Electronic Supporting Information (ESI)

Reinforcement of Nanofibrillar Hydrogels via Cyclodextrin and Self-Assembling Peptide Interactions for Controlled Drug Delivery

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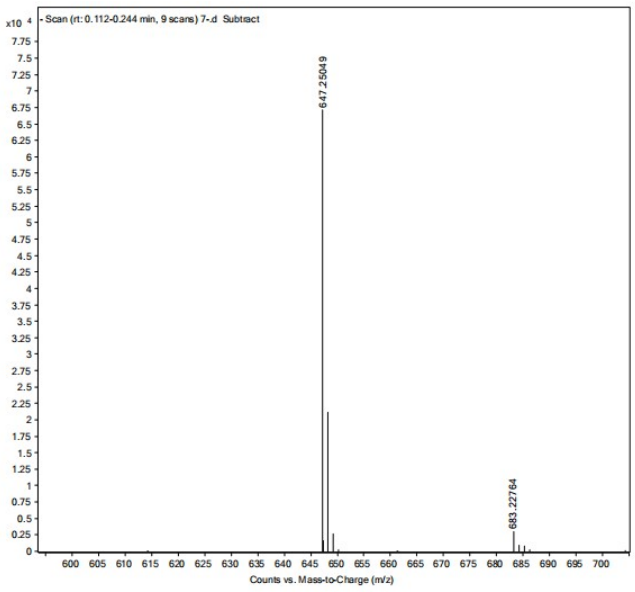

Fig. S1. MS of peptide Fmoc-GFFG. (ESI-MS: $C_{37}H_{36}N_4O_7$, cal.MW = 648, obsvd.$[M-H]^-$ = 647.2)

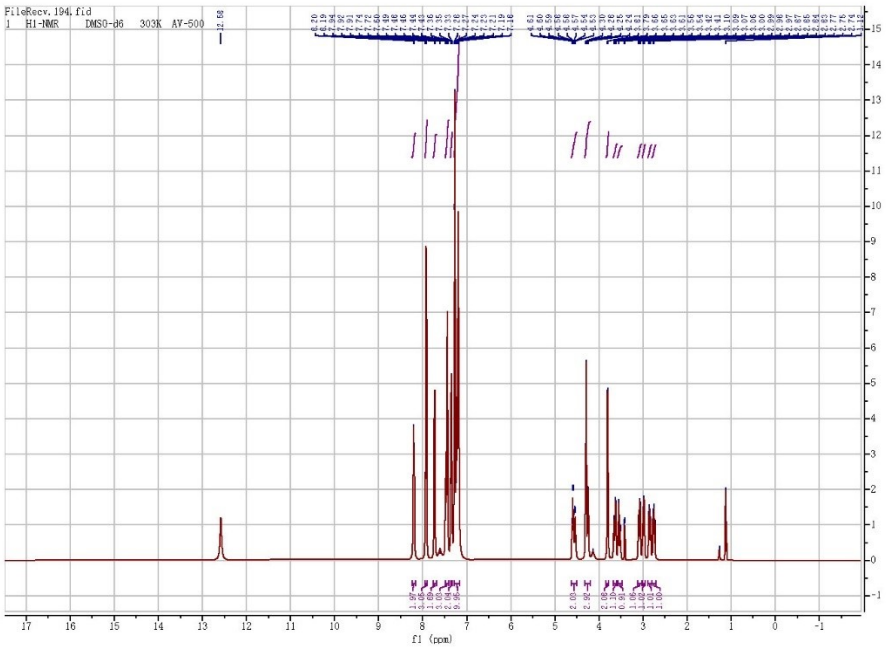

Fig. S2. ^{1}H NMR spectrum of peptide Fmoc-GFFG

δ 12.37 (d, J = 170.3 Hz, 1H), 7.90 (d, J = 8.3 Hz, 2H), 7.69 (d, J = 7.3 Hz, 4H), 7.44 (d, J = 5.6 Hz, 2H), 7.40 (t, J = 7.4 Hz, 5H), 7.31 (t, J = 7.3 Hz, 5H), 3.77 (d, J = 5.1

Hz, 4H),3.60 (dd, J = 16.8, 5.8 Hz, 2H), 3.50 (dd, J = 16.6, 5.7 Hz, 2H), 3.37 (dt, J = 14.0, 7.0 Hz, 1H), 3.05 (dd,J = 13.8, 4.2 Hz, 2H), 2.99 – 2.91 (m, 2H), 2.82 (dd, J = 13.5, 9.6 Hz, 2H), 2.75 – 2.67 (m, 2H).

