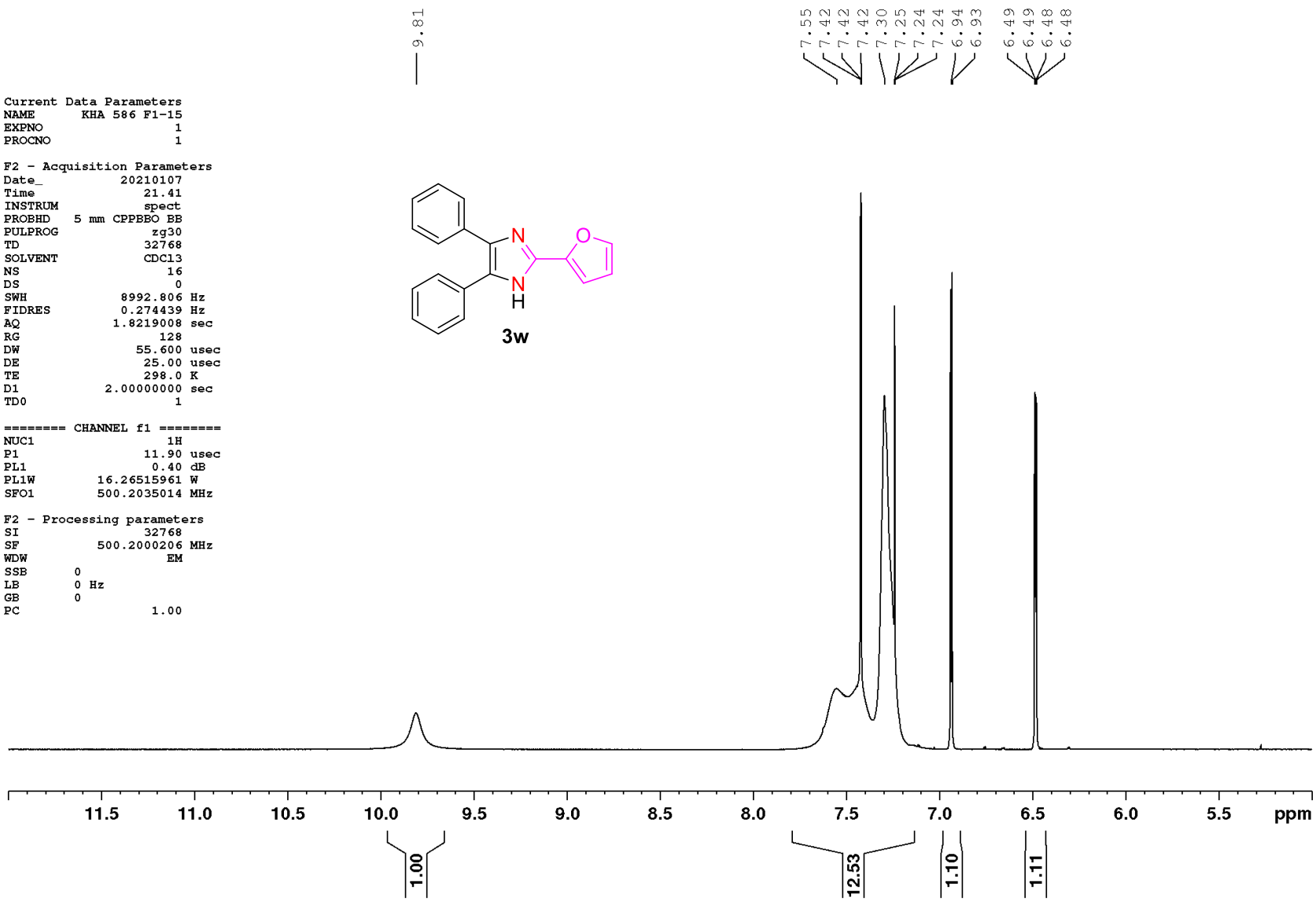


Figure S50. ^{1}H NMR spectrum of compound **3w** (500 MHz, $CDCl_3$, 25 ^{o}C)

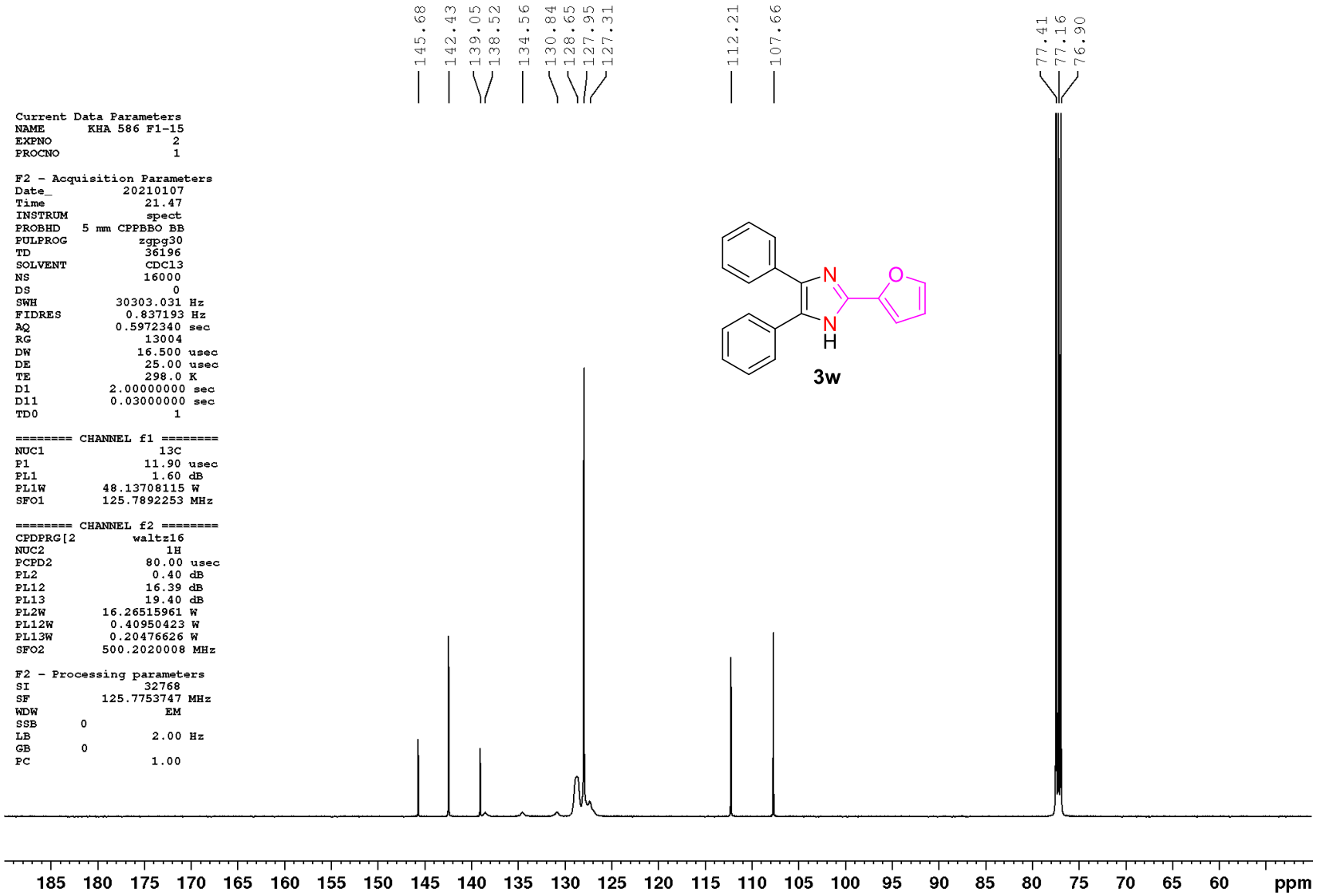


Figure S51. ^{13}C NMR spectrum of compound **3w** (125 MHz, $CDCl_3$, 25 °C)

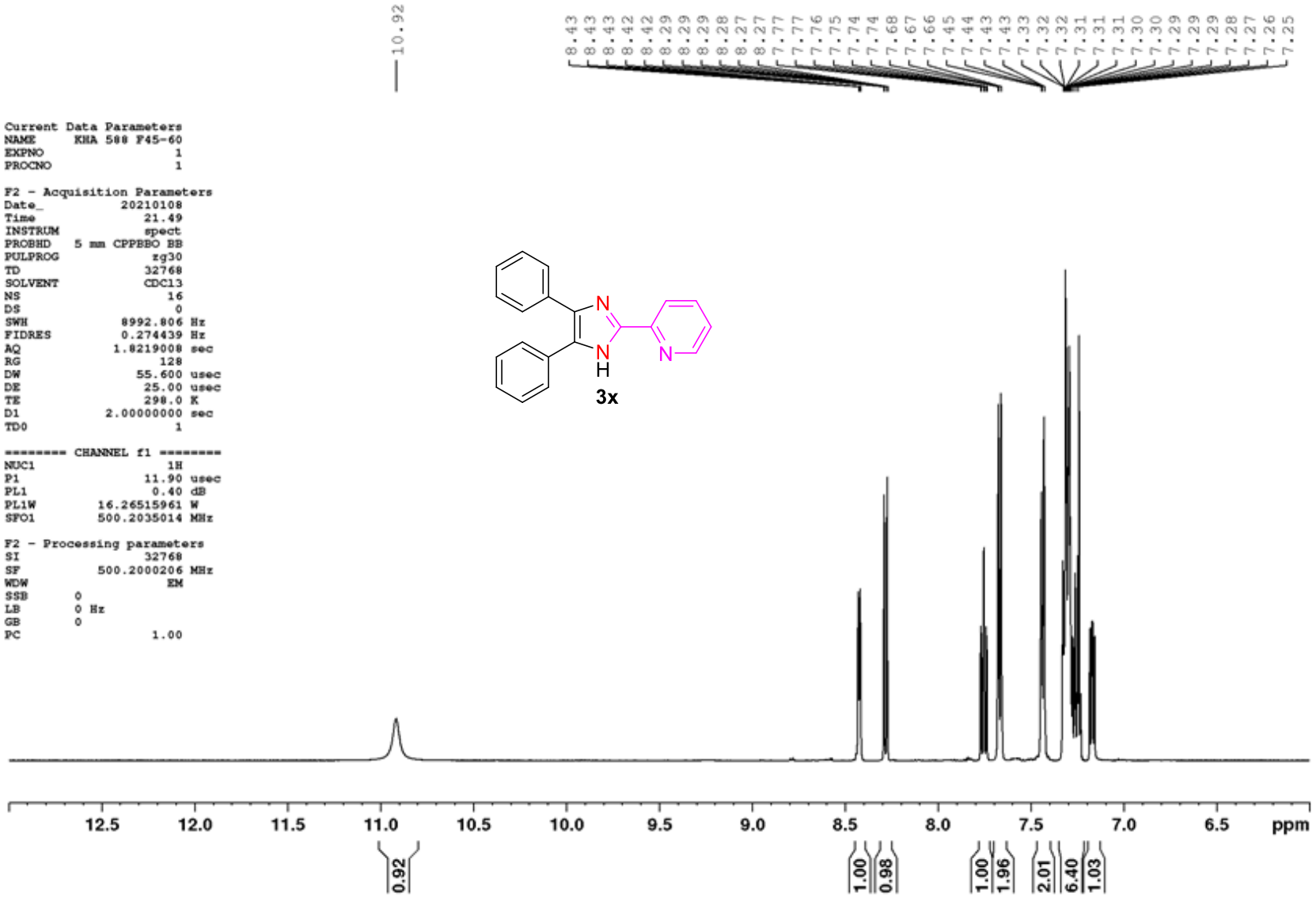


Figure S52. ^{1}H NMR spectrum of compound **3x** (500 MHz, $CDCl_3$, 25 ^{o}C)

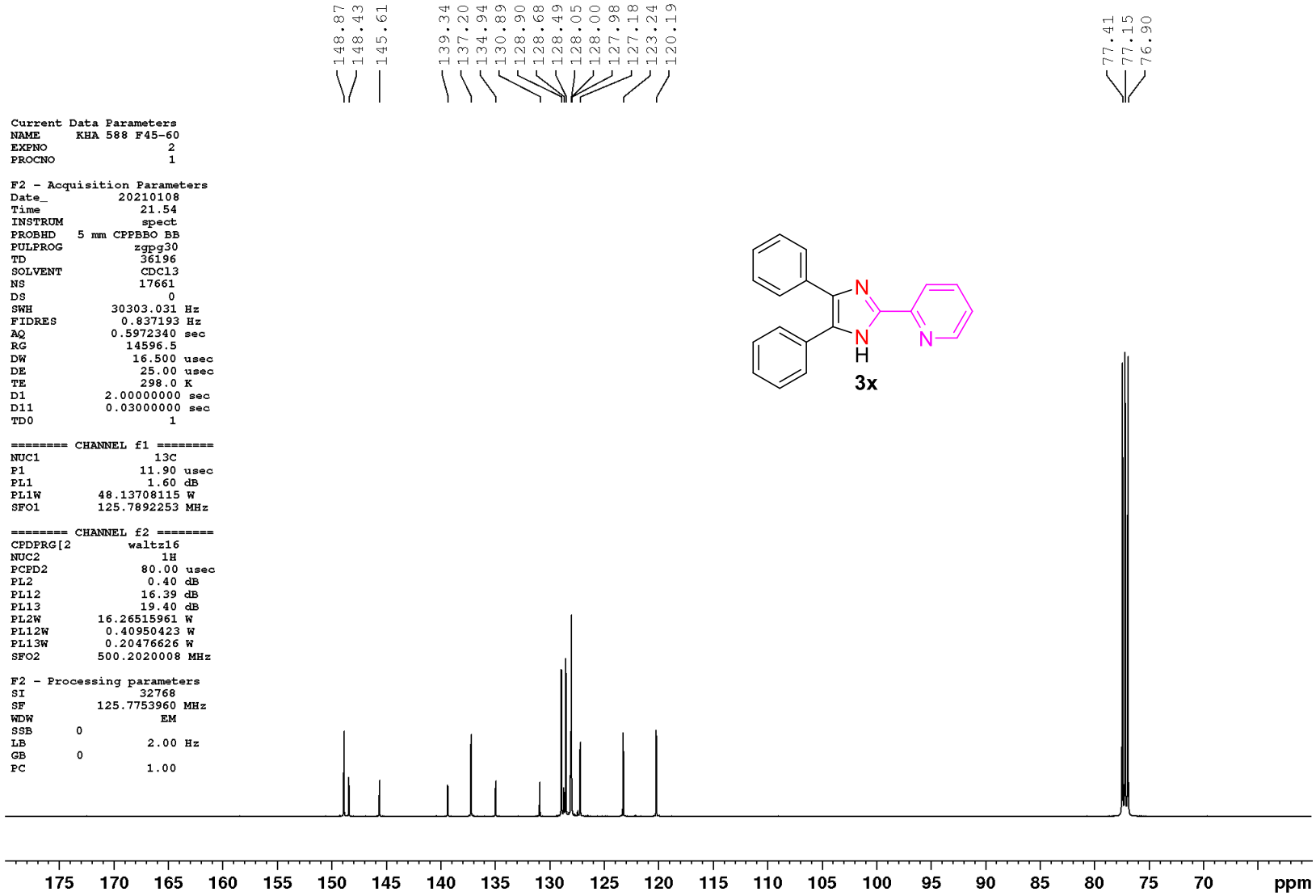


Figure S53. ^{13}C NMR spectrum of compound **3x** (125 MHz, $CDCl_3$, 25 ºC)

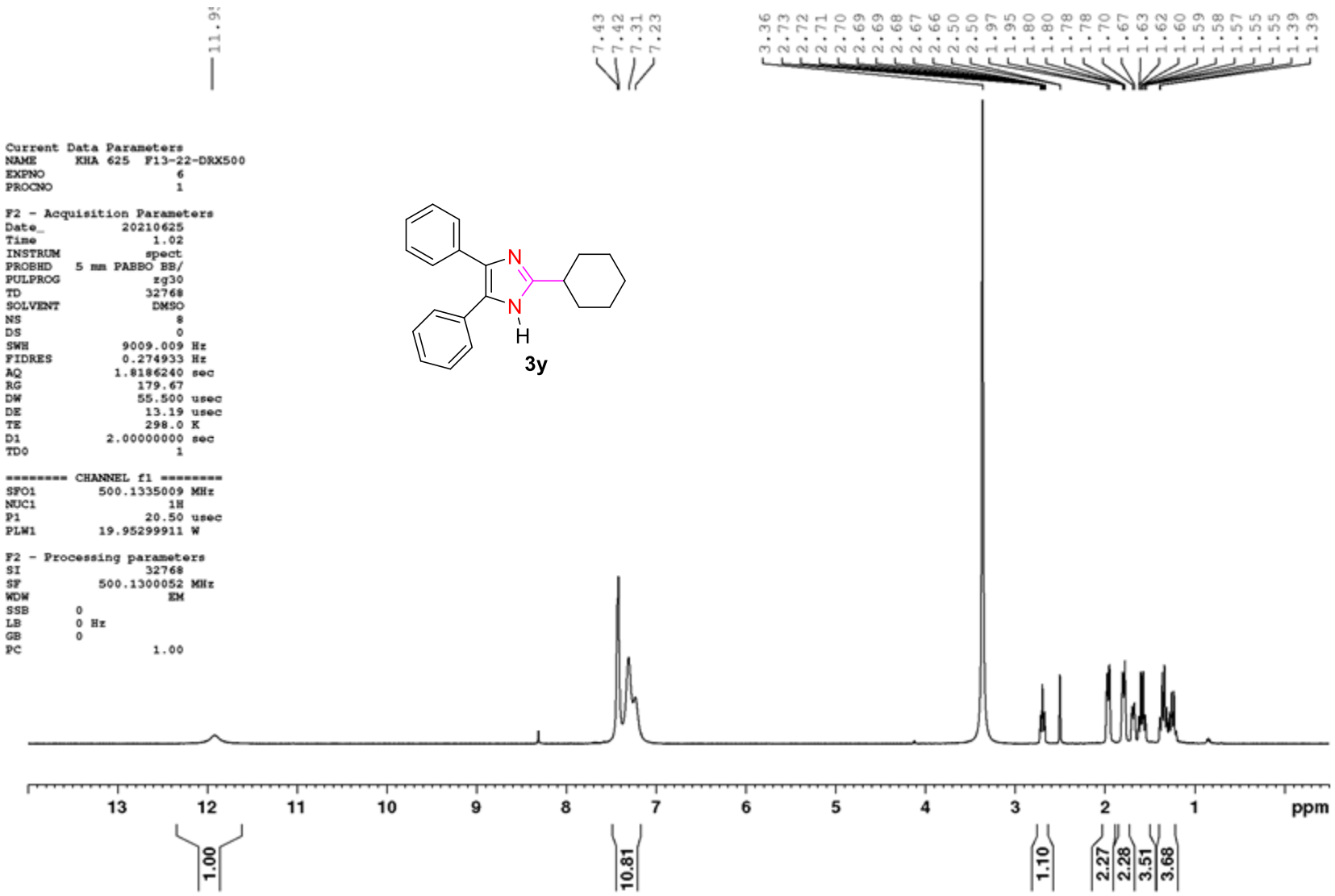


Figure S54. ^{1}H NMR spectrum of compound **3y** (500 MHz, $CDCl_3$, 25 ^{o}C)

