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Supporting information

I_2/DMSO mediated multicomponent reaction for the synthesis of 2-arylbenzo[*d*]imidazo[2,1-*b*] thiazole derivatives

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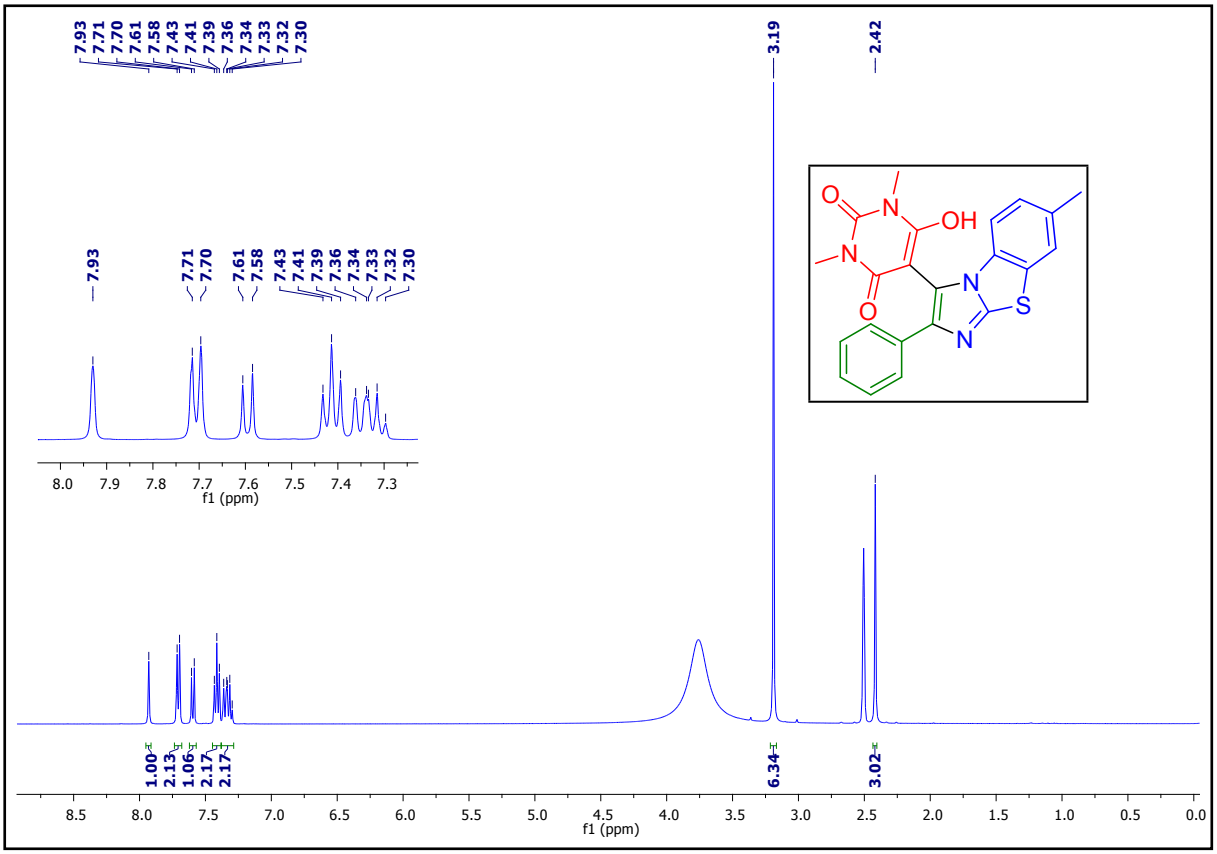

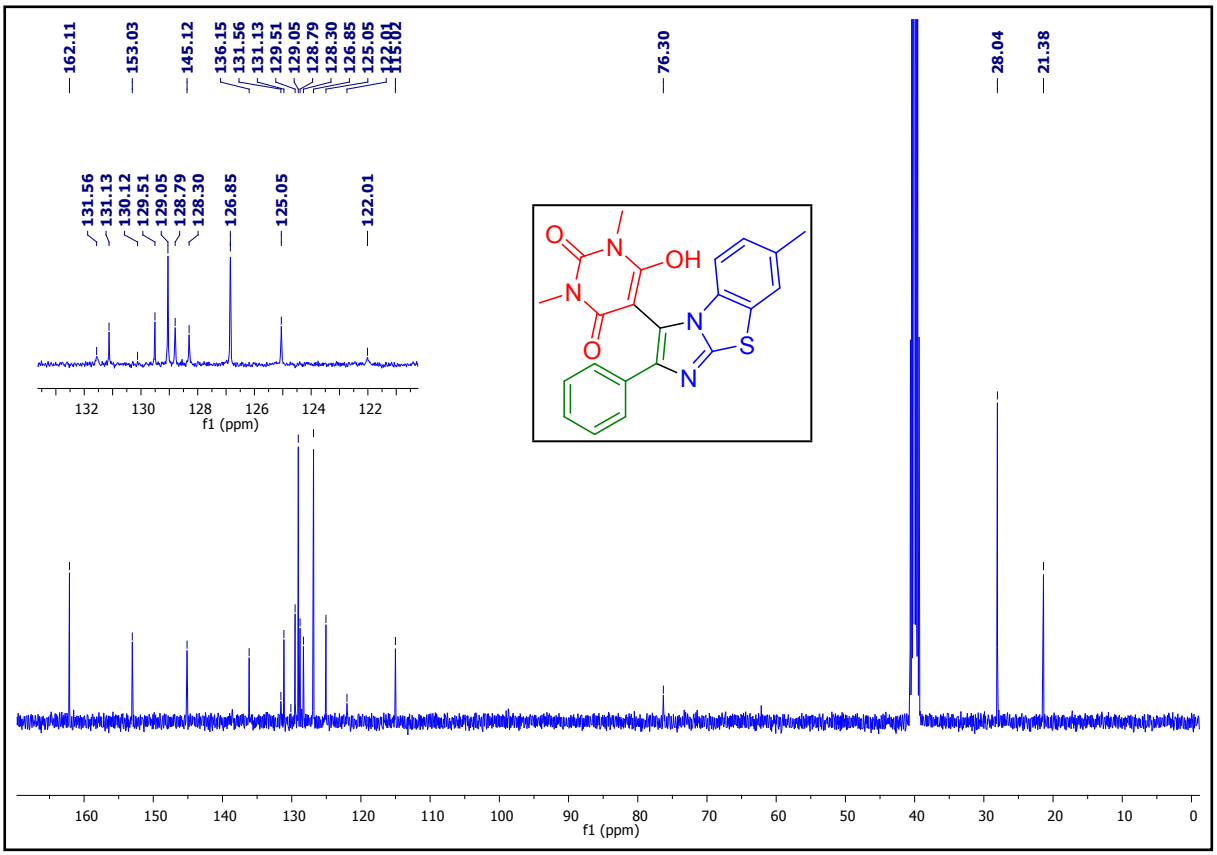

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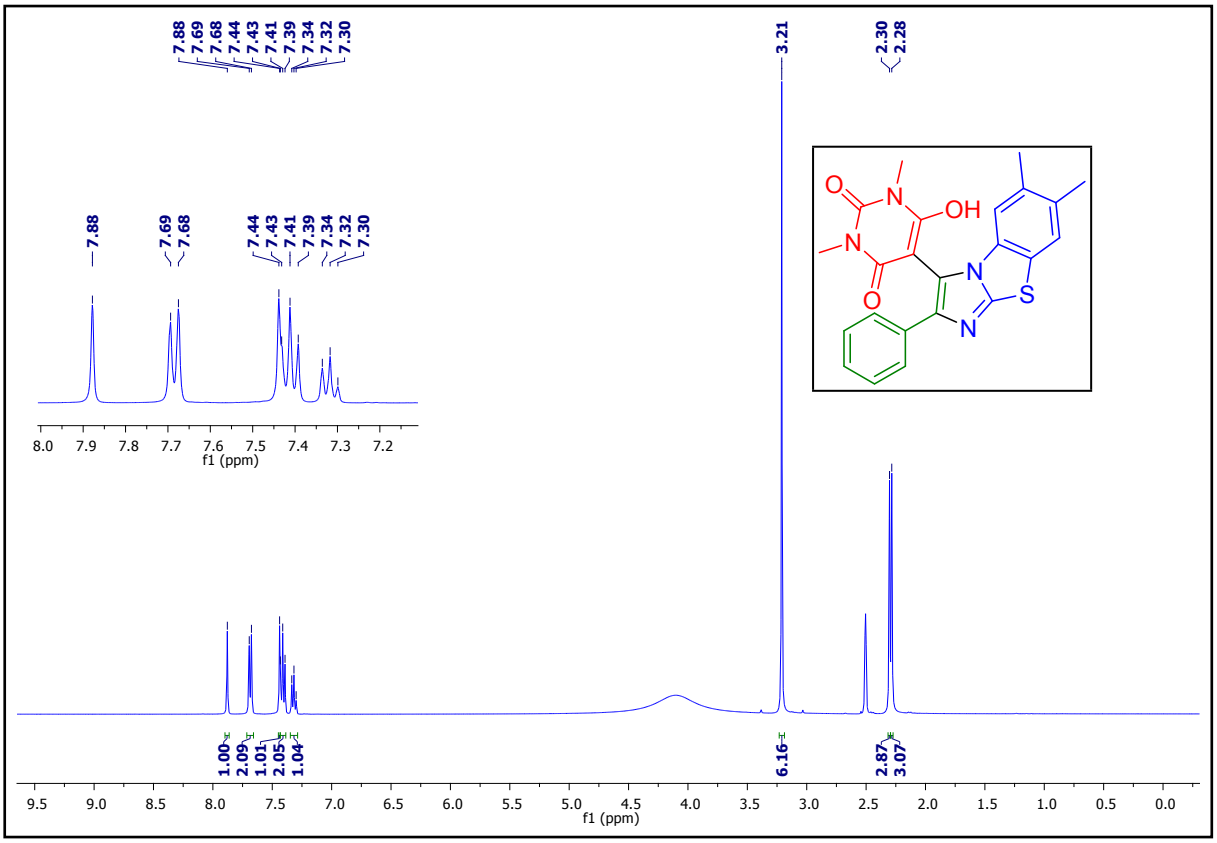

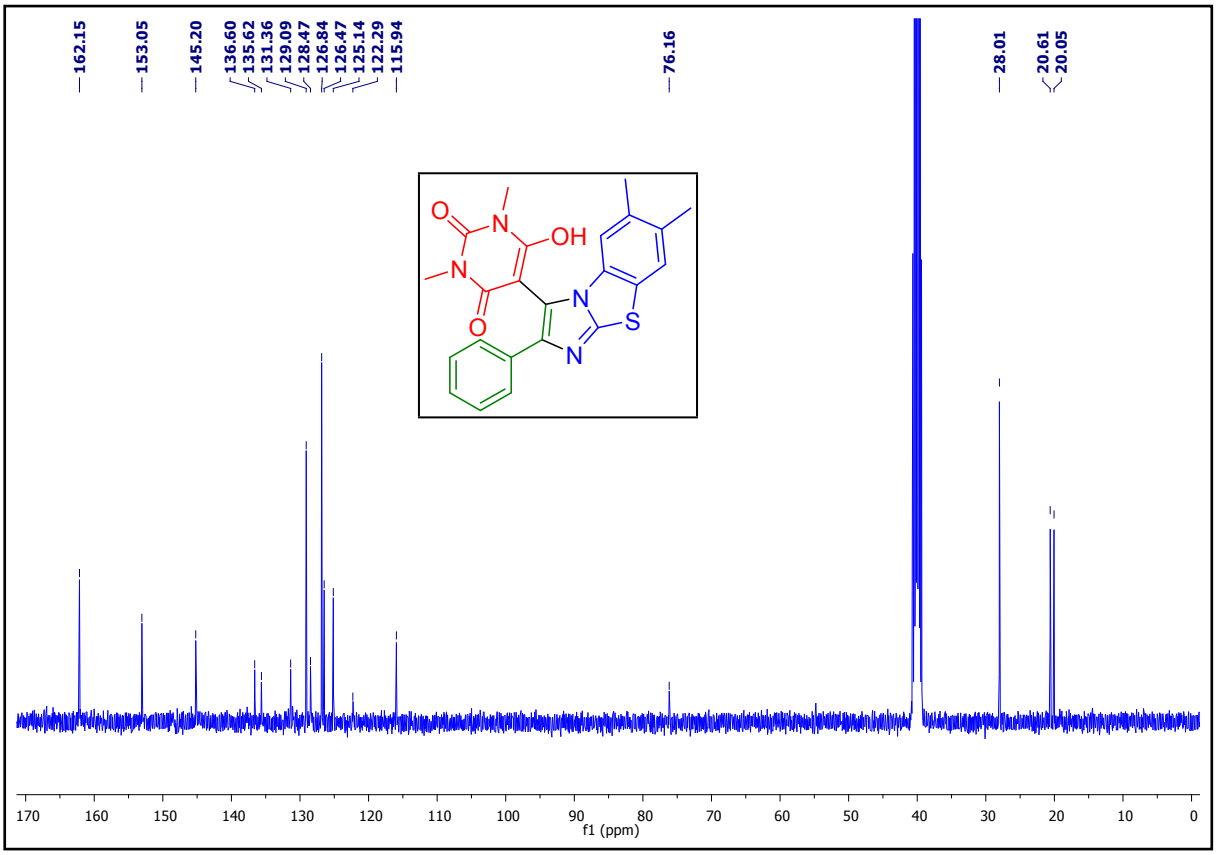

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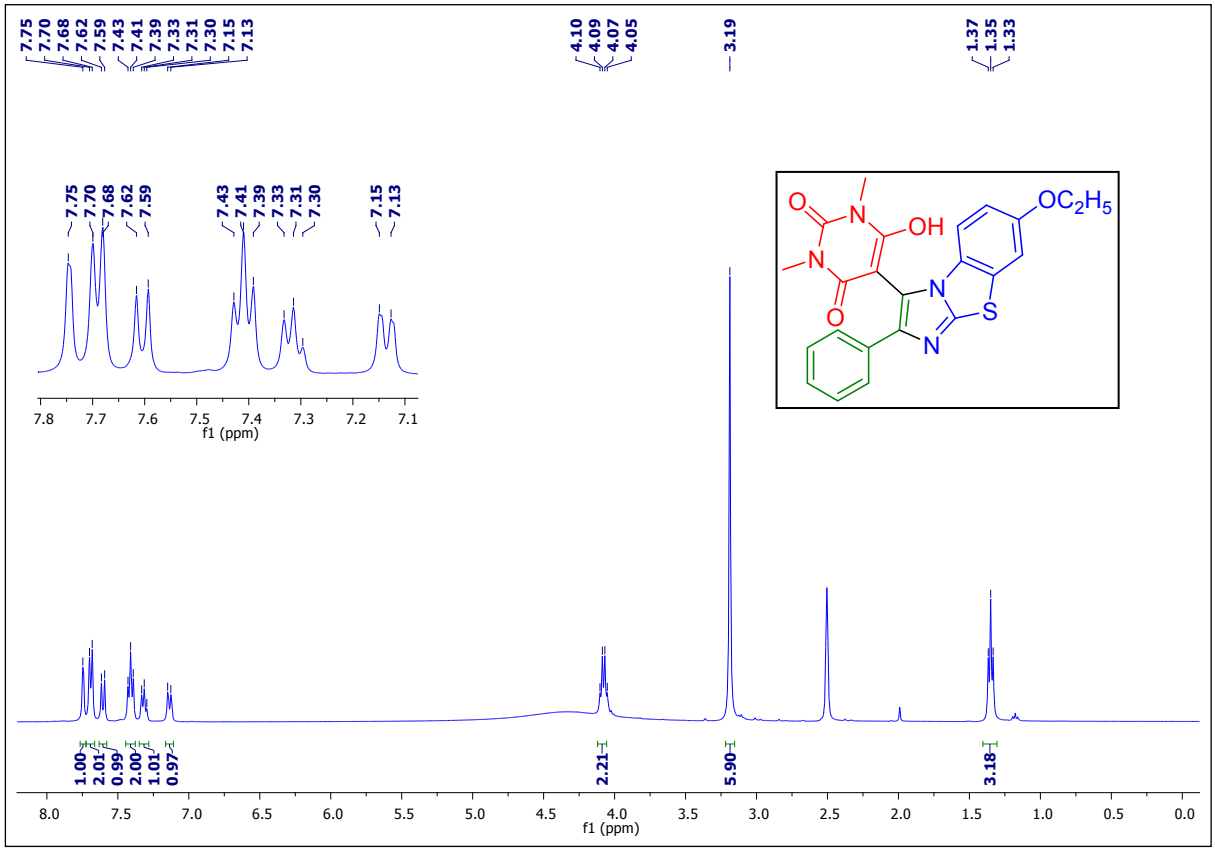

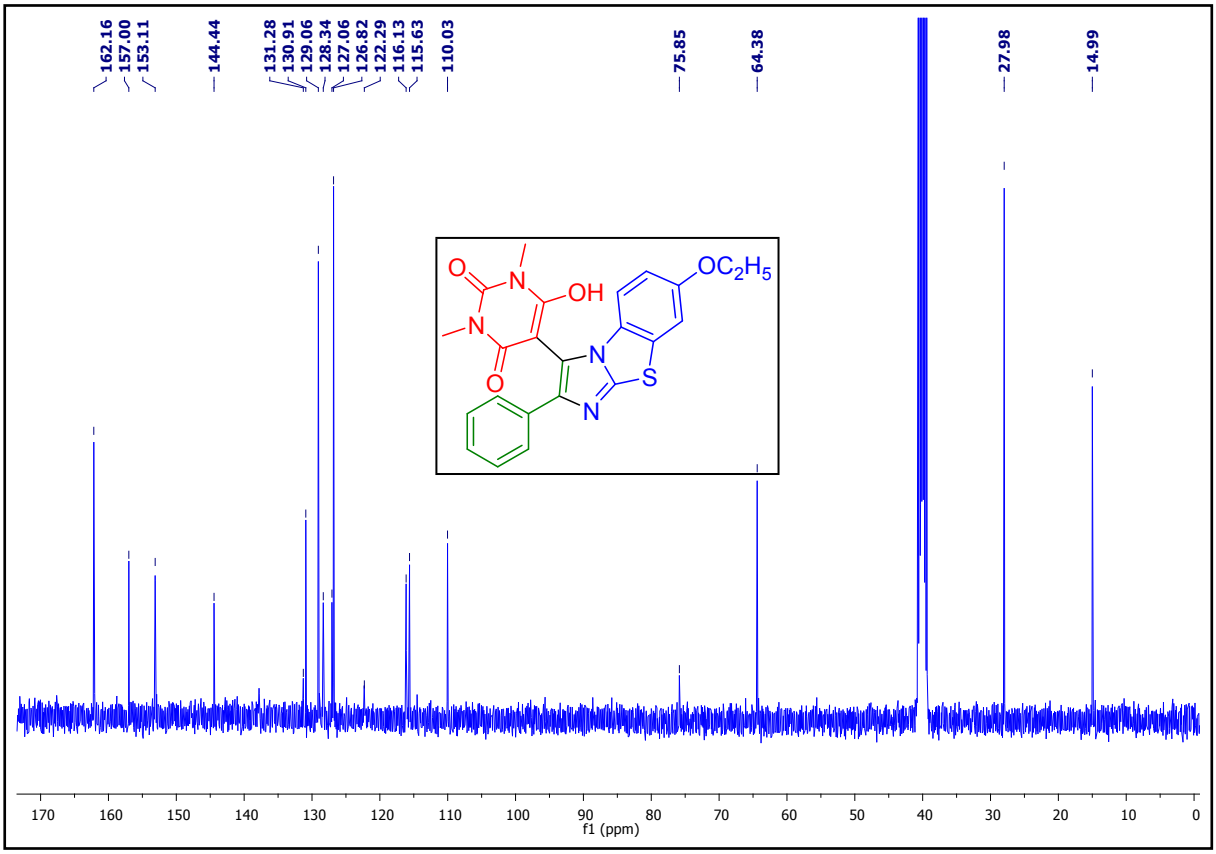

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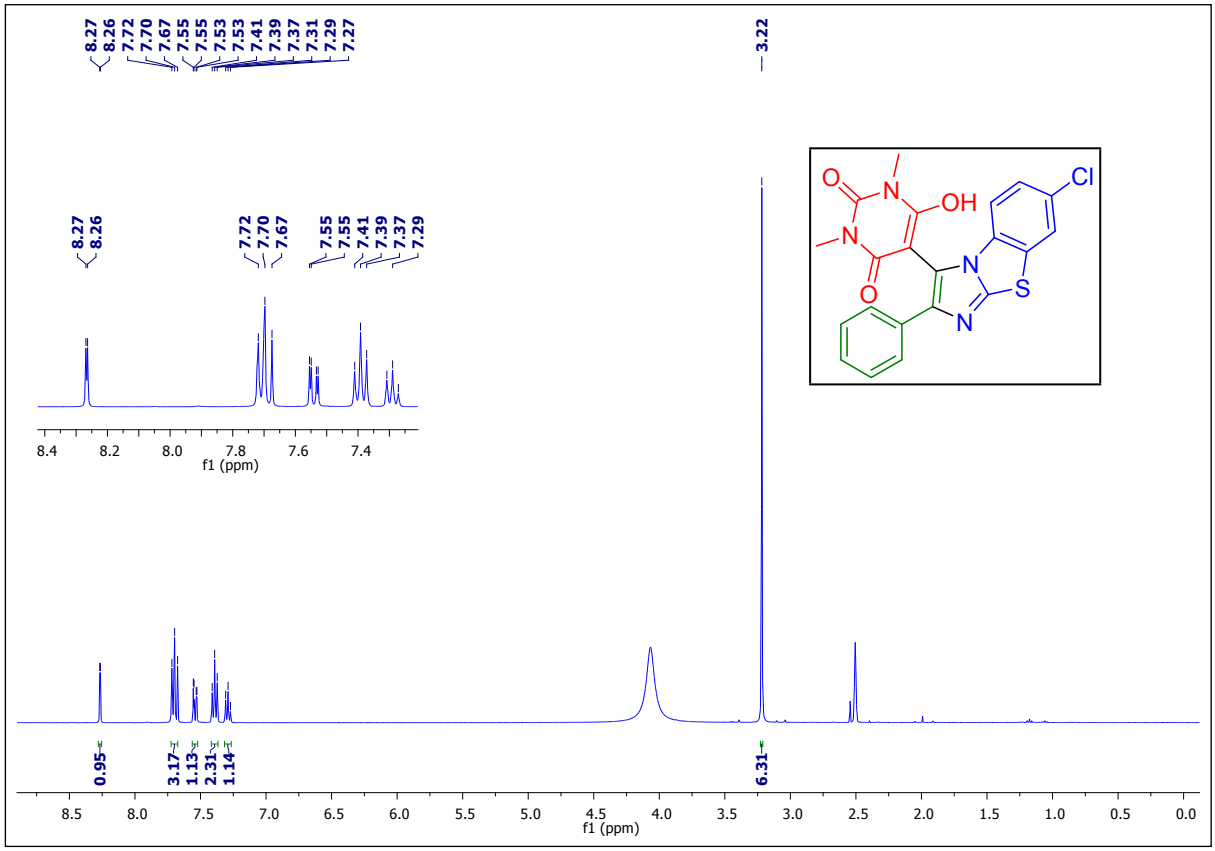

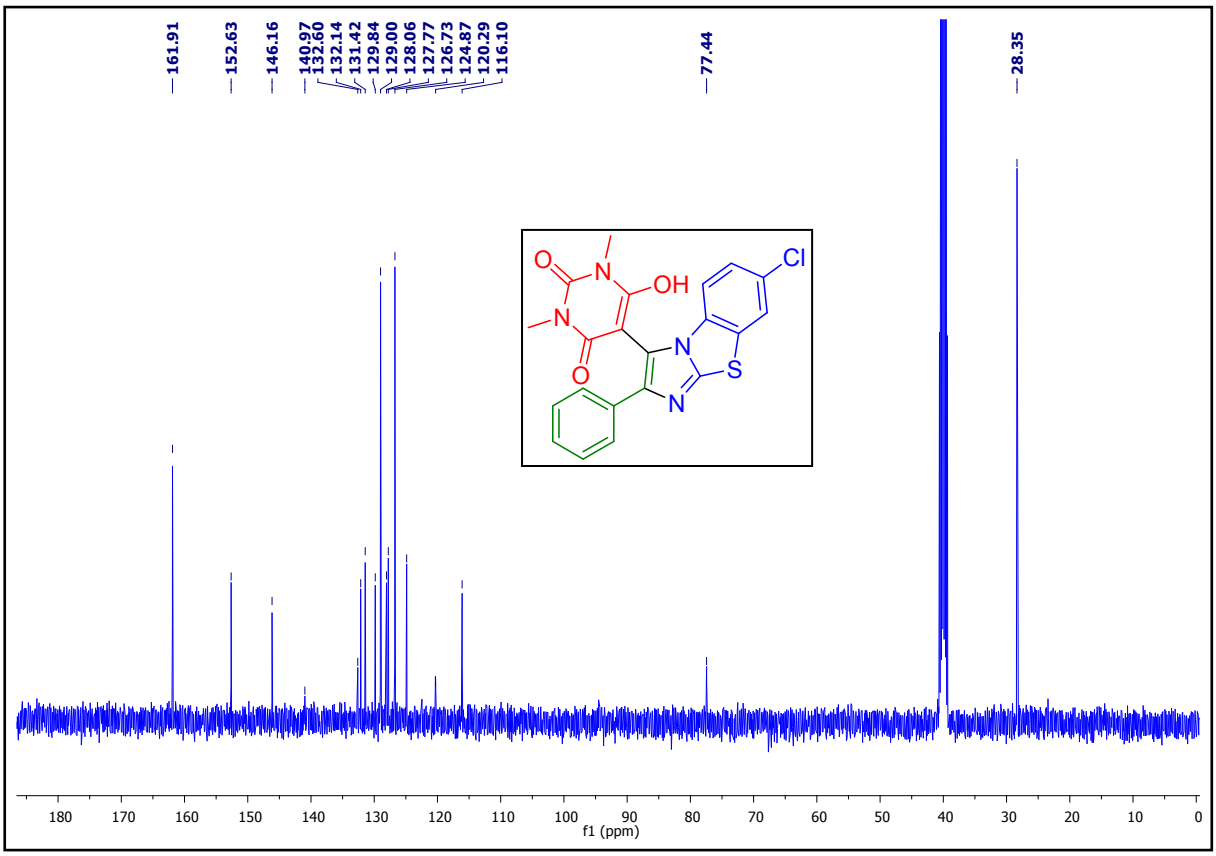

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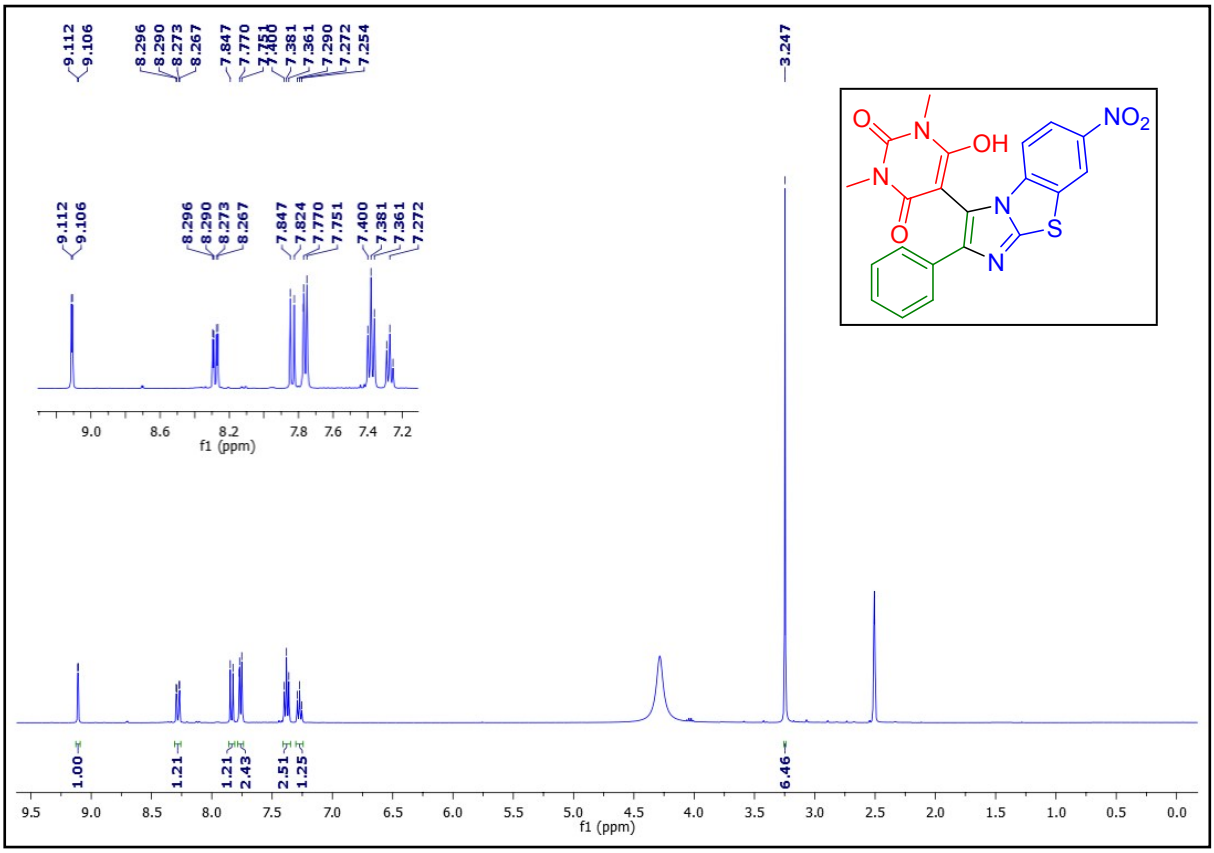

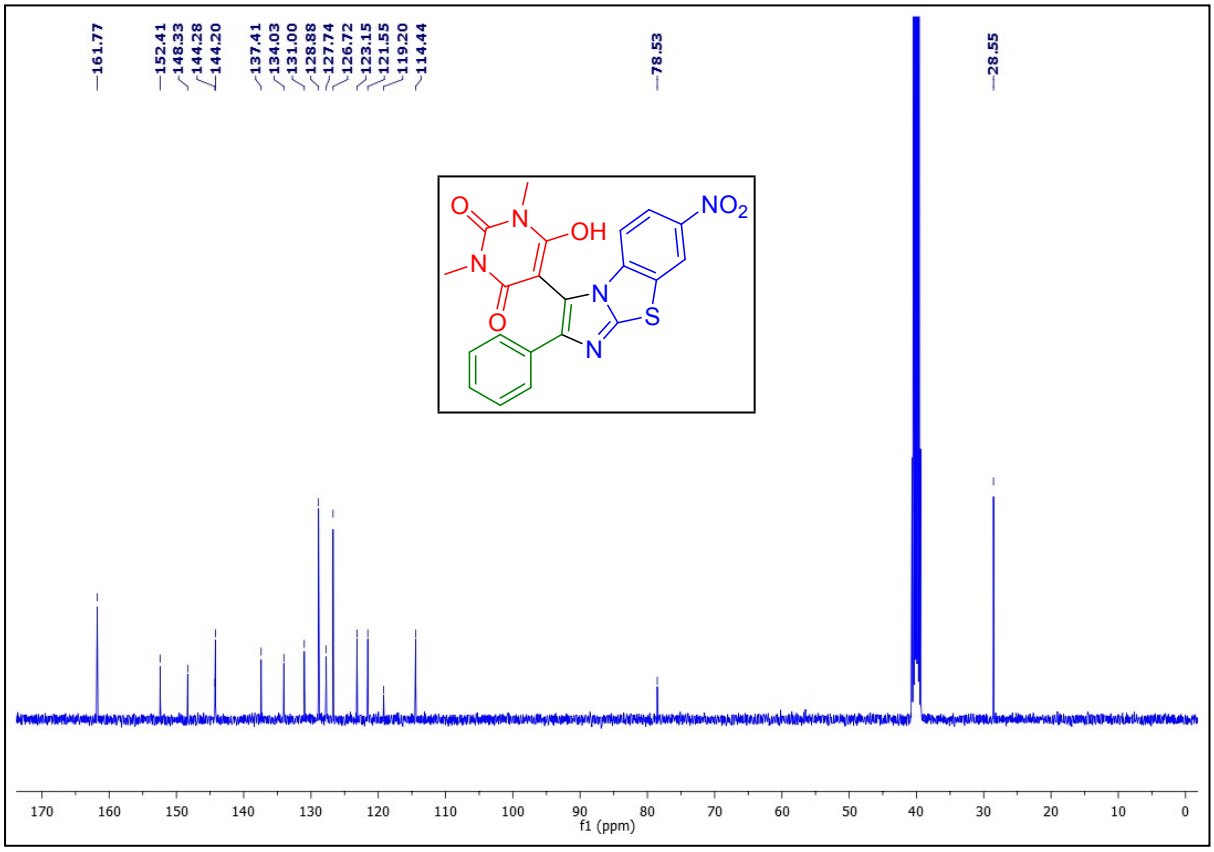

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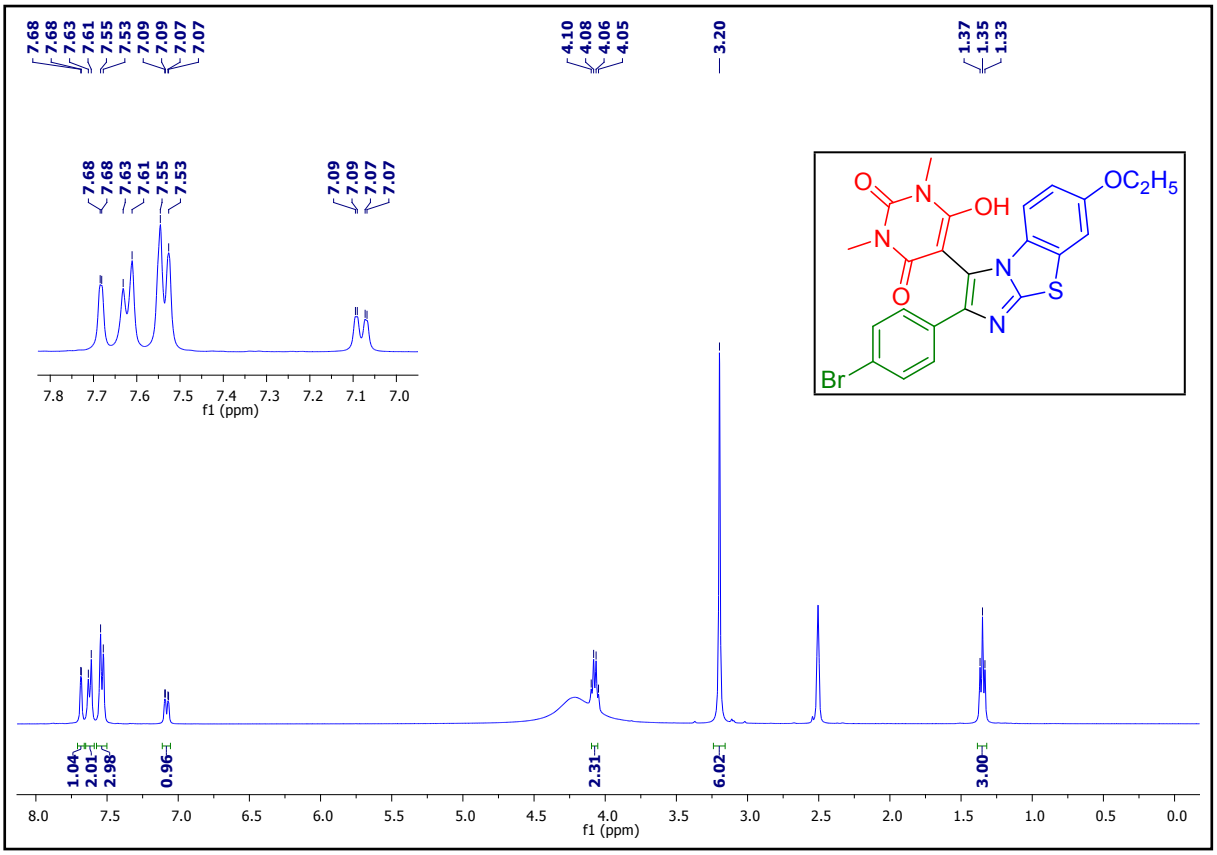

