# Iron complexes with nitrogen bidentate ligands as green catalysts for alcohol oxidation

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# Supplementary information

**Table 1S.** Coordination bond lengths (Å) and angles (°) for complex 1.

| | | | |
|---|---|---|---|
| Fe-N(1) | 1.973(2) | Fe-N(4) | 1.959(2) |
| Fe-N(2) | 1.960(2) | Fe-N(5) | 1.965(2) |
| Fe-N(3) | 1.965(2) | Fe-N(6) | 1.9598(19) |
| | | | |
| N(4)-Fe-N(6) | 88.54(8) | N(2)-Fe-N(5) | 87.77(8) |
| N(4)-Fe-N(2) | 174.63(8) | N(3)-Fe-N(5) | 177.54(8) |
| N(6)-Fe-N(2) | 95.02(8) | N(4)-Fe-N(1) | 94.74(9) |
| N(4)-Fe-N(3) | 81.93(9) | N(6)-Fe-N(1) | 176.12(9) |
| N(6)-Fe-N(3) | 96.39(8) | N(2)-Fe-N(1) | 81.85(9) |
| N(2)-Fe-N(3) | 93.66(8) | N(3)-Fe-N(1) | 86.14(8) |
| N(4)-Fe-N(5) | 96.75(8) | N(5)-Fe-N(1) | 96.05(8) |
| N(6)-Fe-N(5) | 81.49(8) | | |

