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Supporting information for article:

The subatomic resolution study of laccase inhibition by chloride and fluoride anions using single-crystal serial crystallography: insights into the enzymatic reaction mechanism

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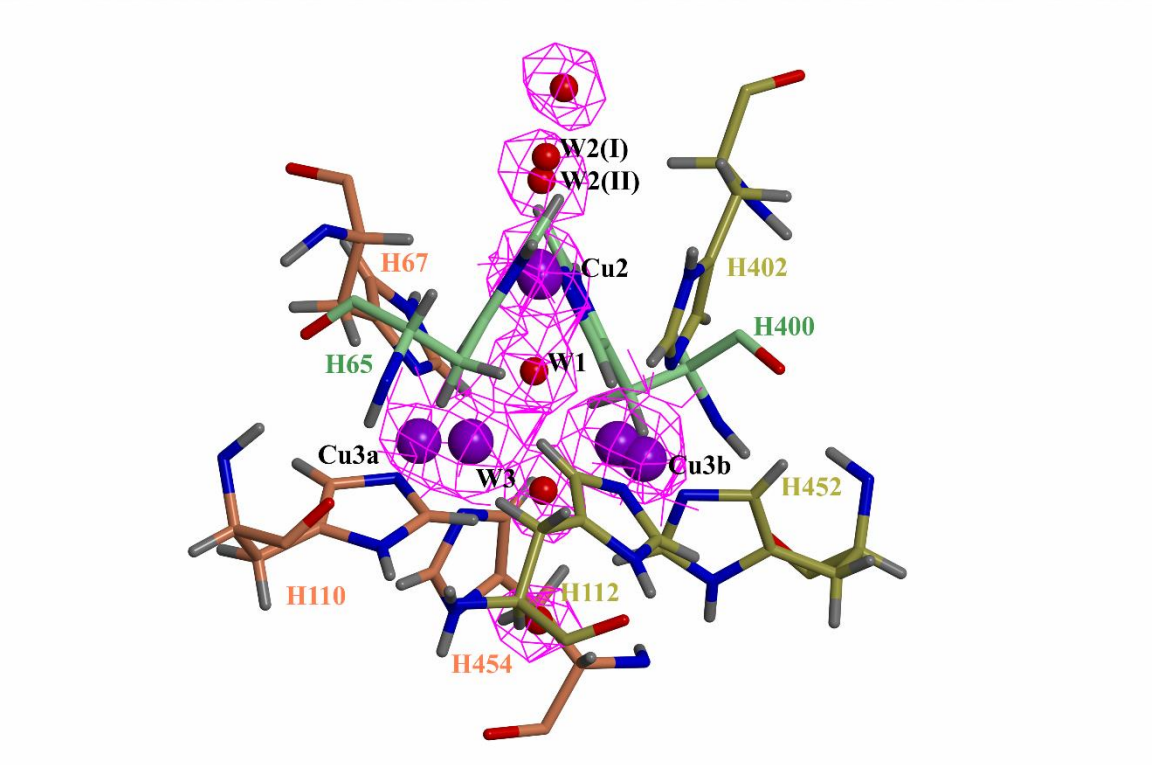

Figure S1 TNC structure for native laccase with 15 kGy dose. The ($2F_{obs}$-F_{calc}) electron density maps at l σ level are shown in magenta. Purple spheres represent positions of the copper ions. Red spheres show positions of the oxygen ligands. The carbon atoms of histidine residues are colored as in Fig. 2.

