In situ generation of functionalized 1,2,4-triazole-5-thiones containing pyridine or pyrazine moieties and their coordination to Hg^{II}

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Table S1. Selected bond lengths and angles for compounds **1**, **2** and ligands in complexes listed.

	HMPytat (**1**)	HMPztat (**2**)	$[Hg(HMPytat)_2Br_2].H_2O$ (**4a**)			
Bond lengths [Å]						
S(1)-C(17)	1.679(3)	1.6819(18)	1.732(18)	1.717(19)	1.70(2)	1.703(19)
N(13)-C(17)	1.336(4)	1.334(2)	1.34(2)	1.30(2)	1.31(2)	1.32(2)
N(14)-C(17)	1.387(3)	1.372(2)	1.36(2)	1.35(2)	1.37(2)	1.36(2)
N(12)-N(13)	1.370(3)	1.365(2)	1.36(2)	1.345(19)	1.39(2)	1.38(2)
Angles [º]						
N(13)-C(17)-N(14)	104.4(2)	103.96(15)	108.0(15)	105.3(16)	105.3(16)	105.4(16)
N(13-C(17)-S(1)	128.3(2)	128.13(14)	125.3(14)	127.2(16)	126.8(14)	126.4(14)
N(14)-(C17)-S(1)	127.2(2)	127.91(14)	126.7(15)	127.2(15)	127.8(14)	127.8(14)
C(16)-N(12)-N(13)	104.2(2)	103.82(14)	107.0(16)	105.1(15)	101.8(16)	102.9(15)
C(17)-N(13)-N(12)	113.5(2)	113.67(15)	109(5(15)	113.4(16)	113.7(16)	113.4(15)

	$[\{Hg(EPytat)(HEPytat)Cl_2\}_2Hg]$ (**6a**)		$[Hg(MPytat)_2]_n$ (**3a**)	$[Hg(EPytat)_2]_n$ (**6b**)	$[Hg(MPztat)_2]_n$ (**10a**)		$[Hg(EPztat)_2]_n$ (**11a**)*	
Bond lengths [Å]								
S(1)-C(17)	1.741(5)	1.704(5)	1.720(5)	1.735(9)	1.745(8)	1.735(8)	1.739(6)	1.739(5)
N(13)-C(17)	1.308(6)	1.324(6)	1.320(8)	1.311(11)	1.306(10)	1.323(11)	1.315(7)	1.314(6)[a]
N(14)-C(17)	1.374(6)	1.368(6)	1.354(6)	1.364(12)	1.370(10)	1.370(10)	1.362(7)	1.367(6)[a]
N(12)-N(13)	1.379(5)	1.358(5)	1.379(6)	1.377(11)	1.375(9)	1.381(9)	1.386(7)	1.389(6)
Angles [º]								
N(13)-C(17)-N(14)	109.4(4)	105.3(4)	108.4(4)	108.8(8)	111.4(7)	108.8(6)	110.3(5)	111.1(4)[b]
N(13-C(17)-S(1)	128.0(4)	130.9(4)	124.9(4)	125.4(8)	124.5(6)	127.7(6)	126.0(4)	126.2(4)[b]
N(14)-(C17)-S(1)	122.5(3)	123.8(2)	126.5(5)	125.7(7)	123.9(6)	123.4(6)	123.6(4)	122.7(4)[b]
C(16)-N(12)-N(13)	107.0(4)	104.6(4)	105.3(4)	107.3(8)	107.5(6)	106.6(6)	107.7(5)	107.7(4)
C(17)-N(13)-N(12)	108.5(4)	112.8(4)	109.4(4)	108.5(8)	107.0(6)	108.4(6)	106.6(5)	107.1(4)[a]

*) Symmetry transformations: a) C(27) -x+1/2, y+1/2, -z+3/2; b) N(23), N(24) -x+1/2, y-1/2, -z+3/2

Table S2. Non classical hydrogen bond parameters [Å, º] for compounds **1**,**2** and complexes. The letters in superscript refer to the symmetry codes shown in the text and figures.

