

Supporting information: New *tris*(hydroxypyridinone) bifunctional chelators containing isothiocyanate groups provide a versatile a platform for rapid one-step labeling and PET imaging with $^{68}\text{Ga}^{3+}$

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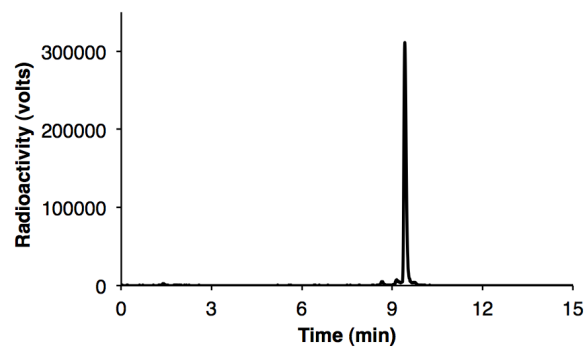
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Table S2. Biodistribution data of Balb/c nu/nu mice bearing U87MG tumours 1 h PI of [^{68}Ga (THP-PhNCS-RGD)] **Page 6**

Figure S1. Exemplar RP-HPLC traces (sodium iodide scintillation detector) of (a) [$^{68}\text{Ga}(\text{THP-NCS-RGD})$] and (b) [$^{68}\text{Ga}(\text{THP-PhNCS-RGD})$] labeled at radiochemical yields > 95% and specific activities of 60-80 MBq nmol $^{-1}$, for radiolabeling conjugates for in vivo studies.

(a)



(b)

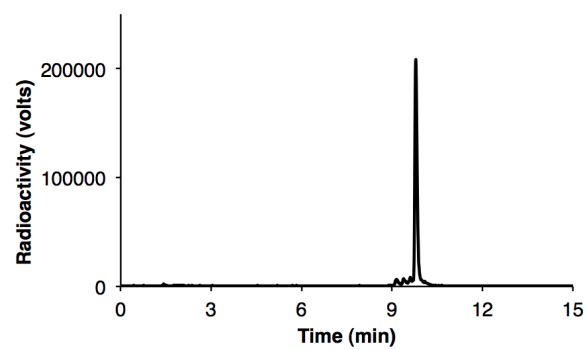


Figure S2. Size exclusion HPLC chromatograms of (a) a sample of [$^{68}\text{Ga}(\text{acetate})_3$] incubated in human serum for 1 h; (b) [$^{68}\text{Ga}(\text{THP-NCS-RGD})$]; (c) [$^{68}\text{Ga}(\text{THP-NCS-RGD})$] after 1 h (black trace) and 4 h (red trace) incubation in human serum at 37 °C; (d) [$^{68}\text{Ga}(\text{THP-PhNCS-RGD})$]; (e) [$^{68}\text{Ga}(\text{THP-PhNCS-RGD})$] after 1 h (black trace) and 4 h (red trace) incubation in human serum at 37 °C.