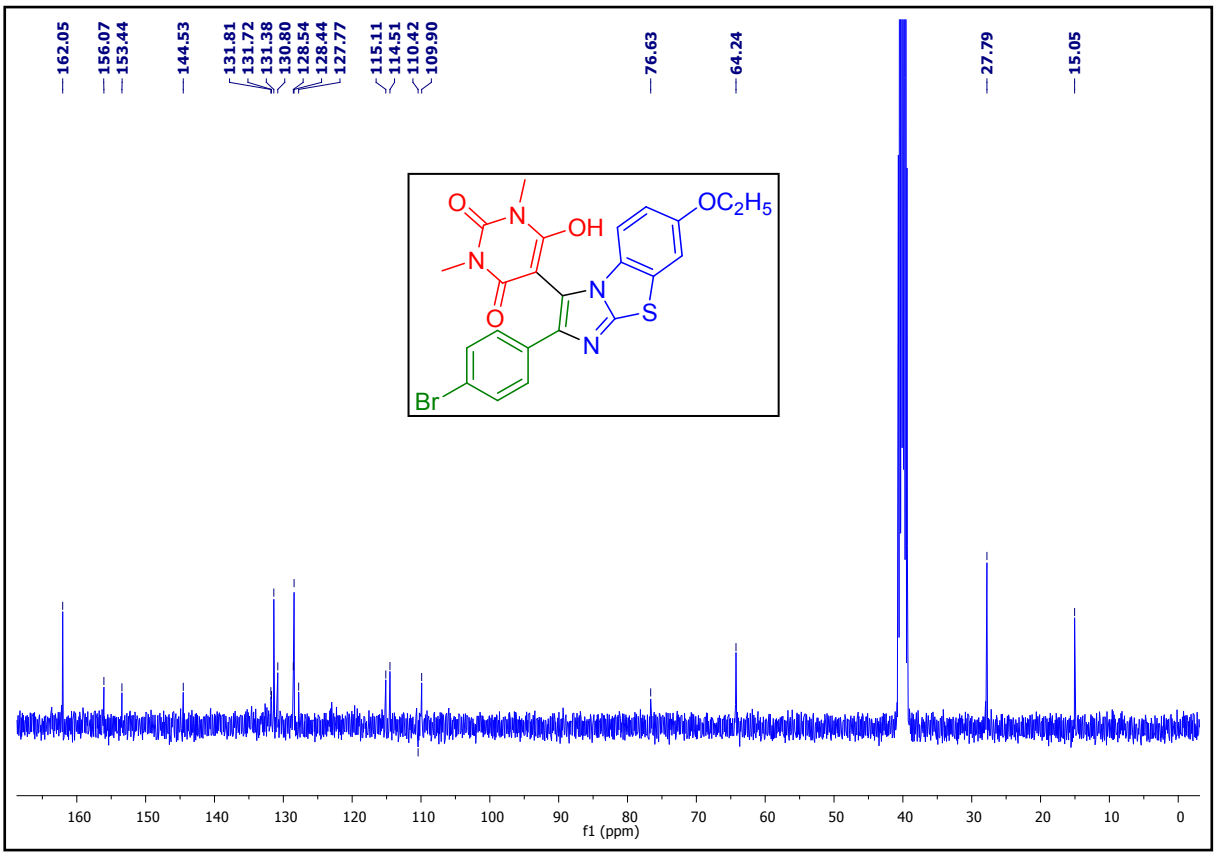

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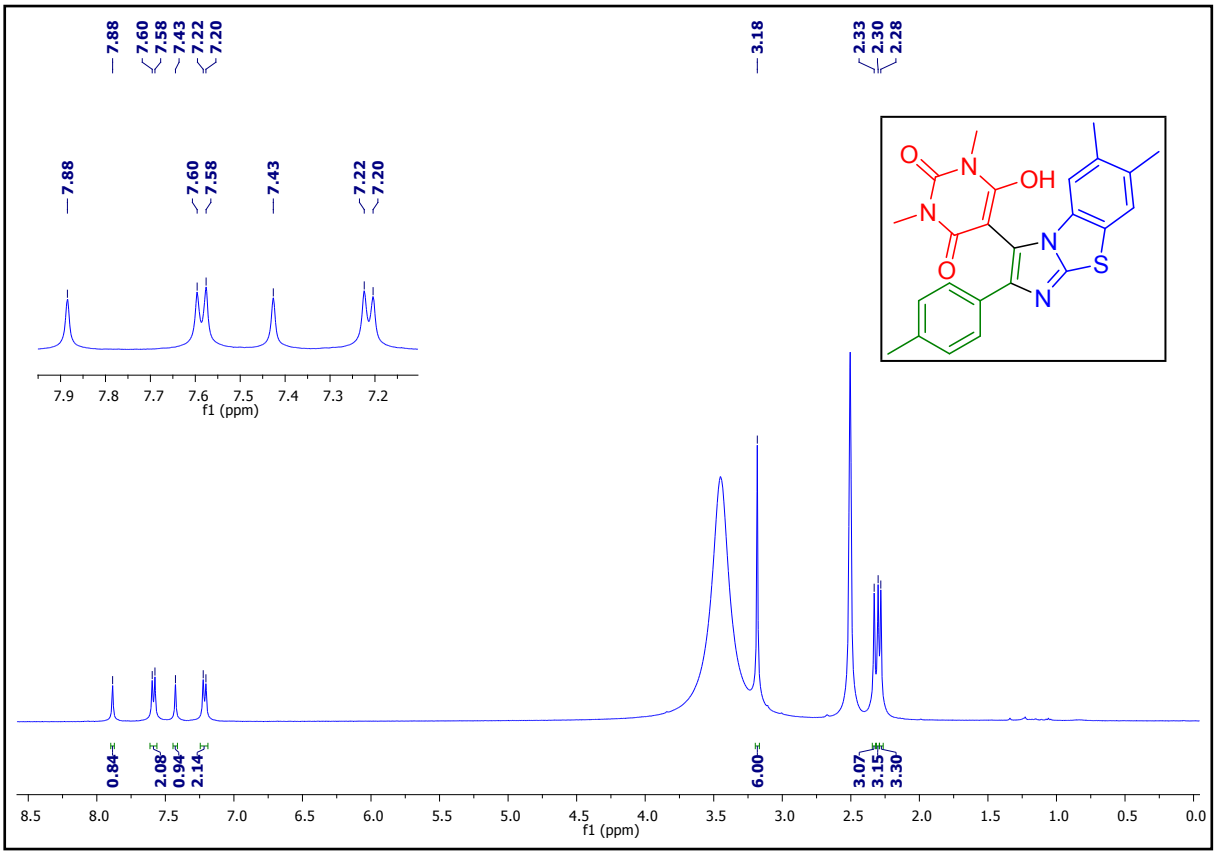

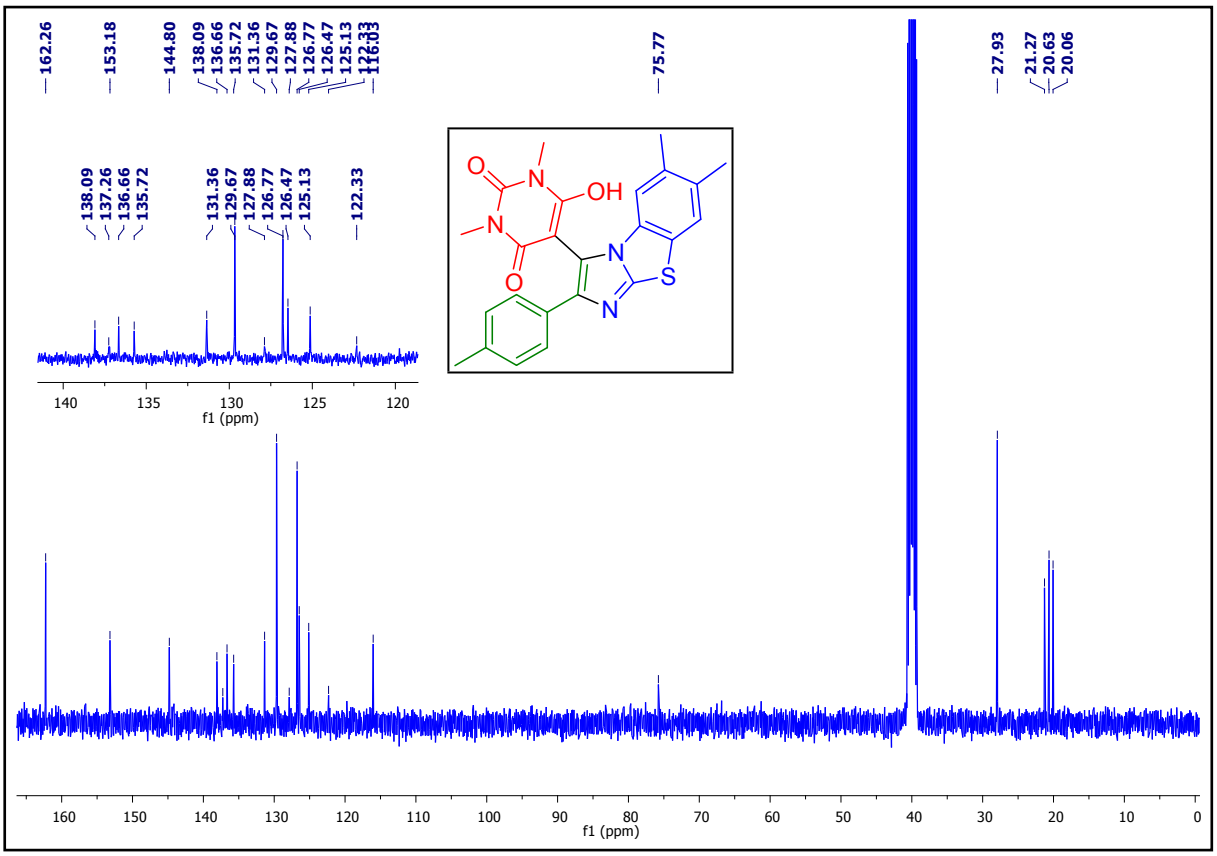

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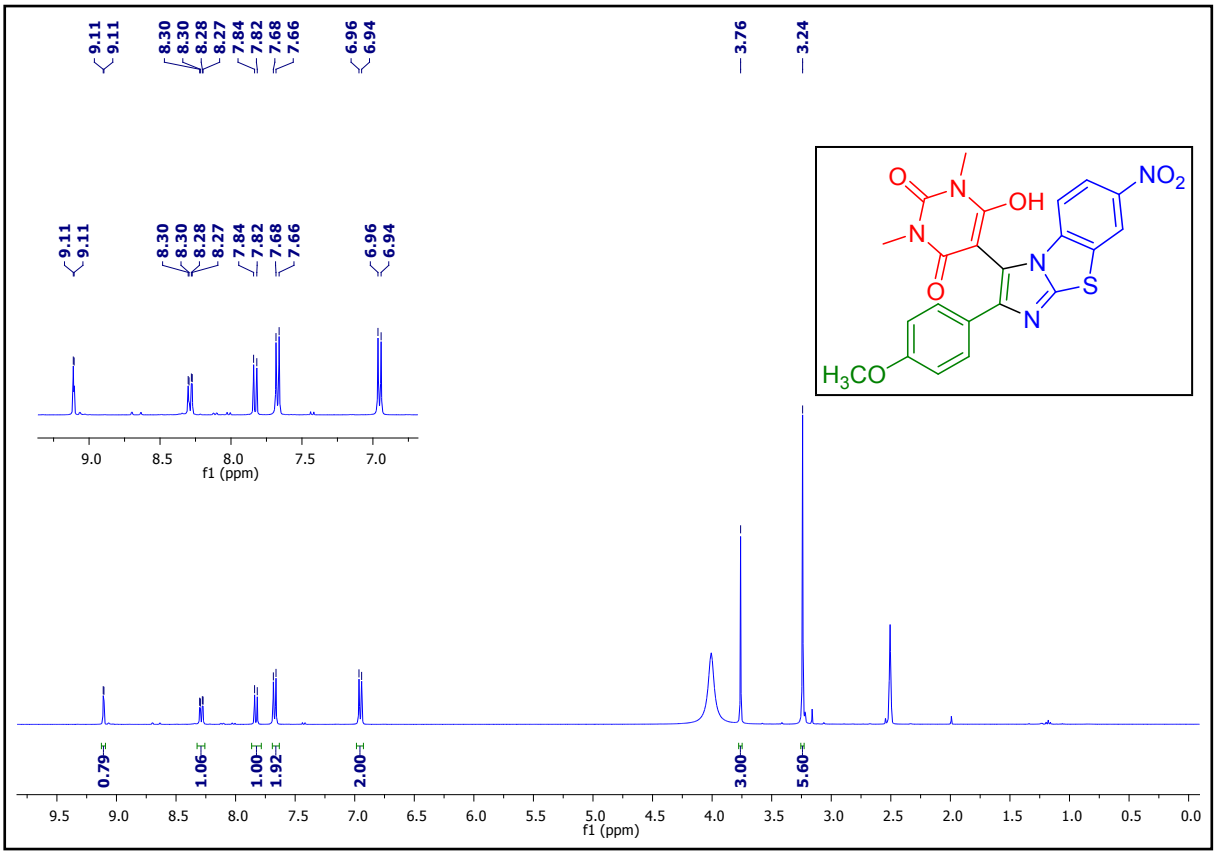

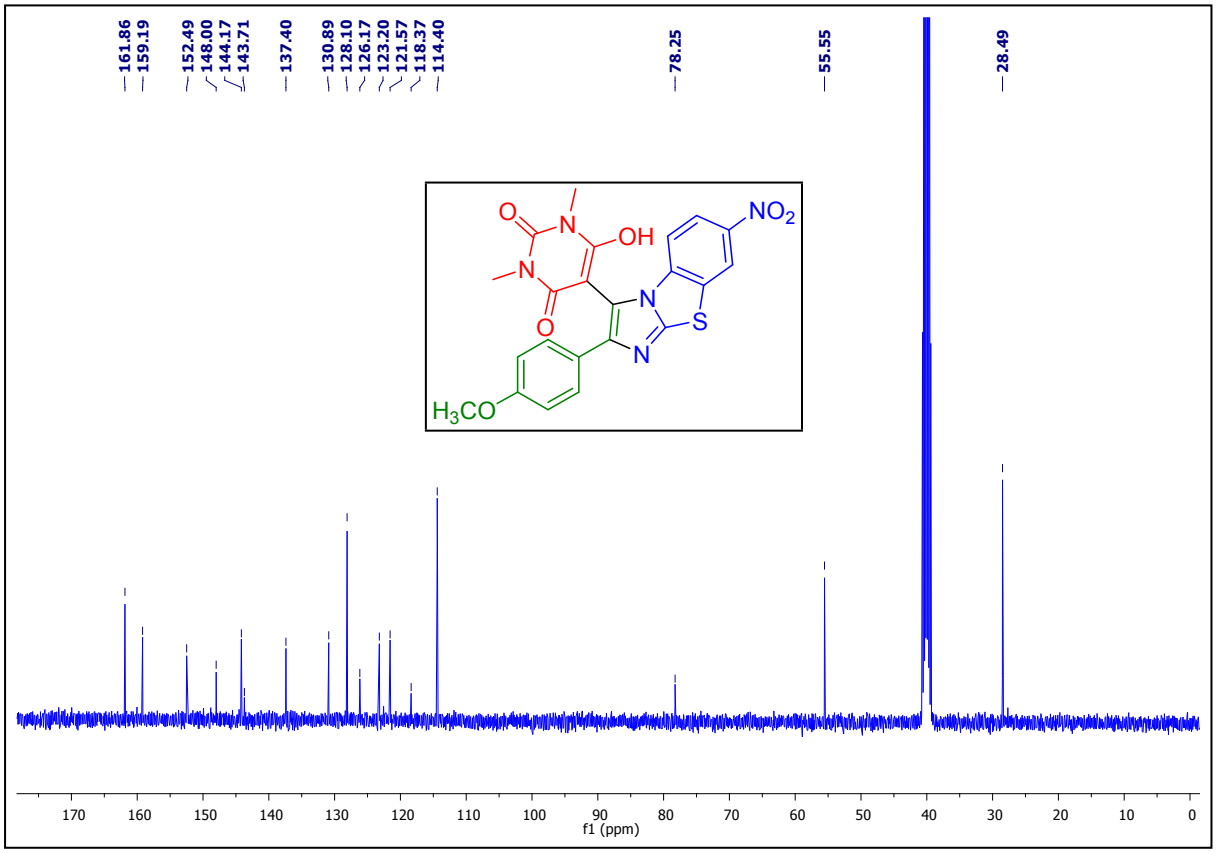

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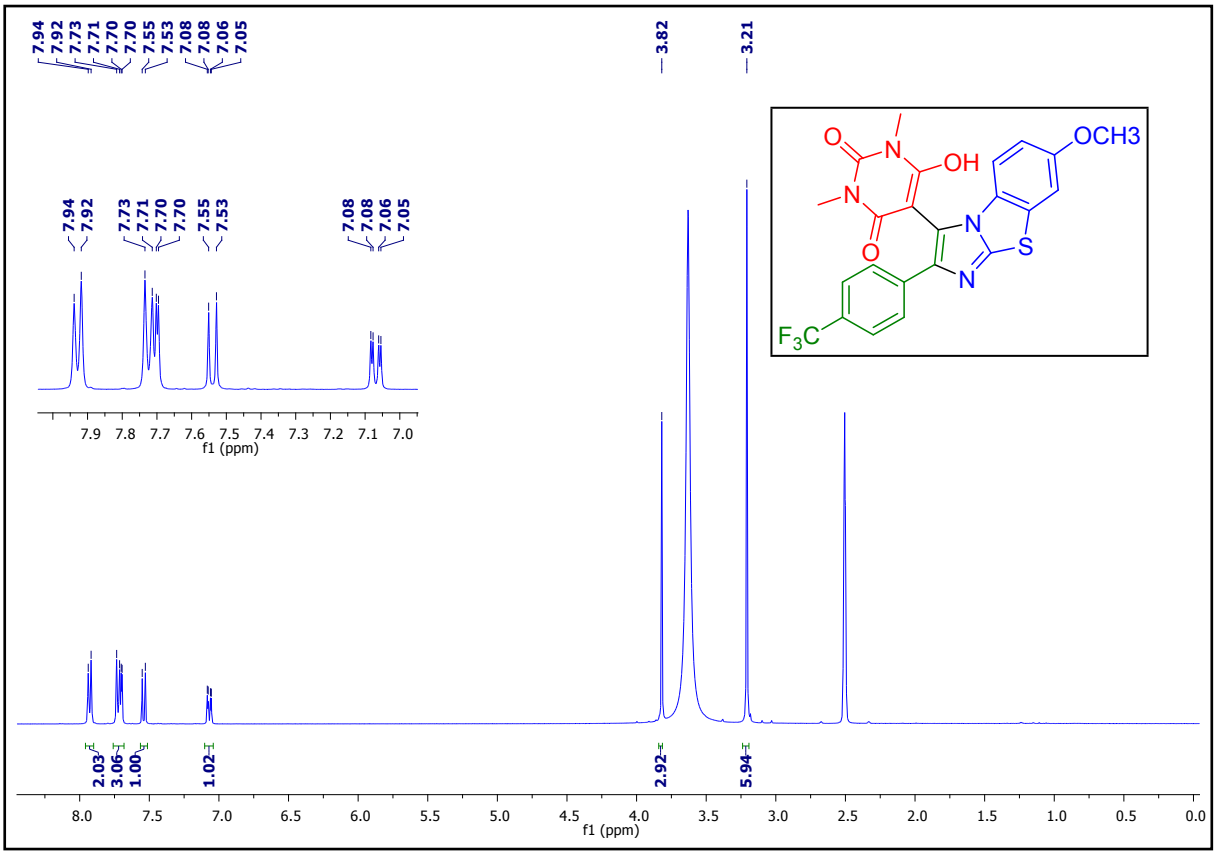

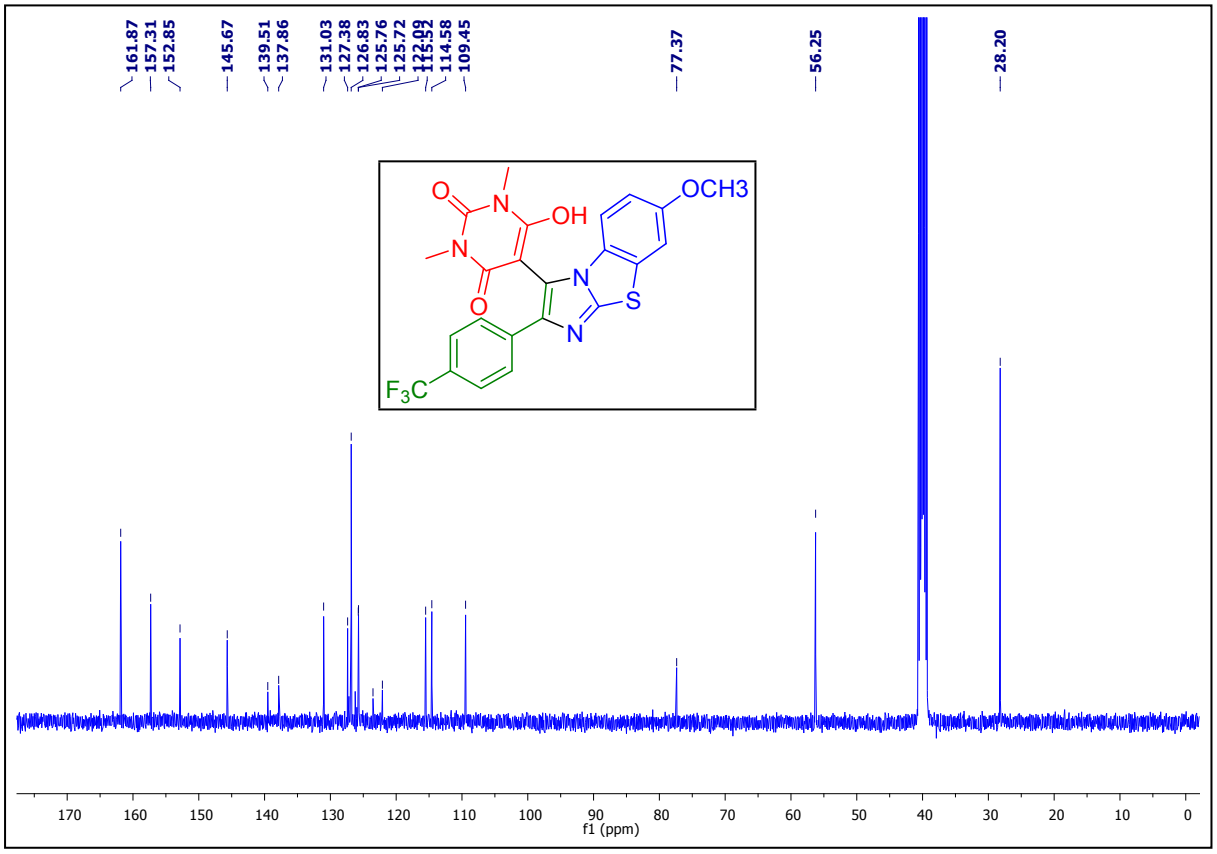

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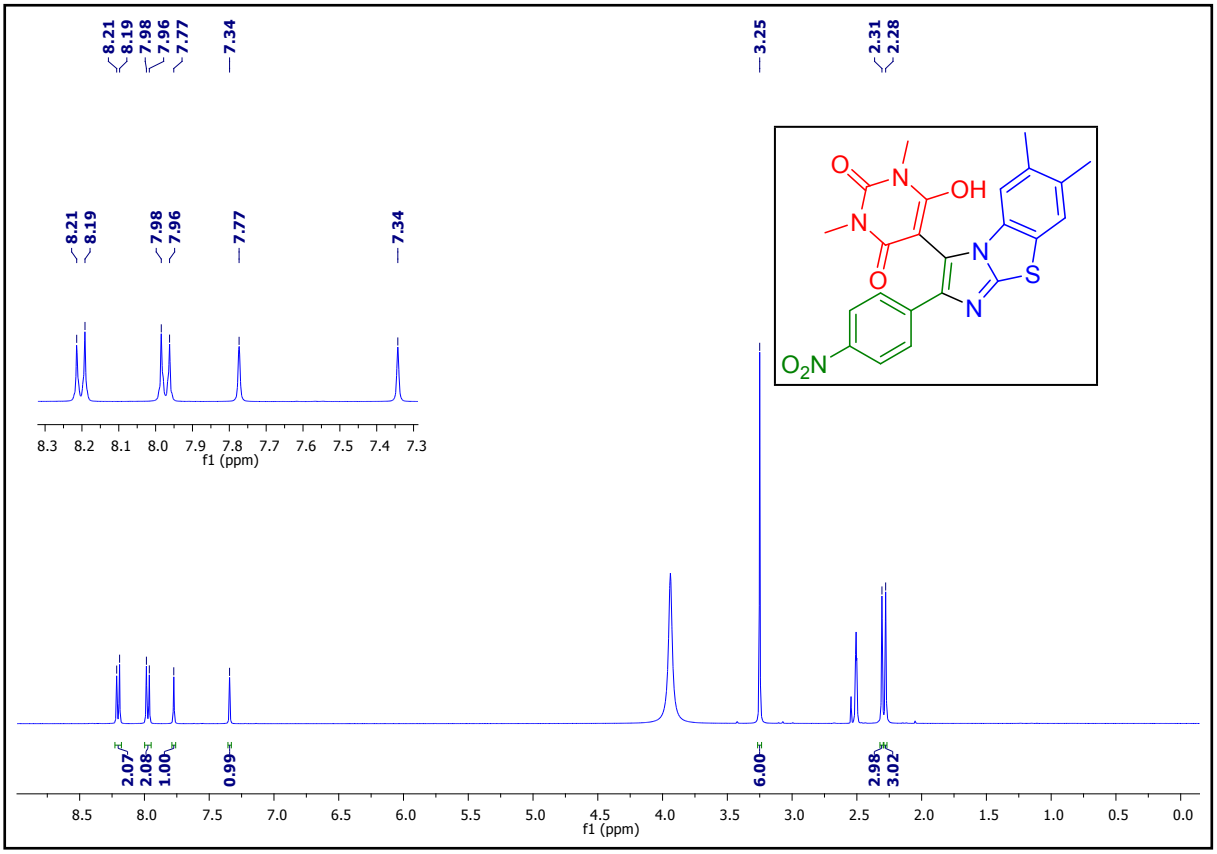

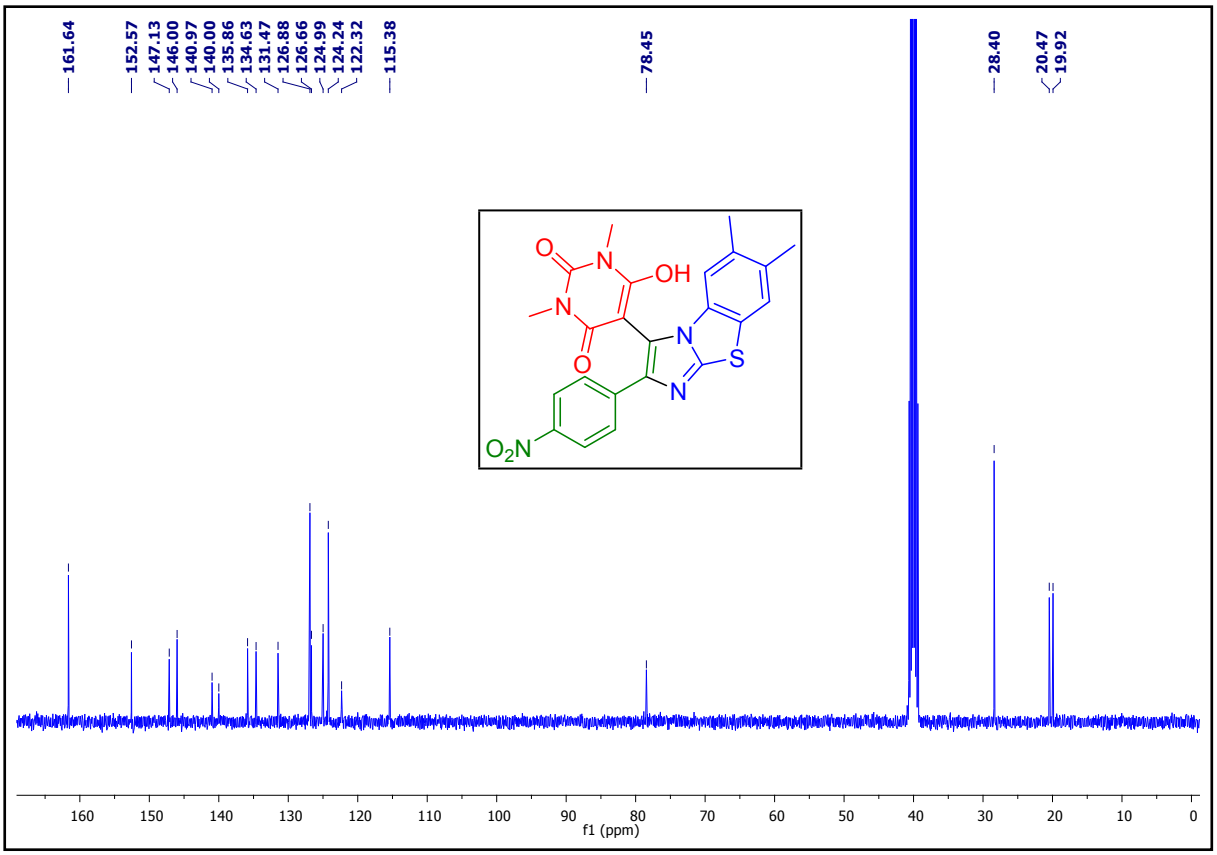

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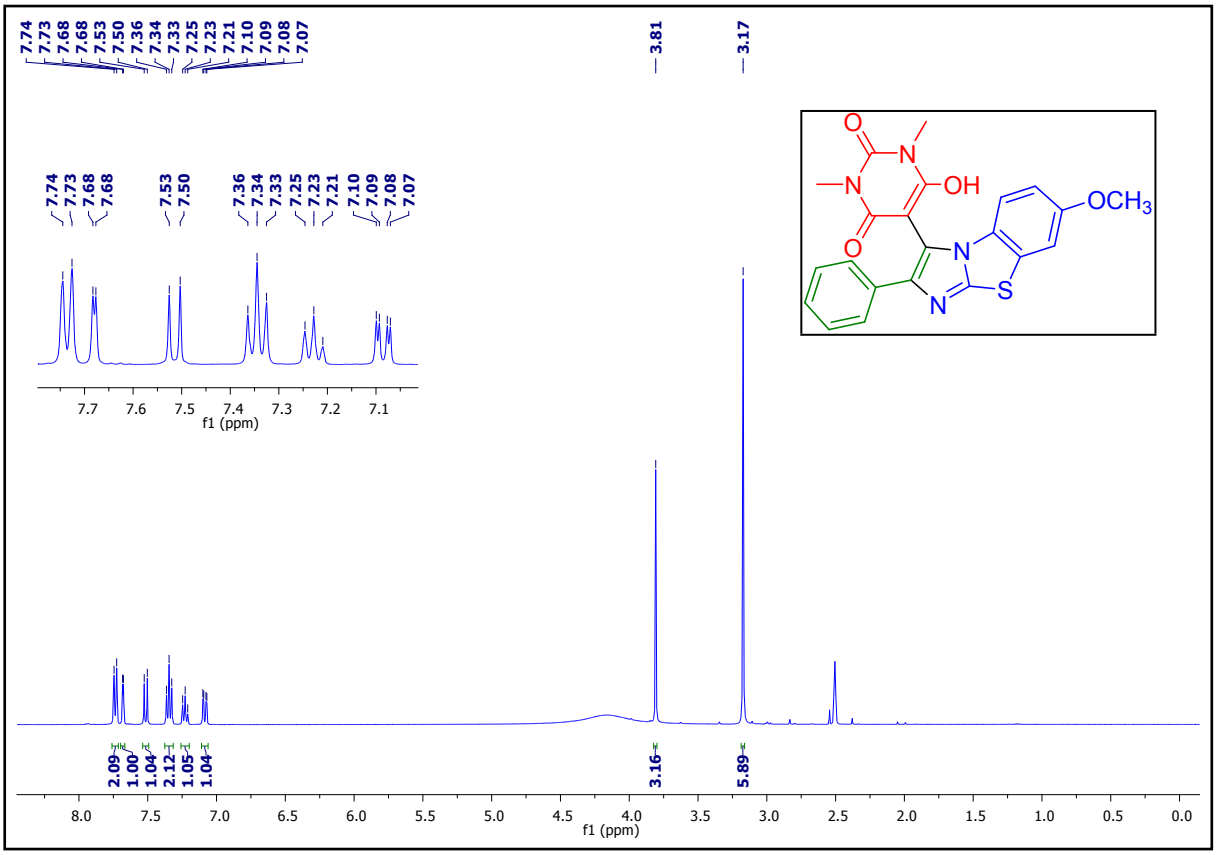