Compound	D–H···A	D–H	H···A	D···A	∠DHA	Symmetry code
1	C18-H18C···S1	1.04	2.69	3.196(3)	110.2	
2	C11-H11···N16[b]	0.93	2.72	3.449(3)	135.7	x+1/2, -y+1/2, z+1/2
	C12-H12···S1[c]	0.93	3.120	3.926(2)	149.4	-x+3/1, y-1/2, -z+1/2
3a	C1-H1···S1[d]	0.93	3.02	3.664(6)	127.4	x+1/2, -y+1/2, z+1/2
	C2-H2···S1[d]	0.93	2.94	3.602(6)	129.1	x+1/2, -y+1/2, z+1/2
	C8-H8B…S1	0.96	2.71	3.207(6)	111.8	
4a	C11-H11···Br11[a]	0.93	2.98	3.90(2)	174.6	-x+1. –y, -z+1
	C18-H18A···S21[b]	0.96	2.95	3.88(2)	163.4	x-1, y, z
	C18-H18B···N11	0.96	2.53	3.04(2)	113.6	
	C18-H18B···N22[a]	0.96	2.63	3.45(3)	144.1	-x+1. –y, -z+1
	C21-H21···Br21[c]	0.93	3.50	3.82(2)	140.6	x, y-1, z
	C24-H24···Br22[d]	0.93	3.18	3.75(2)	121.5	-x+2, -y, -z+1
	C28-H28B···N21	0.96	2.43	2.94(3)	113.0	
	C31-H31···r21[f]	0.93	3.01	3.92(2)	168.6	-x+2, -y+1, -z
	C32-H32···N21[g]	0.93	2.65	3.56(3)	165.8	-x+2, -y, -z
	C38-H38C···S21	0.96	2.73	3.22(2)	112.2	
	C48-H48B···N41	0.96	2.45	2.91(3)	102.9	
6a	C12-H12···Cl2[b]	0.93	2.93	3.644(6)	134.3	x+1, y, z+1
	C14-H14···N22	0.93	2.65	3.564(7)	166.3	
	C18-H18B···N11	0.97	2.41	2.938(6)	113.9	
	C19-H19A···S2[c]	0.96	3-01	3.849(6)	146.3	-x+1, -y, -z
	C28-H28A···N21	0.97	2.41	2.992(7)	118.0	
6b	C1-H1···S1[d]	0.93	2.82	3.64(1)	148.0	-x+1/2, y-1/2, -z-1/2
	C9-H9A···N1	0.96	2.65	3.25(2)	120.7	
10a	C12-H12···N26[c]	0.95	2.68	3.558(11)	153.8	-x+3/2, y-1/2, z-1/2
	C18-H18A···S1	0.98	2.73	3.229(9)	112.0	
	C18-H18B···N12[b]	0.98	2.58	3.310(11)	131.0	x+1/2, -y+1/2, z
	C18-H18B···N13[b]	0.98	2.57	3.154(11)	117.9	x+1/2, -y+1/2, z
	C18-H18C···N12[d]	0.98	2.44	3.192(11)	133.5	x, y-1, z
	C28-H28A···N24[e]	0.98	2.56	3.309(10)	132.9	x-1/2, -y-1/2, z
	C28-H28B···N21[e]	0.98	2.66	3.418(11)	134.7	x-1/2, -y-1/2, z
	C28-H28C···N22[d]	0.98	2.58	3.487(11)	145.2	x, y-1, z
11a	C12-H12···S2[d]	0.93	2.96	3.593(9)	126.8	x+1/2, -y+3/2, z-1/2
	C18-H18A···N11	0.97	2.48	3.008(11)	114.0	
	C24-H24···S1	0.93	2.97	3.531(6)	120.1	
	C28-H28B···N21[b]	0.97	2.52	3.021(8)	112.1	-x, -y+1, -z+1