

DNA interactions and biological activity of 2,9-disubstituted 1,10-phenanthroline thiosemicarbazone-based ligands and a 4-phenylthiazole derivative

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DMSO-d₆

— 11.99

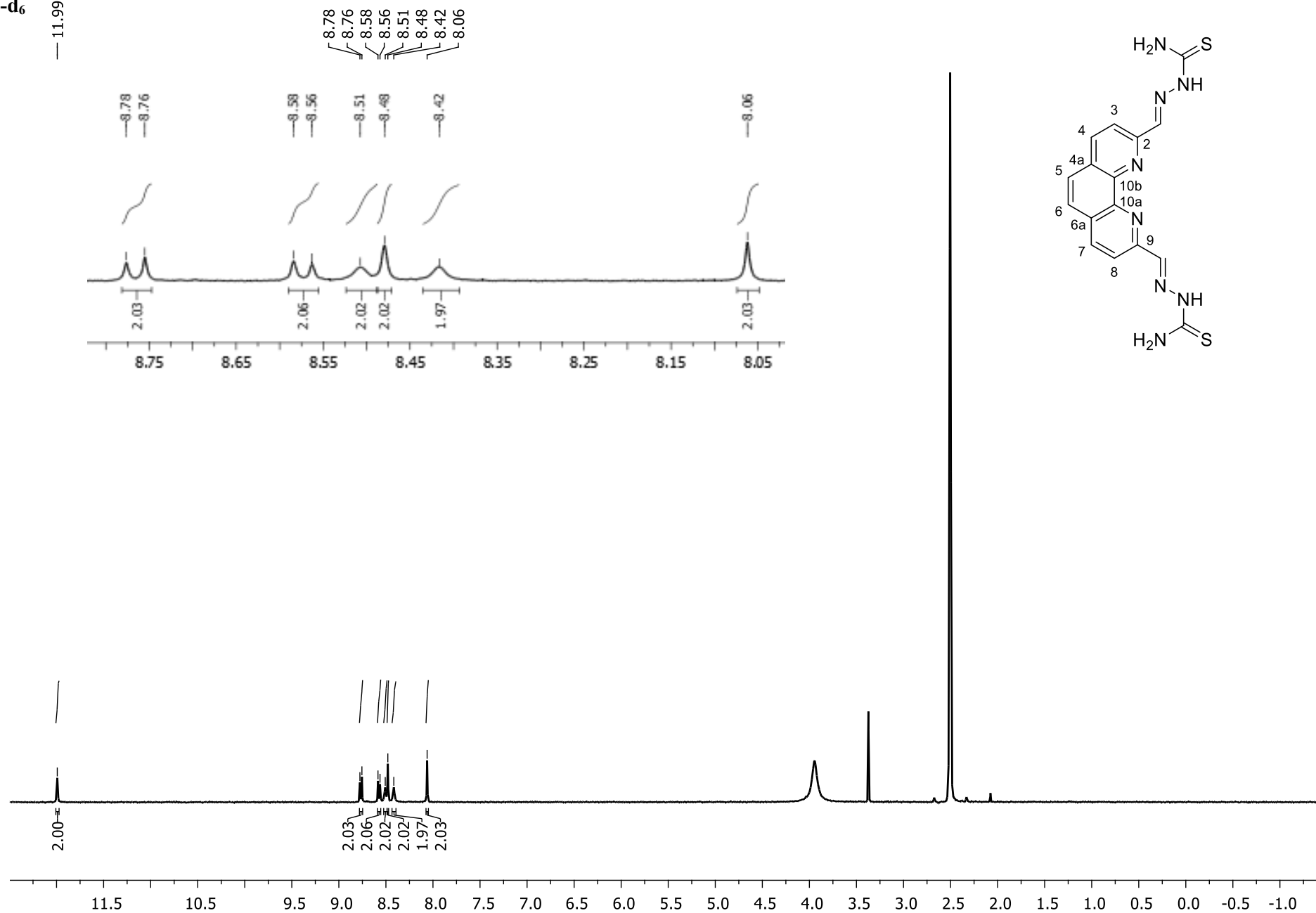


Figure S1. ¹H NMR (400 MHz, DMSO-d₆) of **1**

DMSO-d₆

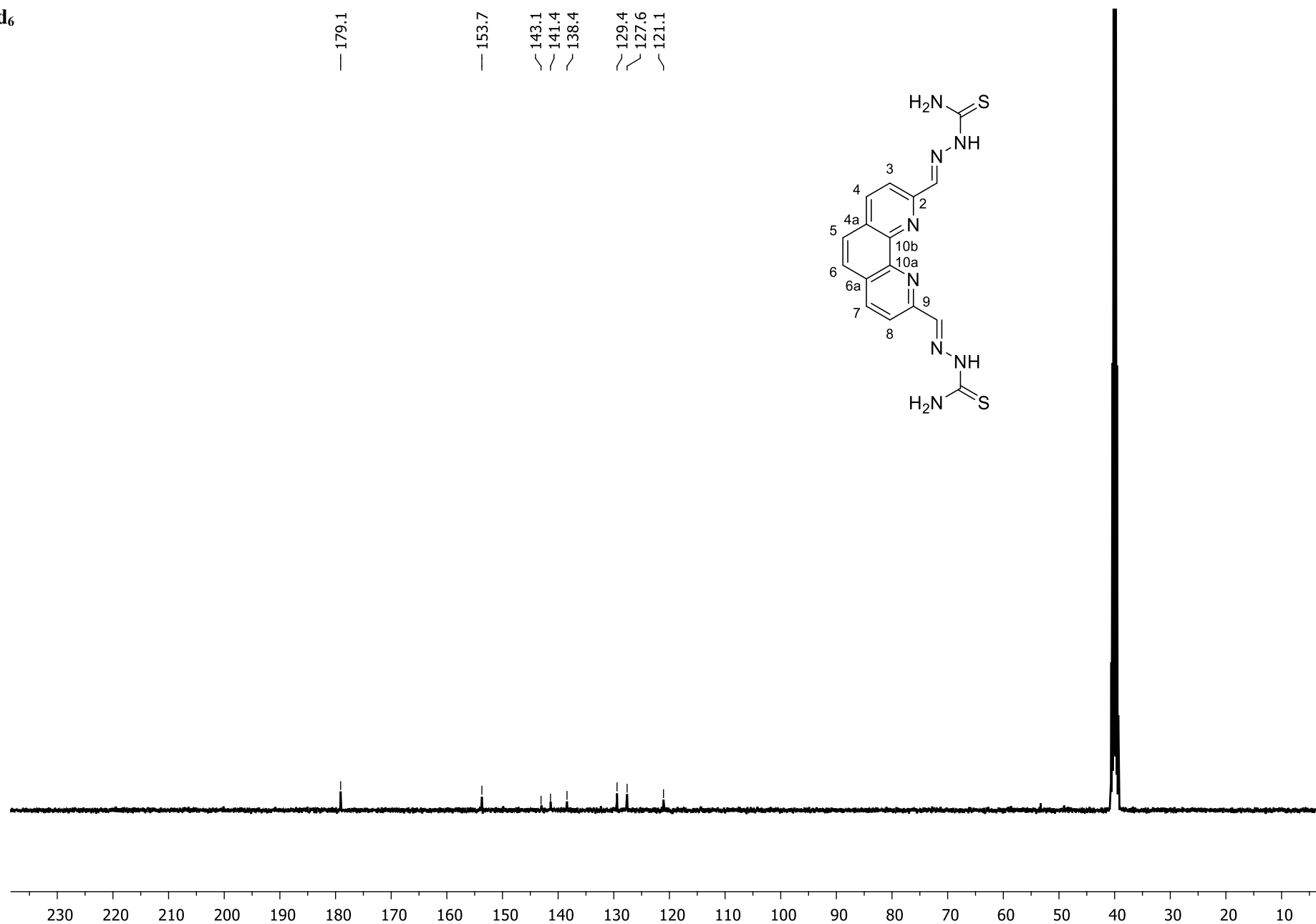


