

Synthesis and preclinical investigation of lactosamine-based radiopharmaceuticals for the detection of galectin-3-expressing melanoma cells

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Part 1: ^1H NMR and ^{13}C NMR spectra of compound 2, 3 and 4.

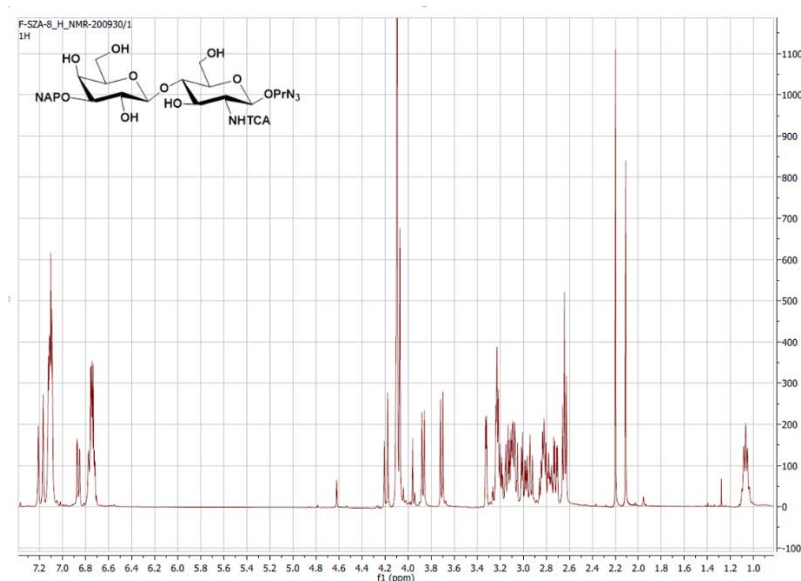


