Electronic Supplementary Information:

The Effect of Chalcogen Substitution on the Structure and Spectroscopy of 4,7-Dimethyl-2*H*-chromen-2-one/thione Analogues

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Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for 4,7-dimethyl-chromen-2-thione. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
C(1)	7925(2)	0	538(2)	67(1)
C(2)	9136(2)	0	1307(2)	69(1)
C(3)	9276(2)	0	2324(2)	67(1)
C(4)	8157(2)	0	2668(2)	63(1)
C(5)	8139(3)	0	3699(2)	75(1)
C(6)	7025(3)	0	3948(2)	80(1)
C(7)	5858(3)	0	3175(2)	71(1)
C(8)	5848(3)	0	2154(2)	65(1)
C(9)	6983(2)	0	1918(2)	58(1)
C(10)	4636(4)	0	3458(3)	94(1)
C(11)	10569(3)	0	3106(3)	89(1)
O	6884(2)	0	879(1)	65(1)
S(1)	7696(1)	0	-712(1)	101(1)

Table S2. Anisotropic displacement parameters ($Å^2$ x 10^3) for 4,7-dimethyl-chromen-2-thione. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	51(1)	81(2)	70(2)	0	22(1)	0
C(2)	51(1)	77(2)	79(2)	0	19(1)	0
C(3)	55(1)	66(2)	74(2)	0	10(1)	0
C(4)	61(1)	57(1)	65(2)	0	10(1)	0
C(5)	75(2)	83(2)	60(2)	0	7(1)	0
C(6)	95(2)	87(2)	60(2)	0	25(2)	0
C(7)	78(2)	74(2)	66(2)	0	30(1)	0
C(8)	61(1)	70(2)	66(2)	0	21(1)	0
C(9)	57(1)	58(1)	60(1)	0	17(1)	0
C(10)	95(2)	119(3)	81(2)	0	48(2)	0
C(11)	58(2)	109(3)	88(2)	0	2(2)	0
O	50(1)	87(1)	59(1)	0	17(1)	0
S(1)	63(1)	176(1)	67(1)	0	25(1)	0

Table S3. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for 4,7-dimethyl-chromen-2-thione.

Atom	x	y	z	U(eq)
H(2)	9820(20)	0	1010(30)	84(10)
H(5)	8920(20)	0	4240(20)	104(12)
H(6)	7040(40)	0	4660(12)	91(11)
H(8)	5088(19)	0	1579(17)	75(9)
H(10A)	3890(40)	0	2880(40)	190(30)
H(10B)	4580(40)	1120(7)	3860(17)	147(13)
H(11A)	11190(40)	0	2740(30)	128(16)
H(11B)	10680(30)	1110(30)	3545(19)	116(10)

Table S4. Analysis of Short Intermolecular Contacts for **1** and **2** [Å and °]

Donor --- H....Acceptor	**d(D – H)**	**d(H...A)**	**d(D...A)**	**∠(D - H...A)**	**Symmetry**	**Label Fig. 4**
Compound **1**						
C(2) --H(2A) ..O(2)	0.93	2.50	3.4044(7)	165	-x,1-y,-z	1
C(11) --H(11A) ..O(2)	0,96	2,61	3,525	160	1-x,2-y,1-z	2
C(10) --H(10C) ..O(2)	0,96	2,71	3,4634	135	x,y-1,z	3
Compound **2**						
C(2) --H(2) ..S(1)	0.98	2.87	3.8169(3)	165	2-x,y,-z	1
C(8) --H(8) ..S(1)	0.94	2.96	3.8230	152	-x+1,+y,-z	2

