

SUPPORTING INFORMATION

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Title: Synthesis, Characterization, and in vitro Testing of a Bacteria-Targeted MR Contrast Agent

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^1H and ^{13}C NMR of **4-10**: S2-S8

MS (ESI-positive) of **8-10**: S9-S10

Analytical HPLC and HPLC-MS of Zn-**1** compounds: S11-S13

Luminescence Decay of Zn-**1**-Tb in H_2O and D_2O : S14

Relaxivity of Zn-**1**: S14-S15

^1H NMR of Zn-**1**-Eu: S15-S16

T_2 imaging data: S16

Figure S2: ¹H NMR of 4

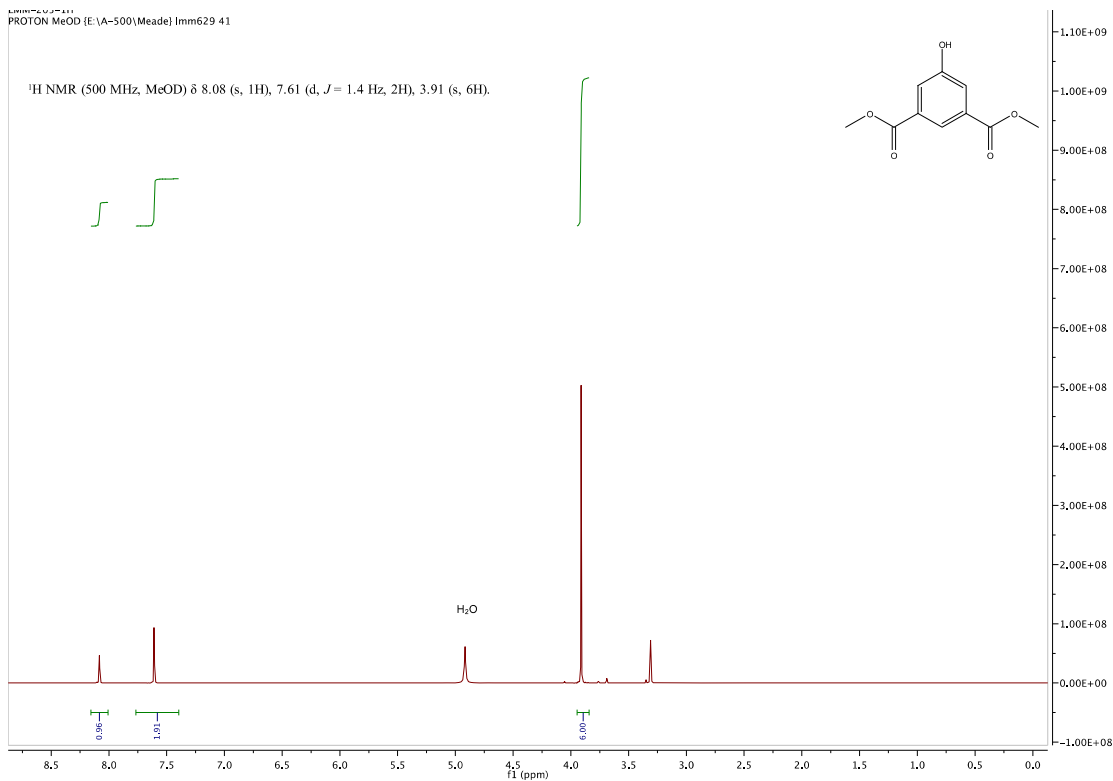


Figure S1: ¹³C NMR of 4

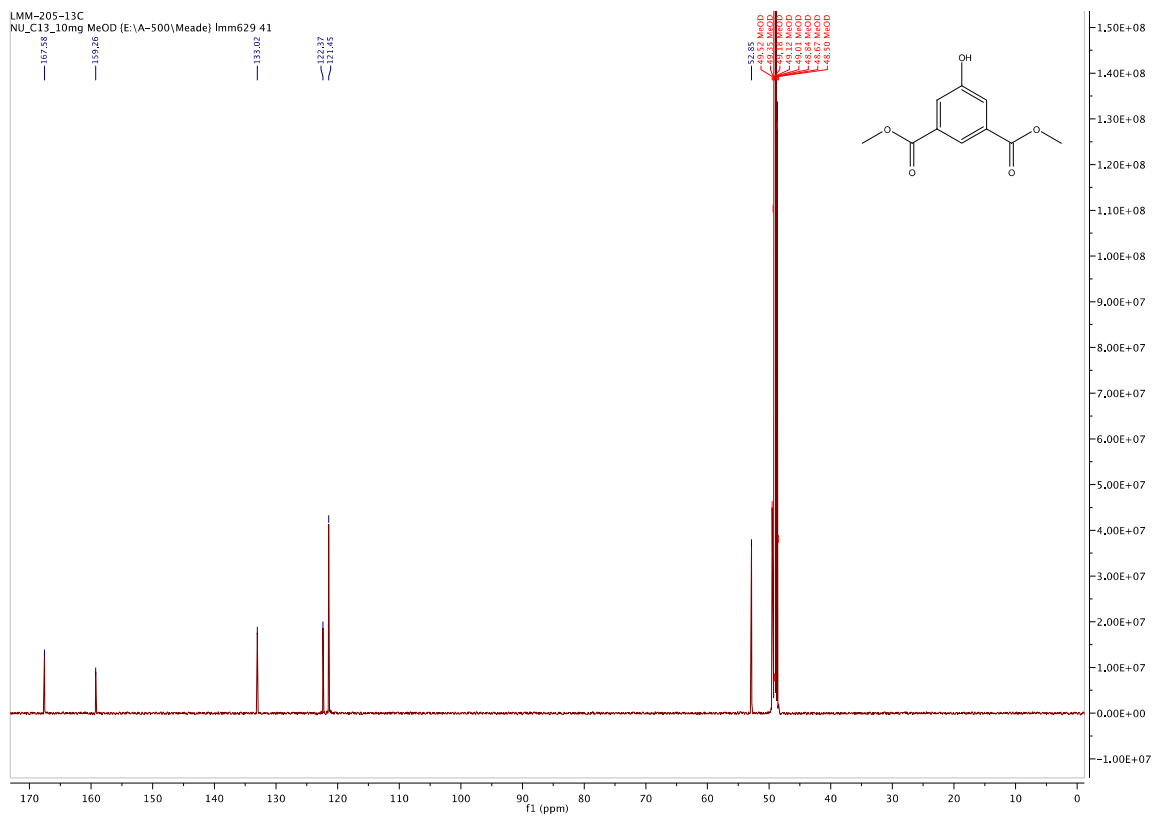


Figure S3: ¹H NMR of 5

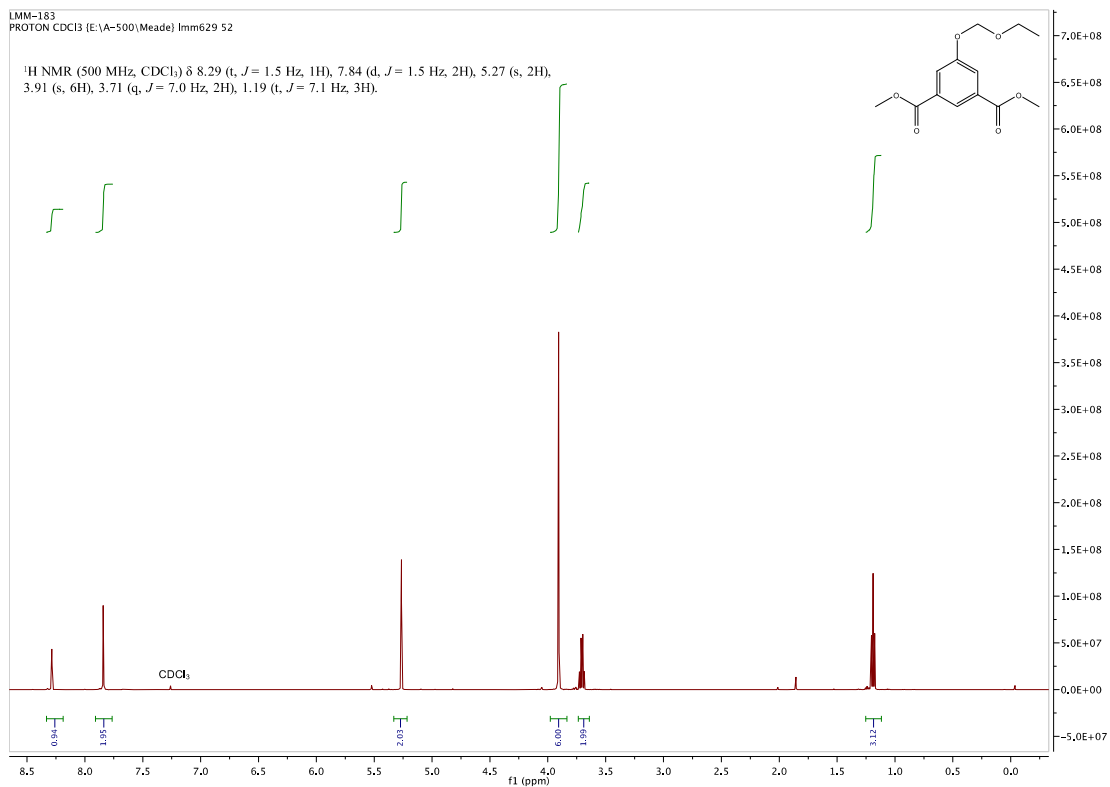


Figure S4: ¹³C NMR of 5

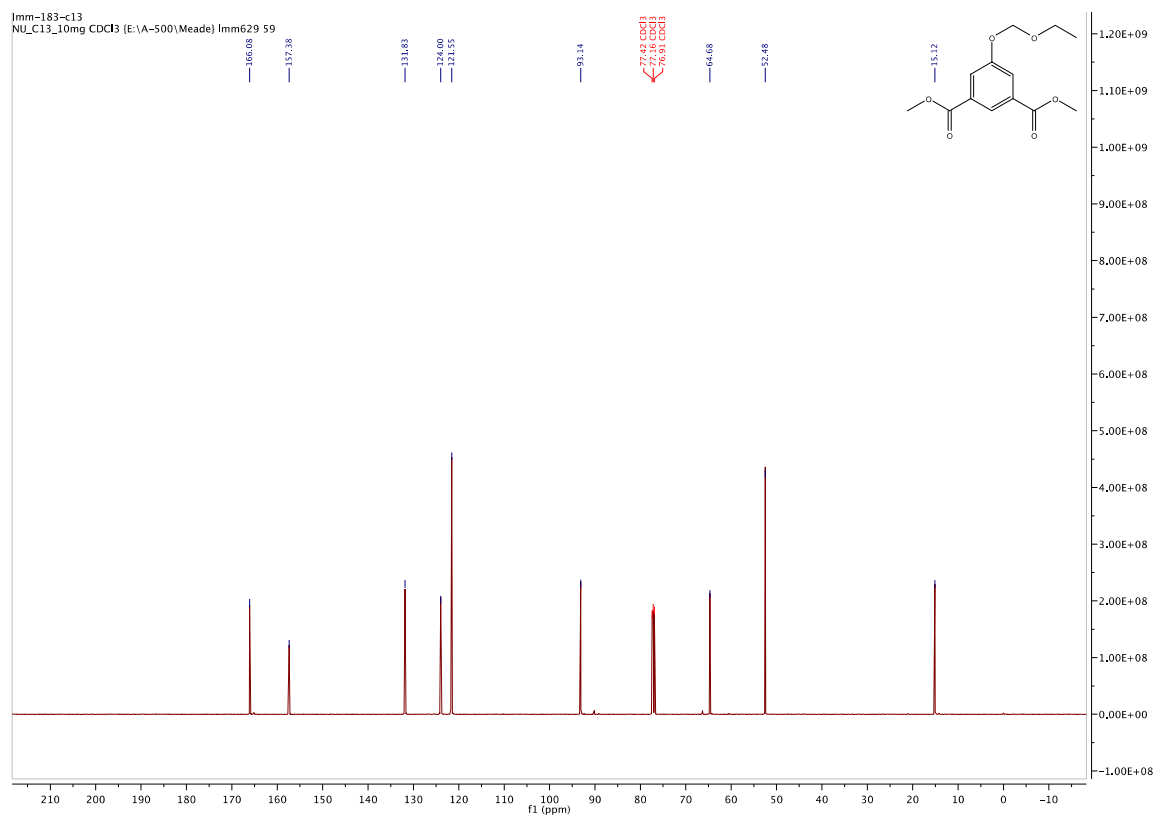


Figure S5: ¹H NMR of 6

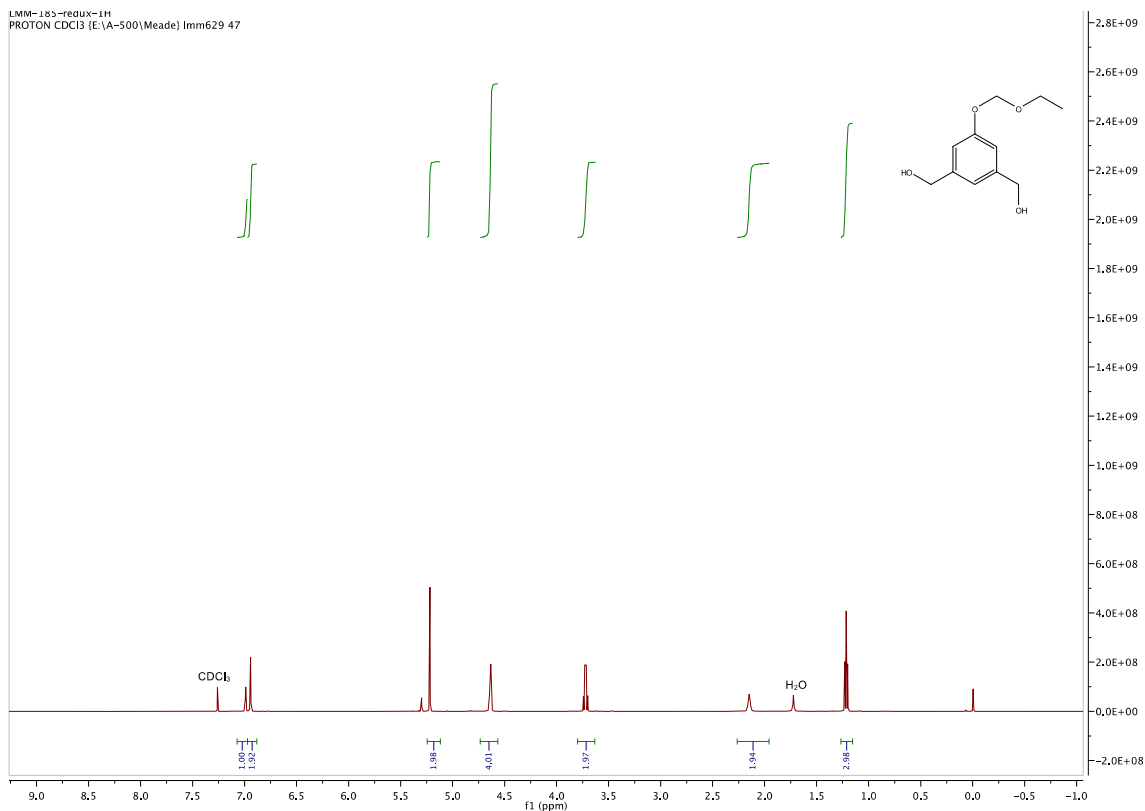


Figure S6: ¹³C of 6

