

## **Supporting Information**

**for**

### **Selectively Attacking Tumor Cells of Ru/Ir-Arene Complexes Based on Meclofenamic Acid via Cyclooxygenase-2 Inhibition**

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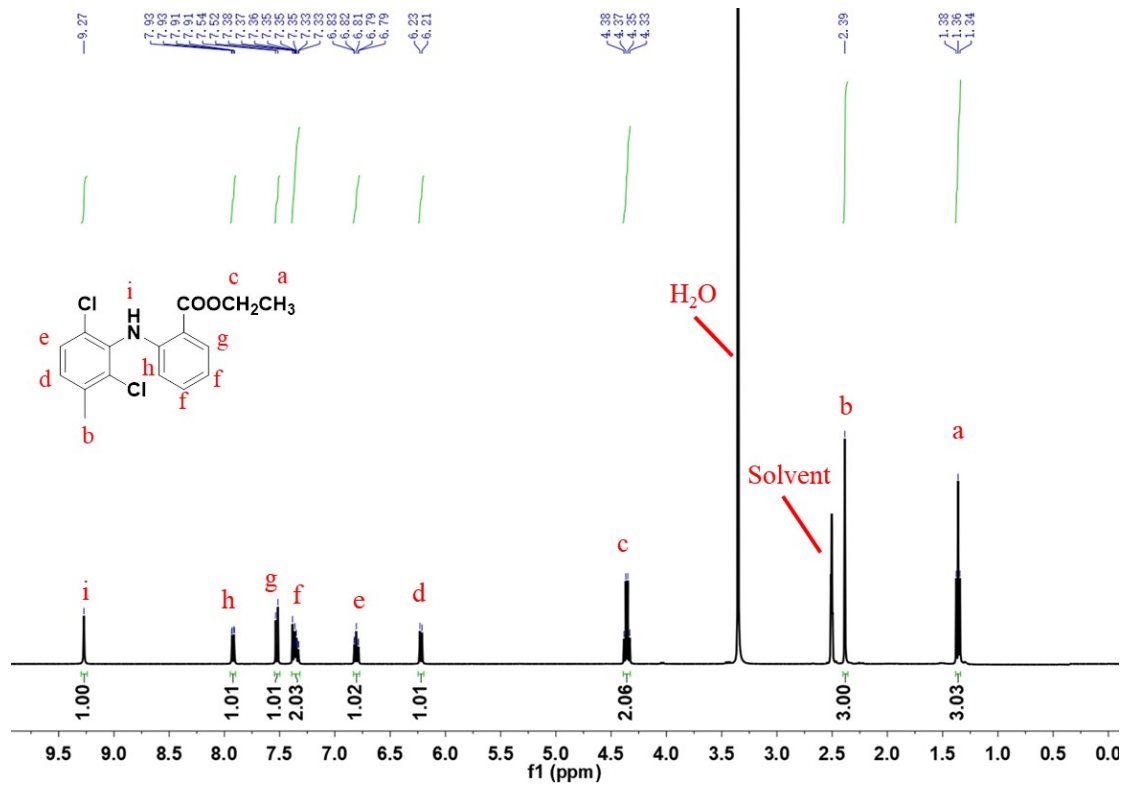


Fig. S1 <sup>1</sup>H NMR spectrum (400 MHz, DMSO-d<sub>6</sub>) of Ethyl melofenarate.

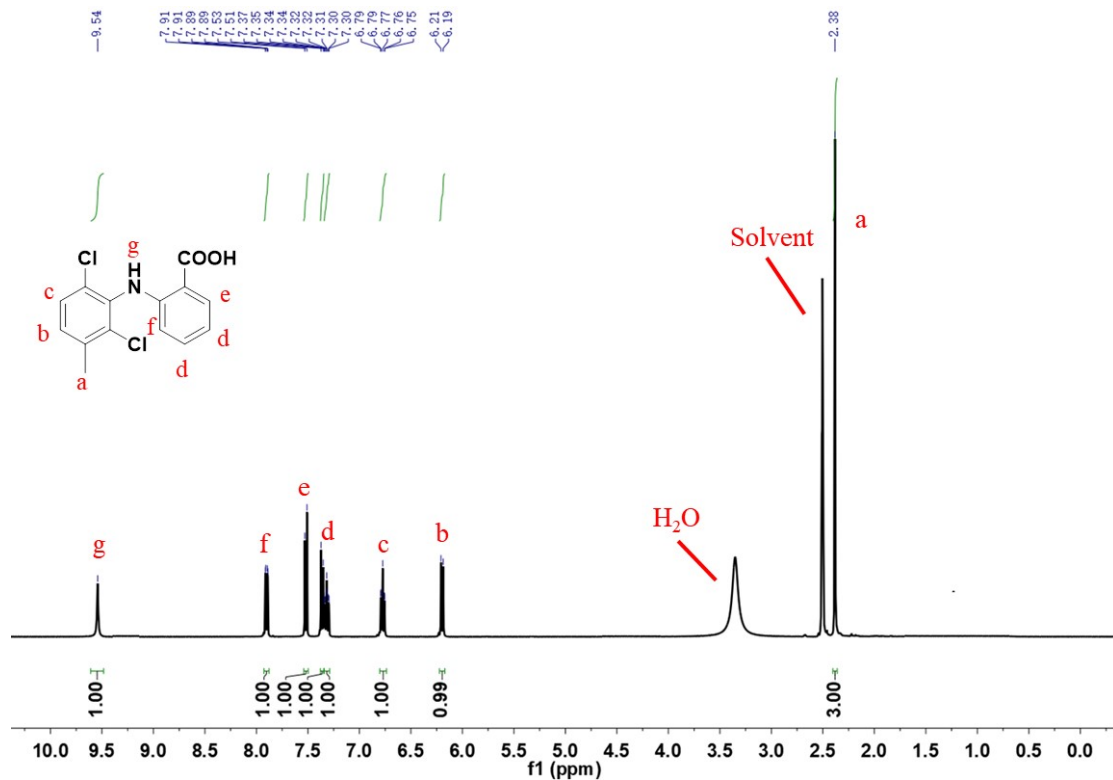


Fig. S2 <sup>1</sup>H NMR spectrum (400 MHz, DMSO-d<sub>6</sub>) of MA.

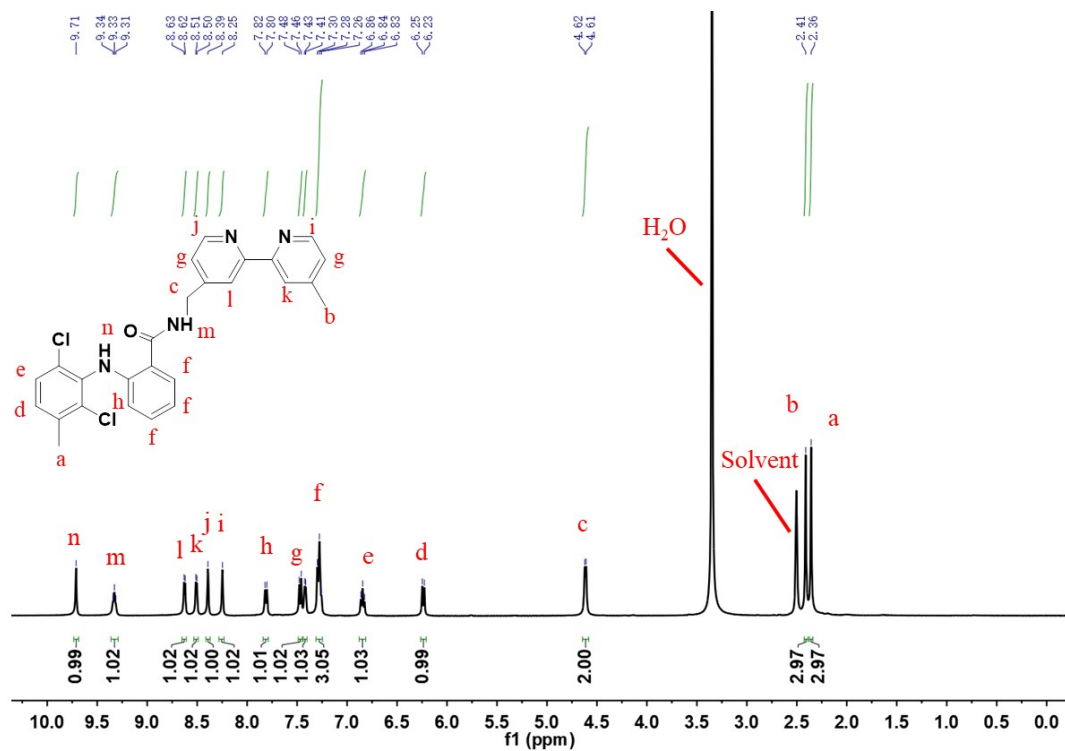


Fig. S3.  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{DMSO-d}_6$ ) of MA-bpy.

