

## Supplementary Material

### Synthesis, characterization and biological evaluation of zinc and copper azasterol complexes against *Sporothrix brasiliensis*

Rodrigo M. S. Justo,<sup>a</sup> Luana Pereira Borba-Santos,<sup>b</sup> Youssef Bacila Sade,<sup>c</sup> Frederico Henrique C. Ferreira,<sup>d</sup> Nathália M. P. Rosa,<sup>d</sup> Luiz Antônio S. Costa,<sup>d</sup> Gonzalo Visbal,<sup>\*c</sup> Sonia Rozental,<sup>b</sup> Maribel Navarro<sup>\*a</sup>

---

<sup>a.</sup> *Universidade Federal de Juiz de Fora, Departamento de Química, Rua José Lourenço Kelmer S/N, 36060-900 Juiz De Fora, MG, Brazil.*

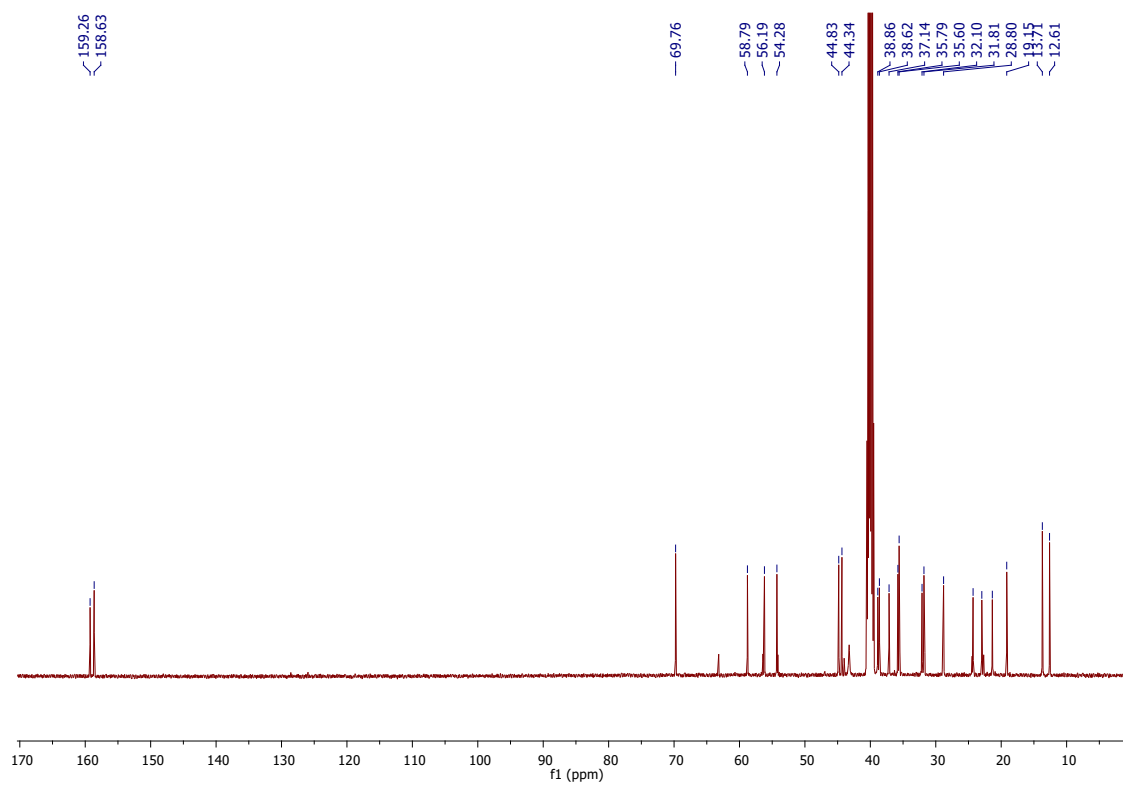
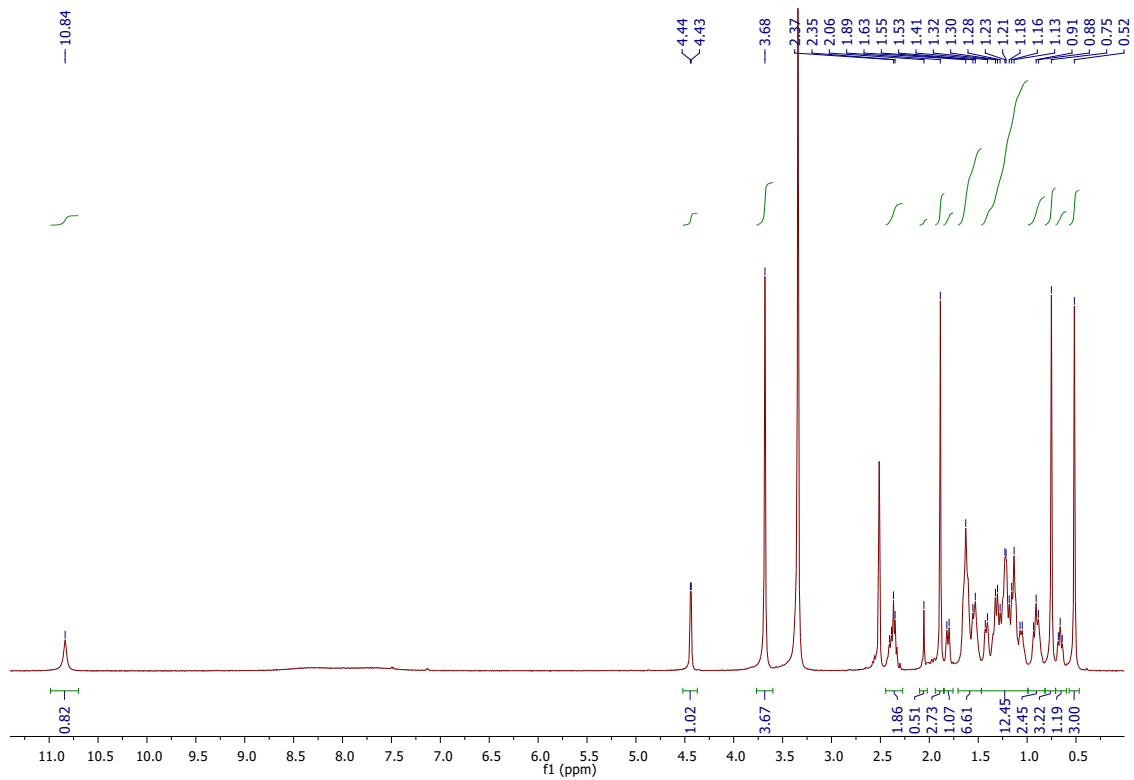
<sup>b.</sup> *Laboratório de Biologia celular de Fungos, Instituto de Biofísica Carlos Chagas Filho, Universidade Federal do Rio de Janeiro, Rio de Janeiro, RJ, Brazil.*

<sup>c.</sup> *Instituto Nacional de Metrologia, Qualidade e Tecnologia (INMETRO), Rio de Janeiro, Brazil*

<sup>d.</sup> *NEQC – Núcleo de Estudos em Química Computacional, Departamento de Química, ICE, Universidade Federal de Juiz de Fora, Juiz de Fora, MG, Brazil.*

