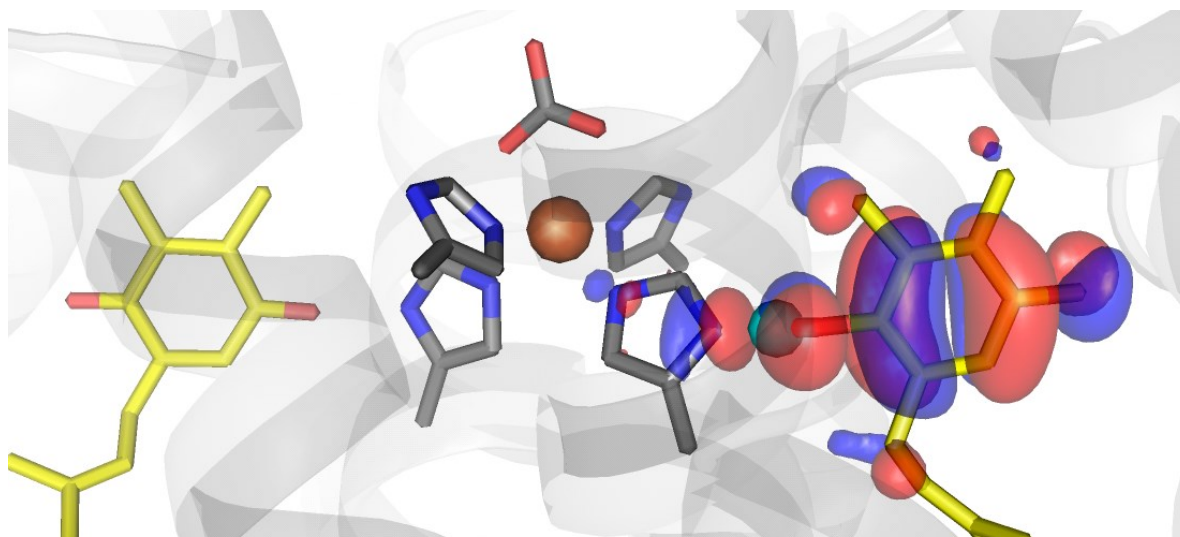


## Supporting Information



**Figure S1.** HOMO population of the D1-His215...Q<sub>B</sub> moiety (Q<sub>B</sub> : D1-His215 = 94.5 : 4.3) when  $N_{\text{His215}\dots\text{H}} = 1.44 \text{ \AA}$ . The HOMO is populated over Q<sub>B</sub> and D1-His215 with the ratio of 94.5 and 4.3.