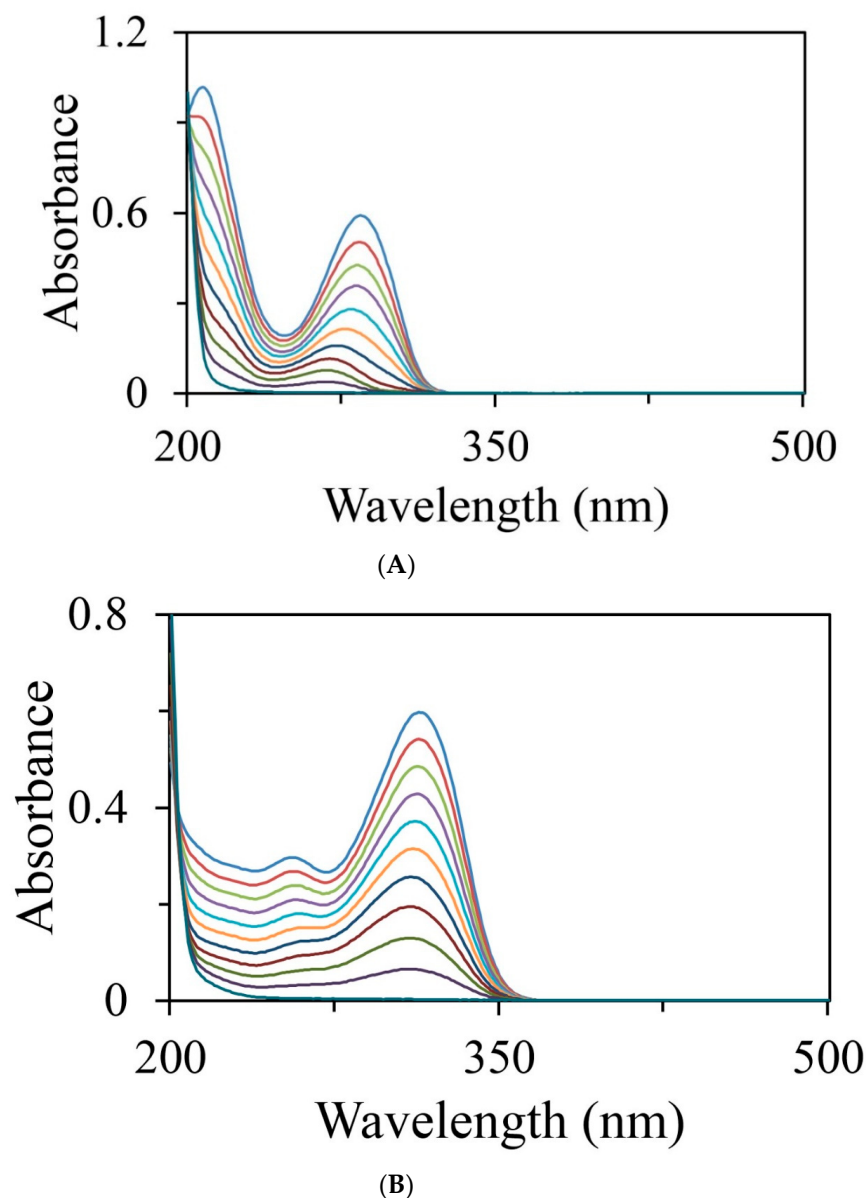
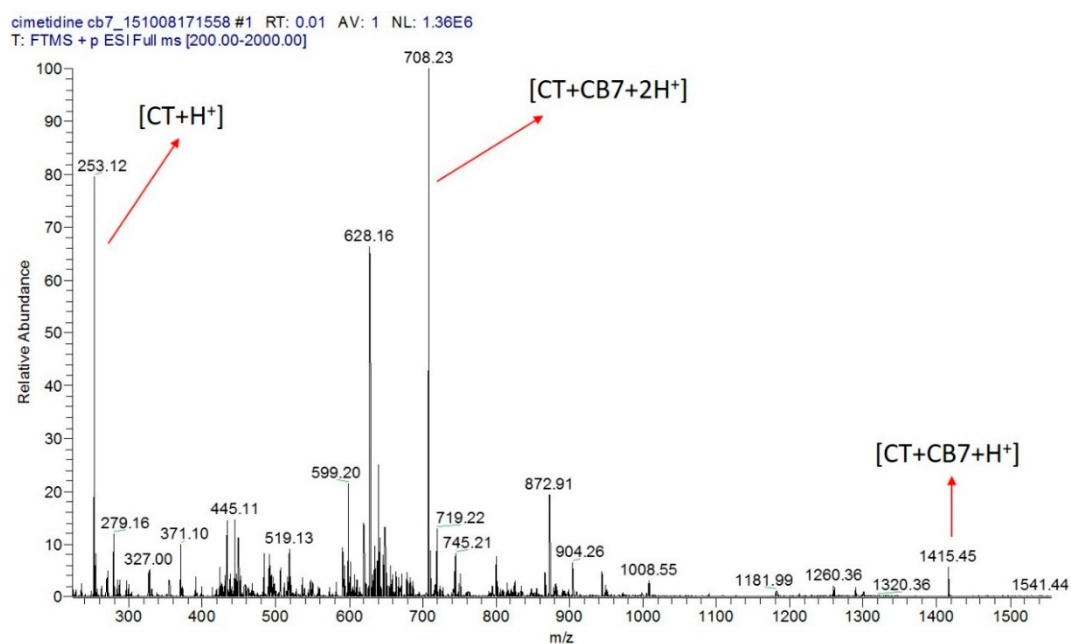


