

Supplementary Materials: Towards Facile Radiolabeling and Preparation of Gallium-68-/Bismuth-213-DOTA-[Thi⁸, Met(O₂)¹¹]-Substance P for Future Clinical Application: First Experiences

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Table S1: Overview of the ⁶⁸Ga/⁶⁸Ge- and the ²²⁵Ac/²¹³Bi-generator systems.

Figure S1: Representative HPLC-UV analysis (signals at 254 nm wavelength).

Figure S2: Radio-chromatograms of generator-derived ⁶⁸Ga-activity at different pH values (adjusted with 2.5 M sodium acetate).

Figure S3: Radio-ITLC-SG analysis of a crude sample of [⁶⁸Ga]Ga-DOTA-[Thi⁸, Met(O₂)¹¹]SP.

Figure S4: Radio-ITLC-SG chromatograms for analysis of [⁶⁸Ga]Ga-DOTA-[Thi⁸, Met(O₂)¹¹]SP quality over time.

Table S1. Overview of the ⁶⁸Ga/⁶⁸Ge- and ²²⁵Ac/²¹³Bi-generator systems.

Generators	⁶⁸ Ga/ ⁶⁸ Ge	²²⁵ Ac/ ²¹³ Bi
Manufacturer	iThemba LABS	ITM Medical Isotopes GmbH
Mother radionuclide	⁶⁸ Ge	²²⁵ Ac
Mother half-life (days)	271	10
Daughter radionuclide	⁶⁸ Ga	²¹³ Bi
Daughter half-life (min)	67.7	45.6
Matrix of resin	Tin dioxide	AG-MP-50
Eluent	0.6 M HCl	0.1 M NaI/0.1 M HCl
Energy (keV; type)	1900; β ⁺ ; EC	435; β ⁻ ; α (high LET)

LET = linear energy transfer; EC = Electron Capture.

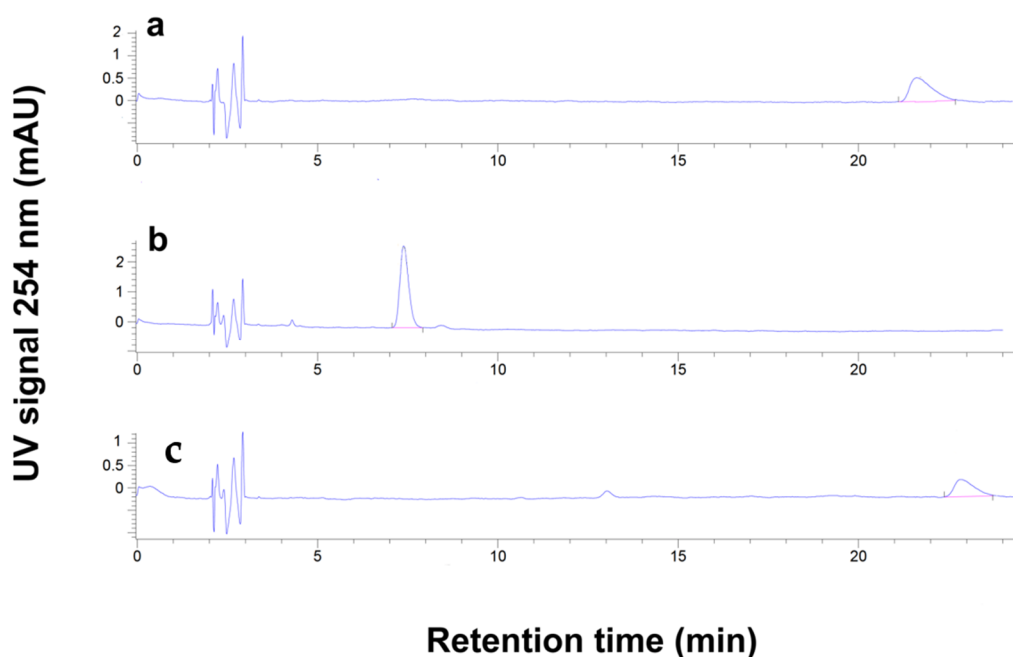


Figure S1. Representative HPLC-UV analysis (signal intensity at 254 nm wavelength). The UV signal was detected for retention times of a) DSP (21.8 ± 0.4 min), b) DOTA-[Thi⁸, Met(O₂)¹¹]SP (7.5 ± 0.2 min), and c) SP (22.8 ± 0.4 min). Isocratic HPLC elution was performed using 75% solvent A (0.1% TFA in water) / 25% solvent B (0.1% TFA in acetonitrile); Zorbax SB C18 (4.6 mm x 250 mm; 5 μm) column (40 °C, 1.0 mL/min).

