

**Characterization of the interaction between acotiamide  
hydrochloride and human serum albumin:  $^1\text{H}$  STD NMR  
spectroscopy, electrochemical measurement, and docking  
investigations Supporting information**

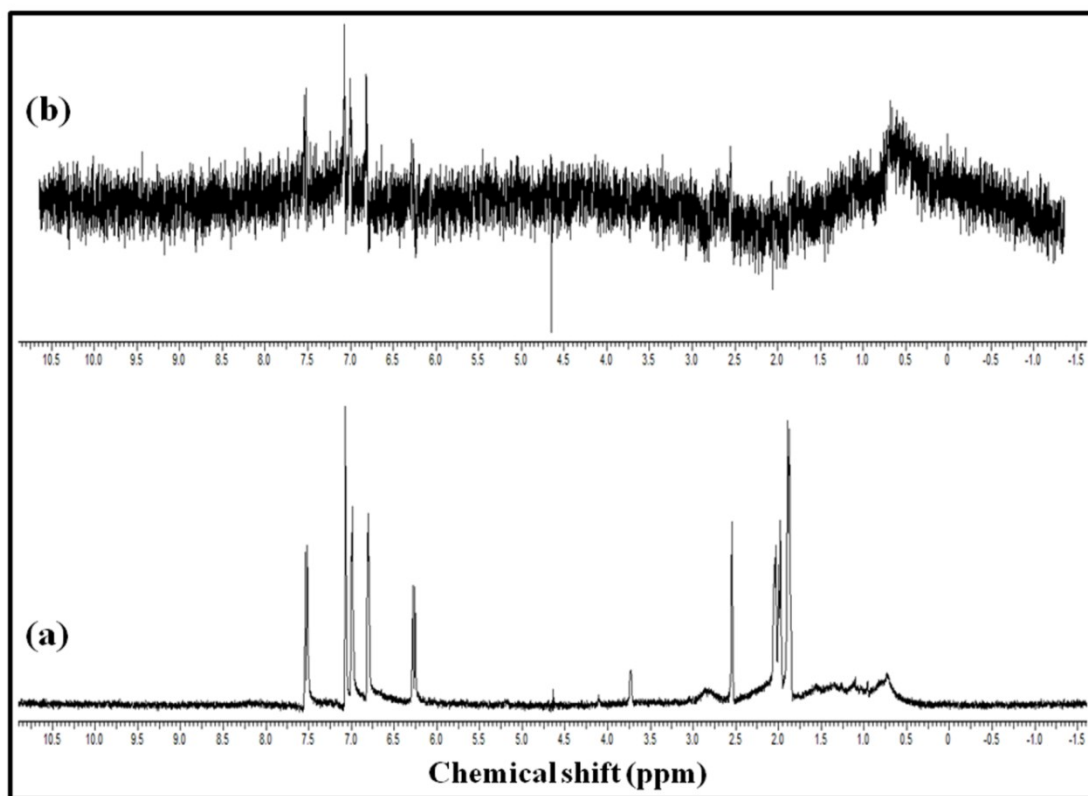
Jiawei He, Hongqin Yang, Shanshan Li, Kailin Xu, Qing Wang, Yanmei Huang, Hui Li\*

College of Chemical Engineering, Sichuan University, Chengdu  
Sichuan, China.

