



Supporting Information

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SUPPLEMENTARY INFORMATION

Solid Phase Synthesis, Characterization, and Antibacterial Activities of Metallocene Peptide Bioconjugates

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1. HPLC

Reverse-phase HPLC was performed on a Varian ProStar instrument equipped with a 410 autosampler, and a 330 PDA detector. The compounds were purified on a semi-preparative Varian C18 column (60Å / 8 µm, 250 × 10.0 mm), while an analytical Varian C18 column (60 Å / 8 µm, 250 × 4.60 mm) was used for analyses. The eluents contained 0.1% (v/v) trifluoroacetic acid (Tables 1, 2). The purities of all HPLC traces were greater than 97%.

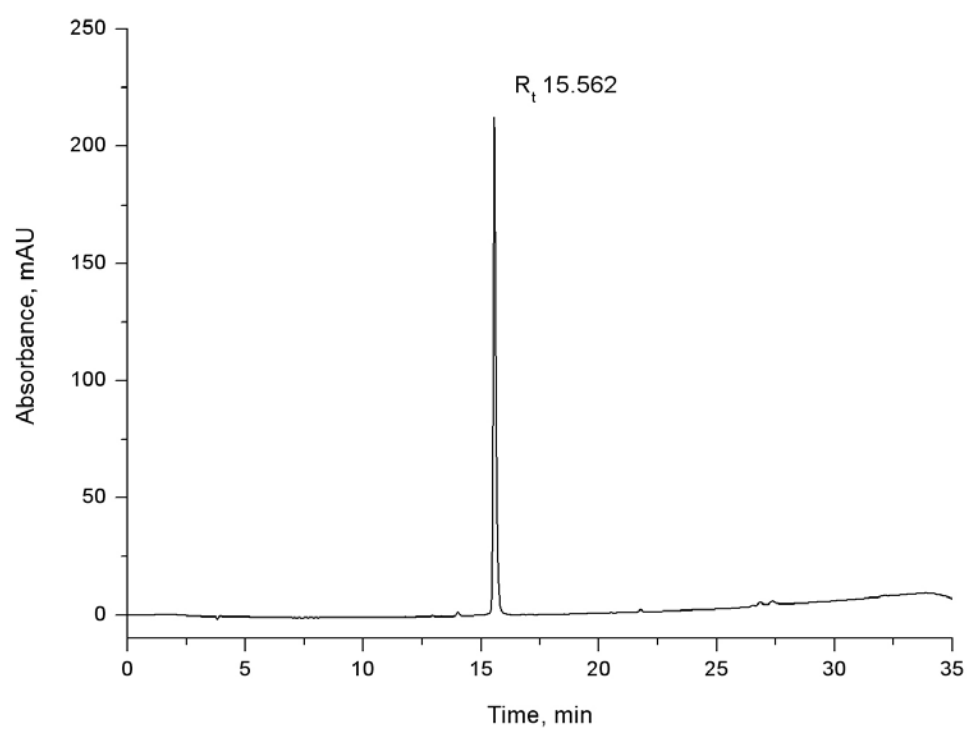
Table 1. Solvent delivery method for analytical HPLC

Time (min)	% H ₂ O	% MeCN	Flow rate (mL min ⁻¹)
0	95	5	1
30	5	95	1
35	95	5	1

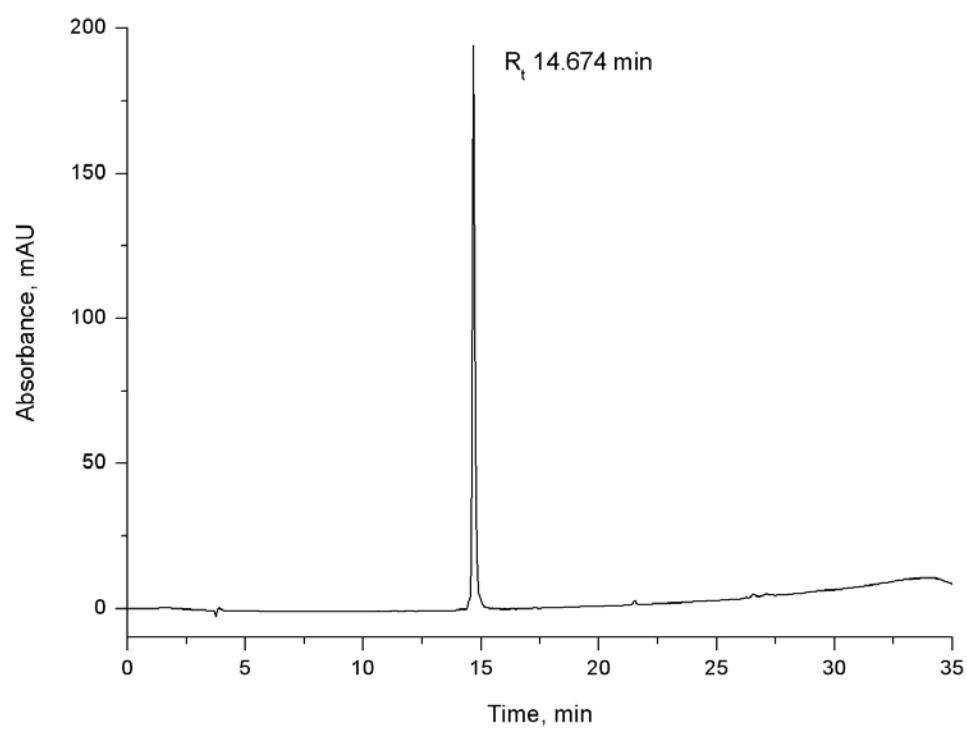
Table 2. General Solvent delivery method for preparative HPLC

Time (min)	% H ₂ O	% MeCN	Flow rate (mL min ⁻¹)
0	90	10	5
50	50	50	5
55	50	100	5
60	90	10	5

