SUPPORTING INFORMATION

One-pot construction of diverse and functionalized isochromenoquinolinediones by Rh(III)-catalyzed annulation of unprotected arylamides with 3-diazoquinolinediones and their application for fluorescence sensor

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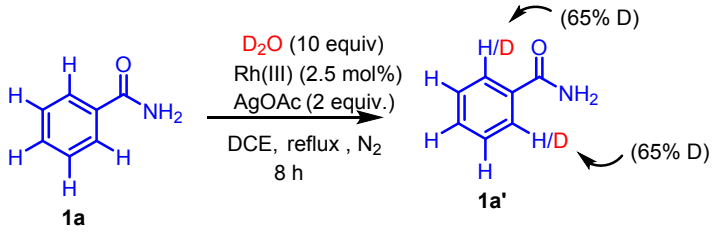
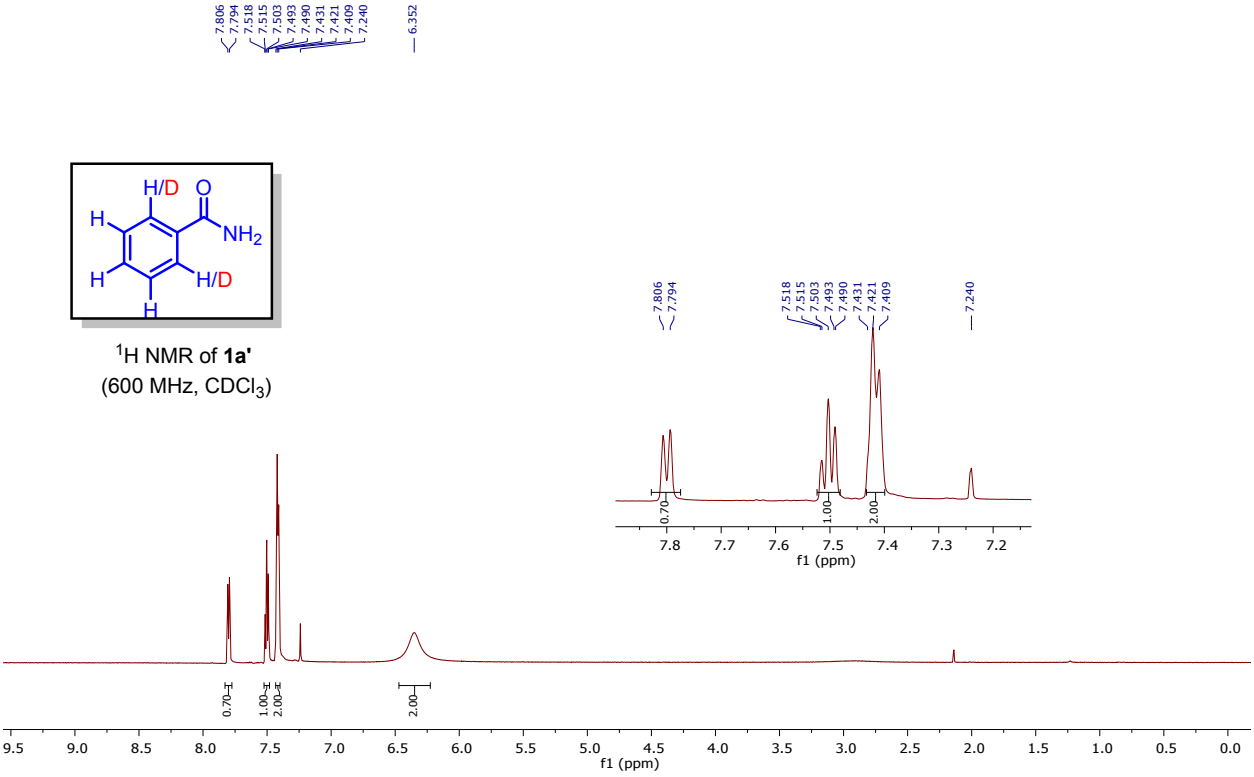
H/D exchange experiment

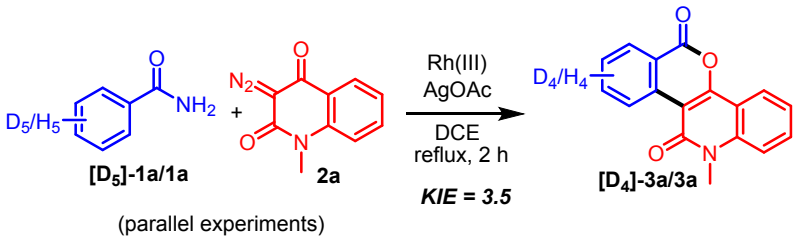


Scheme S1. Control experiment of H/D exchange.

Benzamide (**1a**) (0.2 mmol) was taken in an oven dried two-necked round bottomed flask and dissolved in 3 mL of anhydrous 1,2-dichloroethane (DCE). This was then followed by the addition of $[RhCp^*Cl_2]_2$ (2.5 mol%), AgOAc (2 equiv) and D_2O (10 equiv) under nitrogen atmosphere. The reaction mixture was stirred under reflux condition for 8 h. Then, the solvent was removed *in vacuo* and the residue was purified by silica gel column chromatography (Hex: EtOAc = 1:1) to obtain **1a'**. The two ortho-H were deuterated with 65% each.

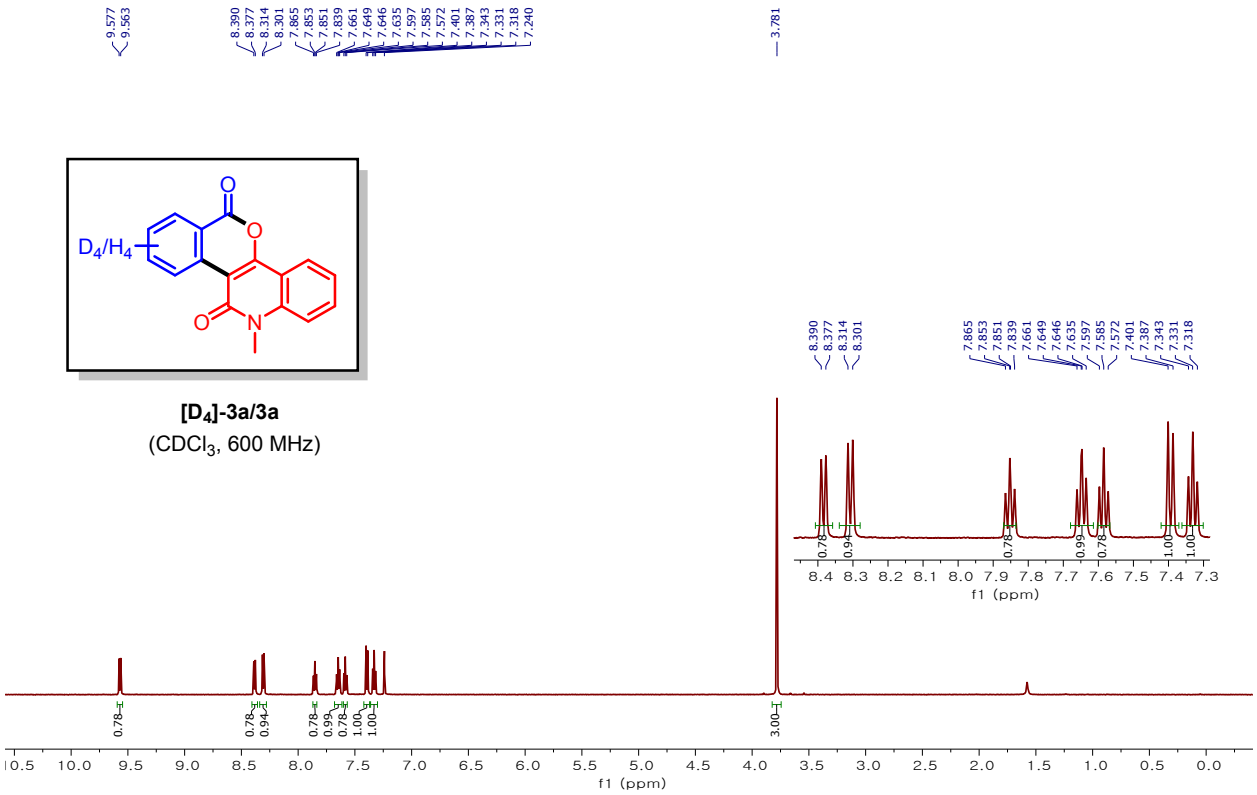


Kinetic Isotope Effect (KIE) Study

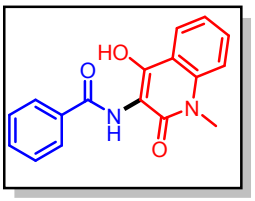


Scheme S2. Kinetic isotope effect study.

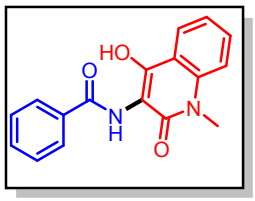
In an oven dried two-necked flask, a mixture of benazamide (**1a**) (0.2 mmol), and 3-diazo-1-methylquinoline-2,4(1*H*,3*H*)-dione (**2a**) (0.2 mmol) were dissolved in DCE (2 mL). This was then followed by addition of $[RhCp^*Cl_2]_2$ (2.5 mol%), and AgOAc (2.0 equiv.) under nitrogen atmosphere. In another reaction flask, benzamide-2,3,4,5,6-d_5 (**[D$_5$]-1a**) (0.2 mmol) was used instead of **1a**. The two reaction mixtures were stirred under reflux condition for 2 h. The reaction mixture were then cooled to room temperature. The reaction mixtures were combined, the volatiles were removed *in vacuo* and the product **[D$_4$]-3a/3a** was isolated by silica gel column chromatography (Hex: EtOAc = 1:5) in 30% combined yield (34 mg). The value of K_H/K_D was calculated based on ^{1}H NMR. Here, K_H/K_D = 0.78/(1.0-0.78) = 3.5. HRMS was measured for **[D$_4$]-3a/3a**. HRMS *m/z* (M^+): calcd for $C_{17}H_7D_4NO_3$: 281.0990; found: 281.0992.



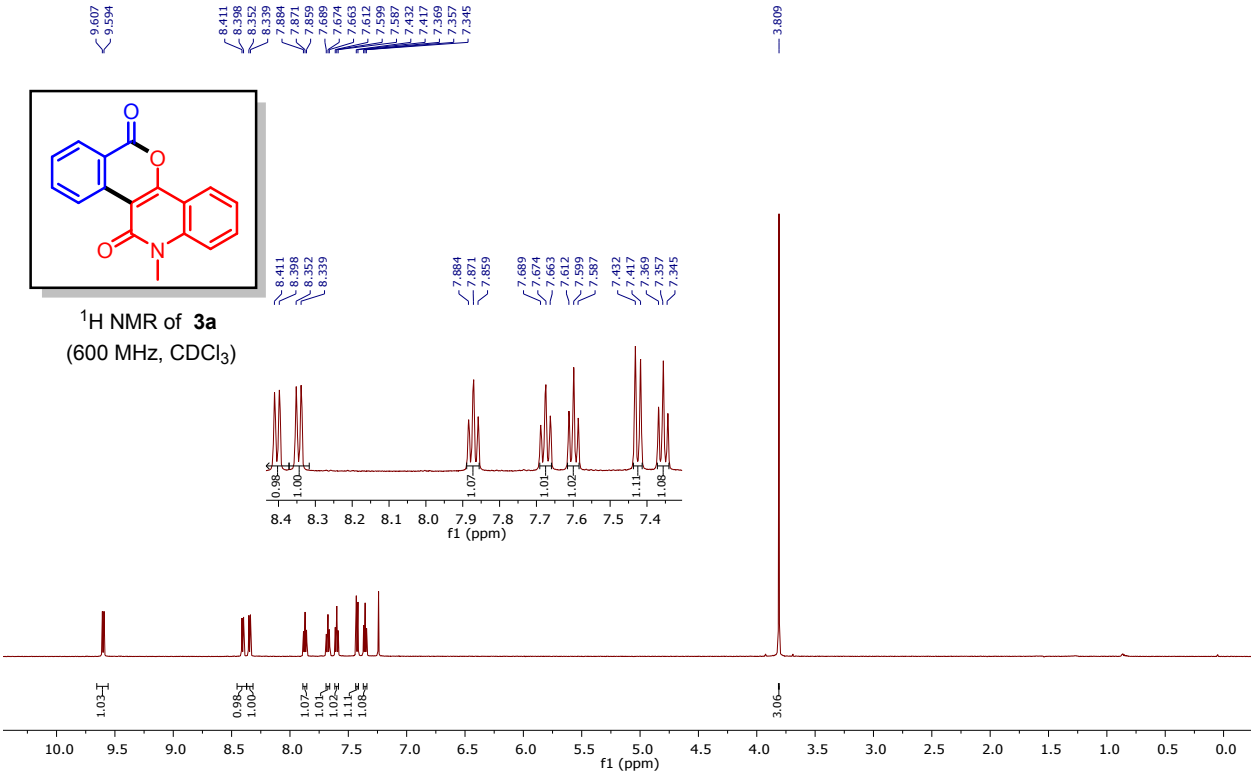
^{1}H NMR and ^{13}C NMR spectra of synthesized compounds (3-11)



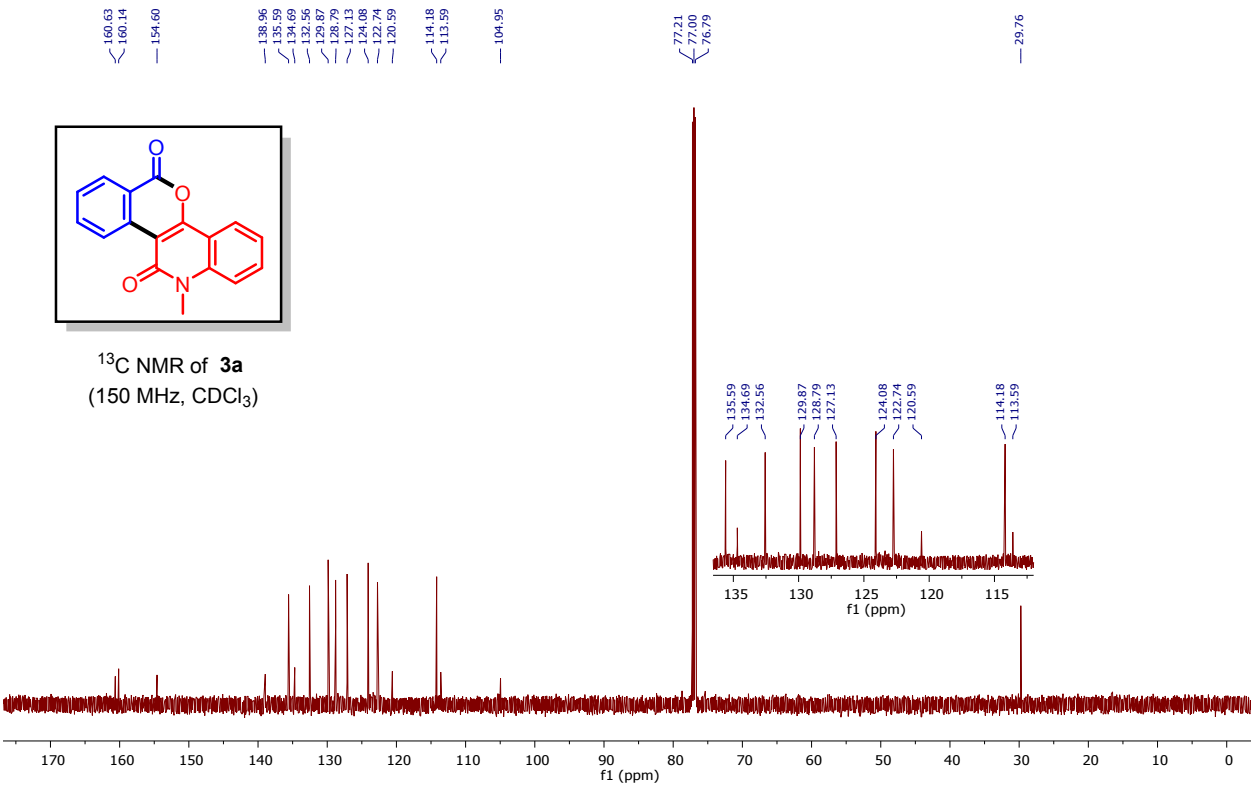
^{1}H NMR of **3a'**
(600 MHz in $CDCl_3$)



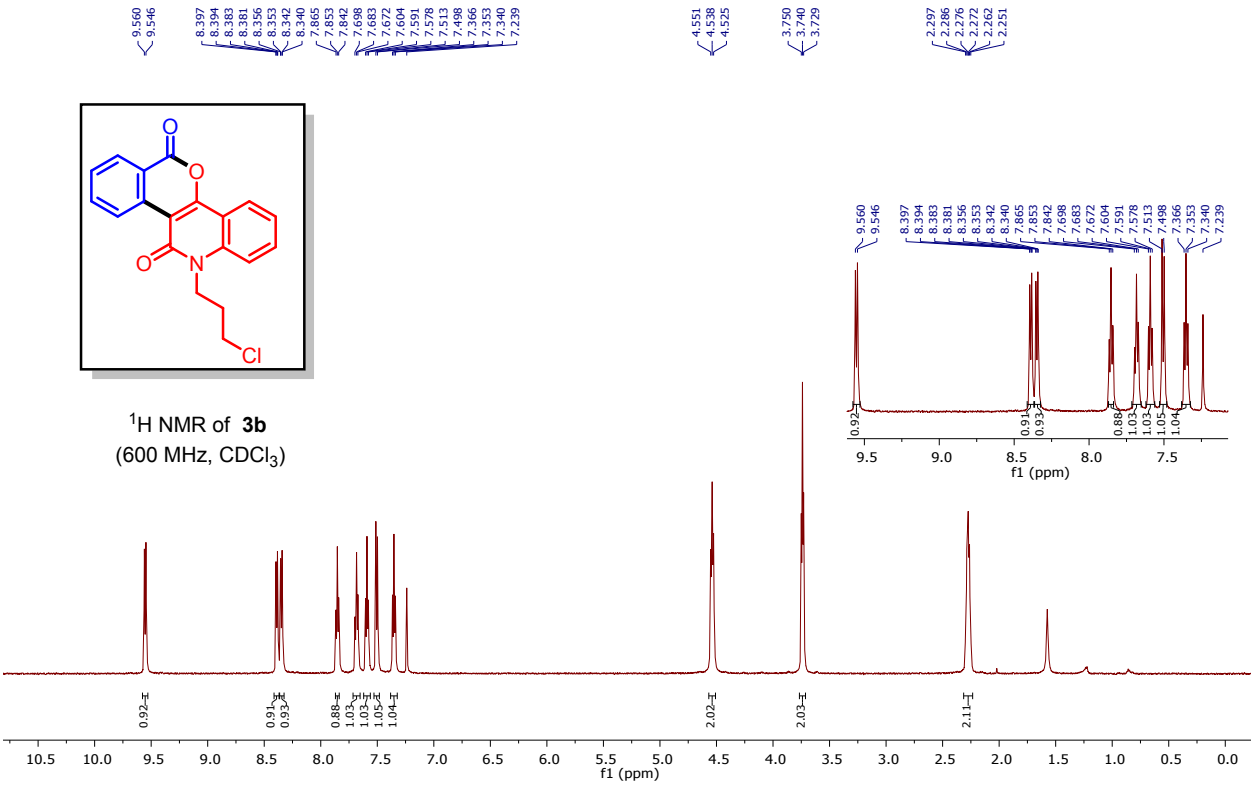
^{13}C NMR of **3a'**
(150 MHz in $CDCl_3$)



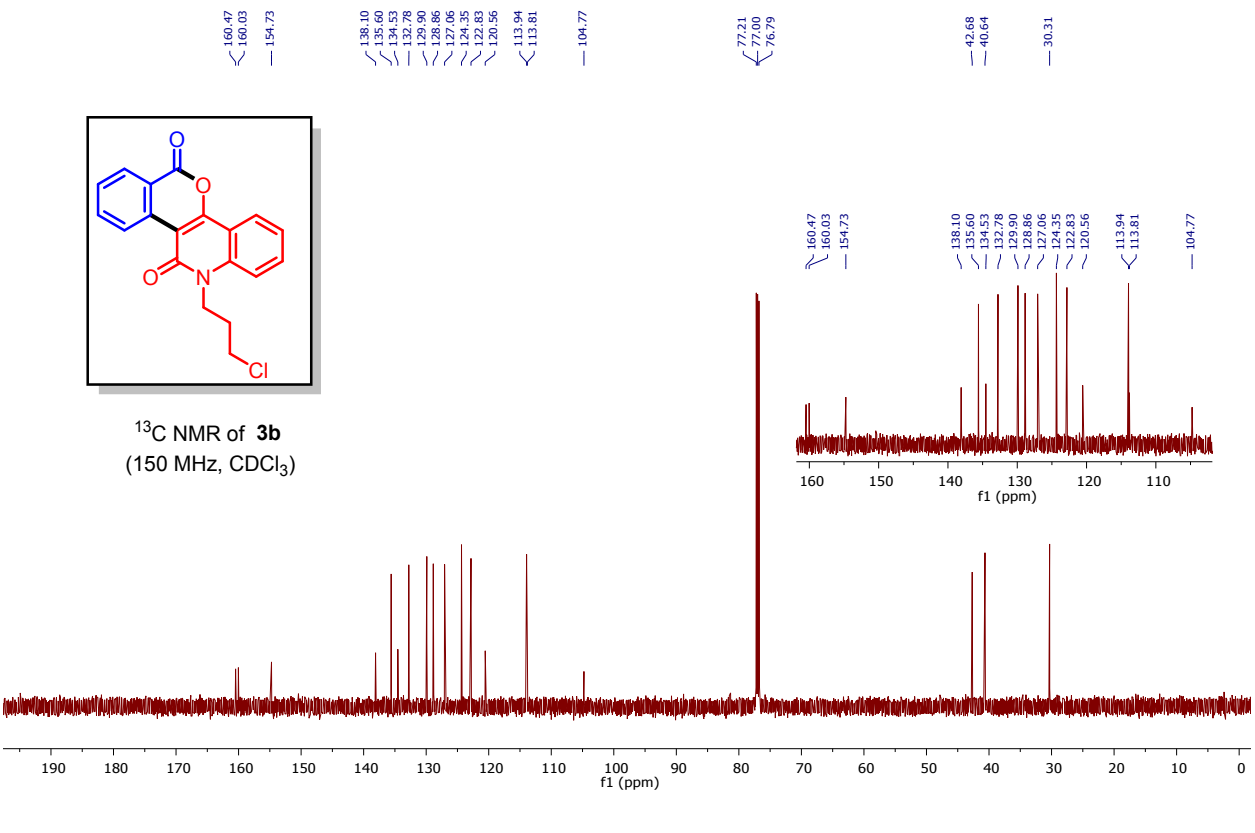
^{1}H NMR of **3a**
(600 MHz, $CDCl_3$)



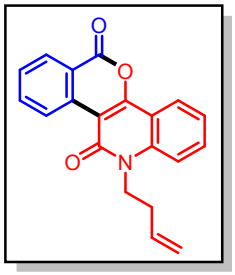
^{13}C NMR of **3a**
(150 MHz, $CDCl_3$)



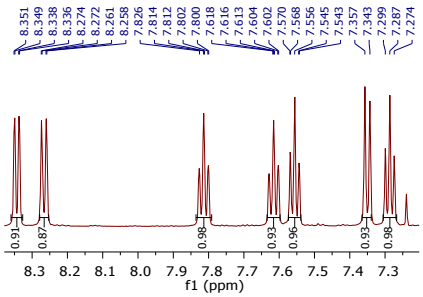
^{1}H NMR of **3b**
(600 MHz, $CDCl_3$)

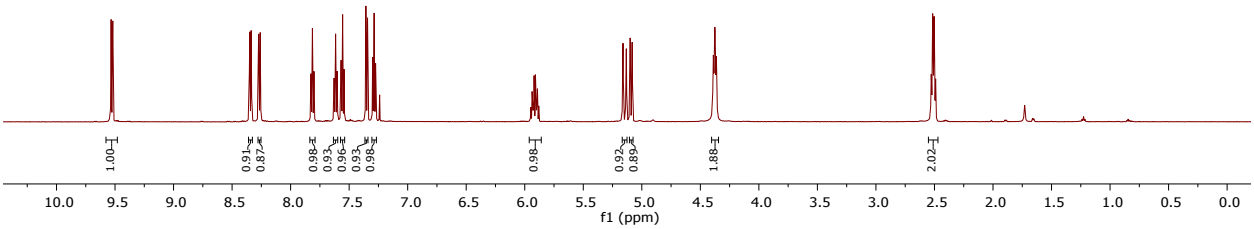


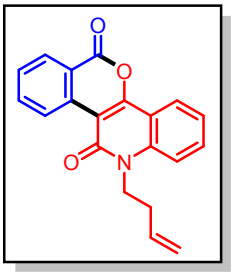
^{13}C NMR of **3b**
(150 MHz, $CDCl_3$)



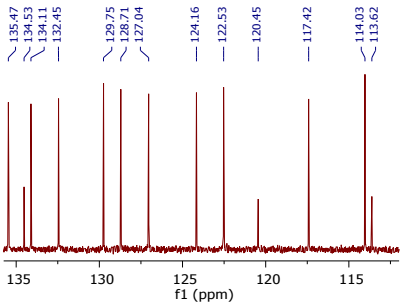
^{1}H NMR of **3c**
(600 MHz, $CDCl_3$)

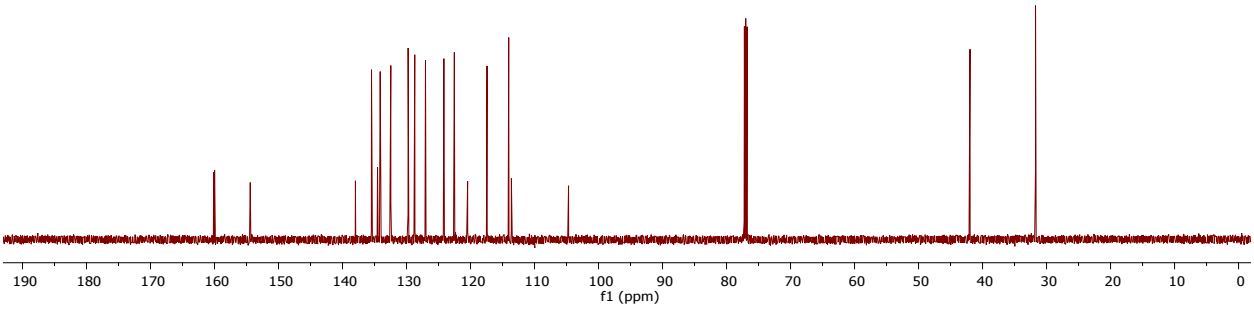


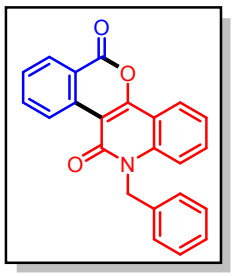




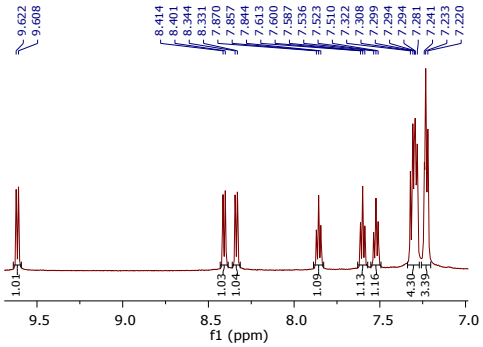
^{13}C NMR of **3c**
(150 MHz, $CDCl_3$)

