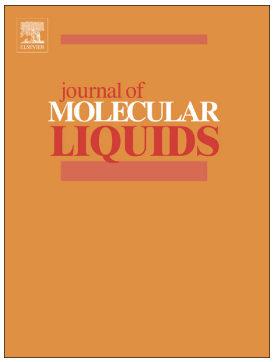

Probing the interaction of doxycycline to trypsin and bovine hemoglobin by using multi-spectral techniques and molecular docking

Qing Fang, Mai Xing, Chenhui Guo, Ying Liu

PII: S0167-7322(17)31725-7
DOI: doi: 10.1016/j.molliq.2017.07.032
Reference: MOLLIQ 7609

To appear in: *Journal of Molecular Liquids*

Received date: 22 April 2017
Revised date: 8 July 2017
Accepted date: 11 July 2017

Please cite this article as: Qing Fang, Mai Xing, Chenhui Guo, Ying Liu , Probing the interaction of doxycycline to trypsin and bovine hemoglobin by using multi-spectral techniques and molecular docking, *Journal of Molecular Liquids* (2017), doi: 10.1016/j.molliq.2017.07.032

Probing the interaction of doxycycline to trypsin and bovine hemoglobin by using multi-spectral techniques and molecular docking

Qing Fang[1], Mai Xing[1], Chenhui Guo[1], Ying Liu[* 1,2]

1. College of Life and Environmental Sciences, Minzu University of China, Beijing 100081, China

2. Beijing Engineering Research Center of Food Environment and Public Health, Minzu University of China, Beijing 100081, China

* Corresponding author. Tel.:+86 15810128921; fax: +86 10 68450641

E-mail address: liuying4300@163.com

Abstract: The interactions of doxycycline (DC) with digestive enzyme (trypsin) and intracellular protein (bovine hemoglobin, BHb) were investigated by using multi-spectral techniques and molecular docking. Fluorescence studies suggested that DC quenched trypsin fluorescence in a static quenching and BHb fluorescence in a combined quenching (dynamic and static quenching) with binding constants of 0.22 and 1.45 × 10^4 L·mol^{-1} at 298 K, respectively. The thermodynamic parameters demonstrated that the main forces of BHb-DC and trypsin-DC systems were hydrophobic forces, hydrogen bonds and van der Waals forces in the binding processes. Based on the results of FRET, the binding distances between DC and the inner tryptophan residues of trypsin and BHb were calculated to be 4.09 and 3.86 nm, respectively. Furthermore, the results of circular dichroism spectra (CD) indicated the secondary structures of trypsin and BHb were partially changed by DC with the α-helix percentage of trypsin-DC system increased (6.3%–7.3%) and that of BHb-DC system also increased (38.5%–46.2%), the β-sheet percentage of trypsin-DC system decreased from 43.3% to 41.0%. UV-vis and three-dimensional fluorescence spectra results showed these binding interactions could cause conformational and some