

## Supporting Information

### Development of a homotrimeric PSMA radioligand based on the NOTI chelating platform

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## HPLC chromatograms

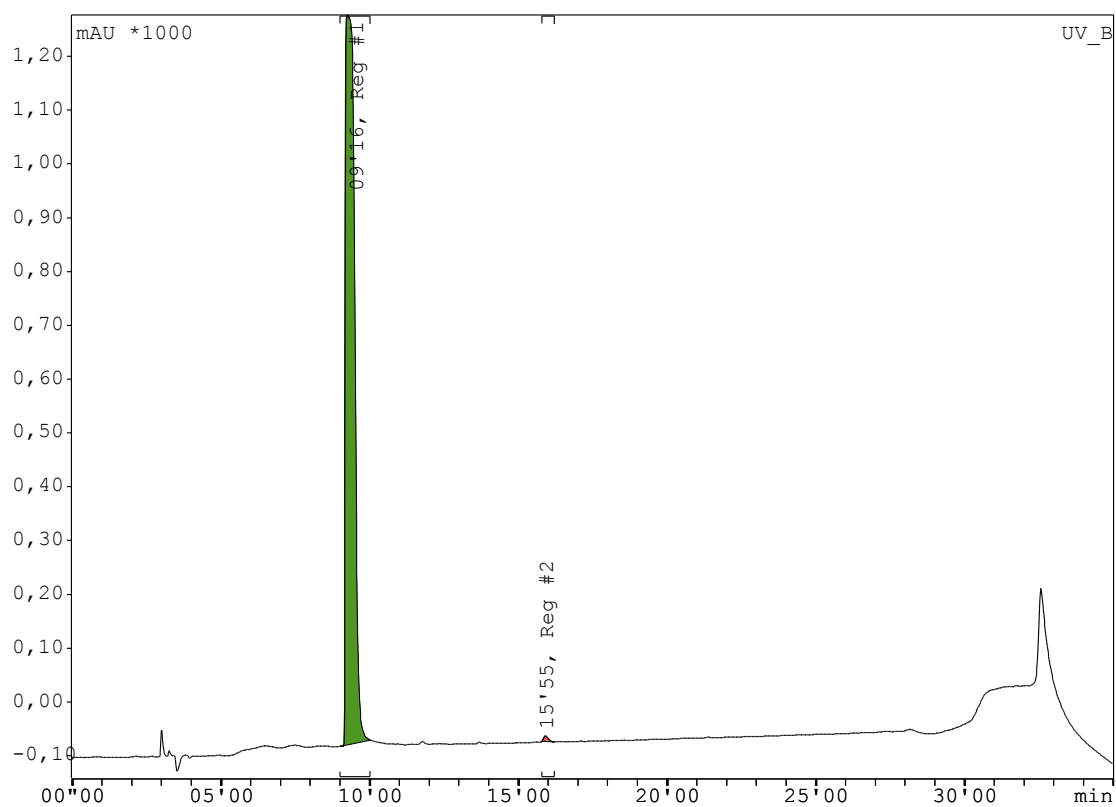


Figure S1. Representative UV/vis RP-HPLC chromatogram of **1**.

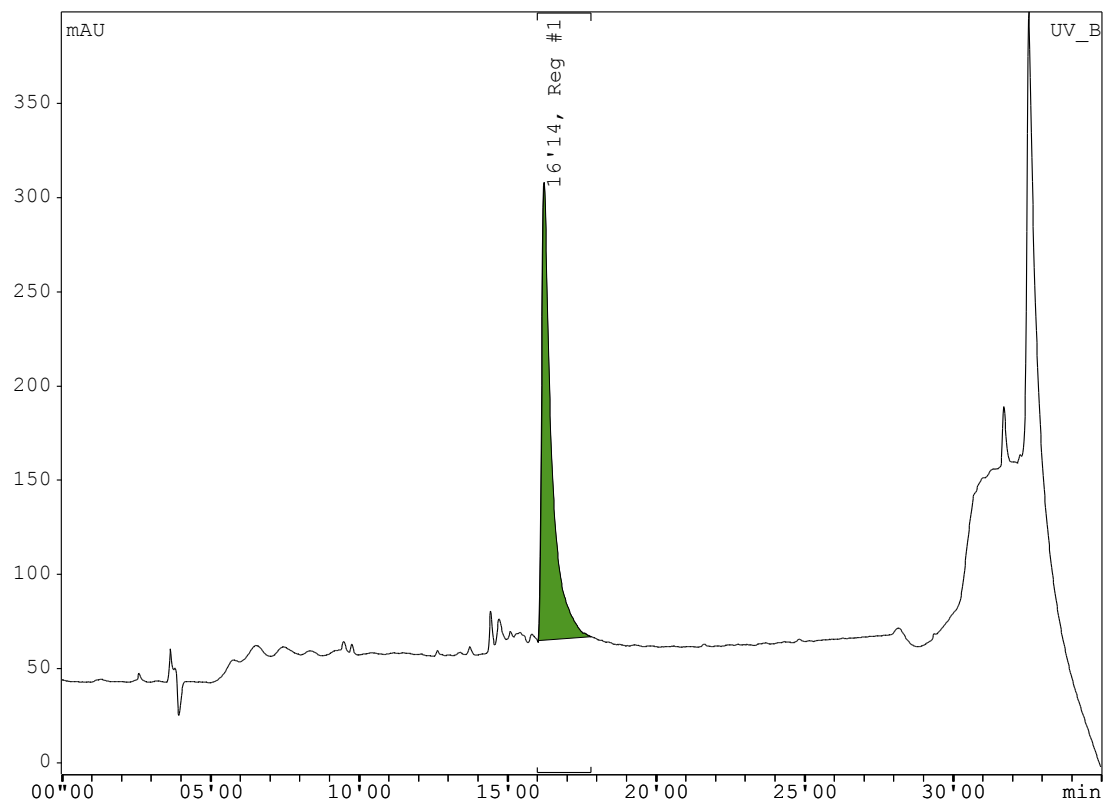


Figure S2. Representative UV/vis RP-HPLC chromatogram of **2**.

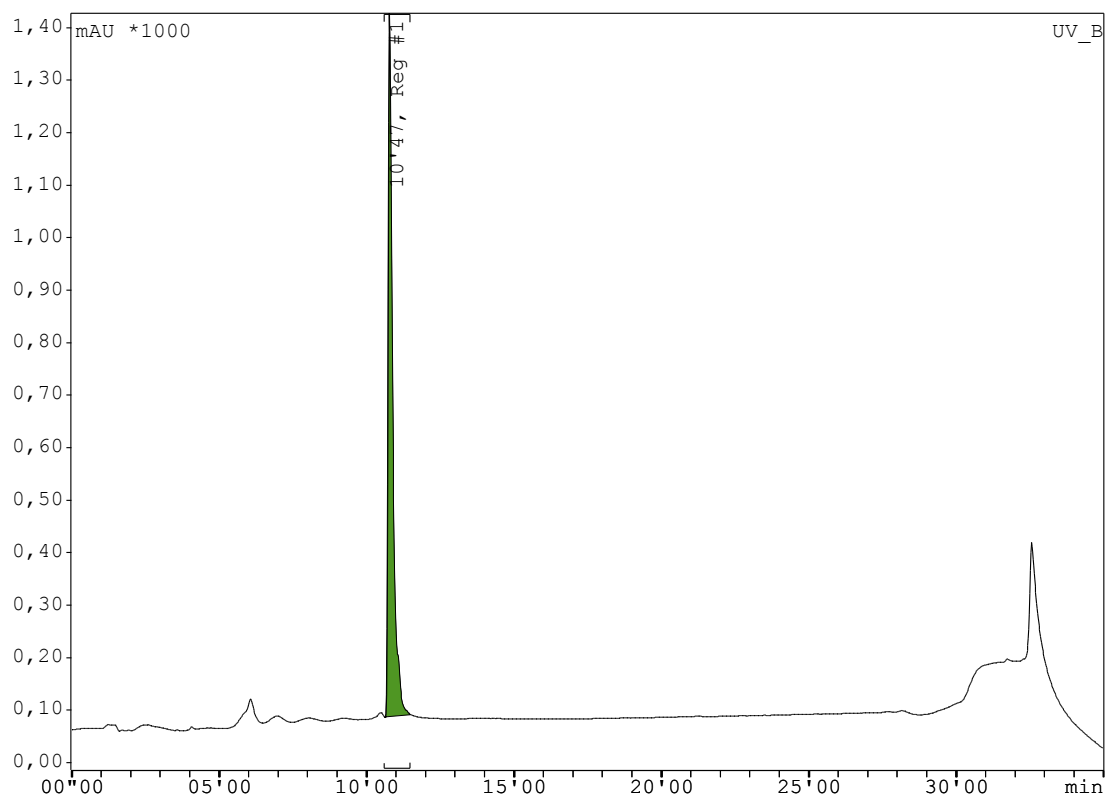


Figure S3. Representative UV/vis RP-HPLC chromatogram of **3**.

