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Synthesis of 4-arylethyl-6-arylpyrimidine-2-thiols through aza-Michael addition/nucleophilic addition/aromatization tandem reactions

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Abstract: An efficient method for the synthesis of the title compounds by reactions of divinyl ketones with thiourea is described. This protocol has the advantages of high yields, mild reaction conditions and simple work-up procedure.

Keywords: 4-arylethyl-6-arylpyrimidine-2-thiol; divinyl ketone; tandem reaction; thiourea.

Introduction

Pyrimidine-2-thiols are widely used in medicinal chemistry because of their broad spectrum of biological activities [1, 2]. They are precursors to important organic compounds [3–5] and organometallic complexes [6–8]. In addition, they can also be utilized in the determination of many metal ions (Pb, Ru, Bi, Pd, Pt) as selective and sensitive ligands in analytical chemistry [9–14].

The traditional method for the synthesis of unsubstituted pyrimidine-2-thiol is based on the reaction of 1,1,3,3-tetraethoxypropane with thiourea in a strong acidic medium [15]. Synthesis of substituted pyrimidine-2-thiols involves the reactions of β -enaminoamides with thiourea under basic conditions [16] and the reactions of chalcones with thiourea [17–20]. In this paper, we report a facile preparation of 4-arylethyl-6-arylpyrimidine-2-thiols by reactions of divinyl ketones with thiourea through aza-Michael addition/nucleophilic addition/aromatization tandem processes.

Results and discussion

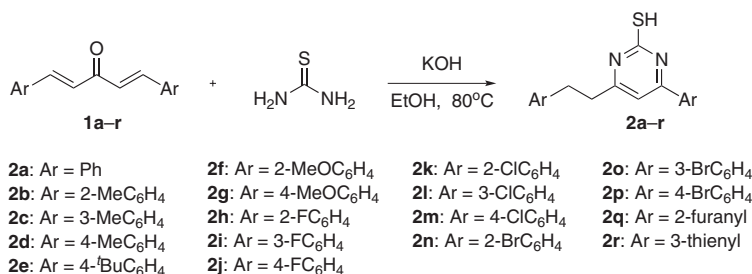
Initially, (1*E*,4*E*)-1,5-diphenylpenta-1,4-dien-3-one (**1a**) was allowed to react with thiourea in ethanol in the presence of potassium hydroxide as a base (Scheme 1). The isolated product was 4-phenethyl-6-phenylpyrimidine-2-thiol (**2a**), the structure of which was confirmed by spectral methods and elemental analysis. The reactions conducted in MeCN, *N,N*-dimethylformamide, dimethyl sulfoxide and *n*-PrOH were inefficient, and a moderate yield of 42% was obtained in MeOH. However, the best yield of 86% was obtained using EtOH as solvent. Inorganic bases, such as Na₂CO₃, K₂CO₃ and Cs₂CO₃, and organic bases, such as 1,8-diazabicyclo[5.4.0]undec-7-ene, 1,4-diazabicyclo[2.2.2]octane, 4-dimethylaminopyridine and Et₃N, had little or no effect on the reaction. However, high yields of **2a** in the range of 79–86% were obtained for the reaction conducted in the presence of strong bases including NaOH, KOH and KOBu^t. The highest yield of 86% was obtained in the presence of KOH. This optimal yield was observed by using 2 equiv of KOH based on **1a** at 80°C for 8 h.

The reactions of other substrates containing a wide range of functional groups including electron-donating groups (Me and MeO) and electron-withdrawing groups (F, Cl and Br) on aromatic rings of divinyl ketones **1a–p** furnished the corresponding products **2a–p** in good to high yields. In addition, divinyl ketones containing heterocycles, such as 2-furanyl and 3-thienyl, were also transformed into the corresponding products **2q–r** in good yields. Unfortunately, the reactions of divinyl ketones bearing nitro group on aromatic rings and aliphatic divinyl ketones were not successful. All products **2a–r** were characterized by proton nuclear magnetic resonance (¹H NMR), carbon-13 nuclear magnetic resonance (¹³C NMR), infrared (IR) and elemental analysis.

