



Supplementary materials

NHS-functionalized THP derivative for efficient synthesis of kit-based precursors for ^{68}Ga labelled PET probes

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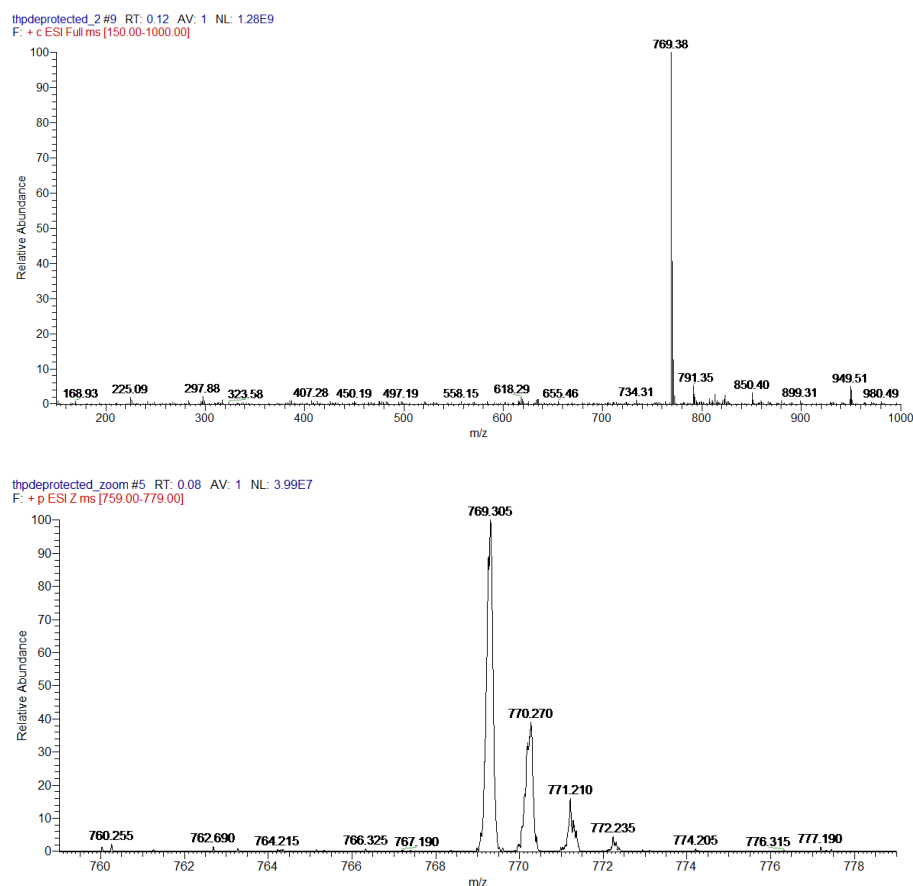


Figure S1. ESI⁺ MS spectra of deprotected THP (5).

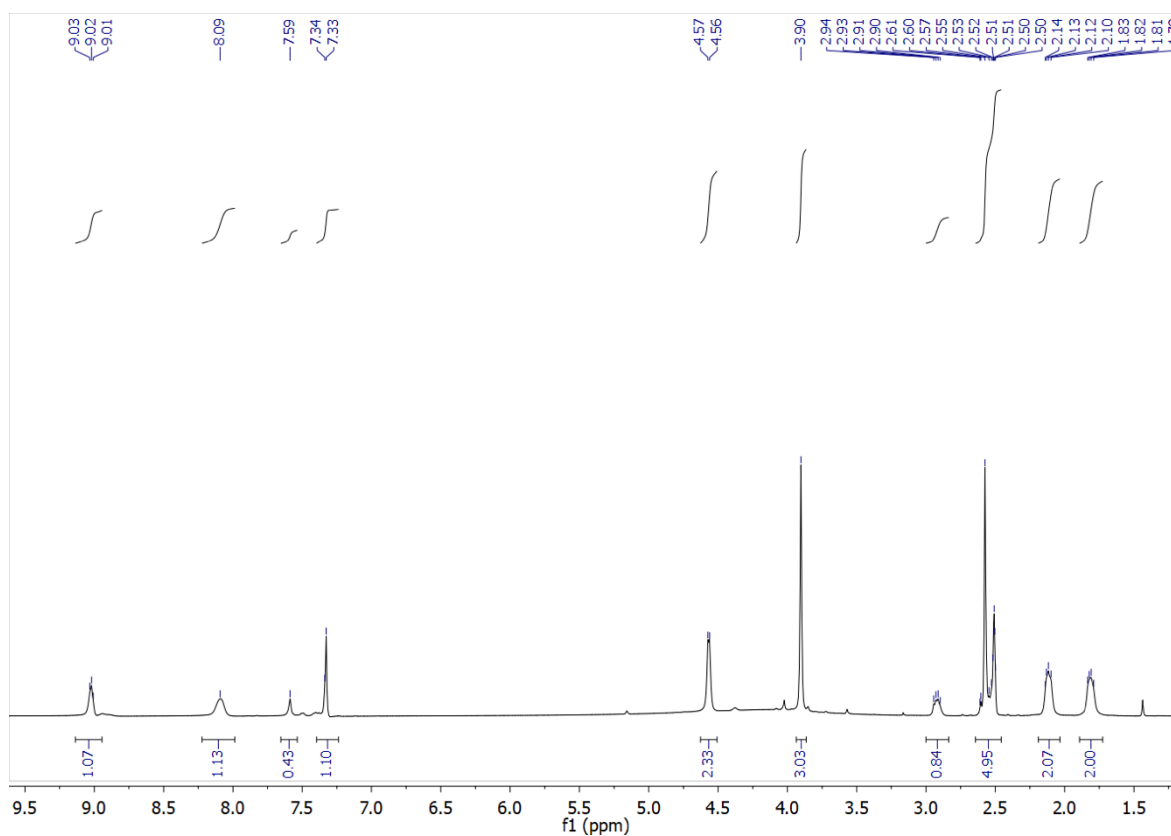


Figure S2. ¹H NMR of deprotected THP (5).

