

Figure S1 The ^1H NMR spectrum of ZW800-1 in DMSO- d_6 . Y-axis is the intensity of the peak.

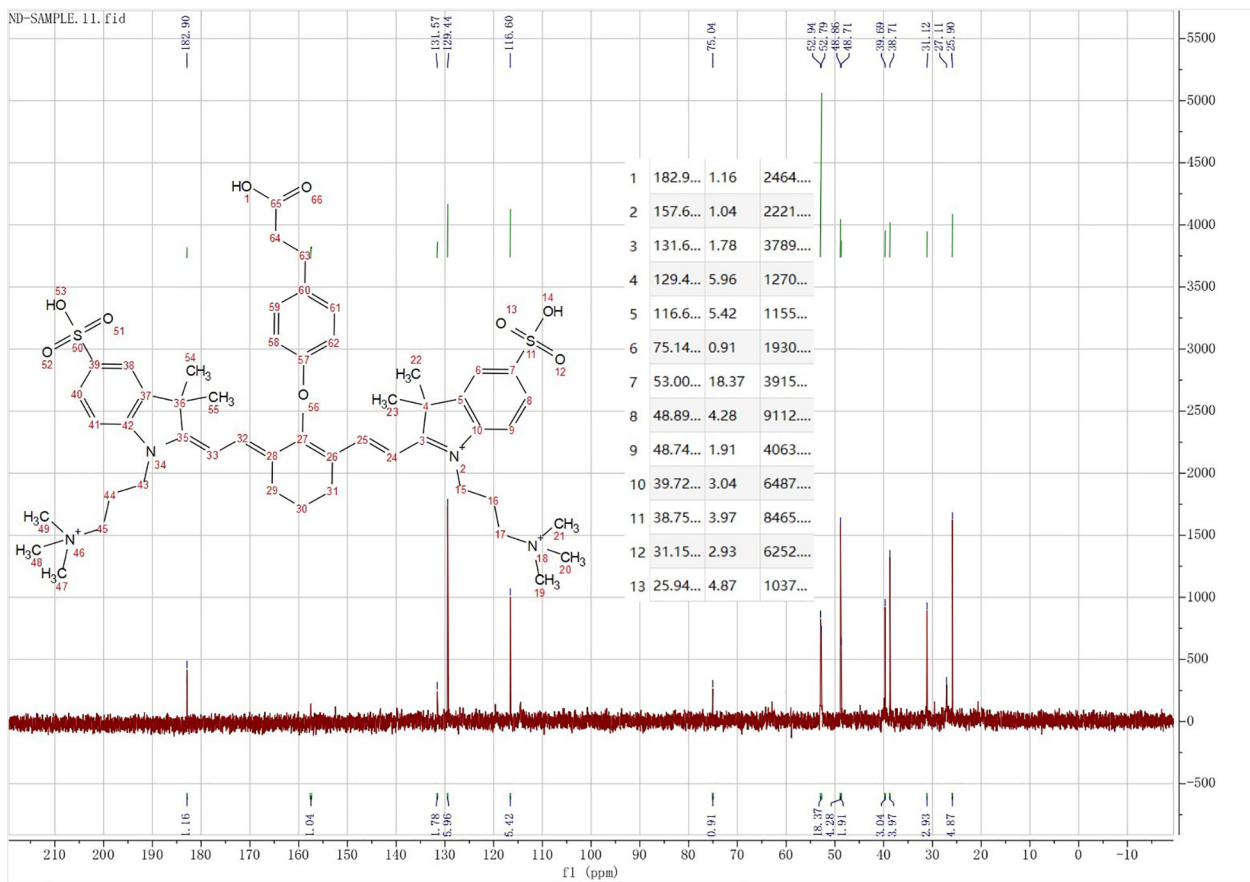
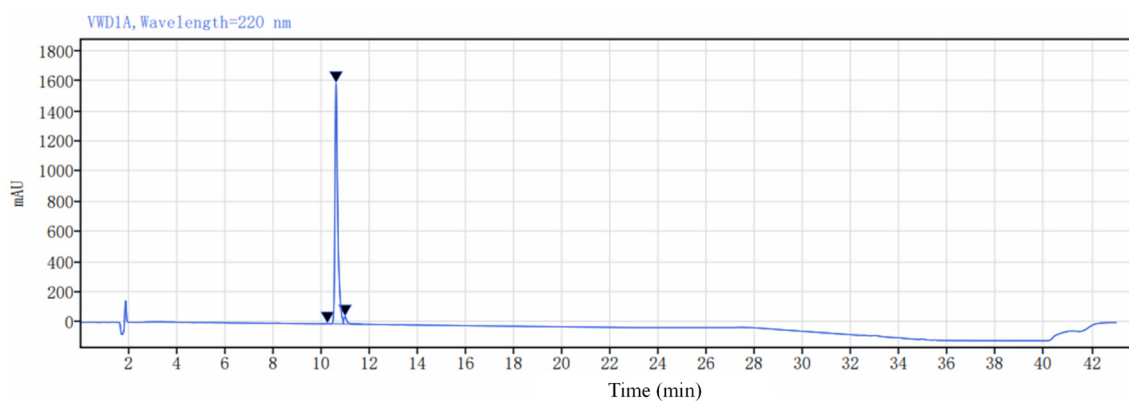