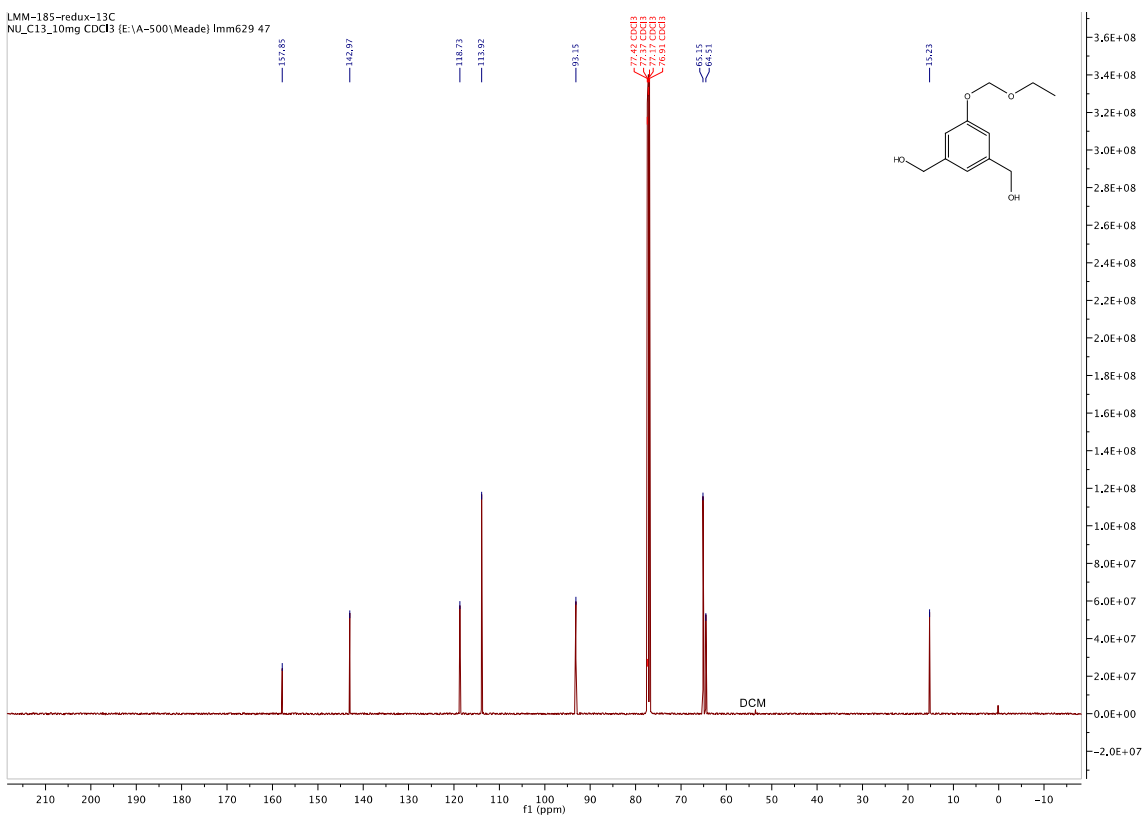


Figure S7: ¹H NMR of 7

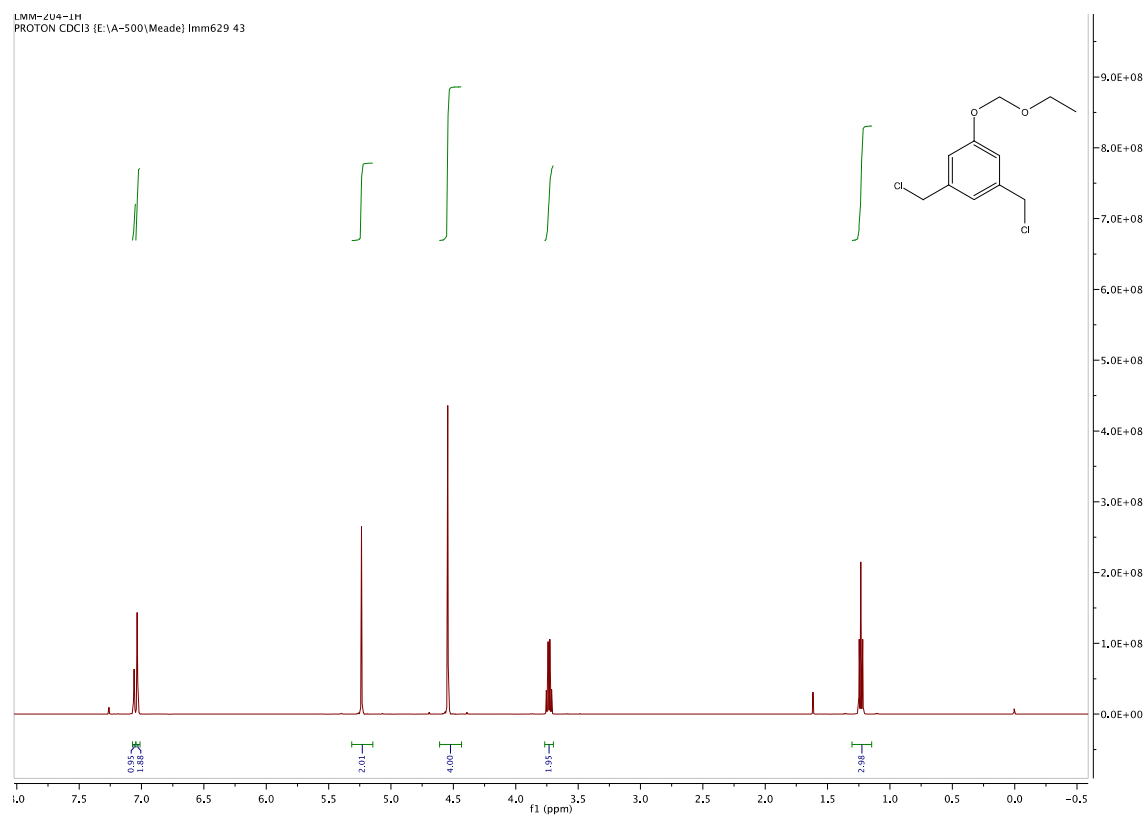


Figure S8: ¹³C NMR of 7

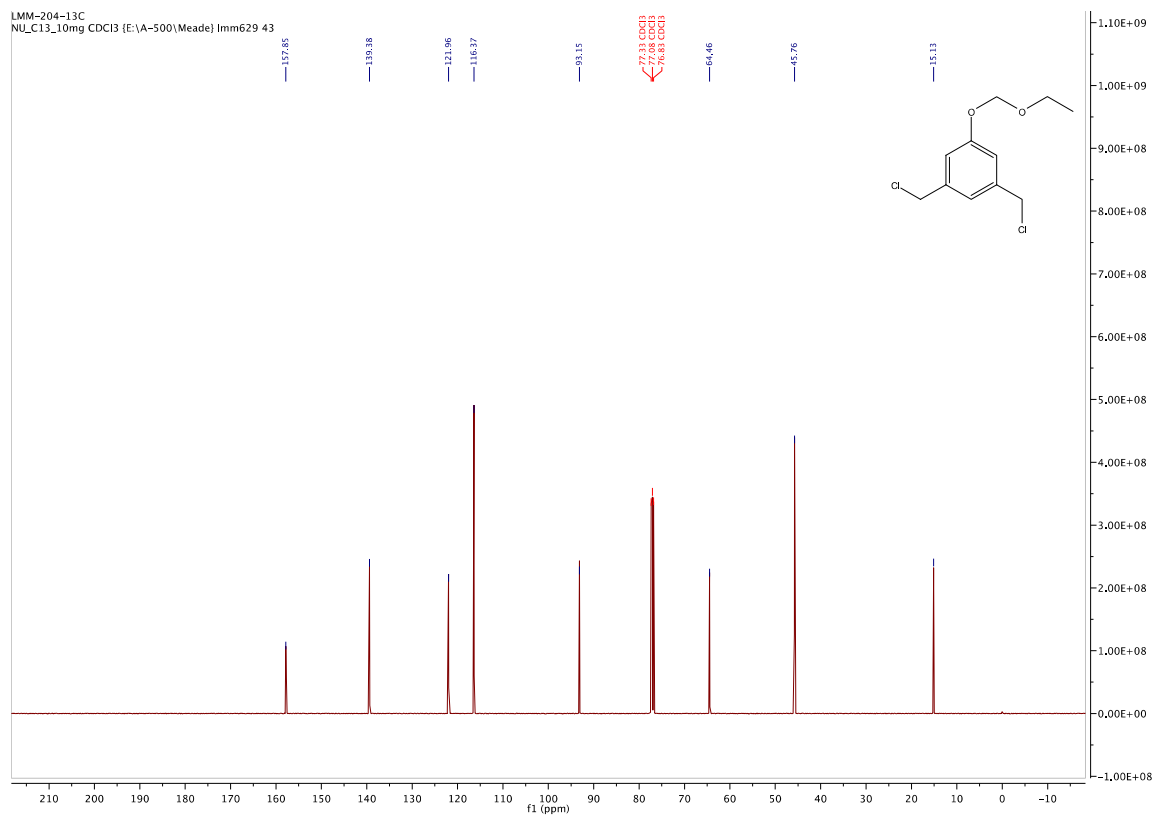


Figure S9: ¹H NMR of 8

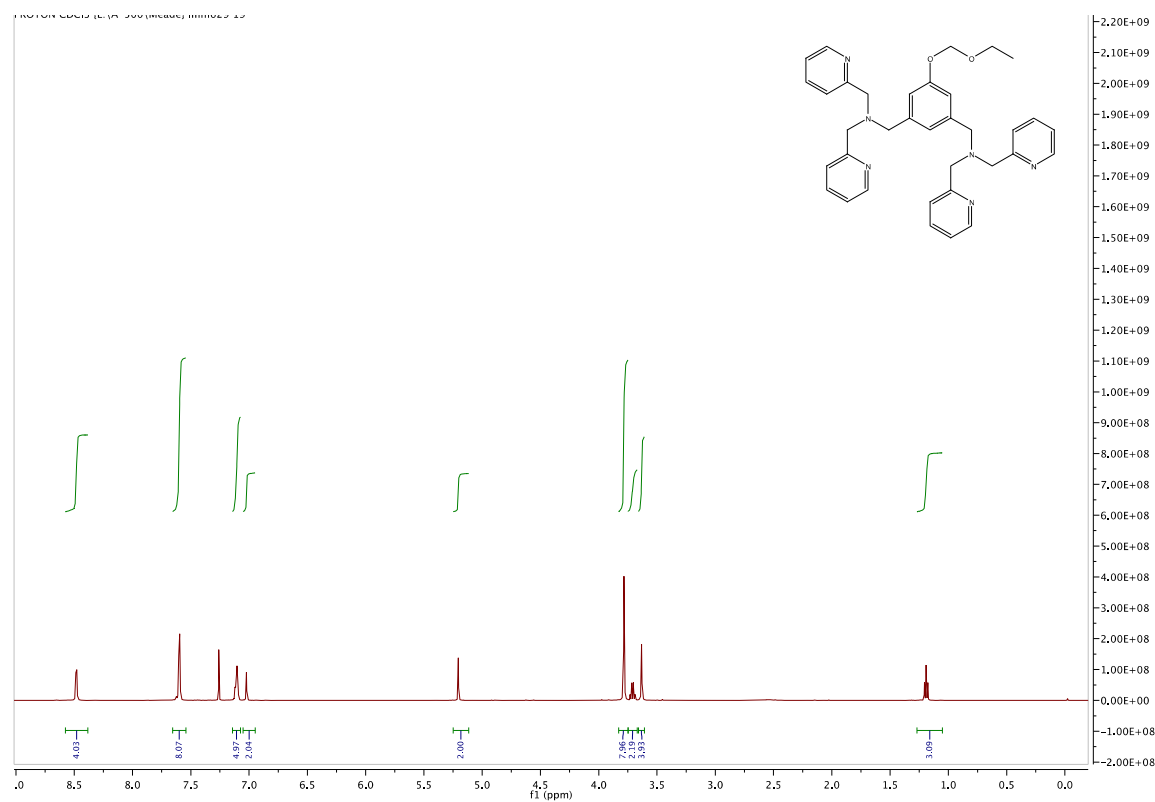


Figure S10: ¹³C NMR of 8

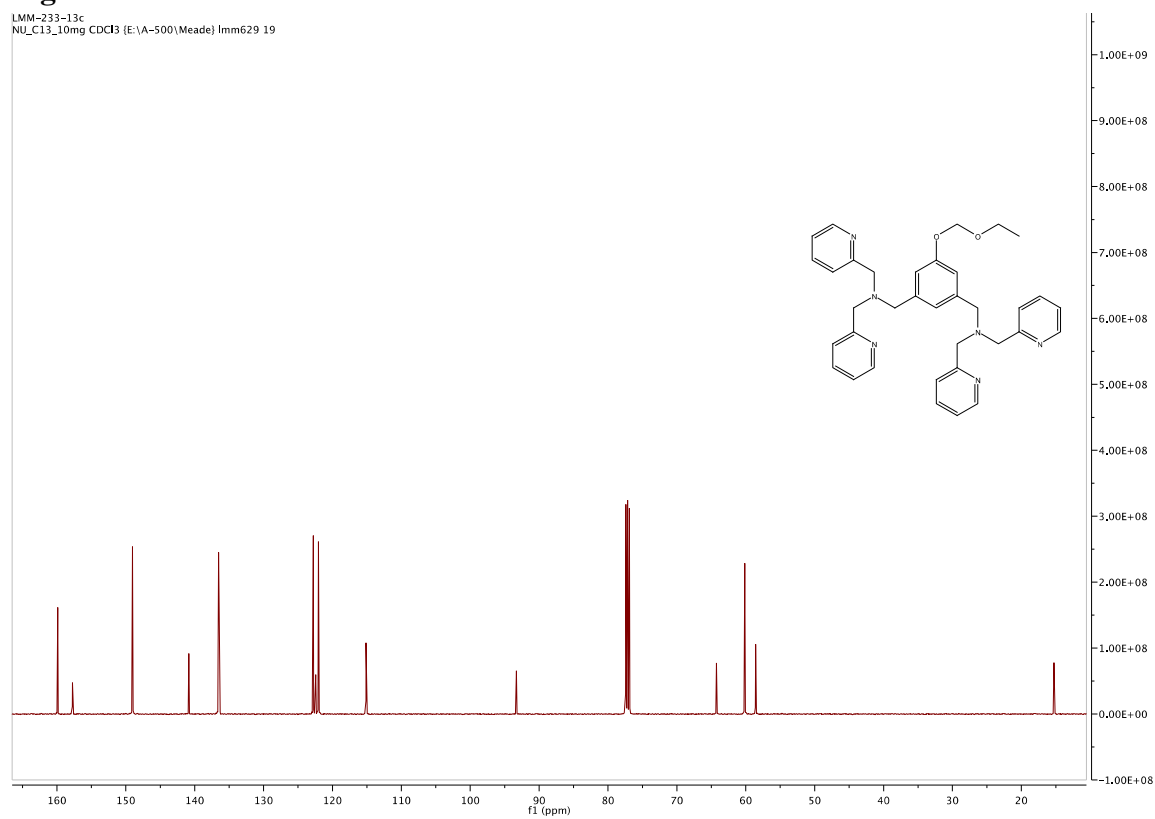


Figure S11: ¹H NMR of 9



Figure S12: ¹³C NMR of 9

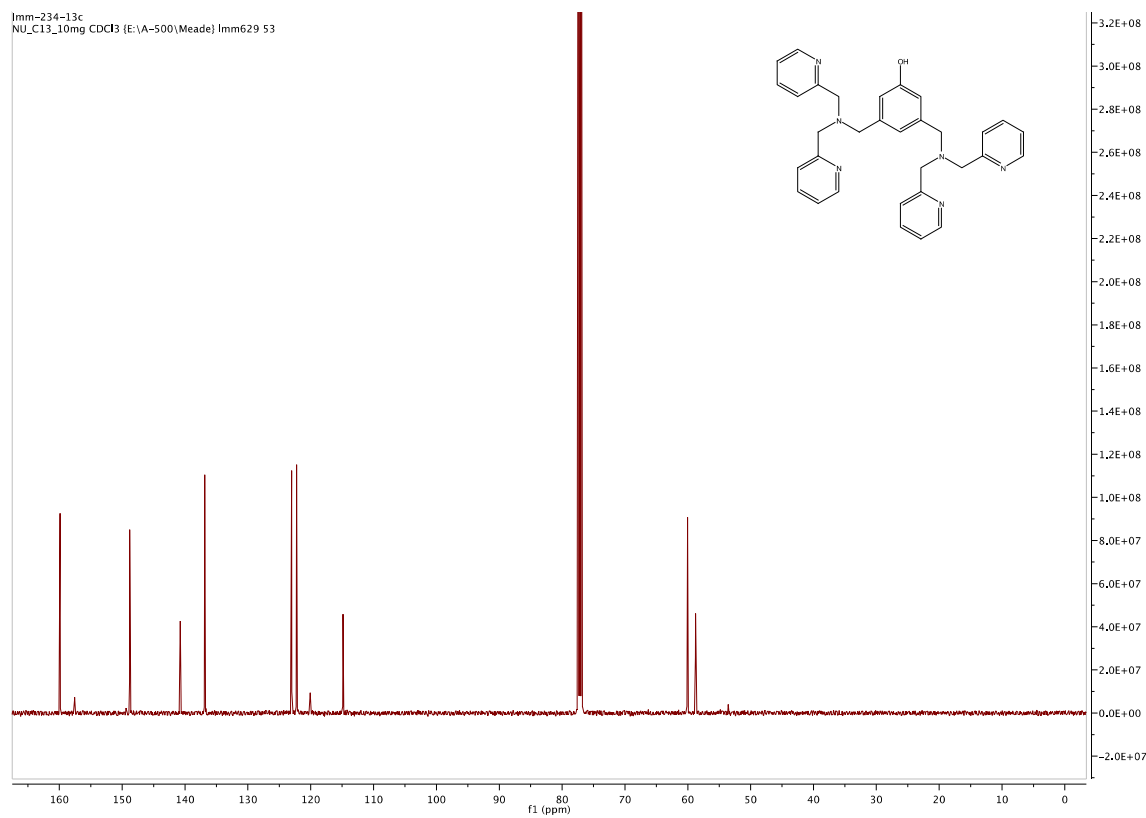


Figure S13: ¹H NMR of 10

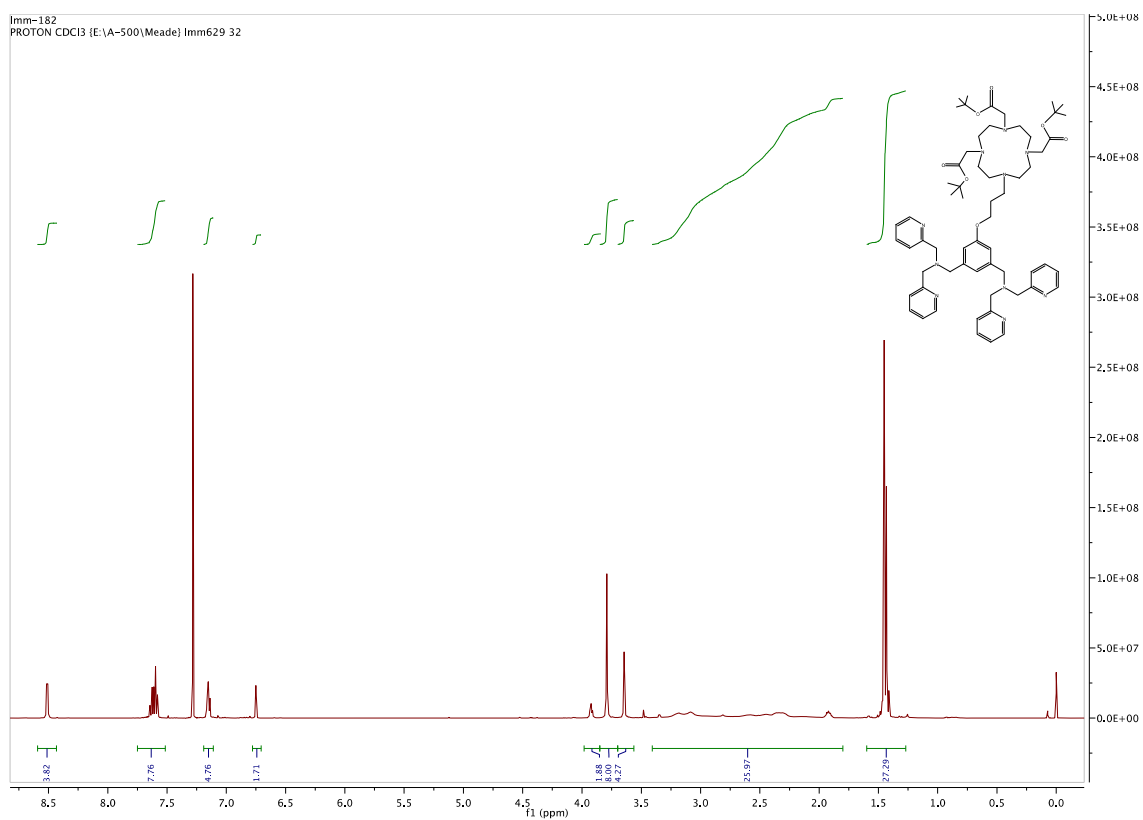