# ESI-MS spectra

**Figure 1S.** ESI-MS positive spectrum of $[Fe(bipy)_3](OTf)_2$ (solution in $CD_3CN$).

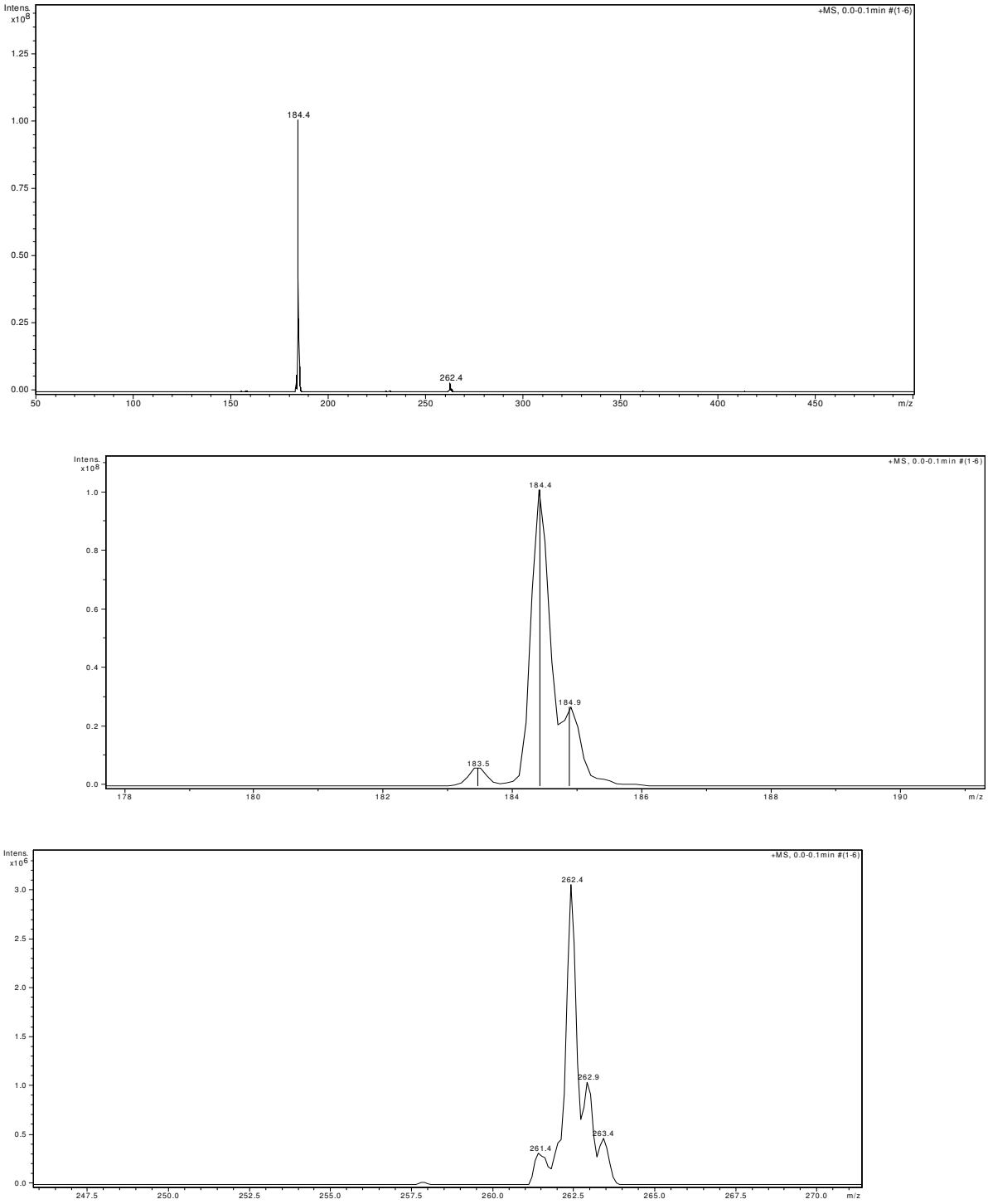
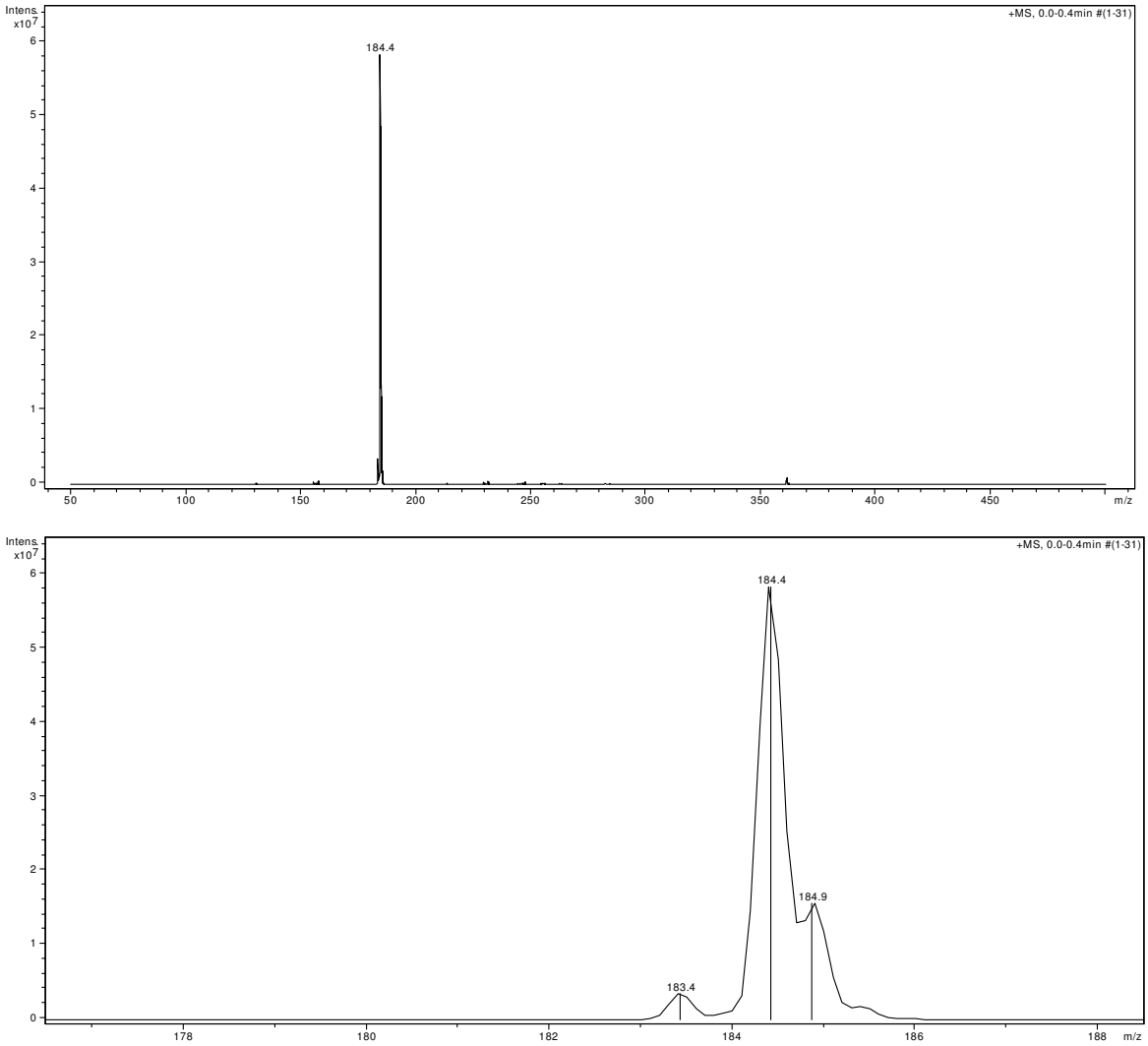


