STRUCTURAL
CHEMISTRY

Volume 76 (2020)

Supporting information for article:

Synthesis, crystal structure and conformational analysis of an unexpected [1,5]dithiocine product of aminopyridine and thio-vanillin

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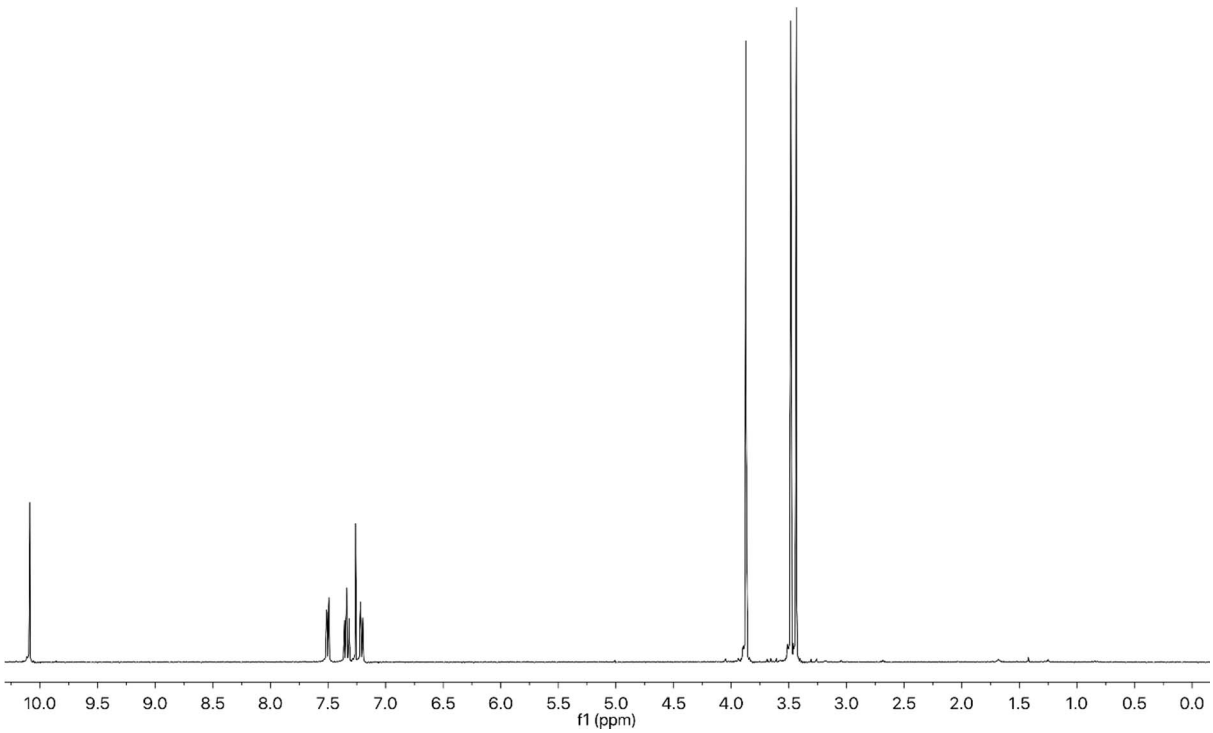

Figure S1 ^{1}H-NMR spectrum of compound O- (2-formyl-6-methoxyphenyl) dimethylcarbamothioate