Figure S14: ¹³C NMR of 10

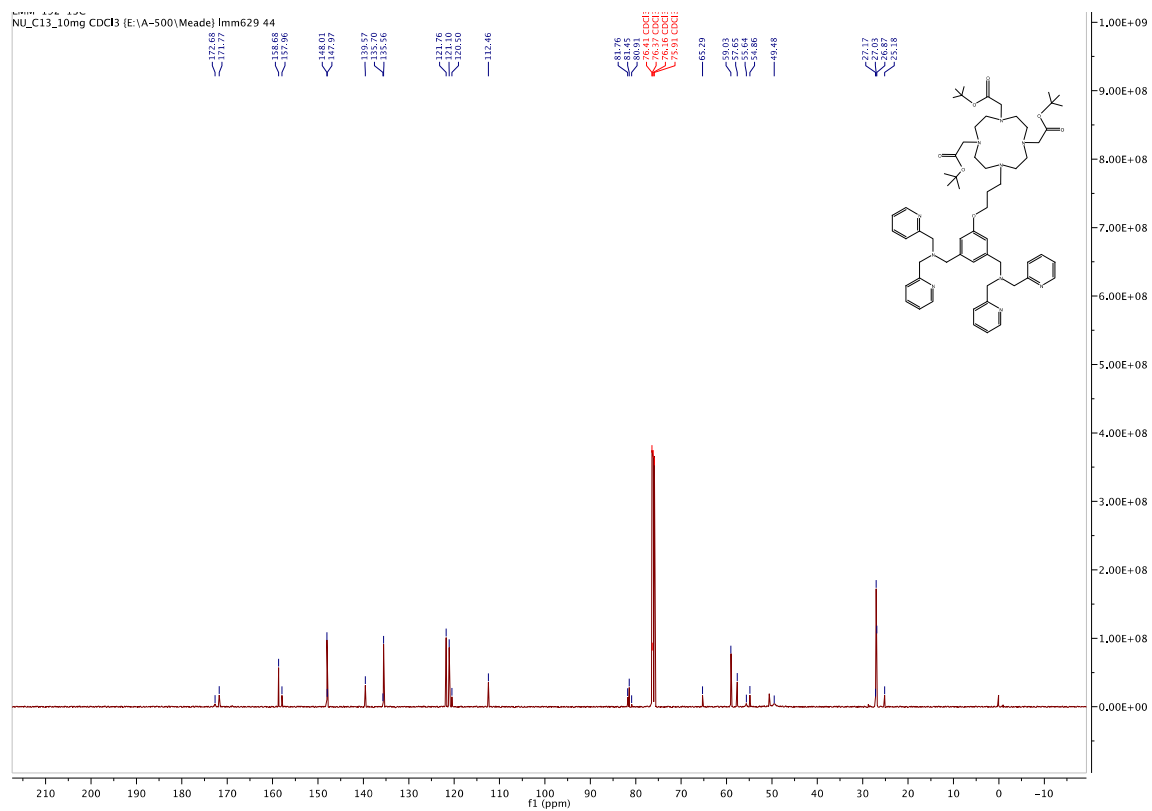


Figure S15: MS (ESI-positive) of 8

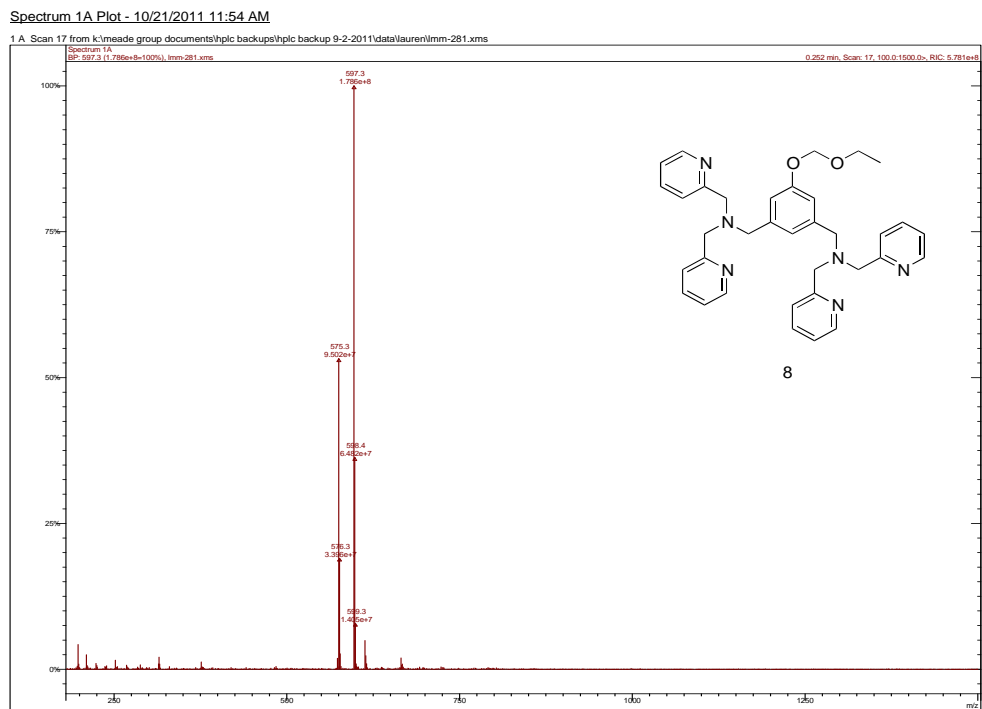


Figure S16: MS (ESI-positive) of 9

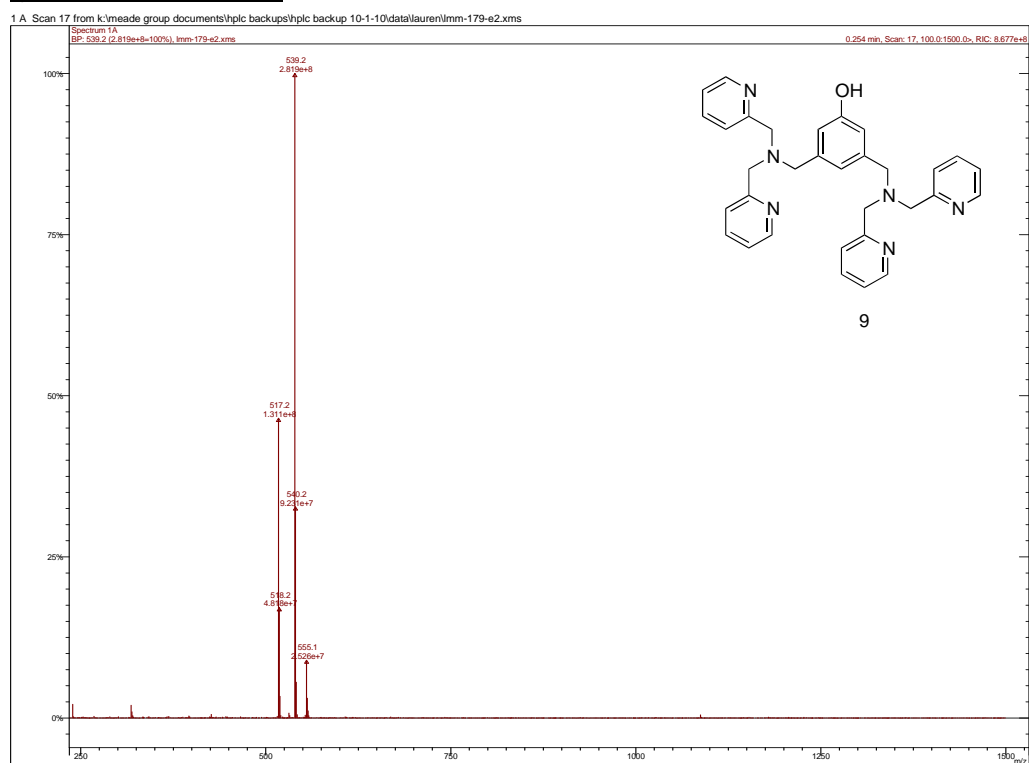


Figure S17: MS (ESI-positive) of **10**

Spectrum 1A Plot - 10/25/2011 3:59 PM

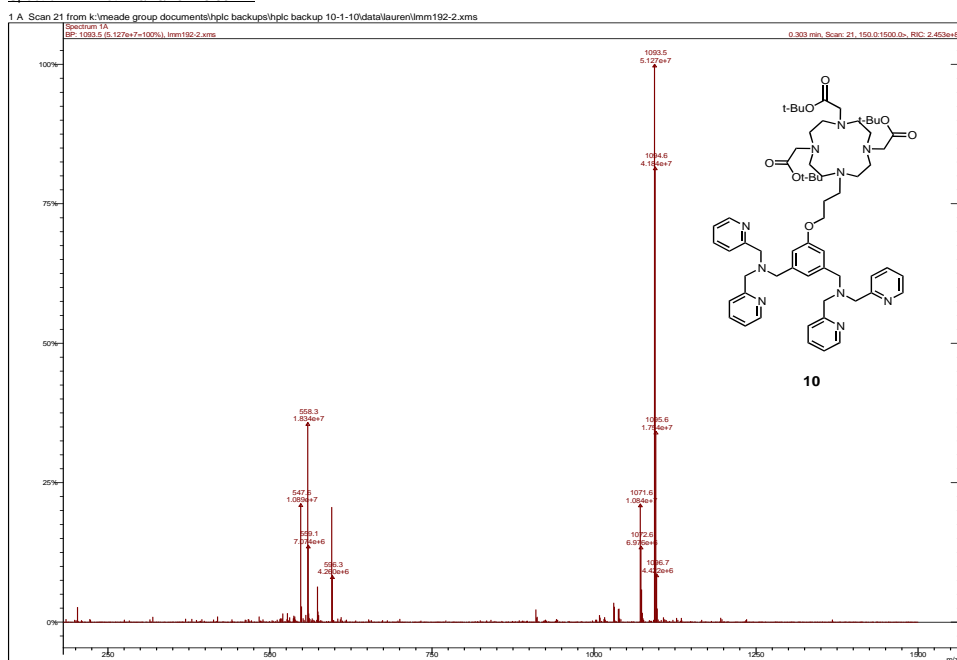


Figure S18: MS (ESI-positive) of **10** after deprotection with TFA

