Supplementary Information

for

One-pot Synthesis of 1, 5-Diketones under Transition-Metal-free Condition: Application in the Synthesis of 2,4,6-Triaryl Pyridine Derivatives

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

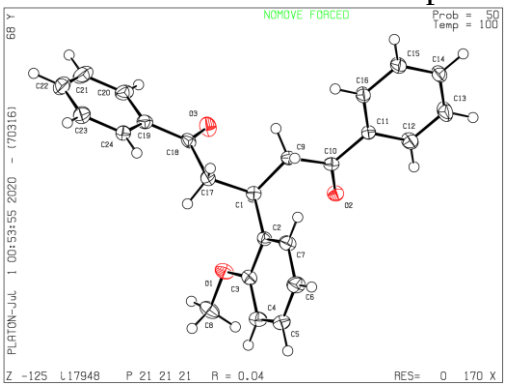


Figure S1. Single X-ray crystal structure of 1, 5-dicarbonyls **3o** (the thermal ellipsoid was drawn at the 50% probability level)

Table S1. Crystal data and structure refinement for i17948

CCDC	2031225	
Identification code	i17948	
Empirical formula	C24 H22 O3	
Formula weight	358.41	
Temperature	100.0(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 5.2961(2) Å	α= 90°.
	b = 17.1066(5) Å	β= 90°.
	c = 20.7005(6) Å	γ = 90°.
Volume	1875.43(10) $Å^3$	
Z, Density (calculated)	4, 1.269 Mg/m^3	
Absorption coefficient	0.658 mm^{-1}	
F(000)	760	
Crystal size	0.272 x 0.156 x 0.116 mm^3	
Theta range for data collection	3.351 to 66.664°.	
Index ranges	-6<=h<=5, -20<=k<=20, -24<=l<=24	
Reflections collected	13354	
Independent reflections	3308 [R(int) = 0.0638]	
Completeness to theta = 66.664°	99.6 %	
Absorption correction	Numerical	
Max. and min. transmission	1 and 0.7968	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3308 / 0 / 249	
Goodness-of-fit on F^2	1.056	
Final R indices [I>2sigma(I)]	R1 = 0.0353, wR2 = 0.0855	

R indices (all data)	R1 = 0.0397, wR2 = 0.0879
Absolute structure parameter	0.4(3)
Extinction coefficient	n/a
Largest diff. peak and hole	0.146 and -0.151 e.Å^{-3}

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for i17948. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	66(3)	3522(1)	4372(1)	25(1)
O(2)	-166(3)	5877(1)	4024(1)	23(1)
O(3)	2518(3)	5121(1)	5904(1)	30(1)
C(1)	3104(4)	4808(1)	4595(1)	19(1)
C(2)	3220(4)	4357(1)	3961(1)	19(1)
C(3)	1636(4)	3711(1)	3865(1)	20(1)
C(4)	1720(4)	3281(1)	3295(1)	25(1)
C(5)	3465(5)	3485(1)	2816(1)	26(1)
C(6)	5083(5)	4106(1)	2906(1)	29(1)
C(7)	4932(5)	4539(1)	3479(1)	24(1)
C(8)	-1625(4)	2887(1)	4282(1)	29(1)
C(9)	3822(4)	5669(1)	4528(1)	18(1)
C(10)	1864(4)	6156(1)	4186(1)	18(1)
C(11)	2421(4)	7001(1)	4064(1)	18(1)
C(12)	754(5)	7431(1)	3684(1)	30(1)
C(13)	1168(5)	8225(1)	3576(2)	36(1)
C(14)	3249(4)	8591(1)	3843(1)	26(1)
C(15)	4918(5)	8167(1)	4218(1)	30(1)
C(16)	4511(4)	7370(1)	4326(1)	26(1)
C(17)	4771(4)	4411(1)	5099(1)	20(1)
C(18)	4234(4)	4668(1)	5786(1)	20(1)
C(19)	5787(4)	4342(1)	6321(1)	22(1)
C(20)	5006(5)	4486(1)	6956(1)	28(1)
C(21)	6358(5)	4182(2)	7471(1)	38(1)
C(22)	8505(5)	3735(2)	7363(1)	37(1)
C(23)	9300(5)	3585(2)	6733(1)	33(1)
C(24)	7939(5)	3888(1)	6216(1)	24(1)

Table S3. Bond lengths [Å] and angles [°] for i17948.

O(1)-C(3)	1.378(3)
O(1)-C(8)	1.420(3)
O(2)-C(10)	1.224(3)
O(3)-C(18)	1.220(3)
C(1)-C(2)	1.522(3)
C(1)-C(17)	1.527(3)
C(1)-C(9)	1.527(3)
C(1)-H(1)	1.0000
C(2)-C(7)	1.385(3)
C(2)-C(3)	1.401(3)
C(3)-C(4)	1.391(3)
C(4)-C(5)	1.400(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.378(3)
C(5)-H(5)	0.9500
C(6)-C(7)	1.399(3)
C(6)-H(6)	0.9500
C(7)-H(7)	0.9500
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-C(10)	1.506(3)
C(9)-H(9A)	0.9900
C(9)-H(9AB)	0.9900
C(10)-C(11)	1.497(3)
C(11)-C(16)	1.385(3)
C(11)-C(12)	1.393(3)
C(12)-C(13)	1.394(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.383(3)
C(13)-H(13)	0.9500
C(14)-C(15)	1.383(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.399(3)
C(15)-H(15)	0.9500
C(16)-H(16)	0.9500

C(17)-C(18)	1.515(3)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-C(19)	1.487(3)
C(19)-C(24)	1.396(3)
C(19)-C(20)	1.401(3)
C(20)-C(21)	1.386(4)
C(20)-H(20)	0.9500
C(21)-C(22)	1.389(4)
C(21)-H(21)	0.9500
C(22)-C(23)	1.395(4)
C(22)-H(22)	0.9500
C(23)-C(24)	1.390(3)
C(23)-H(23)	0.9500
C(24)-H(24)	0.9500
C(3)-O(1)-C(8)	117.37(18)
C(2)-C(1)-C(17)	109.86(17)
C(2)-C(1)-C(9)	113.65(18)
C(17)-C(1)-C(9)	110.28(18)
C(2)-C(1)-H(1)	107.6
C(17)-C(1)-H(1)	107.6
C(9)-C(1)-H(1)	107.6
C(7)-C(2)-C(3)	117.8(2)
C(7)-C(2)-C(1)	122.25(19)
C(3)-C(2)-C(1)	119.90(19)
O(1)-C(3)-C(4)	122.82(19)
O(1)-C(3)-C(2)	115.93(19)
C(4)-C(3)-C(2)	121.2(2)
C(3)-C(4)-C(5)	119.4(2)
C(3)-C(4)-H(4)	120.3
C(5)-C(4)-H(4)	120.3
C(6)-C(5)-C(4)	120.4(2)
C(6)-C(5)-H(5)	119.8
C(4)-C(5)-H(5)	119.8
C(5)-C(6)-C(7)	119.2(2)
C(5)-C(6)-H(6)	120.4
C(7)-C(6)-H(6)	120.4
C(2)-C(7)-C(6)	122.0(2)

C(2)-C(7)-H(7)	119.0
C(6)-C(7)-H(7)	119.0
O(1)-C(8)-H(8A)	109.5
O(1)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
O(1)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(10)-C(9)-C(1)	113.85(17)
C(10)-C(9)-H(9A)	108.8
C(1)-C(9)-H(9A)	108.8
C(10)-C(9)-H(9AB)	108.8
C(1)-C(9)-H(9AB)	108.8
H(9A)-C(9)-H(9AB)	107.7
O(2)-C(10)-C(11)	120.24(19)
O(2)-C(10)-C(9)	121.19(18)
C(11)-C(10)-C(9)	118.56(18)
C(16)-C(11)-C(12)	119.17(19)
C(16)-C(11)-C(10)	122.06(19)
C(12)-C(11)-C(10)	118.76(19)
C(11)-C(12)-C(13)	120.4(2)
C(11)-C(12)-H(12)	119.8
C(13)-C(12)-H(12)	119.8
C(14)-C(13)-C(12)	120.1(2)
C(14)-C(13)-H(13)	119.9
C(12)-C(13)-H(13)	119.9
C(15)-C(14)-C(13)	119.7(2)
C(15)-C(14)-H(14)	120.1
C(13)-C(14)-H(14)	120.1
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(11)-C(16)-C(15)	120.3(2)
C(11)-C(16)-H(16)	119.9
C(15)-C(16)-H(16)	119.9
C(18)-C(17)-C(1)	113.83(17)
C(18)-C(17)-H(17A)	108.8
C(1)-C(17)-H(17A)	108.8

C(18)-C(17)-H(17B)	108.8
C(1)-C(17)-H(17B)	108.8
H(17A)-C(17)-H(17B)	107.7
O(3)-C(18)-C(19)	120.1(2)
O(3)-C(18)-C(17)	120.8(2)
C(19)-C(18)-C(17)	119.07(19)
C(24)-C(19)-C(20)	119.0(2)
C(24)-C(19)-C(18)	123.0(2)
C(20)-C(19)-C(18)	118.0(2)
C(21)-C(20)-C(19)	120.3(2)
C(21)-C(20)-H(20)	119.9
C(19)-C(20)-H(20)	119.9
C(20)-C(21)-C(22)	120.4(2)
C(20)-C(21)-H(21)	119.8
C(22)-C(21)-H(21)	119.8
C(21)-C(22)-C(23)	120.0(2)
C(21)-C(22)-H(22)	120.0
C(23)-C(22)-H(22)	120.0
C(24)-C(23)-C(22)	119.6(3)
C(24)-C(23)-H(23)	120.2
C(22)-C(23)-H(23)	120.2
C(23)-C(24)-C(19)	120.7(2)
C(23)-C(24)-H(24)	119.6
C(19)-C(24)-H(24)	119.6

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2$x 10^3) for i17948. 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)	21(1)	23(1)	31(1)	-3(1)	6(1)	-5(1)
O(2)	17(1)	24(1)	28(1)	0(1)	-2(1)	-4(1)
O(3)	34(1)	27(1)	28(1)	1(1)	10(1)	9(1)
C(1)	16(1)	20(1)	20(1)	-1(1)	2(1)	-1(1)
C(2)	18(1)	18(1)	20(1)	-1(1)	0(1)	1(1)
C(3)	18(1)	19(1)	24(1)	0(1)	1(1)	0(1)
C(4)	22(1)	24(1)	29(1)	-5(1)	-1(1)	-1(1)
C(5)	32(1)	26(1)	21(1)	-5(1)	-1(1)	-1(1)
C(6)	35(1)	29(1)	22(1)	-3(1)	7(1)	-3(1)
C(7)	29(1)	22(1)	22(1)	-2(1)	5(1)	-4(1)
C(8)	23(1)	21(1)	43(2)	-2(1)	4(1)	-4(1)
C(9)	16(1)	19(1)	20(1)	0(1)	1(1)	-2(1)
C(10)	16(1)	20(1)	18(1)	-3(1)	3(1)	-2(1)
C(11)	16(1)	19(1)	18(1)	0(1)	0(1)	0(1)
C(12)	23(1)	23(1)	42(1)	2(1)	-13(1)	-3(1)
C(13)	33(1)	25(1)	51(2)	10(1)	-16(1)	-2(1)
C(14)	26(1)	20(1)	31(1)	3(1)	-3(1)	-2(1)
C(15)	32(1)	23(1)	35(1)	5(1)	-11(1)	-9(1)
C(16)	26(1)	21(1)	32(1)	5(1)	-10(1)	-5(1)
C(17)	22(1)	20(1)	20(1)	0(1)	3(1)	1(1)
C(18)	24(1)	16(1)	21(1)	1(1)	6(1)	-3(1)
C(19)	27(1)	21(1)	19(1)	-2(1)	3(1)	-5(1)
C(20)	34(1)	30(1)	20(1)	-2(1)	3(1)	-11(1)
C(21)	45(2)	47(2)	21(1)	2(1)	-3(1)	-19(1)
C(22)	43(2)	39(1)	28(1)	8(1)	-12(1)	-16(1)
C(23)	35(1)	30(1)	34(2)	3(1)	-11(1)	-6(1)
C(24)	29(1)	22(1)	23(1)	1(1)	-5(1)	-4(1)

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

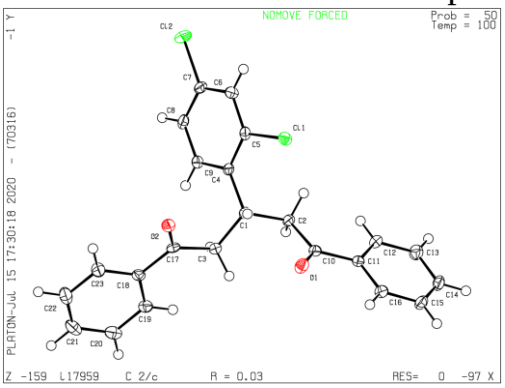


Figure S2. Single X-ray crystal structure of 1, 5-dicarbonyls **3q** (the thermal ellipsoid was drawn at the 50% probability level)

Table S5. Crystal data and structure refinement for i17959.

CCDC	2031234	
Identification code	i17959	
Empirical formula	C23 H18 Cl2 O2	
Formula weight	397.27	
Temperature	100.0(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 22.7208(6) Å	α= 90°.
	b = 4.89590(10) Å	β= 91.140(2)°.
	c = 34.0185(10) Å	γ = 90°.
Z, Volume,	8, 3783.43(17) $Å^3$	
Density (calculated)	1.395 Mg/m^3	
Absorption coefficient	3.207 mm^{-1}	
F(000)	1648	
Crystal size	0.194 x 0.081 x 0.043 mm^3	
Theta range for data collection	3.892 to 65.204°.	
Index ranges	-26<=h<=26, -5<=k<=5, -40<=l<=40	
Reflections collected	38496	
Independent reflections	3231 [R(int) = 0.0713]	
Completeness to theta = 65.204°	99.9 %	
Absorption correction	Numerical	
Max. and min. transmission	1 and 0.8202	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3231 / 0 / 244	
Goodness-of-fit on F^2	1.049	
Final R indices [I>2sigma(I)]	R1 = 0.0302, wR2 = 0.0724	

R indices (all data)	R1 = 0.0383, wR2 = 0.0770
Extinction coefficient	n/a
Largest diff. peak and hole	0.241 and -0.284 e.Å^{-3}

Table S6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for i17959. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	4795(1)	8545(1)	4502(1)	19(1)
Cl(2)	6684(1)	3518(1)	5133(1)	33(1)
O(1)	3913(1)	7291(3)	3466(1)	22(1)
O(2)	5856(1)	7442(2)	3366(1)	19(1)
C(1)	4944(1)	5024(3)	3775(1)	15(1)
C(2)	4339(1)	3838(3)	3877(1)	15(1)
C(3)	5143(1)	3881(3)	3382(1)	16(1)
C(4)	5387(1)	4587(3)	4110(1)	14(1)
C(5)	5355(1)	6130(3)	4454(1)	15(1)
C(6)	5746(1)	5844(3)	4769(1)	19(1)
C(7)	6187(1)	3910(4)	4741(1)	19(1)
C(8)	6237(1)	2303(4)	4411(1)	19(1)
C(9)	5838(1)	2657(3)	4100(1)	16(1)
C(10)	3829(1)	5317(3)	3677(1)	16(1)
C(11)	3220(1)	4303(3)	3748(1)	16(1)
C(12)	3105(1)	2213(4)	4014(1)	19(1)
C(13)	2531(1)	1346(4)	4070(1)	23(1)
C(14)	2072(1)	2520(4)	3858(1)	22(1)
C(15)	2181(1)	4605(4)	3593(1)	21(1)
C(16)	2752(1)	5513(4)	3541(1)	19(1)
C(17)	5683(1)	5281(3)	3225(1)	16(1)
C(18)	5996(1)	4018(3)	2889(1)	17(1)
C(19)	5750(1)	1855(4)	2674(1)	20(1)
C(20)	6036(1)	795(4)	2352(1)	24(1)
C(21)	6574(1)	1849(4)	2246(1)	26(1)
C(22)	6830(1)	3956(4)	2462(1)	26(1)
C(23)	6542(1)	5054(4)	2780(1)	21(1)

Table S7. Bond lengths [Å] and angles [°] for i17959.

Cl(1)-C(5)	1.7457(16)
Cl(2)-C(7)	1.7421(16)
O(1)-C(10)	1.221(2)
O(2)-C(17)	1.223(2)
C(1)-C(4)	1.520(2)
C(1)-C(3)	1.529(2)
C(1)-C(2)	1.537(2)
C(1)-H(1)	1.0000
C(2)-C(10)	1.516(2)
C(2)-H(2A)	0.9900
C(2)-H(2AB)	0.9900
C(3)-C(17)	1.513(2)
C(3)-H(3A)	0.9900
C(3)-H(3AB)	0.9900
C(4)-C(9)	1.396(2)
C(4)-C(5)	1.397(2)
C(5)-C(6)	1.386(2)
C(6)-C(7)	1.382(2)
C(6)-H(6)	0.9500
C(7)-C(8)	1.376(2)
C(8)-C(9)	1.390(2)
C(8)-H(8)	0.9500
C(9)-H(9)	0.9500
C(10)-C(11)	1.495(2)
C(11)-C(12)	1.393(2)
C(11)-C(16)	1.397(2)
C(12)-C(13)	1.389(2)
C(12)-H(12)	0.9500
C(13)-C(14)	1.383(2)
C(13)-H(13)	0.9500
C(14)-C(15)	1.385(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.386(2)
C(15)-H(15)	0.9500
C(16)-H(16)	0.9500
C(17)-C(18)	1.491(2)

C(18)-C(19)	1.396(2)
C(18)-C(23)	1.398(2)
C(19)-C(20)	1.387(2)
C(19)-H(19)	0.9500
C(20)-C(21)	1.382(3)
C(20)-H(20)	0.9500
C(21)-C(22)	1.388(3)
C(21)-H(21)	0.9500
C(22)-C(23)	1.384(2)
C(22)-H(22)	0.9500
C(23)-H(23)	0.9500
C(4)-C(1)-C(3)	113.67(13)
C(4)-C(1)-C(2)	111.08(12)
C(3)-C(1)-C(2)	109.91(13)
C(4)-C(1)-H(1)	107.3
C(3)-C(1)-H(1)	107.3
C(2)-C(1)-H(1)	107.3
C(10)-C(2)-C(1)	113.36(13)
C(10)-C(2)-H(2A)	108.9
C(1)-C(2)-H(2A)	108.9
C(10)-C(2)-H(2AB)	108.9
C(1)-C(2)-H(2AB)	108.9
H(2A)-C(2)-H(2AB)	107.7
C(17)-C(3)-C(1)	113.58(13)
C(17)-C(3)-H(3A)	108.9
C(1)-C(3)-H(3A)	108.9
C(17)-C(3)-H(3AB)	108.9
C(1)-C(3)-H(3AB)	108.9
H(3A)-C(3)-H(3AB)	107.7
C(9)-C(4)-C(5)	115.92(14)
C(9)-C(4)-C(1)	123.62(14)
C(5)-C(4)-C(1)	120.46(14)
C(6)-C(5)-C(4)	123.35(15)
C(6)-C(5)-Cl(1)	116.94(12)
C(4)-C(5)-Cl(1)	119.70(12)
C(7)-C(6)-C(5)	118.07(15)
C(7)-C(6)-H(6)	121.0
C(5)-C(6)-H(6)	121.0

C(8)-C(7)-C(6)	121.30(15)
C(8)-C(7)-Cl(2)	119.88(13)
C(6)-C(7)-Cl(2)	118.82(13)
C(7)-C(8)-C(9)	119.10(15)
C(7)-C(8)-H(8)	120.4
C(9)-C(8)-H(8)	120.4
C(8)-C(9)-C(4)	122.25(15)
C(8)-C(9)-H(9)	118.9
C(4)-C(9)-H(9)	118.9
O(1)-C(10)-C(11)	120.87(15)
O(1)-C(10)-C(2)	121.07(14)
C(11)-C(10)-C(2)	118.06(14)
C(12)-C(11)-C(16)	119.21(15)
C(12)-C(11)-C(10)	122.39(15)
C(16)-C(11)-C(10)	118.41(15)
C(13)-C(12)-C(11)	120.23(16)
C(13)-C(12)-H(12)	119.9
C(11)-C(12)-H(12)	119.9
C(14)-C(13)-C(12)	120.09(16)
C(14)-C(13)-H(13)	120.0
C(12)-C(13)-H(13)	120.0
C(13)-C(14)-C(15)	120.14(16)
C(13)-C(14)-H(14)	119.9
C(15)-C(14)-H(14)	119.9
C(14)-C(15)-C(16)	120.08(16)
C(14)-C(15)-H(15)	120.0
C(16)-C(15)-H(15)	120.0
C(15)-C(16)-C(11)	120.24(16)
C(15)-C(16)-H(16)	119.9
C(11)-C(16)-H(16)	119.9
O(2)-C(17)-C(18)	120.47(14)
O(2)-C(17)-C(3)	120.53(14)
C(18)-C(17)-C(3)	118.99(14)
C(19)-C(18)-C(23)	119.04(15)
C(19)-C(18)-C(17)	121.58(15)
C(23)-C(18)-C(17)	119.36(15)
C(20)-C(19)-C(18)	120.58(16)
C(20)-C(19)-H(19)	119.7

C(18)-C(19)-H(19)	119.7
C(21)-C(20)-C(19)	119.77(17)
C(21)-C(20)-H(20)	120.1
C(19)-C(20)-H(20)	120.1
C(20)-C(21)-C(22)	120.28(16)
C(20)-C(21)-H(21)	119.9
C(22)-C(21)-H(21)	119.9
C(23)-C(22)-C(21)	120.19(17)
C(23)-C(22)-H(22)	119.9
C(21)-C(22)-H(22)	119.9
C(22)-C(23)-C(18)	120.11(17)
C(22)-C(23)-H(23)	119.9
C(18)-C(23)-H(23)	119.9

Symmetry transformations used to generate equivalent atoms:

Table S8. Anisotropic displacement parameters ($Å^2$x 10^3)for i17959. 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)	20(1)	20(1)	17(1)	0(1)	1(1)	5(1)
Cl(2)	23(1)	52(1)	22(1)	1(1)	-11(1)	7(1)
O(1)	17(1)	25(1)	24(1)	9(1)	-2(1)	-2(1)
O(2)	19(1)	21(1)	18(1)	-2(1)	0(1)	-2(1)
C(1)	12(1)	17(1)	15(1)	1(1)	-1(1)	-1(1)
C(2)	13(1)	18(1)	15(1)	1(1)	-1(1)	-1(1)
C(3)	15(1)	20(1)	14(1)	0(1)	-2(1)	0(1)
C(4)	12(1)	16(1)	14(1)	2(1)	1(1)	-4(1)
C(5)	13(1)	16(1)	17(1)	2(1)	3(1)	1(1)
C(6)	20(1)	22(1)	14(1)	-1(1)	0(1)	-2(1)
C(7)	14(1)	28(1)	16(1)	4(1)	-3(1)	-2(1)
C(8)	11(1)	22(1)	23(1)	4(1)	1(1)	2(1)
C(9)	14(1)	18(1)	16(1)	0(1)	2(1)	-2(1)
C(10)	16(1)	18(1)	14(1)	-2(1)	-1(1)	1(1)
C(11)	15(1)	19(1)	13(1)	-4(1)	-1(1)	0(1)
C(12)	15(1)	22(1)	19(1)	0(1)	-3(1)	0(1)
C(13)	20(1)	24(1)	24(1)	1(1)	1(1)	-3(1)
C(14)	13(1)	26(1)	26(1)	-5(1)	1(1)	-3(1)
C(15)	14(1)	25(1)	24(1)	-3(1)	-3(1)	3(1)
C(16)	18(1)	22(1)	17(1)	-2(1)	-2(1)	1(1)
C(17)	16(1)	19(1)	13(1)	3(1)	-5(1)	2(1)
C(18)	18(1)	20(1)	13(1)	3(1)	-2(1)	4(1)
C(19)	20(1)	23(1)	16(1)	1(1)	-2(1)	1(1)
C(20)	31(1)	24(1)	17(1)	-1(1)	-3(1)	5(1)
C(21)	34(1)	26(1)	17(1)	2(1)	6(1)	11(1)
C(22)	23(1)	30(1)	25(1)	2(1)	8(1)	3(1)
C(23)	20(1)	24(1)	20(1)	1(1)	2(1)	0(1)

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

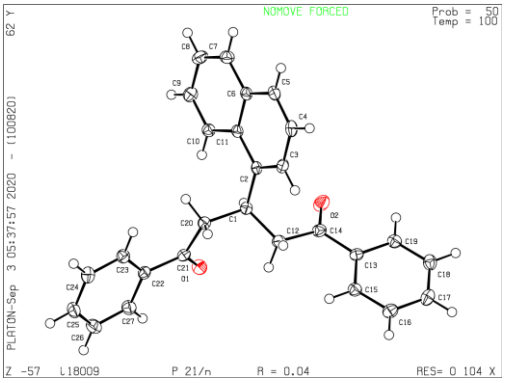


Figure S3. Single X-ray crystal structure of 1, 5-dicarbonyls **3t** (the thermal ellipsoid was drawn at the 50% probability level)

Table S9. Crystal data and structure refinement for i18009.

CCDC	2031246	
Identification code	i18009	
Empirical formula	C27 H22 O2	
Formula weight	378.44	
Temperature	100.0(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 13.3568(5) Å	α= 90°.
	b = 10.1409(3) Å	β= 96.328(2)°.
	c = 14.6406(5) Å	γ = 90°.
Z, Volume	4, 1970.99(12) $Å^3$	
Density (calculated)	1.275 Mg/m^3	
Absorption coefficient	0.079 mm^{-1}	
F(000)	800	
Crystal size	0.150 x 0.125 x 0.125 mm^3	
Theta range for data collection	1.959 to 27.105°.	
Index ranges	-17<=h<=17, -12<=k<=12, -18<=l<=18	
Reflections collected	83535	
Independent reflections	4341 [R(int) = 0.0721]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Numerical	
Max. and min. transmission	0.9988 and 0.9689	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4341 / 0 / 262	
Goodness-of-fit on F^2	1.058	
Final R indices [I>2sigma(I)]	R1 = 0.0384, wR2 = 0.0865	

R indices (all data)	R1 = 0.0530, wR2 = 0.0949
Extinction coefficient	n/a
Largest diff. peak and hole	0.267 and -0.219 e.Å^{-3}

Table S10. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for i18009. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	4534(1)	7404(1)	3042(1)	23(1)
O(2)	5892(1)	11210(1)	2168(1)	32(1)
C(1)	6331(1)	8902(1)	3152(1)	18(1)
C(2)	7285(1)	9578(1)	3585(1)	17(1)
C(3)	8126(1)	9700(1)	3130(1)	20(1)
C(4)	9017(1)	10303(1)	3541(1)	22(1)
C(5)	9067(1)	10784(1)	4415(1)	20(1)
C(6)	8233(1)	10655(1)	4927(1)	18(1)
C(7)	8287(1)	11108(1)	5846(1)	22(1)
C(8)	7485(1)	10973(1)	6344(1)	25(1)
C(9)	6594(1)	10364(1)	5947(1)	23(1)
C(10)	6519(1)	9915(1)	5059(1)	19(1)
C(11)	7331(1)	10047(1)	4513(1)	16(1)
C(12)	6224(1)	8904(1)	2099(1)	20(1)
C(13)	6228(1)	10486(1)	703(1)	18(1)
C(14)	6102(1)	10283(1)	1698(1)	20(1)
C(15)	6334(1)	9435(1)	103(1)	20(1)
C(16)	6440(1)	9677(1)	-815(1)	24(1)
C(17)	6453(1)	10961(1)	-1138(1)	25(1)
C(18)	6357(1)	12012(1)	-545(1)	23(1)
C(19)	6238(1)	11774(1)	368(1)	20(1)
C(20)	6304(1)	7482(1)	3526(1)	19(1)
C(21)	5281(1)	6824(1)	3392(1)	18(1)
C(22)	5217(1)	5412(1)	3683(1)	18(1)
C(23)	6022(1)	4771(1)	4189(1)	20(1)
C(24)	5956(1)	3439(1)	4395(1)	24(1)
C(25)	5093(1)	2743(1)	4098(1)	25(1)
C(26)	4278(1)	3375(1)	3614(1)	28(1)
C(27)	4337(1)	4707(1)	3411(1)	24(1)

Table S11. Bond lengths [Å] and angles [°] for i18009.

O(1)-C(21)	1.2206(15)
O(2)-C(14)	1.2158(16)
C(1)-C(2)	1.5220(17)
C(1)-C(12)	1.5313(17)
C(1)-C(20)	1.5423(17)
C(1)-H(1)	1.0000
C(2)-C(3)	1.3735(18)
C(2)-C(11)	1.4342(17)
C(3)-C(4)	1.4123(19)
C(3)-H(3)	0.9500
C(4)-C(5)	1.3637(19)
C(4)-H(4)	0.9500
C(5)-C(6)	1.4156(18)
C(5)-H(5)	0.9500
C(6)-C(7)	1.4168(18)
C(6)-C(11)	1.4273(17)
C(7)-C(8)	1.366(2)
C(7)-H(7)	0.9500
C(8)-C(9)	1.4091(19)
C(8)-H(8)	0.9500
C(9)-C(10)	1.3702(18)
C(9)-H(9)	0.9500
C(10)-C(11)	1.4230(18)
C(10)-H(10)	0.9500
C(12)-C(14)	1.5189(18)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(19)	1.3964(18)
C(13)-C(15)	1.3973(18)
C(13)-C(14)	1.4990(18)
C(15)-C(16)	1.3886(19)
C(15)-H(15)	0.9500
C(16)-C(17)	1.386(2)
C(16)-H(16)	0.9500
C(17)-C(18)	1.389(2)
C(17)-H(17)	0.9500

C(18)-C(19)	1.3849(19)
C(18)-H(18)	0.9500
C(19)-H(19)	0.9500
C(20)-C(21)	1.5142(17)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-C(22)	1.4991(18)
C(22)-C(27)	1.3951(18)
C(22)-C(23)	1.3966(18)
C(23)-C(24)	1.3889(19)
C(23)-H(23)	0.9500
C(24)-C(25)	1.381(2)
C(24)-H(24)	0.9500
C(25)-C(26)	1.388(2)
C(25)-H(25)	0.9500
C(26)-C(27)	1.3876(19)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500
C(2)-C(1)-C(12)	113.58(10)
C(2)-C(1)-C(20)	108.89(10)
C(12)-C(1)-C(20)	110.80(10)
C(2)-C(1)-H(1)	107.8
C(12)-C(1)-H(1)	107.8
C(20)-C(1)-H(1)	107.8
C(3)-C(2)-C(11)	118.51(12)
C(3)-C(2)-C(1)	122.02(11)
C(11)-C(2)-C(1)	119.40(11)
C(2)-C(3)-C(4)	121.89(12)
C(2)-C(3)-H(3)	119.1
C(4)-C(3)-H(3)	119.1
C(5)-C(4)-C(3)	120.44(12)
C(5)-C(4)-H(4)	119.8
C(3)-C(4)-H(4)	119.8
C(4)-C(5)-C(6)	120.22(12)
C(4)-C(5)-H(5)	119.9
C(6)-C(5)-H(5)	119.9
C(5)-C(6)-C(7)	120.84(12)
C(5)-C(6)-C(11)	119.45(12)

C(7)-C(6)-C(11)	119.70(12)
C(8)-C(7)-C(6)	120.90(13)
C(8)-C(7)-H(7)	119.6
C(6)-C(7)-H(7)	119.6
C(7)-C(8)-C(9)	119.99(13)
C(7)-C(8)-H(8)	120.0
C(9)-C(8)-H(8)	120.0
C(10)-C(9)-C(8)	120.46(12)
C(10)-C(9)-H(9)	119.8
C(8)-C(9)-H(9)	119.8
C(9)-C(10)-C(11)	121.43(12)
C(9)-C(10)-H(10)	119.3
C(11)-C(10)-H(10)	119.3
C(10)-C(11)-C(6)	117.51(11)
C(10)-C(11)-C(2)	123.02(11)
C(6)-C(11)-C(2)	119.45(11)
C(14)-C(12)-C(1)	112.63(10)
C(14)-C(12)-H(12A)	109.1
C(1)-C(12)-H(12A)	109.1
C(14)-C(12)-H(12B)	109.1
C(1)-C(12)-H(12B)	109.1
H(12A)-C(12)-H(12B)	107.8
C(19)-C(13)-C(15)	119.15(12)
C(19)-C(13)-C(14)	118.41(11)
C(15)-C(13)-C(14)	122.44(12)
O(2)-C(14)-C(13)	120.14(12)
O(2)-C(14)-C(12)	120.95(12)
C(13)-C(14)-C(12)	118.91(11)
C(16)-C(15)-C(13)	120.10(12)
C(16)-C(15)-H(15)	119.9
C(13)-C(15)-H(15)	119.9
C(17)-C(16)-C(15)	120.18(13)
C(17)-C(16)-H(16)	119.9
C(15)-C(16)-H(16)	119.9
C(16)-C(17)-C(18)	120.15(13)
C(16)-C(17)-H(17)	119.9
C(18)-C(17)-H(17)	119.9
C(19)-C(18)-C(17)	119.81(13)

C(19)-C(18)-H(18)	120.1
C(17)-C(18)-H(18)	120.1
C(18)-C(19)-C(13)	120.60(12)
C(18)-C(19)-H(19)	119.7
C(13)-C(19)-H(19)	119.7
C(21)-C(20)-C(1)	114.97(10)
C(21)-C(20)-H(20A)	108.5
C(1)-C(20)-H(20A)	108.5
C(21)-C(20)-H(20B)	108.5
C(1)-C(20)-H(20B)	108.5
H(20A)-C(20)-H(20B)	107.5
O(1)-C(21)-C(22)	120.69(11)
O(1)-C(21)-C(20)	121.69(11)
C(22)-C(21)-C(20)	117.60(11)
C(27)-C(22)-C(23)	119.21(12)
C(27)-C(22)-C(21)	118.74(11)
C(23)-C(22)-C(21)	122.01(11)
C(24)-C(23)-C(22)	120.27(12)
C(24)-C(23)-H(23)	119.9
C(22)-C(23)-H(23)	119.9
C(25)-C(24)-C(23)	119.94(13)
C(25)-C(24)-H(24)	120.0
C(23)-C(24)-H(24)	120.0
C(24)-C(25)-C(26)	120.40(13)
C(24)-C(25)-H(25)	119.8
C(26)-C(25)-H(25)	119.8
C(27)-C(26)-C(25)	119.87(13)
C(27)-C(26)-H(26)	120.1
C(25)-C(26)-H(26)	120.1
C(26)-C(27)-C(22)	120.26(13)
C(26)-C(27)-H(27)	119.9
C(22)-C(27)-H(27)	119.9

Symmetry transformations used to generate equivalent atoms:

Table S12. Anisotropic displacement parameters ($Å^2$x 10^3)for i18009. 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)	20(1)	22(1)	27(1)	2(1)	0(1)	2(1)
O(2)	55(1)	22(1)	20(1)	-2(1)	4(1)	9(1)
C(1)	20(1)	17(1)	17(1)	1(1)	2(1)	0(1)
C(2)	21(1)	13(1)	17(1)	3(1)	1(1)	1(1)
C(3)	24(1)	21(1)	16(1)	3(1)	3(1)	1(1)
C(4)	19(1)	23(1)	24(1)	7(1)	7(1)	1(1)
C(5)	18(1)	18(1)	25(1)	5(1)	0(1)	-2(1)
C(6)	20(1)	14(1)	20(1)	3(1)	0(1)	1(1)
C(7)	23(1)	21(1)	22(1)	-1(1)	-2(1)	-1(1)
C(8)	30(1)	28(1)	18(1)	-4(1)	1(1)	1(1)
C(9)	23(1)	26(1)	21(1)	-1(1)	6(1)	1(1)
C(10)	19(1)	18(1)	20(1)	0(1)	2(1)	0(1)
C(11)	18(1)	13(1)	18(1)	2(1)	1(1)	1(1)
C(12)	22(1)	18(1)	18(1)	-1(1)	0(1)	0(1)
C(13)	14(1)	21(1)	18(1)	0(1)	-2(1)	1(1)
C(14)	21(1)	20(1)	19(1)	-1(1)	-2(1)	1(1)
C(15)	19(1)	20(1)	21(1)	0(1)	0(1)	0(1)
C(16)	25(1)	25(1)	21(1)	-3(1)	4(1)	2(1)
C(17)	24(1)	31(1)	20(1)	4(1)	5(1)	2(1)
C(18)	21(1)	23(1)	26(1)	6(1)	1(1)	1(1)
C(19)	18(1)	20(1)	22(1)	0(1)	-1(1)	1(1)
C(20)	19(1)	18(1)	18(1)	1(1)	0(1)	0(1)
C(21)	19(1)	20(1)	15(1)	-2(1)	3(1)	1(1)
C(22)	20(1)	19(1)	15(1)	-1(1)	5(1)	0(1)
C(23)	19(1)	22(1)	20(1)	1(1)	3(1)	-1(1)
C(24)	24(1)	24(1)	25(1)	5(1)	4(1)	2(1)
C(25)	31(1)	19(1)	27(1)	3(1)	5(1)	-2(1)
C(26)	27(1)	26(1)	31(1)	1(1)	-2(1)	-8(1)
C(27)	21(1)	24(1)	25(1)	2(1)	-1(1)	-2(1)

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

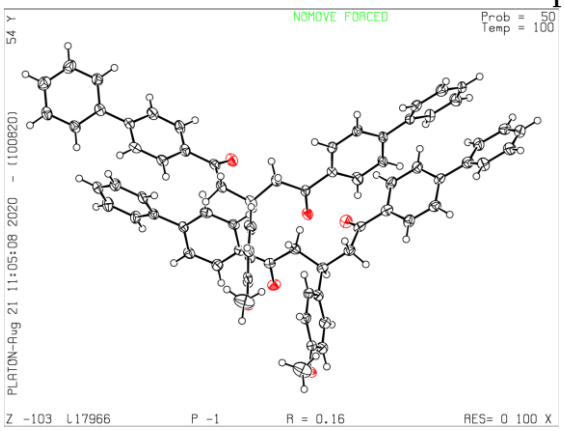


Figure S4. Single X-ray crystal structure of 1, 5-dicarbonyls **4e** (the thermal ellipsoid was drawn at the 50% probability level).

Table S13. Crystal data and structure refinement for i17966.

CCDC	2031242	
Identification code	i17966	
Empirical formula	C36 H30 O3	
Formula weight	510.60	
Temperature	100.0(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 10.2451(10) Å	α= 89.086(4)°.
	b = 10.3941(9) Å	β= 89.020(4)°.
	c = 26.429(2) Å	γ = 77.645(4)°.
Z, Volume	4, 2748.6(4) $Å^3$	
Density (calculated)	1.234 Mg/m^3	
Absorption coefficient	0.077 mm^{-1}	
F(000)	1080	
Crystal size	0.167 x 0.110 x 0.063 mm^3	
Theta range for data collection	2.035 to 27.193°.	
Index ranges	-13<=h<=13, -13<=k<=13, -33<=l<=33	
Reflections collected	132589	
Independent reflections	12176 [R(int) = 0.1739]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Numerical	
Max. and min. transmission	0.9787 and 0.8859	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12176 / 0 / 706	
Goodness-of-fit on F^2	1.091	

Final R indices [I>2sigma(I)]	R1 = 0.1599, wR2 = 0.4169
R indices (all data)	R1 = 0.2009, wR2 = 0.4372
Extinction coefficient	0.0104(15)
Largest diff. peak and hole	0.739 and -0.558 e.Å^{-3}

Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for i17966. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	7207(6)	-901(6)	8007(2)	38(2)
O(2)	4654(5)	4821(6)	7034(2)	27(1)
O(3)	5075(6)	7312(6)	8306(2)	32(1)
O(4)	2064(6)	-1085(6)	7186(2)	36(1)
O(5)	319(6)	7064(6)	6559(2)	32(1)
O(6)	-420(5)	4682(6)	7870(2)	30(1)
C(1)	5943(7)	4716(8)	7953(3)	27(2)
C(2)	6296(7)	3211(8)	7950(3)	21(2)
C(3)	7632(8)	2530(8)	7902(3)	29(2)
C(4)	7974(8)	1159(8)	7932(3)	29(2)
C(5)	6990(8)	461(8)	7993(3)	26(2)
C(6)	5652(8)	1112(8)	8054(3)	28(2)
C(7)	5345(7)	2466(8)	8023(3)	23(2)
C(8)	8545(11)	-1610(10)	7999(5)	58(3)
C(9)	6453(8)	5361(8)	7482(3)	26(2)
C(10)	5630(7)	5320(7)	7018(3)	20(1)
C(11)	6023(7)	5904(7)	6531(3)	21(2)
C(12)	7214(8)	6330(8)	6465(3)	26(2)
C(13)	7528(8)	6869(8)	6007(3)	25(2)
C(14)	6634(8)	7059(7)	5606(3)	23(2)
C(15)	5438(8)	6655(8)	5674(3)	28(2)
C(16)	5136(8)	6078(9)	6132(3)	31(2)
C(17)	6979(8)	7638(7)	5117(3)	24(2)
C(18)	8312(8)	7418(8)	4940(3)	27(2)
C(19)	8616(9)	7916(9)	4474(3)	32(2)
C(20)	7607(9)	8639(9)	4169(3)	34(2)
C(21)	6294(9)	8870(9)	4341(3)	34(2)
C(22)	5965(8)	8383(8)	4812(3)	29(2)
C(23)	6474(8)	5196(8)	8437(3)	25(2)

C(24)	5892(8)	6621(8)	8568(3)	26(2)
C(25)	6301(8)	7119(8)	9057(3)	27(2)
C(26)	5975(9)	8439(9)	9154(3)	32(2)
C(27)	6326(8)	8930(8)	9604(3)	29(2)
C(28)	7017(8)	8082(8)	9982(3)	24(2)
C(29)	7318(8)	6734(8)	9879(3)	27(2)
C(30)	6985(8)	6257(8)	9426(3)	26(2)
C(31)	7396(8)	8574(8)	10468(3)	26(2)
C(32)	7863(10)	9725(8)	10481(3)	34(2)
C(33)	8249(10)	10171(9)	10941(4)	39(2)
C(34)	8210(10)	9460(9)	11388(4)	38(2)
C(35)	7779(9)	8289(9)	11373(3)	32(2)
C(36)	7376(8)	7842(8)	10911(3)	28(2)
C(37)	995(7)	4493(7)	6960(3)	23(2)
C(38)	1317(7)	2997(8)	7033(3)	22(2)
C(39)	2599(7)	2314(7)	7139(3)	23(2)
C(40)	2898(8)	942(8)	7188(3)	24(2)
C(41)	1907(8)	244(7)	7141(3)	23(2)
C(42)	612(8)	916(8)	7021(3)	28(2)
C(43)	328(8)	2283(8)	6971(3)	27(2)
C(44)	3405(11)	-1812(10)	7248(5)	53(3)
C(45)	1604(8)	4877(7)	6456(3)	25(2)
C(46)	1089(8)	6293(8)	6293(3)	26(2)
C(47)	1535(8)	6742(7)	5792(3)	25(2)
C(48)	1981(8)	5897(8)	5394(3)	29(2)
C(49)	2279(8)	6361(8)	4926(3)	29(2)
C(50)	2193(8)	7694(8)	4834(3)	26(2)
C(51)	1778(9)	8556(8)	5235(3)	29(2)
C(52)	1447(8)	8081(8)	5708(3)	28(2)
C(53)	2497(8)	8216(8)	4327(3)	30(2)
C(54)	3462(9)	7497(9)	4011(3)	32(2)
C(55)	3750(10)	7991(10)	3538(3)	40(2)
C(56)	3090(10)	9209(10)	3383(3)	39(2)
C(57)	2110(10)	9962(9)	3684(3)	37(2)
C(58)	1831(9)	9475(8)	4160(3)	32(2)
C(59)	1431(8)	5186(8)	7409(3)	26(2)
C(60)	614(7)	5082(7)	7889(3)	23(2)
C(61)	1077(7)	5463(7)	8381(3)	23(2)

C(62)	2173(8)	6039(7)	8426(3)	23(2)
C(63)	2514(8)	6462(8)	8885(3)	27(2)
C(64)	1761(7)	6299(7)	9321(3)	21(2)
C(65)	667(7)	5722(8)	9281(3)	25(2)
C(66)	321(8)	5305(8)	8812(3)	27(2)
C(67)	2105(7)	6776(8)	9818(3)	24(2)
C(68)	3446(8)	6743(8)	9940(3)	28(2)
C(69)	3751(9)	7232(9)	10397(3)	31(2)
C(70)	2761(9)	7755(8)	10745(3)	31(2)
C(71)	1425(9)	7768(9)	10634(3)	35(2)
C(72)	1116(8)	7279(8)	10175(3)	28(2)

Table S15. Bond lengths [Å] and angles [°] for i17966.

O(1)-C(5)	1.385(10)
O(1)-C(8)	1.410(12)
O(2)-C(10)	1.221(9)
O(3)-C(24)	1.201(10)
O(4)-C(41)	1.359(9)
O(4)-C(44)	1.430(11)
O(5)-C(46)	1.220(10)
O(6)-C(60)	1.220(9)
C(1)-C(2)	1.528(11)
C(1)-C(23)	1.530(11)
C(1)-C(9)	1.540(10)
C(1)-H(1)	1.0000
C(2)-C(7)	1.378(10)
C(2)-C(3)	1.405(10)
C(3)-C(4)	1.394(12)
C(3)-H(3)	0.9500
C(4)-C(5)	1.370(11)
C(4)-H(4)	0.9500
C(5)-C(6)	1.401(11)
C(6)-C(7)	1.376(11)
C(6)-H(6)	0.9500
C(7)-H(7)	0.9500
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-C(10)	1.506(10)
C(9)-H(9A)	0.9900
C(9)-H(9AB)	0.9900
C(10)-C(11)	1.501(10)
C(11)-C(16)	1.387(11)
C(11)-C(12)	1.392(10)
C(12)-C(13)	1.385(11)
C(12)-H(12)	0.9500
C(13)-C(14)	1.398(10)
C(13)-H(13)	0.9500
C(14)-C(15)	1.385(11)

C(14)-C(17)	1.487(10)
C(15)-C(16)	1.403(11)
C(15)-H(15)	0.9500
C(16)-H(16)	0.9500
C(17)-C(18)	1.408(11)
C(17)-C(22)	1.411(11)
C(18)-C(19)	1.384(12)
C(18)-H(18)	0.9500
C(19)-C(20)	1.400(13)
C(19)-H(19)	0.9500
C(20)-C(21)	1.385(13)
C(20)-H(20)	0.9500
C(21)-C(22)	1.400(12)
C(21)-H(21)	0.9500
C(22)-H(22)	0.9500
C(23)-C(24)	1.517(11)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-C(25)	1.499(11)
C(25)-C(26)	1.368(12)
C(25)-C(30)	1.404(11)
C(26)-C(27)	1.385(12)
C(26)-H(26)	0.9500
C(27)-C(28)	1.417(11)
C(27)-H(27)	0.9500
C(28)-C(29)	1.400(11)
C(28)-C(31)	1.478(11)
C(29)-C(30)	1.378(11)
C(29)-H(29)	0.9500
C(30)-H(30)	0.9500
C(31)-C(32)	1.381(12)
C(31)-C(36)	1.387(11)
C(32)-C(33)	1.400(12)
C(32)-H(32)	0.9500
C(33)-C(34)	1.388(13)
C(33)-H(33)	0.9500
C(34)-C(35)	1.382(13)
C(34)-H(34)	0.9500

C(35)-C(36)	1.413(12)
C(35)-H(35)	0.9500
C(36)-H(36)	0.9500
C(37)-C(59)	1.519(11)
C(37)-C(38)	1.528(11)
C(37)-C(45)	1.545(11)
C(37)-H(37)	1.0000
C(38)-C(39)	1.384(10)
C(38)-C(43)	1.391(10)
C(39)-C(40)	1.397(11)
C(39)-H(39)	0.9500
C(40)-C(41)	1.377(10)
C(40)-H(40)	0.9500
C(41)-C(42)	1.400(11)
C(42)-C(43)	1.393(12)
C(42)-H(42)	0.9500
C(43)-H(43)	0.9500
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(45)-C(46)	1.512(11)
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900
C(46)-C(47)	1.494(11)
C(47)-C(48)	1.387(11)
C(47)-C(52)	1.389(11)
C(48)-C(49)	1.375(12)
C(48)-H(48)	0.9500
C(49)-C(50)	1.387(11)
C(49)-H(49)	0.9500
C(50)-C(51)	1.400(11)
C(50)-C(53)	1.489(11)
C(51)-C(52)	1.400(11)
C(51)-H(51)	0.9500
C(52)-H(52)	0.9500
C(53)-C(54)	1.382(12)
C(53)-C(58)	1.408(11)
C(54)-C(55)	1.396(12)

C(54)-H(54)	0.9500
C(55)-C(56)	1.361(14)
C(55)-H(55)	0.9500
C(56)-C(57)	1.382(14)
C(56)-H(56)	0.9500
C(57)-C(58)	1.396(12)
C(57)-H(57)	0.9500
C(58)-H(58)	0.9500
C(59)-C(60)	1.523(10)
C(59)-H(59A)	0.9900
C(59)-H(59B)	0.9900
C(60)-C(61)	1.480(11)
C(61)-C(62)	1.389(10)
C(61)-C(66)	1.395(11)
C(62)-C(63)	1.372(11)
C(62)-H(62)	0.9500
C(63)-C(64)	1.404(10)
C(63)-H(63)	0.9500
C(64)-C(65)	1.386(10)
C(64)-C(67)	1.485(10)
C(65)-C(66)	1.395(11)
C(65)-H(65)	0.9500
C(66)-H(66)	0.9500
C(67)-C(72)	1.395(11)
C(67)-C(68)	1.410(11)
C(68)-C(69)	1.384(11)
C(68)-H(68)	0.9500
C(69)-C(70)	1.385(12)
C(69)-H(69)	0.9500
C(70)-C(71)	1.401(13)
C(70)-H(70)	0.9500
C(71)-C(72)	1.391(12)
C(71)-H(71)	0.9500
C(72)-H(72)	0.9500
C(5)-O(1)-C(8)	117.4(7)
C(41)-O(4)-C(44)	115.9(7)
C(2)-C(1)-C(23)	109.0(6)
C(2)-C(1)-C(9)	113.8(6)

C(23)-C(1)-C(9)	110.8(7)
C(2)-C(1)-H(1)	107.7
C(23)-C(1)-H(1)	107.7
C(9)-C(1)-H(1)	107.7
C(7)-C(2)-C(3)	117.2(7)
C(7)-C(2)-C(1)	122.1(7)
C(3)-C(2)-C(1)	120.6(7)
C(4)-C(3)-C(2)	121.1(7)
C(4)-C(3)-H(3)	119.5
C(2)-C(3)-H(3)	119.5
C(5)-C(4)-C(3)	119.6(7)
C(5)-C(4)-H(4)	120.2
C(3)-C(4)-H(4)	120.2
C(4)-C(5)-O(1)	124.5(7)
C(4)-C(5)-C(6)	120.6(8)
O(1)-C(5)-C(6)	114.8(7)
C(7)-C(6)-C(5)	118.4(7)
C(7)-C(6)-H(6)	120.8
C(5)-C(6)-H(6)	120.8
C(6)-C(7)-C(2)	123.1(7)
C(6)-C(7)-H(7)	118.5
C(2)-C(7)-H(7)	118.5
O(1)-C(8)-H(8A)	109.5
O(1)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
O(1)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(10)-C(9)-C(1)	113.5(6)
C(10)-C(9)-H(9A)	108.9
C(1)-C(9)-H(9A)	108.9
C(10)-C(9)-H(9AB)	108.9
C(1)-C(9)-H(9AB)	108.9
H(9A)-C(9)-H(9AB)	107.7
O(2)-C(10)-C(11)	119.9(6)
O(2)-C(10)-C(9)	121.0(6)
C(11)-C(10)-C(9)	119.2(6)
C(16)-C(11)-C(12)	118.2(7)

C(16)-C(11)-C(10)	118.6(7)
C(12)-C(11)-C(10)	123.1(7)
C(13)-C(12)-C(11)	120.9(7)
C(13)-C(12)-H(12)	119.5
C(11)-C(12)-H(12)	119.5
C(12)-C(13)-C(14)	121.1(7)
C(12)-C(13)-H(13)	119.4
C(14)-C(13)-H(13)	119.4
C(15)-C(14)-C(13)	117.9(7)
C(15)-C(14)-C(17)	121.3(7)
C(13)-C(14)-C(17)	120.8(7)
C(14)-C(15)-C(16)	120.9(7)
C(14)-C(15)-H(15)	119.6
C(16)-C(15)-H(15)	119.6
C(11)-C(16)-C(15)	120.9(7)
C(11)-C(16)-H(16)	119.6
C(15)-C(16)-H(16)	119.6
C(18)-C(17)-C(22)	118.8(7)
C(18)-C(17)-C(14)	120.9(7)
C(22)-C(17)-C(14)	120.3(7)
C(19)-C(18)-C(17)	120.4(8)
C(19)-C(18)-H(18)	119.8
C(17)-C(18)-H(18)	119.8
C(18)-C(19)-C(20)	120.8(8)
C(18)-C(19)-H(19)	119.6
C(20)-C(19)-H(19)	119.6
C(21)-C(20)-C(19)	119.3(8)
C(21)-C(20)-H(20)	120.4
C(19)-C(20)-H(20)	120.4
C(20)-C(21)-C(22)	120.9(8)
C(20)-C(21)-H(21)	119.5
C(22)-C(21)-H(21)	119.5
C(21)-C(22)-C(17)	119.8(8)
C(21)-C(22)-H(22)	120.1
C(17)-C(22)-H(22)	120.1
C(24)-C(23)-C(1)	115.3(6)
C(24)-C(23)-H(23A)	108.5
C(1)-C(23)-H(23A)	108.5