# Supplementary Materials: Molecular Encapsulations of Histamine H<sub>2</sub>-Receptor Antagonists by Macrocyclic Cucurbit[7]uril: An Experimental and Computational Study

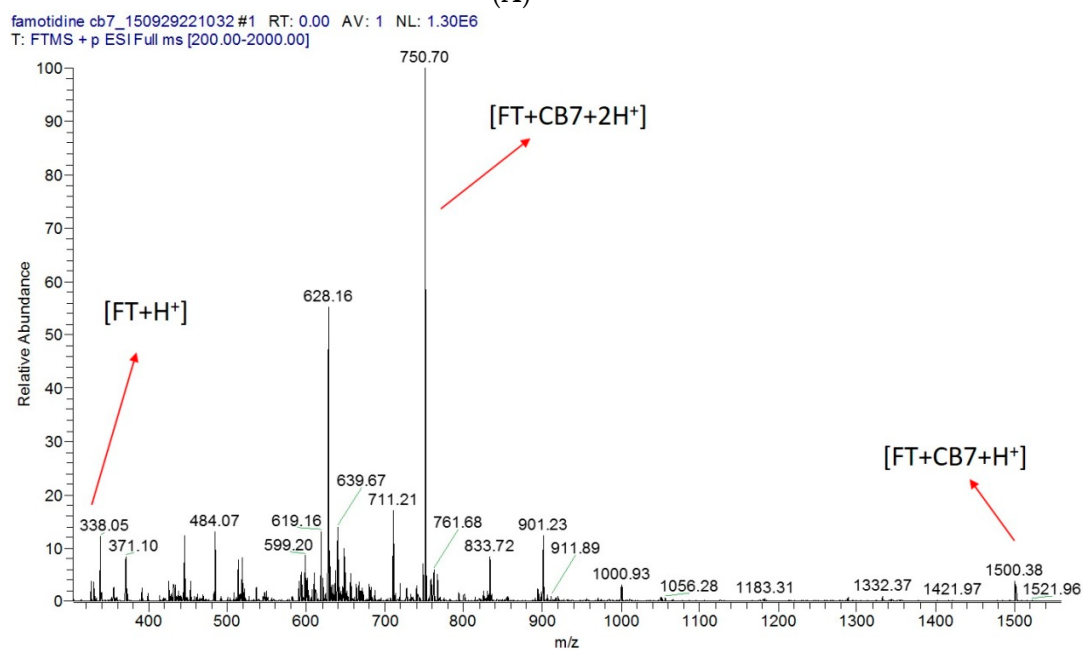
Hang Yin, Runmiao Wang, Jianbo Wan, Ying Zheng, Defang Ouyang and Ruibing Wang



**Figure S1.** UV-Visible absorbance spectra of FT and CB[7] under Job plot titration (A); UV-Visible absorbance of NT and CB[7] under Job plot titration (B).