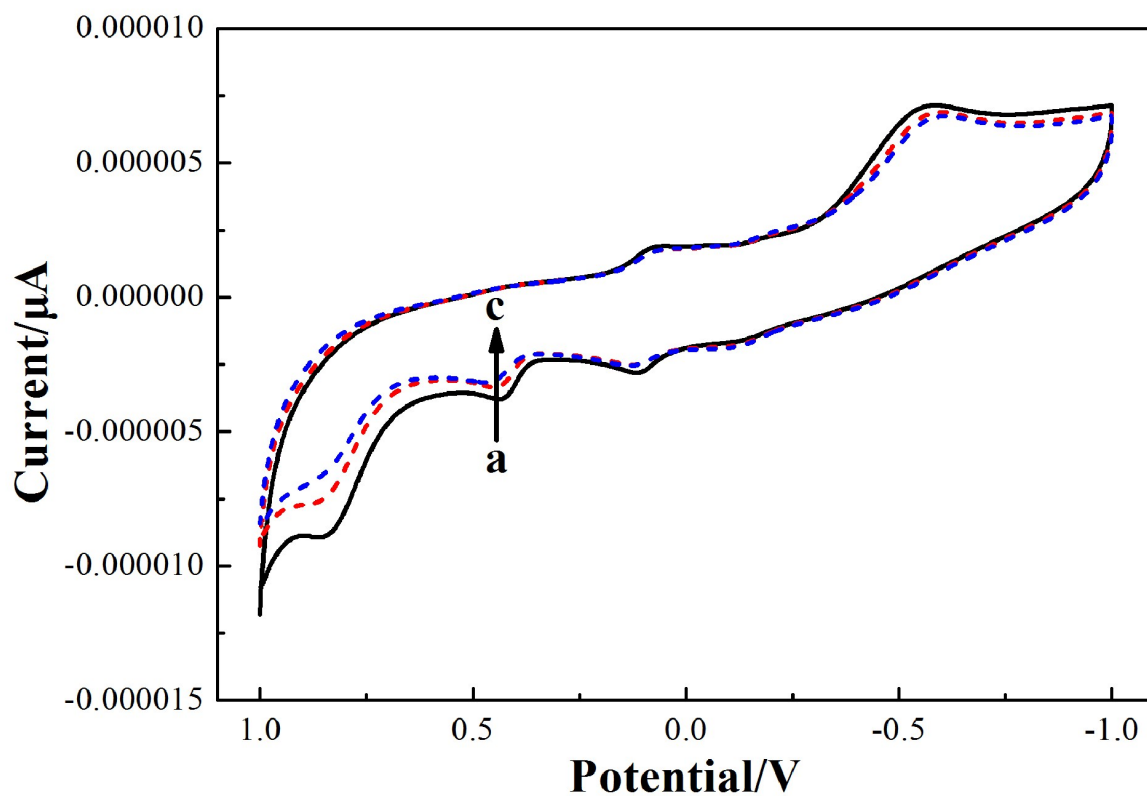
E-mail: [lihuilab@sina.com](mailto:lihuilab@sina.com);

Fax: +86 028 85401207;

