

ESI for:

**Metal-directed assembly of chiral bis-Zn(II) Schiff base structures**

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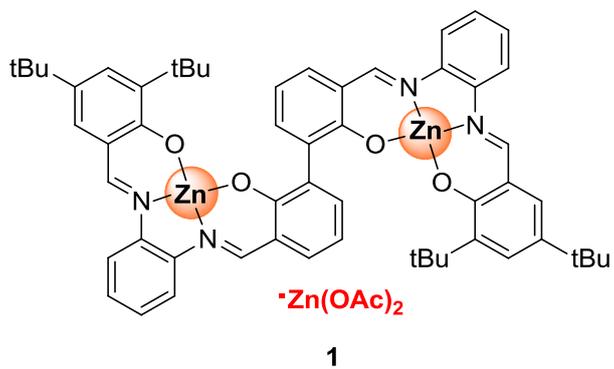
<sup>b</sup>*Catalan Institute for Research and Advanced Studies (ICREA), Pg. Lluís*

*Companys 23, 08010, Barcelona, Spain.*

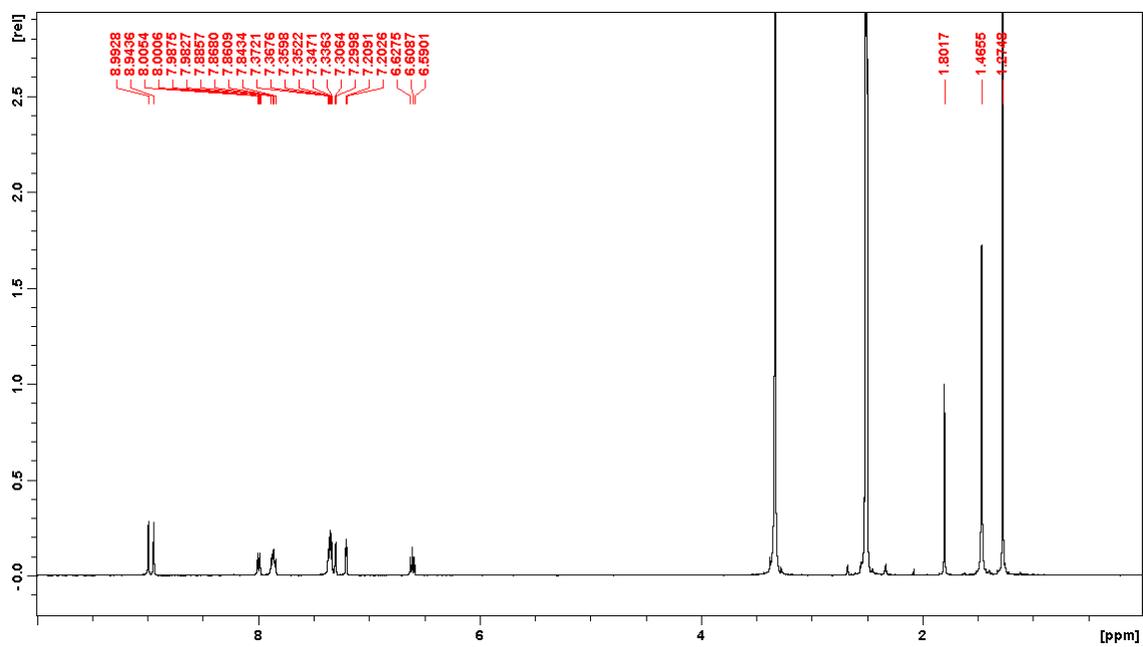
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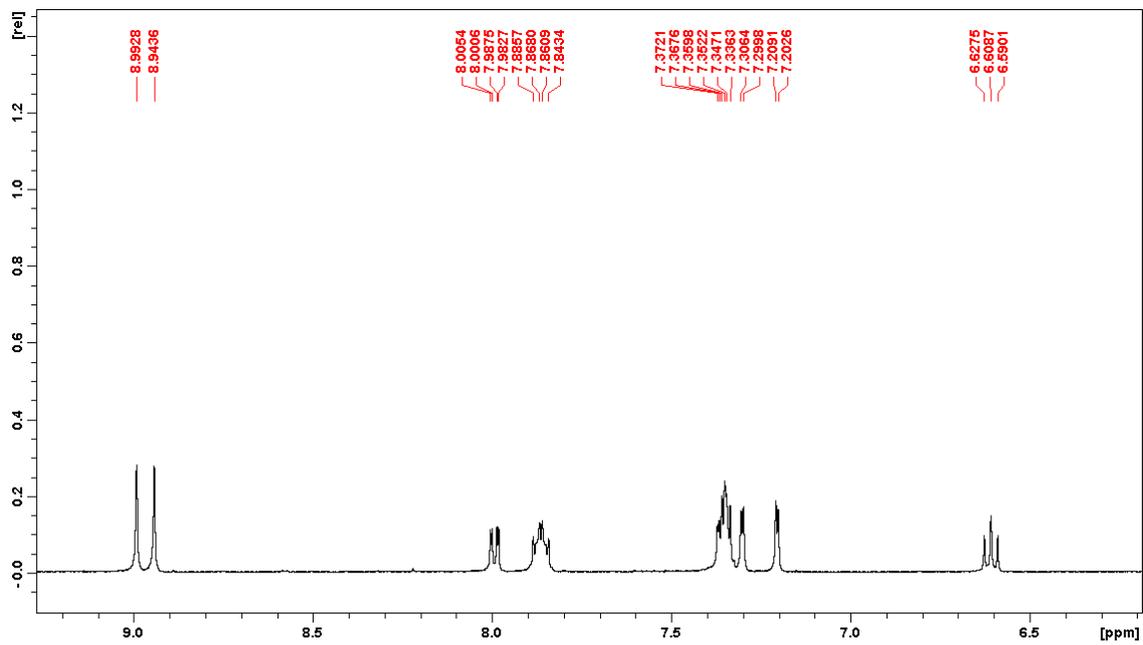
### Copies of NMR and MS spectra for complex **1**:



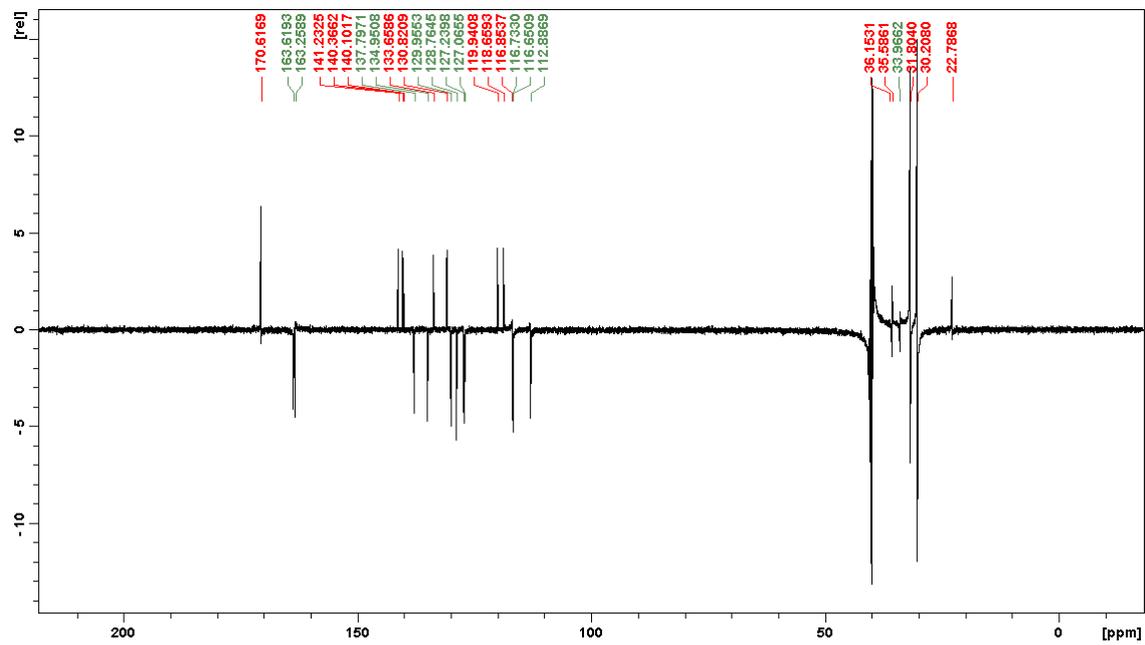
$^1\text{H}$  NMR in  $\text{DMSO-}d_6$ :



