

Supplementary Material

Lemon juice mediated multicomponent reactions for the synthesis of fused imidazoles

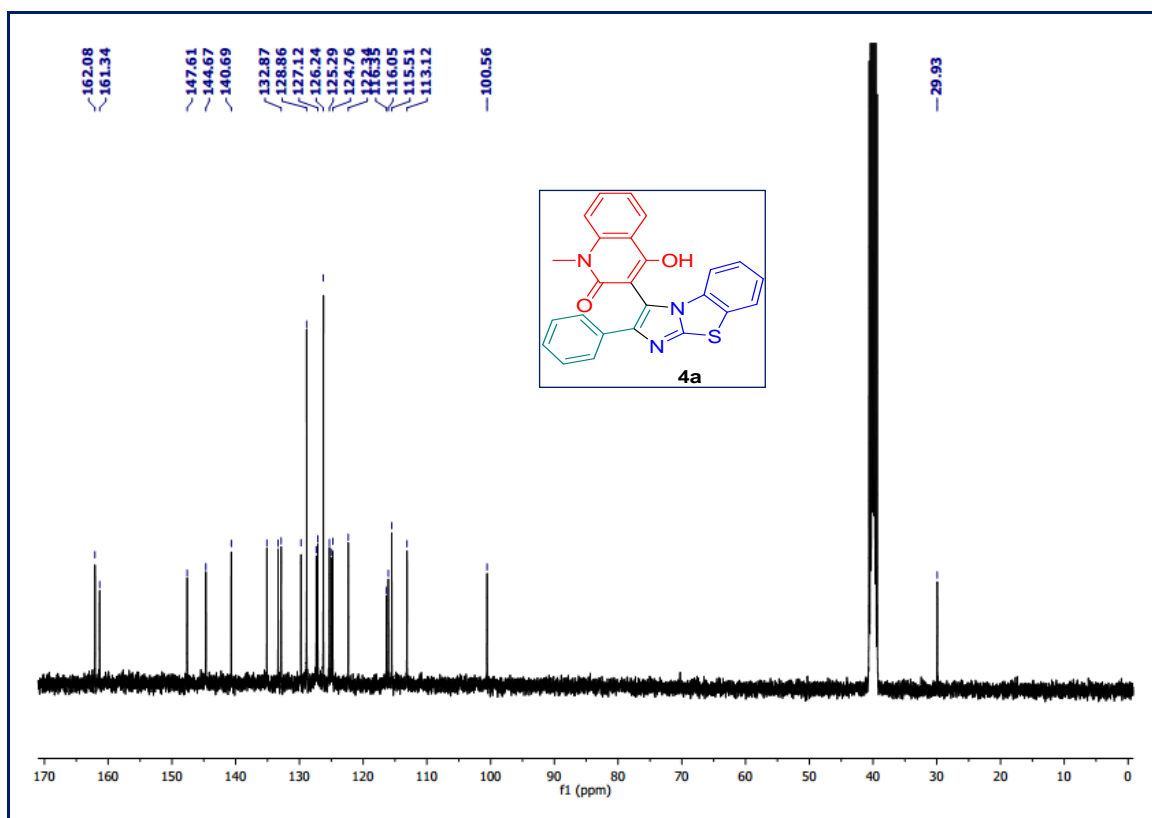
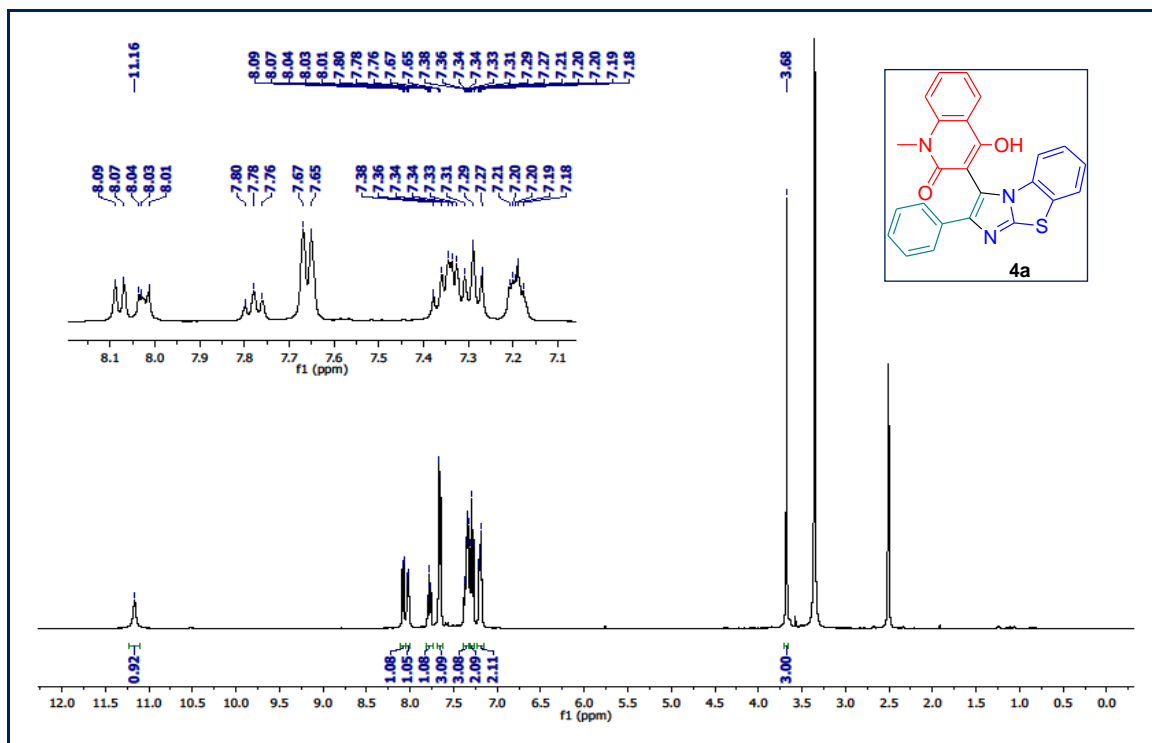
Argha Saha, Asim Jana and Lokman H. Choudhury*

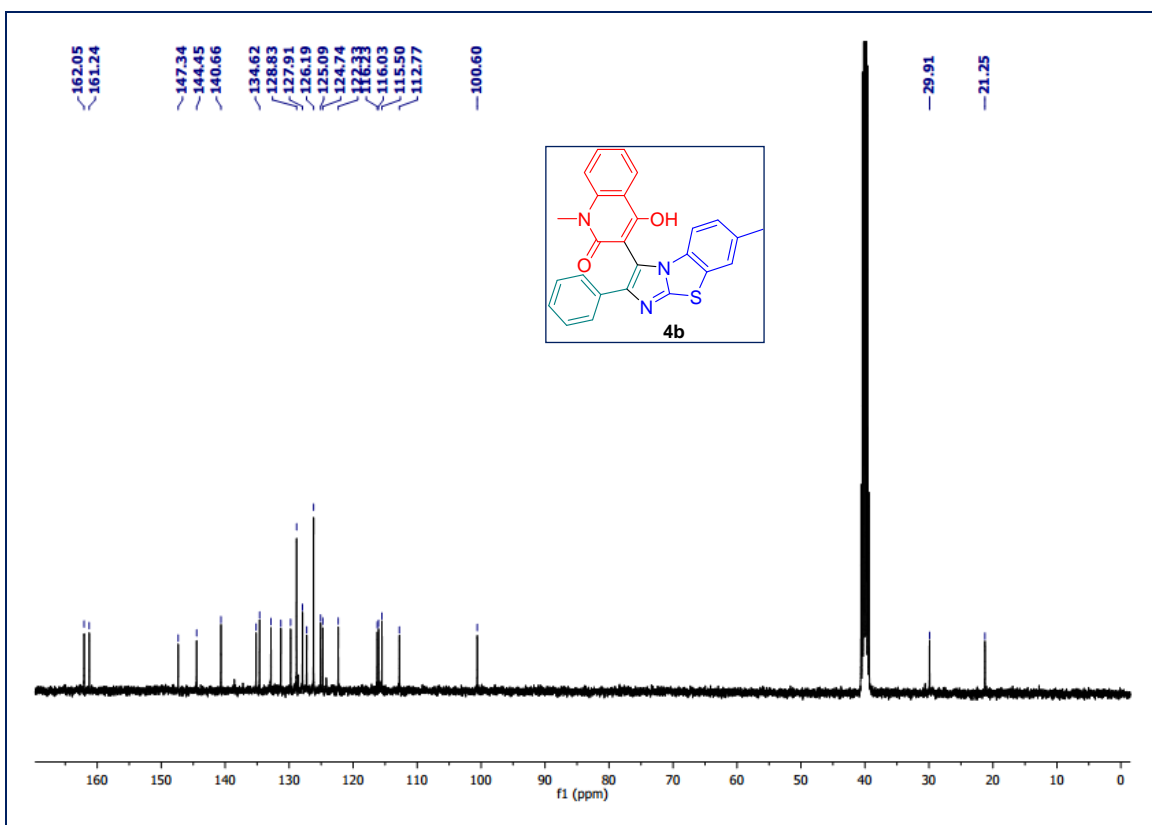
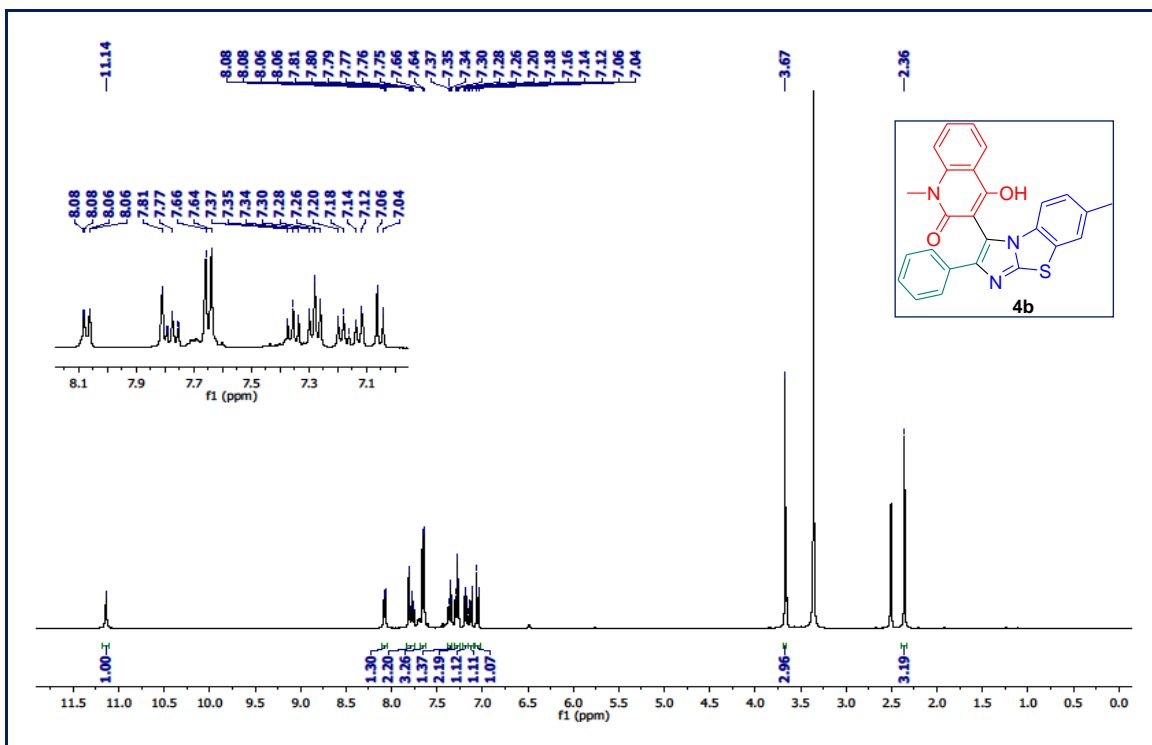
Department of Chemistry, Indian Institute of Technology Patna, Bihta, Patna-801103

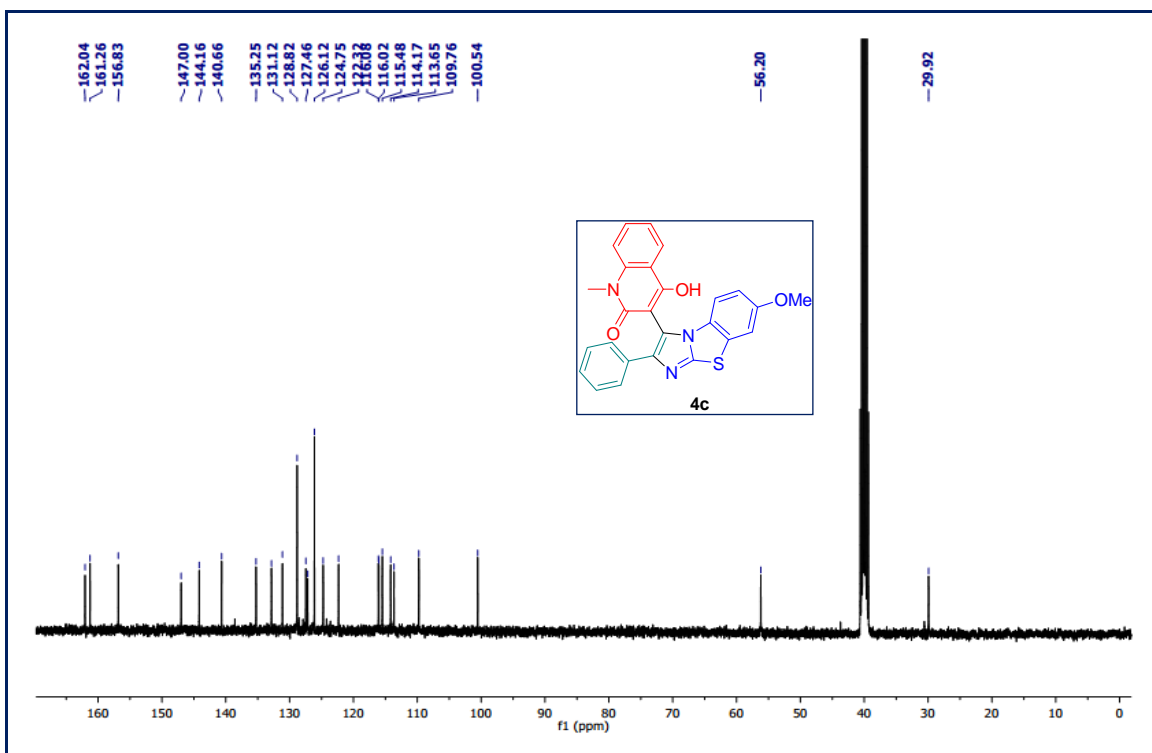
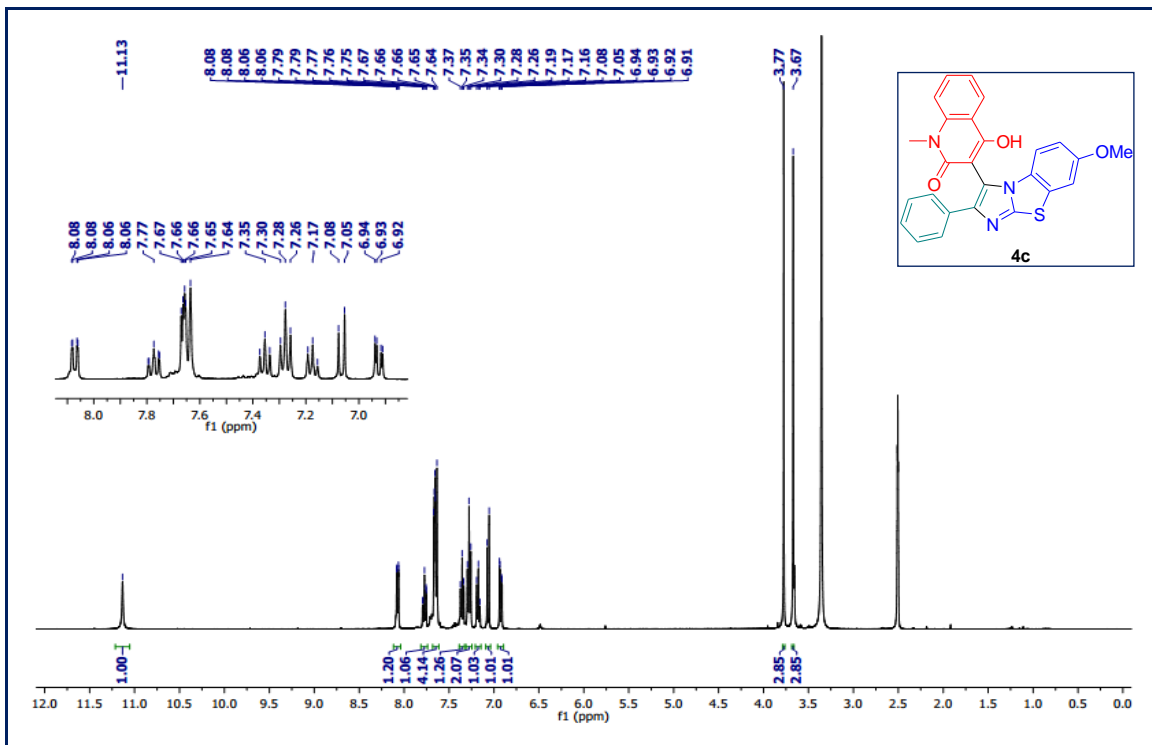
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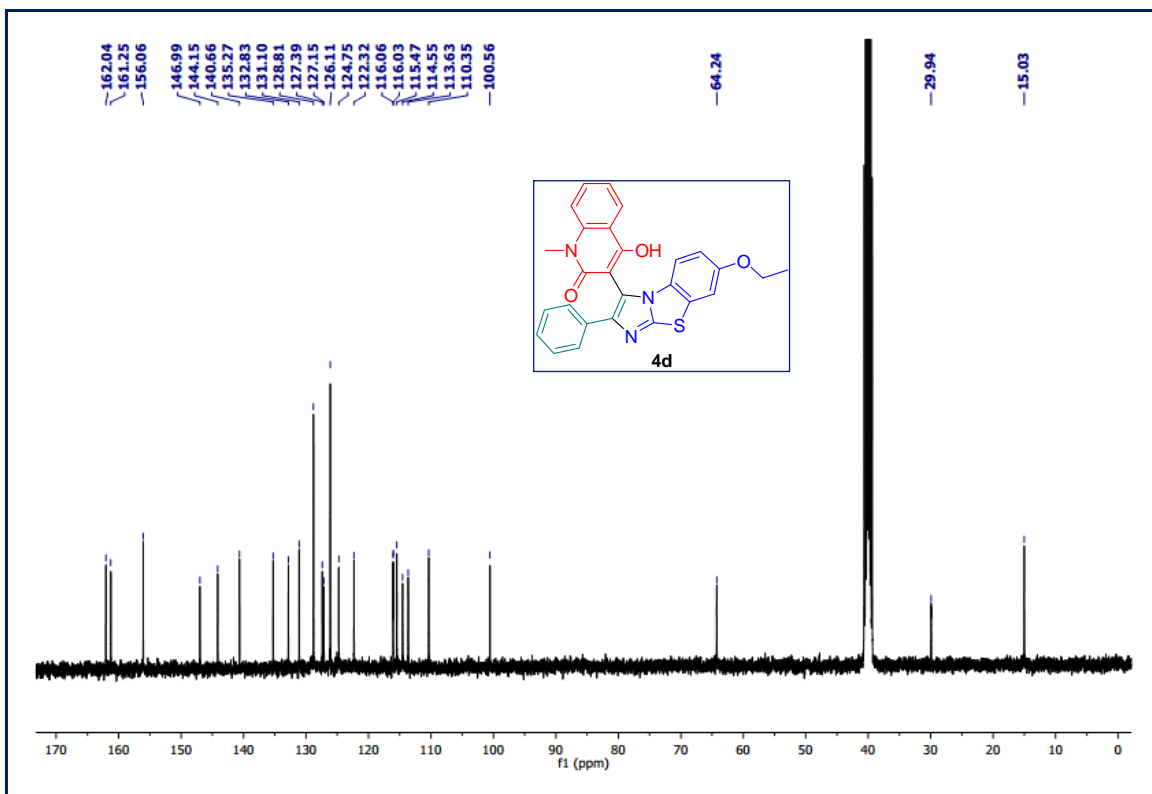
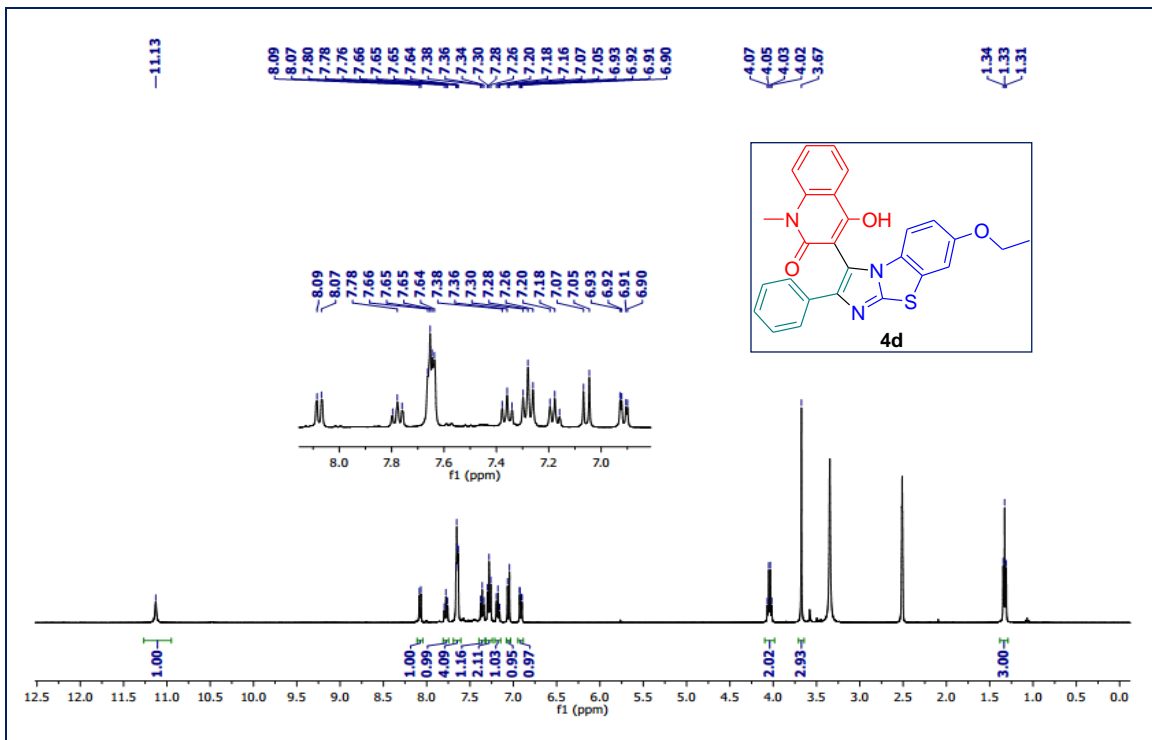
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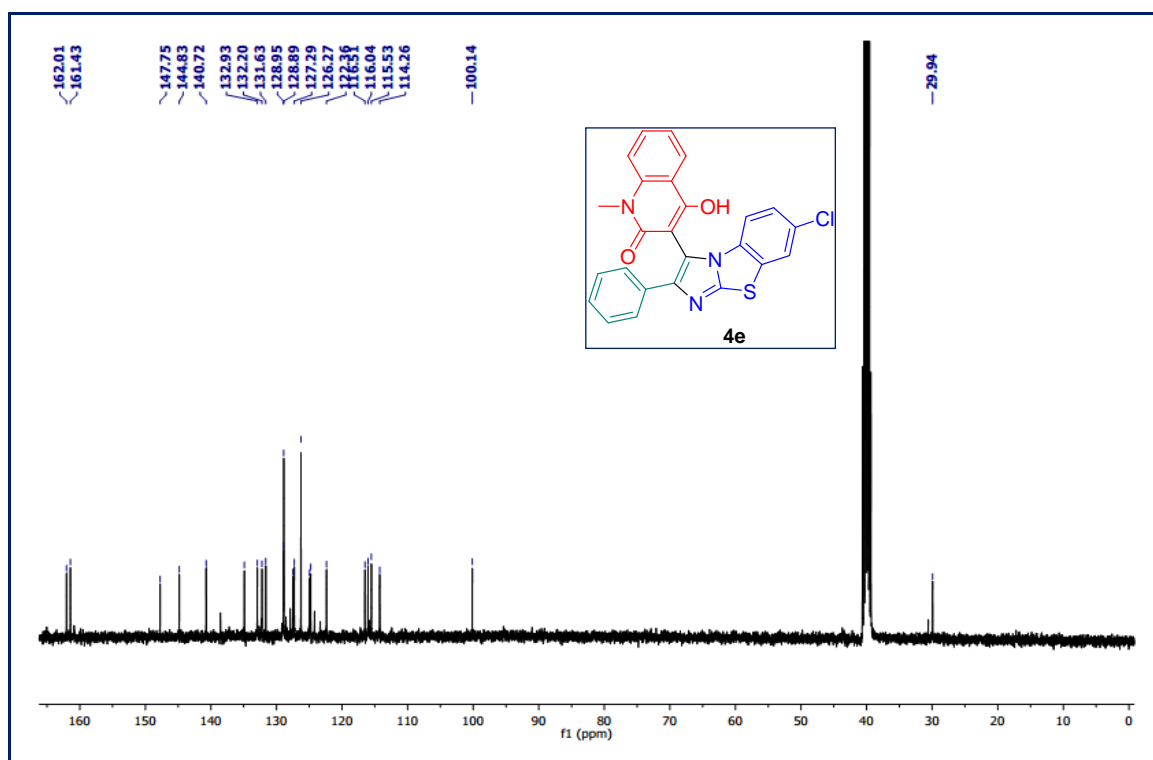
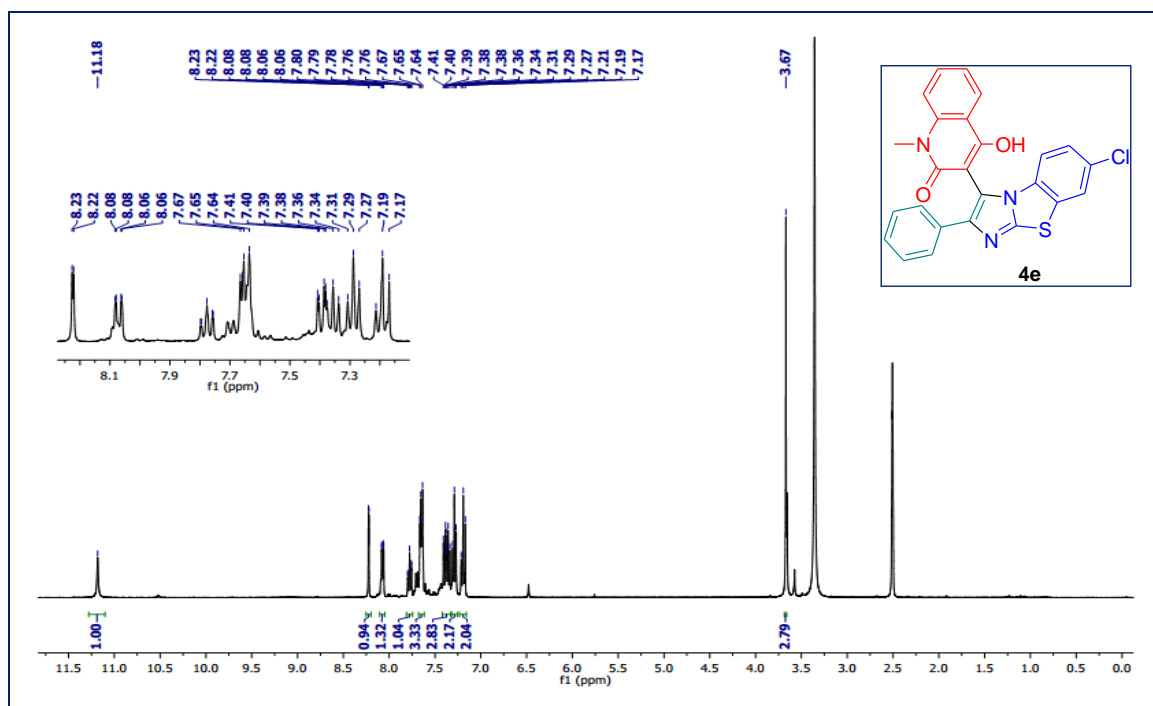
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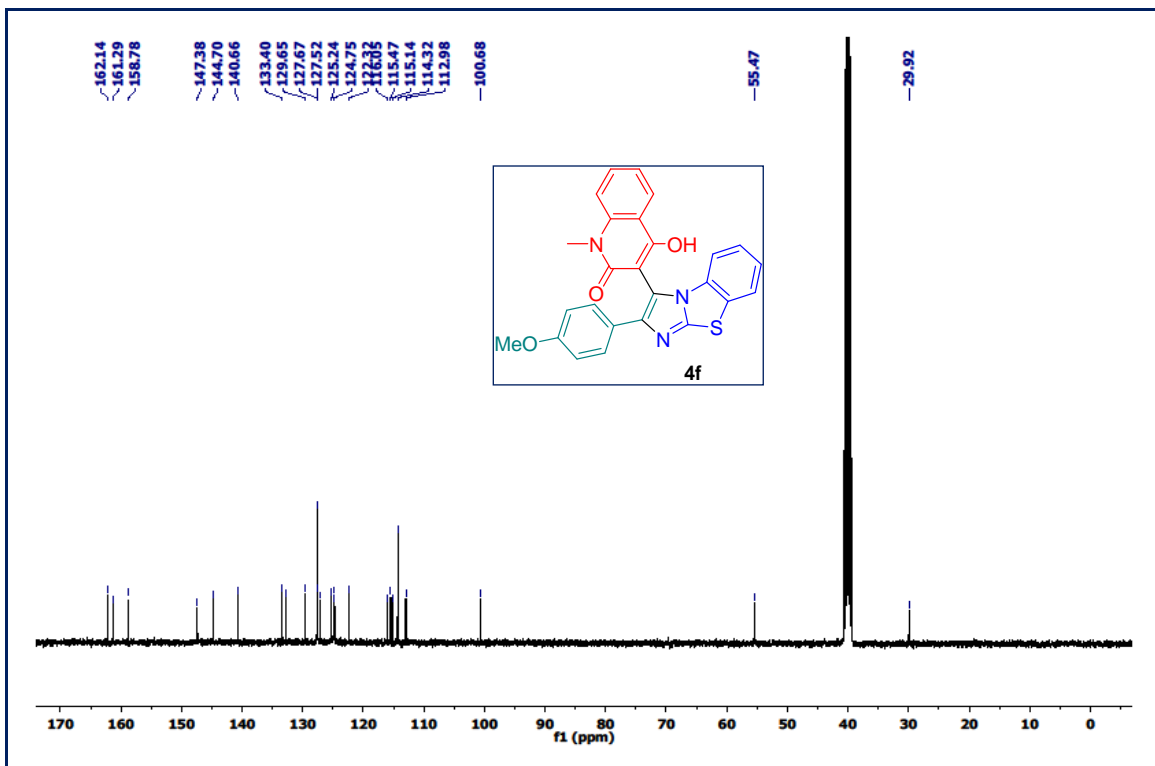
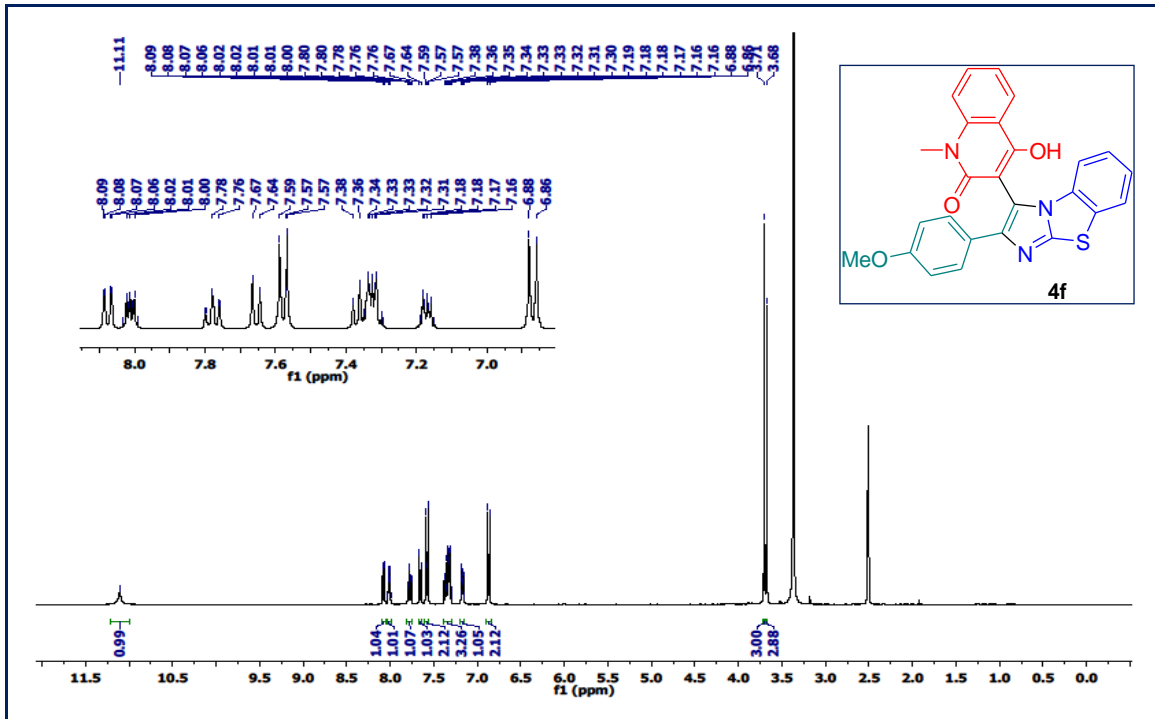


