Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information for

Efficient biodegradation of malachite green by an artificial enzyme designed in myoglobin

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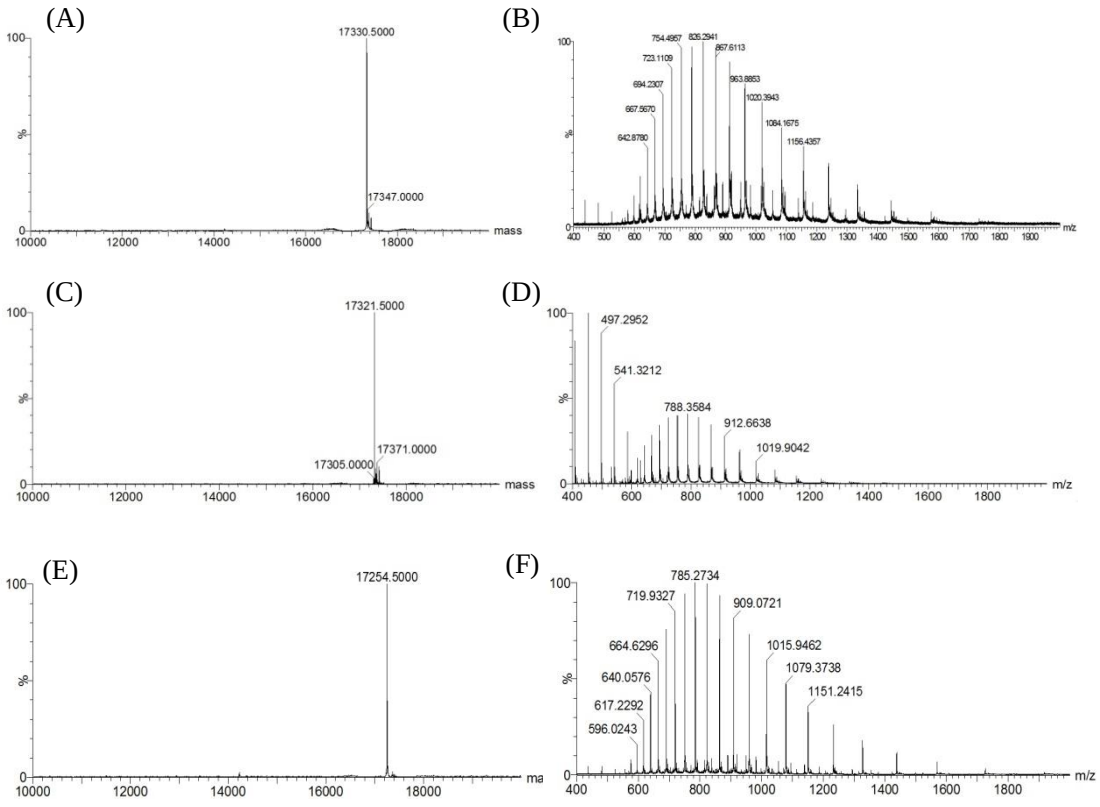

Figure S1. Mass spectra of WT Mb (A, B), F43H Mb (C, D) and F43H/H64A Mb (E, F), and the calculated molecular weight is 17,330.50 Da, 17321.05 Da and 17254.99 Da, respectively. The observed molecular weight is 17331 ±0.5 Da, 17321.5 ±0.5 Da and 17254.0 ±0.5 Da, respectively.