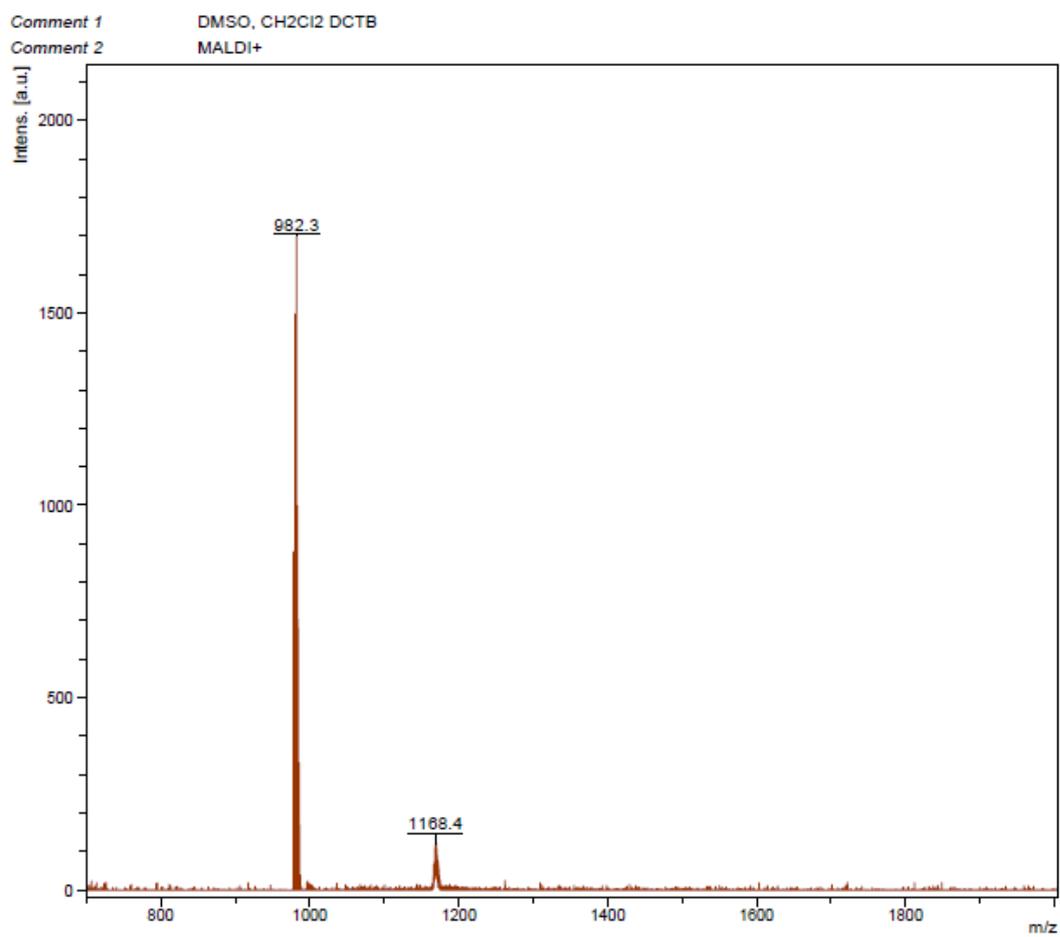
Extension of the aromatic region ( $^1\text{H}$  NMR for **1**,  $\text{DMSO-}d_6$ ):



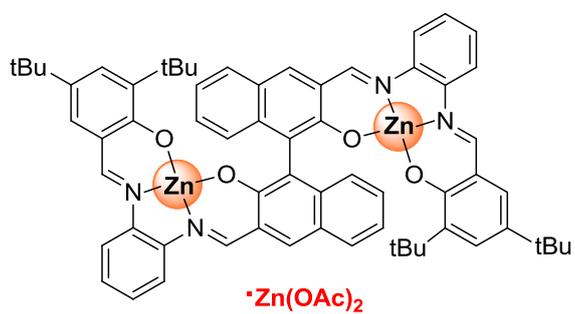
$^{13}\text{C}\{^1\text{H}\}$  NMR (DEPT-Q) in  $\text{DMSO-}d_6$ :



MS spectrum recorded for **1** (MALDI+, dctb):