Figure S1 ^1H NMR spectrum of compound 2

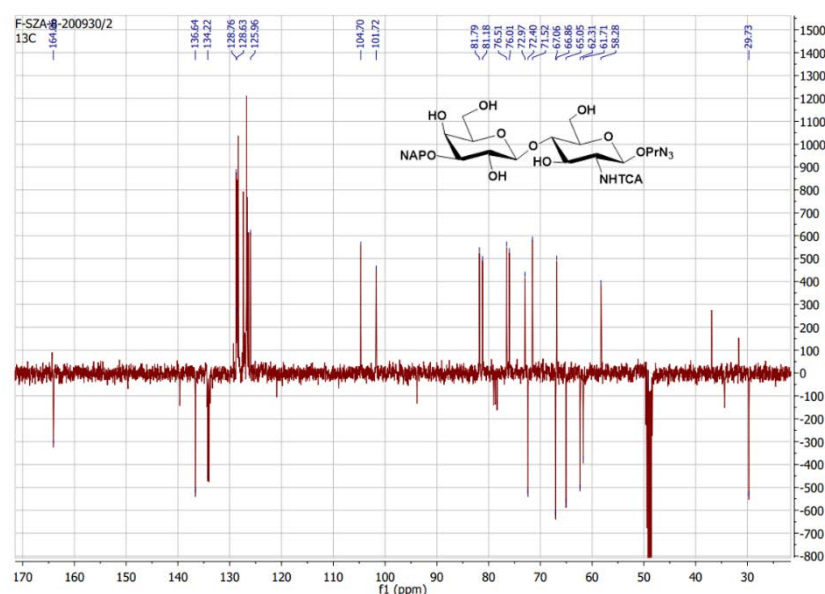


Figure S2 ^{13}C NMR spectrum of compound 2

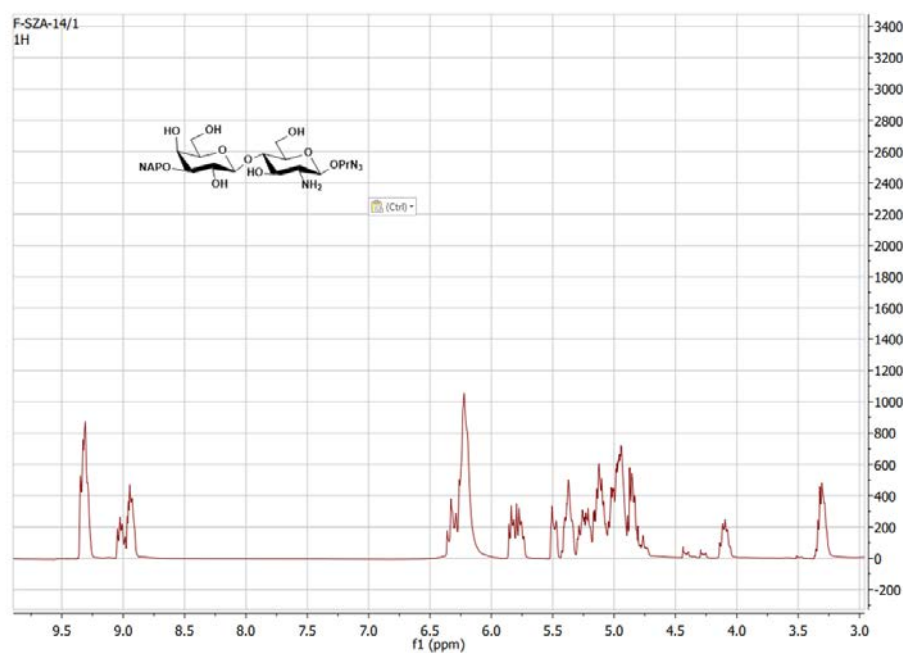


Figure S3 ¹H NMR spectrum of compound 3

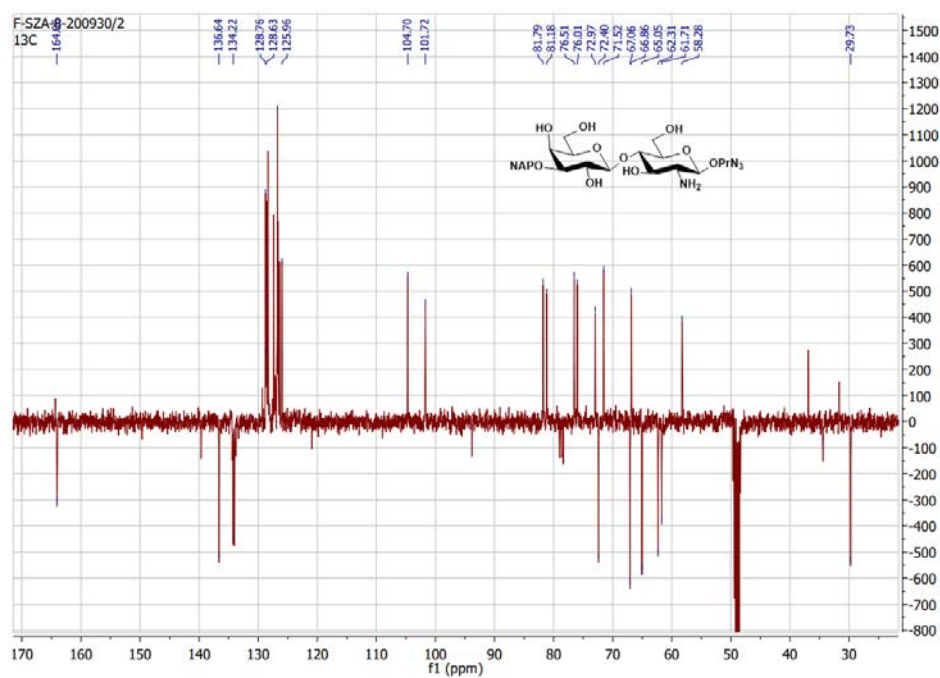
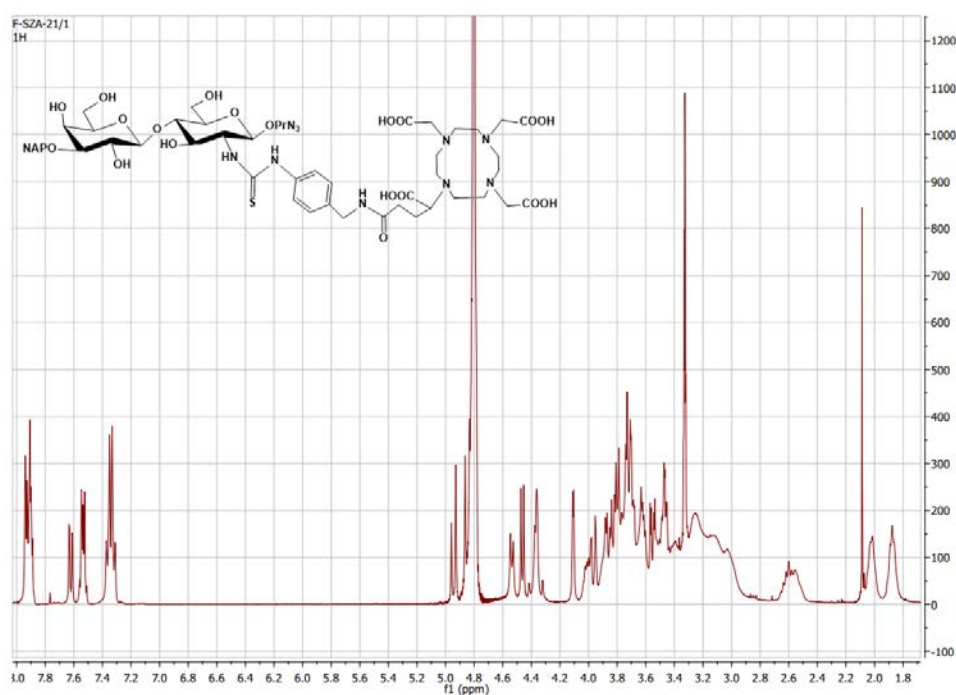