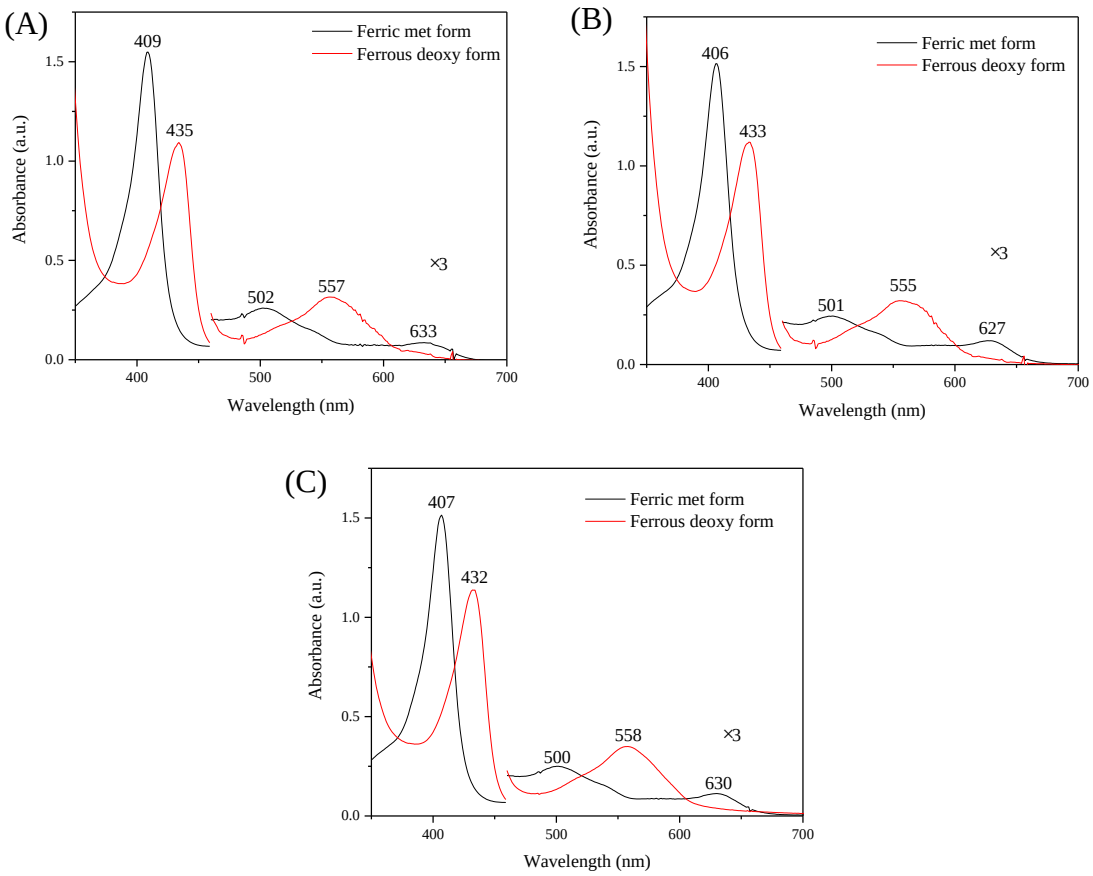

Figure S2. UV-Vis spectra of WT Mb (A), F43H Mb (B) and F43H/H64A Mb (C) in the ferric met form (black) and ferrous doxy form (red), respectively.

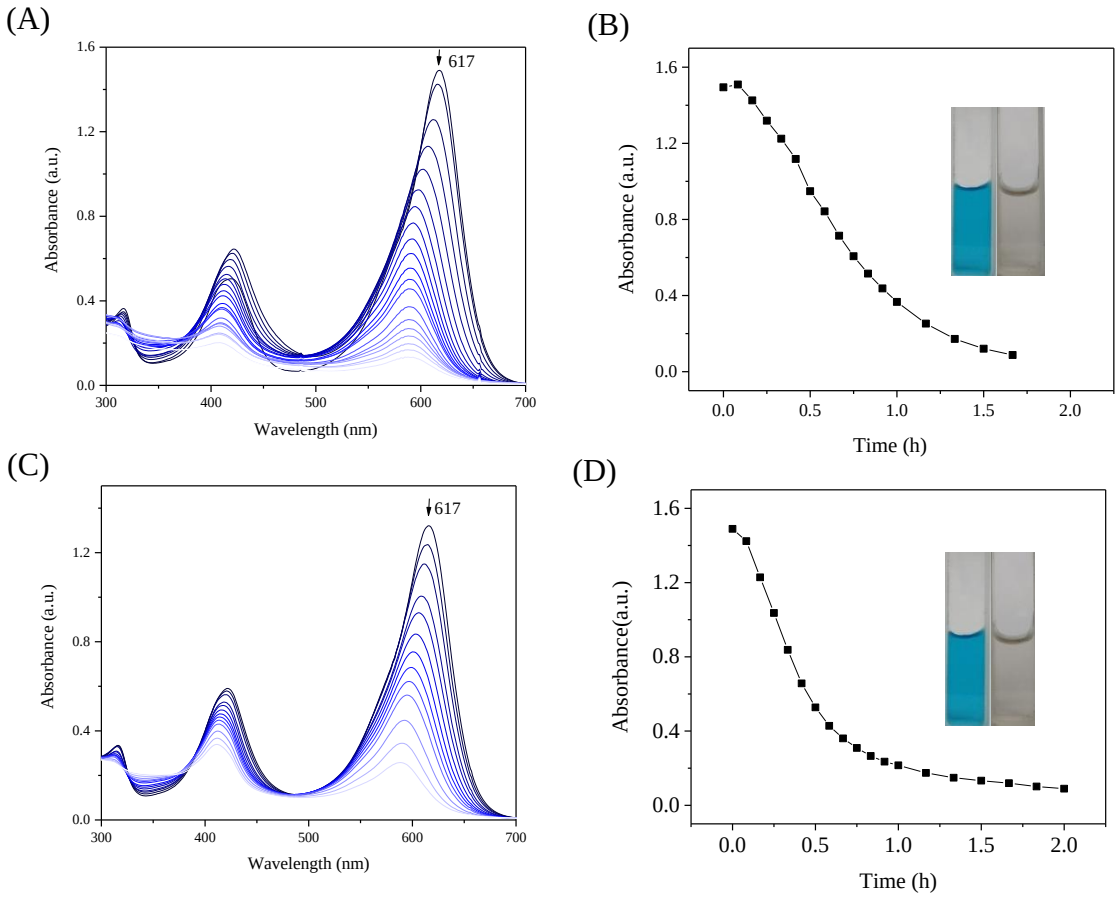

Figure S3. UV-Vis spectra of MG (10 μM) oxidized by WT Mb (A) and F43H Mb (C) (2 μM) with H_2O_2 (200 μM) in KPi buffer (100 mM, pH 6.0) at 25 ^{o}C for 2 h. Kinetic changes of absorption at 617 nm upon oxidation of MG catalyzed by WT Mb (B) and F43H Mb (D). The digital photos of the solution before and after reaction were shown as insets.

Table S1 Docking results of MG to F43H/H64A Mb AutoDock program

Model	$E_{binding}$ [a]	$E_{inter\text{-}mol}$ [b]	E_{vdw} [c]	E_{elec} [d]
1	-5.35	-6.54	-0.30	0.01
2	-5.35	-6.54	-0.27	0.01
3	-5.35	-6.54	-0.32	0.00
4	-5.35	-6.54	-0.28	0.01
5	-5.35	-6.55	-0.27	0.02
6	-5.35	-6.54	-0.31	0.01
7	-5.34	-6.54	-0.29	0.01
8	-5.34	-6.54	-0.32	0.00
9	-5.34	-6.54	-0.36	0.00
10	-5.33	-6.53	-0.33	0.01

[a] Binding energy. [b] Intermolecular energy. [c] van der Waals energies. [d] Electrostatic interactions.