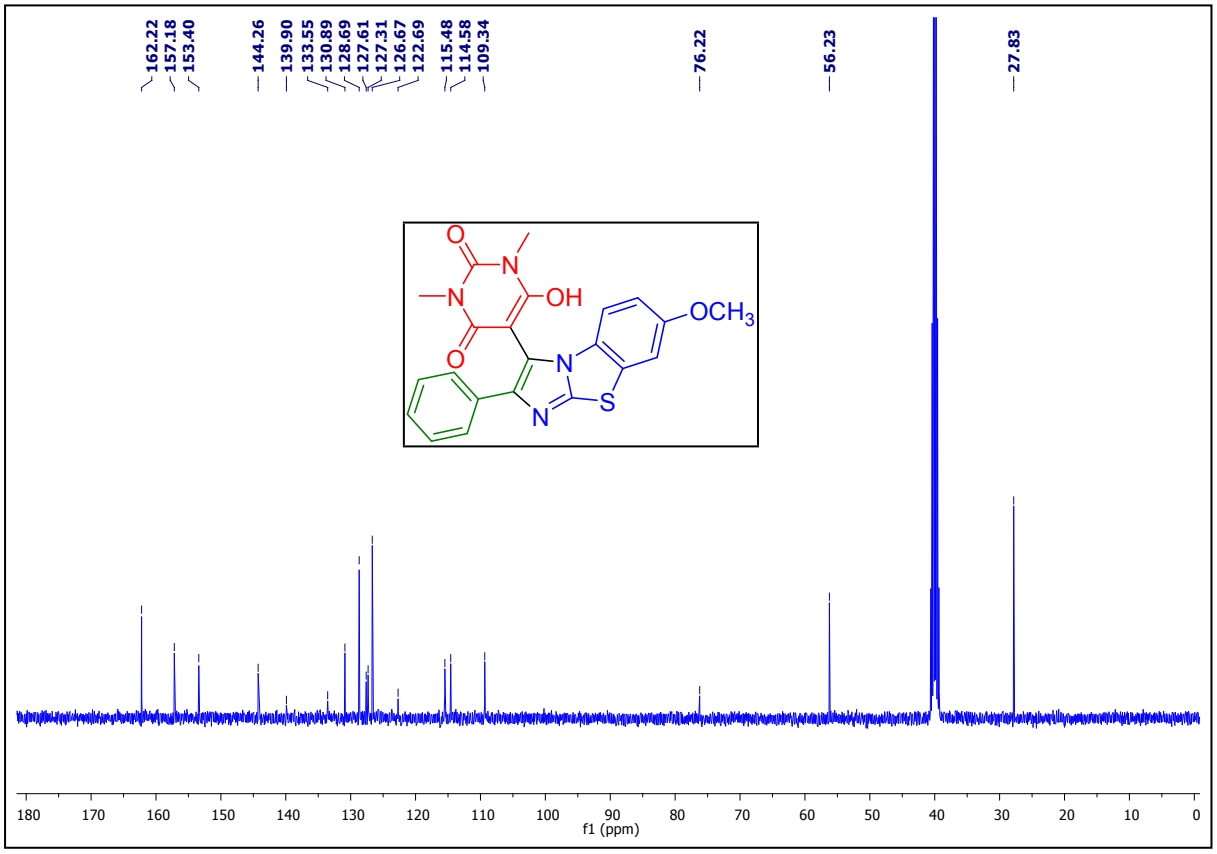

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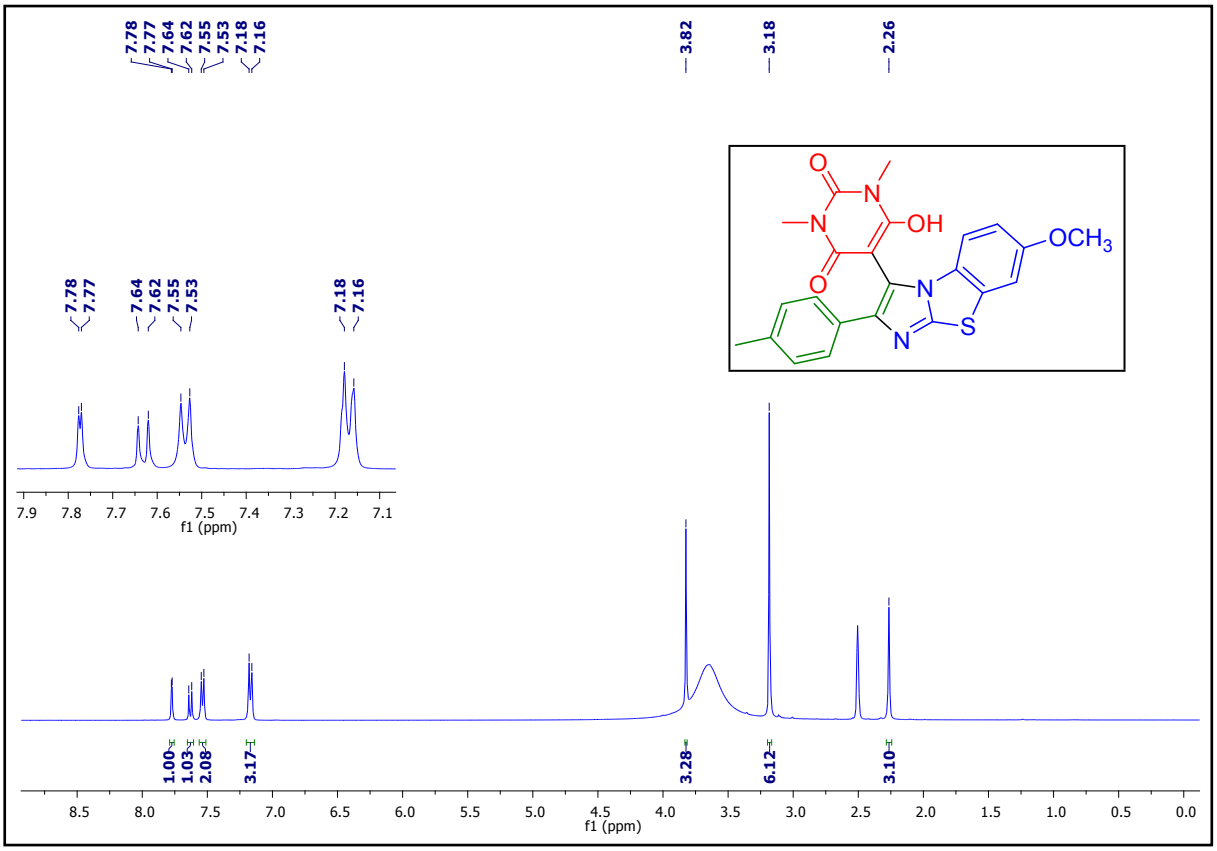

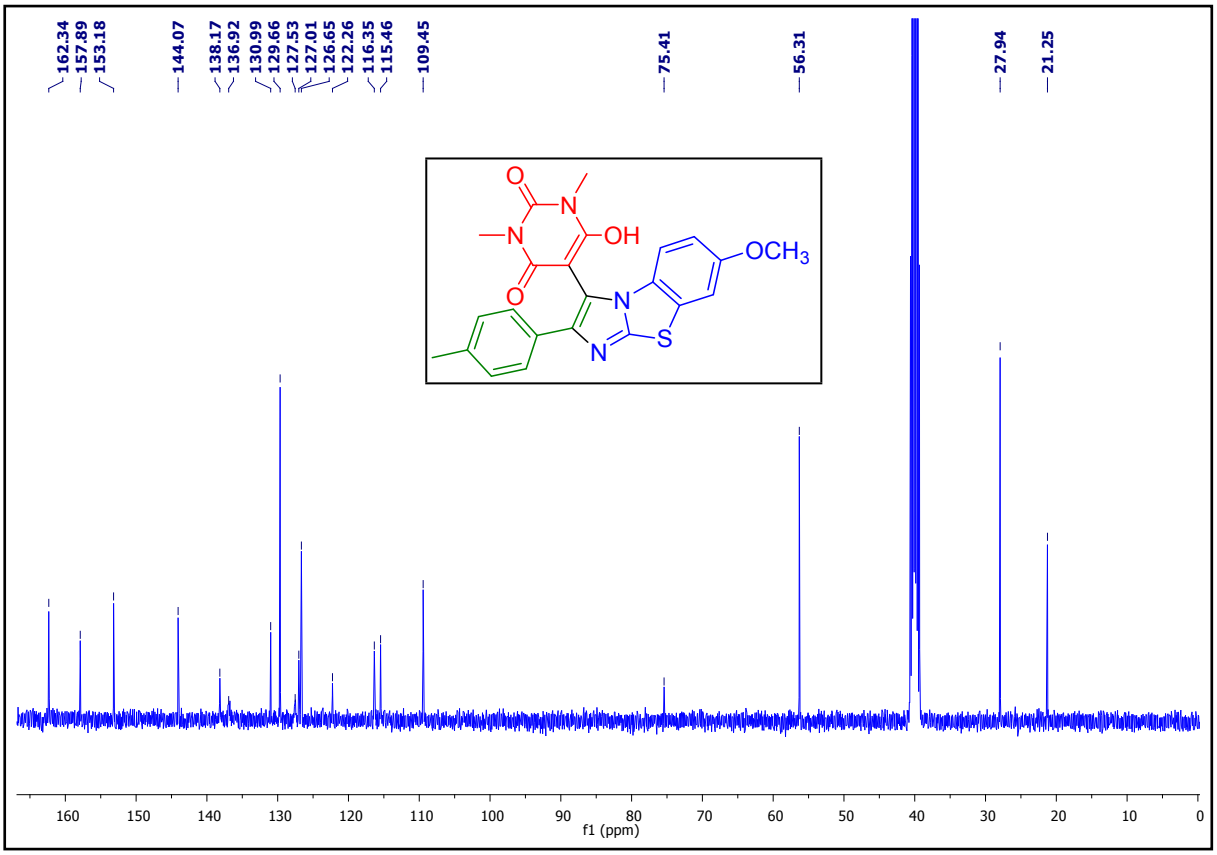

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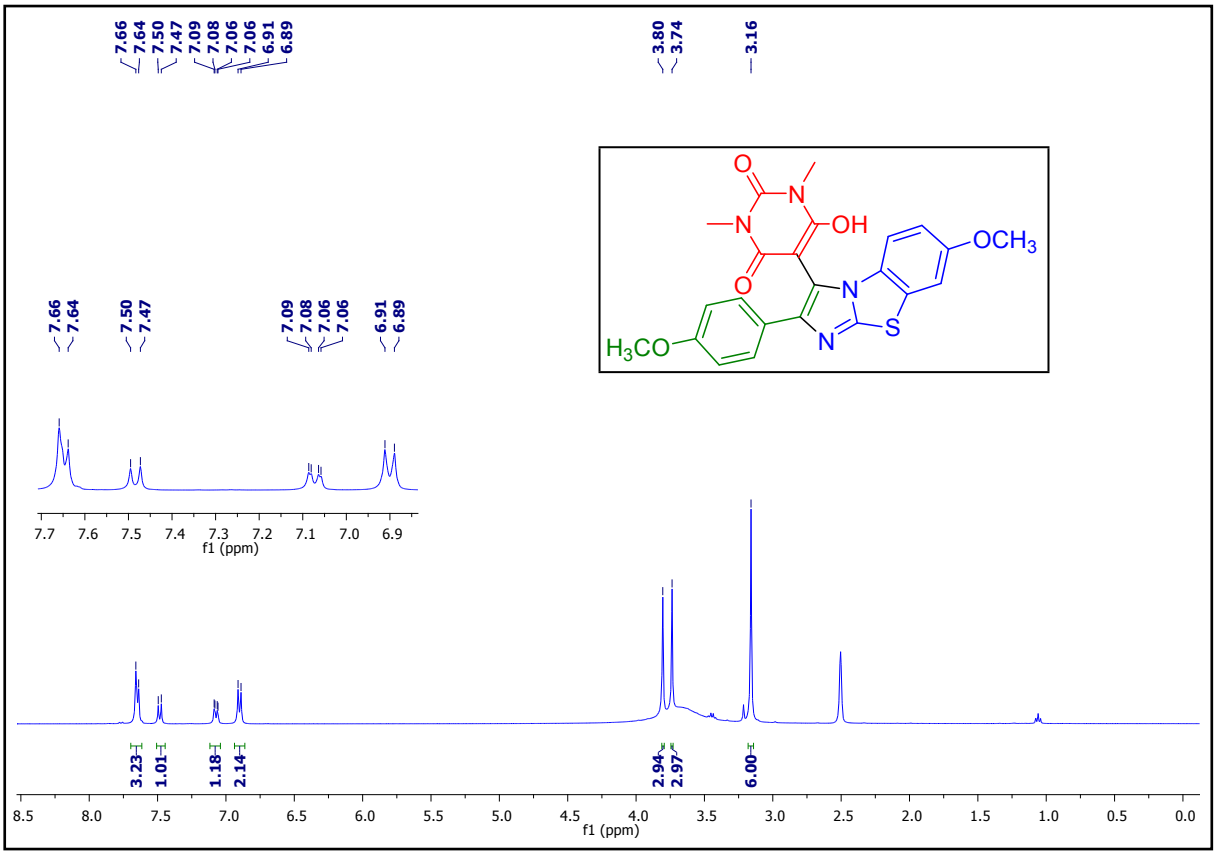

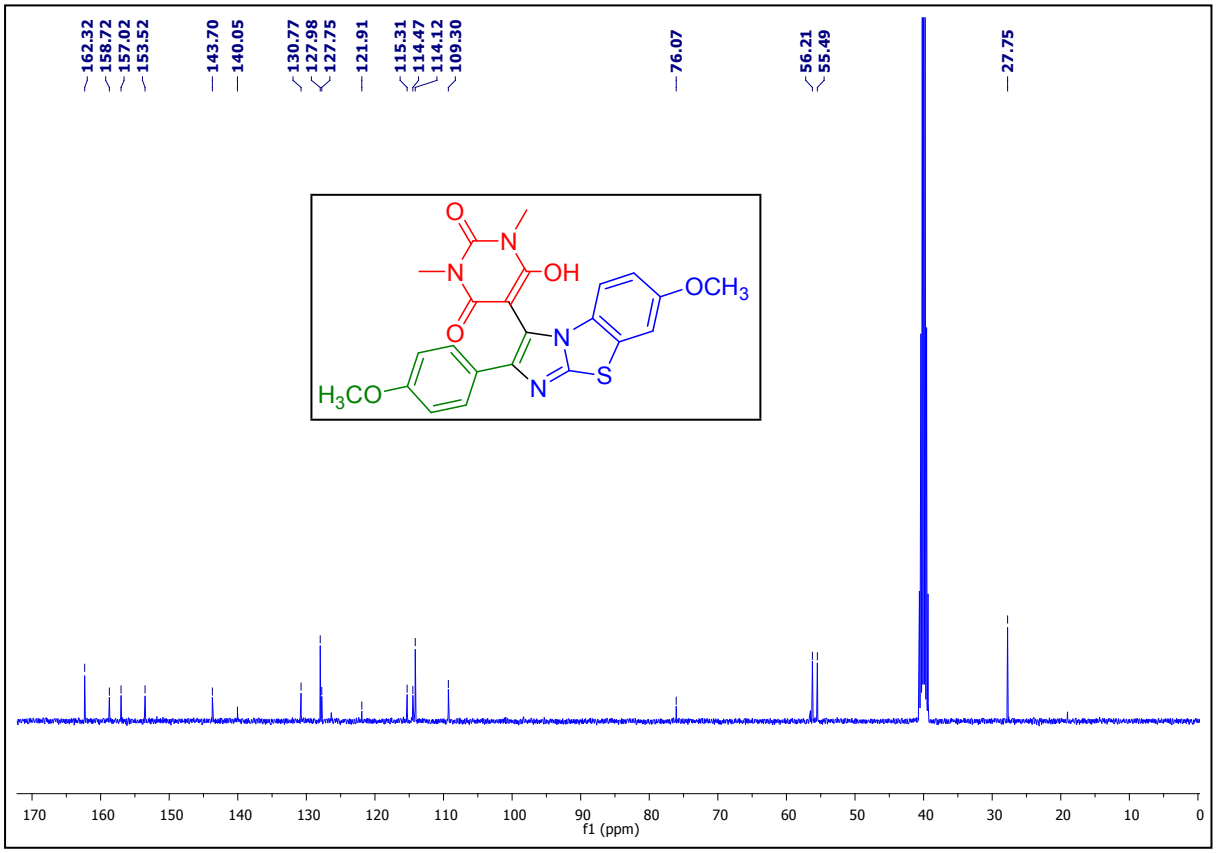

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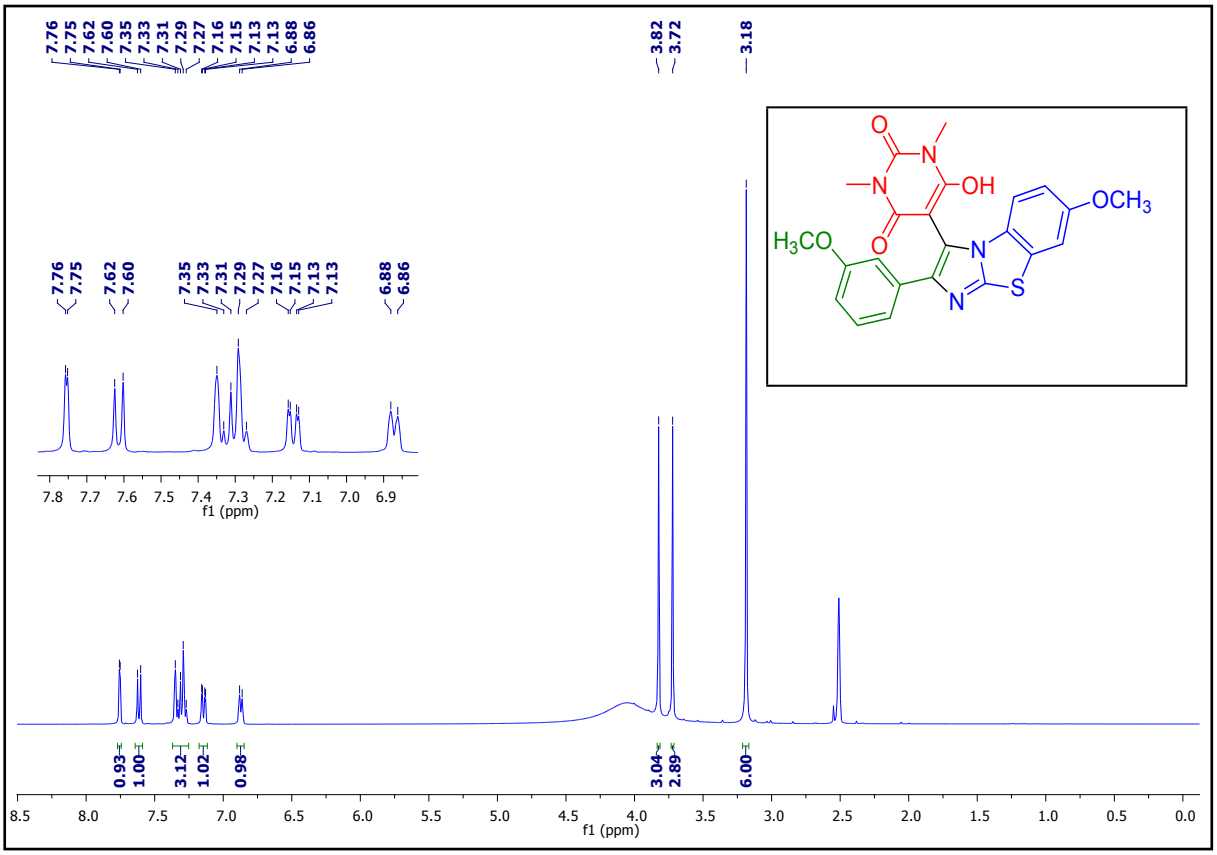

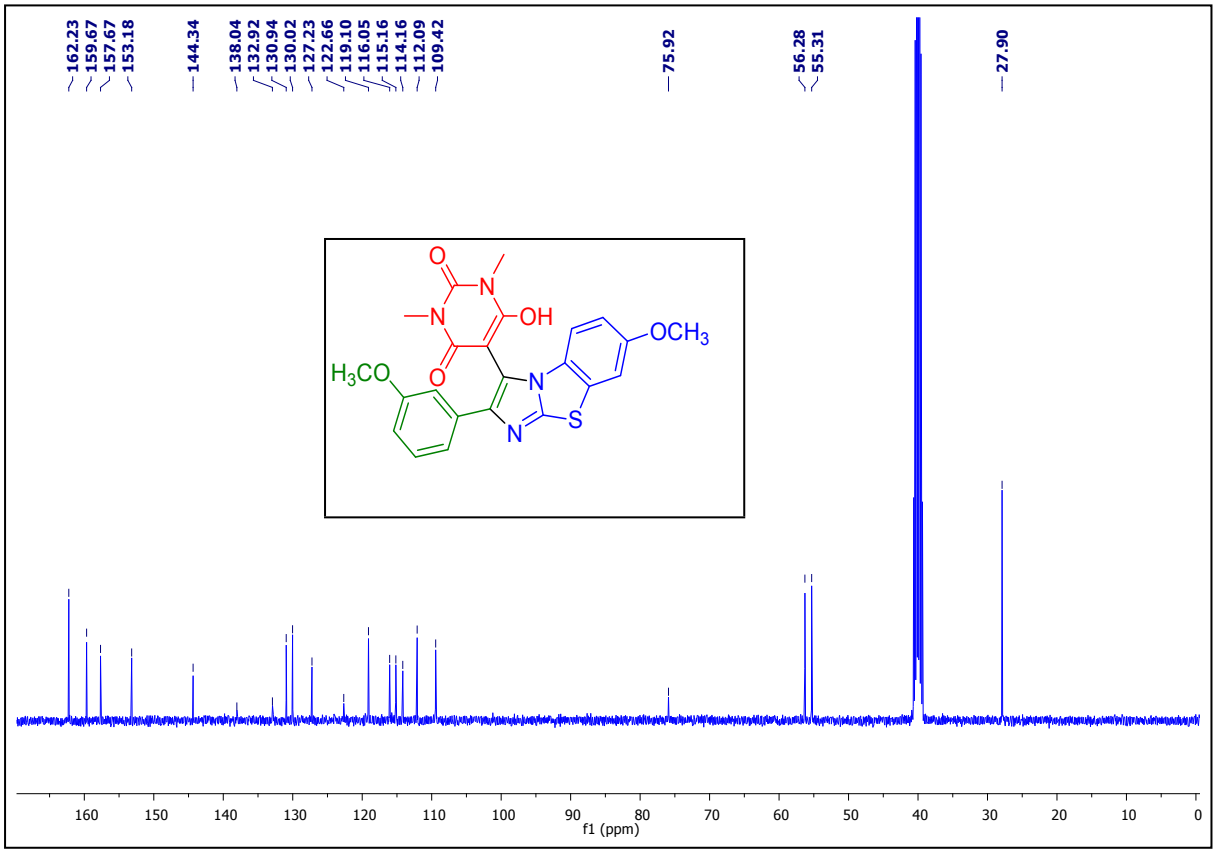

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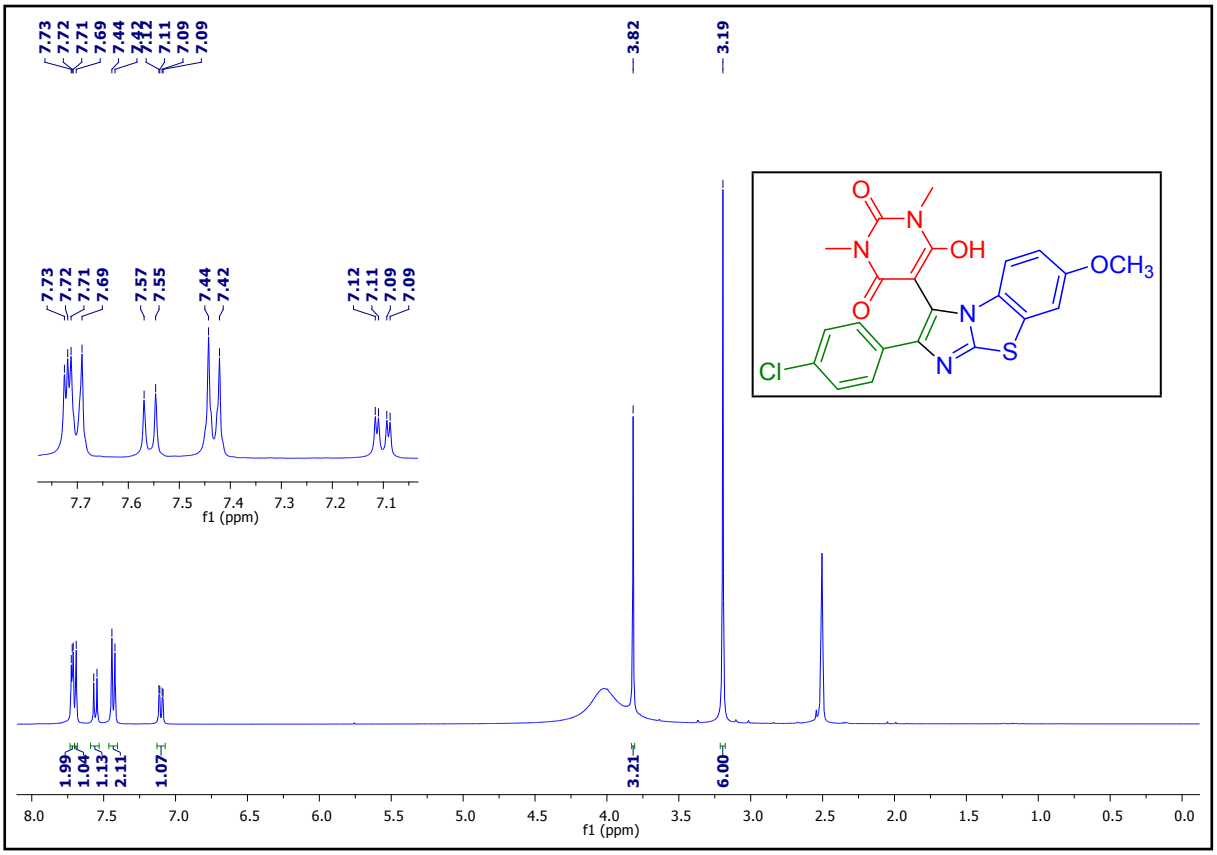

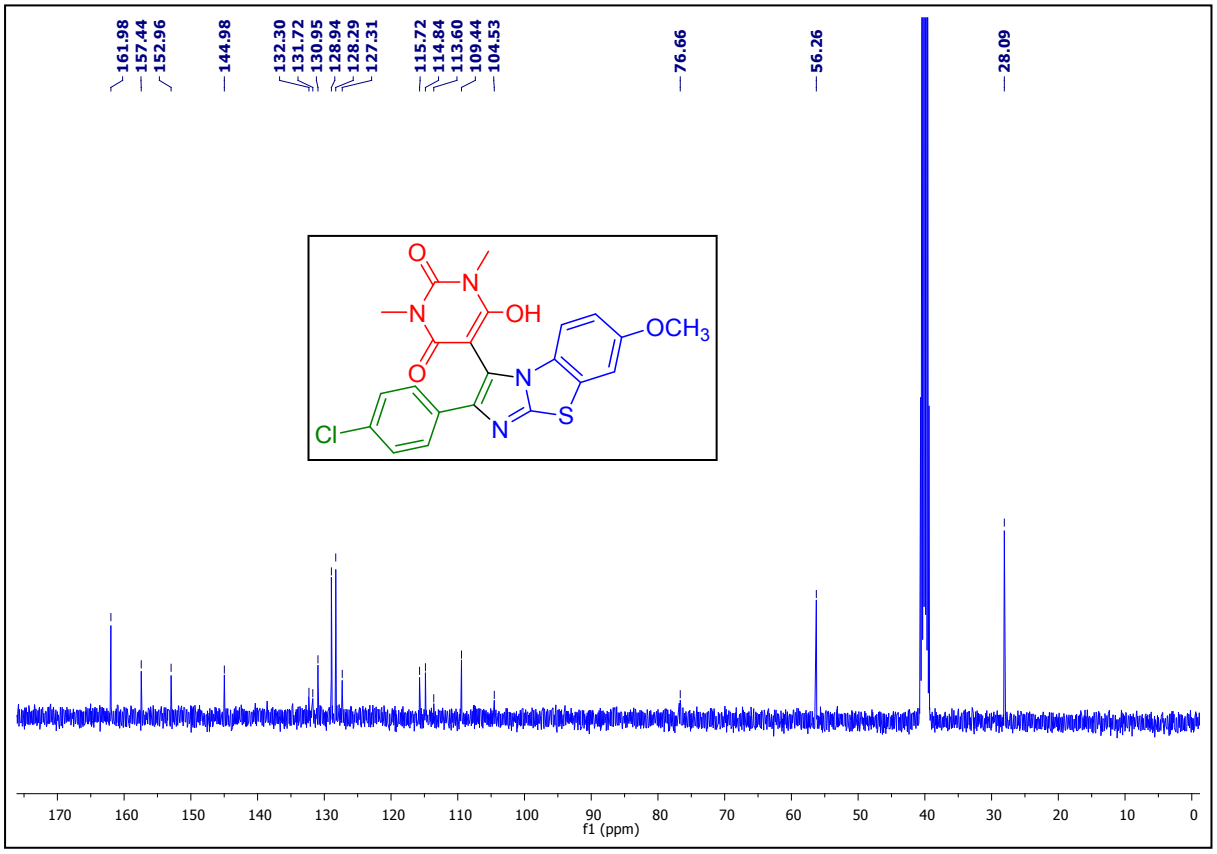

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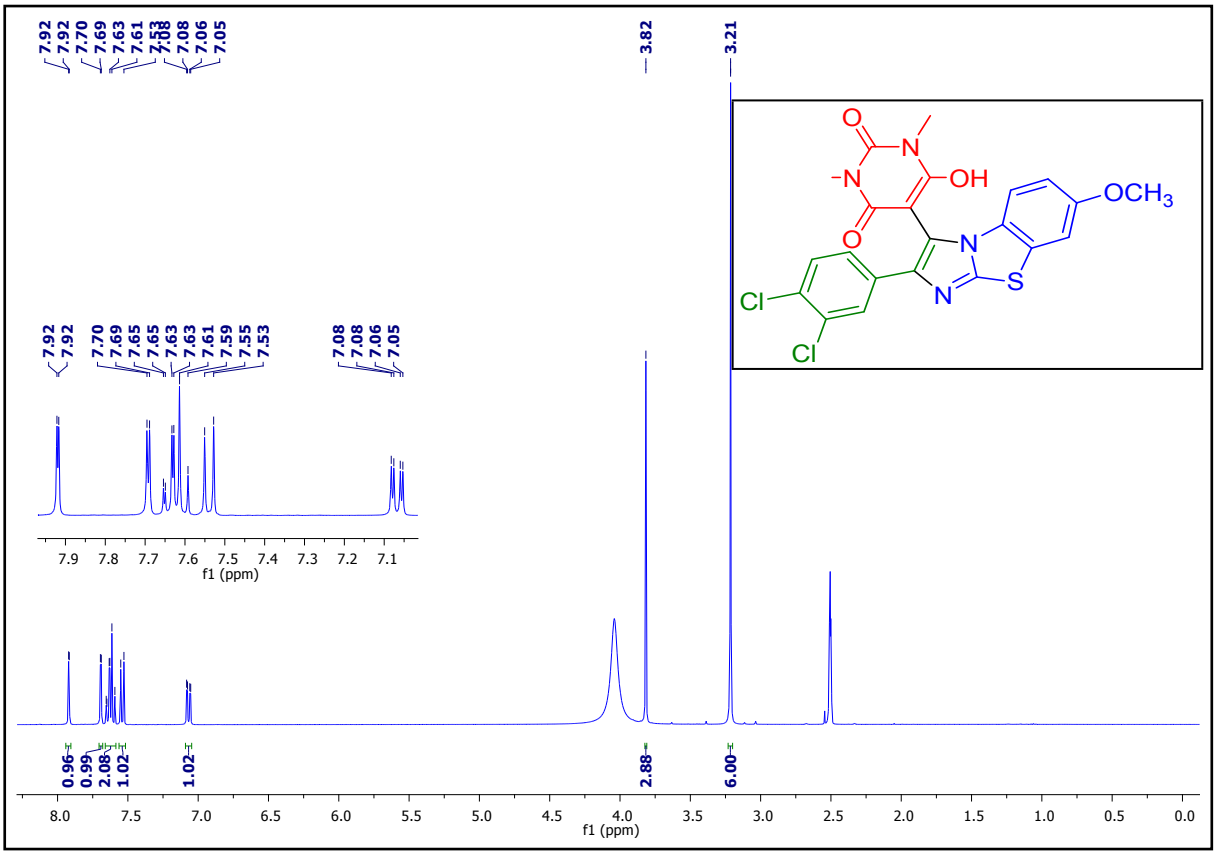