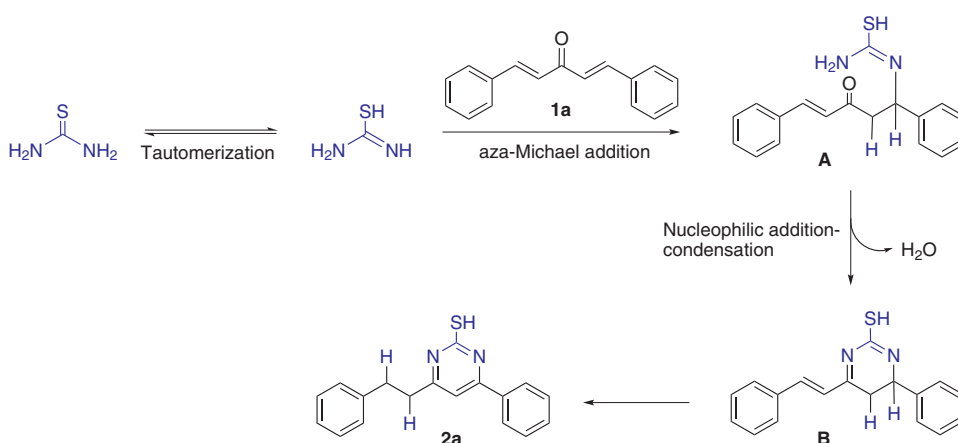
A plausible mechanism is illustrated for the synthesis of **2a** in Scheme 2 [16, 18, 20]. As can be seen, the initial aza-Michael addition reaction generates the intermediate product **A**. Compound **A** undergoes intramolecular cyclization, which is followed by dehydration to afford intermediate product **B**. The intermediate product **B** is a direct precursor to the observed final product **2a**.

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Scheme 1 Synthesis of 4-arylethyl-6-arylpyrimidine-2-thiols.

Scheme 2 Proposed mechanism for the reaction **1a** with thiourea.

Conclusion

An efficient method for the synthesis of 4-arylethyl-6-arylpyrimidine-2-thiols by reactions of divinyl ketones with thiourea through aza-Michael addition/nucleophilic addition/aromatization tandem processes was developed.

Experimental

¹H NMR (600 MHz) and ¹³C NMR (150 MHz) spectra were obtained with a Mercury-600B instrument using deuterated chloroform (CDCl₃) as solvent and tetramethylsilane (Me₄Si) as the internal standard. IR spectra were recorded as KBr pellets. Elemental analyses were performed on a Vario El Elemental Analysis instrument. Melting points were observed on an Electrothermal melting point apparatus. Divinyl ketones were synthesized according to the literature procedure [21, 22].

General procedure for synthesis of 4-arylethyl-6-arylpyrimidine-2-thiols (**2a-r**)

A mixture of divinyl ketone (**1**, 1 mmol), thiourea (1.5 mmol) and potassium hydroxide (2 mmol) in ethanol (5 mL) was stirred at 80°C for 8 h.

The reaction progress was monitored by thin-layer chromatography (TLC). After the completion of the reaction, the mixture was extracted with ethyl acetate (3 × 10 mL). The extract was washed with saturated brine (3 × 10 mL), dried over anhydrous sodium sulfate and concentrated under reduced pressure. The residue of **2a-r** was purified by column chromatography eluting with a mixture of petroleum ether and ethyl acetate (10:1).

4-Phenethyl-6-phenylpyrimidine-2-thiol (2a) Yellow oil; yield 86%; ¹H NMR: δ 7.93 (d, *J* = 6.8 Hz, 2H), 7.43–7.33 (m, 4H), 7.17–7.13 (m, 4H), 7.07 (s, 1H), 3.02 (t, *J* = 6.0 Hz, 2H), 2.97 (t, *J* = 6.0 Hz, 2H), SH signal was not observed; ¹³C NMR: δ 171.1, 169.6, 164.2, 140.7, 136.2, 131.0, 128.8, 128.5, 128.4, 127.2, 126.1, 112.5, 39.6, 34.5; IR: ν 2921, 2849, 1515, 1229, 829 cm⁻¹. Anal. Calcd for C₁₈H₁₆N₂S: C, 73.94; H, 5.52; N, 9.58. Found: C, 74.03; H, 5.50; N, 9.54.