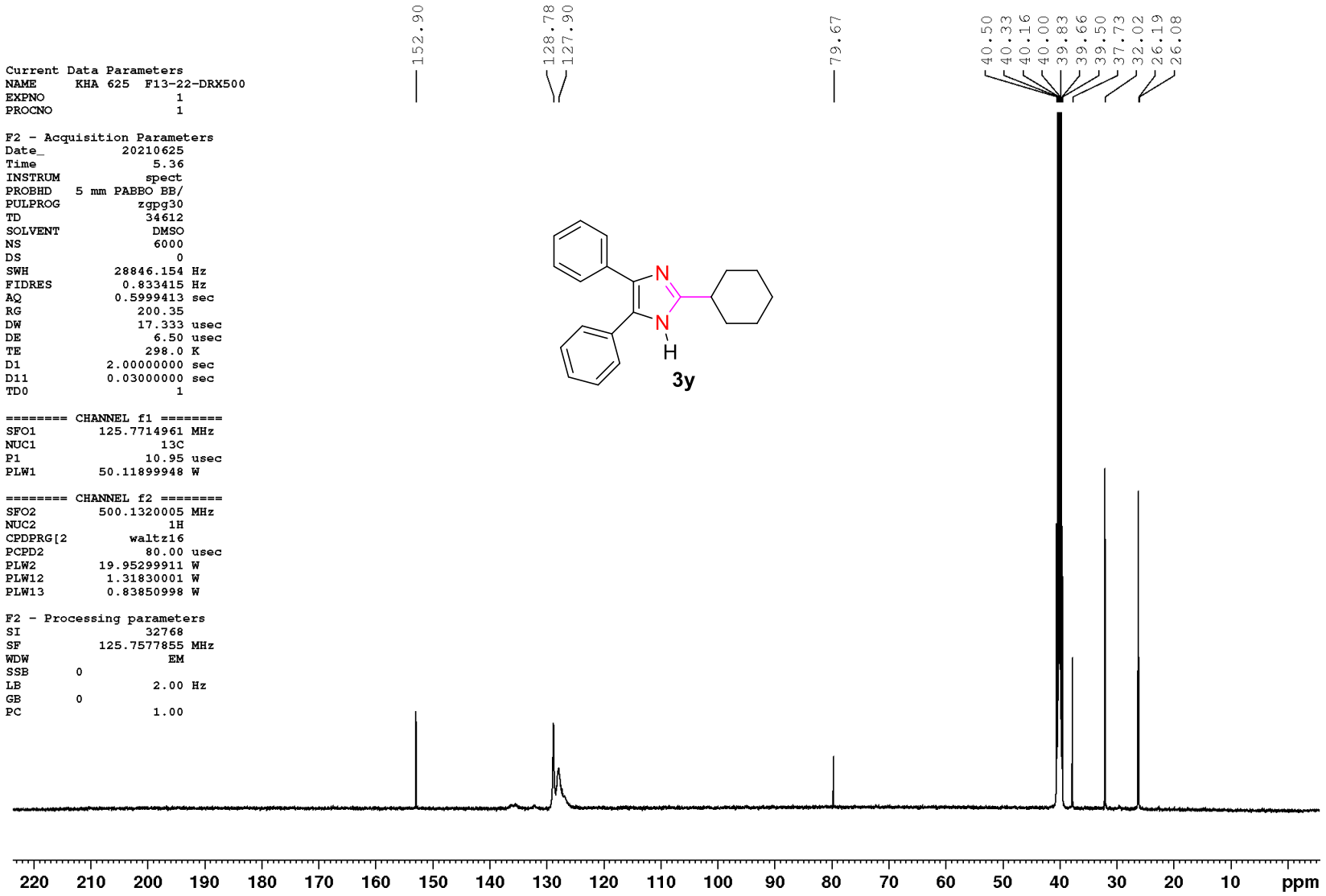


Figure S55. ^{13}C NMR spectrum of compound **3y** (125 MHz, $CDCl_3$, 25 ^oC)

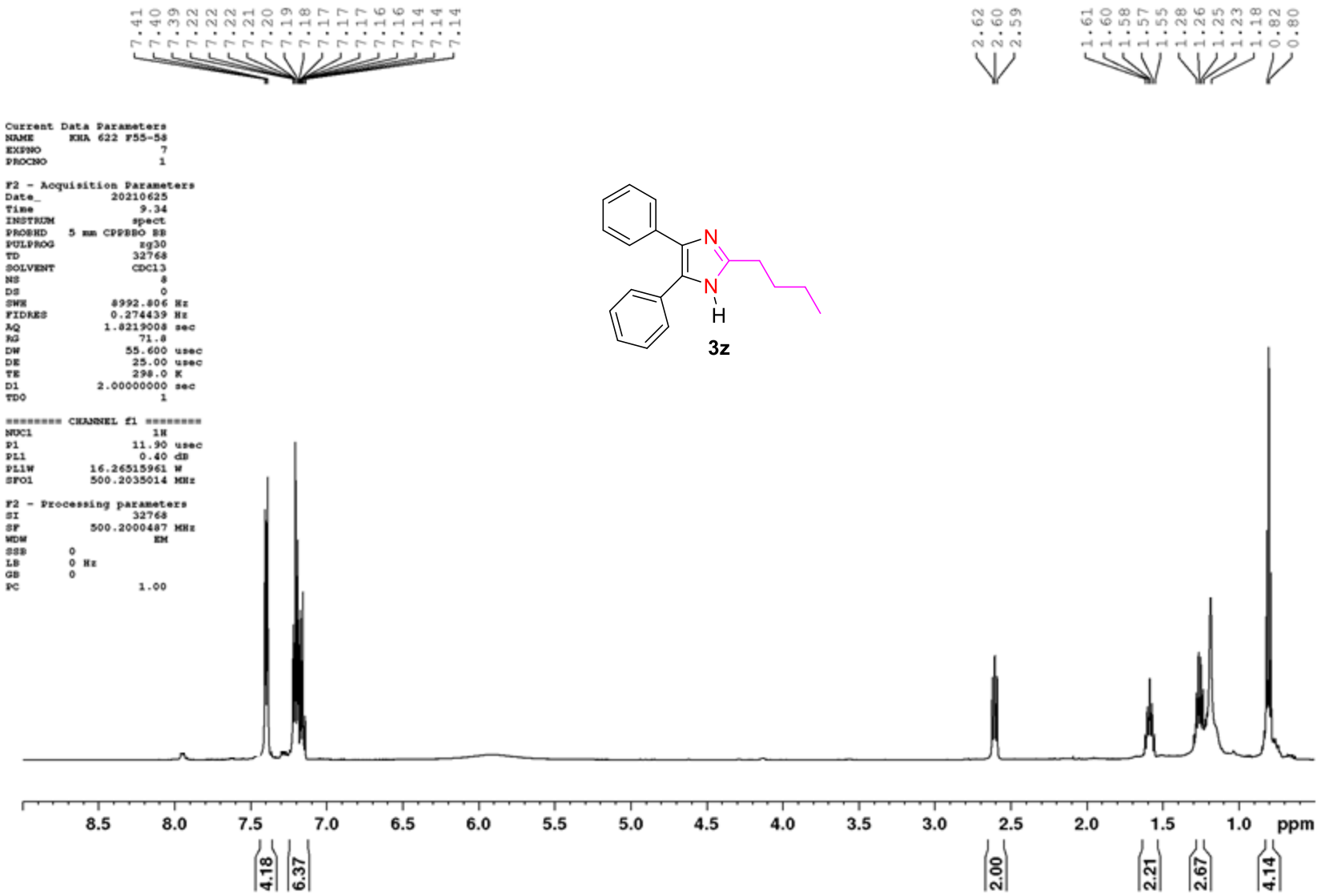


Figure S56. ^{1}H NMR spectrum of compound **3z** (500 MHz, $CDCl_3$, 25 ^{o}C)

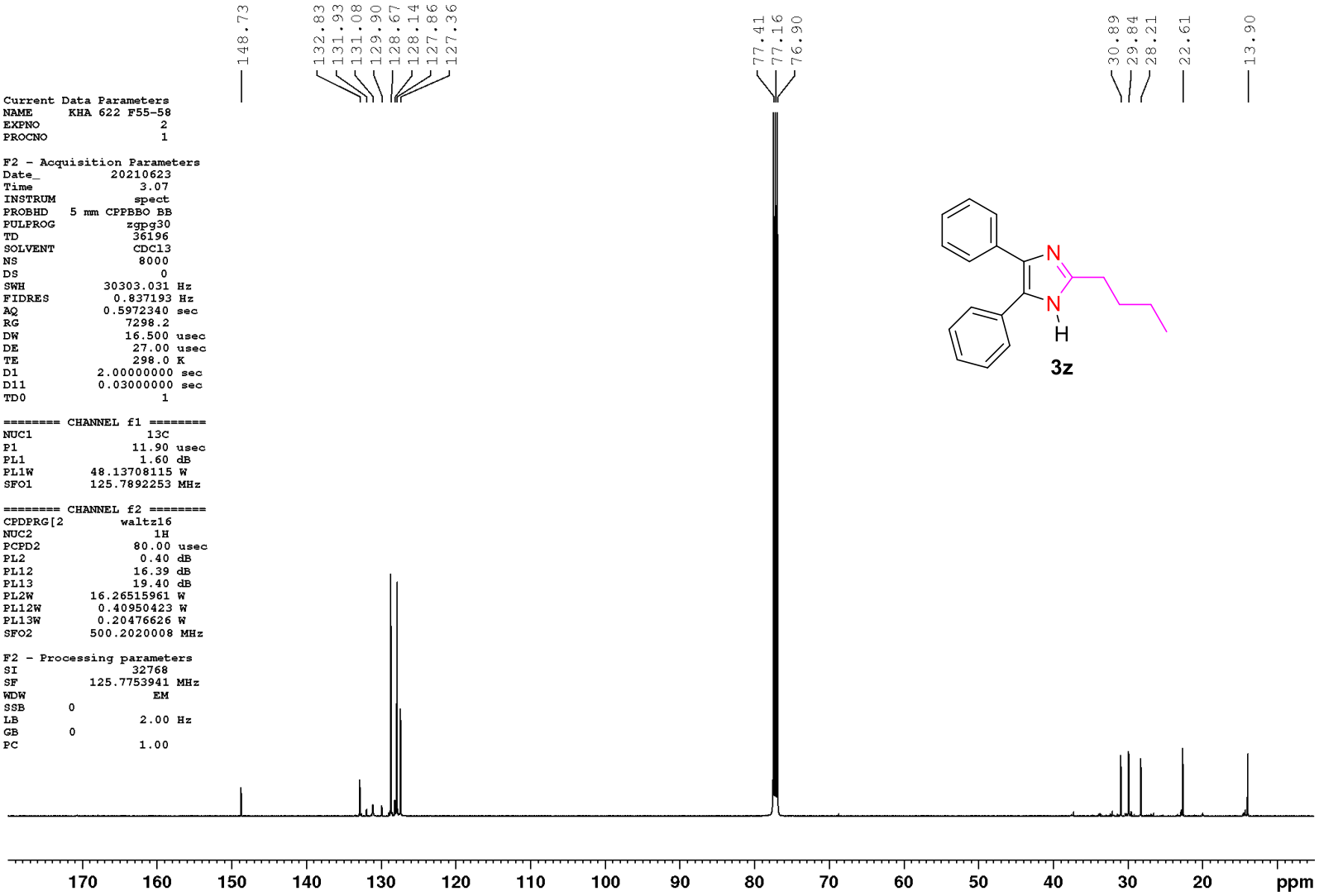


Figure S57. ^{13}C NMR spectrum of compound **3z** (125 MHz, $CDCl_3$, 25 ^oC)

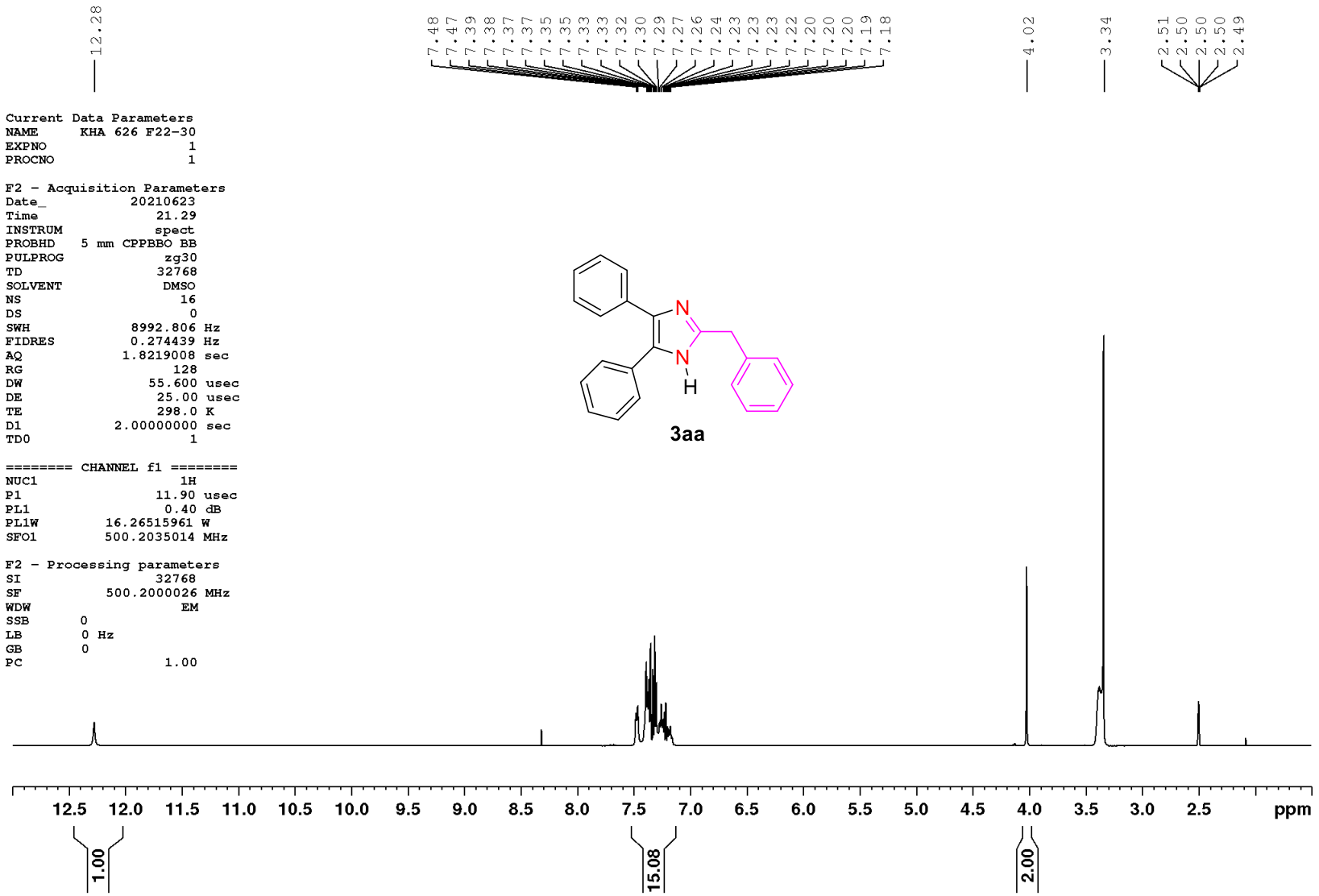


Figure S58. ^{1}H NMR spectrum of compound **3aa** (500 MHz, $CDCl_3$, 25 ^{o}C)

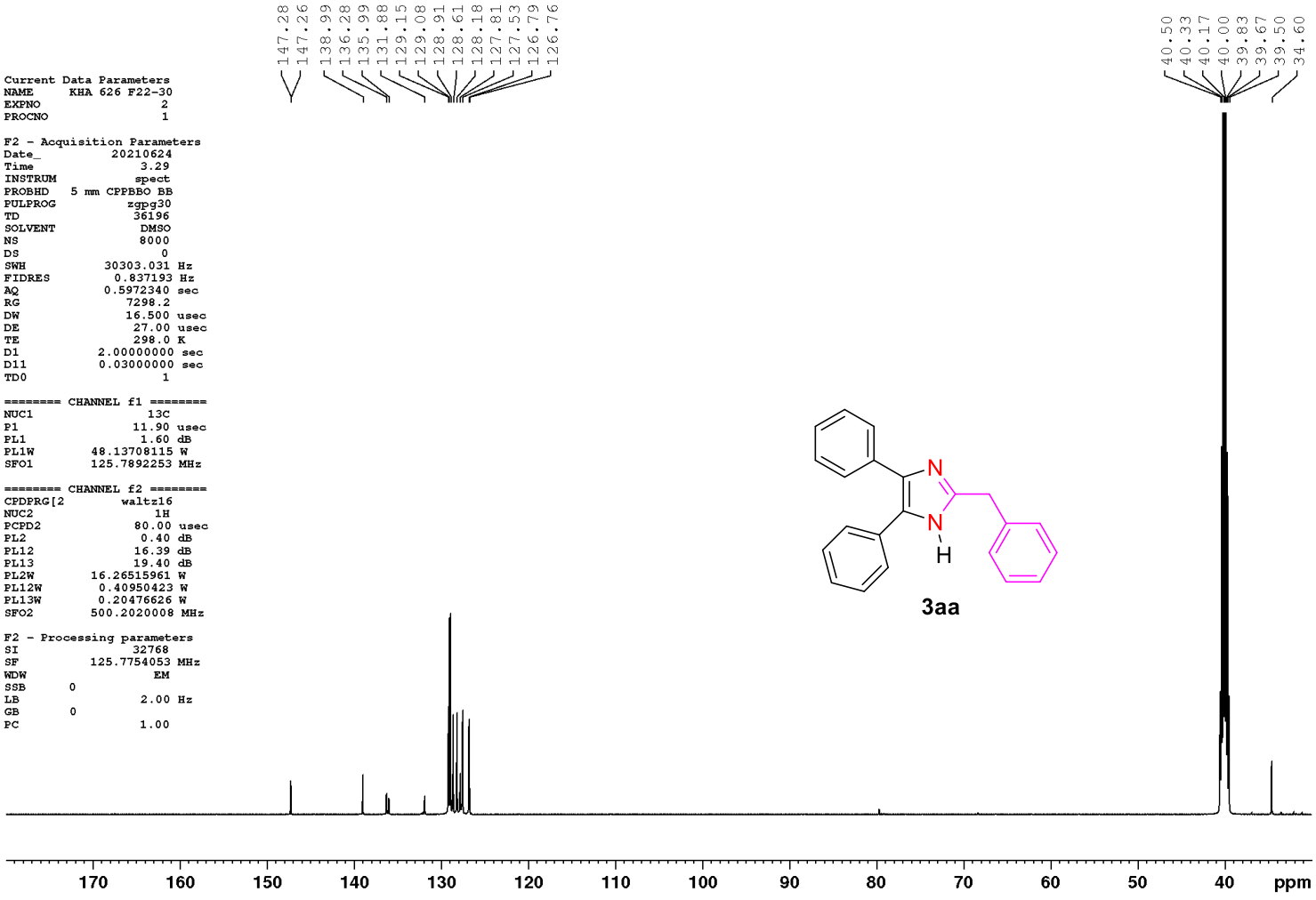


Figure S59. ^{13}C NMR spectrum of compound **3y** (125 MHz, $CDCl_3$, 25 ^{o}C)