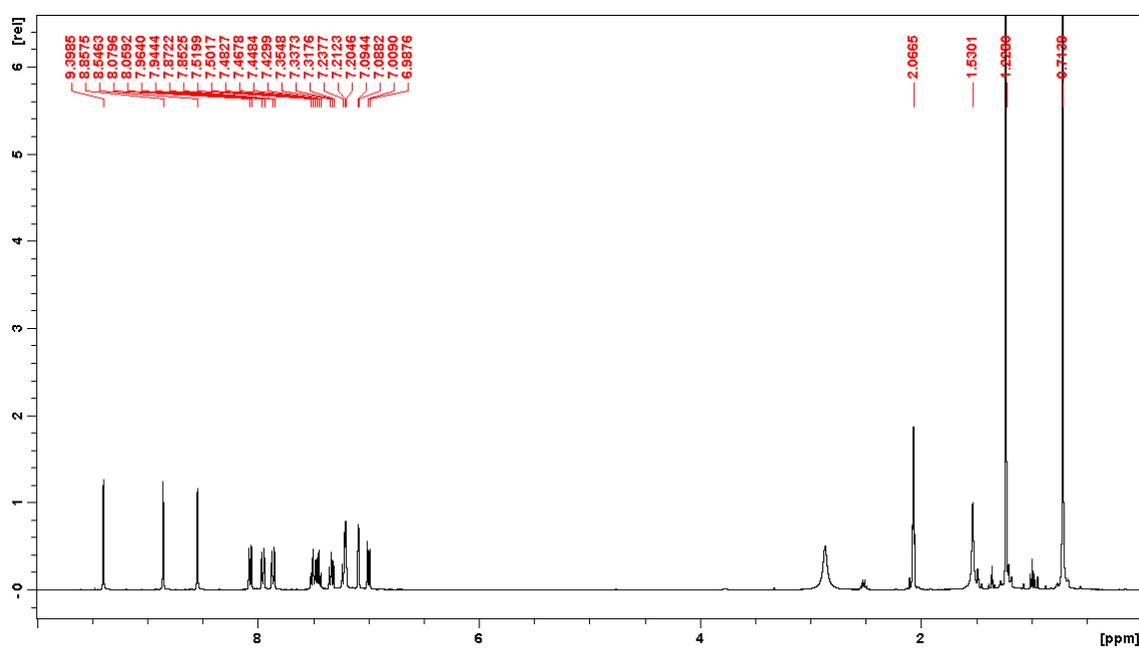


## Copies of NMR and MS spectra for complex **2**:

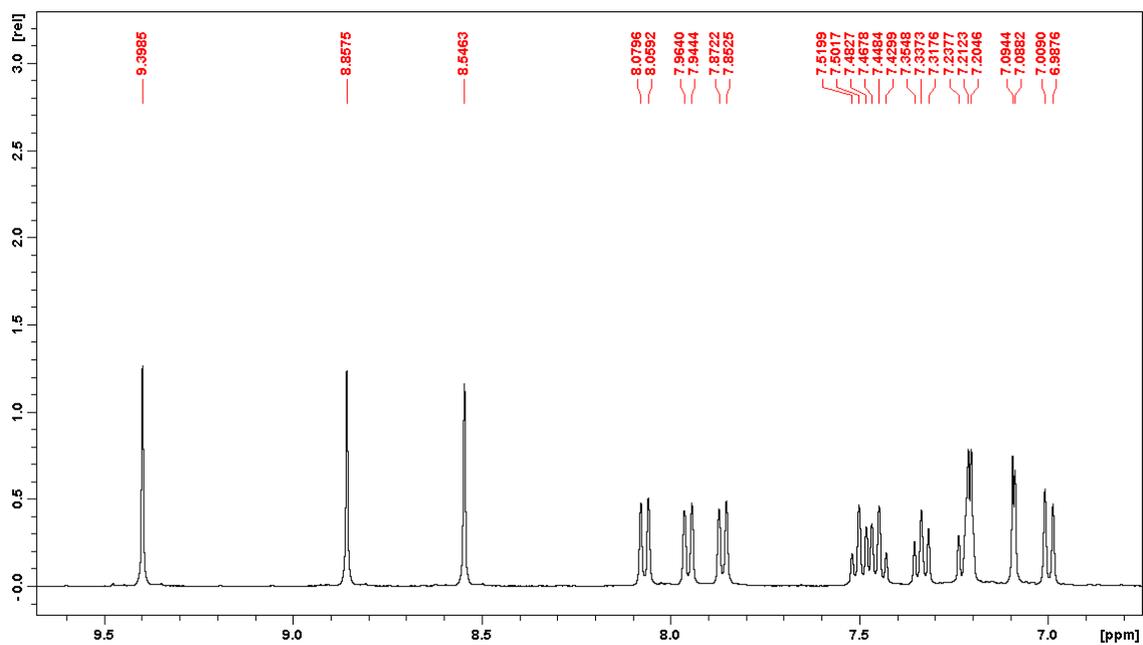


**2**

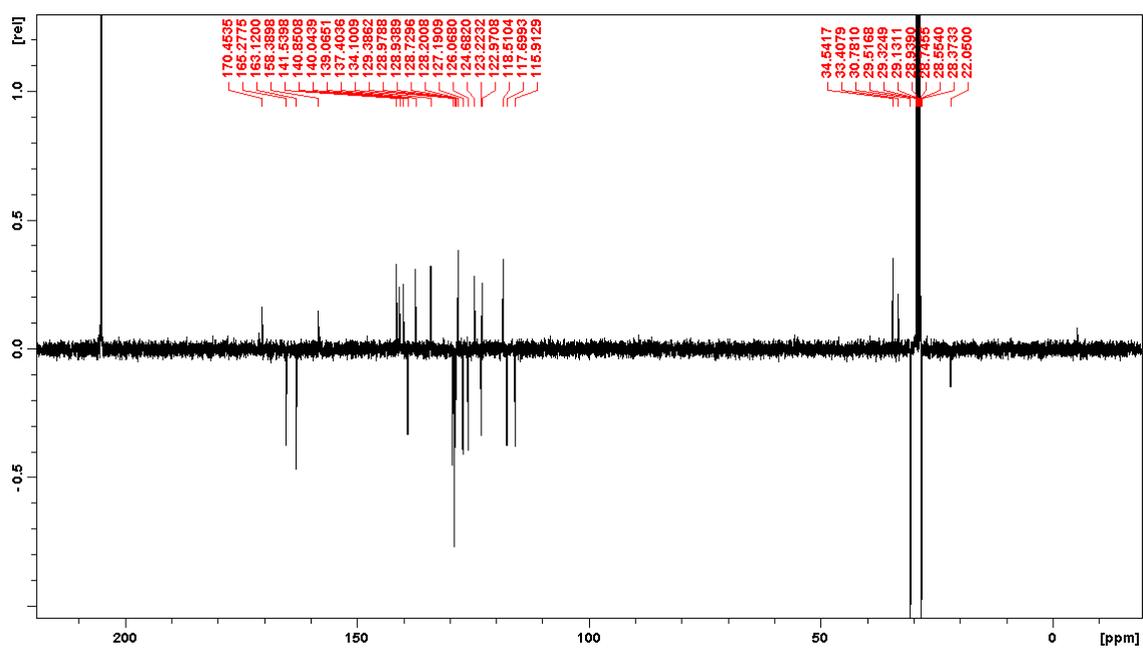
$^1\text{H}$  NMR in Acetone- $d_6$ :



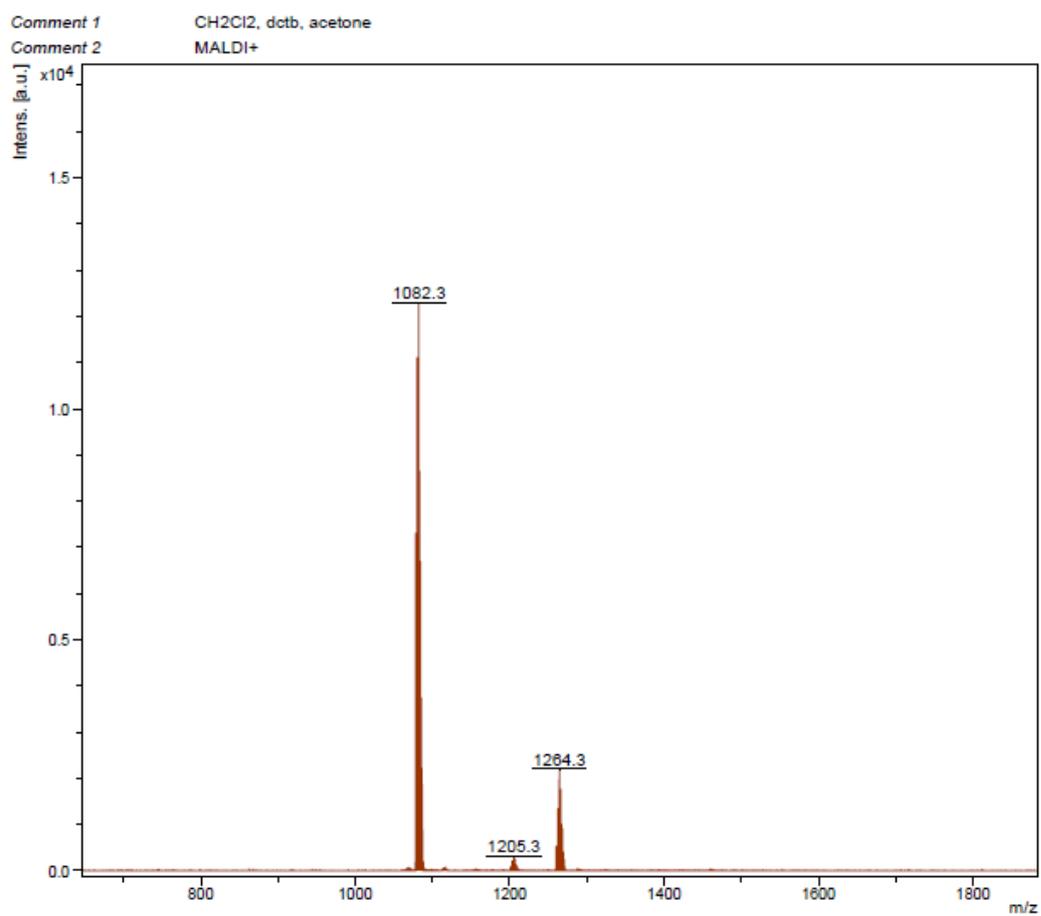
Extension of the aromatic region ( $^1\text{H}$  NMR for **2**, Acetone- $d_6$ ):



