## **Electronic Supplementary Information**

## Structural characterization and pharmacological assessment in

## vitro / in vivo on a new copper(II)-based derivative of enrofloxacin

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Figure S1. The FT-IR spectra of Enrofloxacin (H-EFX) (upper) and EFX-Cu (bottom).



Figure S2. The packing diagram of the crystal structure of the EFX-Cu.



Figure S3. The ESI-MS spectrum of EFX.



**Figure S3**. The ESI-MS spectra of the EFX-Cu in the low resolution (upper) and high resolution (lower) mode, respectively, both of which indicating the coordinated species of EFX-Cu.



**Figure S4**. The time-dependent UV-Vis spectra of the EFX-Cu to indicate its stability in aqueous solution at room temperature.



Figure S5-A. The in vitro antibacterial effect of EFX towards five typical pathogenic bacteria .



Figure S5-B. The in vitro antibacterial effect of EFX-Cu towards five typical pathogenic bacteria.



**Figure S6**. The antibacterial activity of EFX and its copper(II) complex, EFX-Cu, represented by the MIC and MBC values ( $\mu$ g/mL).



**Figure S7**. The development status of the wild-type AB zebrafish in each group incubated with different concentration of EFX-Na.





**Figure S8**. The ROS production in the hepatocyte cell line HL-7702 (upper) and the lung fibroblast cell line L-929 (lower) induced different concentrations of EFX-Na, reflected by the quantitative emission intensity of the green fluorescence.

|         | Incubated concentrations of EFX-Cu for each group (µmol/L) |       |       |       |       |        |
|---------|--|-------|-------|-------|-------|--------|
| EFX-Na  | Control  | 0.01  | 0.1   | 1     | 10    | 20     |
|         | Survival (death) of zebrafish                              |       |       |       |       |        |
| 24 hpf  | 28(2)  | 30(0) | 26(4) | 28(2) | 30(0) | 30(0)  |
| 48 hpf  | 28(2)  | 30(0) | 26(4) | 26(4) | 30(0) | 26(4)  |
| 72 hpf  | 28(2)  | 30(0) | 26(4) | 24(6) | 30(0) | 10(20) |
| 96 hpf  | 28(2)  | 30(0) | 26(4) | 24(6) | 30(0) | 10(20) |
| 120 hpf | 28(2)  | 30(0) | 26(4) | 24(6) | 30(0) | 6(24)  |

**Table S1**. The survival and death of the tested zebrafish in each group incubated with different concentrations of EFX-Na.