

# 2-[[bis(propan-2-yl)carbamoithioyl]sulfanyl]acetic acid

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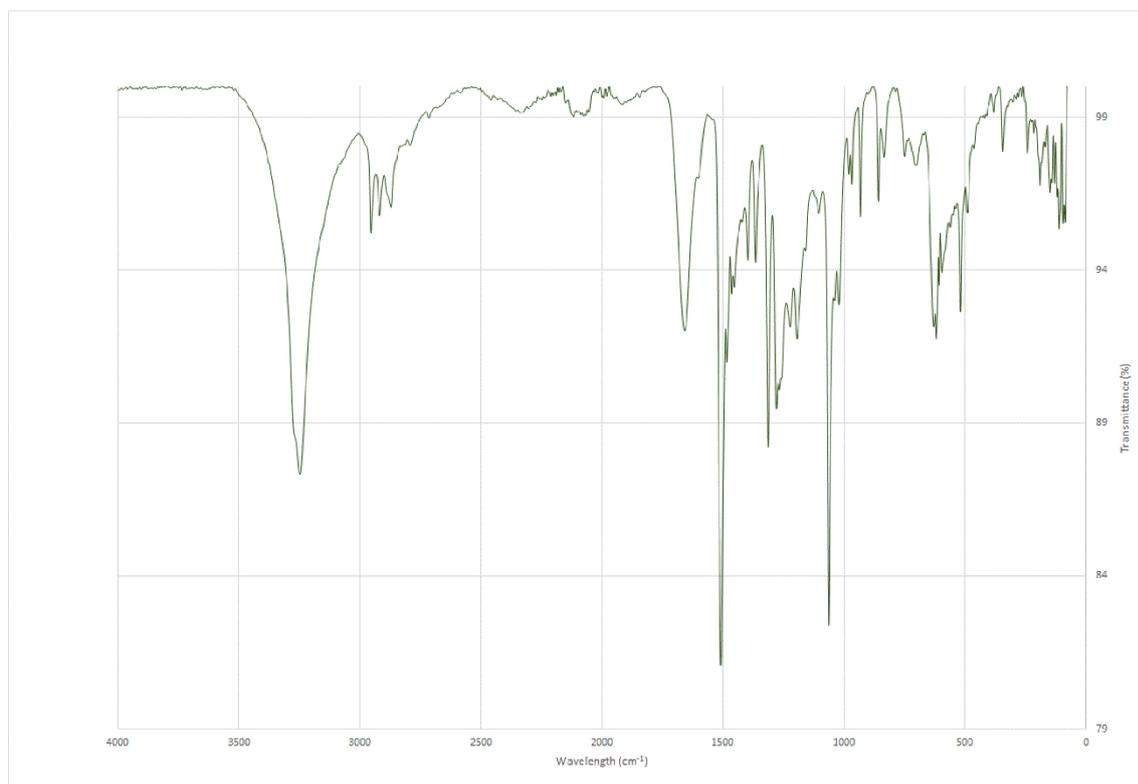
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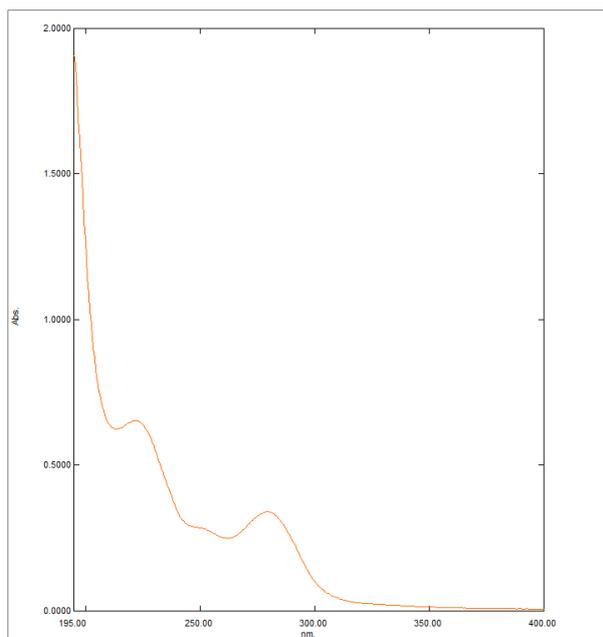
## SUPPLEMENTARY MATERIALS

Contents:

