

Supplementary Material:

Diverse Cobalt(II) and Iron(II/III) Coordination Complexes/Polymers Based on 4'-Pyridyl: 2,2';6',2''-Terpyridine: Synthesis, Structures, Catalytic and Anticancer Activities

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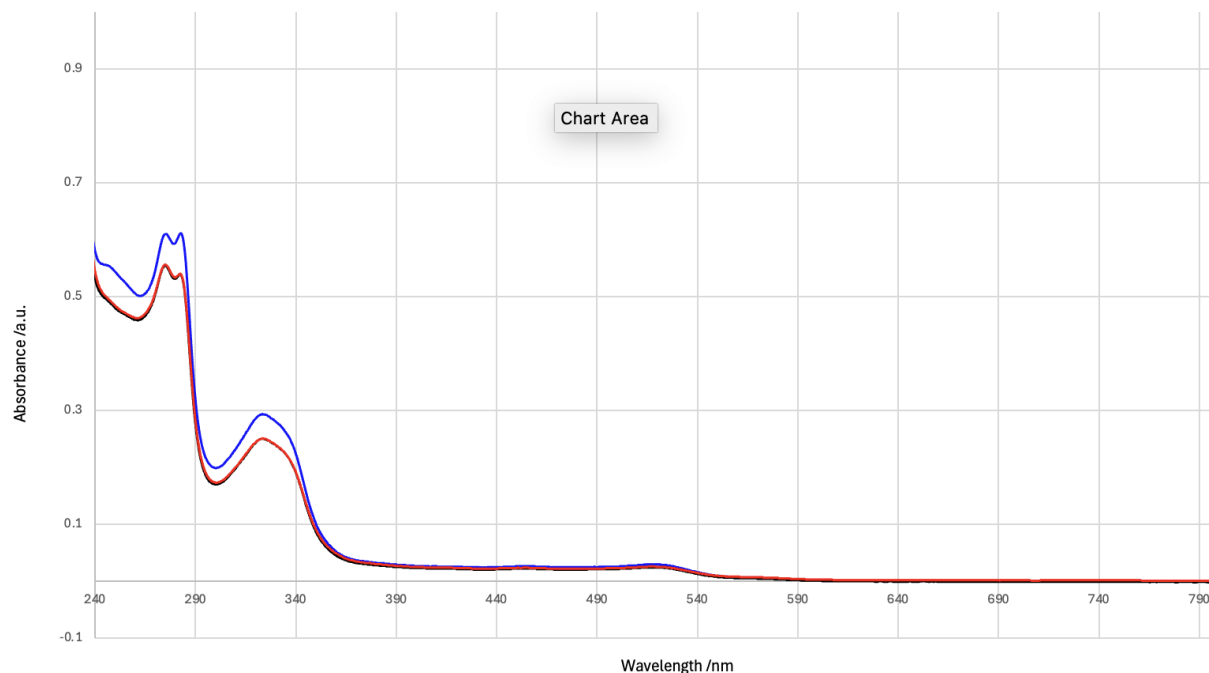


Figure S1. The UV-Vis spectra of compound **1** in water (concentration: 1×10^{-5} M) as prepared (blue), after 24 h (red) and after being warmed up to 37 °C for 2 h (black).