Figure S2 The ^{13}C NMR spectrum of ZW800-1 in DMSO- d_6 . Y-axis is the intensity of the peak.



Signal VWD1A, Wavelength=220 nm

Ret.Time (min)	Height	Area	Area%
10.245	1.38	19.247	0.15
10.604	1600.17	12776.281	96.52
10.979	49.44	441.070	3.33
Total		13236.60	

Figure S3 The HPLC spectrum of ZW800-1. HPLC, high-performance-liquid-chromatography.

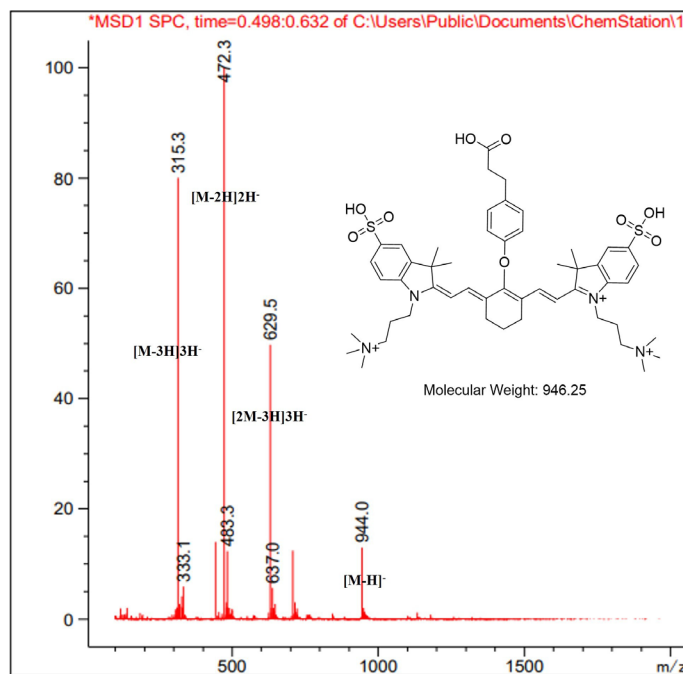


Figure S4 The mass spectrometry of ZW800-1. Y-axis is relative abundance of ions.

