

Electronic Supplementary Information (ESI) for:

A New Tetrapodal 3-Hydroxy-4-Pyridinone Ligand for Complexation of ⁸⁹Zirconium for Positron Emission Tomography (PET) Imaging

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Supplementary Information Contents

Fig. S1. ¹ H-NMR of THPN.....	S-2
Fig. S2. ¹³ C-NMR of THPN.....	S-3
Fig. S3. HR-MS (+) of THPN.....	S-4
Fig. S4. HR-MS (–) of THPN.....	S-5
Fig. S5. HPLC chromatogram (λ ₂₅₄) of THPN	S-5
Fig. S6. MALDI-MS of Zr-THPN.	S-6
Fig. S7. FT-IR comparison of Zr-THPN and THPN	S-7
Fig. S8. ¹ H-NMR comparison of Zr-THPN and THPN	S-8
Fig. S9. ITLC comparison.....	S-8
Fig. S10. ITLCs of transchelation competition.....	S-9
Fig. S11. Coronal SPECT/CT images of all four mice injected with ⁸⁹ Zr-THPN	S-10
Fig. S12. Coronal SPECT/CT image of the mouse injected with ⁸⁹ Zr-DFO.....	S-11

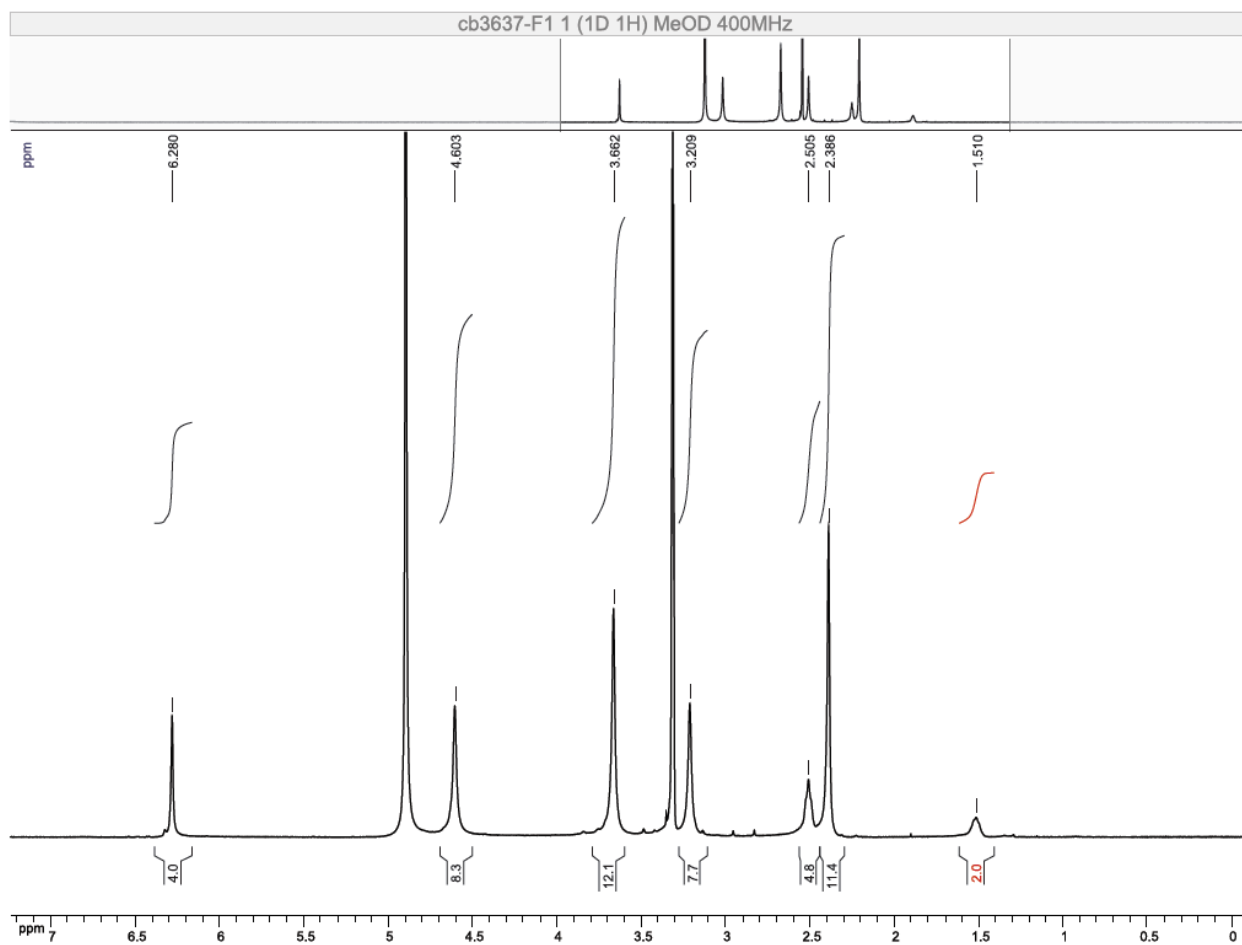


Fig. S1. ^1H -NMR of THPN.