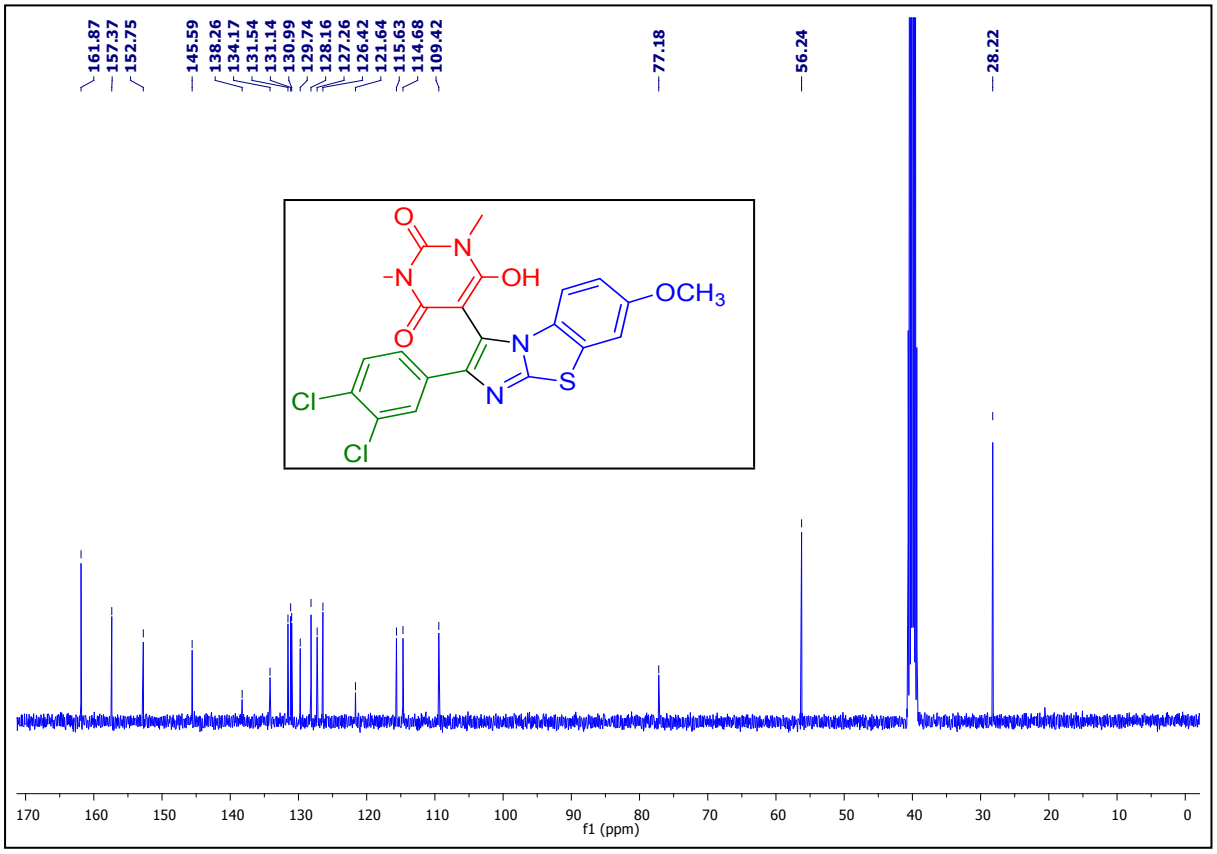

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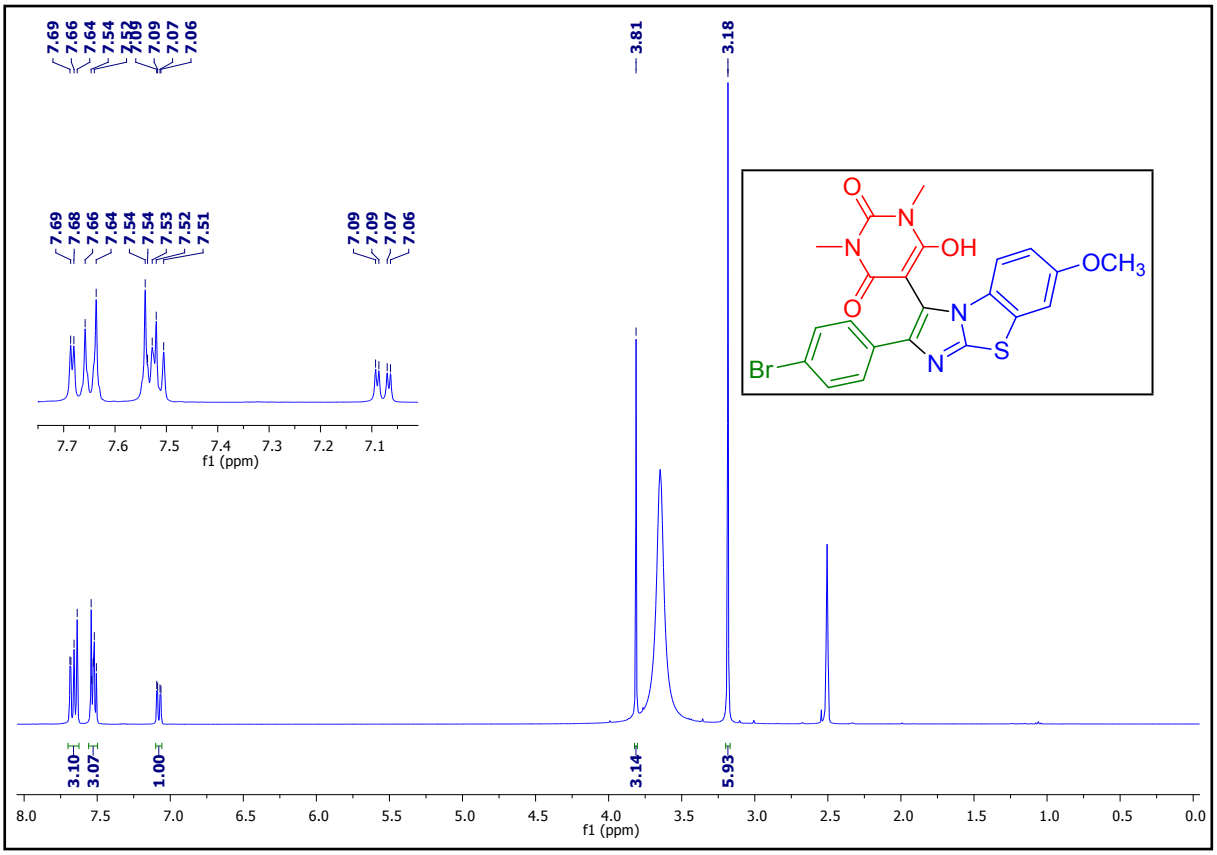

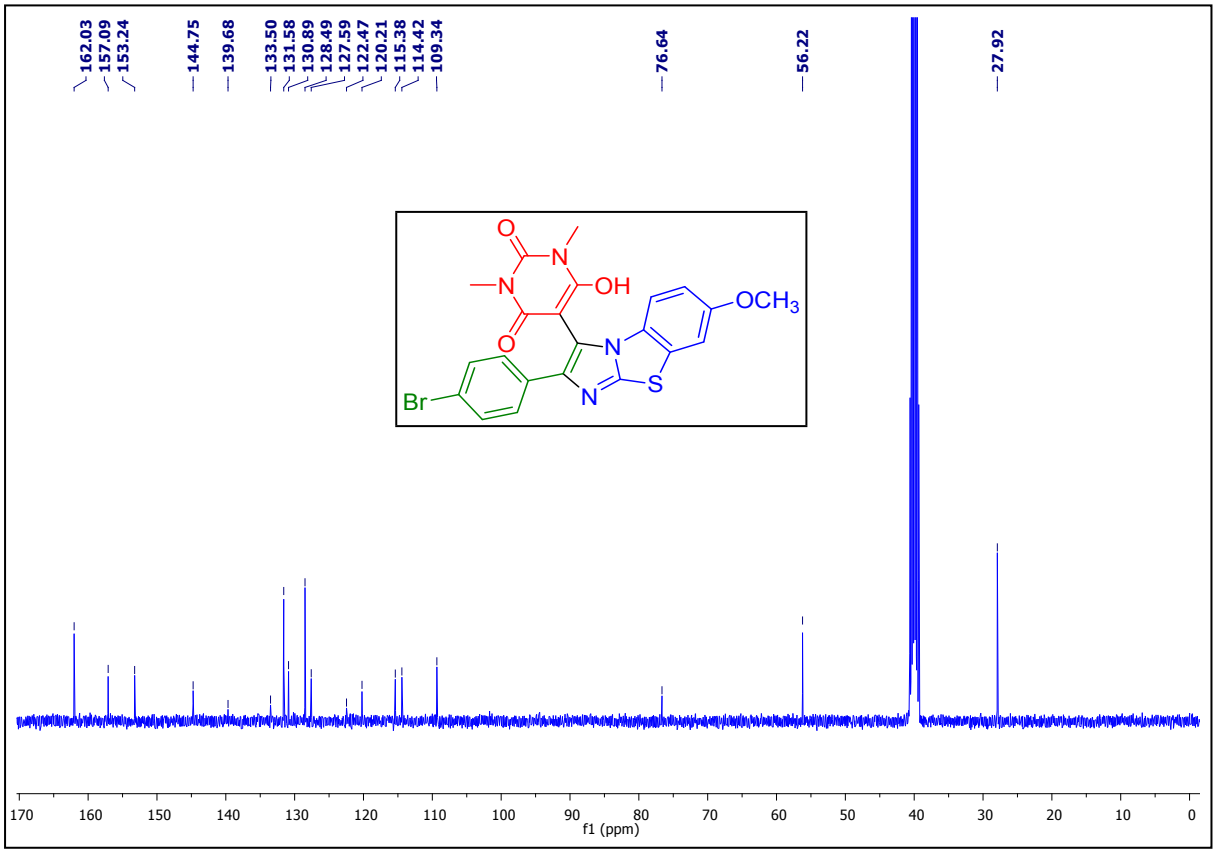

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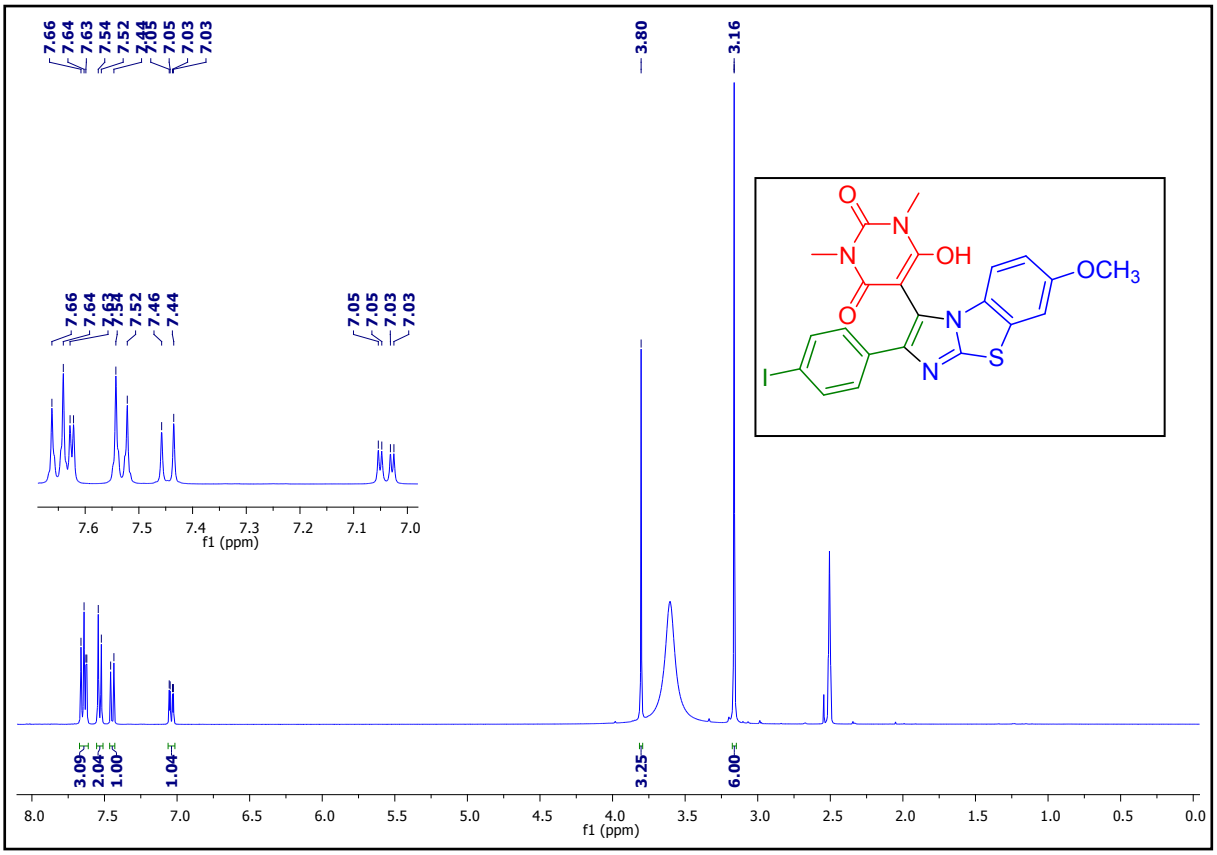

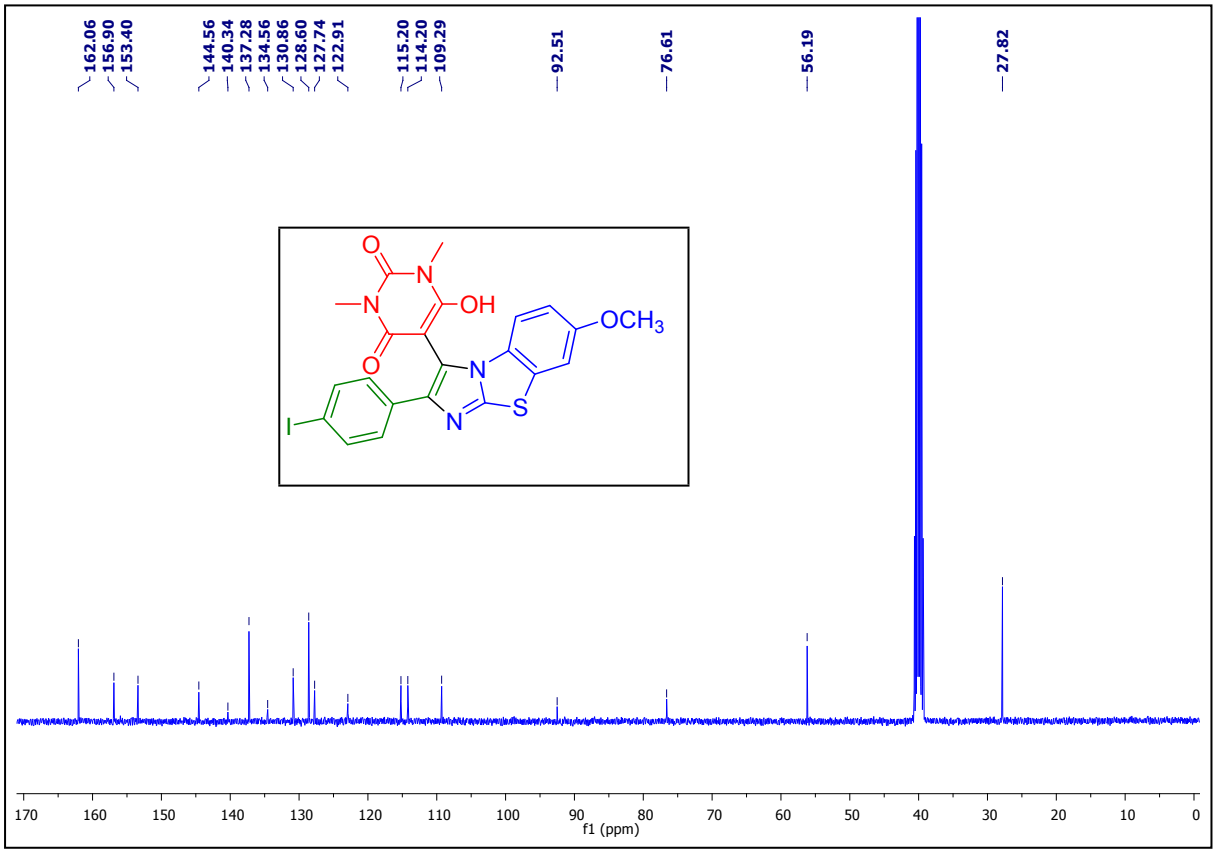

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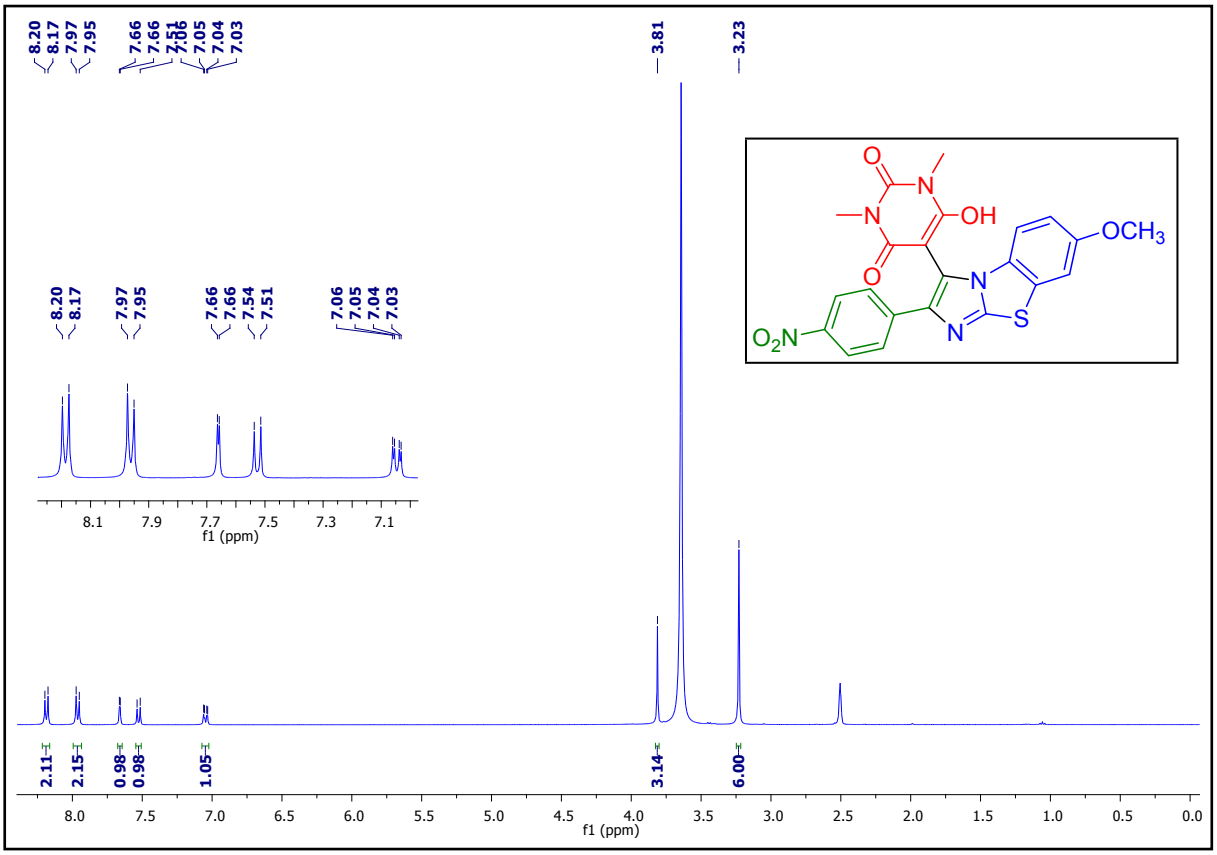

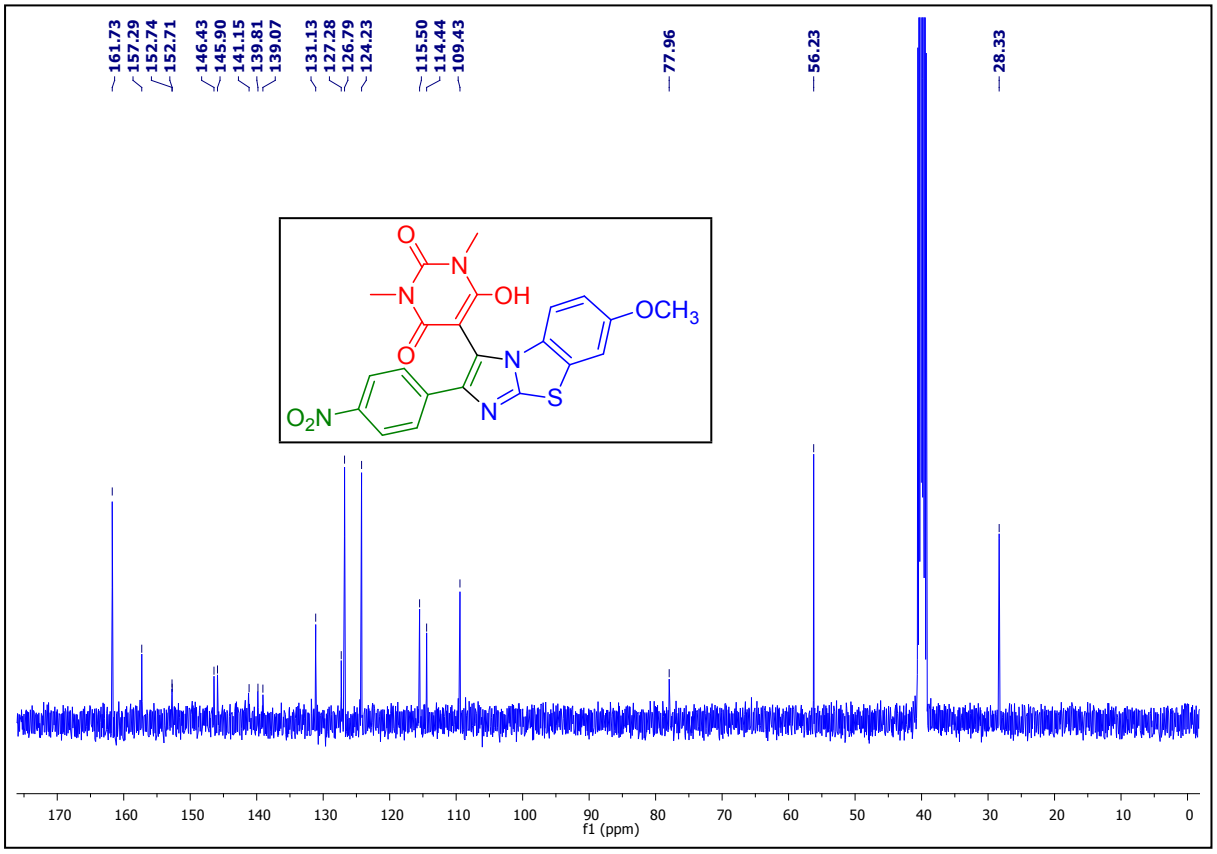

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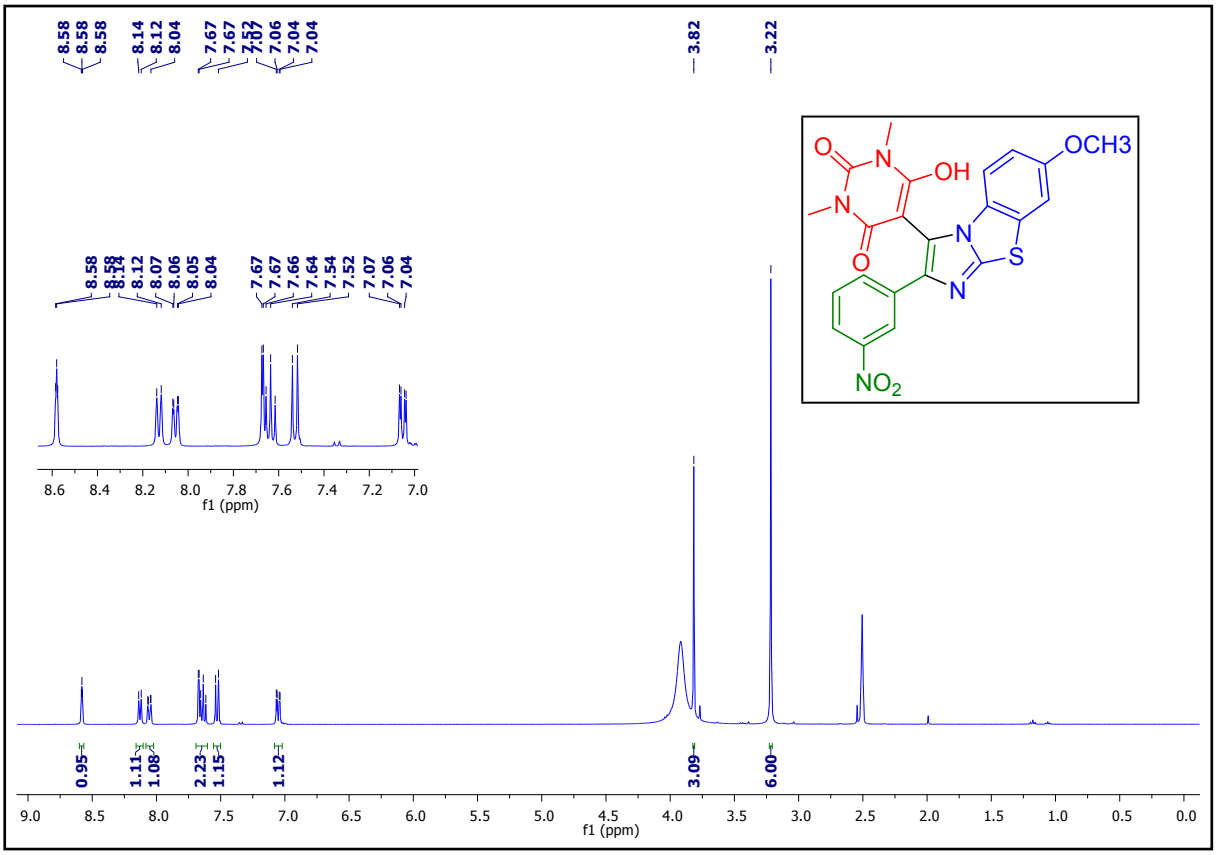

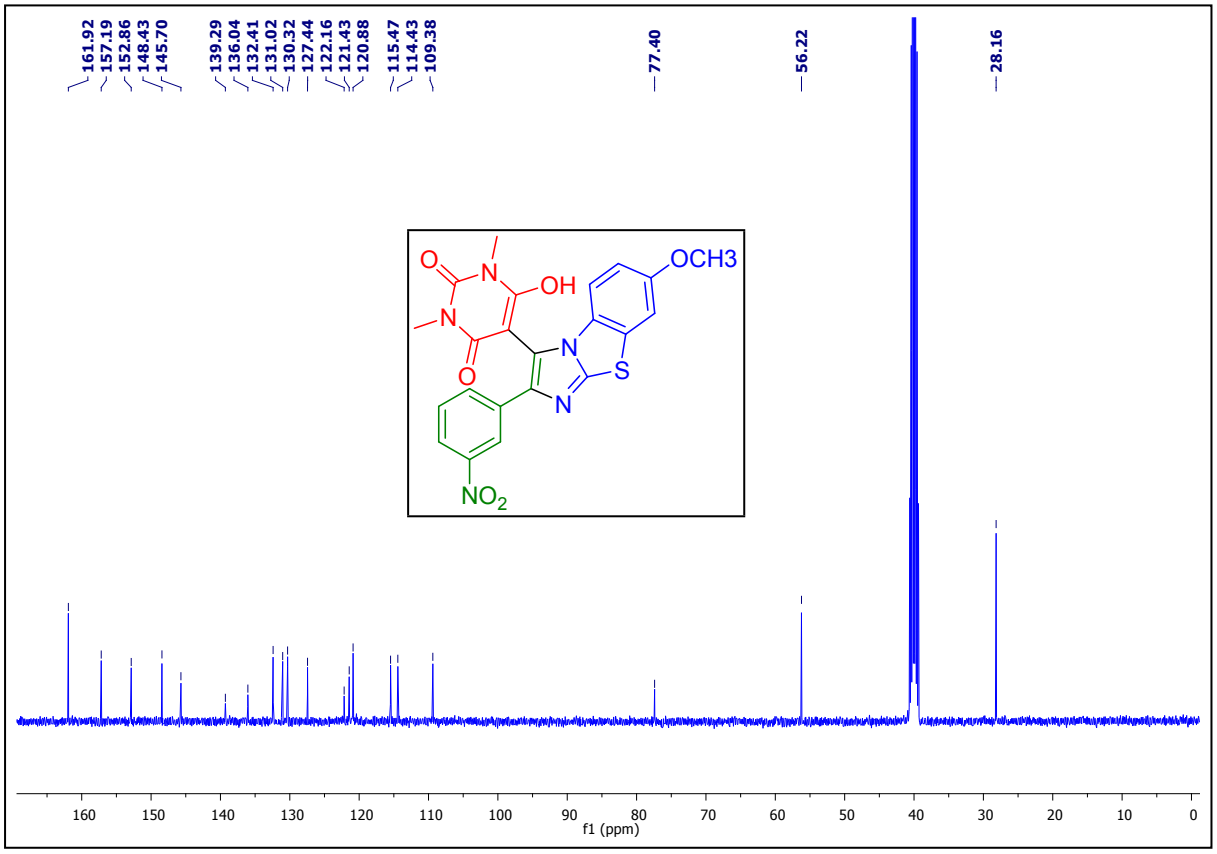

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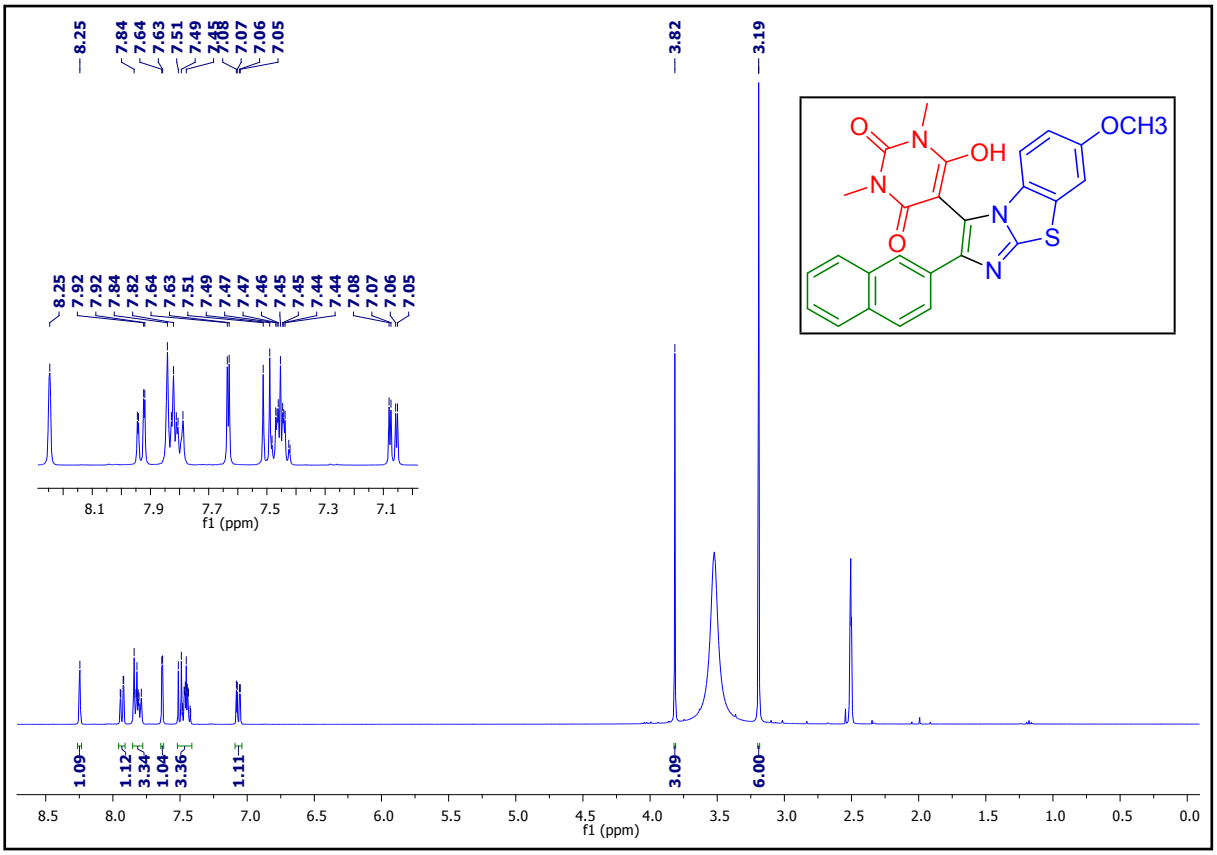