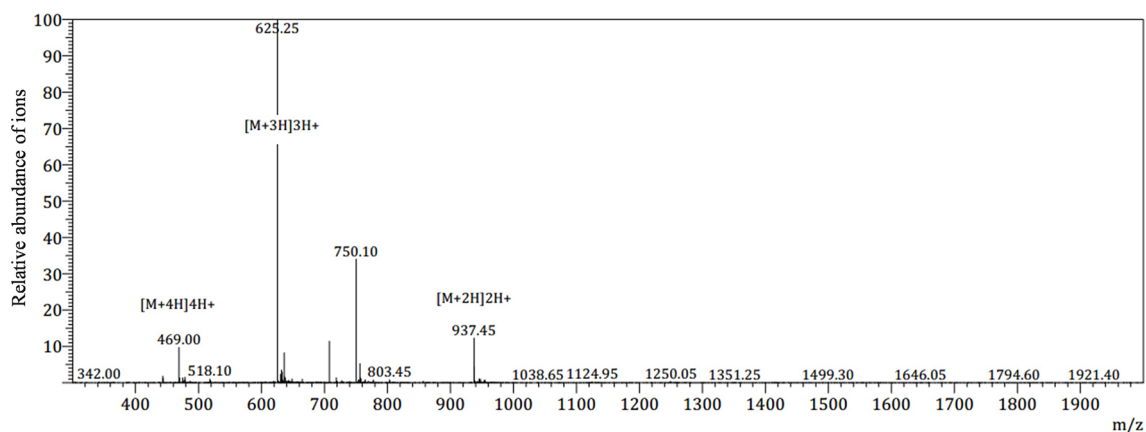
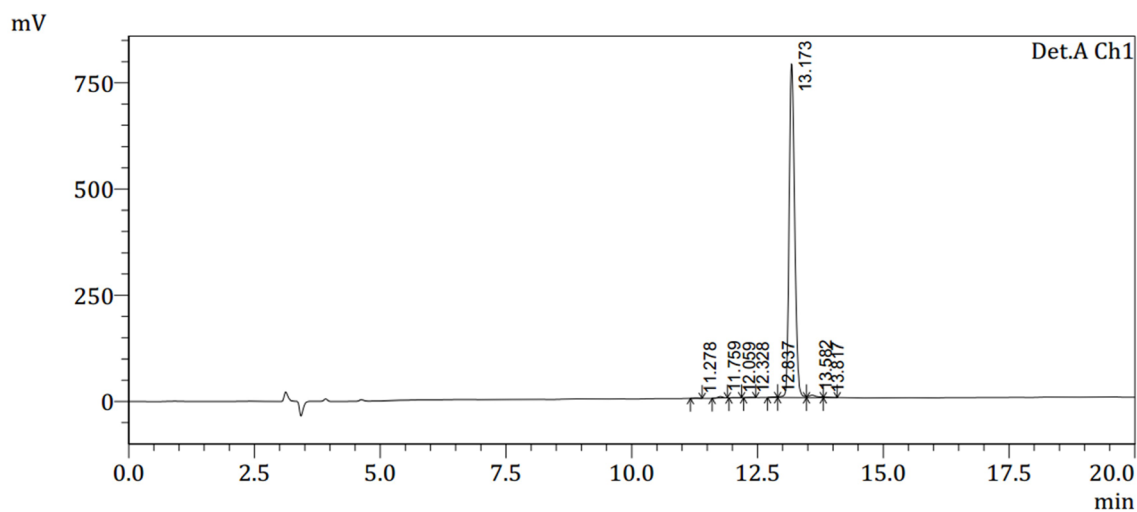


Figure S5 The mass spectrometry of iRGD-ZW800.



Detector A Ch1 220nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.278	8317	1195	0.135	0.149
2	11.759	25759	3653	0.420	0.456
3	12.059	2893	331	0.047	0.041
4	12.328	5105	728	0.083	0.091
5	12.837	12259	1596	0.200	0.199
6	13.173	6008485	786215	97.865	98.179
7	13.582	65274	5851	1.063	0.731
8	13.817	11504	1229	0.187	0.153
Total		6139596	800798	100.000	100.000

Figure S6 The HPLC spectrum of iRGD-ZW800. HPLC, high-performance-liquid-chromatography.