Figure S4 ¹³C NMR spectrum of compound 3

Figure S5 ^1H NMR spectrum of compound 4

Part 2: Mass spectra of compound 2, 3, 4, 7, 8 and 9

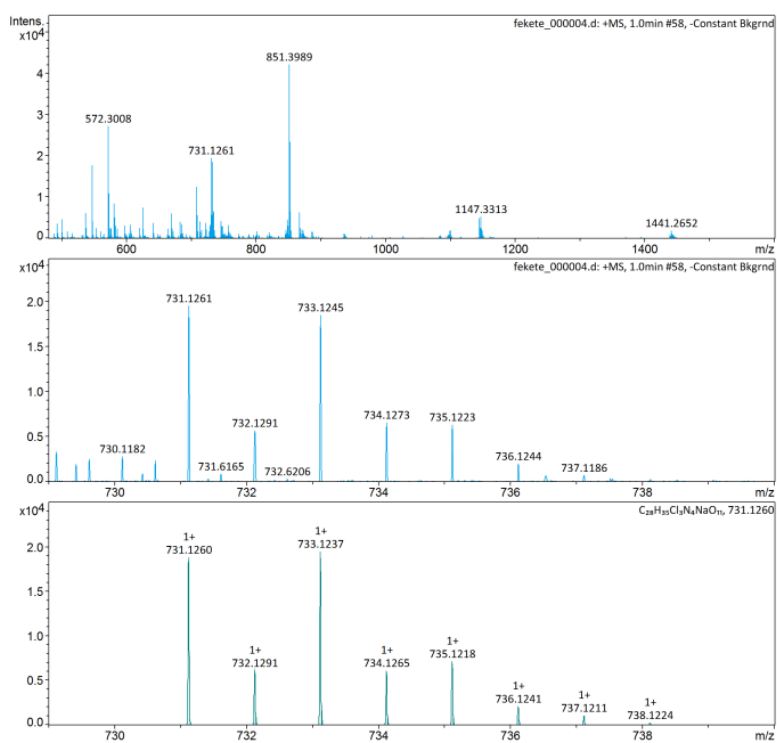


Figure S6 Mass spectrum of compound 2

