Electronic Supplementary Material (ESI) for RSC Advances.

Comprehensive study of the adsorption of an acylhydrazone derivative by serum albumin: An unclassical static quenching

Content:

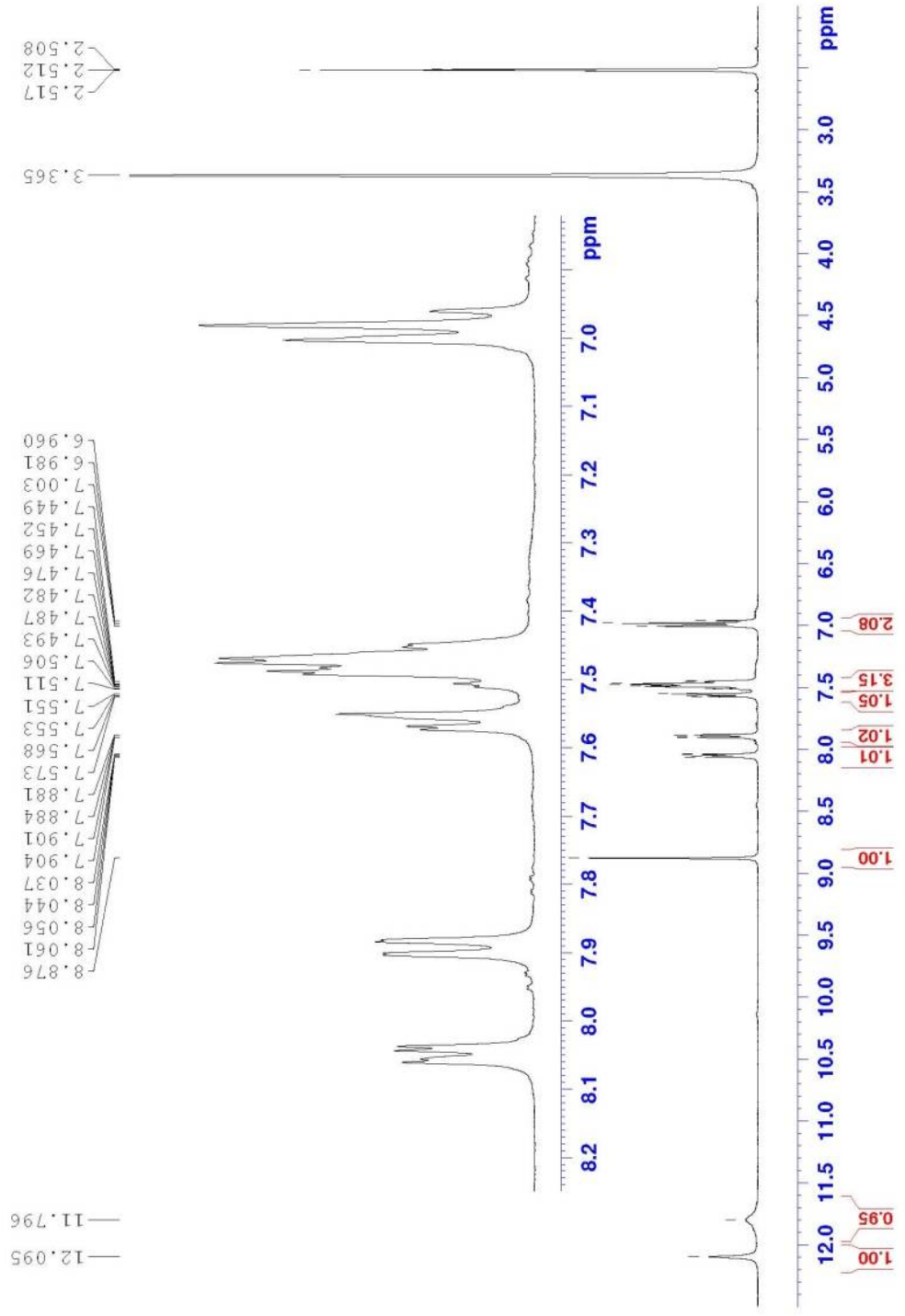


Figure 1. The ^{1}H NMR for NCH.

