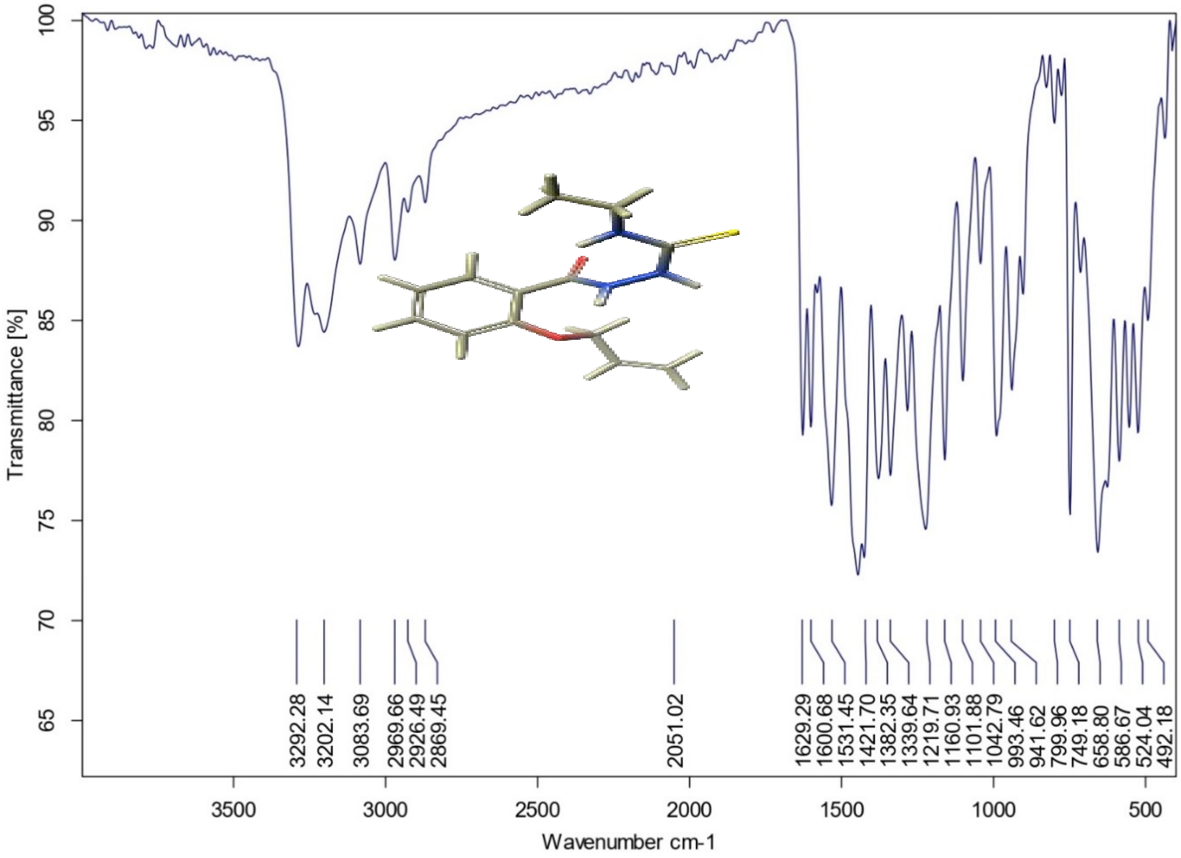