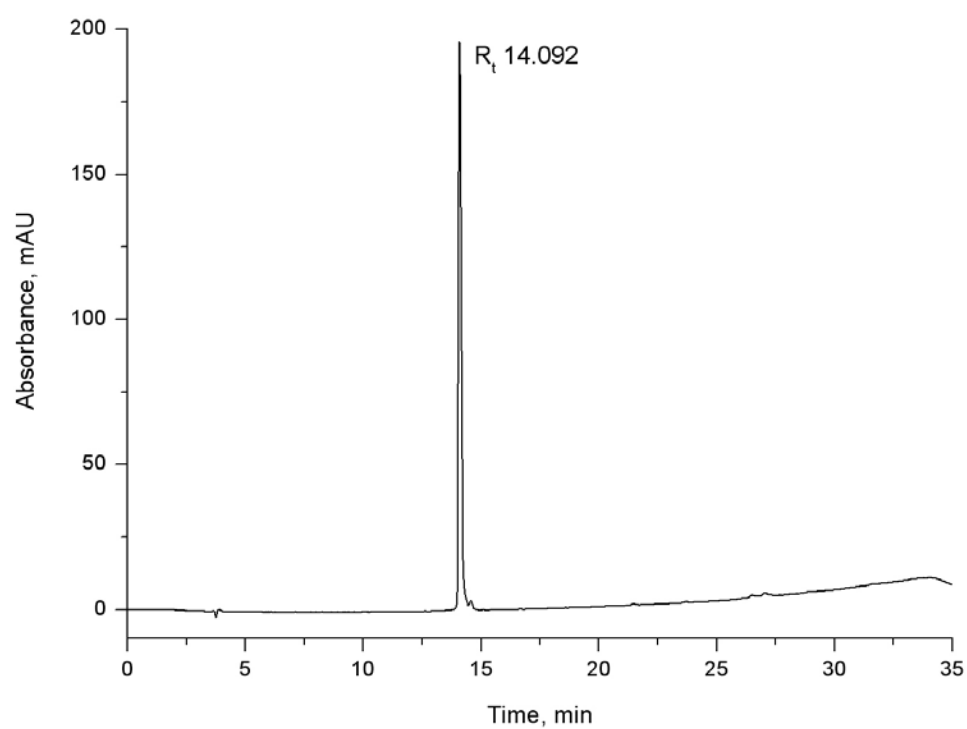
Compound **1** HPLC Analytical trace at 254 nm



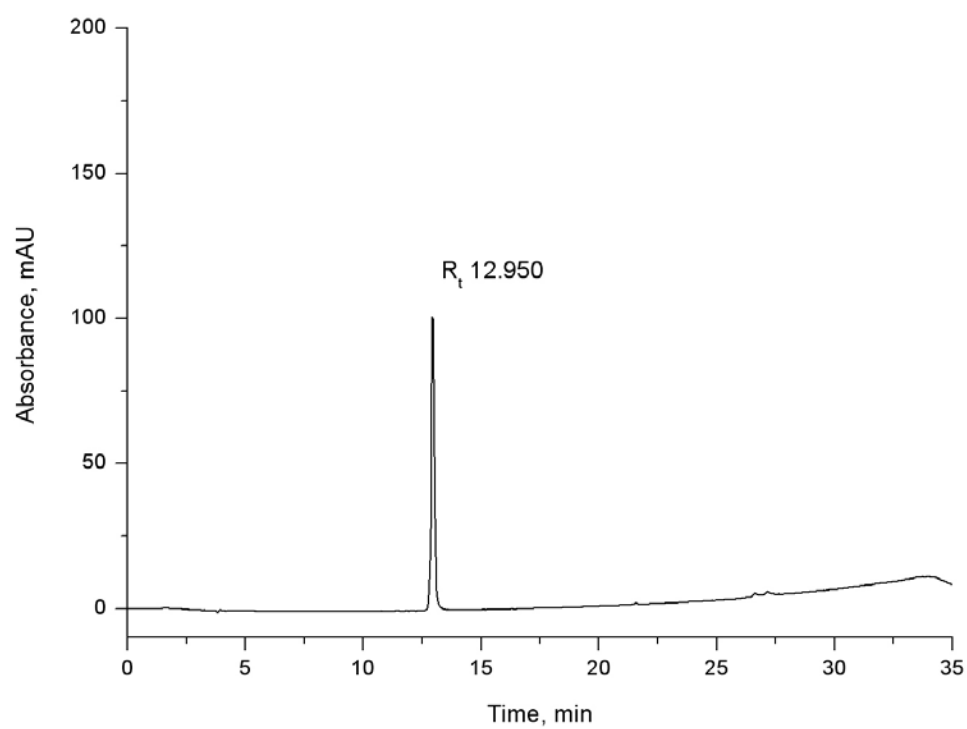
Compound **4** HPLC Analytical trace at 254 nm



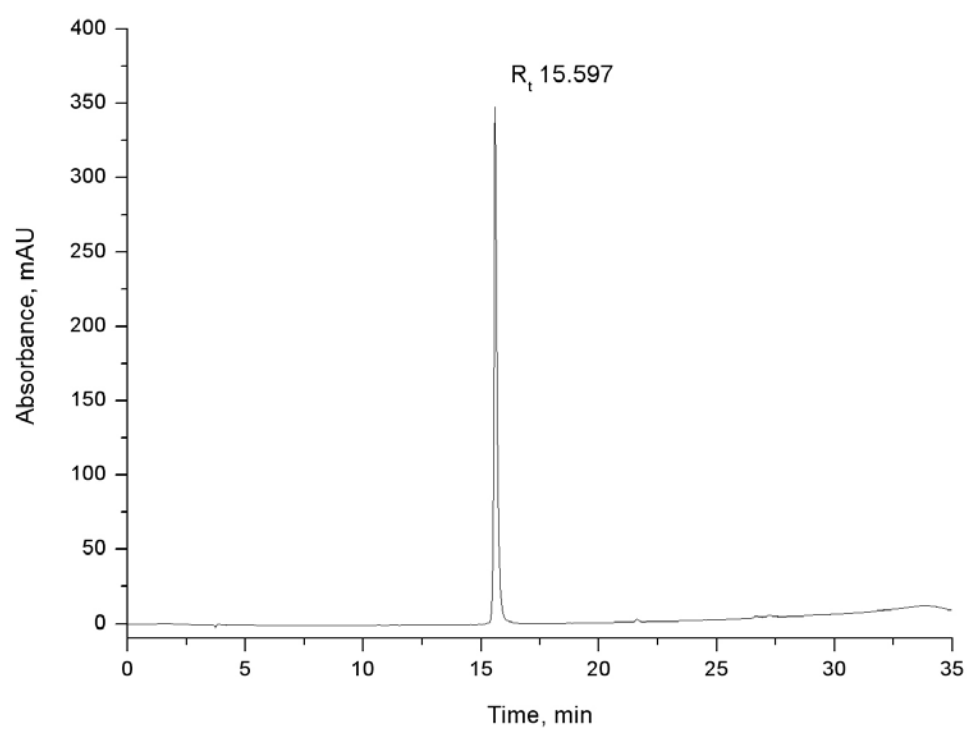
Compound **5** HPLC Analytical trace at 254 nm