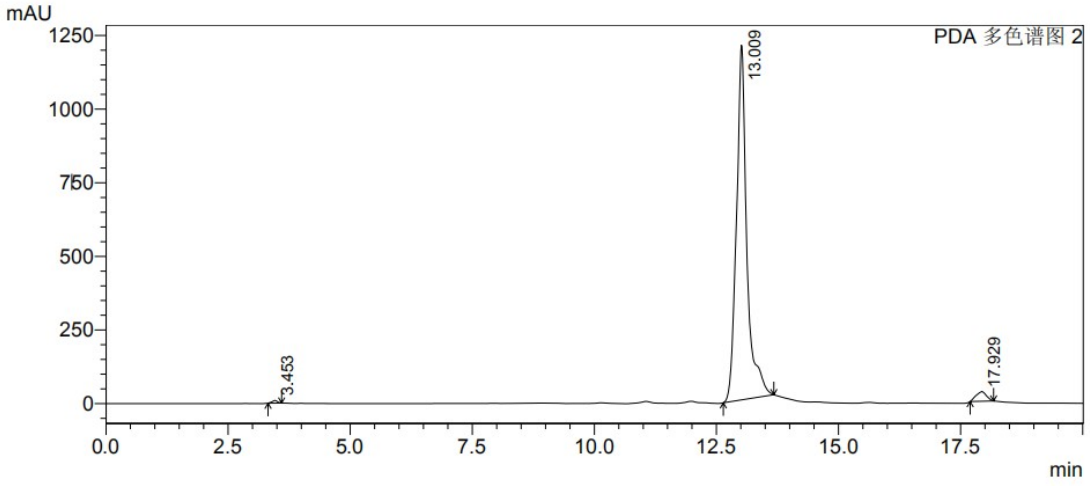

Fig. S3. HPLC spectrum of peptide Fmoc-GFFG.

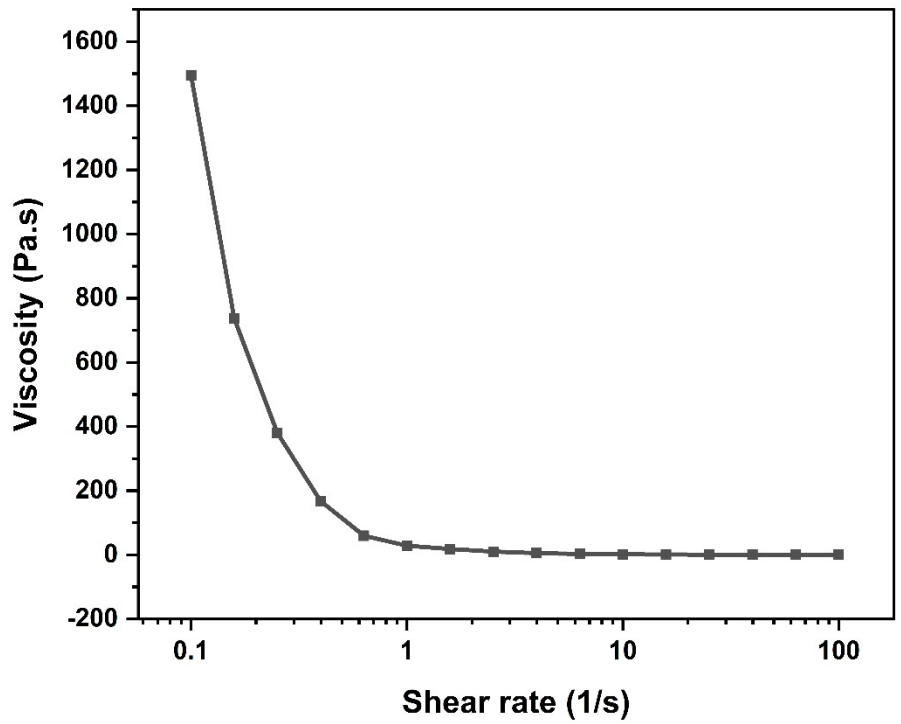

Fig. S4. Flow sweep of Fmoc-GFFG/SBE-β-CD (1%/2 eq) hydrogel.