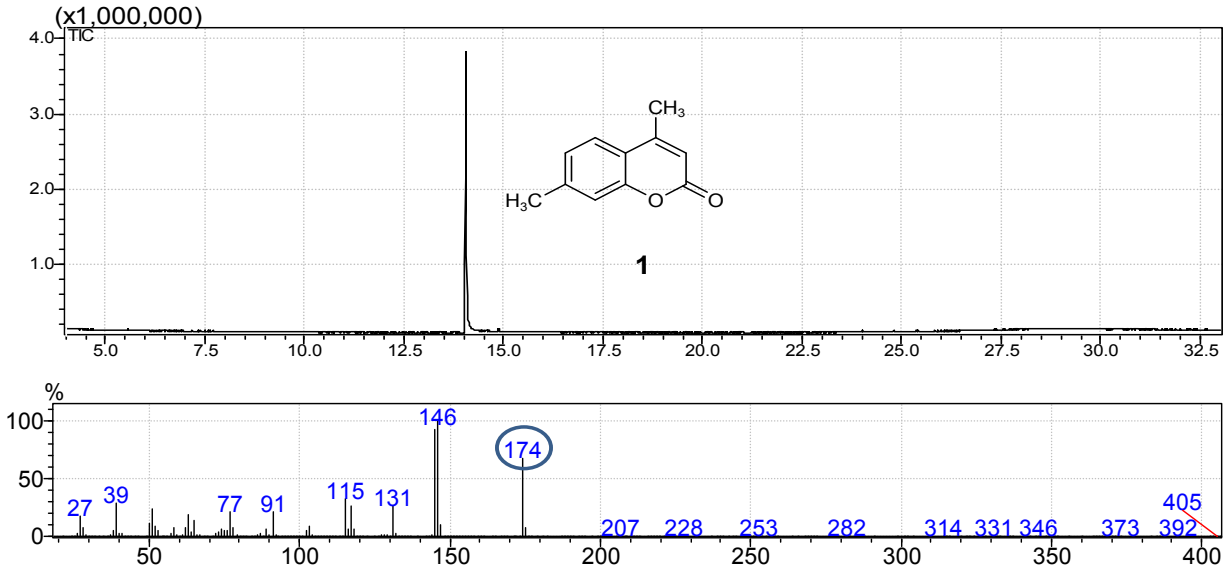

Figure S1. CG/MS Chromatografy for 4,7-Dimethyl-2H-chromen-2-one (**1**).

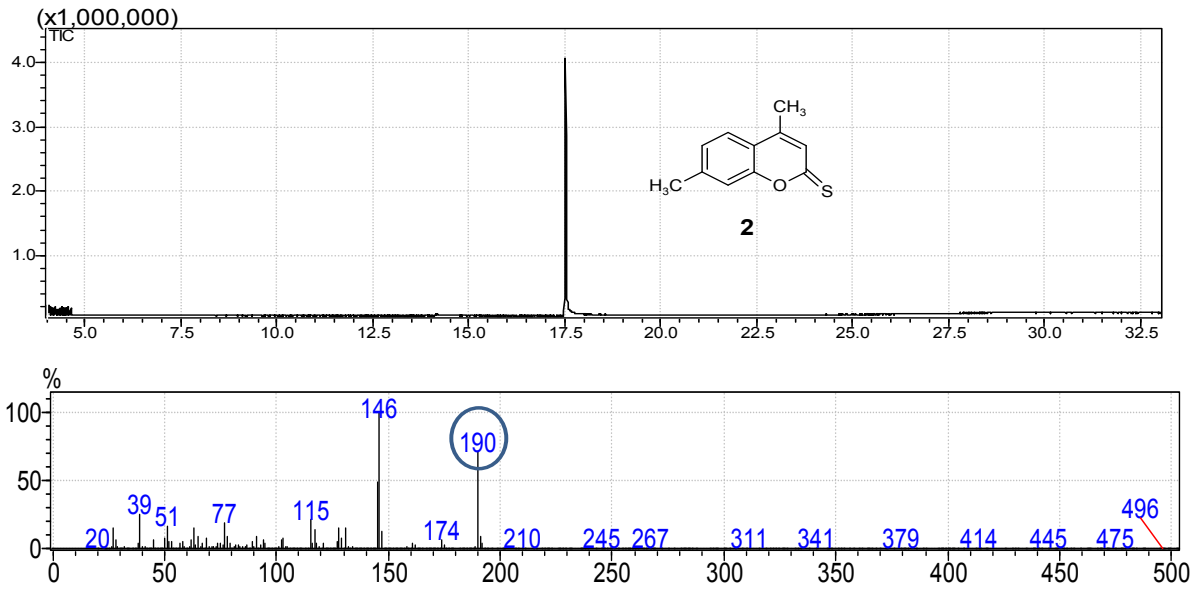

Figure S2. CG/MS Chromatografy for 4,7-Dimethyl-2H-chromen-2-thione (**2**).