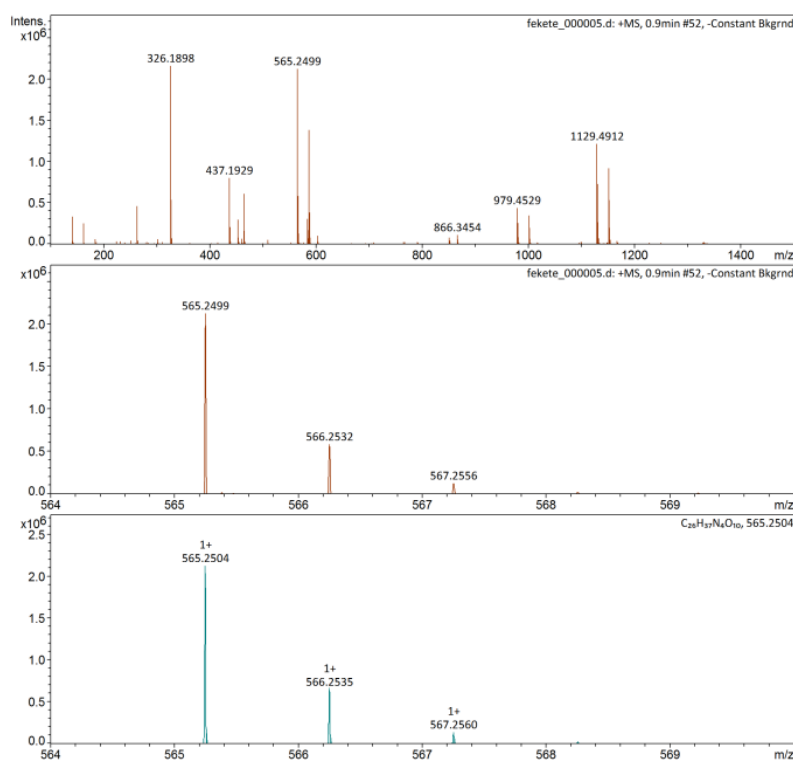


Figure S7 Mass spectrum of compound 3

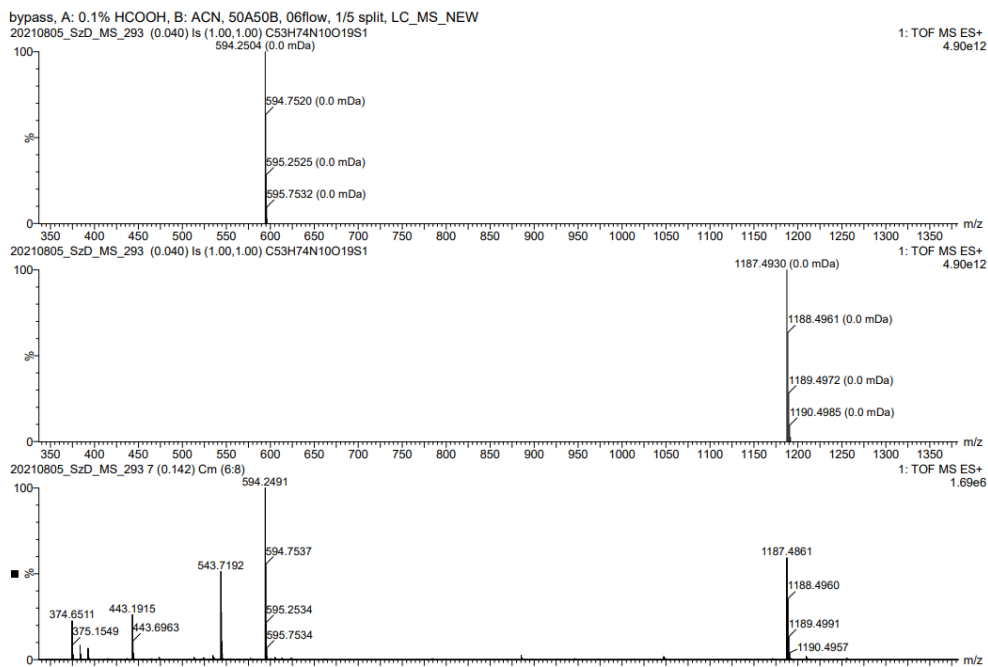


Figure S8 Mass spectrum of compound 4

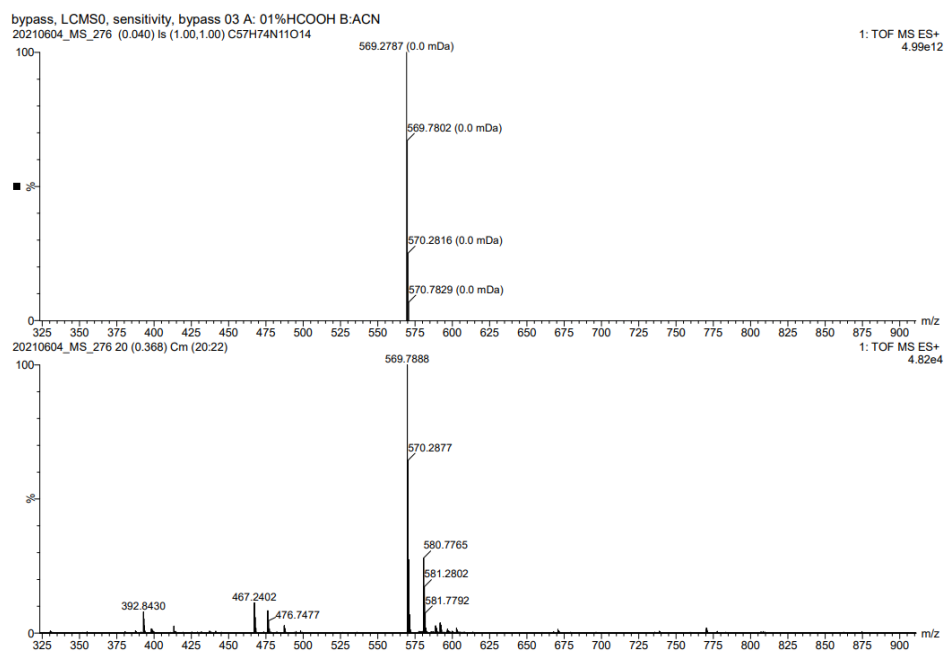