Figure S2. ¹³C NMR (101 MHz, DMSO-d₆) of **1**

DMSO-d₆

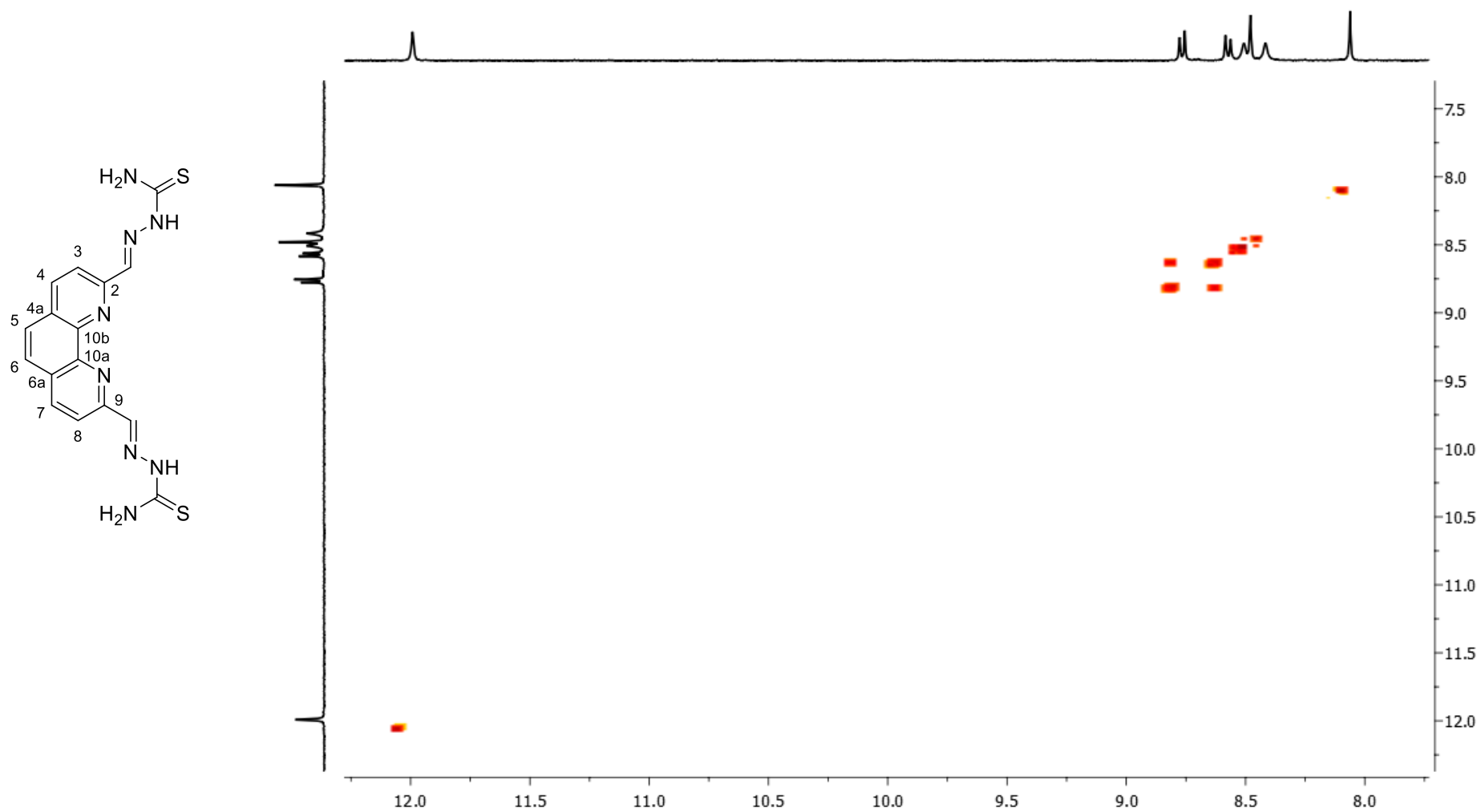


Figure S3. ¹H-¹H-COSY (400 MHz, DMSO-d₆) of **1**

DMSO-d₆

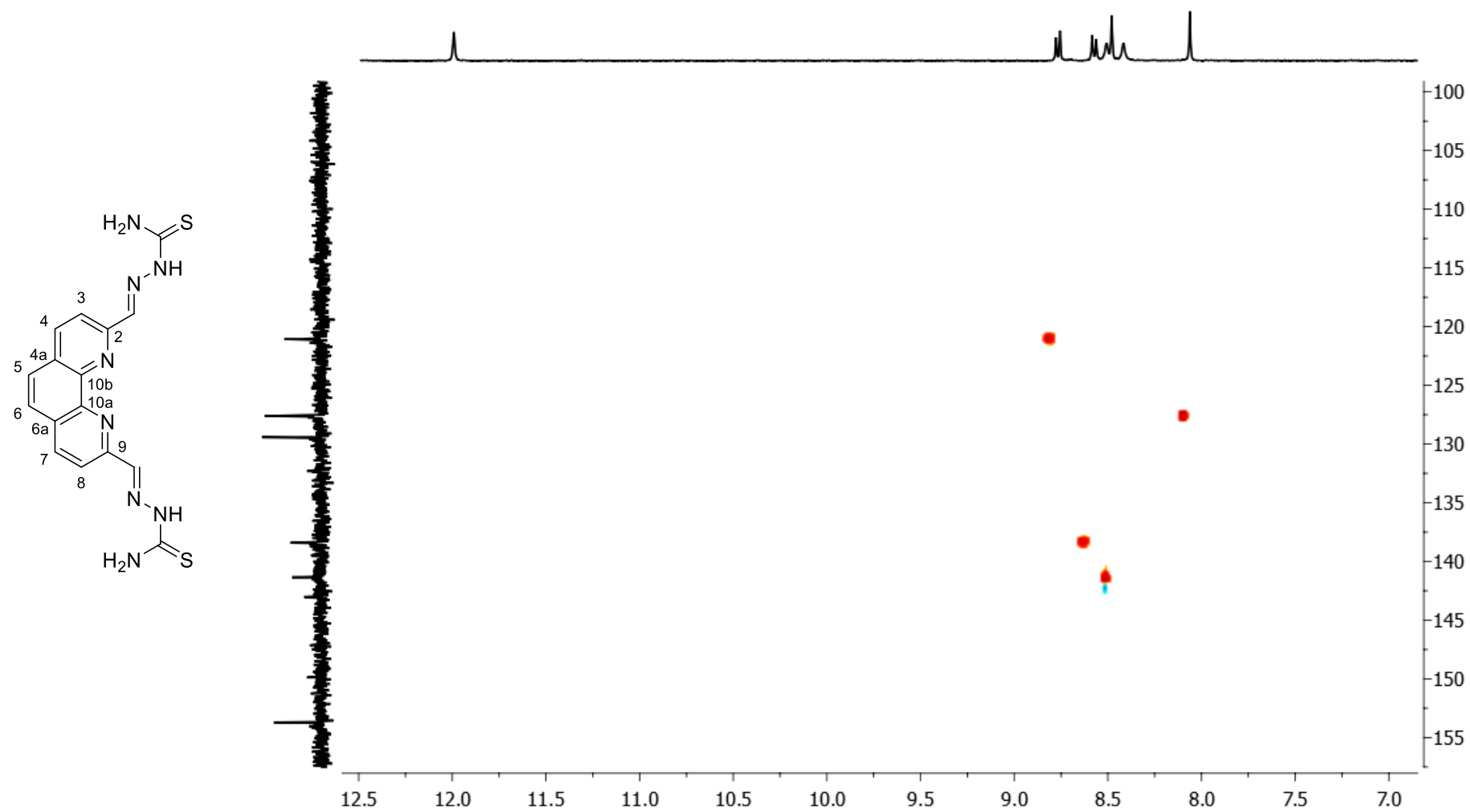


Figure S4. ¹H-¹³C-HSQC (400 MHz, DMSO-d₆) of **1**

DMSO-d₆

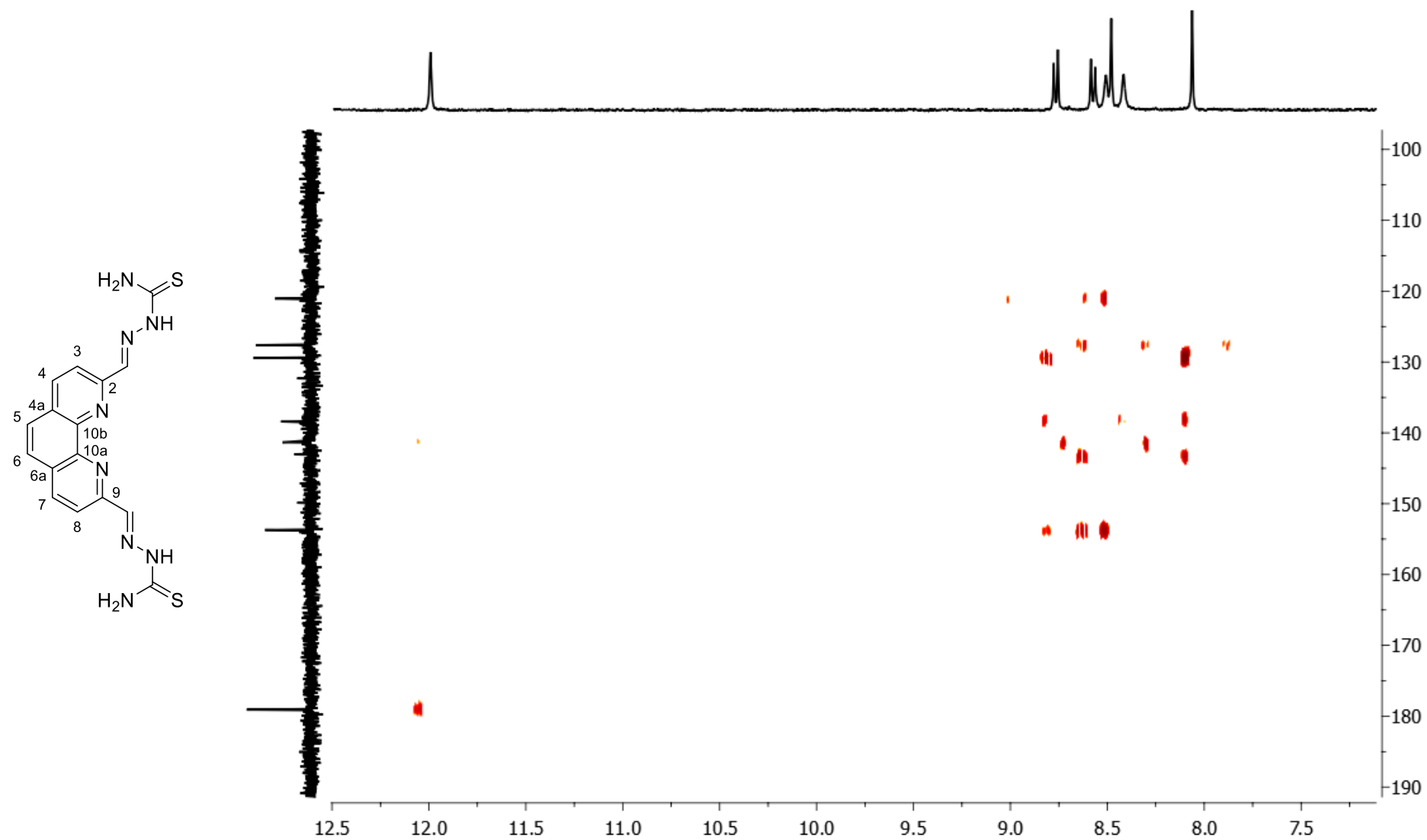


