Supporting Information

Yoon et al. 10.1073/pnas.0902127106

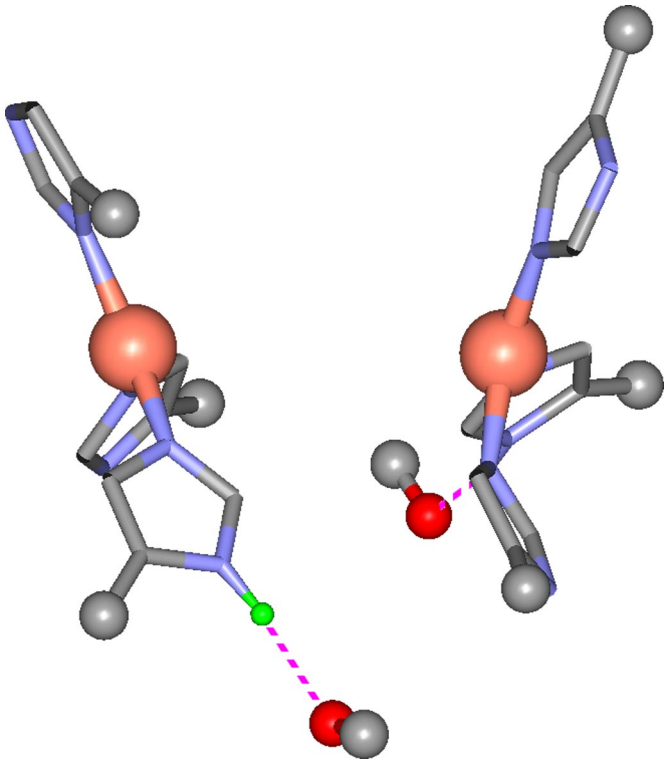

Fig. S1. Optimized structure of deoxy Lc^{T3} with additional hydrogen bonds between two His ligands and backbone carbonyl groups. The backbone carbonyl groups are part of the HXH loops in the Lc^{T3} site. The carbonyl groups were modeled with CH_2O, and the positions of C and O atoms were fixed during the geometry optimization. The resulting Cu–Cu distance is 5.797 Å.

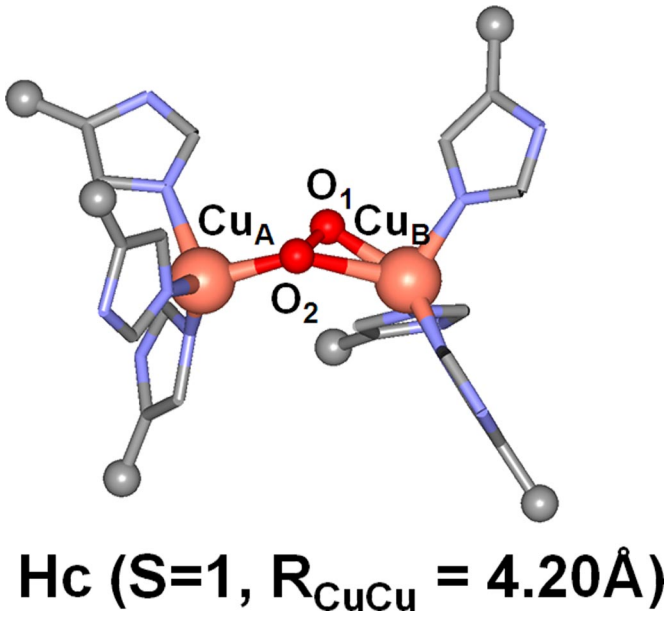

Fig. S2. Optimized structure of oxy hemocyanin at S = 1 spin state with R(Cu–Cu) fixed at 4.20 Å.