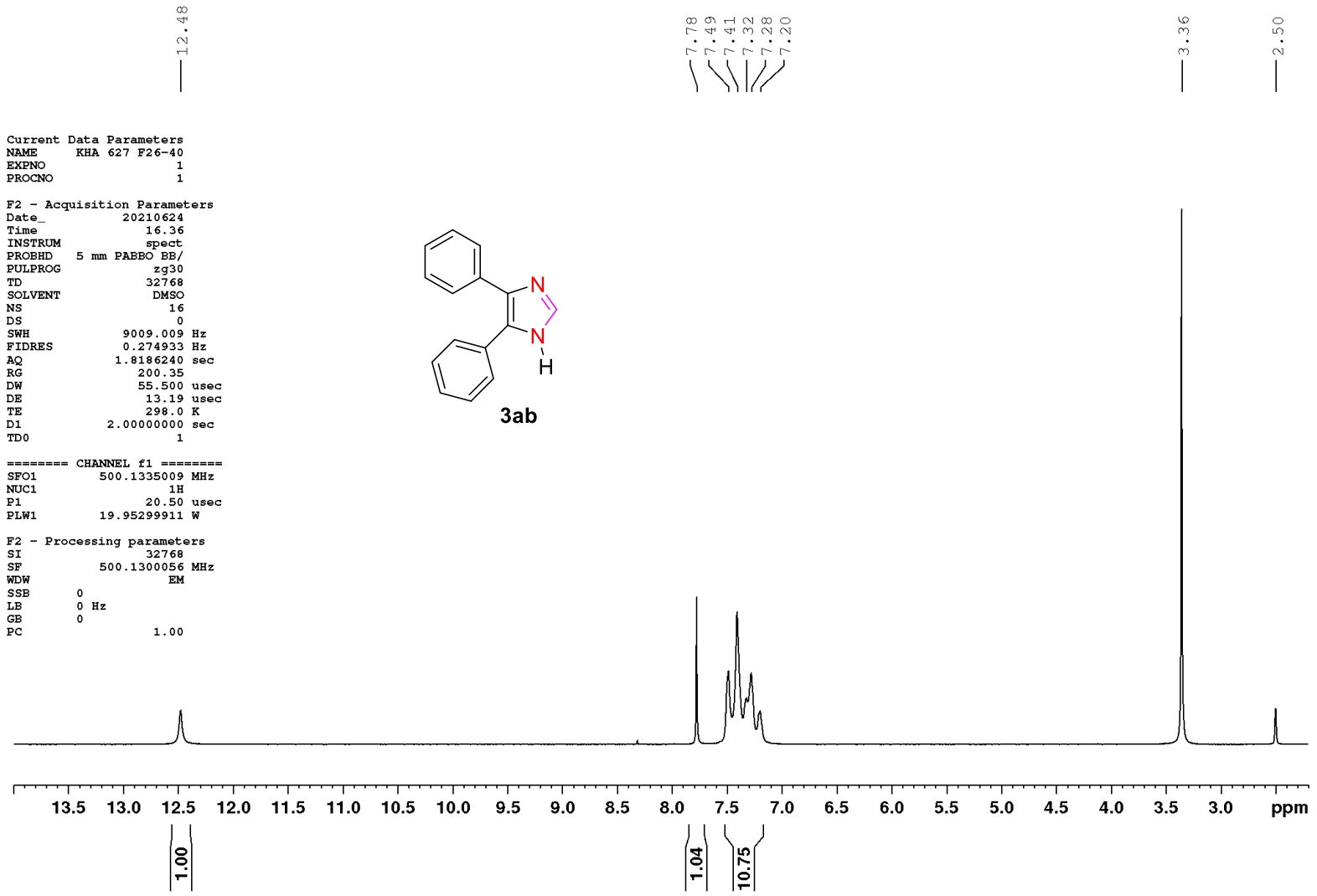


Figure S60. ^{1}H NMR spectrum of compound **3ab** (500 MHz, $CDCl_3$, 25 ^{o}C)

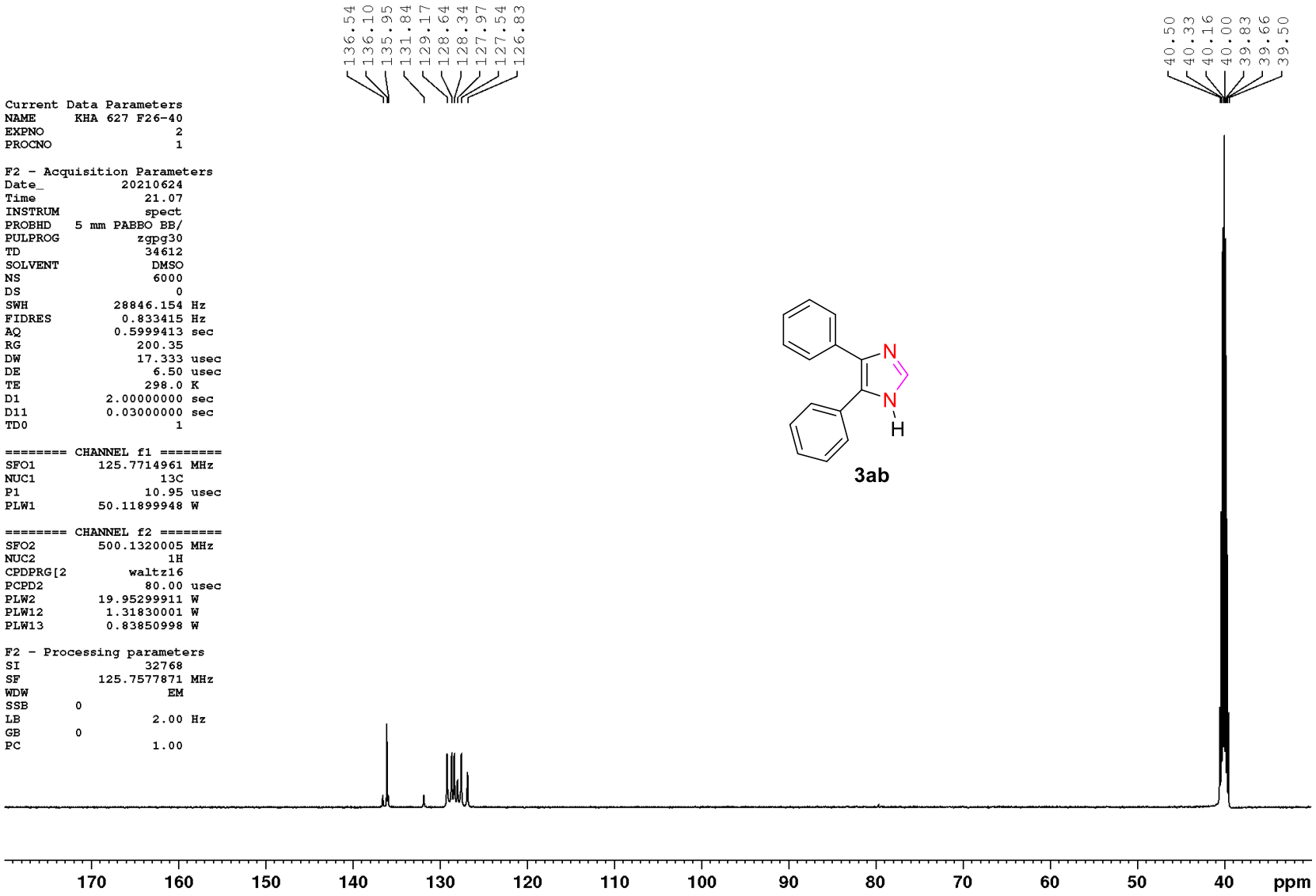


Figure S61. ^{13}C NMR spectrum of compound **3ab** (125 MHz, $CDCl_3$, 25 ^oC)

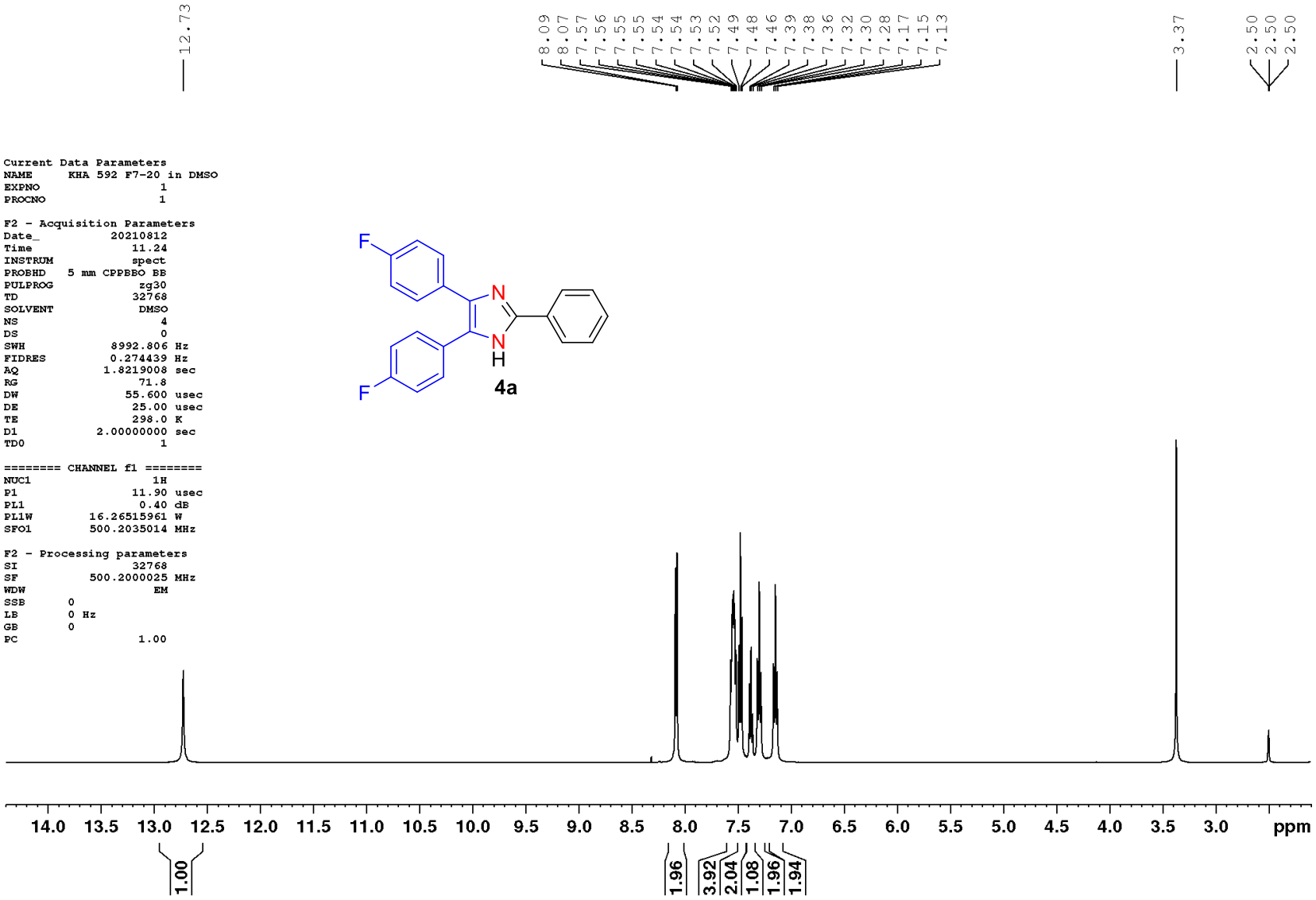


Figure S62. ^{1}H NMR spectrum of compound **4a** (500 MHz, DMSO-d_6, 25 ^{o}C)

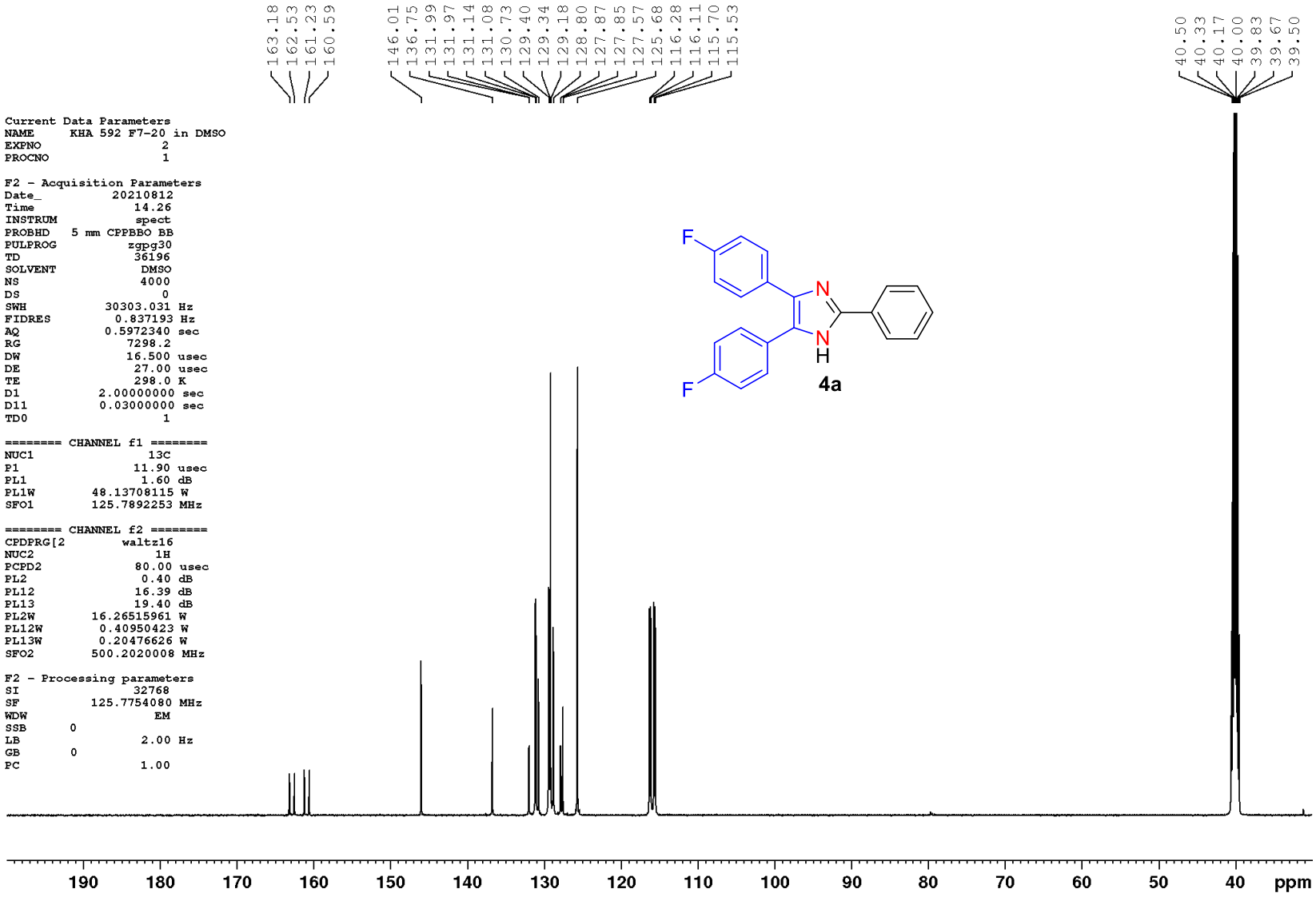


Figure S63. ^{13}C NMR spectrum of compound **4a** (125 MHz, DMSO-d_6, 25 ^{o}C)

