

Supporting Information for

Bis(thiosemicarbazone) Complexes of Cobalt(III). Synthesis, Characterization, and Anticancer Potential

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Contents

Figures S1–S9. ^1H NMR Spectra of $[\text{Co}(\text{BTSC})(\text{L})_2]^+$ Complexes

Figures S10–S18. $^{13}\text{C}\{^1\text{H}\}$ NMR Spectra of $[\text{Co}(\text{BTSC})(\text{L})_2]^+$ Complexes

Figures S19–S27. ^{59}Co NMR Spectra of $[\text{Co}(\text{BTSC})(\text{L})_2]^+$ Complexes

Figures S28–S36. IR Spectra of $[\text{Co}(\text{BTSC})(\text{L})_2]^+$ Complexes

Figures S37–S45. HPLC Chromatograms of $[\text{Co}(\text{BTSC})(\text{L})_2]^+$ Complexes

Figures S46–S54. UV-Vis Spectra of $[\text{Co}(\text{BTSC})(\text{L})_2]^+$ Complexes

Figures S55–S63. Cyclic Voltammograms of $[\text{Co}(\text{BTSC})(\text{L})_2]^+$ Complexes

Figure S64. Uptake of $[\text{Co}(\text{BTSC})(\text{Im})_2]^+$ Complexes in HeLa and A549 Cells

Figures S65–S73. Dose-Response Curves of $[\text{Co}(\text{BTSC})(\text{L})_2]^+$ Complexes

Figures S74–S75. ^1H NMR Spectrum of $[\text{Co}(\text{GTS})(\text{NH}_3)_2]^+$ in the Presence of Tetrathiomolybdate

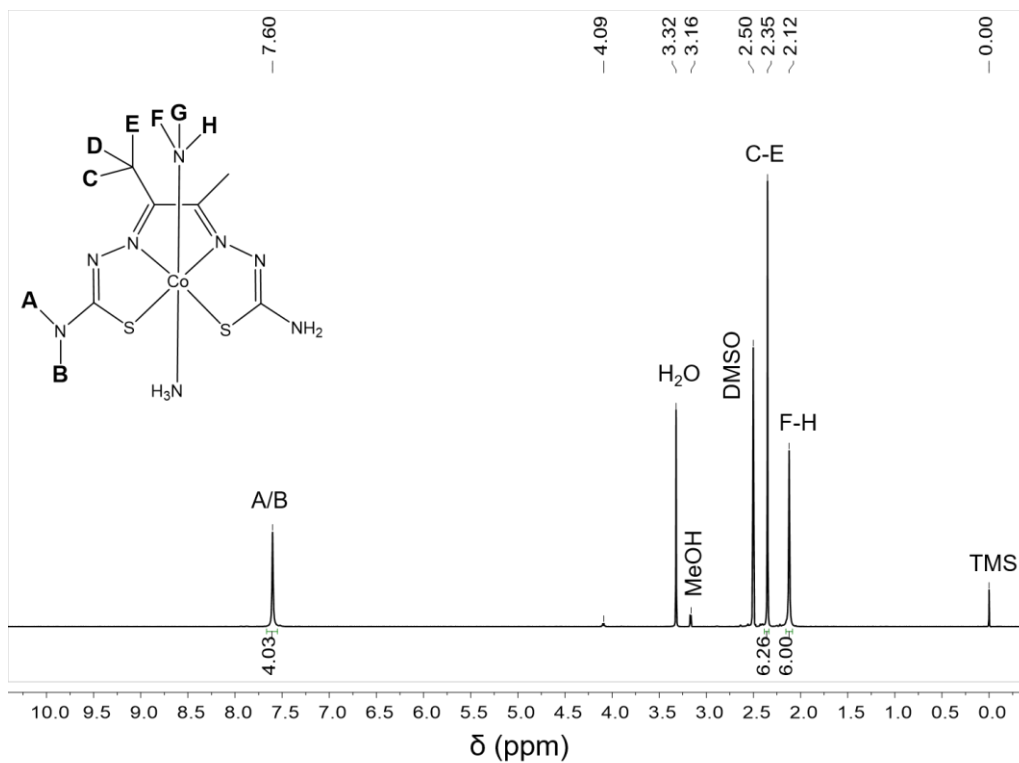


Figure S1. ^1H NMR spectrum of $[\text{Co}(\text{ATS})(\text{NH}_3)_2]^+$ ($\text{DMSO-}d_6$, 500 MHz, 298 K)

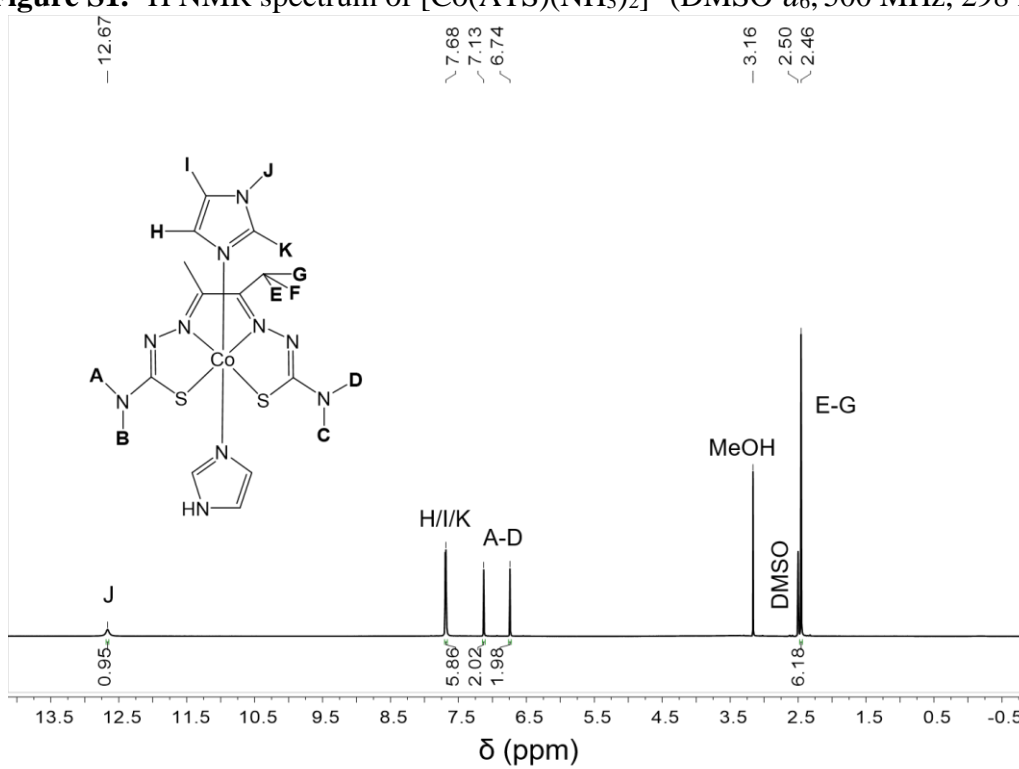


Figure S2. ^1H NMR spectrum of $[\text{Co}(\text{ATS})(\text{Im})_2]^+$ ($\text{DMSO-}d_6$ 500 MHz, 298 K)

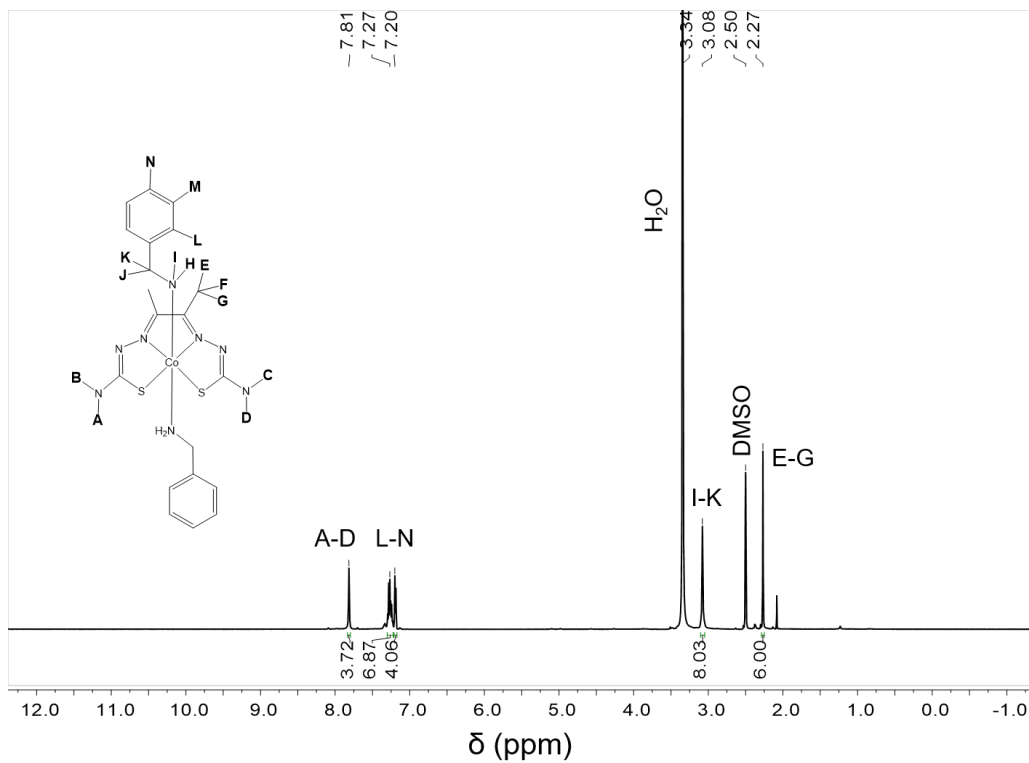


Figure S3. ^1H NMR spectrum of $[\text{Co}(\text{ATS})(\text{BnA})_2]^+$ ($\text{DMSO}-d_6$ 500 MHz, 298 K)

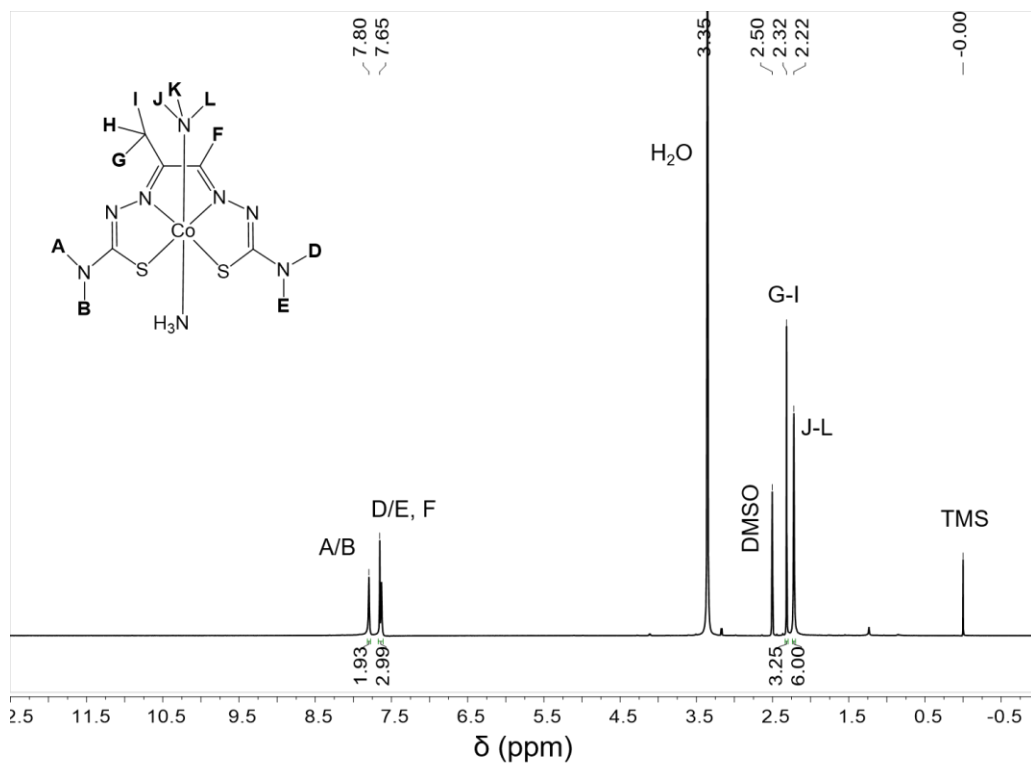


Figure S4. ^1H NMR spectrum of $[\text{Co}(\text{PTS})(\text{NH}_3)_2]^+$ ($\text{DMSO}-d_6$ 500 MHz, 298 K)

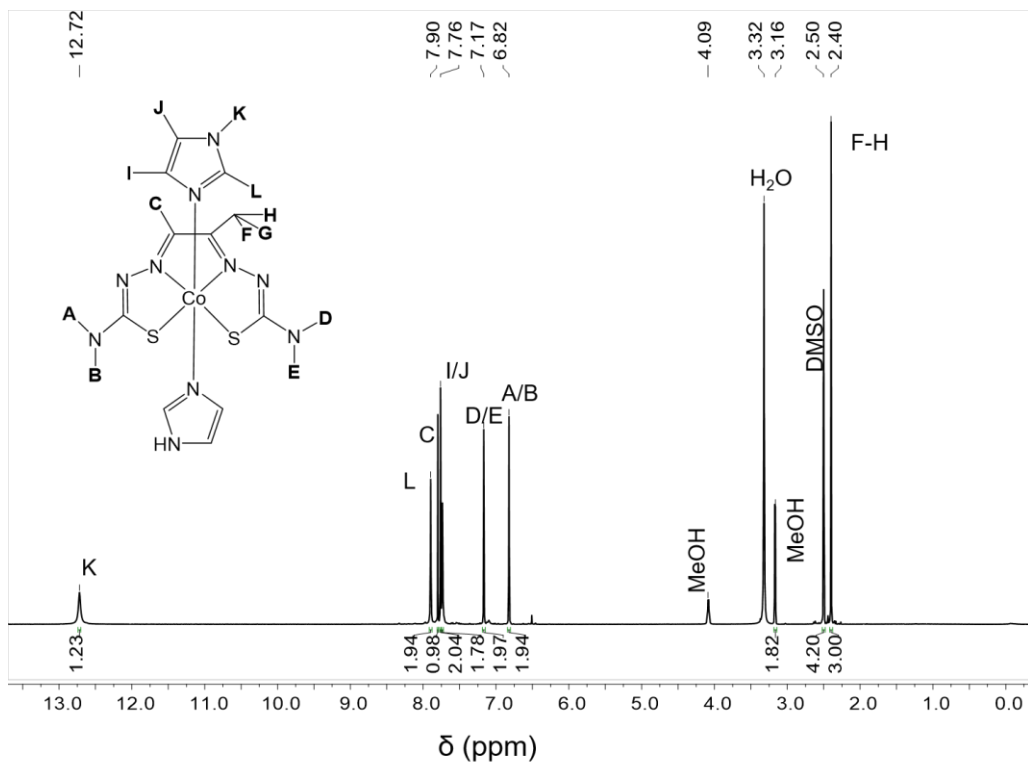


Figure S5. ^1H NMR spectrum of $[\text{Co}(\text{PTS})(\text{Im})_2]^+$ (DMSO- d_6 500 MHz, 298 K)

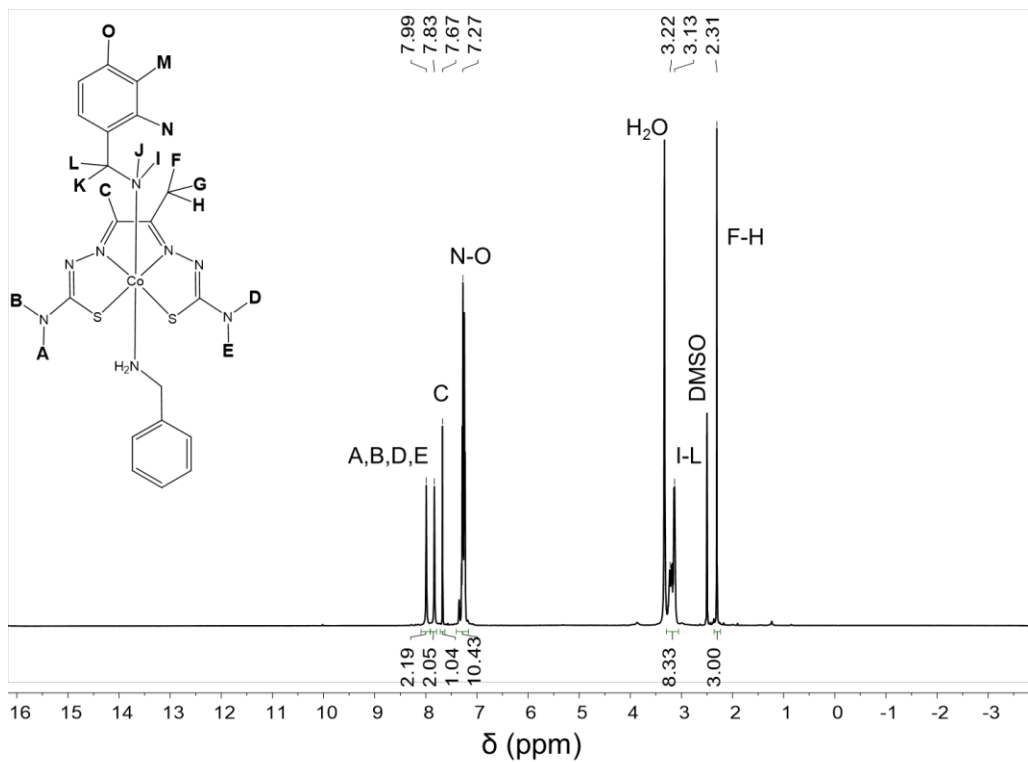


Figure S6. ^1H NMR spectrum of $[\text{Co}(\text{PTS})(\text{BnA})_2]^+$ (DMSO- d_6 500 MHz, 298 K)

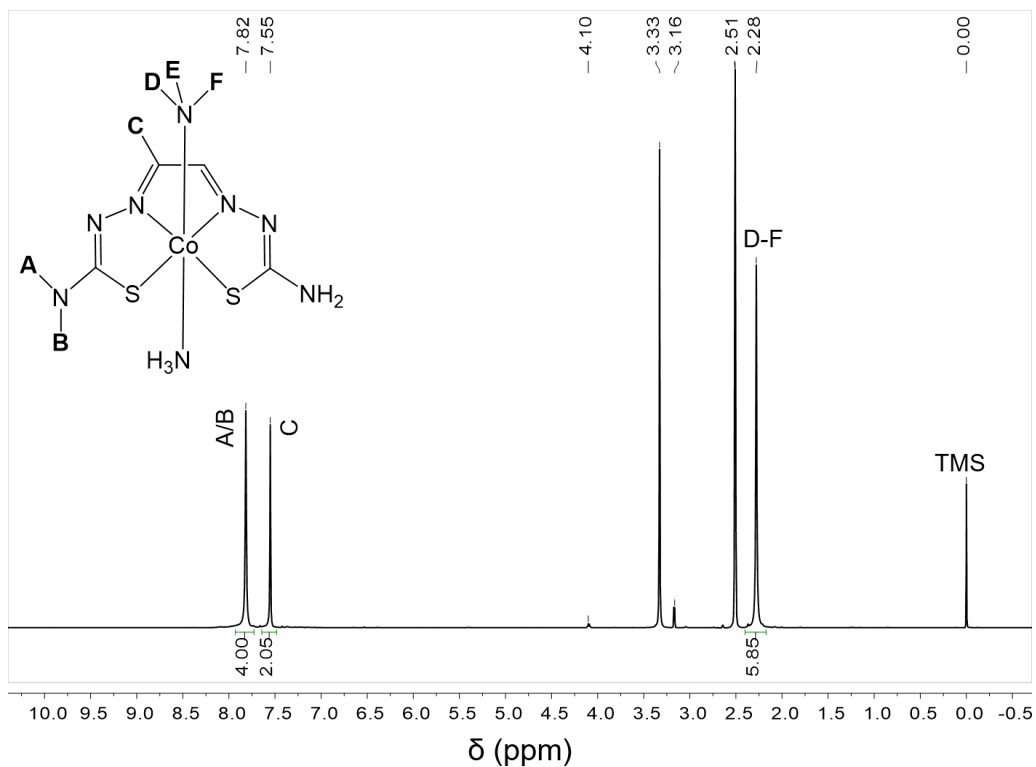


Figure S7. ^1H NMR spectrum of $[\text{Co}(\text{GTS})(\text{NH}_3)_2]^+$ ($\text{DMSO-}d_6$ 500 MHz, 298 K)

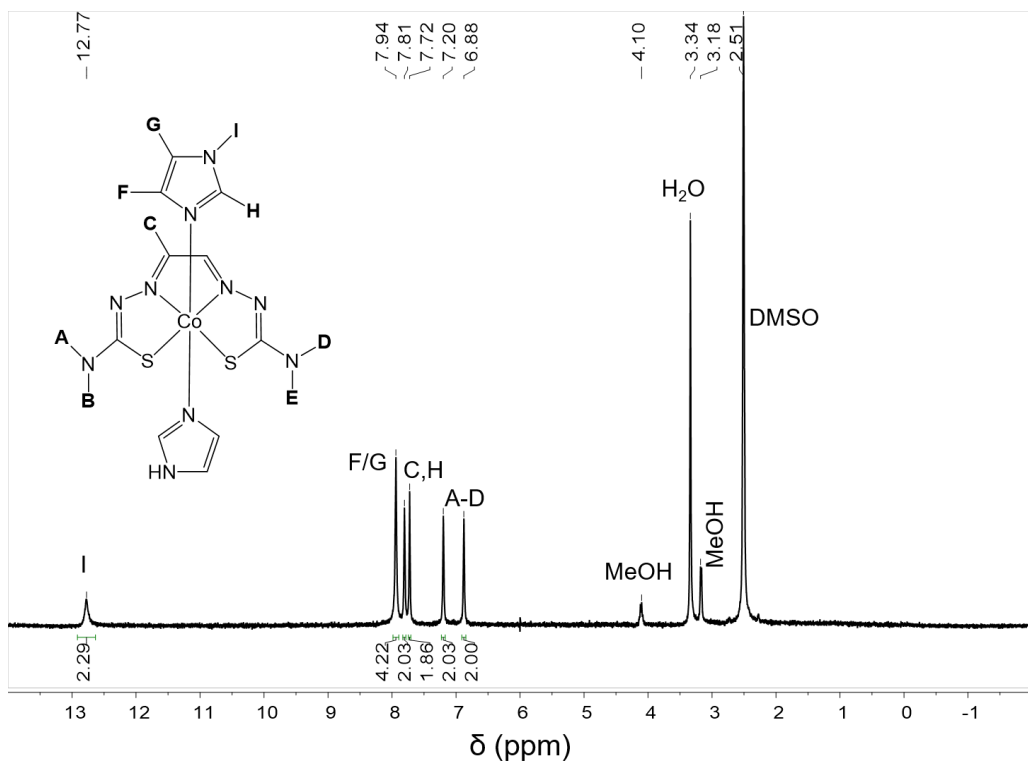


Figure S8. ^1H NMR spectrum of $[\text{Co}(\text{GTS})(\text{Im})_2]^+$ ($\text{DMSO-}d_6$ 500 MHz, 298 K)