Figure S5. ¹H-¹³C-HMBC (400 MHz, DMSO-d₆) of **1**

DMSO-d₆

— 12.02

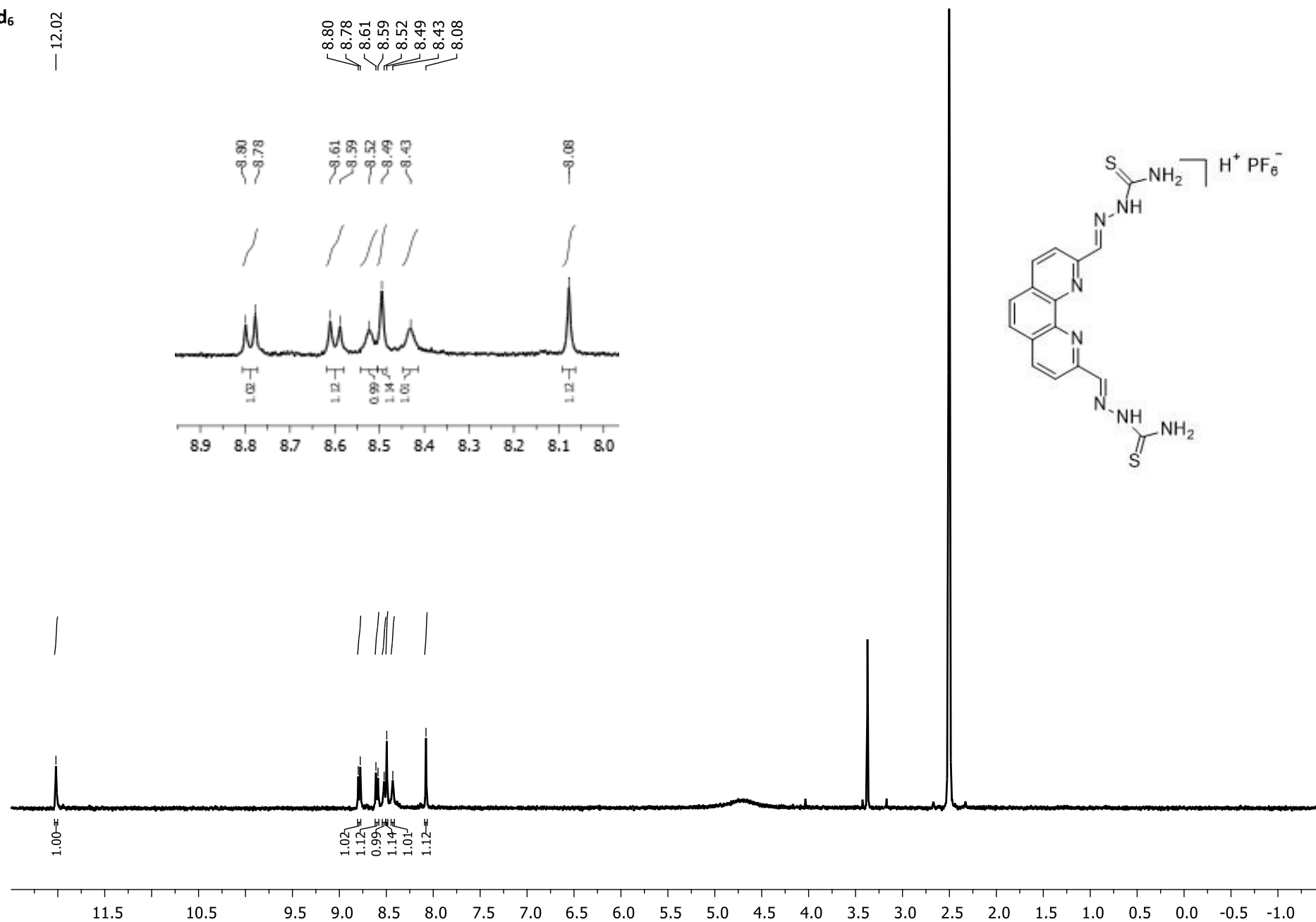


Figure S6. ¹H NMR (400 MHz, DMSO-d₆) of **2**

DMSO-d₆

— 179.0

— 154.0

— 144.5

— 142.4

— 137.6

— 129.3

— 127.5

— 120.7

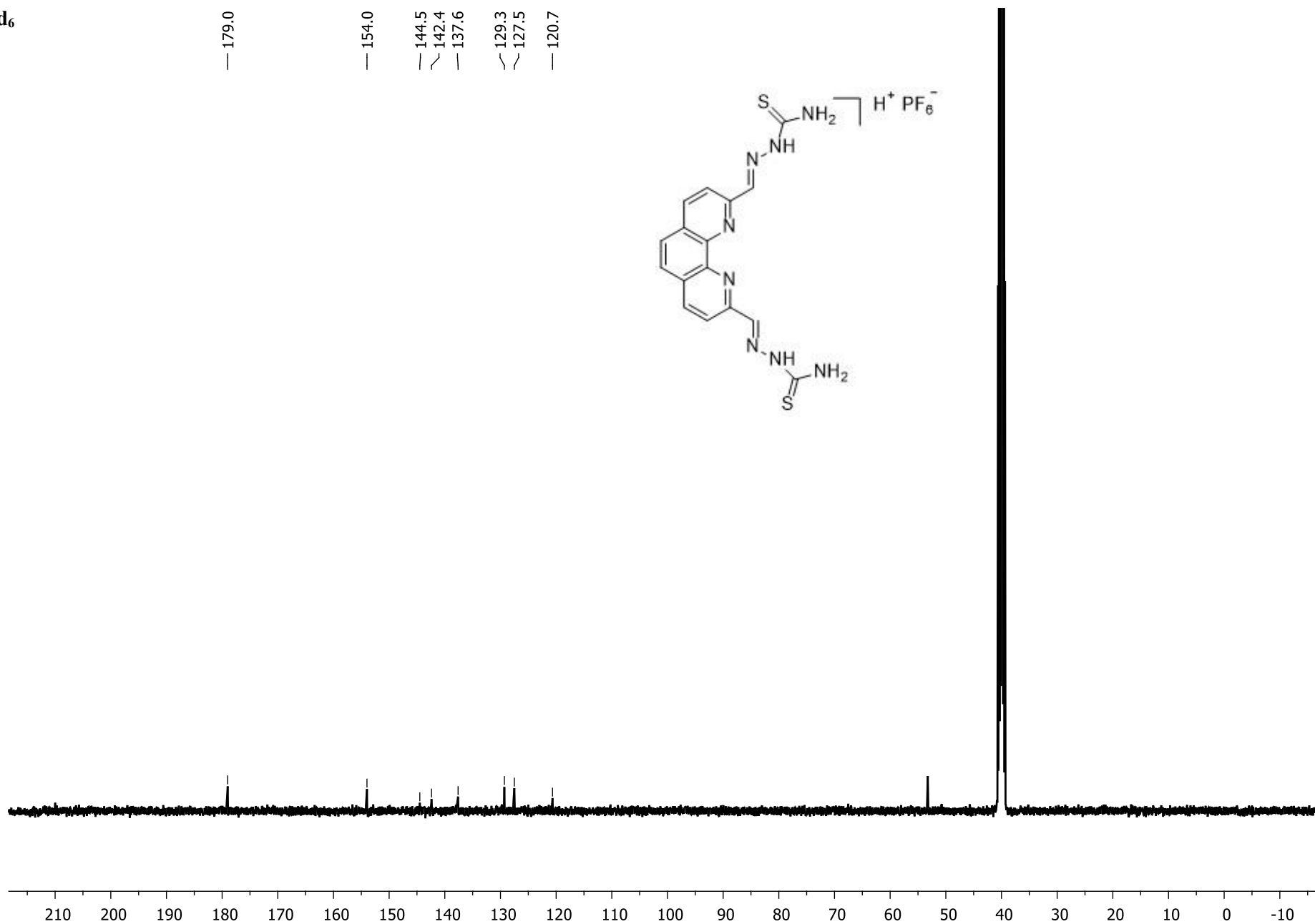
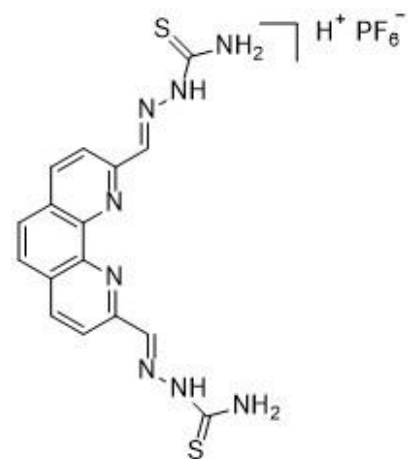
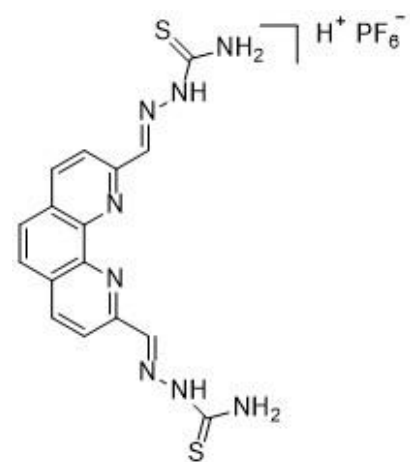


