Supplementary Information (SI) for Organic & Biomolecular Chemistry.
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Supporting Information

Synthesis of Alkynyl Cyclopropa[*c*]coumarins via Propargyl Sulfonium Salts as C1 Synthon

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1. Stereochemical study of 3a and 3a' (Figure S1)

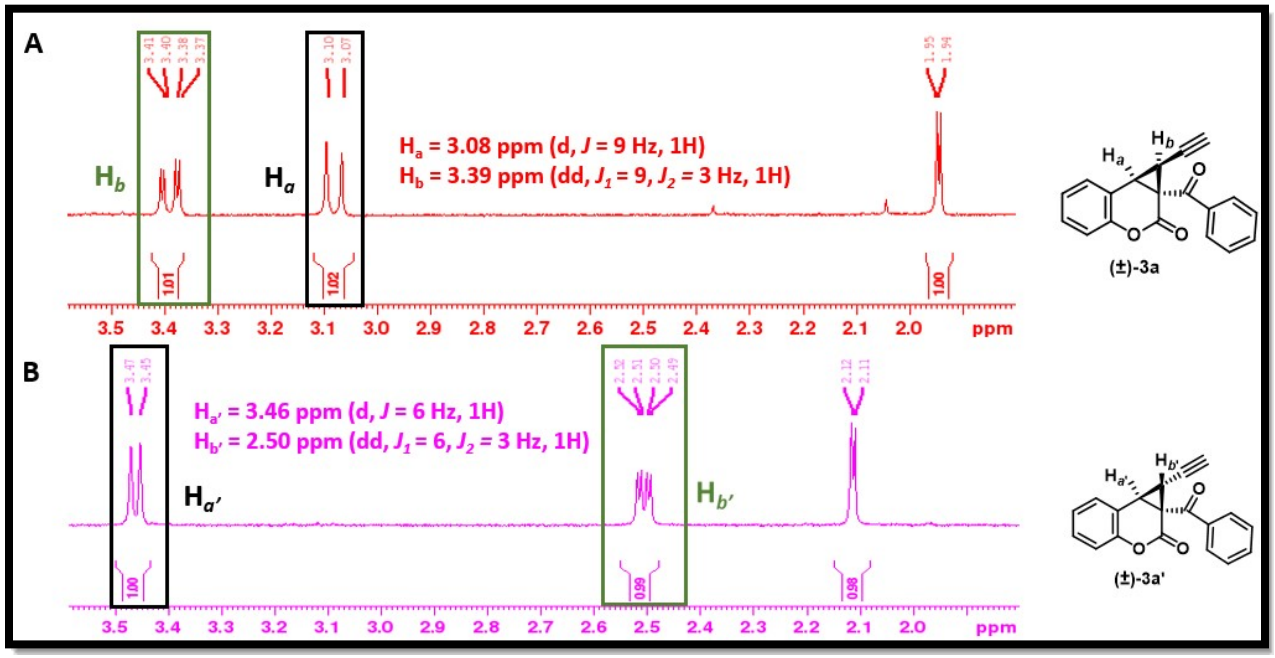


Figure S1. Zoom-in between 1.8 and 3.6 ppm of the ^{1}H NMR spectra of isolated compound **3a** (A) and isolated compound **3a'**(B).

2. Time dependent NMR studies of tetrahydrothiophene sulfonium salts under alkaline condition

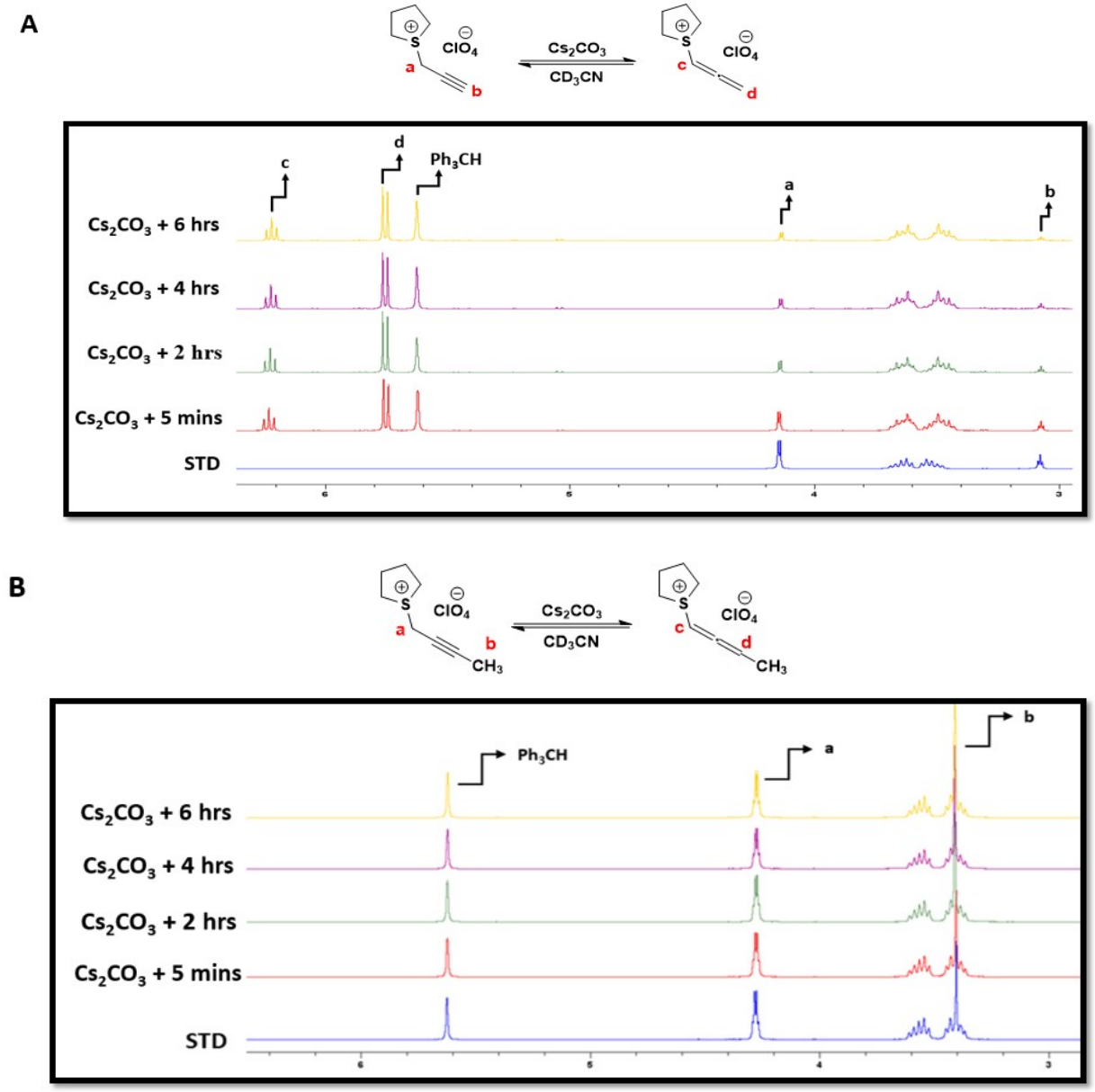


Figure S2. The time-dependent NMR studies were performed over 6 hours, with measurements taken at 2-hour intervals. This observation is made using triphenylmethane (Ph_3CH) as an internal standard and CD_3CN as solvent. A) The figure illustrates that propargyl sulfonium salt **2b**, under alkaline conditions, undergoes isomerization. The ratio of isomerization of allenic sulfonium salt and propargyl sulfonium ylide is 2:1. The STD spectrum represents the initial spectrum of the sulfonium ylide **2b**. B) The figure indicates that sulfonium salt **2c**, under alkaline conditions, does not show characteristic allenic peaks for isomerization. The STD spectrum corresponds to the initial spectrum of the sulfonium ylide **2c**.

3. Stereochemical study of 3l and 3l' (Figure S3)

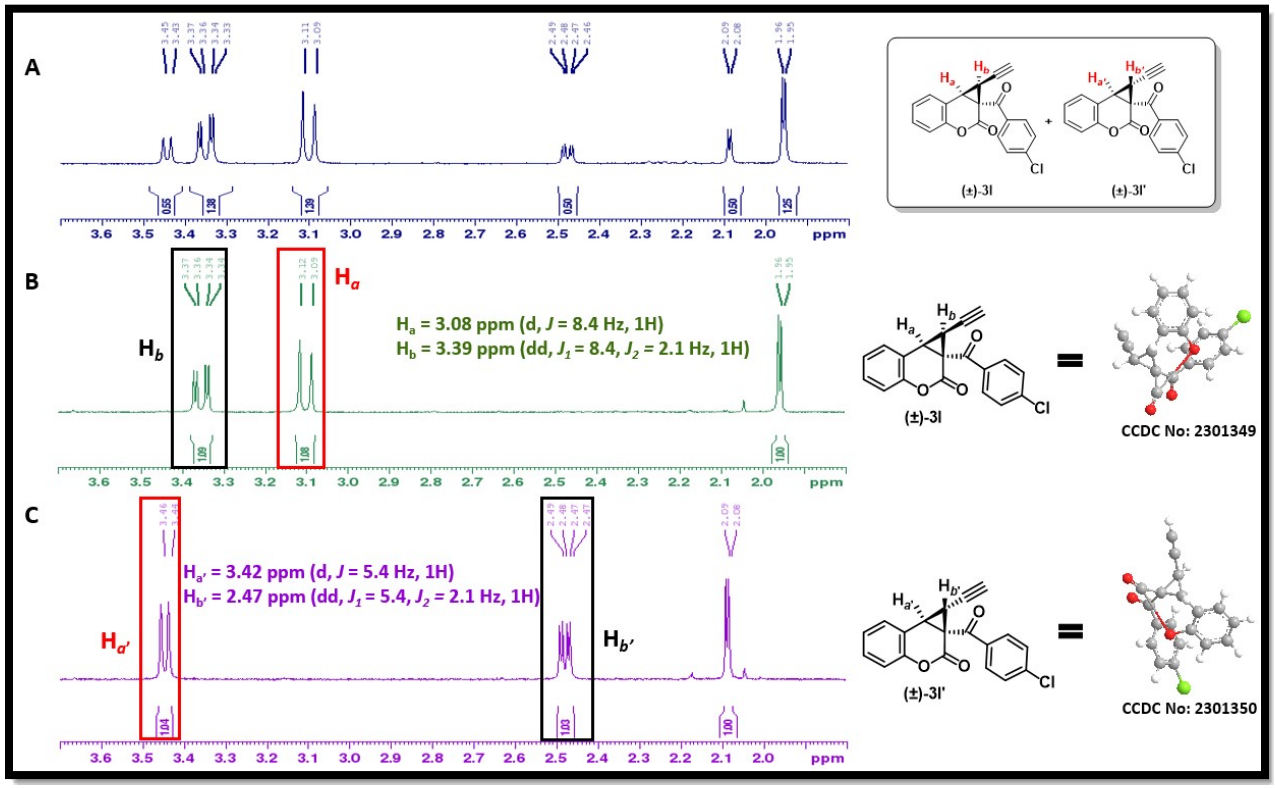
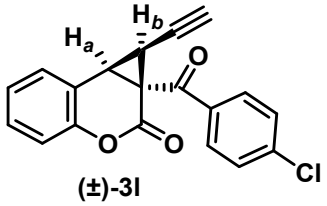


Figure S3. Zoom-in between 1.8 and 3.7 ppm of the ^{1}H NMR spectra of the mixture of **3l** and **3l'** (A), isolated compound **3l** (B), and isolated compound **3l'**(C).

4. X-Ray Crystallography Data of 3l and 3l'



(±)-3l

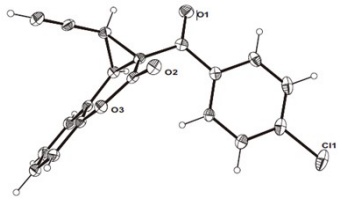


Table 1. Crystal data and structure refinement for d24730.

Identification code	d24730	
Empirical formula	C19 H11 Cl O3	
Formula weight	322.73	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P b c a	
Unit cell dimensions	a = 7.1577(3) Å	α= 90°.
	b = 19.5983(8) Å	β= 90°.
	c = 21.4037(10) Å	γ = 90°.
Volume	3002.5(2) $Å^3$	
Z	8	
Density (calculated)	1.428 Mg/m^3	
Absorption coefficient	2.363 mm^{-1}	
F(000)	1328	
Crystal size	0.72 x 0.55 x 0.09 mm^3	
Theta range for data collection	4.51 to 66.80°.	
Index ranges	-6<=h<=8, -23<=k<=22, -19<=l<=25	
Reflections collected	9534	
Independent reflections	2623 [R(int) = 0.0441]	
Completeness to theta = 66.80°	98.3 %	
Absorption correction	None	
Max. and min. transmission	0.8155 and 0.2810	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2623 / 0 / 208	
Goodness-of-fit on F^2	1.047	
Final R indices [I>2sigma(I)]	R1 = 0.0535, wR2 = 0.1451	

R indices (all data)	R1 = 0.0575, wR2 = 0.1492
Largest diff. peak and hole	0.592 and -0.696 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for d24730. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	8743(4)	6274(1)	6401(1)	50(1)
C(2)	8523(3)	6075(1)	5789(1)	44(1)
C(3)	6863(3)	6227(1)	5488(1)	36(1)
C(4)	5431(3)	6579(1)	5795(1)	36(1)
C(5)	5712(4)	6787(1)	6412(1)	47(1)
C(6)	7362(4)	6634(1)	6715(1)	54(1)
C(7)	3654(3)	6758(1)	5481(1)	38(1)
C(8)	3207(3)	6423(1)	4865(1)	33(1)
C(9)	3220(3)	5663(1)	4854(1)	33(1)
C(10)	4284(3)	5683(1)	3782(1)	36(1)
C(11)	4854(3)	5266(1)	3296(1)	47(1)
C(12)	5570(3)	5564(2)	2764(1)	55(1)
C(13)	5735(3)	6267(2)	2721(1)	55(1)
C(14)	5161(3)	6673(1)	3212(1)	46(1)
C(15)	4393(3)	6385(1)	3749(1)	36(1)
C(16)	3695(3)	6804(1)	4271(1)	36(1)
C(17)	1675(3)	6752(1)	4472(1)	37(1)
C(18)	361(3)	6324(1)	4148(1)	41(1)
C(19)	-700(3)	5953(2)	3898(1)	56(1)
Cl(1)	10788(1)	6057(1)	6793(1)	77(1)
O(1)	2617(3)	7192(1)	5694(1)	55(1)
O(2)	2819(2)	5324(1)	5299(1)	43(1)
O(3)	3617(2)	5342(1)	4311(1)	38(1)

Table 3. Bond lengths [Å] and angles [°] for d24730.

C(1)-C(2)	1.375(3)
C(1)-C(6)	1.390(4)
C(1)-Cl(1)	1.741(3)
C(2)-C(3)	1.384(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.398(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.397(3)
C(4)-C(7)	1.481(3)
C(5)-C(6)	1.380(4)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-O(1)	1.217(3)
C(7)-C(8)	1.506(3)
C(8)-C(9)	1.490(3)
C(8)-C(16)	1.517(3)
C(8)-C(17)	1.526(3)
C(9)-O(2)	1.197(3)
C(9)-O(3)	1.351(2)
C(10)-C(15)	1.380(3)
C(10)-C(11)	1.384(3)
C(10)-O(3)	1.397(3)
C(11)-C(12)	1.380(4)
C(11)-H(11)	0.9500
C(12)-C(13)	1.385(4)
C(12)-H(12)	0.9500
C(13)-C(14)	1.382(4)
C(13)-H(13)	0.9500
C(14)-C(15)	1.393(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.474(3)
C(16)-C(17)	1.512(3)
C(16)-H(16)	1.0000
C(17)-C(18)	1.437(3)

C(17)-H(17)	1.0000
C(18)-C(19)	1.180(4)
C(19)-H(19)	0.9500

C(2)-C(1)-C(6)	121.6(2)
C(2)-C(1)-Cl(1)	119.1(2)
C(6)-C(1)-Cl(1)	119.26(19)
C(1)-C(2)-C(3)	118.7(2)
C(1)-C(2)-H(2)	120.6
C(3)-C(2)-H(2)	120.6
C(2)-C(3)-C(4)	121.1(2)
C(2)-C(3)-H(3)	119.5
C(4)-C(3)-H(3)	119.5
C(5)-C(4)-C(3)	118.9(2)
C(5)-C(4)-C(7)	118.9(2)
C(3)-C(4)-C(7)	122.23(19)
C(6)-C(5)-C(4)	120.3(2)
C(6)-C(5)-H(5)	119.8
C(4)-C(5)-H(5)	119.8
C(5)-C(6)-C(1)	119.4(2)
C(5)-C(6)-H(6)	120.3
C(1)-C(6)-H(6)	120.3
O(1)-C(7)-C(4)	121.3(2)
O(1)-C(7)-C(8)	120.2(2)
C(4)-C(7)-C(8)	118.37(18)
C(9)-C(8)-C(7)	116.73(16)
C(9)-C(8)-C(16)	118.48(17)
C(7)-C(8)-C(16)	118.03(16)
C(9)-C(8)-C(17)	114.67(16)
C(7)-C(8)-C(17)	116.83(17)
C(16)-C(8)-C(17)	59.61(13)
O(2)-C(9)-O(3)	118.53(18)
O(2)-C(9)-C(8)	122.68(19)
O(3)-C(9)-C(8)	118.72(17)
C(15)-C(10)-C(11)	122.2(2)
C(15)-C(10)-O(3)	122.46(18)

C(11)-C(10)-O(3)	115.33(19)
C(12)-C(11)-C(10)	118.7(2)
C(12)-C(11)-H(11)	120.6
C(10)-C(11)-H(11)	120.6
C(11)-C(12)-C(13)	120.5(2)
C(11)-C(12)-H(12)	119.8
C(13)-C(12)-H(12)	119.8
C(14)-C(13)-C(12)	119.8(2)
C(14)-C(13)-H(13)	120.1
C(12)-C(13)-H(13)	120.1
C(13)-C(14)-C(15)	120.7(2)
C(13)-C(14)-H(14)	119.6
C(15)-C(14)-H(14)	119.6
C(10)-C(15)-C(14)	118.0(2)
C(10)-C(15)-C(16)	119.86(18)
C(14)-C(15)-C(16)	122.2(2)
C(15)-C(16)-C(17)	120.11(18)
C(15)-C(16)-C(8)	116.06(17)
C(17)-C(16)-C(8)	60.50(13)
C(15)-C(16)-H(16)	116.2
C(17)-C(16)-H(16)	116.2
C(8)-C(16)-H(16)	116.2
C(18)-C(17)-C(16)	121.89(19)
C(18)-C(17)-C(8)	119.38(17)
C(16)-C(17)-C(8)	59.89(13)
C(18)-C(17)-H(17)	114.9
C(16)-C(17)-H(17)	114.9
C(8)-C(17)-H(17)	114.9
C(19)-C(18)-C(17)	177.3(3)
C(18)-C(19)-H(19)	180.0
C(9)-O(3)-C(10)	123.13(16)

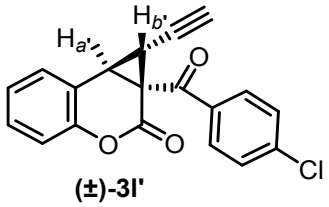
Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3)for d24730. 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}
C(1)	53(1)	52(1)	44(1)	15(1)	-14(1)	-20(1)
C(2)	43(1)	40(1)	50(1)	4(1)	-8(1)	-9(1)
C(3)	40(1)	33(1)	36(1)	0(1)	-6(1)	-6(1)
C(4)	42(1)	30(1)	37(1)	2(1)	-1(1)	-10(1)
C(5)	57(1)	49(1)	36(1)	-3(1)	6(1)	-15(1)
C(6)	66(2)	63(2)	34(1)	5(1)	-9(1)	-29(1)
C(7)	40(1)	29(1)	44(1)	1(1)	4(1)	-5(1)
C(8)	30(1)	28(1)	40(1)	3(1)	-2(1)	1(1)
C(9)	26(1)	30(1)	43(1)	1(1)	-7(1)	0(1)
C(10)	26(1)	41(1)	42(1)	-4(1)	-5(1)	-1(1)
C(11)	36(1)	52(1)	53(1)	-16(1)	-5(1)	1(1)
C(12)	36(1)	80(2)	49(1)	-21(1)	-3(1)	1(1)
C(13)	36(1)	86(2)	42(1)	0(1)	2(1)	-6(1)
C(14)	36(1)	56(1)	45(1)	5(1)	0(1)	-5(1)
C(15)	27(1)	42(1)	39(1)	1(1)	-5(1)	-2(1)
C(16)	38(1)	28(1)	42(1)	4(1)	-1(1)	-2(1)
C(17)	36(1)	33(1)	44(1)	6(1)	-1(1)	8(1)
C(18)	30(1)	50(1)	44(1)	7(1)	-2(1)	9(1)
C(19)	34(1)	76(2)	57(2)	-2(1)	-5(1)	-2(1)
Cl(1)	68(1)	93(1)	68(1)	25(1)	-37(1)	-21(1)
O(1)	55(1)	47(1)	64(1)	-18(1)	0(1)	10(1)
O(2)	46(1)	33(1)	49(1)	9(1)	-4(1)	-4(1)
O(3)	40(1)	28(1)	46(1)	-2(1)	-4(1)	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for d24730.

	x	y	z	U(eq)
H(2)	9491	5837	5577	53
H(3)	6693	6091	5066	43
H(5)	4763	7035	6623	57
H(6)	7551	6775	7135	65
H(11)	4753	4784	3328	56
H(12)	5952	5286	2424	66
H(13)	6243	6469	2355	66
H(14)	5290	7155	3184	55
H(16)	4300	7260	4326	43
H(17)	1135	7180	4650	45
H(19)	-1554	5654	3697	67



(±)-3l'

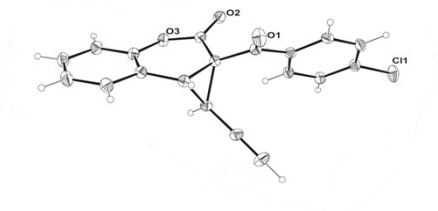


Table 1. Crystal data and structure refinement for d24731.

Identification code	d24731	
Empirical formula	C19 H11 Cl O3	
Formula weight	322.73	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 9.5190(3) Å	α= 90°.

	b = 14.8049(4) Å	β= 90.7470(10)°.
	c = 21.6031(6) Å	γ = 90°.
Volume	3044.22(15) $Å^3$	
Z	8	
Density (calculated)	1.408 Mg/m^3	
Absorption coefficient	2.330 mm^{-1}	
F(000)	1328	
Crystal size	0.57 x 0.20 x 0.11 mm^3	
Theta range for data collection	3.62 to 66.54°.	
Index ranges	-11<=h<=10, -17<=k<=17, -25<=l<=24	
Reflections collected	16059	
Independent reflections	5295 [R(int) = 0.0445]	
Completeness to theta = 66.54°	98.6 %	
Absorption correction	None	
Max. and min. transmission	0.7836 and 0.3501	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5295 / 0 / 415	
Goodness-of-fit on F^2	0.440	
Final R indices [I>2sigma(I)]	R1 = 0.0471, wR2 = 0.1169	
R indices (all data)	R1 = 0.0523, wR2 = 0.1247	
Largest diff. peak and hole	0.210 and -0.565 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for d24731. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	133(2)	664(2)	7604(1)	42(1)
C(2)	706(2)	1347(1)	7250(1)	41(1)
C(3)	2126(2)	1534(1)	7305(1)	37(1)
C(4)	2978(2)	1038(1)	7711(1)	34(1)
C(5)	2376(2)	336(1)	8047(1)	37(1)
C(6)	961(2)	150(1)	8000(1)	41(1)
C(7)	4465(2)	1274(1)	7852(1)	37(1)
C(8)	5212(2)	1972(1)	7462(1)	32(1)
C(9)	5474(2)	1726(1)	6808(1)	35(1)
C(10)	7499(2)	2724(1)	6786(1)	37(1)
C(11)	8560(2)	3034(2)	6410(1)	46(1)
C(12)	9654(2)	3516(2)	6676(1)	52(1)
C(13)	9688(2)	3673(2)	7309(1)	52(1)
C(14)	8611(2)	3357(2)	7676(1)	46(1)
C(15)	7487(2)	2882(1)	7417(1)	36(1)
C(16)	6268(2)	2589(1)	7781(1)	36(1)
C(17)	4852(2)	2973(1)	7589(1)	37(1)
C(18)	3804(2)	3188(2)	8041(1)	44(1)
C(19)	2931(3)	3381(2)	8401(1)	58(1)
C(20)	-348(3)	894(2)	5503(1)	68(1)
C(21)	1021(3)	827(2)	5735(1)	57(1)
C(22)	2044(2)	1373(2)	5483(1)	46(1)
C(23)	1719(2)	1955(2)	4994(1)	45(1)
C(24)	341(2)	1988(2)	4763(1)	61(1)
C(25)	-684(3)	1462(2)	5019(1)	74(1)
C(26)	2797(2)	2508(1)	4687(1)	41(1)
C(27)	4127(2)	2780(1)	5034(1)	35(1)
C(28)	3961(2)	3255(1)	5639(1)	39(1)
C(29)	6057(2)	4146(1)	5441(1)	40(1)
C(30)	6867(2)	4853(2)	5670(1)	51(1)
C(31)	7967(3)	5163(2)	5319(1)	55(1)

C(32)	8257(3)	4776(2)	4752(1)	56(1)
C(33)	7432(3)	4071(2)	4534(1)	49(1)
C(34)	6306(2)	3753(1)	4873(1)	39(1)
C(35)	5388(2)	3018(1)	4650(1)	37(1)
C(36)	5390(2)	2124(1)	4986(1)	33(1)
C(37)	5209(2)	1306(1)	4631(1)	35(1)
C(38)	5088(2)	644(1)	4330(1)	44(1)
Cl(1)	-1660(1)	445(1)	7564(1)	66(1)
Cl(2)	-1649(1)	241(1)	5834(1)	103(1)
O(1)	5079(2)	953(1)	8297(1)	59(1)
O(2)	4867(2)	1133(1)	6536(1)	47(1)
O(3)	6442(2)	2209(1)	6492(1)	41(1)
O(4)	2664(2)	2739(1)	4148(1)	57(1)
O(5)	3000(2)	3145(1)	5986(1)	55(1)
O(6)	4968(2)	3855(1)	5820(1)	49(1)

Table 3. Bond lengths [Å] and angles [°] for d24731.

C(1)-C(2)	1.385(3)
C(1)-C(6)	1.383(3)
C(1)-Cl(1)	1.738(2)
C(2)-C(3)	1.383(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.395(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.395(3)
C(4)-C(7)	1.486(3)
C(5)-C(6)	1.378(3)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-O(1)	1.215(2)
C(7)-C(8)	1.516(3)
C(8)-C(9)	1.484(3)
C(8)-C(16)	1.517(3)
C(8)-C(17)	1.547(3)
C(9)-O(2)	1.201(2)
C(9)-O(3)	1.358(2)
C(10)-C(15)	1.384(3)
C(10)-C(11)	1.383(3)
C(10)-O(3)	1.407(2)
C(11)-C(12)	1.382(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.388(4)
C(12)-H(12)	0.9500
C(13)-C(14)	1.385(3)
C(13)-H(13)	0.9500
C(14)-C(15)	1.392(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.476(3)
C(16)-C(17)	1.517(3)
C(16)-H(16)	1.0000
C(17)-C(18)	1.441(3)

C(17)-H(17)	1.0000
C(18)-C(19)	1.181(3)
C(19)-H(19)	0.9500
C(20)-C(25)	1.376(5)
C(20)-C(21)	1.395(4)
C(20)-Cl(2)	1.732(3)
C(21)-C(22)	1.383(3)
C(21)-H(21)	0.9500
C(22)-C(23)	1.394(3)
C(22)-H(22)	0.9500
C(23)-C(24)	1.398(3)
C(23)-C(26)	1.477(3)
C(24)-C(25)	1.370(4)
C(24)-H(24)	0.9500
C(25)-H(25)	0.9500
C(26)-O(4)	1.218(3)
C(26)-C(27)	1.518(3)
C(27)-C(28)	1.494(3)
C(27)-C(35)	1.511(3)
C(27)-C(36)	1.551(3)
C(28)-O(5)	1.201(3)
C(28)-O(6)	1.360(2)
C(29)-C(30)	1.388(3)
C(29)-C(34)	1.381(3)
C(29)-O(6)	1.397(3)
C(30)-C(31)	1.380(4)
C(30)-H(30)	0.9500
C(31)-C(32)	1.382(4)
C(31)-H(31)	0.9500
C(32)-C(33)	1.386(3)
C(32)-H(32)	0.9500
C(33)-C(34)	1.389(3)
C(33)-H(33)	0.9500
C(34)-C(35)	1.472(3)
C(35)-C(36)	1.511(3)
C(35)-H(35)	1.0000

C(36)-C(37)	1.443(3)
C(36)-H(36)	1.0000
C(37)-C(38)	1.182(3)
C(38)-H(38)	0.9500

C(2)-C(1)-C(6)	121.19(19)
C(2)-C(1)-Cl(1)	120.16(17)
C(6)-C(1)-Cl(1)	118.65(16)
C(3)-C(2)-C(1)	119.32(19)
C(3)-C(2)-H(2)	120.3
C(1)-C(2)-H(2)	120.3
C(2)-C(3)-C(4)	120.56(18)
C(2)-C(3)-H(3)	119.7
C(4)-C(3)-H(3)	119.7
C(3)-C(4)-C(5)	118.69(18)
C(3)-C(4)-C(7)	123.38(18)
C(5)-C(4)-C(7)	117.65(17)
C(6)-C(5)-C(4)	121.21(19)
C(6)-C(5)-H(5)	119.4
C(4)-C(5)-H(5)	119.4
C(5)-C(6)-C(1)	118.99(19)
C(5)-C(6)-H(6)	120.5
C(1)-C(6)-H(6)	120.5
O(1)-C(7)-C(4)	121.20(18)
O(1)-C(7)-C(8)	118.77(18)
C(4)-C(7)-C(8)	119.90(16)
C(9)-C(8)-C(16)	117.50(16)
C(9)-C(8)-C(7)	116.56(16)
C(16)-C(8)-C(7)	118.10(16)
C(9)-C(8)-C(17)	116.34(16)
C(16)-C(8)-C(17)	59.34(13)
C(7)-C(8)-C(17)	116.71(16)
O(2)-C(9)-O(3)	117.64(17)
O(2)-C(9)-C(8)	124.06(19)
O(3)-C(9)-C(8)	118.30(16)
C(15)-C(10)-C(11)	122.56(19)

C(15)-C(10)-O(3)	121.40(17)
C(11)-C(10)-O(3)	116.01(18)
C(12)-C(11)-C(10)	118.7(2)
C(12)-C(11)-H(11)	120.7
C(10)-C(11)-H(11)	120.7
C(11)-C(12)-C(13)	120.3(2)
C(11)-C(12)-H(12)	119.9
C(13)-C(12)-H(12)	119.9
C(14)-C(13)-C(12)	120.0(2)
C(14)-C(13)-H(13)	120.0
C(12)-C(13)-H(13)	120.0
C(13)-C(14)-C(15)	120.7(2)
C(13)-C(14)-H(14)	119.6
C(15)-C(14)-H(14)	119.6
C(10)-C(15)-C(14)	117.77(19)
C(10)-C(15)-C(16)	119.53(17)
C(14)-C(15)-C(16)	122.62(18)
C(15)-C(16)-C(8)	117.09(16)
C(15)-C(16)-C(17)	116.41(17)
C(8)-C(16)-C(17)	61.31(12)
C(15)-C(16)-H(16)	116.8
C(8)-C(16)-H(16)	116.8
C(17)-C(16)-H(16)	116.8
C(18)-C(17)-C(16)	121.13(17)
C(18)-C(17)-C(8)	119.17(18)
C(16)-C(17)-C(8)	59.35(12)
C(18)-C(17)-H(17)	115.3
C(16)-C(17)-H(17)	115.3
C(8)-C(17)-H(17)	115.3
C(19)-C(18)-C(17)	178.1(3)
C(18)-C(19)-H(19)	180.0
C(25)-C(20)-C(21)	121.6(3)
C(25)-C(20)-Cl(2)	119.6(2)
C(21)-C(20)-Cl(2)	118.7(3)
C(22)-C(21)-C(20)	118.4(3)
C(22)-C(21)-H(21)	120.8

C(20)-C(21)-H(21)	120.8
C(21)-C(22)-C(23)	120.6(2)
C(21)-C(22)-H(22)	119.7
C(23)-C(22)-H(22)	119.7
C(22)-C(23)-C(24)	119.3(2)
C(22)-C(23)-C(26)	122.32(19)
C(24)-C(23)-C(26)	118.3(2)
C(25)-C(24)-C(23)	120.4(3)
C(25)-C(24)-H(24)	119.8
C(23)-C(24)-H(24)	119.8
C(24)-C(25)-C(20)	119.6(2)
C(24)-C(25)-H(25)	120.2
C(20)-C(25)-H(25)	120.2
O(4)-C(26)-C(23)	121.43(19)
O(4)-C(26)-C(27)	118.3(2)
C(23)-C(26)-C(27)	120.28(18)
C(28)-C(27)-C(26)	117.43(17)
C(28)-C(27)-C(35)	117.74(17)
C(26)-C(27)-C(35)	116.97(16)
C(28)-C(27)-C(36)	116.36(16)
C(26)-C(27)-C(36)	116.28(16)
C(35)-C(27)-C(36)	59.13(12)
O(5)-C(28)-O(6)	116.67(18)
O(5)-C(28)-C(27)	124.95(19)
O(6)-C(28)-C(27)	118.38(18)
C(30)-C(29)-C(34)	122.3(2)
C(30)-C(29)-O(6)	115.91(19)
C(34)-C(29)-O(6)	121.83(18)
C(29)-C(30)-C(31)	118.5(2)
C(29)-C(30)-H(30)	120.8
C(31)-C(30)-H(30)	120.8
C(32)-C(31)-C(30)	120.7(2)
C(32)-C(31)-H(31)	119.6
C(30)-C(31)-H(31)	119.6
C(31)-C(32)-C(33)	119.7(2)
C(31)-C(32)-H(32)	120.1