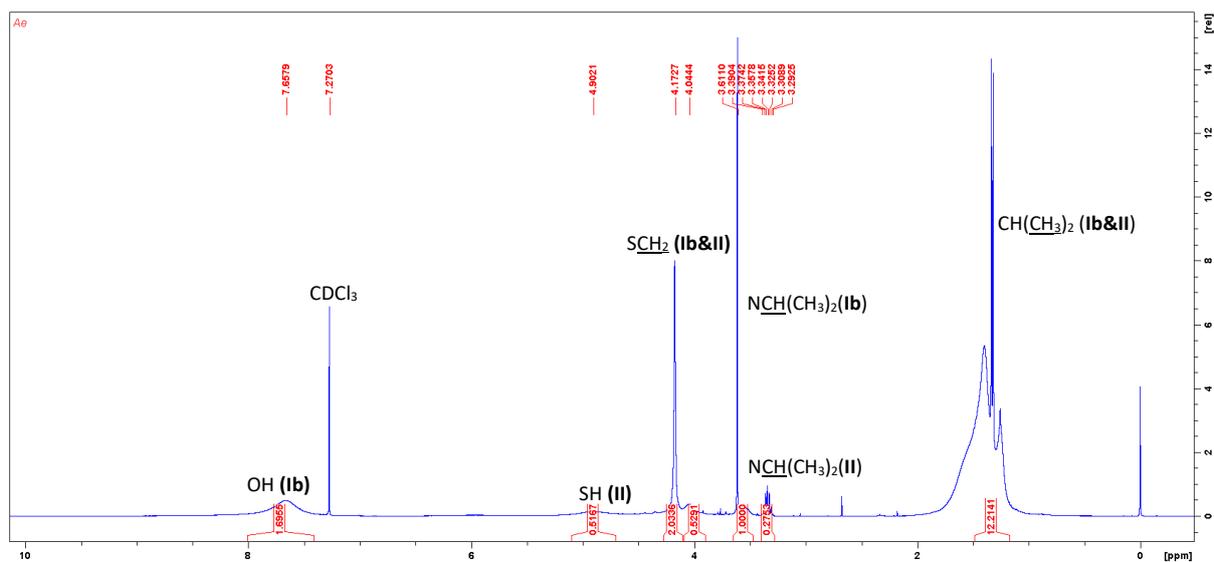
- Figure S1.** IR spectrum of Compound 1.
- Figure S2.** UV spectrum of Compound 1 recorded in acetonitrile solution.
- Figure S3.**  $^1\text{H}$  NMR spectrum (25 °C) of Compound 1: (a) full spectrum and (b) expanded.
- Figure S4.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum (25 °C) of Compound 1: (a) full spectrum and (b) expanded.
- Figure S5.** Overlay of DEPT-135 NMR spectra of Compound 1 measured at different temperatures.
- Figure S6.** Overlay of  $^1\text{H}$  NMR spectra of Compound 1 measured at different temperatures: (a) full spectrum and (b) expanded.



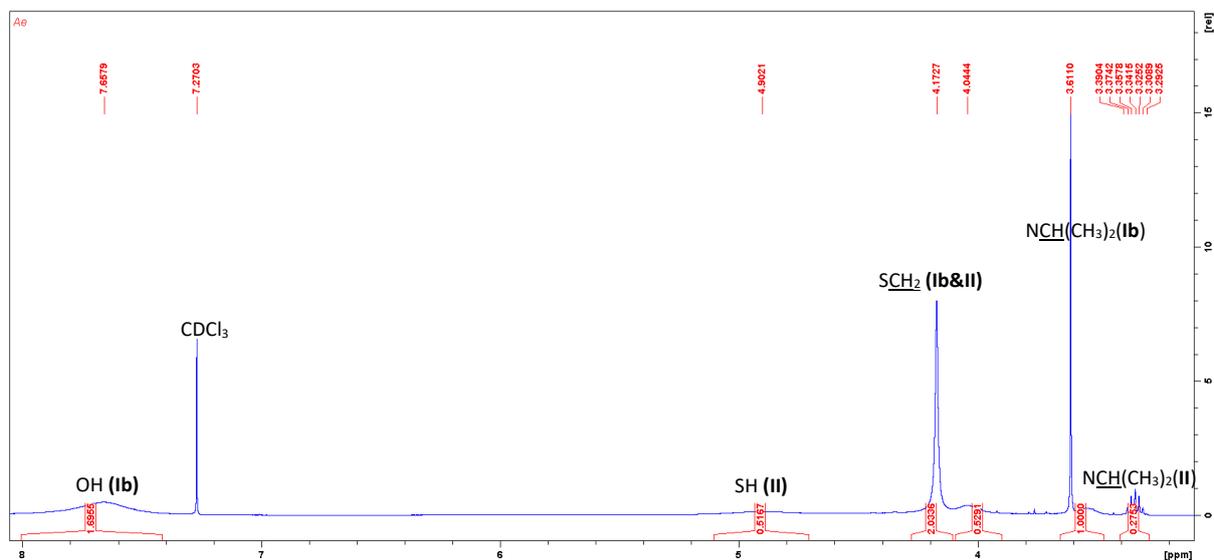
**Figure S1.** IR spectrum of Compound 1.