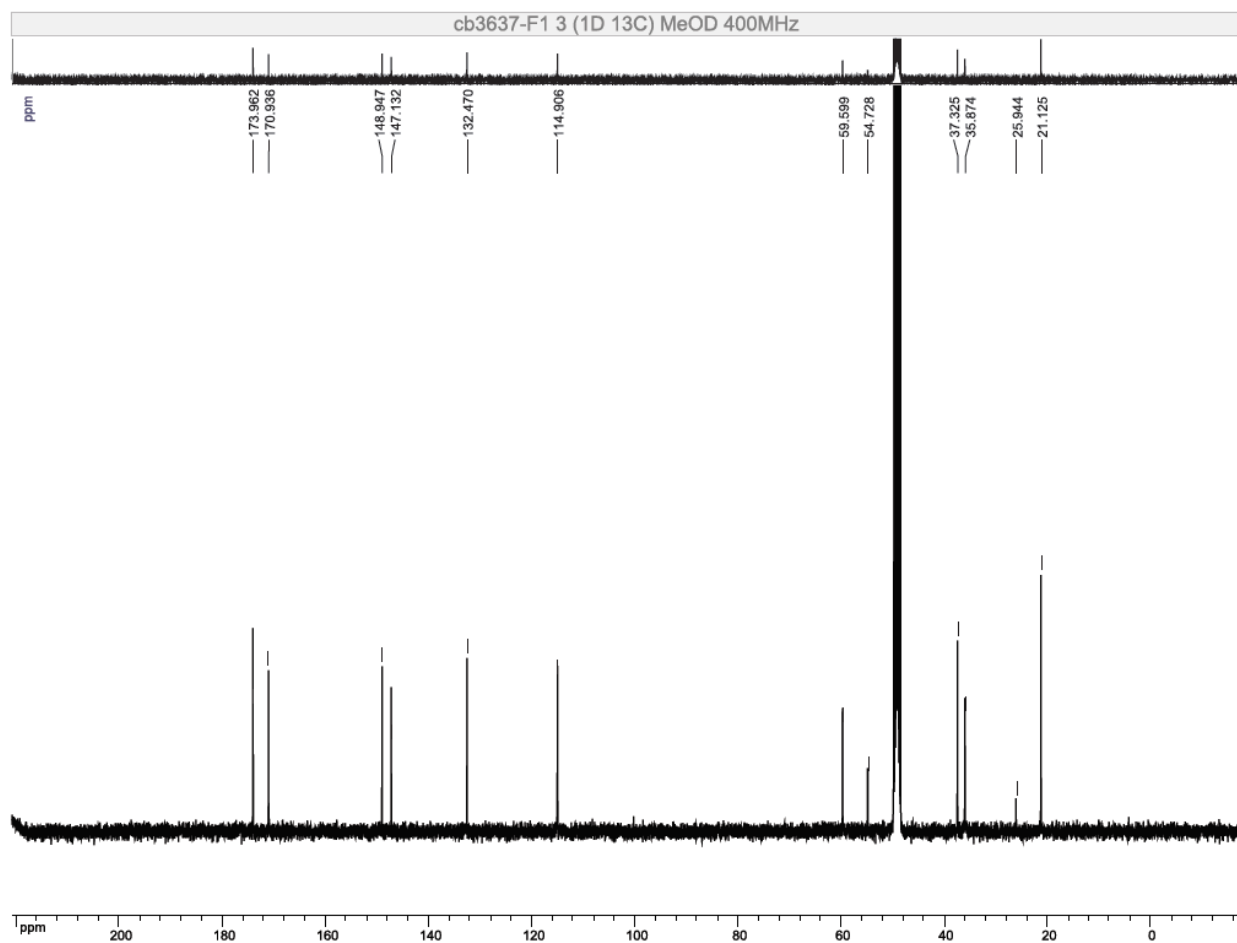


Fig. S2. ^{13}C -NMR of THPN.

cb3556_50perM-1_HRPos #82 RT: 0.37 AV: 1 NL: 3.35E7
T: FTMS + p ESI Full ms [133.40-2000.00]

