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Supplementary Material

Aggregation of hydrogen bonded dimeric triorganotin amino substituted pyrimidine-2-thiolates

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Table S1. ^{1}H NMR for the studied compounds.

compound	Thiol skeleton			Organotin skeleton			
	NH_2	**H5**	**H6**	**1***	**2***	**3***	**4***
1a	6.05 br	6.65	7.73	0.45 (60.3)	-	-	-
1b	5.96 br	6.56	7.62	1.68 – 0.89 m (27H)			
1c	6.01 br	6.75	7.68	-	7.89 -7.41 m (15H)		
2a	5.93 br	5.24		0.51 (63.6)	-	-	-
2b	5.84 br	5.13		1.60 – 0.85 m (27H)			
2c	5.83 br	5.16		-	7.83 -7.46 m (15H)		

Table S2. ^{13}C NMR for the studied compounds.

compound	Thiol skeleton				Organotin skeleton			
	C2	**C4**	**C5**	**C6**	**α***	**β***	**γ***	**δ***
1a	177.6	163.0	100.3	154.8	- 1.40 (412.5/399.8)	-	-	-
1b	178.9	163.7	101.1	154.8	16.44 (323.0)	27.8 (25.4)	26.9 (62.4)	13.5
1c	177.6	163.0	101.4	154.8	138.4	136.9	128.8	129.2
2a	170.5	163.8	78.9	163.8	- 1.43 (411.4/393.6)	-	-	-
2b	171.1	163.4	78.7	163.4	15.79 (315.8)	28.8 (22.3)	26.8 (62.3)	13.8
2c	169.4	163.3	79.0	163.3	141.82	136.4 (40.5)	128.9	129.3

Table S3. Geometrical parameters (Å,°) of hydrogen bonds in the crystals of **2a** and **2c**

D-H...A	d(D-H)	d(H…A)	d(D-A)	<(D-H…A)
2a				
N4-H1N4···N3^{i}	0.89	2.13	3.022(3)	175
N4-H2N4···S1^{ii}	0.89	2.81	3.491(2)	134
N6-H1N6···S1^{iii}	0.89	2.72	3.535(2)	154
2c				
N4-H1N4···N3^{iv}	0.84	2.36	3.201(3)	179
N4-H2N4···Cg1^{v}	0.84	2.69	3.505(4)	163
N6-H1N6···Cg2^{v}	0.84	3.00	3.792(5)	158

(symmetry codes: (i) -x-1, -y+1, -z+1; (ii) x-1, y, z; (iii) x, -y+1/2, z+1/2; (iv) -x+2, -y+1, -z+1; (v) x, -y+1/2, z+1/2. Cg1 and Cg2 are the centroid of the C7-C12 and C19-C24 rings, respectively.