4-(2-Methylphenethyl)-6-(*o*-tolyl)pyrimidine-2-thiol (2b) Yellow oil; yield 74%; ¹H NMR: δ 7.31–7.27 (m, 2H), 7.21 (t, *J* = 7.3 Hz, 2H), 7.13–7.04 (m, 4H), 6.89 (s, 1H), 3.00 (s, 4H), 2.26 (s, 3H), 2.23 (s, 3H), SH signal was not observed; ¹³C NMR: δ 170.8, 169.1, 167.9, 138.9, 137.2, 136.7, 135.9, 131.2, 130.3, 129.6, 128.8, 126.3, 126.0, 116.7, 38.2, 20.4, 19.2; IR: ν 2930, 2850, 1563, 1517, 1237, 698 cm⁻¹. Anal. Calcd for C₂₀H₂₀N₂S: C, 74.96; H, 6.29; N, 8.74. Found: C, 74.88; H, 6.32; N, 8.77.

4-(3-Methylphenethyl)-6-(*m*-tolyl)pyrimidine-2-thiol (2c) Yellow oil; yield 88%; ¹H NMR: δ 7.71 (s, 2H), 7.26–7.22 (m, 2H), 7.15 (s, 1H), 7.07 (t, *J* = 6.9 Hz, 1H), 6.98–6.93 (m, 2H), 6.89 (d, *J* = 5.6 Hz, 1H), 3.01 (t, *J* = 7.9 Hz, 2H), 2.90 (t, *J* = 7.9 Hz, 2H), 2.32 (s, 3H), 2.26 (s, 3H), SH signal

was not observed; ^{13}C NMR: δ 171.1, 169.5, 164.4, 140.8, 138.4, 138.0, 136.2, 131.7, 129.2, 128.6, 128.3, 127.8, 126.8, 125.4, 124.3, 112.5, 39.6, 34.5, 21.4, 21.3. IR: ν 2938, 2850, 1563 cm^{-1} , 1514, 1254, 689 cm^{-1} . Anal. Calcd for $\text{C}_{20}\text{H}_{20}\text{N}_2\text{S}$: C, 74.96; H, 6.29; N, 8.74. Found: C, 75.07; H, 6.27; N, 8.72.

4-(4-Methylphenethyl)-6-(*p*-tolyl)pyrimidine-2-thiol (2d) Yellow solid; mp 120–122°C; yield 75%; ^1H NMR: δ 7.83 (d, $J=8.0$ Hz, 2H), 7.17 (d, $J=8.0$ Hz, 2H), 7.09 (s, 1H), 6.97 (s, 4H), 2.99 (t, $J=7.5$ Hz, 2H), 2.92 (t, $J=7.5$ Hz, 2H), 2.36 (s, 3H), 2.26 (s, 3H), SH signal was not observed; ^{13}C NMR: δ 171.0, 169.4, 164.1, 141.4, 137.8, 135.5, 133.5, 129.5, 129.0, 128.3, 127.1, 112.1, 39.7, 34.1, 21.4, 20.9. IR: ν 2921, 2856, 1563, 1506, 1237, 820 cm^{-1} . Anal. Calcd for $\text{C}_{20}\text{H}_{20}\text{N}_2\text{S}$: C, 74.96; H, 6.29; N, 8.74. Found: C, 74.90; H, 6.30; N, 8.72.