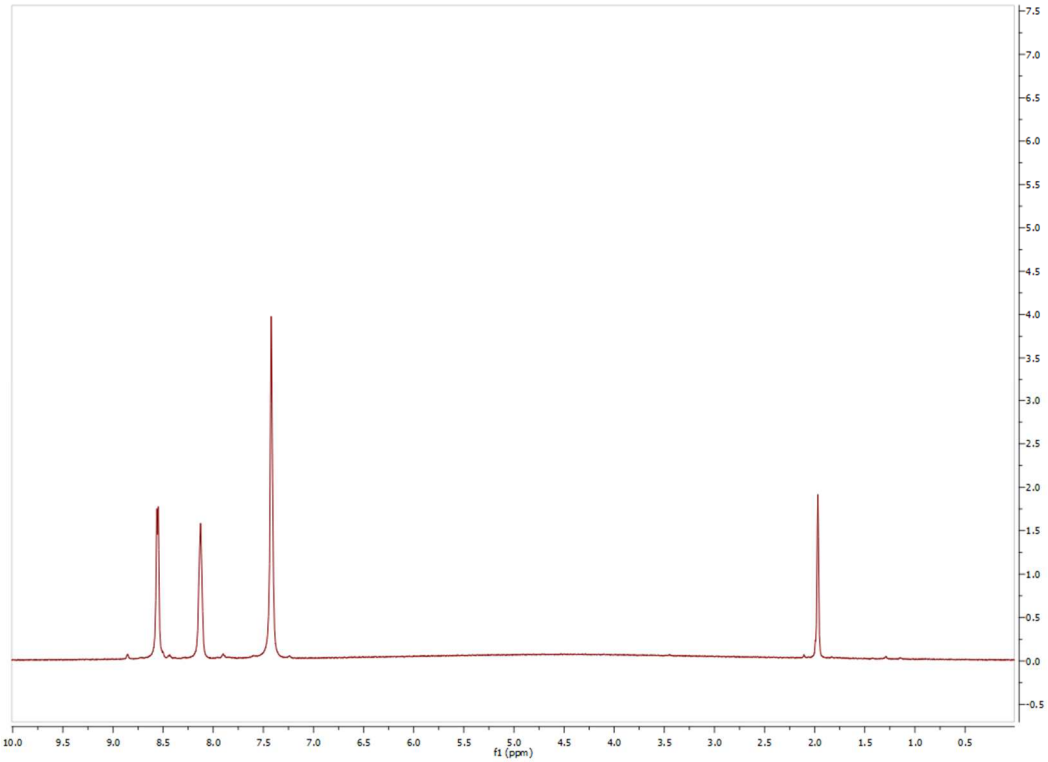
**Figure 2S.** ESI-MS positive spectrum of the final reaction mixture ($CD_3CN$) of oxidation of cyclohexanol catalyzed by $[Fe(bipy)_3](OTf)_2$ .



# NMR data

$^{1}H$ and $^{13}C$ NMR spectra were recorded either on a Varian 500 spectrometer operating at 500 MHz and 125.68 MHz, respectively, or on a Jeol EX400 spectrometer operating at 400 MHz and 100.4 MHz, respectively; chemical shifts were measured relative to the residual solvent signal. Resonances were assigned with reference to COSY and HSQC spectra.