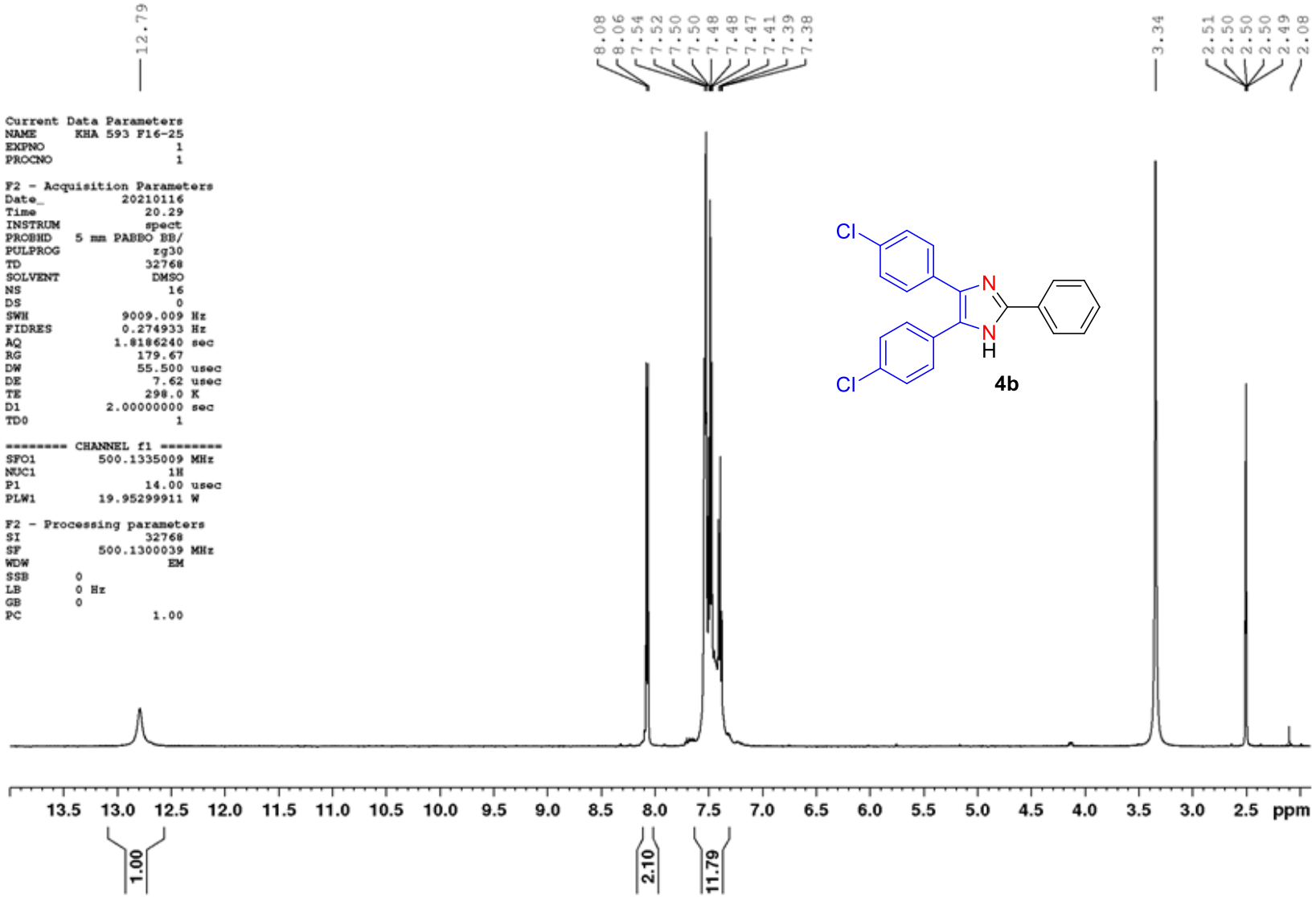
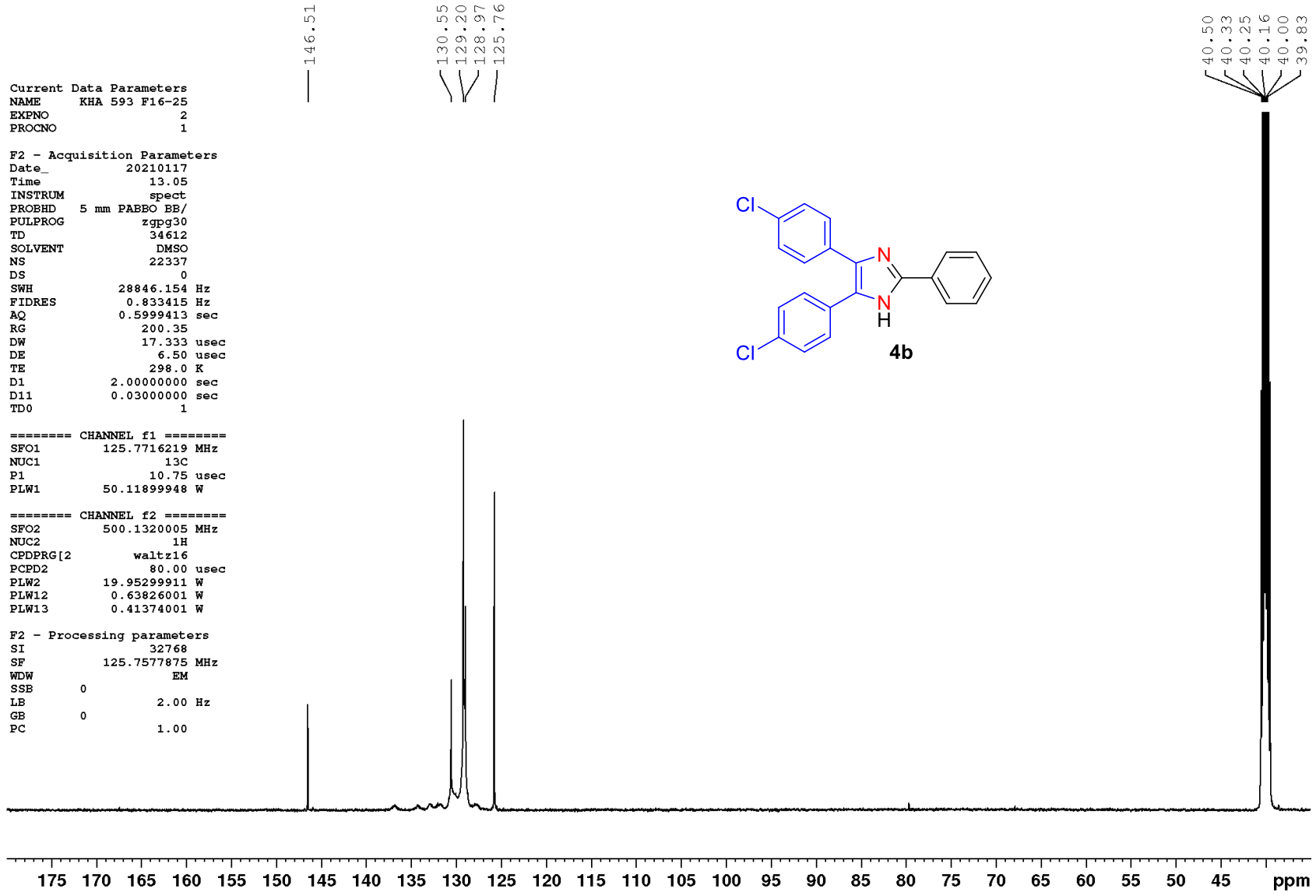


Figure S64. ^{1}H NMR spectrum of compound **4b** (500 MHz, DMSO-d_6, 25 ^{o}C)

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PLW13         0.41374001 W

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Figure S65. ^{13}C NMR spectrum of compound **4b** (125 MHz, DMSO-d_6, 25 ^{o}C)

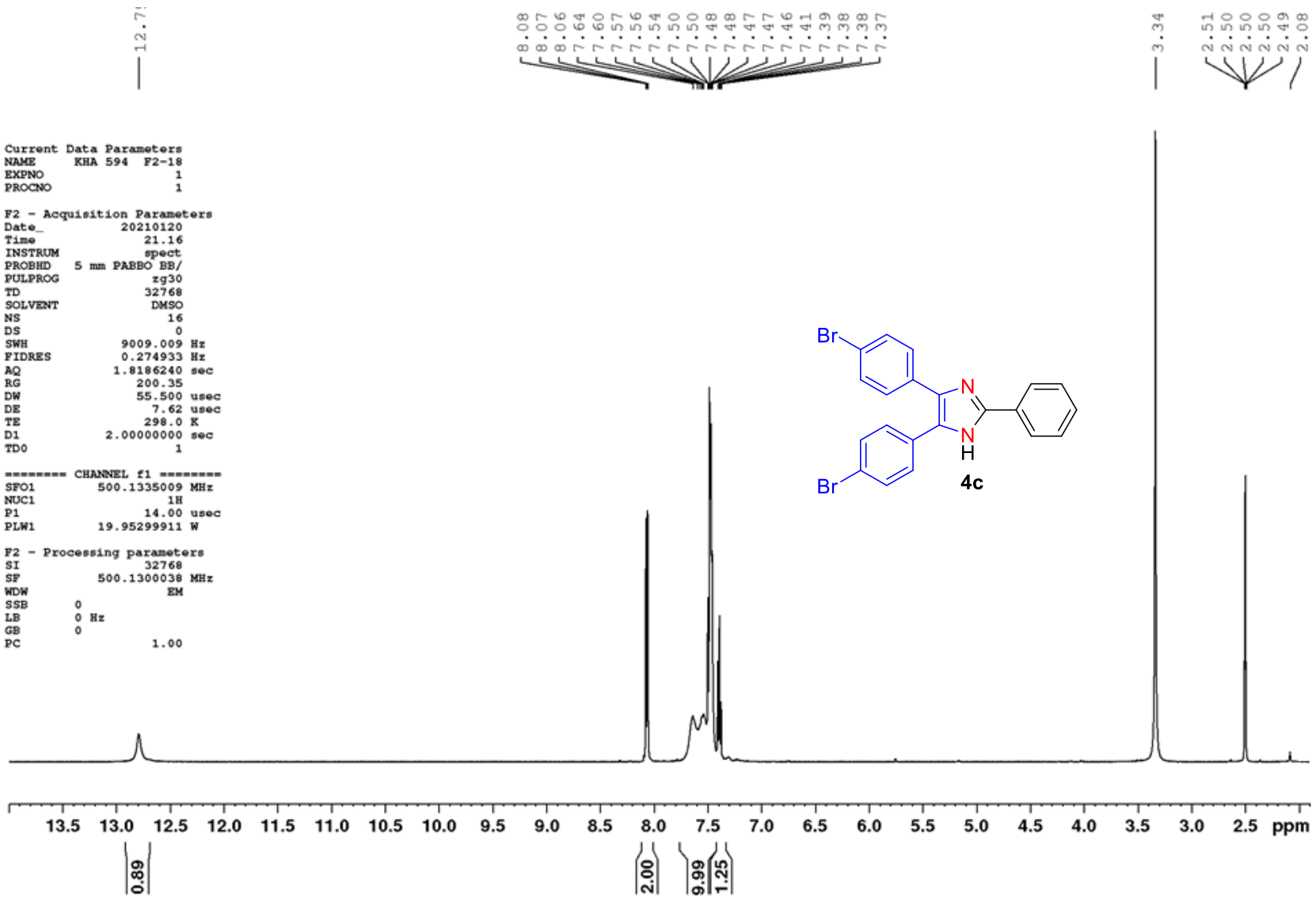
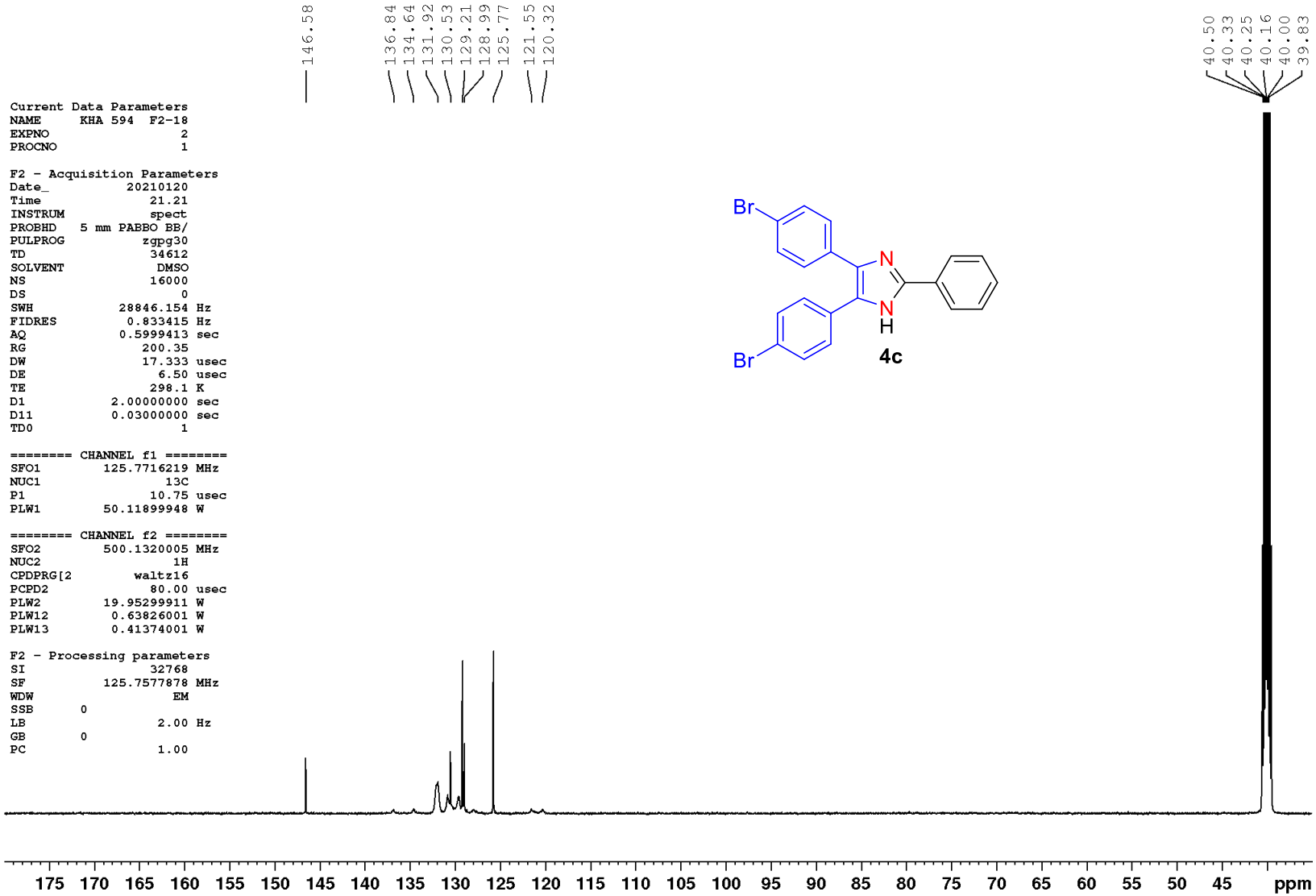


Figure S66. ^{1}H NMR spectrum of compound **4c** (500 MHz, DMSO-d_6, 25 ^{o}C)

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PLW12        0.63826001 W
PLW13        0.41374001 W

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Figure S67. ^{13}C NMR spectrum of compound **4c** (125 MHz, DMSO-d_6, 25 ^{o}C)

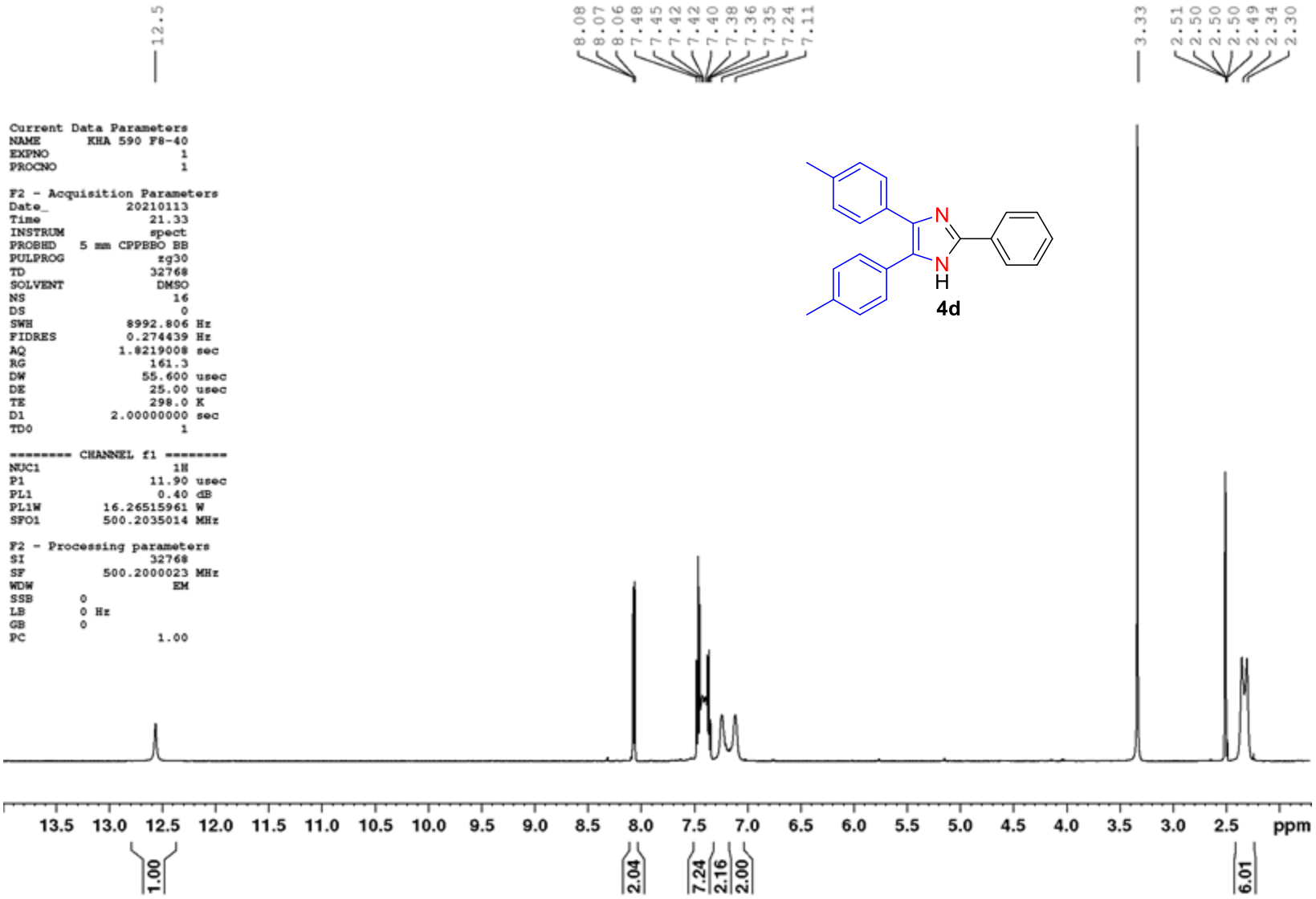


Figure S68. ^{1}H NMR spectrum of compound **4d** (500 MHz, DMSO-d_6, 25 ^{o}C)

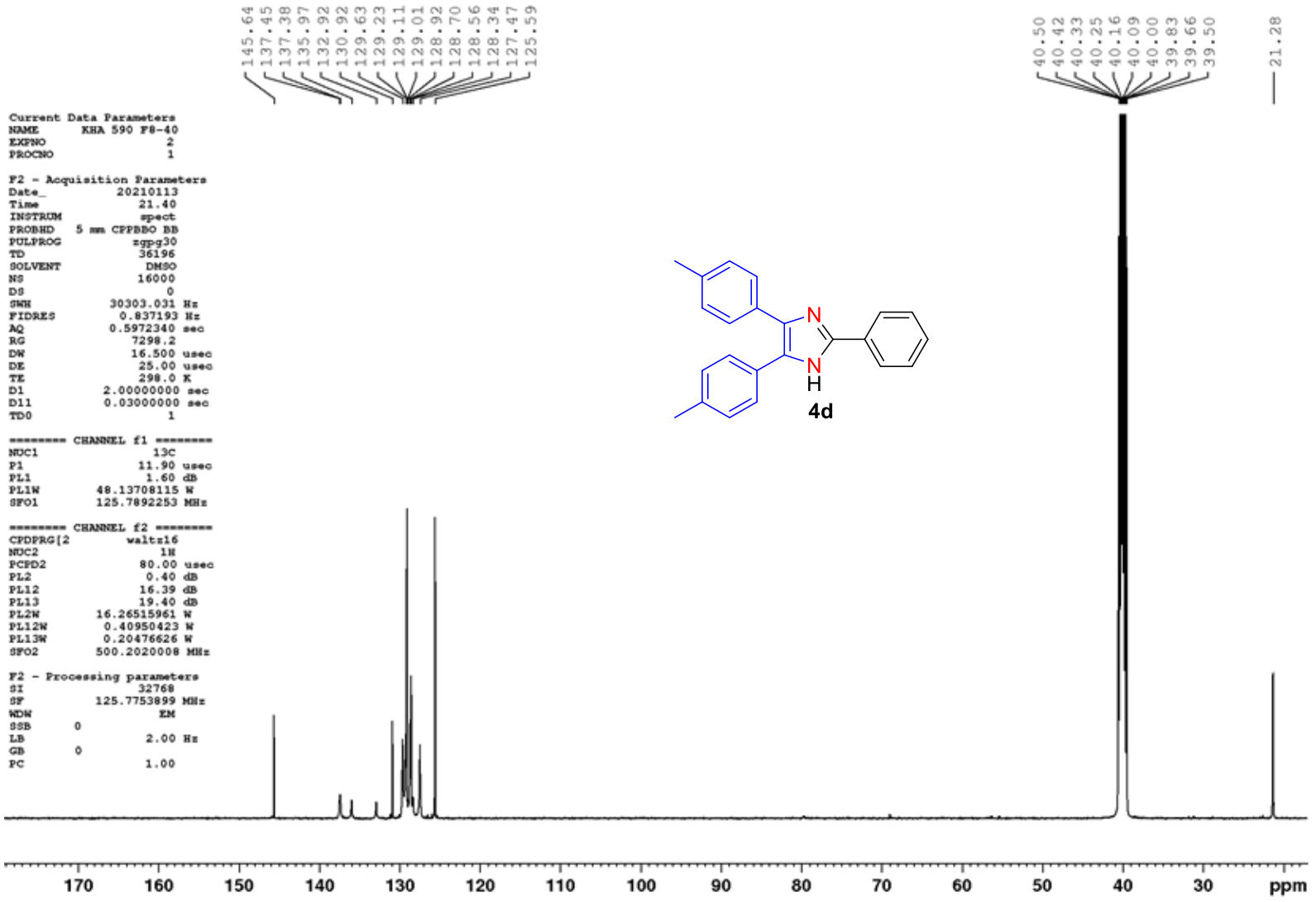


Figure S69. ^{13}C NMR spectrum of compound **4d** (125 MHz, DMSO-d_6, 25 ^{o}C)