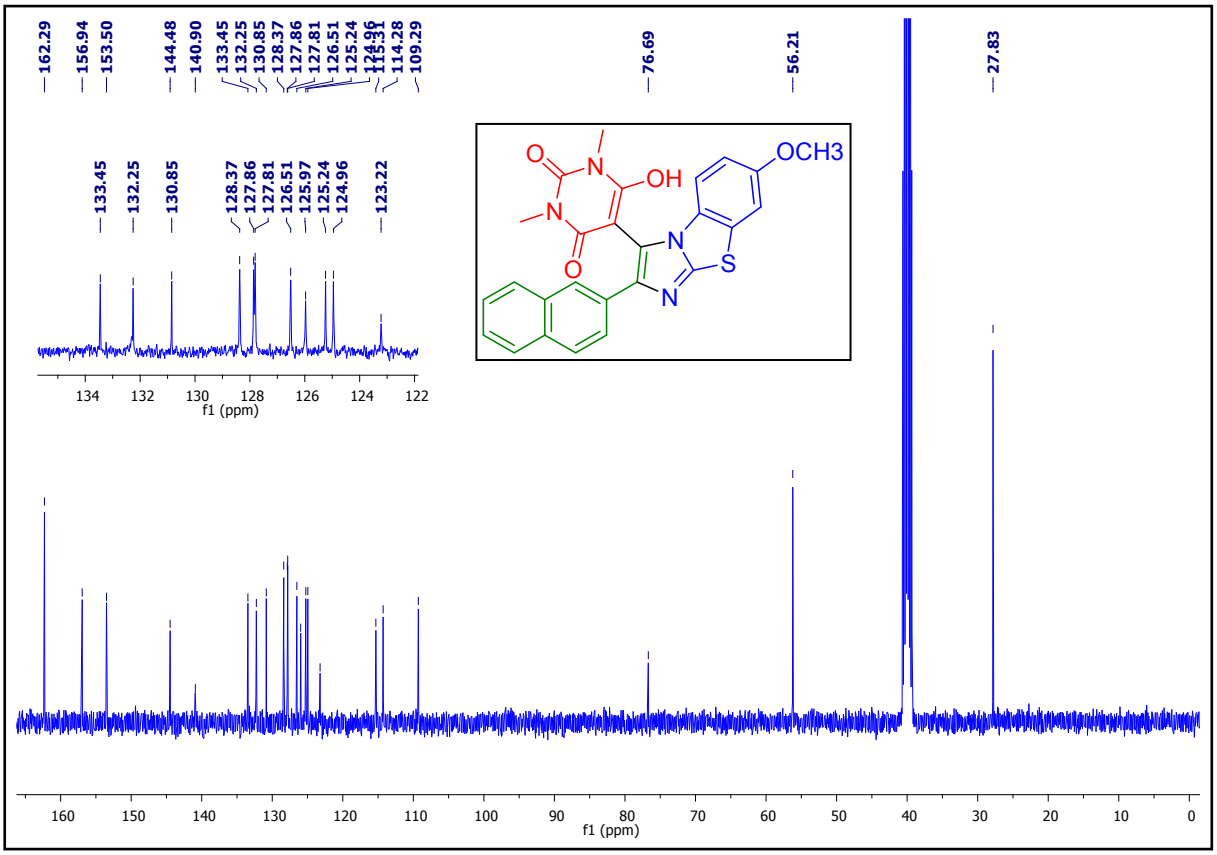

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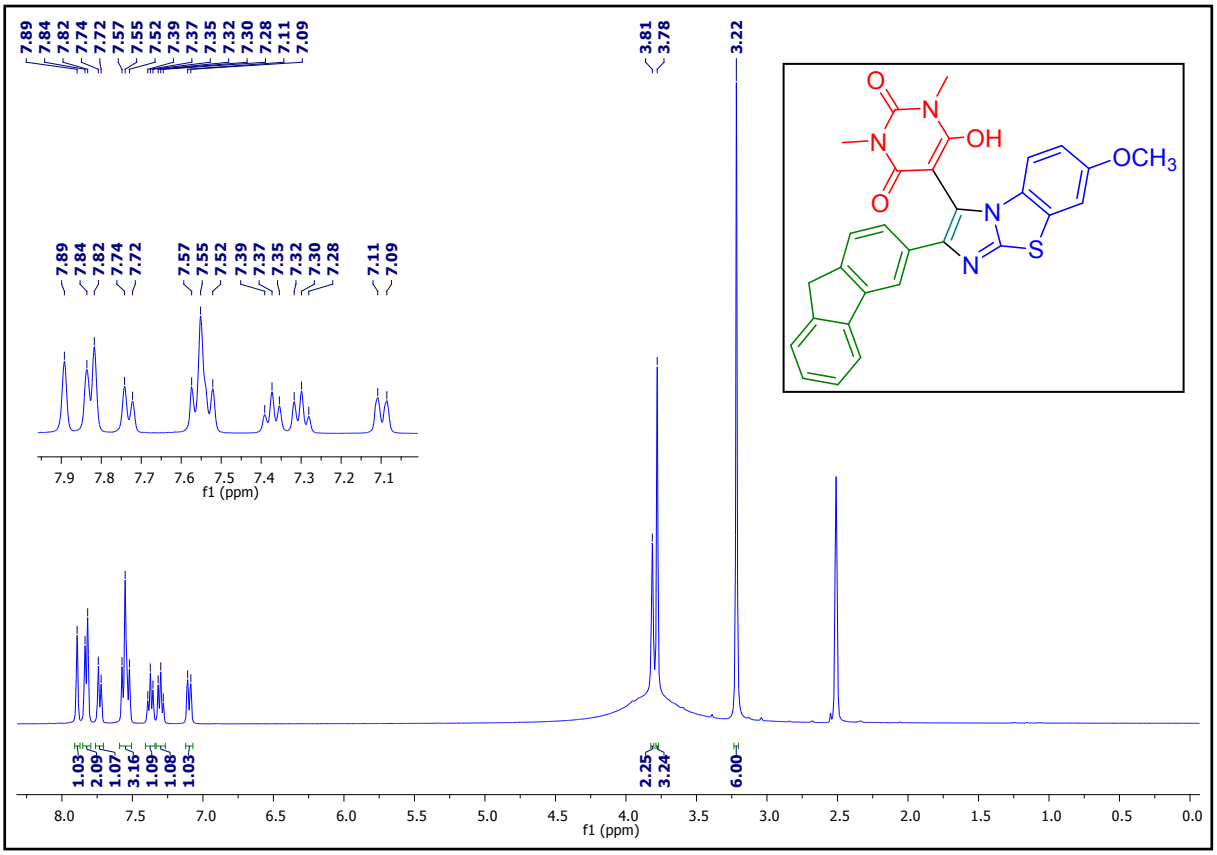

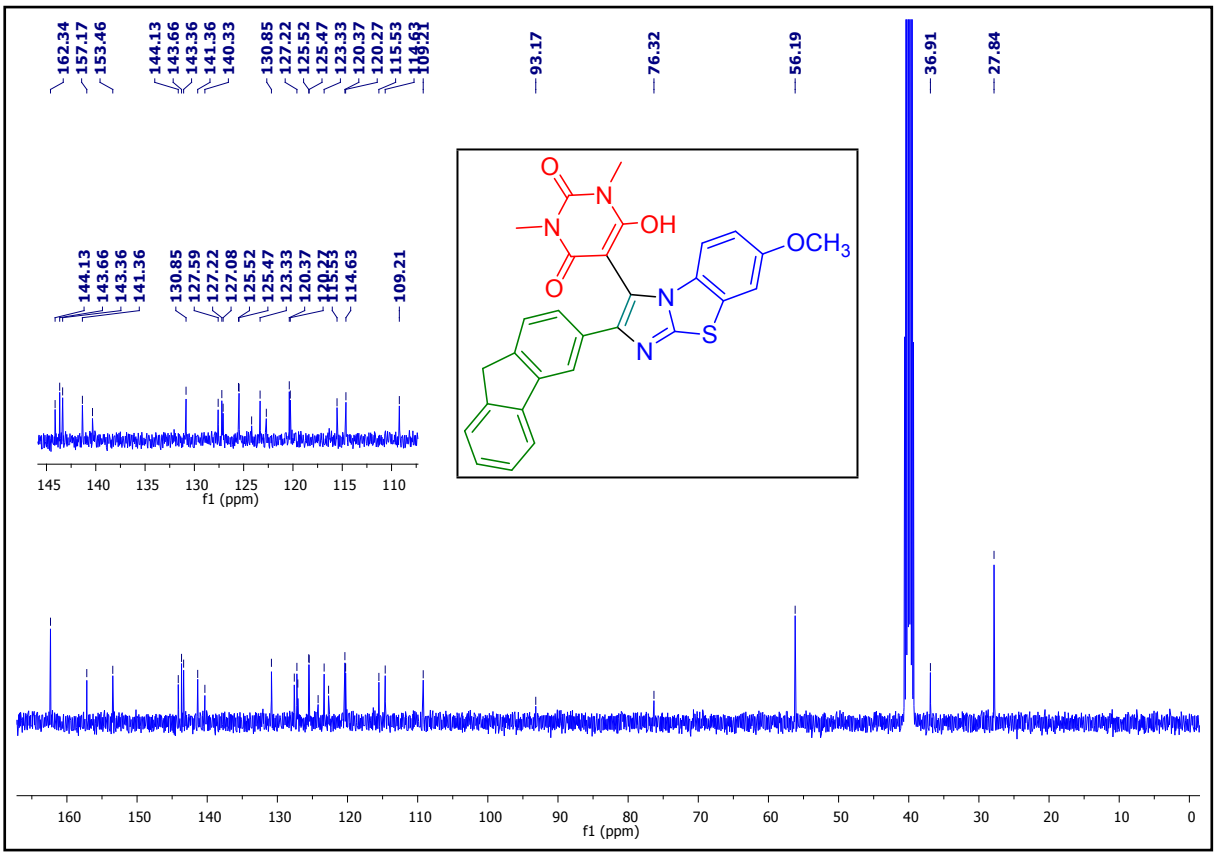

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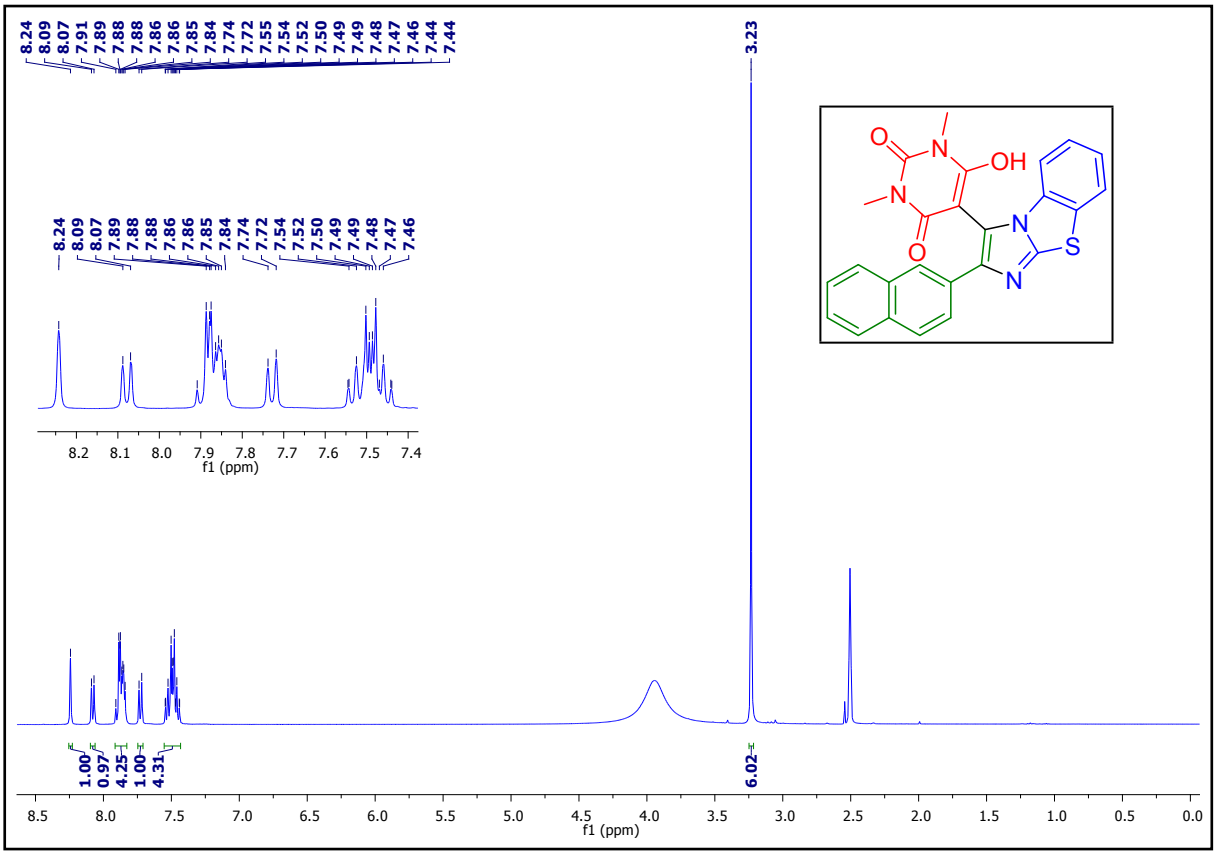

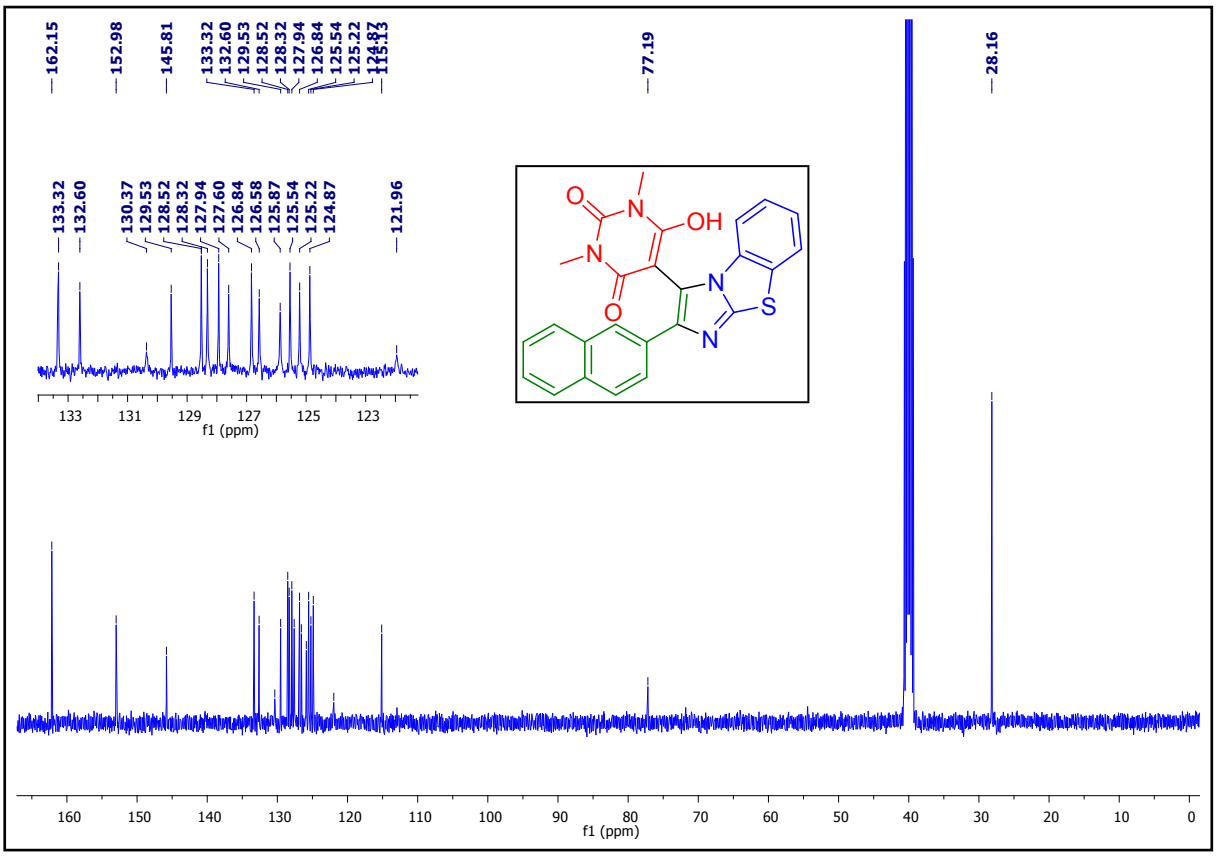

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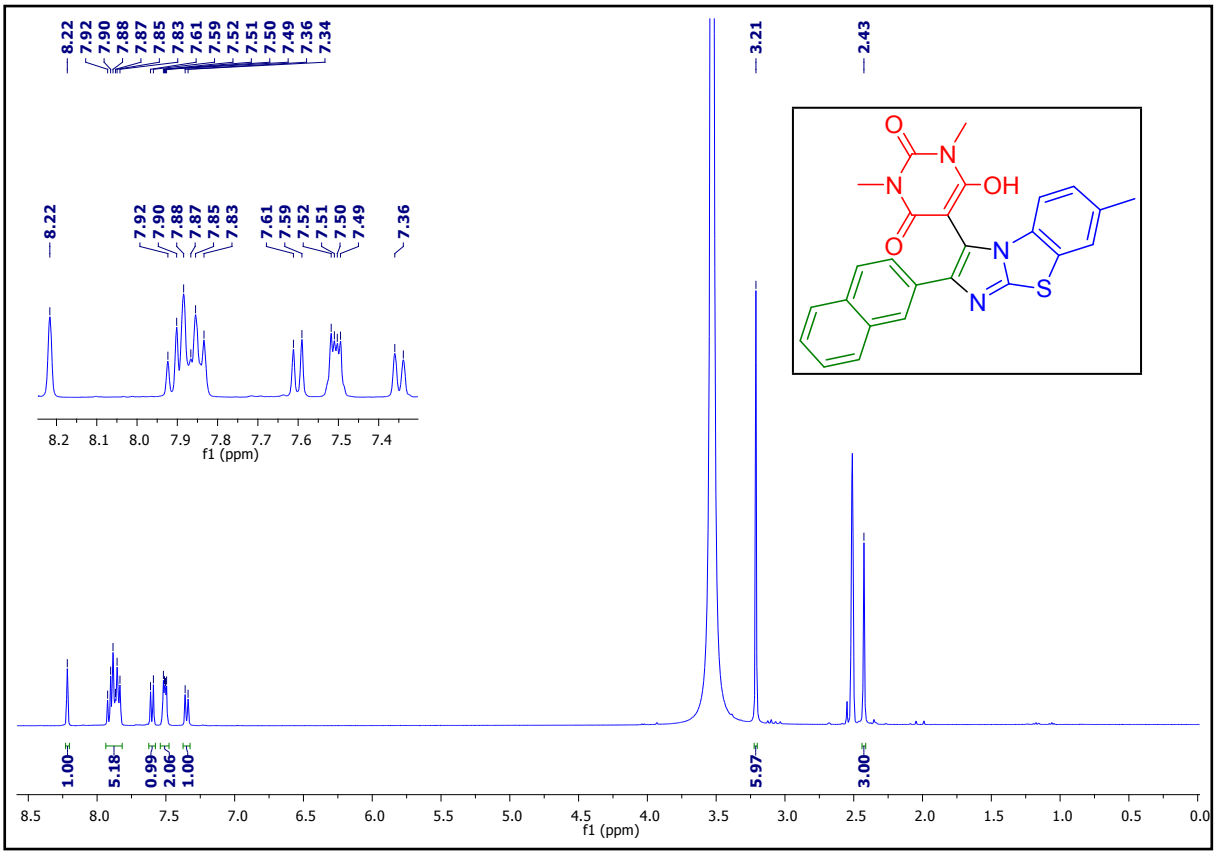

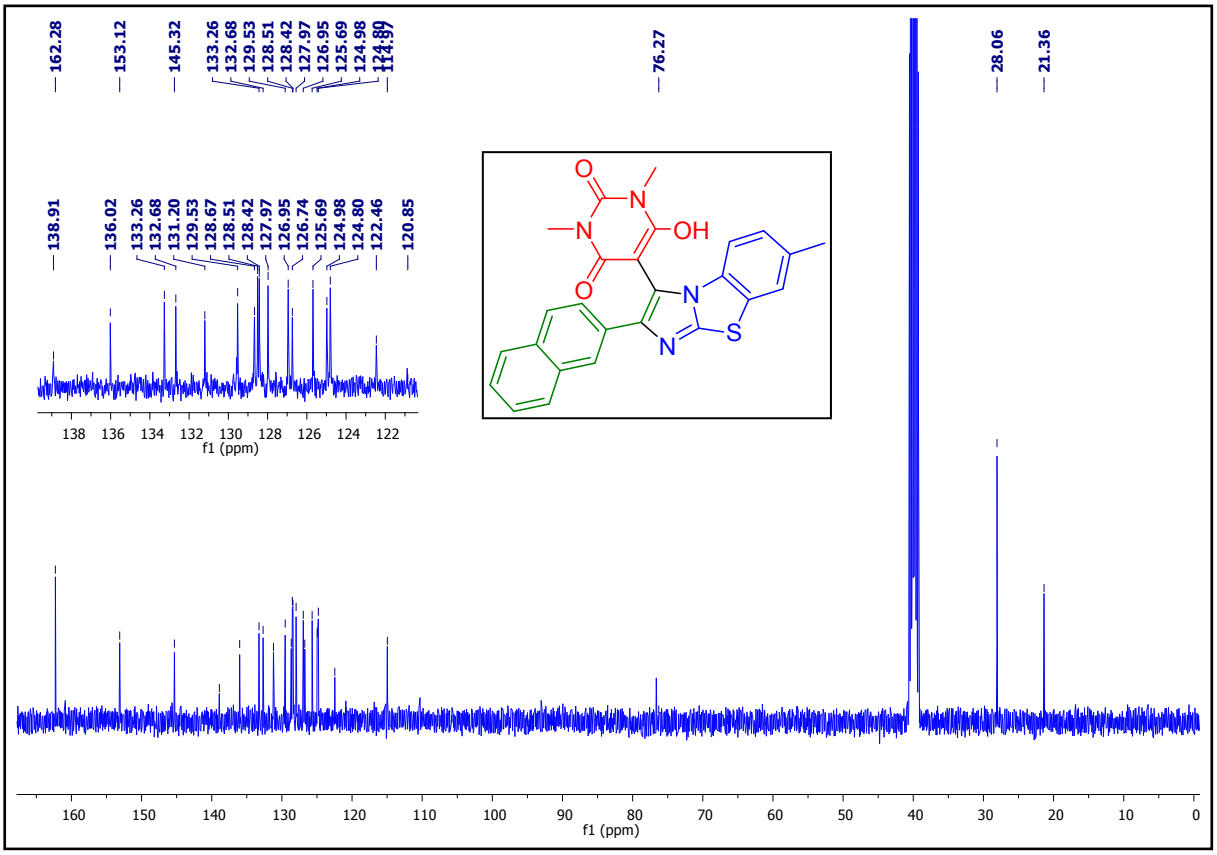

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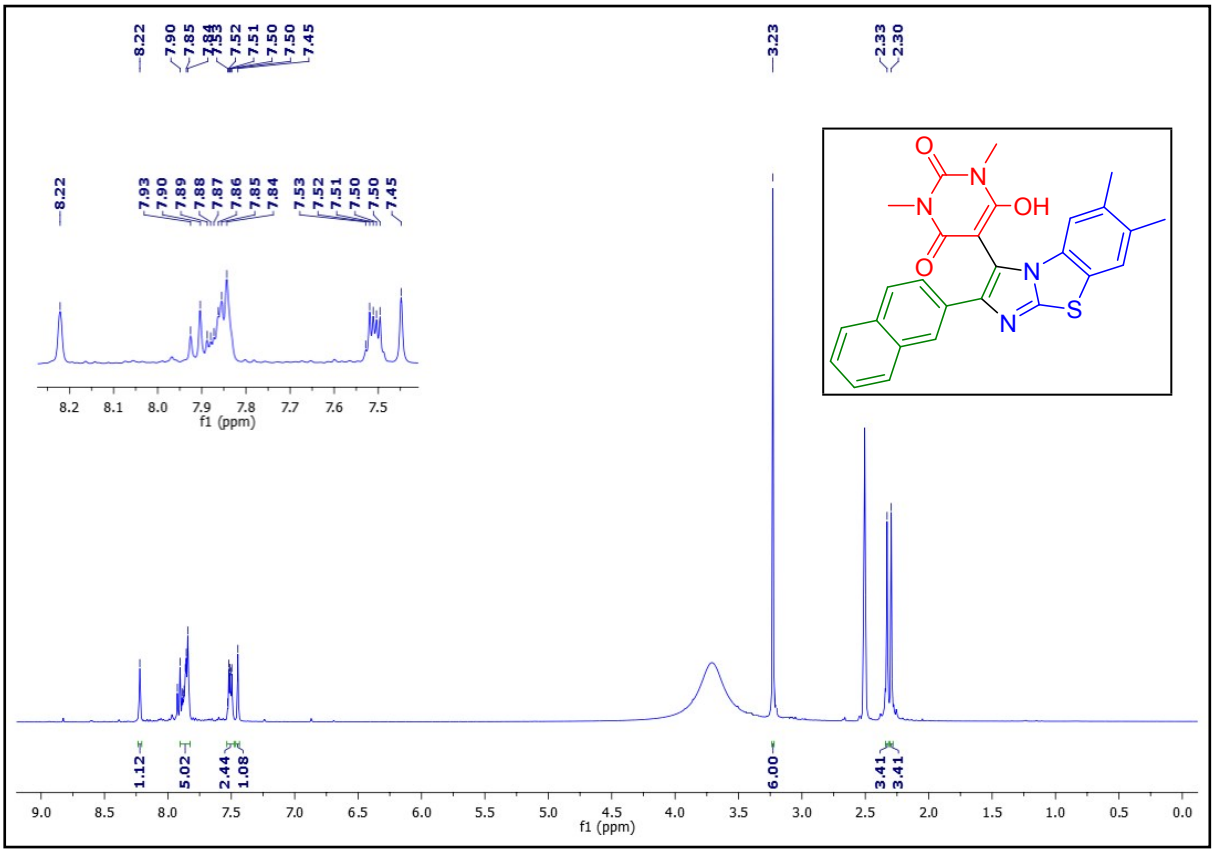

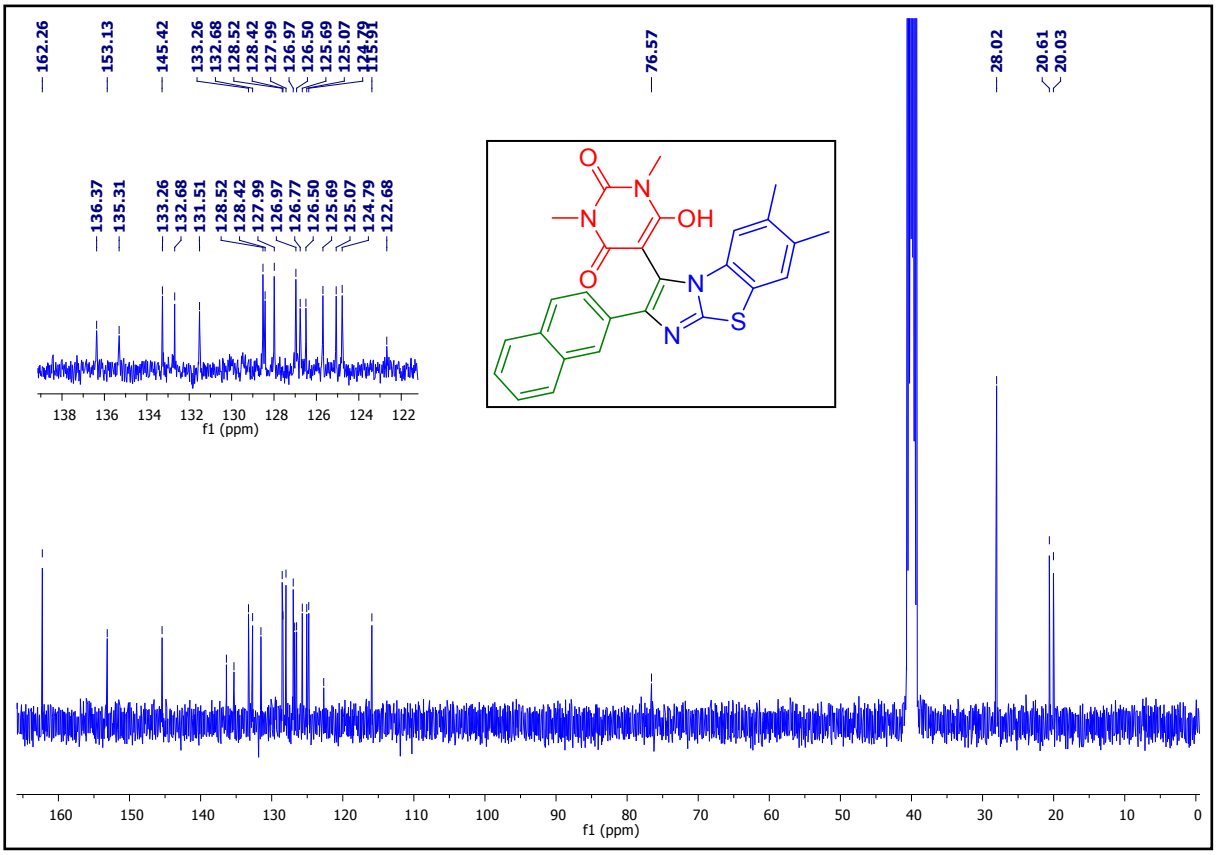

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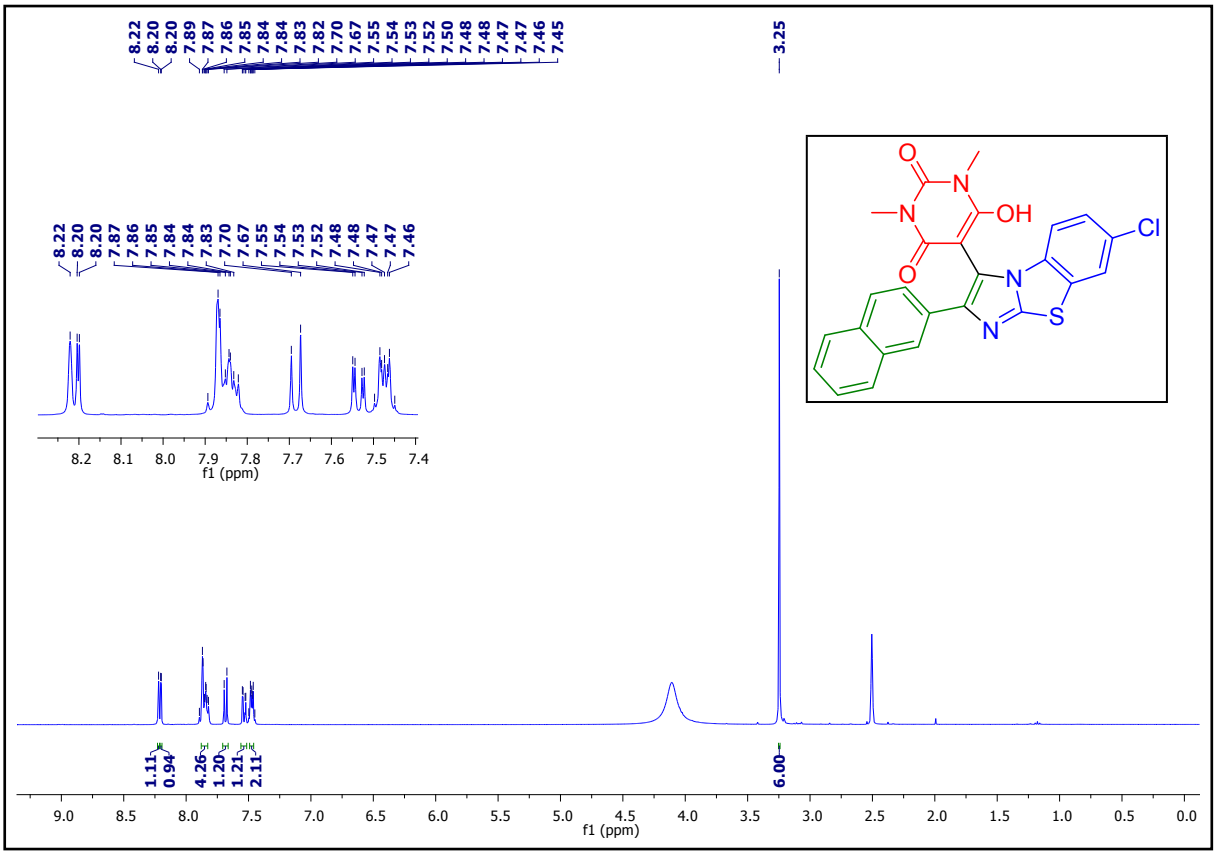

