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Title	NMR basis for interprotein electron transfer gating between cytochrome c and cytochrome c oxidase
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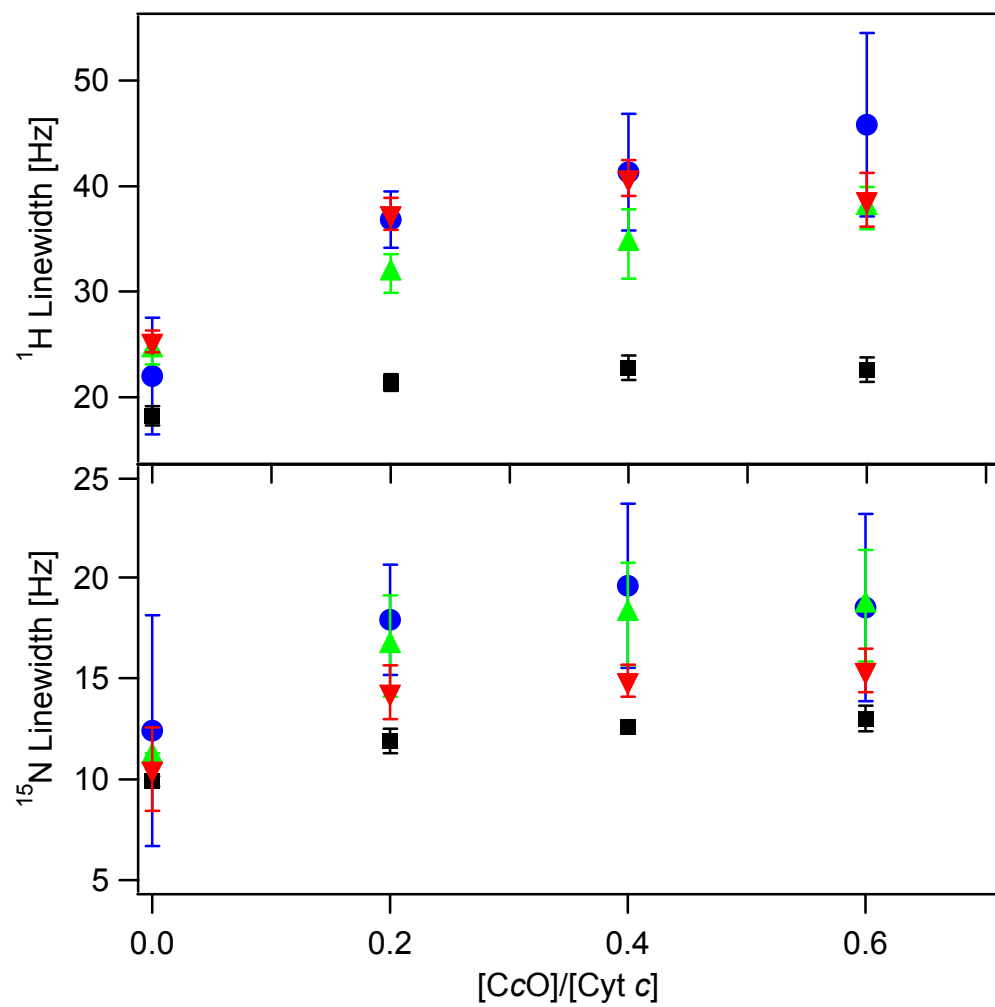