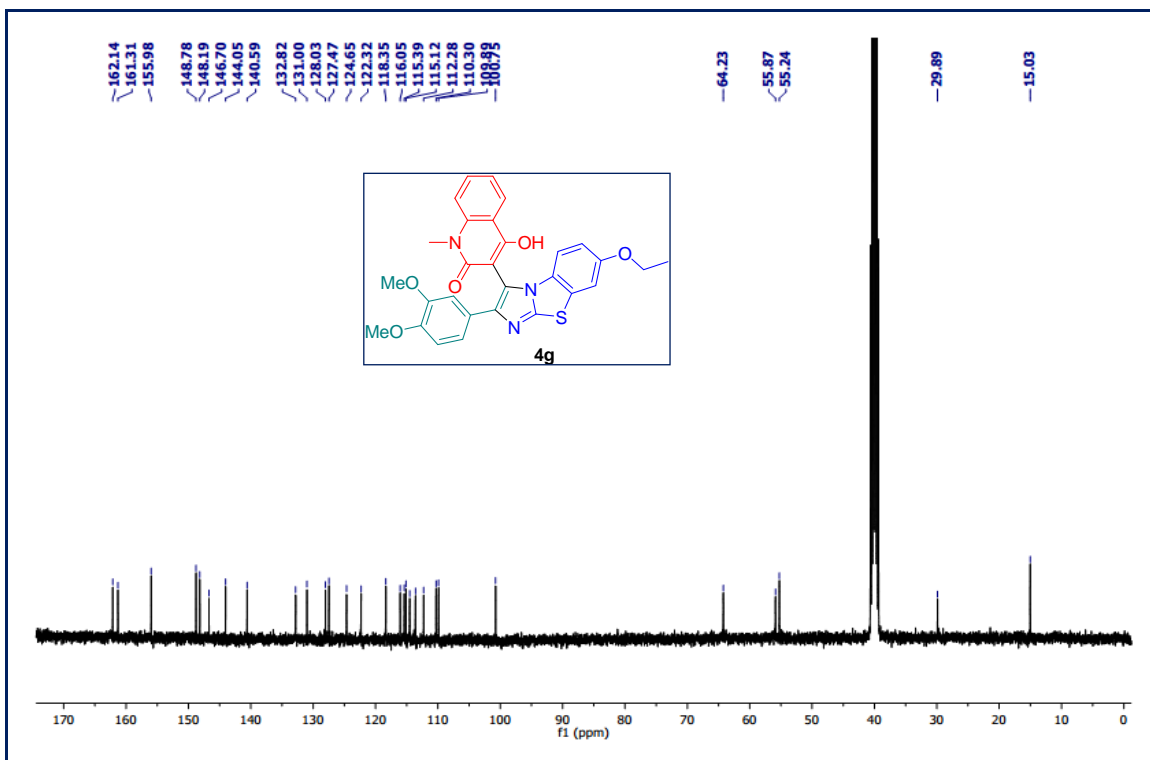
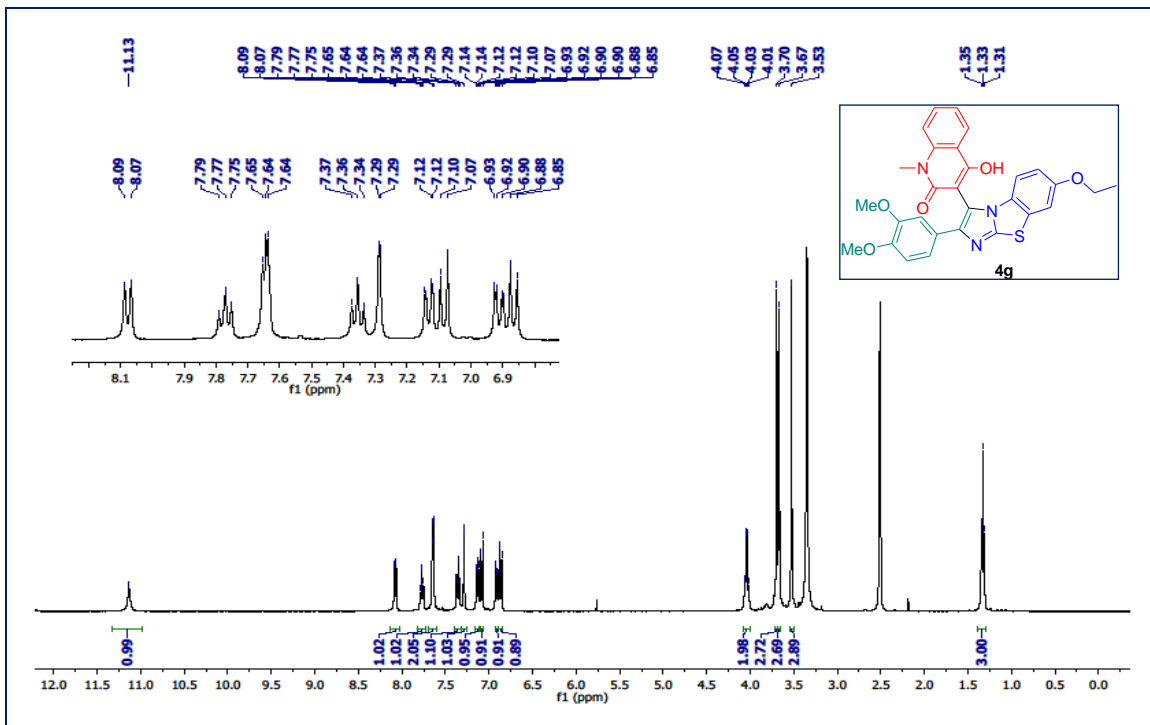


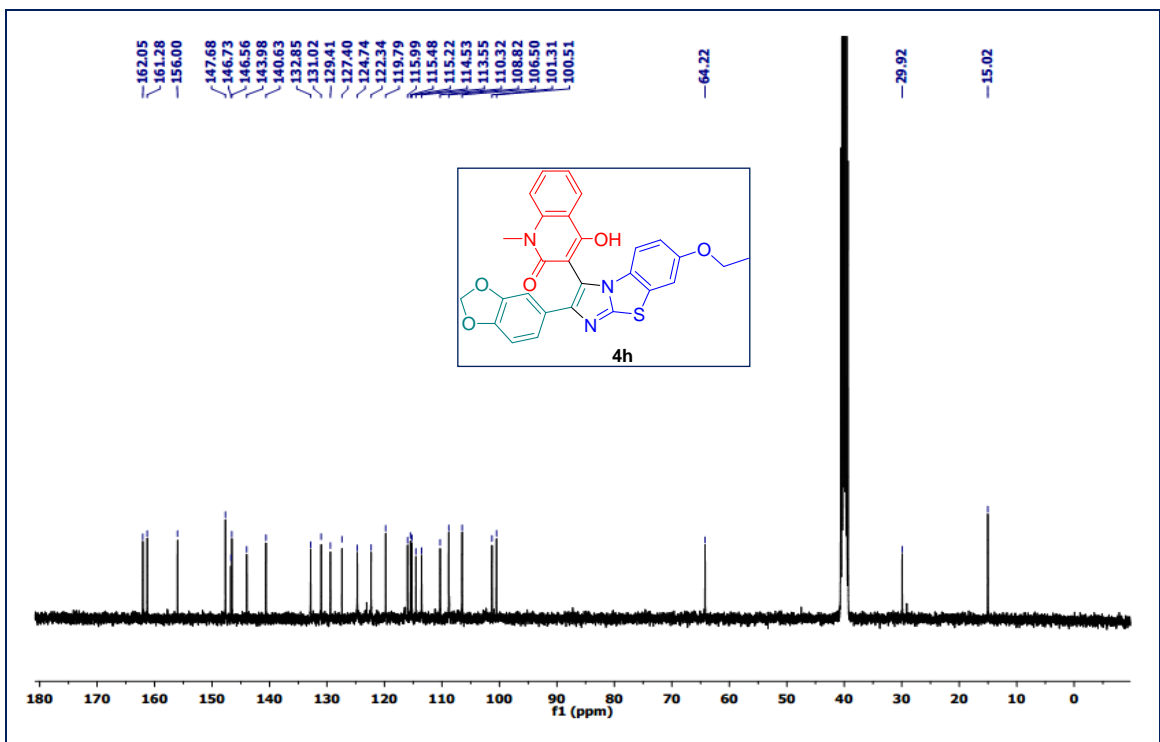
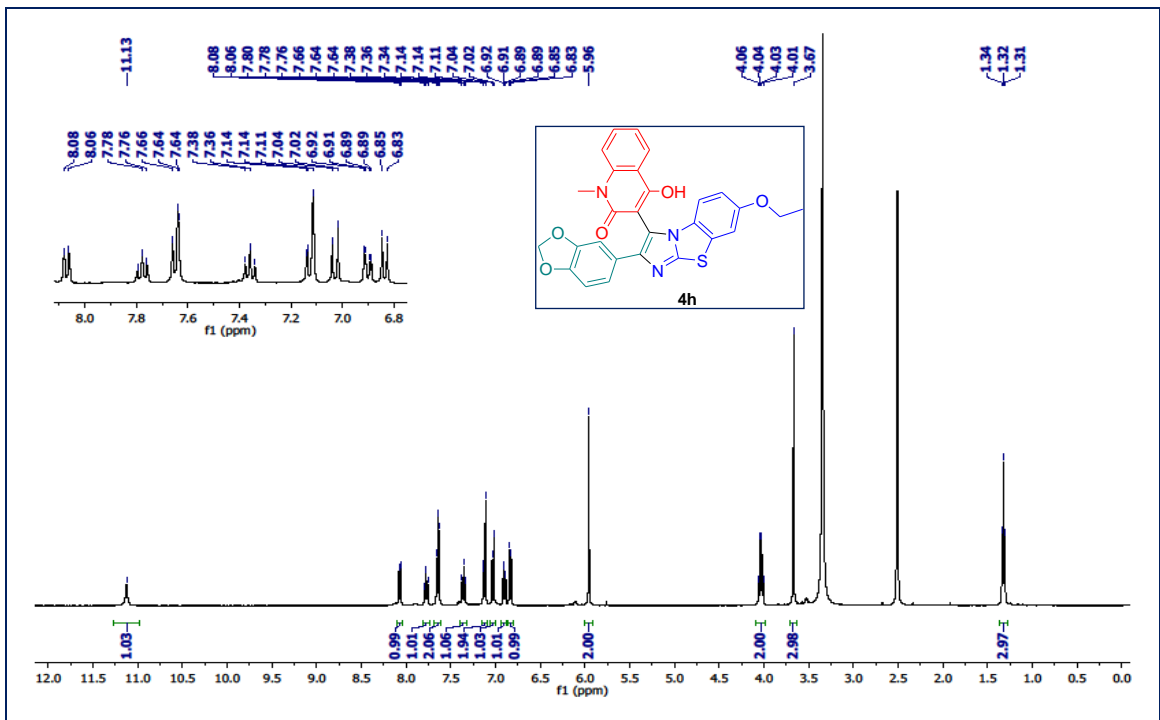


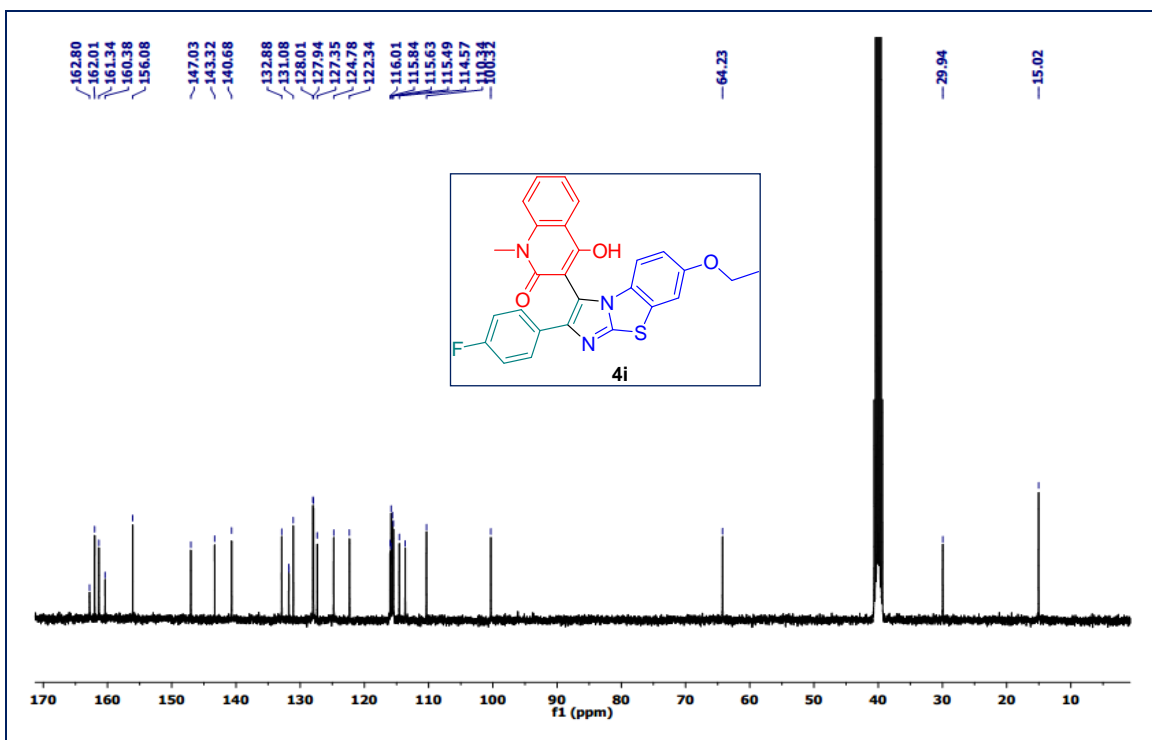
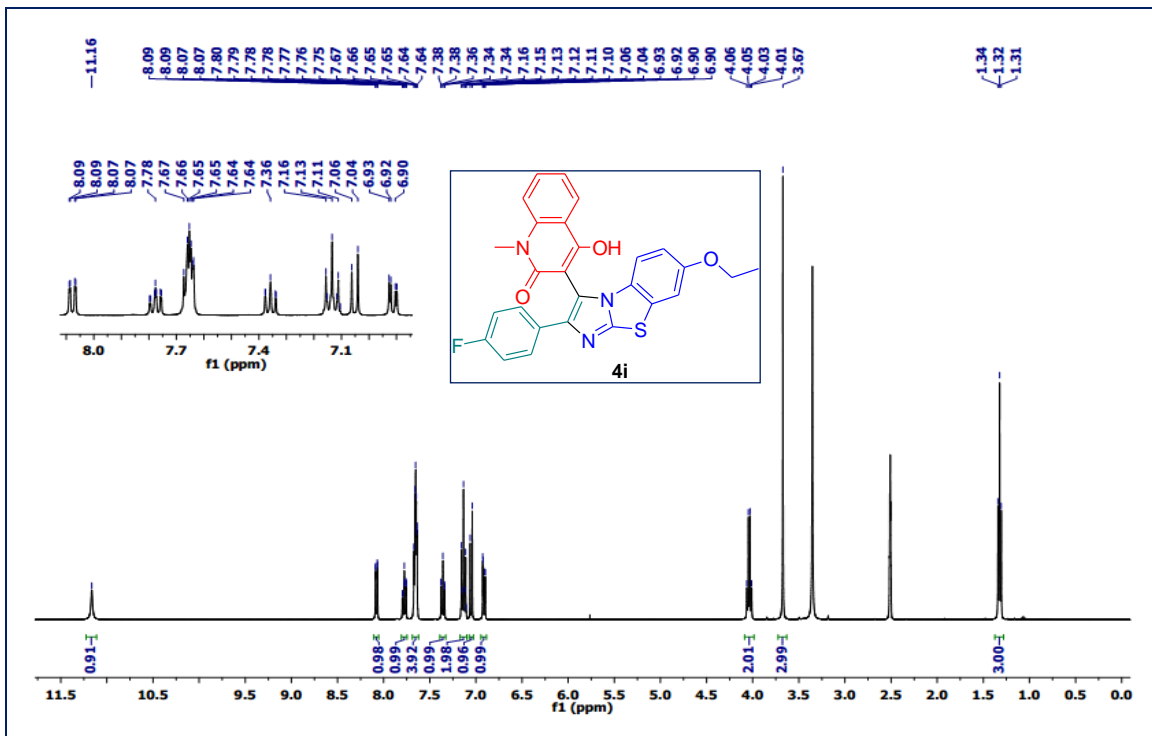


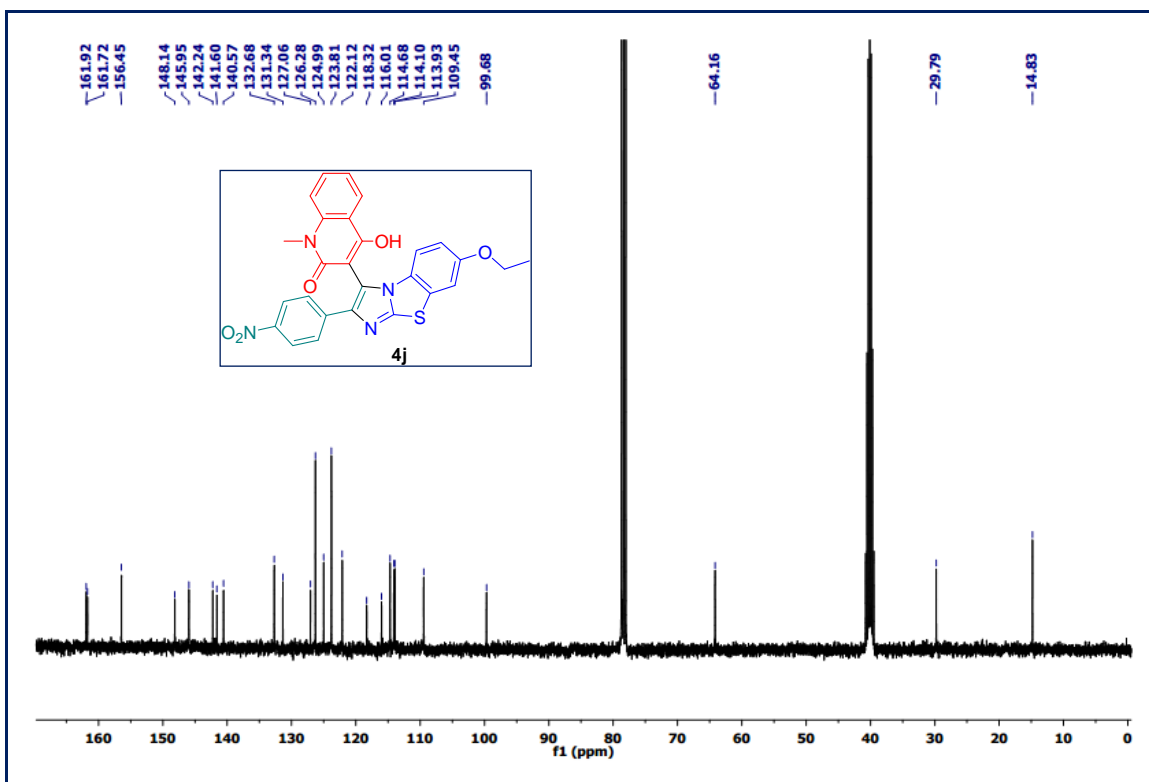
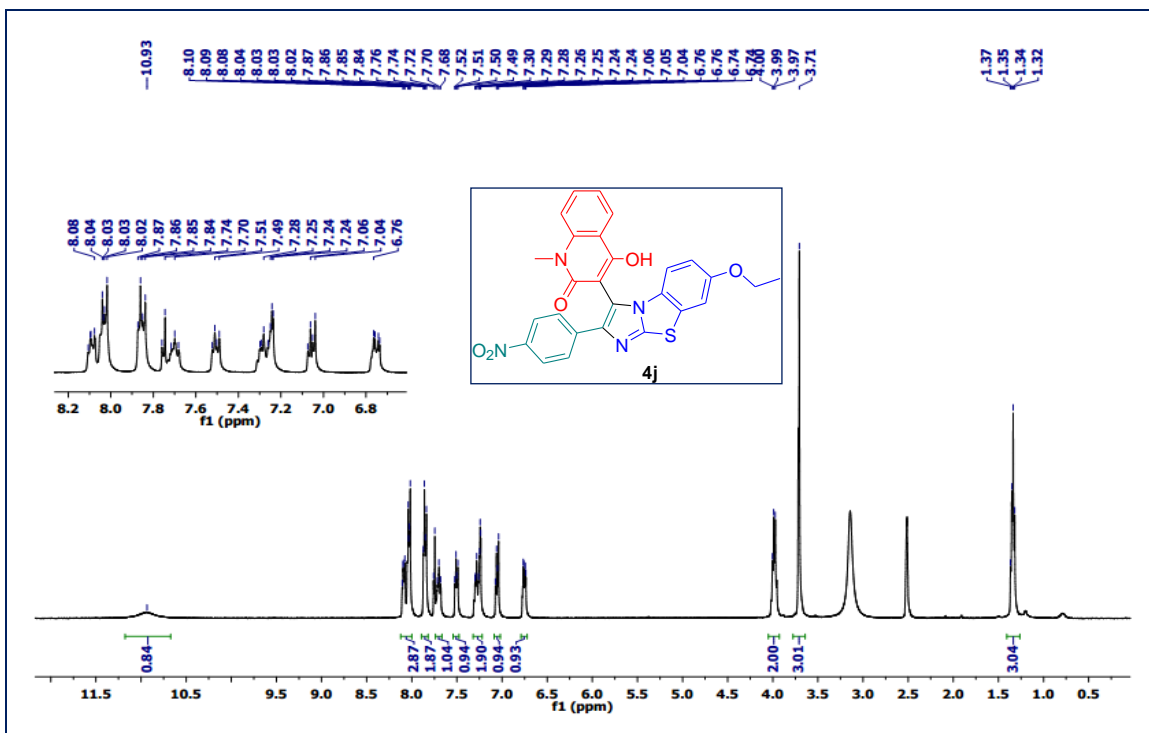


