Supporting Information

Interaction between Histidine and Zn(II) Metal Ions over a Wide pH as Revealed by Solid-State NMR Spectroscopy and DFT Calculations

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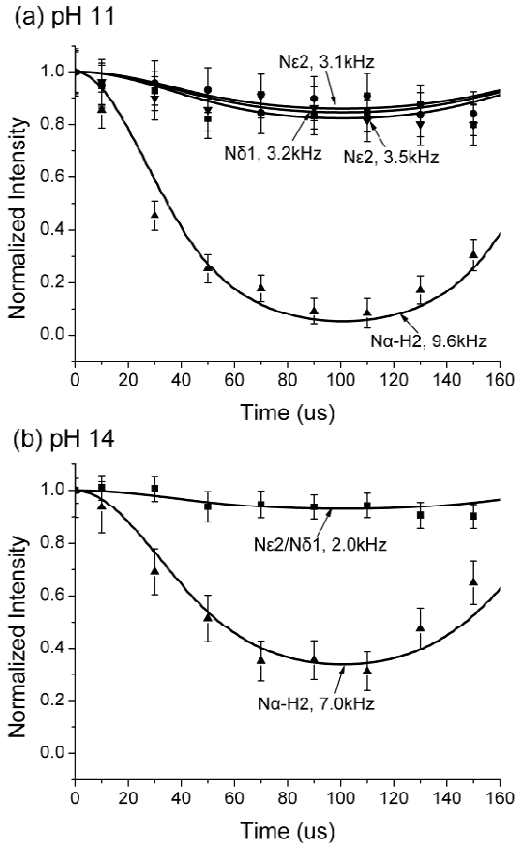

Figure S1. ^{15}N-^{1}H dipolar couplings, which are obtained from DIPSHIFT experiment in double version, of 25% diluted U-^{13}C, ^{15}N-labeled histidine upon Zn(II) binding prepared at (a) pH 11, (b) pH 14. The simulated coupling strengths are indicated. The real ^{15}N-^{1}H dipole couplings are deduced after taking into account the PMLG scaling factor.

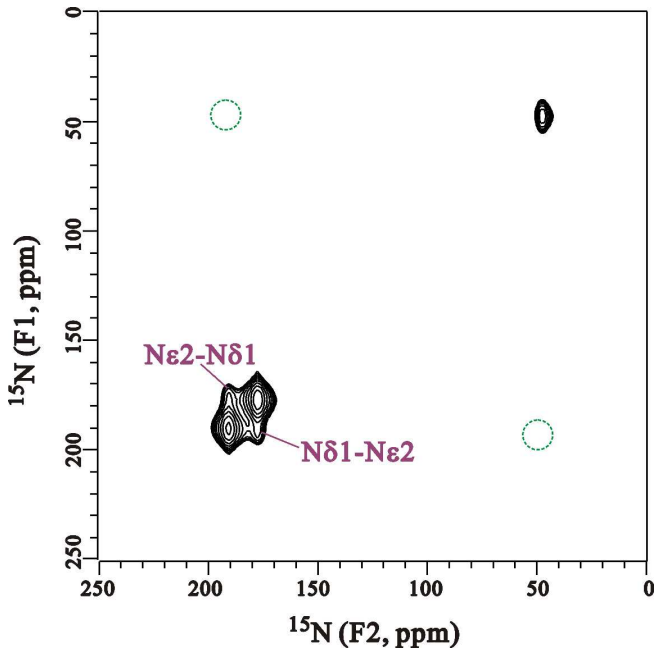

Figure S2. 2D ^{15}N-^{15}N homo-nuclear correlation NMR spectrum of U-^{13}C, ^{15}N-labeled histidine hydrochloride monohydrate. The PDSD mixing time was set to 4 s.

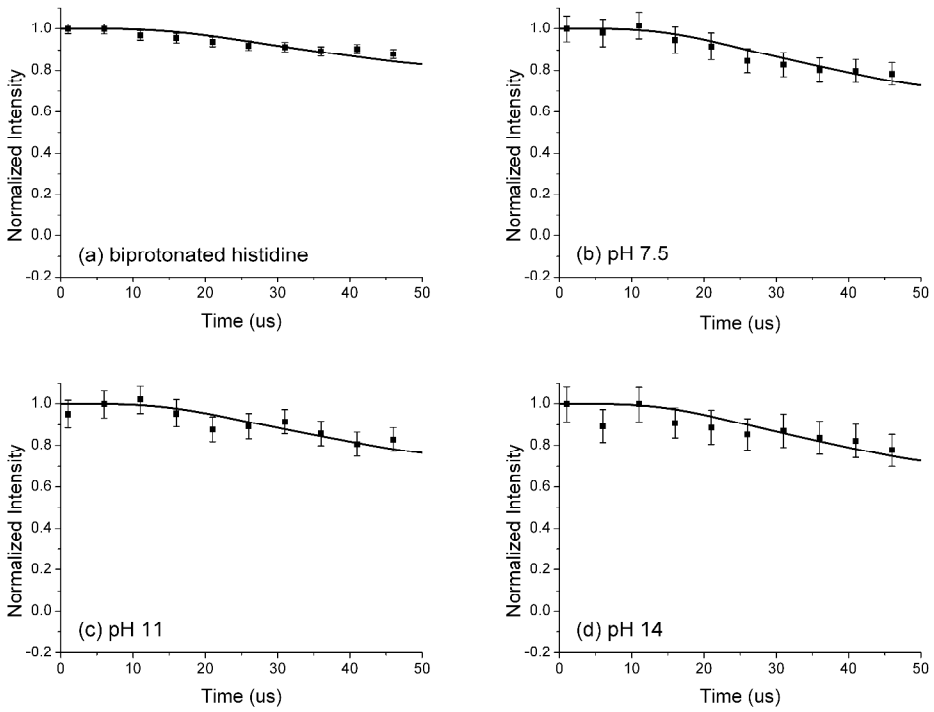

Figure S3. CSA dephasing curves for $^{15}N_{\alpha}$ site of (a) biprotonated histidine, and 25% diluted U-^{13}C, ^{15}N-labeled histidine upon Zn(II) binding prepared at (b) pH 7.5, (c) pH 11, and (d) pH 14.

