

Supplementary Information

Figure S1. ^1H and ^{13}C NMR spectra of compounds **2a–2n**, **3a–3k**.

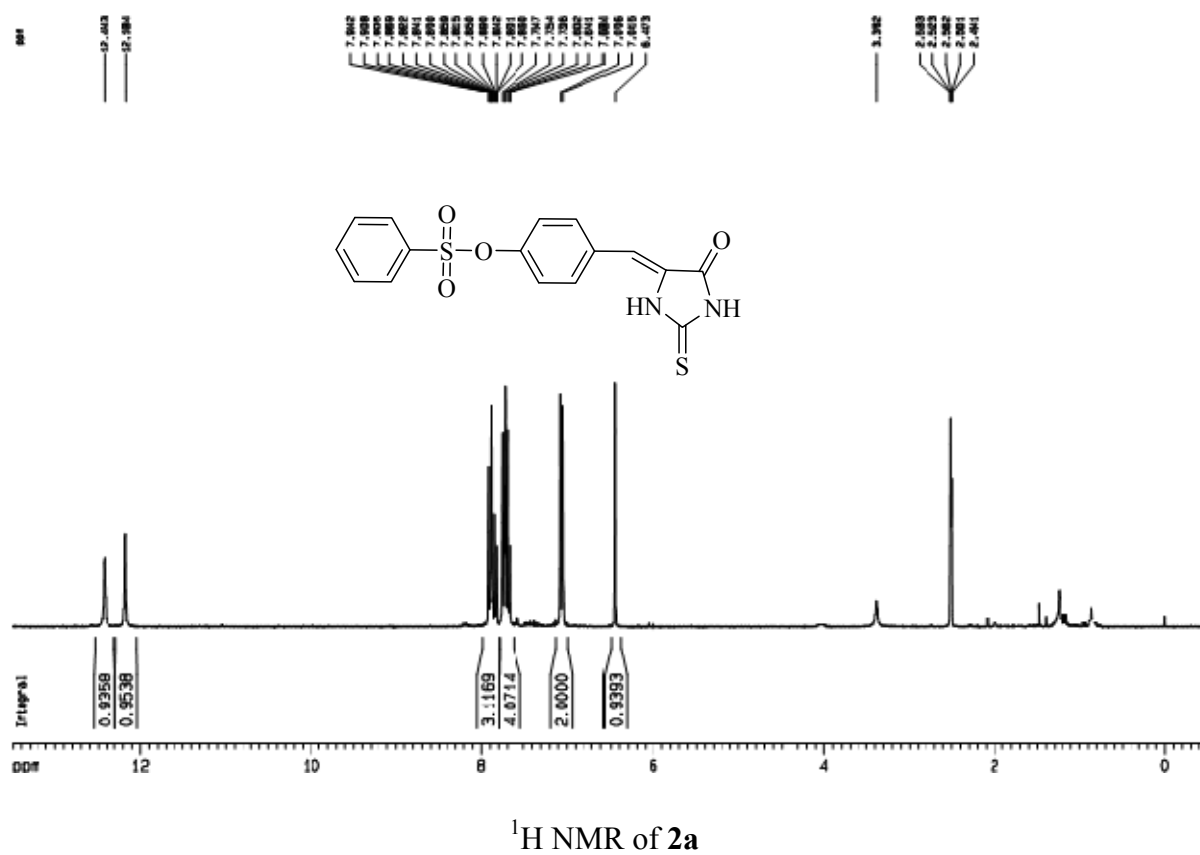


Figure S1. Cont.

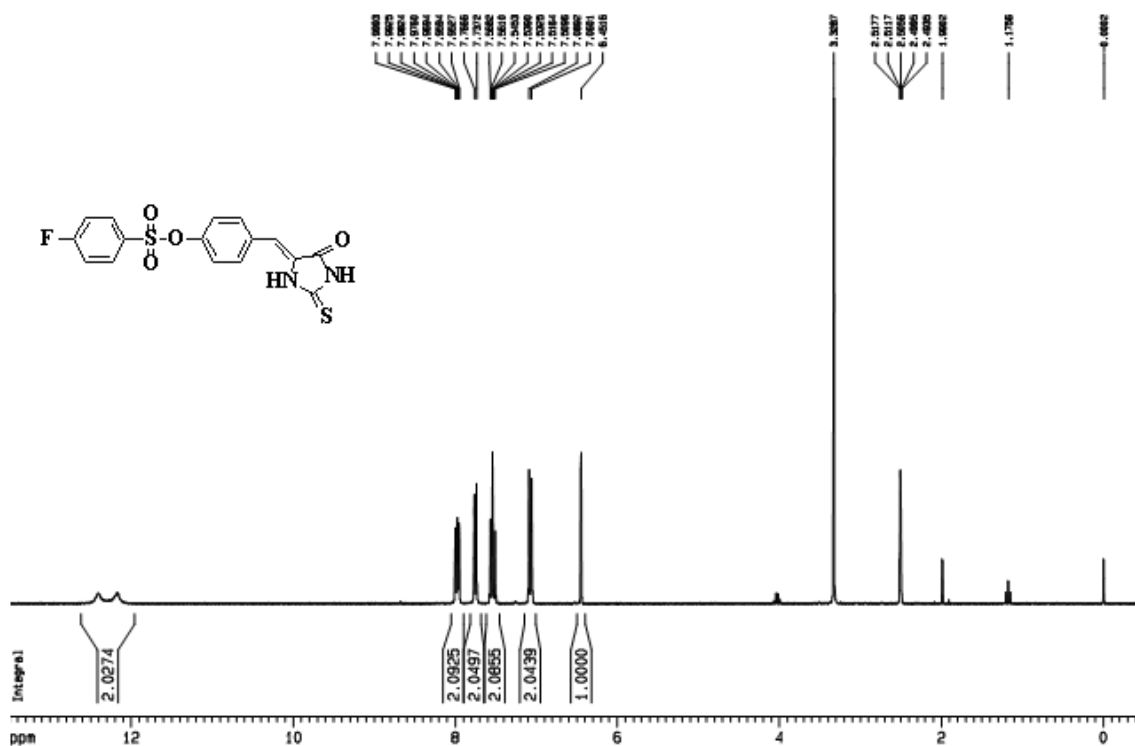
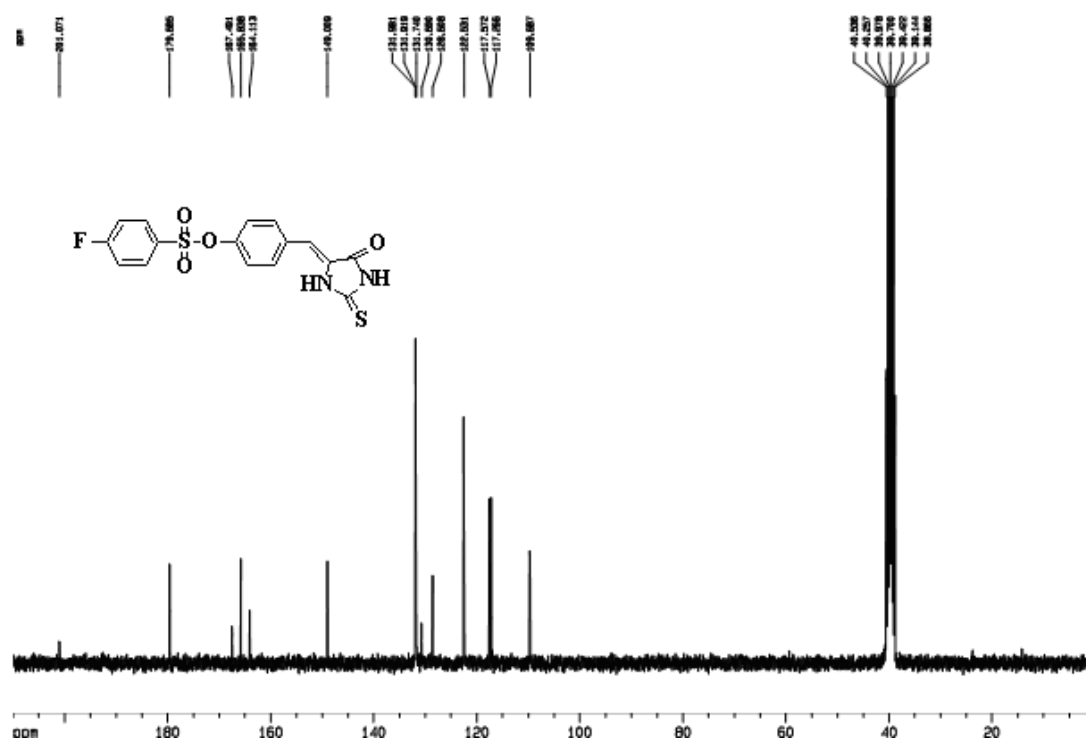
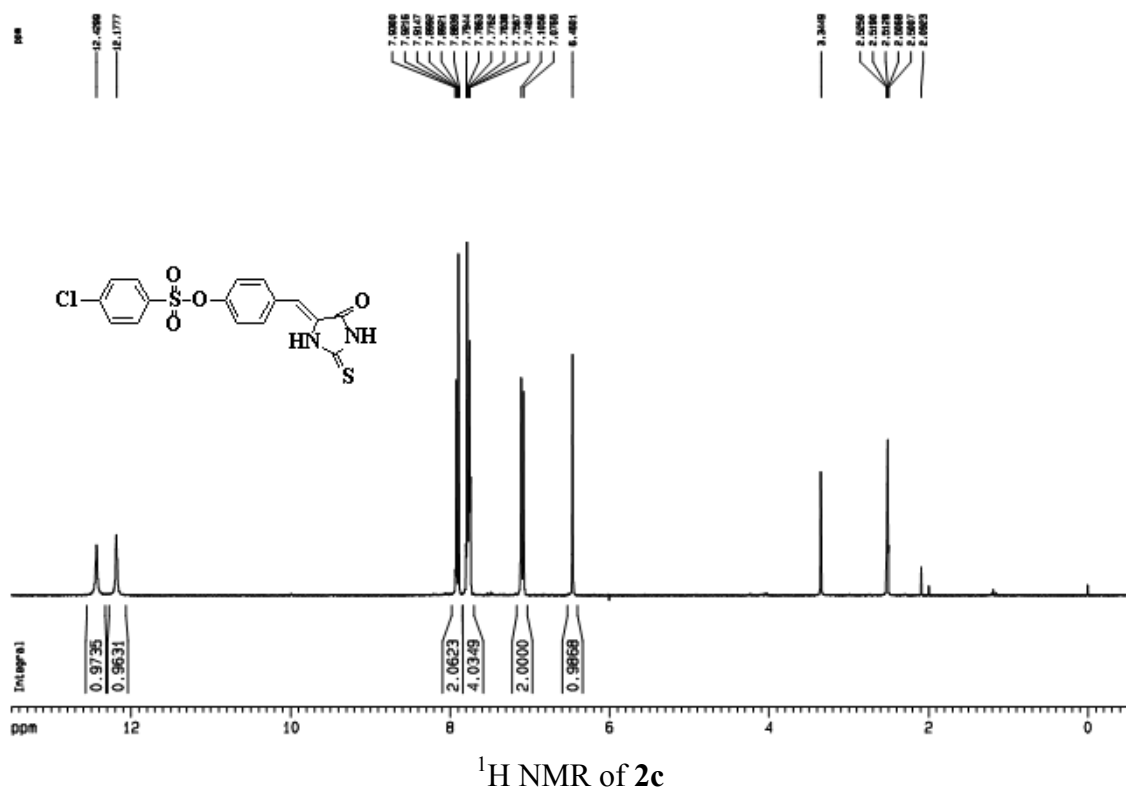
¹H NMR of **2b**¹³C NMR of **2b**

Figure S1. Cont.