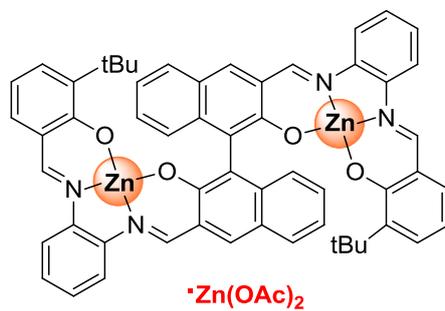
$^{13}\text{C}\{^1\text{H}\}$  NMR (DEPT-Q) in Acetone- $d_6$ :



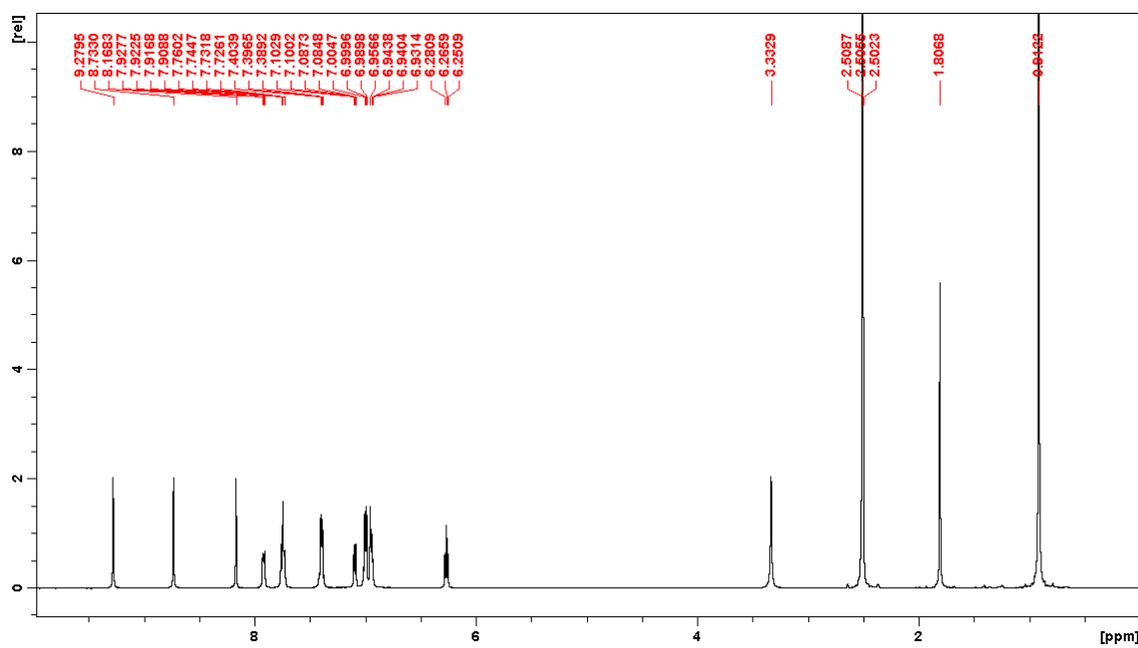
MS spectrum recorded for **2** (MALDI+, dctb):



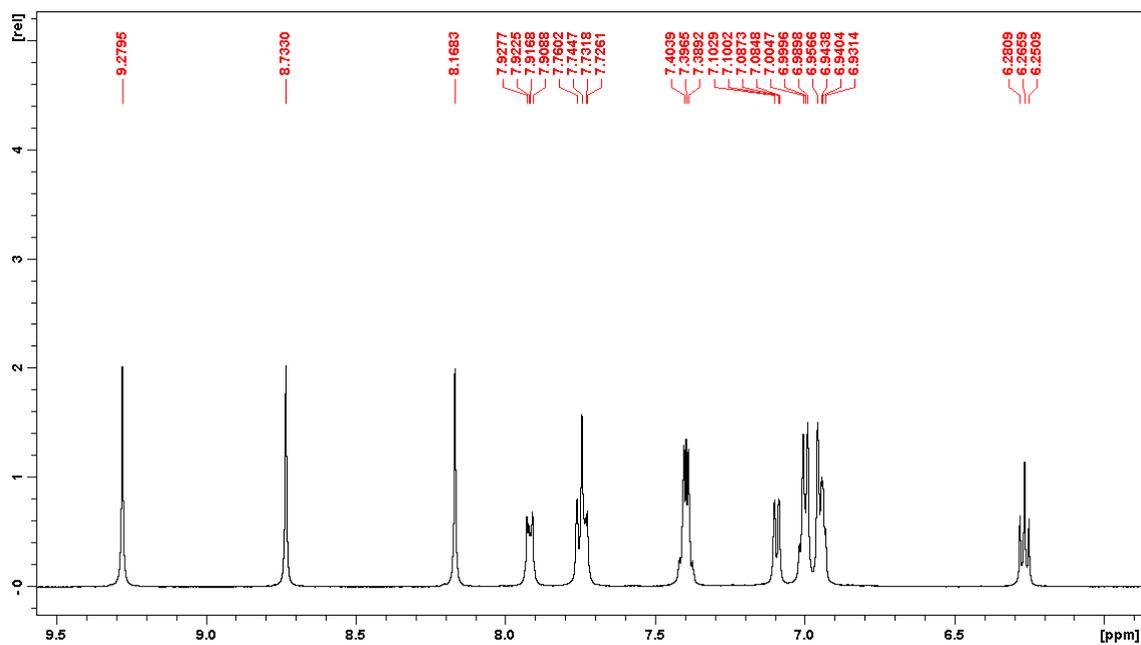
### Copies of NMR and MS spectra for complex **3**:



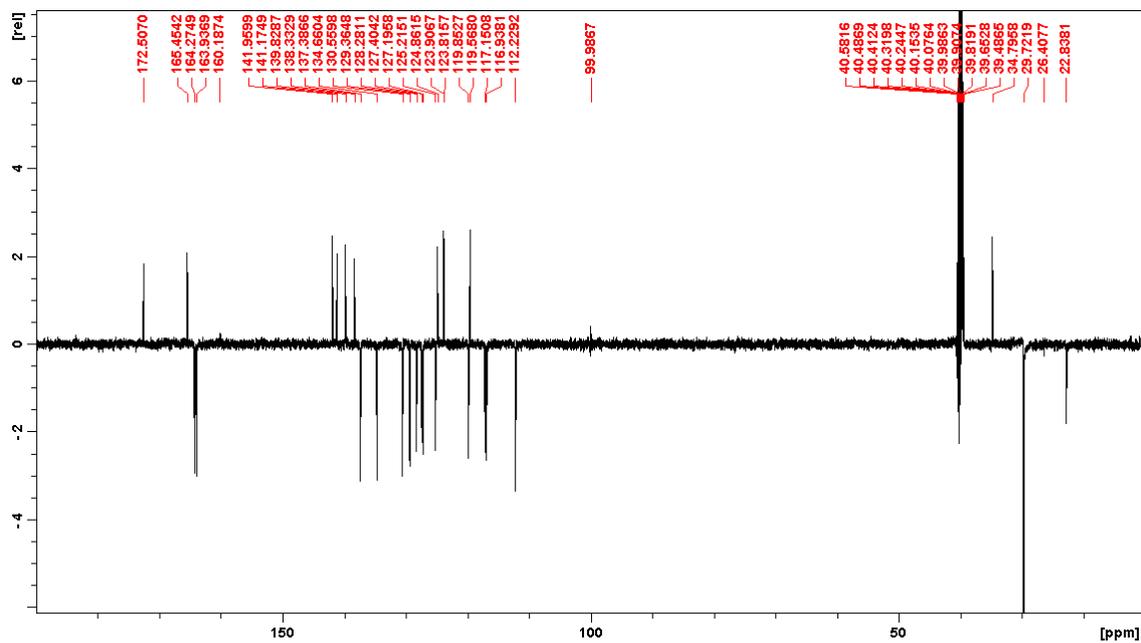
$^1\text{H}$  NMR in Acetone- $d_6$ :