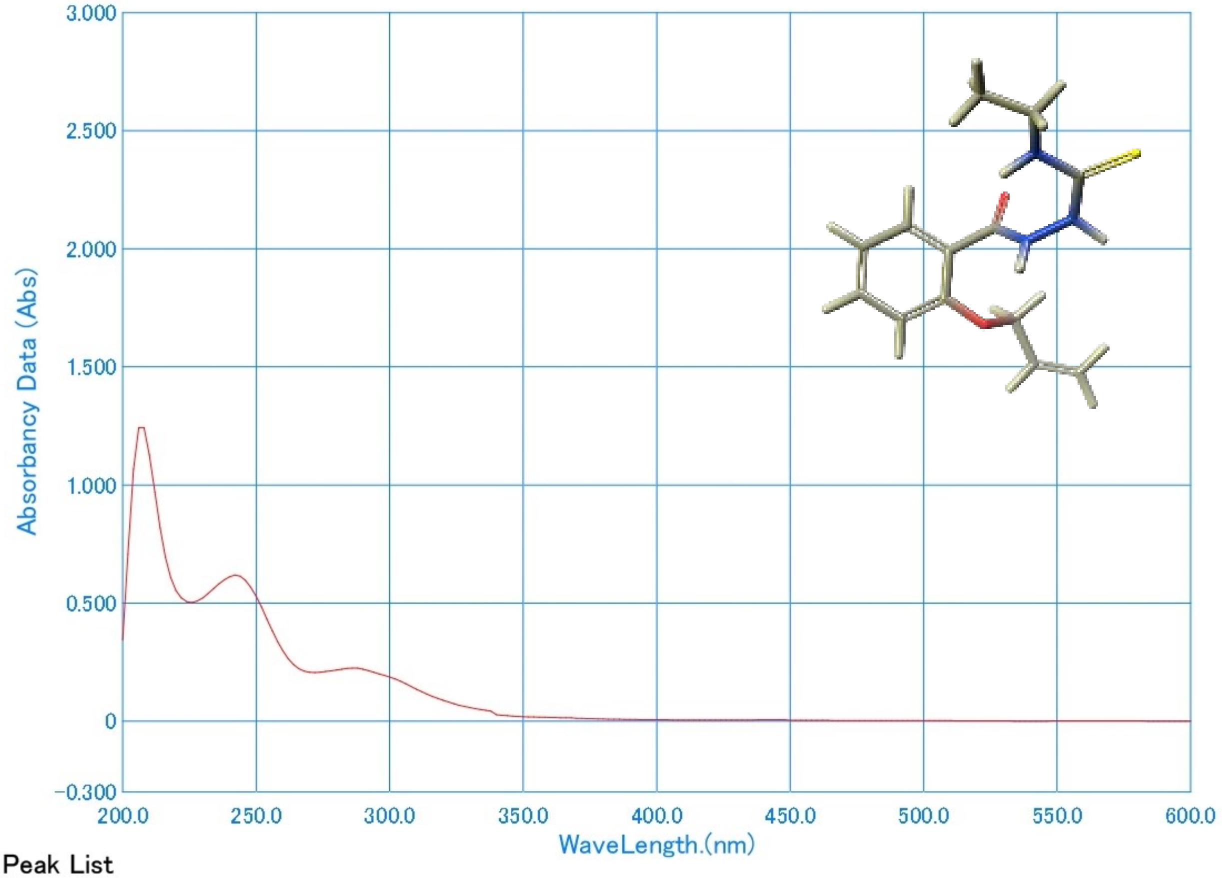