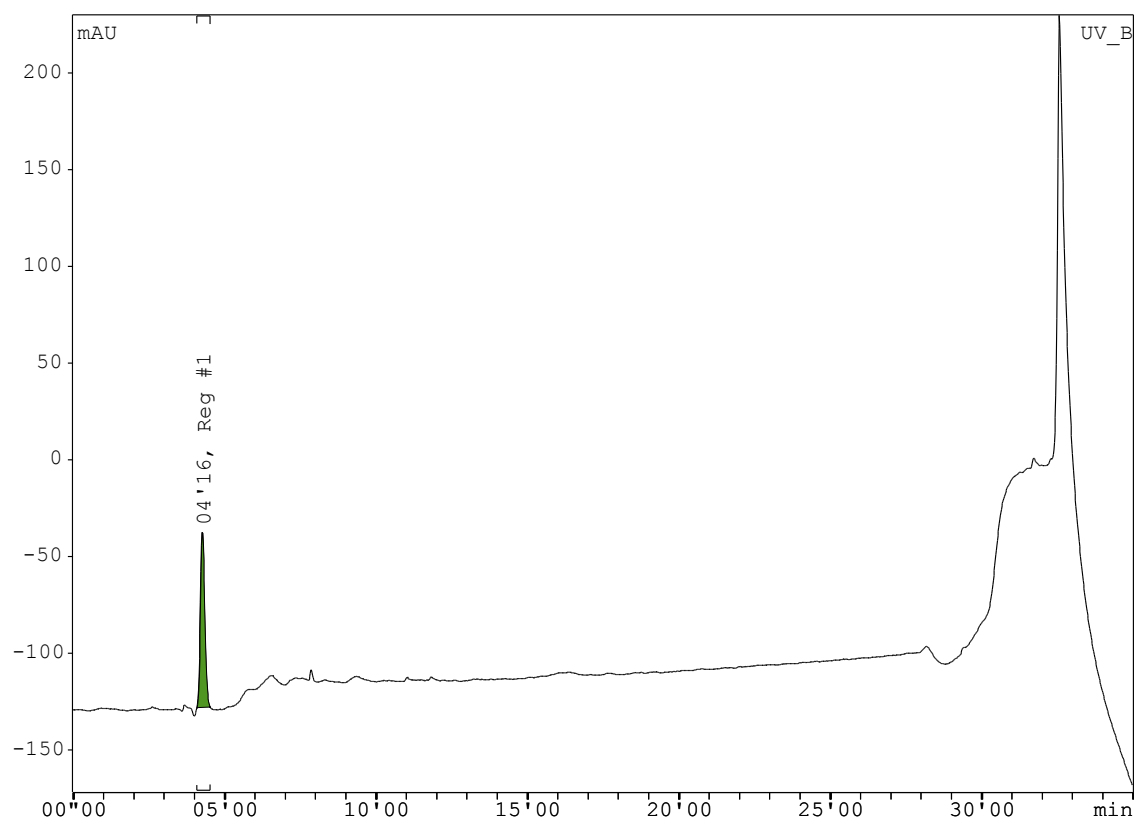


Figure S4. Representative UV/vis RP-HPLC chromatogram of **4**.

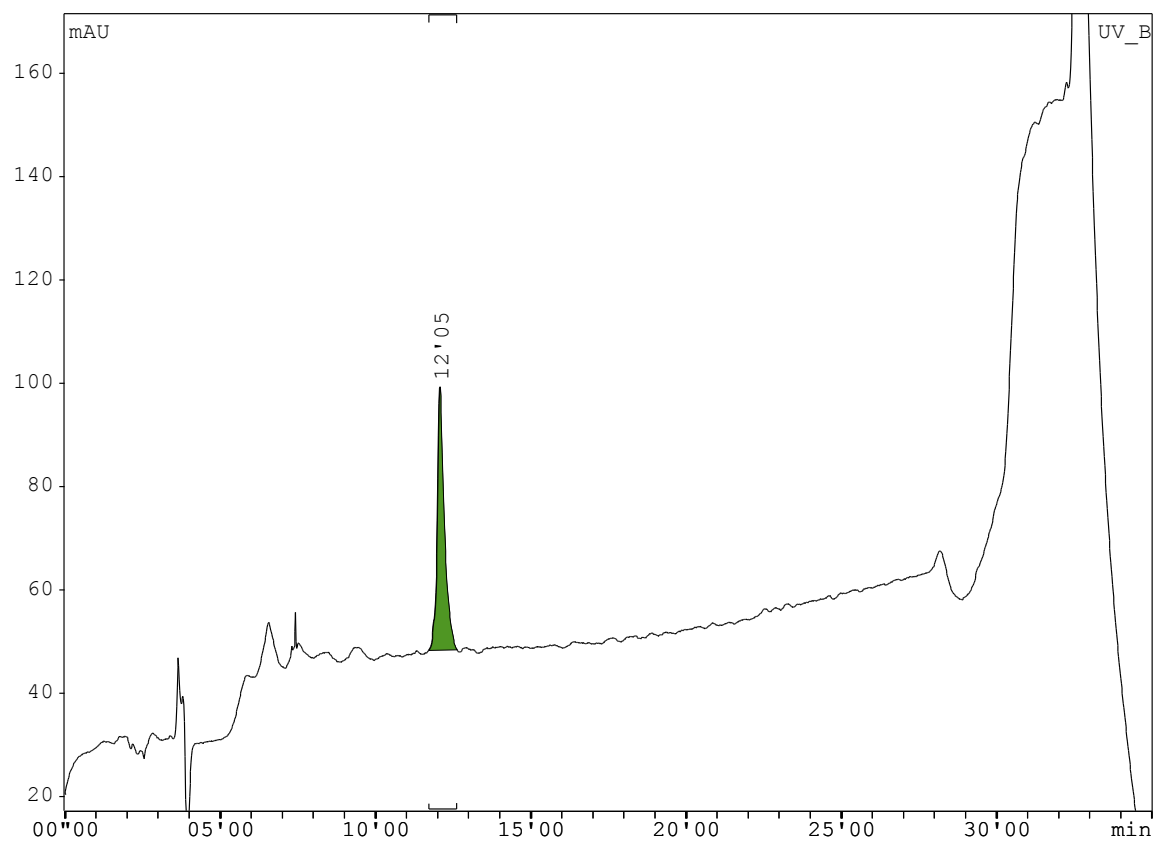


Figure S5. Representative UV/vis RP-HPLC chromatogram of **7**.

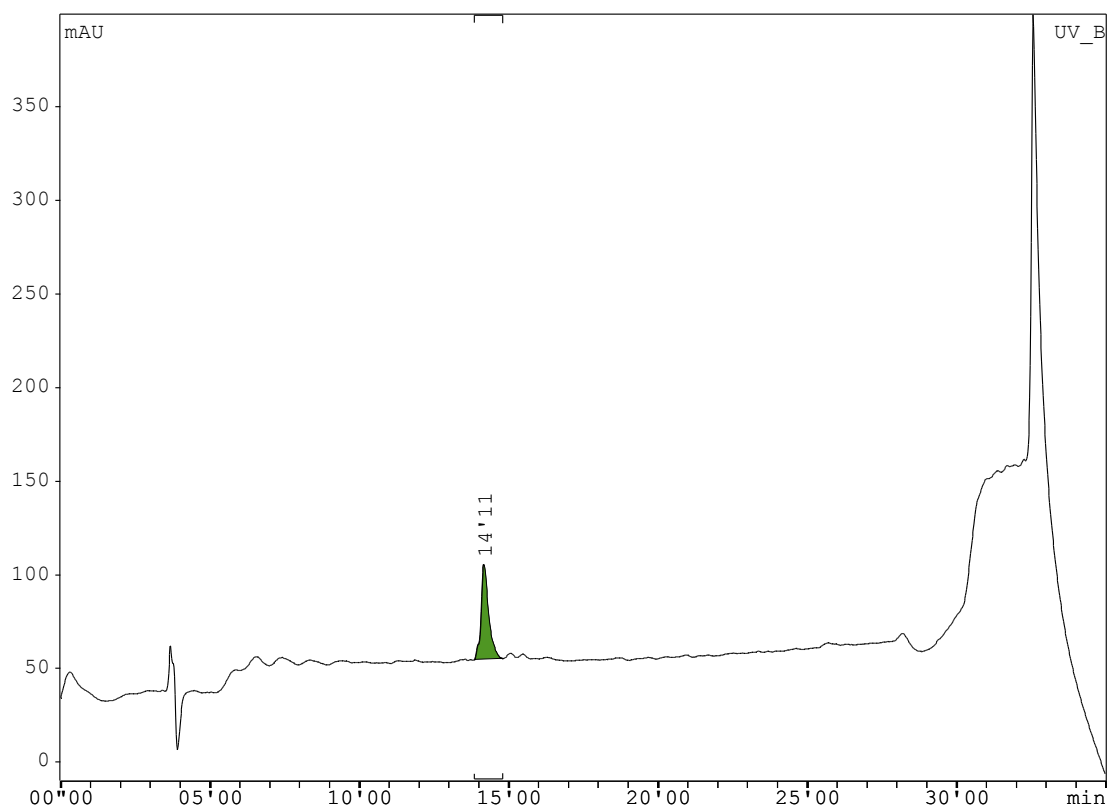


Figure S6. Representative UV/vis RP-HPLC chromatogram of **8**.