Figure S2

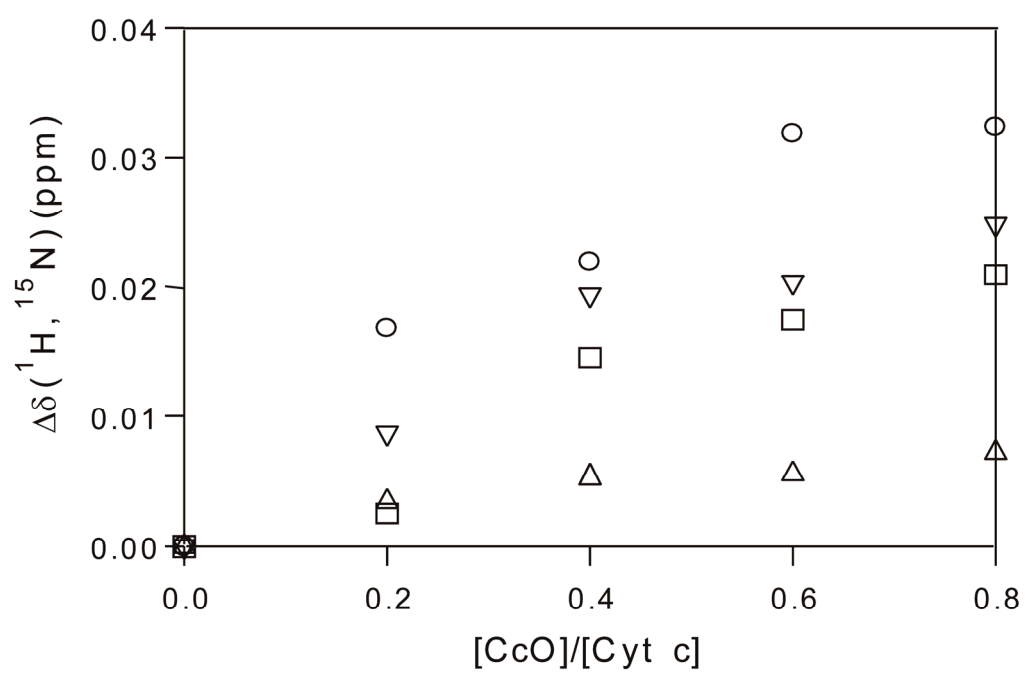


Figure S3

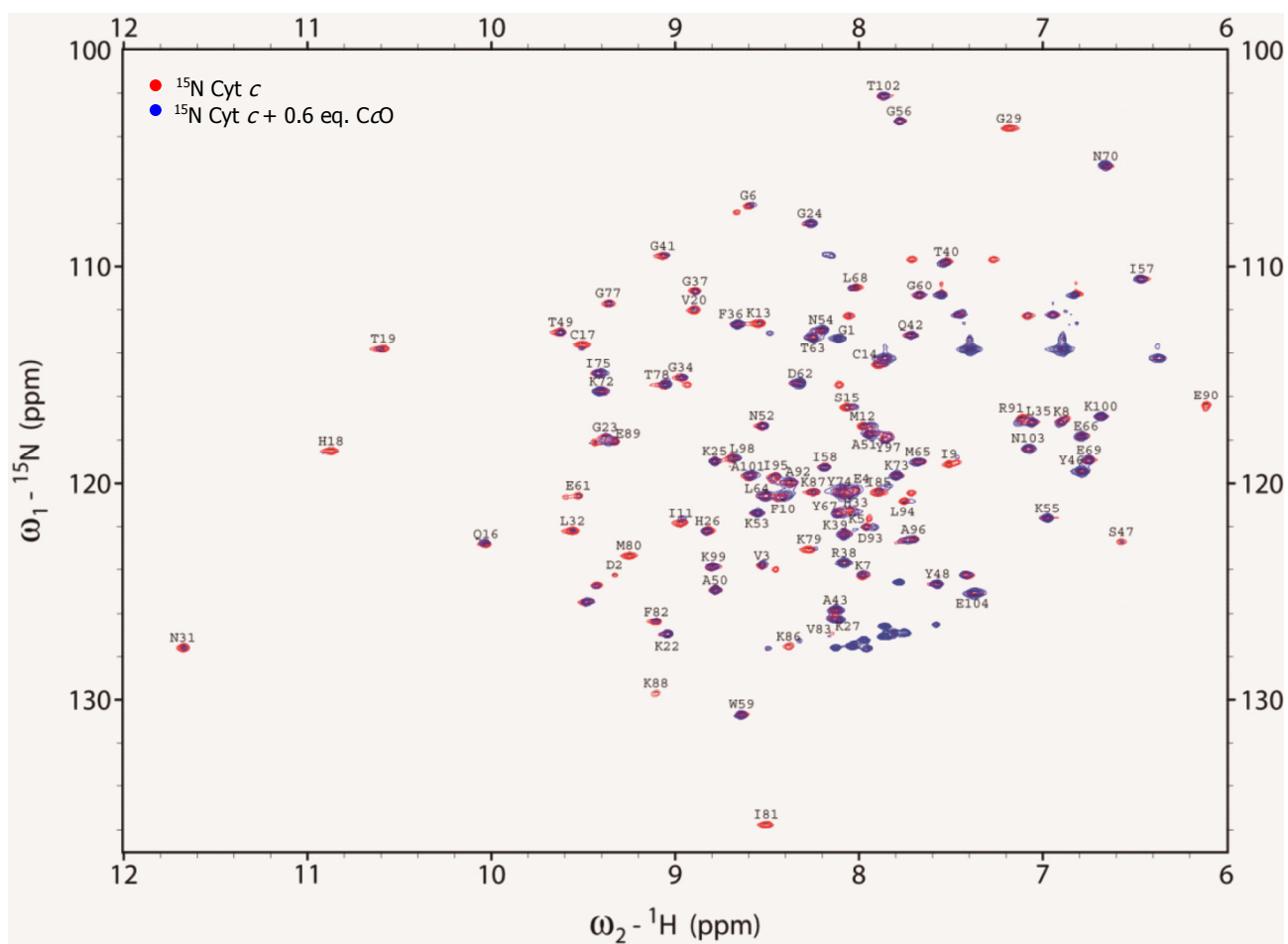
