

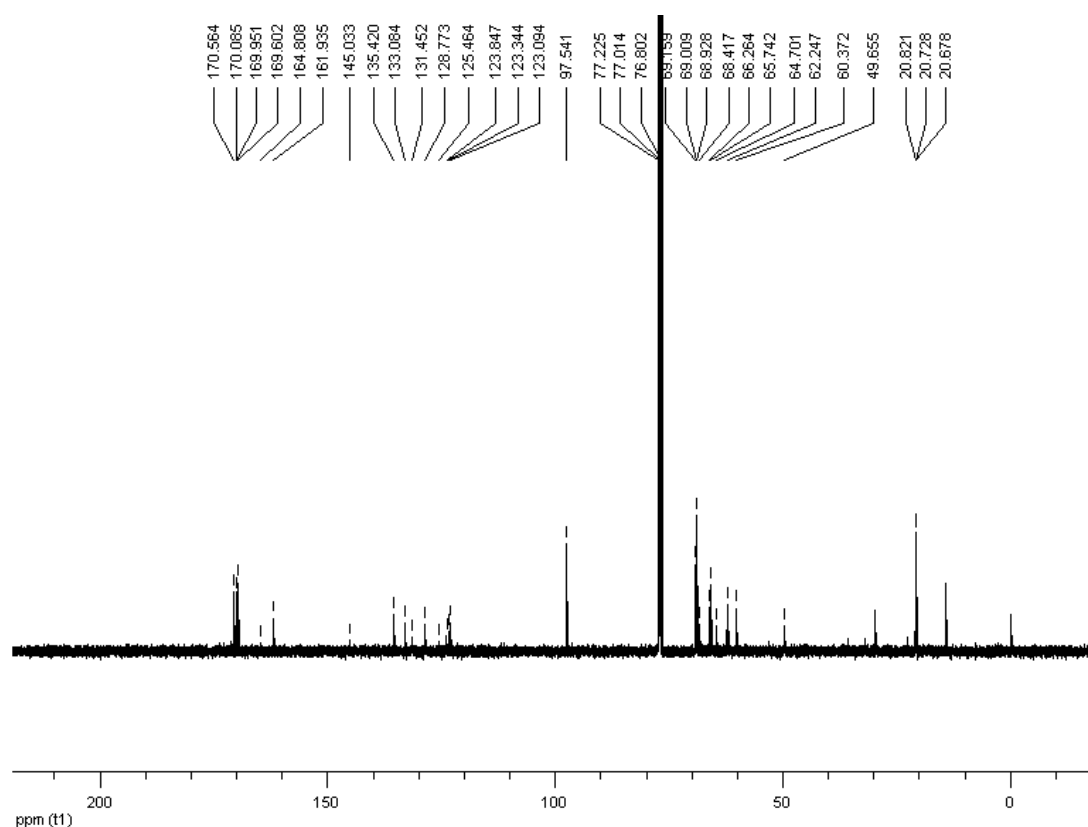


Figure S2. ^{13}C NMR (CDCl_3 , 150 MHz) of compound **PBI-Cl-AcMan**.