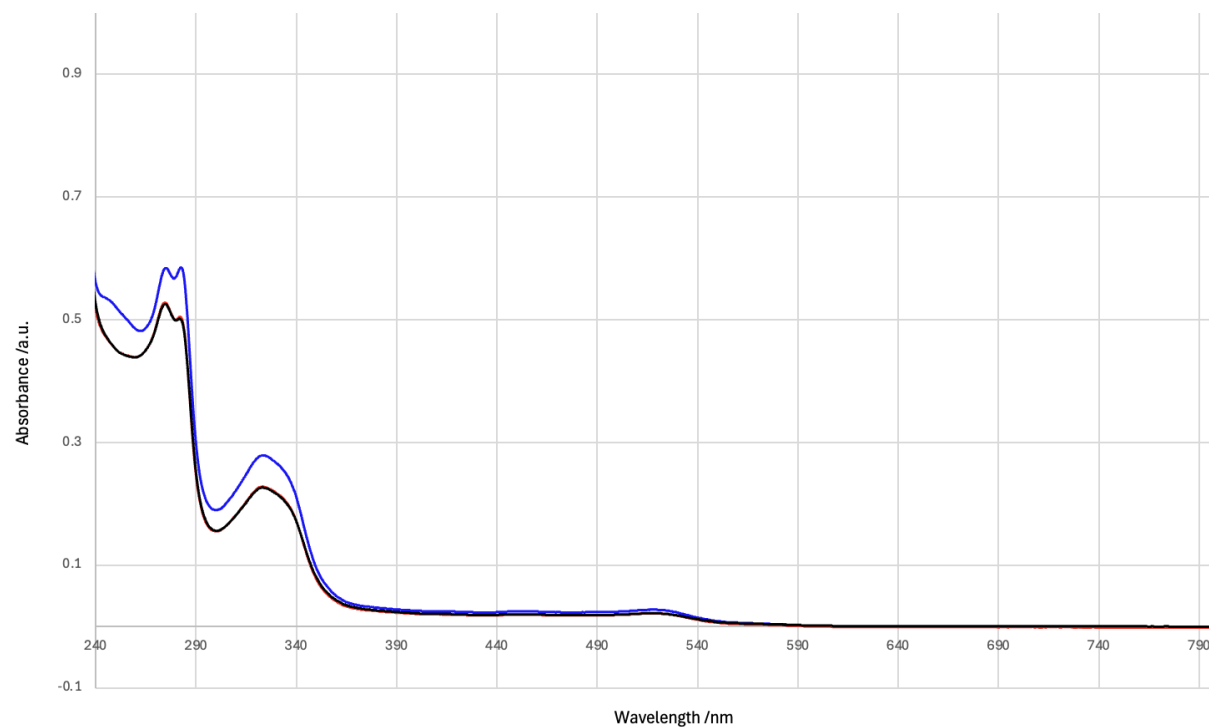


Figure S2. The UV-Vis spectra of compound **2** in water (concentration: 1×10^{-5} M) as prepared (blue), after 24 h (red) and after being warmed up to 37 °C for 2 h (black).