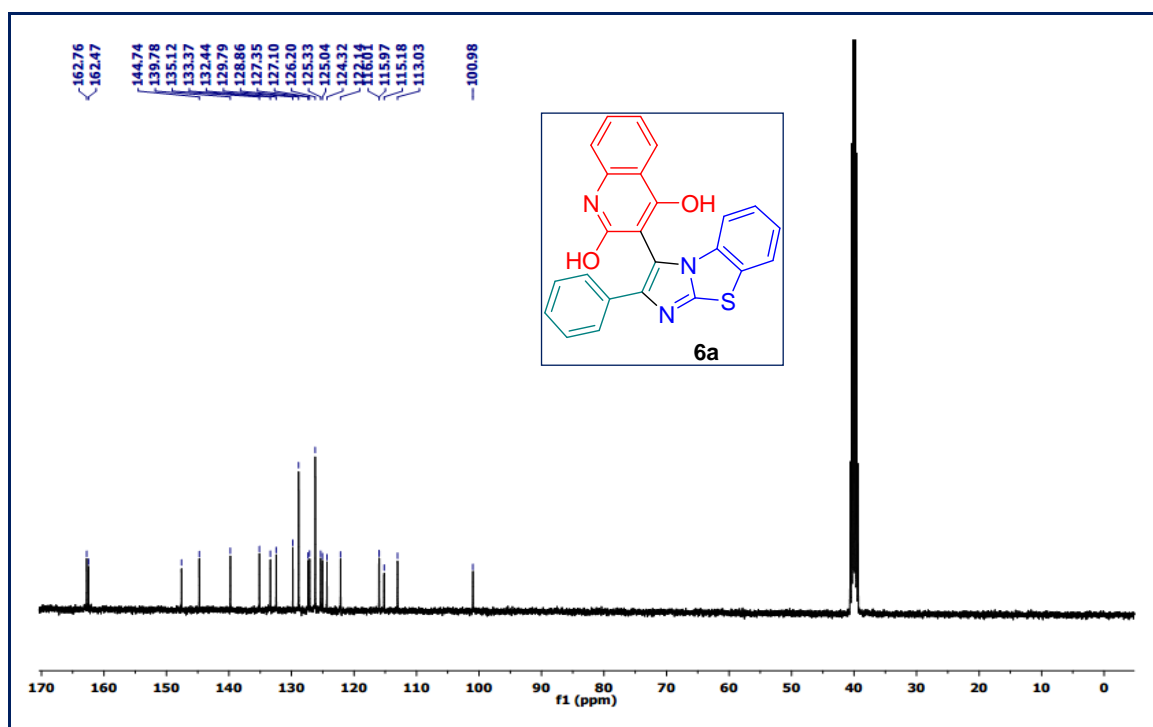
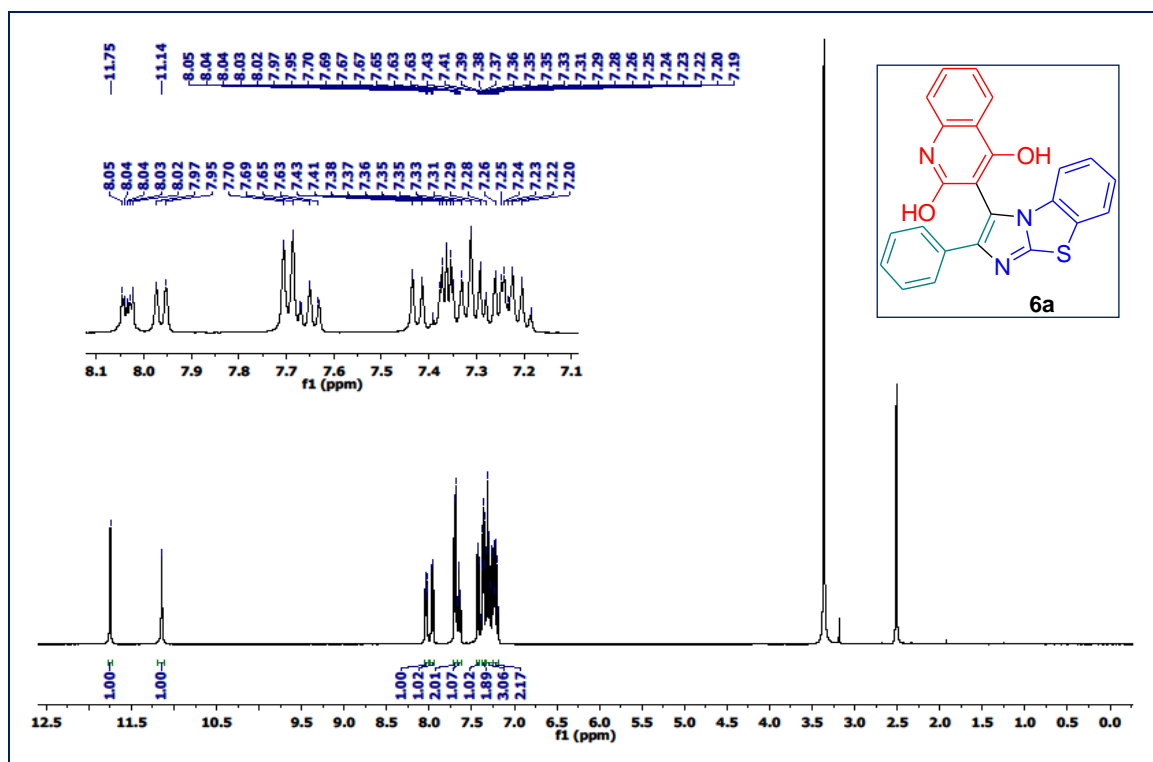


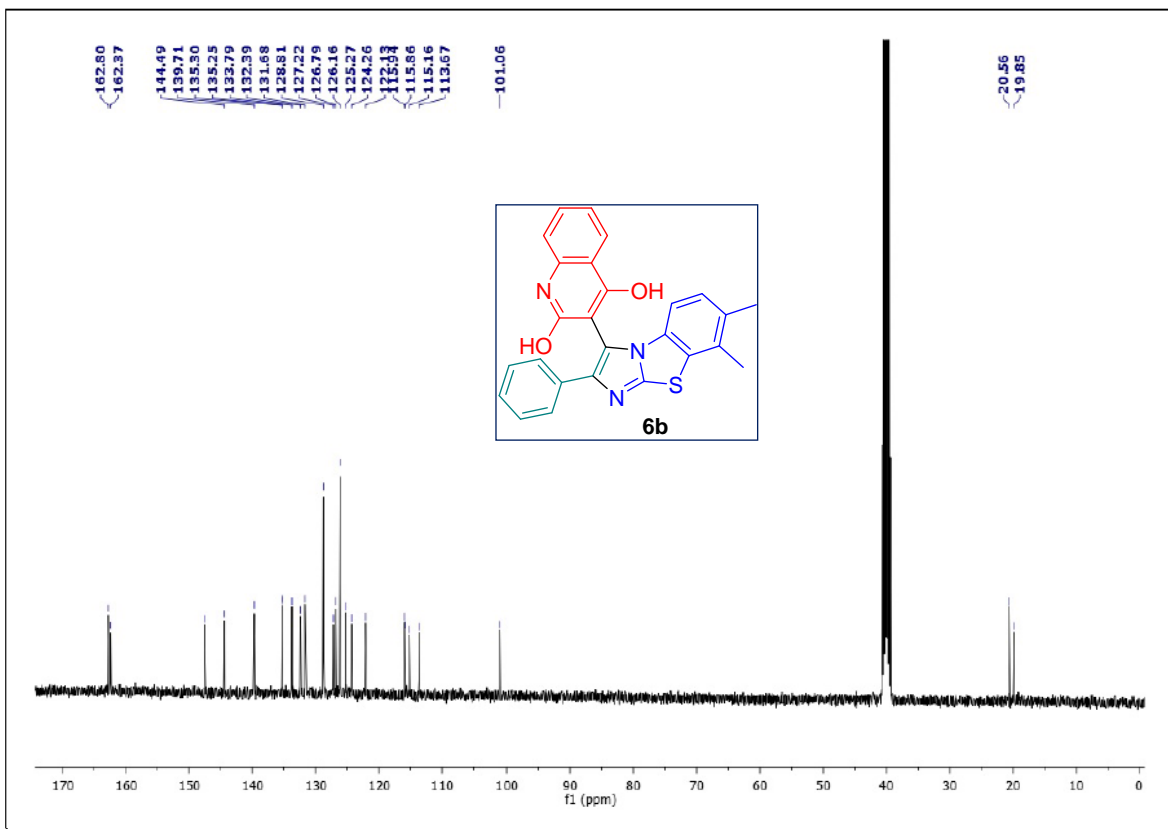
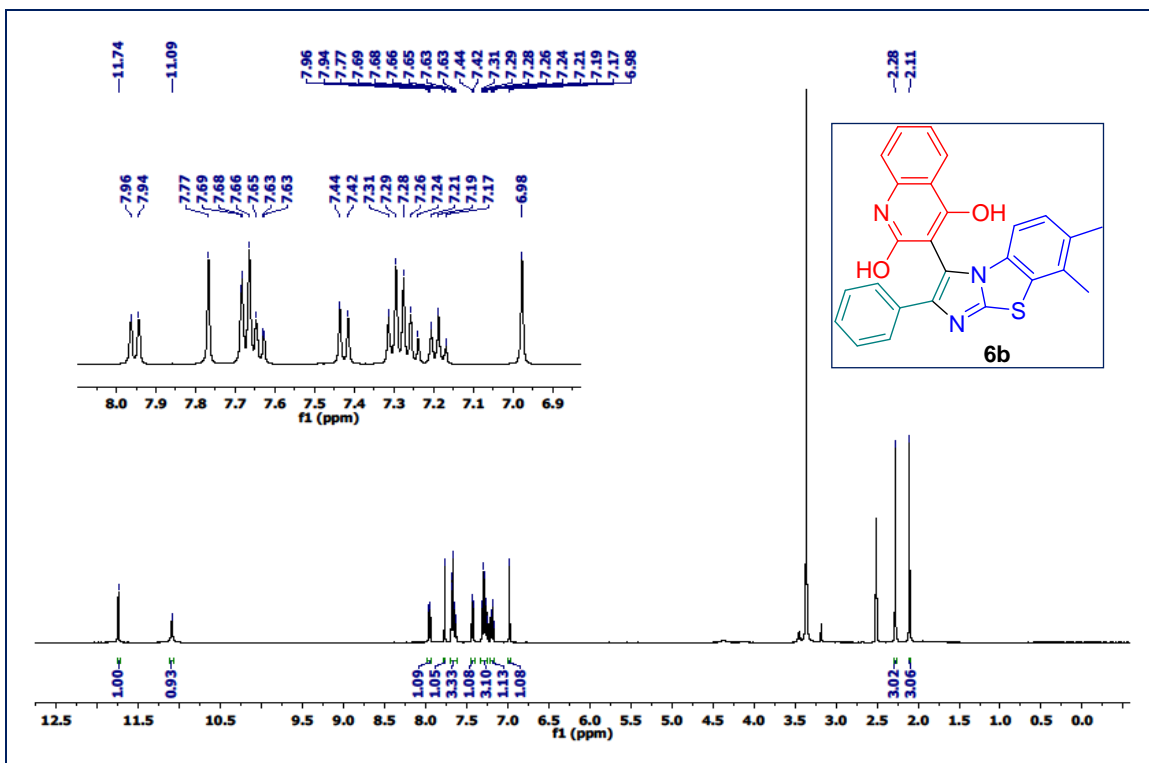


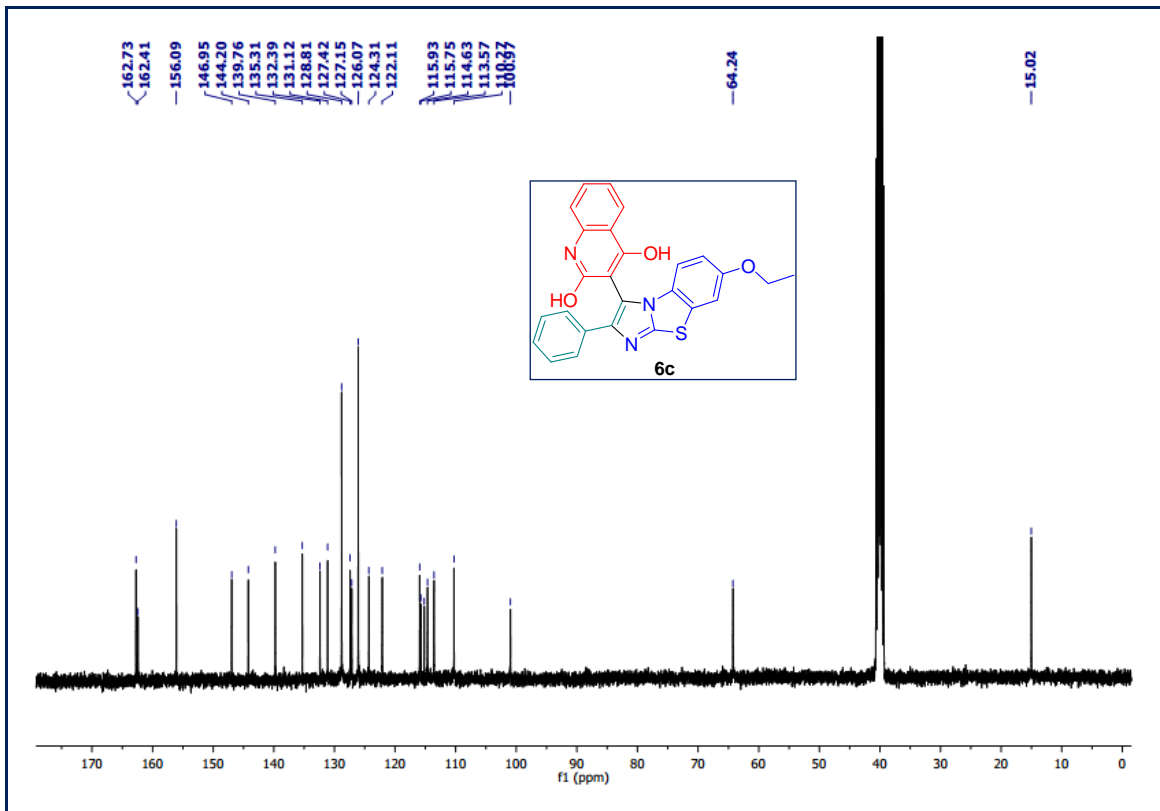
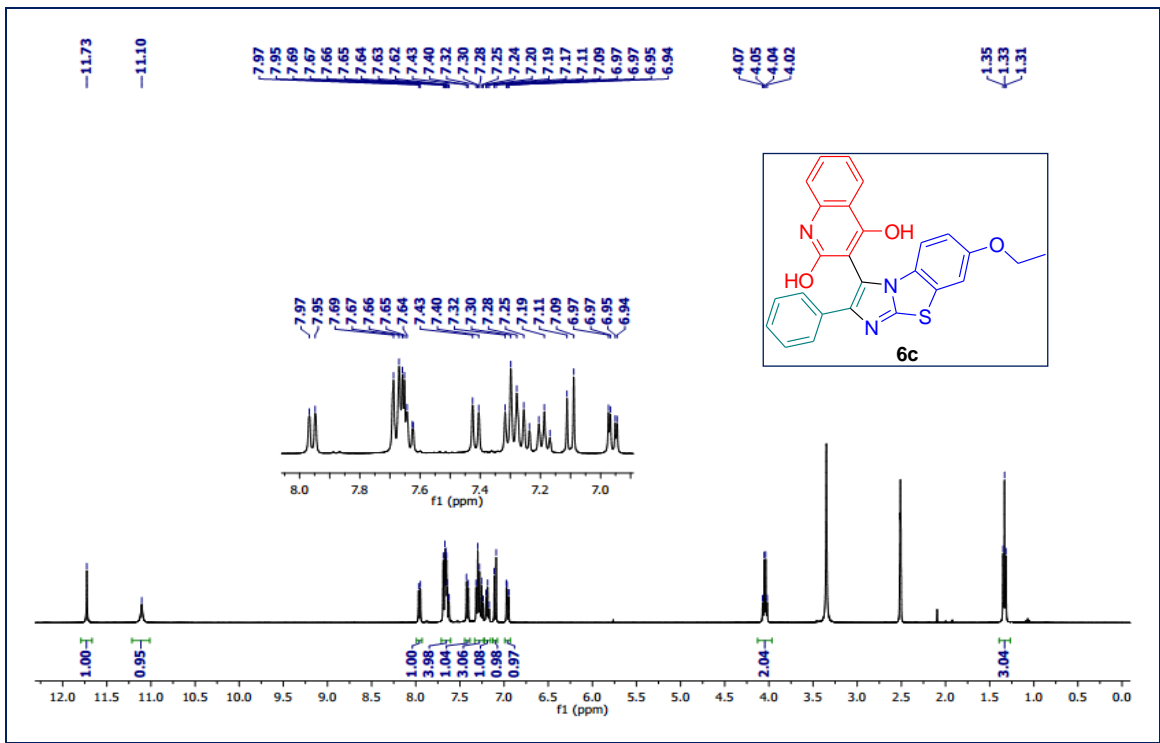


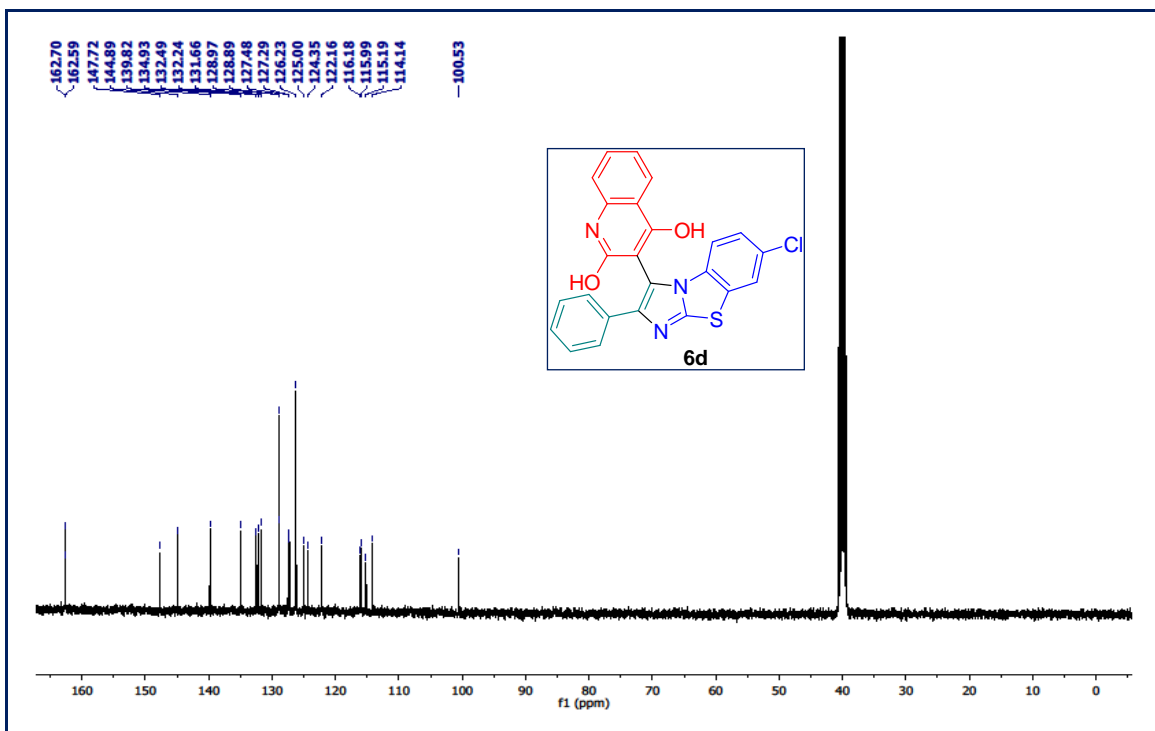
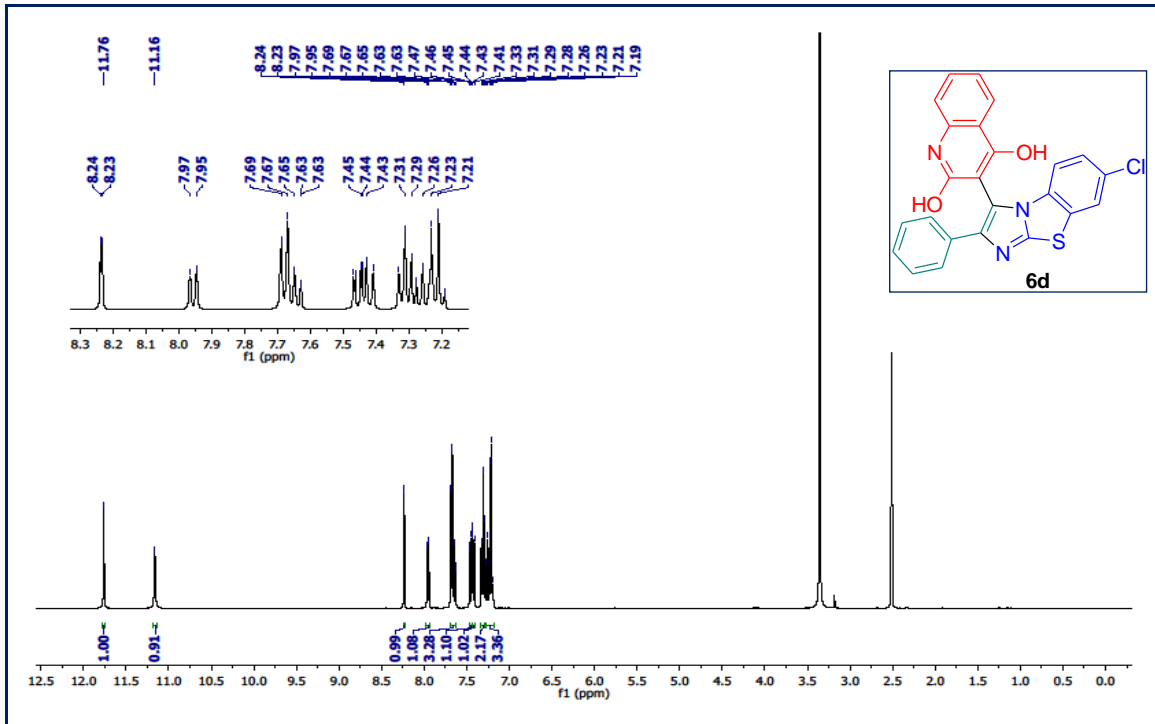


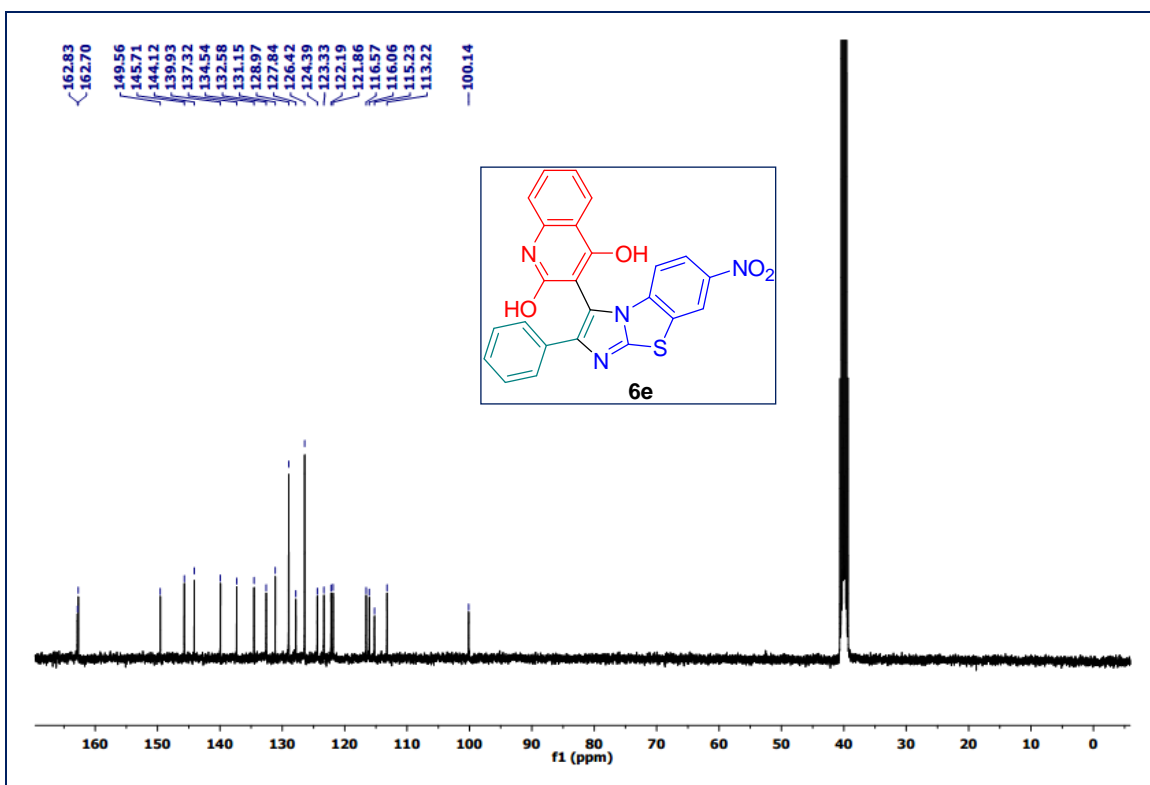
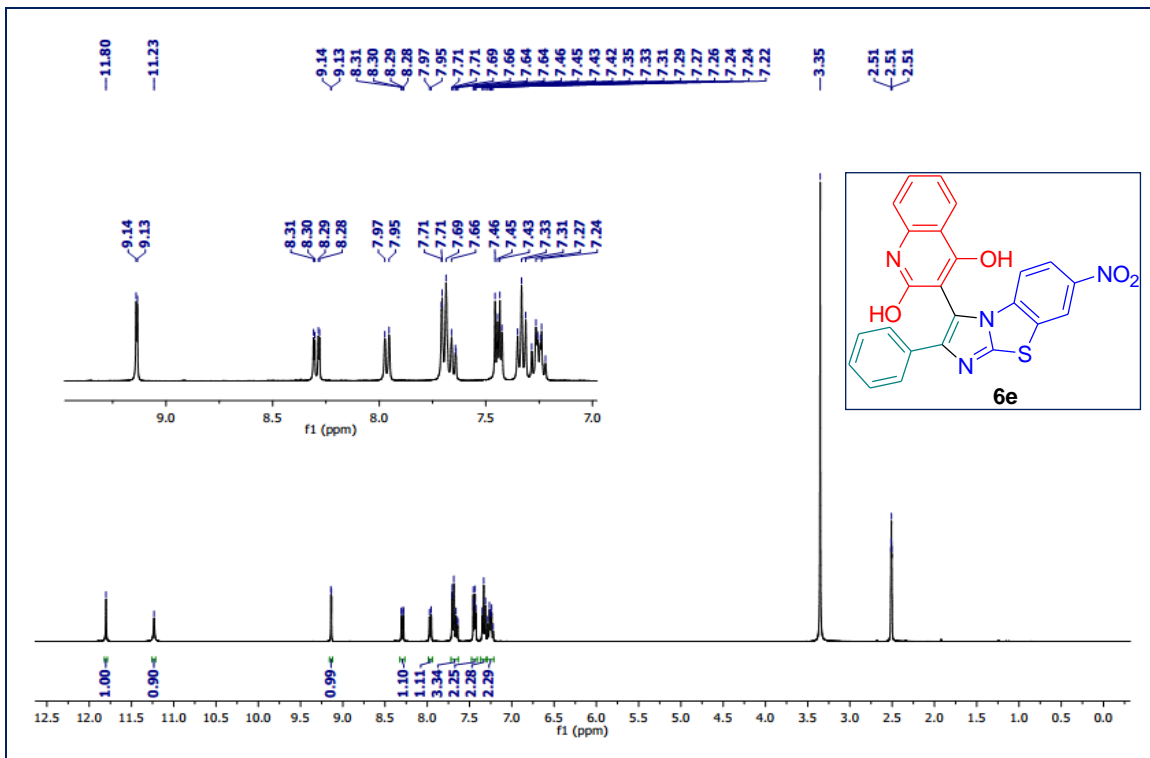


