Supporting Information for

Original article

Whole-body PET tracking of a D-dodecapeptide and its radiotheranostic potential for PD-L1 overexpressing tumors

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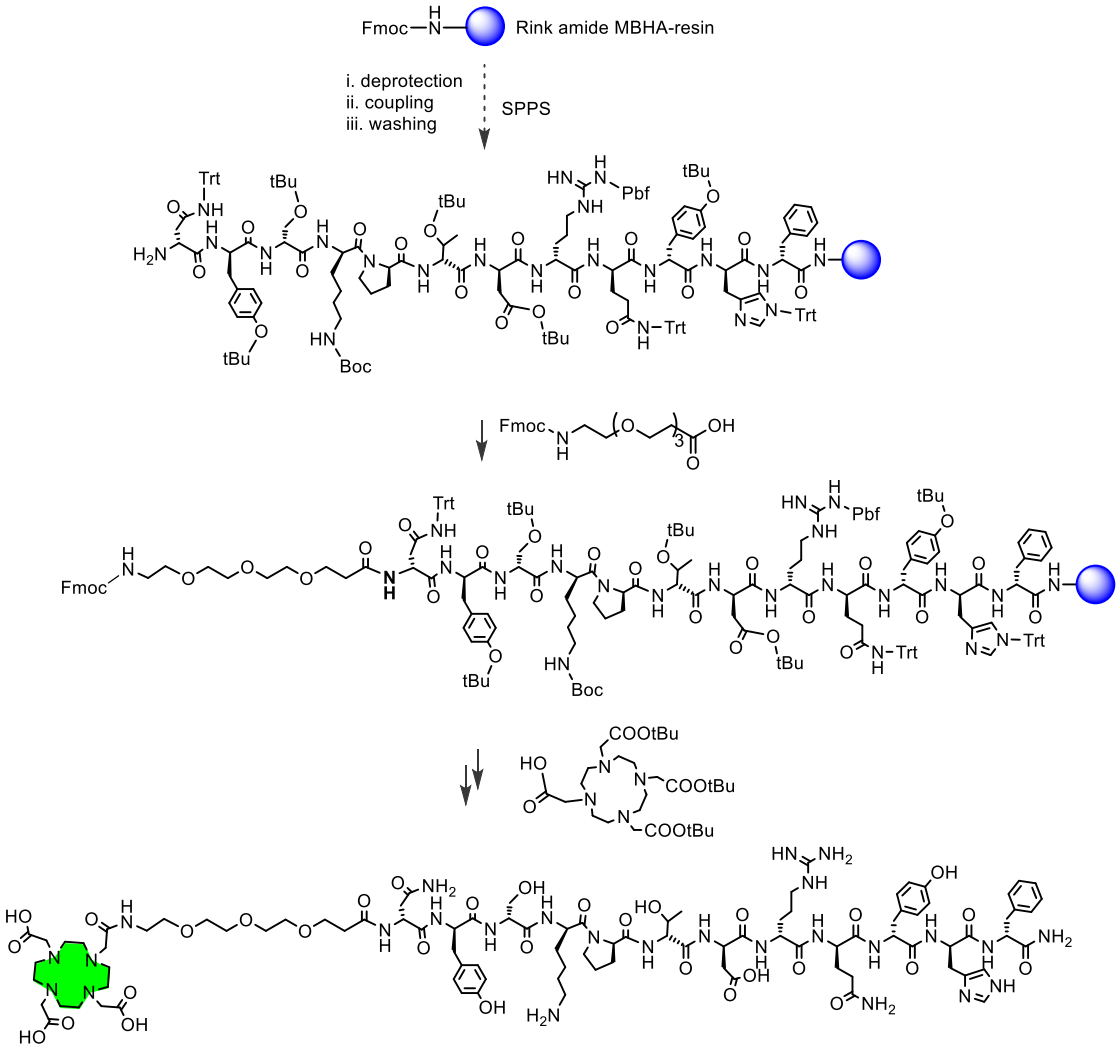
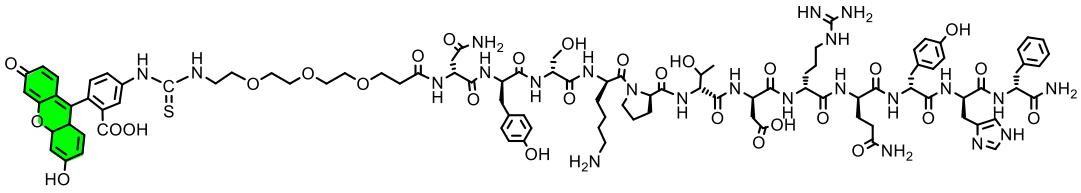


Scheme S1 Fmoc-based solid-phase peptide synthesis of DPA-DOTA.