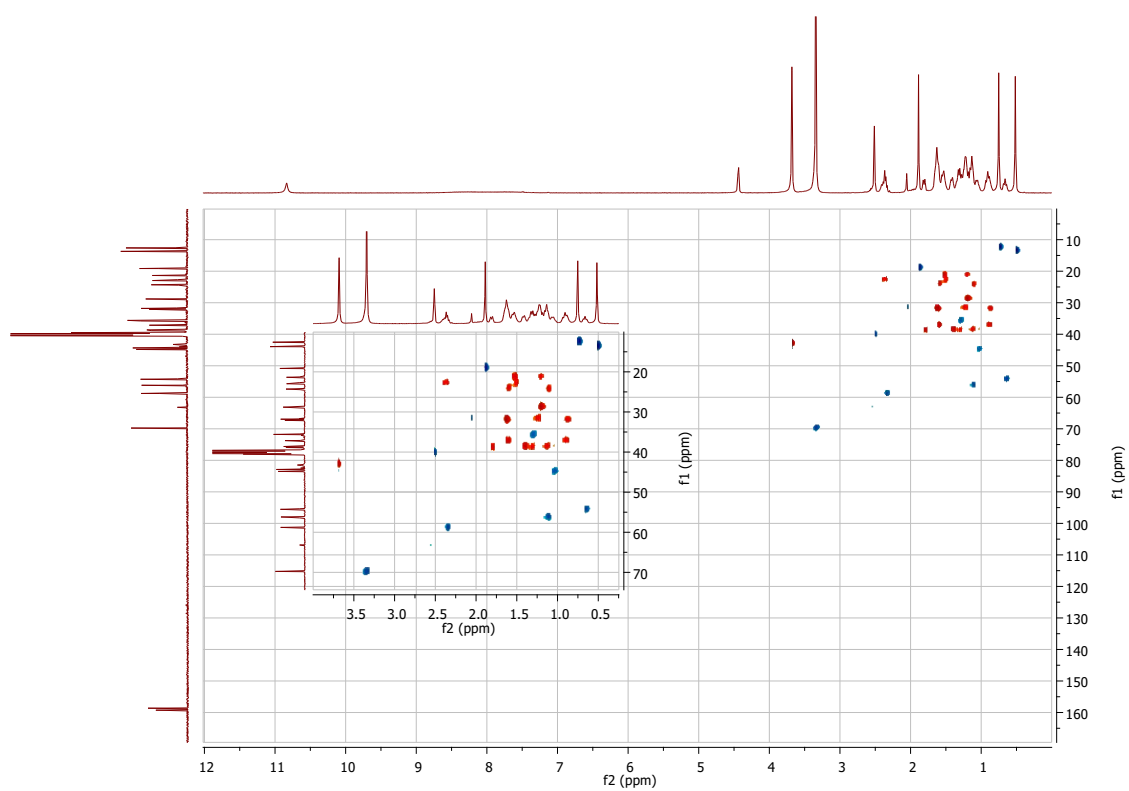
---

# NMR Data

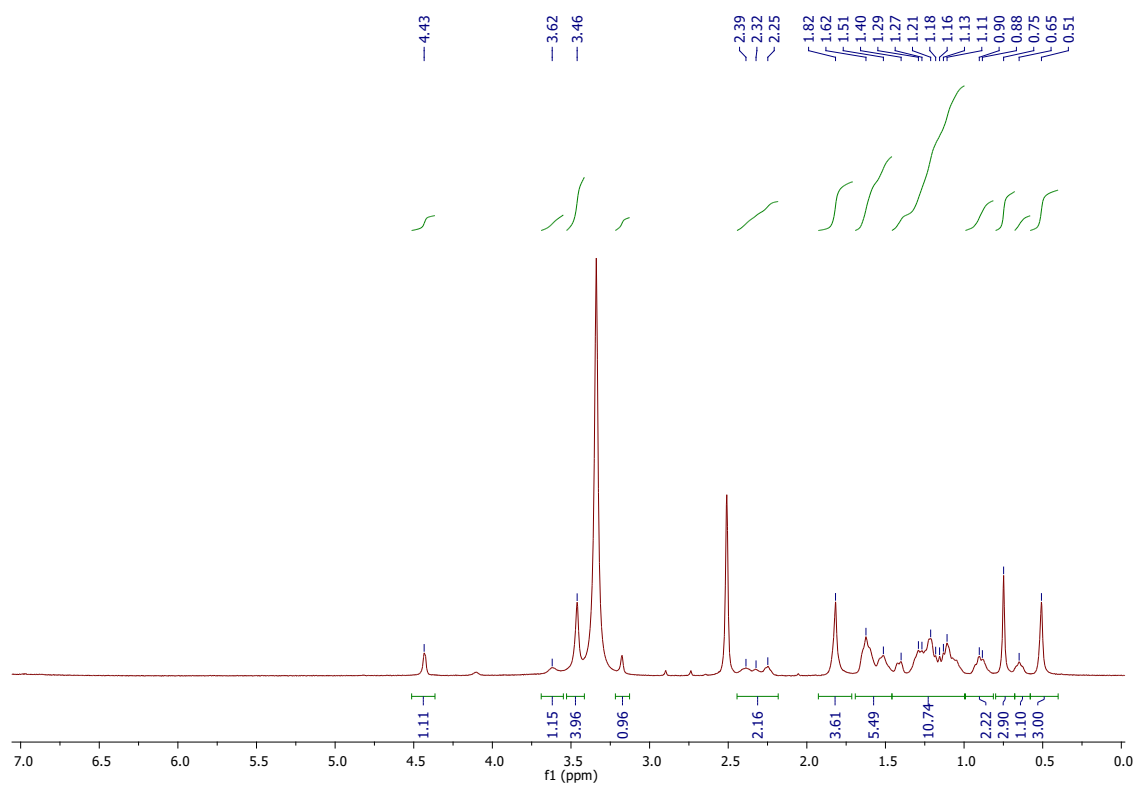


**Figure S1**  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ) spectrum of the free ligand H1.

**Figure S2**  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ) spectrum of the free ligand H1.



**Figure S3** 2D HSQC NMR spectra of the free ligand H1.



**Figure S4**  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ) spectrum of compound **1**.

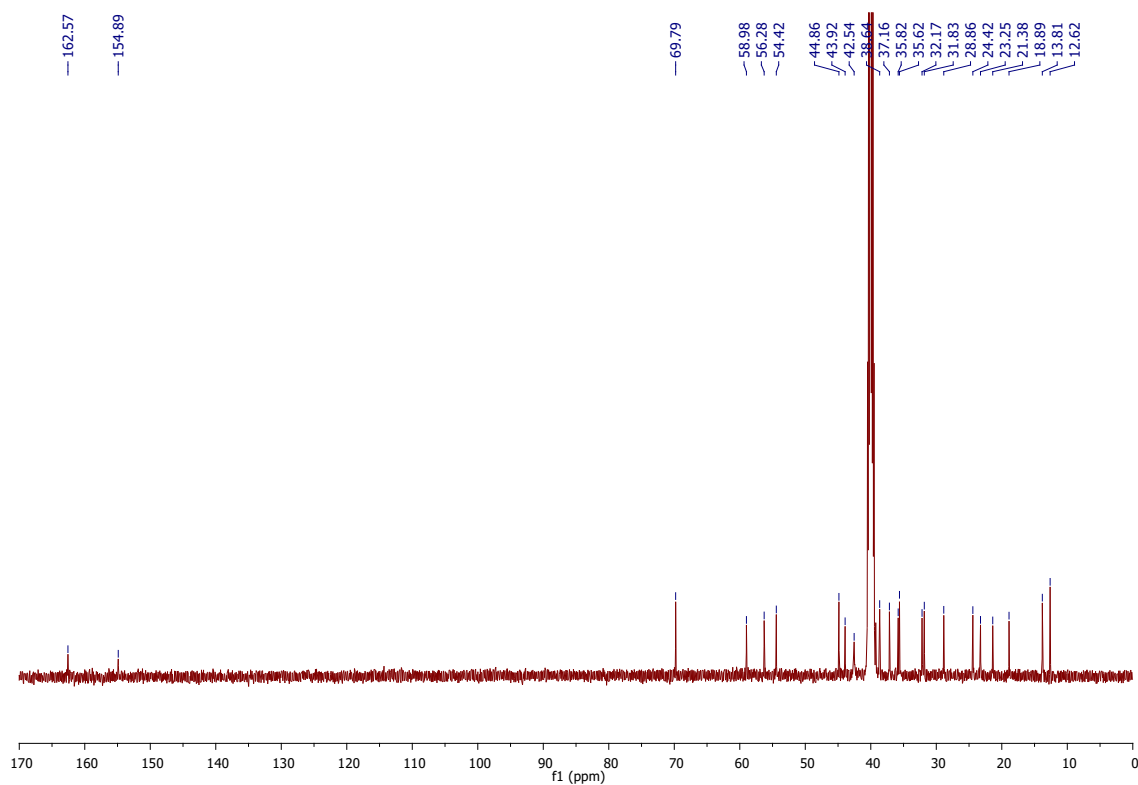


Figure S5  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ) spectrum of compound 1.

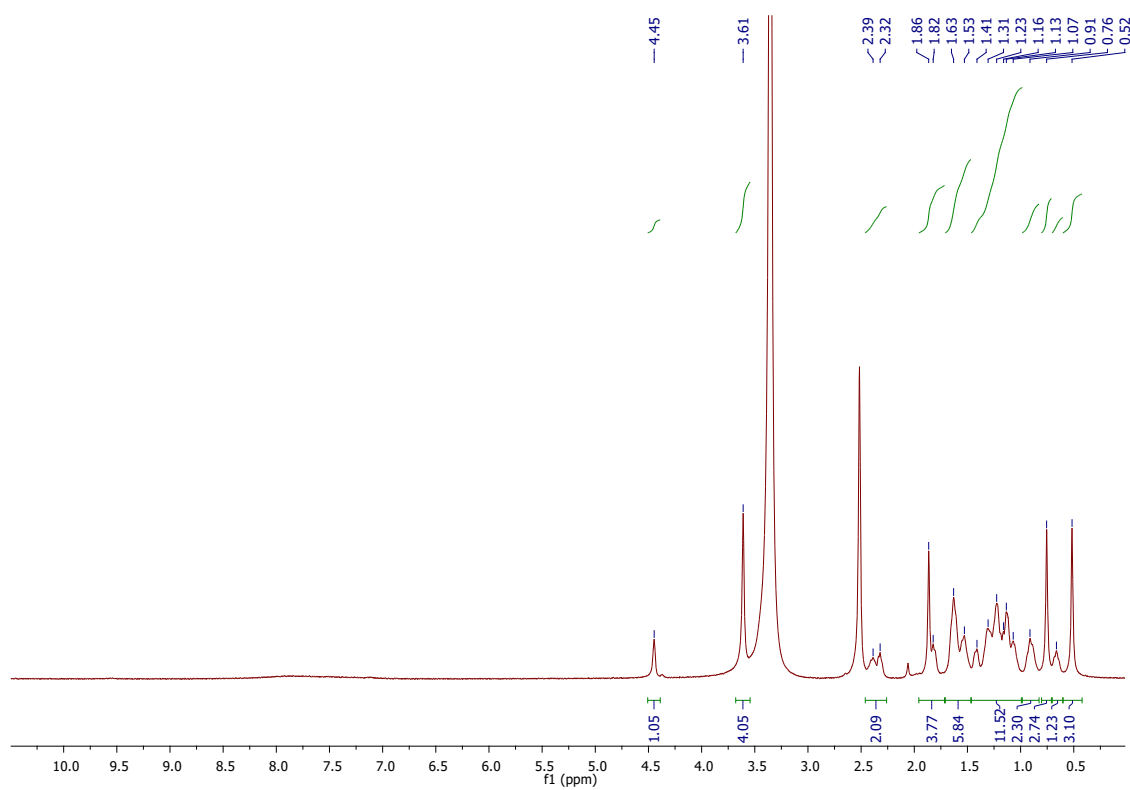


Figure S6  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ) spectrum of compound 2.