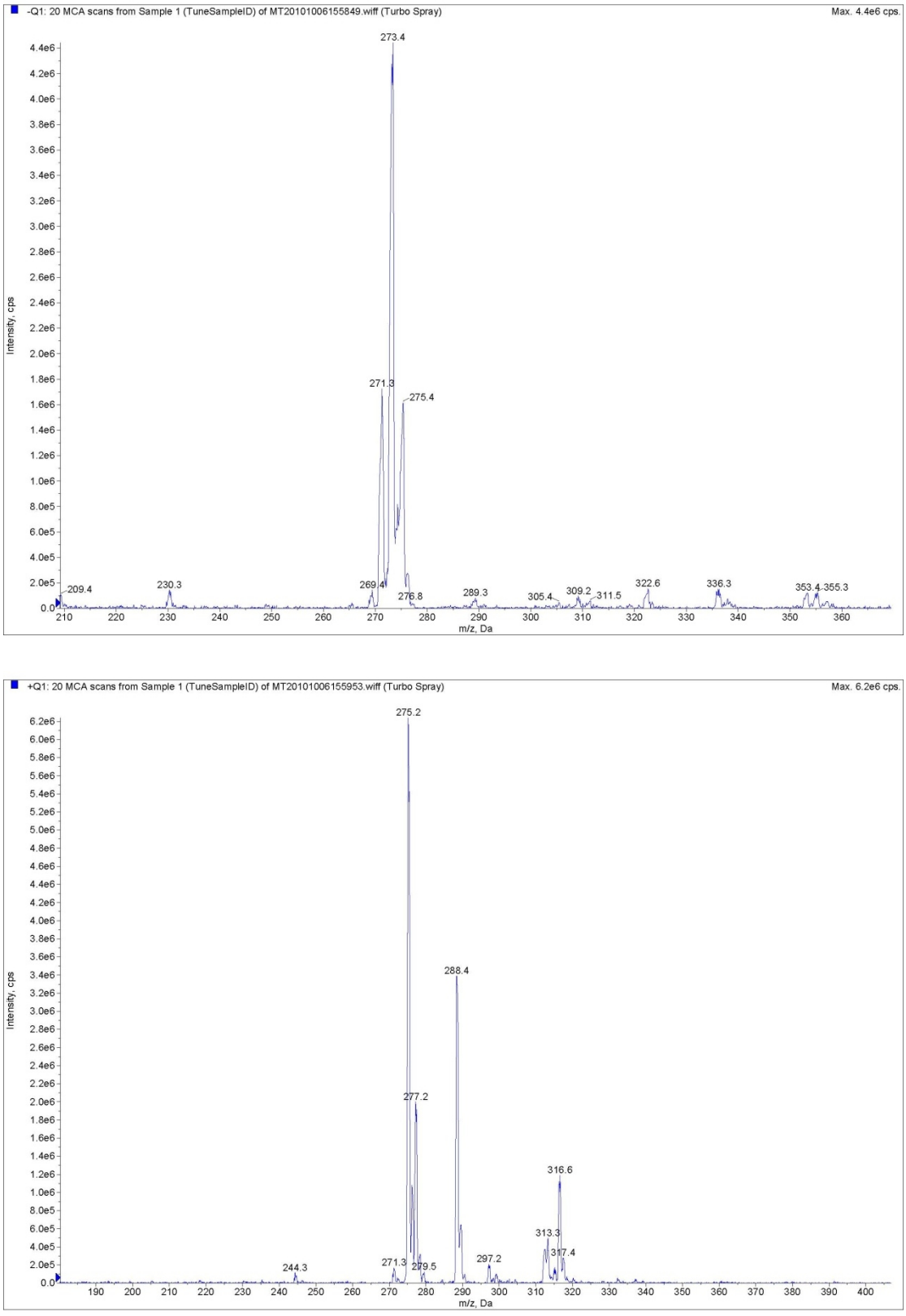


Figure 2. The ESI-MS spectra of NCH.
Up: the negative mode; Down: the positive mode.