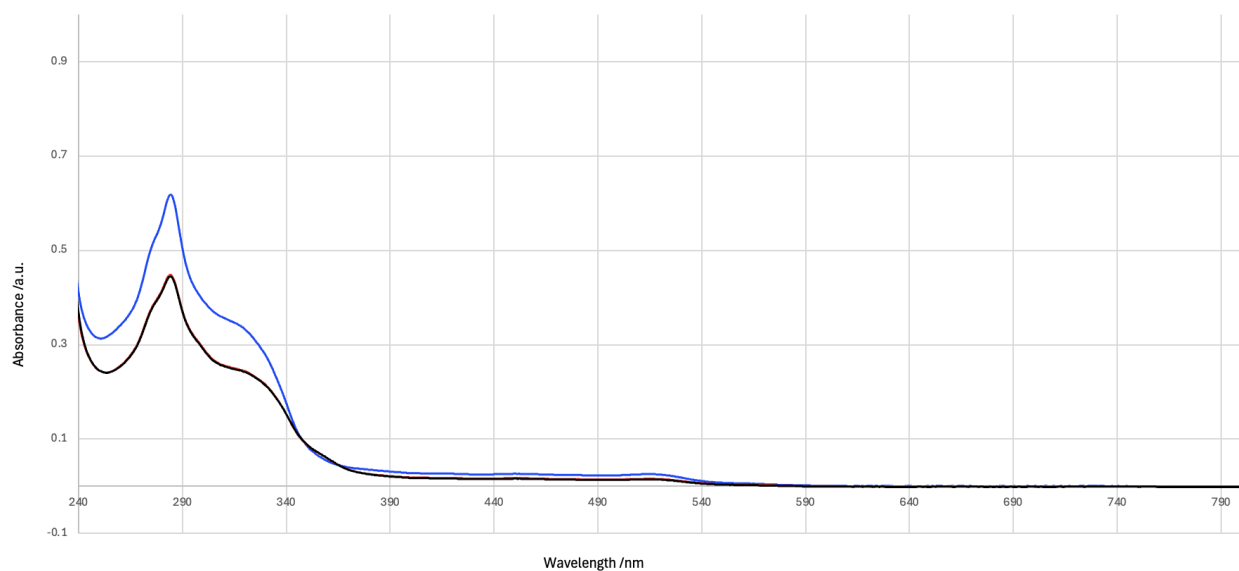


Figure S3. The UV-Vis spectra of compound **3** in water (concentration: 1×10^{-5} M) as prepared (blue), after 24 h (red) and after being warmed up to 37 °C for 2 h (black).

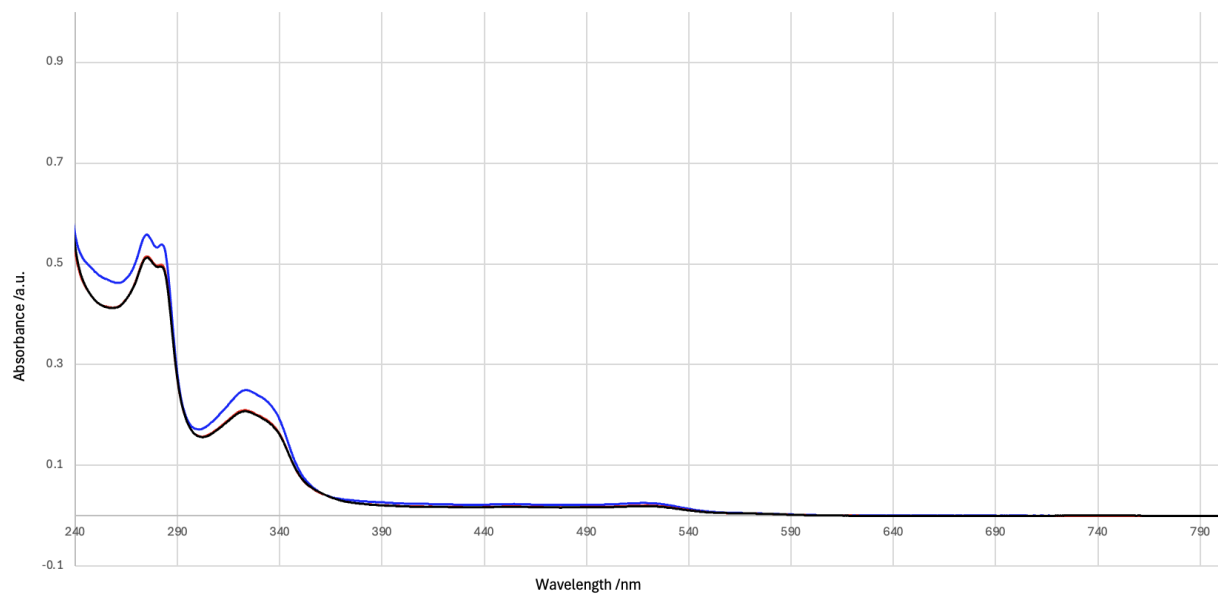


Figure S4. The UV-Vis spectra of compound **4** in water (concentration: 1×10^{-5} M) as prepared (blue), after 24 h (red) and after being warmed up to 37 °C for 2 h (black).