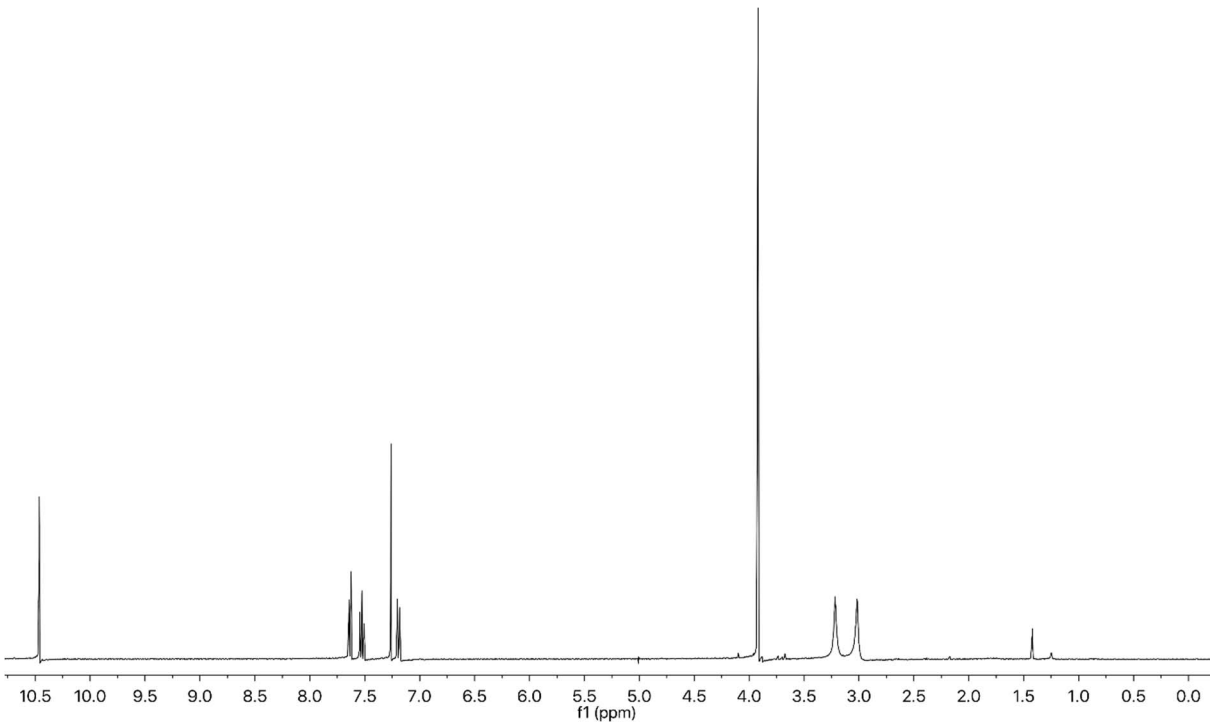

Figure S2 ^{1}H-NMR spectrum of compound S- (2-formyl-6-methoxyphenyl) dimethylcarbamothioate

