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Synthesis of fused pyrroles containing 4-hyroxycoumarins by regioselective metal-free multicomponent reactions

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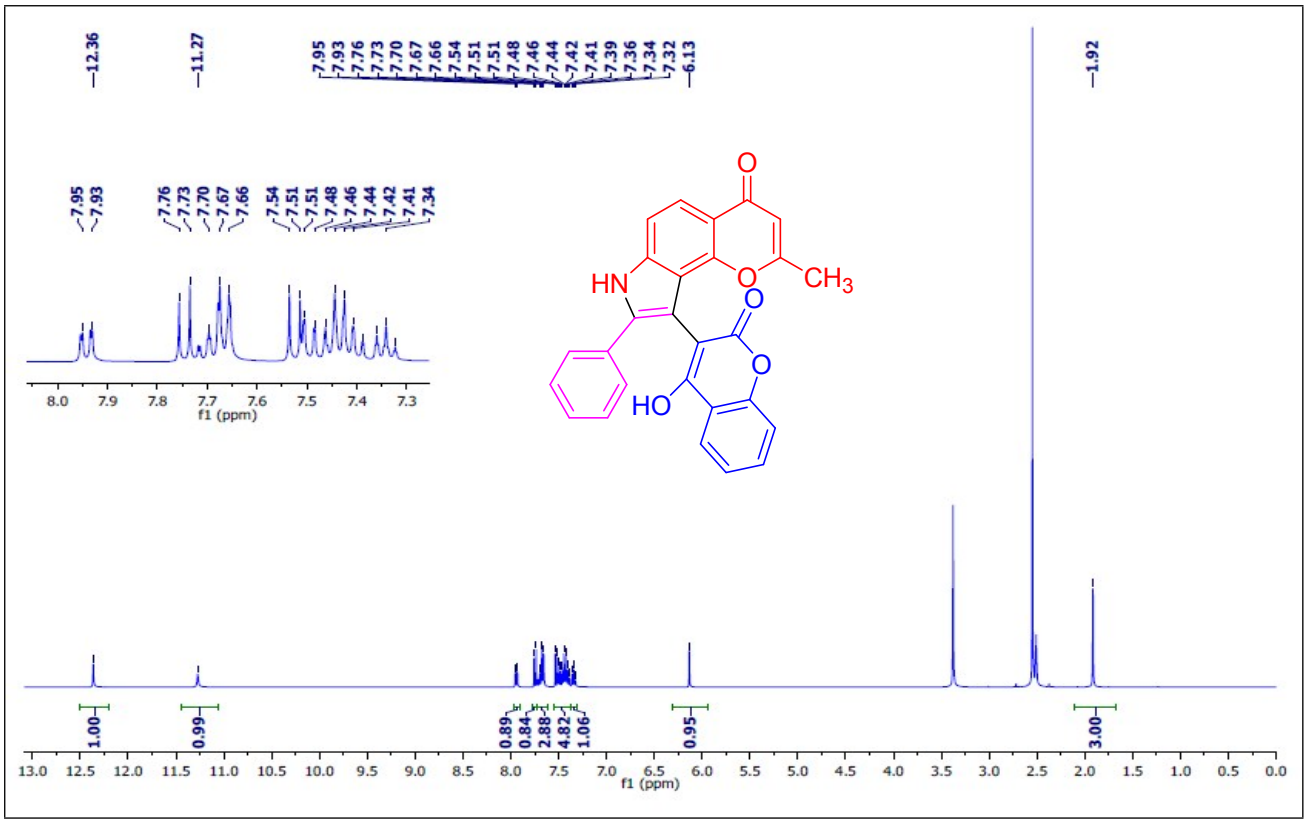
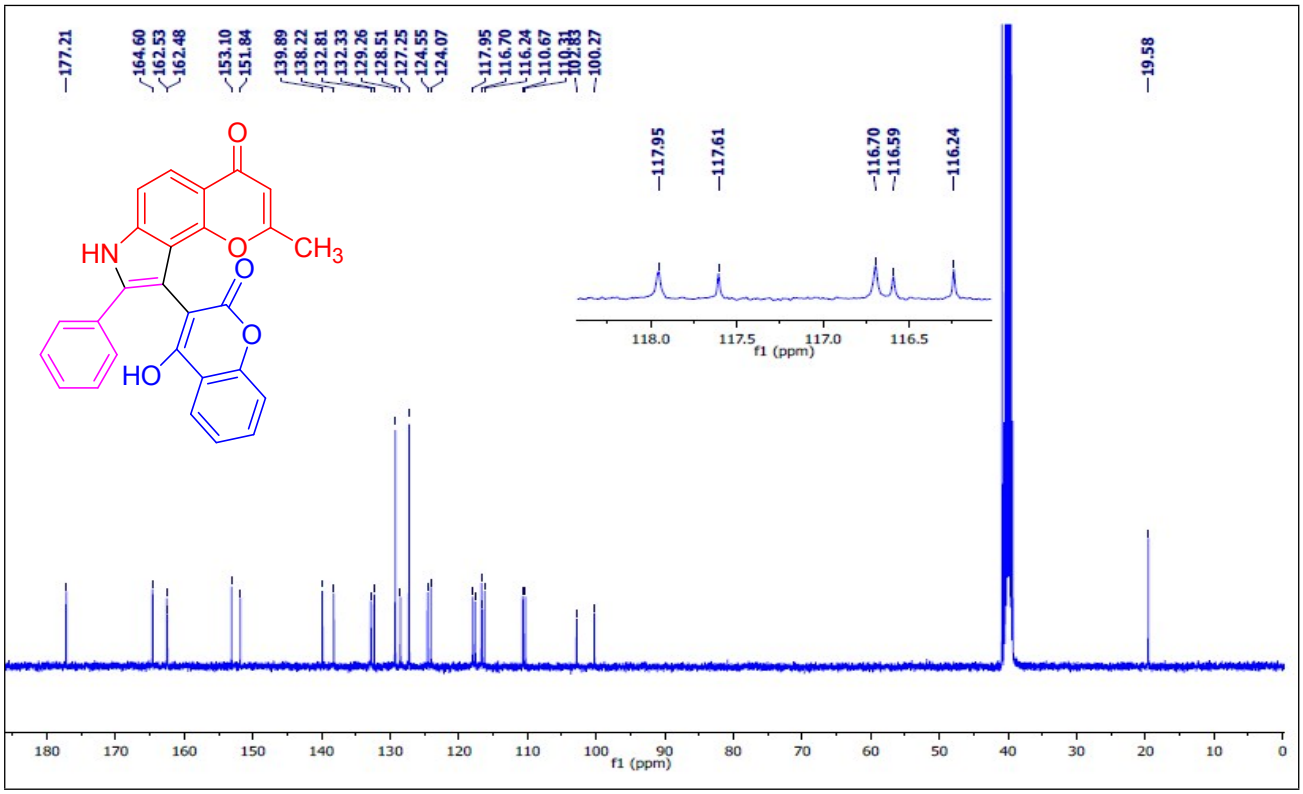
^{1}H and ^{13}C NMR spectra of (4a)





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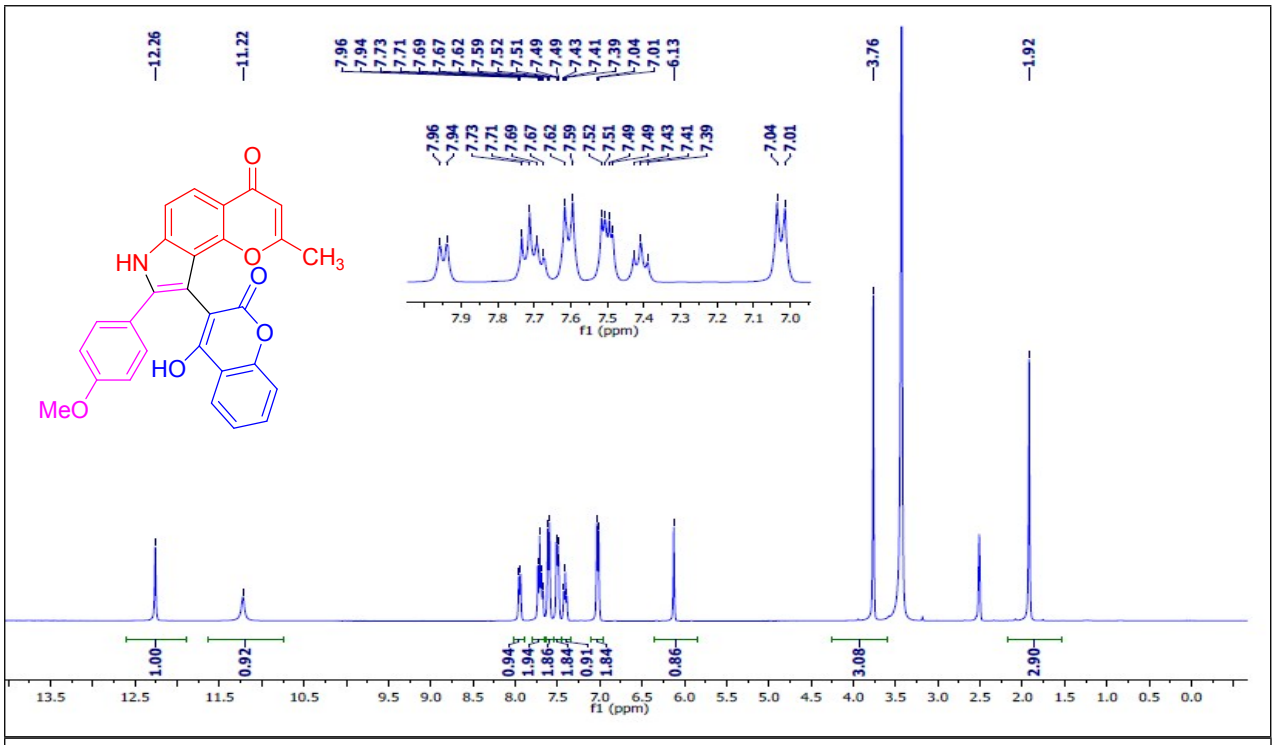

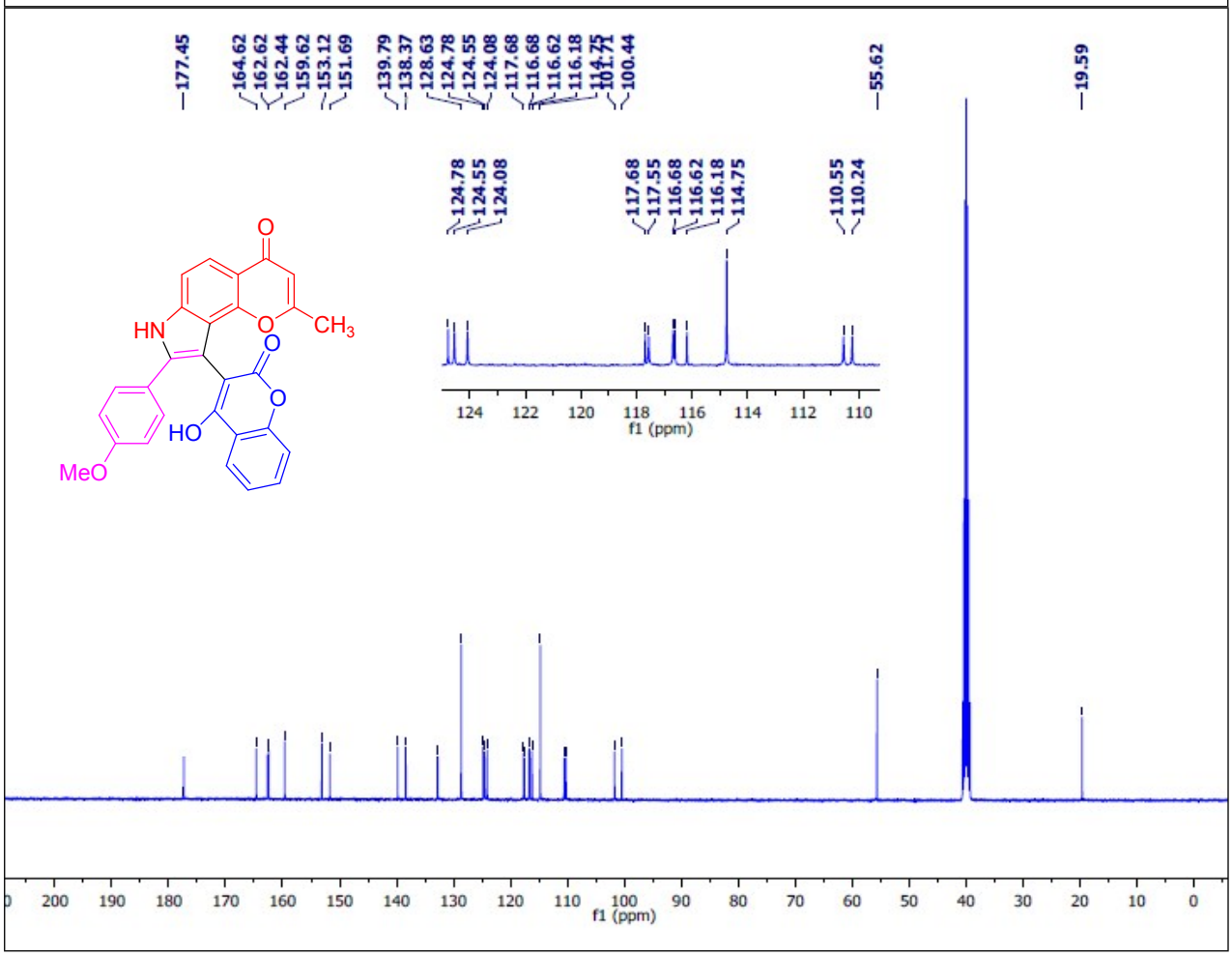

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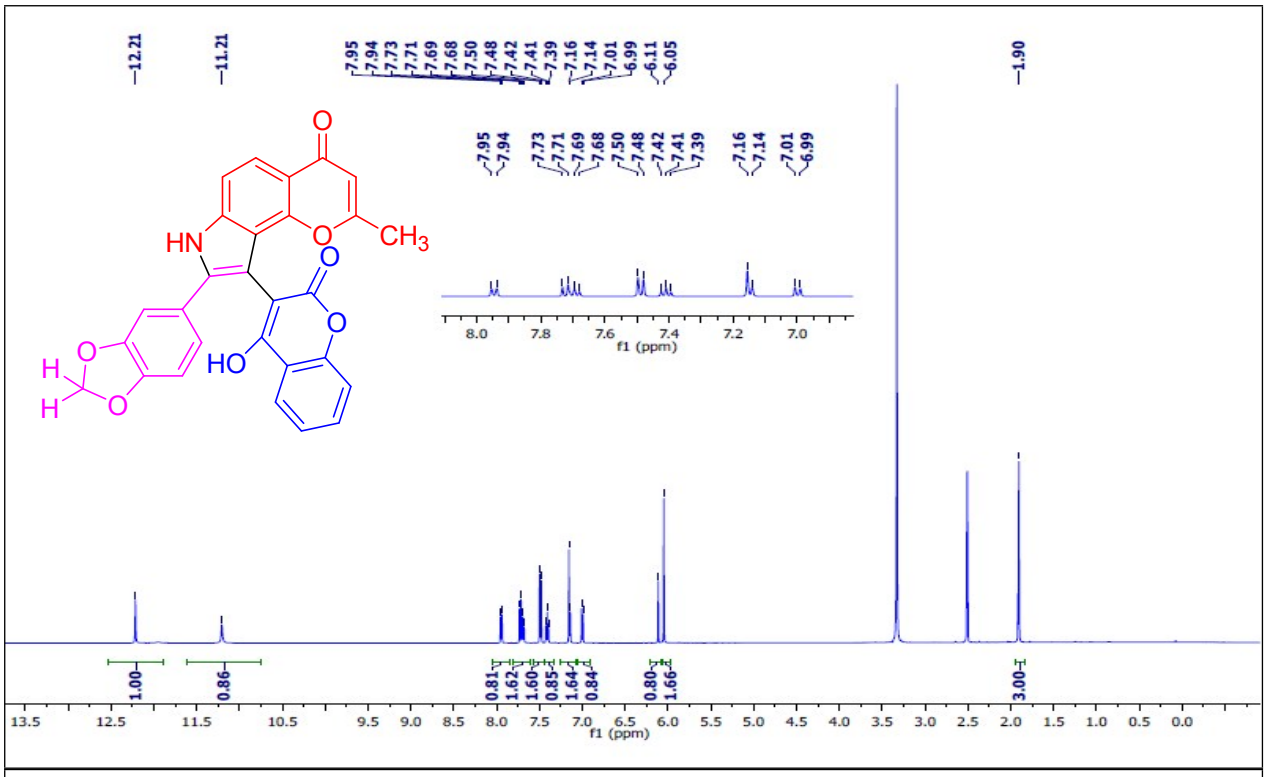

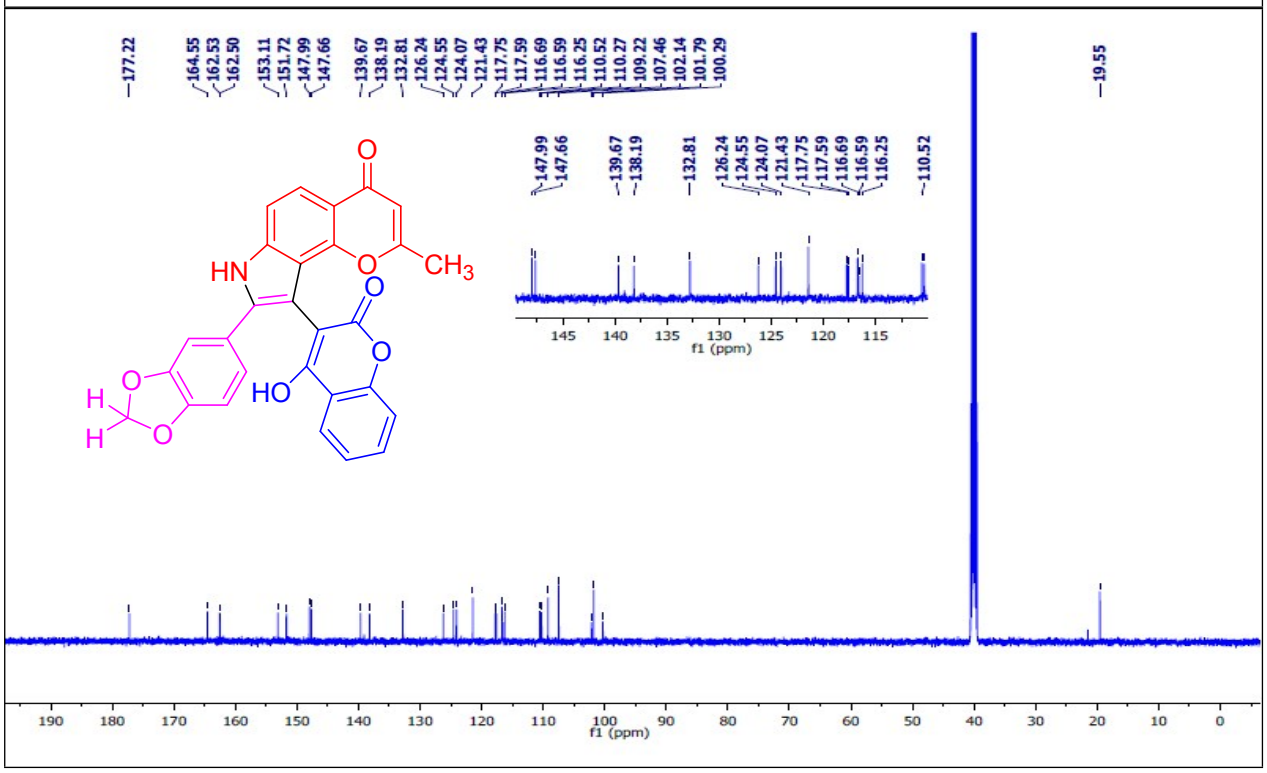

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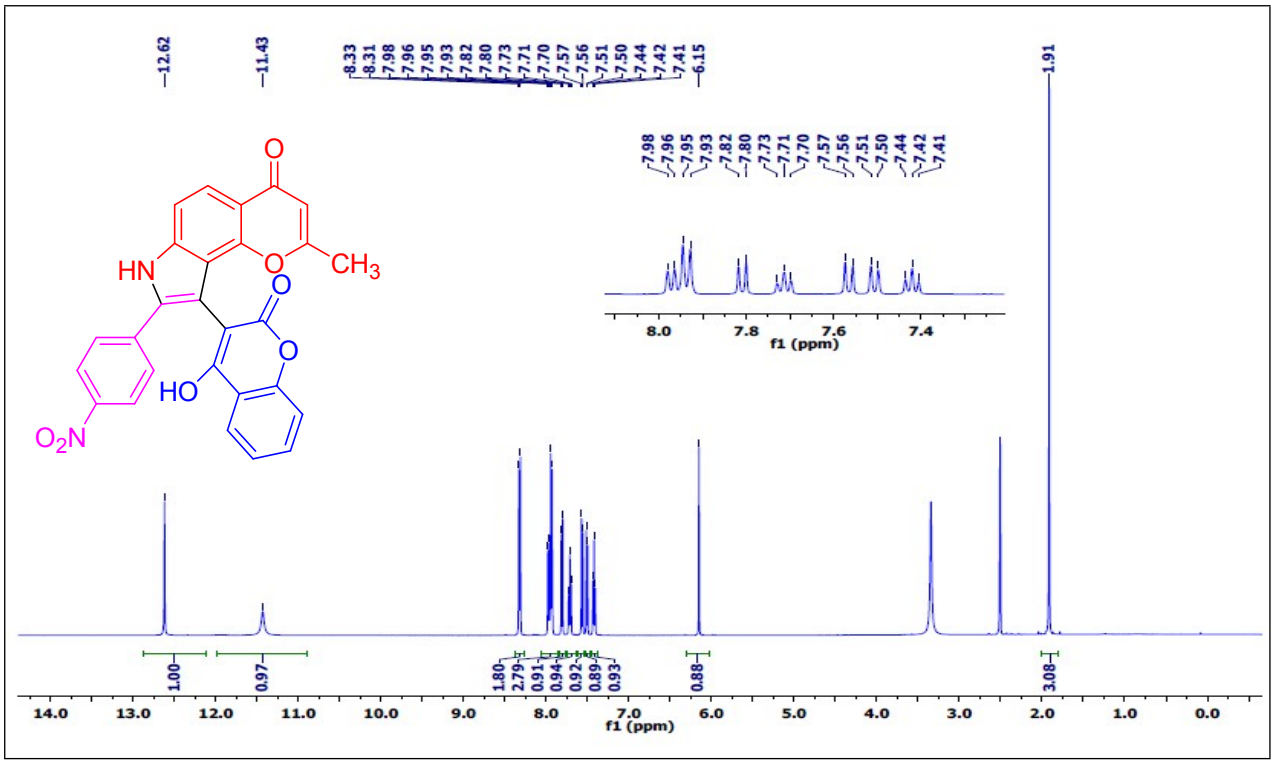

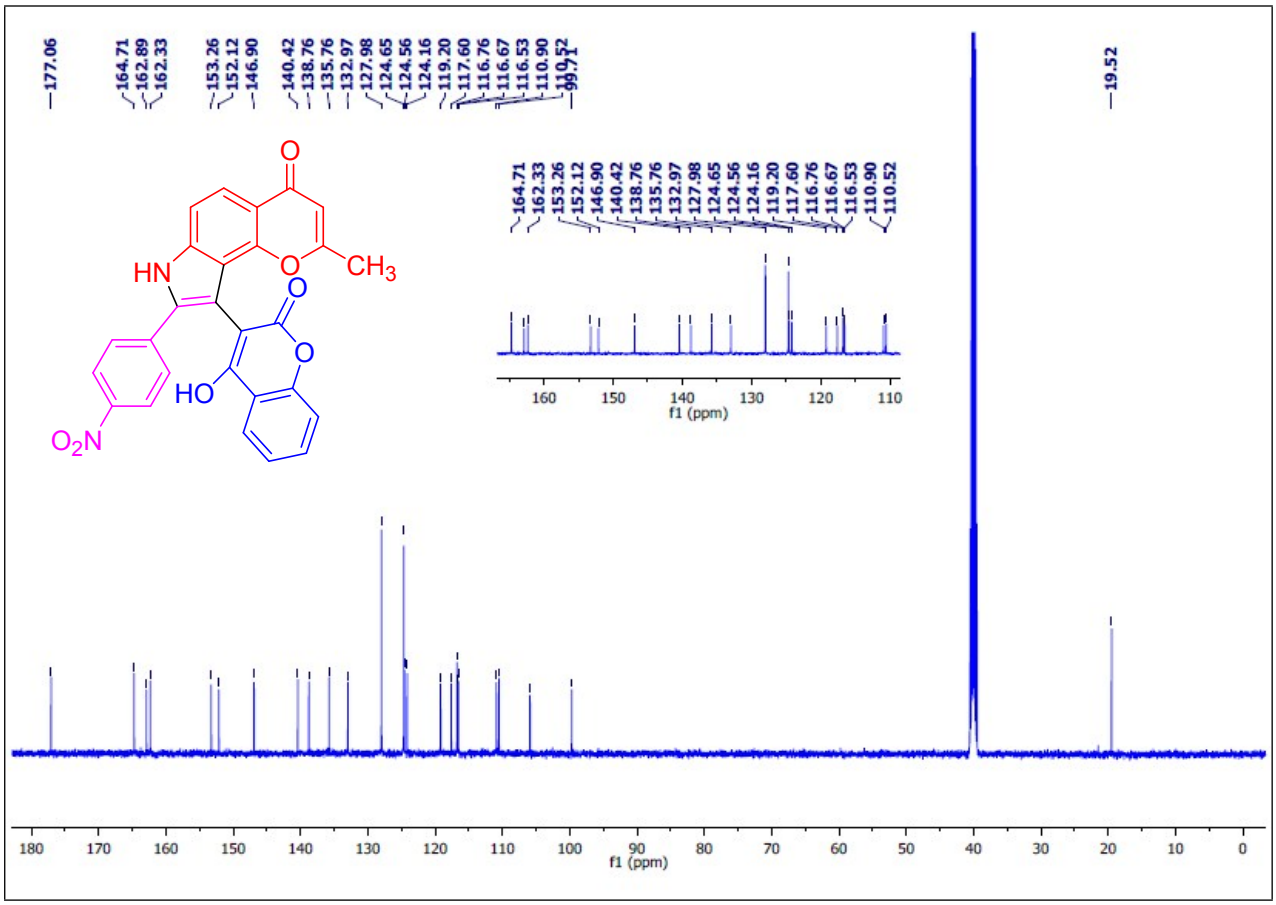

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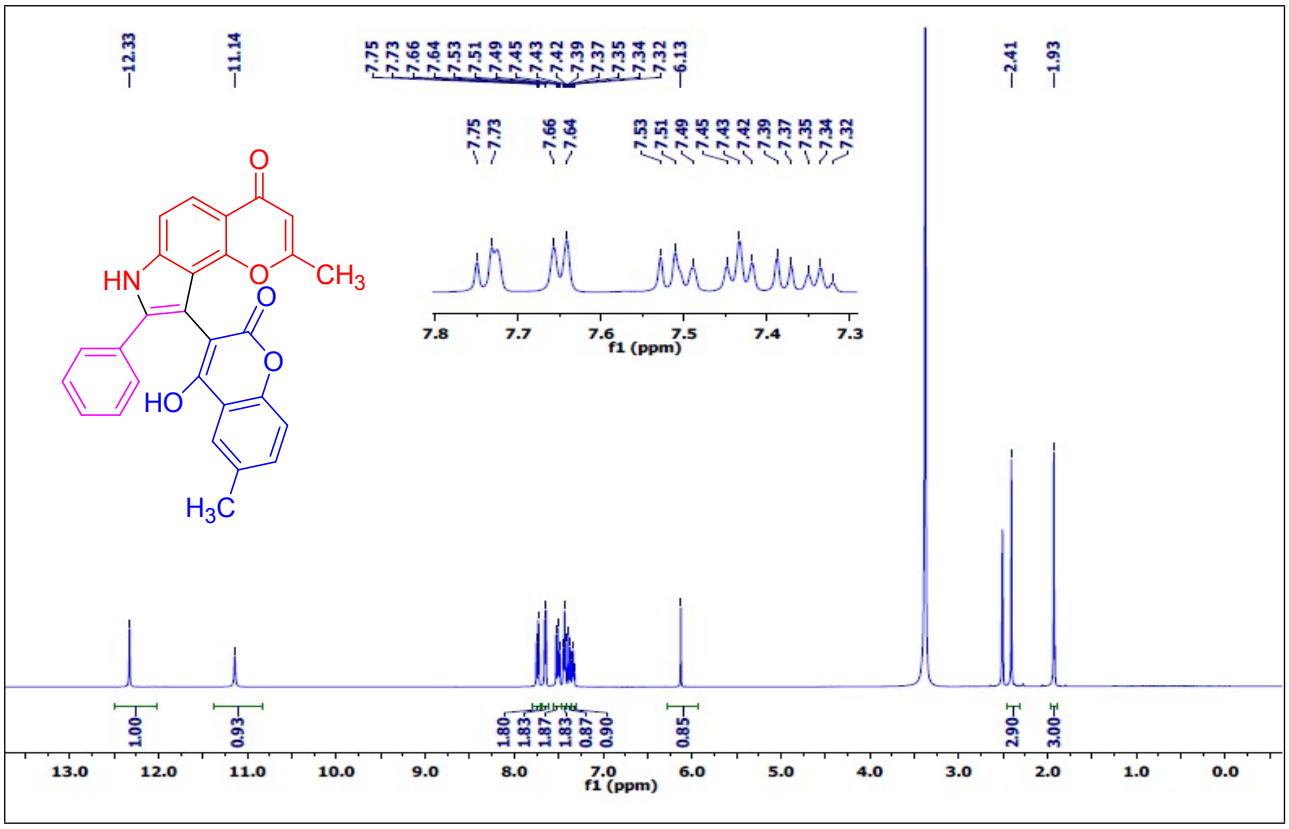