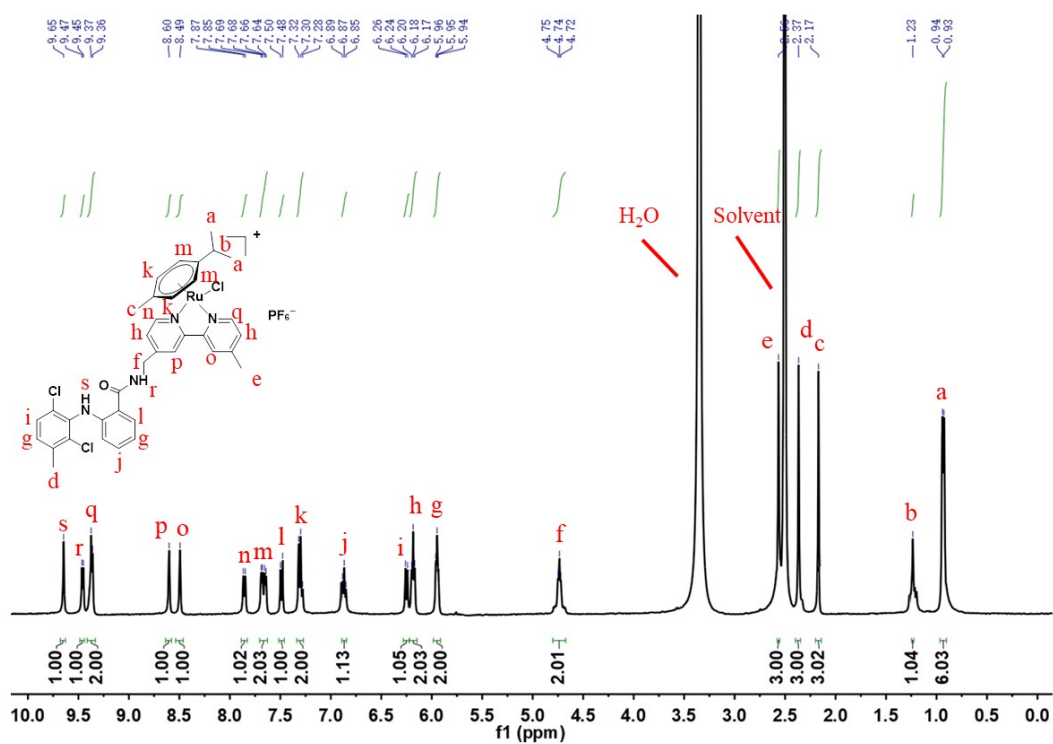


Fig. S4  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{DMSO-d}_6$ ) of MA-bpy-Ru.

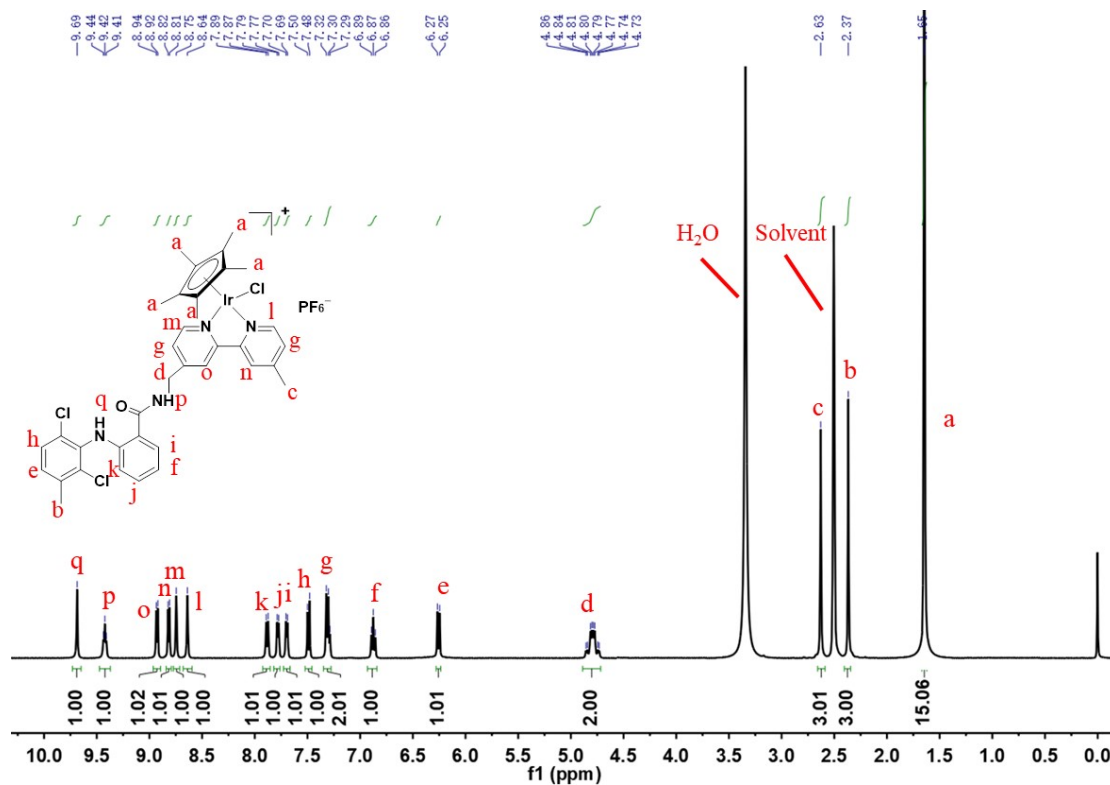


Fig. S5  $^1\text{H}$  NMR spectrum (400 MHz, DMSO- $d_6$ ) of MA-bpy-Ir.

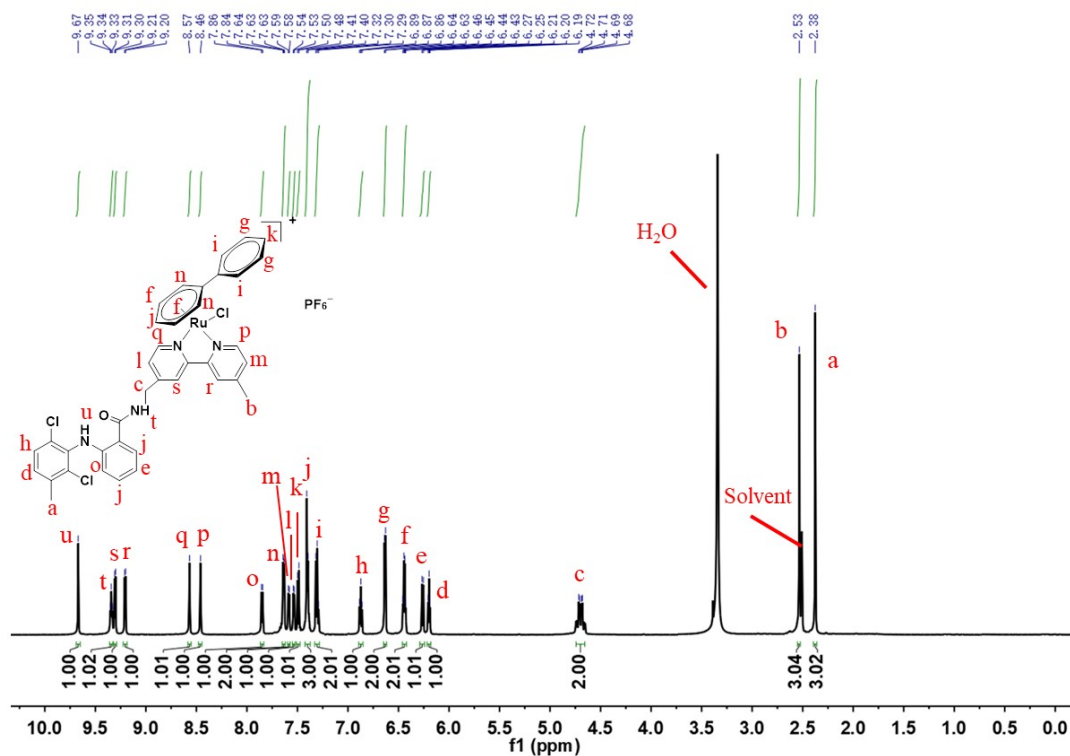


Fig. S6  $^1\text{H}$  NMR spectrum (600 MHz, DMSO- $d_6$ ) of MA-bip-Ru.