C(33)-C(32)-H(32)	120.1
C(32)-C(33)-C(34)	120.9(2)
C(32)-C(33)-H(33)	119.6
C(34)-C(33)-H(33)	119.6
C(29)-C(34)-C(33)	117.9(2)
C(29)-C(34)-C(35)	119.65(19)
C(33)-C(34)-C(35)	122.42(19)
C(34)-C(35)-C(27)	117.68(17)
C(34)-C(35)-C(36)	119.49(16)
C(27)-C(35)-C(36)	61.75(13)
C(34)-C(35)-H(35)	115.7
C(27)-C(35)-H(35)	115.7
C(36)-C(35)-H(35)	115.7
C(37)-C(36)-C(35)	118.69(16)
C(37)-C(36)-C(27)	118.30(16)
C(35)-C(36)-C(27)	59.11(13)
C(37)-C(36)-H(36)	116.2
C(35)-C(36)-H(36)	116.2
C(27)-C(36)-H(36)	116.2
C(38)-C(37)-C(36)	178.2(2)
C(37)-C(38)-H(38)	180.0
C(9)-O(3)-C(10)	122.97(15)
C(28)-O(6)-C(29)	124.00(16)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3)for d24731. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

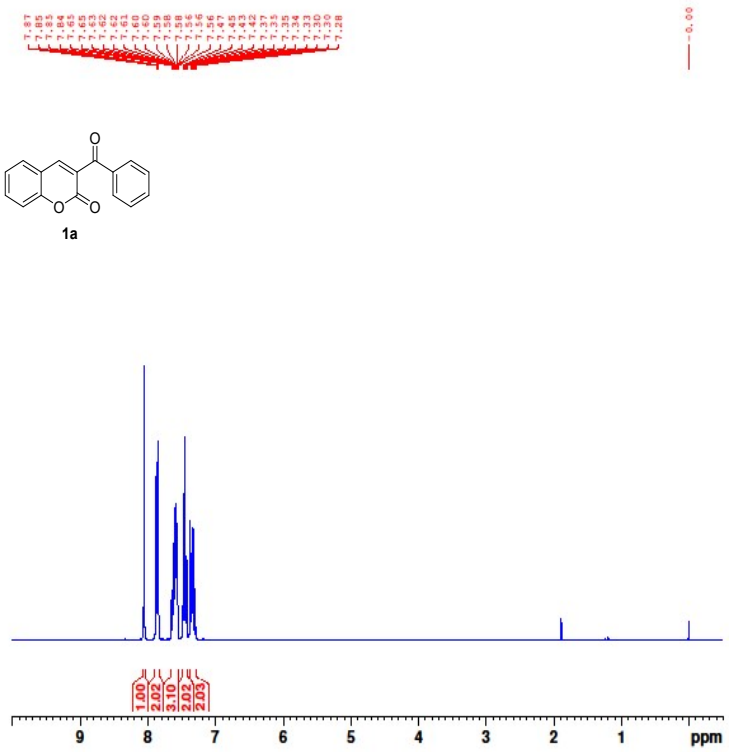
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	40(1)	43(1)	44(1)	-3(1)	3(1)	-9(1)
C(2)	37(1)	43(1)	43(1)	6(1)	-4(1)	1(1)
C(3)	38(1)	35(1)	37(1)	5(1)	1(1)	-3(1)
C(4)	38(1)	33(1)	32(1)	-2(1)	2(1)	1(1)
C(5)	45(1)	32(1)	35(1)	1(1)	0(1)	3(1)
C(6)	48(1)	34(1)	41(1)	3(1)	4(1)	-8(1)
C(7)	38(1)	39(1)	34(1)	2(1)	0(1)	4(1)
C(8)	31(1)	35(1)	28(1)	-1(1)	-2(1)	2(1)
C(9)	33(1)	40(1)	33(1)	-4(1)	-2(1)	4(1)
C(10)	35(1)	40(1)	35(1)	2(1)	-3(1)	0(1)
C(11)	46(1)	51(1)	39(1)	8(1)	5(1)	1(1)
C(12)	43(1)	50(1)	63(2)	14(1)	5(1)	-7(1)
C(13)	43(1)	50(1)	62(2)	5(1)	-7(1)	-12(1)
C(14)	45(1)	48(1)	44(1)	-2(1)	-7(1)	-6(1)
C(15)	36(1)	37(1)	36(1)	0(1)	-4(1)	0(1)
C(16)	38(1)	41(1)	29(1)	-4(1)	-2(1)	-2(1)
C(17)	42(1)	35(1)	33(1)	-3(1)	1(1)	2(1)
C(18)	45(1)	44(1)	41(1)	-8(1)	-1(1)	4(1)
C(19)	52(1)	73(2)	50(1)	-14(1)	9(1)	12(1)
C(20)	42(1)	91(2)	71(2)	-45(2)	20(1)	-22(1)
C(21)	55(1)	62(2)	55(1)	-21(1)	11(1)	-12(1)
C(22)	38(1)	54(1)	47(1)	-15(1)	0(1)	-4(1)
C(23)	36(1)	56(1)	43(1)	-17(1)	-7(1)	5(1)
C(24)	36(1)	91(2)	57(1)	-23(1)	-8(1)	8(1)
C(25)	36(1)	117(3)	69(2)	-39(2)	-3(1)	1(1)
C(26)	43(1)	41(1)	40(1)	-9(1)	-9(1)	10(1)
C(27)	38(1)	37(1)	31(1)	-4(1)	-3(1)	6(1)
C(28)	39(1)	40(1)	38(1)	-9(1)	-1(1)	5(1)
C(29)	40(1)	36(1)	44(1)	-4(1)	-1(1)	2(1)
C(30)	51(1)	43(1)	60(1)	-15(1)	-6(1)	2(1)
C(31)	52(1)	37(1)	75(2)	-4(1)	-10(1)	-3(1)

C(32)	56(1)	50(1)	63(2)	13(1)	-2(1)	-11(1)
C(33)	58(1)	46(1)	43(1)	6(1)	1(1)	-6(1)
C(34)	47(1)	33(1)	37(1)	3(1)	-4(1)	1(1)
C(35)	46(1)	37(1)	28(1)	-2(1)	-2(1)	1(1)
C(36)	35(1)	37(1)	28(1)	-3(1)	0(1)	2(1)
C(37)	37(1)	37(1)	32(1)	1(1)	4(1)	2(1)
C(38)	51(1)	37(1)	43(1)	-6(1)	7(1)	-2(1)
Cl(1)	41(1)	78(1)	78(1)	16(1)	-3(1)	-18(1)
Cl(2)	70(1)	131(1)	110(1)	-56(1)	45(1)	-50(1)
O(1)	48(1)	72(1)	56(1)	28(1)	-14(1)	-7(1)
O(2)	42(1)	55(1)	43(1)	-18(1)	0(1)	-5(1)
O(3)	40(1)	55(1)	28(1)	-3(1)	0(1)	-7(1)
O(4)	65(1)	64(1)	43(1)	-1(1)	-19(1)	2(1)
O(5)	53(1)	64(1)	49(1)	-20(1)	13(1)	-7(1)
O(6)	48(1)	55(1)	44(1)	-22(1)	4(1)	-7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for d24731.

	x	y	z	U(eq)
H(2)	130	1685	6972	49
H(3)	2524	2003	7064	44
H(5)	2954	-20	8313	45
H(6)	561	-324	8235	49
H(11)	8538	2917	5977	55
H(12)	10386	3742	6424	62
H(13)	10451	3996	7491	62
H(14)	8639	3467	8109	55
H(16)	6433	2490	8234	43
H(17)	4862	3377	7217	44
H(19)	2228	3537	8690	70
H(21)	1246	415	6059	68
H(22)	2977	1351	5644	56
H(24)	114	2377	4427	73
H(25)	-1621	1488	4862	89
H(30)	6668	5118	6060	62
H(31)	8531	5648	5467	65
H(32)	9019	4992	4514	68
H(33)	7639	3802	4146	59
H(35)	5244	2986	4191	44
H(36)	6017	2081	5360	40
H(38)	4992	111	4087	52

5. NMR Spectra

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EXPNO                  1
PROCNO                 1

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PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    16
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              2.7262976 sec
RG                 72.74
DW                83.200 usec
DE                12.63 usec
TE                296.8 K
D1              2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          300.1318008 MHz
NUC1                  1H
P1                 14.00 usec
PLW1           7.69999981 W

F2 - Processing parameters
SI                 16384
SF            300.1299999 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
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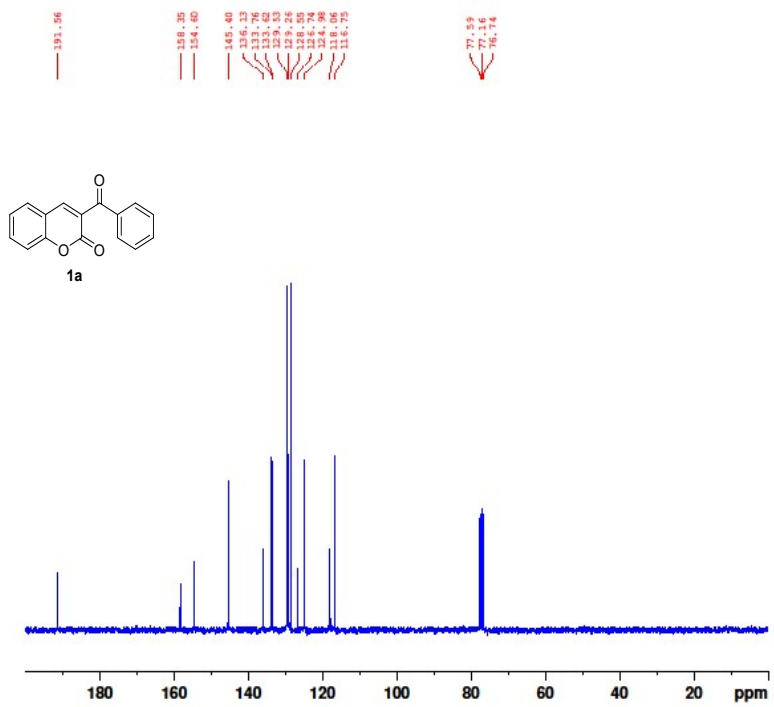


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EXPNO                  2
PROCNO                 1

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PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                    64
DS                     0
SWH            18028.846 Hz
FIDRES          0.550197 Hz
AQ              0.9087659 sec
RG                219.17
DW                27.733 usec
DE                 6.50 usec
TE                296.8 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          75.4756726 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          28.29999924 W

======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                  1H
CPDPRG[2 bi_waltz65_256
PCPD2              90.00 usec
PLW2           8.30000019 W
PLW12          0.20084000 W
PLW13          0.16268000 W

F2 - Processing parameters
SI                 32768
SF            75.4677540 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
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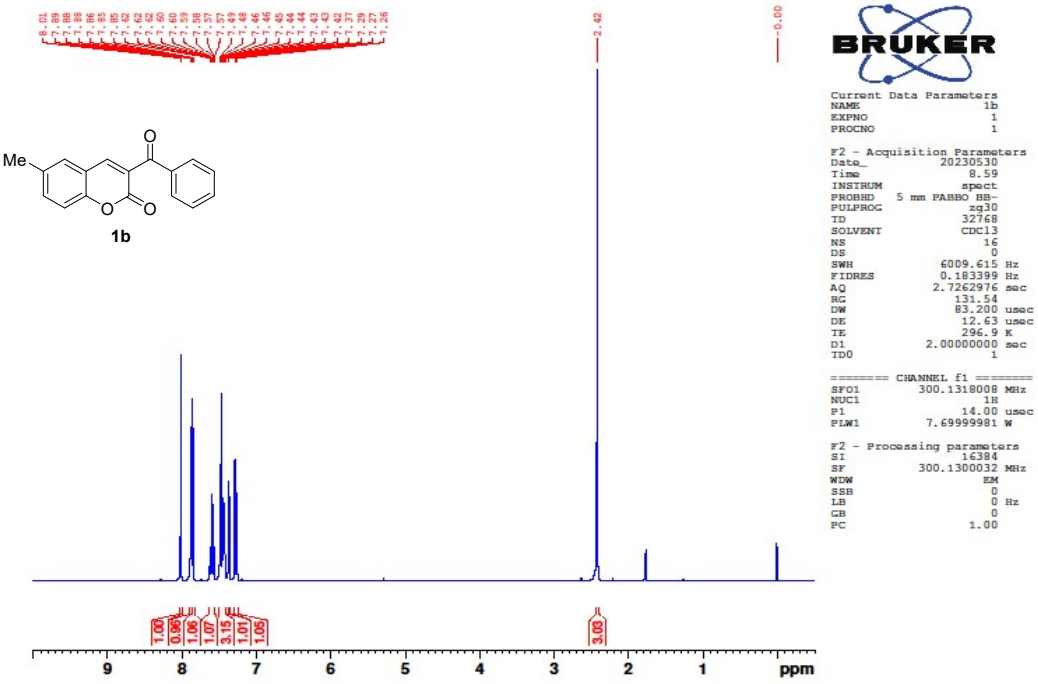


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Current Data Parameters
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EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230530
Time                8.59
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              2.7262976 sec
RG                131.54
DW                83.200 usec
DE                12.63 usec
TE                296.9 K
D1              2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          300.1318008 MHz
NUC1                  1H
P1                 14.00 usec
PLW1           7.69999981 W

F2 - Processing parameters
SI                 16384
SF            300.1300032 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
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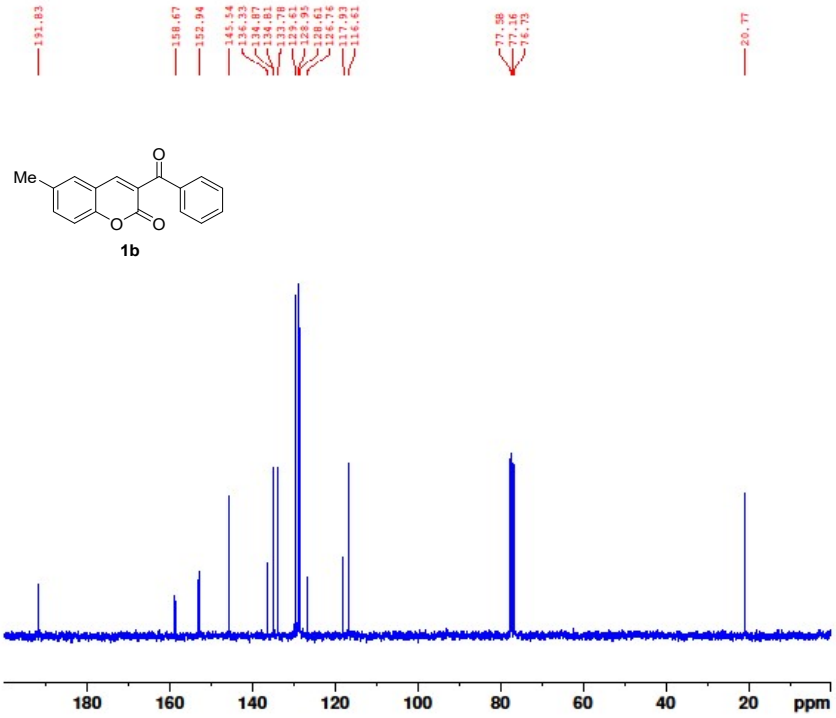


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EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
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Time                9.00
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   128
DS                     0
SWH            18028.846 Hz
FIDRES          0.550197 Hz
AQ              0.9087659 sec
RG                219.17
DW                27.733 usec
DE                 6.50 usec
TE                297.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          75.4756726 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          28.29999924 W

======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                  1H
CPDPRG[2 bi_waltz65_256
PCPD2              90.00 usec
PLW2           8.30000019 W
PLW12          0.20084000 W
PLW13          0.16268000 W

F2 - Processing parameters
SI                 32768
SF            75.4677470 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
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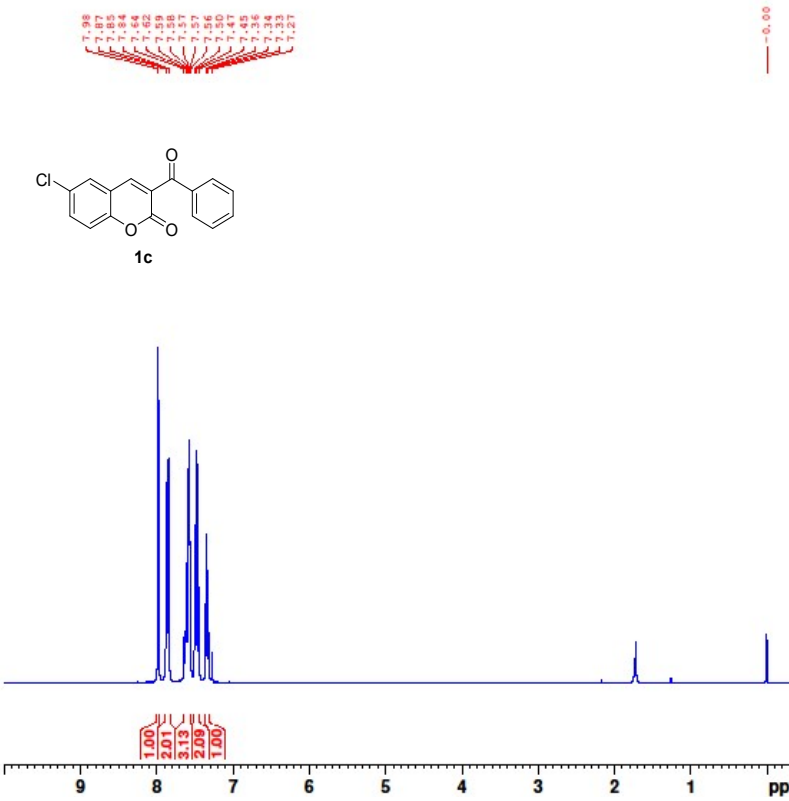

BRUKER

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EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
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Time               20.01
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              2.7262976 sec
RG                194.81
DW                83.200 usec
DE                12.63 usec
TE                296.0 K
D1              2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          300.1318008 MHz
NUC1                  1H
P1                 14.00 usec
PLW1          7.69999981 W

F2 - Processing parameters
SI                 16384
SF            300.1300037 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
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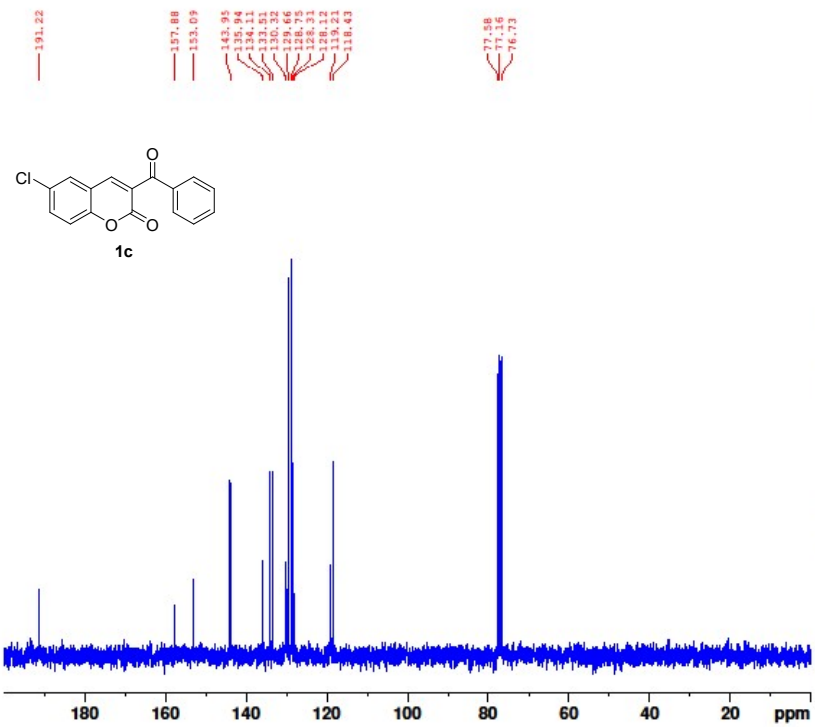

BRUKER

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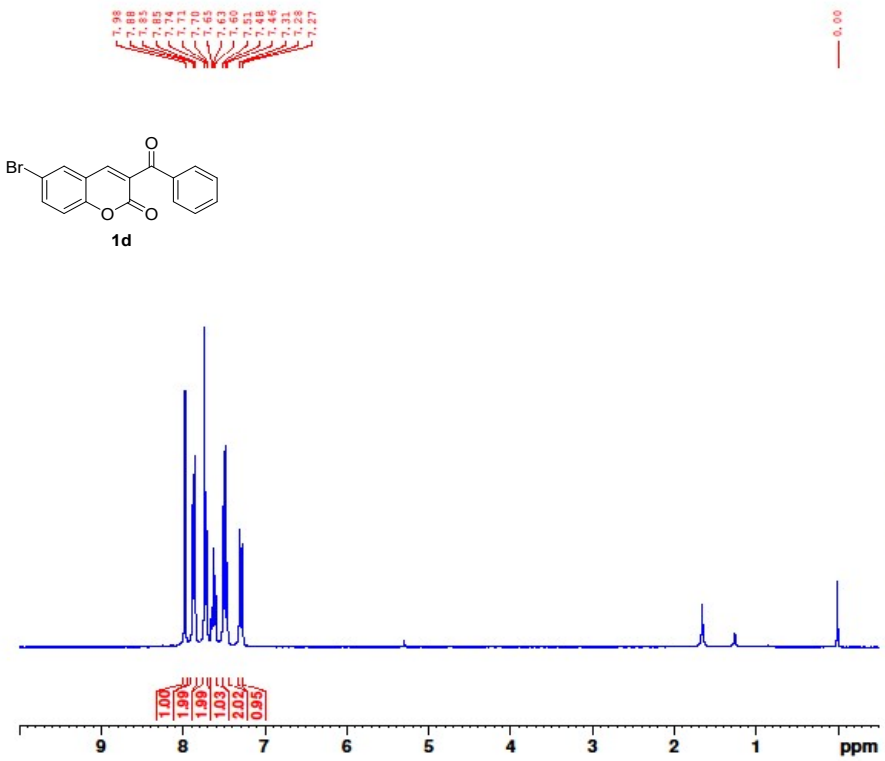
Current Data Parameters
NAME                  1c
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230531
Time               20.03
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   128
DS                     0
SWH            18028.846 Hz
FIDRES          0.550197 Hz
AQ              0.9087659 sec
RG                219.17
DW                27.733 usec
DE                 6.50 usec
TE                296.2 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          75.4756726 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          28.29999924 W

======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                  1H
CPDPRG[2 bi_waltz65_256
PCPD2              90.00 usec
PLW2          8.30000019 W
PLW12         0.20084000 W
PLW13         0.16268000 W

F2 - Processing parameters
SI                 32768
SF            75.4677450 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```



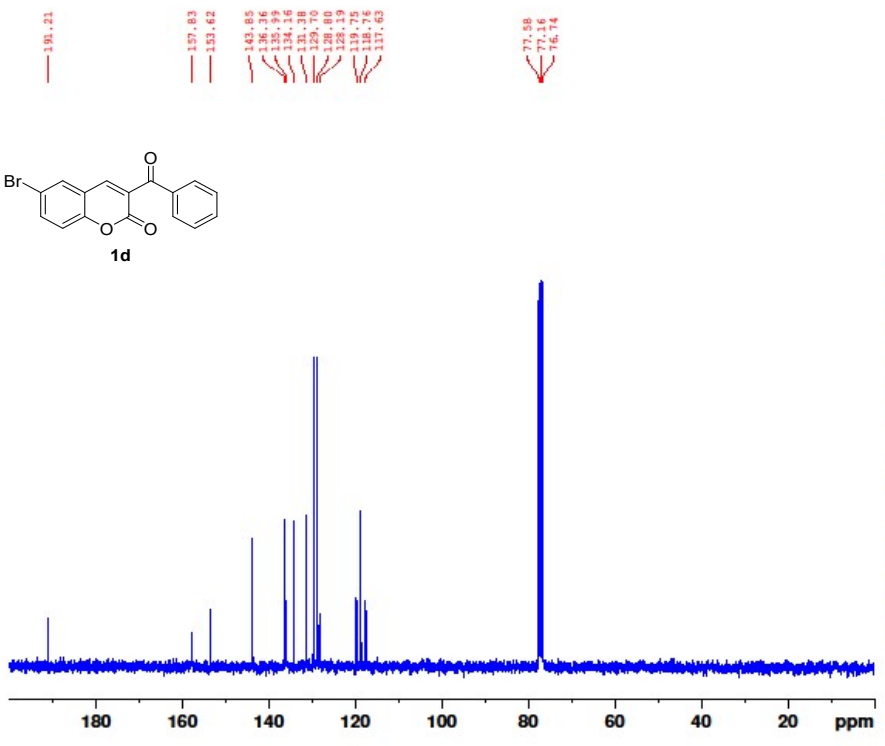
BRUKER

```
Current Data Parameters
NAME                  1d
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230605
Time               20.53
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   64
DS                    0
SWH            6009.615 Hz
FIDRES        0.183399 Hz
AQ            2.7262976 sec
RG               219.17
DW               83.200 usec
DE               12.63 usec
TE               295.1 K
D1            2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         300.1318008 MHz
NUC1                 1H
P1                14.00 usec
PLW1          7.69999981 W

F2 - Processing parameters
SI                16384
SF           300.1300050 MHz
WDW                  EM
SSB                   0
LB                 0 Hz
GB                    0
PC                 1.00
```



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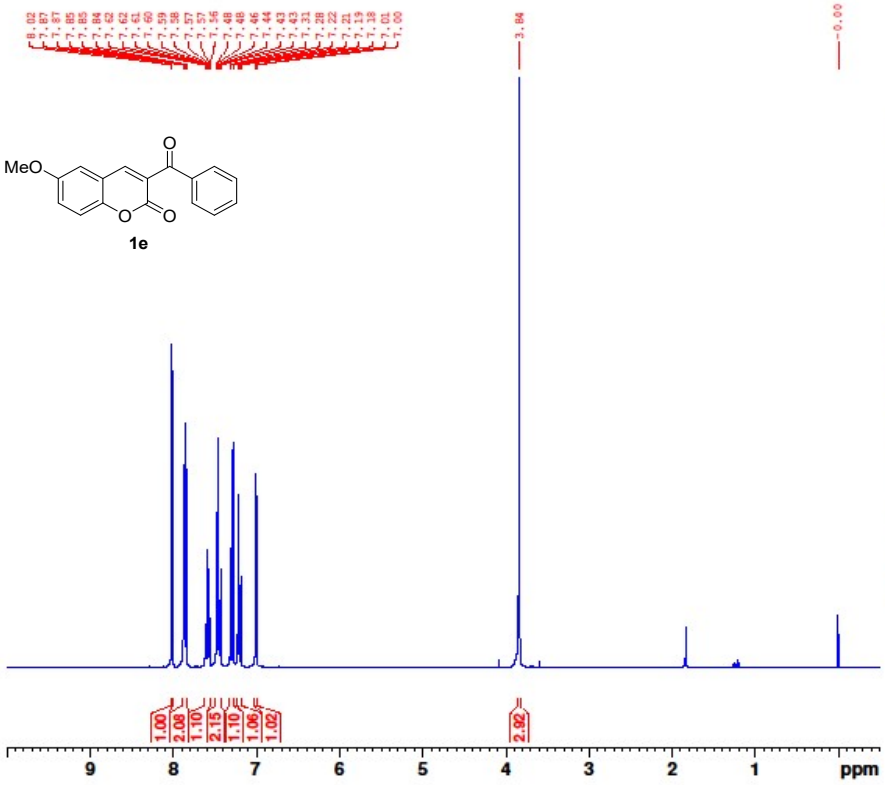
```
Current Data Parameters
NAME                  1d
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230605
Time               21.07
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  256
DS                    0
SWH           18028.846 Hz
FIDRES        0.550197 Hz
AQ            0.9087659 sec
RG               219.17
DW               27.733 usec
DE                6.50 usec
TE               296.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         75.4756726 MHz
NUC1                13C
P1                10.00 usec
PLW1         28.29999924 W

======== CHANNEL f2 ========
SFO2         300.1312005 MHz
NUC2                 1H
CPDPRG[2 bi_waltz65_256
PCPD2             90.00 usec
PLW2          8.30000019 W
PLW12         0.20084000 W
PLW13         0.16268000 W

F2 - Processing parameters
SI                32768
SF           75.4677419 MHz
WDW                  EM
SSB                   0
LB                 2.00 Hz
GB                    0
PC                 1.00
```



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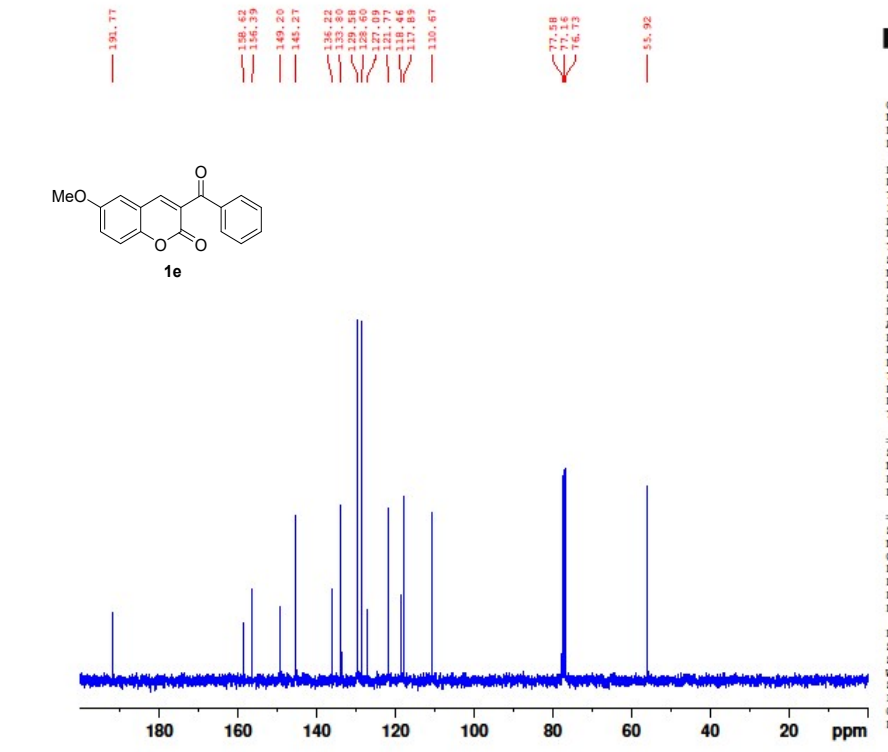
```
Current Data Parameters
NAME                  1e
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230530
Time                6.58
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              2.7262976 sec
RG                106.61
DW                83.200 usec
DE                12.63 usec
TE                296.6 K
D1              2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          300.1318008 MHz
NUC1                  1H
P1                 14.00 usec
PLW1           7.69999981 W

F2 - Processing parameters
SI                 16384
SF            300.1300008 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```



BRUKER

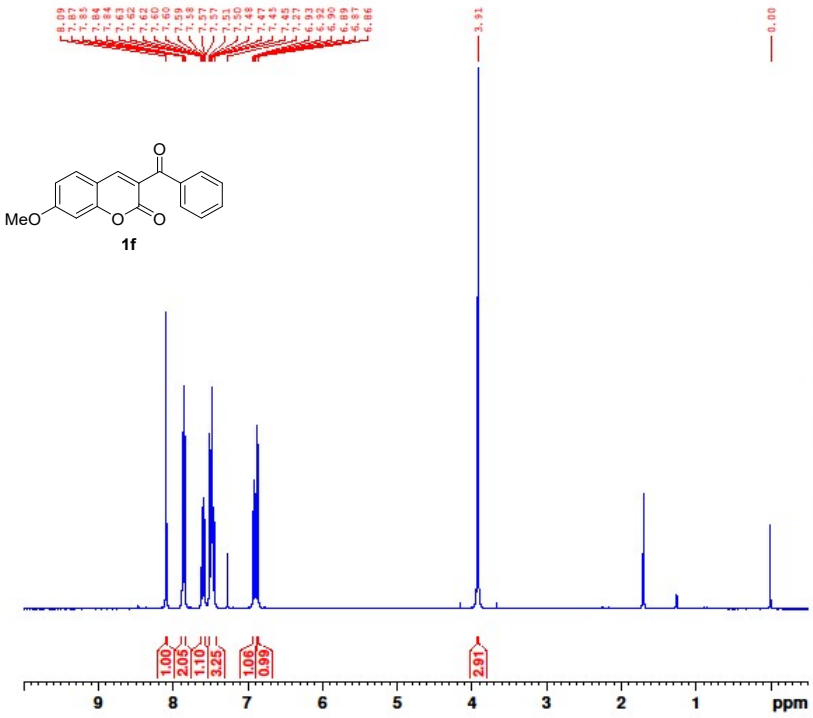
```
Current Data Parameters
NAME                  1e
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230530
Time                7.01
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   512
DS                     0
SWH            18028.846 Hz
FIDRES          0.550197 Hz
AQ              0.9087659 sec
RG                219.17
DW                27.733 usec
DE                 6.50 usec
TE                296.8 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

