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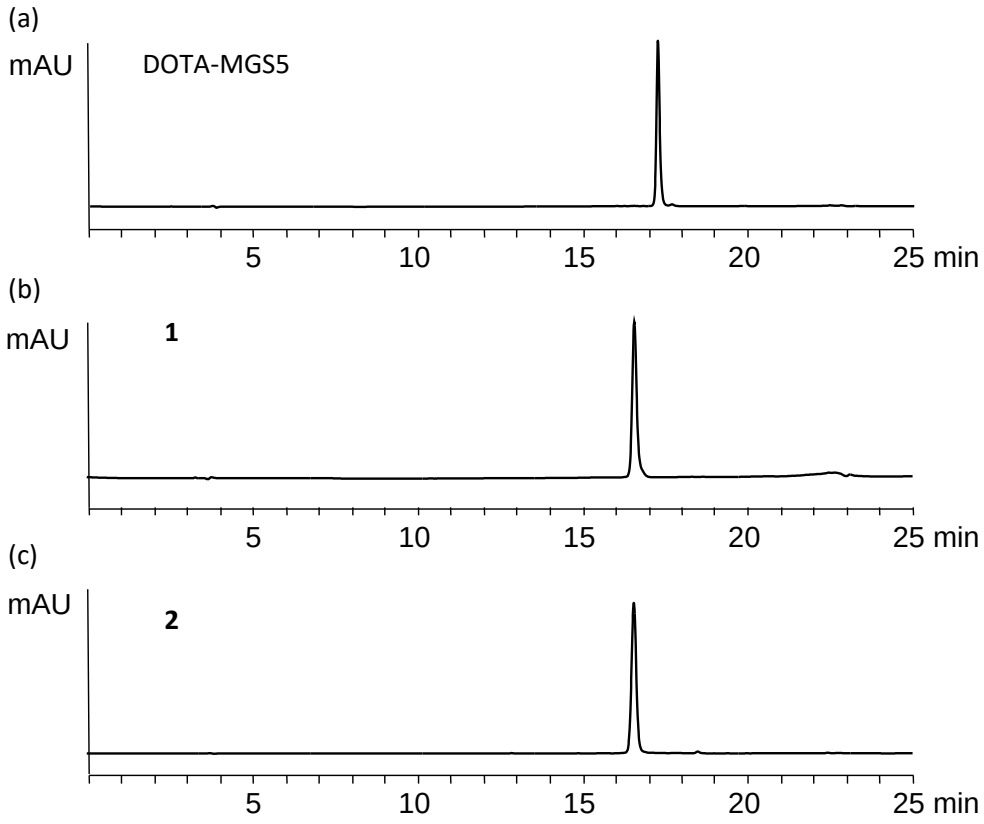

Figure S1. UV-chromatograms of (a) DOTA-MGS5, (b) **1** and (c) **2** after HPLC purification.