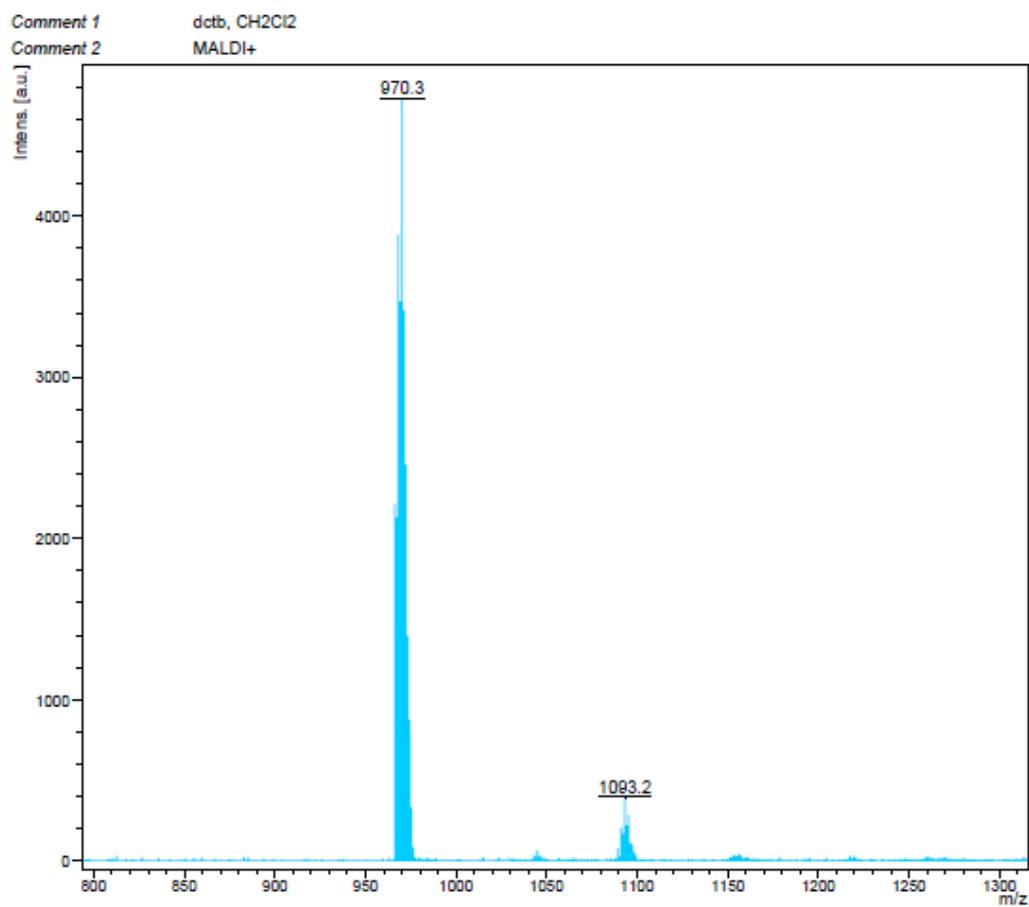
Extension of the aromatic region ( $^1\text{H}$  NMR for **3**, Acetone- $d_6$ ):



$^{13}\text{C}\{^1\text{H}\}$  NMR (DEPT-Q) in Acetone- $d_6$ :

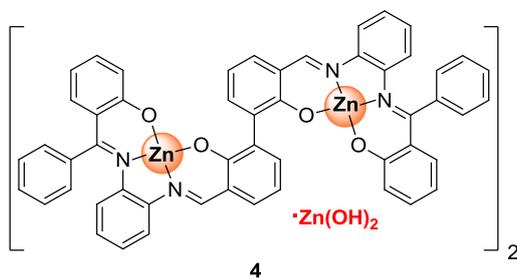


MS spectrum recorded for **3** (MALDI+, dctb):

