

## Supplementary Information

### Cellular Uptake and Photo-Cytotoxicity of a Gadolinium(III)-DOTA-Naphthalimide Complex “Clicked” to a Lipidated Tat Peptide

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## NMR Spectra of Reported Compounds

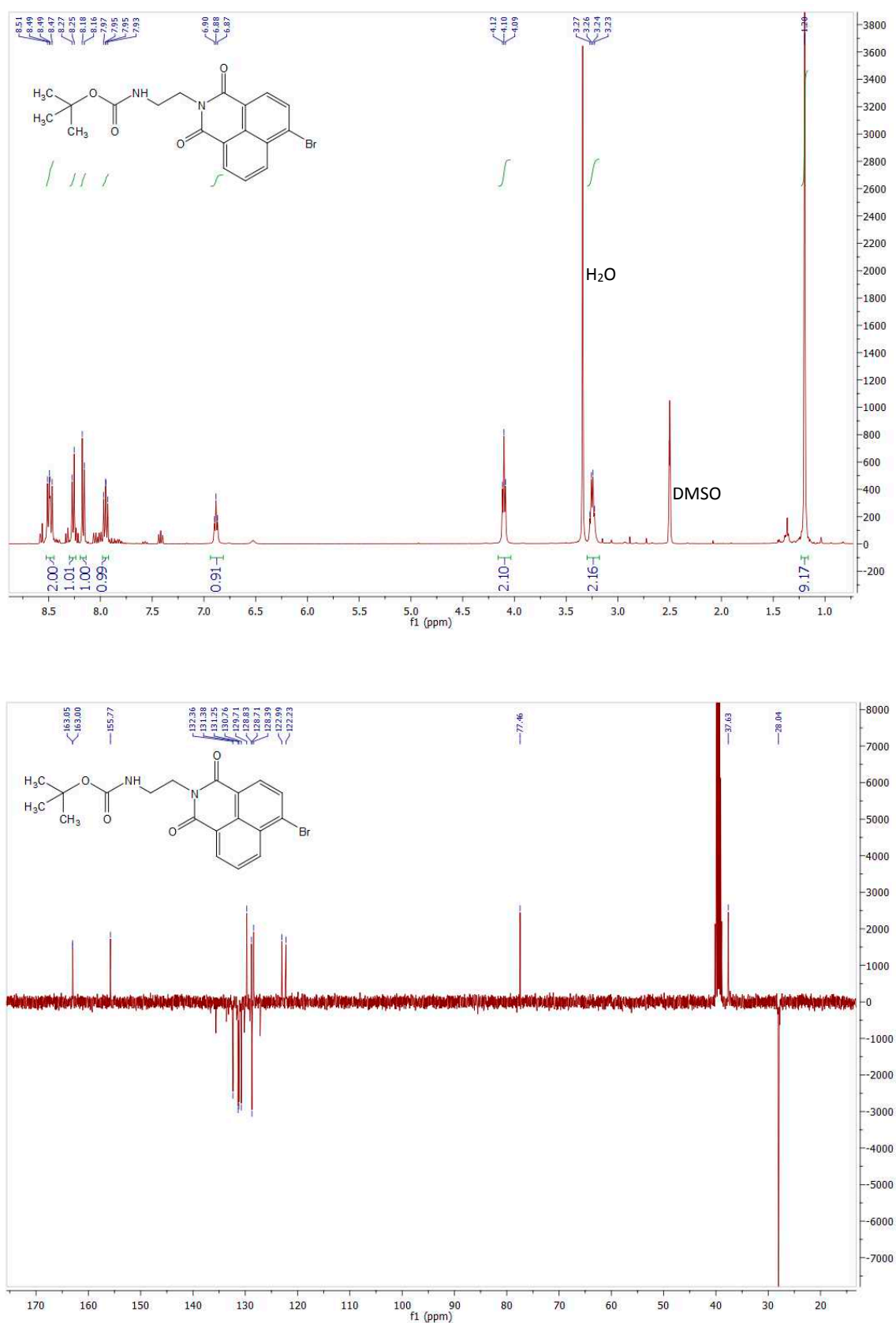