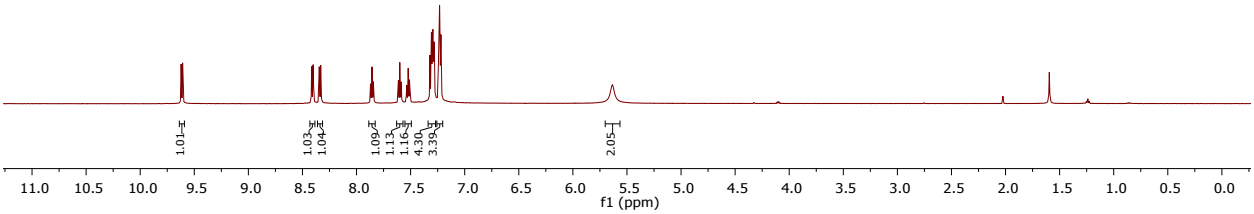


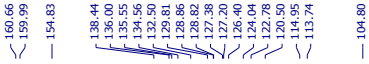


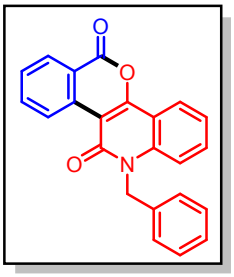


^{1}H NMR of **3d**
(600 MHz, $CDCl_3$)

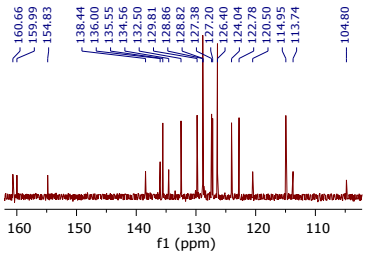


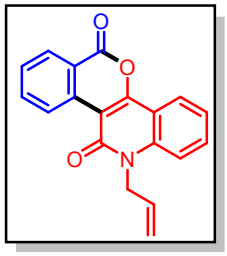




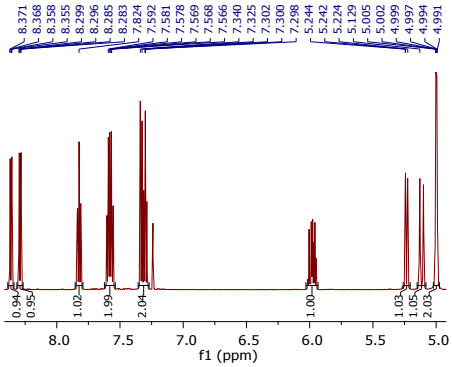


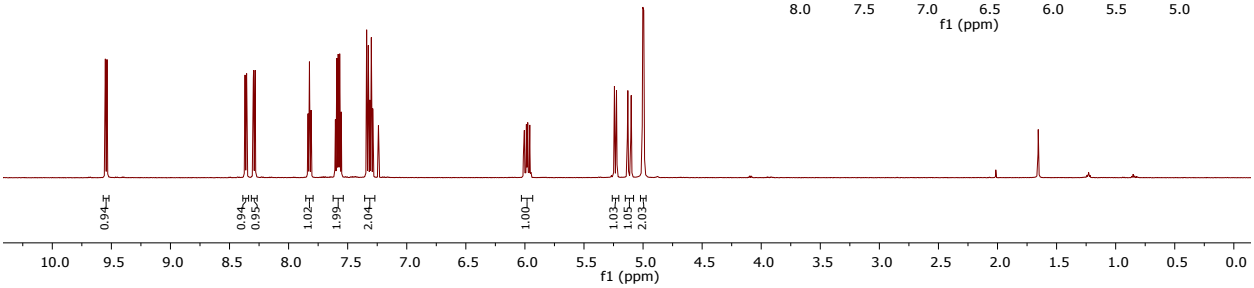
^{13}C NMR of **3d**
(150 MHz, $CDCl_3$)

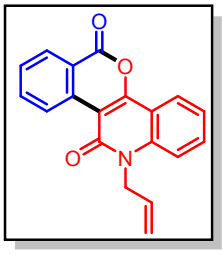




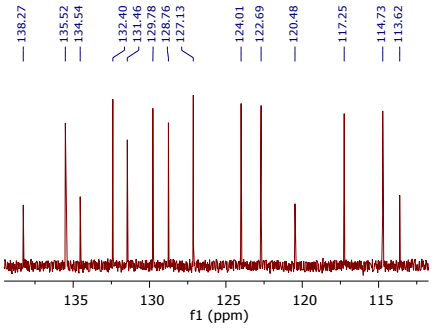
^{1}H NMR of **3e**
(600 MHz, $CDCl_3$)

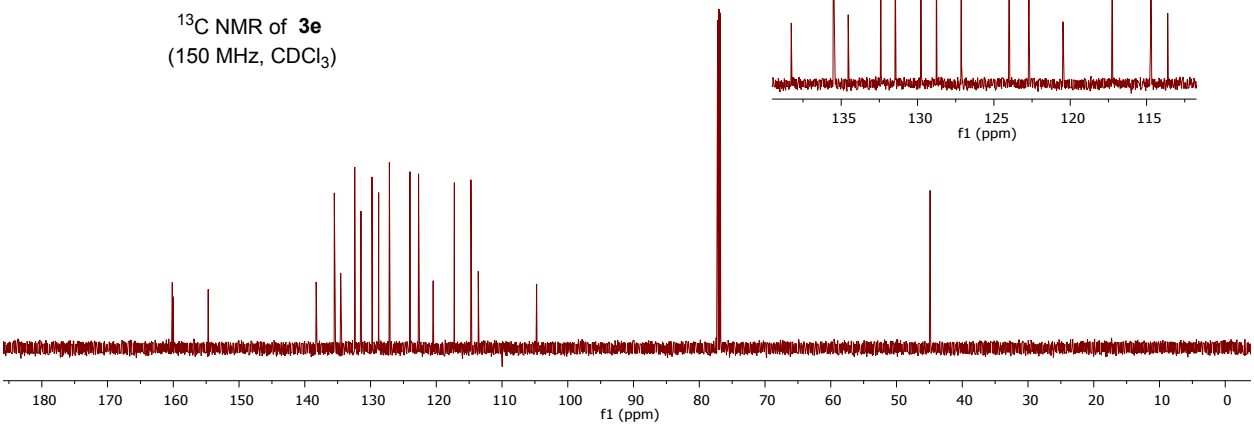


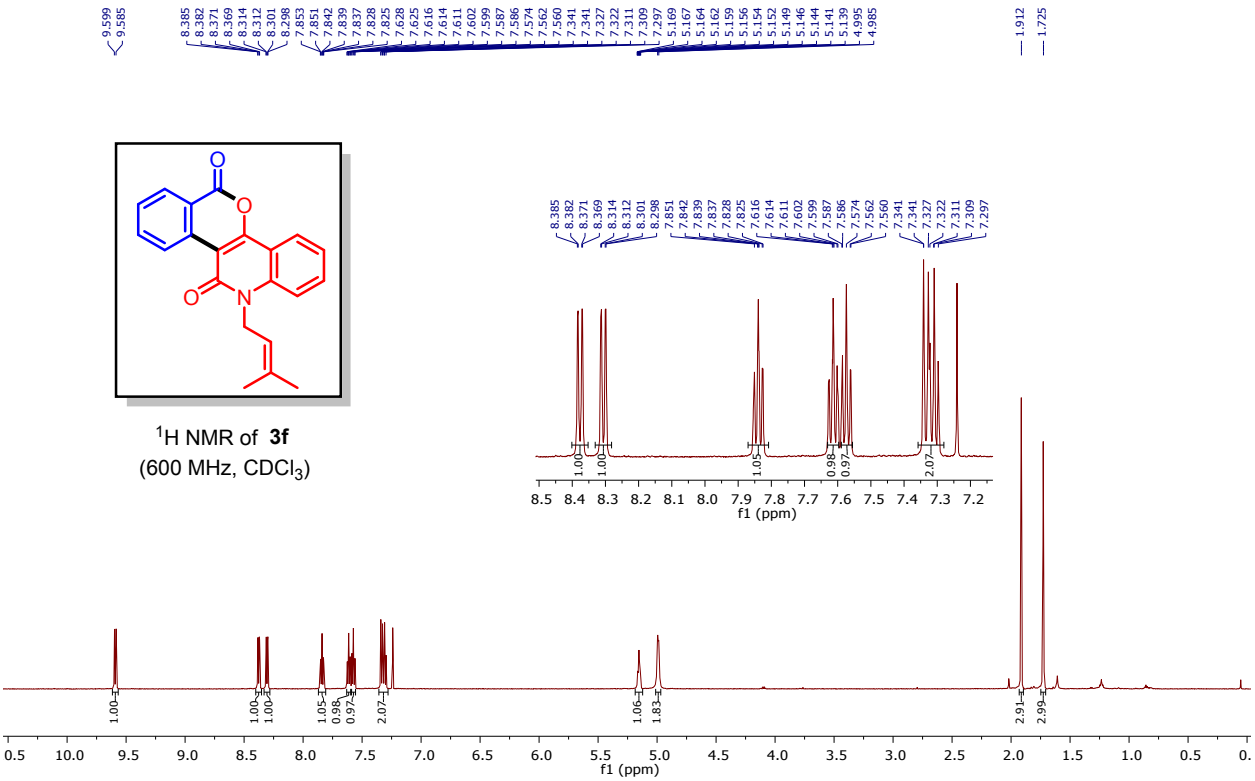




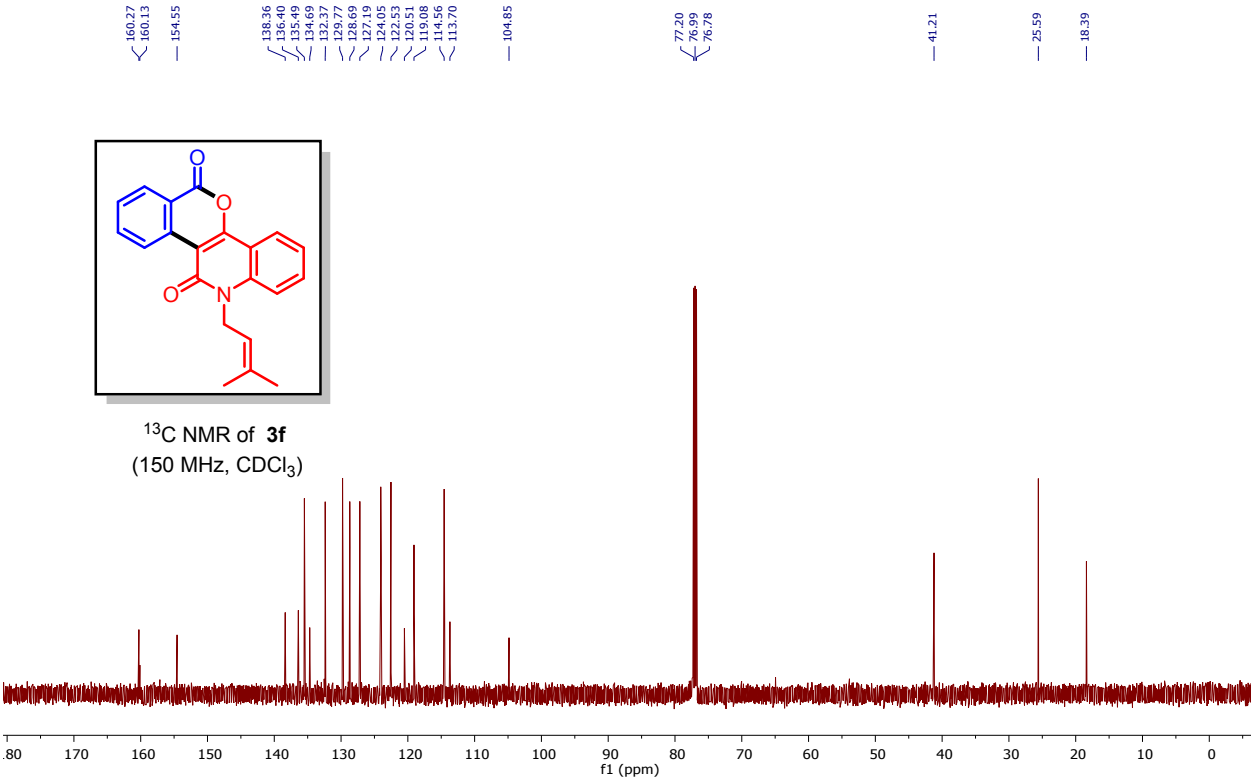
^{13}C NMR of **3e**
(150 MHz, $CDCl_3$)



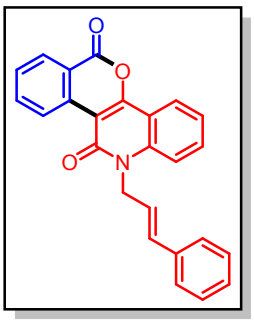




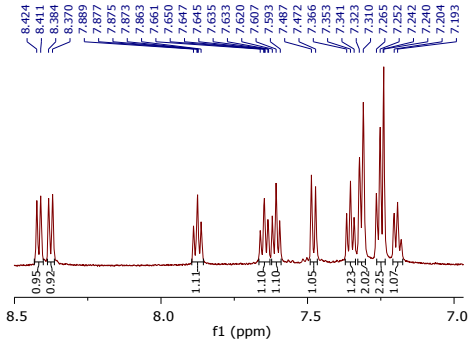
^{1}H NMR of **3f**
(600 MHz, $CDCl_3$)

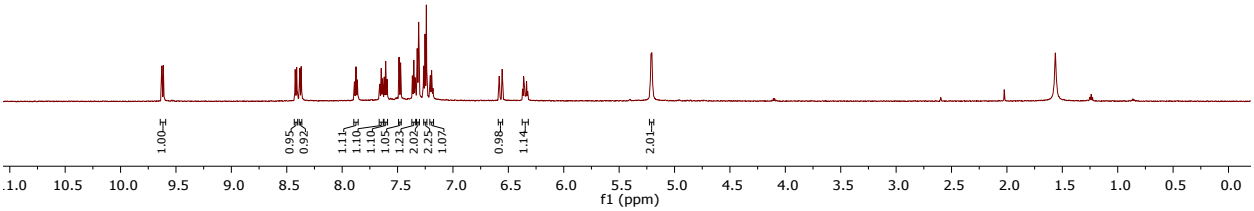


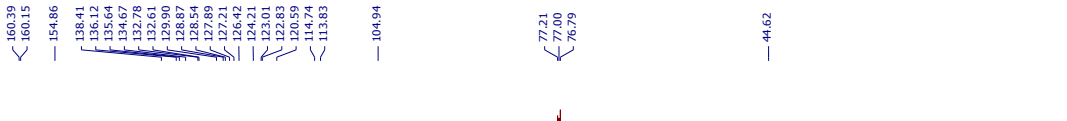
^{13}C NMR of **3f**
(150 MHz, $CDCl_3$)

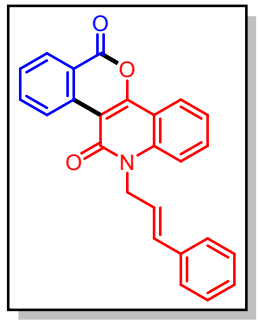


^{1}H NMR of **3g**
(600 MHz, $CDCl_3$)

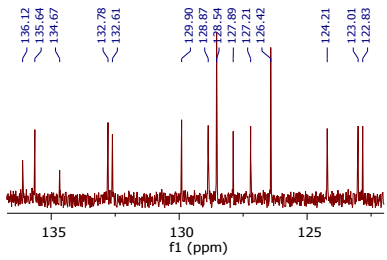


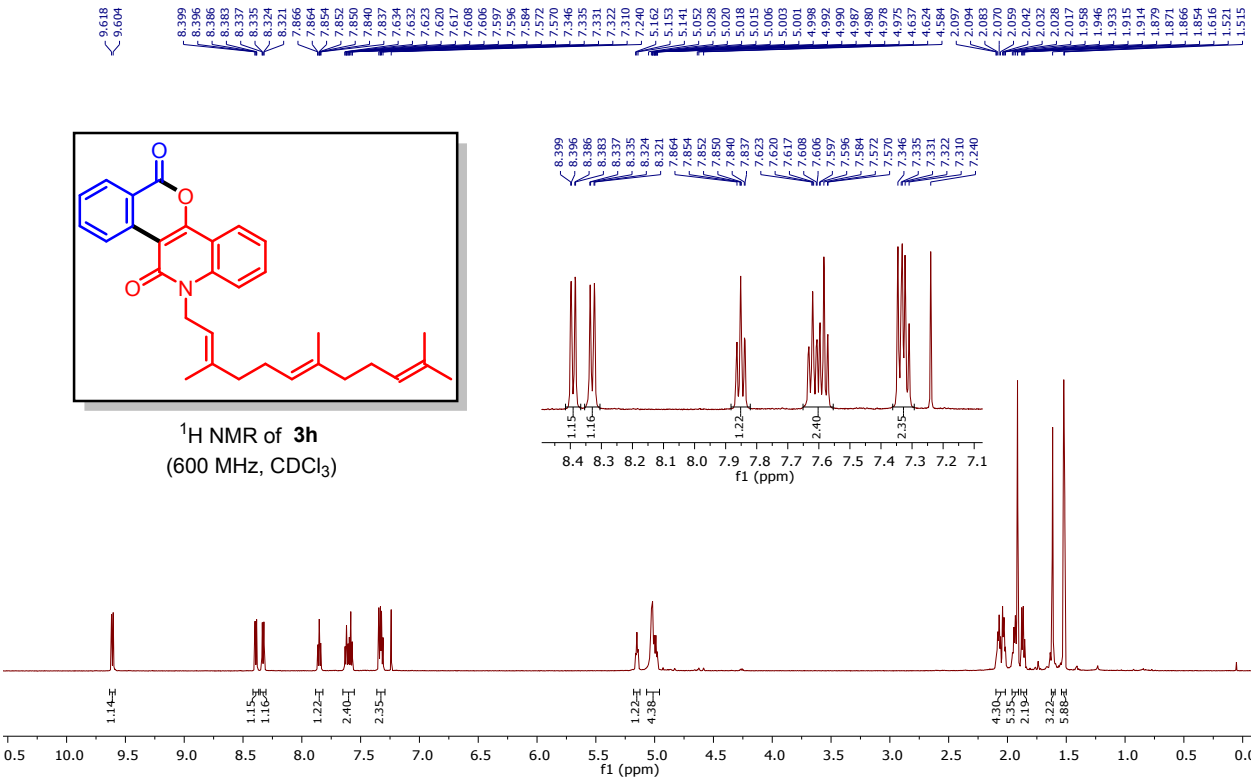




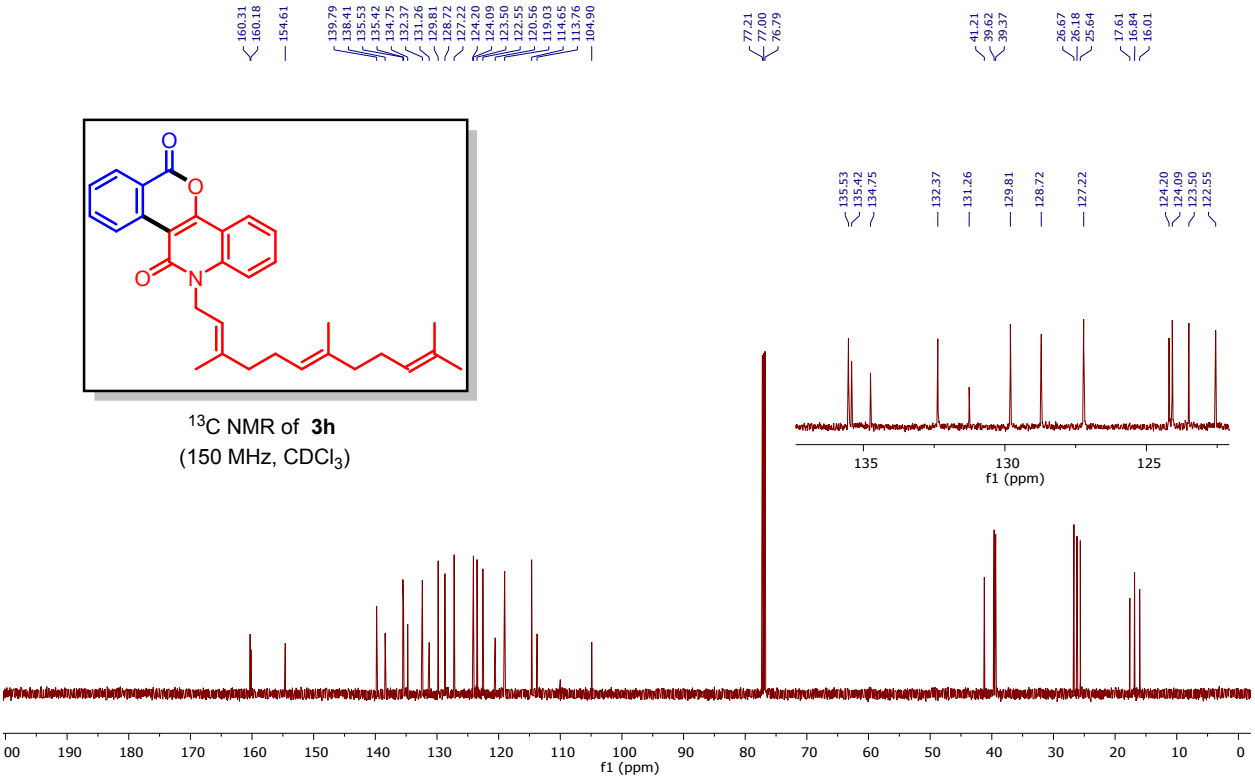


^{13}C NMR of **3g**
(150 MHz, $CDCl_3$)

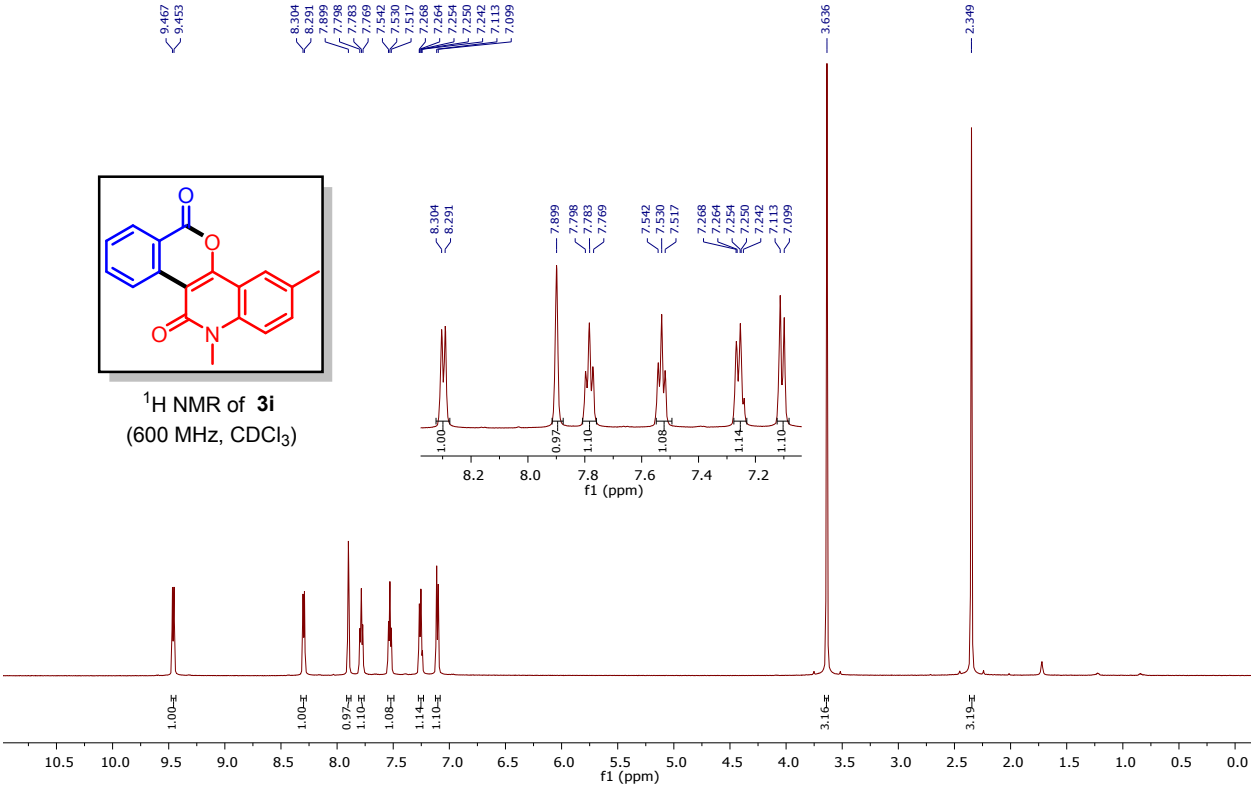




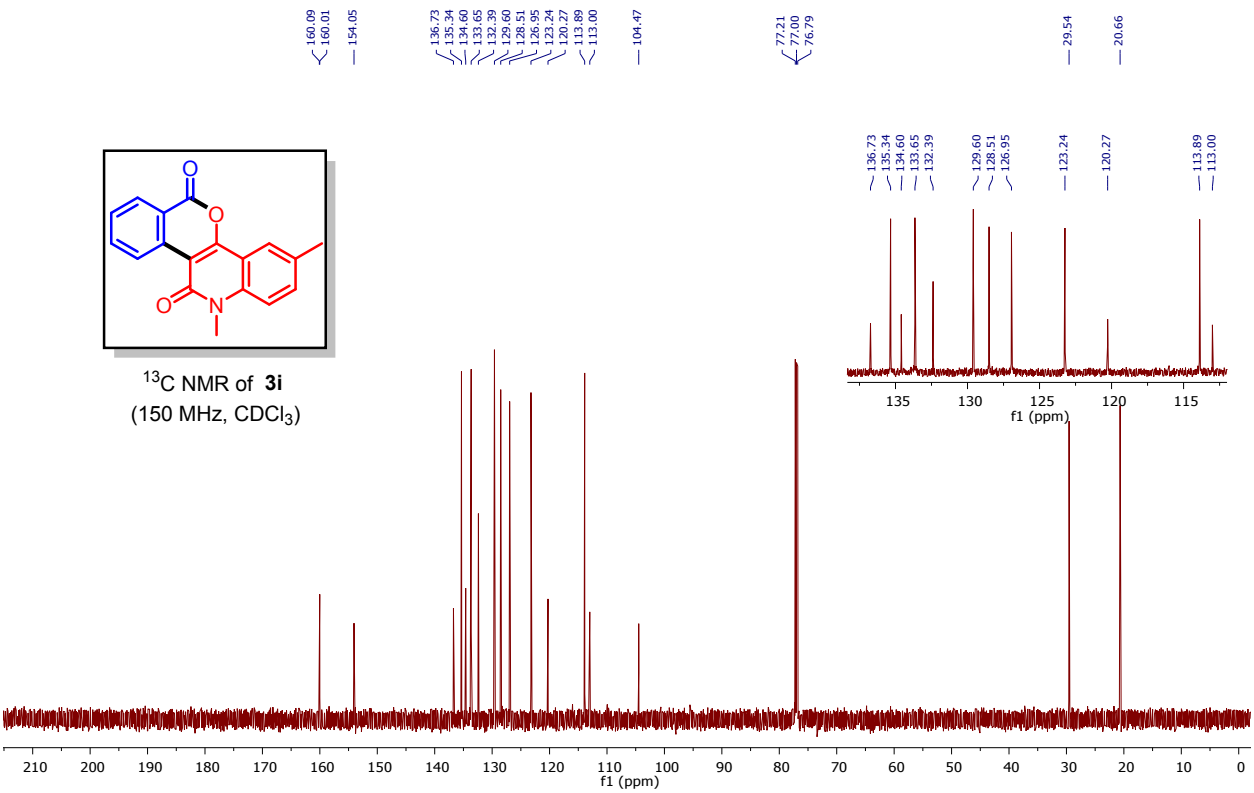
^{1}H NMR of **3h**
(600 MHz, $CDCl_3$)



