

Supplementary Materials

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

Alyssa C. Pollard ^{1,2}, Jorge de la Cerda ², F. William Schuler ², Tyler R. Pollard ³, Aikaterini Kotrotsou ², Federica Pisaneschi ² and Mark D. Pagel ^{2,*}

¹ Department of Chemistry, Rice University, Houston, TX 77005, USA; acp4@rice.edu

² Department of Cancer Systems Imaging, MD Anderson Cancer Center, Houston, TX 77054, USA; jorge.de-lacerda@mdanderson.org (J.d.l.C.); fschuler@mdanderson.org (F.W.S.); aikaterini.kotrotsou@gmail.com (A.K.); fpisaneschi@mdanderson.org (F.P.)

³ Department of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA 30332, USA; polko987@outlook.com

* Correspondence: mdpagel@mdanderson.org; Tel.: +001-(713)-205-8515

1. NMR Spectra of Synthesized Compounds

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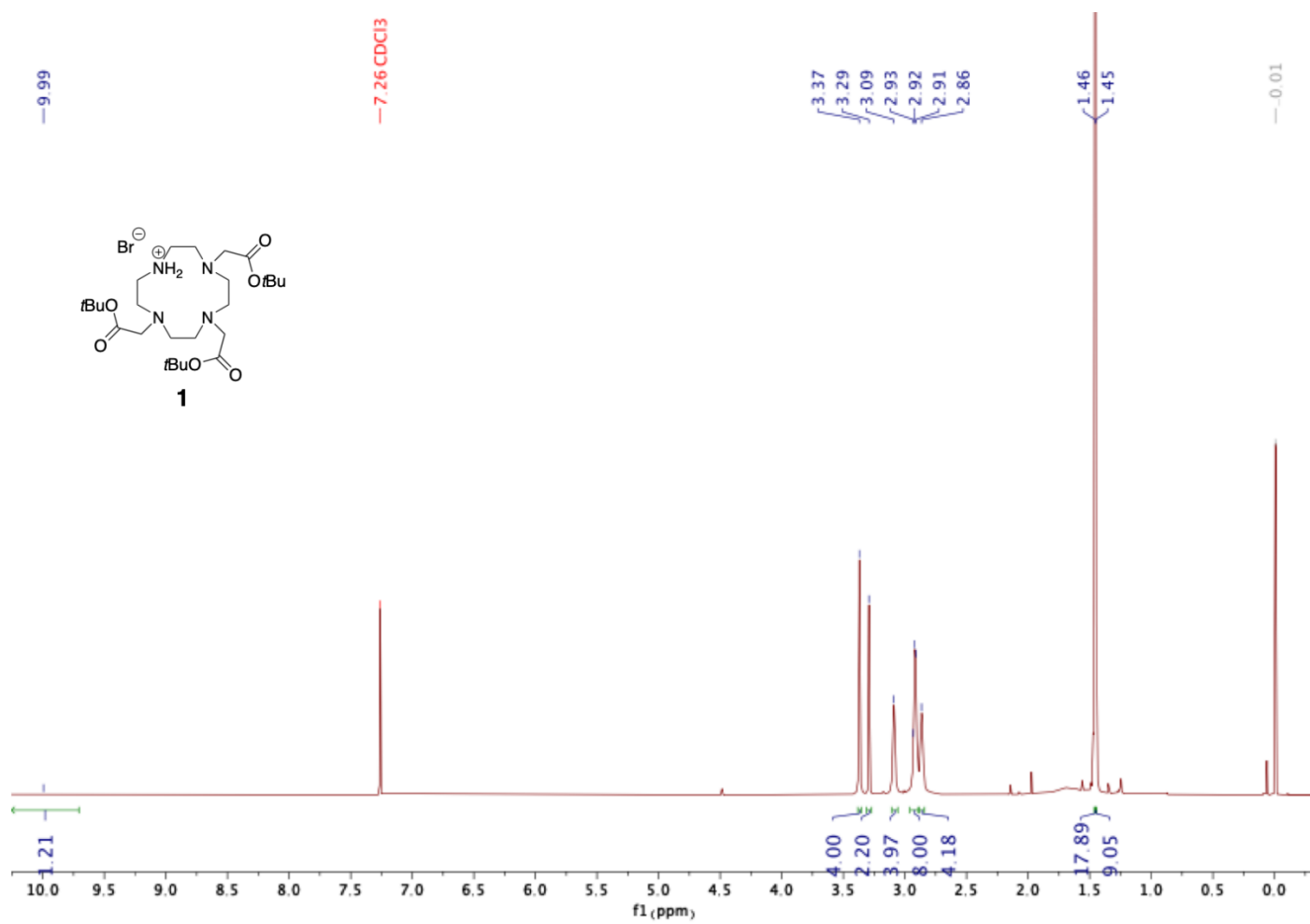


Figure S1. NMR spectrum of compound **1**.