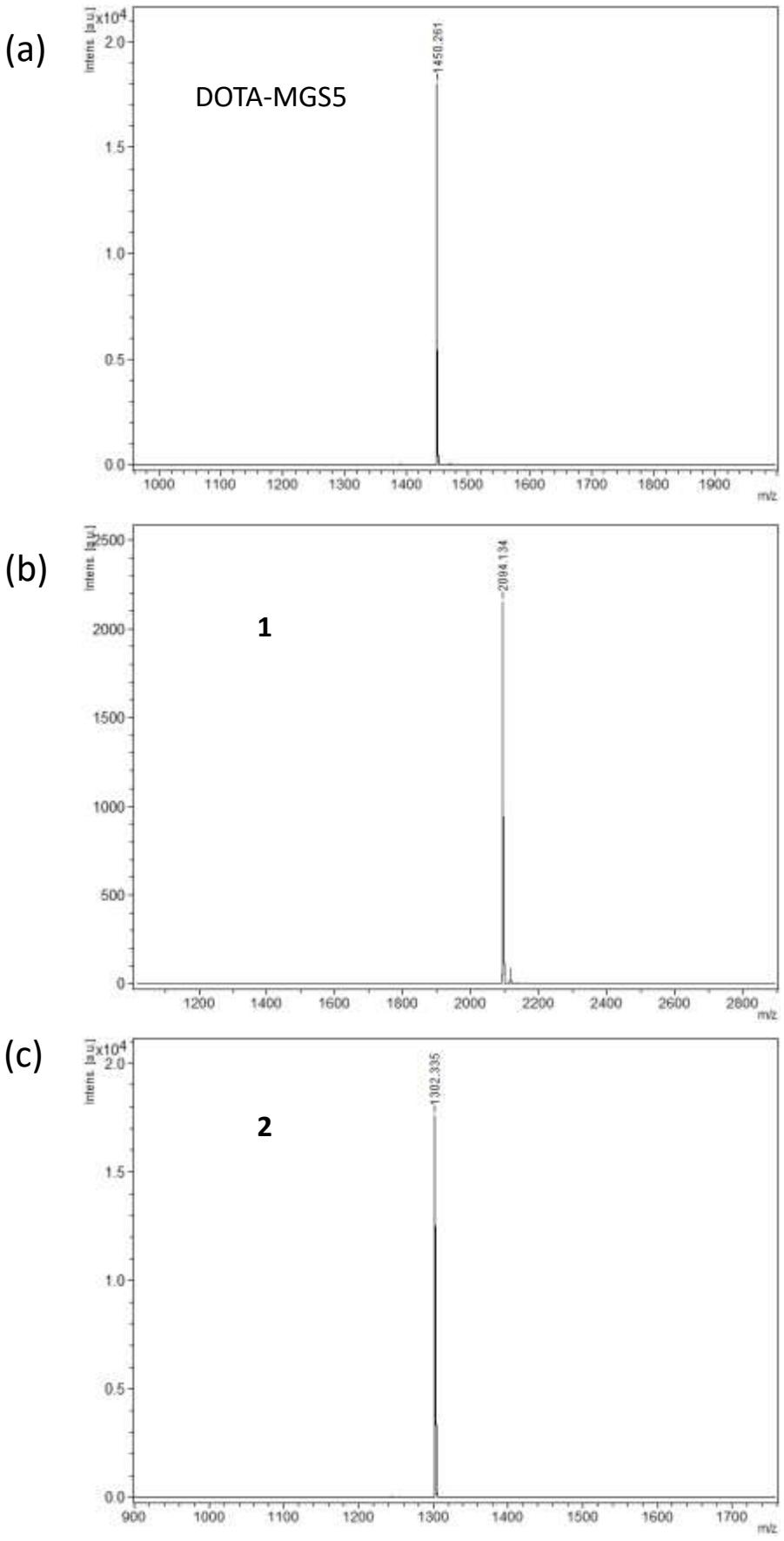

Figure S2. Mass spectra of (a) DOTA-MGS5, (b) **1** and (c) **2** after HPLC purification