C(24)-C(23)-H(23B)	108.5
C(1)-C(23)-H(23B)	108.5
H(23A)-C(23)-H(23B)	107.5
O(3)-C(24)-C(25)	120.6(8)
O(3)-C(24)-C(23)	121.7(7)
C(25)-C(24)-C(23)	117.6(7)
C(26)-C(25)-C(30)	118.9(7)
C(26)-C(25)-C(24)	119.6(7)
C(30)-C(25)-C(24)	121.5(7)
C(25)-C(26)-C(27)	121.1(8)
C(25)-C(26)-H(26)	119.5
C(27)-C(26)-H(26)	119.5
C(26)-C(27)-C(28)	121.2(8)
C(26)-C(27)-H(27)	119.4
C(28)-C(27)-H(27)	119.4
C(29)-C(28)-C(27)	116.7(7)
C(29)-C(28)-C(31)	120.7(7)
C(27)-C(28)-C(31)	122.5(7)
C(30)-C(29)-C(28)	121.6(7)
C(30)-C(29)-H(29)	119.2
C(28)-C(29)-H(29)	119.2
C(29)-C(30)-C(25)	120.5(7)
C(29)-C(30)-H(30)	119.7
C(25)-C(30)-H(30)	119.7
C(32)-C(31)-C(36)	119.1(8)
C(32)-C(31)-C(28)	120.2(7)
C(36)-C(31)-C(28)	120.6(7)
C(31)-C(32)-C(33)	120.0(8)
C(31)-C(32)-H(32)	120.0
C(33)-C(32)-H(32)	120.0
C(34)-C(33)-C(32)	121.3(9)
C(34)-C(33)-H(33)	119.3
C(32)-C(33)-H(33)	119.3
C(35)-C(34)-C(33)	118.7(9)
C(35)-C(34)-H(34)	120.7
C(33)-C(34)-H(34)	120.7
C(34)-C(35)-C(36)	120.1(8)
C(34)-C(35)-H(35)	119.9

C(36)-C(35)-H(35)	119.9
C(31)-C(36)-C(35)	120.7(8)
C(31)-C(36)-H(36)	119.7
C(35)-C(36)-H(36)	119.7
C(59)-C(37)-C(38)	111.9(6)
C(59)-C(37)-C(45)	112.1(6)
C(38)-C(37)-C(45)	110.4(6)
C(59)-C(37)-H(37)	107.4
C(38)-C(37)-H(37)	107.4
C(45)-C(37)-H(37)	107.4
C(39)-C(38)-C(43)	118.3(7)
C(39)-C(38)-C(37)	121.4(7)
C(43)-C(38)-C(37)	120.3(7)
C(38)-C(39)-C(40)	121.2(7)
C(38)-C(39)-H(39)	119.4
C(40)-C(39)-H(39)	119.4
C(41)-C(40)-C(39)	120.2(7)
C(41)-C(40)-H(40)	119.9
C(39)-C(40)-H(40)	119.9
O(4)-C(41)-C(40)	125.9(7)
O(4)-C(41)-C(42)	114.7(7)
C(40)-C(41)-C(42)	119.3(7)
C(43)-C(42)-C(41)	119.8(8)
C(43)-C(42)-H(42)	120.1
C(41)-C(42)-H(42)	120.1
C(38)-C(43)-C(42)	121.0(7)
C(38)-C(43)-H(43)	119.5
C(42)-C(43)-H(43)	119.5
O(4)-C(44)-H(44A)	109.5
O(4)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
O(4)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(46)-C(45)-C(37)	114.3(6)
C(46)-C(45)-H(45A)	108.7
C(37)-C(45)-H(45A)	108.7
C(46)-C(45)-H(45B)	108.7

C(37)-C(45)-H(45B)	108.7
H(45A)-C(45)-H(45B)	107.6
O(5)-C(46)-C(47)	119.9(7)
O(5)-C(46)-C(45)	121.5(7)
C(47)-C(46)-C(45)	118.6(7)
C(48)-C(47)-C(52)	117.9(8)
C(48)-C(47)-C(46)	123.4(7)
C(52)-C(47)-C(46)	118.7(7)
C(49)-C(48)-C(47)	121.6(8)
C(49)-C(48)-H(48)	119.2
C(47)-C(48)-H(48)	119.2
C(48)-C(49)-C(50)	121.5(8)
C(48)-C(49)-H(49)	119.3
C(50)-C(49)-H(49)	119.3
C(49)-C(50)-C(51)	117.5(8)
C(49)-C(50)-C(53)	122.2(7)
C(51)-C(50)-C(53)	120.3(7)
C(52)-C(51)-C(50)	120.8(7)
C(52)-C(51)-H(51)	119.6
C(50)-C(51)-H(51)	119.6
C(47)-C(52)-C(51)	120.8(7)
C(47)-C(52)-H(52)	119.6
C(51)-C(52)-H(52)	119.6
C(54)-C(53)-C(58)	117.8(8)
C(54)-C(53)-C(50)	121.2(7)
C(58)-C(53)-C(50)	120.9(8)
C(53)-C(54)-C(55)	121.1(8)
C(53)-C(54)-H(54)	119.4
C(55)-C(54)-H(54)	119.4
C(56)-C(55)-C(54)	120.0(9)
C(56)-C(55)-H(55)	120.0
C(54)-C(55)-H(55)	120.0
C(55)-C(56)-C(57)	121.0(9)
C(55)-C(56)-H(56)	119.5
C(57)-C(56)-H(56)	119.5
C(56)-C(57)-C(58)	119.0(9)
C(56)-C(57)-H(57)	120.5
C(58)-C(57)-H(57)	120.5

C(57)-C(58)-C(53)	121.0(8)
C(57)-C(58)-H(58)	119.5
C(53)-C(58)-H(58)	119.5
C(37)-C(59)-C(60)	113.3(6)
C(37)-C(59)-H(59A)	108.9
C(60)-C(59)-H(59A)	108.9
C(37)-C(59)-H(59B)	108.9
C(60)-C(59)-H(59B)	108.9
H(59A)-C(59)-H(59B)	107.7
O(6)-C(60)-C(61)	119.7(7)
O(6)-C(60)-C(59)	120.3(7)
C(61)-C(60)-C(59)	119.9(6)
C(62)-C(61)-C(66)	119.0(7)
C(62)-C(61)-C(60)	123.1(7)
C(66)-C(61)-C(60)	117.8(7)
C(63)-C(62)-C(61)	121.3(7)
C(63)-C(62)-H(62)	119.4
C(61)-C(62)-H(62)	119.4
C(62)-C(63)-C(64)	120.0(7)
C(62)-C(63)-H(63)	120.0
C(64)-C(63)-H(63)	120.0
C(65)-C(64)-C(63)	119.3(7)
C(65)-C(64)-C(67)	120.2(7)
C(63)-C(64)-C(67)	120.5(7)
C(64)-C(65)-C(66)	120.3(7)
C(64)-C(65)-H(65)	119.8
C(66)-C(65)-H(65)	119.8
C(61)-C(66)-C(65)	120.1(7)
C(61)-C(66)-H(66)	119.9
C(65)-C(66)-H(66)	119.9
C(72)-C(67)-C(68)	118.1(7)
C(72)-C(67)-C(64)	121.2(7)
C(68)-C(67)-C(64)	120.7(7)
C(69)-C(68)-C(67)	120.1(8)
C(69)-C(68)-H(68)	119.9
C(67)-C(68)-H(68)	119.9
C(68)-C(69)-C(70)	121.4(8)
C(68)-C(69)-H(69)	119.3

C(70)-C(69)-H(69)	119.3
C(69)-C(70)-C(71)	119.2(8)
C(69)-C(70)-H(70)	120.4
C(71)-C(70)-H(70)	120.4
C(72)-C(71)-C(70)	119.5(8)
C(72)-C(71)-H(71)	120.2
C(70)-C(71)-H(71)	120.2
C(71)-C(72)-C(67)	121.6(8)
C(71)-C(72)-H(72)	119.2
C(67)-C(72)-H(72)	119.2

Symmetry transformations used to generate equivalent atoms:

Table S16. Anisotropic displacement parameters ($Å^2$x 10^3)for i17966. 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)	40(4)	32(3)	42(4)	2(3)	3(3)	-6(3)
O(2)	22(3)	35(3)	24(3)	6(2)	-3(2)	-8(2)
O(3)	30(3)	36(3)	30(3)	8(2)	-2(2)	-6(3)
O(4)	39(3)	22(3)	45(4)	11(3)	-6(3)	-4(3)
O(5)	30(3)	30(3)	33(3)	-1(2)	-3(2)	-1(2)
O(6)	20(3)	37(3)	35(3)	-6(3)	6(2)	-13(2)
C(1)	17(4)	32(4)	28(4)	8(3)	2(3)	1(3)
C(2)	14(3)	33(4)	17(3)	2(3)	0(3)	-7(3)
C(3)	21(4)	34(4)	32(4)	6(3)	1(3)	-9(3)
C(4)	24(4)	33(4)	26(4)	1(3)	5(3)	-1(3)
C(5)	33(4)	31(4)	16(3)	3(3)	2(3)	-8(3)
C(6)	28(4)	37(5)	21(4)	4(3)	-1(3)	-12(3)
C(7)	17(3)	33(4)	21(4)	4(3)	-1(3)	-6(3)
C(8)	48(6)	35(5)	86(9)	3(5)	19(6)	-3(5)
C(9)	25(4)	34(4)	21(4)	3(3)	0(3)	-10(3)
C(10)	16(3)	24(4)	20(3)	2(3)	-3(3)	-2(3)
C(11)	21(4)	21(4)	21(4)	2(3)	1(3)	-4(3)
C(12)	24(4)	28(4)	24(4)	3(3)	-7(3)	-7(3)
C(13)	21(4)	34(4)	22(4)	-3(3)	-2(3)	-10(3)
C(14)	24(4)	25(4)	19(3)	3(3)	-3(3)	-5(3)
C(15)	27(4)	39(5)	21(4)	9(3)	-8(3)	-14(3)
C(16)	22(4)	44(5)	30(4)	9(4)	-7(3)	-11(4)
C(17)	33(4)	19(4)	19(3)	0(3)	-3(3)	-5(3)
C(18)	26(4)	29(4)	26(4)	-3(3)	-5(3)	-7(3)
C(19)	32(4)	34(4)	31(4)	-9(3)	6(3)	-9(4)
C(20)	50(5)	42(5)	16(4)	-2(3)	2(3)	-26(4)
C(21)	35(5)	37(5)	31(4)	7(4)	-7(4)	-10(4)
C(22)	30(4)	31(4)	24(4)	-1(3)	-2(3)	-3(3)
C(23)	24(4)	29(4)	21(4)	4(3)	5(3)	-3(3)
C(24)	25(4)	31(4)	23(4)	6(3)	1(3)	-10(3)
C(25)	26(4)	33(4)	21(4)	2(3)	3(3)	-6(3)
C(26)	37(5)	33(4)	23(4)	7(3)	-3(3)	-2(4)
C(27)	36(4)	24(4)	26(4)	1(3)	6(3)	-1(3)

C(28)	23(4)	27(4)	22(4)	5(3)	1(3)	-5(3)
C(29)	26(4)	25(4)	30(4)	6(3)	3(3)	-6(3)
C(30)	28(4)	19(4)	26(4)	2(3)	5(3)	1(3)
C(31)	24(4)	27(4)	25(4)	2(3)	3(3)	-1(3)
C(32)	52(5)	24(4)	26(4)	1(3)	-2(4)	-7(4)
C(33)	52(6)	28(4)	37(5)	-5(4)	-9(4)	-5(4)
C(34)	43(5)	36(5)	36(5)	-9(4)	2(4)	-7(4)
C(35)	33(4)	40(5)	23(4)	2(3)	5(3)	-8(4)
C(36)	33(4)	24(4)	24(4)	1(3)	5(3)	-1(3)
C(37)	16(3)	26(4)	27(4)	-1(3)	-2(3)	-6(3)
C(38)	19(3)	28(4)	21(3)	-2(3)	7(3)	-5(3)
C(39)	22(4)	24(4)	24(4)	2(3)	-6(3)	-5(3)
C(40)	23(4)	26(4)	24(4)	-1(3)	-5(3)	-5(3)
C(41)	25(4)	23(4)	21(4)	1(3)	-2(3)	-6(3)
C(42)	26(4)	31(4)	28(4)	-2(3)	3(3)	-6(3)
C(43)	20(4)	33(4)	27(4)	-3(3)	4(3)	-6(3)
C(44)	47(6)	32(5)	74(8)	9(5)	5(5)	6(4)
C(45)	24(4)	22(4)	28(4)	0(3)	-5(3)	-5(3)
C(46)	24(4)	24(4)	32(4)	-5(3)	-5(3)	-7(3)
C(47)	20(4)	21(4)	33(4)	0(3)	-8(3)	0(3)
C(48)	31(4)	25(4)	27(4)	-5(3)	-3(3)	1(3)
C(49)	32(4)	23(4)	32(4)	-4(3)	-1(3)	-5(3)
C(50)	25(4)	25(4)	27(4)	-5(3)	-6(3)	-6(3)
C(51)	38(5)	22(4)	27(4)	3(3)	-11(3)	-3(3)
C(52)	32(4)	25(4)	26(4)	-6(3)	-6(3)	0(3)
C(53)	33(4)	25(4)	31(4)	-1(3)	-5(3)	-6(3)
C(54)	33(4)	30(4)	30(4)	1(3)	2(3)	-1(3)
C(55)	52(6)	40(5)	31(5)	-6(4)	12(4)	-20(4)
C(56)	49(6)	47(5)	27(4)	0(4)	-5(4)	-23(5)
C(57)	50(6)	28(4)	34(5)	3(4)	-9(4)	-15(4)
C(58)	37(5)	31(4)	26(4)	3(3)	-6(3)	-6(4)
C(59)	26(4)	29(4)	26(4)	0(3)	4(3)	-10(3)
C(60)	20(4)	20(4)	28(4)	-1(3)	0(3)	-4(3)
C(61)	21(4)	19(3)	27(4)	2(3)	3(3)	-4(3)
C(62)	24(4)	21(4)	24(4)	0(3)	6(3)	-5(3)
C(63)	24(4)	26(4)	31(4)	1(3)	5(3)	-7(3)
C(64)	19(3)	21(4)	21(3)	4(3)	-2(3)	-1(3)
C(65)	18(4)	32(4)	26(4)	4(3)	1(3)	-7(3)

C(66)	21(4)	34(4)	28(4)	4(3)	-6(3)	-8(3)
C(67)	22(4)	28(4)	21(4)	2(3)	2(3)	-7(3)
C(68)	28(4)	37(4)	20(4)	6(3)	0(3)	-10(3)
C(69)	29(4)	42(5)	26(4)	2(3)	-2(3)	-13(4)
C(70)	43(5)	30(4)	23(4)	8(3)	-5(3)	-10(4)
C(71)	36(5)	43(5)	25(4)	-2(4)	6(3)	-6(4)
C(72)	26(4)	38(5)	22(4)	-2(3)	1(3)	-9(3)

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

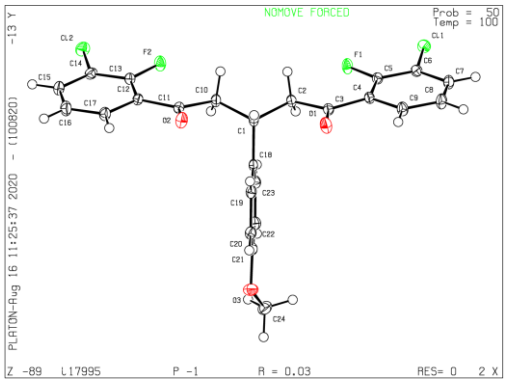


Figure S5. Single X-ray crystal structure of 1, 5-dicarbonyls **4r** (the thermal ellipsoid was drawn at the 50% probability level)

Table S17. Crystal data and structure refinement for i17995

CCDC	2031245	
Identification code	i17995	
Empirical formula	C24 H18 Cl2 F2 O3	
Formula weight	463.28	
Temperature	100.0(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.9911(2) Å	α= 88.9720(10)°.
	b = 10.8950(3) Å	β= 73.5650(10)°.
	c = 11.8009(3) Å	γ = 66.1240(10)°.
Z, Volume	2, 1007.71(4) $Å^3$	
Density (calculated)	1.527 Mg/m^3	
Absorption coefficient	0.366 mm^{-1}	
F(000)	476	
Crystal size	0.288 x 0.227 x 0.182 mm^3	
Theta range for data collection	1.810 to 30.508°.	
Index ranges	-12<=h<=12, -15<=k<=15, -16<=l<=16	

Reflections collected	52936
Independent reflections	6134 [R(int) = 0.0380]
Completeness to theta = 25.242°	99.7 %
Absorption correction	Numerical
Max. and min. transmission	1 and 0.9675
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6134 / 0 / 281
Goodness-of-fit on F^2	1.022
Final R indices [I>2sigma(I)]	R1 = 0.0330, wR2 = 0.0811
R indices (all data)	R1 = 0.0405, wR2 = 0.0860
Extinction coefficient	n/a
Largest diff. peak and hole	0.442 and -0.372 e.Å^{-3}

Table S18. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for i17995. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	12288(1)	-1735(1)	739(1)	19(1)
Cl(2)	6259(1)	9717(1)	978(1)	23(1)
F(1)	9606(1)	900(1)	1640(1)	20(1)
F(2)	6384(1)	7197(1)	1880(1)	21(1)
O(1)	5078(1)	1829(1)	4383(1)	22(1)
O(2)	2673(1)	6687(1)	4619(1)	21(1)
O(3)	-460(1)	3998(1)	1613(1)	21(1)
C(1)	4790(1)	4156(1)	3337(1)	14(1)
C(2)	6453(1)	2867(1)	2914(1)	15(1)
C(3)	6318(1)	1678(1)	3544(1)	15(1)
C(4)	7724(1)	278(1)	3149(1)	14(1)
C(5)	9239(1)	-61(1)	2228(1)	15(1)
C(6)	10427(1)	-1393(1)	1884(1)	15(1)
C(7)	10132(2)	-2428(1)	2463(1)	19(1)
C(8)	8634(2)	-2115(1)	3387(1)	21(1)
C(9)	7457(2)	-787(1)	3722(1)	18(1)
C(10)	5133(1)	5408(1)	3000(1)	16(1)
C(11)	3735(1)	6705(1)	3718(1)	15(1)
C(12)	3640(1)	8049(1)	3321(1)	14(1)
C(13)	4901(1)	8248(1)	2441(1)	15(1)
C(14)	4684(2)	9524(1)	2102(1)	17(1)

C(15)	3197(2)	10639(1)	2659(1)	21(1)
C(16)	1924(2)	10472(1)	3546(1)	22(1)
C(17)	2147(2)	9193(1)	3867(1)	18(1)
C(18)	3418(1)	4100(1)	2855(1)	14(1)
C(19)	1845(1)	4223(1)	3614(1)	15(1)
C(20)	584(1)	4176(1)	3181(1)	16(1)
C(21)	871(1)	4000(1)	1955(1)	16(1)
C(22)	2440(2)	3852(1)	1173(1)	16(1)
C(23)	3678(1)	3914(1)	1634(1)	16(1)
C(24)	-85(2)	3408(1)	438(1)	23(1)

Table S19. Bond lengths [Å] and angles [°] for i17995.

Cl(1)-C(6)	1.7319(12)
Cl(2)-C(14)	1.7253(12)
F(1)-C(5)	1.3461(13)
F(2)-C(13)	1.3489(13)
O(1)-C(3)	1.2174(14)
O(2)-C(11)	1.2182(14)
O(3)-C(21)	1.3684(14)
O(3)-C(24)	1.4280(15)
C(1)-C(18)	1.5199(16)
C(1)-C(2)	1.5366(15)
C(1)-C(10)	1.5377(15)
C(1)-H(1)	1.0000
C(2)-C(3)	1.5122(15)
C(2)-H(2A)	0.9900
C(2)-H(2AB)	0.9900
C(3)-C(4)	1.5081(15)
C(4)-C(5)	1.3933(15)
C(4)-C(9)	1.4024(15)
C(5)-C(6)	1.3904(15)
C(6)-C(7)	1.3856(16)
C(7)-C(8)	1.3890(17)
C(7)-H(7)	0.9500
C(8)-C(9)	1.3843(17)
C(8)-H(8)	0.9500
C(9)-H(9)	0.9500
C(10)-C(11)	1.5163(15)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.5057(15)
C(12)-C(13)	1.3913(16)
C(12)-C(17)	1.3982(16)
C(13)-C(14)	1.3912(16)
C(14)-C(15)	1.3829(17)
C(15)-C(16)	1.3863(18)
C(15)-H(15)	0.9500
C(16)-C(17)	1.3870(17)

C(16)-H(16)	0.9500
C(17)-H(17)	0.9500
C(18)-C(23)	1.3972(16)
C(18)-C(19)	1.3977(15)
C(19)-C(20)	1.3883(16)
C(19)-H(19)	0.9500
C(20)-C(21)	1.3974(16)
C(20)-H(20)	0.9500
C(21)-C(22)	1.3977(16)
C(22)-C(23)	1.3954(16)
C(22)-H(22)	0.9500
C(23)-H(23)	0.9500
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(21)-O(3)-C(24)	117.57(10)
C(18)-C(1)-C(2)	111.66(9)
C(18)-C(1)-C(10)	111.35(9)
C(2)-C(1)-C(10)	110.30(9)
C(18)-C(1)-H(1)	107.8
C(2)-C(1)-H(1)	107.8
C(10)-C(1)-H(1)	107.8
C(3)-C(2)-C(1)	112.16(9)
C(3)-C(2)-H(2A)	109.2
C(1)-C(2)-H(2A)	109.2
C(3)-C(2)-H(2AB)	109.2
C(1)-C(2)-H(2AB)	109.2
H(2A)-C(2)-H(2AB)	107.9
O(1)-C(3)-C(4)	118.57(10)
O(1)-C(3)-C(2)	120.87(10)
C(4)-C(3)-C(2)	120.56(10)
C(5)-C(4)-C(9)	116.95(10)
C(5)-C(4)-C(3)	125.74(10)
C(9)-C(4)-C(3)	117.26(10)
F(1)-C(5)-C(6)	117.52(10)
F(1)-C(5)-C(4)	120.77(10)
C(6)-C(5)-C(4)	121.70(10)
C(7)-C(6)-C(5)	120.29(10)

C(7)-C(6)-Cl(1)	120.67(9)
C(5)-C(6)-Cl(1)	119.03(9)
C(6)-C(7)-C(8)	119.08(11)
C(6)-C(7)-H(7)	120.5
C(8)-C(7)-H(7)	120.5
C(9)-C(8)-C(7)	120.27(11)
C(9)-C(8)-H(8)	119.9
C(7)-C(8)-H(8)	119.9
C(8)-C(9)-C(4)	121.71(11)
C(8)-C(9)-H(9)	119.1
C(4)-C(9)-H(9)	119.1
C(11)-C(10)-C(1)	113.00(9)
C(11)-C(10)-H(10A)	109.0
C(1)-C(10)-H(10A)	109.0
C(11)-C(10)-H(10B)	109.0
C(1)-C(10)-H(10B)	109.0
H(10A)-C(10)-H(10B)	107.8
O(2)-C(11)-C(12)	118.76(10)
O(2)-C(11)-C(10)	121.19(10)
C(12)-C(11)-C(10)	120.05(10)
C(13)-C(12)-C(17)	117.12(10)
C(13)-C(12)-C(11)	125.49(10)
C(17)-C(12)-C(11)	117.38(10)
F(2)-C(13)-C(14)	117.57(10)
F(2)-C(13)-C(12)	120.70(10)
C(14)-C(13)-C(12)	121.73(11)
C(15)-C(14)-C(13)	119.97(11)
C(15)-C(14)-Cl(2)	119.88(9)
C(13)-C(14)-Cl(2)	120.15(9)
C(14)-C(15)-C(16)	119.52(11)
C(14)-C(15)-H(15)	120.2
C(16)-C(15)-H(15)	120.2
C(15)-C(16)-C(17)	119.99(11)
C(15)-C(16)-H(16)	120.0
C(17)-C(16)-H(16)	120.0
C(16)-C(17)-C(12)	121.66(11)
C(16)-C(17)-H(17)	119.2
C(12)-C(17)-H(17)	119.2

C(23)-C(18)-C(19)	117.17(10)
C(23)-C(18)-C(1)	121.40(10)
C(19)-C(18)-C(1)	121.43(10)
C(20)-C(19)-C(18)	121.76(11)
C(20)-C(19)-H(19)	119.1
C(18)-C(19)-H(19)	119.1
C(19)-C(20)-C(21)	119.97(10)
C(19)-C(20)-H(20)	120.0
C(21)-C(20)-H(20)	120.0
O(3)-C(21)-C(20)	115.75(10)
O(3)-C(21)-C(22)	124.57(11)
C(20)-C(21)-C(22)	119.68(11)
C(23)-C(22)-C(21)	119.04(11)
C(23)-C(22)-H(22)	120.5
C(21)-C(22)-H(22)	120.5
C(22)-C(23)-C(18)	122.37(10)
C(22)-C(23)-H(23)	118.8
C(18)-C(23)-H(23)	118.8
O(3)-C(24)-H(24A)	109.5
O(3)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
O(3)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S20. Anisotropic displacement parameters ($Å^2$x 10^3)for i17995. 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)	15(1)	19(1)	19(1)	-1(1)	-1(1)	-6(1)
Cl(2)	25(1)	24(1)	24(1)	8(1)	-7(1)	-15(1)
F(1)	18(1)	14(1)	25(1)	7(1)	0(1)	-6(1)
F(2)	17(1)	15(1)	25(1)	1(1)	1(1)	-5(1)
O(1)	17(1)	17(1)	24(1)	6(1)	1(1)	-5(1)
O(2)	22(1)	16(1)	19(1)	1(1)	1(1)	-8(1)
O(3)	17(1)	25(1)	23(1)	-2(1)	-5(1)	-9(1)
C(1)	14(1)	10(1)	16(1)	2(1)	-3(1)	-4(1)
C(2)	13(1)	11(1)	17(1)	3(1)	-2(1)	-4(1)
C(3)	14(1)	13(1)	17(1)	3(1)	-5(1)	-5(1)
C(4)	14(1)	12(1)	16(1)	3(1)	-5(1)	-5(1)
C(5)	15(1)	13(1)	17(1)	5(1)	-5(1)	-6(1)
C(6)	14(1)	15(1)	15(1)	0(1)	-3(1)	-5(1)
C(7)	19(1)	12(1)	23(1)	2(1)	-6(1)	-5(1)
C(8)	23(1)	14(1)	24(1)	6(1)	-4(1)	-7(1)
C(9)	17(1)	14(1)	20(1)	5(1)	-3(1)	-6(1)
C(10)	14(1)	11(1)	18(1)	1(1)	-2(1)	-4(1)
C(11)	15(1)	12(1)	16(1)	1(1)	-5(1)	-6(1)
C(12)	16(1)	12(1)	16(1)	1(1)	-5(1)	-6(1)
C(13)	15(1)	12(1)	17(1)	0(1)	-5(1)	-4(1)
C(14)	19(1)	18(1)	19(1)	4(1)	-7(1)	-11(1)
C(15)	24(1)	13(1)	26(1)	5(1)	-10(1)	-8(1)
C(16)	21(1)	13(1)	28(1)	0(1)	-5(1)	-4(1)
C(17)	17(1)	14(1)	20(1)	0(1)	-3(1)	-5(1)
C(18)	13(1)	9(1)	16(1)	2(1)	-2(1)	-3(1)
C(19)	15(1)	12(1)	14(1)	0(1)	-1(1)	-5(1)
C(20)	14(1)	14(1)	18(1)	-1(1)	0(1)	-5(1)
C(21)	14(1)	11(1)	20(1)	1(1)	-4(1)	-4(1)
C(22)	17(1)	15(1)	15(1)	2(1)	-3(1)	-6(1)
C(23)	13(1)	14(1)	16(1)	2(1)	-1(1)	-4(1)
C(24)	28(1)	22(1)	24(1)	2(1)	-11(1)	-14(1)

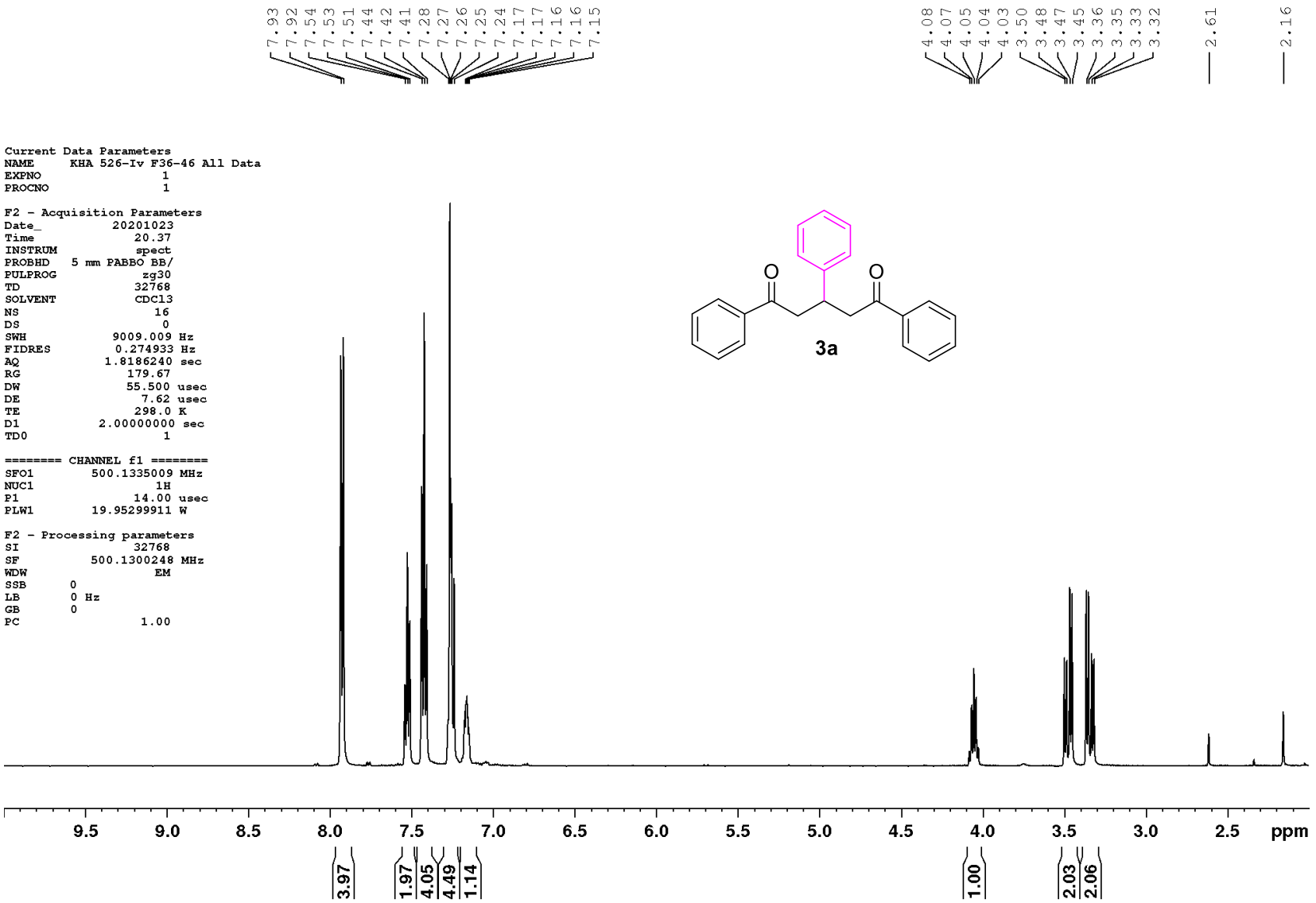
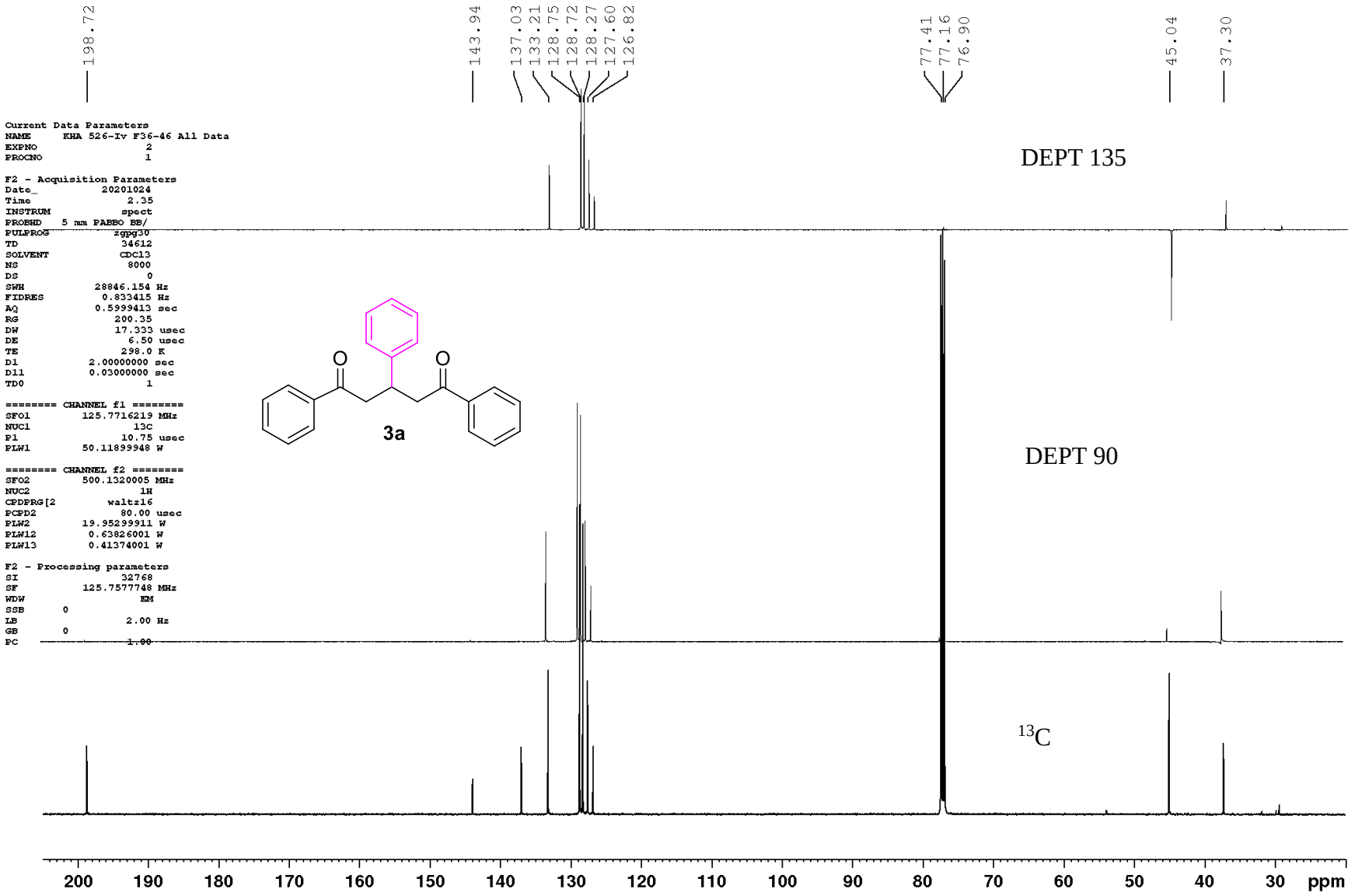


Figure S6. ^{1}H NMR spectrum of compound **3a** (500 MHz, $CDCl_3$, 25 ^{o}C)

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DE                6.50 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
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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
SSB       0
LB               2.00 Hz
GB        0
PC               1.00
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Figure S7. ^{13}C NMR spectrum of compound **3a** (125 MHz, $CDCl_3$, 25 ^{o}C)

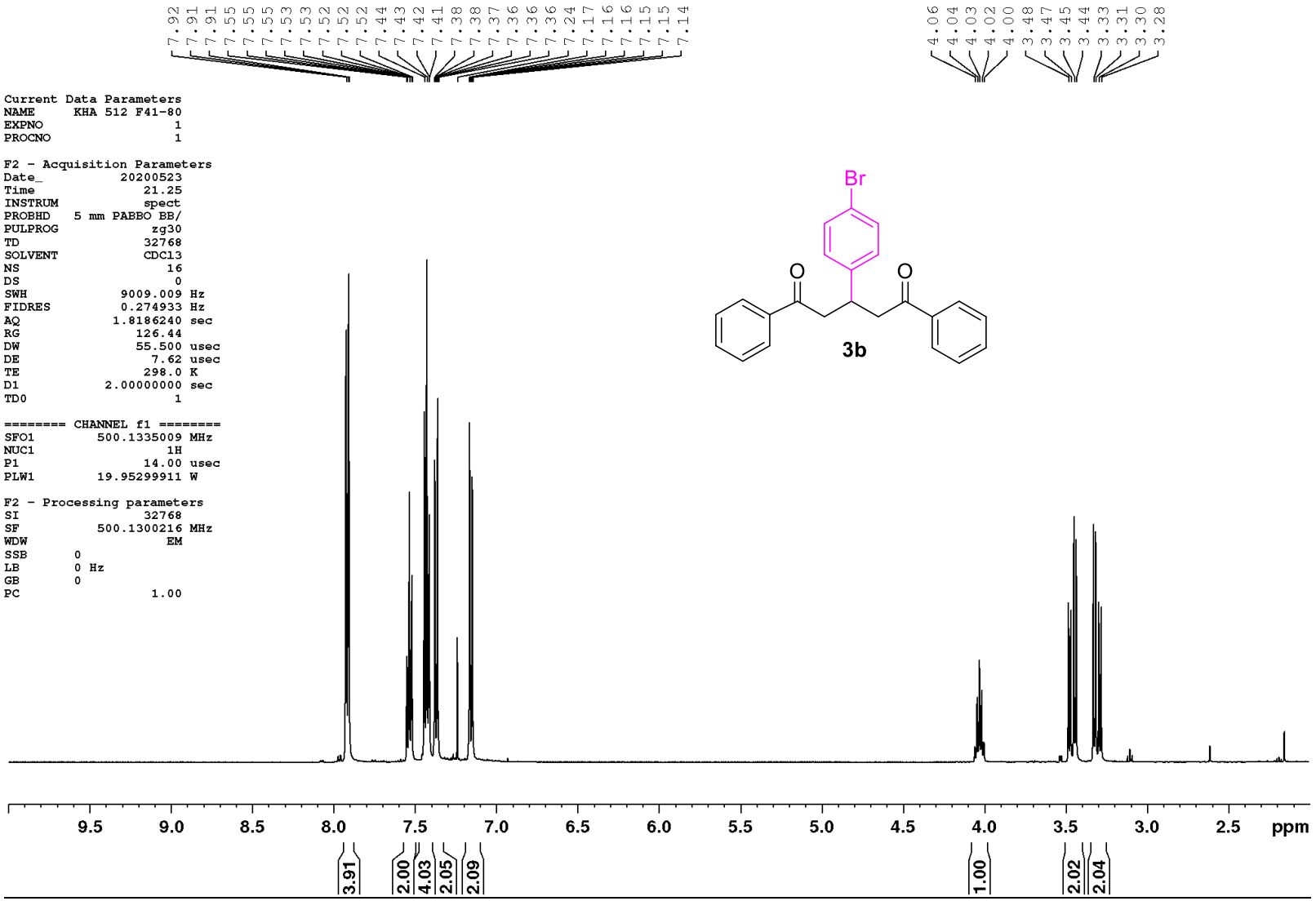


Figure S8. ^{1}H NMR spectrum of compound **3b** (500 MHz, $CDCl_3$, 25 ^{o}C)

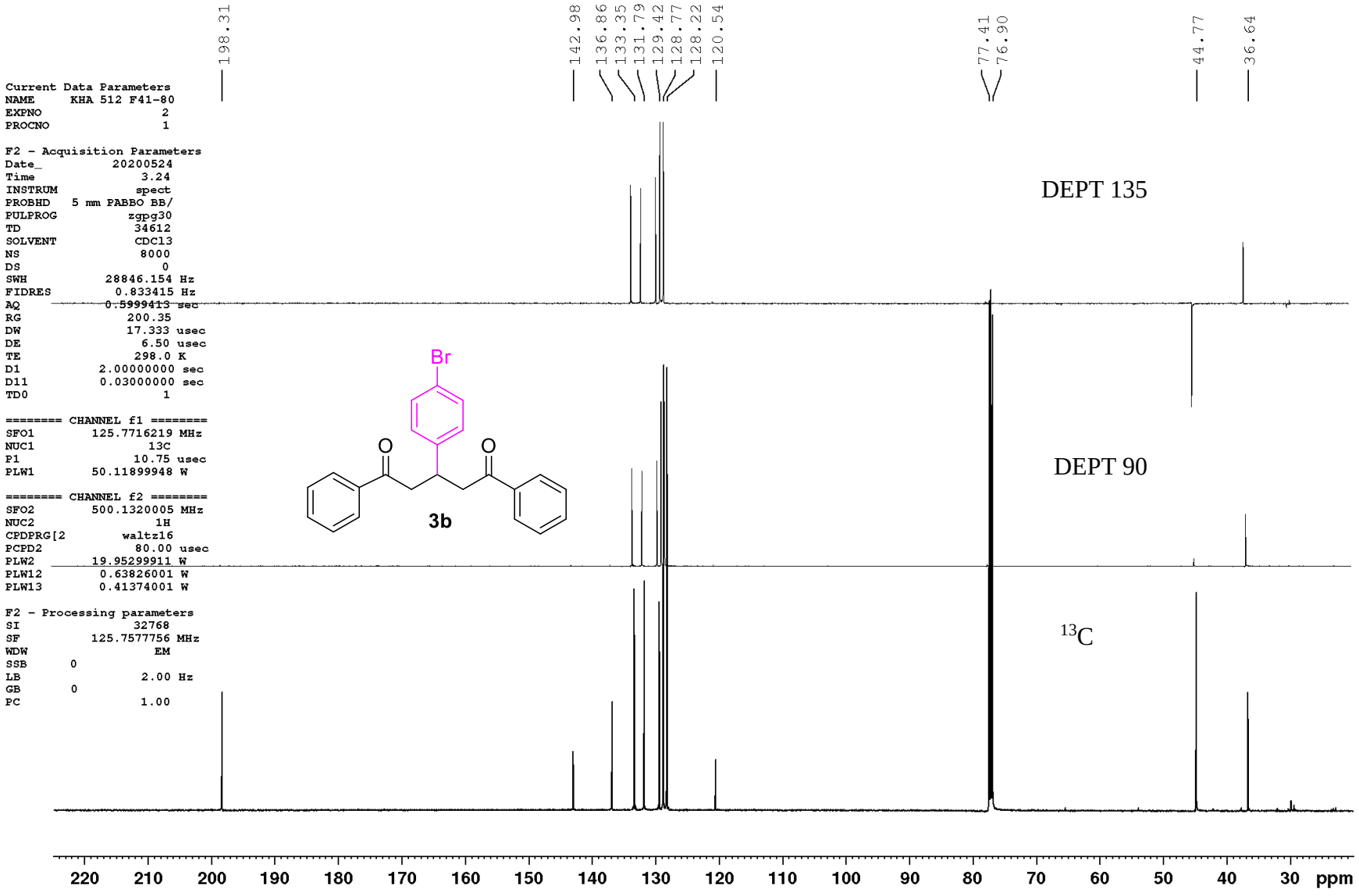


Figure S9. ^{13}C NMR spectrum of compound **3b** (125 MHz, $CDCl_3$, 25 ^oC)

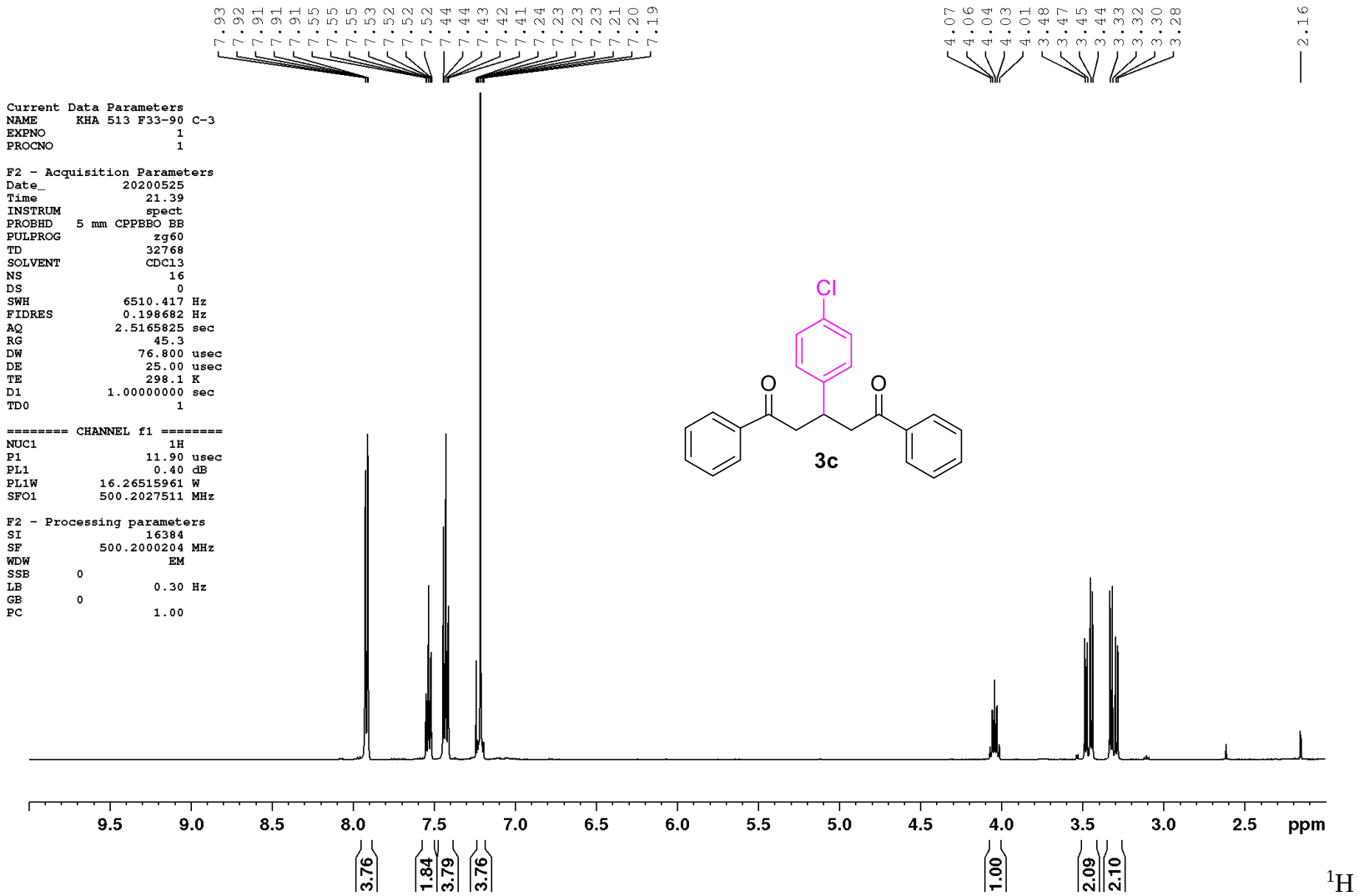


Figure S10. ^{1}H NMR spectrum of compound **3c** (500 MHz, $CDCl_3$, 25 ^{o}C)

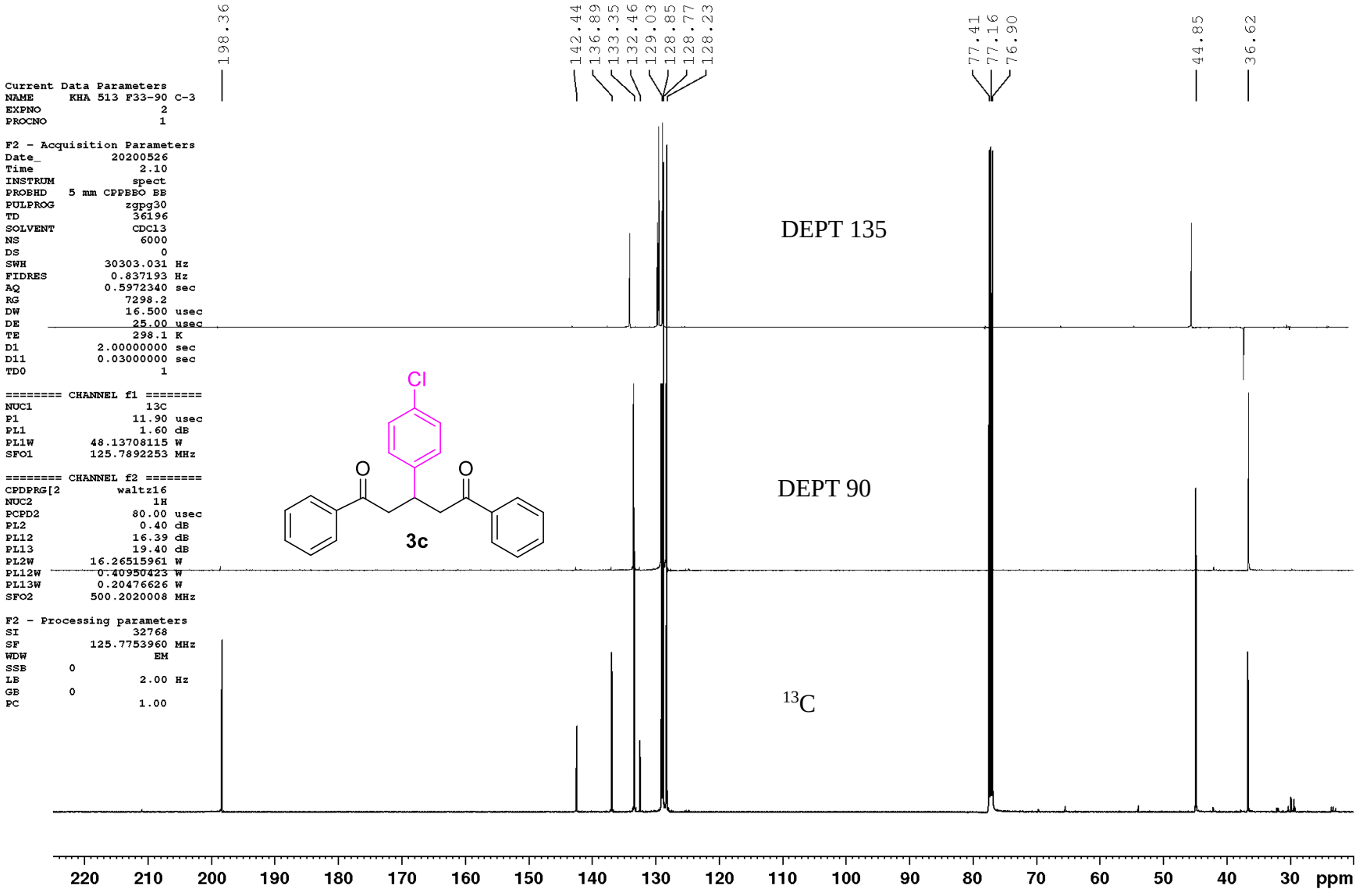


Figure S11. ^{13}C NMR spectrum of compound **3c** (125 MHz, $CDCl_3$, 25 ºC)

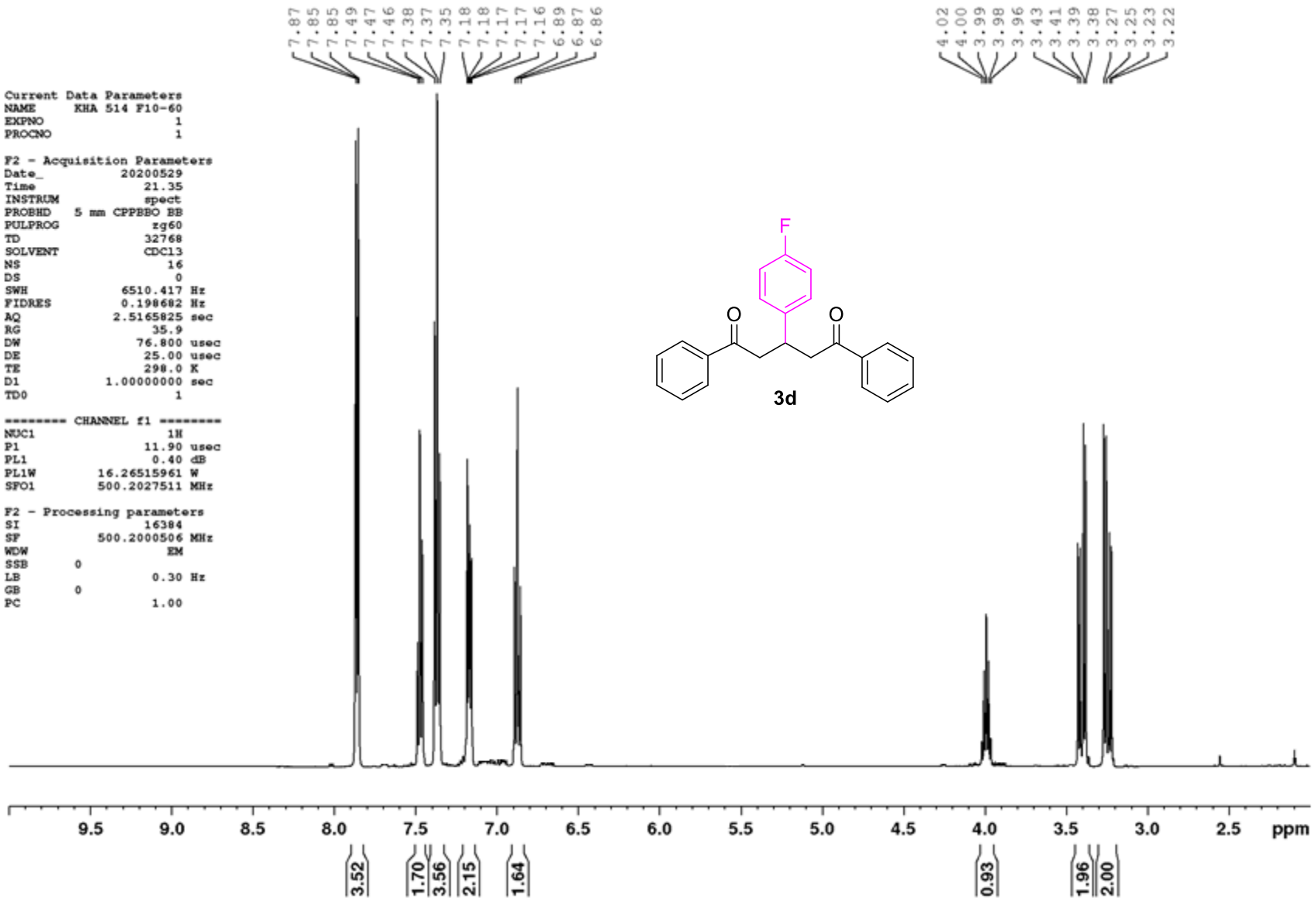


Figure S12. ^{1}H NMR spectrum of compound **3d** (500 MHz, $CDCl_3$, 25 ^{o}C)