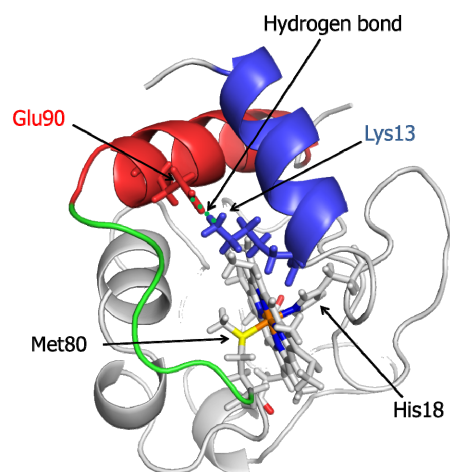
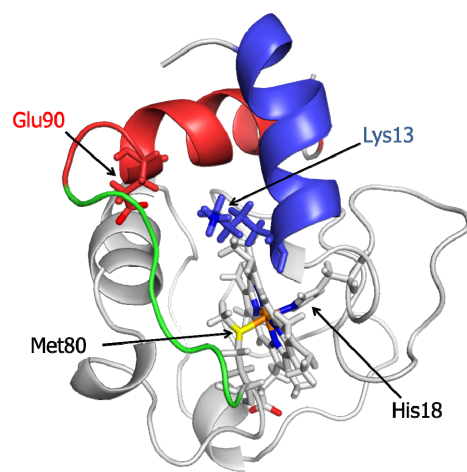