(A)



(B)

nizatidine cb7\_150929221032 #1 RT: 0.01 AV: 1 NL: 1.25E6  
T: FTMS + p ESI Full ms [200.00-2000.00]

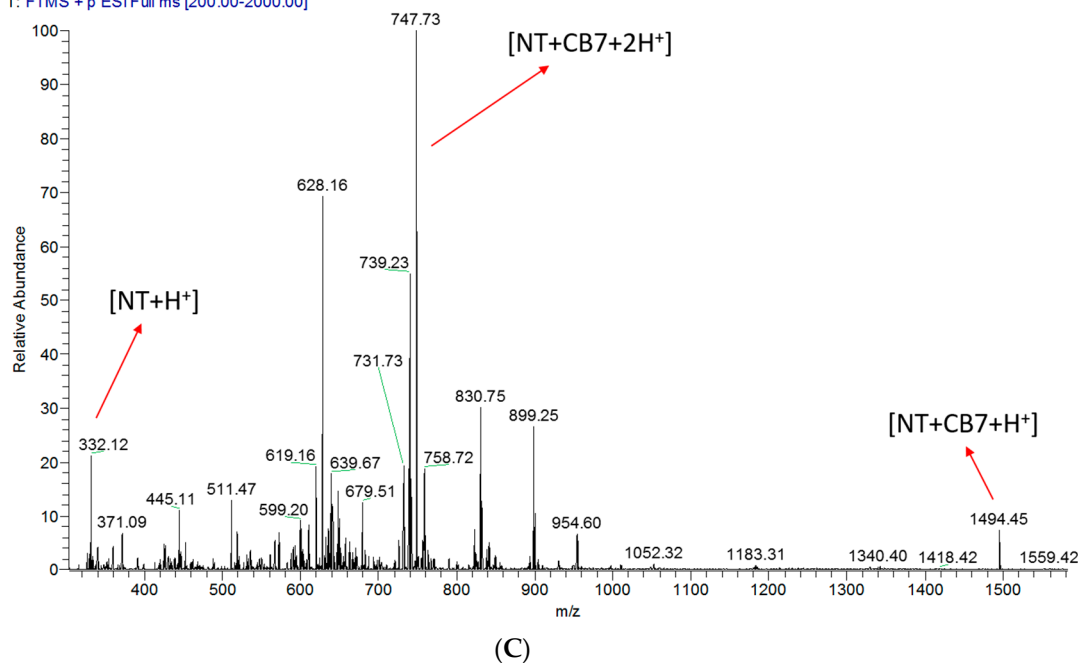


Figure S2. ESI-MS spectra of CT@CB[7] (A), FT@CB[7] (B) and NT@CB[7] (C).