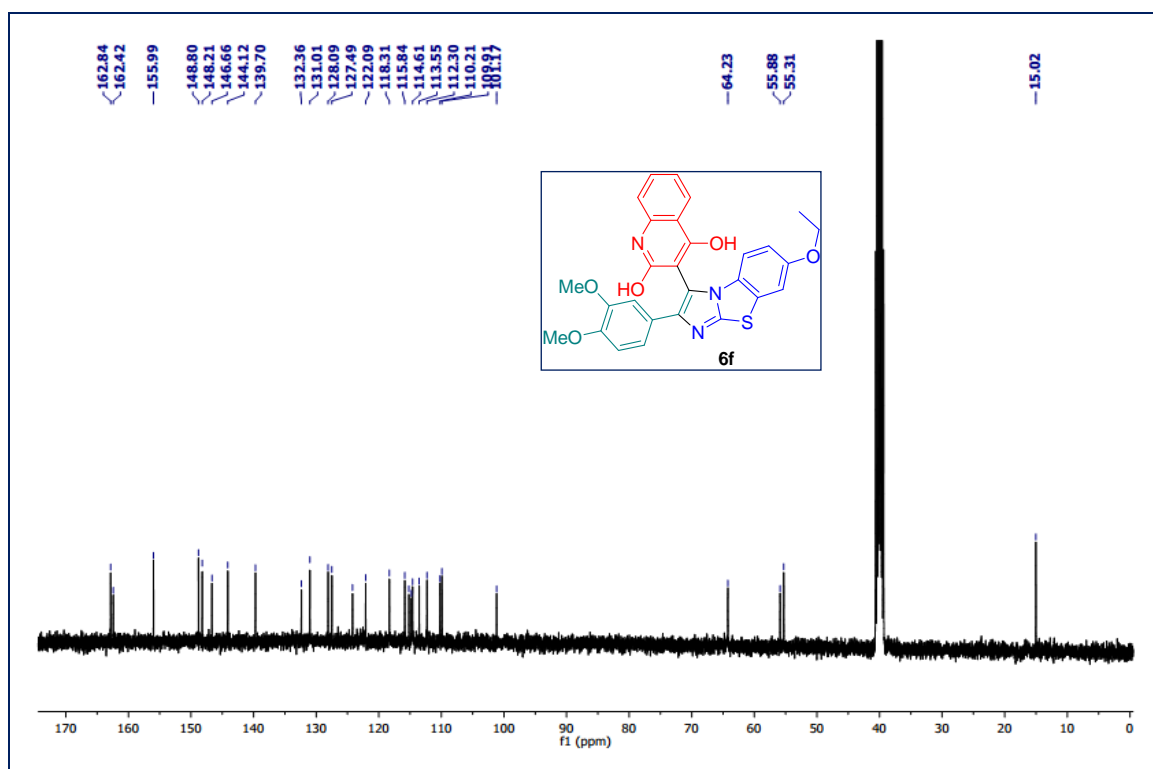
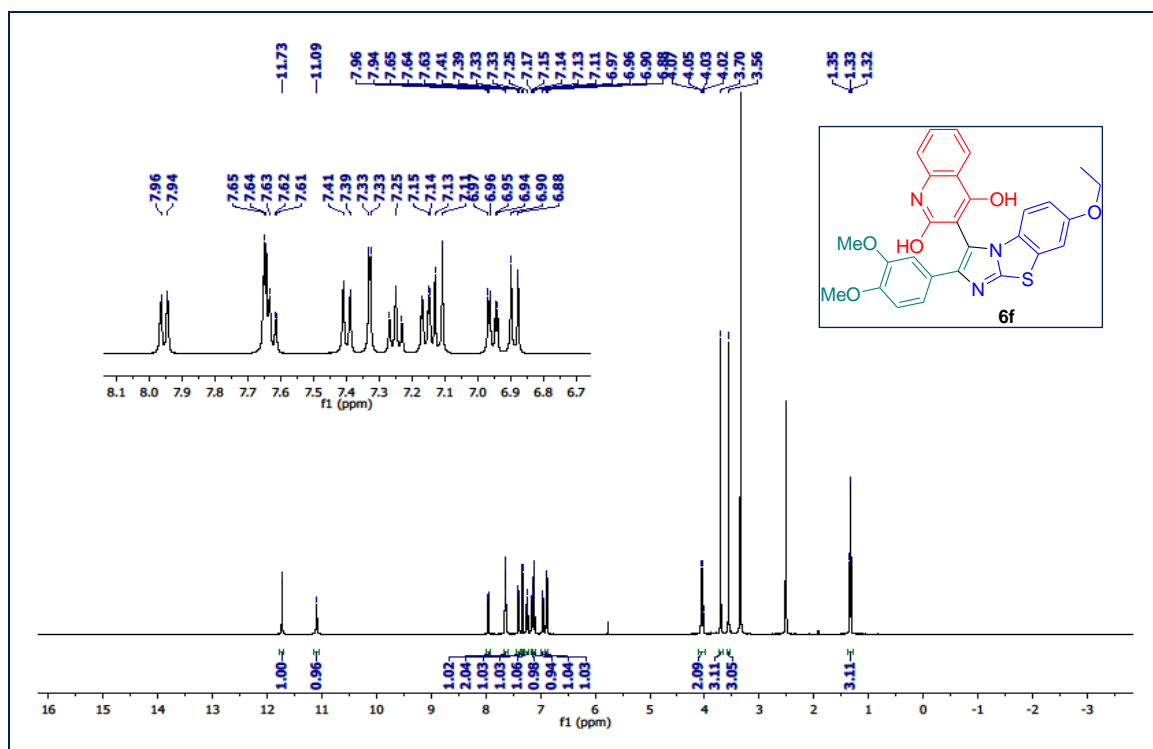


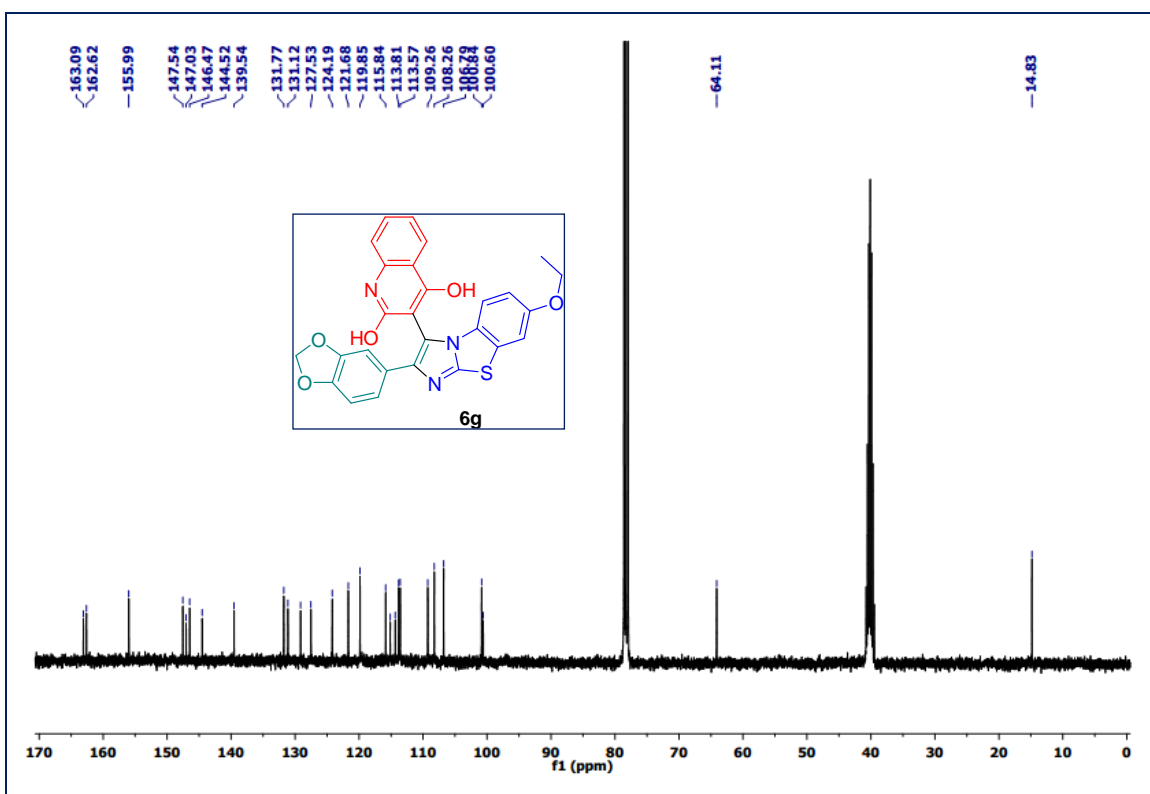
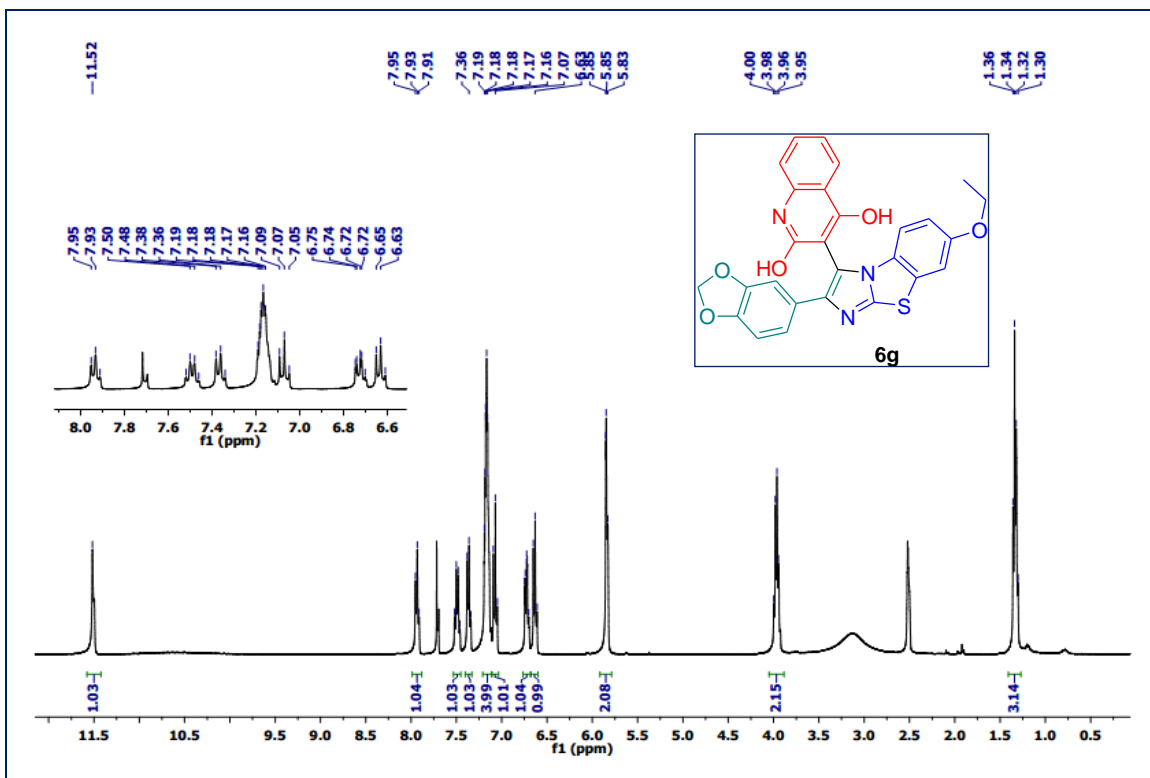


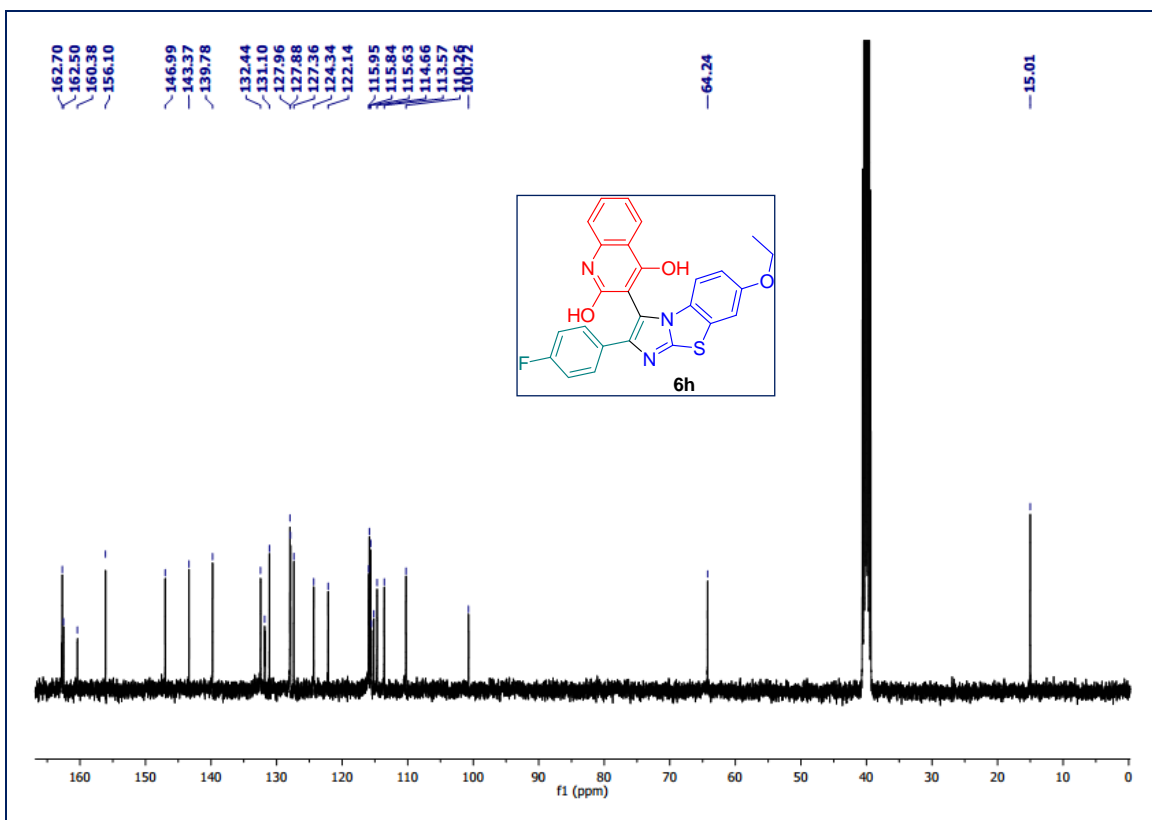
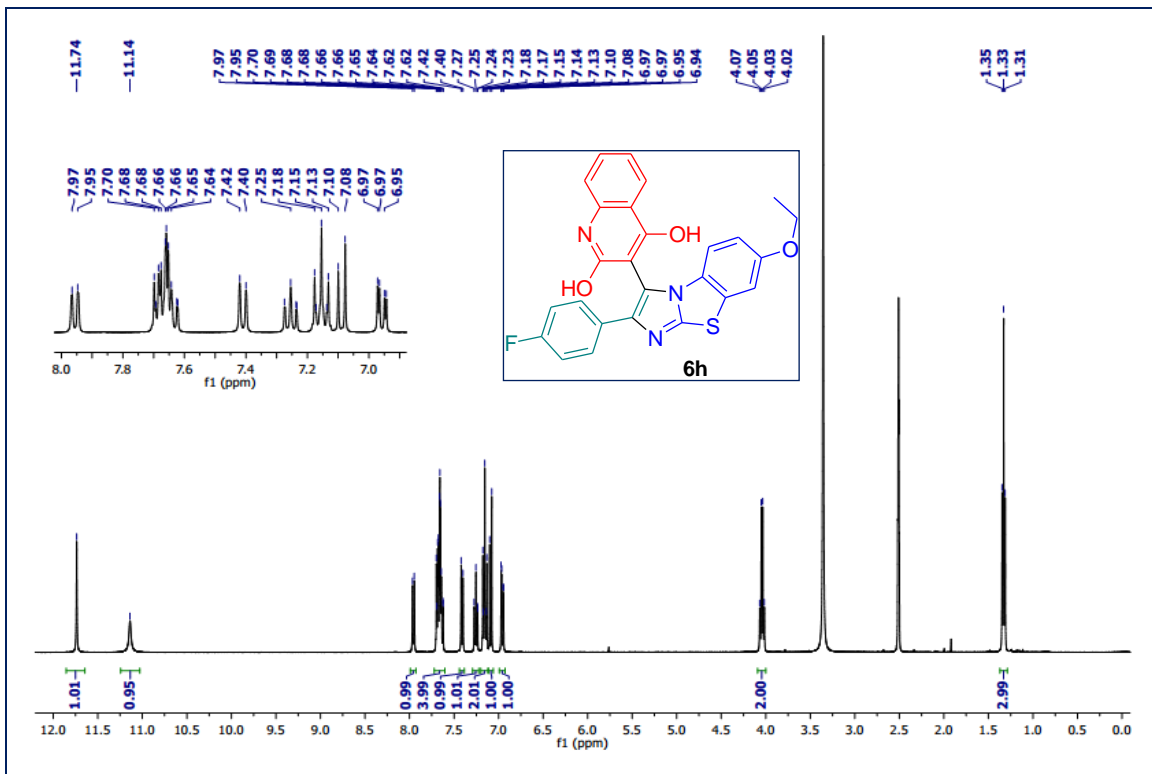


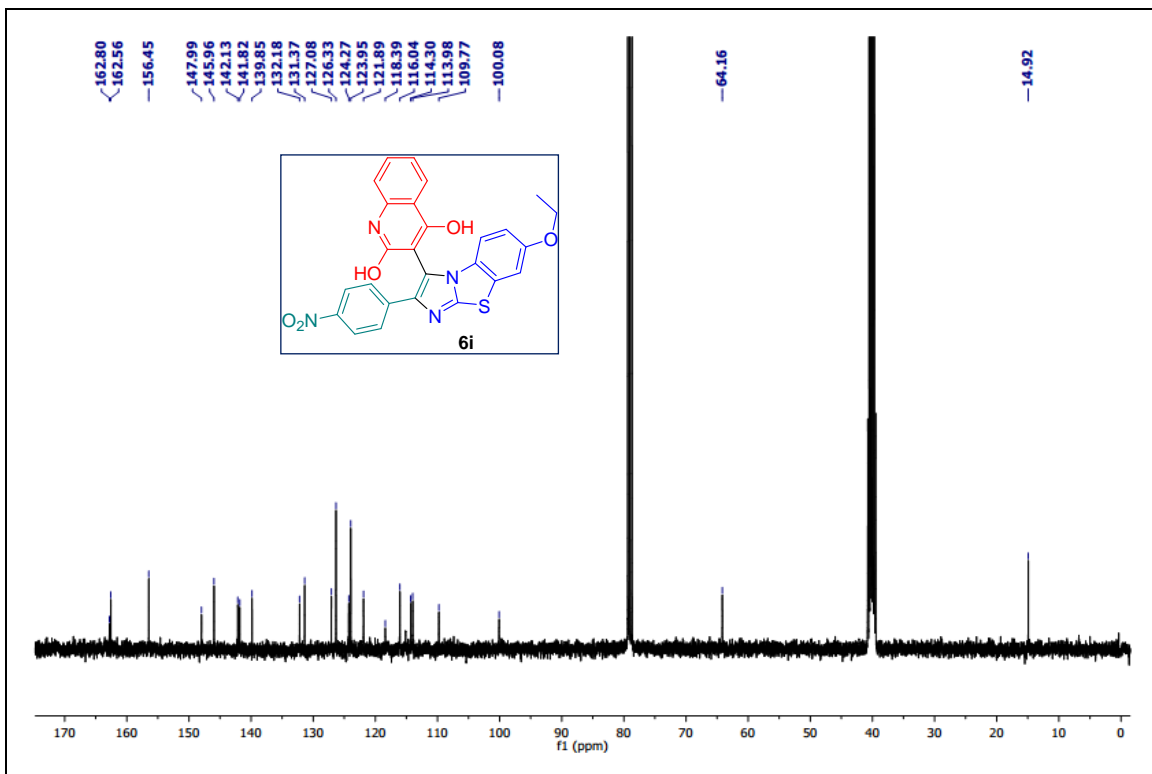
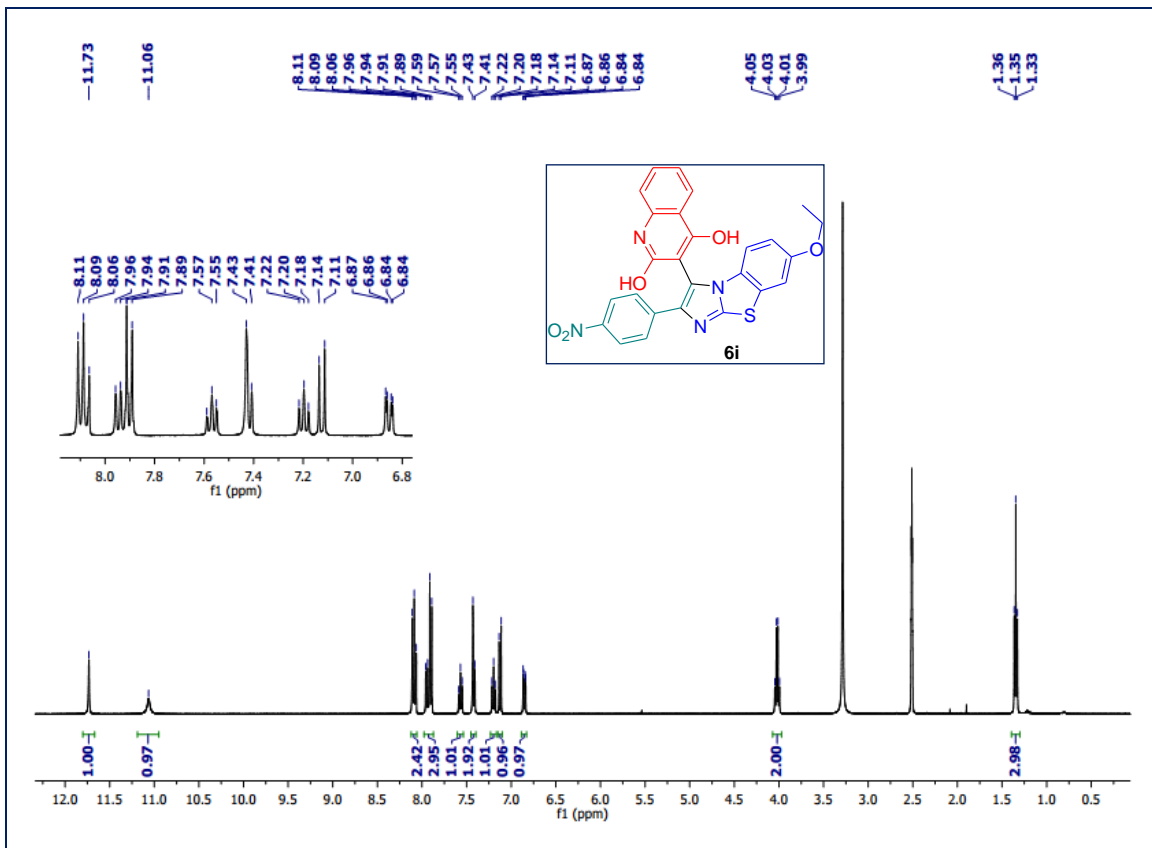


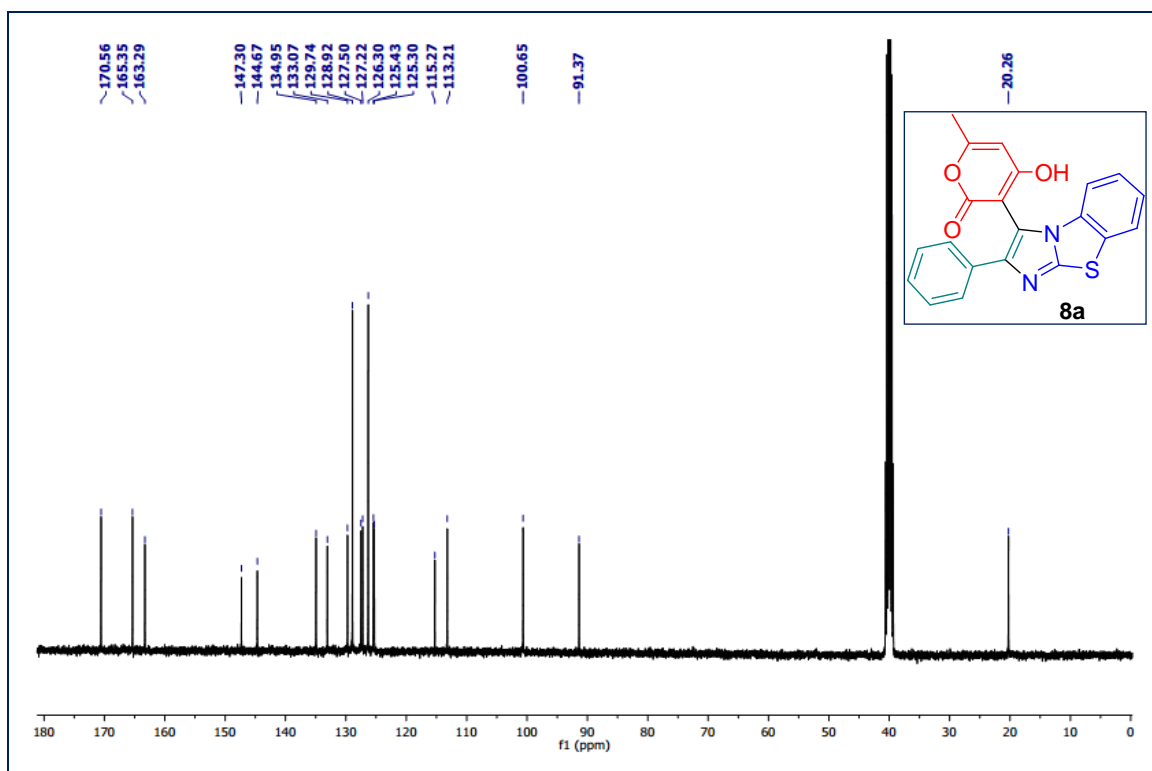
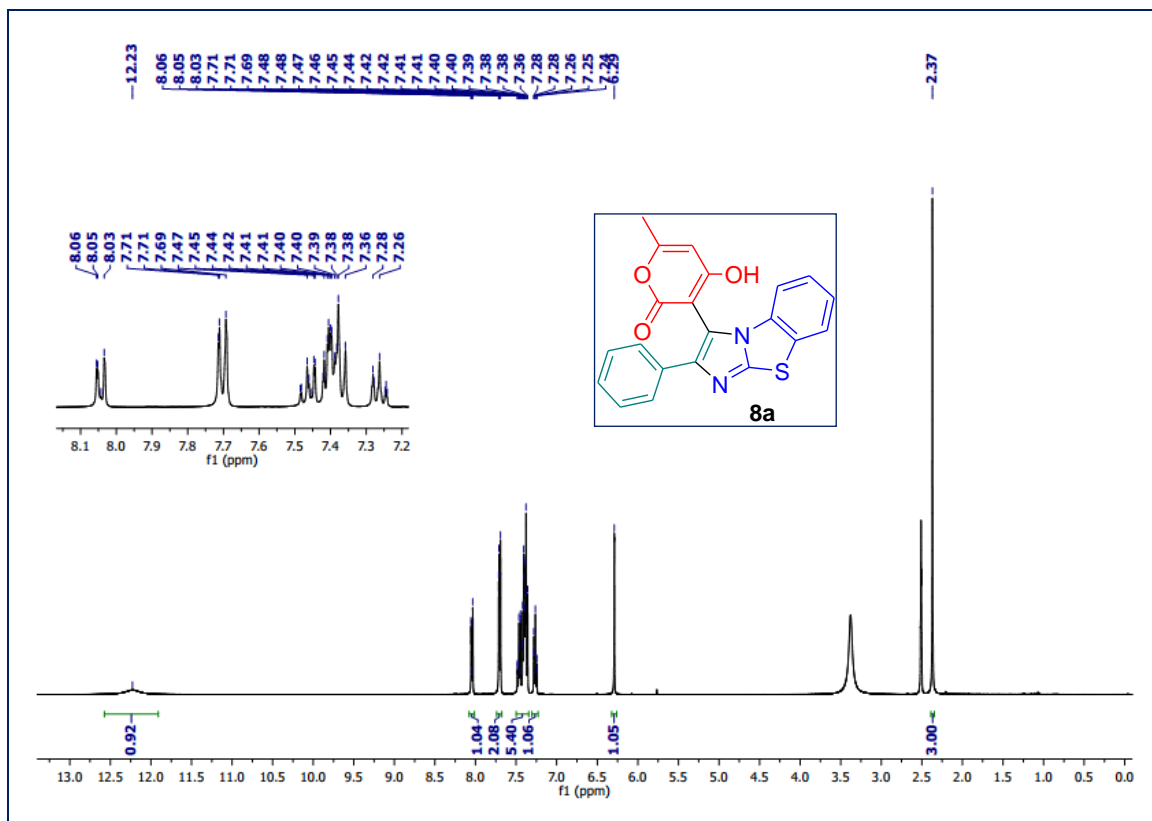