Scheme S2 Chemical structure of FITC-DPA.

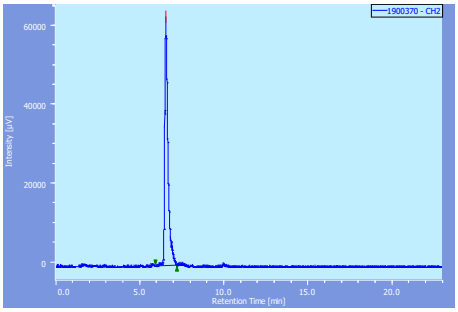


Figure S1 HPLC spectrum of [^{64}Cu]DPA after 24 h incubation in mouse serum.

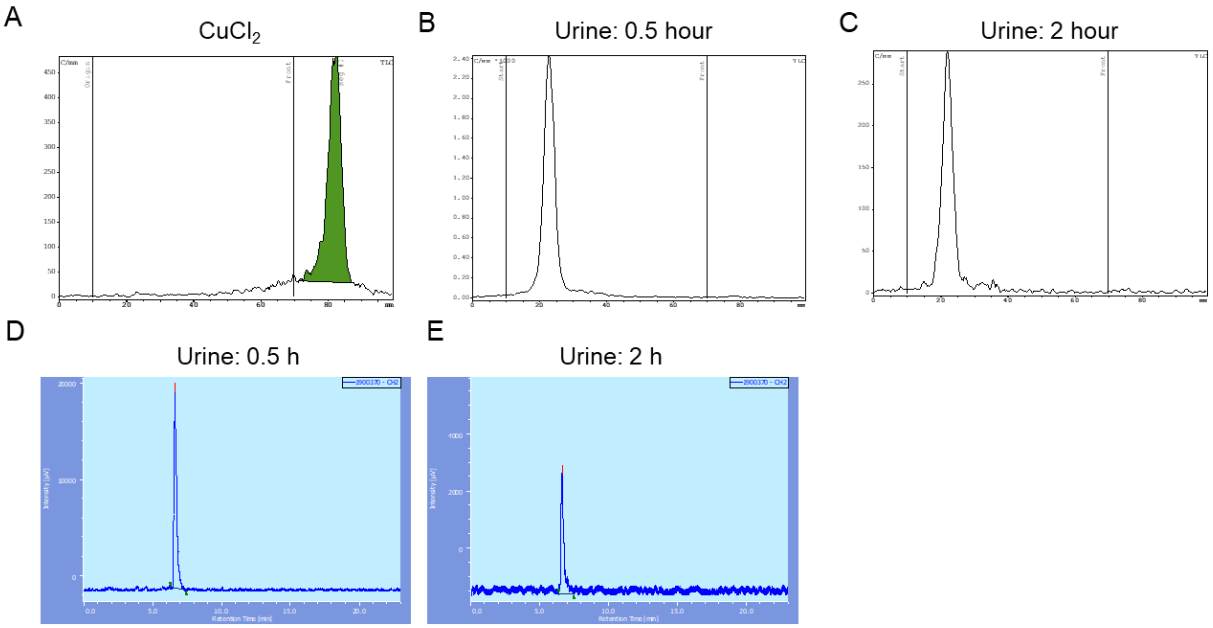


Figure S2 Metabolite study of [^{64}Cu]DPA. (A) Radio TLC curve of $^{64}CuCl_2$. (B and C) Radio TLC curves of mouse urine samples that were collected at 0.5 and 2 h after intravenous injection of [^{64}Cu]DPA. (D and E) HPLC spectra of mouse urine samples that were collected at 0.5 and 2 h after intravenous injection of [^{64}Cu]DPA.

