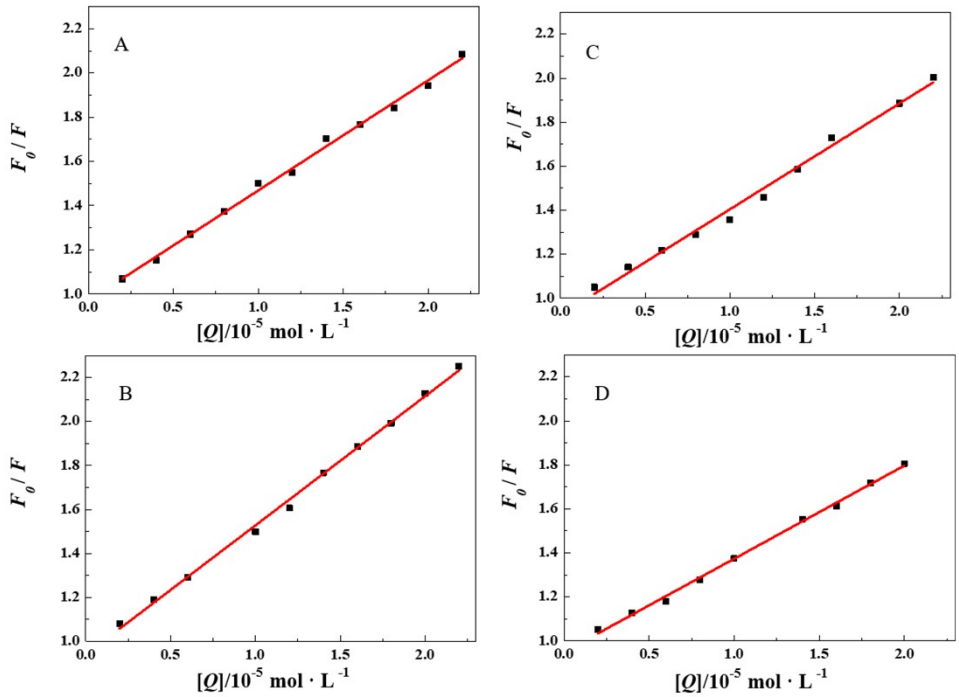

Fig. S1. Stern–Volmer plots for the quenching of lysozyme by OXY (A) or PIC (B) and trypsin by OXY (C) or PIC (D) at 298.2 K.