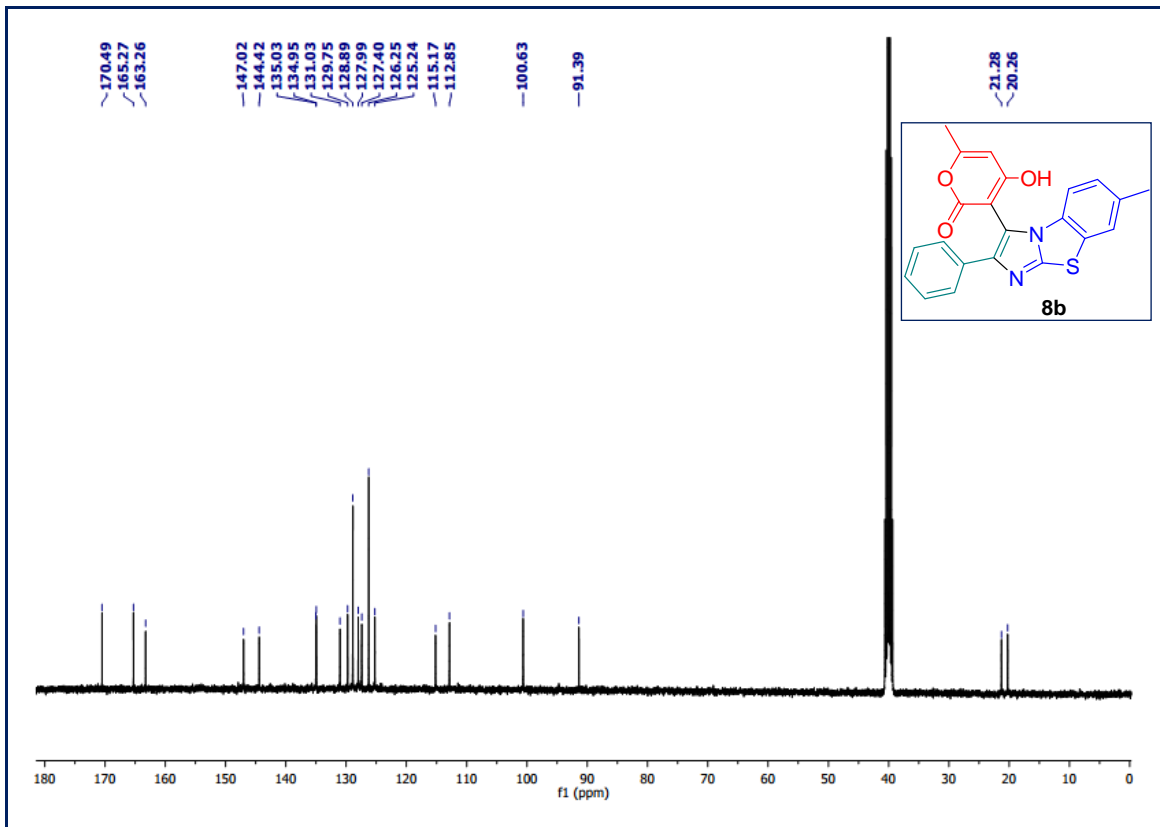
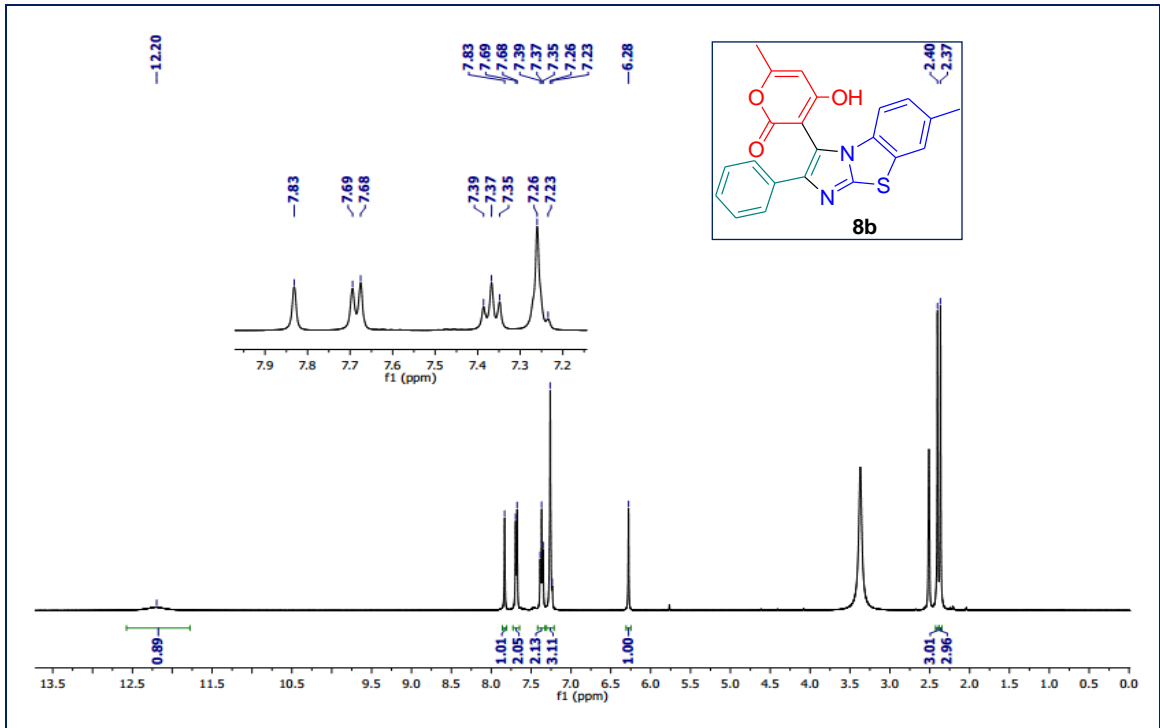


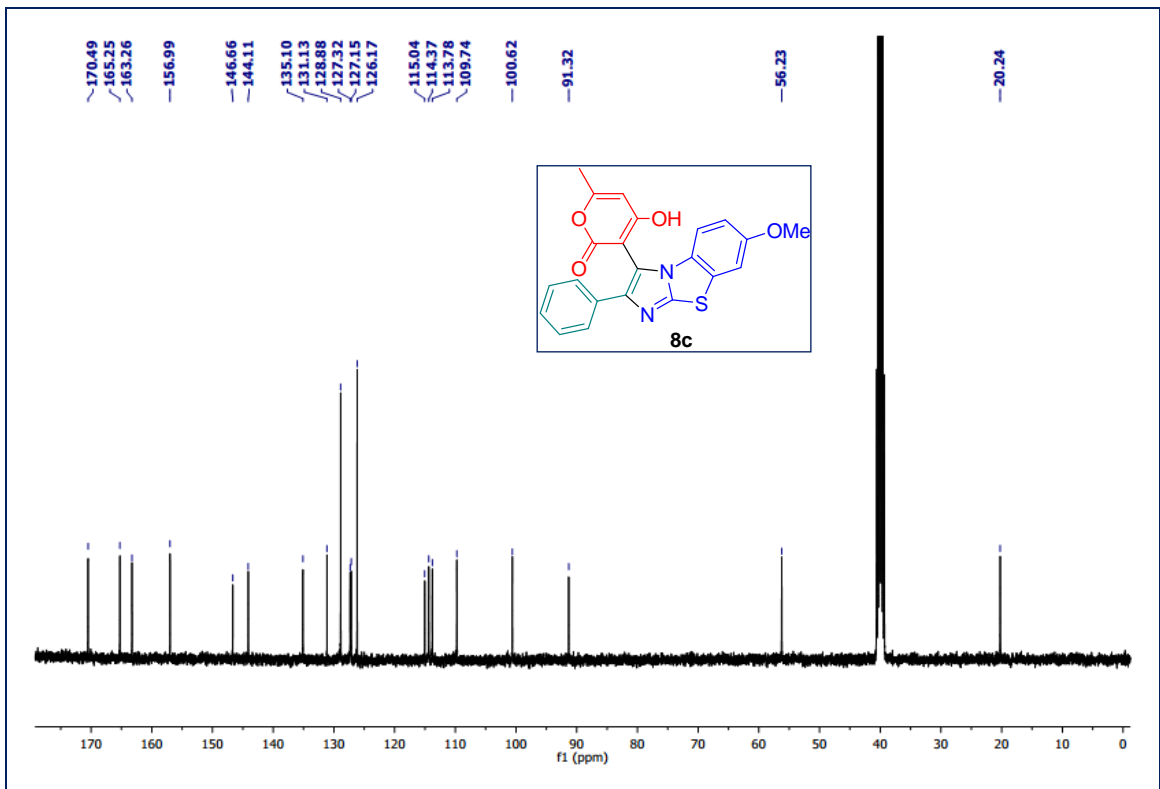
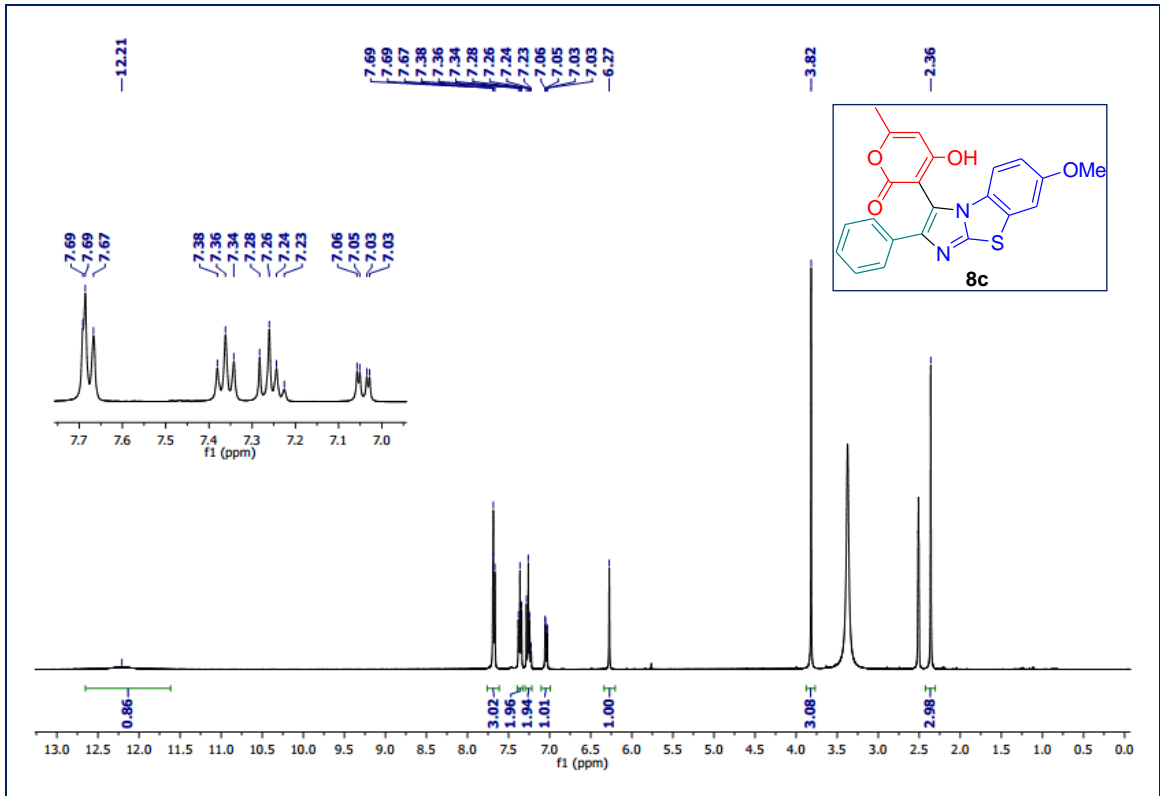


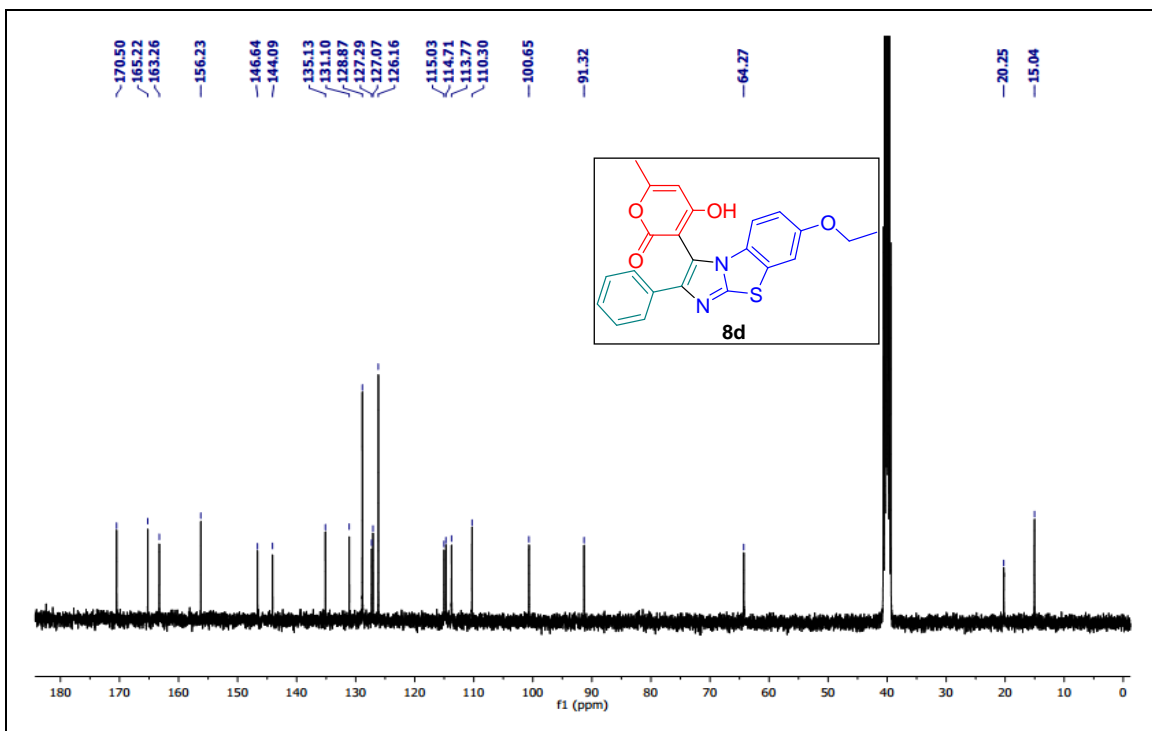
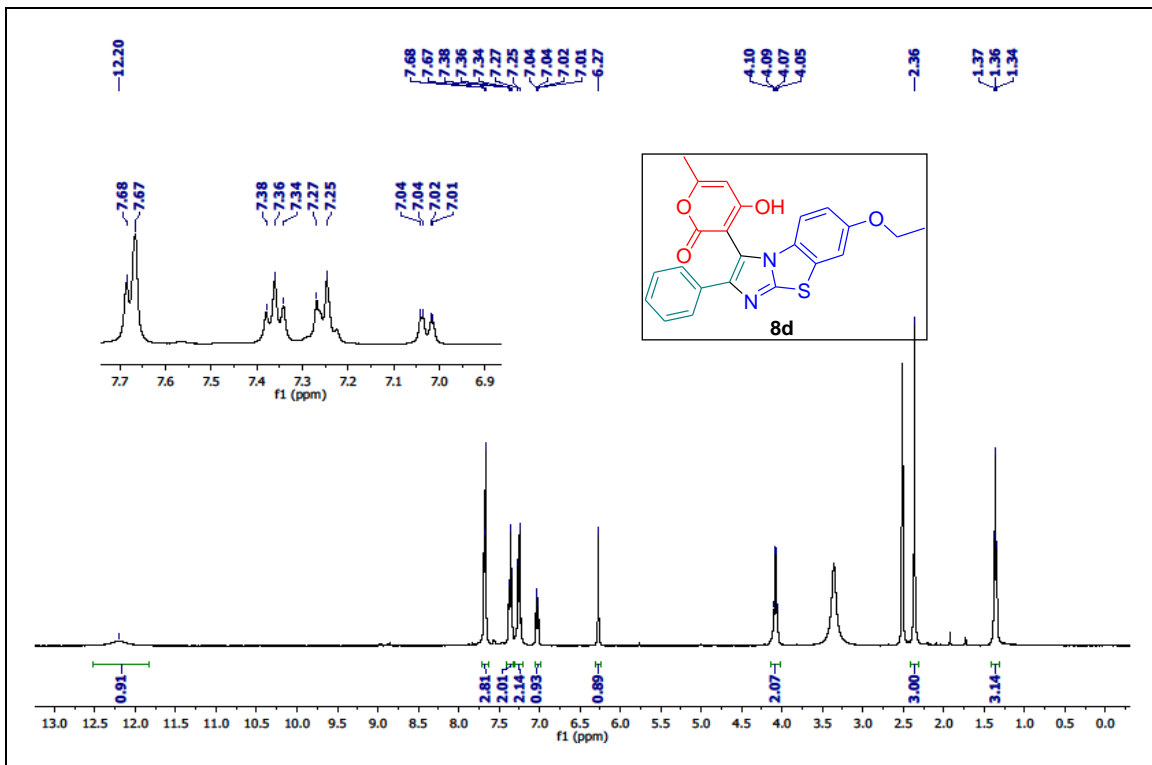


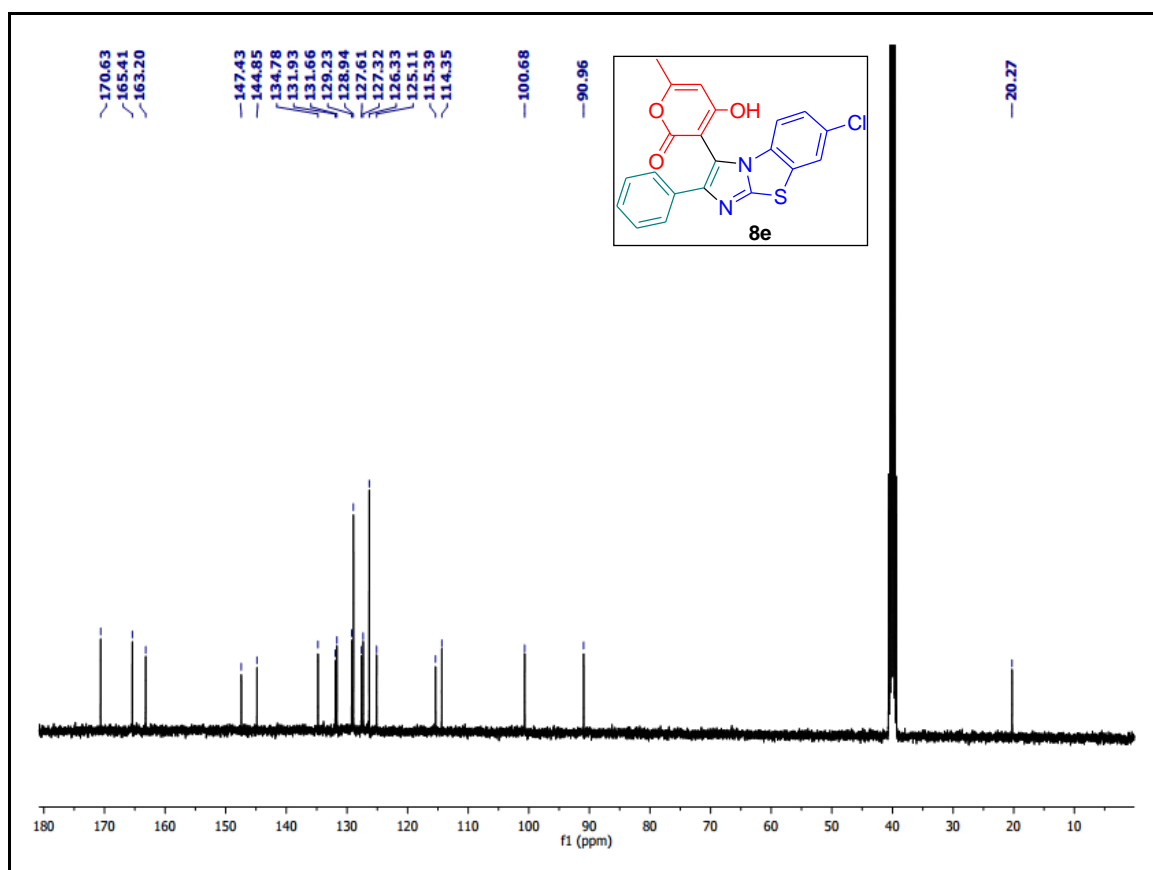
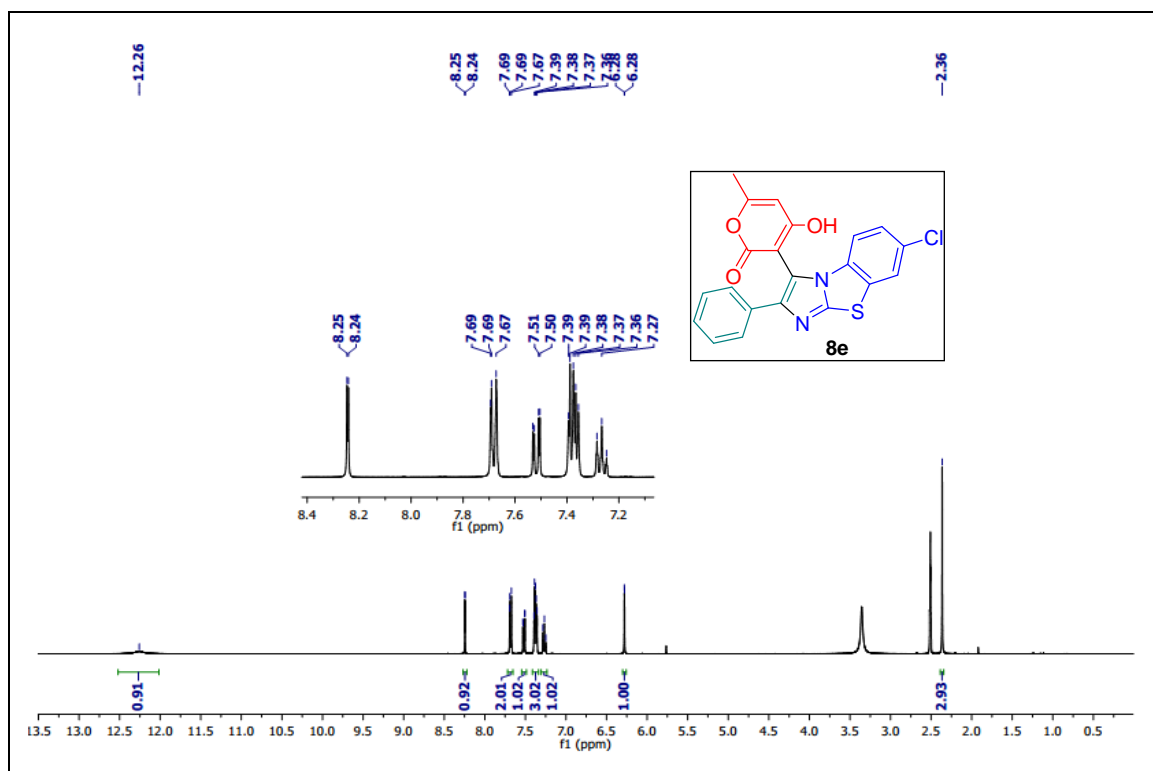