======= CHANNEL f1 =======
SFO1          75.4756726 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          28.29999924 W

======= CHANNEL f2 =======
SFO2          300.1312005 MHz
NUC2                  1H
CPDPRG[2 bi_waltz65_256
PCPD2              90.00 usec
PLW2           8.30000019 W
PLW12          0.20084000 W
PLW13          0.16268000 W

F2 - Processing parameters
SI                 32768
SF            75.4677491 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```

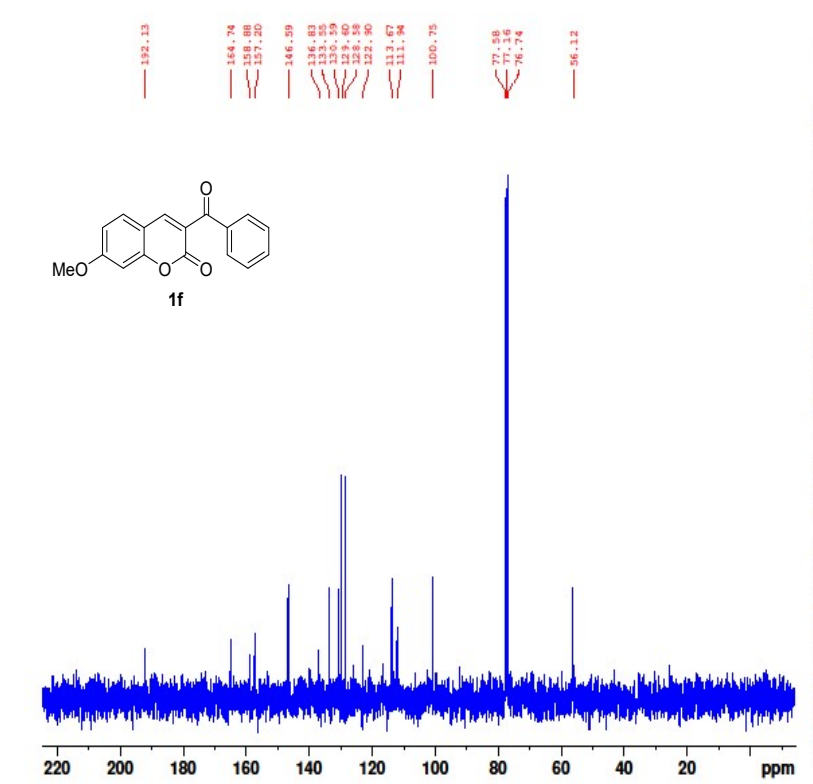


```
Current Data Parameters
NAME                  1f
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230604
Time               15.14
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    64
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              2.7262976 sec
RG                219.17
DW                83.200 usec
DE                12.63 usec
TE                295.5 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          300.1318008 MHz
NUC1                   1H
P1                 14.00 usec
PLW1           7.69999981 W

F2 - Processing parameters
SI                 16384
SF            300.1300042 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```



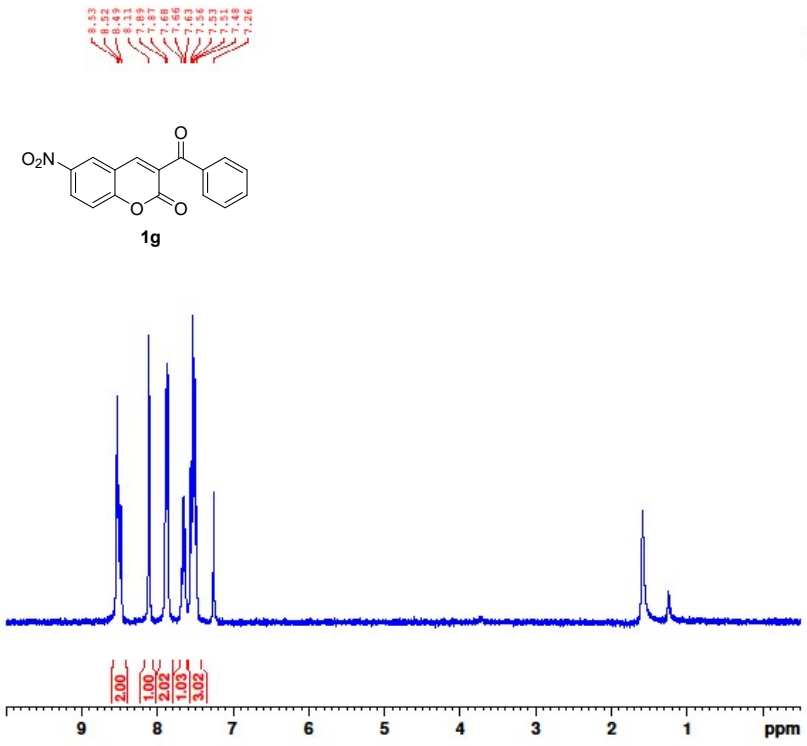
```
Current Data Parameters
NAME                  1f
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230604
Time               15.15
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   500
DS                     0
SWH            18028.846 Hz
FIDRES          0.550197 Hz
AQ              0.9087659 sec
RG                219.17
DW                27.733 usec
DE                 6.50 usec
TE                295.6 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          75.4756726 MHz
NUC1                   13C
P1                 10.00 usec
PLW1          28.29999924 W

======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                   1H
CPDPRG[2 bi_waltz65_256
PCPD2              90.00 usec
PLW2           8.30000019 W
PLW12          0.20084000 W
PLW13          0.16268000 W

F2 - Processing parameters
SI                 32768
SF            75.4677428 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```



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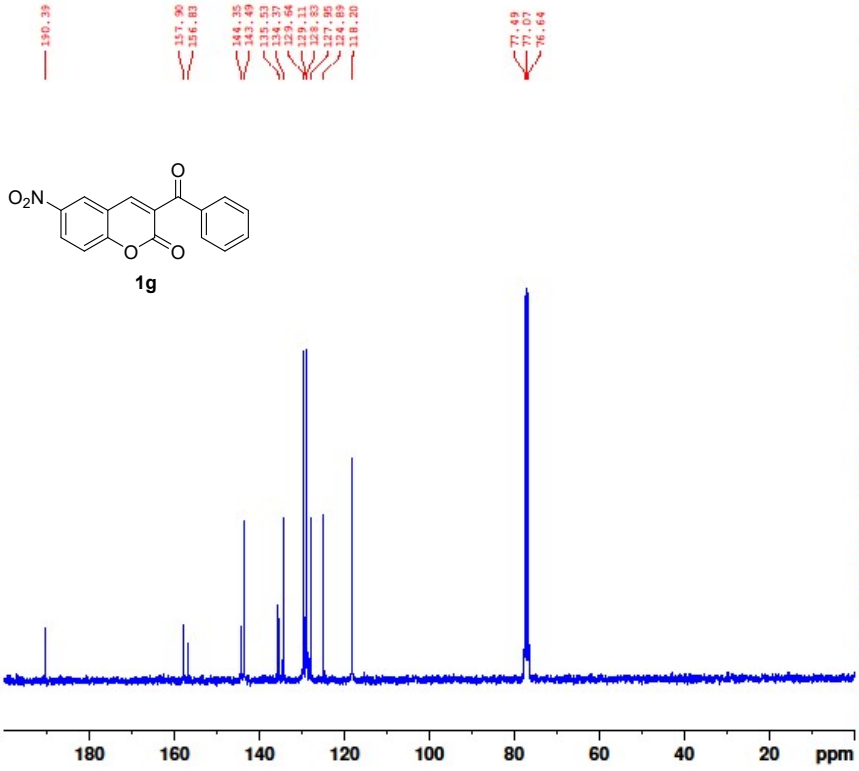
```
Current Data Parameters
NAME                  1g
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230411
Time               11.35
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    64
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              2.7262976 sec
RG                 219.17
DW                 83.200 usec
DE                 12.63 usec
TE                 295.5 K
D1              2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          300.1318008 MHz
NUC1                  1H
P1                 14.00 usec
PLW1           7.69999981 W

F2 - Processing parameters
SI                 16384
SF            300.1300079 MHz
WDW                   EM
SSB                    0
LB                  0 Hz
GB                     0
PC                  1.00
```



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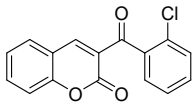
```
Current Data Parameters
NAME                  1g
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240427
Time               19.18
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  1652
DS                     0
SWH            18028.846 Hz
FIDRES          0.550197 Hz
AQ              0.9087659 sec
RG                 219.17
DW                 27.733 usec
DE                  6.50 usec
TE                 297.7 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

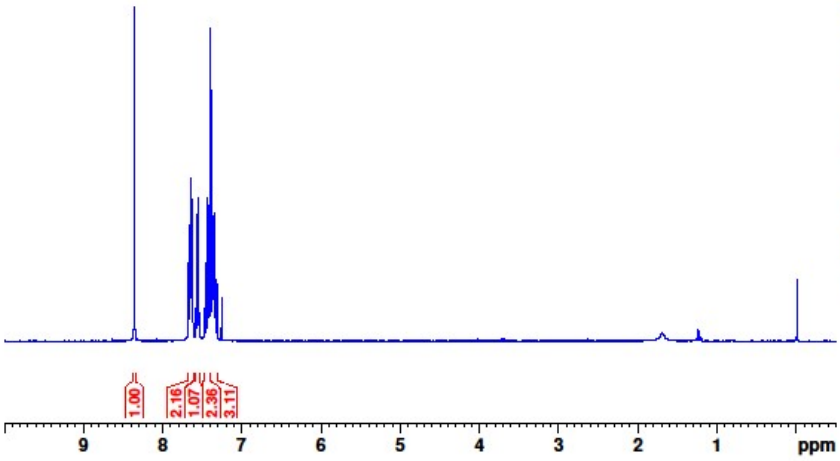
======== CHANNEL f1 ========
SFO1          75.4756726 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          28.29999924 W

======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                  1H
CPDPRG[2 bi_waltz65_256
PCPD2              90.00 usec
PLW2           8.30000019 W
PLW12          0.20084000 W
PLW13          0.16268000 W

F2 - Processing parameters
SI                 32768
SF            75.4677485 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```



1h

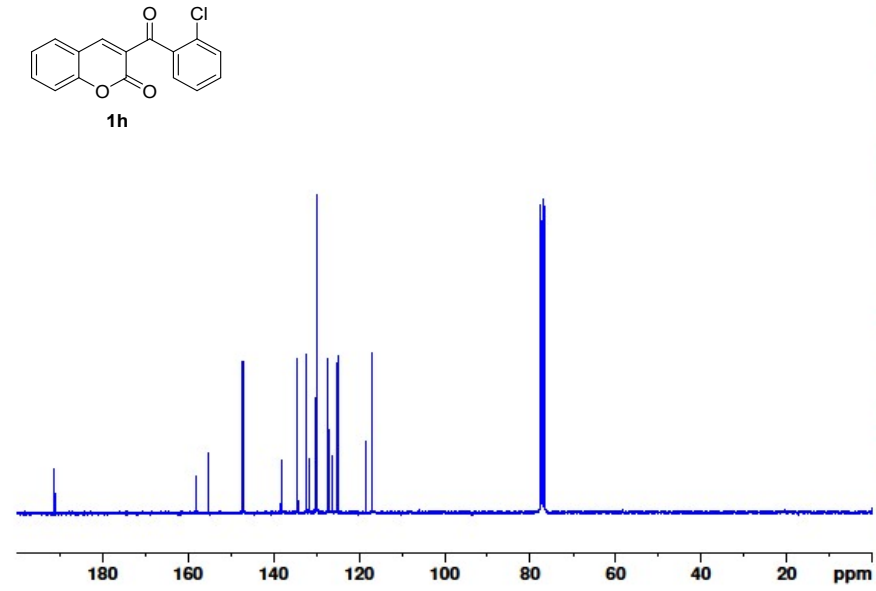


```
Current Data Parameters
NAME                  1h
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240204
Time               19.25
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ             2.7262976 sec
RG                219.17
DW                83.200 usec
DE                12.63 usec
TE                296.0 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         300.1318008 MHz
NUC1                   1H
P1                  14.00 usec
PLW1          7.69999981 W

F2 - Processing parameters
SI                 16384
SF           300.1300079 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```



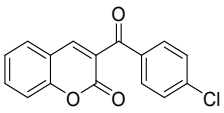
```
Current Data Parameters
NAME                  1h
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240204
Time               21.02
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  1972
DS                     0
SWH            18028.846 Hz
FIDRES          0.550197 Hz
AQ             0.9087659 sec
RG                219.17
DW                27.733 usec
DE                 6.50 usec
TE                297.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

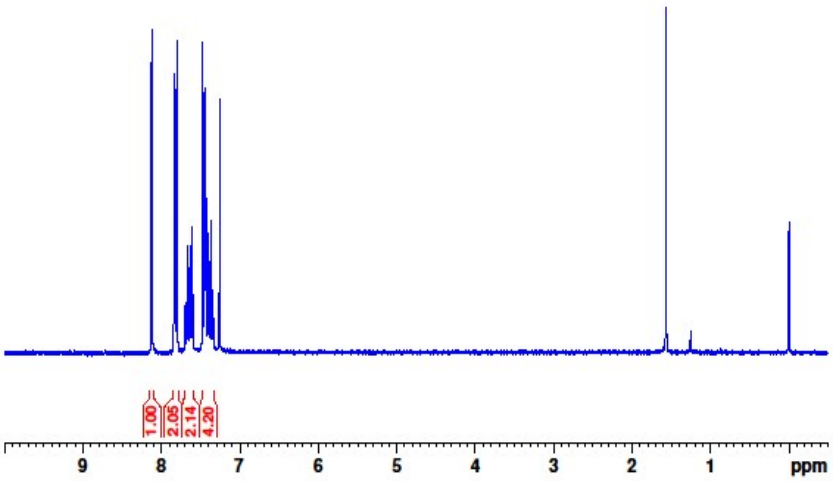
======== CHANNEL f1 ========
SFO1          75.4756726 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          28.29999924 W

======== CHANNEL f2 ========
SFO2         300.1312005 MHz
NUC2                   1H
CPDPRG[2 bi_waltz65_256
PCPD2              90.00 usec
PLW2           8.30000019 W
PLW12          0.20084000 W
PLW13          0.16268000 W

F2 - Processing parameters
SI                 32768
SF           75.4677485 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```



1i

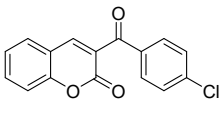



```
Current Data Parameters
NAME                  S15
EXPNO                   1
PROCNO                  1

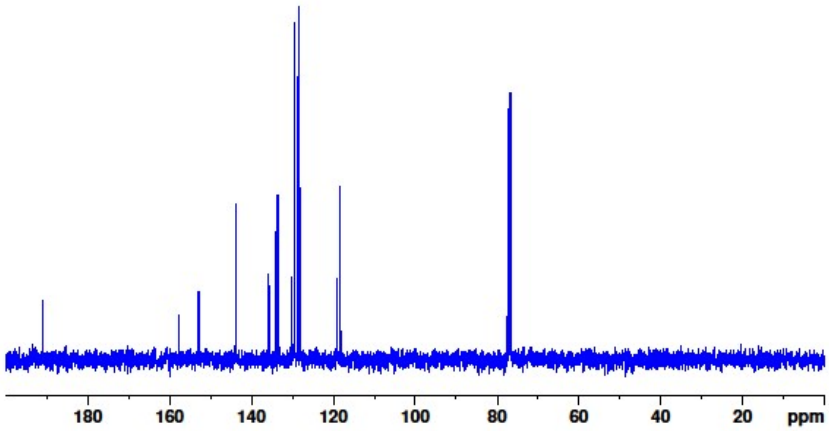
F2 - Acquisition Parameters
Date_           20230731
Time                8.56
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              2.7262976 sec
RG                 219.17
DW                83.200 usec
DE                12.63 usec
TE                296.7 K
D1              2.00000000 sec
TD0                    1

======== CHANNEL f1 =======
SFO1          300.1318008 MHz
NUC1                1H
P1                14.00 usec
PLW1           7.69999981 W

F2 - Processing parameters
SI                 16384
SF            300.1300079 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```



1i



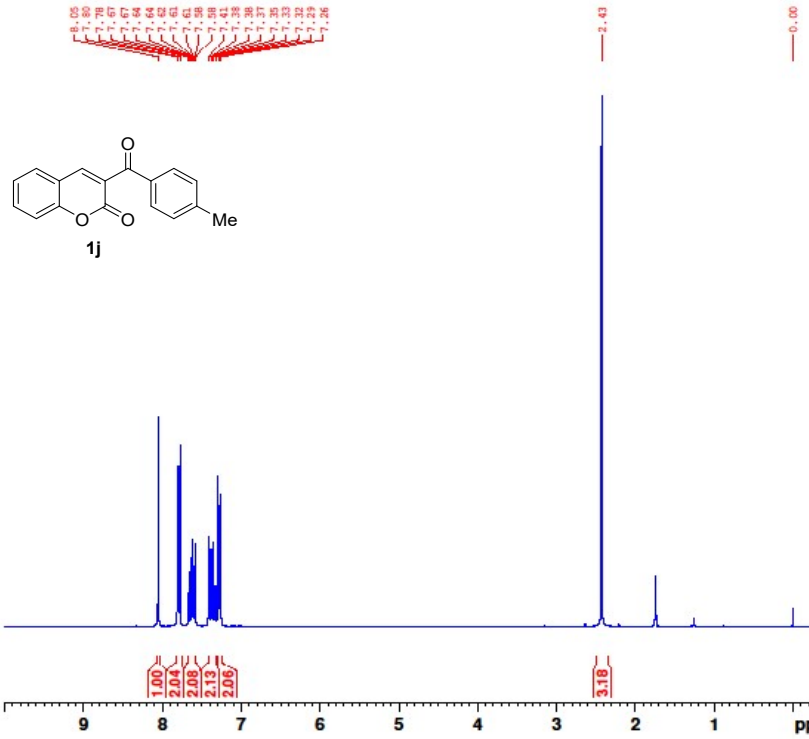

```
Current Data Parameters
NAME                  1i
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230531
Time               20.03
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   128
DS                     0
SWH            18028.846 Hz
FIDRES          0.550197 Hz
AQ              0.9087659 sec
RG                 219.17
DW                27.733 usec
DE                 6.50 usec
TE                296.2 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 =======
SFO1           75.4756726 MHz
NUC1                13C
P1                10.00 usec
PLW1           28.29999924 W

======== CHANNEL f2 =======
SFO2          300.1312005 MHz
NUC2                1H
CPDPRG[2 bi_waltz65_256
PCPD2             90.00 usec
PLW2           8.30000019 W
PLW12          0.20084000 W
PLW13          0.16268000 W

F2 - Processing parameters
SI                 32768
SF            75.4677599 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```



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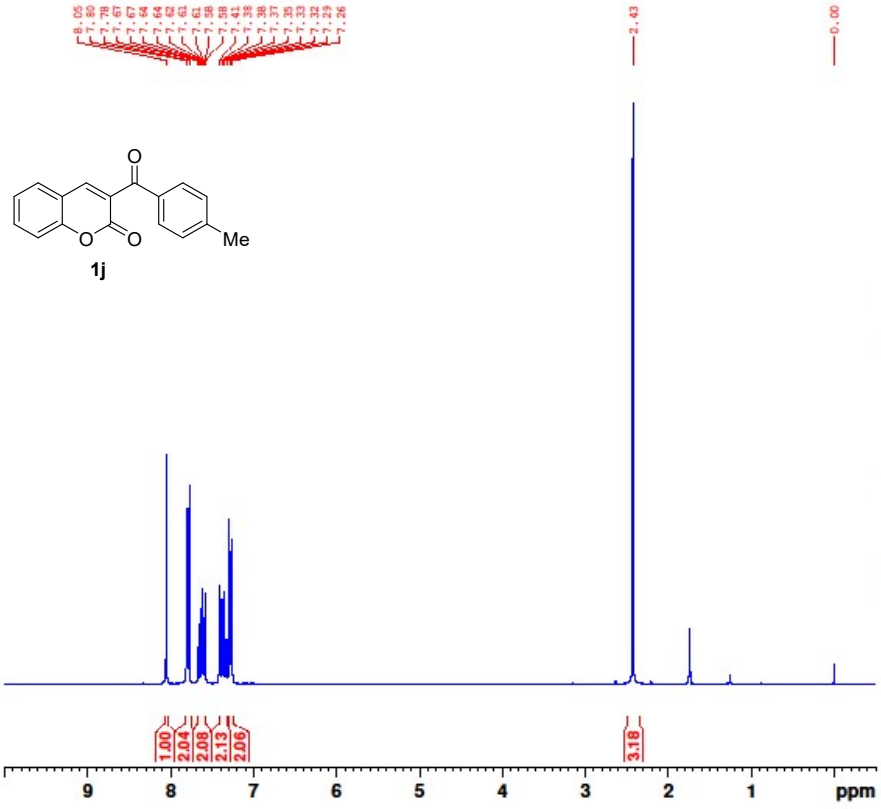
```
Current Data Parameters
NAME                  1j
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240211
Time              17.08
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   64
DS                    0
SWH            6009.615 Hz
FIDRES        0.183399 Hz
AQ            2.7262976 sec
RG               194.81
DW               83.200 usec
DE               12.63 usec
TE               292.1 K
D1            2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         300.1318008 MHz
NUC1                1H
P1                14.00 usec
PLW1          7.69999981 W

F2 - Processing parameters
SI                16384
SF           300.1300040 MHz
WDW                  EM
SSB                   0
LB                    0 Hz
GB                    0
PC                 1.00
```



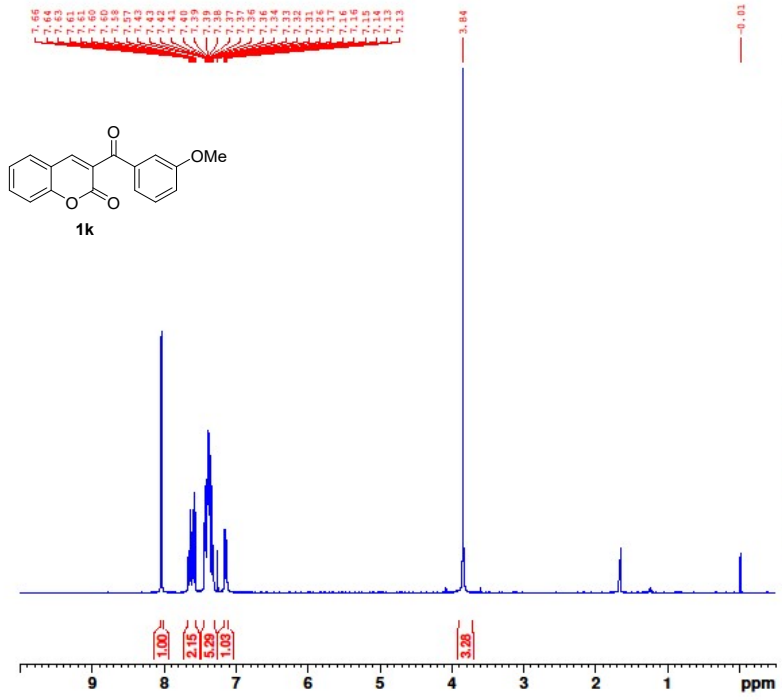
BRUKER

```
Current Data Parameters
NAME                  1j
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240211
Time              17.08
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   64
DS                    0
SWH            6009.615 Hz
FIDRES        0.183399 Hz
AQ            2.7262976 sec
RG               194.81
DW               83.200 usec
DE               12.63 usec
TE               292.1 K
D1            2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         300.1318008 MHz
NUC1                1H
P1                14.00 usec
PLW1          7.69999981 W

F2 - Processing parameters
SI                16384
SF           300.1300040 MHz
WDW                  EM
SSB                   0
LB                    0 Hz
GB                    0
PC                 1.00
```



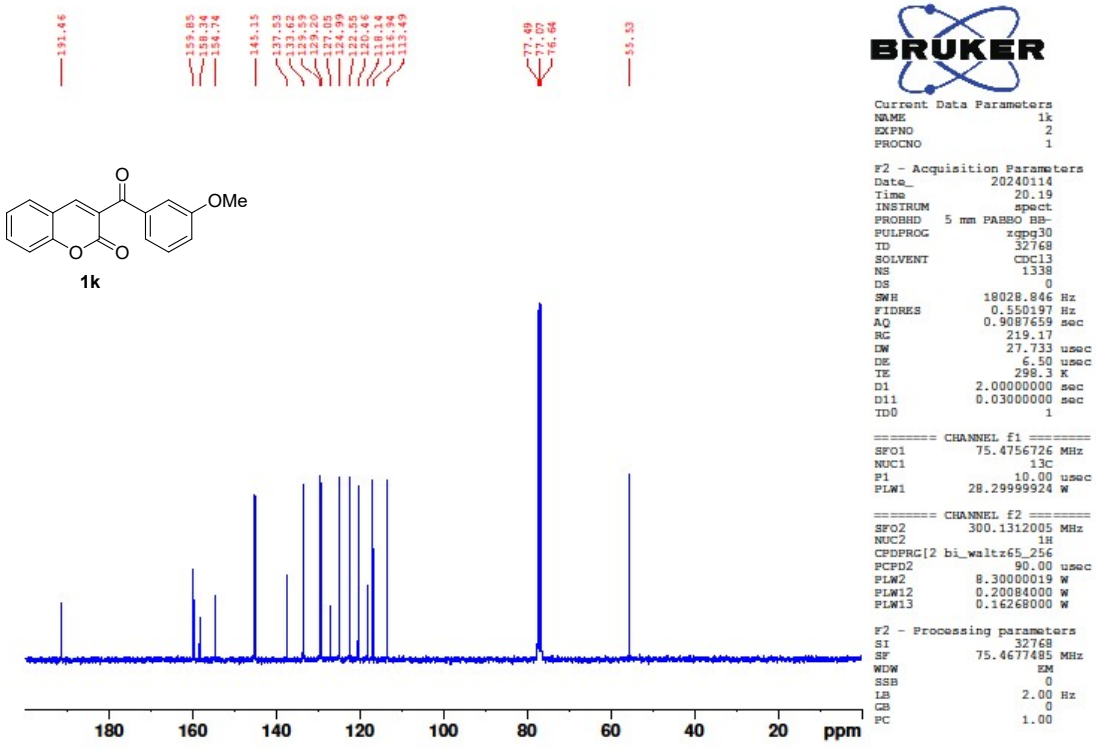
BRUKER

```
Current Data Parameters
NAME                  1k
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240114
Time              19.11
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               32768
SOLVENT           CDCl3
NS                   64
DS                    0
SWH            6009.615 Hz
FIDRES         0.183399 Hz
AQ             2.7262976 sec
RG               219.17
DW               83.200 usec
DE               12.63 usec
TE               297.2 K
D1             2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         300.1318008 MHz
NUC1               1H
P1               14.00 usec
PLW1          7.69999981 W

F2 - Processing parameters
SI                16384
SF           300.1300079 MHz
WDW                  EM
SSB                   0
LB                    0 Hz
GB                    0
PC                 1.00
```



BRUKER

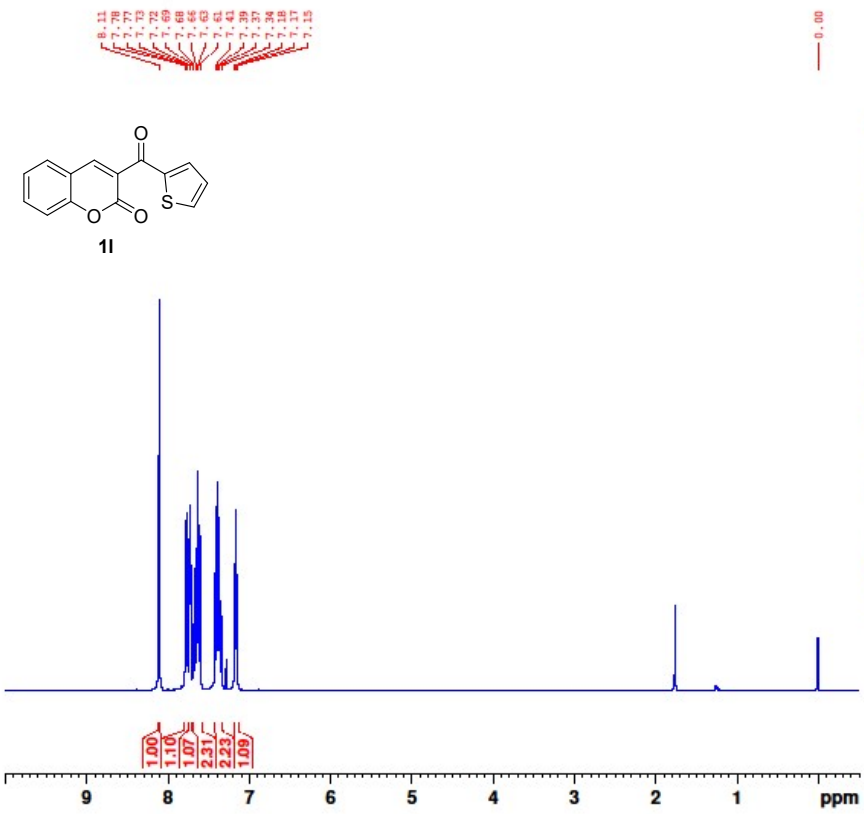
```
Current Data Parameters
NAME                  1k
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240114
Time              20.19
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               32768
SOLVENT           CDCl3
NS                 1338
DS                    0
SWH           18028.846 Hz
FIDRES         0.550197 Hz
AQ             0.9087659 sec
RG               219.17
DW               27.733 usec
DE                6.50 usec
TE               298.3 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1          75.4756726 MHz
NUC1               13C
P1               10.00 usec
PLW1          28.29999924 W

======== CHANNEL f2 ========
SFO2         300.1312005 MHz
NUC2               1H
CPDPRG[2 bi_waltz65_256
PCPD2            90.00 usec
PLW2          8.30000019 W
PLW12         0.20084000 W
PLW13         0.16268000 W

F2 - Processing parameters
SI                32768
SF           75.4677485 MHz
WDW                  EM
SSB                   0
LB                 2.00 Hz
GB                    0
PC                 1.00
```

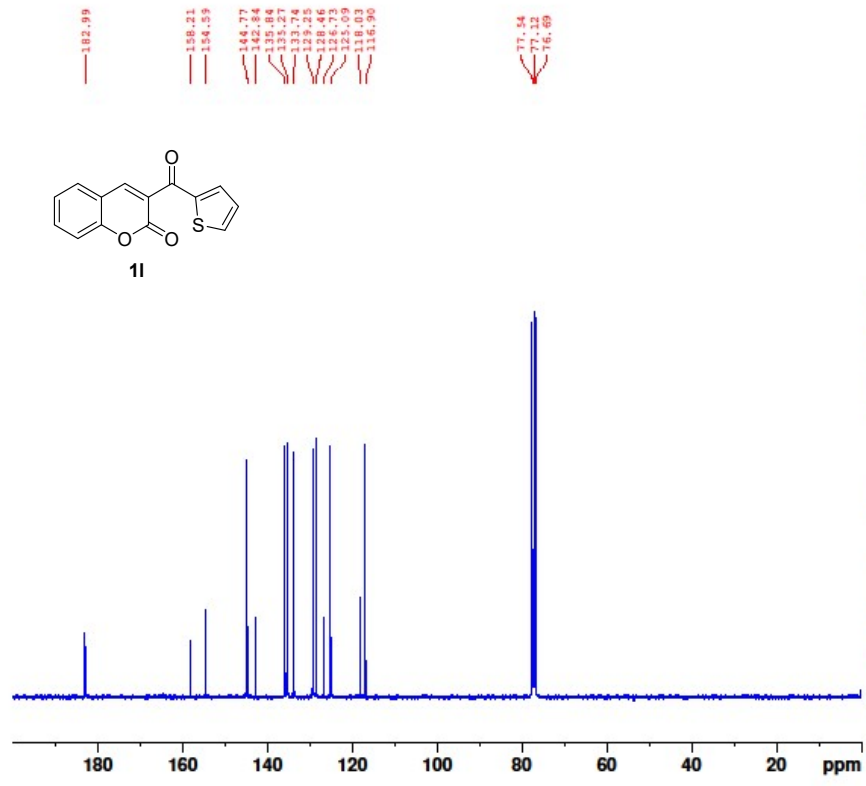


Current Data Parameters
NAME 11
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240301
Time 14.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 194.81
DW 83.200 usec
DE 12.63 usec
TE 292.9 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 300.1318008 MHz
NUC1 1H
P1 14.00 usec
PLW1 7.69999981 W

F2 - Processing parameters
SI 16384
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



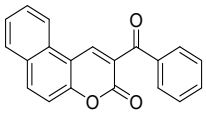
Current Data Parameters
NAME 11
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240301
Time 16.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1898
DS 0
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 219.17
DW 27.733 usec
DE 6.50 usec
TE 294.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

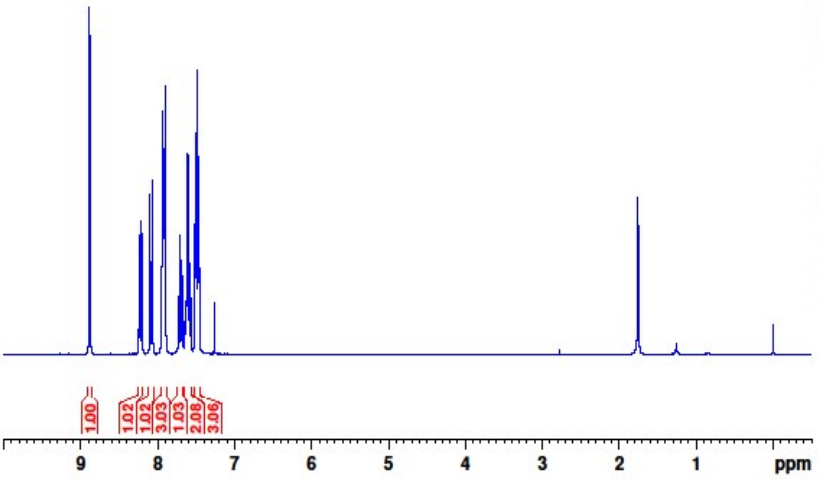
======== CHANNEL f1 ========
SFO1 75.4756726 MHz
NUC1 13C
P1 10.00 usec
PLW1 28.29999924 W

======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 bi_waltz65_256
PCPD2 90.00 usec
PLW2 8.30000019 W
PLW12 0.20084000 W
PLW13 0.16268000 W

F2 - Processing parameters
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00



1m