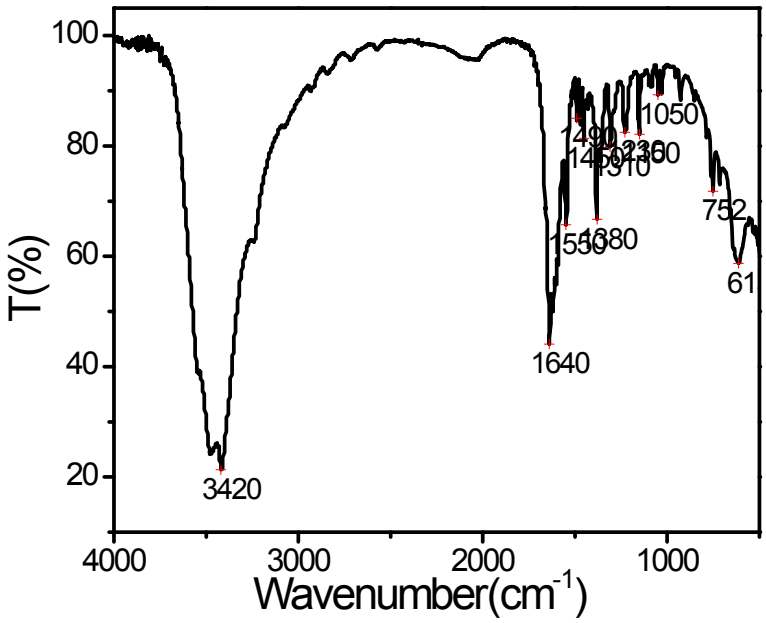


Figure 3. The IR spectrum of NCH.

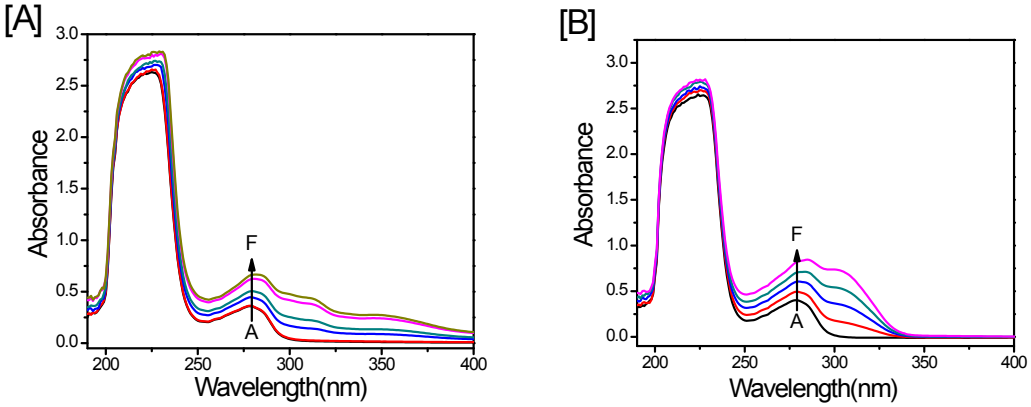


Figure 4. The addition UV-visible spectra of HSA-NCH[A] and BSA-NCH[B] system.

c(HSA) = *c*(BSA) = 10μM, the concentration of NCH from A to F: 0, 2.5, 5, 10, 15, 20μM.