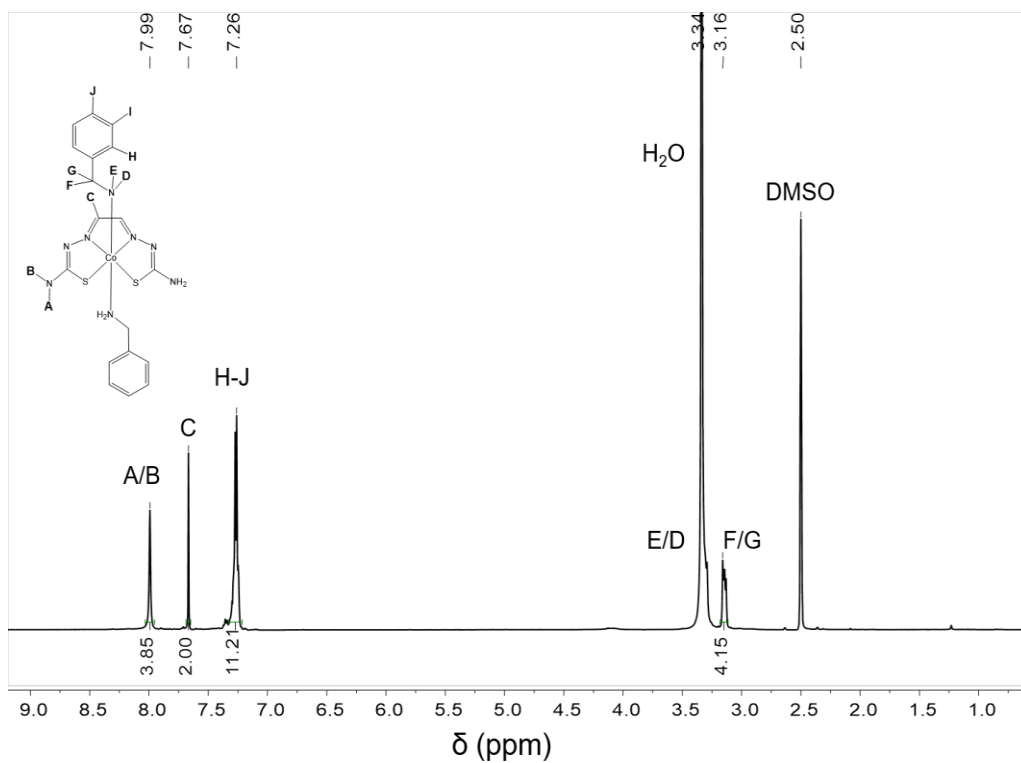


Figure S9. ^1H NMR spectrum of $[\text{Co}(\text{GTS})(\text{BnA})_2]^+$ ($\text{DMSO-}d_6$ 500 MHz, 298 K)

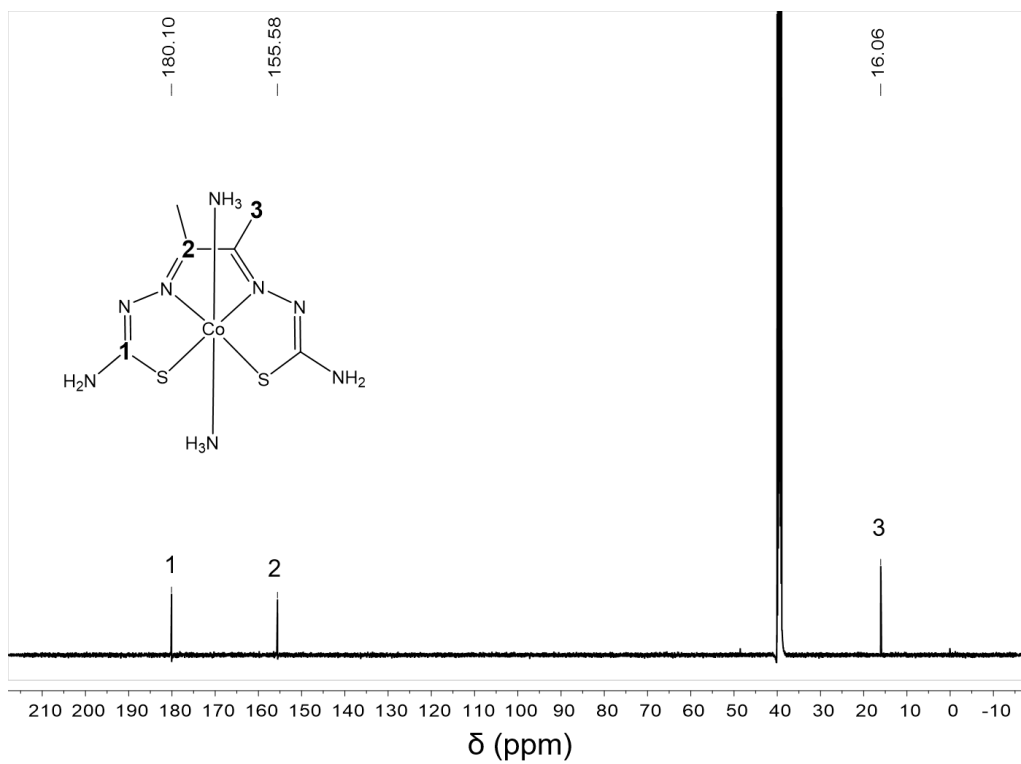


Figure S10. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[\text{Co}(\text{ATS})(\text{NH}_3)_2]^+$ ($\text{DMSO-}d_6$, 125 MHz, 298 K)

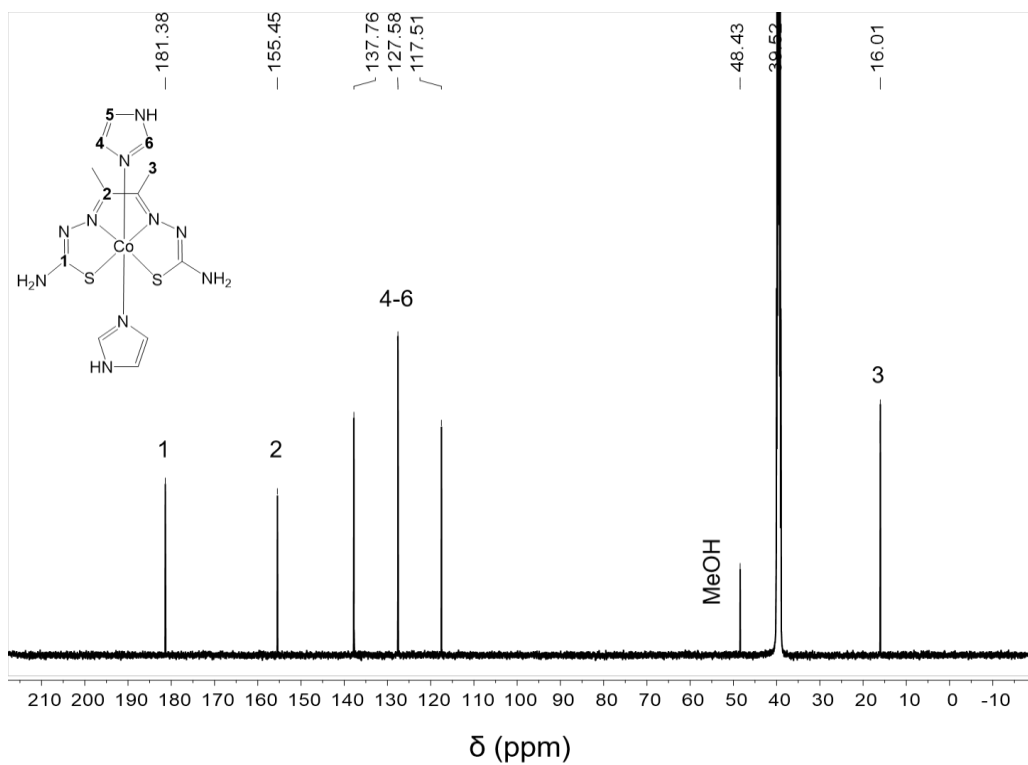


Figure S11. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[\text{Co}(\text{ATS})(\text{Im})_2]^+$ ($\text{DMSO-}d_6$ 125 MHz, 298 K)

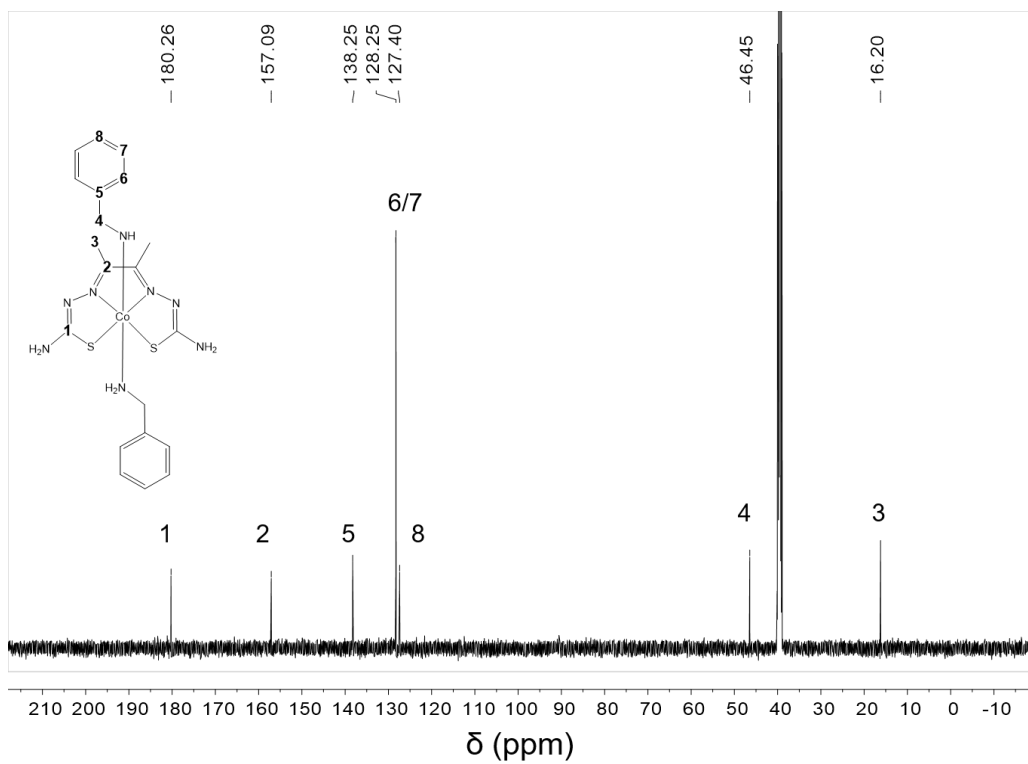


Figure S12. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[\text{Co}(\text{ATS})(\text{BnA})_2]^+$ ($\text{DMSO-}d_6$ 125 MHz, 298 K)

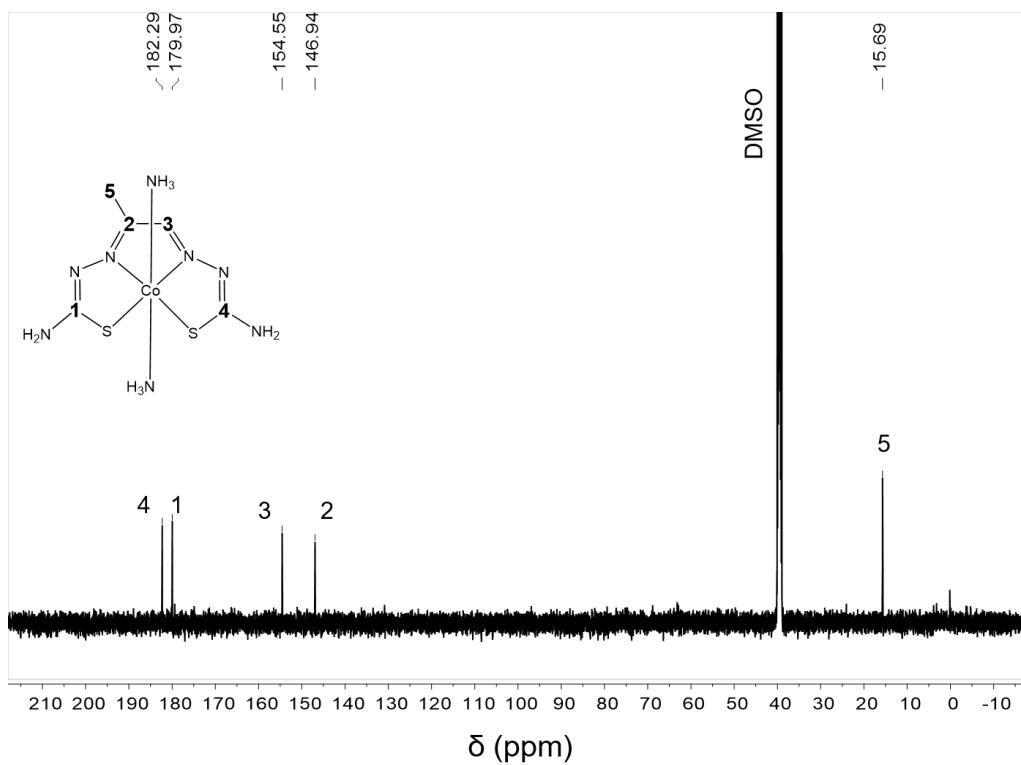


Figure S13. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[\text{Co}(\text{PTS})(\text{NH}_3)_2]^+$ ($\text{DMSO-}d_6$ 125 MHz, 298 K)

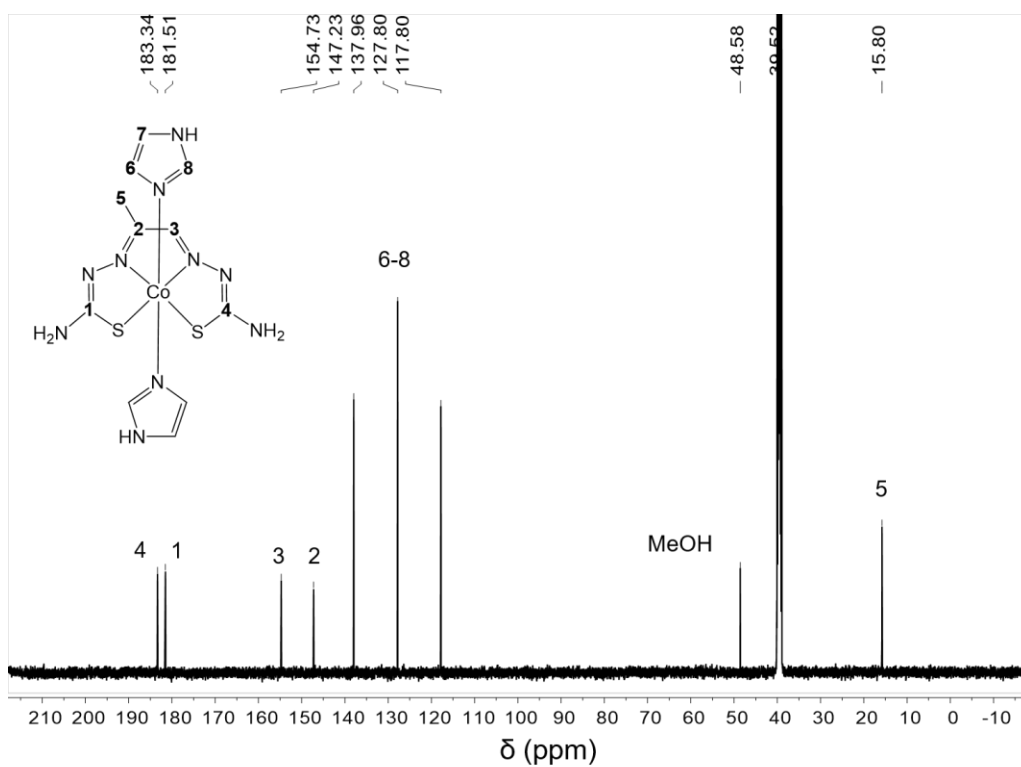
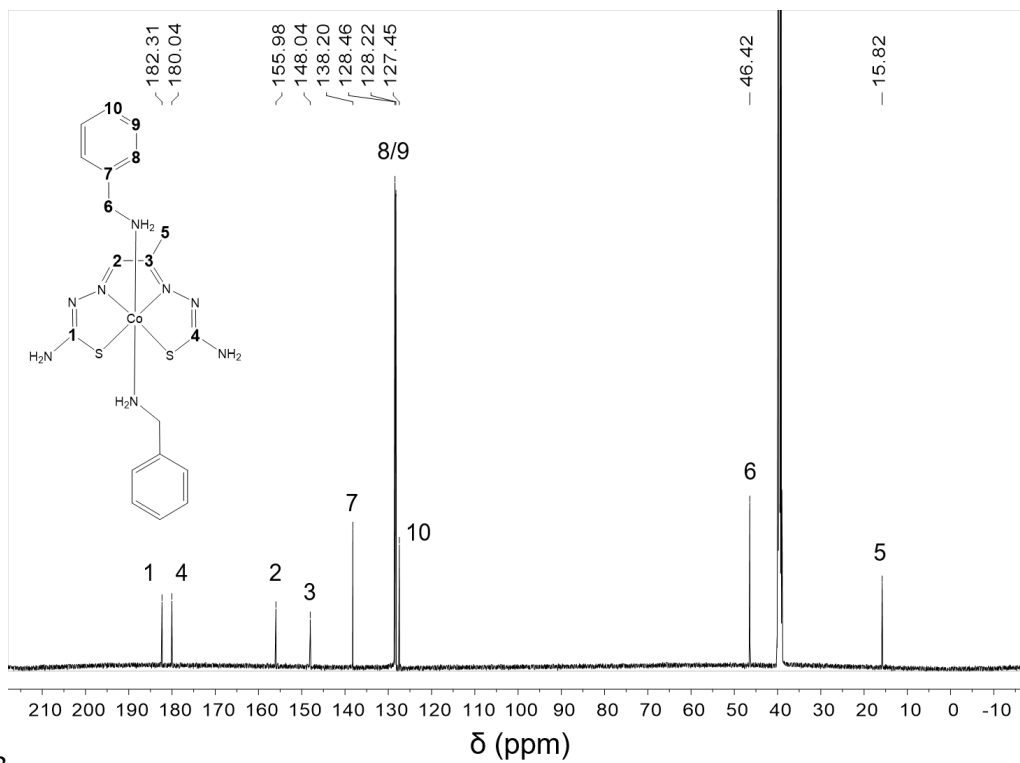


Figure S14. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[\text{Co}(\text{PTS})(\text{Im})_2]^+$ ($\text{DMSO-}d_6$ 125 MHz, 298 K)



3

Figure S15. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[\text{Co}(\text{PTS})(\text{BnA})_2]^+$ (DMSO- d_6 125 MHz, 298 K)

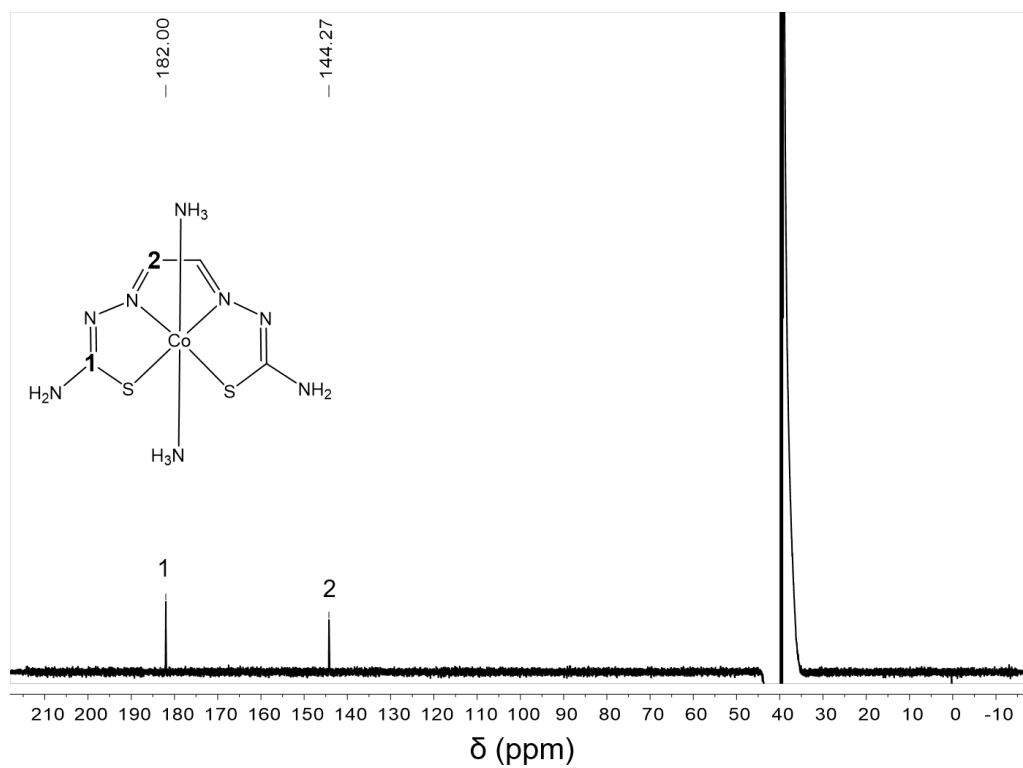


Figure S16. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[\text{Co}(\text{GTS})(\text{NH}_3)_2]^+$ (DMSO- d_6 125 MHz, 298 K)

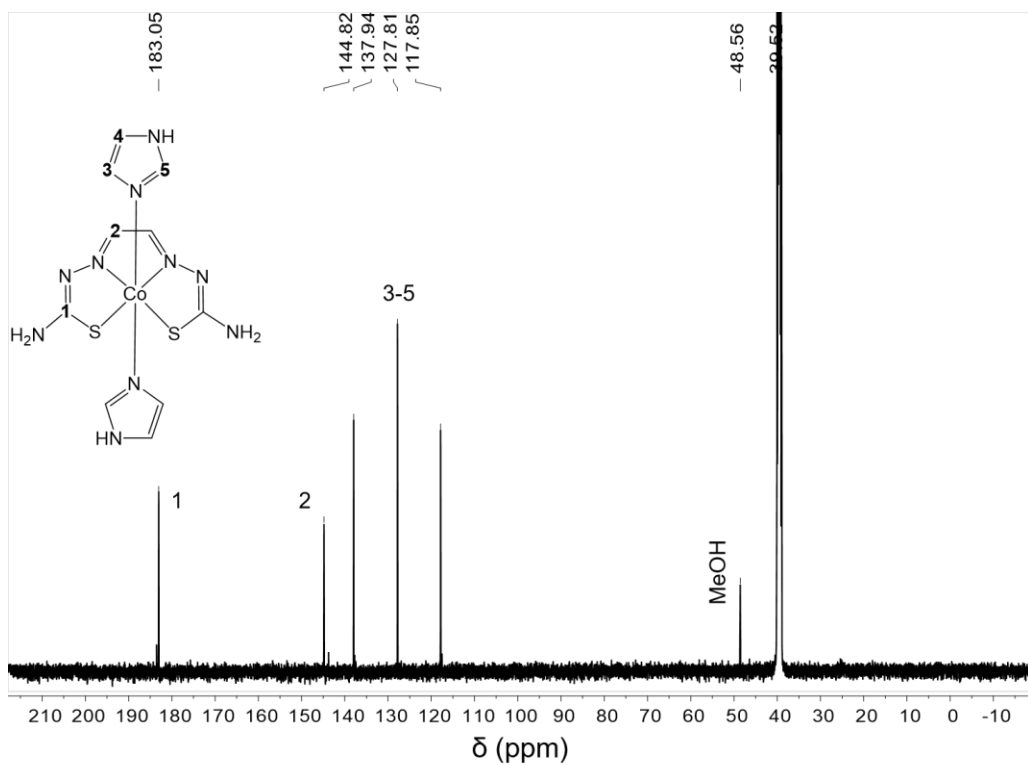


Figure S17. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[\text{Co}(\text{GTS})(\text{Im})_2]^+$ (DMSO- d_6 125 MHz, 298 K)