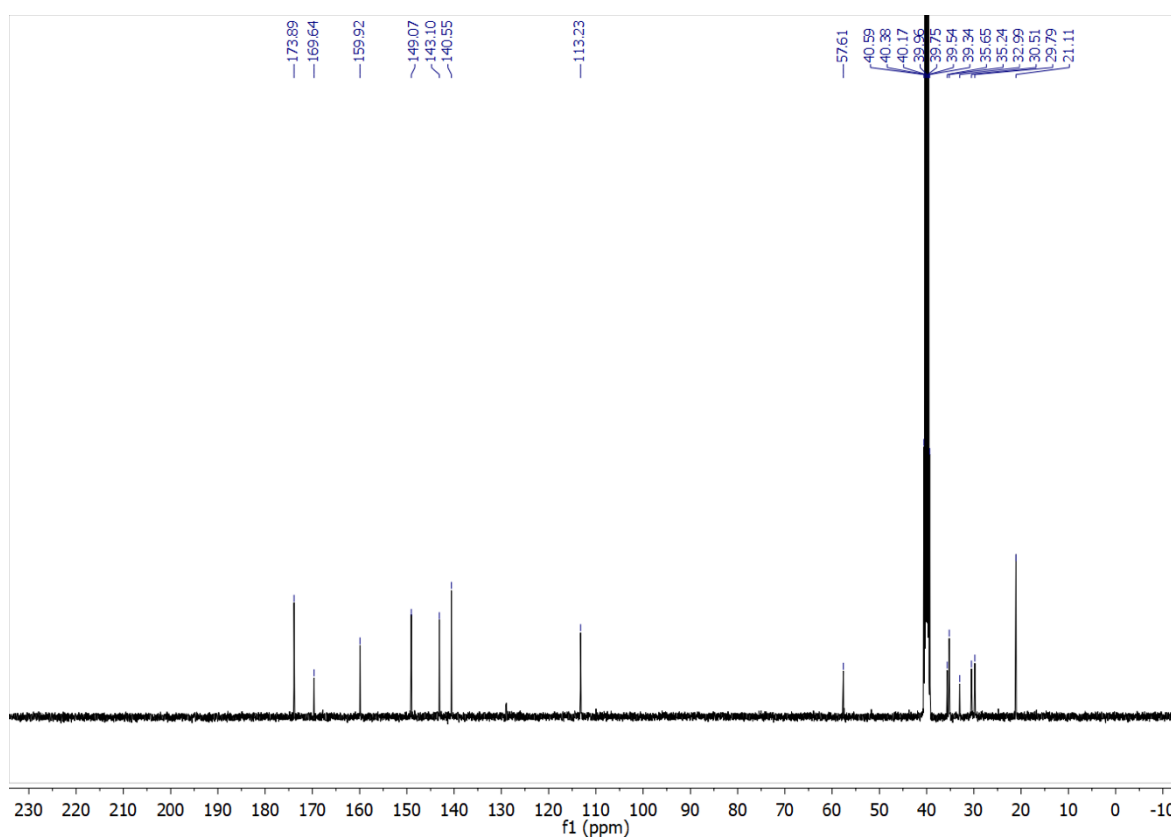


Figure S3. ¹³C NMR of deprotected THP (5).