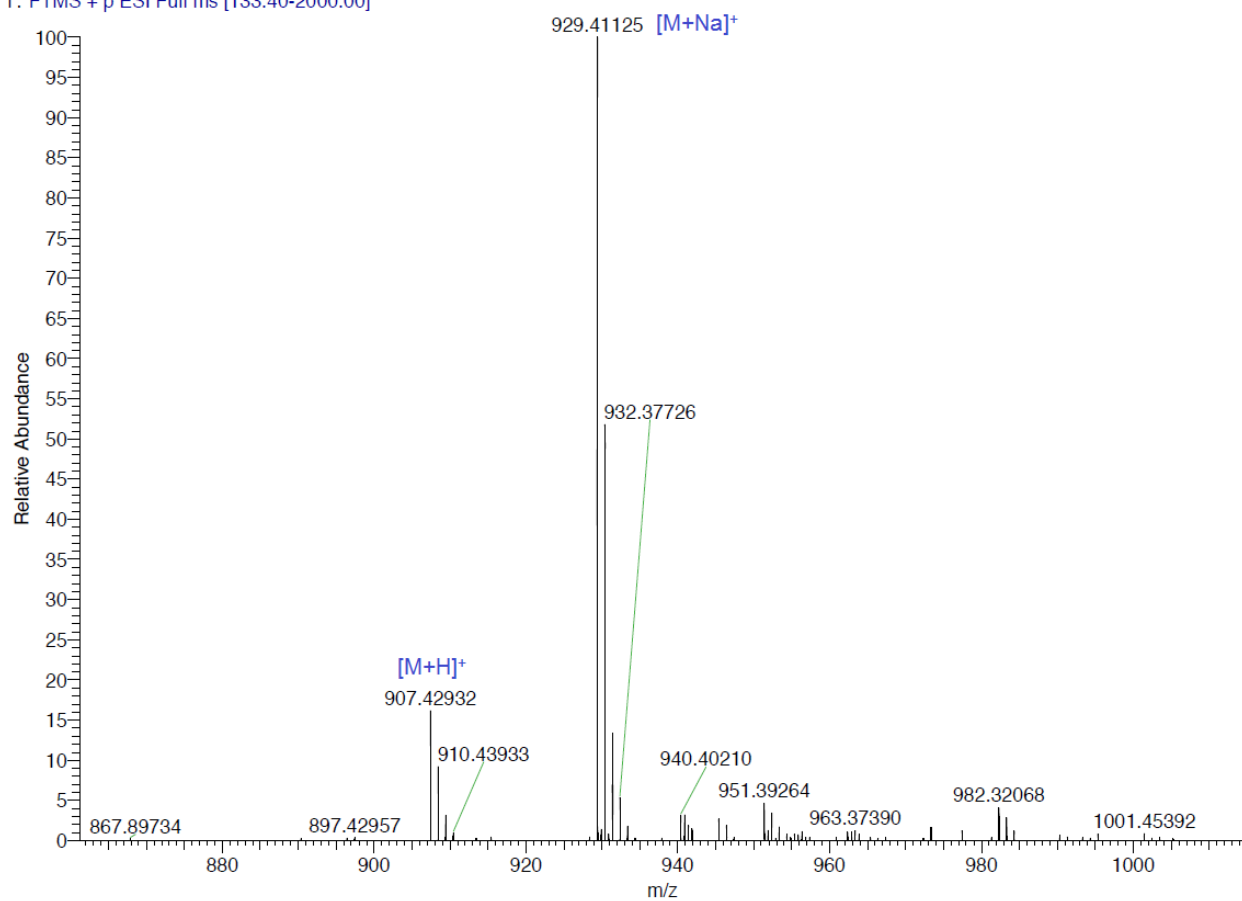


Fig. S3. HR-MS (+) of THPN.

cb3556_50perM-1_HRNeg #111 RT: 0.49 AV: 1 NL: 1.13E7
T: FTMS - p ESI Full ms [133.40-2000.00]