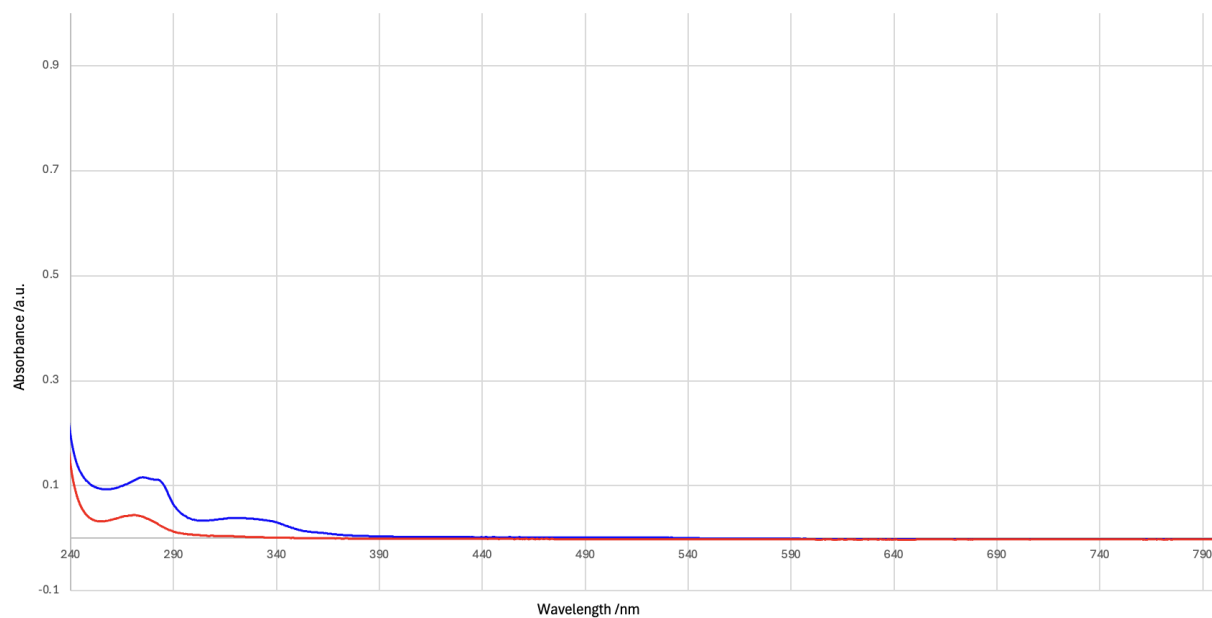


Figure S5. The UV-Vis spectra of compound **5** in water (concentration: 1×10^{-5} M, based on the $[\text{Co}^{\text{II}}(\text{pytpy})(\text{NO}_3)_2]$ unit) as prepared (blue) and after 24 h (red).