**Figure S2.** UV spectrum of Compound **1** recorded in acetonitrile solution.



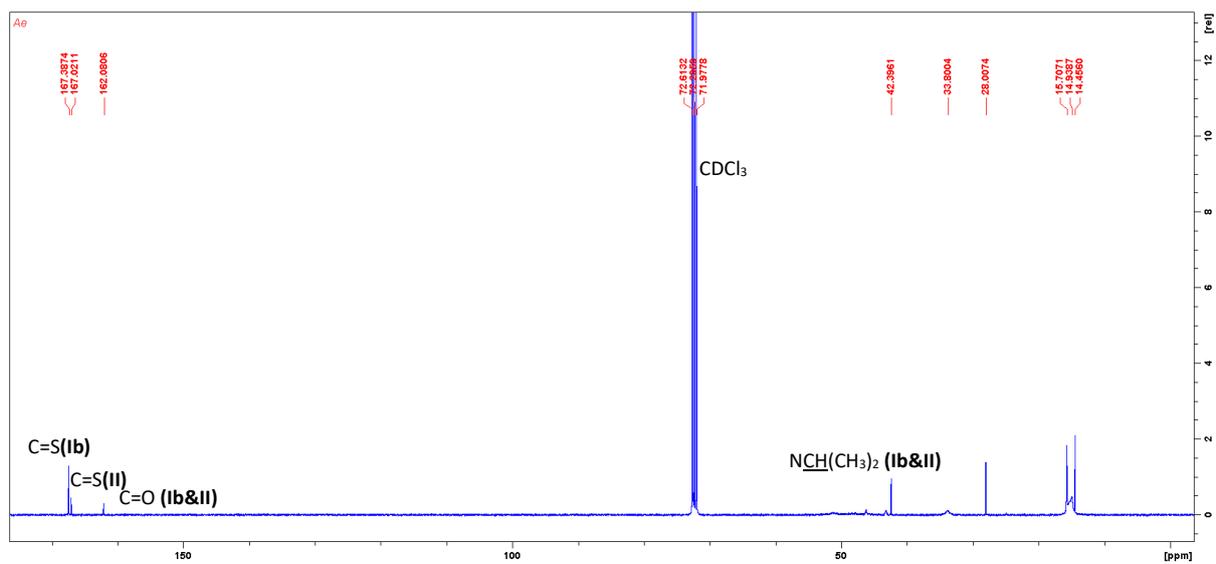
(a)



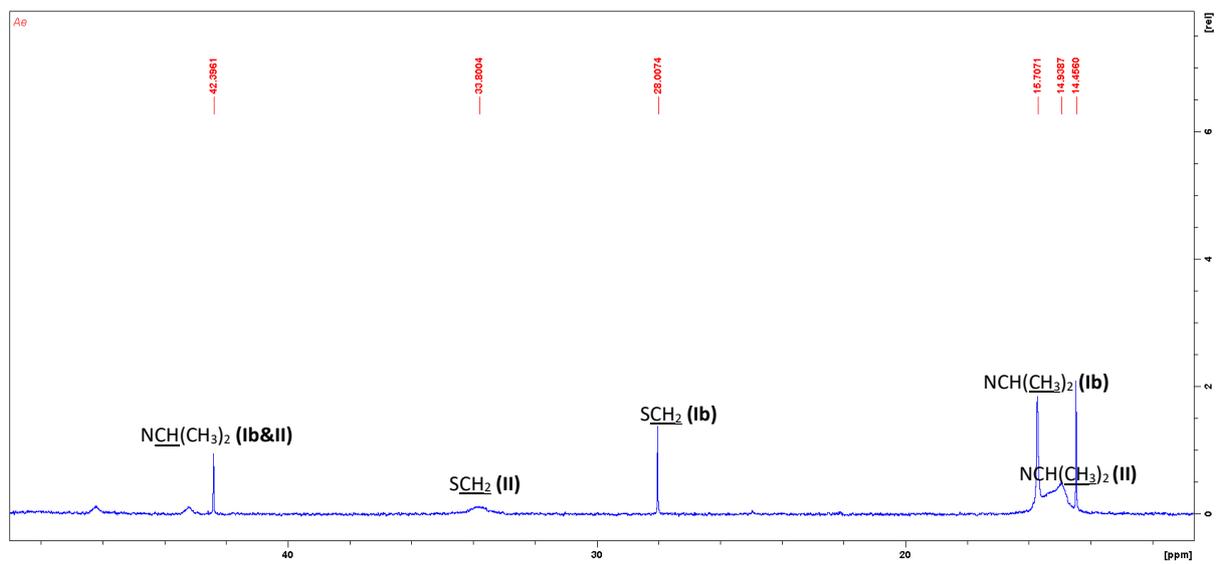
(b)