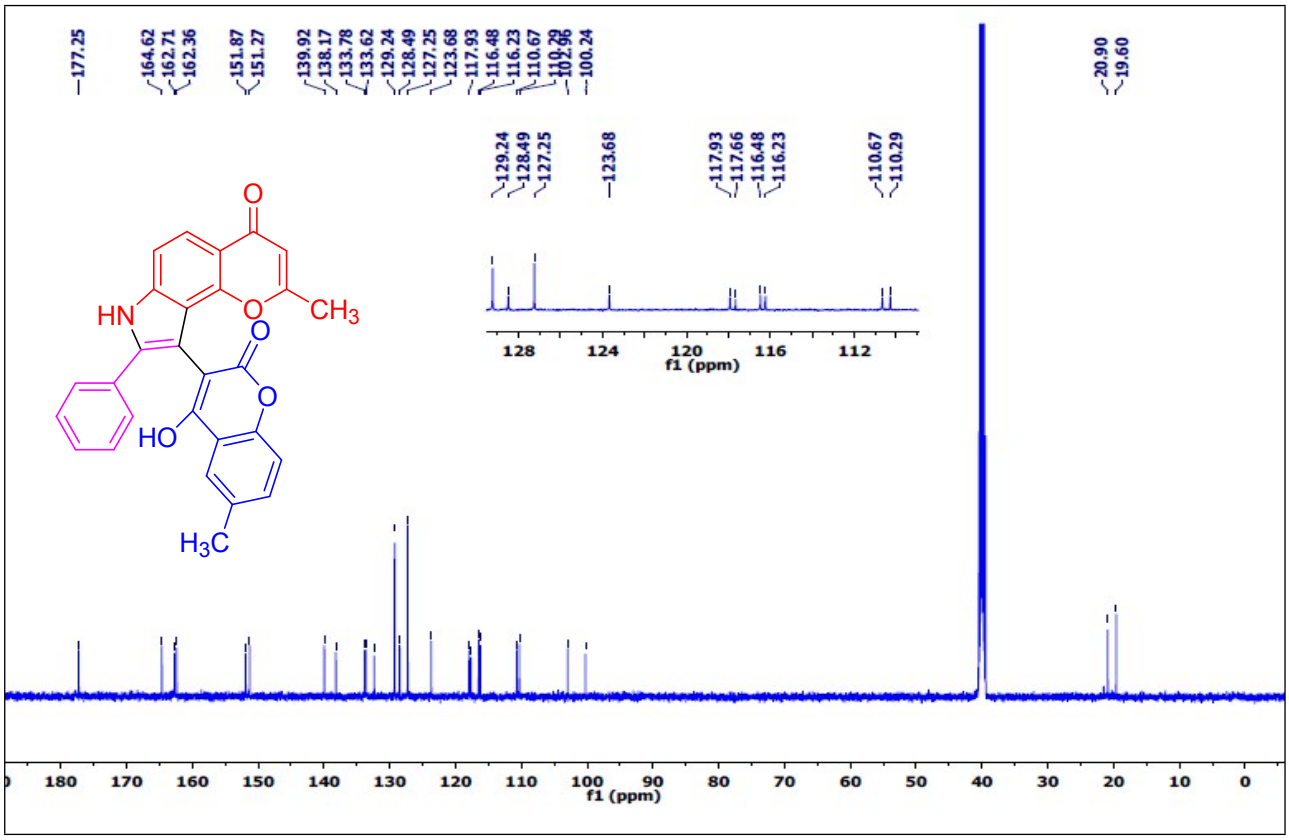

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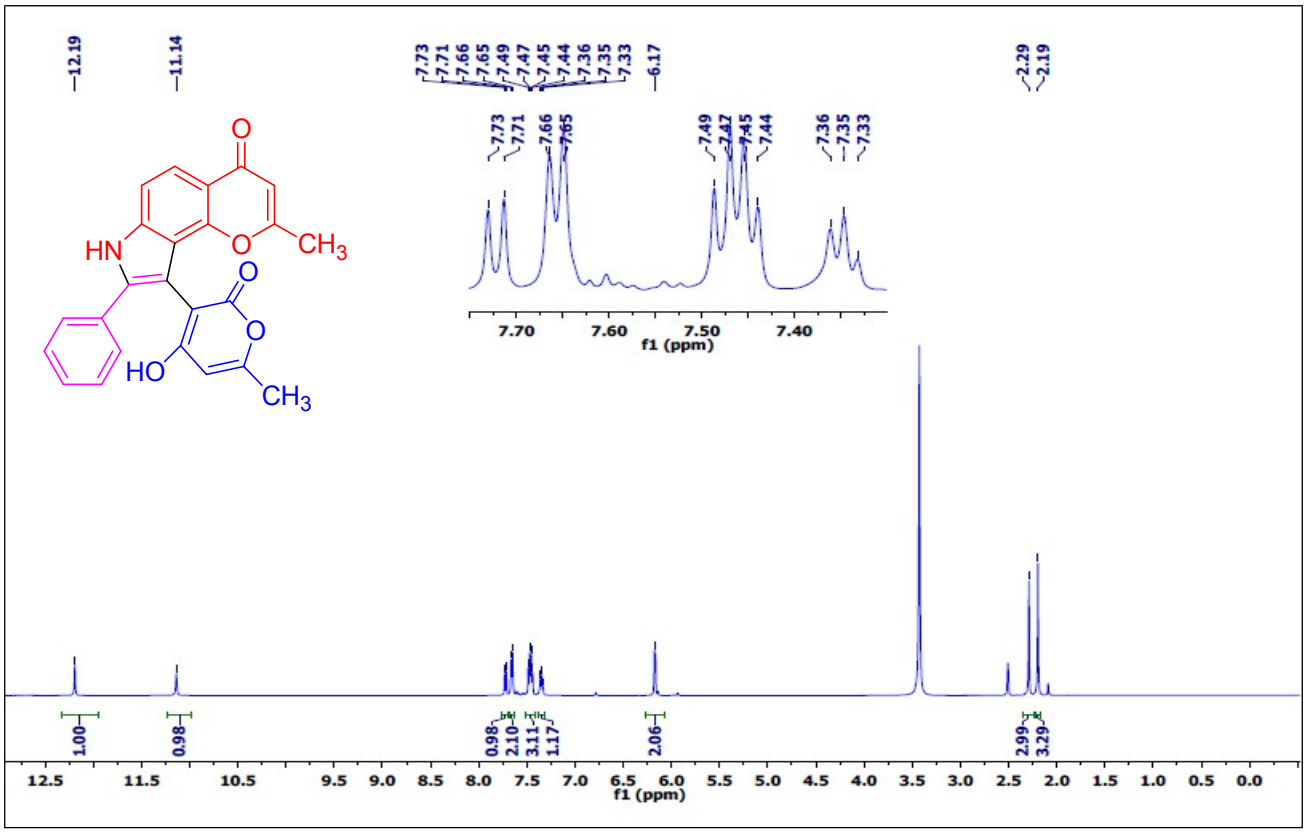

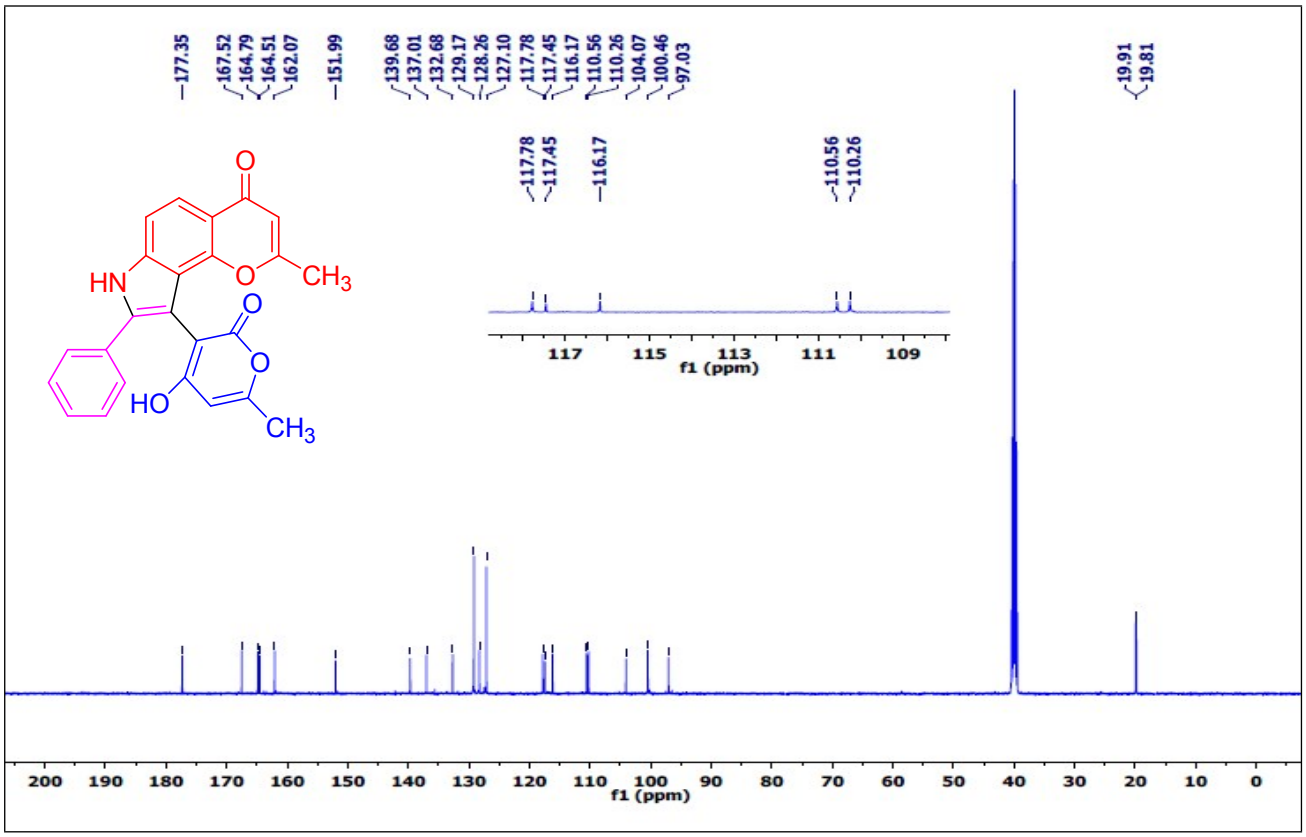

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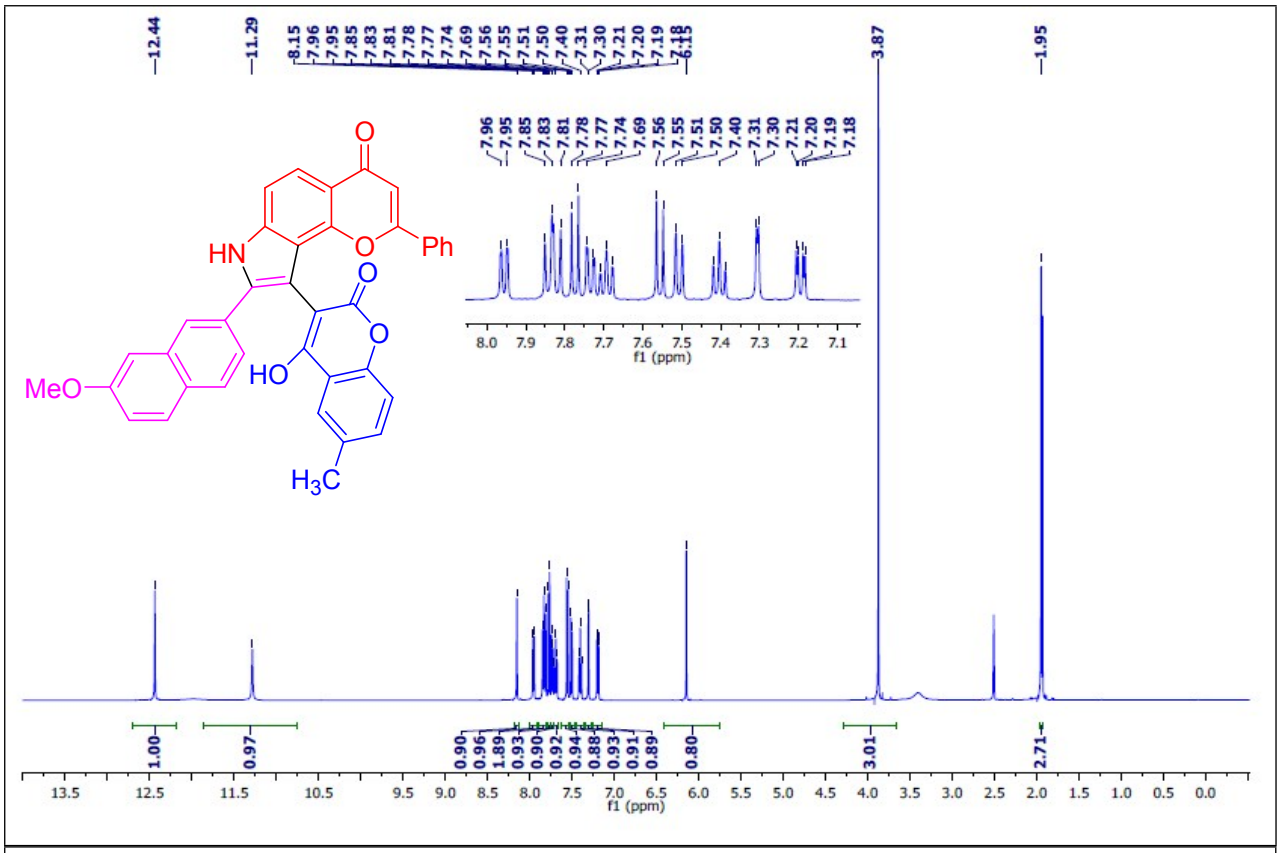

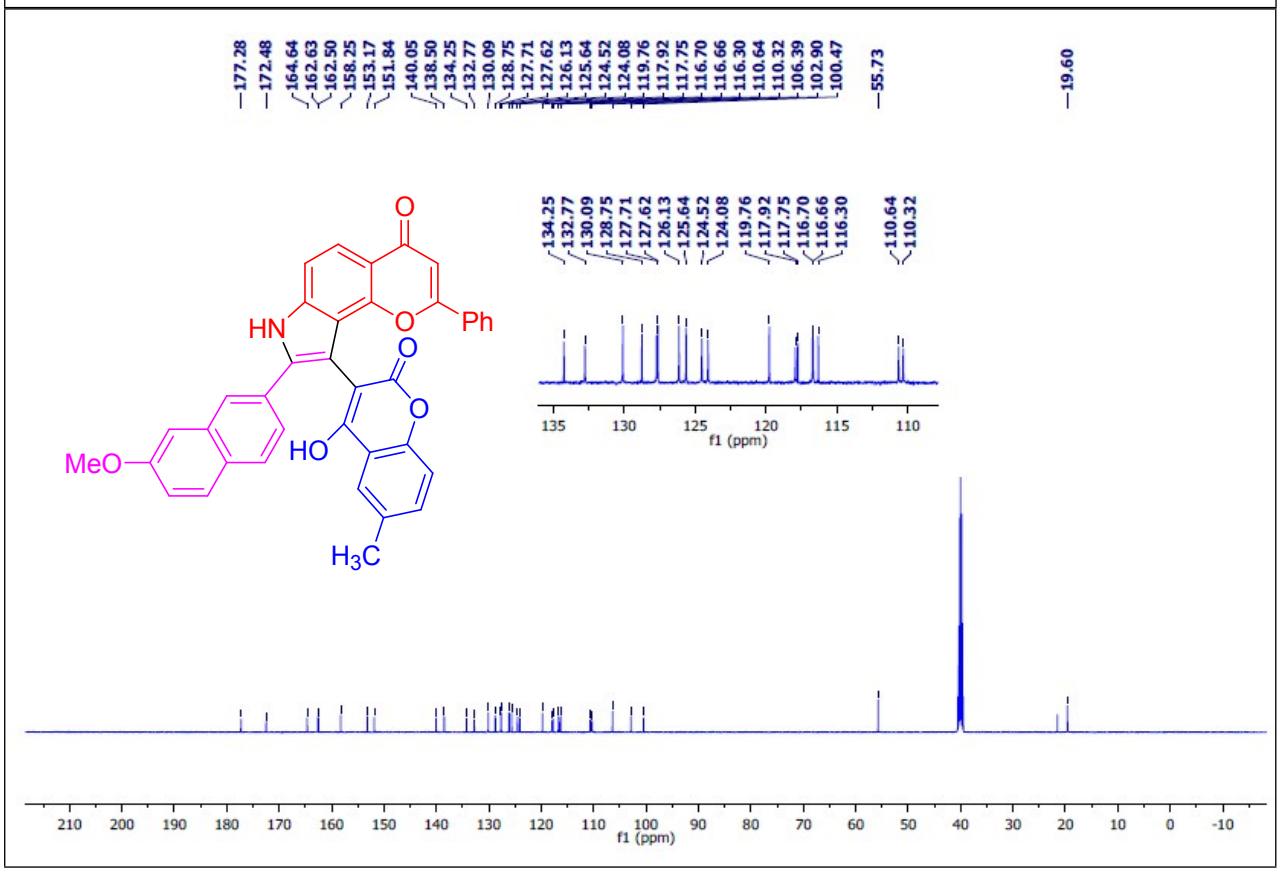

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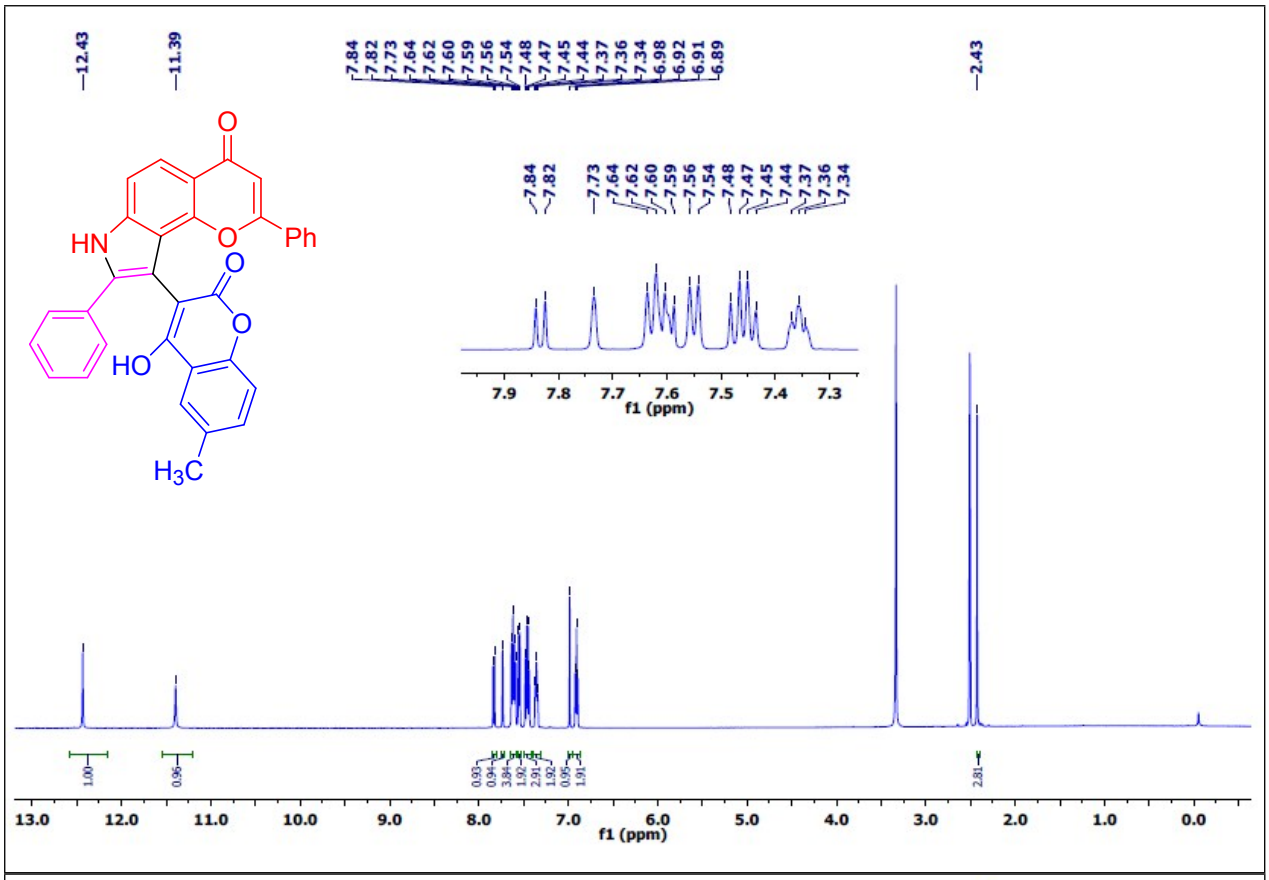

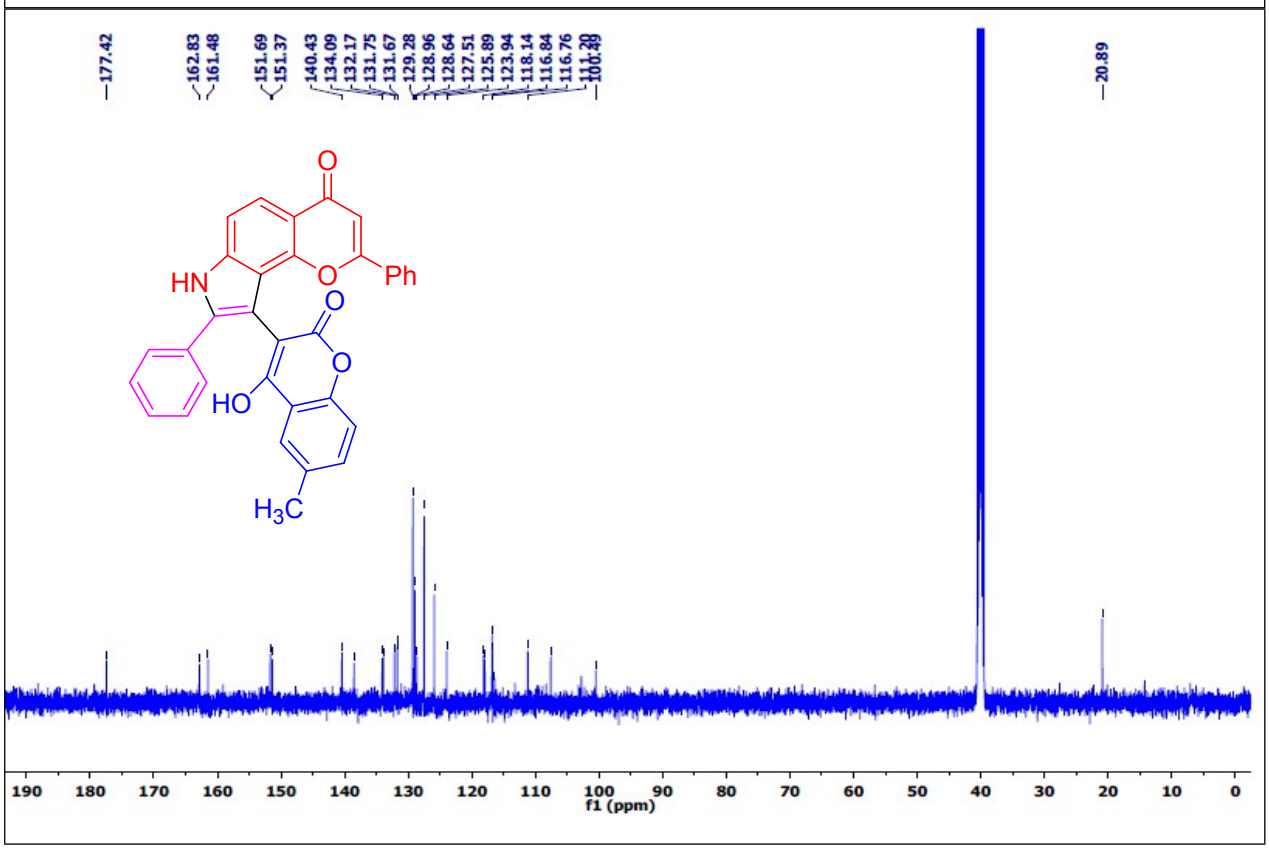

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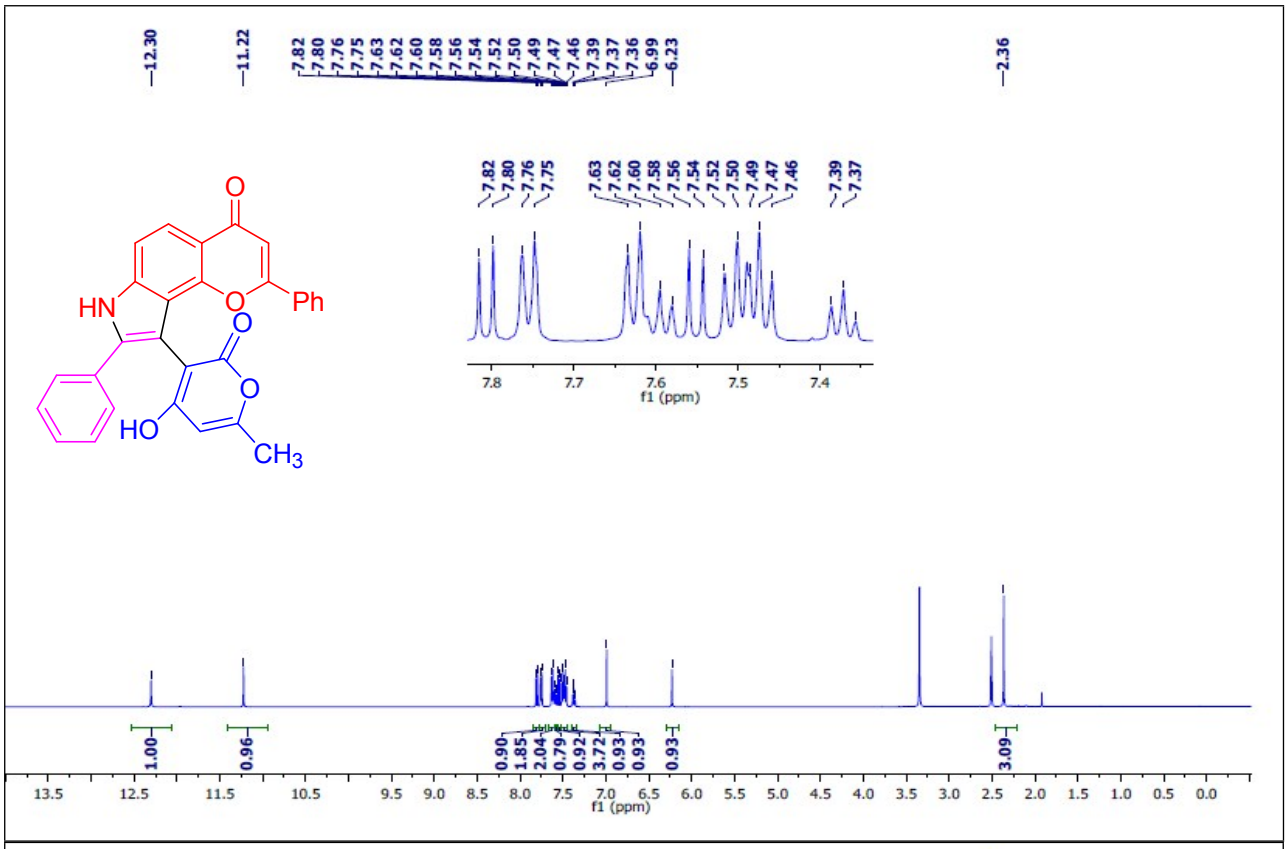