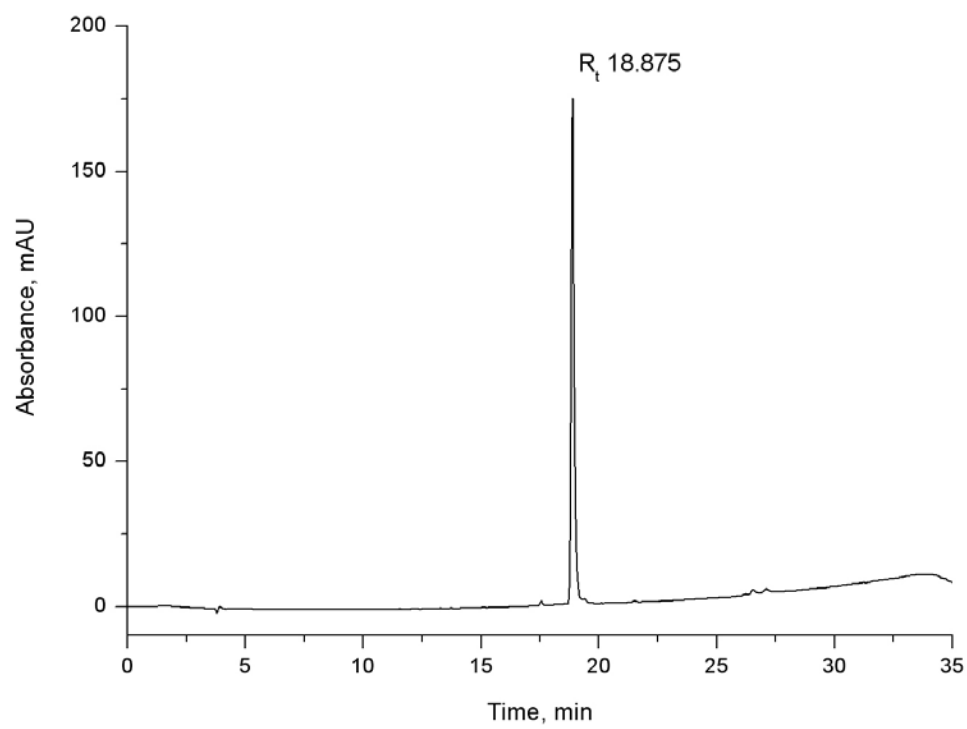
Compound **2** HPLC Analytical trace at 254 nm



Compound **3** HPLC Analytical trace at 254 nm



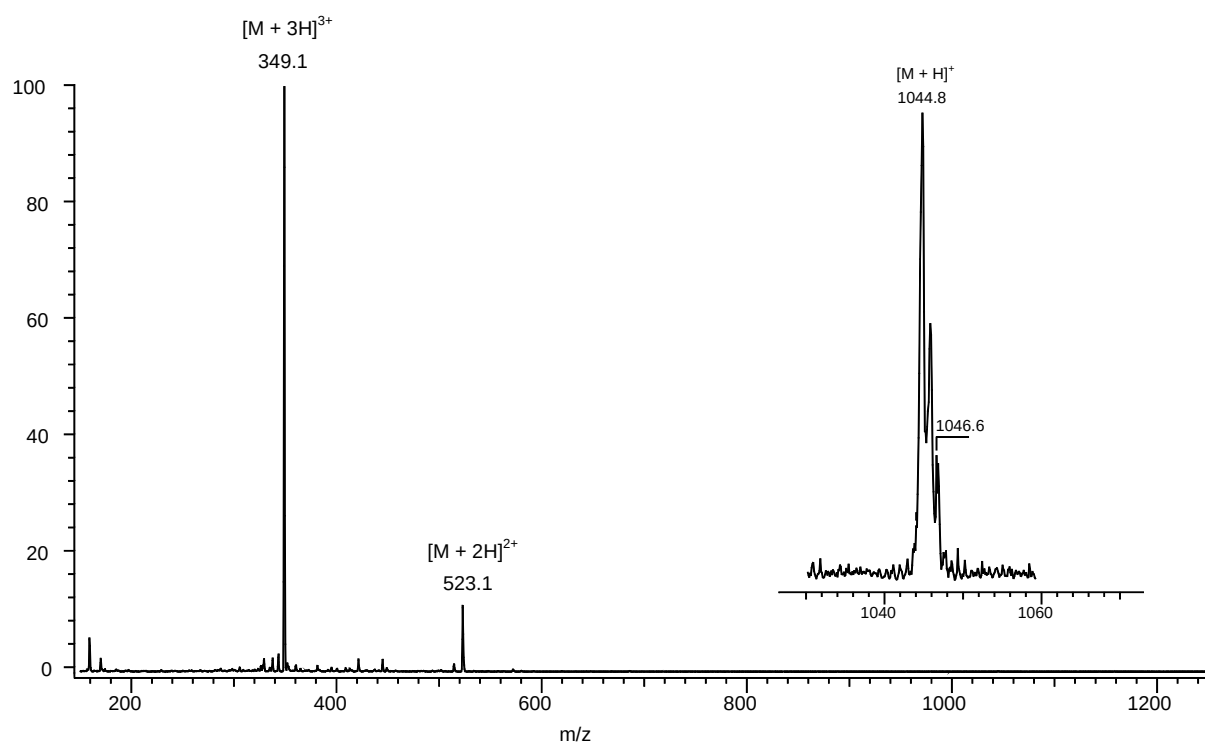
Compound **6** HPLC Analytical trace at 254 nm



