

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

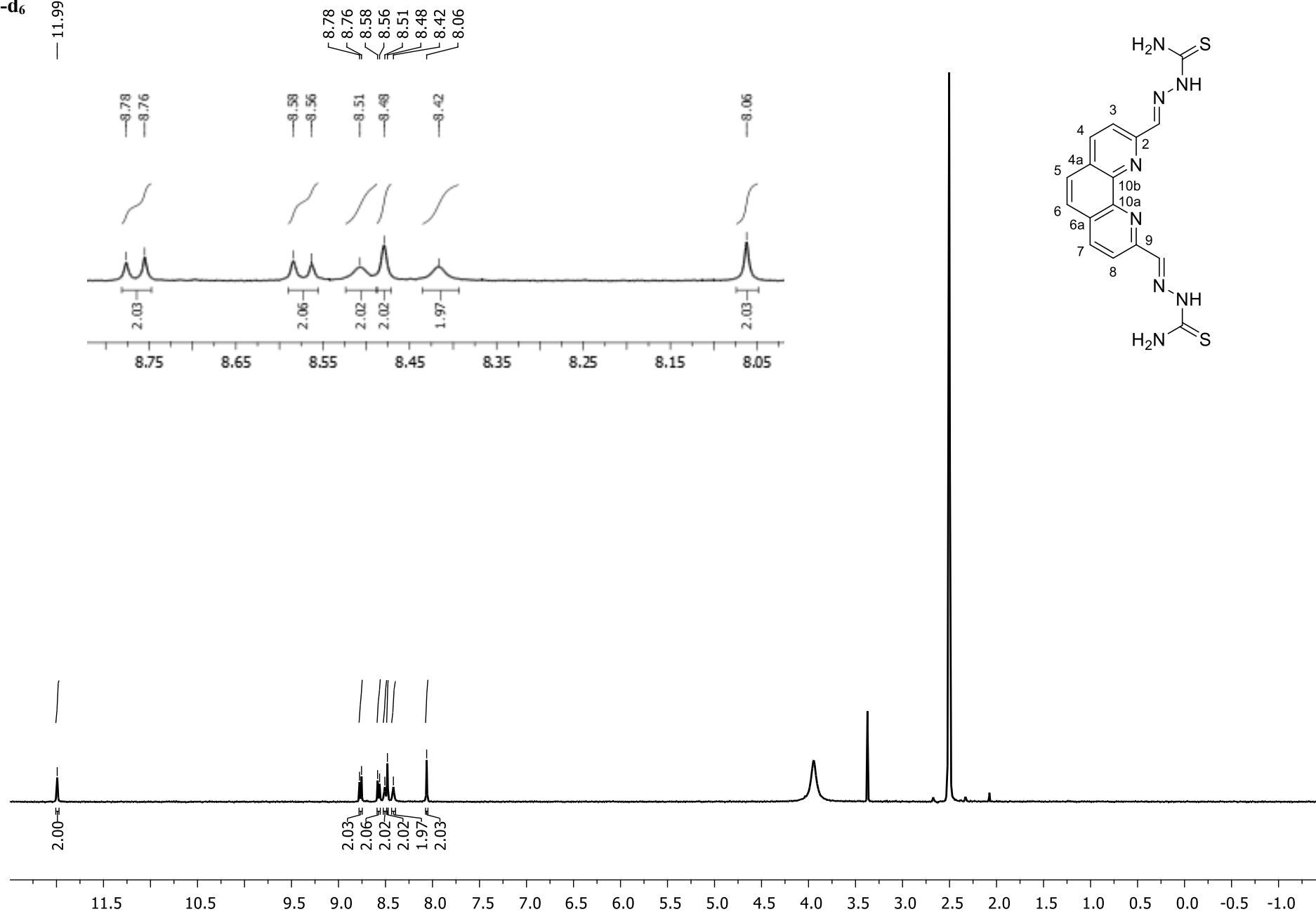


Figure S1. ¹H NMR (400 MHz, DMSO-d₆) of **1**

DMSO-d₆

— 179.1
— 153.7
~ 143.1
~ 141.4
~ 138.4
~ 129.4
~ 127.6
~ 121.1

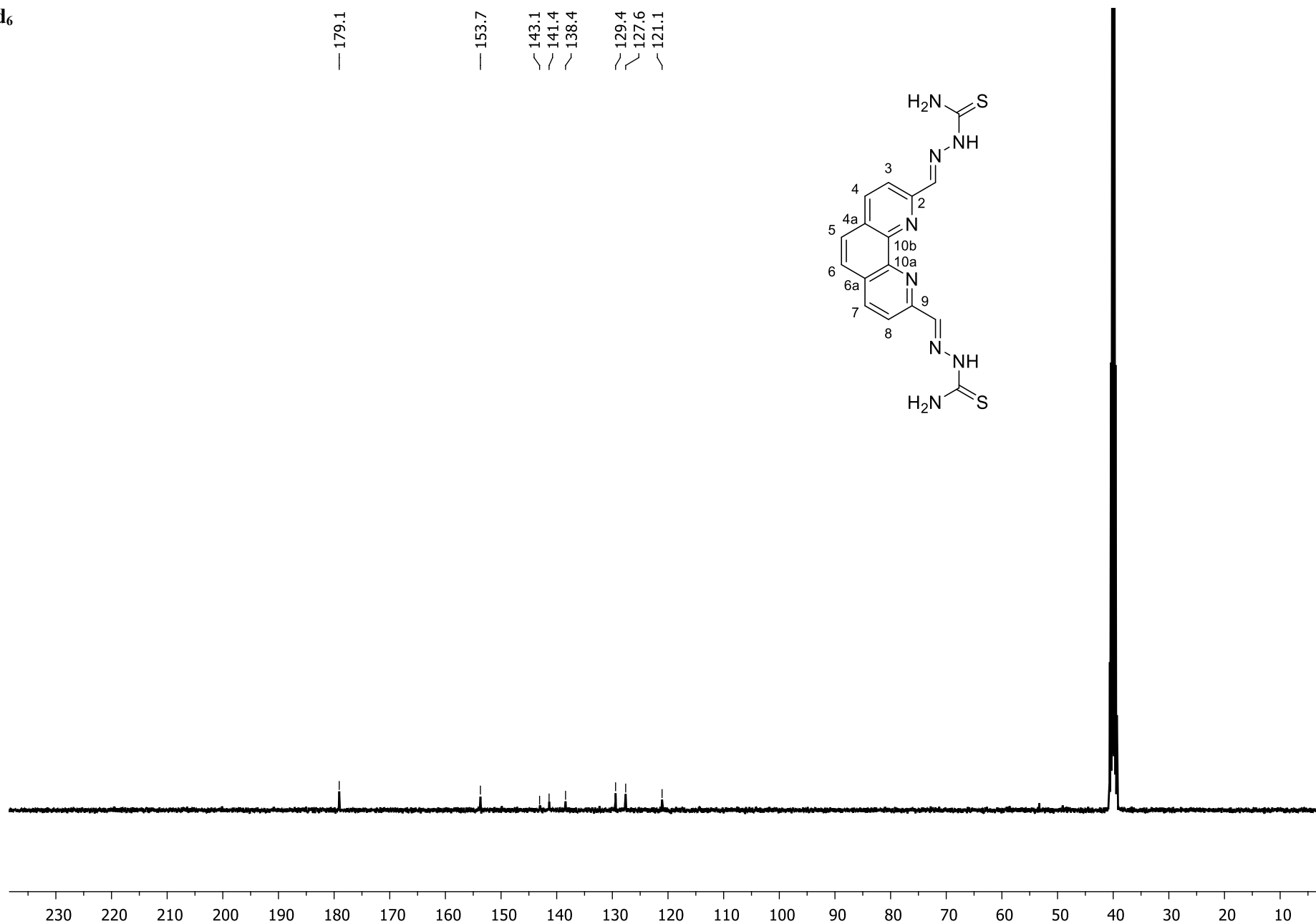
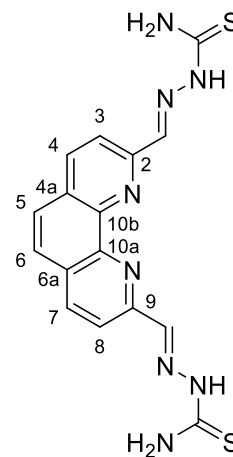