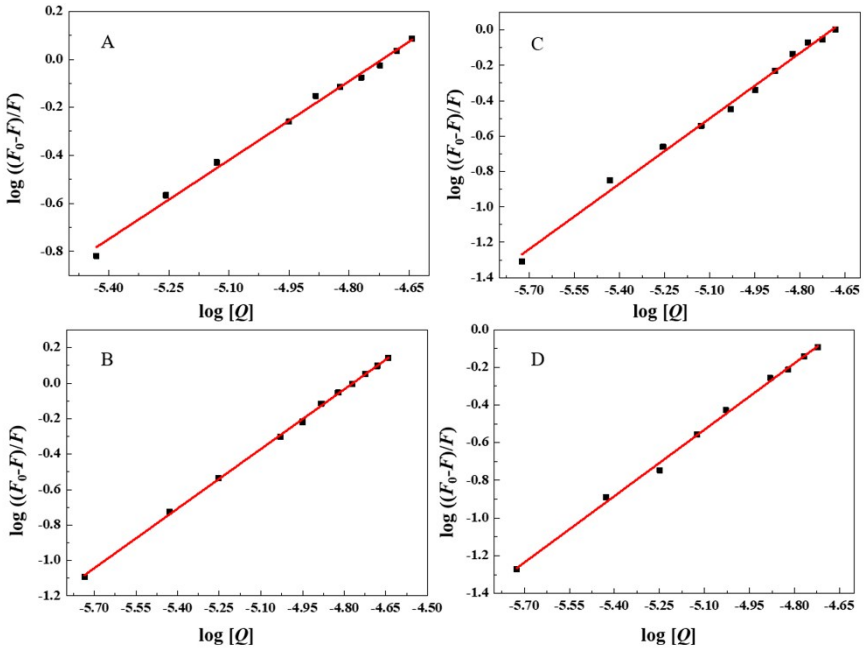

Fig. S2. Log ((F_0-F)/F) versus log [Q] plots for (A) OXY + lysozyme, (B) PIC + lysozyme, (C) OXY + trypsin and (D) PIC + trypsin at 298.2 K. [Q] is the free concentration of the ligand, which can be expressed as $[Q] = [Q]_0 - n(F_0 - F)\,[P]_0/F_0$.

