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Supporting information for article:

Copper(II)- and gold(III)-mediated cyclization of a thiourea to a substituted 2-aminobenzothiazole

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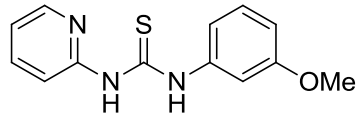
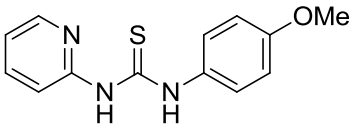
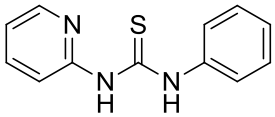
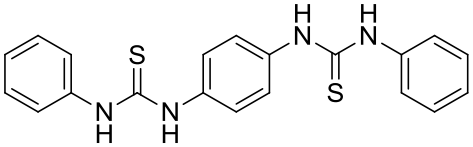
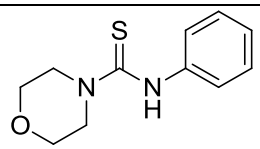
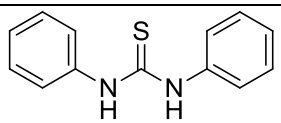
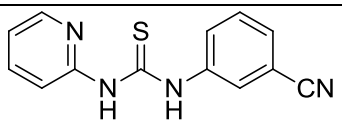
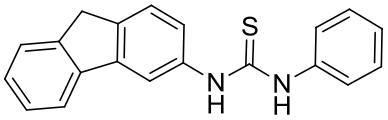
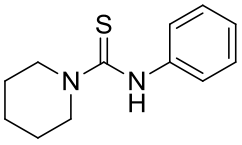
S1. General procedure for the conversion of thiourea to benzothiazole

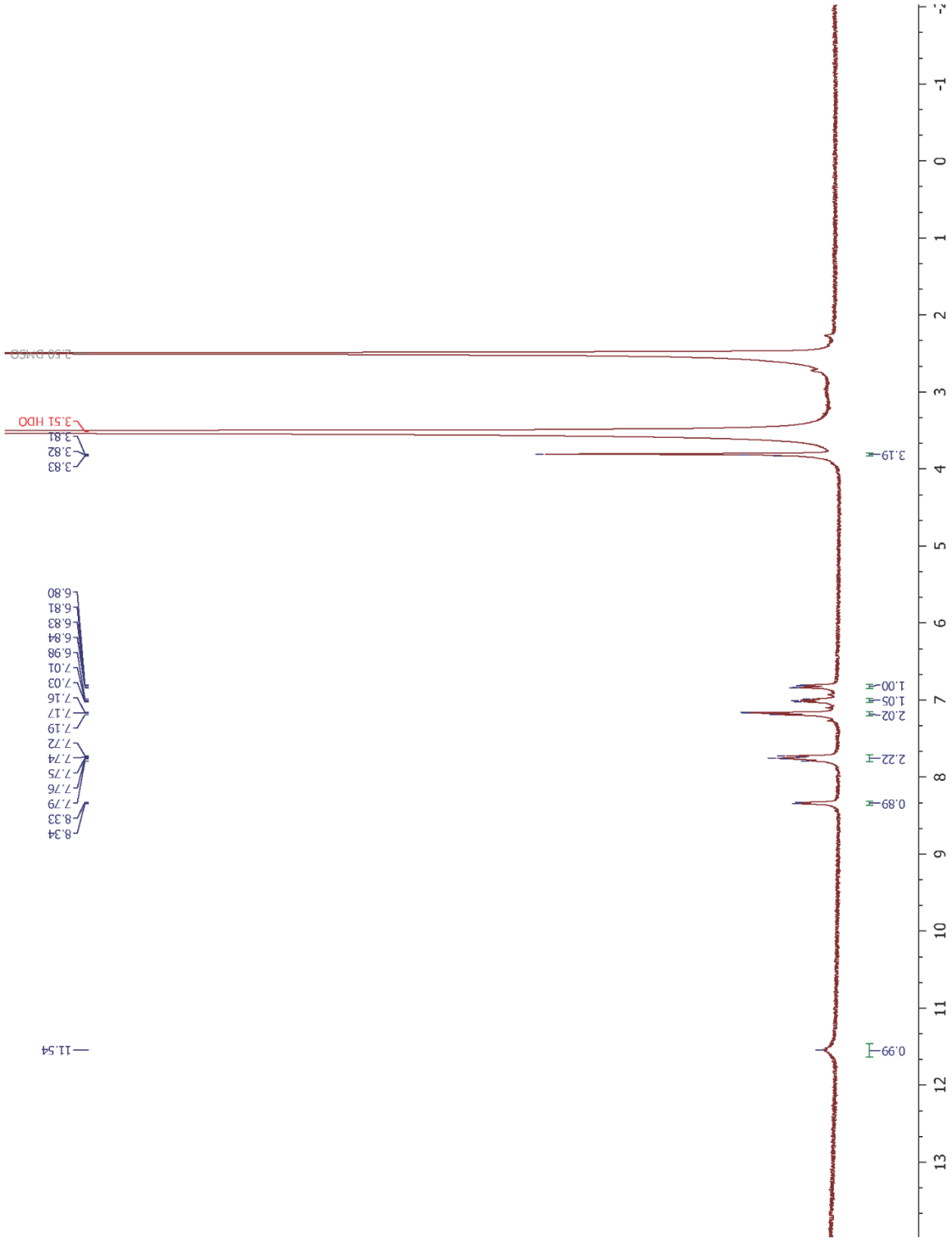
L (1 equiv.) and $Cu(NO_3)_2{\cdot}3H_2O$ (1 equiv.) were separately dissolved in 10 mL of methanol. The solution of $Cu(NO_3)_2$ was added dropwise to the solution of **L**. The resulting solution was stirred vigorously with heating (~60 ºC) for 20 minutes. Solvent was then removed *in vacuo* and the light green/yellow residue was subsequently dissolved in CH_2Cl_2, and transferred to a separatory funnel. The organic layer was then washed with dilute aqueous ammonium chloride (2x10 mL), with sodium thiosulfate (2x10 mL), and deionized water (1x25 mL). CH_2Cl_2 was then removed , and the remaining white power was analyzed *via* IR spectroscopy, ^1H and ^{13}C NMR, and compared to the starting thiourea, in order to determine if a successful cyclization to the corresponding benzothiazole was achieved. For all attempted reactions, only those with electron donating substituents (-OMe) on the phenyl rings were successful. Attempts are summarized in Table S1.