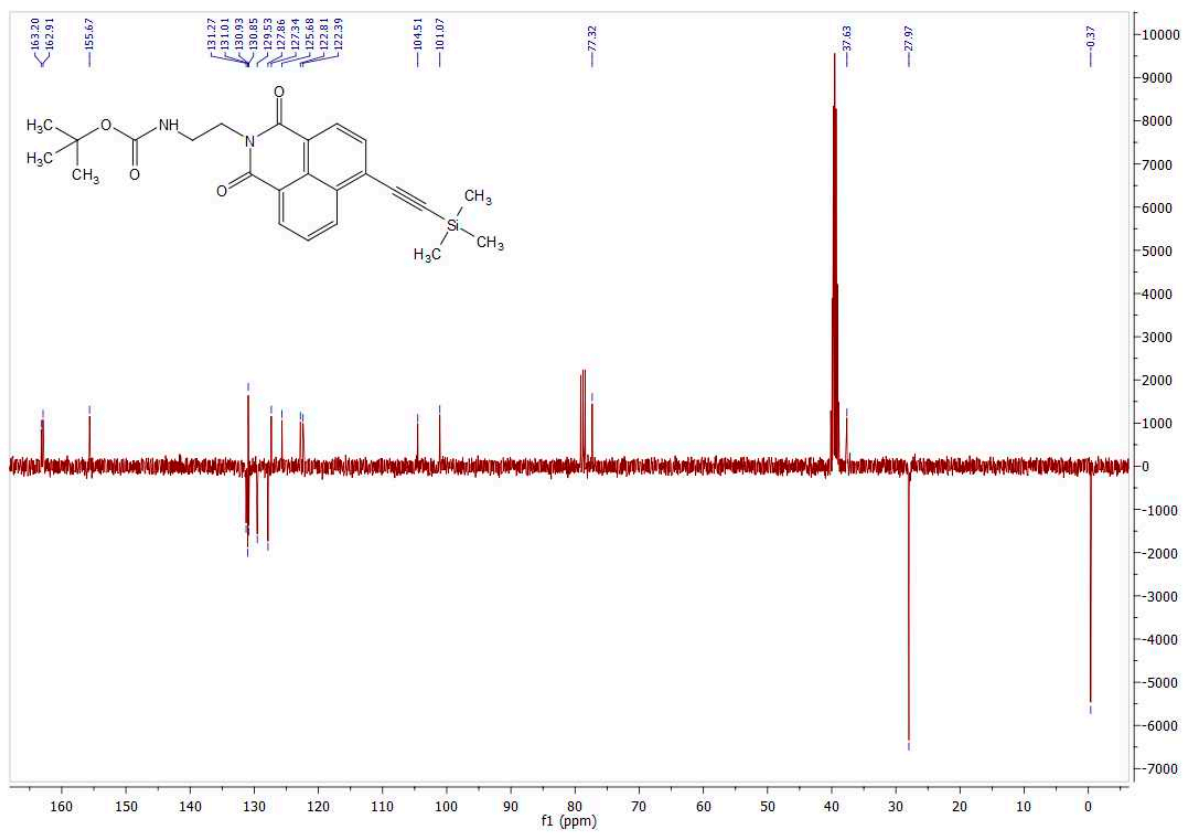
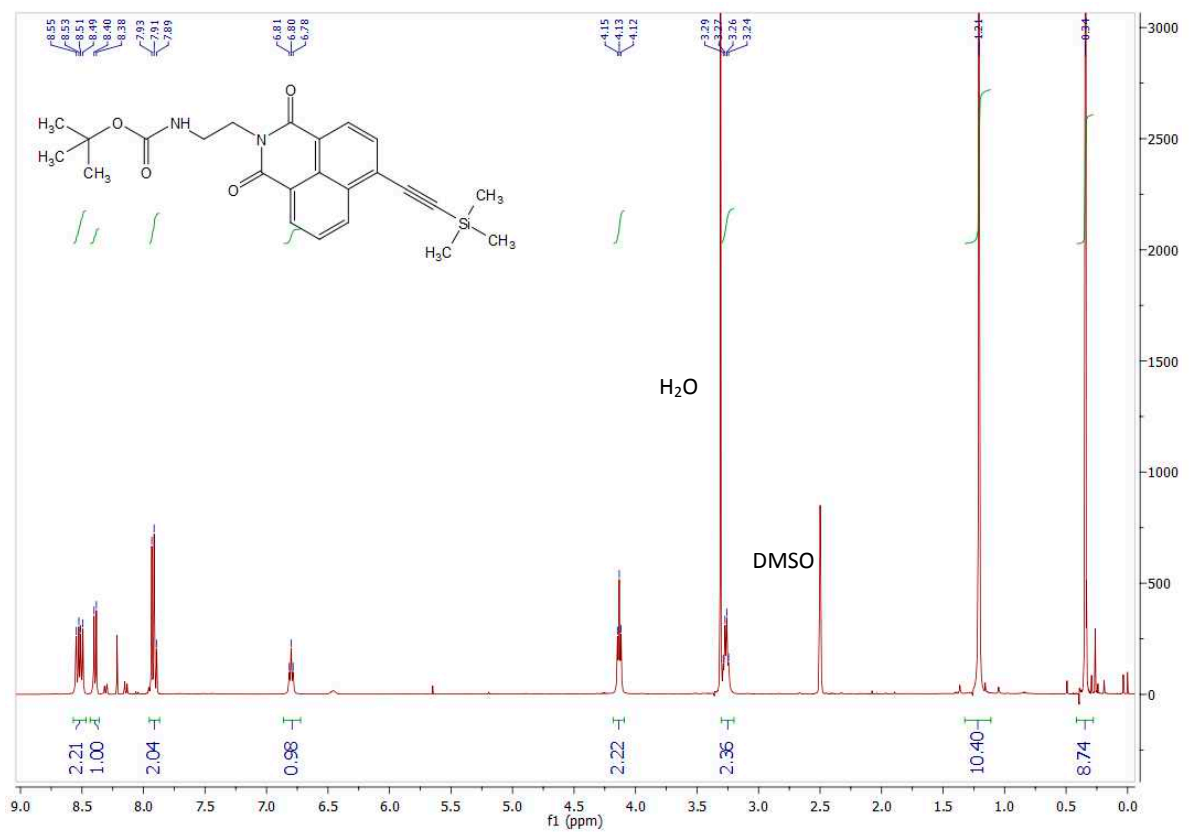
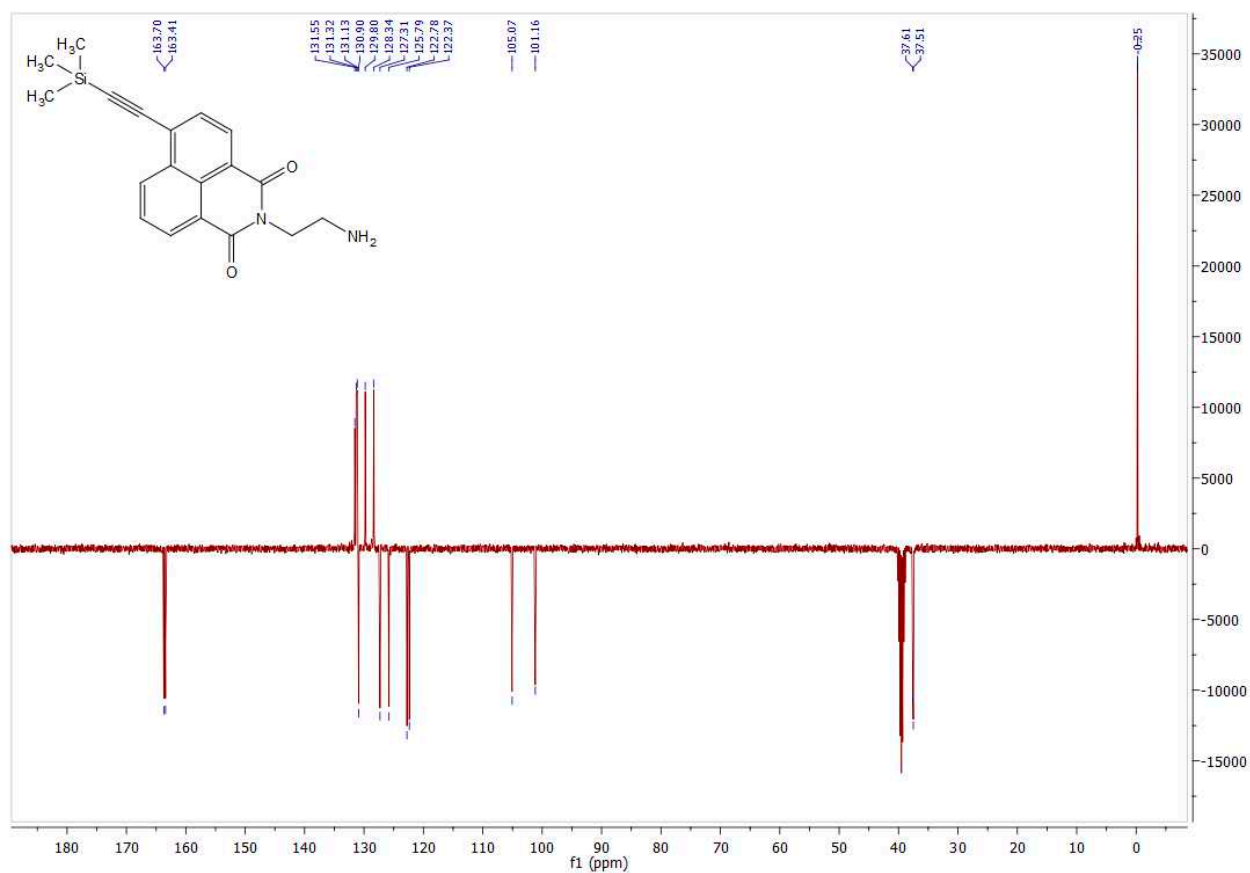
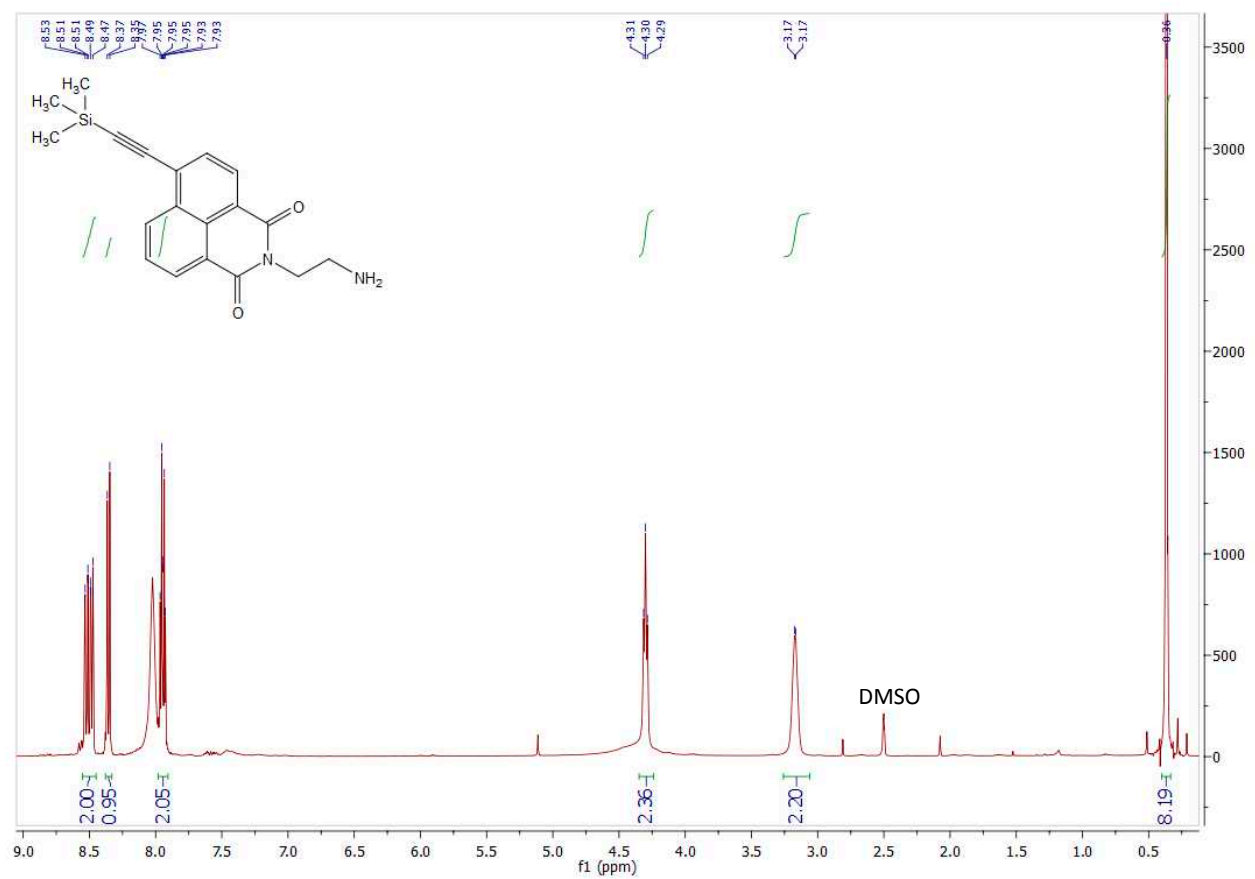