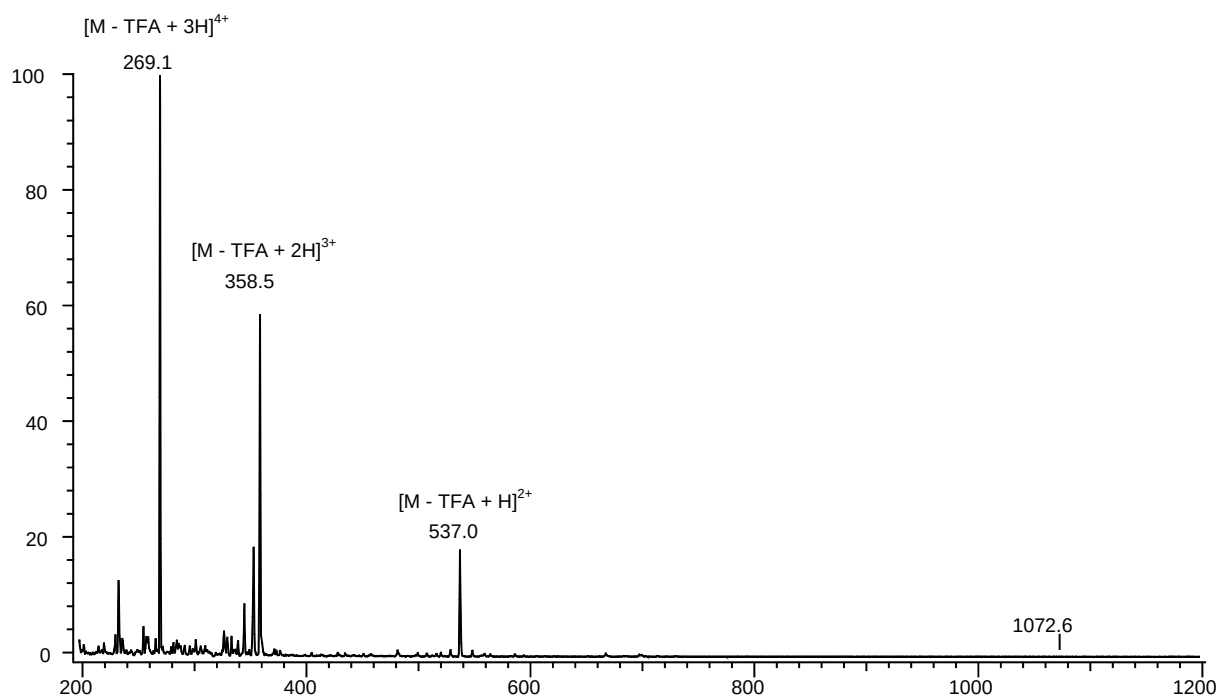
2. MS

Mass spectra were measured by positive ion electrospray mass spectrometry on a Finnigan TSQ 700 spectrometer (4.5 kV, 40 psi, 130 – 200°C). Note: TFA = CF_3CO_2

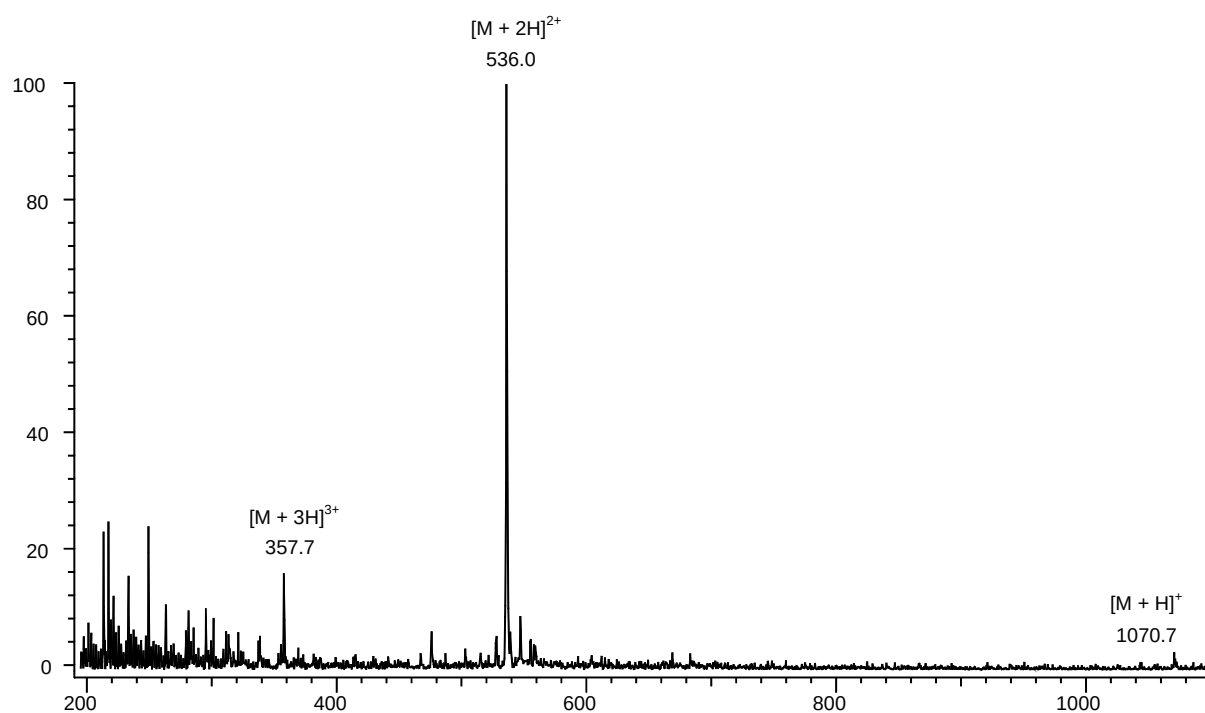
Compound **1** ESI-MS (Exact mass = 1043.57)