Spectrum 1A Plot - 10/21/2011 12:20 PM

1 A Scan 17 from k:\meade group documents\hplc backups\hplc backup 5-27-2011\data\lauren\deprotected-ig.xms

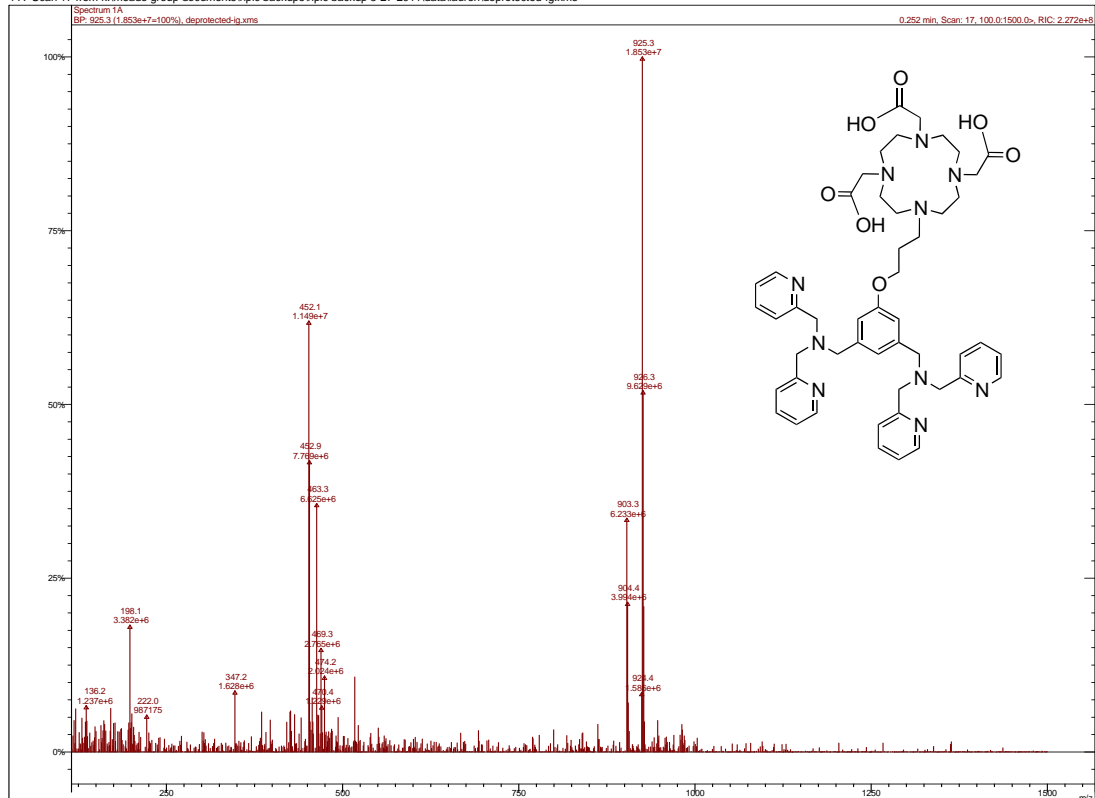


Figure S19: Analytical HPLC trace (ELSD) of Zn-1-Eu

Chromatogram Plot 1 - 10/21/2011 7:14 PM

File: c:\varianw\data\lauren\no seriously retard_10-21-2011_5-53-51 pm.run
Sample: Operator:
Scan Range: 0 - 0 Time Range: 0.00 - 49.98 min. Date: 10/21/2011 5:53 PM