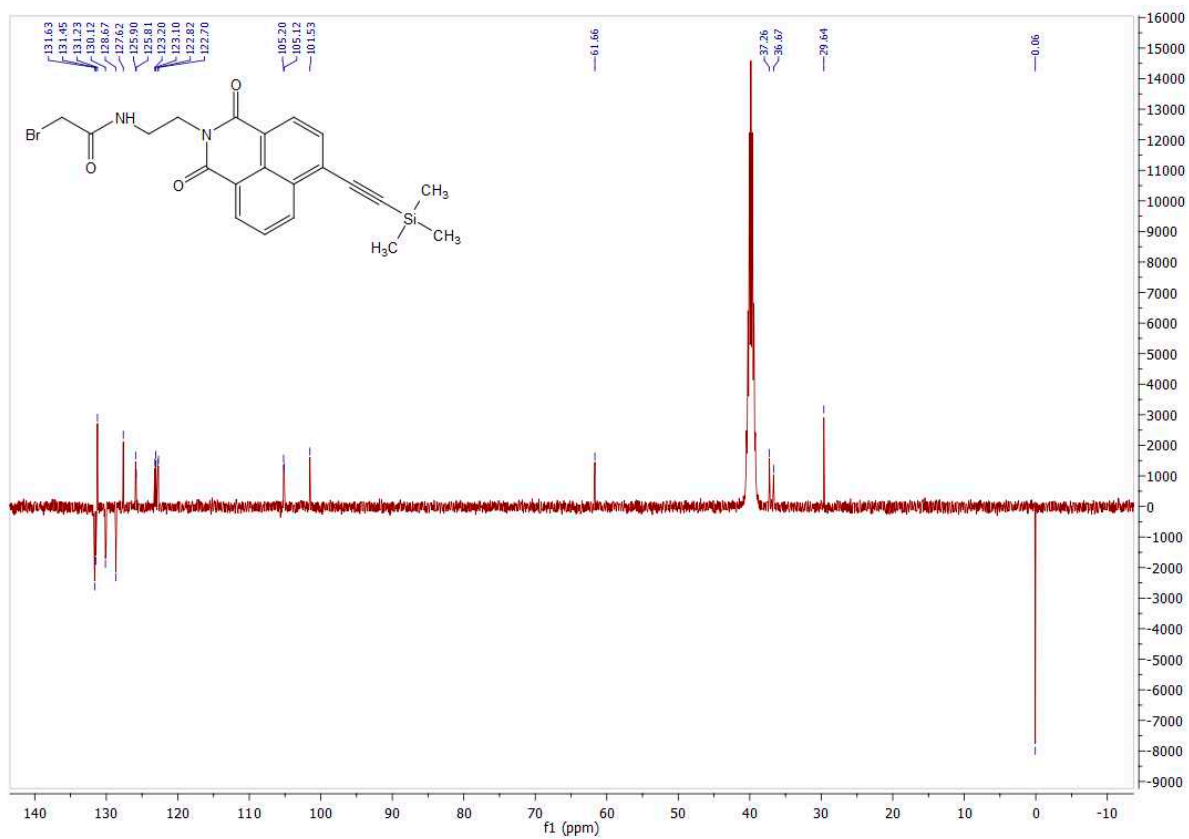
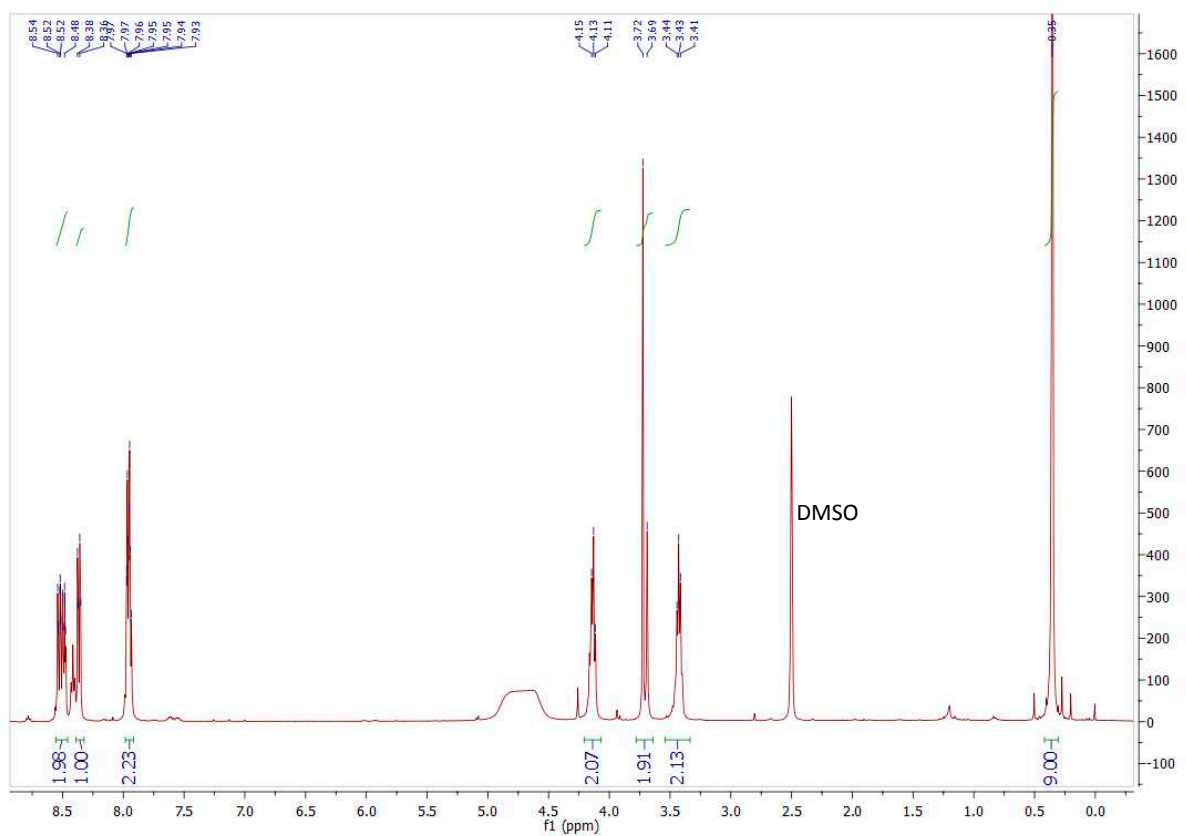
Figure S1.  $^1\text{H}$ - and  $^{13}\text{C}$ -NMR spectra of compound 1 in DMSO- $d_6$ .