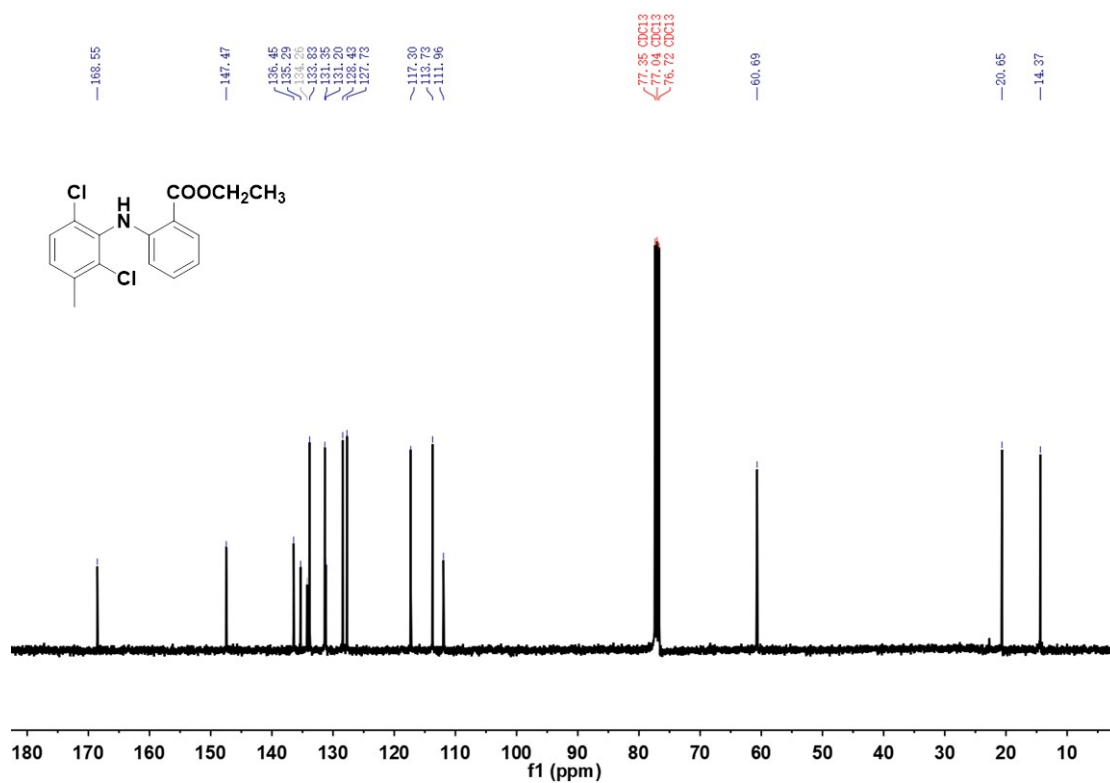


Fig. S7  $^{13}\text{C}$  NMR spectrum (101 MHz,  $\text{CDCl}_3$ ) of Ethyl melofenarate.

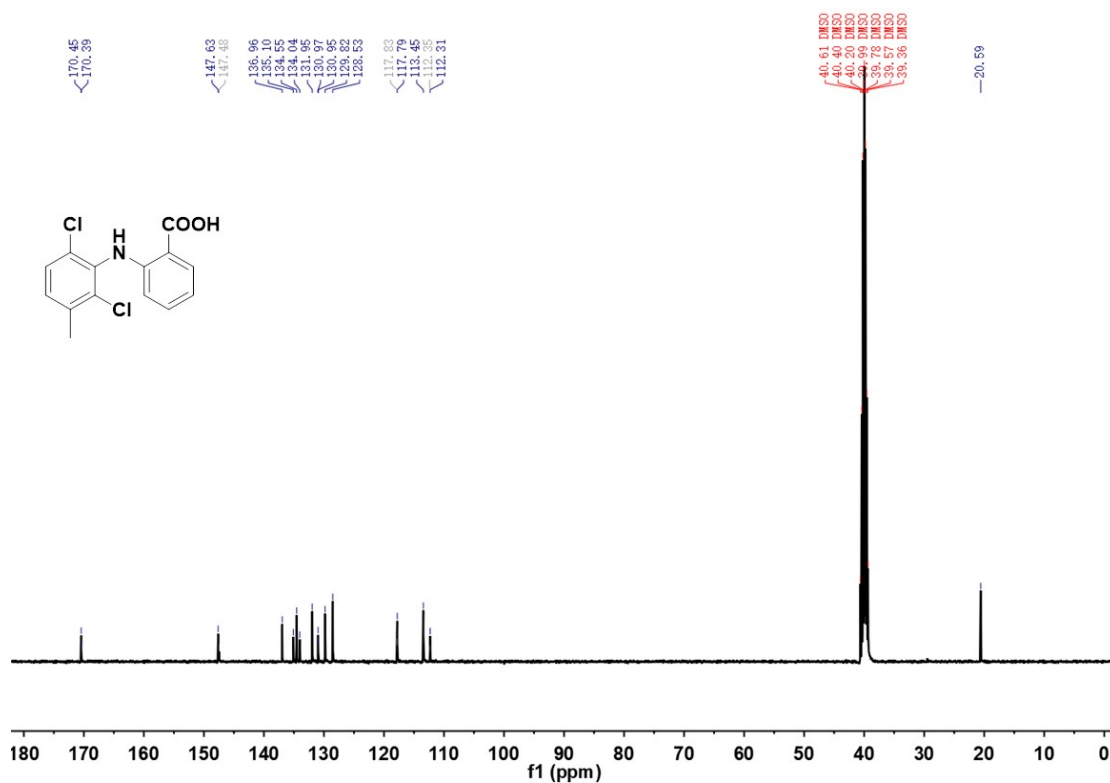


Fig. S8  $^{13}\text{C}$  NMR spectrum (101 MHz,  $\text{DMSO-d}_6$ ) of MA.

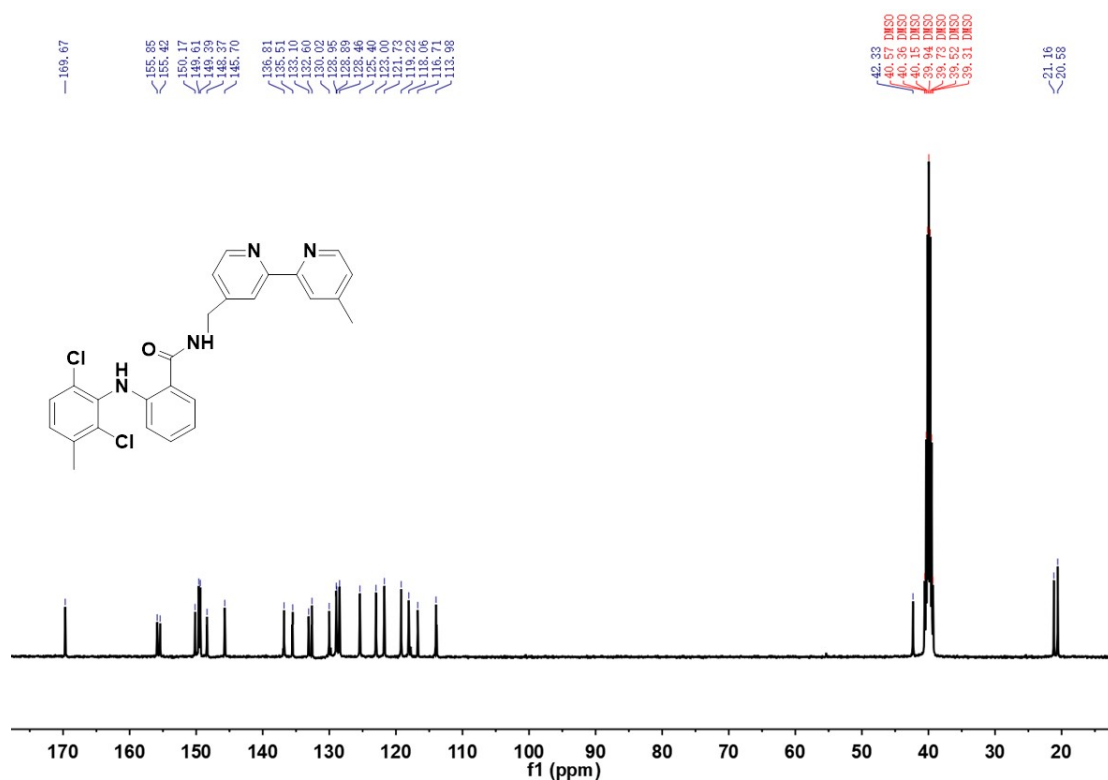


Fig. S9  $^{13}\text{C}$  NMR spectrum (101 MHz, DMSO- $d_6$ ) of MA-bpy.