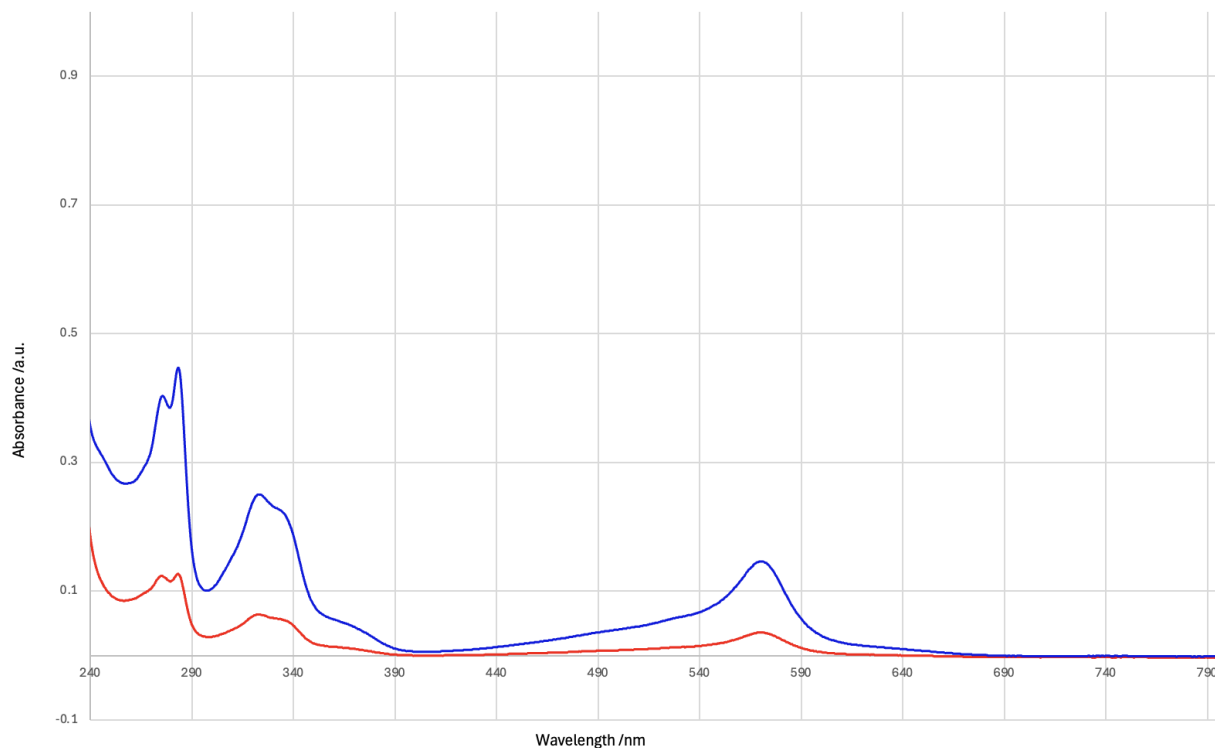


Figure S6. The UV-Vis spectra of compound **6** in water (concentration: 1×10^{-5} M) as prepared (blue) and after 24 h (red).

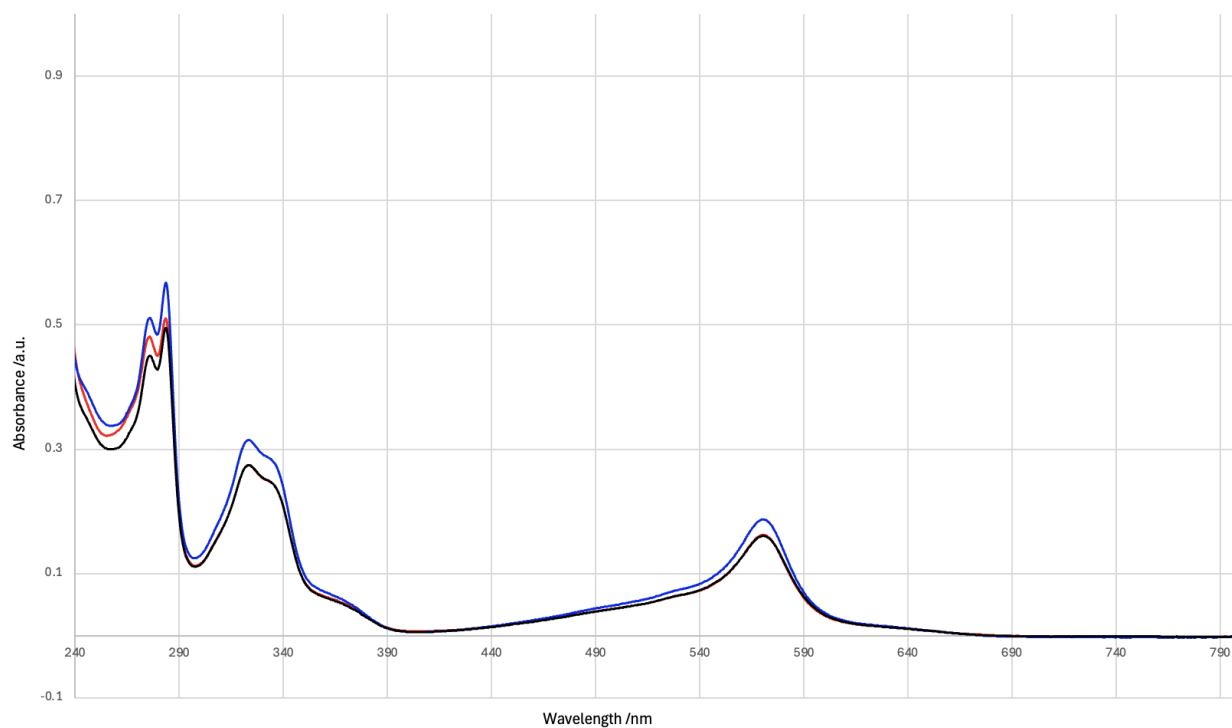


Figure S7. The UV-Vis spectra of compound **7** in water (concentration: 1×10^{-5} M) as prepared (blue), after 24 h (red) and after being warmed up to 37 °C for 2 h (black).