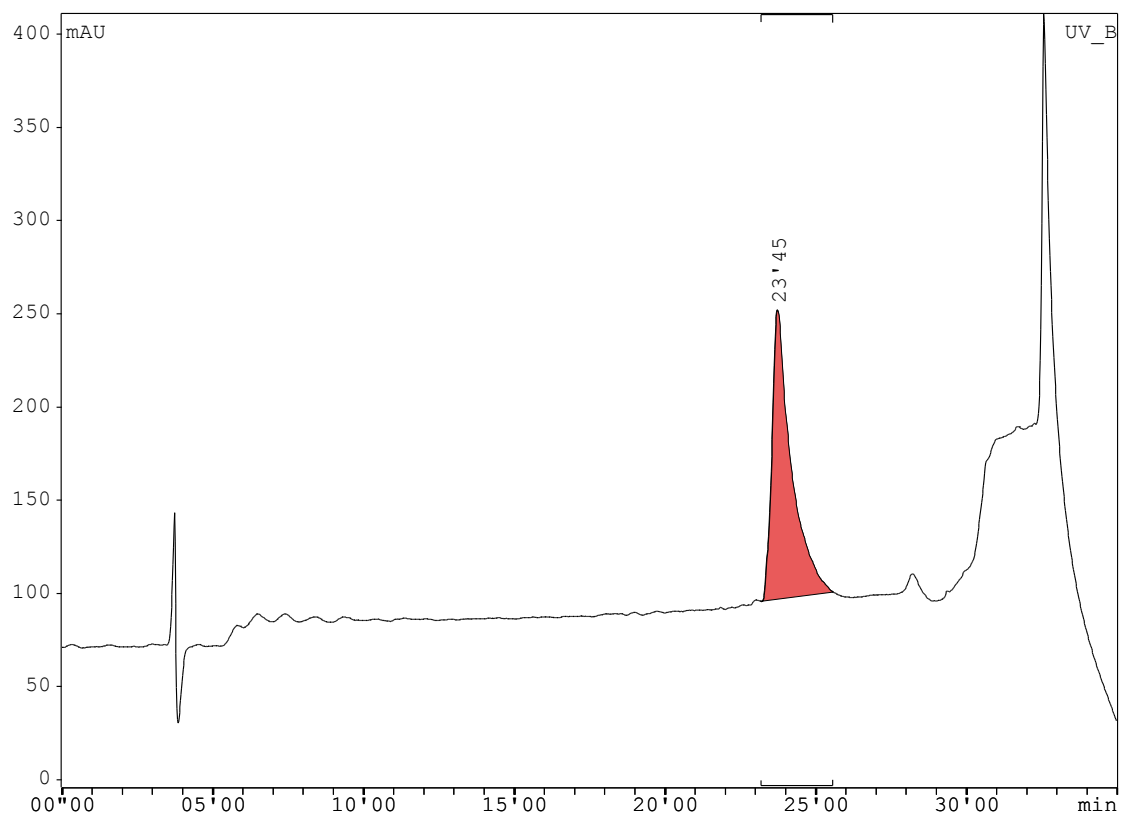


Figure S7. Representative UV/vis RP-HPLC chromatogram of **9**.

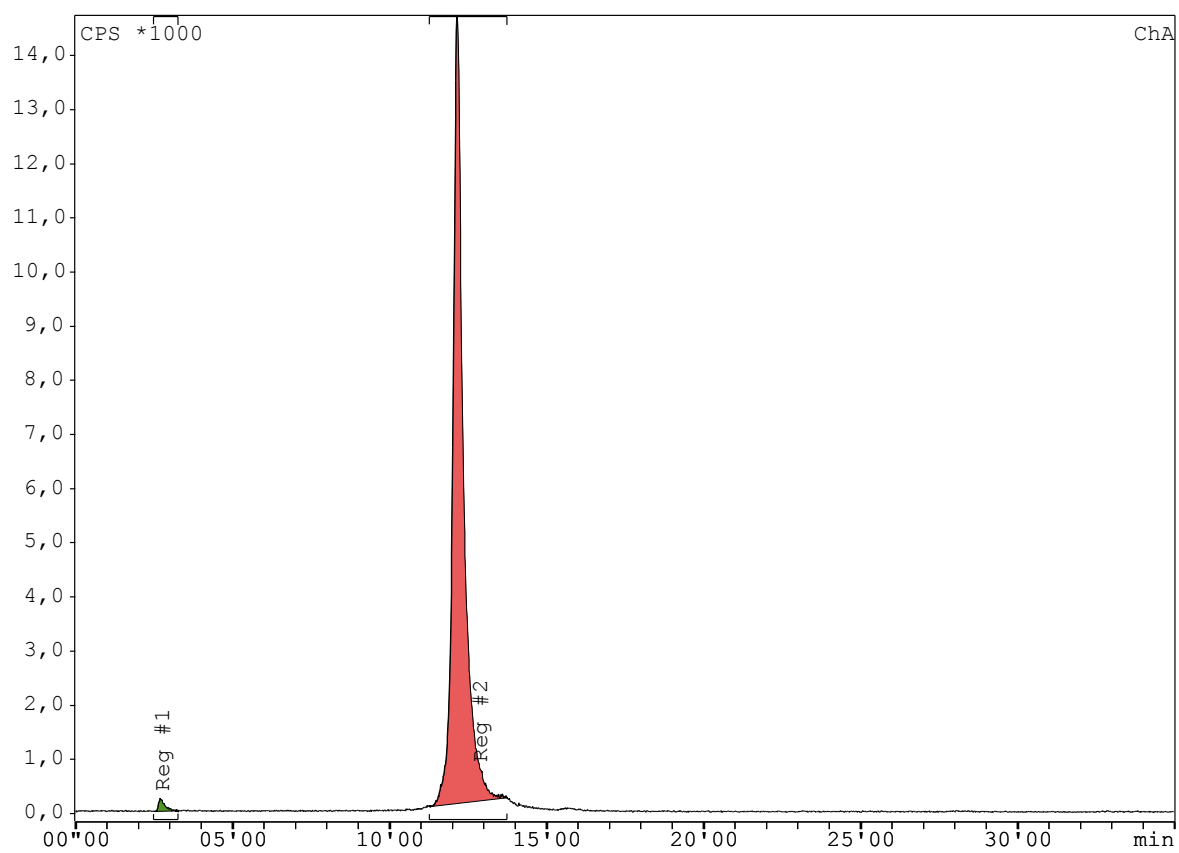


Figure S8. Representative radio-RP-HPLC chromatogram of [<sup>68</sup>Ga]Ga-7.

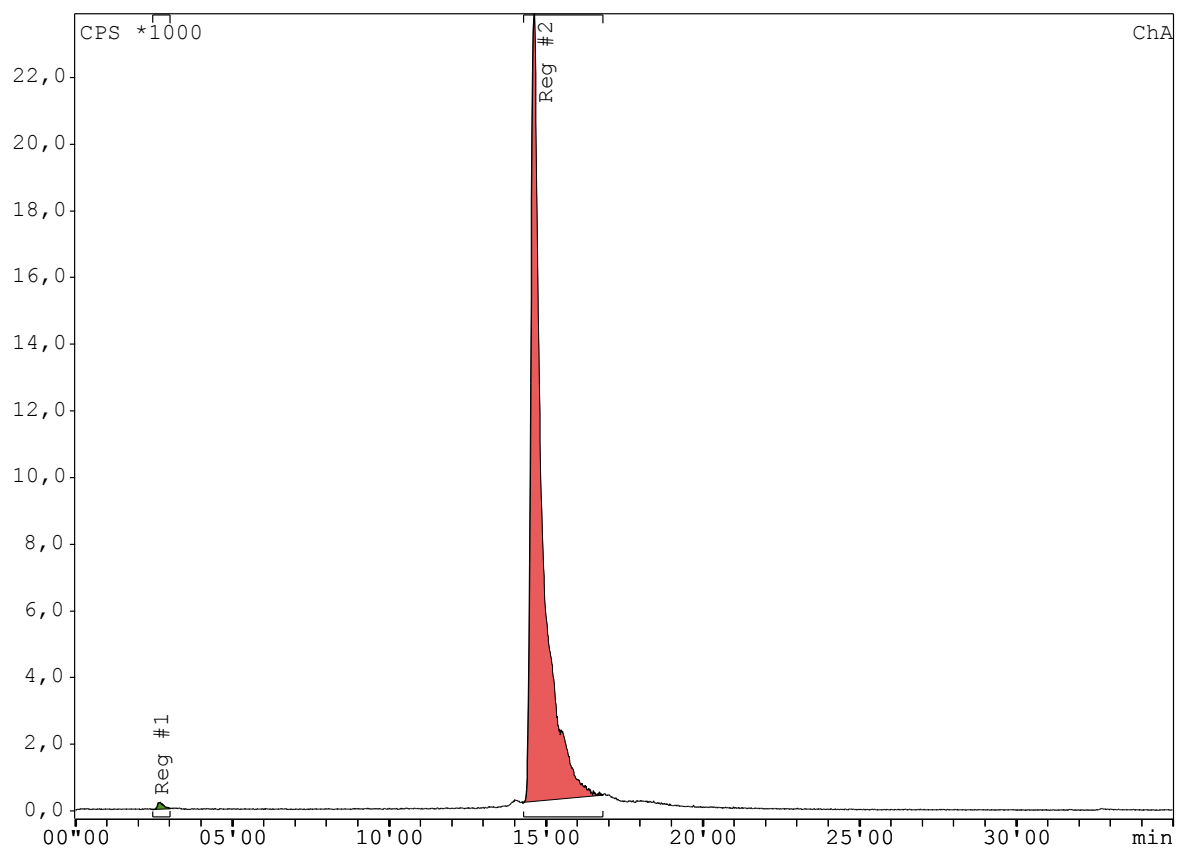


Figure S9. Representative radio-RP-HPLC chromatogram of [ $^{68}\text{Ga}$ ]Ga-8.