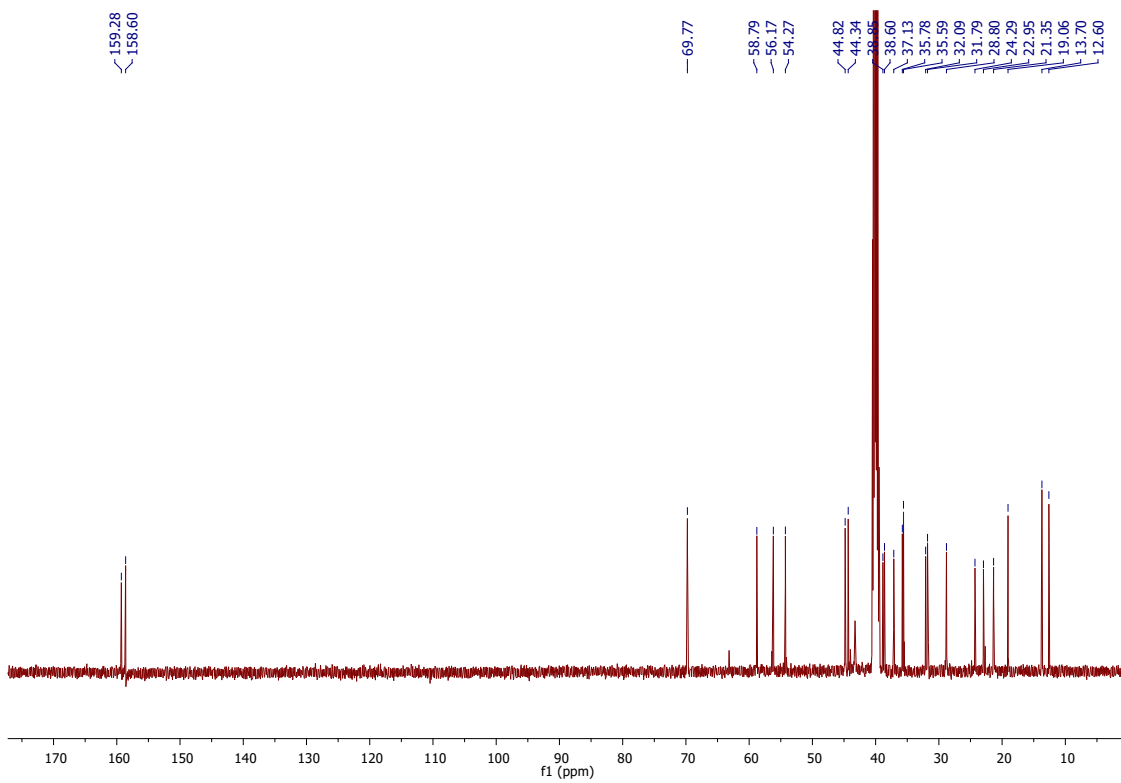


Figure S7  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ) spectrum of compound 2.

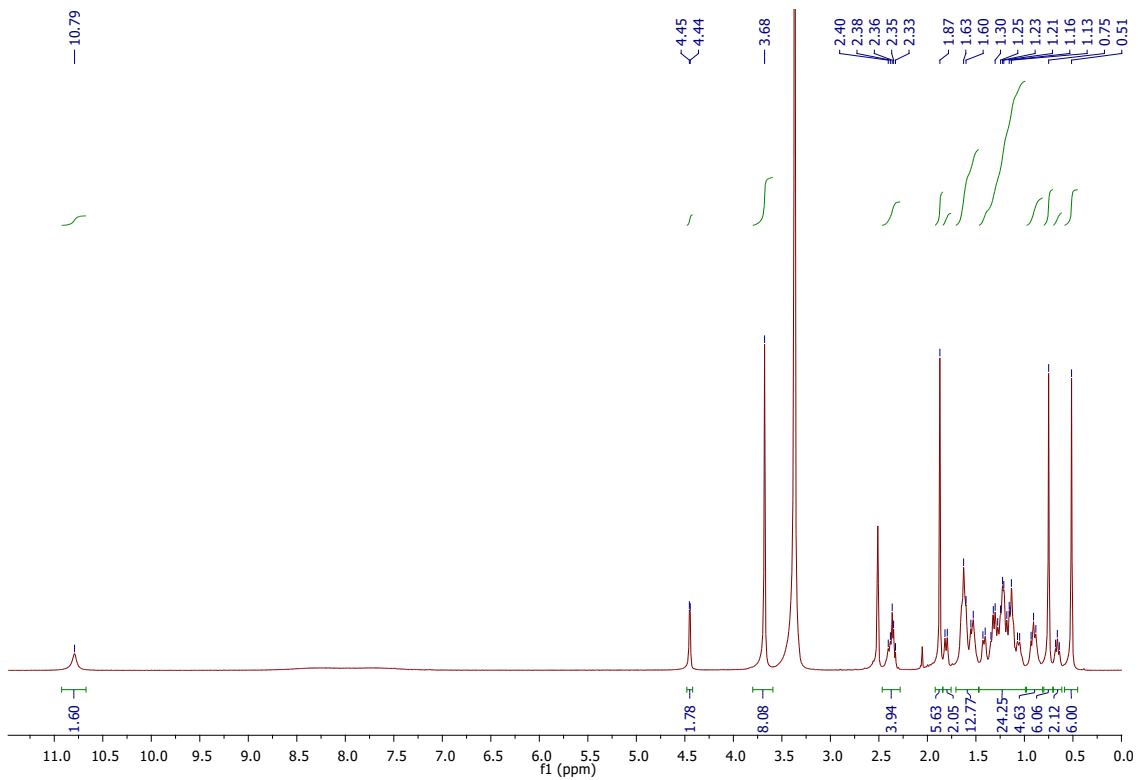


Figure S8  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ) spectrum of compound 3.

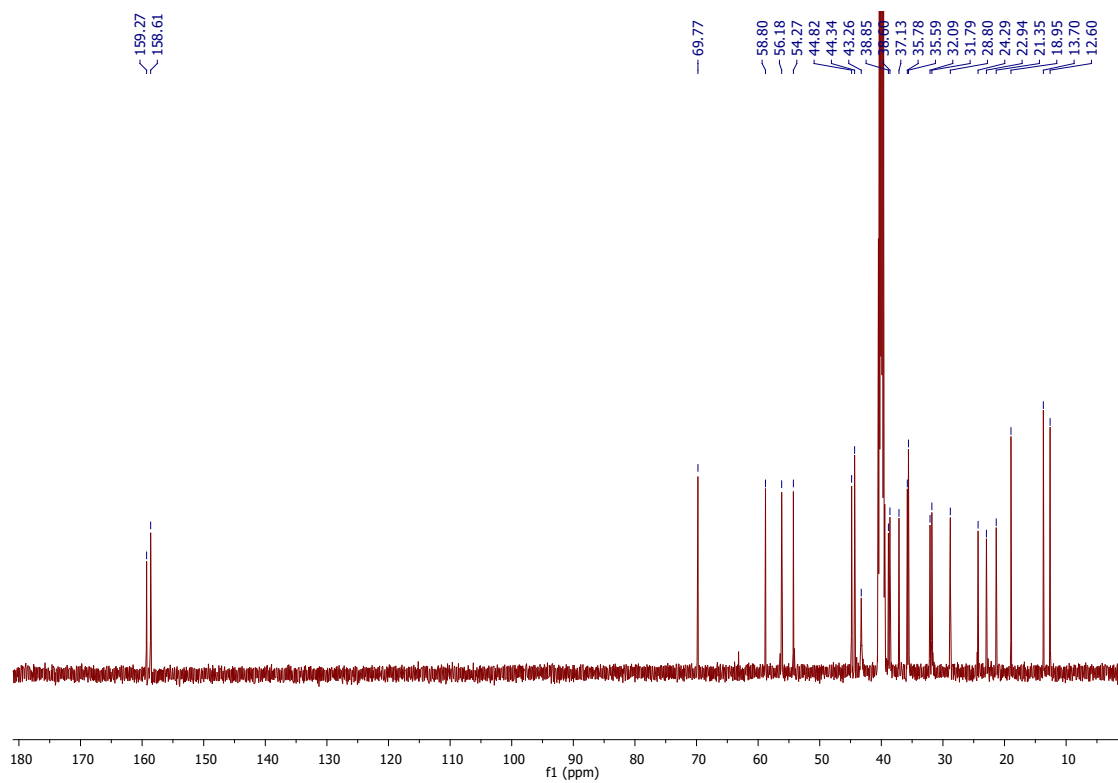


Figure S9  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ) spectrum of compound **3**.