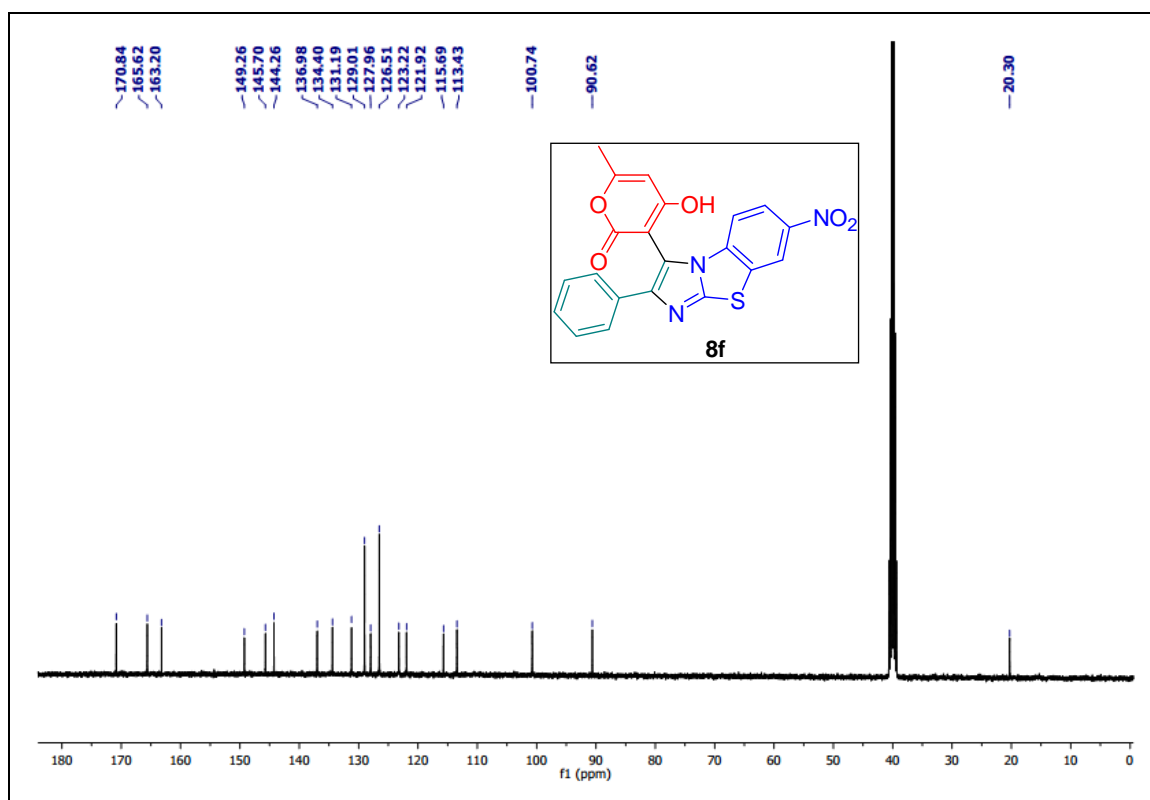
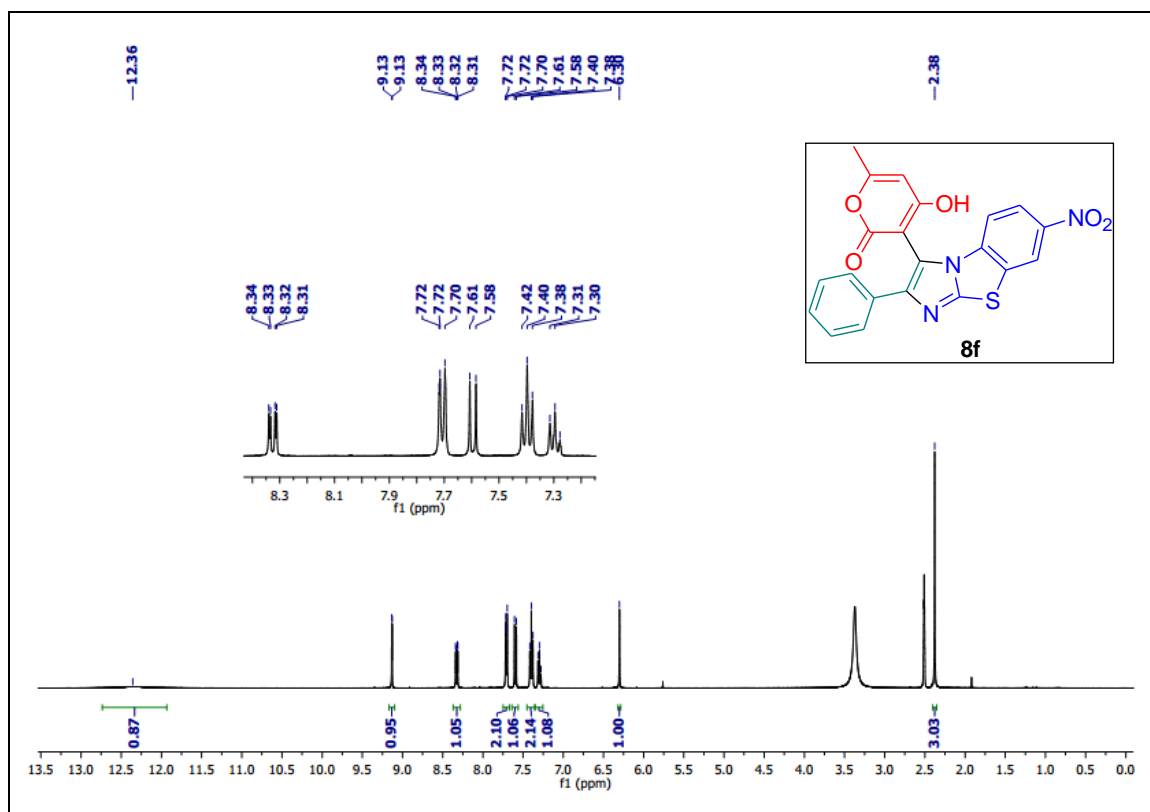


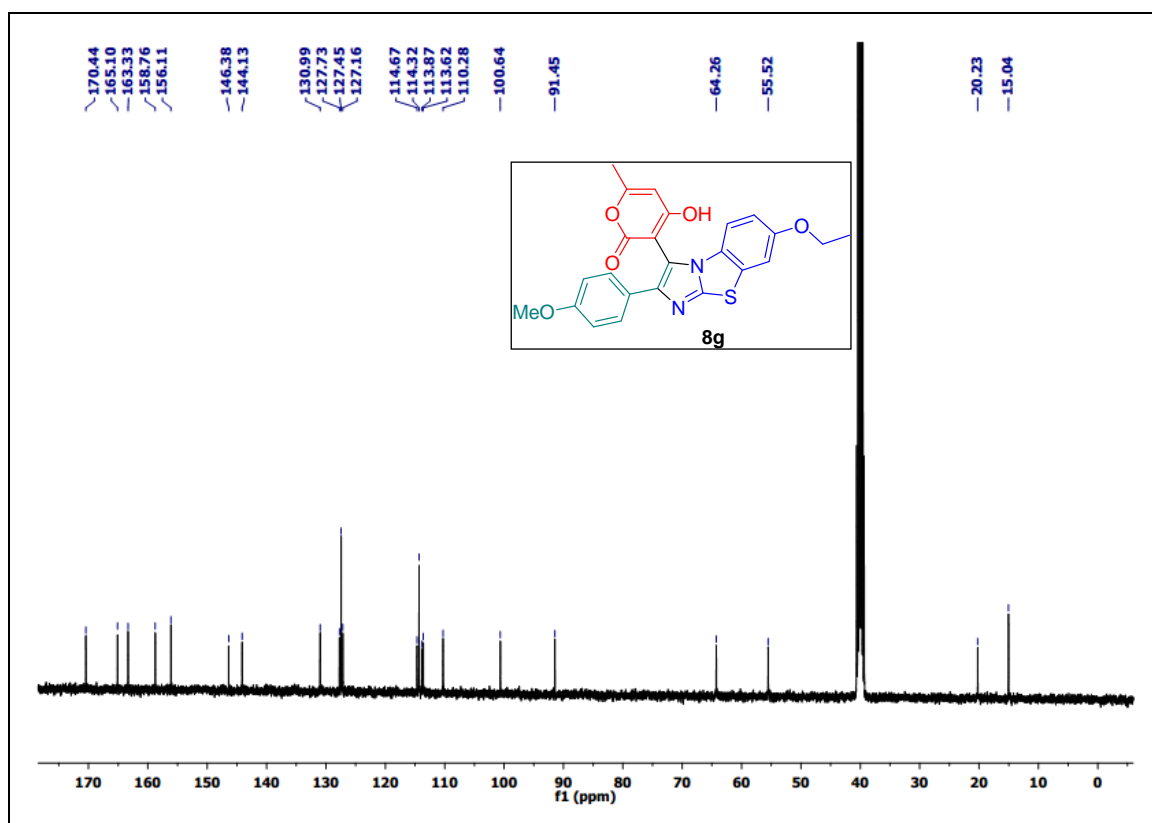
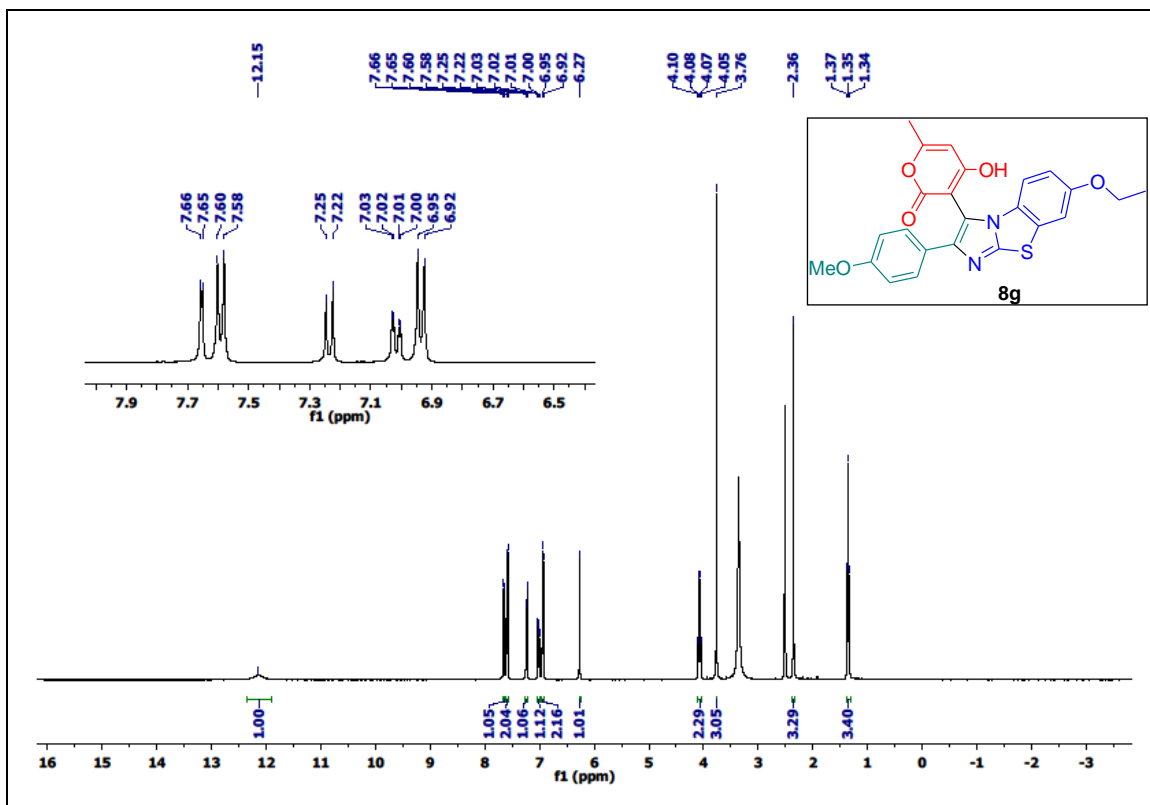


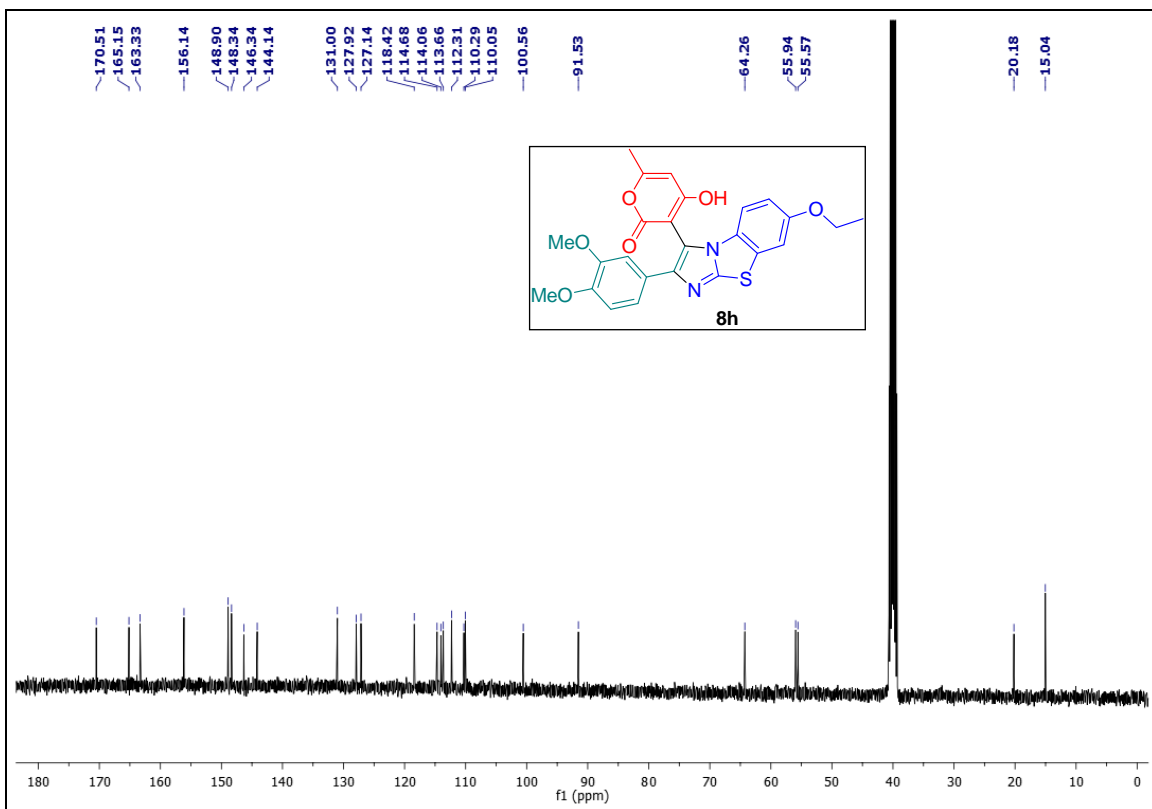
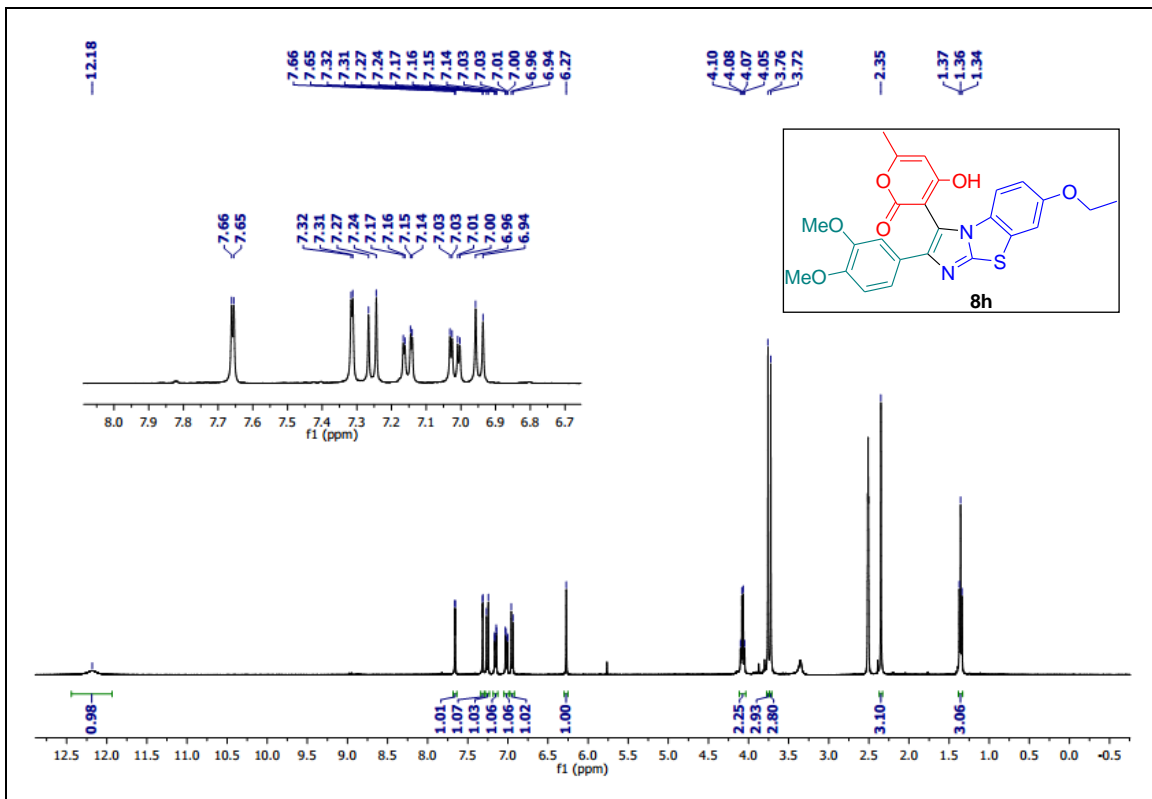


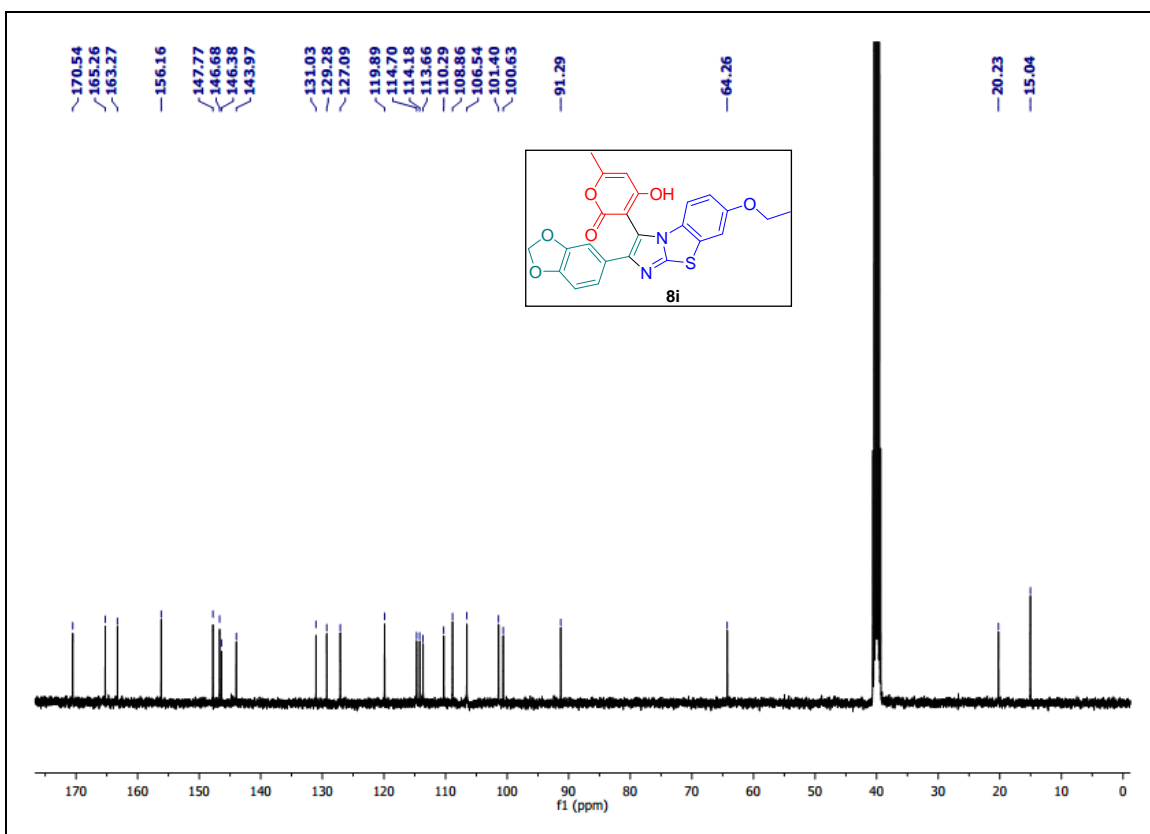
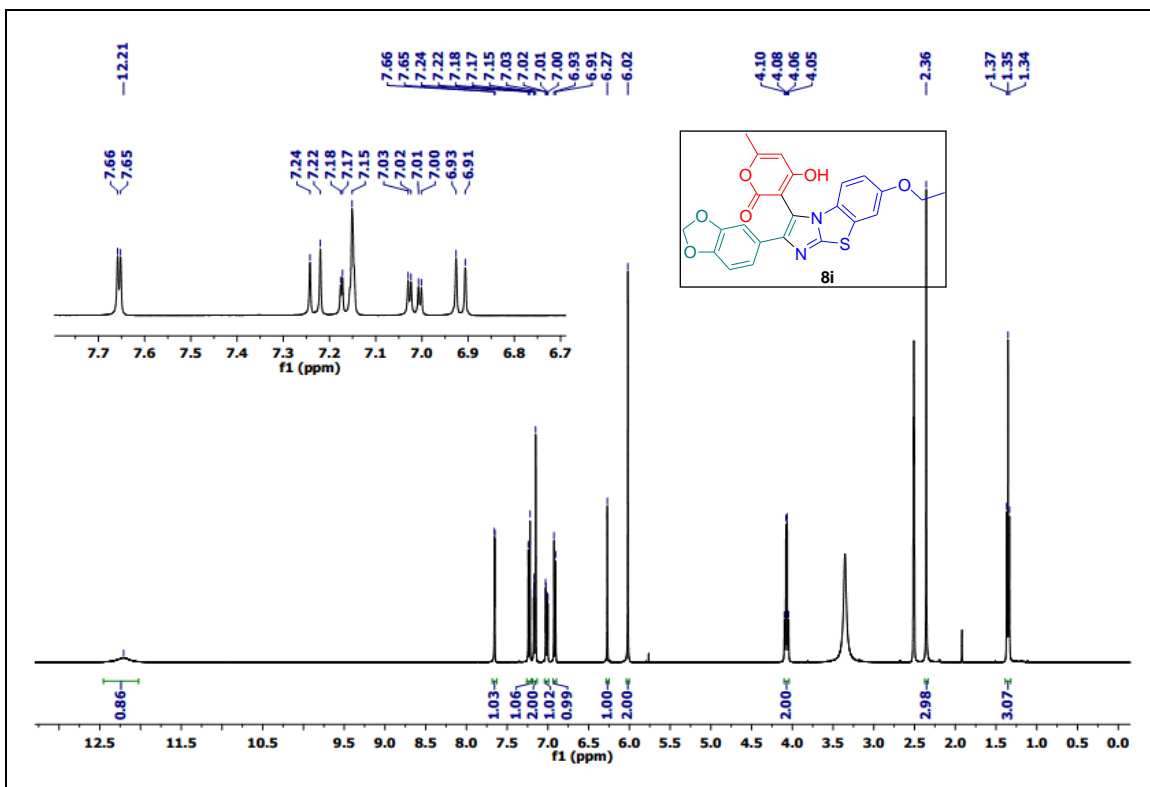


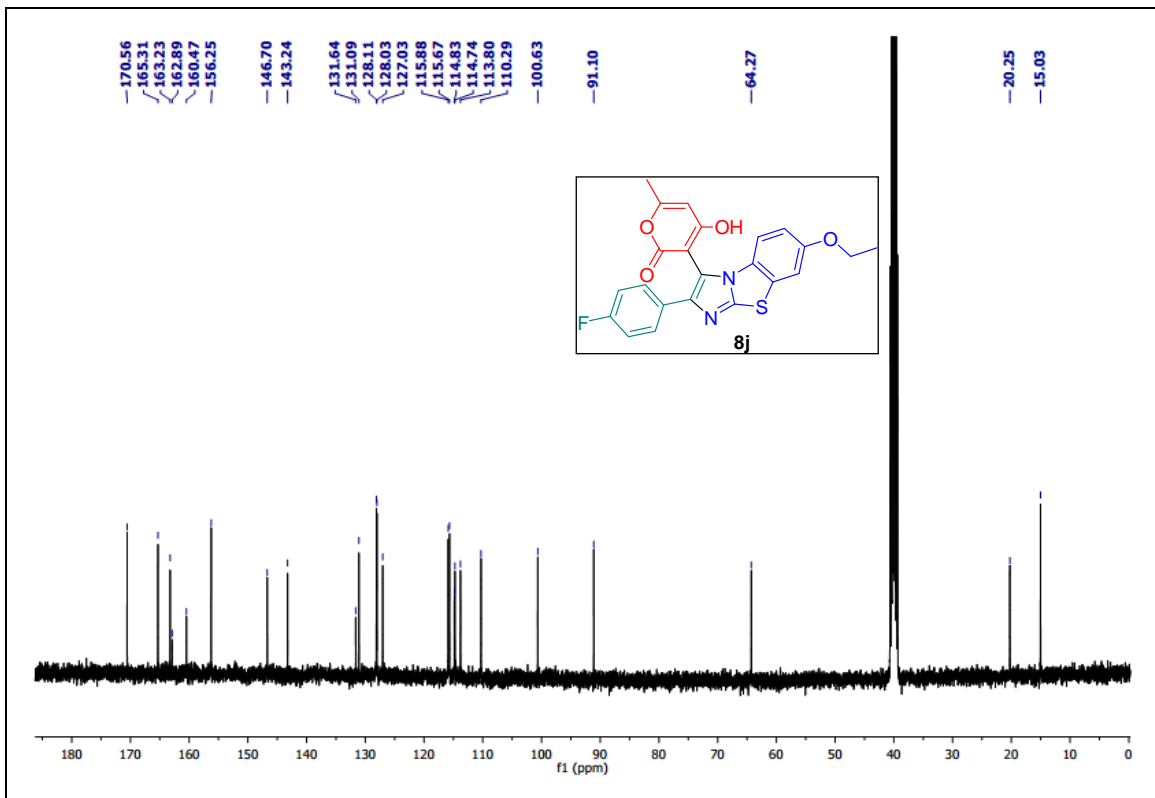
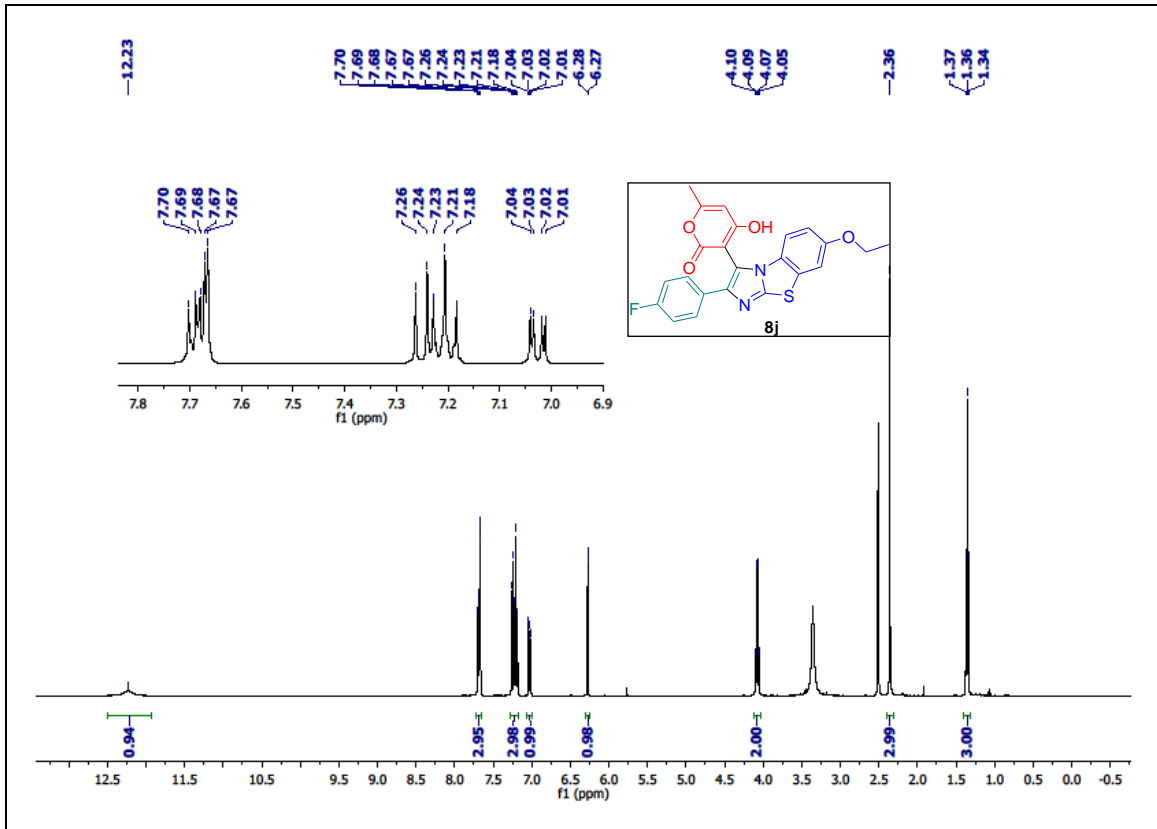