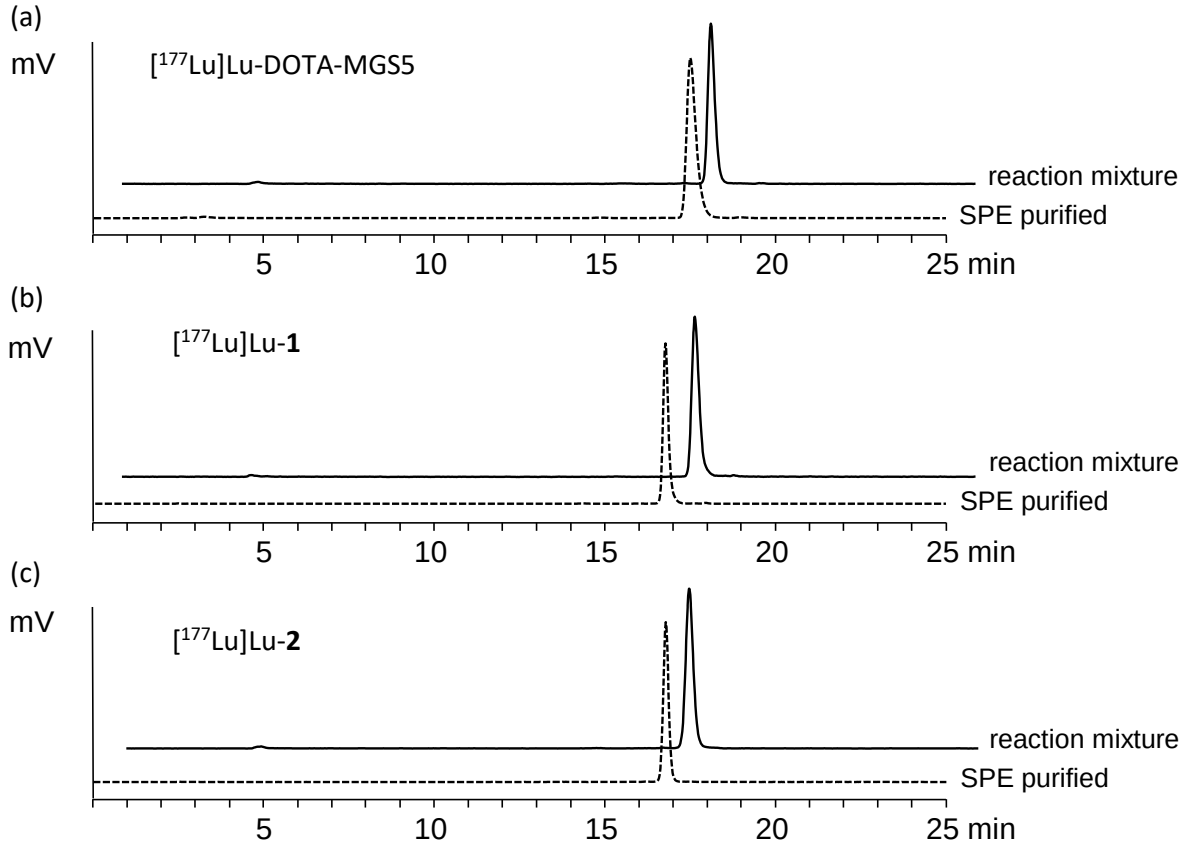

Figure S3. Radiochromatograms of ^{177}Lu-labeled (a) DOTA-MGS5, (b) **1** and (c) **2**: reaction mixture after radiolabeling with minor presence (≤2%) of free lutetium-177 (solid line) and after removal of hydrophilic impurities by solid phase extraction (dashed line), respectively.

Table S1. Results of biodistribution studies evaluated in A431-CCK2R/A431-mock xenografted BALB/c nude mice of the ^{177}Lu-labeled peptide derivatives (~0.5 MBq, 20 pmol, 4 h p.i.). Values expressed as percentage of injected activity per gram tissue (% IA/g); mean ± SD (n=5).

radiopeptide	**[^{177}Lu]Lu-DOTA-MGS5**	**[^{177}Lu]Lu-1**	**[^{177}Lu]Lu-2**
blood	0.11±0.11	0.02±0.00	0.03±0.01
lung	0.17±0.14	0.12 ±0.04	0.22±0.06
heart	0.10±0.06	0.06±0.01	0.07±0.02
femur	0.36±0.35	0.21±0.05	0.22±0.15
muscle	0.10±0.02	0.04±0.02	0.06±0.03
spleen	0.27±0.18	1.86±0.62	0.96±0.30
intestine	1.02±0.23	0.42±0.07	0.60±0.12
liver	1.02±0.80	2.48±0.39	1.43±0.18
kidneys	3.45±0.91	21.60±2.11	1.96±0.29
stomach	6.26±4.28	4.77±1.10	4.30±0.95
pancreas	1.91±0.91	1.25±0.27	0.72±0.14
A431-CCK2R	22.8±4.67	22.18±6.23	32.10±4.05
A431-mock	0.19±0.03	0.14±0.04	0.22±0.06

Table S2. Results of the additional biodistribution study with 1000-fold excess of non-radiolabeled peptide (blocking experiment) in A431-CCK2R/A431-mock xenografted BALB/c nude mice of the ^{177}Lu-labeled peptide derivatives (~0.5 MBq, 20 pmol, 4 h p.i.). Values expressed as percentage of injected activity per gram tissue (% IA/g; n=1).

radiopeptide	**[^{177}Lu]Lu-DOTA-MGS5**	**[^{177}Lu]Lu-1**	**[^{177}Lu]Lu-2**
blood	0.09	0.03	0.02
lung	0.08	0.06	0.20
heart	0.08	0.05	0.04
femur	0.04	0.18	0.09
muscle	0.03	0.02	0.04
spleen	0.16	1.13	0.70
intestine	0.79	0.17	0.45
liver	0.54	2.86	1.13
kidneys	2.95	9.21	1.47
stomach	0.09	0.06	0.09
pancreas	0.11	0.05	0.05
A431-CCK2R	0.54	0.45	0.39
A431-mock	0.34	0.12	0.16