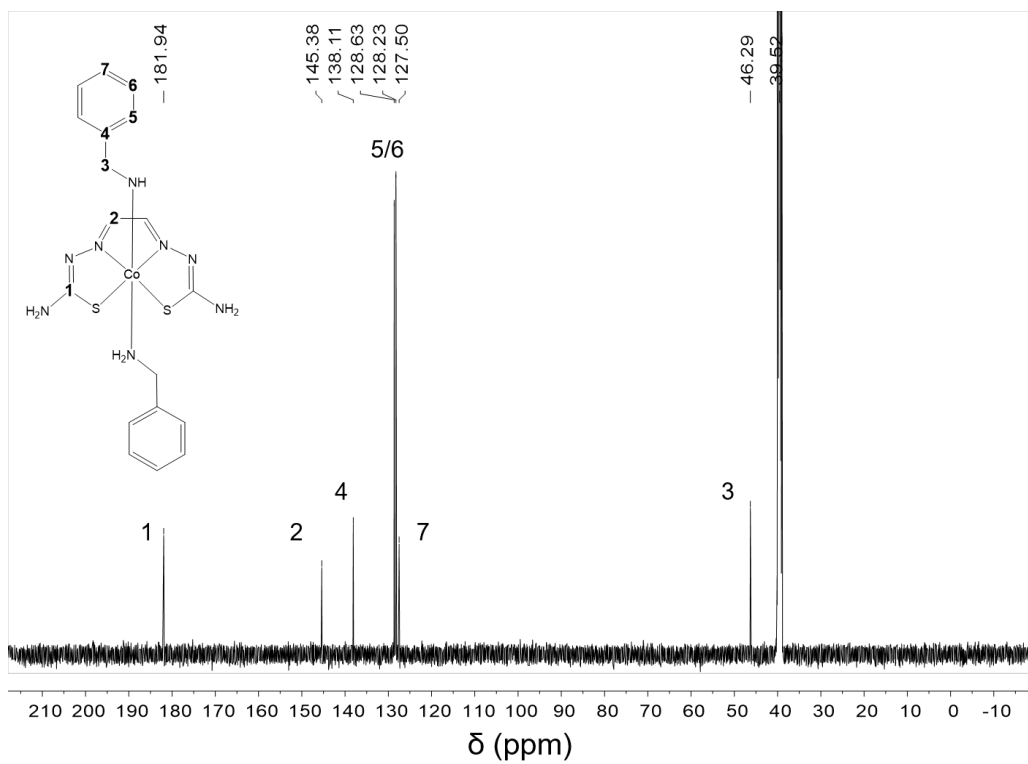


Figure S18. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[\text{Co}(\text{GTS})(\text{BnA})_2]^+$ (DMSO- d_6 125 MHz, 298 K)

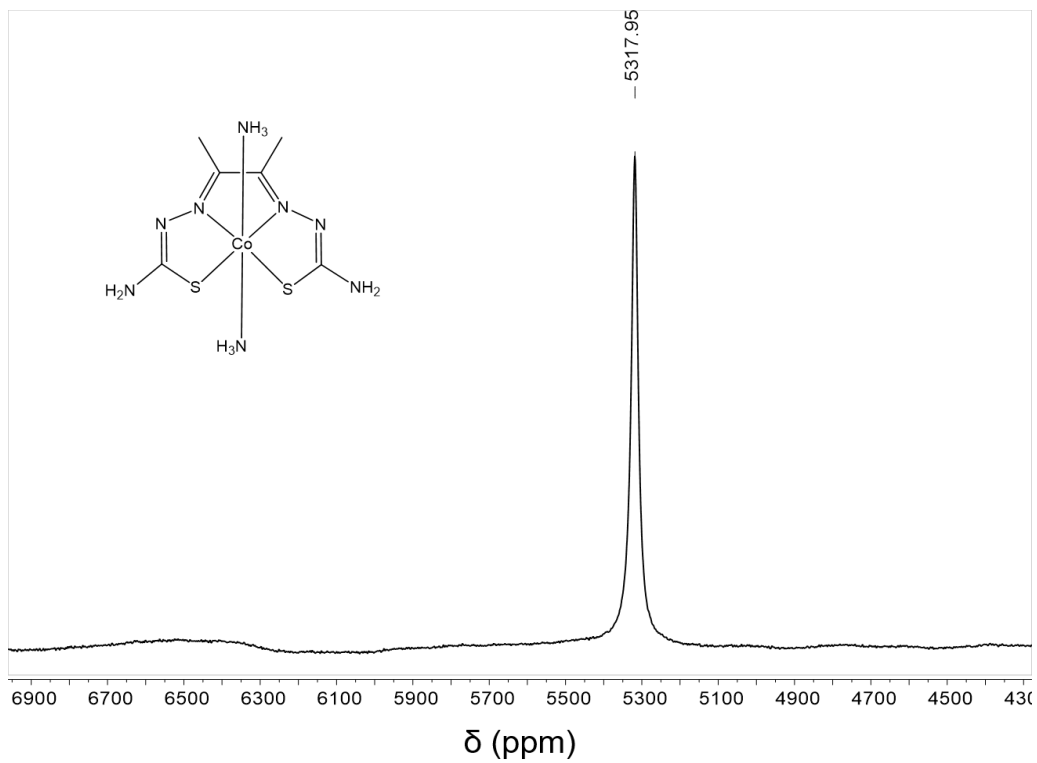


Figure S19. ^{59}Co NMR spectrum of $[\text{Co}(\text{ATS})(\text{NH}_3)_2]^+$ (DMSO- d_6 , 119 MHz, 298 K)

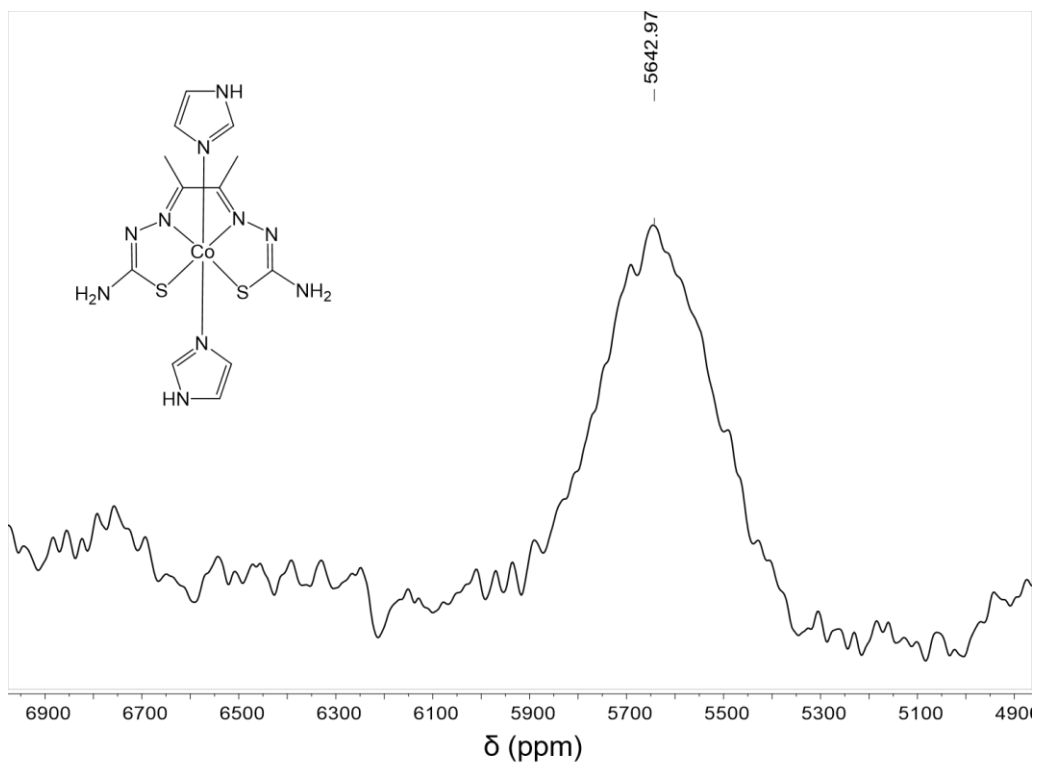


Figure S20. ^{59}Co NMR spectrum of $[\text{Co}(\text{ATS})(\text{Im})_2]^+$ (DMSO- d_6 , 119 MHz, 298 K)

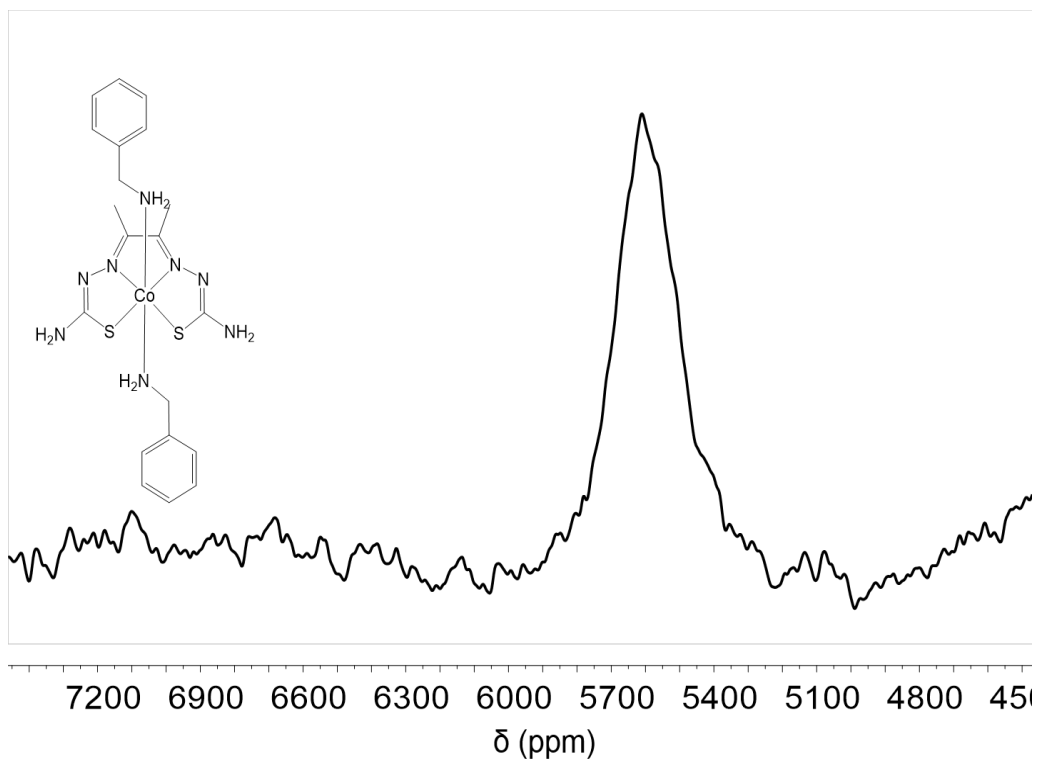


Figure S21. ^{59}Co NMR spectrum of $[\text{Co}(\text{ATS})(\text{BnA})_2]^+$ ($\text{DMSO-}d_6$ 119 MHz, 298 K)

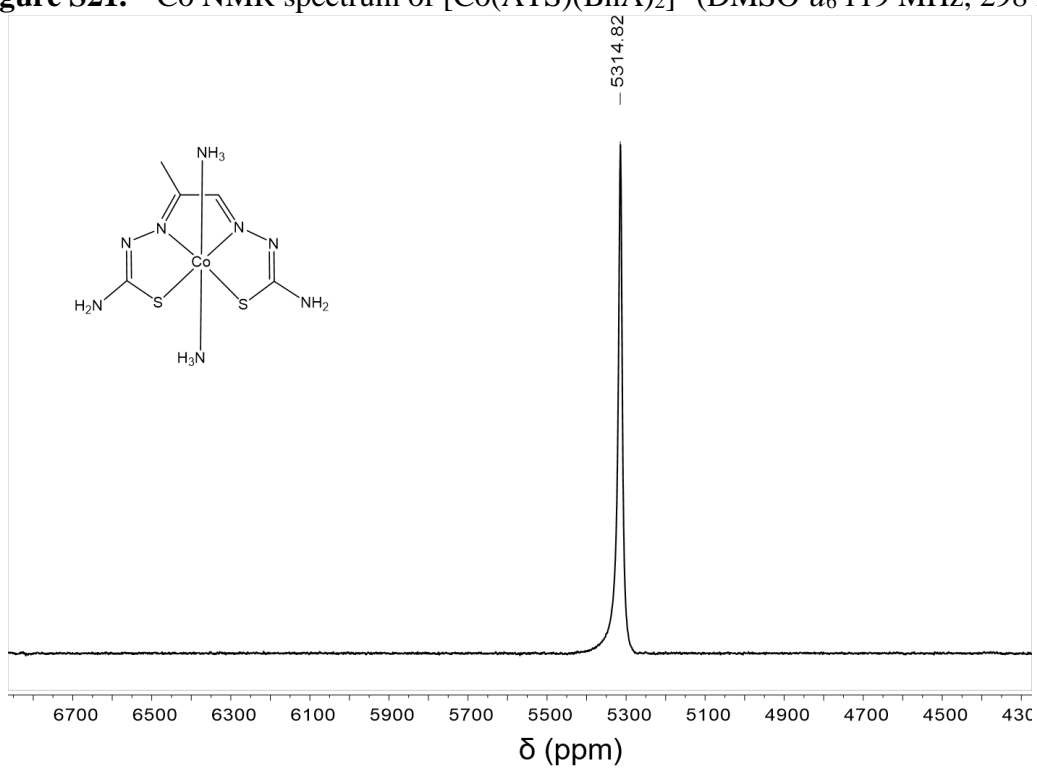


Figure S22. ^{59}Co NMR spectrum of $[\text{Co}(\text{PTS})(\text{NH}_3)_2]^+$ ($\text{DMSO-}d_6$ 119 MHz, 298 K)

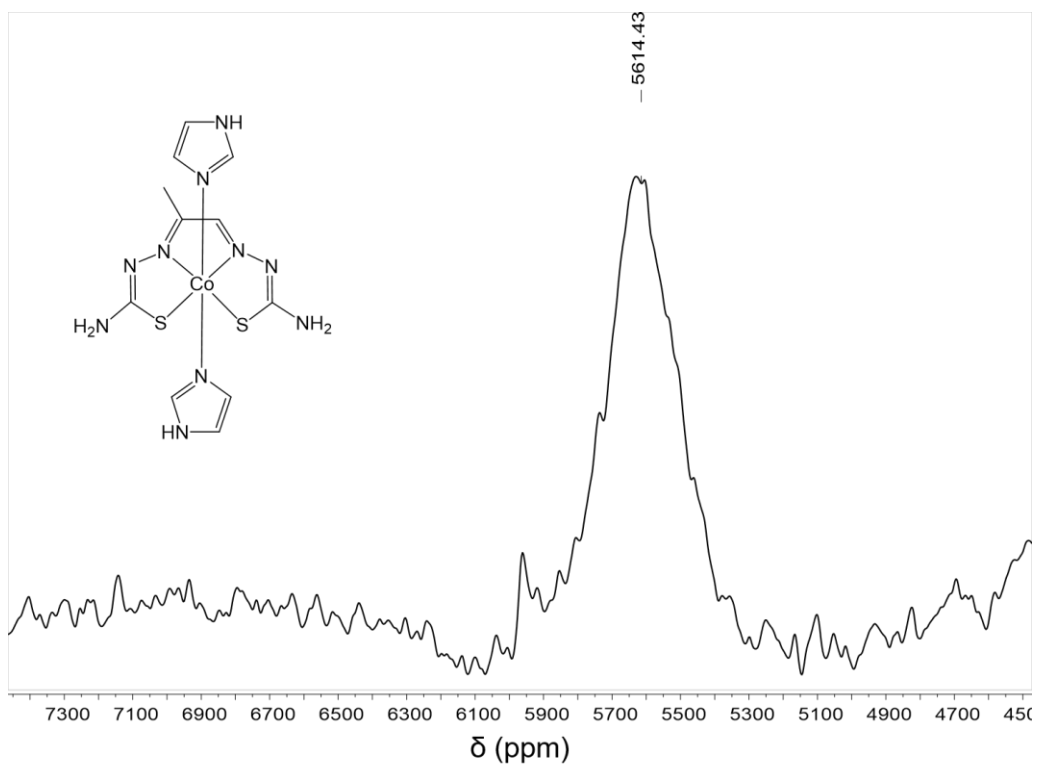


Figure S23. ^{59}Co NMR spectrum of $[\text{Co}(\text{PTS})(\text{Im})_2]^+$ (DMSO- d_6 119 MHz, 298 K)

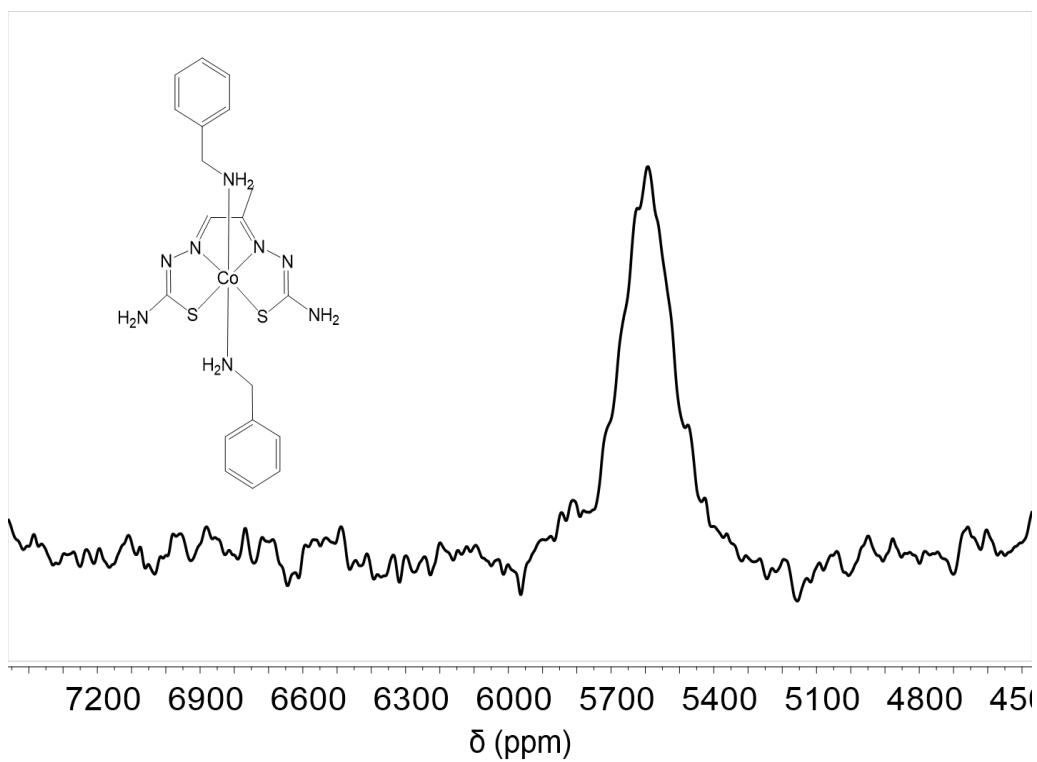


Figure S24. ^{59}Co NMR spectrum of $[\text{Co}(\text{PTS})(\text{BnA})_2]^+$ (DMSO- d_6 119 MHz, 298 K)

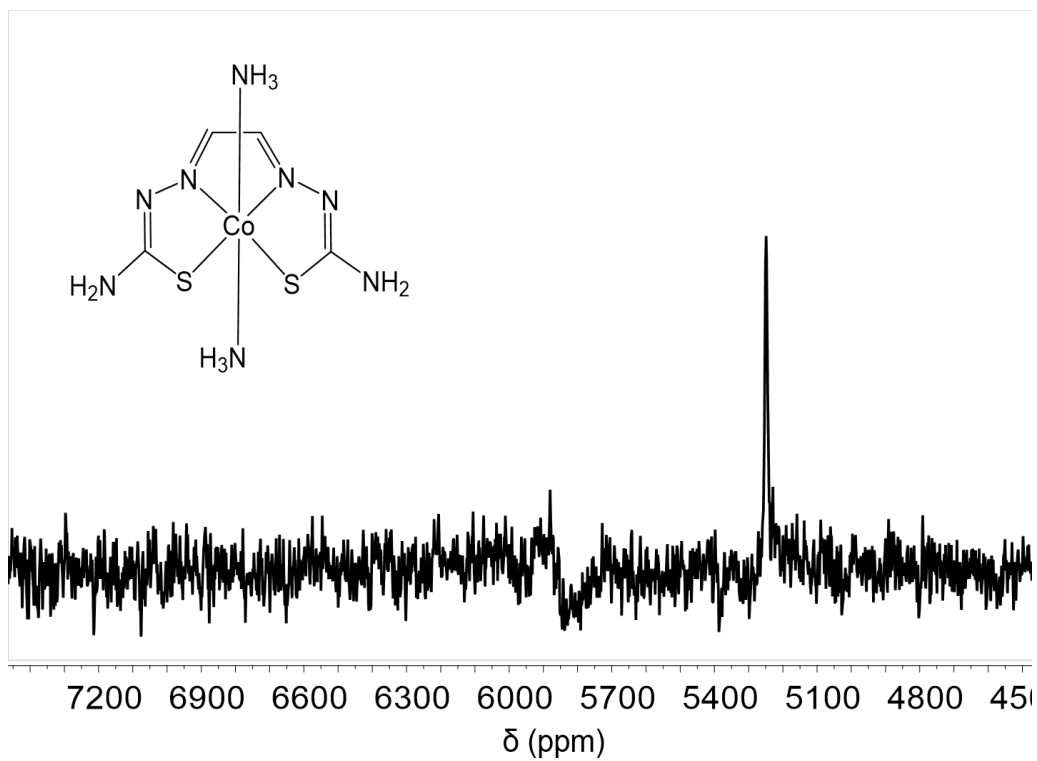


Figure S25. ^{59}Co NMR spectrum of $[\text{Co}(\text{GTS})(\text{NH}_3)_2]^+$ (DMSO- d_6 119 MHz, 298 K)

