Electronic Supplementary Material (ESI) for Biomaterials Science.

Supplementary Figures and data

Injectable pH and redox dual responsive hydrogel based on self-assembled peptides for anti-tumor drug delivery

Ying Zhu[a], Liying Wang[b],Yiping Li[a], Zhewei Huang[a], Shiyao Luo[a], Han Han[a], Yue He[a], Faisal Raza[a], Jun Wu[b]*, and Liang Ge[a]*

[a] *State Key Laboratory of Natural Medicines, China Pharmaceutical University, No.24 Tongjia Xiang, Nanjing, 210009, China*

[b] *Key Laboratory of Sensing Technology and Biomedical Instrument of Guangdong Province, School of Biomedical Engineering, Sun Yat-sen University, Guangzhou 510006, China*

* Corresponding authors. E-mail address: wujun29@mail.sysu.edu.cn (J. Wu), geliang1981@hotmail.com (Liang Ge)

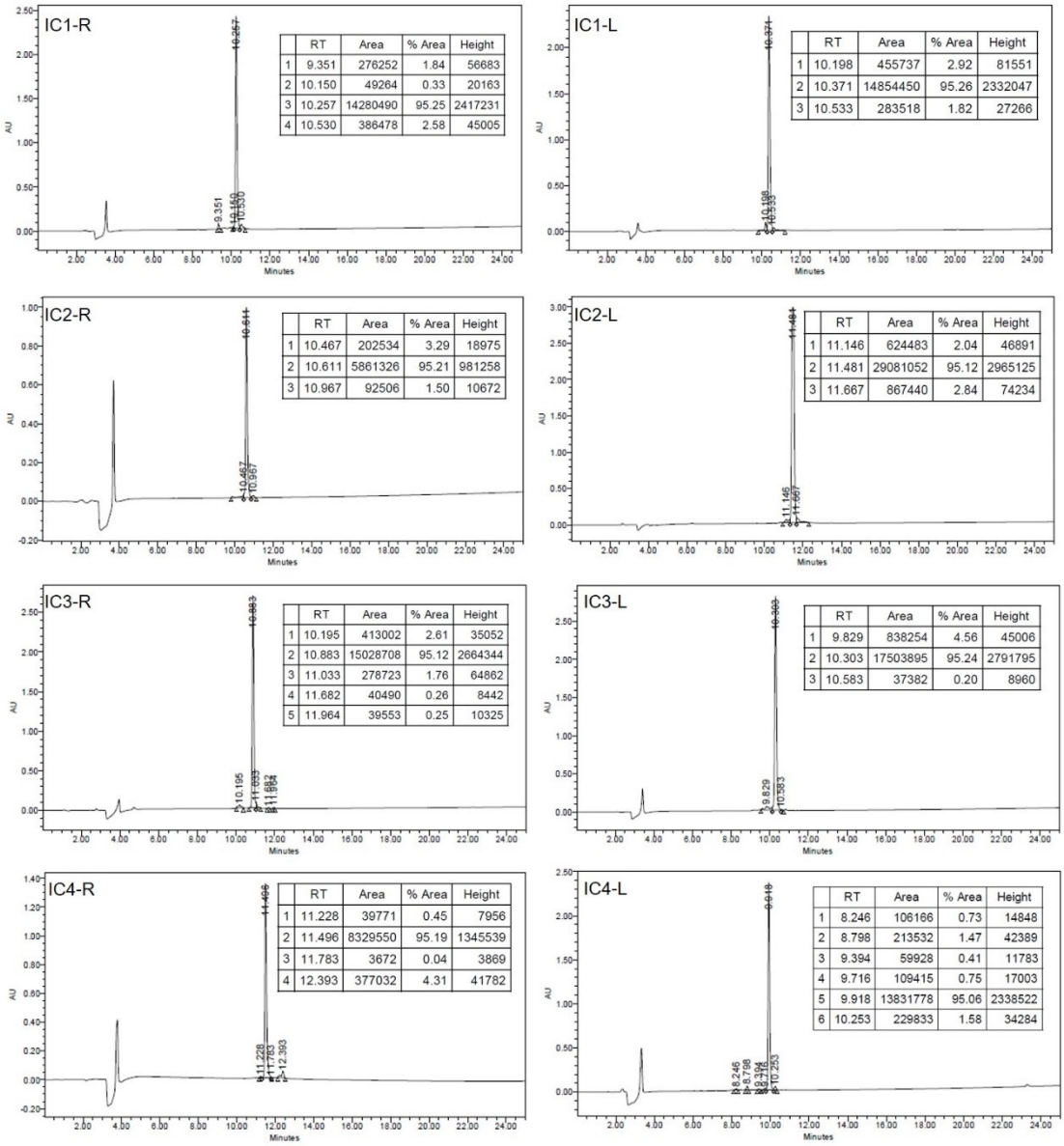

Fig. S1. The UHPLC chromatograms and peak data of designed peptides.

The purity of IC1-R, IC1-L, IC2-R, IC2-L, IC3-R, IC3-L, IC4-R and IC4-L were 95.25%,95.26%,95.21%,95.12%,95.12%,95.24%,95.19% and 95.06%, respectively, according to the uplc-hplc and peak data of the eight peptides, which all met the purity requirements of hydrogel preparation and evaluation in the later stage.