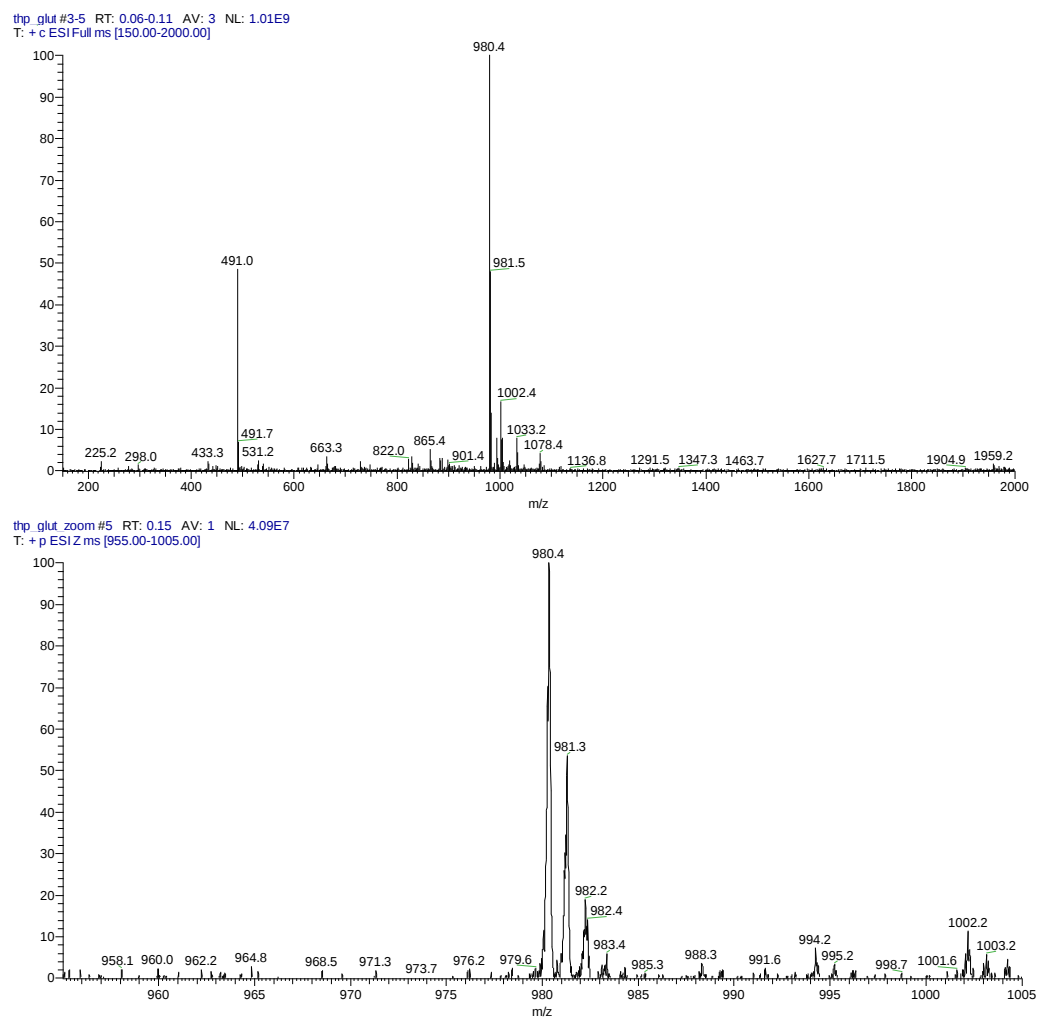


Figure S4. ESI+ MS spectra of NHS-THP-glutaric (7).

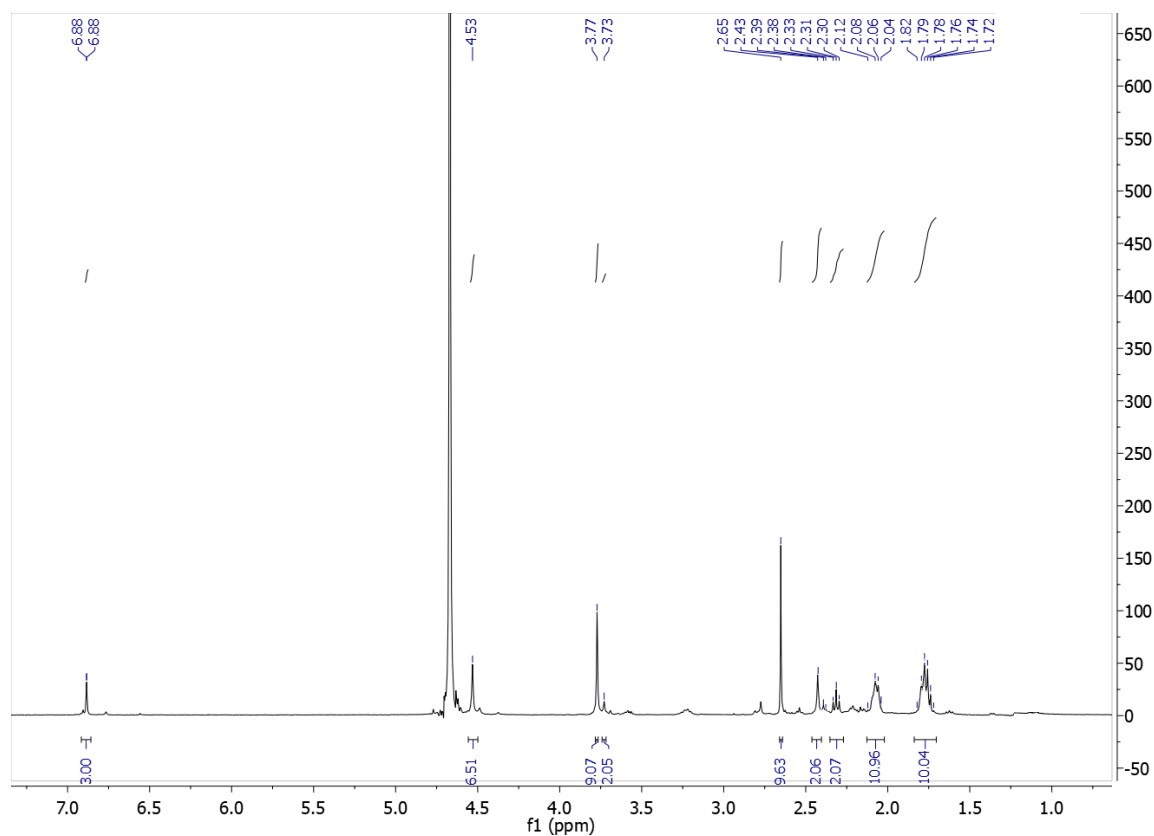


Figure S5. ^1H NMR of NHS-THP-glutaric (7).