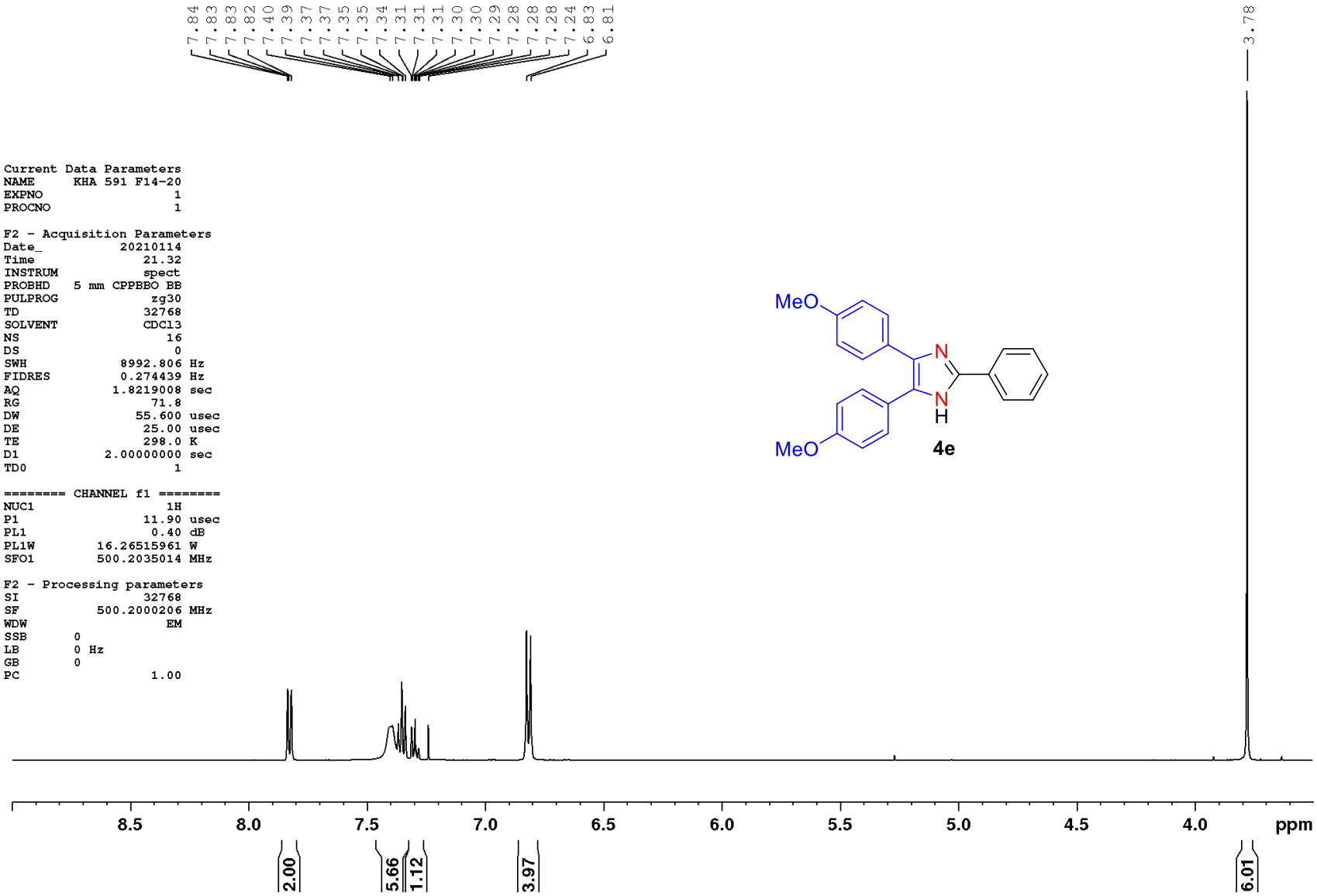


Figure S70. ^{1}H NMR spectrum of compound **4e** (500 MHz, $CDCl_3$, 25 ^{o}C)

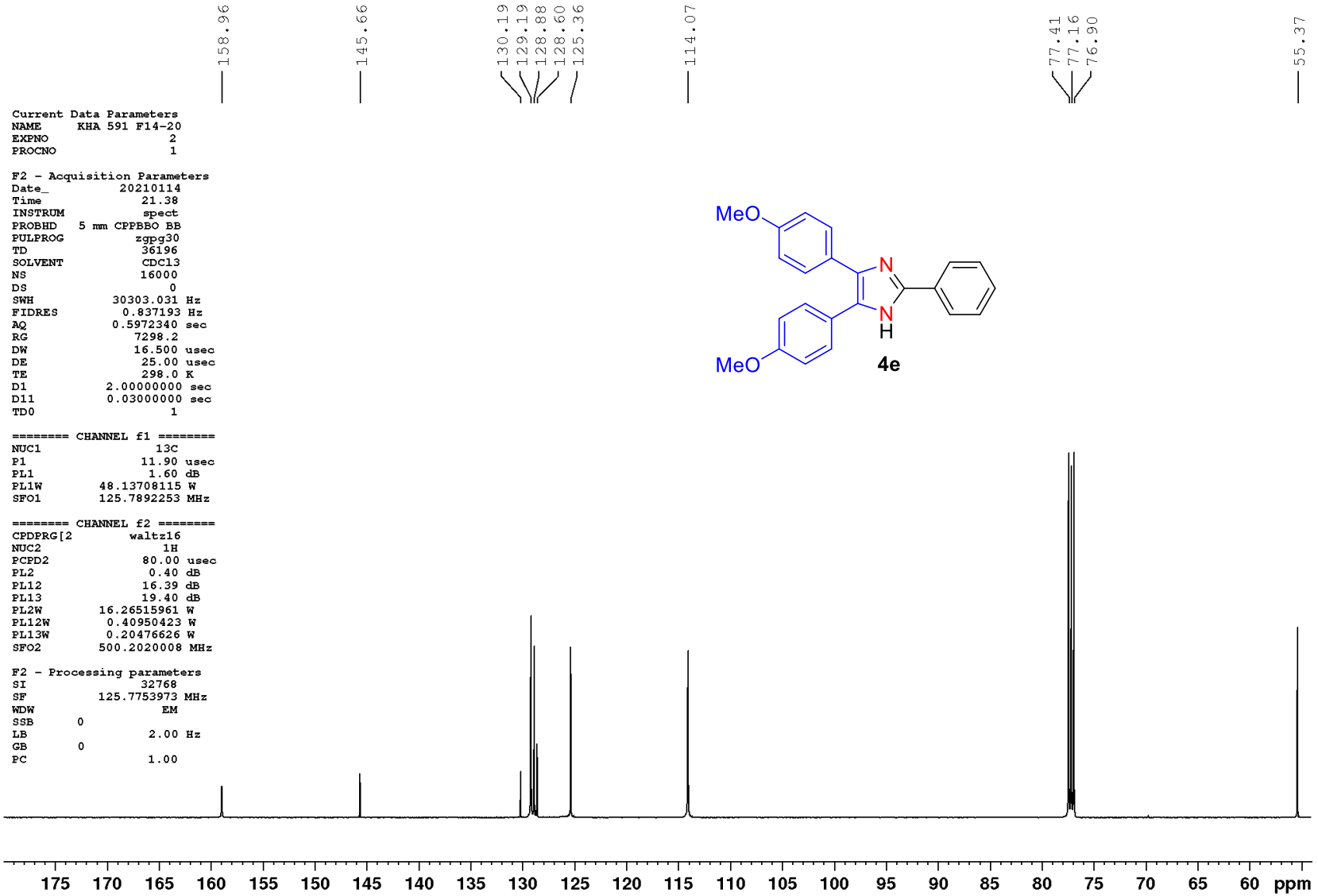


Figure S71. ^{13}C NMR spectrum of compound **4e** (125 MHz, $CDCl_3$, 25 ^oC)

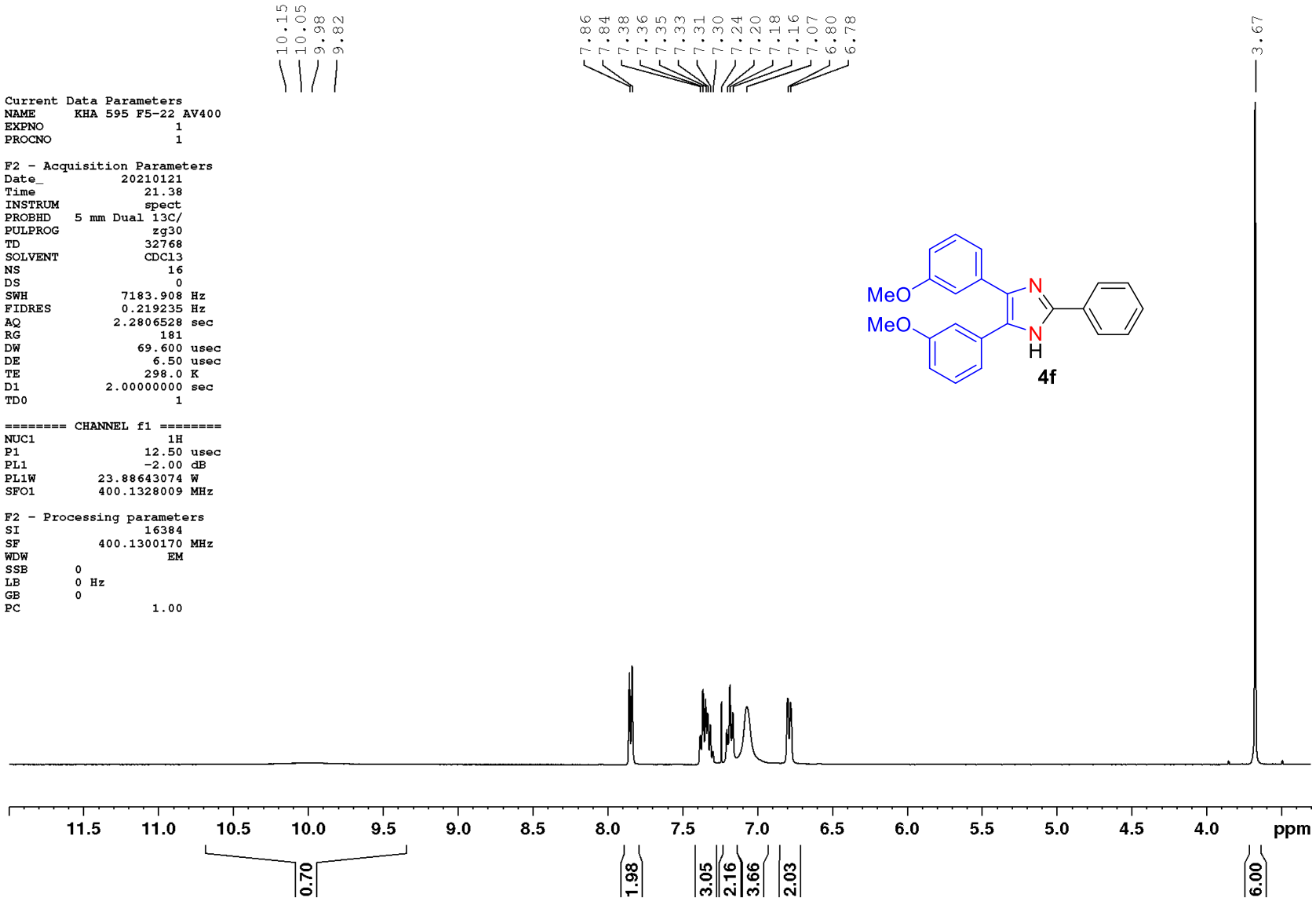


Figure S72. ^{1}H NMR spectrum of compound **4f** (400 MHz, $CDCl_3$, 25 ^{o}C)

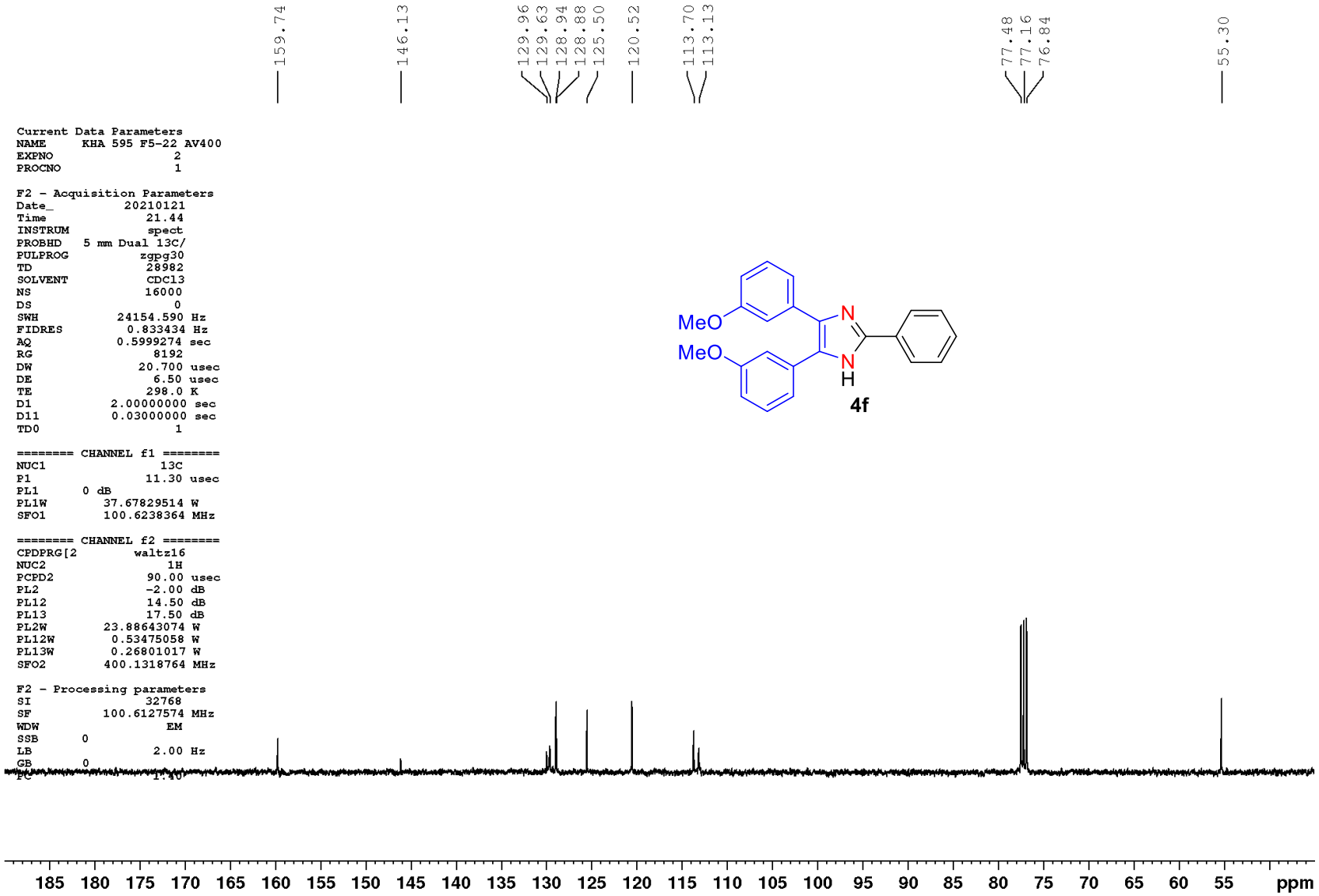


Figure S73. ^{13}C NMR spectrum of compound **4f** (100 MHz, $CDCl_3$, 25 ^oC)