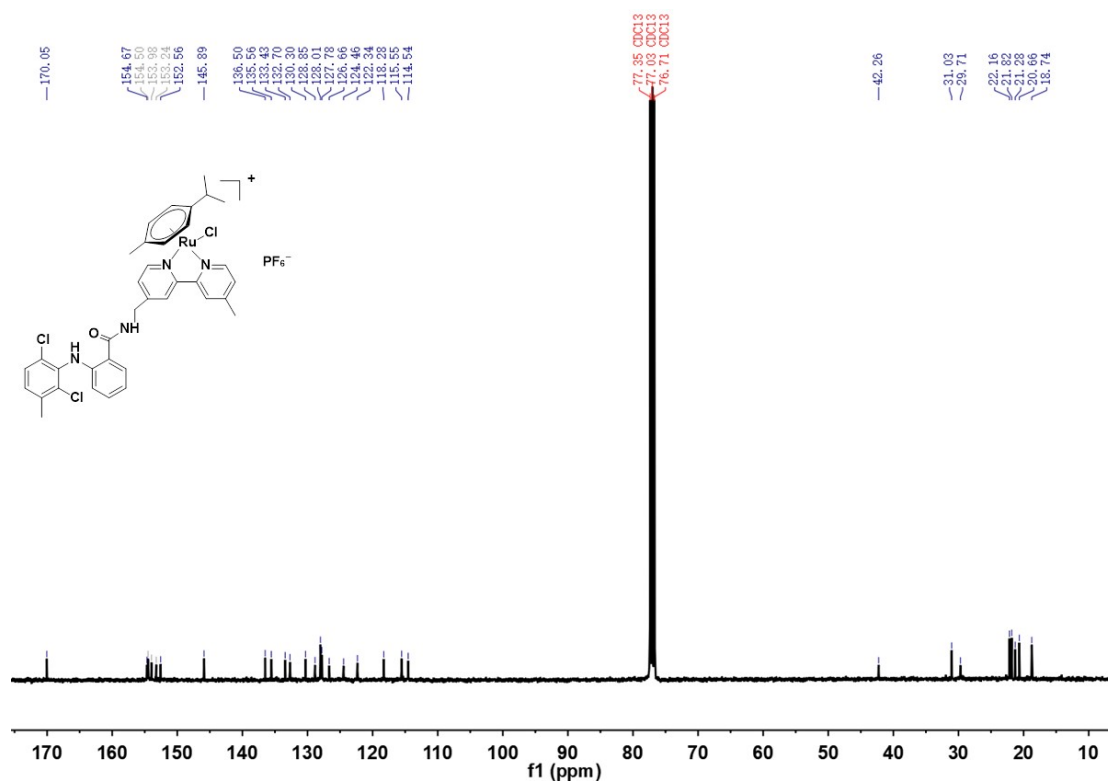


Fig. S10  $^{13}\text{C}$  NMR spectrum (101 MHz,  $\text{CDCl}_3$ ) of MA-bpy-Ru.

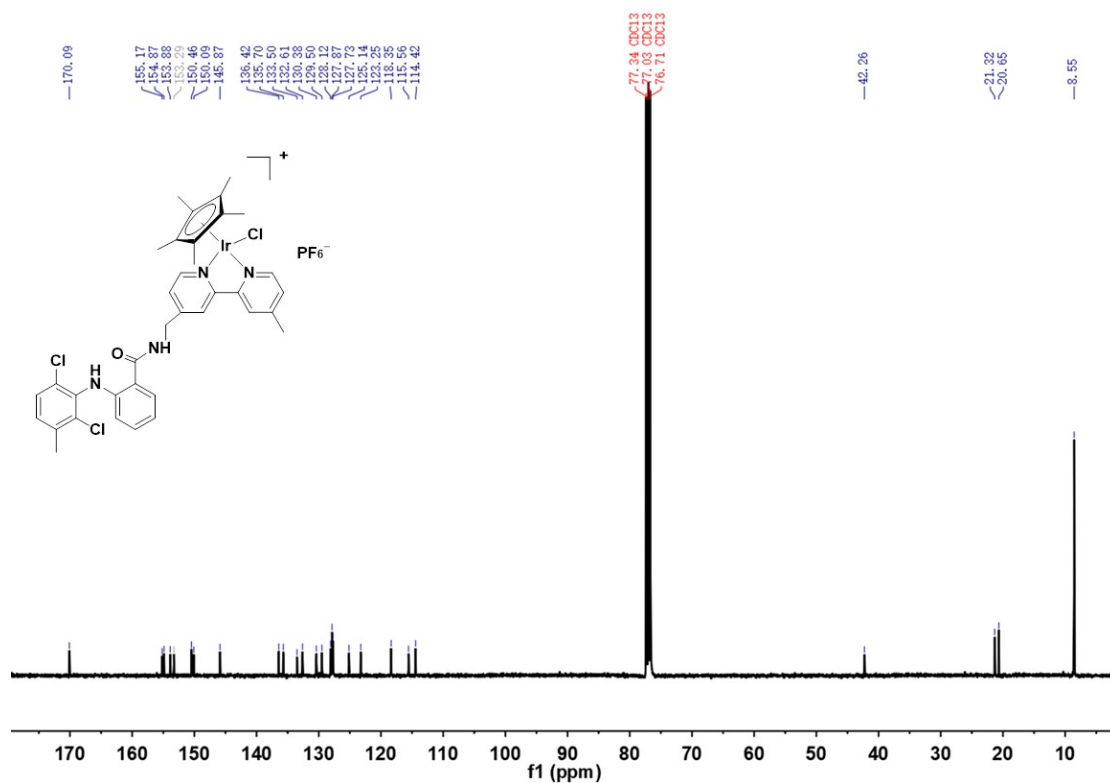


Fig. S11  $^{13}\text{C}$  NMR spectrum (101 MHz,  $\text{CDCl}_3$ ) of MA-bpy-Ir.

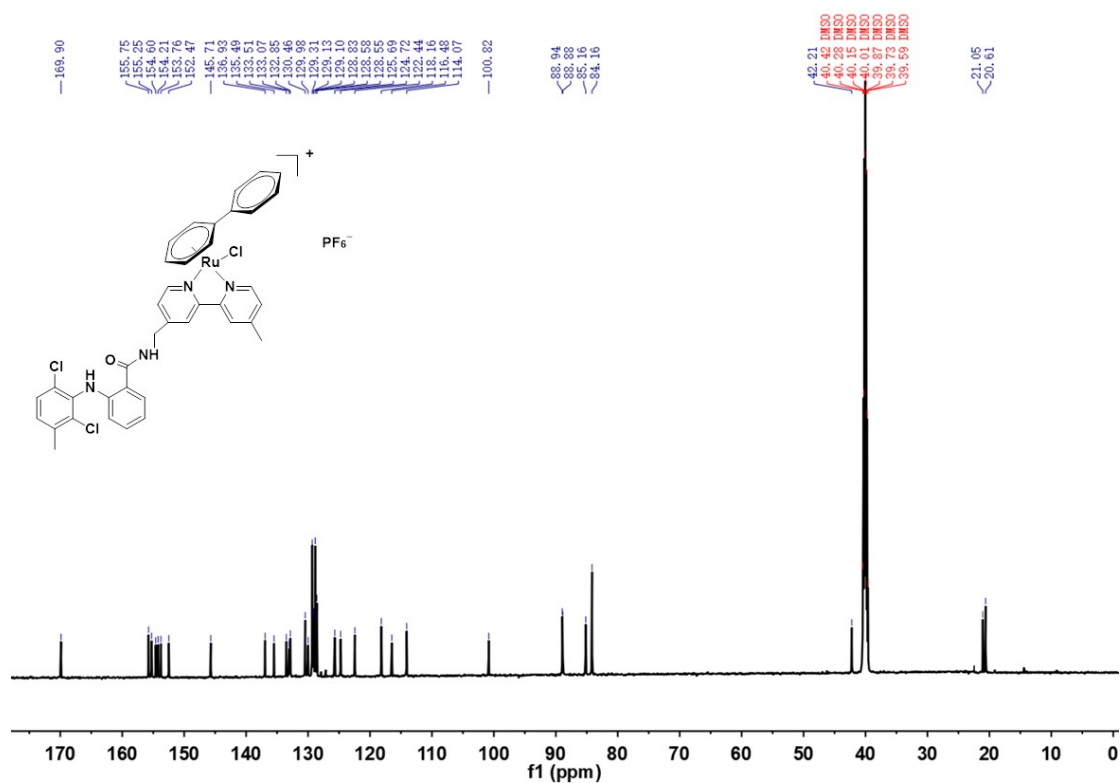


Fig. S12  $^{13}\text{C}$  NMR spectrum (151 MHz,  $\text{DMSO-d}_6$ ) of MA-bip-Ru.