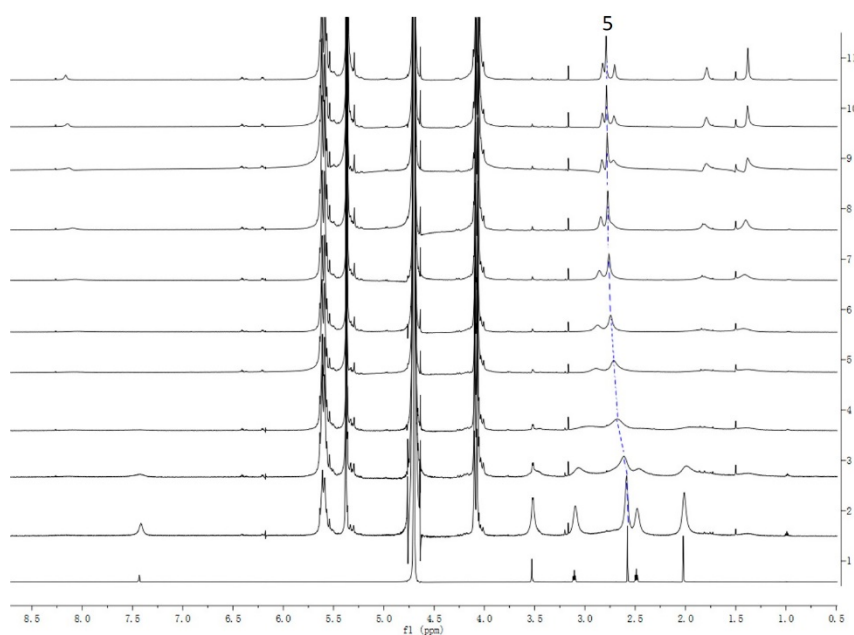
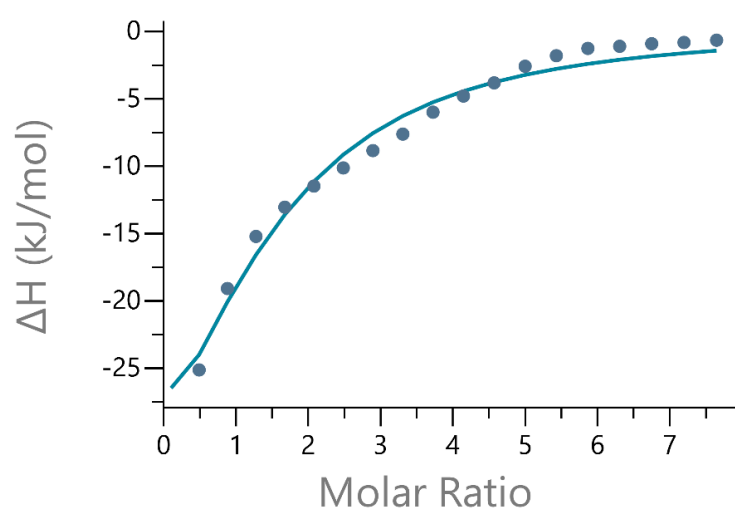
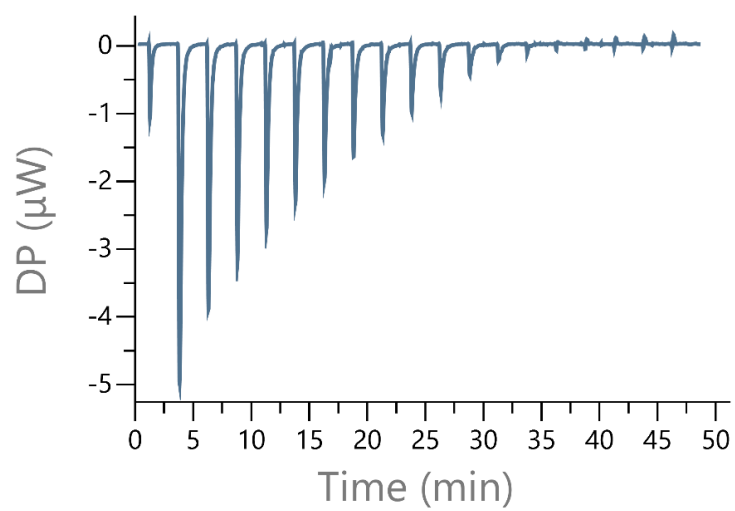
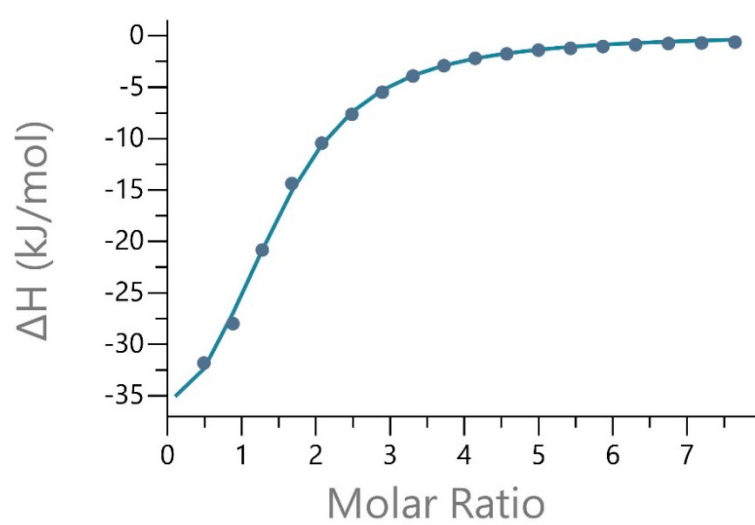
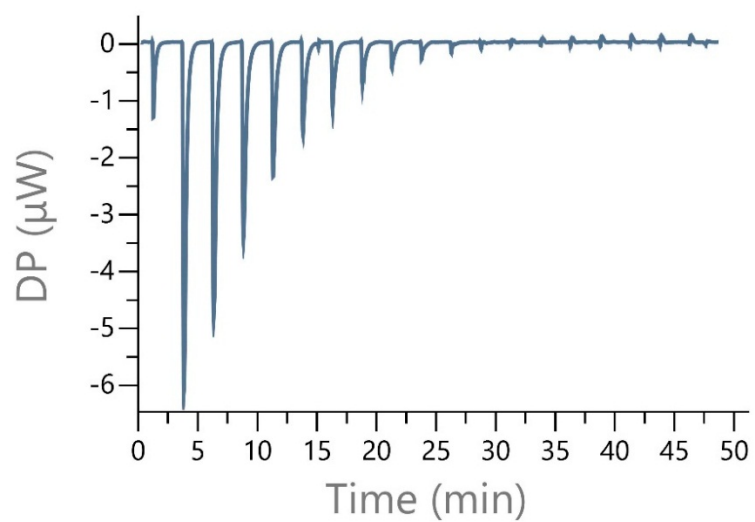