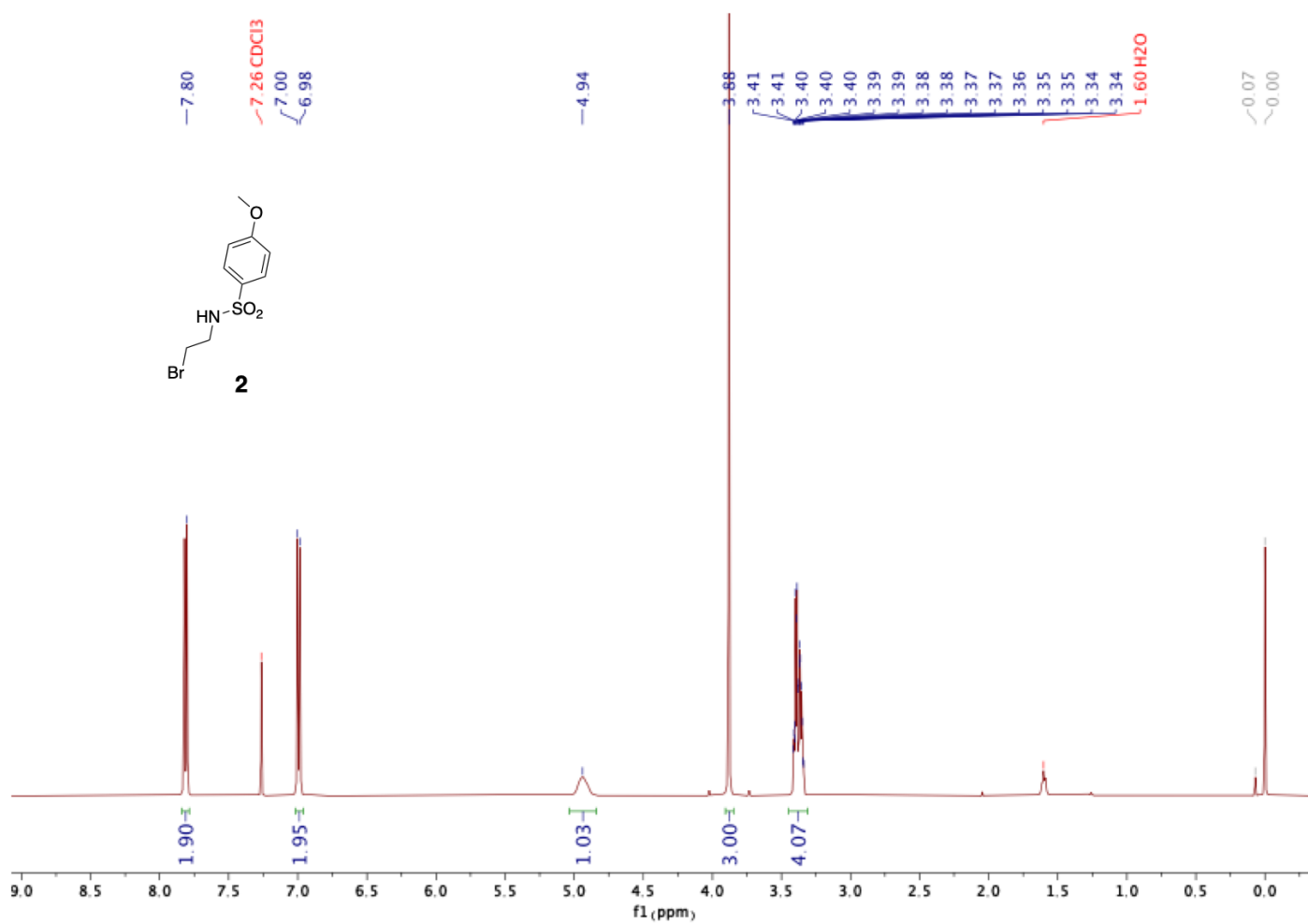
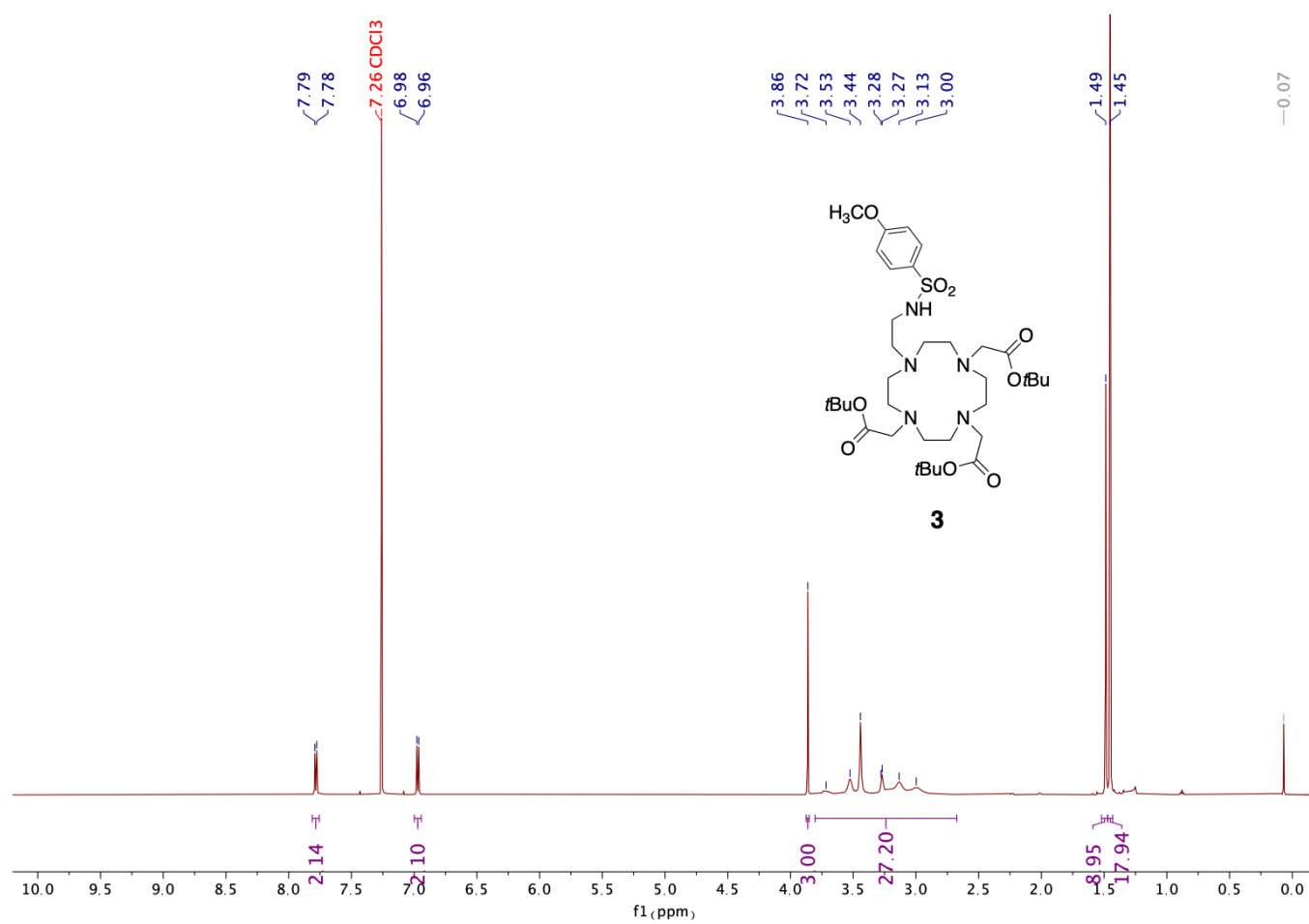