**Figure 3S.** $^{1}H$ and $^{13}C$ NMR spectra ($CD_3CN$, 25°C) of $[Fe(bipy)_3](OTf)_2$ (**1**).



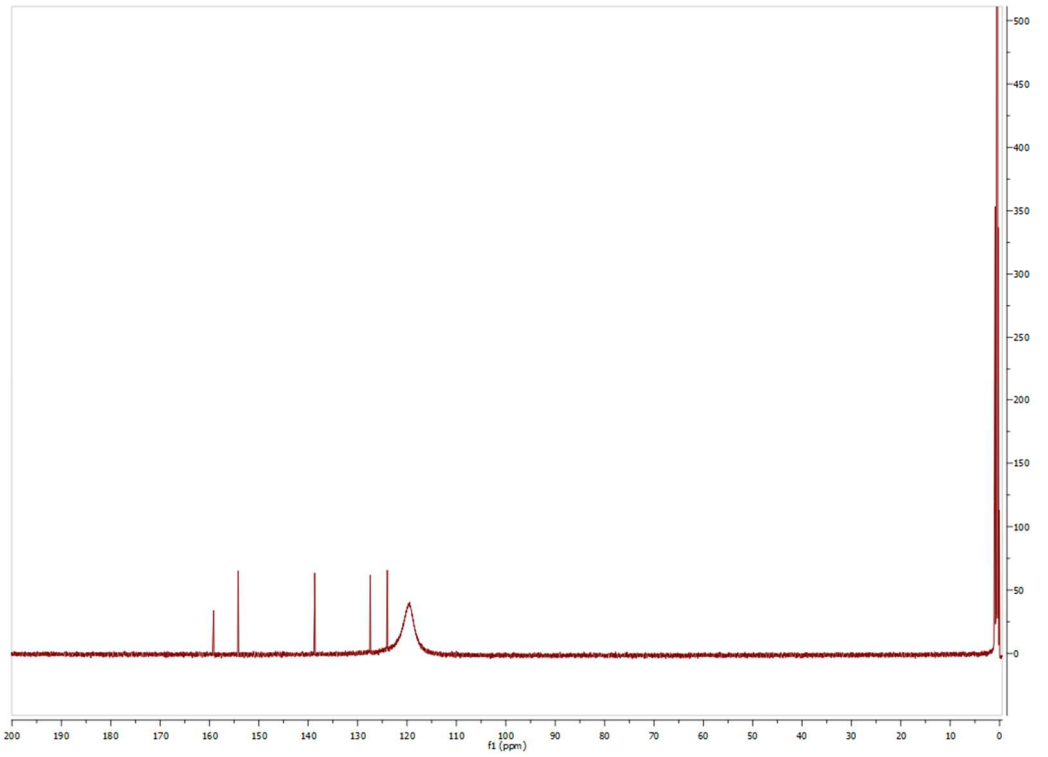
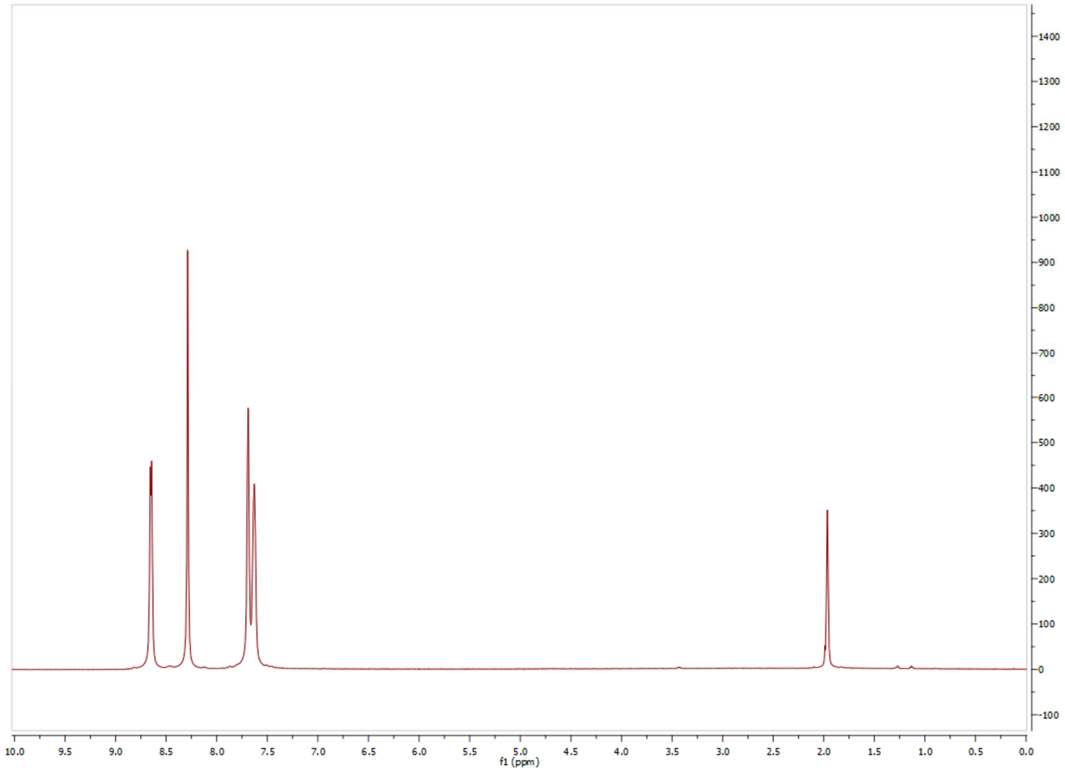