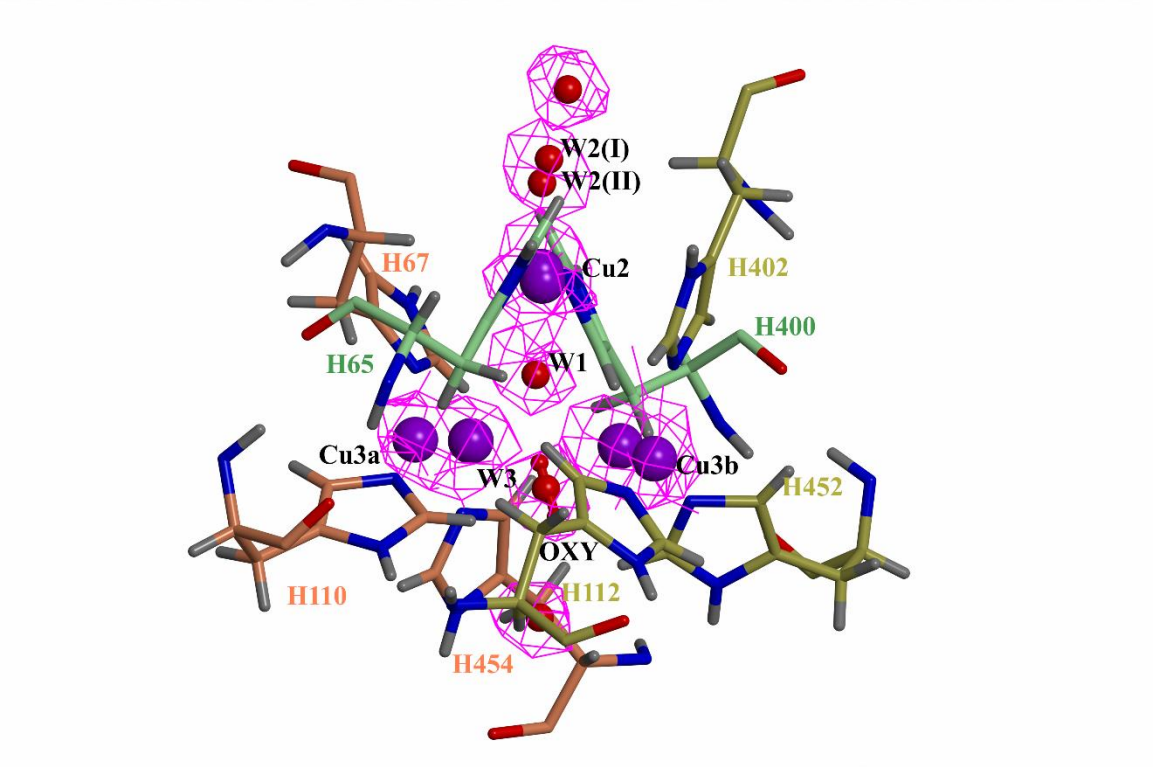

Figure S2 TNC structure for native laccase with 165 kGy dose. The ($2F_{obs}$-F_{calc}) electron density maps at l σ level are shown in magenta. Purple spheres represent positions of the copper ions. Red spheres show positions of the oxygen ligands. The carbon atoms of histidine residues are colored as in Fig. 2.