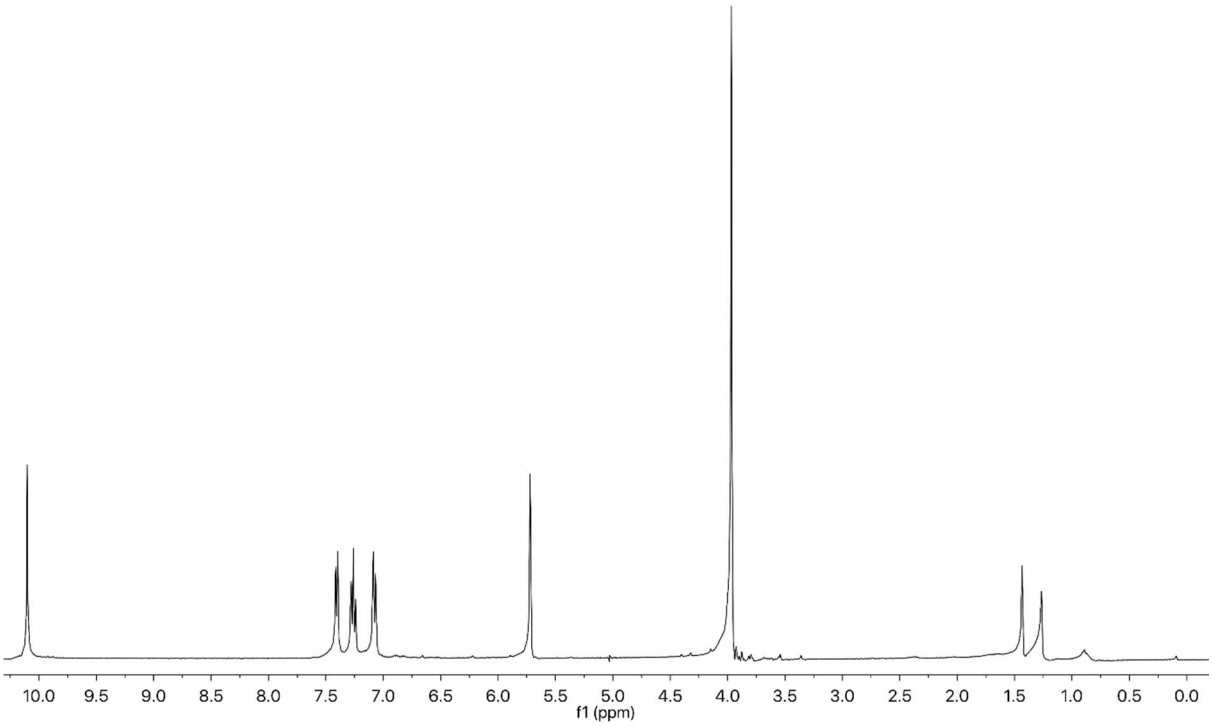

Figure S3 ^{1}H-NMR spectrum of compound 2-mercapto-3-methoxybenzaldehyde **2b**

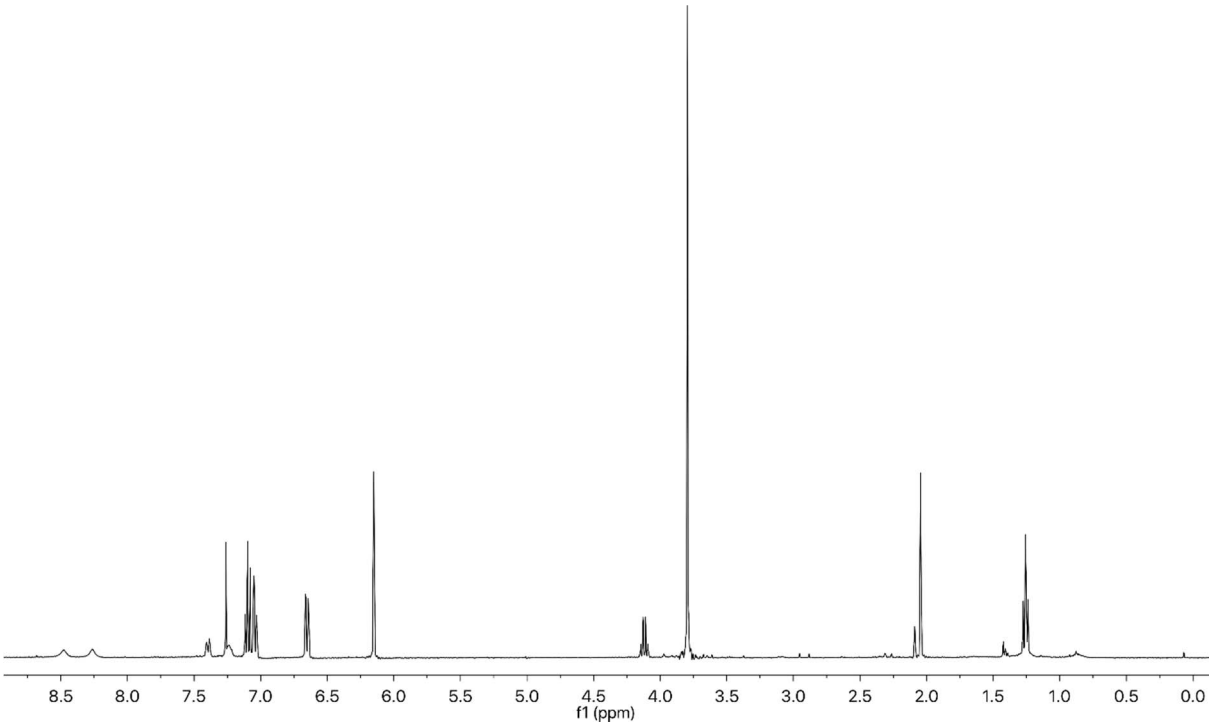

Figure S4 ^{1}H-NMR spectrum of compound 4,10-dimethoxy-13-(pyridin-3-yl)-6H,12H-6,12-epiminodibenzo[b,f] [1,5]dithiocin **4**