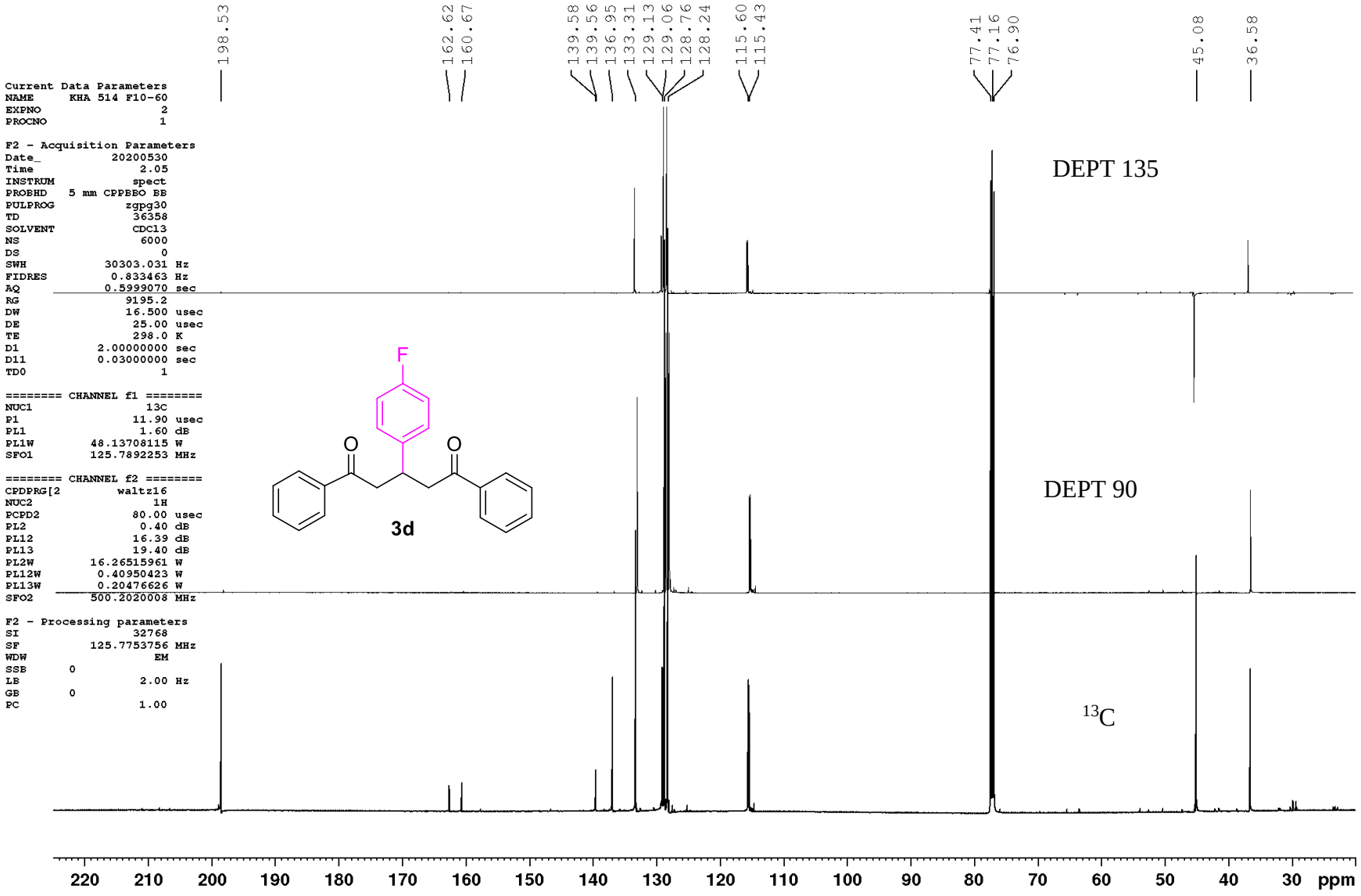


Figure S13. ^{13}C NMR spectrum of compound **3d** (125 MHz, $CDCl_3$, 25 °C)

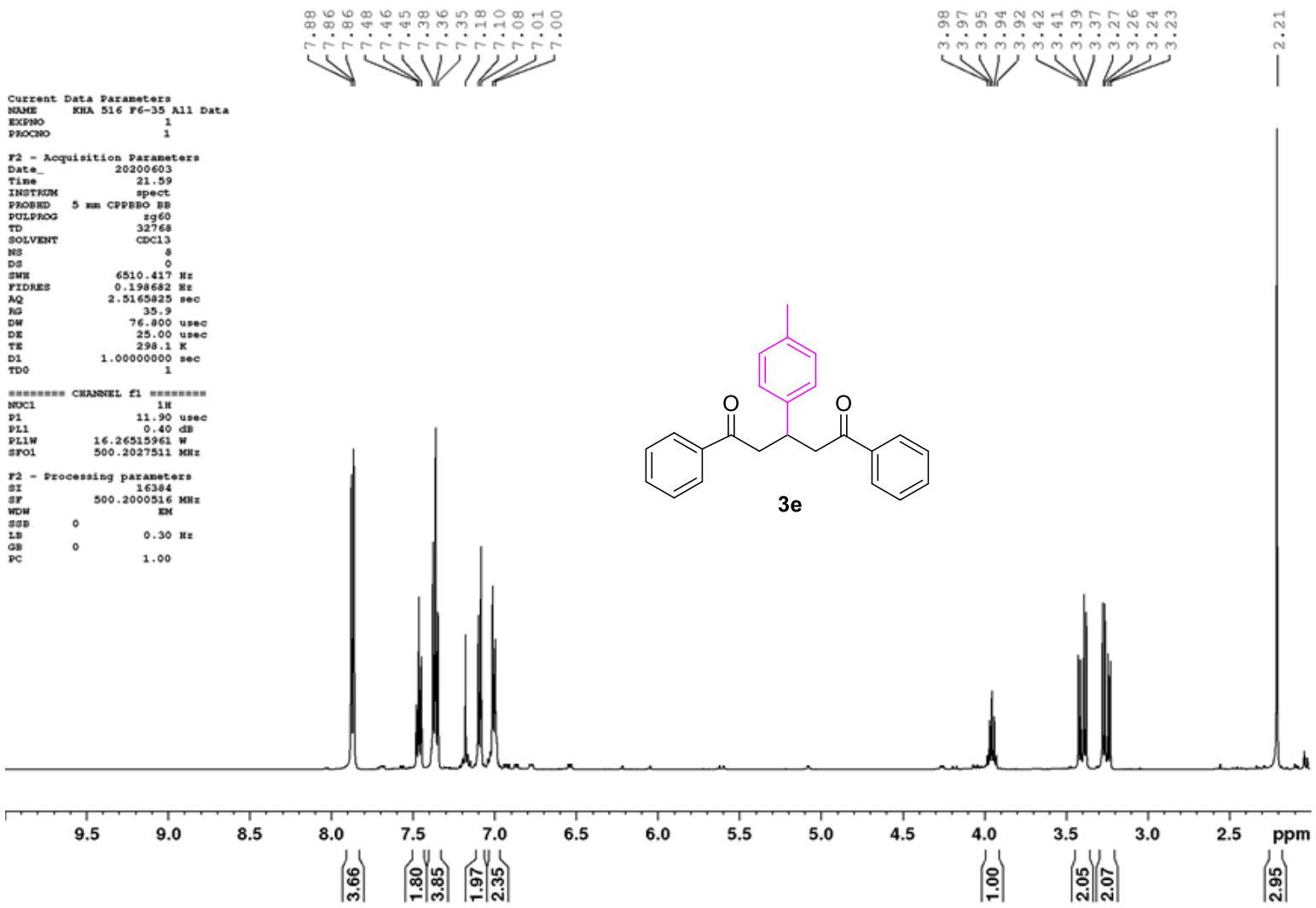


Figure S14. ^{1}H NMR spectrum of compound **3e** (500 MHz, $CDCl_3$, 25 ^{o}C)

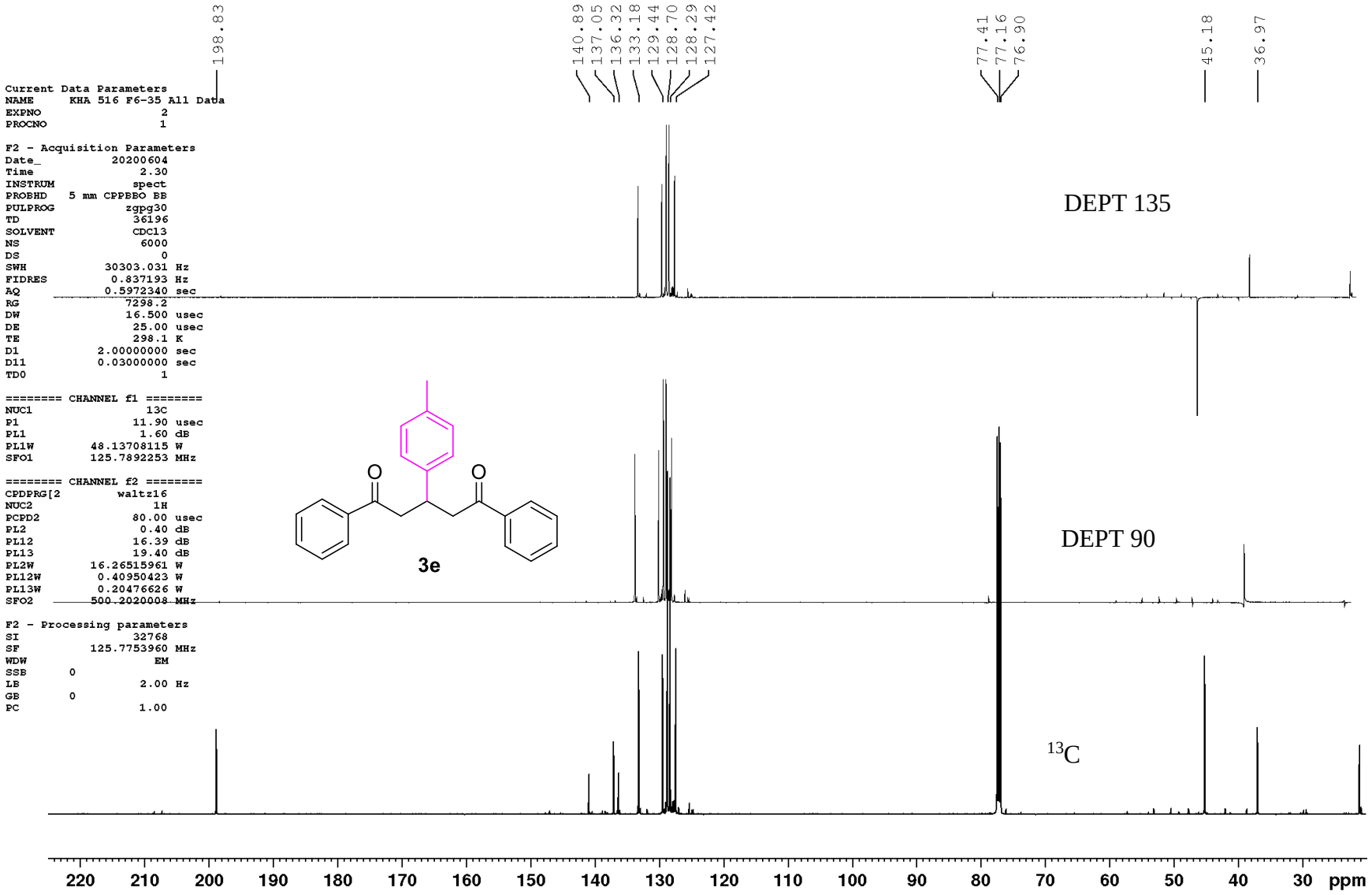


Figure S15. ^{13}C NMR spectrum of compound **3e** (125 MHz, $CDCl_3$, 25 ^oC)

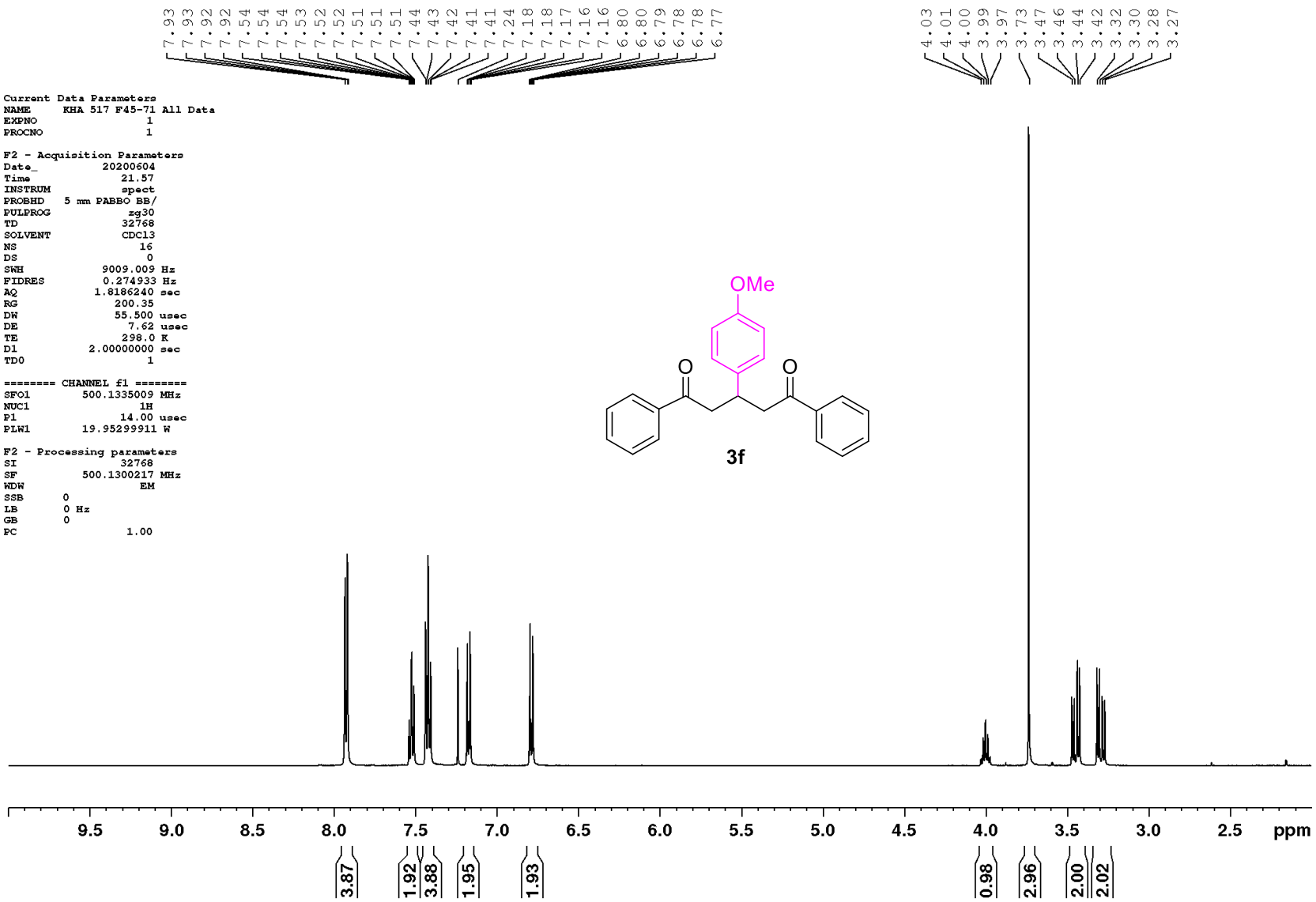


Figure S16. ^{1}H NMR spectrum of compound **3f** (500 MHz, $CDCl_3$, 25 ^{o}C)

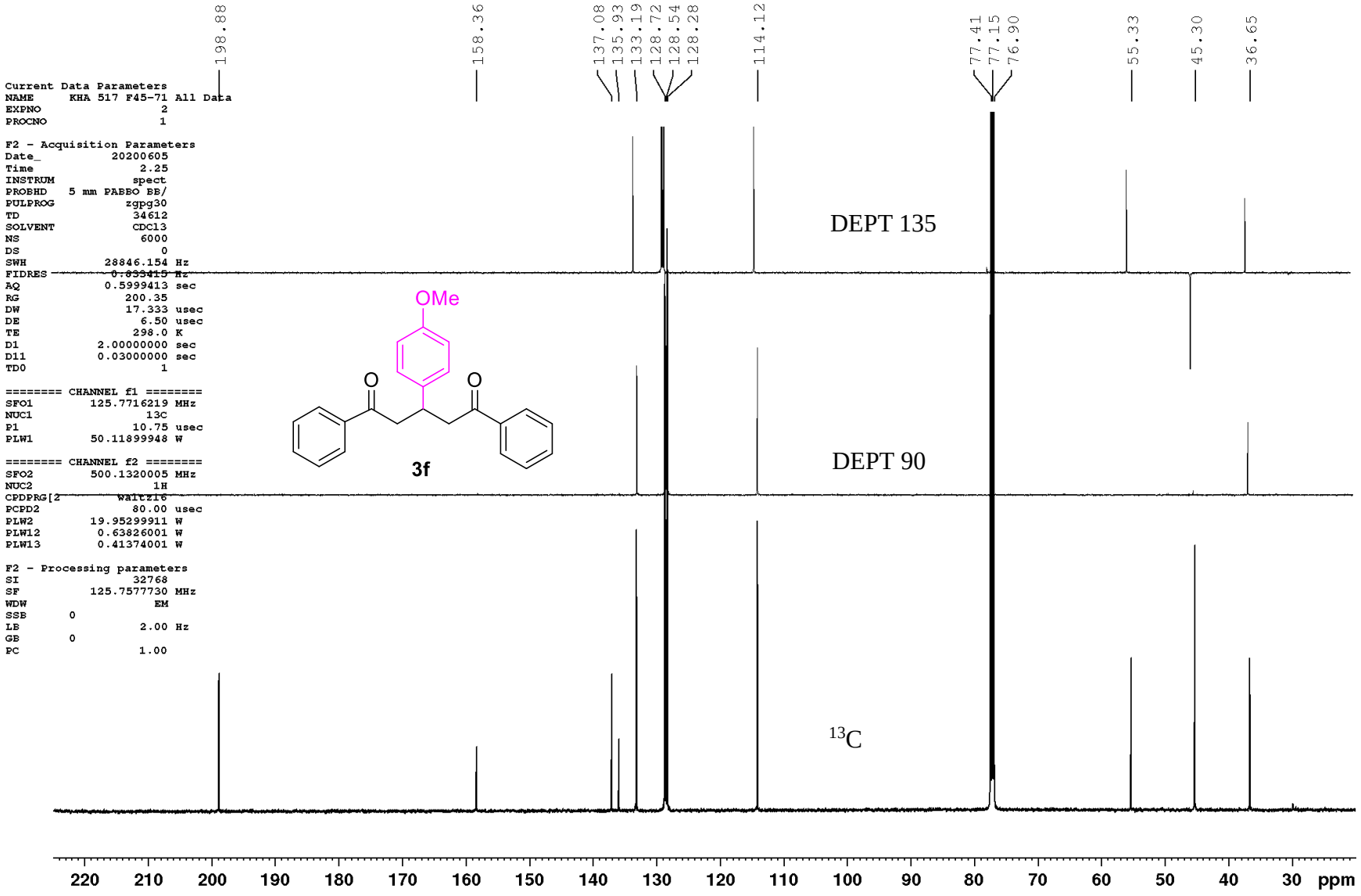


Figure S17. ^{13}C NMR spectrum of compound **3f** (125 MHz, $CDCl_3$, 25 ^oC)

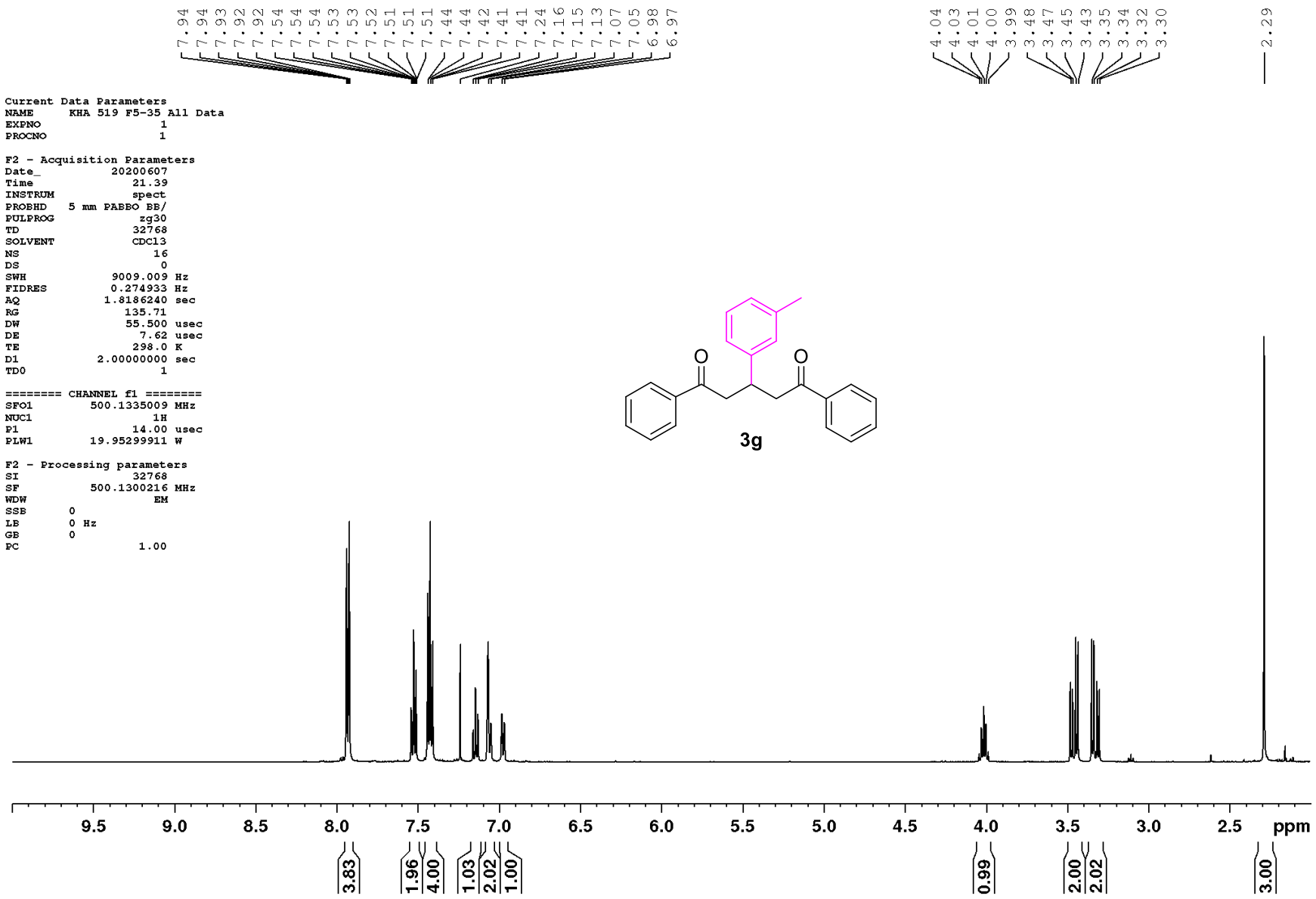


Figure S18. ^{1}H NMR spectrum of compound **3g** (500 MHz, $CDCl_3$, 25 ^{o}C)

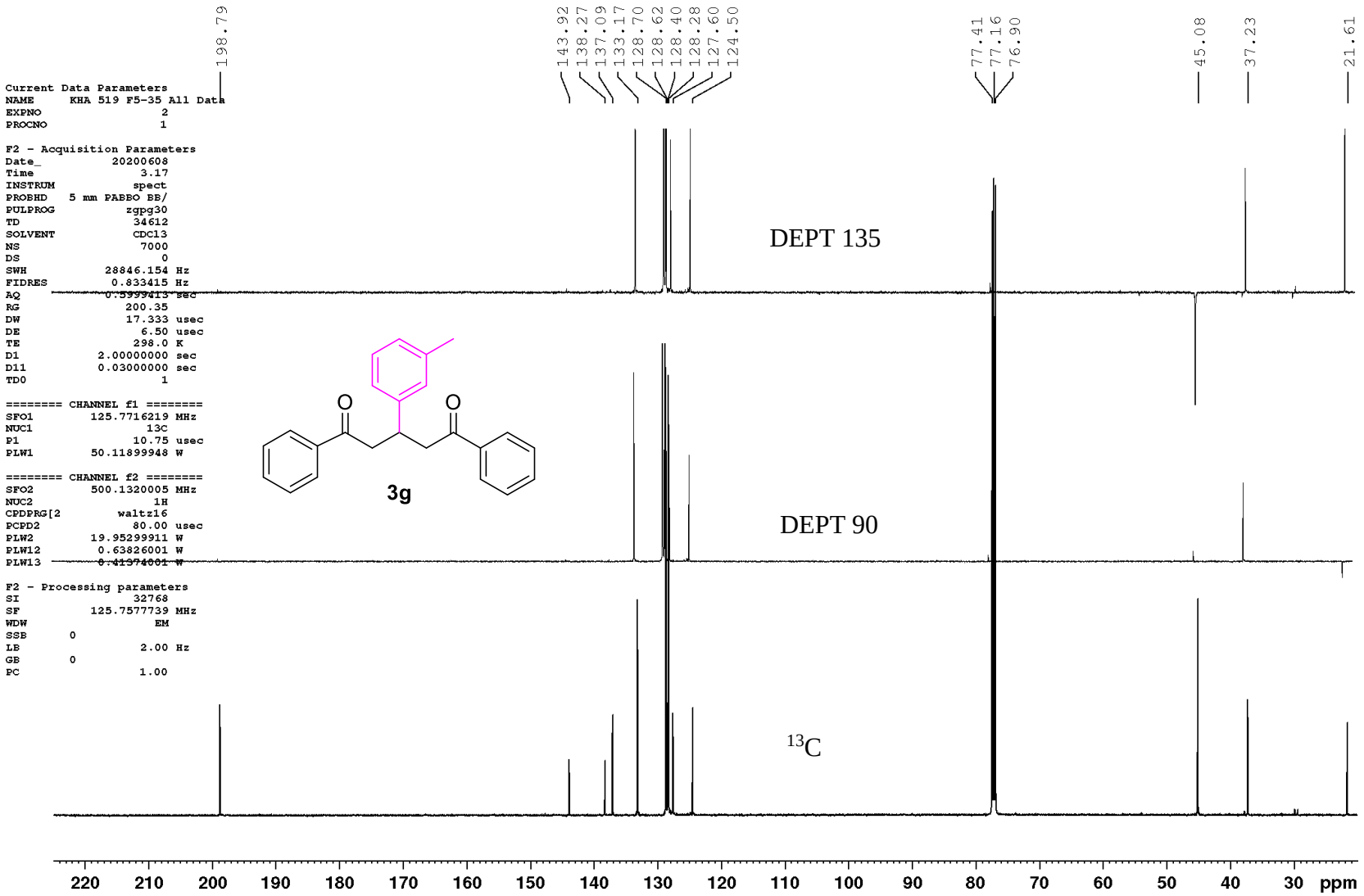


Figure S19. ^{13}C NMR spectrum of compound **3g** (125 MHz, $CDCl_3$, 25 ^oC)

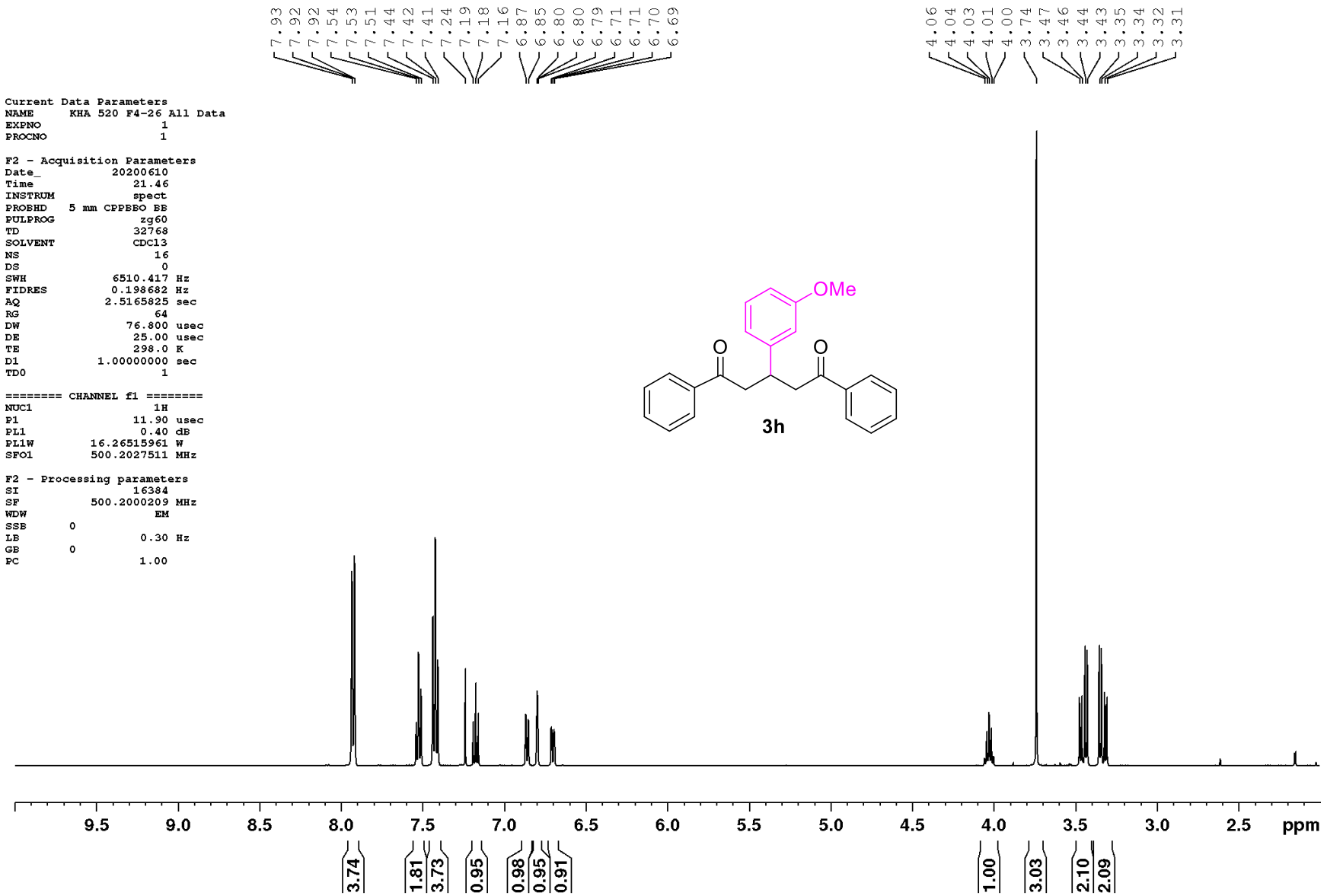


Figure S20. ^{1}H NMR spectrum of compound **3h** (500 MHz, $CDCl_3$, 25 ^{o}C)

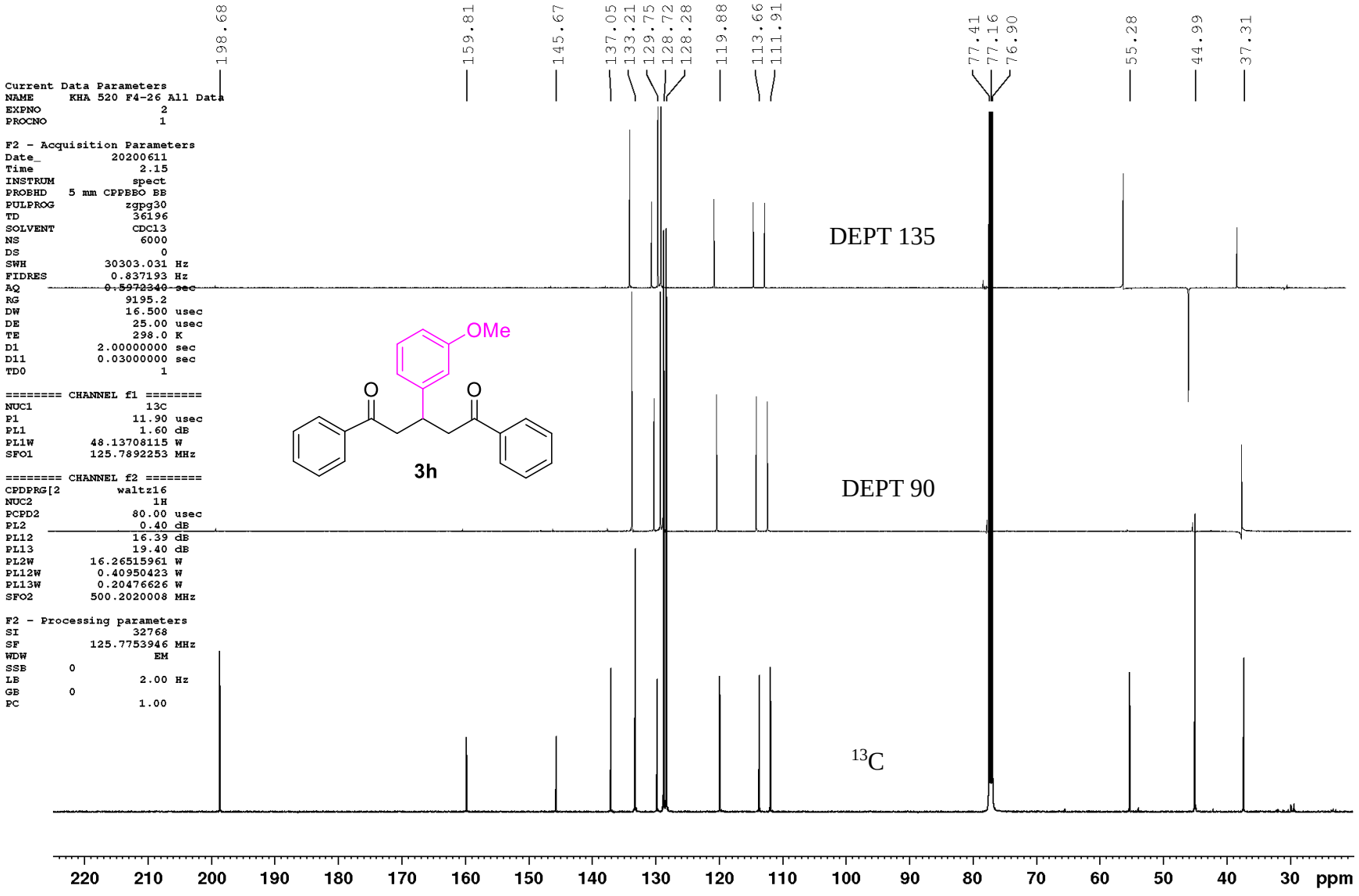


Figure S21. ^{13}C NMR spectrum of compound **3h** (125 MHz, $CDCl_3$, 25 °C)

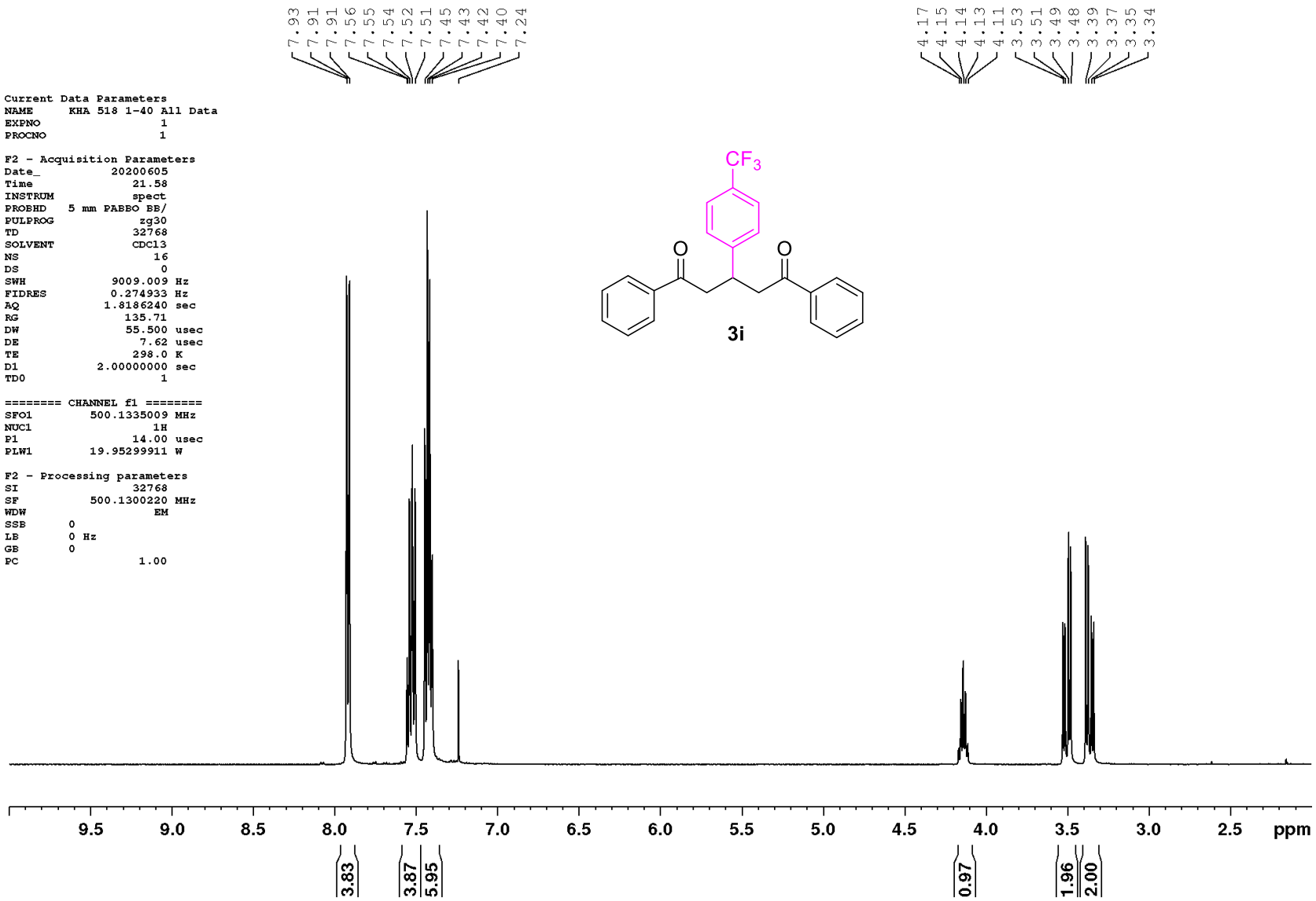


Figure S22. ^{1}H NMR spectrum of compound **3i** (500 MHz, $CDCl_3$, 25 ^{o}C)

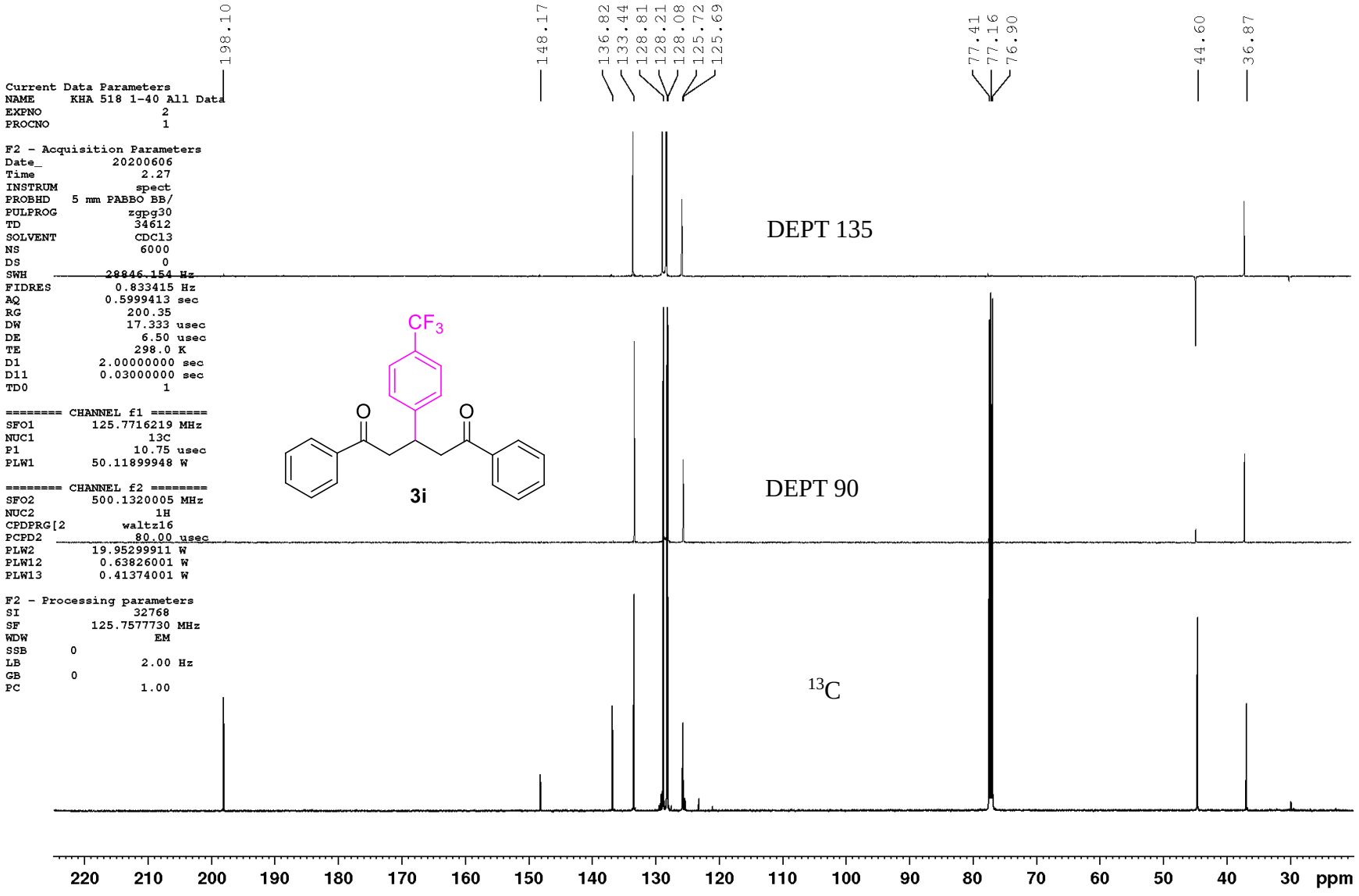


Figure S23. ^{13}C NMR spectrum of compound **3i** (125 MHz, $CDCl_3$, 25 °C)

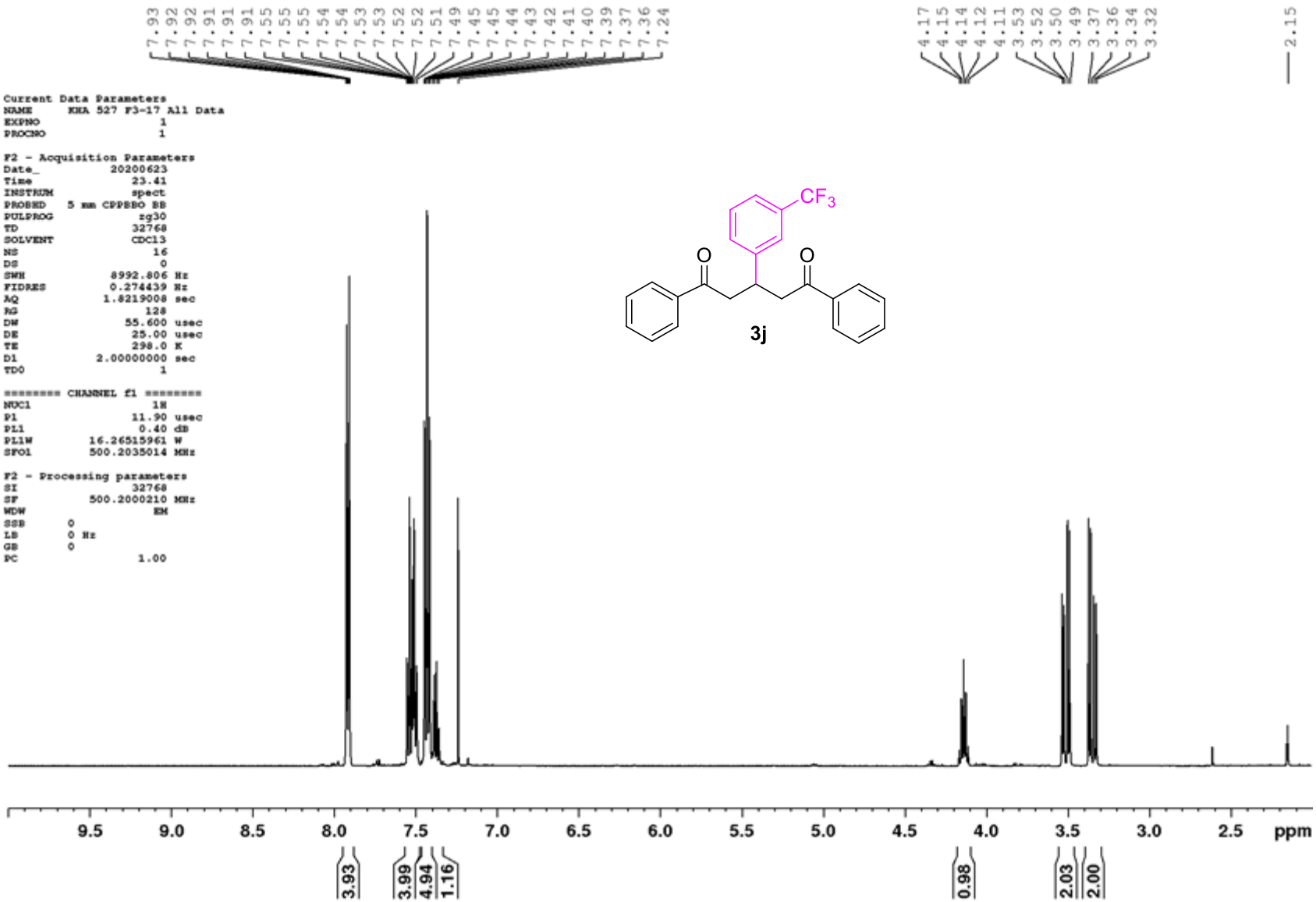


Figure S24. ^{1}H NMR spectrum of compound **3j** (500 MHz, $CDCl_3$, 25 ^{o}C)

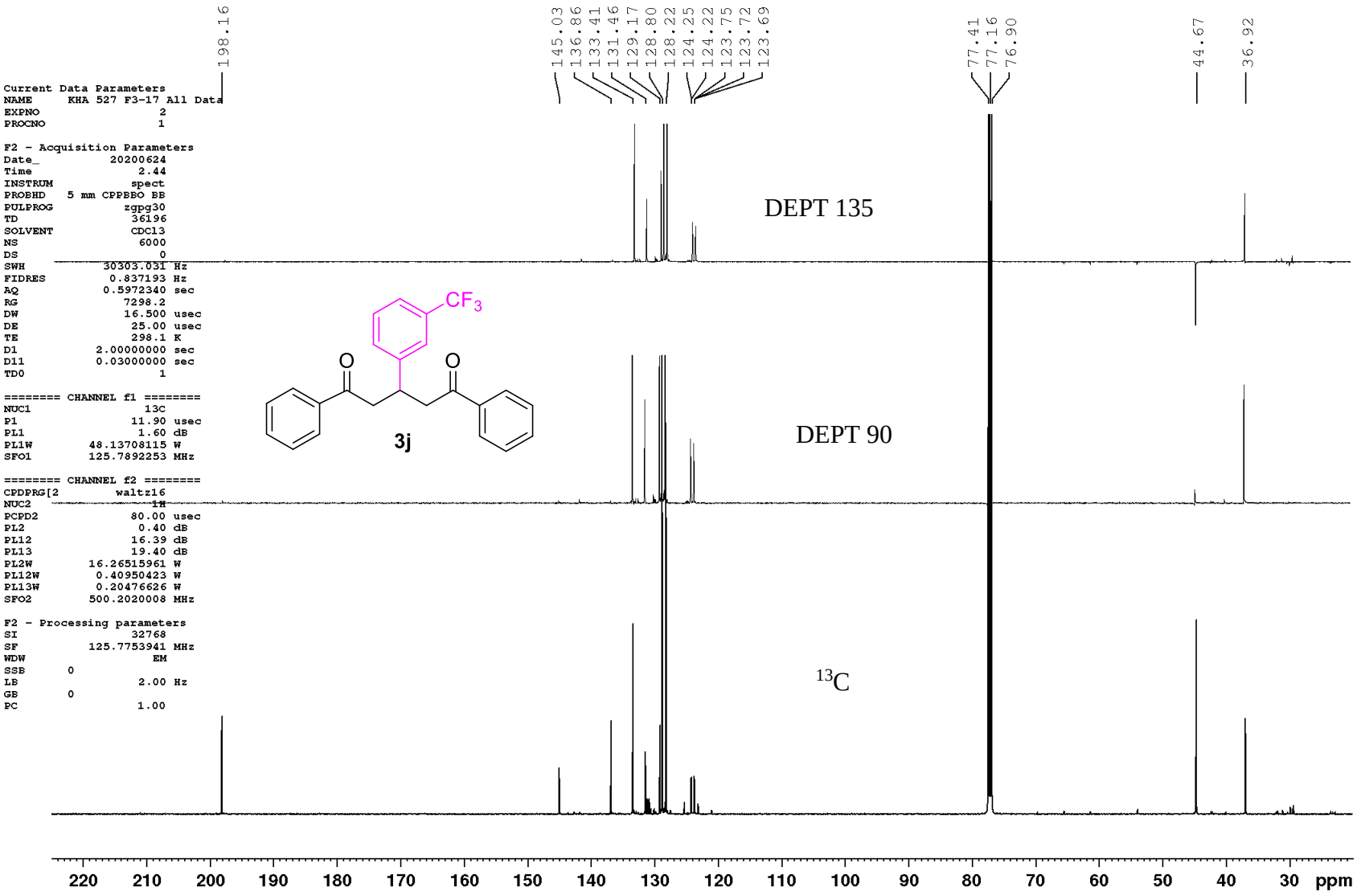


Figure S25. ^{13}C NMR spectrum of compound **3j** (125 MHz, $CDCl_3$, 25 ^oC)

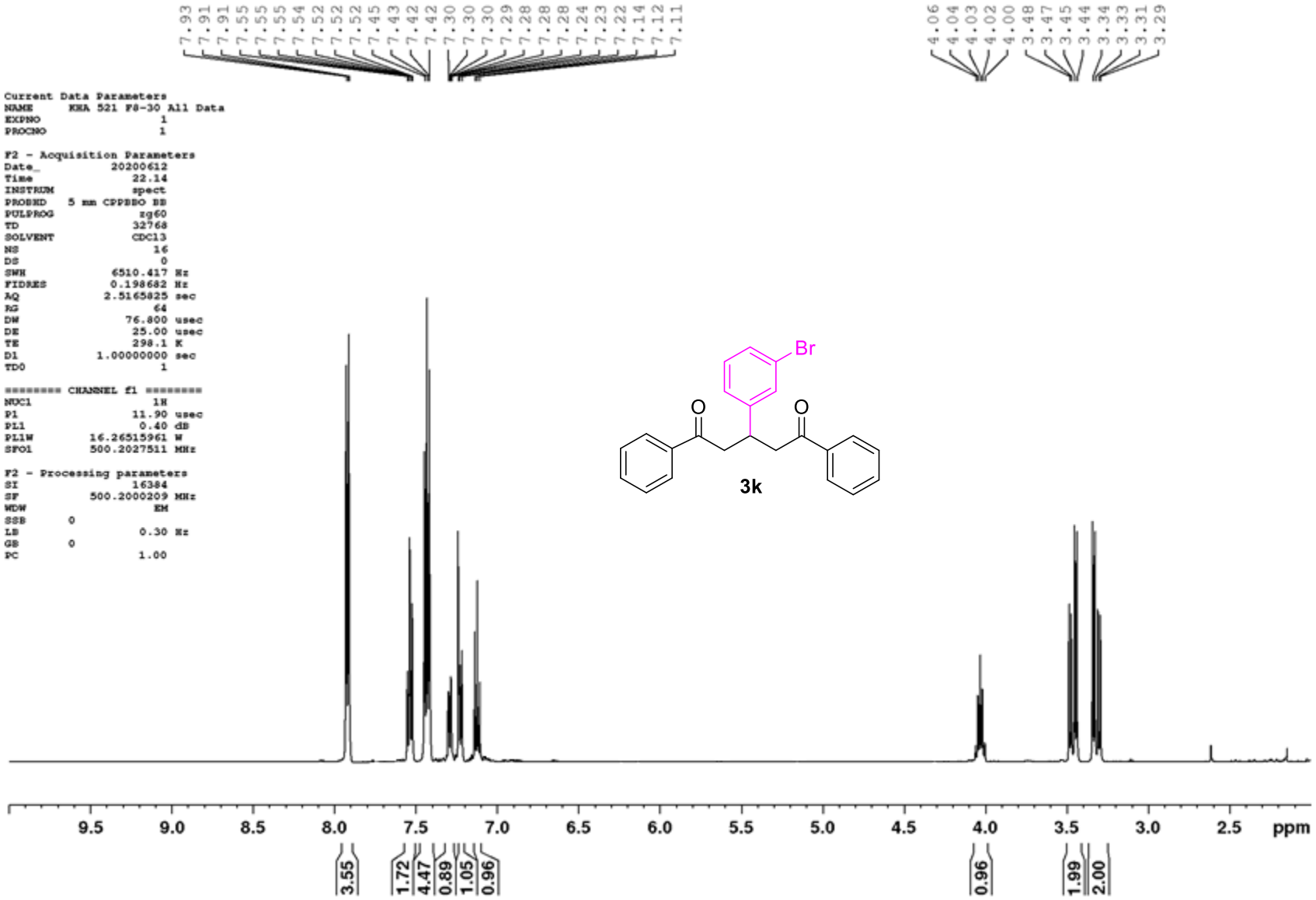


Figure S26. ^{1}H NMR spectrum of compound **3k** (500 MHz, $CDCl_3$, 25 ^{o}C)