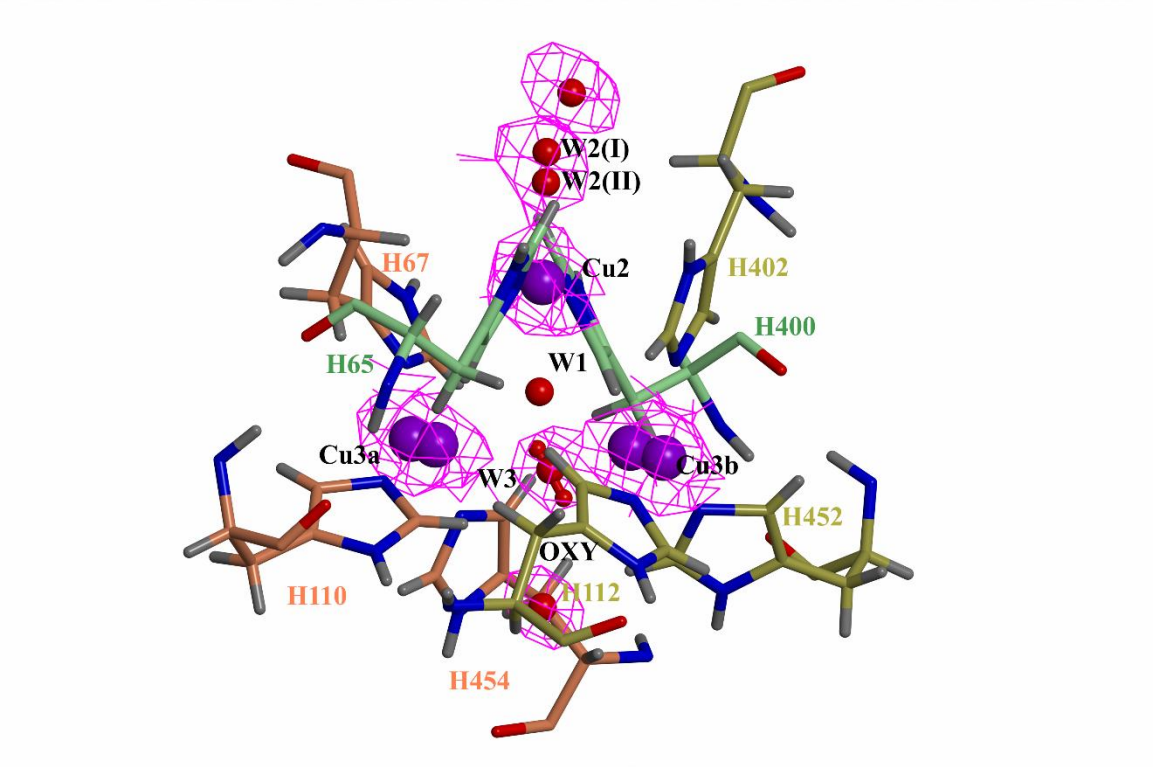

Figure S3 TNC structure for native laccase with 1215 kGy dose. The ($2F_{obs}$-F_{calc}) electron density maps at l σ level are shown in magenta. Purple spheres represent positions of the copper ions. Red spheres show position of the oxygen ligands. The carbon atoms of histidine residues are colored as in Fig. 2.