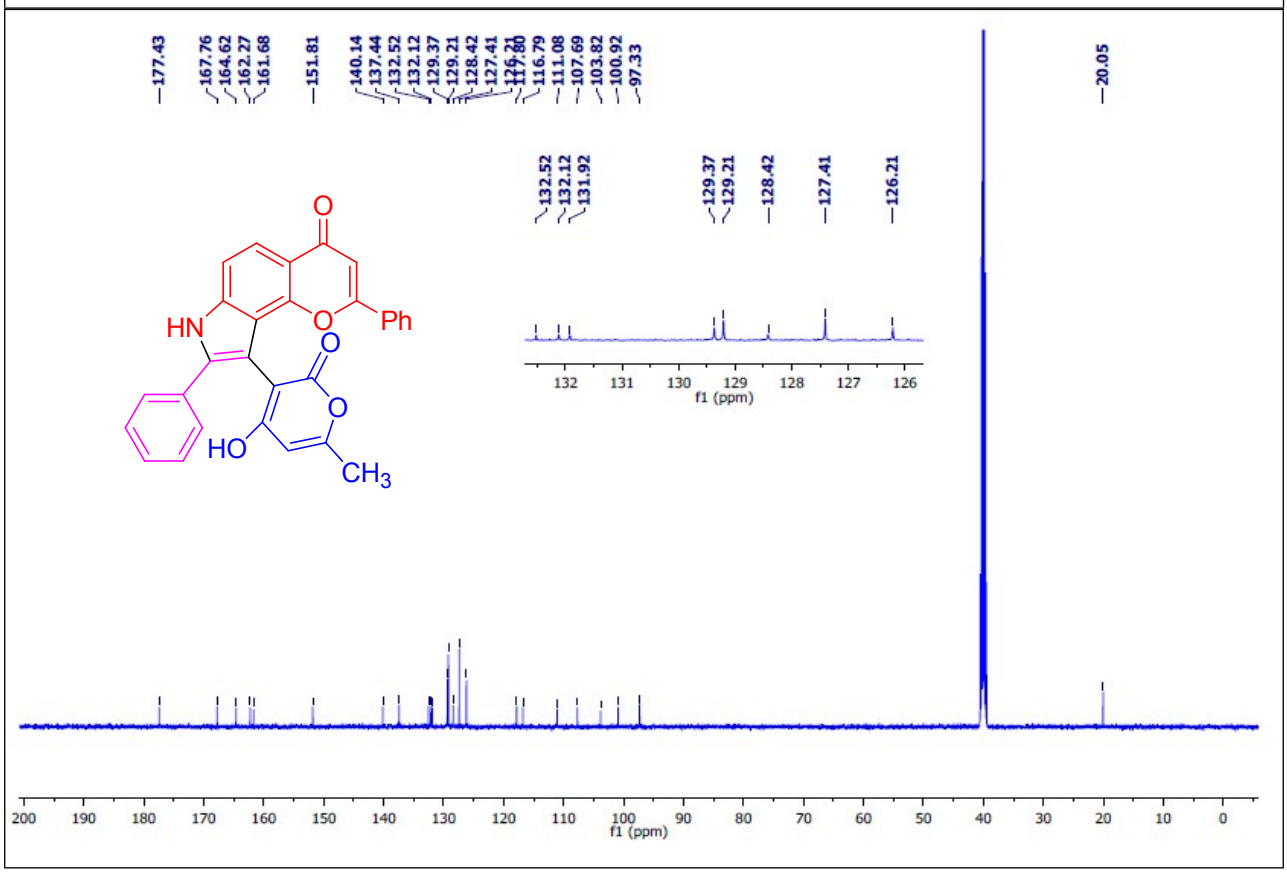

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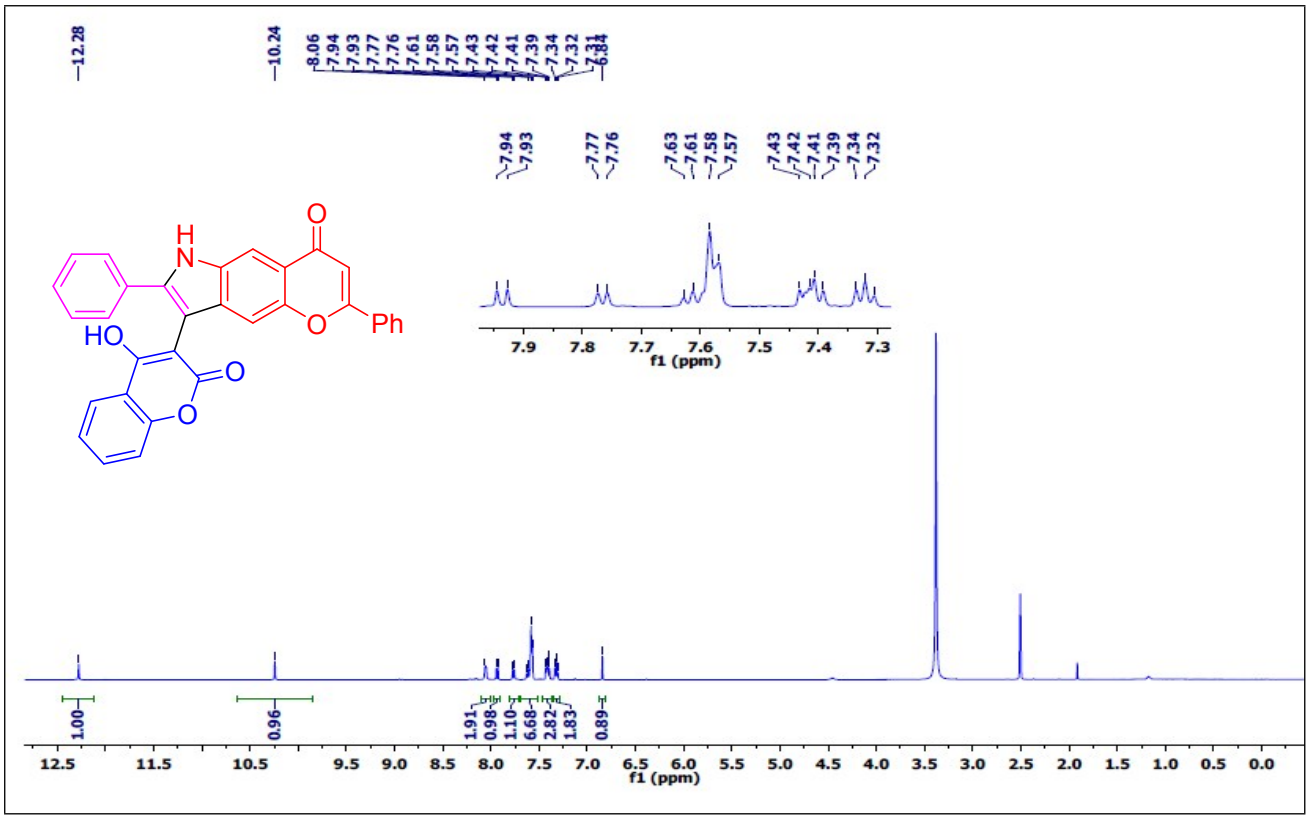

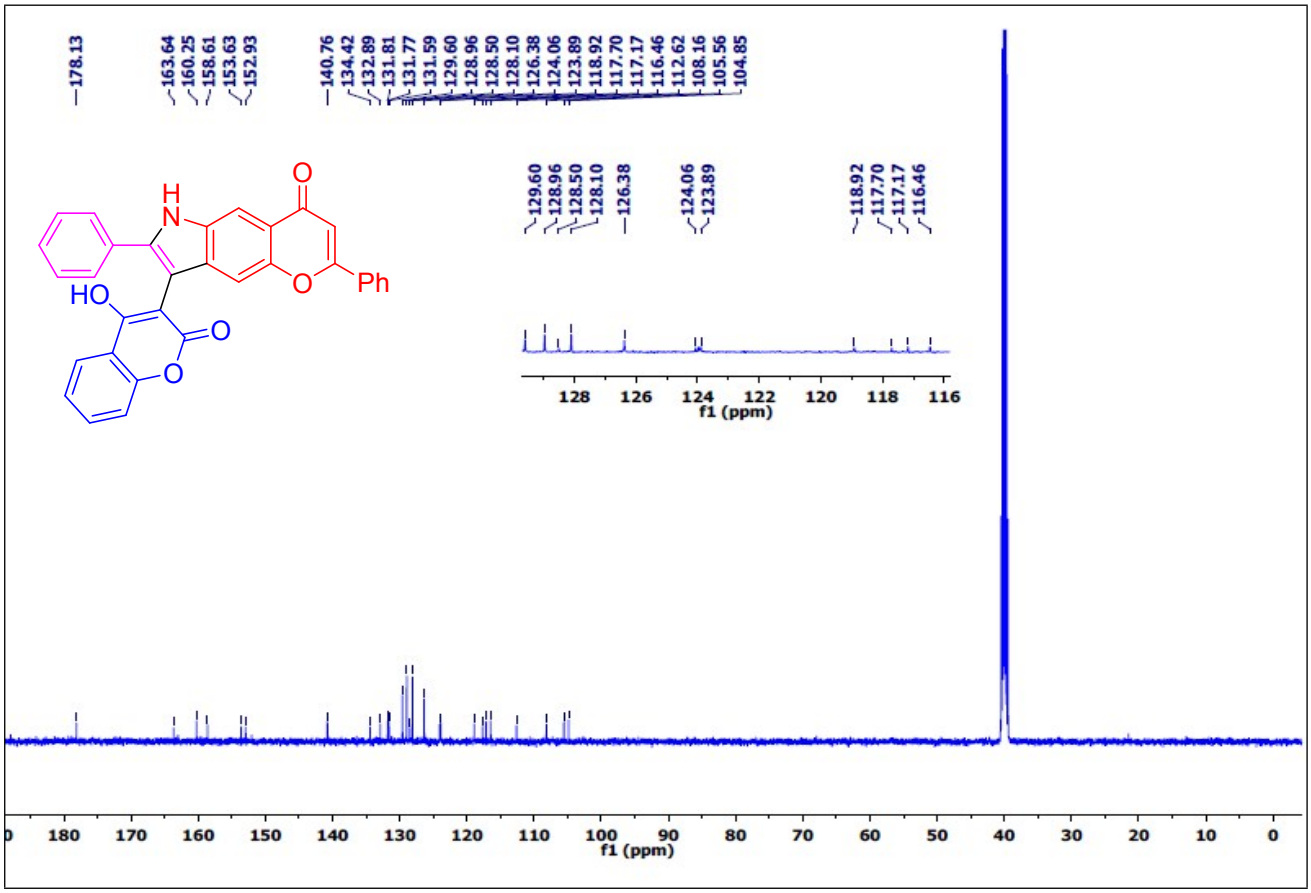

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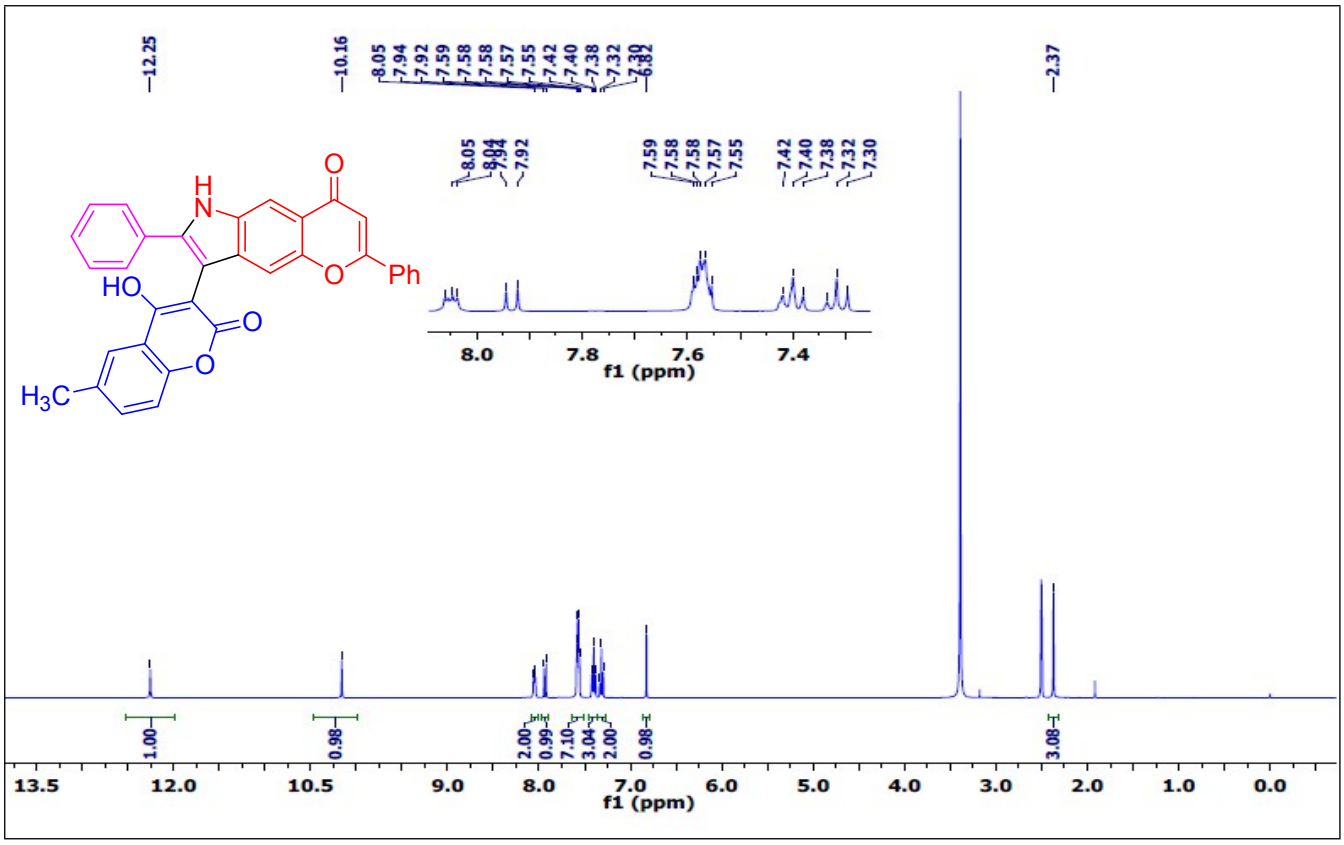

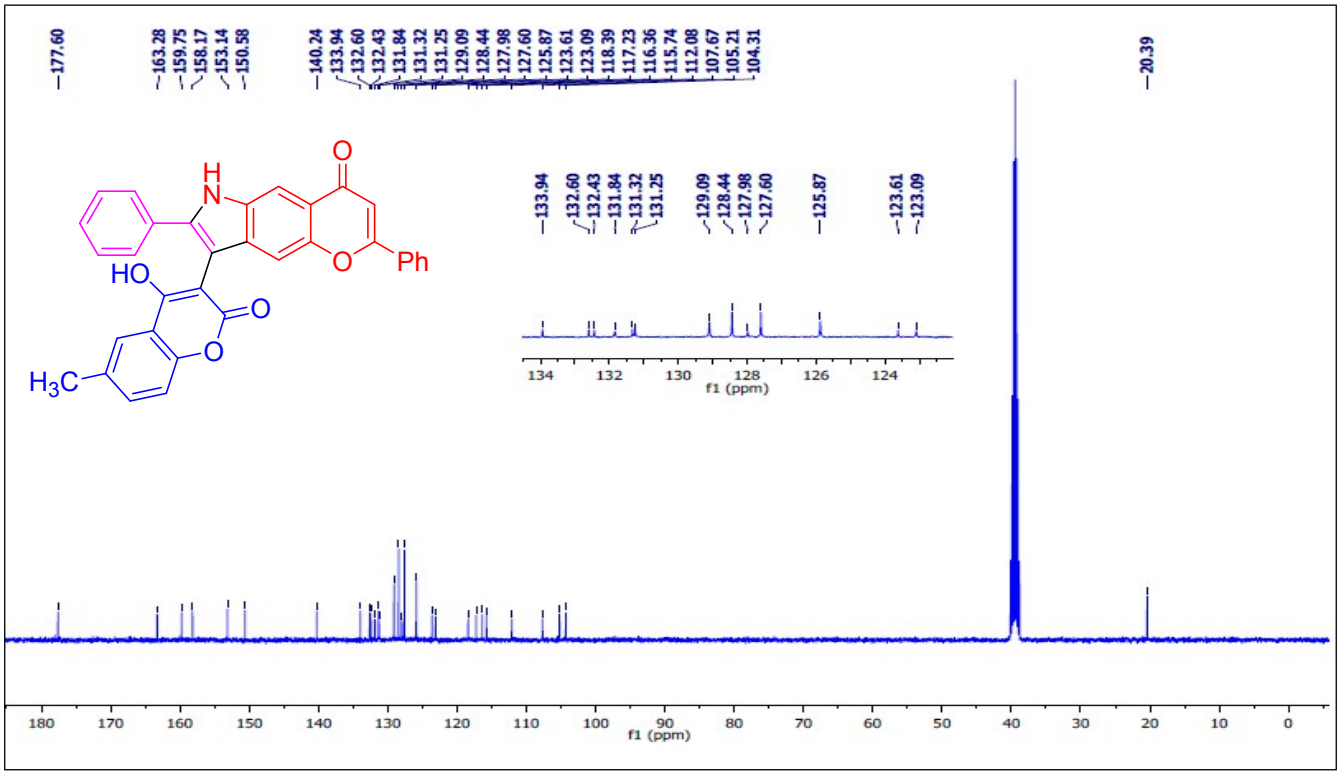

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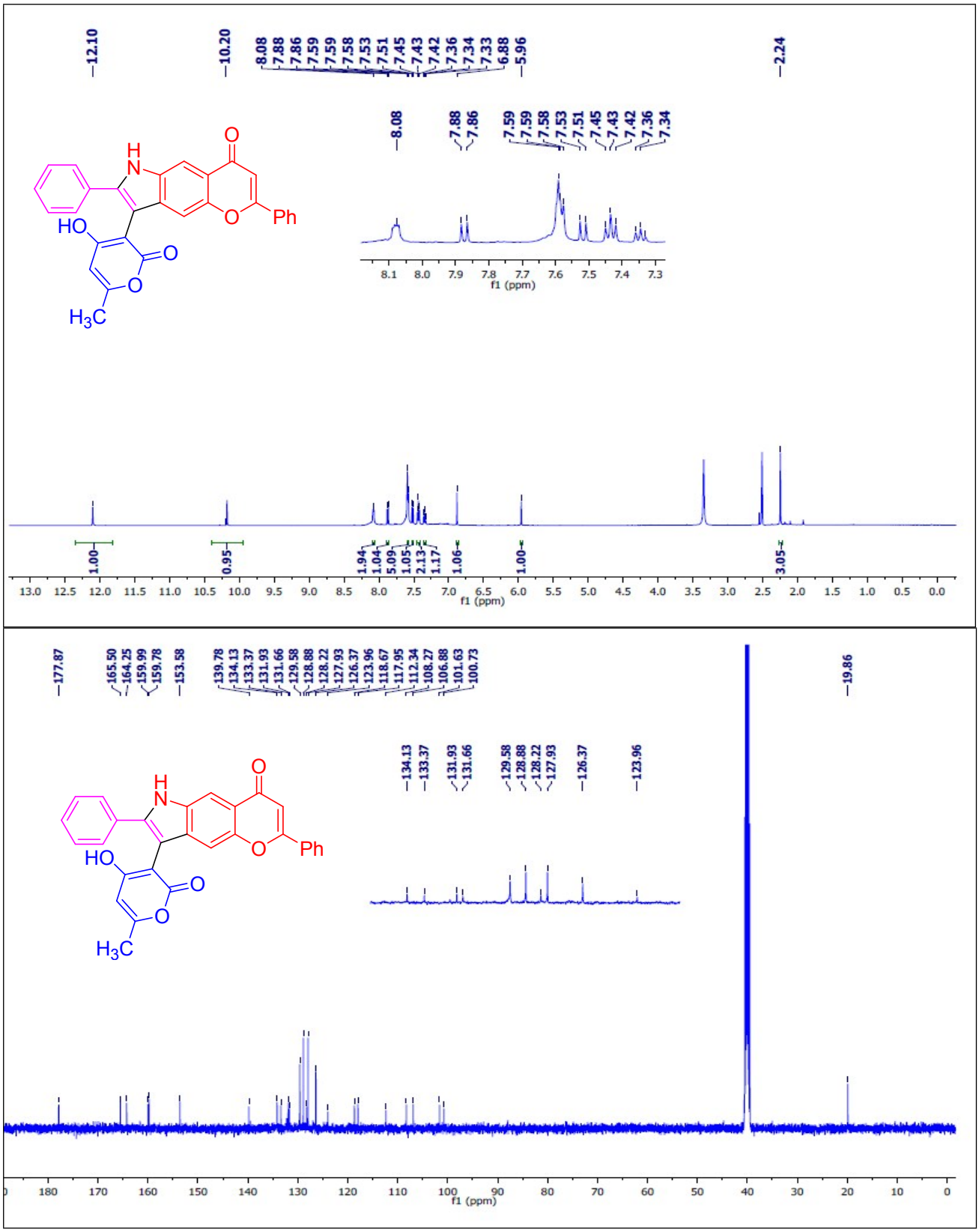
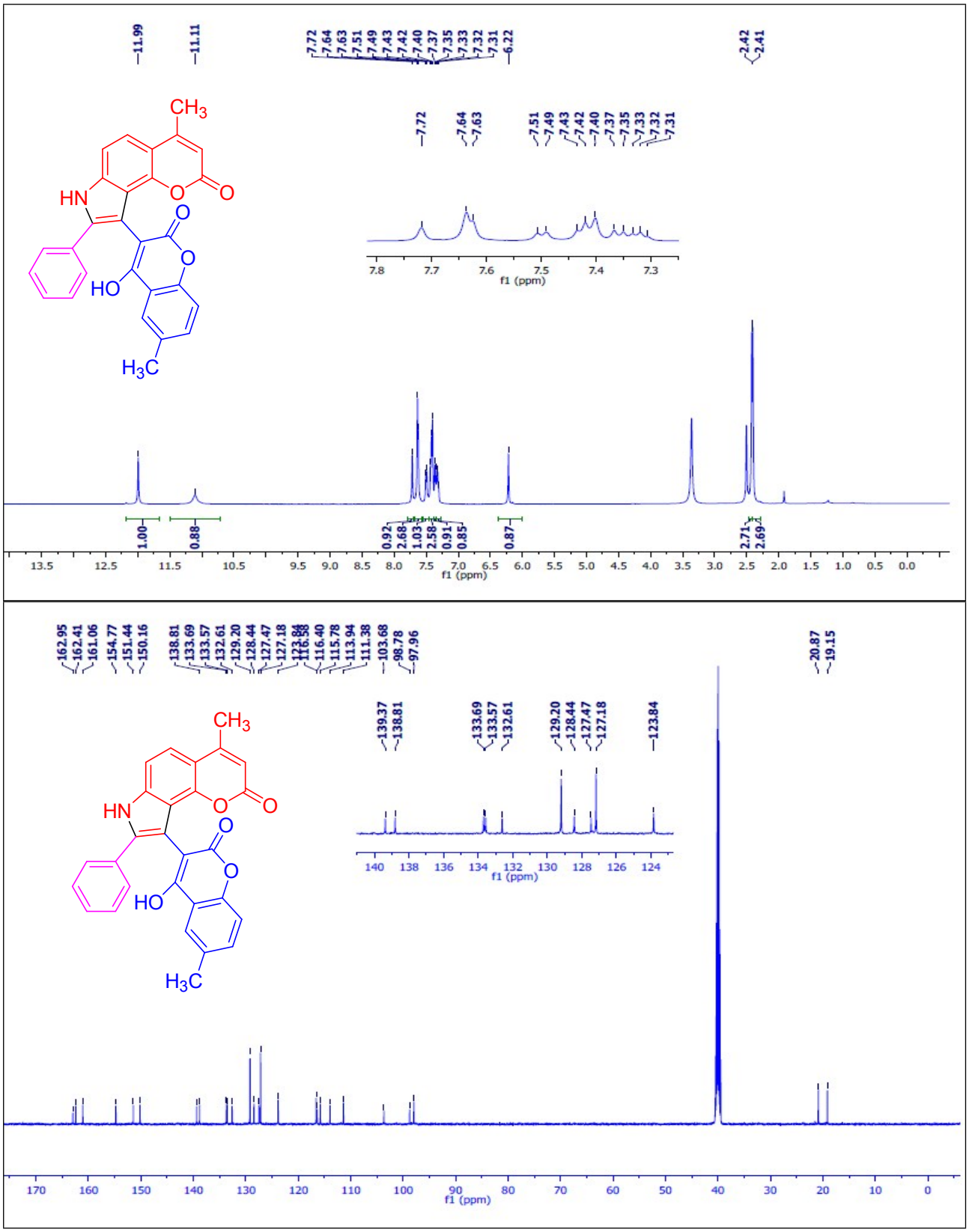


^{1}H and ^{13}C NMR spectra of (8a)



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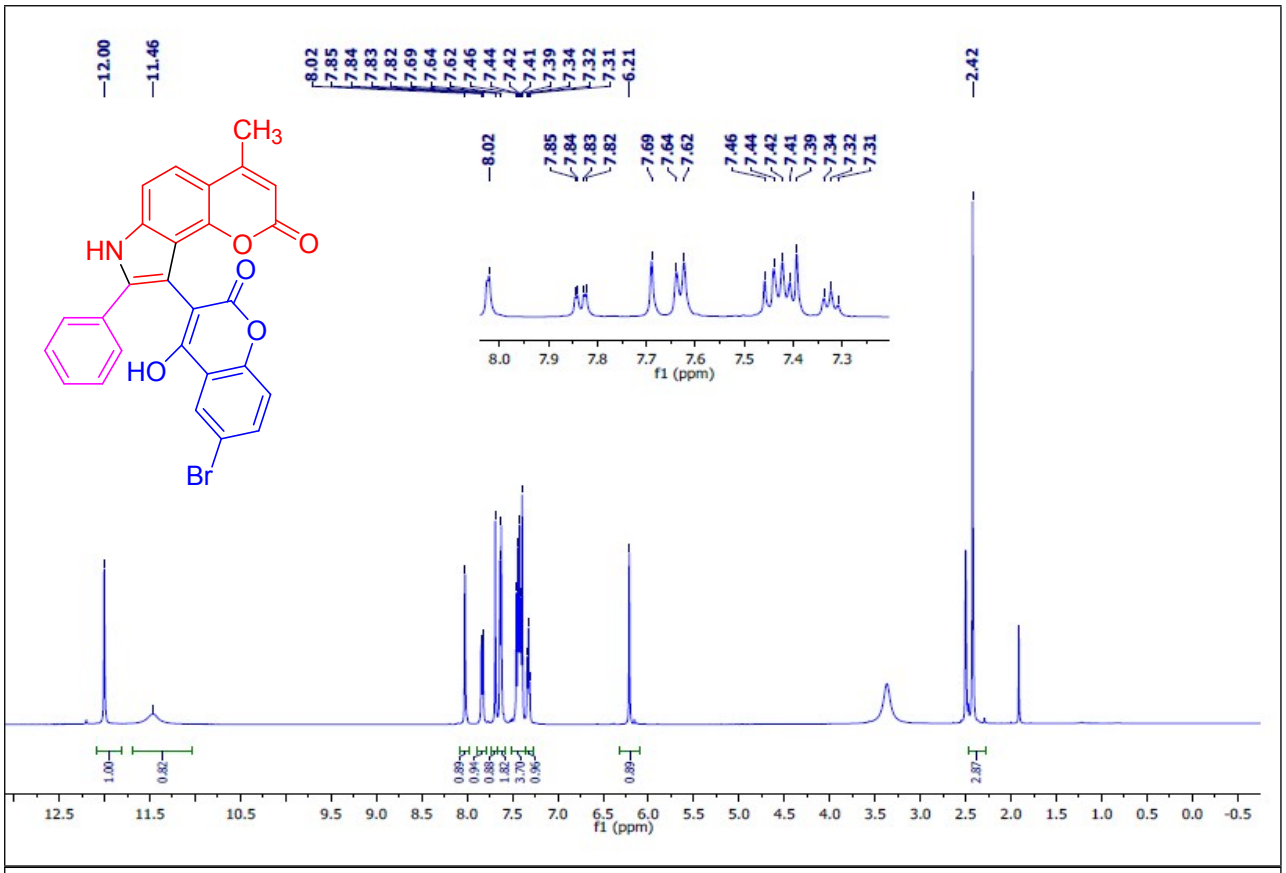

