

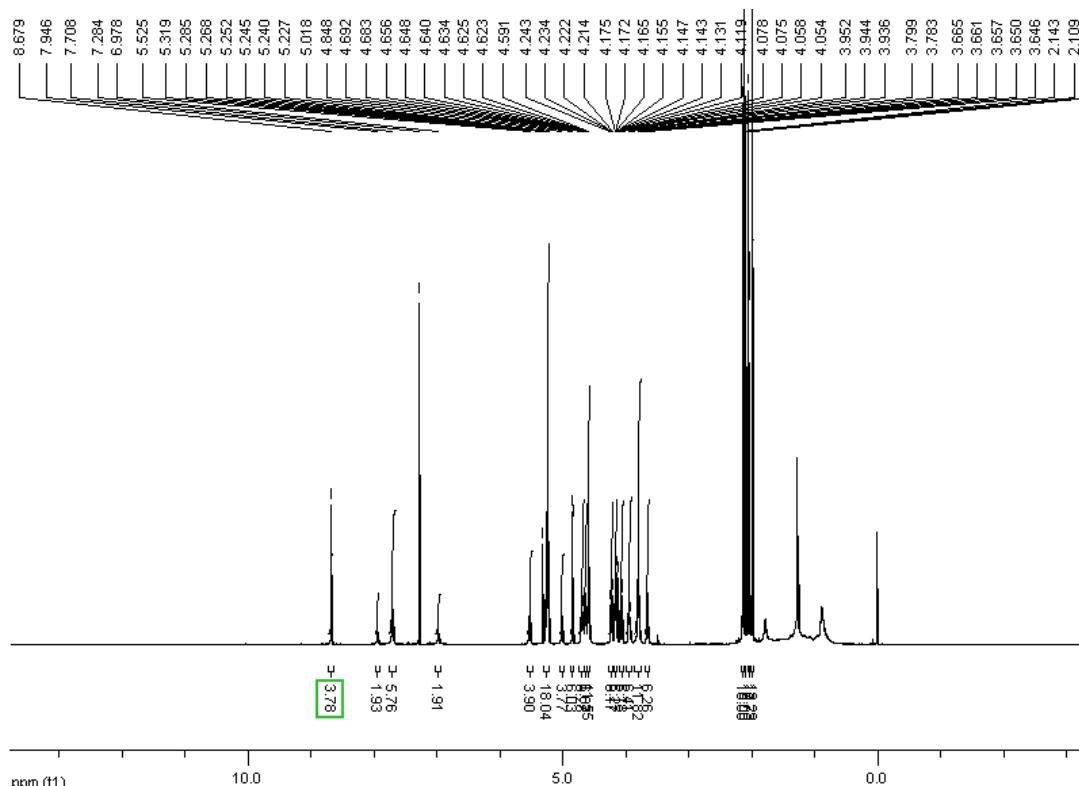
**Supporting Information**  
**for**  
**Synthesis, Optical Properties and Binding Interactions of**  
**Multivalent Glycocluster