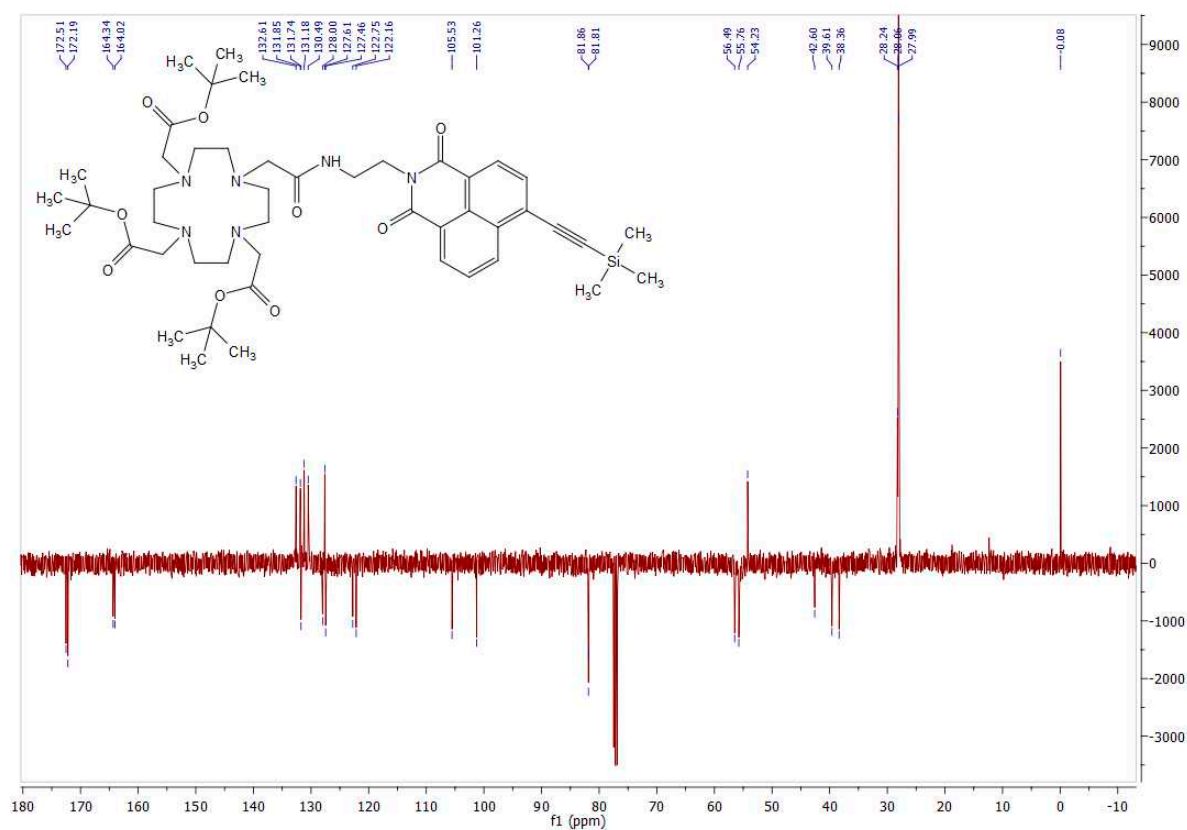
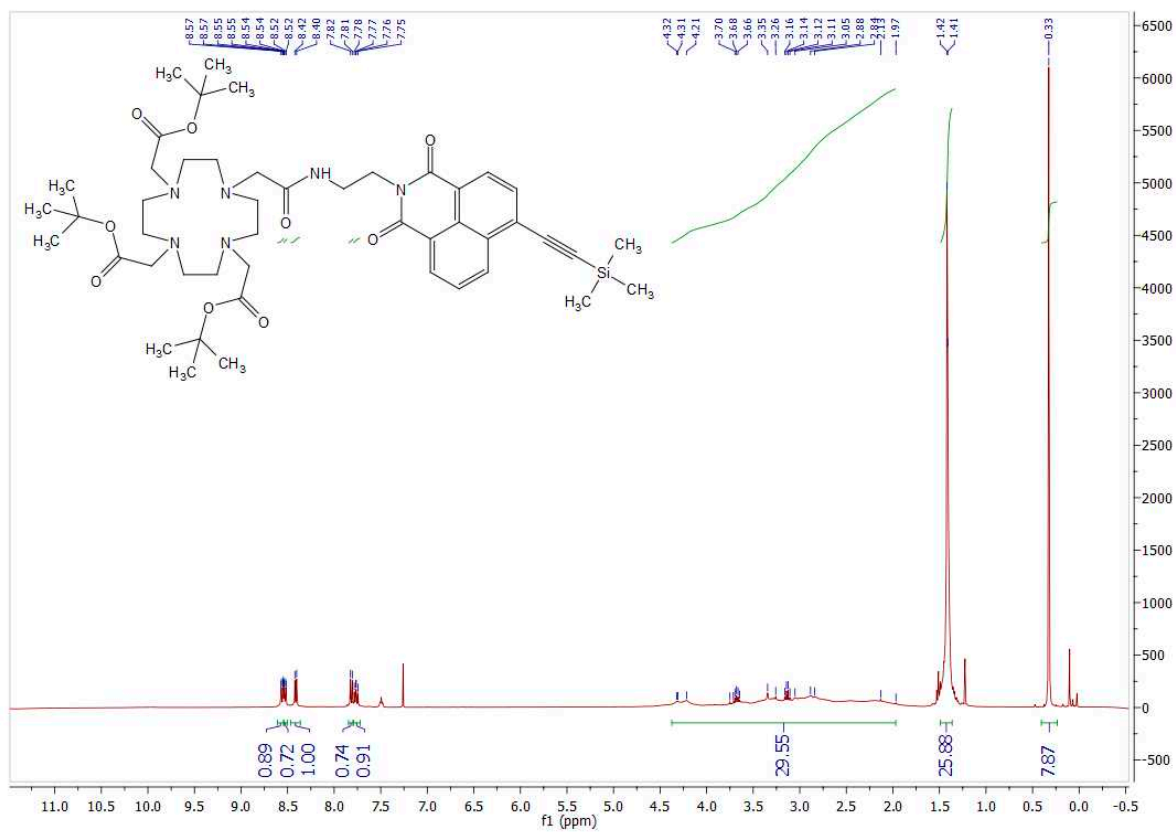
**Figure S2.** <sup>1</sup>H- and <sup>13</sup>C-NMR spectra of compound 2 in DMSO-*d*<sub>6</sub>.