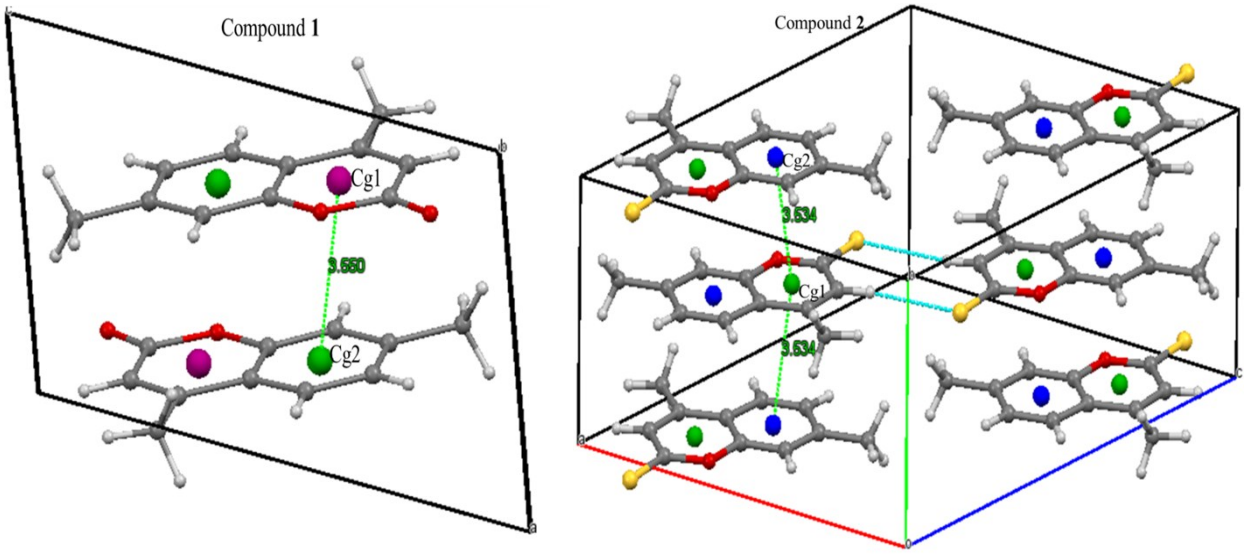

Figure S3. A view of the π-π stacking interactions showing *C*g1···*C*g2 contacts, for compounds **1** and **2**.

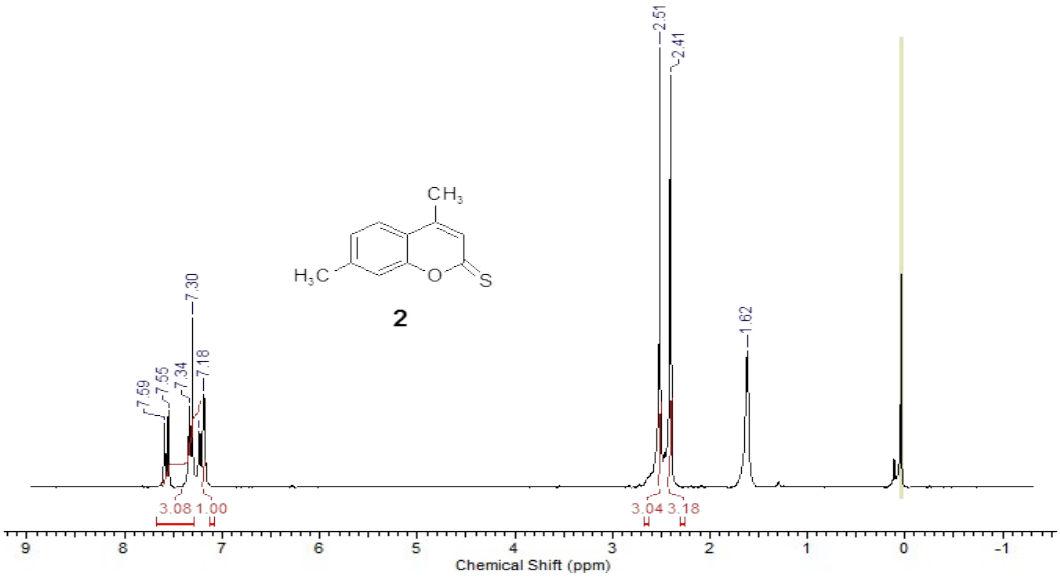

Figure S4. ^{1}H NMR spectrum for 4,7-Dimethyl-2*H*-chromen-2-thione (**2**).