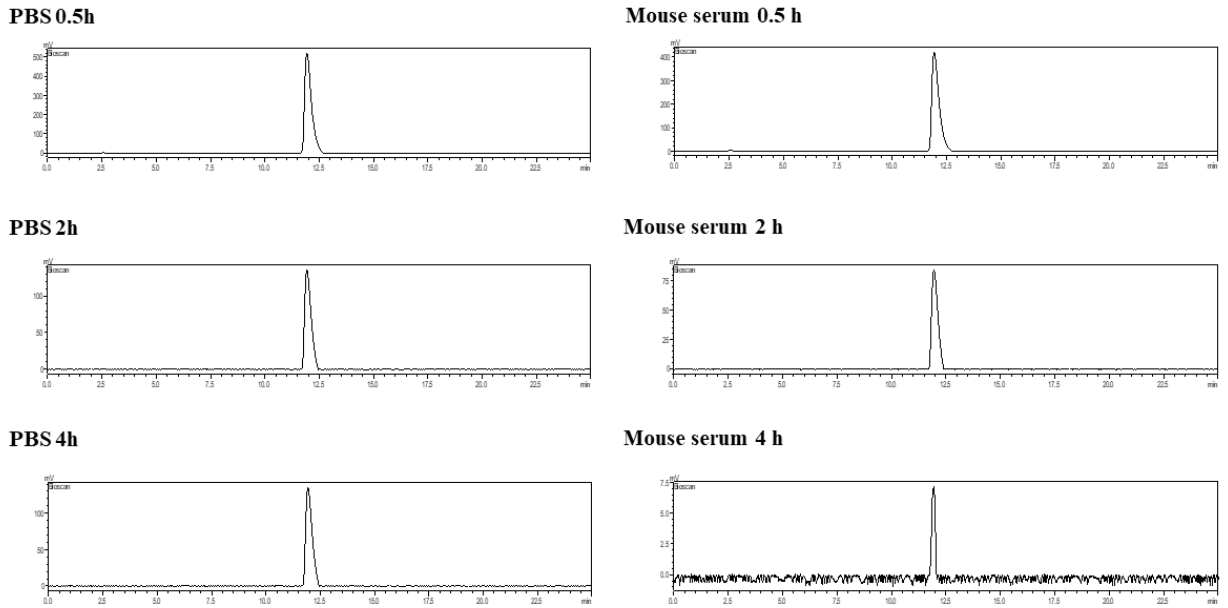


Figure S3 HPLC curves of [^{68}Ga]DPA after incubation for 0.5, 2, and 4 h in PBS or mouse serum.

Table S1. Radiolabeling and quality control of [^{64}Cu]DPA and [^{68}Ga]DPA. Radiochemical yield (RCY), molar activity, and radiochemical purity of the as-prepared tracers. Data represent mean SD (*n* =7).

Tracers	[^{64}Cu]DPA	[^{68}Ga]DPA
Radiochemical yield (%)	>99	>95
Molar activity (GBq μmol^{-1})	74 ± 5	37 ± 8
Radiochemical purity[a] (%)[a]	>95	>95

[a]The radiochemical purity was determined by HPLC under conditions as follows: YMC-Triat-C18 column (4.6 mm i.d. 150 mm, 5 mm); solvent gradient of 10%–90% acetonitrile (0.1% trifluoroacetic acid (TFA)), 20 min; flow rate of 1 mL/min.

Table S2 Biodistribution of [^{64}Cu]DPA at 20, 40, 60, and 80 min after i.v. injection (*n* = 3 per time point) in C57BL/6J mice.

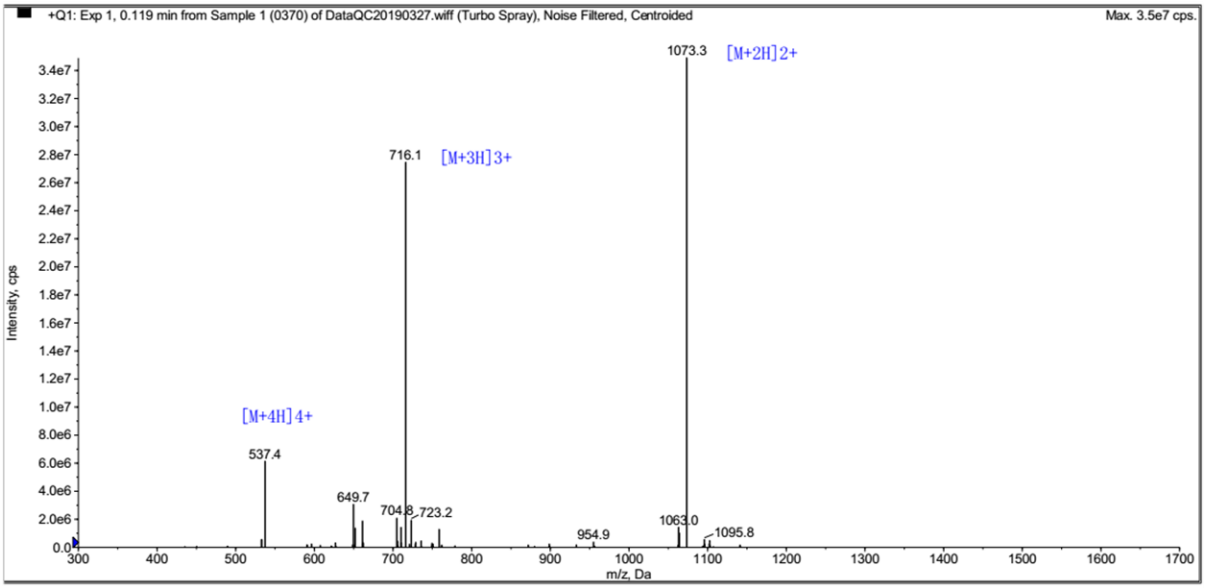
	[^{64}Cu]DPA			
	20 min	40 min	60 min	80 min
Blood	2.34 ± 0.38	0.97 ± 0.13	0.20 ± 0.01	0.14 ± 0.03
Heart	0.81 ± 0.15	0.56 ± 0.14	0.21 ± 0.02	0.18 ± 0.01
Lung	1.78 ± 0.29	1.31 ± 0.07	0.78 ± 0.06	0.75 ± 0.02