4-(4-*tert*-Butylphenethyl)-6-(4-*tert*-butylphenyl)pyrimidine-2-thiol (2e) Yellow solid; mp 113–115°C; yield 81%; ^1H NMR: δ 7.87 (d, $J=8.3$ Hz, 2H), 7.38 (d, $J=8.3$ Hz, 2H), 7.18 (d, $J=8.1$ Hz, 2H), 7.07 (s, 1H), 7.00 (d, $J=8.1$ Hz, 2H), 3.02 (t, $J=7.6$ Hz, 2H), 2.93 (t, $J=7.6$ Hz, 2H), 1.29 (s, 9H), 1.25 (s, 9H), SH signal was not observed; ^{13}C NMR: δ 171.0, 169.6, 164.1, 154.4, 148.8, 137.7, 133.5, 128.1, 127.0, 125.7, 125.2, 112.4, 39.6, 34.8, 34.3, 34.1, 31.3, 31.1; IR: ν 2917, 2910, 2851, 1568, 1516, 1217, 827 cm^{-1} . Anal. Calcd for $\text{C}_{26}\text{H}_{32}\text{N}_2\text{S}$: C, 77.18; H, 7.97; N, 6.92. Found: C, 77.23; H, 8.00; N, 6.89.

4-(2-Methoxyphenethyl)-6-(2-methoxyphenyl)pyrimidine-2-thiol (2f) Yellow oil; yield 73%; ^1H NMR: δ 7.85 (d, $J=6.0$ Hz, 1H), 7.53 (s, 1H), 7.34 (t, $J=7.8$ Hz, 1H), 7.13 (t, $J=8.6$ Hz, 1H), 7.03 (d, $J=7.3$ Hz, 1H), 6.94–6.91 (m, 2H), 6.80–6.74 (m, 2H), 3.79 (s, 3H), 3.75 (s, 3H), 3.02–2.98 (m, 4H), SH signal was not observed; ^{13}C NMR: δ 170.9, 168.7, 162.7, 158.1, 157.4, 131.5, 131.4, 129.9, 129.4, 127.2, 125.8, 121.1, 120.3, 117.3, 111.4, 110.1, 55.5, 55.1, 37.8, 29.4; IR: ν 2930, 2849, 1563, 1506, 1237, 759 cm^{-1} . Anal. Calcd for $\text{C}_{20}\text{H}_{20}\text{N}_2\text{O}_2\text{S}$: C, 68.16; H, 5.72; N, 7.95. Found: C, 68.09; H, 5.74; N, 7.99.

4-(4-Methoxyphenethyl)-6-(4-methoxyphenyl)pyrimidine-2-thiol (2g) Brown oil; yield 63%; ^1H NMR: δ 7.93 (d, $J=8.8$ Hz, 2H), 7.03 (s, 1H), 6.96 (d, $J=8.4$ Hz, 2H), 6.87 (d, $J=8.8$ Hz, 2H), 6.67 (d, $J=8.4$ Hz, 2H), 3.80 (s, 3H), 3.70 (s, 3H), 2.98 (t, $J=7.4$ Hz, 2H), 2.91 (t, $J=7.4$ Hz, 2H), SH signal was not observed; ^{13}C NMR: δ 170.8, 169.4, 163.7, 162.1, 157.9, 130.0, 129.3, 128.8, 128.7, 114.1, 113.7, 111.7, 55.3, 55.1, 39.8, 33.6; IR: ν 2938, 2850, 1563, 1514, 1237, 838 cm^{-1} . Anal. Calcd for $\text{C}_{20}\text{H}_{20}\text{N}_2\text{O}_2\text{S}$: C, 68.16; H, 5.72; N, 7.95. Found: C, 68.21; H, 5.71; N, 7.92.

4-(2-Fluorophenethyl)-6-(2-fluorophenyl)pyrimidine-2-thiol (2h) Yellow solid; mp 108–110°C; yield 91%; ^1H NMR: δ 8.02 (t, $J=7.0$ Hz, 1H), 7.38 (s, 2H), 7.16–7.04 (m, 4H), 6.98–6.94 (t, $J=9.2$ Hz, 1H), 6.91 (t, $J=7.5$ Hz, 1H), 3.07–3.01 (m, 4H), SH signal was not observed; ^{13}C NMR: δ 171.0, 169.3, 162.7, 161.9, 160.6, 160.4, 160.3, 132.3, 130.9, 130.6, 127.9, 124.6, 123.9, 116.8, 116.4, 115.3, 37.8, 27.7; IR: ν 2921, 2850, 1569, 1840, 1237, 751 cm^{-1} . Anal. Calcd for $\text{C}_{18}\text{H}_{14}\text{F}_2\text{N}_2\text{S}$: C, 65.84; H, 4.30; N, 8.53. Found: C, 65.96; H, 4.28; N, 8.49.