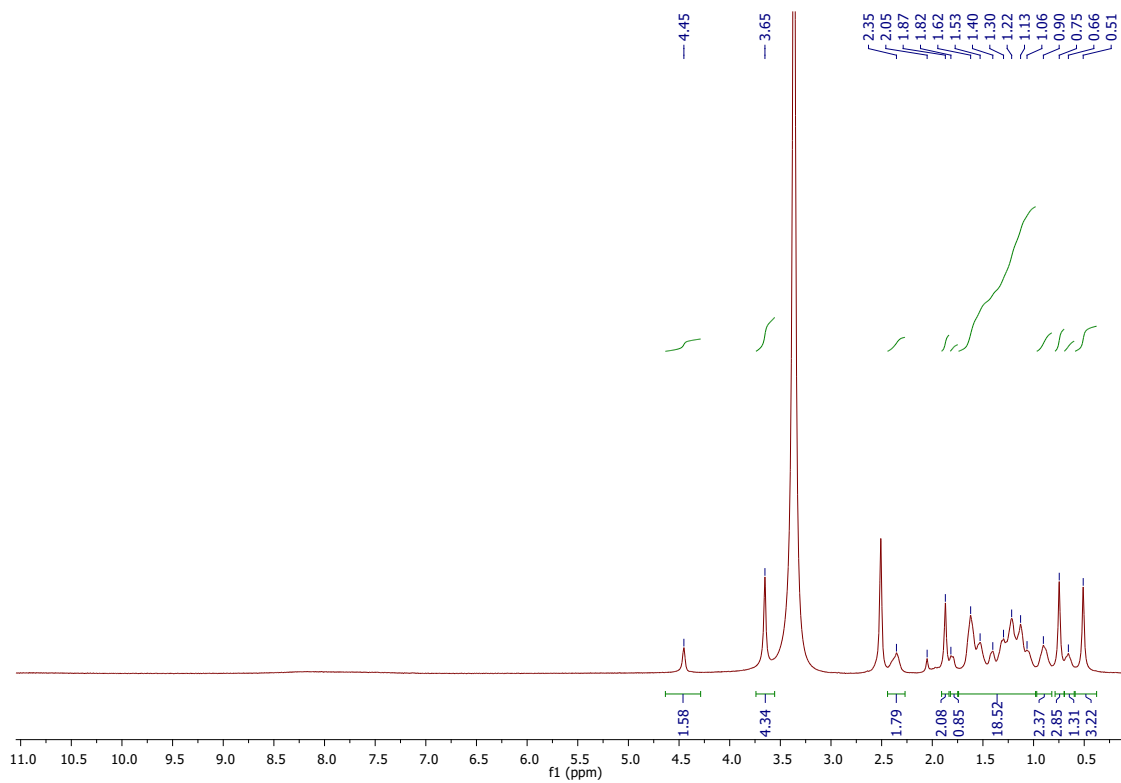


Figure S10  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ) spectrum of compound **5**.

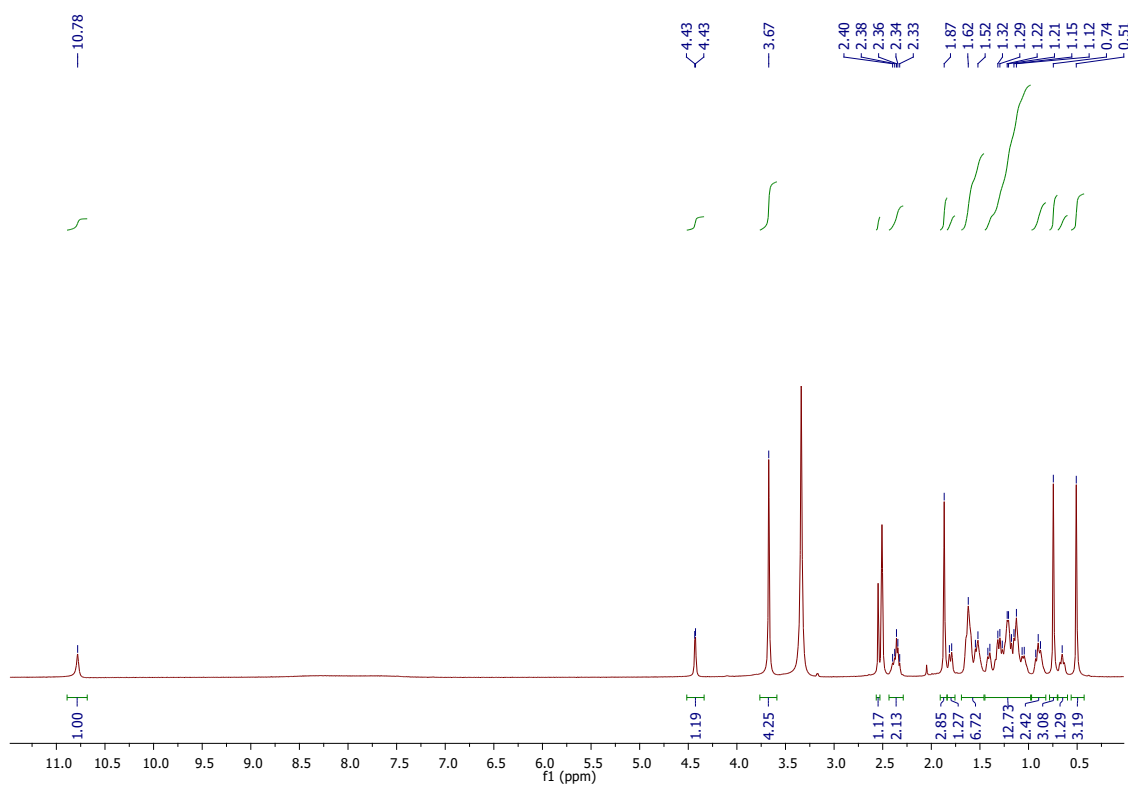


Figure S11  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ ) spectrum of compound **6**.

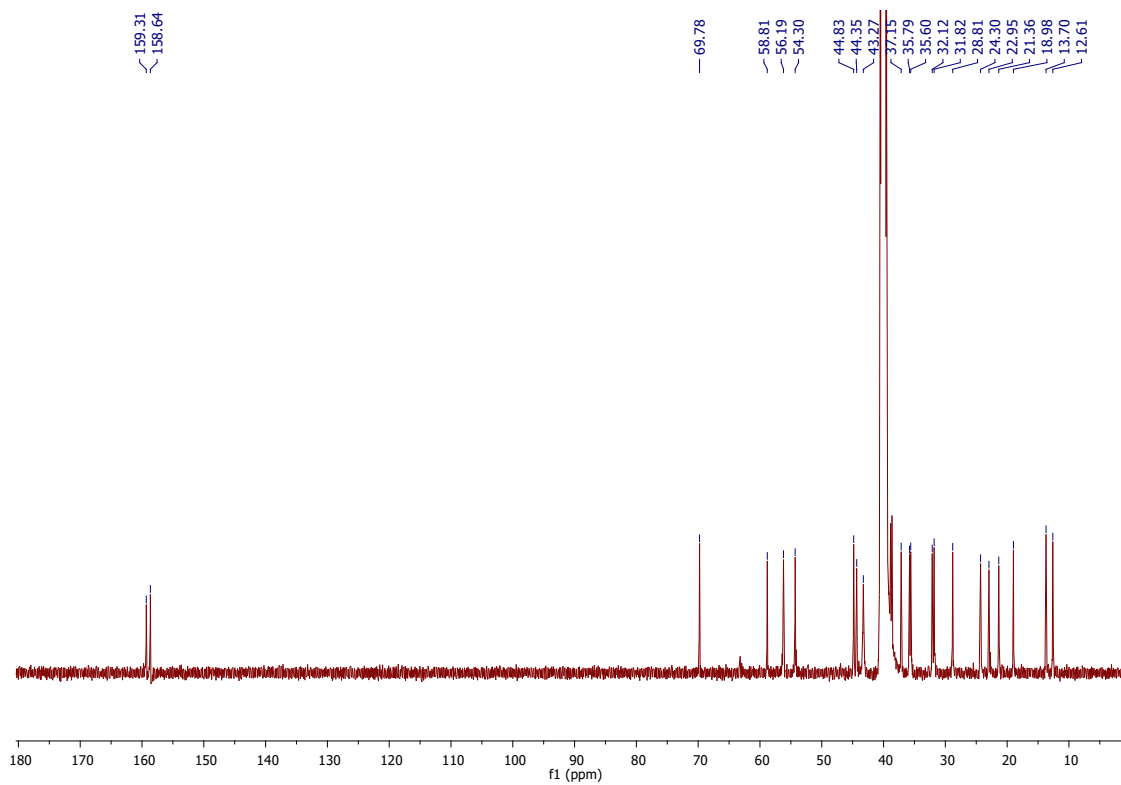
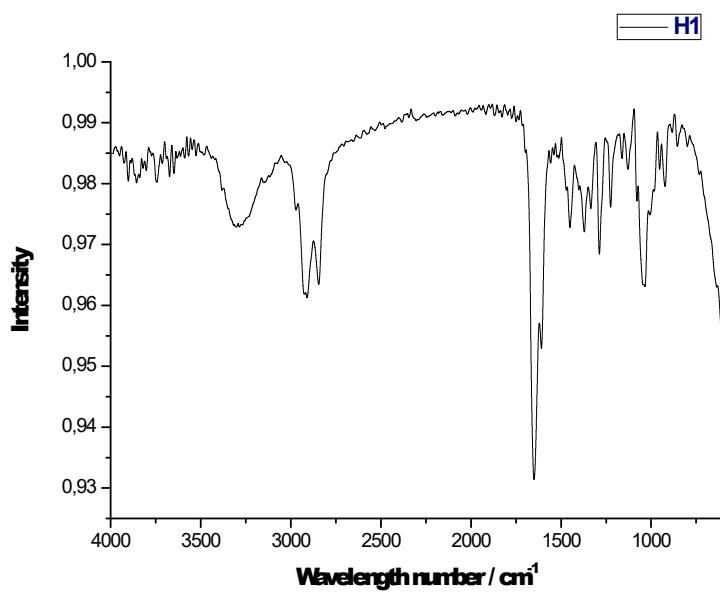