Figure S7. ¹³C NMR (101 MHz, DMSO-d₆) of **2**

DMSO-d₆



-69.20
-71.08

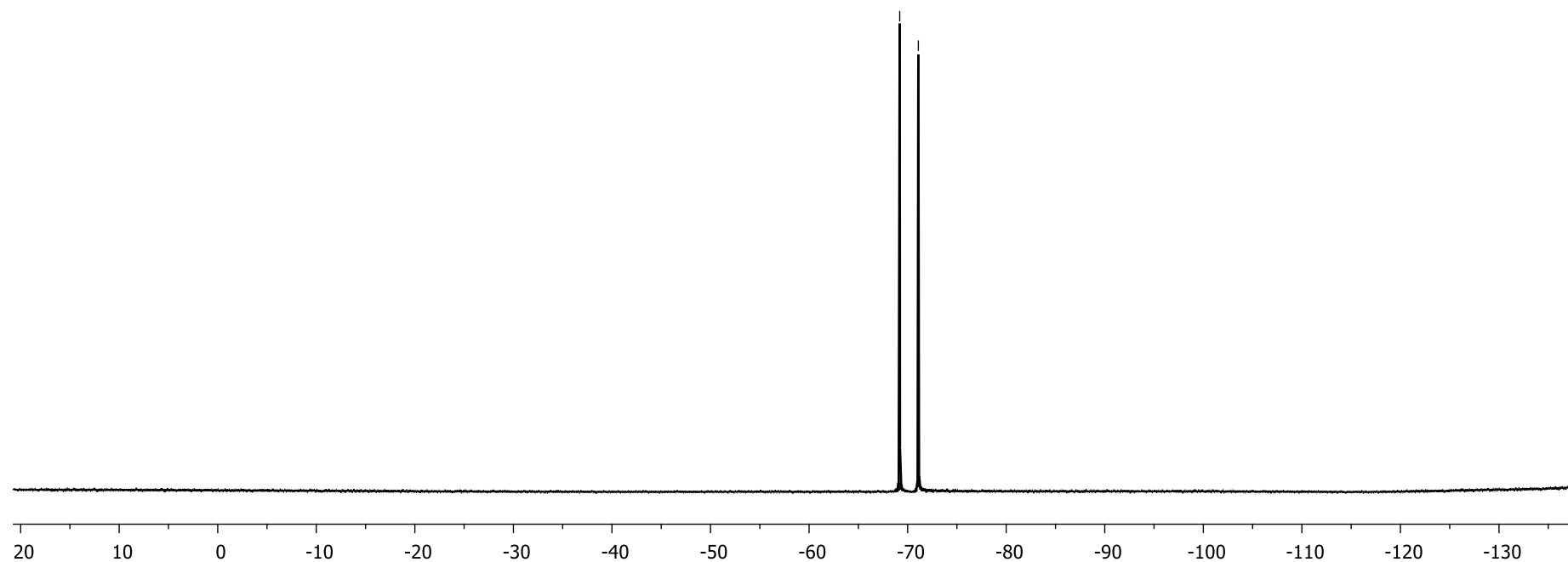


Figure S8. ¹⁹F NMR (376 MHz, DMSO-d₆) of **2**

DMSO-d₆

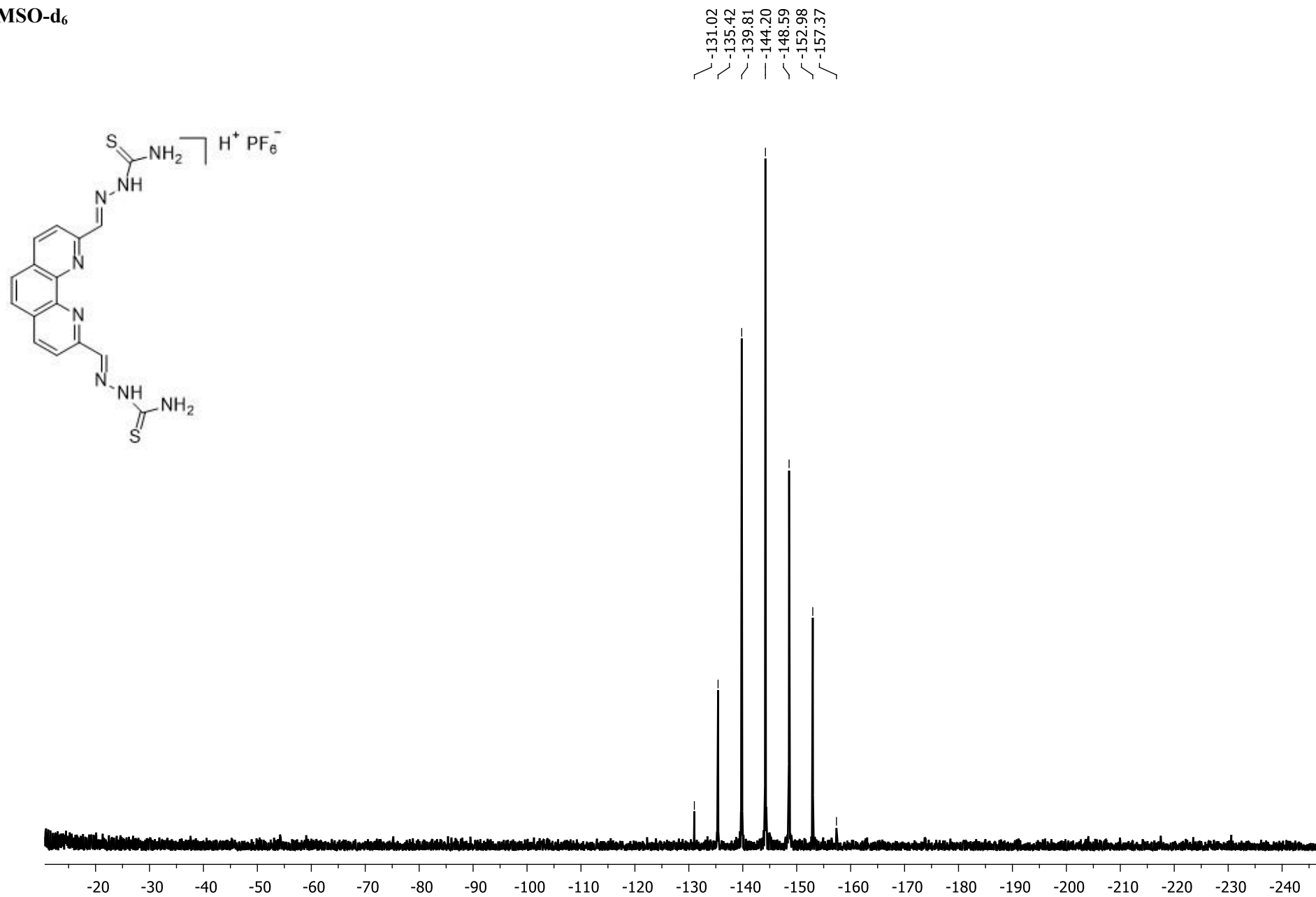


Figure S9. ³¹P NMR (162 MHz, DMSO-d₆) of **2**

DMSO-d₆

— 12.01

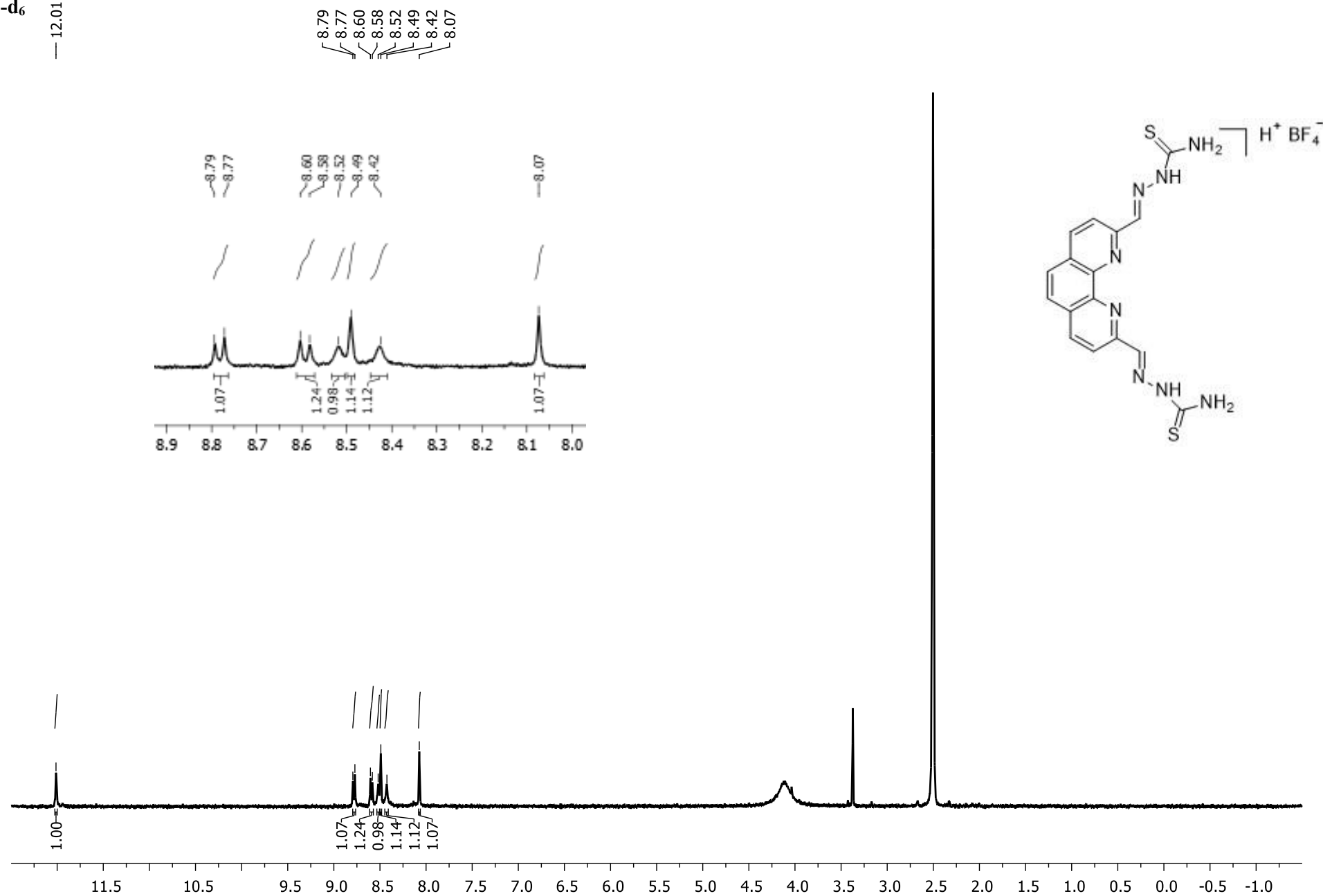