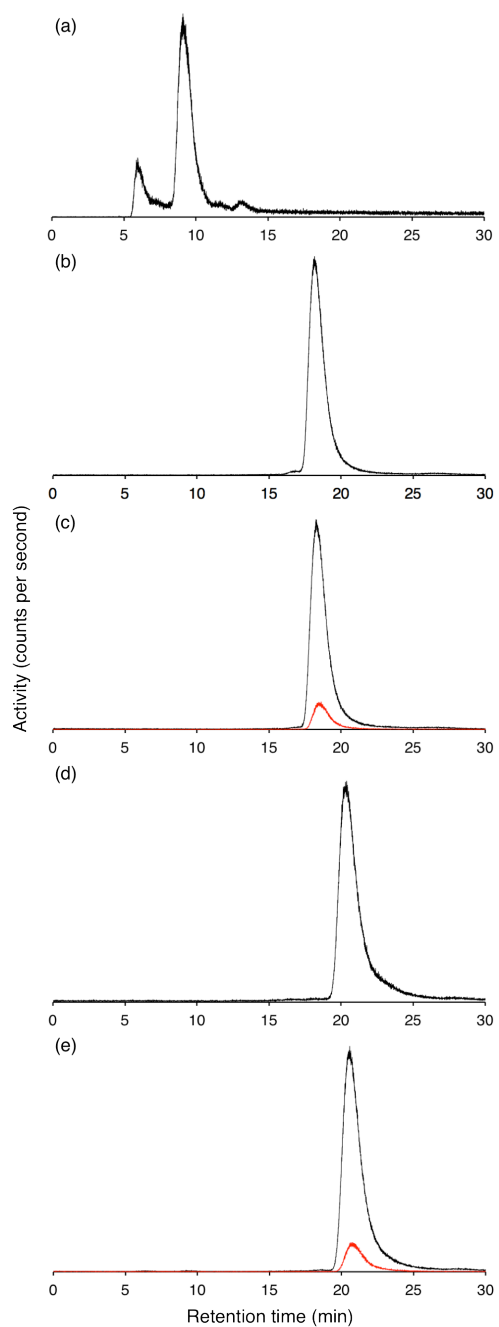


Figure S3. Radio-HPLC chromatograms of (a) [^{68}Ga (THP-NCS-RGD)]; (b) an ex vivo sample extracted from serum 20 min PI of [^{68}Ga (THP-NCS-RGD)]; (c) an ex vivo sample extracted from serum 90 min PI of [^{68}Ga (THP-NCS-RGD)]; and (d) an ex vivo sample extracted from urine 20 min PI of [^{68}Ga (THP-NCS-RGD)].

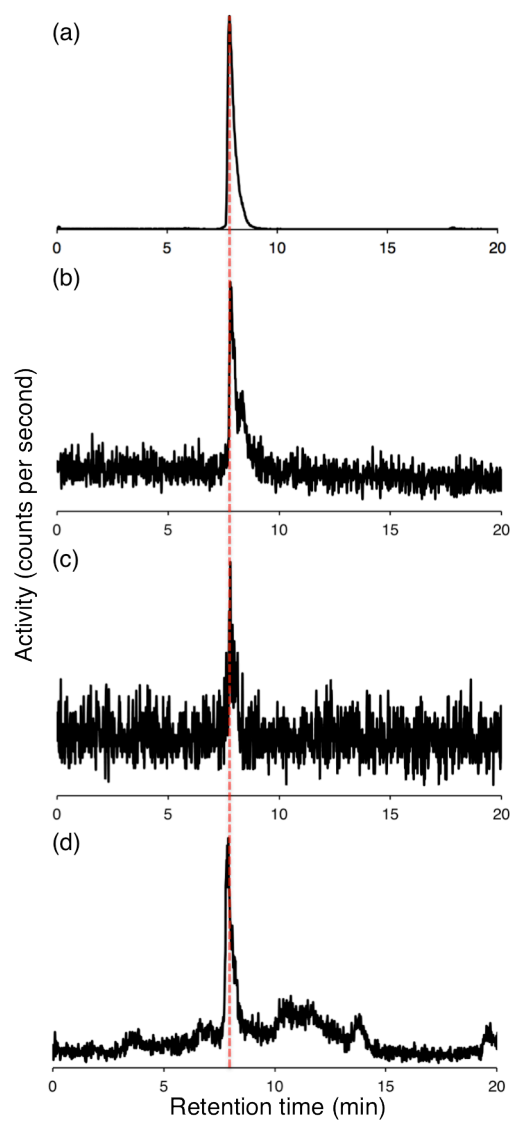


Figure S4. Radio-HPLC chromatograms of (a) [$^{68}\text{Ga}(\text{THP-PhNCS-RGD})$]; (b) an ex vivo sample extracted from serum 20 min PI of [$^{68}\text{Ga}(\text{THP-PhNCS-RGD})$]; (c) an ex vivo sample extracted from serum 90 min PI of [$^{68}\text{Ga}(\text{THP-PhNCS-RGD})$]; and (d) an ex vivo sample extracted from urine 90 min PI of [$^{68}\text{Ga}(\text{THP-PhNCS-RGD})$].