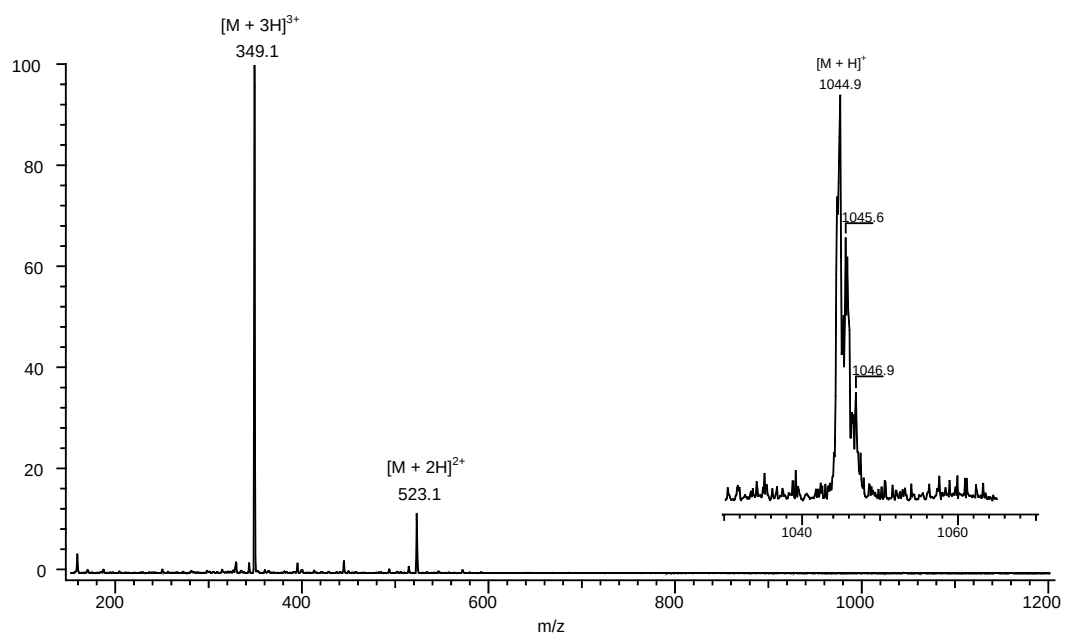
Compound **2** ESI-MS (Exact mass = 1185.46)



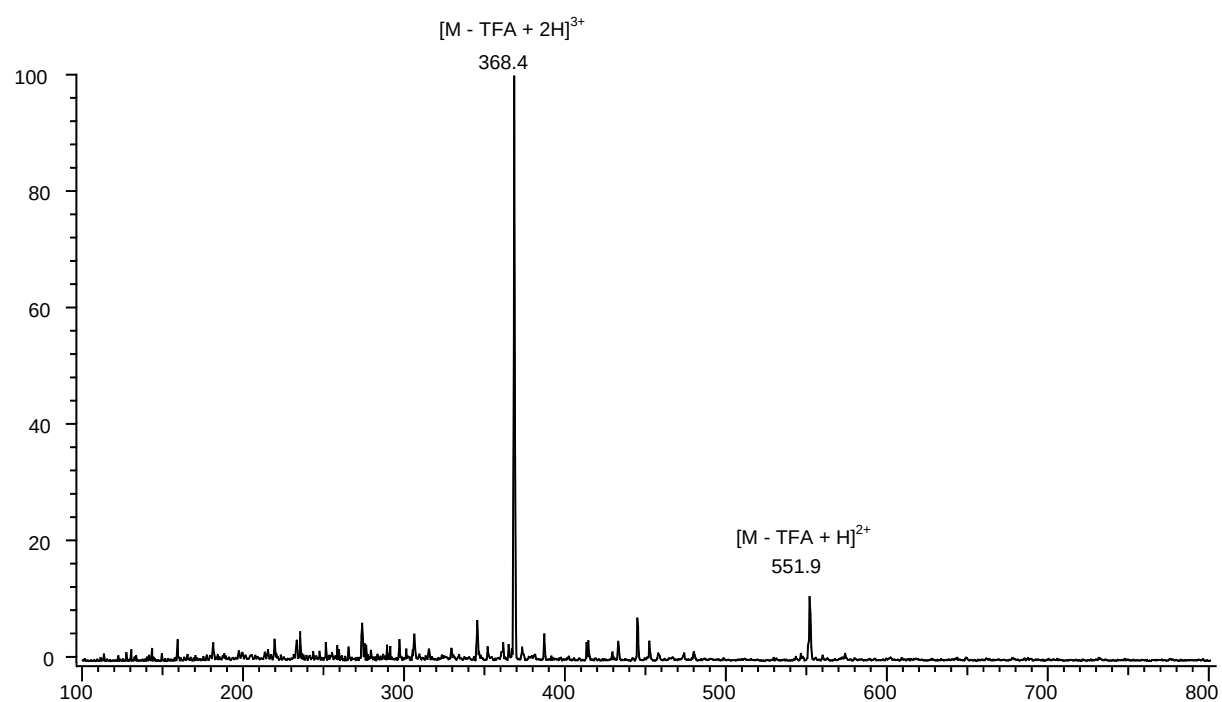
Compound **3** ESI-MS (Exact mass = 1069.48)



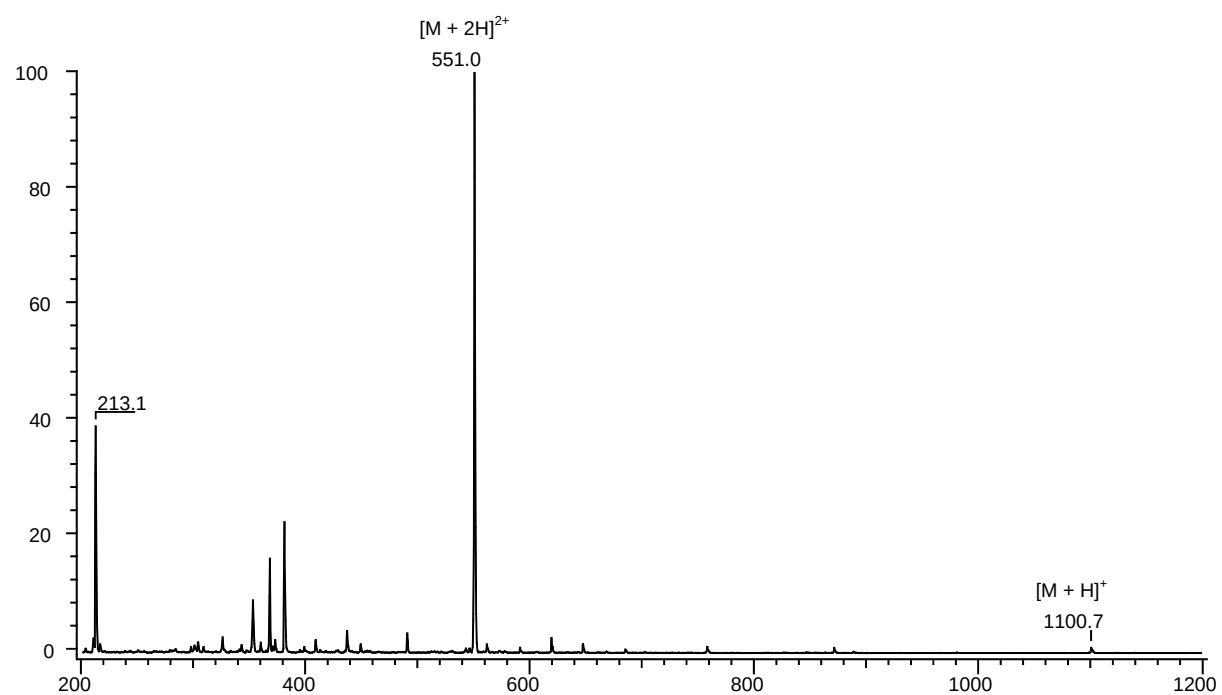
Compound **4** ESI-MS (Exact mass = 1043.57)