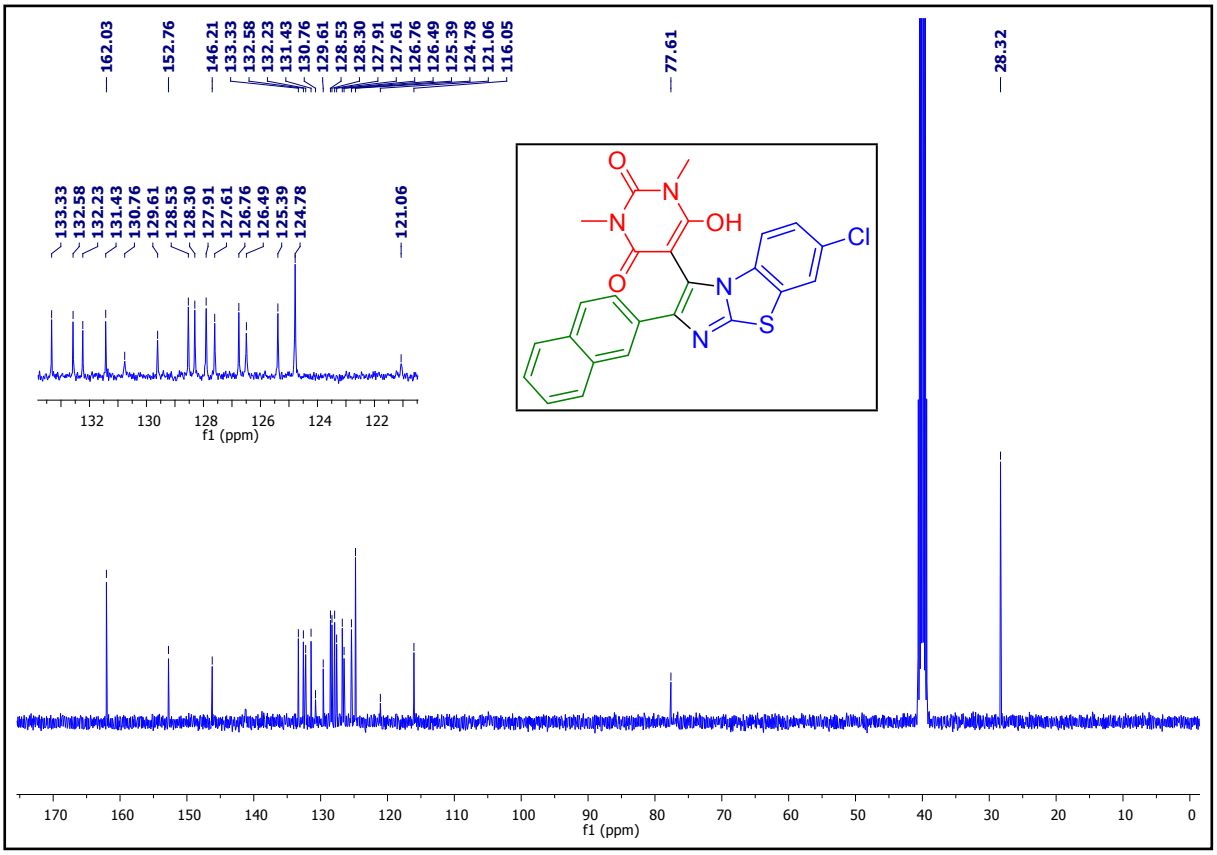

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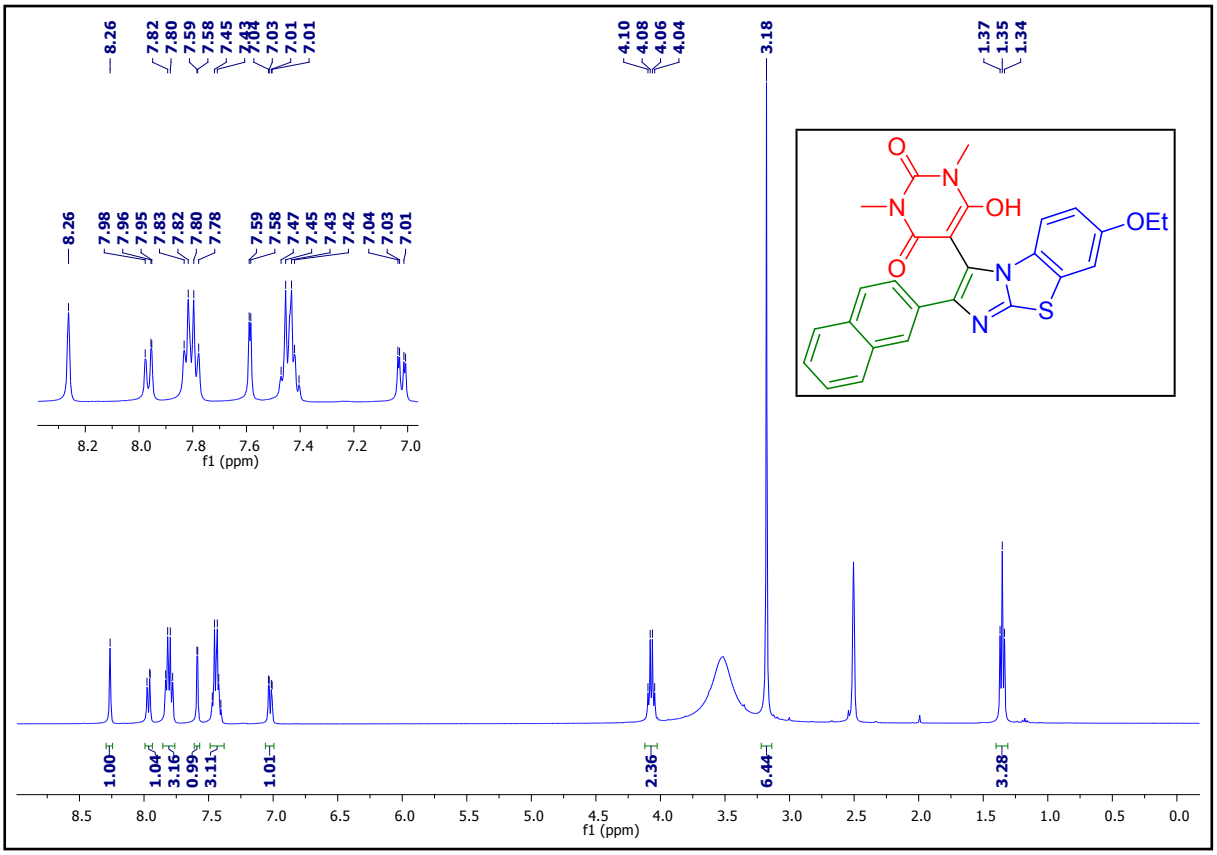

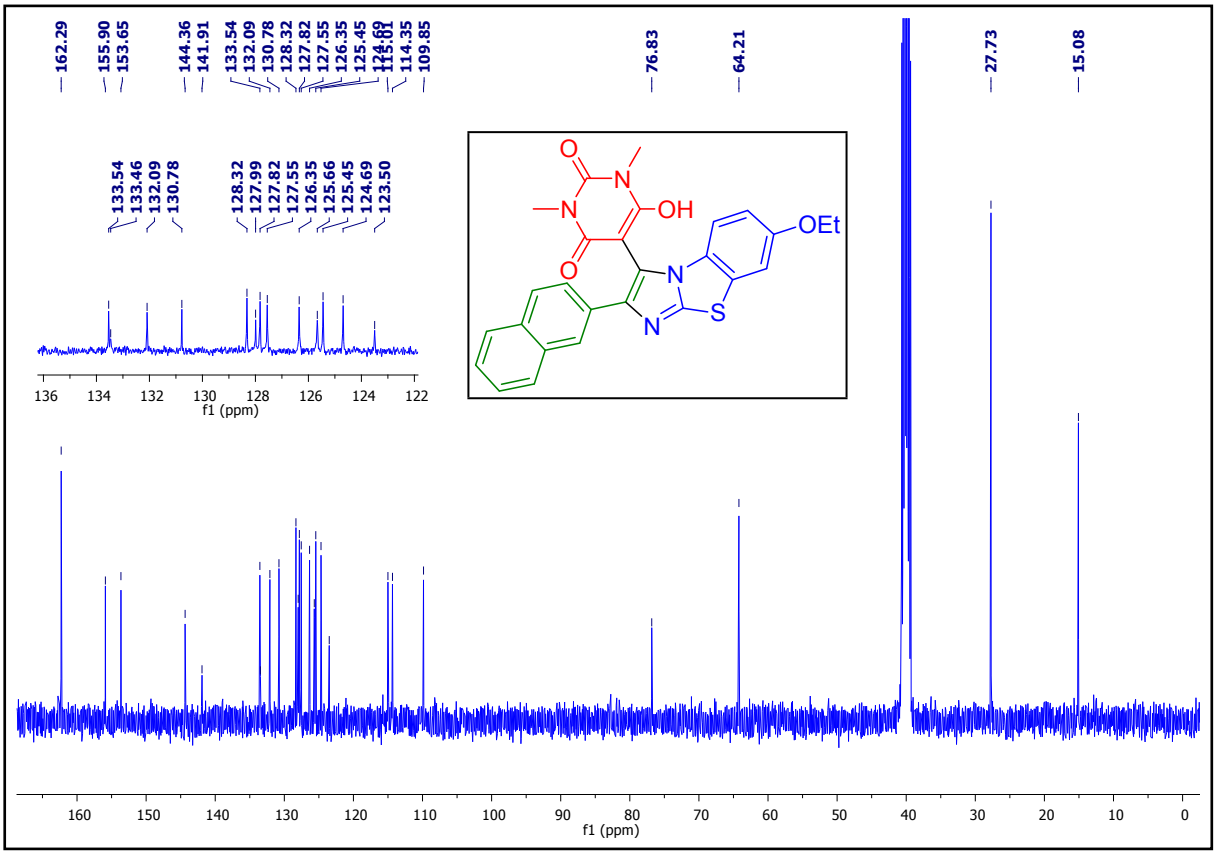

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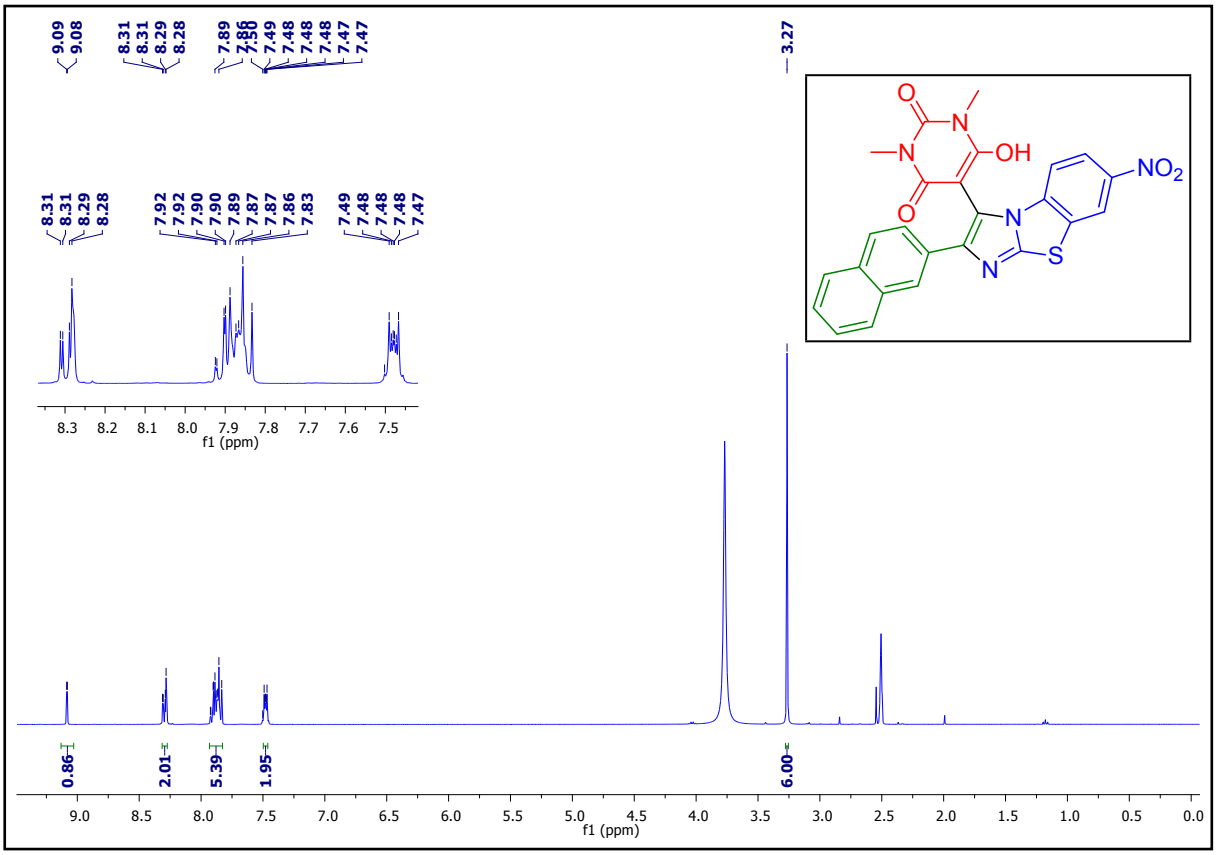
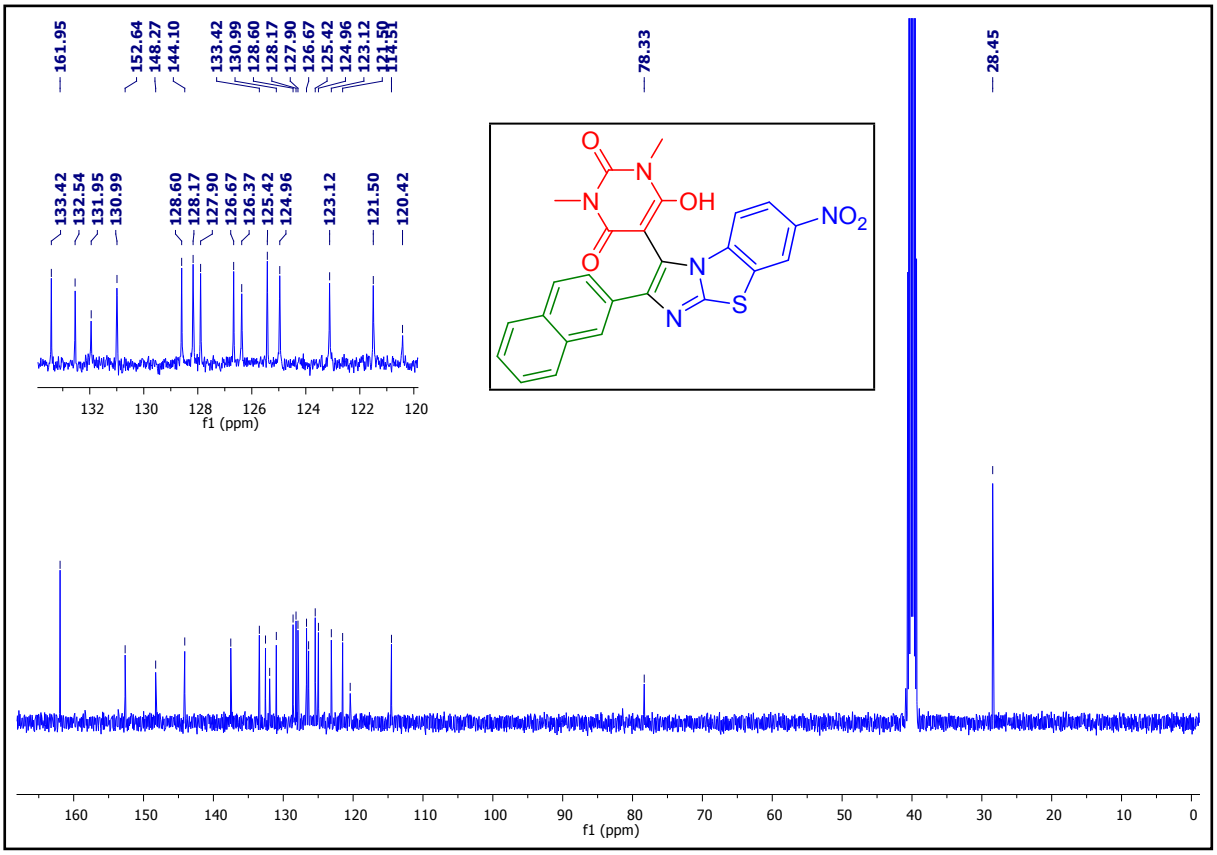
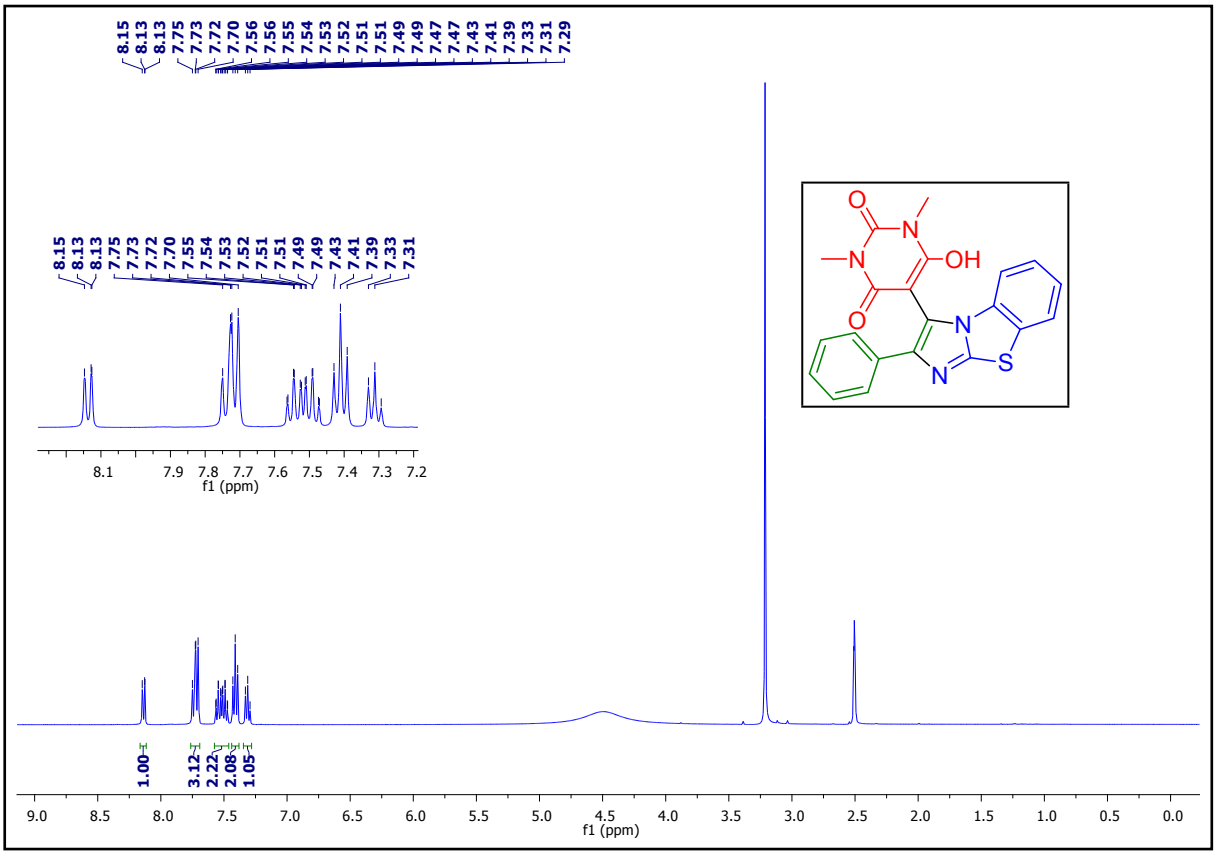
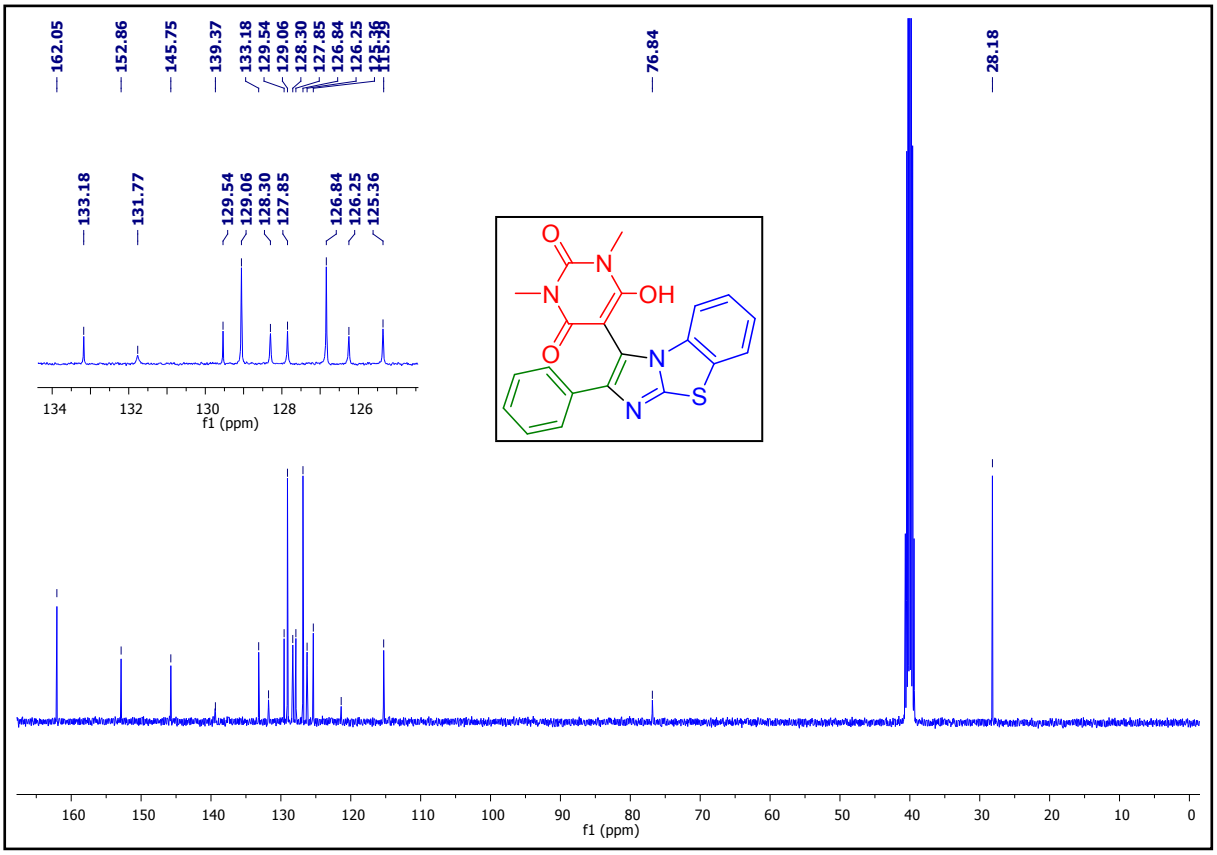