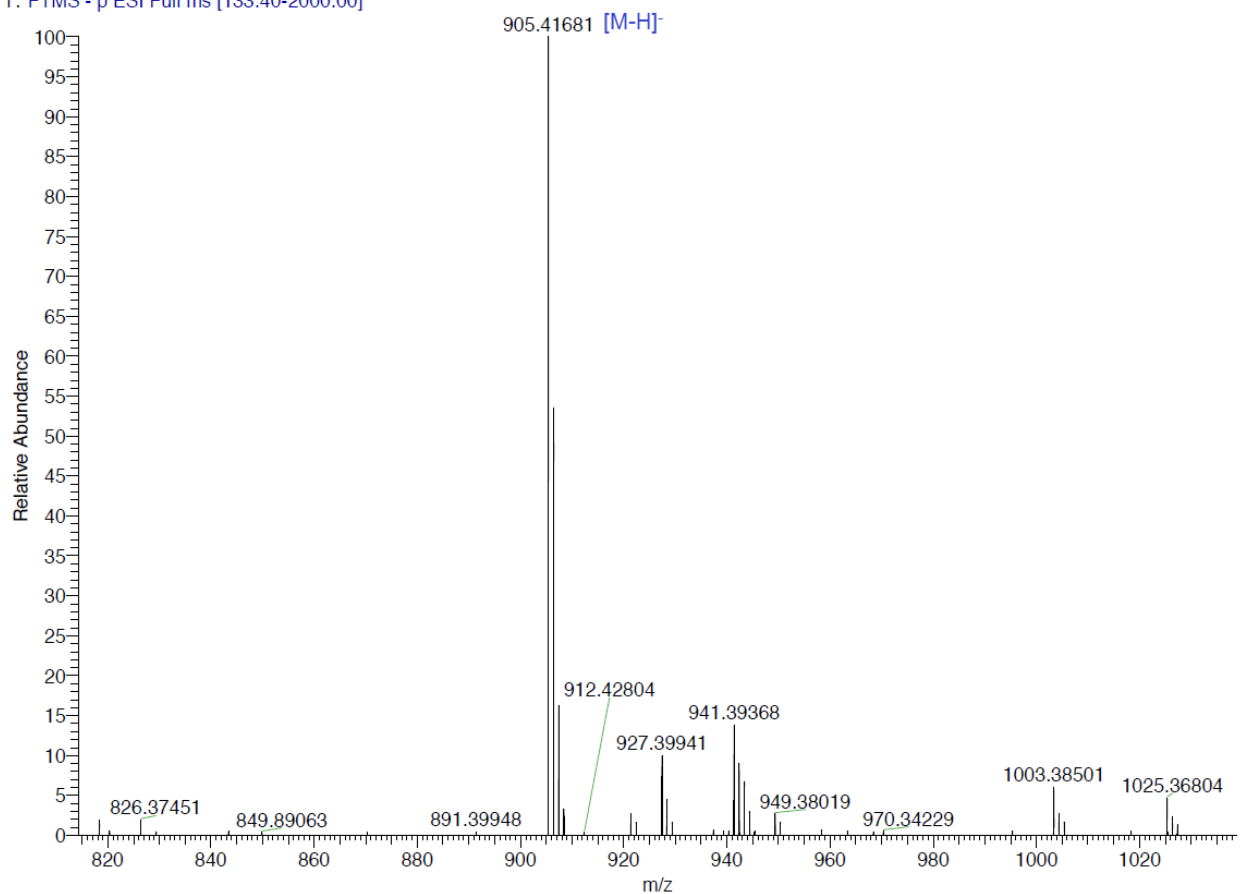


Fig. S4. HR-MS (-) of THPN.

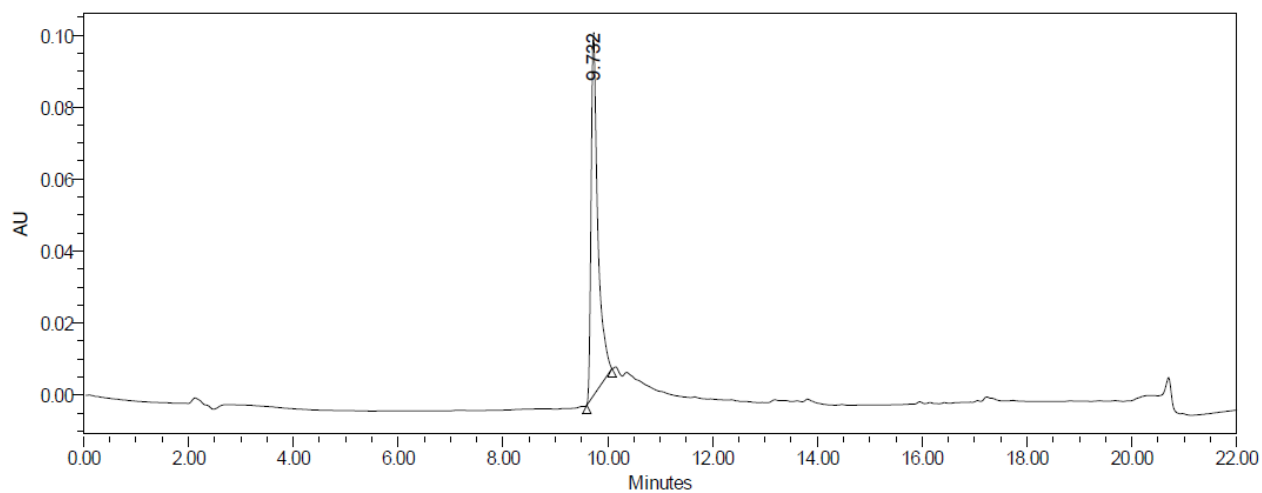


Fig. S5. HPLC chromatogram (λ_{254}) of THPN.

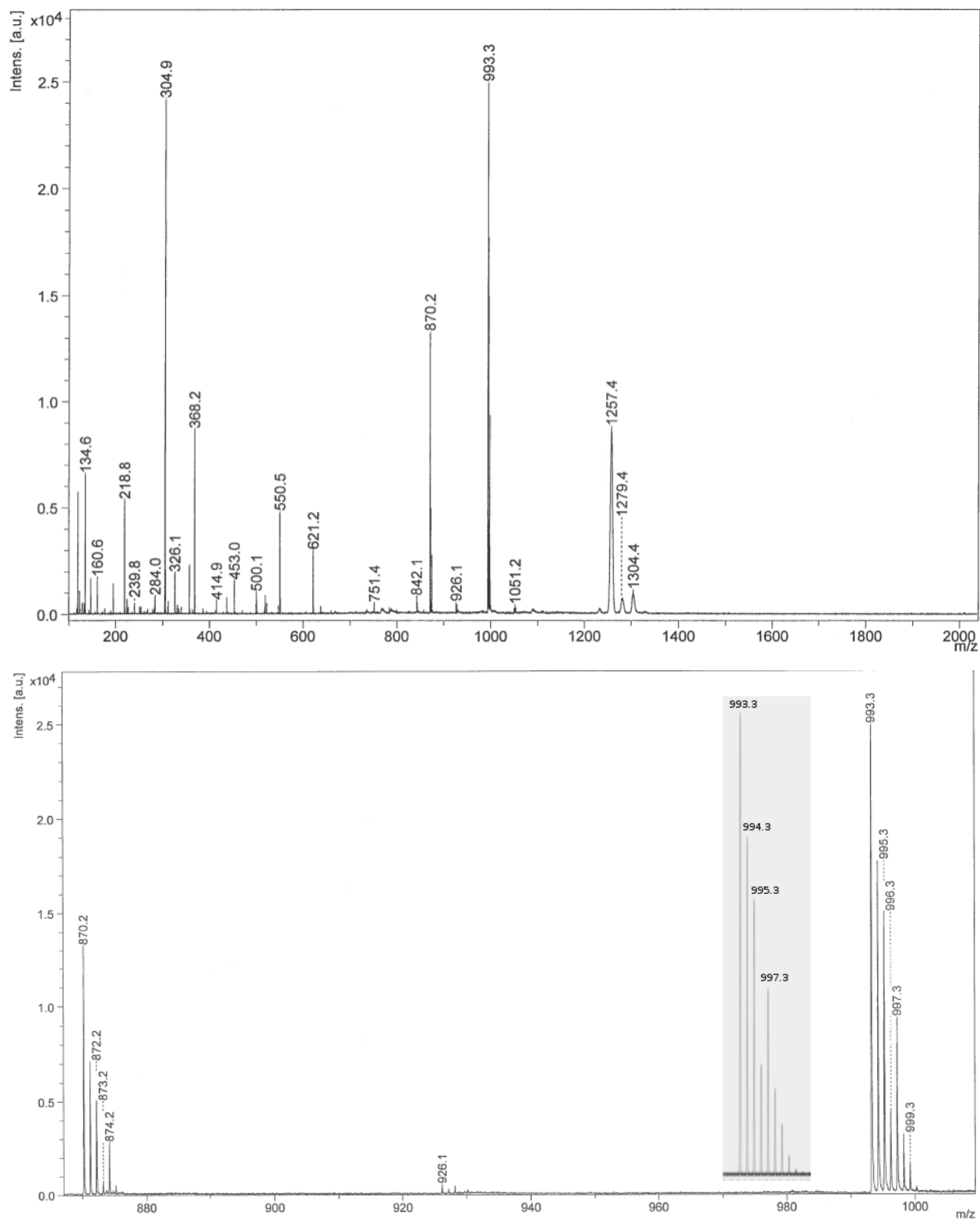


Fig. S6. MALDI-MS of Zr-THPN. The monometallic complex shows the expected $[M+H]^+$ peak and isotope pattern at m/z 993.3 that matches the predicted pattern (inset).

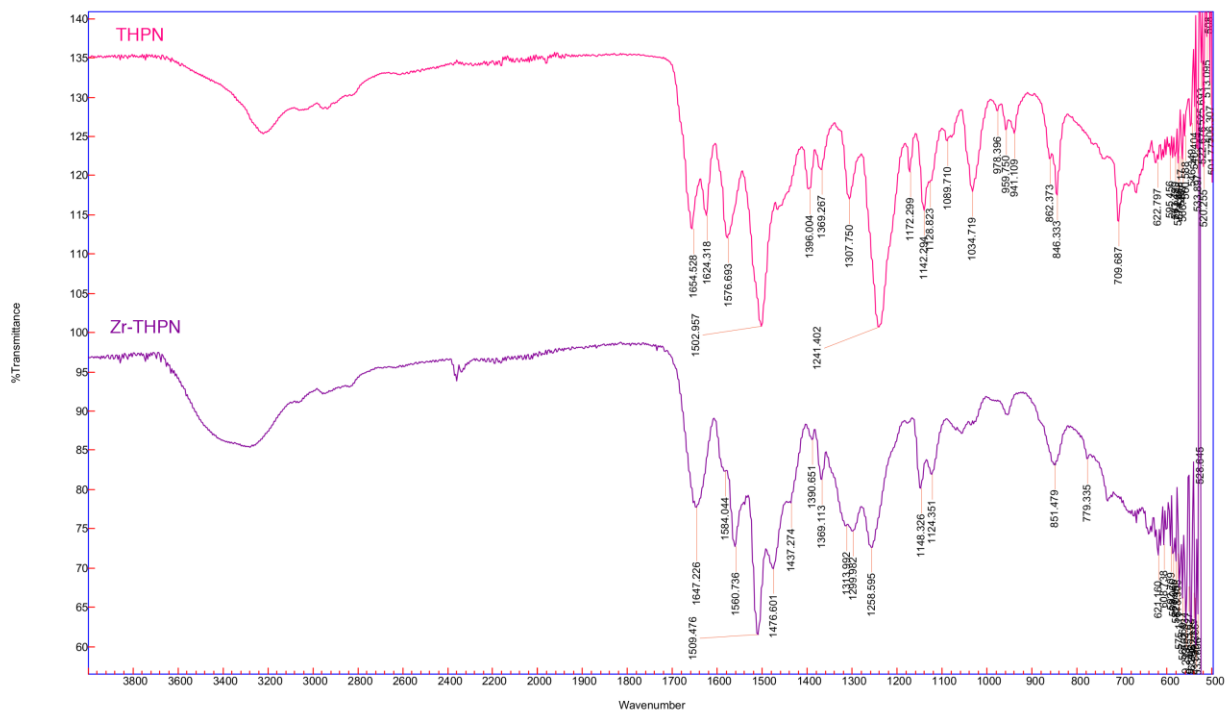


Fig. S7. FT-IR comparison of Zr-THPN and THPN.

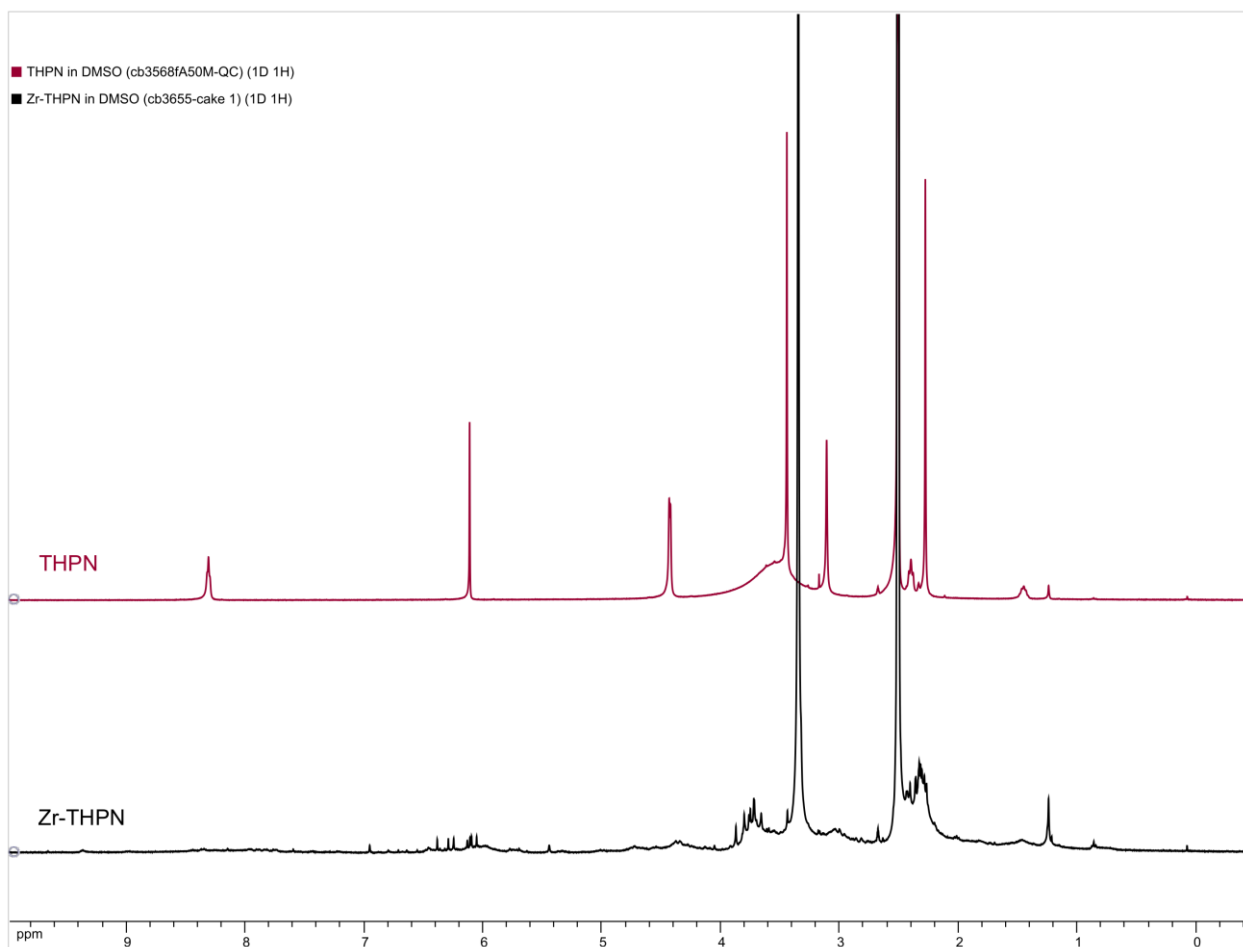


Fig. S8. ^1H -NMR comparison of Zr-THPN and THPN (in DMSO- d_6 , 400 MHz).