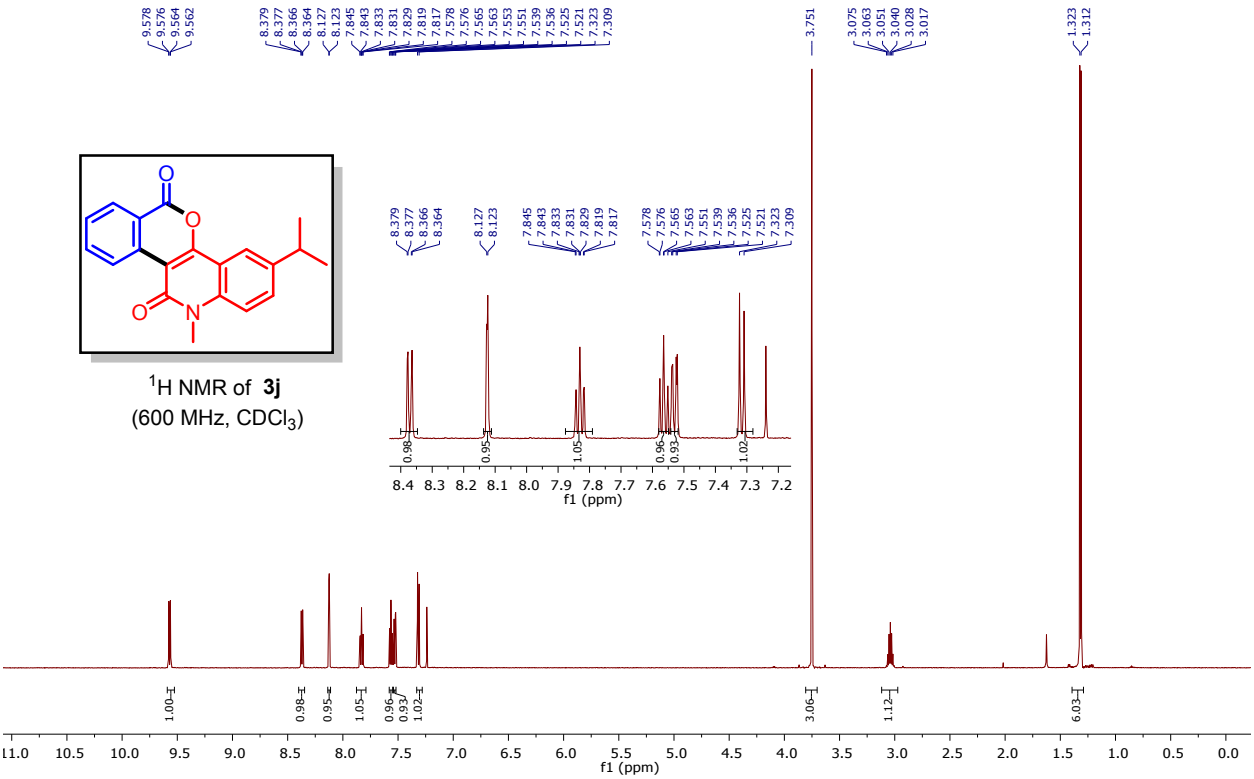
^{13}C NMR of **3h**
(150 MHz, $CDCl_3$)



^{1}H NMR of **3i**
(600 MHz, $CDCl_3$)



^{13}C NMR of **3i**
(150 MHz, $CDCl_3$)



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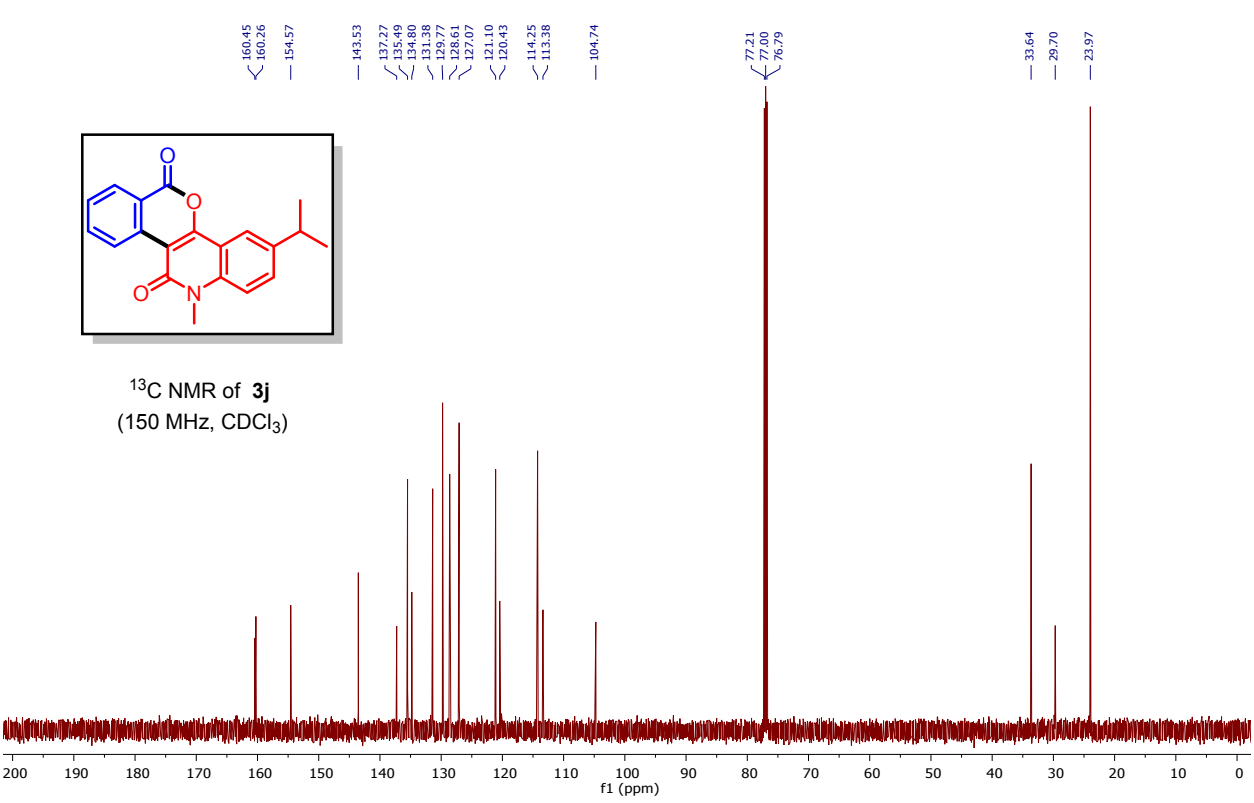
(600 MHz, $CDCl_3$)



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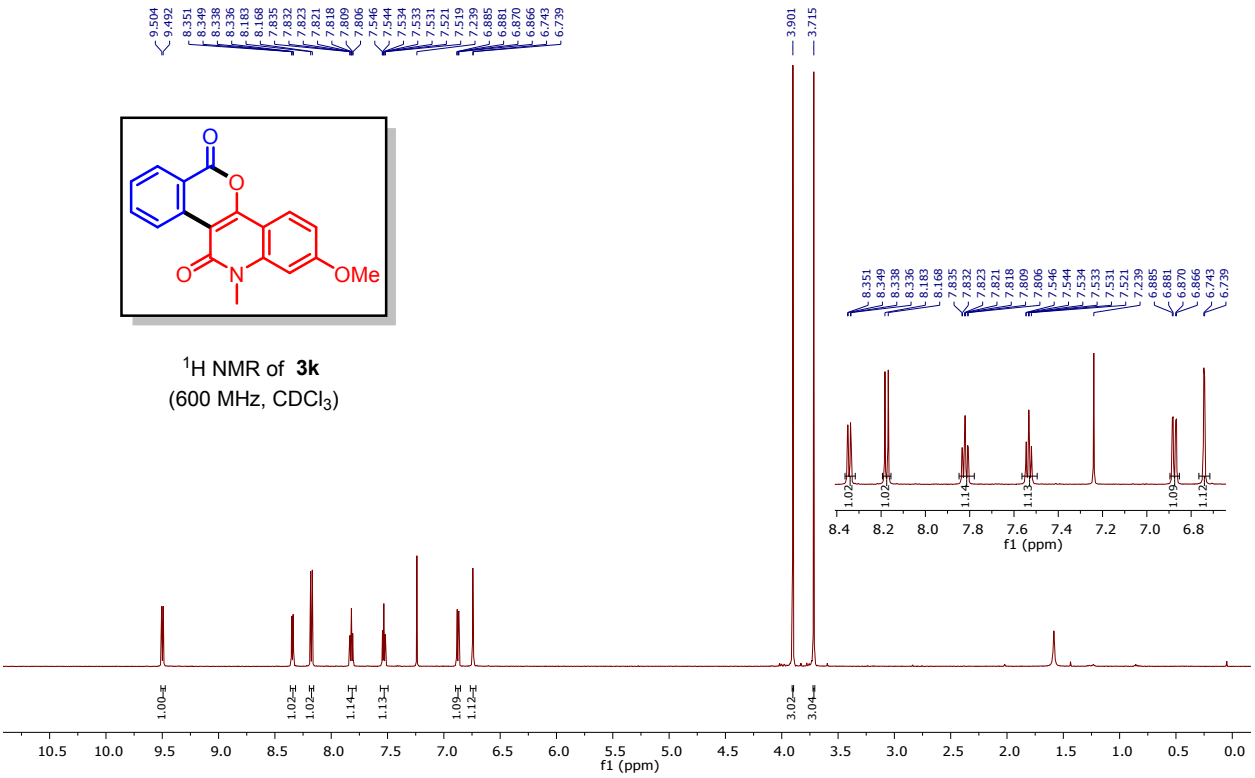
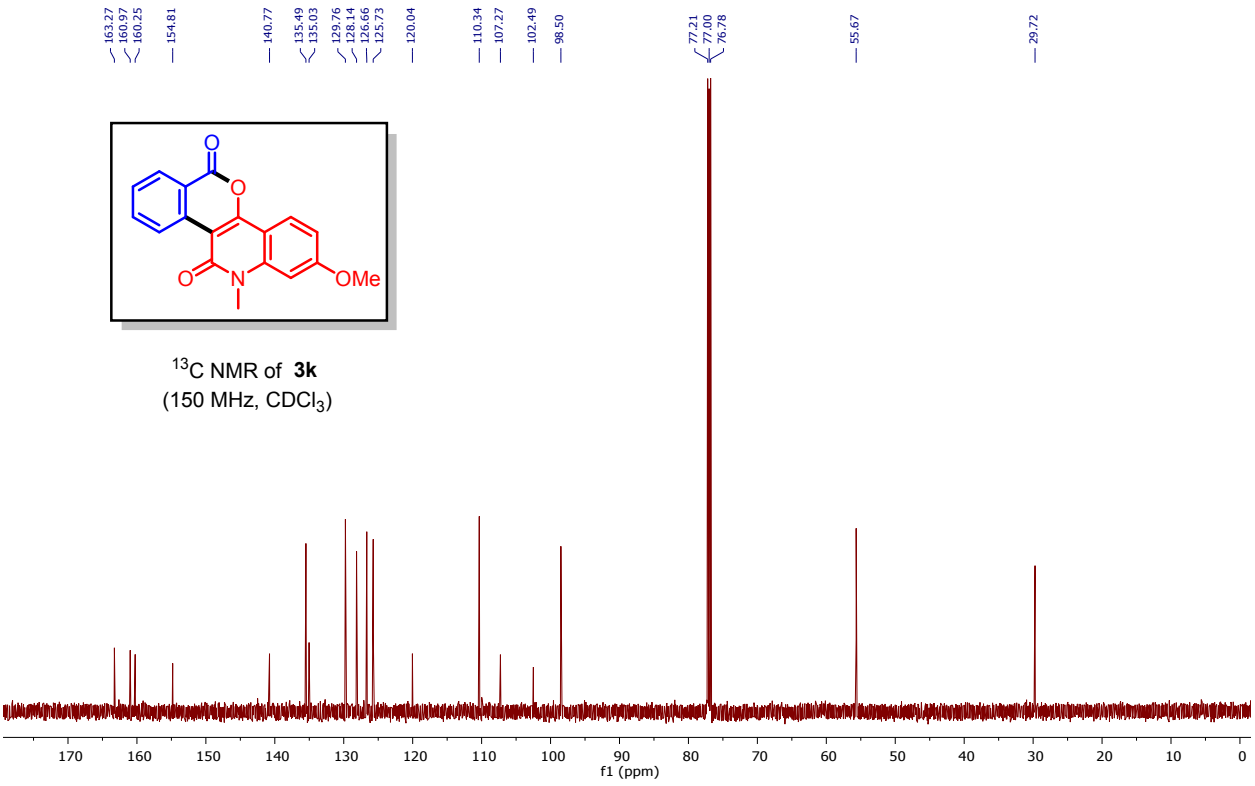
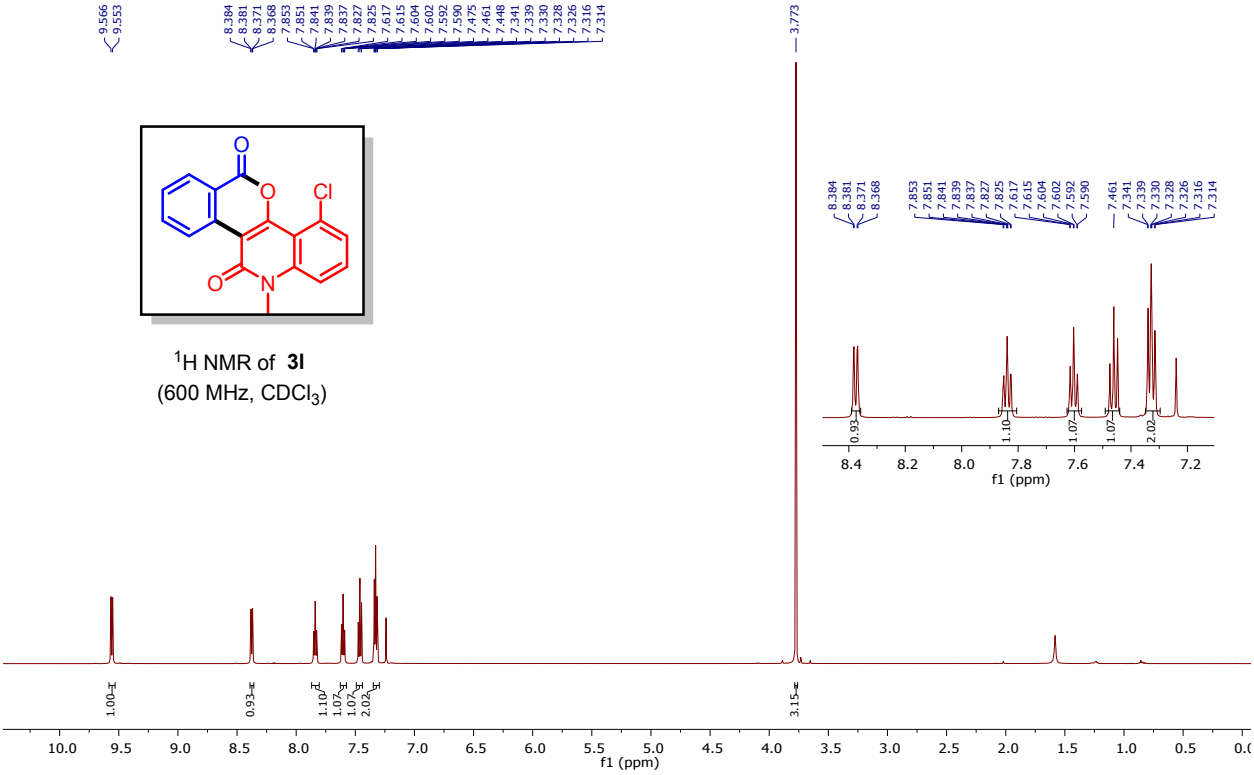
(150 MHz, $CDCl_3$)



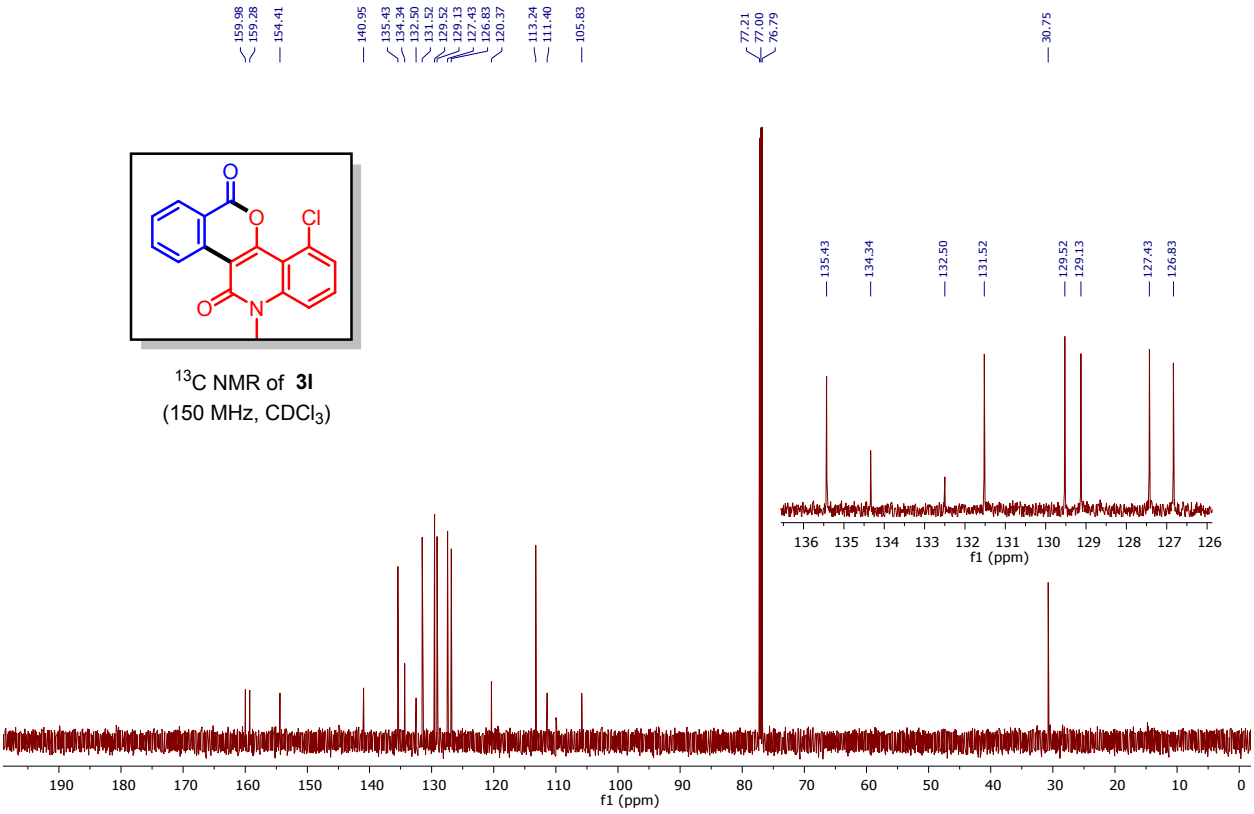
^{1}H NMR of **3k**
(600 MHz, $CDCl_3$)



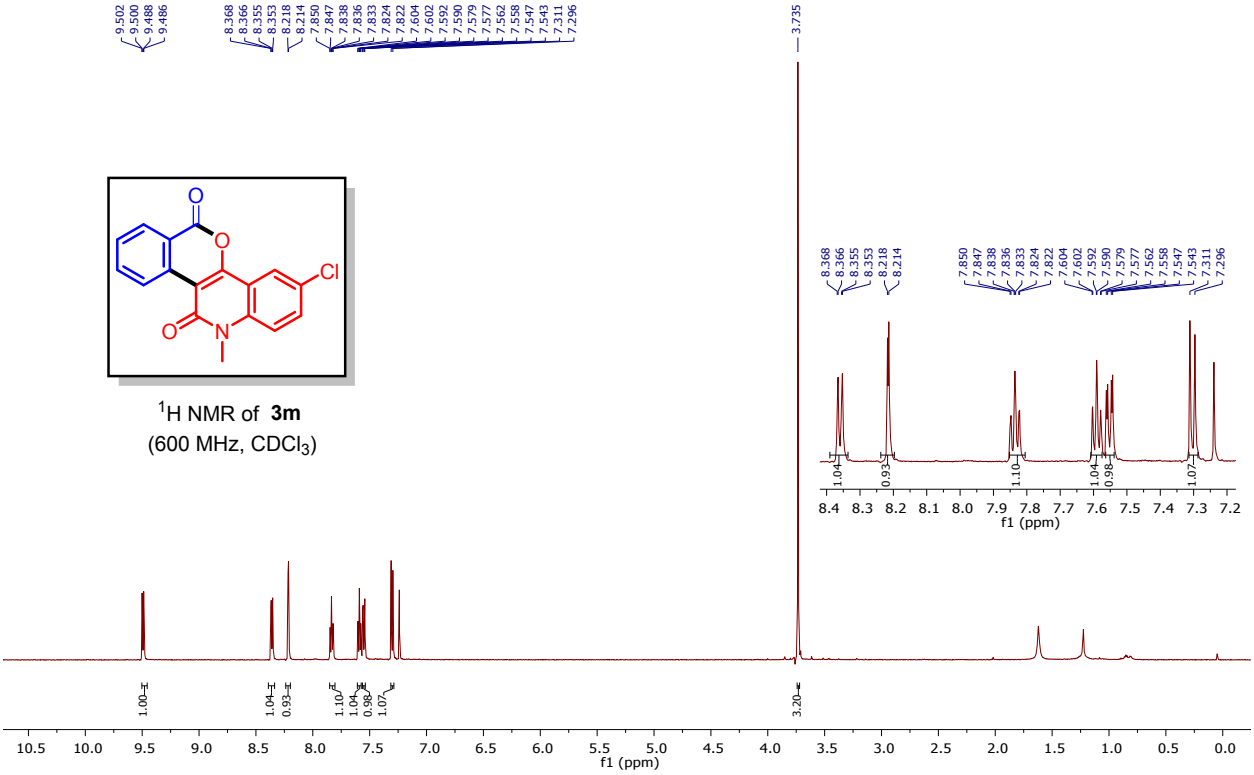
^{13}C NMR of **3k**
(150 MHz, $CDCl_3$)



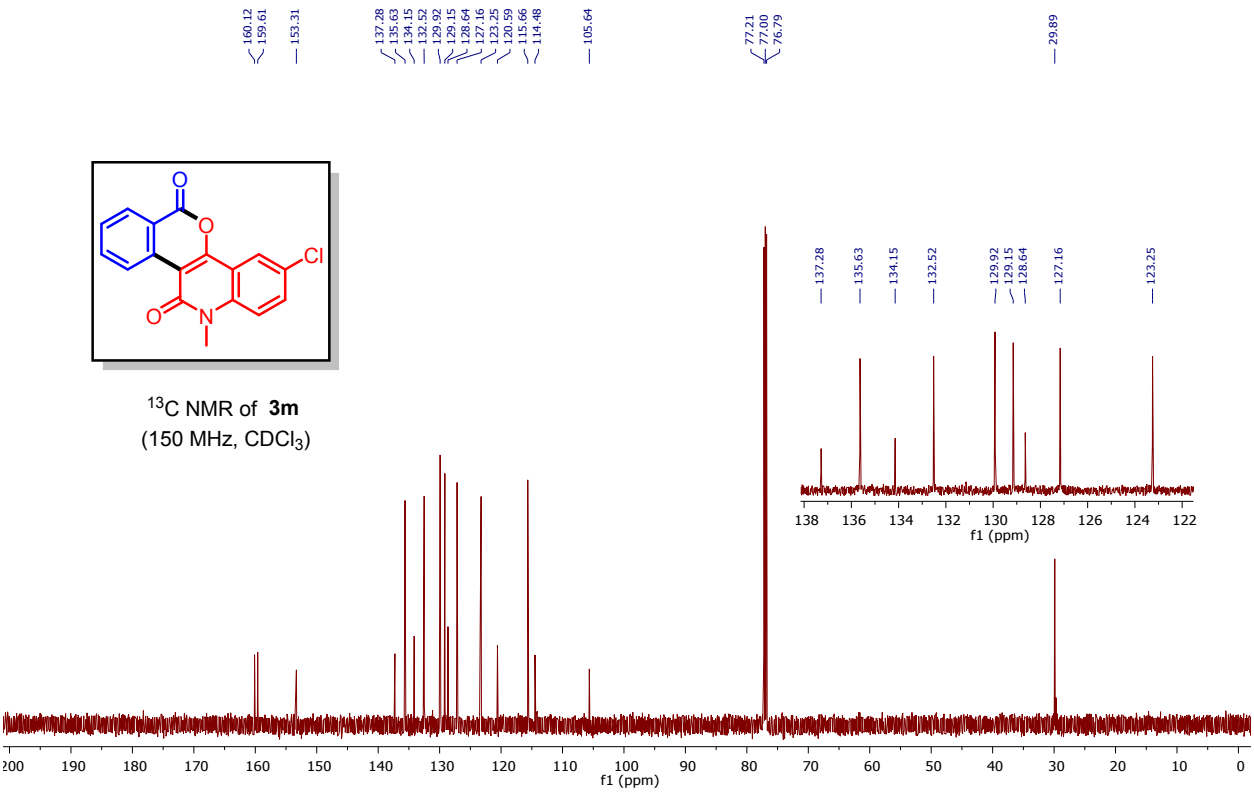
^{1}H NMR of **3l**
(600 MHz, $CDCl_3$)



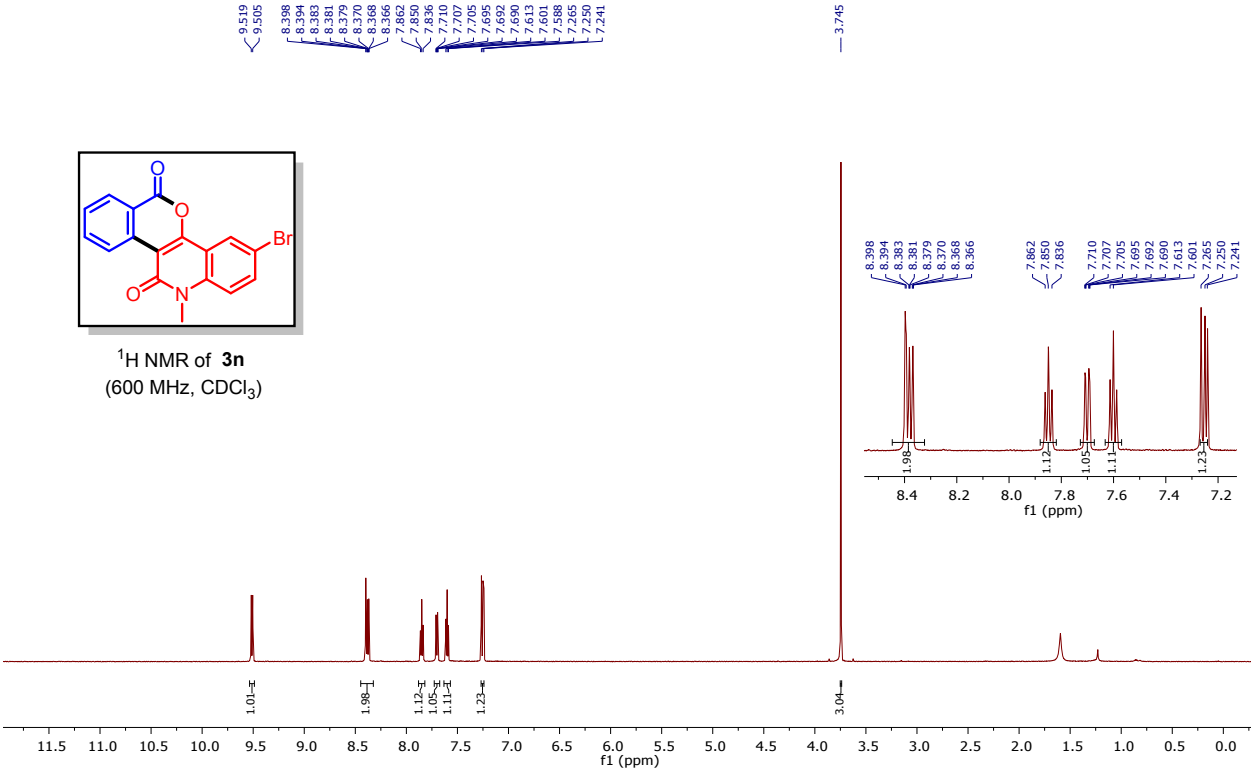
^{13}C NMR of **3l**
(150 MHz, $CDCl_3$)