Figure S2. ¹³C NMR (101 MHz, DMSO-d₆) of **1**

DMSO-d₆

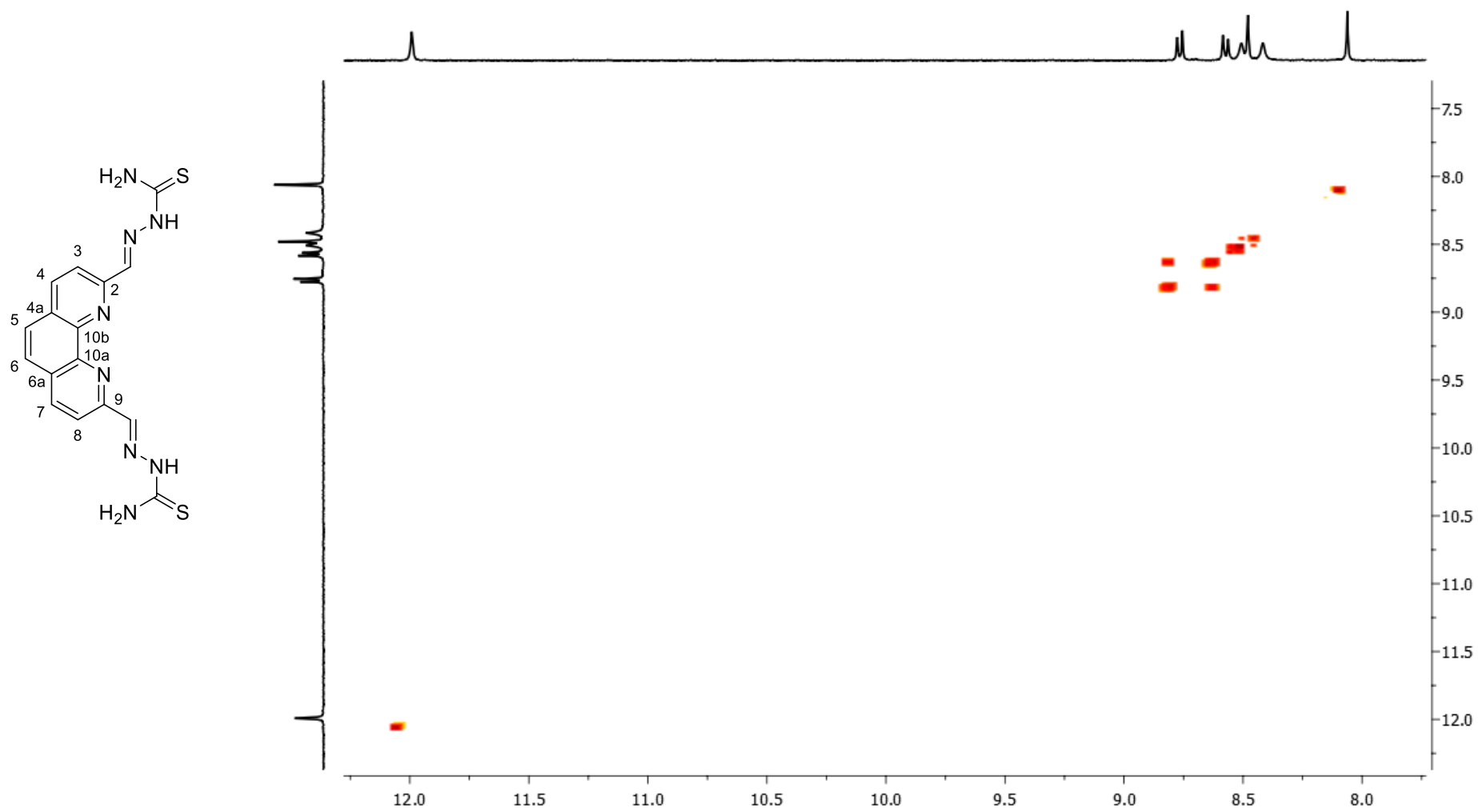


Figure S3. ¹H-¹H-COSY (400 MHz, DMSO-d₆) of **1**

DMSO-d₆

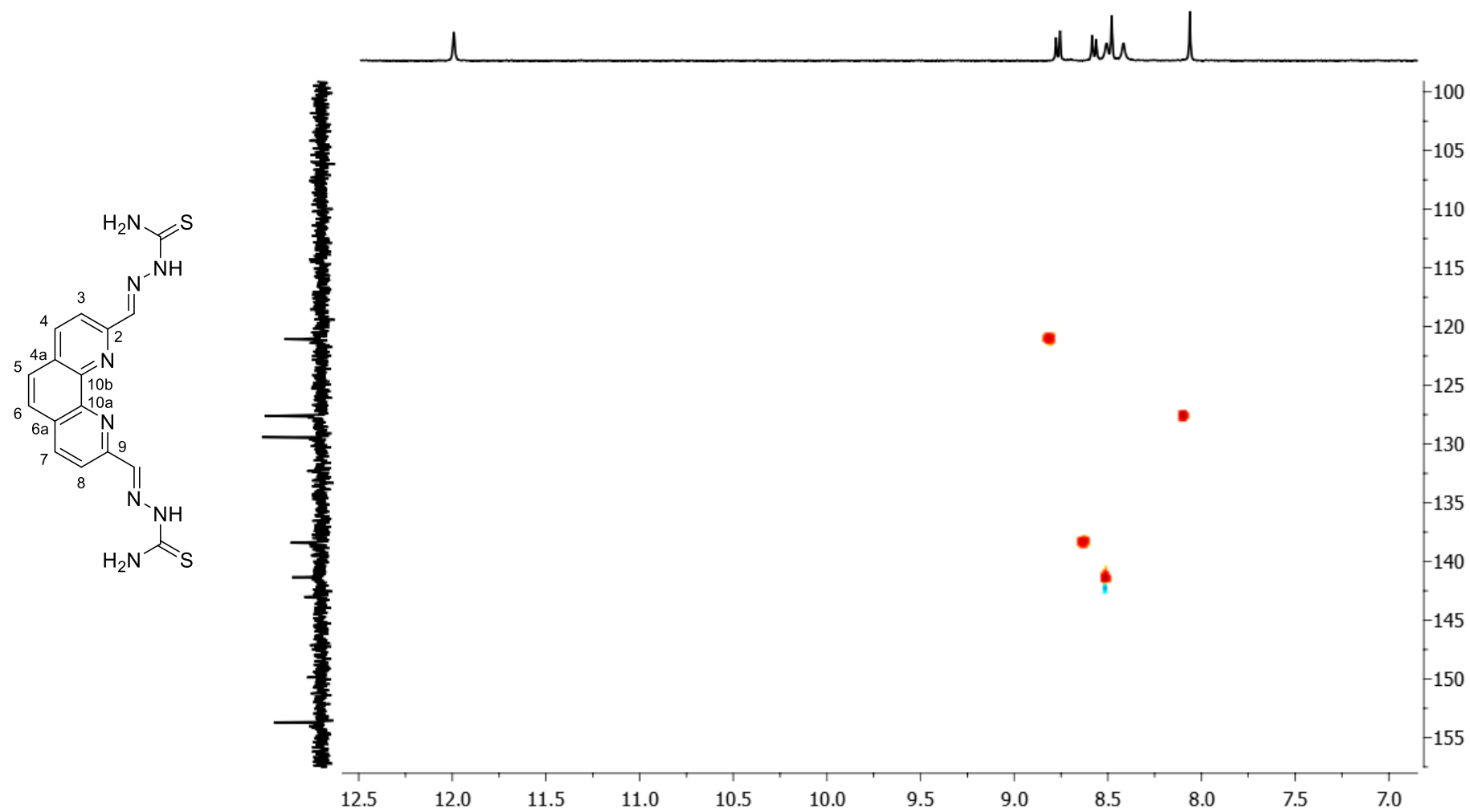


Figure S4. ¹H-¹³C-HSQC (400 MHz, DMSO-d₆) of **1**

DMSO-d₆

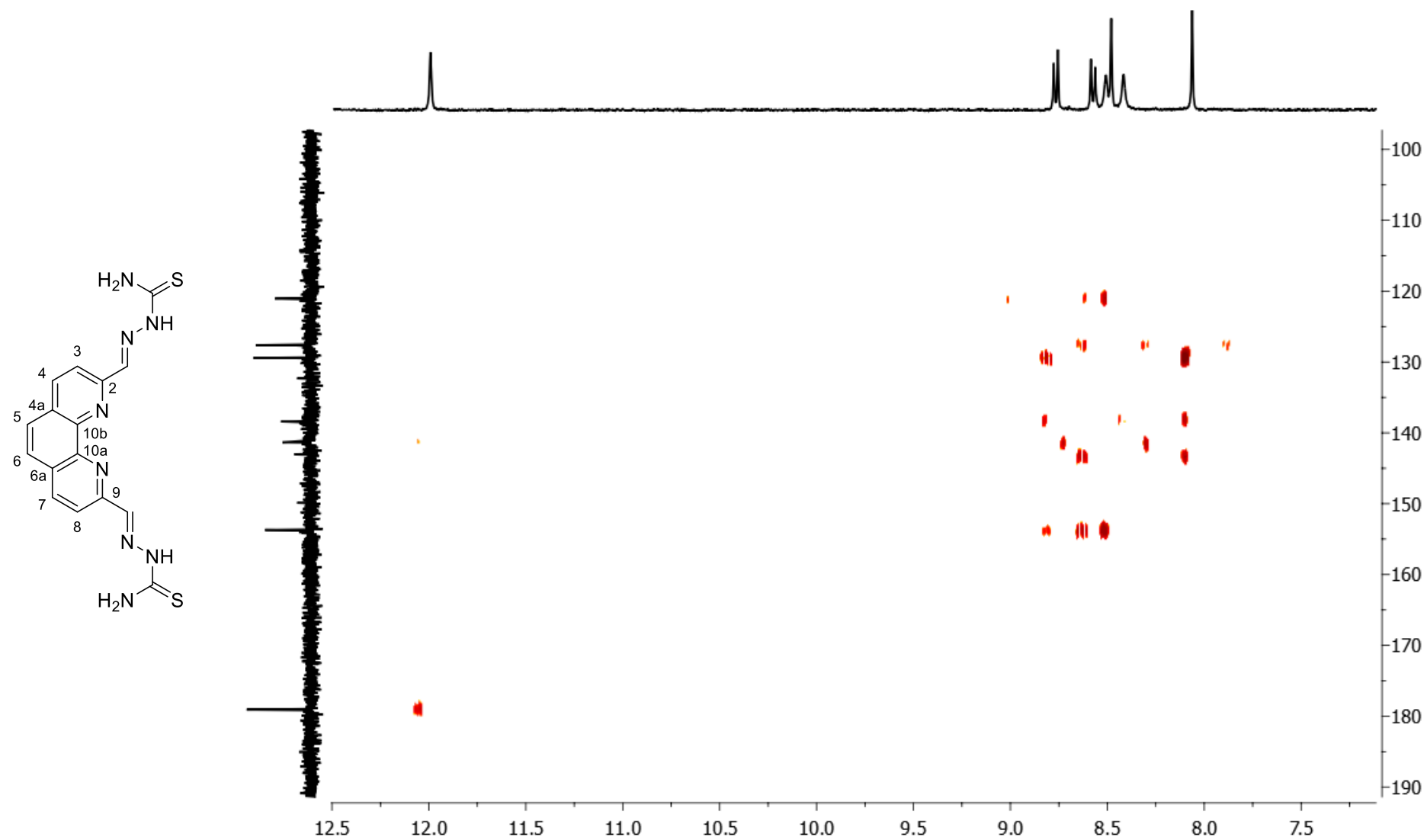


Figure S5. ¹H-¹³C-HMBC (400 MHz, DMSO-d₆) of **1**