Figure S9 Mass spectrum of compound 7

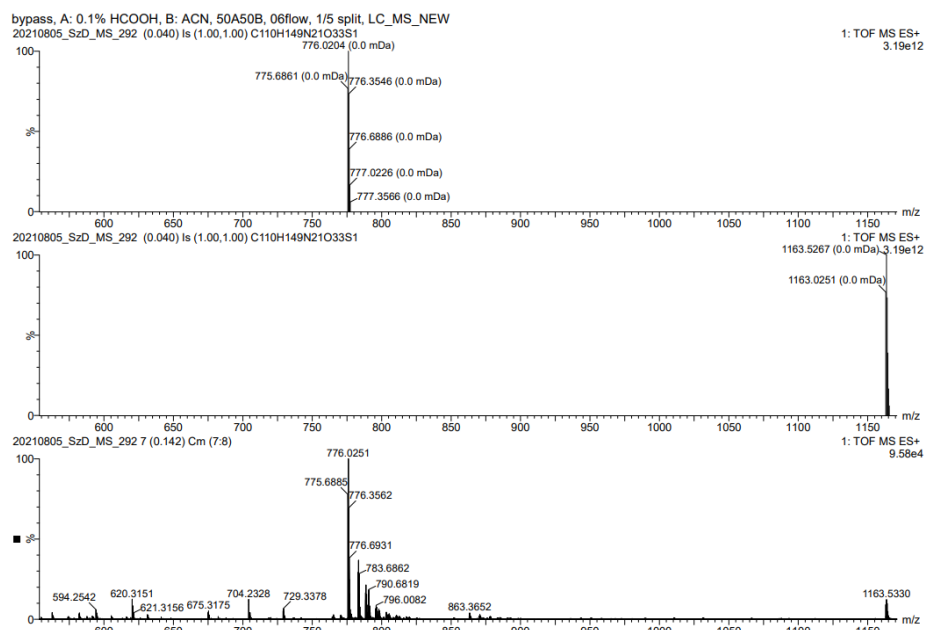


Figure S10 Mass spectrum of compound 8

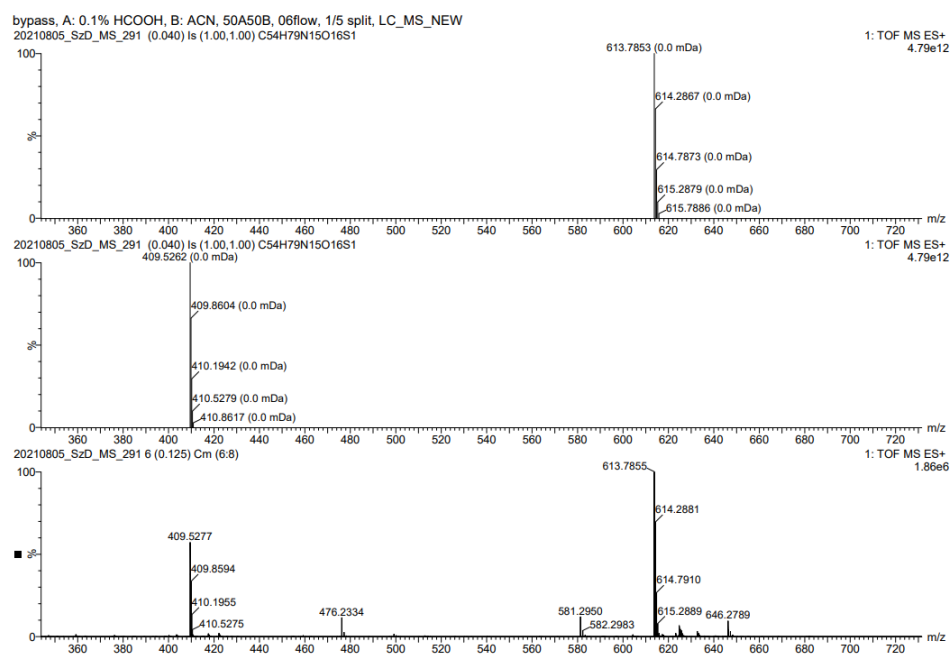
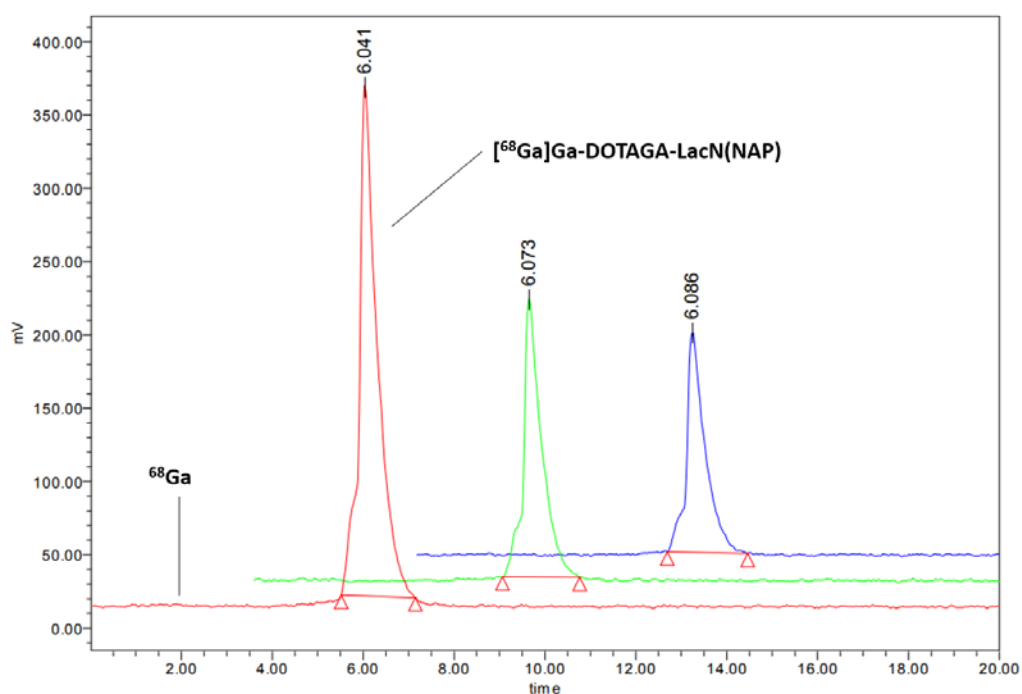