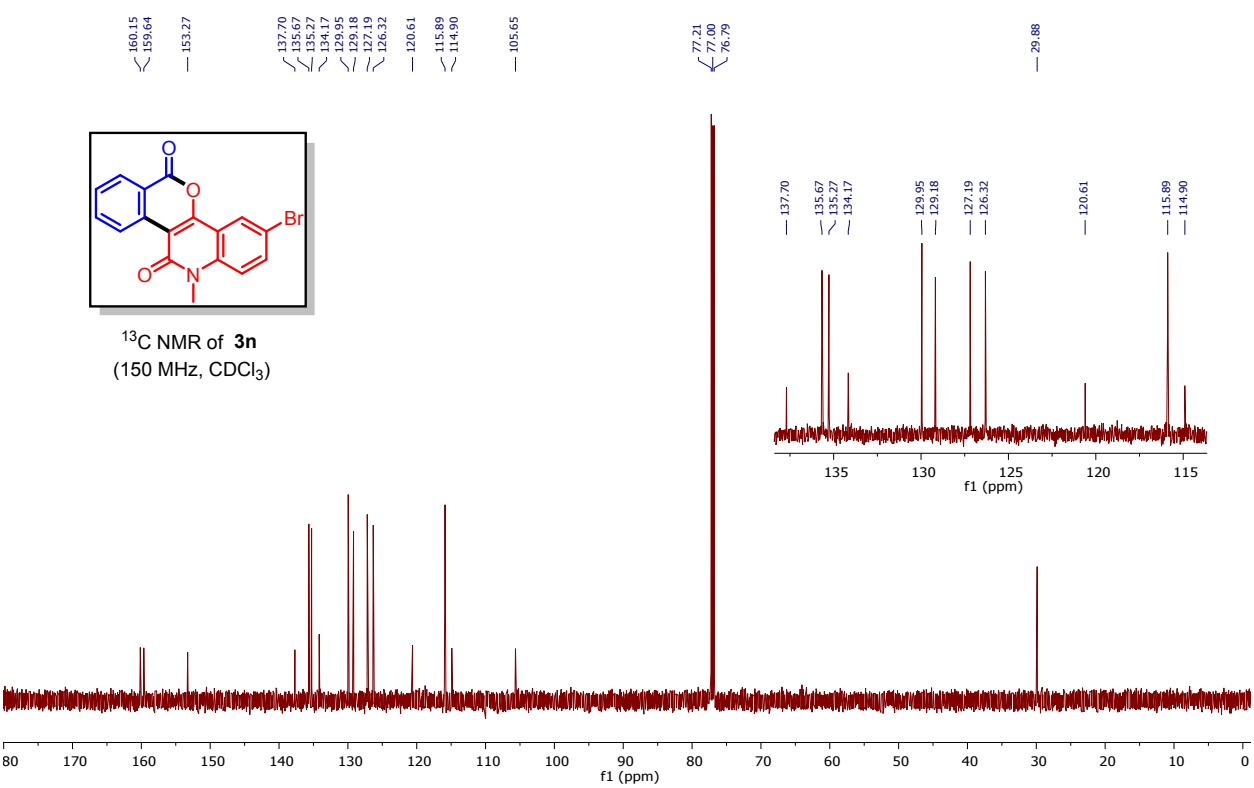
^{1}H NMR of **3m**
(600 MHz, $CDCl_3$)



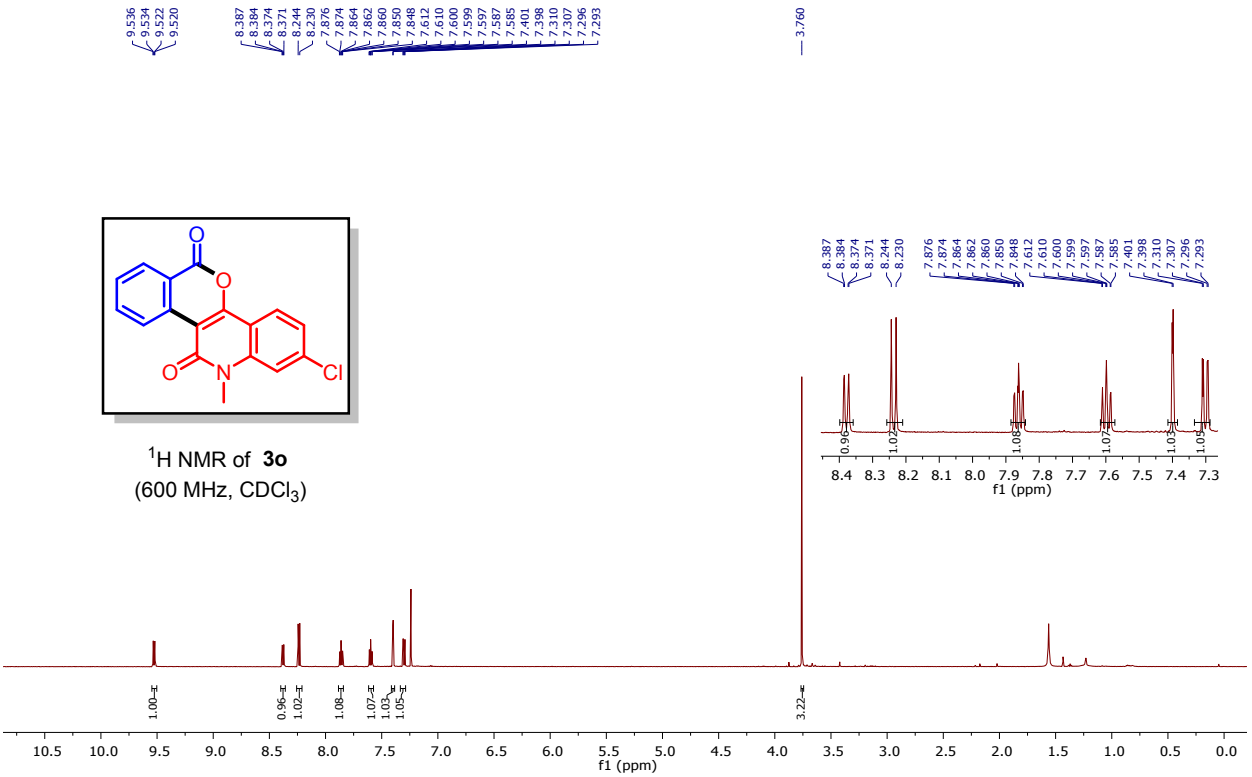
^{13}C NMR of **3m**
(150 MHz, $CDCl_3$)



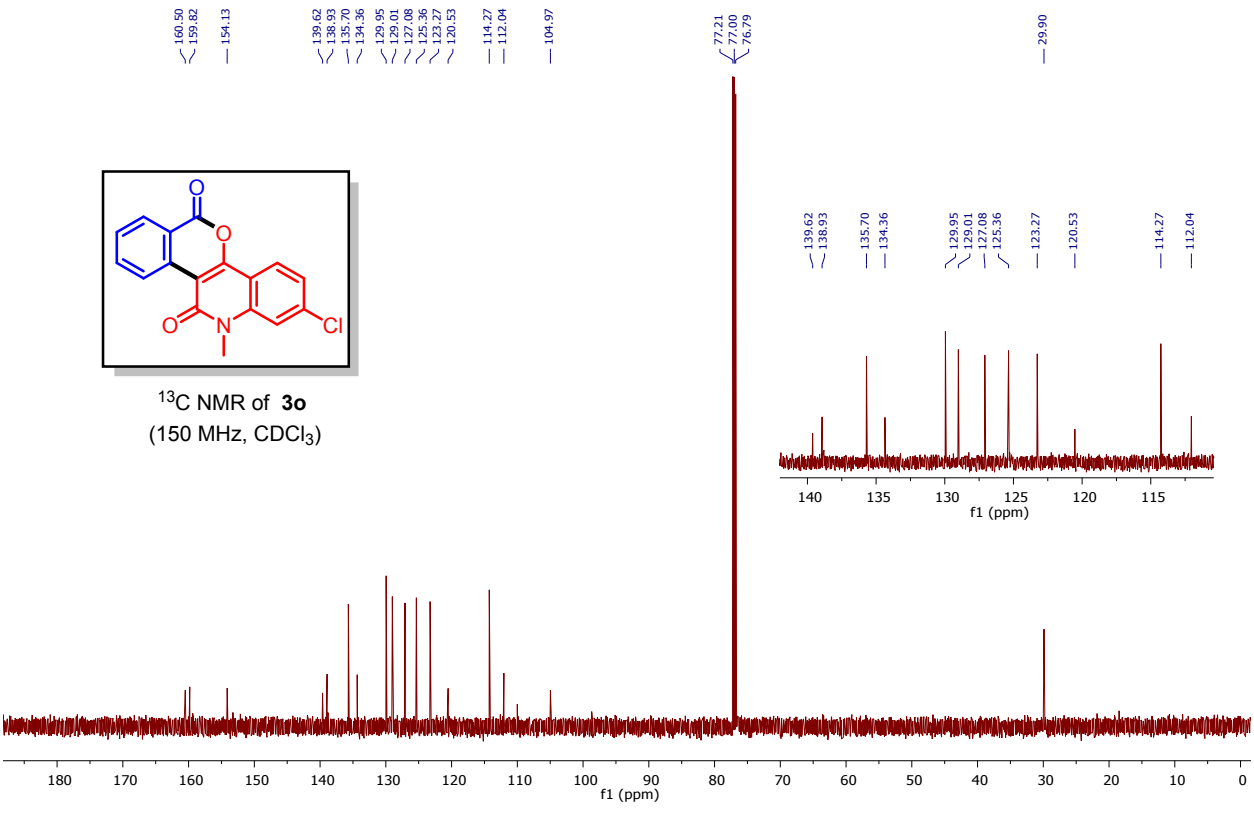
^{1}H NMR of **3n**
(600 MHz, $CDCl_3$)



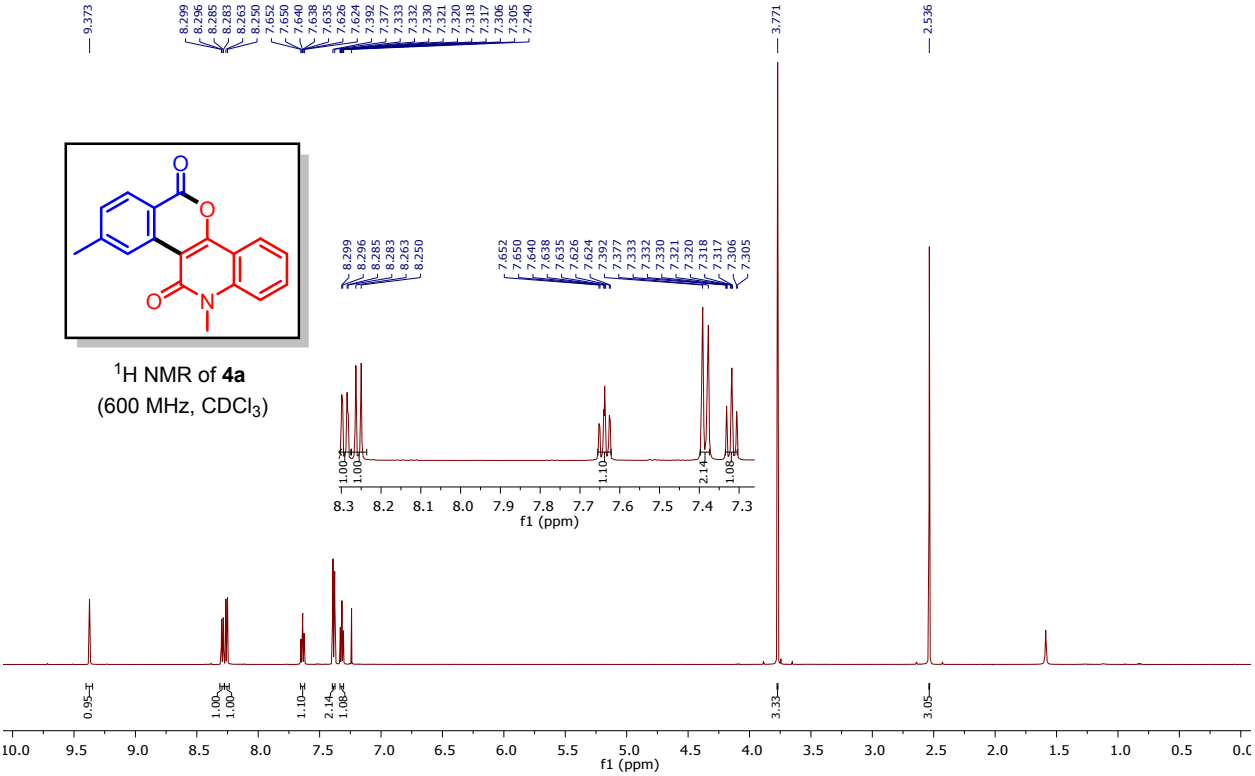
^{13}C NMR of **3n**
(150 MHz, $CDCl_3$)



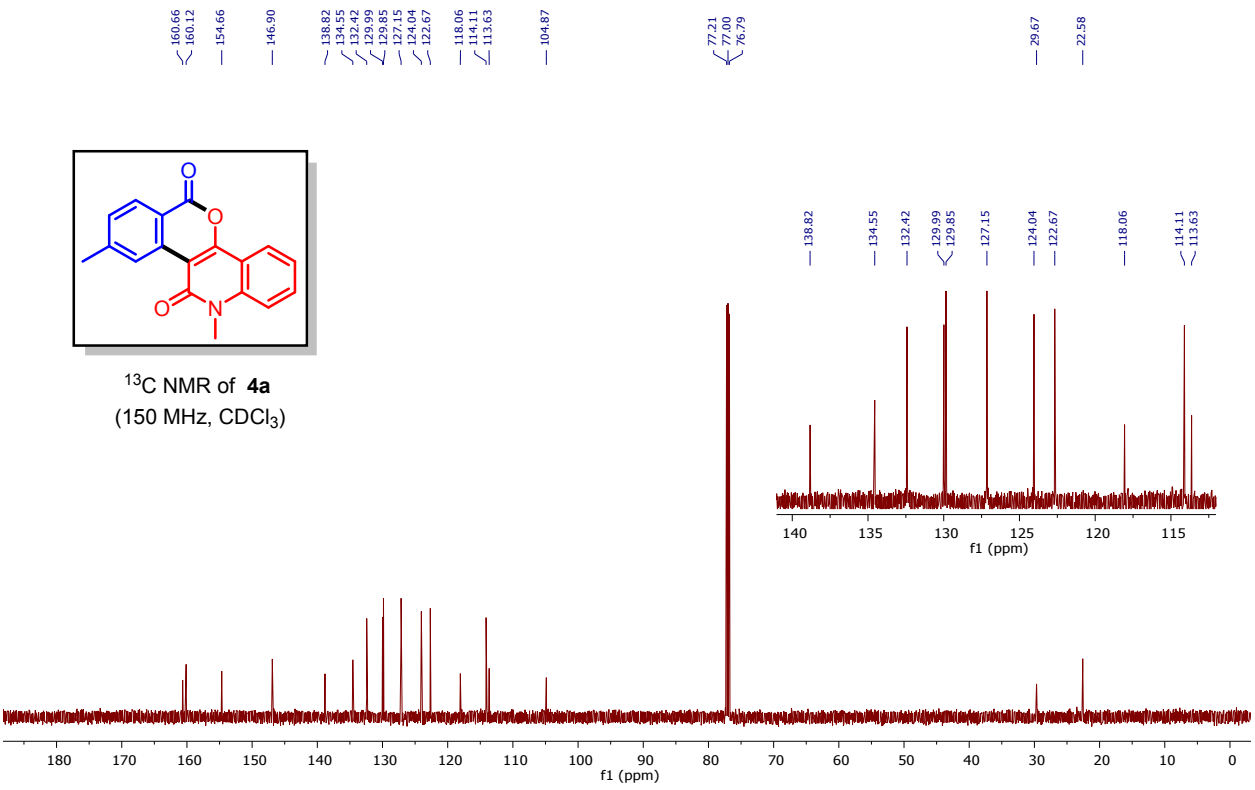
^{1}H NMR of **3o**
(600 MHz, $CDCl_3$)



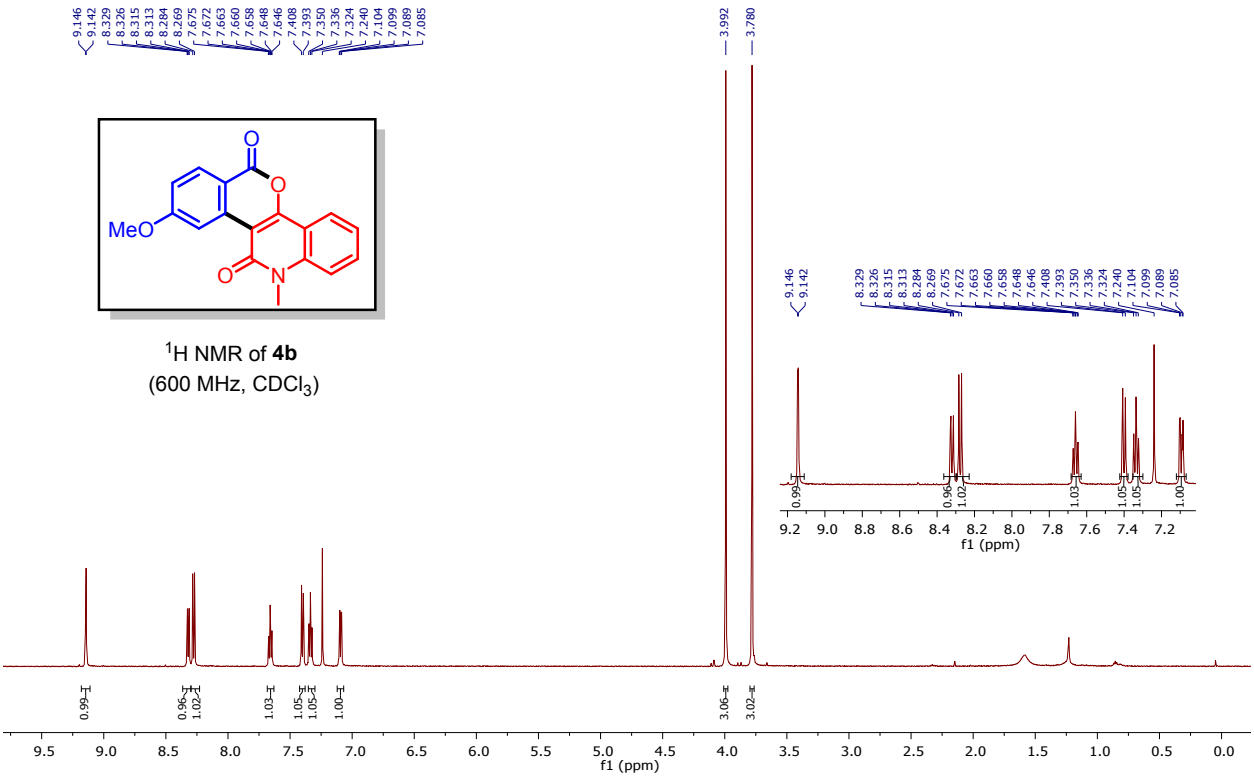
^{13}C NMR of **3o**
(150 MHz, $CDCl_3$)



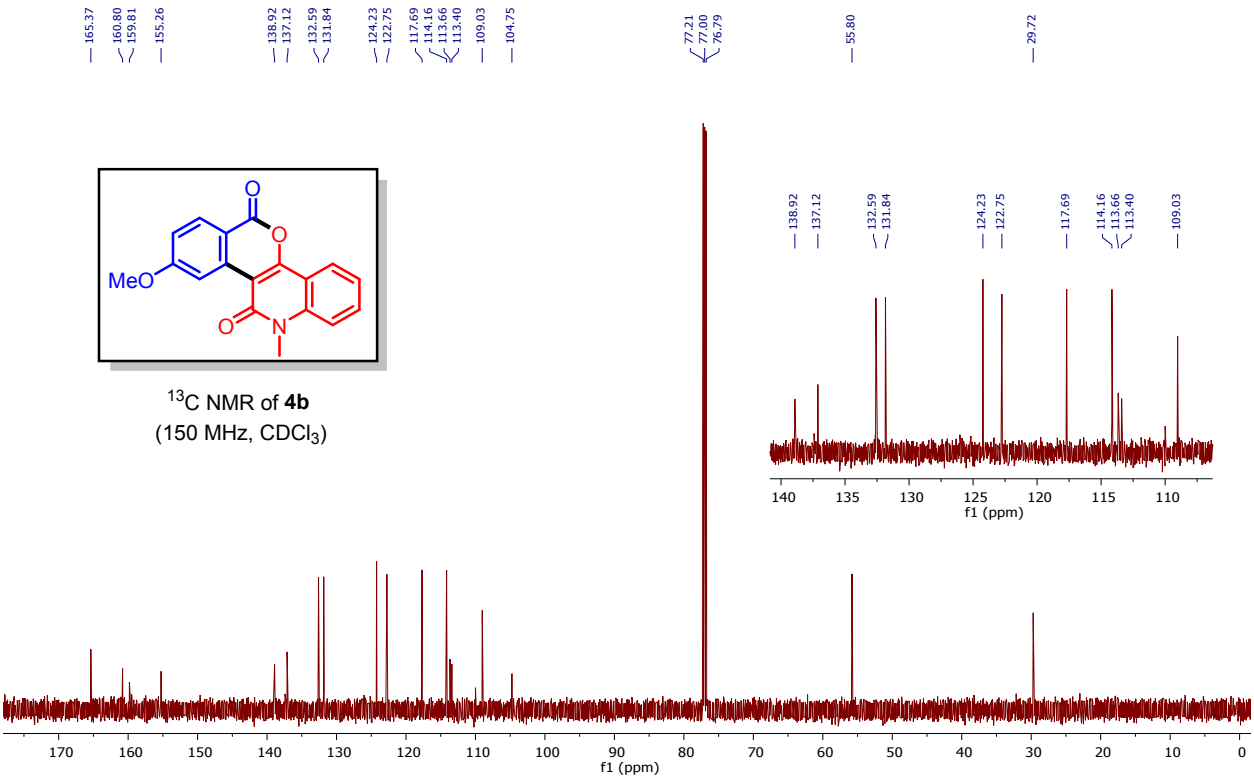
^{1}H NMR of **4a**
(600 MHz, $CDCl_3$)



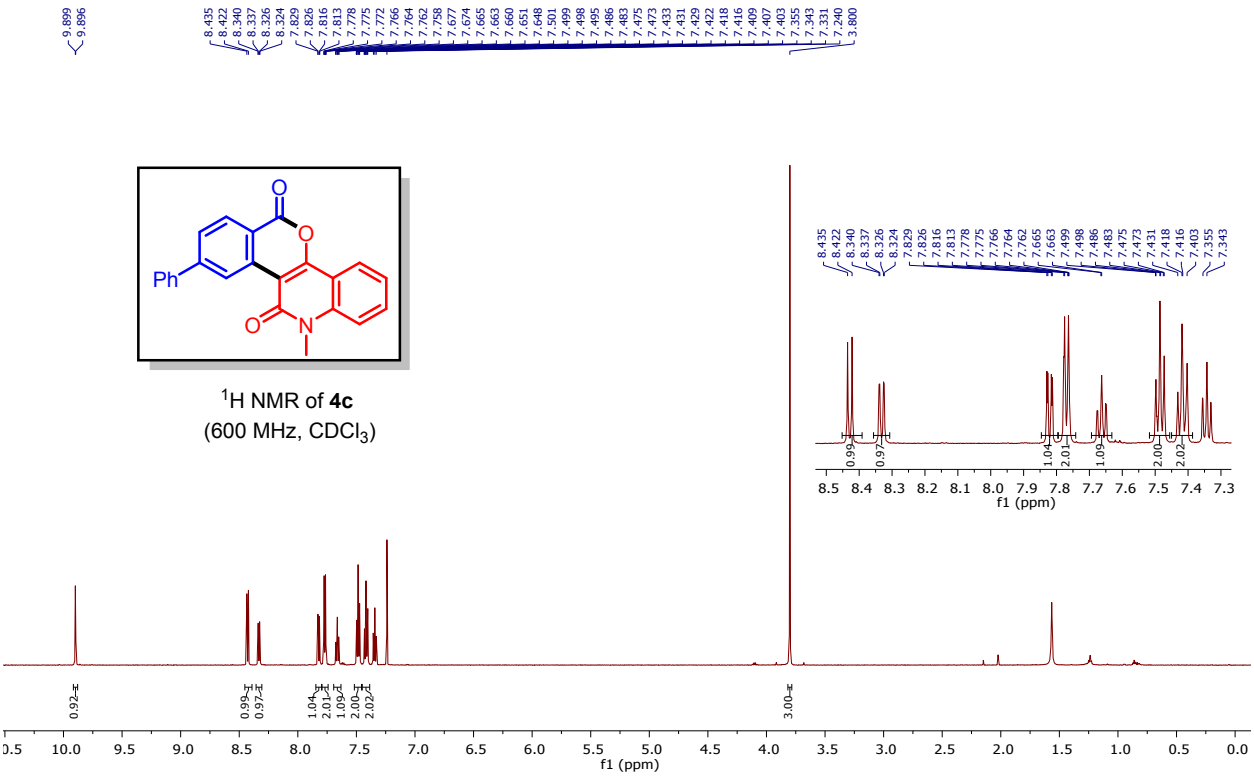
^{13}C NMR of **4a**
(150 MHz, $CDCl_3$)



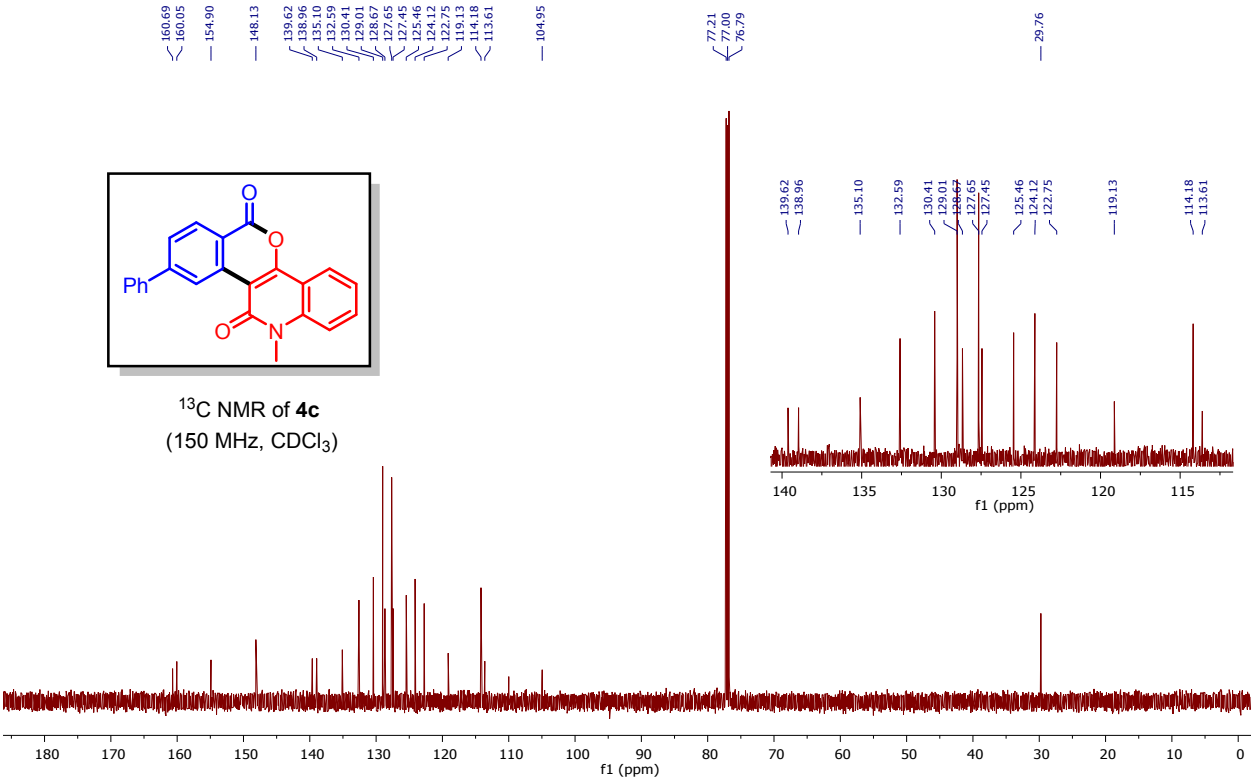
^{1}H NMR of **4b**
(600 MHz, $CDCl_3$)