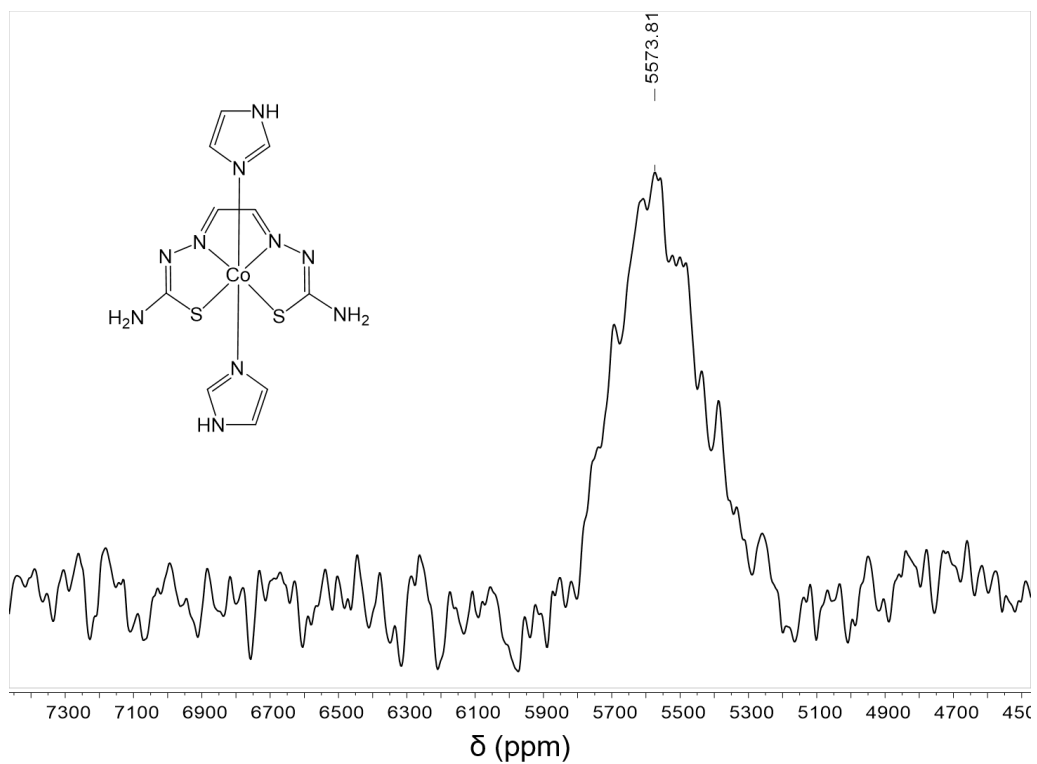


Figure S26. ^{59}Co NMR spectrum of $[\text{Co}(\text{GTS})(\text{Im})_2]^+$ (DMSO- d_6 119 MHz, 298 K)

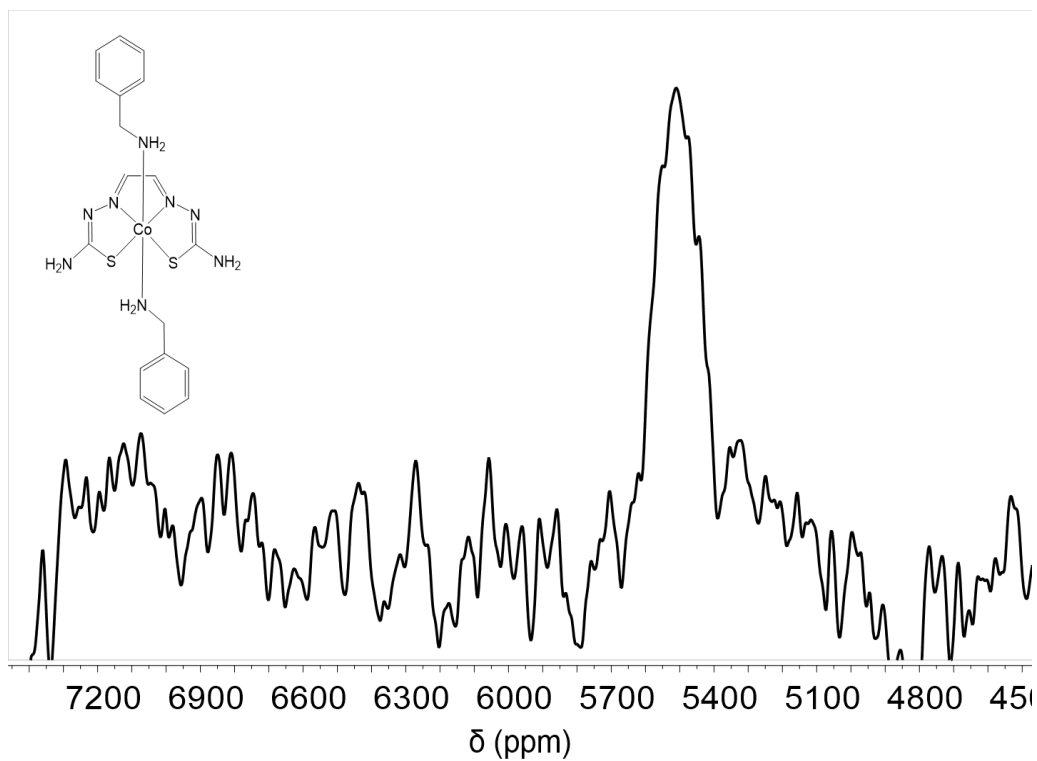


Figure S27. ^{59}Co NMR spectrum of $[\text{Co}(\text{GTS})(\text{BnA})_2]^+$ ($\text{DMSO-}d_6$ 119 MHz, 298 K)

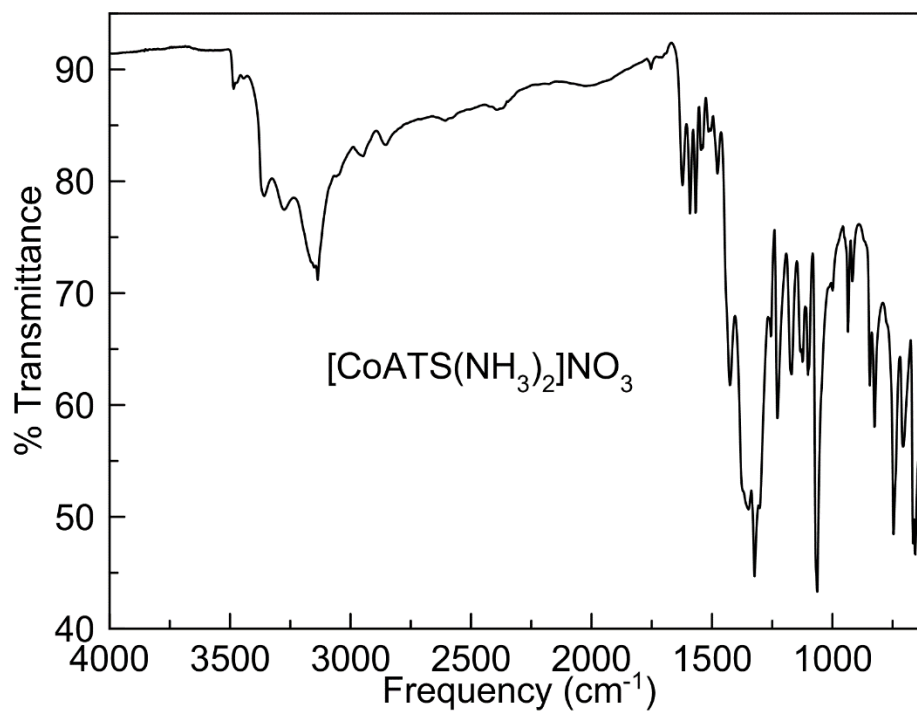


Figure S28. IR Spectrum of $[\text{Co}(\text{ATS})(\text{NH}_3)_2](\text{NO}_3)$.

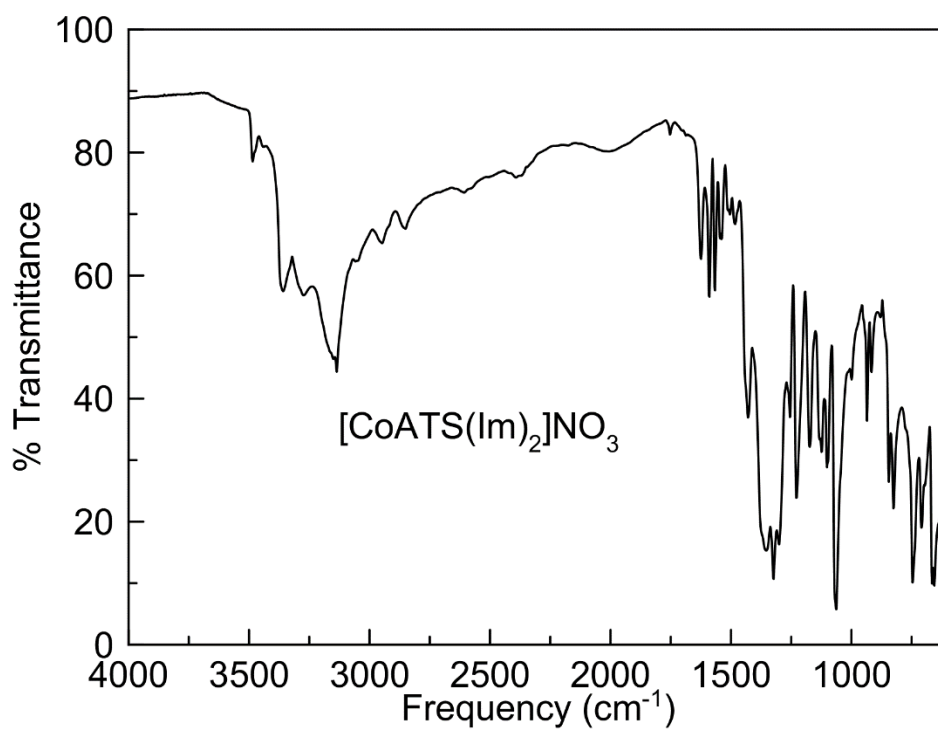


Figure S29. IR Spectrum of [Co(ATS)(Im)₂](NO₃).

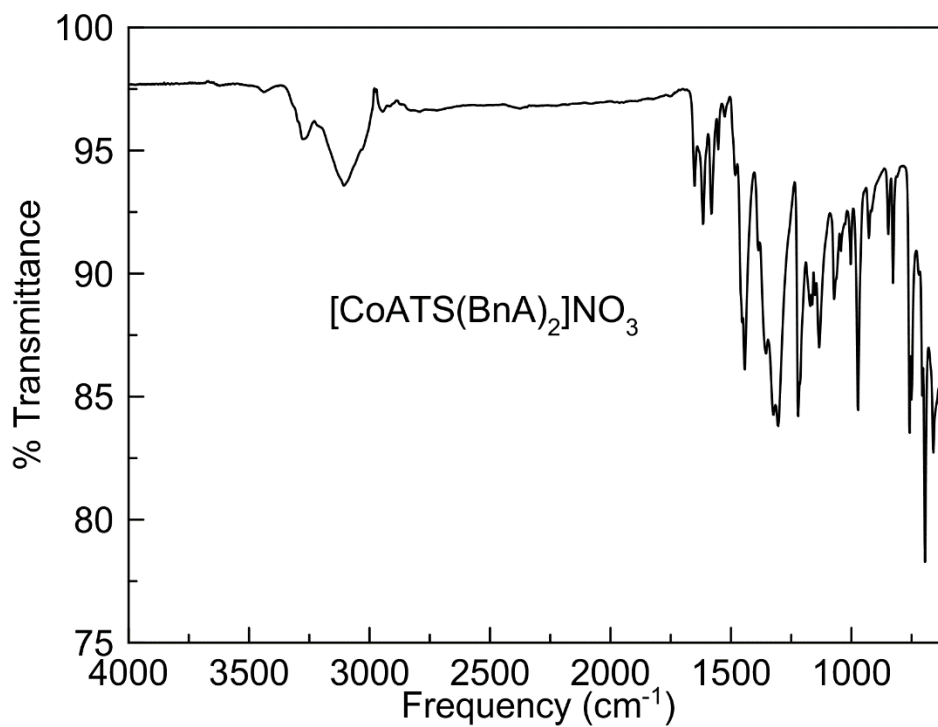


Figure S30. IR Spectrum of [Co(ATS)(BnA₂)](NO₃).

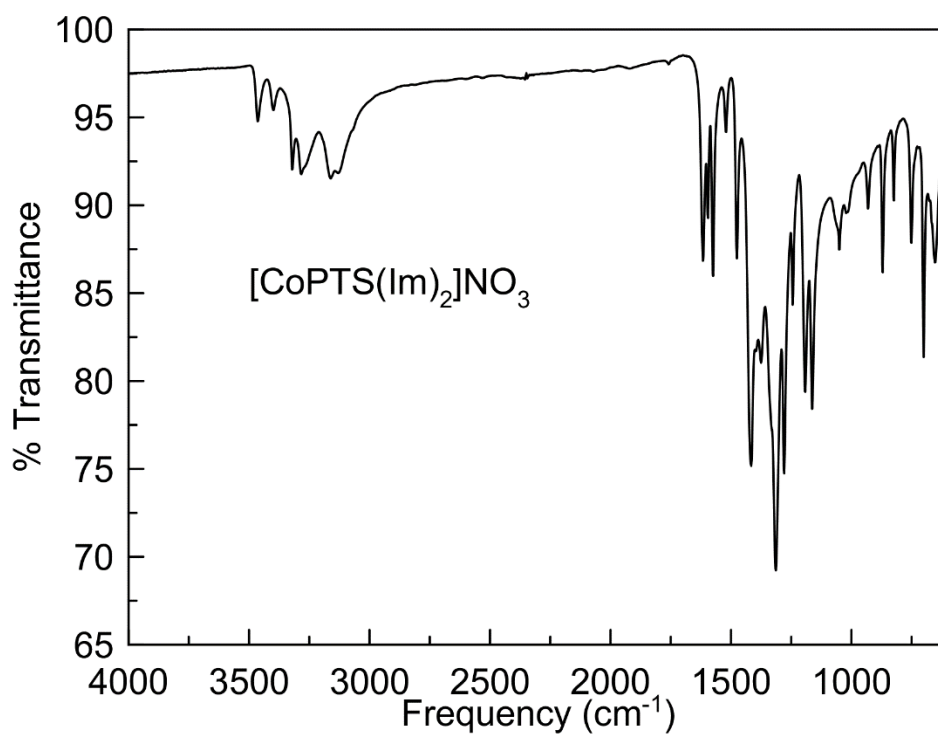


Figure S31. IR Spectrum of $[\text{Co}(\text{PTS})(\text{NH}_3)_2](\text{NO}_3)$.

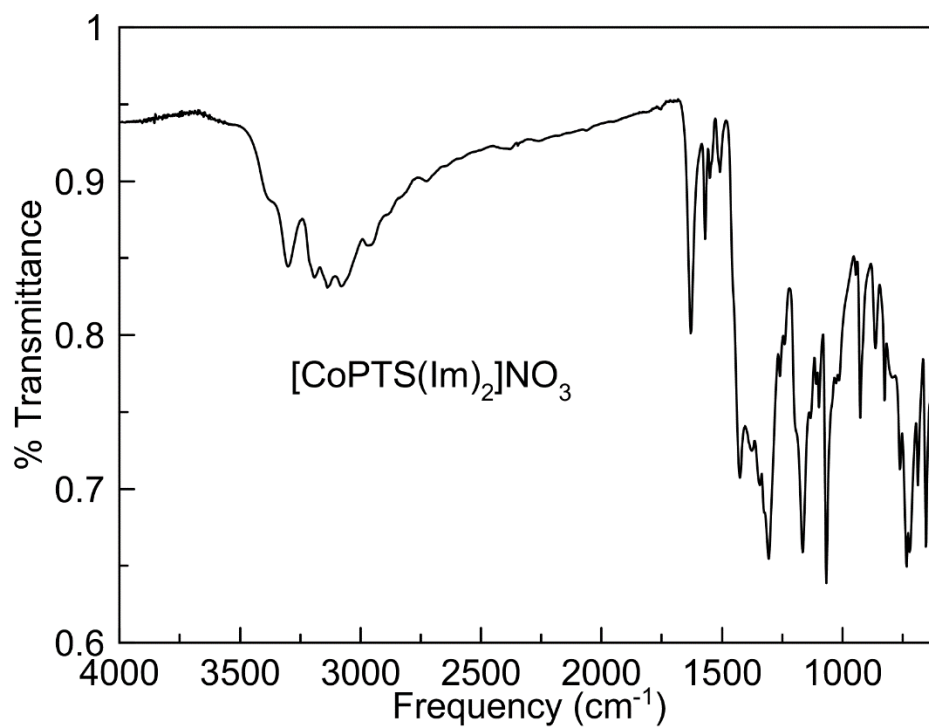


Figure S32. IR Spectrum of $[\text{Co}(\text{PTS})(\text{Im})_2](\text{NO}_3)$.

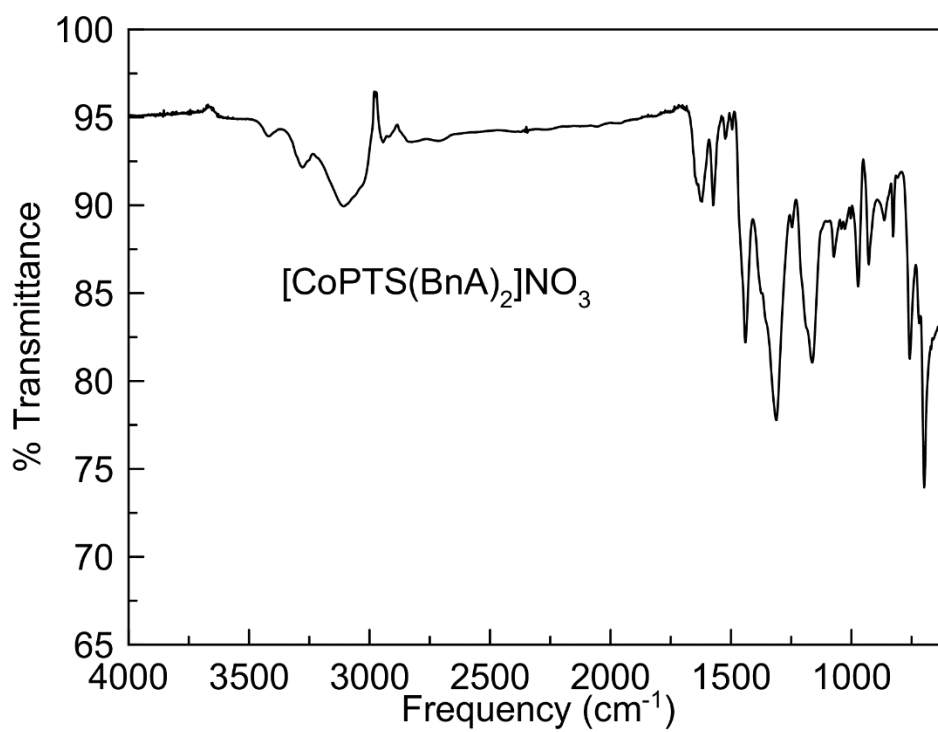


Figure S33. IR Spectrum of [Co(PTS)(BnA)₂](NO₃).

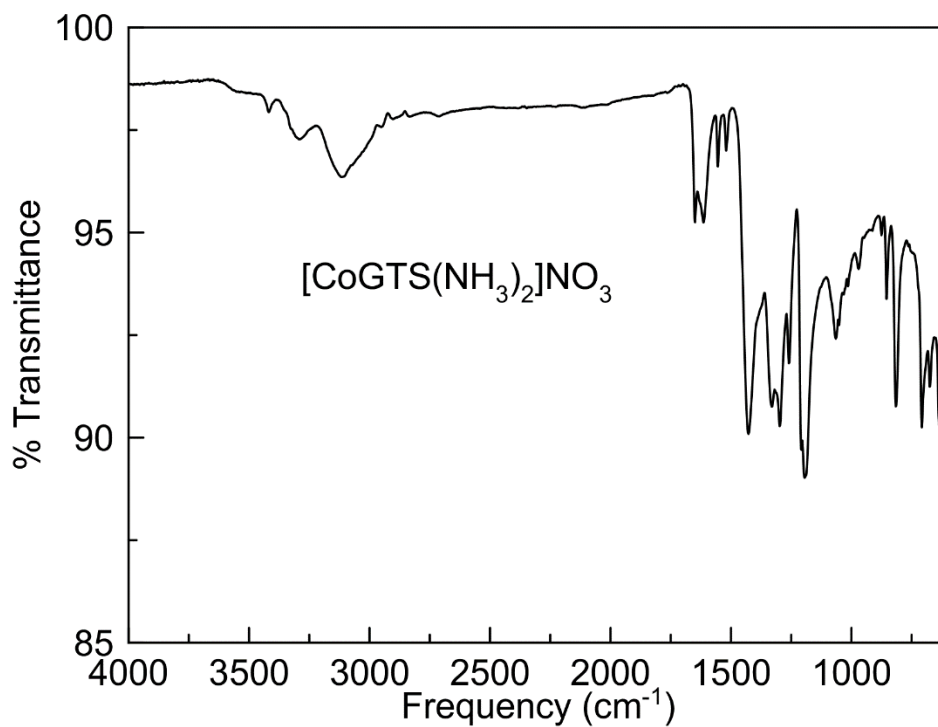


Figure S34. IR Spectrum of [Co(GTS)(NH₃)₂](NO₃).

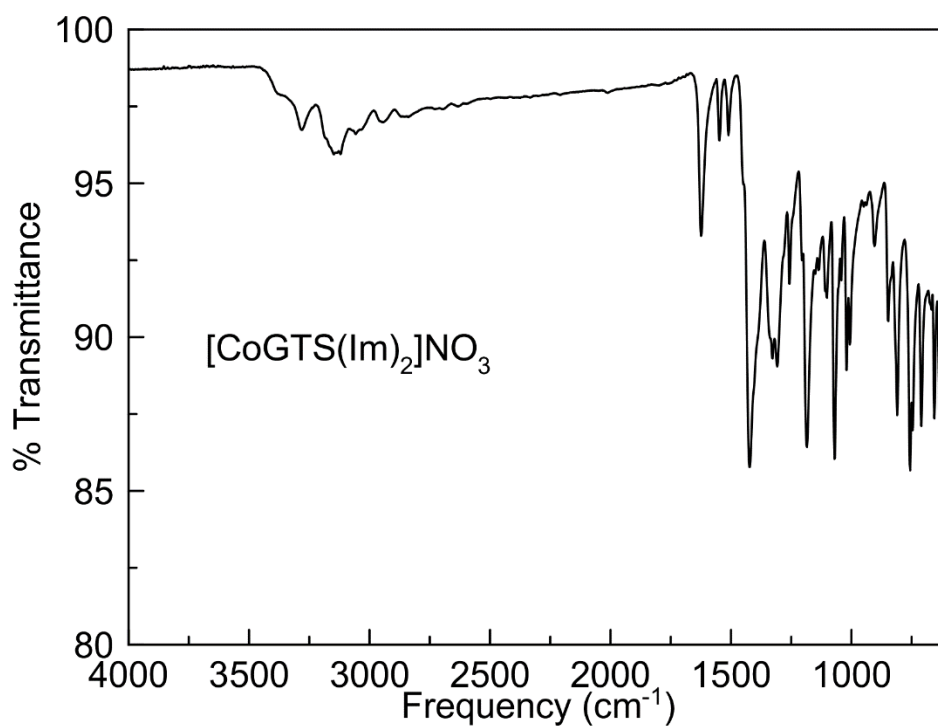


Figure S35. IR Spectrum of [Co(GTS)(Im)₂]₂(NO₃).