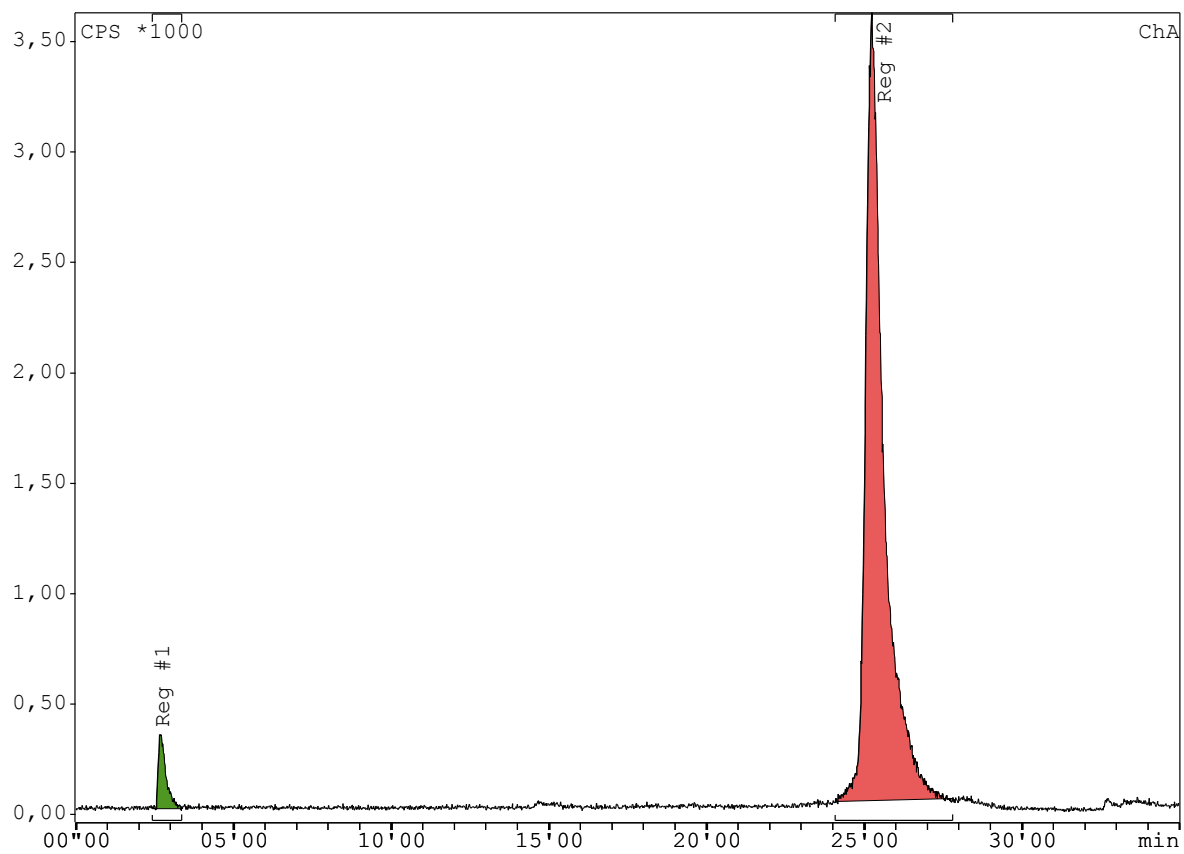


Figure S10. Representative radio-RP-HPLC chromatogram of [ $^{68}\text{Ga}$ ]Ga-9.



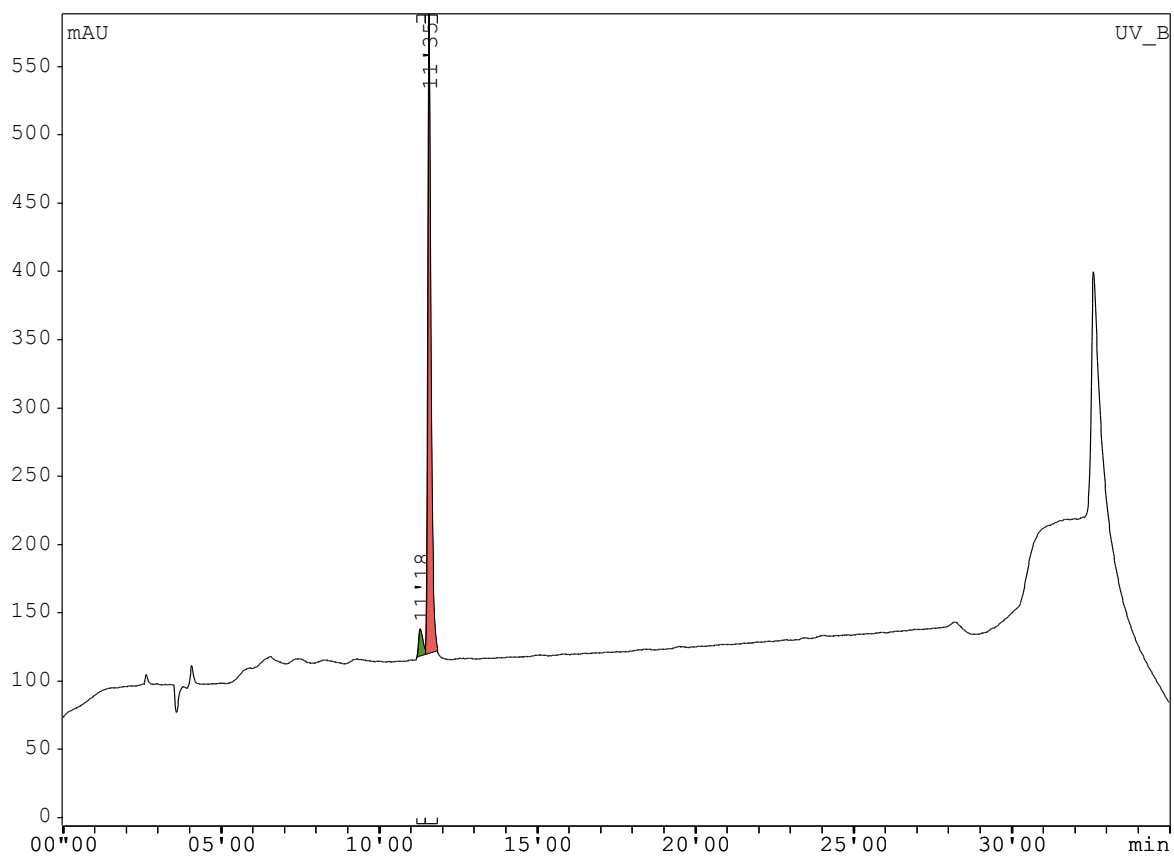


Figure S11. Representative UV/vis RP-HPLC chromatogram of <sup>nat</sup>Ga-7.

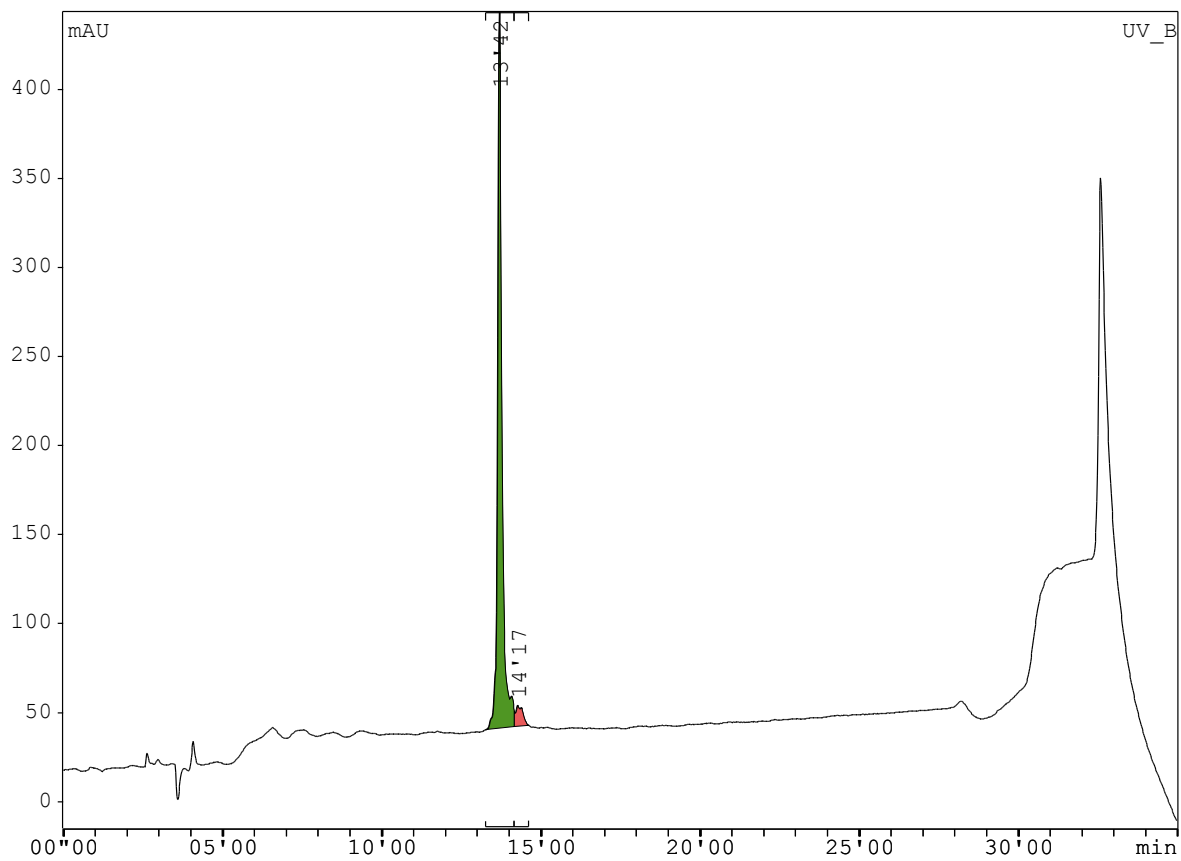


Figure S12. Representative UV/vis RP-HPLC chromatogram of <sup>nat</sup>Ga-8.