Chemical structure: COc1ccc(cc1)S(=O)(=O)Oc2ccc(cc2)/C=C3NC(=O)NC(=O)S3

¹H NMR spectrum (CDCl₃) data:

Chemical Shift (ppm)	Integration
12.119, 12.100	1.9827
7.858, 7.856, 7.855, 7.853, 7.852, 7.847, 7.834, 7.827, 7.825, 7.823, 7.809, 7.807	4.0280
7.554, 7.550, 7.548, 7.545, 7.543, 7.529, 7.527	2.0153
7.554, 7.550, 7.548, 7.545, 7.543, 7.529, 7.527	2.0159
6.985	0.9854
3.974	3.0000
3.939	-
2.958, 2.956, 2.955, 2.953, 2.952, 2.947, 2.945	-

Chemical structure of the compound is shown above the spectrum. The spectrum displays peaks corresponding to the chemical structure, with the following chemical shifts (ppm) labeled above the peaks:

179.873, 165.873, 164.316, 149.099, 133.873, 133.782, 133.745, 133.698, 133.654, 133.586, 119.825, 119.885, 56.164, 40.000, 39.975, 39.950, 39.925, 39.900, 39.875, 39.850.

¹³C NMR of **2d**

Figure S1. Cont.

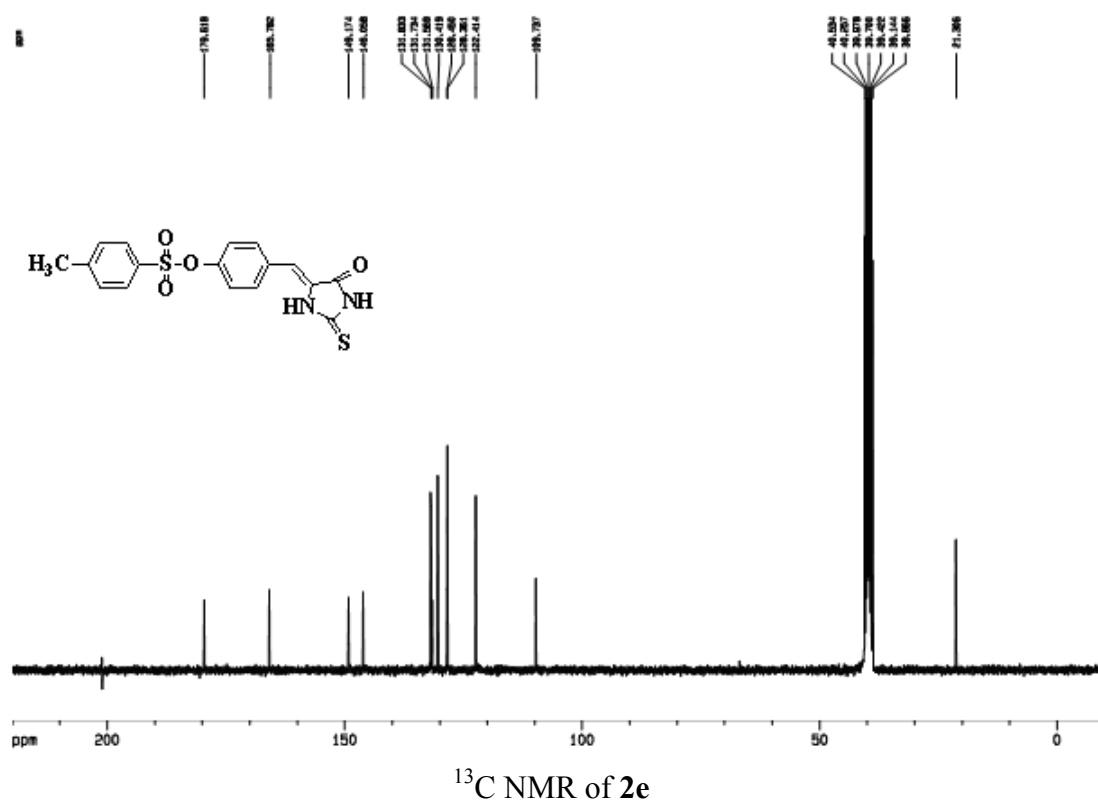
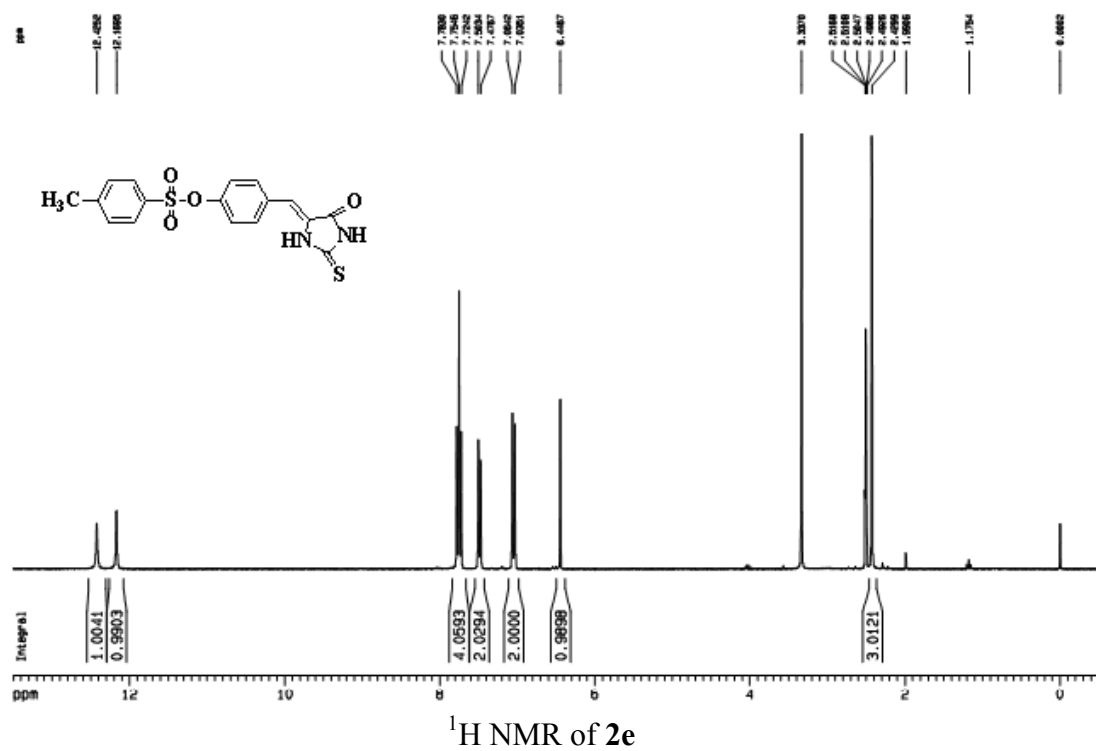


Figure S1. Cont.

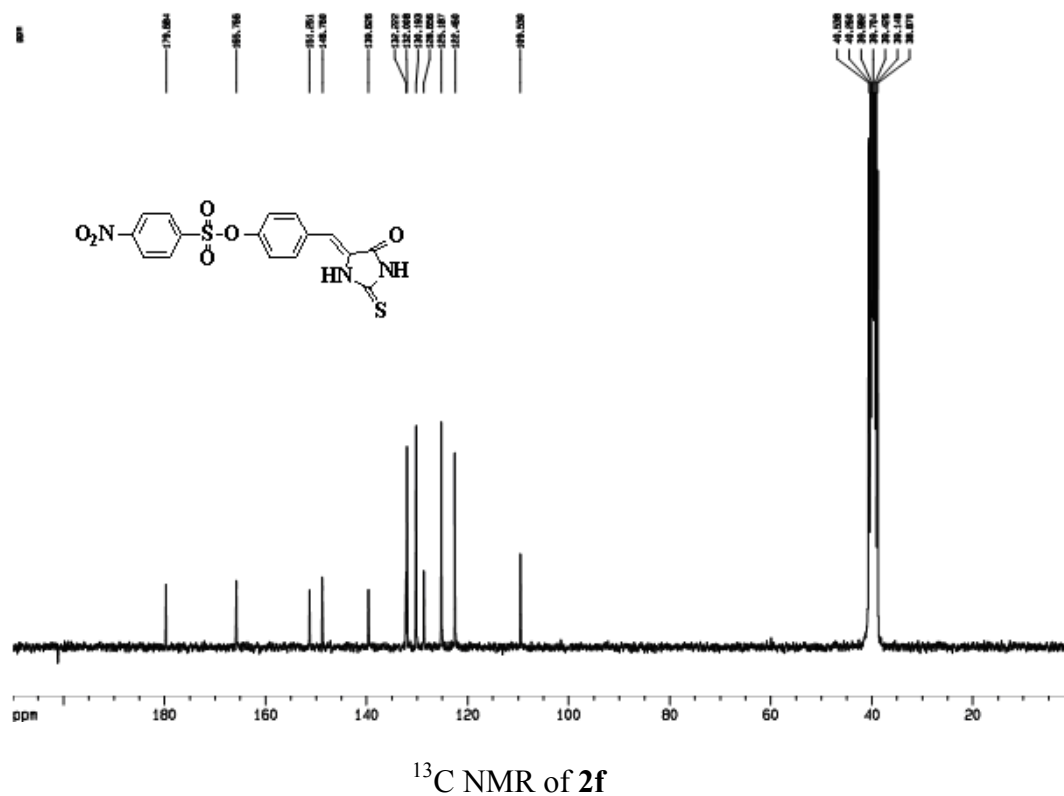
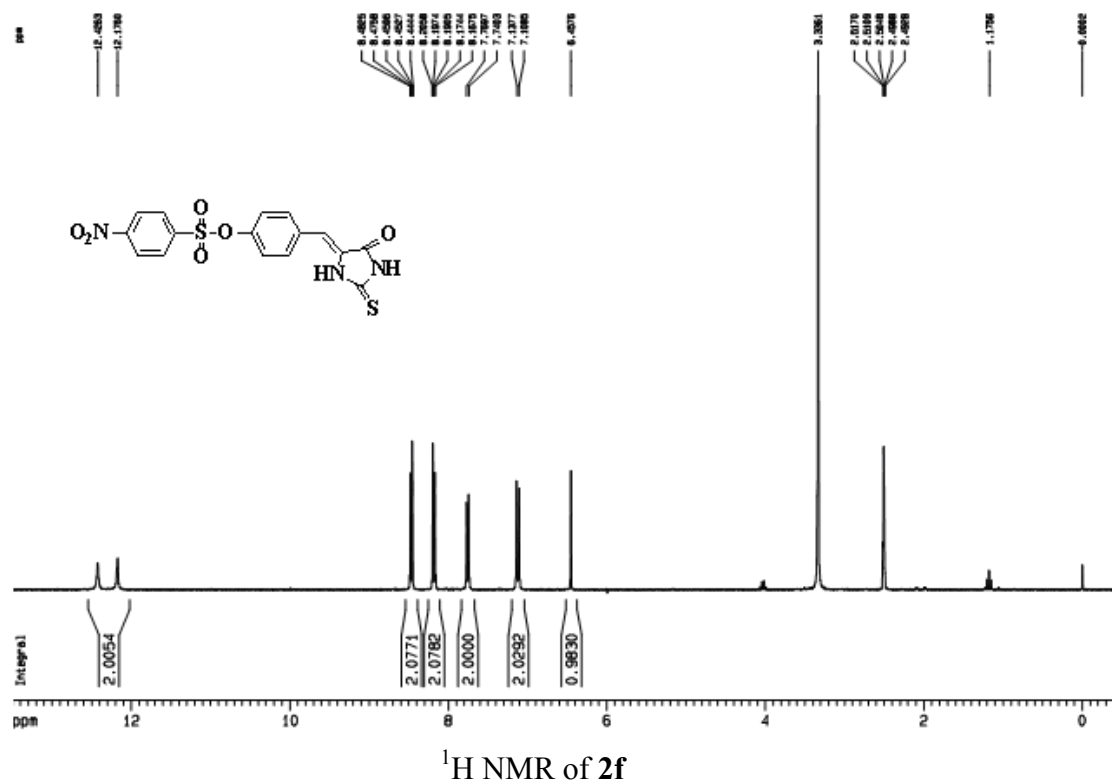