Based on Fluorescent Perylene**  
**Bisimide Derivative**

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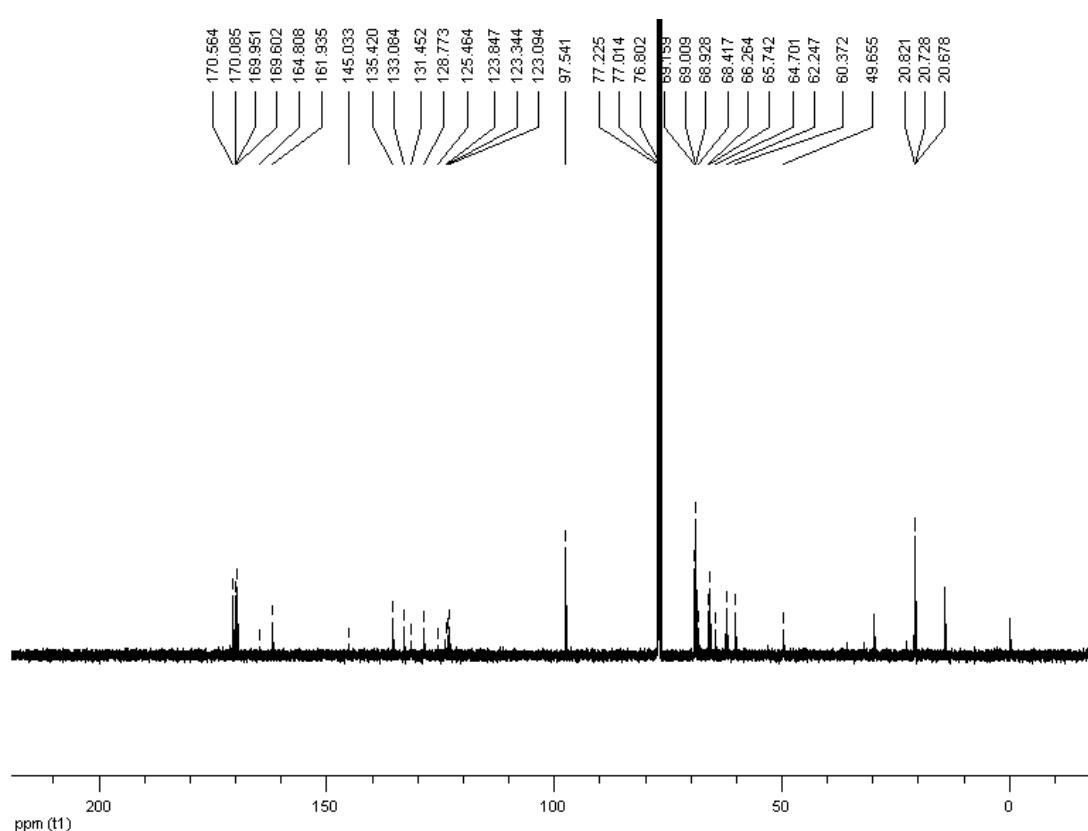