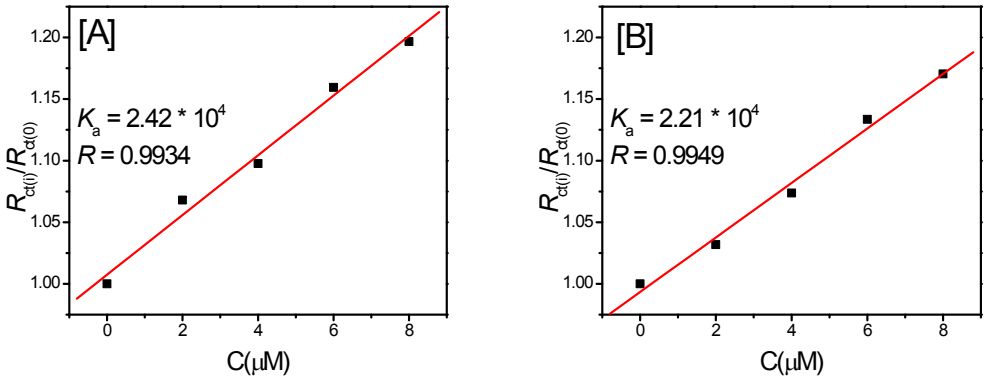
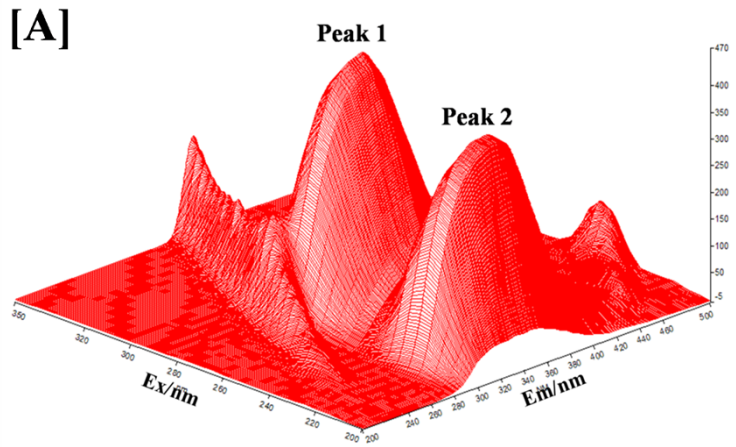
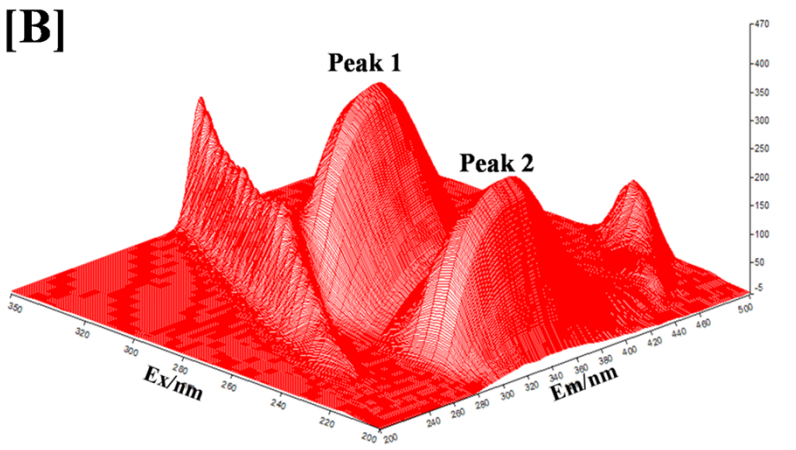
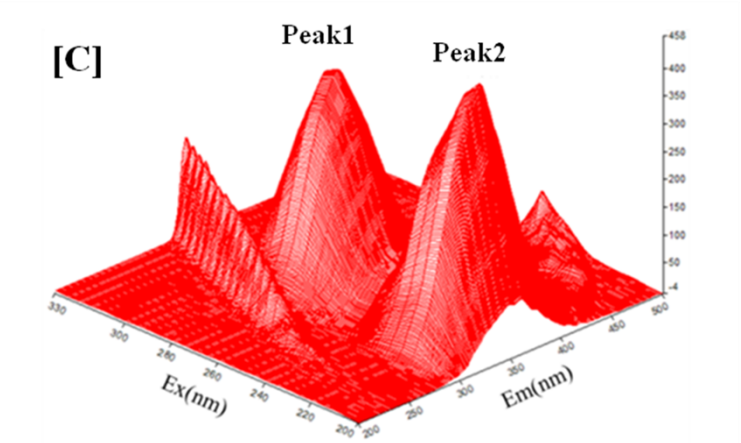


Figure 5. The Langmuir isotherm plots for HSA-NCH[A] and BSA-NCH[B] system.


[A]
Peak 1
Peak 2
Ex/nm
Em/nm


[B]
Peak 1
Peak 2
Ex/nm
Em/nm


[C]
Peak1
Peak2
Ex(nm)
Em(nm)