Figure S1. Cont.

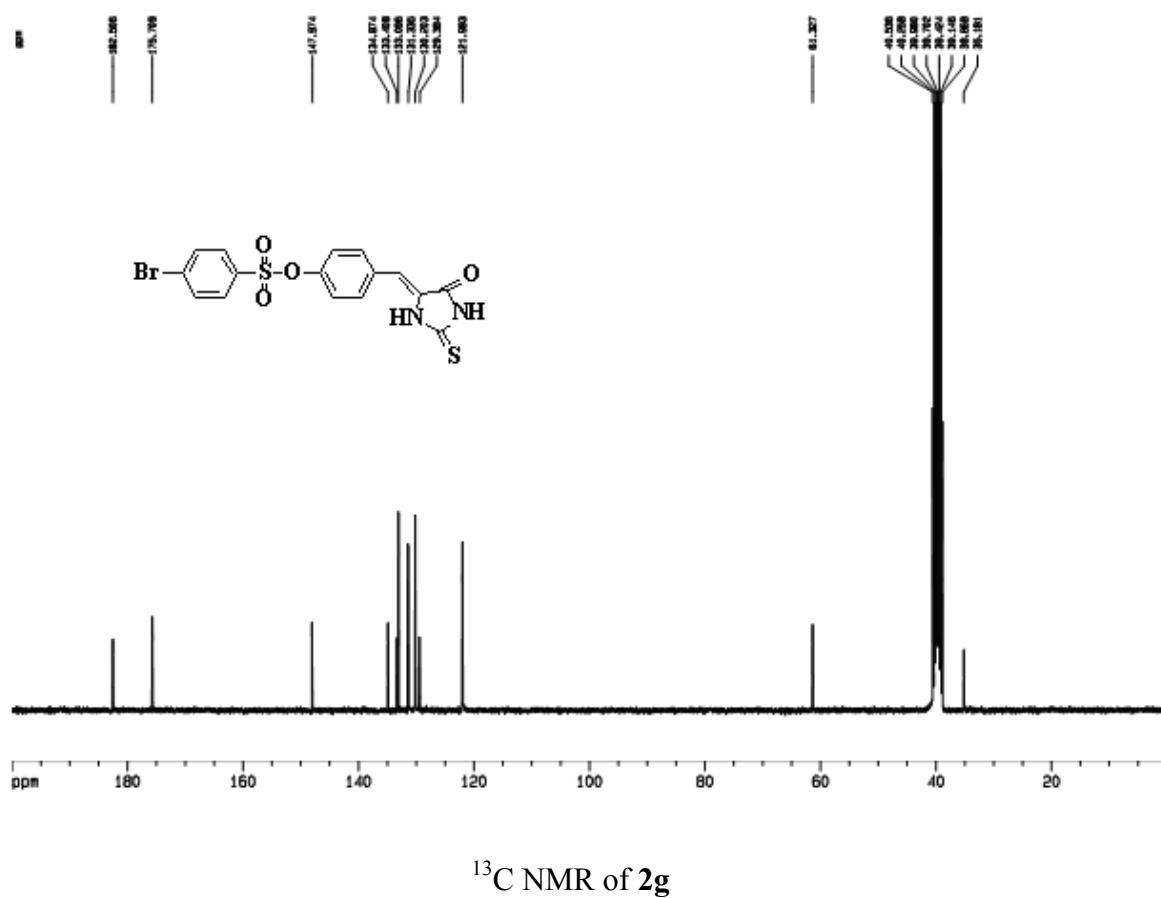
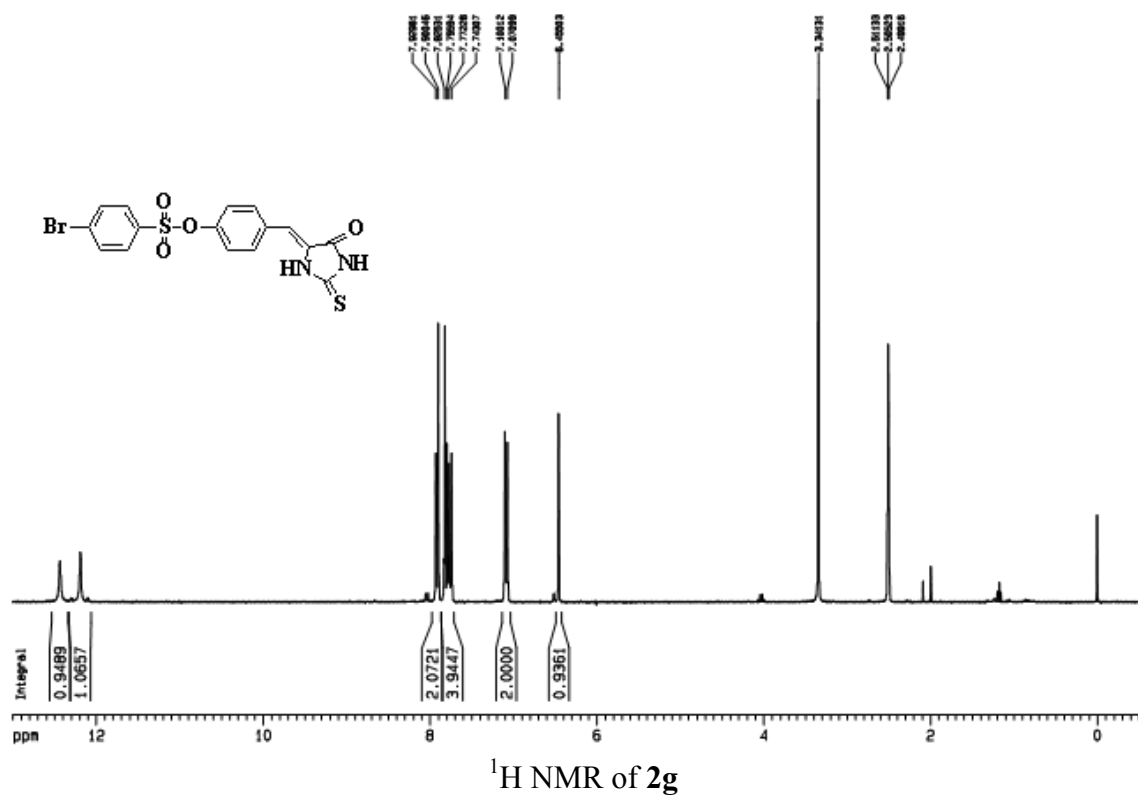
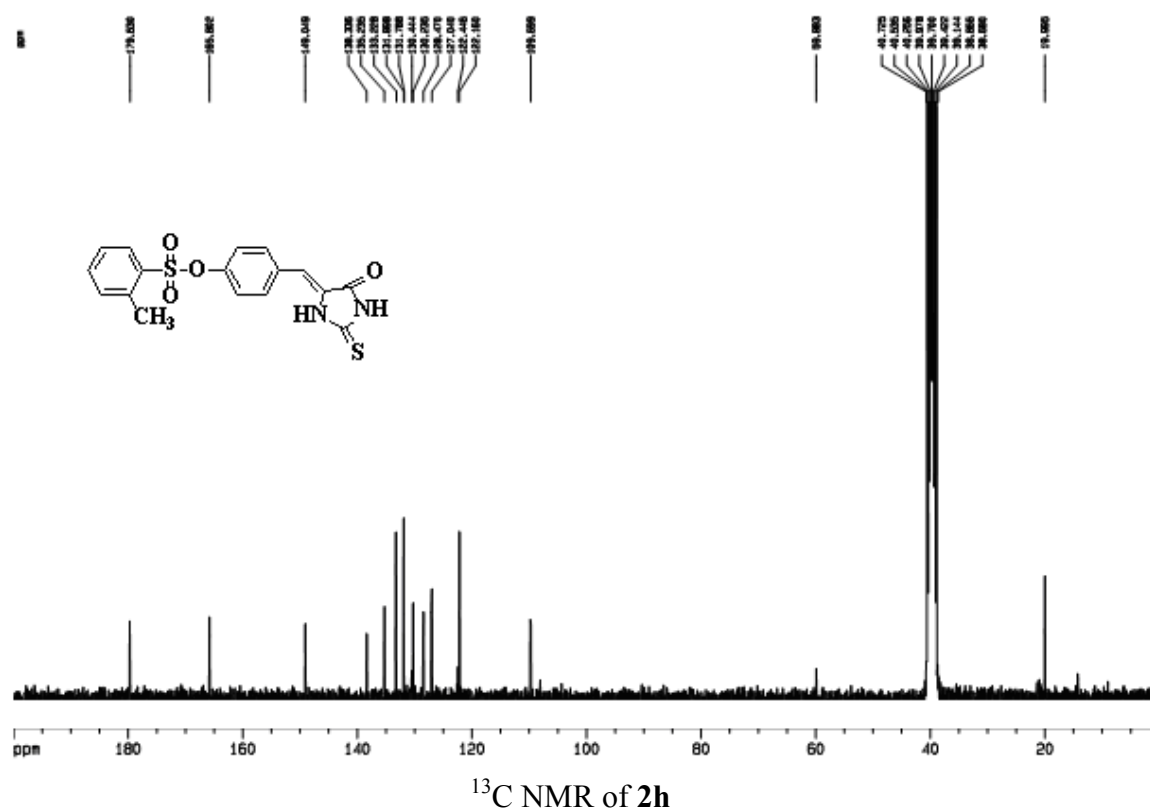
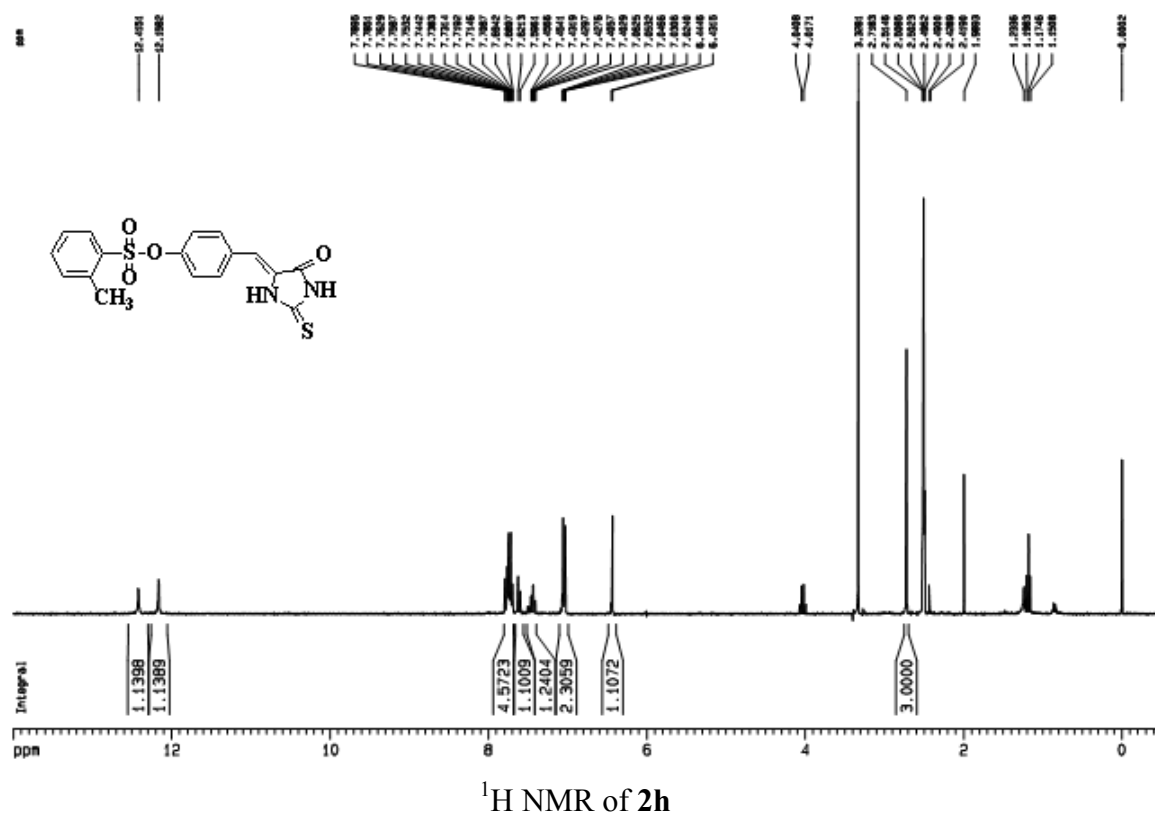