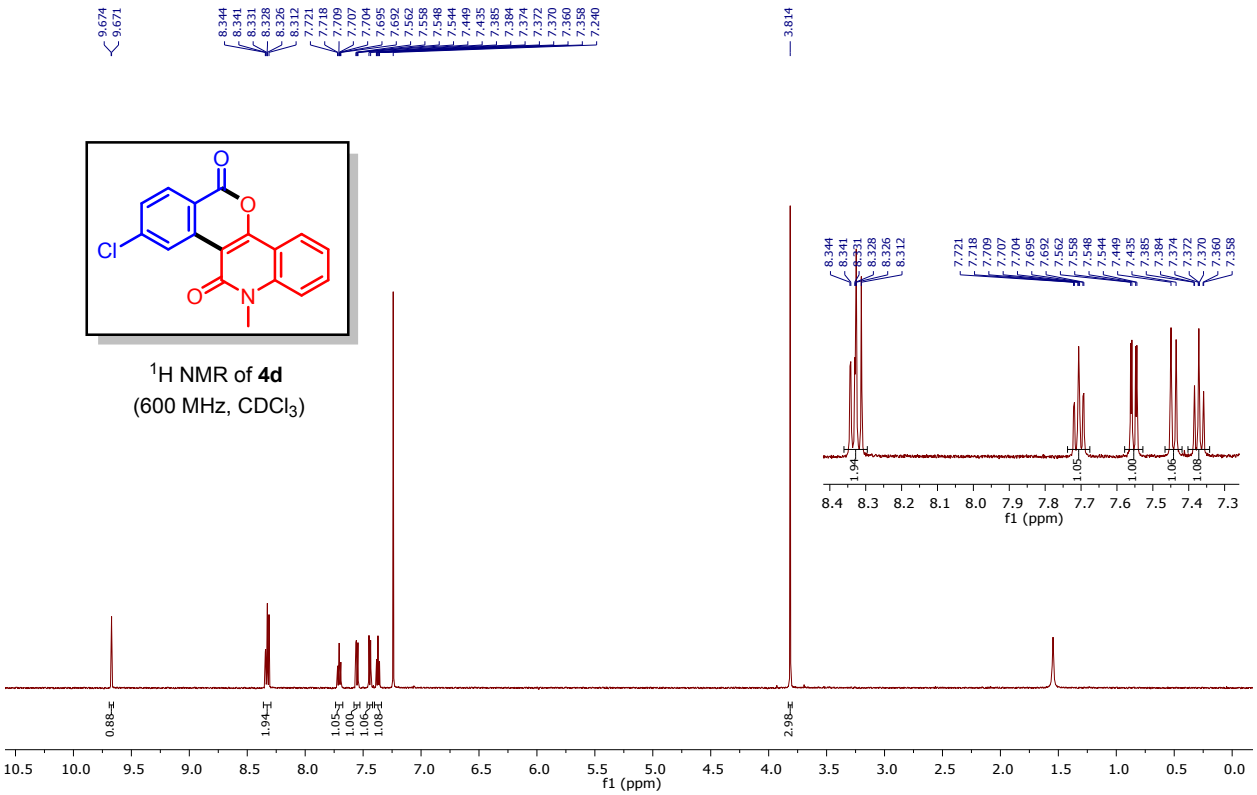
^{13}C NMR of **4b**
(150 MHz, $CDCl_3$)



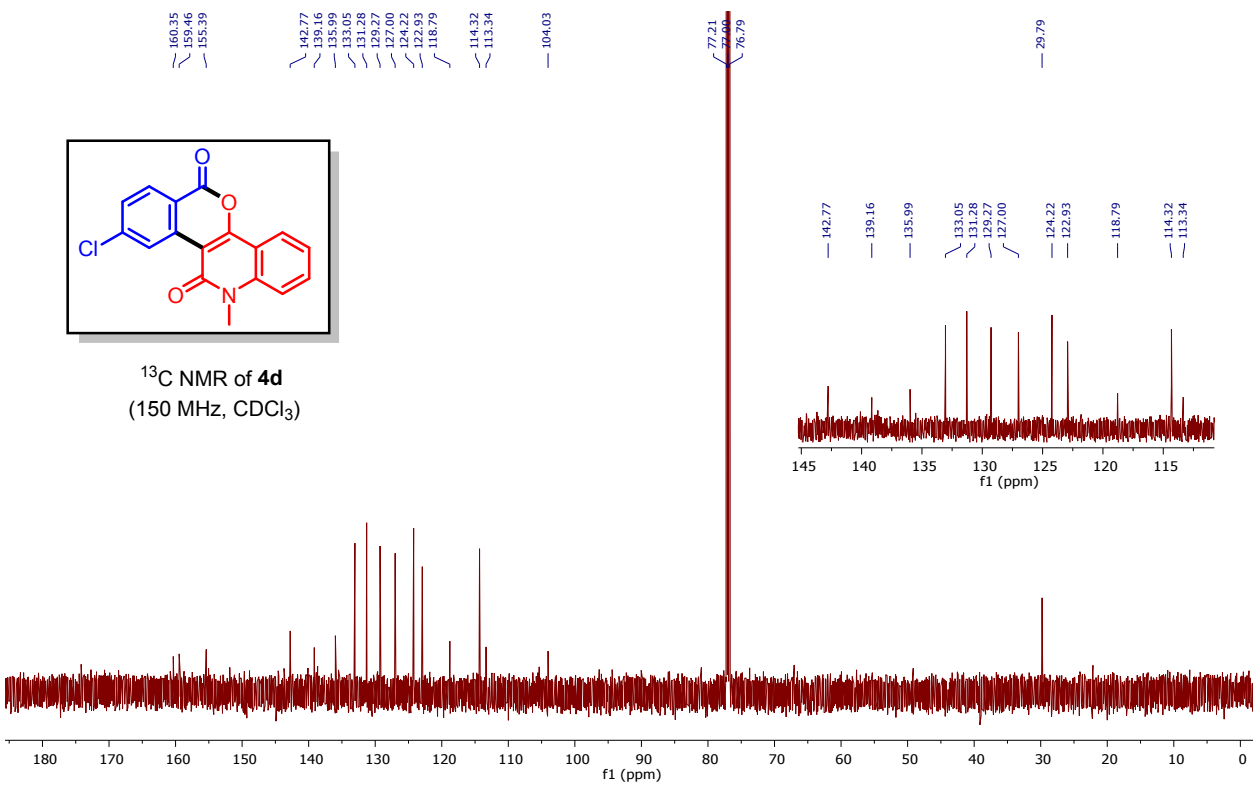
^{1}H NMR of **4c**
(600 MHz, $CDCl_3$)



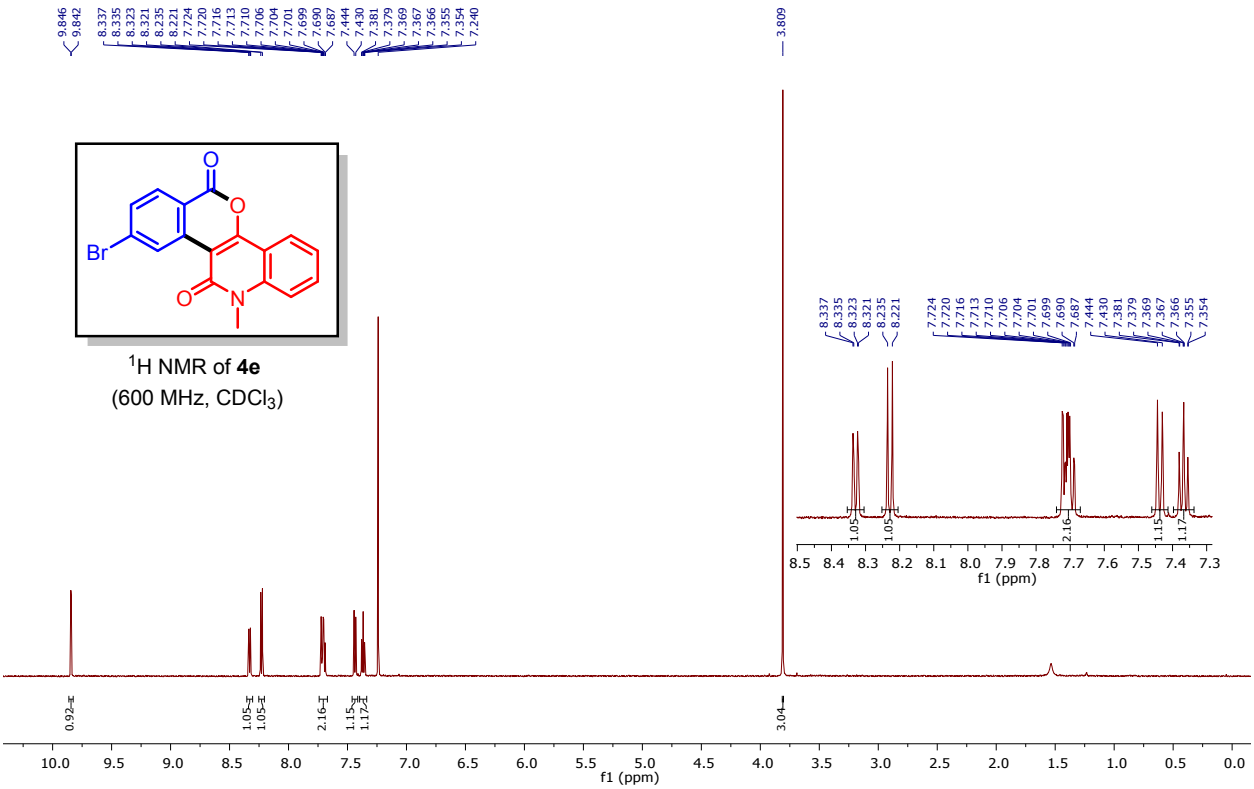
^{13}C NMR of **4c**
(150 MHz, $CDCl_3$)



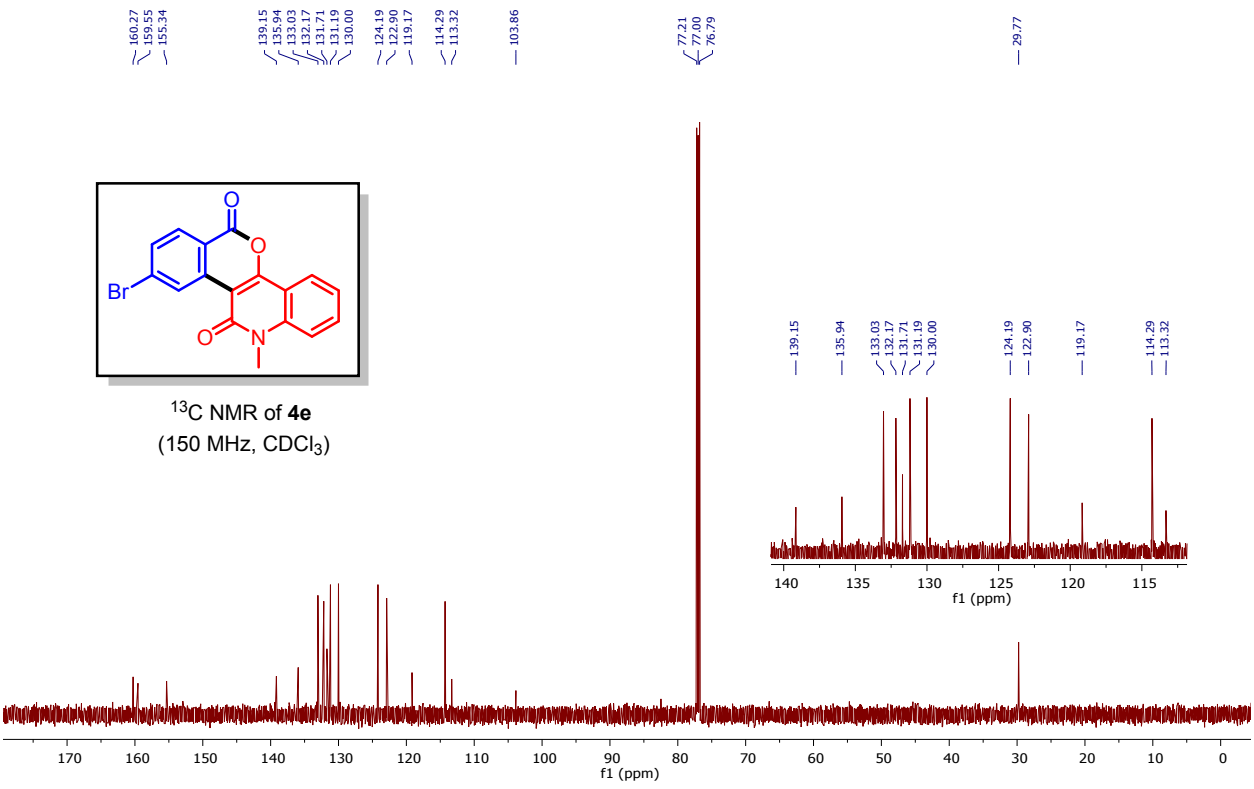
^{1}H NMR of **4d**
(600 MHz, $CDCl_3$)



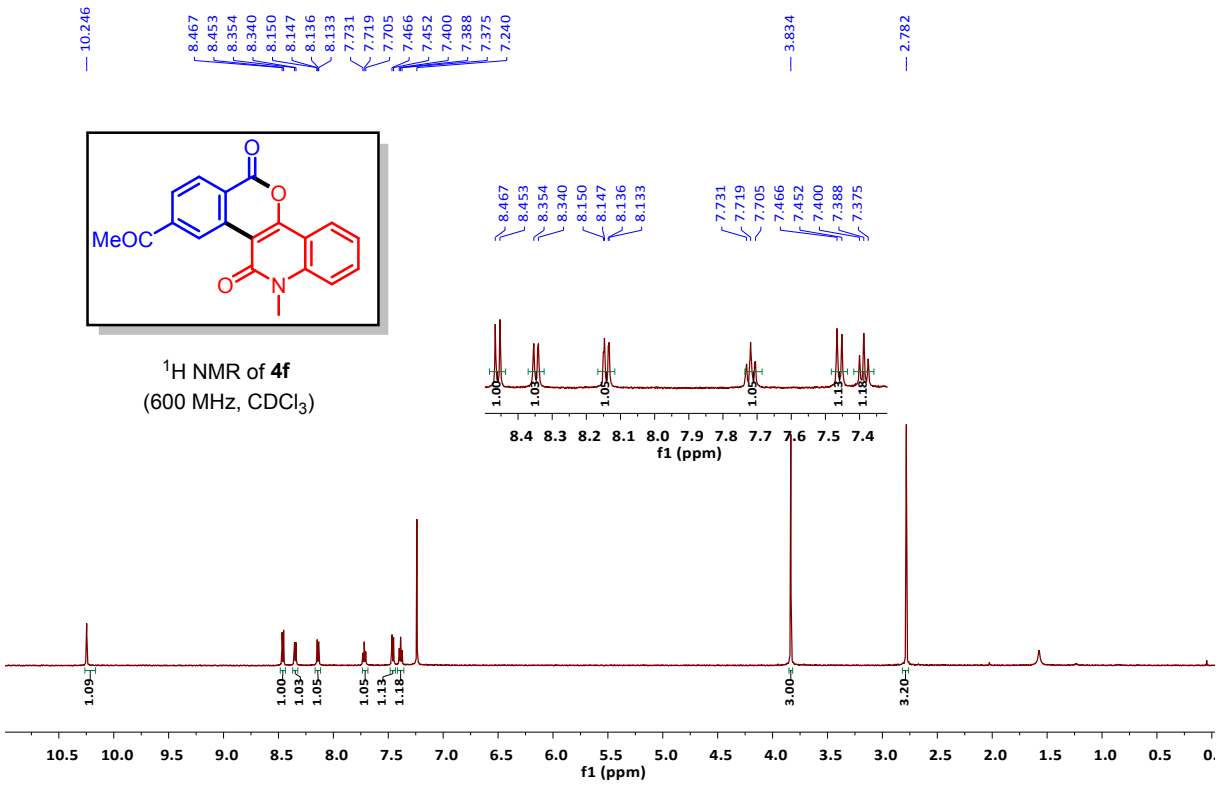
^{13}C NMR of **4d**
(150 MHz, $CDCl_3$)



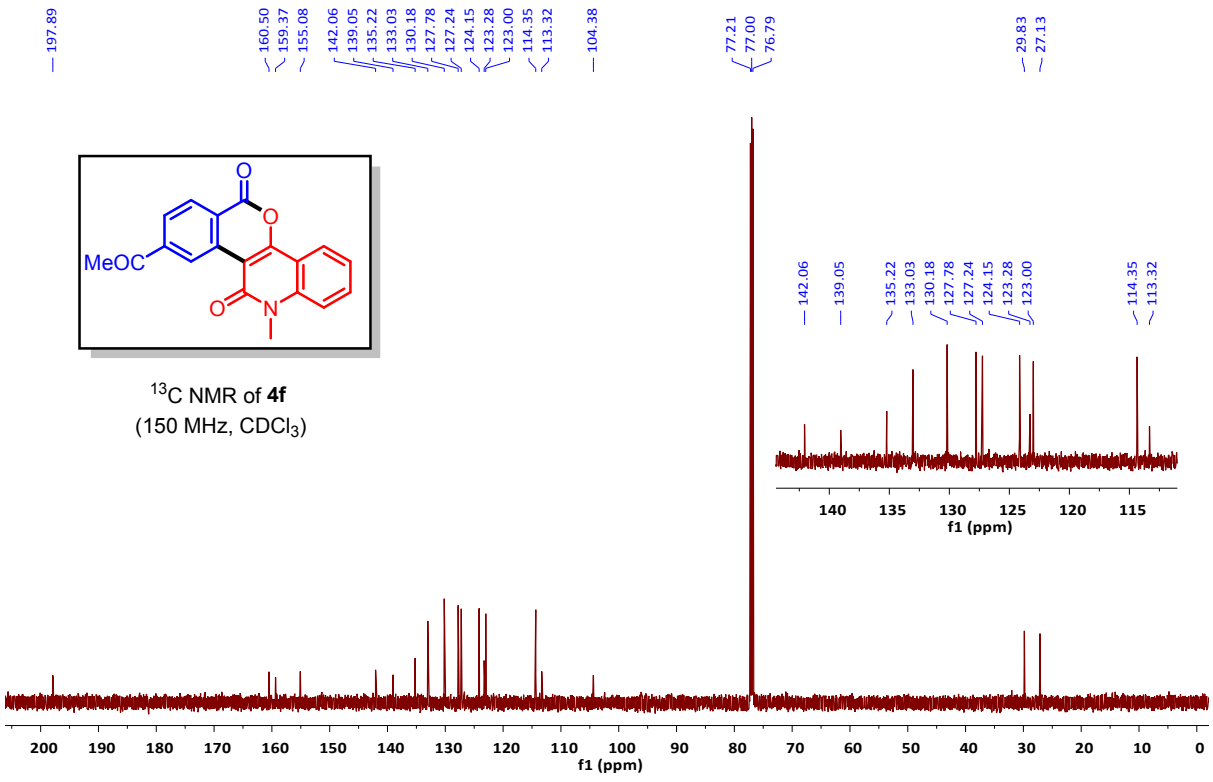
^{1}H NMR of **4e**
(600 MHz, $CDCl_3$)



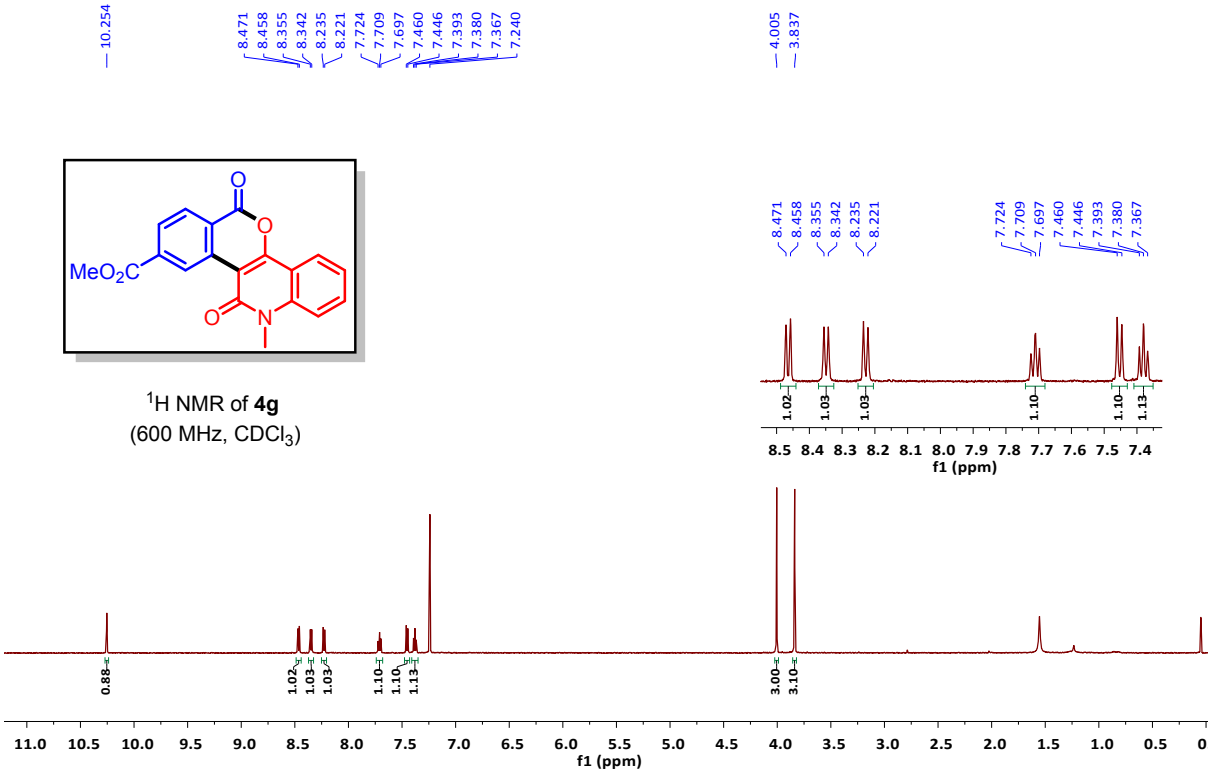
^{13}C NMR of **4e**
(150 MHz, $CDCl_3$)



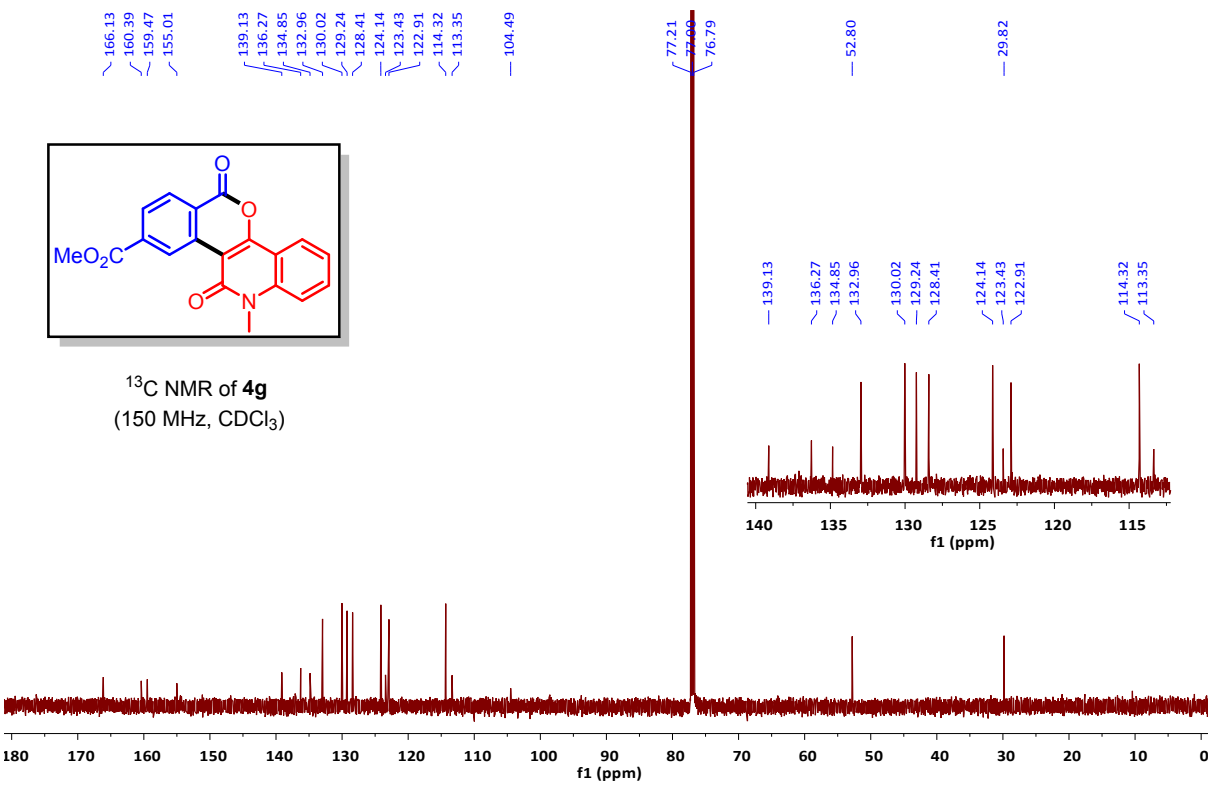
^{1}H NMR of **4f**
(600 MHz, $CDCl_3$)



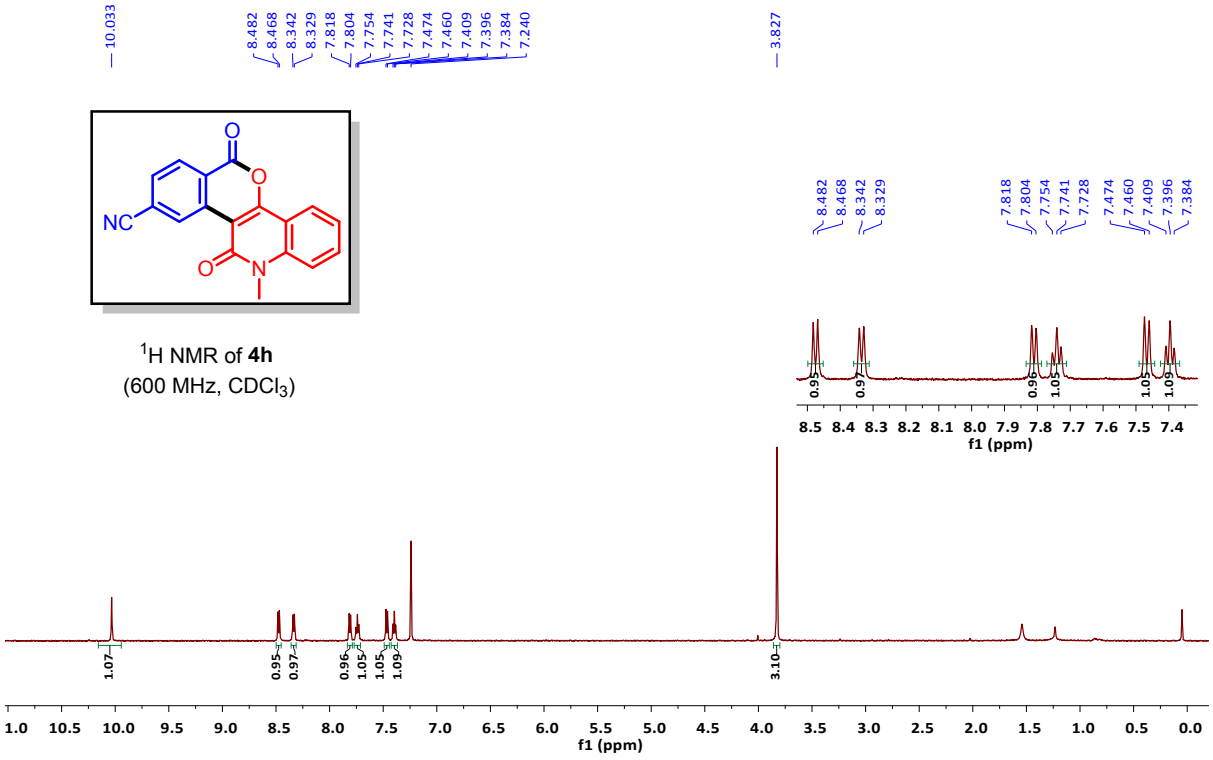
^{13}C NMR of **4f**
(150 MHz, $CDCl_3$)