4-(3-Fluorophenethyl)-6-(3-fluorophenyl)pyrimidine-2-thiol (2i) Yellow solid; mp 122–124°C; yield 96%; ^1H NMR: δ 7.85 (s, 1H), 7.80 (d, $J=7.8$ Hz, 1H), 7.39 (d, $J=8.0$ Hz, 1H), 7.32 (t, $J=7.9$ Hz, 1H), 7.18–7.05 (m, 4H), 6.94 (d, $J=7.4$ Hz, 1H), 3.04 (t, $J=7.8$ Hz, 2H), 2.98–2.95 (t, $J=7.8$ Hz, 2H), SH signal was not observed; ^{13}C NMR: δ 171.0, 169.8, 163.0, 142.6, 137.9, 135.0, 134.2, 131.0, 130.1, 129.7, 128.5, 127.3, 126.5, 126.4, 125.2, 112.7, 39.0, 33.8; IR: ν 2921, 2853, 1568, 1514, 1237,

759 cm^{-1} . Anal. Calcd for $\text{C}_{18}\text{H}_{14}\text{F}_2\text{N}_2\text{S}$: C, 65.84; H, 4.30; N, 8.53. Found: C, 65.77; H, 4.31; N, 8.57.

4-(4-Fluorophenethyl)-6-(4-fluorophenyl)pyrimidine-2-thiol (2j) Yellow solid; mp 134–136°C; yield 90%; ^1H NMR: δ 7.96 (d, $J=5.4$ Hz, 1H), 7.95 (d, $J=5.4$ Hz, 1H), 7.08 (s, 1H), 7.06 (d, $J=8.6$ Hz, 2H), 7.02–6.99 (m, 2H), 6.82 (t, $J=8.6$ Hz, 2H), 3.00 (t, $J=7.0$ Hz, 2H), 2.95 (t, $J=7.0$ Hz, 2H), SH signal was not observed; ^{13}C NMR: δ 170.9, 169.7, 165.5, 163.9, 163.2, 162.1, 160.5, 136.2, 132.2, 129.7, 129.2, 115.9, 115.1, 112.2, 39.5, 33.4; IR: ν 2921, 2856, 1573, 1224, 846 cm^{-1} . Anal. Calcd for $\text{C}_{18}\text{H}_{14}\text{F}_2\text{N}_2\text{S}$: C, 65.84; H, 4.30; N, 8.53. Found: C, 65.80; H, 4.32; N, 8.55.

4-(2-Chlorophenethyl)-6-(2-chlorophenyl)pyrimidine-2-thiol (2k) Orange solid; mp 119–121°C; yield 87%; ^1H NMR: δ 7.47 (d, $J=7.5$ Hz, 1H), 7.40 (d, $J=8.1$ Hz, 1H), 7.33–7.26 (m, 3H), 7.25 (s, 1H), 7.11–7.05 (m, 3H), 3.10–3.06 (m, 4H), SH signal was not observed; ^{13}C NMR: δ 170.2, 169.4, 164.3, 138.2, 136.2, 133.9, 132.3, 131.6, 130.8, 130.5, 130.4, 129.5, 127.7, 127.1, 126.8, 117.6, 37.4, 32.3. IR: ν 2935, 2861, 1565, 1514, 1228, 759 cm^{-1} . Anal. Calcd for $\text{C}_{18}\text{H}_{14}\text{Cl}_2\text{N}_2\text{S}$: C, 59.84; H, 3.91; N, 7.75. Found: C, 59.77; H, 3.92; N, 7.78.