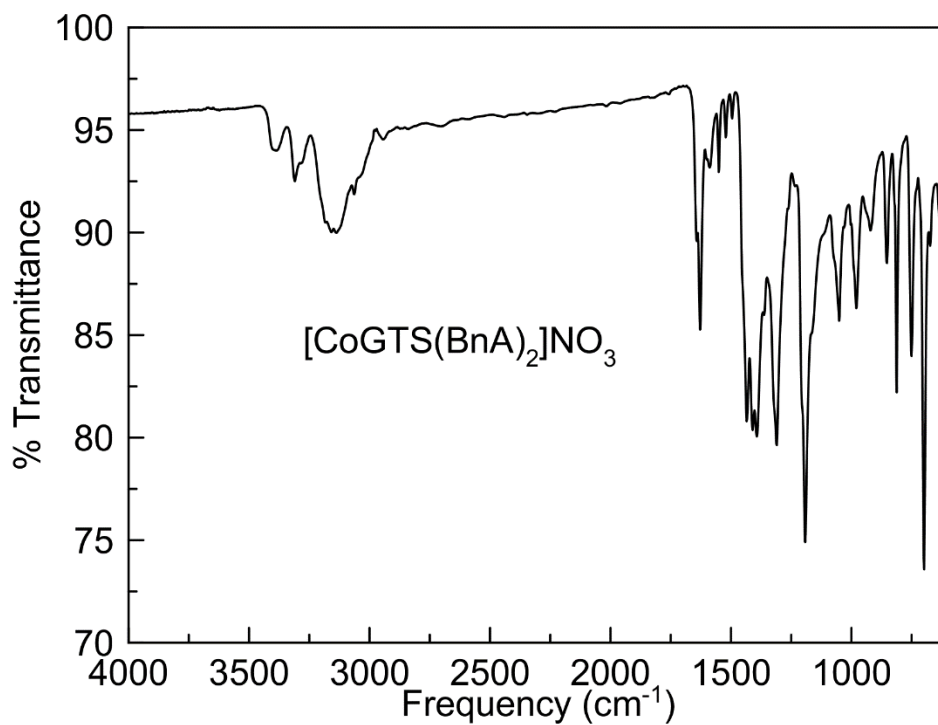


Figure S36. IR Spectrum of [Co(GTS)(BnA)₂]₂(NO₃).

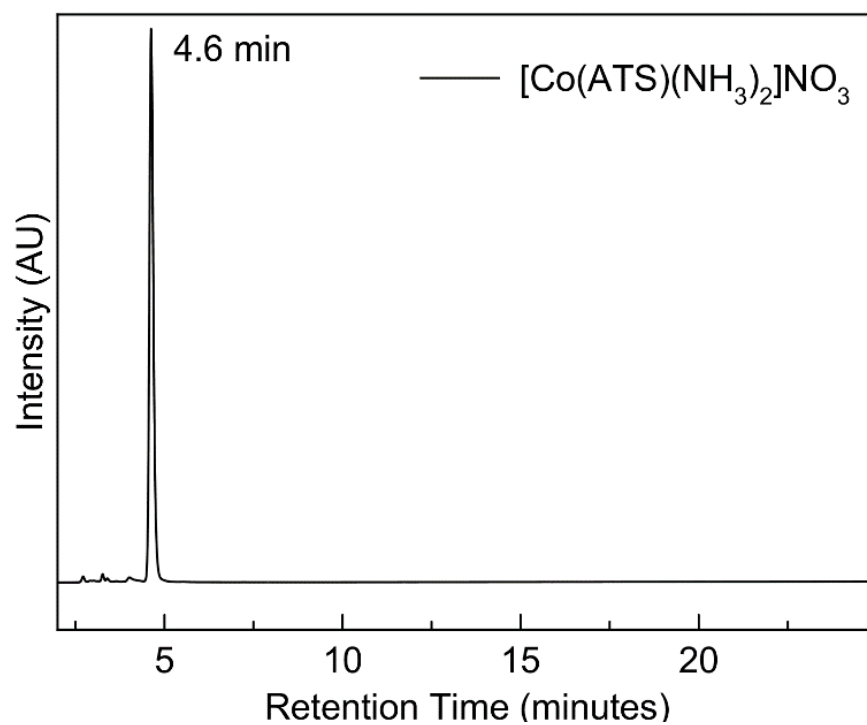


Figure S37. HPLC Chromatogram of $[\text{Co}(\text{ATS})(\text{NH}_3)_2]^+$

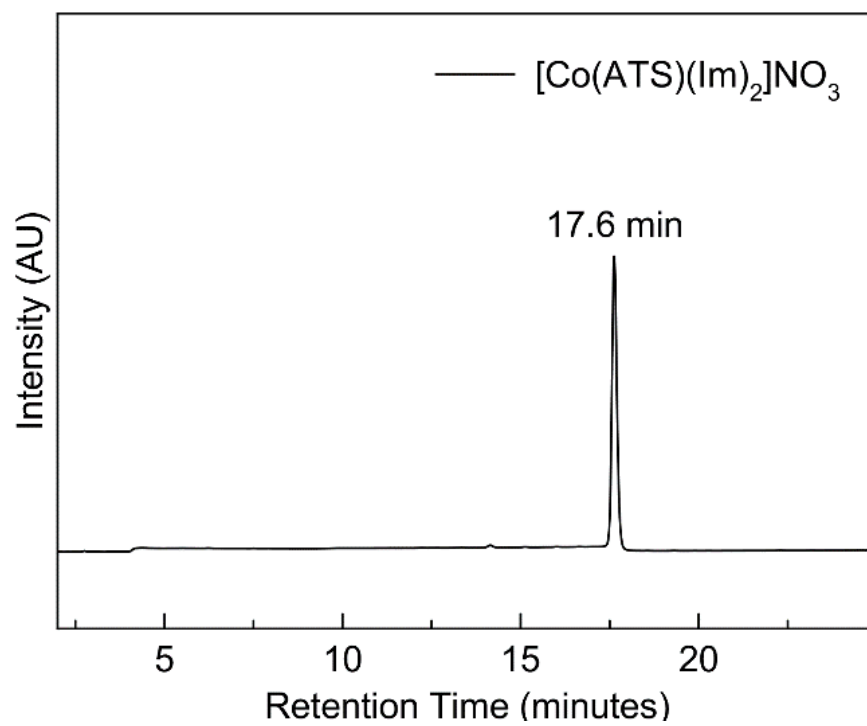


Figure S38. HPLC Chromatogram of $[\text{Co}(\text{ATS})(\text{Im})_2]^+$

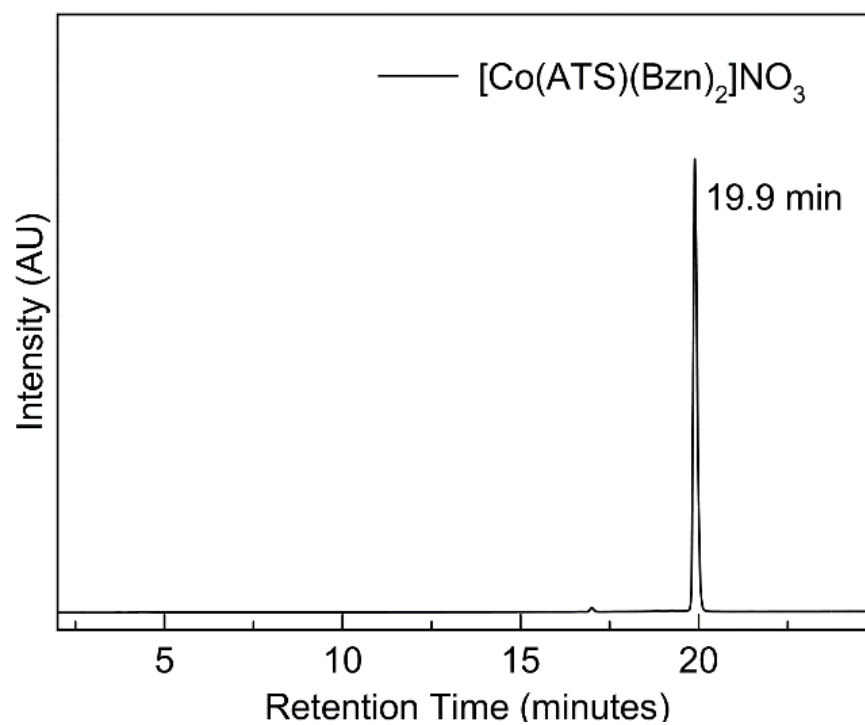


Figure S39. HPLC Chromatogram of $[\text{Co}(\text{ATS})(\text{BnA})_2]^+$

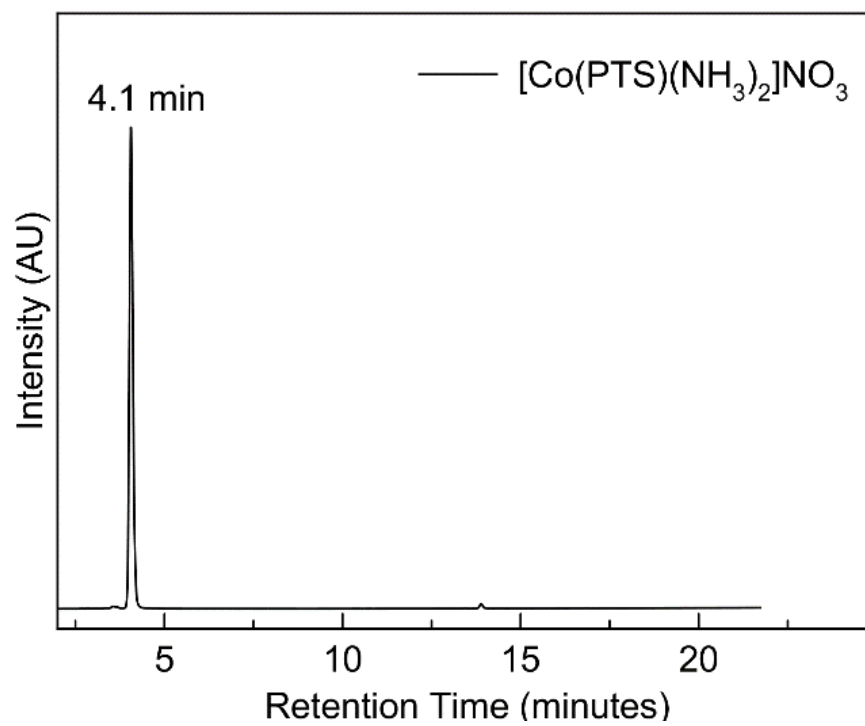


Figure S40. HPLC Chromatogram of $[\text{Co}(\text{PTS})(\text{NH}_3)_2]^+$

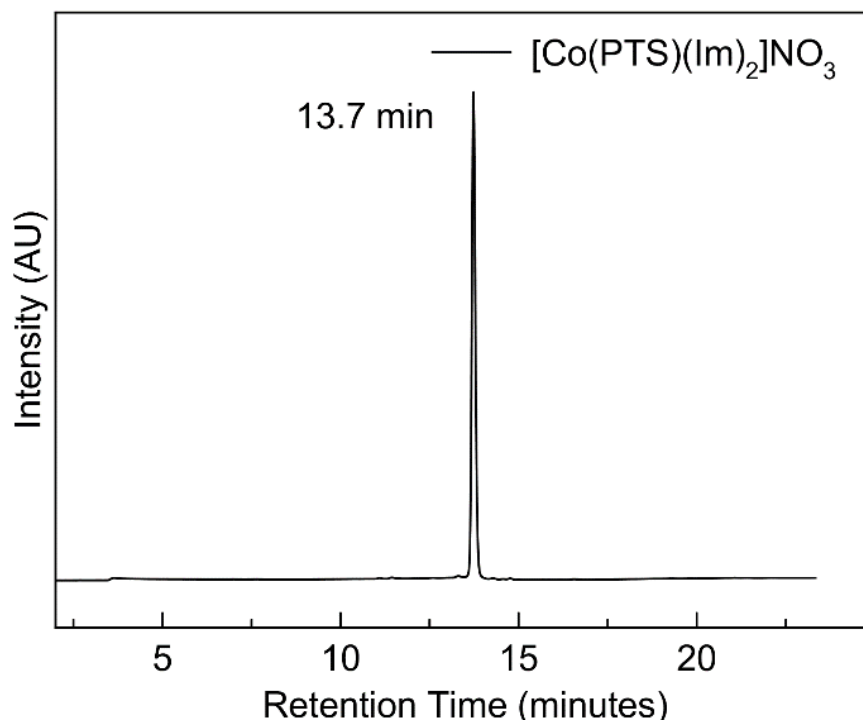


Figure S41. HPLC Chromatogram of $[\text{Co}(\text{PTS})(\text{Im})_2]^+$

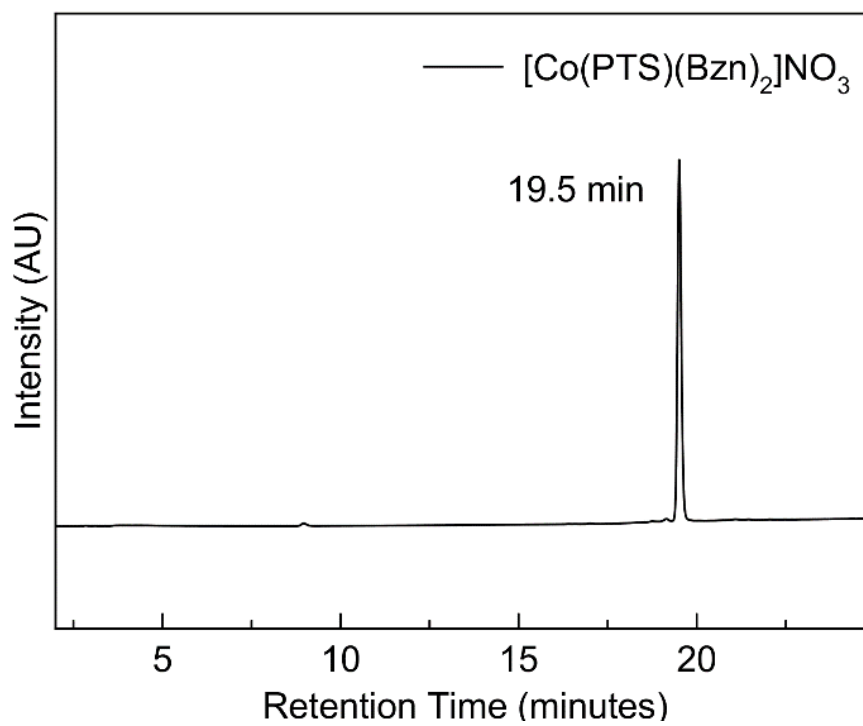


Figure S42. HPLC Chromatogram of $[\text{Co}(\text{PTS})(\text{BnA})_2]^+$

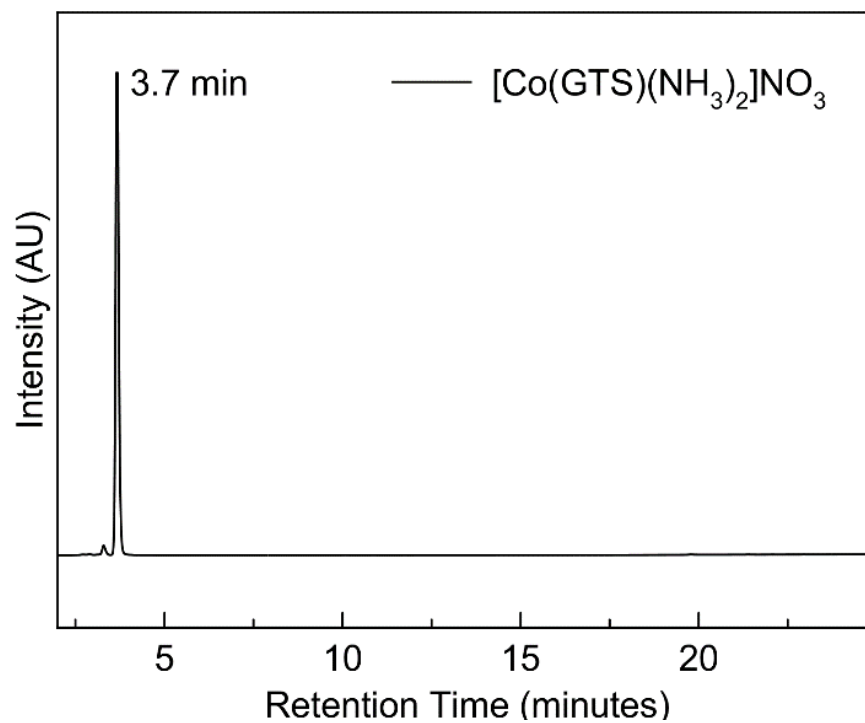


Figure S43. HPLC Chromatogram of $[\text{Co}(\text{GTS})(\text{NH}_3)_2]^+$

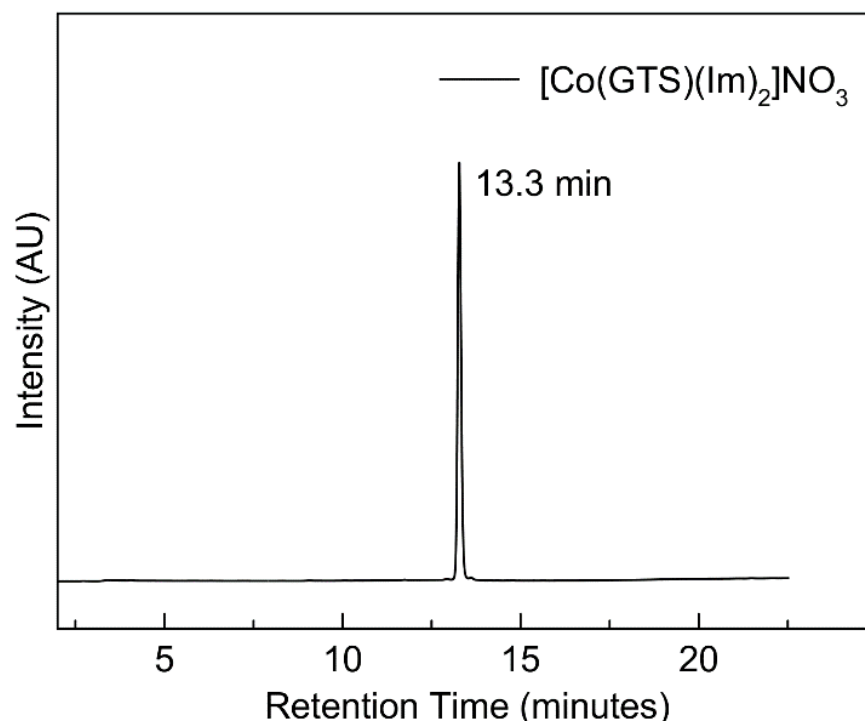


Figure S44. HPLC Chromatogram of $[\text{Co}(\text{GTS})(\text{Im})_2]^+$

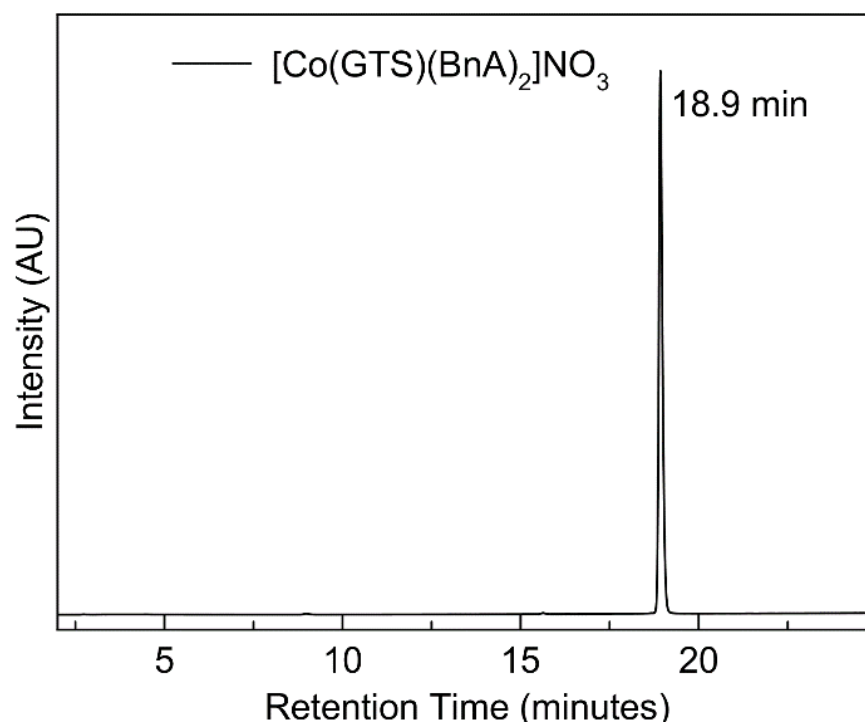


Figure S45. HPLC Chromatogram of $[\text{Co}(\text{GTS})(\text{BnA})_2]^+$

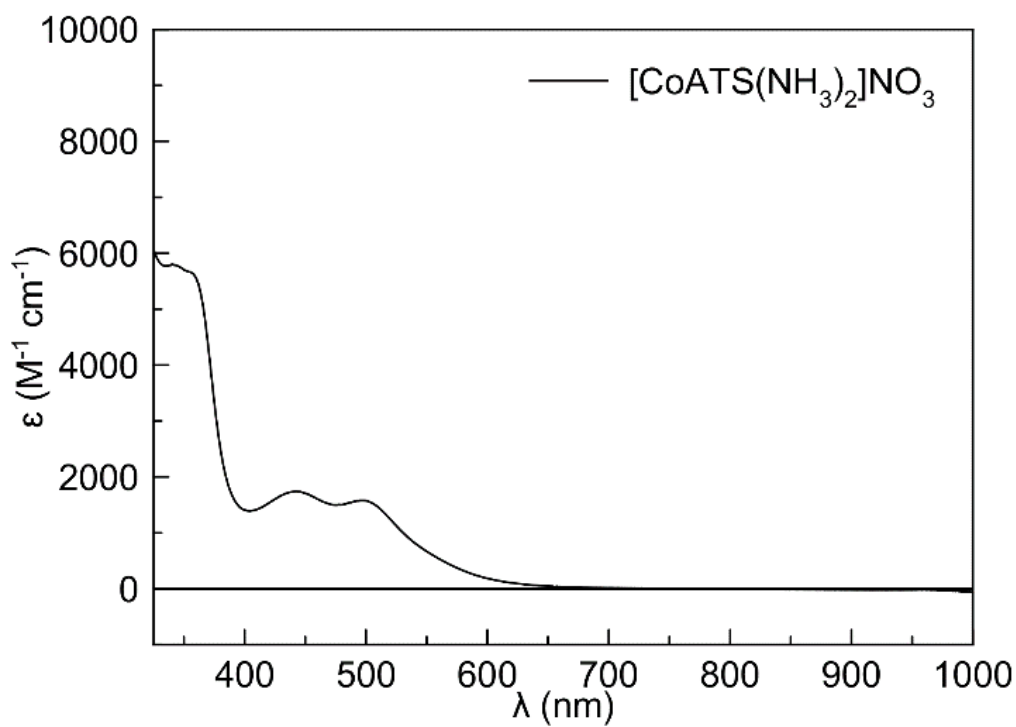


Figure S46. UV-Vis Spectrum of $[\text{Co}(\text{ATS})(\text{NH}_3)_2]^+$ in pH 7.4 phosphate-buffered saline.