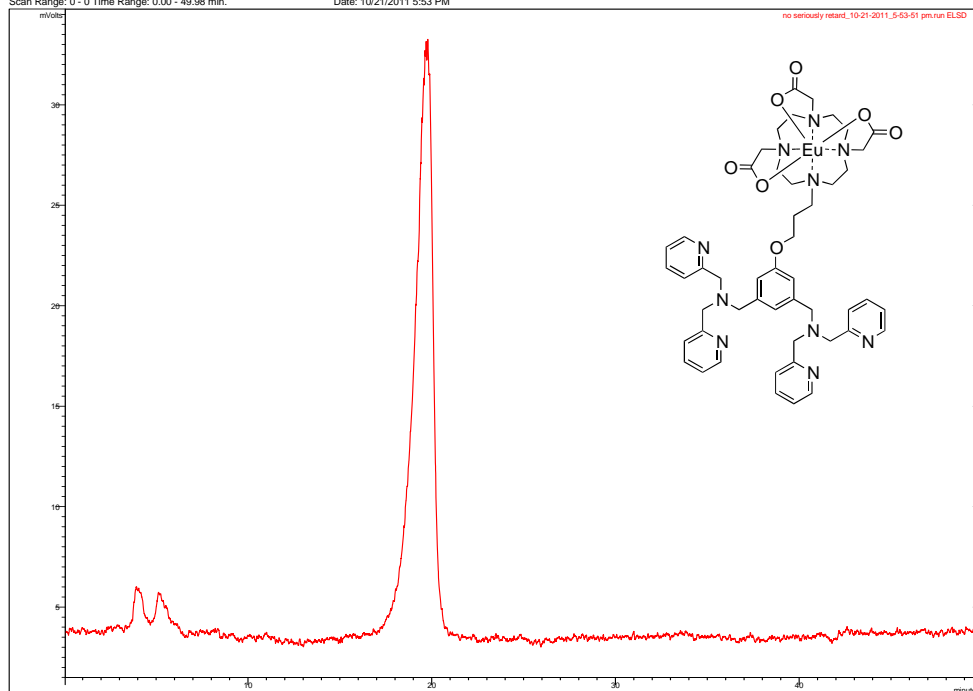


Figure S20: HPLC-MS (ESI-positive) of Zn-1-Eu

Spectrum 1A Plot - 10/21/2011 7:18 PM

1 A Scan 1294 from c:\varianw\data\lauren\eu-iguana.xms

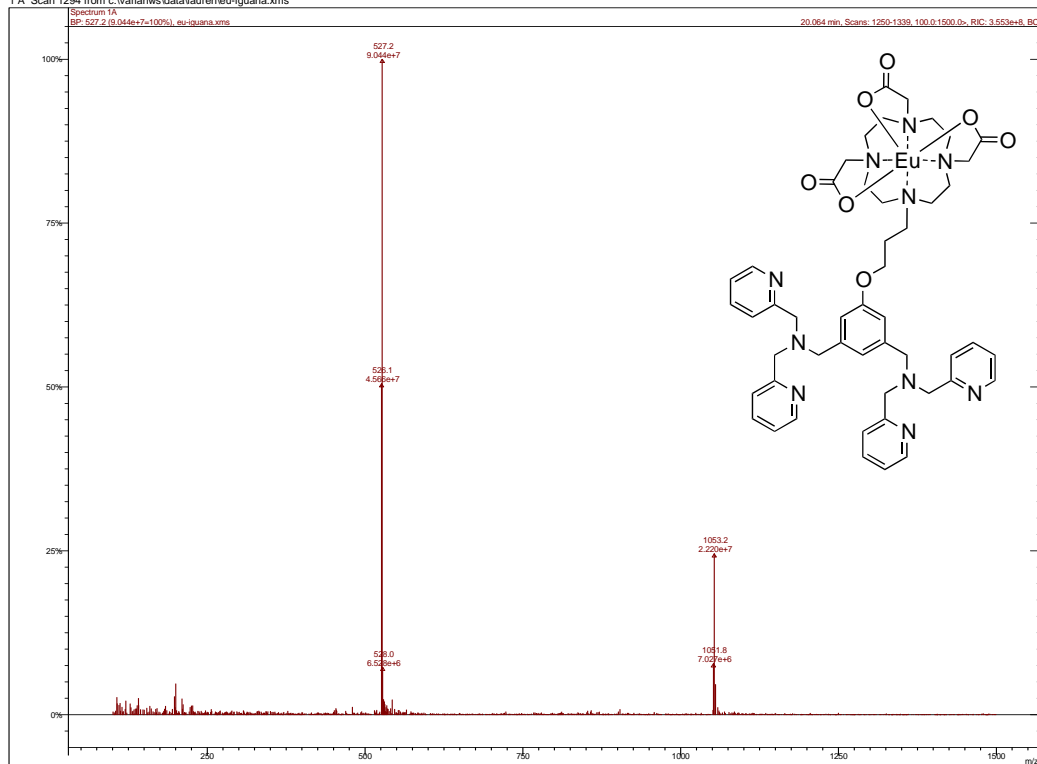


Figure S21: Analytical HPLC trace (ELSD) of Zn-1

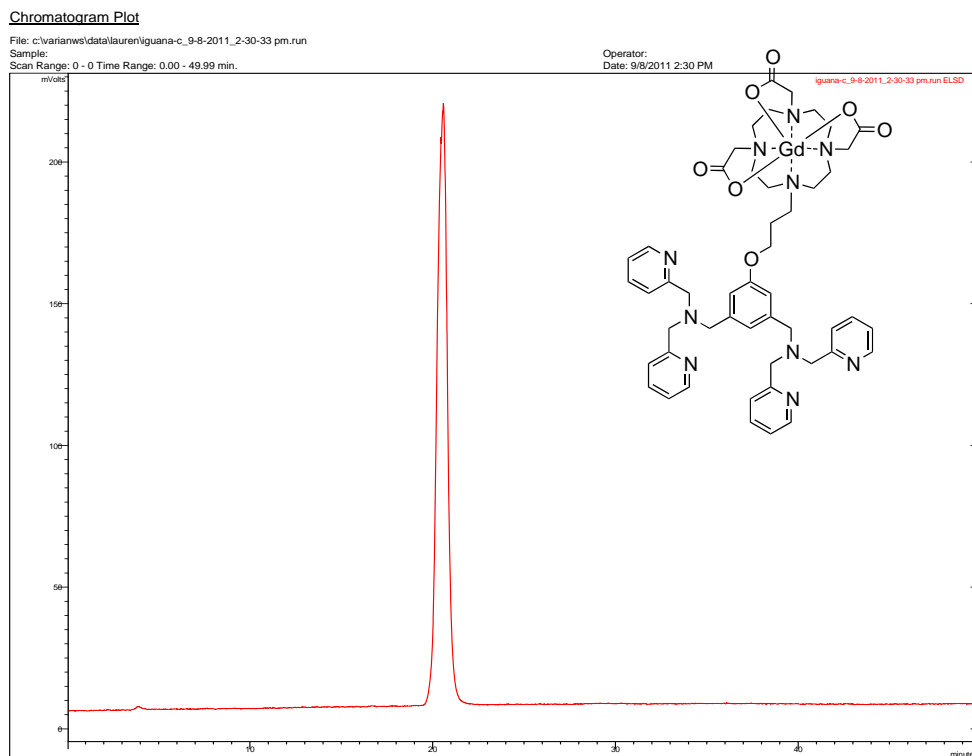


Figure S22: HPLC MS of Zn-1

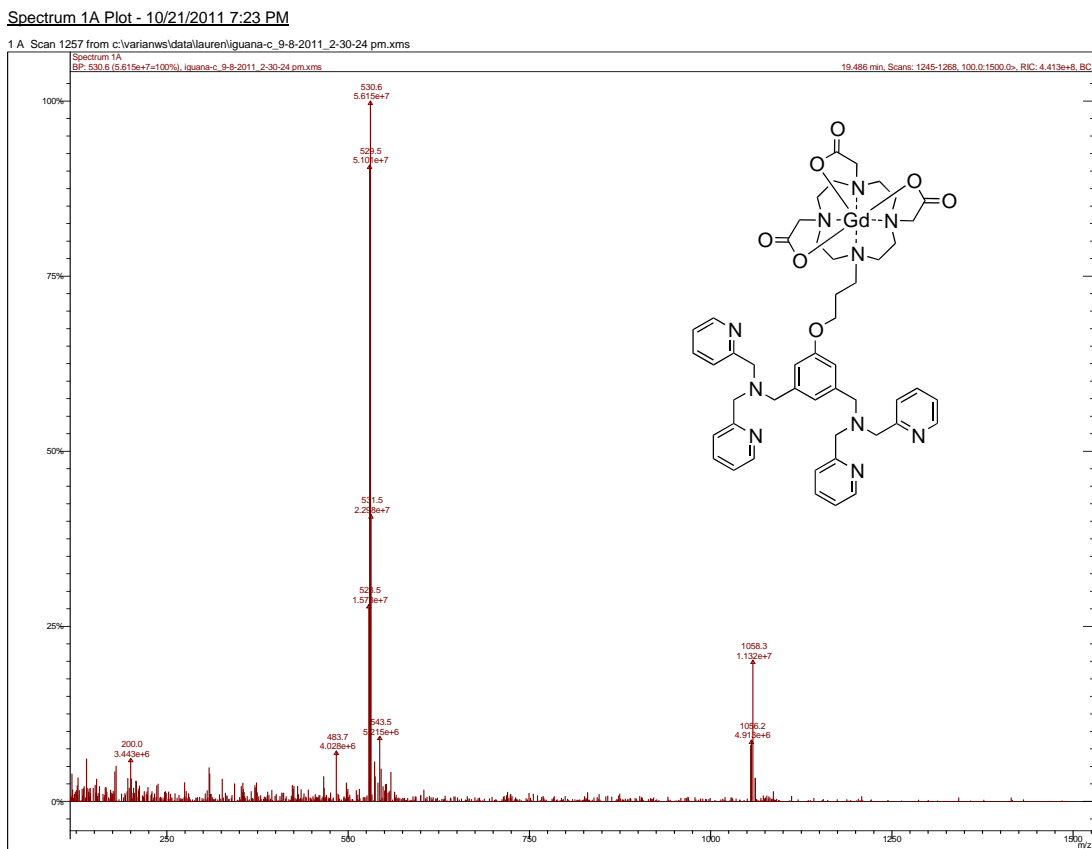


Figure S23: Analytical HPLC trace (ELSD) of Zn-1-Tb

Chromatogram Plot 1 - 10/25/2011 3:53 PM

File: k:\meade group documents\hplc backups\hplc backup 5-27-2011\data\lauren\hplc-imm-186\tb-iguana-with elsd_12-8-2010_5-06-10 pm.run

Sample:

Operator:

Scan Range: 0 - 0 Time Range: 0.00 - 49.99 min.