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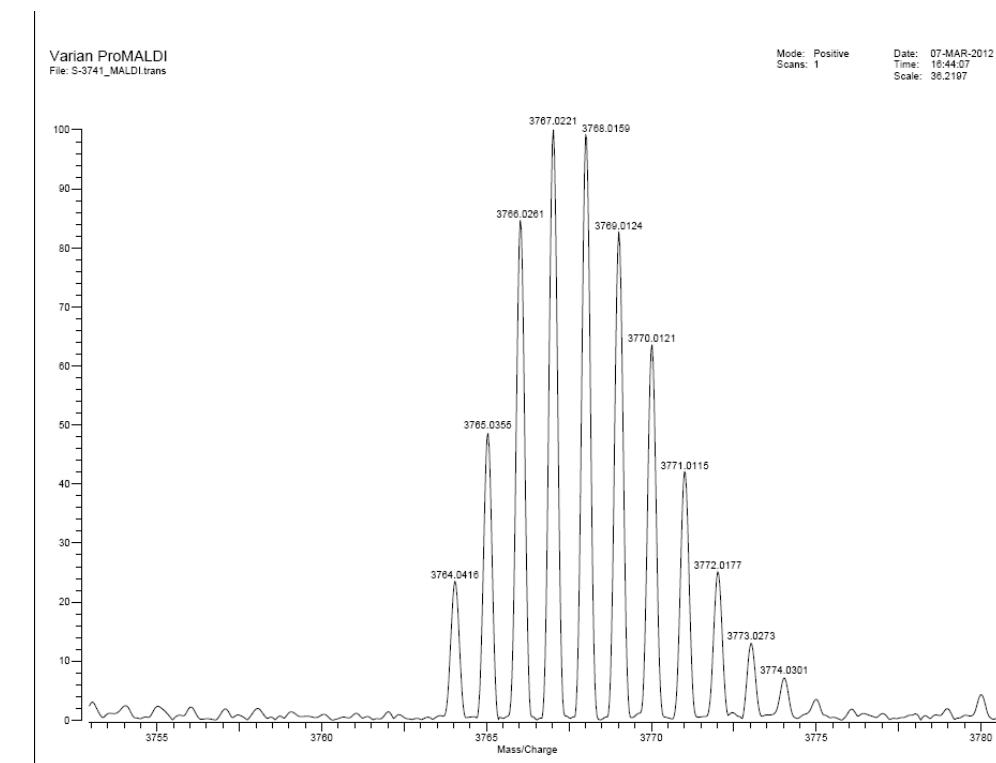
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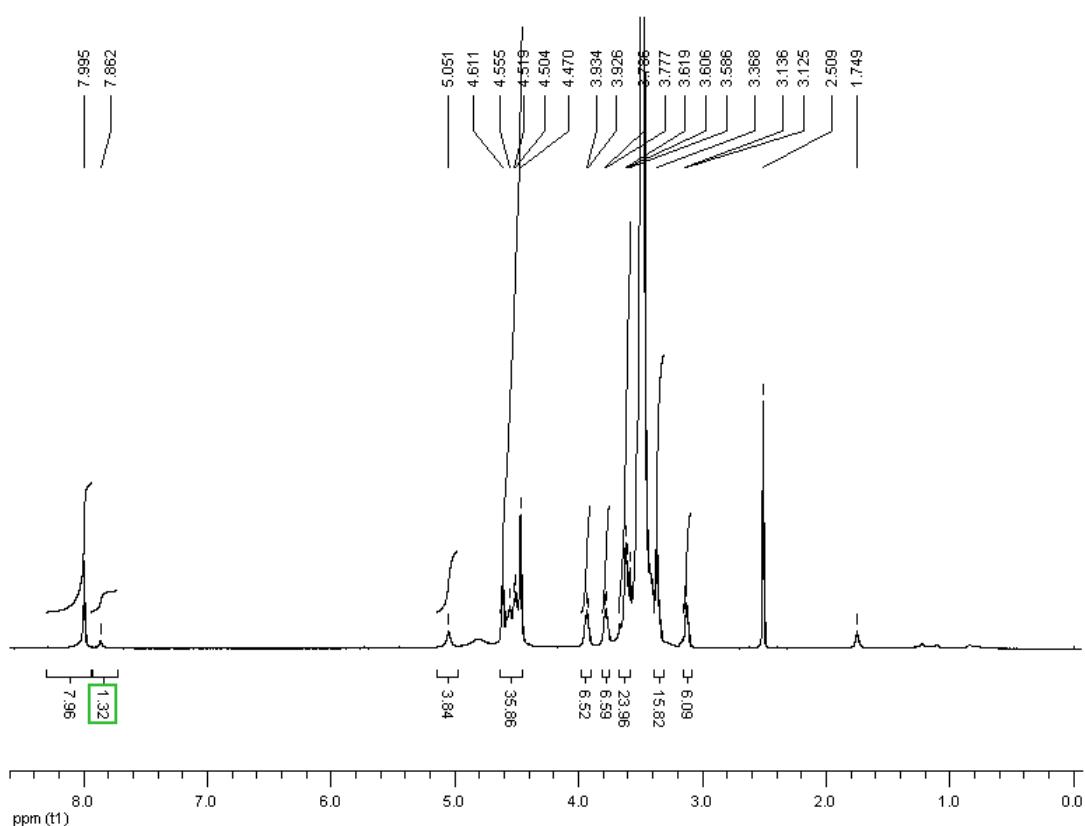