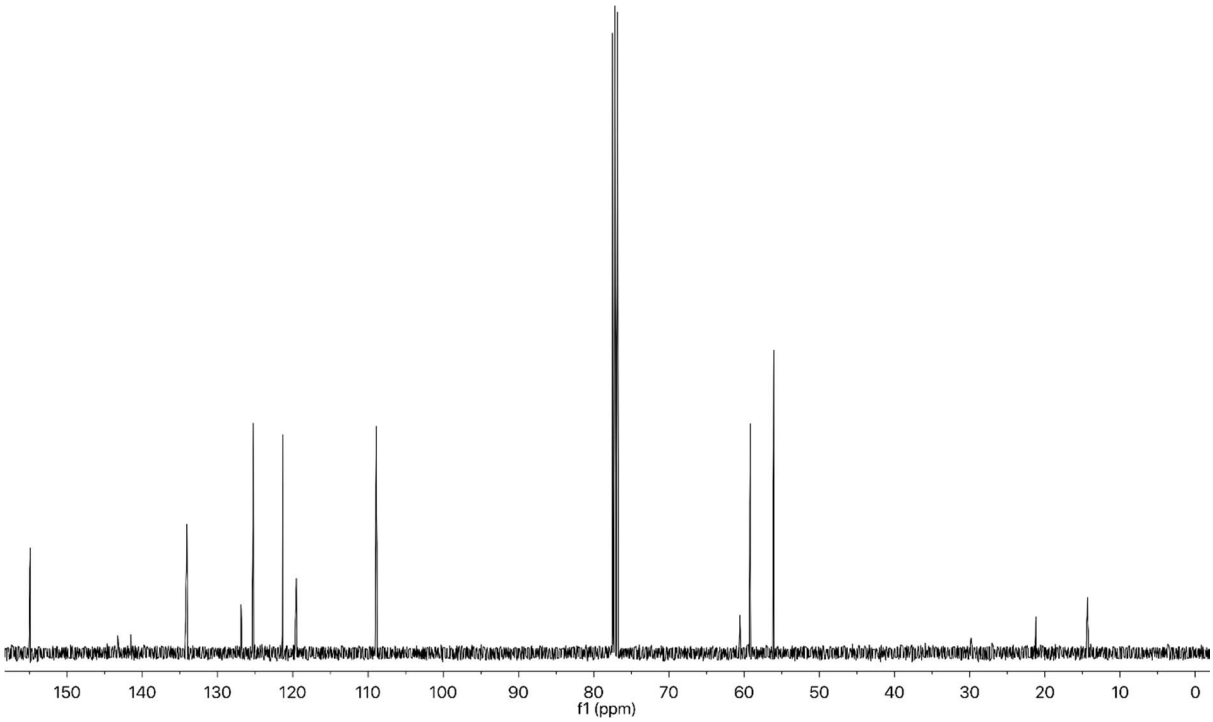

Figure S5 ^{13}C-NMR spectrum of compound 4,10-dimethoxy-13-(pyridin-3-yl)-6H,12H-6,12-epiminodibenzo[b,f] [1,5]dithiocin **4**