Figure S11 Mass spectrum of compound 9

Part 3: Stability studies of [^{68}Ga]Ga-DOTAGA-LacN(NAP) and [^{68}Ga]Ga-DOTAGA-LacN(NAP)-cRGDfK

Figure S12 Stability test of [^{68}Ga]Ga-DOTAGA-LacN(NAP) in 0.01 M Na_2EDTA solution.

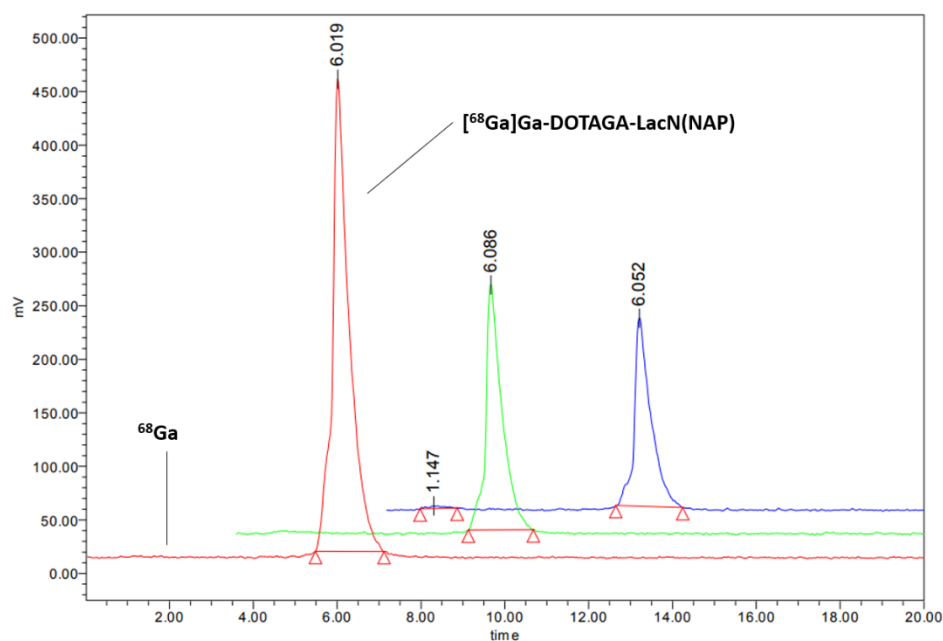


Figure S13 Stability test of $[^{68}\text{Ga}]\text{Ga-DOTAGA-LacN(NAP)}$ in 0.01 M oxalic acid solution.