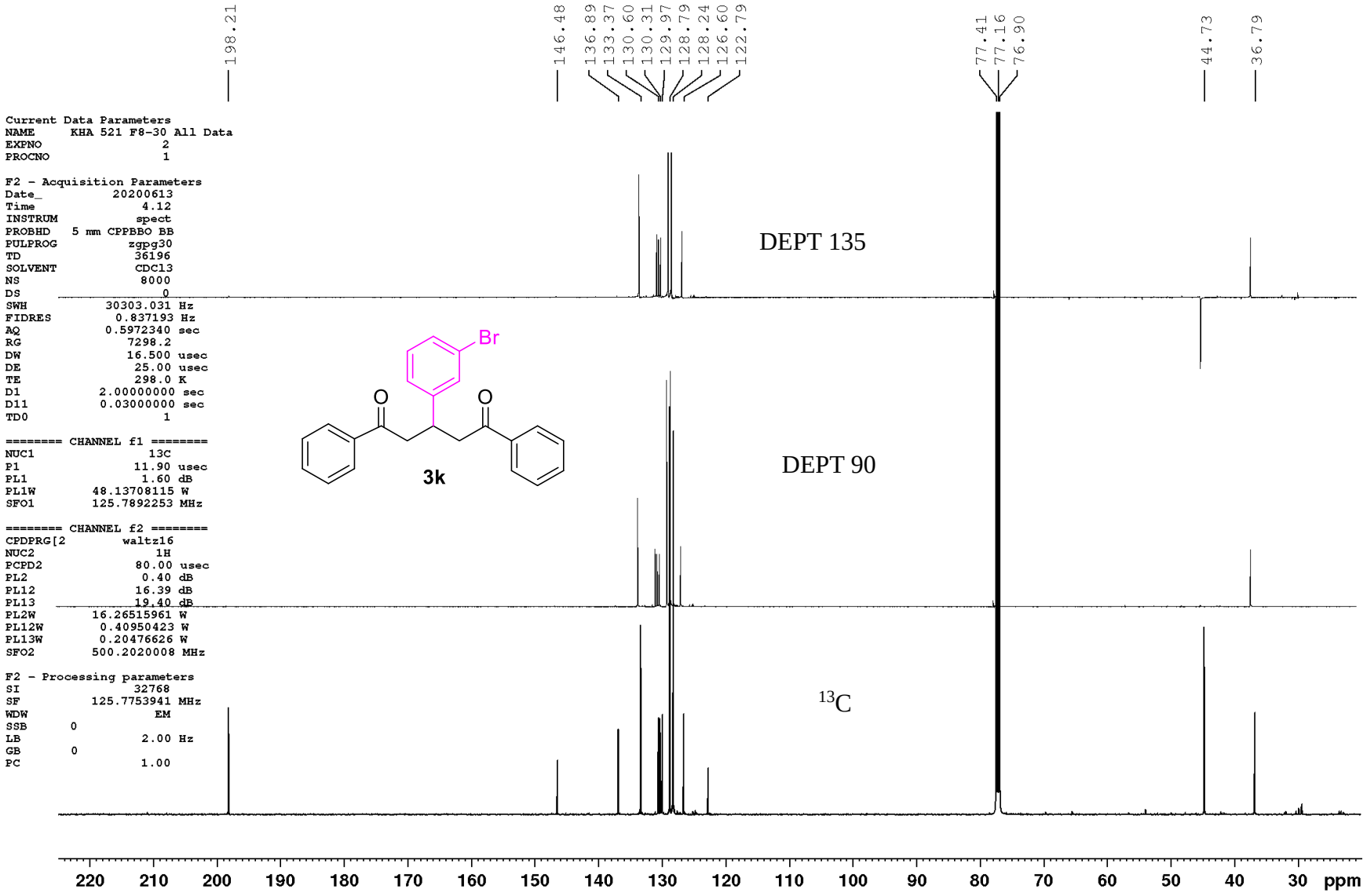


Figure S27. ^{13}C NMR spectrum of compound **3k** (125 MHz, $CDCl_3$, 25 °C)

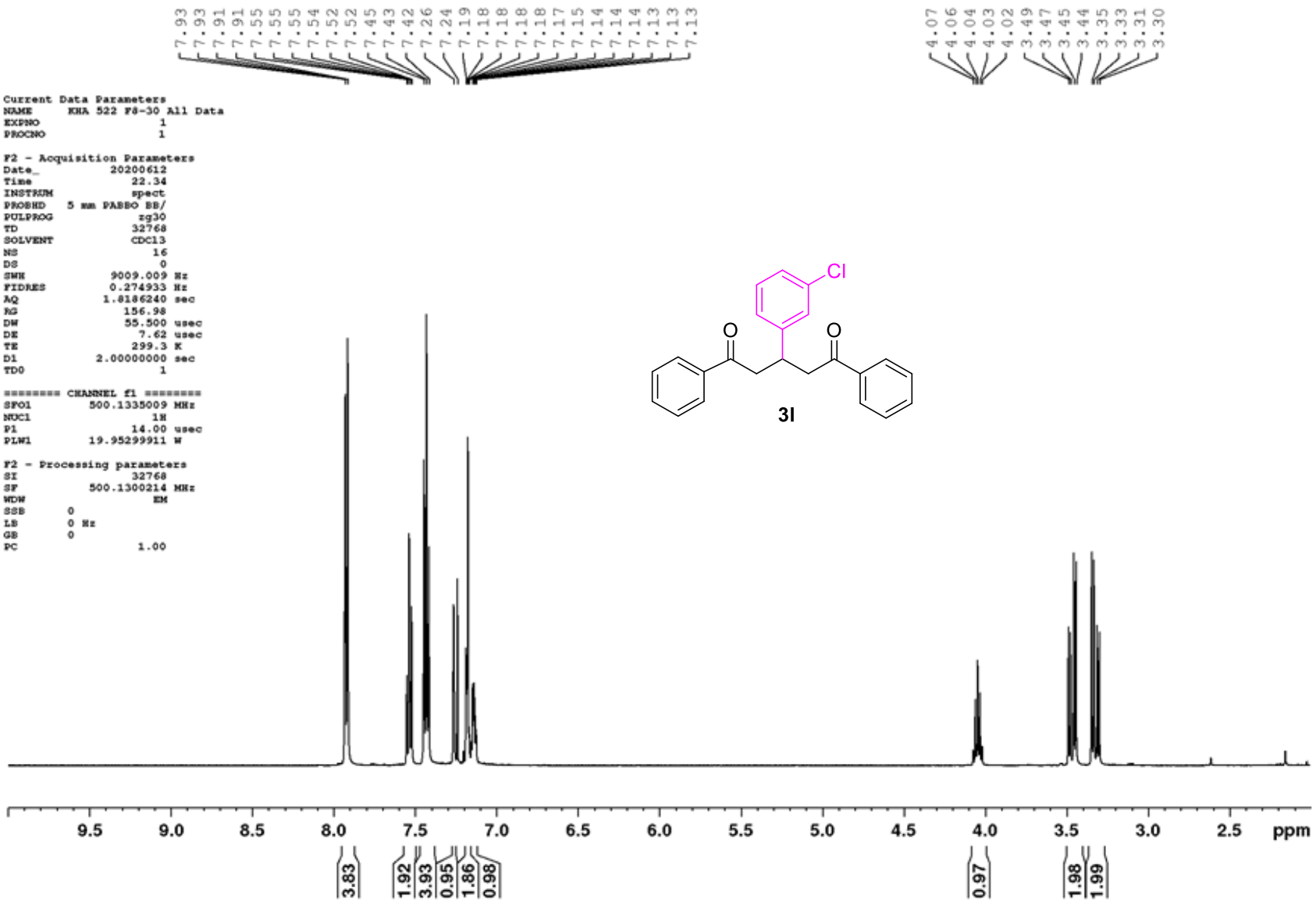


Figure S28. ^{1}H NMR spectrum of compound **3l** (500 MHz, $CDCl_3$, 25 ^{o}C)

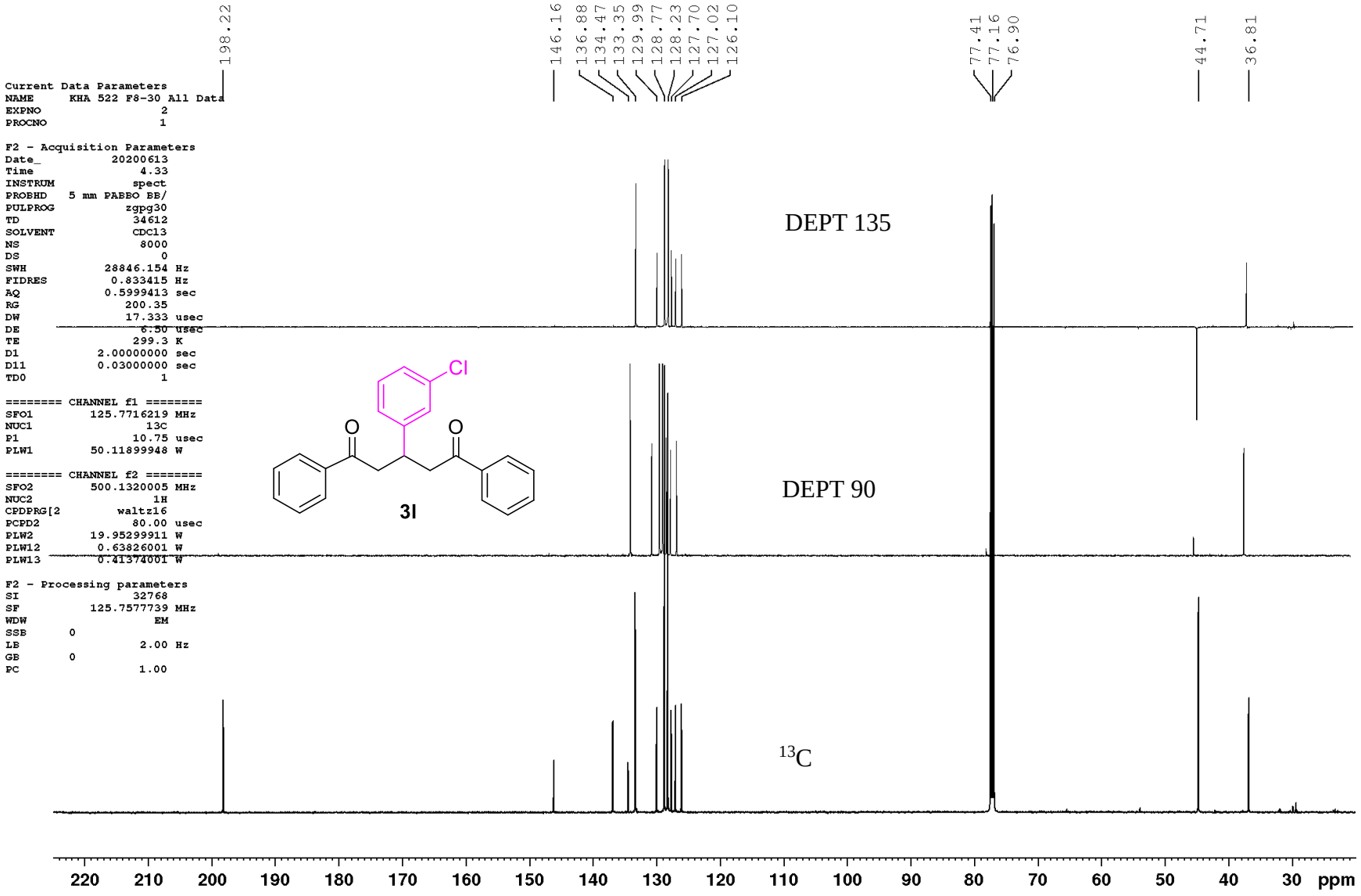


Figure S29. ^{13}C NMR spectrum of compound **3l** (125 MHz, $CDCl_3$, 25 °C)

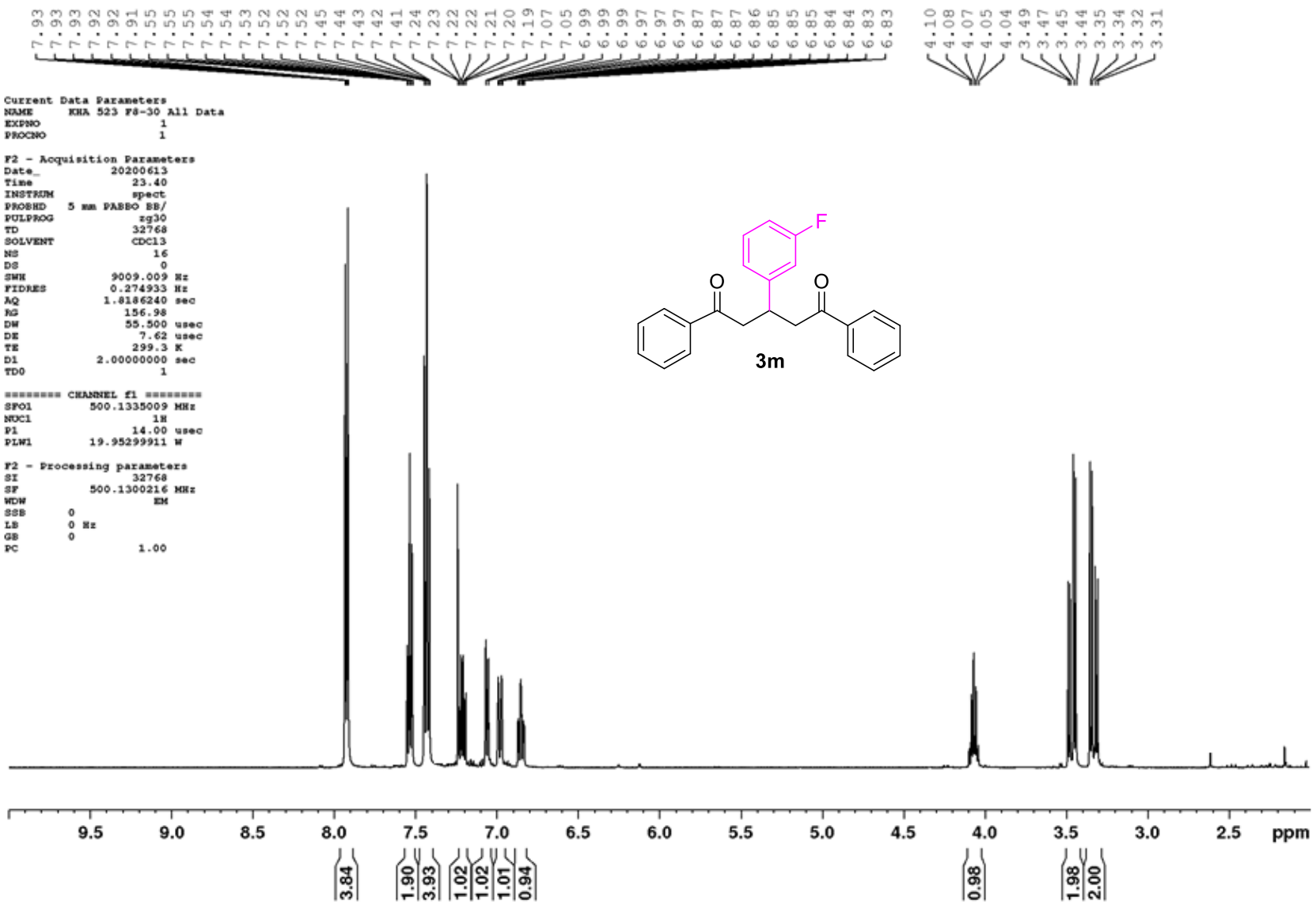


Figure S30. ^{1}H NMR spectrum of compound **3m** (500 MHz, $CDCl_3$, 25 ^{o}C)

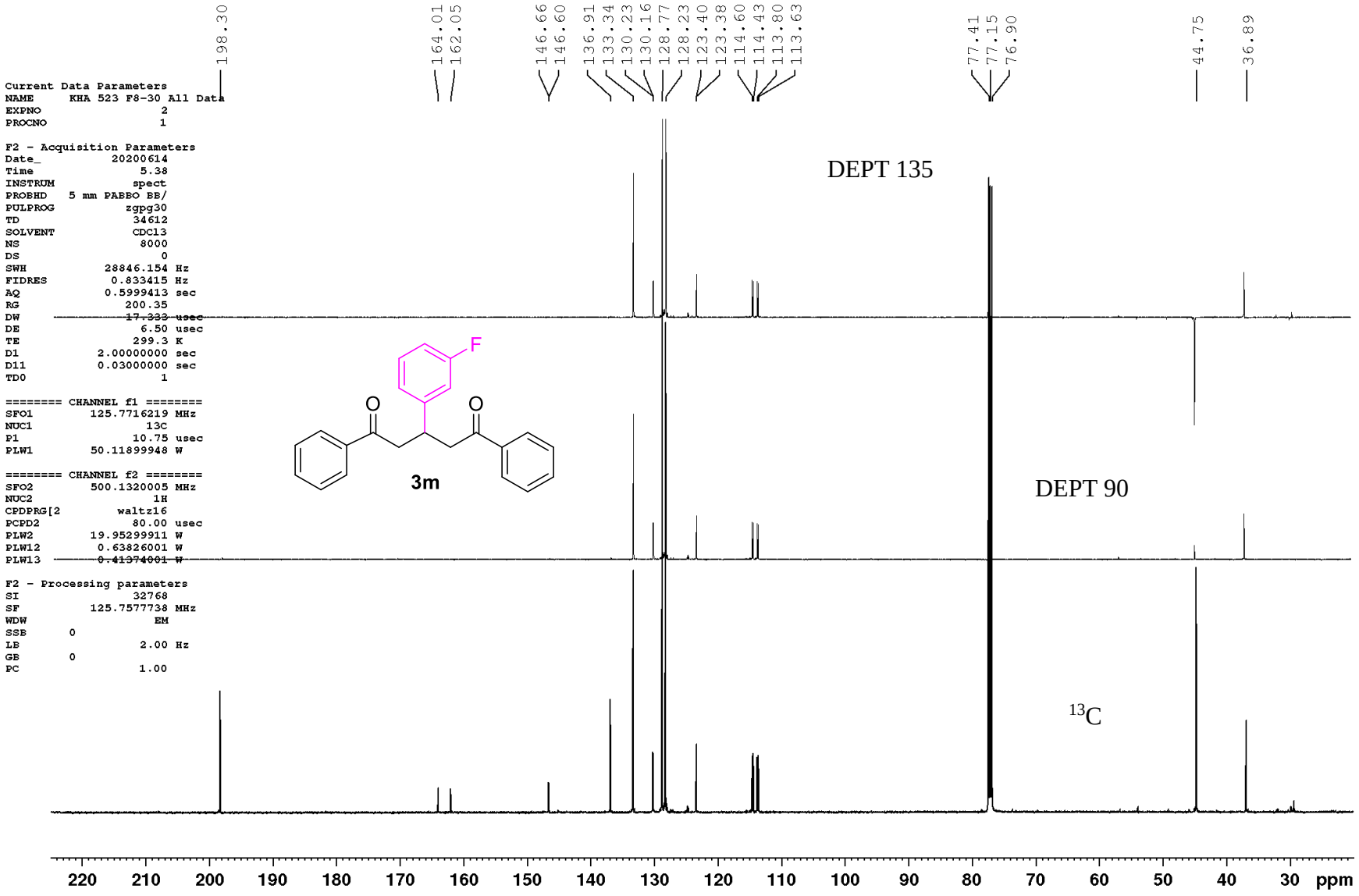


Figure S31. ^{13}C NMR spectrum of compound **3m** (125 MHz, $CDCl_3$, 25 ^oC)

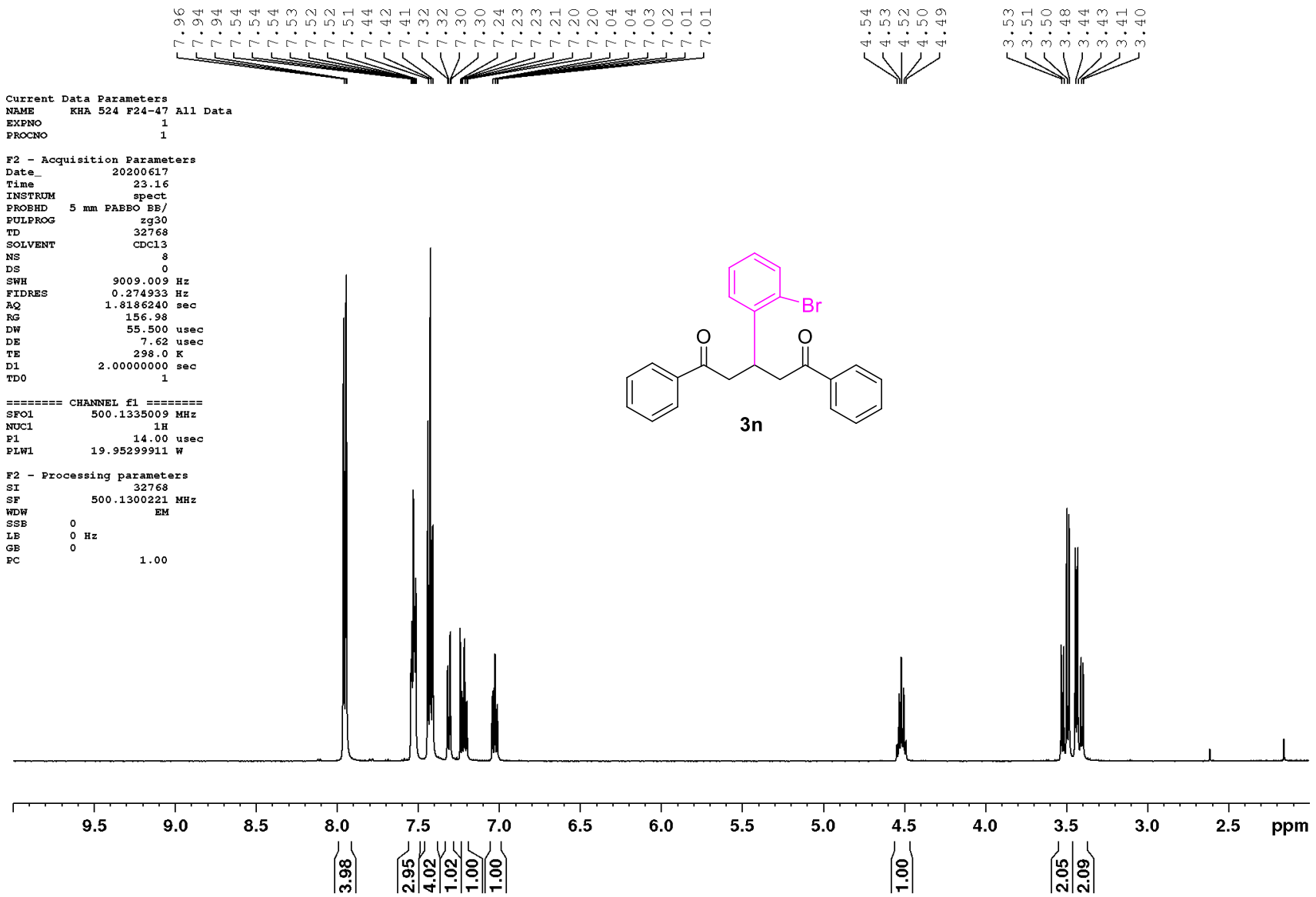


Figure S32. ^{1}H NMR spectrum of compound **3n** (500 MHz, $CDCl_3$, 25 ^{o}C)

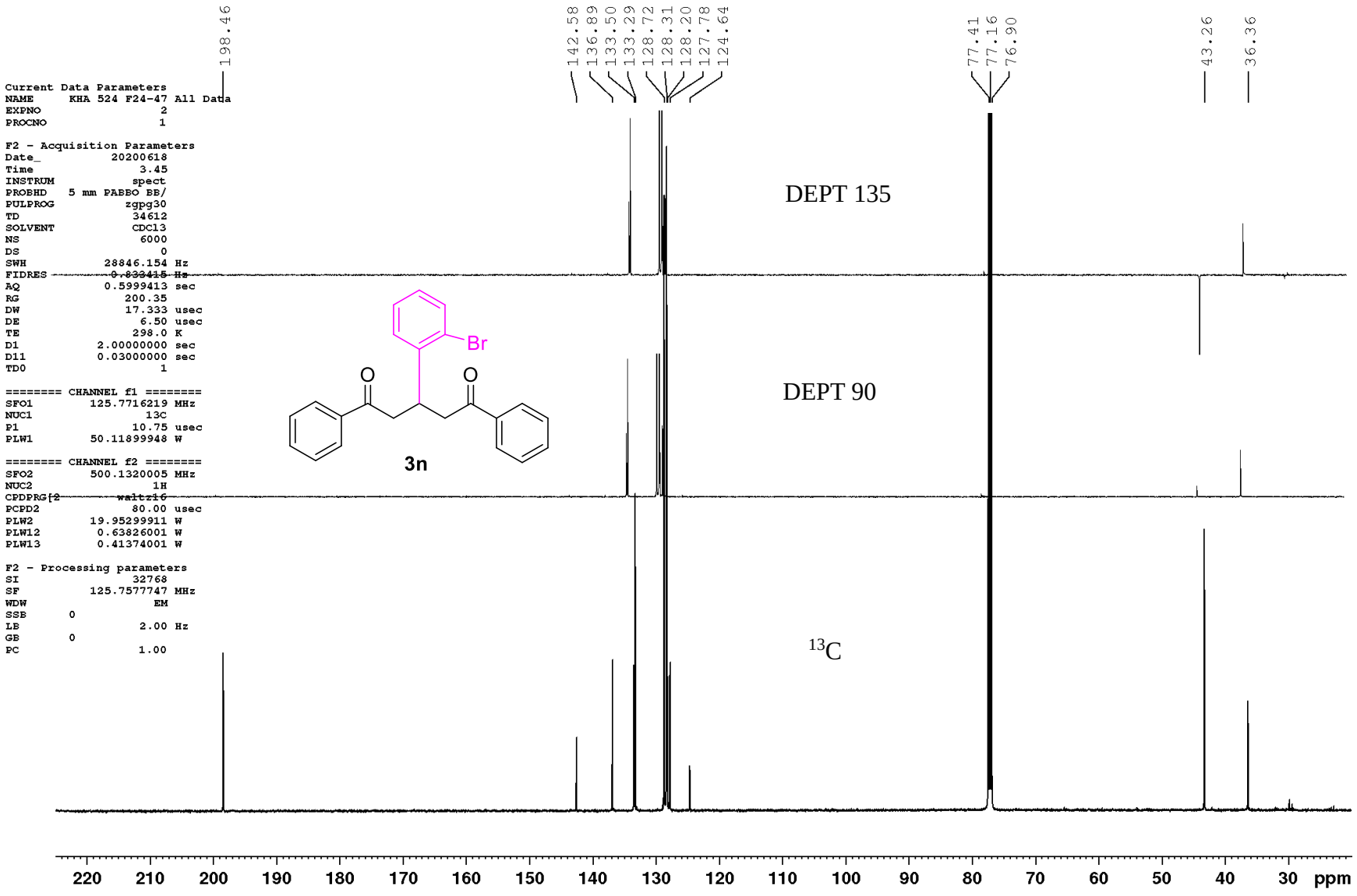


Figure S33. ^{13}C NMR spectrum of compound **3n** (125 MHz, $CDCl_3$, 25 ^oC)

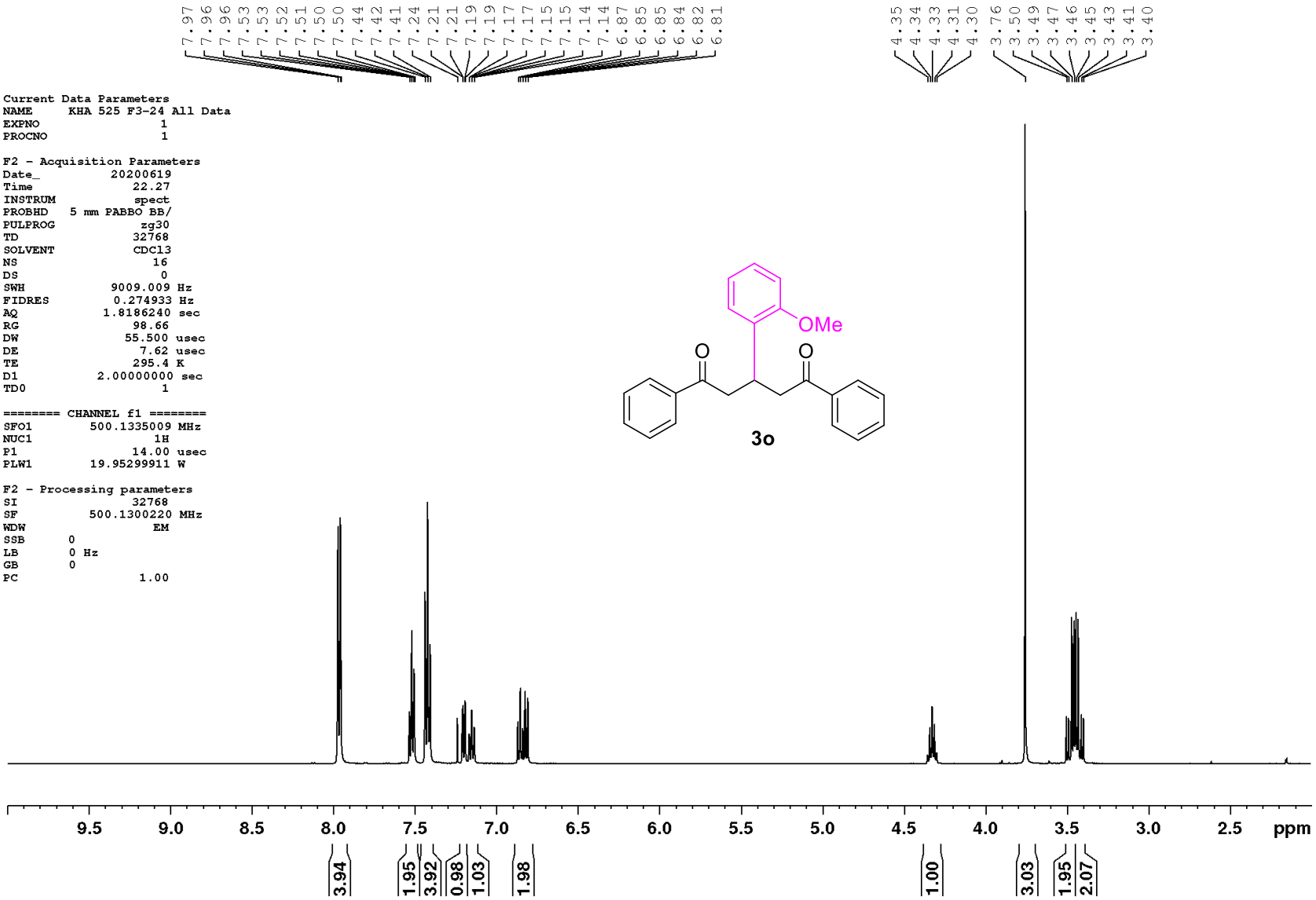


Figure S34. ^{1}H NMR spectrum of compound **3o** (500 MHz, $CDCl_3$, 25 ^{o}C)

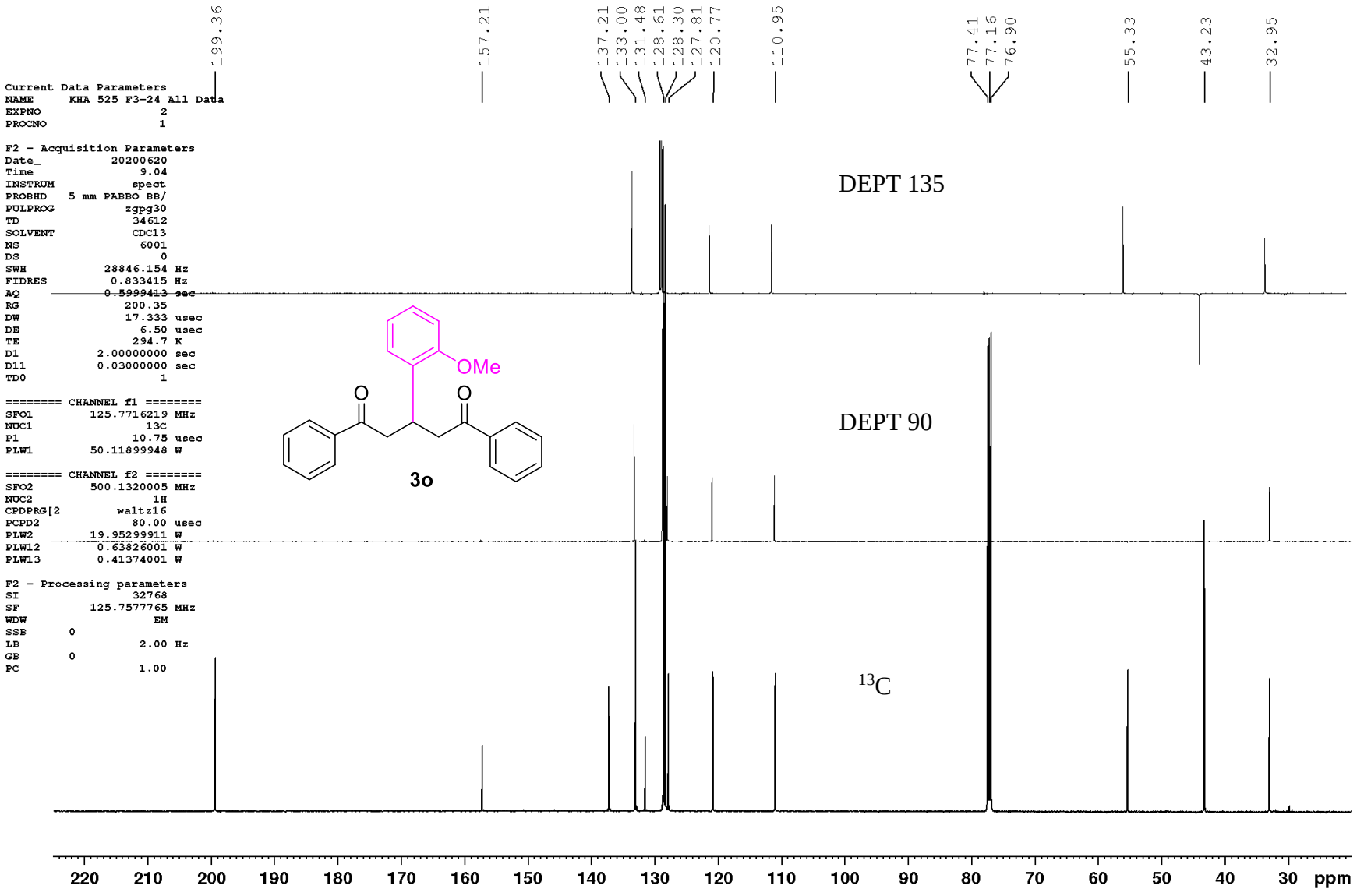


Figure S35. ^{13}C NMR spectrum of compound **3o** (125 MHz, $CDCl_3$, 25 ºC)

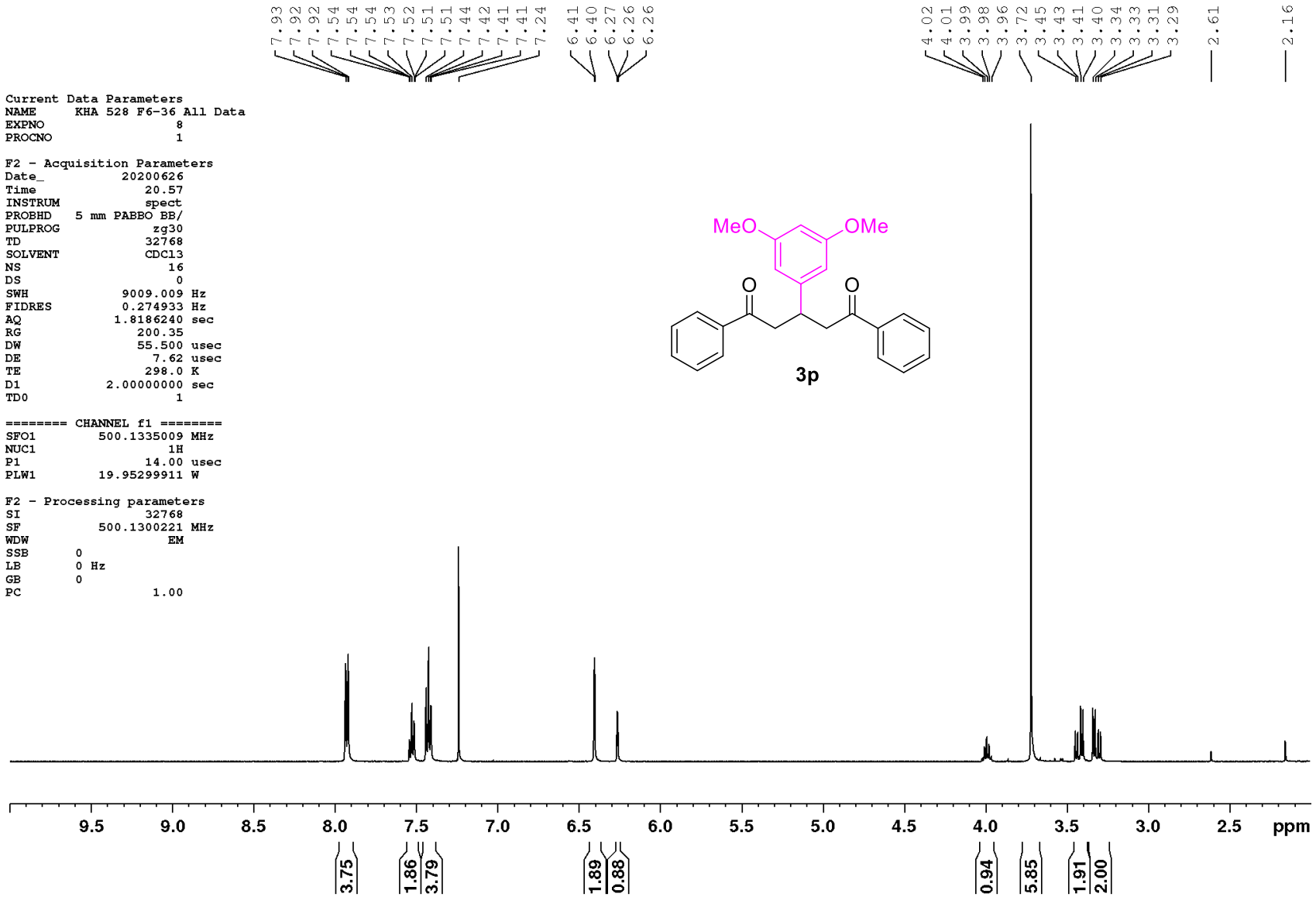


Figure S36. ^{1}H NMR spectrum of compound **3p** (500 MHz, $CDCl_3$, 25 ^{o}C)

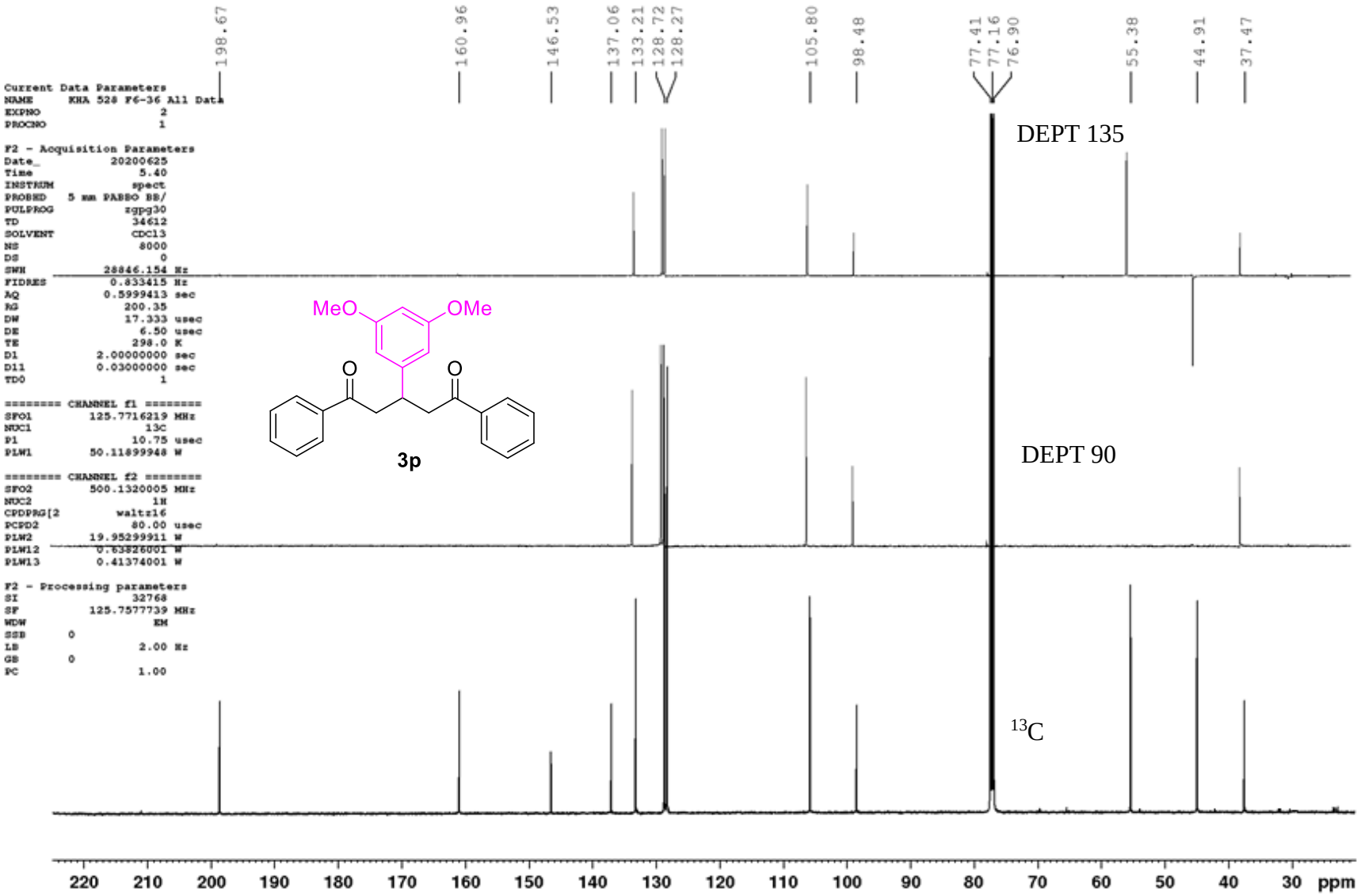


Figure S37. ^{13}C NMR spectrum of compound **3p** (125 MHz, $CDCl_3$, 25 °C)

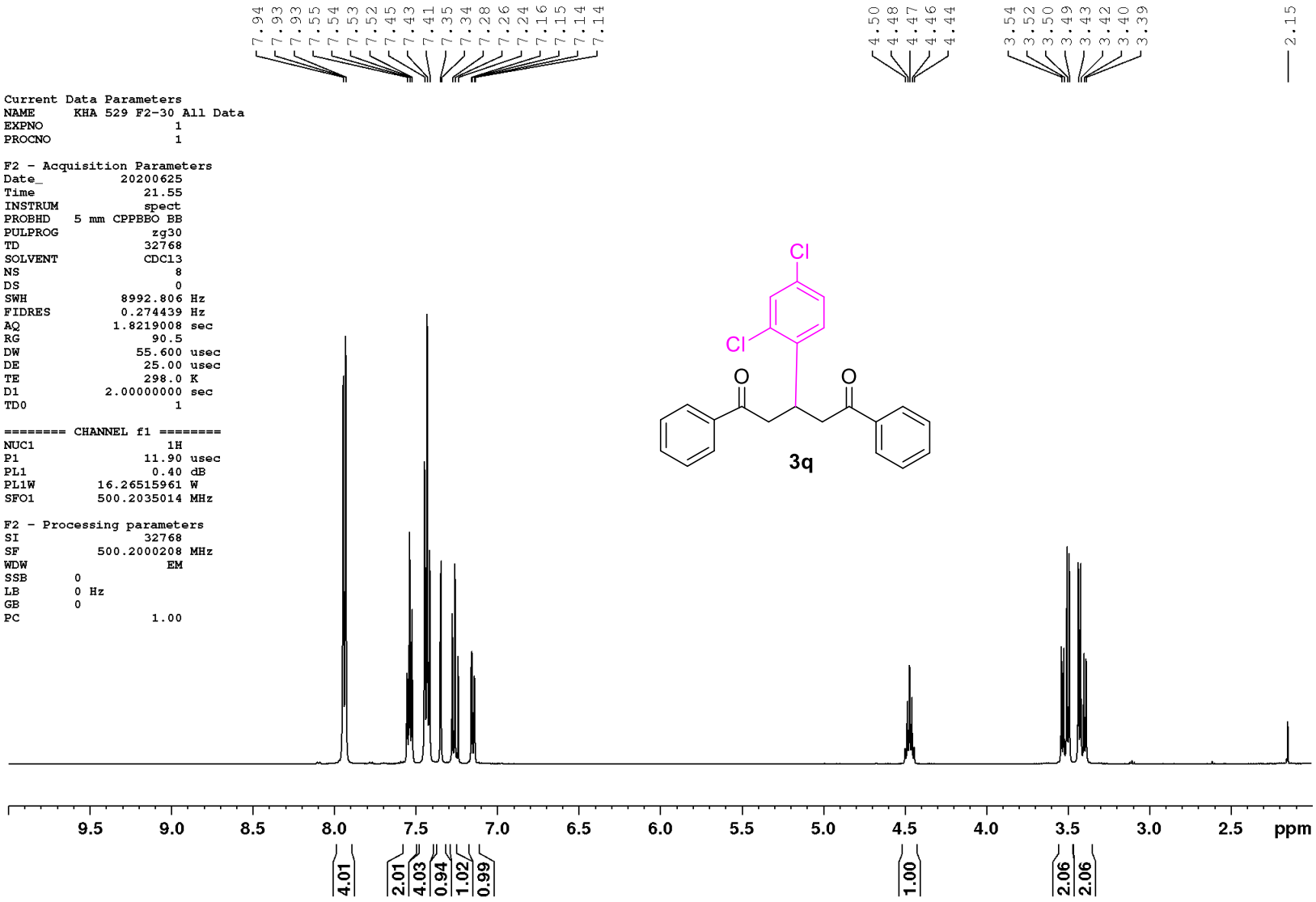


Figure S38. ^{1}H NMR spectrum of compound **3q** (500 MHz, $CDCl_3$, 25 ^{o}C)

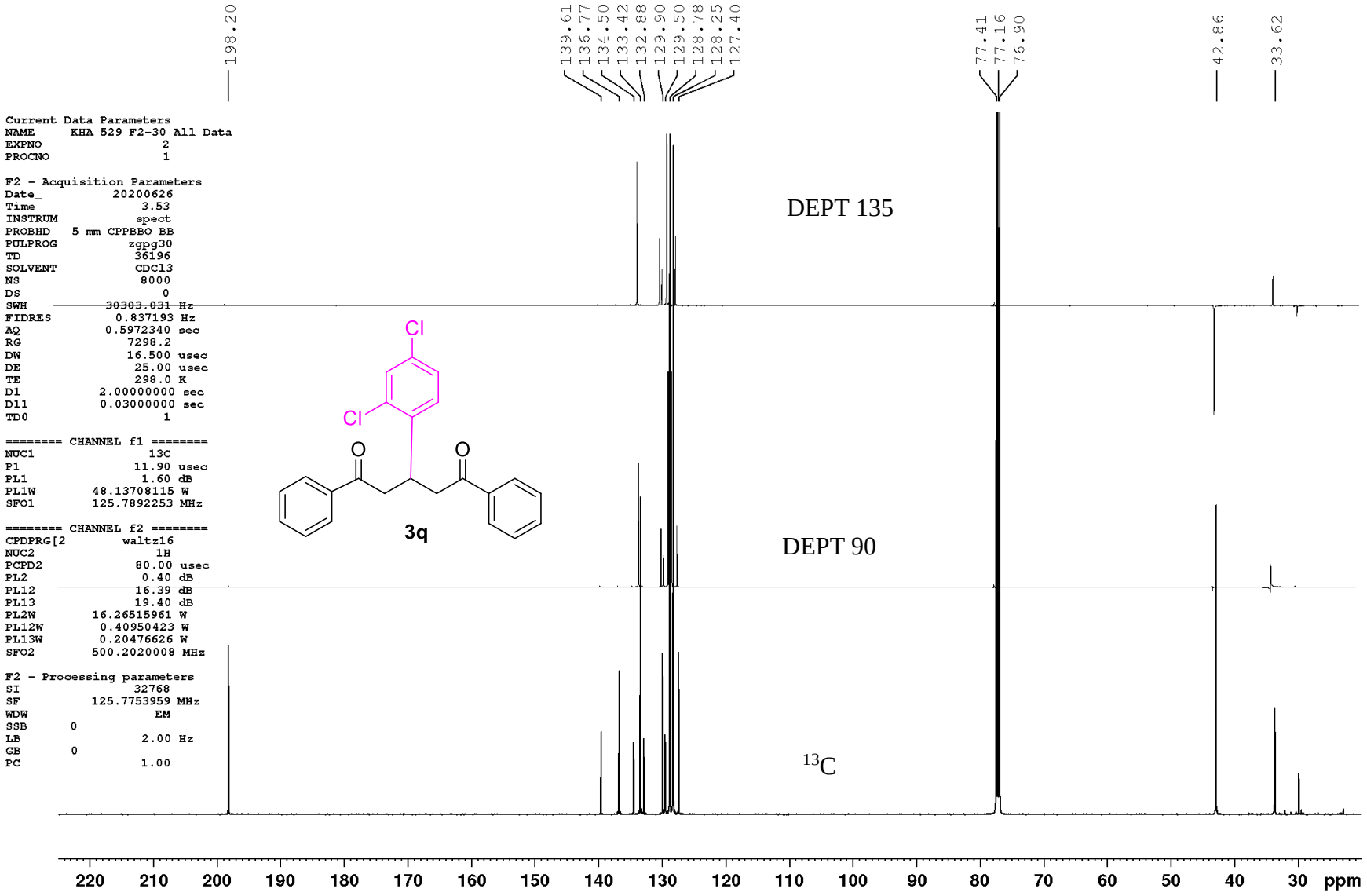


Figure S39. ^{13}C NMR spectrum of compound **3q** (125 MHz, $CDCl_3$, 25 °C)