Figure S1 FTIR spectra of S3 Ligand



Peak List

No.	Wavelength(nm)	Abs	Trans(%T)
No Peak Data!			

Max Record 200.0 nm − 600.0 nm

No.	Wavelength(nm)	Abs	Trans(%T)
1	208.0	1.154	7.0

Figure S2 UV-Vis spectra of S3 Ligand

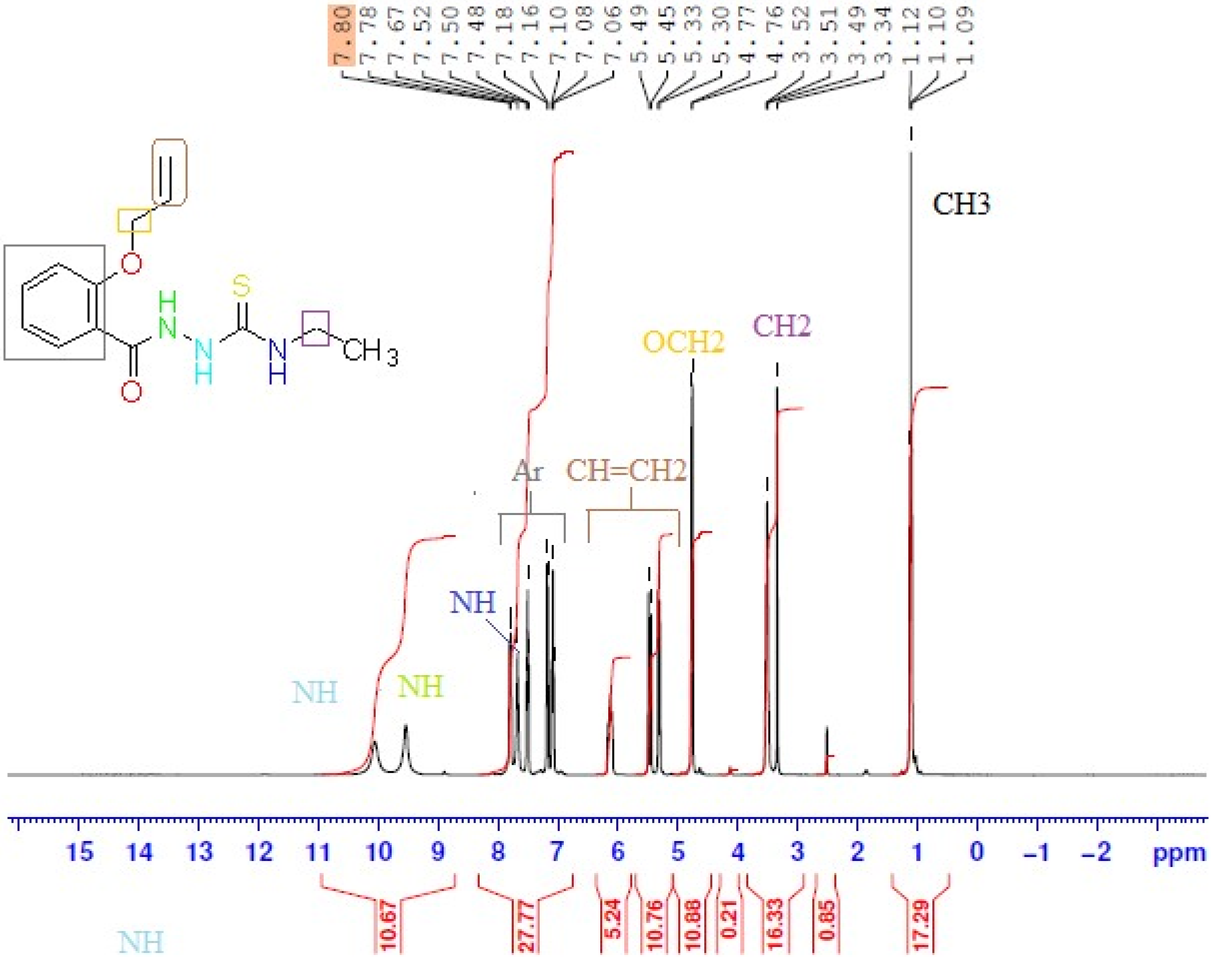