Figure S1. Cont.



Chemical structure of **2i** is shown above the spectrum. The spectrum displays peaks corresponding to the protons in the molecule, with chemical shifts ranging from approximately 0.5 to 12.5 ppm. Key features include a broad peak around 12.5 ppm (NH), aromatic signals between 7.0 and 8.0 ppm, a singlet at 6.5 ppm, a multiplet at 3.0 ppm, and a sharp peak at 2.5 ppm. Integration values are provided below the baseline, and chemical shift values are indicated above the peaks.

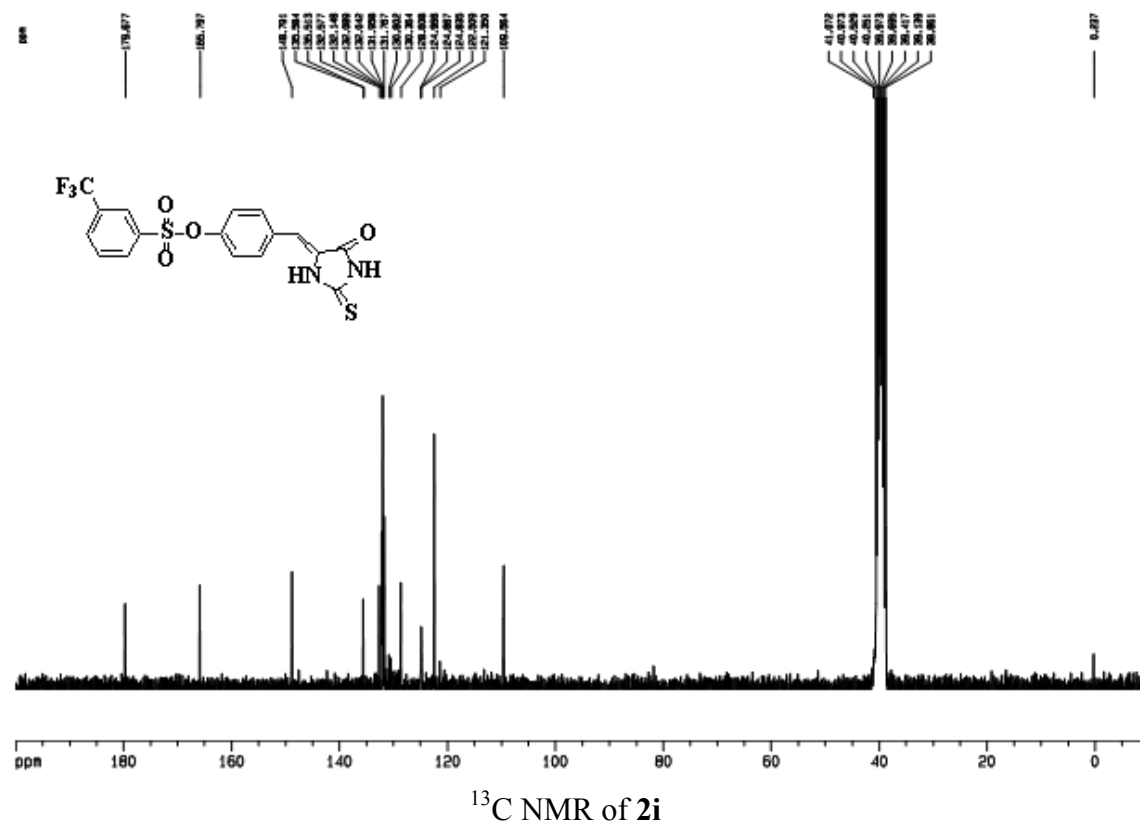


Figure S1. Cont.

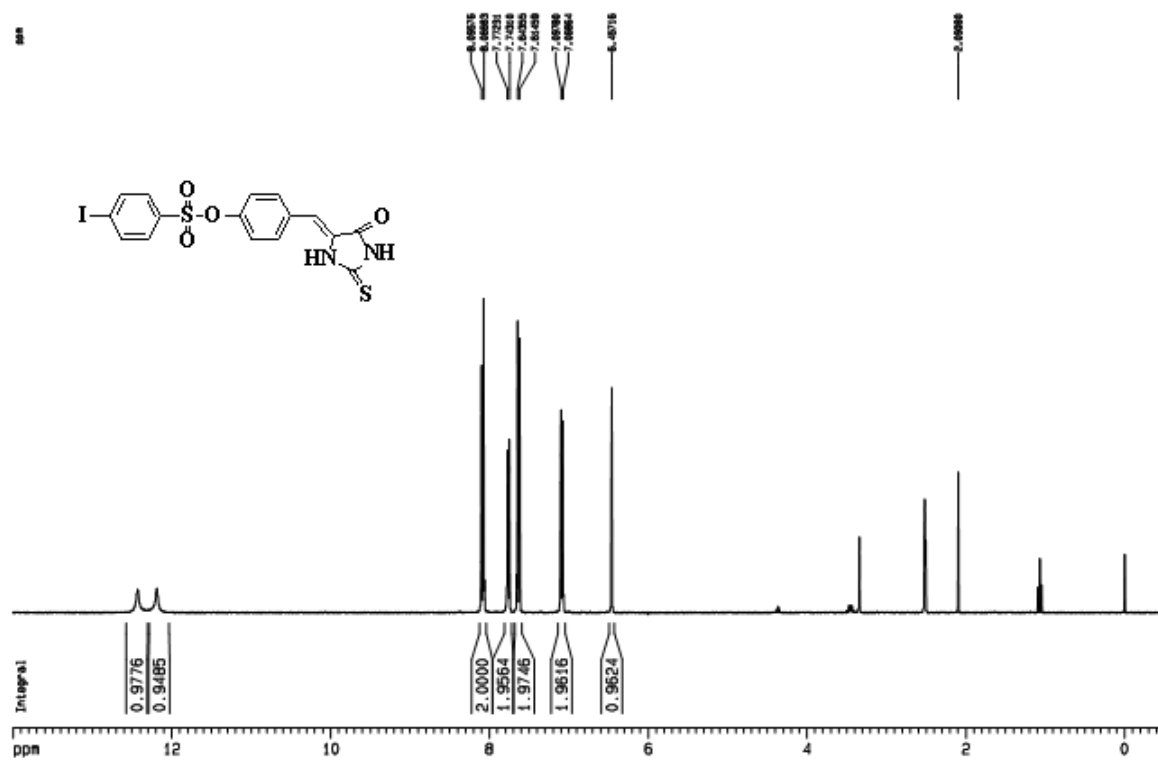
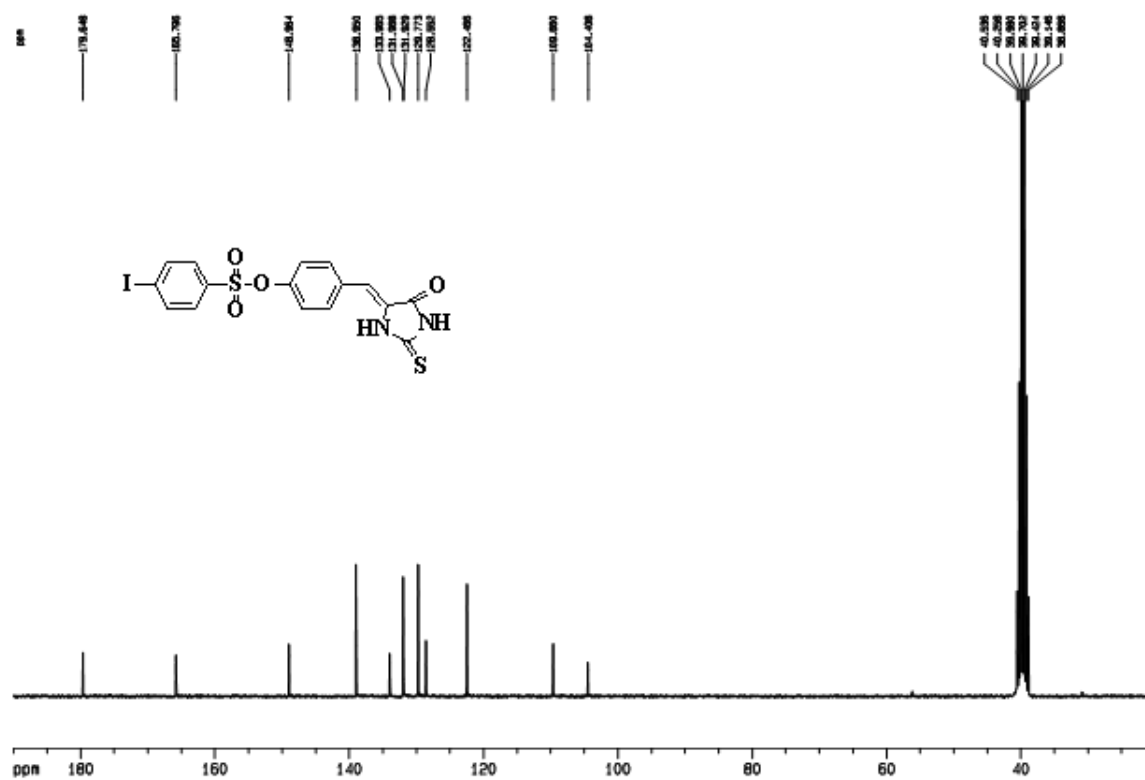
¹H NMR of **2j**

Figure S1. Cont.