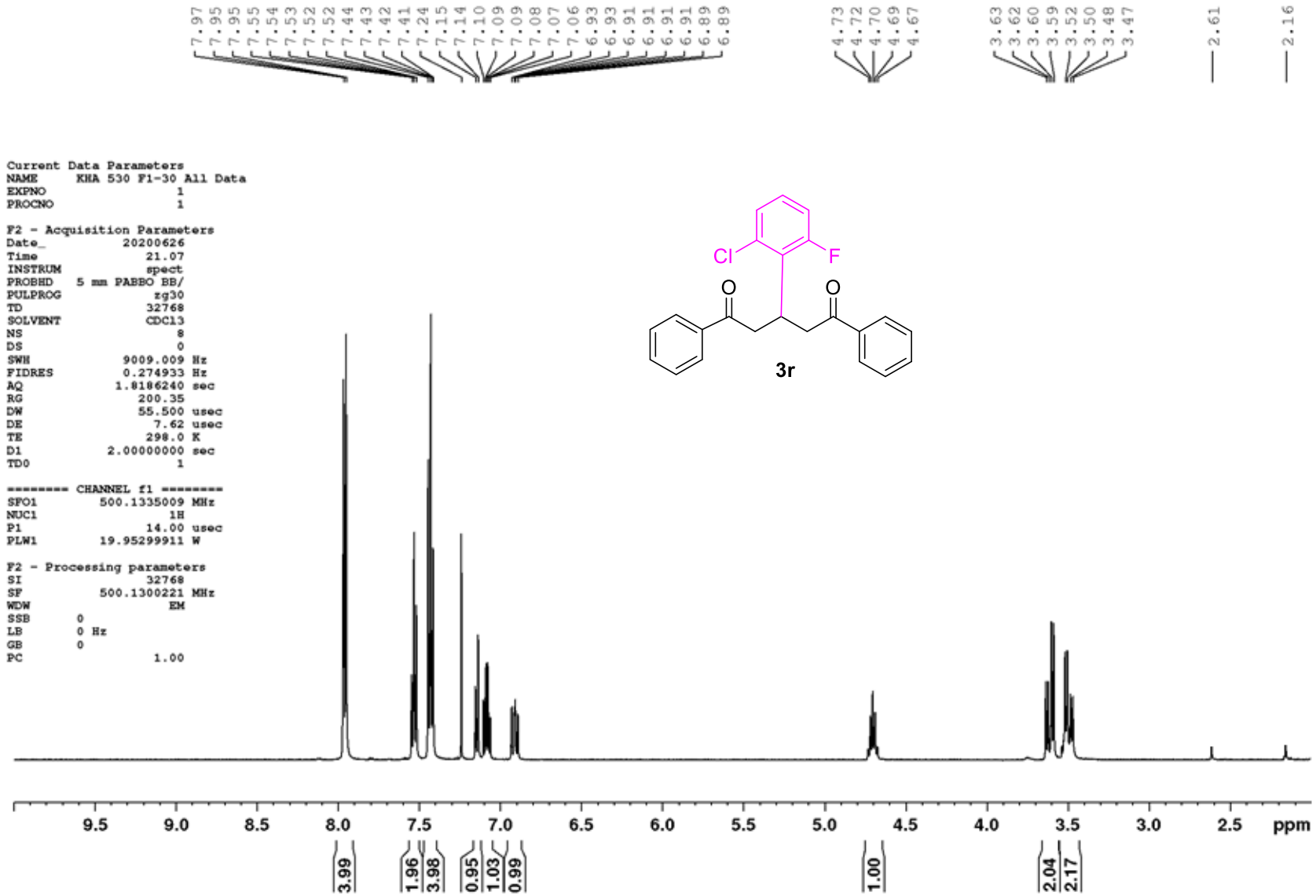
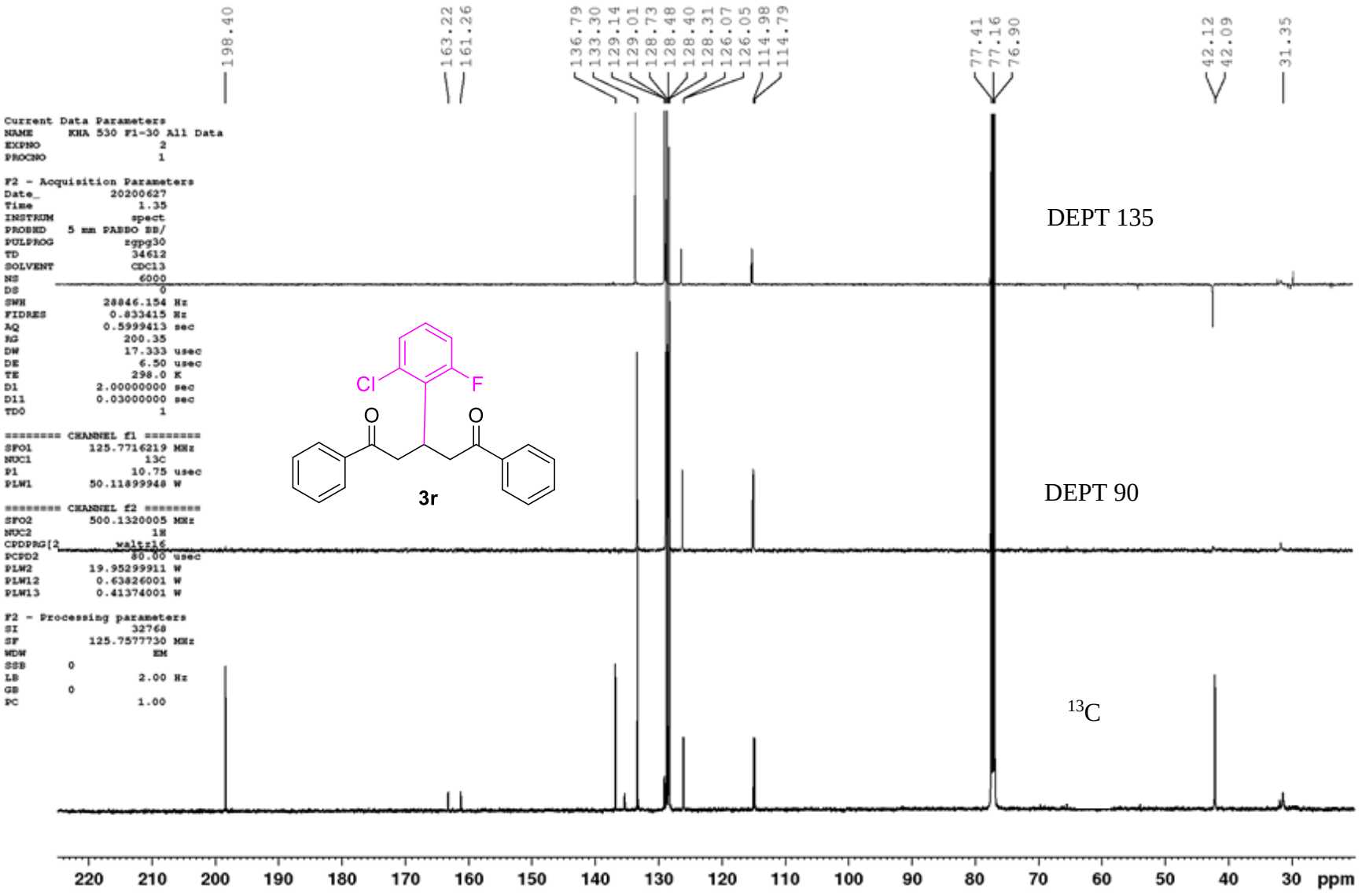


Figure S40. ^{1}H NMR spectrum of compound **3r** (500 MHz, $CDCl_3$, 25 ^{o}C)

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TD                34612
SOLVENT           CDCl3
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SWH           28846.154 Hz
FIDRES        0.833415 Hz
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RG               200.35
DW               17.333 usec
DE                6.50 usec
TE               298.0 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
SSB       0
LB                2.00 Hz
GB        0
PC                1.00
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Figure S41. ^{13}C NMR spectrum of compound **3r** (125 MHz, $CDCl_3$, 25 ºC)

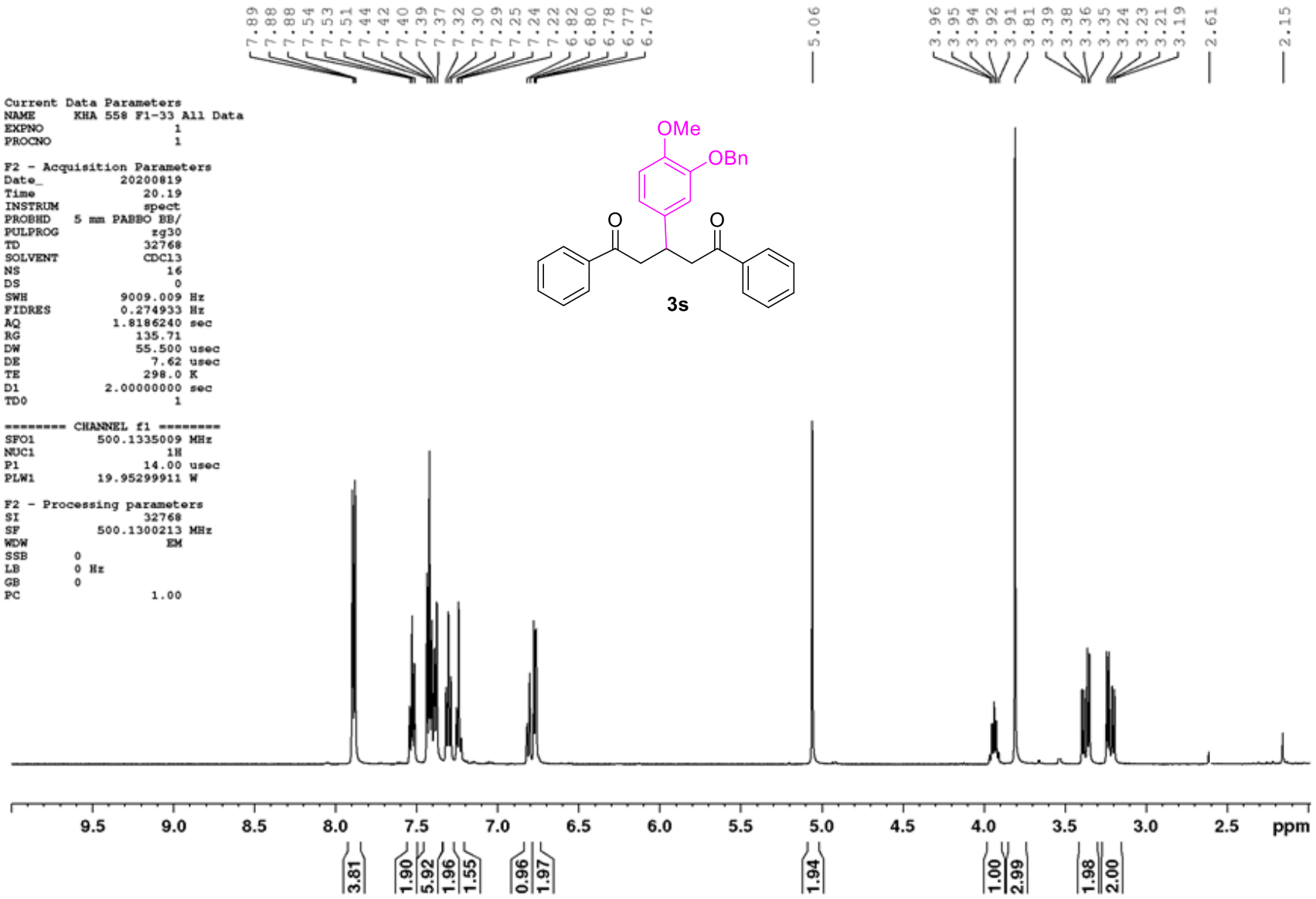


Figure S42. ^{1}H NMR spectrum of compound **3s** (500 MHz, $CDCl_3$, 25 ^{o}C)

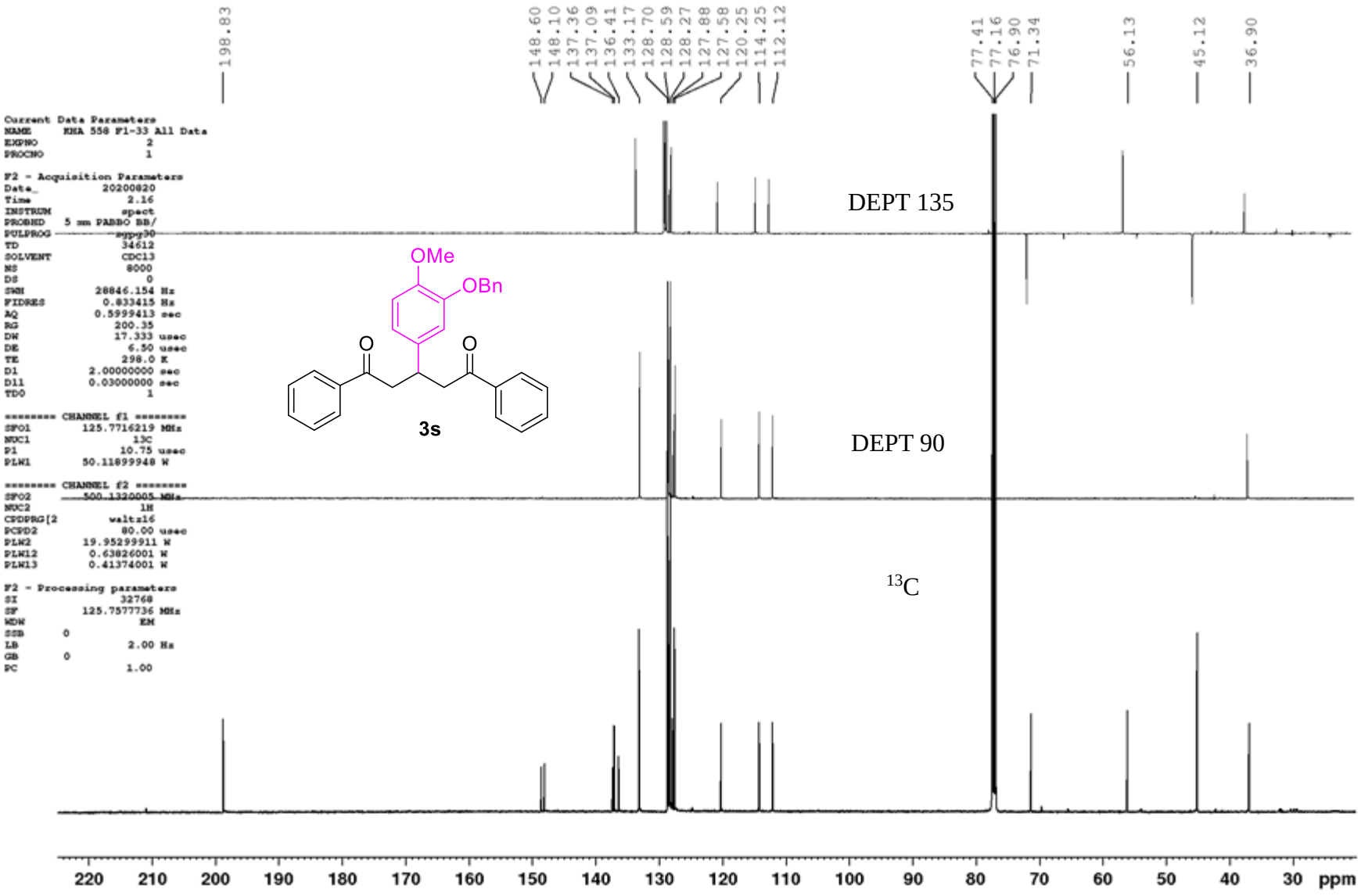


Figure S43. ^{13}C NMR spectrum of compound **3s** (125 MHz, $CDCl_3$, 25 °C)

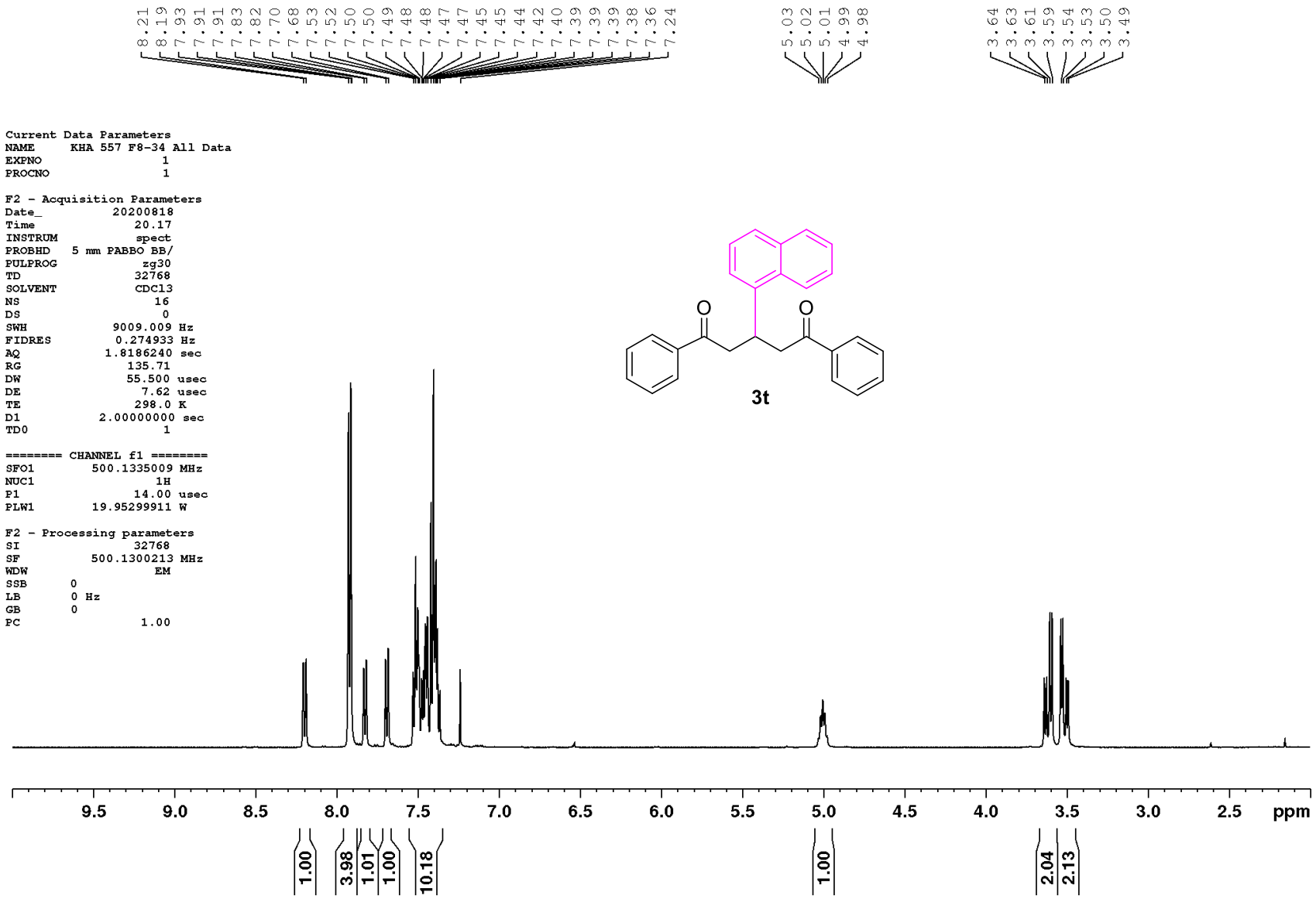


Figure S44. ^{1}H NMR spectrum of compound **3t** (500 MHz, $CDCl_3$, 25 ^{o}C)

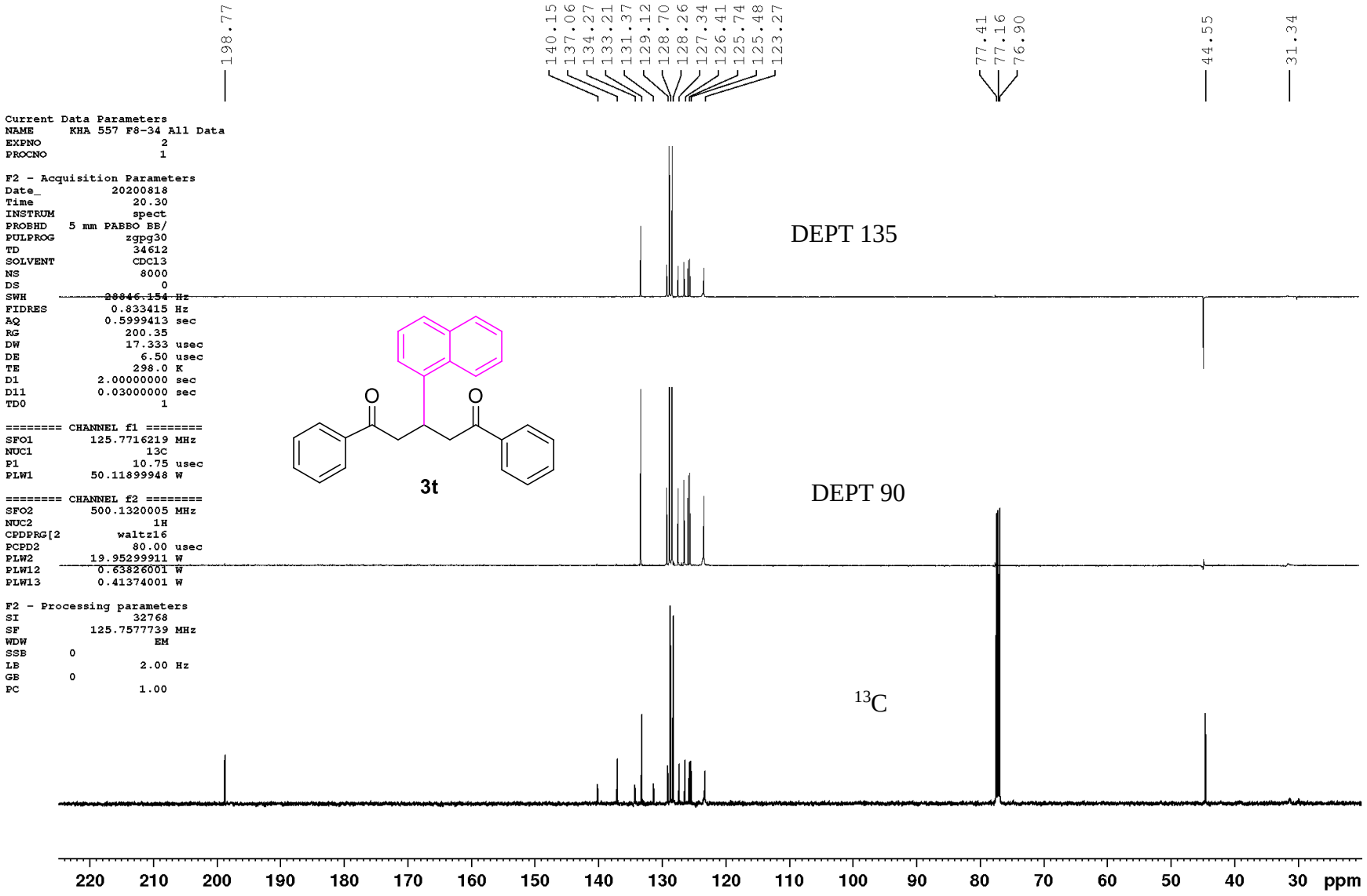


Figure S45. ^{13}C NMR spectrum of compound **3t** (125 MHz, $CDCl_3$, 25 ^oC)

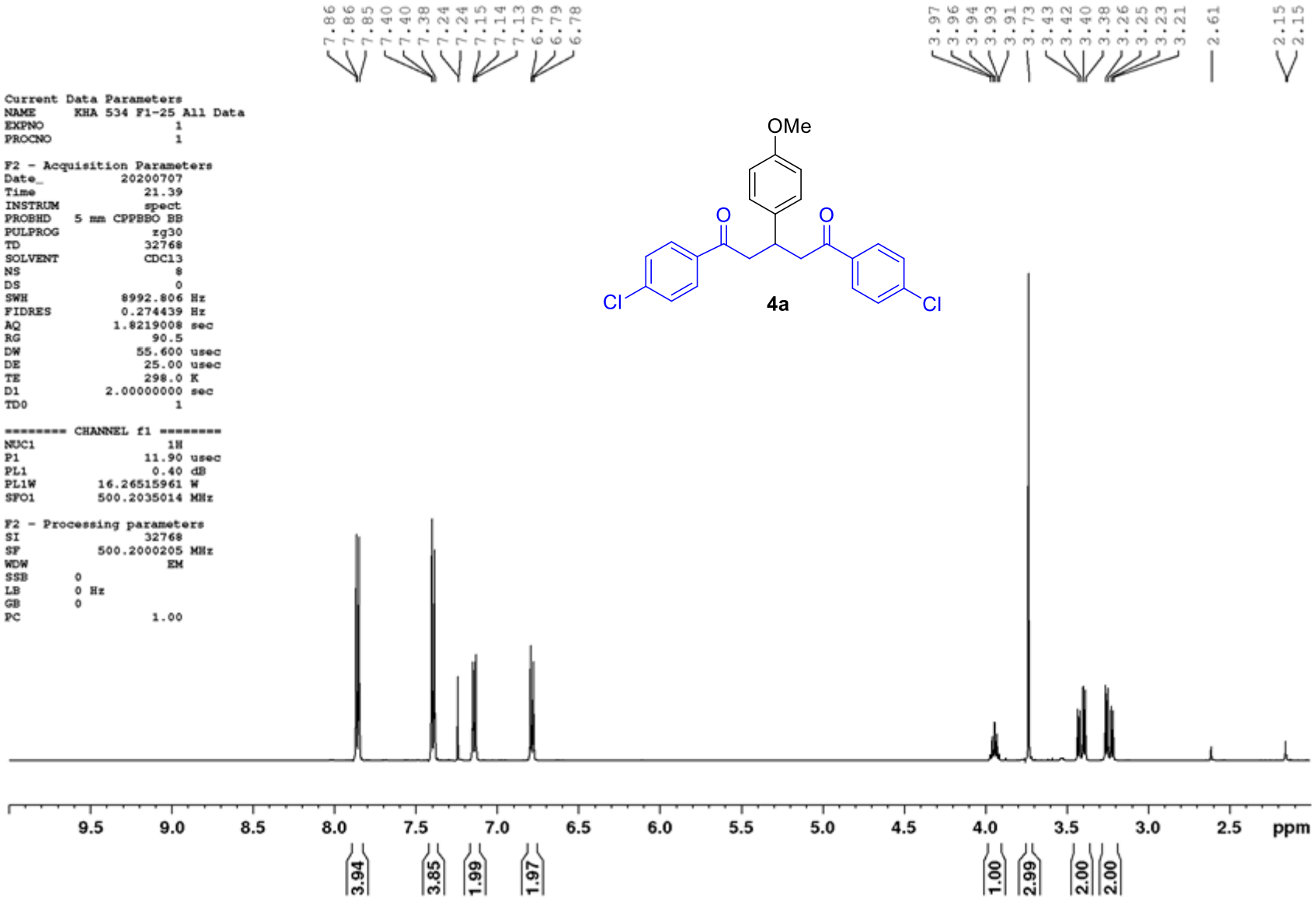


Figure S46. ^{1}H NMR spectrum of compound **4a** (500 MHz, $CDCl_3$, 25 ^{o}C)

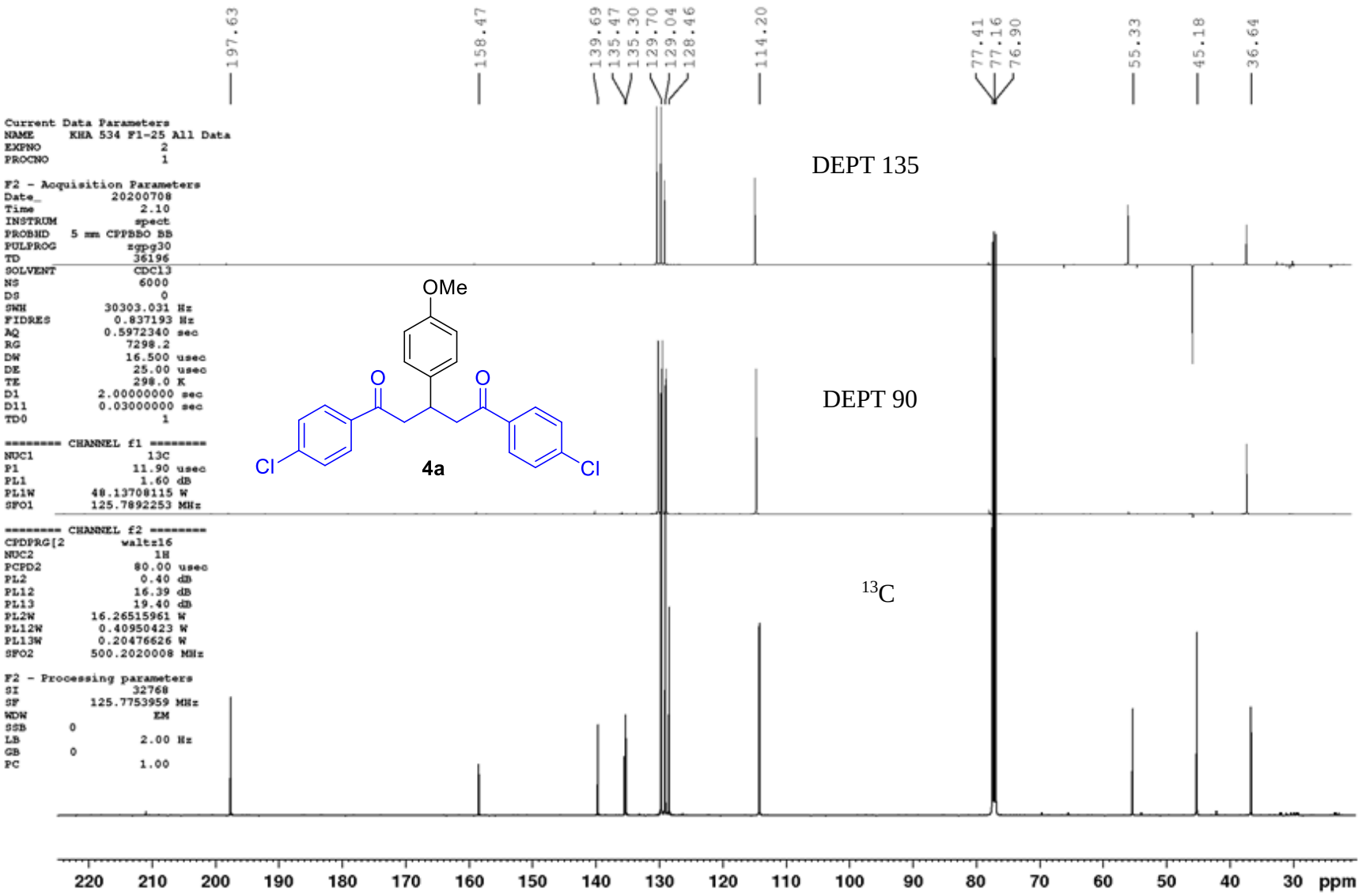


Figure S47. ^{13}C NMR spectrum of compound **4a** (125 MHz, $CDCl_3$, 25 °C)

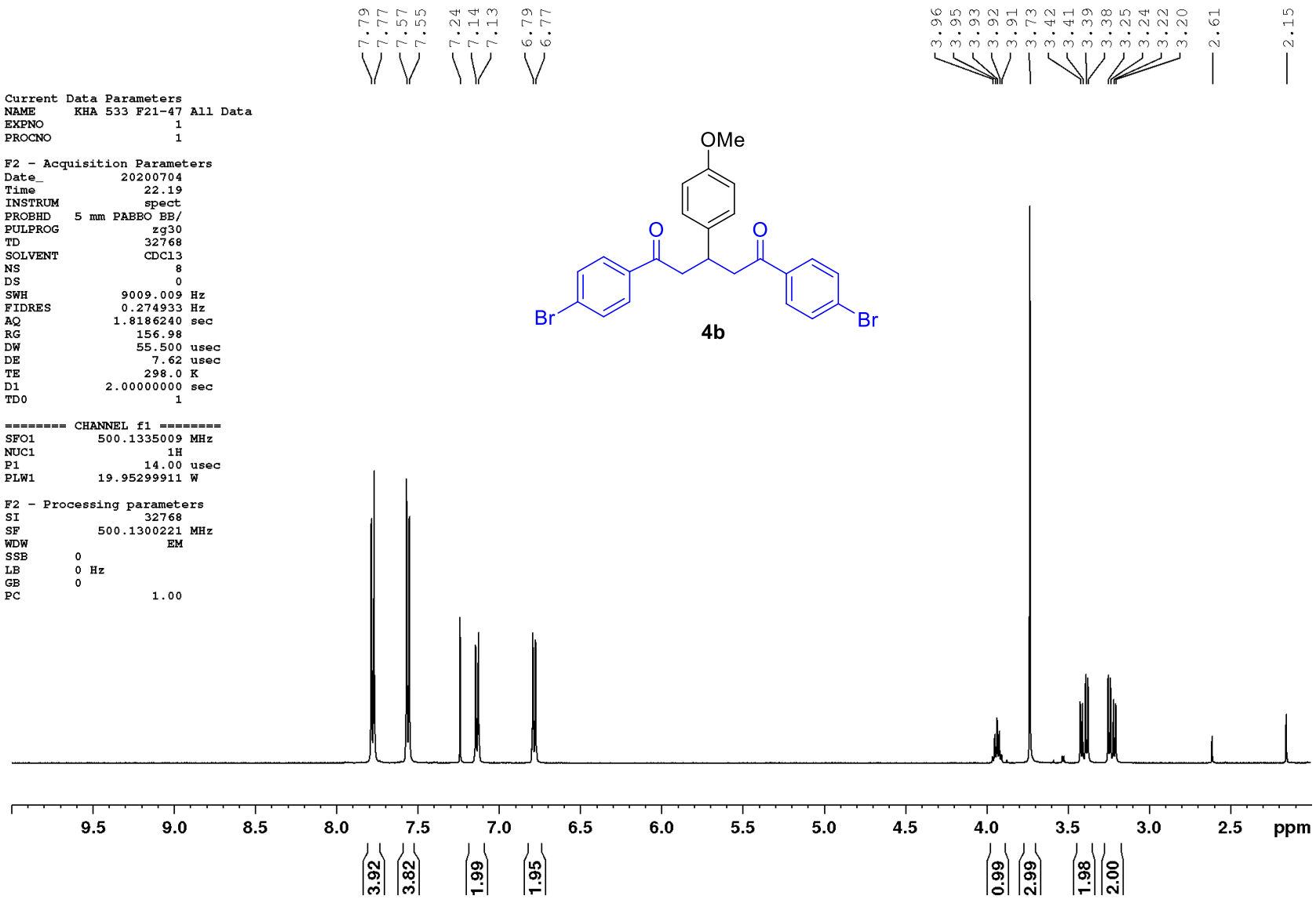


Figure S48. ^{1}H NMR spectrum of compound **4b** (500 MHz, $CDCl_3$, 25 ^{o}C)

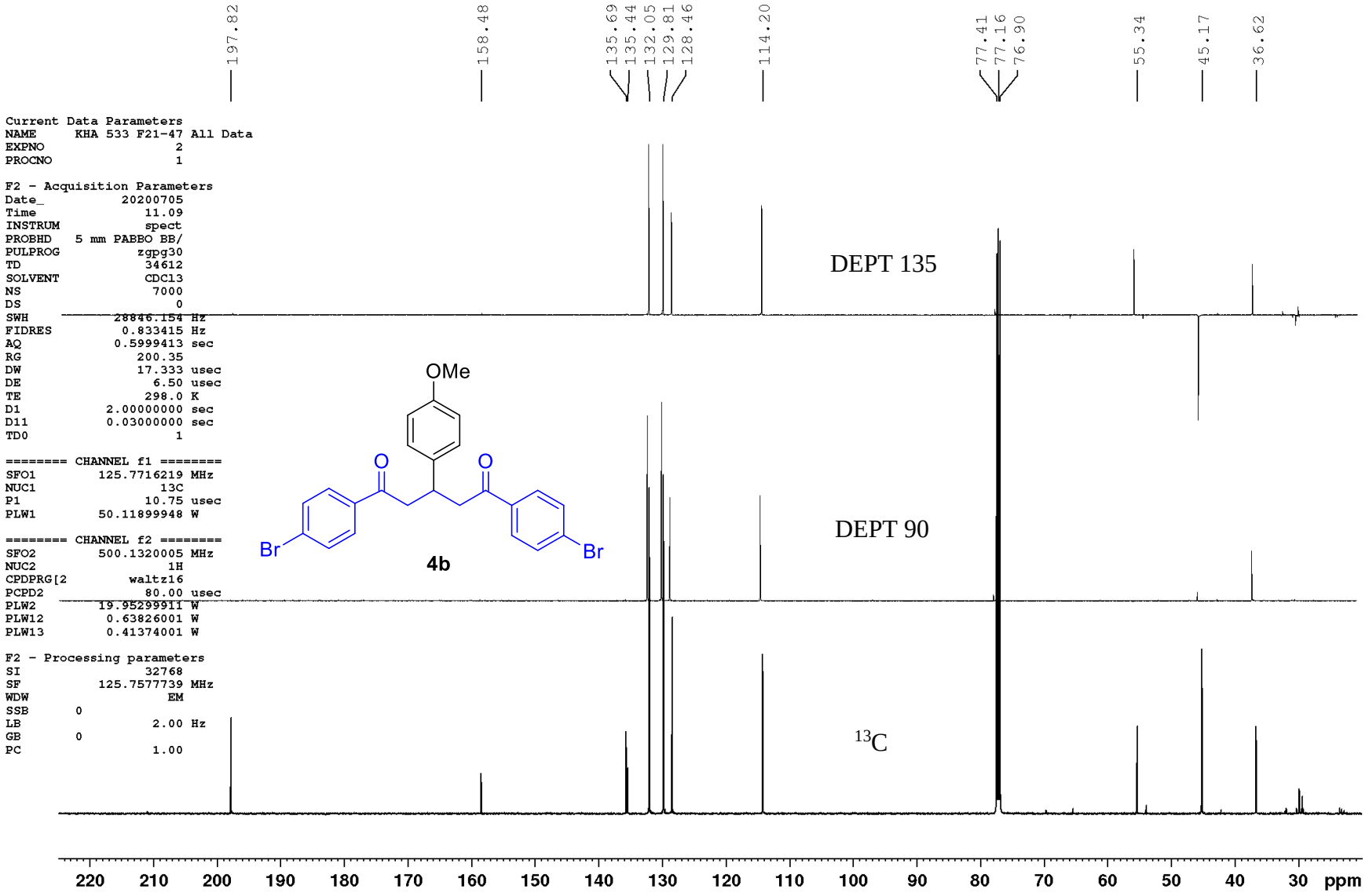


Figure S49. ^{13}C NMR spectrum of compound **4b** (125 MHz, $CDCl_3$, 25 °C)

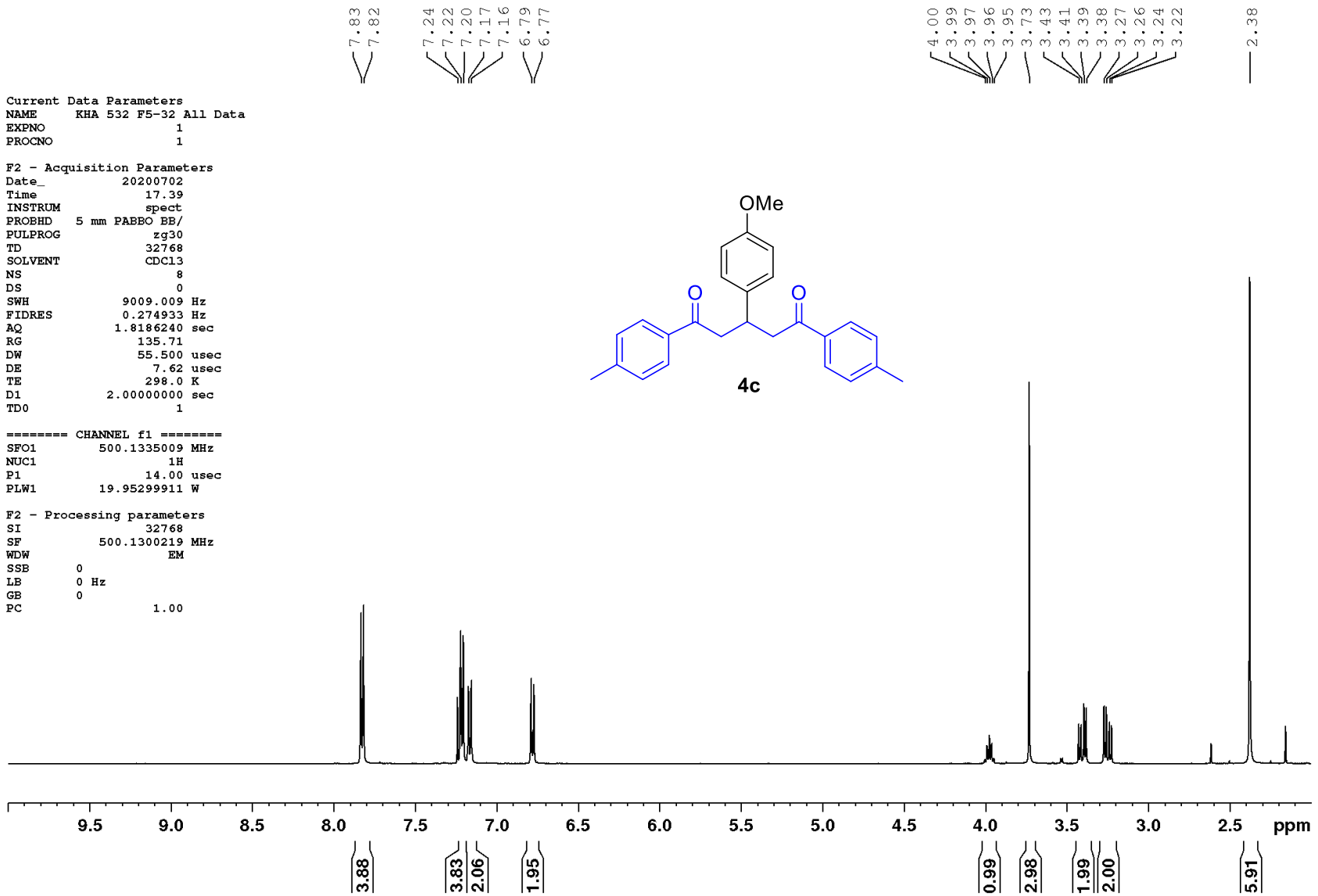


Figure S50. ^{1}H NMR spectrum of compound **4c** (500 MHz, $CDCl_3$, 25 ^{o}C)

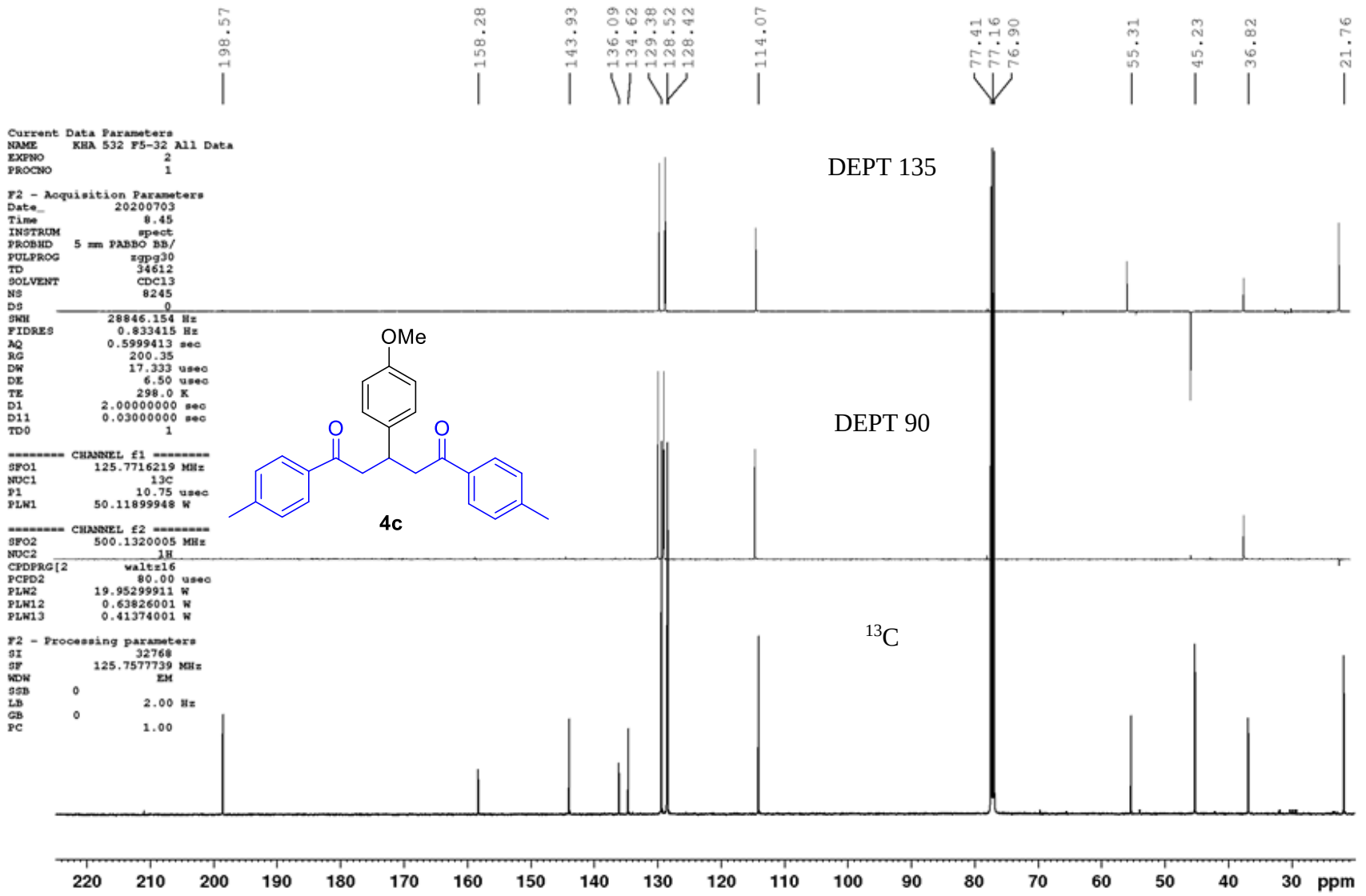


Figure S51. ^{13}C NMR spectrum of compound **4c** (125 MHz, $CDCl_3$, 25 ºC)

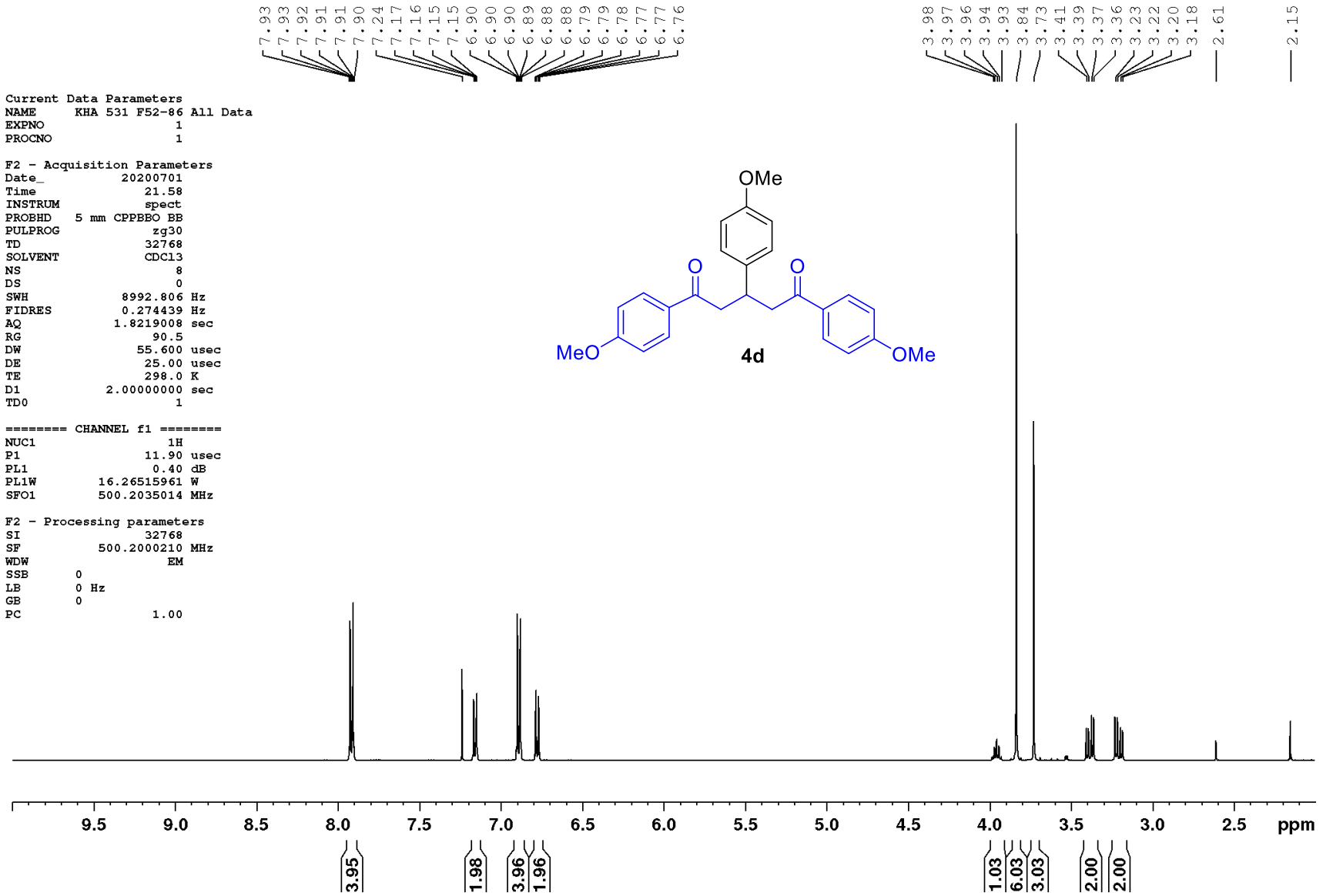


Figure S52. ^{1}H NMR spectrum of compound **4d** (500 MHz, $CDCl_3$, 25 ^{o}C)

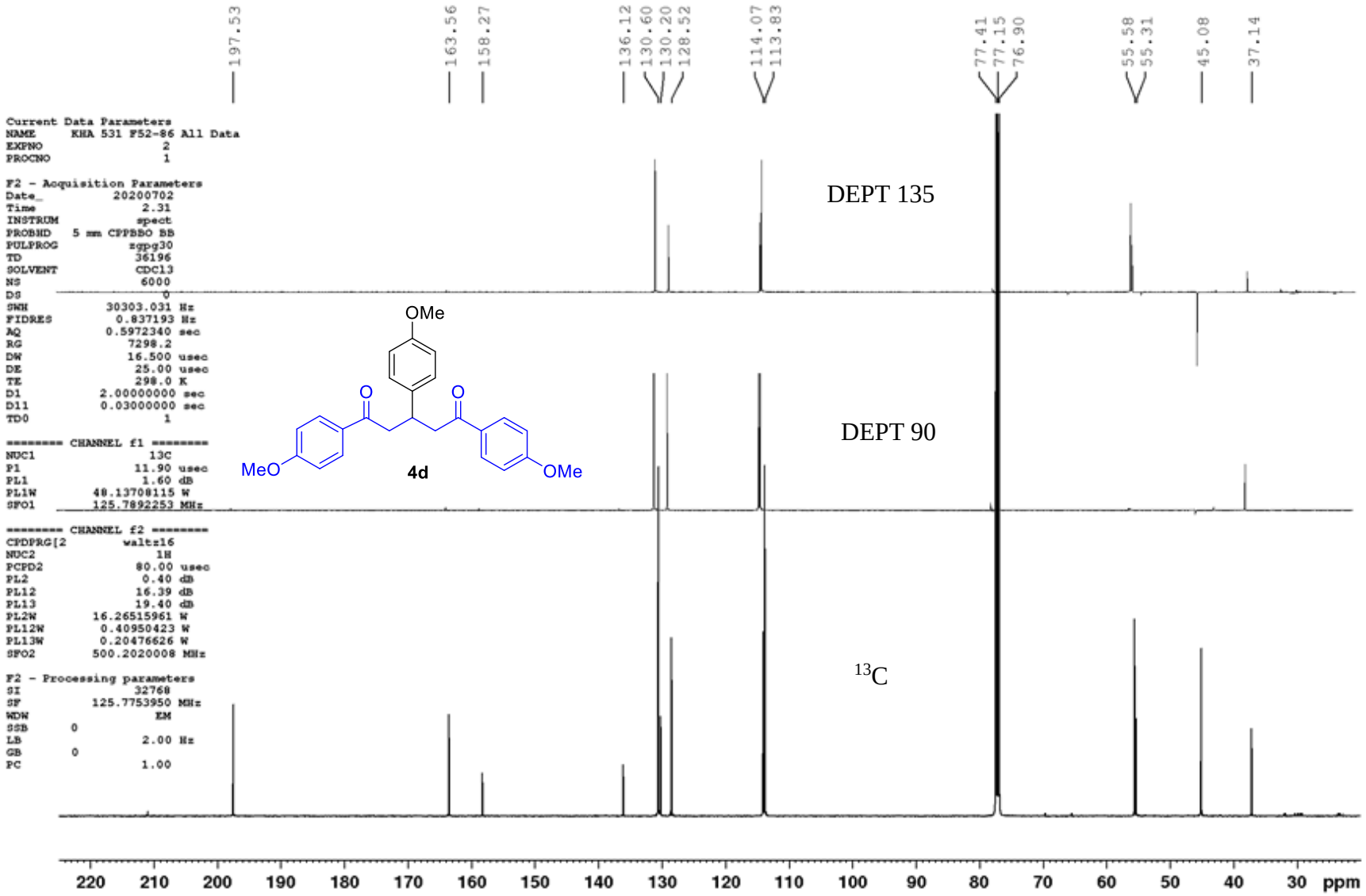


Figure S53. ^{13}C NMR spectrum of compound **4d** (125 MHz, $CDCl_3$, 25 °C)