**Figure 4S.** $^{1}H$ and $^{13}C$ NMR spectra ($CD_3CN$, 25°C) of $[Fe(phen)_3](OTf)_2$ (**2**).



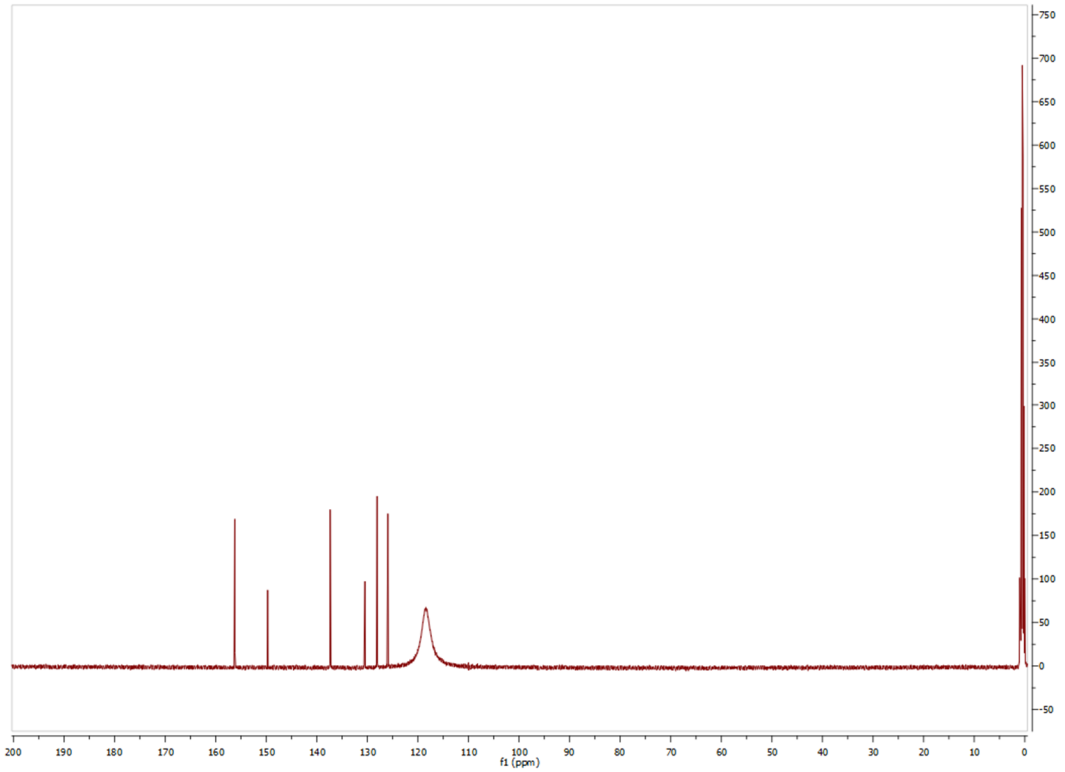



**Figure 5S.** $^{1}H$ and $^{13}C$ NMR spectra ($CD_3CN$, 25°C) of $[Fe(DMbipy)_3](OTf)_2$ (**3**).

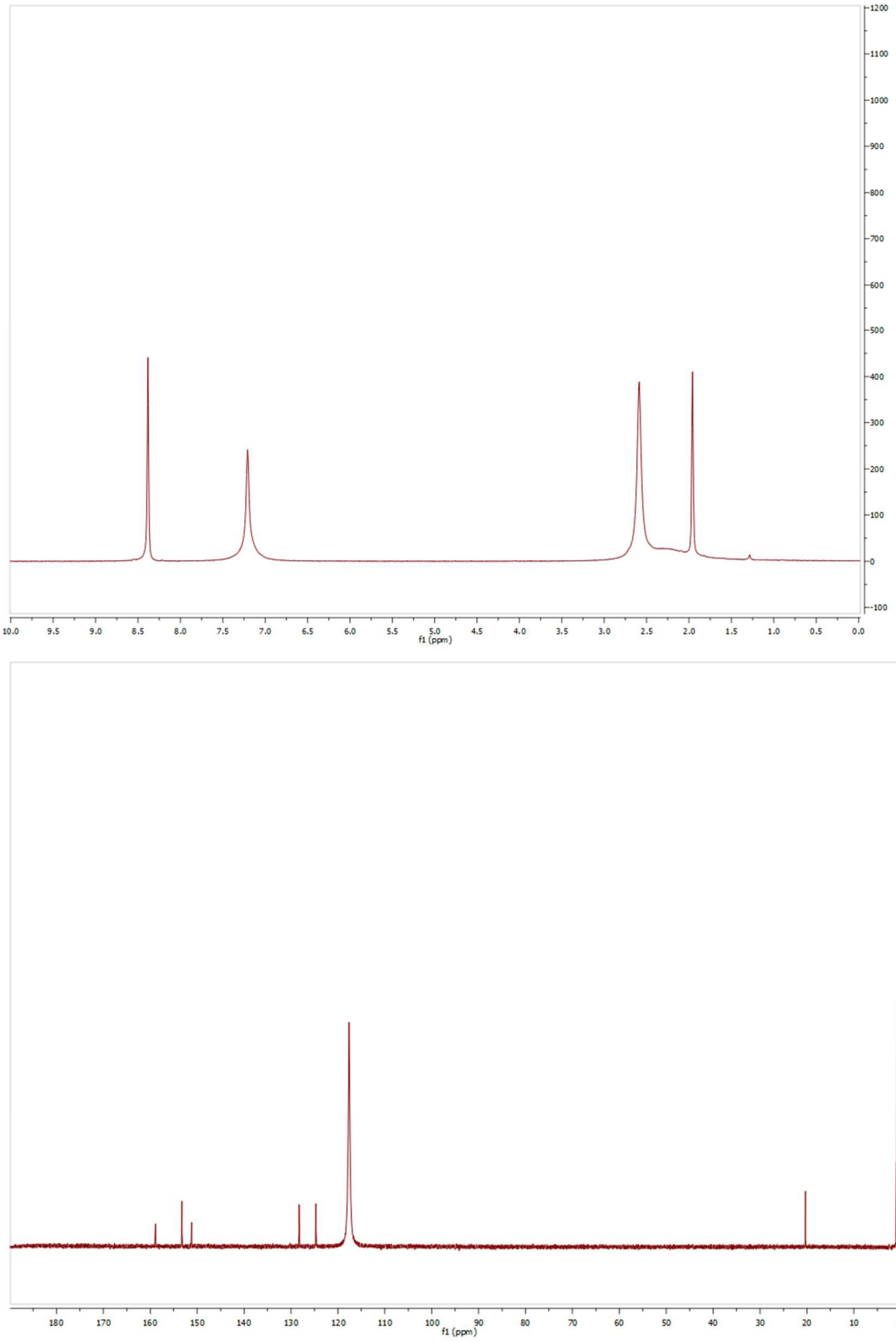