DMSO-d₆

— 12.02

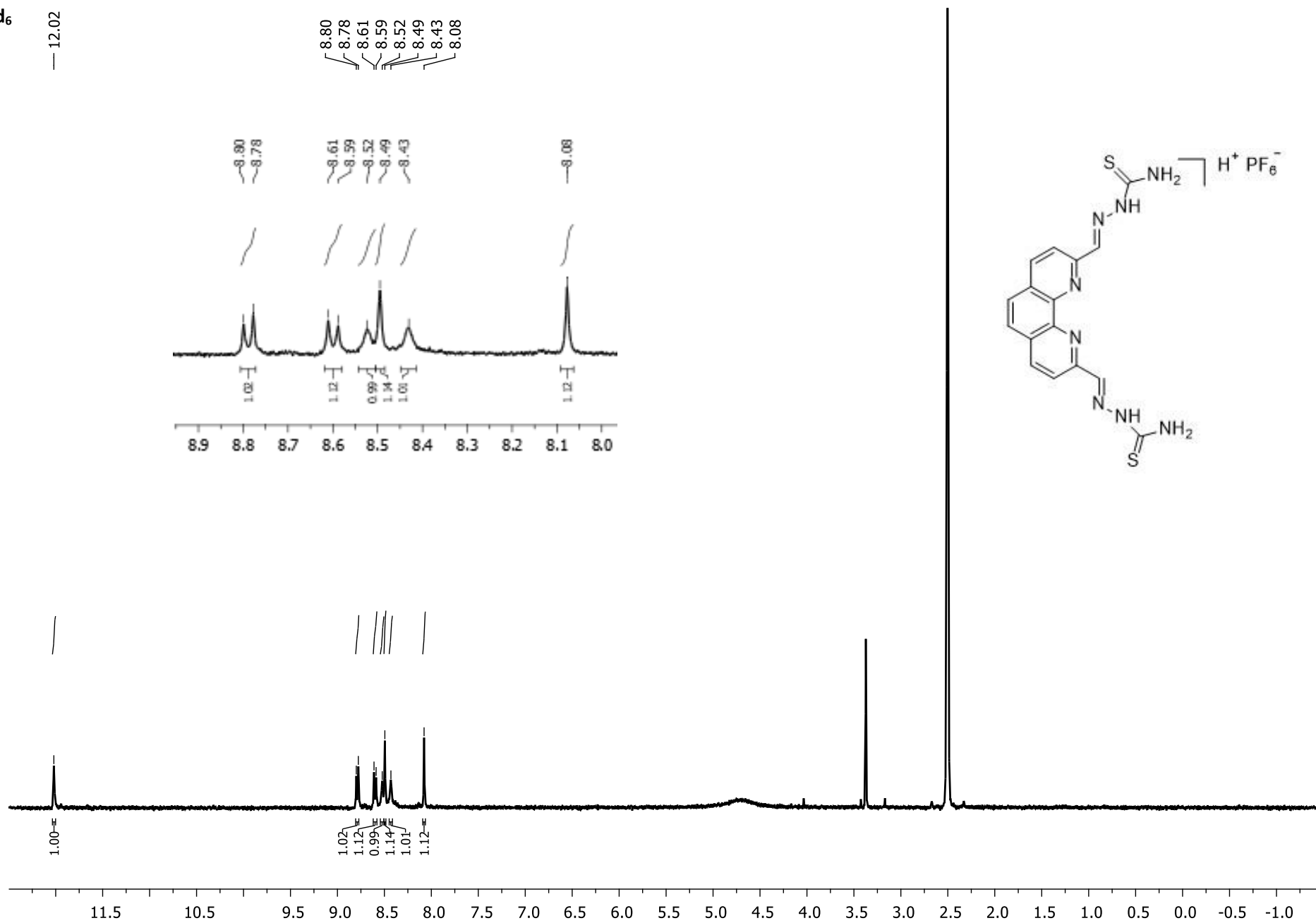


Figure S6. ¹H NMR (400 MHz, DMSO-d₆) of 2

DMSO-d₆

— 179.0

— 154.0

— 144.5

— 142.4

— 137.6

— 129.3

— 127.5

— 120.7

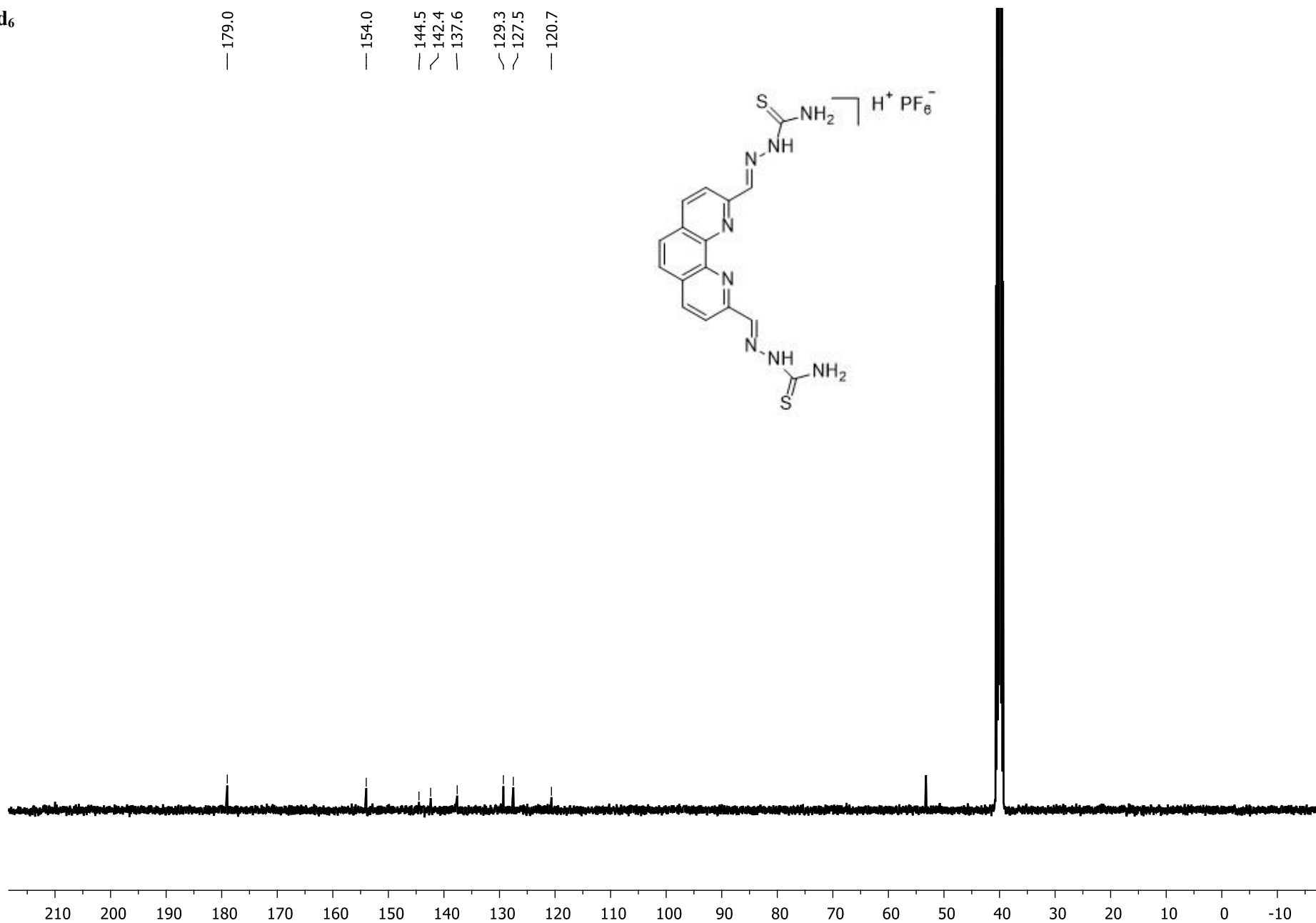
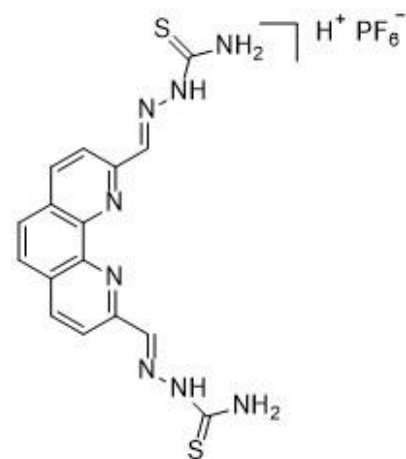
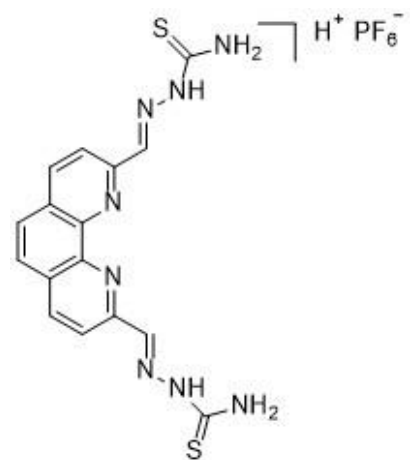