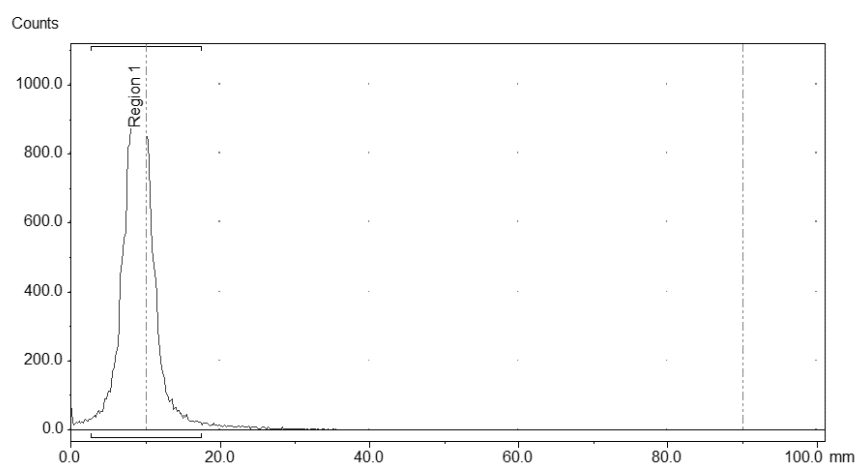


Figure S6. ITLC acetate unbound ^{68}Ga .

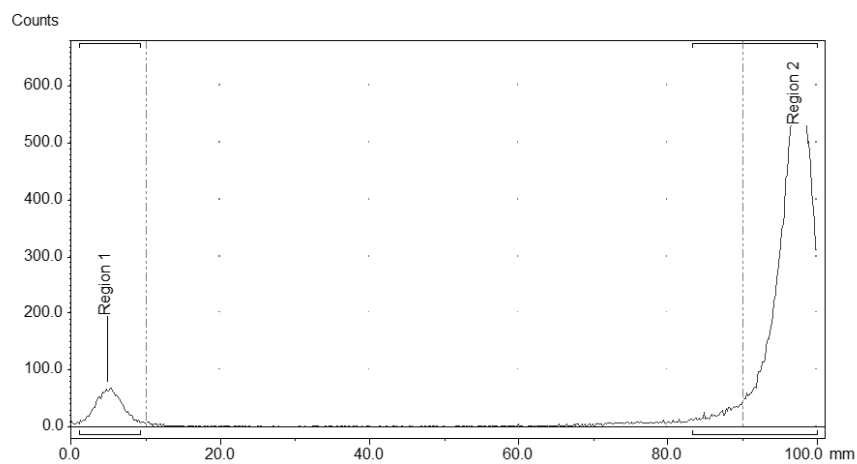
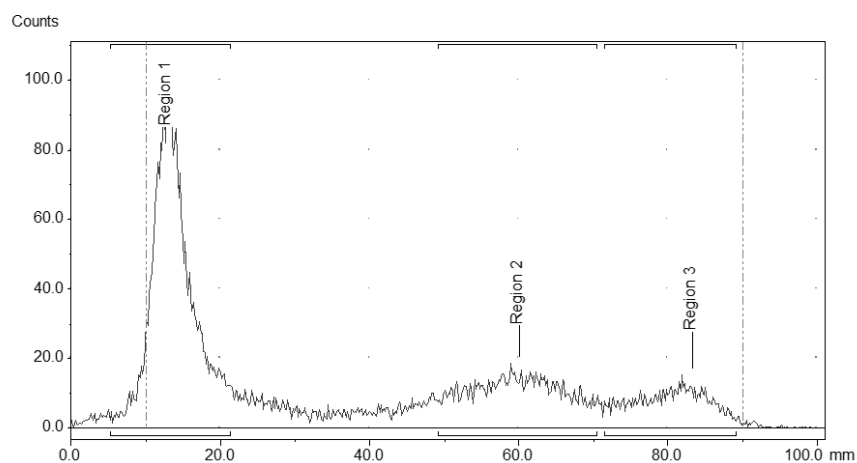
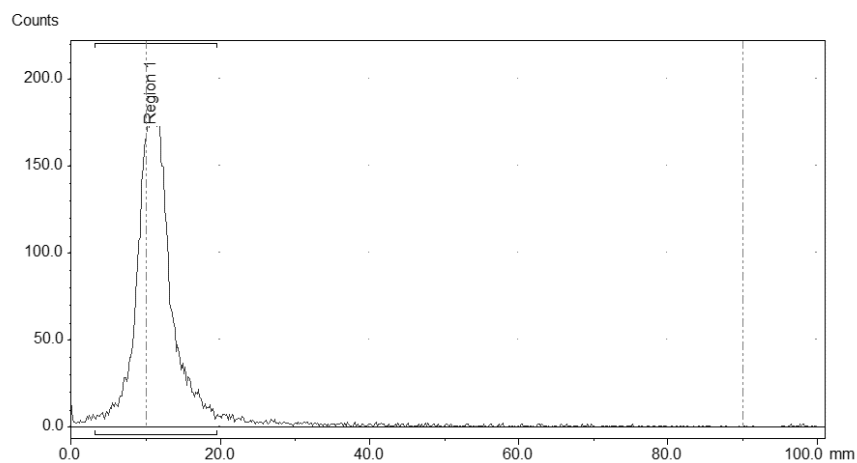
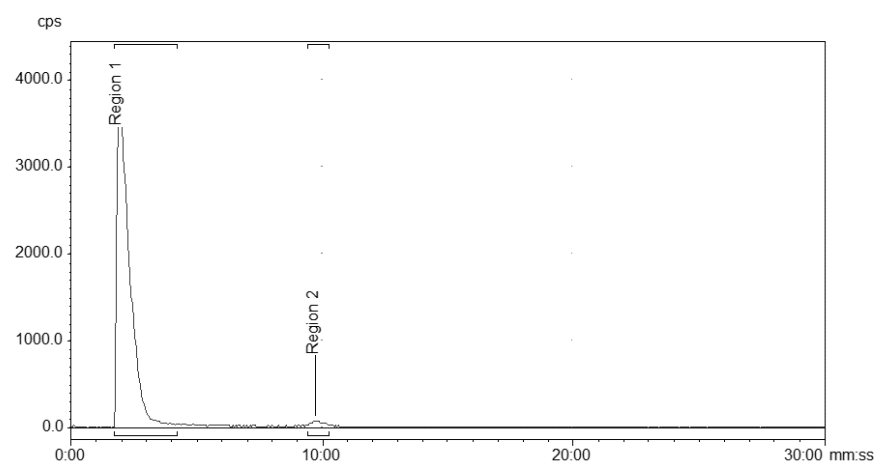