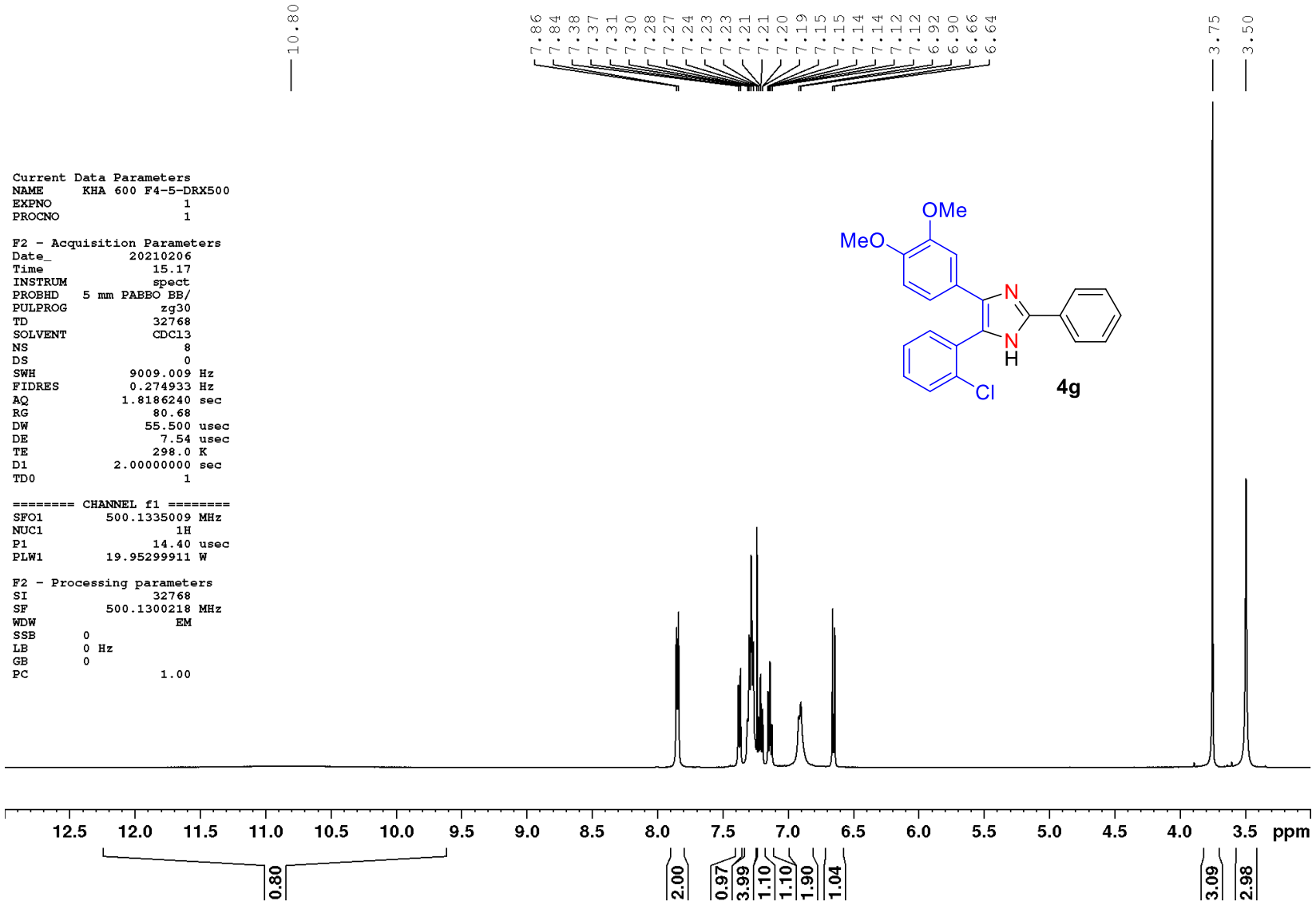


Figure S74. ^{1}H NMR spectrum of compound **4g** (500 MHz, $CDCl_3$, 25 ^{o}C)

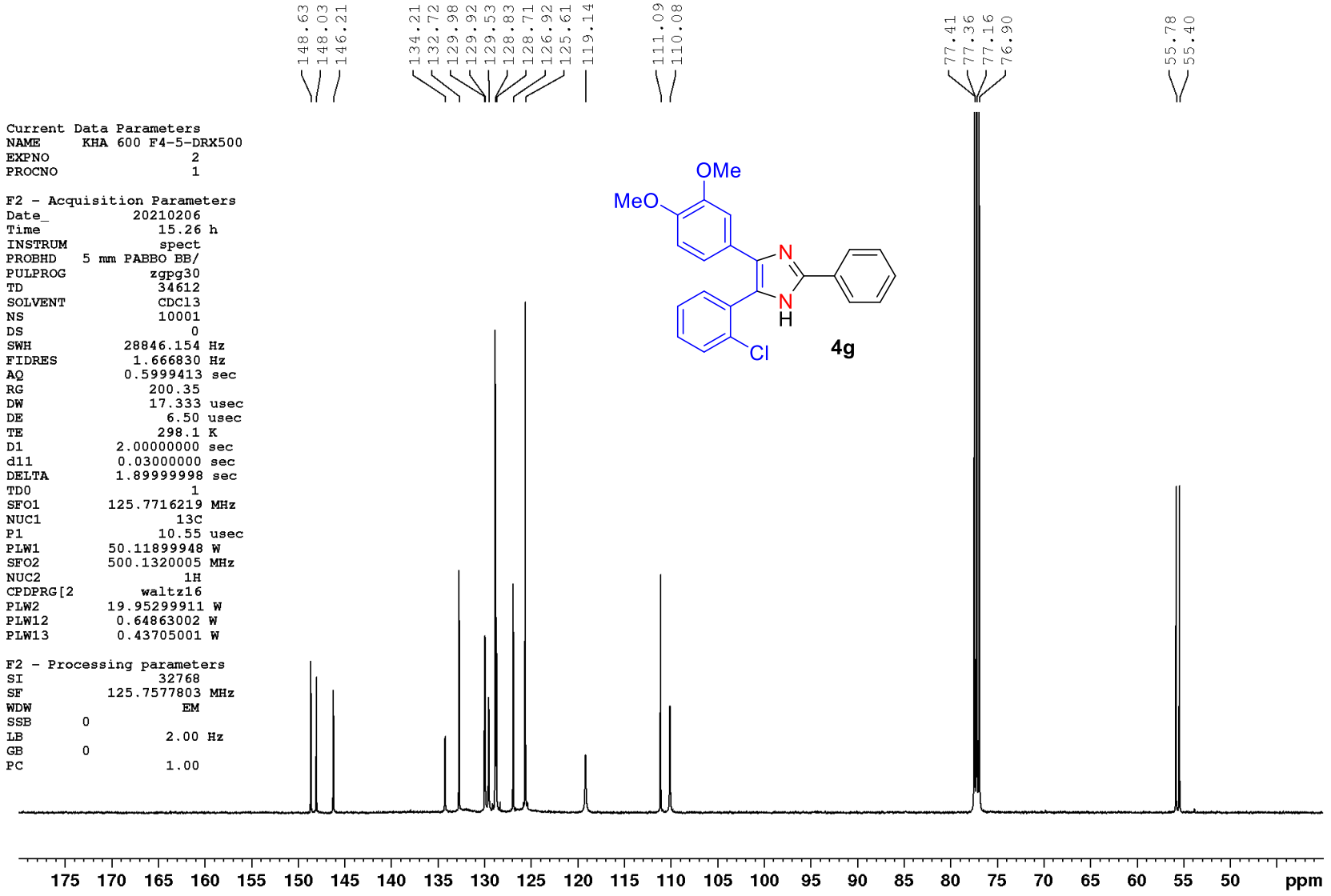


Figure S75. ^{13}C NMR spectrum of compound **4g** (125 MHz, $CDCl_3$, 25 ^{o}C)

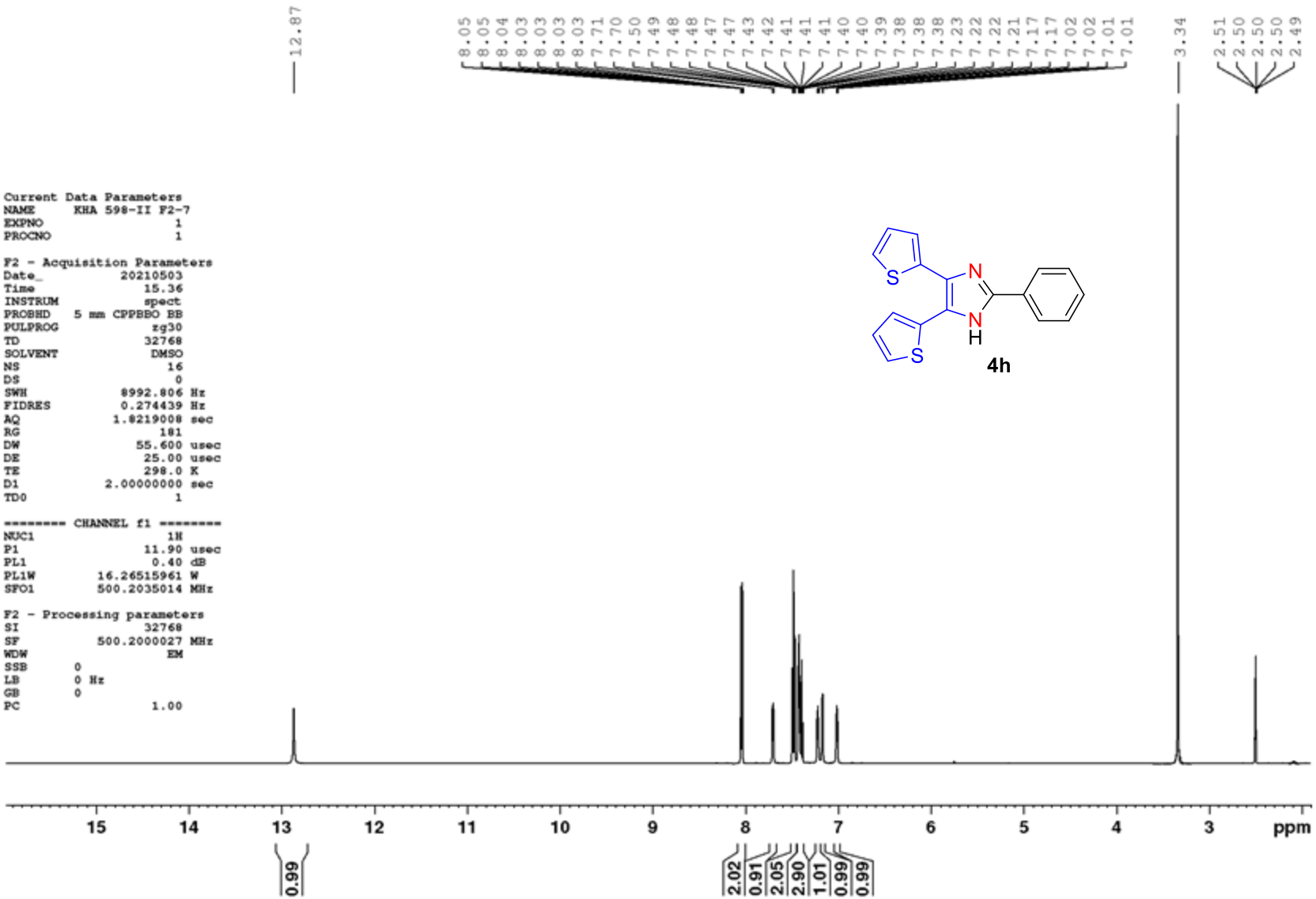


Figure S76. ^{1}H NMR spectrum of compound **4h** (500 MHz, DMSO-d_6, 25 ^{o}C)

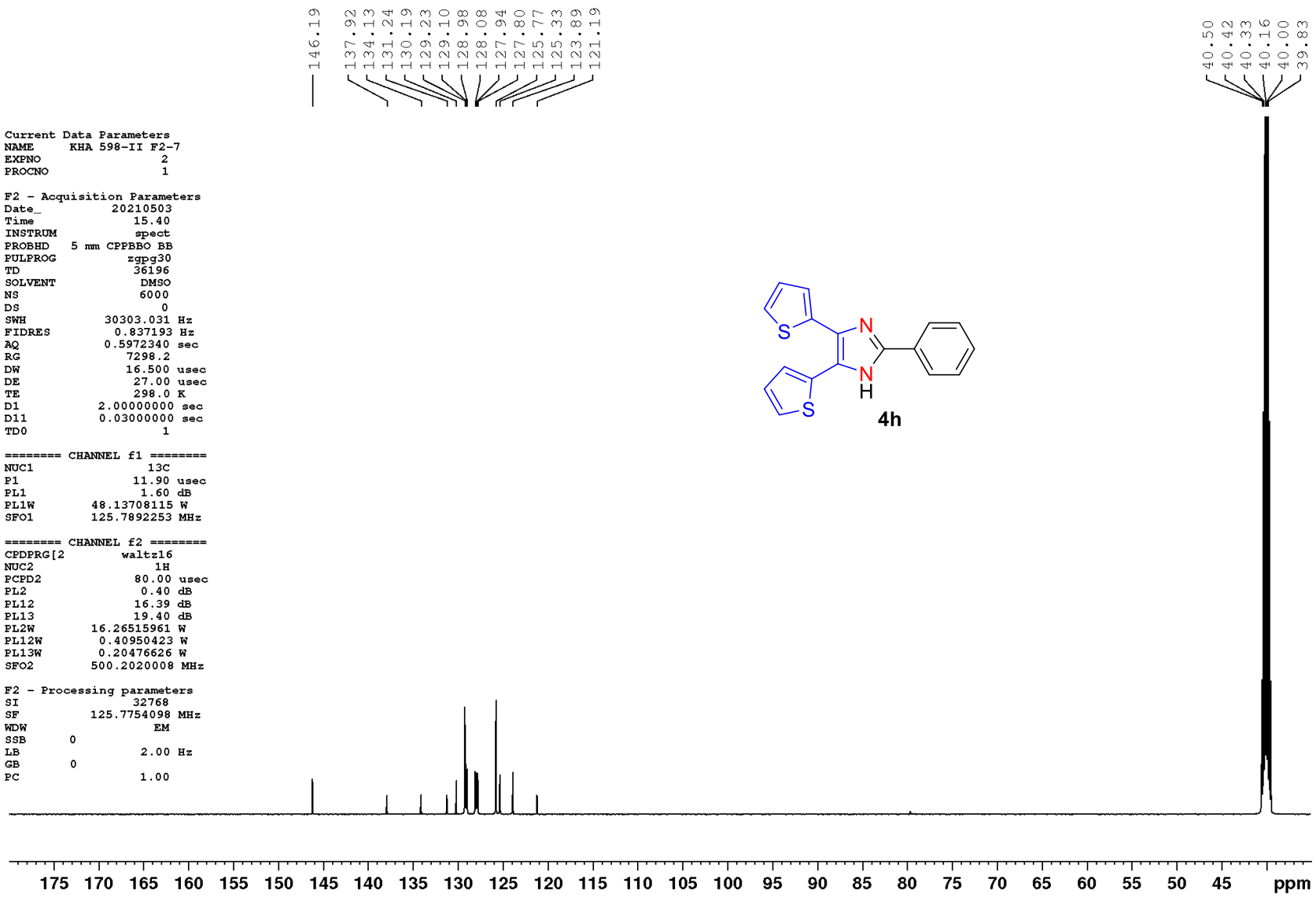


Figure S77. ^{13}C NMR spectrum of compound **4h** (125 MHz, DMSO-d_6, 25 ^{o}C)

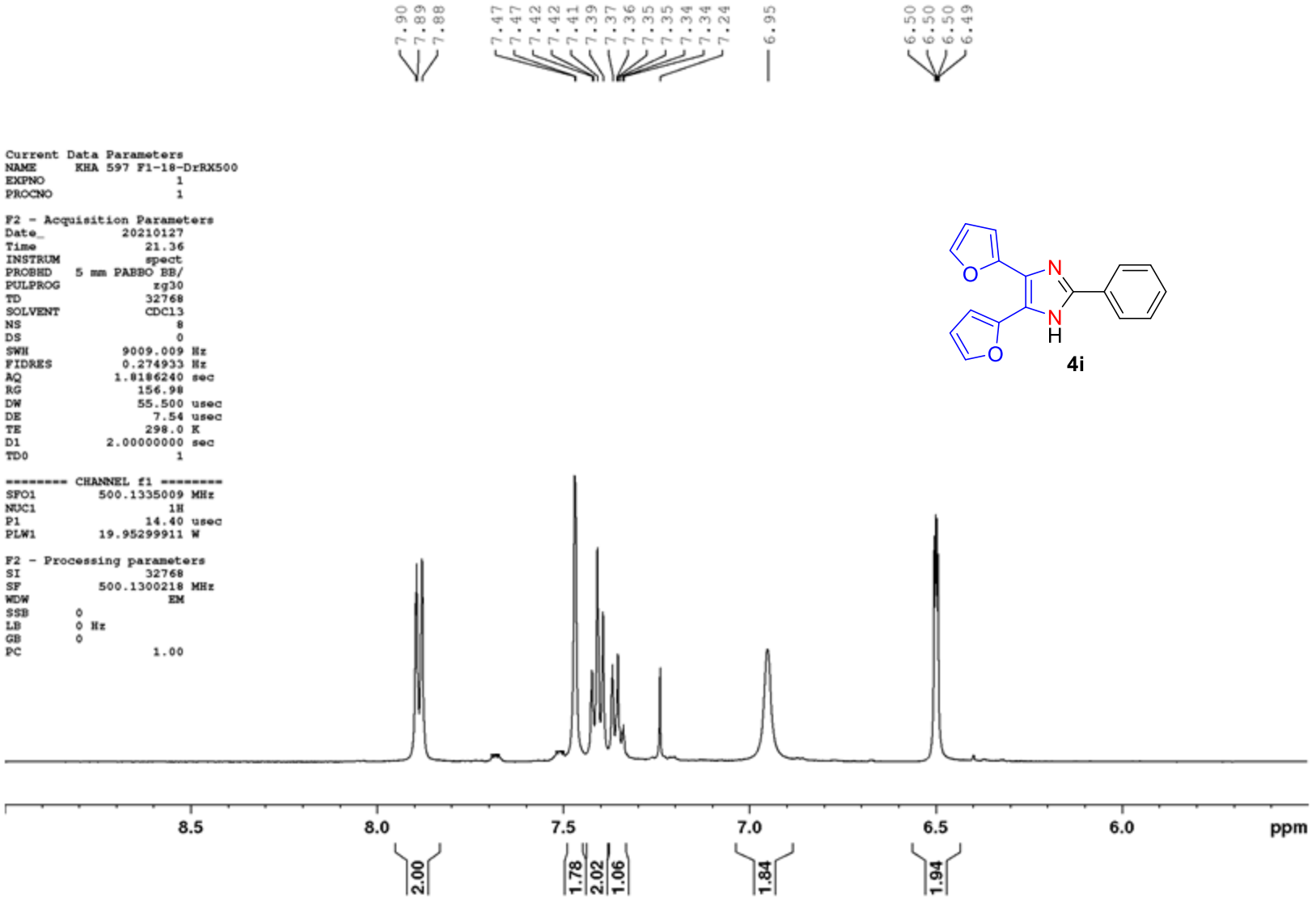


Figure S78. ^{1}H NMR spectrum of compound **4i** (500 MHz, $CDCl_3$, 25 ^{o}C)