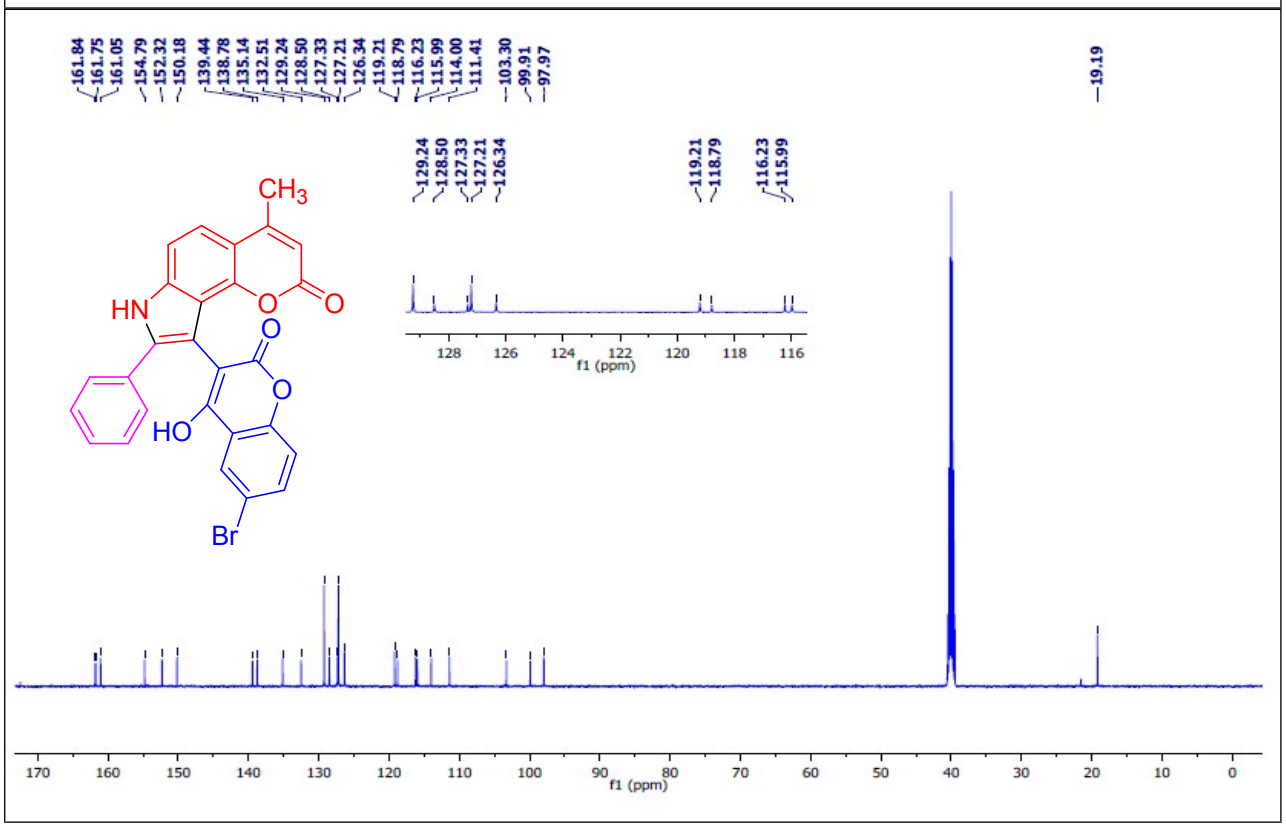

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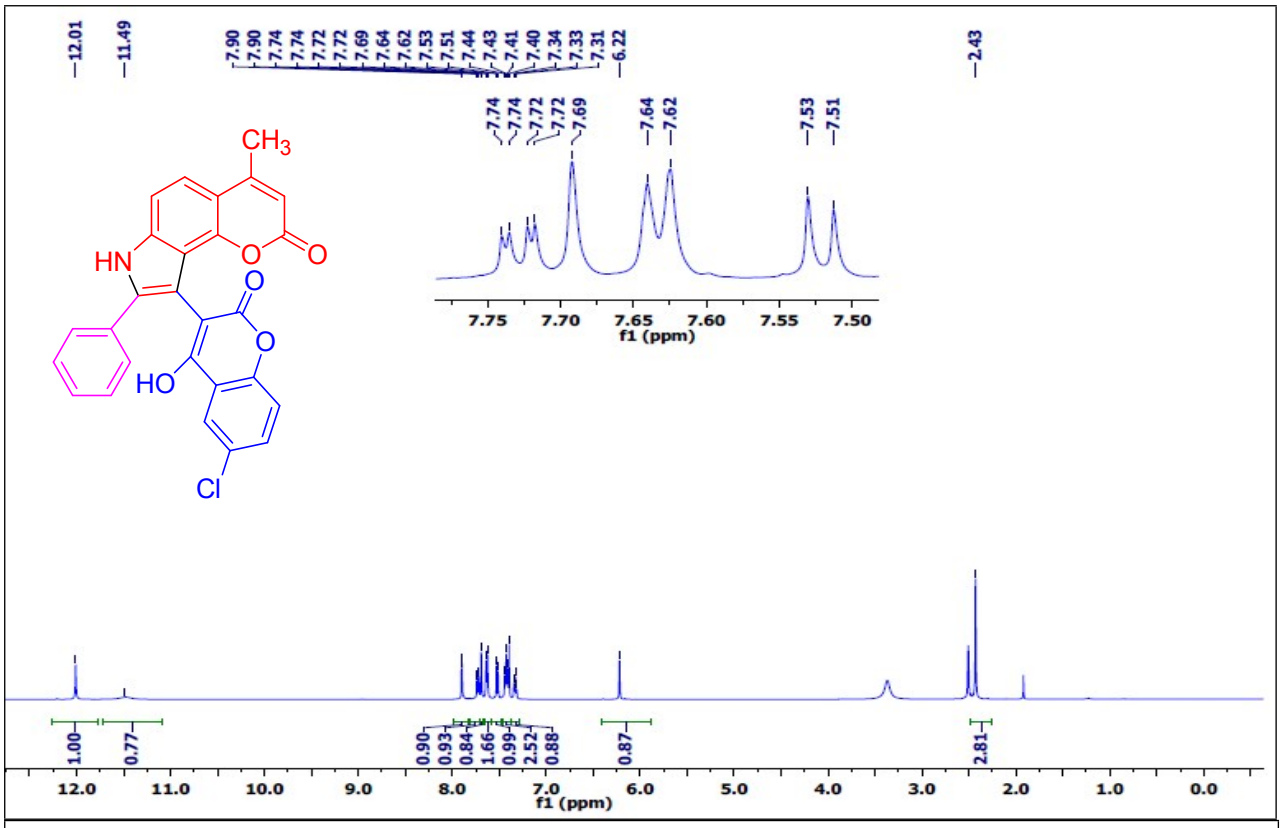

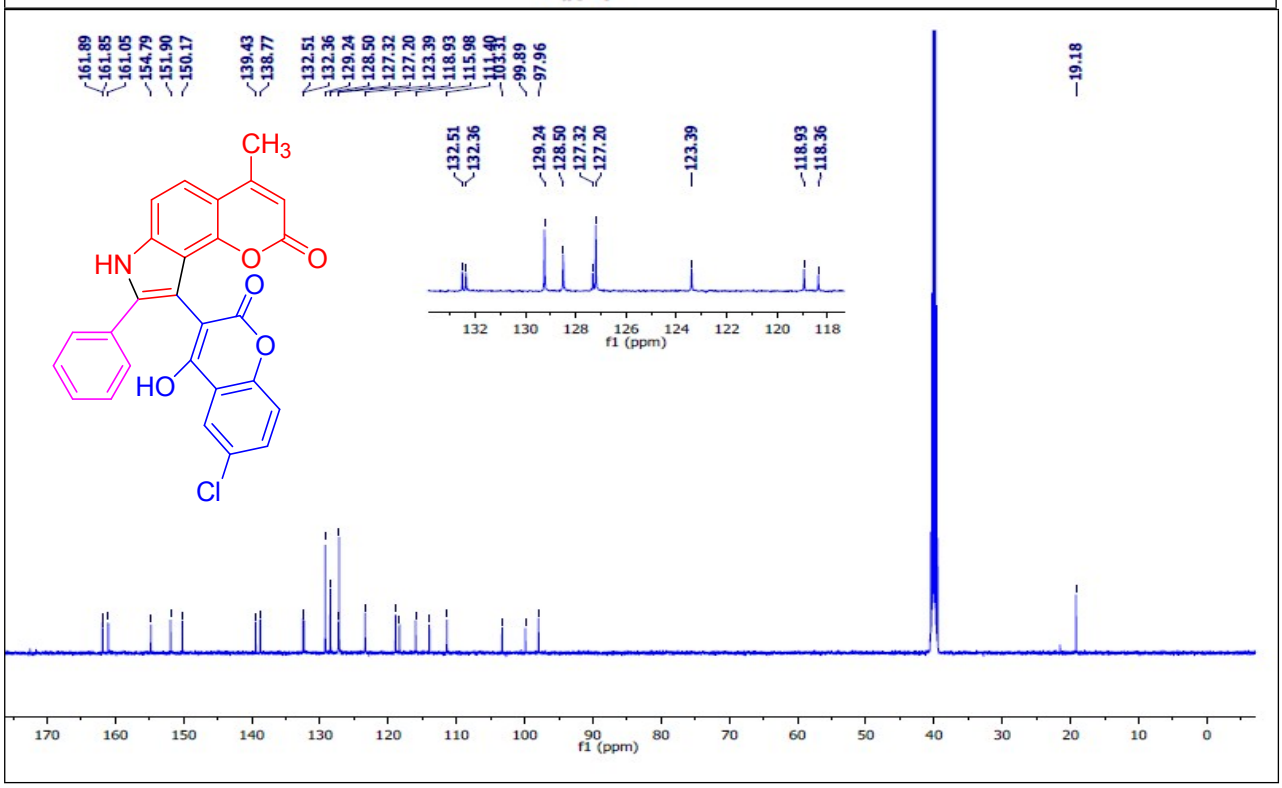

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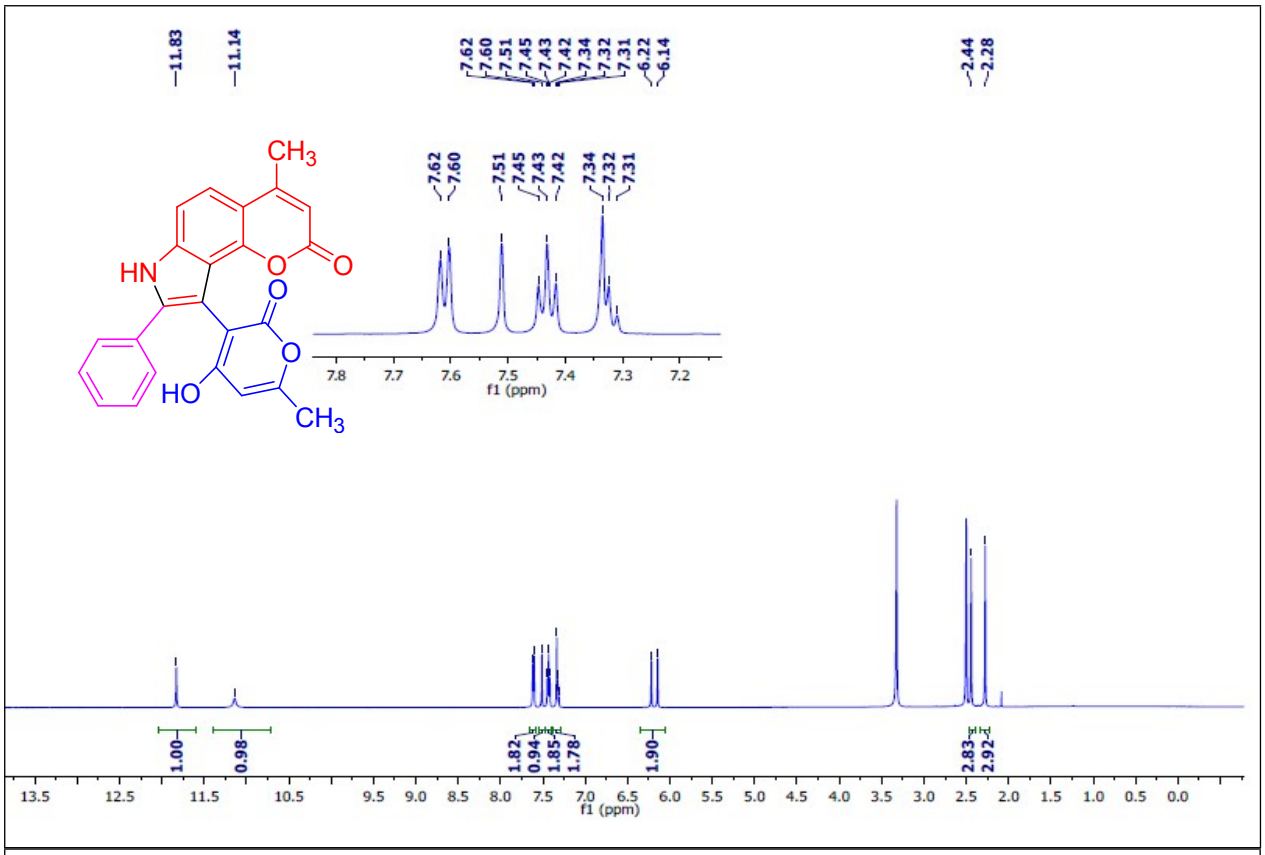

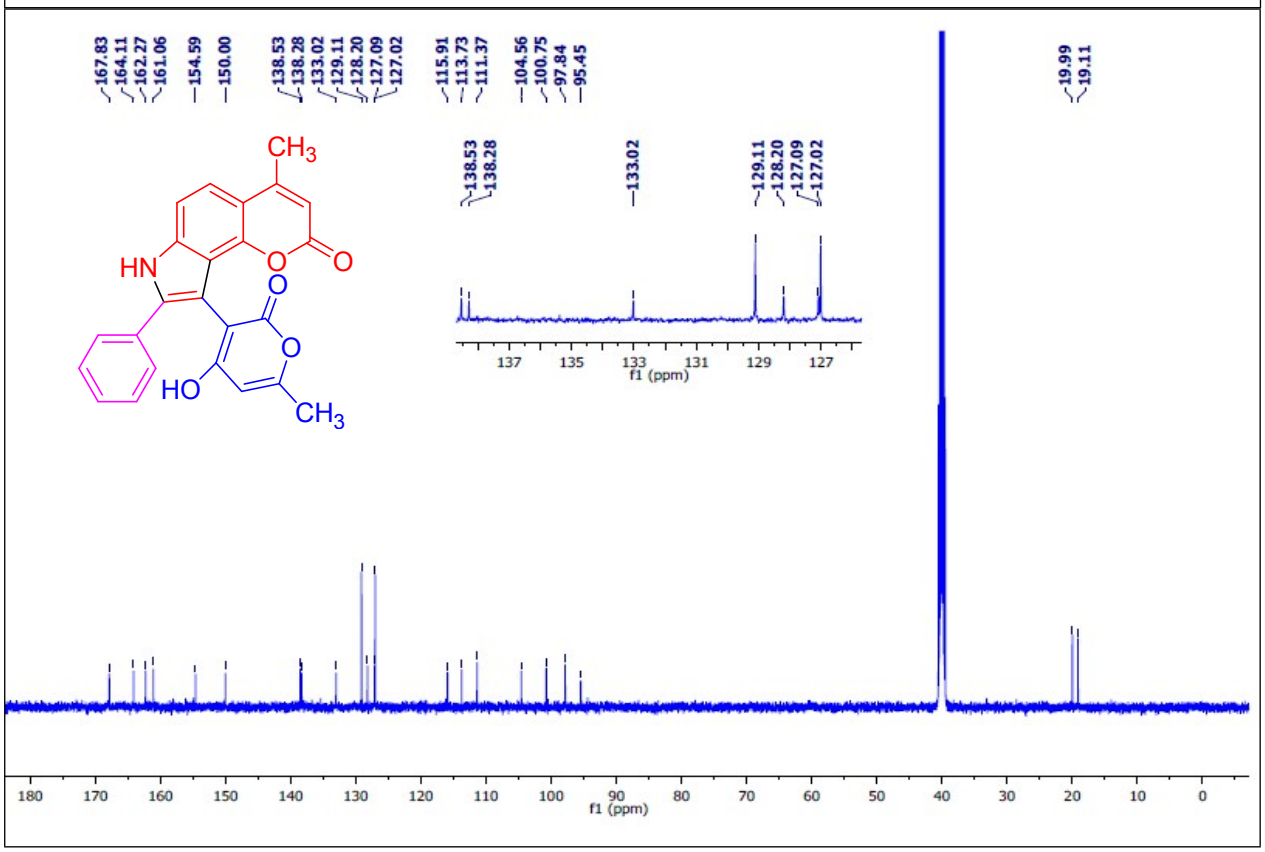

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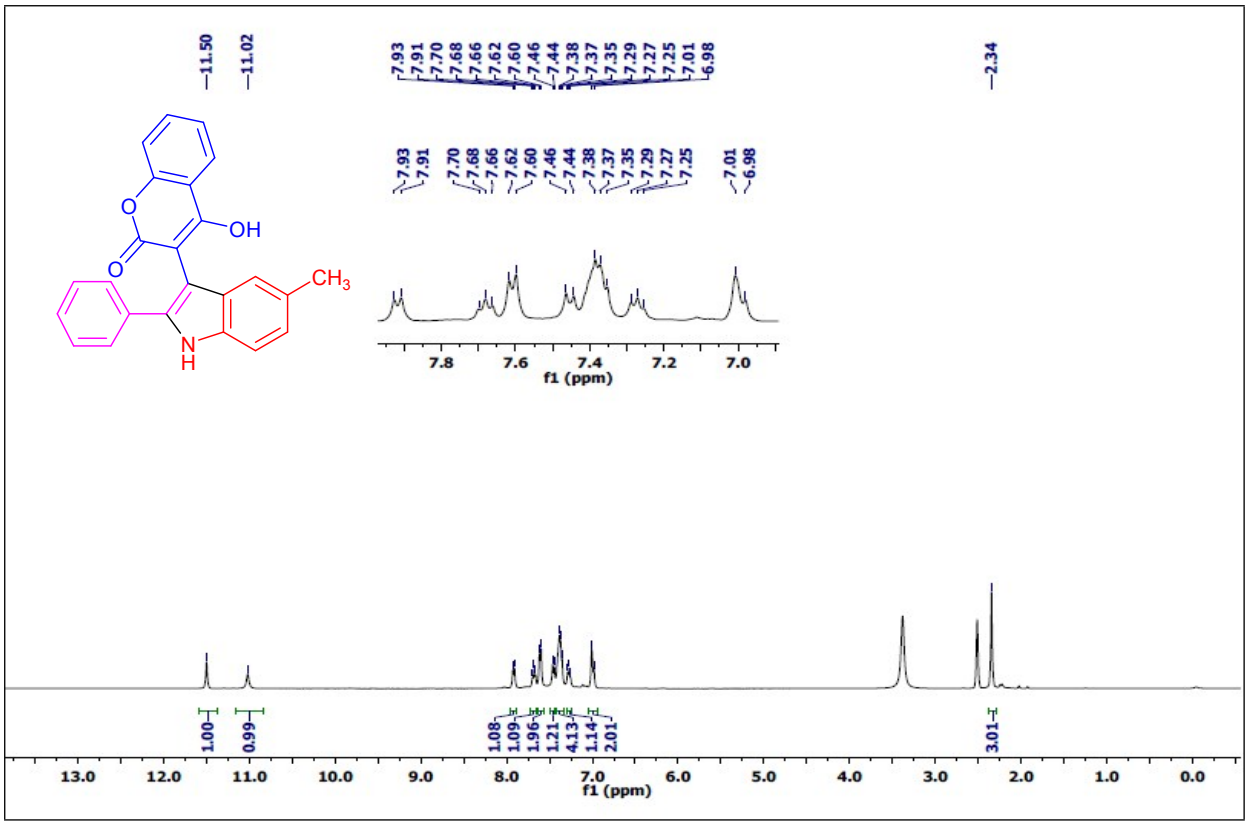

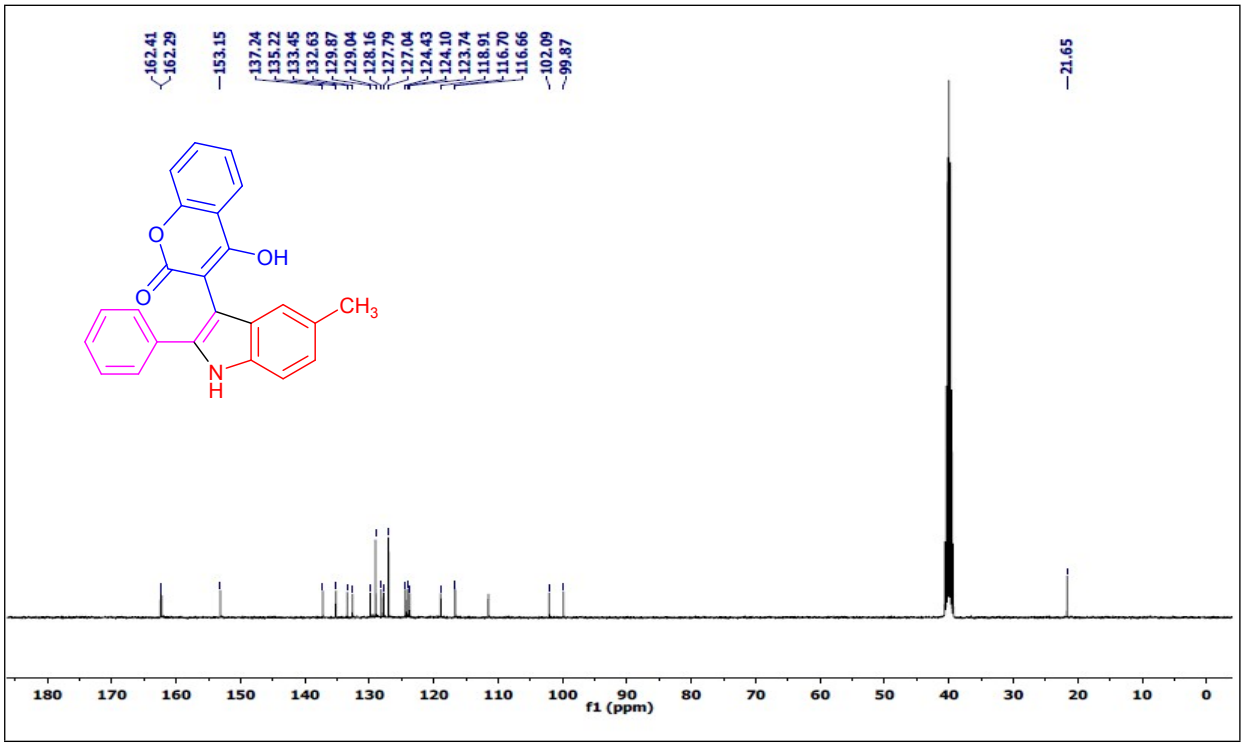

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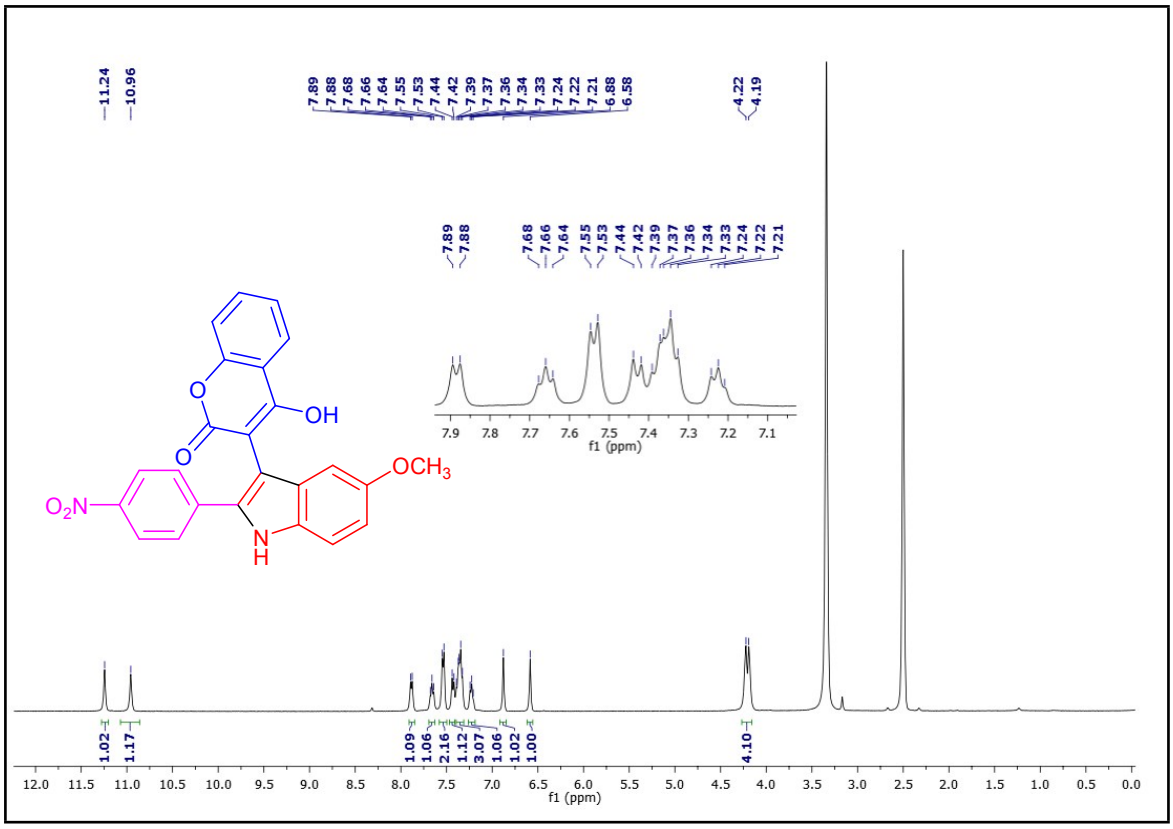