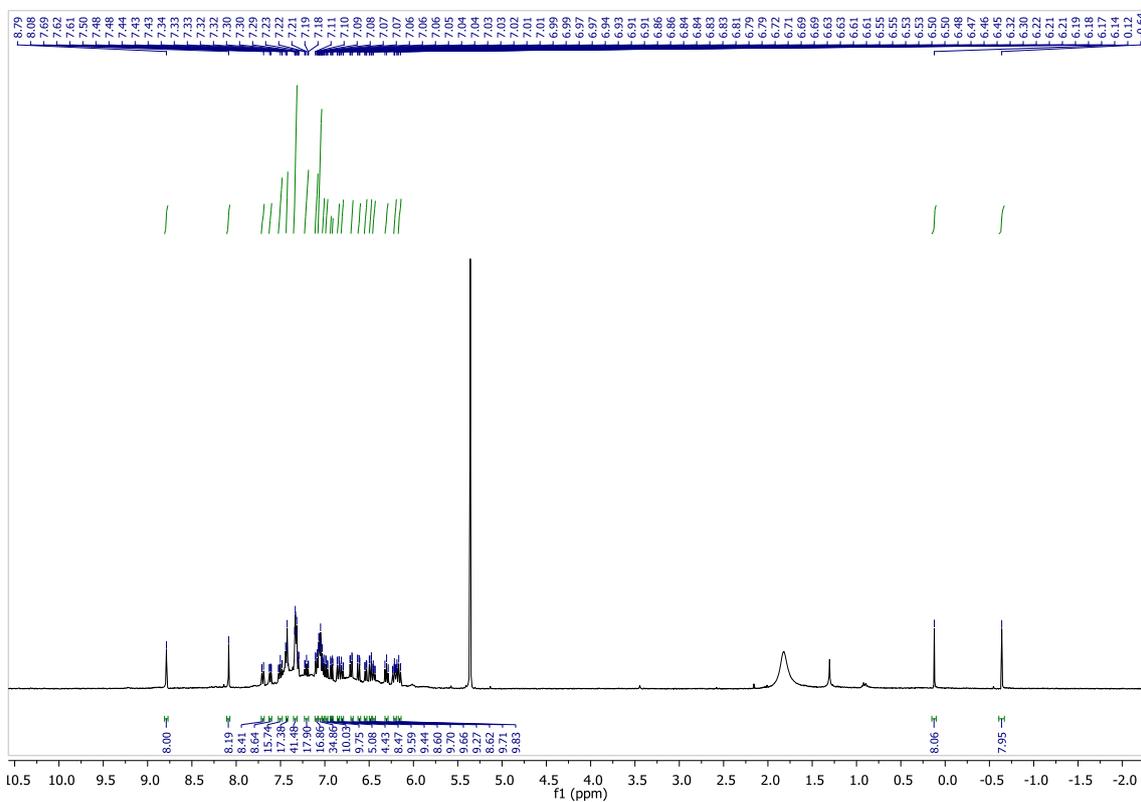


### Copies of NMR and MS spectra for complex **4**:

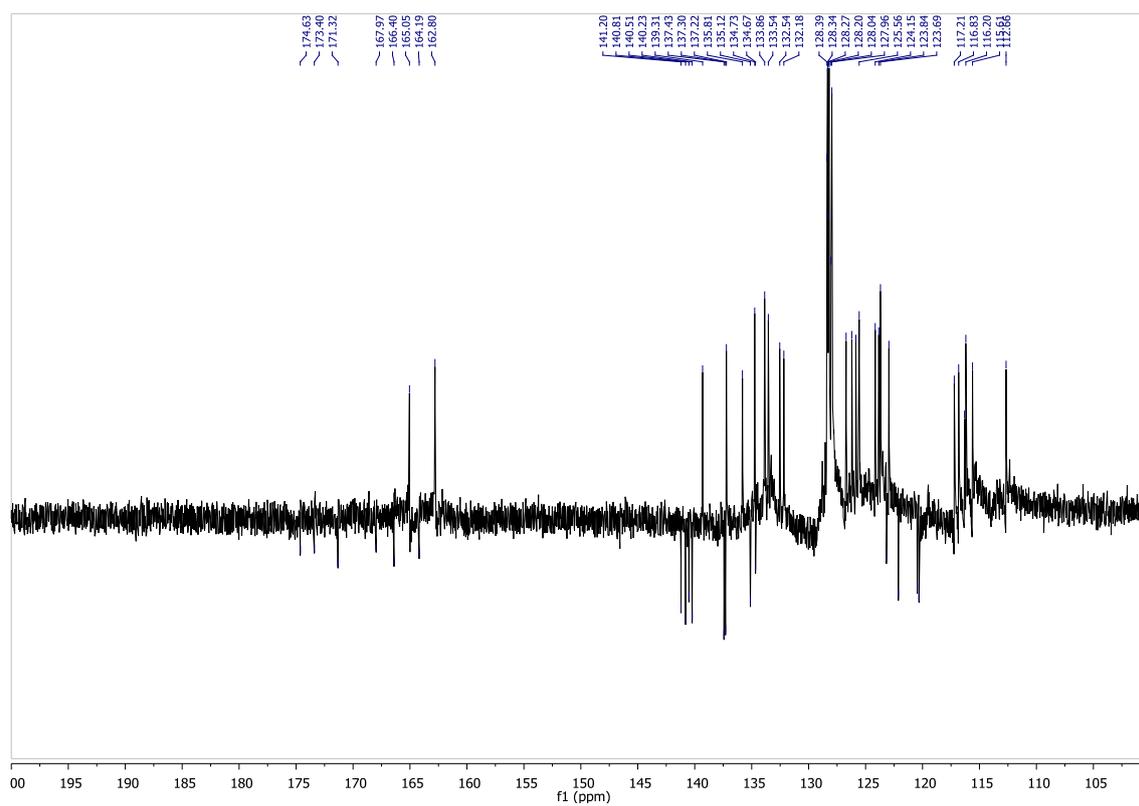
#### Zn<sub>6</sub>



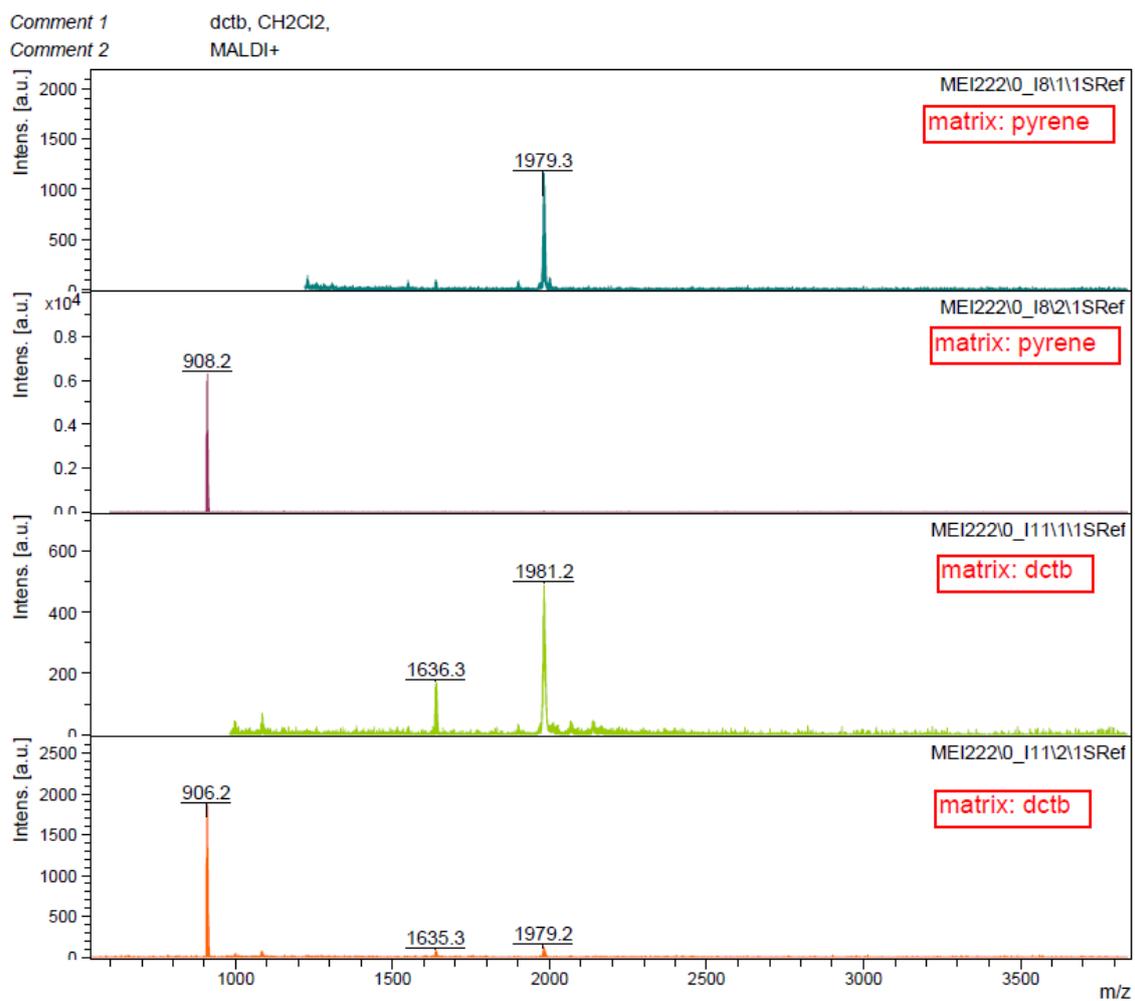
#### <sup>1</sup>H NMR in CD<sub>2</sub>Cl<sub>2</sub>:



$^{13}\text{C}$  NMR spectrum (DEPTQ) in  $\text{CD}_2\text{Cl}_2$ :

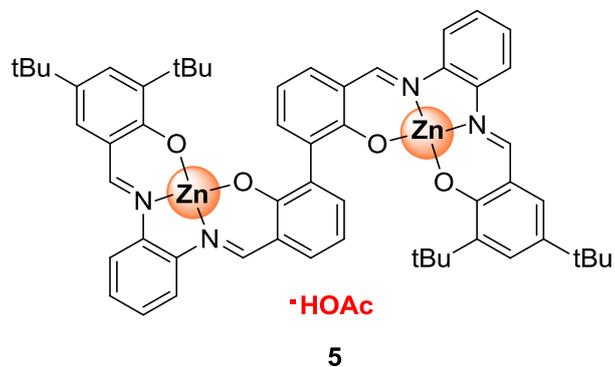


MS spectrum recorded for **4** (MALDI+, dctb or pyrene):