4-(3-Chlorophenethyl)-6-(3-chlorophenyl)pyrimidine-2-thiol (2l) Yellow solid; mp 121–122°C; yield 90%; ^1H NMR: δ 7.85 (s, 1H), 7.80 (d, $J=7.8$ Hz, 1H), 7.40 (d, $J=7.8$ Hz, 1H), 7.32 (t, $J=7.2$ Hz, 1H), 7.16 (s, 1H), 7.13–7.07 (m, 3H), 6.94 (d, $J=7.4$ Hz, 1H), 3.04 (t, $J=7.6$ Hz, 2H), 2.96 (t, $J=7.6$ Hz, 2H), SH signal was not observed; ^{13}C NMR: δ 171.0, 169.8, 163.0, 142.6, 137.9, 135.0, 134.2, 131.0, 130.1, 129.7, 128.5, 127.3, 126.5, 126.4, 125.2, 112.7, 39.0, 33.8; IR: ν 2921, 2850, 1560, 1514, 1217, 749 cm^{-1} . Anal. Calcd for $\text{C}_{18}\text{H}_{14}\text{Cl}_2\text{N}_2\text{S}$: C, 59.84; H, 3.91; N, 7.75. Found: C, 59.90; H, 3.89; N, 7.72.

4-(4-Chlorophenethyl)-6-(4-chlorophenyl)pyrimidine-2-thiol (2m) White solid; mp 115–117°C; yield 88%; ^1H NMR: δ 7.87 (d, $J=8.5$ Hz, 2H), 7.35 (d, $J=8.5$ Hz, 2H), 7.09 (d, $J=8.3$ Hz, 3H), 6.96 (d, $J=8.3$ Hz, 2H), 2.99 (t, $J=7.2$ Hz, 2H), 2.94 (t, $J=7.2$ Hz, 2H), SH signal was not observed; ^{13}C NMR: δ 170.9, 169.8, 163.1, 139.0, 137.5, 134.4, 131.9, 129.7, 129.1, 128.5, 128.4, 112.3, 39.1, 33.4; IR: ν 2930, 2856, 1579, 1560, 1514, 828 cm^{-1} . Anal. Calcd for $\text{C}_{18}\text{H}_{14}\text{Cl}_2\text{N}_2\text{S}$: C, 59.84; H, 3.91; N, 7.75. Found: C, 59.89; H, 3.90; N, 7.73.

4-(2-Bromophenethyl)-6-(2-bromophenyl)pyrimidine-2-thiol (2n) Orange solid; mp 117–119°C; yield 88%; ^1H NMR: δ 7.60 (d, $J=7.9$ Hz, 1H), 7.49 (d, $J=6.8$ Hz, 1H), 7.40 (d, $J=7.6$ Hz, 1H), 7.32 (t, $J=7.4$ Hz, 1H), 7.24 (t, $J=7.4$ Hz, 1H), 7.21 (s, 1H), 7.13–7.08 (m, 2H), 7.02 (t, $J=6.6$ Hz, 1H), 3.10 (t, $J=7.6$ Hz, 2H), 3.06 (t, $J=7.6$ Hz, 2H), SH signal was not observed; ^{13}C NMR: δ 170.0, 169.4, 165.7, 139.9, 138.3, 133.6, 132.8, 131.5, 130.8, 130.6, 127.9, 127.6, 127.5, 124.4, 121.4, 117.6, 37.6, 34.8. IR: ν 2921, 2856, 1573, 1506, 1219, 751 cm^{-1} . Anal. Calcd for $\text{C}_{18}\text{H}_{14}\text{Br}_2\text{N}_2\text{S}$: C, 48.02; H, 3.13; N, 6.22. Found: C, 47.92; H, 3.15; N, 6.25.