Figure S10. ¹H NMR (400 MHz, DMSO-d₆) of **3**

DMSO-d₆

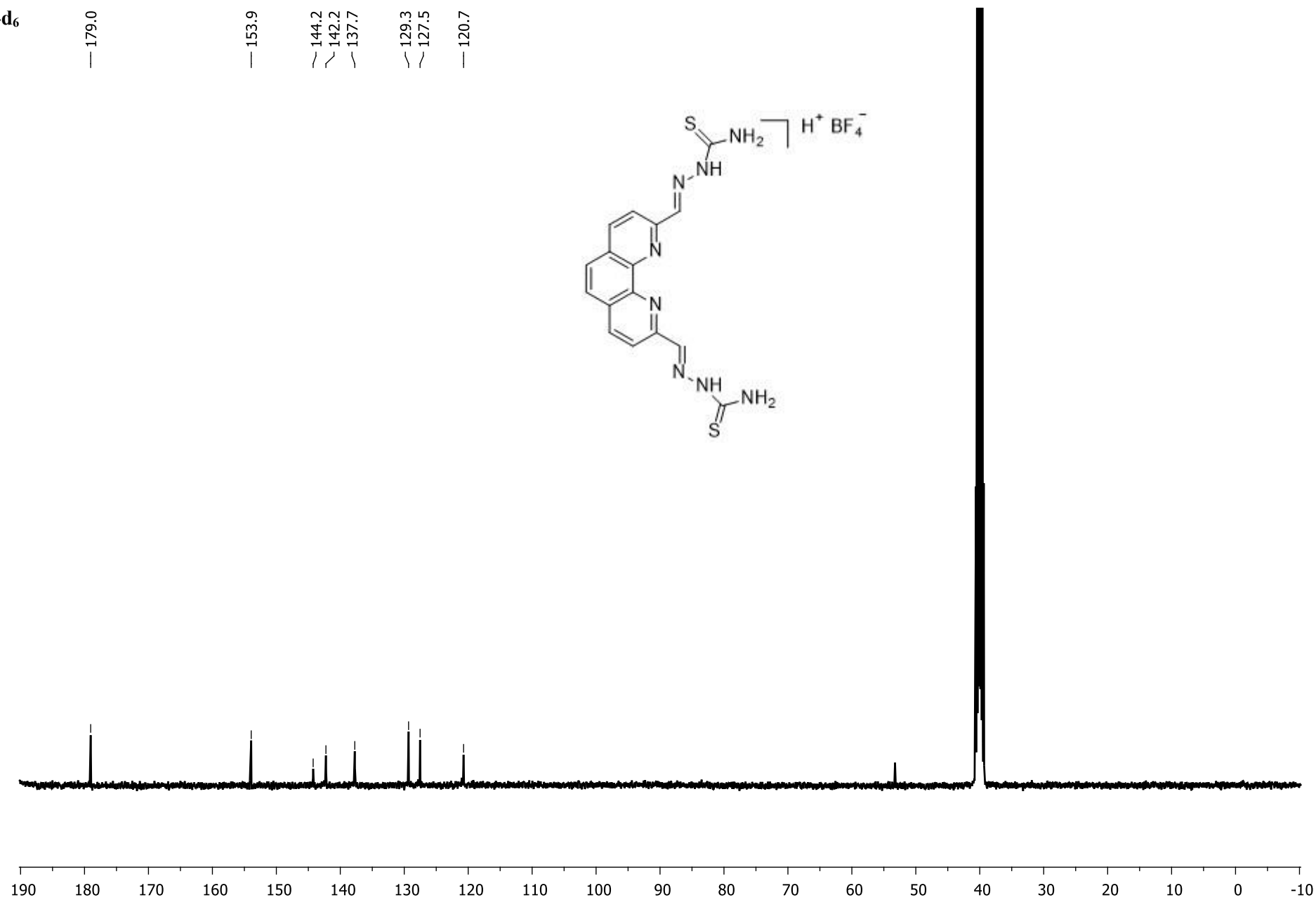


Figure S11. ¹³C NMR (101 MHz, DMSO-d₆) of **3**

DMSO-d₆

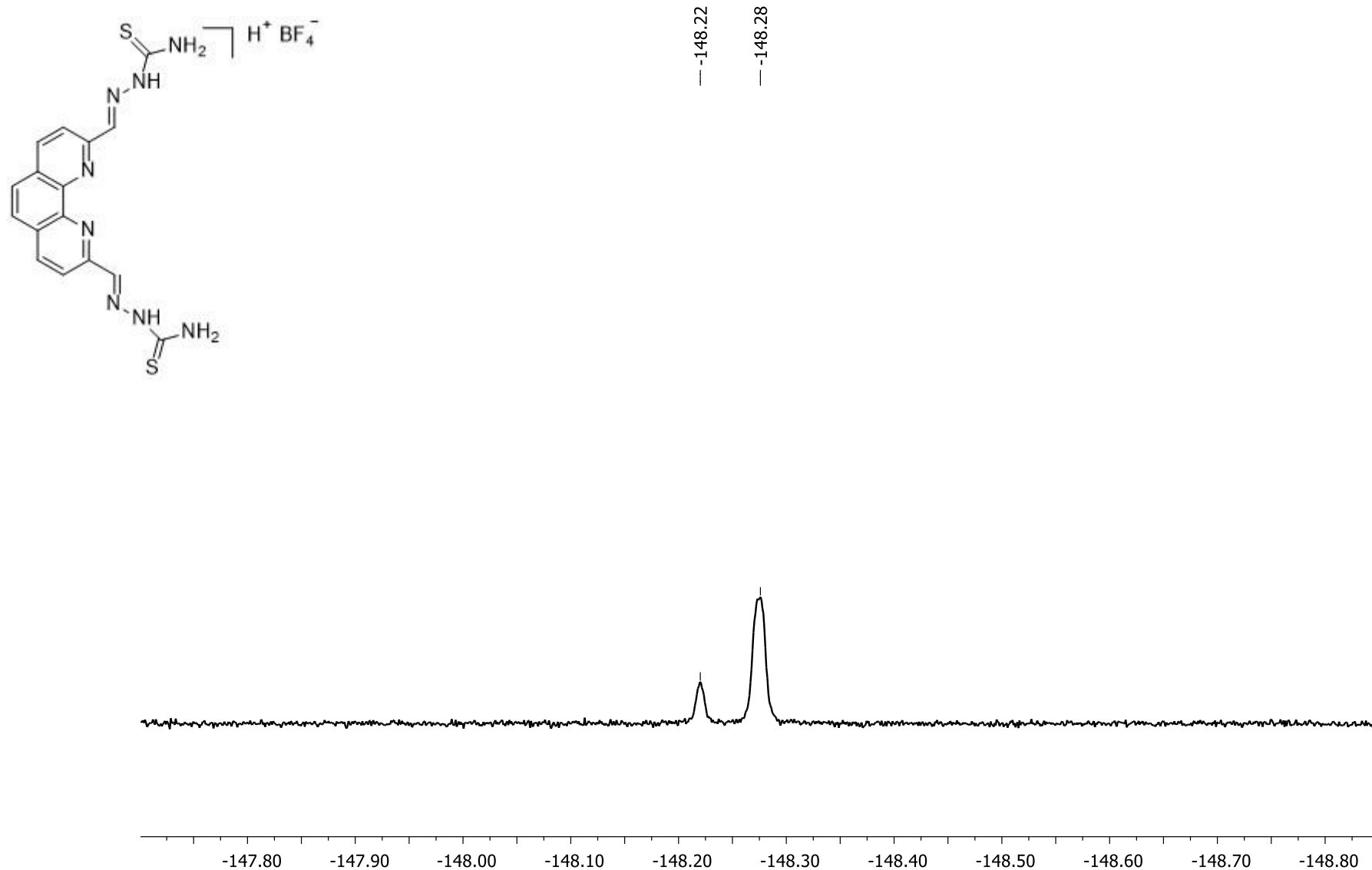


Figure S12. ¹⁹F NMR ((376 MHz, DMSO-d₆) of **3**

DMSO-d₆

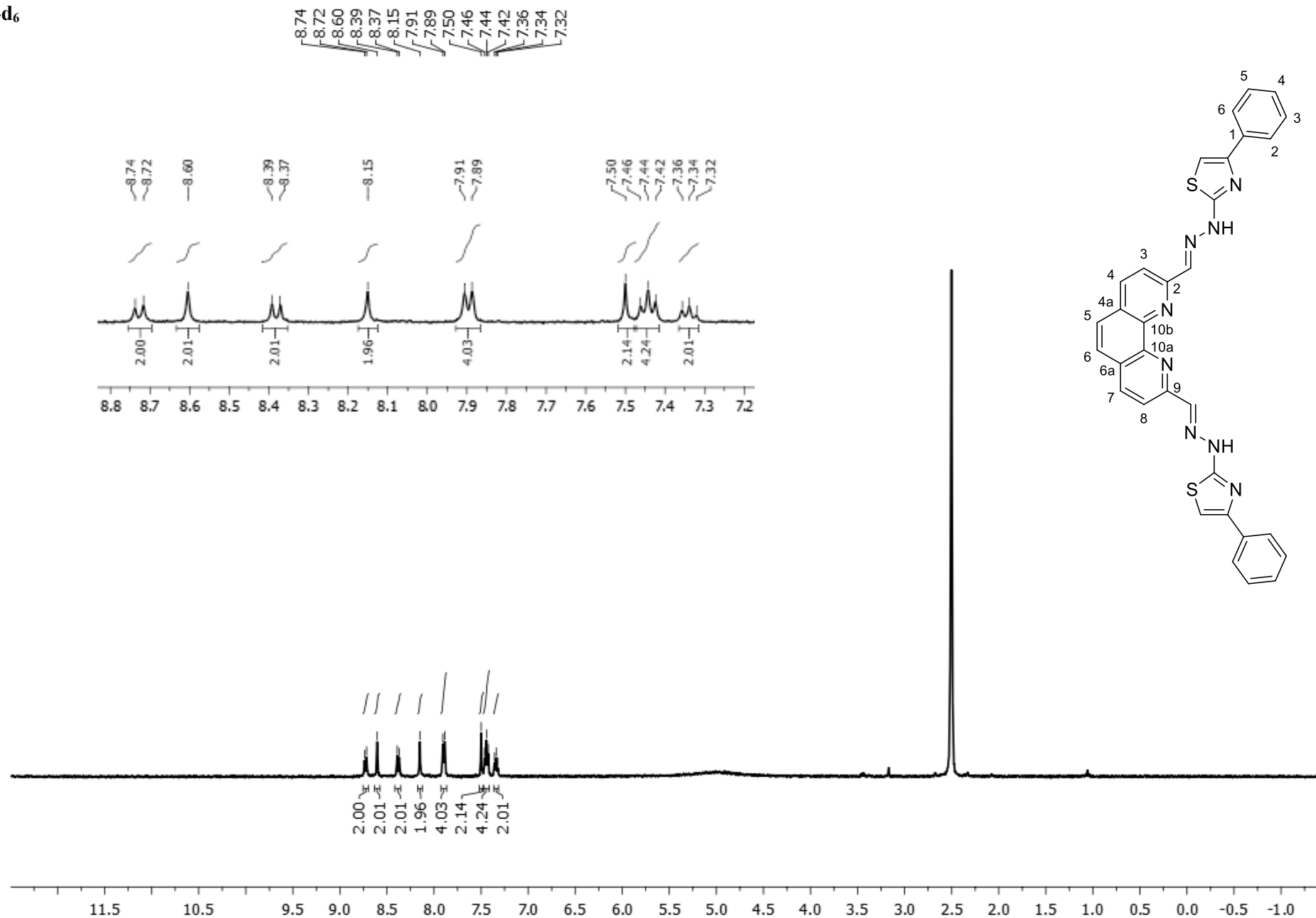