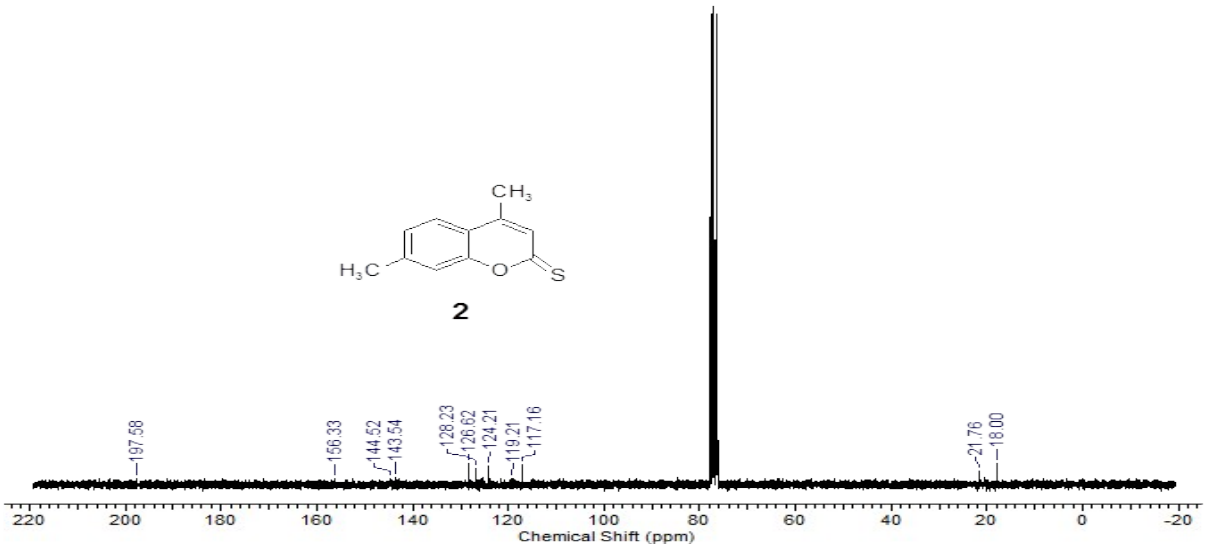

Figure S5. ^{13}C NMR spectrum for 4,7-Dimethyl-2*H*-chromen-2-thione (**2**).

