

## Electronic Supplementary Information

### Computer-Aided Design of Short Peptide Ligands Targeting Tumor Necrosis Factor-Alpha for Adsorbents Applications

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#### Supporting figures and tables

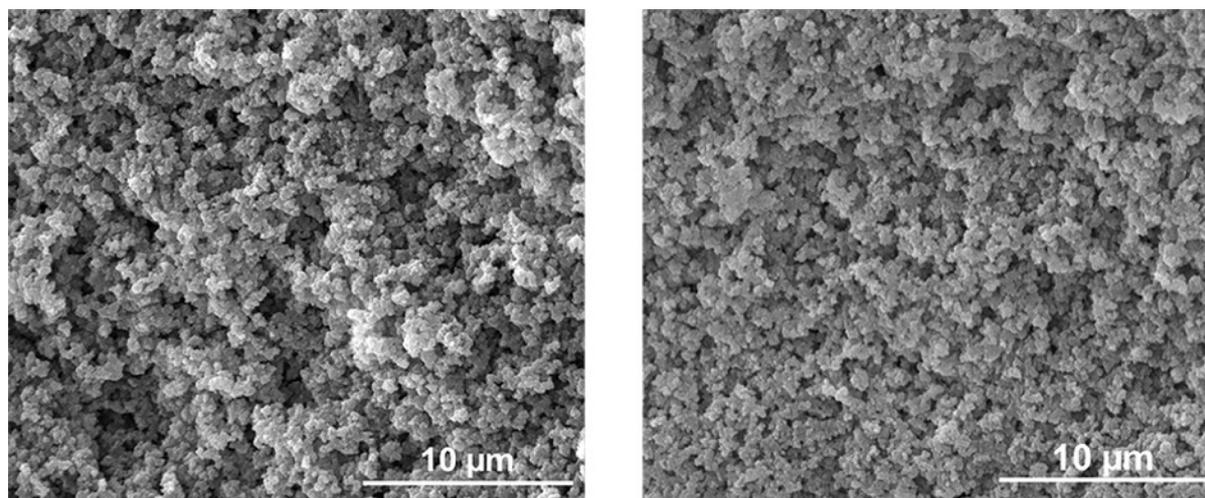


Figure S1. SEM micrographs of internal morphology in PVA microspheres.

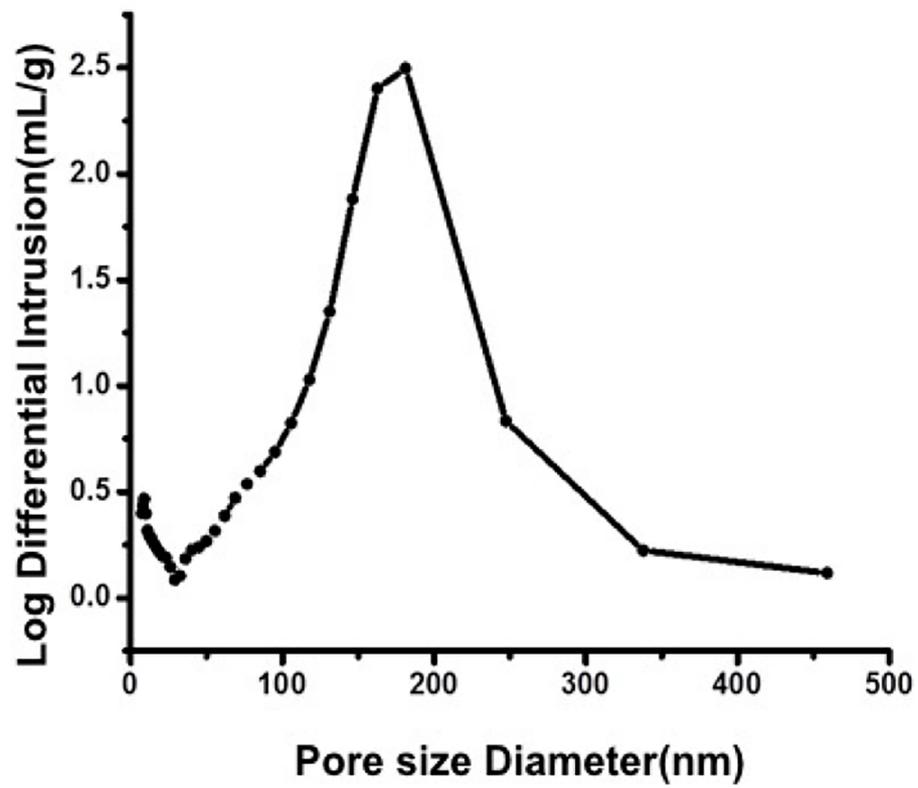
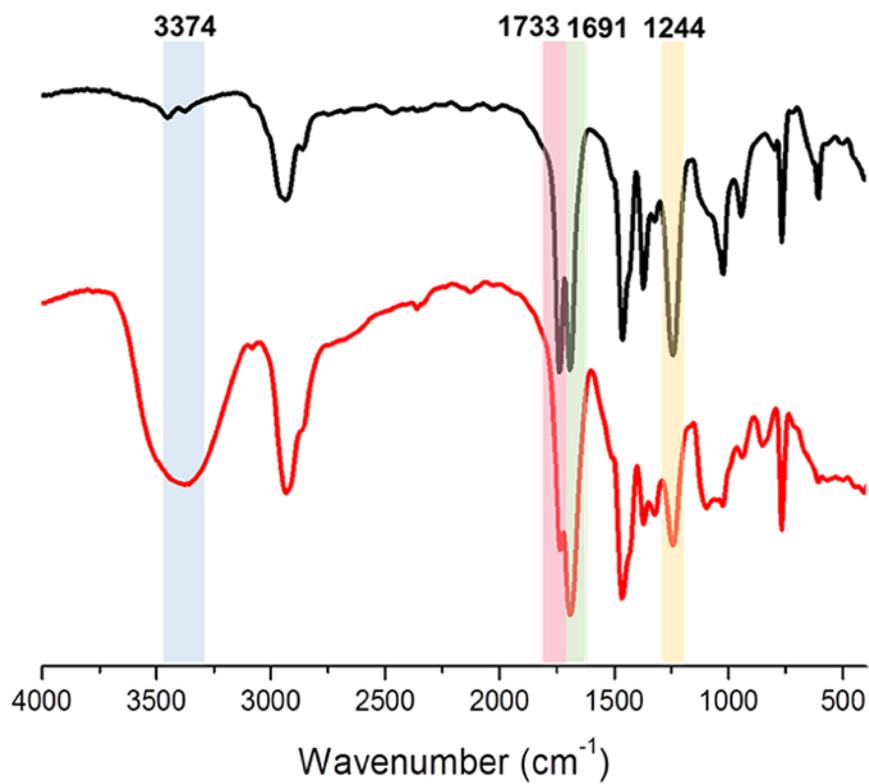