Figure S7. ITLC citrate unbound ^{68}Ga .**Figure S8.** ITLC acetate [^{68}Ga]Ga-GLP-1-peptide-THP (9).**Figure S9.** ITLC citrate [^{68}Ga]Ga-GLP-1-peptide-THP (9).**Figure S10.** Reverse phase HPLC unbound gallium.

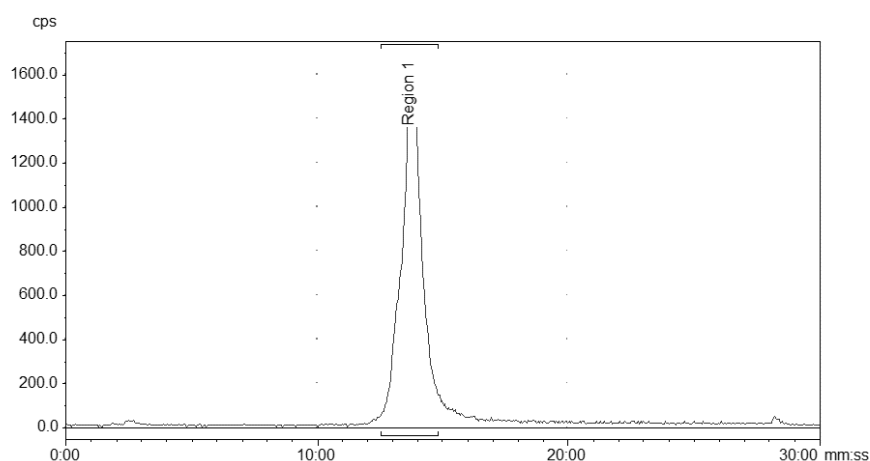


Figure S11. Reverse phase HPLC $[^{68}\text{Ga}]\text{Ga-GLP-1-peptide-THP}$ (9).

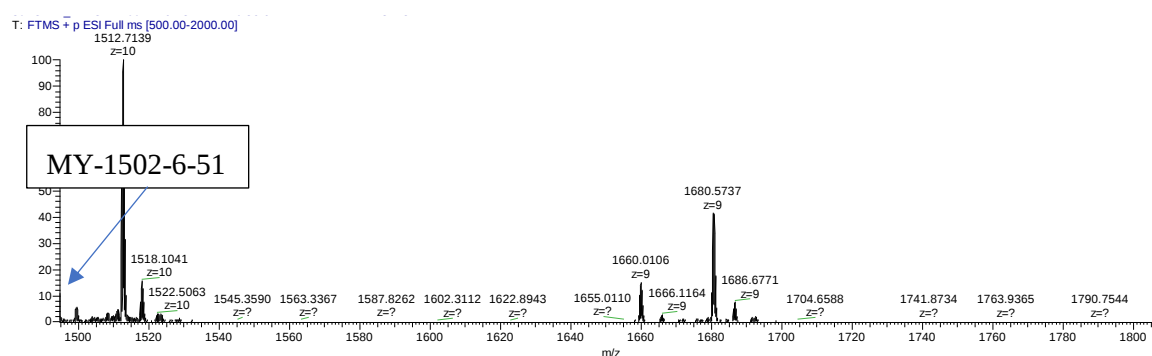


Figure S12. ESI+ mass spectrum of MY-1502-6-51. The peak at m/z 1518 corresponds to the $[\text{M}+10\text{H}]^{10+}$ of MY-1502-6-51.