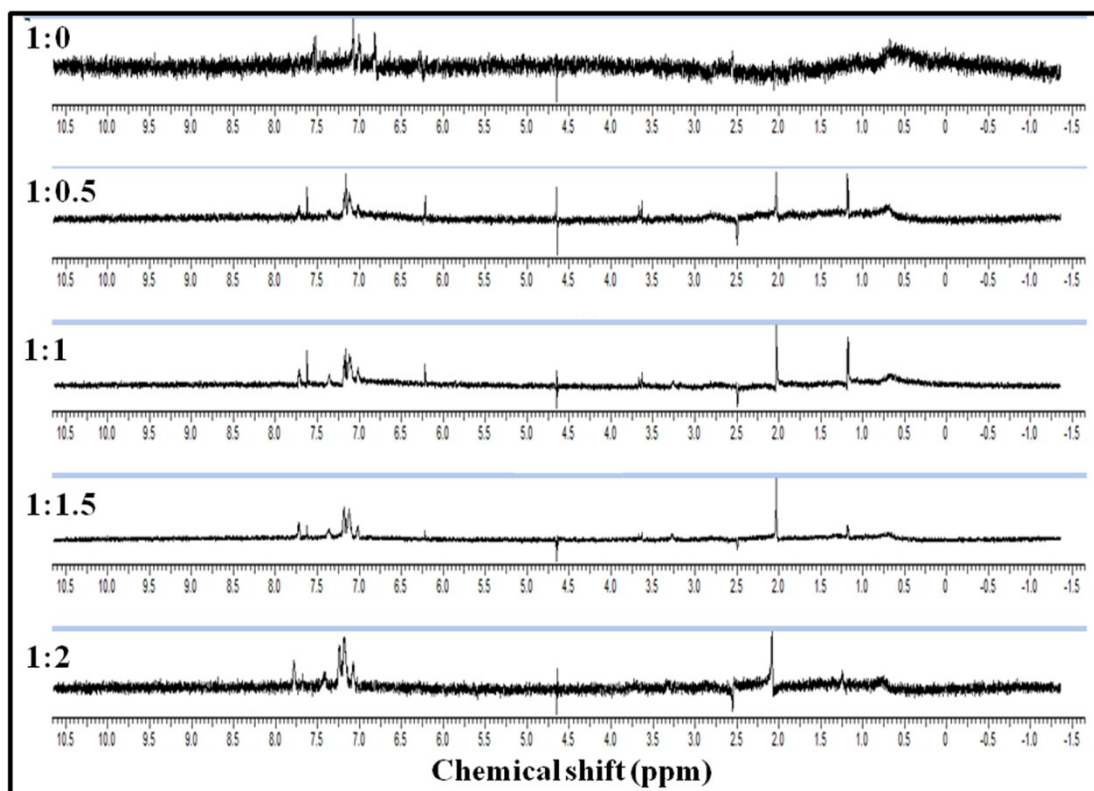
Tel: +86 028 85405149



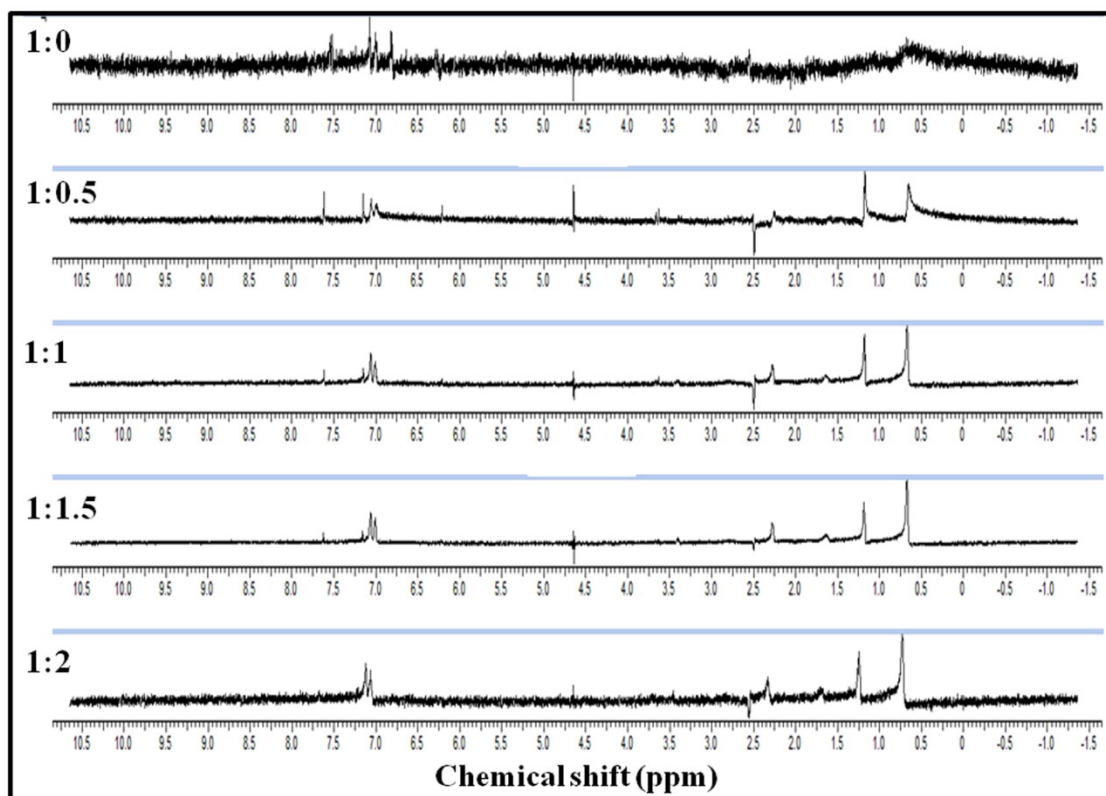
**Fig. S1** The full  $^1\text{H}$  NMR spectrum of Z-338 and HSA in 40 : 1 ratio obtained with a Watergate scheme for solvent suppression (a) and the corresponding STD spectrum (b).



**Fig. S2** CV curves of Z-338 in the absence and presence of HSA.  $[\text{Z-338}] = 5.0 \times 10^{-4} \text{ M}$ .  $[\text{HSA}] = 0, 1.0 \times 10^{-5} \text{ M}$  and  $2.0 \times 10^{-5} \text{ M}$  (a–c, respectively).



**Fig. S3** The full STD NMR spectra of HSA-Z-338 system without and with warfarin. The concentration of HSA ( $1.0 \times 10^{-5}$  M) and Z-338 ( $4.0 \times 10^{-4}$  M) was keep constant. The concentration of warfarin was 0,  $2.0 \times 10^{-4}$  M,  $4.0 \times 10^{-4}$  M,  $6.0 \times 10^{-4}$  M and  $8.0 \times 10^{-4}$  M, respectively.



**Fig. S4** The full STD NMR spectra of HSA-Z-338 system without and with ibuprofen. The concentration of HSA ( $1.0 \times 10^{-5}$  M) and Z-338 ( $4.0 \times 10^{-4}$  M) was keep constant. The concentration of ibuprofen was 0,  $2.0 \times 10^{-4}$  M,  $4.0 \times 10^{-4}$  M,  $6.0 \times 10^{-4}$  M and  $8.0 \times 10^{-4}$  M, respectively.