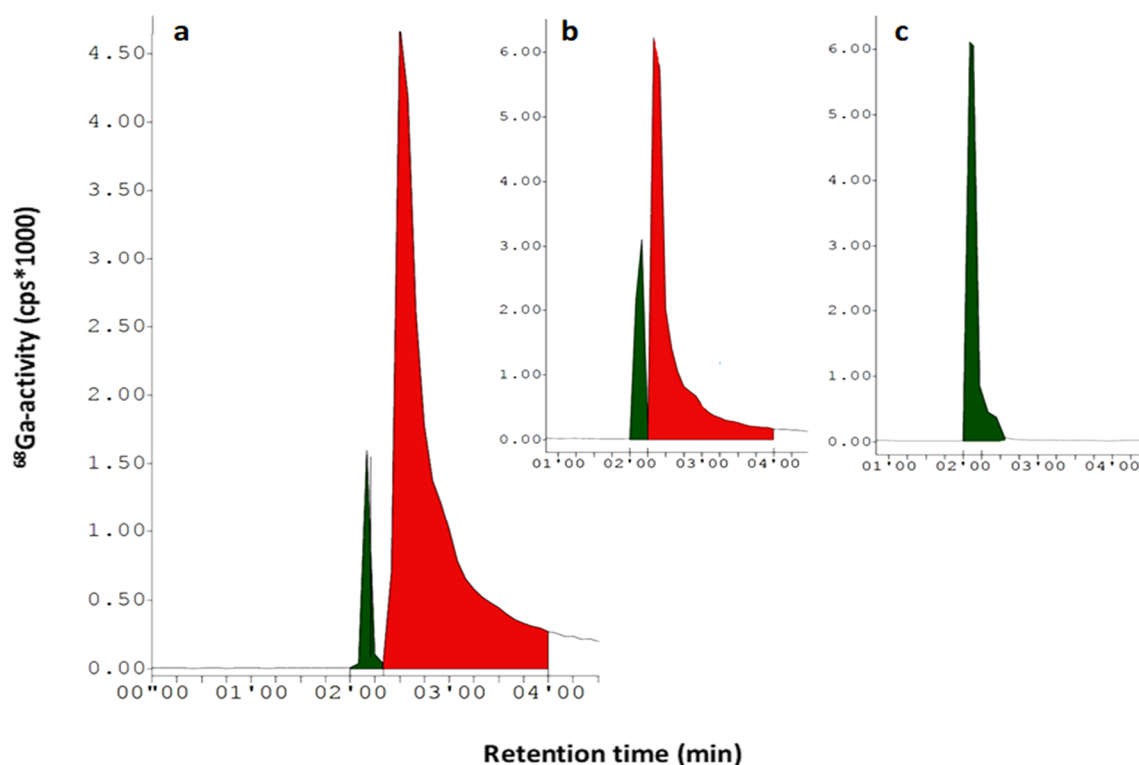


Figure S2. Radio-chromatograms of generator-derived ^{68}Ga -activity adjusted with 2.5 M sodium acetate to obtain different pH: a) pH 3.7, b) pH 3.3, and c) pH 2.3 ($n=2$). Isocratic HPLC elution: 75% solvent A (0.1% TFA in water) / 25% solvent B (0.1% TFA in acetonitrile); Zorbax SB C18 (4.6 mm x 250 mm; 5 μm) column (40 $^{\circ}\text{C}$, 1.0 mL/min).