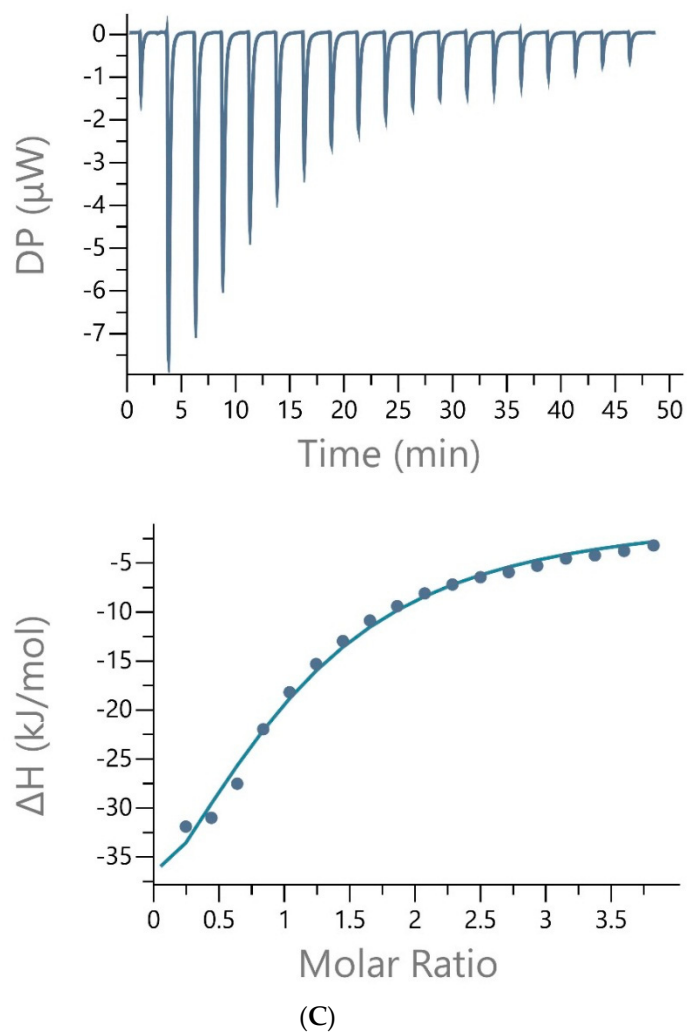
Figure S3. <sup>1</sup>H-NMR spectra of CT in the presence of increasing concentration of CB[7] (increased from 0 to 3.0 eqv. of CT).



(A)



(B)



**Figure S4.** ITC raw plots and integrated heat plots of (A) CT with CB[7], (B) FT with CB[7], and (C) NT with CB[7].