Figure S7. ¹³C NMR (101 MHz, DMSO-d₆) of **2**

DMSO-d₆



-69.20
-71.08

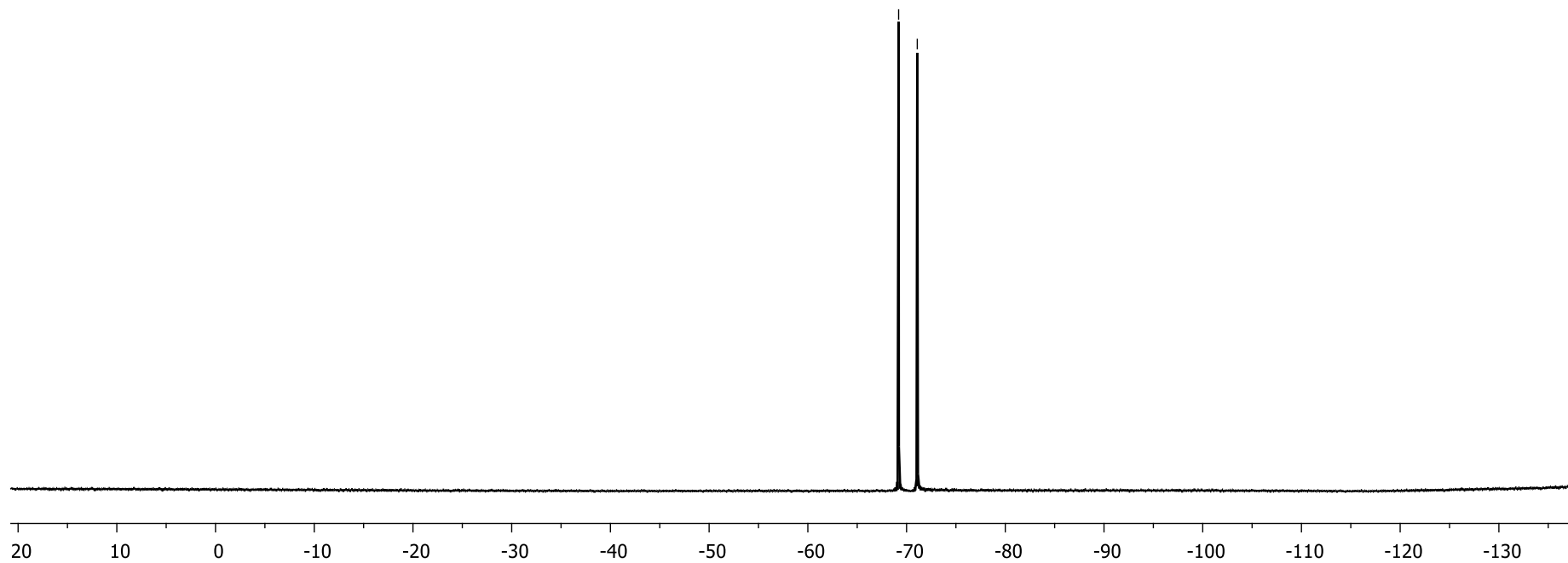
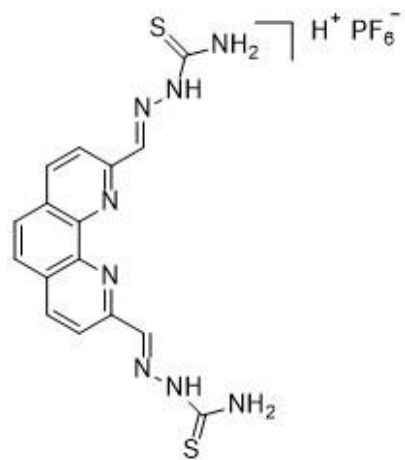