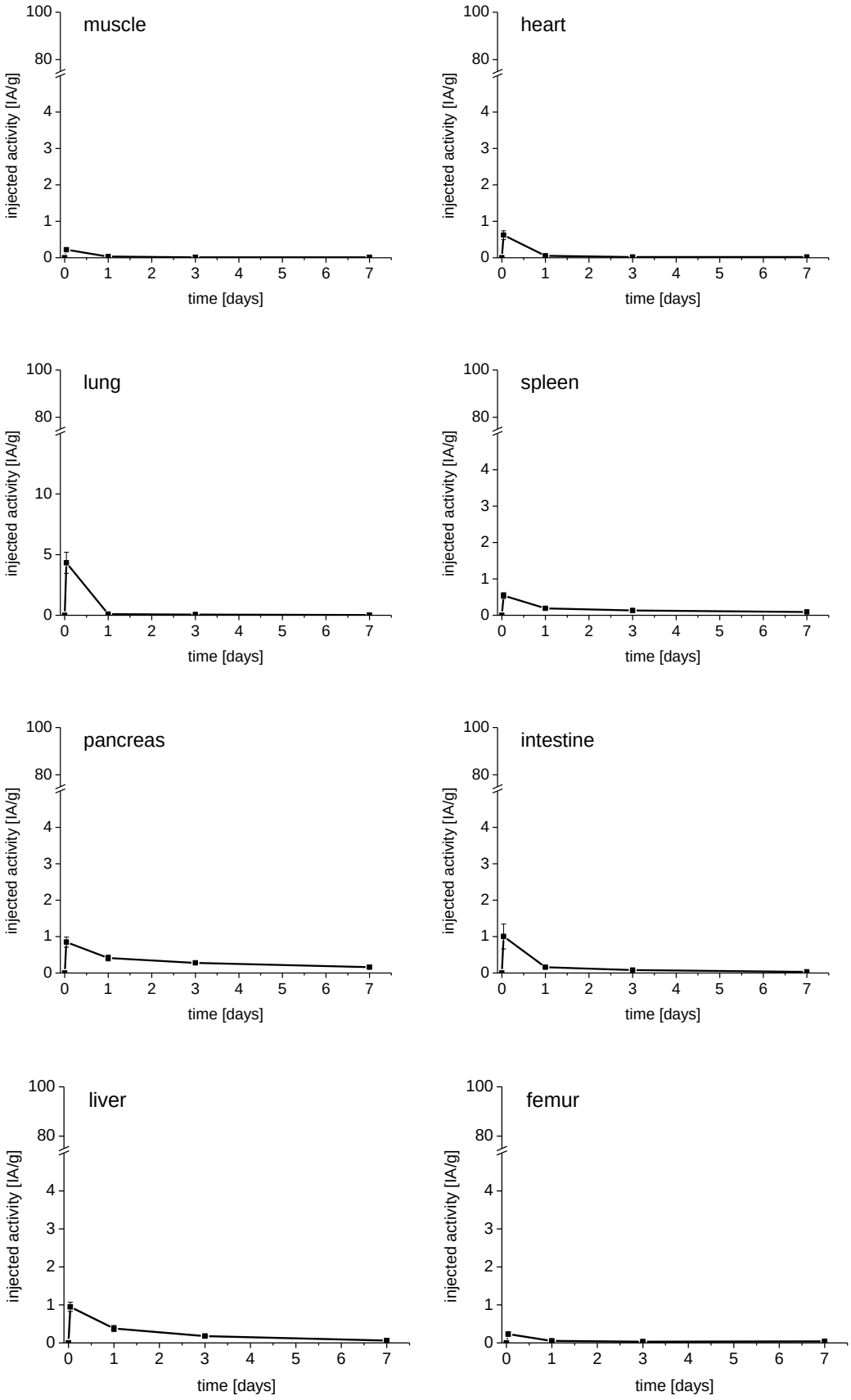

Figure S3. Uptake of [^{177}Lu]Lu-**2** in different tissues dissected from A431-CCK2R xenografted BALB/c nude mice for up to 7 days after injection (n=5).

Table S3. Uptake values of [^{177}Lu]Lu-**2** in A431-CCK2R tumor xenograft for up to 7 days after injection (n=5).

Timepoint p.i.	**1 h**	**24 h**	**3 days**	**7 days**
	[% IA/g]	**[% IA/g]**	**[% IA/g]**	**[% IA/g]**
blood	1.45±0.30	0.01±0.00	0.00±0.00	0.01±0.00
lung	4.33±0.87	0.09±0.02	0.06±0.01	0.02±0.01
heart	0.62±0.12	0.05±0.01	0.02±0.00	0.02±0.00
femur	0.23±0.05	0.05±0.01	0.03±0.01	0.04±0.02
muscle	0.22±0.05	0.03±0.00	0.01±0.00	0.01±0.01
spleen	0.54±0.08	0.19±0.03	0.13±0.02	0.09±0.04
intestine	1.00±0.34	0.16±0.02	0.08±0.00	0.03±0.00
liver	0.95±0.12	0.38±0.08	0.18±0.01	0.06±0.01
kidneys	2.84±0.42	1.32±0.23	0.72±0.10	0.31±0.03
stomach	5.43±1.05	3.66±0.38	2.28±0.33	0.88±0.12
pancreas	0.85±0.14	0.41±0.08	0.28±0.04	0.16±0.04
A431-CCK2R	56.29±9.14	33.61±2.95	12.52±0.96	1.23±0.53