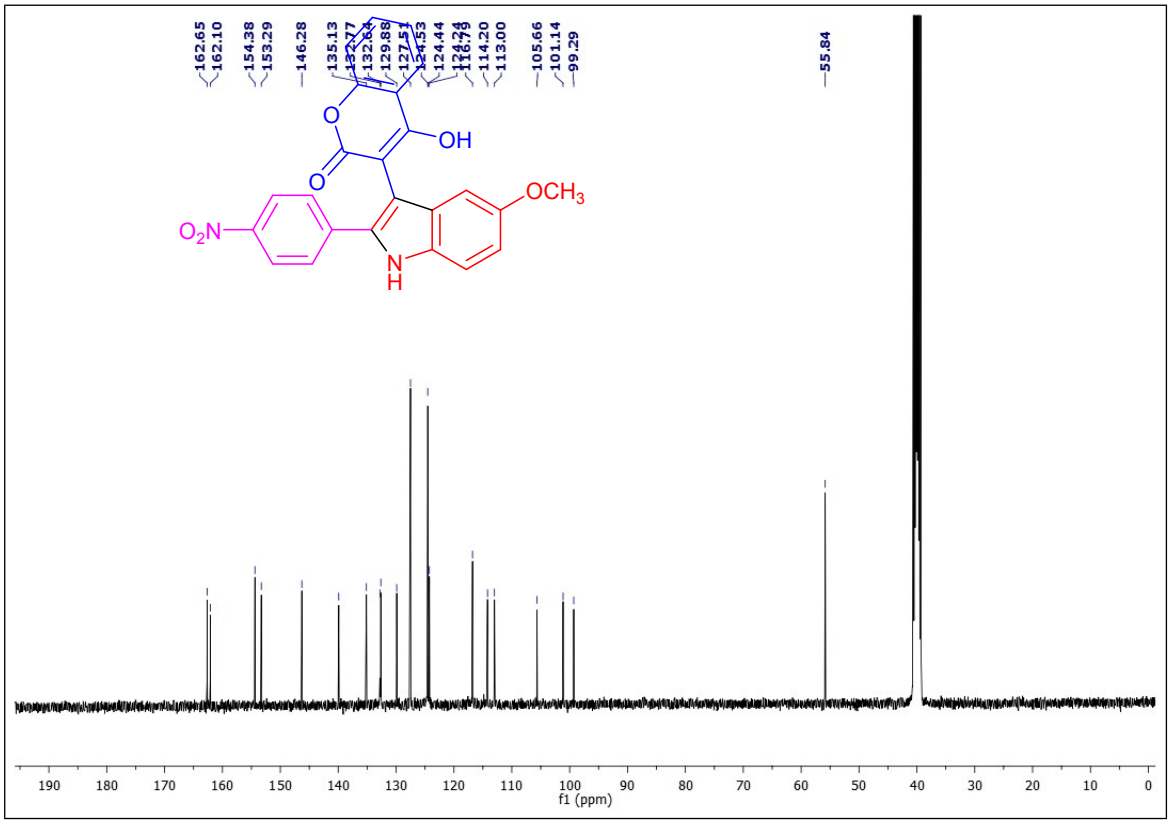

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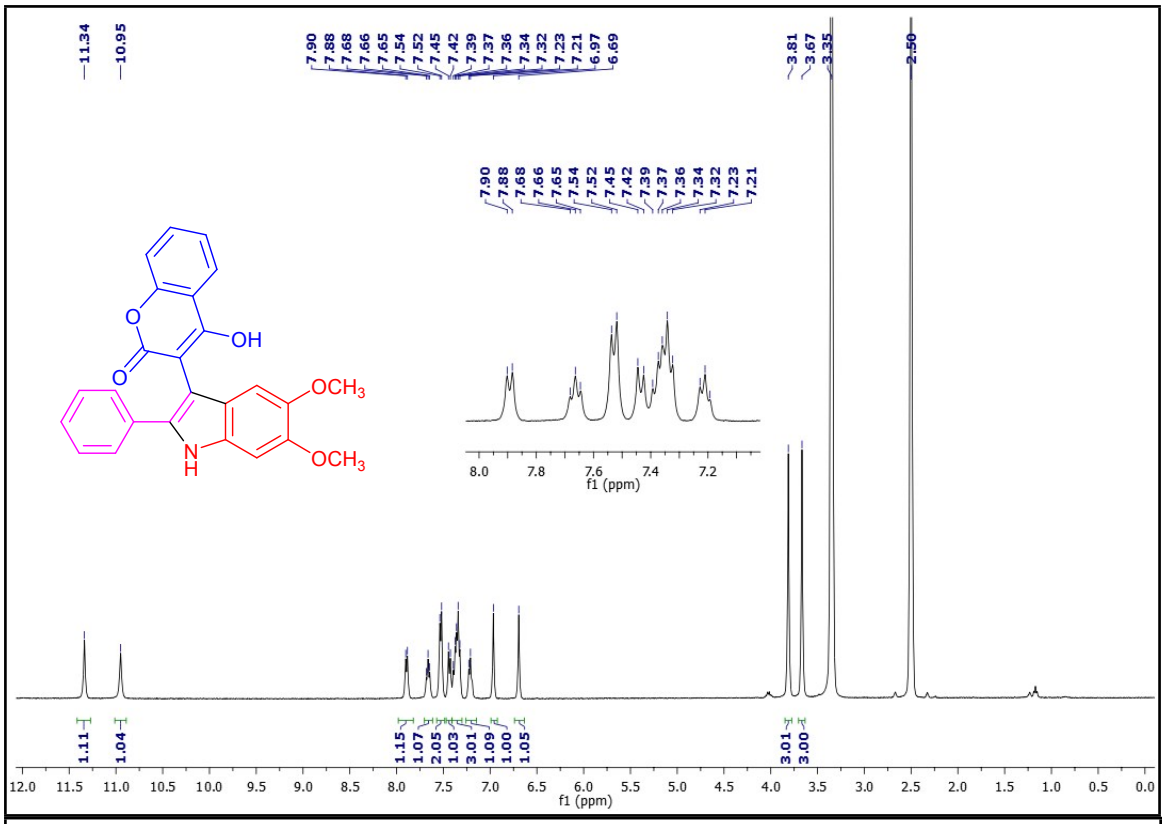

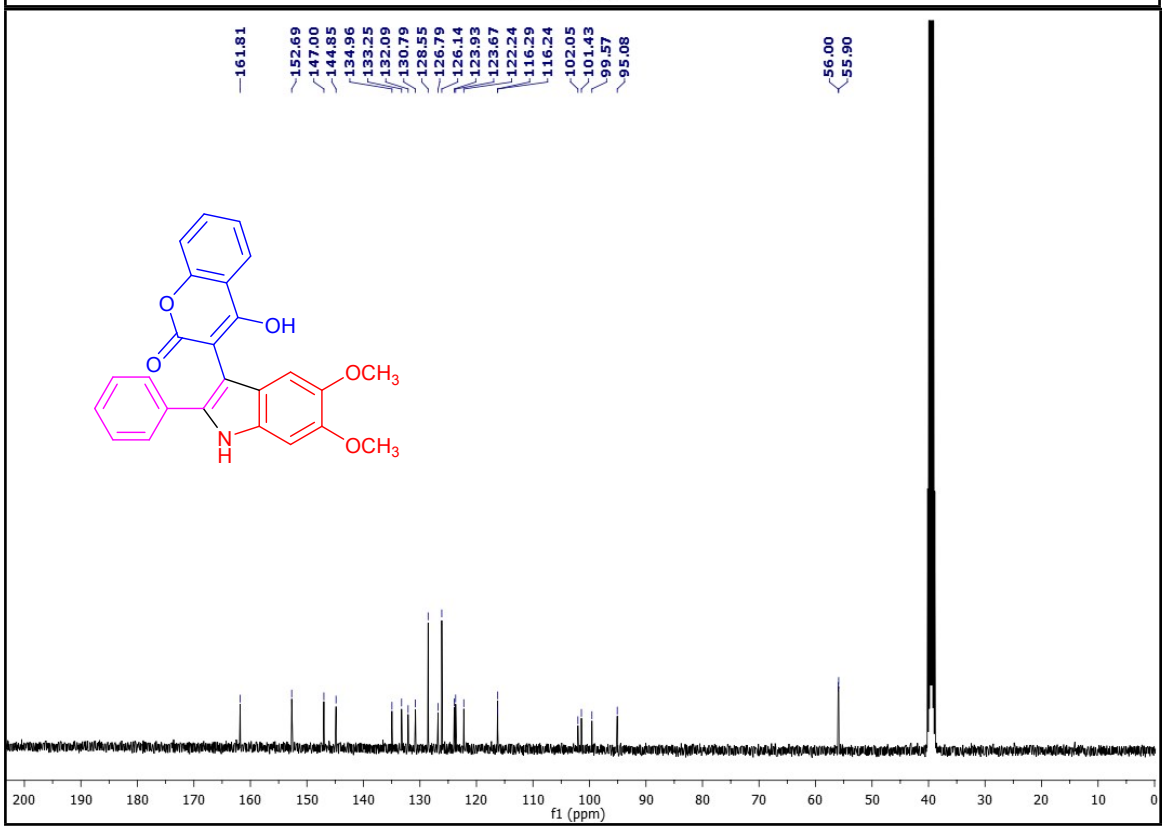

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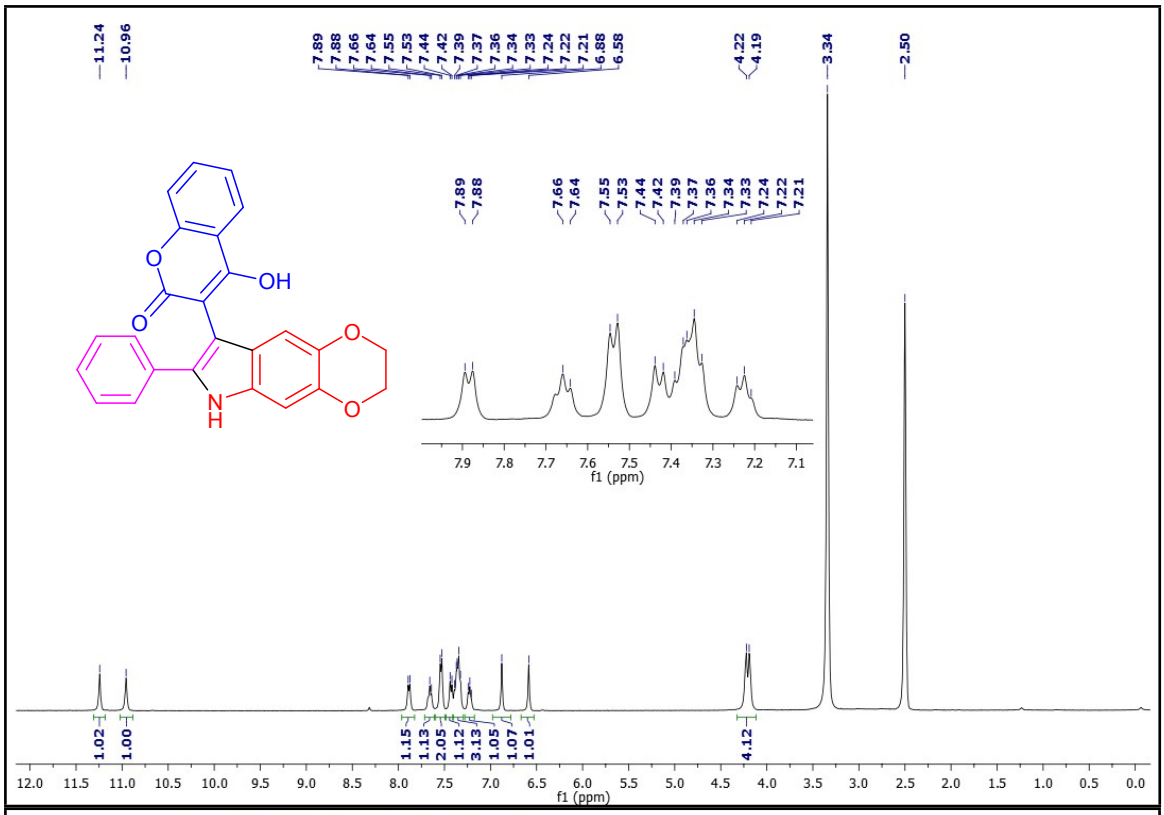

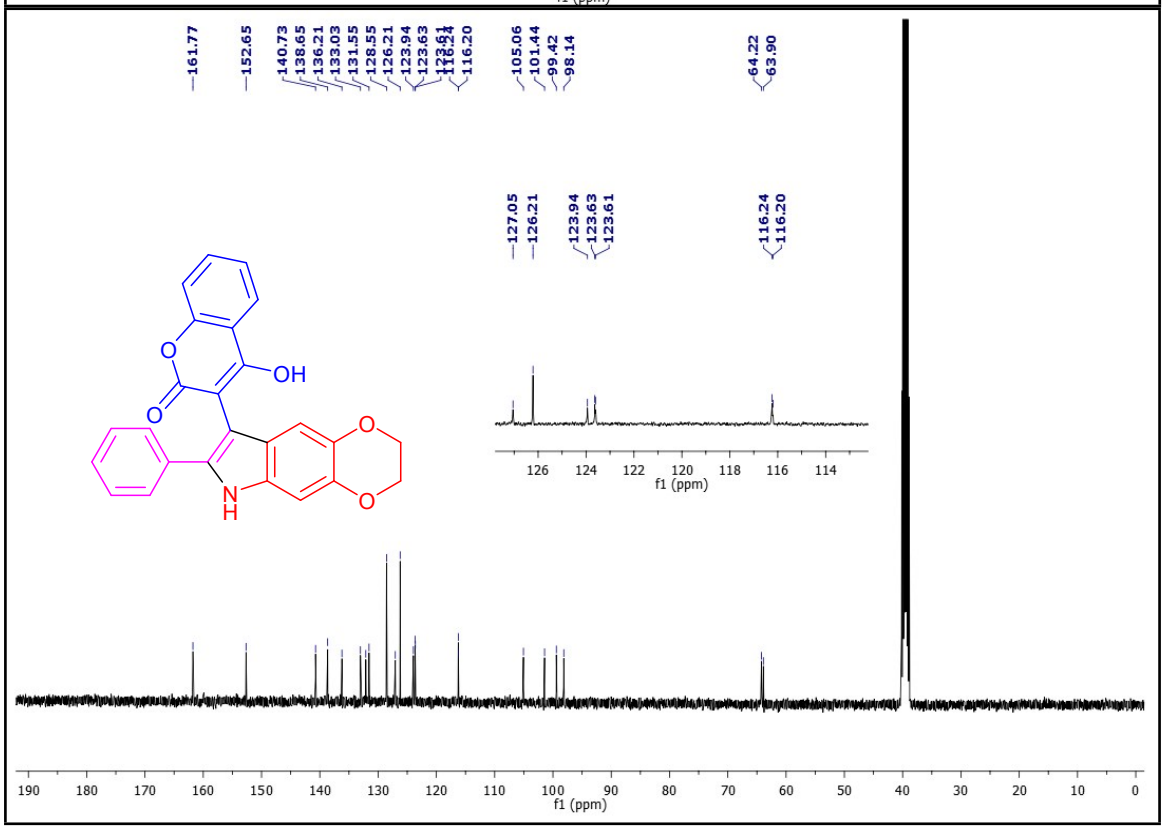

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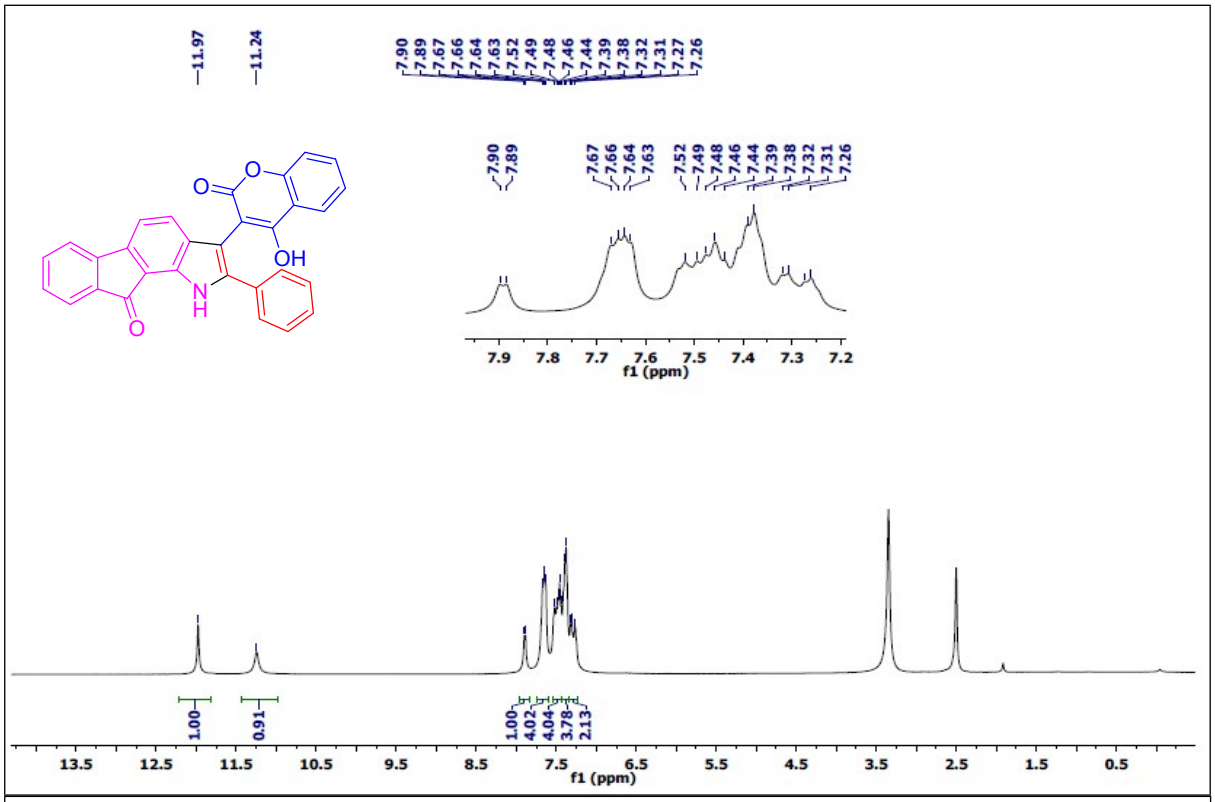

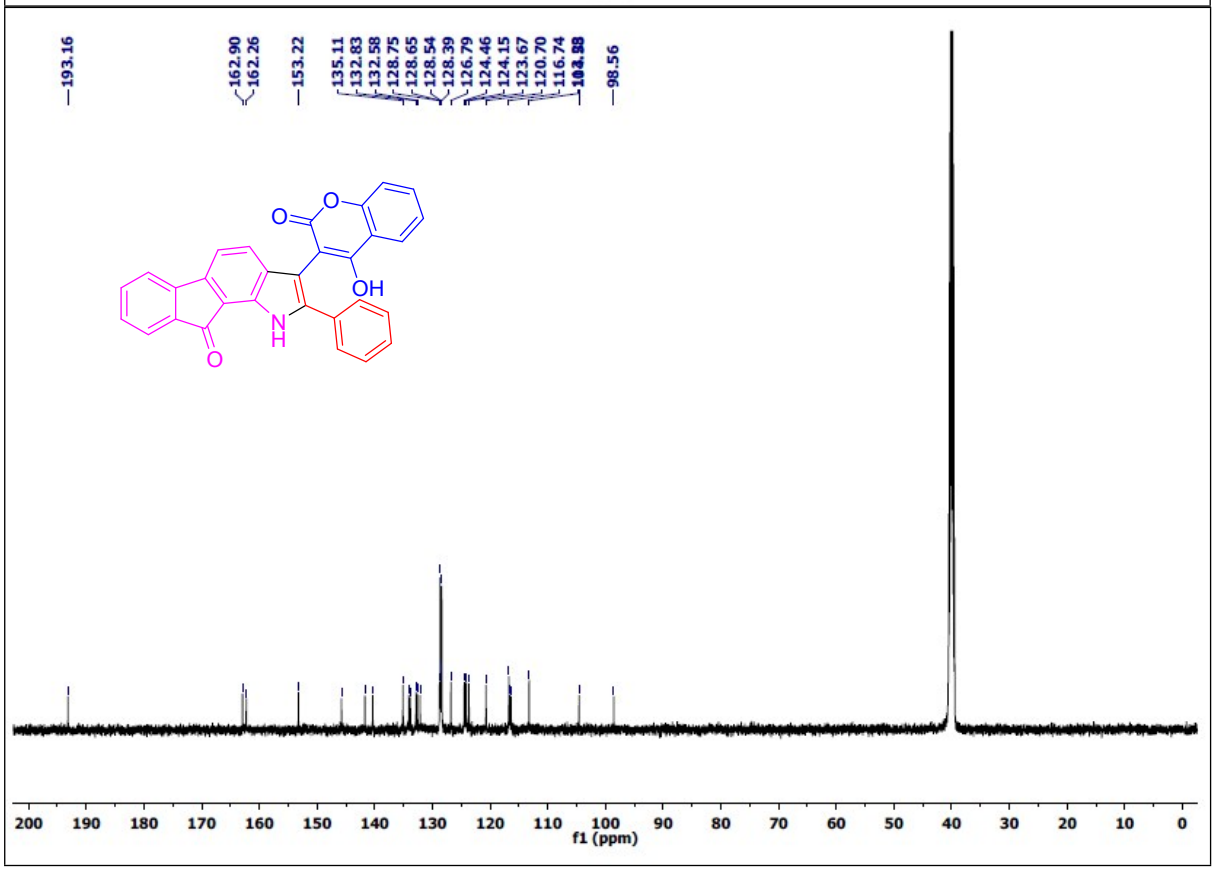

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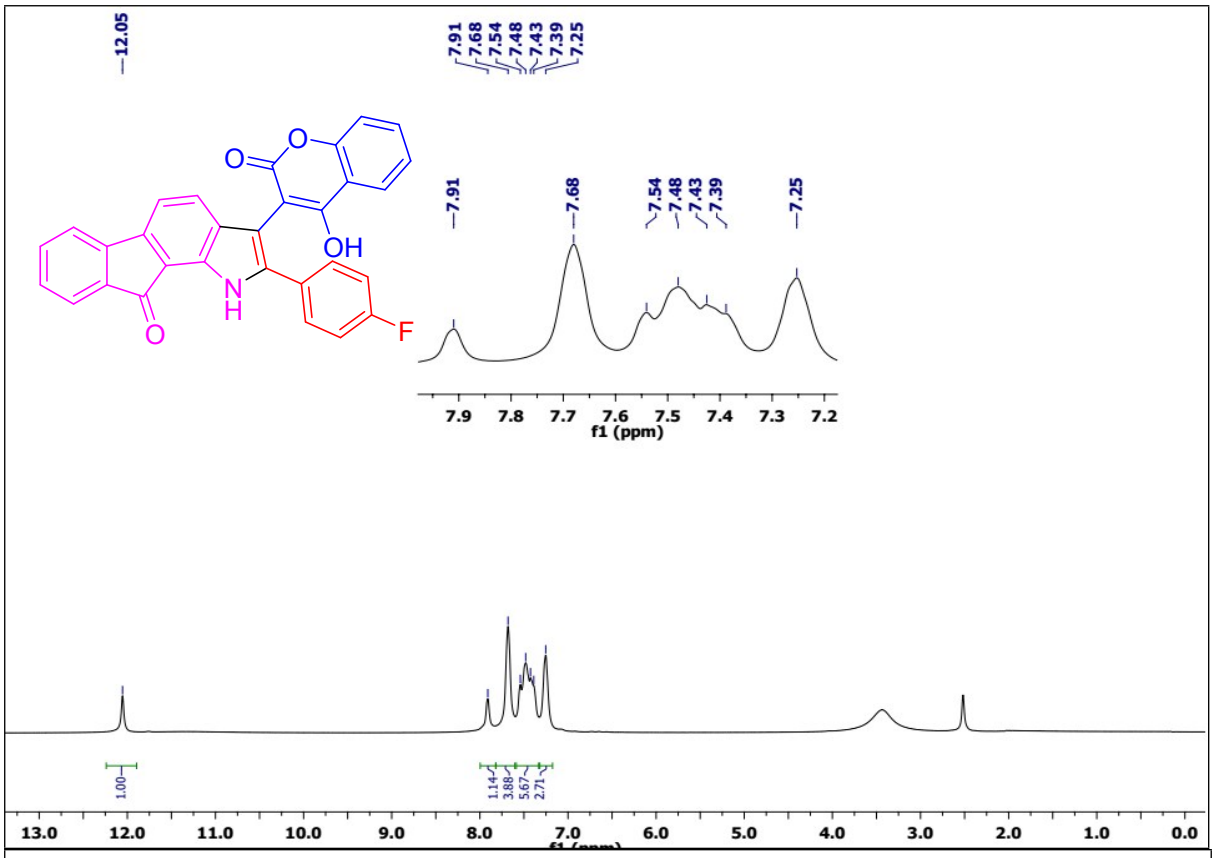

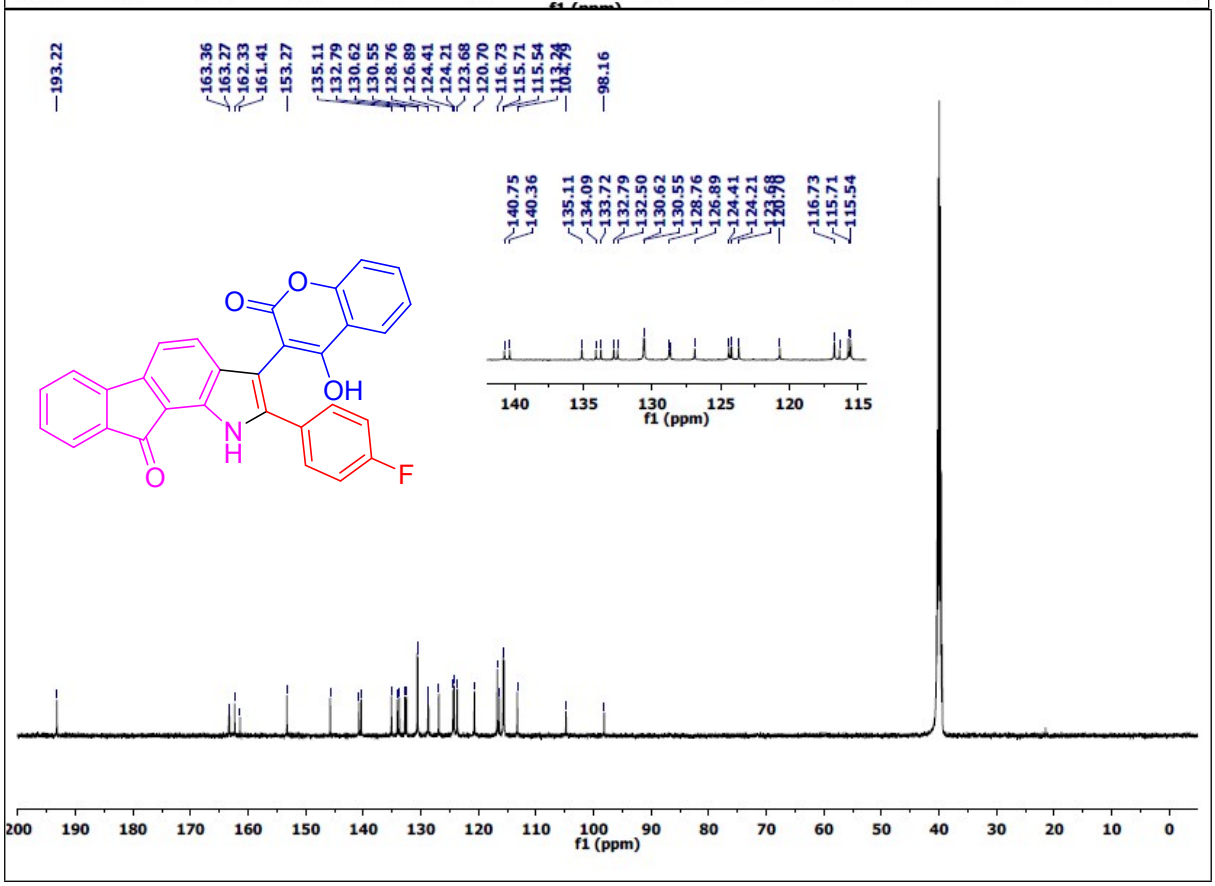

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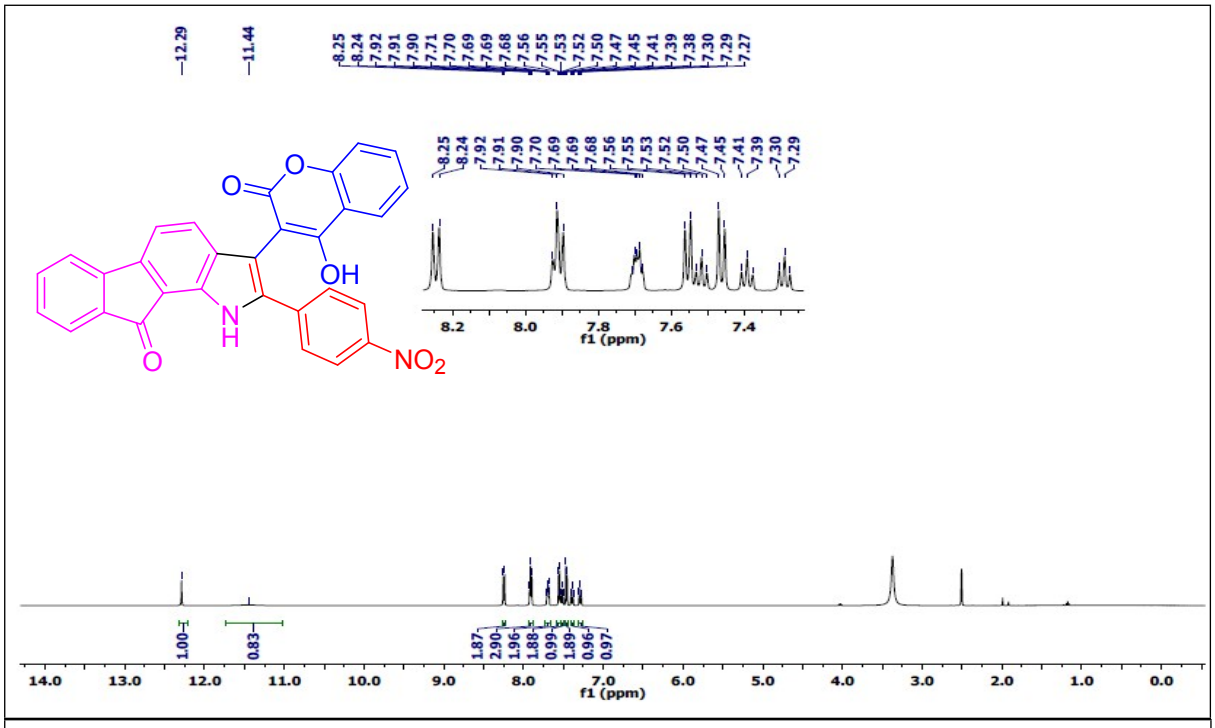