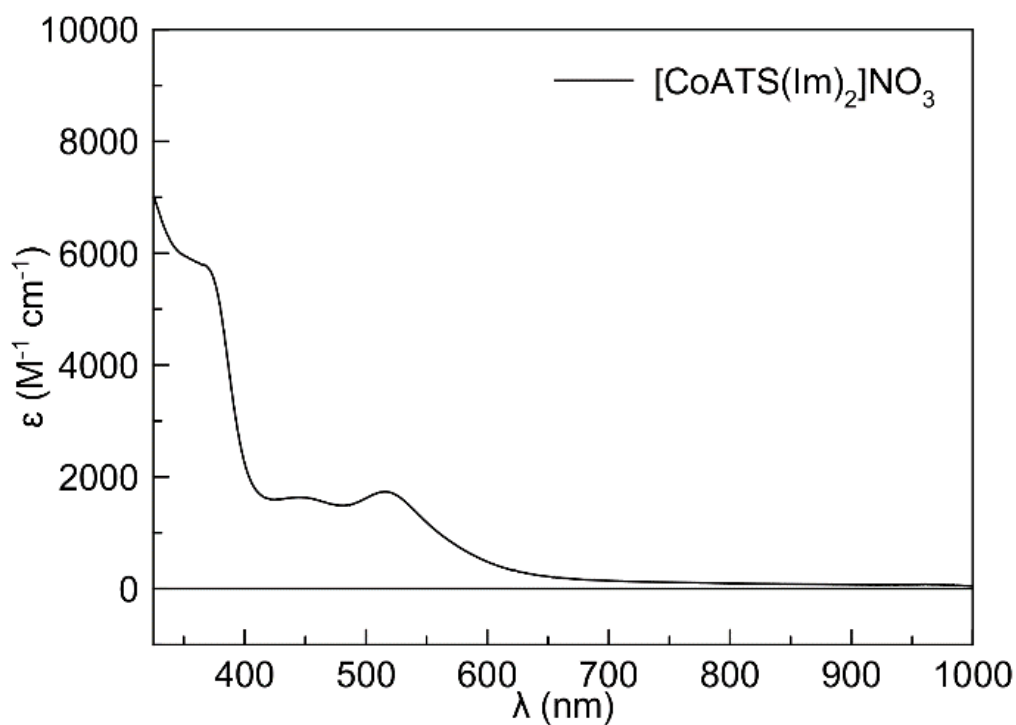


Figure S47. UV-Vis Spectrum of [Co(ATS)(Im)₂]⁺ in pH 7.4 phosphate-buffered saline.

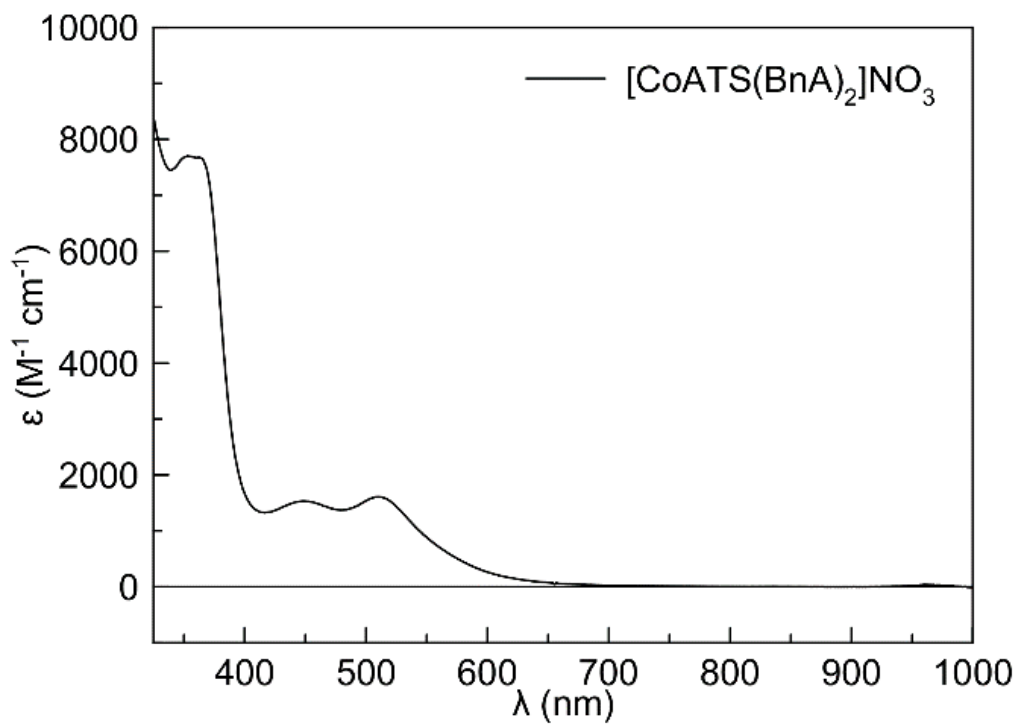


Figure S48. UV-Vis Spectrum of [Co(ATS)(BnA)₂]⁺ in pH 7.4 phosphate-buffered saline.

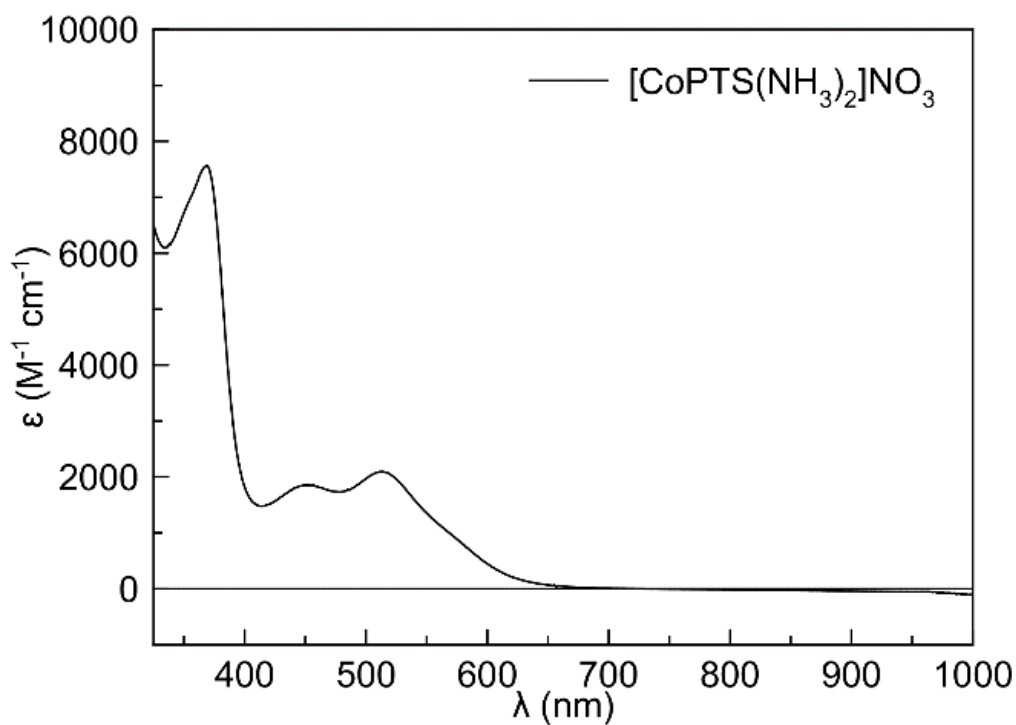


Figure S49. UV-Vis Spectrum of $[\text{Co}(\text{PTS})(\text{NH}_3)_2]^+$ in pH 7.4 phosphate-buffered saline.

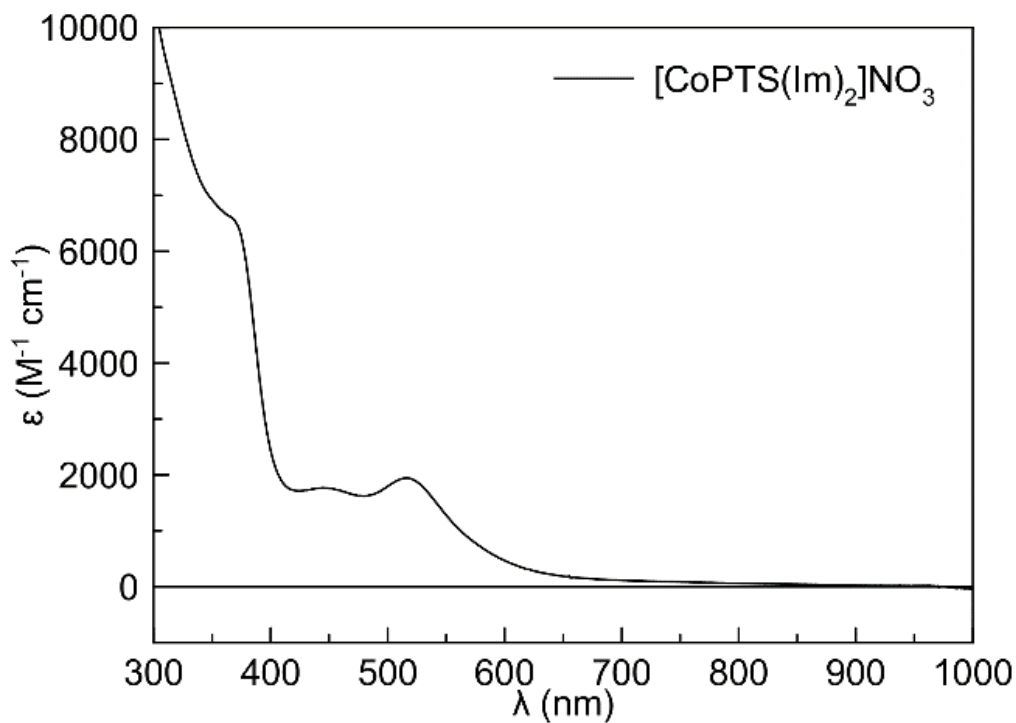


Figure S50. UV-Vis Spectrum of $[\text{Co}(\text{PTS})(\text{Im})_2]^+$ in pH 7.4 phosphate-buffered saline.

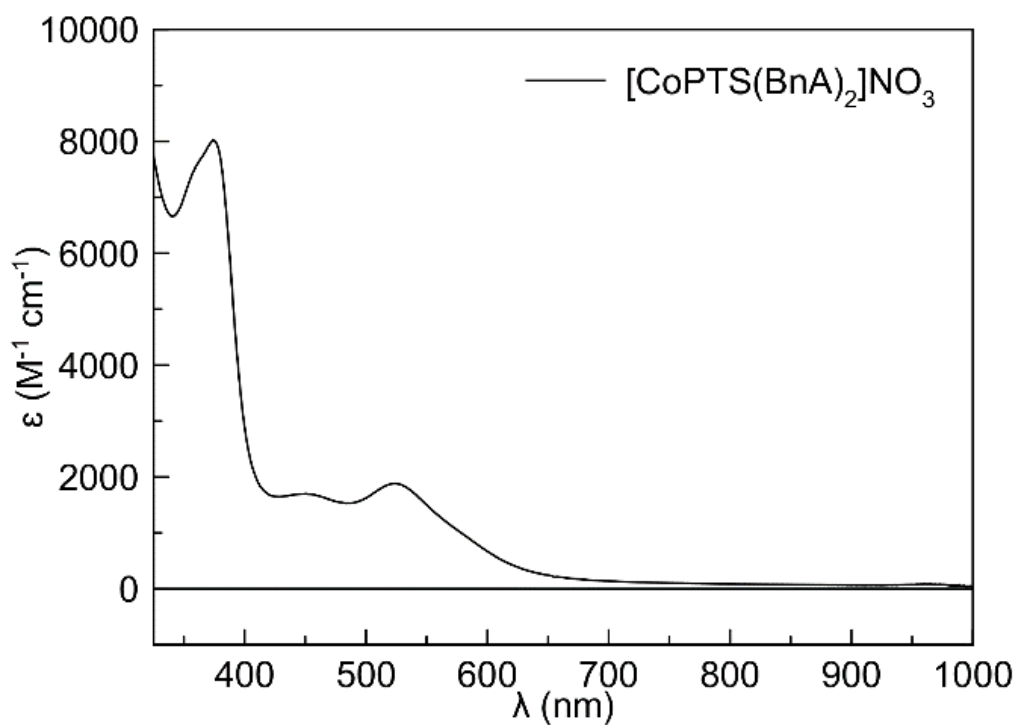


Figure S51. UV-Vis Spectrum of $[\text{Co}(\text{PTS})(\text{BnA})_2]^+$ in pH 7.4 phosphate-buffered saline.

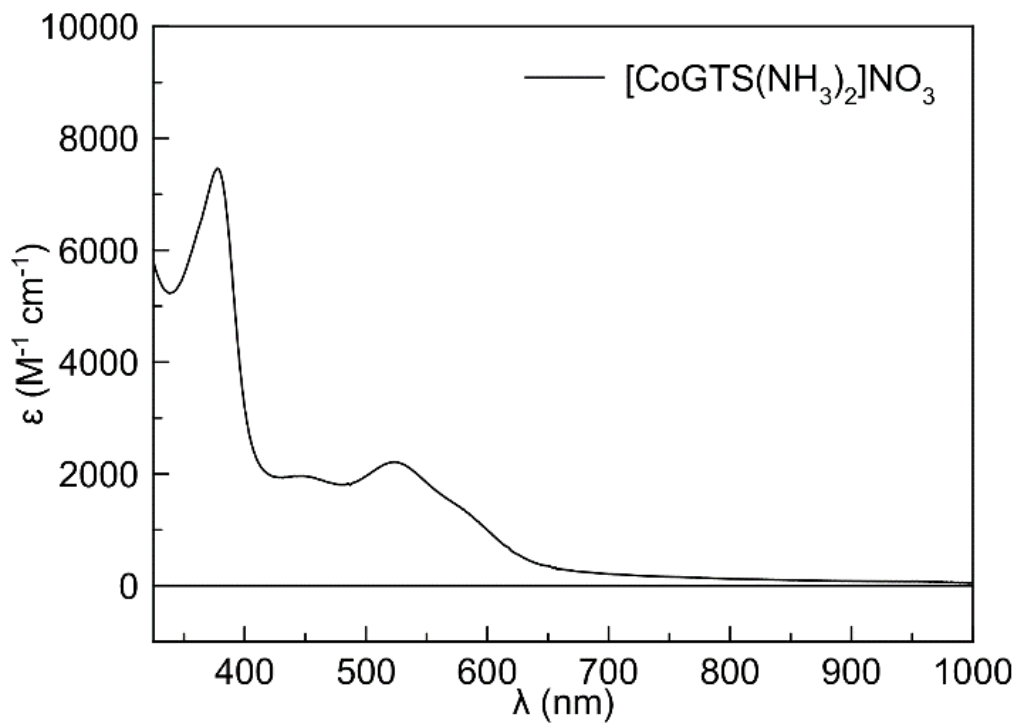


Figure S52. UV-Vis Spectrum of $[\text{Co}(\text{GTS})(\text{NH}_3)_2]^+$ in pH 7.4 phosphate-buffered saline.

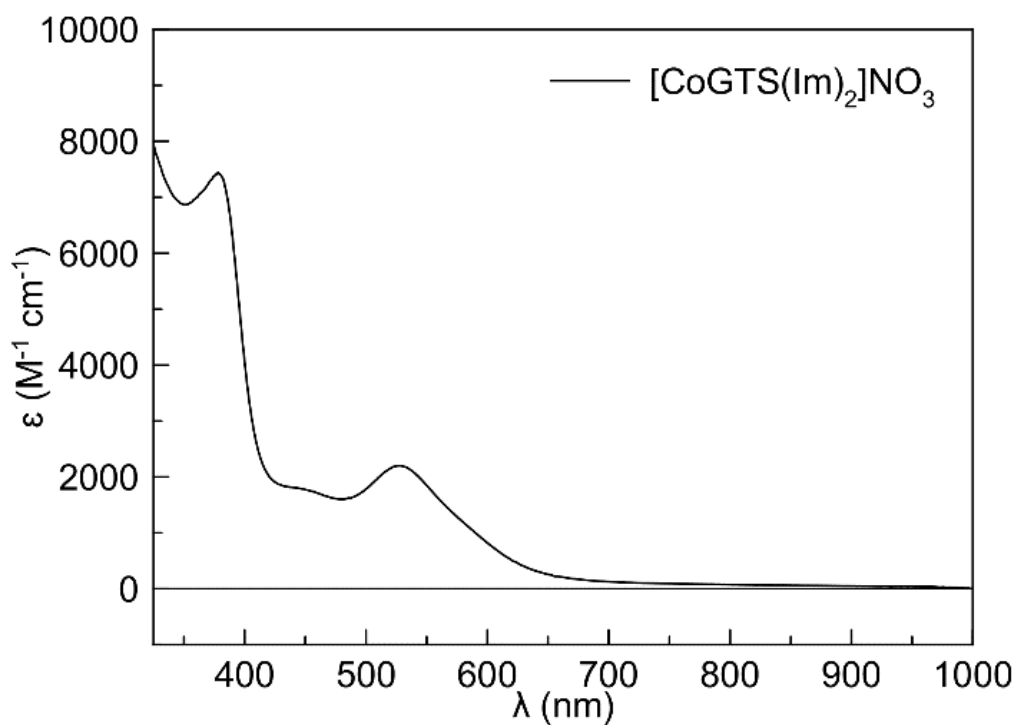


Figure S53. UV-Vis Spectrum of $[\text{Co}(\text{GTS})(\text{Im})_2]^+$ in pH 7.4 phosphate-buffered saline.

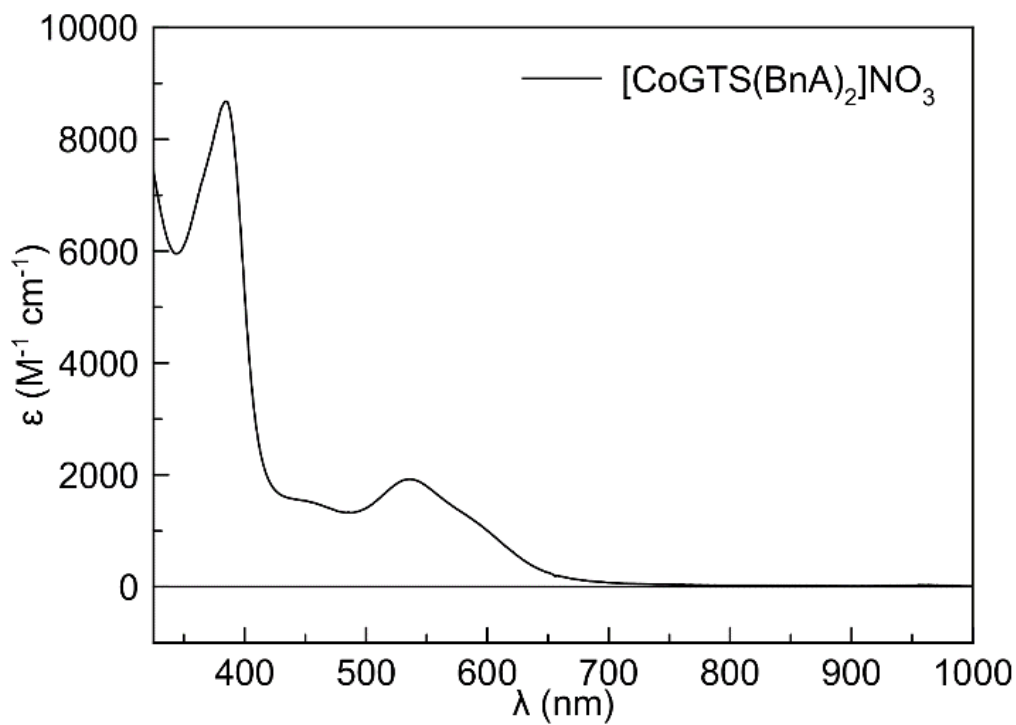


Figure S54. UV-Vis Spectrum of $[\text{Co}(\text{GTS})(\text{BnA})_2]^+$ in pH 7.4 phosphate-buffered saline.

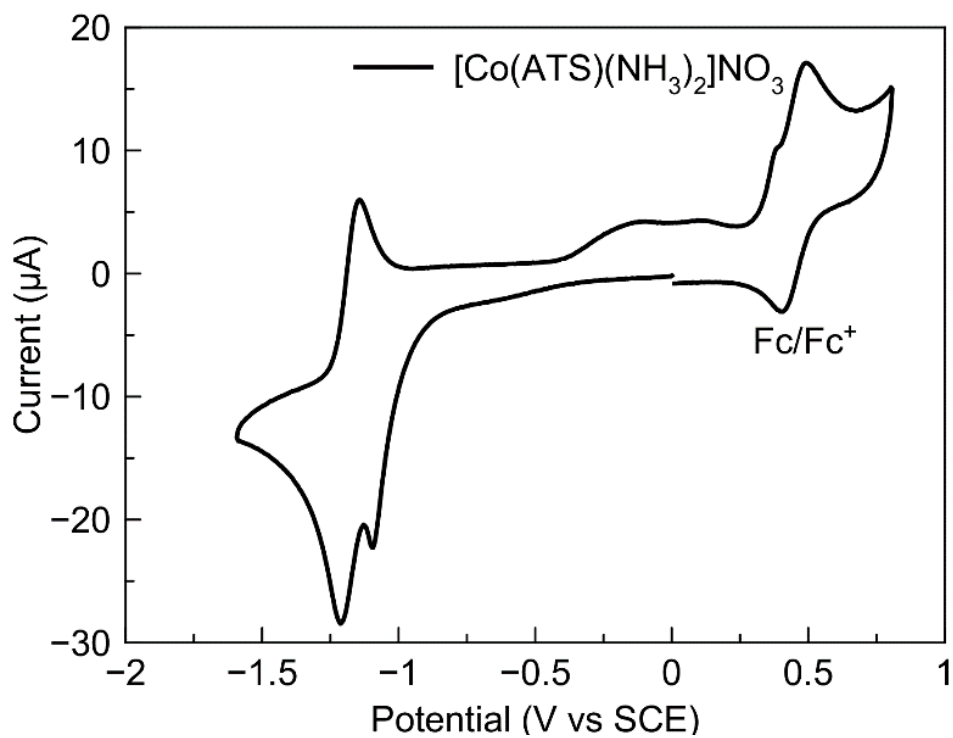


Figure S55. CV of $[\text{Co}(\text{ATS})(\text{NH}_3)_2]^+$ in DMF with 0.1 M $[\text{N}(\text{Bu})_4]\text{PF}_6$

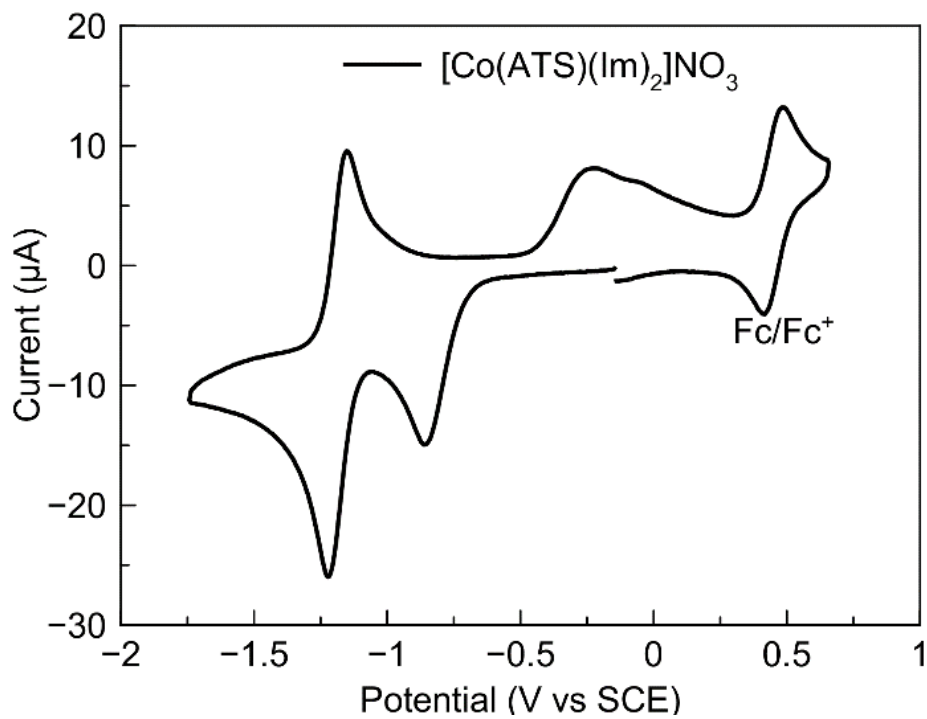


Figure S56. CV of $[\text{Co}(\text{ATS})(\text{Im})_2]^+$ in DMF with 0.1 M $[\text{N}(\text{Bu})_4]\text{PF}_6$

