

## Supporting Information

# <sup>44</sup>Sc: an attractive isotope for peptide-based PET imaging

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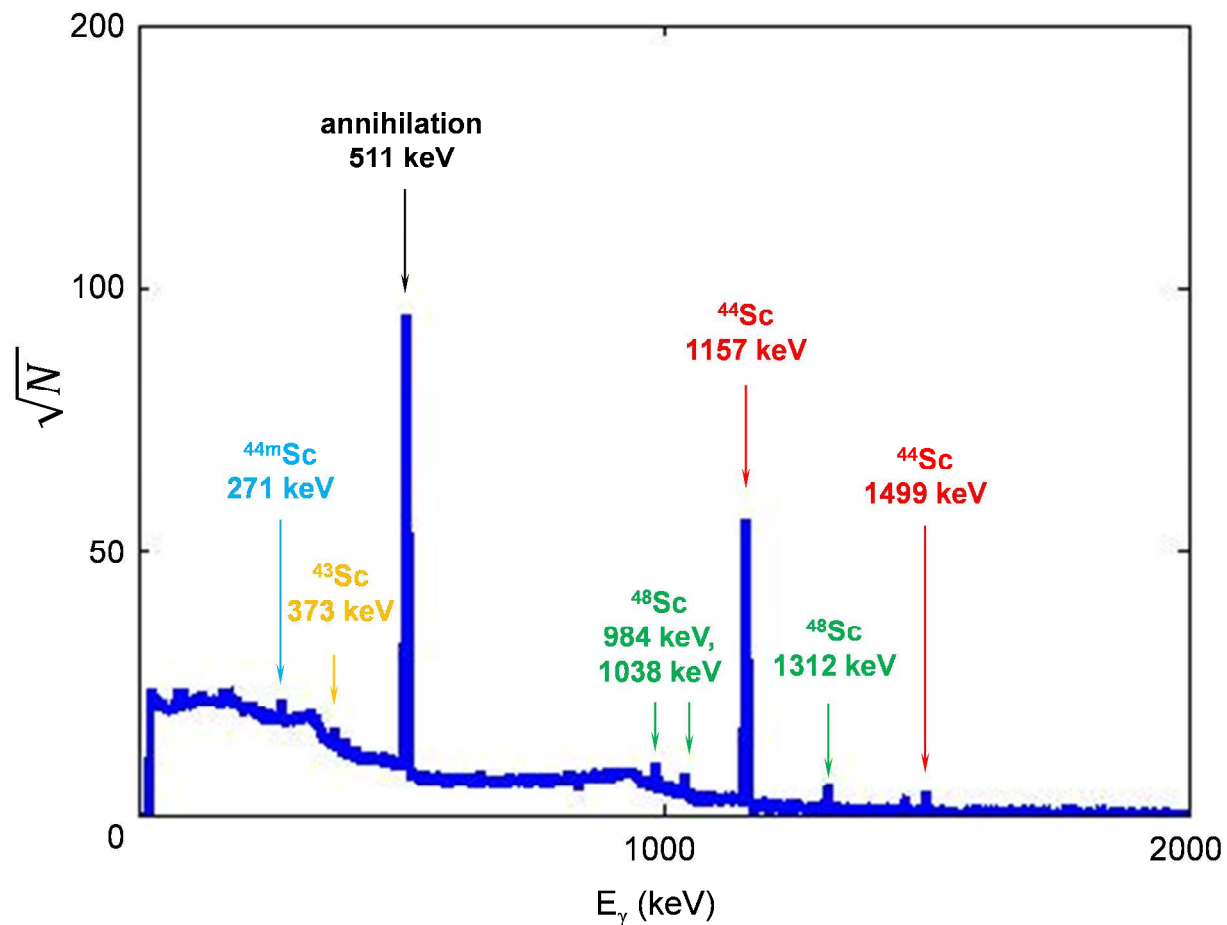