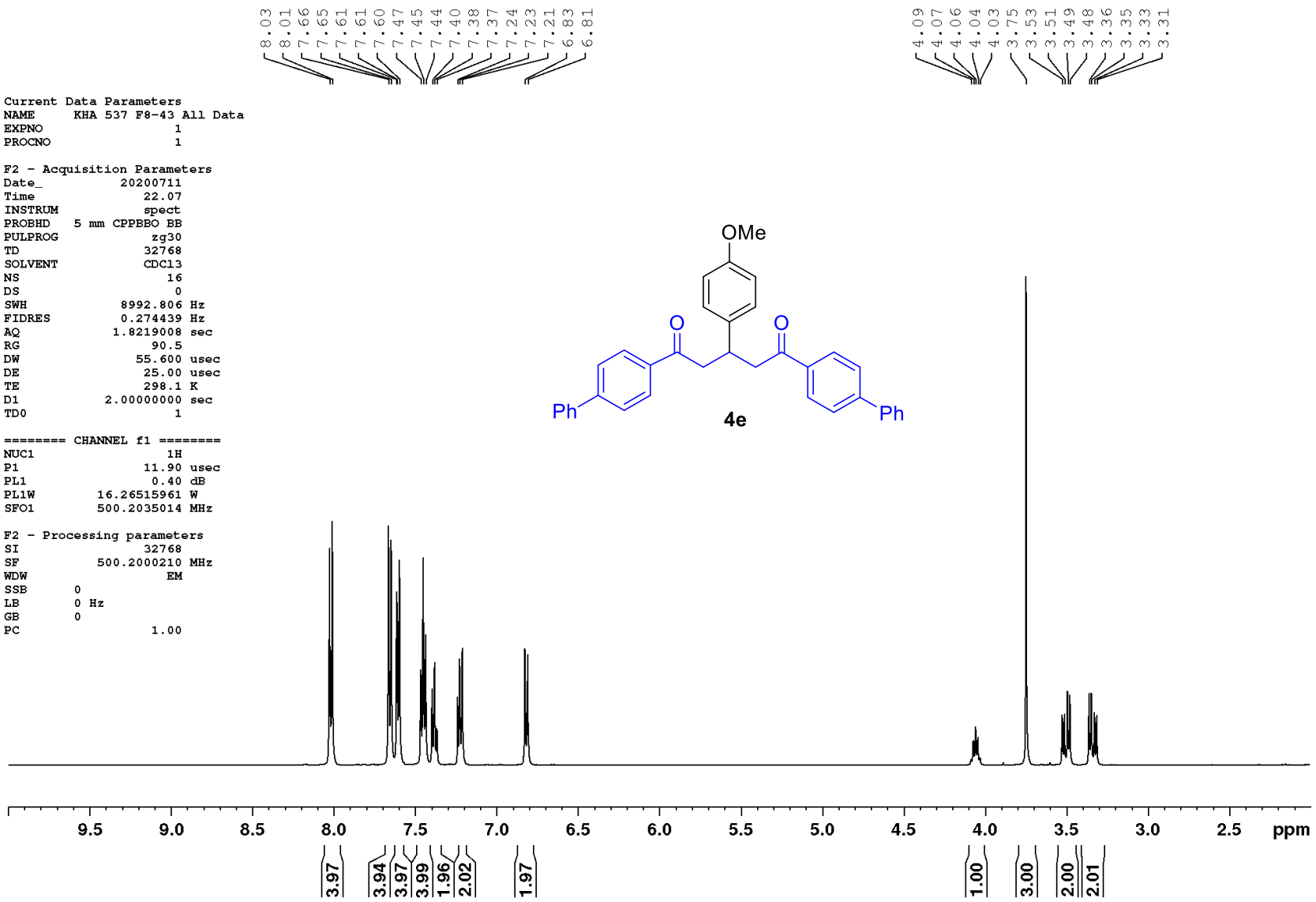


Figure S54. ^{1}H NMR spectrum of compound **4e** (500 MHz, $CDCl_3$, 25 ^{o}C)

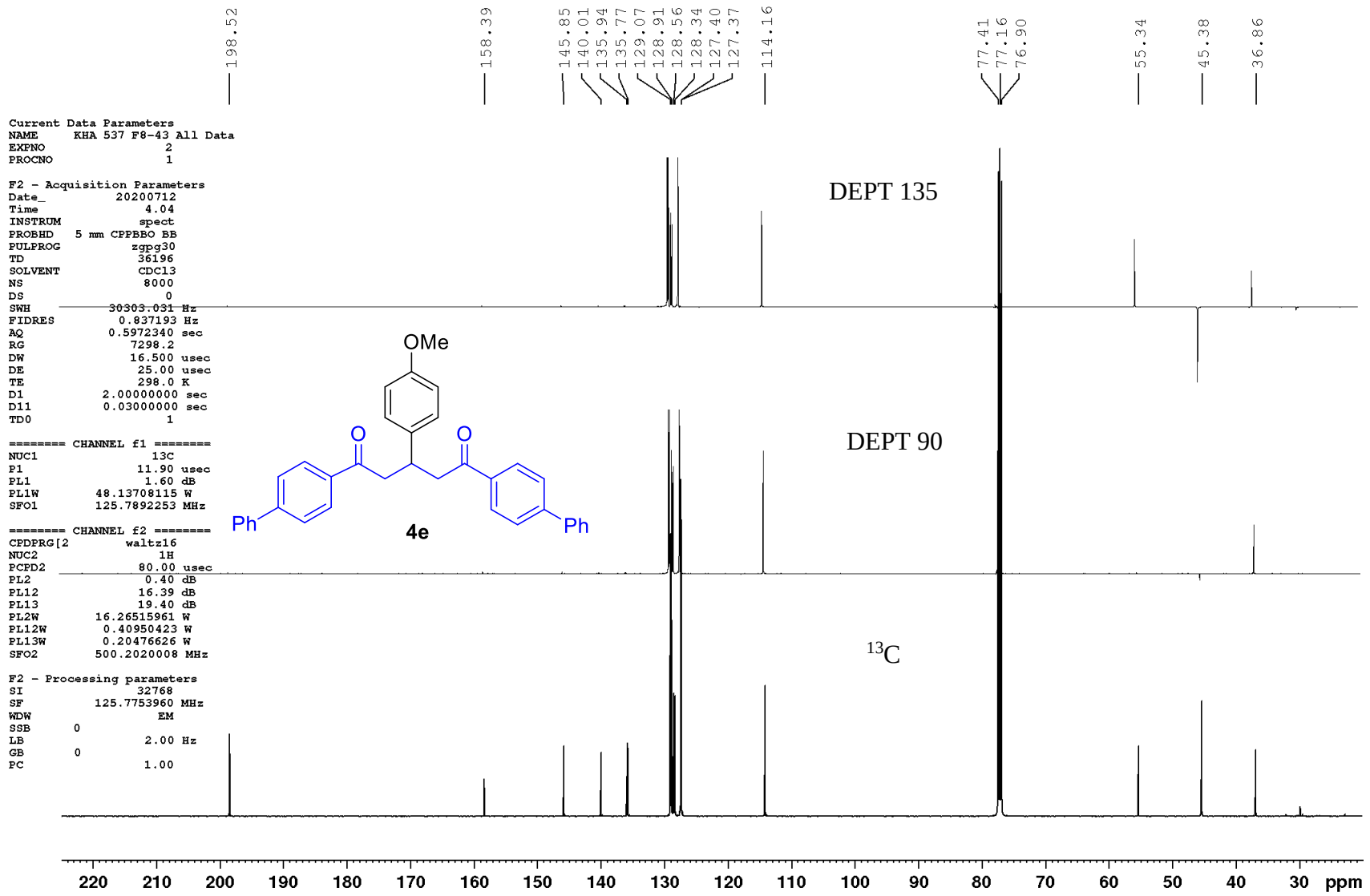


Figure S55. ^{13}C NMR spectrum of compound **4e** (125 MHz, $CDCl_3$, 25 ^oC)

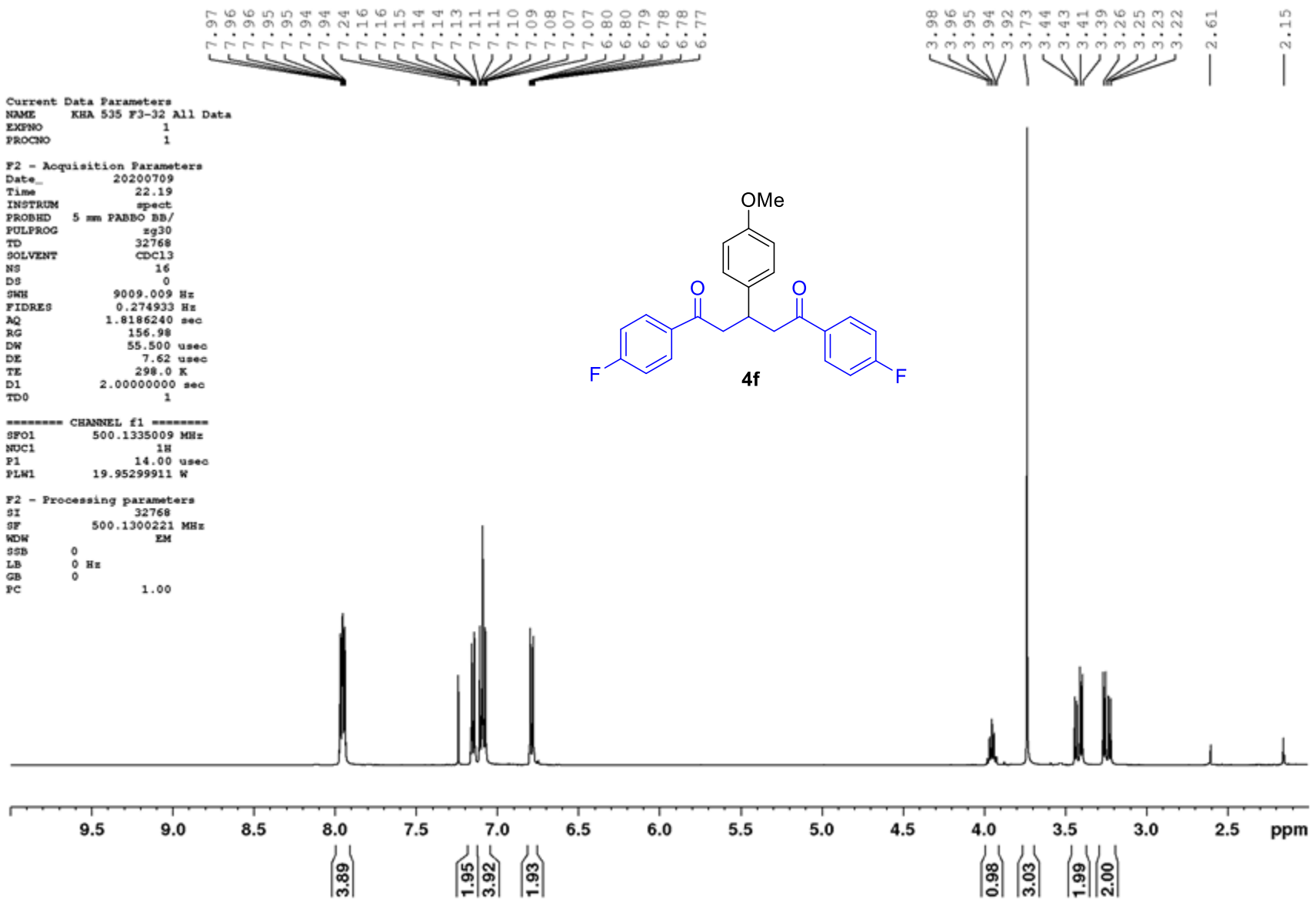


Figure S56. ^{1}H NMR spectrum of compound **4f** (500 MHz, $CDCl_3$, 25 ^{o}C)

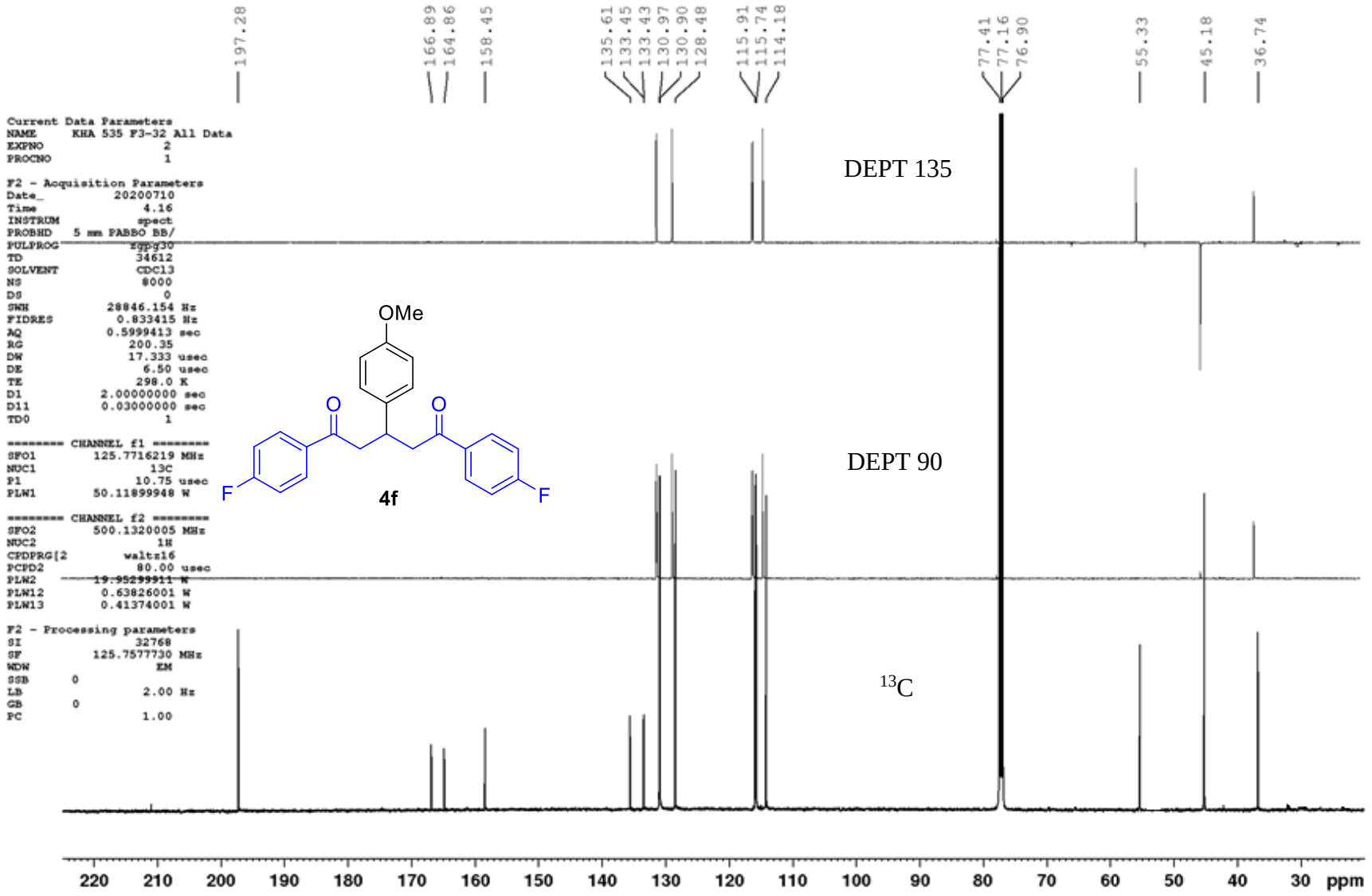


Figure S57. ^{13}C NMR spectrum of compound **4f** (125 MHz, $CDCl_3$, 25 °C)

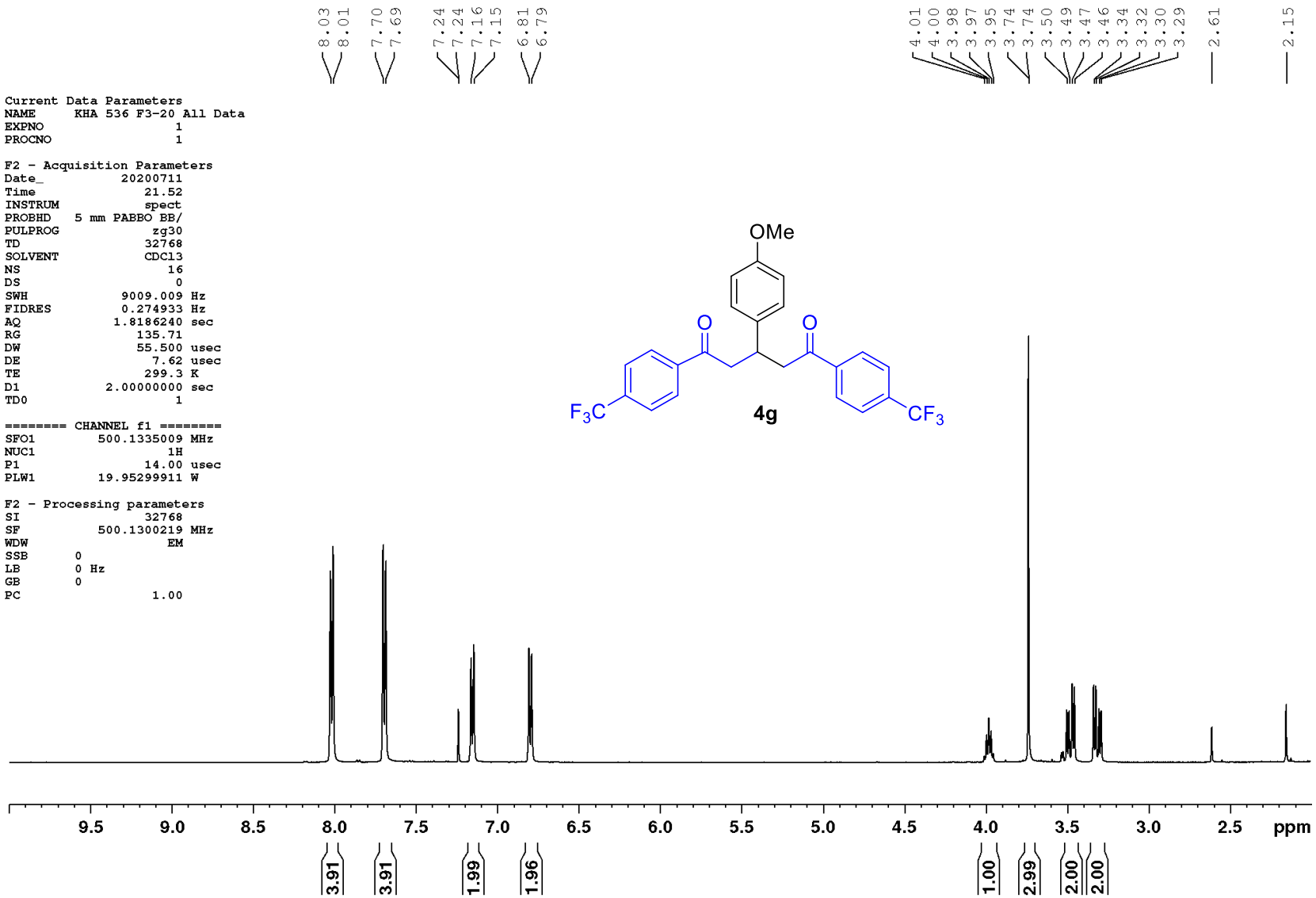


Figure S58. ^{1}H NMR spectrum of compound **4g** (500 MHz, $CDCl_3$, 25 ^{o}C)

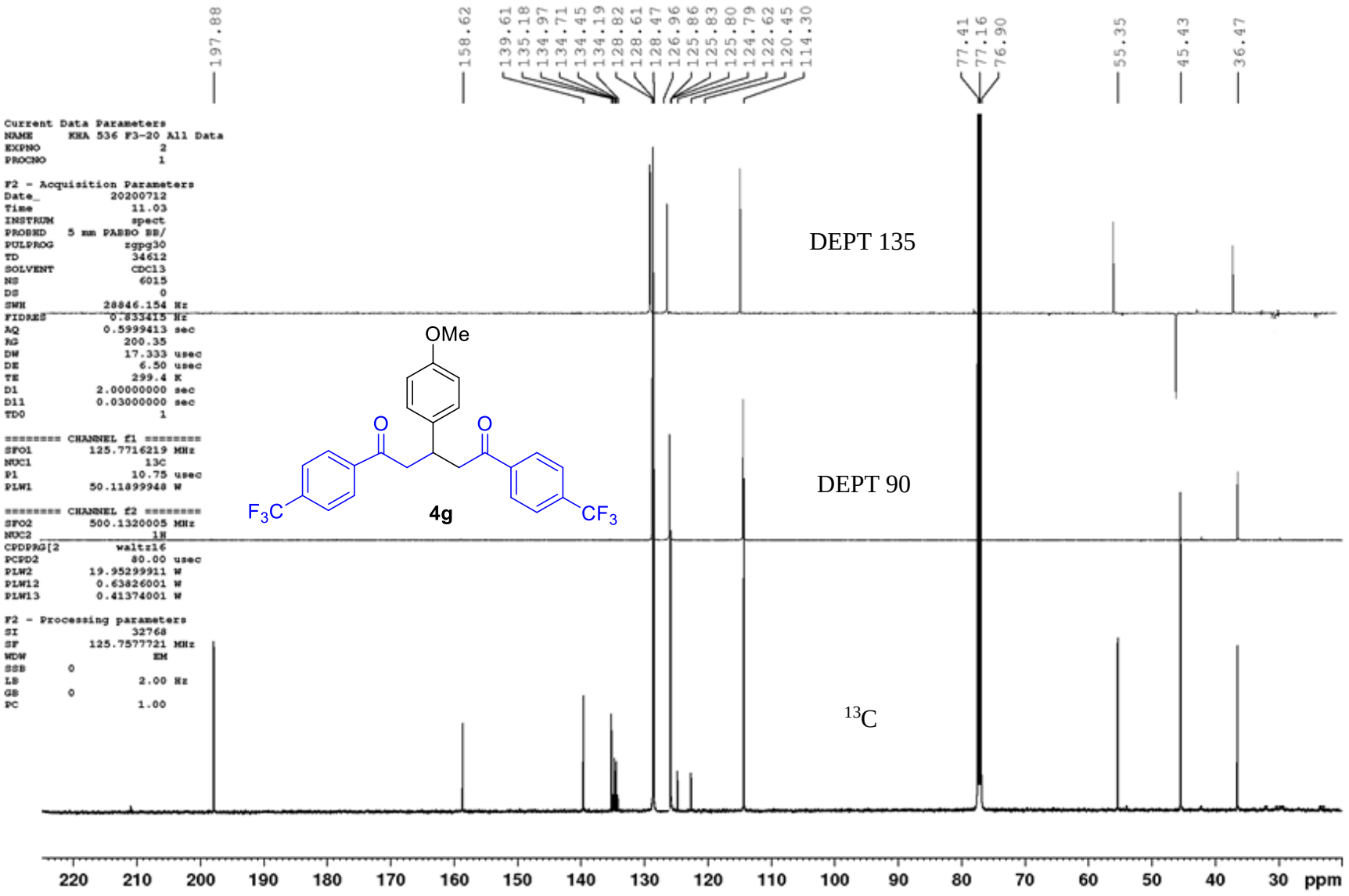


Figure S59. ^{13}C NMR spectrum of compound **4g** (125 MHz, $CDCl_3$, 25 ºC)

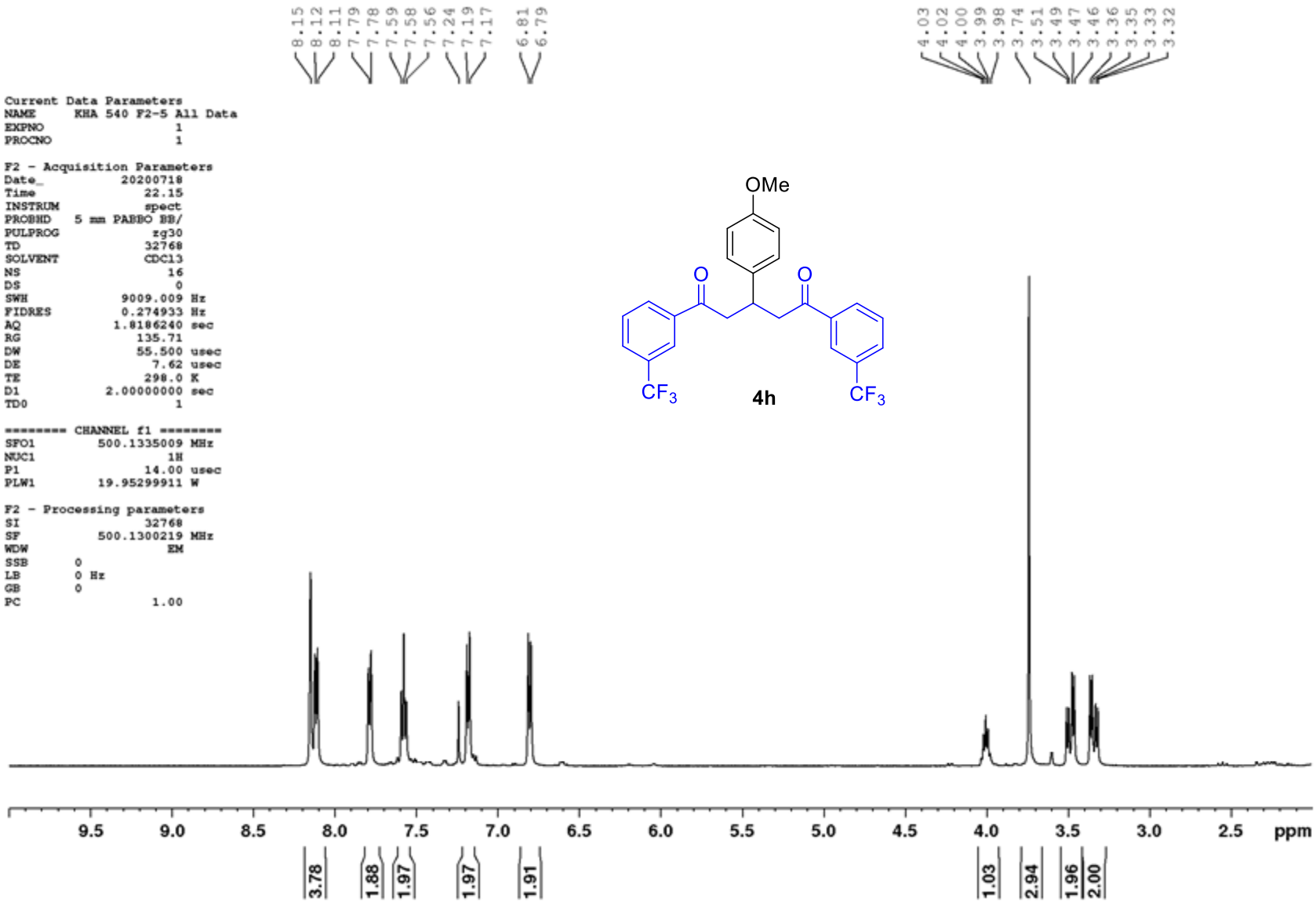


Figure S60. ^{1}H NMR spectrum of compound **4h** (500 MHz, $CDCl_3$, 25 ^{o}C)

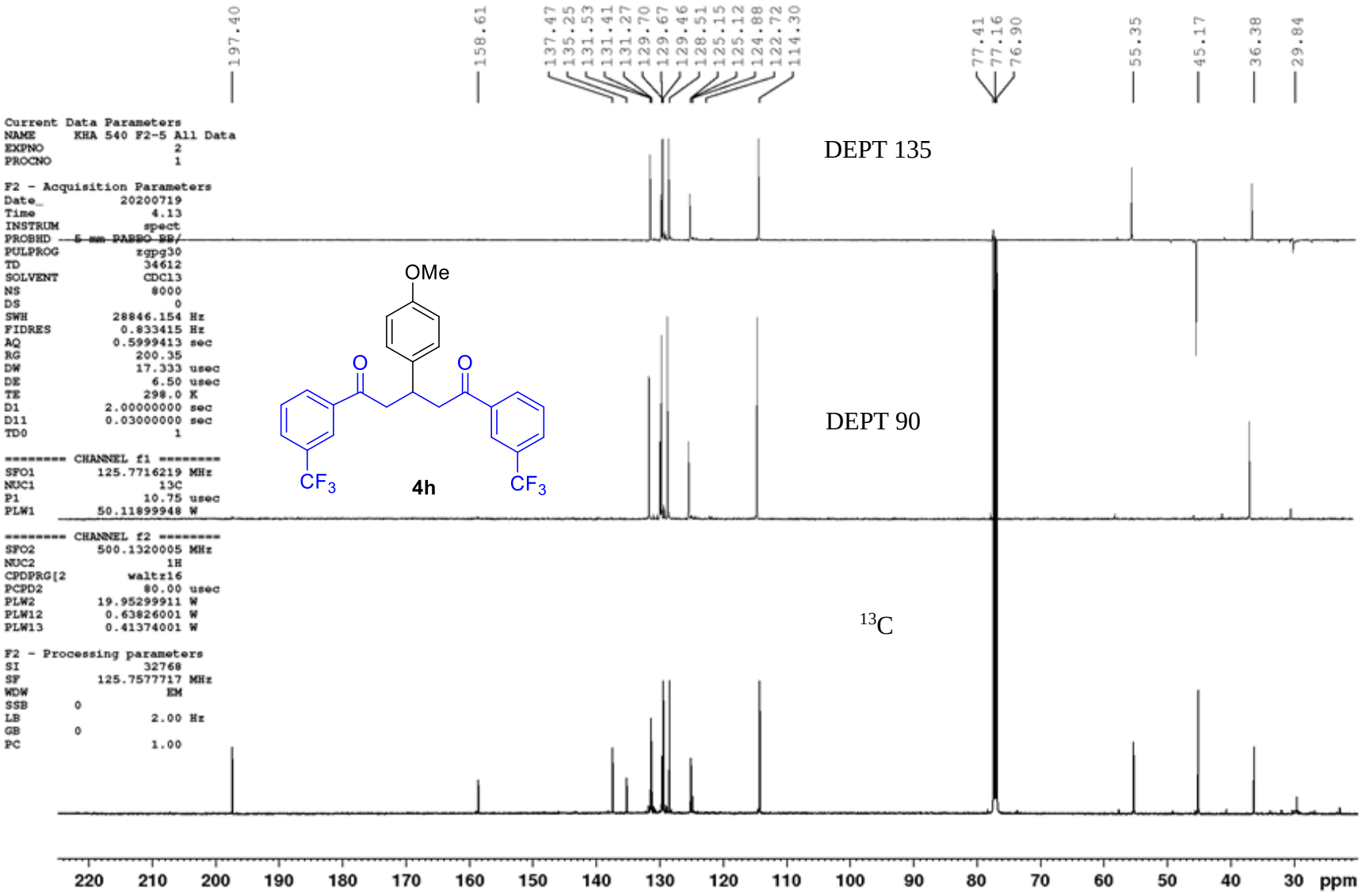


Figure S61. ^{13}C NMR spectrum of compound **4h** (125 MHz, $CDCl_3$, 25 ^oC)

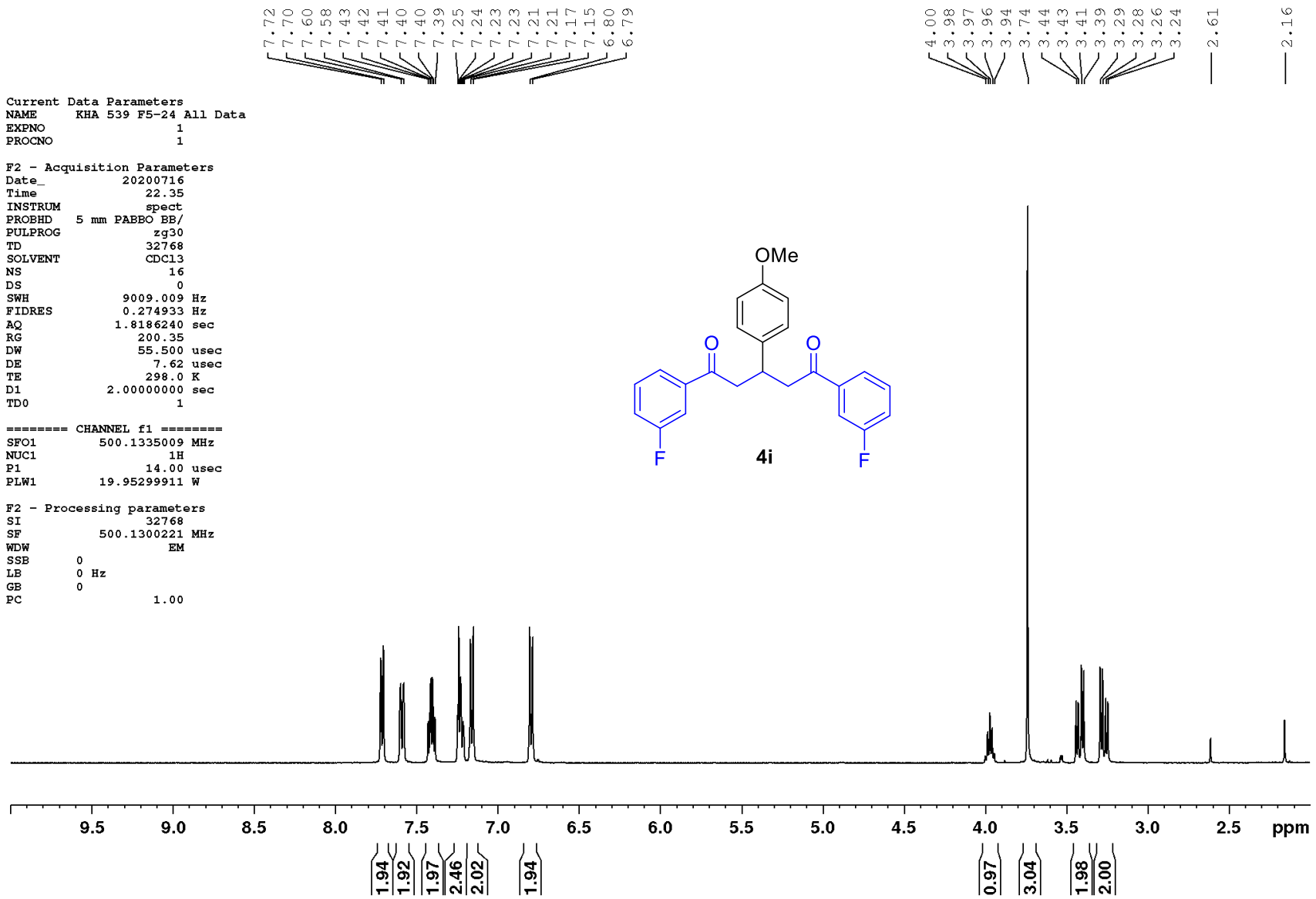


Figure S62. ^{1}H NMR spectrum of compound **4i** (500 MHz, $CDCl_3$, 25 ^{o}C)

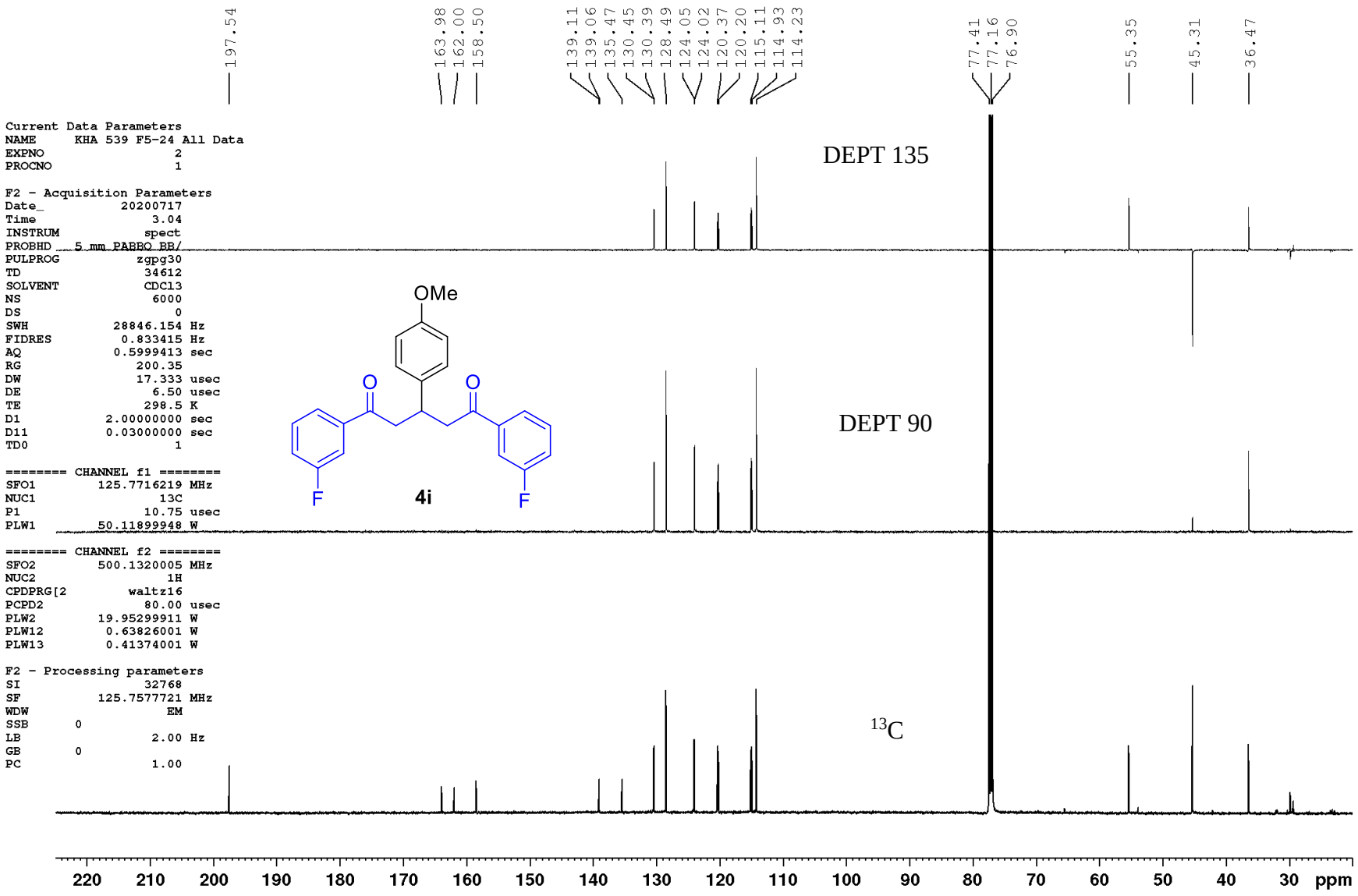


Figure S63. ^{13}C NMR spectrum of compound **4i** (125 MHz, $CDCl_3$, 25 °C)

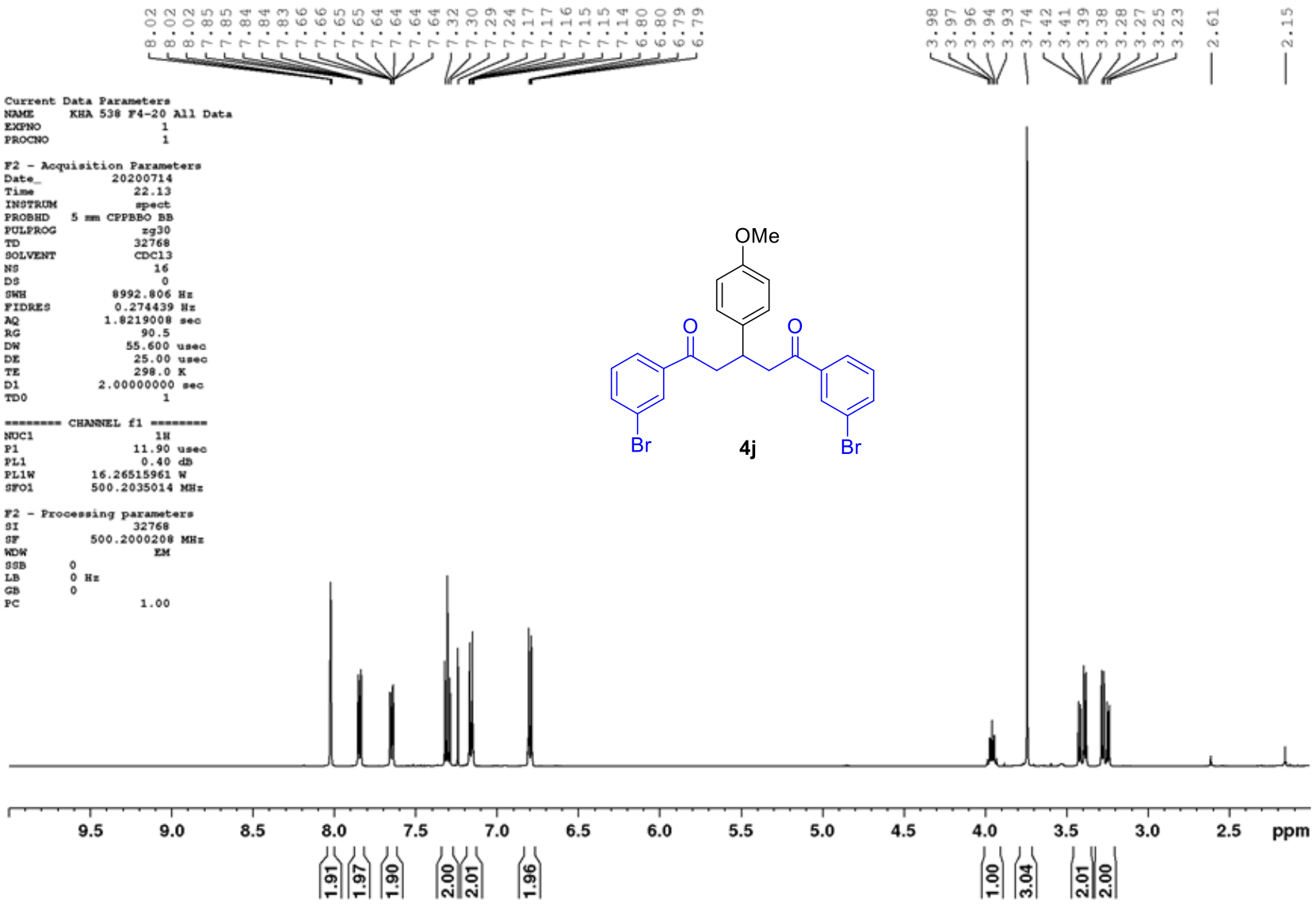


Figure S64. ^{1}H NMR spectrum of compound **4j** (500 MHz, $CDCl_3$, 25 ^{o}C)

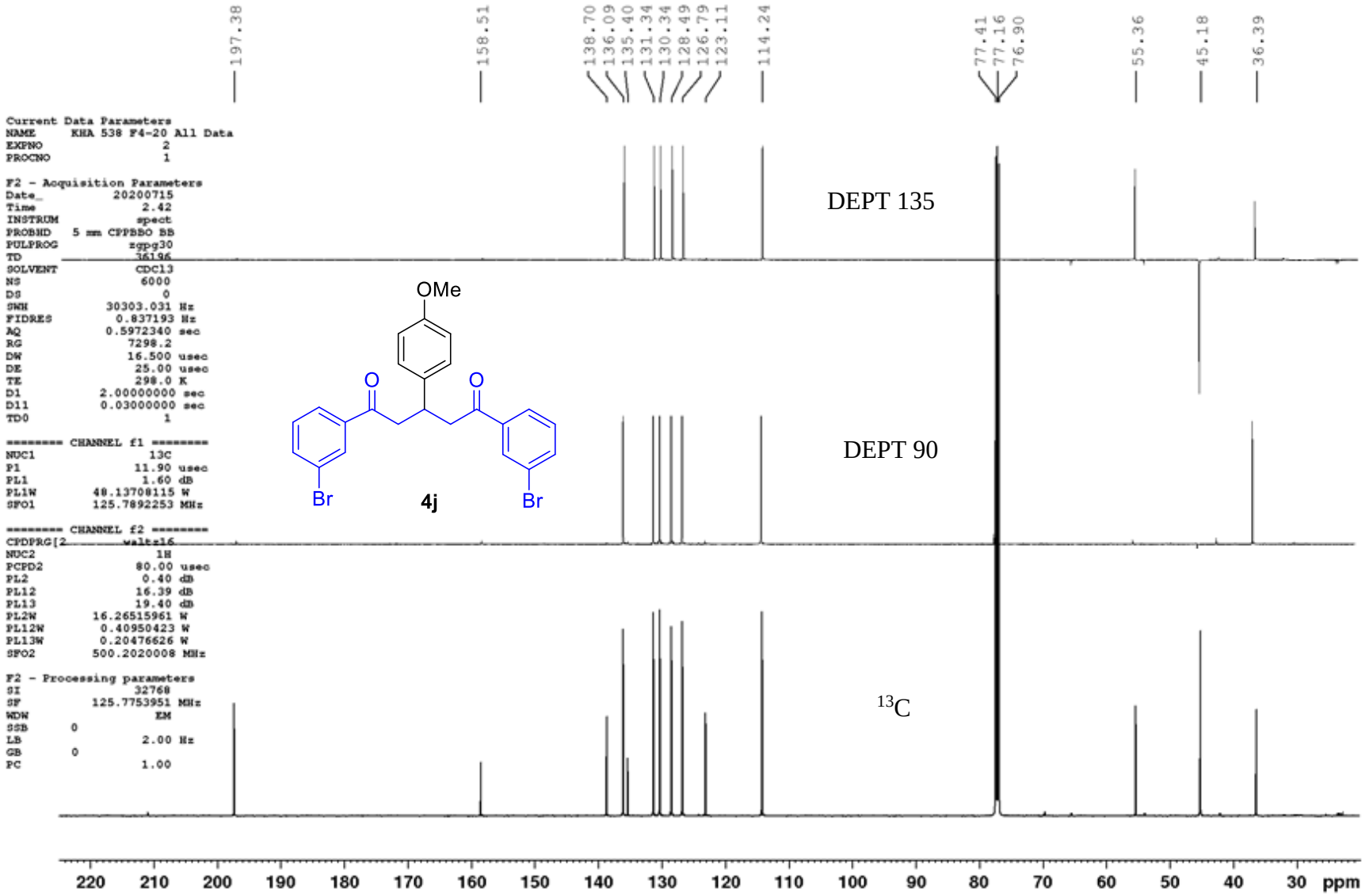


Figure S65. ^{13}C NMR spectrum of compound **4j** (125 MHz, $CDCl_3$, 25 °C)

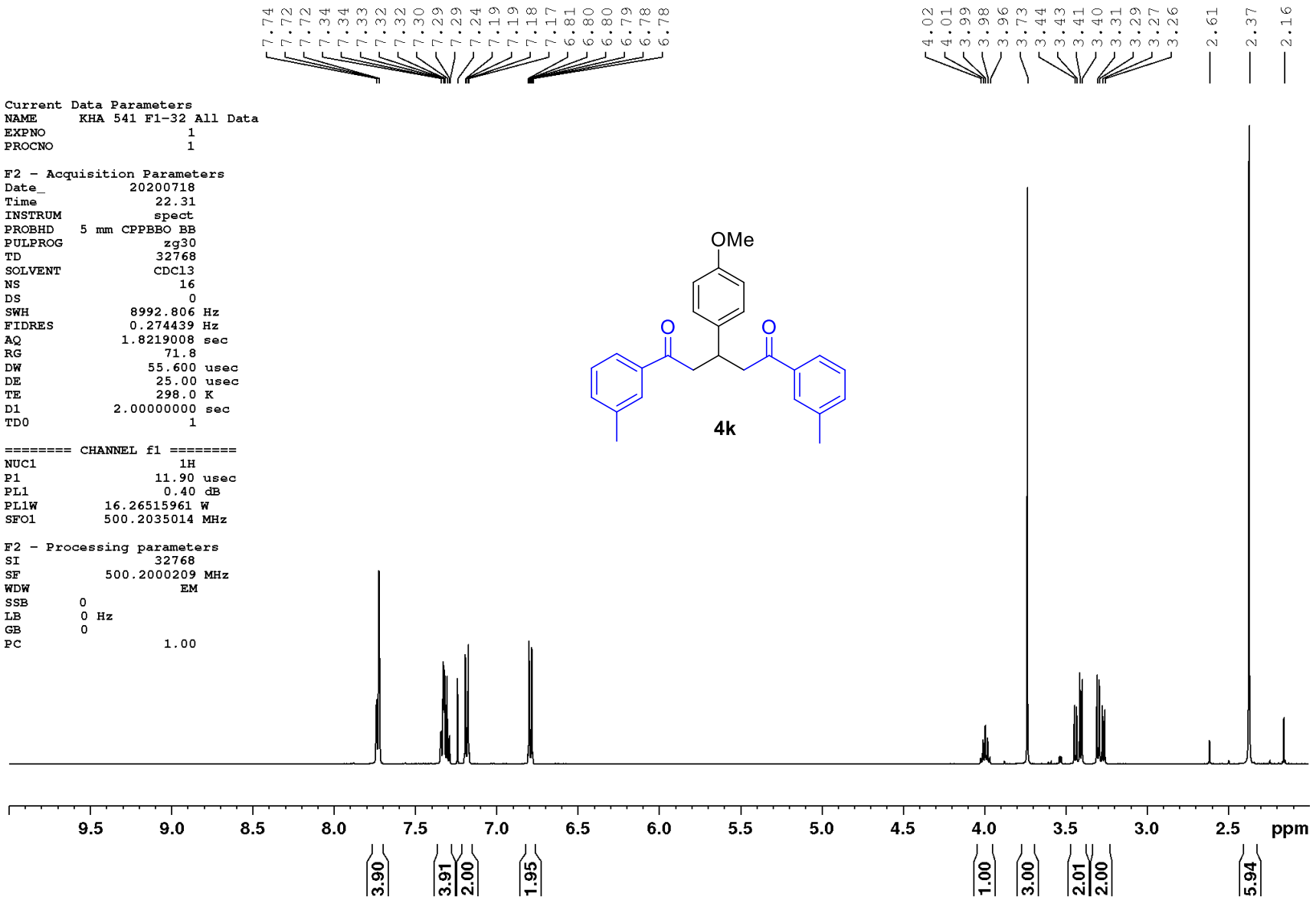


Figure S66. ^{1}H NMR spectrum of compound **4k** (500 MHz, $CDCl_3$, 25 ^{o}C)

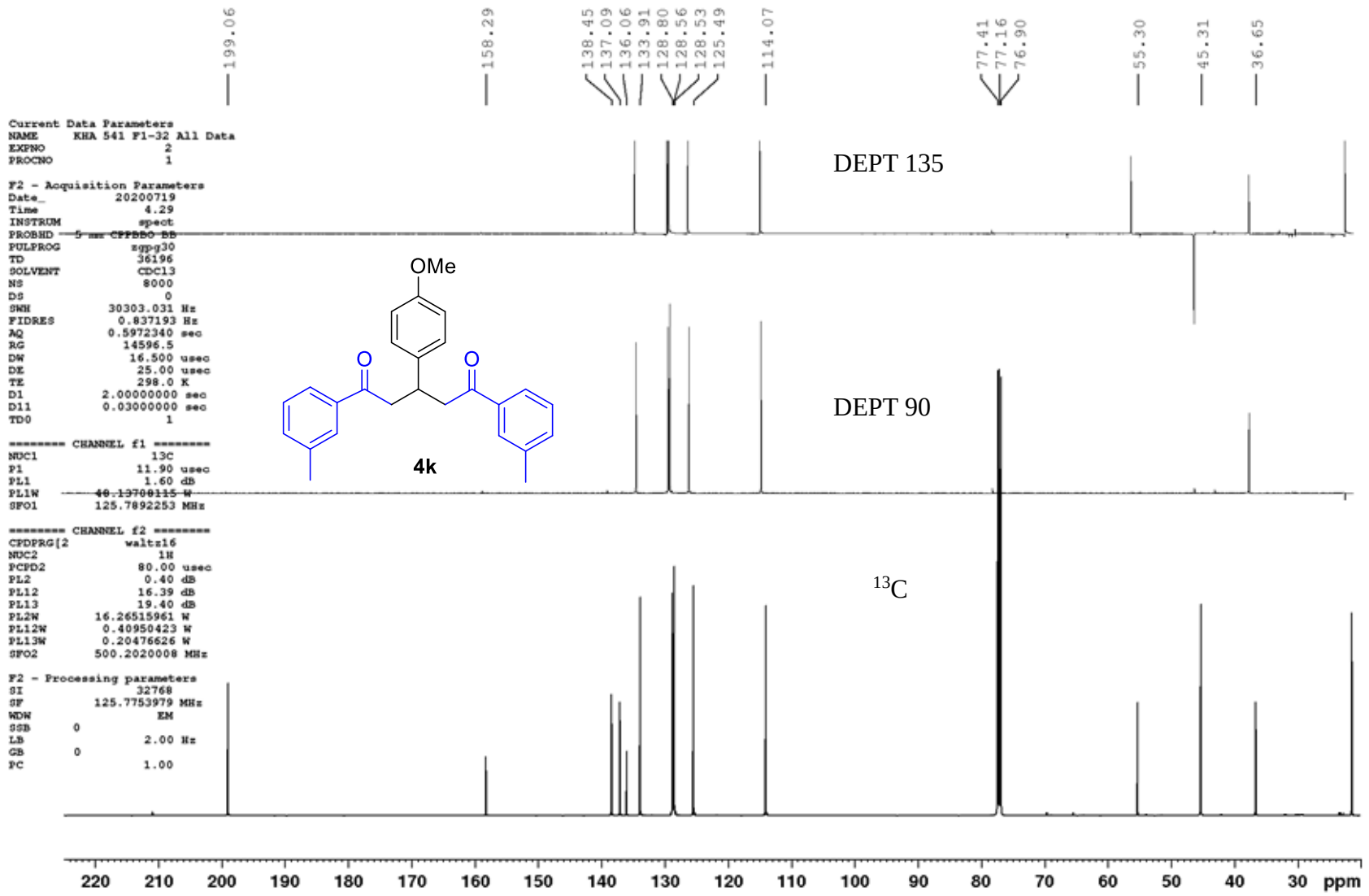


Figure S67. ^{13}C NMR spectrum of compound **4k** (125 MHz, $CDCl_3$, 25 °C)