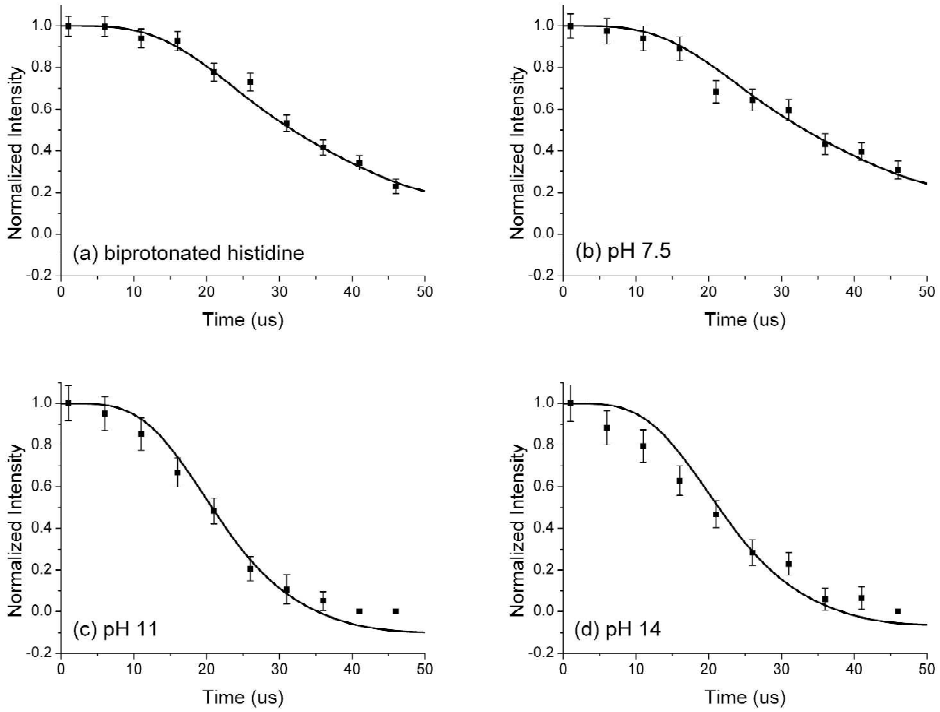

Figure S4. CSA dephasing curves for imidazole $^{15}N_{\varepsilon 2}$ site of (a) biprotonated histidine, and 25% diluted U-^{13}C, ^{15}N-labeled histidine upon Zn(II) binding prepared at (b) pH 7.5, (c) pH 11, and (d) pH 14.

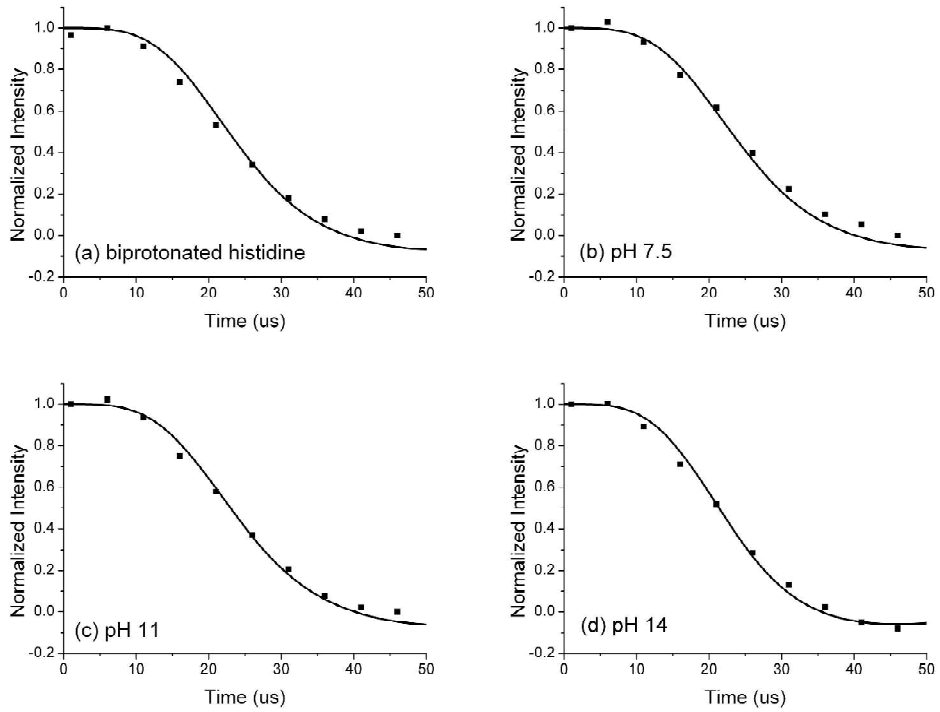

Figure S5. CSA dephasing curves for imidazole $^{13}C_{\varepsilon 1}$ site of (a) biprotonated histidine, and 25% diluted U-^{13}C, ^{15}N-labeled histidine upon Zn(II) binding prepared at (b) pH 7.5, (c) pH 11, and (d) pH 14.