A Dual Modality ^{99m}Tc/Re(I)-Labelled T140 Analogue for Imaging of CXCR4 Expression

William L. Turnbull, Lihai Yu, Emily Murrell, Mark Milne, Carlie Charron, Leonard G. Luyt

Table of Contents

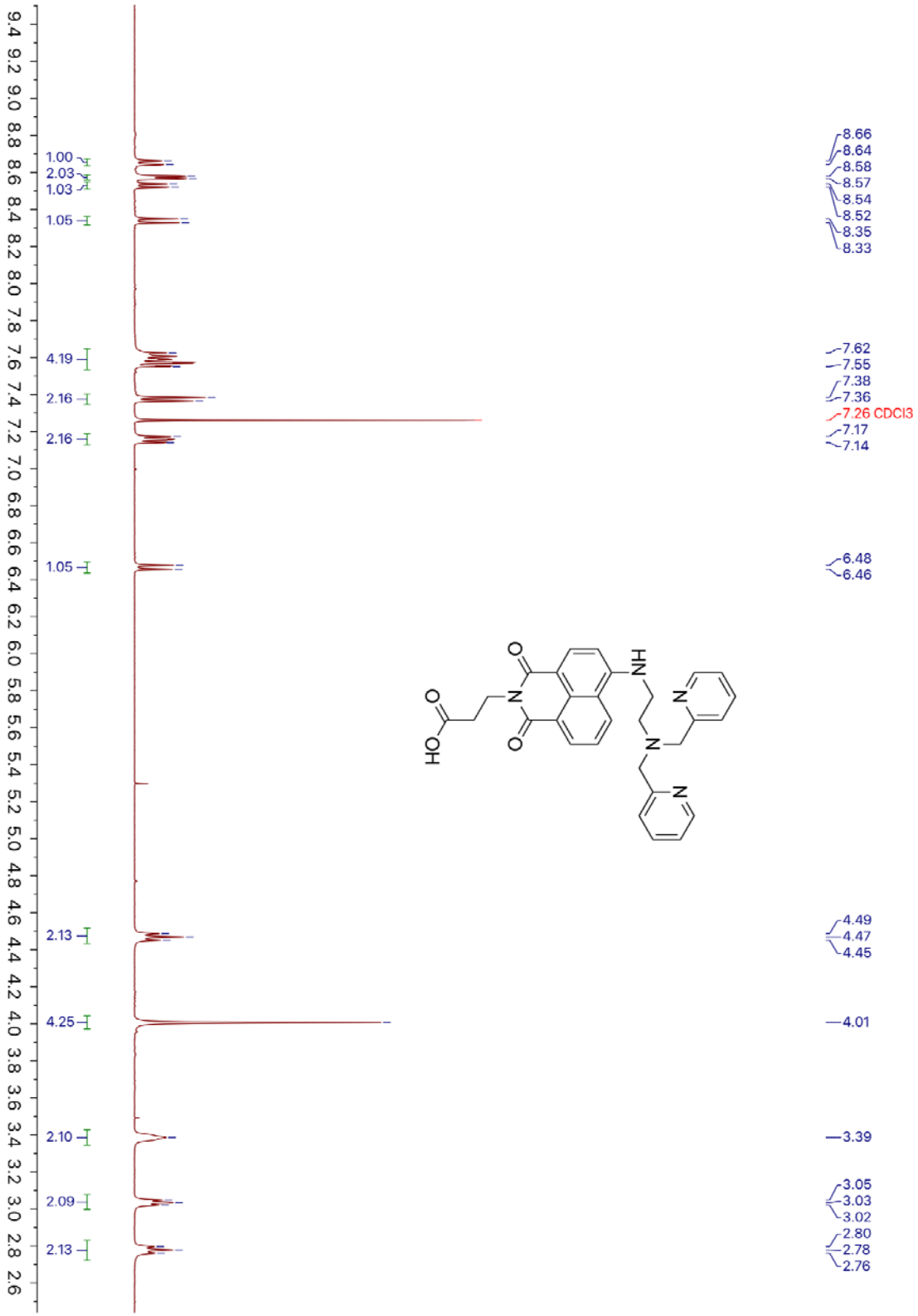

Figure S1 – ^{1}H NMR spectrum (400 MHz; $CDCl_3$) of compound **5** (DPA-Naph-OH).

