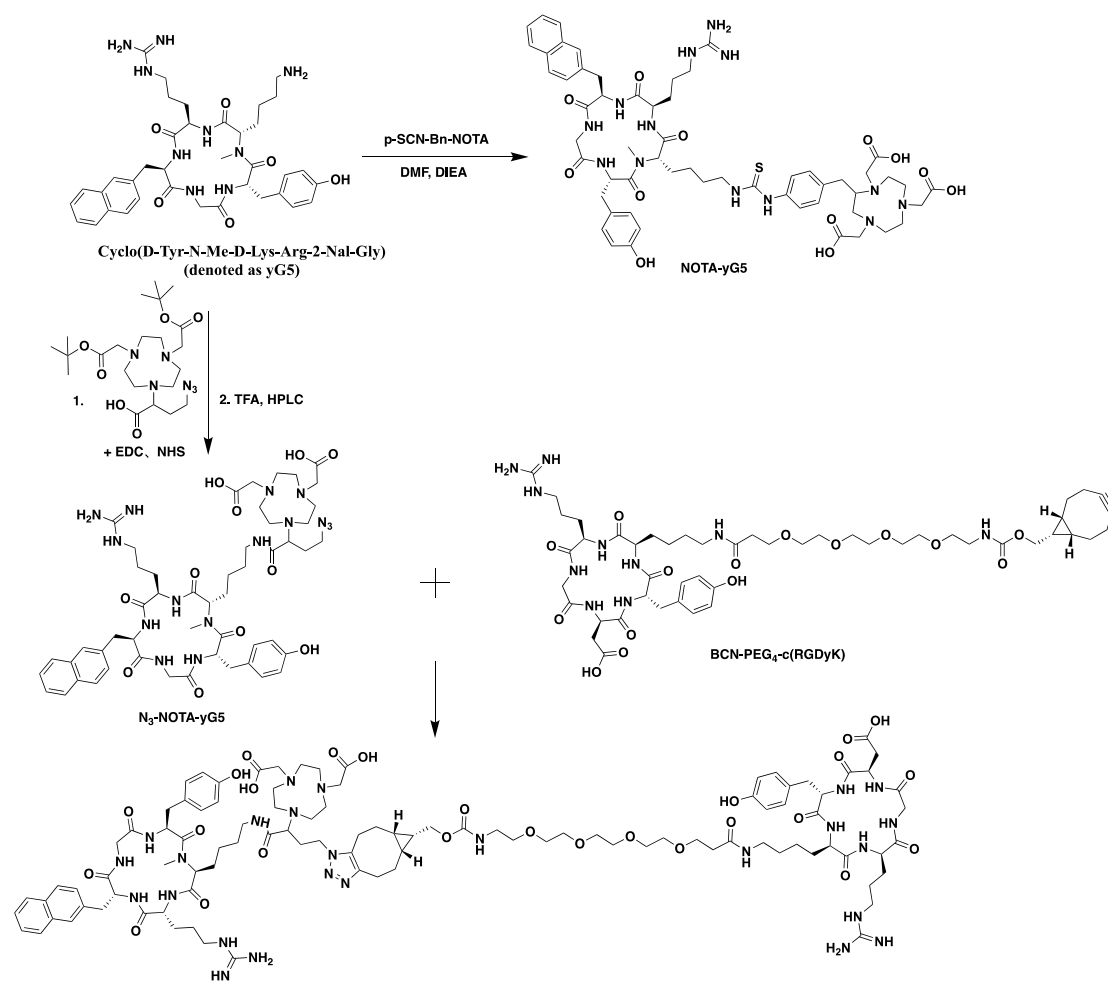
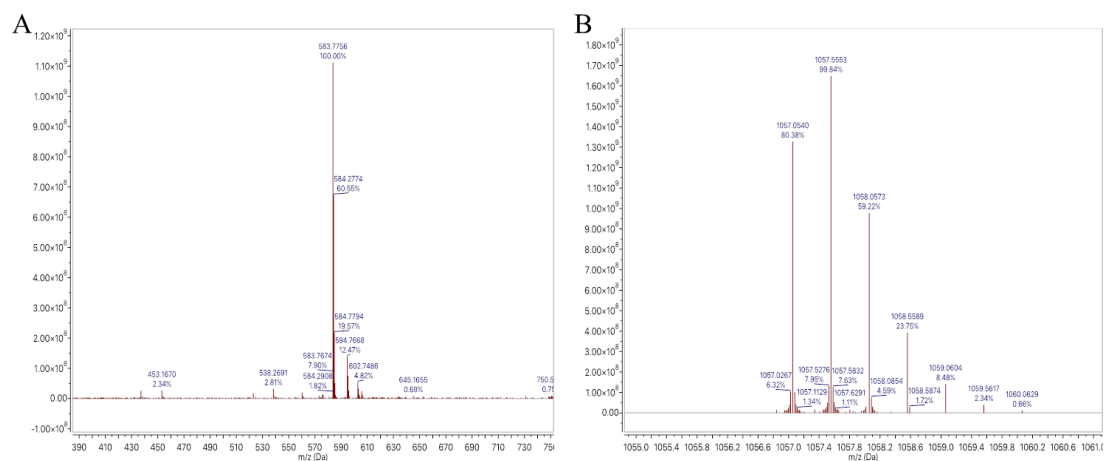