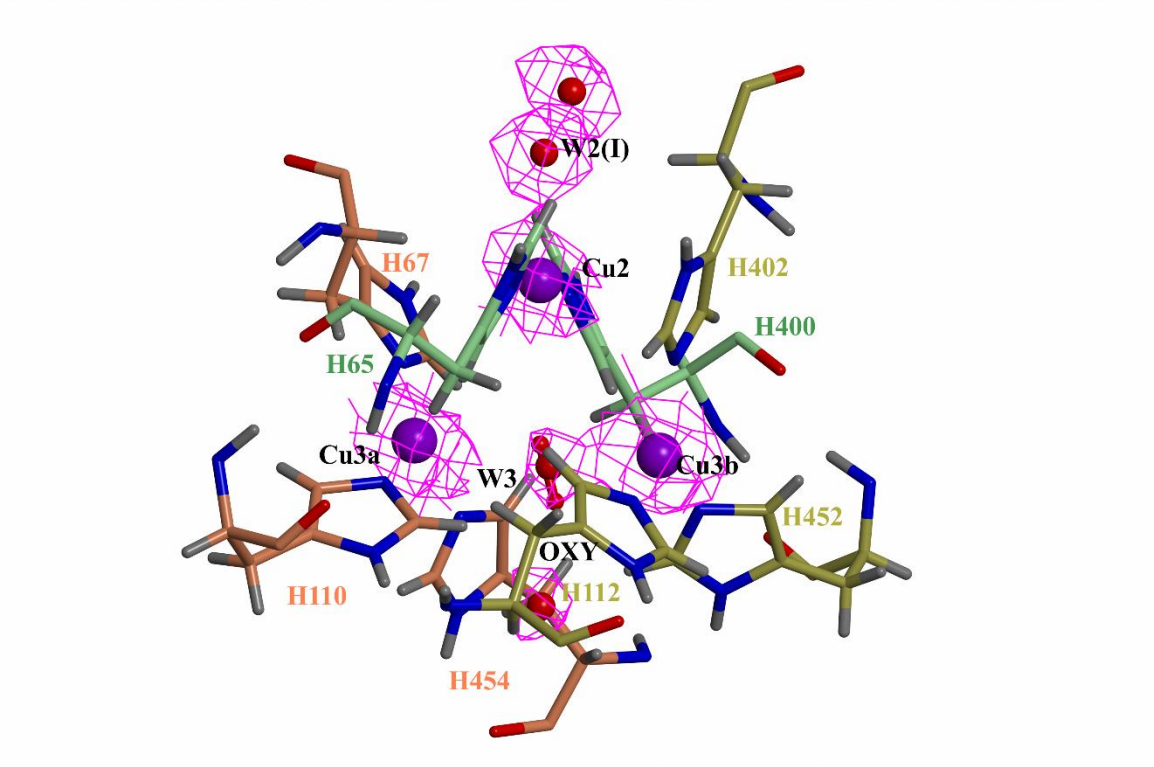

Figure S4 TNC structure for native laccase with 4065 kGy dose. The ($2F_{obs}$-F_{calc}) electron density maps at l σ level are shown in magenta. Purple spheres represent the positions of the copper ions. Red spheres show position of the oxygen ligands. The carbon atoms of histidine residues are colored as in Fig. 2.

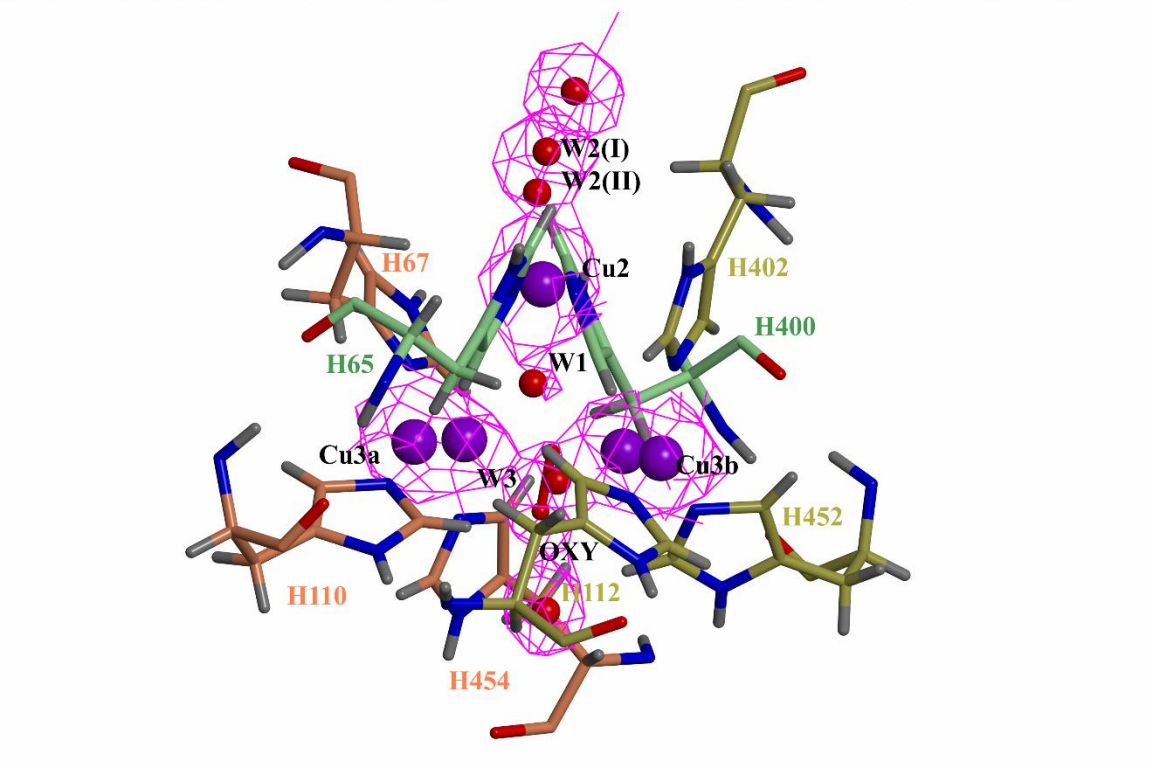

Figure S5 TNC structure for native laccase with 4415 kGy dose (after recooling). The ($2F_{obs}$-F_{calc}) electron density maps at l σ level are shown in magenta. Purple spheres represent positions of the copper ions. Red spheres show the positions of the oxygen ligands. The carbon atoms of histidine residues are colored as in Fig. 2.