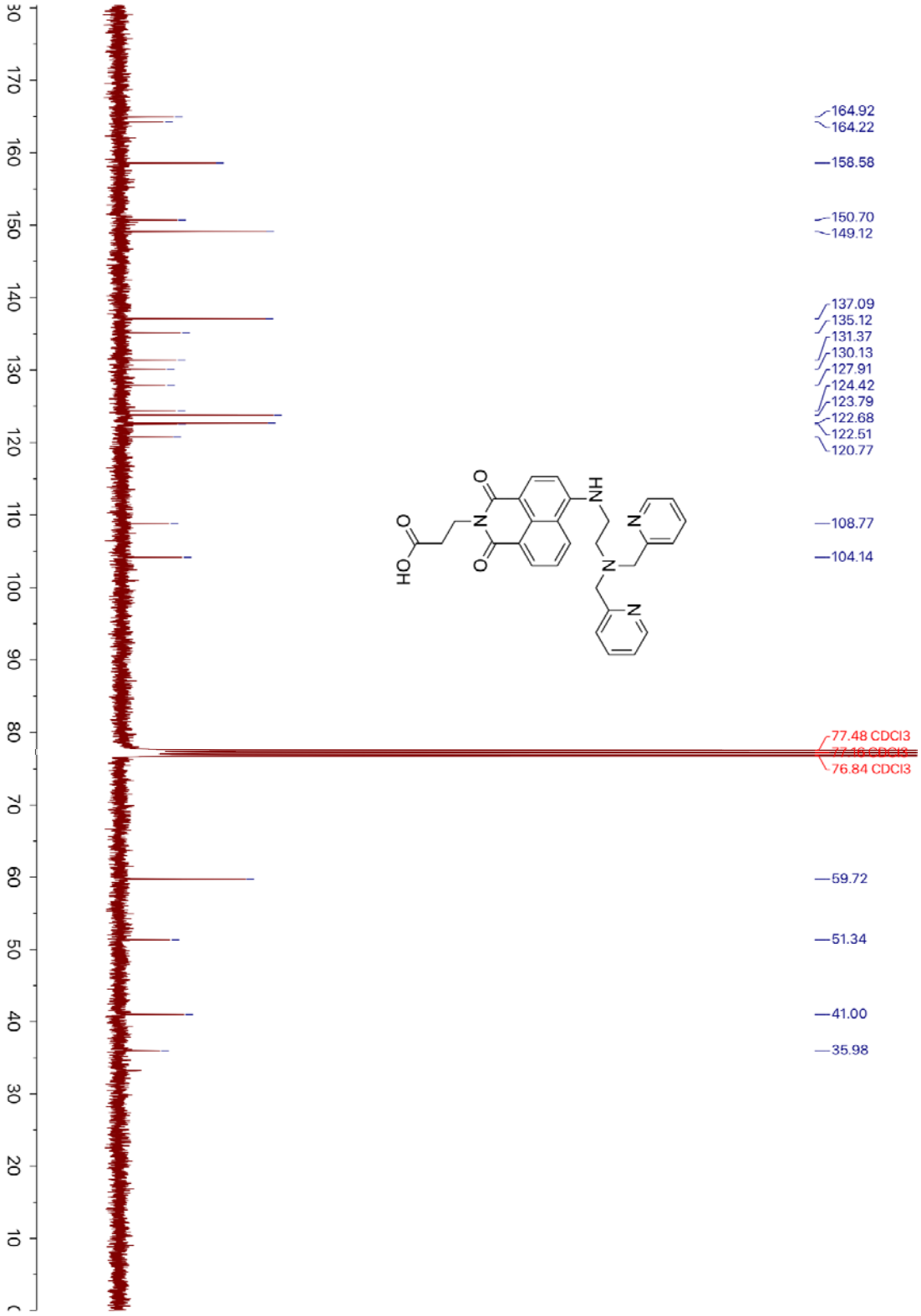

Figure S2 – ^{13}C NMR spectrum (100 MHz; $CDCl_3$) of compound **5** (DPA-Naph-OH).