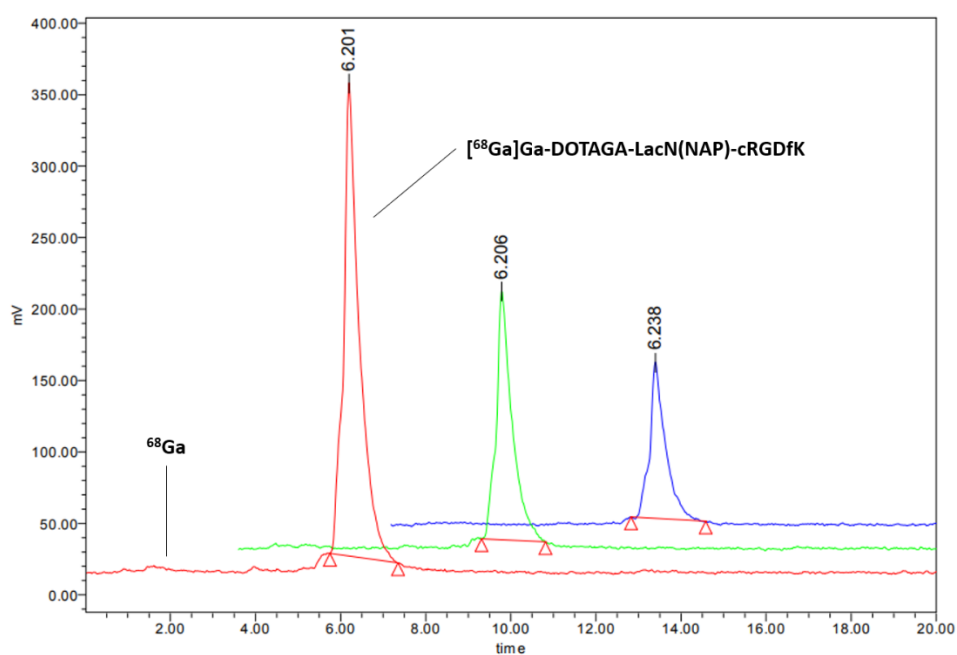


Figure S14 Stability test of $[^{68}\text{Ga}]\text{Ga-DOTAGA-LacN(NAP)-cRGDfK}$ in 0.01 M Na_2EDTA solution.



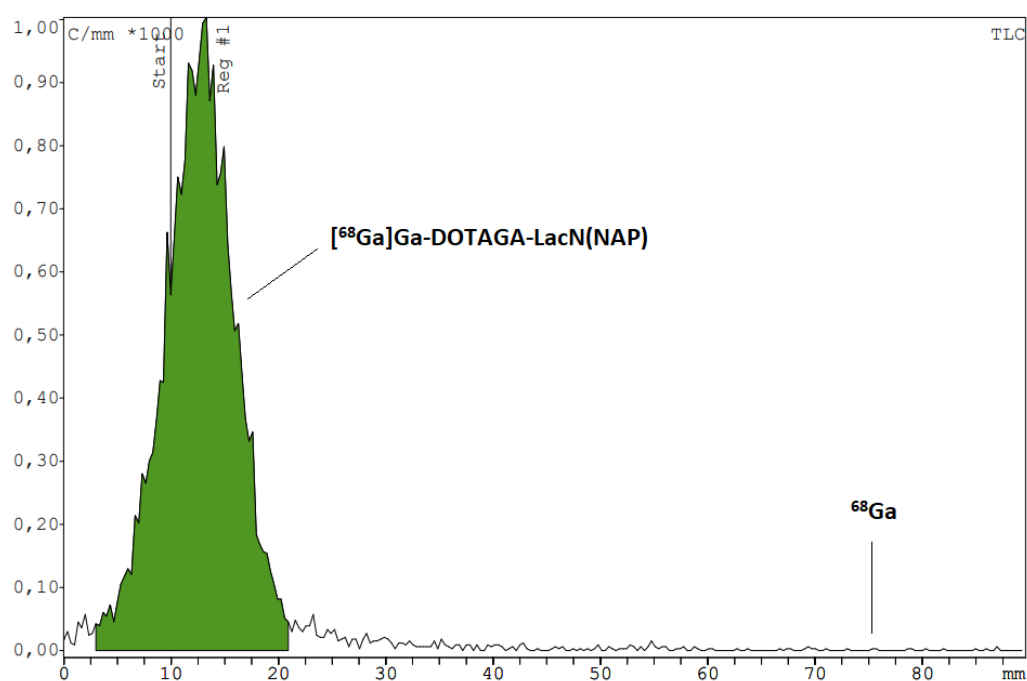


Figure S17 Stability test of $[^{68}\text{Ga}]\text{Ga-DOTAGA-LacN(NAP)}$ in human serum after 2 hours.