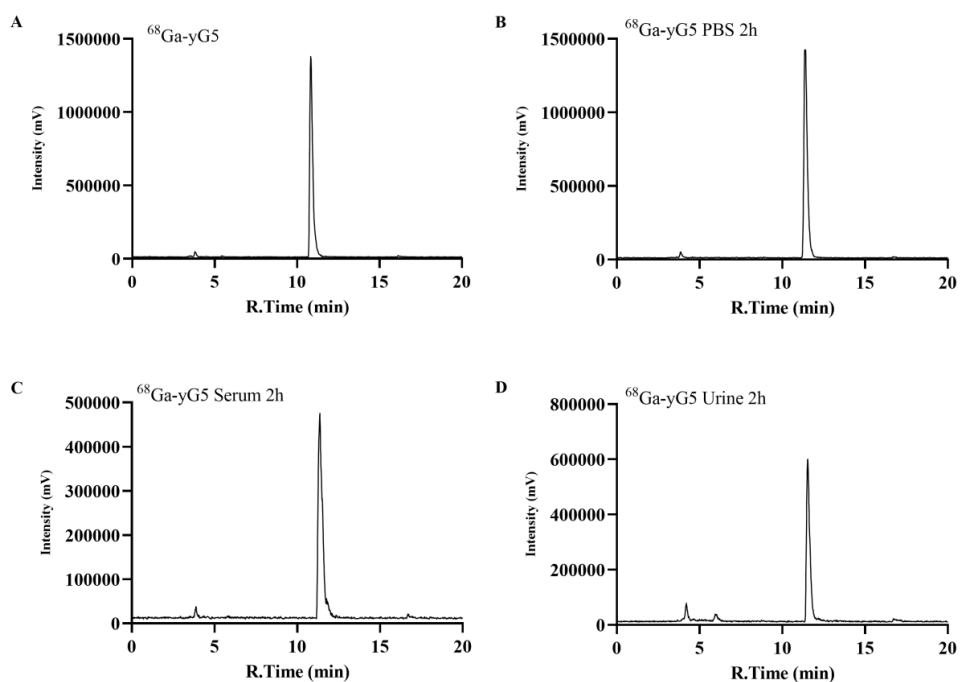
## Supplementary materials



**Scheme S1.** Synthesis route of NOTA-yG5 and NOTA-yG5-RGD.



**Figure S1.** Mass spectra of NOTA-yG5 (A) and NOTA-yG5-RGD (B).



**Figure S2.** Identification and stability study of  $^{68}\text{Ga}$ -yG5. Analytic radio-HPLC chromatograms of  $^{68}\text{Ga}$ -yG5 (A). 2 h *in vitro* stability of  $^{68}\text{Ga}$ -yG5 in PBS (B), and serum (C). 2 h *in vivo* stability of  $^{68}\text{Ga}$ -yG5 in urine (D).

**Table S1.** Biodistribution results of  $^{68}\text{Ga}$ -yG5-RGD,  $^{68}\text{Ga}$ -yG5 and  $^{68}\text{Ga}$ -RGD in BxPC3 xenograft mice at 90 min p.i.