Figure S13. ¹H NMR (400 MHz, DMSO-d₆) of 4

DMSO-d₆

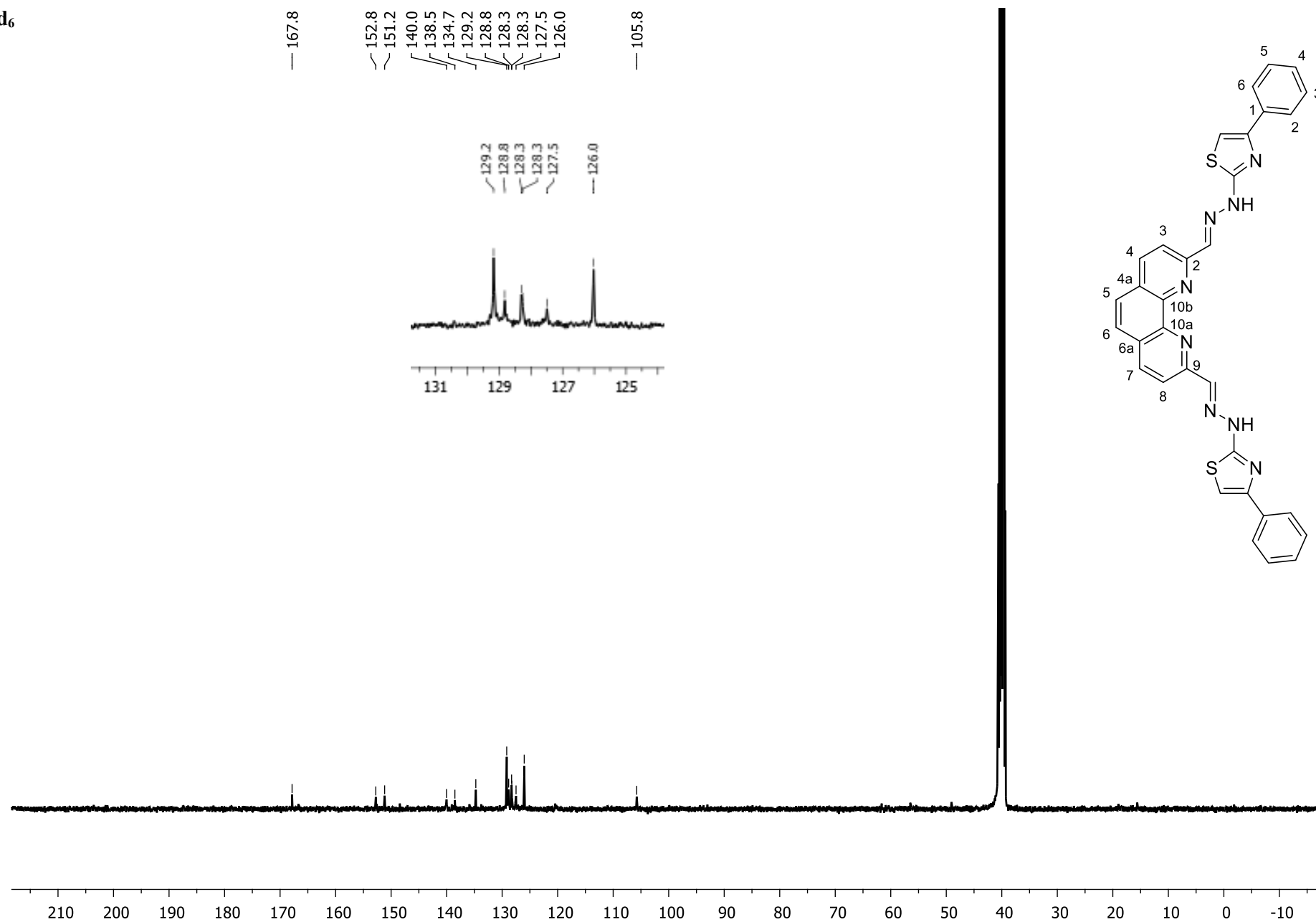


Figure S14. ¹³C NMR (101 MHz, DMSO-d₆) of **4**

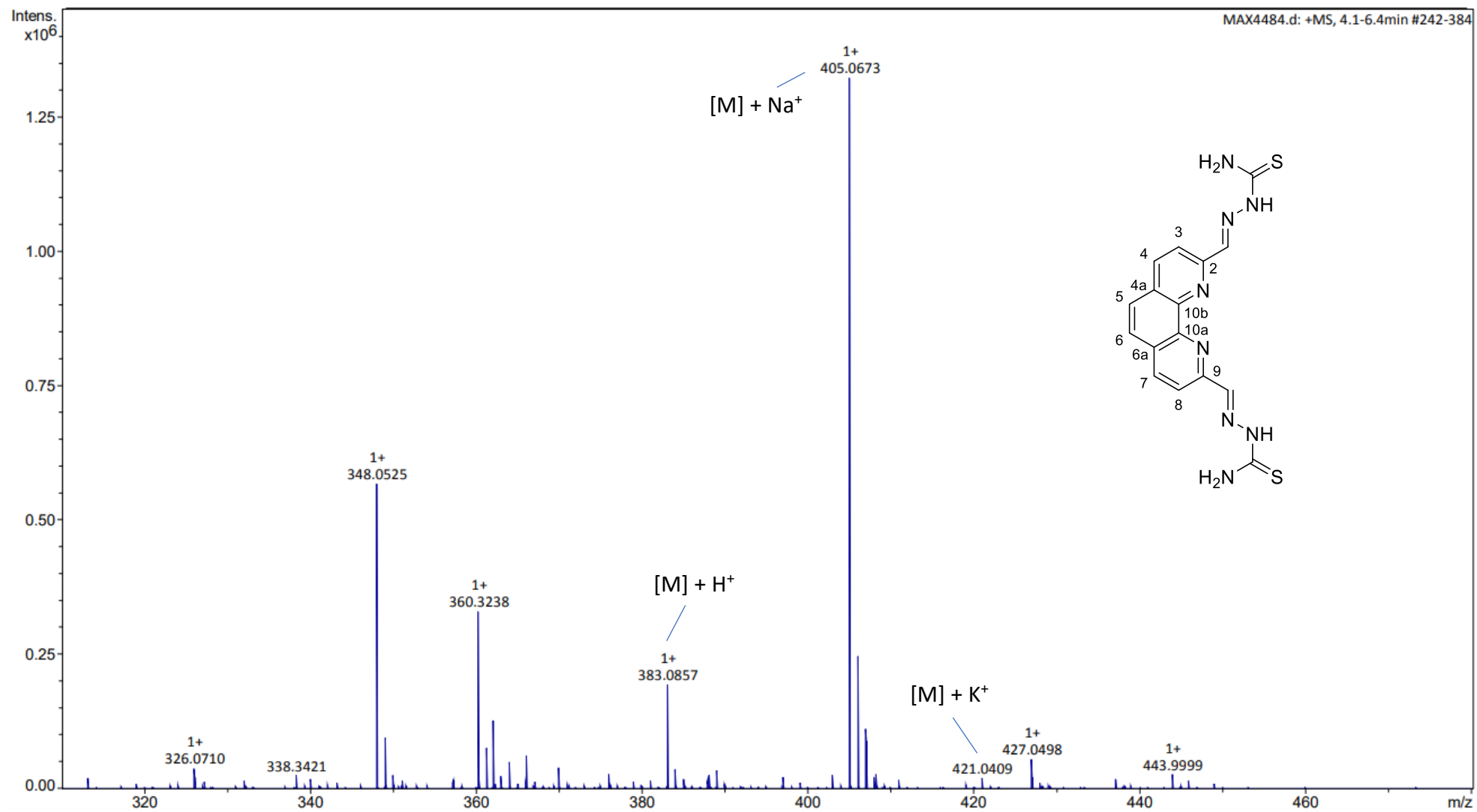


Figure S15. Zoomed view of high-resolution electrospray ionization mass spectrum (ESI-HRMS-pos) of **1** (MeOH, 1% formic acid)