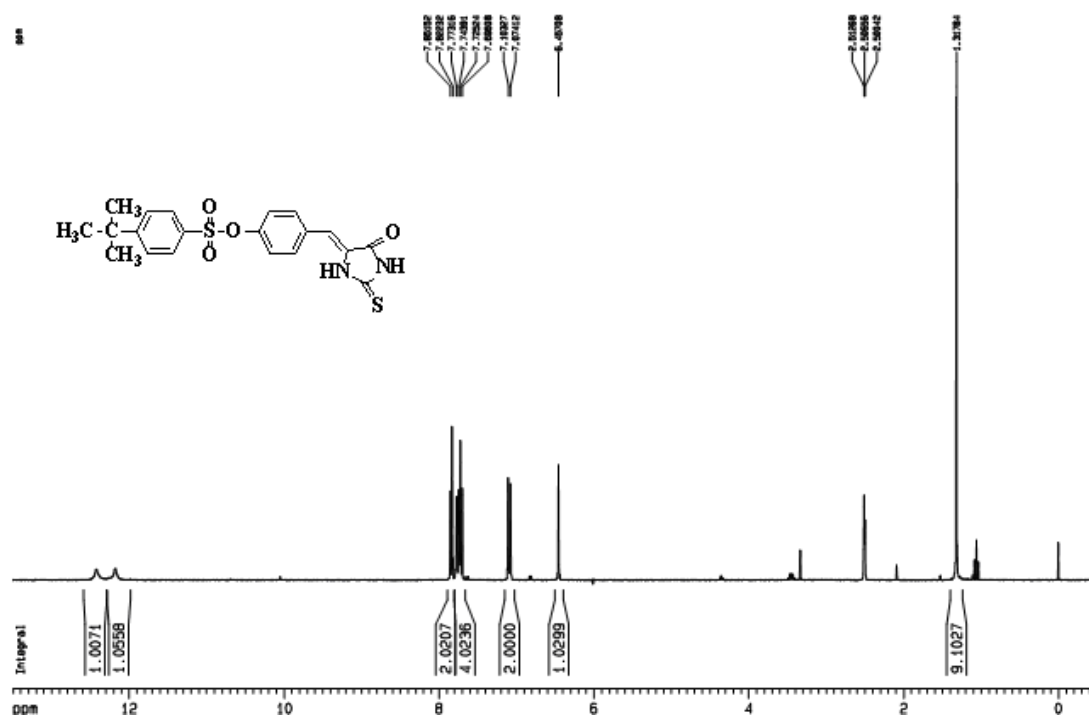
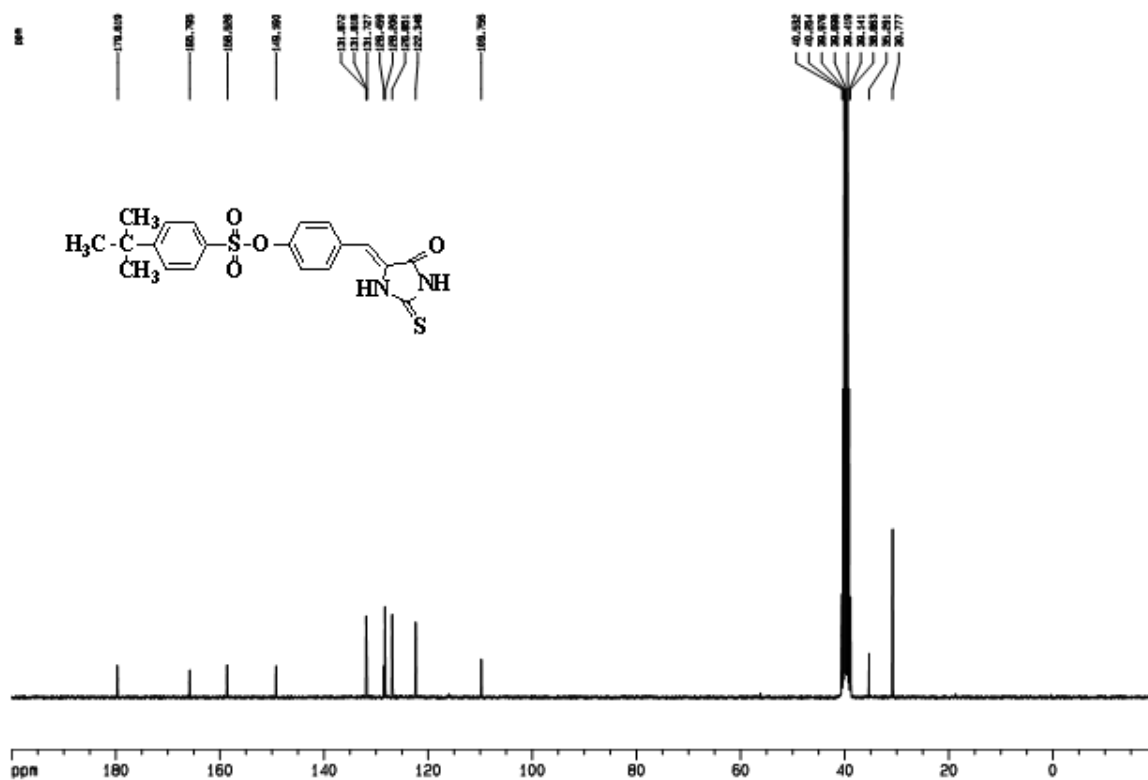
¹H NMR of **2k**¹³C NMR of **2k**

Figure S1. Cont.

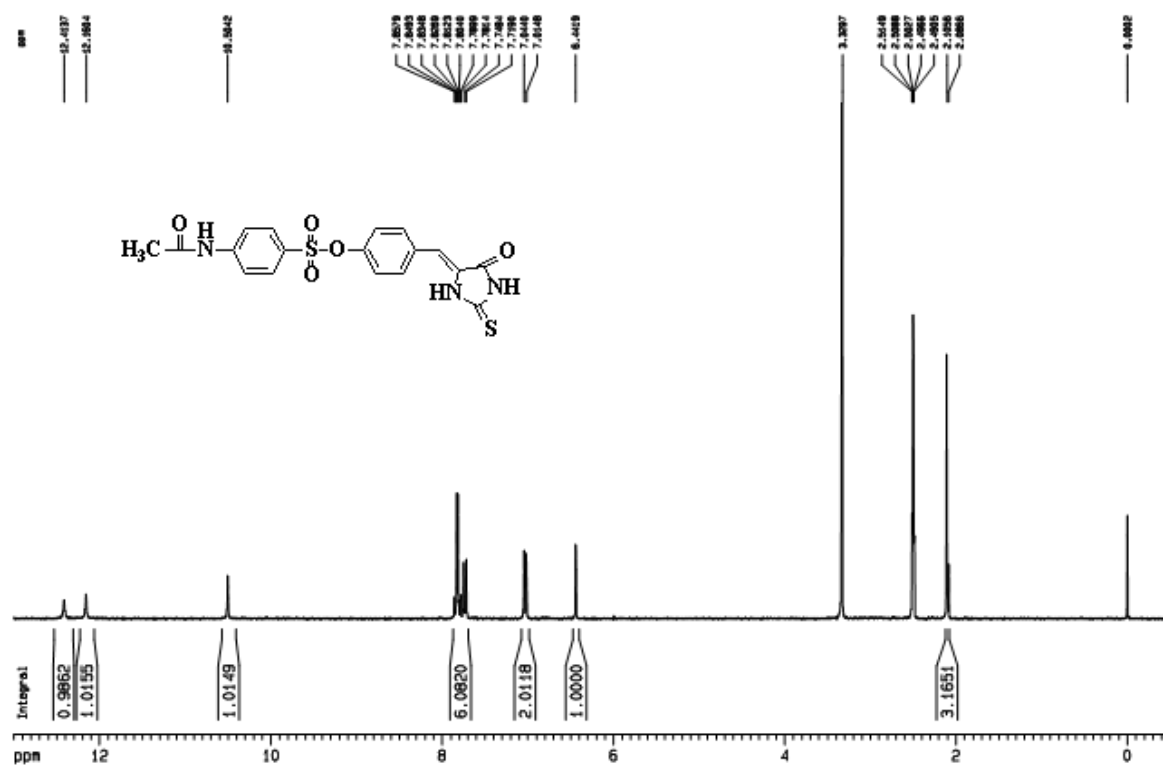


Figure S1. Cont.