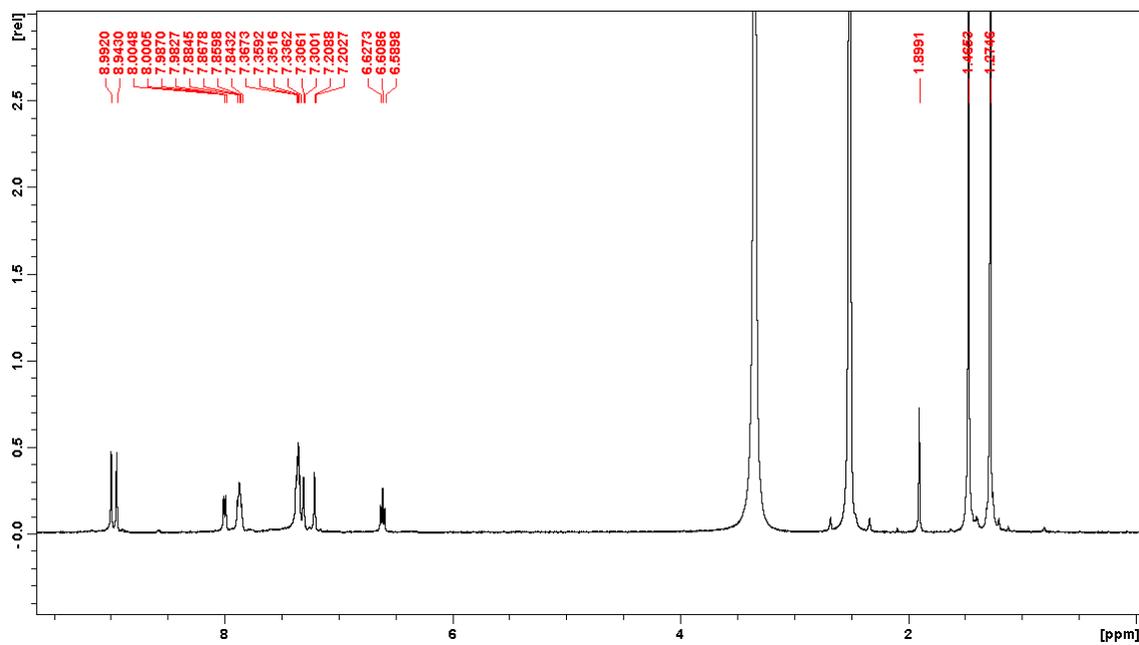


Note that the matrix has a large impact on the ms analysis (dctb versus pyrene).

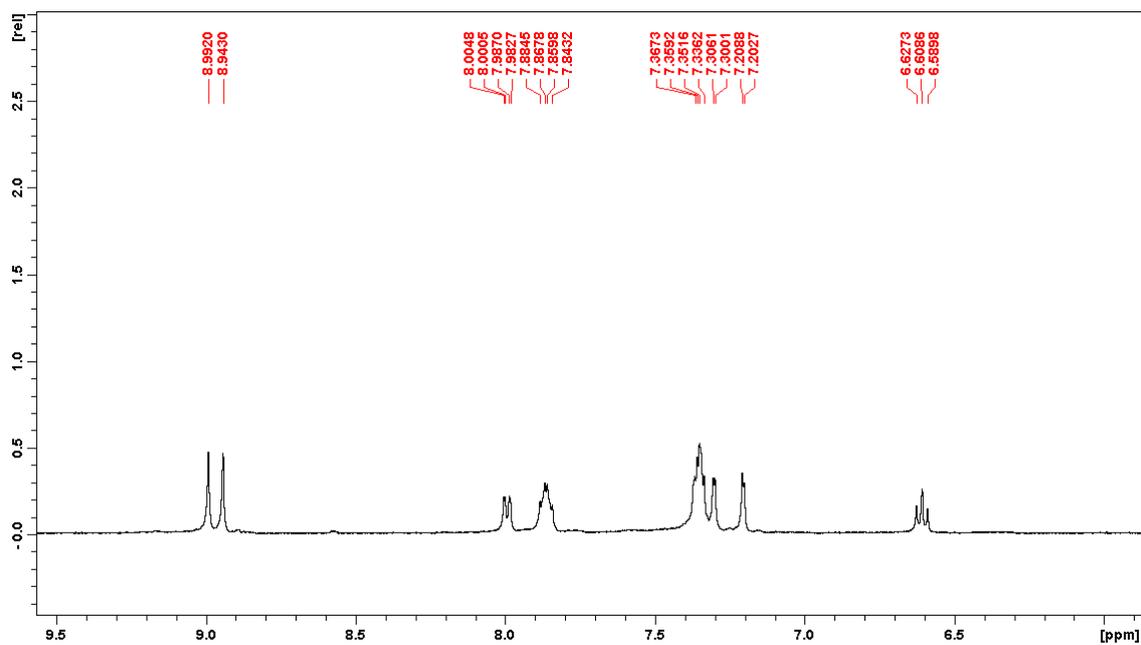
### Copies of NMR and MS spectra for complex **5**:



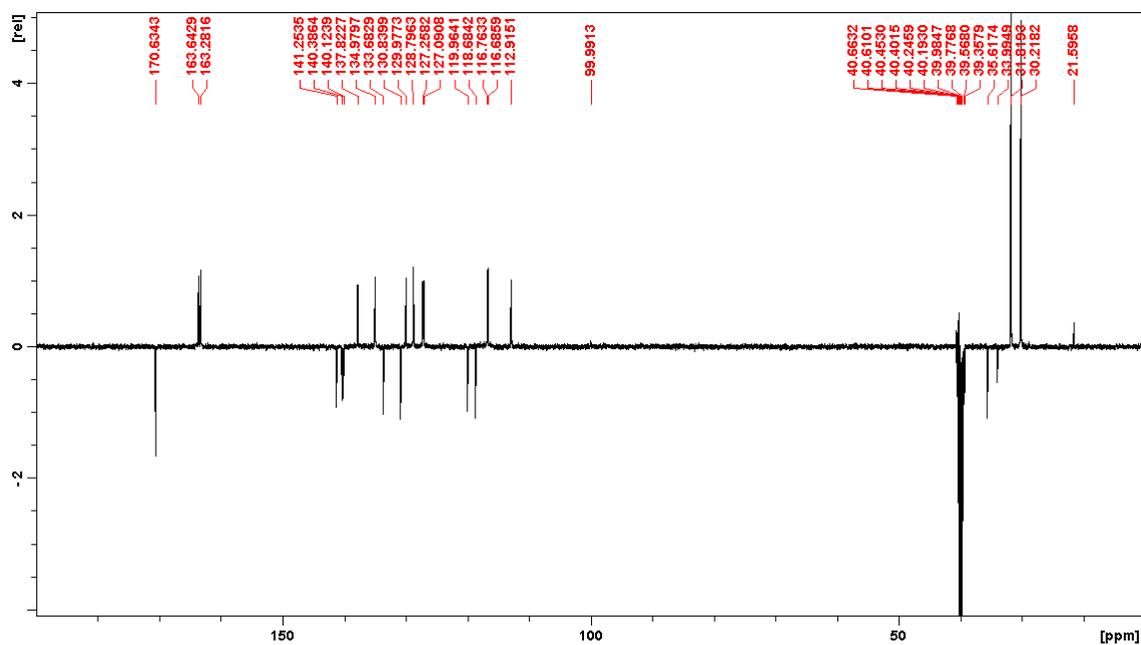
$^1\text{H}$  NMR in  $\text{DMSO-}d_6$ :