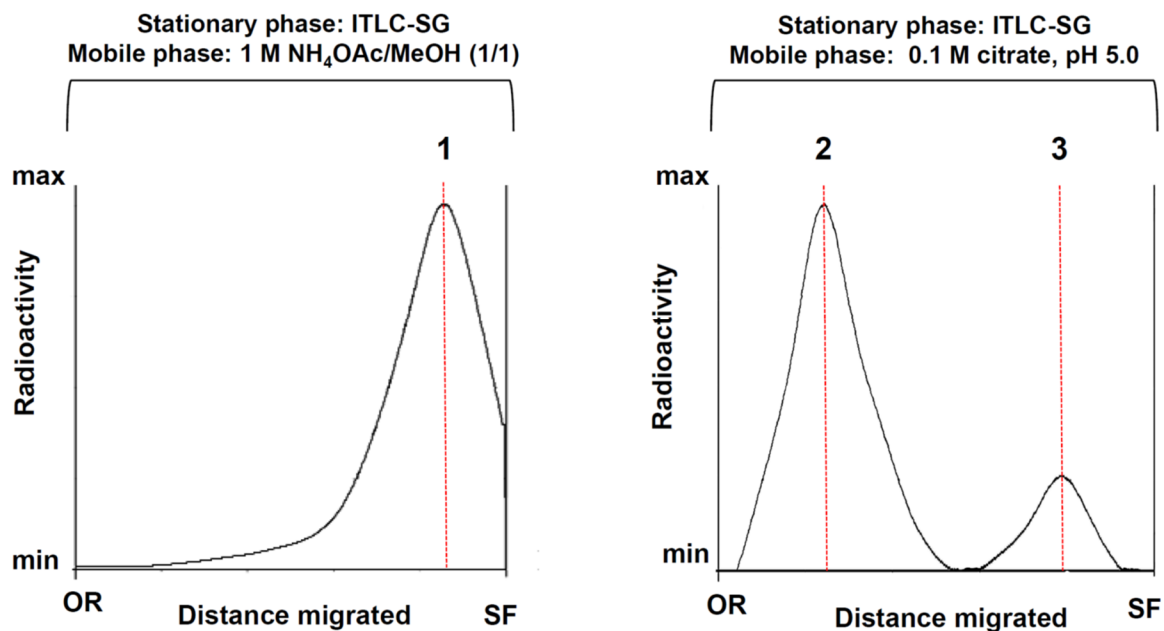


Figure S3. Representative crude radio-ITLC chromatograms for ^{68}Ga -DOTA-[Thi⁸, Met(O₂)¹¹]SP determining the radiolabeling quality of the tracer (right) and presence of ^{68}Ga -colloids (left). Peak for 1) and 2) ^{68}Ga -DOTA-[Thi⁸, Met(O₂)¹¹]SP, 3) uncomplexed ^{68}Ga -activity; SF – solvent front and OR – origin.

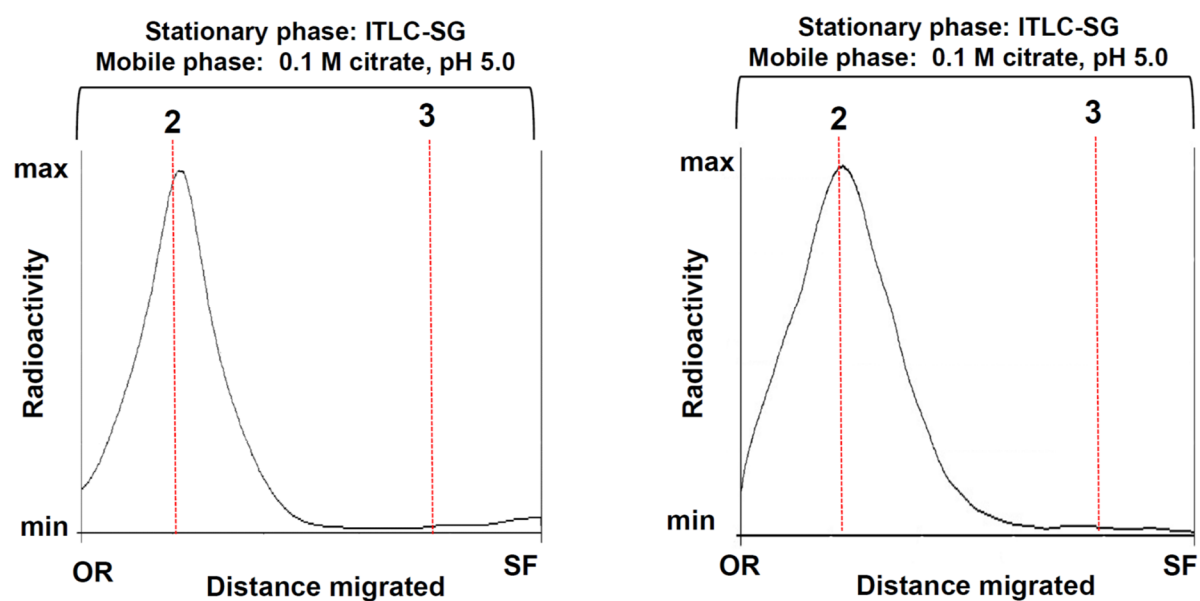


Figure S4. Radio-ITLC chromatograms for analysis of product quality over time of [⁶⁸Ga]Ga-DOTA-[Thi⁸, Met(O₂)¹¹]SP immediately after preparation (left) and after 120 min incubation (right) at 37 °C (pH 6.5). Peak for 2) [⁶⁸Ga]Ga-DOTA-[Thi⁸, Met(O₂)¹¹]SP and 3) uncomplexed ⁶⁸Ga-activity; SF – solvent front and OR – origin.