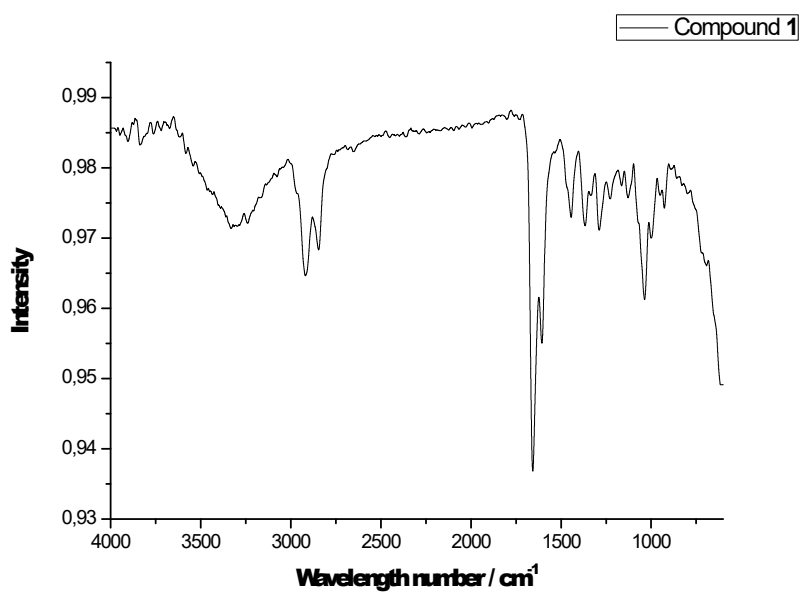
Figure S12  $^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ) spectrum of compound **6**.



# IR Data



**Figure S13** IR spectrum (cm<sup>-1</sup>) of the free ligand H1.



**Figure S14** IR spectrum (cm<sup>-1</sup>) of compound 1.

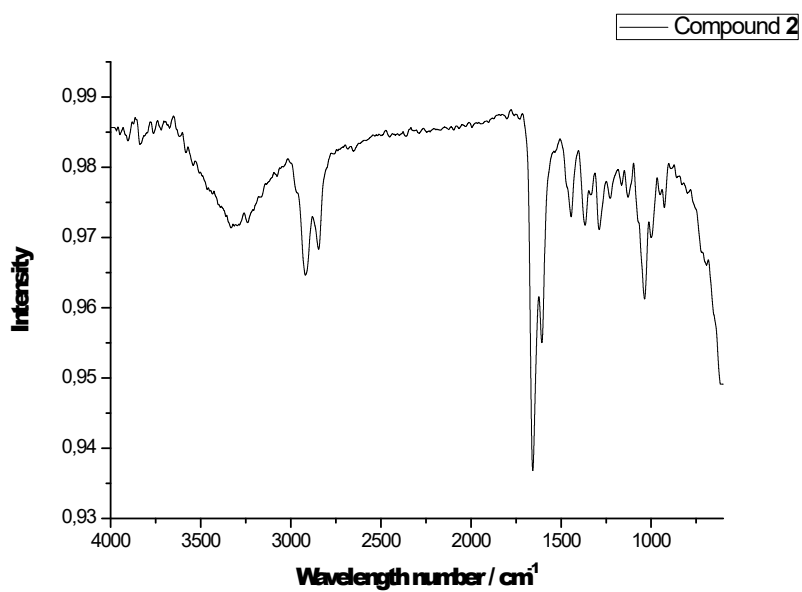


Figure S15 IR spectrum (cm<sup>-1</sup>) of compound 2.

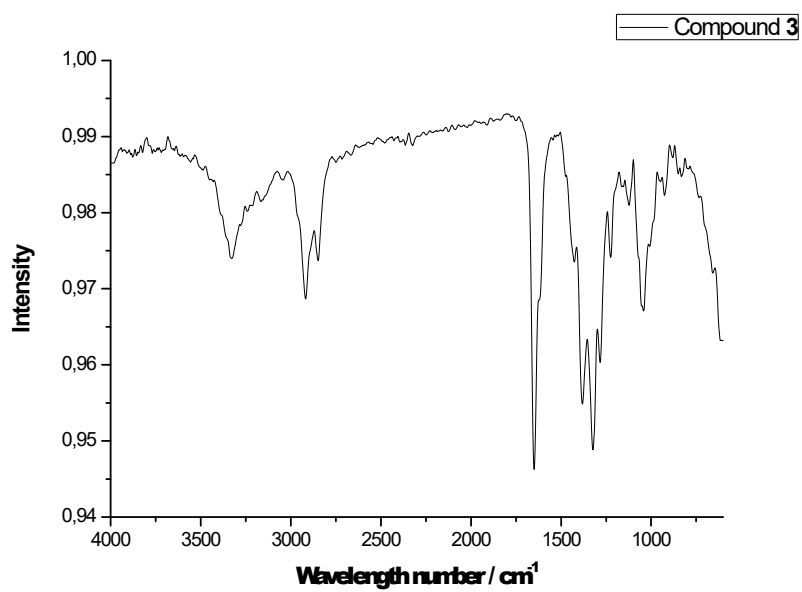


Figure S16 IR spectrum (cm<sup>-1</sup>) of compound 3.

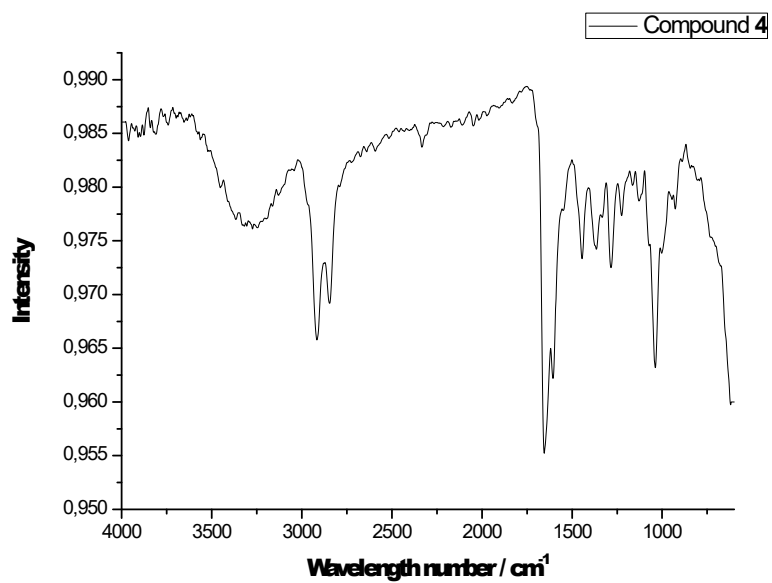


Figure S17 IR spectrum (cm<sup>-1</sup>) of compound 4.