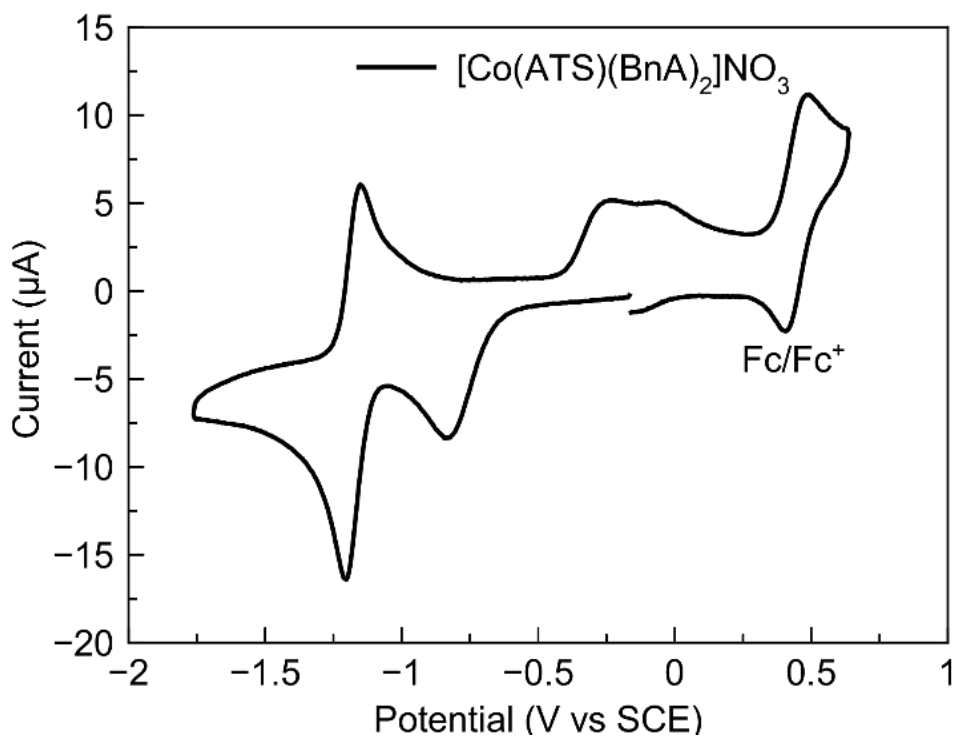


Figure S57. CV of $[\text{Co}(\text{ATS})(\text{BnA})_2]^+$ in DMF with 0.1 M $[\text{N}(\text{Bu})_4]\text{PF}_6$

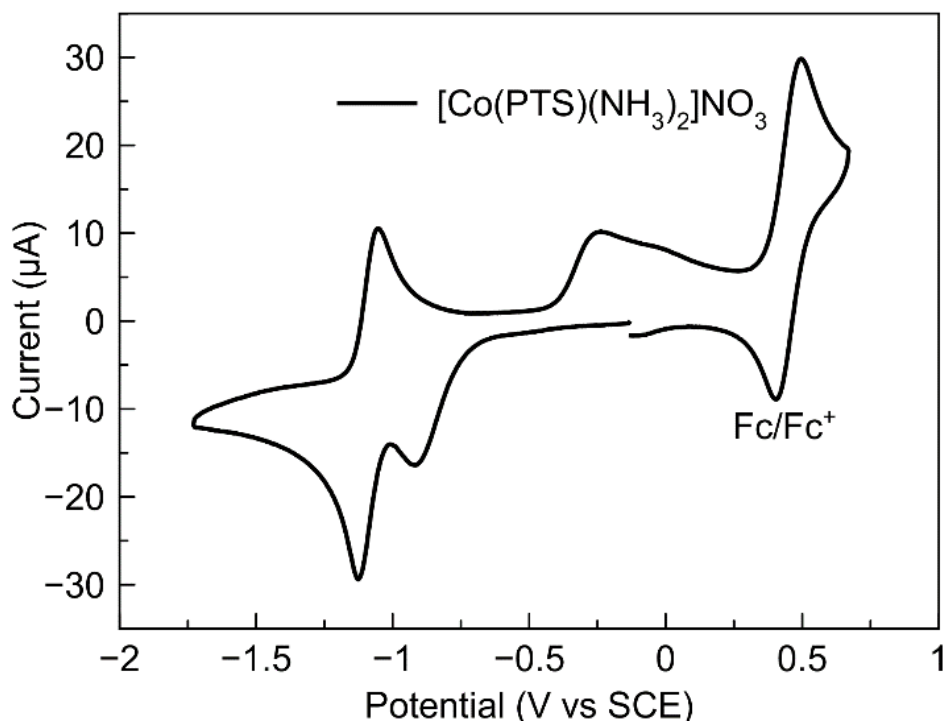


Figure S58. CV of $[\text{Co}(\text{PTS})(\text{NH}_3)_2]^+$ in DMF with 0.1 M $[\text{N}(\text{Bu})_4]\text{PF}_6$

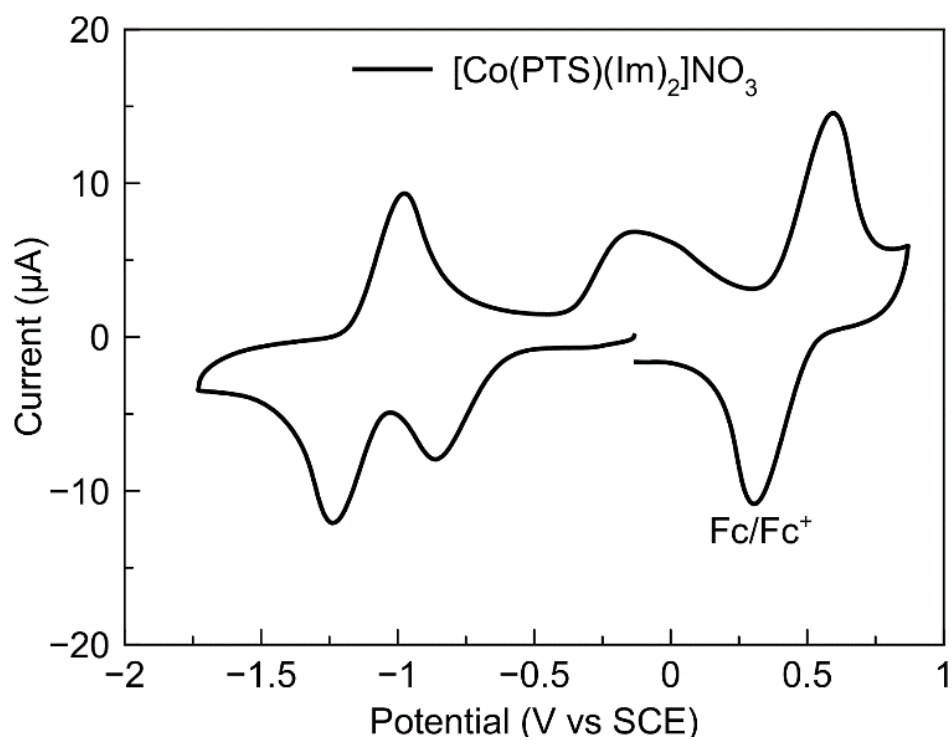


Figure S59. CV of $[\text{Co}(\text{PTS})(\text{Im})_2]^+$ in DMF with 0.1 M $[\text{N}(\text{Bu})_4]\text{PF}_6$

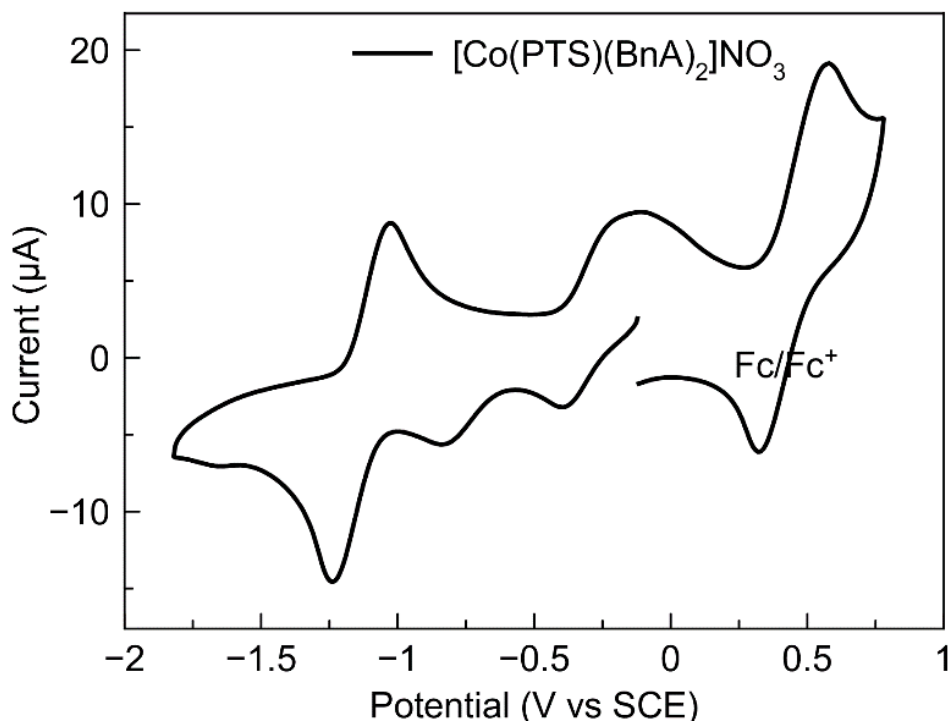


Figure S60. CV of $[\text{Co}(\text{PTS})(\text{BnA})_2]^+$ in DMF with 0.1 M $[\text{N}(\text{Bu})_4]\text{PF}_6$

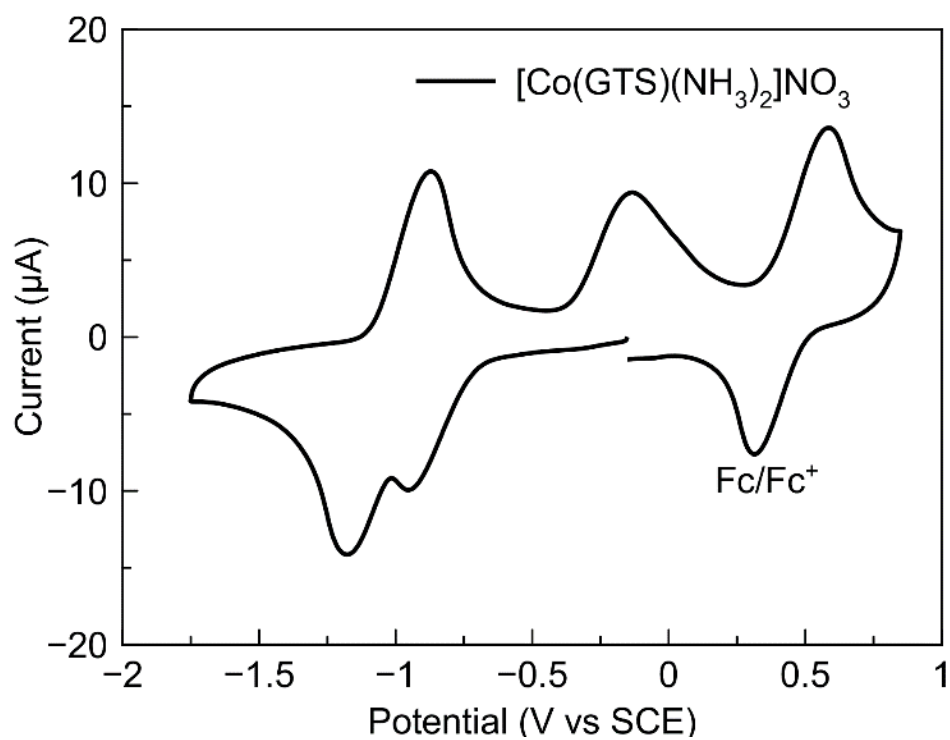


Figure S61. CV of $[\text{Co}(\text{GTS})(\text{NH}_3)_2]^+$ in DMF with 0.1 M $[\text{N}(\text{Bu})_4]\text{PF}_6$

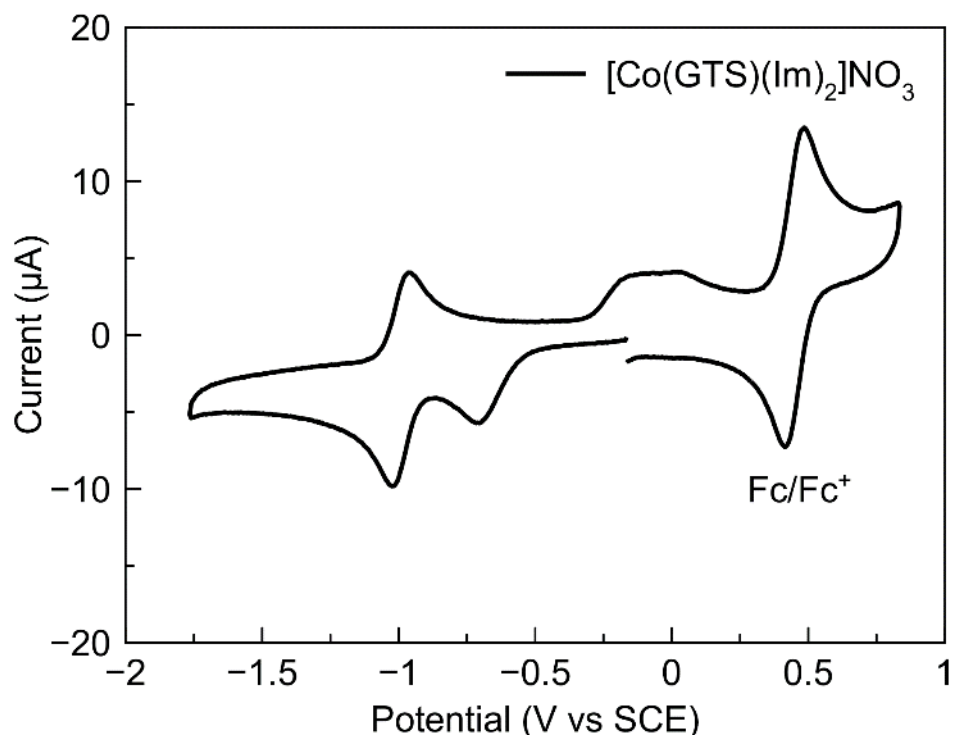


Figure S62. CV of $[\text{Co}(\text{GTS})(\text{Im})_2]^+$ in DMF with 0.1 M $[\text{N}(\text{Bu})_4]\text{PF}_6$

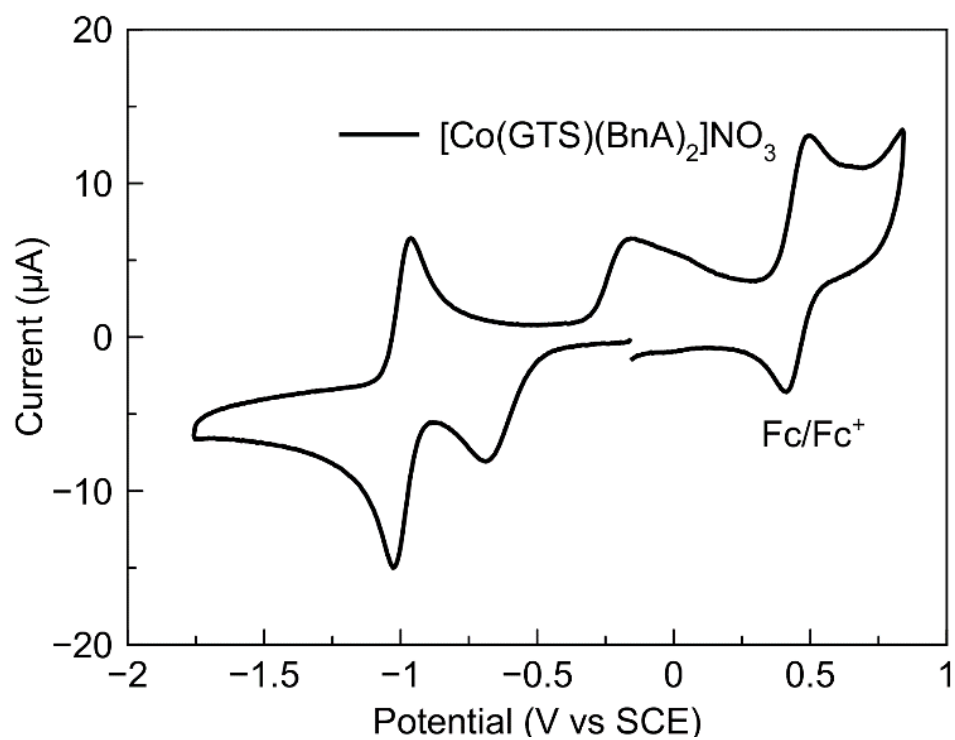


Figure S63. CV of $[\text{Co}(\text{GTS})(\text{BnA})_2]^+$ in DMF with 0.1 M $[\text{N}(\text{Bu})_4]\text{PF}_6$

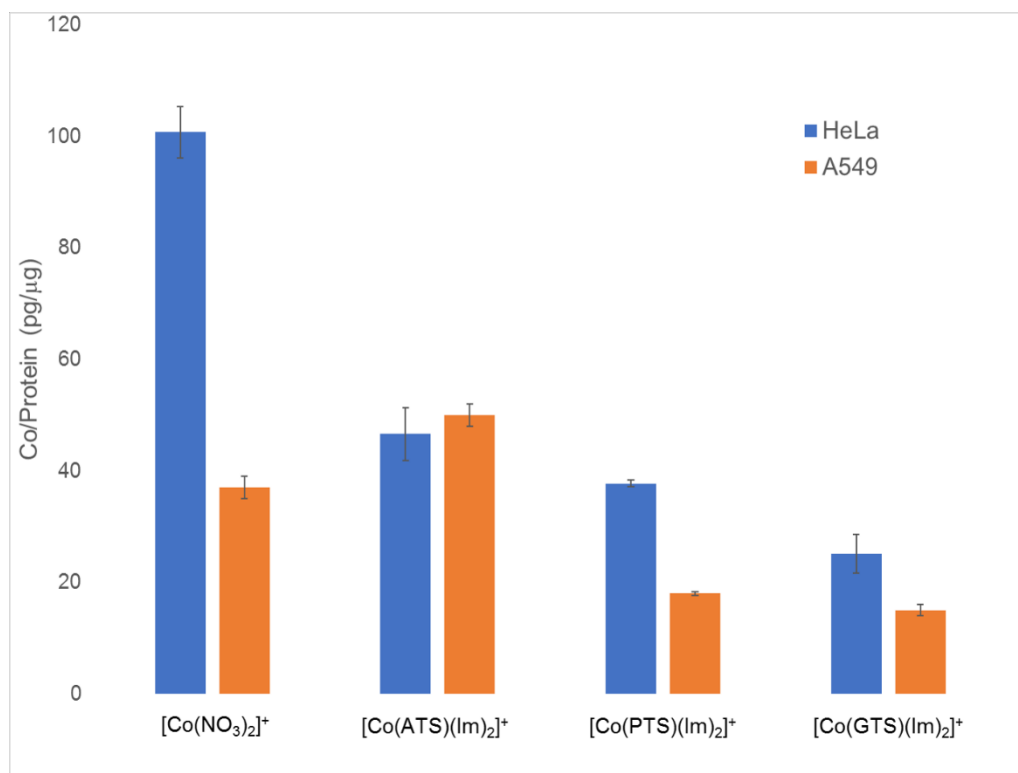


Figure S64. Uptake of $[\text{Co}(\text{BTSC})(\text{Im})_2]^+$ Complexes in HeLa and A549 Cells

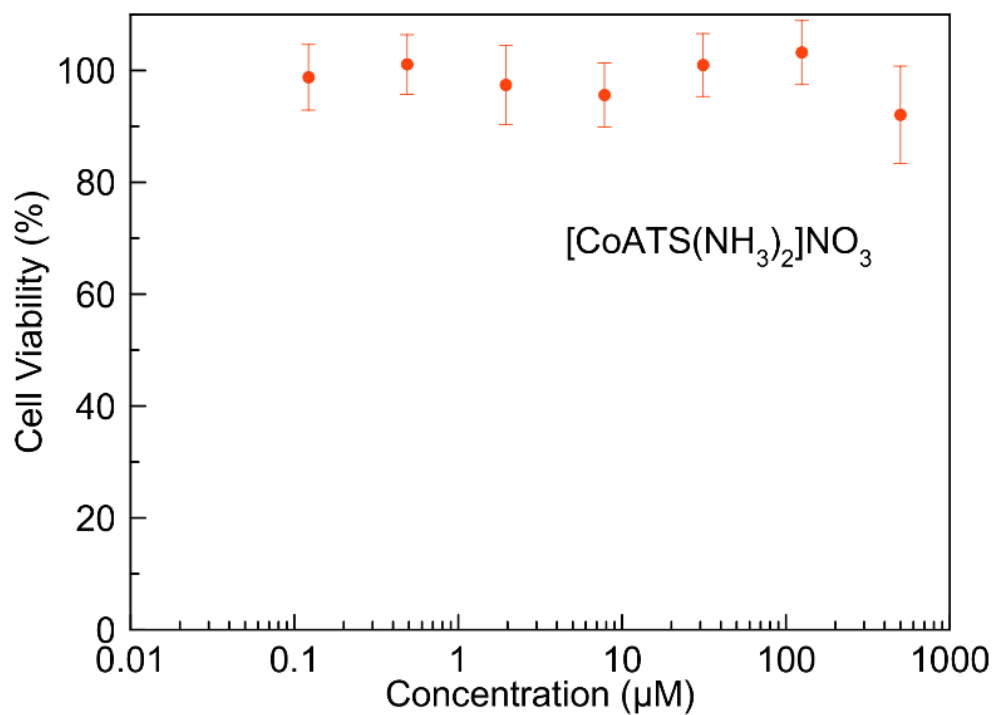


Figure S65. Dose-Response Curve of $[\text{Co}(\text{ATS})(\text{NH}_3)_2]^+$ in A549 Cells