```
Current Data Parameters
NAME                  1m
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230530
Time                8.26
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ             2.7262976 sec
RG                194.81
DW                83.200 usec
DE                12.63 usec
TE                296.9 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          300.1318008 MHz
NUC1                   1H
P1                  14.00 usec
PLW1           7.69999981 W

F2 - Processing parameters
SI                 16384
SF            300.1300065 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

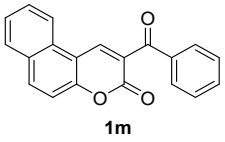
```
Current Data Parameters
NAME                  1m
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230530
Time                8.27
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   128
DS                     0
SWH            18028.846 Hz
FIDRES          0.550197 Hz
AQ             0.9087659 sec
RG                219.17
DW                27.733 usec
DE                 6.50 usec
TE                296.9 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

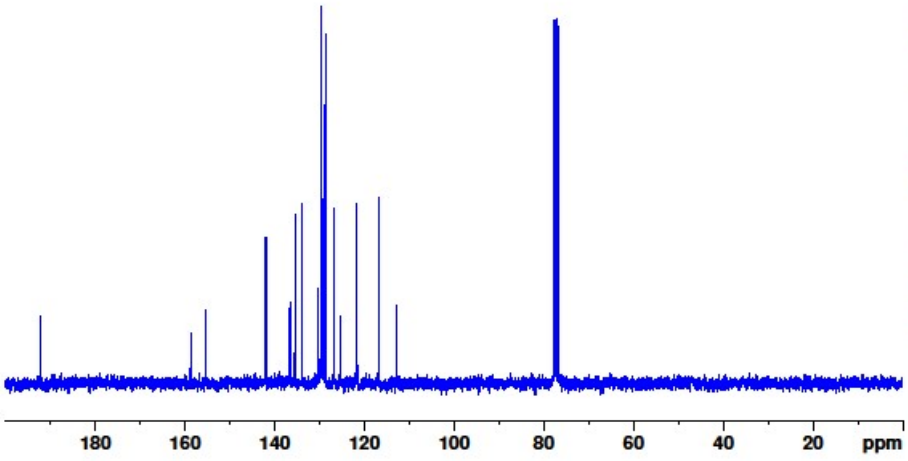
======== CHANNEL f1 ========
SFO1          75.4756726 MHz
NUC1                   13C
P1                  10.00 usec
PLW1          28.29999924 W

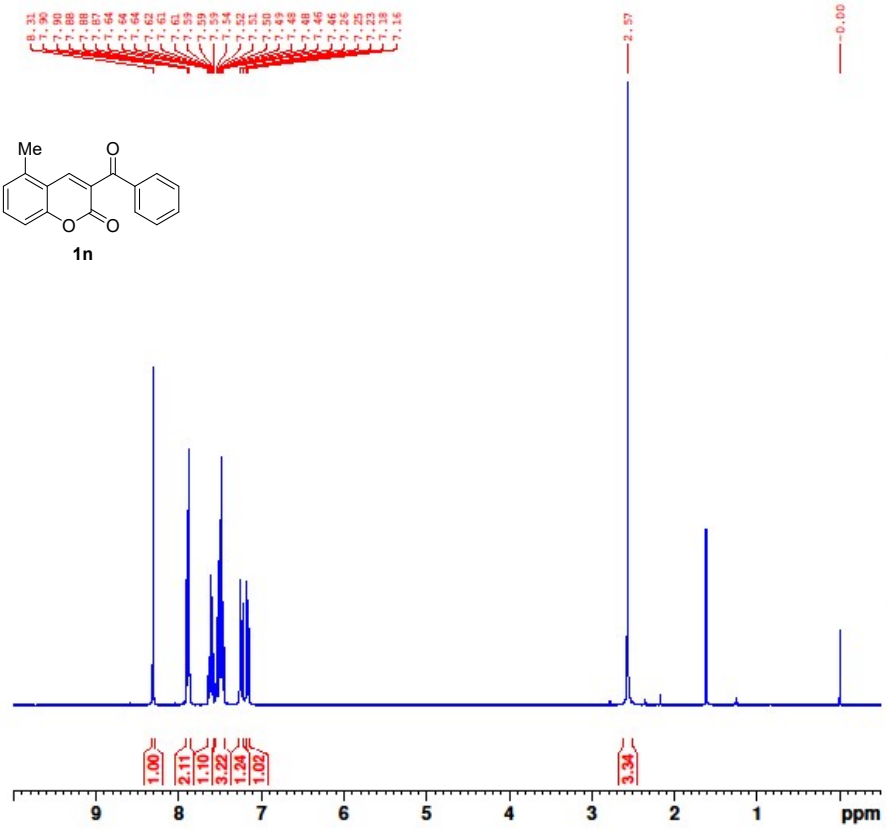
======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                   1H
CPDPRG[2 bi_waltz65_256
PCPD2               90.00 usec
PLW2           8.30000019 W
PLW12          0.20084000 W
PLW13          0.16268000 W

F2 - Processing parameters
SI                 32768
SF            75.4677442 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```



1m



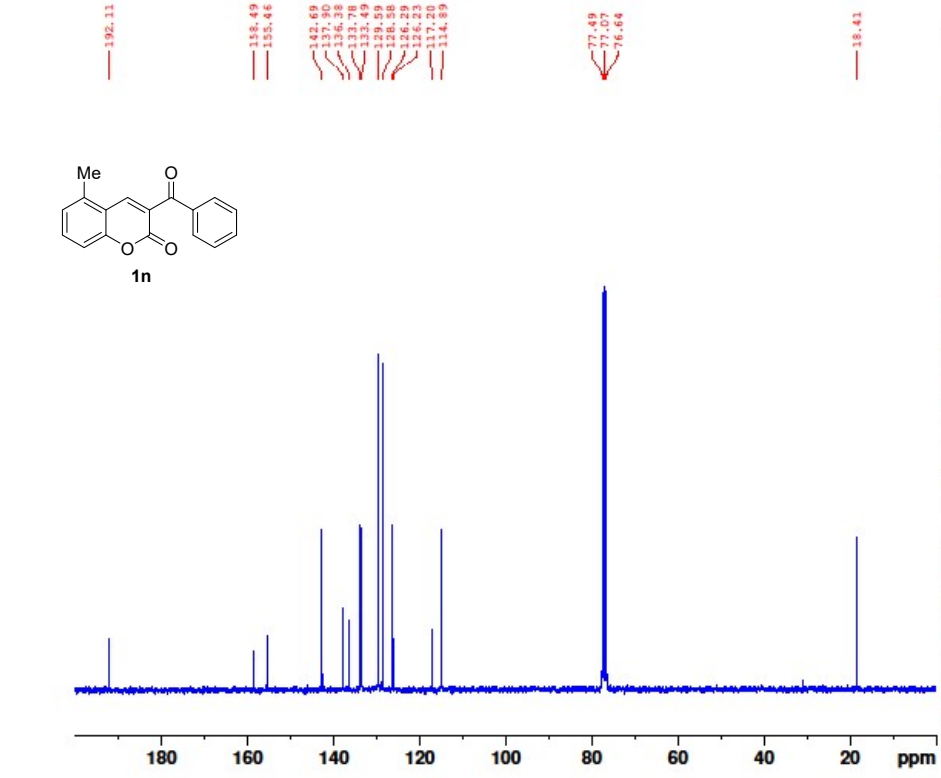



```
Current Data Parameters
NAME                  1n
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240105
Time               17.55
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    64
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              2.7262976 sec
RG                 219.17
DW                 83.200 usec
DE                 12.63 usec
TE                 297.1 K
D1              2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          300.1318008 MHz
NUC1                  1H
P1                 14.00 usec
PLW1           7.69999981 W

F2 - Processing parameters
SI                 16384
SF            300.1300068 MHz
WDW                   EM
SSB                    0
LB                  0 Hz
GB                     0
PC                  1.00
```



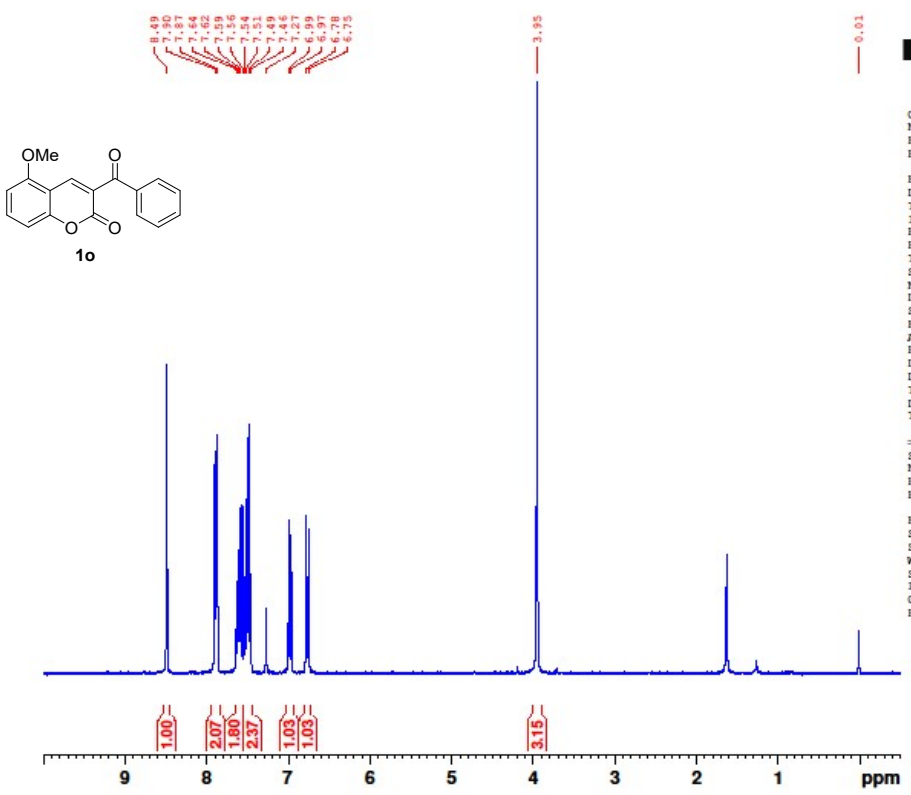

```
Current Data Parameters
NAME                  1n
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240112
Time               16.49
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  1424
DS                     0
SWH            18028.846 Hz
FIDRES          0.550197 Hz
AQ              0.9087659 sec
RG                 219.17
DW                 27.733 usec
DE                  6.50 usec
TE                 297.6 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1           75.4756726 MHz
NUC1                  13C
P1                 10.00 usec
PLW1           28.29999924 W

======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                  1H
CPDPRG[2 bi_waltz65_256
PCPD2              90.00 usec
PLW2           8.30000019 W
PLW12          0.20084000 W
PLW13          0.16268000 W

F2 - Processing parameters
SI                 32768
SF            75.4677485 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```



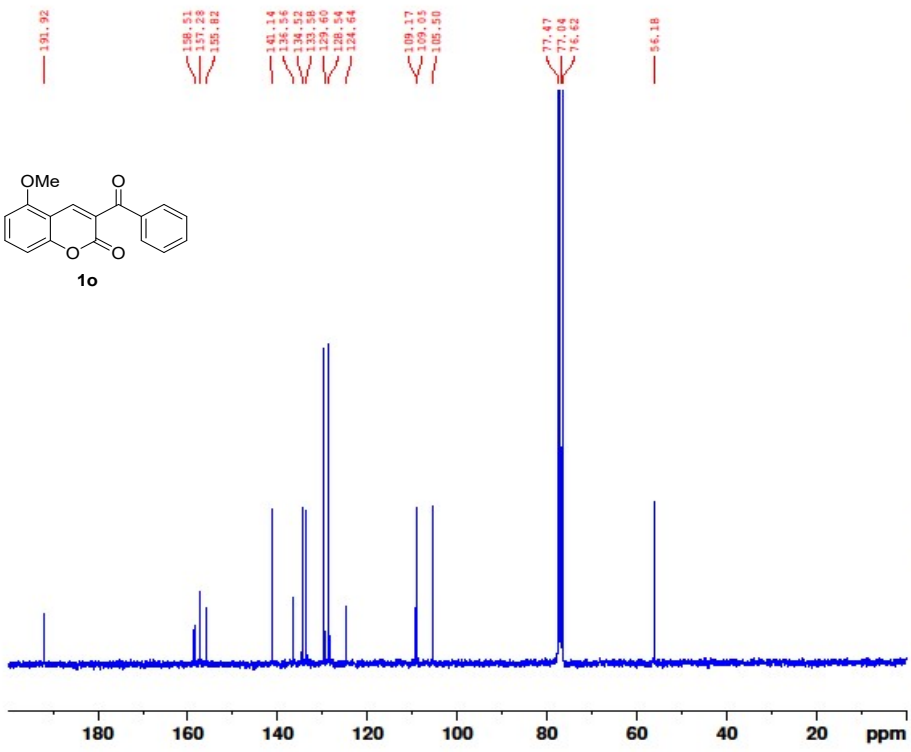
BRUKER

```
Current Data Parameters
NAME                  1o
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240115
Time               12.06
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    64
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              2.7262976 sec
RG                 219.17
DW                 83.200 usec
DE                 12.63 usec
TE                 297.7 K
D1              2.00000000 sec
TD0                    1

======== CHANNEL f1 =======
SFO1          300.1318008 MHz
NUC1                   1H
P1                  14.00 usec
PLW1           7.69999981 W

F2 - Processing parameters
SI                 16384
SF            300.1300035 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```



BRUKER

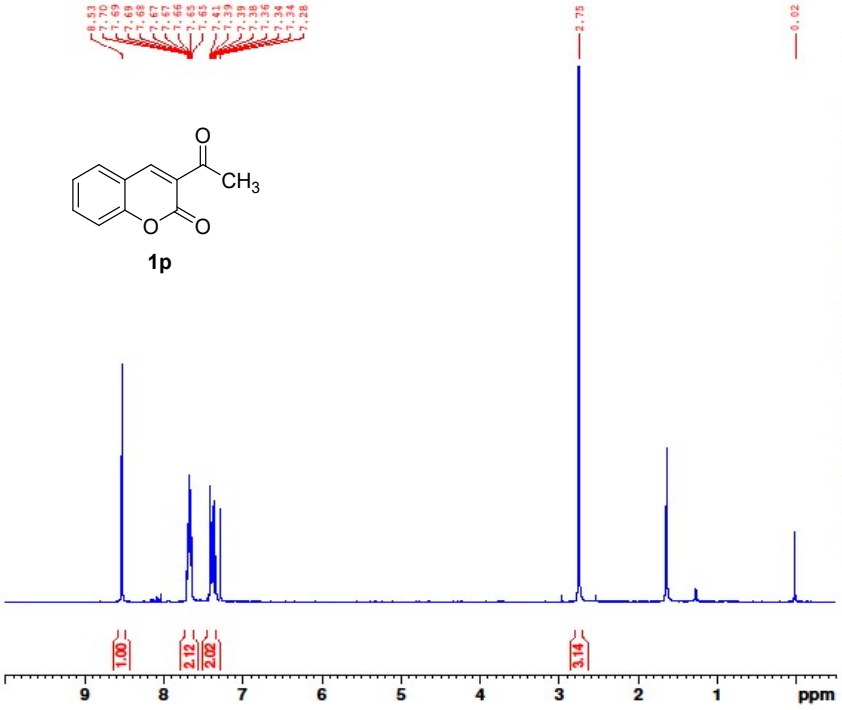
```
Current Data Parameters
NAME                  1o
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240115
Time               13.50
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  2048
DS                     0
SWH            18028.846 Hz
FIDRES          0.550197 Hz
AQ              0.9087659 sec
RG                 219.17
DW                 27.733 usec
DE                  6.50 usec
TE                 298.5 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          75.4756726 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          28.29999924 W

======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                   1H
CPDPRG[2 bi_waltz65_256
PCPD2              90.00 usec
PLW2           8.30000019 W
PLW12          0.20084000 W
PLW13          0.16268000 W

F2 - Processing parameters
SI                 32768
SF            75.4677485 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```



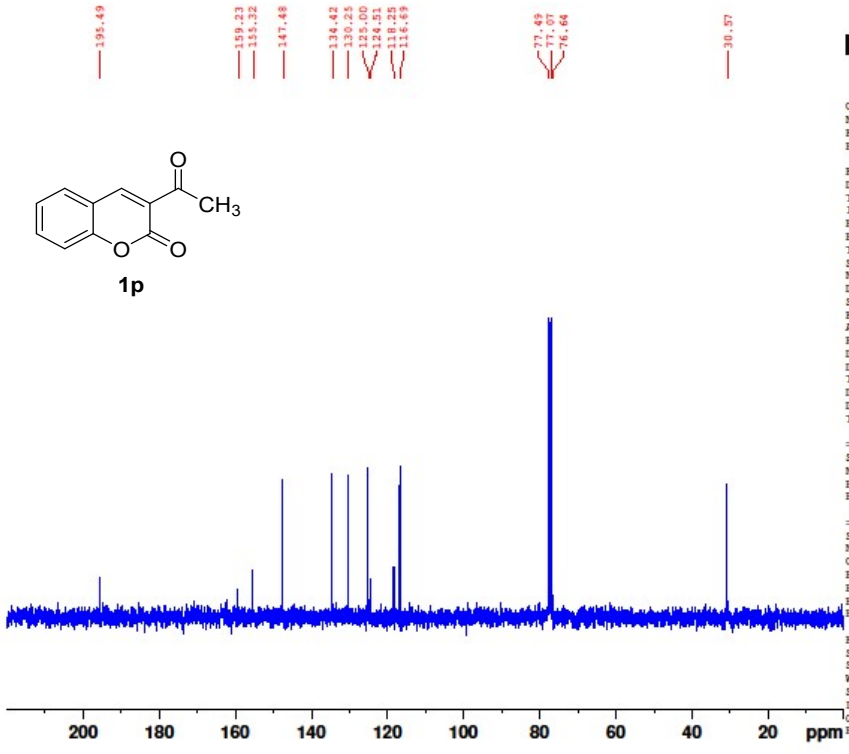
1p

```
Current Data Parameters
NAME          240809-LA-1P
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20240809
Time                 18.26
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     64
DS                      0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              2.7262976 sec
RG                 219.17
DW                 83.200 usec
DE                 12.63 usec
TE                 297.8 K
D1              2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          300.1318008 MHz
NUC1                    1H
P1                  14.00 usec
PLW1           7.69999981 W

F2 - Processing parameters
SI                  16384
SF            300.1300000 MHz
WDW                    EM
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.00
```



1p

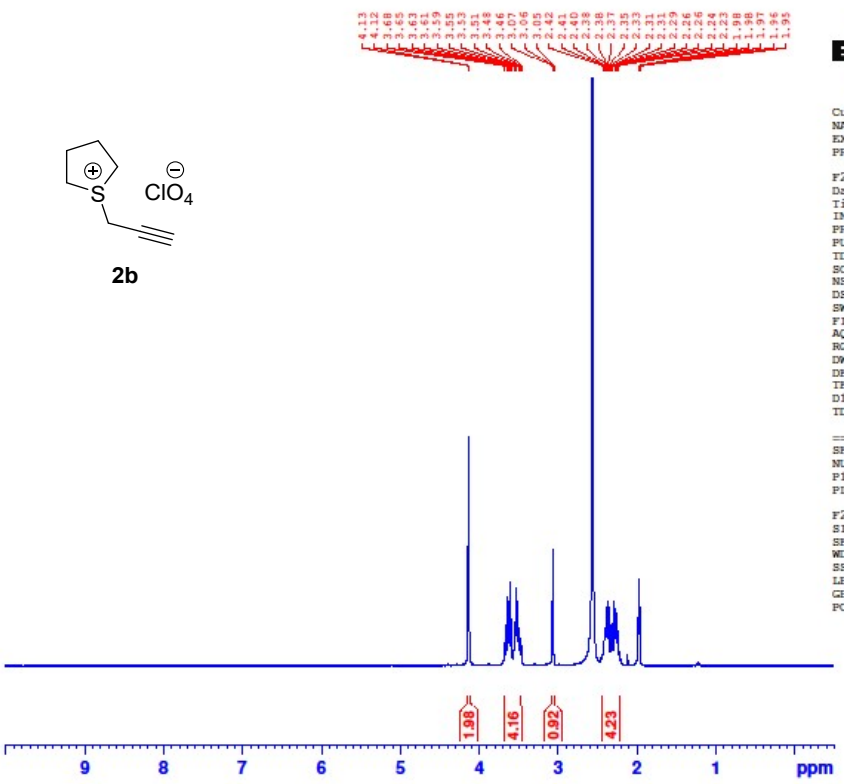
```
Current Data Parameters
NAME       240809-LA-1P-13C
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20240809
Time                 18.36
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                  32768
SOLVENT             CDCl3
NS                     64
DS                      0
SWH            18028.846 Hz
FIDRES          0.550197 Hz
AQ              0.9087659 sec
RG                 219.17
DW                 27.733 usec
DE                  6.50 usec
TE                 298.1 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          75.4756726 MHz
NUC1                   13C
P1                  10.00 usec
PLW1          28.29999924 W

======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                    1H
CPDPRG[2 bi_waltz65_256
PCPD2               90.00 usec
PLW2           8.30000019 W
PLW12          0.20084000 W
PLW13          0.16268000 W

F2 - Processing parameters
SI                  32768
SF            75.4677485 MHz
WDW                    EM
SSB                     0
LB                   2.00 Hz
GB                      0
PC                   1.00
```



2b

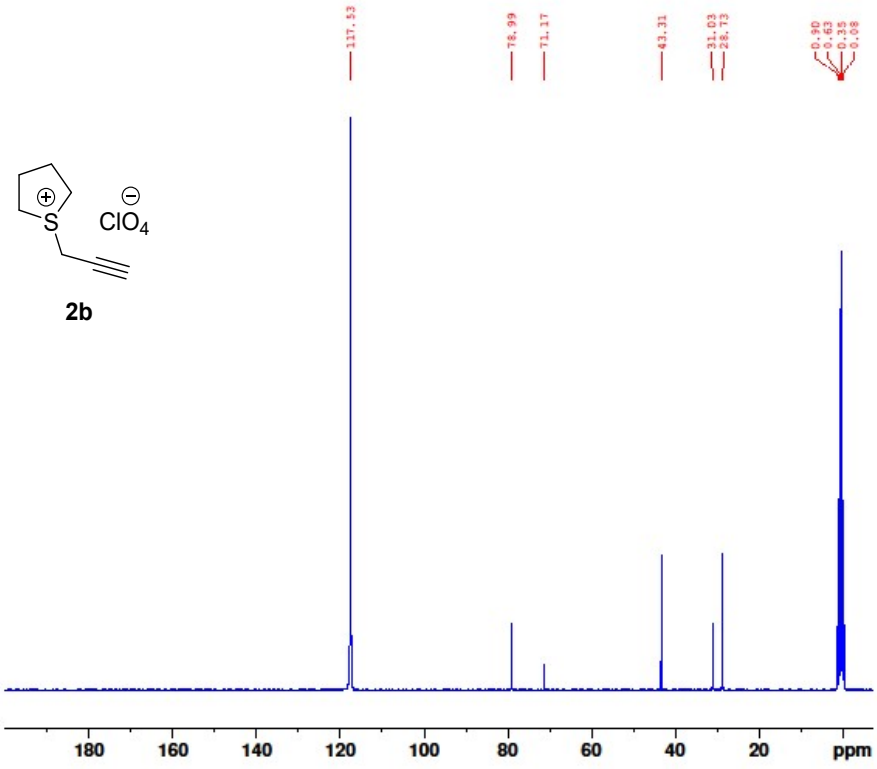
BRUKER

```
Current Data Parameters
NAME      240131-PSY-longtime
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20240131
Time                 22.46
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CD3CN
NS                      64
DS                       0
SWH               6009.615 Hz
FIDRES           0.183399 Hz
AQ                2.7262976 sec
RG                   148.08
DW                 83.200 usec
DE                  12.63 usec
TE                  296.1 K
D1              2.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            300.1318008 MHz
NUC1                    1H
P1                   14.00 usec
PLW1             7.69999981 W

F2 - Processing parameters
SI                   16384
SF              300.1300000 MHz
WDW                     EM
SSB                      0
LB                       0 Hz
GB                       0
PC                    1.00
```



2b

BRUKER

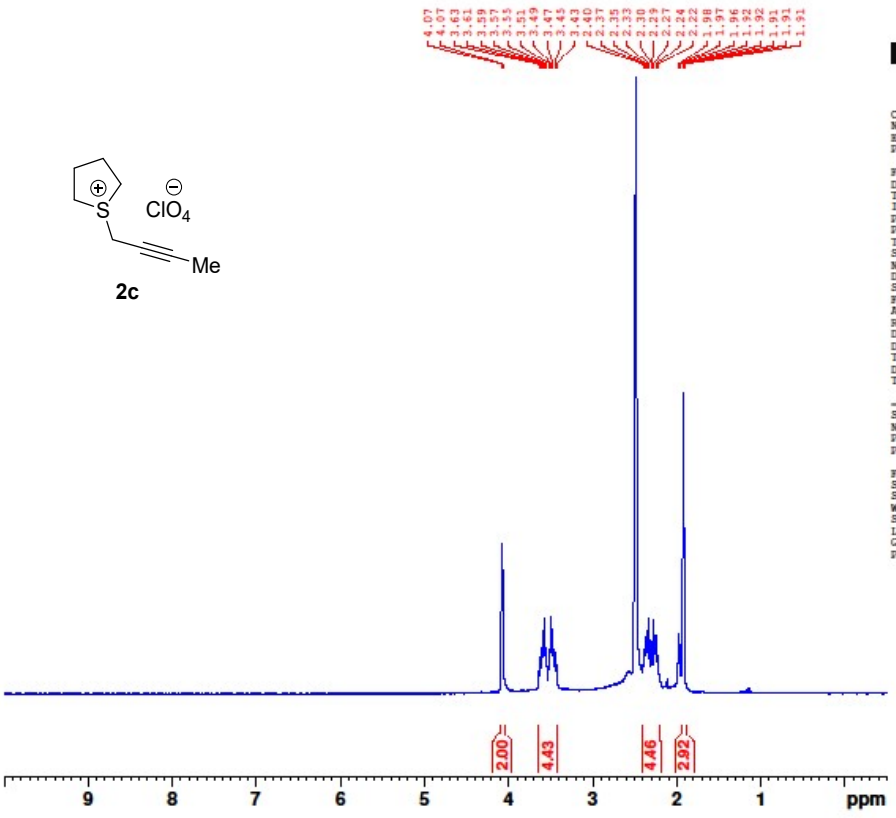
```
Current Data Parameters
NAME      240131-PSY-longtime
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20240201
Time                  5.37
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                   32768
SOLVENT              CD3CN
NS                    8192
DS                       0
SWH              18028.846 Hz
FIDRES           0.550197 Hz
AQ                0.9087659 sec
RG                   219.17
DW                 27.733 usec
DE                   6.50 usec
TE                  297.2 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            75.4756726 MHz
NUC1                    13C
P1                   10.00 usec
PLW1            28.29999924 W

======== CHANNEL f2 ========
SFO2           300.1312005 MHz
NUC2                    1H
CPDPRG[2 bi_waltz65_256
PCPD2                90.00 usec
PLW2            8.30000019 W
PLW12           0.20084000 W
PLW13           0.16268000 W

F2 - Processing parameters
SI                   32768
SF              75.4677485 MHz
WDW                     EM
SSB                      0
LB                    2.00 Hz
GB                       0
PC                    1.00
```



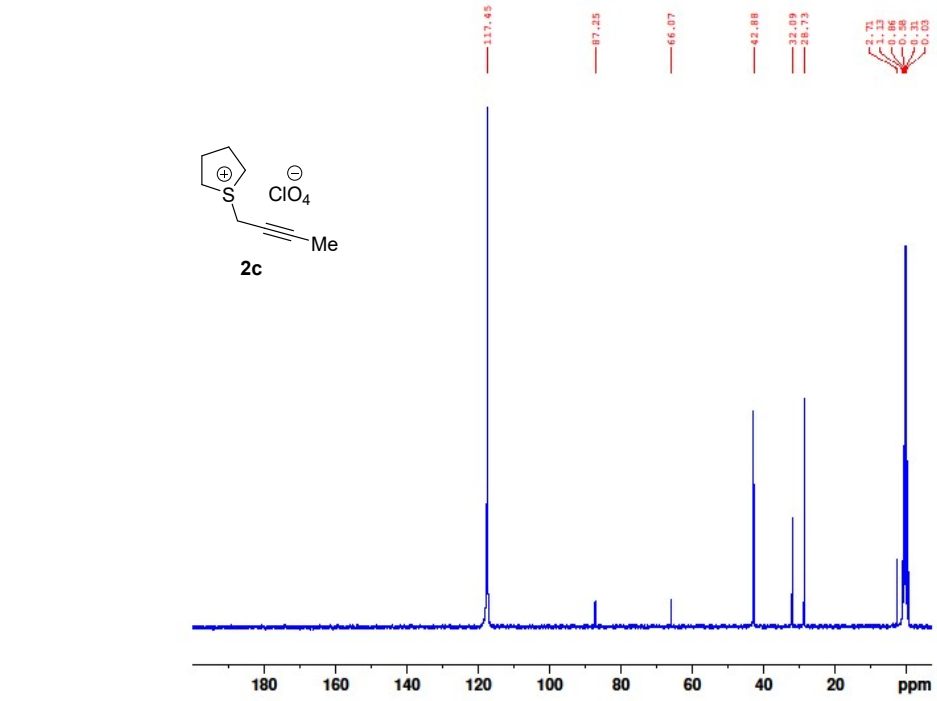
BRUKER

```
Current Data Parameters
NAME      240425-LA-PSYME-LONGTIME
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20240425
Time              15.17
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               32768
SOLVENT          CD3CN
NS                  64
DS                   0
SWH           6009.615 Hz
FIDRES        0.183399 Hz
AQ            2.7262976 sec
RG              121.85
DW              83.200 usec
DE              12.63 usec
TE              299.0 K
D1            2.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        300.1318008 MHz
NUC1               1H
P1                14.00 usec
PLW1         7.69999981 W

F2 - Processing parameters
SI               16384
SF          300.1300000 MHz
WDW                EM
SSB                 0
LB                  0 Hz
GB                  0
PC               1.00
```