Figure S2. NMR of compound 2.

Figure S3. NMR of compound **3**.

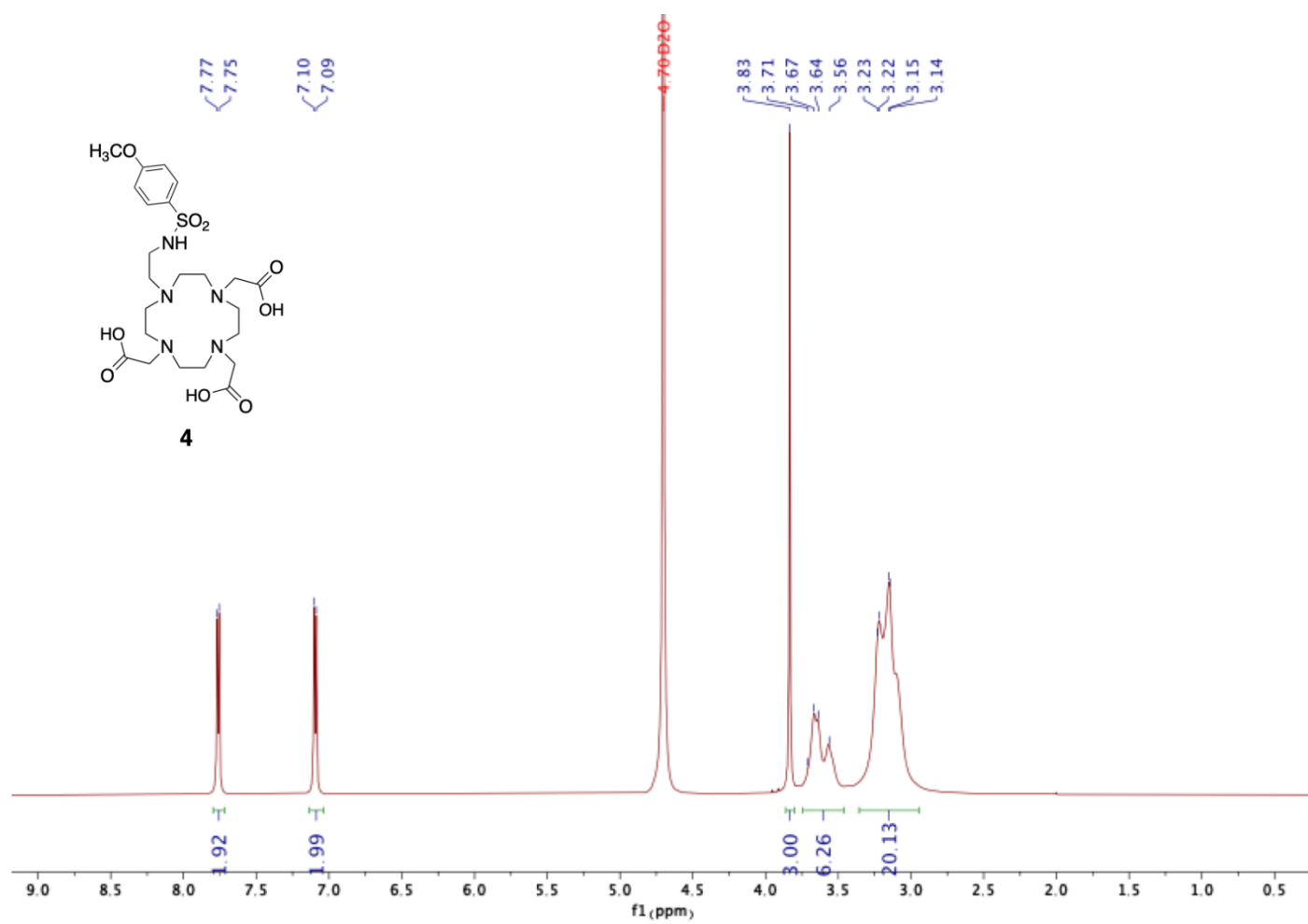
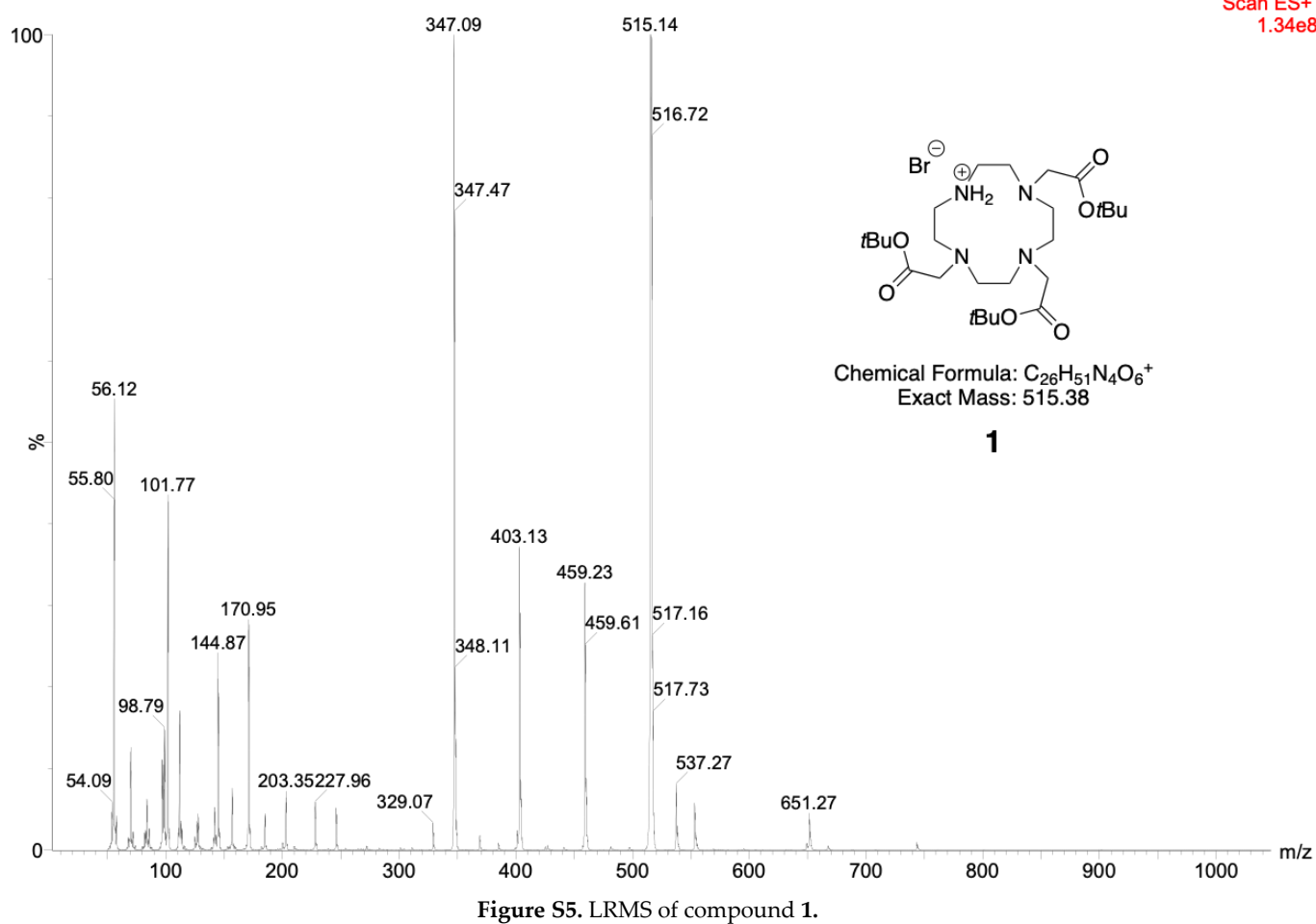