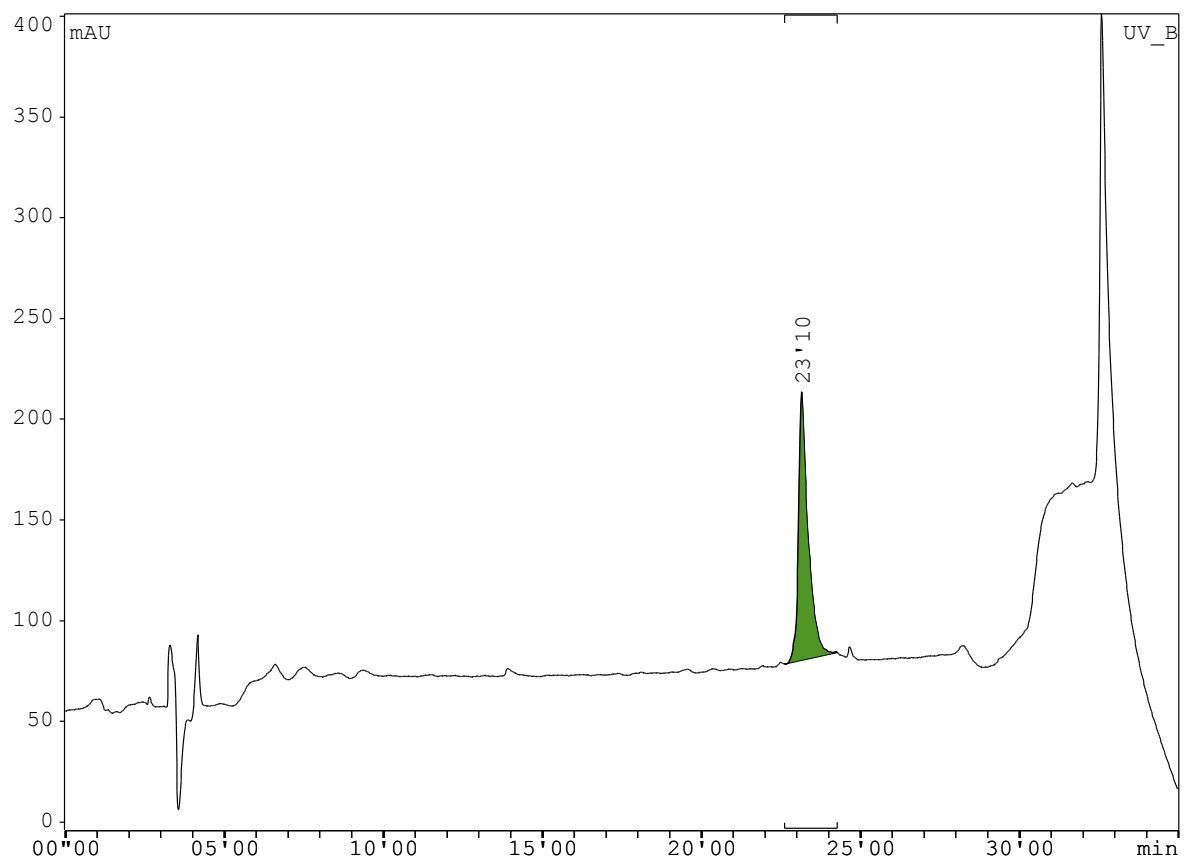


Figure S13. Representative UV/vis RP-HPLC chromatogram of <sup>nat</sup>Ga-9.

## NMR data

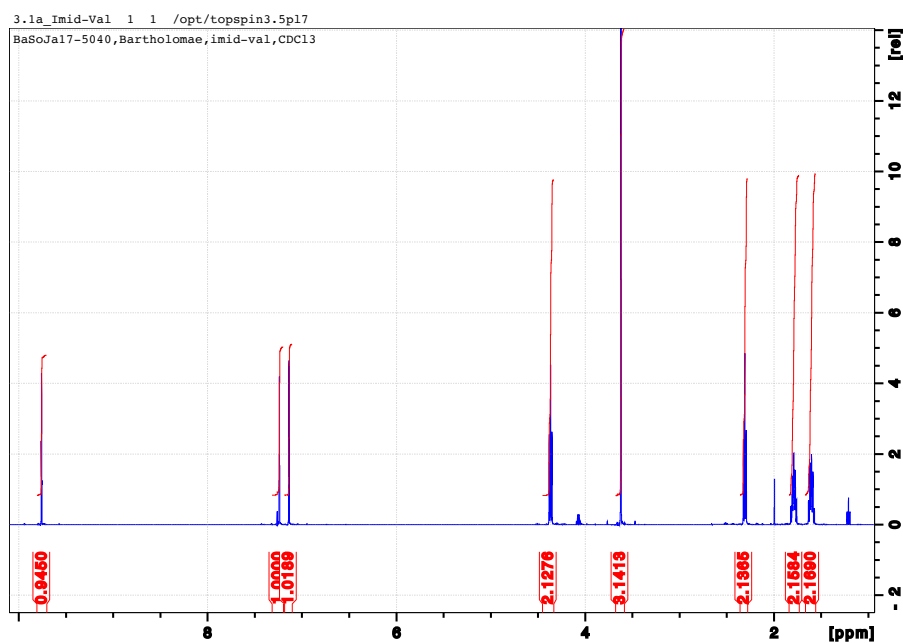


Figure S14.  $^1\text{H}$ -NMR of compound **1** in  $\text{CDCl}_3$ .

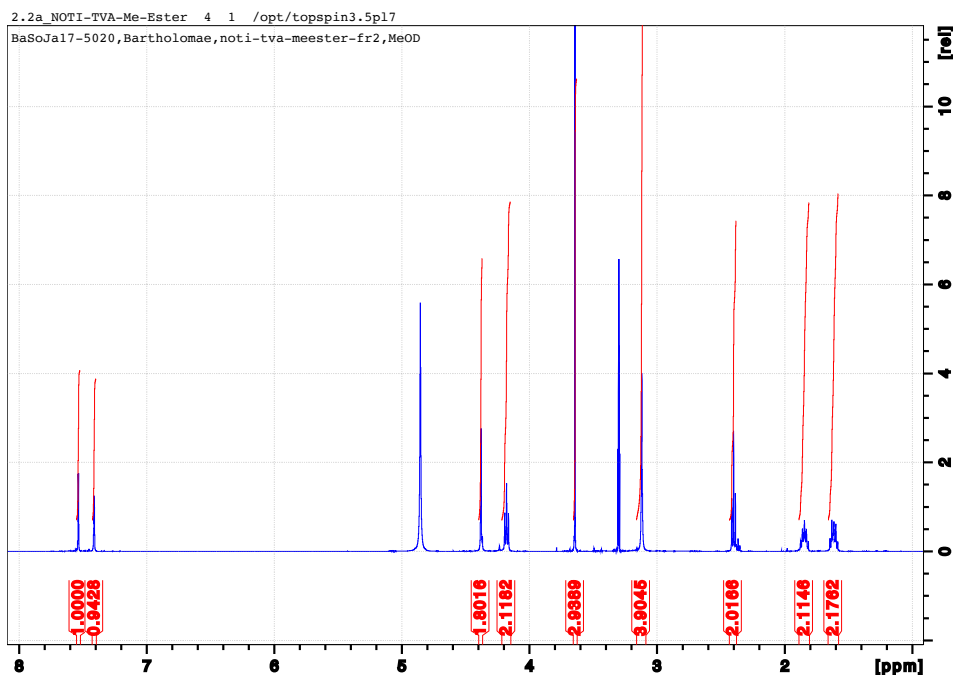


Figure S15.  $^1\text{H}$ -NMR of compound **2** in  $d_4\text{-MeOD}$ .

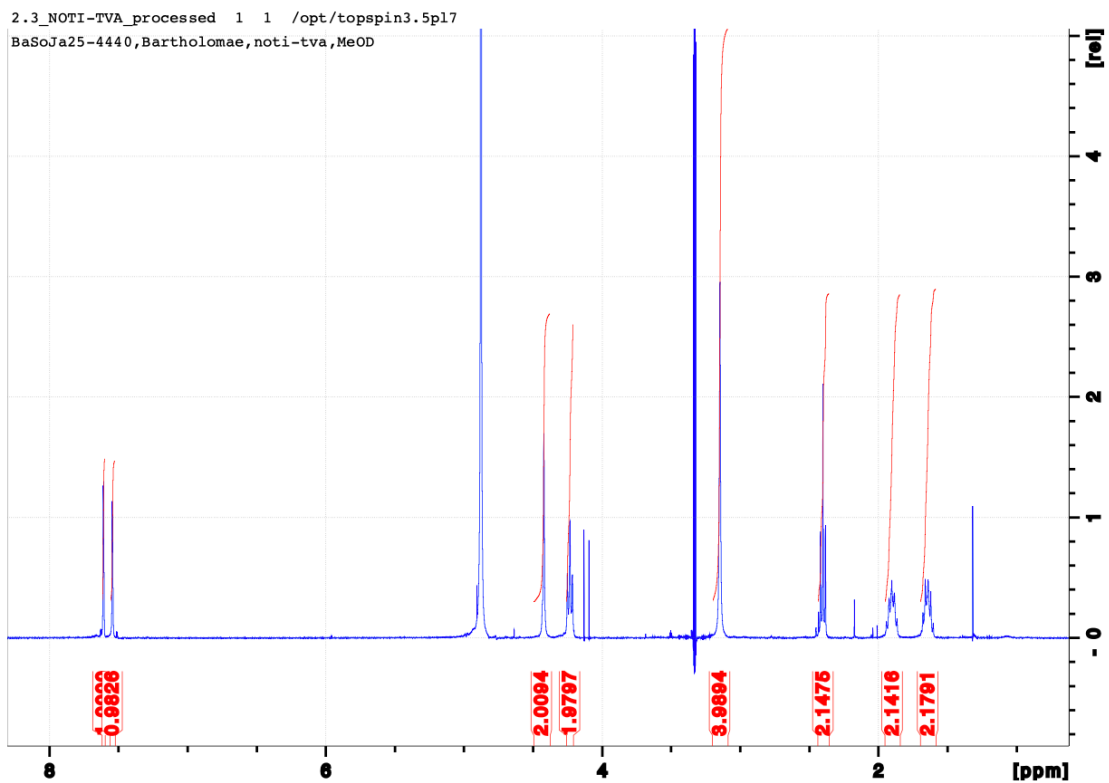


Figure S16.  $^1\text{H-NMR}$  of compound 3 in  $\text{d}_4\text{-MeOD}$ .