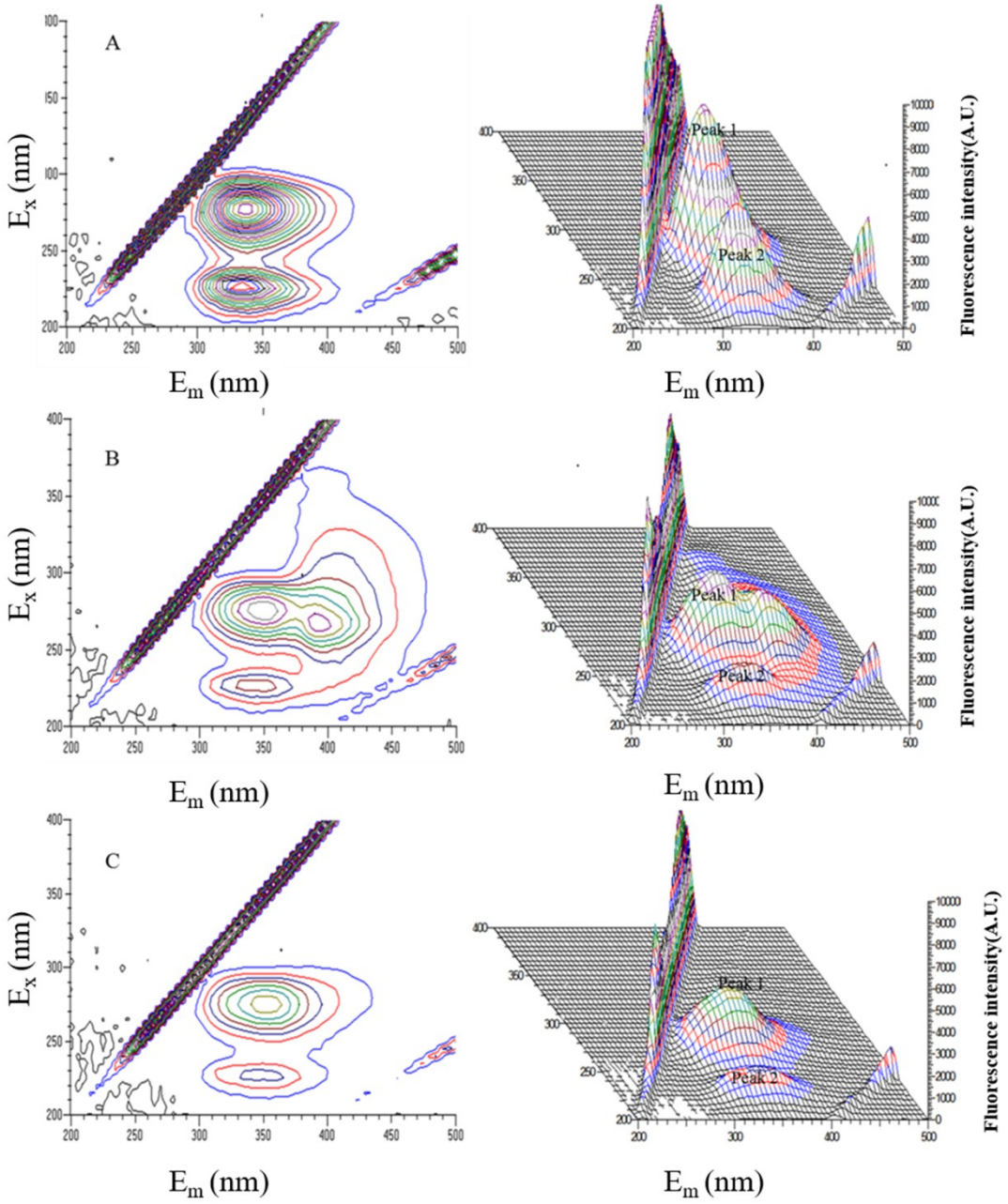

Fig.S3. The three-dimensional fluorescence spectrum of trypsin (2 μM) (A), PIC- trypsin (10:1) (B), OXY- trypsin (10:1) (C).

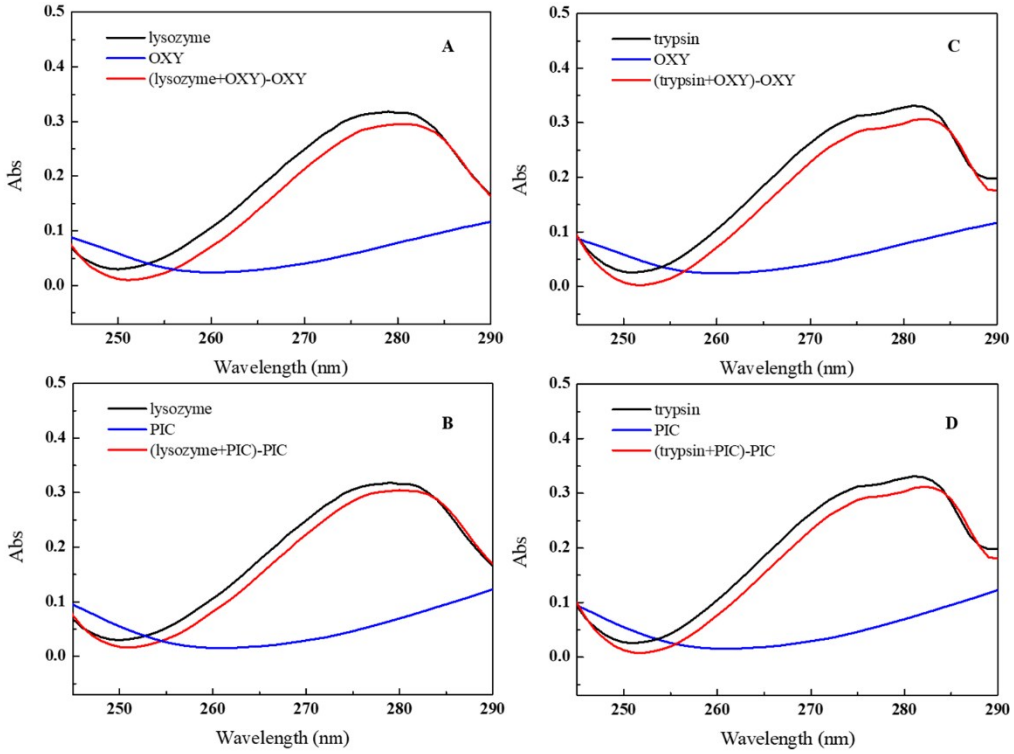

Fig.S4. (A) The absorption spectra of lysozyme, OXY and the difference absorption spectrum between lysozyme + OXY and OXY. (B) Absorption spectra of lysozyme, PIC and the difference absorption spectrum between lysozyme + PIC and PIC. (C) Absorption spectra of trypsin, OXY and the difference absorption spectrum between trypsin + OXY and OXY. (D) Absorption spectra of trypsin, PIC and the difference absorption spectrum between trypsin + PIC and PIC. The concentrations of lysozyme, trypsin, OXY and PIC were all 8 μM.