**Figure S1.** <sup>1</sup>H NMR ( $\text{CDCl}_3$ , 600 MHz) of compound PBI-Cl-AcMan.



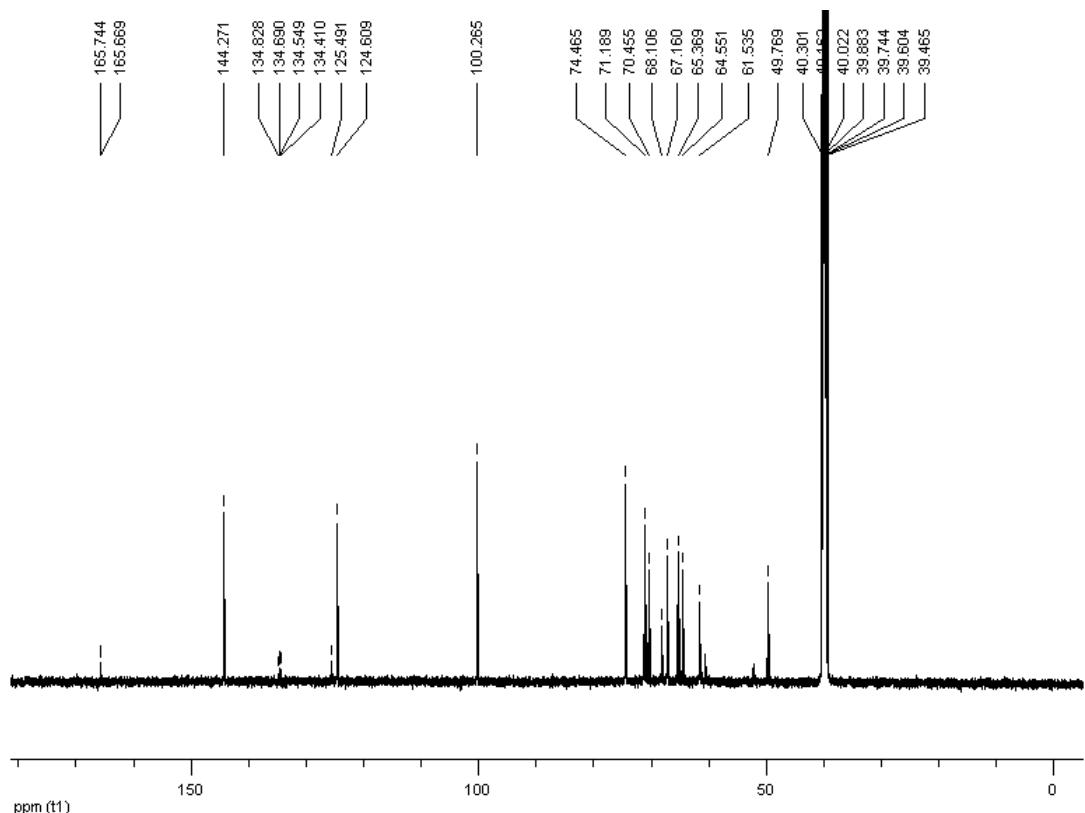
**Figure S2.** <sup>13</sup>C NMR ( $\text{CDCl}_3$ , 150 MHz) of compound **PBI-Cl-AcMan**.