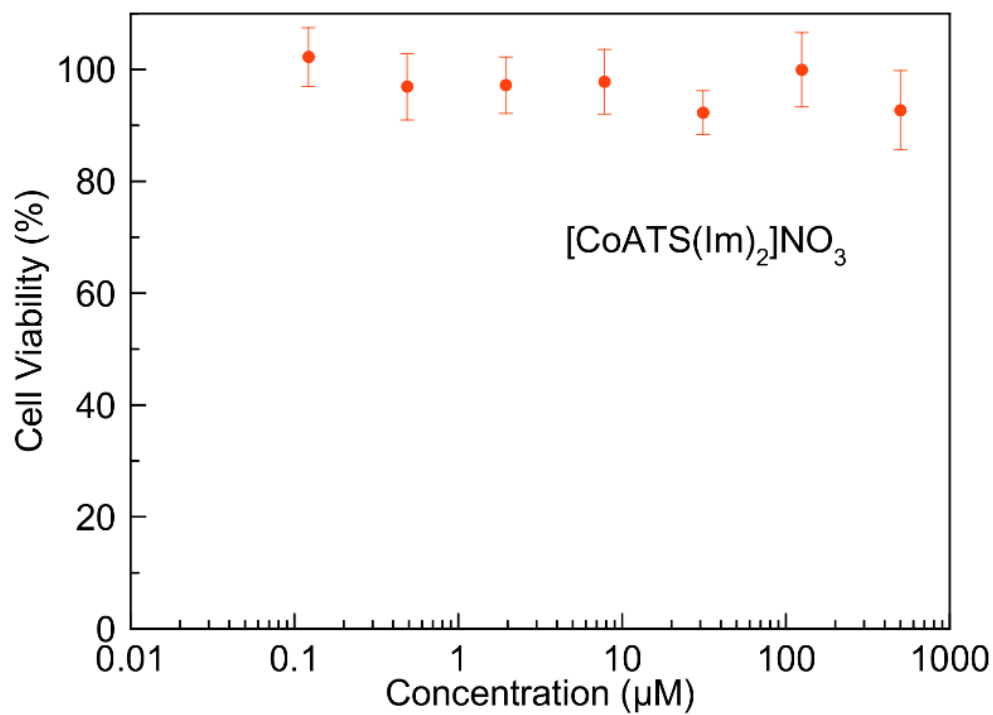


Figure S66. Dose-Response Curve of $[\text{Co}(\text{ATS})(\text{Im})_2]^+$ in A549 Cells

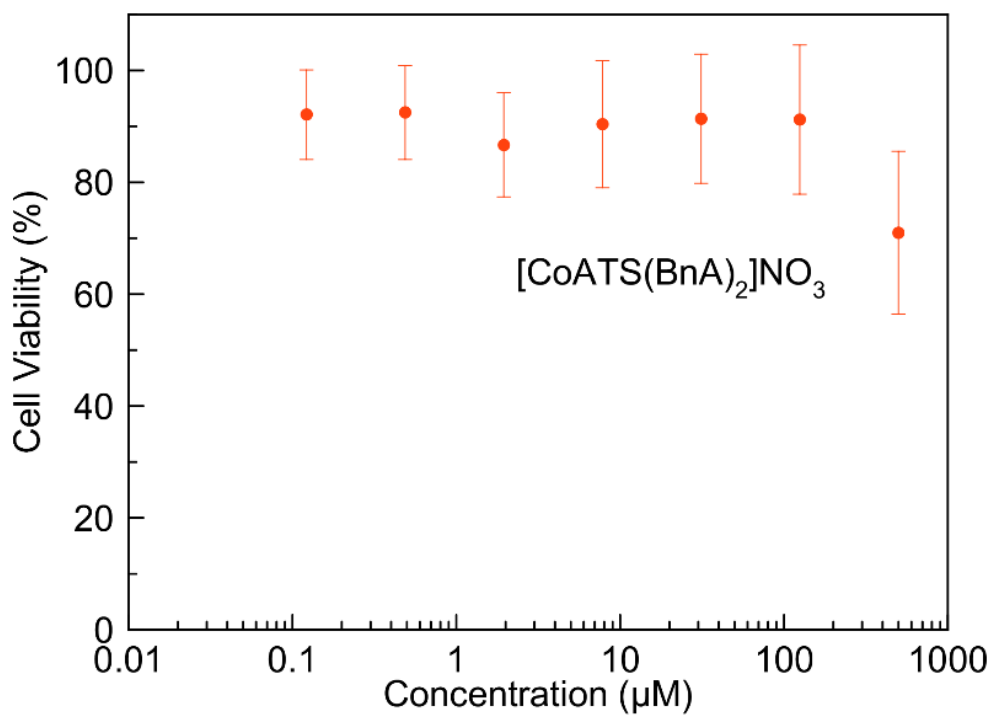


Figure S67. Dose-Response Curve of $[\text{Co}(\text{ATS})(\text{BnA})_2]^+$ in A549 Cells

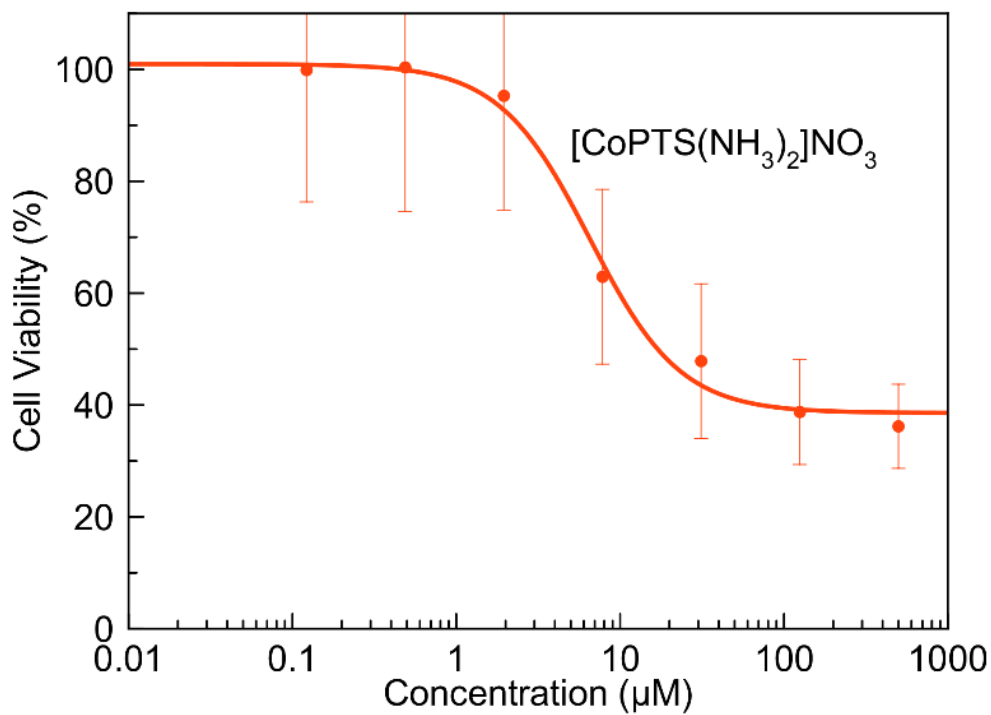


Figure S68. Dose-Response Curve of $[\text{Co}(\text{PTS})(\text{NH}_3)_2]^+$ in A549 Cells

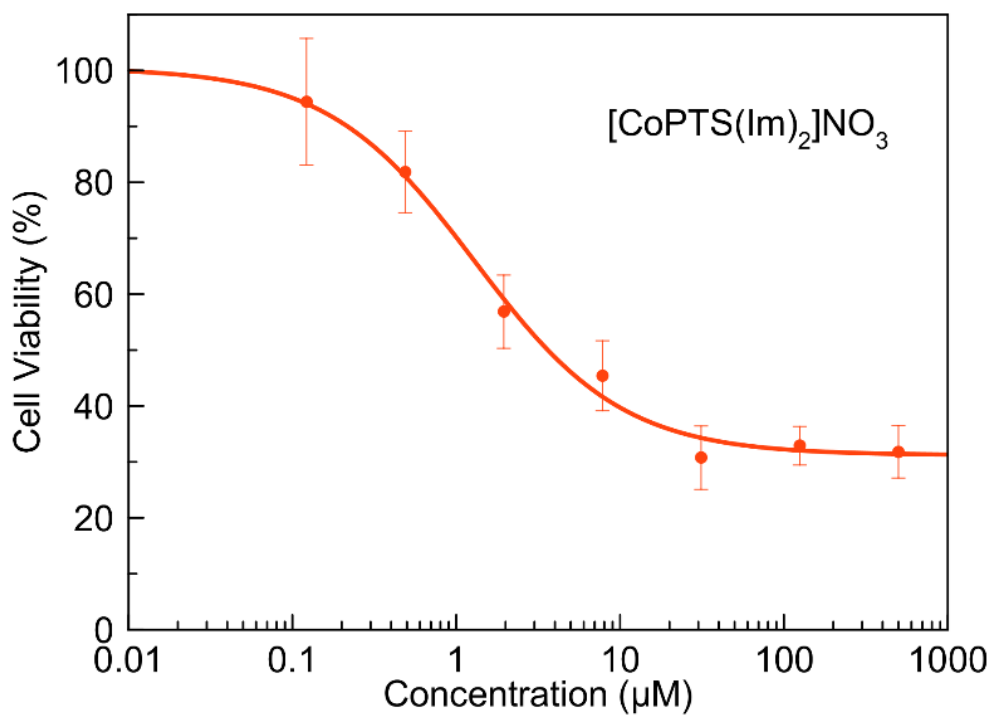


Figure S69. Dose-Response Curve of [Co(PTS)(Im)₂]⁺ in A549 Cells

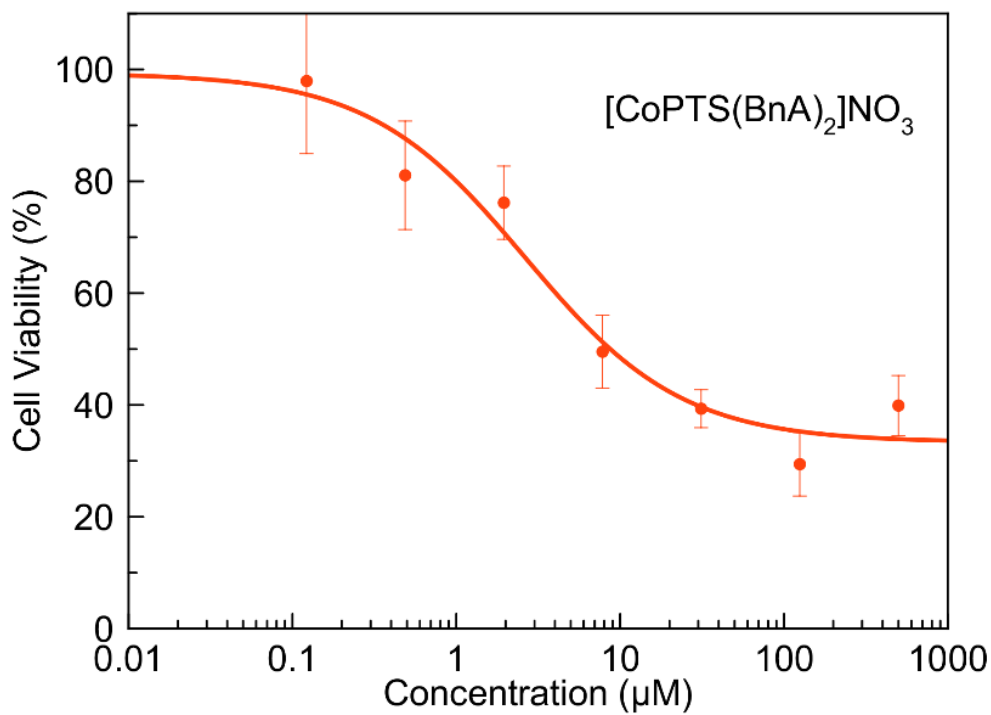


Figure S70. Dose-Response Curve of [Co(PTS)(BnA)₂]⁺ in A549 Cells

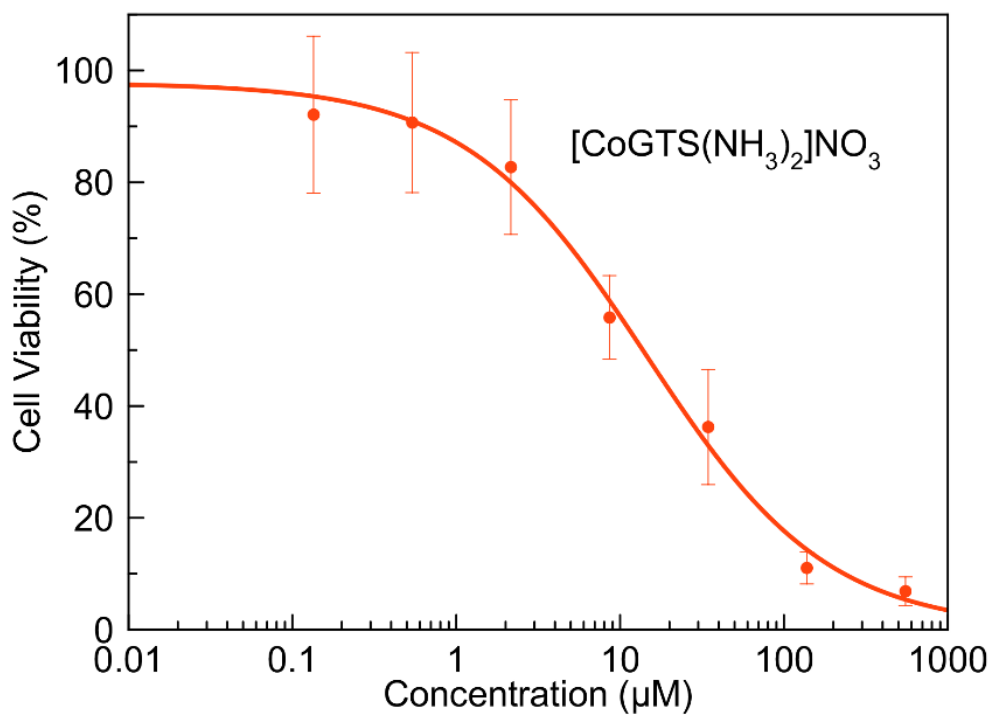


Figure S71. Dose-Response Curve of $[\text{Co}(\text{GTS})(\text{NH}_3)_2]^+$ in A549 Cells

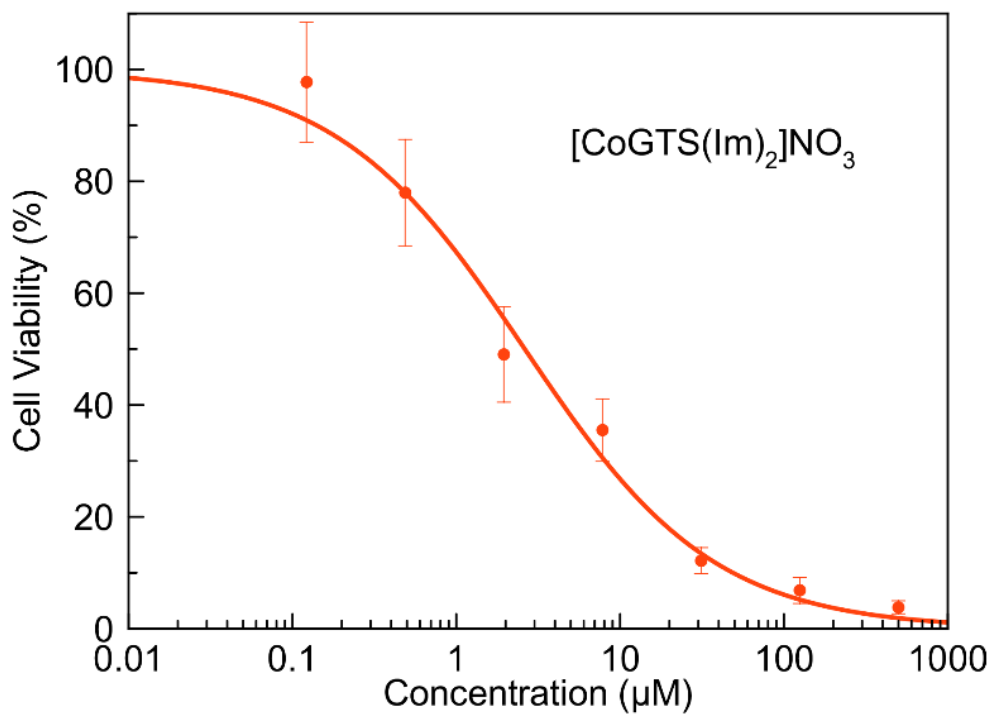


Figure S72. Dose-Response Curve of $[\text{Co}(\text{GTS})(\text{Im})_2]^+$ in A549 Cells

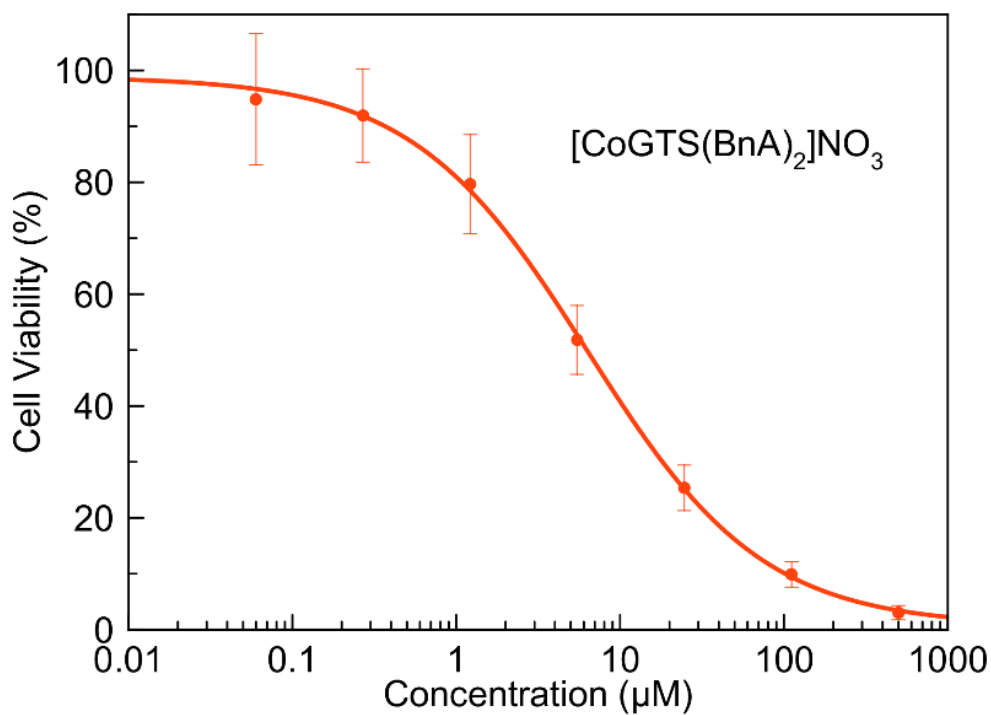


Figure S73. Dose-Response Curve of $[\text{Co}(\text{GTS})(\text{BnA})_2]^+$ in A549 Cells

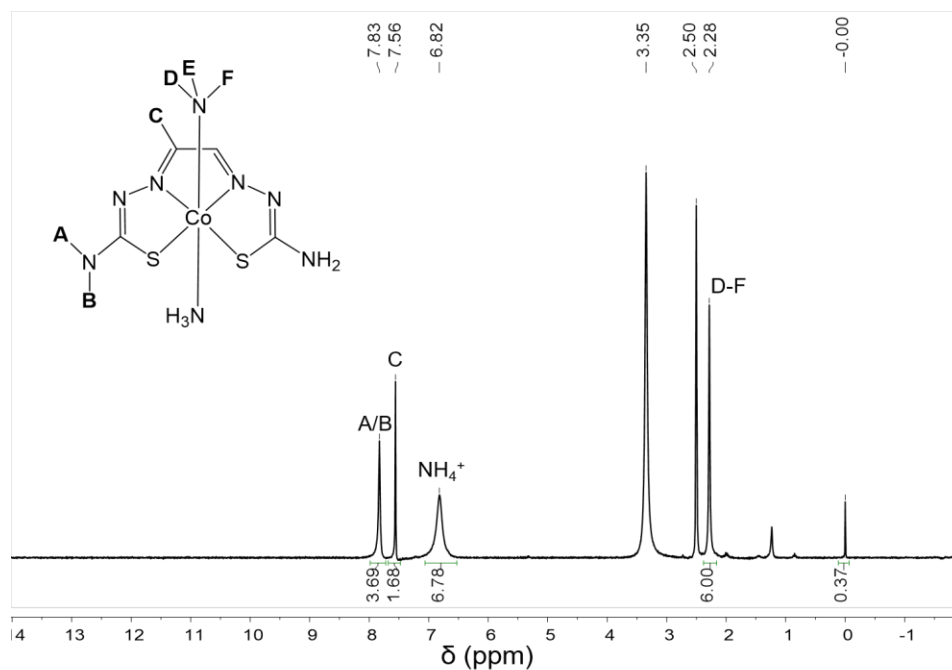


Figure S74. ^1H NMR spectrum of $[\text{Co}(\text{GTS})(\text{NH}_3)_2]^+$ and ammonium tetrathiomolybdate immediately after mixing ($\text{DMSO}-d_6$, 400 MHz, 298 K)

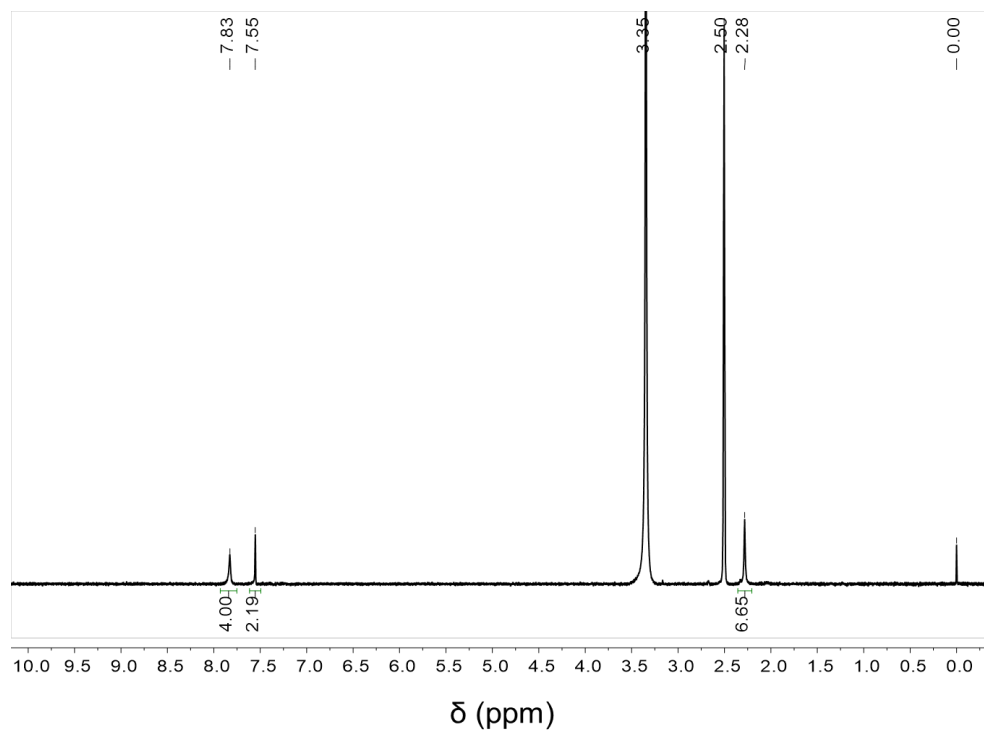


Figure S75. ¹H NMR spectrum of [Co(GTS)(NH₃)₂]⁺ and ammonium tetrathiomolybdate 1 day after mixing (DMSO-*d*₆, 400 MHz, 298 K)