MA-bpy-Ru #12-15 RT: 0.13-0.16 AV: 4 NL: 5.14E8  
T: FTMS + p ESI Full ms [200.0000-1600.0000]

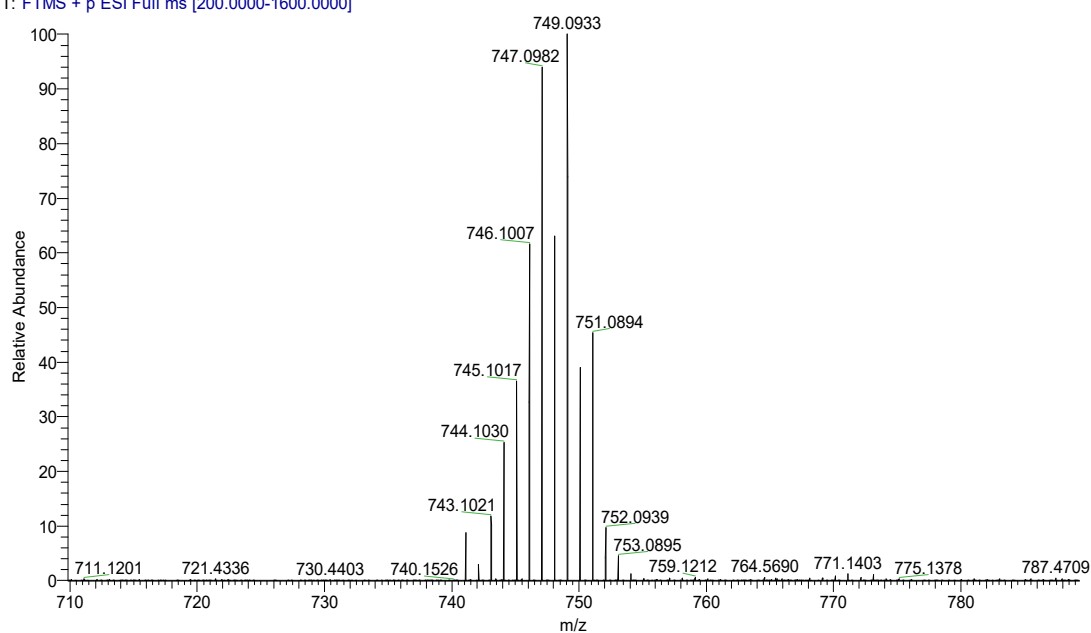


Fig. S13 HR-MS spectra of MA-bpy-Ru in methanol solution.

MA-bpy-Ir #11 RT: 0.13 AV: 1 NL: 7.64E8  
T: FTMS + p ESI Full ms [200.0000-1600.0000]

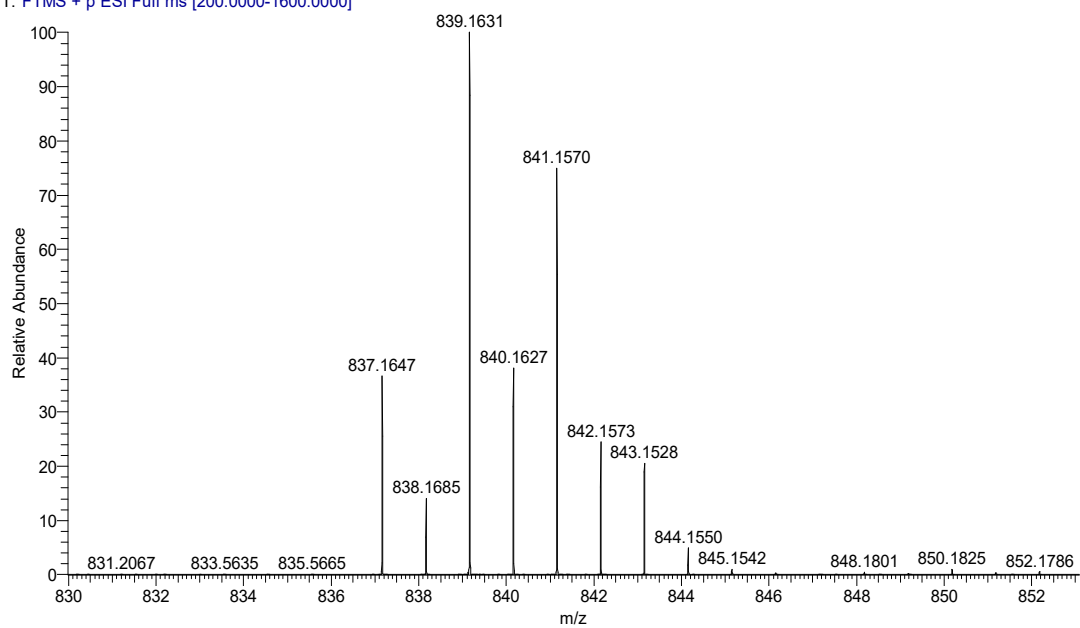


Fig. S14 HR-MS spectra of MA-bpy-Ir in methanol solution.

MA-bipRu #14 RT: 0.15 AV: 1 NL: 3.86E8  
T: FTMS + p ESI Full ms [200.0000-1600.0000]

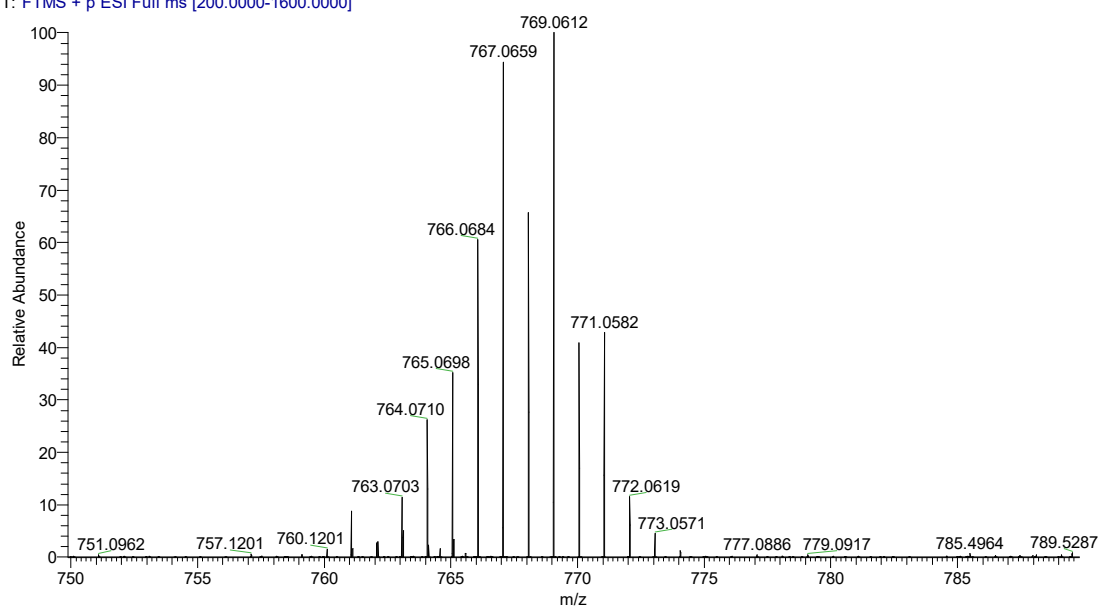


Fig. S15 HR-MS spectra of MA-bip-Ru in methanol solution.