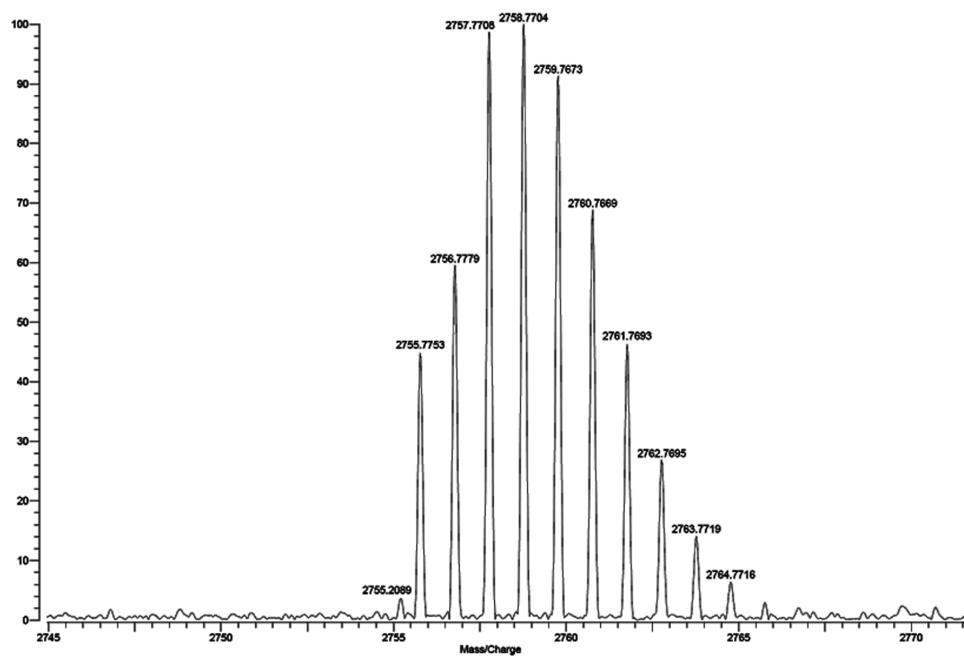
**Figure S3.** HRMS of compound **PBI-Cl-AcMan**.



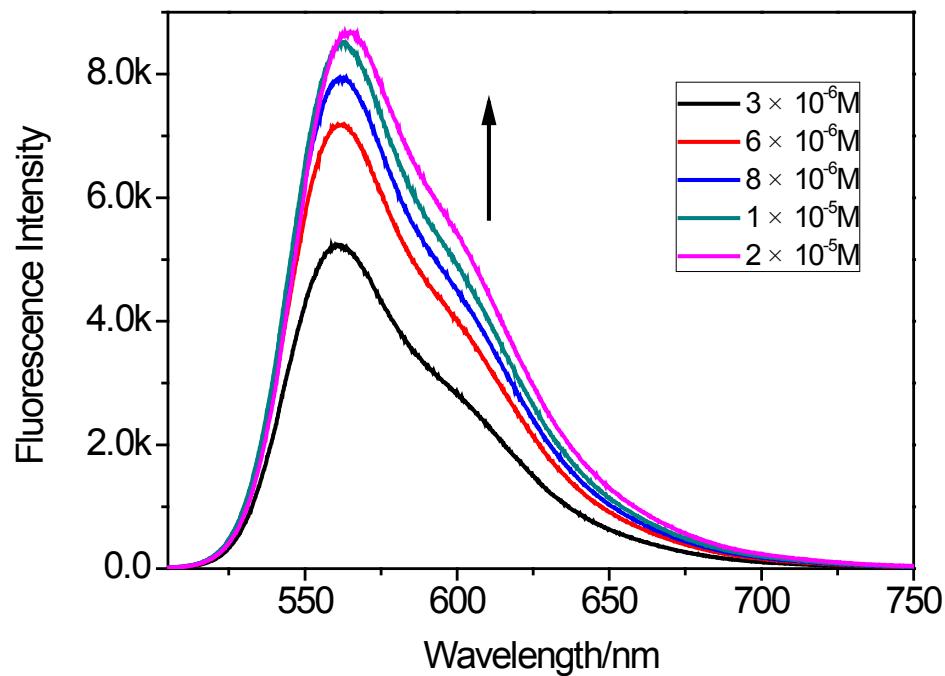
**Figure S4.**  $^1\text{H}$  NMR (DMSO- $d_6$ +D<sub>2</sub>O, 600 MHz) of compound **PBI-Cl-Man**.



