Supporting Information for

Oxovanadium(IV) based Hypocrellin B Complexes with Enhanced

Photodynamic Activity

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Figure S1. The high-resolution mass spectra of complex 1 (a), 2 (b), and 3 (c). For each spectrum, the upper panel shows the experimental results and the lower one shows the simulated spectrum obtained using the software of Bruker Daltonics Data Analysis 3.4.



Figure S2. UV-vis absorption spectra of complex **1-3** solutions (25 μ M) in DMF/(Tris-CH₃COOH/EDTA buffer) (pH = 7.4) before and after irradiation (\geq 550 nm, 40 min).



Figure S3. Cyclic voltammograms of HB (a) and complex 1-3 (b-d) in DMF (vs SCE). The supporting electrolyte is 0.1 M of tetra-*n*-butylammonium hexafluorophosphate, and the scan speed is 50 mV/s.





Figure S4. Absorption spectra of HB (a), complex **1** (b) and complex **3** (c) (13 μ M) in PBS buffer (pH = 7.4) in the presence of varied concentrations of CT-DNA. The inset shows the plot of ($\varepsilon_a - \varepsilon_f$)/(ε_b - ε_f) vs. [DNA]. [HB] = [VO²⁺-HB] = 2 × 10⁻⁴ M; The maximum DNA concentration is 55.48 μ M for (a), 25.60 μ M for (b), 20.95 μ M for (c).



Figure S5. Fluorescence quenching of EB bound to CT-DNA by HB (a), complex 1 (b), and complex 3 (c). Inset is the plot of I/I_0 *vs.* [complex]. $\lambda_{ex} = 510$ nm. The maximum concentration is 22.5 μ M for HB, 17.5 μ M for 1, and 8.8 μ M for 3.