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# Supplementary Materials: Toward Stability Enhancement of NTS1R-Targeted Radioligands: Structural Interventions on [$^{99m}$Tc]Tc-DT1

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## Analytical data for DT7, DT8 and DT9

Analytical data for the DT1 ($N_4$-Gly$^7$-Arg-Arg-Pro-Tyr-Ile-Leu-OH; $N_4$, 6-(carboxy)-1,4,8,11-tetraazaundecane) mimics DT7 ([DAsn$^{14}$]DT1), DT8 ([β-Homoleucine$^{13}$]DT1) and DT9 ([(palmitoyl)Lys$^7$]DT1) from PiChem Forschungs- und Entwicklungs GmbH (Raaba-Grambach, Austria), comprising purity via HPLC analysis and MALDI-TOF data is summarized in Table S1.

**Table S1.** Analytical data for DT7, DT8 and DT9.[a]

| | HPLC | | | | MW [d] calcd | MW found [e], m/z |
|---|---|---|---|---|---|---|
| | $t_R$ (min) | | % Purity | | | |
| DT7 | 13.7 [a] | 17.1 [c] | >95 [a] | >99 [c] | 1174.4 | 1175.2 |
| DT8 | 8.7 [b] | 19.1 [c] | >95 [b] | >99 [c] | 1076.3 | 1076.2 |
| DT9 | 19.2 [a] | 37.7 [c] | >90 [a] | >99 [c] | 1367.8 | 1368.8 |

[a] A Nucleosil C18 (5 µm, 4 mm × 150 mm) column (MACHEREY-NAGEL GmbH & Co. KG; Dueren, Germany) was eluted at 1 mL/min flow rate with the following gradient: 90%A/10%B to 50%A/50%B in 30 min, UV trace at 215 nm, while in [b] 90%A/10%B to 10%A/90%B in 50 min was applied; A: 0.1% TFA, B: 0.1%TFA in MeCN. In an additional analysis system, a Waters Symmetry Shield RP-18 (5 µm, 4.6 mm × 150 mm) cartridge column (Waters, Vienna, Austria) was eluted at a 1 mL/min flow rate with the following linear gradient: from 100%A/0%B to 40%A/60%B in 60 min; A = 0.01% TFA and B = MeCN – UV trace at 220 nm; [d] average mass; [e] verification on MALDI TOF mass spectrometry.