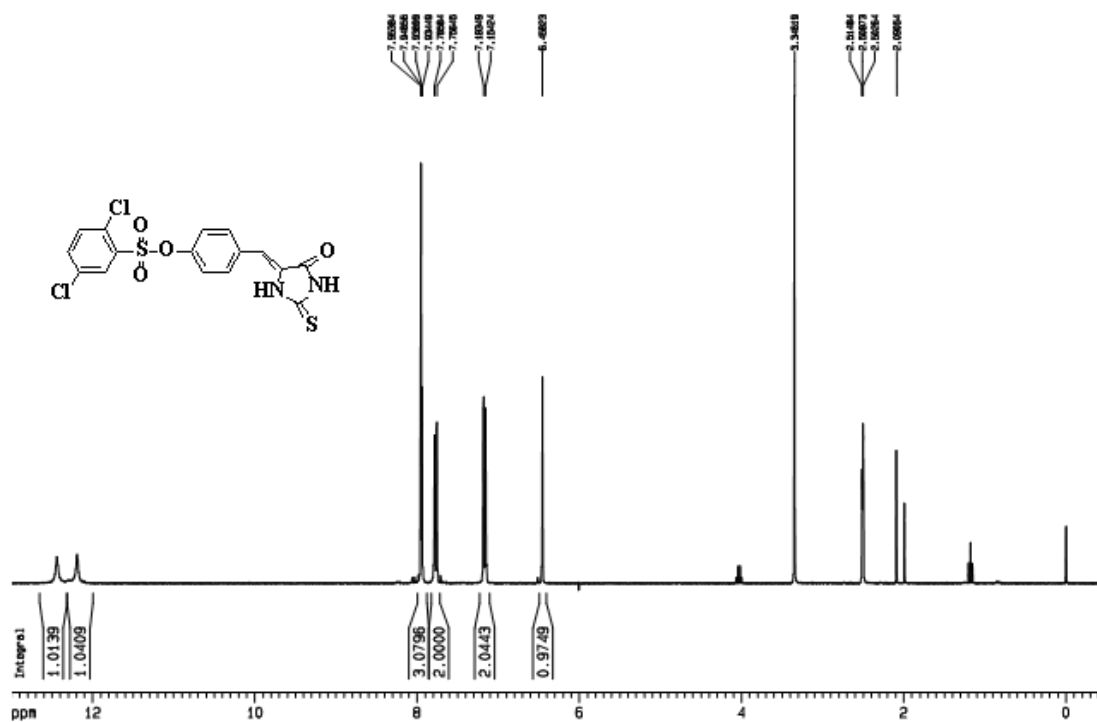
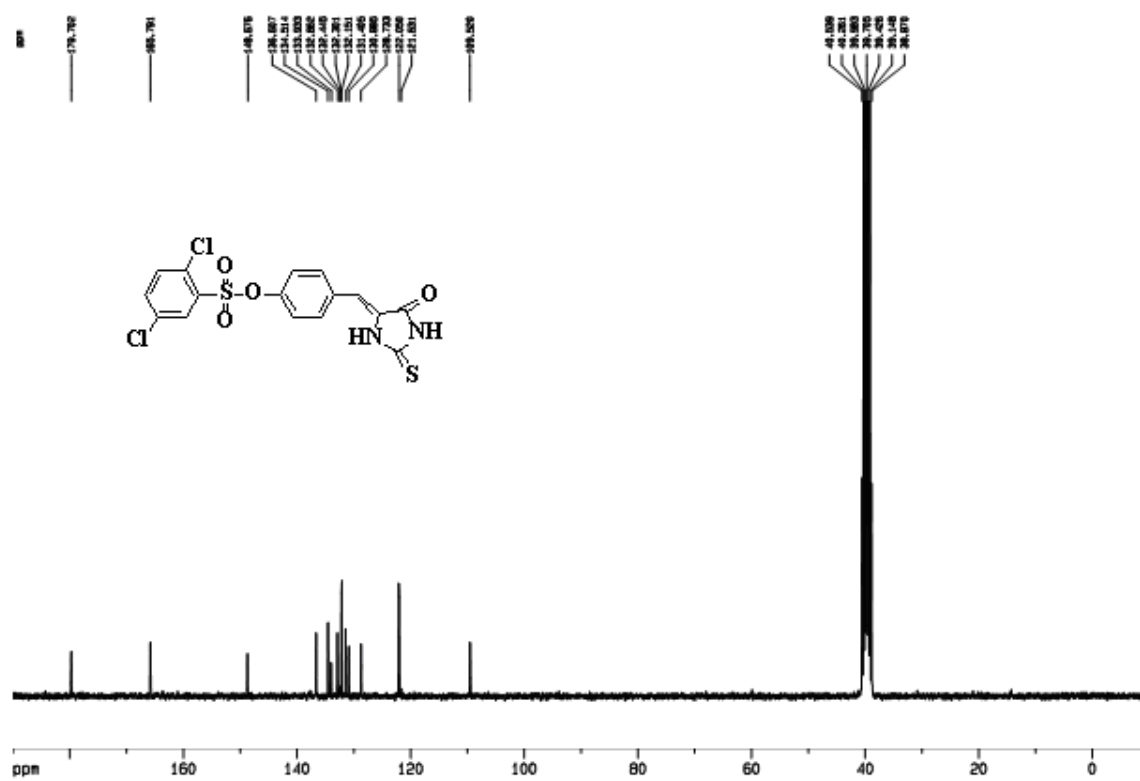
 ^1H NMR of 2m ^{13}C NMR of 2m

Figure S1. Cont.

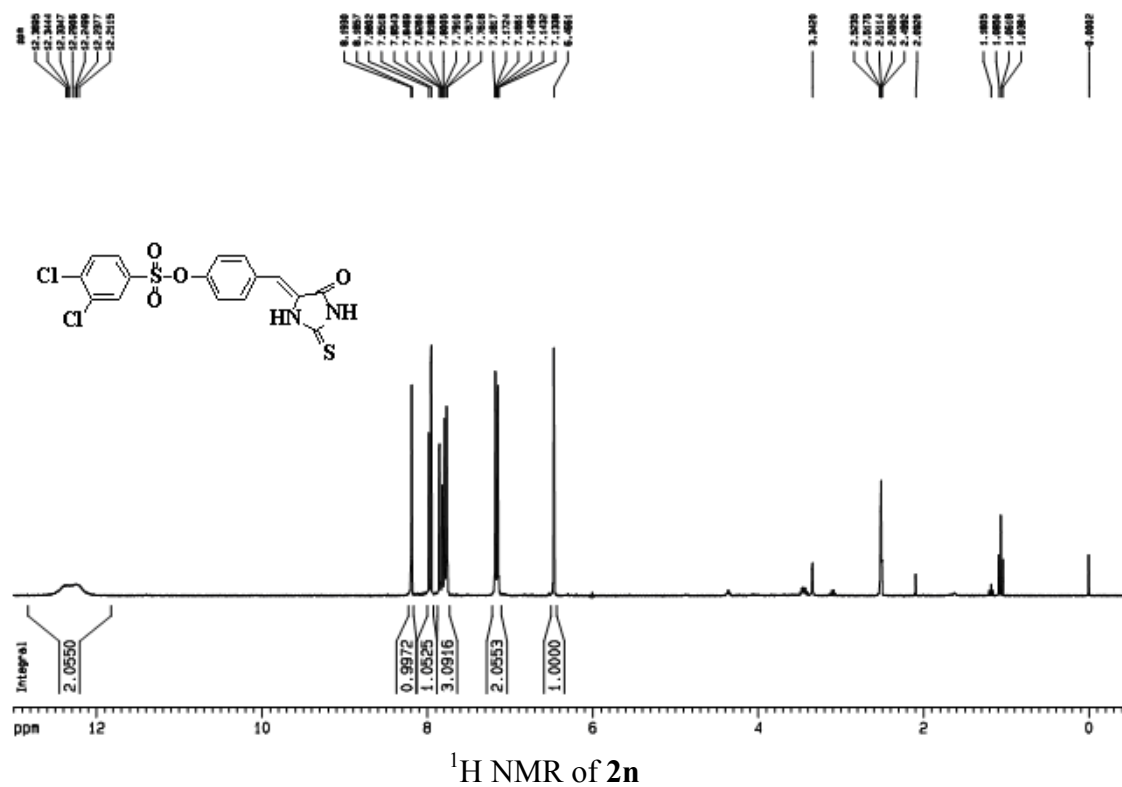
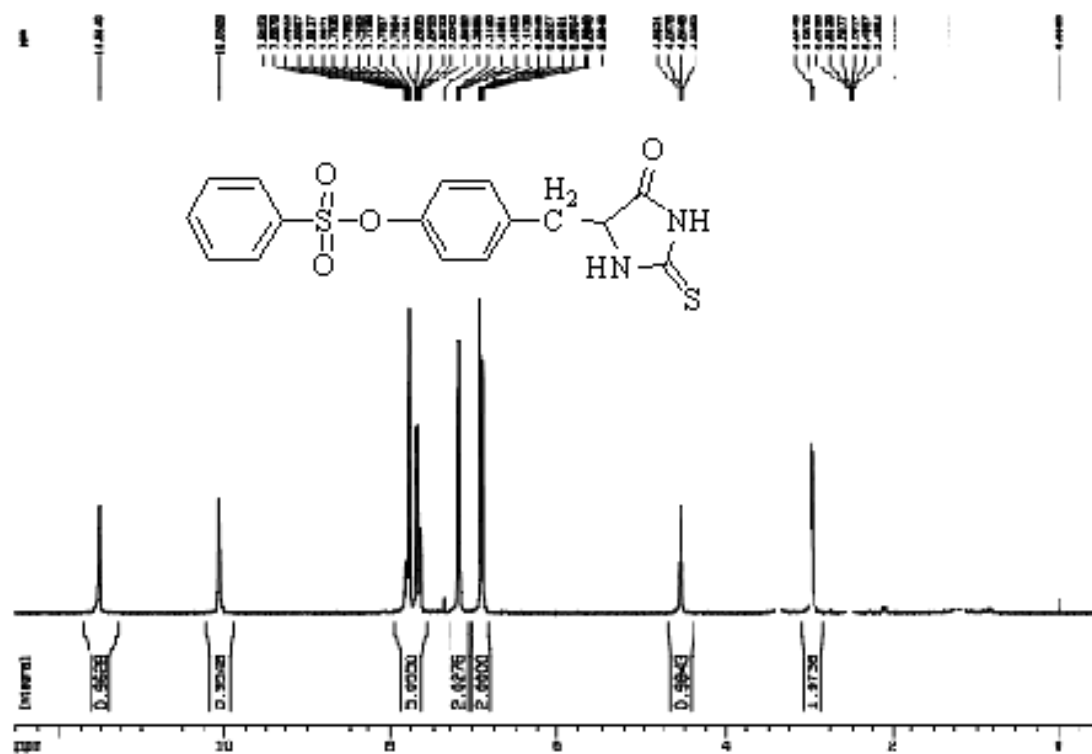
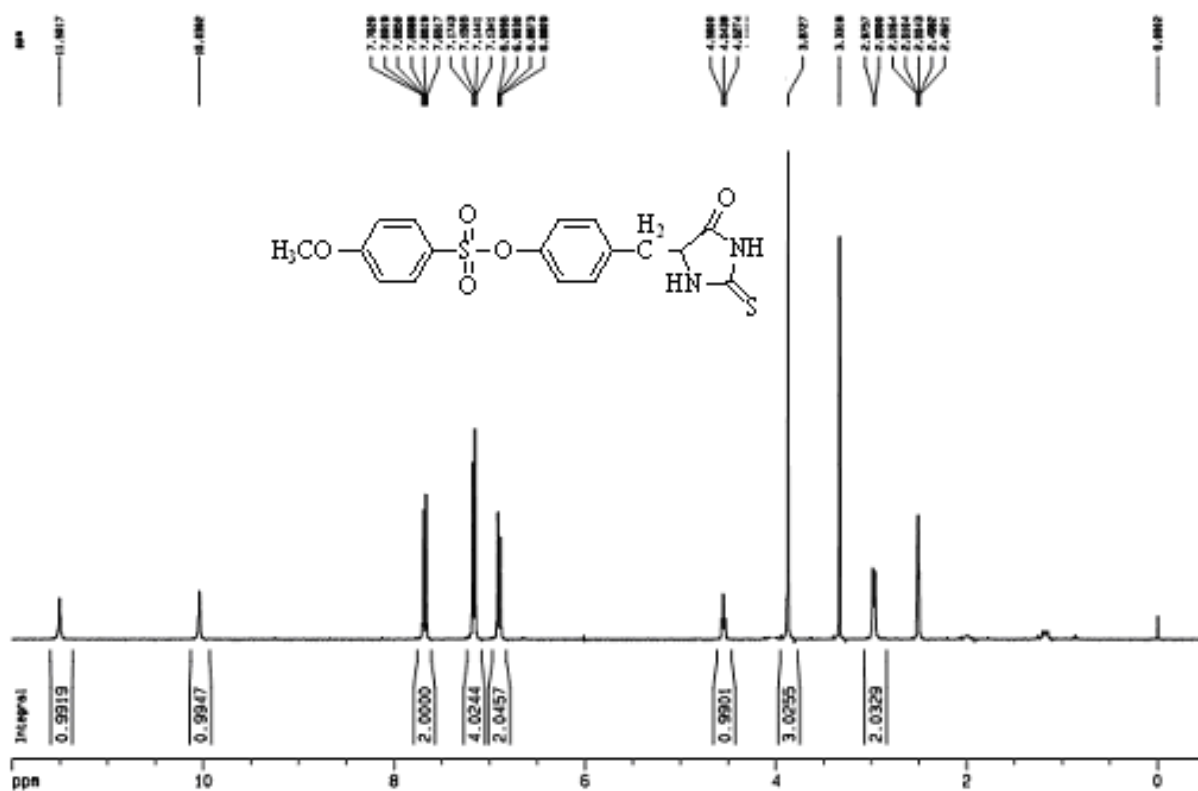