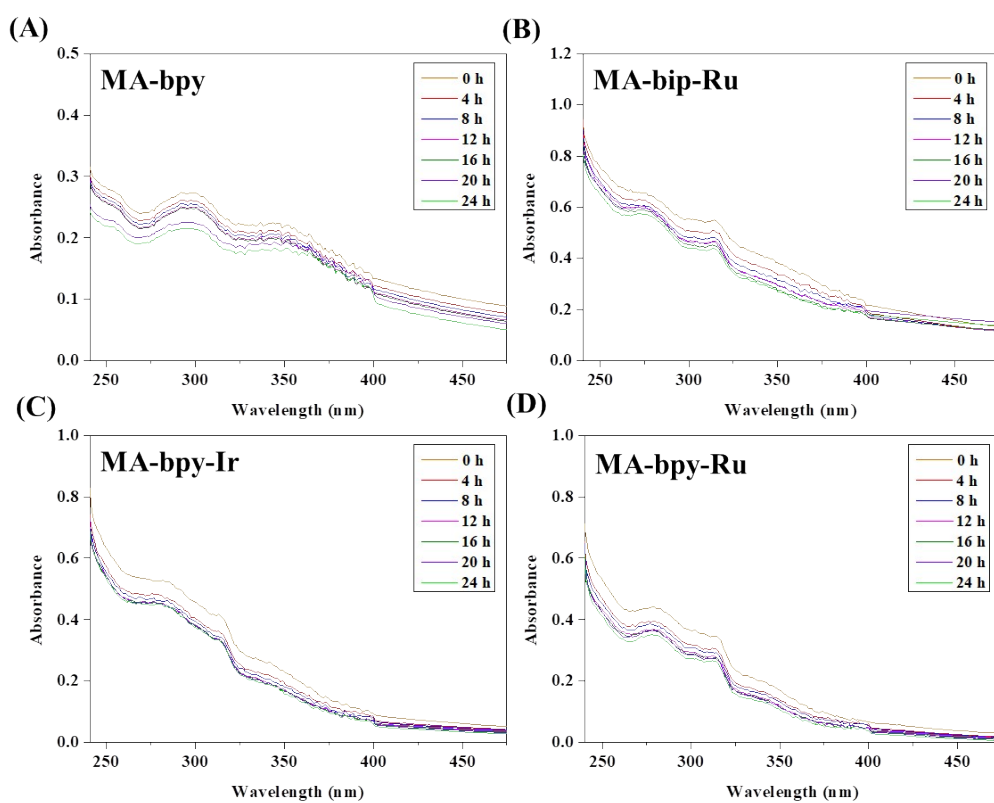


Fig. S16 Stability properties of MA-bpy, MA-bpy-Ru, MA-bpy-Ir and MA-bip-Ru was studied in DMSO/H<sub>2</sub>O solution (5% DMSO) at room temperature.

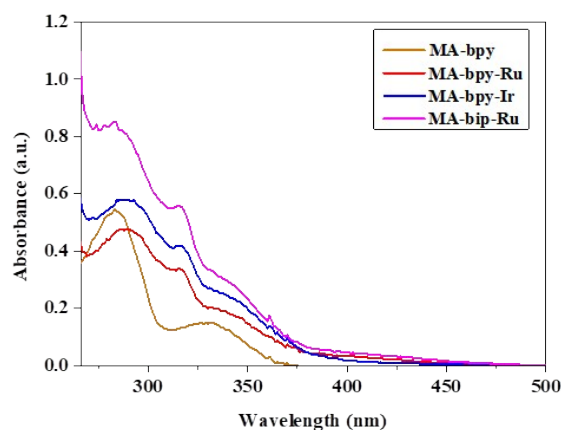


Fig. S17 UV-vis spectra for 30  $\mu\text{M}$  solution of MA-bpy, MA-bpy-Ru, MA-bpy-Ir and MA-bip-Ru in DMSO at room temperature.

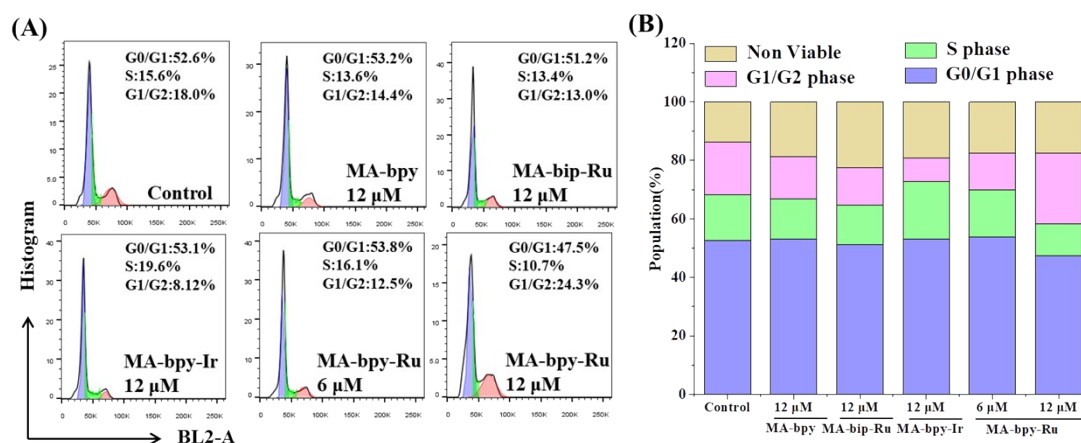


Fig. S18 (A) Cell cycle assay of MCF-7 cells by flow cytometry after incubation with MA-bpy (12  $\mu\text{M}$ ), MA-bip-Ru (12  $\mu\text{M}$ ), MA-bpy-Ir (12  $\mu\text{M}$ ) and MA-bpy-Ru (6  $\mu\text{M}$ , 12  $\mu\text{M}$ ) for 24 h and staining with PI; (B) Corresponding percentages of each phase of the cell cycle.