Figure S4. NMR of compound 4.

2. LRMS of Synthesized Compounds



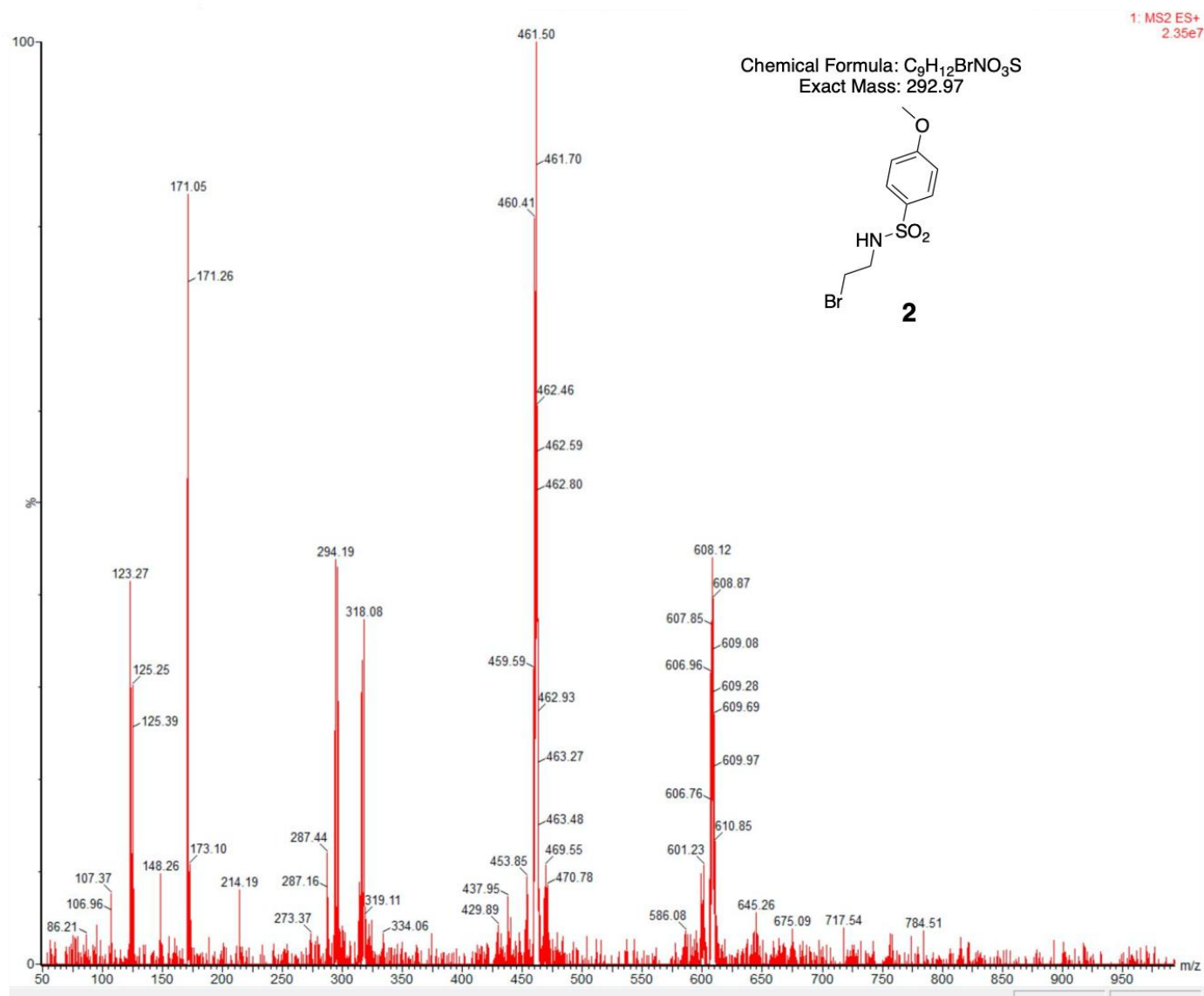


Figure S6. LRMS of compound 2.