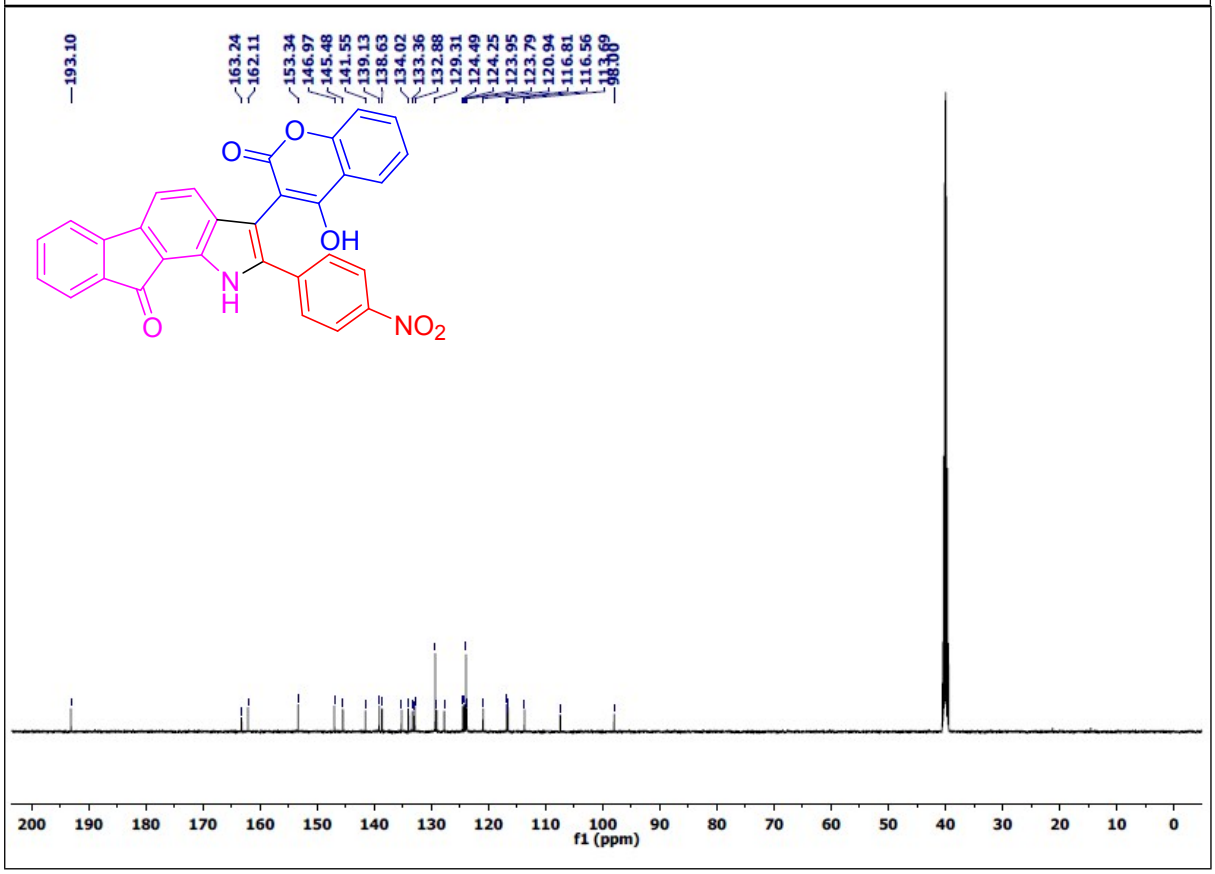

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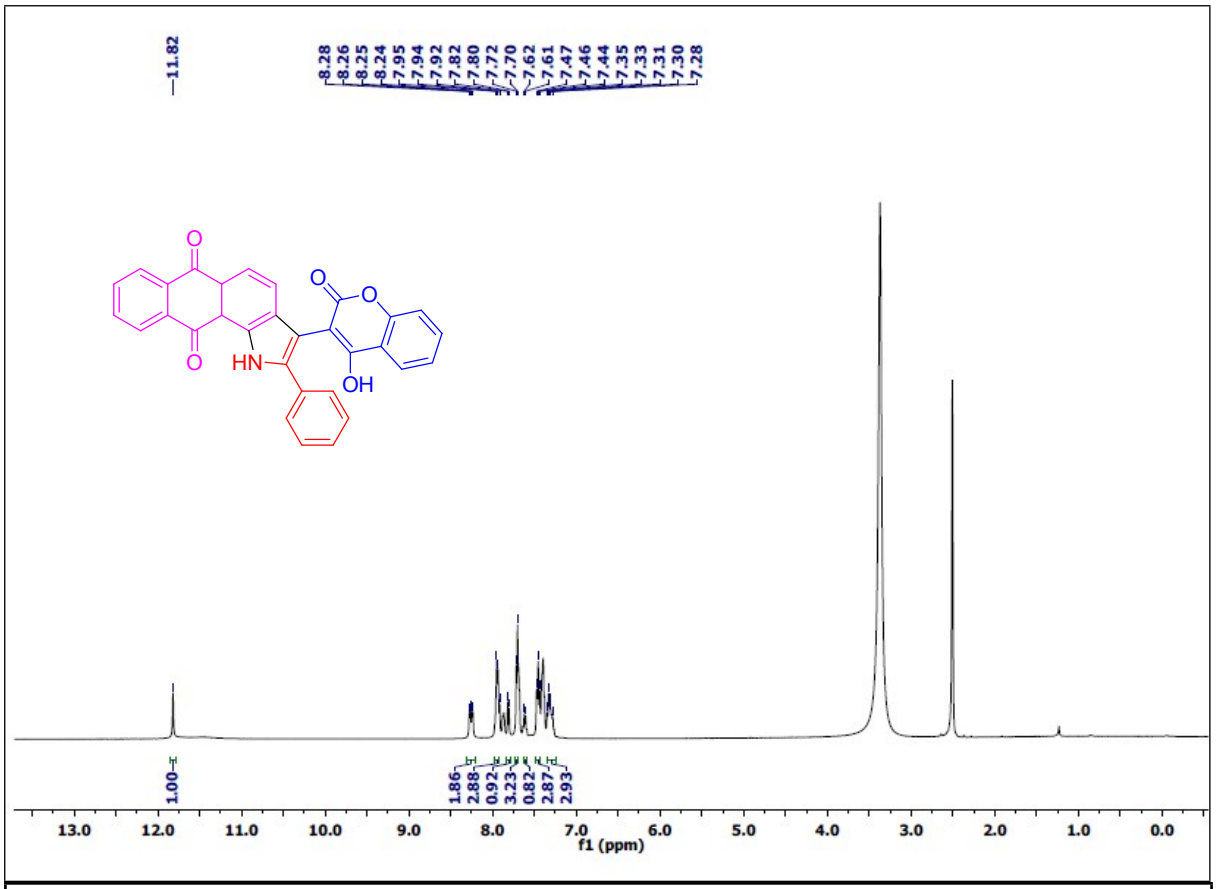

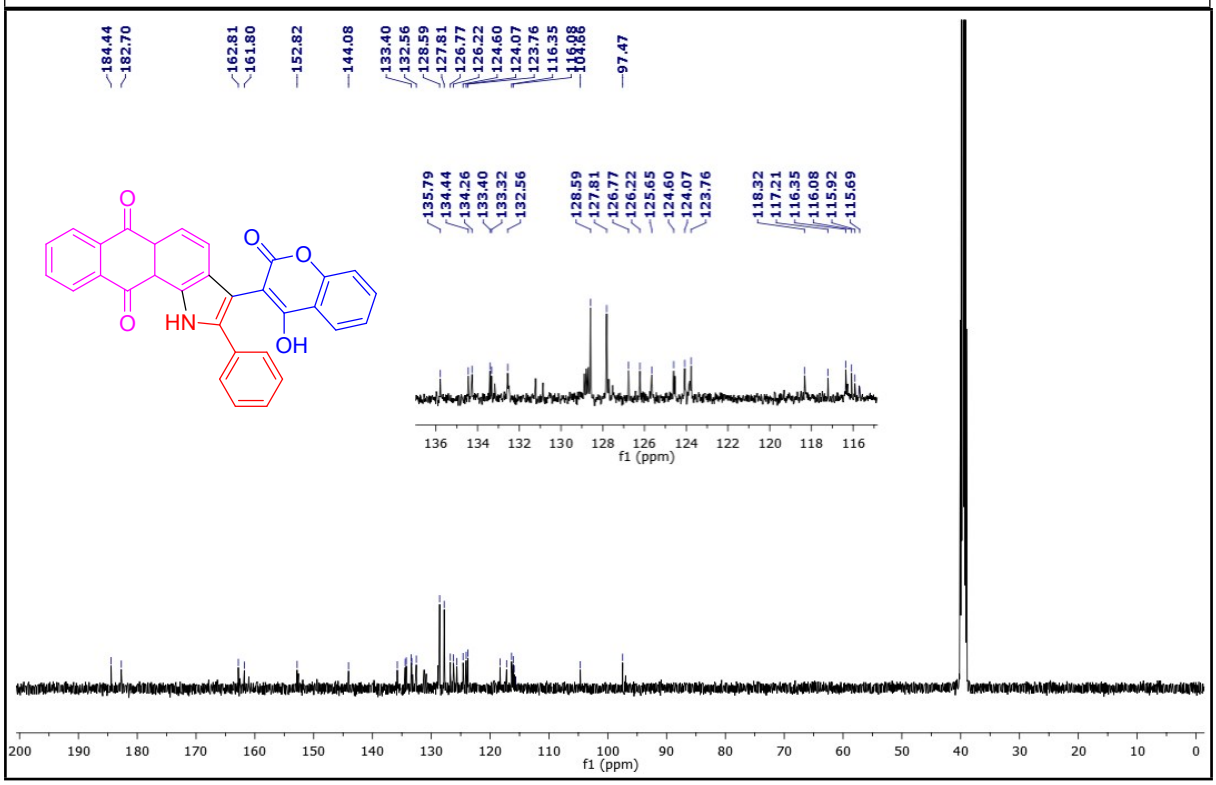

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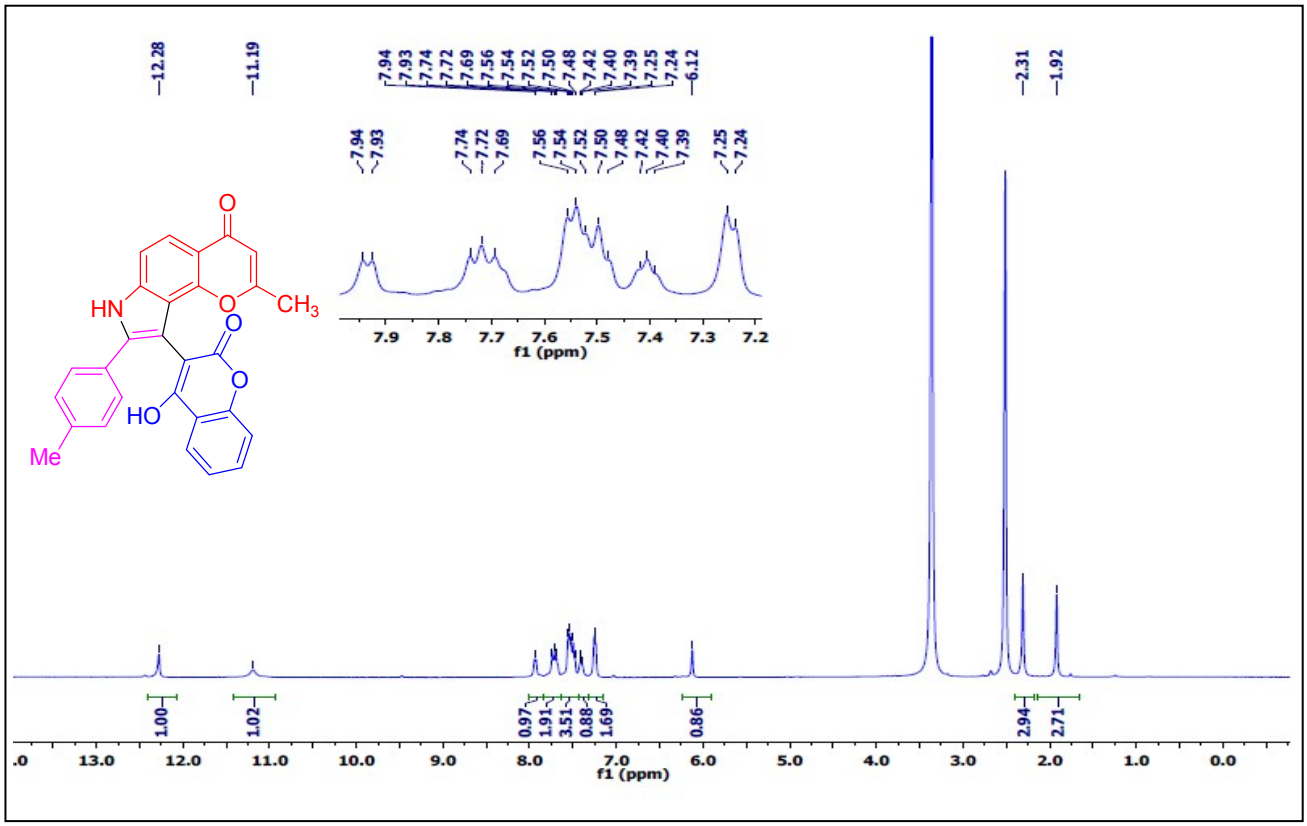

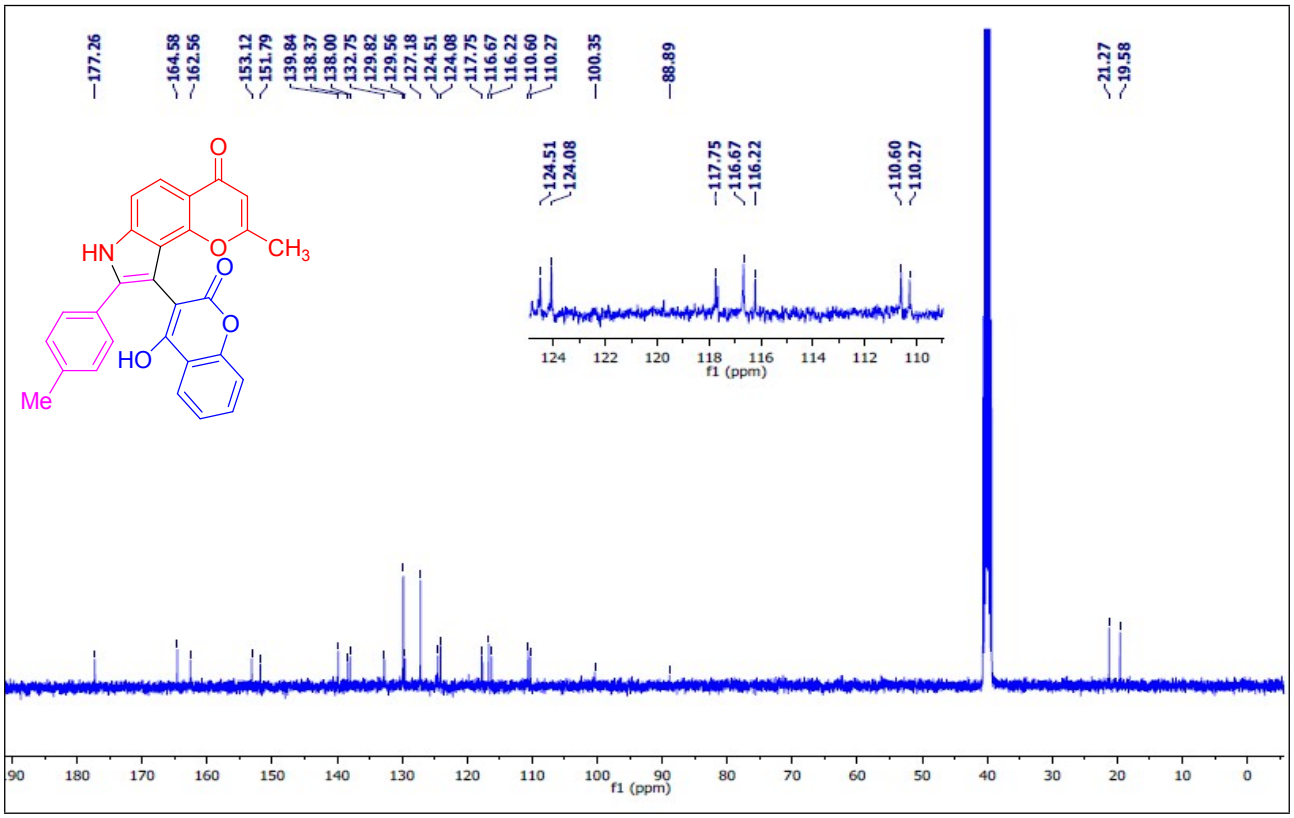

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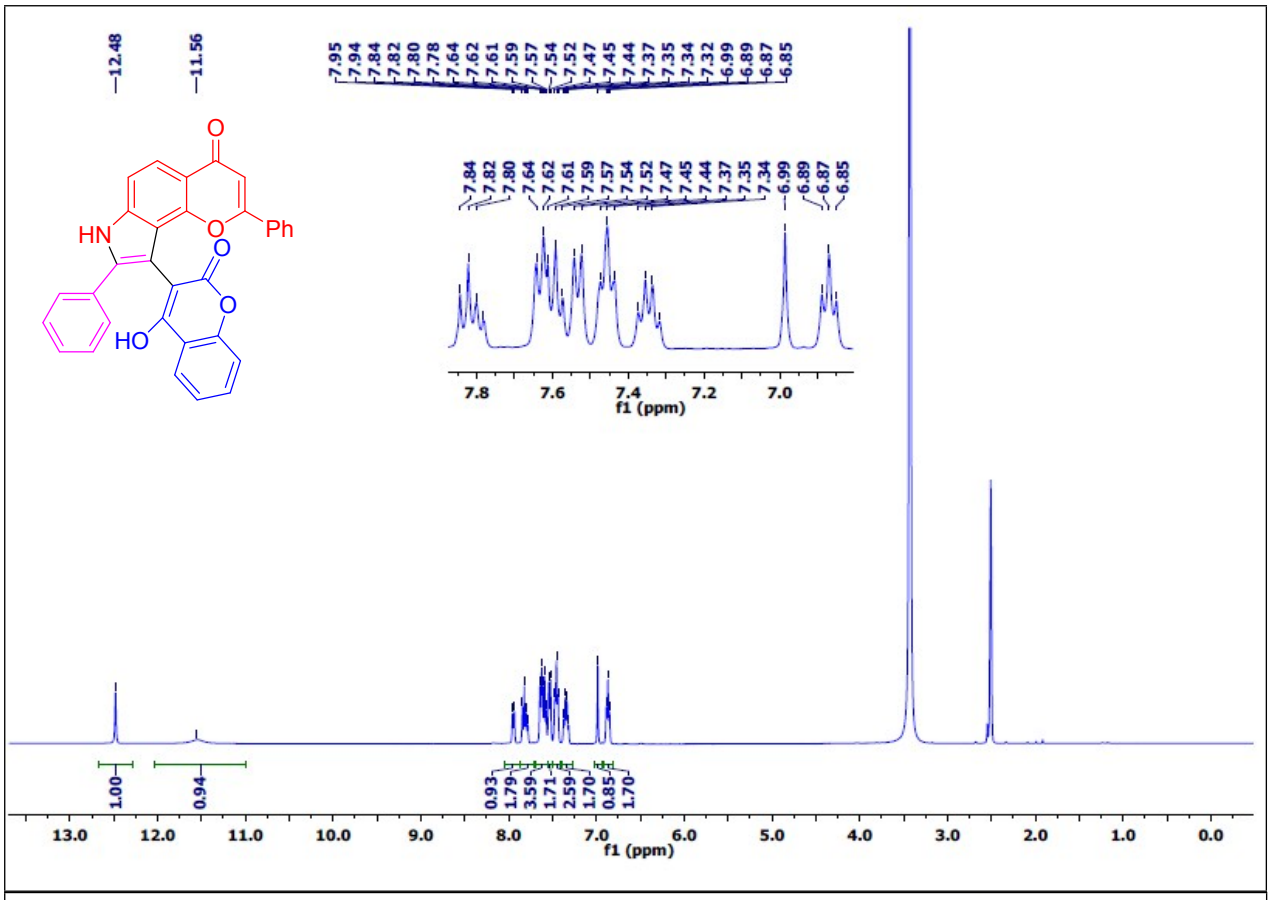