Figure S3 NMR spectra of S3 ligand

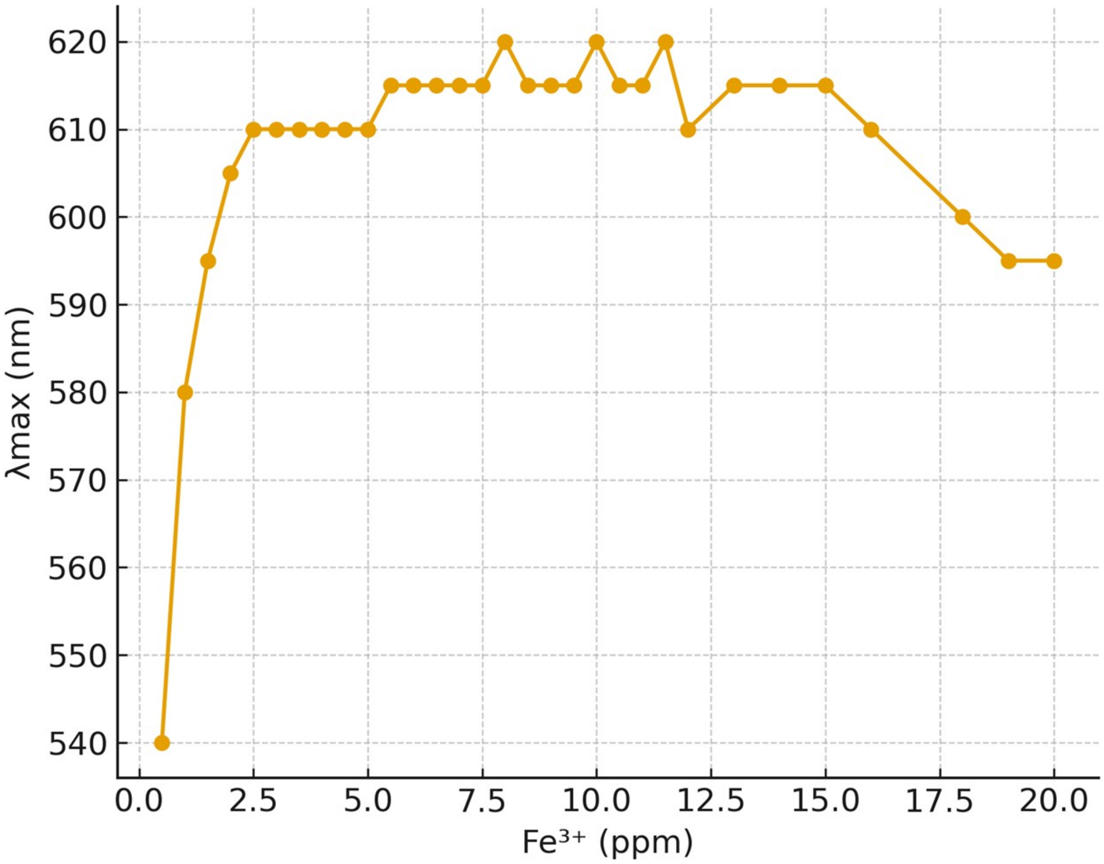


Figure S4 Bathochromic shift of the visible band (450–650 nm) as Fe^{3+} increases. The progressive red shift toward ~620 nm reflects strengthening LMCT character as Fe^{3+} coordination saturates.