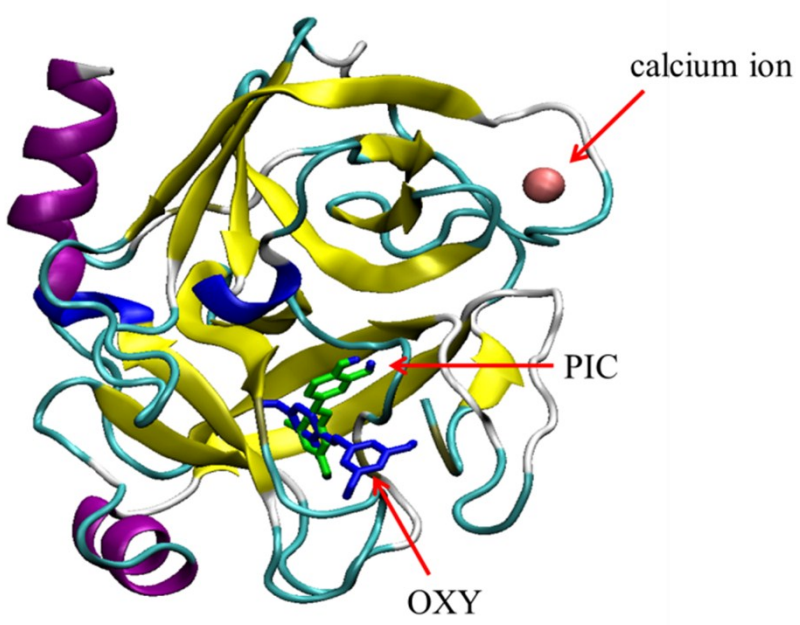

Fig.S5. The docking comparison of the binding sites of the calcium ion, PIC, and OXY in trypsin

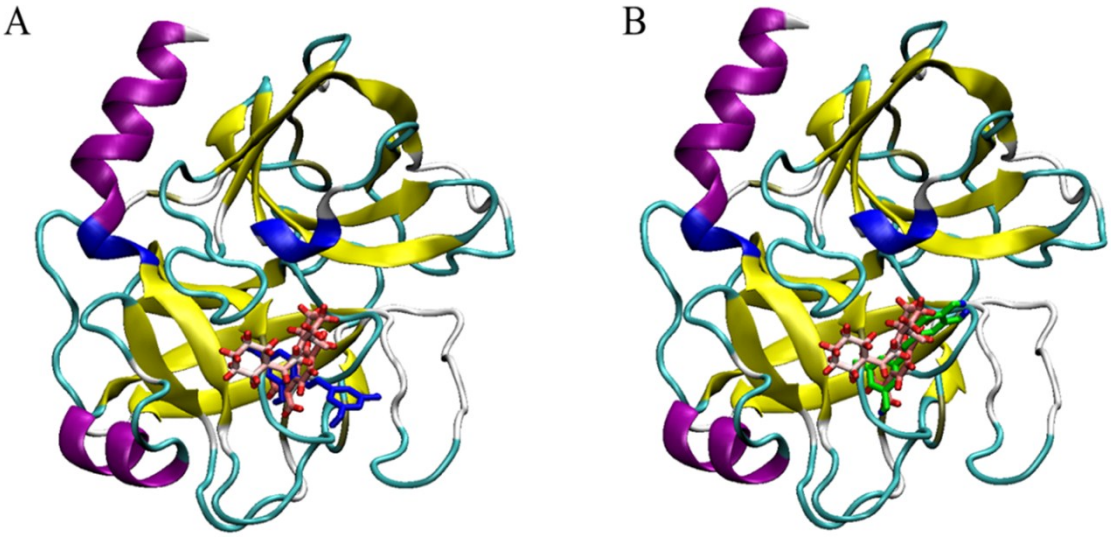

Fig.S6. (A) The docking comparison of the binding sites of the cocrystal ligand (red color) and OXY (blue color) in trypsin. (B) The docking comparison of the binding sites of the cocrystal ligand (red color) and PIC (green color) in trypsin.