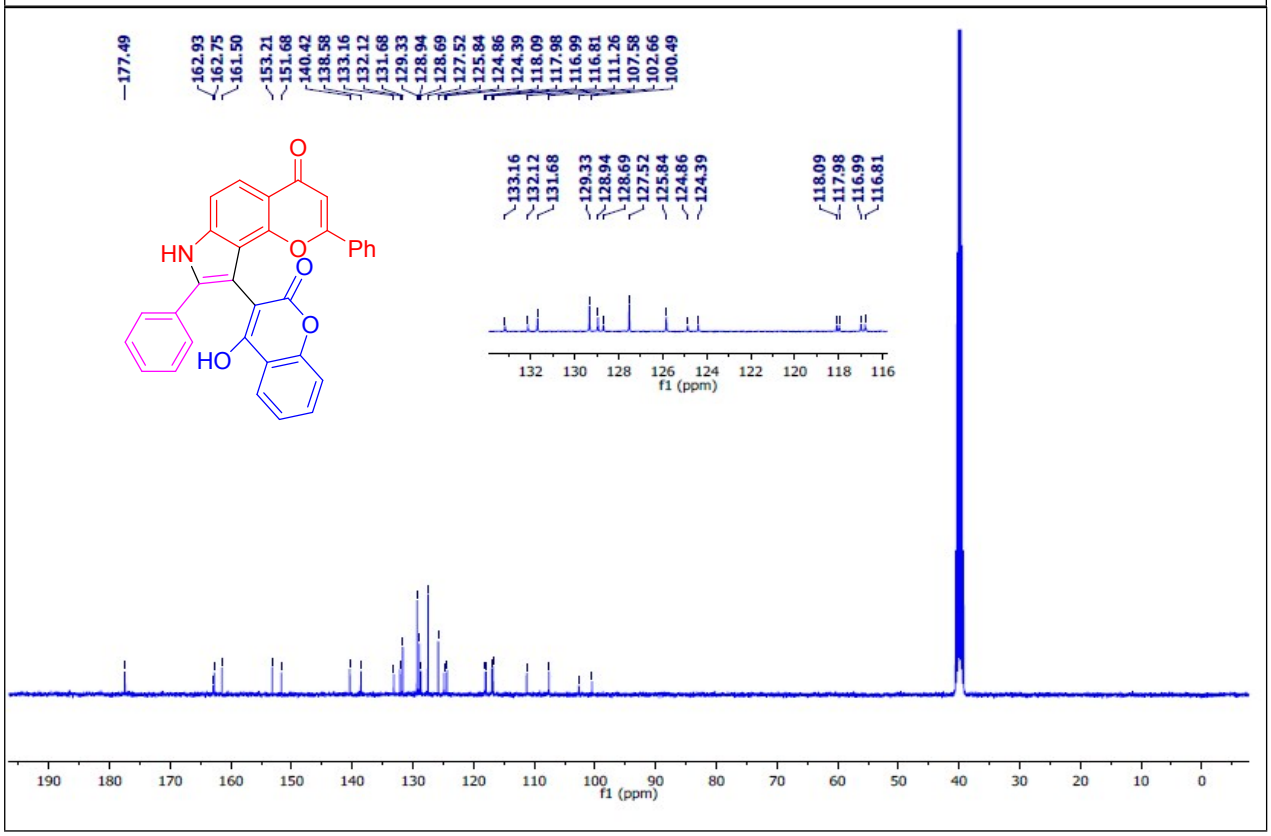

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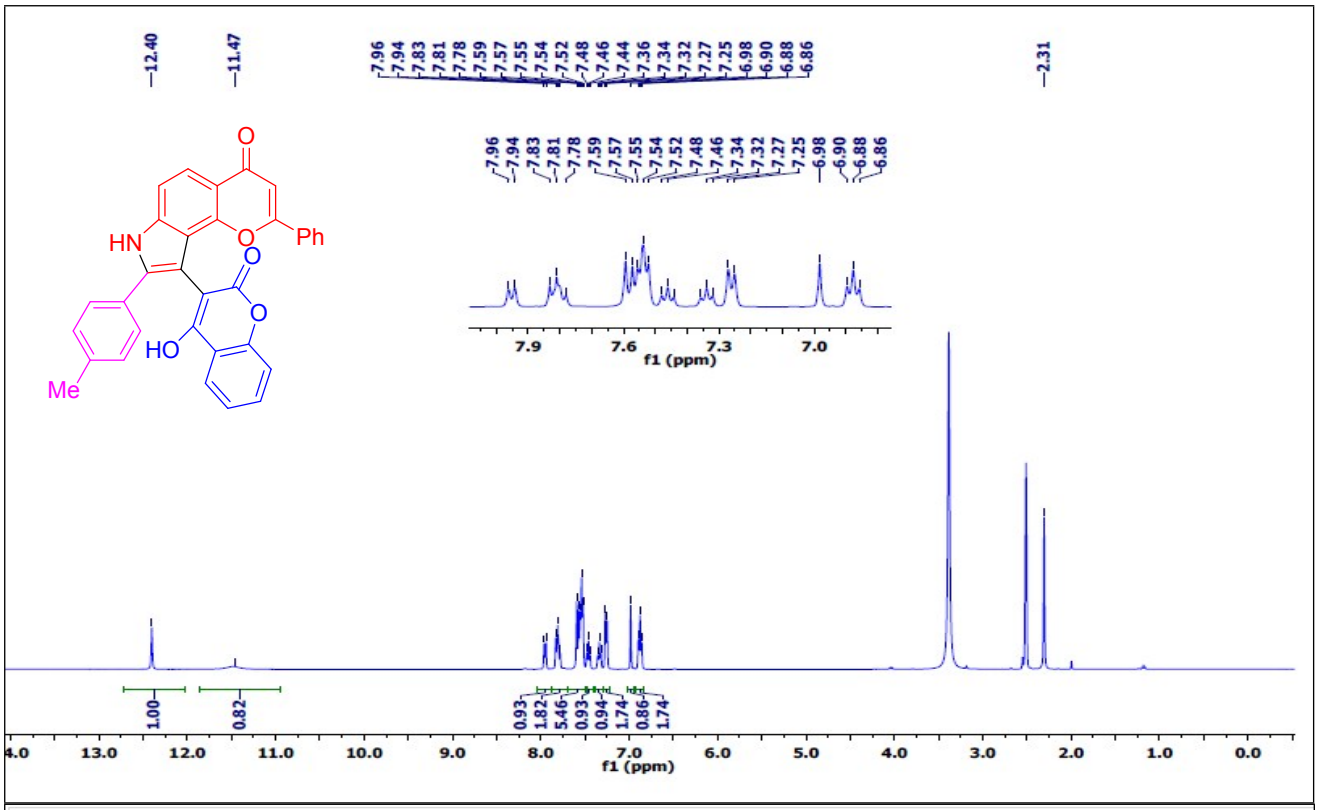
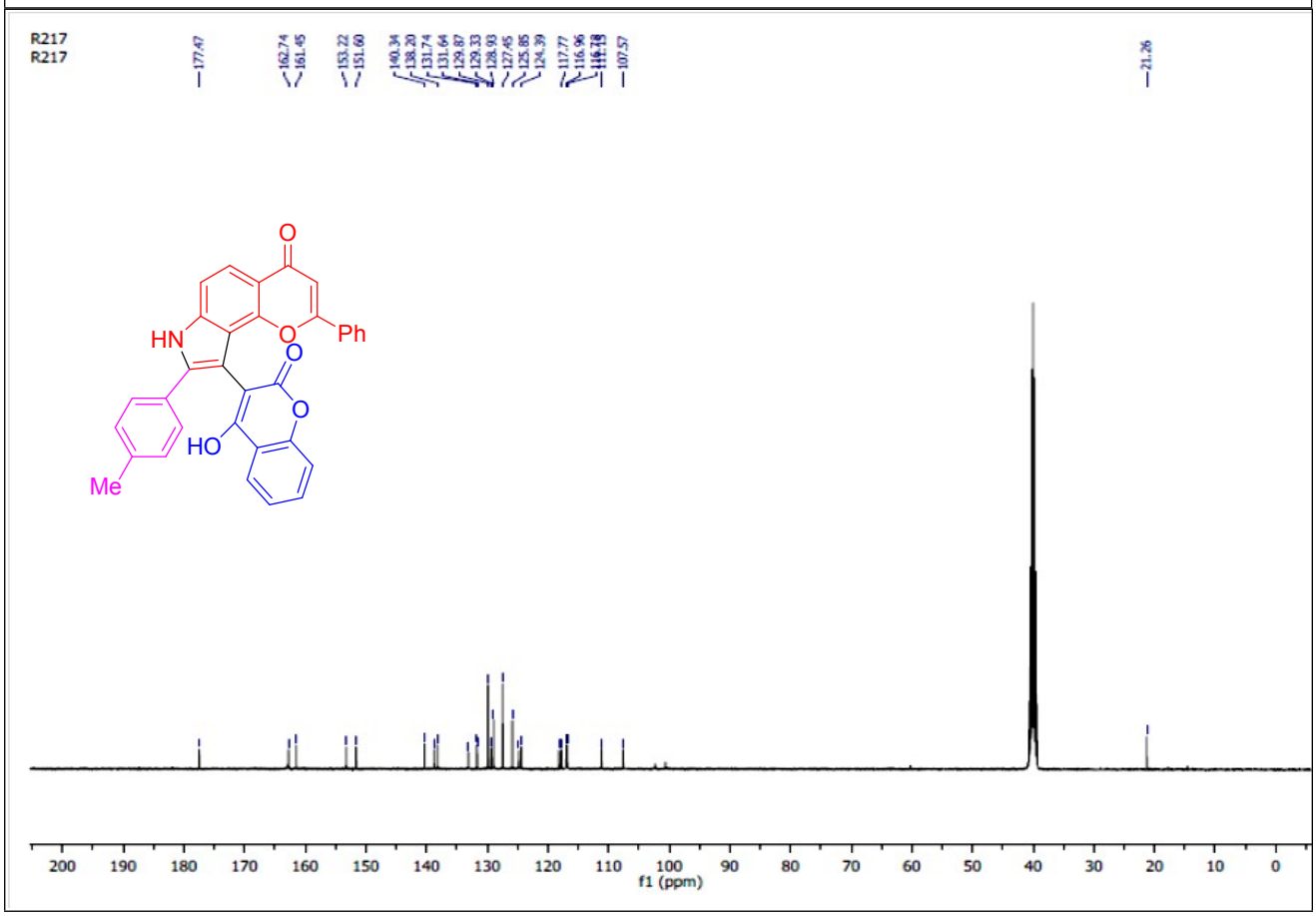
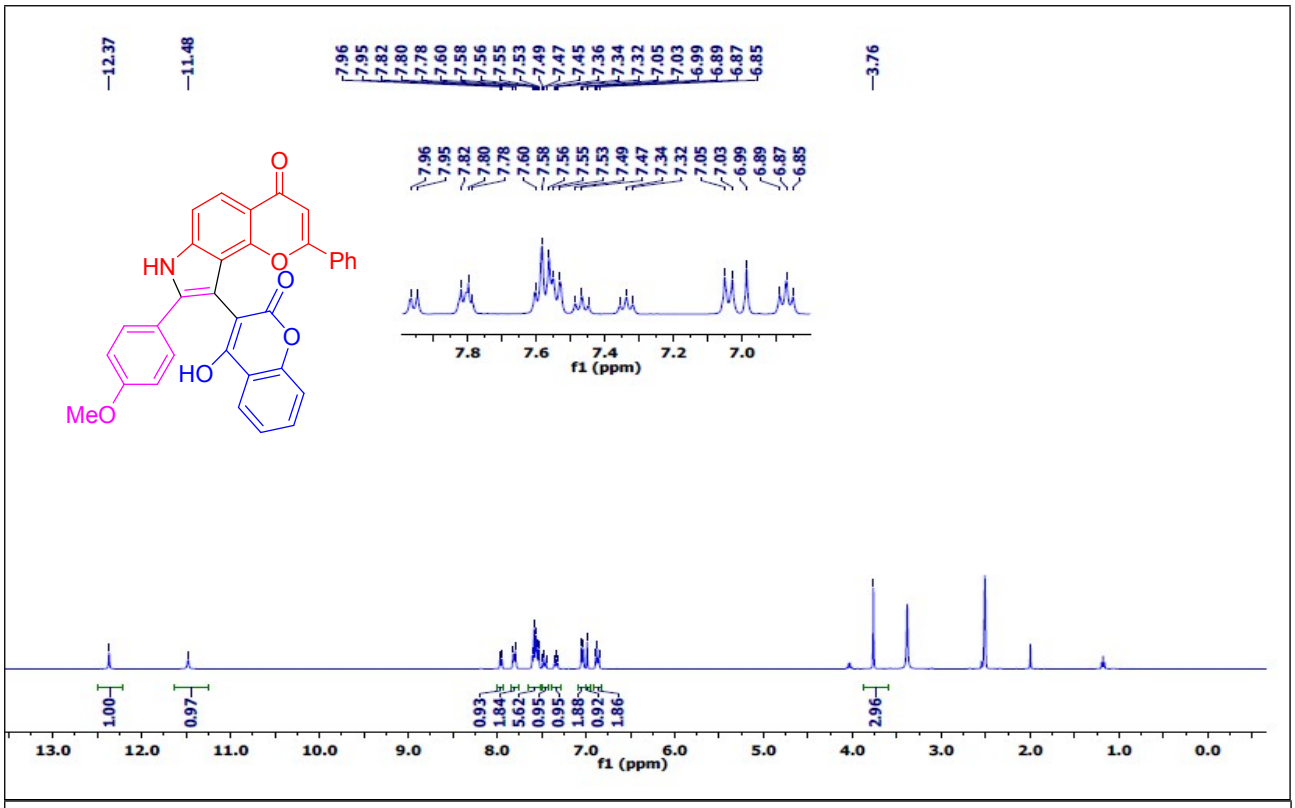
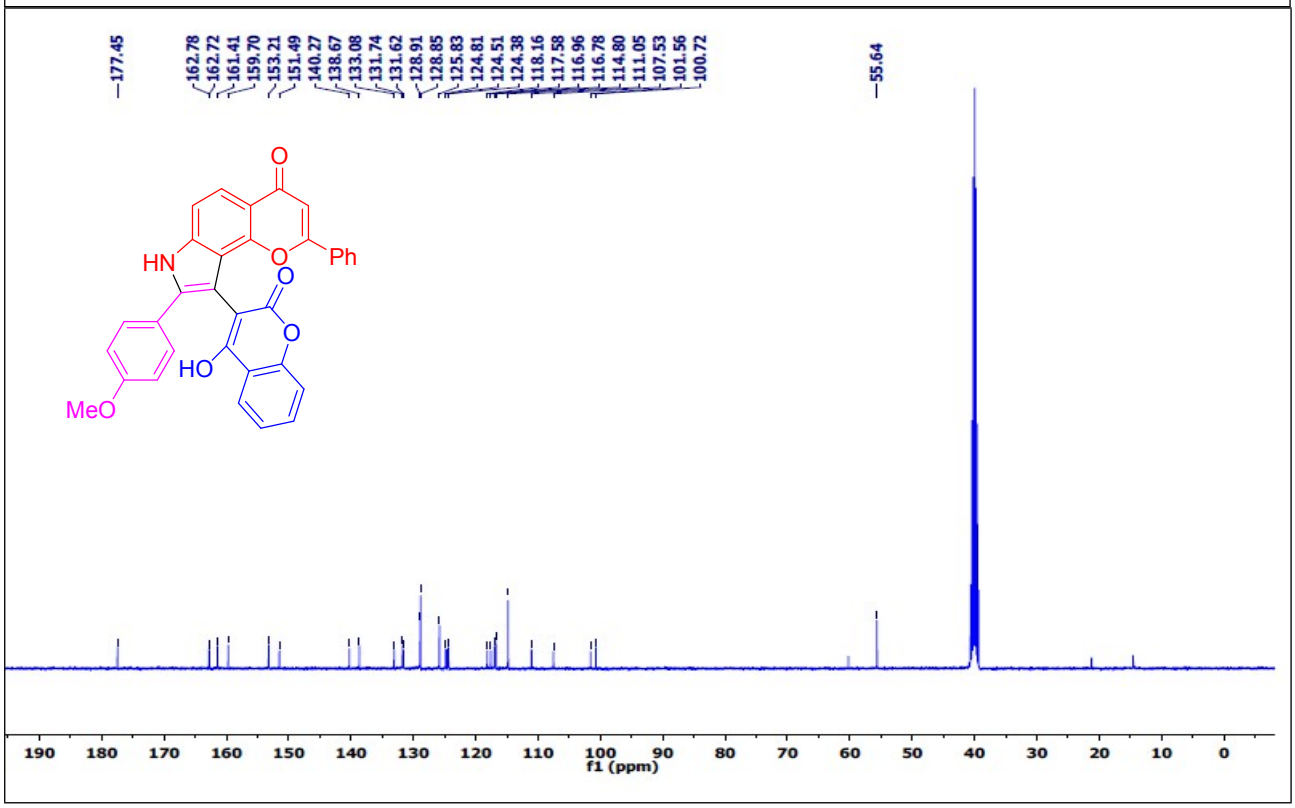


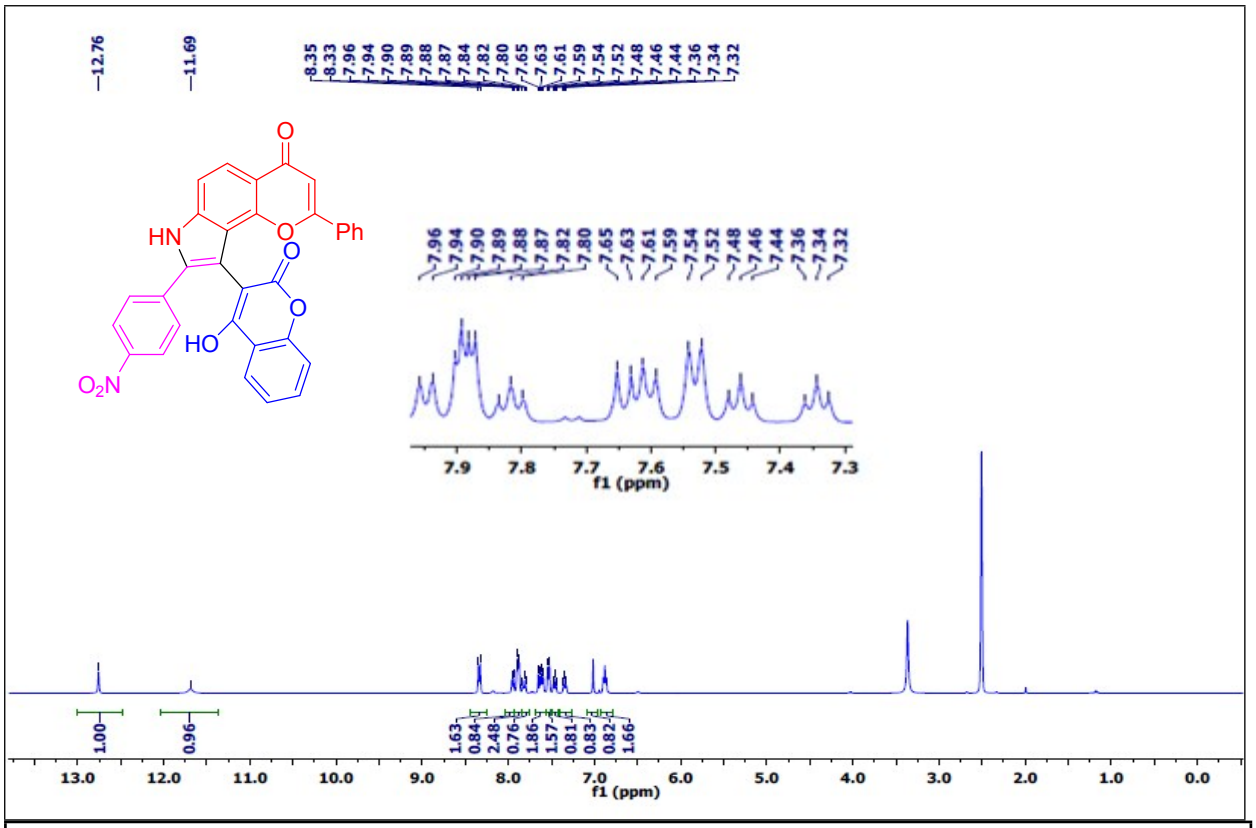


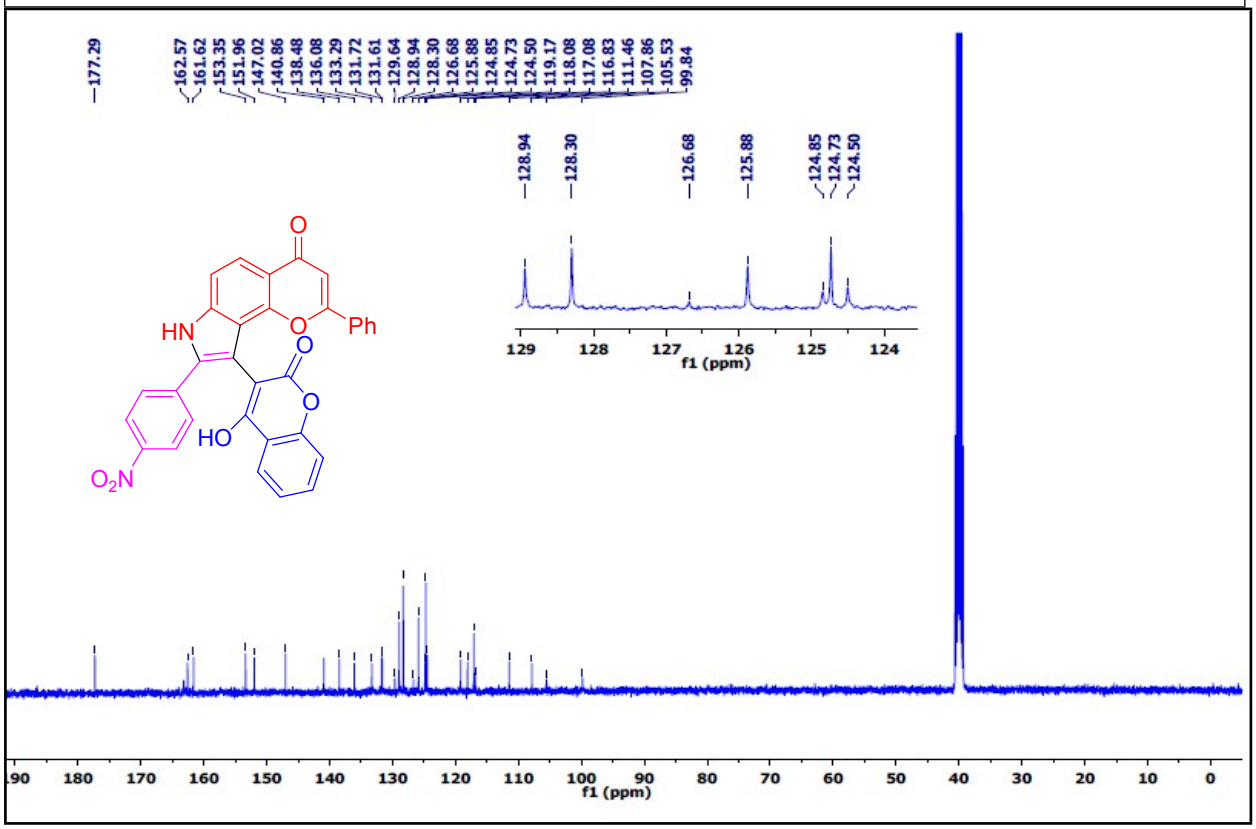
^{1}H and ^{13}C NMR spectra of (4m)



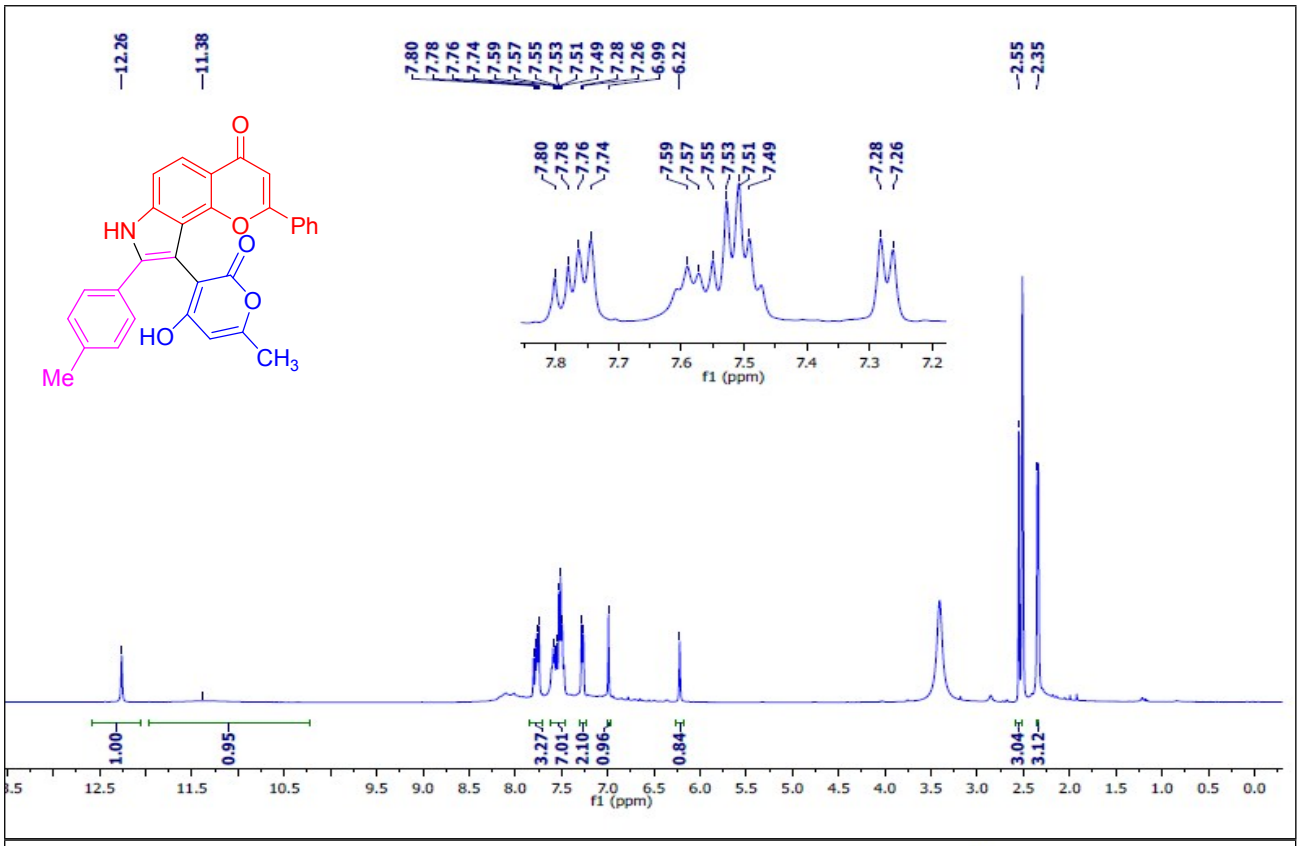


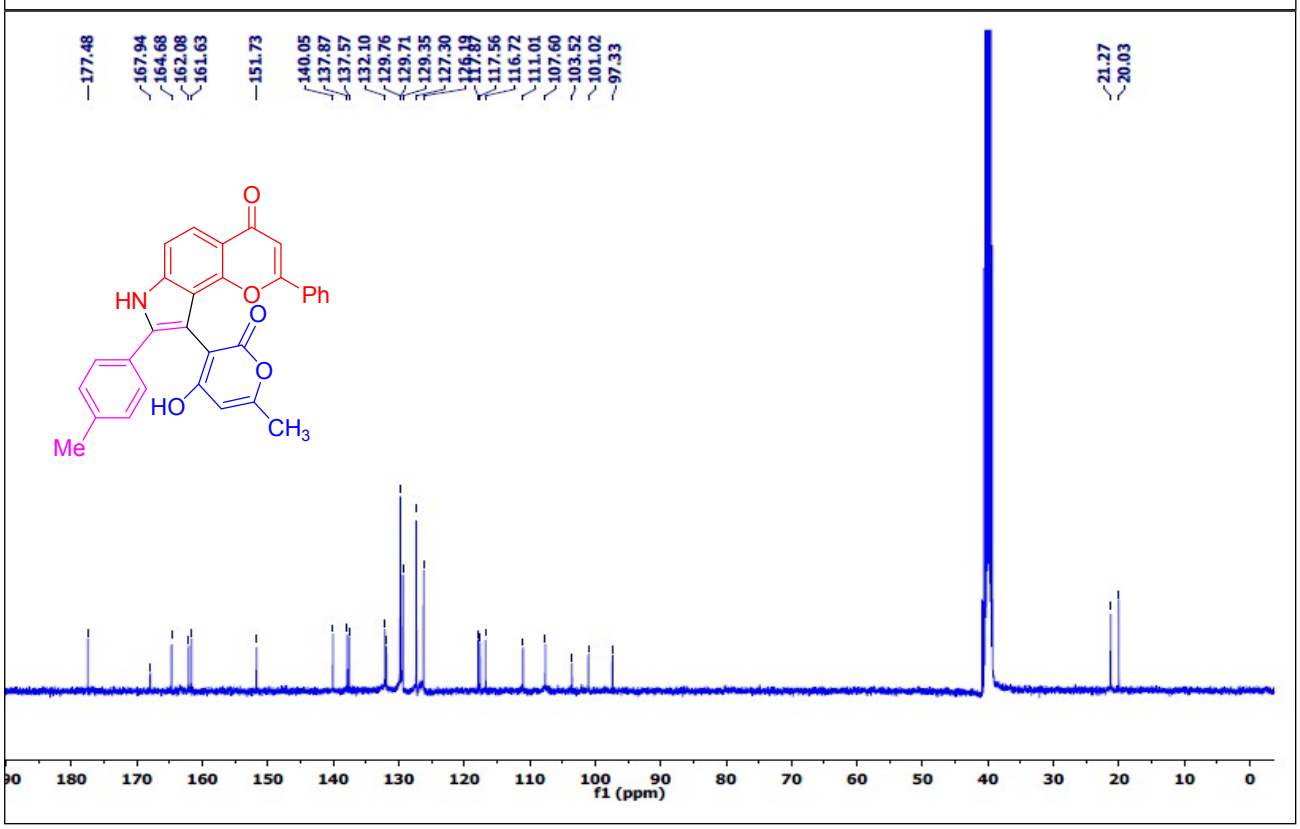
^{1}H and ^{13}C NMR spectra of (4n)





^{1}H and ^{13}C NMR spectra of (4o)





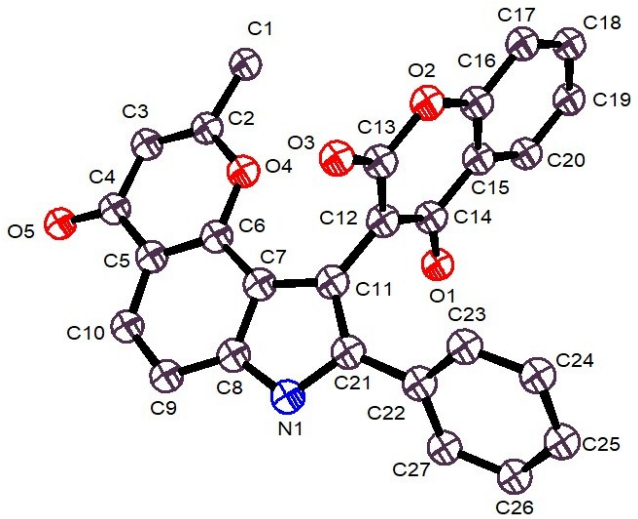


Table S1. Crystal data and structure refinement for **4a** (**CCDC 1579680)**

Identification code	rrnew_a
Empirical formula	$C_{60}\ H_{50}\ N_2\ O_{14}\ S_3$
Formula weight	1119.20
Temperature	295(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 20.451(2) Å α= 90°.
b = 29.075(3) Å	β= 103.894(2)°.
c = 9.8797(9) Å	γ = 90°.
Volume	5702.8(9) $Å^3$
Z	4
Density (calculated)	1.304 g/cm^3
Absorption coefficient	0.197 mm^{-1}
F(000)	2336
Crystal size	0.150 x 0.100 x 0.100 mm^3
Theta range for data collection	2.544 to 21.161°.
Index ranges	-20<=h<=20, -29<=k<=29, -10<=l<=10
Reflections collected	46182
Independent reflections	6209 [R(int) = 0.0350]
Completeness to theta = 21.161°	99.6 %

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7446 and 0.6666
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6209 / 332 / 824
Goodness-of-fit on F^2	1.060
Final R indices [I>2sigma(I)]	R1 = 0.0647, wR2 = 0.1840
R indices (all data)	R1 = 0.0735, wR2 = 0.1938
Extinction coefficient	0.0056(7)
Largest diff. peak and hole	0.913 and -0.400 e.$Å^{-3}$

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

	x	y	z	U(eq)
C(1)	137(3)	3967(2)	6459(5)	63(1)
C(2)	255(2)	4419(2)	7192(4)	47(1)
C(3)	5(2)	4820(2)	6685(4)	48(1)
C(4)	125(2)	5236(2)	7495(4)	45(1)
C(5)	537(2)	5182(1)	8896(4)	40(1)
C(6)	774(2)	4748(1)	9354(4)	38(1)
C(7)	1135(2)	4673(1)	10726(4)	37(1)
C(8)	1243(2)	5054(1)	11632(4)	40(1)
C(9)	1026(2)	5497(1)	11201(4)	45(1)
C(10)	681(2)	5557(1)	9853(4)	45(1)
C(11)	1405(2)	4276(1)	11522(4)	39(1)
C(12)	1368(2)	3792(1)	11054(4)	41(1)
C(13)	1854(2)	3637(2)	10319(4)	52(1)
C(14)	903(2)	3496(1)	11305(4)	46(1)
C(15)	888(2)	3023(1)	10838(5)	54(1)
C(16)	1361(3)	2891(2)	10128(5)	60(1)
C(17)	1396(3)	2441(2)	9669(6)	81(2)
C(18)	944(4)	2128(2)	9936(7)	102(2)
C(19)	460(4)	2256(2)	10631(8)	104(2)