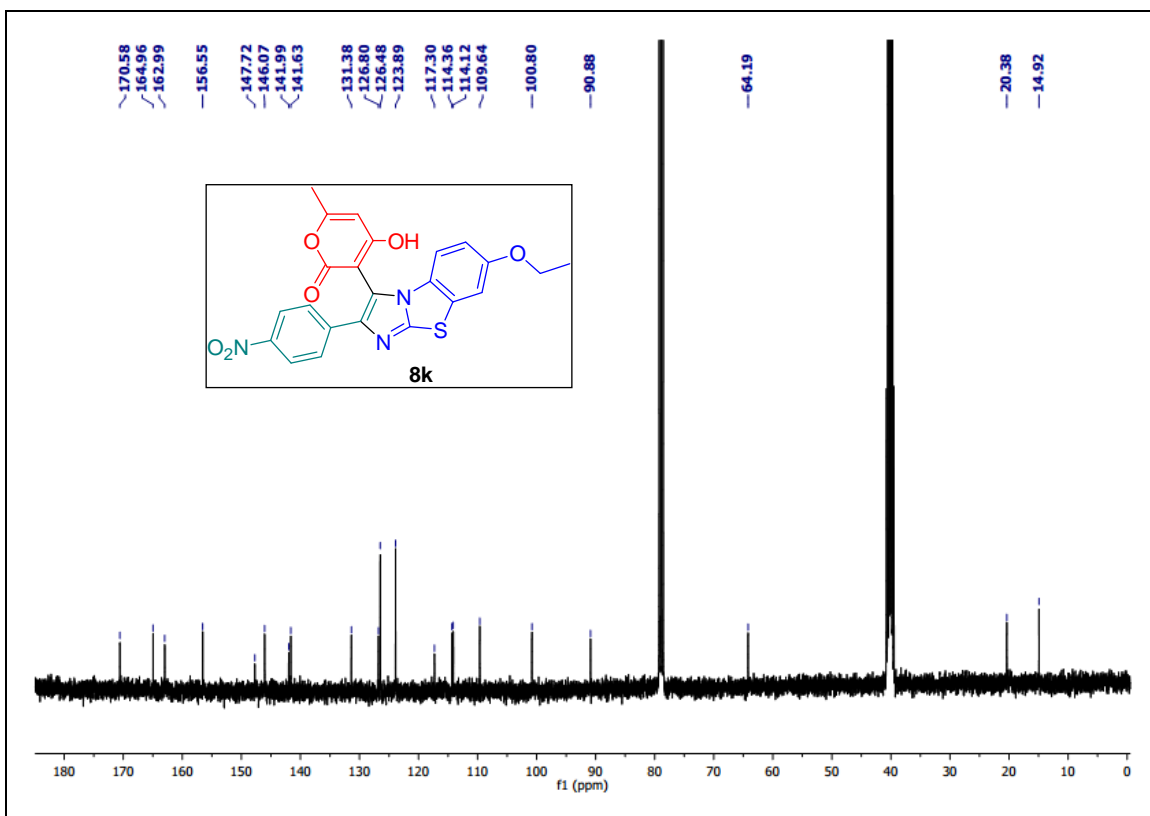
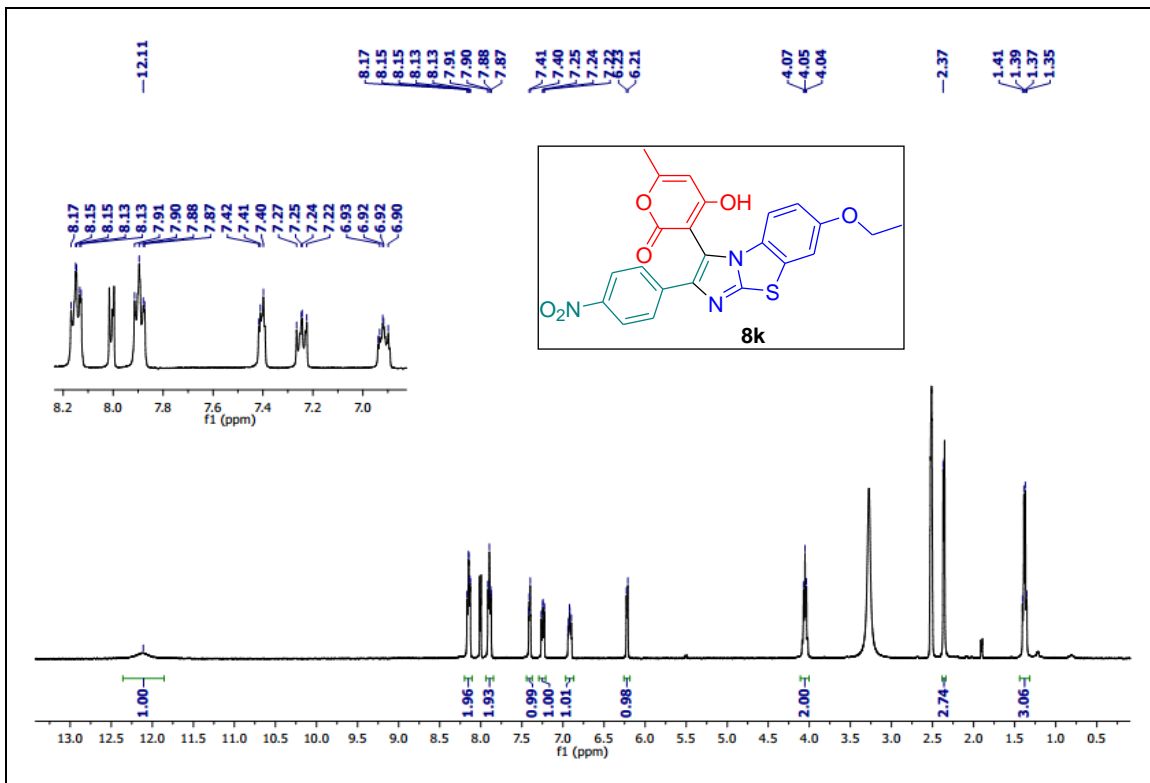


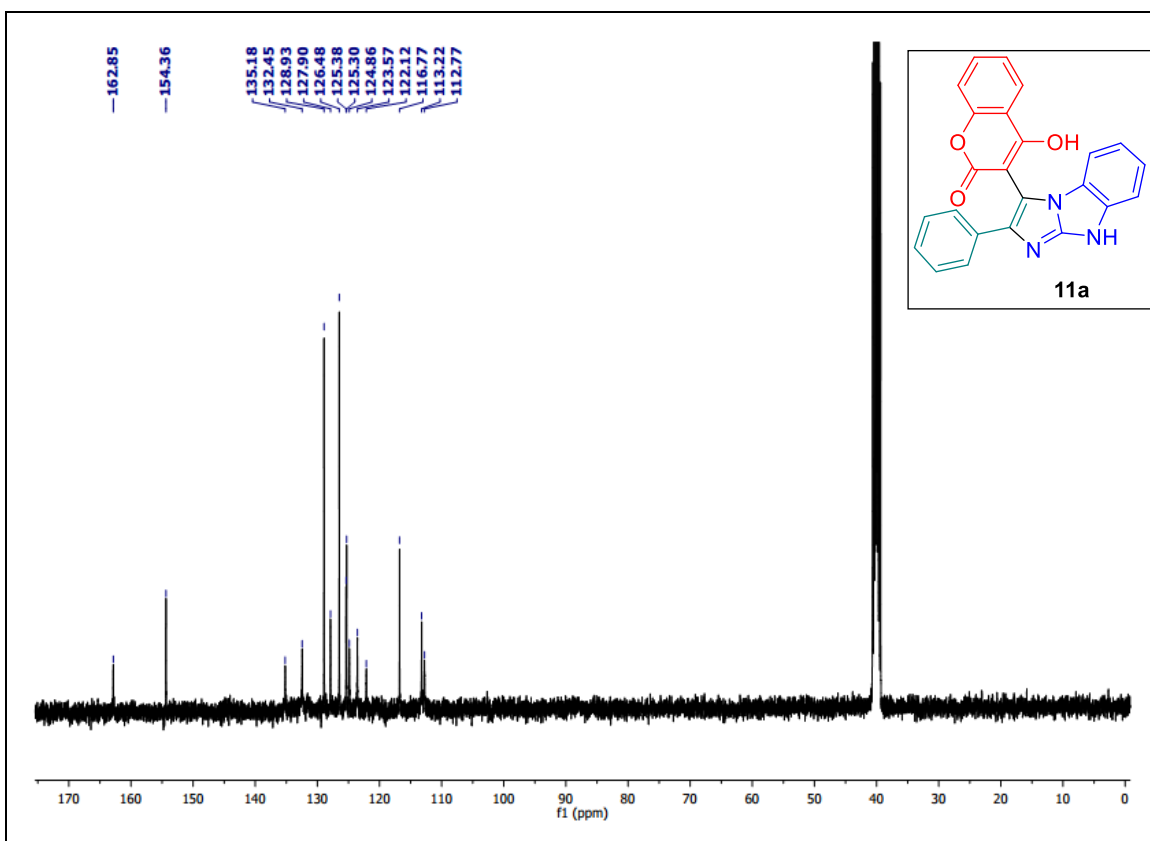
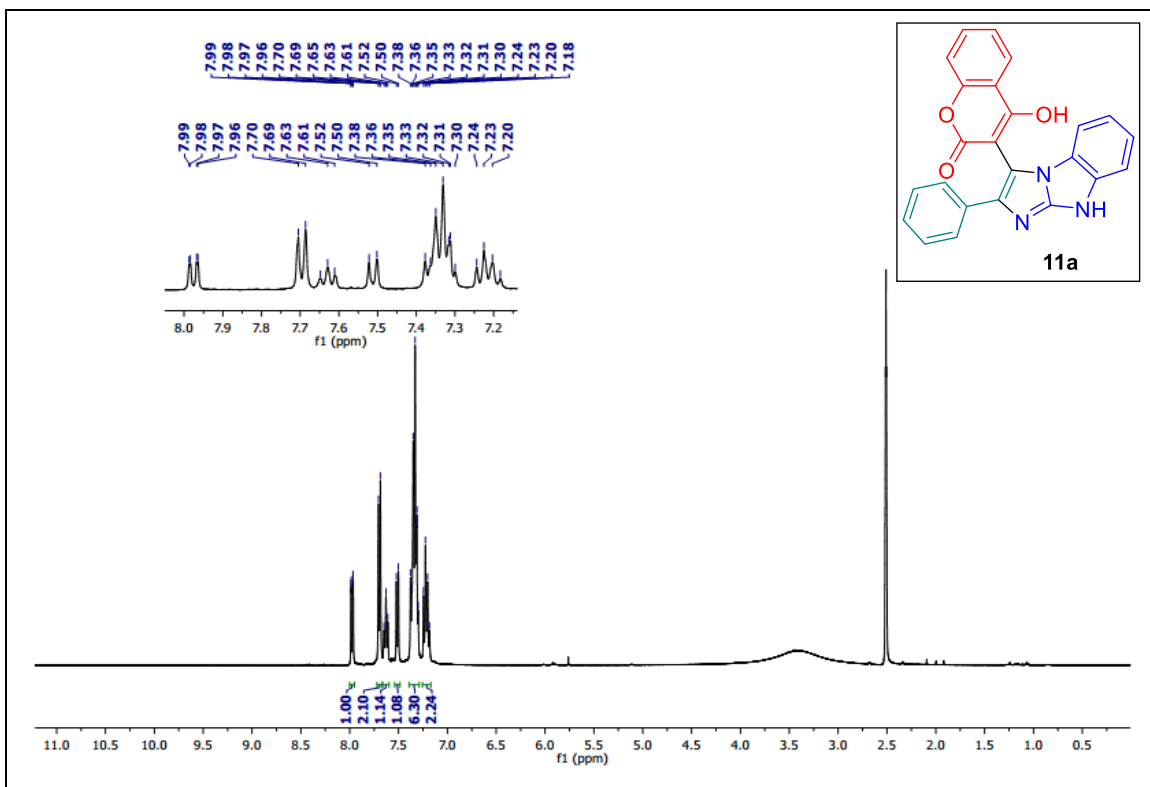


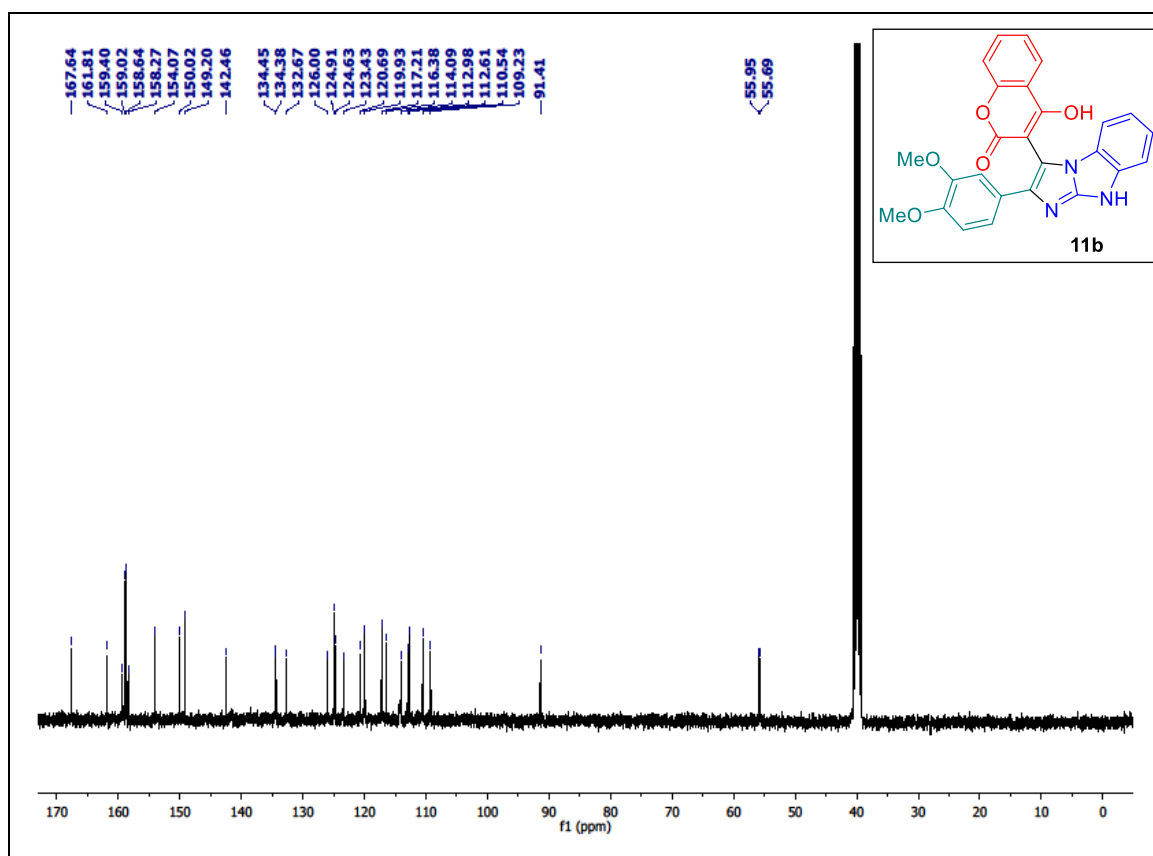
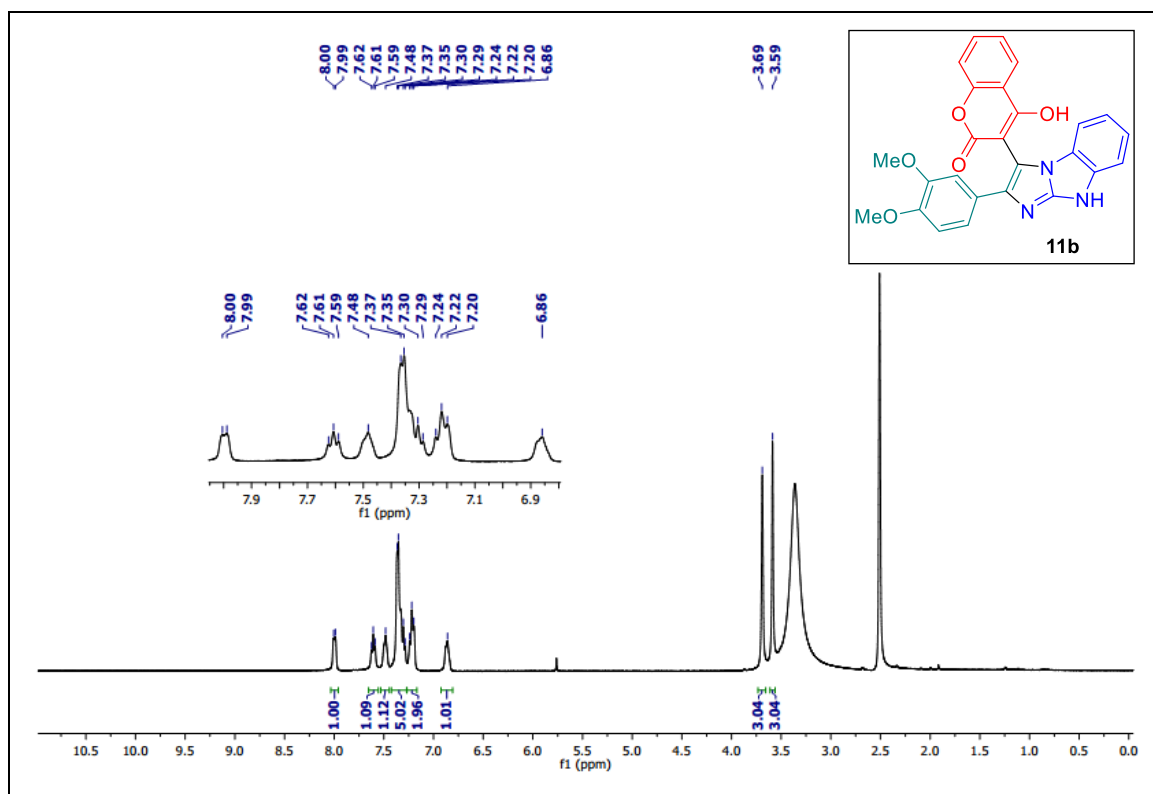


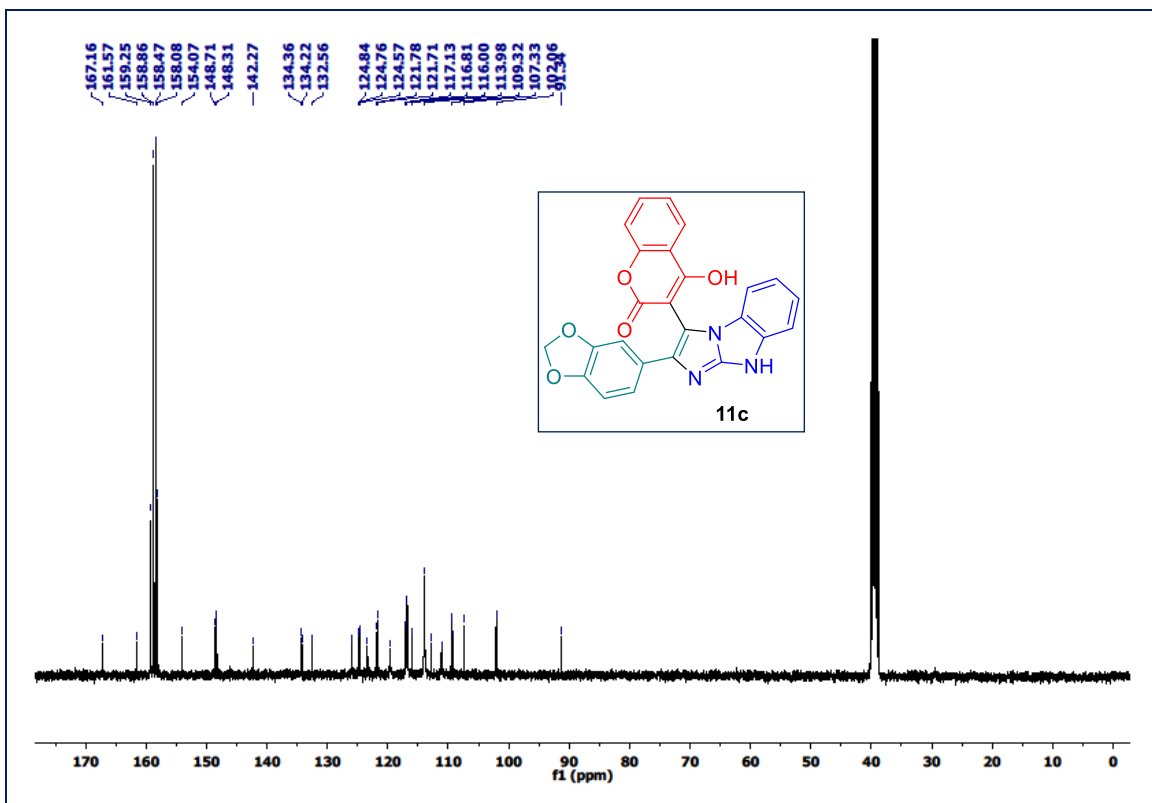
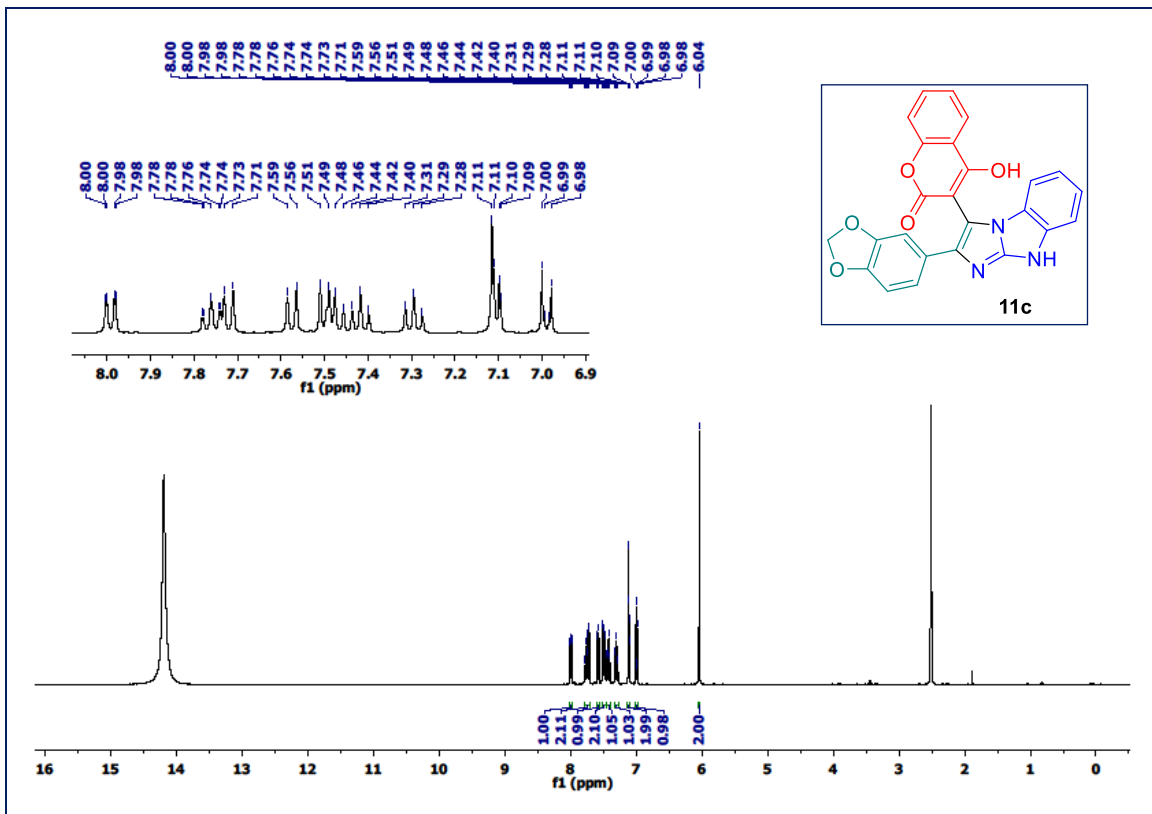


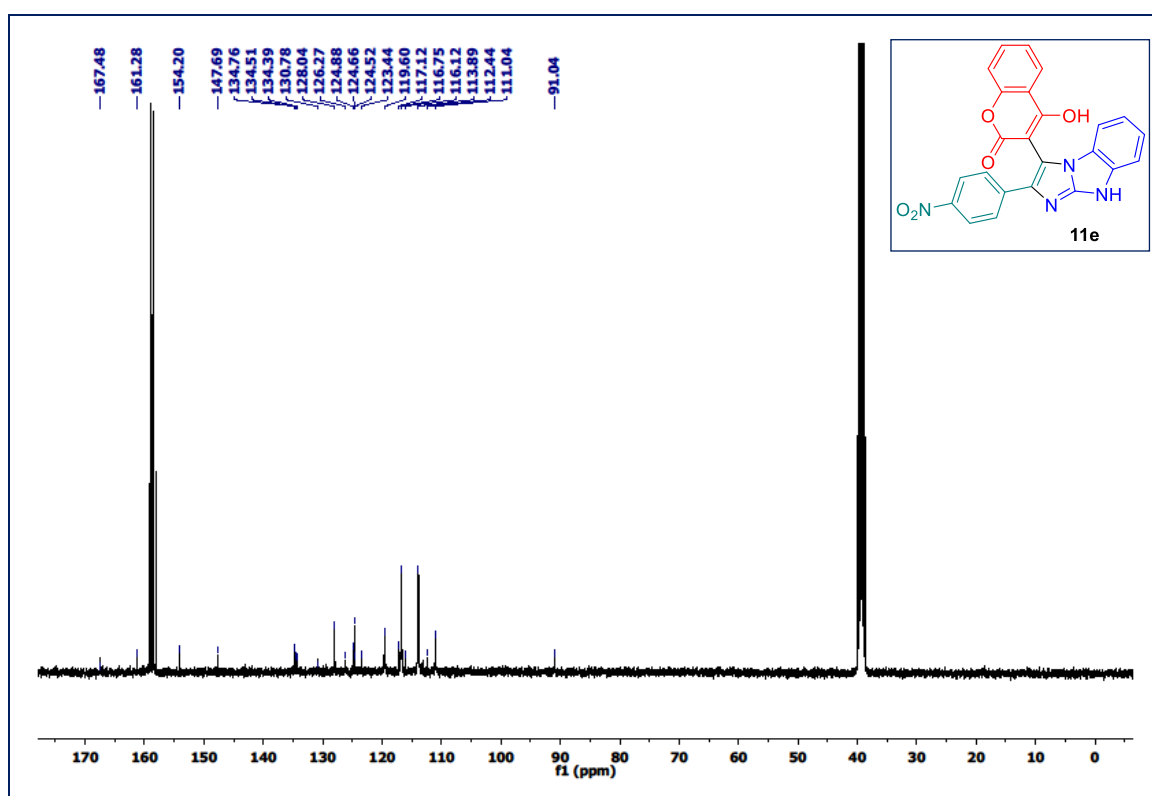
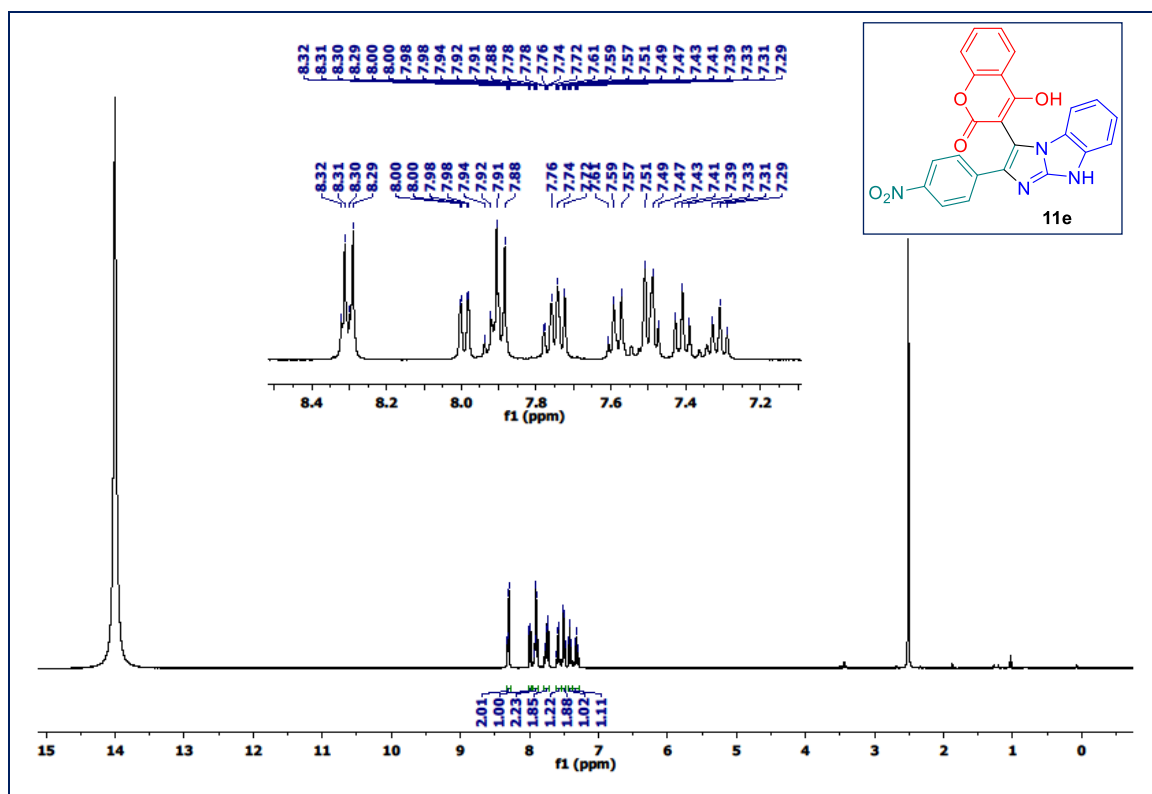












Crystal structure description of **4b**.