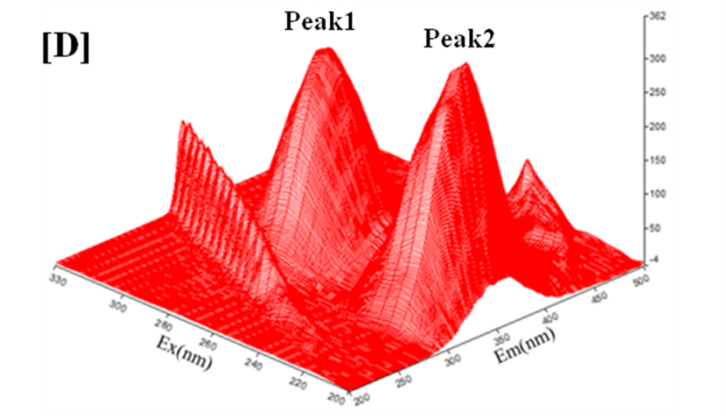
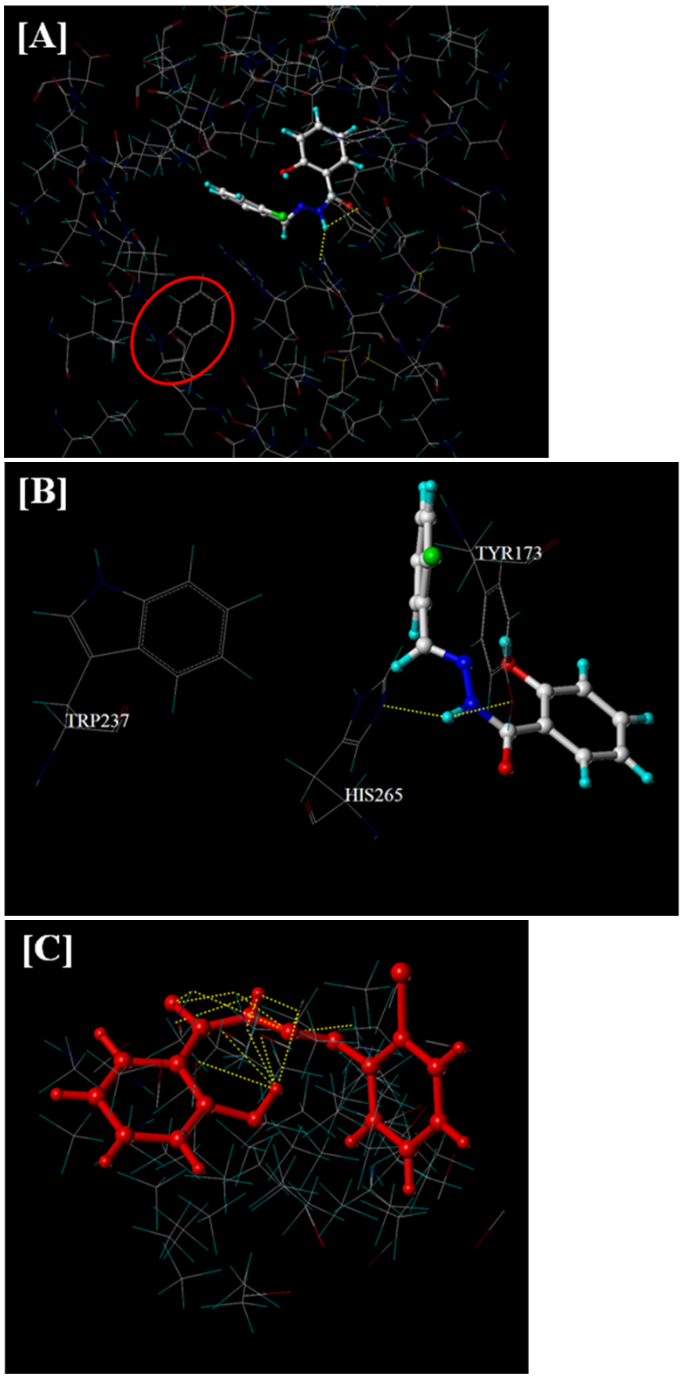

[D]
Peak1
Peak2
Ex(nm)
Em(nm)

Figure 6. 3D fluorescence spectra of HSA[A], NCH-HSA[B], BSA[C] and BSA-NCH[D].

c(HSA) = c(BSA) = c(NCH) = 2 μM; λ_{ex} = 200 – 350 nm, λ_{em} = 200 – 500 nm.



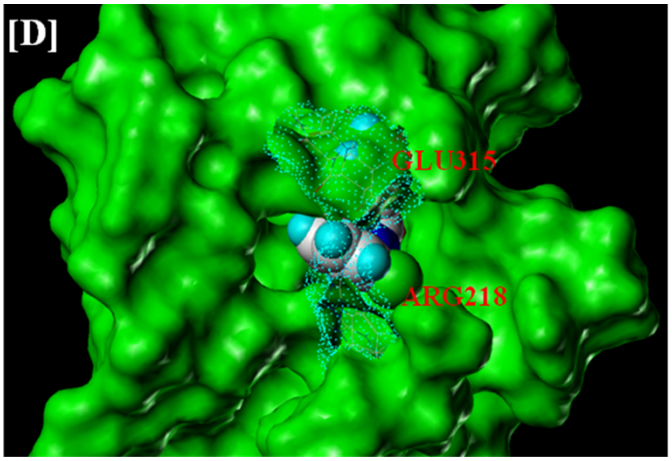


Figure 7. The detailed docking results of NCH and BSA.

[A]: The configuration of NCH in binding site of BSA. NCH is shown in ball-stick model, while Trp237 we concerned are showed in the red circle. All hydrogen bonds are showed as yellow dashed lines. [B]: The illustration of hydrogen bonds and the conformation of Trp237 and NCH. NCH is shown in ball-stick model. [C]:The align of NCH with the protomol. There are three kinds of probe: CH_4 for the hydrophobicity, C=O for hydrophilicity and hydrogen bond acceptor and N-H for hydrophilicity and hydrogen bond donor and acceptor. [D]:The illustration of the obstacle (blue dot ARG218 and GLU315 surface) in the entrance pathway of NCH into the binding site.