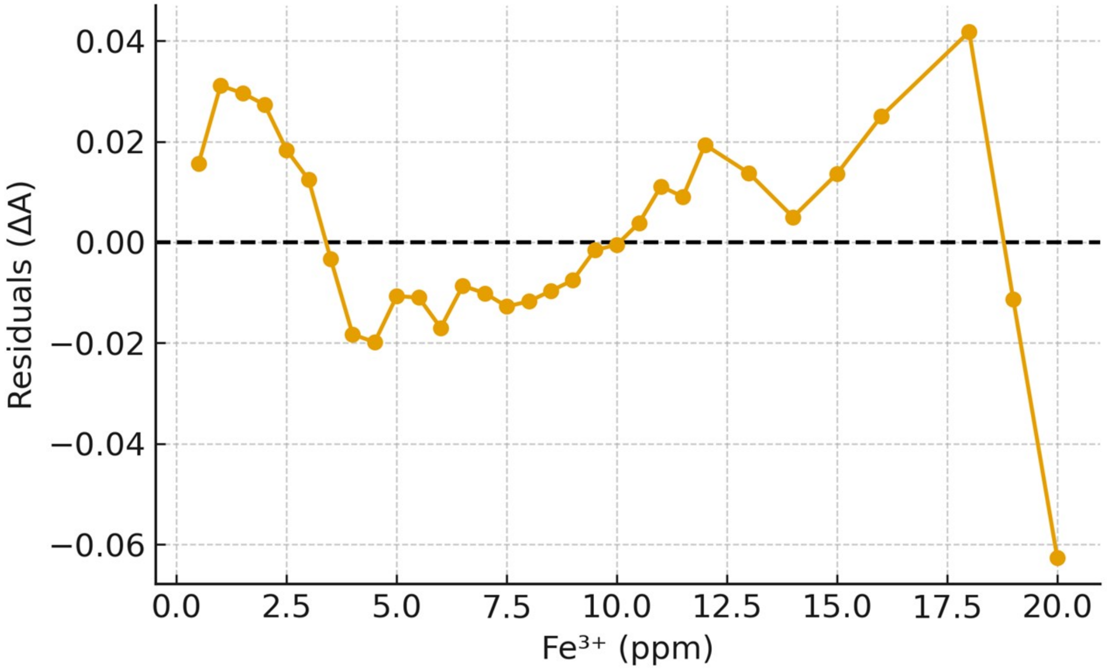


Figure S 5: Residuals vs Fe^{3+} concentration for the Hill model. The plot shows the difference between observed and fitted values (residuals) from a nonlinear regression analysis of Fe^{3+} titration data. The residuals are represented as orange dots, and the dashed line indicates zero residuals, which highlights the fit quality.

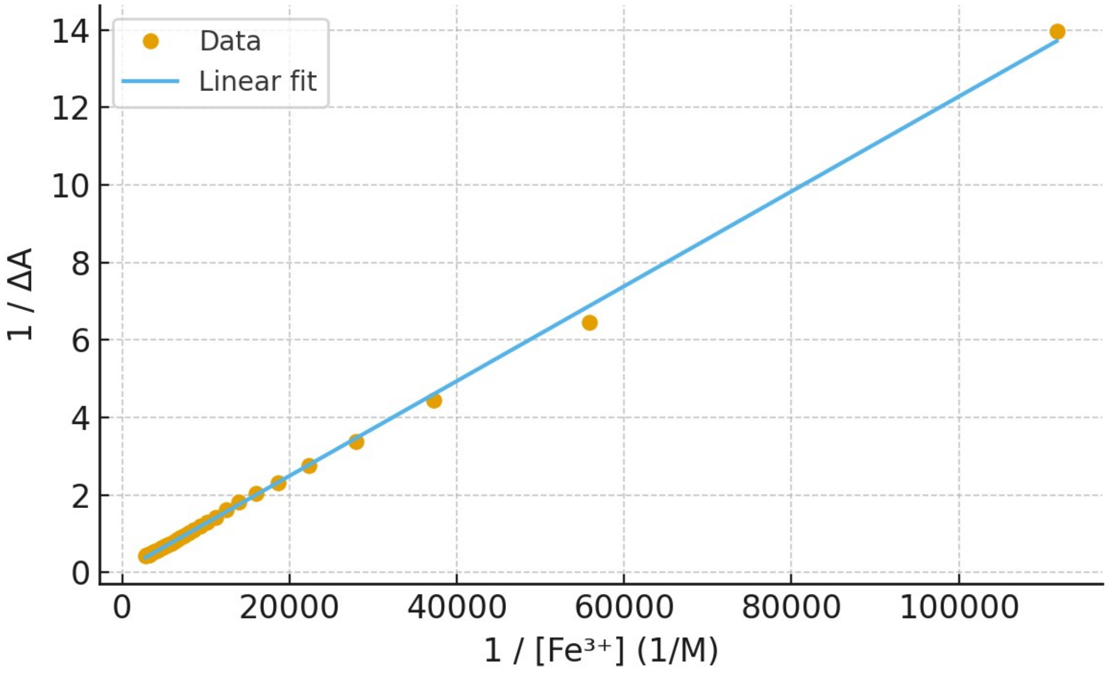


Figure S 6 Benesi–Hildebrand linearization of the calibration region (≤10 ppm) assuming a 1:1 equilibrium: $1/\Delta A=1/A_{max}+(1/(KA_{max}))\,(1/[M])$. The fit gives Amax ≈ 40.9 a.u., $K \approx 5.0\times10^{-3}\ M^{-1}$, $R^2 = 0.9985$. The apparent K is inconsistent with the non-linear global fits ($\approx10^3\ M^{-1}$), underscoring the known sensitivity of BH plots to baseline error and slight deviations from strict 1:1 behavior. We therefore report Hill/1:1 non-linear parameters in the main text and include BH in the SI for completeness.