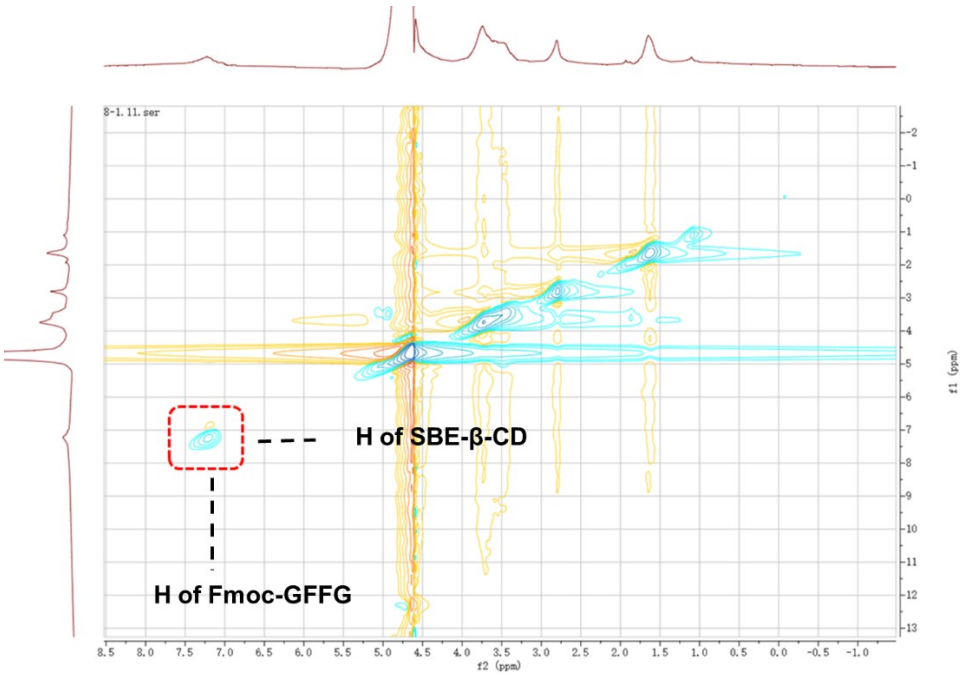

Fig. S5. 2D NOESY spectrum of the Fmoc-GFFG/SBE-β-CD inclusion complex.

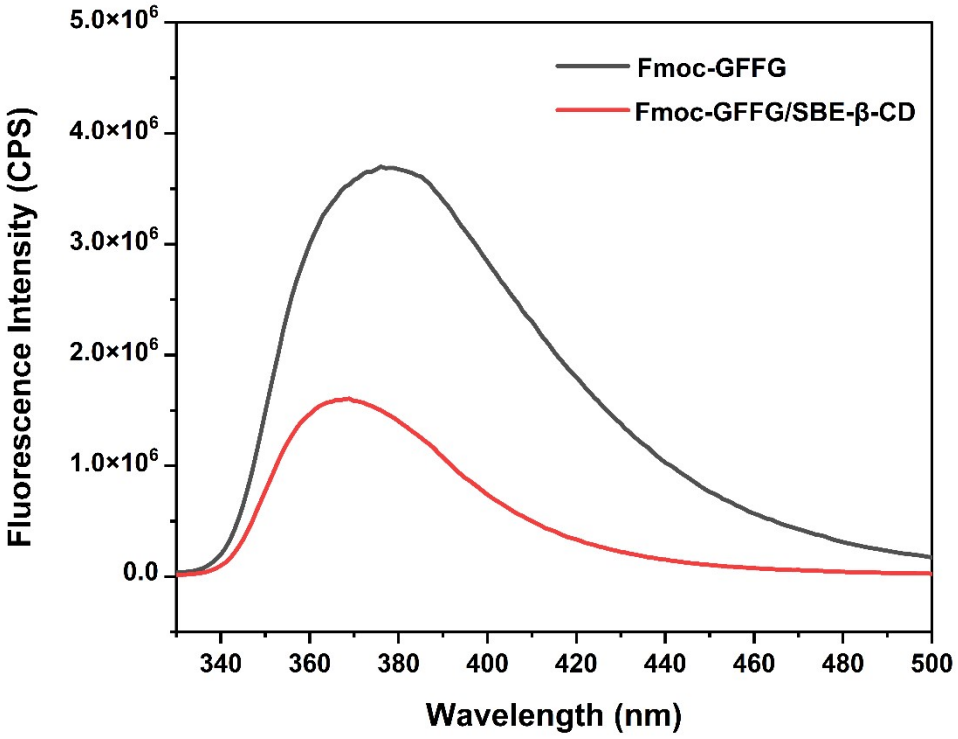

Fig. S6. Fluorescence spectra of Fmoc-GFFG with or without SBE-β-CD.

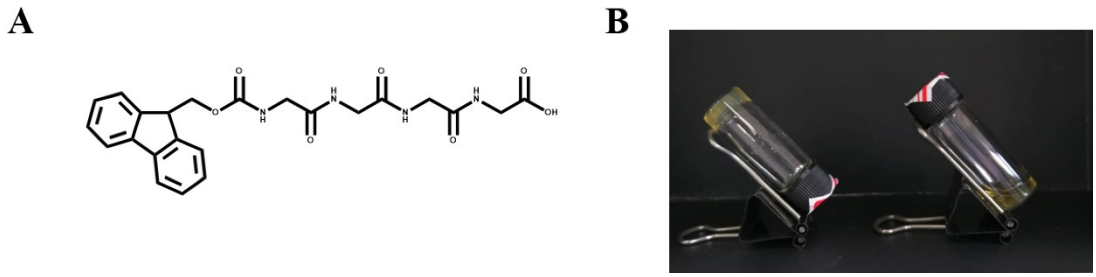

Figure. S7. Molecular structure of Fmoc-GGGG. (B) Gel pictures of Fmoc-GGGG (2%) without (left) or with 2 eq SEB-β-CD (right).