Compound **5** ESI-MS (Exact mass = 1215.44)



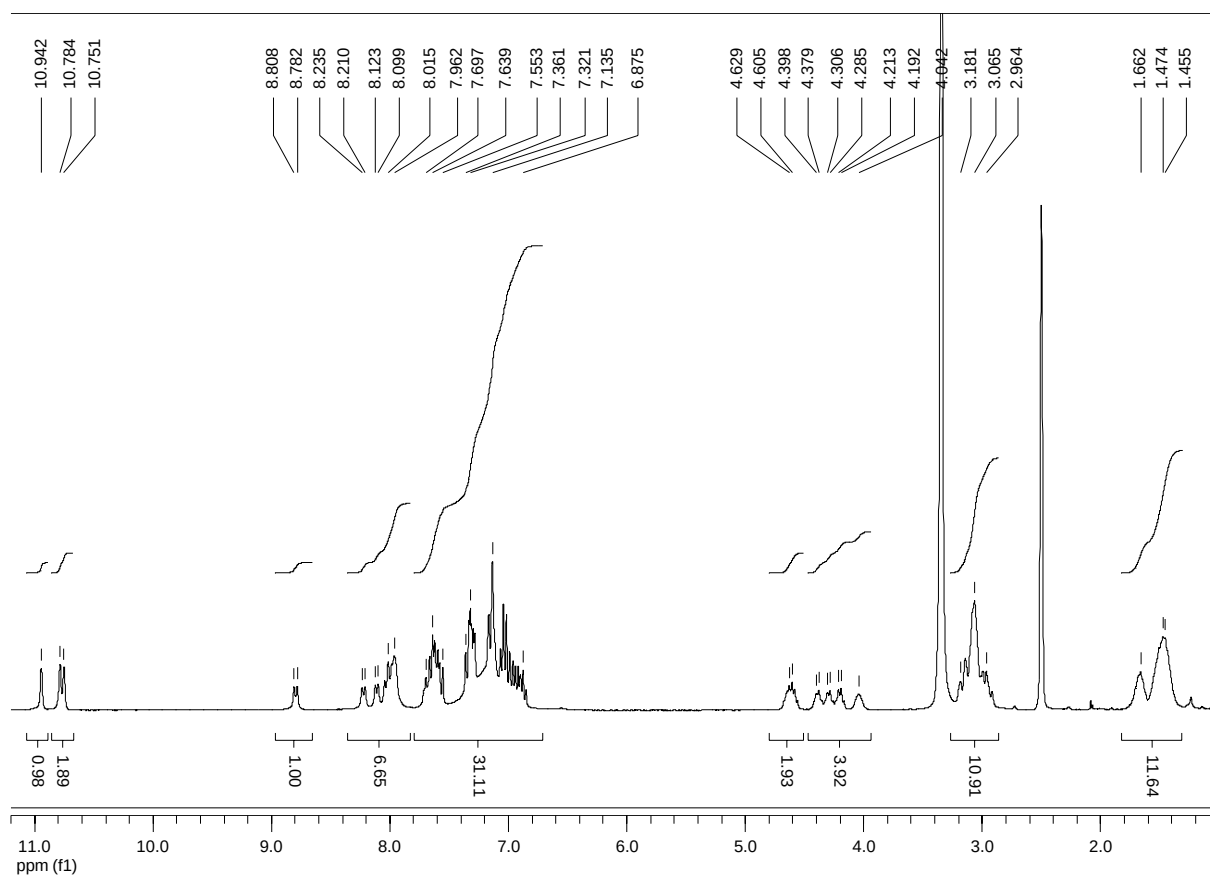
Compound **6** ESI-MS (Exact mass = 1099.46)