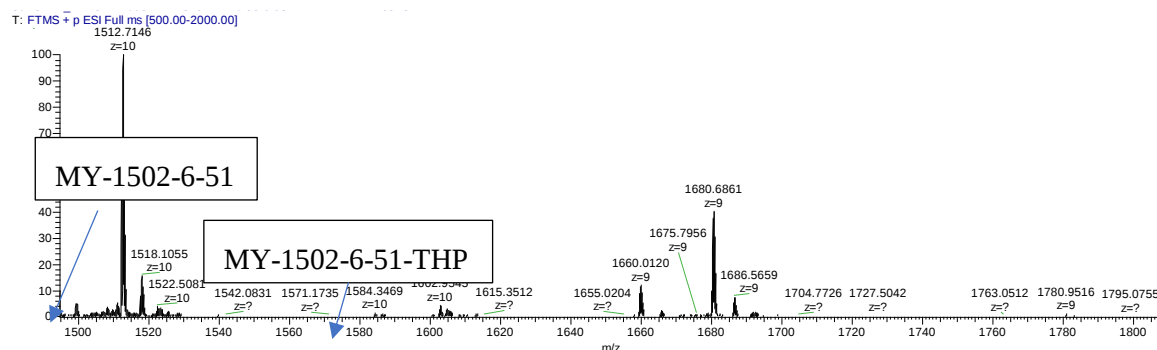


Figure S13. ESI+ mass spectrum of MY-1502-6-51-THP (10) (20-fold molar excess of 7). The peak at m/z 1518 corresponds to the $[\text{M}+10\text{H}]^{10+}$ of MY-1502-6-51. The peak at 1603 corresponds to $[\text{M}+10\text{H}]^{10+}$ of 1MY-1502-6-51-THP.

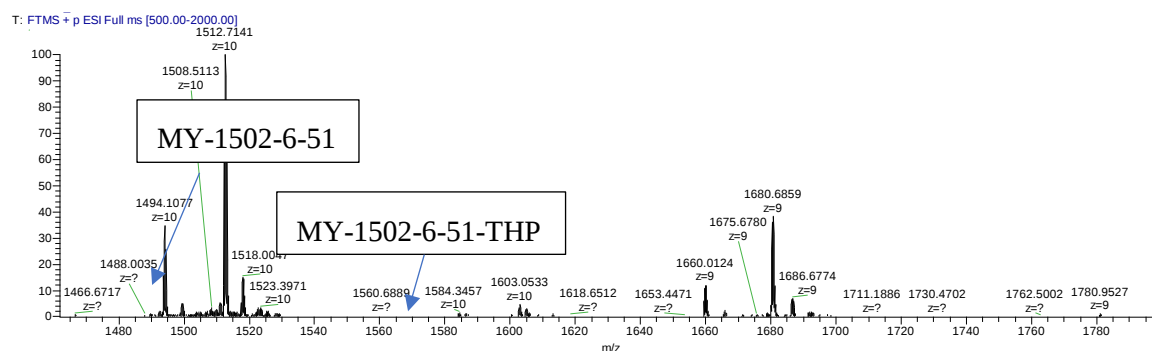


Figure S14. ESI+ mass spectrum of MY-1502-6-51-THP (10) (40-fold molar excess of 7). The peak at m/z 1518 corresponds to the $[\text{M}+10\text{H}]^{10+}$ of MY-1502-6-51. The peak at 1603 corresponds to $[\text{M}+10\text{H}]^{10+}$ of MY-1502-6-51-THP.

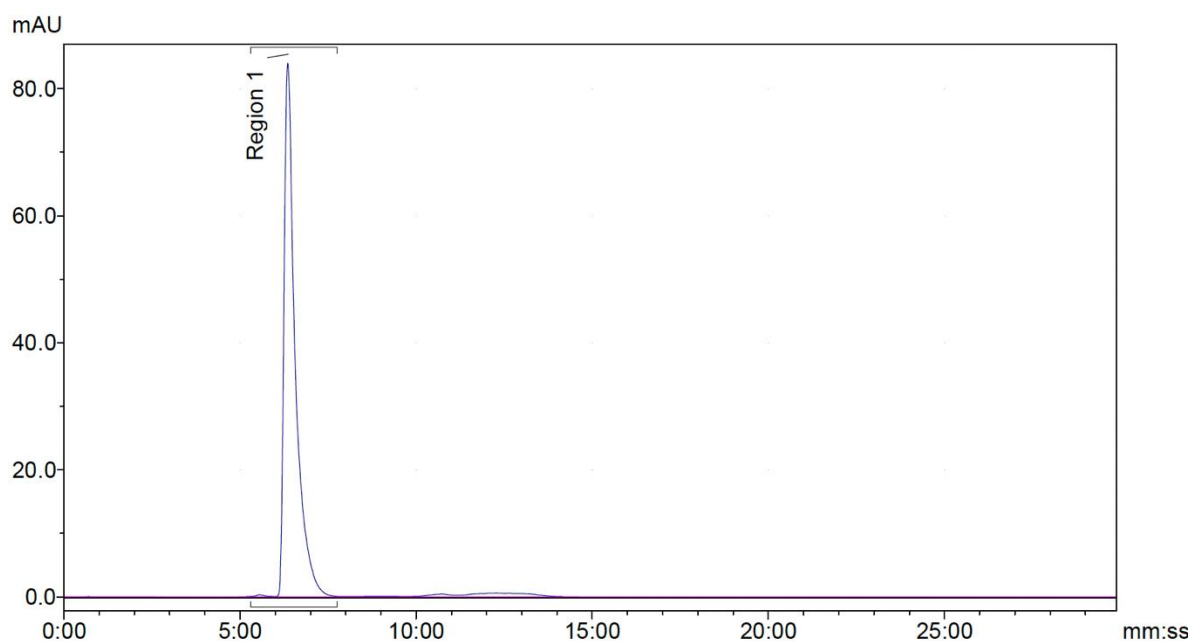


Figure S15. HPLC UV chromatogram (Method 2) of MY-1502-6-51-THP (**10**) (20-fold molar excess of **7**). Region 1 ($R_t=6.4$ min, 100%) represents MY-1502-6-51-THP. .