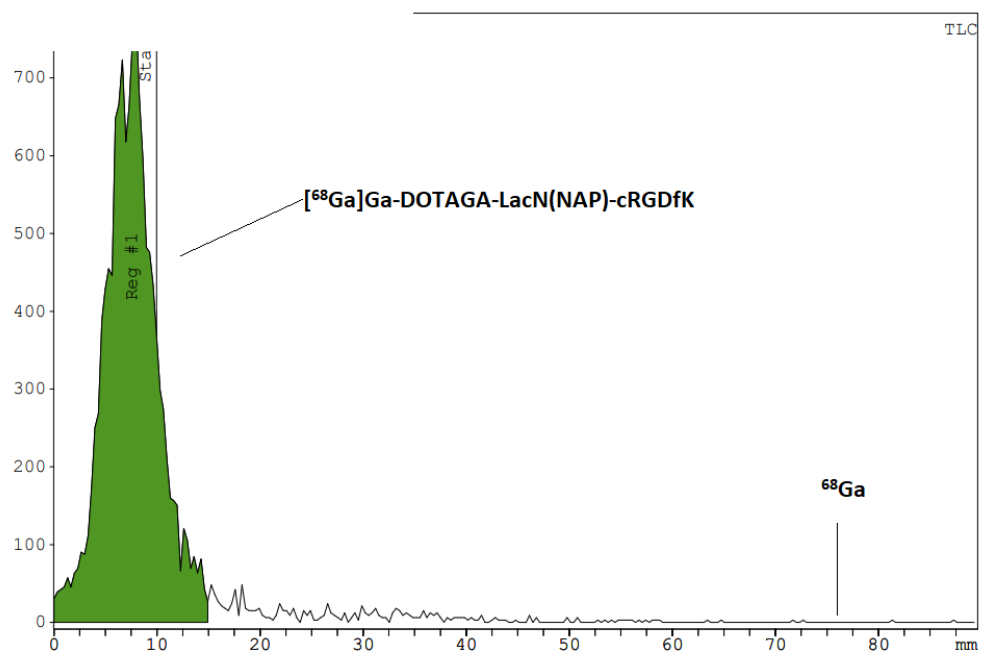


Figure S18 Stability test of $[^{68}\text{Ga}]\text{Ga-DOTAGA-LacN(NAP)-cRGDfK}$ in human serum after 2 hours.

TableS1 *Ex vivo* biodistribution of ^{68}Ga -labeled DOTAGA-LacN(NAP), DOTAGA-LacN(NAP)-cRGDfK, and DOTAGA-cRGDfK in B16-F10 tumor-bearing mice (n=5/radiopharmaceutical) 100 min after intravenous injection of the radiotracers. %ID/g tissue values are presented as mean \pm SD.

	^{68}Ga]Ga-DOTAGA-LacN(NAP)	^{68}Ga]Ga-DOTAGA-LacN(NAP)-cRGDfK	^{68}Ga]Ga-DOTAGA-cRGDfK
blood	0.29 \pm 0.01	0.58 \pm 0.14	0.37 \pm 0.05
liver	0.33 \pm 0.19	2.19 \pm 0.73	1.00 \pm 0.25
spleen	0.17 \pm 0.02	1.60 \pm 1.17	0.80 \pm 0.09
kidney	8.19 \pm 1.36	6.14 \pm 1.14	2.43 \pm 0.26
small intestine	0.27 \pm 0.9	1.77 \pm 0.96	0.78 \pm 0.20
large intestine	0.13 \pm 0.01	1.74 \pm 0.70	0.55 \pm 0.16
stomach	0.14 \pm 0.04	1.70 \pm 0.72	0.69 \pm 0.21
muscle	0.05 \pm 0.01	0.27 \pm 0.07	0.10 \pm 0.01
fat	0.11 \pm 0.08	0.17 \pm 0.13	0.19 \pm 0.08
lungs	0.35 \pm 0.06	1.54 \pm 0.62	0.66 \pm 0.18
heart	0.12 \pm 0.02	0.61 \pm 0.17	0.26 \pm 0.06
brain	0.02 \pm 0.01	0.06 \pm 0.01	0.03 \pm 0.01
bone (femur)	0.07 \pm 0.02	0.54 \pm 0.21	0.26 \pm 0.04
salivary glands	0.11 \pm 0.02	1.34 \pm 0.50	0.54 \pm 0.18
gall bladder	0.43 \pm 0.38	3.07 \pm 2.10	0.84 \pm 0.29
pancreas	0.11 \pm 0.06	0.43 \pm 0.12	0.18 \pm 0.06