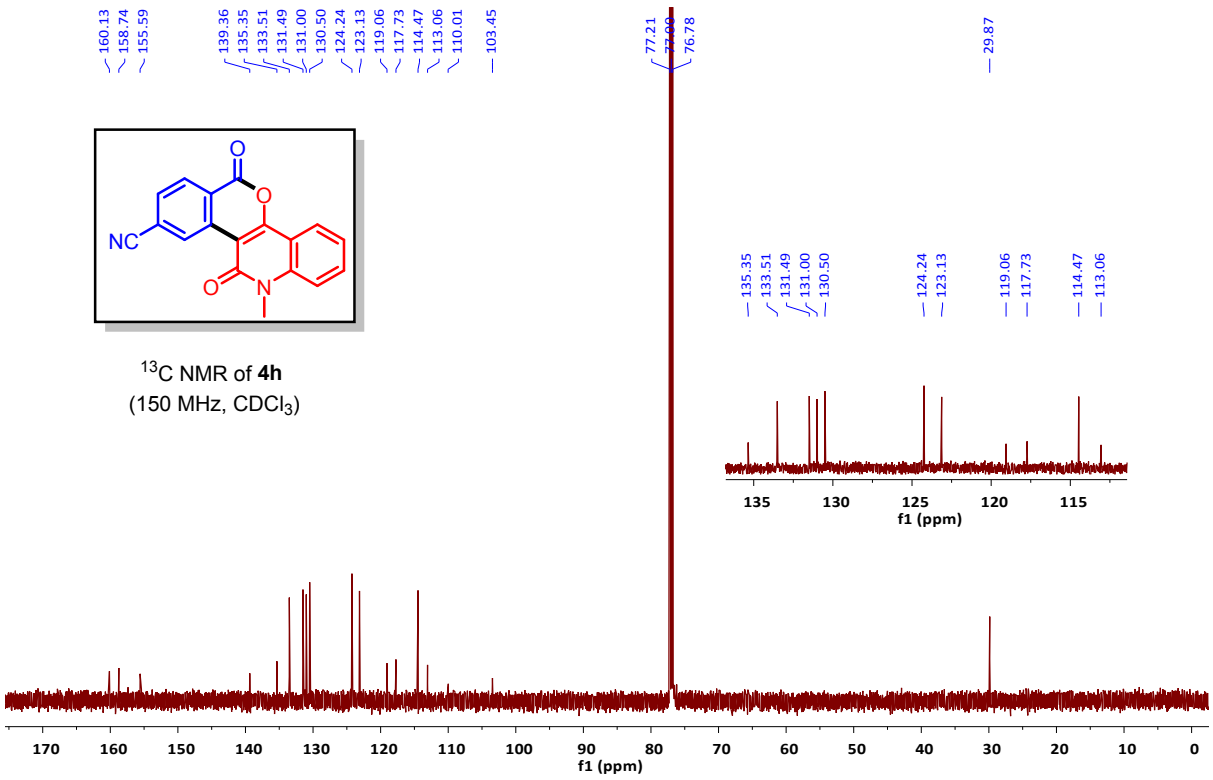
^{1}H NMR of **4g**
(600 MHz, $CDCl_3$)



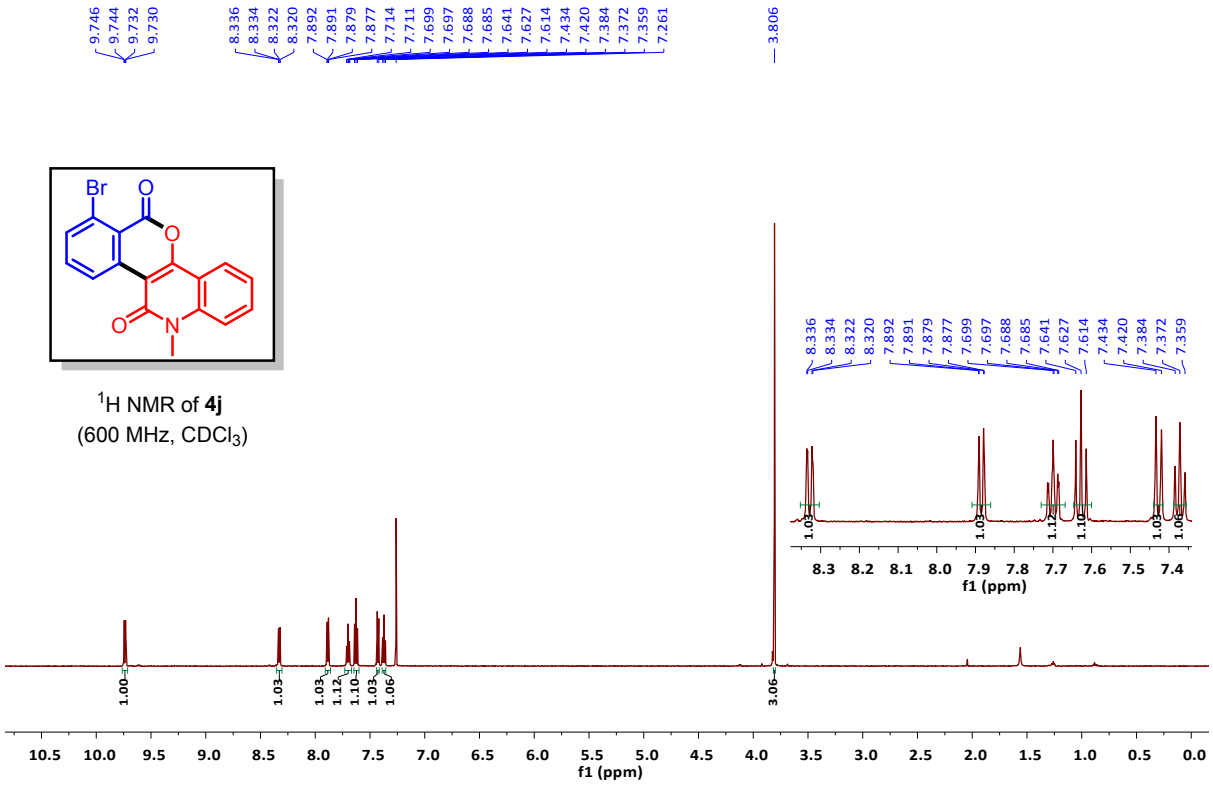
^{13}C NMR of **4g**
(150 MHz, $CDCl_3$)



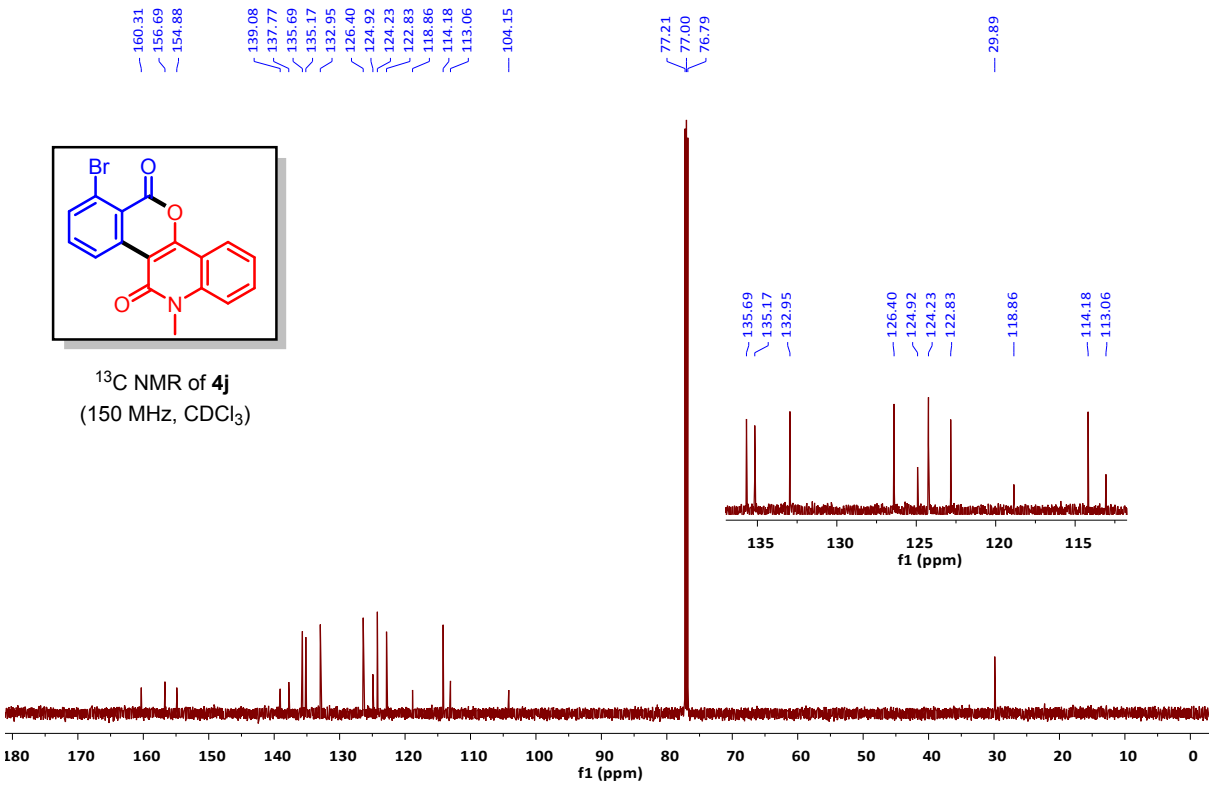
^{1}H NMR of **4h**
(600 MHz, $CDCl_3$)



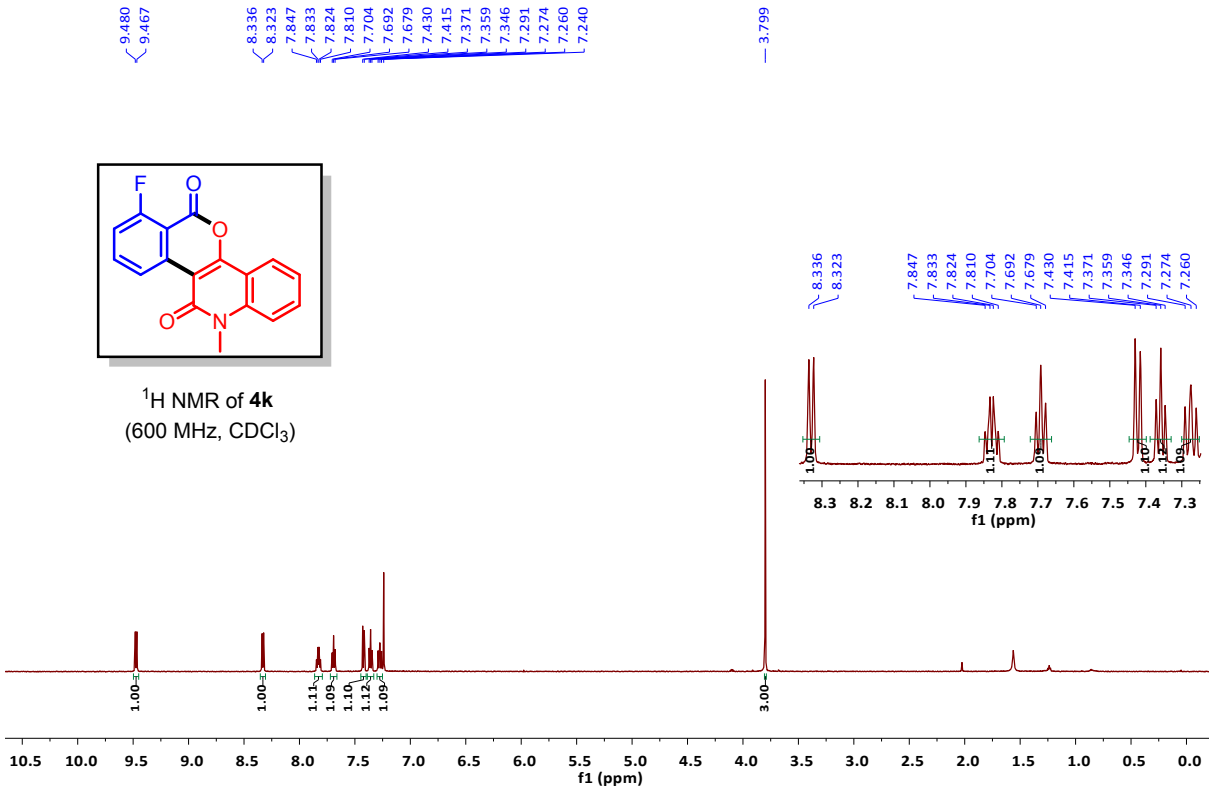
^{13}C NMR of **4h**
(150 MHz, $CDCl_3$)



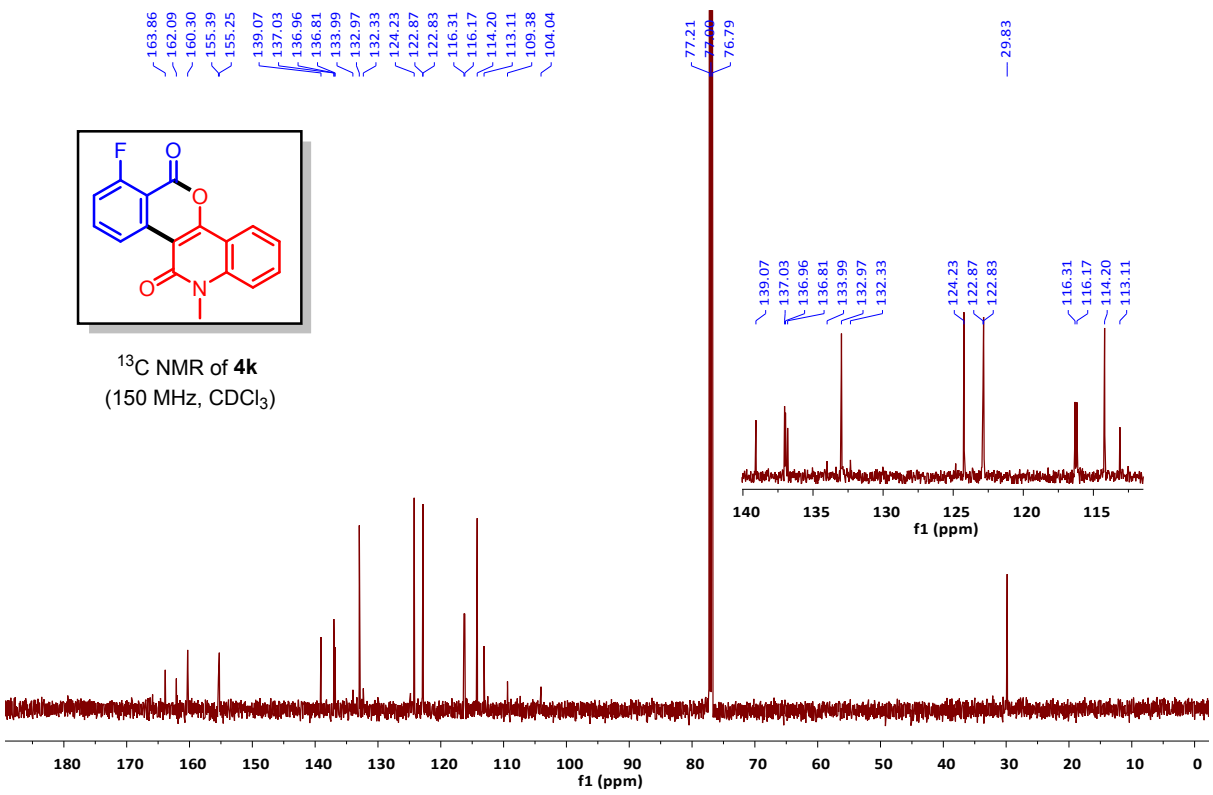
^{1}H NMR of **4j**
(600 MHz, $CDCl_3$)



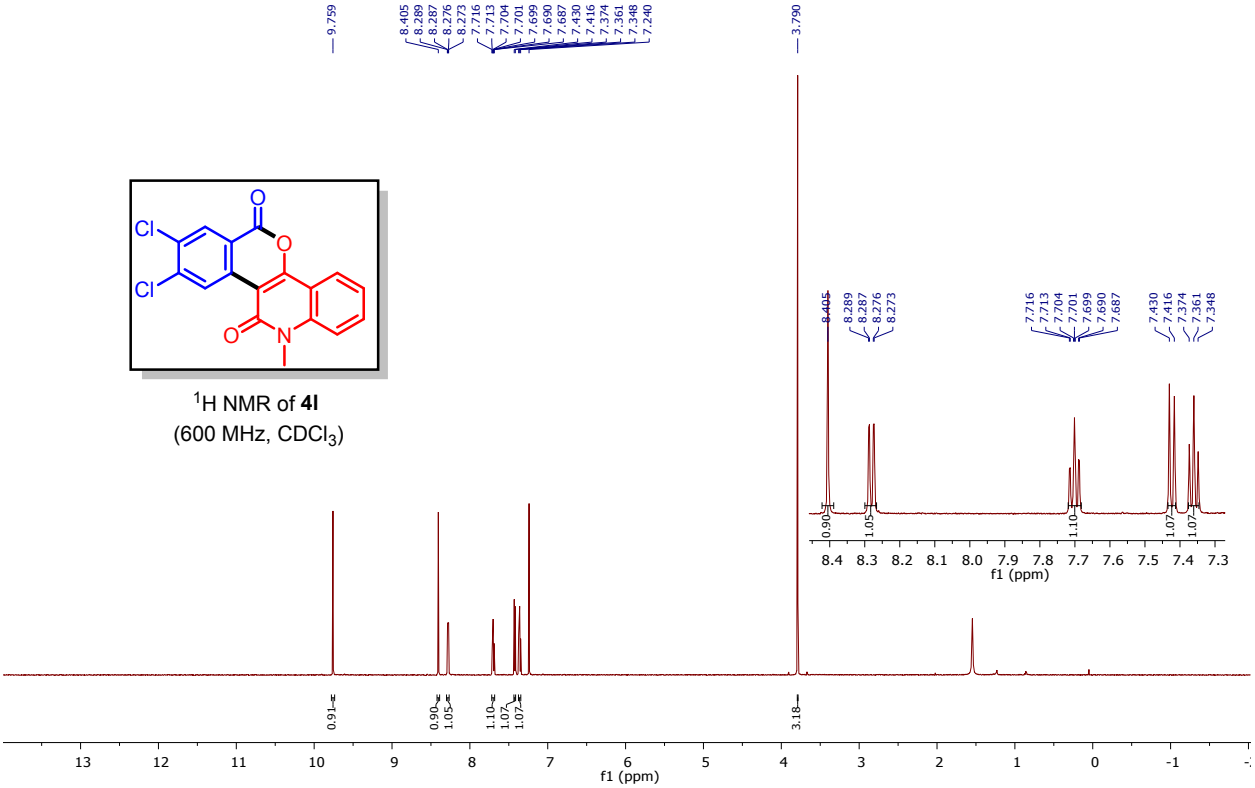
^{13}C NMR of **4j**
(150 MHz, $CDCl_3$)



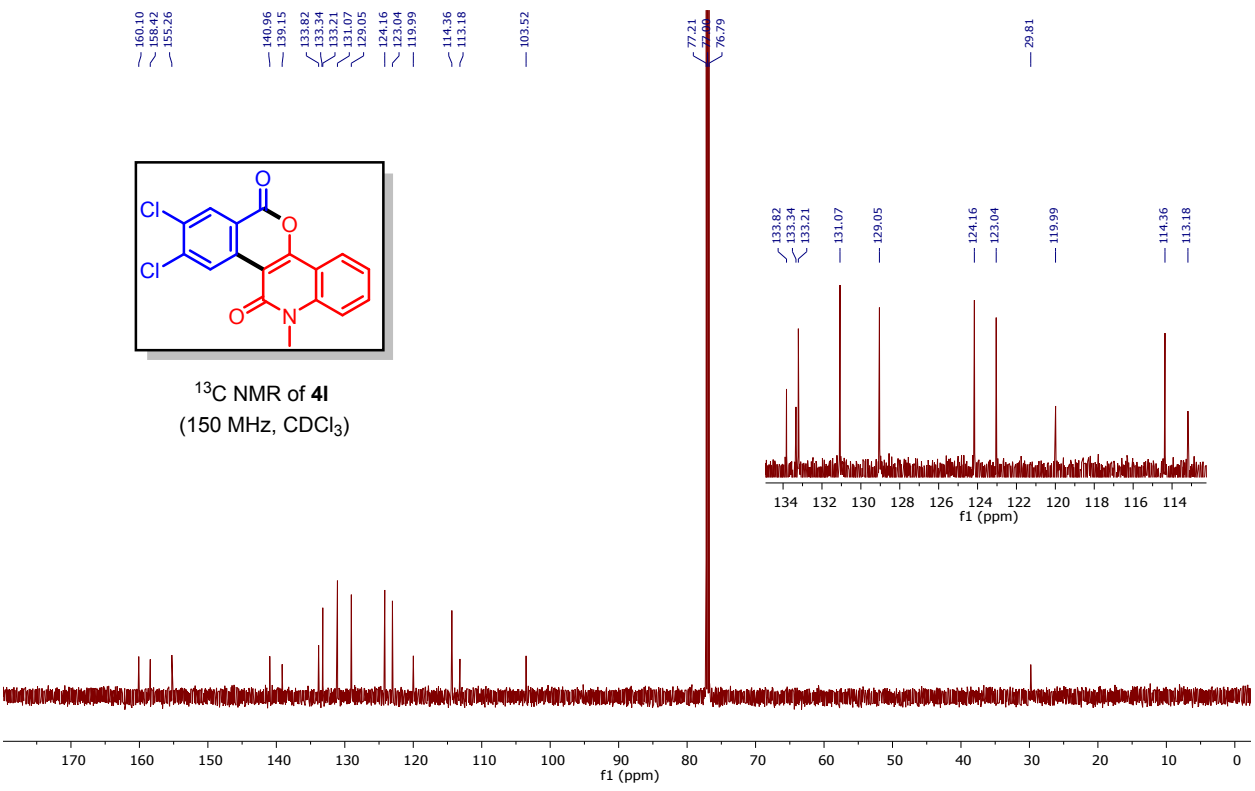
^{1}H NMR of **4k**
(600 MHz, $CDCl_3$)



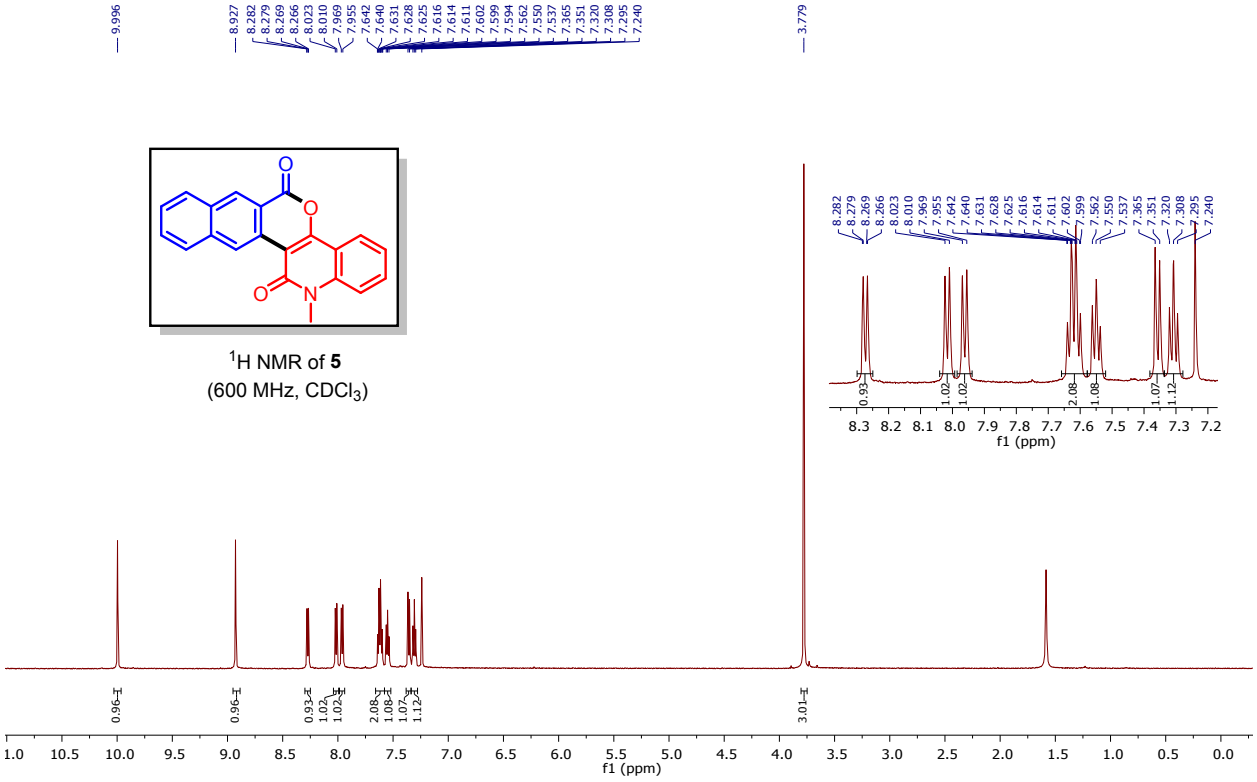
^{13}C NMR of **4k**
(150 MHz, $CDCl_3$)



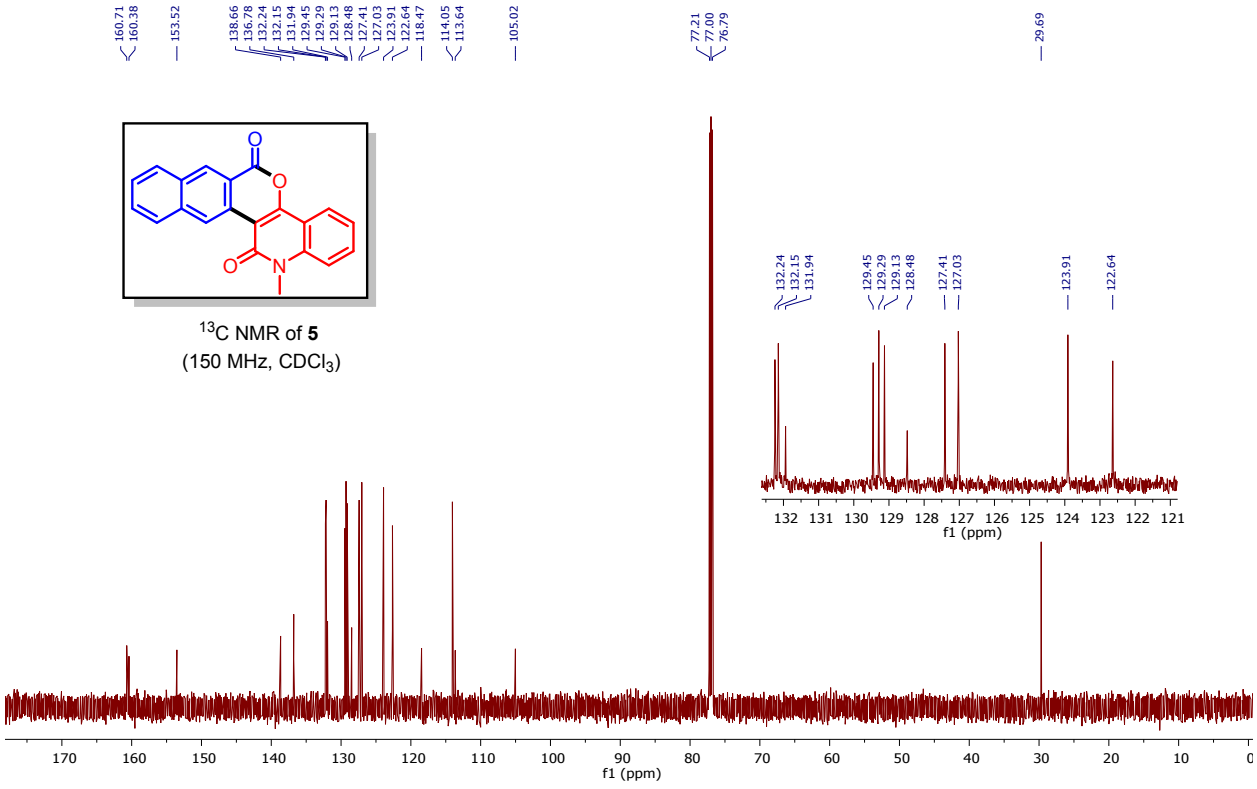
^{1}H NMR of **4l**
(600 MHz, $CDCl_3$)