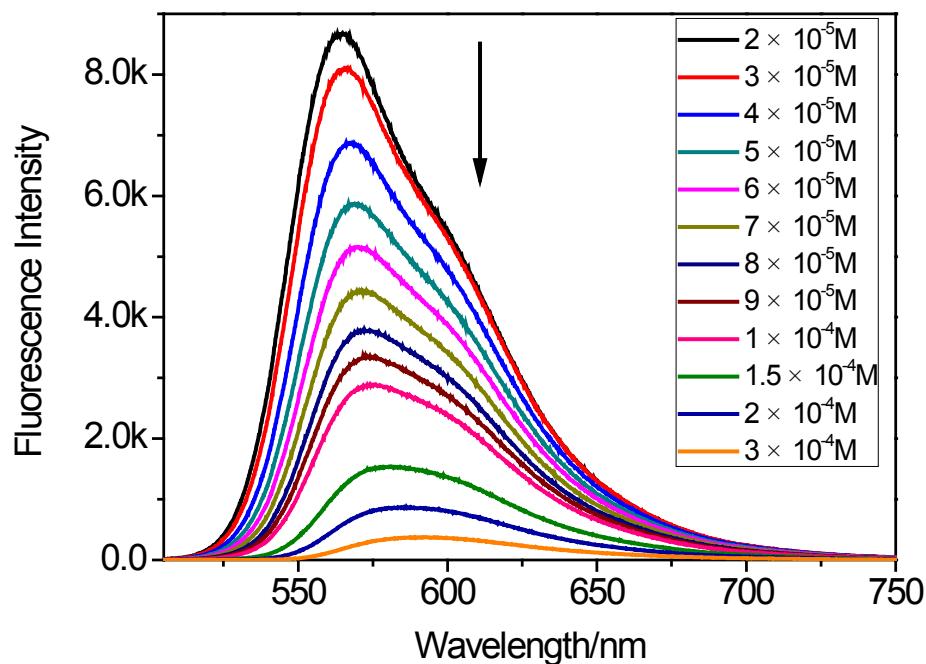
**Figure S5.**  $^{13}\text{C}$  NMR (DMSO- $d_6$ +D<sub>2</sub>O, 150 MHz) of compound **PBI-Cl-Man**.



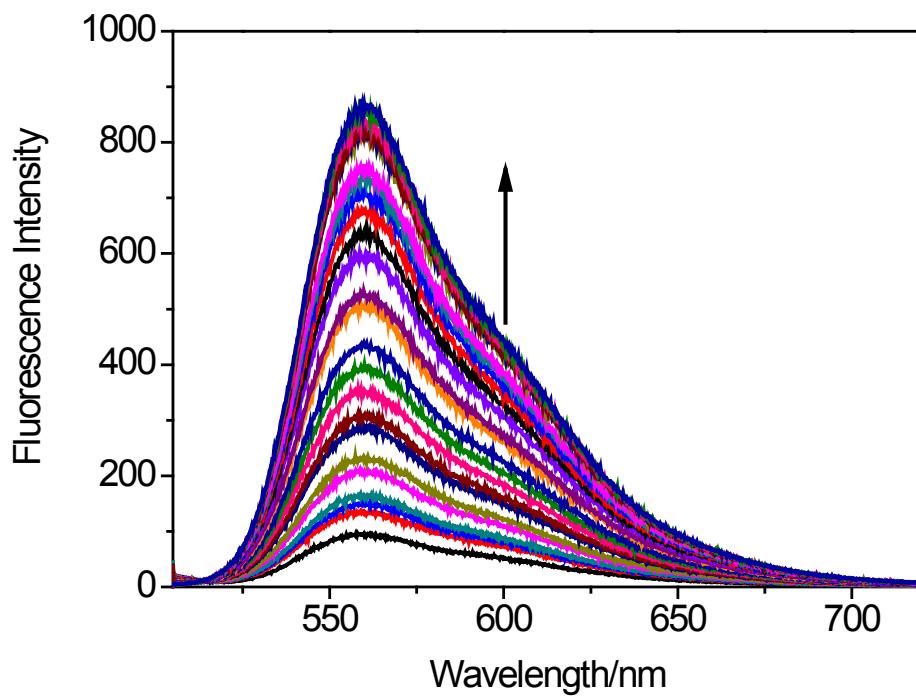
**Figure S6.** HRMS of compound **PBI-Cl-Man**.



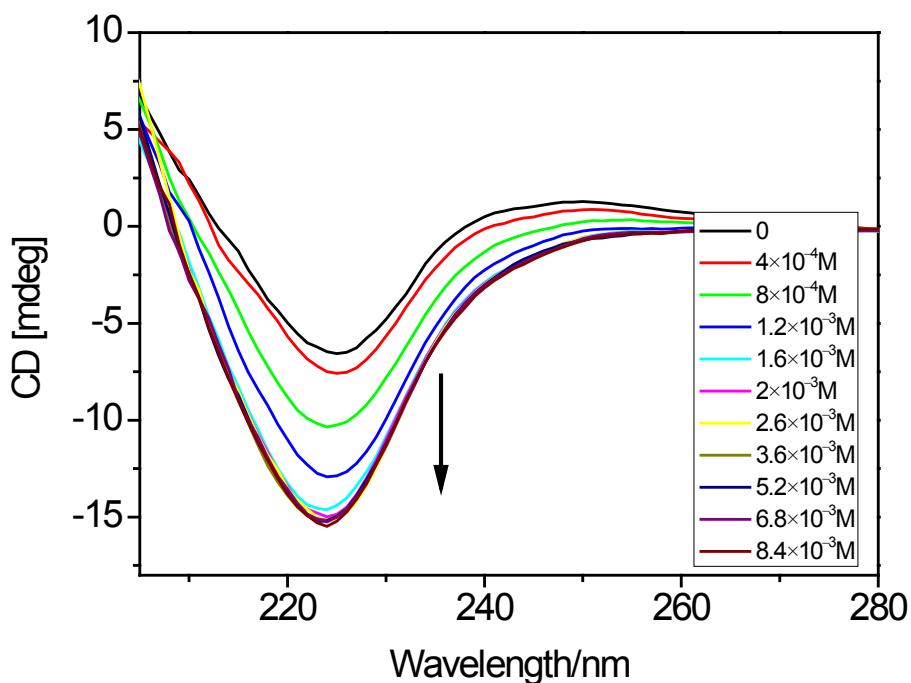
**Figure S7.** Fluorescence spectra of **PBI-Cl-Man** ( $\lambda_{\text{ex}} = 495$  nm, from  $3.0 \times 10^{-6}$  M to  $2.0 \times 10^{-5}$  M) in PBS buffer (pH = 7.2, 10 mM, 0.1 mM CaCl<sub>2</sub>, 0.1 mM MnCl<sub>2</sub>).



