

## Supporting information

### Binding Mode Investigations on the Interaction of lead (II) Acetate with Human Chorionic Gonadotropin

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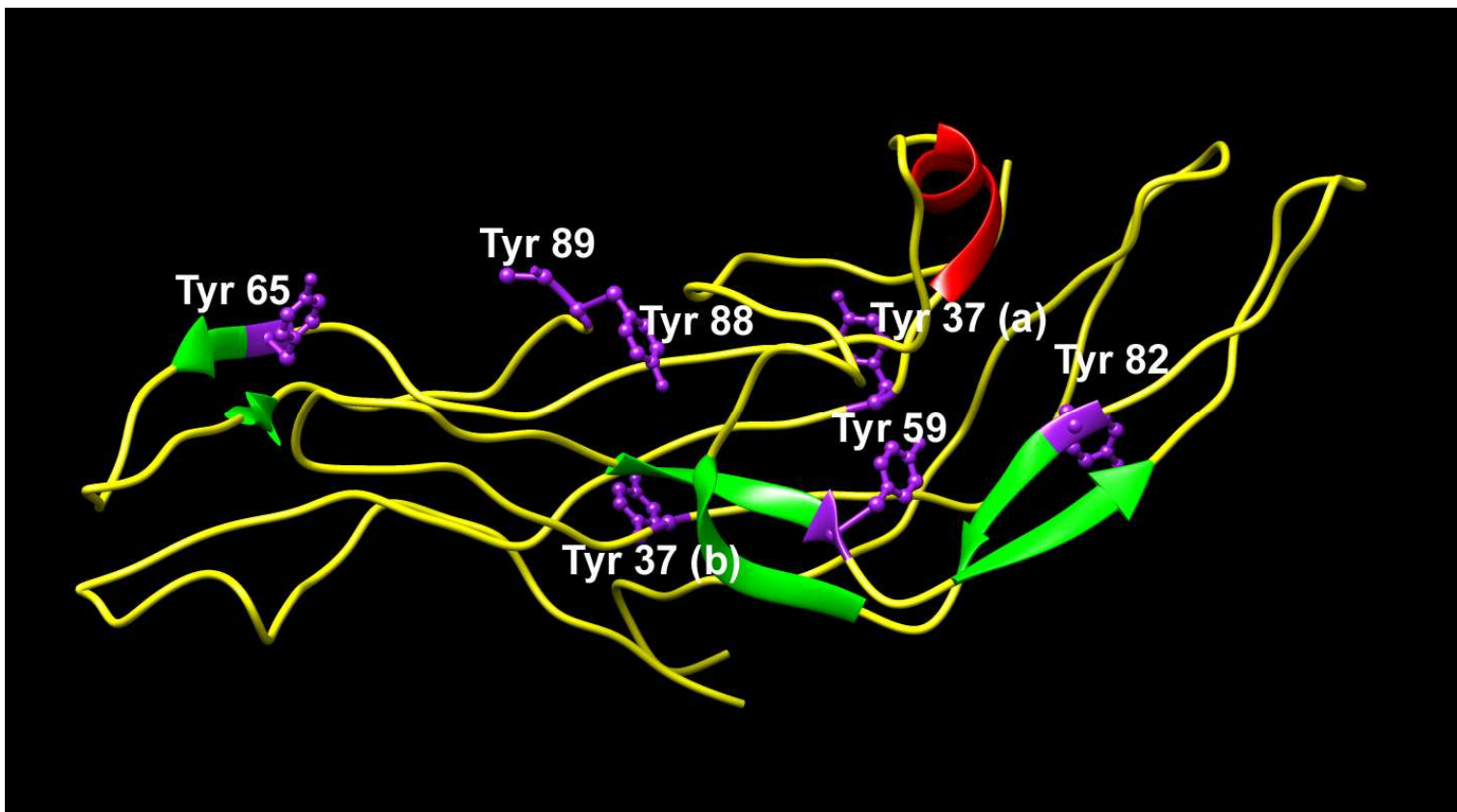
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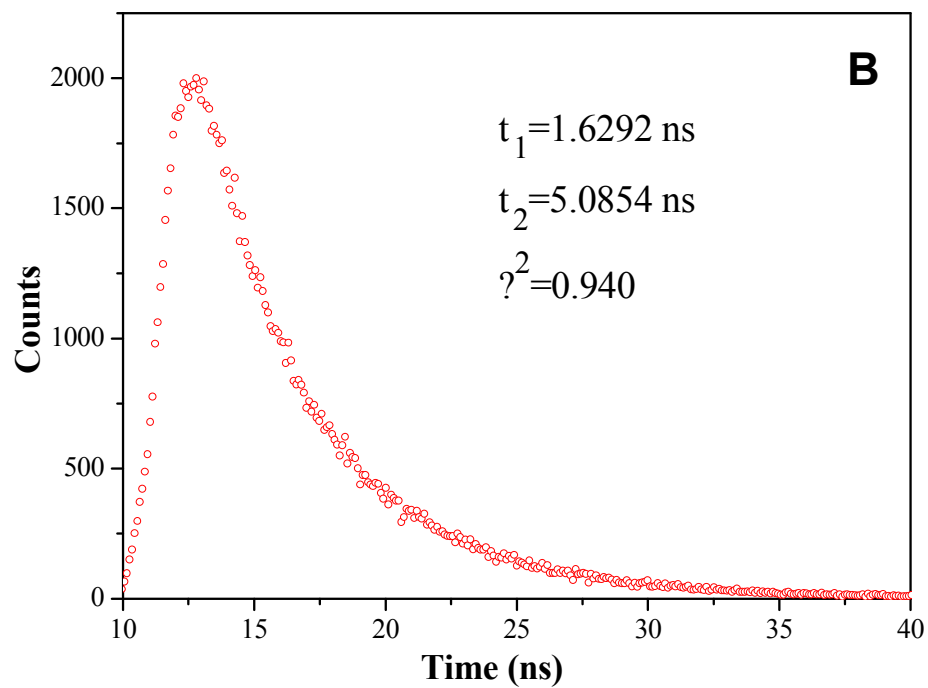
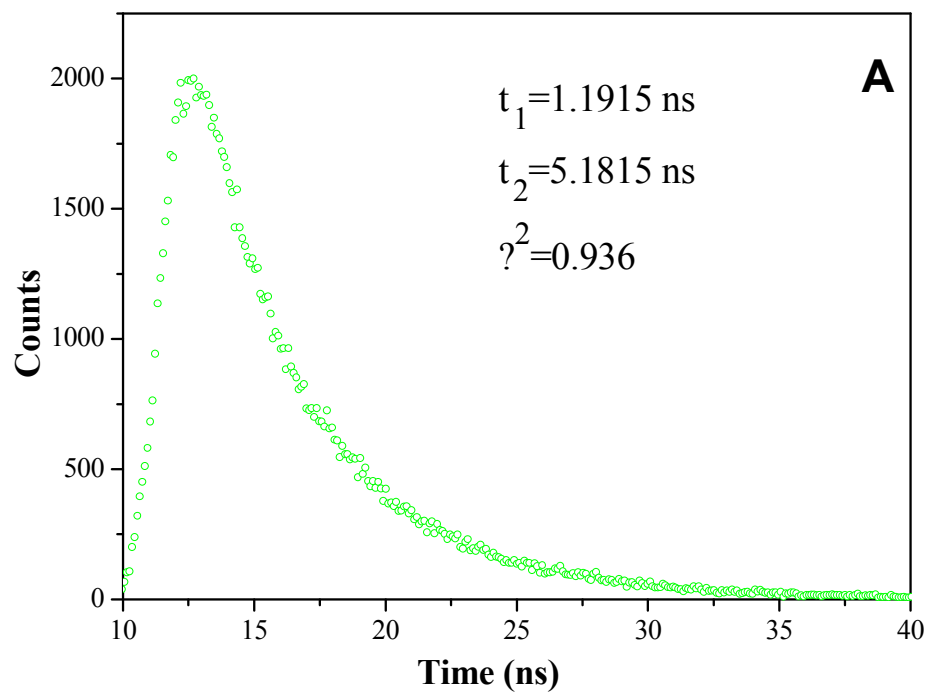