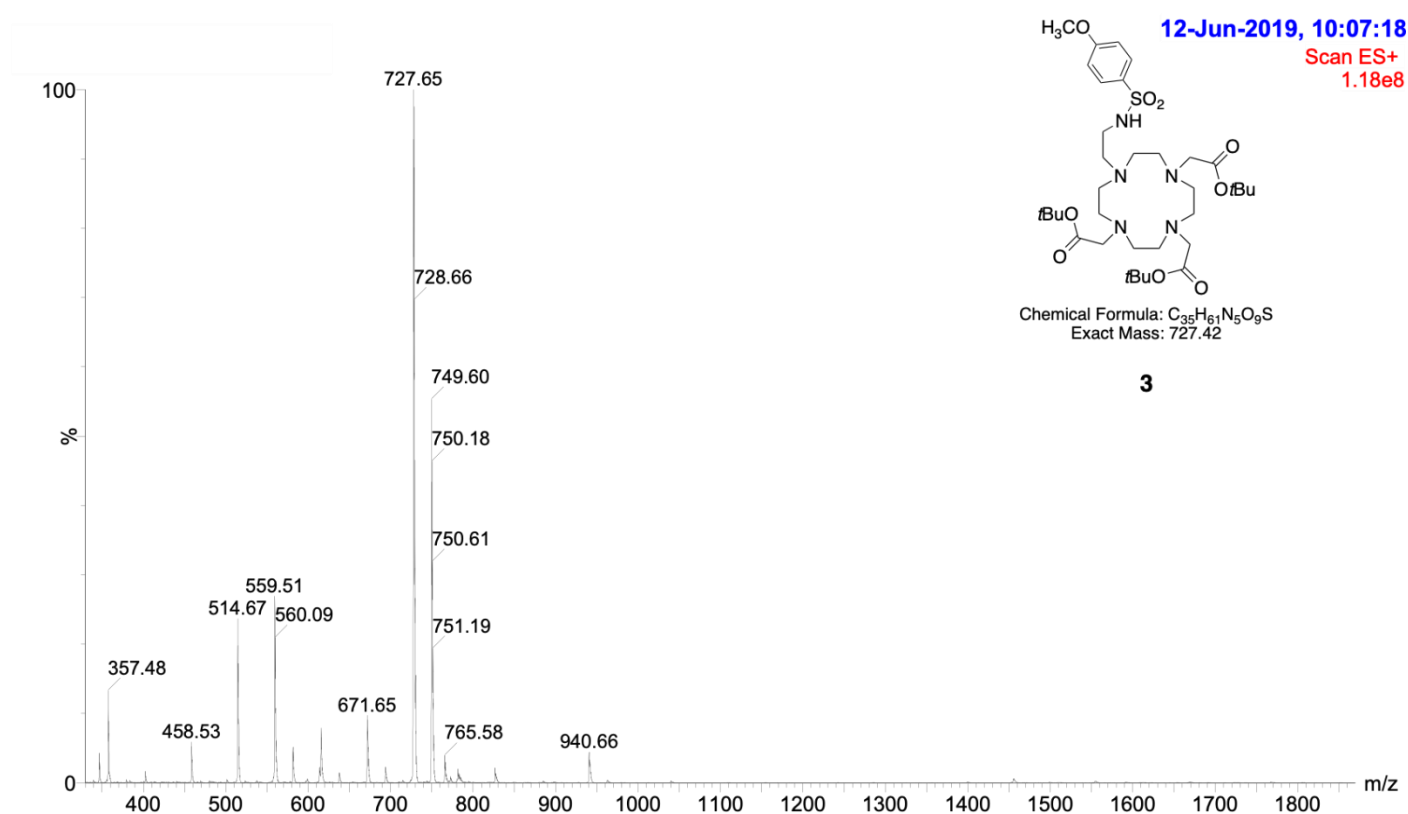


Figure S7. LRMS of compound 3.