Figure S4



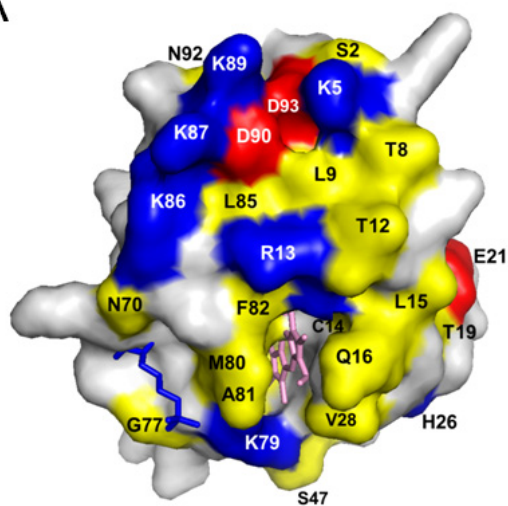
(a) Reduced Cyt *c*



(b) Oxidized Cyt *c*

Figure S5

A



B

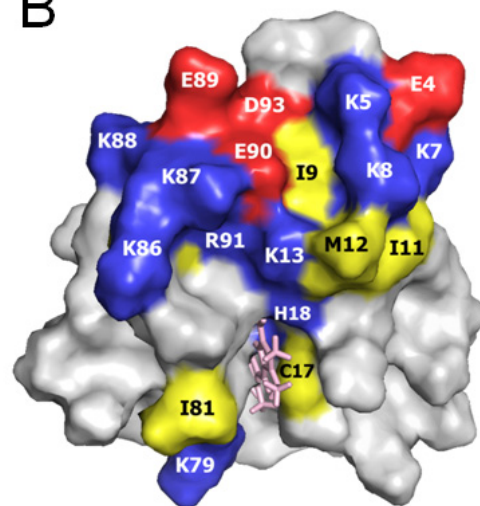


Figure S6

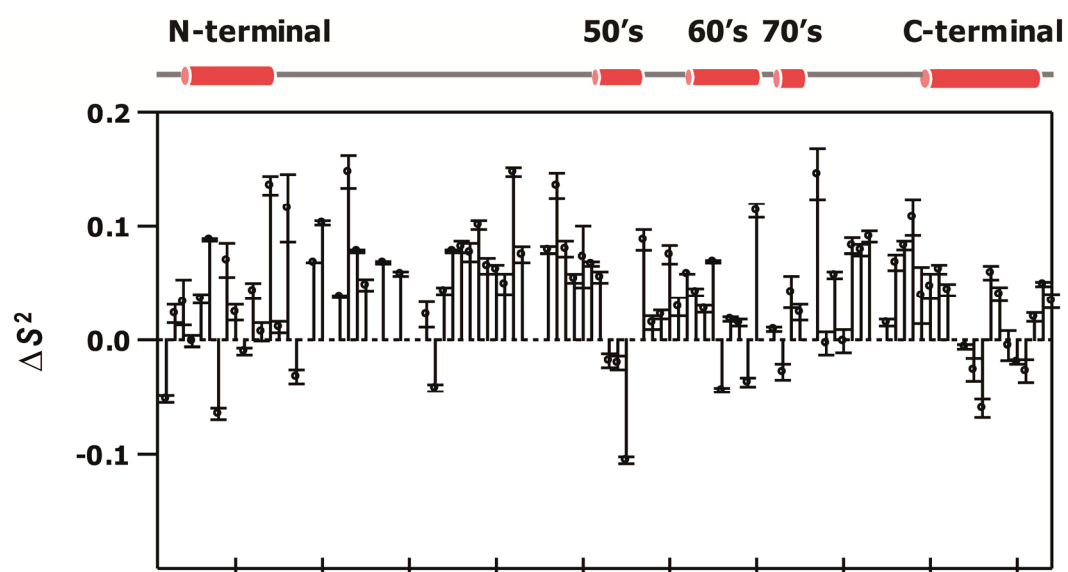
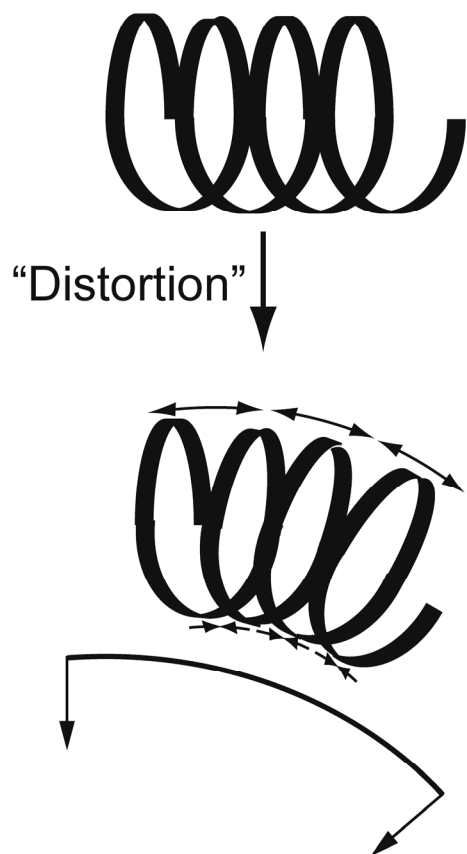