Figure S8. ¹⁹F NMR (376 MHz, DMSO-d₆) of **2**

DMSO-d₆



-131.02
-135.42
-139.81
-144.20
-148.59
-152.98
-157.37

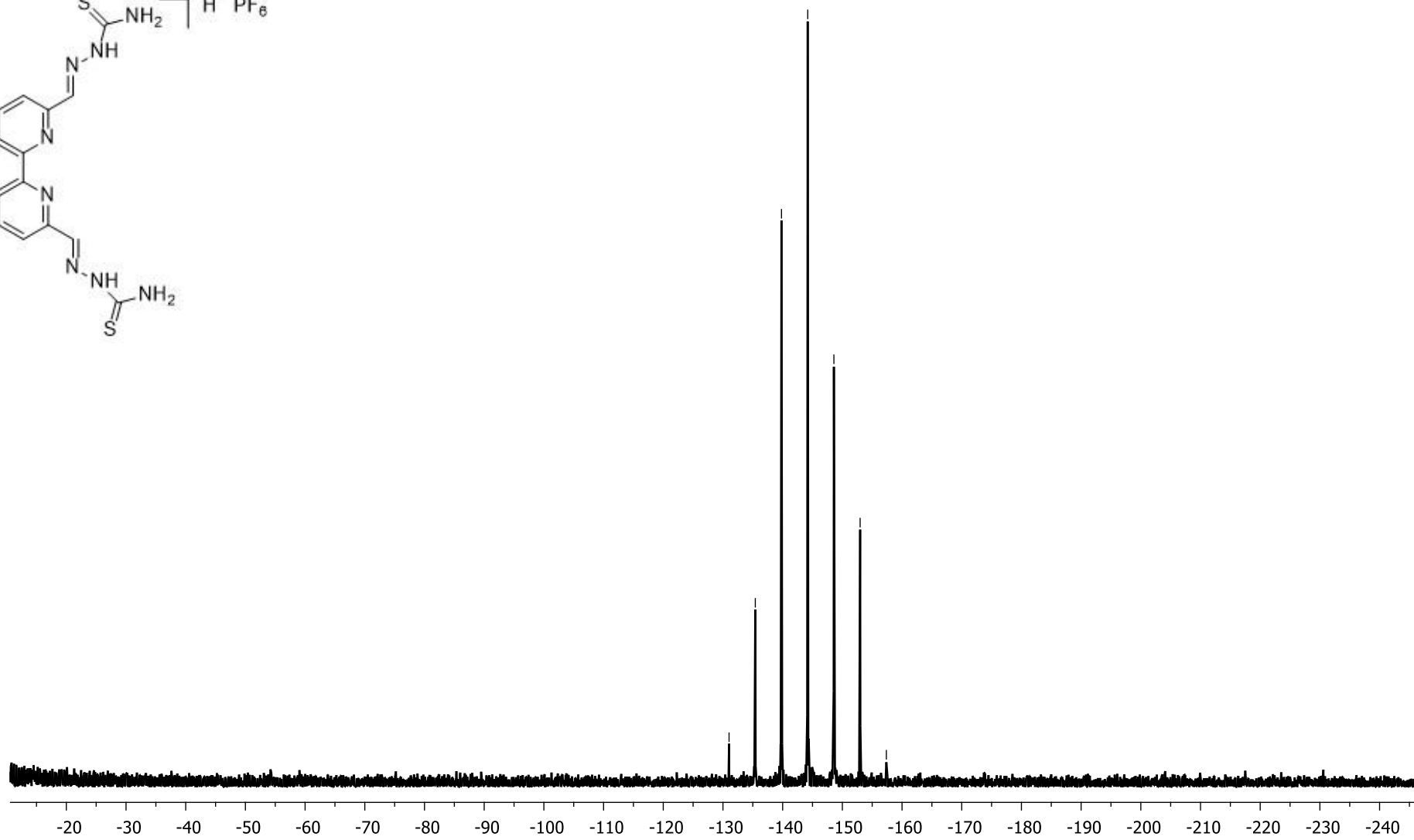


Figure S9. ³¹P NMR (162 MHz, DMSO-d₆) of 2

DMSO-d₆

—12.01

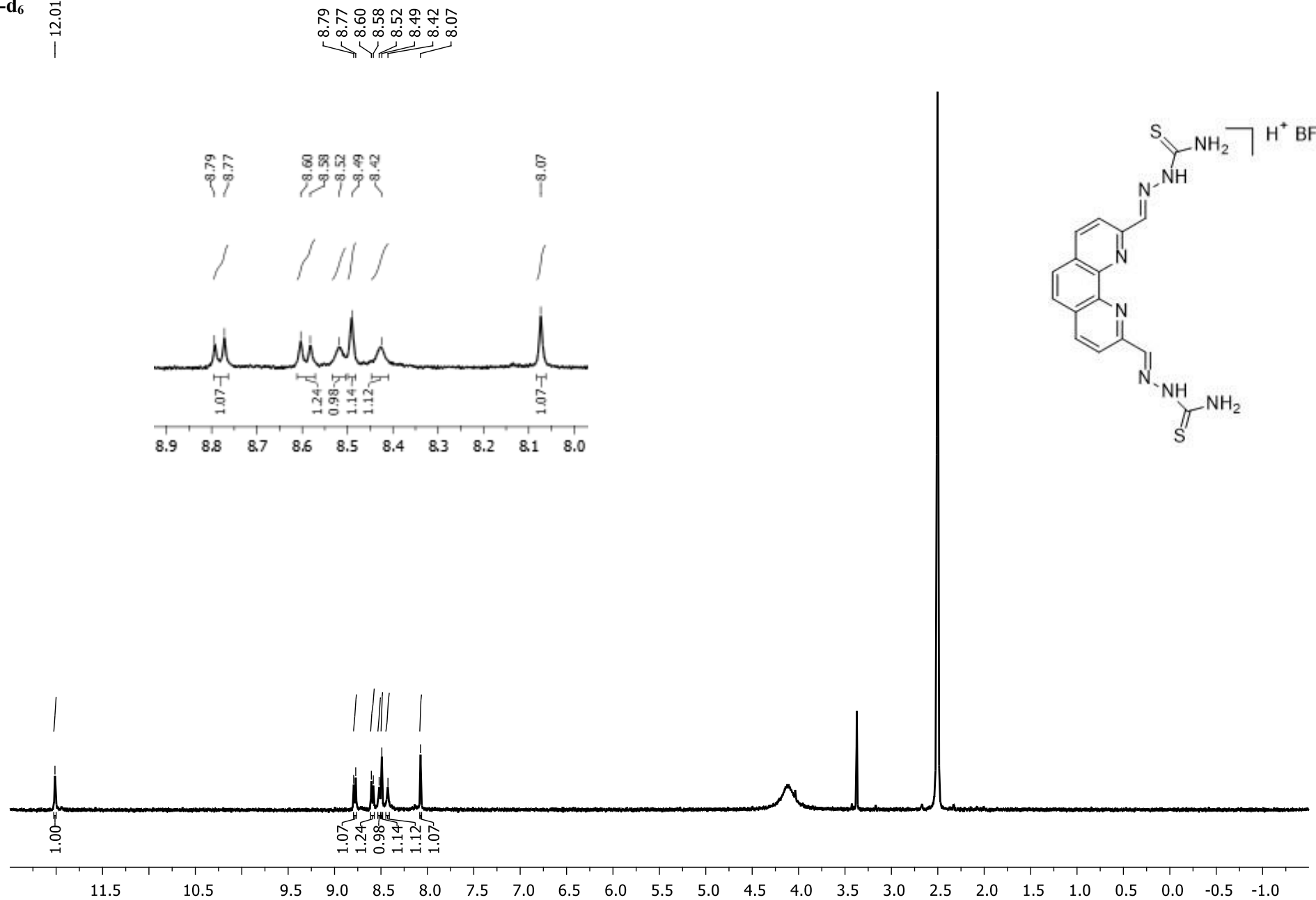


Figure S10. ¹H NMR (400 MHz, DMSO-d₆) of **3**

DMSO-d₆

— 179.0

— 153.9

— 144.2

— 142.2

— 137.7

— 129.3

— 127.5

— 120.7

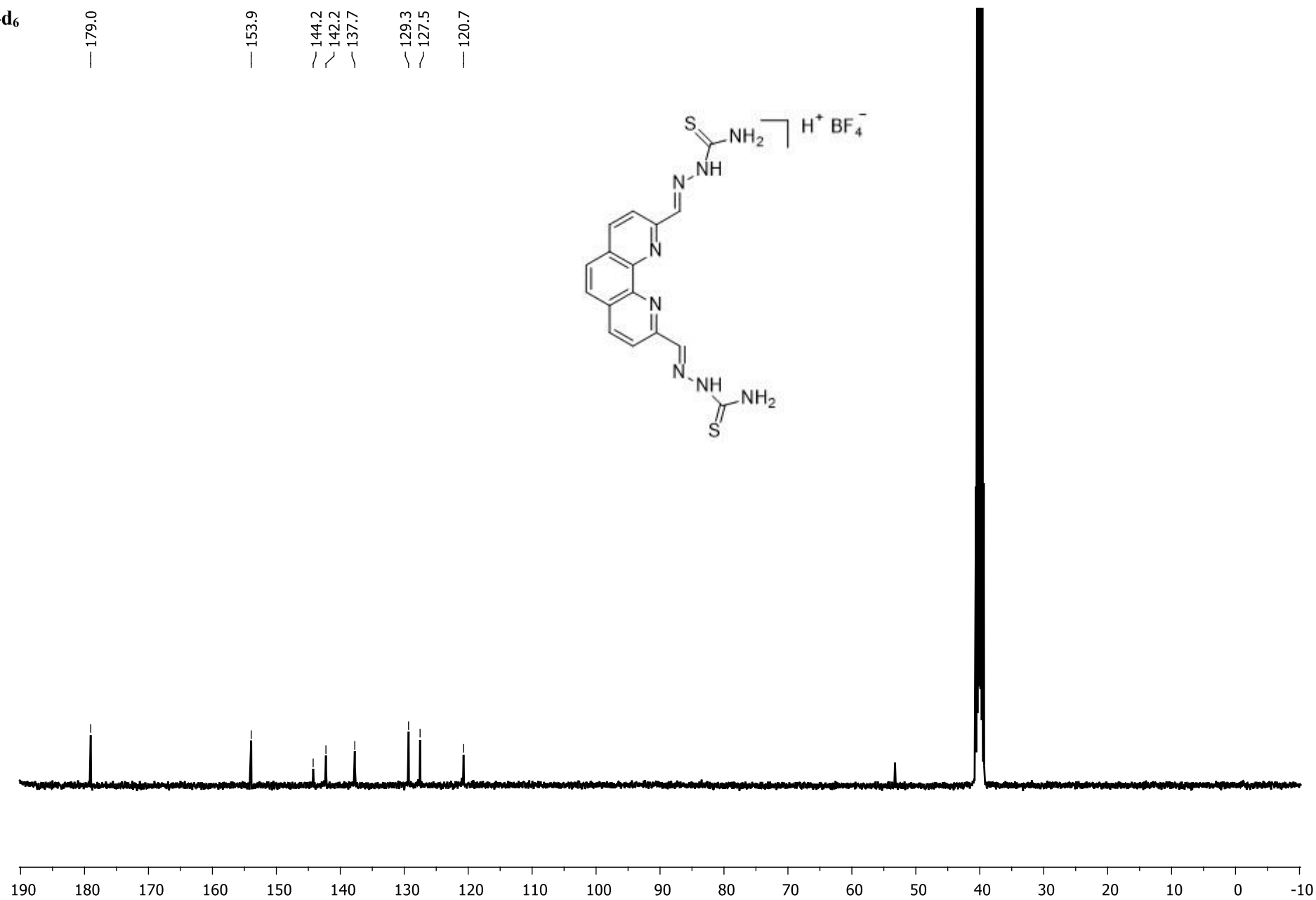
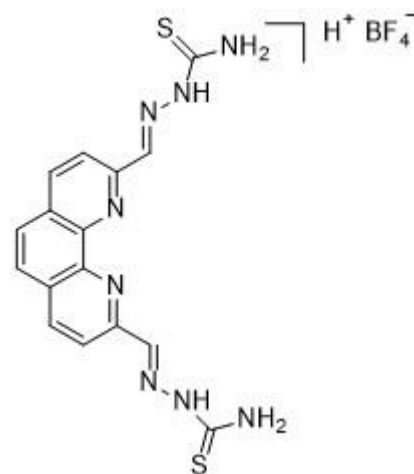