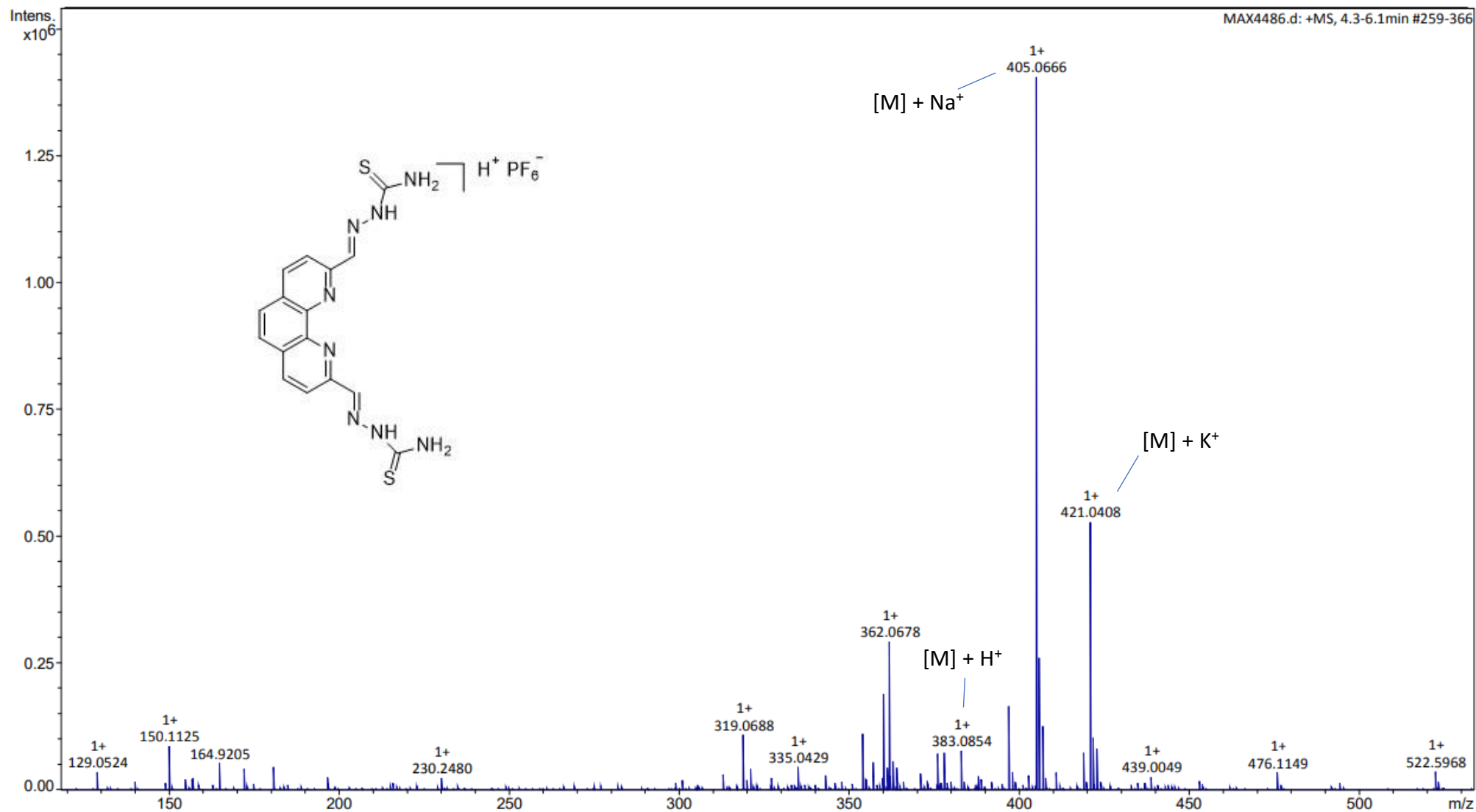


Figure S16. Zoomed view of high-resolution electrospray ionization mass spectrum (ESI-HRMS-pos) of **2** (MeOH, 1% formic acid)

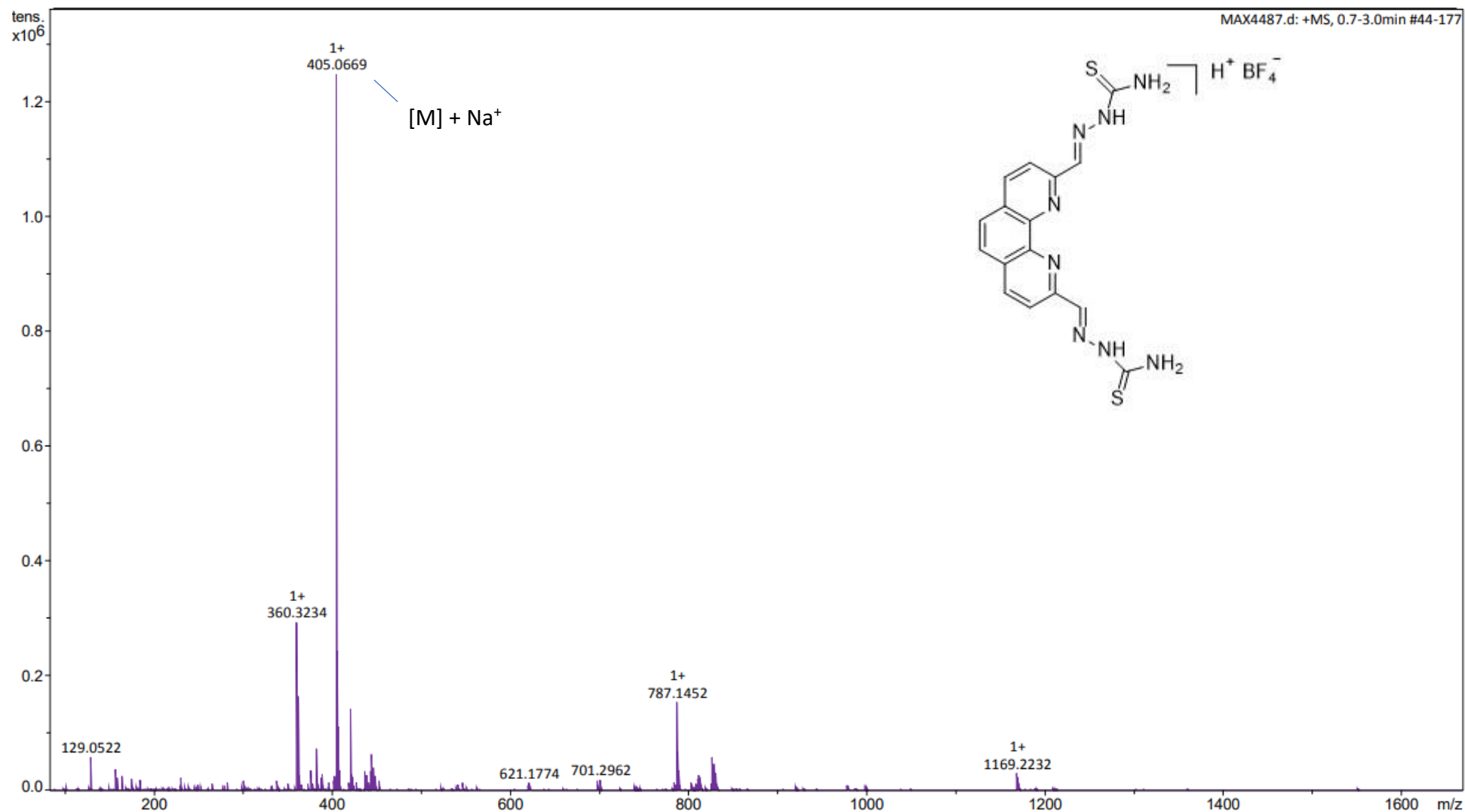


Figure S17. High-resolution electrospray ionization mass spectrum (ESI-HRMS-pos) of **3** (MeOH, 1% formic acid)