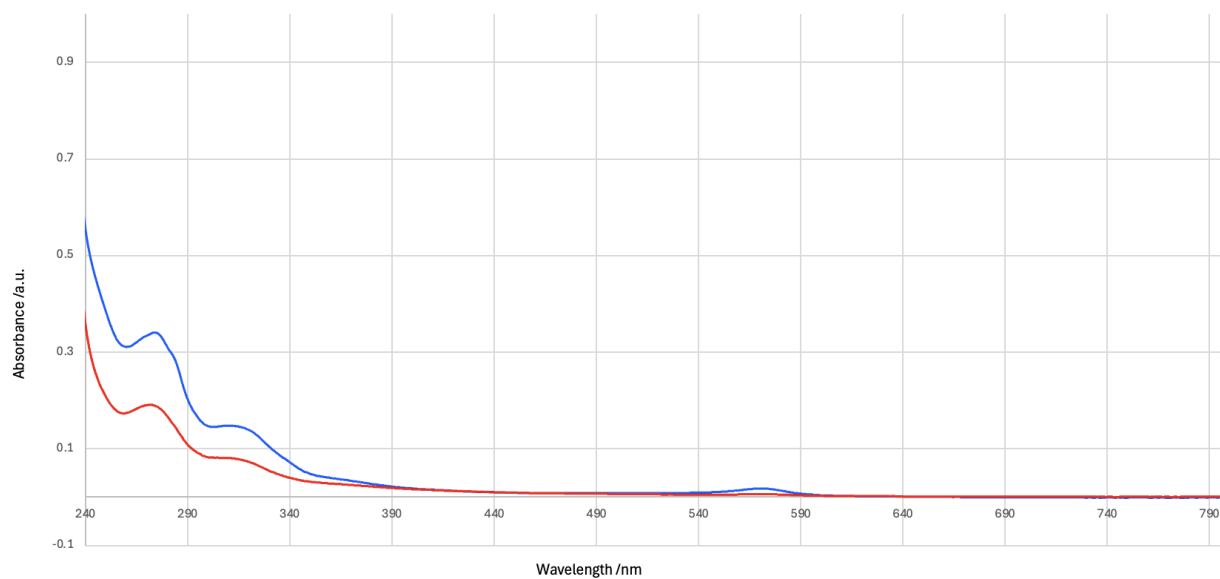


Figure S8. The UV-Vis spectra of compound **8** in water (concentration: 1×10^{-5} M) as prepared (blue) and after 24 h (red).