Figure S11. ¹³C NMR (101 MHz, DMSO-d₆) of **3**

DMSO-d₆

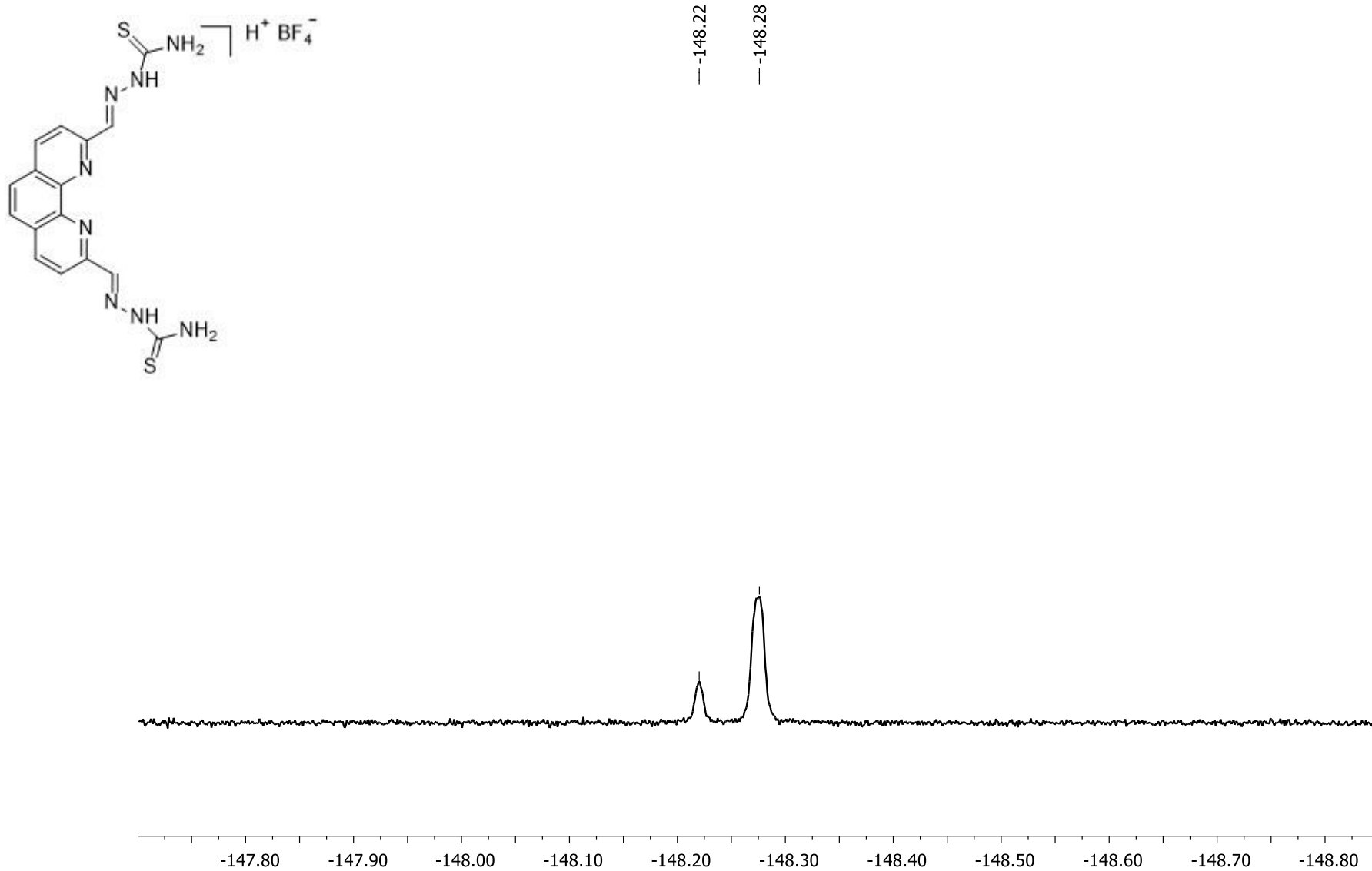


Figure S12. ¹⁹F NMR ((376 MHz, DMSO-d₆) of 3

DMSO-d₆

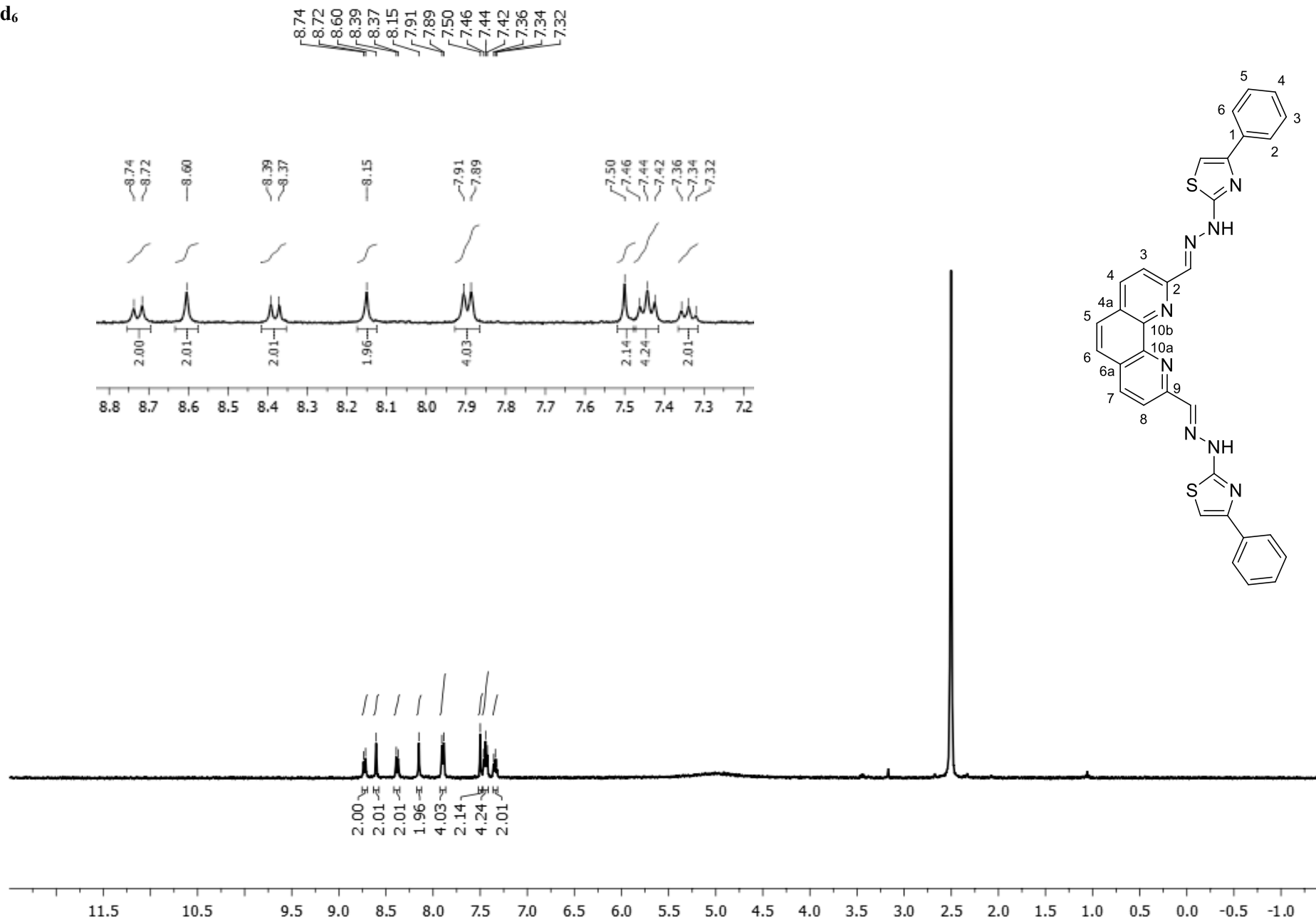


Figure S13. ¹H NMR (400 MHz, DMSO-d₆) of 4

DMSO-d₆

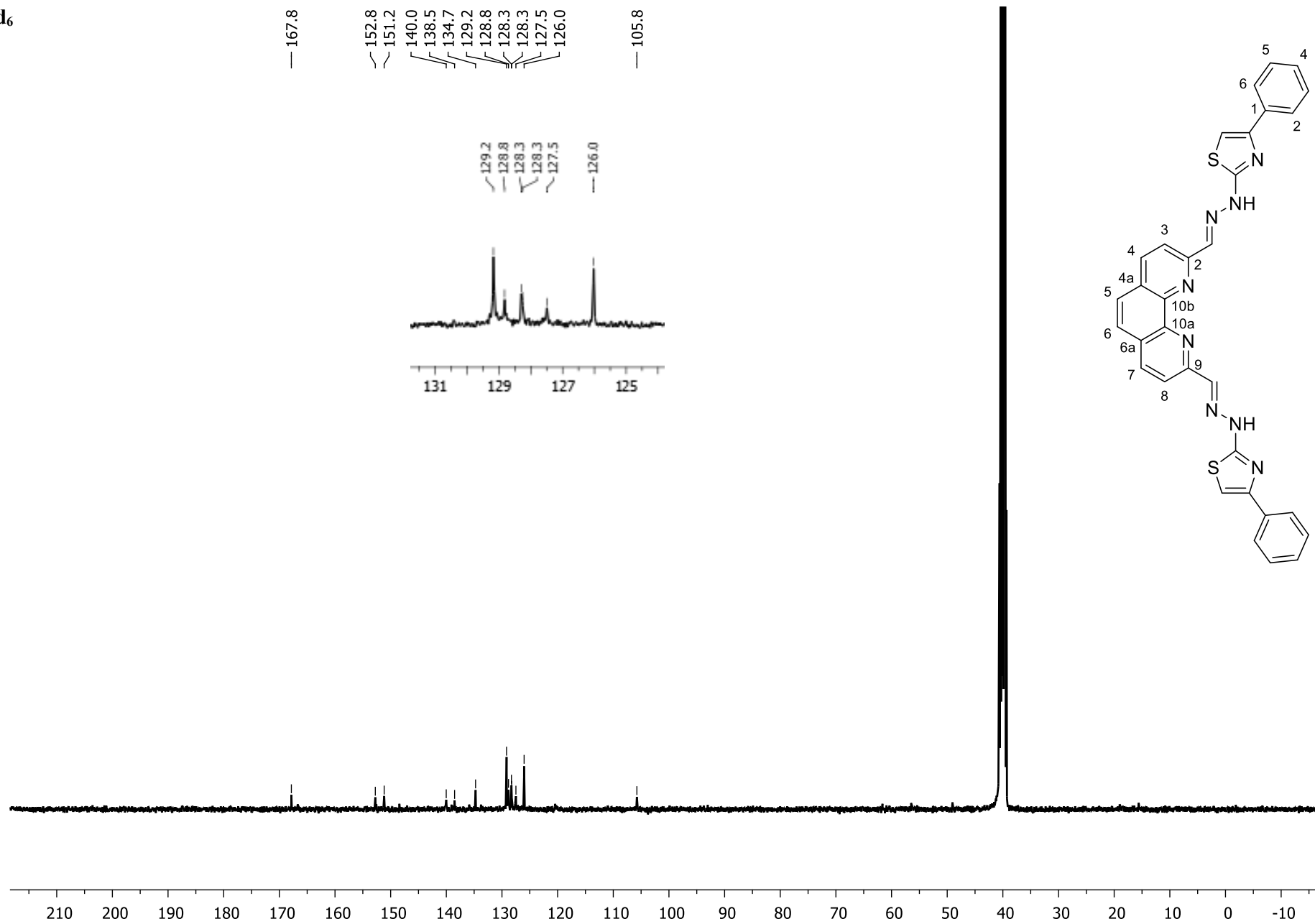


Figure S14. ¹³C NMR (101 MHz, DMSO-d₆) of 4