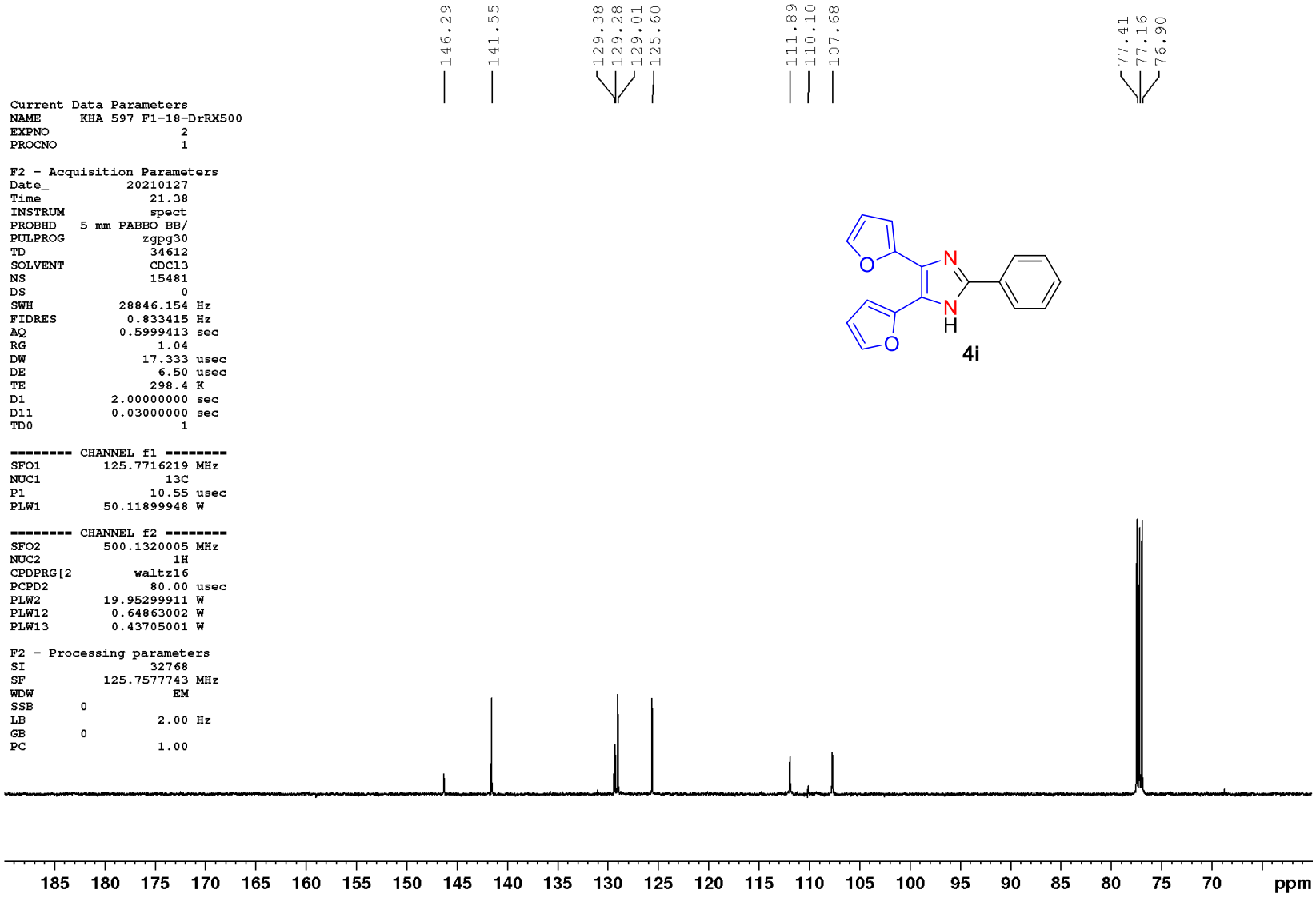


Figure S79. ^{13}C NMR spectrum of compound **4i** (125 MHz, $CDCl_3$, 25 ^oC)

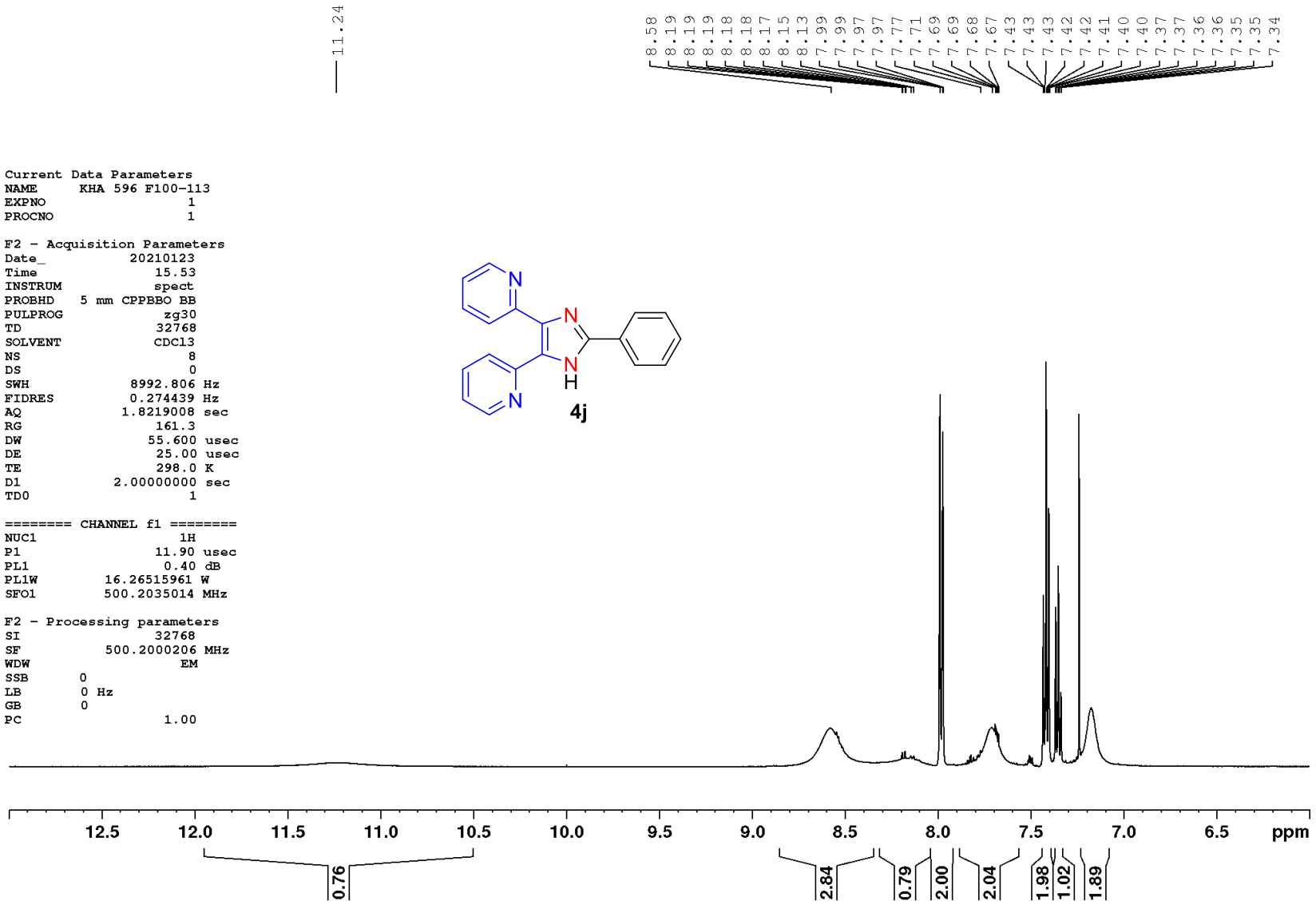


Figure S80. ^{1}H NMR spectrum of compound **4j** (500 MHz, $CDCl_3$, 25 ^{o}C)

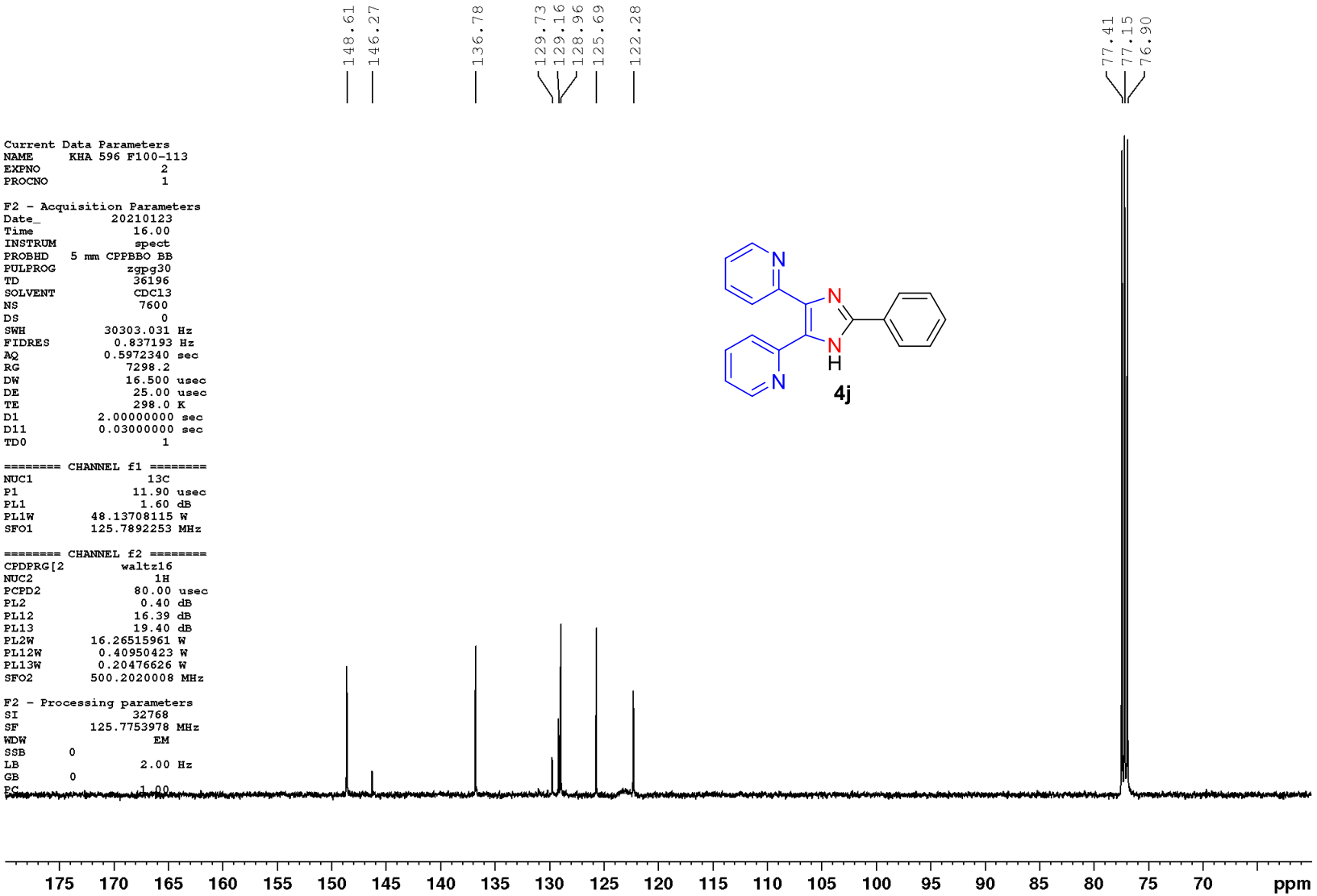


Figure S81. ^{13}C NMR spectrum of compound **4j** (125 MHz, $CDCl_3$, 25 ^oC)

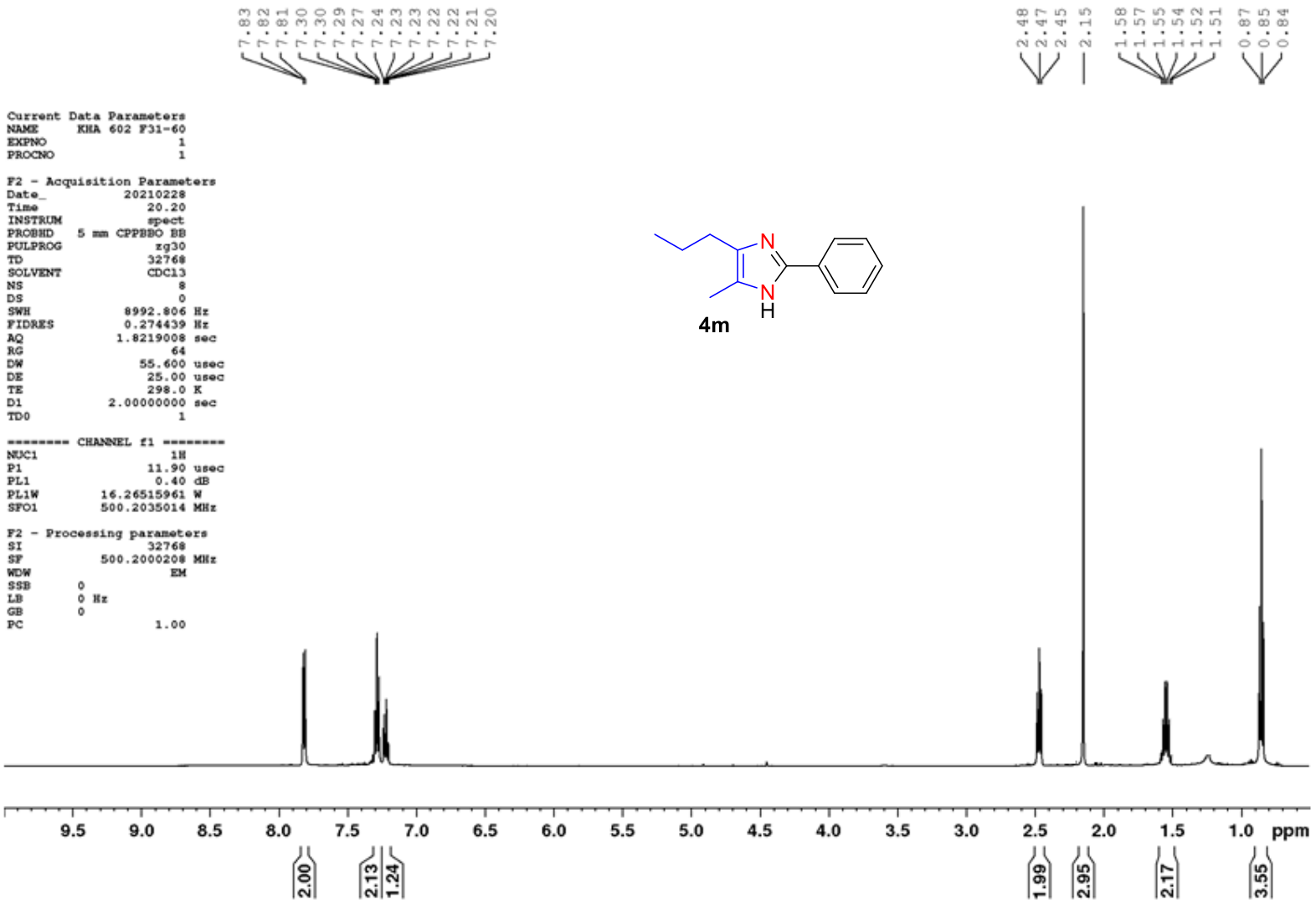


Figure S82. ^{1}H NMR spectrum of compound **4m** (500 MHz, $CDCl_3$, 25 ^{o}C)

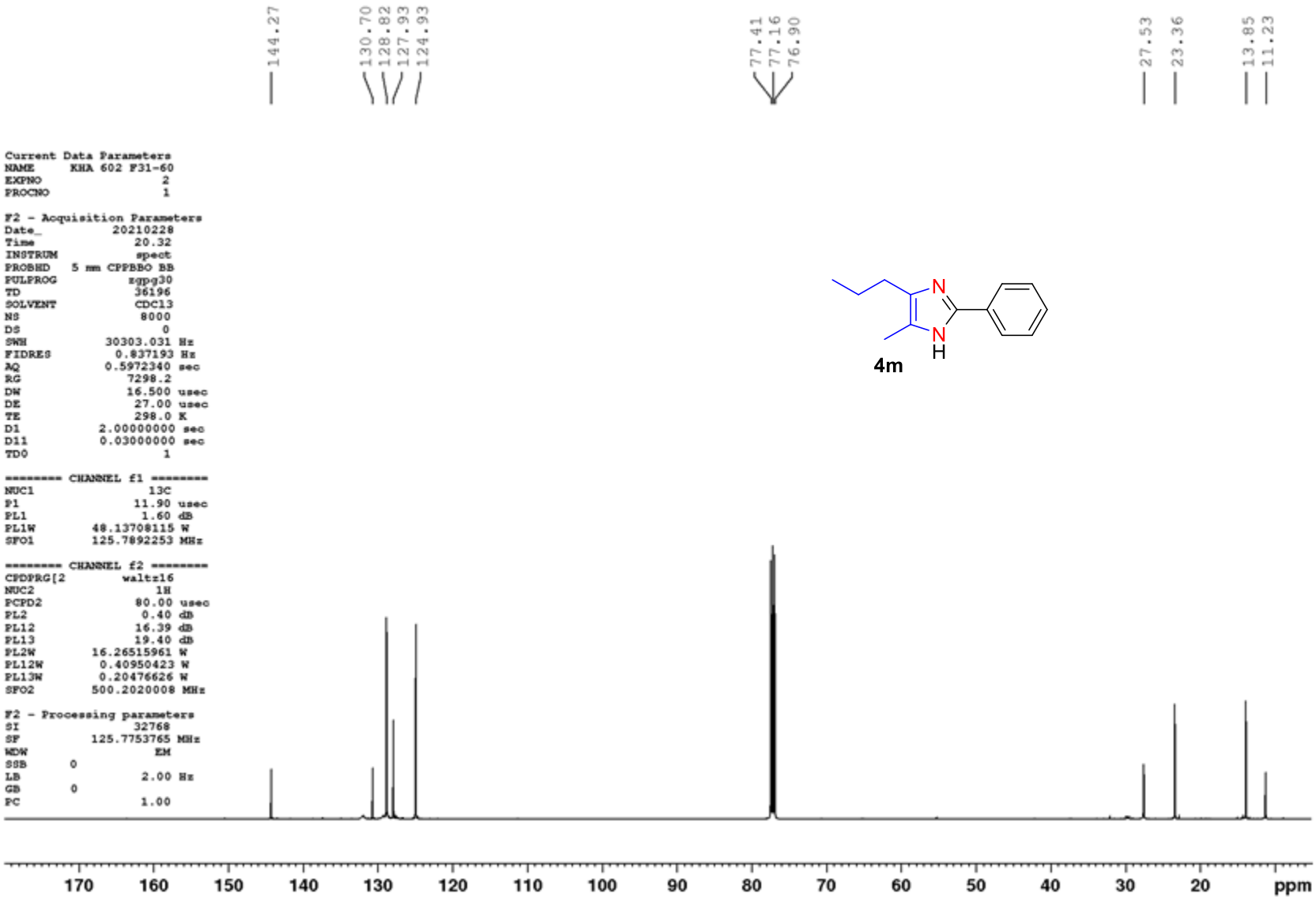


Figure S83. ^{13}C NMR spectrum of compound **4m** (125 MHz, $CDCl_3$, 25 ^oC)