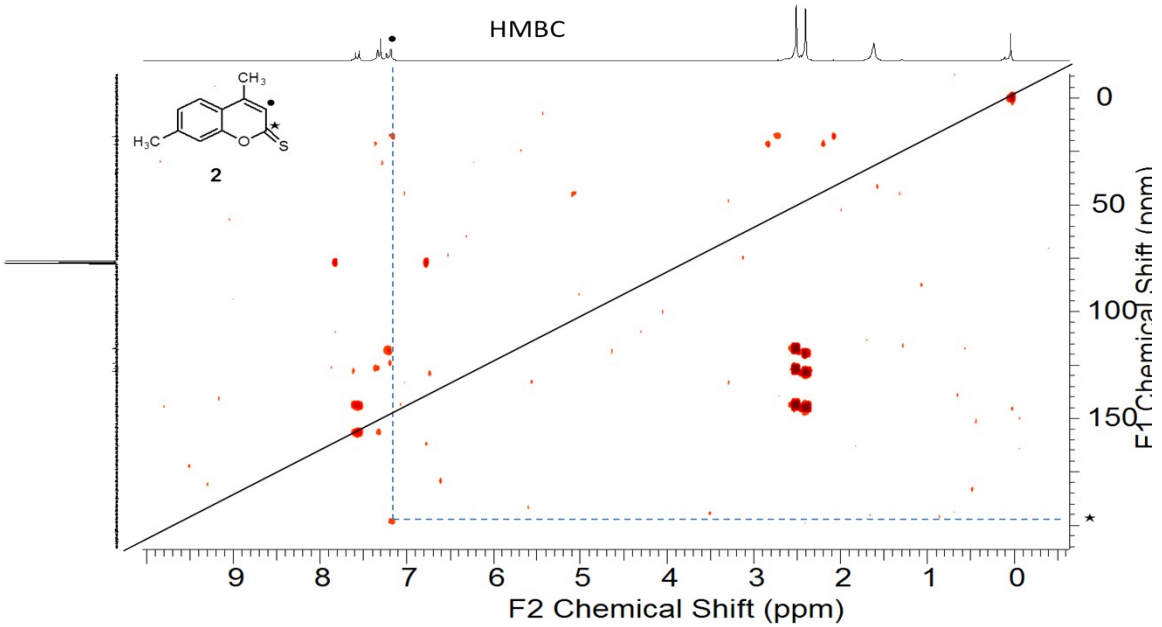

Figure S6. HMBC 2D-NMR spectrum for 4,7-Dimethyl-2*H*-chromen-2-thione (**2**).

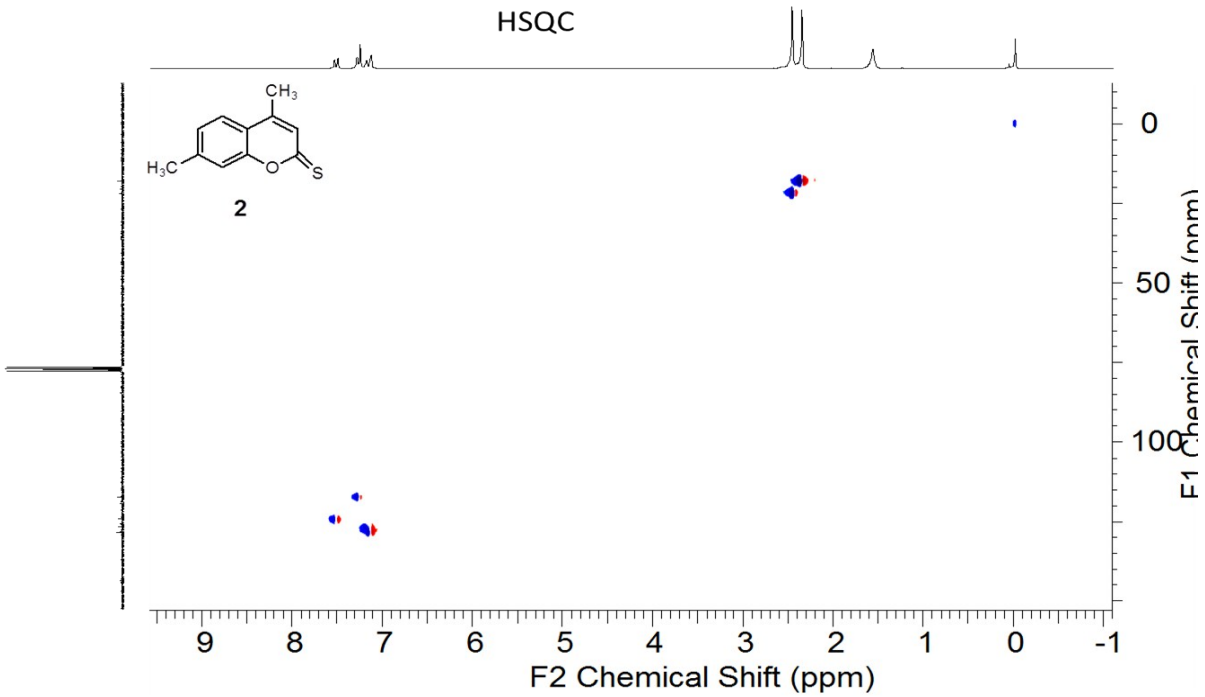

Figure S7. HSQC 2D-NMR Spectrum for 4,7-Dimethyl-2*H*-chromen-2-thione (**2**).