Thymus	0.72	±	0.17	0.78	±	0.47	0.17	±	0.01	0.15	±	0.01
Liver	1.40	±	0.19	1.44	±	0.06	1.29	±	0.11	1.29	±	0.08
Pancreas	0.51	±	0.08	0.33	±	0.01	0.22	±	0.05	0.19	±	0.04
Spleen	0.63	±	0.16	1.27	±	1.32	0.17	±	0.01	0.17	±	0.03
Kidney	28.64	±	3.04	29.31	±	1.05	24.42	±	0.50	28.52	±	3.22
Stomach	1.15	±	0.71	1.07	±	0.44	0.49	±	0.10	0.62	±	0.24
S. intestine	1.36	±	0.36	1.32	±	0.23	0.89	±	0.08	0.82	±	0.10
Int. lym. node	3.90	±	0.23	0.87	±	0.05	0.59	±	0.46	0.39	±	0.15
Muscle	0.90	±	0.30	0.32	±	0.02	0.23	±	0.16	0.15	±	0.11
Bone	1.08	±	0.57	0.36	±	0.08	0.41	±	0.18	0.19	±	0.02
Testis	0.66	±	0.05	0.30	±	0.01	0.12	±	0.01	0.14	±	0.05
Brain	0.11	±	0.02	0.05	±	0.01	0.04	±	0.01	0.02	±	0.00

Table S3 Biodistribution of [^{68}Ga]DPA at 5, 30, 60, and 120 min after i.v. injection (n = 3 per time point) in BALB/c nude mice bearing U87MG tumors.

	[^{68}Ga]DPA							
	5 min			30 min			60 min			120 min		
blood	3.89	±	0.43	1.55	±	1.07	0.11	±	0.02	0.05	±	0.01
heart	1.19	±	0.39	0.52	±	0.33	0.06	±	0.02	0.05	±	0.02
liver	1.06	±	0.26	0.59	±	0.43	0.19	±	0.02	0.16	±	0.04
spleen	0.98	±	0.14	0.68	±	0.67	0.14	±	0.06	0.09	±	0.03
lung	1.64	±	0.42	1.03	±	0.90	0.13	±	0.05	0.09	±	0.02
kidney	19.23	±	1.95	16.13	±	1.51	11.50	±	0.44	5.20	±	0.31
stomach	1.54	±	0.10	0.61	±	0.35	0.08	±	0.01	0.08	±	0.03
intestinal	0.72	±	0.27	0.47	±	0.35	0.08	±	0.02	0.06	±	0.03
pancreas	1.88	±	0.28	0.77	±	0.75	0.16	±	0.03	0.13	±	0.03
muscle	2.21	±	0.27	0.71	±	0.37	0.18	±	0.02	0.14	±	0.04
bone	2.18	±	0.11	0.85	±	0.51	0.26	±	0.09	0.14	±	0.06
brain	0.19	±	0.04	0.11	±	0.08	0.03	±	0.01	0.02	±	0.01
tumor	4.50	±	0.32	3.77	±	0.27	2.99	±	0.03	0.89	±	0.19
fat	2.09	±	0.49	0.81	±	0.12	0.27	±	0.07	0.10	±	0.07

Mass spectrum of DOTA-DPA.



HPLC curve of DOTA-DPA.