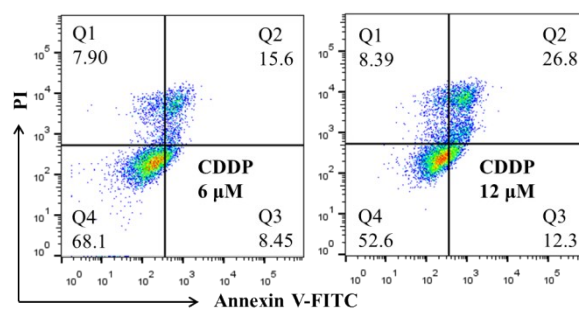
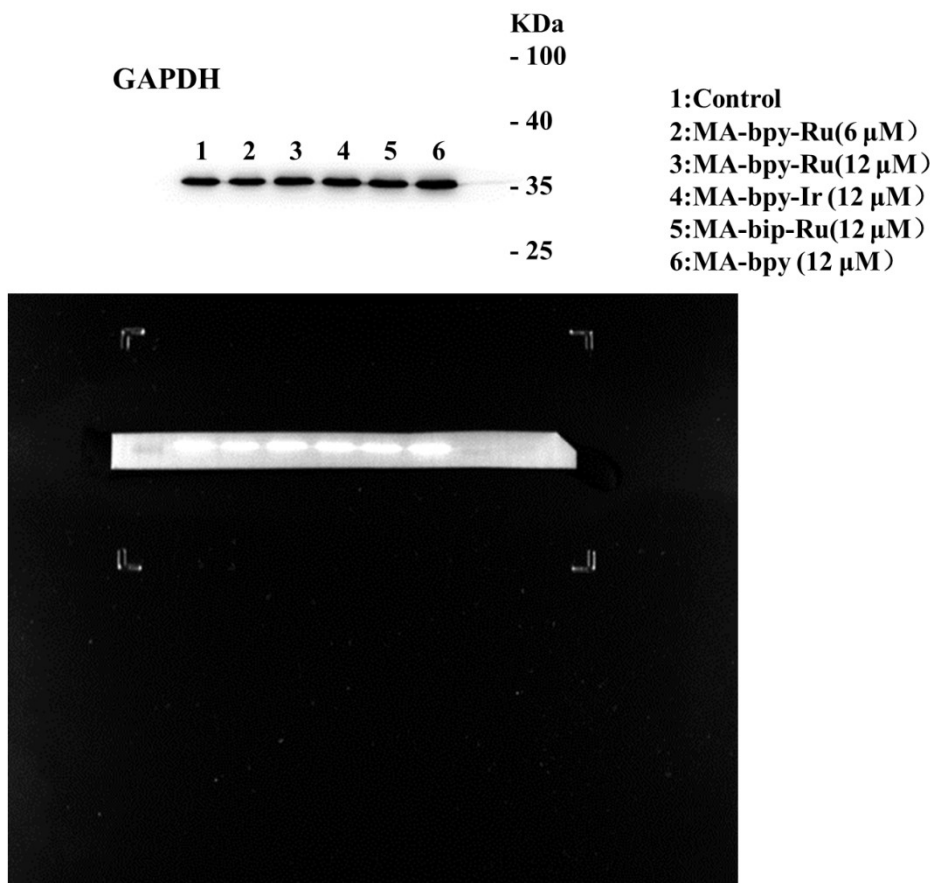
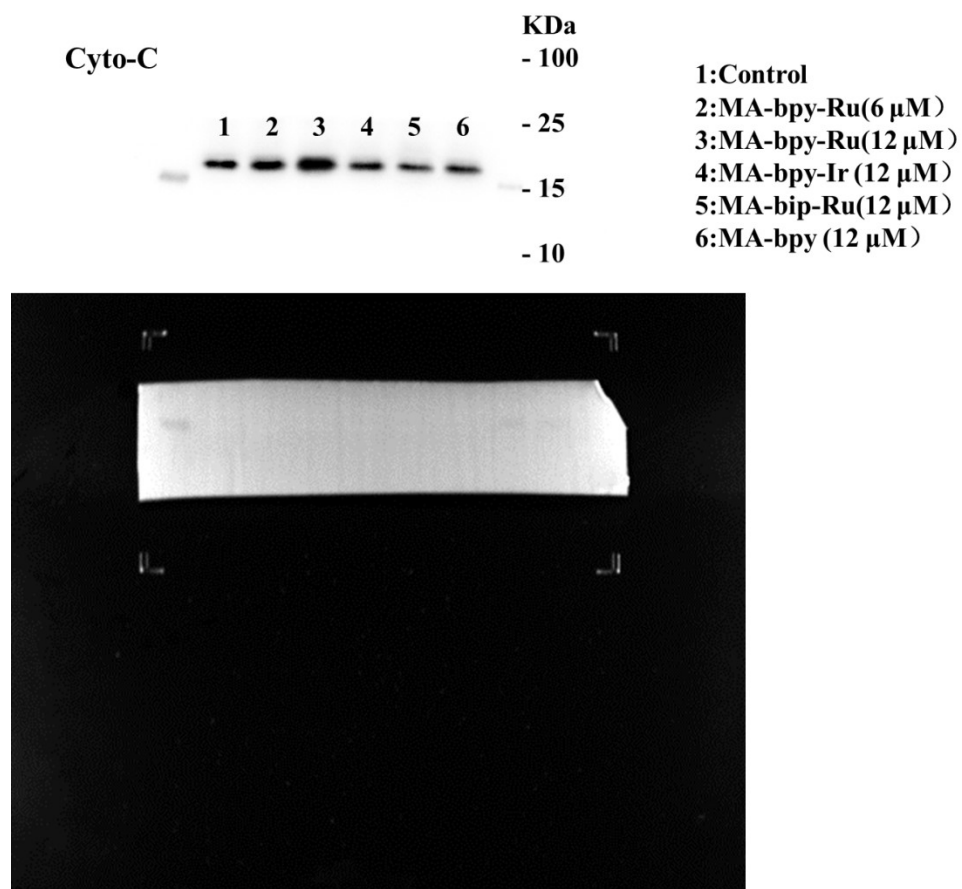
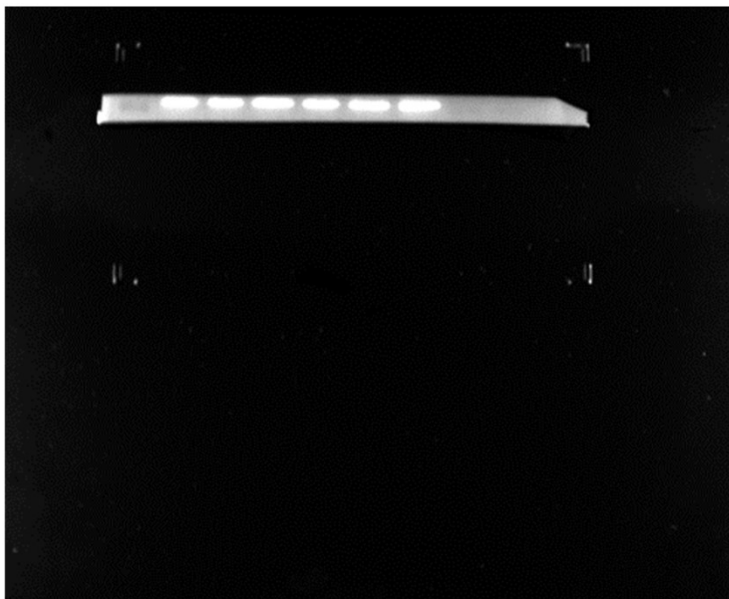
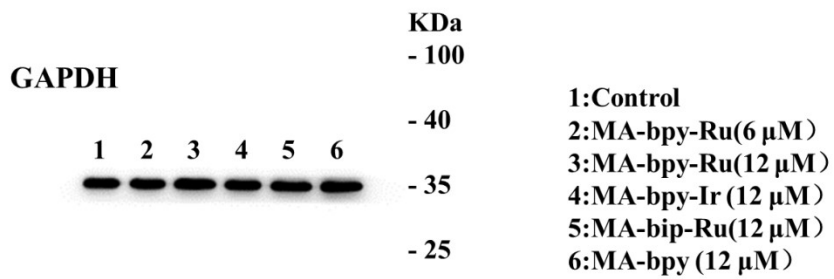
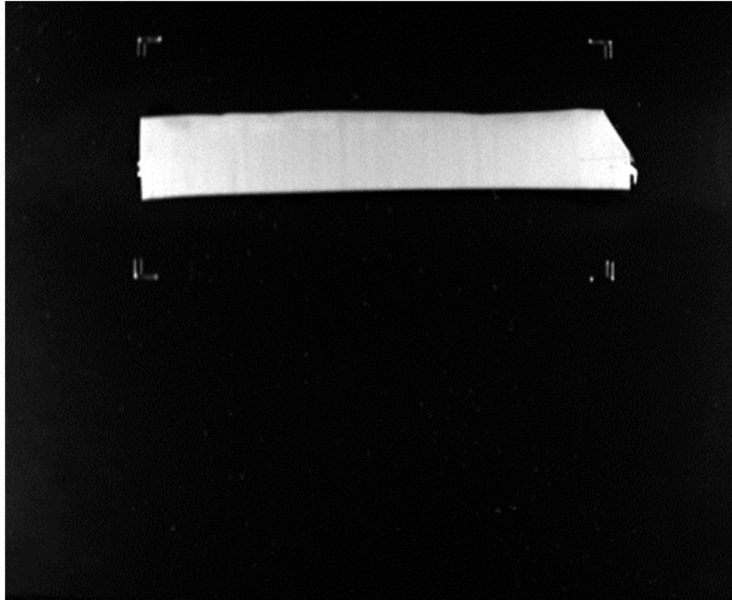
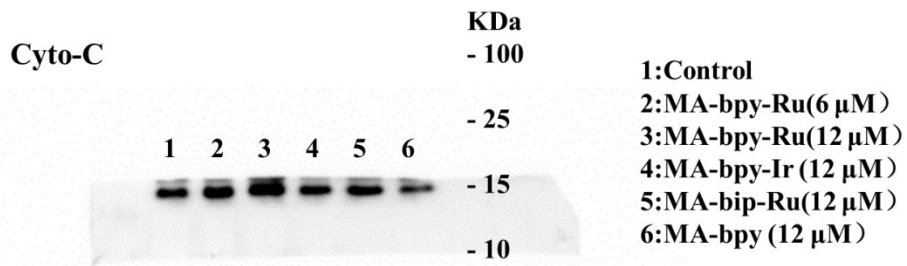


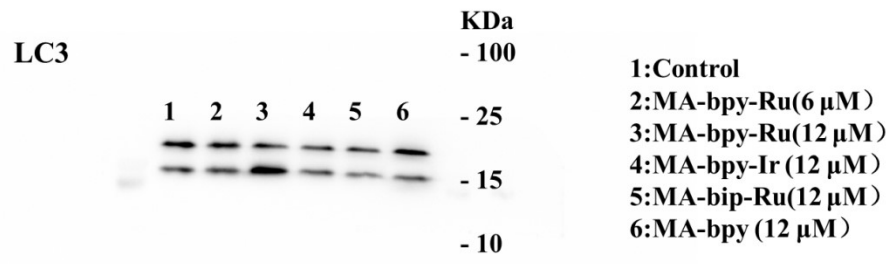
Fig. S19 Apoptotic assays of MCF-7 cells by flow cytometry after incubation with CDDP (6  $\mu\text{M}$ , 12  $\mu\text{M}$ ) for 24 h and staining with Annexin V-FITC and PI.