Table S1 Attempted conversions of thioreas to benzothiazoles

Thiourea (L)	Benzothiazole
 1-(3-methoxyphenyl)-3-(pyridin-2-yl)thiourea Molecular Weight: 259.33	Confirmed (reported herein)
 1-(4-methoxyphenyl)-3-(pyridin-2-yl)thiourea Molecular Weight: 259.33	Confirmed spectroscopically
 1-phenyl-3-(pyridin-2-yl)thiourea Molecular Weight: 229.30	Uncertain; difficulty in separating cation from reaction product in work-up
 1,1'-(1,4-phenylene)bis(3-phenylthiourea) Molecular Weight: 378.51	No. Further attempts with mixed solvents for reaction, and *via* microwave synthesis, were also unsuccessful.

 *N*-phenylmorpholine-4-carbothioamide Molecular Weight: 222.31	No. Further attempts with ethanol as the reaction solvent were also unsuccessful.
 1,3-diphenylthiourea Molecular Weight: 228.31	No
 1-(3-cyanophenyl)-3-(pyridin-2-yl)thiourea Molecular Weight: 254.31	No
 1-(9*H*-fluoren-3-yl)-3-phenylthiourea Molecular Weight: 316.42	No
 *N*-phenylpiperidine-1-carbothioamide Molecular Weight: 220.33	No

S2. NMR of ([(HBL1)$_2$(AuCl$_2$)]Cl·H$_2$O) Crystals


2.50 DMSO
3.51 HDO
3.81
3.82
3.83
6.80
6.81
6.83
6.84
6.98
7.01
7.03
7.16
7.17
7.19
7.72
7.74
7.75
7.76
7.79
8.33
8.34
11.54
3.19
1.00
1.05
2.02
2.22
0.89
0.99