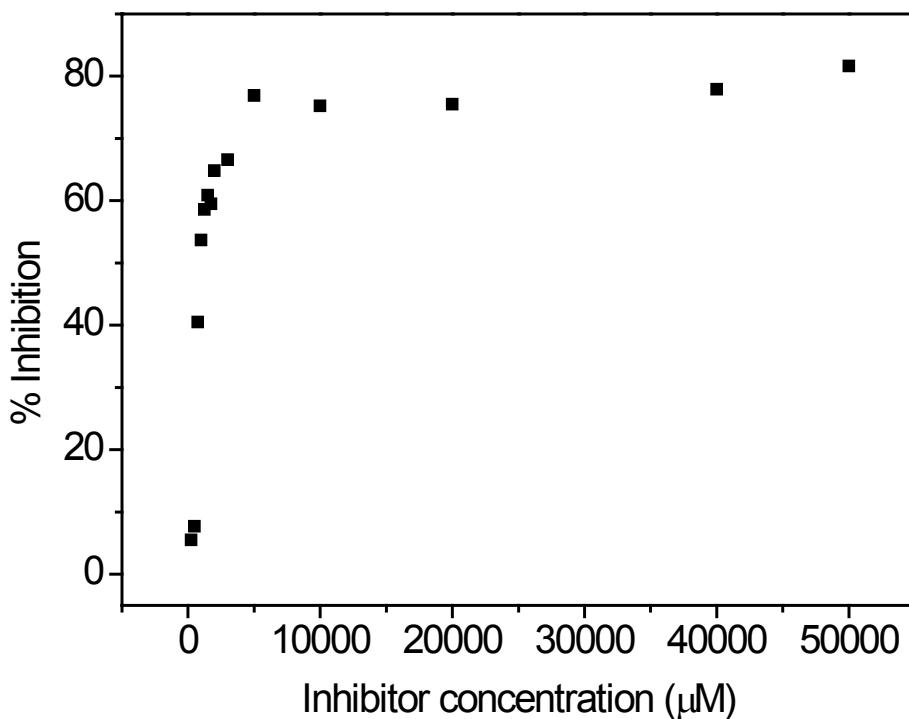
**Figure S8.** Concentration-dependent fluorescence spectra of **PBI-Cl-Man** ( $\lambda_{\text{ex}} = 495$  nm, from  $2.0 \times 10^{-5}$  M to  $3.0 \times 10^{-4}$  M) in PBS buffer (pH = 7.2, 10 mM, 0.1 mM CaCl<sub>2</sub>, 0.1 mM MnCl<sub>2</sub>).



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



**Figure S10.** CD spectra of the complexes of Con A ( $4 \times 10^{-7}$  M) and compound PBI-Cl-Man ( $1 \times 10^{-6}$  M) upon addition of  $\alpha$ -MMP in PBS buffer (pH = 7.2, 10 mM, 0.1 mM  $\text{CaCl}_2$ , 0.1 mM  $\text{MnCl}_2$ ).



**Figure S11.** Inhibition curve of  $\alpha$ -MMP for determination of the  $\text{IC}_{50}$ .