### 1. Raw blot for Fig. 4 (Cyto-C and LC3)

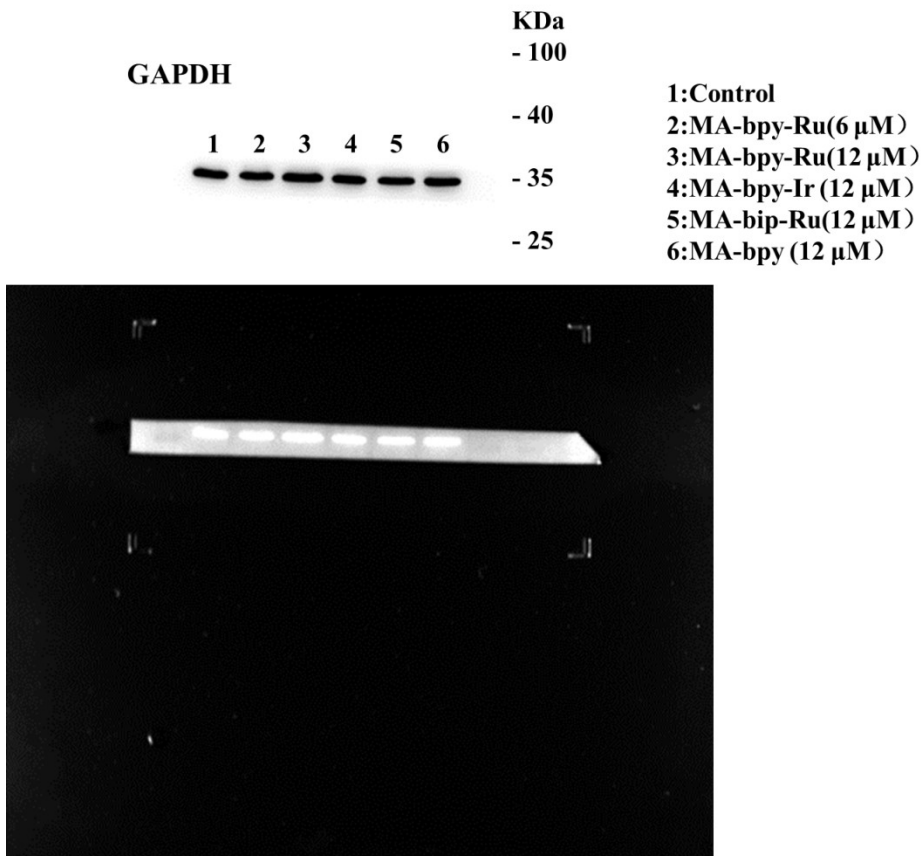
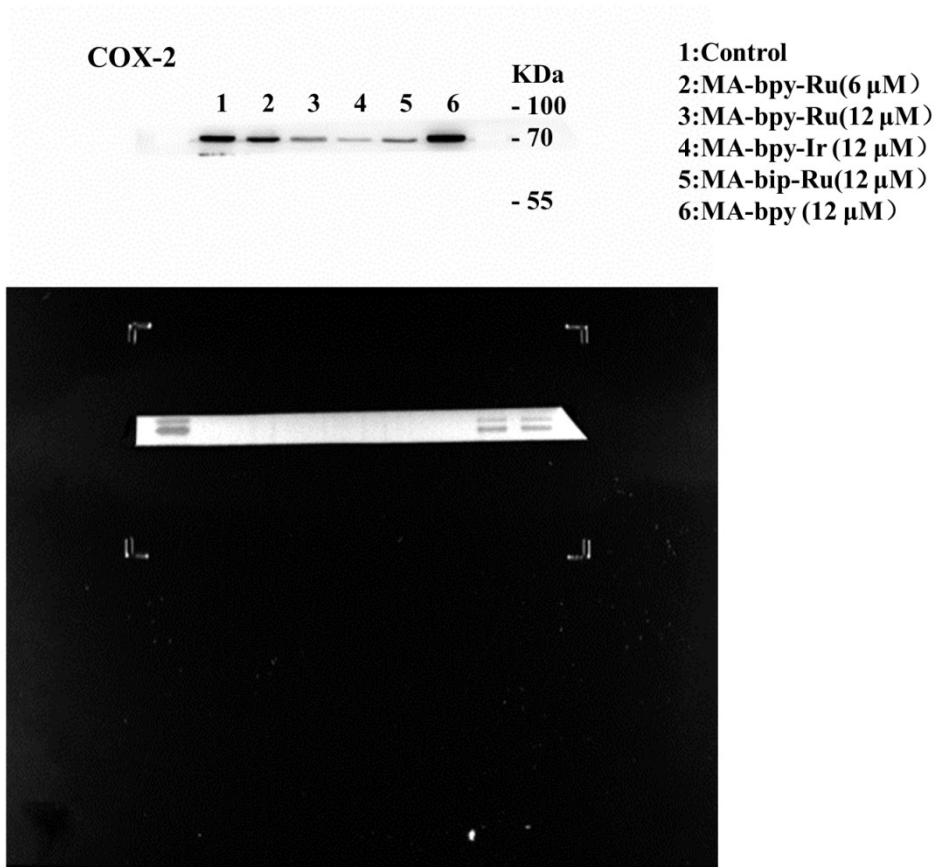








## 2. Raw blot for Fig. 5 (COX-2)



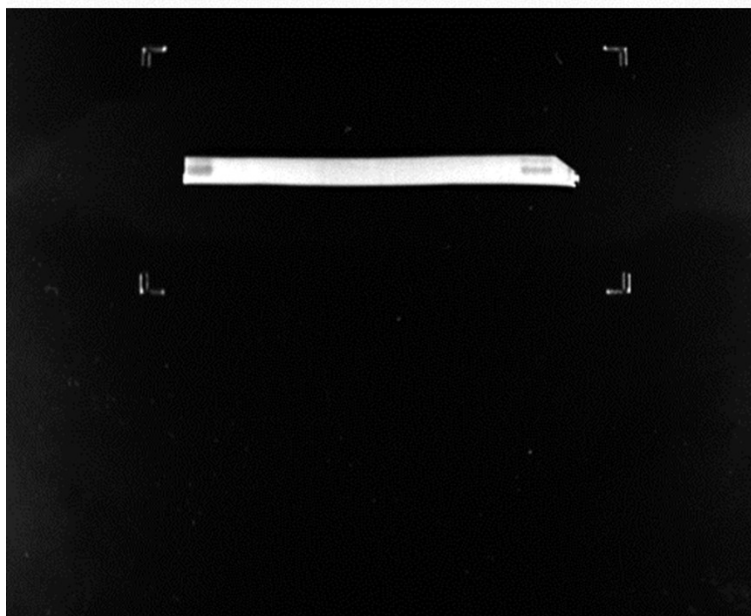


**COX-2**

1 2 3 4 5 6

**KDa**  
- 100  
- 70  
- 55

**1:Control**  
**2:MA-bpy-Ru(6 μM)**  
**3:MA-bpy-Ru(12 μM)**  
**4:MA-bpy-Ir (12 μM)**  
**5:MA-bip-Ru(12 μM)**  
**6:MA-bpy (12 μM)**



**GAPDH**

1 2 3 4 5 6

**KDa**  
- 100  
- 40  
- 35  
- 25

**1:Control**  
**2:MA-bpy-Ru(6 μM)**  
**3:MA-bpy-Ru(12 μM)**  
**4:MA-bpy-Ir (12 μM)**  
**5:MA-bip-Ru(12 μM)**  
**6:MA-bpy (12 μM)**