**Figure S3.**  $^1\text{H}$  NMR spectrum (25 °C) of Compound 1: (a) full spectrum and (b) expanded.

[Note: Exact 1H:1H integration of  $\text{NCH}$  is not observed for II and 1b, due to the fast exchange of the proton. Exact integration value of  $\text{SH}$  (1H for II) is not observed due to low percentage of (II). The exact integration of  $\text{NCH(CH}_3)_2$  (1H:1H) and  $\text{SCH}_2$  (2H:2H) cannot be measured because of the overlapping of signals of (Ib & II)].

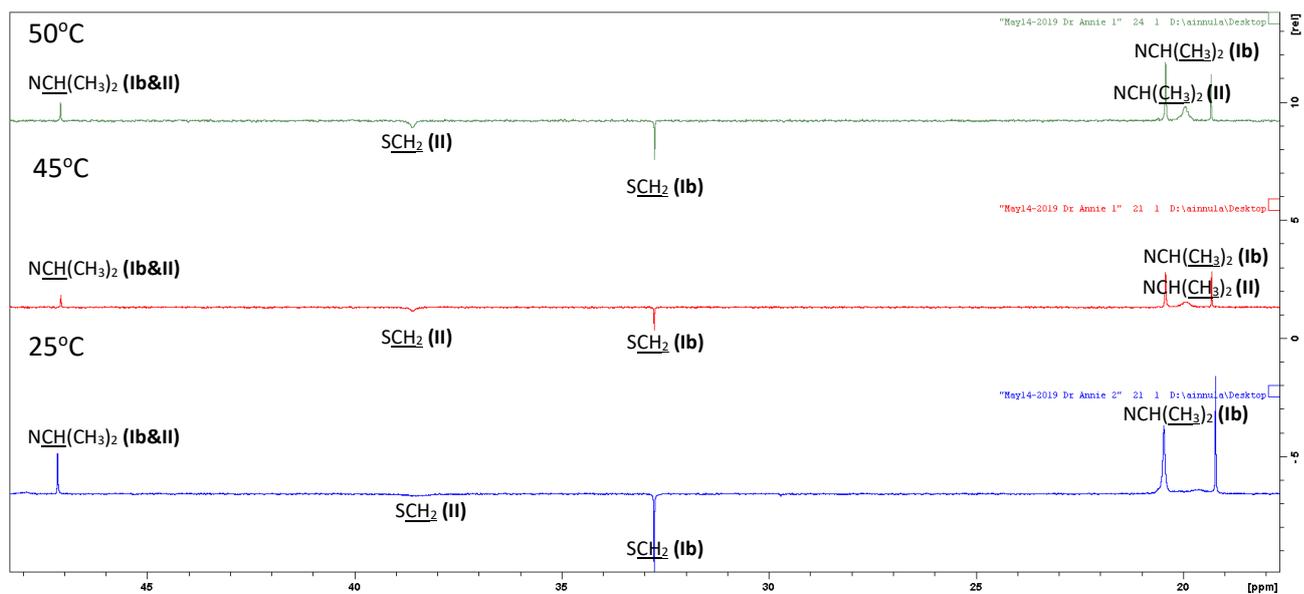


(a)