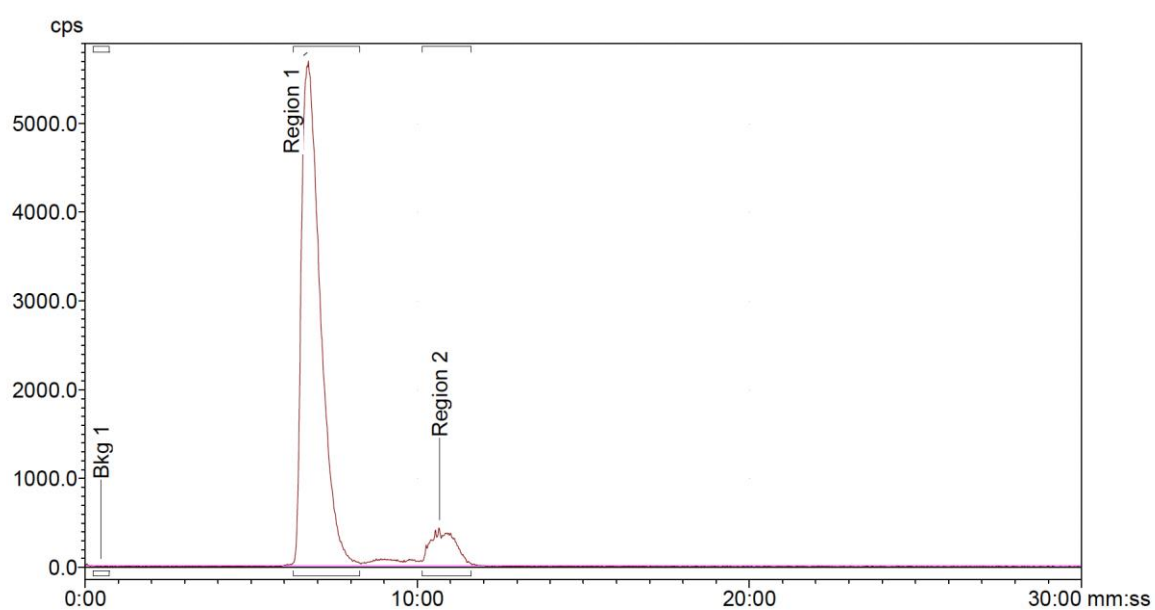


Figure S16. HPLC radiochromatogram (Method 2) of ^{68}Ga -MY-1502-6-51-THP (**11**) (20-fold molar excess of **7**). Region 1 ($R_t=6.7$ min, 91%) represents ^{68}Ga -MY-1502-6-51-THP, region 2 ($R_t=10.7$ min, 9%) represents free ^{68}Ga .

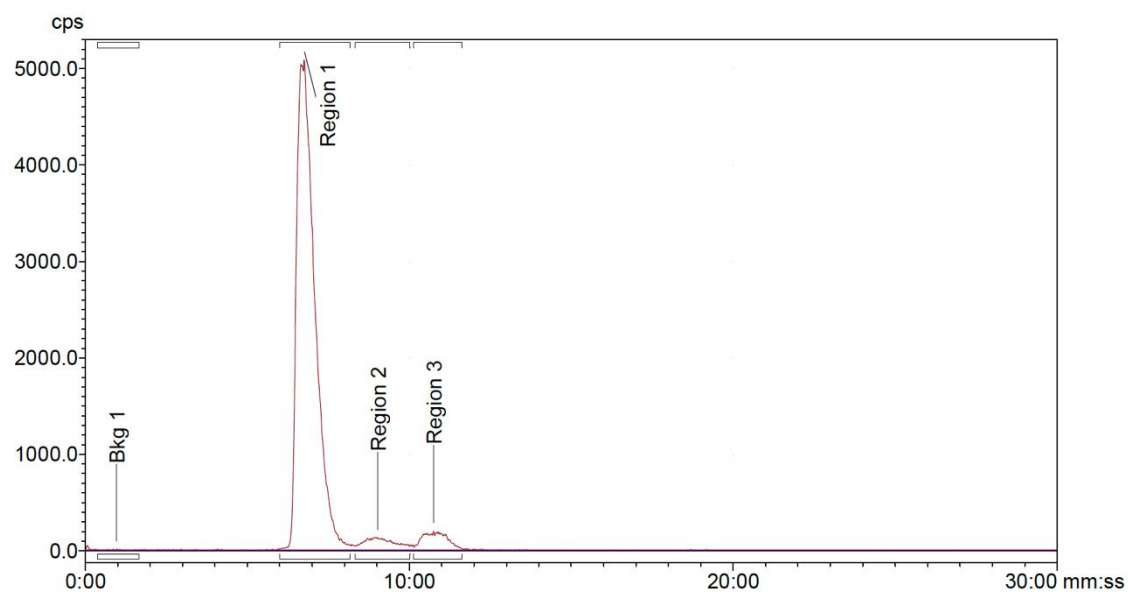
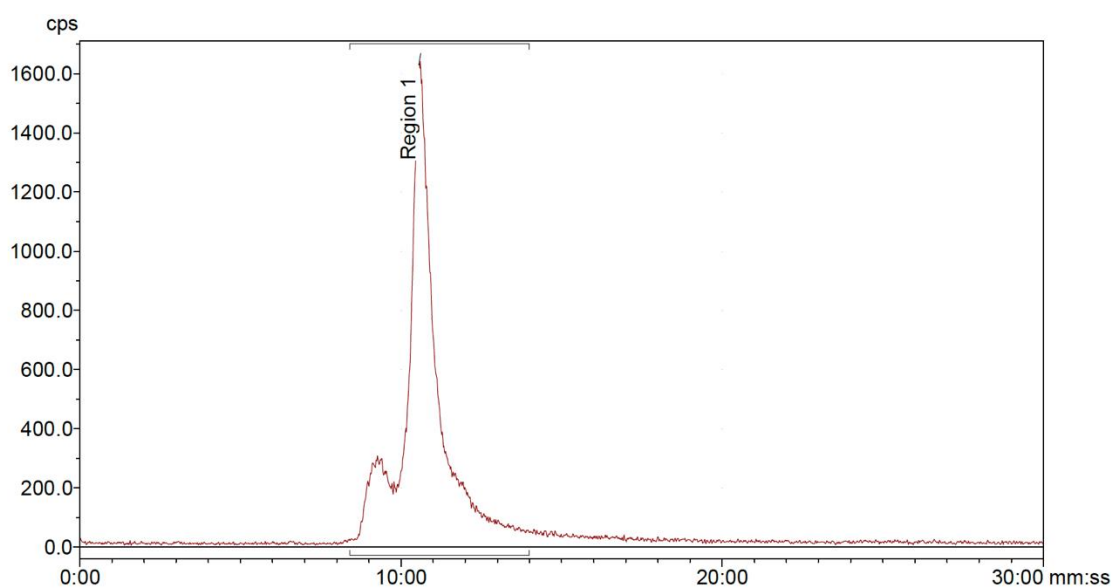