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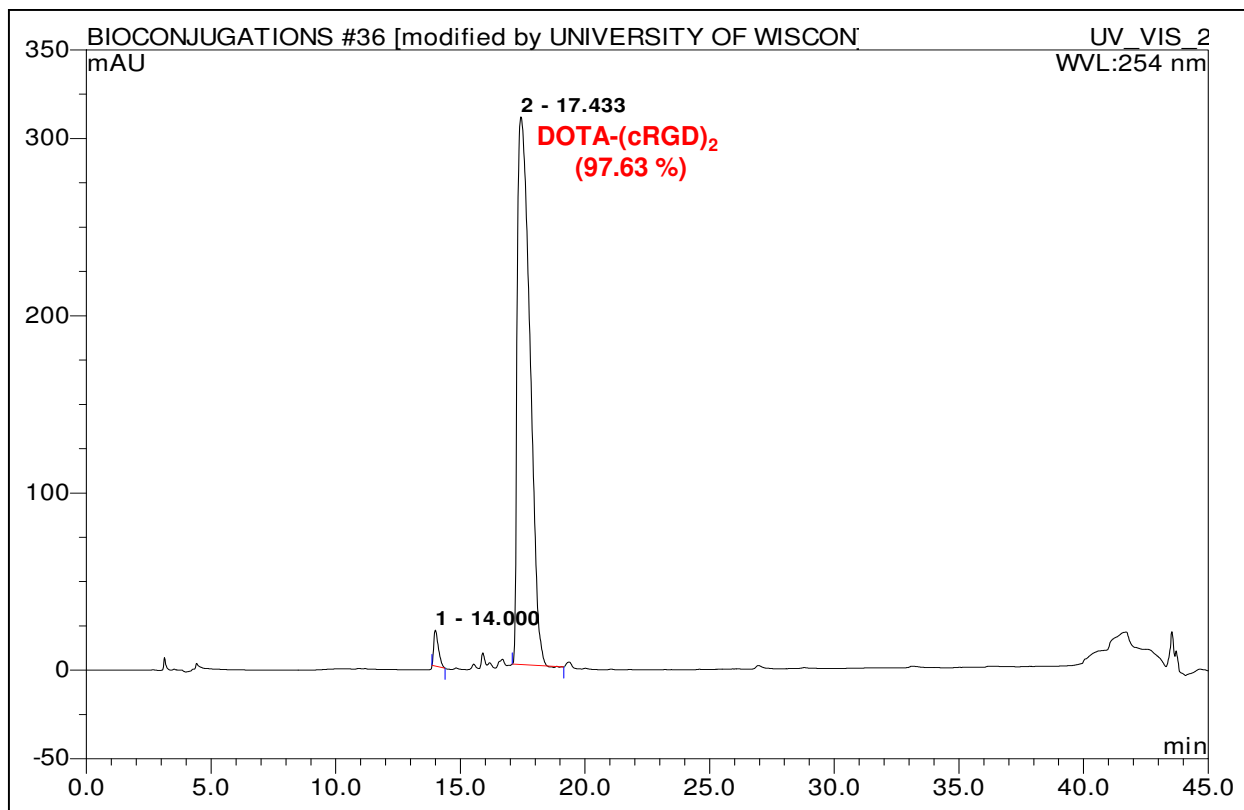
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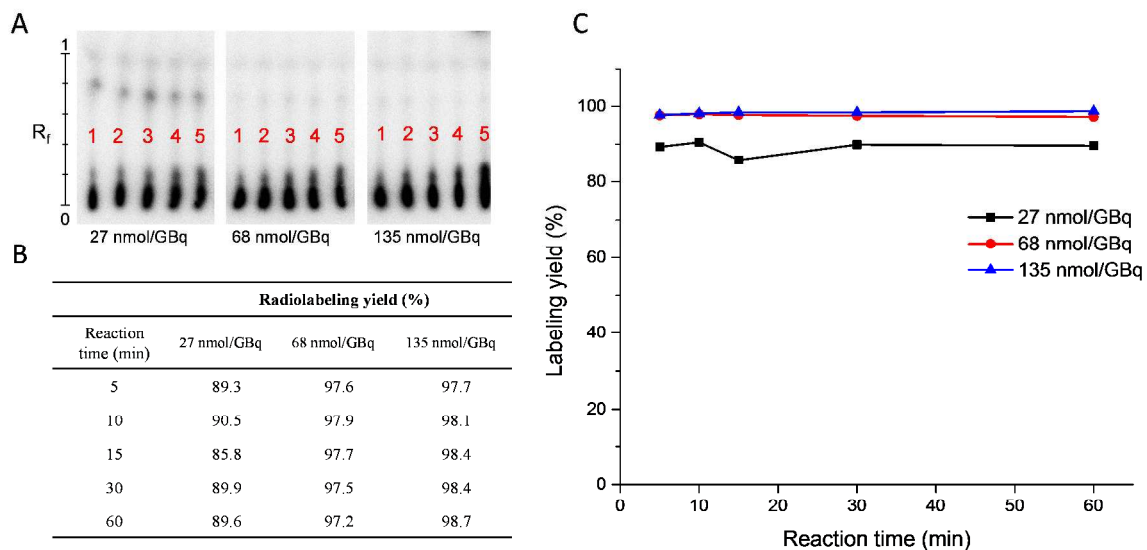
## Supplementary Figures and Tables