BRUKER

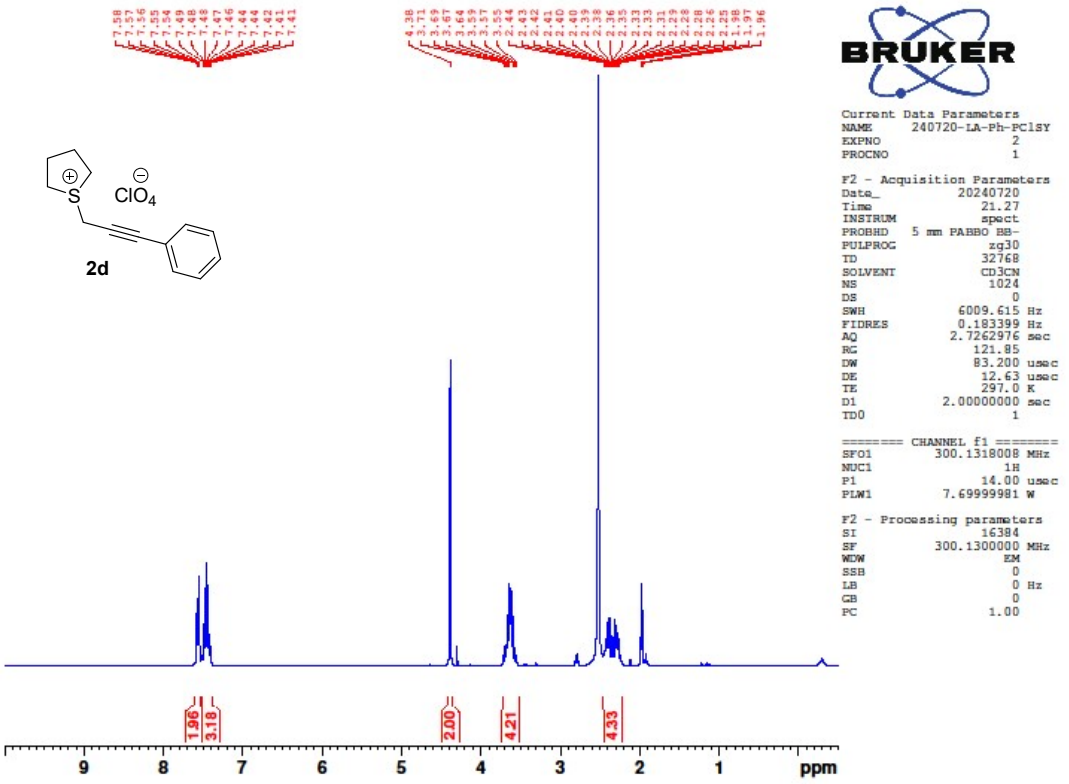
```
Current Data Parameters
NAME      240425-LA-PSYME-LONGTIME
EXPNO                2
PROCNO               1

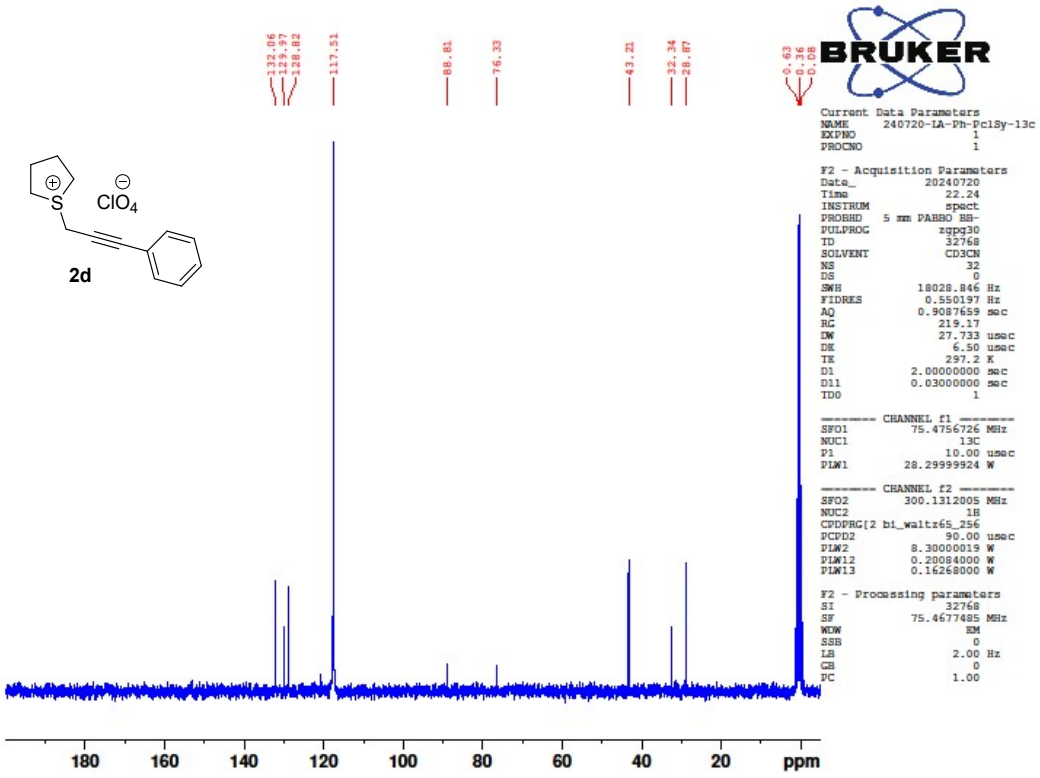
F2 - Acquisition Parameters
Date_          20240425
Time              16.56
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               32768
SOLVENT          CD3CN
NS                1933
DS                   0
SWH          18028.846 Hz
FIDRES        0.550197 Hz
AQ            0.9087659 sec
RG              219.17
DW              27.733 usec
DE               6.50 usec
TE              303.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

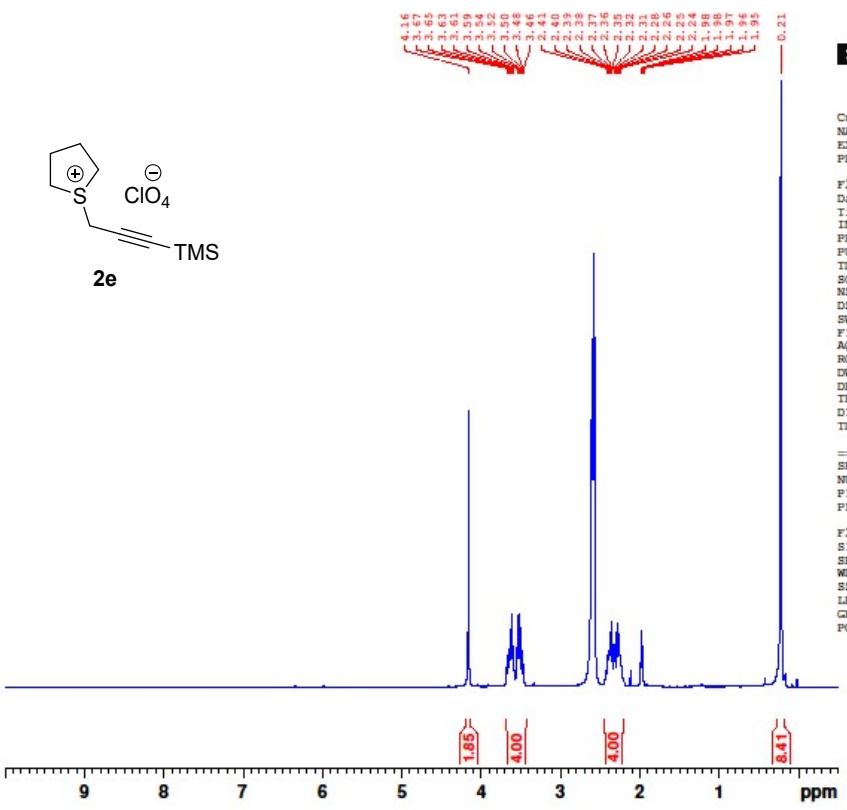
======== CHANNEL f1 ========
SFO1         75.4756726 MHz
NUC1               13C
P1                10.00 usec
PLW1         28.29999924 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2               1H
CPDPRG[2 bi_waltz65_256
PCPD2             90.00 usec
PLW2          8.30000019 W
PLW12         0.20084000 W
PLW13         0.16268000 W

F2 - Processing parameters
SI               32768
SF          75.4677485 MHz
WDW                EM
SSB                 0
LB               2.00 Hz
GB                  0
PC               1.00
```


7.58
7.57
7.56
7.55
7.54
7.49
7.48
7.48
7.47
7.46
7.44
7.44
7.42
7.41
7.41
4.38
3.71
3.69
3.67
3.64
3.59
3.57
3.55
2.44
2.43
2.42
2.41
2.40
2.40
2.39
2.38
2.36
2.35
2.33
2.33
2.31
2.29
2.28
2.28
2.26
2.25
1.98
1.97
1.96
ClO4
2d
1.96
3.18
2.00
4.21
4.33
9
8
7
6
5
4
3
2
1
ppm
BRUKER
Current Data Parameters
NAME 240720-LA-Ph-PClSY
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20240720
Time 21.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CD3CN
NS 1024
DS 0
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 121.85
DW 83.200 usec
DE 12.63 usec
TE 297.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318008 MHz
NUC1 1H
P1 14.00 usec
PLW1 7.69999981 W
F2 - Processing parameters
SI 16384
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00


132.06
129.97
128.82
117.51
88.61
76.33
43.21
32.34
28.87
0.63
0.36
0.08
ClO4
2d
180
160
140
120
100
80
60
40
20
ppm
BRUKER
Current Data Parameters
NAME 240720-LA-Ph-PClSy-13c
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20240720
Time 22.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CD3CN
NS 32
DS 0
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 219.17
DW 27.733 usec
DE 6.50 usec
TE 297.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 75.4756726 MHz
NUC1 13C
P1 10.00 usec
PLW1 28.29999924 W
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 bi_waltz65_256
PCPD2 90.00 usec
PLW2 8.30000019 W
PLW12 0.20084000 W
PLW13 0.16268000 W
F2 - Processing parameters
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00



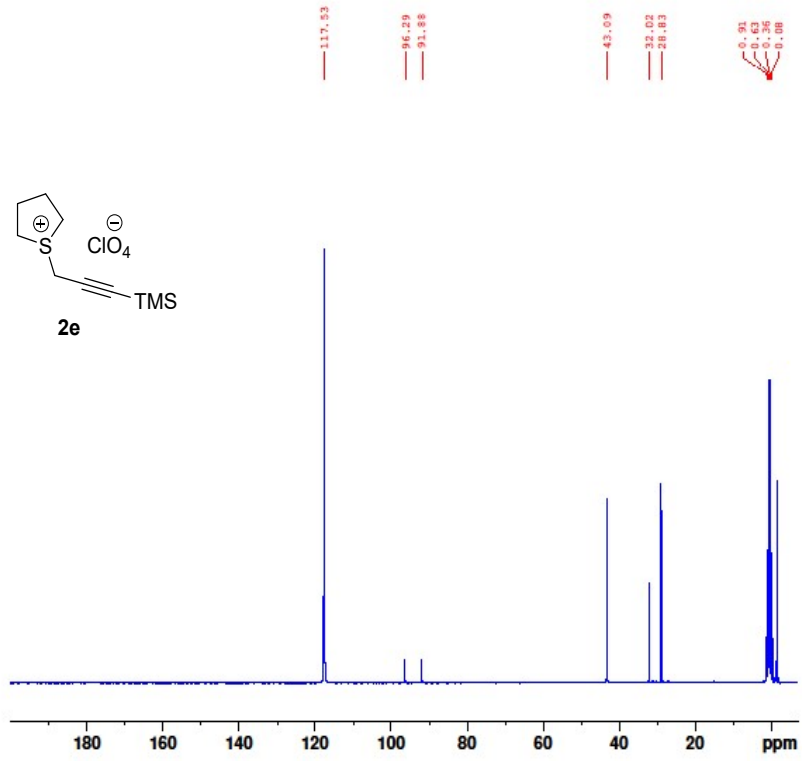
2e


```
Current Data Parameters
NAME      240426-LA-PSYTMS
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20240426
Time                 23.46
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CD3CN
NS                     64
DS                      0
SWH               6009.615 Hz
FIDRES           0.183399 Hz
AQ               2.7262976 sec
RG                   96.06
DW                 83.200 usec
DE                 12.63 usec
TE                 296.8 K
D1              2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          300.1318008 MHz
NUC1                    1H
P1                  14.00 usec
PLW1           7.69999981 W

F2 - Processing parameters
SI                  16384
SF            300.1300000 MHz
WDW                    EM
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.00
```



2e

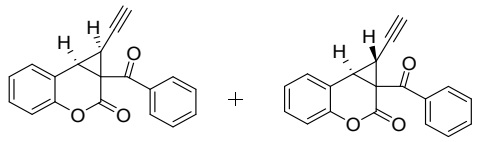

```
Current Data Parameters
NAME      240426-LA-PSYTMS
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_              20240427
Time                  9.55
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                  32768
SOLVENT             CD3CN
NS                  12288
DS                      0
SWH              18028.846 Hz
FIDRES           0.550197 Hz
AQ               0.9087659 sec
RG                  219.17
DW                 27.733 usec
DE                  6.50 usec
TE                 297.9 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

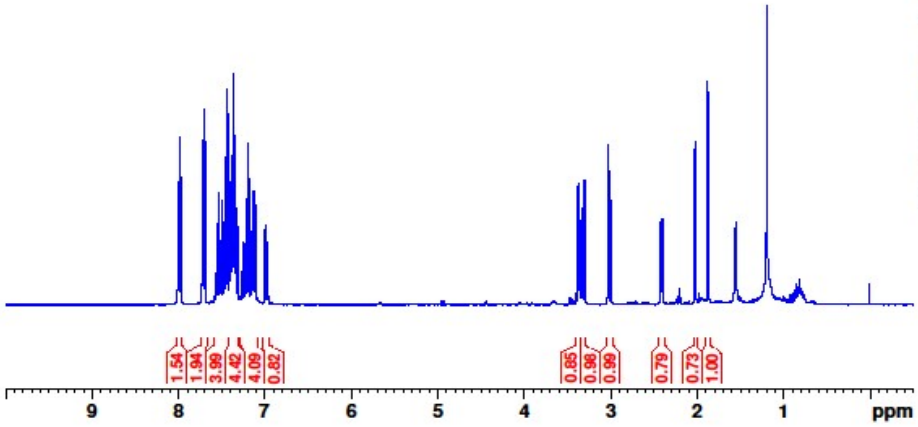
======== CHANNEL f1 ========
SFO1          75.4756726 MHz
NUC1                    13C
P1                  10.00 usec
PLW1           28.29999924 W

======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                    1H
CPDPRG[2 bi_waltz65_256
PCPD2               90.00 usec
PLW2           8.30000019 W
PLW12          0.20084000 W
PLW13          0.16268000 W

F2 - Processing parameters
SI                  32768
SF            75.4677485 MHz
WDW                    EM
SSB                     0
LB                   2.00 Hz
GB                      0
PC                   1.00
```



3a 3a'

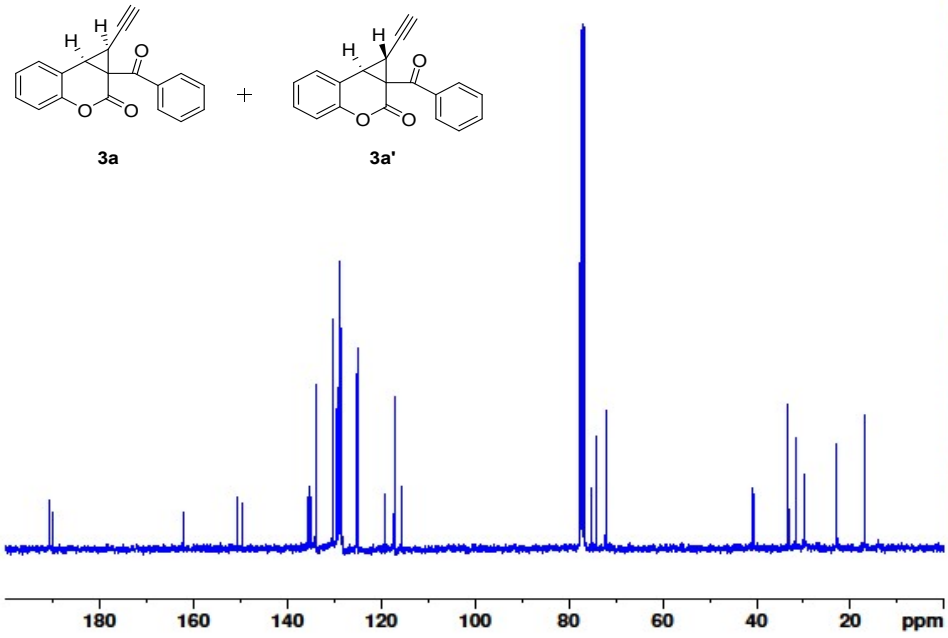


```
Current Data Parameters
NAME      230512-LA-L1-OVERNIGHT
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20230513
Time                       21.05
INSTRUM                    spect
PROBHD   5 mm PABBO BB-
PULPROG                     zg30
TD                         32768
SOLVENT                    CDCl3
NS                            13
DS                             0
SWH                     6009.615 Hz
FIDRES                  0.183399 Hz
AQ                      2.7262976 sec
RG                         194.81
DW                         83.200 usec
DE                         12.63 usec
TE                         296.6 K
D1                      2.00000000 sec
TD0                            1

======== CHANNEL f1 ========
SFO1                  300.1318008 MHz
NUC1                          1H
P1                         14.00 usec
PLW1                   7.69999981 W

F2 - Processing parameters
SI                         16384
SF                    300.1300278 MHz
WDW                           EM
SSB                            0
LB                             0 Hz
GB                             0
PC                          1.00
```



3a 3a'

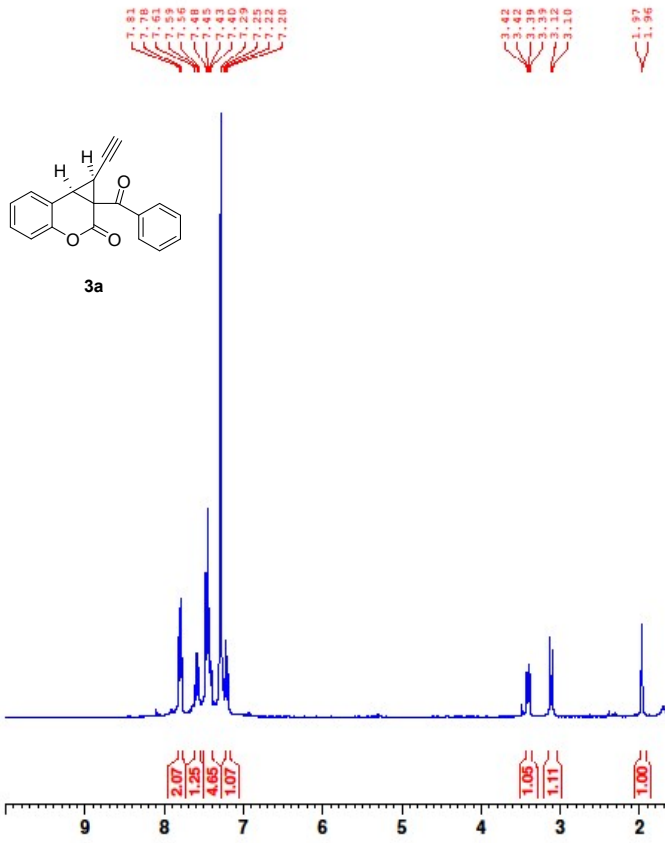
```
Current Data Parameters
NAME      230512-LA-L1-OVERNIGHT
EXPNO                          3
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20230514
Time                       1.29
INSTRUM                    spect
PROBHD   5 mm PABBO BB-
PULPROG                 zgpg30
TD                         32768
SOLVENT                    CDCl3
NS                          2048
DS                             0
SWH                    18028.846 Hz
FIDRES                  0.550197 Hz
AQ                      0.9087659 sec
RG                         219.17
DW                         27.733 usec
DE                          6.50 usec
TE                         297.5 K
D1                      2.00000000 sec
D11                     0.03000000 sec
TD0                            1

======== CHANNEL f1 ========
SFO1                  75.4756726 MHz
NUC1                          13C
P1                         10.00 usec
PLW1                   28.29999924 W

======== CHANNEL f2 ========
SFO2                  300.1312005 MHz
NUC2                          1H
CPDPRG[2 bi_waltz65_256
PCPD2                      90.00 usec
PLW2                   8.30000019 W
PLW12                  0.20084000 W
PLW13                  0.16268000 W

F2 - Processing parameters
SI                         32768
SF                    75.4677485 MHz
WDW                           EM
SSB                            0
LB                          2.00 Hz
GB                             0
PC                          1.00
```



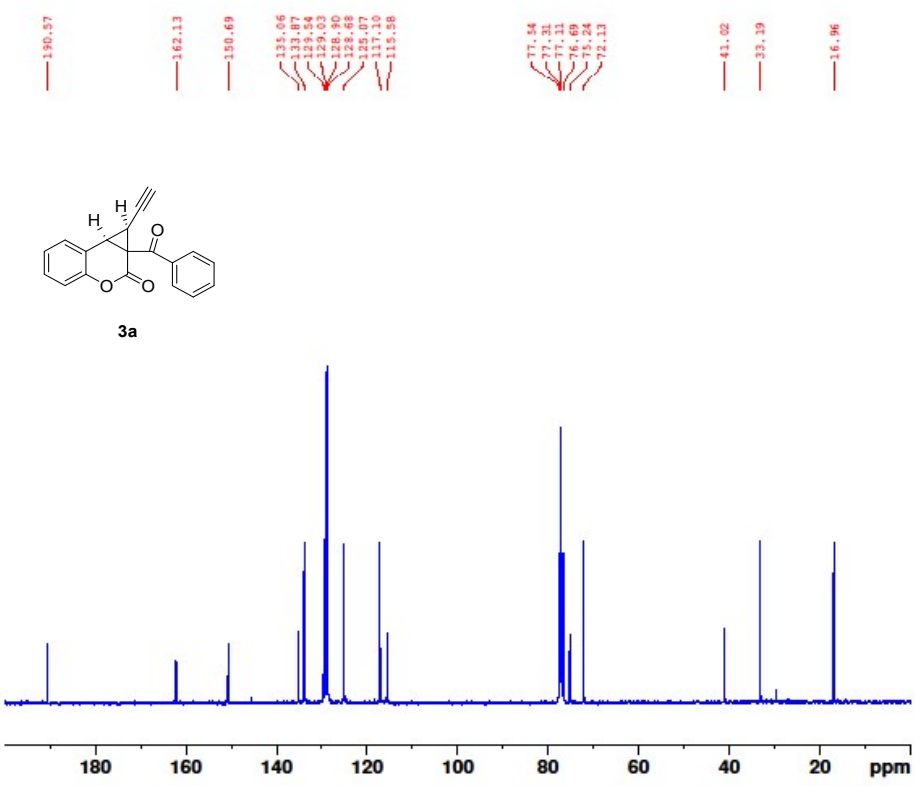
BRUKER

```
Current Data Parameters
NAME      240429-LA-L1-a
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240429
Time              14.04
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ             2.7262976 sec
RG                106.61
DW                83.200 usec
DE                12.63 usec
TE                297.1 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         300.1318008 MHz
NUC1                   1H
P1                 14.00 usec
PLW1          7.69999981 W

F2 - Processing parameters
SI                 16384
SF            300.1300000 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```



BRUKER

```
Current Data Parameters
NAME      240429-LA-L1-a
EXPNO                  2
PROCNO                 1

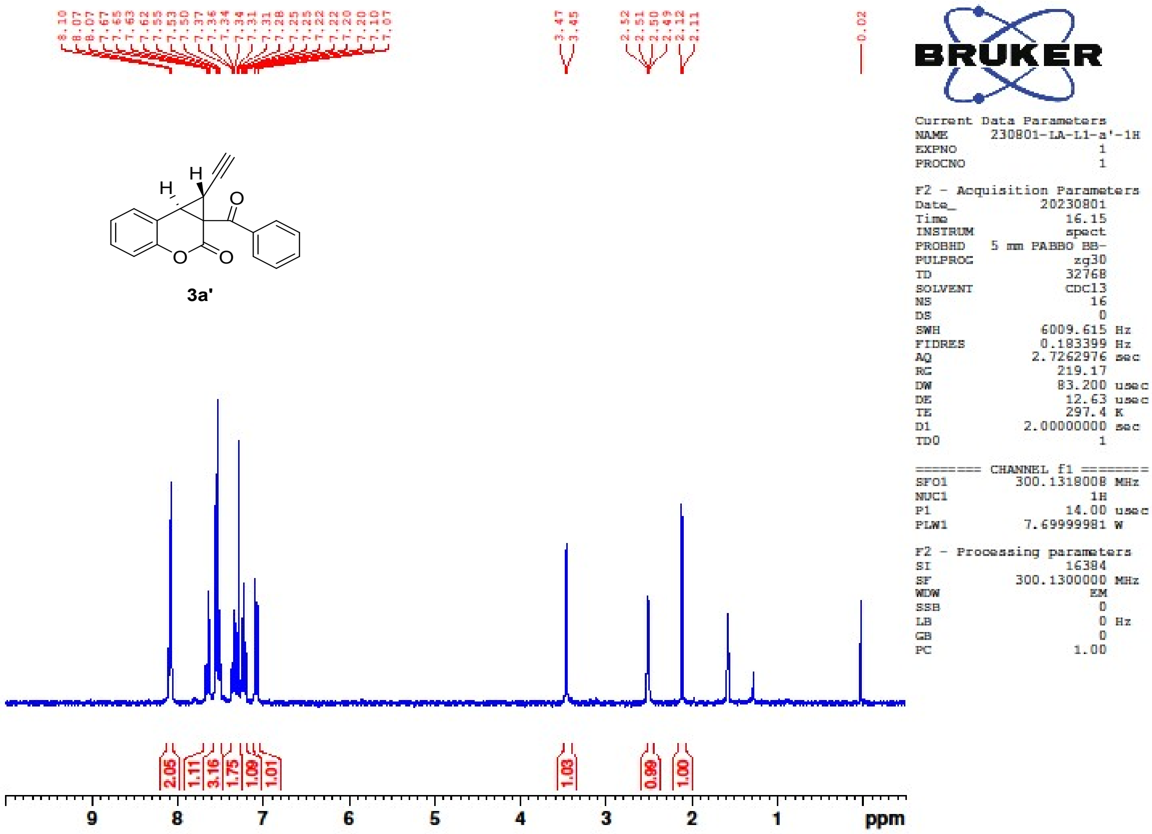
F2 - Acquisition Parameters
Date_           20240429
Time              15.45
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  2048
DS                     0
SWH            18028.846 Hz
FIDRES          0.550197 Hz
AQ             0.9087659 sec
RG                219.17
DW                27.733 usec
DE                 6.50 usec
TE                298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         75.4756726 MHz
NUC1                  13C
P1                10.00 usec
PLW1         28.29999924 W

======== CHANNEL f2 ========
SFO2         300.1312005 MHz
NUC2                   1H
CPDPRG[2 bi_waltz65_256
PCPD2             90.00 usec
PLW2           8.30000019 W
PLW12          0.20084000 W
PLW13          0.16268000 W

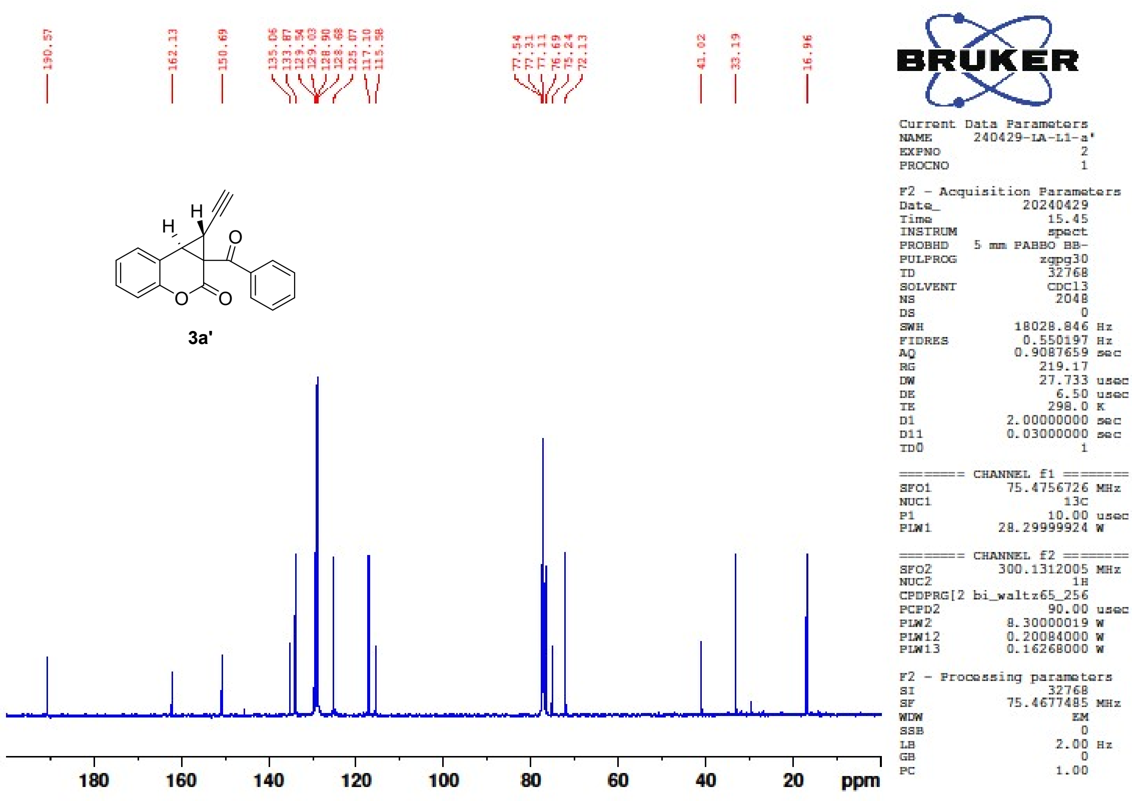
F2 - Processing parameters
SI                 32768
SF            75.4677485 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```

3a'

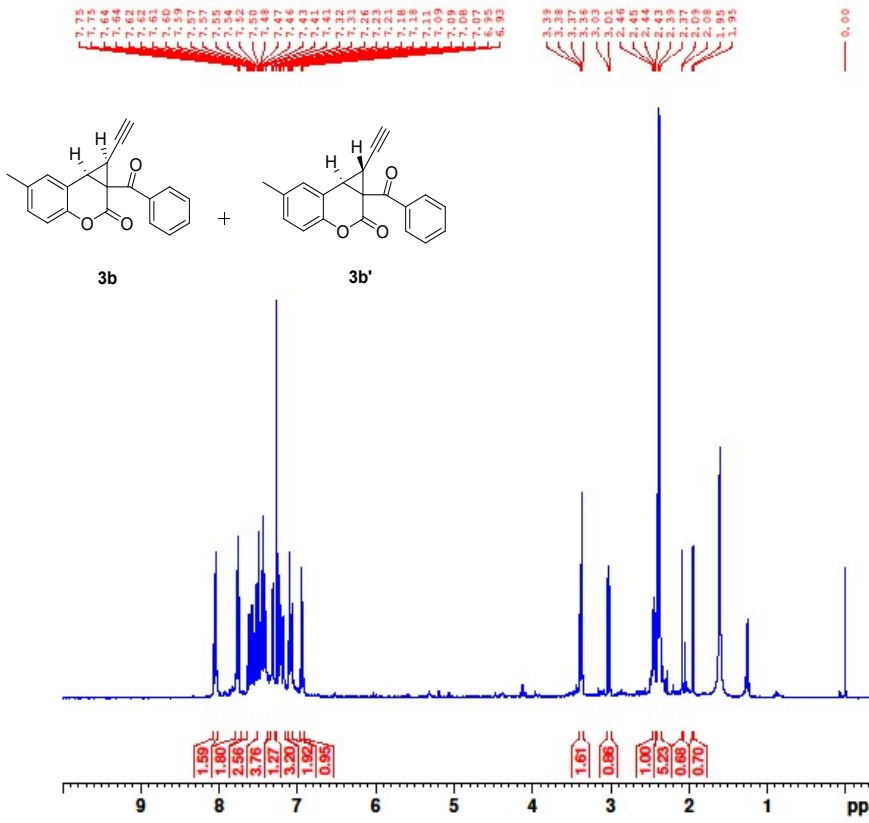


8.10
8.07
8.07
7.67
7.65
7.63
7.62
7.55
7.53
7.50
7.37
7.36
7.34
7.34
7.31
7.31
7.28
7.25
7.25
7.22
7.22
7.20
7.20
7.10
7.07
3.47
3.45
2.52
2.51
2.50
2.49
2.12
2.11
0.02
2.05
1.11
3.16
1.75
1.09
1.01
1.03
0.99
1.00
9
8
7
6
5
4
3
2
1
ppm
BRUKER
Current Data Parameters
NAME 230801-LA-L1-a'-1H
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230801
Time 16.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 219.17
DW 83.200 usec
DE 12.63 usec
TE 297.4 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.1318008 MHz
NUC1 1H
P1 14.00 usec
PLW1 7.69999981 W
F2 - Processing parameters
SI 16384
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

3a'



190.57
162.13
150.69
135.06
133.87
129.54
129.03
128.90
128.68
125.07
117.10
115.58
77.54
77.31
77.11
76.69
75.24
72.13
41.02
33.19
16.96
180
160
140
120
100
80
60
40
20
ppm
BRUKER
Current Data Parameters
NAME 240429-LA-L1-a'
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20240429
Time 15.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2048
DS 0
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 219.17
DW 27.733 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======= CHANNEL f1 =======
SFO1 75.4756726 MHz
NUC1 13C
P1 10.00 usec
PLW1 28.29999924 W
======= CHANNEL f2 =======
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 bi_waltz65_256
PCPD2 90.00 usec
PLW2 8.30000019 W
PLW12 0.20084000 W
PLW13 0.16268000 W
F2 - Processing parameters
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

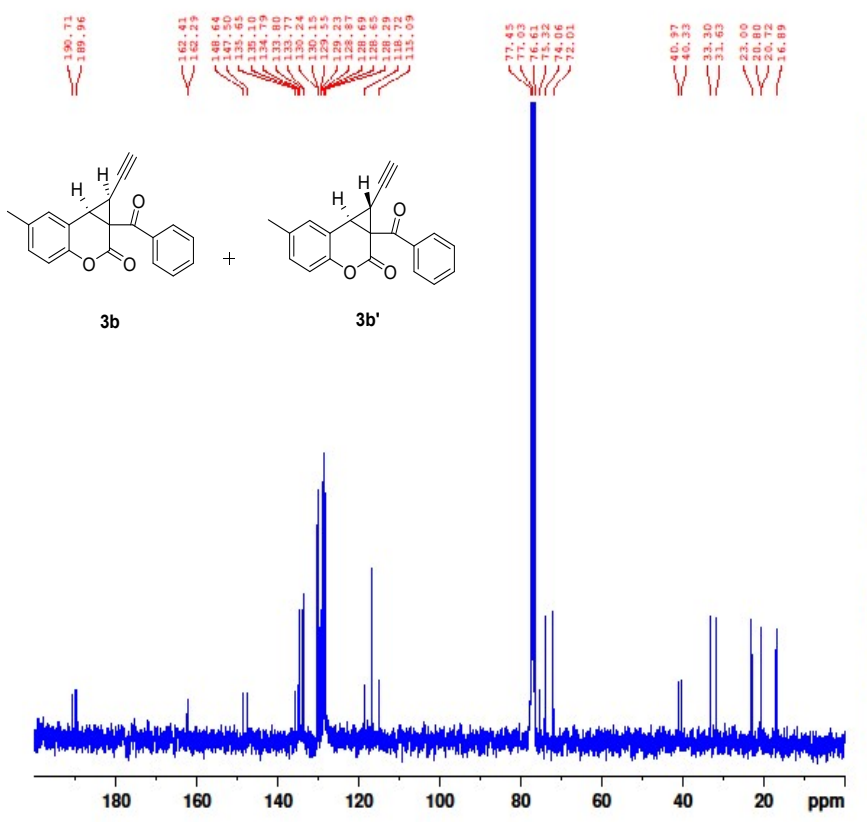



```
Current Data Parameters
NAME      231105-LA-03988-L2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231105
Time              11.30
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   64
DS                    0
SWH            6009.615 Hz
FIDRES         0.183399 Hz
AQ             2.7262976 sec
RG               219.17
DW               83.200 usec
DE               12.63 usec
TE               296.1 K
D1             2.00000000 sec
TD0                   1

======== CHANNEL f1 =======
SFO1         300.1318008 MHz
NUC1               1H
P1               14.00 usec
PLW1          7.69999981 W

F2 - Processing parameters
SI                16384
SF           300.1300070 MHz
WDW                EM
SSB                   0
LB                 0 Hz
GB                    0
PC                 1.00
```