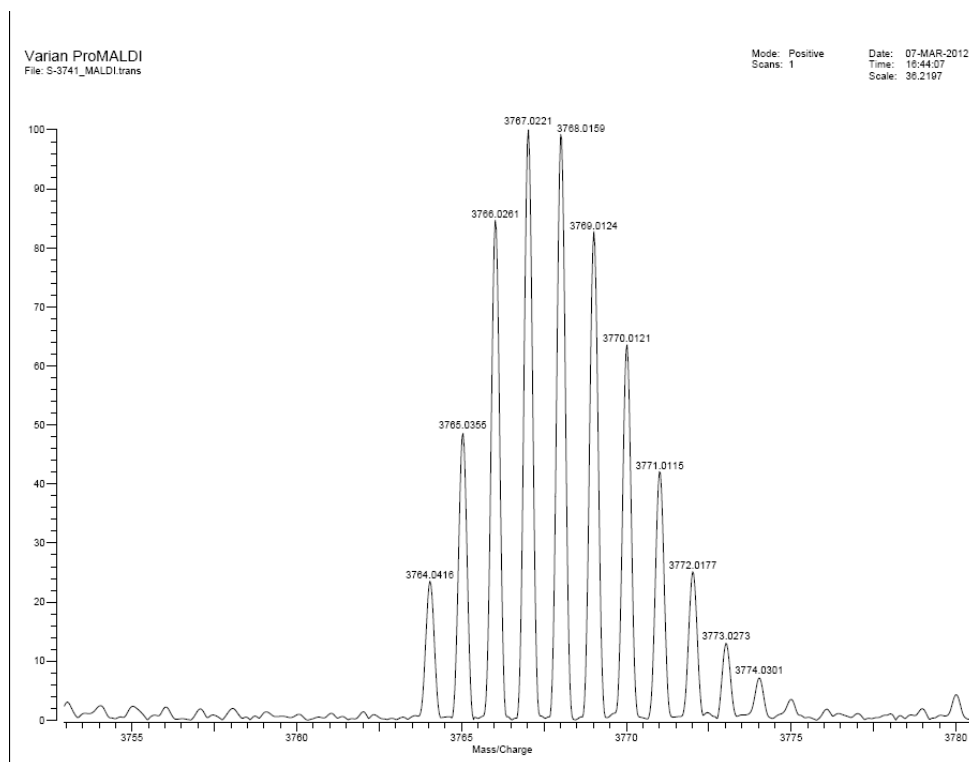


Figure S3. HRMS of compound **PBI-Cl-AcMan**.

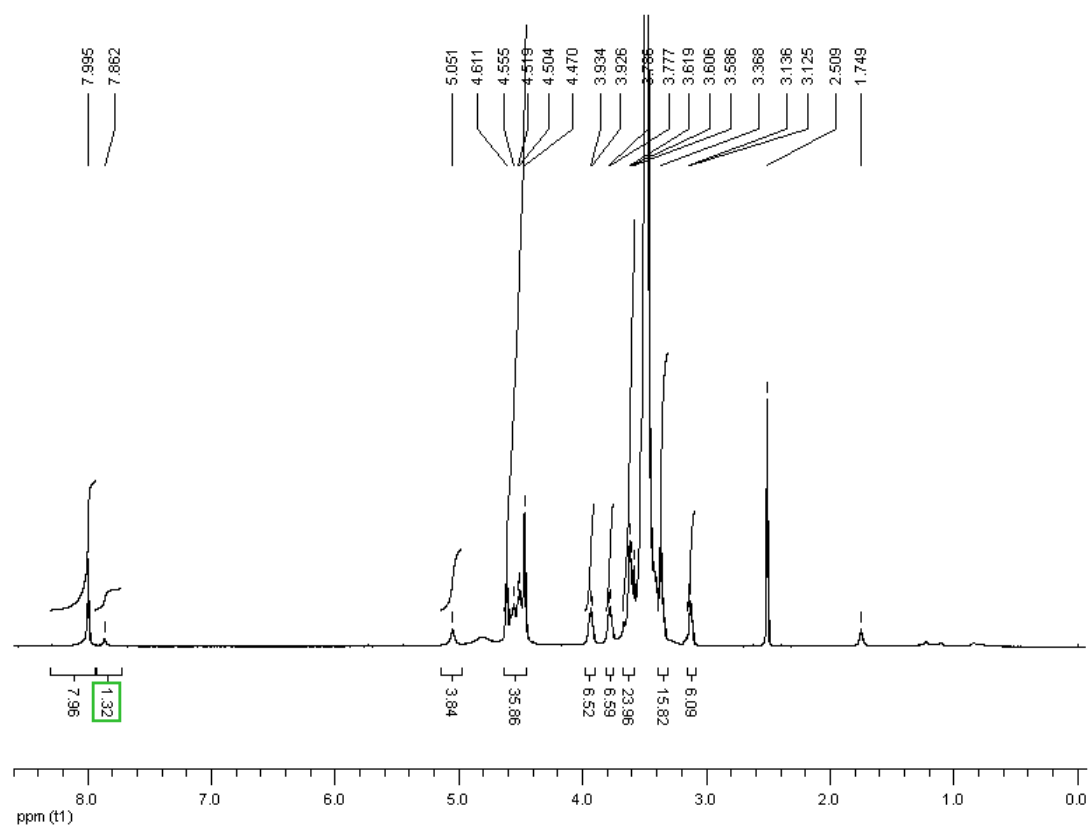


Figure S4. ¹H NMR (DMSO-*d*₆+D₂O, 600 MHz) of compound **PBI-Cl-Man**.