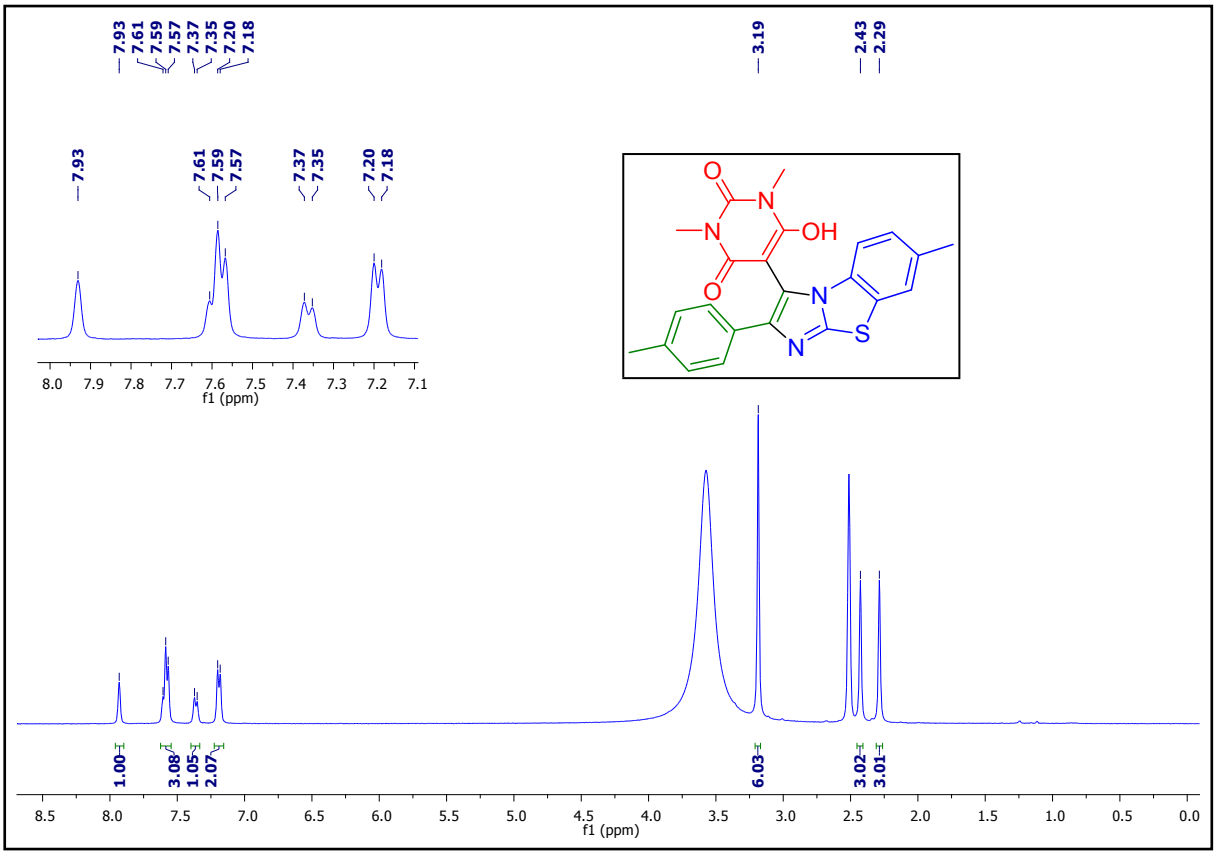


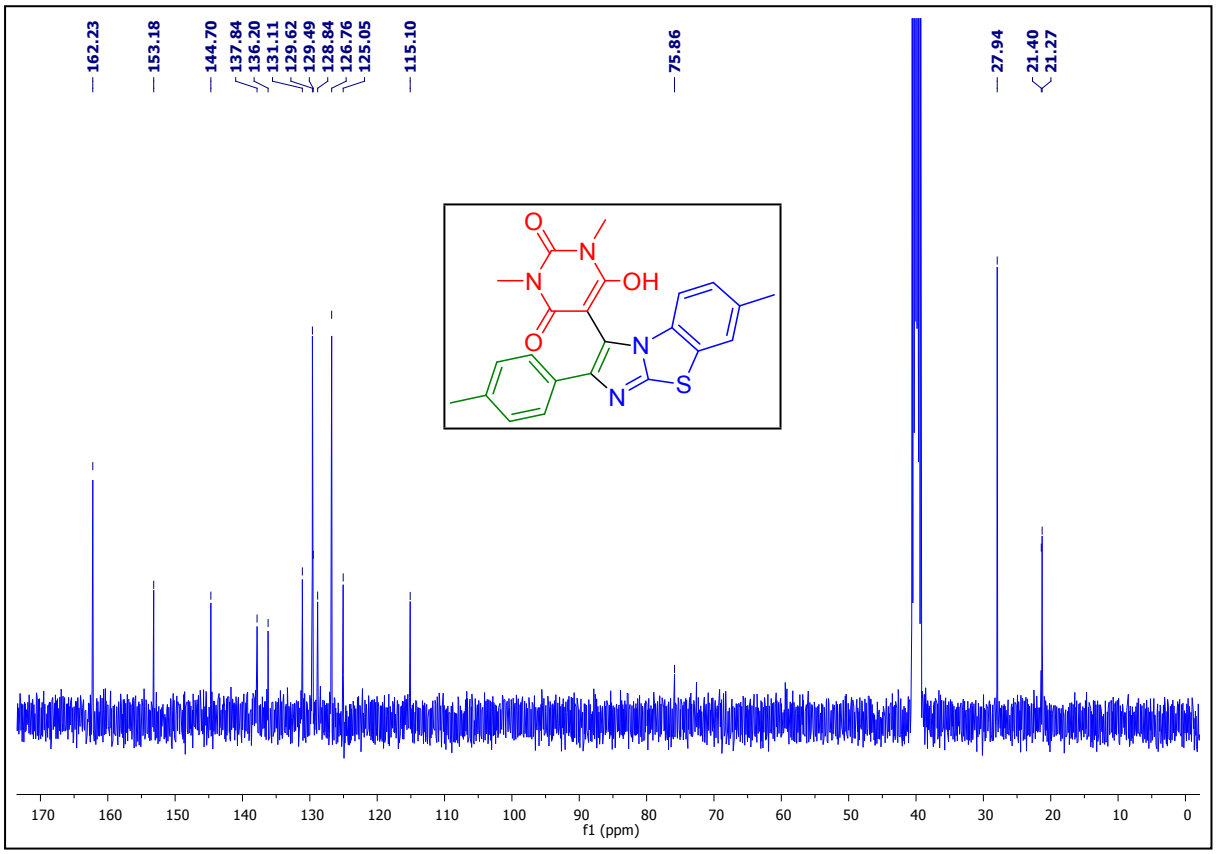
^{1}H and ^{13}C NMR spectra of 6s



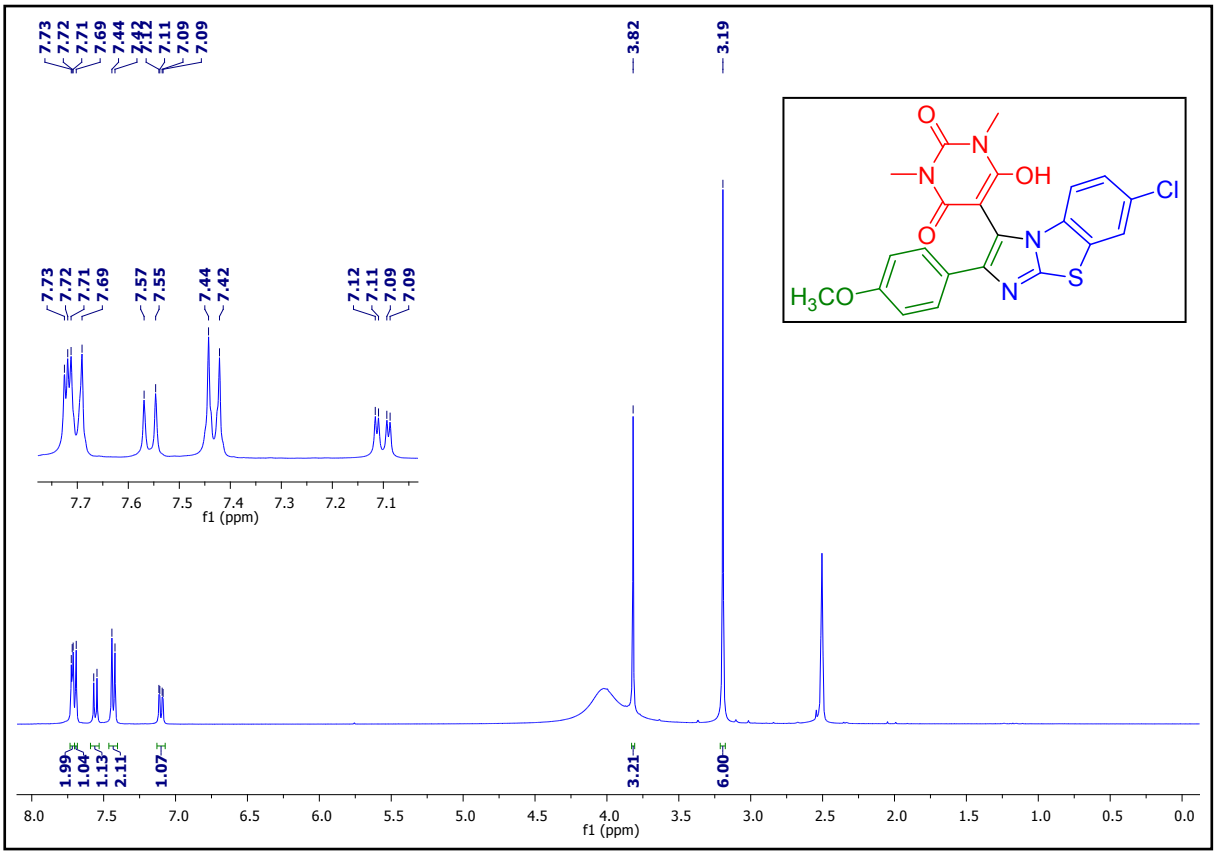


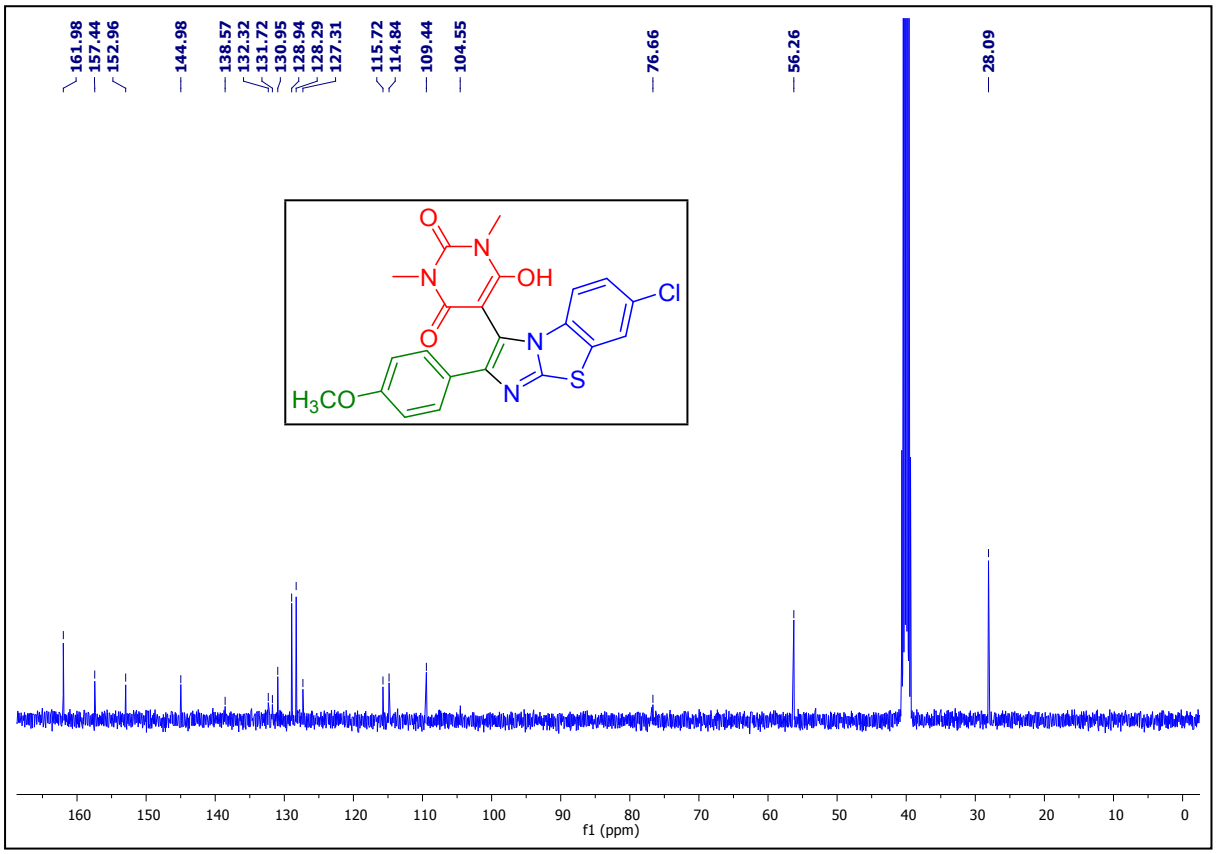
^{1}H and ^{13}C NMR spectra of 6t



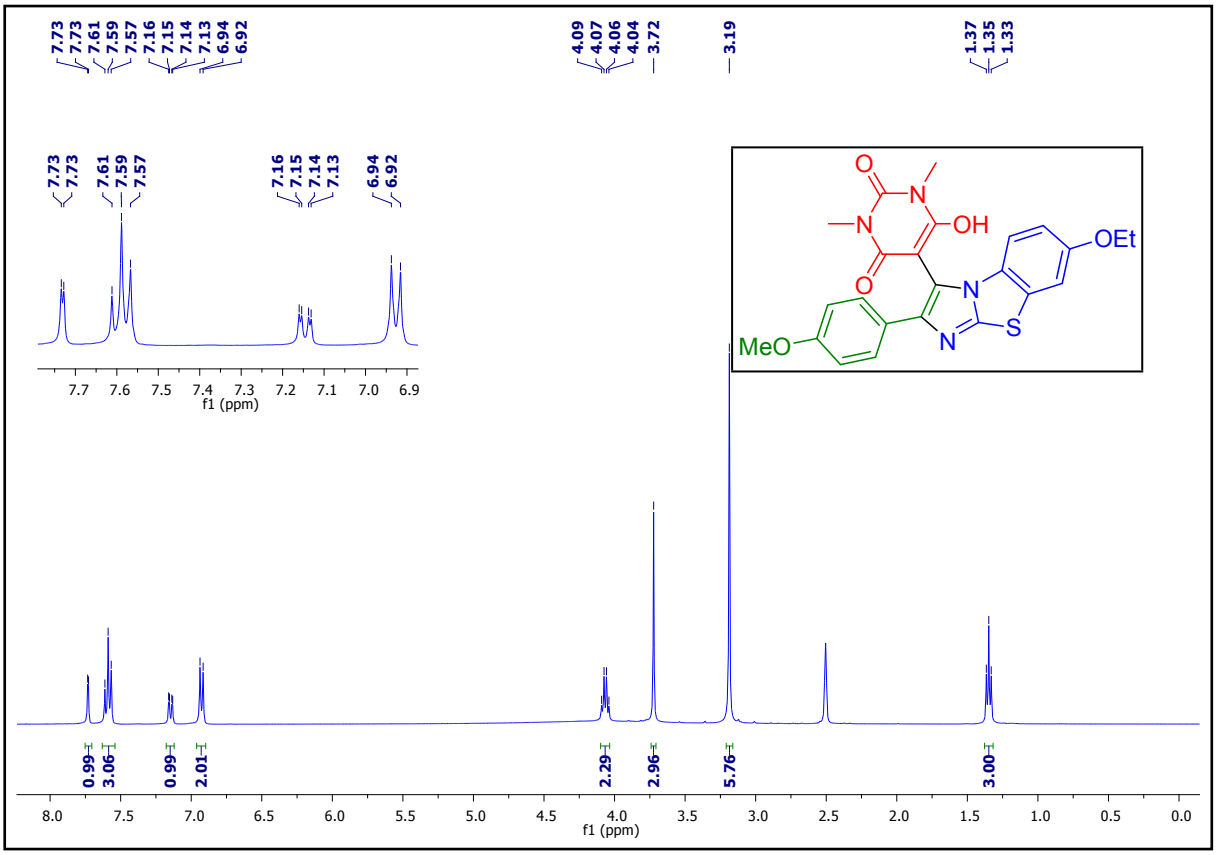


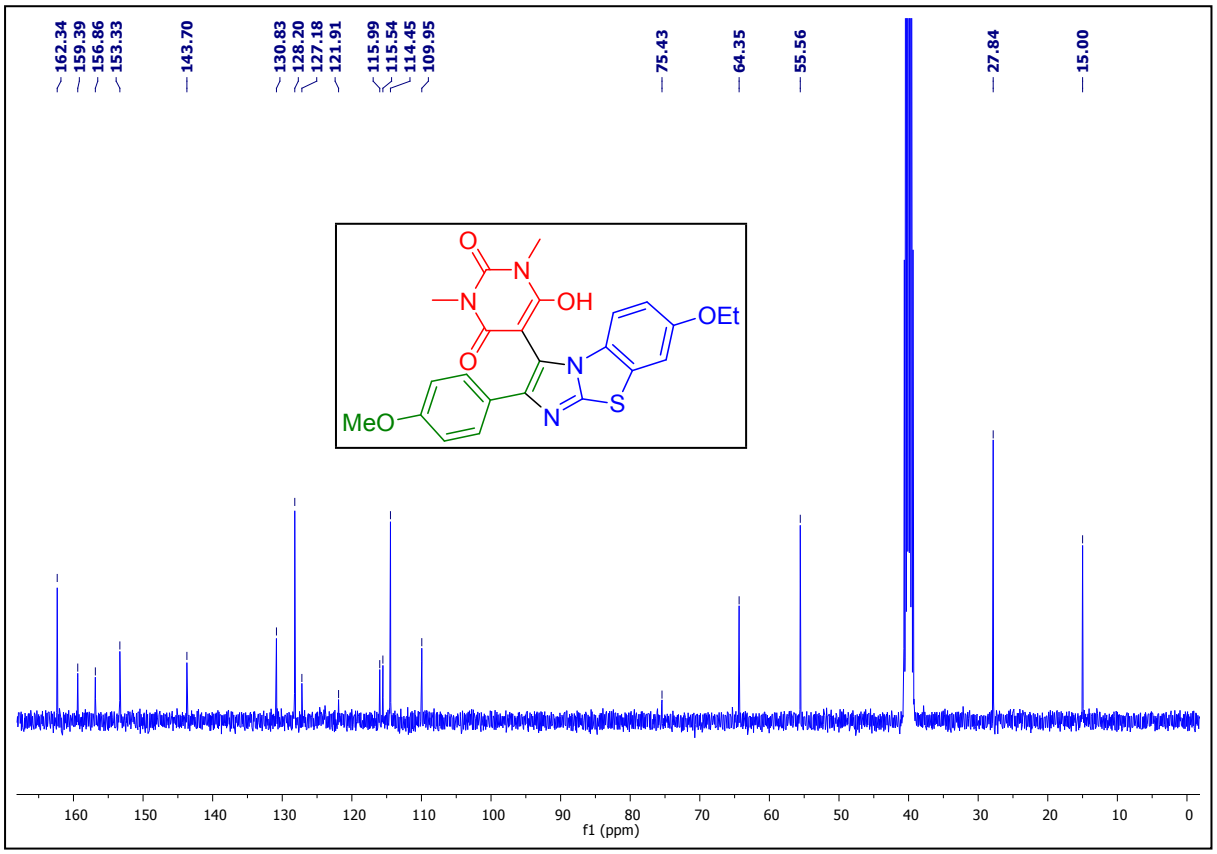
^{1}H and ^{13}C NMR spectra of 6u



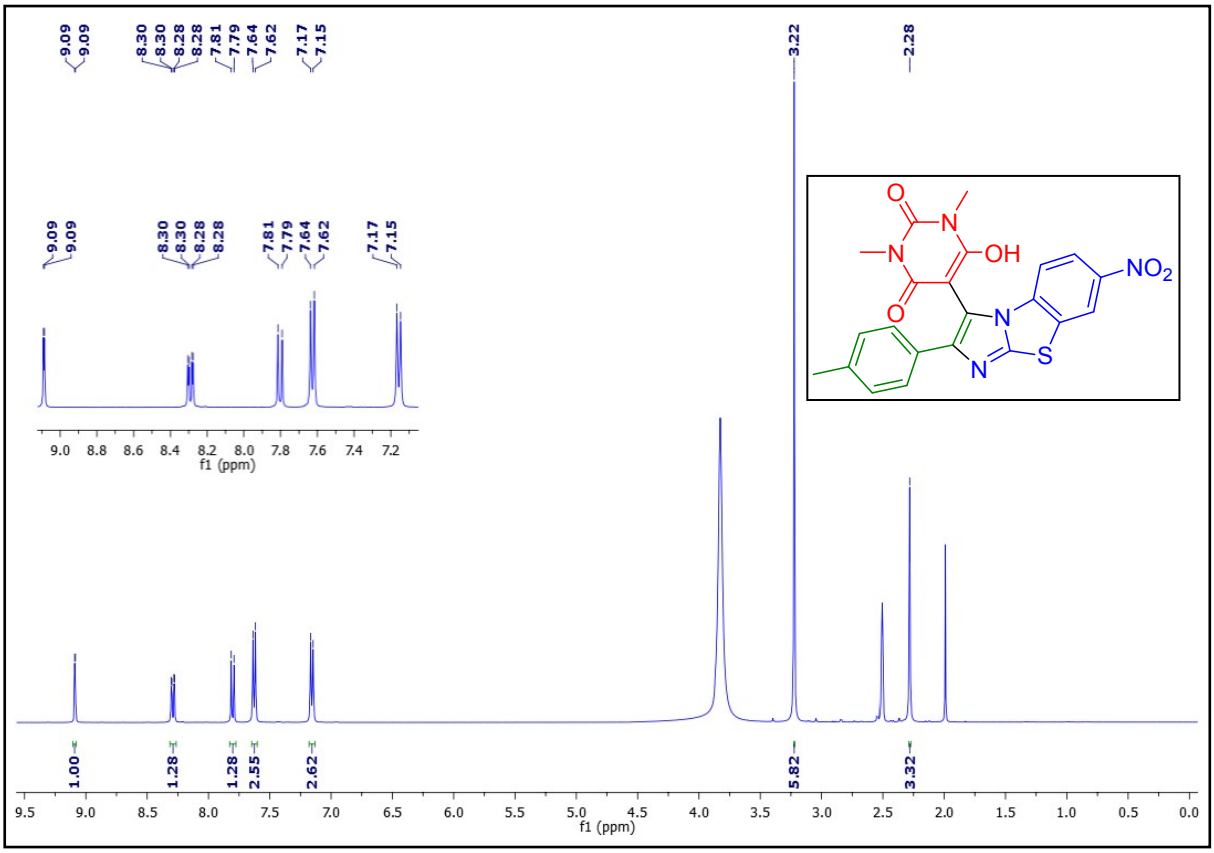


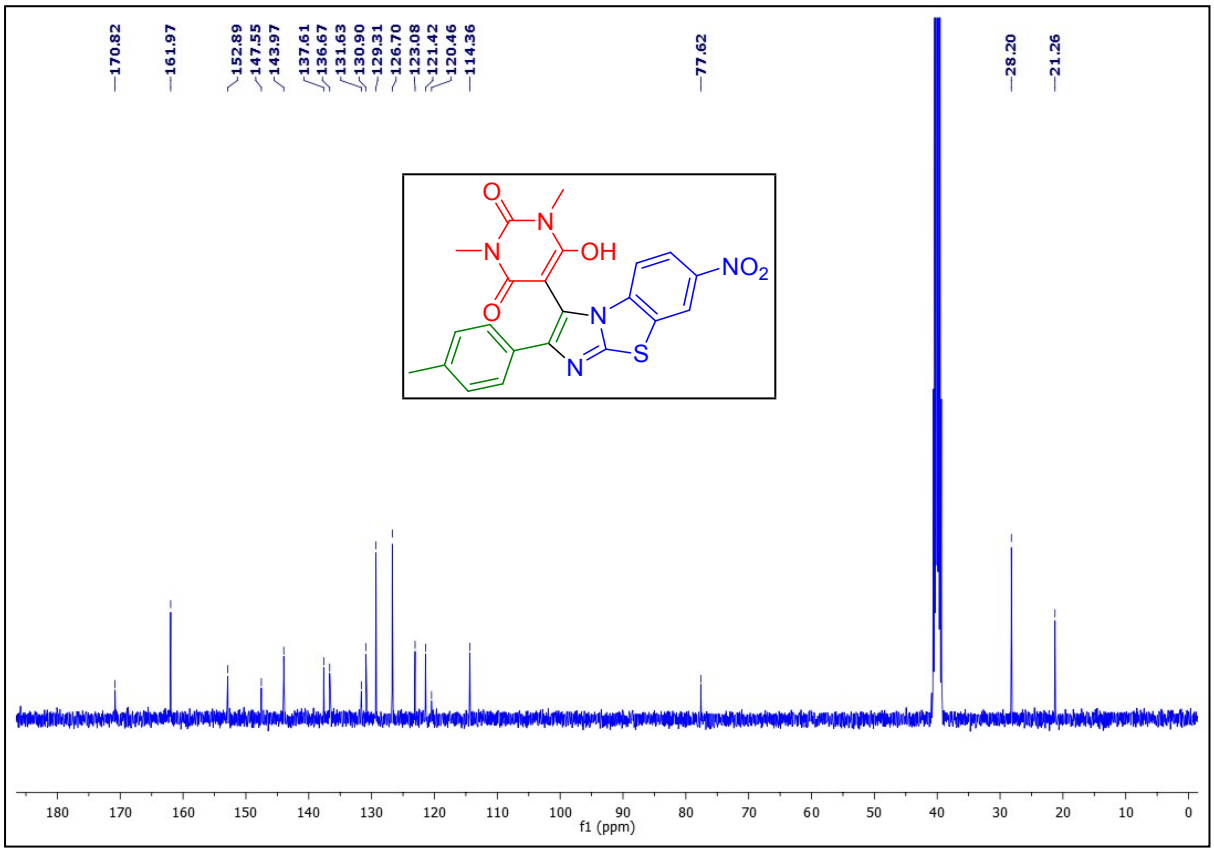
^{1}H and ^{13}C NMR spectra of 6v



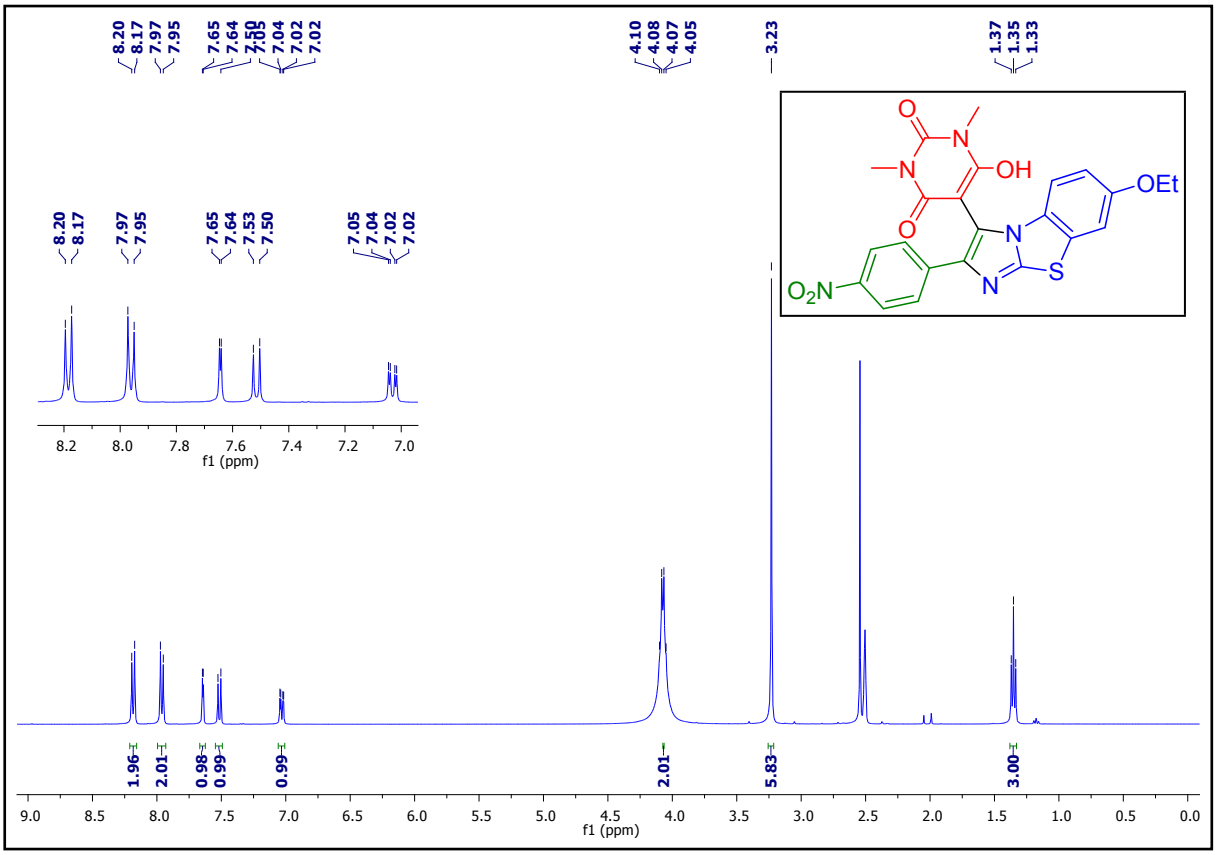


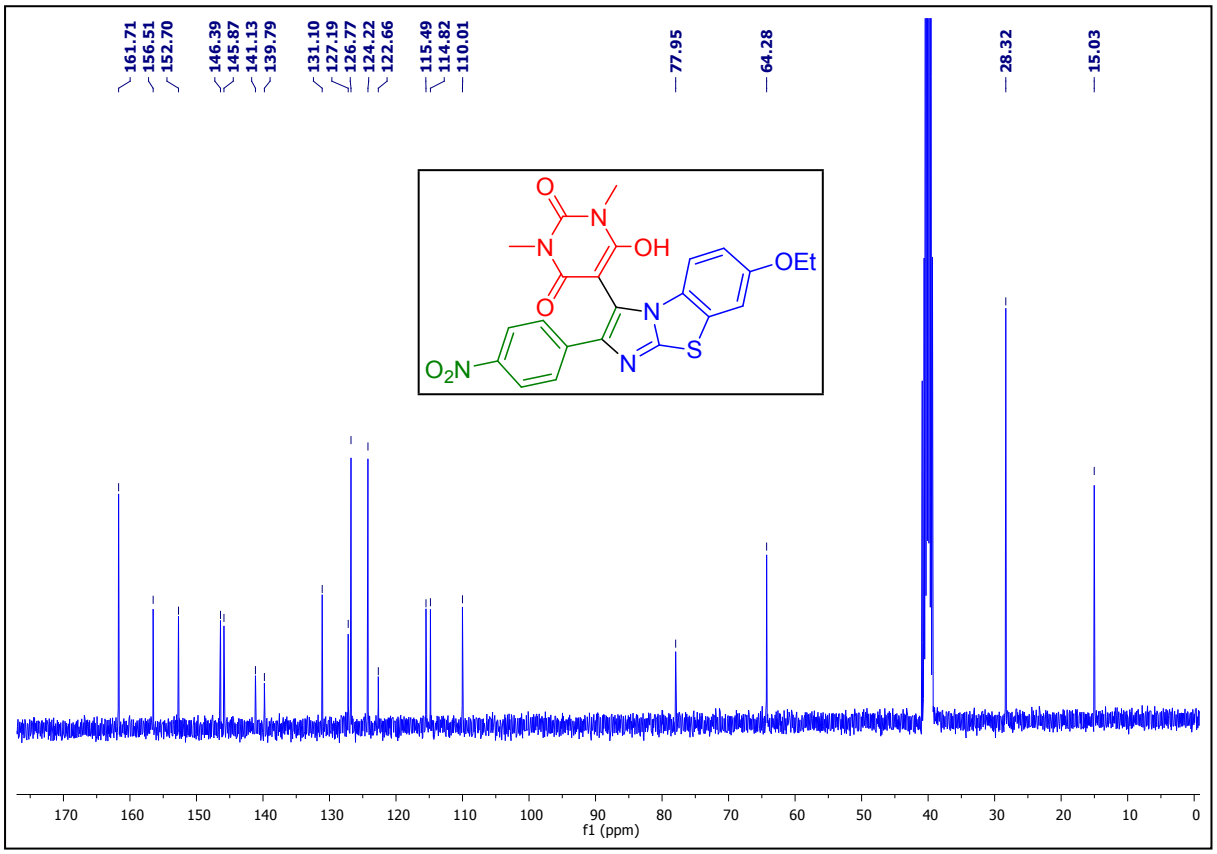
^{1}H and ^{13}C NMR spectra of 6w



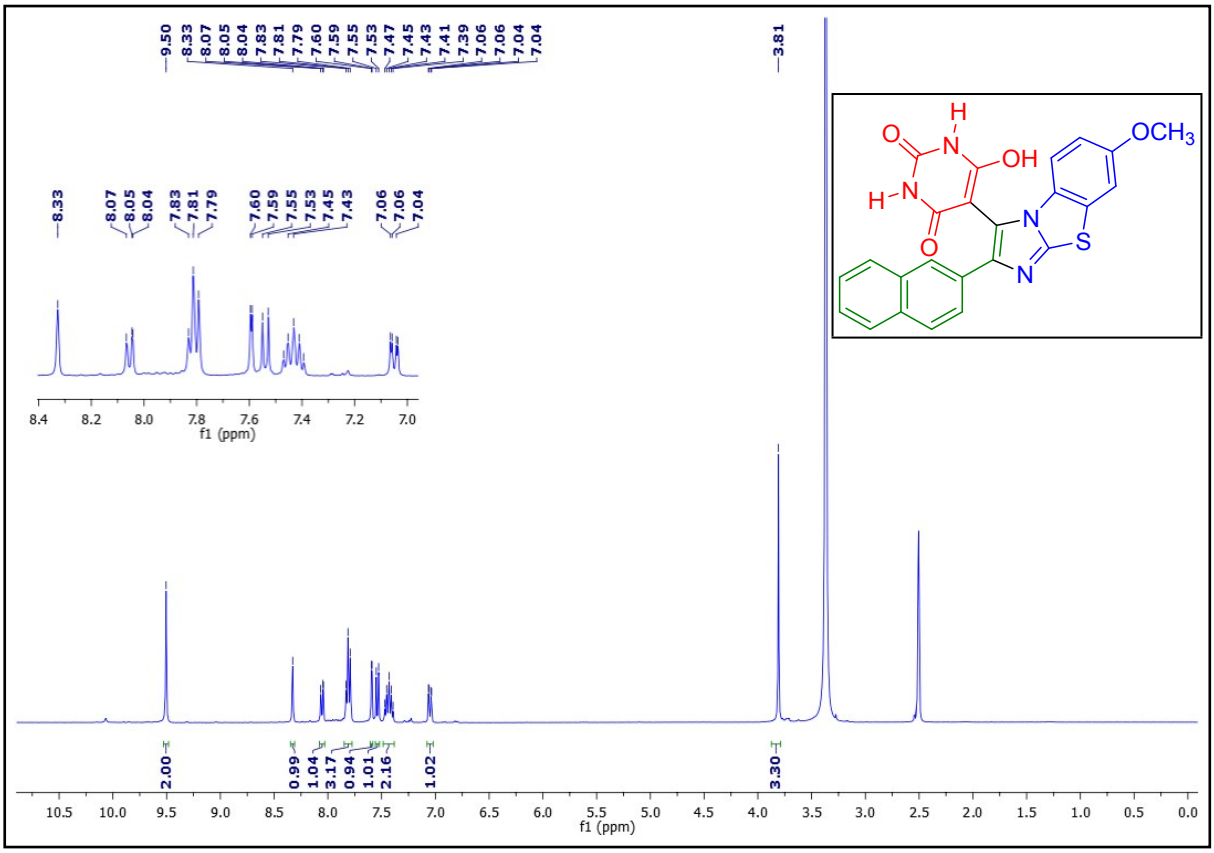


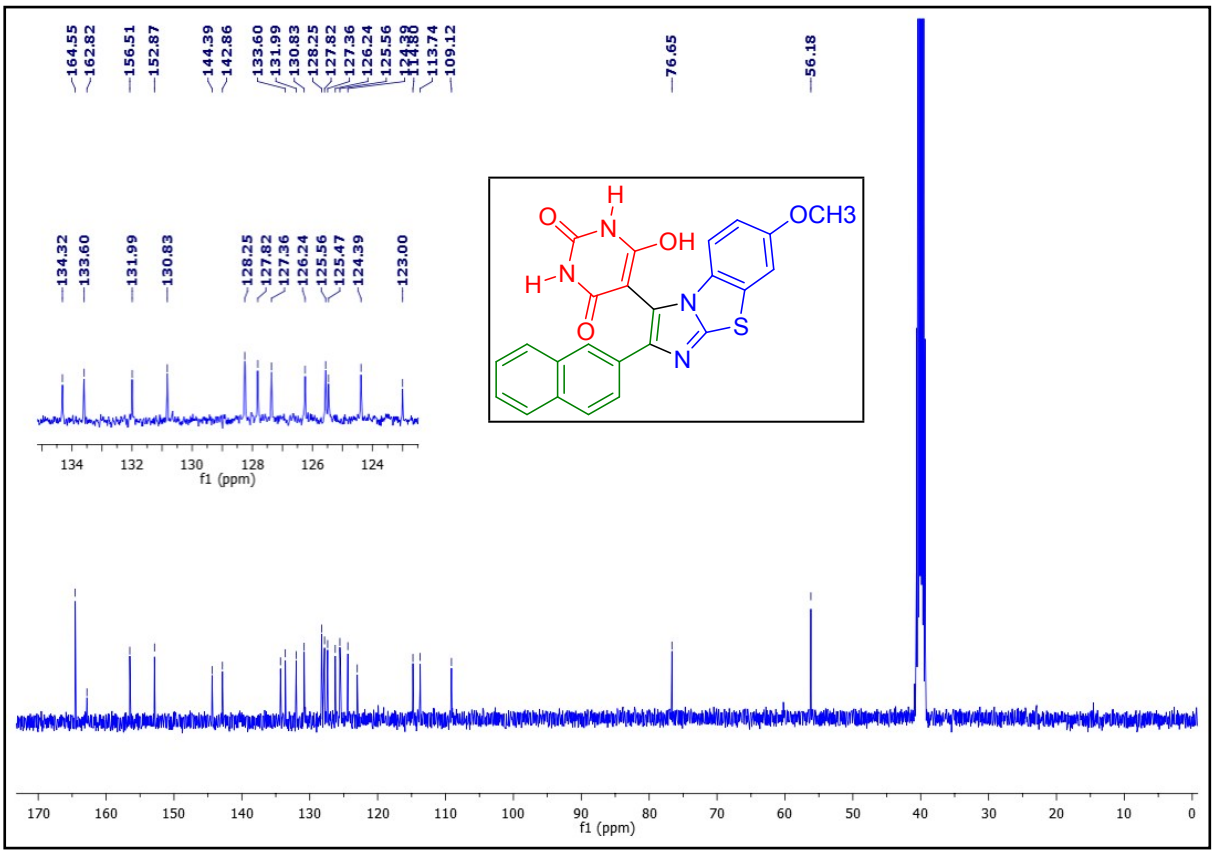
^{1}H and ^{13}C NMR spectra of 6x



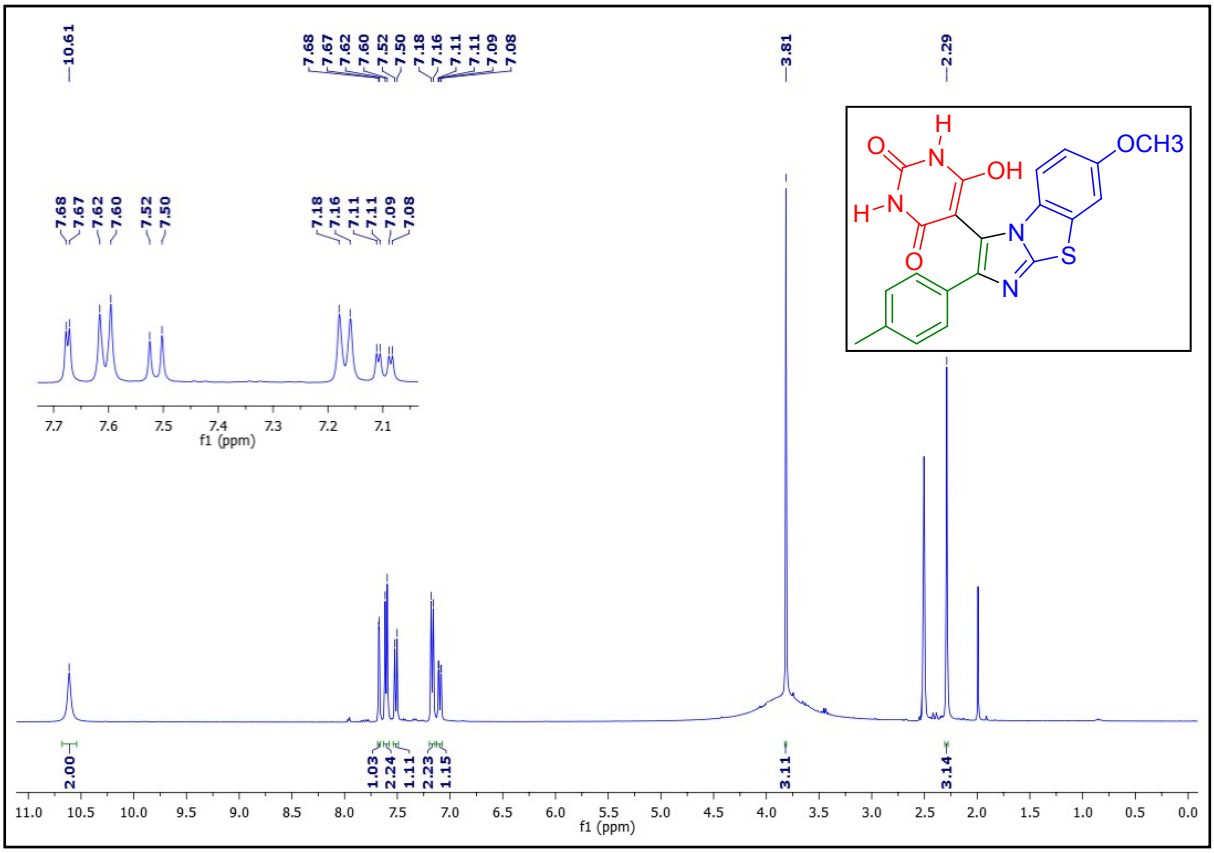


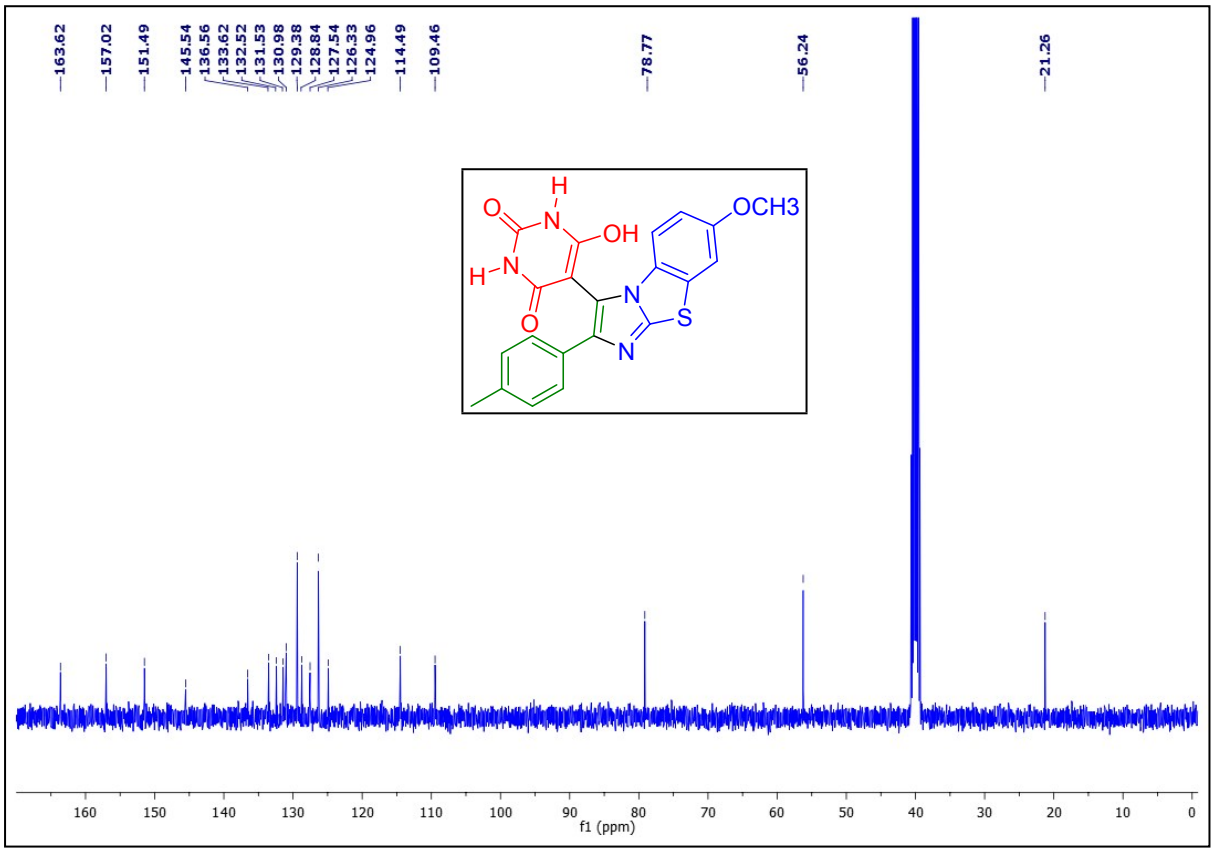
^{1}H and ^{13}C NMR spectra of 6y



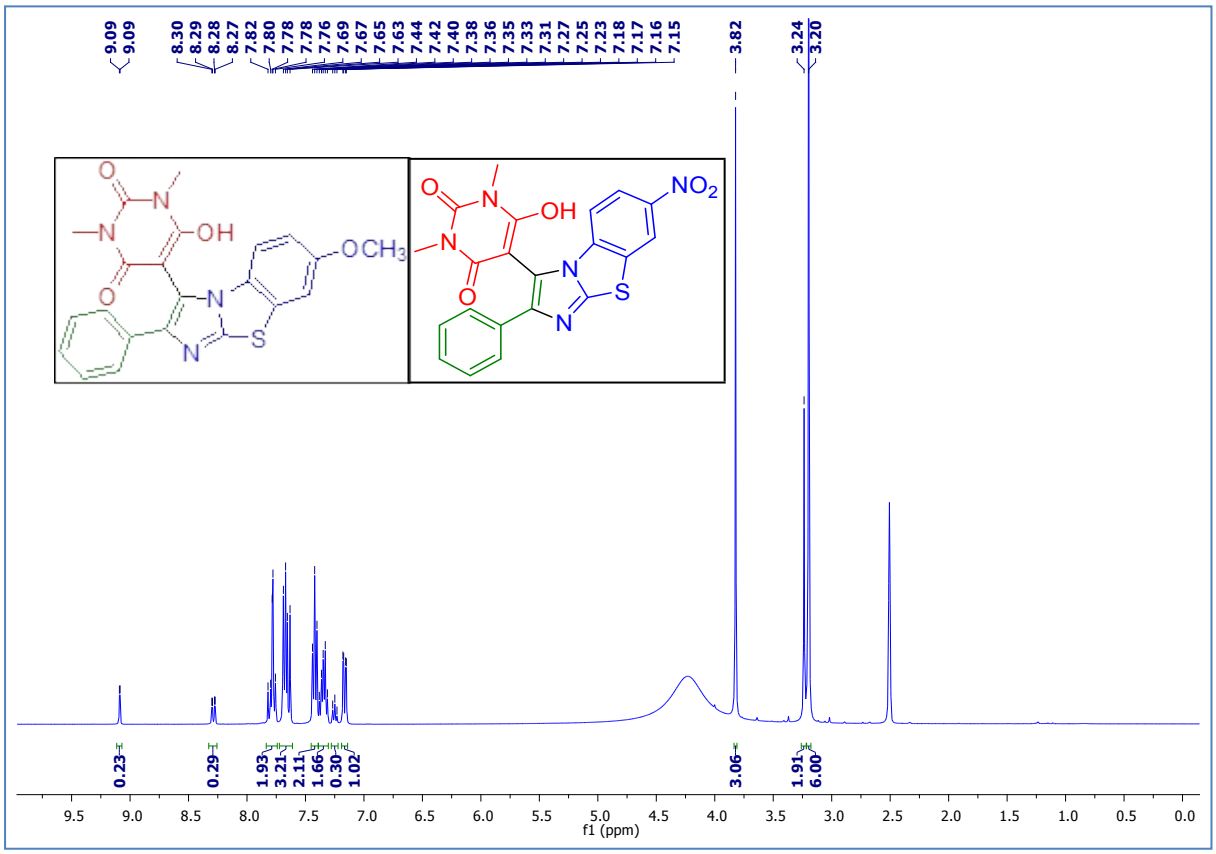


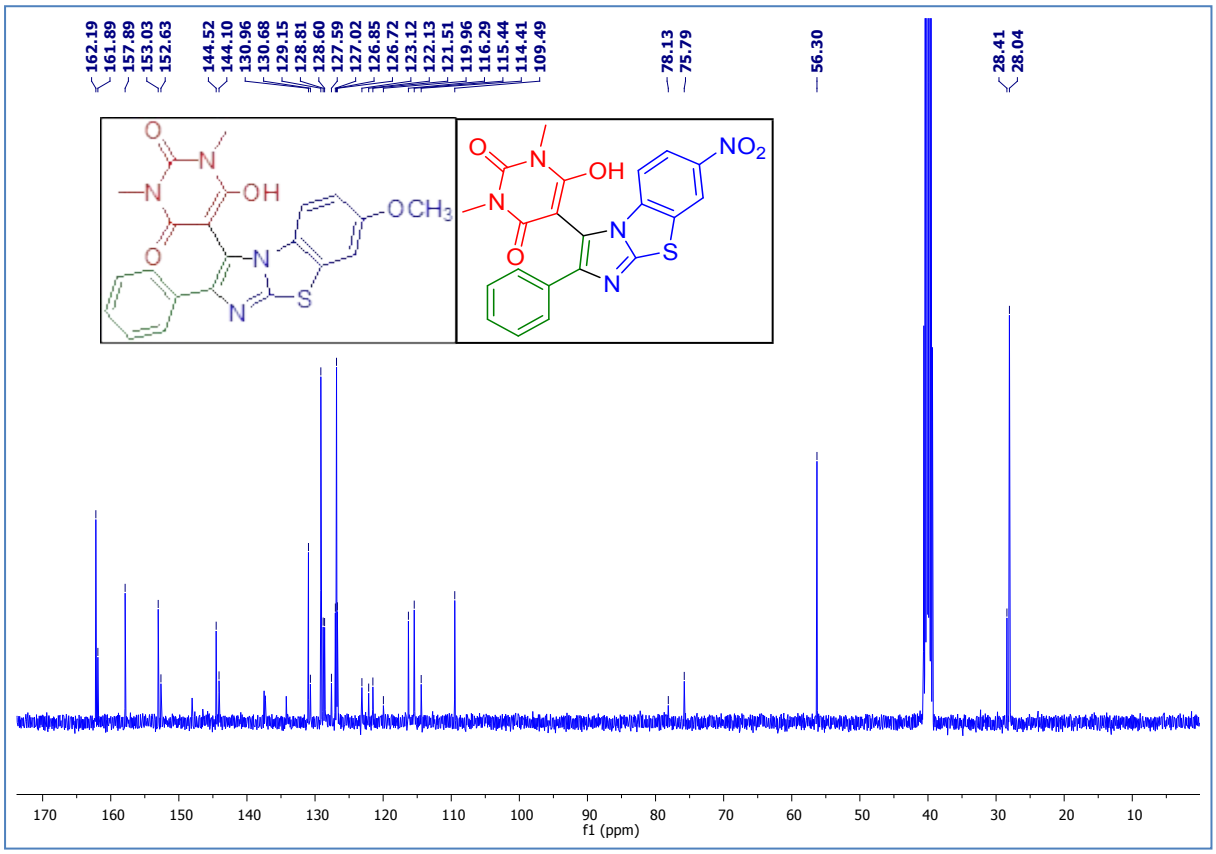
^{1}H and ^{13}C NMR spectra of 6z



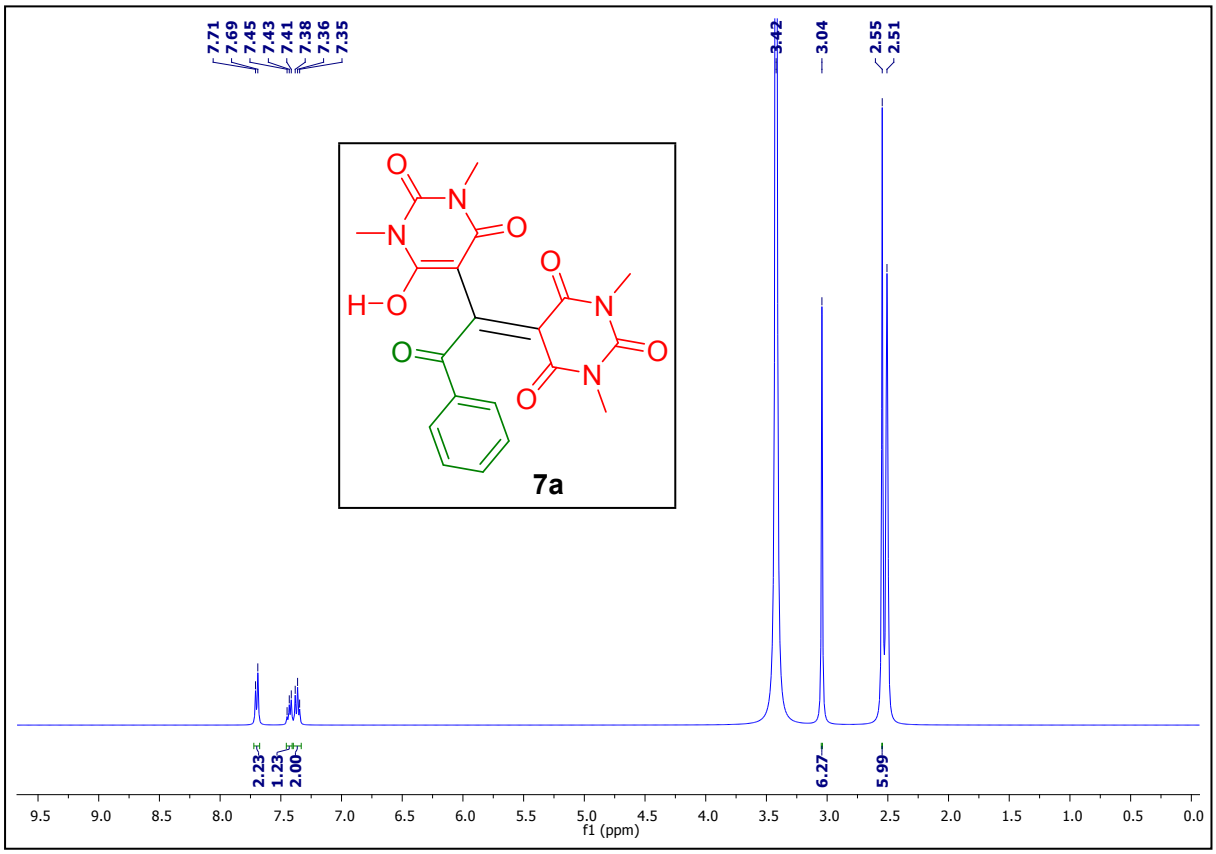


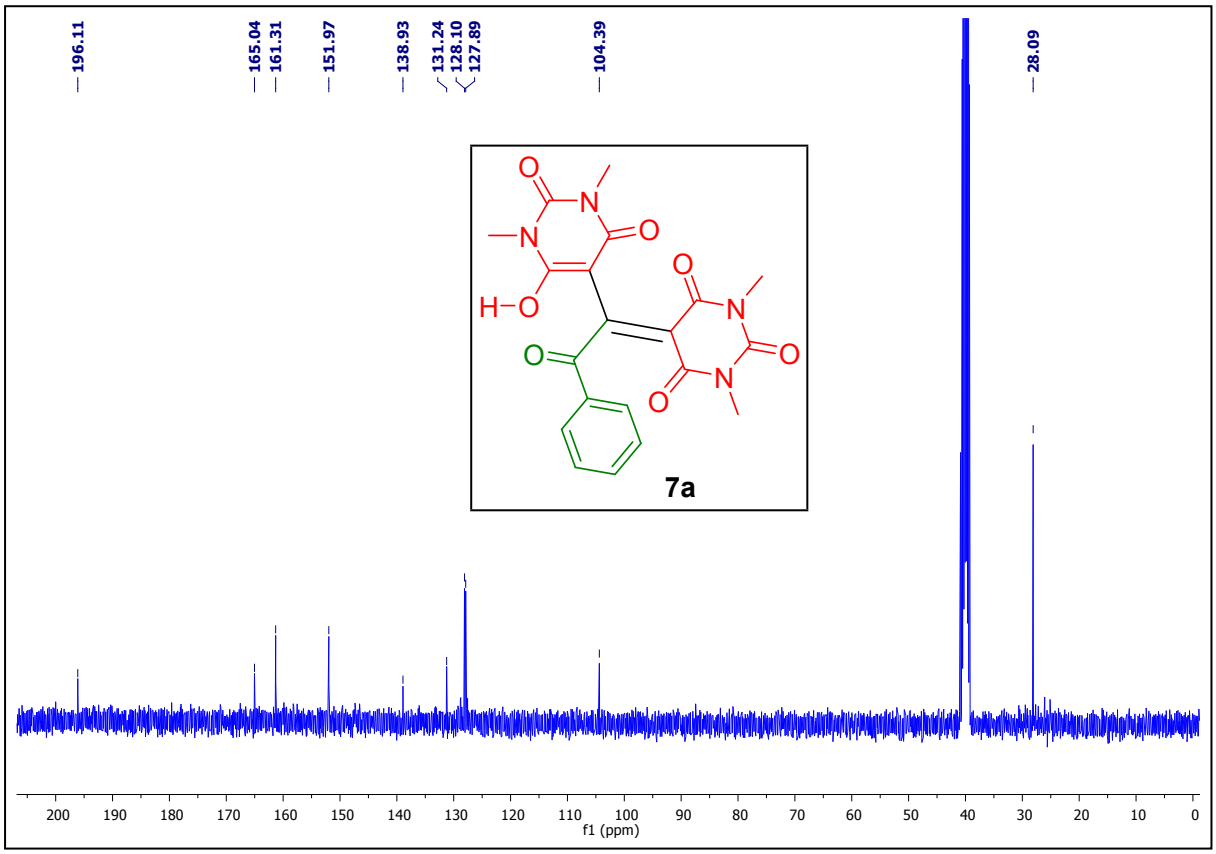
^{1}H and ^{13}C NMR spectra of 6a&4e (competition experiment)





^{1}H and ^{13}C NMR spectra of7a





Crystal structure description of 6o.

A specimen of $C_{27}H_{22}N_4O_3S$, approximate dimensions 0.300 mm x 0.300 mm x 0.300 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.The integration of the data using a monoclinic unit cell yielded a total of 35307 reflections to a maximum θ angle of 25.00° (0.84 Å resolution), of which 4189 were independent (average redundancy 8.429, completeness = 99.9%, R_{int} = 7.66%, R_{sig} = 5.23%) and 2724 (65.03%) were greater than $2\sigma(F^2)$. The final cell constants of a = 11.638(4) Å, b = 14.774(6) Å, c = 14.105(5) Å, β = 101.385(10)°, volume = 2377.5(15) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9500 and 0.9500.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 1 21/n 1, with Z = 4 for the formula unit, $C_{27}H_{22}N_4O_3S$. The final anisotropic full-matrix least-squares refinement on F^2 with 322 variables converged at R1 = 5.42%, for the observed data and wR2 = 14.64% for all data. The goodness-of-fit was 1.053. The largest peak in the final difference electron density synthesis was 0.470 $e^-/Å^3$ and the largest hole was -0.386 $e^-/Å^3$ with an RMS deviation of 0.055 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.348 g/cm^3 and F(000), 1008 e^-.

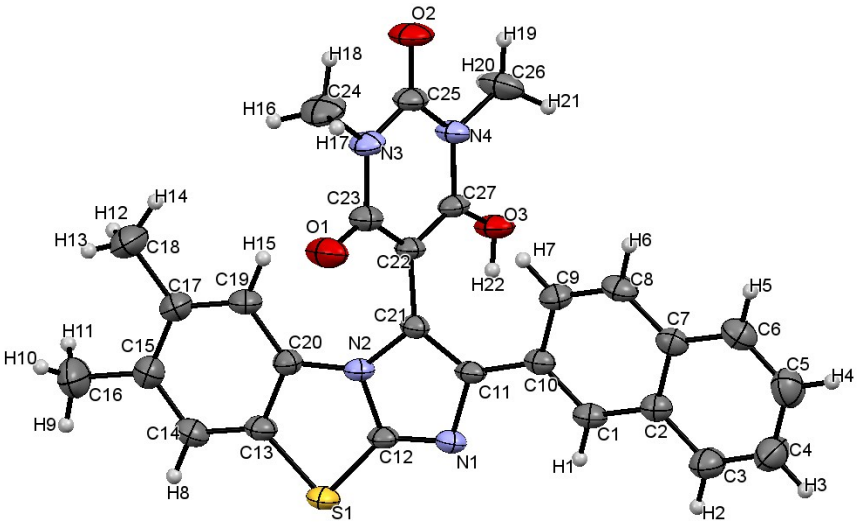


Figure S1. ORTEP view of **6o**with 50% ellipsoidal probability (CCDC 1895624).

Table S1. Sample and crystal information for 6o.

Chemical formula	$C_{27}H_{22}N_4O_3S$	
Formula weight	482.54 g/mol	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal size	0.300 x 0.300 x 0.300 mm	
Crystal system	monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 11.638(4) Å	α = 90°
	b = 14.774(6) Å	β = 101.385(10)°
	c = 14.105(5) Å	γ = 90°
Volume	2377.5(15) $Å^3$	
Z	4	
Density (calculated)	1.348 g/cm^3	
Absorption coefficient	0.174 mm^{-1}	
F(000)	1008	

Table S2. Data collection and structure refinement for 6o.

Theta range for data collection	2.53 to 25.00°
Index ranges	-13<=h<=13, -17<=k<=17, -16<=l<=16
Reflections collected	35307
Independent reflections	4189 [R(int) = 0.0766]
Max. and min. transmission	0.9500 and 0.9500
Structure solution technique	direct methods
Structure solution program	SHELXS-97 (Sheldrick 2008)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014 (Sheldrick 2014)
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	4189 / 0 / 322
Goodness-of-fit on F^2	1.053
Δ/σ_{max}	0.010
Final R indices	2724 data; I>2σ(I) R1 = 0.0542, wR2 = 0.1230
	all data R1 = 0.0998, wR2 = 0.1464
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0613P)^2+1.6611P]$ where $P=(F_o^2+2F_c^2)/3$
Extinction coefficient	0.0024(6)
Largest diff. peak and hole	0.470 and -0.386 $eÅ^{-3}$
R.M.S. deviation from mean	0.055 $eÅ^{-3}$

Table S3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 6o.

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	0.79191(6)	0.58897(6)	0.67106(6)	0.0393(3)
O3	0.29216(18)	0.45779(15)	0.60164(17)	0.0450(6)
O2	0.04719(18)	0.59847(16)	0.76763(18)	0.0566(7)
N2	0.57178(19)	0.60111(16)	0.68066(17)	0.0304(6)
O1	0.38399(19)	0.74586(16)	0.74446(18)	0.0558(7)
N1	0.58721(19)	0.60245(16)	0.52741(18)	0.0319(6)
N4	0.1706(2)	0.52982(17)	0.68330(19)	0.0369(7)
N3	0.2174(2)	0.67091(18)	0.75892(19)	0.0406(7)
C21	0.4559(2)	0.60759(19)	0.6264(2)	0.0291(7)
C11	0.4671(2)	0.61115(19)	0.5315(2)	0.0302(7)
C10	0.3813(2)	0.62733(19)	0.4421(2)	0.0311(7)
C27	0.2762(2)	0.5276(2)	0.6489(2)	0.0312(7)
C20	0.6295(2)	0.5977(2)	0.7785(2)	0.0322(7)
C2	0.3327(2)	0.6388(2)	0.2659(2)	0.0340(7)
C12	0.6465(2)	0.5972(2)	0.6187(2)	0.0306(7)
C7	0.2157(2)	0.6631(2)	0.2700(2)	0.0336(7)
C22	0.3509(2)	0.6027(2)	0.6698(2)	0.0309(7)
C1	0.4128(2)	0.6215(2)	0.3529(2)	0.0351(8)
C13	0.7511(2)	0.5902(2)	0.7848(2)	0.0343(8)
C23	0.3230(3)	0.6774(2)	0.7244(2)	0.0380(8)
C9	0.2640(2)	0.6536(2)	0.4449(2)	0.0382(8)
C19	0.5823(3)	0.6014(2)	0.8611(2)	0.0393(8)
C8	0.1858(3)	0.6707(2)	0.3616(2)	0.0401(8)
C14	0.8243(3)	0.5847(2)	0.8744(2)	0.0429(8)
C6	0.1361(3)	0.6787(2)	0.1827(2)	0.0441(9)
C17	0.6561(3)	0.5965(2)	0.9505(2)	0.0451(9)
C15	0.7783(3)	0.5870(2)	0.9579(2)	0.0457(9)
C3	0.3655(3)	0.6328(2)	0.1744(2)	0.0484(9)
C5	0.1694(3)	0.6715(2)	0.0955(3)	0.0529(10)
C26	0.0866(3)	0.4549(2)	0.6580(3)	0.0548(10)
C4	0.2860(3)	0.6483(3)	0.0915(3)	0.0552(10)
C24	0.1844(3)	0.7471(3)	0.8152(3)	0.0616(11)
C16	0.8590(3)	0.5787(3)	0.0551(3)	0.0754(13)
C18	0.6052(3)	0.6033(3)	0.0407(3)	0.0778(14)
C25	0.1392(2)	0.5998(2)	0.7382(2)	0.0389(8)

Table S4. Bond lengths (Å) for 6o.

S1-C12	1.712(3)	S1-C13	1.760(3)
O3-C27	1.262(3)	O3-H22	0.82
O2-C25	1.223(3)	N2-C12	1.350(3)

N2-C20	1.412(4)	N2-C21	1.416(3)
O1-C23	1.237(4)	N1-C12	1.338(4)
N1-C11	1.417(3)	N4-C25	1.384(4)
N4-C27	1.407(3)	N4-C26	1.473(4)
N3-C25	1.382(4)	N3-C23	1.412(4)
N3-C24	1.471(4)	C21-C11	1.371(4)
C21-C22	1.473(4)	C11-C10	1.466(4)
C10-C1	1.380(4)	C10-C9	1.427(4)
C27-C22	1.405(4)	C20-C19	1.384(4)
C20-C13	1.405(4)	C2-C1	1.411(4)
C2-C3	1.418(4)	C2-C7	1.421(4)
C7-C6	1.406(4)	C7-C8	1.407(4)
C22-C23	1.418(4)	C1-H1	0.93
C13-C14	1.380(4)	C9-C8	1.360(4)
C9-H7	0.93	C19-C17	1.380(4)
C19-H15	0.93	C8-H6	0.93
C14-C15	1.387(4)	C14-H8	0.93
C6-C5	1.365(5)	C6-H5	0.93
C17-C15	1.413(4)	C17-C18	1.509(5)
C15-C16	1.507(5)	C3-C4	1.360(5)
C3-H2	0.93	C5-C4	1.410(5)
C5-H4	0.93	C26-H20	0.96
C26-H21	0.96	C26-H19	0.96
C4-H3	0.93	C24-H18	0.96
C24-H17	0.96	C24-H16	0.96
C16-H9	0.96	C16-H11	0.96
C16-H10	0.96	C18-H14	0.96
C18-H13	0.96	C18-H12	0.96

Table S5. Bond angles (°) for 6o.

C12-S1-C13	88.32(14)	C27-O3-H22	109.5
C12-N2-C20	112.9(2)	C12-N2-C21	108.6(2)
C20-N2-C21	138.6(2)	C12-N1-C11	106.9(2)
C25-N4-C27	123.7(3)	C25-N4-C26	117.5(2)
C27-N4-C26	118.8(3)	C25-N3-C23	124.0(3)
C25-N3-C24	117.7(2)	C23-N3-C24	118.2(3)
C11-C21-N2	105.5(2)	C11-C21-C22	130.9(3)
N2-C21-C22	123.5(3)	C21-C11-N1	108.7(2)
C21-C11-C10	131.8(2)	N1-C11-C10	119.3(2)
C1-C10-C9	118.1(3)	C1-C10-C11	121.0(3)
