

Supplementary Materials

Table S1. Summary of crystal data and intensity collection and structure refinement parameters for **1**.

Compound	1
Chemical formula	C ₂₈ H ₂₁ N ₅ S ₂
Formula weight	491.64
Crystal system	monoclinic
Space group	P-1 21/c1
<i>a</i> (Å)	12.378(2)
<i>b</i> (Å)	16.2178(5)
<i>c</i> (Å)	19.947(3)
α (°)	90.0
β (°)	143.00(4)
γ (°)	90.0
Volume (Å ³)	2409.6(6)
<i>Z</i>	4
Calc. density (g cm ⁻³)	1.355
Temperature (K)	293(2)
Abs. coeff. (mm ⁻¹)	0.249
<i>F</i> (0 0 0)	1024
Obs. reflections	6038
Goodness-of-fit	1.024
<i>R</i> ₁ ^a	0.0442
<i>wR</i> ₂	0.1150

^a $w = 1/[\sigma^2(F_o^2) + (\alpha P)^2 + bP]$ and $P = (\max(F_o^2, 0) + 2F_c^2)/3$; $R_1 = \Sigma(|F_o| - |F_c|)/\Sigma(|F_o|)$ and $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$.

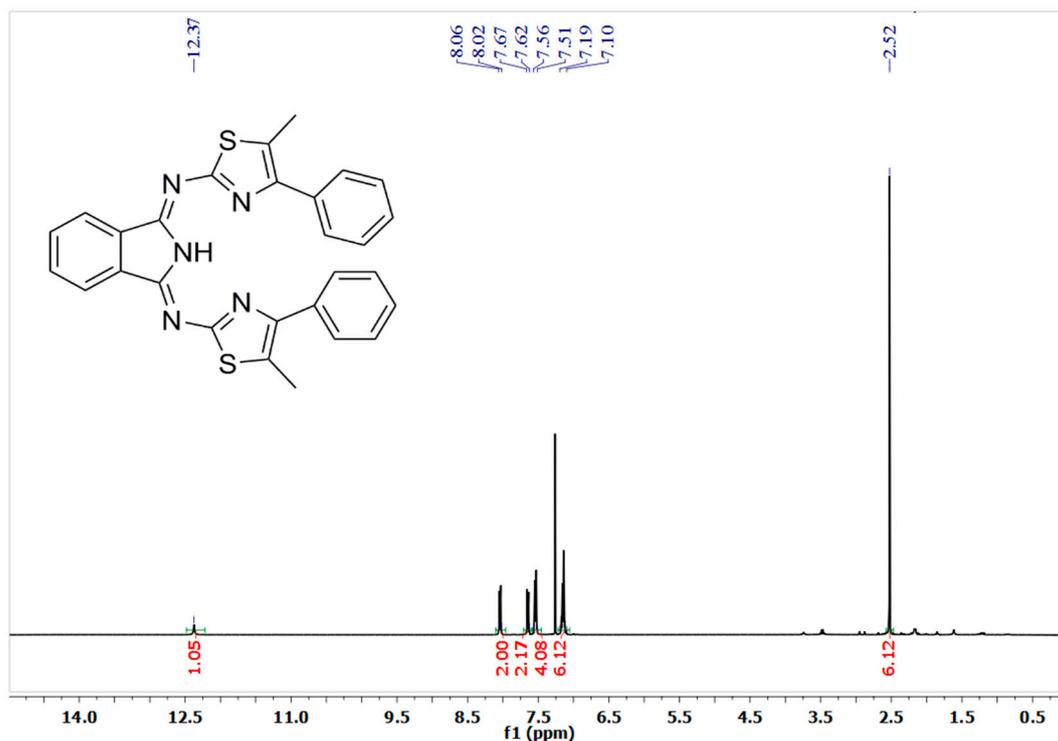


Figure S1. ¹H-NMR spectrum of **1**.