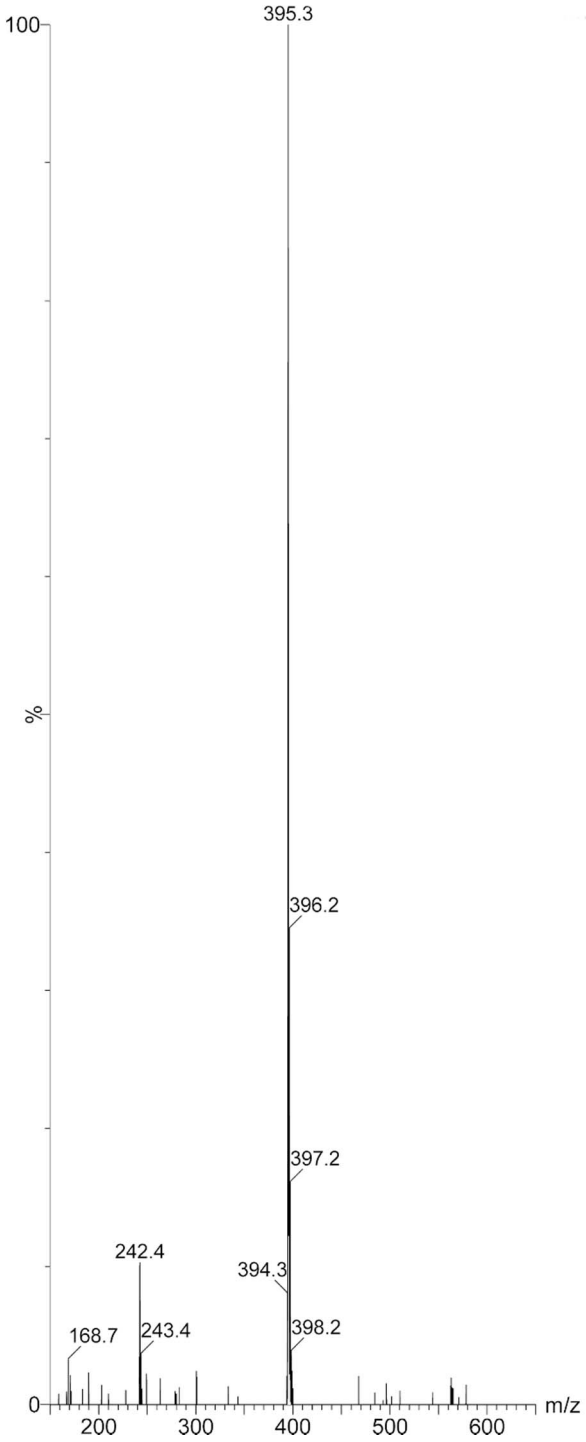

Figure S6 LC-MS spectrum of compound 4,10-dimethoxy-13-(pyridin-3-yl)-6H,12H-6,12-epiminodibenzo[b,f] [1,5]dithiocin **4**

Table S1 Hydrogen-bond geometry (Å, º)

D*—H···*A	***D*—H**	**H···*A***	***D*···*A***	***D*—H···*A***
C28—H28···O9^{i}	0.98	2.41	3.222 (3)	140.3
C29—H29···S2^{ii}	0.98	2.88	3.601 (2)	131.1
C41—H41A···O2^{iii}	0.96	2.51	3.367 (3)	148.1
O10—H10A···N6	0.82	2.11	2.804 (5)	143.0
O9—H9···O10	0.82	1.76	2.569 (5)	166.9

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*, −*y*+1, −*z*+1; (iii) *x*, *y*+1, *z*-1

