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Supporting Information

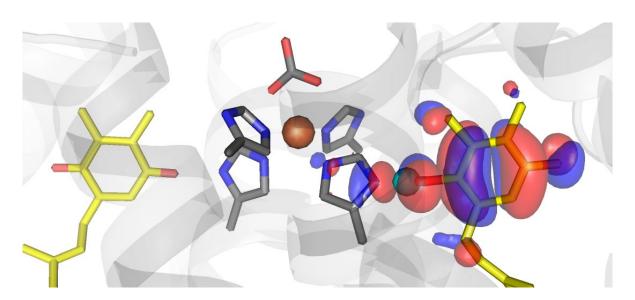


Figure S1. HOMO population of the D1-His215... Q_B moiety (Q_B : D1-His215 = 94.5 : 4.3) when $N_{His215}...H = 1.44$ Å. The HOMO is populated over Q_B and D1-His215 with the ratio of 94.5 and 4.3.