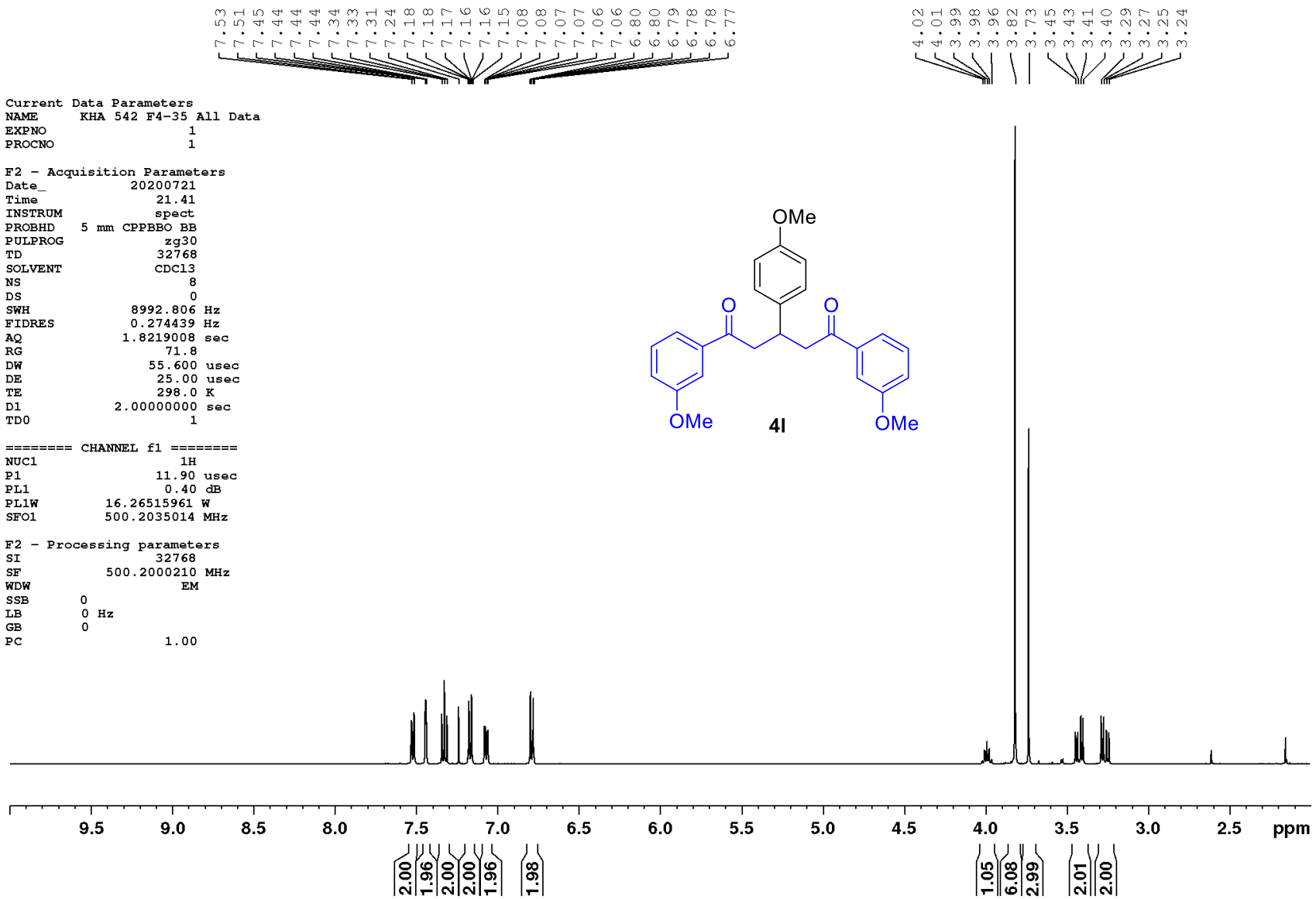


Figure S68. ^{1}H NMR spectrum of compound **4l** (500 MHz, $CDCl_3$, 25 ^{o}C)

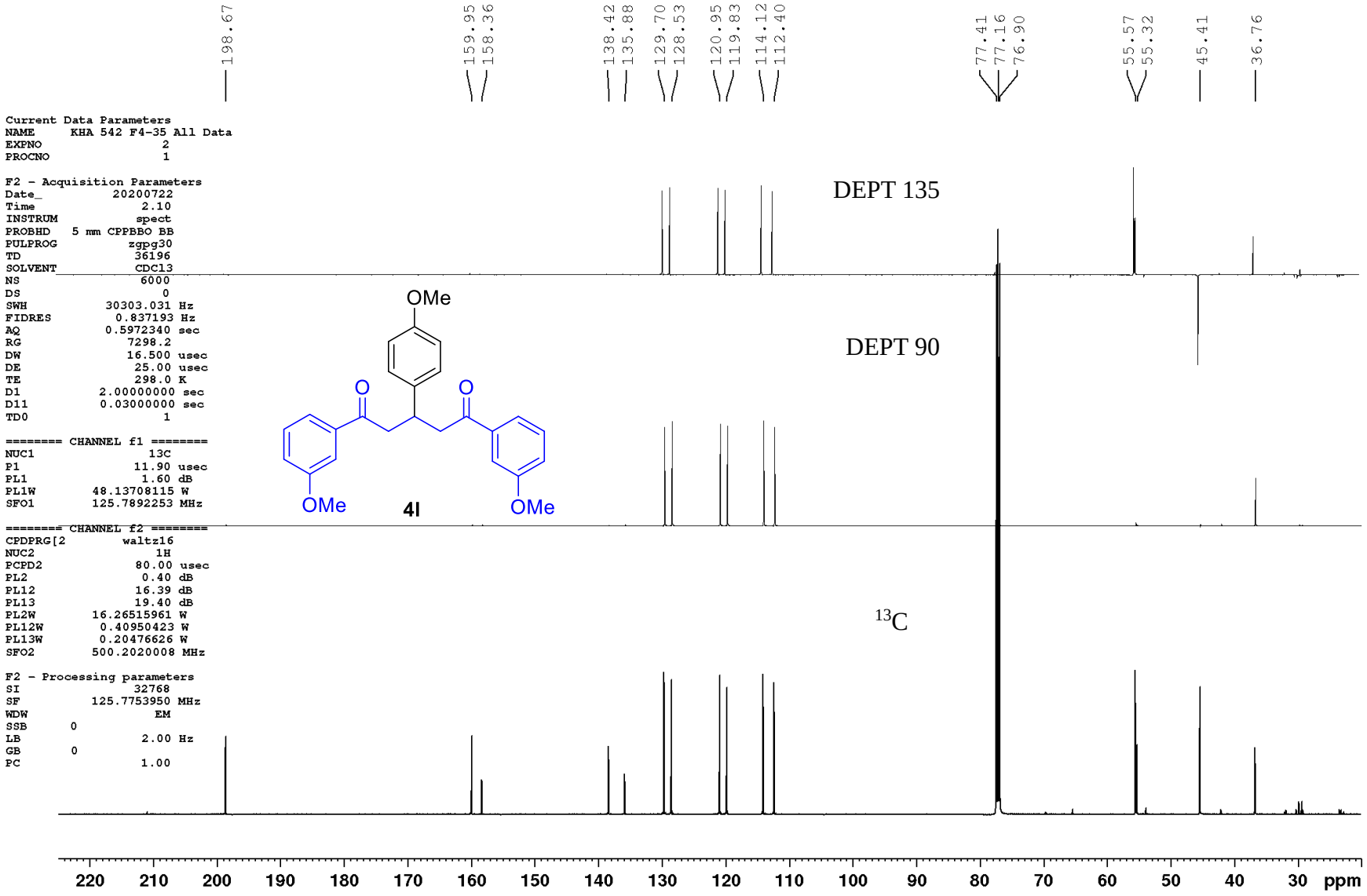


Figure S69. ^{13}C NMR spectrum of compound **4l** (125 MHz, $CDCl_3$, 25 ^oC)

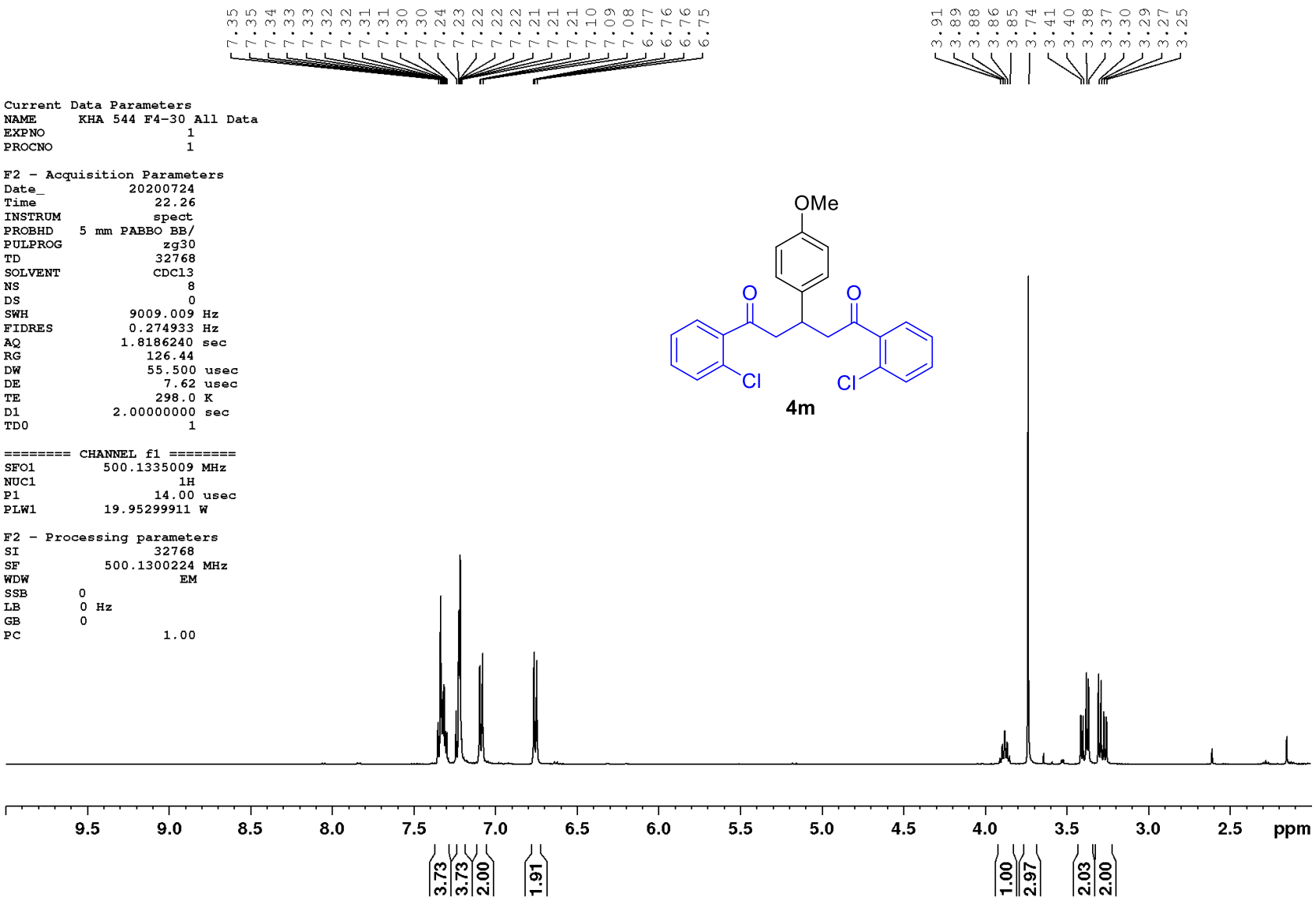


Figure S70. ^{1}H NMR spectrum of compound **4m** (500 MHz, $CDCl_3$, 25 ^{o}C)

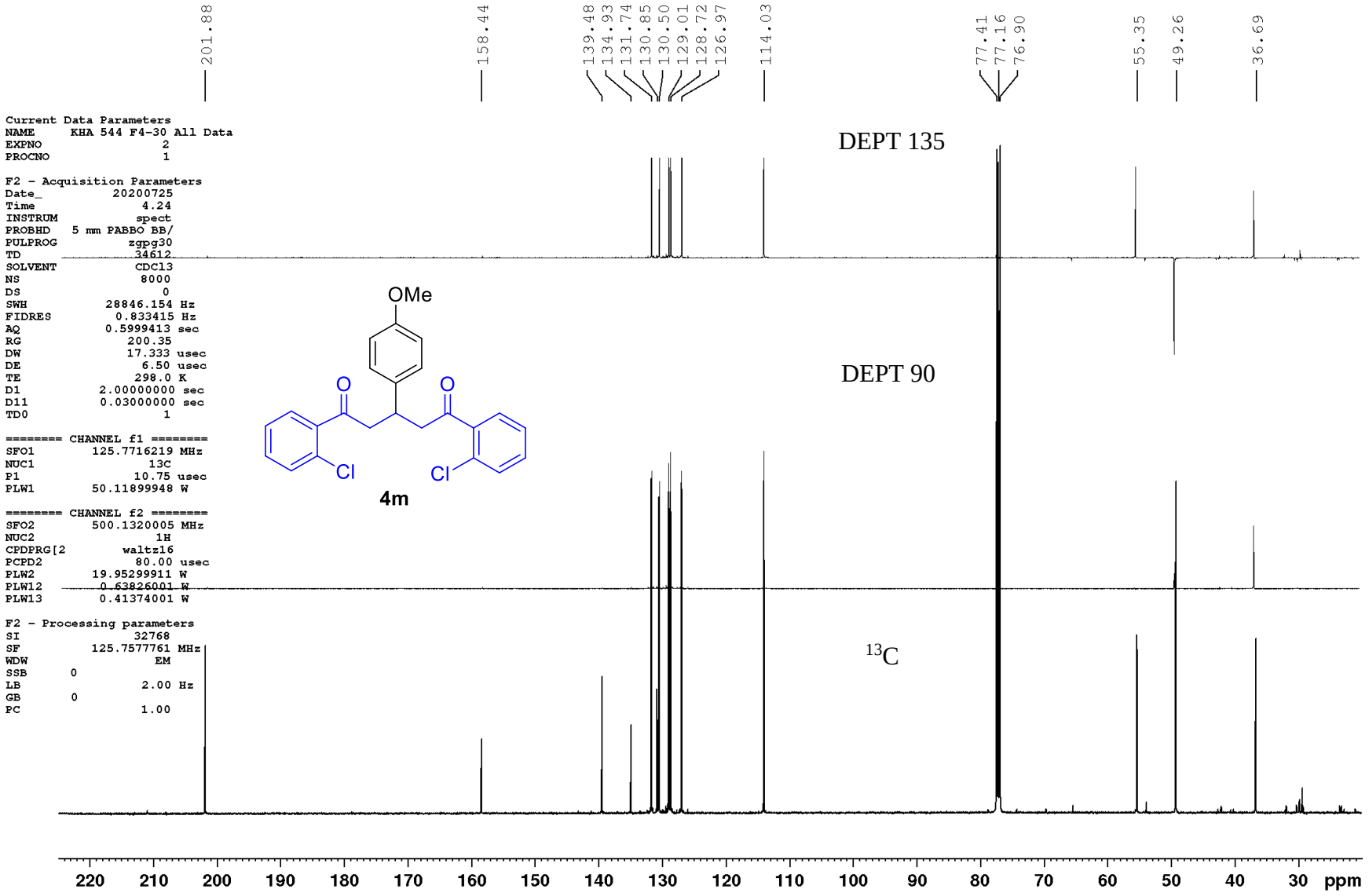


Figure S71. ^{13}C NMR spectrum of compound **4m** (125 MHz, $CDCl_3$, 25 ^oC)

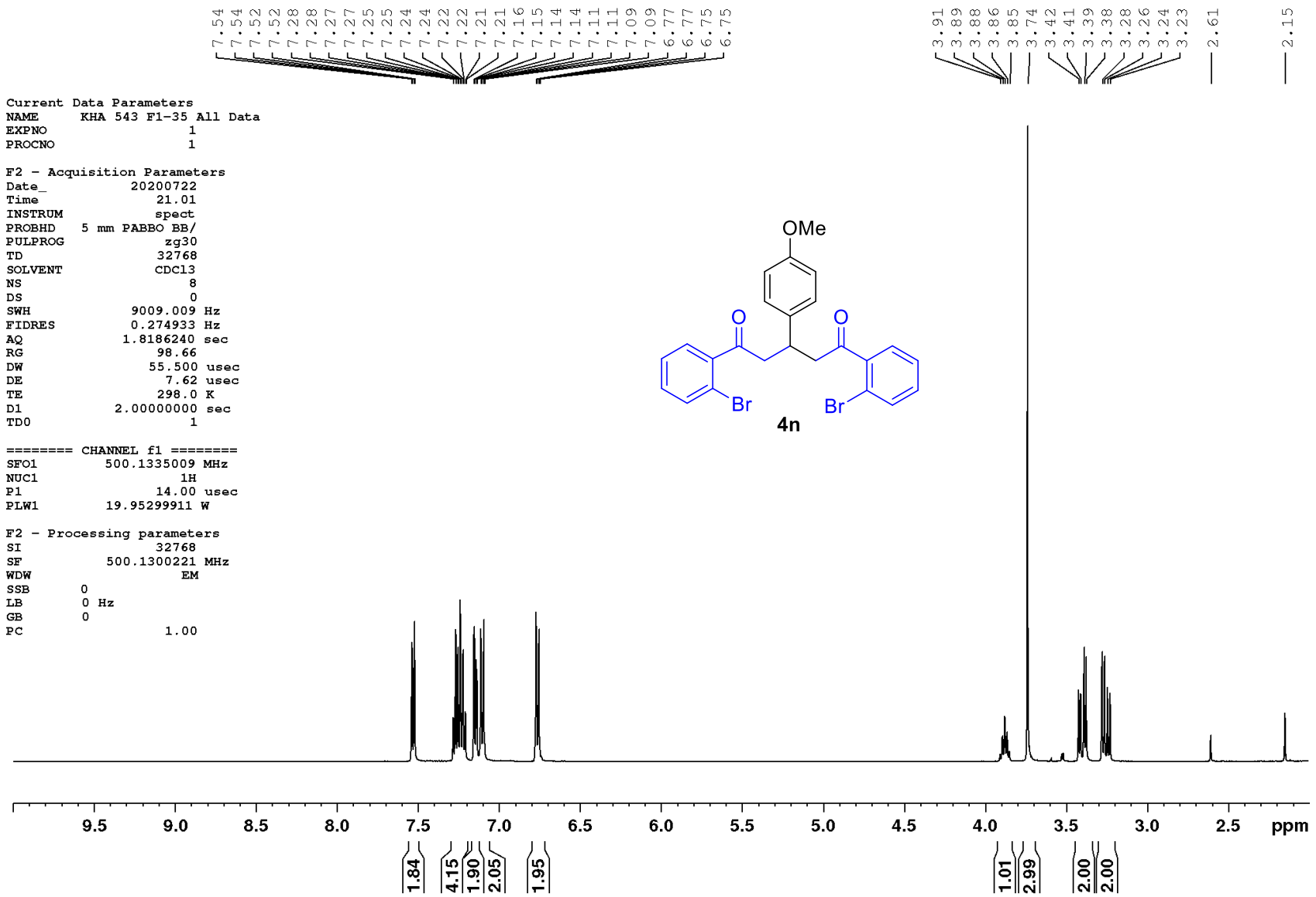


Figure S72. ^{1}H NMR spectrum of compound **4n** (500 MHz, $CDCl_3$, 25 ^{o}C)

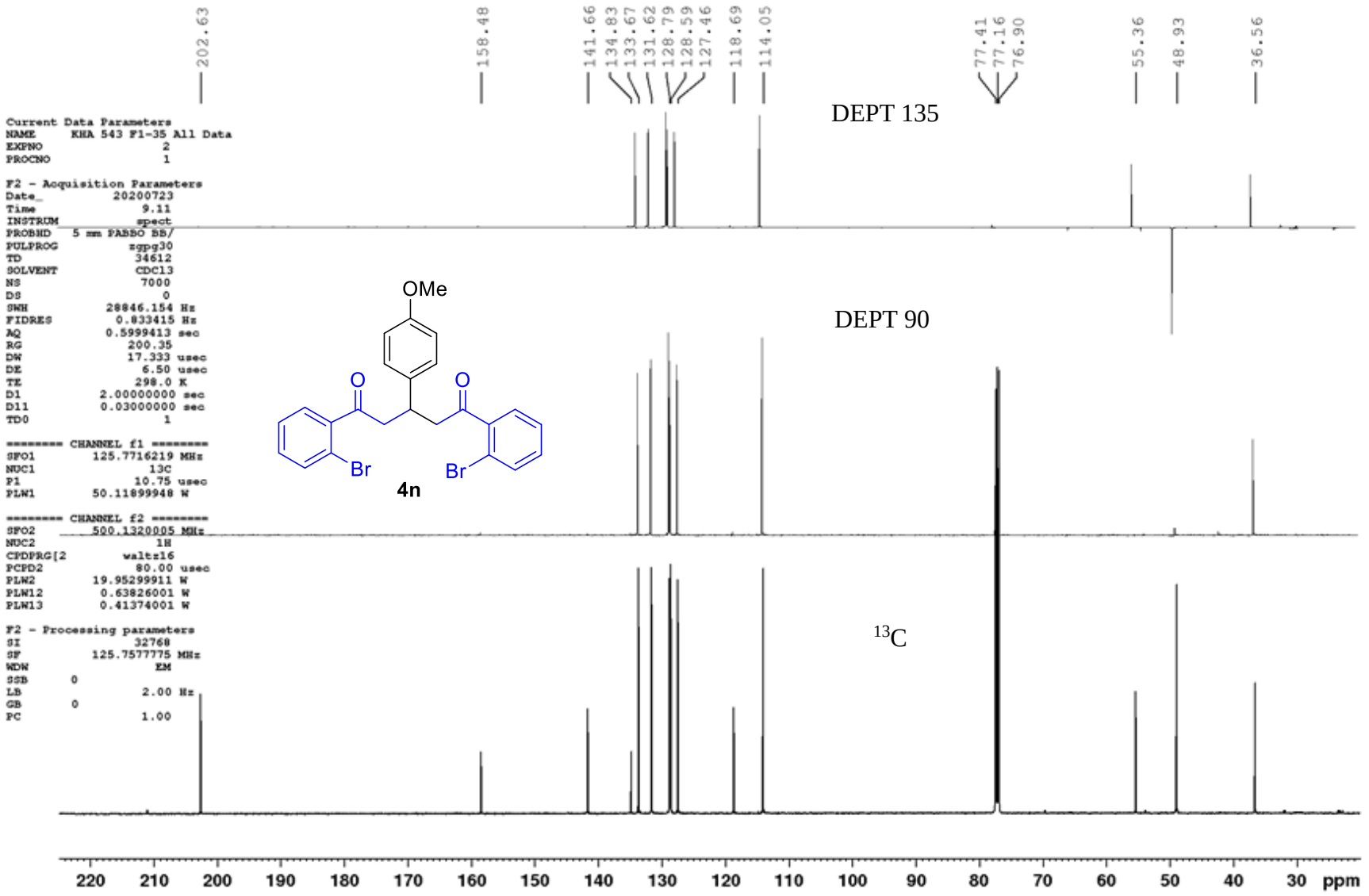


Figure S73. ^{13}C NMR spectrum of compound **4n** (125 MHz, $CDCl_3$, 25 °C)

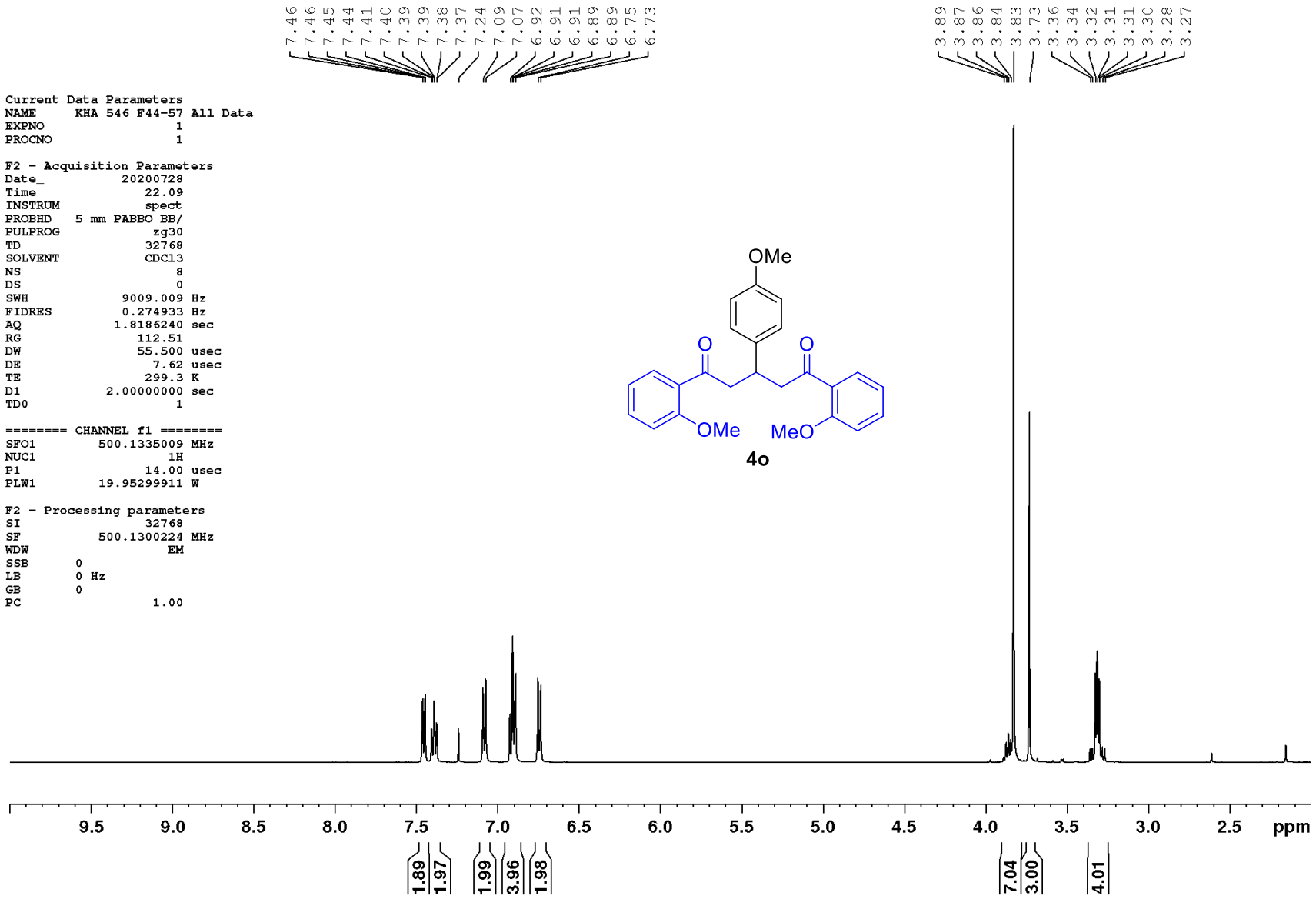
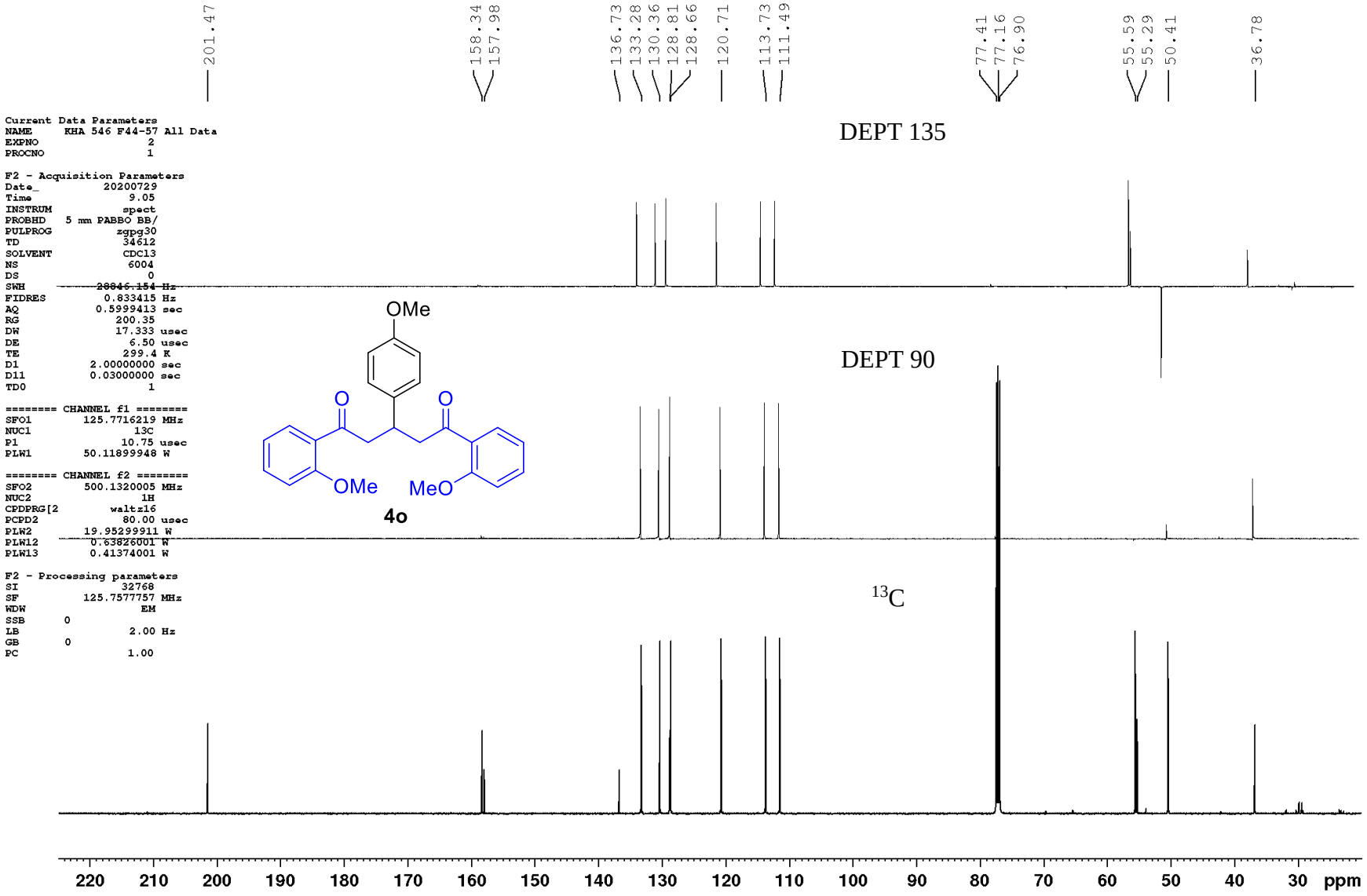


Figure S74. ^{1}H NMR spectrum of compound **4o** (500 MHz, $CDCl_3$, 25 ^{o}C)

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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                299.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        125.7716219 MHz
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
SSB       0
LB                 2.00 Hz
GB        0
PC                 1.00
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Figure S75. ^{13}C NMR spectrum of compound **4o** (125 MHz, $CDCl_3$, 25 ^oC)

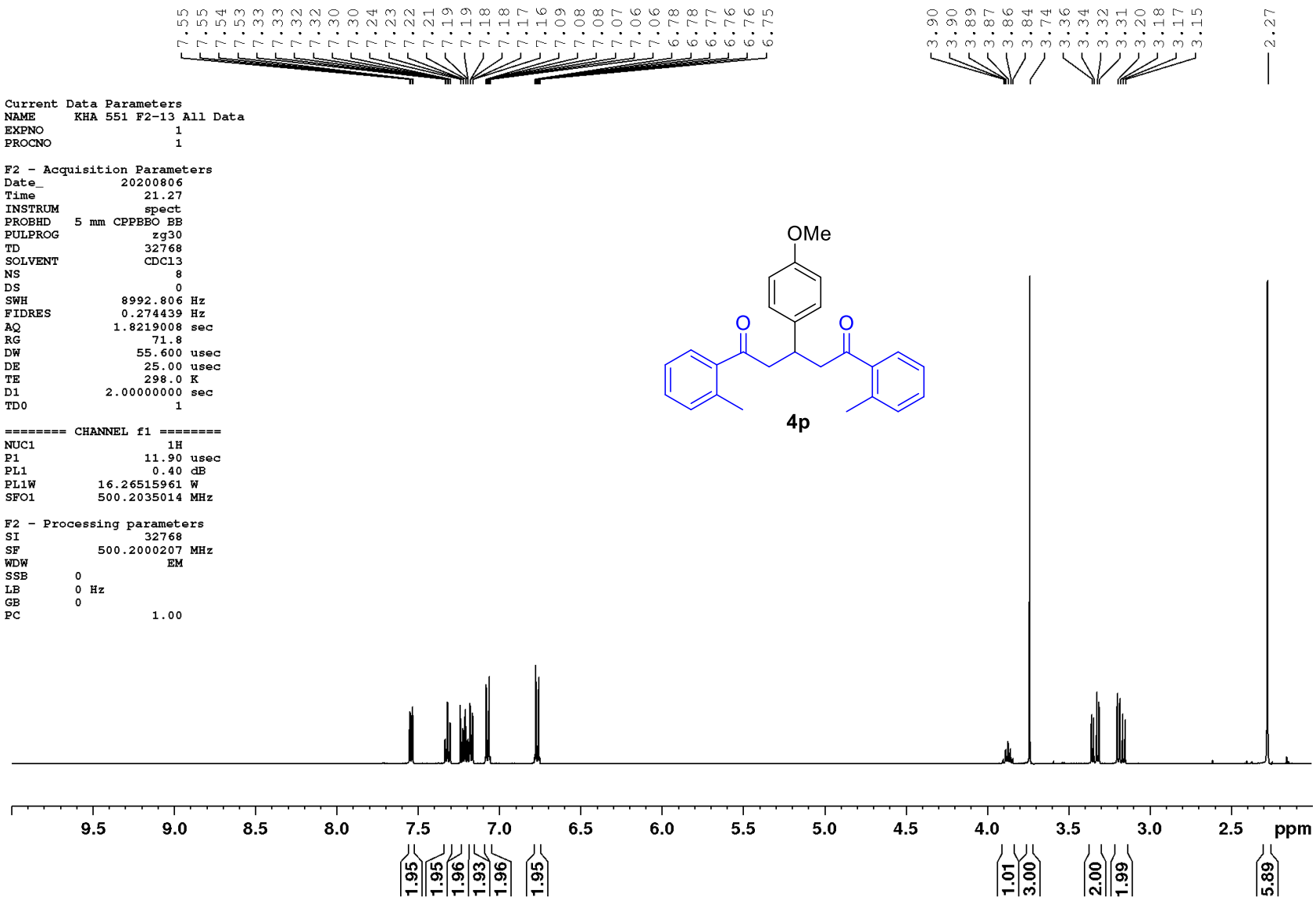


Figure S76. ^{1}H NMR spectrum of compound **4p** (500 MHz, $CDCl_3$, 25 ^{o}C)

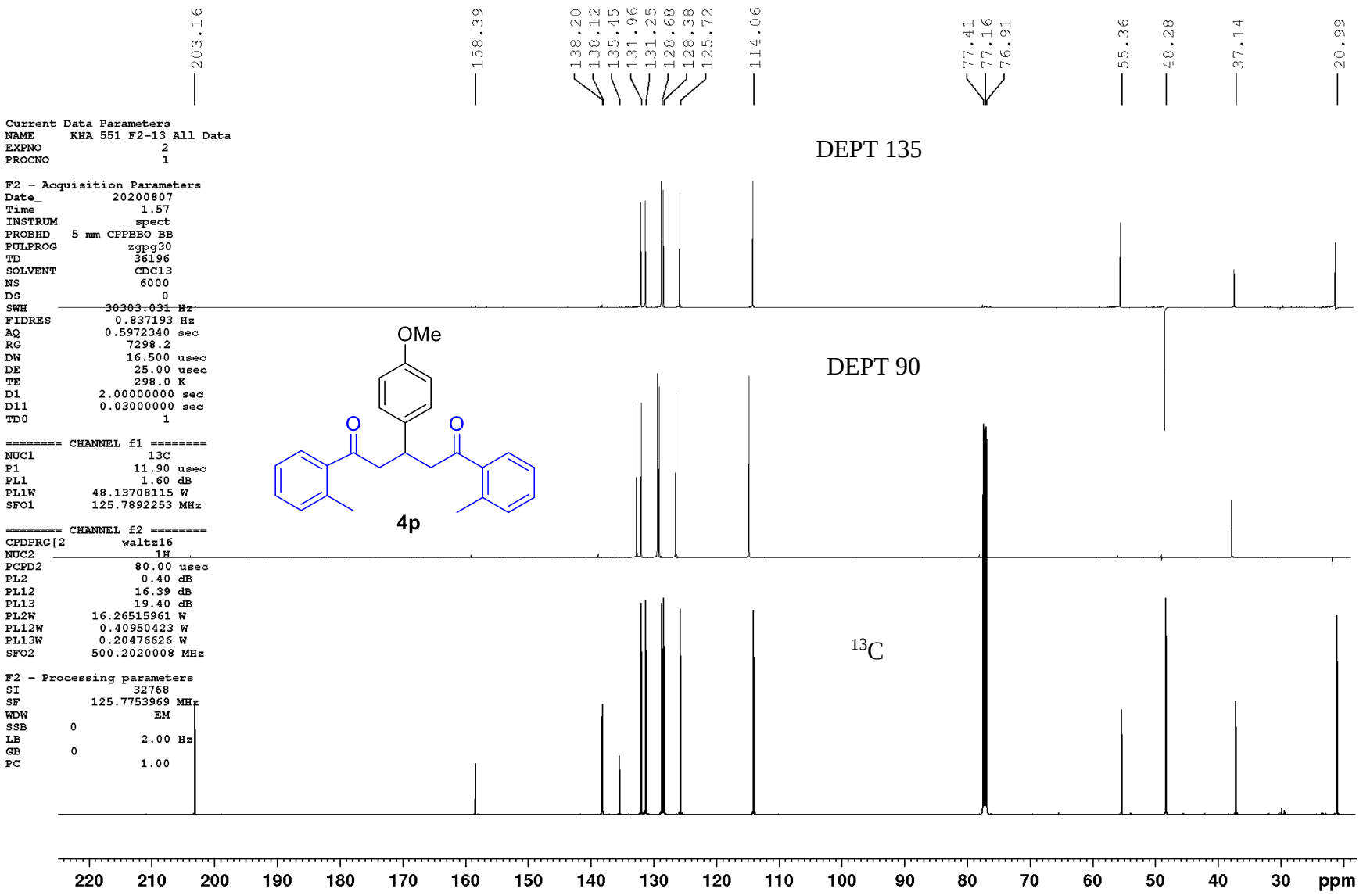


Figure S77. ^{13}C NMR spectrum of compound **4p** (125 MHz, $CDCl_3$, 25 °C)

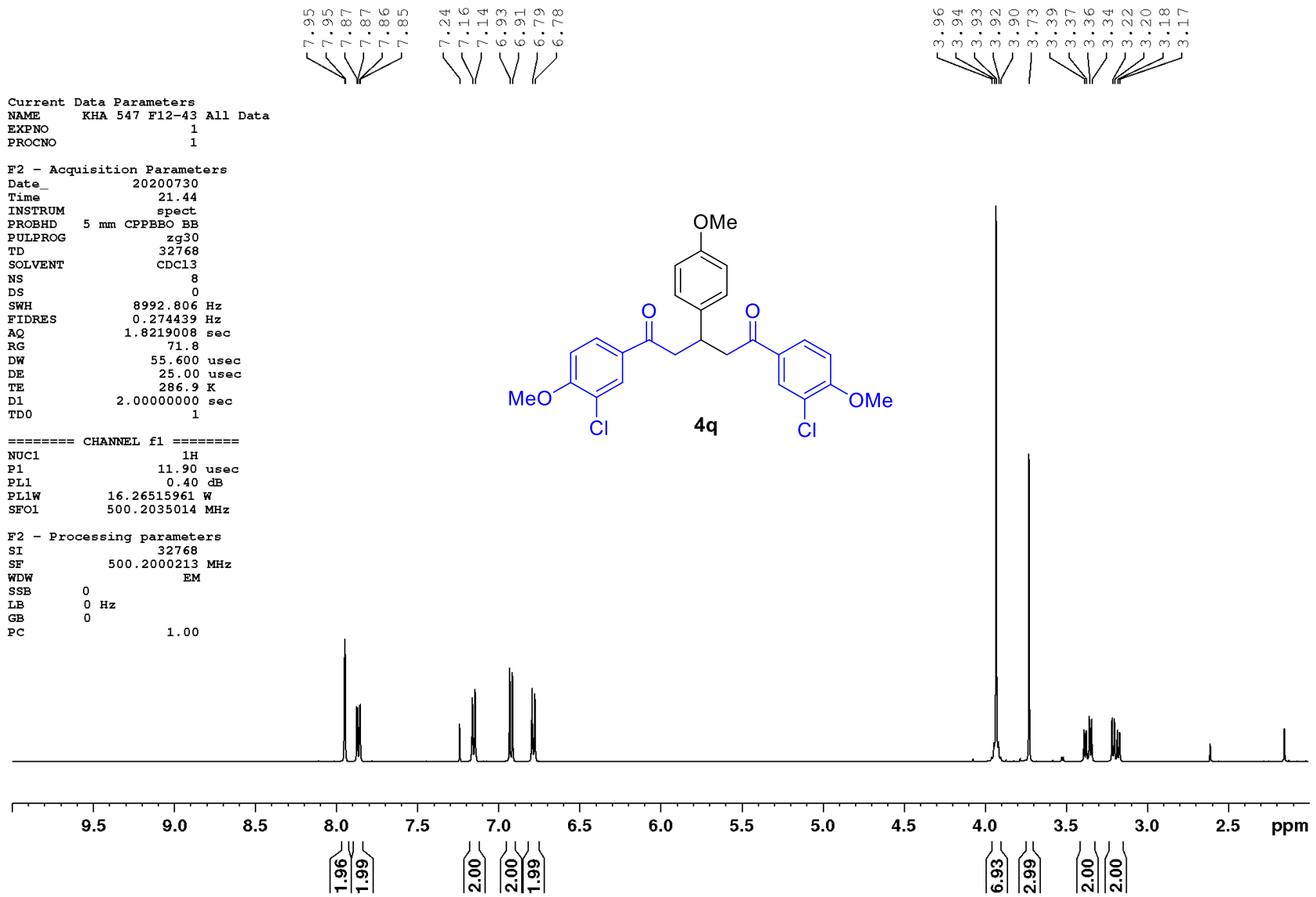


Figure S78. ^{1}H NMR spectrum of compound **4q** (500 MHz, $CDCl_3$, 25 ^{o}C)

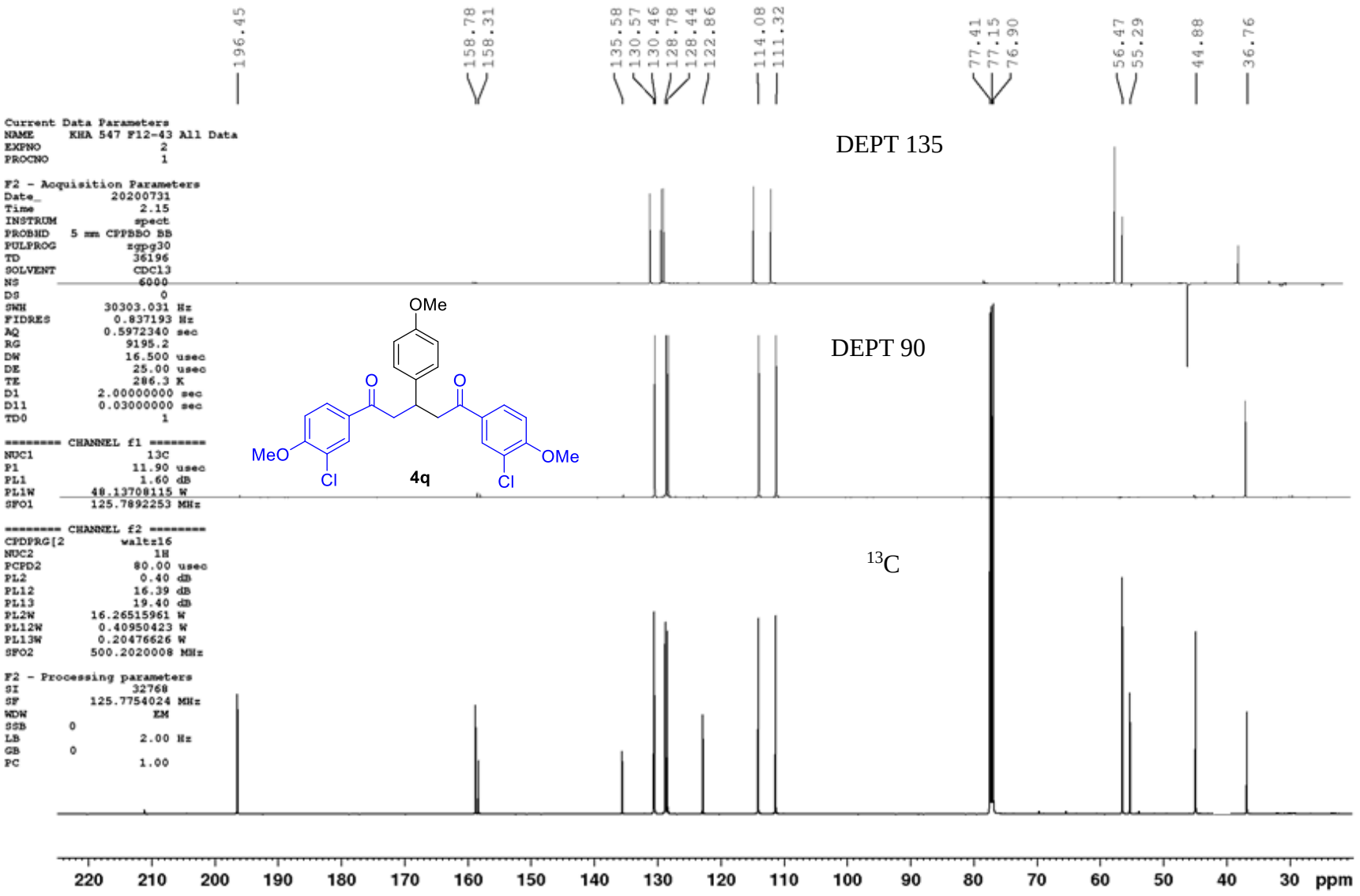


Figure S79. ^{13}C NMR spectrum of compound **4q** (125 MHz, $CDCl_3$, 25 °C)

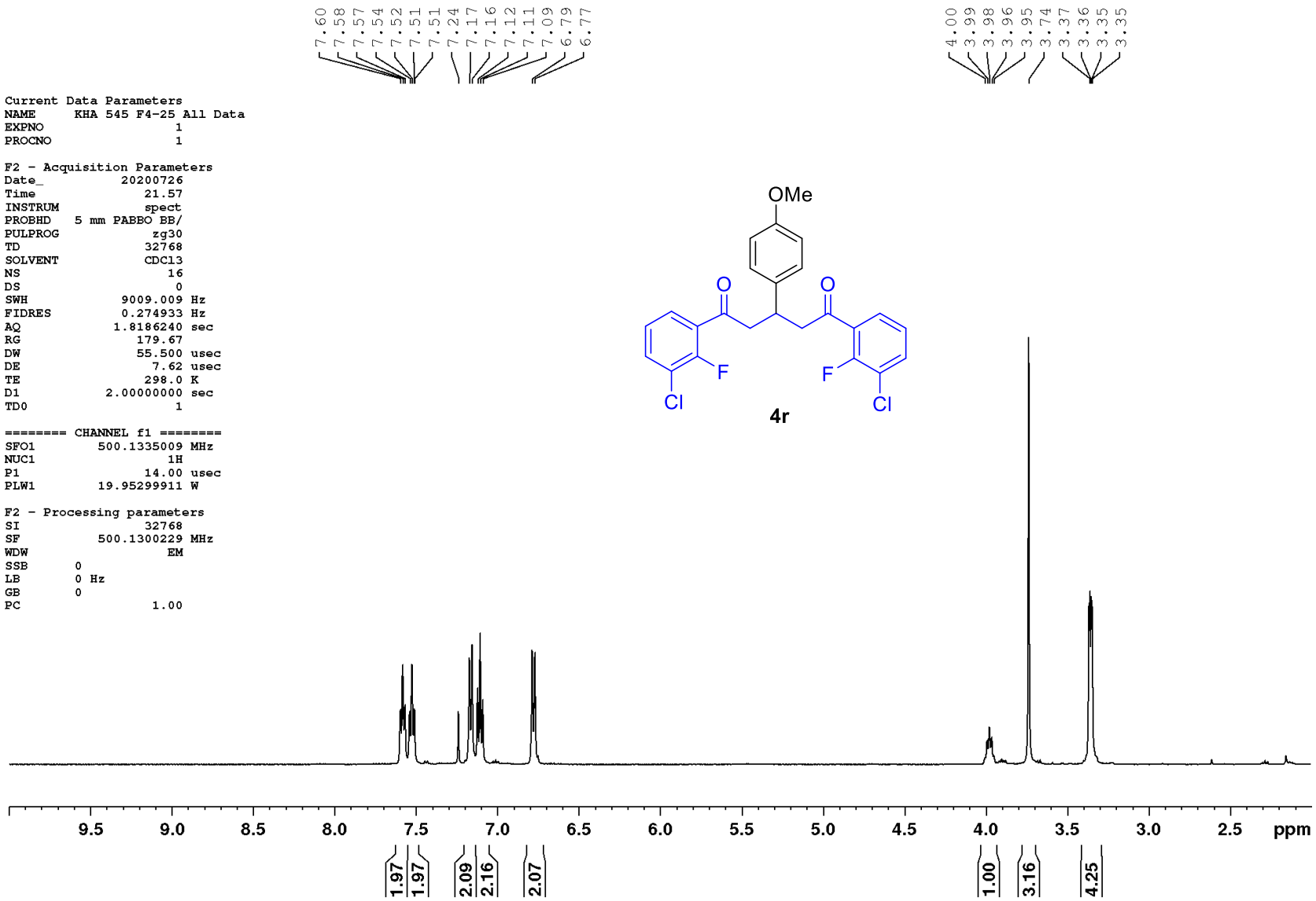


Figure S80. ^{1}H NMR spectrum of compound **4r** (500 MHz, $CDCl_3$, 25 ^{o}C)

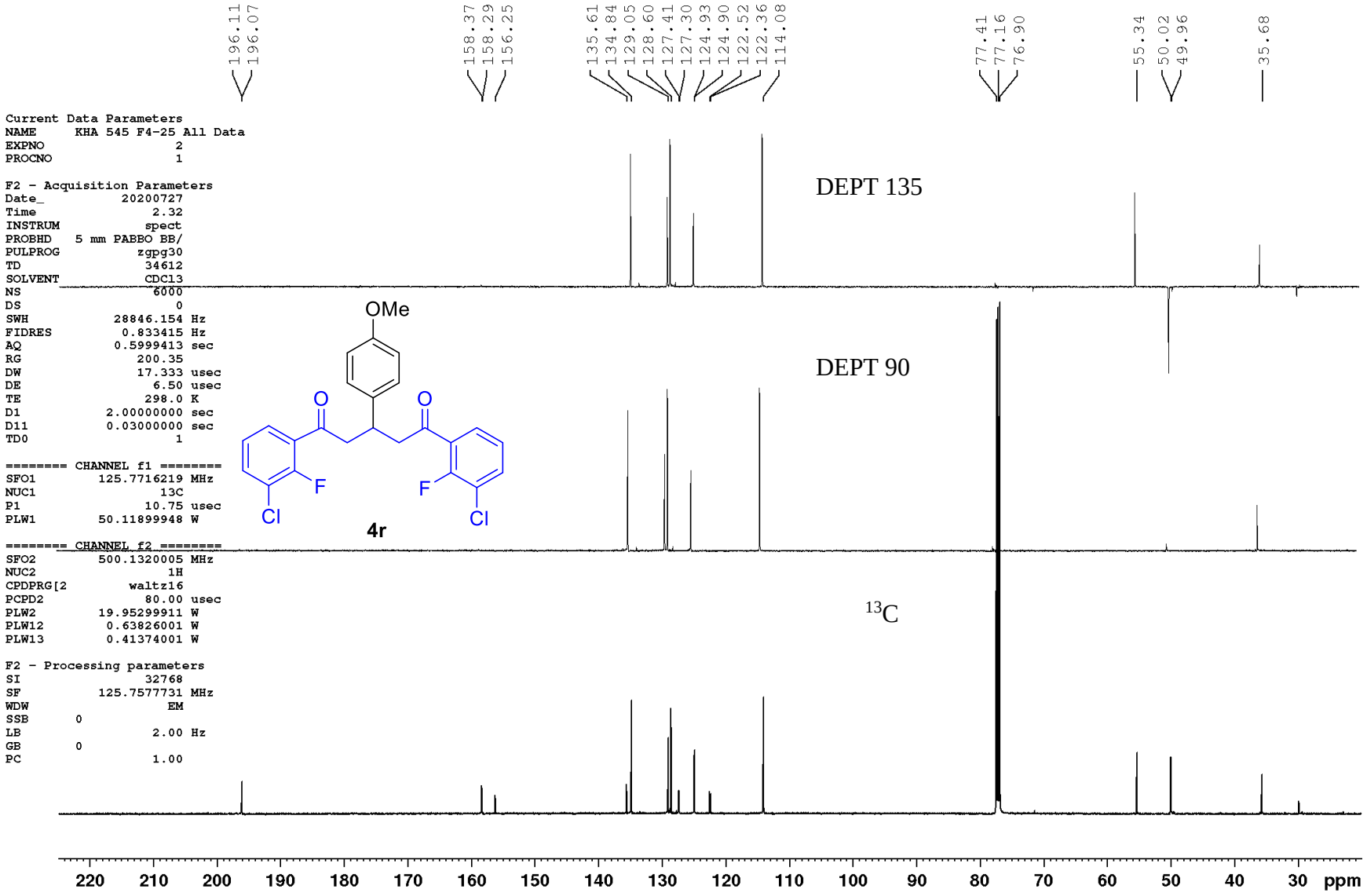


Figure S81. ^{13}C NMR spectrum of compound **4r** (125 MHz, $CDCl_3$, 25 °C)