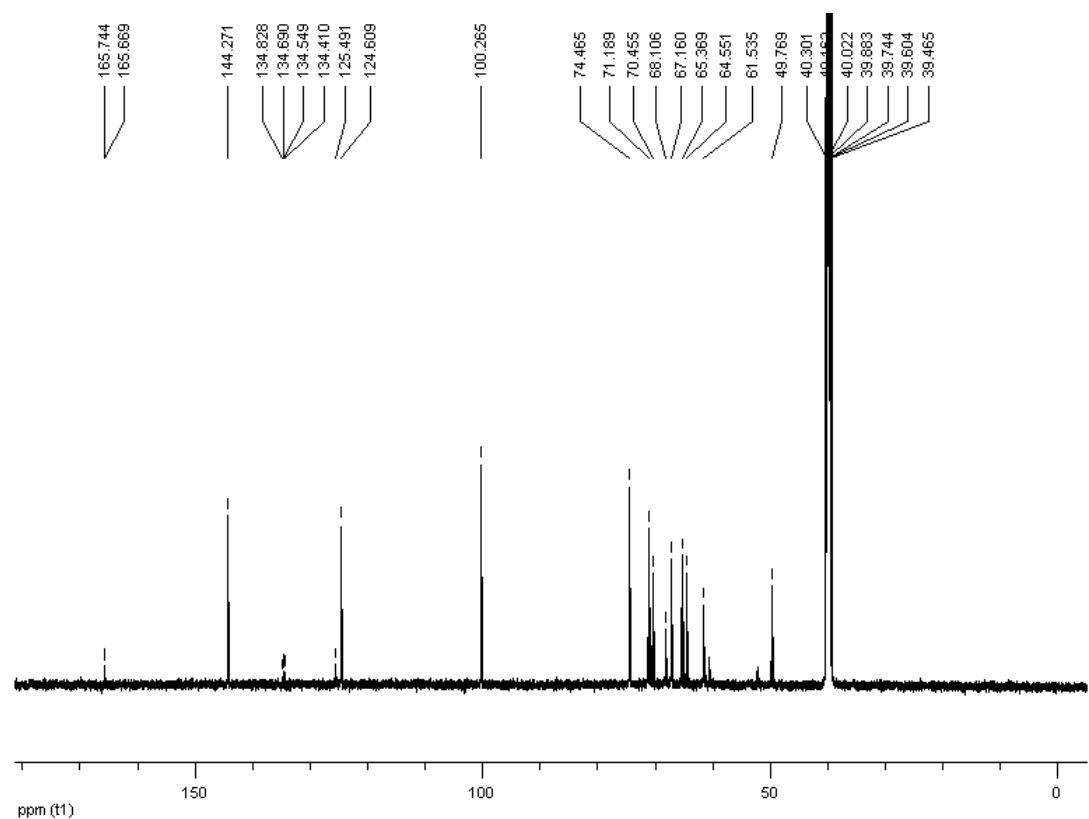


Figure S5. ¹³C NMR (DMSO-*d*₆+D₂O, 150 MHz) of compound **PBI-Cl-Man**.