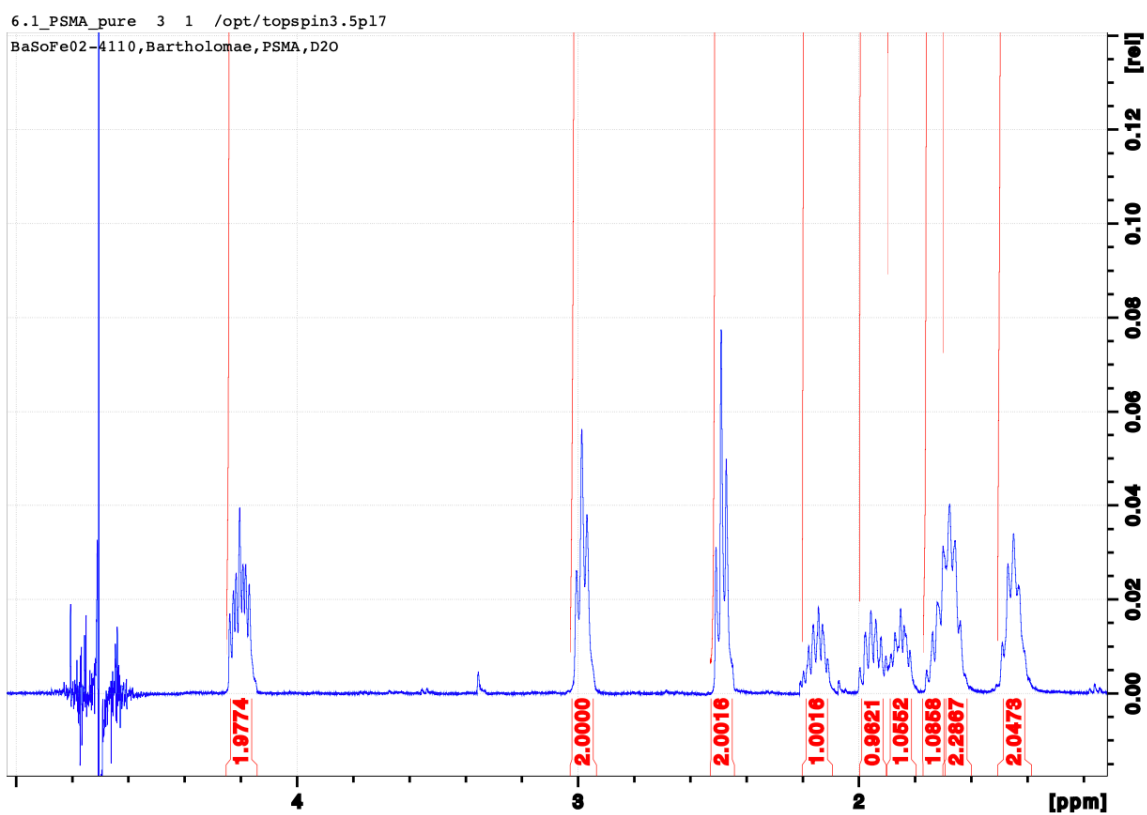


Figure S17.  $^1\text{H-NMR}$  of compound 4 in  $\text{D}_2\text{O}$ .

# Mass spectrometry data

D:\data\_2018\klind32s\_hr03

2/15/2018 2:54:48 PM

ms.ms.vnl

klind32s\_hr03 #1 RT: 0.00 AV: 1 NL: 6.14E7  
T: FTMS + p ESI Full lock ms [50.00-700.00]

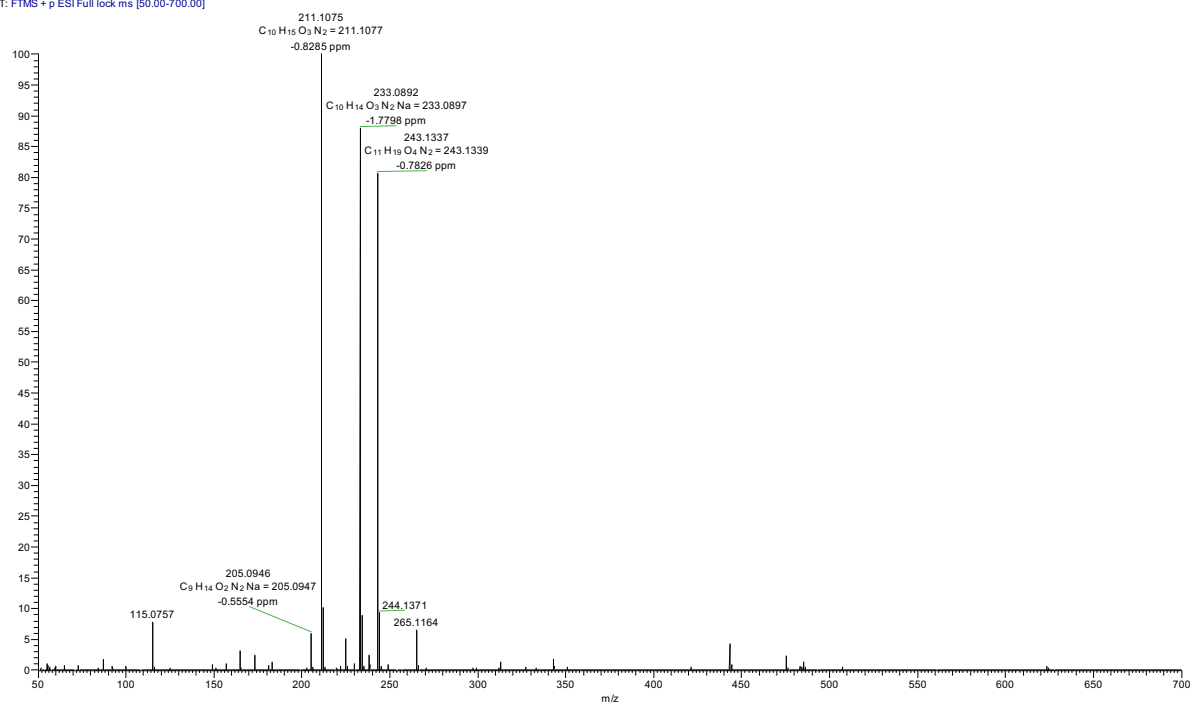


Figure S18. HR-ESI-MS of compound 1.

D:\data\_2018\klind23s\_hr04

1/29/2018 10:26:51 AM

ms.ms.est

klind23s\_hr04 #1 RT: 0.00 AV: 1 NL: 8.20E7  
T: FTMS + p ESI Full ms [100.00-2000.00]

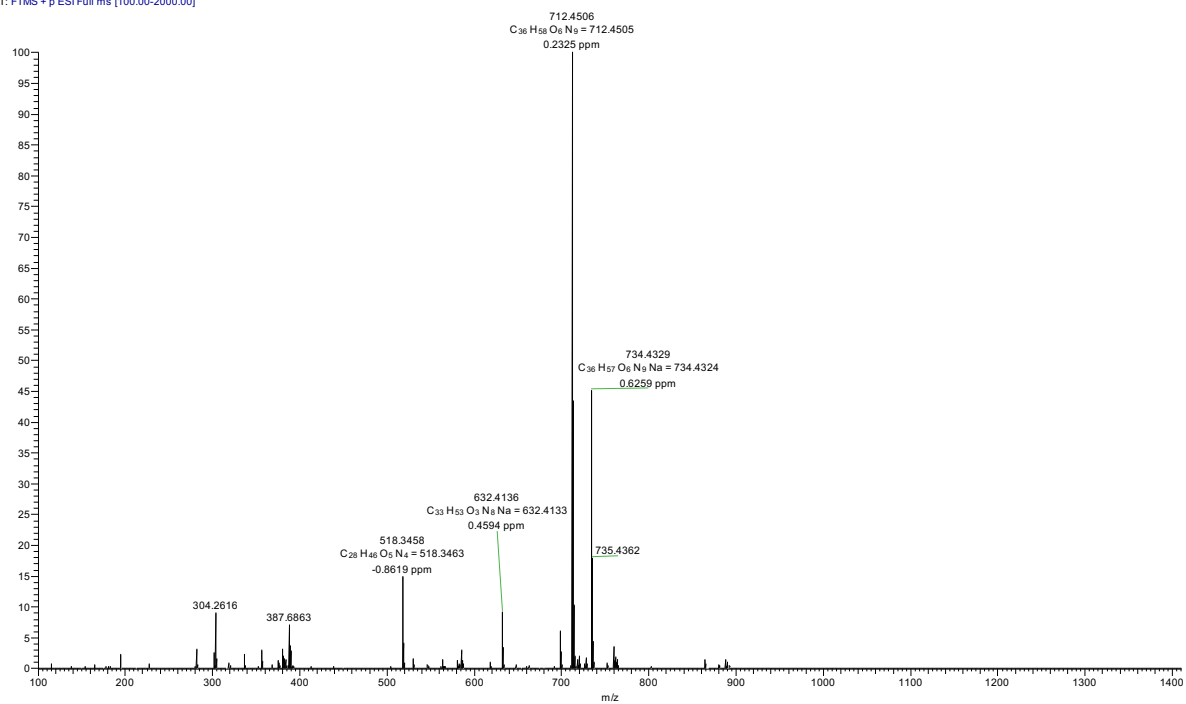


Figure S19. HR-ESI-MS of compound 2.