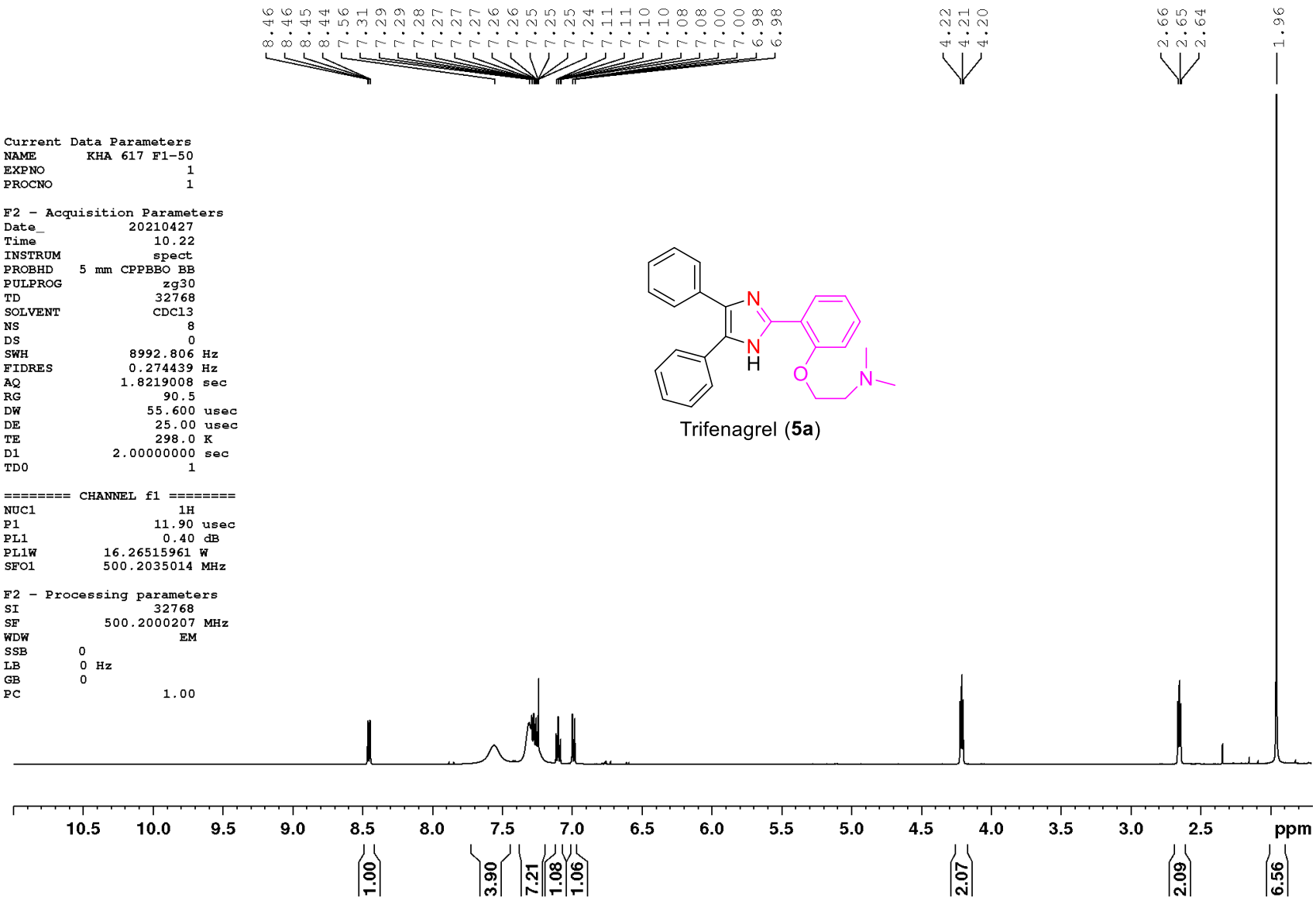


Figure S84. ^{1}H NMR spectrum of compound **5a** (500 MHz, $CDCl_3$, 25 ^{o}C)

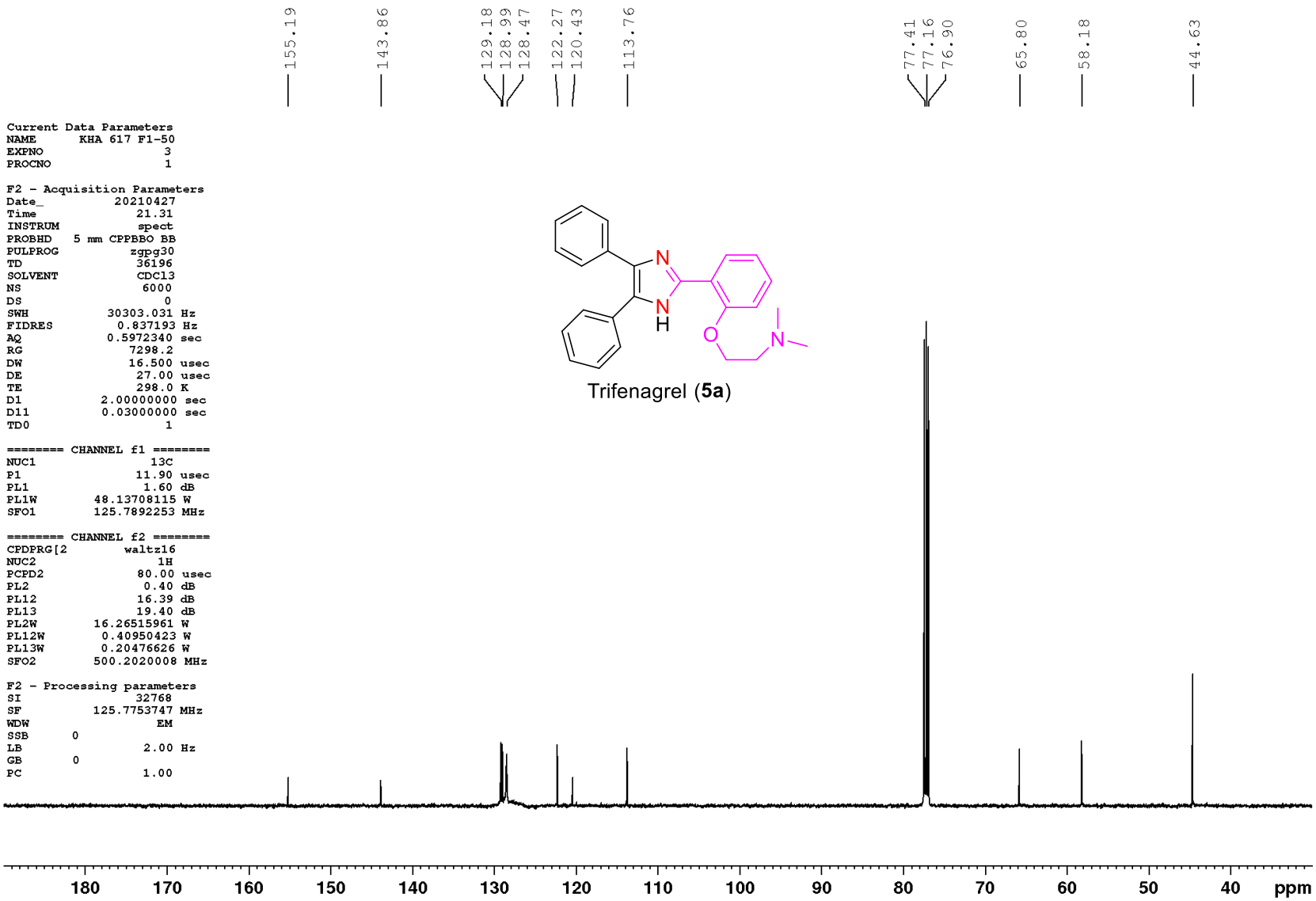


Figure S85. ^{13}C NMR spectrum of compound **5a** (125 MHz, $CDCl_3$, 25 ^oC)

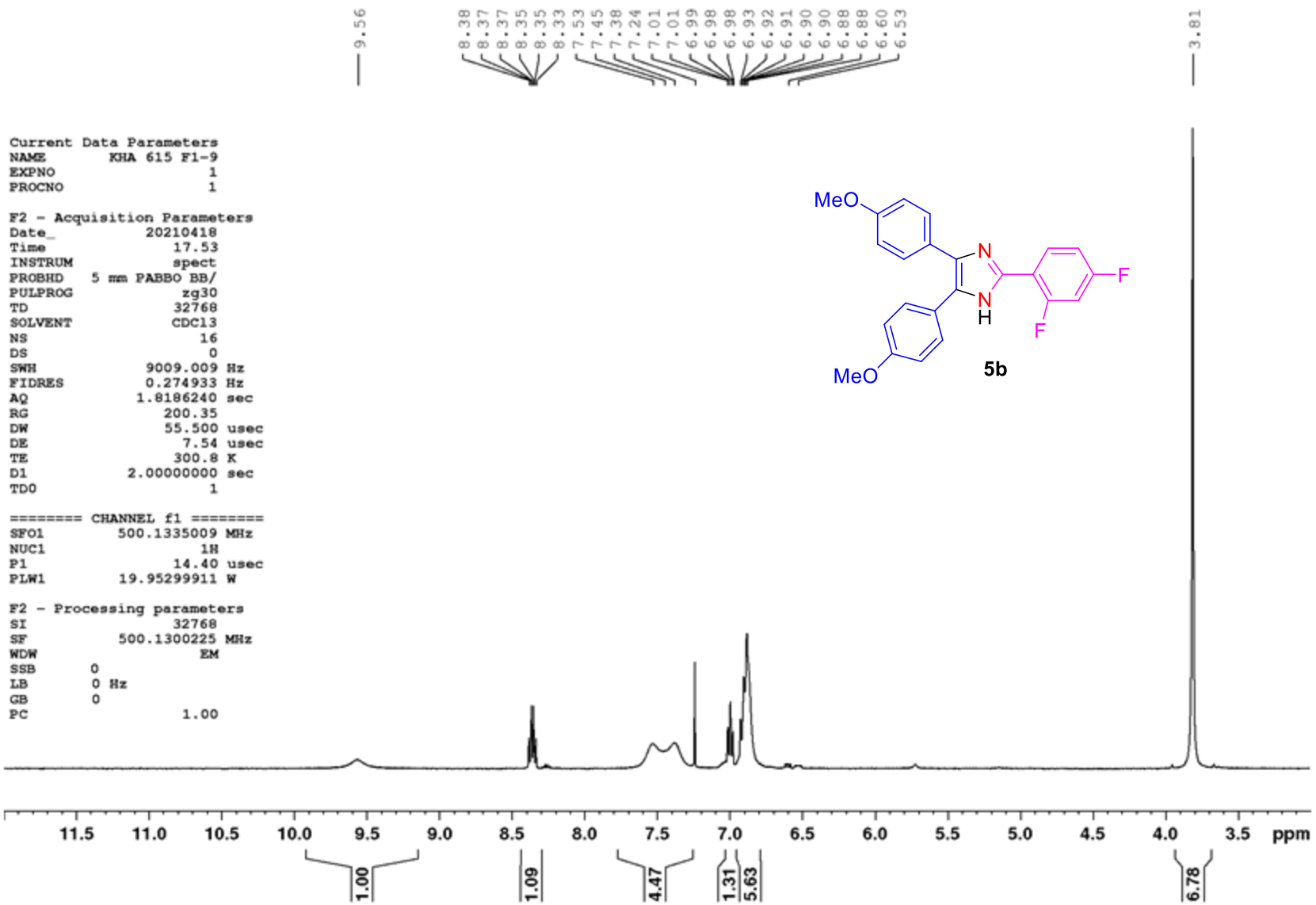


Figure S86. ^{1}H NMR spectrum of compound **5b** (500 MHz, $CDCl_3$, 25 ^{o}C)

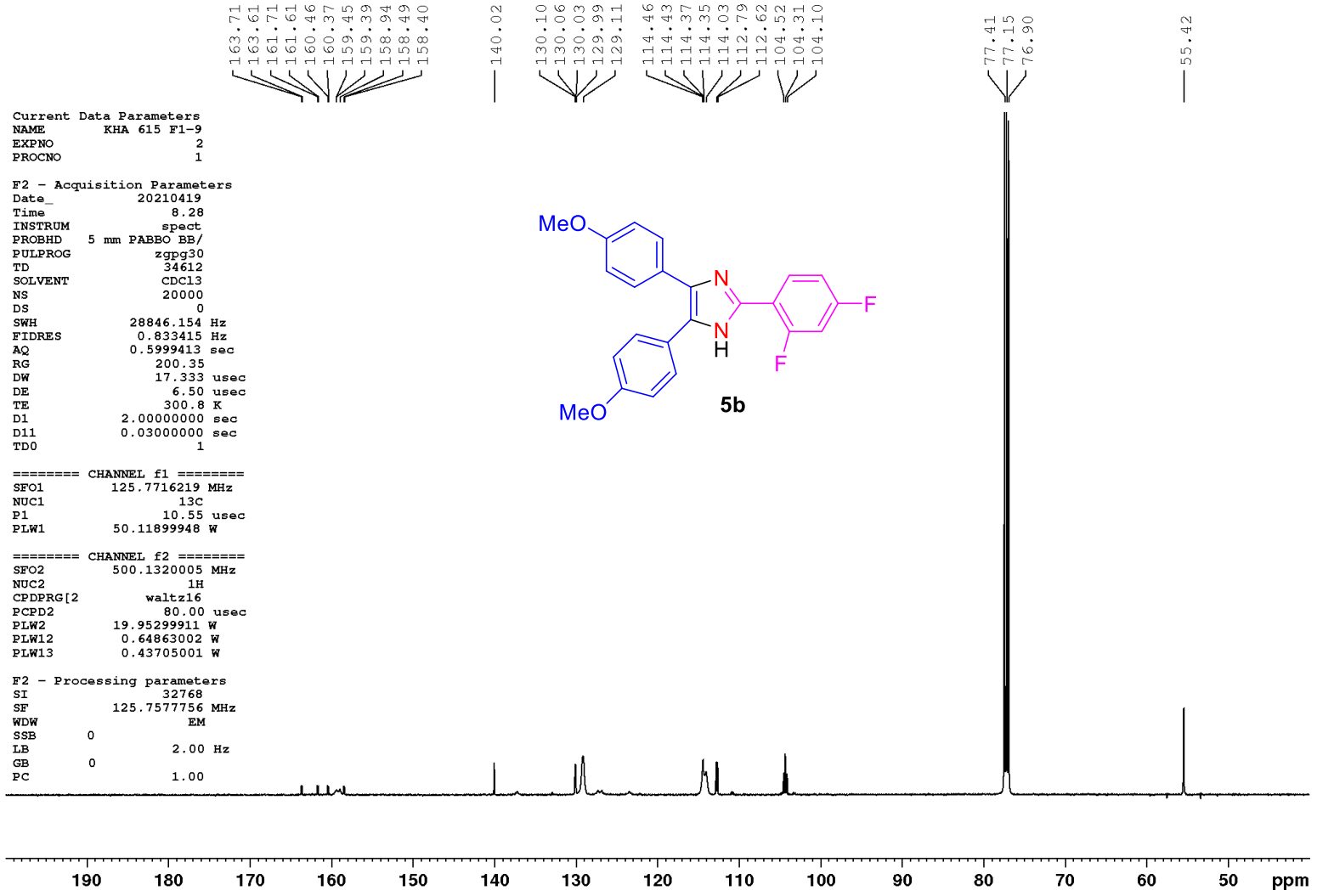
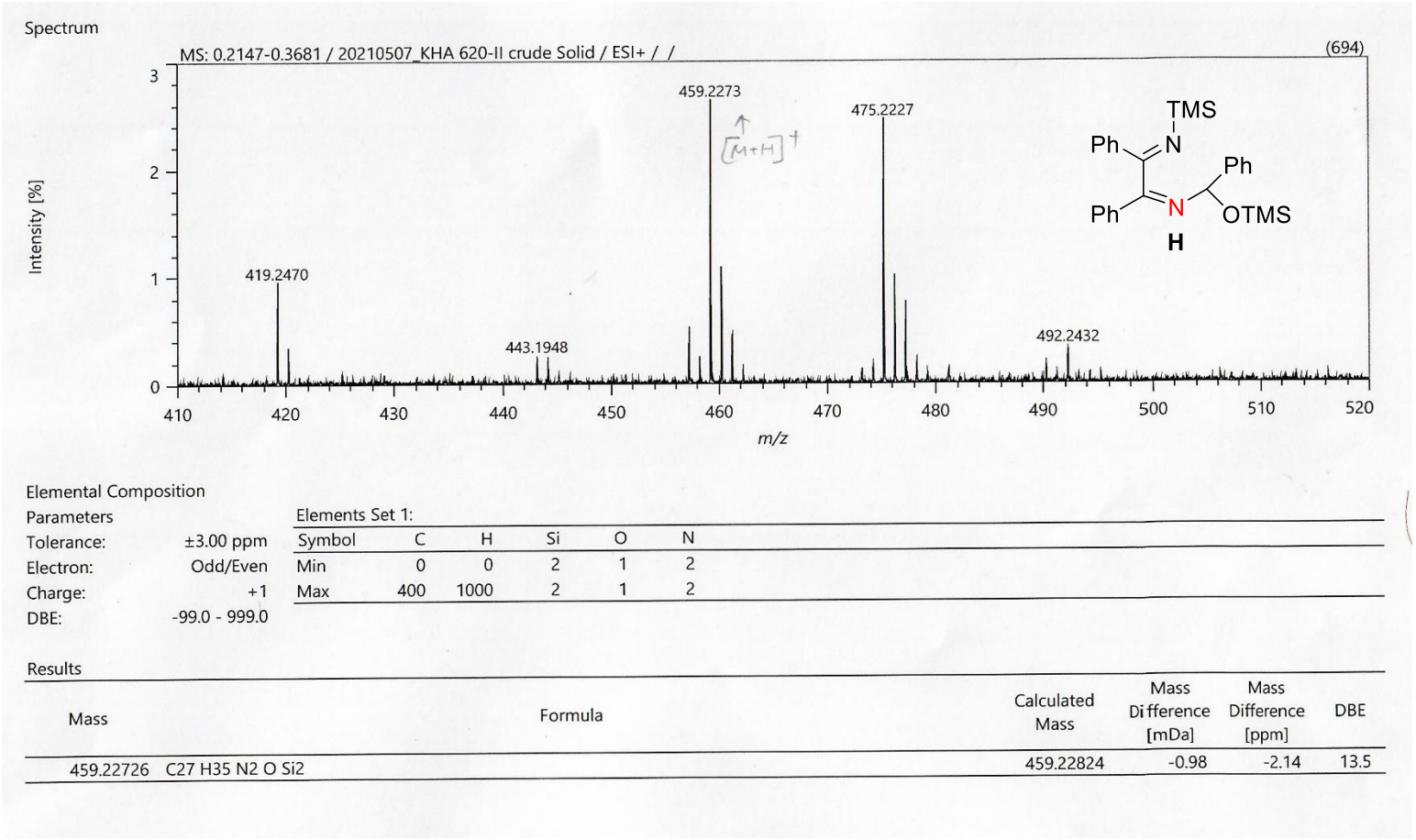


Figure S87. ^{13}C NMR spectrum of compound **5b** (125 MHz, $CDCl_3$, 25 °C)



Elemental Composition

Parameters		Elements Set 1:					
Tolerance:	±3.00 ppm	Symbol	C	H	Si	O	N
Electron:	Odd/Even	Min	0	0	2	1	2
Charge:	+1	Max	400	1000	2	1	2
DBE:	-99.0 - 999.0						

Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
459.22726	C27 H35 N2 O Si2	459.22824	-0.98	-2.14	13.5

Figure S88. HRMS of ethane-1,2-diimine intermediate **H**