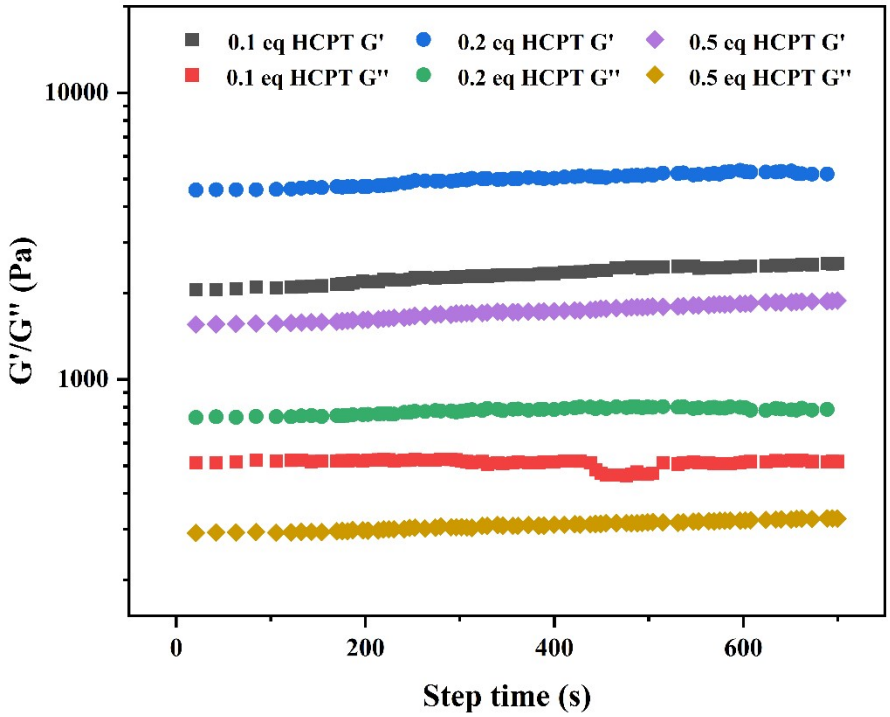

Fig. S8. Dynamic time sweep of Fmoc-GFFG/SBE-β-CD hydrogels with different HCPT equivalent.

Table S1. Gelation time of Fmoc-GFFG with different types of β-CD.

Formulation	Fmoc-GFFG	+ β-CD	+ HP-β-CD	+ SBE-β-CD
GelationTime	60 min	—	24 h	10 min

—, no gelation

Table S2. Gelation time of Fmoc-GFFG with various ratios of SBE-β-CD.

SBE-β-CD	0 eq	0.5 eq	2 eq	4 eq	6 eq	8 eq
Gelation Time	60 min	40 min	10 min	24 h	—	—

—, no gelation

Table S3. The association constants between SBE-β-CD and various anti-tumor drugs.

Anti-tumor drug	SBE-β-CD（mol/L）	Inclusion Complex（μg/ml）	Slope	Intercede	Complexation Constant
Gem	0.0000	0.05979	0.5138483	0.0585215	18.06
	0.0411	0.07856			
	0.0657	0.09035			
	0.0986	0.11096			
	0.1315	0.12606			
CDDP	0.0164	2601.5	0.0534851	0.0080247	7.040
	0.0247	2807.25			
	0.0370	3032.25			
	0.0493	3174.75			
	0.0740	3549.75			
HCPT	0.0000	0.000007	0.0023623	0.0000064	368.1
	0.0205	0.000056			
	0.0288	0.000071			
	0.0329	0.000083			
	0.0411	0.000106			
Cur	0.0329	0.000003	0.0006263	0.0000189	33.09
	0.0657	0.000022			
	0.0986	0.000041			
	0.1315	0.000061			
	0.1643	0.000087			

Table S4. The calculated parameters for the HCPT release from various hydrogel formulations using a Ritger-Peppas model.

Formulation	n	k	R^2
Fmoc-GFFG@HCPT	0.3500	0.1063	0.9844
Fmoc-GFFG/SBE-β-CD@HCPT	0.5467	0.0961	0.9977

Table S5. IC_{50} values of HCPT, SBE-β-CD@HCPT and Fmoc-GFFG/SBE-β-CD@HCPT.

Formulation	IC_{50}
HCPT	0.25
SBE-β-CD@HCPT	0.36
Fmoc-GFFG/SBE-β-CD@HCPT	0.58