organs \ probes	$^{68}\text{Ga}$ -yG5-RGD	$^{68}\text{Ga}$ -yG5	$^{68}\text{Ga}$ -RGD
blood	0.18±0.03	0.45±0.07	0.11±0.02
brain	0.02±0.00	0.03±0.00	0.02±0.00
heart	0.34±0.04	0.35±0.05	0.35±0.06
lung	0.85±0.06	0.87±0.12	0.34±0.03
liver	5.58±0.24	7.08±0.88	1.27±0.15
spleen	1.15±0.41	1.49±0.13	0.59±0.08
kidney	2.89±0.40	2.67±0.10	1.58±0.11
stomach	0.85±0.07	0.76±0.06	0.84±0.04
small intestine	0.68±0.34	1.35±0.19	0.71±0.03
large intestine	0.70±0.06	0.63±0.10	0.74±0.04
muscle	0.19±0.02	0.24±0.05	0.14±0.02

bone	0.56±0.08	0.41±0.04	0.31±0.06
tumor	2.54±0.44	0.90±0.18**	1.21±0.06**
pancreas	0.20±0.02	0.21±0.00	0.27±0.07
<b>uptake ratio</b>			
tumor/blood	14.48±0.80	2.01±0.43***	10.76±2.04*
tumor/muscle	13.58±0.81	3.86±1.29***	8.61±0.61**
tumor/kidney	0.90±0.29	0.34±0.06*	0.77±0.06 <sup>ns</sup>
tumor/liver	0.46±0.10	0.13±0.04*	0.96±0.15 <sup>ns</sup>

(Note: each 5.55–7.4 MBq. Data are presented as mean ± SD (%ID/g, n = 4). ns  $P > 0.05$ , \* $P < 0.05$ , \*\* $P < 0.01$ , \*\*\* $P < 0.001$ )

**Table S2.** Biodistribution results of *in vivo* blocking assays.

<b>organs</b> <b>blocking</b>	<b>AMD3100</b> <b>blocking</b>	<b>RGD</b> <b>blocking</b>	<b>Dual</b> <b>blocking</b>
blood	0.15±0.02	0.25±0.03	0.34±0.06
brain	0.02±0.01	0.01±0.00	0.02±0.00
heart	0.22±0.05	0.16±0.05	0.48±0.07
lung	0.67±0.25	1.01±0.31	0.80±0.32
liver	4.46±0.73	5.59±1.06	2.78±0.19
spleen	0.76±0.10	0.70±0.08	0.75±0.09
kidney	1.93±0.25	2.04±0.31	3.29±0.69
stomach	0.63±0.15	0.26±0.11	0.57±0.08
small intestine	0.35±0.08	0.22±0.03	0.52±0.11
large intestine	0.45±0.08	0.27±0.08	0.53±0.12
muscle	0.14±0.05	0.14±0.06	0.28±0.08
bone	0.49±0.05	0.50±0.06	0.81±0.18
tumor	0.89±0.28**	0.47±0.05**	0.37±0.07**
pancreas	0.16±0.03	0.10±0.03	0.25±0.06

(Note: Each mouse was co-injected of excess amount of unlabeled AMD3100 (10mg/kg), RGD (10mg/kg), and AMD3100 (10mg/kg) + RGD (10mg/kg) at 30 min p.i. each 5.55–7.4 MBq. Data

are presented as mean  $\pm$  SD (%ID/g, n = 4). ns  $P>0.05$ , \*\* $P<0.01$ )

**Table S3.** Biodistribution results of  $^{68}\text{Ga}$ -yG5-RGD in BxPC3 and MX-1 xenograft mice at 90 min p.i.

<del>organs</del>	<del>models</del>	BxPC3	MX-1
	blood	0.18 $\pm$ 0.03	0.15 $\pm$ 0.03
	brain	0.02 $\pm$ 0.00	0.03 $\pm$ 0.01
	heart	0.34 $\pm$ 0.04	0.42 $\pm$ 0.09
	lung	0.85 $\pm$ 0.06	0.86 $\pm$ 0.21
	liver	5.58 $\pm$ 0.24	6.08 $\pm$ 0.96
	spleen	1.15 $\pm$ 0.41	1.39 $\pm$ 0.23
	kidney	2.89 $\pm$ 0.40	4.30 $\pm$ 0.84
	stomach	0.85 $\pm$ 0.07	1.15 $\pm$ 0.28
	small intestine	0.68 $\pm$ 0.34	0.76 $\pm$ 0.18
	large intestine	0.70 $\pm$ 0.06	0.83 $\pm$ 0.13
	muscle	0.19 $\pm$ 0.02	0.27 $\pm$ 0.06
	bone	0.56 $\pm$ 0.08	0.87 $\pm$ 0.19
	tumor	2.54 $\pm$ 0.44	0.42 $\pm$ 0.11***
	pancreas	0.20 $\pm$ 0.02	0.22 $\pm$ 0.05

(Note: each 5.55–7.4 MBq. Data are presented as mean  $\pm$  SD (%ID/g, n = 4). ns  $P>0.05$ , \*\*\* $P<0.001$ )