Figure S7

A



B

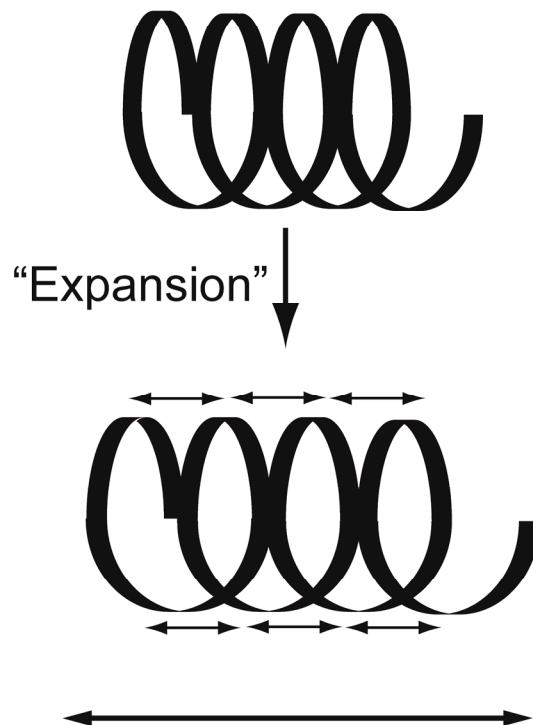


Figure S8

FIGURE LEGENDS

Figure S1. Superposition of the amide region of the ^1H - ^{15}N HSQC spectra of ^{15}N -enriched reduced Cyt *c* alone (red) and in the presence of unlabeled CcO (blue). Assignments of the backbone resonances of human reduced Cyt *c* were achieved by sets of triple resonance experiments.

Figure S2. Line broadening of some peaks from Cyt *c* by addition of CcO. The specific line broadening was observed for the signals from Ile9 (blue circle), Lys13 (green triangle), and Lys79 (red triangle), which were significantly different from the non-specific line broadening (Tyr48; black square). The experimental error in the signal width was estimated from the Gaussian peak fitting. Enhanced error was observed for the NMR signals (Ile9, Lys13 and Lys79) from the interaction sites due to the association with CcO. We measured the HSQC spectra for Cyt *c* in the presence of the 0.8 and 1 equivalent amount of CcO, but the heavily broadened NMR signals prevented us from estimating the reliable line width.

Figure S3. Chemical shift changes of some peaks from Cyt *c* by addition of CcO. The chemical shift changes observed for the peaks from Lys5(∇), Cys17($\square$), and Lys86($\circ$) are specific and significant, while typical non-specific chemical shift changes due to the experimental error and/or indirect weak interactions are less than 0.01 ppm (Lys39; $\triangle$). The typical experimental error in the ^1H - ^{15}N chemical shifts is less than ± 0.005 ppm. We measured the HSQC spectra for Cyt *c* in the presence of an equivalent amount of CcO, but the heavily broadened NMR signals prevented us from determining the chemical shift.

Figure S4. Superposition of the amide region of the ^1H - ^{15}N HSQC spectra of ^{15}N -labeled oxidized Cyt *c* alone (red) and in the presence of unlabeled CcO (blue). Assignments of the cross peaks were achieved by sets of triple resonance experiments.

Figure S5. Structures of reduced (a) (1) and oxidized Cyt *c* (b) (2). N-terminal helix (H1: 3-13), loop 7 (L7: 81-87), and C-terminal helix (H5: 88-101) is highlighted in blue, green, and red, respectively.

Figure S6. Interaction site for CcP on yeast Cyt *c* (3) (A) and CcO on human Cyt *c* (B). Positively charged, negatively charged, and non-polar residues are shown in blue, red, and yellow,

respectively.

Figure S7. Plots of difference S^2 between the oxidized and reduced forms ($\Delta S^2 = S^2_{\text{ox}} - S^2_{\text{red}}$) as a function of residue number for Cyt *c* (4). The redox dependence of the dynamic behavior of the N-terminal helix is comparable with that of the C-terminal helix, which is not prominent, compared with those of other regions.

Figure S8. Schematic representation of “distorted” (A) and “expanded” helix structures (B).

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