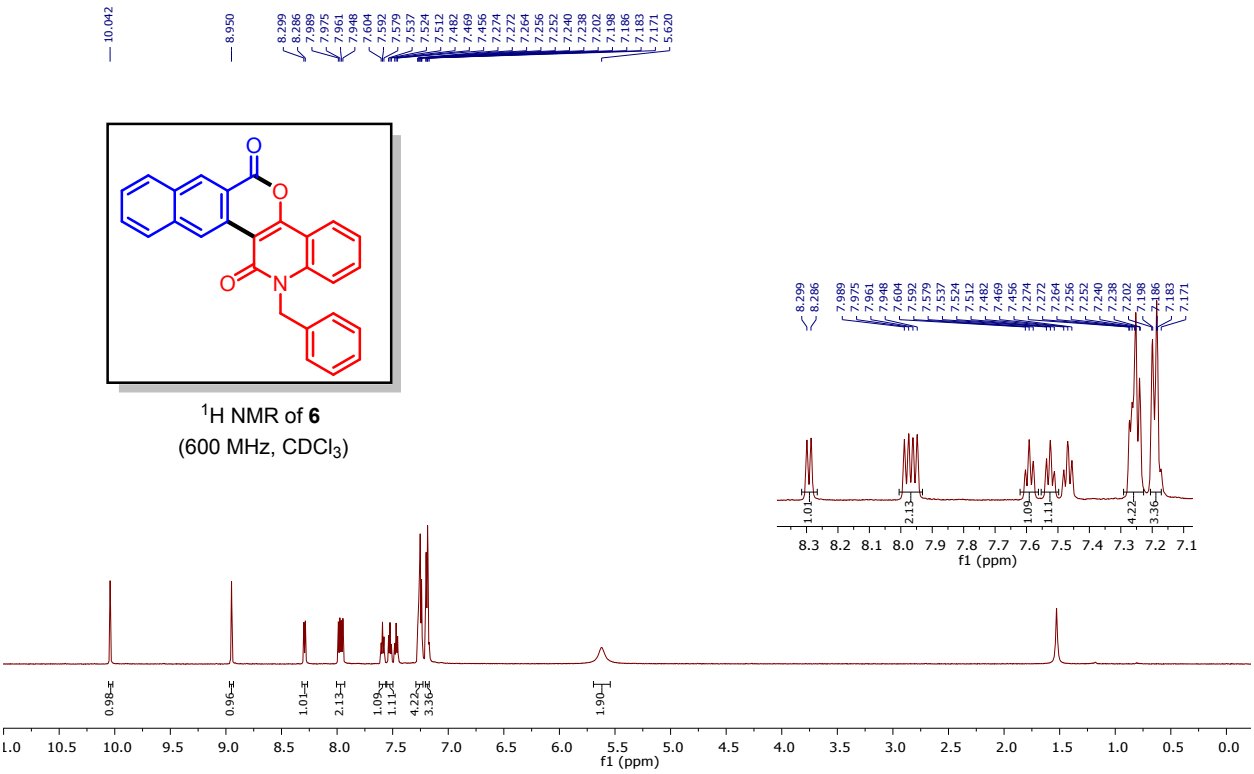
^{13}C NMR of **4l**
(150 MHz, $CDCl_3$)



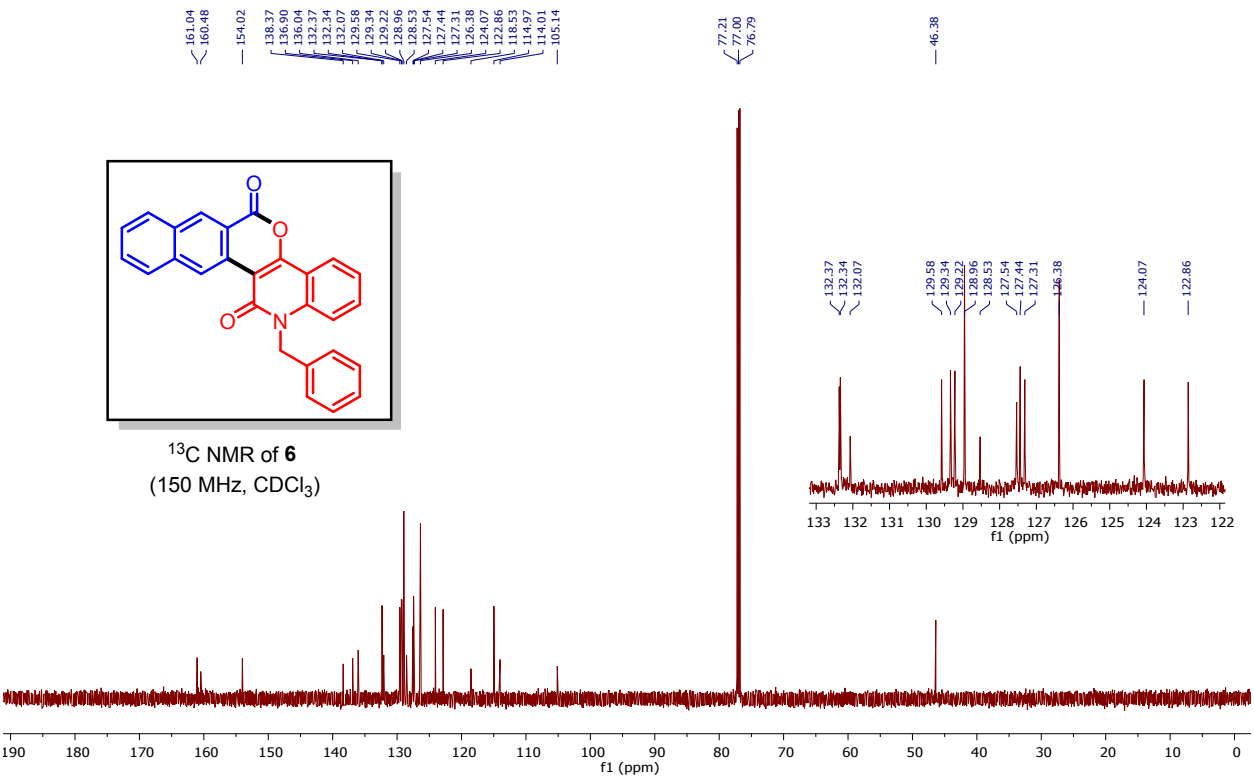
^{1}H NMR of **5**
(600 MHz, $CDCl_3$)



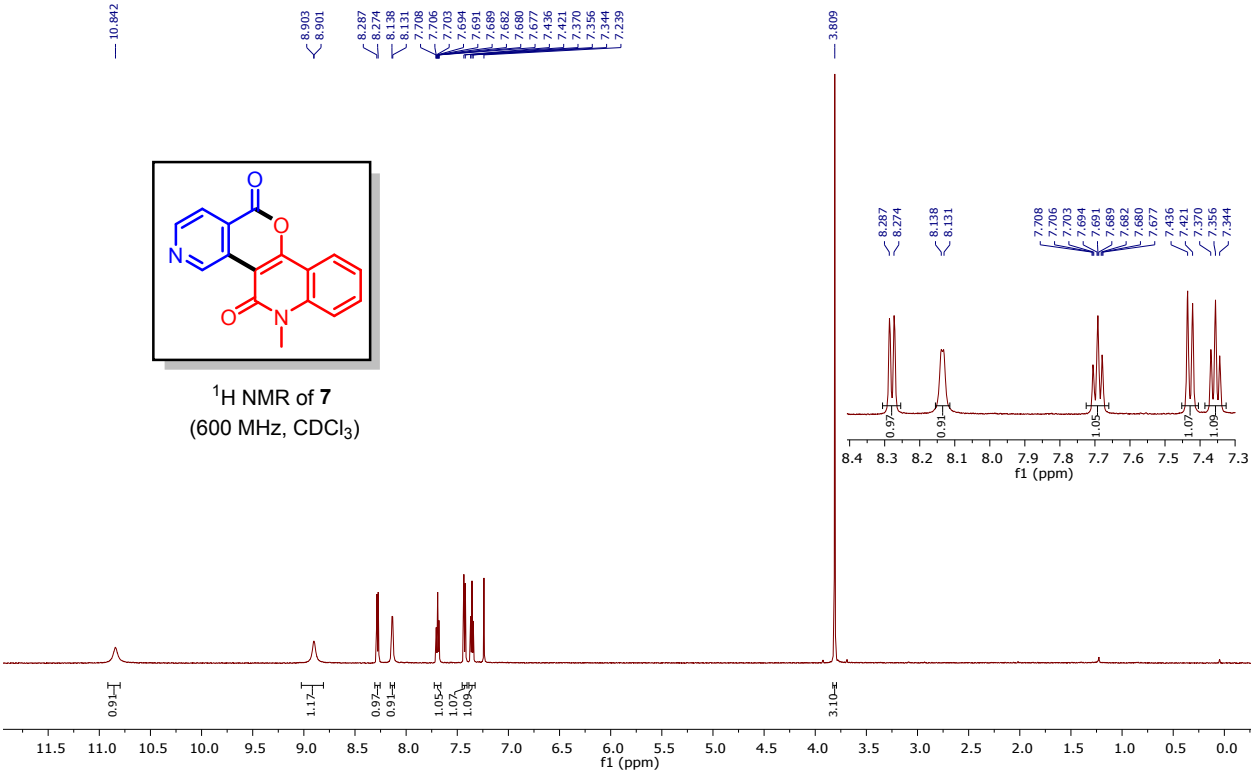
^{13}C NMR of **5**
(150 MHz, $CDCl_3$)



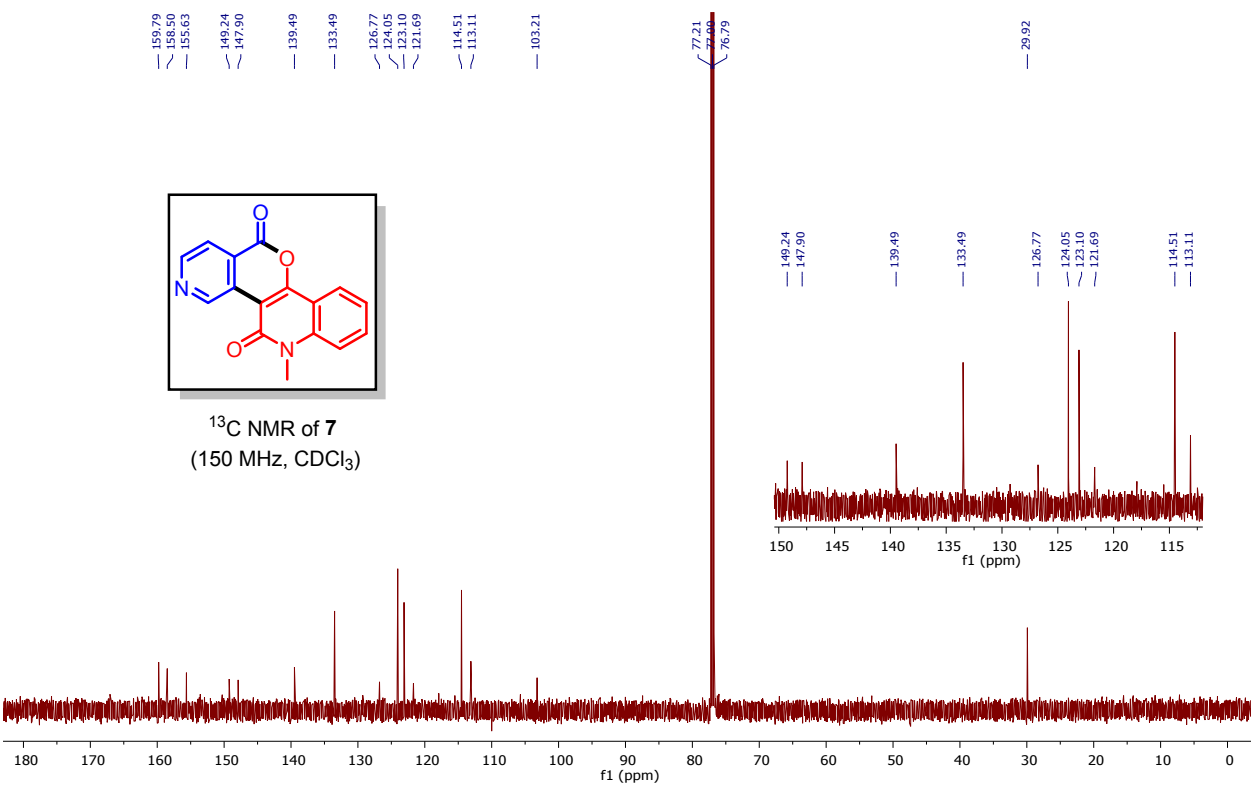
^{1}H NMR of **6**
(600 MHz, $CDCl_3$)



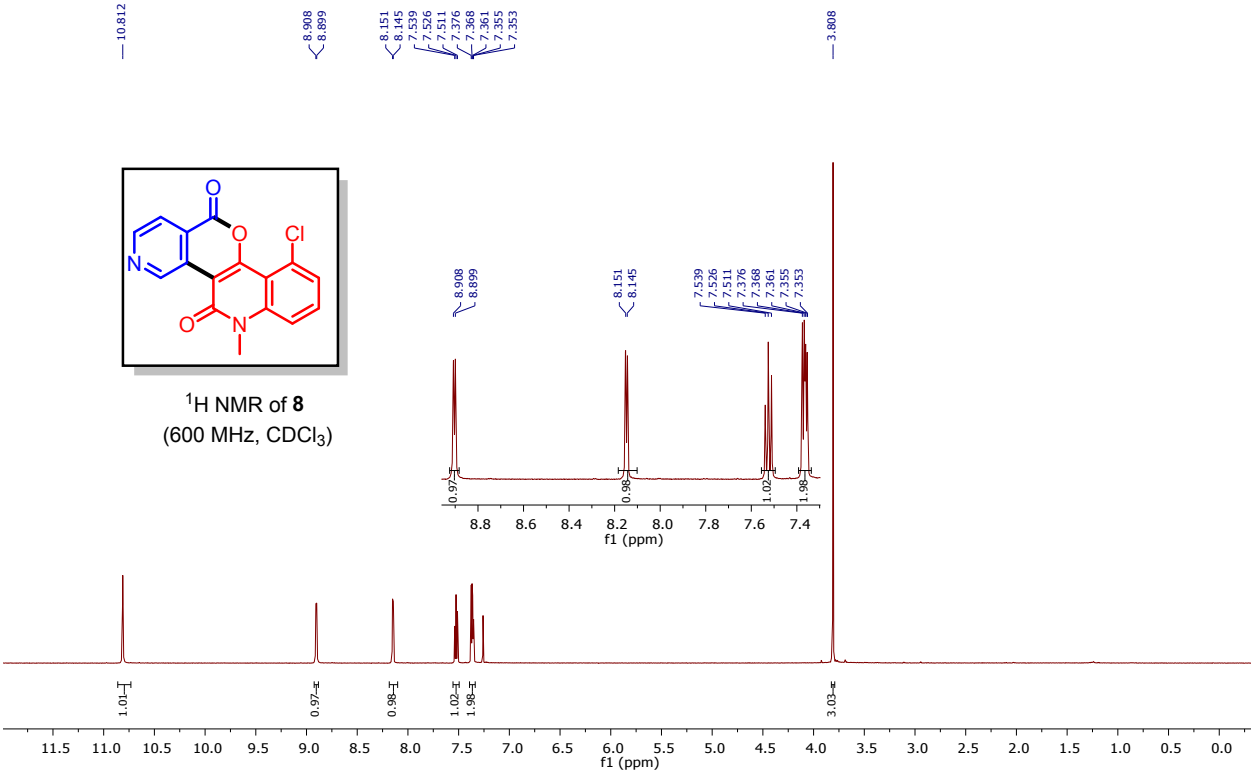
^{13}C NMR of **6**
(150 MHz, $CDCl_3$)



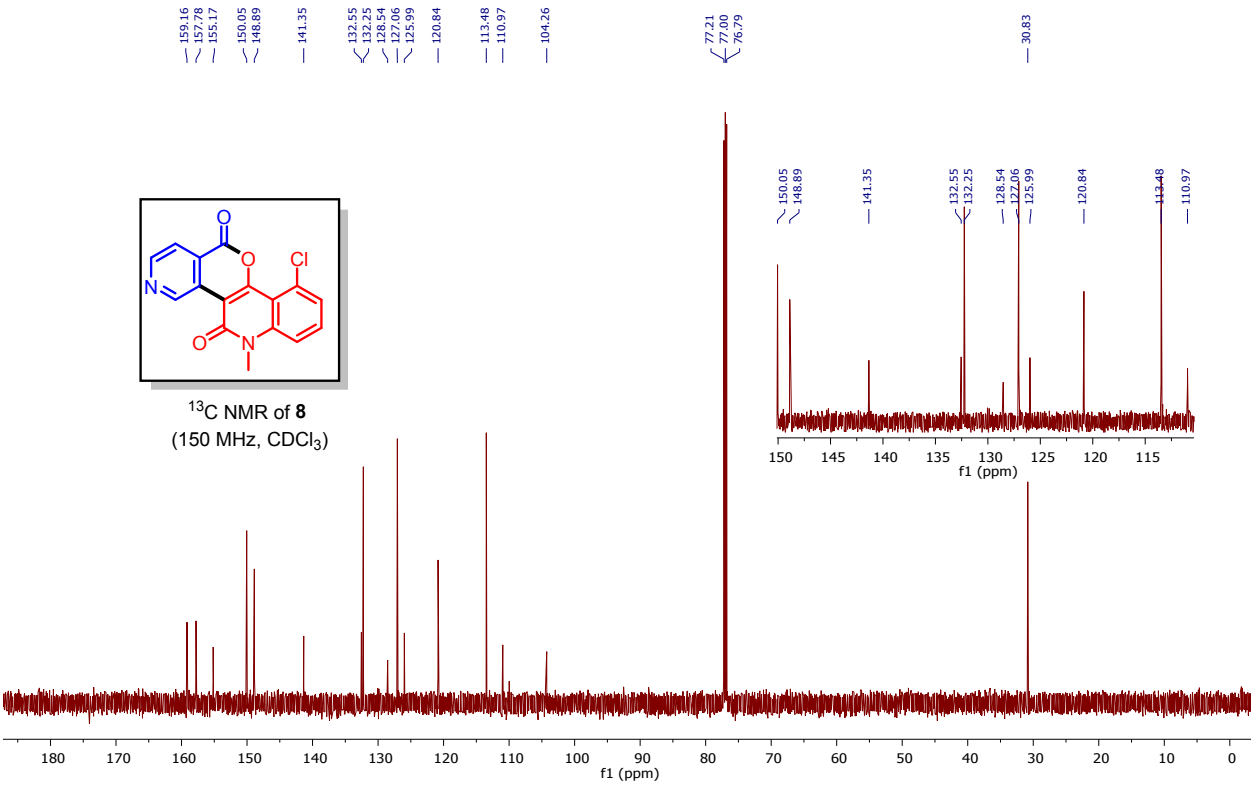
^{1}H NMR of **7**
(600 MHz, $CDCl_3$)



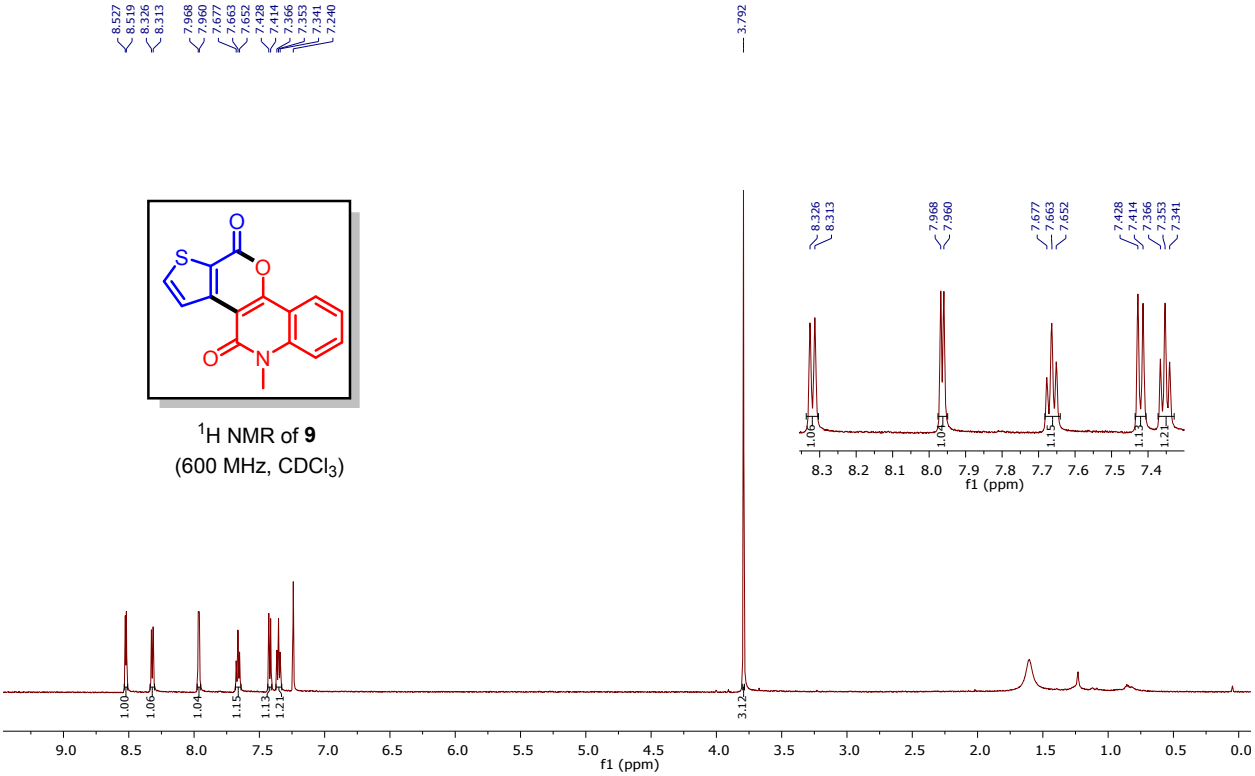
^{13}C NMR of **7**
(150 MHz, $CDCl_3$)



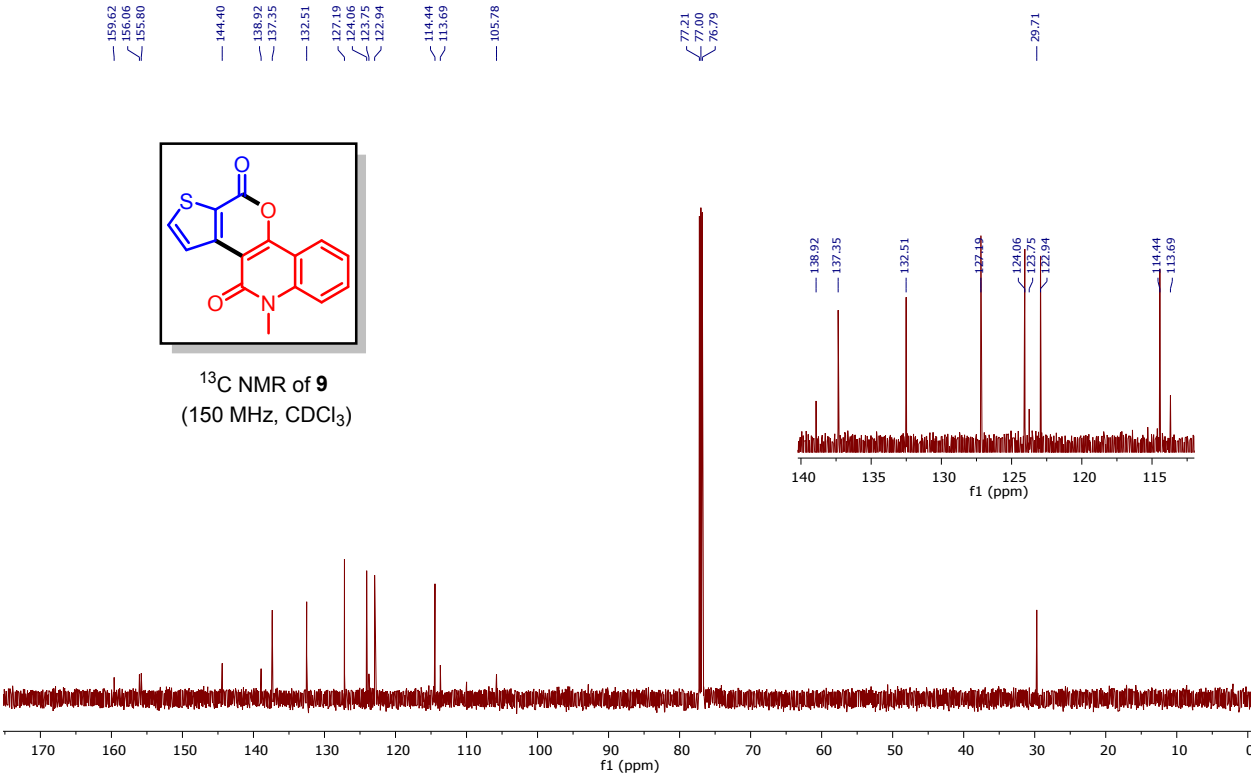
^{1}H NMR of **8**
(600 MHz, $CDCl_3$)



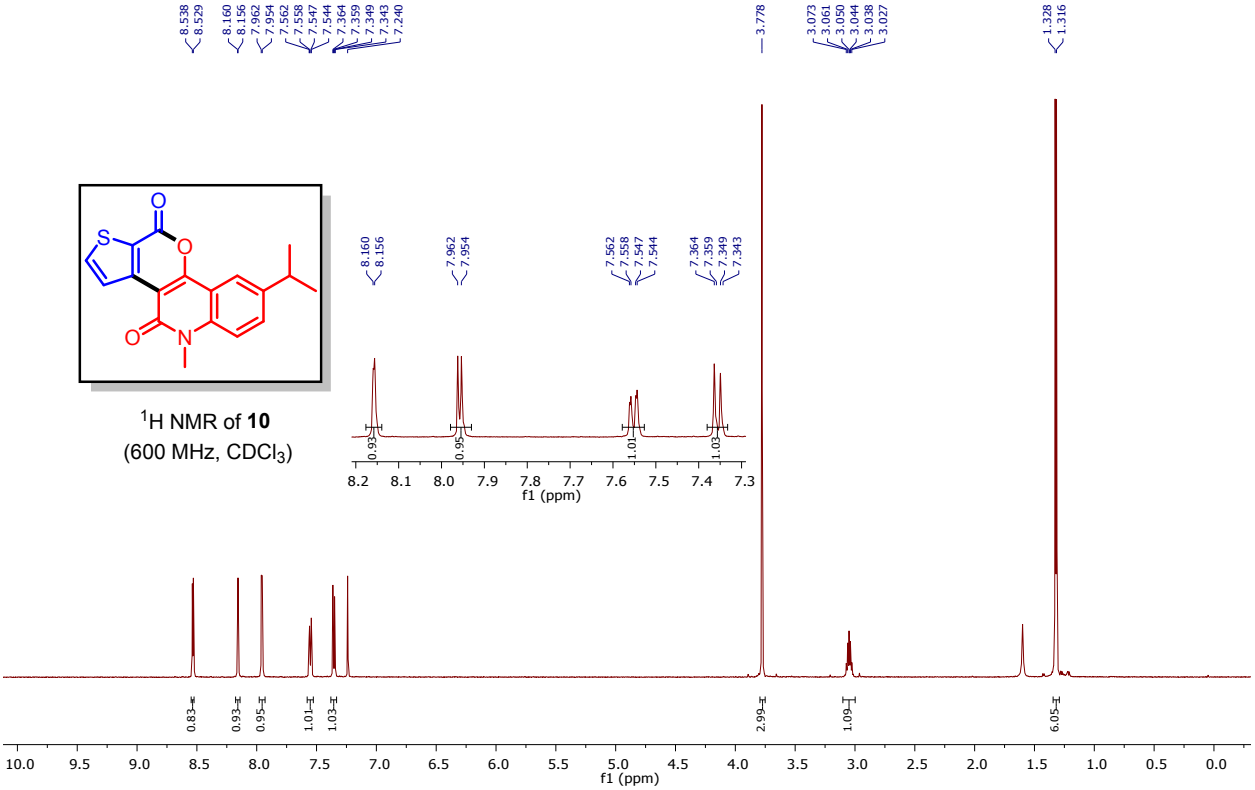
^{13}C NMR of **8**
(150 MHz, $CDCl_3$)