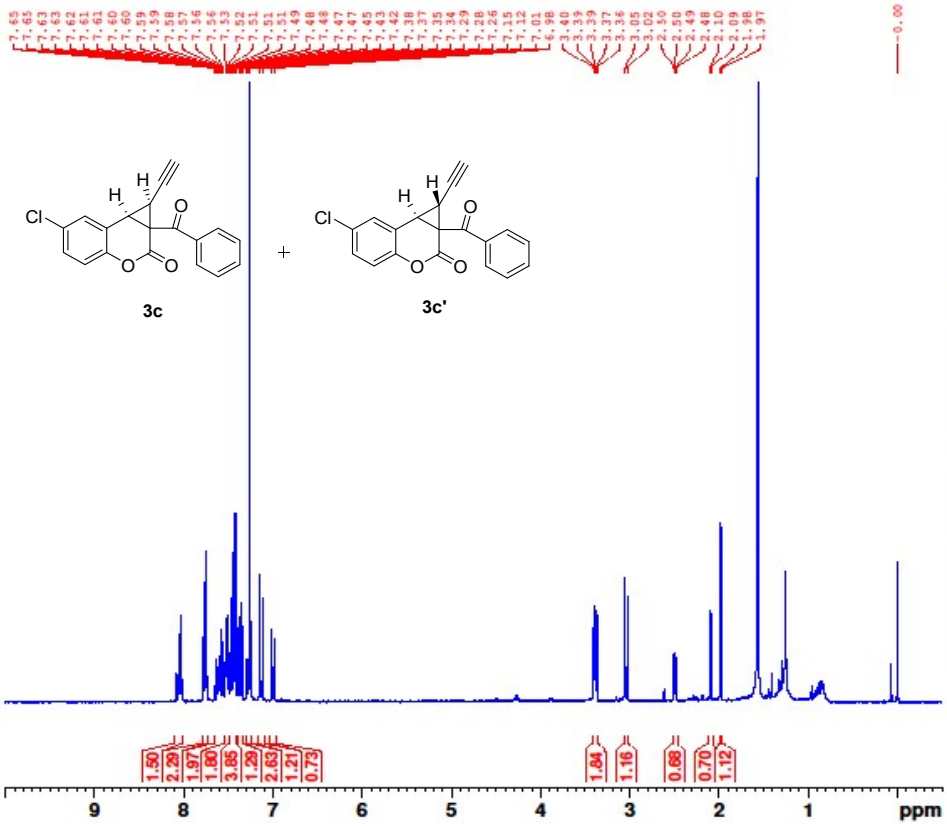

```
Current Data Parameters
NAME      231105-LA-03988-L2
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231105
Time              13.12
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 2048
DS                    0
SWH           18028.846 Hz
FIDRES         0.550197 Hz
AQ             0.9087659 sec
RG               219.17
DW               27.733 usec
DE                6.50 usec
TE               296.6 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                   1

======== CHANNEL f1 =======
SFO1         75.4756726 MHz
NUC1               13C
P1               10.00 usec
PLW1         28.29999924 W

======== CHANNEL f2 =======
SFO2         300.1312005 MHz
NUC2               1H
CPDPRG[2 bi_waltz65_256
PCPD2            90.00 usec
PLW2          8.30000019 W
PLW12         0.20084000 W
PLW13         0.16268000 W

F2 - Processing parameters
SI                32768
SF           75.4677485 MHz
WDW                EM
SSB                   0
LB                2.00 Hz
GB                    0
PC                 1.00
```

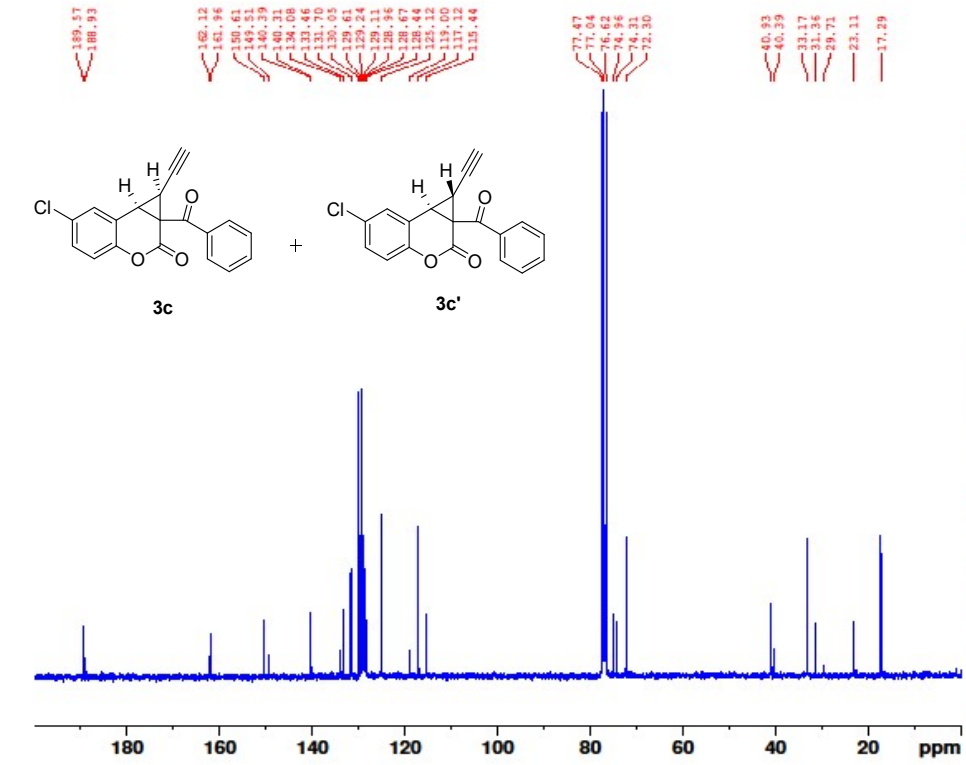



```
Current Data Parameters
NAME                  L7
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231112
Time               14.12
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   64
DS                    0
SWH           6009.615 Hz
FIDRES        0.183399 Hz
AQ            2.7262976 sec
RG                219.17
DW              83.200 usec
DE               12.63 usec
TE               297.9 K
D1            2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        300.1318008 MHz
NUC1                1H
P1                14.00 usec
PLW1         7.69999981 W

F2 - Processing parameters
SI                16384
SF          300.1300079 MHz
WDW                  EM
SSB                   0
LB                 0 Hz
GB                    0
PC                 1.00
```



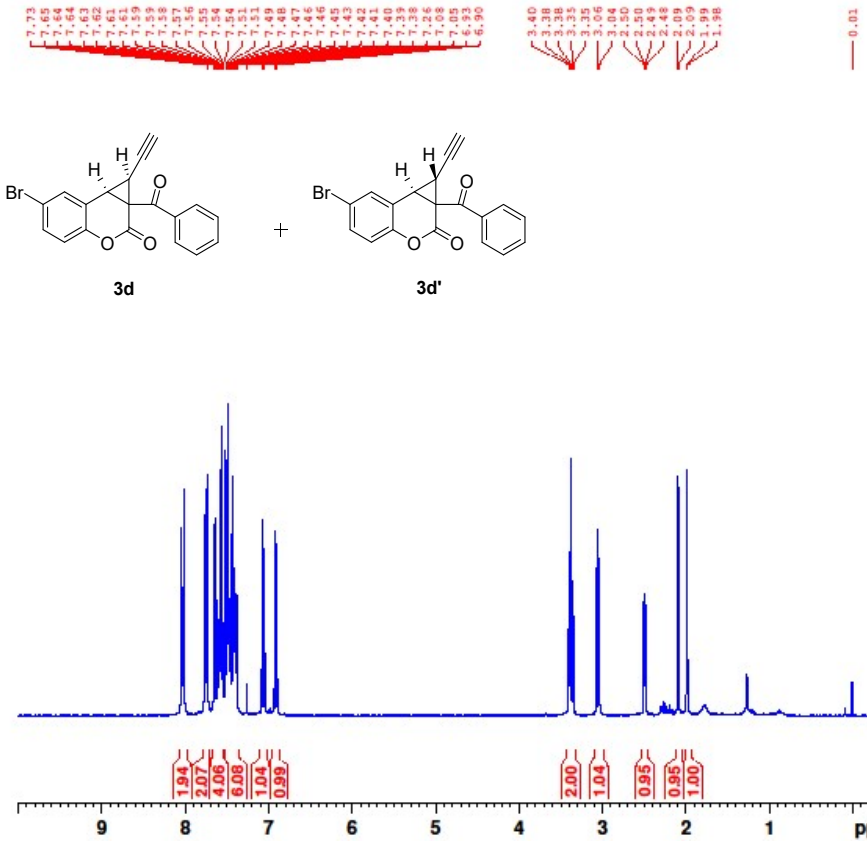

```
Current Data Parameters
NAME                  L7
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240101
Time               18.49
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 2048
DS                    0
SWH          18028.846 Hz
FIDRES        0.550197 Hz
AQ            0.9087659 sec
RG                219.17
DW              27.733 usec
DE                6.50 usec
TE               298.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         75.4756726 MHz
NUC1                13C
P1                10.00 usec
PLW1         28.29999924 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2                1H
CPDPRG[2 bi_waltz65_256
PCPD2             90.00 usec
PLW2          8.30000019 W
PLW12         0.20084000 W
PLW13         0.16268000 W

F2 - Processing parameters
SI                32768
SF          75.4677485 MHz
WDW                  EM
SSB                   0
LB                 2.00 Hz
GB                    0
PC                 1.00
```

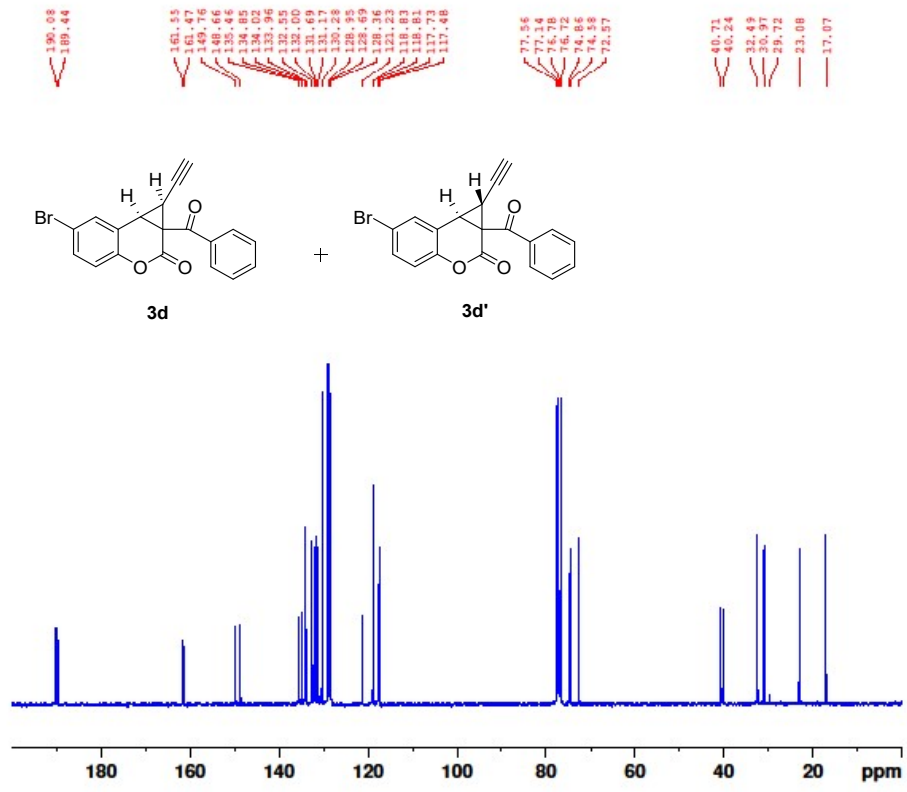



```
Current Data Parameters
NAME         240101-LA-L8
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_             20240101
Time                 15.05
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     64
DS                      0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              2.7262976 sec
RG                 106.61
DW                 83.200 usec
DE                 12.63 usec
TE                 297.5 K
D1              2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          300.1318008 MHz
NUC1                    1H
P1                  14.00 usec
PLW1          7.69999981 W

F2 - Processing parameters
SI                  16384
SF            300.1300071 MHz
WDW                    EM
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.00
```



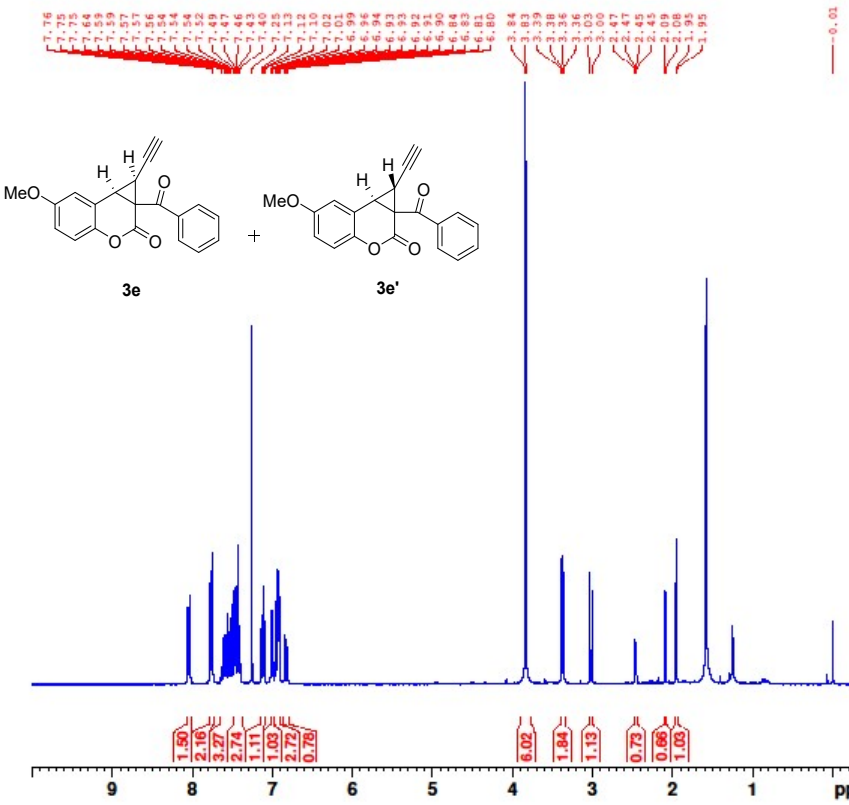

```
Current Data Parameters
NAME         240101-LA-L8
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_             20240101
Time                 16.51
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                  32768
SOLVENT             CDCl3
NS                   2048
DS                      0
SWH            18028.846 Hz
FIDRES          0.550197 Hz
AQ              0.9087659 sec
RG                 219.17
DW                 27.733 usec
DE                  6.50 usec
TE                 298.5 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          75.4756726 MHz
NUC1                   13C
P1                  10.00 usec
PLW1          28.29999924 W

======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                    1H
CPDPRG[2 bi_waltz65_256
PCPD2               90.00 usec
PLW2          8.30000019 W
PLW12         0.20084000 W
PLW13         0.16268000 W

F2 - Processing parameters
SI                  32768
SF            75.4677485 MHz
WDW                    EM
SSB                     0
LB                   2.00 Hz
GB                      0
PC                   1.00
```

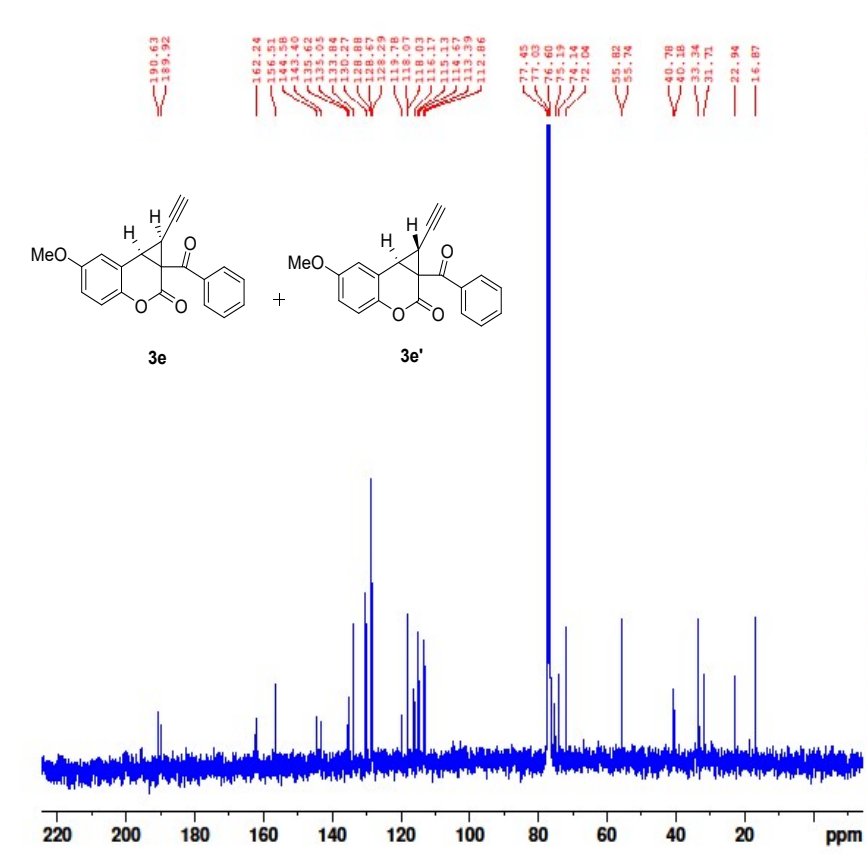



```
Current Data Parameters
NAME                  L3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231103
Time               15.59
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    64
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ             2.7262976 sec
RG                219.17
DW                83.200 usec
DE                12.63 usec
TE                295.8 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 =======
SFO1          300.1318008 MHz
NUC1                  1H
P1                 14.00 usec
PLW1           7.69999981 W

F2 - Processing parameters
SI                 16384
SF            300.1300089 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```



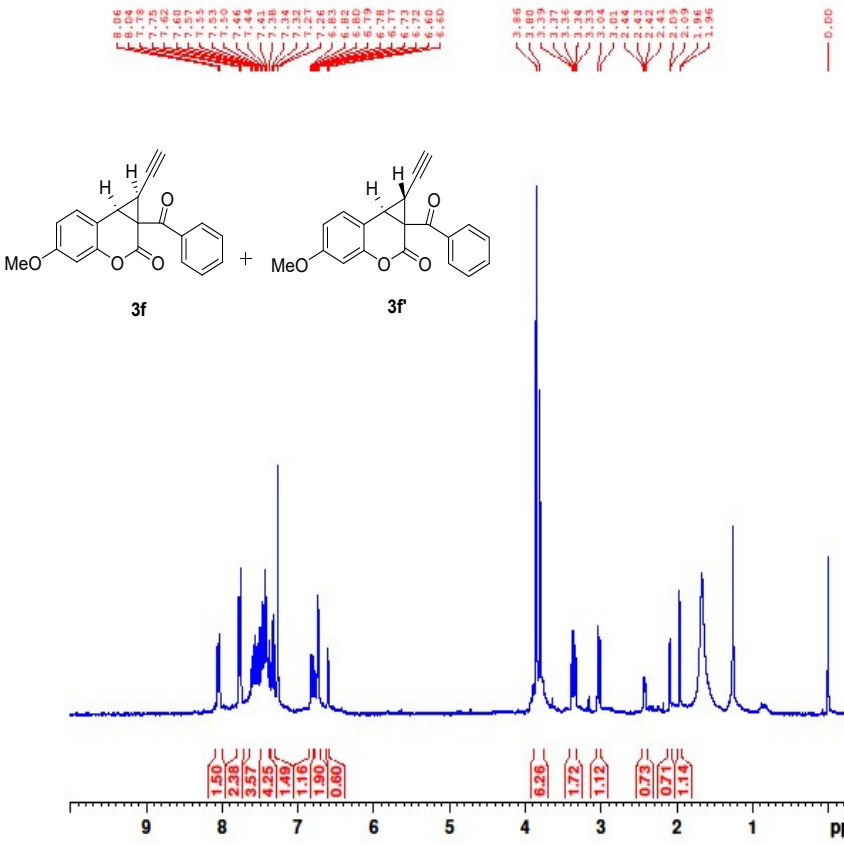

```
Current Data Parameters
NAME                  L3
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231103
Time               17.41
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  2048
DS                     0
SWH            18028.846 Hz
FIDRES          0.550197 Hz
AQ             0.9087659 sec
RG                219.17
DW                27.733 usec
DE                 6.50 usec
TE                296.9 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 =======
SFO1           75.4756726 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          28.29999924 W

======== CHANNEL f2 =======
SFO2          300.1312005 MHz
NUC2                  1H
CPDPRG[2 bi_waltz65_256
PCPD2              90.00 usec
PLW2           8.30000019 W
PLW12          0.20084000 W
PLW13          0.16268000 W

F2 - Processing parameters
SI                 32768
SF             75.4677485 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```

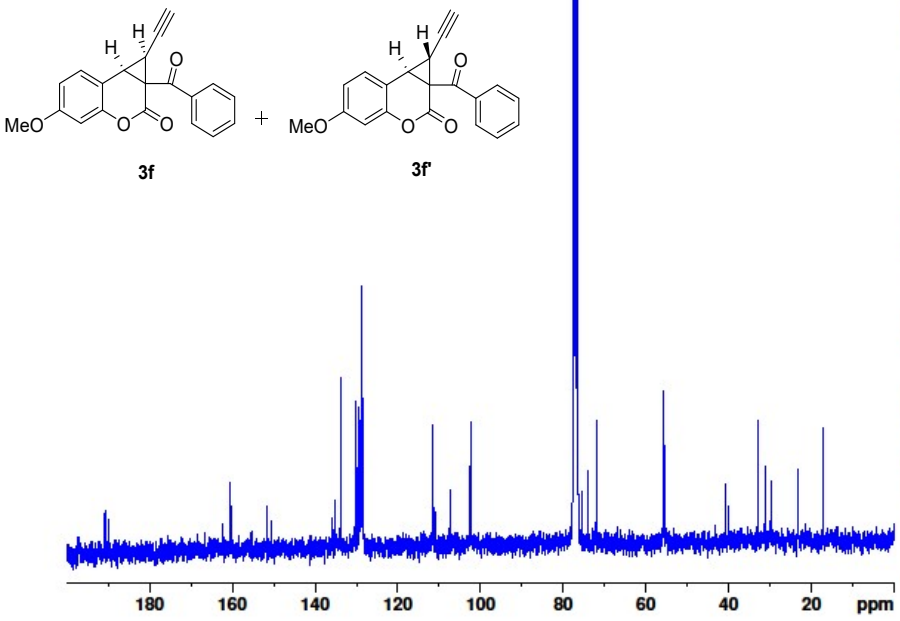



```
Current Data Parameters
NAME          240102-LA-L4
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20240101
Time                 20.00
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     64
DS                      0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              2.7262976 sec
RG                 219.17
DW                 83.200 usec
DE                 12.63 usec
TE                 297.8 K
D1              2.00000000 sec
TD0                     1

======== CHANNEL f1 =======
SFO1          300.1318008 MHz
NUC1                  1H
P1                 14.00 usec
PLW1           7.69999981 W

F2 - Processing parameters
SI                  16384
SF            300.1300064 MHz
WDW                    EM
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.00
```



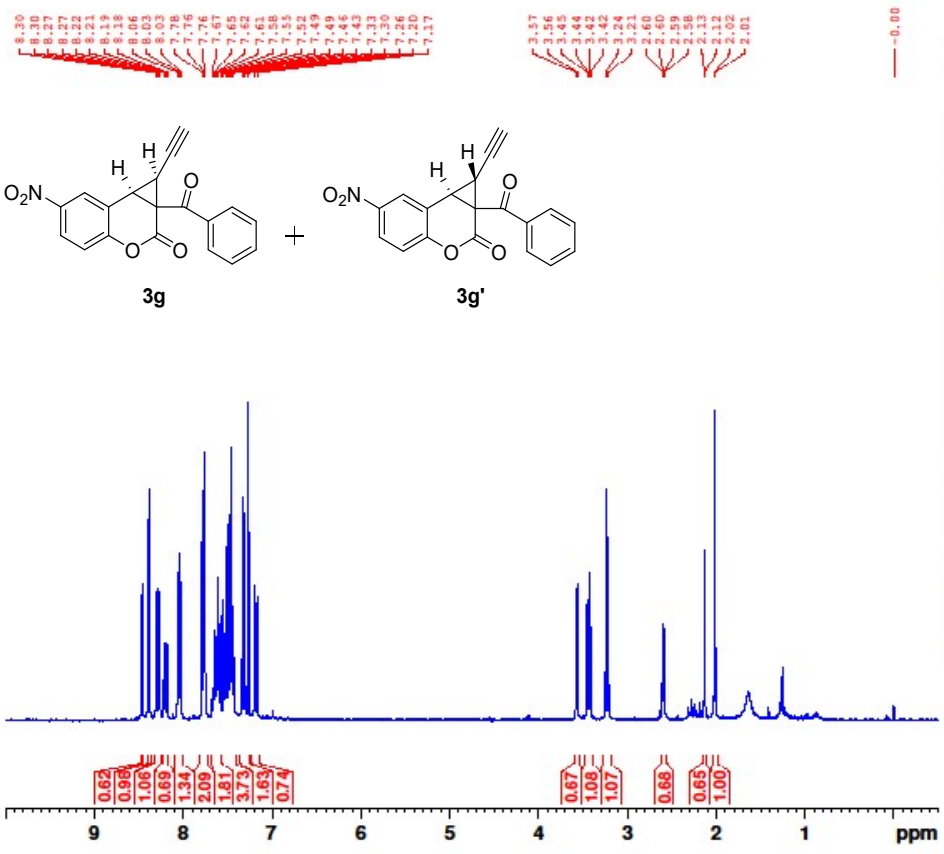

```
Current Data Parameters
NAME          240102-LA-L4
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_              20240102
Time                  7.55
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                  32768
SOLVENT             CDCl3
NS                  14336
DS                      0
SWH            18028.846 Hz
FIDRES          0.550197 Hz
AQ              0.9087659 sec
RG                 219.17
DW                 27.733 usec
DE                  6.50 usec
TE                 299.9 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 =======
SFO1          75.4756726 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          28.29999924 W

======== CHANNEL f2 =======
SFO2          300.1312005 MHz
NUC2                  1H
CPDPRG[2 bi_waltz65_256
PCPD2              90.00 usec
PLW2           8.30000019 W
PLW12          0.20084000 W
PLW13          0.16268000 W

F2 - Processing parameters
SI                  32768
SF            75.4677485 MHz
WDW                    EM
SSB                     0
LB                   2.00 Hz
GB                      0
PC                   1.00
```

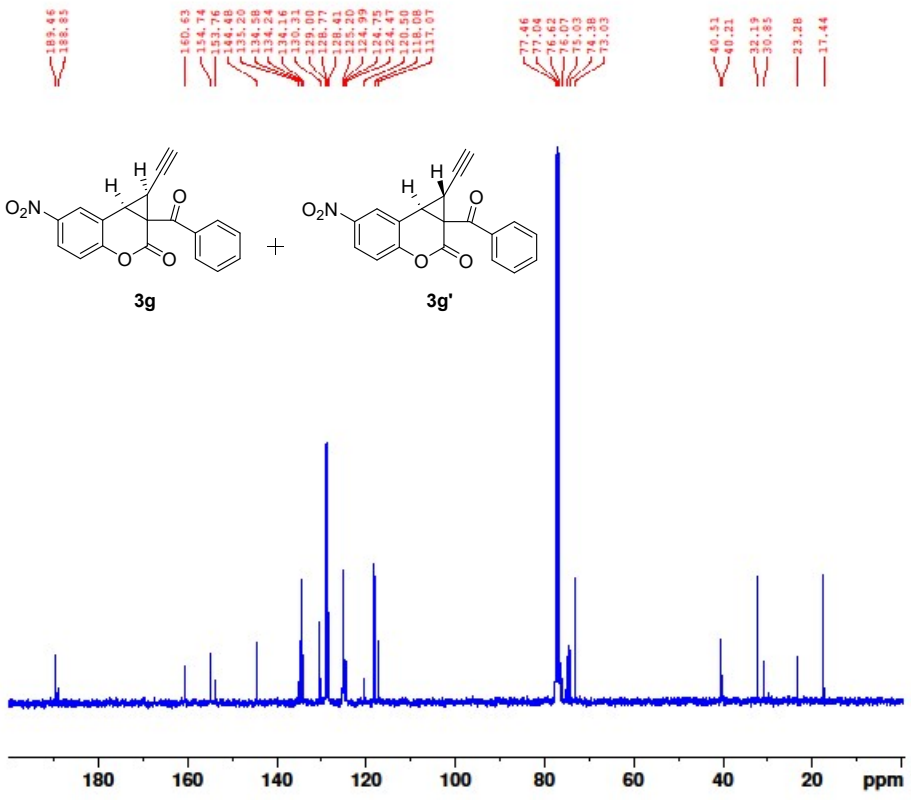


Current Data Parameters
NAME 231216-LA-L13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231126
Time 17.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 219.17
DW 83.200 usec
DE 12.63 usec
TE 297.7 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 300.1318008 MHz
NUC1 1H
P1 14.00 usec
PLW1 7.69999981 W

F2 - Processing parameters
SI 16384
SF 300.1300062 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



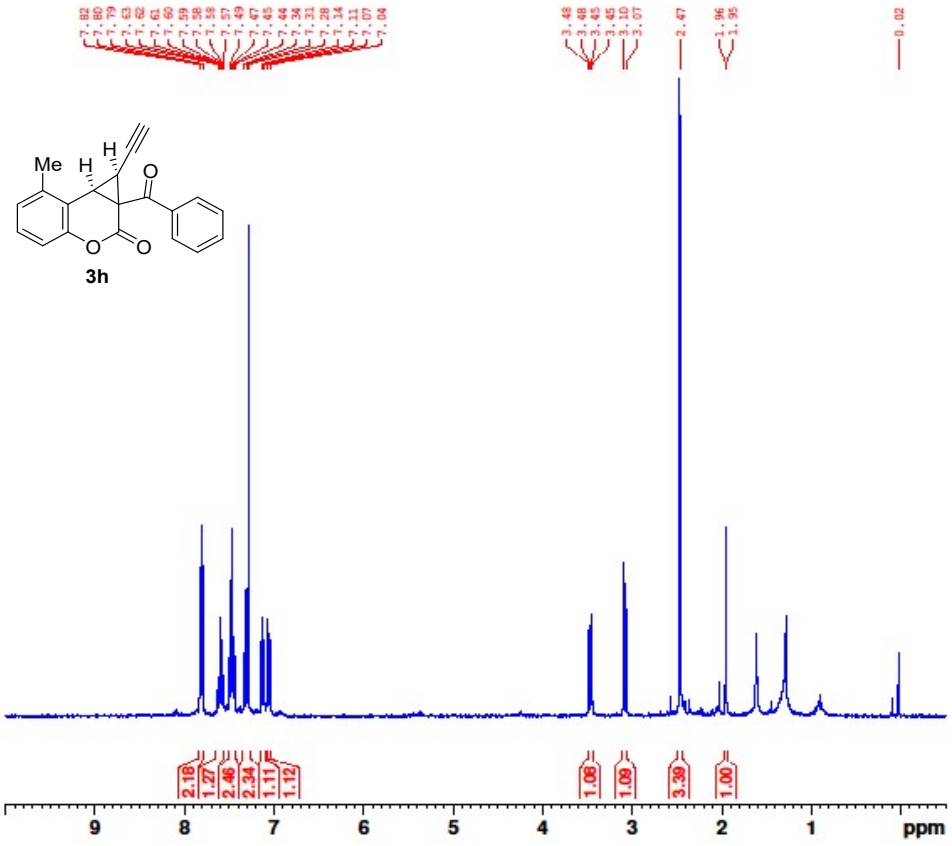
Current Data Parameters
NAME 231216-LA-L13
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231216
Time 17.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2048
DS 0
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 219.17
DW 27.733 usec
DE 6.50 usec
TE 298.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 75.4756726 MHz
NUC1 13C
P1 10.00 usec
PLW1 28.29999924 W

======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 bi_waltz65_256
PCPD2 90.00 usec
PLW2 8.30000019 W
PLW12 0.20084000 W
PLW13 0.16268000 W

F2 - Processing parameters
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00