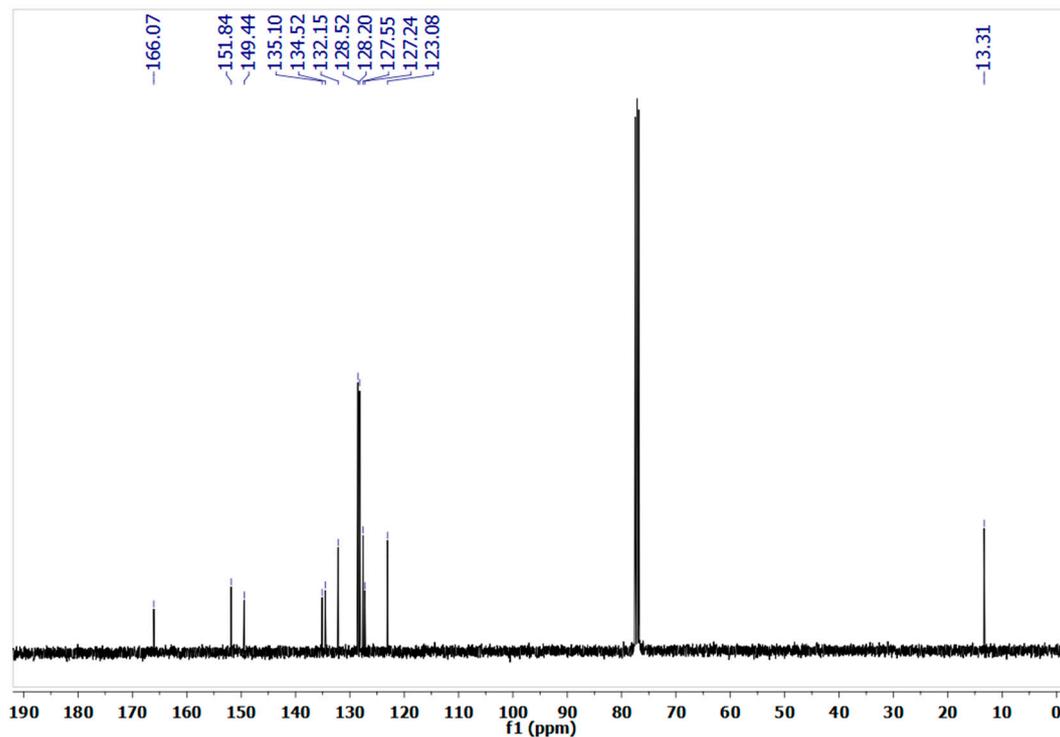


Figure S2. ¹³C-NMR spectrum of 1.

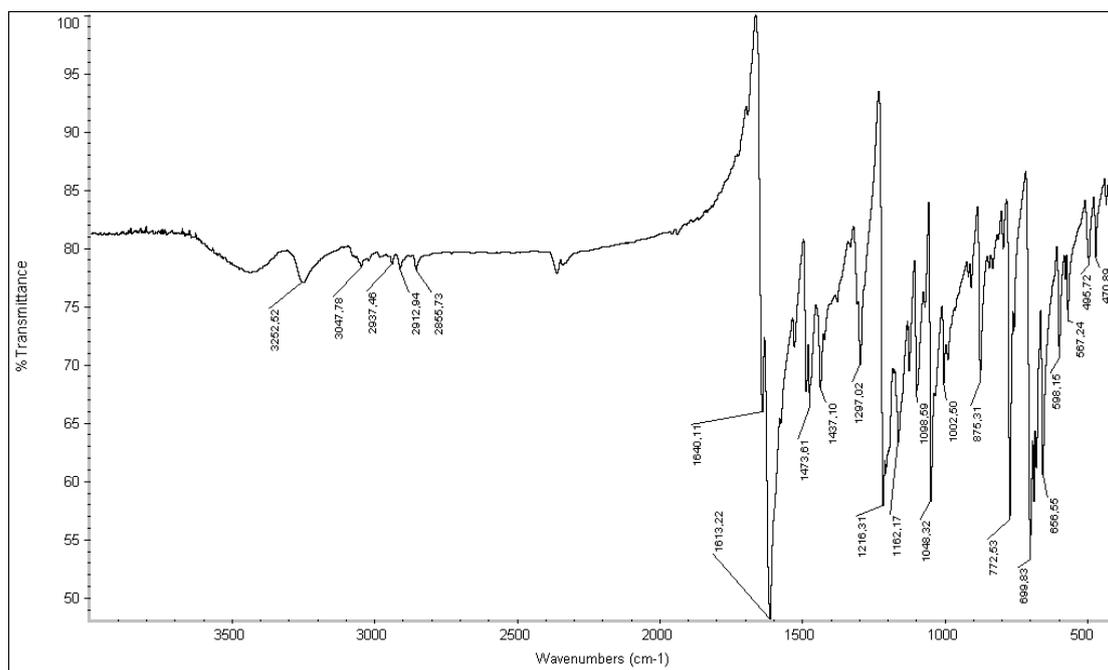


Figure S3. FT-IR spectrum of 1.