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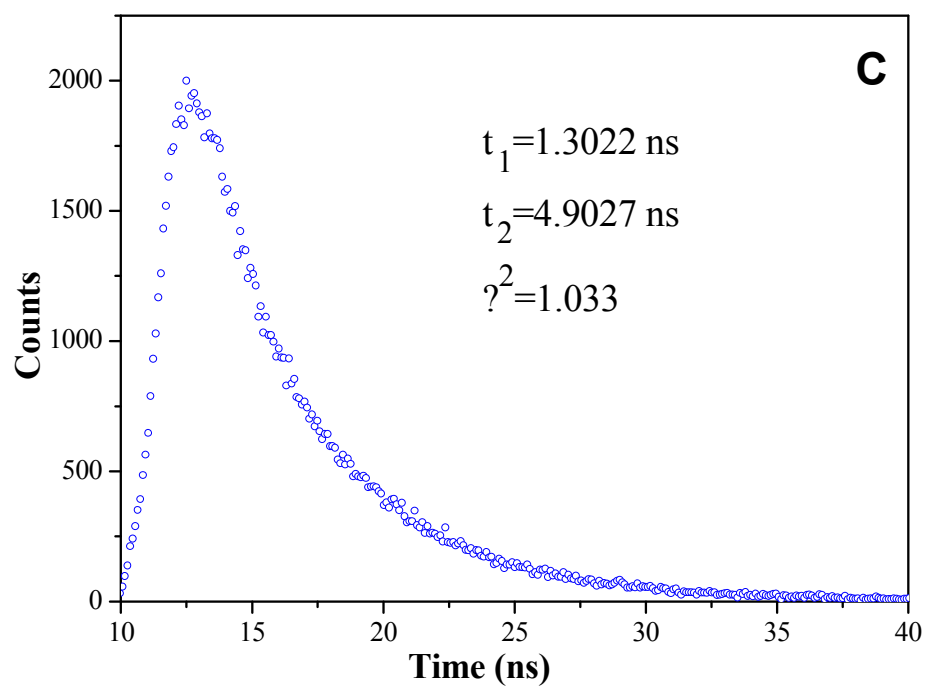
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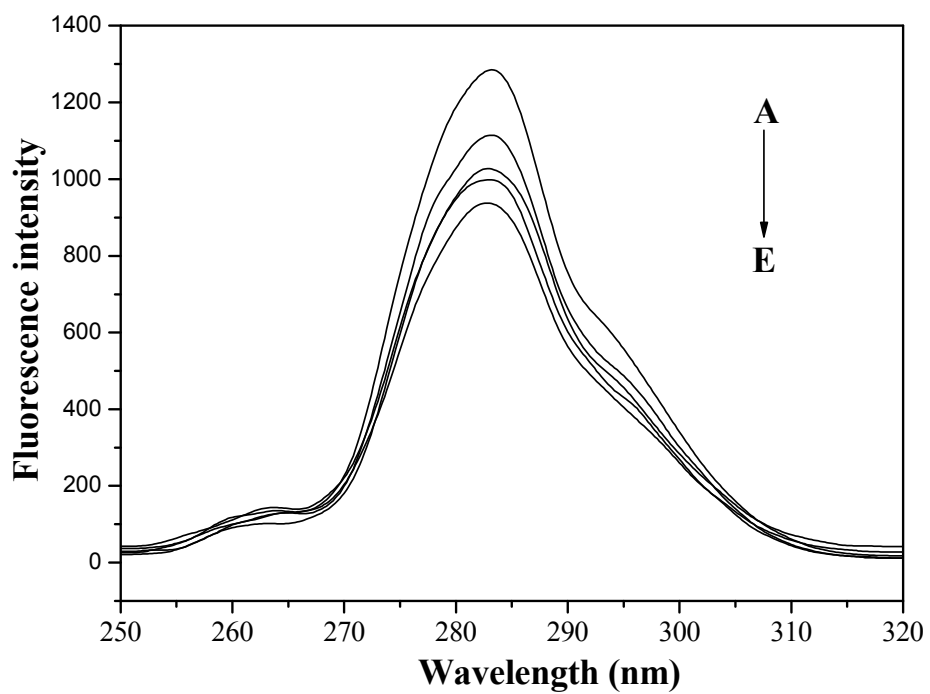