Figure S1. Cont.

¹H NMR of **3a**¹H NMR of **3d**

¹H NMR spectrum of compound **3g** in CDCl₃. The spectrum shows peaks at 11.505, 10.412, 7.353-7.395, 6.357-6.379, 4.534-4.537, 3.345, 2.517-2.519, and 0.000 ppm. The chemical structure of **3g** is shown above the spectrum: Br-C₆H₄-SO₂-O-C₆H₄-CH₂-C(=O)-NH-C(=S)-NH₂. Integration values are provided for each peak group: 1.0012, 0.9905, 4.0357, 2.0203, 2.0067, 1.0000, 2.0394, and 0.0000.

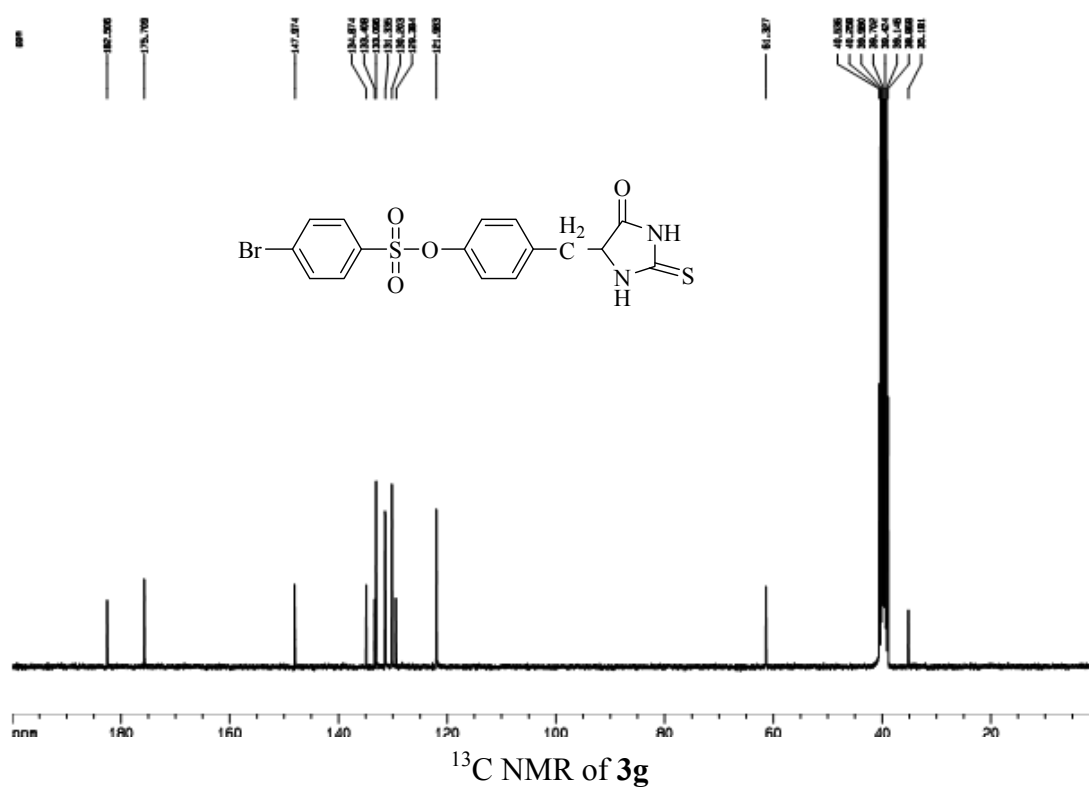


Figure S1. Cont.

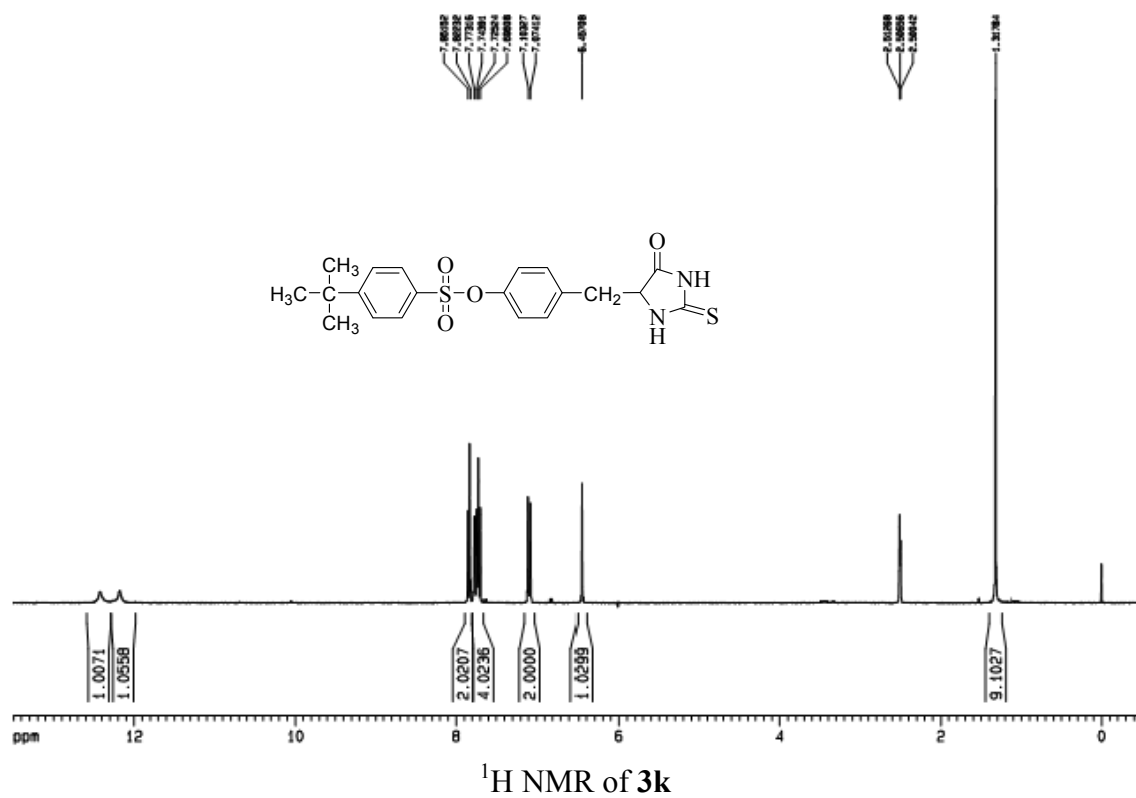


Figure S2. X-ray structure and parameters of **2k**. (a) X-ray structure of **2k**; (b) The packing diagram in the unit cell of **2k**.

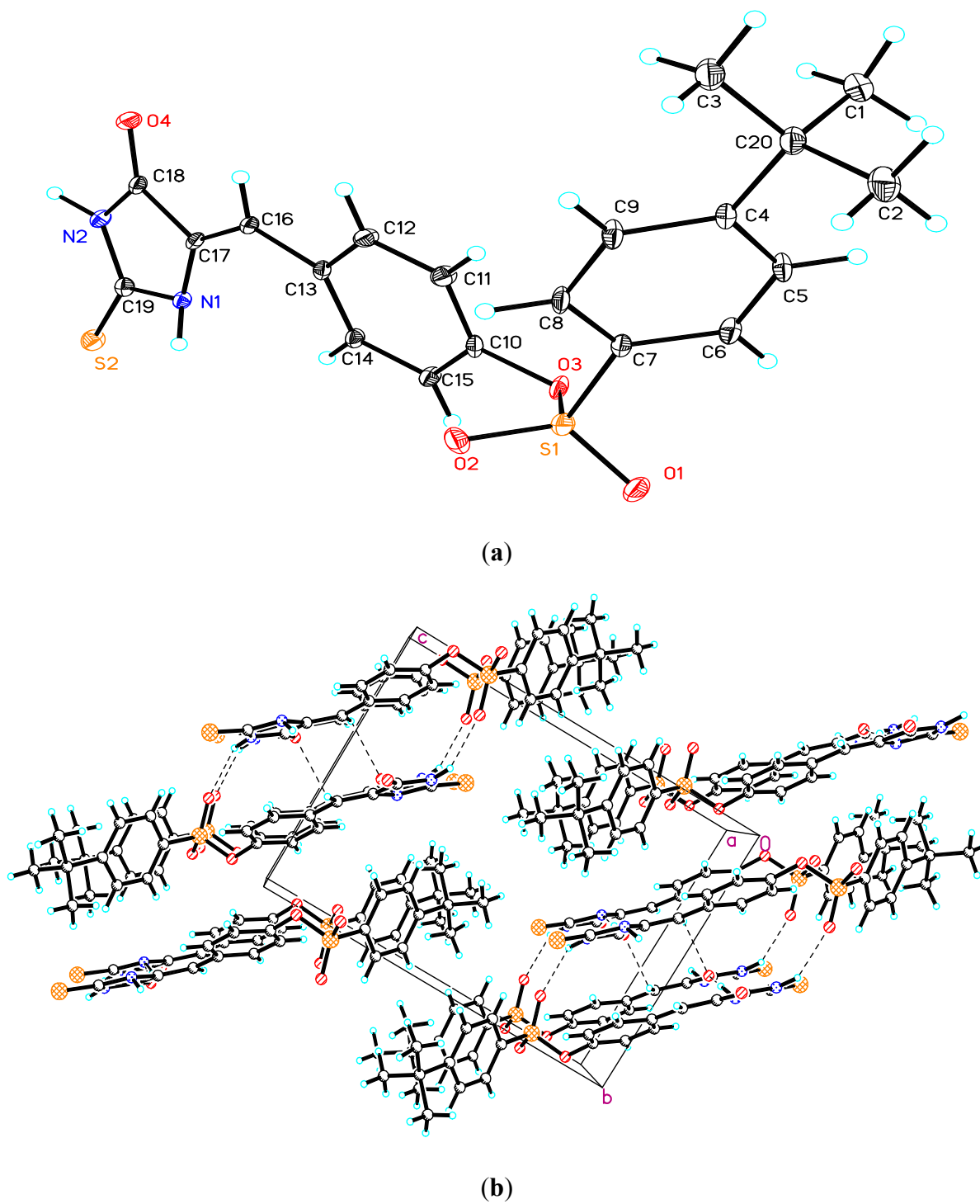


Table S1. Crystal data and structure refinement for **2k**.