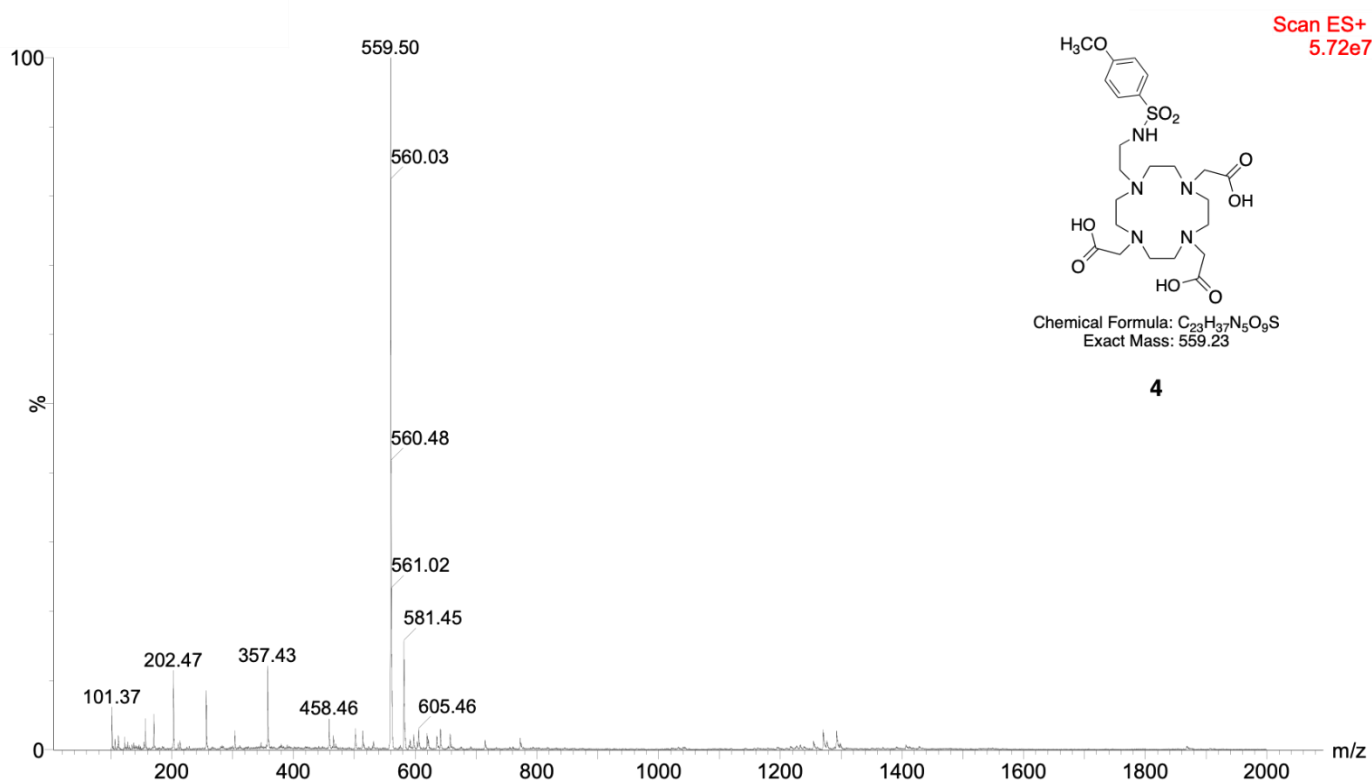


Figure S8. LRMS of compound 4.