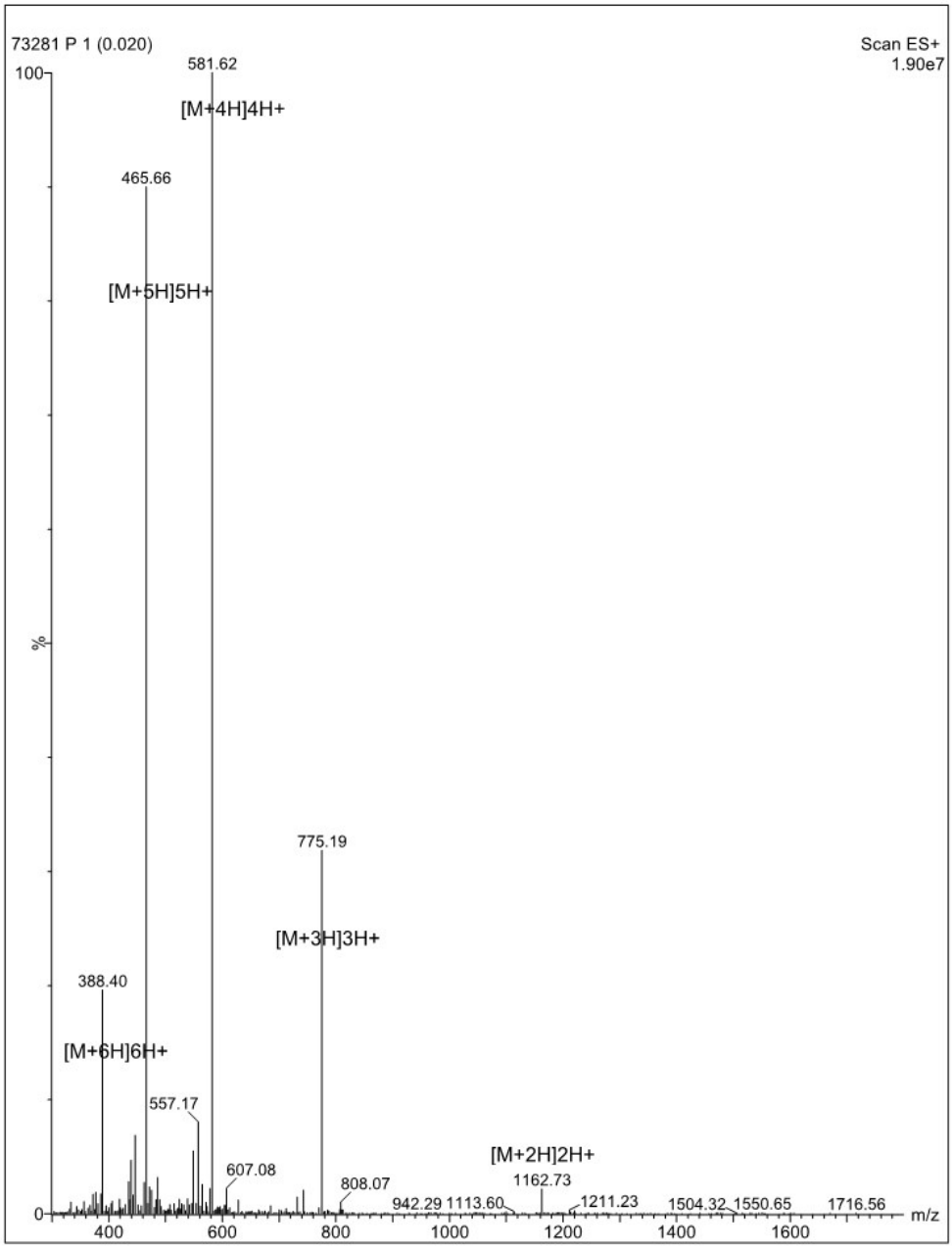

Fig. S2. The mass spectrum of IC1-R peptide.

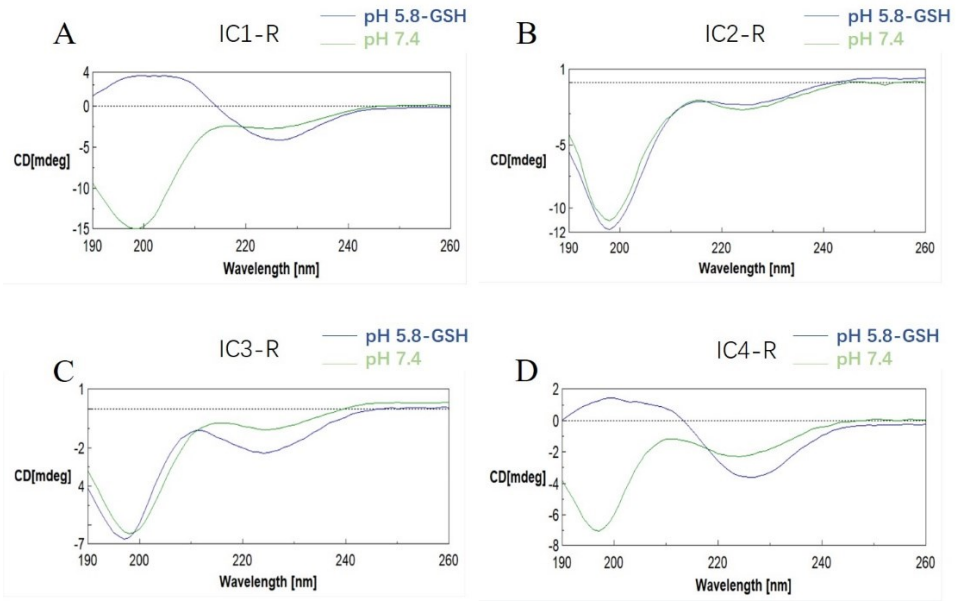

Fig. S3. Circular dichroism spectrum of IC1-R (A), IC2-R (B), IC3-R (C), and IC4-R (D) in different buffer solution

