Electronic supplementary information (ESI) for
Preparation of Dihydroquinazoline Carbohydrazone Fe(II) Complexes
for Spin Crossover

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1. NMR Spectroscopy

2-(pyridin-2-yl)-3-((pyridin-2-ylmethylene)amino)-2,3-dihydroquinazolin-4(1H)-one

Figure S1. $^1$H NMR spectrum of pq-2py in DMSO.
2-amino-N'-(pyridin-2-ylmethylene)benzohydrazide

![NMR spectrum of pq in DMSO](image)

**Figure S2.** $^1$HNMR spectrum of pq in DMSO.
Figure S3. $^1$H NMR spectrum of pq-2OCH$_3$ in DMSO.
Figure S4. $^1$H NMR spectrum of pq-3OCH$_3$ in DMSO.
Figure S5. IR spectrum of [Fe(pq-2py)₂](ClO₄)₂·CH₃OH·2H₂O (1) at room temperature.
Figure S6. IR spectrum of [Fe(pq-2py)2](BF4)2·2CH3CN·1.75H2O (2) at room temperature.
Figure S7. IR spectrum of [Fe(pq-2py)$_2$](CF$_3$SO$_3$)$_2$·CH$_3$CN·CH$_3$OH (3) at room temperature.
Figure S8. IR spectrum of [Fe(pq-2OCH₃)₂](ClO₄)₂·H₂O (4) at room temperature.
Figure S9. IR spectrum of $[\text{Fe(pq-3OCH}_3\text{)}_2](\text{ClO}_4)_2\cdot \text{H}_2\text{O}$ (5) at room temperature.
Figure S10. Crystal packing portion of the crystal structure of 2 (100 K, a) and 3 (200 K, b) at, as viewed along the crystallographic b axis, highlighting the intermolecular π…π stacking.
Figure S11. Crystal packing portion of the crystal structure of 5 as viewed along the crystallographic $b$ axis, highlighting the intermolecular $\pi\ldots\pi$ stacking.
Figure S12. (a) Plots of $\chi_m T$ versus $T$ for compounds 4, 5 and their corresponding desolvated samples.

(b)
Figure S13. TGA curves of complex [Fe(pq-2py)$_2$](BF$_4$)$_2$·2CH$_3$CN·1.75H$_2$O (2).
Figure S14. TGA curves of complexe $[\text{Fe(pq-2py)}_2](\text{CF}_3\text{SO}_3)_2 \cdot \text{CH}_3\text{CN} \cdot \text{CH}_3\text{OH}$ (3)