klind24s\_hr05 #1 RT: 0.00 AV: 1 NL: 3.84E7  
T: FTMS + p ESI Full ms [100.00-1400.00]

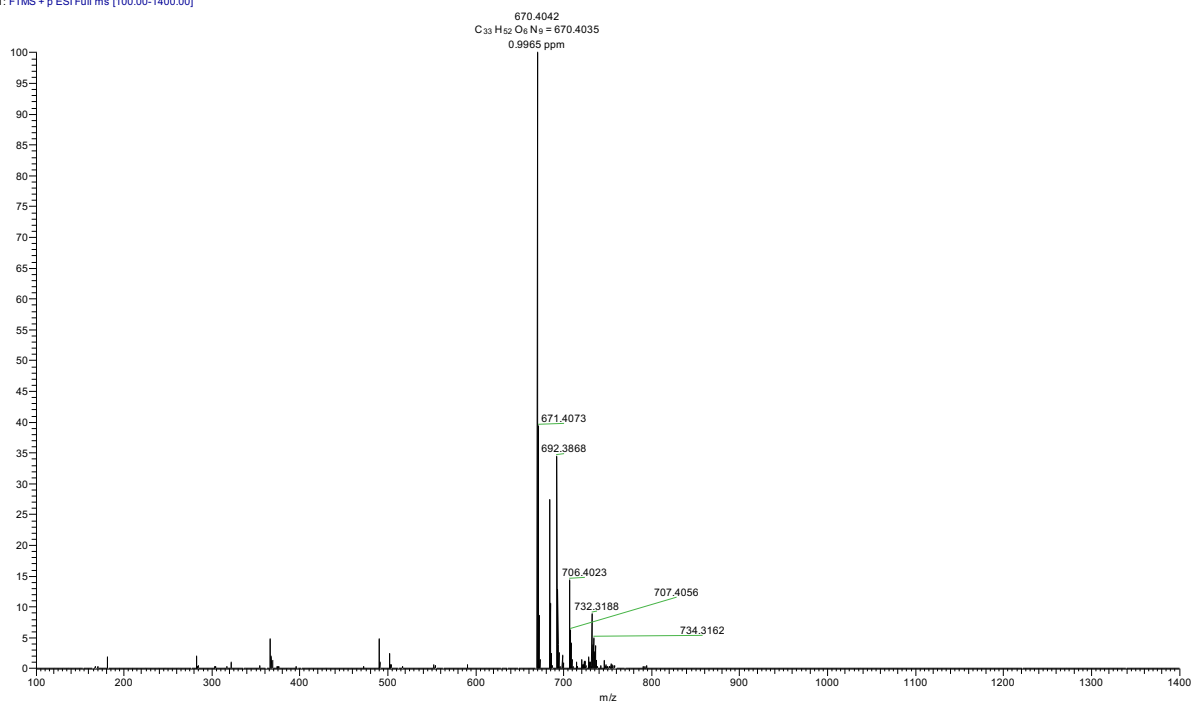


Figure S20. HR-ESI-MS of compound 3.

klind33s\_hr02 #1 RT: 0.02 AV: 1 NL: 1.65E6  
T: FTMS - p ESI Full lock ms [200.00-1000.00]

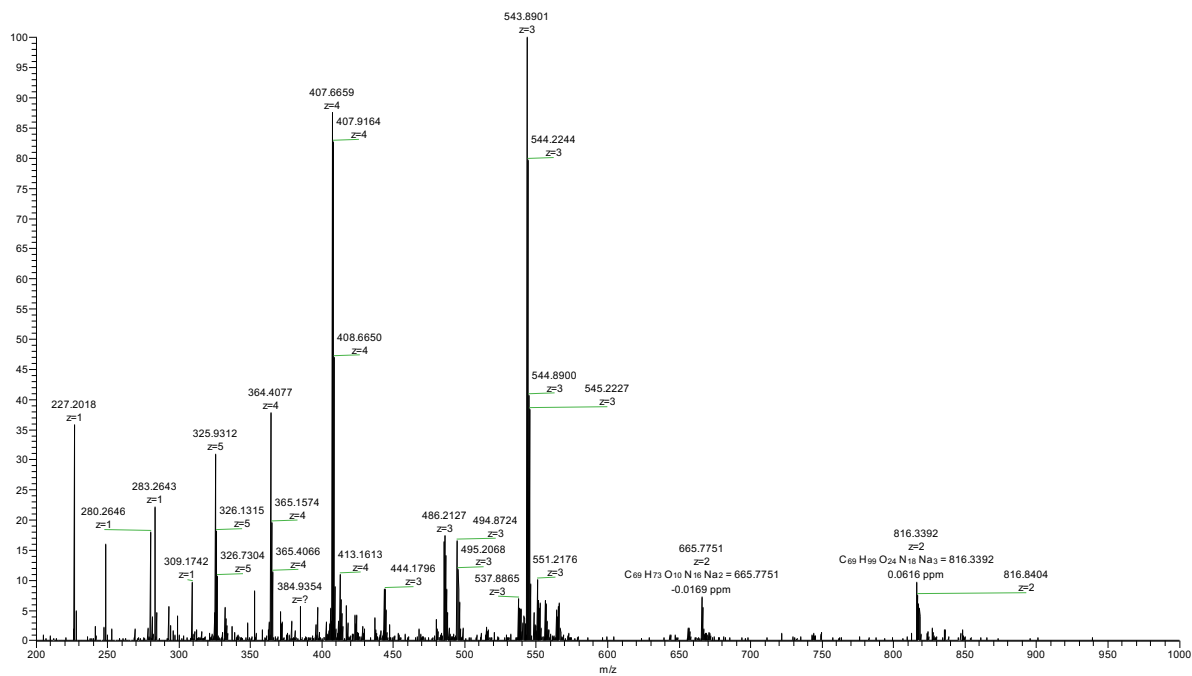


Figure S21. HR-ESI-MS of compound 7.



klind35s\_hr06 #1 RT: 0.02 AV: 1 NL: 3.83E6  
T: FTMS - p ESI Full lock ms [400.00-1200.10]

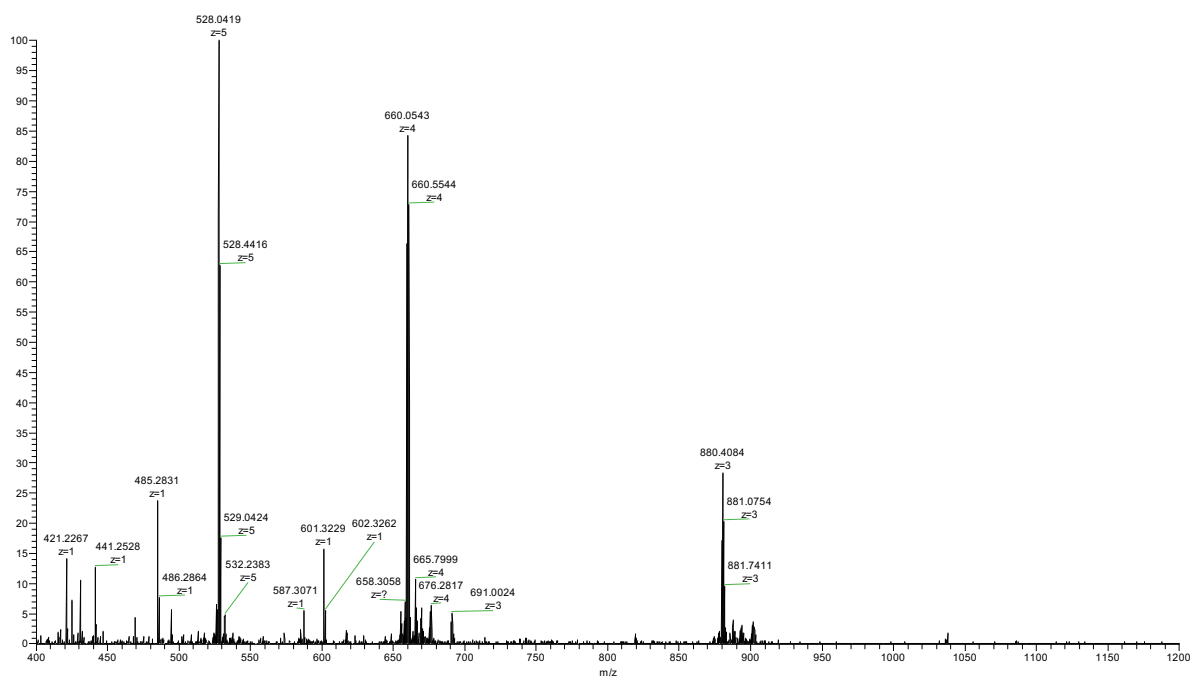


Figure S25. HR-ESI-MS of compound 9.