Figure S2. Pore size distribution of polyvinyl alcohol Beads recorded by mercury intrusion porosimetry (MIP).



**Figure S3.** FT-IR spectra of adsorbent before(a) and after(b) alcoholysis reaction. After alcoholysis reaction, the absorbance peak at 3374 cm<sup>-1</sup> and the absorbance peaks at 1733 cm<sup>-1</sup> and 1244 cm<sup>-1</sup> had disappeared. The absorbance peaks at 1691 cm<sup>-1</sup>.

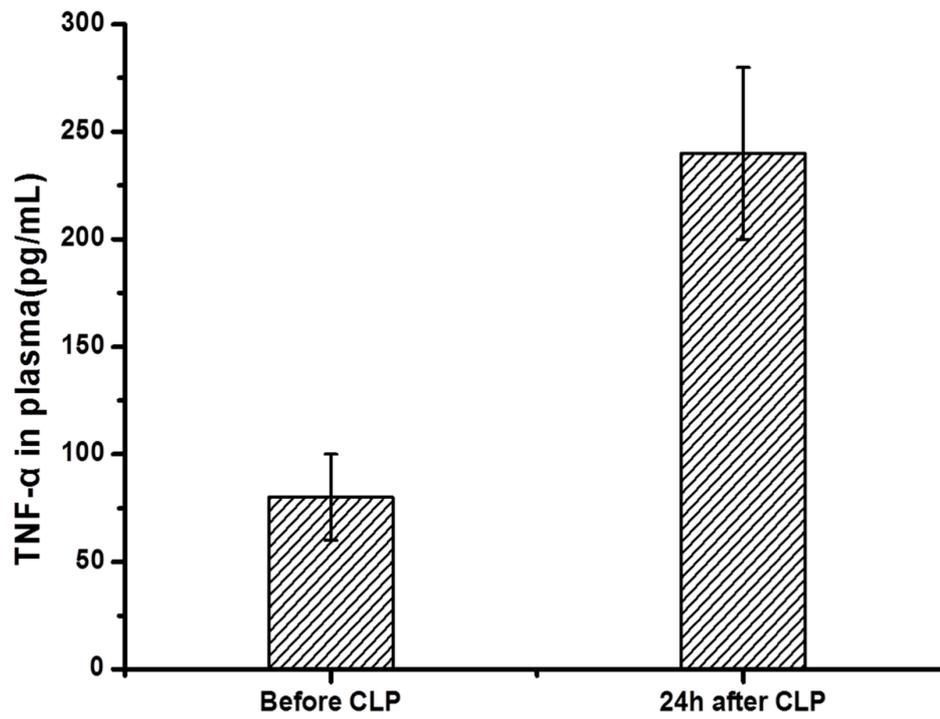


Figure S4. Concentration of TNF- $\alpha$  in plasma of healthy and CLP rats at 24 h after operation.