**Figure S1.** Gamma spectrum of  $^{44}\text{Sc}$  after separation (y axis represents the square root of the count collected for each particular energy channel). The arrows point to the most prominent gamma lines of the isotopes present in the product.



**Figure S2.** HPLC showing high purity of DOTA-(cRGD)<sub>2</sub> (column: Acclaim® 120 C18, 5µm, 4.6 × 250 mm; flow: 1mL/min; mobile phase: linear gradient from 5% EtOH at t = 0 to 65% EtOH at t = 40 min)



**Figure S3.** Optimization of the conditions for  $^{44}\text{Sc}$ -labeling of DOTA-(cRGD) $_2$ . **(A)** Radio-TLC showing the time progression; lanes 1-5 correspond to 5, 10, 15, 30, 60 min of radiolabeling time with different amount of DOTA-(cRGD) $_2$  (27, 68, and 135 nmol/GBq of  $^{44}\text{Sc}$ ). Radio-TLCs were run in 0.1 M sodium citrate (pH 4.5);  $^{44}\text{Sc}$ -DOTA-(cRGD) $_2$  remains at the origin ( $R_f = 0-0.2$ ) whereas free  $^{44}\text{Sc}$  moves with the solvent front ( $R_f = 0.6-1.0$ ). **(B)** Radiolabeling yield (%) calculated from quantitative analysis of radio-TLC. **(C)** The influence of time and amount of precursor on the radiolabeling yield.

**Table S1.** Quantitative data of  $^{44}\text{Sc}$ -DOTA-(cRGD)<sub>2</sub> uptake in U87MG tumor-bearing nude mice

$^{44}\text{Sc}$ -DOTA-(cRGD) <sub>2</sub> tissue uptake*(%ID/g)						
Organ	0.5 h p.i.	0.5 h p.i. with blocking**	2 h p.i.	2 h p.i. with blocking**	4 h p.i.	4 h p.i. with blocking**
Tumor	3.93±1.19	1.02±0.25	3.07±1.17	0.14±0.04	3.00±1.25	0.06±0.01
Heart/Blood	0.98±0.14	1.06±0.26	0.36±0.08	0.05±0.01	0.34±0.07	0.02±0.01
Liver	1.73±0.47	0.65±0.14	1.55±0.53	0.11±0.02	1.46±0.57	0.05±0.01
Kidney	3.53±1.36	3.17±0.40	1.63±0.47	0.63±0.17	1.50±0.44	0.21±0.05
Muscle	0.60±0.13	0.41±0.12	0.35±0.17	0.04±0.02	0.31±0.15	0.03±0.01

\*Values shown represent mean±SD (n=3)  
\*\*Blocking group was co-injected with a 50mg/kg dose of (cRGD)<sub>2</sub>

**Table S2.** *Ex vivo* biodistribution of  $^{44}\text{Sc}$ -DOTA-(cRGD) $_2$  in U87MG tumor-bearing nude mice

Organ	$^{44}\text{Sc}$ -DOTA-(cRGD) $_2$ tissue uptake*(%ID/g)	
	4 h p.i.	4 h p.i. with blocking
Tumor	2.48±0.76	0.128±0.020
Blood	0.02±0.00	0.008±0.002
Skin	0.64±0.33	0.117±0.025
Muscle	0.15±0.09	0.023±0.003
Bone	0.35±0.24	0.025±0.004
Heart	0.18±0.09	0.024±0.006
Lung	0.44±0.23	0.058±0.007
Liver	1.07±0.65	0.106±0.027
Kidney	1.56±0.48	1.287±0.261
Spleen	0.83±0.45	0.064±0.016
Pancreas	0.15±0.06	0.019±0.005
Stomach	0.71±0.30	0.042±0.010
Intestine	1.58±1.02	0.055±0.013
Brain	0.03±0.01	0.008±0.002

\*Values shown represent mean±SD (n=3)