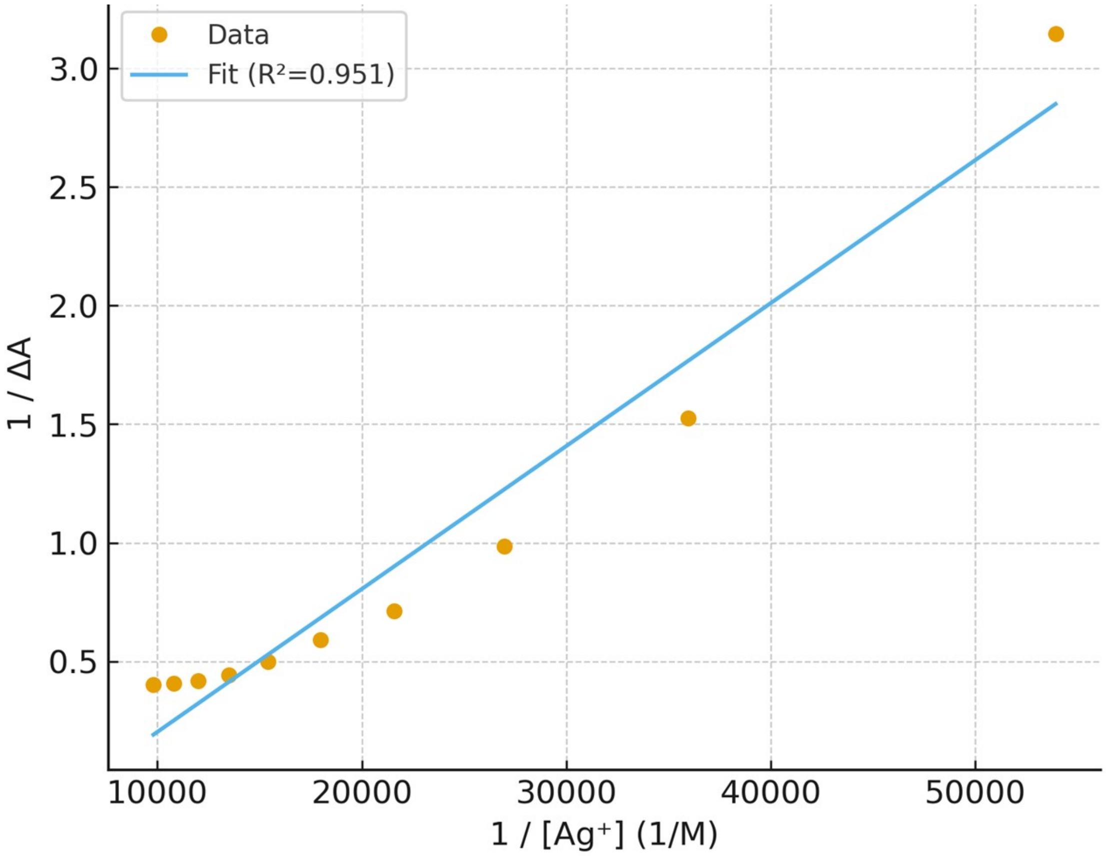


Figure S 7 Benesi–Hildebrand linearization of the Ag^+–S3 binding equilibrium at pH 4. The plot of 1/ΔA vs. 1/[Ag^+] yields a straight line ($R^2 = 0.951$), consistent with a 1:1 complexation model and allowing estimation of the binding constant.