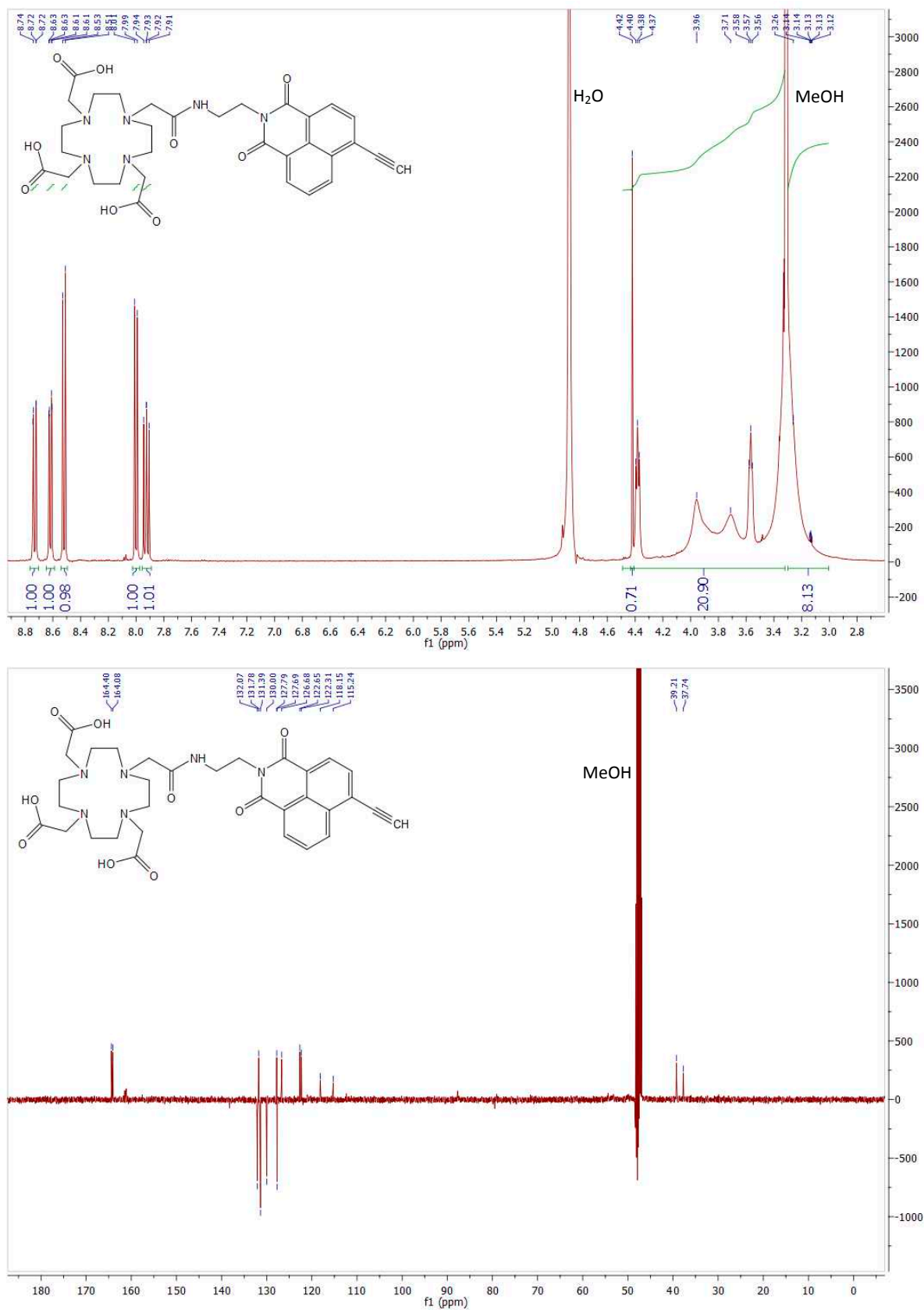
**Figure S3.** <sup>1</sup>H- and <sup>13</sup>C-NMR spectra of compound 3 in DMSO-*d*<sub>6</sub>.