Figure S17. HPLC radiochromatogram (Method 2) of ^{68}Ga -MY-1502-6-51-THP (**11**) (40-fold molar excess of **7**). Region 1 ($R_t=6.8$ min, 92%) represents ^{68}Ga -MY-1502-6-51-THP, region 2 ($R_t=9.0$ min, 4%) represents a small ^{68}Ga containing species, potentially ^{68}Ga -**7** and region 3 ($R_t=10.8$ min, 4%) represents free ^{68}Ga .



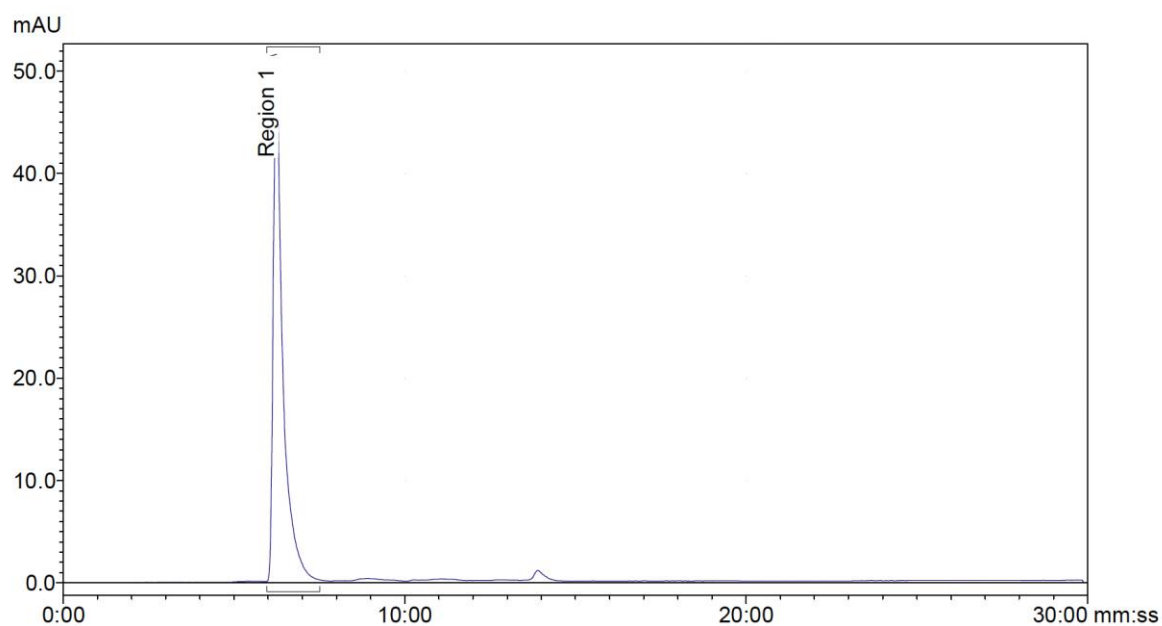


Figure S18. HPLC radiochromatogram (Method 2) and corresponding UV chromatograms (bottom) of ^{68}Ga labeled MY-1502-6-51 (20-fold molar excess of **5**). The peak in the radiochromatogram ($R_t=10.8$ min) represents free ^{68}Ga with no protein-associated radioactivity present. The UV chromatogram confirmed the presence of MY-1502-6-51 ($R_t=6.3$ min).