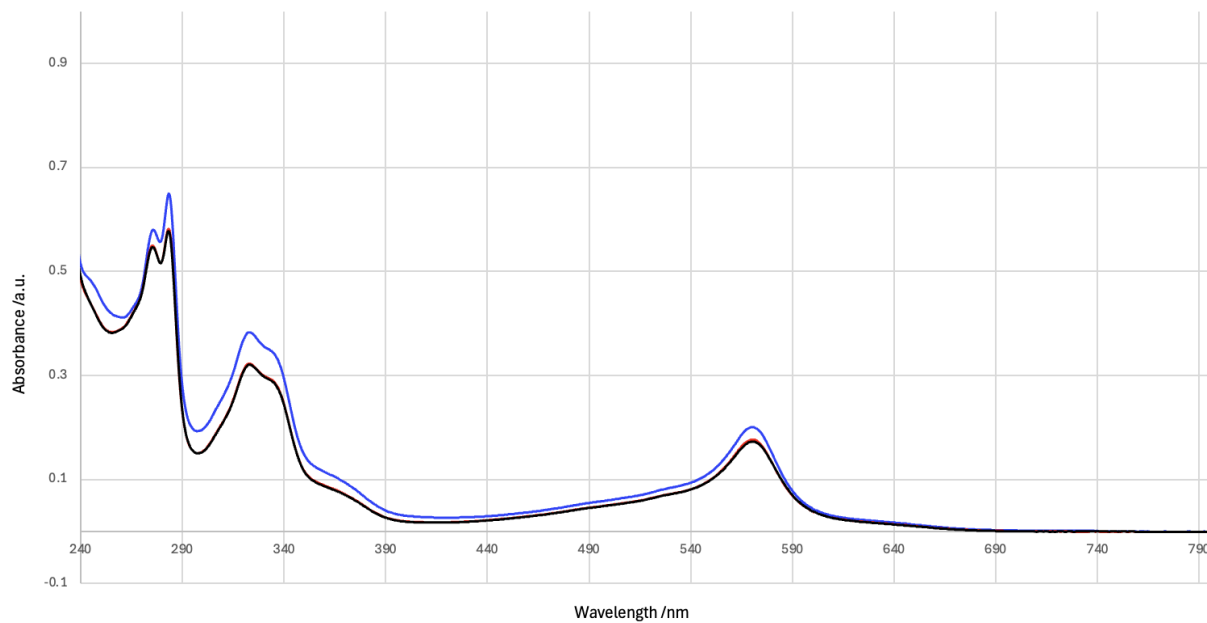


Figure S9. The UV-Vis spectra of compound **9** in water (concentration: 1×10^{-5} M) as prepared (blue), after 24 h (red) and after being warmed up to 37 °C for 2 h (black).

Table S1. X-ray crystallographic data for compounds **2**, **5**, **6** and **8**.

| | 2 | 5 | 6 | 8•H₂O |
|--|--|---|---|---|
| lattice | Monoclinic | Triclinic | Monoclinic | Triclinic |
| formula | C ₄₀ H ₂₈ B ₂ CoF ₈ N ₈ | C ₂₀ H ₁₄ CoN ₆ O ₆ | C ₄₆ H ₃₄ B ₃ ClF ₁₂ FeN ₈ | C ₄₀ H ₃₆ Fe ₂ N ₁₄ O ₂₂ |
| formula weight | 853.25 | 493.30 | 1050.54 | 1176.53 |
| space group | <i>P</i> 2 ₁ / <i>c</i> | <i>P</i> -1 | <i>C</i> 2/ <i>c</i> | <i>P</i> -1 |
| <i>a</i> /Å | 8.8470(3) | 8.2424(14) | 13.4537(4) | 9.2589(3) |
| <i>b</i> /Å | 8.9342(3) | 11.1514(19) | 16.8582(5) | 9.3932(3) |
| <i>c</i> /Å | 45.4437(14) | 11.1680(19) | 20.3828(6) | 14.2734(5) |
| α /° | 90 | 73.843(3) | 90 | 98.432(2) |
| β /° | 95.0000(10) | 75.035(3) | 103.8880(10) | 93.553(2) |
| γ /° | 90 | 84.237(3) | 90 | 112.234(2) |
| <i>V</i> /Å ³ | 3578.2(2) | 952.1(3) | 4487.8(2) | 1127.26(7) |
| <i>Z</i> | 4 | 2 | 4 | 1 |
| temperature (K) | 130(2) | 130(2) | 130(2) | 130(2) |
| radiation (λ , Å) | 1.54178 | 0.71073 | 0.71073 | 1.54178 |
| ρ (calcd.) g cm ⁻³ | 1.584 | 1.721 | 1.555 | 1.733 |
| μ (Mo/Cu K α), mm ⁻¹ | 4.523 | 0.958 | 0.491 | 6.097 |
| θ max, deg. | 74.565 | 33.406 | 30.550 | 75.434 |
| no. of data collected | 83183 | 45031 | 62092 | 25337 |
| no. of data | 7253 | 6971 | 6876 | 4546 |
| no. of parameters | 632 | 299 | 391 | 410 |
| <i>R</i> _I [<i>I</i> > 2 σ (<i>I</i>)] | 0.0402 | 0.0394 | 0.0350 | 0.0453 |
| <i>wR</i> ₂ [<i>I</i> > 2 σ (<i>I</i>)] | 0.1066 | 0.0832 | 0.0921 | 0.1197 |
| <i>R</i> _I [all data] | 0.0417 | 0.0562 | 0.0386 | 0.0506 |
| <i>wR</i> ₂ [all data] | 0.1080 | 0.0899 | 0.0949 | 0.1238 |
| GOF | 1.032 | 1.042 | 1.044 | 1.069 |
| <i>R</i> _{int} | 0.0425 | 0.0594 | 0.0355 | 0.0523 |