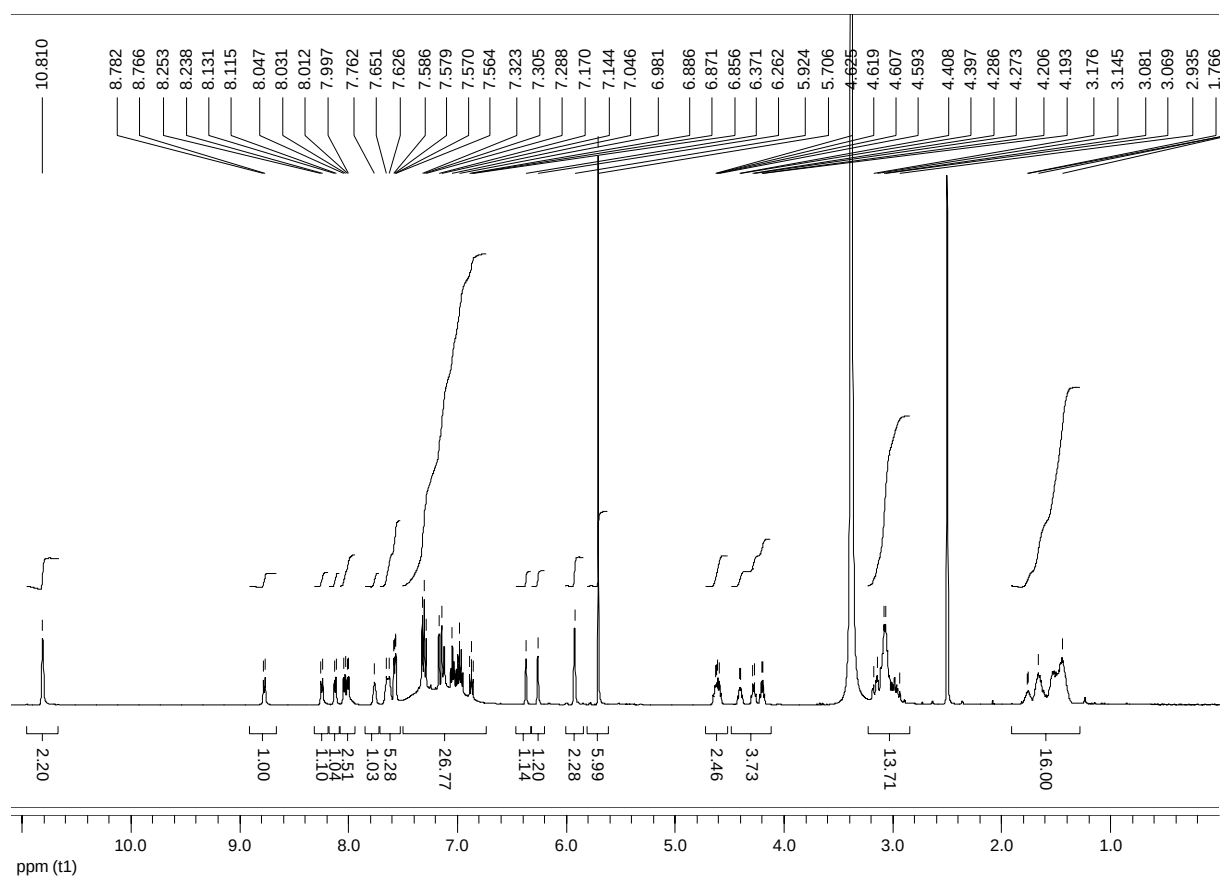
3. NMR

NMR spectra were recorded on a Bruker DRX 300 spectrometer. The ^1H chemical shifts were referenced to residual solvent ($\text{D}_6[\text{DMSO}]$) protons.

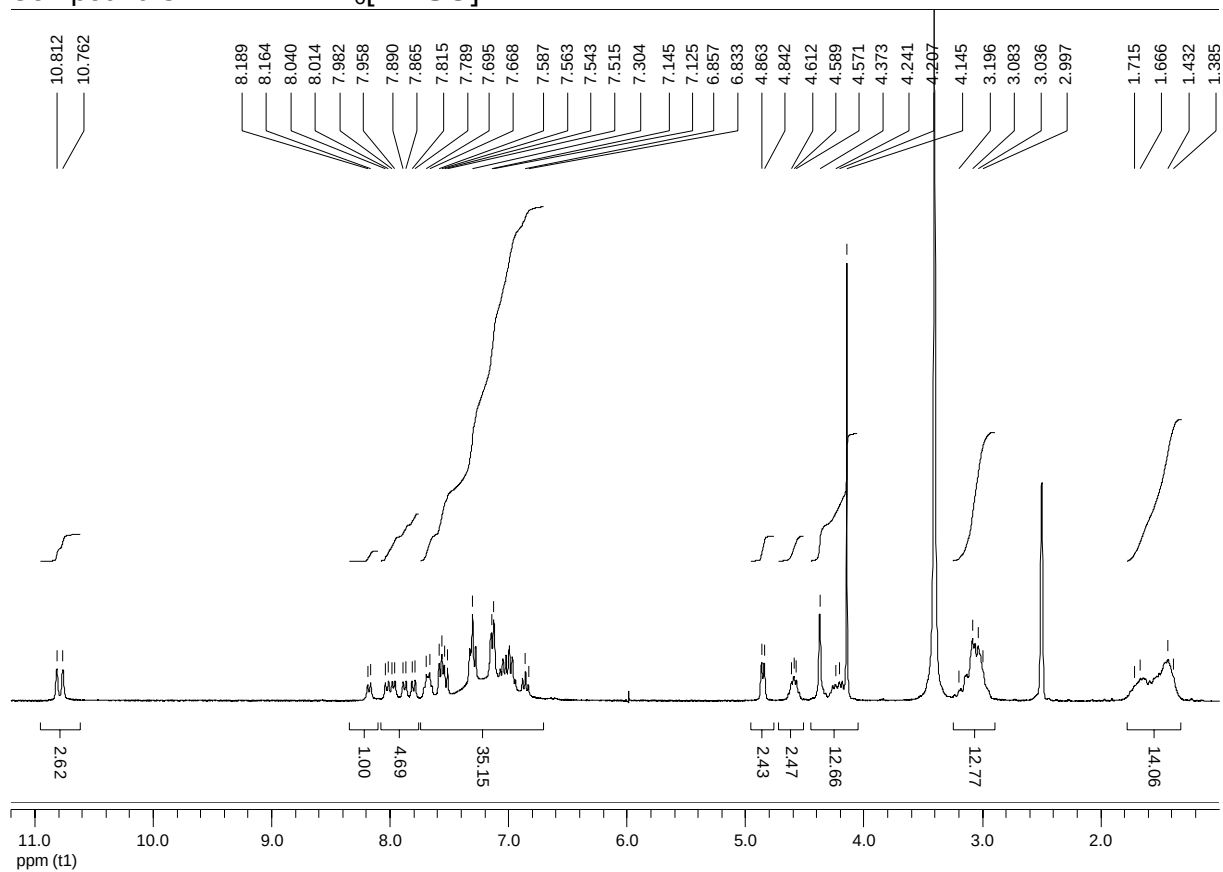
Compound **1** ^1H NMR in $\text{D}_6[\text{DMSO}]$