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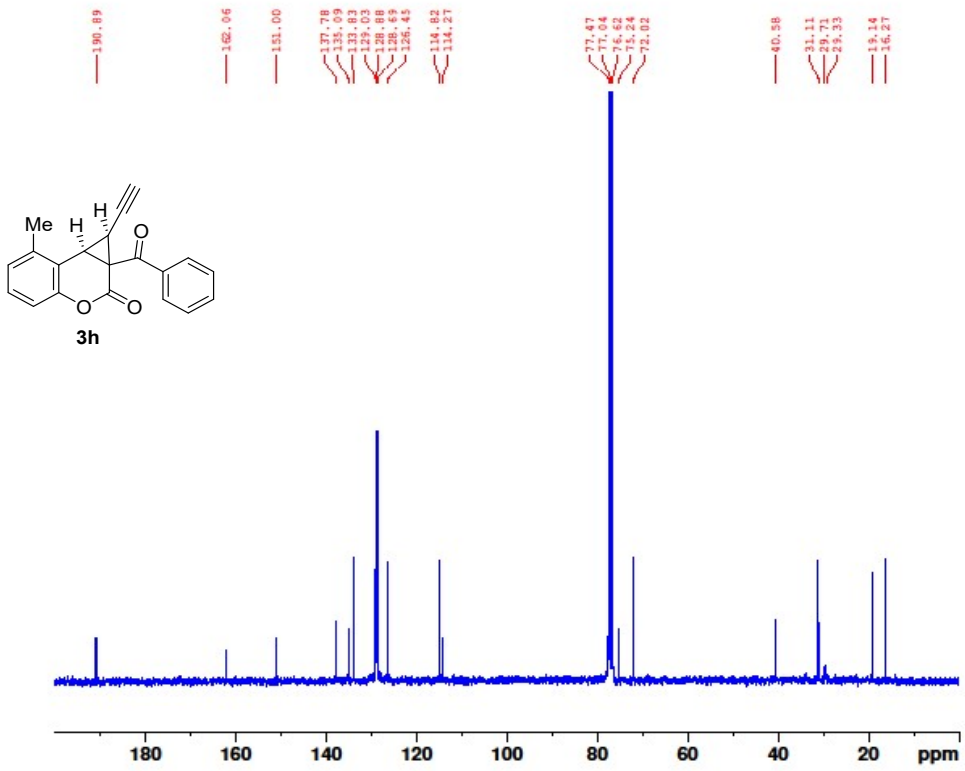
```
Current Data Parameters
NAME        240111-LA-L22
EXPNO               1
PROCNO              1

F2 - Acquisition Parameters
Date_          20240108
Time              12.44
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                  64
DS                   0
SWH           6009.615 Hz
FIDRES        0.183399 Hz
AQ            2.7262976 sec
RG               219.17
DW               83.200 usec
DE               12.63 usec
TE               296.7 K
D1            2.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1         300.1318008 MHz
NUC1               1H
P1               14.00 usec
PLW1          7.69999981 W

F2 - Processing parameters
SI               16384
SF           300.1300000 MHz
WDW                EM
SSB                 0
LB                  0 Hz
GB                  0
PC               1.00
```



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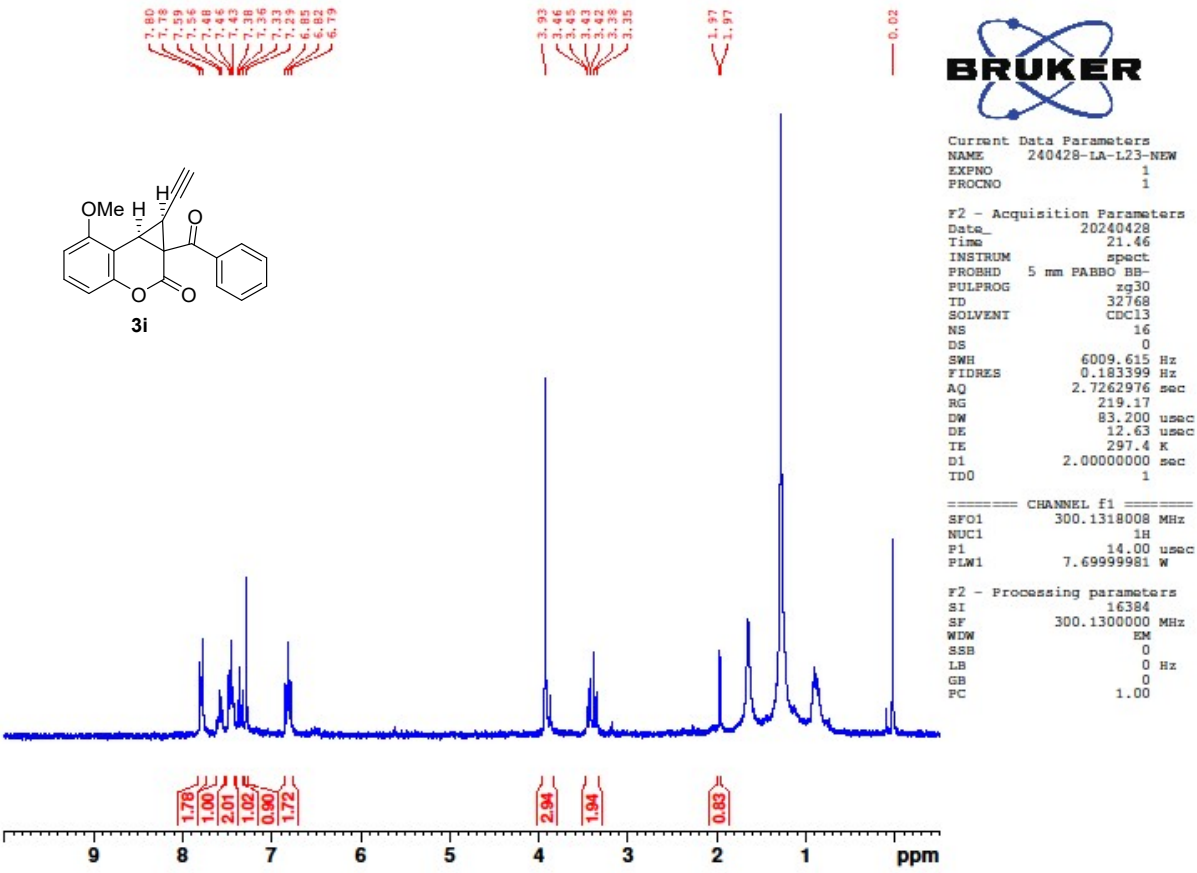
```
Current Data Parameters
NAME        240111-LA-L22
EXPNO               2
PROCNO              1

F2 - Acquisition Parameters
Date_          20240111
Time              16.51
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               32768
SOLVENT          CDCl3
NS                1737
DS                   0
SWH          18028.846 Hz
FIDRES        0.550197 Hz
AQ            0.9087659 sec
RG               219.17
DW               27.733 usec
DE                6.50 usec
TE               297.6 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1         75.4756726 MHz
NUC1               13C
P1               10.00 usec
PLW1         28.29999924 W

======== CHANNEL f2 ========
SFO2         300.1312005 MHz
NUC2               1H
CPDPRG[2 bi_waltz65_256
PCPD2            90.00 usec
PLW2          8.30000019 W
PLW12         0.20084000 W
PLW13         0.16268000 W

F2 - Processing parameters
SI               32768
SF           75.4677485 MHz
WDW                EM
SSB                 0
LB                2.00 Hz
GB                  0
PC               1.00
```



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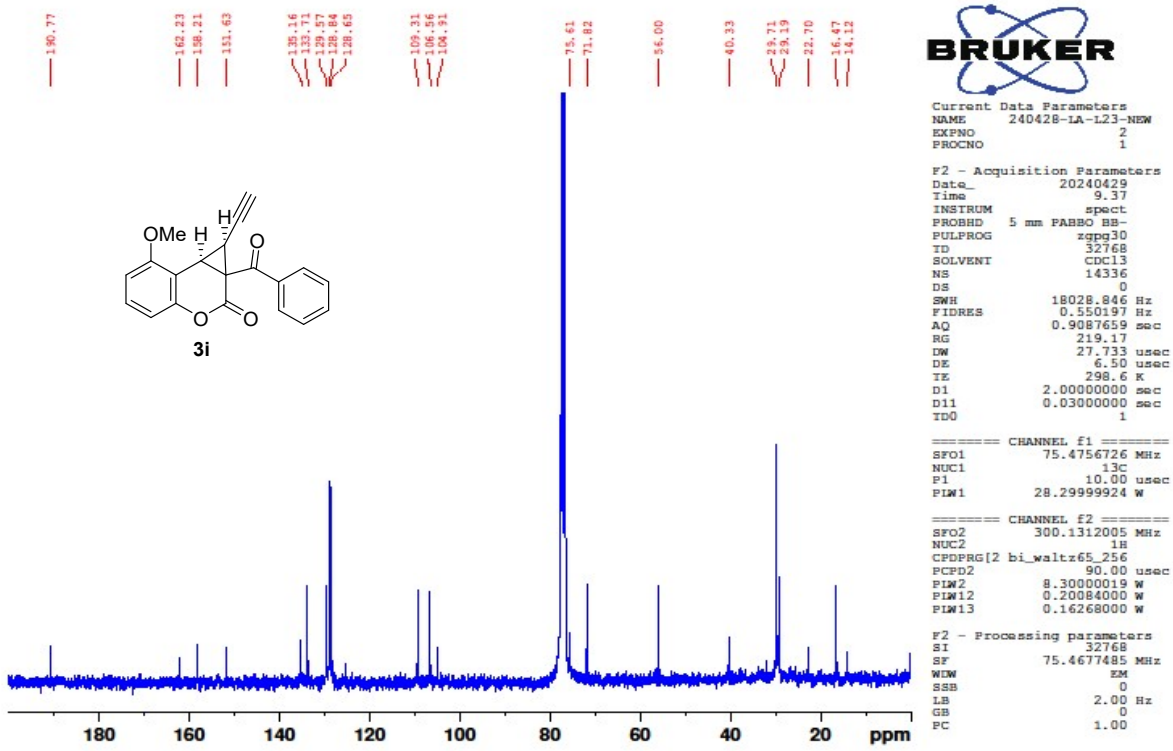
```
Current Data Parameters
NAME      240428-LA-L23-NEW
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20240428
Time                  21.46
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       16
DS                        0
SWH                6009.615 Hz
FIDRES            0.183399 Hz
AQ                2.7262976 sec
RG                   219.17
DW                   83.200 usec
DE                   12.63 usec
TE                   297.4 K
D1                2.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1             300.1318008 MHz
NUC1                       1H
P1                      14.00 usec
PLW1              7.69999981 W

F2 - Processing parameters
SI                        16384
SF               300.1300000 MHz
WDW                          EM
SSB                           0
LB                            0 Hz
GB                            0
PC                         1.00
```



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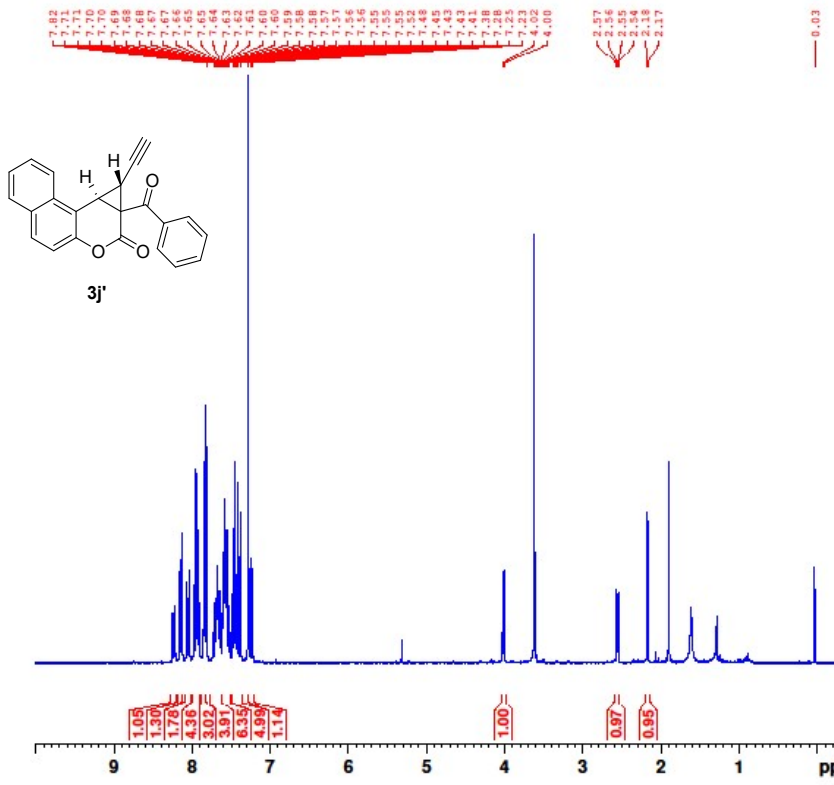
```
Current Data Parameters
NAME      240428-LA-L23-NEW
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20240429
Time                  9.37
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                    32768
SOLVENT               CDCl3
NS                    14336
DS                        0
SWH               18028.846 Hz
FIDRES            0.550197 Hz
AQ                0.9087659 sec
RG                   219.17
DW                   27.733 usec
DE                    6.50 usec
TE                   298.6 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1             75.4756726 MHz
NUC1                      13C
P1                    10.00 usec
PLW1             28.29999924 W

======== CHANNEL f2 ========
SFO2             300.1312005 MHz
NUC2                       1H
CPDPRG[2 bi_waltz65_256
PCPD2                 90.00 usec
PLW2              8.30000019 W
PLW12             0.20084000 W
PLW13             0.16268000 W

F2 - Processing parameters
SI                        32768
SF               75.4677485 MHz
WDW                          EM
SSB                           0
LB                         2.00 Hz
GB                            0
PC                         1.00
```

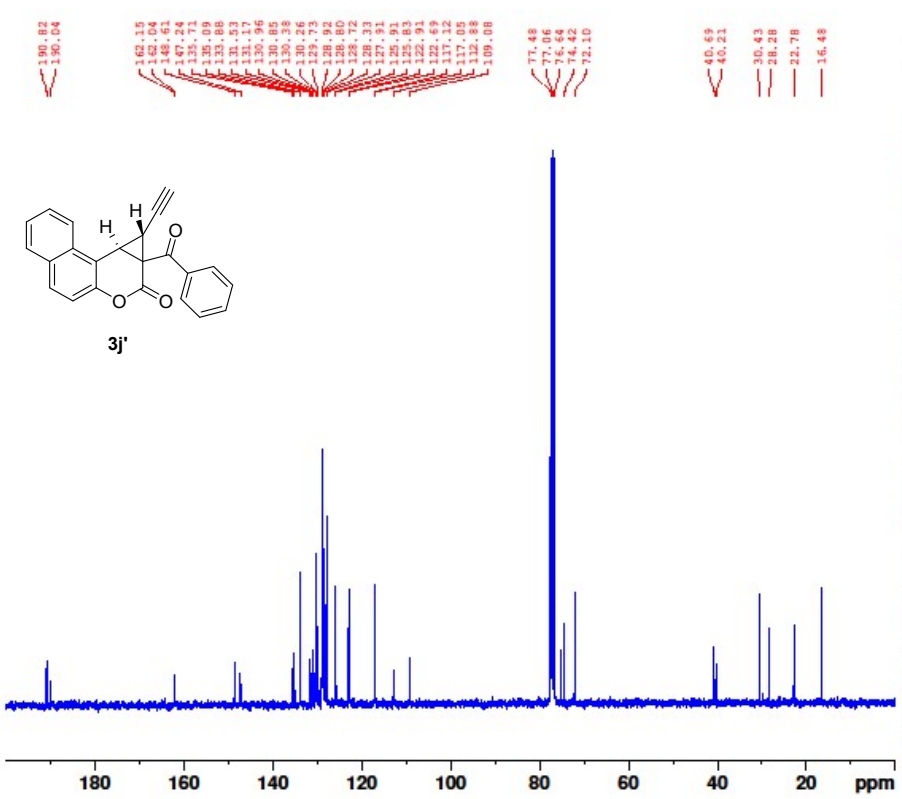



```
Current Data Parameters
NAME       240110-LA-L11
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240110
Time               14.04
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    64
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              2.7262976 sec
RG                 219.17
DW                 83.200 usec
DE                 12.63 usec
TE                 297.3 K
D1              2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          300.1318008 MHz
NUC1                  1H
P1                 14.00 usec
PLW1           7.69999981 W

F2 - Processing parameters
SI                 16384
SF            300.1300000 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```



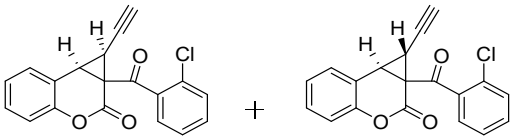

```
Current Data Parameters
NAME       240110-LA-L11
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231217
Time               18.31
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  2048
DS                     0
SWH            18028.846 Hz
FIDRES          0.550197 Hz
AQ              0.9087659 sec
RG                 219.17
DW                 27.733 usec
DE                  6.50 usec
TE                 298.2 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

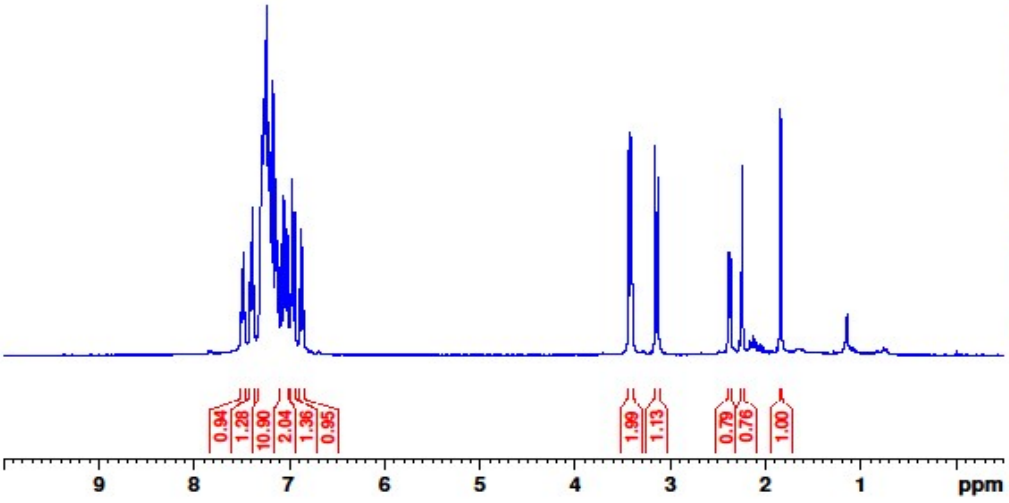
======== CHANNEL f1 ========
SFO1          75.4756726 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          28.29999924 W

======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                  1H
CPDPRG[2 bi_waltz65_256
PCPD2              90.00 usec
PLW2           8.30000019 W
PLW12          0.20084000 W
PLW13          0.16268000 W

F2 - Processing parameters
SI                 32768
SF            75.4677485 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```



3k 3k'

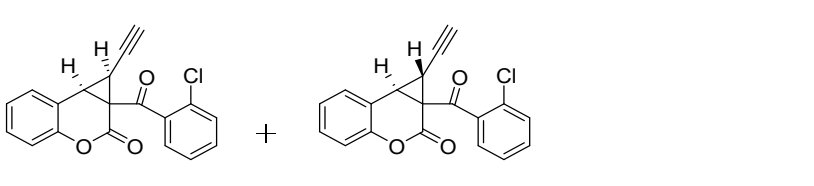


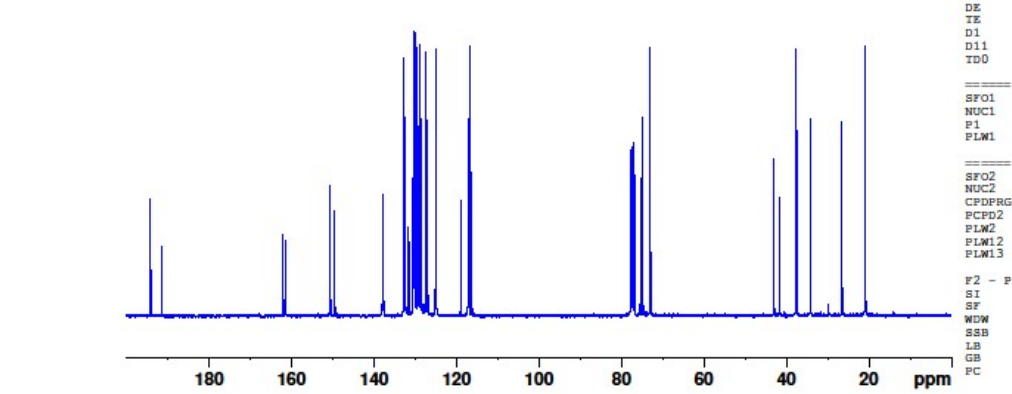

```
Current Data Parameters
NAME       231205-LA-L14
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231205
Time               19.52
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              2.7262976 sec
RG                  36.7
DW                83.200 usec
DE                12.63 usec
TE                297.8 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          300.1318008 MHz
NUC1                  1H
P1                 14.00 usec
PLW1           7.69999981 W

F2 - Processing parameters
SI                 16384
SF            300.1300477 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```





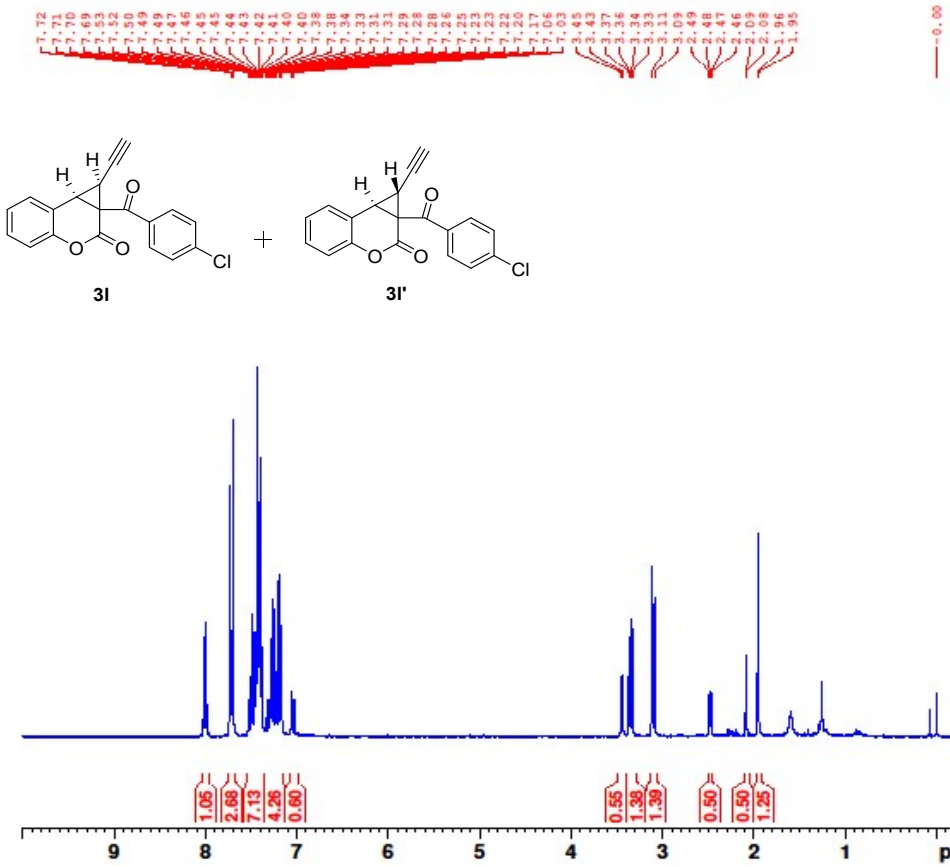
```
Current Data Parameters
NAME       231205-LA-L14
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231205
Time               21.36
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  2048
DS                     0
SWH            18028.846 Hz
FIDRES          0.550197 Hz
AQ              0.9087659 sec
RG                 219.17
DW                27.733 usec
DE                 6.50 usec
TE                299.3 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1           75.4756726 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          28.29999924 W

======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                  1H
CPDPRG[2 bi_waltz65_256
PCPD2              90.00 usec
PLW2           8.30000019 W
PLW12          0.20084000 W
PLW13          0.16268000 W

F2 - Processing parameters
SI                 32768
SF            75.4677485 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```



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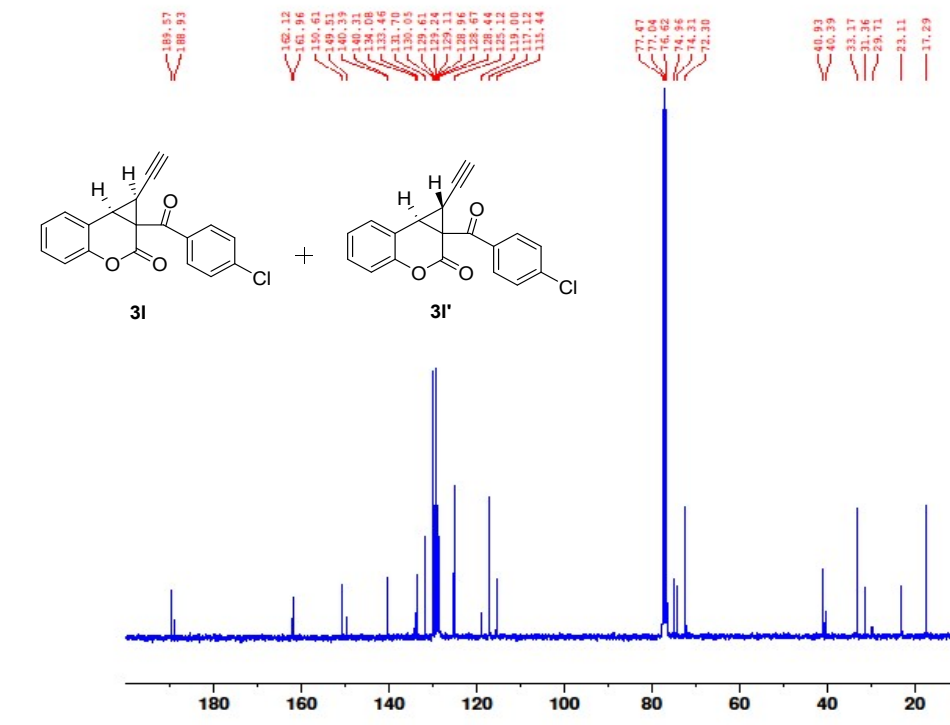
```
Current Data Parameters
NAME          240101-LA-L15
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20240101
Time                  17.02
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                      64
DS                       0
SWH                6009.615 Hz
FIDRES            0.183399 Hz
AQ                2.7262976 sec
RG                   219.17
DW                   83.200 usec
DE                   12.63 usec
TE                   297.8 K
D1                2.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1             300.1318008 MHz
NUC1                      1H
P1                     14.00 usec
PLW1              7.69999981 W

F2 - Processing parameters
SI                       16384
SF                300.1300076 MHz
WDW                      EM
SSB                       0
LB                        0 Hz
GB                        0
PC                     1.00
```



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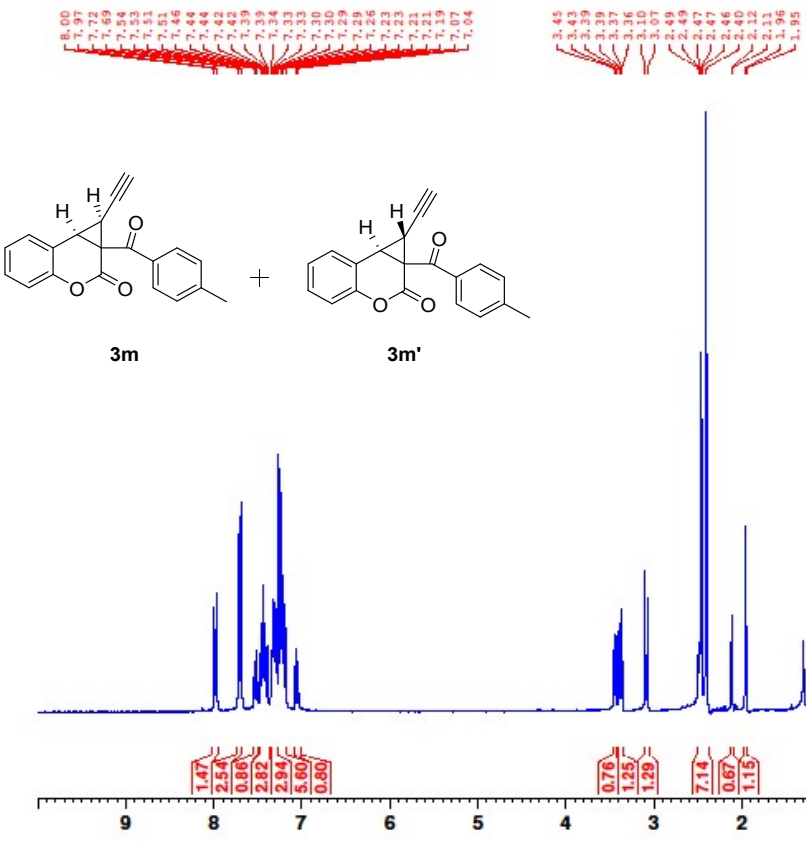
```
Current Data Parameters
NAME          240101-LA-L15
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20240101
Time                  18.49
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                    2048
DS                       0
SWH               18028.846 Hz
FIDRES            0.550197 Hz
AQ                0.9087659 sec
RG                   219.17
DW                   27.733 usec
DE                    6.50 usec
TE                   298.5 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1             75.4756726 MHz
NUC1                     13C
P1                     10.00 usec
PLW1             28.29999924 W

======== CHANNEL f2 ========
SFO2            300.1312005 MHz
NUC2                     1H
CPDPRG[2 bi_waltz65_256
PCPD2                  90.00 usec
PLW2             8.30000019 W
PLW12            0.20084000 W
PLW13            0.16268000 W

F2 - Processing parameters
SI                       32768
SF                75.4677485 MHz
WDW                      EM
SSB                       0
LB                     2.00 Hz
GB                        0
PC                     1.00
```

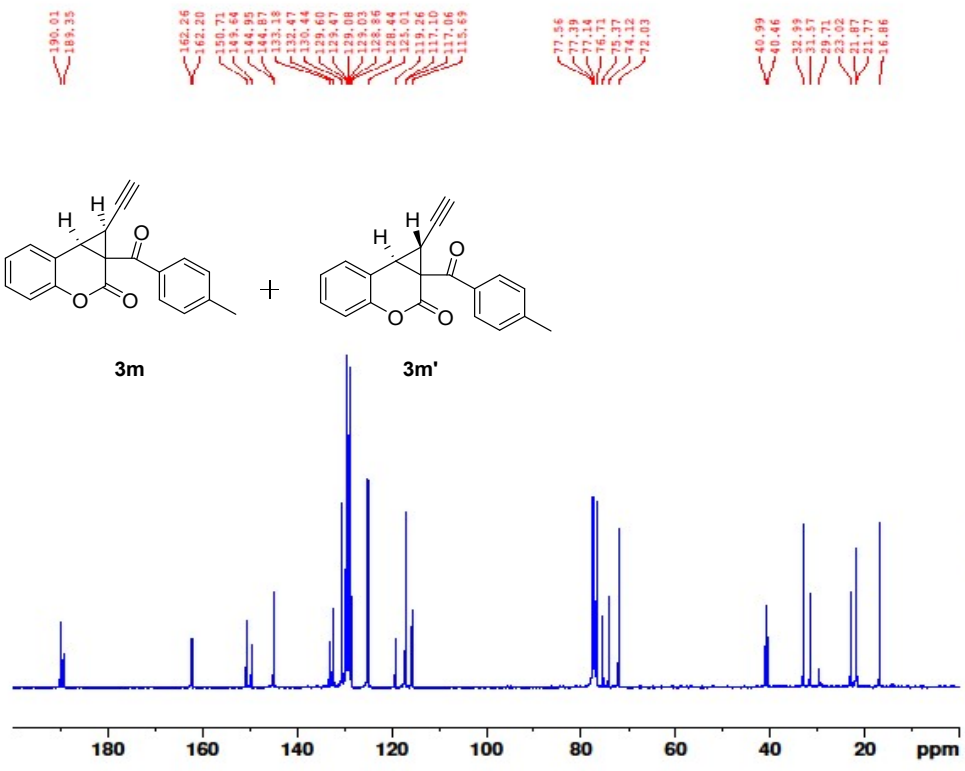



```
Current Data Parameters
NAME       231205-LA-L16
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Data_              20231205
Time                  22.08
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                      16
DS                       0
SWH               6009.615 Hz
FIDRES            0.183399 Hz
AQ               2.7262976 sec
RG                   96.06
DW                 83.200 usec
DE                 12.63 usec
TE                 298.5 K
D1              2.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          300.1318008 MHz
NUC1                    1H
P1                  14.00 usec
PLW1          7.69999981 W

F2 - Processing parameters
SI                   16384
SF            300.1300000 MHz
WDW                     EM
SSB                      0
LB                    0 Hz
GB                       0
PC                    1.00
```