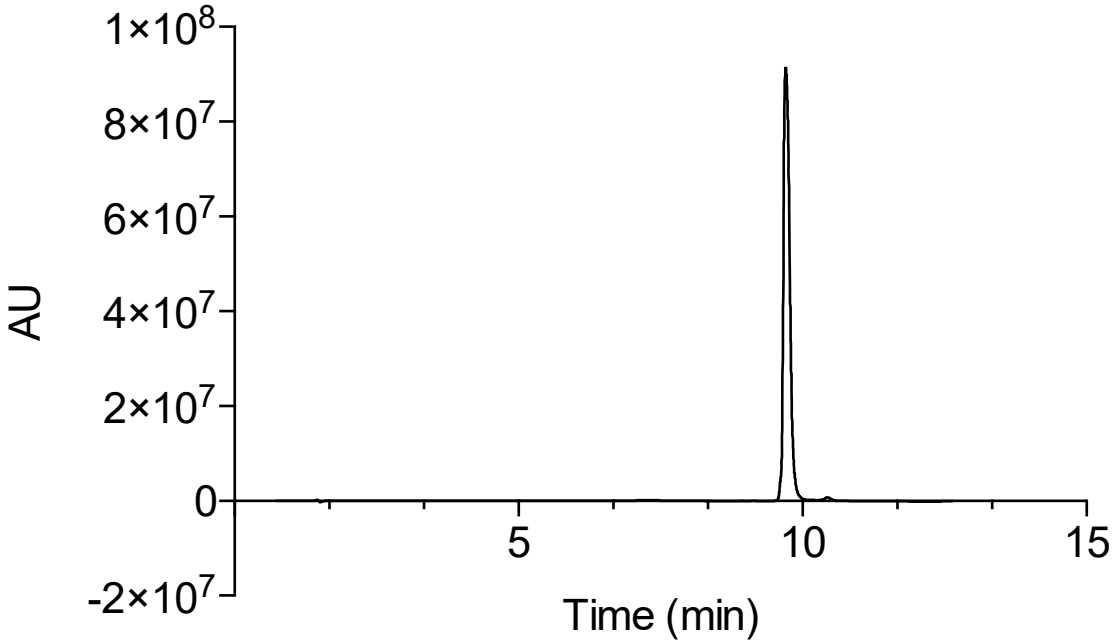

Figure S3 – HPLC chromatogram (10-70% CH_3CN/H_2O + 0.1% TFA) of peptide **6** (T140).

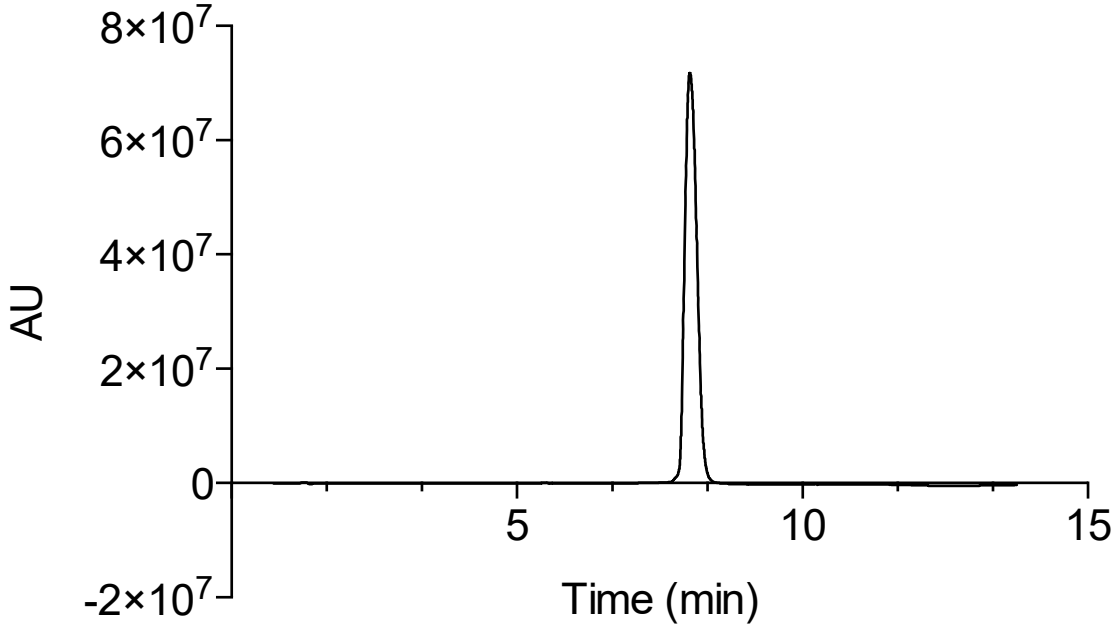

Figure S4 – HPLC chromatogram (20-80% CH_3CN/H_2O + 0.1% TFA) of peptide **7** (DPA-Naph-T140).

