### **Supporting Information**

# Synthesis, Characterization and Derivatization of Hydroxyl-Functionalized Iron(II) bis(NHC) Complexes

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1. NMR spectrum of 2,2-dibromoethanol

Br Br

Figure S1. Structure of 2,2-dibromoethanol.



Figure S2. <sup>1</sup>H NMR spectrum of 2,2-dibromoethanol in CDCl<sub>3</sub> at 400.13 MHz.

#### 2. NMR spectra of compound P1



Figure S3. Structure of compound P1.



Figure S4. <sup>1</sup>H NMR spectrum of ligand precursor **P1** in DMSO-d<sub>6</sub> at 400.13 MHz.



Figure S5.  ${}^{13}C{}^{1}H$  NMR spectrum of ligand precursor **P1** in DMSO-d<sub>6</sub> at 100.62 MHz.

#### 3. NMR spectra of compound C1



Figure S6. Structure of compound C1.



Figure S7. <sup>1</sup>H NMR spectrum of complex **C1** in CD<sub>3</sub>CN at 400.13 MHz.



Figure S8.  ${}^{13}C{}^{1}H$  NMR spectrum of complex **C1** in CD<sub>3</sub>CN at 100.62 MHz.

4. NMR spectra of compound C2



C2

Figure S9. Structure of compound C2.



Figure S10. <sup>1</sup>H NMR spectrum of complex **C2** in CD<sub>3</sub>CN at 400.13 MHz.



Figure S11.  ${}^{13}C{}^{1}H$  NMR spectrum of complex **C2** in CD<sub>3</sub>CN at 100.62 MHz.

5. NMR spectra of compound C3



Figure S12. Structure of compound **C3**.



Figure S13. <sup>1</sup>H NMR spectrum of complex C3 in CD<sub>3</sub>CN at 400.13 MHz.



Figure S14.  $^{13}C{^{1}H}$  NMR spectrum of complex C3 in CD<sub>3</sub>CN at 100.62 MHz.

6. NMR spectra of compound P2a



P2a

Figure S15. Structure of compound **P2a**.



Figure S16. <sup>1</sup>H NMR spectrum of ligand precursor **P2a** in DMSO-d<sub>6</sub> at 400.13 MHz.



Figure S17. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of ligand precursor **P2a** in DMSO-d<sub>6</sub> at 100.62 MHz.

7. NMR spectra of compound P2b



P2b





Figure S19. <sup>1</sup>H NMR spectrum of ligand precursor **P2b** in DMSO-d<sub>6</sub> at 400.13 MHz.



Figure S20. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of ligand precursor **P2b** in DMSO-d<sub>6</sub> at 100.62 MHz.

8. NMR spectra of compound P2c



P2c





Figure S22. <sup>1</sup>H NMR spectrum of ligand precursor **P2c** in DMSO-d<sub>6</sub> at 400.13 MHz.



Figure S23.  ${}^{13}C{}^{1}H$  NMR spectrum of ligand precursor **P2c** in DMSO-d<sub>6</sub> at 100.62 MHz.

9. NMR spectra of compound C2a



Figure S24. Structure of compound **C2a**.



Figure S25. <sup>1</sup>H NMR spectrum of complex **C2a** in CD<sub>3</sub>CN at 400.13 MHz.



Figure S26. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of complex **C2a** in CD<sub>3</sub>CN at 100.62 MHz.

#### 10. NMR spectra of compound C2b



C2b

Figure S27. Structure of compound **C2b**.



Figure S28. <sup>1</sup>H NMR spectrum of complex **C2b** in CD<sub>3</sub>CN at 400.13 MHz.



Figure S29.  ${}^{13}C{}^{1}H$  NMR spectrum of complex **C2b** in CD<sub>3</sub>CN at 100.62 MHz.

#### 11. NMR spectra of compound C2c



C2c





Figure S31. <sup>1</sup>H NMR spectrum of complex **C2c** in CD<sub>3</sub>CN at 400.13 MHz.



Figure S32.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of complex **C2c** in CD<sub>3</sub>CN at 100.62 MHz.

#### 12. NMR spectra of compound C2d



C2d





Figure S34. <sup>1</sup>H NMR spectrum of complex **C2d** in CD<sub>3</sub>CN at 400.13 MHz.



Figure S36. <sup>19</sup>F NMR spectrum of complex **C2d** in CD<sub>3</sub>CN at 376.46 MHz.