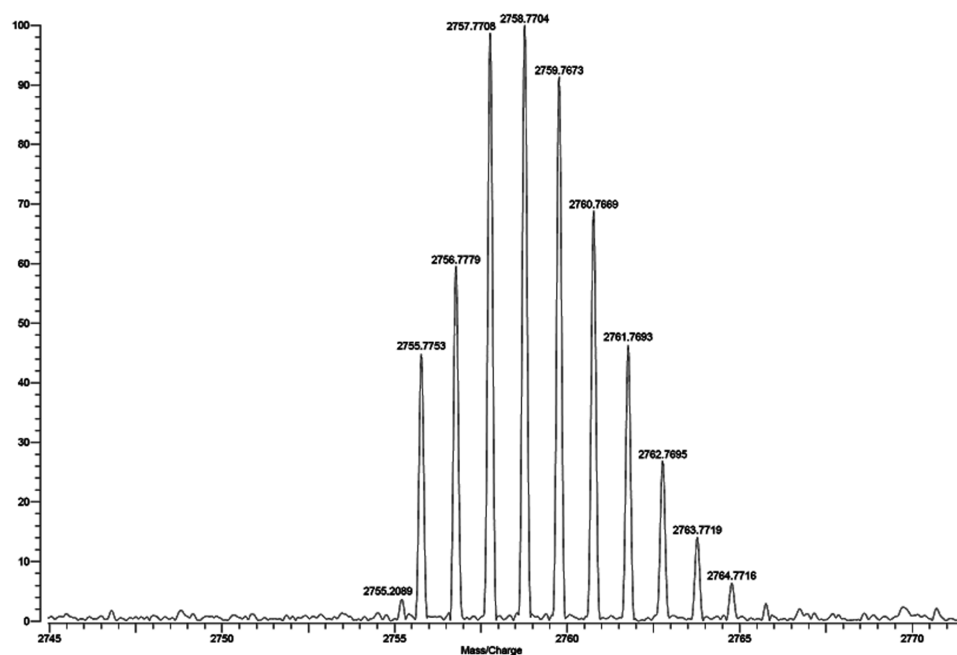


Figure S6. HRMS of compound **PBI-Cl-Man**.

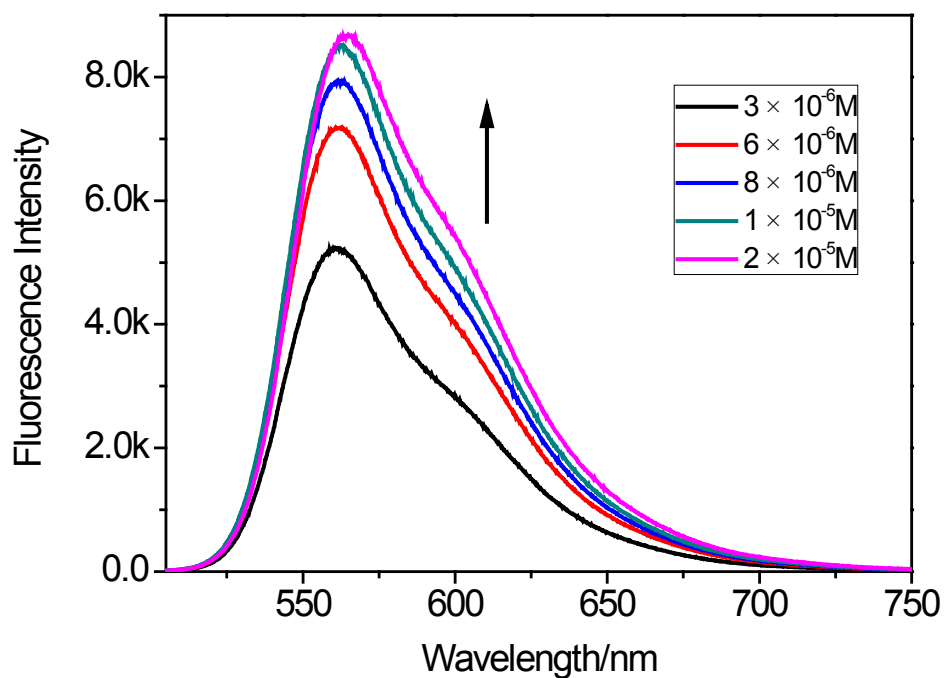


Figure S7. Fluorescence spectra of **PBI-Cl-Man** ($\lambda_{\text{ex}} = 495$ nm, from 3.0×10^{-6} M to 2.0×10^{-5} M) in PBS buffer (pH = 7.2, 10 mM, 0.1 mM CaCl_2 , 0.1 mM MnCl_2).