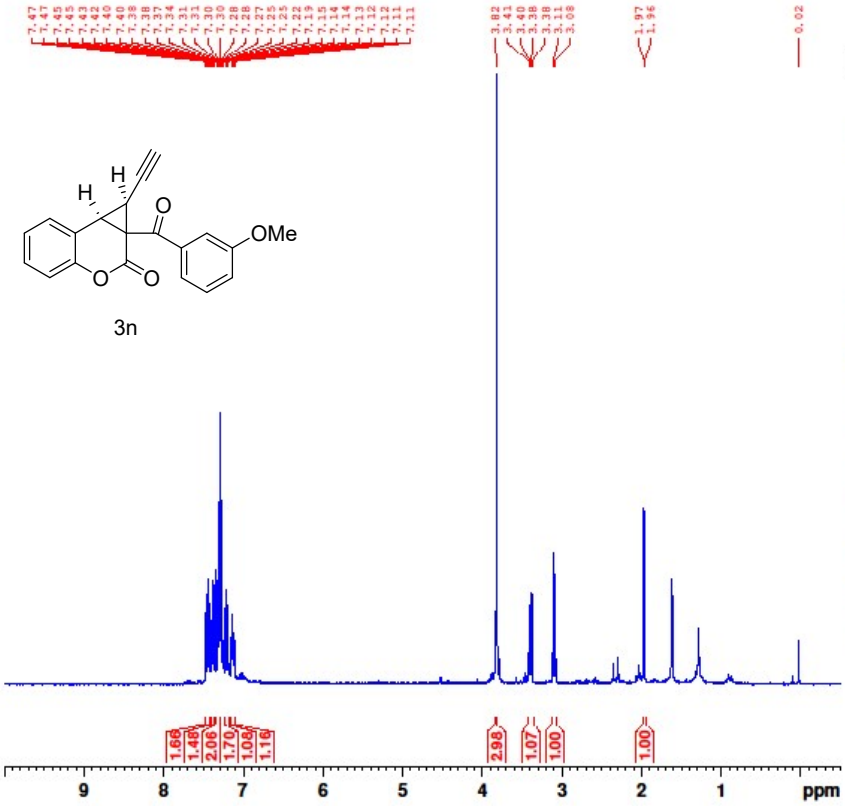

```
Current Data Parameters
NAME       231205-LA-L16
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Data_              20231206
Time                   6.39
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                   10240
DS                       0
SWH              18028.846 Hz
FIDRES            0.550197 Hz
AQ               0.9087659 sec
RG                   219.17
DW                 27.733 usec
DE                  6.50 usec
TE                 298.9 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          75.4756726 MHz
NUC1                   13C
P1                  10.00 usec
PLW1          28.29999924 W

======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                    1H
CPDPRG[2 bi_waltz65_256
PCPD2               90.00 usec
PLW2          8.30000019 W
PLW12         0.20084000 W
PLW13         0.16268000 W

F2 - Processing parameters
SI                   32768
SF            75.4677485 MHz
WDW                     EM
SSB                      0
LB                  2.00 Hz
GB                       0
PC                    1.00
```



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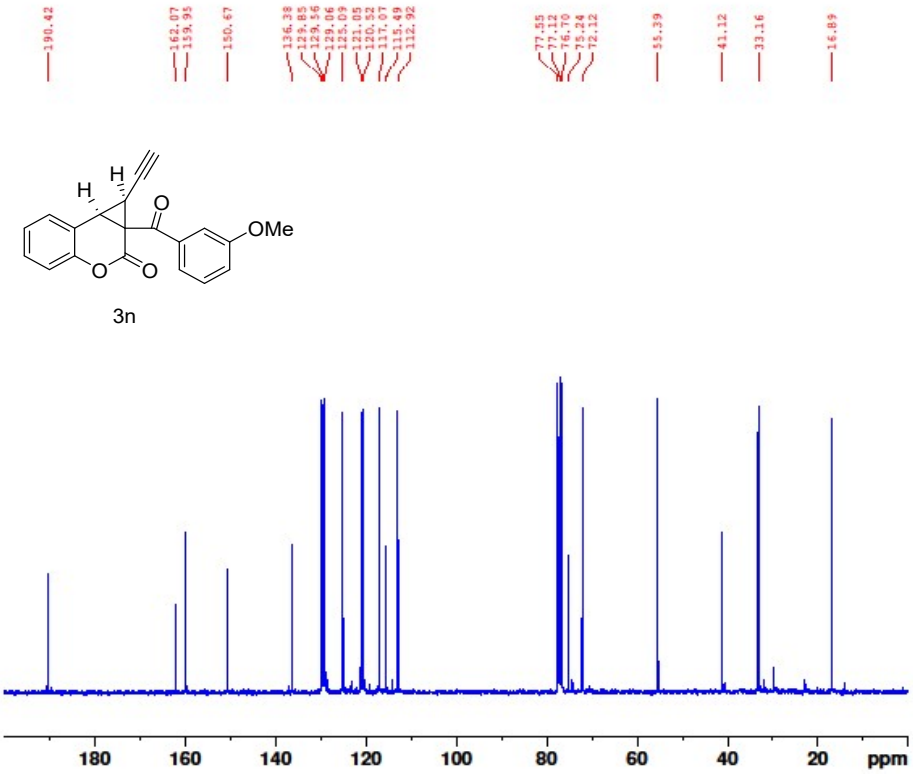
```
Current Data Parameters
NAME                  L17
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20240115
Time               21.35
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              2.7262976 sec
RG                219.17
DW                83.200 usec
DE                12.63 usec
TE                297.5 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          300.1318008 MHz
NUC1                  1H
P1                 14.00 usec
PLW1           7.69999981 W

F2 - Processing parameters
SI                 16384
SF            300.1300000 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```



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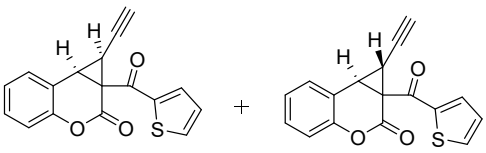
```
Current Data Parameters
NAME                  L17
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20231204
Time               20.12
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  2048
DS                     0
SWH            18028.846 Hz
FIDRES          0.550197 Hz
AQ              0.9087659 sec
RG                219.17
DW                27.733 usec
DE                 6.50 usec
TE                298.6 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          75.4756726 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          28.29999924 W

======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                  1H
CPDPRG[2 bi_waltz65_256
PCPD2              90.00 usec
PLW2           8.30000019 W
PLW12          0.20084000 W
PLW13          0.16268000 W

F2 - Processing parameters
SI                 32768
SF            75.4677485 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```



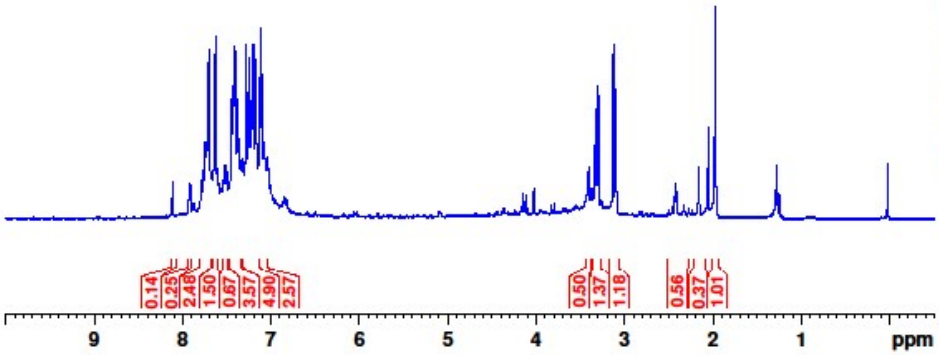
3o + 3o'

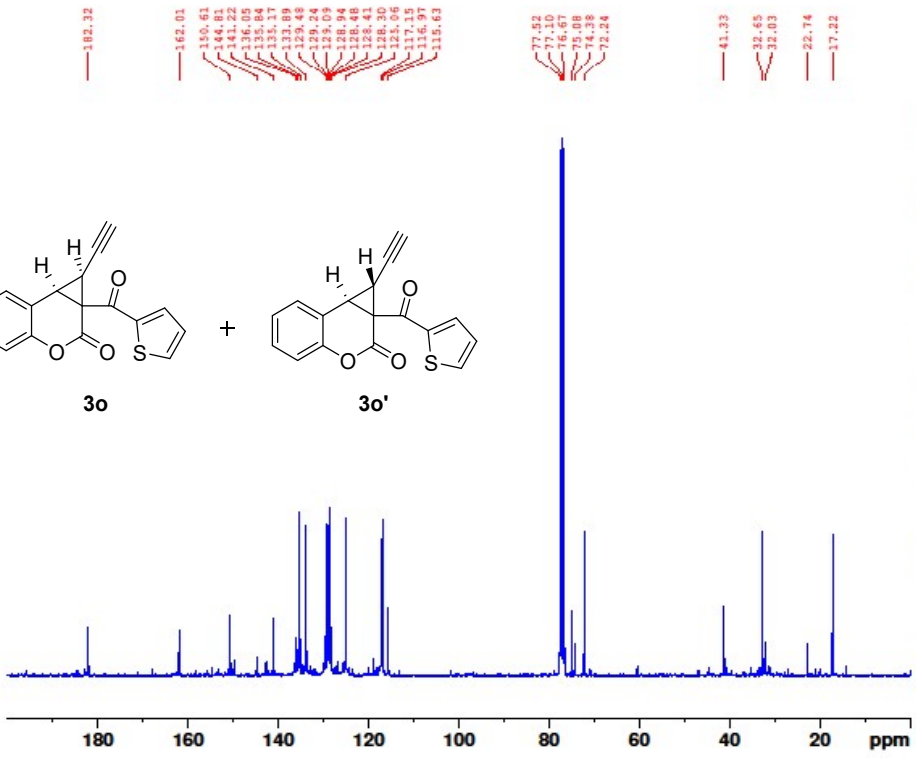
```
Current Data Parameters
NAME      240429-LA-3L-L24
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20240429
Time                 22.08
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     16
DS                      0
SWH             6009.615 Hz
FIDRES          0.183399 Hz
AQ              2.7262976 sec
RG                 148.08
DW                 83.200 usec
DE                 12.63 usec
TE                 297.5 K
D1              2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          300.1318008 MHz
NUC1                    1H
P1                  14.00 usec
PLW1           7.69999981 W

F2 - Processing parameters
SI                  16384
SF            300.1300000 MHz
WDW                    EM
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.00
```





3o + 3o'

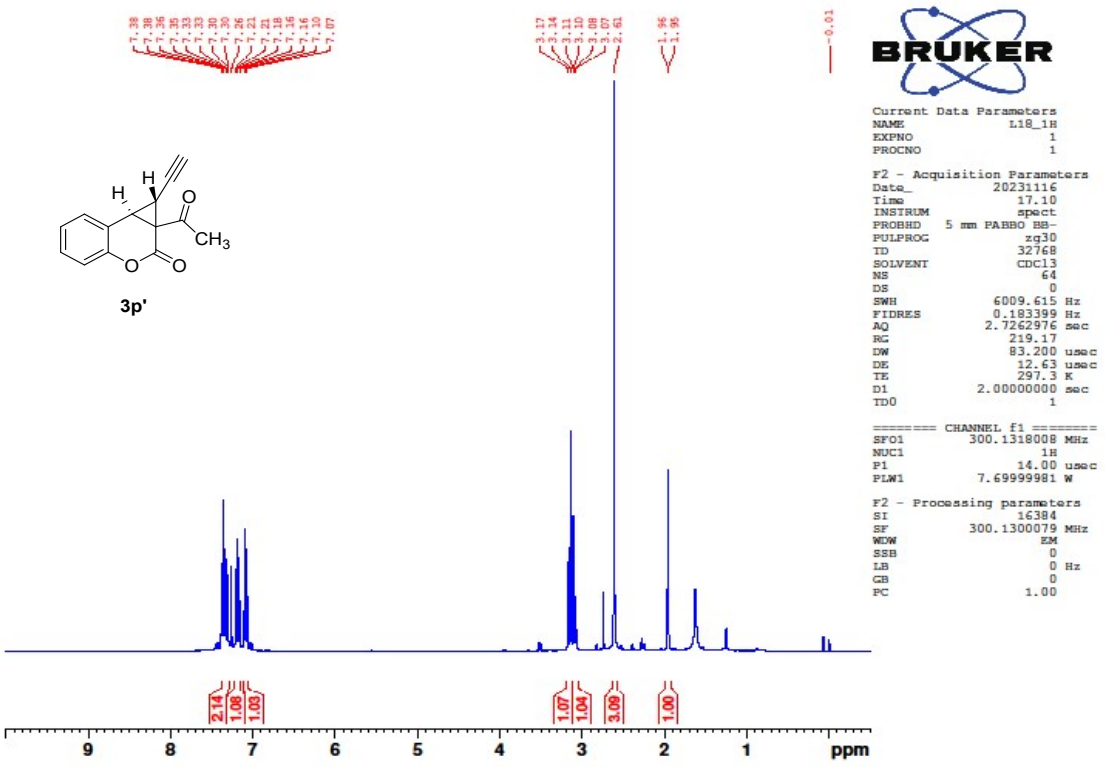
```
Current Data Parameters
NAME      240429-LA-3L-L24
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_              20240430
Time                  8.18
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                  32768
SOLVENT             CDCl3
NS                  12288
DS                      0
SWH            18028.846 Hz
FIDRES          0.550197 Hz
AQ              0.9087659 sec
RG                 219.17
DW                 27.733 usec
DE                  6.50 usec
TE                 297.9 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          75.4756726 MHz
NUC1                    13C
P1                  10.00 usec
PLW1           28.29999924 W

======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                    1H
CPDPRG[2 bi_waltz65_256
PCPD2               90.00 usec
PLW2            8.30000019 W
PLW12           0.20084000 W
PLW13           0.16268000 W

F2 - Processing parameters
SI                  32768
SF            75.4677485 MHz
WDW                    EM
SSB                     0
LB                   2.00 Hz
GB                      0
PC                   1.00
```



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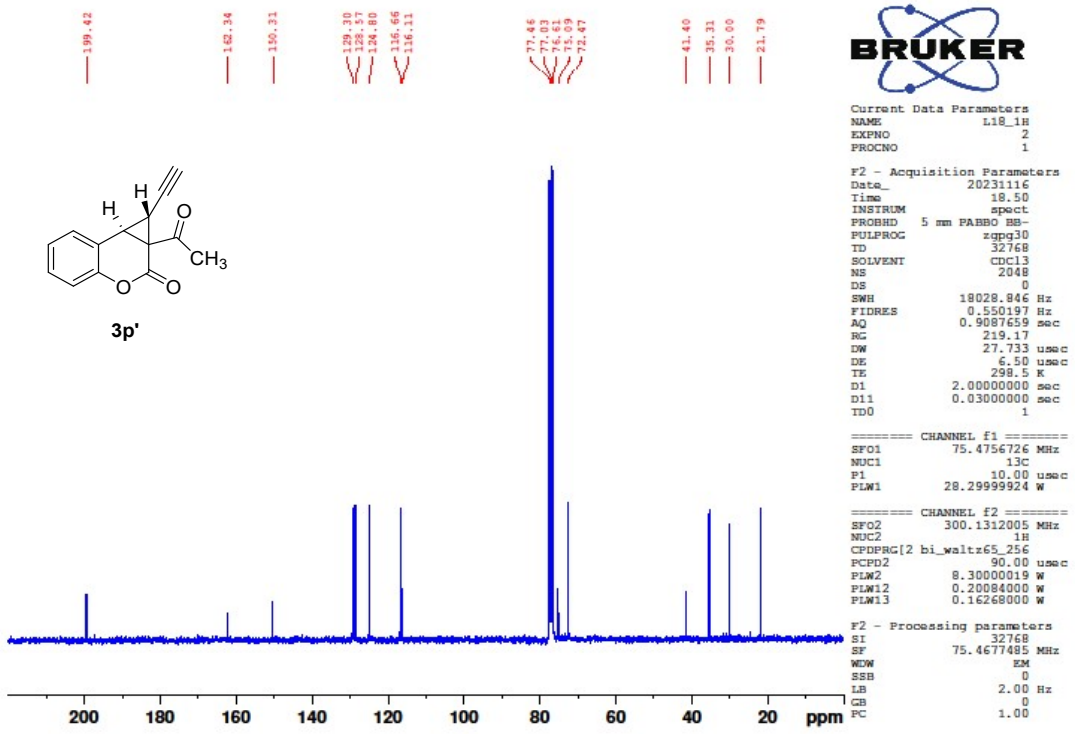
```
Current Data Parameters
NAME                  L18_1H
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20231116
Time                 17.10
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     64
DS                      0
SWH               6009.615 Hz
FIDRES            0.183399 Hz
AQ                2.7262976 sec
RG                   219.17
DW                 83.200 usec
DE                 12.63 usec
TE                  297.3 K
D1                2.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            300.1318008 MHz
NUC1                      1H
P1                     14.00 usec
PLW1             7.69999981 W

F2 - Processing parameters
SI                      16384
SF                300.1300079 MHz
WDW                        EM
SSB                         0
LB                      0 Hz
GB                          0
PC                       1.00
```



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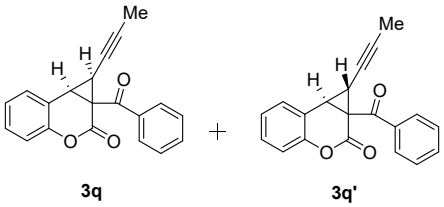
```
Current Data Parameters
NAME                  L18_1H
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20231116
Time                 18.50
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                  32768
SOLVENT             CDCl3
NS                   2048
DS                      0
SWH              18028.846 Hz
FIDRES            0.550197 Hz
AQ                0.9087659 sec
RG                   219.17
DW                 27.733 usec
DE                  6.50 usec
TE                  298.5 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1

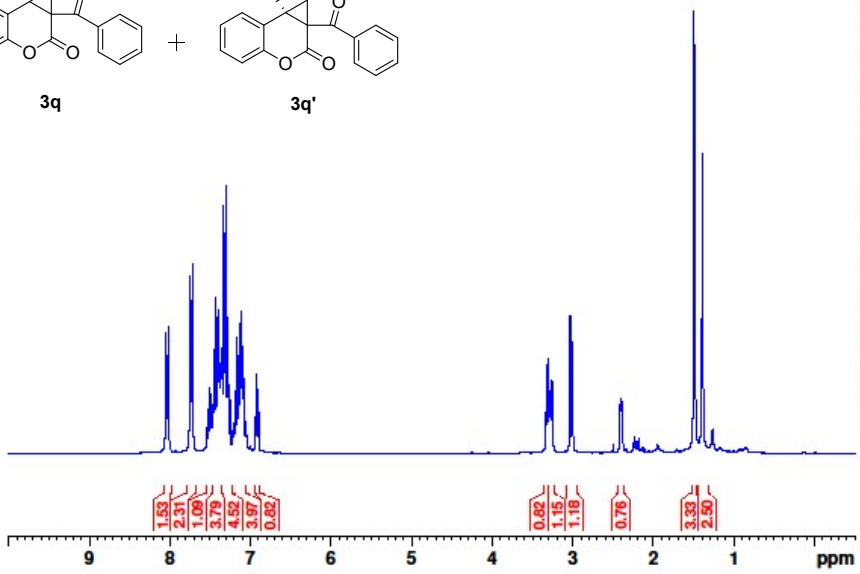
======== CHANNEL f1 ========
SFO1            75.4756726 MHz
NUC1                      13C
P1                     10.00 usec
PLW1            28.29999924 W

======== CHANNEL f2 ========
SFO2           300.1312005 MHz
NUC2                      1H
CPDPRG[2 bi_waltz65_256
PCPD2                  90.00 usec
PLW2            8.30000019 W
PLW12           0.20084000 W
PLW13           0.16268000 W

F2 - Processing parameters
SI                      32768
SF                75.4677485 MHz
WDW                        EM
SSB                         0
LB                     2.00 Hz
GB                          0
PC                       1.00
```



3q 3q'

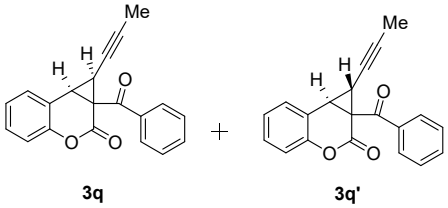


```
Current Data Parameters
NAME        231207-LA-L19
EXPNO                   1
PROCNO                  1

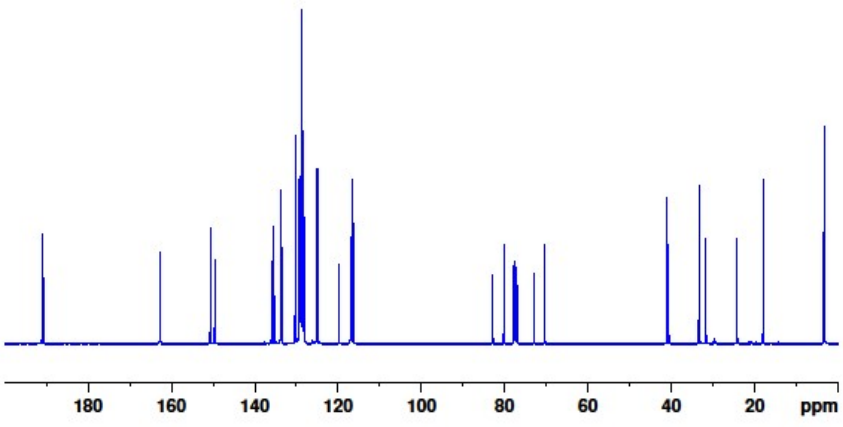
F2 - Acquisition Parameters
Date_            20231207
Time                11.14
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     64
DS                      0
SWH              6009.615 Hz
FIDRES           0.183399 Hz
AQ               2.7262976 sec
RG                  20.26
DW                 83.200 usec
DE                 12.63 usec
TE                 297.6 K
D1              2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          300.1318008 MHz
NUC1                    1H
P1                  14.00 usec
PLW1           7.69999981 W

F2 - Processing parameters
SI                  16384
SF            300.1300082 MHz
WDW                    EM
SSB                     0
LB                   0 Hz
GB                      0
PC                   1.00
```



3q 3q'



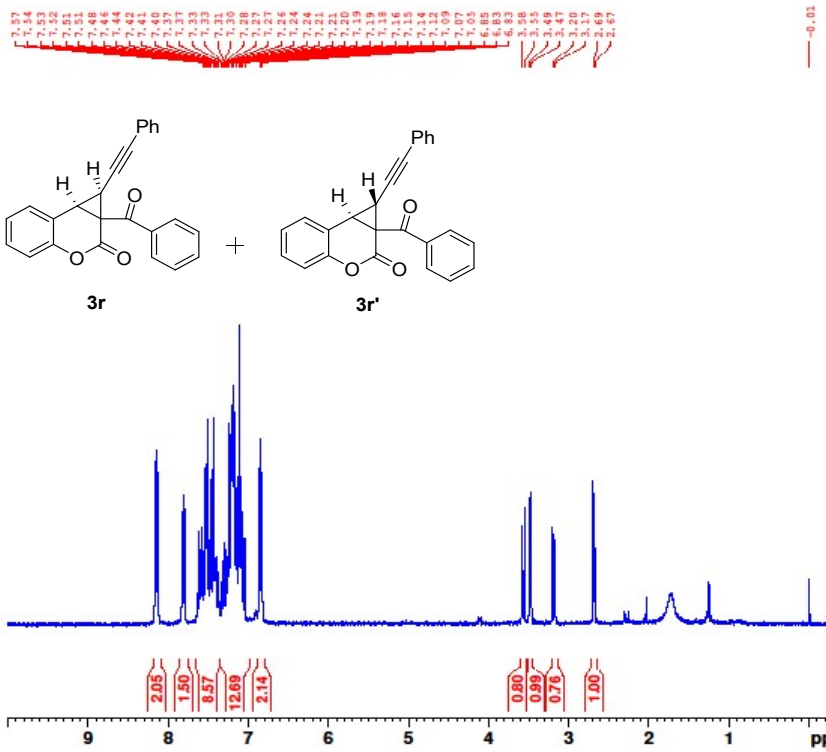
```
Current Data Parameters
NAME        231207-LA-L19
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20231207
Time                12.55
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                  32768
SOLVENT             CDCl3
NS                   2048
DS                      0
SWH             18028.846 Hz
FIDRES           0.550197 Hz
AQ               0.9087659 sec
RG                  219.17
DW                 27.733 usec
DE                  6.50 usec
TE                 297.7 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          75.4756726 MHz
NUC1                    13C
P1                  10.00 usec
PLW1          28.29999924 W

======== CHANNEL f2 ========
SFO2          300.1312005 MHz
NUC2                    1H
CPDPRG[2 bi_waltz65_256
PCPD2               90.00 usec
PLW2           8.30000019 W
PLW12          0.20084000 W
PLW13          0.16268000 W

F2 - Processing parameters
SI                  32768
SF            75.4677485 MHz
WDW                    EM
SSB                     0
LB                   2.00 Hz
GB                      0
PC                   1.00
```



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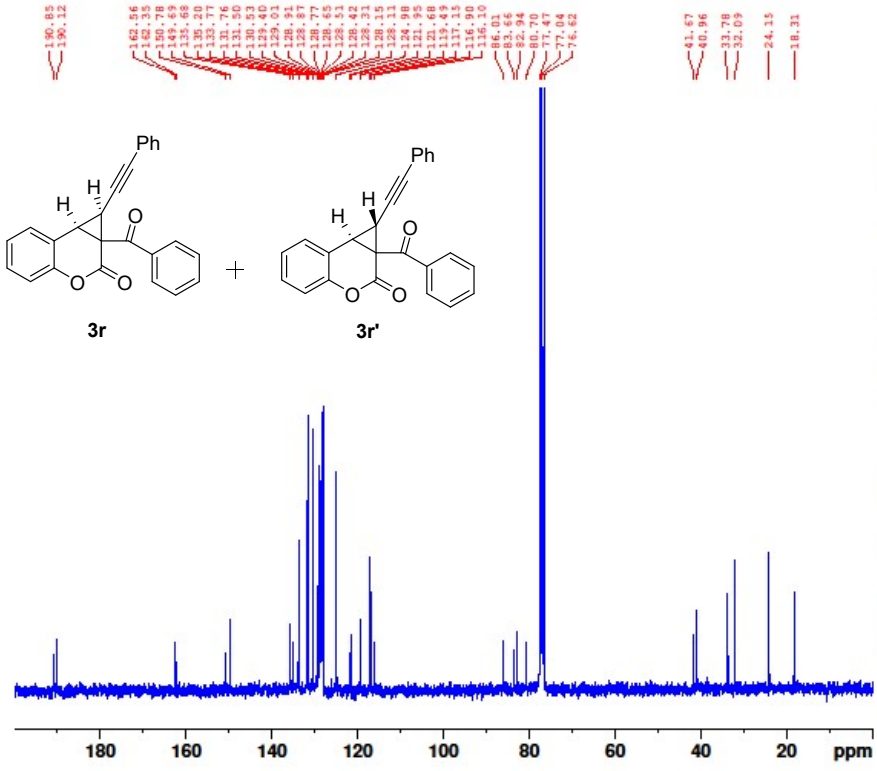
```
Current Data Parameters
NAME          240121-LA-L20
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20240121
Time                  18.15
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                      64
DS                       0
SWH               6009.615 Hz
FIDRES           0.183399 Hz
AQ               2.7262976 sec
RG                  219.17
DW                  83.200 usec
DE                   12.63 usec
TE                  297.8 K
D1               2.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            300.1318008 MHz
NUC1                    1H
P1                   14.00 usec
PLW1            7.69999981 W

F2 - Processing parameters
SI                   16384
SF              300.1300119 MHz
WDW                     EM
SSB                      0
LB                       0 Hz
GB                       0
PC                    1.00
```



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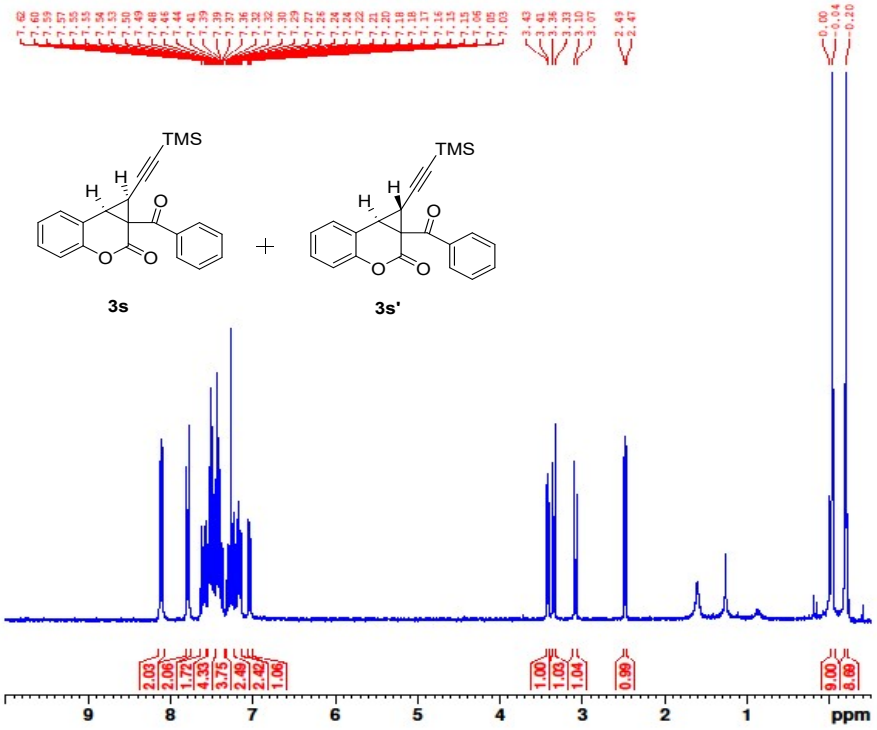
```
Current Data Parameters
NAME          240121-LA-L20
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20240121
Time                  19.50
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                    1912
DS                       0
SWH              18028.846 Hz
FIDRES           0.550197 Hz
AQ               0.9087659 sec
RG                  219.17
DW                  27.733 usec
DE                    6.50 usec
TE                  298.5 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            75.4756726 MHz
NUC1                    13C
P1                   10.00 usec
PLW1           28.29999924 W

======== CHANNEL f2 ========
SFO2           300.1312005 MHz
NUC2                    1H
CPDPRG[2 bi_waltz65_256
PCPD2                90.00 usec
PLW2           8.30000019 W
PLW12          0.20084000 W
PLW13          0.16268000 W

F2 - Processing parameters
SI                   32768
SF              75.4677485 MHz
WDW                     EM
SSB                      0
LB                    2.00 Hz
GB                       0
PC                    1.00
```

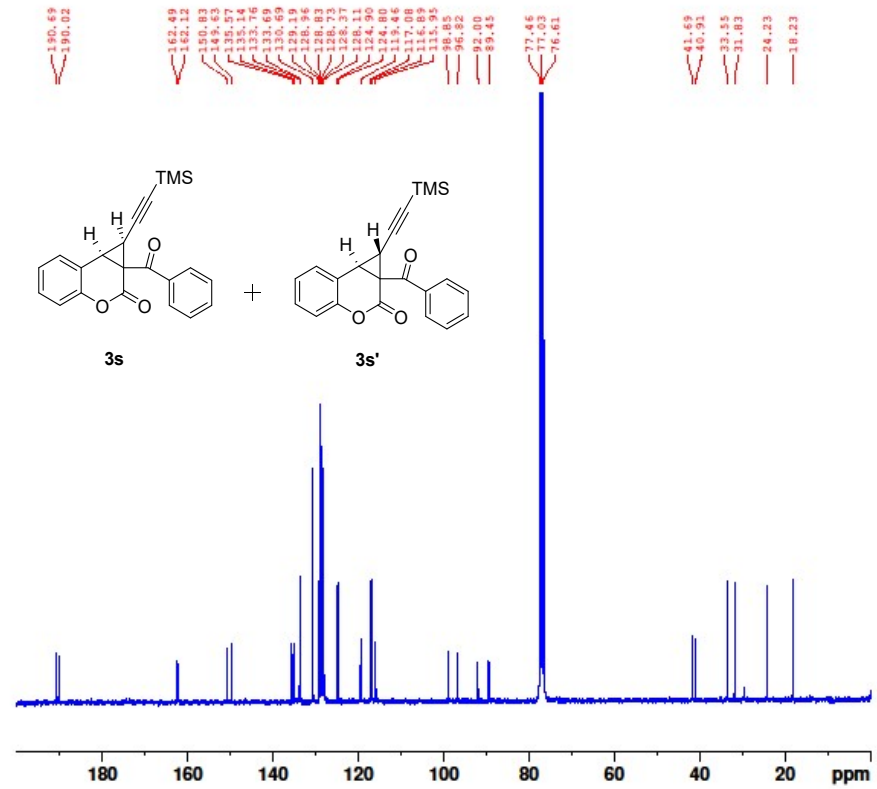



```
Current Data Parameters
NAME          240114-LA-L21
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20240114
Time                  20.25
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                      64
DS                       0
SWH               6009.615 Hz
FIDRES            0.183399 Hz
AQ                2.7262976 sec
RG                   219.17
DW                   83.200 usec
DE                   12.63 usec
TE                   297.8 K
D1                2.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            300.1318008 MHz
NUC1                    1H
P1                   14.00 usec
PLW1           7.69999981 W

F2 - Processing parameters
SI                   16384
SF              300.1300057 MHz
WDW                     EM
SSB                      0
LB                       0 Hz
GB                       0
PC                    1.00
```




```
Current Data Parameters
NAME          240114-LA-L21
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20240115
Time                   6.39
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                   12288
DS                       0
SWH              18028.846 Hz
FIDRES            0.550197 Hz
AQ                0.9087659 sec
RG                   219.17
DW                   27.733 usec
DE                    6.50 usec
TE                   298.3 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            75.4756726 MHz
NUC1                    13C
P1                   10.00 usec
PLW1           28.29999924 W

======== CHANNEL f2 ========
SFO2            300.1312005 MHz
NUC2                    1H
CPDPRG[2 bi_waltz65_256
PCPD2                90.00 usec
PLW2           8.30000019 W
PLW12          0.20084000 W
PLW13          0.16268000 W

F2 - Processing parameters
SI                   32768
SF              75.4677485 MHz
WDW                     EM
SSB                      0
LB                    2.00 Hz
GB                       0
PC                    1.00
```