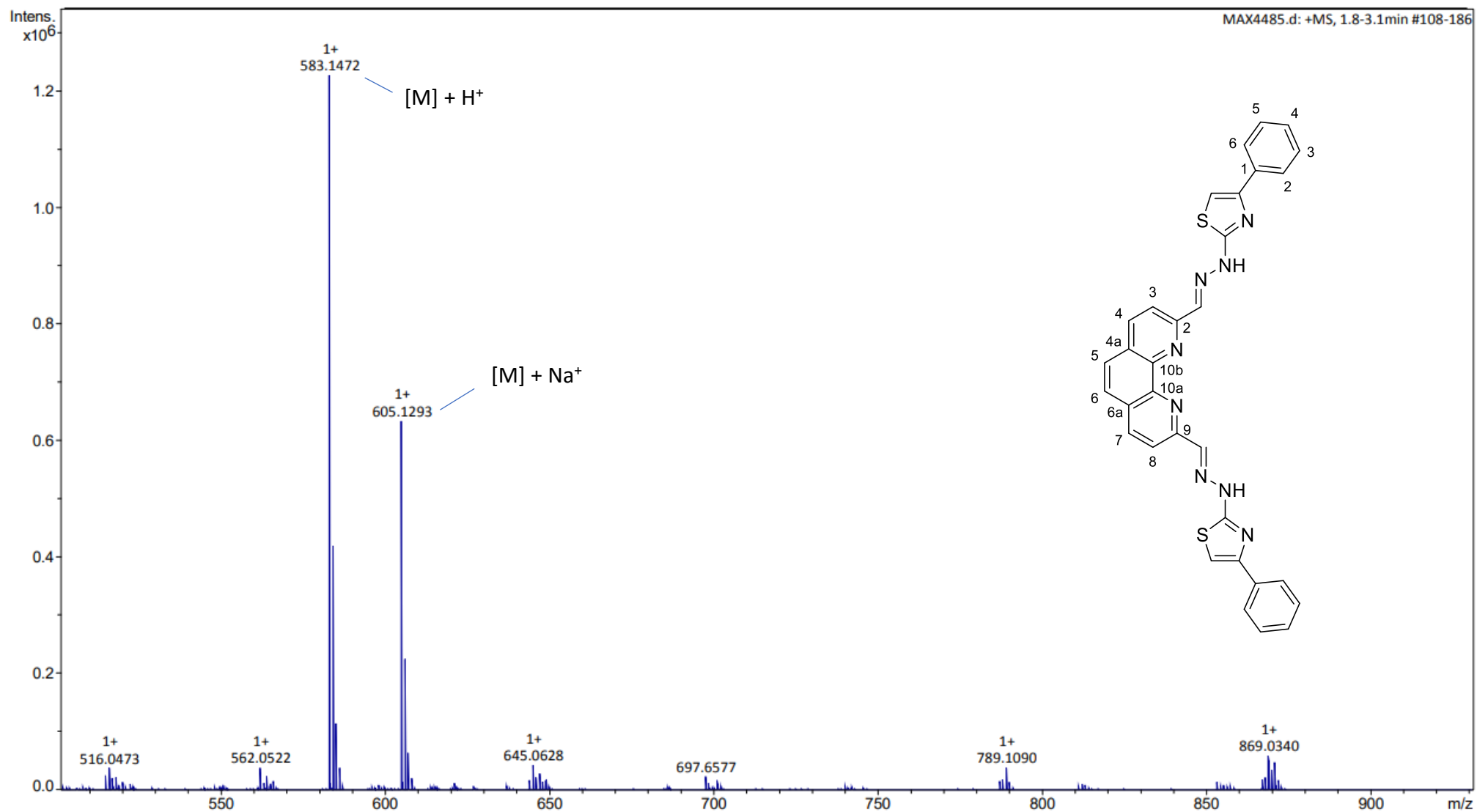


Figure S18. Zoomed view of high-resolution electrospray ionization mass spectrum (ESI-HRMS-pos) of **4** (MeOH, 1% formic acid)

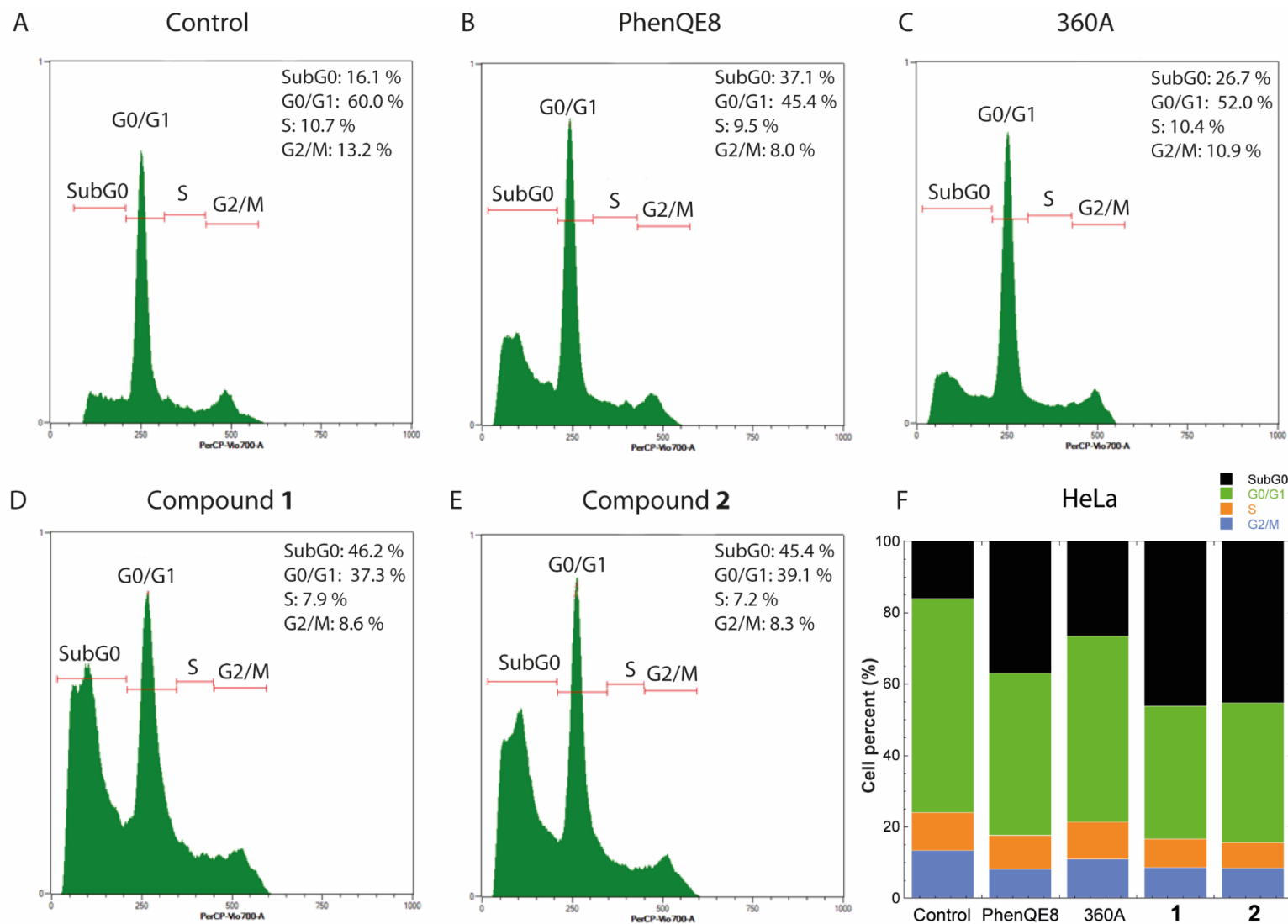


Figure S19. HeLa cell cycle histograms after 72 h treatment with $\frac{1}{2}$ IC₅₀ compound concentration. A) Untreated cells (negative control); B) PhenQE8 (structural analogue with antitumor properties, positive control); C) 360A (antitumor agent, positive control); D) compound **1**; E) compound **2**, and F) Stack bar graph representing averaged cell percents in each cycle phase and SubG0 after compound treatment. Increase in the SubG0 population percent is associated to apoptosis.