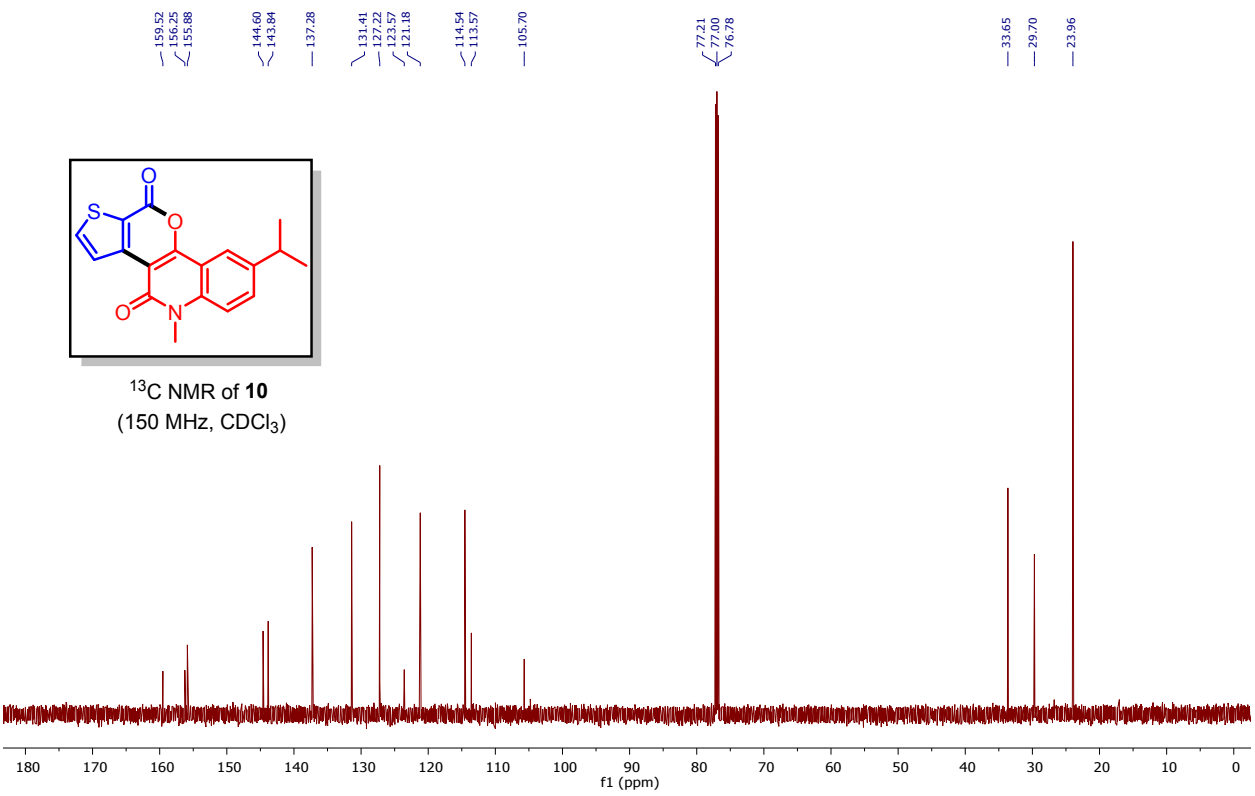
^{1}H NMR of **9**
(600 MHz, $CDCl_3$)



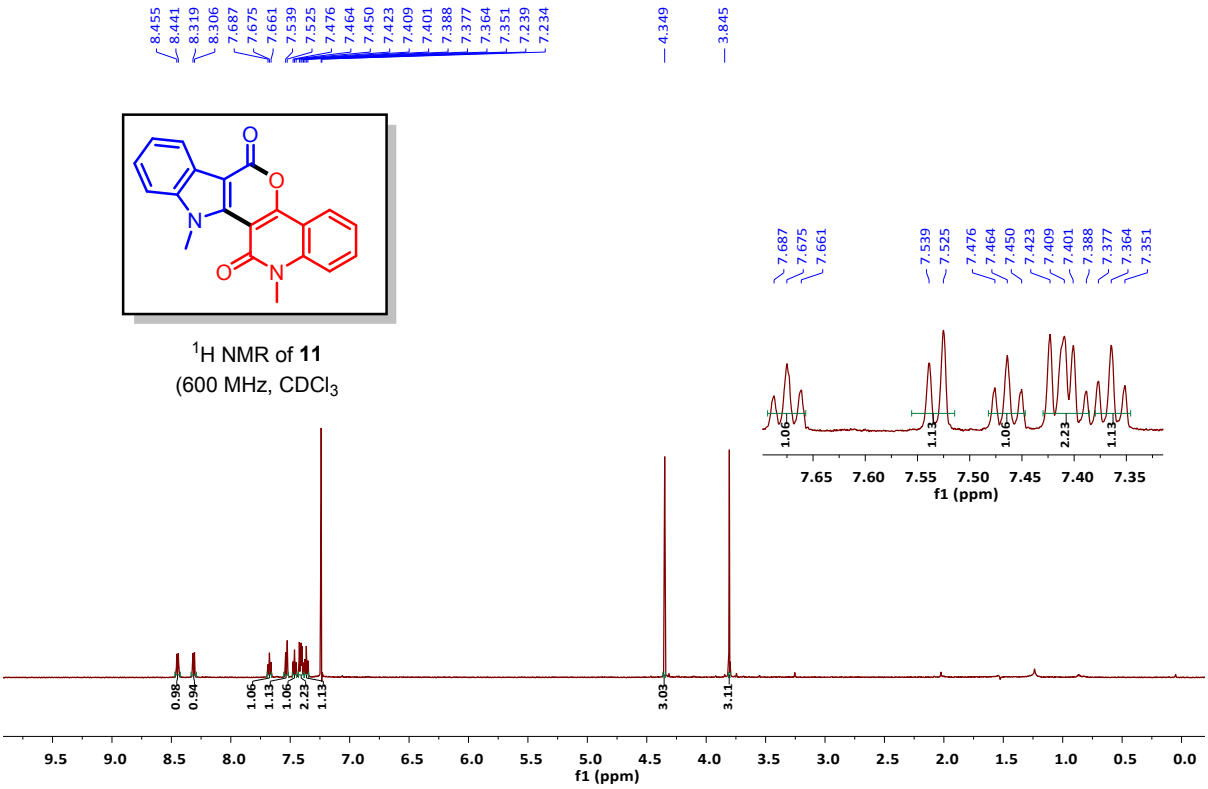
^{13}C NMR of **9**
(150 MHz, $CDCl_3$)



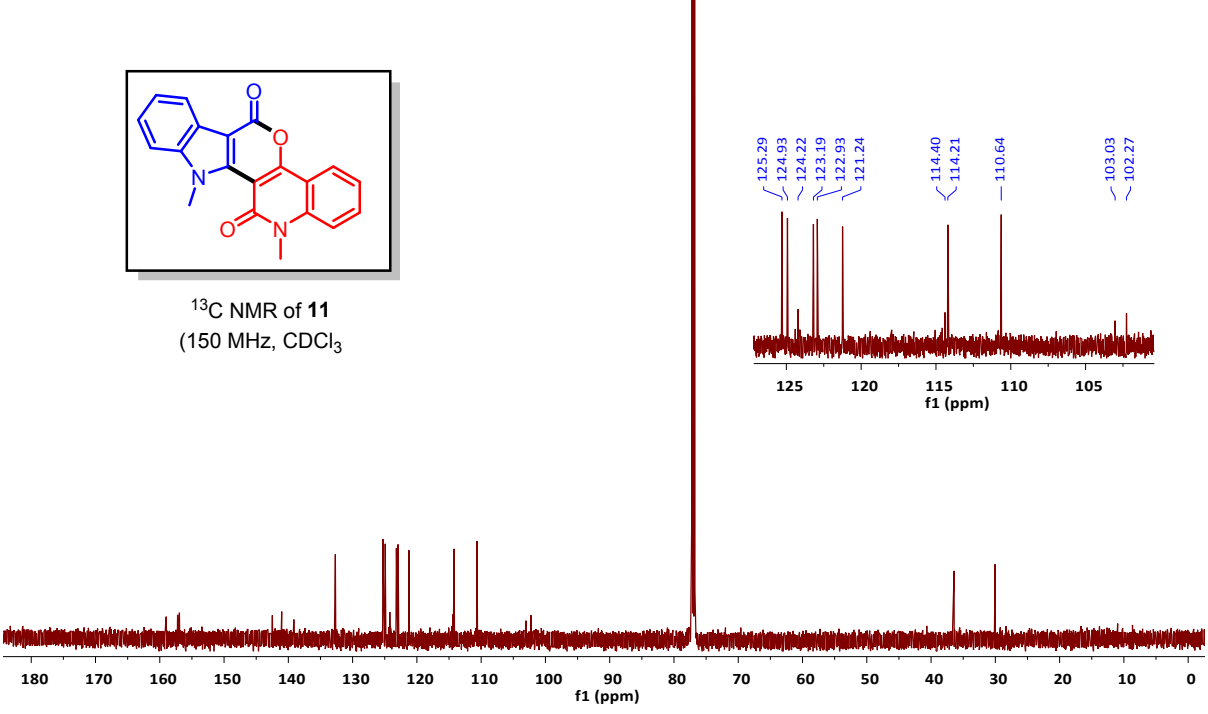
^{1}H NMR of **10**
(600 MHz, $CDCl_3$)



^{13}C NMR of **10**
(150 MHz, $CDCl_3$)



^{1}H NMR of **11**
(600 MHz, $CDCl_3$)



^{13}C NMR of **11**
(150 MHz, $CDCl_3$)

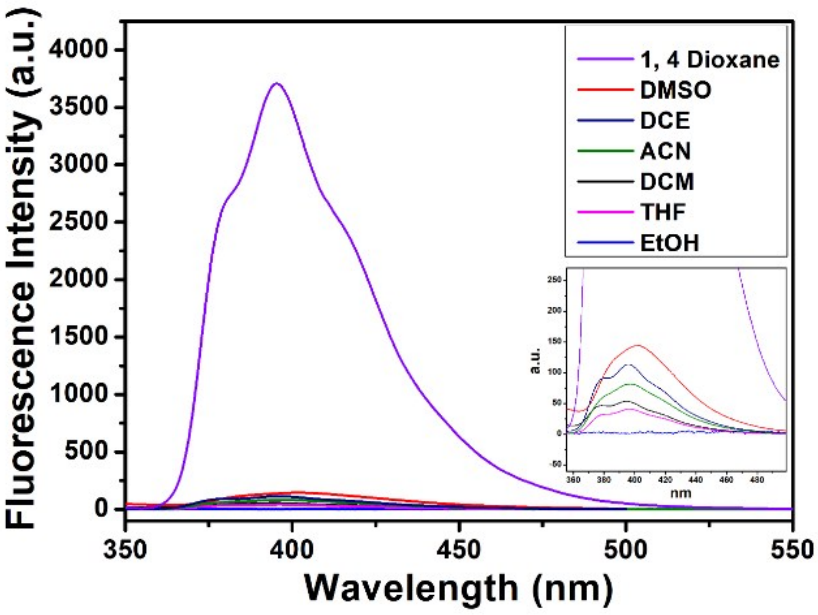


Figure. S1. Fluorescence spectra of **4a** in various solvents.

X-Ray crystallographic structure and data of compound (3j)

X-Ray crystallographic structure and data of compound **3j**: Empirical Formula- $C_{20}H_{17}NO_3$, M = 319.35, Monoclinic, Space group Pbca, a = 12.9877 (7) Å, b = 16.1253 (9) Å, c = 7.4653 (4) Å, V = 1525.43 (14) $Å^3$, Z = 4, T = 223(2) K, ρcalcd = 1.391 Mg/m^3 , 2Θmax. = 25.242° , Refinement of 220 parameters on 3798 independent reflections out of 49338 collected reflections (Rint = 0.0940) led to R1 = 0.0546 [I >2σ(I)], wR_2 = 0.1166 (all data) and S = 1.020 with the largest difference peak and hole of 0.429 and - 0.278 e.$Å^{-3}$ respectively.The crystal structure has been deposited at the Cambridge Crystallographic Data Centre (CCDC 1878962). The data can be obtained free of charge via the Internet at www.ccdc.cam.ac.uk/data_request/cif.

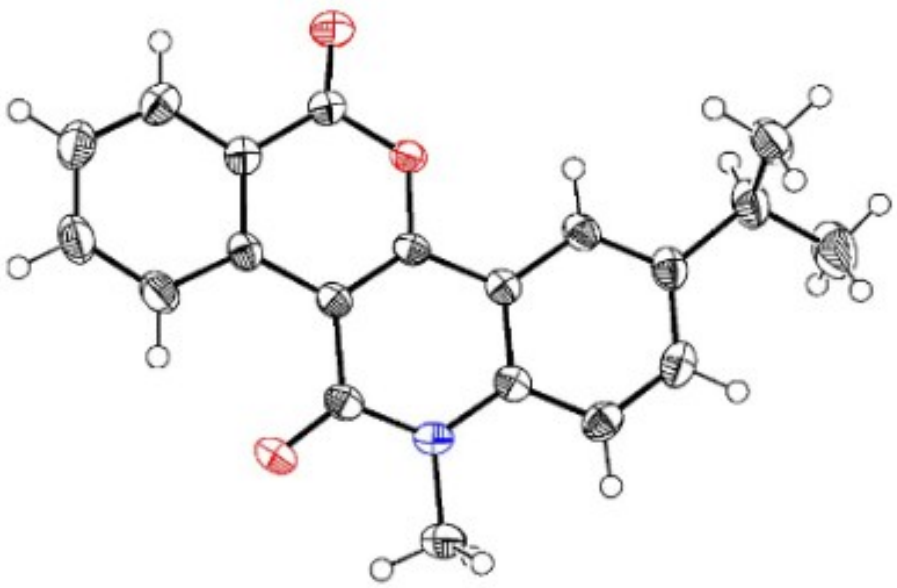


Table 1. Crystal data and structure refinement for No1.

Identification code	No1	
Empirical formula	$C_{20}\ H_{17}\ N\ O_3$	
Formula weight	319.35	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 12.9877(7) Å	α= 90°.
	b = 16.1253(9) Å	β= 102.6634(19)°.
	c = 7.4653(4) Å	γ = 90°.
Volume	1525.43(14) Å^3	
Z	4	
Density (calculated)	1.391 Mg/m^3	
Absorption coefficient	0.094 mm^{-1}	
F(000)	672	
Crystal size	0.200 x 0.160 x 0.100 mm^3	
Theta range for data collection	2.526 to 28.364°.	
Index ranges	-17<=h<=17, -21<=k<=21, -9<=l<=9	
Reflections collected	49338	
Independent reflections	3798 [R(int) = 0.0940]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.7178	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3798 / 0 / 220	
Goodness-of-fit on F^2	1.020	
Final R indices [I>2sigma(I)]	R1 = 0.0546, wR2 = 0.1166	
R indices (all data)	R1 = 0.0987, wR2 = 0.1386	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.429 and -0.278 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for No1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	-696(1)	6661(1)	217(2)	26(1)
C(1)	-1554(1)	7091(1)	-737(2)	27(1)
C(2)	-2591(1)	6757(1)	-712(2)	27(1)
C(3)	-3466(2)	7224(1)	-1565(3)	36(1)
C(4)	-4463(2)	6961(1)	-1508(3)	42(1)
C(5)	-4588(2)	6243(1)	-572(3)	43(1)
C(6)	-3732(2)	5766(1)	255(3)	37(1)
C(7)	-2704(1)	6006(1)	182(2)	26(1)
C(8)	-1747(1)	5554(1)	1002(2)	24(1)
C(9)	-1756(2)	4708(1)	1726(2)	27(1)
N(1)	-788(1)	4364(1)	2539(2)	26(1)
C(10)	167(1)	4785(1)	2758(2)	25(1)
C(11)	1115(2)	4451(1)	3737(3)	32(1)
C(12)	2041(2)	4890(1)	3909(3)	35(1)
C(13)	2084(2)	5673(1)	3110(3)	33(1)
C(14)	1148(1)	5995(1)	2138(3)	29(1)
C(15)	188(1)	5571(1)	1961(2)	24(1)
C(16)	-798(1)	5917(1)	1040(2)	23(1)
O(2)	-1366(1)	7713(1)	-1499(2)	39(1)
O(3)	-2571(1)	4303(1)	1600(2)	39(1)
C(17)	-784(2)	3506(1)	3191(3)	36(1)
C(18)	3086(2)	6192(2)	3301(3)	44(1)
C(19)	4085(2)	5709(2)	3842(4)	65(1)
C(20)	3055(2)	6921(1)	4559(3)	45(1)

Table 3. Bond lengths [Å] and angles [°] for No1.

O(1)-C(16)	1.367(2)
O(1)-C(1)	1.372(2)
C(1)-O(2)	1.203(2)
C(1)-C(2)	1.454(3)
C(2)-C(3)	1.395(3)
C(2)-C(7)	1.405(3)
C(3)-C(4)	1.373(3)
C(3)-H(3)	0.9400
C(4)-C(5)	1.380(3)
C(4)-H(4)	0.9400
C(5)-C(6)	1.380(3)
C(5)-H(5)	0.9400
C(6)-C(7)	1.404(3)
C(6)-H(6)	0.9400
C(7)-C(8)	1.455(2)
C(8)-C(16)	1.359(2)
C(8)-C(9)	1.468(2)
C(9)-O(3)	1.231(2)
C(9)-N(1)	1.387(2)
N(1)-C(10)	1.392(2)
N(1)-C(17)	1.466(2)
C(10)-C(11)	1.395(3)
C(10)-C(15)	1.402(2)
C(11)-C(12)	1.377(3)
C(11)-H(11)	0.9400
C(12)-C(13)	1.402(3)
C(12)-H(12)	0.9400
C(13)-C(14)	1.374(3)
C(13)-C(18)	1.528(3)
C(14)-C(15)	1.402(2)
C(14)-H(14)	0.9400
C(15)-C(16)	1.427(2)
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700

C(17)-H(17C)	0.9700
C(18)-C(19)	1.492(3)
C(18)-C(20)	1.510(3)
C(18)-H(18)	0.9900
C(19)-H(19A)	0.9700
C(19)-H(19B)	0.9700
C(19)-H(19C)	0.9700
C(20)-H(20A)	0.9700
C(20)-H(20B)	0.9700
C(20)-H(20C)	0.9700

C(16)-O(1)-C(1)	122.04(14)
O(2)-C(1)-O(1)	116.21(17)
O(2)-C(1)-C(2)	126.77(18)
O(1)-C(1)-C(2)	117.02(16)
C(3)-C(2)-C(7)	121.50(18)
C(3)-C(2)-C(1)	117.25(17)
C(7)-C(2)-C(1)	121.23(17)
C(4)-C(3)-C(2)	119.9(2)
C(4)-C(3)-H(3)	120.1
C(2)-C(3)-H(3)	120.1
C(3)-C(4)-C(5)	119.5(2)
C(3)-C(4)-H(4)	120.3
C(5)-C(4)-H(4)	120.3
C(6)-C(5)-C(4)	121.4(2)
C(6)-C(5)-H(5)	119.3
C(4)-C(5)-H(5)	119.3
C(5)-C(6)-C(7)	120.6(2)
C(5)-C(6)-H(6)	119.7
C(7)-C(6)-H(6)	119.7
C(6)-C(7)-C(2)	117.09(17)
C(6)-C(7)-C(8)	125.28(18)
C(2)-C(7)-C(8)	117.60(16)
C(16)-C(8)-C(7)	118.70(16)
C(16)-C(8)-C(9)	118.19(16)
C(7)-C(8)-C(9)	123.06(16)

O(3)-C(9)-N(1)	120.23(17)
O(3)-C(9)-C(8)	122.79(17)
N(1)-C(9)-C(8)	116.97(15)
C(9)-N(1)-C(10)	123.69(15)
C(9)-N(1)-C(17)	117.39(16)
C(10)-N(1)-C(17)	118.91(16)
N(1)-C(10)-C(11)	122.30(17)
N(1)-C(10)-C(15)	119.40(16)
C(11)-C(10)-C(15)	118.30(17)
C(12)-C(11)-C(10)	120.20(18)
C(12)-C(11)-H(11)	119.9
C(10)-C(11)-H(11)	119.9
C(11)-C(12)-C(13)	122.57(18)
C(11)-C(12)-H(12)	118.7
C(13)-C(12)-H(12)	118.7
C(14)-C(13)-C(12)	116.87(18)
C(14)-C(13)-C(18)	118.61(19)
C(12)-C(13)-C(18)	124.50(18)
C(13)-C(14)-C(15)	122.06(18)
C(13)-C(14)-H(14)	119.0
C(15)-C(14)-H(14)	119.0
C(14)-C(15)-C(10)	119.99(17)
C(14)-C(15)-C(16)	122.68(17)
C(10)-C(15)-C(16)	117.30(16)
C(8)-C(16)-O(1)	122.97(16)
C(8)-C(16)-C(15)	123.77(16)
O(1)-C(16)-C(15)	113.26(15)
N(1)-C(17)-H(17A)	109.5
N(1)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
N(1)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(19)-C(18)-C(20)	112.23(19)
C(19)-C(18)-C(13)	114.3(2)
C(20)-C(18)-C(13)	110.23(17)

C(19)-C(18)-H(18)	106.5
C(20)-C(18)-H(18)	106.5
C(13)-C(18)-H(18)	106.5
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(18)-C(20)-H(20A)	109.5
C(18)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(18)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for No1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	26(1)	22(1)	31(1)	1(1)	8(1)	-2(1)
C(1)	31(1)	26(1)	24(1)	-1(1)	7(1)	1(1)
C(2)	29(1)	29(1)	24(1)	-4(1)	7(1)	0(1)
C(3)	36(1)	37(1)	34(1)	3(1)	4(1)	6(1)
C(4)	31(1)	45(1)	47(1)	-4(1)	0(1)	6(1)
C(5)	24(1)	44(1)	61(2)	-10(1)	7(1)	-4(1)
C(6)	30(1)	33(1)	50(1)	-6(1)	10(1)	-6(1)
C(7)	26(1)	27(1)	26(1)	-7(1)	6(1)	-2(1)
C(8)	27(1)	24(1)	24(1)	-4(1)	6(1)	-2(1)
C(9)	32(1)	26(1)	26(1)	-4(1)	8(1)	-4(1)
N(1)	32(1)	22(1)	27(1)	0(1)	9(1)	-1(1)
C(10)	30(1)	24(1)	21(1)	-6(1)	7(1)	-1(1)
C(11)	38(1)	31(1)	28(1)	0(1)	5(1)	5(1)
C(12)	30(1)	41(1)	33(1)	-5(1)	1(1)	8(1)
C(13)	26(1)	35(1)	37(1)	-9(1)	6(1)	0(1)
C(14)	28(1)	27(1)	33(1)	-5(1)	9(1)	-3(1)
C(15)	27(1)	24(1)	23(1)	-6(1)	8(1)	-1(1)
C(16)	28(1)	20(1)	23(1)	-4(1)	8(1)	-2(1)
O(2)	42(1)	32(1)	44(1)	11(1)	9(1)	-2(1)
O(3)	34(1)	32(1)	50(1)	5(1)	8(1)	-11(1)
C(17)	42(1)	28(1)	41(1)	6(1)	14(1)	-1(1)
C(18)	27(1)	52(1)	53(1)	-5(1)	7(1)	-3(1)
C(19)	33(1)	62(2)	100(2)	-17(2)	12(1)	2(1)
C(20)	34(1)	42(1)	60(1)	-6(1)	8(1)	-10(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for No1.

	x	y	z	U(eq)
H(3)	-3372	7719	-2177	44
H(4)	-5056	7266	-2103	51
H(5)	-5270	6075	-495	52
H(6)	-3840	5276	871	45
H(11)	1122	3925	4281	39
H(12)	2669	4656	4588	42
H(14)	1151	6516	1574	35
H(17A)	-326	3173	2613	54
H(17B)	-1495	3285	2879	54
H(17C)	-527	3494	4513	54
H(18)	3076	6426	2071	53
H(19A)	4682	6069	3828	98
H(19B)	4079	5257	2982	98
H(19C)	4145	5486	5067	98
H(20A)	3068	6720	5789	68
H(20B)	2414	7236	4115	68
H(20C)	3663	7273	4582	68

Table 6. Torsion angles [°] for No1.

C(16)-O(1)-C(1)-O(2)	-175.52(16)
C(16)-O(1)-C(1)-C(2)	5.0(2)
O(2)-C(1)-C(2)-C(3)	-4.0(3)
O(1)-C(1)-C(2)-C(3)	175.39(16)
O(2)-C(1)-C(2)-C(7)	177.76(18)
O(1)-C(1)-C(2)-C(7)	-2.9(2)
C(7)-C(2)-C(3)-C(4)	1.4(3)
C(1)-C(2)-C(3)-C(4)	-176.87(18)
C(2)-C(3)-C(4)-C(5)	1.3(3)
C(3)-C(4)-C(5)-C(6)	-2.4(3)
C(4)-C(5)-C(6)-C(7)	0.8(3)
C(5)-C(6)-C(7)-C(2)	1.9(3)
C(5)-C(6)-C(7)-C(8)	179.94(18)
C(3)-C(2)-C(7)-C(6)	-3.0(3)
C(1)-C(2)-C(7)-C(6)	175.23(17)
C(3)-C(2)-C(7)-C(8)	178.84(17)
C(1)-C(2)-C(7)-C(8)	-3.0(2)
C(6)-C(7)-C(8)-C(16)	-171.11(18)
C(2)-C(7)-C(8)-C(16)	6.9(2)
C(6)-C(7)-C(8)-C(9)	11.5(3)
C(2)-C(7)-C(8)-C(9)	-170.47(16)
C(16)-C(8)-C(9)-O(3)	-173.29(17)
C(7)-C(8)-C(9)-O(3)	4.1(3)
C(16)-C(8)-C(9)-N(1)	5.2(2)
C(7)-C(8)-C(9)-N(1)	-177.41(15)
O(3)-C(9)-N(1)-C(10)	-179.02(16)
C(8)-C(9)-N(1)-C(10)	2.5(2)
O(3)-C(9)-N(1)-C(17)	1.2(3)
C(8)-C(9)-N(1)-C(17)	-177.28(16)
C(9)-N(1)-C(10)-C(11)	173.69(16)
C(17)-N(1)-C(10)-C(11)	-6.6(2)
C(9)-N(1)-C(10)-C(15)	-6.8(2)
C(17)-N(1)-C(10)-C(15)	172.98(16)
N(1)-C(10)-C(11)-C(12)	179.70(16)

C(15)-C(10)-C(11)-C(12)	0.2(3)
C(10)-C(11)-C(12)-C(13)	-0.8(3)
C(11)-C(12)-C(13)-C(14)	0.4(3)
C(11)-C(12)-C(13)-C(18)	178.46(19)
C(12)-C(13)-C(14)-C(15)	0.7(3)
C(18)-C(13)-C(14)-C(15)	-177.48(17)
C(13)-C(14)-C(15)-C(10)	-1.4(3)
C(13)-C(14)-C(15)-C(16)	176.57(17)
N(1)-C(10)-C(15)-C(14)	-178.66(16)
C(11)-C(10)-C(15)-C(14)	0.9(2)
N(1)-C(10)-C(15)-C(16)	3.3(2)
C(11)-C(10)-C(15)-C(16)	-177.16(16)
C(7)-C(8)-C(16)-O(1)	-5.2(3)
C(9)-C(8)-C(16)-O(1)	172.37(15)
C(7)-C(8)-C(16)-C(15)	173.66(16)
C(9)-C(8)-C(16)-C(15)	-8.8(3)
C(1)-O(1)-C(16)-C(8)	-1.0(2)
C(1)-O(1)-C(16)-C(15)	-179.98(15)
C(14)-C(15)-C(16)-C(8)	-173.41(17)
C(10)-C(15)-C(16)-C(8)	4.6(3)
C(14)-C(15)-C(16)-O(1)	5.5(2)
C(10)-C(15)-C(16)-O(1)	-176.48(14)
C(14)-C(13)-C(18)-C(19)	-161.8(2)
C(12)-C(13)-C(18)-C(19)	20.1(3)
C(14)-C(13)-C(18)-C(20)	70.7(3)
C(12)-C(13)-C(18)-C(20)	-107.4(2)

Symmetry transformations used to generate equivalent atoms: