

Supplementary Materials

Radiometal-Based PET/MRI Contrast Agents for Sensing Tumor Extracellular pH

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1. NMR Spectra of Synthesized Compounds

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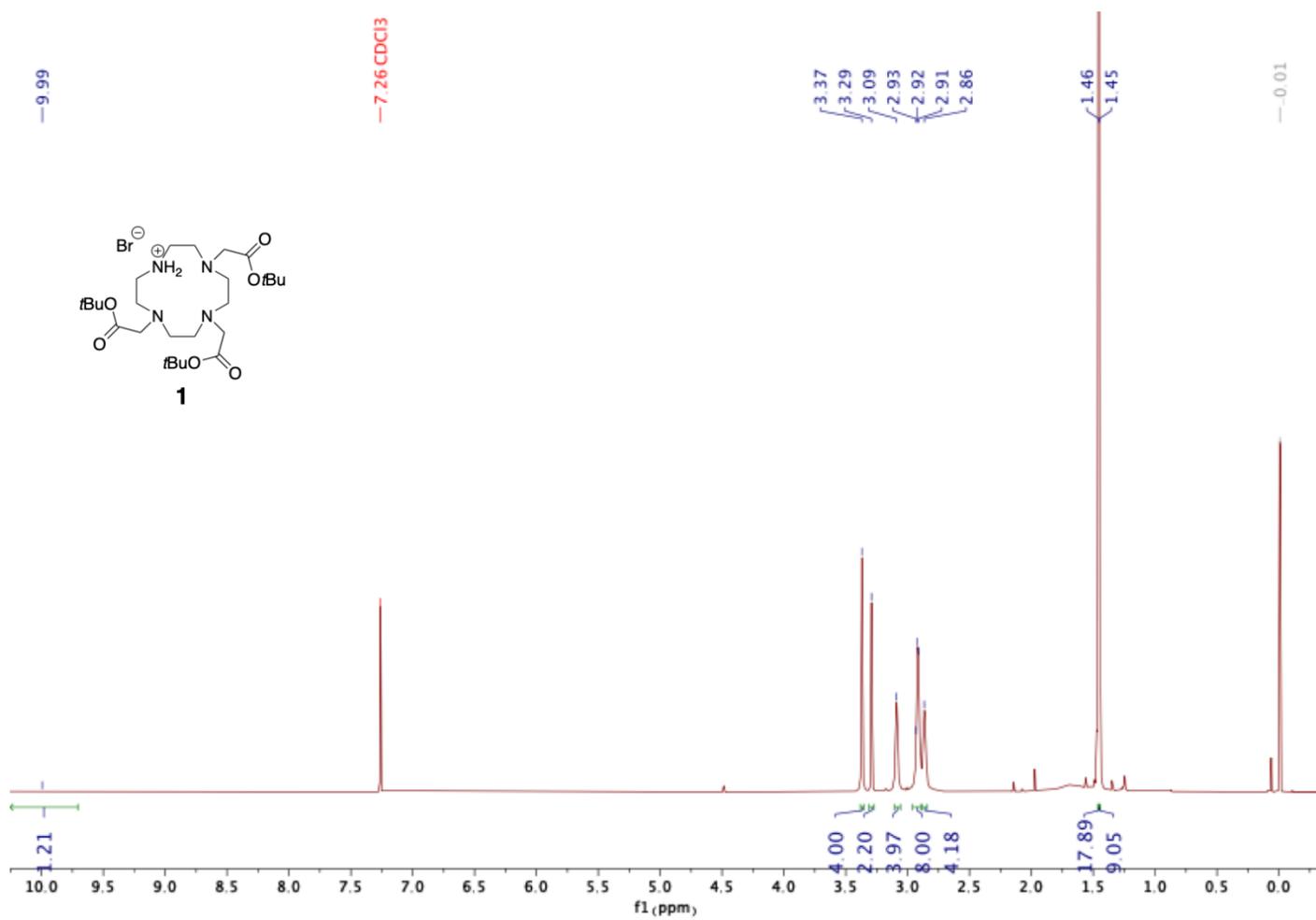


Figure S1. NMR spectrum of compound 1.

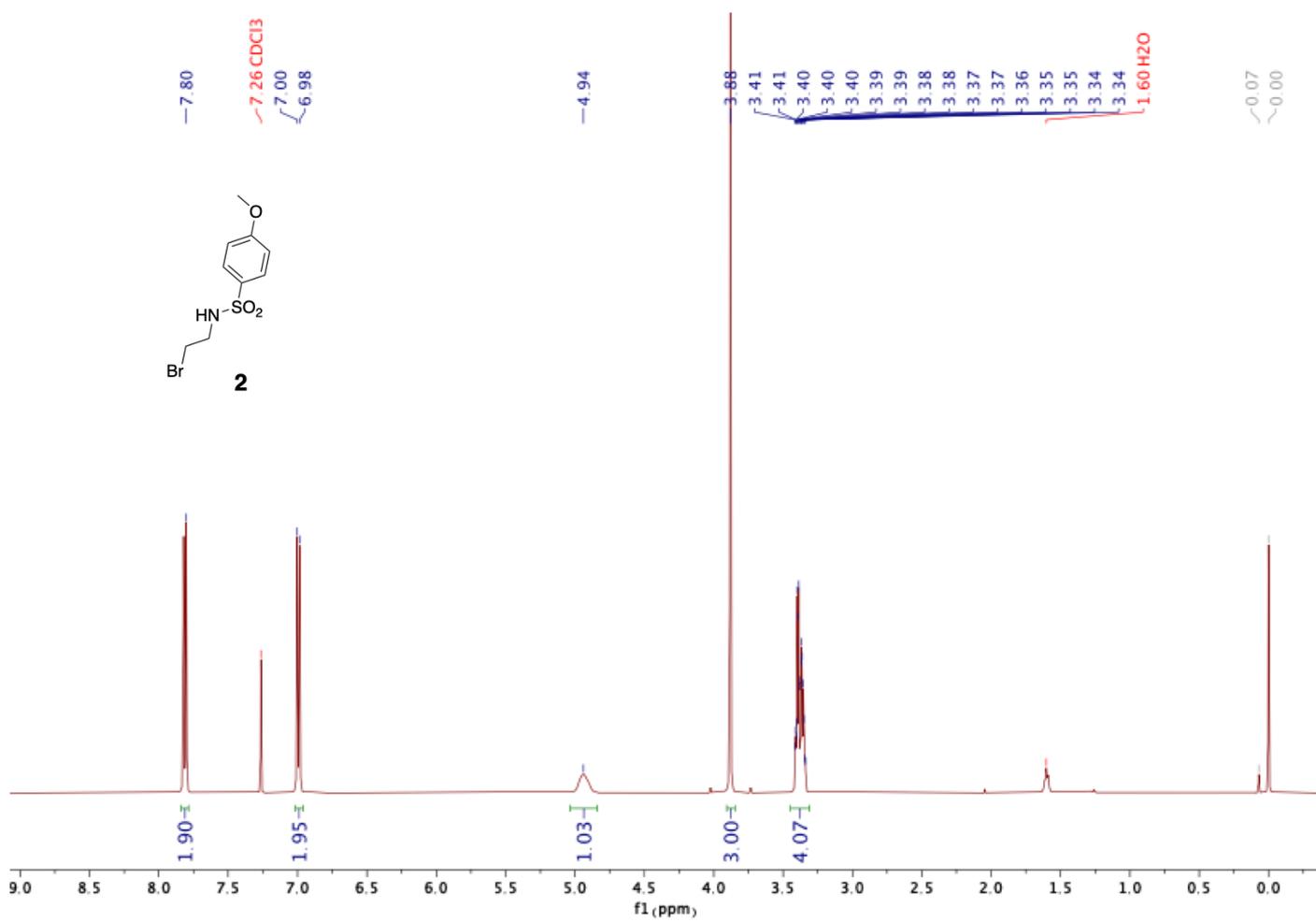


Figure S2. NMR of compound 2.

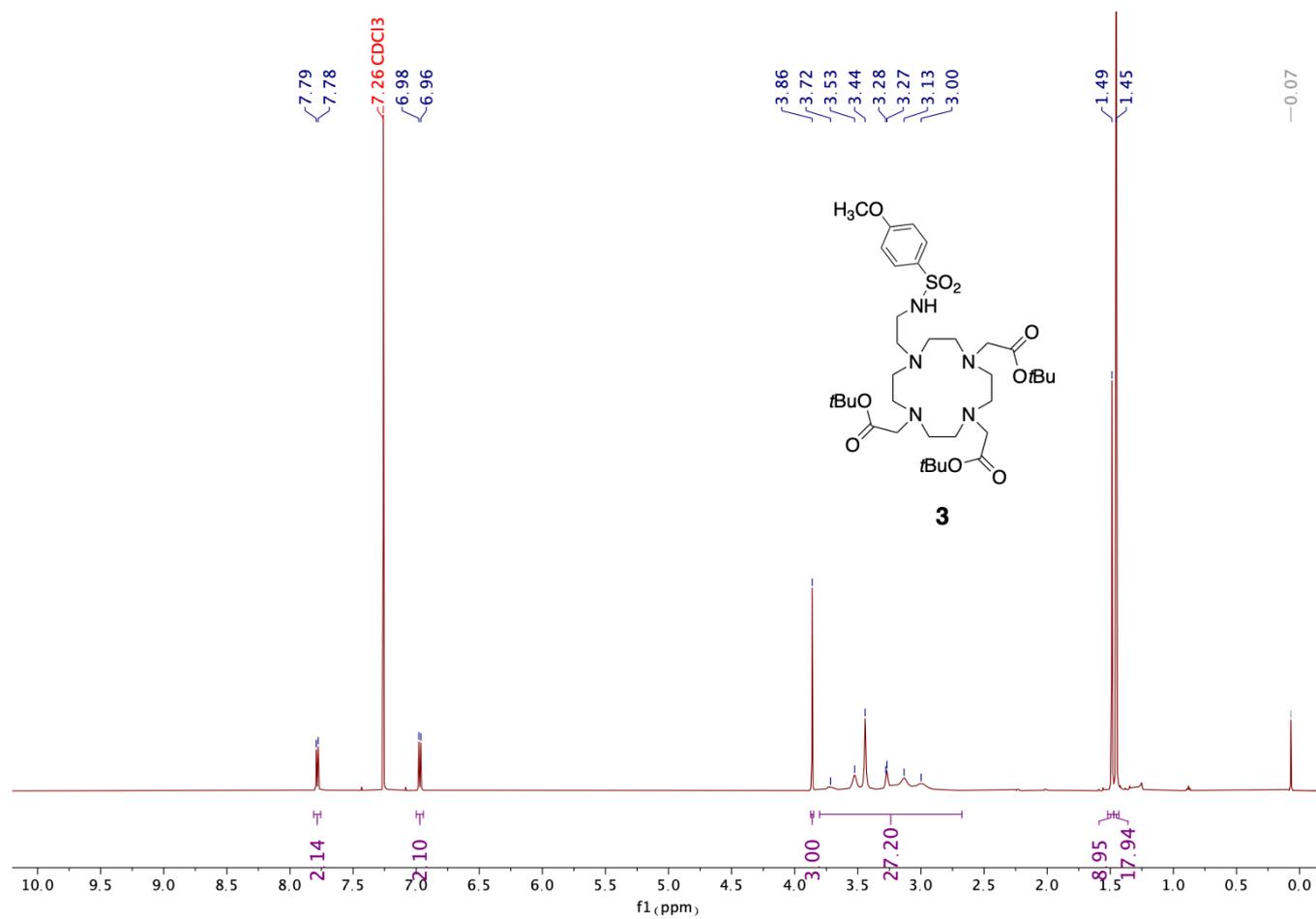


Figure S3. NMR of compound 3.

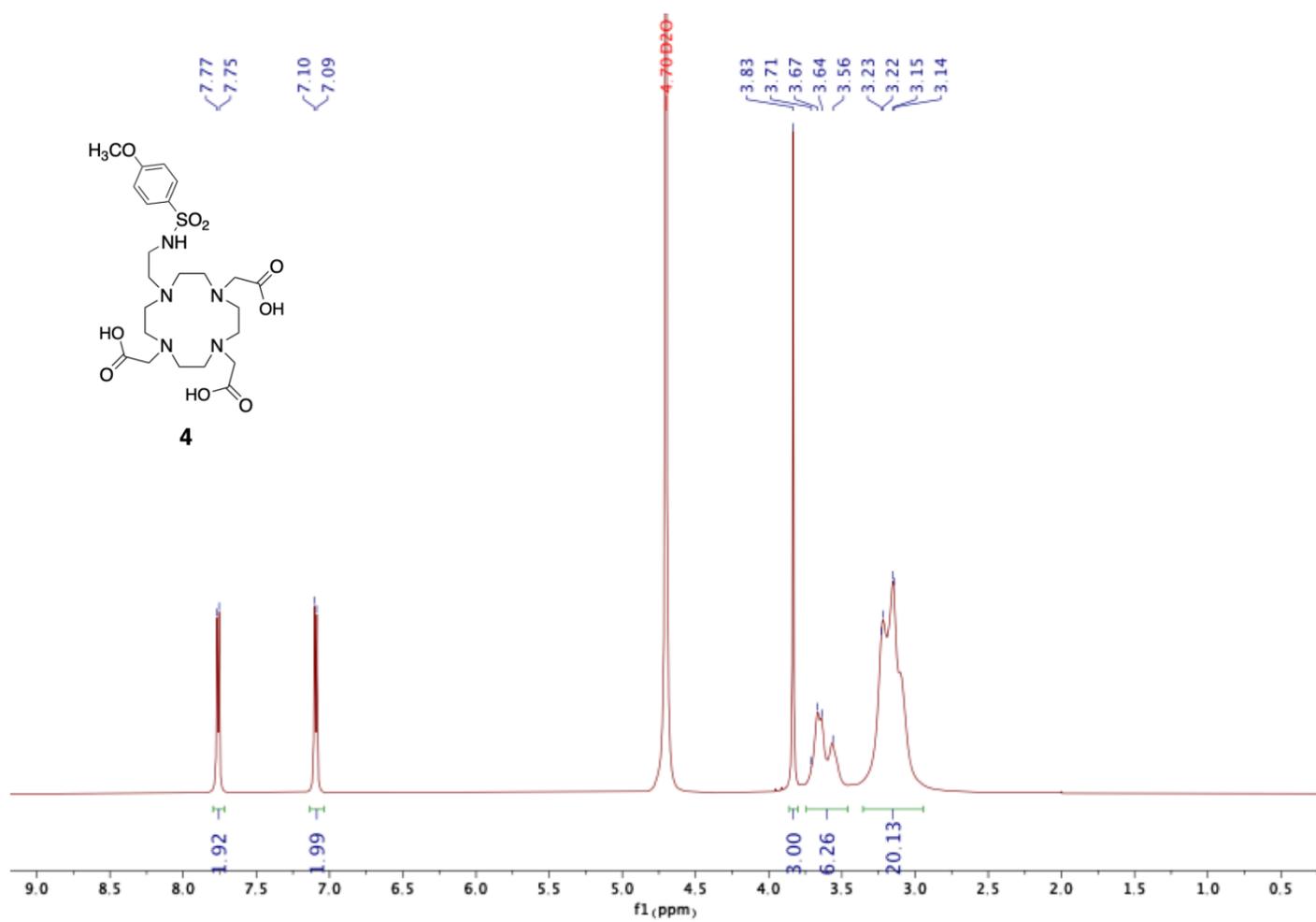


Figure S4. NMR of compound 4.

2. LRMS of Synthesized Compounds

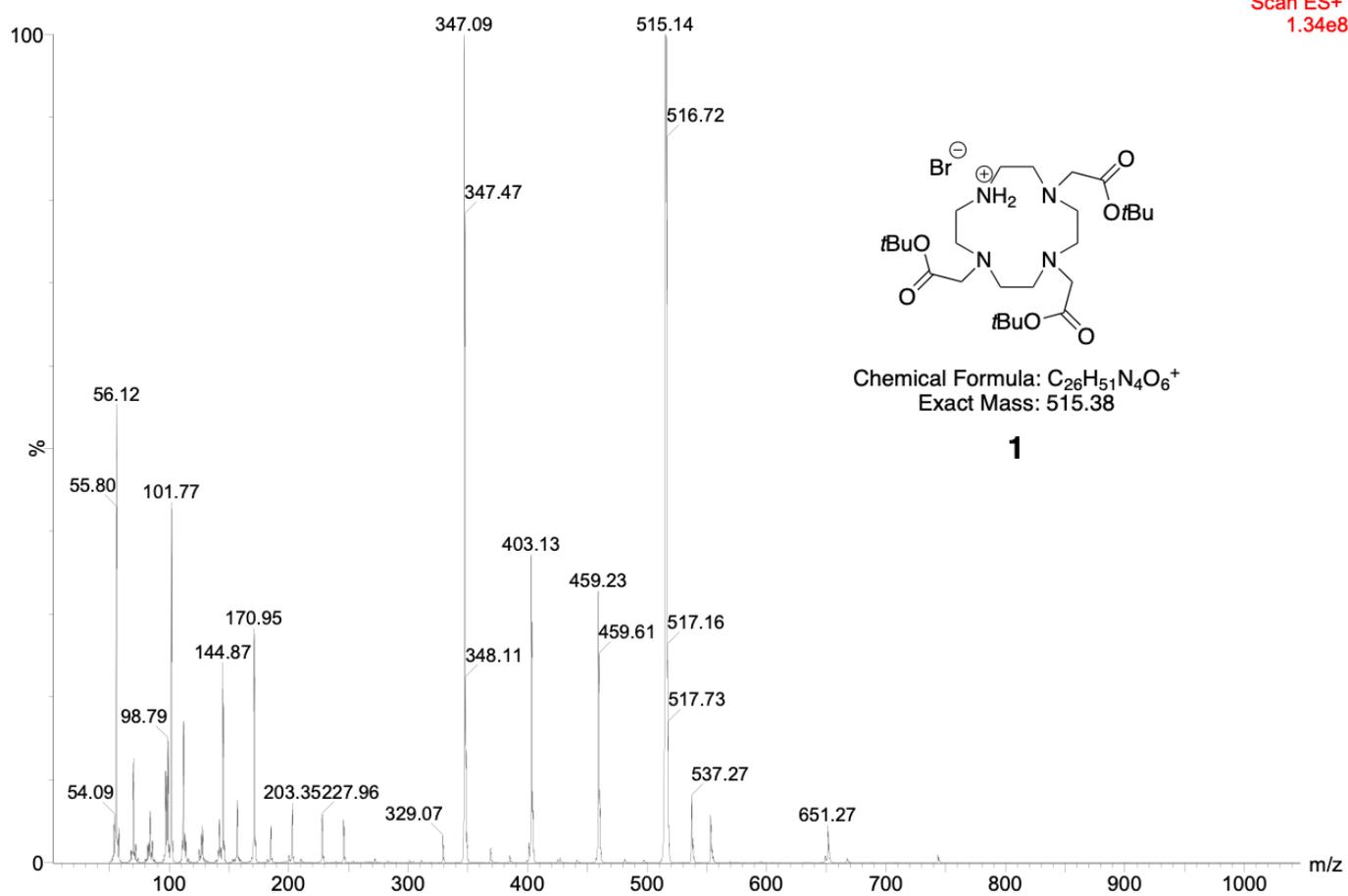


Figure S5. LRMS of compound 1.

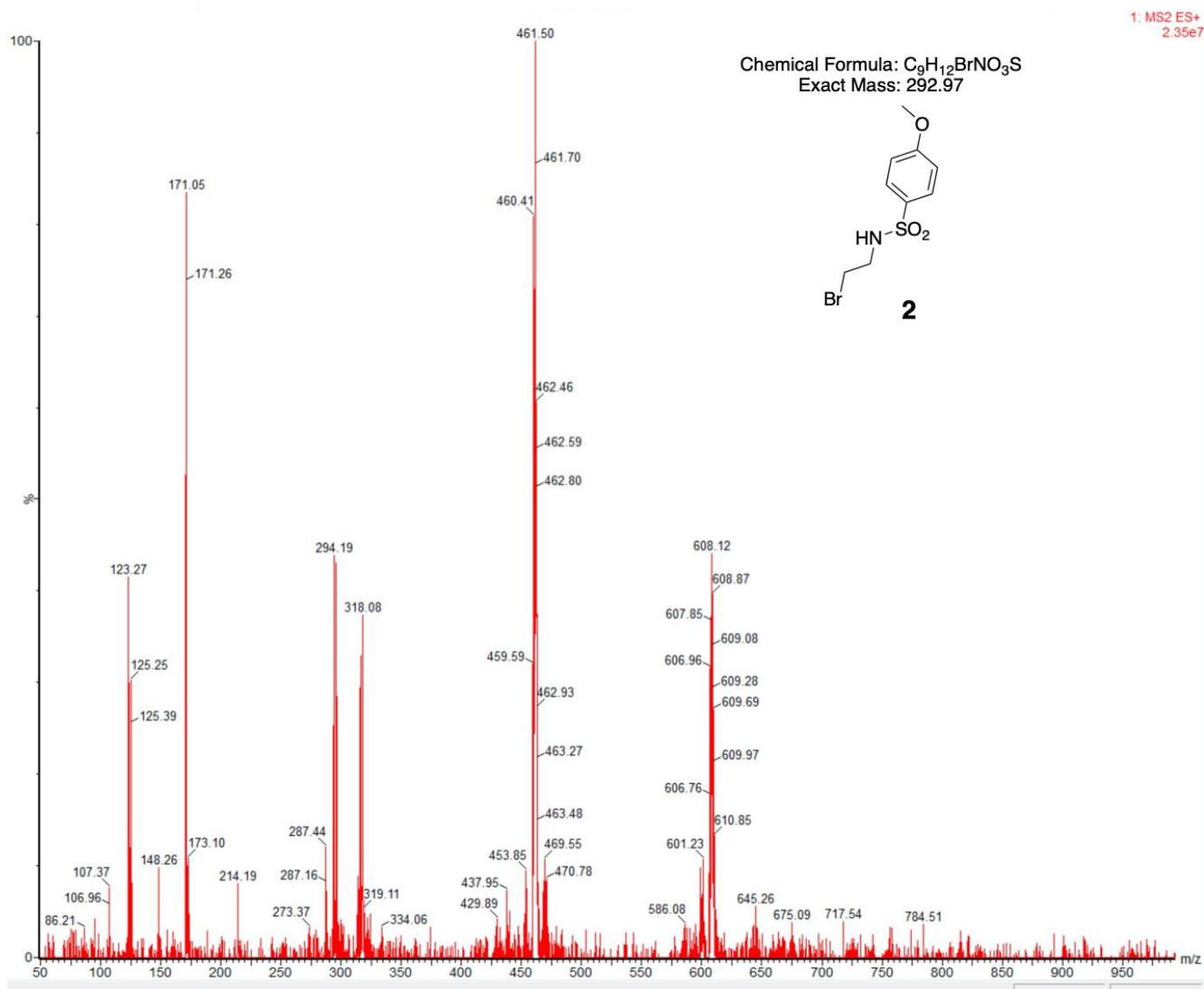


Figure S6. LRMS of compound 2.

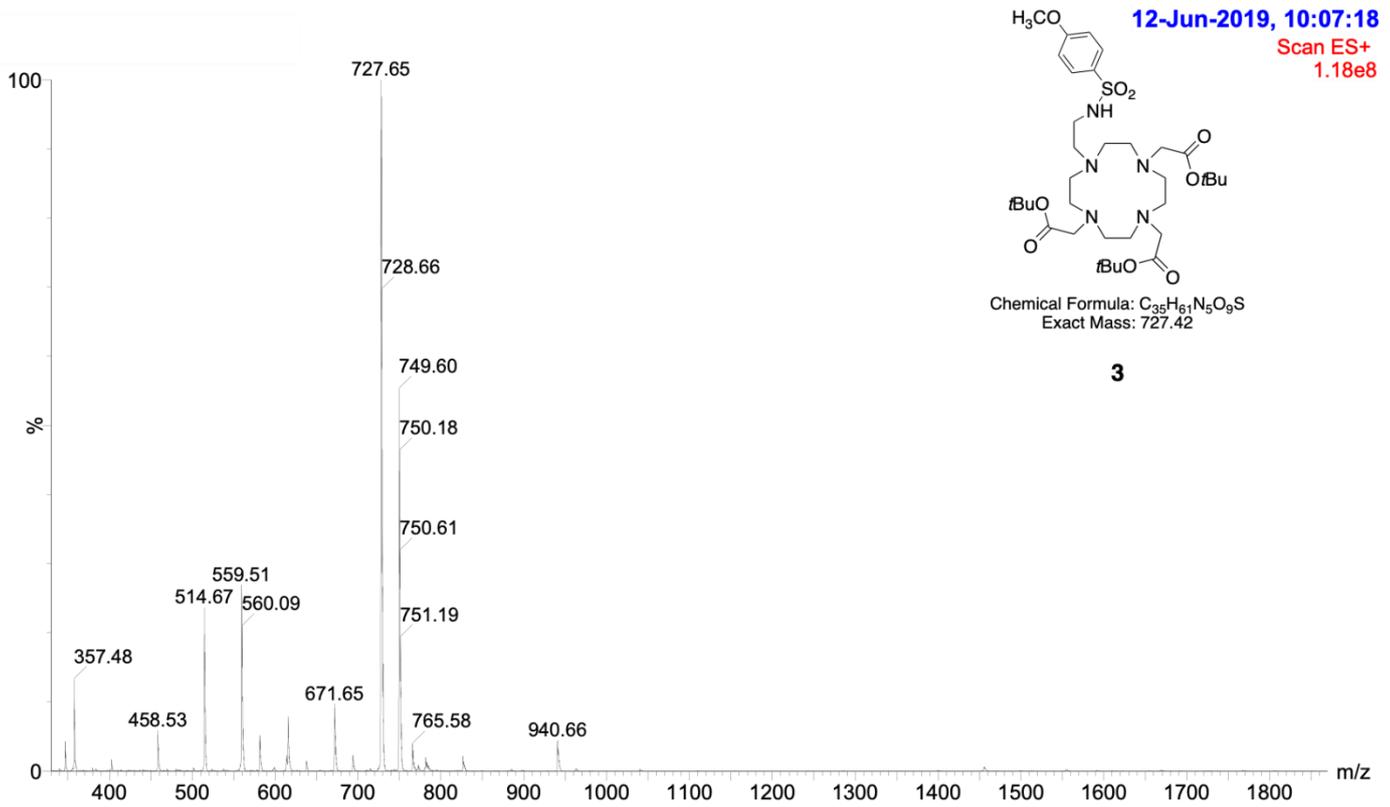


Figure S7. LRMS of compound 3.

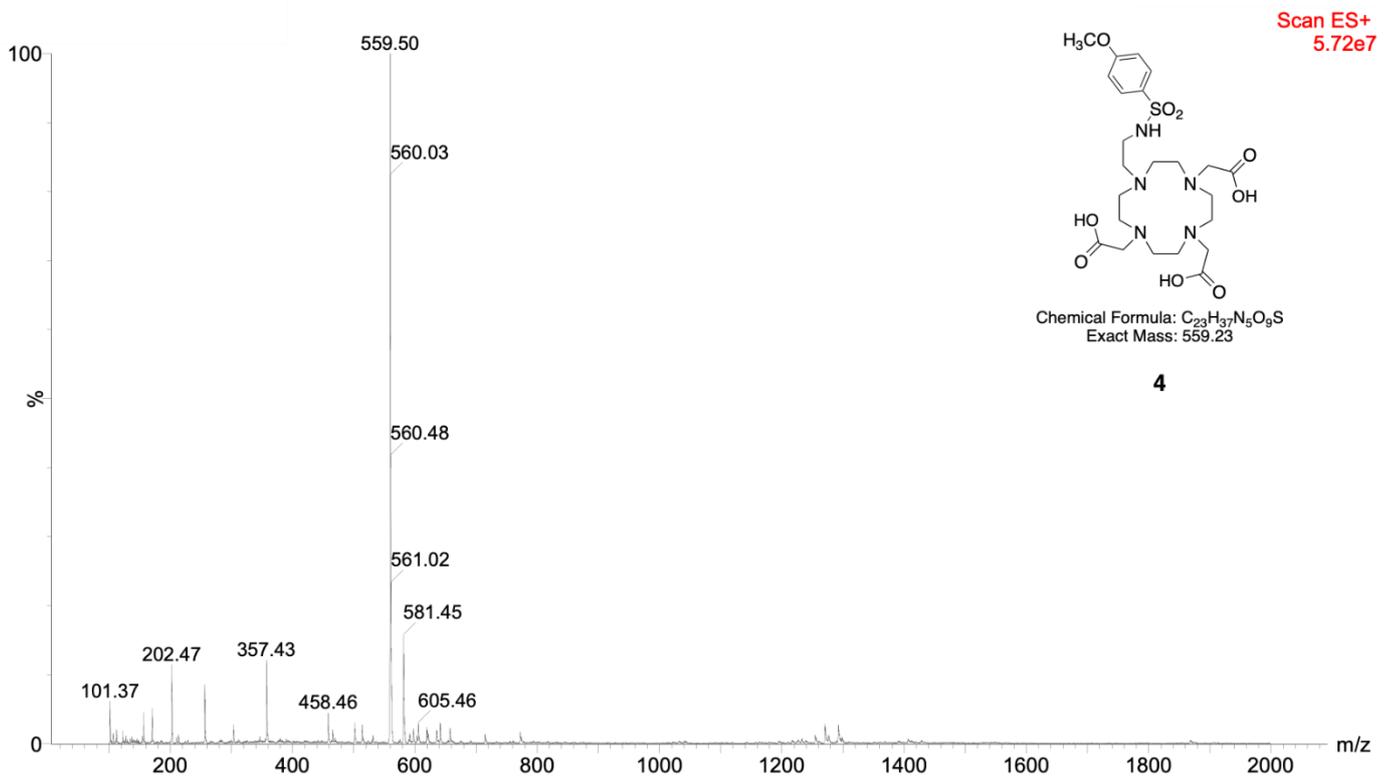
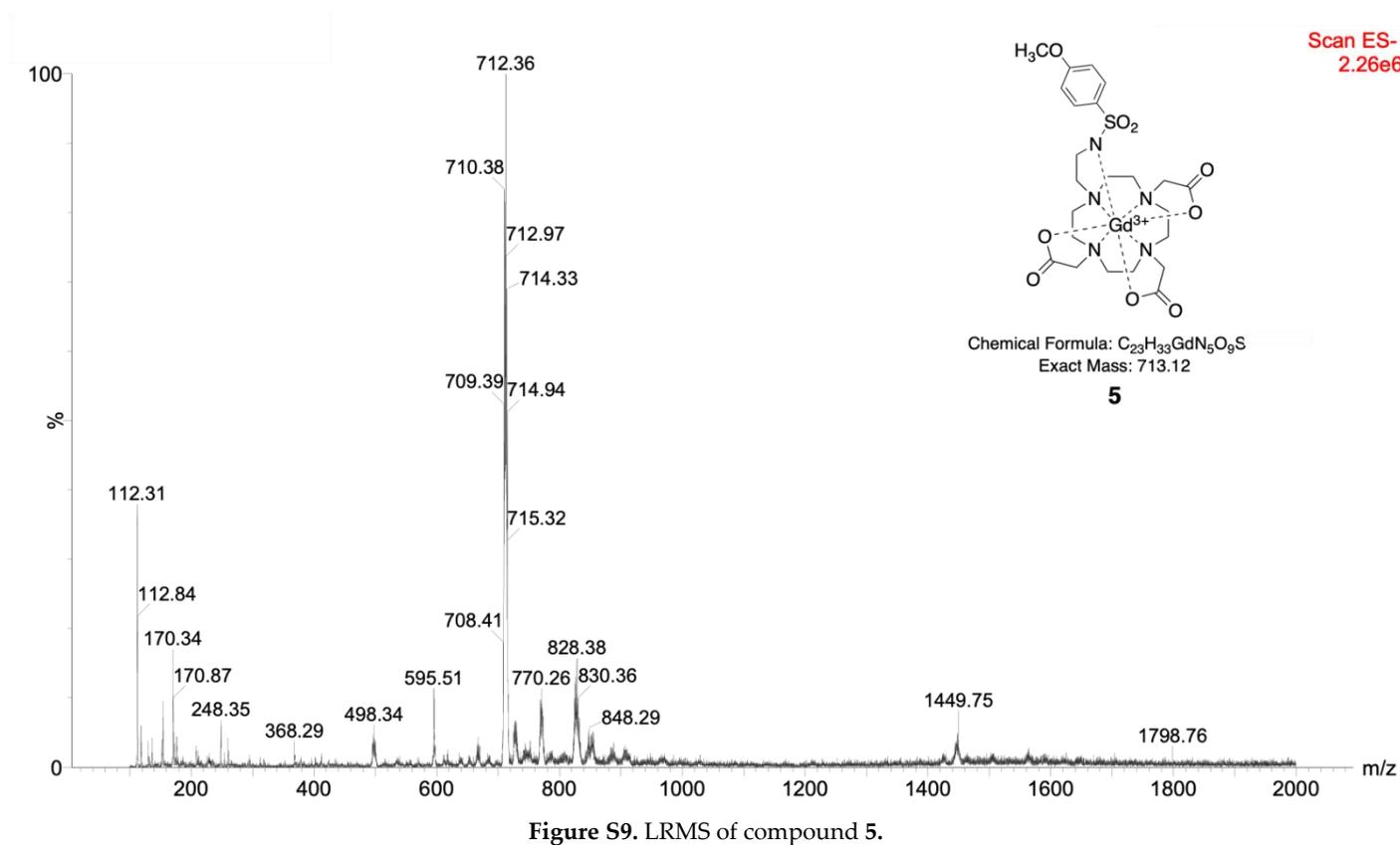
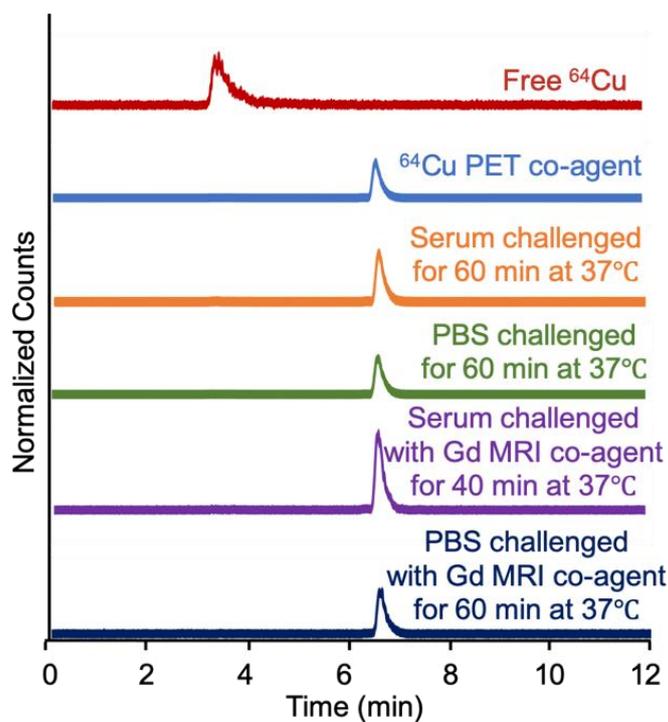


Figure S8. LRMS of compound 4.



3. RadioHPLC Traces of PET Co-Agents



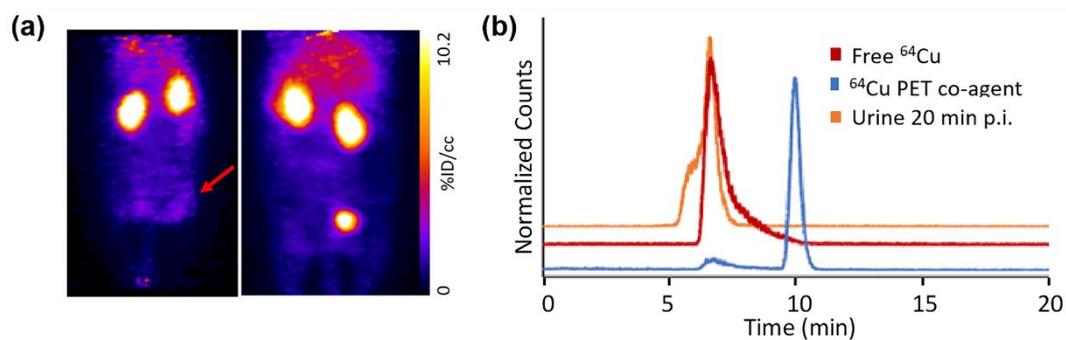


Figure S11. Metabolism of the ^{64}Cu PET co-agent. (a) A PET image from the dynamic PET/MRI scan using the ^{64}Cu PET co-agent showed poor tumor uptake and high liver uptake. (b) RadioHPLC of urine collected from the mouse after the dynamic PET/MRI scan (orange trace) showed the presence of only free ^{64}Cu (red trace) rather than showing the intact ^{64}Cu PET co-agent (blue trace), indicating *in vivo* de-chelation of the ^{64}Cu PET co-agent.