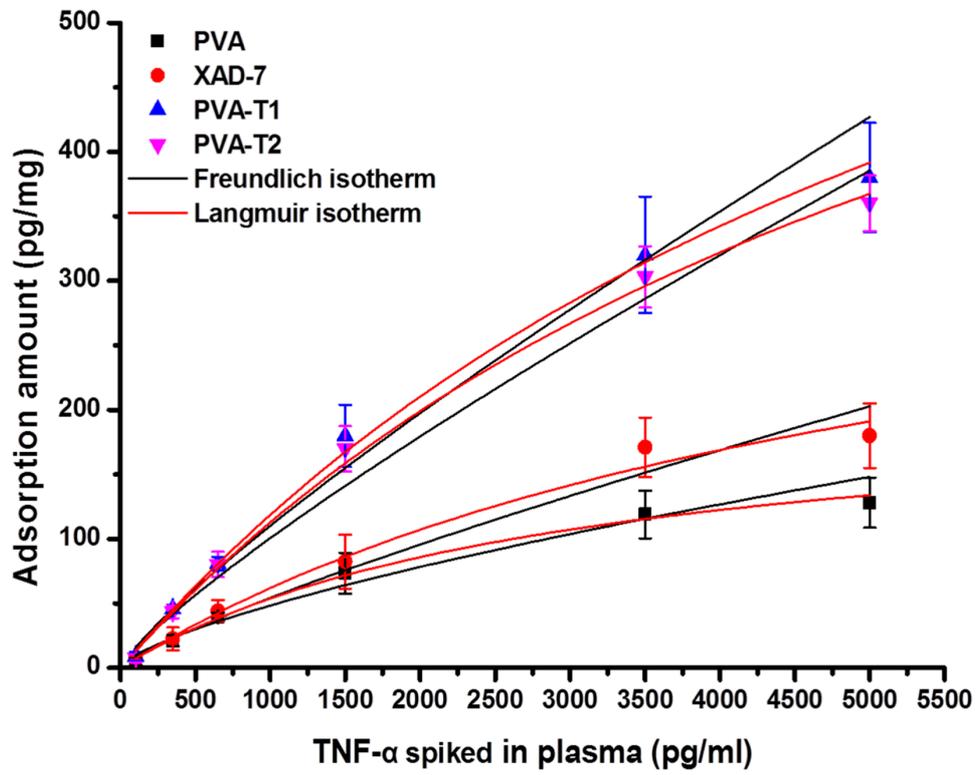
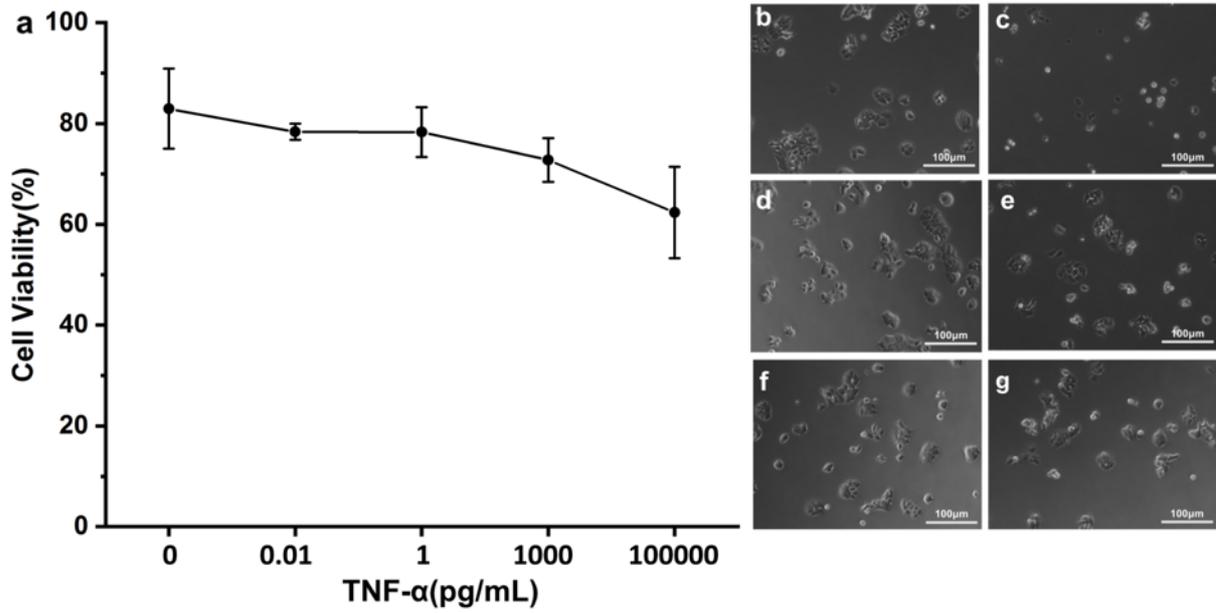
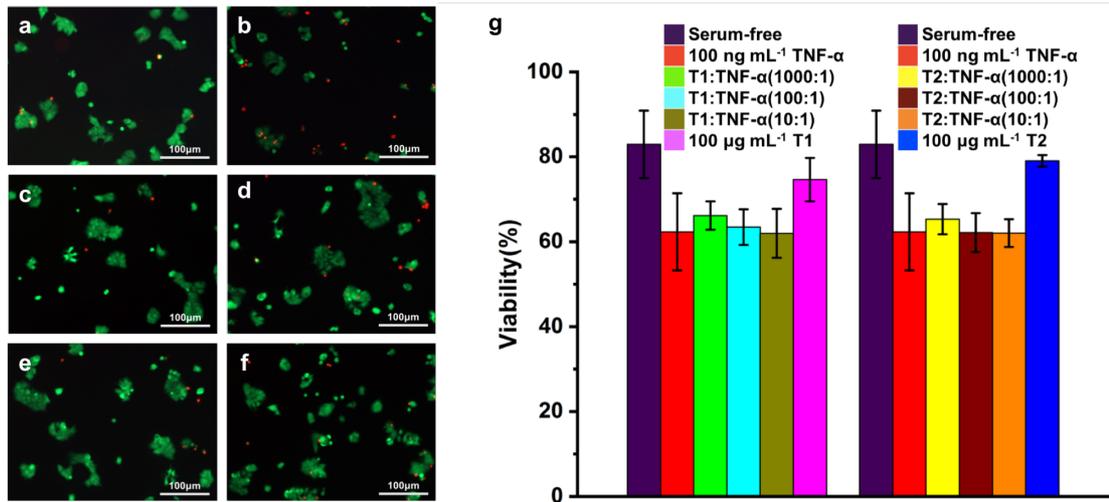