C9-C10-C11	120.9(3)	O3-C27-C22	127.3(3)

O3-C27-N4	115.5(3)	C22-C27-N4	117.2(3)
C19-C20-C13	120.9(3)	C19-C20-N2	129.1(3)
C13-C20-N2	110.1(2)	C1-C2-C3	122.0(3)
C1-C2-C7	118.9(3)	C3-C2-C7	119.1(3)
N1-C12-N2	110.2(2)	N1-C12-S1	134.2(2)
N2-C12-S1	115.6(2)	C6-C7-C8	123.5(3)
C6-C7-C2	118.4(3)	C8-C7-C2	118.1(3)
C27-C22-C23	121.9(3)	C27-C22-C21	118.8(3)
C23-C22-C21	119.0(3)	C10-C1-C2	122.2(3)
C10-C1-H1	118.9	C2-C1-H1	118.9
C14-C13-C20	119.6(3)	C14-C13-S1	127.2(2)
C20-C13-S1	113.2(2)	O1-C23-N3	118.4(3)
O1-C23-C22	125.3(3)	N3-C23-C22	116.3(3)
C8-C9-C10	120.5(3)	C8-C9-H7	119.8
C10-C9-H7	119.8	C17-C19-C20	119.2(3)
C17-C19-H15	120.4	C20-C19-H15	120.4
C9-C8-C7	122.2(3)	C9-C8-H6	118.9
C7-C8-H6	118.9	C13-C14-C15	120.3(3)
C13-C14-H8	119.8	C15-C14-H8	119.8
C5-C6-C7	121.5(3)	C5-C6-H5	119.3
C7-C6-H5	119.3	C19-C17-C15	120.5(3)
C19-C17-C18	119.3(3)	C15-C17-C18	120.2(3)
C14-C15-C17	119.5(3)	C14-C15-C16	119.7(3)
C17-C15-C16	120.8(3)	C4-C3-C2	120.7(3)
C4-C3-H2	119.6	C2-C3-H2	119.6
C6-C5-C4	120.1(3)	C6-C5-H4	120.0
C4-C5-H4	120.0	N4-C26-H20	109.5
N4-C26-H21	109.5	H20-C26-H21	109.5
N4-C26-H19	109.5	H20-C26-H19	109.5
H21-C26-H19	109.5	C3-C4-C5	120.2(3)
C3-C4-H3	119.9	C5-C4-H3	119.9
N3-C24-H18	109.5	N3-C24-H17	109.5
H18-C24-H17	109.5	N3-C24-H16	109.5
H18-C24-H16	109.5	H17-C24-H16	109.5
C15-C16-H9	109.5	C15-C16-H11	109.5
H9-C16-H11	109.5	C15-C16-H10	109.5
H9-C16-H10	109.5	H11-C16-H10	109.5
C17-C18-H14	109.5	C17-C18-H13	109.5
H14-C18-H13	109.5	C17-C18-H12	109.5
H14-C18-H12	109.5	H13-C18-H12	109.5
O2-C25-N3	121.7(3)	O2-C25-N4	121.5(3)
N3-C25-N4	116.8(2)		

Table S6. Torsion angles (°) for 6o.

C12-N2-C21-C11	-2.5(3)	C20-N2-C21-C11	177.5(3)
C12-N2-C21-C22	172.8(3)	C20-N2-C21-C22	-7.2(5)
N2-C21-C11-N1	2.8(3)	C22-C21-C11-N1	-172.0(3)
N2-C21-C11-C10	-172.8(3)	C22-C21-C11-C10	12.4(6)
C12-N1-C11-C21	-2.2(3)	C12-N1-C11-C10	174.1(3)
C21-C11-C10-C1	-175.5(3)	N1-C11-C10-C1	9.3(4)
C21-C11-C10-C9	7.4(5)	N1-C11-C10-C9	-167.9(3)
C25-N4-C27-O3	178.5(3)	C26-N4-C27-O3	-3.0(4)
C25-N4-C27-C22	-2.0(4)	C26-N4-C27-C22	176.4(3)
C12-N2-C20-C19	178.9(3)	C21-N2-C20-C19	-1.1(6)
C12-N2-C20-C13	-0.5(4)	C21-N2-C20-C13	179.5(3)
C11-N1-C12-N2	0.6(3)	C11-N1-C12-S1	-178.0(3)
C20-N2-C12-N1	-178.8(2)	C21-N2-C12-N1	1.2(3)
C20-N2-C12-S1	0.1(3)	C21-N2-C12-S1	-179.9(2)
C13-S1-C12-N1	178.8(3)	C13-S1-C12-N2	0.3(2)
C1-C2-C7-C6	-178.9(3)	C3-C2-C7-C6	1.1(4)
C1-C2-C7-C8	1.3(4)	C3-C2-C7-C8	-178.6(3)
O3-C27-C22-C23	-179.8(3)	N4-C27-C22-C23	0.9(4)
O3-C27-C22-C21	5.9(5)	N4-C27-C22-C21	-173.5(3)
C11-C21-C22-C27	61.6(4)	N2-C21-C22-C27	-112.4(3)
C11-C21-C22-C23	-113.0(4)	N2-C21-C22-C23	73.1(4)
C9-C10-C1-C2	-1.2(4)	C11-C10-C1-C2	-178.4(3)
C3-C2-C1-C10	179.9(3)	C7-C2-C1-C10	0.0(5)
C19-C20-C13-C14	1.3(5)	N2-C20-C13-C14	-179.2(3)
C19-C20-C13-S1	-178.7(2)	N2-C20-C13-S1	0.8(3)
C12-S1-C13-C14	179.3(3)	C12-S1-C13-C20	-0.6(2)
C25-N3-C23-O1	177.2(3)	C24-N3-C23-O1	1.4(5)
C25-N3-C23-C22	-3.7(4)	C24-N3-C23-C22	-179.5(3)
C27-C22-C23-O1	-179.2(3)	C21-C22-C23-O1	-4.8(5)
C27-C22-C23-N3	1.8(4)	C21-C22-C23-N3	176.1(3)
C1-C10-C9-C8	1.2(4)	C11-C10-C9-C8	178.4(3)
C13-C20-C19-C17	-0.9(5)	N2-C20-C19-C17	179.8(3)
C10-C9-C8-C7	0.2(5)	C6-C7-C8-C9	178.8(3)
C2-C7-C8-C9	-1.4(5)	C20-C13-C14-C15	-0.3(5)
S1-C13-C14-C15	179.7(3)	C8-C7-C6-C5	179.3(3)
C2-C7-C6-C5	-0.4(5)	C20-C19-C17-C15	-0.5(5)
C20-C19-C17-C18	178.2(3)	C13-C14-C15-C17	-1.0(5)
C13-C14-C15-C16	178.6(3)	C19-C17-C15-C14	1.5(5)
C18-C17-C15-C14	-177.3(3)	C19-C17-C15-C16	-178.1(3)
C18-C17-C15-C16	3.1(6)	C1-C2-C3-C4	178.8(3)
C7-C2-C3-C4	-1.2(5)	C7-C6-C5-C4	-0.3(5)
C2-C3-C4-C5	0.5(6)	C6-C5-C4-C3	0.2(6)
C23-N3-C25-O2	-177.9(3)	C24-N3-C25-O2	-2.0(5)
C23-N3-C25-N4	2.7(4)	C24-N3-C25-N4	178.5(3)
C27-N4-C25-O2	-179.1(3)	C26-N4-C25-O2	2.4(5)

C27-N4-C25-N3	0.4(4)	C26-N4-C25-N3	-178.1(3)

Table S7. Anisotropic atomic displacement parameters (Å^2) for 6o.

The anisotropic atomic 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}
S1	0.0221(4)	0.0568(6)	0.0418(5)	-0.0005(4)	0.0130(3)	0.0020(4)
O3	0.0342(13)	0.0469(14)	0.0619(16)	-0.0080(12)	0.0290(12)	-0.0039(11)
O2	0.0341(13)	0.0697(17)	0.0757(18)	-0.0060(14)	0.0343(13)	0.0010(12)
N2	0.0224(12)	0.0376(15)	0.0339(15)	-0.0015(12)	0.0119(11)	0.0003(11)
O1	0.0456(14)	0.0513(15)	0.0784(18)	-0.0237(13)	0.0311(13)	-0.0135(12)
N1	0.0212(12)	0.0394(15)	0.0370(16)	-0.0012(12)	0.0103(11)	-0.0013(11)
N4	0.0249(13)	0.0416(16)	0.0488(17)	-0.0017(13)	0.0183(12)	-0.0020(12)
N3	0.0318(14)	0.0461(17)	0.0499(17)	-0.0103(14)	0.0226(13)	0.0019(13)
C21	0.0213(14)	0.0330(18)	0.0348(18)	-0.0041(13)	0.0099(13)	-0.0013(12)
C11	0.0214(14)	0.0335(19)	0.0388(19)	-0.0039(14)	0.0134(13)	-0.0026(12)
C10	0.0260(15)	0.0305(17)	0.0390(19)	-0.0025(14)	0.0116(14)	-0.0014(13)
C27	0.0246(15)	0.0386(19)	0.0343(18)	0.0015(15)	0.0150(13)	0.0035(14)
C20	0.0279(15)	0.0365(18)	0.0343(18)	-0.0049(14)	0.0114(14)	-0.0015(14)
C2	0.0305(16)	0.0356(18)	0.0373(19)	0.0002(15)	0.0102(15)	0.0004(14)
C12	0.0224(15)	0.0355(18)	0.0374(19)	-0.0035(14)	0.0142(14)	0.0010(13)
C7	0.0303(16)	0.0305(18)	0.0407(19)	0.0015(15)	0.0085(15)	-0.0015(13)
C22	0.0218(15)	0.0379(19)	0.0359(18)	-0.0032(14)	0.0129(13)	-0.0009(13)
C1	0.0260(16)	0.0391(19)	0.043(2)	0.0009(15)	0.0133(15)	0.0014(14)
C13	0.0243(15)	0.0405(19)	0.041(2)	-0.0008(15)	0.0122(14)	0.0010(14)
C23	0.0283(16)	0.046(2)	0.043(2)	-0.0010(16)	0.0144(15)	-0.0009(15)
C9	0.0312(17)	0.046(2)	0.040(2)	-0.0040(16)	0.0150(15)	0.0027(15)
C19	0.0274(16)	0.053(2)	0.041(2)	-0.0033(16)	0.0143(15)	-0.0007(15)
C8	0.0249(16)	0.045(2)	0.053(2)	-0.0008(17)	0.0126(16)	0.0045(14)
C14	0.0267(16)	0.056(2)	0.047(2)	-0.0012(17)	0.0080(16)	0.0006(15)
C6	0.0331(18)	0.046(2)	0.052(2)	0.0023(17)	0.0056(17)	0.0017(15)
C17	0.0381(18)	0.064(2)	0.036(2)	-0.0040(17)	0.0136(16)	-0.0034(17)
C15	0.0397(19)	0.061(2)	0.036(2)	-0.0037(17)	0.0075(16)	-0.0027(17)
C3	0.0388(19)	0.063(2)	0.046(2)	0.0011(18)	0.0147(18)	0.0065(17)
C5	0.048(2)	0.061(2)	0.046(2)	0.0046(19)	-0.0010(18)	0.0004(18)
C26	0.0359(19)	0.051(2)	0.083(3)	-0.004(2)	0.0257(19)	-0.0113(17)
C4	0.051(2)	0.076(3)	0.040(2)	0.0017(19)	0.0124(18)	0.009(2)
C24	0.059(2)	0.058(2)	0.079(3)	-0.022(2)	0.040(2)	0.003(2)
C16	0.049(2)	0.128(4)	0.045(2)	-0.006(2)	-0.0012(19)	0.000(2)
C18	0.055(2)	0.139(4)	0.045(2)	-0.007(3)	0.023(2)	-0.002(3)
C25	0.0234(16)	0.052(2)	0.044(2)	0.0033(17)	0.0154(15)	0.0054(15)

Table S8. Hydrogen atomic coordinates and isotropic atomic displacement

parameters (Å^2) for 6o.

	x/a	y/b	z/c	U(eq)
H22	0.3548	0.4620	0.5837	0.067
H1	0.4894	0.6055	0.3502	0.042
H7	0.2410	0.6592	0.5041	0.046
H15	0.5018	0.6072	0.8565	0.047
H6	0.1099	0.6879	0.3653	0.048
H8	0.9048	0.5794	0.8788	0.051
H5	0.0592	0.6943	0.1844	0.053
H2	0.4423	0.6180	0.1711	0.058
H4	0.1152	0.6819	0.0386	0.063
H20	0.1157	0.4021	0.6948	0.082
H21	0.0770	0.4418	0.5903	0.082
H19	0.0124	0.4719	0.6726	0.082
H3	0.3085	0.6437	0.0320	0.066
H18	0.1106	0.7344	0.8330	0.092
H17	0.1778	0.8012	0.7768	0.092
H16	0.2434	0.7554	0.8726	0.092
H9	0.9377	0.5688	1.0463	0.113
H11	0.8347	0.5286	1.0898	0.113
H10	0.8560	0.6334	1.0912	0.113
H14	0.5217	0.6102	1.0230	0.117
H13	0.6382	0.6548	1.0780	0.117
H12	0.6233	0.5493	1.0785	0.117