Date: 12/8/2010 5:06 PM

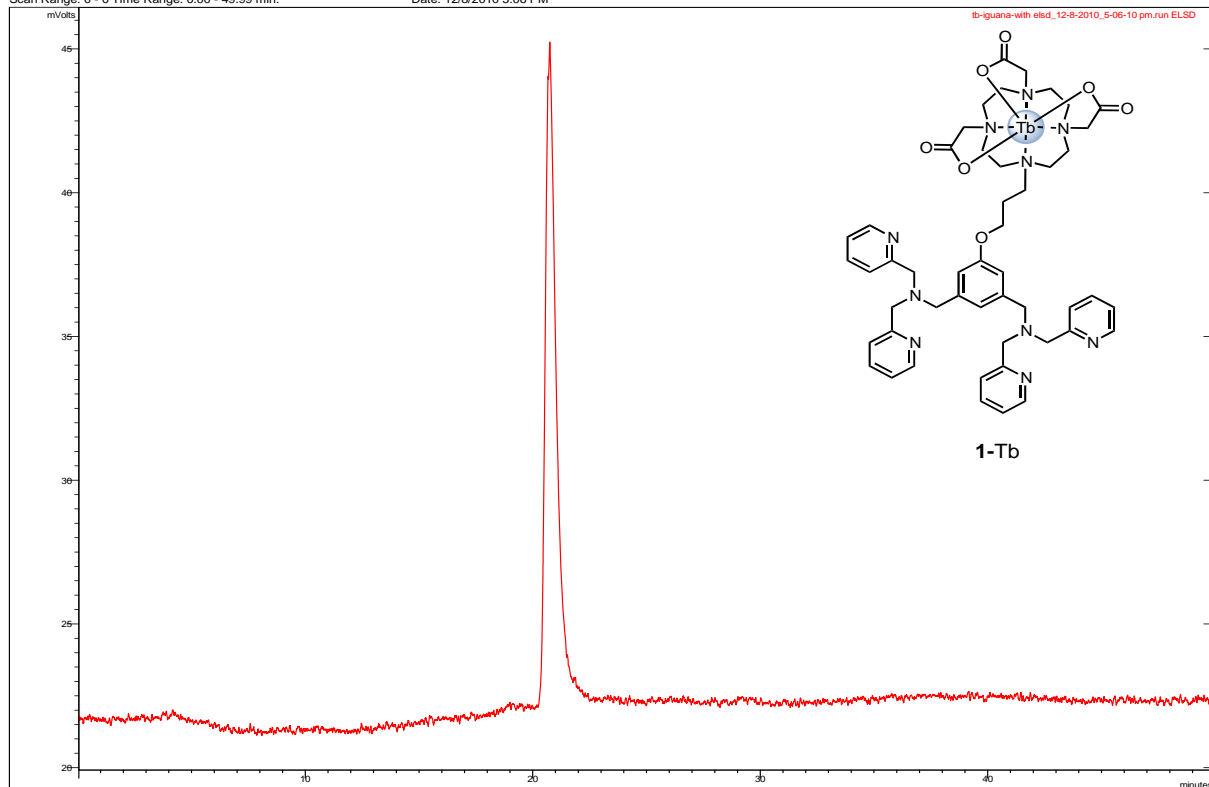


Figure S24: HPLC-MS (ESI positive) of Zn-1-Tb

Spectrum 1A Plot - 10/25/2011 3:50 PM

1 A Scan 1371 from ... \hplc backups\hplc backup 5-27-2011\data\lauren\hplc-imm-186\tb-iguana-with elsd_12-8-2010_5-06-00 pm.xms

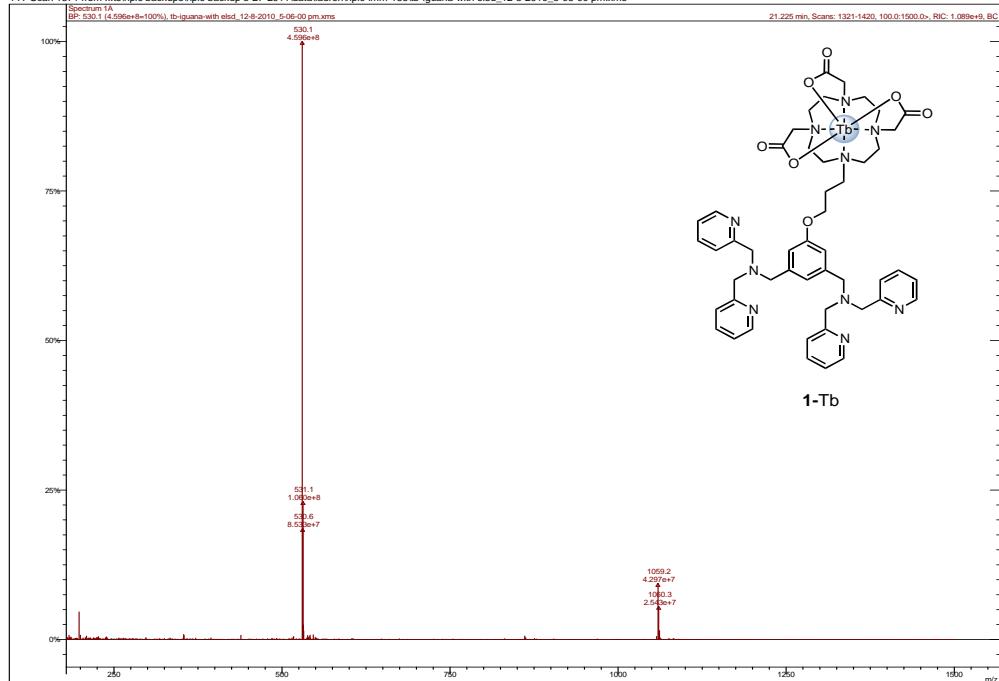


Figure S24: Luminescence lifetime measurements of Zn-1-Tb in H₂O and D₂O

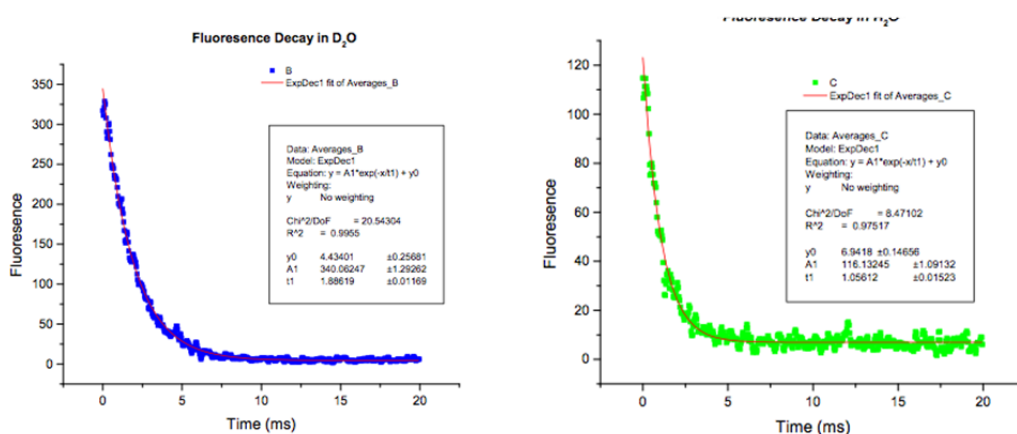


Figure S25: Relaxivity of Zn-1 in 2% DMSO in LB Media at 1.4 T (37 °C)

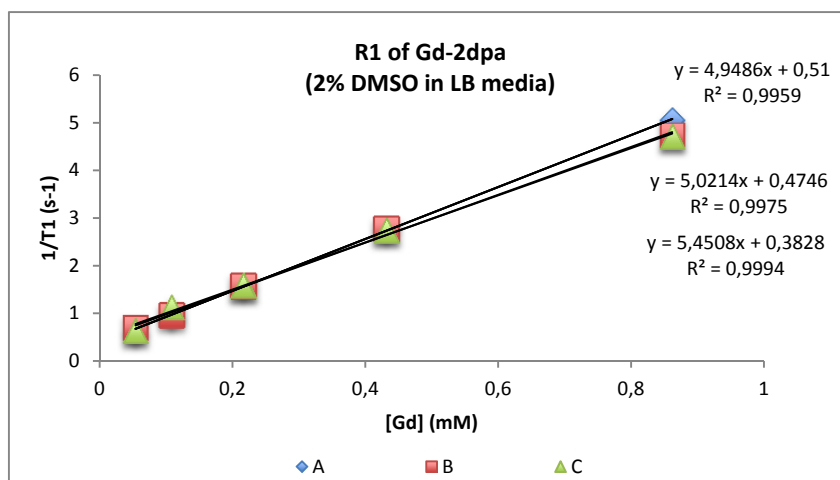


Figure S26: Relaxivity of Zn-1 in agarose gel at 1.4 T (37 °C)