**Figure 6S.** $^{1}H$ and $^{13}C$ NMR spectra ($CD_3CN$, 25°C) of $[Fe(DMphen)_3](OTf)_2$ (**4**).

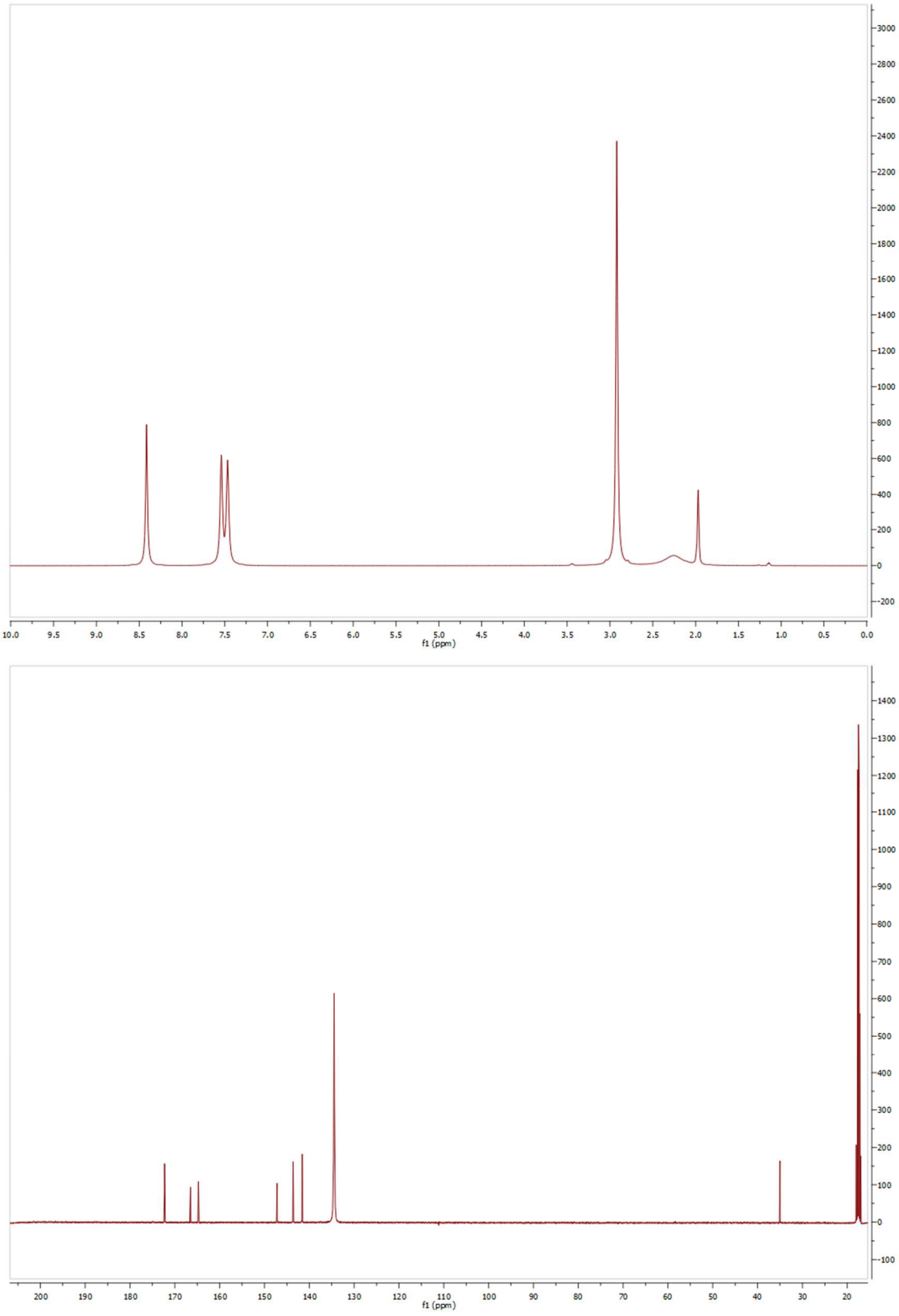


**Figure 7S.** Region of aromatic protons of $^{1}H$ NMR spectrum ($CD_3CN$, 25°C) of the final reaction mixture of oxidation of acetophenone catalyzed by **1** in the presence of 3 equivalents of added bipy (see paragraph 3.5).