Cell parameters	Data
Identification code	2k
Empirical formula	C20 H20 N2 O4 S2
Formula weight	416.50
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 6.1500(12) Å, alpha = 88.33(3) deg.; b = 10.860(2) Å, beta = 88.53(3) deg.; c = 14.610(3) Å, gamma = 81.81(3) deg.
Volume	965.2(3) Å ³
Z, Calculated density	2, 1.433 mg/m ³
Absorption coefficient	0.306 mm ⁻¹
F(000)	436
Crystal size	0.12 × 0.10 × 0.08 mm
Theta range for data collection	1.90 to 24.99 deg.
Limiting indices	-7 ≤ h ≤ 7, -12 ≤ k ≤ 9, -17 ≤ l ≤ 15
Reflections collected/unique	4405/2899 [R(int) = 0.0553]
Completeness to theta = 24.99	85.3%
Absorption correction	None
Max. and min. transmission	0.9760 and 0.9642
Refinement method	Full-matrix least-squares on F ²
Data/restraints/parameters	2899/2/262
Goodness-of-fit on F ²	1.001
Final R indices [I > 2sigma(I)]	R1 = 0.0590, wR2 = 0.1194
R indices (all data)	R1 = 0.0943, wR2 = 0.1312
Largest diff. peak and hole	0.349 and -0.303 e.Å ⁻³

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2k**.

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U(eq)</i>
C(1)	4759(8)	13533(5)	3746(3)	79(1)
C(2)	7286(9)	13316(5)	5052(3)	82(2)
C(3)	4666(9)	11786(5)	4852(3)	83(2)
C(4)	7952(7)	11833(4)	3782(2)	48(1)
C(5)	9218(7)	12445(4)	3157(3)	57(1)
C(6)	10866(7)	11810(4)	2618(3)	54(1)
C(7)	11243(6)	10534(4)	2710(2)	44(1)
C(8)	10042(7)	9907(4)	3318(3)	57(1)
C(9)	8405(7)	10565(4)	3850(3)	58(1)
C(10)	11434(7)	8894(4)	699(2)	47(1)
C(11)	9448(6)	8669(4)	1058(2)	51(1)
C(12)	8371(6)	7795(4)	669(2)	48(1)
C(13)	9285(6)	7135(3)	-92(2)	41(1)
C(14)	11297(6)	7382(4)	-442(3)	46(1)
C(15)	12381(6)	8267(4)	-63(2)	46(1)
C(16)	7953(6)	6276(3)	-477(2)	41(1)
C(17)	8397(6)	5457(3)	-1153(2)	39(1)
C(18)	6660(6)	4781(4)	-1489(2)	44(1)
C(19)	9820(6)	4228(4)	-2311(2)	47(1)
C(20)	6167(7)	12602(4)	4363(3)	58(1)
N(1)	10218(4)	5072(3)	-1698(2)	41(1)
N(2)	7660(5)	4085(3)	-2181(2)	49(1)
O(1)	15139(5)	10459(3)	1997(2)	72(1)
O(2)	13780(5)	8470(3)	2345(2)	65(1)
O(3)	12550(4)	9825(2)	1038(2)	52(1)
O(4)	4722(4)	4852(3)	-1227(2)	60(1)
S(1)	13396(2)	9739(1)	2052(1)	53(1)
S(2)	11564(2)	3526(1)	-3056(1)	64(1)

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

Table S3. Bond lengths [Å] and angles [deg] for 2k.

Bond or angle		Bond or angle		Bond or angle	
C(1)–C(20)	1.524(6)	C(6)–C(7)	1.376(5)	C(14)–H(14)	0.9300
C(1)–H(1A)	0.9600	C(6)–H(6)	0.9300	C(15)–H(15)	0.9300
C(1)–H(1B)	0.9600	C(7)–C(8)	1.368(5)	C(16)–C(17)	1.346(5)
C(1)–H(1C)	0.9600	C(7)–S(1)	1.755(4)	C(16)–H(16)	0.9300
C(2)–C(20)	1.524(6)	C(8)–C(9)	1.384(6)	C(17)–N(1)	1.380(4)
C(2)–H(2A)	0.9600	C(8)–H(8)	0.9300	C(17)–C(18)	1.481(5)
C(2)–H(2B)	0.9600	C(9)–H(9)	0.9300	C(18)–O(4)	1.236(4)
C(2)–H(2C)	0.9600	C(10)–C(11)	1.368(5)	C(18)–N(2)	1.361(5)
C(3)–C(20)	1.520(6)	C(10)–C(15)	1.393(5)	C(19)–N(1)	1.352(5)
C(3)–H(3A)	0.9600	C(10)–O(3)	1.408(4)	C(19)–N(2)	1.367(5)
C(3)–H(3B)	0.9600	C(11)–C(12)	1.376(5)	C(19)–S(2)	1.634(4)
C(3)–H(3C)	0.9600	C(11)–H(11)	0.9300	N(1)–H(1N)	0.9700(4)
C(4)–C(9)	1.367(5)	C(12)–C(13)	1.402(5)	N(2)–H(2N)	0.9701(6)
C(4)–C(5)	1.399(6)	C(12)–H(12)	0.9300	O(1)–S(1)	1.413(3)
C(4)–C(20)	1.534(5)	C(13)–C(14)	1.385(5)	O(2)–S(1)	1.420(3)
C(5)–C(6)	1.384(5)	C(13)–C(16)	1.459(5)	O(3)–S(1)	1.580(3)
C(5)–H(5)	0.9300	C(14)–C(15)	1.382(5)		
C(20)–C(1)–H(1A)	109.5	C(6)–C(7)–S(1)	117.6(3)	C(16)–C(17)–C(18)	120.5(3)
C(20)–C(1)–H(1B)	109.5	C(7)–C(8)–C(9)	119.6(4)	N(1)–C(17)–C(18)	104.8(3)
H(1A)–C(1)–H(1B)	109.5	C(7)–C(8)–H(8)	120.2	O(4)–C(18)–N(2)	127.3(3)
C(20)–C(1)–H(1C)	109.5	C(9)–C(8)–H(8)	120.2	O(4)–C(18)–C(17)	128.4(3)
H(1A)–C(1)–H(1C)	109.5	C(4)–C(9)–C(8)	121.4(4)	N(2)–C(18)–C(17)	104.3(3)
H(1B)–C(1)–H(1C)	109.5	C(4)–C(9)–H(9)	119.3	N(1)–C(19)–N(2)	105.8(3)
C(20)–C(2)–H(2A)	109.5	C(8)–C(9)–H(9)	119.3	N(1)–C(19)–S(2)	127.0(3)
C(20)–C(2)–H(2B)	109.5	C(11)–C(10)–C(15)	121.3(4)	N(2)–C(19)–S(2)	127.2(3)
H(2A)–C(2)–H(2B)	109.5	C(11)–C(10)–O(3)	122.0(3)	C(3)–C(20)–C(2)	110.5(4)
C(20)–C(2)–H(2C)	109.5	C(15)–C(10)–O(3)	116.6(4)	C(3)–C(20)–C(1)	107.9(4)
H(2A)–C(2)–H(2C)	109.5	C(10)–C(11)–C(12)	119.6(4)	C(2)–C(20)–C(1)	108.7(4)
H(2B)–C(2)–H(2C)	109.5	C(10)–C(11)–H(11)	120.2	C(3)–C(20)–C(4)	111.7(4)
C(20)–C(3)–H(3A)	109.5	C(12)–C(11)–H(11)	120.2	C(2)–C(20)–C(4)	108.4(4)
C(20)–C(3)–H(3B)	109.5	C(11)–C(12)–C(13)	120.7(4)	C(1)–C(20)–C(4)	109.5(3)
H(3A)–C(3)–H(3B)	109.5	C(11)–C(12)–H(12)	119.6	C(19)–N(1)–C(17)	112.1(3)
C(20)–C(3)–H(3C)	109.5	C(13)–C(12)–H(12)	119.6	C(19)–N(1)–H(1N)	122(3)
H(3A)–C(3)–H(3C)	109.5	C(14)–C(13)–C(12)	118.5(3)	C(17)–N(1)–H(1N)	111(2)
H(3B)–C(3)–H(3C)	109.5	C(14)–C(13)–C(16)	125.4(3)	C(18)–N(2)–C(19)	112.9(3)
C(9)–C(4)–C(5)	117.5(4)	C(12)–C(13)–C(16)	116.1(3)	C(18)–N(2)–H(2N)	115(2)
C(9)–C(4)–C(20)	123.3(4)	C(15)–C(14)–C(13)	121.3(3)	C(19)–N(2)–H(2N)	130(2)
C(5)–C(4)–C(20)	119.2(4)	C(15)–C(14)–H(14)	119.4	C(10)–O(3)–S(1)	120.8(3)
C(6)–C(5)–C(4)	122.3(4)	C(13)–C(14)–H(14)	119.4	O(2)–S(1)–O(1)	120.52(19)
C(6)–C(5)–H(5)	118.9	C(14)–C(15)–C(10)	118.6(4)	O(2)–S(1)–O(3)	109.09(15)
C(4)–C(5)–H(5)	118.9	C(14)–C(15)–H(15)	120.7	O(1)–S(1)–O(3)	102.50(18)
C(7)–C(6)–C(5)	117.9(4)	C(10)–C(15)–H(15)	120.7	O(2)–S(1)–C(7)	109.69(19)
C(7)–C(6)–H(6)	121.1	C(17)–C(16)–C(13)	130.9(3)	O(1)–S(1)–C(7)	108.52(18)
C(5)–C(6)–H(6)	121.1	C(17)–C(16)–H(16)	114.5	O(3)–S(1)–C(7)	105.35(16)
C(6)–C(5)–C(4)	122.3(4)	C(13)–C(14)–H(14)	119.4	O(2)–S(1)–O(1)	120.52(19)
C(8)–C(7)–C(6)	121.3(4)	C(13)–C(16)–H(16)	114.5		
C(8)–C(7)–S(1)	121.0(3)	C(16)–C(17)–N(1)	134.7(3)		