C(20)	433(3)	2696(2)	11069(6)	82(2)
C(21)	1660(2)	4428(1)	12866(4)	43(1)
C(22)	1950(2)	4162(1)	14129(4)	45(1)
C(23)	2423(2)	3826(2)	14125(5)	59(1)
C(24)	2665(3)	3564(2)	15295(6)	76(2)
C(25)	2454(3)	3636(2)	16477(6)	75(2)
C(26)	1984(3)	3972(2)	16502(5)	70(1)
C(27)	1737(2)	4238(2)	15328(4)	55(1)
C(28)	5579(3)	6144(2)	2003(5)	70(1)
C(29)	5200(2)	5748(2)	2388(4)	48(1)
C(30)	5060(2)	5350(2)	1718(4)	49(1)
C(31)	4680(2)	4992(2)	2184(4)	45(1)
C(32)	4397(2)	5116(1)	3353(4)	43(1)
C(33)	4580(2)	5537(1)	4003(4)	41(1)
C(34)	4346(2)	5670(1)	5159(4)	41(1)
C(35)	3900(2)	5375(1)	5614(4)	42(1)
C(36)	3688(2)	4956(1)	4943(4)	48(1)
C(37)	3943(2)	4832(1)	3852(4)	45(1)
C(38)	4074(2)	5996(1)	7013(4)	43(1)
C(39)	3995(2)	6287(1)	8167(4)	48(1)
C(40)	3987(3)	6763(2)	8062(6)	72(2)
C(41)	3925(3)	7034(2)	9160(7)	90(2)
C(42)	3864(3)	6835(2)	10385(7)	90(2)
C(43)	3869(3)	6367(2)	10506(6)	81(2)
C(44)	3934(2)	6094(2)	9416(5)	63(1)
C(45)	4461(2)	6061(1)	6057(4)	42(1)
C(46)	4911(2)	6451(1)	5965(4)	42(1)
C(47)	5529(2)	6507(1)	6830(4)	42(1)
C(48)	5953(2)	6889(1)	6655(4)	44(1)
C(49)	6594(2)	6973(2)	7499(5)	56(1)
C(50)	6961(3)	7341(2)	7248(5)	68(1)
C(51)	6701(3)	7636(2)	6157(6)	80(2)
C(52)	6073(3)	7564(2)	5317(5)	71(1)
C(53)	5710(2)	7189(2)	5565(4)	50(1)
C(54)	4678(2)	6768(1)	4841(5)	49(1)
N(1)	1566(2)	4899(1)	12931(3)	45(1)

N(2)	3738(2)	5579(1)	6748(3)	47(1)
O(1)	437(2)	3598(1)	11985(4)	67(1)
O(2)	1828(2)	3192(1)	9859(3)	67(1)
O(3)	2302(2)	3870(1)	10063(4)	76(1)
O(4)	652(1)	4371(1)	8505(3)	44(1)
O(5)	-130(2)	5610(1)	7020(3)	57(1)
O(6)	4586(2)	4612(1)	1595(3)	56(1)
O(7)	4990(1)	5844(1)	3558(3)	46(1)
O(8)	5806(1)	6224(1)	7880(3)	58(1)
O(9)	5087(2)	7124(1)	4667(3)	61(1)
O(10)	4137(2)	6751(1)	4003(4)	68(1)
O(14)	1703(2)	5463(1)	5268(4)	107(2)
S(1)	8574(6)	3347(5)	1398(14)	211(5)
C(55)	7840(15)	3452(14)	2030(50)	196(11)
C(56)	9002(12)	3517(10)	3030(20)	136(8)
O(11)	8600(20)	3375(15)	-150(30)	378(15)
S(1')	8256(4)	3106(3)	1980(10)	226(3)
C(56')	8991(10)	3144(9)	3200(20)	222(9)
C(55')	8105(15)	3679(5)	1600(30)	201(8)
O(11')	8468(10)	2879(5)	835(19)	264(7)
S(3)	2525(2)	6430(1)	4428(4)	122(2)
C(59)	2498(10)	6960(6)	3450(30)	194(7)
C(60)	2725(6)	6092(4)	3217(13)	116(4)
O(13)	1783(9)	6357(7)	4330(20)	138(6)
S(3')	2019(6)	6612(4)	3476(13)	201(4)
C(59')	2591(13)	6961(9)	4720(30)	152(8)
C(60')	2581(15)	6389(12)	2650(40)	186(9)
O(13')	1630(20)	6275(15)	4140(50)	158(10)
S(2)	2490(1)	4931(1)	8745(2)	59(1)
C(58)	2679(4)	5166(4)	10475(7)	102(3)
C(57)	3198(3)	4565(3)	8955(9)	88(2)
O(12)	2622(3)	5308(2)	7803(4)	65(2)
S(2')	2464(14)	5113(13)	9100(50)	186(16)
C(58')	2720(40)	5520(20)	10420(70)	200(20)
C(57')	2810(40)	5350(30)	7790(60)	180(20)
O(12')	2980(20)	4721(16)	9620(80)	199(18)

Table S3. Selected Bond lengths [Å] for **4a**

C1—C2	1.491 (6)	C41—C42	1.375 (8)
C1—H1A	0.9600	C41—H41	0.9300
C1—H1B	0.9600	C42—C43	1.364 (8)
C1—H1C	0.9600	C42—H42	0.9300
C2—C3	1.323 (6)	C43—C44	1.369 (7)
C2—O4	1.362 (5)	C43—H43	0.9300
C3—C4	1.438 (6)	C44—H44	0.9300
C3—H3	0.9300	C45—C46	1.478 (6)
C4—O5	1.248 (5)	C46—C47	1.354 (6)
C4—C5	1.446 (6)	C46—C54	1.432 (6)
C5—C6	1.389 (5)	C47—O8	1.338 (5)
C5—C10	1.425 (6)	C47—C48	1.446 (6)
C6—O4	1.366 (5)	C48—C53	1.384 (6)
C6—C7	1.396 (5)	C48—C49	1.396 (6)
C7—C8	1.408 (5)	C49—C50	1.363 (6)
C7—C11	1.431 (5)	C49—H49	0.9300
C8—N1	1.371 (5)	C50—C51	1.379 (7)
C8—C9	1.395 (6)	C50—H50	0.9300
C9—C10	1.360 (6)	C51—C52	1.368 (7)
C9—H9	0.9300	C51—H51	0.9300
C10—H10	0.9300	C52—C53	1.372 (6)
C11—C21	1.377 (6)	C52—H52	0.9300
C11—C12	1.477 (6)	C53—O9	1.380 (5)
C12—C14	1.351 (6)	C54—O10	1.214 (5)
C12—C13	1.436 (6)	C54—O9	1.368 (5)
C13—O3	1.214 (5)	O1—H1	0.8200
C13—O2	1.369 (5)	O8—H8	0.8200
C14—O1	1.325 (5)	S1—O11	1.54 (2)
C14—C15	1.446 (6)	S1—C56	1.714 (17)
C15—C16	1.380 (7)	S1—C55	1.786 (19)
C15—C20	1.387 (7)	C55—H55A	0.9600
C16—O2	1.368 (6)	C55—H55B	0.9600

C16—C17	1.391 (7)	C55—H55C	0.9600
C17—C18	1.369 (9)	C56—H56A	0.9600
C17—H17	0.9300	C56—H56B	0.9600
C18—C19	1.384 (10)	C56—H56C	0.9600
C18—H18	0.9300	S1'—O11'	1.463 (13)
C19—C20	1.358 (8)	S1'—C56'	1.691 (16)
C19—H19	0.9300	S1'—C55'	1.721 (15)
C20—H20	0.9300	C56'—H56D	0.9600
C21—N1	1.387 (5)	C56'—H56E	0.9600
C21—C22	1.466 (6)	C56'—H56F	0.9600
C22—C27	1.374 (6)	C55'—H55D	0.9600
C22—C23	1.375 (6)	C55'—H55E	0.9600
C23—C24	1.374 (7)	C55'—H55F	0.9600
C23—H23	0.9300	S3—O13	1.512 (15)
C24—C25	1.355 (8)	S3—C60	1.672 (11)
C24—H24	0.9300	S3—C59	1.813 (14)
C25—C26	1.375 (7)	C59—H59A	0.9600
C25—H25	0.9300	C59—H59B	0.9600
C26—C27	1.384 (6)	C59—H59C	0.9600
C26—H26	0.9300	C60—H60A	0.9600
C27—H27	0.9300	C60—H60B	0.9600
C28—C29	1.487 (6)	C60—H60C	0.9600
C28—H28A	0.9600	S3'—O13'	1.51 (2)
C28—H28B	0.9600	S3'—C60'	1.693 (18)
C28—H28C	0.9600	S3'—C59'	1.796 (17)
C29—C30	1.331 (6)	C59'—H59D	0.9600
C29—O7	1.355 (5)	C59'—H59E	0.9600
C30—C31	1.438 (6)	C59'—H59F	0.9600
C30—H30	0.9300	C60'—H60D	0.9600
C31—O6	1.244 (5)	C60'—H60E	0.9600
C31—C32	1.455 (6)	C60'—H60F	0.9600
C32—C33	1.390 (6)	S2—O12	1.503 (5)
C32—C37	1.417 (6)	S2—C57	1.770 (7)

C33—O7	1.368 (4)	S2—C58	1.793 (7)
C33—C34	1.396 (5)	C58—H58A	0.9600
C34—C35	1.402 (5)	C58—H58B	0.9600
C34—C45	1.425 (6)	C58—H58C	0.9600
C35—N2	1.376 (5)	C57—H57A	0.9600
C35—C36	1.404 (6)	C57—H57B	0.9600
C36—C37	1.354 (6)	C57—H57C	0.9600
C36—H36	0.9300	S2'—O12'	1.55 (2)
C37—H37	0.9300	S2'—C58'	1.74 (2)
C38—C45	1.383 (5)	S2'—C57'	1.75 (2)
C38—N2	1.389 (5)	C58'—H58D	0.9600
C38—C39	1.458 (6)	C58'—H58E	0.9600
C39—C44	1.387 (6)	C58'—H58F	0.9600
C39—C40	1.389 (6)	C57'—H57D	0.9600
C40—C41	1.372 (7)	C57'—H57E	0.9600
C40—H40	0.9300	C57'—H57F	0.9600

Table S4. Selected Bond angles [°] for **4a**

C2—C1—H1A	109.5	C42—C43—H43	119.7
C2—C1—H1B	109.5	C44—C43—H43	119.7
H1A—C1—H1B	109.5	C43—C44—C39	120.8 (5)
C2—C1—H1C	109.5	C43—C44—H44	119.6
H1A—C1—H1C	109.5	C39—C44—H44	119.6
H1B—C1—H1C	109.5	C38—C45—C34	106.3 (3)
C3—C2—O4	122.5 (4)	C38—C45—C46	127.8 (4)
C3—C2—C1	126.1 (4)	C34—C45—C46	125.9 (3)
O4—C2—C1	111.3 (4)	C47—C46—C54	119.9 (4)
C2—C3—C4	122.2 (4)	C47—C46—C45	123.5 (4)
C2—C3—H3	118.9	C54—C46—C45	116.4 (3)
C4—C3—H3	118.9	O8—C47—C46	125.1 (4)
O5—C4—C3	121.6 (4)	O8—C47—C48	114.2 (4)
O5—C4—C5	123.3 (4)	C46—C47—C48	120.8 (4)
C3—C4—C5	115.1 (4)	C53—C48—C49	117.7 (4)

C6—C5—C10	118.5 (4)	C53—C48—C47	117.7 (4)
C6—C5—C4	119.1 (4)	C49—C48—C47	124.6 (4)
C10—C5—C4	122.2 (4)	C50—C49—C48	120.5 (5)
O4—C6—C5	122.1 (3)	C50—C49—H49	119.8
O4—C6—C7	116.5 (3)	C48—C49—H49	119.8
C5—C6—C7	121.3 (4)	C49—C50—C51	120.3 (5)
C6—C7—C8	117.4 (3)	C49—C50—H50	119.8
C6—C7—C11	134.7 (4)	C51—C50—H50	119.8
C8—C7—C11	107.7 (3)	C52—C51—C50	120.5 (5)
N1—C8—C9	129.5 (4)	C52—C51—H51	119.7
N1—C8—C7	107.6 (3)	C50—C51—H51	119.7
C9—C8—C7	122.8 (4)	C51—C52—C53	118.9 (5)
C10—C9—C8	118.0 (4)	C51—C52—H52	120.6
C10—C9—H9	121.0	C53—C52—H52	120.6
C8—C9—H9	121.0	C52—C53—O9	116.8 (4)
C9—C10—C5	121.9 (4)	C52—C53—C48	122.0 (4)
C9—C10—H10	119.1	O9—C53—C48	121.2 (4)
C5—C10—H10	119.1	O10—C54—O9	115.4 (4)
C21—C11—C7	106.2 (3)	O10—C54—C46	125.5 (4)
C21—C11—C12	125.9 (3)	O9—C54—C46	119.0 (4)
C7—C11—C12	127.8 (3)	C8—N1—C21	108.8 (3)
C14—C12—C13	119.7 (4)	C35—N2—C38	109.0 (3)
C14—C12—C11	122.4 (4)	C14—O1—H1	109.5
C13—C12—C11	117.9 (4)	C16—O2—C13	120.9 (4)
O3—C13—O2	115.5 (4)	C2—O4—C6	118.9 (3)
O3—C13—C12	125.3 (4)	C29—O7—C33	118.9 (3)
O2—C13—C12	119.3 (4)	C47—O8—H8	109.5
O1—C14—C12	125.1 (4)	C54—O9—C53	121.4 (3)
O1—C14—C15	114.3 (4)	O11—S1—C56	141 (2)
C12—C14—C15	120.7 (4)	O11—S1—C55	125 (3)
C16—C15—C20	118.2 (4)	C56—S1—C55	84.4 (18)
C16—C15—C14	117.6 (4)	S1—C55—H55A	109.5
C20—C15—C14	124.2 (5)	S1—C55—H55B	109.5

O2—C16—C15	121.8 (4)	H55A—C55—H55B	109.5
O2—C16—C17	116.4 (5)	S1—C55—H55C	109.5
C15—C16—C17	121.7 (5)	H55A—C55—H55C	109.5
C18—C17—C16	118.2 (6)	H55B—C55—H55C	109.5
C18—C17—H17	120.9	S1—C56—H56A	109.5
C16—C17—H17	120.9	S1—C56—H56B	109.5
C17—C18—C19	120.9 (5)	H56A—C56—H56B	109.5
C17—C18—H18	119.6	S1—C56—H56C	109.5
C19—C18—H18	119.6	H56A—C56—H56C	109.5
C20—C19—C18	120.1 (6)	H56B—C56—H56C	109.5
C20—C19—H19	120.0	O11'—S1'—C56'	101.7 (13)
C18—C19—H19	120.0	O11'—S1'—C55'	109.8 (13)
C19—C20—C15	120.9 (6)	C56'—S1'—C55'	100.1 (13)
C19—C20—H20	119.6	S1'—C56'—H56D	109.5
C15—C20—H20	119.6	S1'—C56'—H56E	109.5
C11—C21—N1	109.7 (3)	H56D—C56'—H56E	109.5
C11—C21—C22	129.4 (4)	S1'—C56'—H56F	109.5
N1—C21—C22	120.8 (4)	H56D—C56'—H56F	109.5
C27—C22—C23	119.0 (4)	H56E—C56'—H56F	109.5
C27—C22—C21	120.1 (4)	S1'—C55'—H55D	109.5
C23—C22—C21	120.8 (4)	S1'—C55'—H55E	109.5
C24—C23—C22	120.2 (5)	H55D—C55'—H55E	109.5
C24—C23—H23	119.9	S1'—C55'—H55F	109.5
C22—C23—H23	119.9	H55D—C55'—H55F	109.5
C25—C24—C23	120.9 (5)	H55E—C55'—H55F	109.5
C25—C24—H24	119.5	O13—S3—C60	106.7 (11)
C23—C24—H24	119.5	O13—S3—C59	100.6 (10)
C24—C25—C26	119.6 (5)	C60—S3—C59	95.7 (9)
C24—C25—H25	120.2	S3—C59—H59A	109.5
C26—C25—H25	120.2	S3—C59—H59B	109.5
C25—C26—C27	119.8 (5)	H59A—C59—H59B	109.5
C25—C26—H26	120.1	S3—C59—H59C	109.5
C27—C26—H26	120.1	H59A—C59—H59C	109.5

C22—C27—C26	120.4 (5)	H59B—C59—H59C	109.5
C22—C27—H27	119.8	S3—C60—H60A	109.5
C26—C27—H27	119.8	S3—C60—H60B	109.5
C29—C28—H28A	109.5	H60A—C60—H60B	109.5
C29—C28—H28B	109.5	S3—C60—H60C	109.5
H28A—C28—H28B	109.5	H60A—C60—H60C	109.5
C29—C28—H28C	109.5	H60B—C60—H60C	109.5
H28A—C28—H28C	109.5	O13'—S3'—C60'	117 (3)
H28B—C28—H28C	109.5	O13'—S3'—C59'	113 (2)
C30—C29—O7	122.0 (4)	C60'—S3'—C59'	98.2 (16)
C30—C29—C28	127.5 (4)	S3'—C59'—H59D	109.5
O7—C29—C28	110.5 (4)	S3'—C59'—H59E	109.5
C29—C30—C31	122.5 (4)	H59D—C59'—H59E	109.5
C29—C30—H30	118.8	S3'—C59'—H59F	109.5
C31—C30—H30	118.8	H59D—C59'—H59F	109.5
O6—C31—C30	121.8 (4)	H59E—C59'—H59F	109.5
O6—C31—C32	123.1 (4)	S3'—C60'—H60D	109.5
C30—C31—C32	115.1 (4)	S3'—C60'—H60E	109.5
C33—C32—C37	118.6 (4)	H60D—C60'—H60E	109.5
C33—C32—C31	118.0 (4)	S3'—C60'—H60F	109.5
C37—C32—C31	123.4 (4)	H60D—C60'—H60F	109.5
O7—C33—C32	123.0 (3)	H60E—C60'—H60F	109.5
O7—C33—C34	116.0 (3)	O12—S2—C57	104.3 (3)
C32—C33—C34	121.0 (3)	O12—S2—C58	106.5 (4)
C33—C34—C35	118.0 (4)	C57—S2—C58	97.7 (4)
C33—C34—C45	133.9 (4)	S2—C58—H58A	109.5
C35—C34—C45	108.2 (3)	S2—C58—H58B	109.5
N2—C35—C34	107.4 (3)	H58A—C58—H58B	109.5
N2—C35—C36	130.5 (4)	S2—C58—H58C	109.5
C34—C35—C36	122.1 (4)	H58A—C58—H58C	109.5
C37—C36—C35	118.2 (4)	H58B—C58—H58C	109.5
C37—C36—H36	120.9	S2—C57—H57A	109.5
C35—C36—H36	120.9	S2—C57—H57B	109.5

C36—C37—C32	122.1 (4)	H57A—C57—H57B	109.5
C36—C37—H37	119.0	S2—C57—H57C	109.5
C32—C37—H37	119.0	H57A—C57—H57C	109.5
C45—C38—N2	109.2 (3)	H57B—C57—H57C	109.5
C45—C38—C39	130.1 (4)	O12'—S2'—C58'	101 (3)
N2—C38—C39	120.7 (4)	O12'—S2'—C57'	100 (3)
C44—C39—C40	117.8 (4)	C58'—S2'—C57'	100.4 (16)
C44—C39—C38	120.9 (4)	S2'—C58'—H58D	109.5
C40—C39—C38	121.3 (4)	S2'—C58'—H58E	109.5
C41—C40—C39	121.0 (5)	H58D—C58'—H58E	109.5
C41—C40—H40	119.5	S2'—C58'—H58F	109.5
C39—C40—H40	119.5	H58D—C58'—H58F	109.5
C40—C41—C42	119.9 (5)	H58E—C58'—H58F	109.5
C40—C41—H41	120.0	S2'—C57'—H57D	109.5
C42—C41—H41	120.0	S2'—C57'—H57E	109.5
C43—C42—C41	119.8 (5)	H57D—C57'—H57E	109.5
C43—C42—H42	120.1	S2'—C57'—H57F	109.5
C41—C42—H42	120.1	H57D—C57'—H57F	109.5
C42—C43—C44	120.6 (5)	H57E—C57'—H57F	109.5

Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4a**. 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}
C(1)	75(3)	60(3)	49(3)	-11(2)	4(2)	3(2)
C(2)	50(3)	51(3)	40(3)	3(2)	12(2)	2(2)
C(3)	56(3)	56(3)	31(2)	5(2)	9(2)	6(2)
C(4)	48(3)	49(3)	40(2)	16(2)	17(2)	8(2)
C(5)	45(2)	37(2)	40(2)	9(2)	13(2)	4(2)
C(6)	40(2)	39(3)	35(2)	1(2)	13(2)	1(2)
C(7)	39(2)	36(2)	37(2)	4(2)	10(2)	1(2)
C(8)	41(2)	38(2)	39(2)	6(2)	9(2)	-1(2)
C(9)	52(3)	33(2)	49(3)	-1(2)	12(2)	-5(2)

C(10)	49(2)	36(2)	49(3)	13(2)	13(2)	3(2)
C(11)	42(2)	36(2)	38(2)	2(2)	7(2)	0(2)
C(12)	48(2)	38(2)	34(2)	4(2)	2(2)	6(2)
C(13)	65(3)	48(3)	41(2)	1(2)	10(2)	2(2)
C(14)	51(3)	39(3)	49(3)	6(2)	11(2)	7(2)
C(15)	60(3)	39(3)	58(3)	2(2)	3(2)	1(2)
C(16)	77(3)	45(3)	47(3)	-4(2)	-3(2)	8(3)
C(17)	109(5)	54(4)	76(4)	-19(3)	13(3)	9(3)
C(18)	140(6)	43(4)	107(5)	-18(3)	0(5)	5(4)
C(19)	124(6)	46(4)	135(6)	0(4)	19(5)	-15(3)
C(20)	90(4)	46(3)	110(5)	-3(3)	25(3)	-10(3)
C(21)	46(2)	39(3)	43(3)	6(2)	6(2)	0(2)
C(22)	51(3)	40(2)	36(2)	1(2)	-2(2)	-2(2)
C(23)	67(3)	57(3)	45(3)	-2(2)	-2(2)	14(3)
C(24)	89(4)	60(3)	64(4)	-2(3)	-10(3)	26(3)
C(25)	97(4)	60(3)	51(3)	15(3)	-14(3)	7(3)
C(26)	88(4)	74(4)	42(3)	8(3)	4(3)	-6(3)
C(27)	65(3)	53(3)	44(3)	6(2)	4(2)	3(2)
C(28)	80(3)	70(3)	72(3)	-3(3)	40(3)	-17(3)
C(29)	46(2)	52(3)	50(3)	4(2)	18(2)	-4(2)
C(30)	54(3)	52(3)	43(2)	0(2)	17(2)	-3(2)
C(31)	48(3)	45(3)	39(2)	-1(2)	3(2)	1(2)
C(32)	46(2)	41(3)	40(2)	0(2)	6(2)	-4(2)
C(33)	38(2)	43(3)	41(2)	4(2)	10(2)	-6(2)
C(34)	42(2)	41(2)	40(2)	-1(2)	7(2)	-5(2)
C(35)	42(2)	44(3)	40(2)	1(2)	9(2)	-6(2)
C(36)	48(3)	45(3)	51(3)	2(2)	13(2)	-14(2)
C(37)	52(3)	41(2)	43(2)	-4(2)	11(2)	-11(2)
C(38)	45(2)	41(3)	42(2)	2(2)	10(2)	-2(2)
C(39)	46(2)	48(3)	51(3)	-6(2)	15(2)	-6(2)
C(40)	90(4)	54(3)	84(4)	-8(3)	45(3)	-5(3)
C(41)	105(5)	58(3)	118(5)	-26(4)	52(4)	-10(3)
C(42)	94(4)	101(5)	82(4)	-40(4)	31(3)	-5(4)
C(43)	100(4)	94(5)	54(3)	-8(3)	26(3)	4(3)
C(44)	75(3)	62(3)	55(3)	-6(3)	20(3)	1(3)
C(45)	42(2)	42(2)	40(2)	0(2)	7(2)	-4(2)

C(46)	43(3)	42(2)	42(2)	0(2)	13(2)	-4(2)
C(47)	51(3)	41(2)	37(2)	-3(2)	15(2)	-2(2)
C(48)	51(3)	45(3)	39(2)	-11(2)	17(2)	-10(2)
C(49)	60(3)	63(3)	47(3)	-15(2)	16(2)	-13(2)
C(50)	65(3)	82(4)	57(3)	-18(3)	14(3)	-35(3)
C(51)	97(4)	76(4)	71(4)	-12(3)	28(3)	-49(3)
C(52)	86(4)	68(3)	58(3)	4(3)	16(3)	-30(3)
C(53)	56(3)	51(3)	46(3)	-6(2)	15(2)	-18(2)
C(54)	52(3)	42(3)	54(3)	-1(2)	12(3)	-13(2)
N(1)	50(2)	40(2)	42(2)	3(2)	4(2)	1(2)
N(2)	51(2)	45(2)	45(2)	-3(2)	15(2)	-7(2)
O(1)	70(2)	42(2)	96(2)	2(2)	36(2)	-3(2)
O(2)	84(2)	52(2)	70(2)	-13(2)	28(2)	4(2)
O(3)	86(3)	77(2)	79(2)	-6(2)	43(2)	-7(2)
O(4)	52(2)	42(2)	35(2)	1(1)	6(1)	5(1)
O(5)	71(2)	53(2)	47(2)	17(2)	13(2)	17(2)
O(6)	76(2)	49(2)	45(2)	-5(2)	16(2)	-6(2)
O(7)	51(2)	44(2)	47(2)	-3(1)	20(1)	-10(1)
O(8)	59(2)	54(2)	55(2)	5(2)	1(2)	-13(2)
O(9)	67(2)	56(2)	57(2)	13(2)	8(2)	-15(2)
O(10)	59(2)	64(2)	72(2)	16(2)	-4(2)	-11(2)
O(14)	148(4)	77(3)	76(3)	-22(2)	-9(3)	6(3)
S(1)	219(9)	205(10)	227(9)	8(8)	88(7)	-56(8)
C(55)	180(20)	140(20)	260(20)	-48(18)	59(18)	50(17)
C(56)	127(15)	170(19)	128(15)	-49(15)	62(12)	-58(15)
O(11)	420(30)	290(20)	380(30)	-10(20)	0(30)	-60(20)
S(1')	230(7)	167(5)	296(8)	-36(5)	92(6)	-23(5)
C(56')	188(15)	237(18)	219(16)	-5(16)	4(13)	42(16)
C(55')	252(18)	116(13)	253(17)	-3(12)	94(15)	26(13)
O(11')	337(16)	177(12)	300(15)	-108(11)	119(13)	-21(12)
S(3)	113(3)	103(2)	142(3)	-2(2)	17(2)	9(2)
C(59)	171(12)	143(11)	270(16)	40(13)	57(13)	-30(10)
C(60)	88(7)	115(9)	145(10)	8(8)	24(7)	-4(7)
O(13)	138(11)	90(8)	212(13)	27(9)	92(11)	-10(7)
S(3')	178(7)	185(7)	240(8)	42(7)	54(7)	-47(6)
C(59')	137(14)	136(15)	186(17)	-24(15)	45(15)	-38(12)

C(60')	187(17)	183(17)	190(17)	-25(15)	48(15)	-33(16)
O(13')	146(15)	131(17)	193(16)	-9(13)	34(13)	-44(12)
S(2)	41(1)	80(2)	59(1)	5(1)	16(1)	-14(1)
C(58)	86(5)	161(8)	64(4)	-19(4)	26(3)	-33(5)
C(57)	53(4)	92(4)	121(6)	12(4)	22(3)	2(3)
O(12)	52(4)	86(3)	59(2)	13(2)	16(2)	-18(2)
S(2')	70(12)	140(20)	360(50)	-30(20)	70(20)	-38(11)
C(58')	110(30)	130(30)	350(50)	-20(30)	70(20)	-40(20)
C(57')	50(30)	150(30)	350(50)	-30(30)	50(30)	-50(20)
O(12')	88(19)	150(20)	370(50)	-30(30)	70(20)	-28(15)