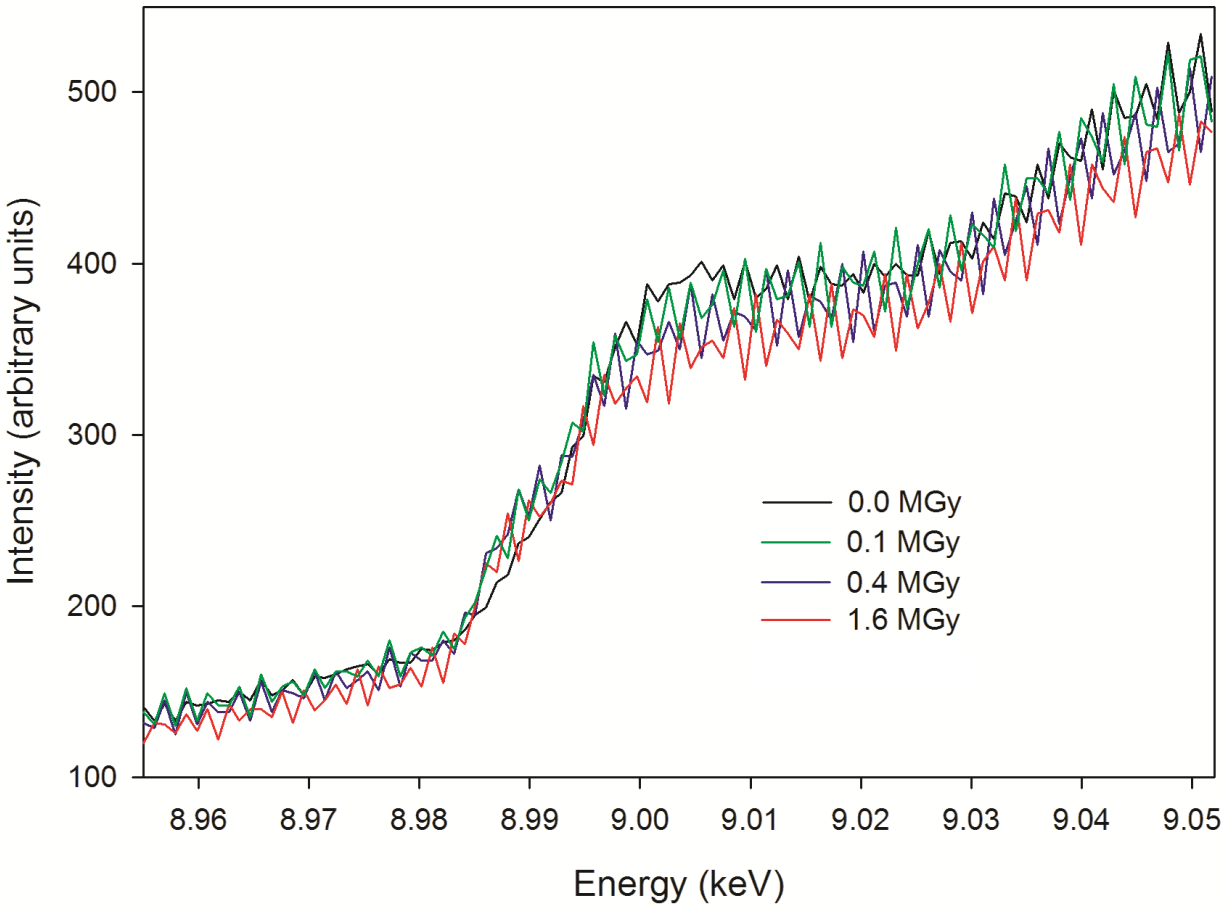

Figure S6 The fluorescence spectra around copper K absorption edge (8.9789 keV) for a crystal of the laccase complex with chloride ions at increasing doses of absorbed X-ray radiation. The fluorescence spectra at doses of 0, 0.1, 0.4 and 1.6 MGy are shown.