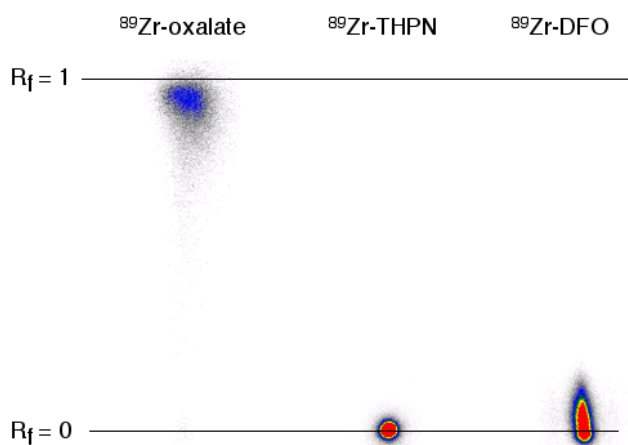


Fig. S9. ITLC comparison of ^{89}Zr -oxalate, ^{89}Zr -THPN, and ^{89}Zr -DFO. Biodex Tec-Control (black #150-005) ITLC strips developed with aqueous DTPA solution (50 mM, pH 7.0).

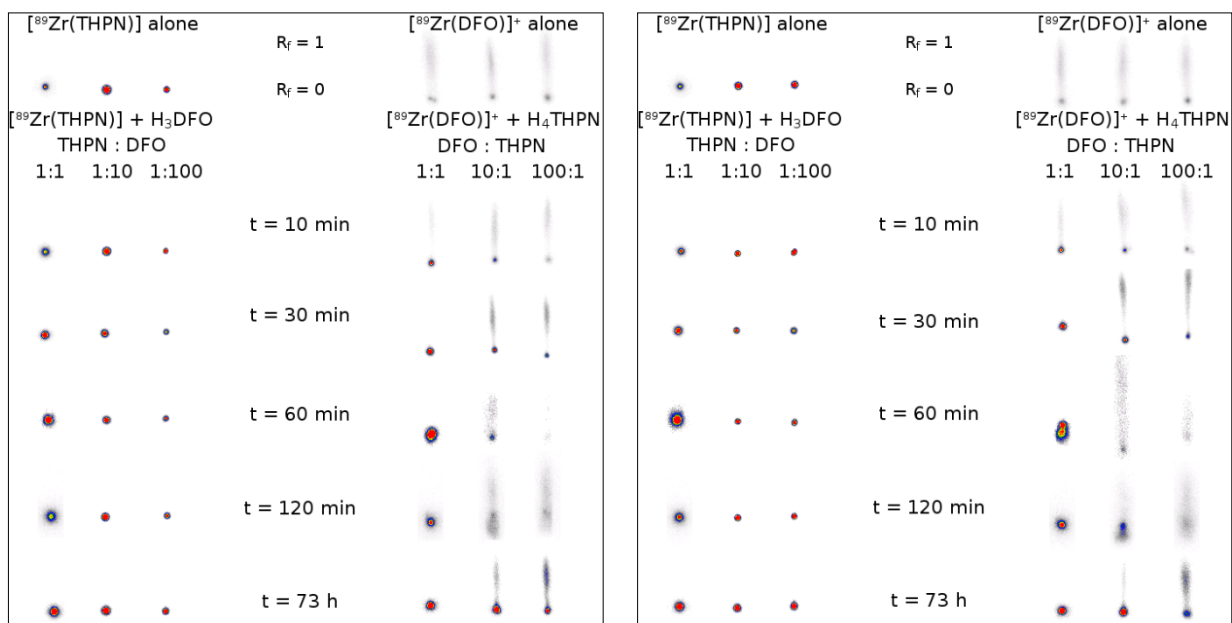


Fig. S10. ITLCs of transchelation competition (repetitions of **Fig. 5** for $n = 3$). Biodex Tec-Control (dark green, #150-771) ITLC strips developed with aqueous sodium citrate solution (100 mM, pH 5.5).