**Fig. S1: Molecular structure of HCG (PDB code 1HRP). Different types of the secondary structure of HCG are color-coded as follows:  $\alpha$ -helix: red,  $\beta$ -pleated sheet: green,  $\beta$ -turn and random coil: yellow. Tyr residues are also marked in purple.**

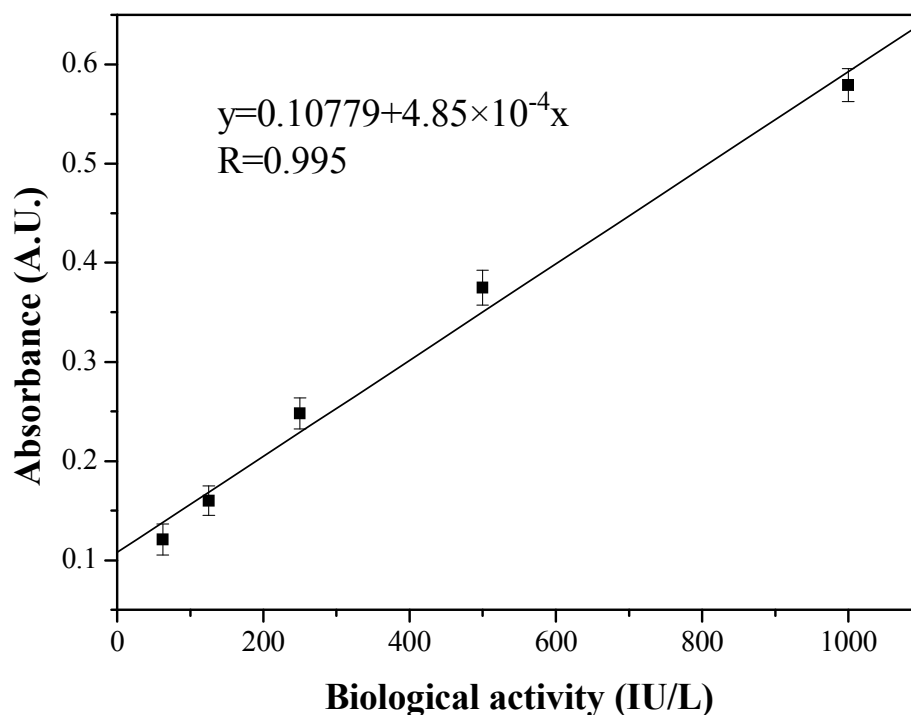




**Fig. S2: Time-resolved fluorescence decay profiles of HCG in the presence of lead.**  
**Conditions: HCG:  $2.7 \times 10^{-6}$  mol/L;  $\text{Pb}(\text{Ac})_2 / (10^{-5}$  mol/L) (a-e): 0, 4, 10; pH=5.5;**  
**T=298 K.**



**Fig. S3:** synchronous fluorescence spectra ( $\Delta\lambda = 15$  nm) of HCG in the presence of lead acetate. Conditions: HCG:  $2.7 \times 10^{-6}$  mol/L;  $\text{Pb}(\text{Ac})_2 / (10^{-5}$  mol/L) (a-e): 0, 1, 4, 7, 10; pH=5.5; T=298 K.



**Fig. S4: Standard curve of HCG biological activities in the range of 0-1000 IU/L by ELISA.**

**S5: Why lead acetate ( $\text{Pb}(\text{Ac})_2$ ) has been chosen for this study?**

There are three soluble lead salts:  $\text{Pb}(\text{Ac})_2$ ,  $\text{PbCl}_2$ ,  $\text{Pb}(\text{NO}_3)_2$ , which can be easily bought. We also need to choose proper buffer solutions to control acidity in the experiments.  $\text{Pb}(\text{NO}_3)_2$  is an explosive and reactive compound, So  $\text{Pb}(\text{Ac})_2$  with HAc-NaAc and  $\text{PbCl}_2$  with Tris-HCl seem the reasonable choices used in this work, because lead toxicity is what we care about.  $\text{PbCl}_2$  is poorly soluble in Tris-HCl (pH=7.4) solution, and  $\text{Pb}(\text{Ac})_2$  is easily soluble in HAc-NaAc buffer. At last we choose  $\text{Pb}(\text{Ac})_2$  in our study.

The isoelectric point of HCG is 2.95, so HCG is negatively charged in our experiments (pH=5.5), and the acetate anion can poorly affect the HCG conformation in our opinion. Considering these factors above,  $\text{Pb}(\text{Ac})_2$  with HAc-NaAc was selected in our study.