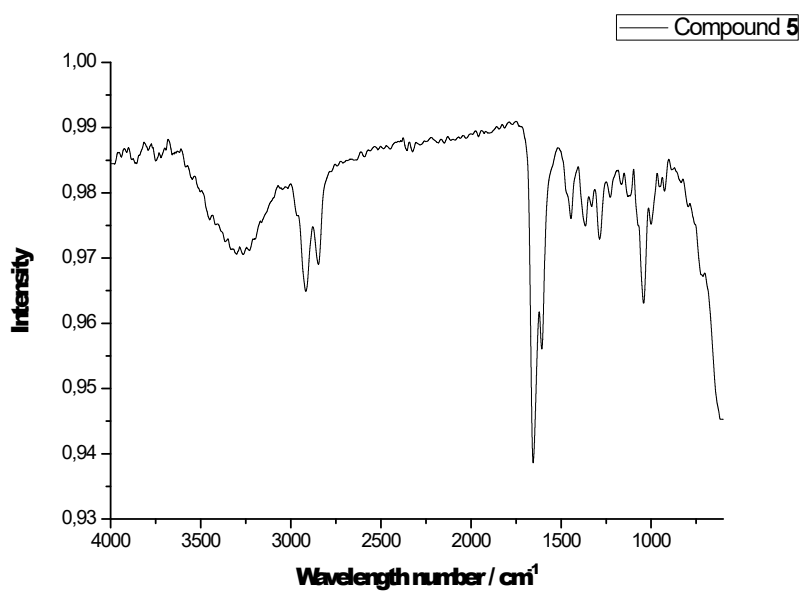


Figure S18 IR spectrum (cm<sup>-1</sup>) of compound 5.

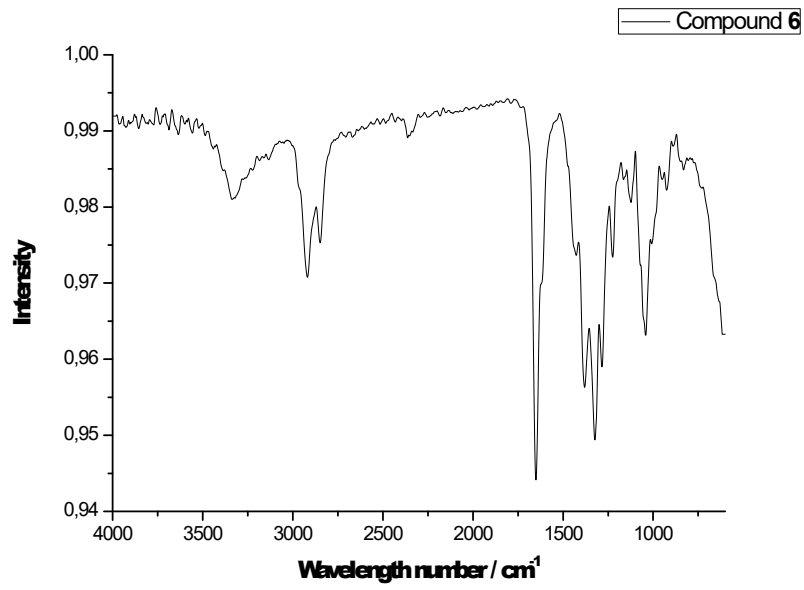


Figure S19 IR spectrum (cm<sup>-1</sup>) of compound 6.

# Mass Spectrometry Data

$[\text{H1}+\text{H}]^+ = 401,2973$   
m/z

[M-OH]

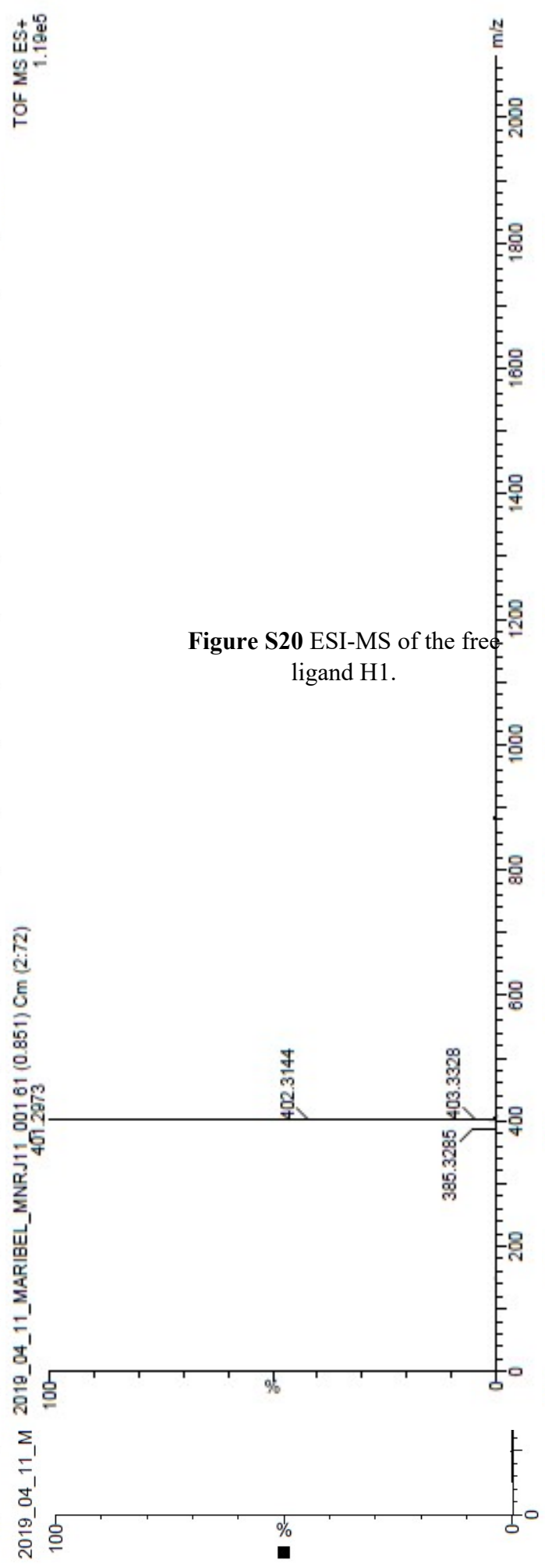


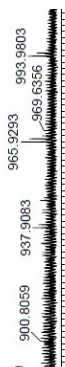
Figure S20 ESI-MS of the free ligand H1.

$[H1+H]^+ = 401,3046$   
m/z

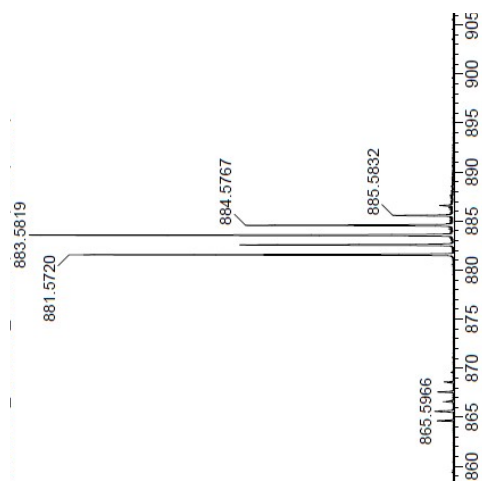
3.91e5

$[M+3H]$

$[H1+H]^+ = 401,3031$   
m/z



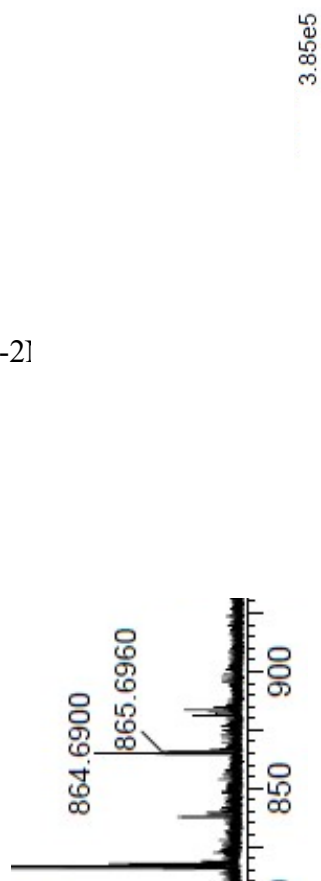
**Figure S22** ESI-MS of compound 2.