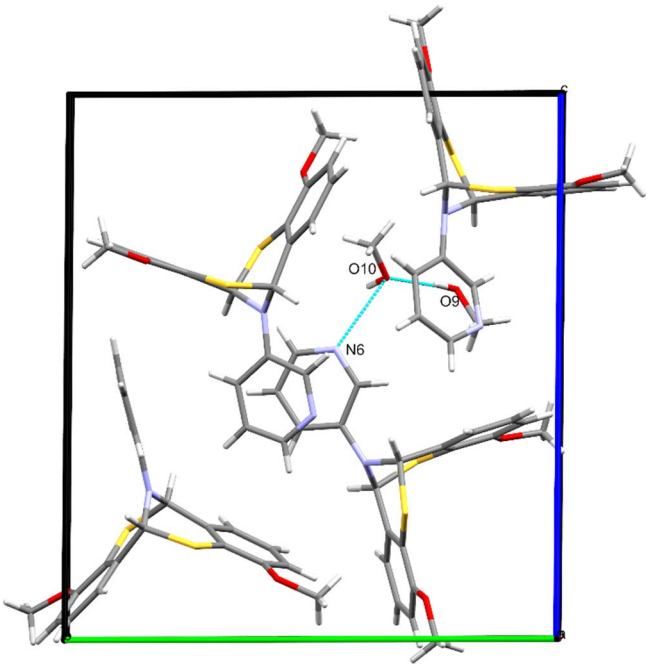

Figure S7 Hydrogen bonds in the asymmetric unit.

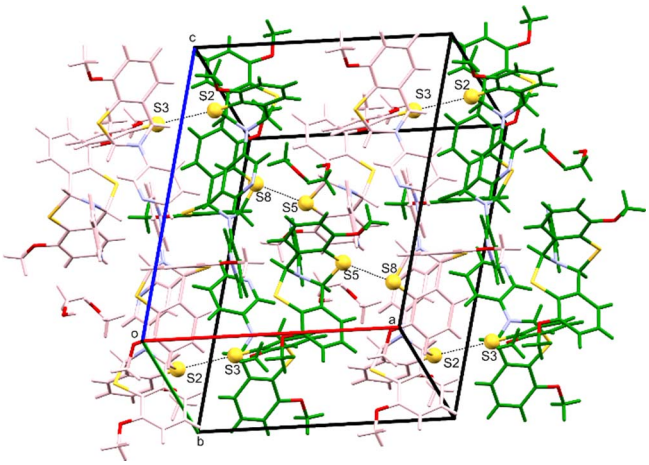

Figure S8 Chalcogen bonds in the structure of four.

Table S2 Occupancy factors of the disordered atoms. * Stands for second component of the disorder.

Atom number	Occupancy factor (ESD)
N_2	0.521 (18)
N_{2A}*	0.479 (18)
N_4	0.570 (2)
N_{4A}*	0.430 (2)
N_6	0.927 (3)
N_{6A}*	0.073 (3)
O_9	0.924 (3)
N_{10}	0.924 (3)

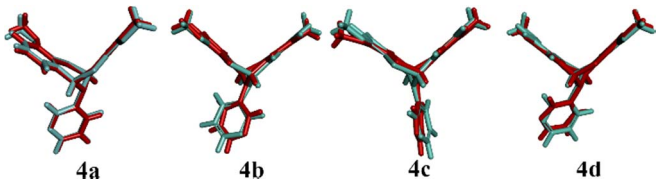

Figure S9 Superposition of crystal structure (red) and the structure after geometry optimisation (blue).

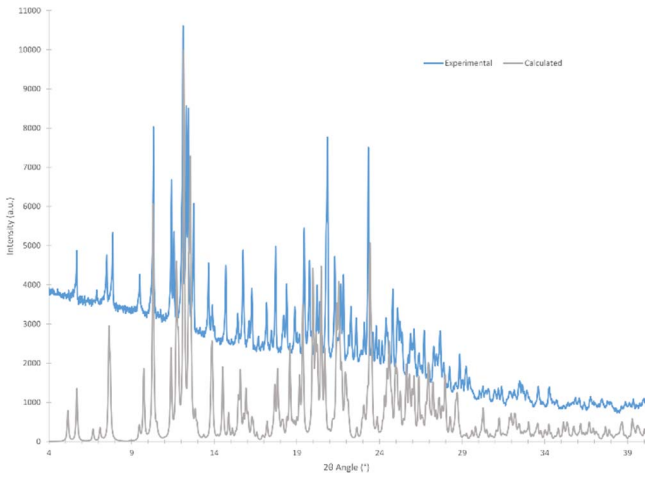

Figure S10 Experimental powder pattern and calculated powder pattern based on the single-crystal structure.