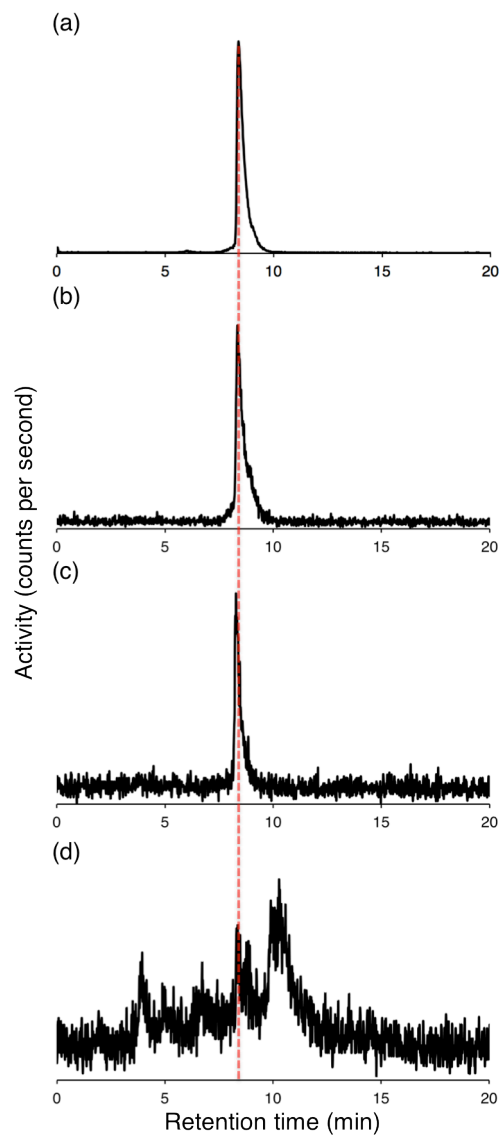


Table S1. Summary of biodistribution data of Balb/c nu/nu mice bearing U87MG tumours 1 h PI of [$^{68}\text{Ga}(\text{THP-NCS-RGD})$] ($n = 3$, except for * where $n = 2$; error corresponds to standard error of the mean).

Organ/tissue	Uptake of [$^{68}\text{Ga}(\text{THP-NCS-RGD})$] (%ID g^{-1})	Uptake in blocked group (%ID g^{-1})	Mean difference (%ID g^{-1})	p-value	95% CI (%ID g^{-1})
Blood	0.84±0.09	0.67±0.05	0.18	1.00×10^{-1}	-0.05-0.41
Tumour	2.35±0.06	0.62±0.10	1.22	6.00×10^{-5}	1.45-1.99
Kidney	4.76±0.36	4.04±0.64	0.72	2.95×10^{-1}	-0.94-2.38
Liver	2.94±0.06	1.30±0.16	1.64	2.81×10^{-4}	1.26-2.03
Heart	0.80±0.04	0.31±0.04*	0.48	1.56×10^{-3}	0.35-0.62
Lungs	1.62±0.14	0.59±0.03*	1.04	6.00×10^{-3}	0.57-1.51
Muscle	0.51±0.10	0.19±0.09*	0.32	7.43×10^{-2}	-0.06-0.69
Spleen	1.40±0.04	0.42±0.09	0.98	2.50×10^{-4}	0.76-1.20

Table S2. Summary of biodistribution data of Balb/c nu/nu mice bearing U87MG tumours 1 h PI of [$^{68}\text{Ga}(\text{THP-PhNCS-RGD})$] ($n = 3$, except for * where $n = 2$; error corresponds to standard error of the mean).

Organ/tissue	Uptake of [$^{68}\text{Ga}(\text{THP-PhNCS-RGD})$] (%ID g^{-1})	Uptake in blocked group (%ID g^{-1})	Mean difference (%ID g^{-1})	p-value	95% CI (%ID g^{-1})
Blood	0.57±0.02	1.29±0.10	0.72	1.20×10^{-3}	0.48-0.96
Tumour	2.86±0.43	0.99±0.12	1.88	6.89×10^{-3}	0.86-2.89
Kidney	4.91±0.73	7.39±1.85	2.48	2.02×10^{-1}	-2.03-6.99
Liver	4.09±0.33	2.68±0.11	1.41	7.93×10^{-3}	0.62-2.21
Heart	0.92±0.11	0.72±0.02	0.20	9.53×10^{-2}	-0.06-0.46
Lungs	1.77±0.16	1.38±0.34	0.39	1.74×10^{-1}	-0.27-1.04
Muscle	0.56±0.05	0.38±0.05*	0.18	6.42×10^{-2}	-0.02-0.38