**Figure S21** ESI-MS of compound 1.



[M-H1-2]



[H1+H]<sup>+</sup>

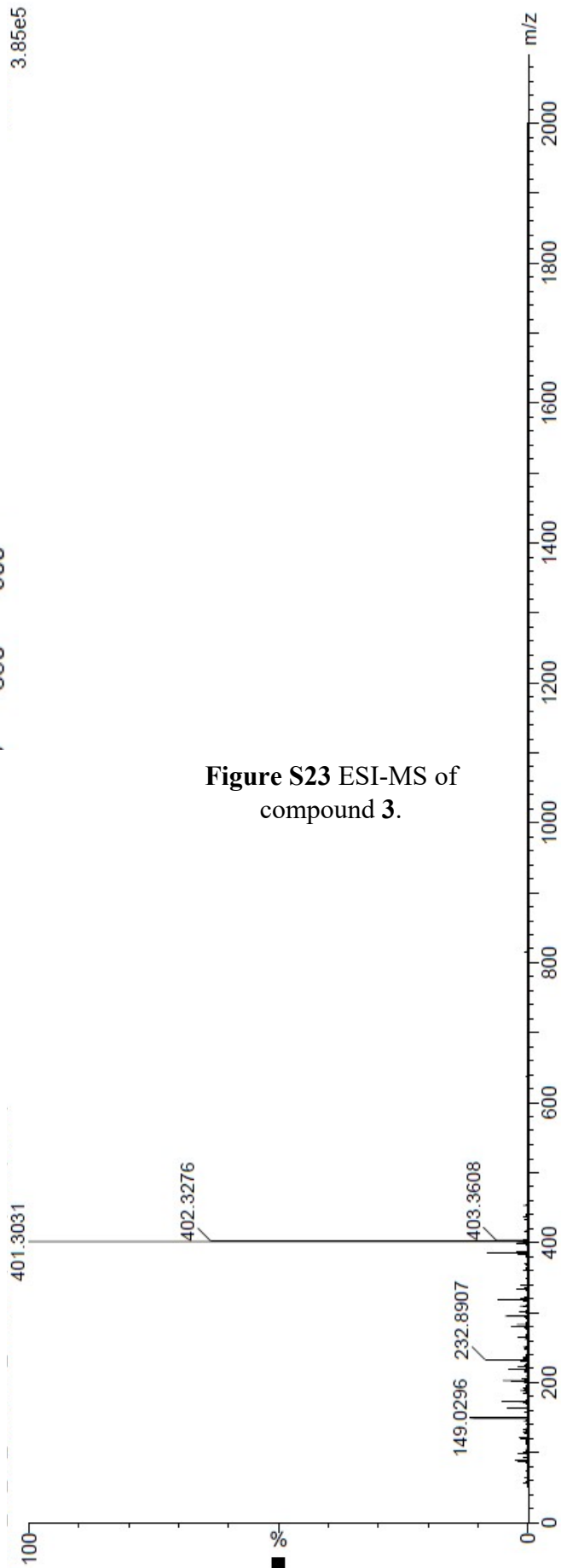


Figure S23 ESI-MS of compound 3.

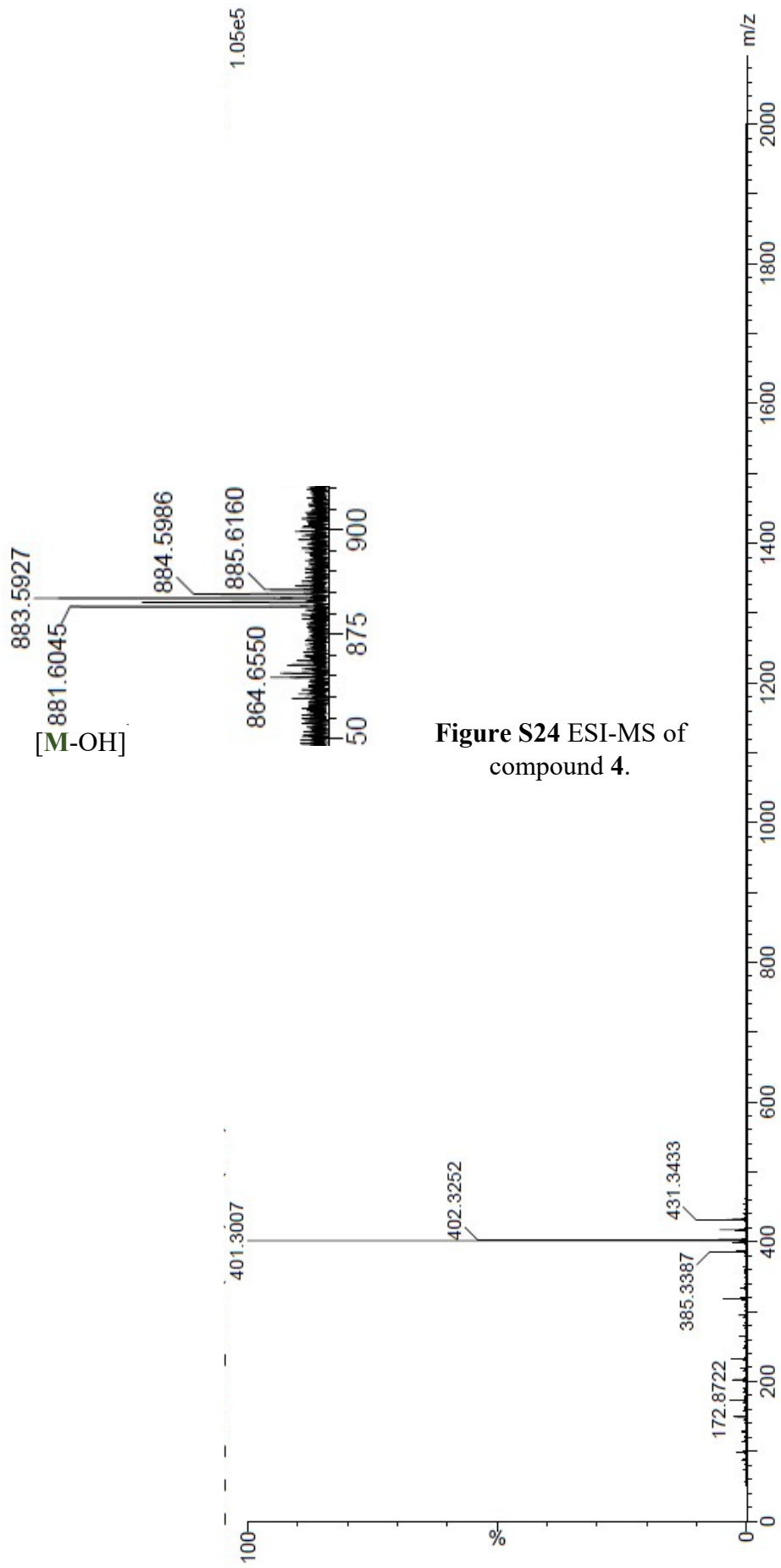
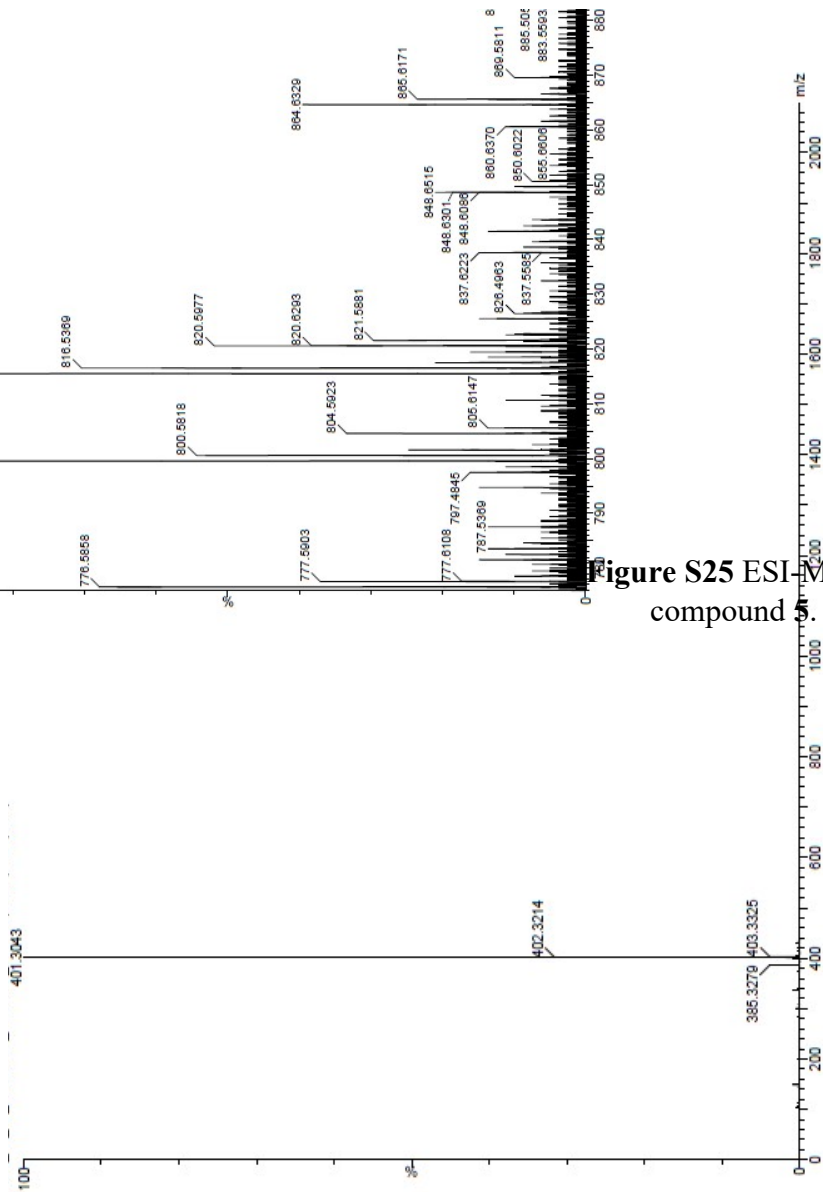


Figure S24 ESI-MS of compound 4.