Spectrum RT 0:32 - 0:52 (49 scans) - Background Subtracted 0:04 - 0:20  
2024\_8\_6\_16\_10\_18\_NOTI-TVA-tPSMA.datx;  
ESI + Max: 1.8E6

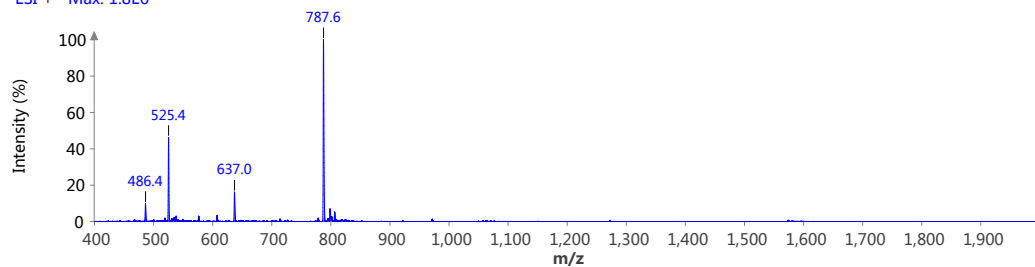


Figure S26. LR-ESI-MS of compound 9.



klind36s\_hr03 #1 RT: 0.02 AV: 1 NL: 5.02E6  
T: FTMS + p ESI Full lock ms [100.00-2000.00]

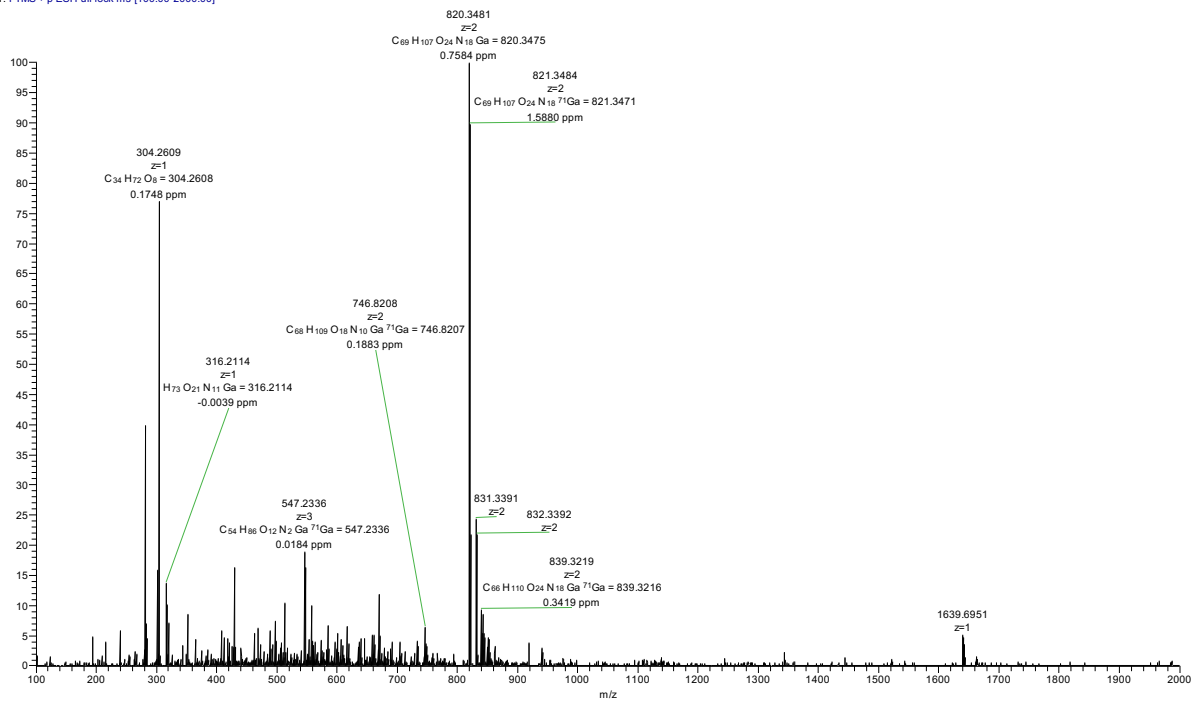


Figure S27. HR-ESI-MS of  $^{nat}\text{Ga-7}$ .

klind37s\_hr03 #1 RT: 0.02 AV: 1 NL: 7.80E6  
T: FTMS + p ESI Full lock ms [100.00-2000.00]

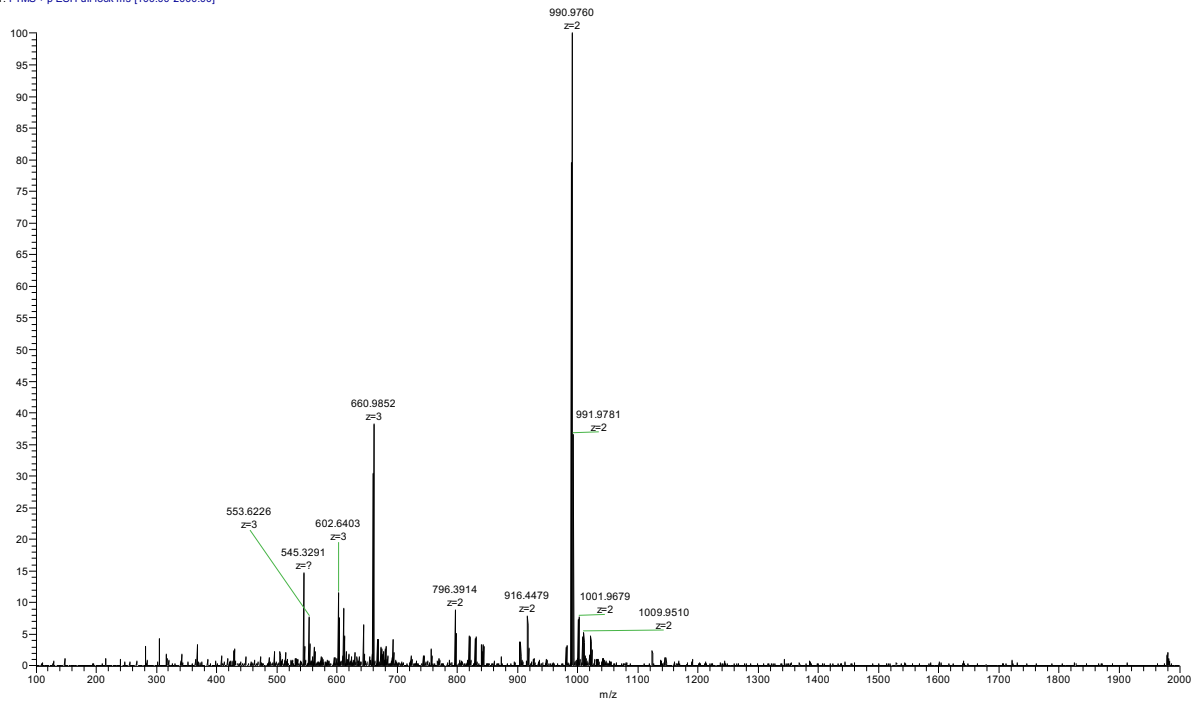


Figure S28. HR-ESI-MS of  $^{nat}\text{Ga-8}$ .

klind38s\_hr04 #1 RT: 0.03 AV: 1 NL: 2.16E5  
T: FTMS + p ESI Full lock ms [150.00-3000.00]

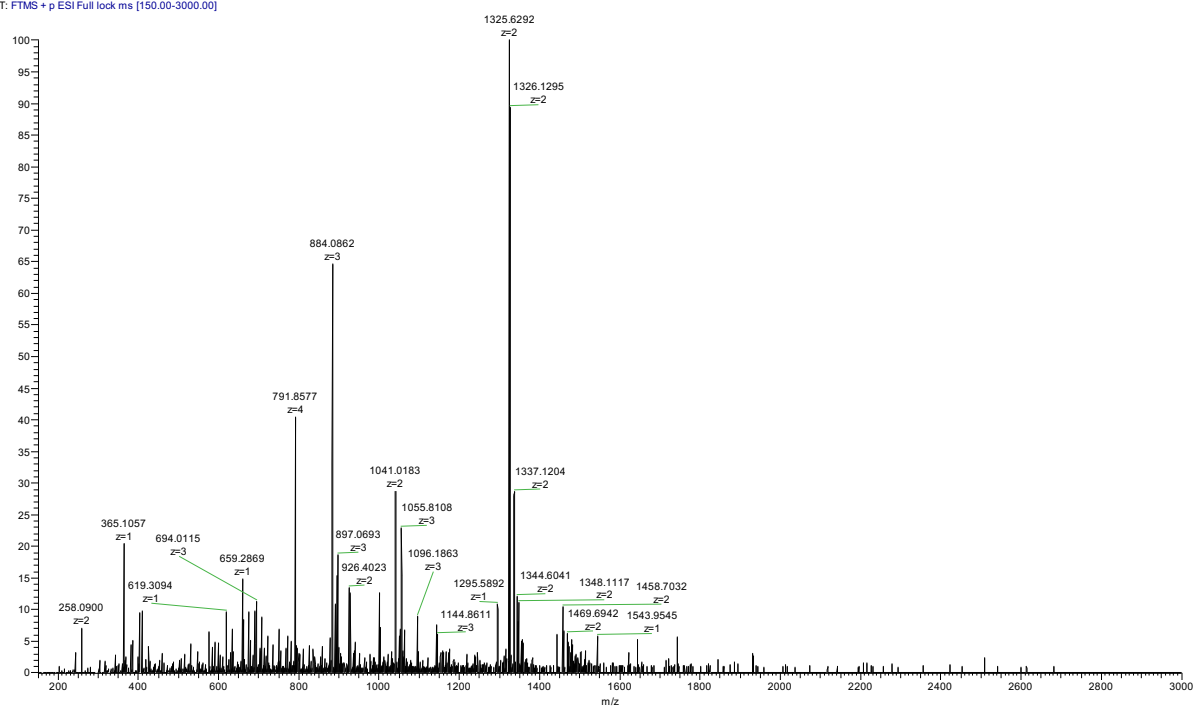


Figure S29. HR-ESI-MS of  $^{nat}\text{Ga-9}$ .