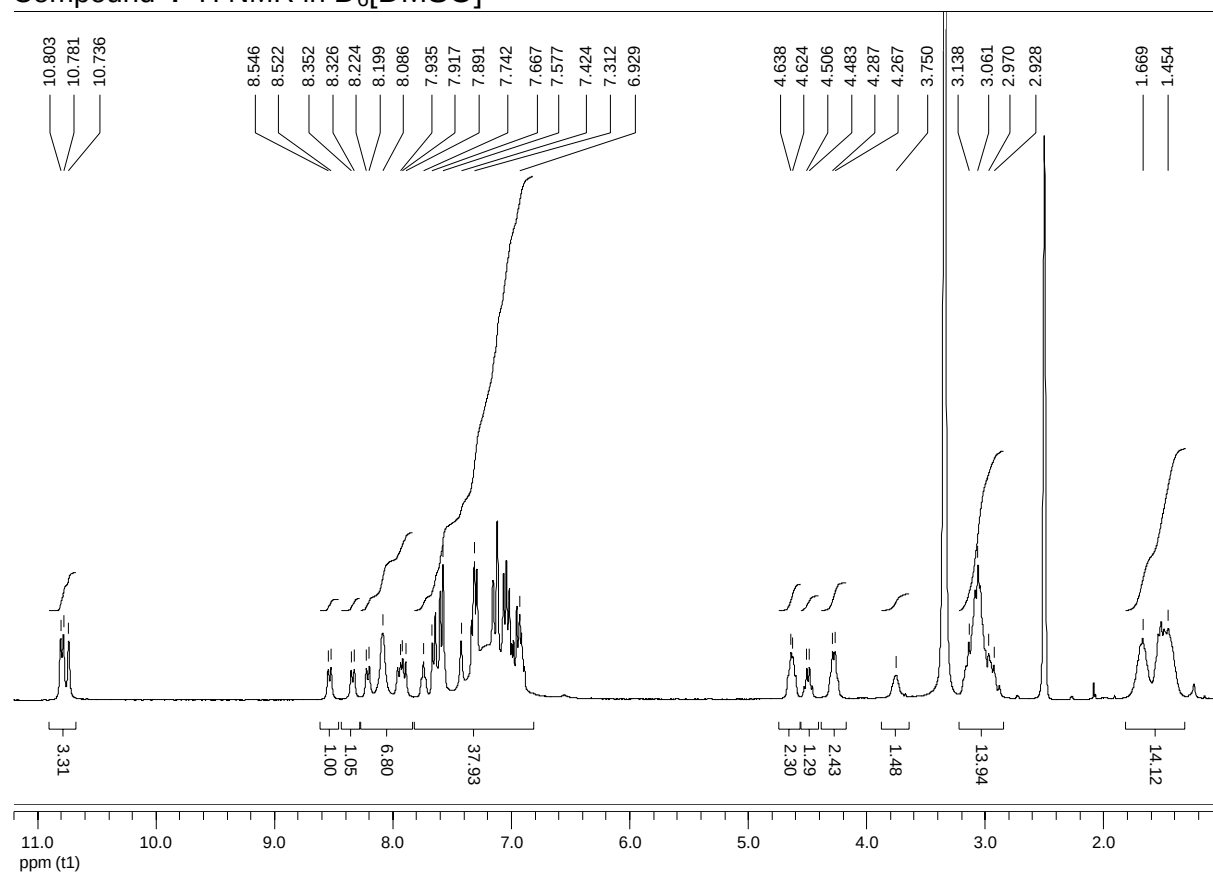
Compound **2** ^1H NMR in $\text{D}_6[\text{DMSO}]$



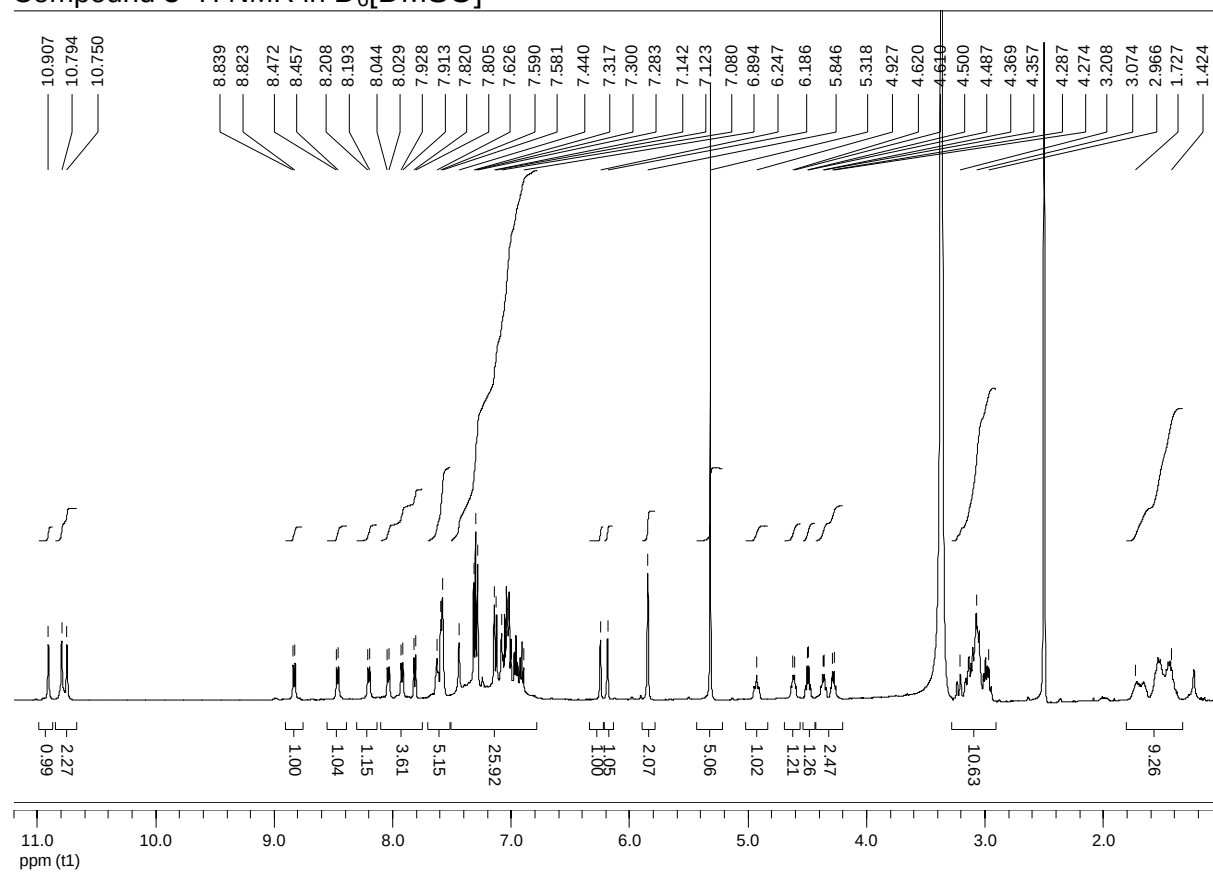
Compound **3** ^1H NMR in $\text{D}_6[\text{DMSO}]$



Compound **4** ^1H NMR in $\text{D}_6[\text{DMSO}]$



Compound **5** ^1H NMR in $\text{D}_6[\text{DMSO}]$



Compound **6** ^1H NMR in $\text{D}_6[\text{DMSO}]$