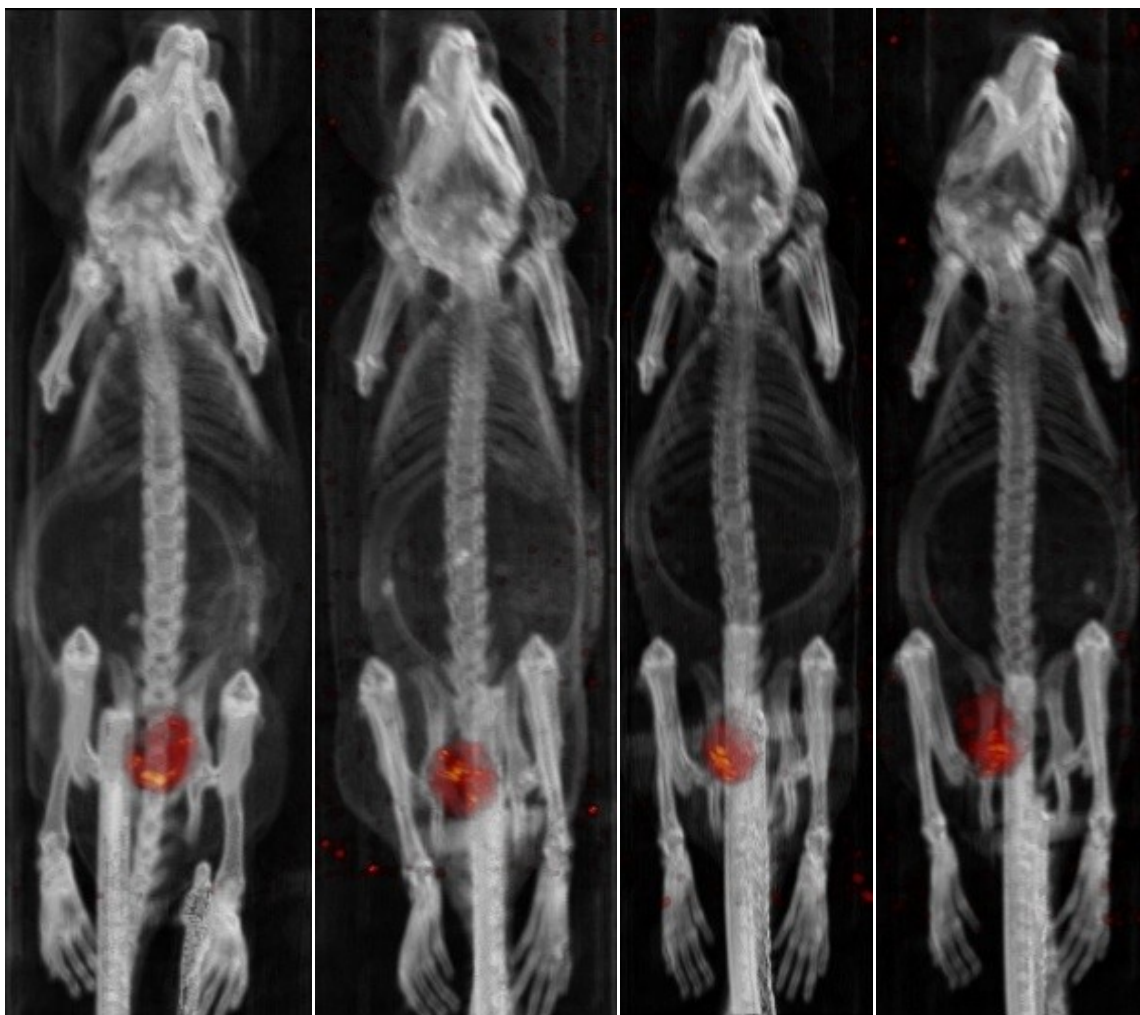


Fig. S11. Coronal SPECT/CT images of all four mice injected with ^{89}Zr -THPN (0-30 min post injection).

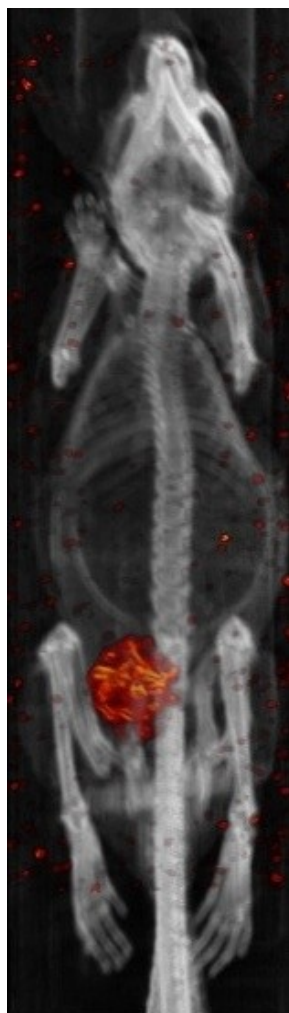


Fig. S12. Coronal SPECT/CT image of the mouse injected with ^{89}Zr -DFO (0-30 min post injection).