Figure S5. Adsorption isotherm of TNF- $\alpha$  spiked in human plasma (T=37 °C).



**Figure S6.** (a) Different amounts (0, 0.01, 1, 1000 and 100000 pg mL<sup>-1</sup>) of TNF-α in serum free cell culture medium induced MCF7 cells death. (Error bars represent standard deviations, n=5.) (b-g) The cytomorphology changes of MCF7 cells in different medium. MCF7 cells were treated with serum free cell culture medium(b), 100 ng mL<sup>-1</sup> TNF-α(c), 100 μg mL<sup>-1</sup> T1(d), a combination of TNF-α and T1(1000:1) (e), 100 μg mL<sup>-1</sup> T2(f) and a combination of TNF-α and T2(1000:1) (g). Cells were photographed in bright field after 24 hr treatment.



**Figure S7.** TNF-induced cytotoxicity was slightly suppressed by peptide T1 and T2. (a-f) Fluorescence images of MCF7 cells treated with serum free cell culture medium(a), 100 ng mL<sup>-1</sup> TNF-α(b), 100 μg mL<sup>-1</sup> T1(c), a combination of TNF-α and T1(1000:1) (d), 100 μg mL<sup>-1</sup> T2(e) and a combination of TNF-α and T2(1000:1) (f) for 24 hr. Cells were stained with Calcein AM (green) and PI (red) by live/dead assay kit. (g) MCF7 cell viability cultured for 24 hr in different medium measured by CCK8 assay. The control group was in RPMI1640 cell culture medium with 10% FBS. (Error bars represent standard deviations, n=5.)

**Table S1.** Values of adsorption isotherm parameters and correlation coefficients.

Adsorbent	Langmuir isotherm			Freundlich isotherm		
	Q (mg/g)	K (L/mg)	R <sup>2</sup>	K <sub>F</sub> ((mg/g) (L/mg) <sup>1/n</sup> )	n	R <sup>2</sup>
PVA	213.04	3.38 10 <sup>-4</sup>	0.99	0.39588	1.44	0.94
XAD-7	399.33	1.83 10 <sup>-4</sup>	0.99	0.18992	1.22	0.97
PVA-T1	920.12	1.48 10 <sup>-4</sup>	0.99	0.32921	1.19	0.96
PVA-T2	842.33	1.55 10 <sup>-4</sup>	0.99	0.31632	1.20	0.97