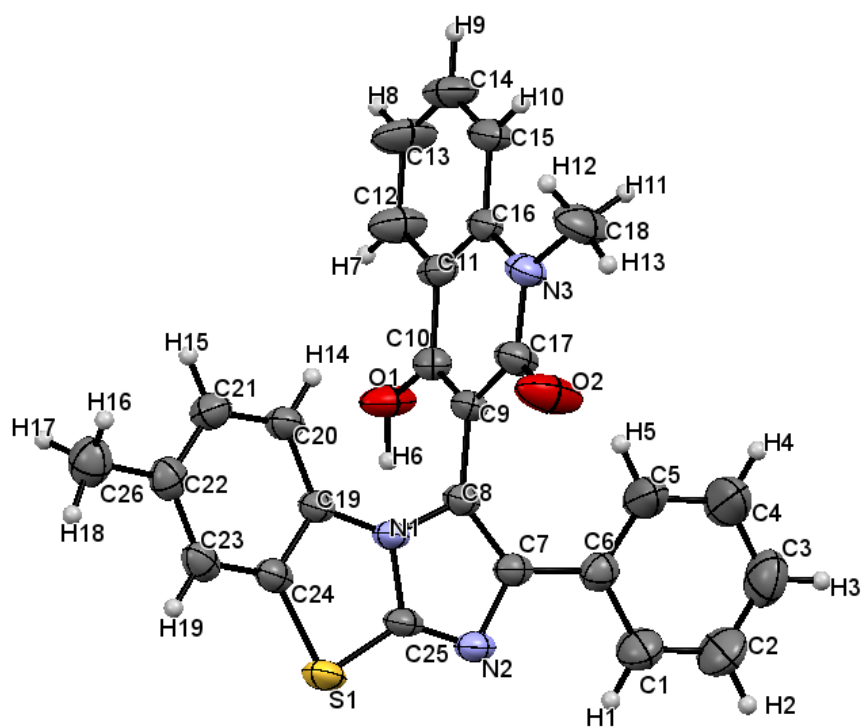


Figure S1. ORTEP view of **4b** with 50% ellipsoidal probability.

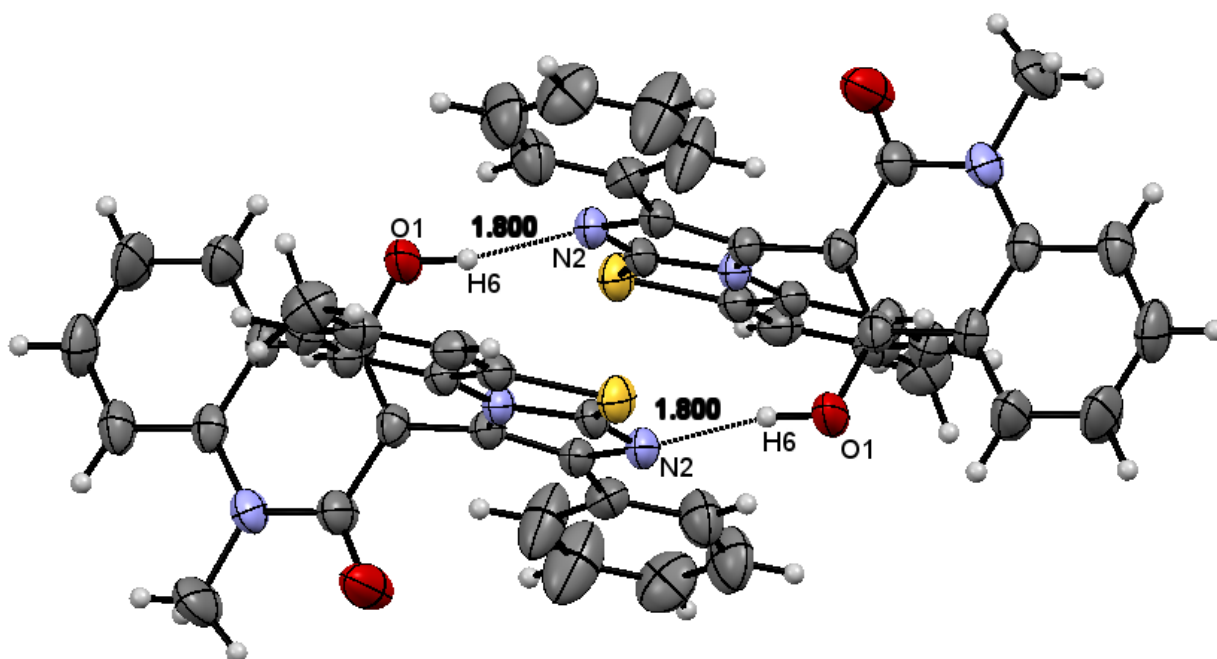


Figure S2. ORTEP view of **4b** with intermolecular hydrogen bonding

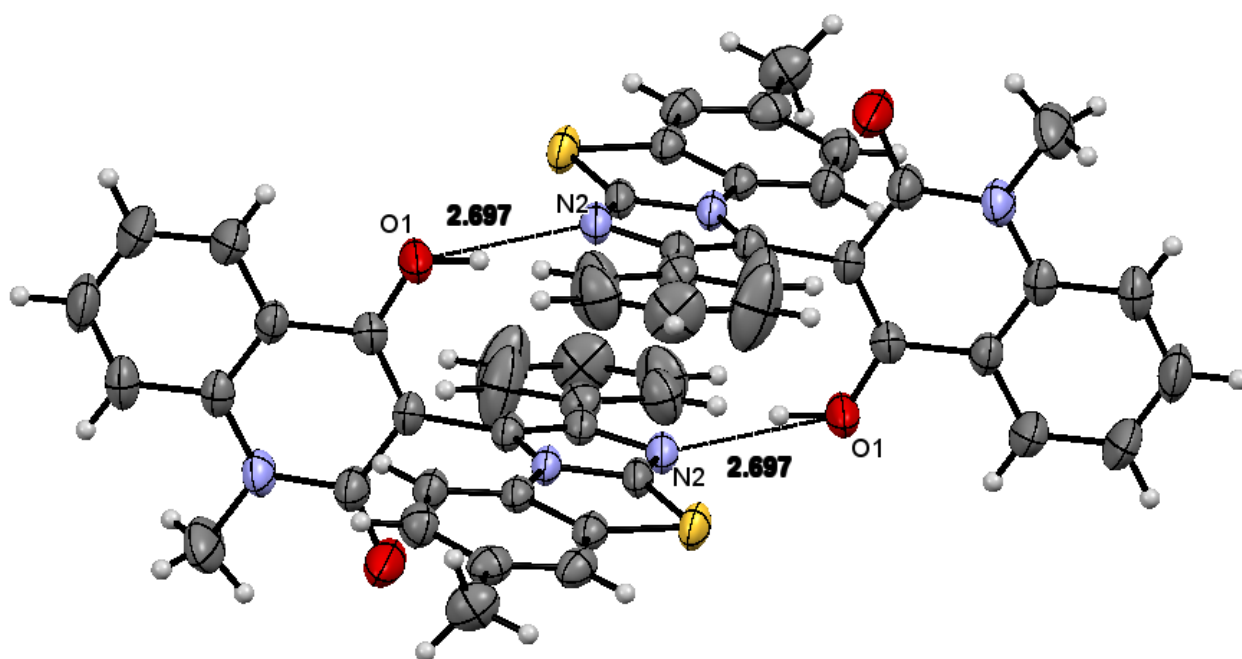


Figure S3. ORTEP view of **4b** with the distance between O...N (Donor-Acceptor) is 2.697 Å.

Table S1. Sample and crystal data for 4b

Chemical formula	C ₂₆ H ₁₉ N ₃ O ₂ S	
Formula weight	437.50 g/mol	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.4053(8) Å	α = 104.180(2)°
	b = 10.2781(9) Å	β = 101.225(2)°
	c = 11.6661(10) Å	γ = 93.954(2)°
Volume	1064.37(16) Å ³	
Z	2	
Density (calculated)	1.365 g/cm ³	
Absorption coefficient	0.182 mm ⁻¹	
F(000)	456	

Table S2. Data collection and structure refinement for 4b

Theta range for data collection	2.56 to 26.08°		
Index ranges	-11 ≤ h ≤ 11, -1 ≤ k ≤ 12, -14 ≤ l ≤ 14		
Reflections collected	19518		
Independent reflections	4225 [R(int) = 0.0321]		
Structure solution technique	direct methods		
Structure solution program	XT, VERSION 2014/5		
Refinement method	Full-matrix least-squares on F ²		
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)		
Function minimized	Σ w(F _o ² - F _c ²) ²		
Data / restraints / parameters	4225 / 0 / 296		
Goodness-of-fit on F ²	1.026		
Δ/σ _{max}	0.001		
Final R indices	3259 data; I > 2σ(I)	R1 = 0.0415, wR2 = 0.1020	
	all data	R1 = 0.0618, wR2 = 0.1129	
Weighting scheme	w=1/[σ ² (F _o ²)+(0.0550P) ² +0.3070P]		
where P=(F _o ² +2F _c ²)/3	where P=(F _o ² +2F _c ²)/3		
Extinction coefficient	0.0130(20)		
Largest diff. peak and hole	0.204 and -0.165 eÅ ⁻³		
R.M.S. deviation from mean	0.043 eÅ ⁻³		

Table S3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å²) for 4b

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
S1	0.70747(5)	0.55696(5)	0.66047(4)	0.04270(16)
O1	0.94771(15)	0.19371(13)	0.29994(13)	0.0555(4)
N1	0.73645(15)	0.42929(13)	0.44736(11)	0.0321(3)
N2	0.87853(15)	0.62633(14)	0.50701(12)	0.0369(3)
N3	0.61172(17)	0.24235(15)	0.03504(12)	0.0426(4)

O2	0.57629(19)	0.43988(16)	0.15682(13)	0.0774(5)
C9	0.76521(18)	0.32776(16)	0.23701(14)	0.0334(4)
C8	0.79992(18)	0.43712(16)	0.35058(14)	0.0327(4)
C19	0.63339(18)	0.34278(16)	0.47412(14)	0.0322(4)
C7	0.88548(18)	0.56059(16)	0.38878(15)	0.0351(4)
C10	0.83664(18)	0.21661(16)	0.22020(15)	0.0348(4)
C24	0.60329(19)	0.39910(16)	0.58685(14)	0.0354(4)
C25	0.78641(18)	0.54577(16)	0.53654(14)	0.0347(4)
C16	0.67738(18)	0.12481(17)	0.01814(14)	0.0360(4)
C23	0.5001(2)	0.33370(18)	0.62963(16)	0.0405(4)
C11	0.79131(18)	0.10924(17)	0.10928(15)	0.0370(4)
C20	0.56437(19)	0.21684(17)	0.40516(15)	0.0383(4)
C6	0.96878(19)	0.62865(17)	0.32164(16)	0.0400(4)
C22	0.4279(2)	0.20823(18)	0.56056(17)	0.0417(4)
C17	0.6450(2)	0.34225(18)	0.14346(16)	0.0439(4)
C21	0.4633(2)	0.15181(18)	0.45016(16)	0.0429(4)
C15	0.6336(2)	0.02068(19)	0.91099(16)	0.0481(5)
C26	0.3127(2)	0.1364(2)	0.6040(2)	0.0568(5)
C1	0.0528(2)	0.7514(2)	0.3774(2)	0.0568(5)
C12	0.8582(2)	0.9912(2)	0.09116(19)	0.0589(6)
C14	0.7020(3)	0.9065(2)	0.89550(19)	0.0620(6)
C18	0.5014(3)	0.2645(2)	0.93616(18)	0.0693(7)
C13	0.8146(3)	0.8908(2)	0.9848(2)	0.0712(7)
C3	0.1207(3)	0.7666(3)	0.1955(2)	0.0717(7)
C2	0.1268(3)	0.8187(3)	0.3145(2)	0.0717(7)
C5	0.9641(3)	0.5777(2)	0.2002(2)	0.0825(9)
C4	0.0392(4)	0.6462(3)	0.1385(2)	0.0979(10)

Table S4. Bond lengths (Å) for 4b

S1-C25	1.7329(18)	S1-C24	1.7609(18)
O1-C10	1.332(2)	O1-H6	0.93(3)
N1-C25	1.363(2)	N1-C8	1.392(2)
N1-C19	1.401(2)	N2-C25	1.308(2)
N2-C7	1.396(2)	N3-C16	1.383(2)
N3-C17	1.385(2)	N3-C18	1.467(2)
O2-C17	1.225(2)	C9-C10	1.357(2)
C9-C17	1.454(2)	C9-C8	1.475(2)
C8-C7	1.378(2)	C19-C20	1.384(2)
C19-C24	1.393(2)	C7-C6	1.466(3)
C10-C11	1.447(2)	C24-C23	1.381(3)
C16-C15	1.400(2)	C16-C11	1.403(2)
C23-C22	1.389(3)	C23-H19	0.93
C11-C12	1.395(3)	C20-C21	1.380(3)
C20-H14	0.93	C6-C5	1.376(3)
C6-C1	1.378(3)	C22-C21	1.390(3)
C22-C26	1.505(3)	C21-H15	0.93
C15-C14	1.367(3)	C15-H10	0.93
C26-H16	0.96	C26-H18	0.96
C26-H17	0.96	C1-C2	1.373(3)
C1-H1	0.93	C12-C13	1.374(3)
C12-H7	0.93	C14-C13	1.382(3)
C14-H9	0.93	C18-H12	0.96
C18-H11	0.96	C18-H13	0.96
C13-H8	0.93	C3-C2	1.348(3)
C3-C4	1.352(4)	C3-H3	0.93
C2-H2	0.93	C5-C4	1.375(3)
C5-H5	0.93	C4-H4	0.93

Table S5. Bond angles (°) for 4b

C25-S1-C24	89.52(8)	C10-O1-H6	118.7(15)
C25-N1-C8	107.06(14)	C25-N1-C19	114.22(14)
C8-N1-C19	138.56(13)	C25-N2-C7	104.87(13)
C16-N3-C17	122.54(15)	C16-N3-C18	120.01(15)
C17-N3-C18	117.45(16)	C10-C9-C17	120.79(15)
C10-C9-C8	122.88(15)	C17-C9-C8	116.30(14)
C7-C8-N1	104.79(14)	C7-C8-C9	134.23(16)
N1-C8-C9	120.95(14)	C20-C19-C24	120.22(16)
C20-C19-N1	128.78(15)	C24-C19-N1	111.00(14)
C8-C7-N2	110.55(15)	C8-C7-C6	129.45(16)
N2-C7-C6	119.88(15)	O1-C10-C9	125.45(15)
O1-C10-C11	114.50(15)	C9-C10-C11	120.04(15)
C23-C24-C19	120.97(16)	C23-C24-S1	126.58(13)
C19-C24-S1	112.44(13)	N2-C25-N1	112.68(15)
N2-C25-S1	134.45(13)	N1-C25-S1	112.80(13)
N3-C16-C15	121.41(16)	N3-C16-C11	119.72(14)
C15-C16-C11	118.88(17)	C24-C23-C22	119.49(16)
C24-C23-H19	120.3	C22-C23-H19	120.3
C12-C11-C16	119.46(16)	C12-C11-C10	121.54(17)
C16-C11-C10	119.00(15)	C21-C20-C19	118.03(16)
C21-C20-H14	121.0	C19-C20-H14	121.0
C5-C6-C1	116.31(19)	C5-C6-C7	122.76(18)
C1-C6-C7	120.89(17)	C23-C22-C21	118.55(17)
C23-C22-C26	120.44(17)	C21-C22-C26	121.00(18)
O2-C17-N3	120.01(16)	O2-C17-C9	122.40(16)
N3-C17-C9	117.56(15)	C20-C21-C22	122.67(17)
C20-C21-H15	118.7	C22-C21-H15	118.7
C14-C15-C16	120.32(19)	C14-C15-H10	119.8
C16-C15-H10	119.8	C22-C26-H16	109.5

C22-C26-H18	109.5	H16-C26-H18	109.5
C22-C26-H17	109.5	H16-C26-H17	109.5
H18-C26-H17	109.5	C2-C1-C6	121.5(2)
C2-C1-H1	119.3	C6-C1-H1	119.3
C13-C12-C11	120.7(2)	C13-C12-H7	119.6
C11-C12-H7	119.6	C15-C14-C13	121.05(18)
C15-C14-H9	119.5	C13-C14-H9	119.5
N3-C18-H12	109.5	N3-C18-H11	109.5
H12-C18-H11	109.5	N3-C18-H13	109.5
H12-C18-H13	109.5	H11-C18-H13	109.5
C12-C13-C14	119.6(2)	C12-C13-H8	120.2
C14-C13-H8	120.2	C2-C3-C4	118.6(2)
C2-C3-H3	120.7	C4-C3-H3	120.7
C3-C2-C1	121.1(2)	C3-C2-H2	119.4
C1-C2-H2	119.4	C4-C5-C6	121.5(2)
C4-C5-H5	119.2	C6-C5-H5	119.2
C3-C4-C5	120.9(2)	C3-C4-H4	119.5
C5-C4-H4	119.5		

Table S6. Torsion angles (°) for 4b

C25-N1-C8-C7	-0.10(17)	C19-N1-C8-C7	174.87(17)
C25-N1-C8-C9	-178.33(14)	C19-N1-C8-C9	-3.4(3)
C10-C9-C8-C7	96.4(2)	C17-C9-C8-C7	-85.8(2)
C10-C9-C8-N1	-86.0(2)	C17-C9-C8-N1	91.83(19)
C25-N1-C19-C20	-178.43(16)	C8-N1-C19-C20	6.8(3)
C25-N1-C19-C24	1.43(19)	C8-N1-C19-C24	-173.30(17)
N1-C8-C7-N2	1.47(18)	C9-C8-C7-N2	179.35(17)
N1-C8-C7-C6	-174.49(16)	C9-C8-C7-C6	3.4(3)
C25-N2-C7-C8	-2.30(18)	C25-N2-C7-C6	174.10(15)

C17-C9-C10-O1	180.00(17)	C8-C9-C10-O1	-2.3(3)
C17-C9-C10-C11	-1.4(3)	C8-C9-C10-C11	176.29(15)
C20-C19-C24-C23	-2.8(2)	N1-C19-C24-C23	177.30(14)
C20-C19-C24-S1	178.12(13)	N1-C19-C24-S1	-1.76(17)
C25-S1-C24-C23	-177.72(16)	C25-S1-C24-C19	1.28(13)
C7-N2-C25-N1	2.25(18)	C7-N2-C25-S1	-174.27(14)
C8-N1-C25-N2	-1.41(19)	C19-N1-C25-N2	-177.77(13)
C8-N1-C25-S1	175.90(10)	C19-N1-C25-S1	-0.46(17)
C24-S1-C25-N2	176.05(18)	C24-S1-C25-N1	-0.47(12)
C17-N3-C16-C15	174.89(17)	C18-N3-C16-C15	-4.7(3)
C17-N3-C16-C11	-5.8(3)	C18-N3-C16-C11	174.66(18)
C19-C24-C23-C22	1.7(2)	S1-C24-C23-C22	-179.40(13)
N3-C16-C11-C12	-179.27(17)	C15-C16-C11-C12	0.1(3)
N3-C16-C11-C10	0.7(3)	C15-C16-C11-C10	-179.90(16)
O1-C10-C11-C12	1.5(3)	C9-C10-C11-C12	-177.24(18)
O1-C10-C11-C16	-178.52(15)	C9-C10-C11-C16	2.8(3)
C24-C19-C20-C21	1.7(2)	N1-C19-C20-C21	-178.46(15)
C8-C7-C6-C5	4.6(3)	N2-C7-C6-C5	-171.0(2)
C8-C7-C6-C1	-177.76(18)	N2-C7-C6-C1	6.6(3)
C24-C23-C22-C21	0.5(3)	C24-C23-C22-C26	-178.66(16)
C16-N3-C17-O2	-174.65(18)	C18-N3-C17-O2	4.9(3)
C16-N3-C17-C9	7.0(3)	C18-N3-C17-C9	-173.43(18)
C10-C9-C17-O2	178.38(19)	C8-C9-C17-O2	0.5(3)
C10-C9-C17-N3	-3.3(3)	C8-C9-C17-N3	178.84(16)
C19-C20-C21-C22	0.5(3)	C23-C22-C21-C20	-1.6(3)
C26-C22-C21-C20	177.53(17)	N3-C16-C15-C14	178.79(18)
C11-C16-C15-C14	-0.6(3)	C5-C6-C1-C2	0.3(3)
C7-C6-C1-C2	-177.43(19)	C16-C11-C12-C13	0.6(3)
C10-C11-C12-C13	-179.4(2)	C16-C15-C14-C13	0.4(3)
C11-C12-C13-C14	-0.8(4)	C15-C14-C13-C12	0.3(4)

C4-C3-C2-C1	0.3(4)	C6-C1-C2-C3	-0.4(4)
C1-C6-C5-C4	-0.1(4)	C7-C6-C5-C4	177.6(3)
C2-C3-C4-C5	-0.2(5)	C6-C5-C4-C3	0.1(5)

Table S7. Anisotropic atomic displacement parameters (Å²) for 4b

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
S1	0.0575(3)	0.0363(3)	0.0266(2)	- 0.00369(18)	0.0059(2)	0.0065(2)
O1	0.0582(8)	0.0386(8)	0.0478(8)	-0.0084(6)	-0.0171(7)	0.0128(6)
N1	0.0408(8)	0.0264(7)	0.0235(7)	0.0002(5)	0.0014(6)	0.0046(6)
N2	0.0432(8)	0.0300(7)	0.0292(7)	0.0001(6)	-0.0014(6)	0.0041(7)
N3	0.0530(9)	0.0413(9)	0.0256(7)	0.0022(6)	-0.0013(6)	0.0052(7)
O2	0.0955(12)	0.0663(10)	0.0486(9)	-0.0099(7)	-0.0161(8)	0.0457(9)
C9	0.0406(9)	0.0312(9)	0.0243(8)	0.0014(7)	0.0062(7)	0.0008(7)
C8	0.0400(9)	0.0303(9)	0.0249(8)	0.0036(7)	0.0034(7)	0.0069(7)
C19	0.0378(9)	0.0294(9)	0.0263(8)	0.0043(7)	0.0017(7)	0.0083(7)
C7	0.0397(9)	0.0296(9)	0.0306(8)	0.0031(7)	0.0001(7)	0.0068(7)
C10	0.0369(9)	0.0324(9)	0.0305(8)	0.0038(7)	0.0039(7)	0.0001(7)
C24	0.0438(9)	0.0321(9)	0.0279(8)	0.0053(7)	0.0029(7)	0.0112(8)
C25	0.0421(9)	0.0300(9)	0.0241(8)	-0.0005(7)	-0.0026(7)	0.0069(8)
C16	0.0415(9)	0.0349(9)	0.0283(8)	0.0026(7)	0.0101(7)	-0.0046(8)
C23	0.0526(11)	0.0403(10)	0.0316(9)	0.0103(8)	0.0111(8)	0.0173(9)
C11	0.0400(9)	0.0308(9)	0.0337(9)	-0.0012(7)	0.0071(8)	-0.0012(7)
C20	0.0465(10)	0.0338(9)	0.0301(9)	0.0017(7)	0.0062(8)	0.0058(8)
C6	0.0419(10)	0.0348(9)	0.0425(10)	0.0107(8)	0.0062(8)	0.0063(8)
C22	0.0440(10)	0.0419(10)	0.0432(10)	0.0156(8)	0.0105(8)	0.0128(8)
C17	0.0554(11)	0.0410(10)	0.0291(9)	0.0013(8)	0.0029(8)	0.0113(9)
C21	0.0477(10)	0.0335(10)	0.0429(10)	0.0046(8)	0.0071(9)	0.0014(8)
C15	0.0570(12)	0.0460(11)	0.0308(9)	-0.0024(8)	0.0048(9)	-0.0060(9)
C26	0.0607(13)	0.0550(13)	0.0614(13)	0.0192(10)	0.0234(11)	0.0102(10)

C1	0.0525(12)	0.0573(13)	0.0521(12)	0.0093(10)	0.0044(10)	-0.0113(10)
C12	0.0589(12)	0.0430(12)	0.0572(13)	-0.0088(10)	-0.0028(10)	0.0126(10)
C14	0.0755(15)	0.0454(12)	0.0464(12)	-0.0153(10)	0.0075(11)	-0.0024(11)
C18	0.0865(16)	0.0681(15)	0.0368(11)	0.0031(10)	-0.0155(11)	0.0201(13)
C13	0.0788(16)	0.0434(12)	0.0683(15)	-0.0187(11)	0.0006(13)	0.0162(11)
C3	0.0789(16)	0.0657(16)	0.0828(18)	0.0303(14)	0.0366(14)	-0.0003(13)
C2	0.0641(14)	0.0654(15)	0.0772(17)	0.0158(13)	0.0103(13)	-0.0236(12)
C5	0.139(2)	0.0491(13)	0.0545(14)	-0.0002(11)	0.0404(15)	-0.0235(15)
C4	0.164(3)	0.0669(17)	0.0666(17)	0.0062(14)	0.0605(19)	-0.0165(19)

Table S8. Hydrogen atomic coordinates and isotropic atomic displacement parameters (\AA^2) for 4b

	x/a	y/b	z/c	U(eq)
H19	0.4790	0.3733	0.7041	0.049
H14	0.5855	0.1772	0.3307	0.046
H15	0.4169	0.0668	0.4048	0.052
H10	0.5576	0.0292	-0.1499	0.058
H16	0.2227	0.1177	0.5442	0.085
H18	0.2982	0.1927	0.6787	0.085
H17	0.3436	0.0531	0.6170	0.085
H1	1.0595	0.7895	0.4596	0.068
H7	0.9332	-0.0198	0.1517	0.071
H9	0.6722	-0.1617	-0.1763	0.074
H12	0.4180	0.1975	-0.0825	0.104
H11	0.5419	0.2573	-0.1343	0.104
H13	0.4722	0.3529	-0.0394	0.104
H8	0.8606	-0.1872	-0.0270	0.085
H3	1.1715	0.8125	0.1534	0.086
H2	1.1820	0.9017	0.3546	0.086
H5	0.9090	0.4950	0.1589	0.099
H4	1.0338	0.6092	0.0564	0.117

H6	0.990(3)	0.263(3)	0.368(2)	0.086(8)
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Table S9. Hydrogen bond distances (Å) and angles (°) for 4b

Atoms	Donor-H	Acceptor-H	Donor-Acceptor	Angle
O1-H6...N2	0.93(3)	1.80(3)	2.6969(18)	162.(2)
C23-H19...O2	0.93	2.35	3.198(2)	151.2