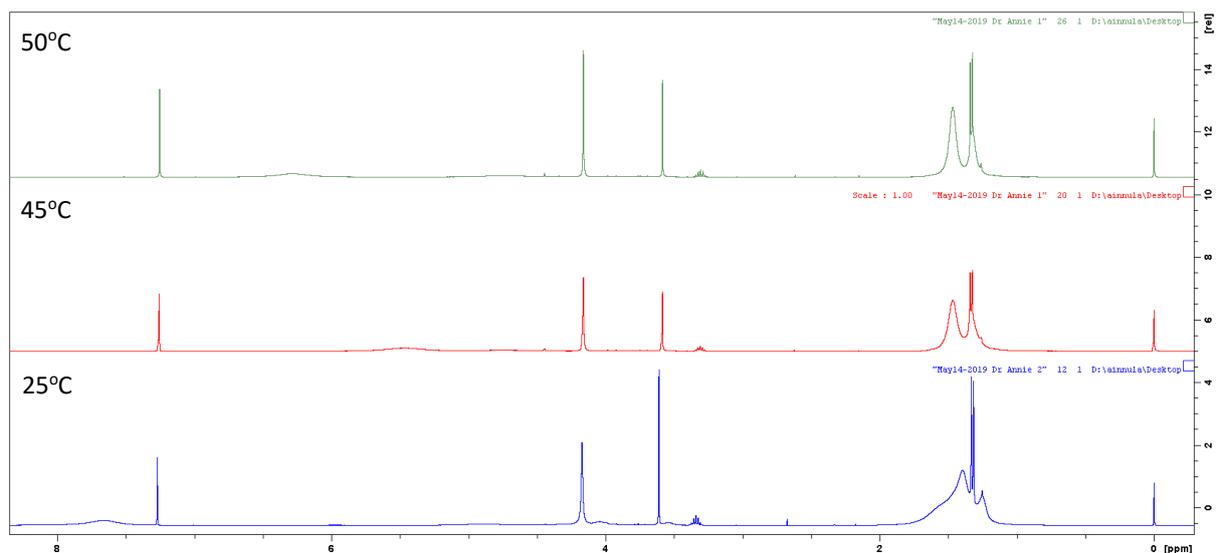


(b)

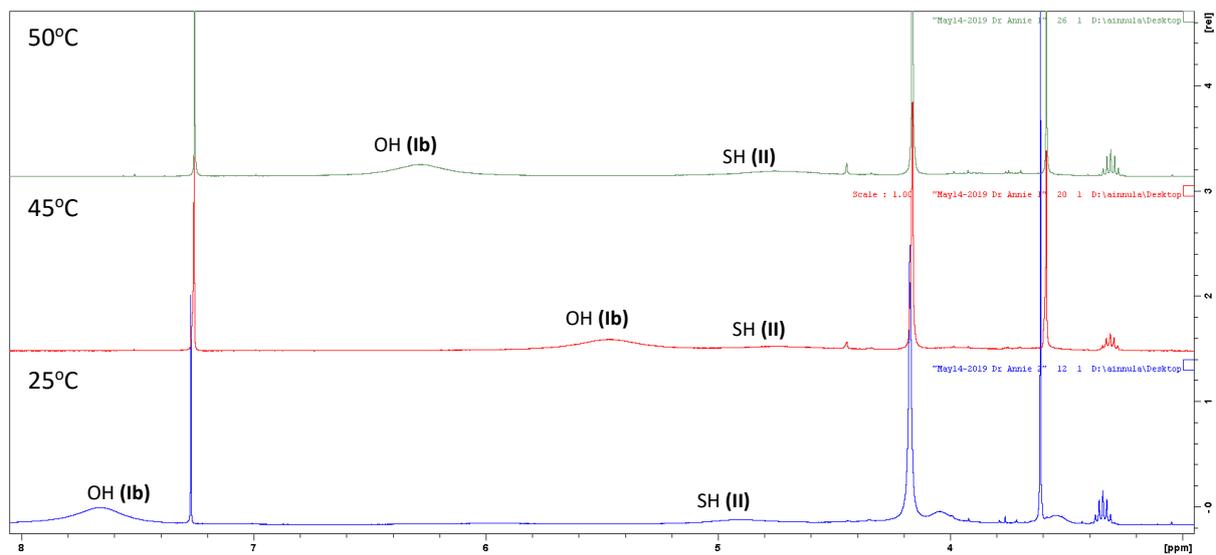
**Figure S4.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum (25 °C) of Compound 1: (a) full spectrum and (b) expanded.



**Figure S5.** Overlay of DEPT-135 NMR spectra of Compound 1 measured at different temperatures.



(a)



(b)

**Figure S6.** Overlay of  $^1\text{H}$  NMR spectra of Compound 1 measured at different temperatures: (a) full spectrum and (b) expanded.