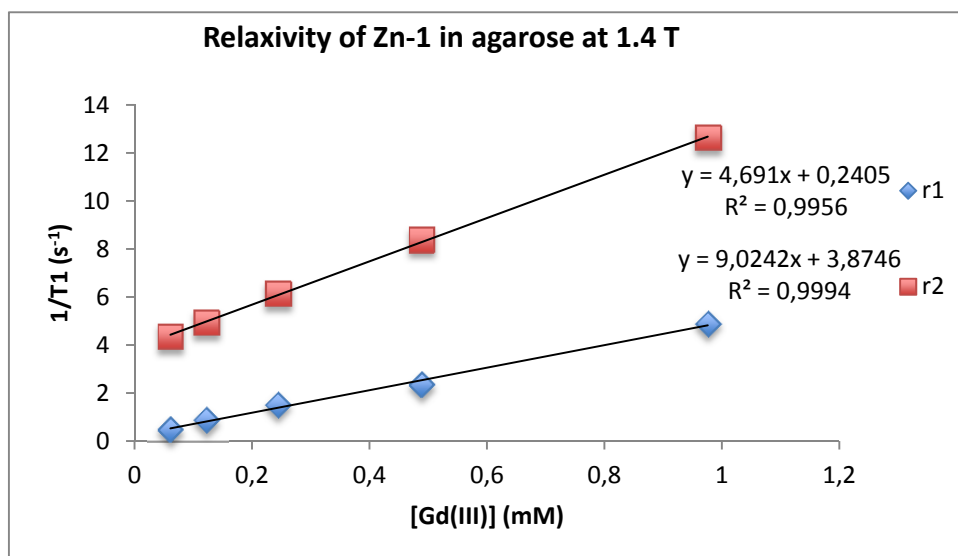


Figure S27: Relaxivity of Zn-1 in agarose gel at 7T (25 °C)

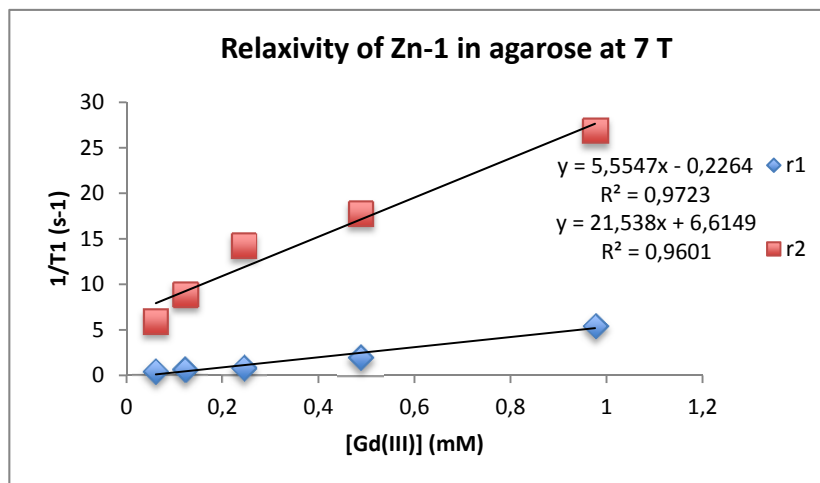


Figure S28: Full ^1H spectrum of Zn-1-Eu at 60 °C in d_6 -DMSO at 600 MHz.

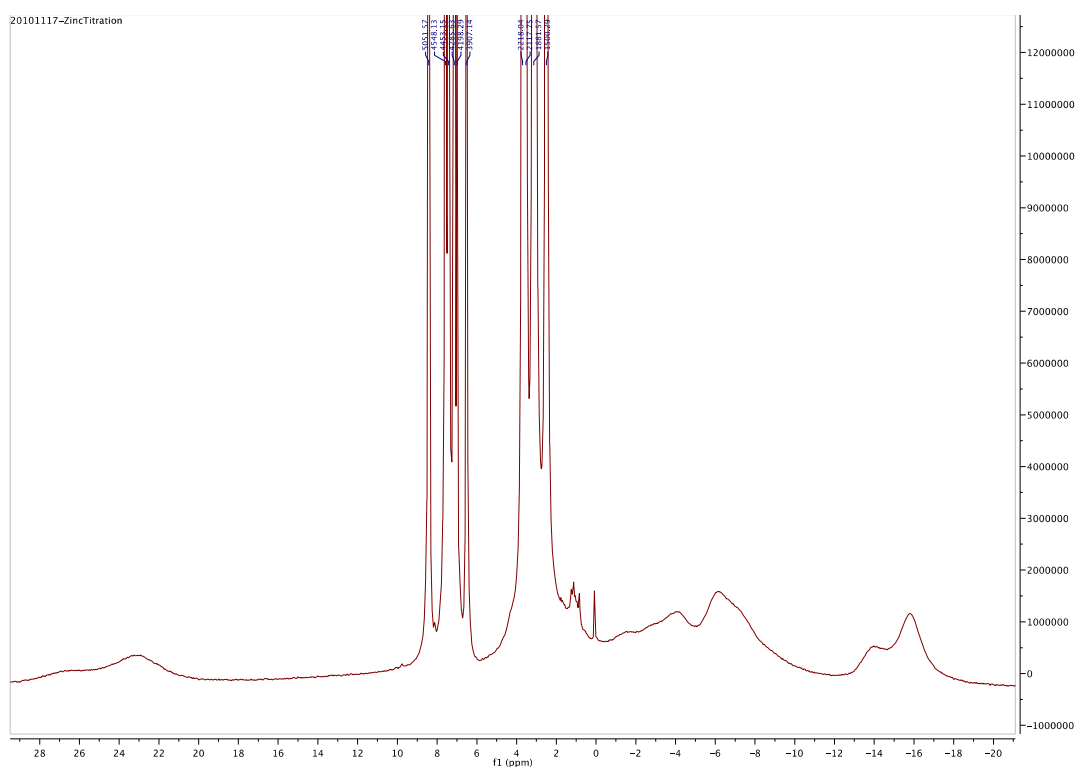


Figure S29: Close up of ^1H NMR of **1-Eu** with increasing equivalents of Zn.

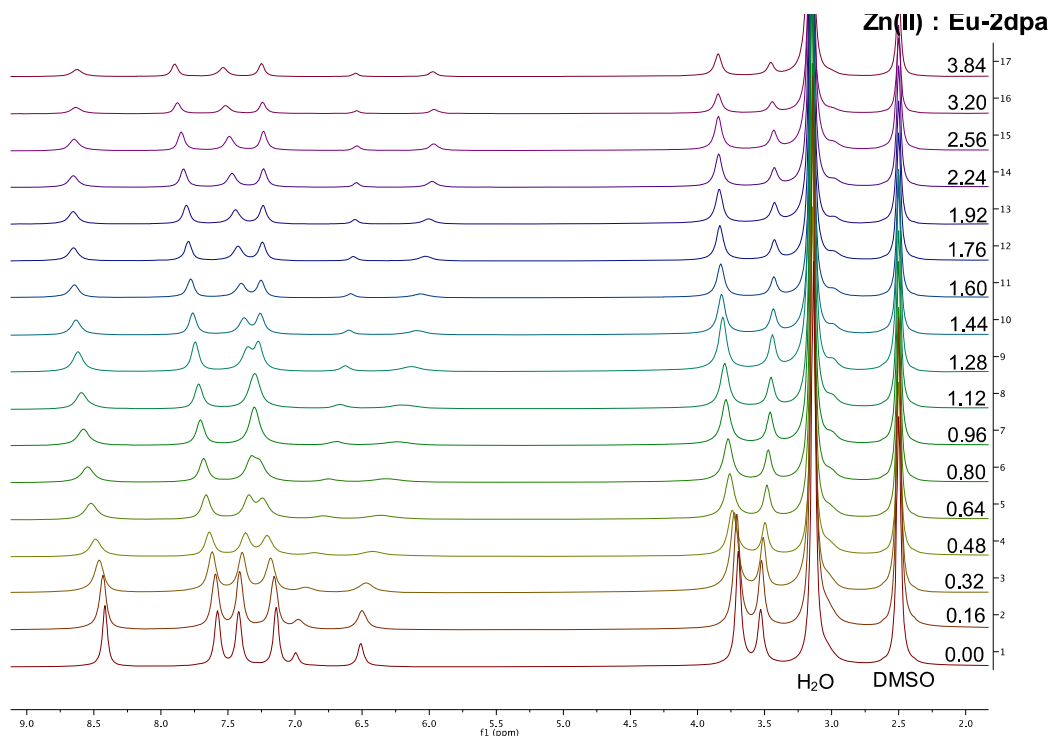


Figure S30: Top - T_2 -weighted phantom images of *S. Aureus* incubated with Zn-1, Zn-2, and Zn3. Images were acquired at 7T at 25 °C. Bottom: T_2 map of phantoms.

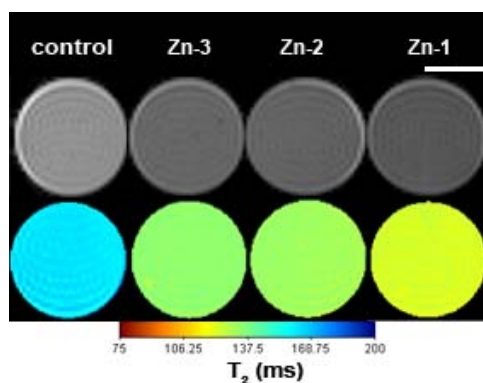


Figure S31: T_2 relaxation times: T_2 relaxation times were acquired at 1.41 (37 °C) and 7 T (25 °C). Data are presented as the percent reduction in T_2 versus bacteria incubated with LB media, washed, and suspended in agarose.

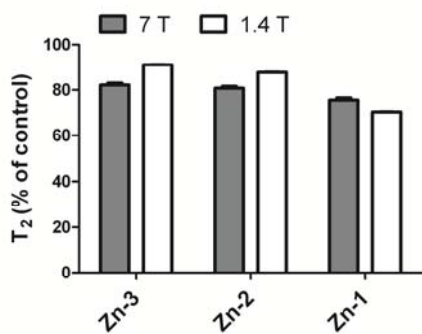


Figure S32: T_1 weighted phantom images of *S. Aureus* incubated with Zn-1, Zn-2, and Zn-3. Images were acquired at 7T (25 °C).