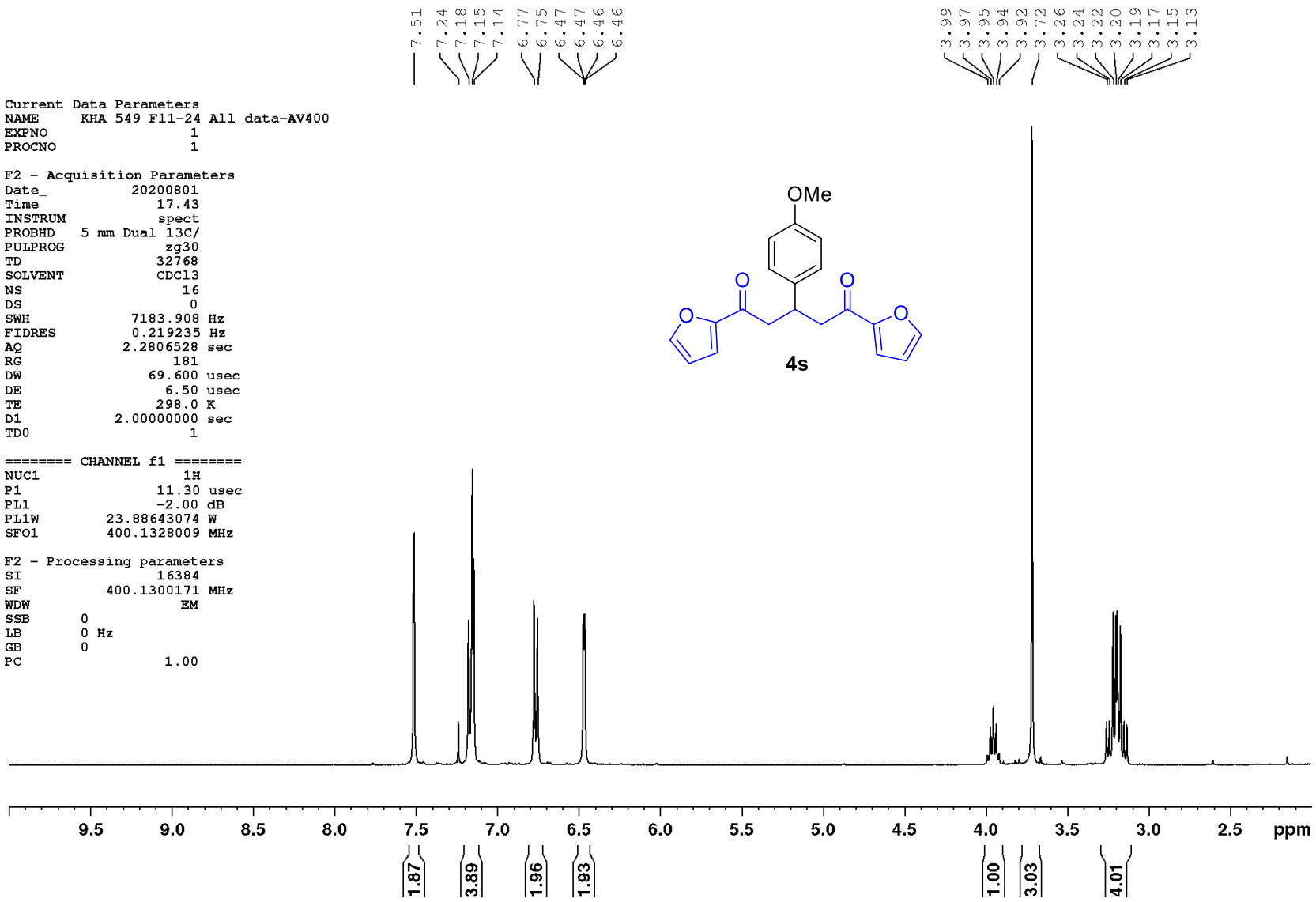
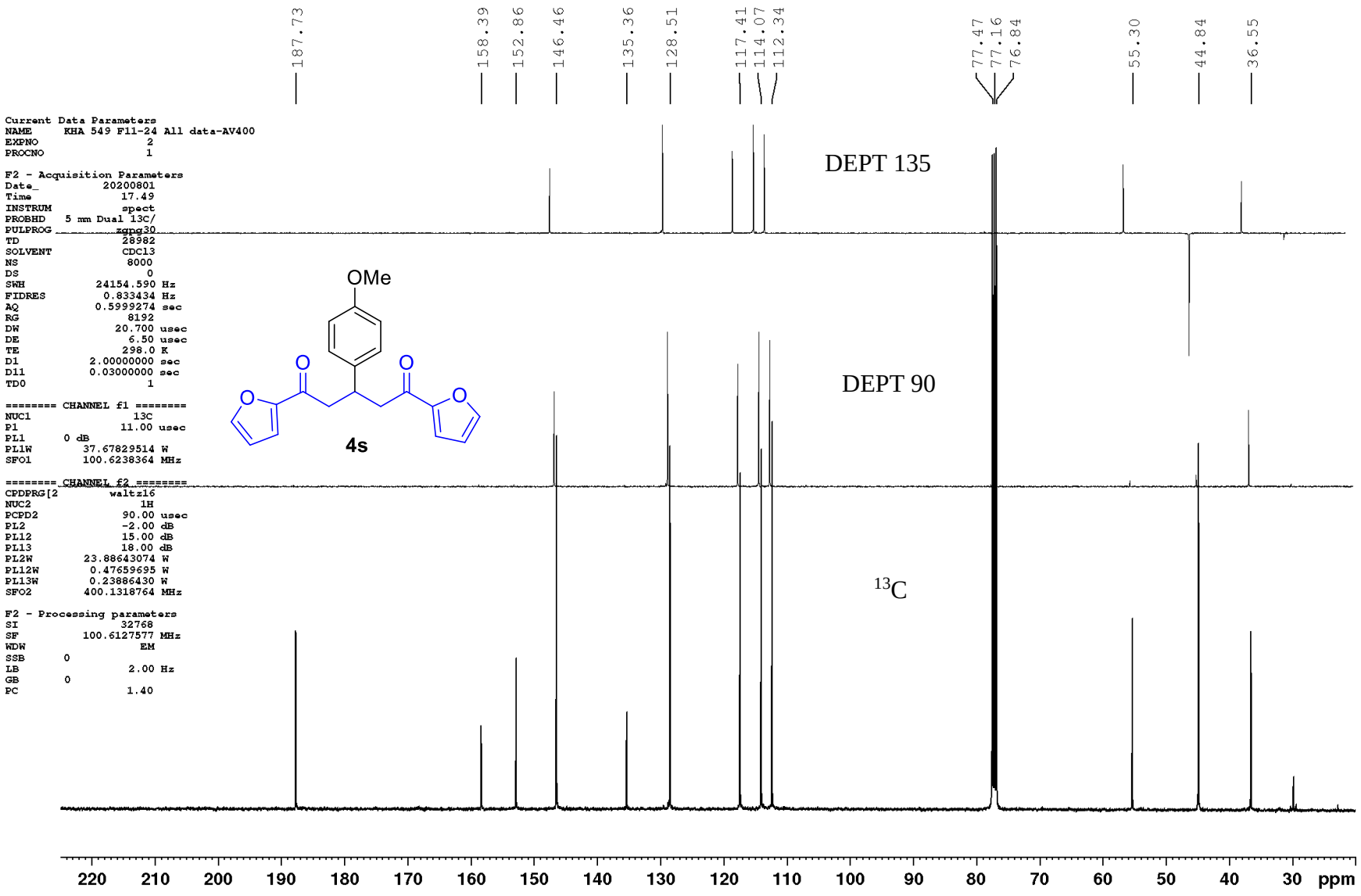


Figure S82. ^{1}H NMR spectrum of compound **4s** (500 MHz, $CDCl_3$, 25 ^{o}C)

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TD                28982
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DS                    0
SWH           24154.590 Hz
FIDRES            0.833434 Hz
AQ            0.5999274 sec
RG                 8192
DW               20.700 usec
DE                6.50 usec
TE                298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                11.00 usec
PL1       0 dB
PL1W        37.67829514 W
SFO1        100.6238364 MHz

======== CHANNEL f2 ========
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PCPD2             90.00 usec
PL2               -2.00 dB
PL12              15.00 dB
PL13              18.00 dB
PL2W        23.88643074 W
PL12W        0.47659695 W
PL13W        0.23886430 W
SFO2        400.1318764 MHz

F2 - Processing parameters
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WDW                  EM
SSB       0
LB                2.00 Hz
GB        0
PC                1.40
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Figure S83. ^{13}C NMR spectrum of compound **4s** (125 MHz, $CDCl_3$, 25 ^oC)

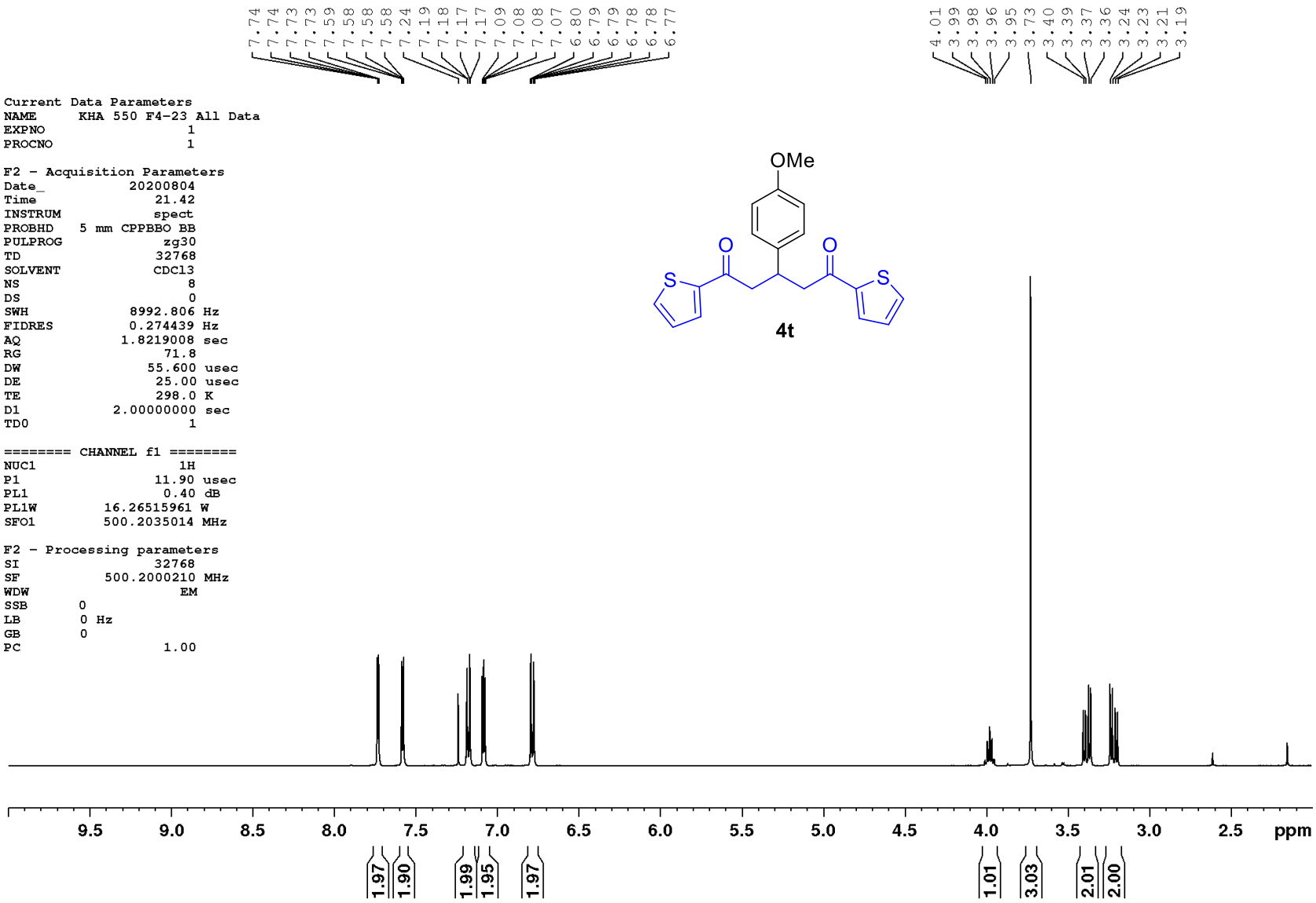

Figure S84. ^{1}H NMR spectrum of compound **4t** (500 MHz, $CDCl_3$, 25 ^{o}C)

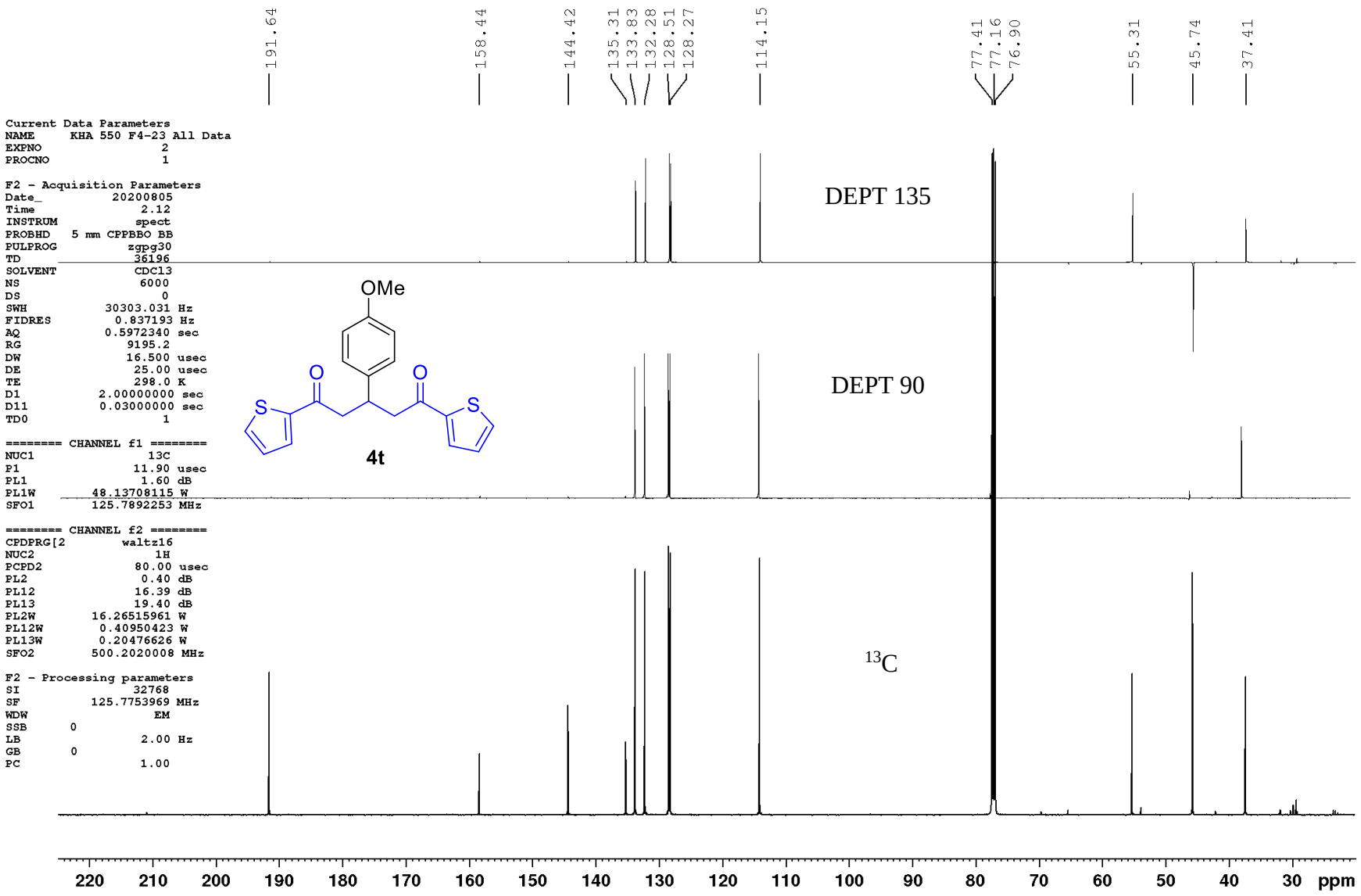

Figure S85. ^{13}C NMR spectrum of compound **4t** (125 MHz, $CDCl_3$, 25 ^oC)

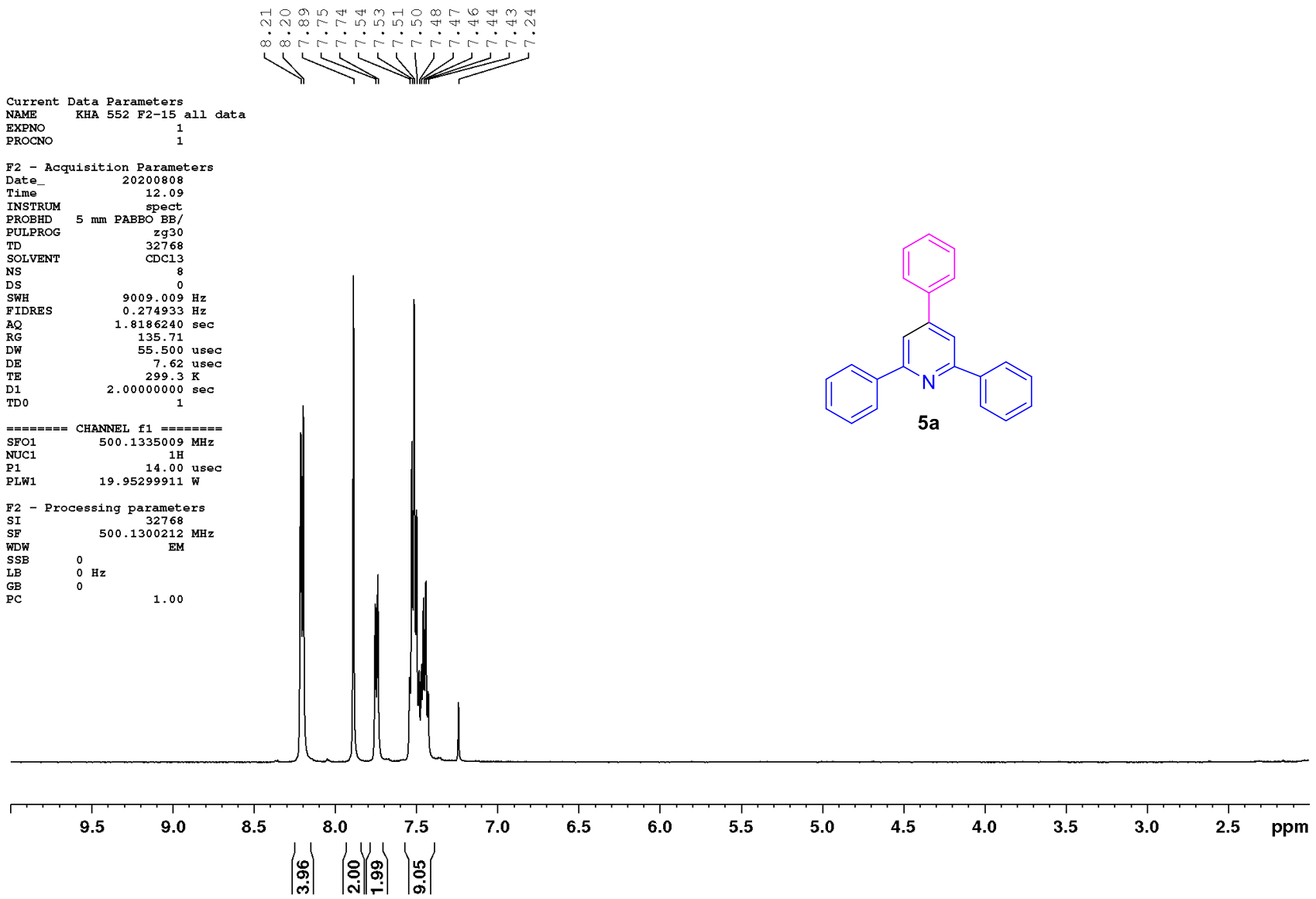

Figure S86. ^{1}H NMR spectrum of compound **5a** (500 MHz, $CDCl_3$, 25 ^{o}C)

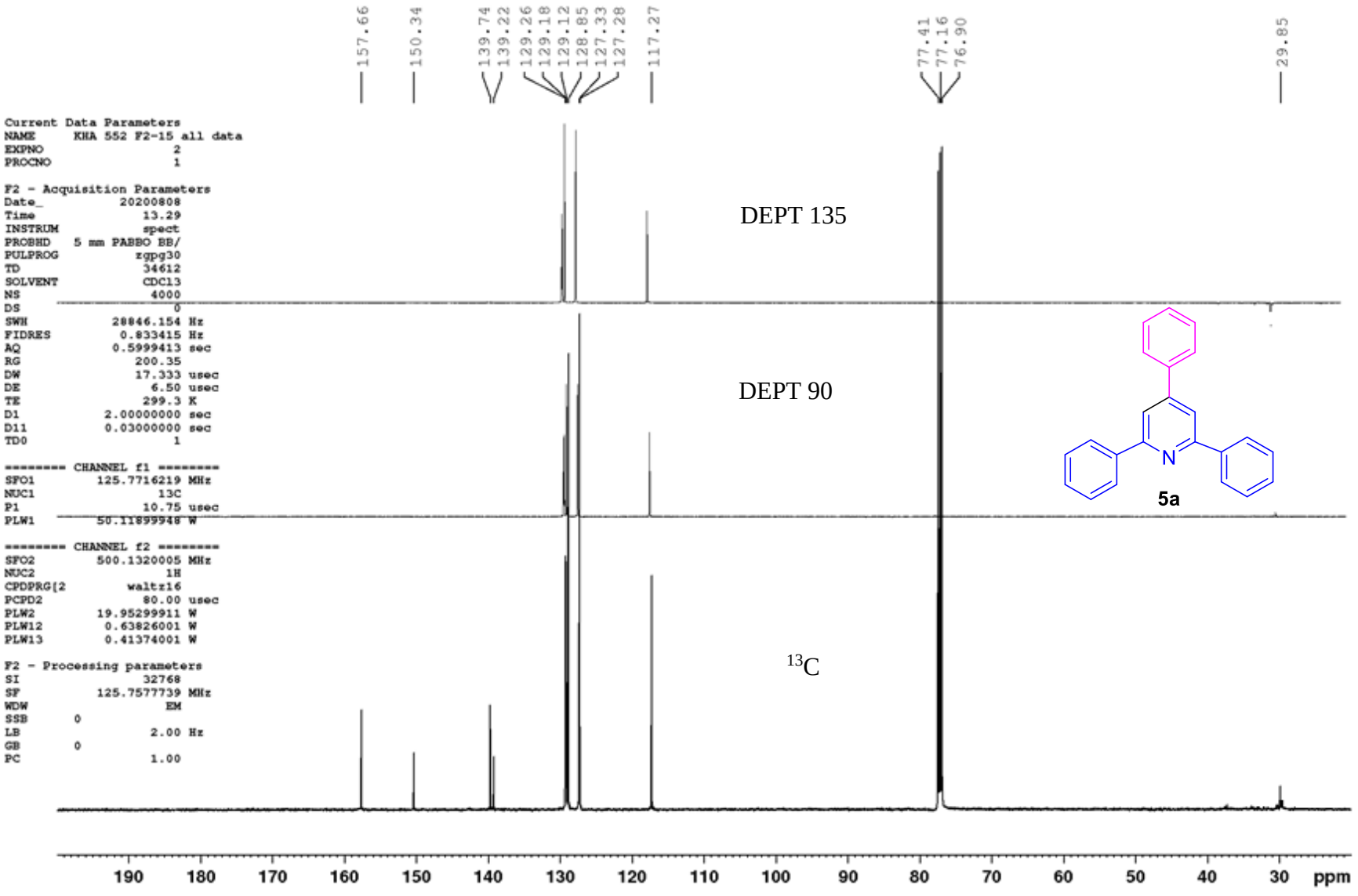

Figure S87. ^{13}C NMR spectrum of compound **5a** (125 MHz, $CDCl_3$, 25 °C)

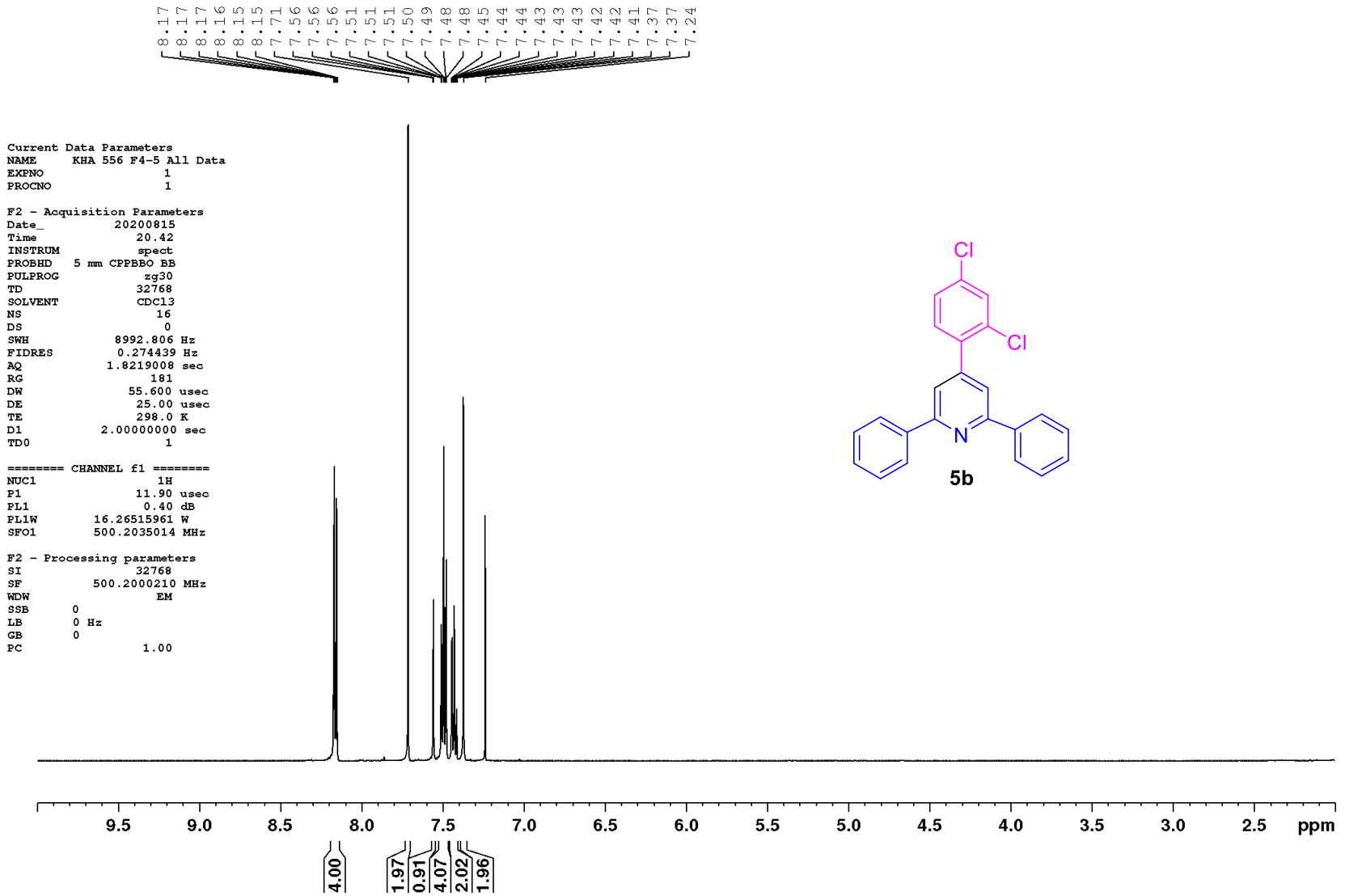

Figure S88. ^{1}H NMR spectrum of compound **5b** (500 MHz, $CDCl_3$, 25 ^{o}C)

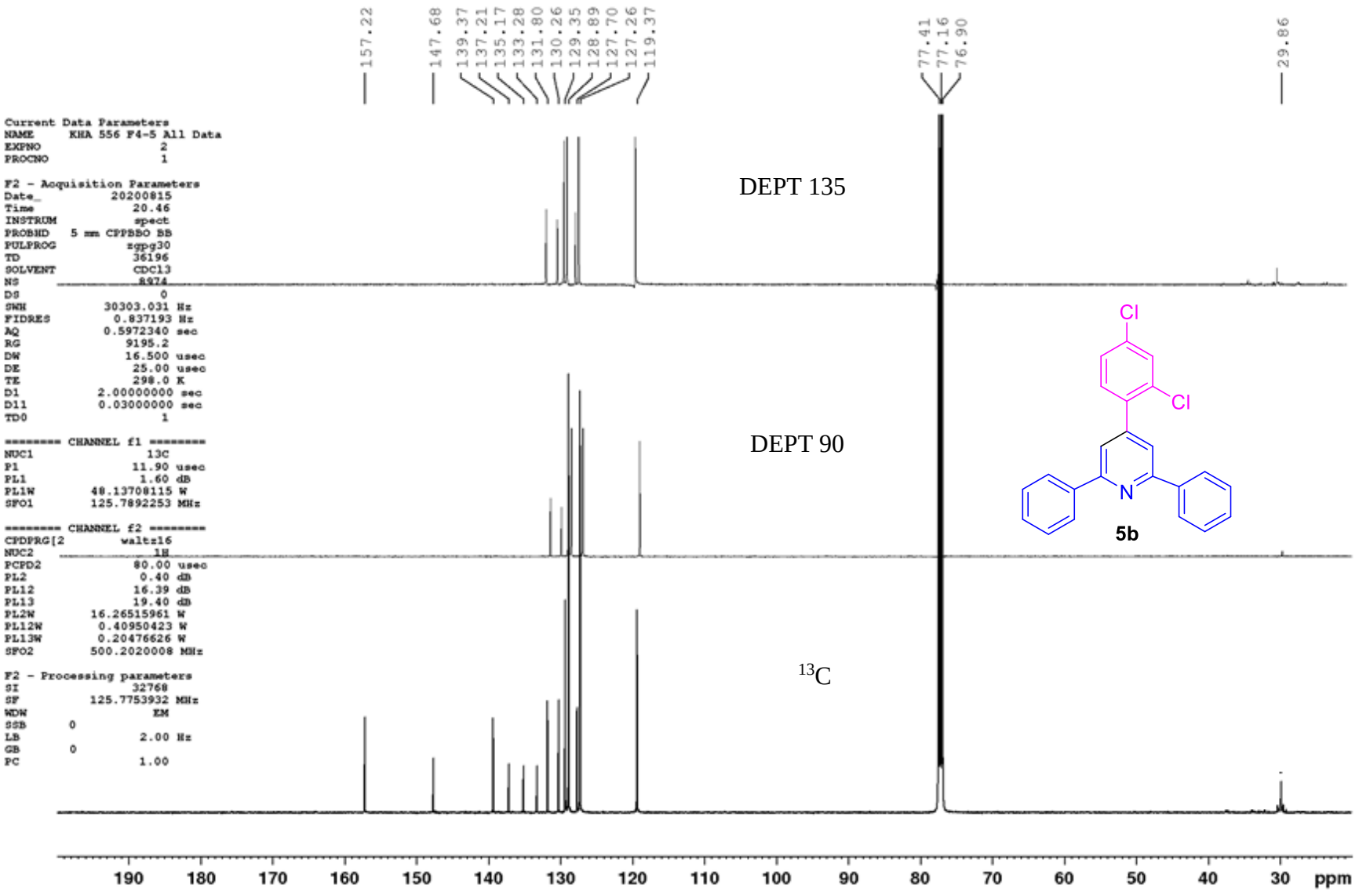

Figure S89. ^{13}C NMR spectrum of compound **5b** (125 MHz, $CDCl_3$, 25 °C)

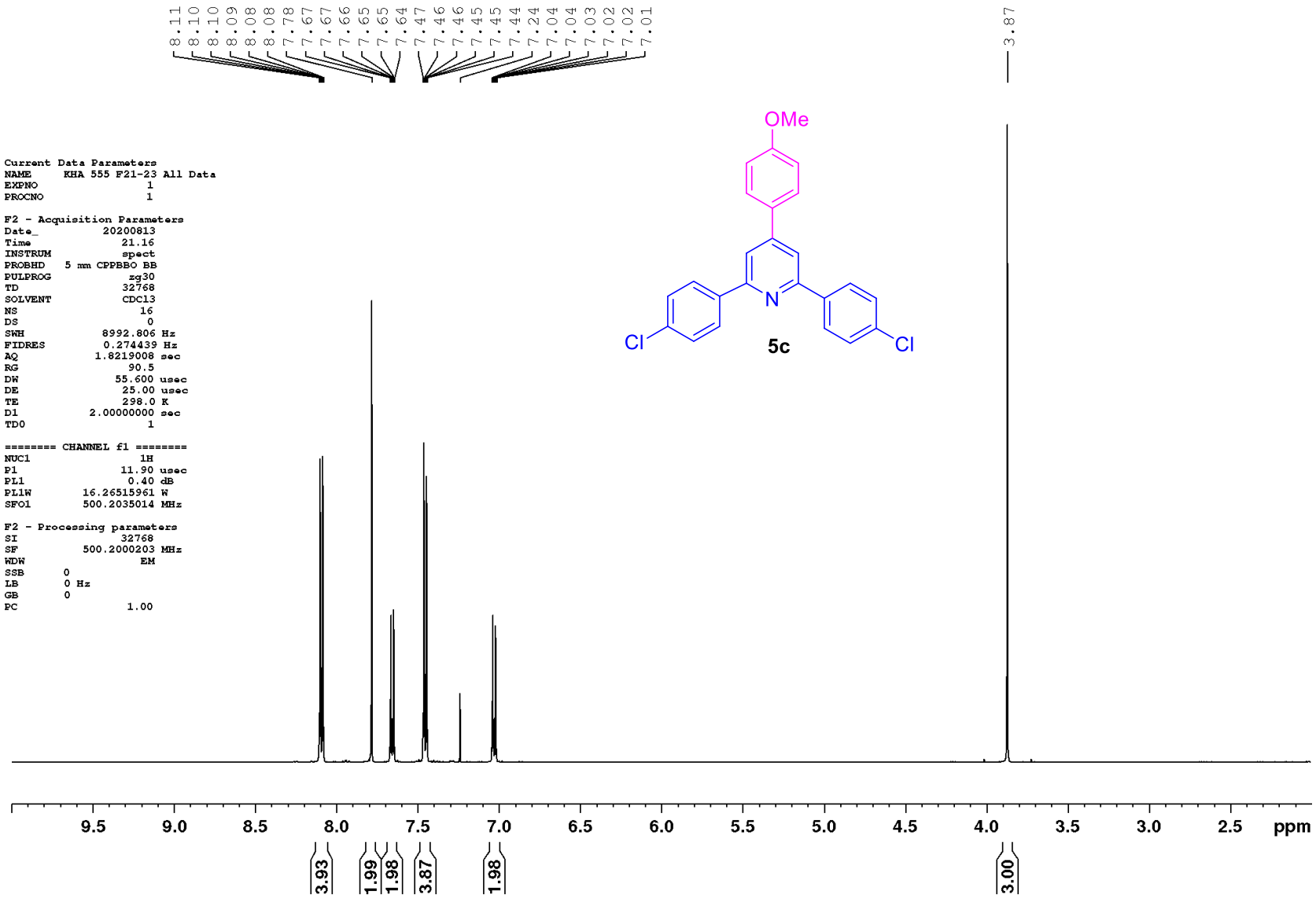

Figure S90. ^{1}H NMR spectrum of compound **5c** (500 MHz, $CDCl_3$, 25 ^{o}C)

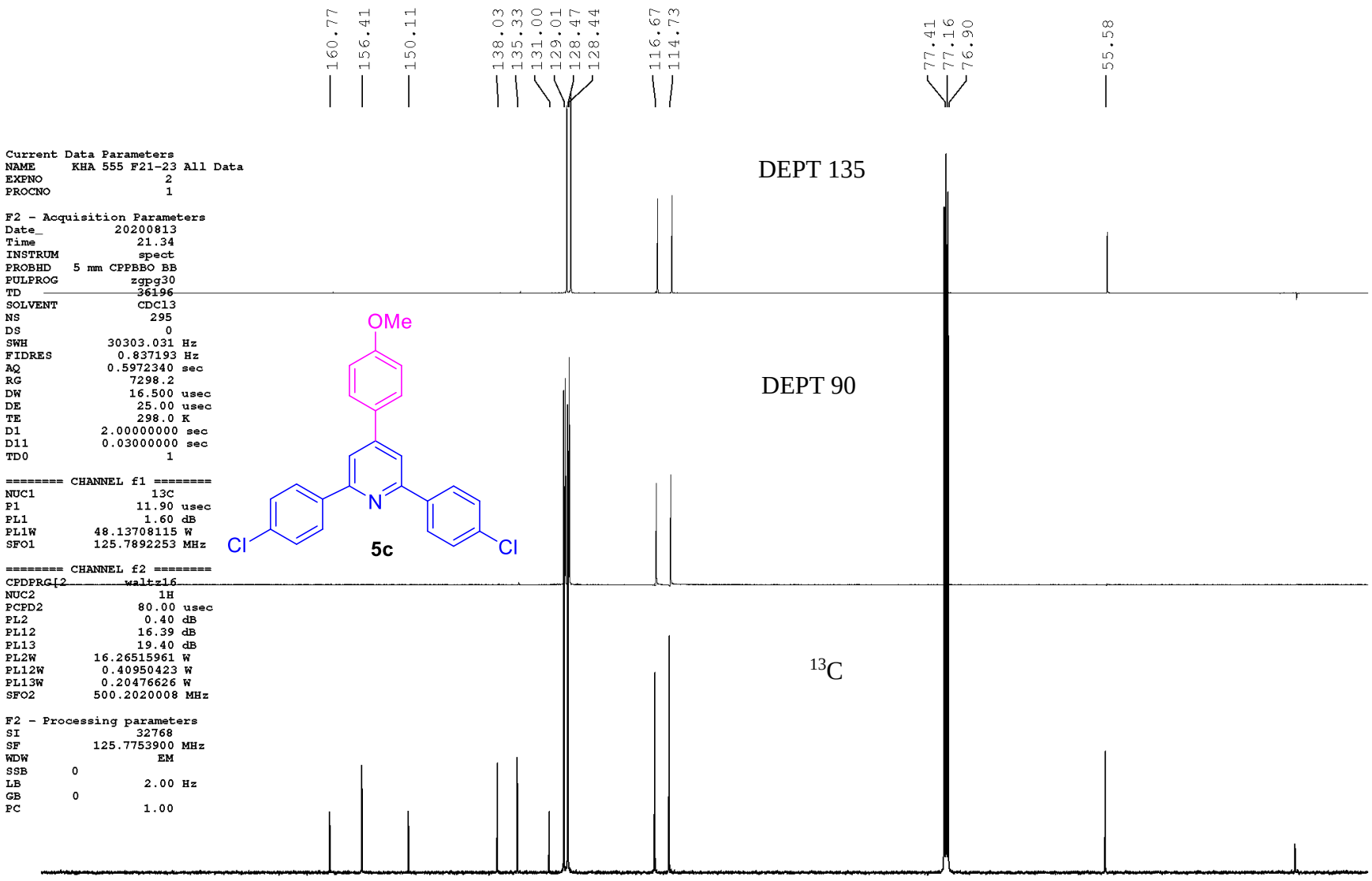

Figure S91. ^{13}C NMR spectrum of compound **5c** (125 MHz, $CDCl_3$, 25 ^oC)

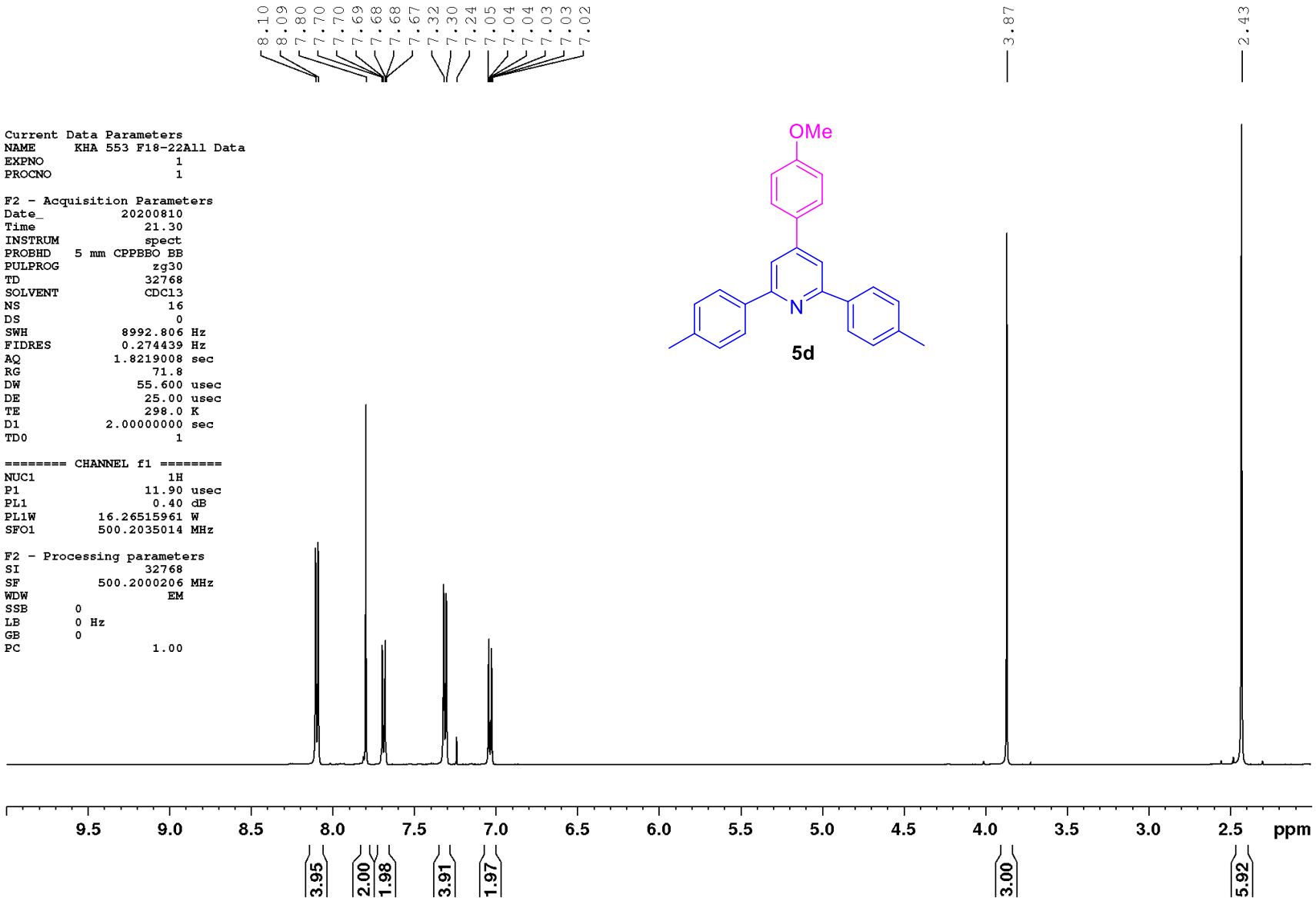

Figure S92. ^{1}H NMR spectrum of compound **5d** (500 MHz, $CDCl_3$, 25 ^{o}C)

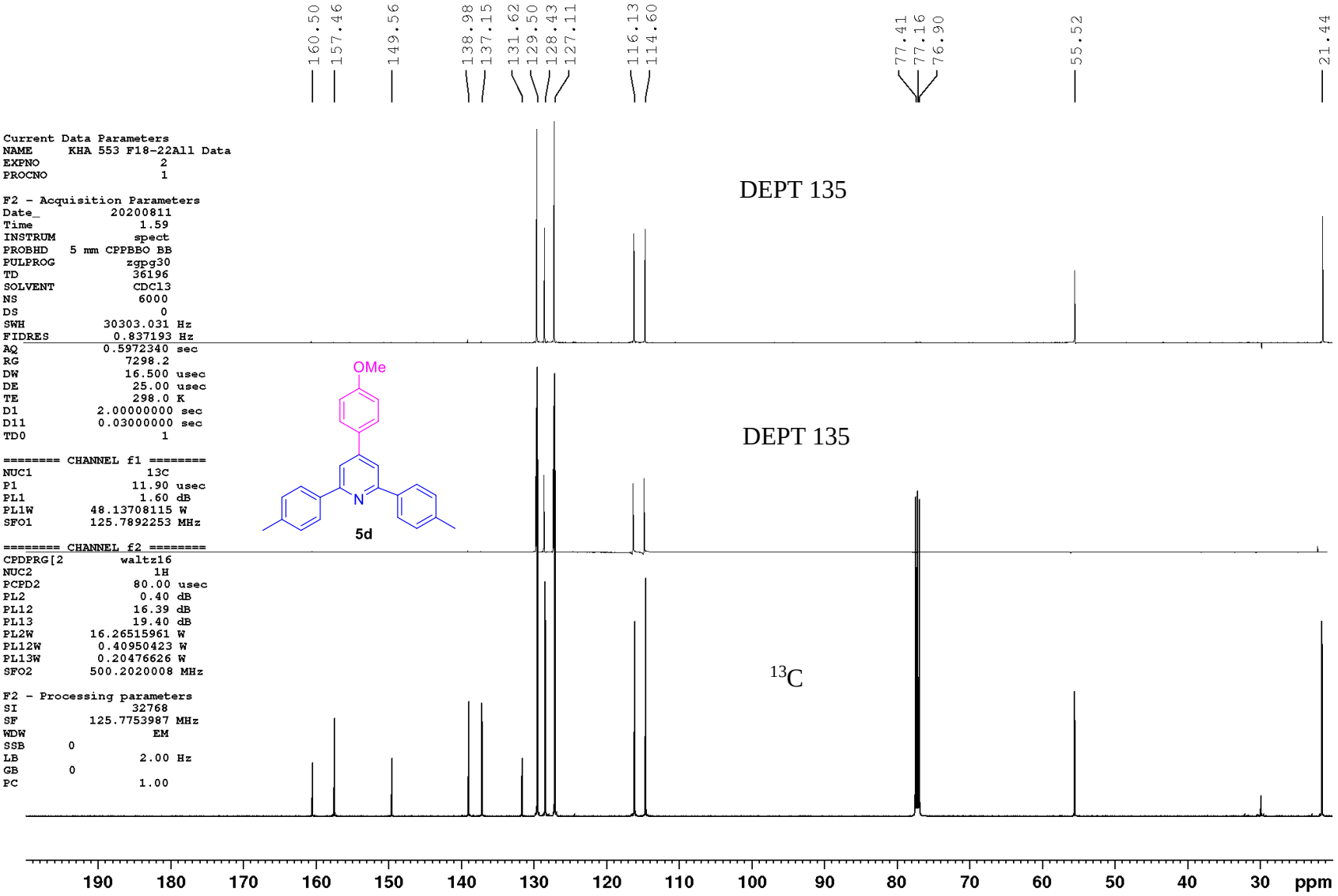

Figure S93. ^{13}C NMR spectrum of compound **5d** (125 MHz, $CDCl_3$, 25 °C)

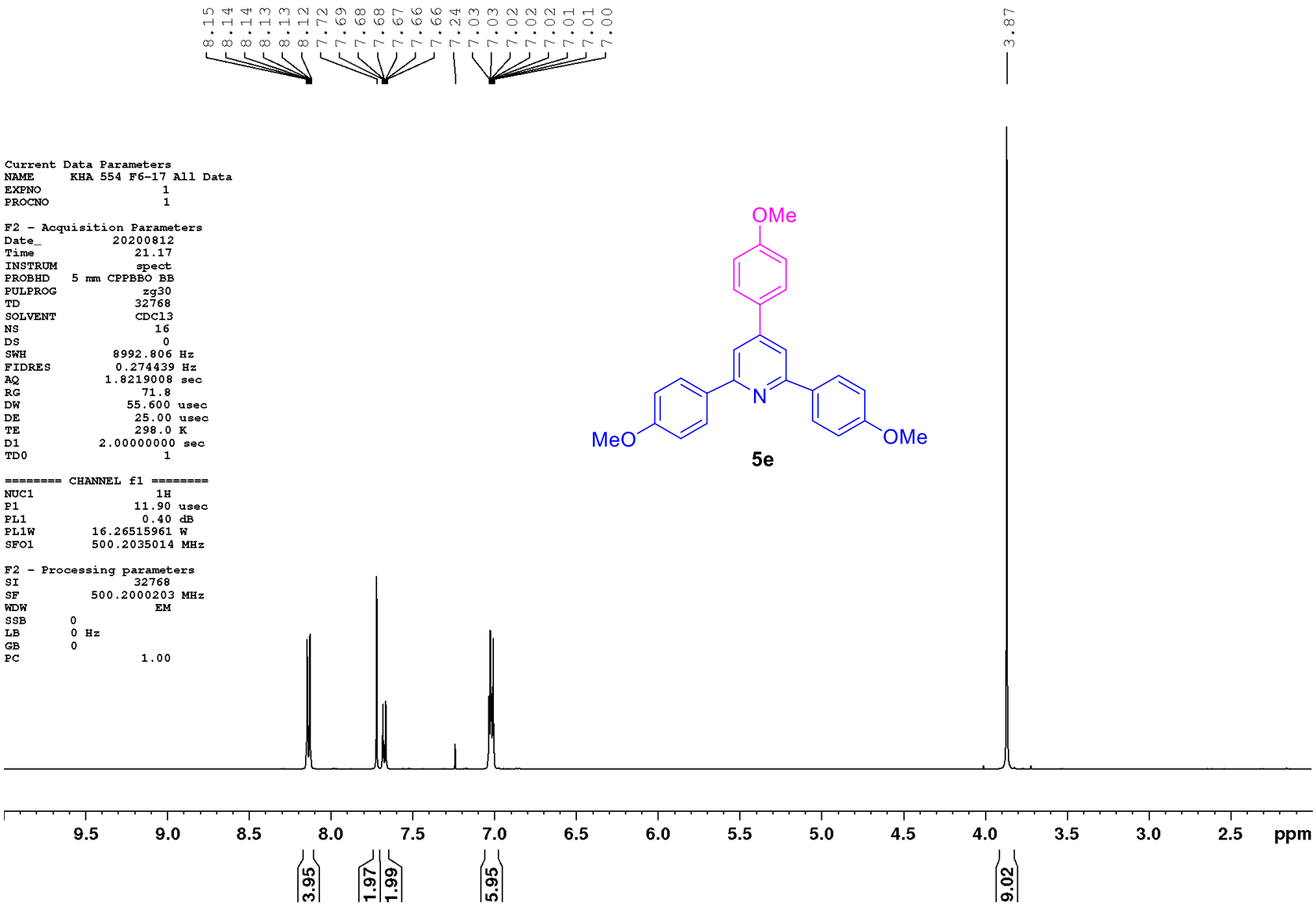

Figure S94. ^{1}H NMR spectrum of compound **5e** (500 MHz, $CDCl_3$, 25 ^{o}C)

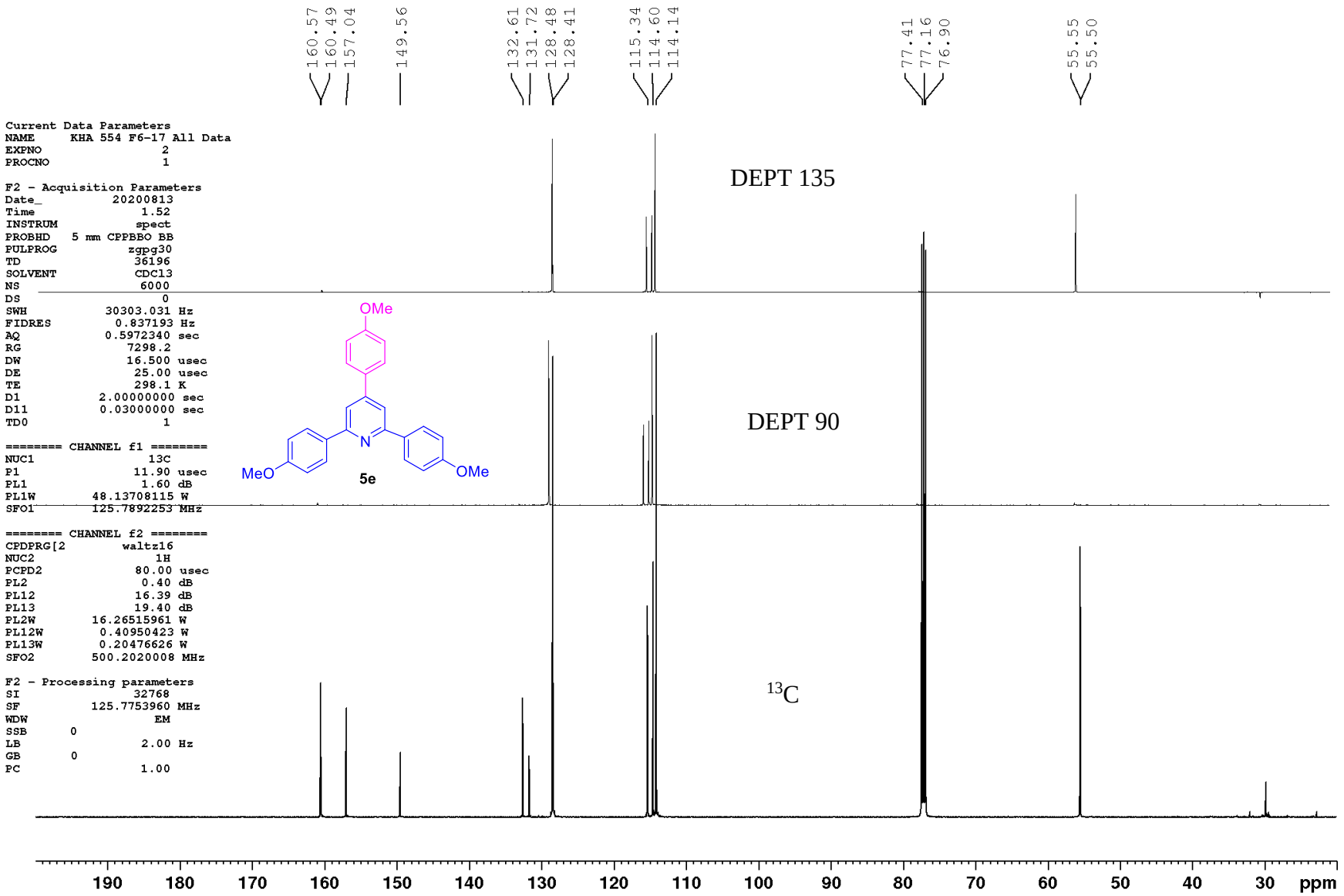

Figure S95. ^{13}C NMR spectrum of compound **5e** (125 MHz, $CDCl_3$, 25 °C)