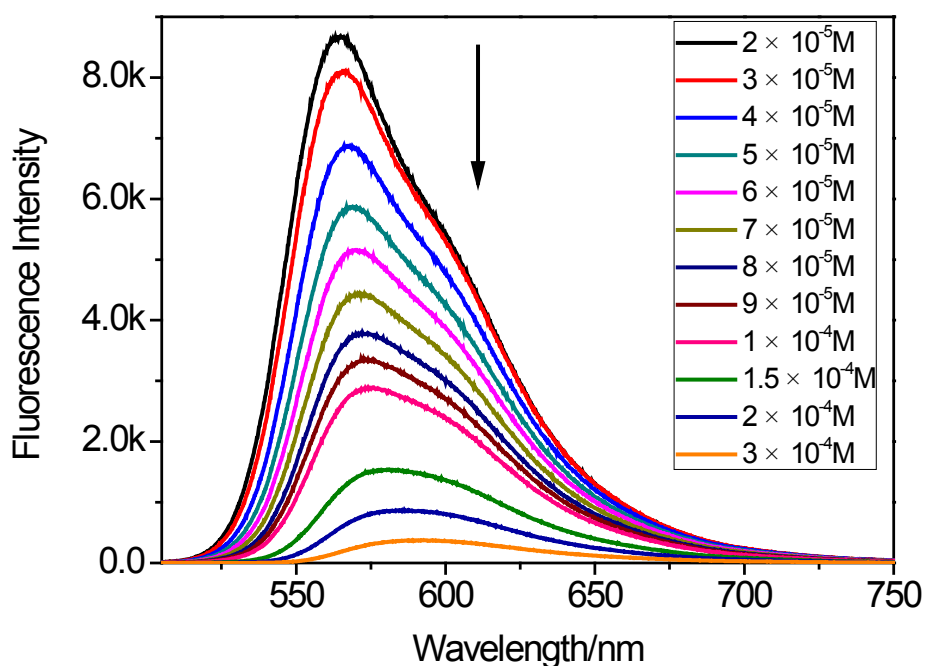


Figure S8. Concentration-dependent fluorescence spectra of **PBI-Cl-Man** ($\lambda_{\text{ex}} = 495$ nm, from $2.0 \times 10^{-5} \text{ M}$ to $3.0 \times 10^{-4} \text{ M}$) in PBS buffer (pH = 7.2, 10 mM, 0.1 mM CaCl_2 , 0.1 mM MnCl_2).

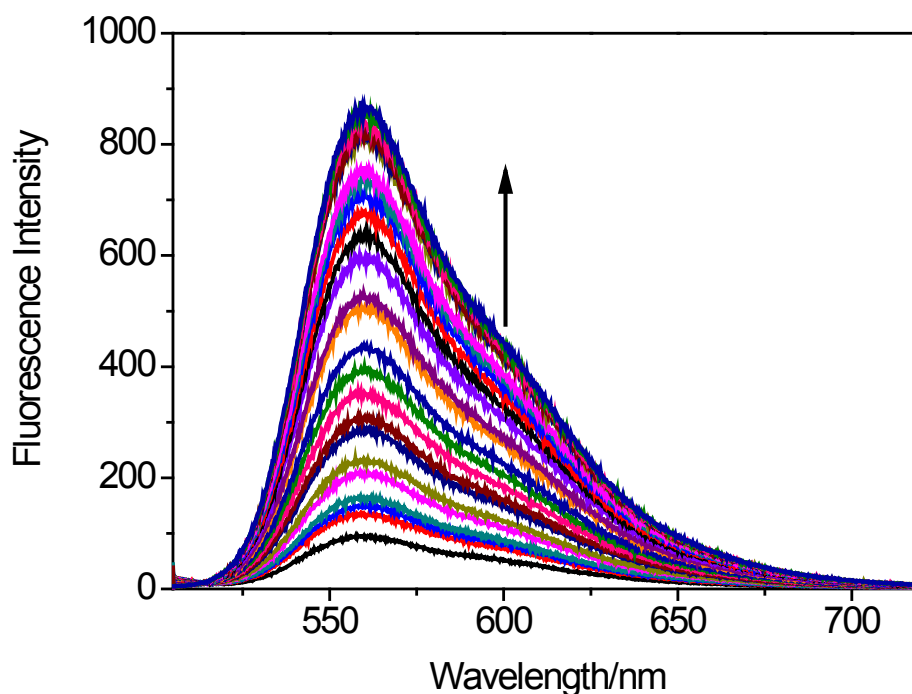


Figure S9. Fluorescence spectra of the complexes of **PBI-Cl-Man** ($\lambda_{\text{ex}} = 495$ nm, $2 \times 10^{-7} \text{ M}$) and Con A ($1 \times 10^{-6} \text{ M}$) upon addition of $\alpha\text{-MMP}$ (from $4 \times 10^{-5} \text{ M}$ to $9.4 \times 10^{-4} \text{ M}$) in PBS buffer (pH = 7.2, 10 mM, 0.1 mM CaCl_2 , 0.1 mM MnCl_2).