**Figure S4.** <sup>1</sup>H- and <sup>13</sup>C-NMR spectra of compound 4 in DMSO-*d*<sub>6</sub>.



**Figure S5.** <sup>1</sup>H- and <sup>13</sup>C-NMR spectra of compound 5 in CDCl<sub>3</sub>.



**Figure S6.** <sup>1</sup>H- and <sup>13</sup>C-NMR spectra of ligand L in CD<sub>3</sub>OD.

## LC Traces for Final Ligand and Gd(III) Complexes

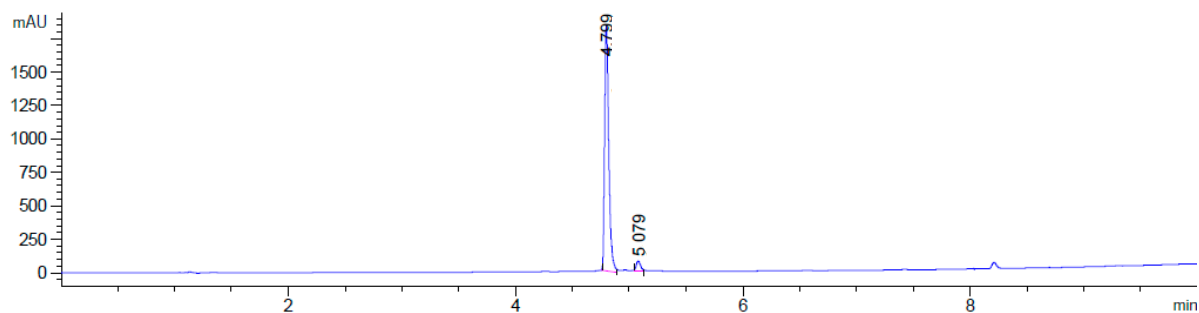


Figure S7. LC trace for ligand L (254nm).