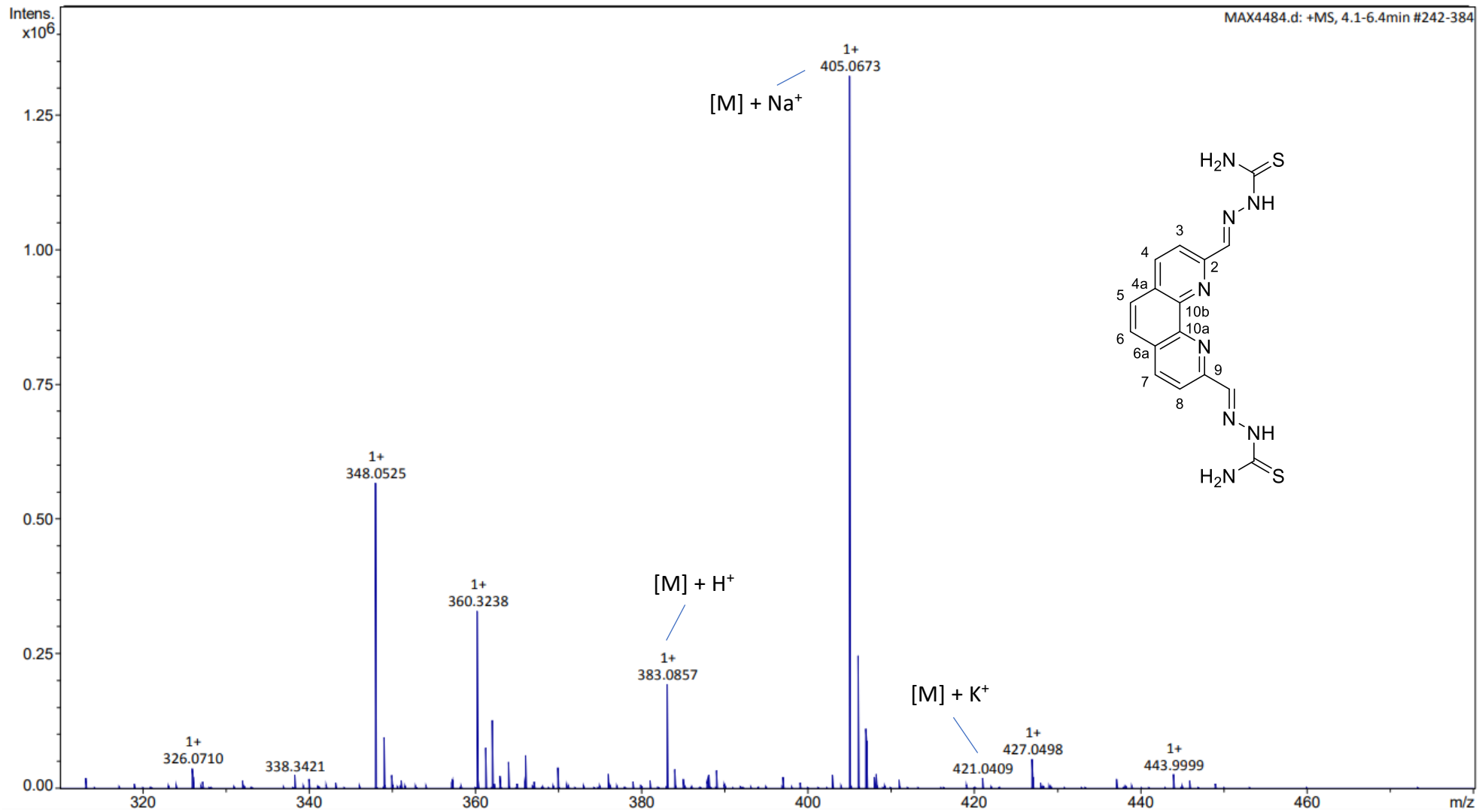


Figure S15. Zoomed view of high-resolution electrospray ionization mass spectrum (ESI-HRMS-pos) of **1** (MeOH, 1% formic acid)

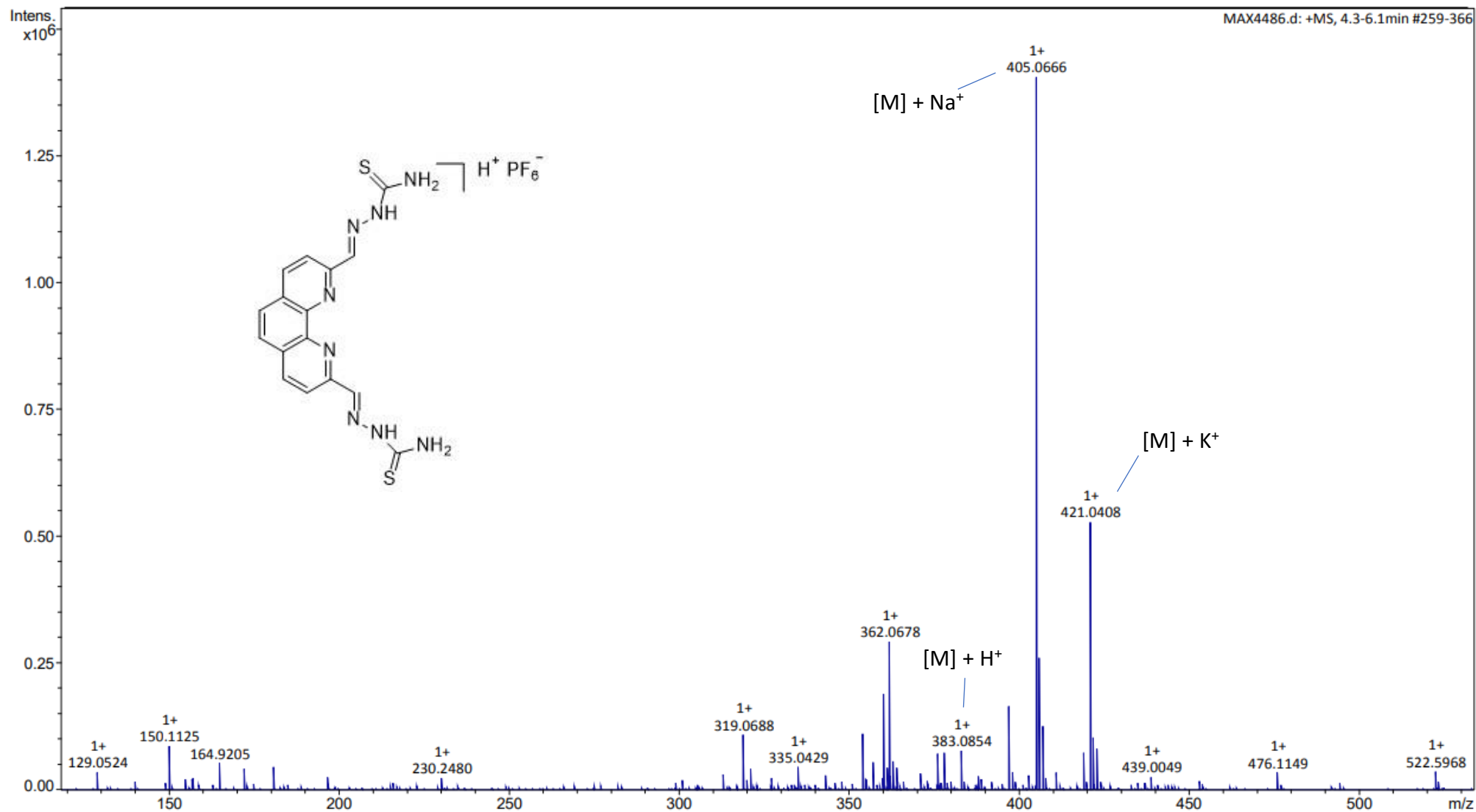


Figure S16. Zoomed view of high-resolution electrospray ionization mass spectrum (ESI-HRMS-pos) of **2** (MeOH, 1% formic acid)