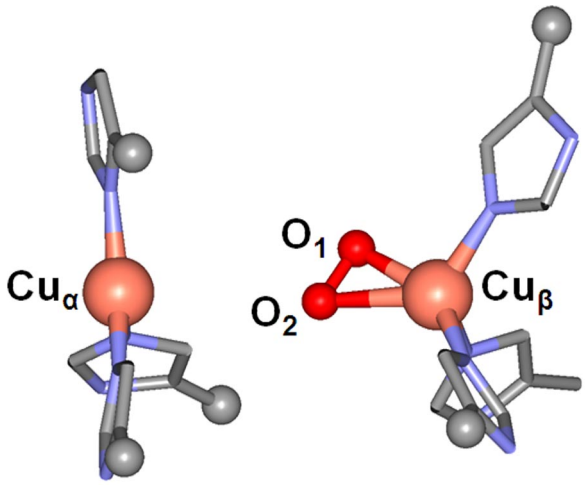

Fig. S3. Optimized structure of oxy laccase (type 3) at the broken-symmetry ($M_S = 0$) spin state with R(Cu–Cu) optimized to 6.13 Å and R(O–O) to 1.29 Å.

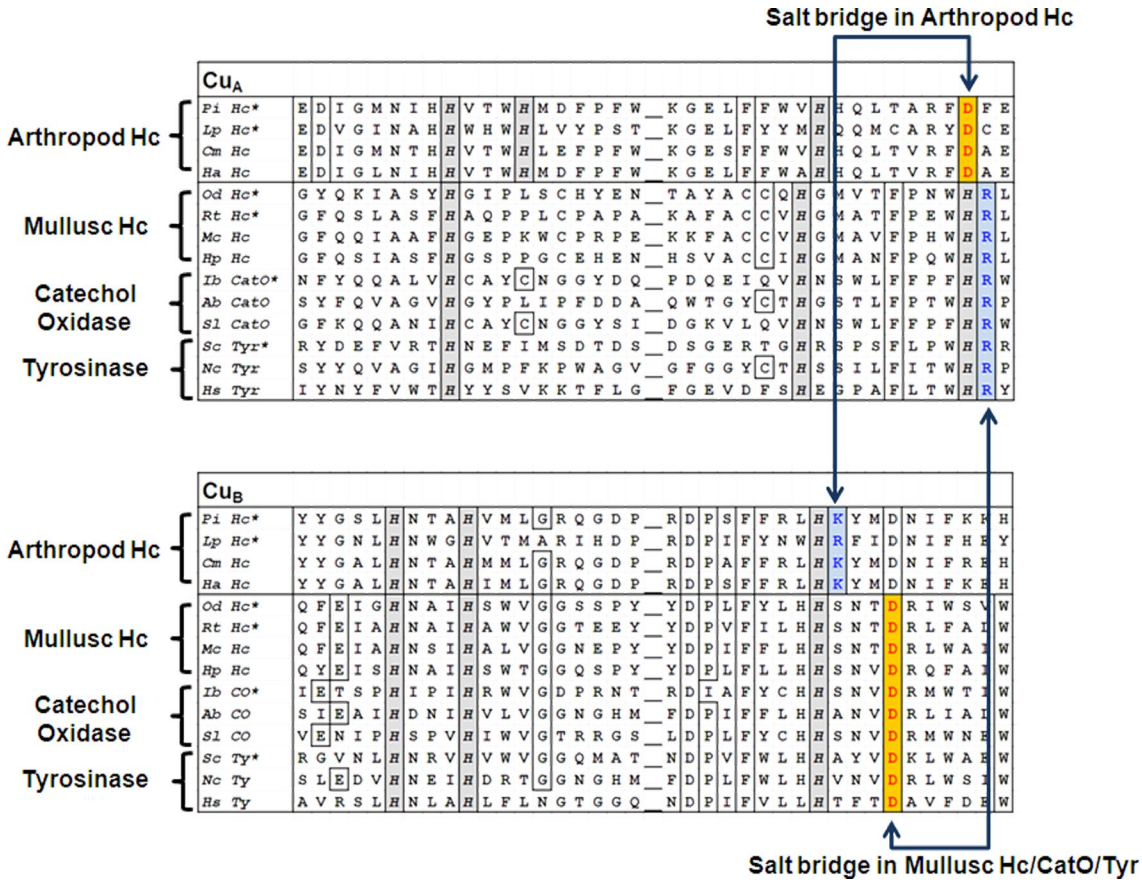

Fig. S4. Sequence alignment of various arthropod and mollusk hemocyanins, catechol oxidase, and tyrosinase. His ligands of Cu_A (*Upper*) and Cu_B (*Lower*) centers are indicated by gray boxes, and the conserved Arg/Lys and Asp that form salt bridges are indicated in blue and red, respectively. Proteins with X-ray structural data are indicated by asterisks.