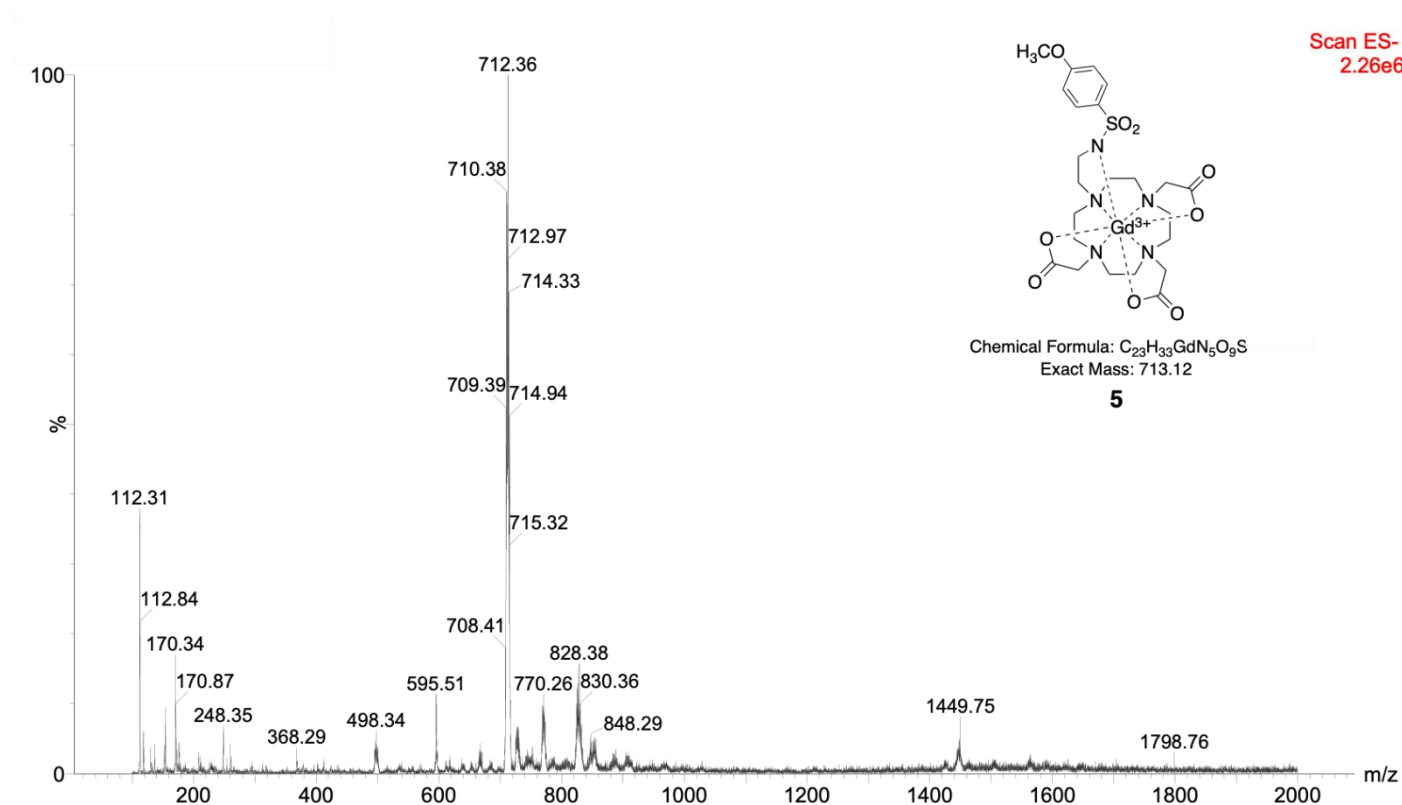


Figure S9. LRMS of compound 5.

3. RadioHPLC Traces of PET Co-Agents

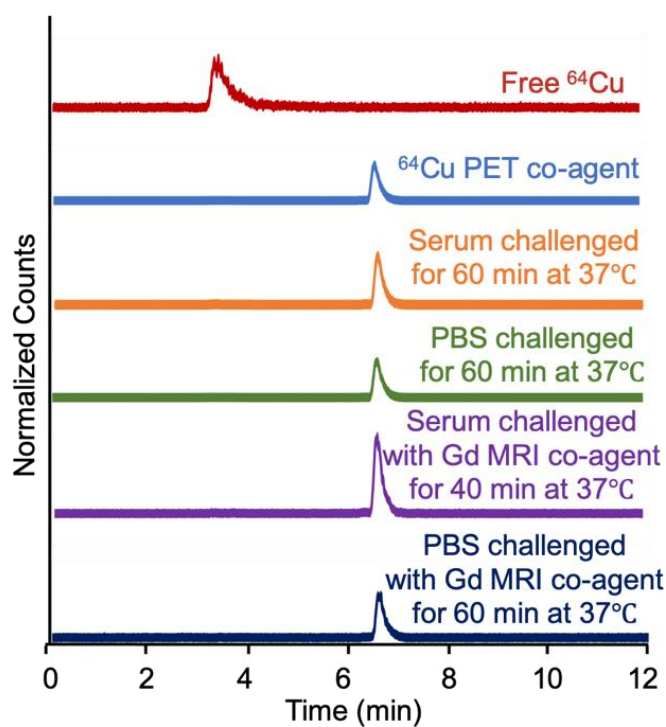


Figure S10. RadioHPLC trace of ^{64}Cu PET co-agent when challenged in solution. The ^{64}Cu PET co-agent (blue trace) was incubated in human serum (orange trace) and PBS (green trace) for one hour at 37°C and showed complete stability with no presence of free ^{64}Cu (red trace). The ^{64}Cu PET co-agent was also incubated in the presence of the MRI co-agent in serum (purple trace) and PBS (dark blue trace) and showed complete stability.

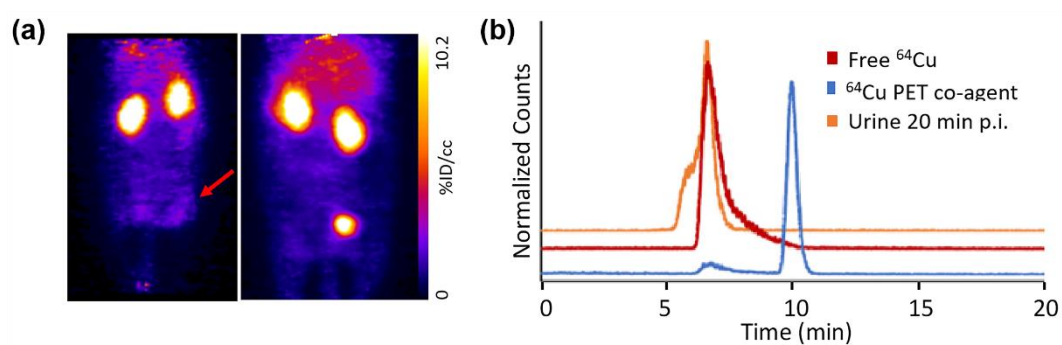


Figure S11. Metabolism of the ^{64}Cu PET co-agent. (a) A PET image from the dynamic PET/MRI scan using the ^{64}Cu PET co-agent showed poor tumor uptake and high liver uptake. (b) RadioHPLC of urine collected from the mouse after the dynamic PET/MRI scan (orange trace) showed the presence of only free ^{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.