

Table S1 Copper-copper and copper-ligand coordination distances and angles among bacterial laccases and other selected MCOs.

Cu centres coordination distances (Å) and angles (°)								
Enzyme	PDB	r.m.s.d. (Å) ^a	Sequence ID (%)	Type 1 Cu(1) (occ: 1.00) ^b	Type 2 Cu(4) (occ: 0.20) ^b	Type 3 Cu(2) (occ: 0.60) ^b	Type 3 Cu(3) (occ: 0.30) ^b	Cu2-Cu3
McoC	-	-	-	His ⁴³⁹ (2.03) Cys ⁴⁹⁵ (2.29) His ⁵⁰⁰ (2.00) Met ⁵⁰⁵ (3.37)	His ¹³⁹ (1.94) His ⁴⁴² (1.93) O2(Oxy) (2.48) HOH (3.18)	His ¹⁸⁰ (1.99) His ⁴⁹⁶ (2.17) His ¹⁴¹ (1.98) O1(Oxy) (2.65) O2(Oxy) (2.19)	His ¹⁸² (2.00) His ⁴⁹⁴ (2.00) His ⁴⁴⁴ (1.96) O1(Oxy) (2.06) O2(Oxy) (2.30)	Cu(2)-Cu(3) – 4.44 Cu(2)-Cu(4) – 3.60 Cu(3)-Cu(4) – 3.58 Cu(2)-O1-Cu(3) angle – 140.8° Cu(2)-O2-Cu(3) angle – 161.0°
CueO	1KV7	1.712	28.2	His ⁴⁴³ (2.02) Cys ⁵⁰⁰ (2.19) His ⁵⁰⁵ (1.98) Met ⁵¹⁰ (3.23)	His ¹⁰¹ (1.92) His ⁴⁴⁶ (1.83) O1(OH) (3.12) HOH (2.96)	His ¹⁴¹ (1.97) His ⁵⁰¹ (2.09) His ¹⁰³ (1.96) OH (2.43)	His ¹⁴³ (2.02) His ⁴⁹⁹ (2.02) His ⁴⁴⁸ (1.94) OH (2.29)	Cu(2)-Cu(3) – 4.70 Cu(2)-Cu(4) – 3.98 Cu(3)-Cu(4) – 3.54 Cu(2)-O-Cu(3) angle – 169.3°
CotA	1W6L	1.670	26.6	His ⁴¹⁹ (2.02) Cys ⁴⁹² (2.22) His ⁴⁹⁷ (1.98) Met ⁵⁰² (3.26)	His ¹⁰⁵ (1.96) His ⁴²² (2.03) O2(Oxy) (2.42) HOH (2.98)	His ¹⁵³ (2.08) His ⁴⁹³ (2.13) His ¹⁰⁷ (2.07) O1(Oxy) (2.57) O2(Oxy) (2.59)	His ¹⁵⁵ (2.11) His ⁴⁹¹ (2.07) His ⁴²⁴ (2.04) O1(Oxy) (2.31) O2(Oxy) (2.29)	Cu(2)-Cu(3) – 4.73 Cu(2)-Cu(4) – 3.99 Cu(3)-Cu(4) – 3.66 Cu(2)-O1-Cu(3) angle – 151.4° Cu(2)-O2-Cu(3) angle – 151.8°
AO (chain A)	1AOZ	1.886	26.8	His ⁴⁴⁵ (2.09) Cys ⁵⁰⁷ (2.13) His ⁵¹² (2.05) Met ⁵¹⁷ (2.90)	His ⁶⁰ (2.00) His ⁴⁴⁸ (2.09) OH (2.02)	His ¹⁰⁴ (2.19) His ⁵⁰⁸ (2.14) His ⁶² (1.98) OH (2.06)	His ¹⁰⁶ (2.16) His ⁵⁰⁶ (2.07) His ⁴⁵⁰ (2.06) OH (1.99)	Cu(2)-Cu(3) – 3.69 Cu(2)-Cu(4) – 3.66 Cu(3)-Cu(4) – 3.79 Cu(2)-O-Cu(3) angle – 130.9°
MaLa (chain A)	1GW0	1.898	24.7	His ⁴³¹ (1.91) Cys ⁵⁰³ (2.20) His ⁵⁰⁸ (1.93) Leu ⁵¹³ (3.68)	His ⁹³ (1.89) His ⁴³⁴ (1.92) O1(Oxy) (2.62) Cl (2.48)	His ¹³⁸ (1.94) His ⁵⁰⁴ (1.95) His ⁹⁵ (1.90) O1(Oxy) (2.48) O2(Oxy) (2.66)	His ¹⁴⁰ (1.96) His ⁵⁰² (1.97) His ⁴³⁶ (1.92) O1(Oxy) (2.59) O2(Oxy) (2.38)	Cu(2)-Cu(3) – 4.91 Cu(2)-Cu(4) – 4.16 Cu(3)-Cu(4) – 3.92 Cu(2)-O1-Cu(3) angle – 153.4° Cu(2)-O2-Cu(3) angle – 151.5°
TvLa	1GYC	2.114	23.0	His ³⁹⁵ (2.02) Cys ⁴⁵³ (2.19) His ⁴⁵⁸ (2.04) Phe ⁴⁶³ (---)	His ⁶⁴ (2.01) His ³⁹⁸ (1.97) HOH (2.35)	His ¹⁰⁹ (2.12) His ⁴⁵⁴ (2.17) His ⁶⁶ (2.15) OH (2.08)	His ¹¹¹ (2.23) His ⁴⁵² (2.16) His ⁴⁰⁰ (2.12) OH (2.19)	Cu(2)-Cu(3) – 3.91 Cu(2)-Cu(4) – 3.81 Cu(3)-Cu(4) – 3.82 Cu(2)-O-Cu(3) angle – 132.9°

McoC *Campylobacter jejuni*; CueO *Escherichia coli* [18]; CotA *Bacillus subtilis* [15]; Ascorbate oxidase (AO) *Cucurbita pepo* [61]; MaLa *Melanocarpus albomyces* [62]; TvLa *Trametes versicolor* [63]

^a Determined by structural superposition with McoC by Secondary Structure Matching [39]; ^b Copper occupancy in McoC copper centres.

CueO structure (PDB:1KV7) was considered as deposited, that is, with a monoatomic oxygen species in between both type 3 Cu ions, although later reports by Roberts *et al* [19] have claimed to believe that this should in fact be considered a chlorine atom.