4-(3-Bromophenethyl)-6-(3-bromophenyl)pyrimidine-2-thiol (2o) Orange oil; yield 91%; ^1H NMR: δ 8.00 (s, 1H), 7.85 (d, $J=8.0$ Hz, 1H), 7.55 (d, $J=8.0$ Hz, 1H), 7.28–7.27 (m, 2H), 7.25 (d, $J=5.9$ Hz, 1H), 7.15 (s, 1H), 7.04–6.97 (m, 2H), 3.04 (t, $J=7.7$ Hz, 2H), 2.95 (t, $J=7.7$ Hz, 2H), SH signal was not observed. ^{13}C NMR: δ 170.9, 169.8, 162.9, 142.9, 138.1, 133.9, 131.4, 130.3, 130.2, 130.0, 129.3, 127.0, 125.6, 123.1, 122.5, 112.7, 39.1, 33.8. IR: ν 2921, 2850, 1575, 1514, 1237, 751 cm^{-1} . Anal. Calcd for $\text{C}_{18}\text{H}_{14}\text{Br}_2\text{N}_2\text{S}$: C, 48.02; H, 3.13; N, 6.22. Found: C, 48.09; H, 3.13; N, 6.20.

4-(4-Bromophenethyl)-6-(4-bromophenyl)pyrimidine-2-thiol (2p) Yellow solid; mp 70–72°C; yield 89%; ¹H NMR: δ 7.80 (d, *J* = 8.6 Hz, 2H), 7.51 (d, *J* = 8.6 Hz, 2H), 7.24 (d, *J* = 8.3 Hz, 2H), 7.08 (s, 1H), 6.91 (d, *J* = 8.3 Hz, 2H), 3.00 (t, *J* = 7.7 Hz, 2H), 2.93 (t, *J* = 7.7 Hz, 2H), SH signal was not observed; ¹³C NMR: δ 170.9, 169.8, 163.2, 139.5, 134.9, 132.1, 131.4, 130.1, 128.6, 125.9, 119.9, 112.3, 39.0, 33.4. IR: ν 2921, 2850, 1573, 1514, 1237 828 cm⁻¹. Anal. Calcd for C₁₈H₁₄Br₂N₂S: C, 48.02; H, 3.13; N, 6.22. Found: C, 48.11; H, 3.11; N, 6.19.

4-(Furan-2-yl)-6-(2-(furan-2-yl)ethyl)pyrimidine-2-thiol (2q) Yellow solid; mp 64–66°C; yield 74%; ¹H NMR: δ 7.64 (d, *J* = 3.7 Hz, 1H), 7.41 (d, *J* = 5.0 Hz, 1H), 7.07–7.02 (m, 3H), 6.80–6.78 (m, 1H), 6.67 (s, 1H), 3.20 (t, *J* = 7.6 Hz, 2H), 3.06 (t, *J* = 7.6 Hz, 2H), SH signal was not observed; ¹³C NMR: δ 170.0, 169.4, 159.3, 143.3, 142.0, 130.3, 128.2, 127.7, 126.7, 124.7, 123.3, 110.9, 39.4, 28.2. IR: ν 2921, 2849, 1573, 1428, 689 cm⁻¹. Anal. Calcd for C₁₄H₁₂N₂O₂S: C, 61.75; H, 4.44; N, 10.29. Found: C, 61.81; H, 4.42; N, 10.25.

4-(Thiophen-3-yl)-6-(2-(thiophen-3-yl)ethyl)pyrimidine-2-thiol (2r) Black solid; mp 92–94°C; yield 63%; ¹H NMR: δ 7.53 (s, 1H), 7.23 (s, 1H), 7.16 (m, 1H), 7.12 (s, 1H), 6.49 (s, 1H), 6.16 (s, 1H), 5.86 (s, 1H), 3.02 (t, *J* = 6.8 Hz, 2H), 2.98 (t, *J* = 6.8 Hz, 2H), SH signal was not observed; ¹³C NMR: δ 170.6, 169.4, 155.7, 154.4, 151.5, 145.0, 141.0, 113.0, 112.5, 110.2, 110.0, 105.4, 35.9, 26.3. IR: ν 2921, 2845, 1600, 1262, 1011, 724 cm⁻¹. Anal. Calcd for C₁₄H₁₂N₂S₂: C, 55.23; H, 3.97; N, 9.20. Found: C, 55.16; H, 3.99; N, 9.23.

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