[H1+H]<sup>+</sup>



[M-Cl+H]

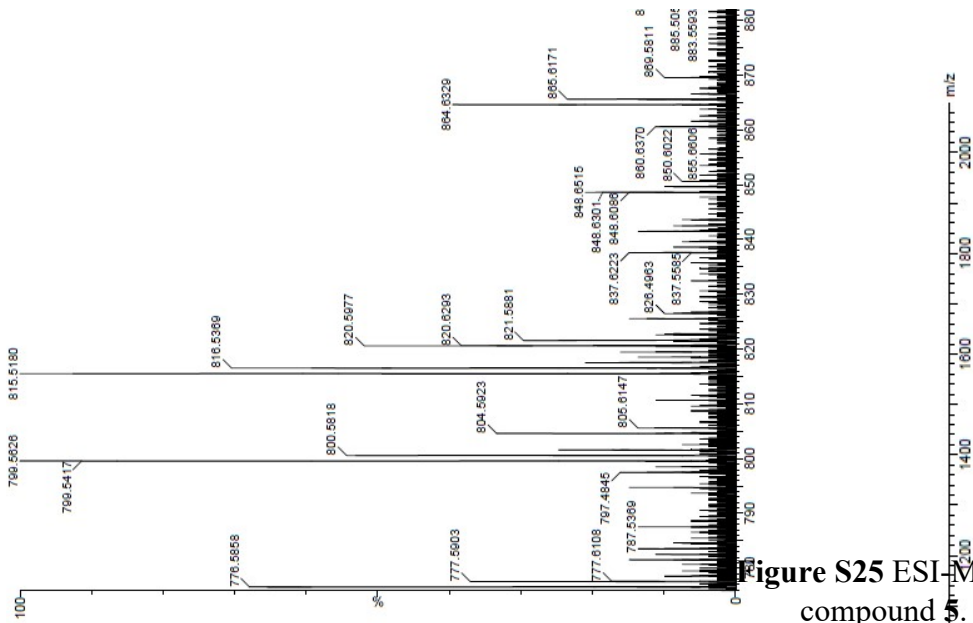


Figure S25 ESI-MS of compound 5.

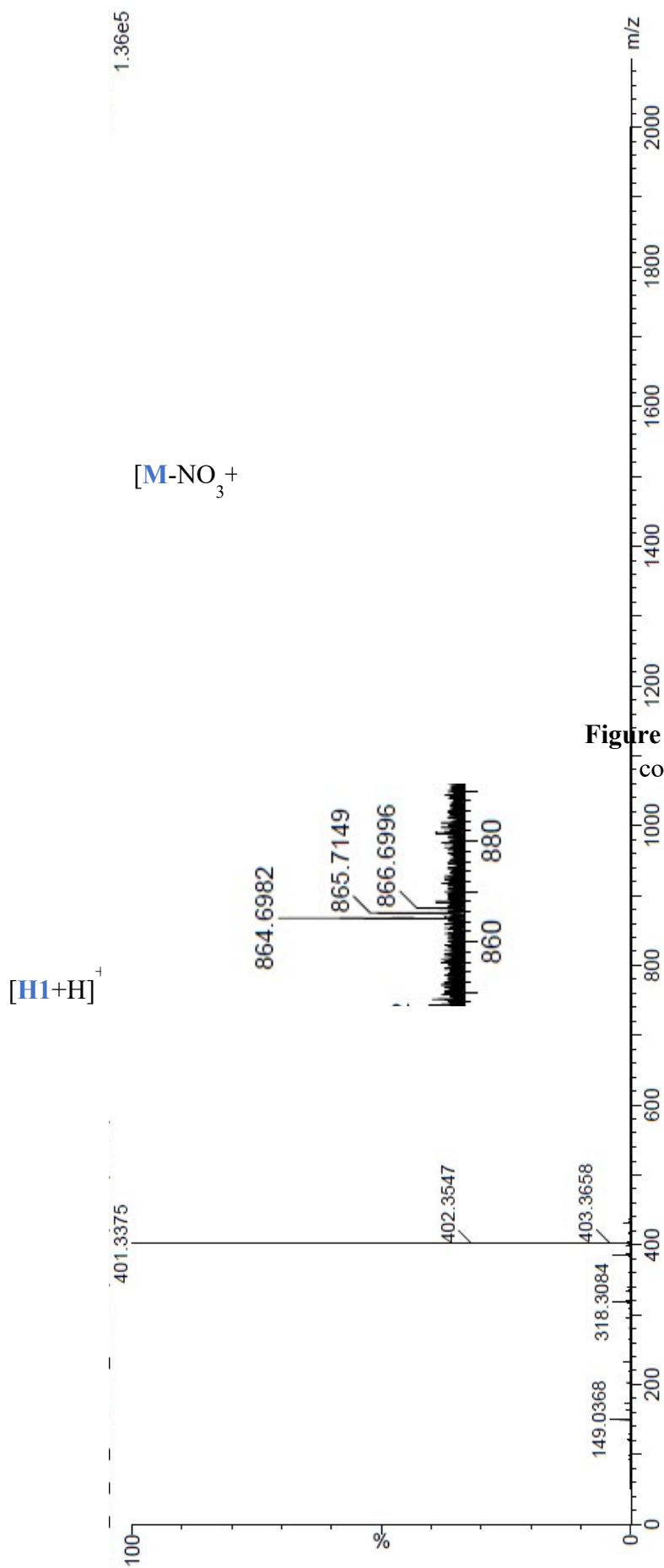
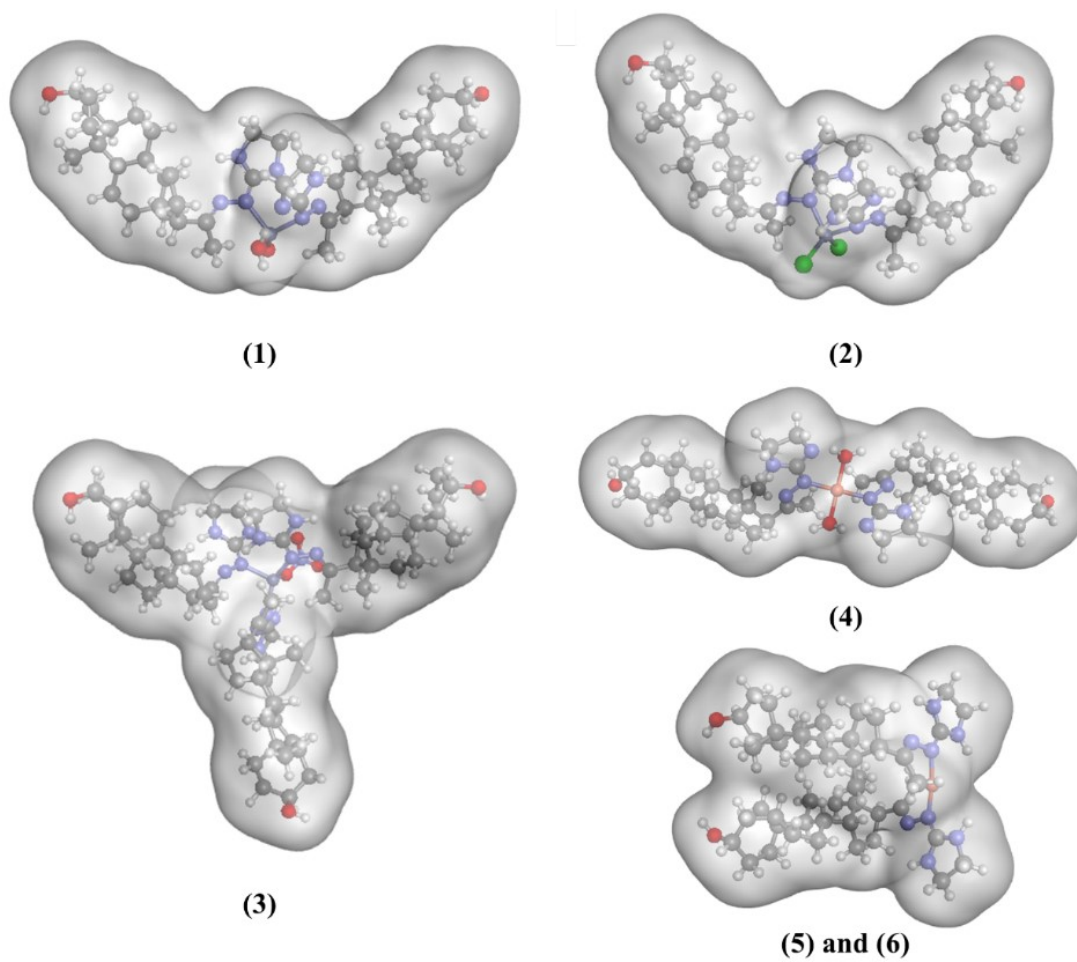


Figure S26 ESI-MS of compound 6.

# Computational data



**Figure S27** Van der Waals surfaces. These surfaces provide a reasonable view of the volume occupied by each complex.