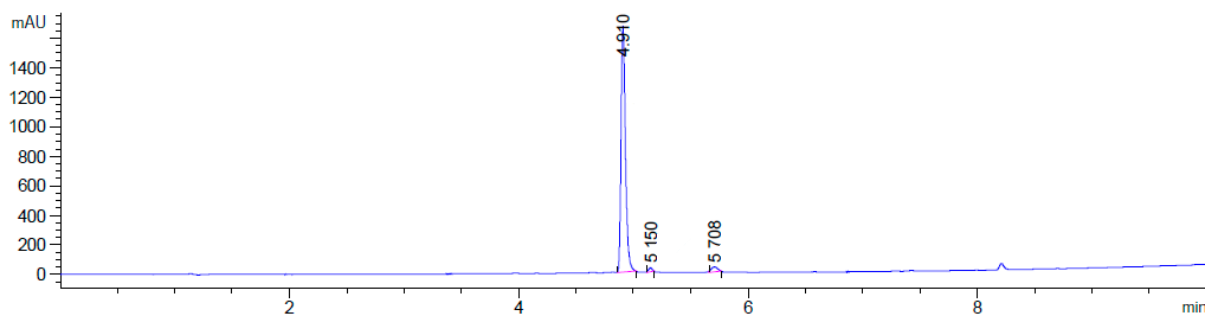


Figure S8. LC trace for Gd-L (254nm).

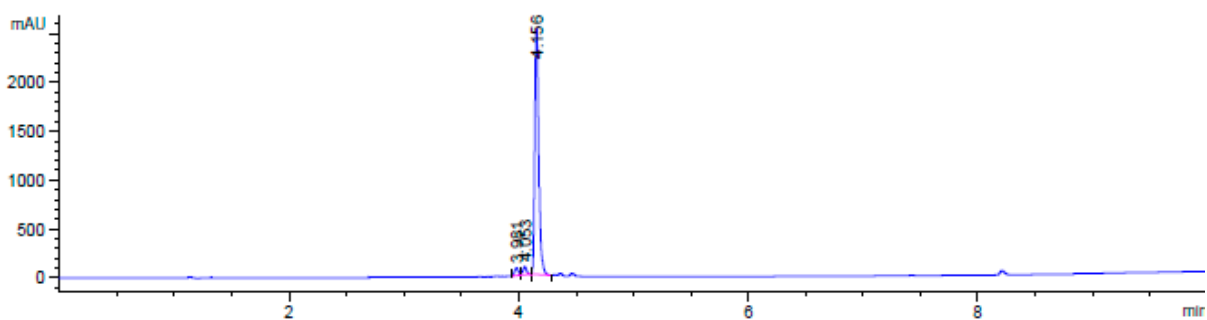
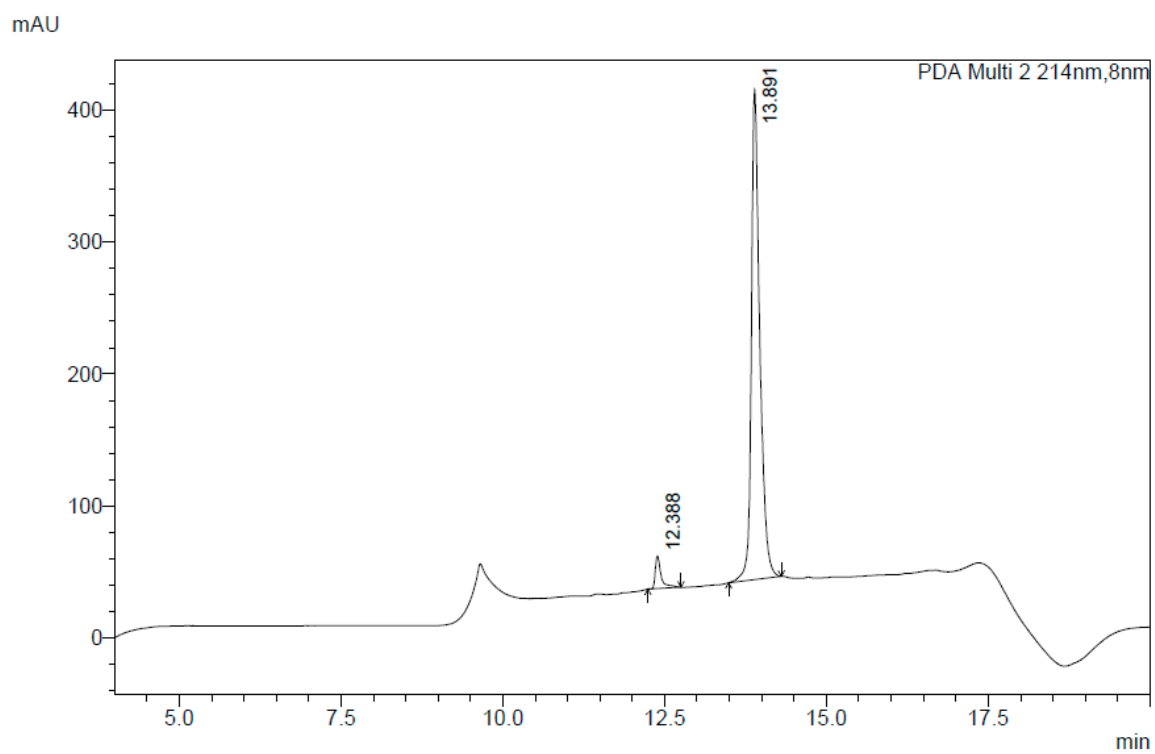


Figure S9. LC trace for "clicked" Gd-L (254nm).



## LC Trace for Peptide Conjugate



**Figure S10.** LC trace for Gd-L-Tat peptide conjugate (214 nm).