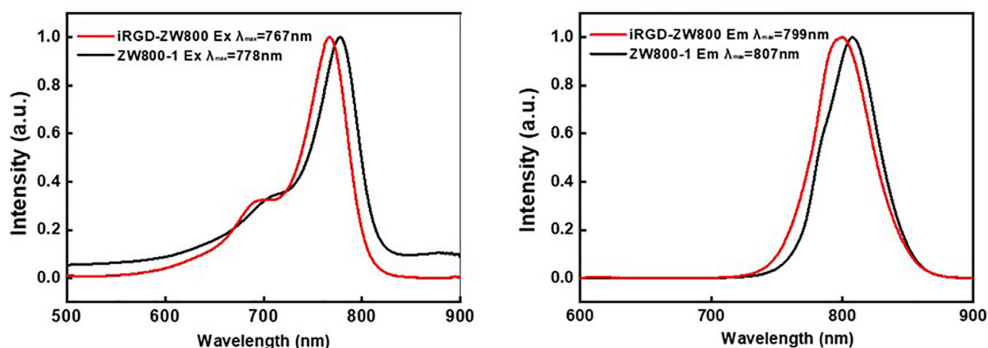


Figure S7 The excitation and emission spectrum of iRGD-ZW800.

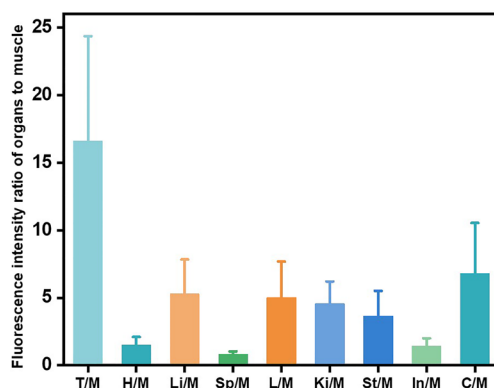


Figure S8 The fluorescence intensity ratio of organs (T, tumor; H, heart; L, lung; Sp, spleen; St, stomach; Li, liver; Ki, kidney; In, intestine; C, colon) to muscle.

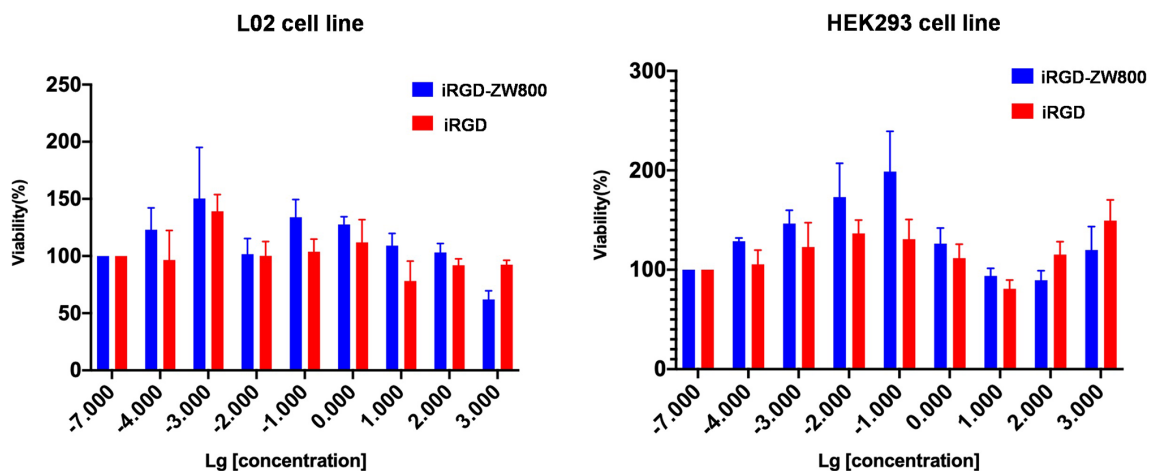


Figure S9 Assessment of cell biocompatibility of the fluorescent molecular imaging probe iRGD-ZW800 and iRGD.