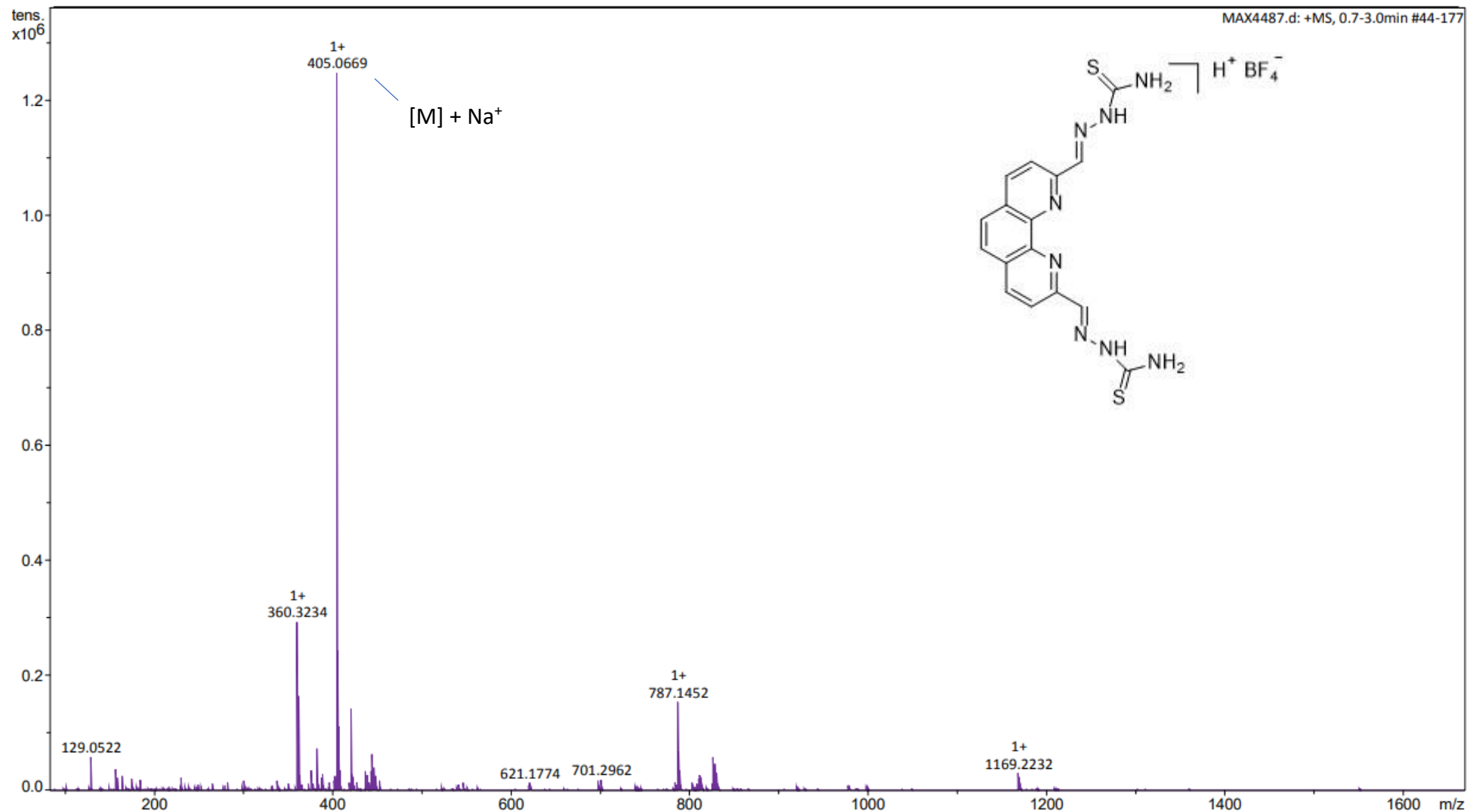


Figure S17. High-resolution electrospray ionization mass spectrum (ESI-HRMS-pos) of **3** (MeOH, 1% formic acid)

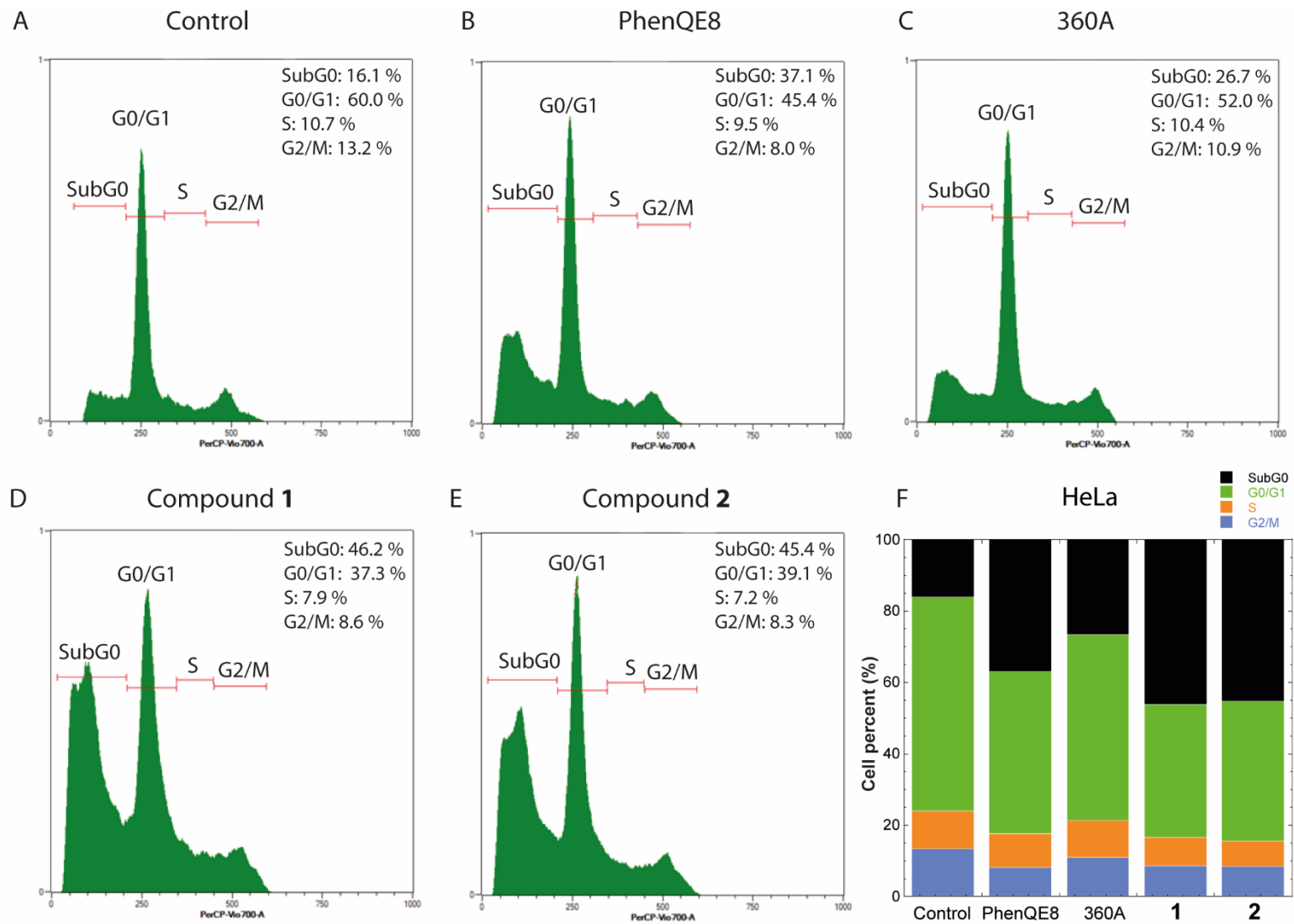


Figure S19. Cell cycle histograms of HeLa cells treated with selected compounds **1**, **2** or reference compounds PhenQE8 or 360A at $\frac{1}{2}$ IC₅₀ concentrations for 72 h.