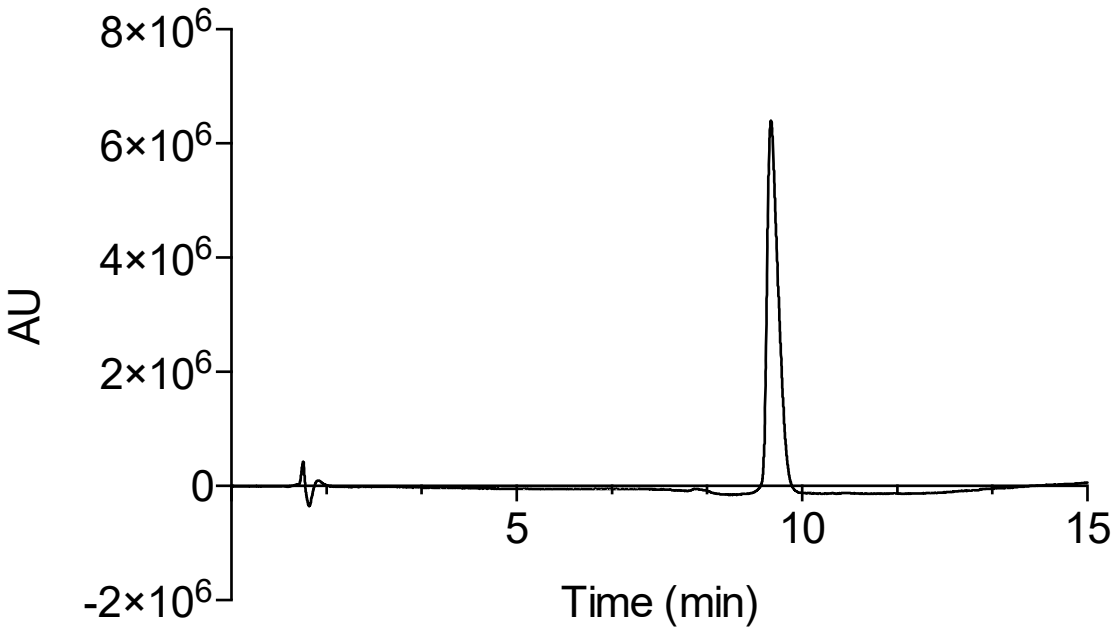

Figure S5 – HPLC chromatogram (20-80% CH_3CN/H_2O + 0.1% TFA) of peptide **Re-7** ($Re(CO)_3$-DPA-Naph-T140).

Table S1 – *Ex vivo* biodistribution data for **[^{99m}Tc]Tc-7** in NOD/SCID mice two hours post-injection

Tissue	Uptake (% ID/g ± SD)
blood	1.91 ± 0.16
heart	0.93 ± 0.04
lung	2.80 ± 0.63
liver	22.67 ± 5.02
spleen	2.05 ± 1.37
pancreas	1.15 ± 0.54
stomach	4.67 ± 0.99
intestine	2.36 ± 1.40
kidney	25.69 ± 15.19
tumor	0.51 ± 0.09
muscle	0.26 ± 0.07
brain	0.10 ± 0.02

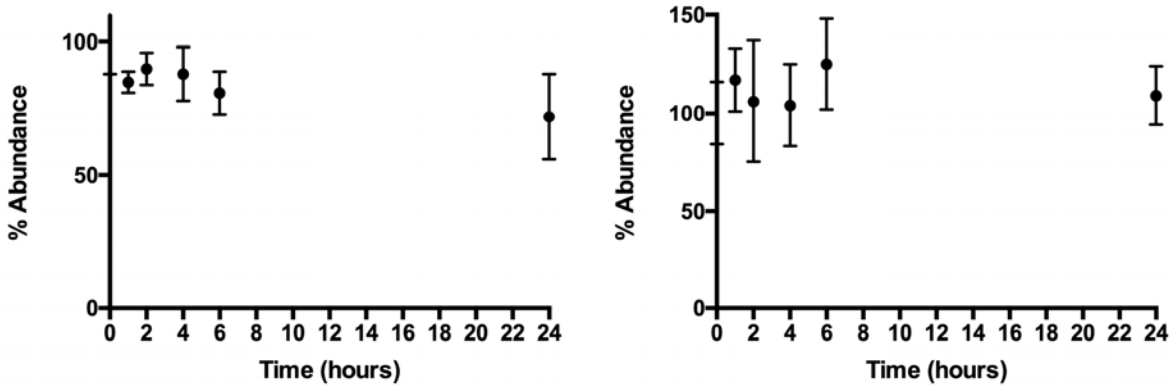

Figure S6 – Serum stability of **7** (left) and **Re-7** (right).

Serum Stability Procedure

Peptides were dissolved to a 1 mM final concentration in 25% human serum in PBS (pH 7.4, 450 μL final volume, DMSO final concentration 0.5%) and incubated at 37 °C. At 0, 1, 2, 4, 6, and 24 hours, 15 μL aliquots of peptide solution was removed and mixed with 40 μL of 4% ammonium hydroxide (pH 11-13) to dissociate peptide interactions with components of human serum. Peptides were isolated from human serum by column separation on Oasis® HLB sorbent 96-well μElution plate and eluted using 20% methanol in water. The extracted peptide was quantified on an Acquity UHPLC-MS system (Waters Co.). Intact peptide was quantified by measuring the peak area of a peptide specific $[M]^{3+}$ ion peak (average of 3 replicates). Percent abundance of peptide peak area relative to peptide peak abundance at T_0 was calculated and plotted as a function of time.