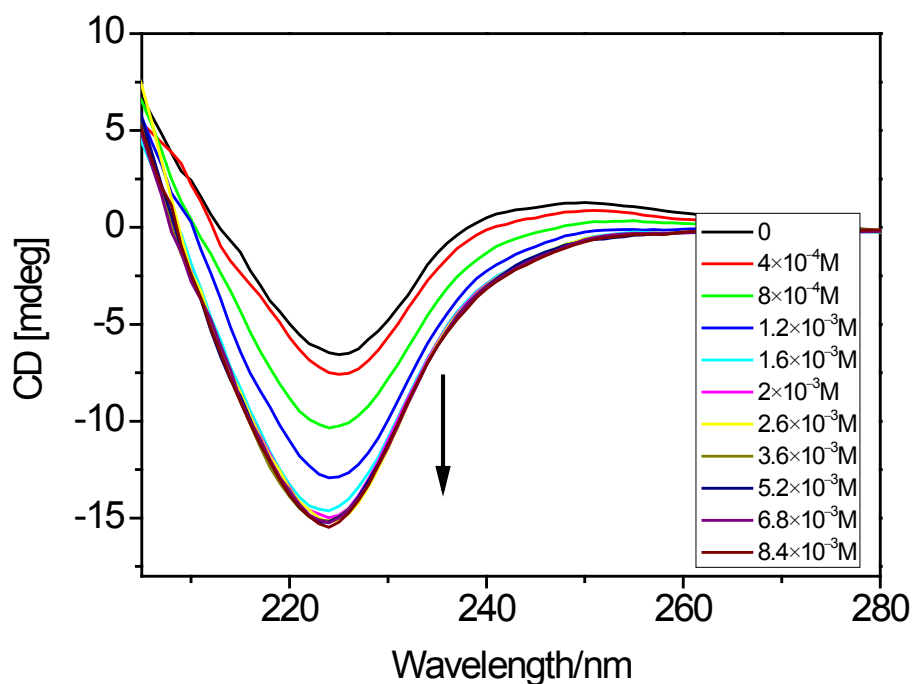


Figure S10. CD spectra of the complexes of Con A (4×10^{-7} M) and compound PBI-Cl-Man (1×10^{-6} M) upon addition of α -MMP in PBS buffer (pH = 7.2, 10 mM, 0.1 mM CaCl_2 , 0.1 mM MnCl_2).

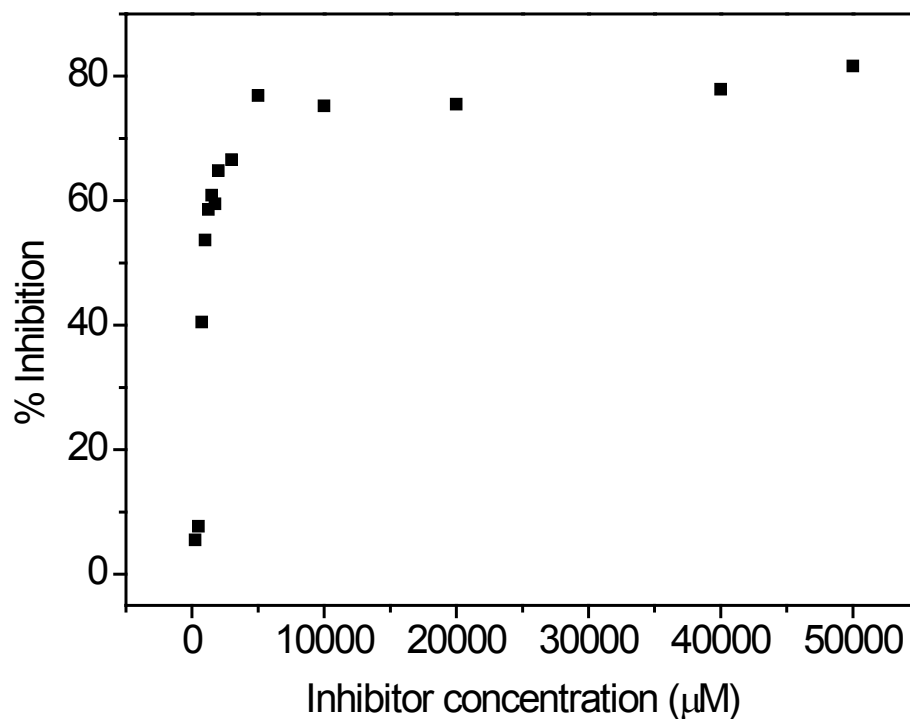


Figure S11. Inhibition curve of α -MMP for determination of the IC_{50} .