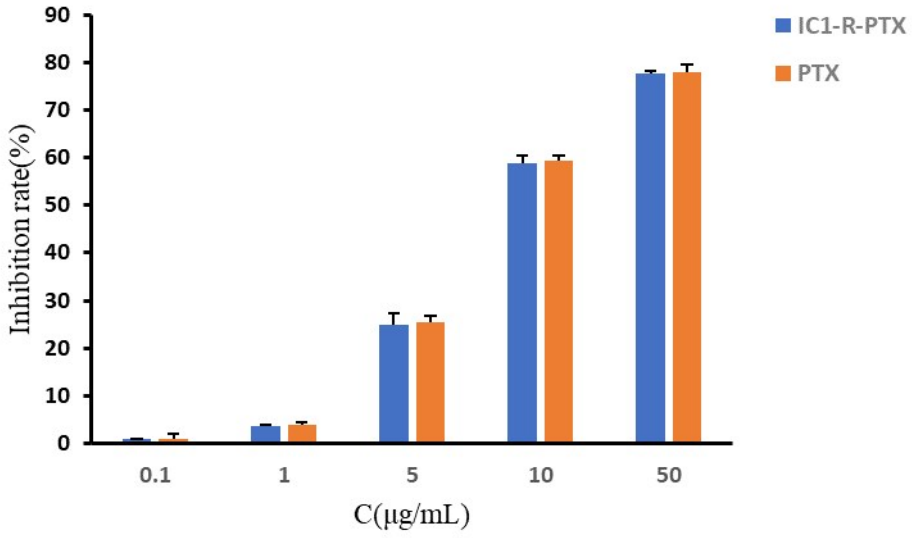

Fig. S4 The cell inhibition rate of drug-loaded peptide hydrogel and free PTX (n=5)

Table S1

Mass spectrometry confirmation of IC1-R peptide.

Peptide	Molecular weight	Theoretical value	Measured value

IC1-R	2322.17	$[M+2H]^{2+}$：1162.09 $[M+3H]^{3+}$：775.06 $[M+4H]^{4+}$：581.54 $[M+5H]^{5+}$：465.43 $[M+6H]^{6+}$：388.03	$[M+2H]^{2+}$：1162.73 $[M+3H]^{3+}$：775.19 $[M+4H]^{4+}$：581.62 $[M+5H]^{5+}$：465.66 $[M+6H]^{6+}$：388.40

Table S2

Gelation of different concentrations of IC peptides (VL: the time peptide solution began to be viscous liquid; SG: the time of stable gel formation; UG: unable to form a stable gel).

Peptide	Concentration of peptide(mg/mL)				
	10	15	20	25	30
IC1-R	VL:5 min; SG:10 min	VL:1 min; SG:7 min	VL:1 min; SG:5 min	Gelation instantly	Gelation instantly
IC1-L	VL:7 min; SG:20 min	VL:3 min; SG:13 min	VL:3 min; SG:12 min	VL:2 min; SG:12 min	VL:1 min; SG:8 min
IC2-R	UG	UG	UG	UG	UG
IC2-L	UG	UG	UG	UG	UG
IC3-R	UG	UG	UG	UG	UG
IC3-L	UG	UG	UG	UG	UG
IC4-R	UG	VL:16 min; SG:25 min	VL:10 min; SG:20 min	VL:7 min; SG:18 min	VL:6 min; SG:15 min
IC4-L	UG	VL:28 min; SG:40 min	VL:28 min; SG:38 min	VL:23 min; SG:31 min	VL:15 min; SG:25 min

Table S3

Gelation of peptides under different pH (VL: the time peptide solution began to be viscous liquid; SG: the time of stable gel formation; UG: unable to form a stable gel).

Peptide	pH			
	6.4	7.4	8.5	9.2
IC1-R	UG	VL:1 min; SG:7 min		
IC1-L	UG	VL:3 min; SG:13 min		
IC2-R	UG	UG	VL:2 min; SG:30 min	
IC2-L	UG	UG	VL:3 min; SG:41 min	
IC3-R	UG	UG	UG	VL:13 min; SG:25 min
IC3-L	UG	UG	UG	VL:17 min; SG:34 min
IC4-R	UG	VL:16 min; SG:25 min		
IC4-L	UG	VL:28 min; SG:40 min		

Table S4

Secondary conformation ratios of IC peptides in different buffer solution.

Peptide	**α**	**β**	**Turn**	**Random**
IC1-R (pH 7.4)	0	63.4	14.8	21.8
IC1-R (pH 5.8-GSH)	0	9.7	23.1	67.2
IC2-R (pH 7.4)	0	10.3	24.9	64.8
IC2-R (pH 5.8-GSH)	0	10.9	23.6	65.5
IC3-R (pH 7.4)	0	9.9	24.0	66.1
IC3-R (pH 5.8-GSH)	0	10.1	26.3	63.6
IC4-R (pH 7.4)	0	56.6	17.1	26.3
IC4-R (pH 5.8-GSH)	0	11.3	21.7	67.0

Table S5

IC50 of PTX and IC1-R-PTX.

Group	PTX	IC1-R-PTX
IC50 (μg/mL)	8.231	8.477