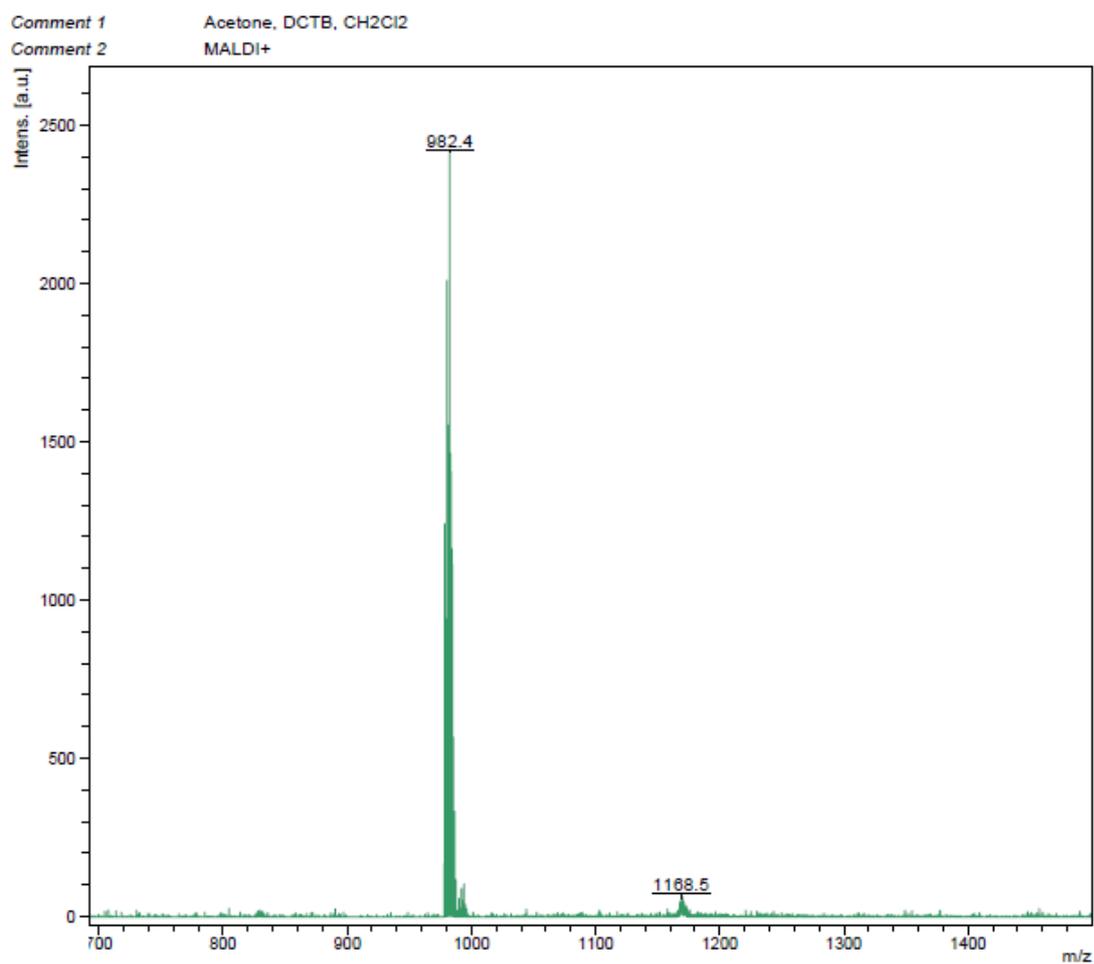
Extension of the aromatic region ( $^1\text{H}$  NMR for **5**, Acetone- $d_6$ ):



$^{13}\text{C}\{^1\text{H}\}$  NMR (DEPT-Q) in DMSO- $d_6$ :



MS spectrum recorded for **5** (MALDI+, dctb):

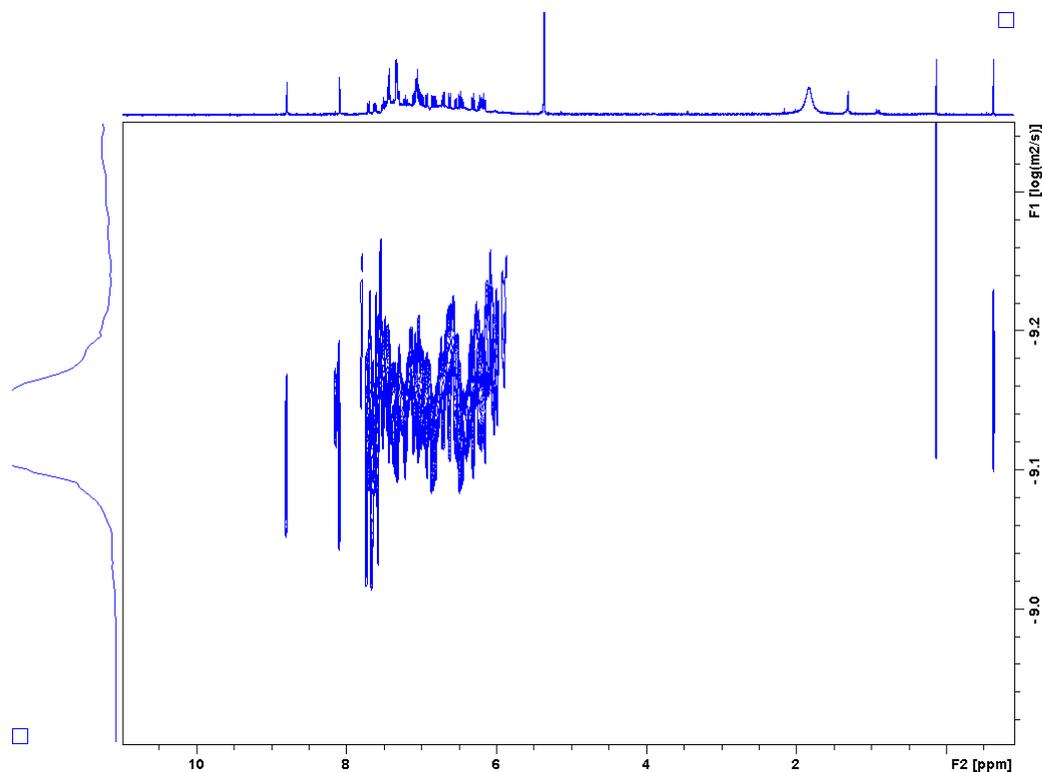


## DOSY NMR of complex 4:

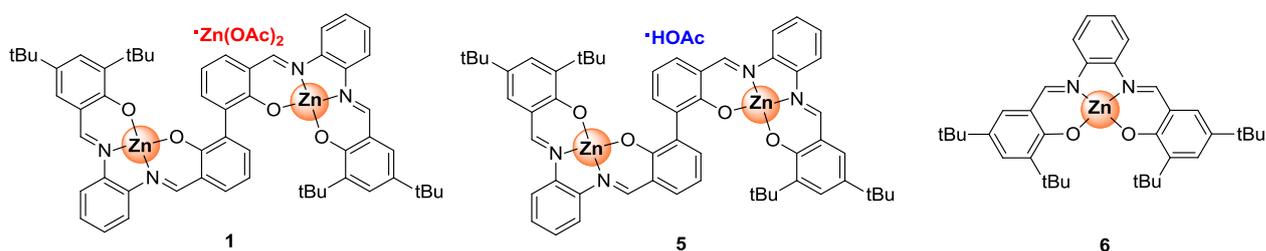
Solvent = CD<sub>2</sub>Cl<sub>2</sub>,  $r_{\text{calc}} = 7.04 \text{ \AA}$  using Stokes-Einstein equation for spherical particles:

$$D = \frac{k_B T}{6\pi \eta R}$$

where  $\eta$  is the viscosity of the medium and  $k_B$  is the Boltzmann's constant and  $R$  is the radius of the species.

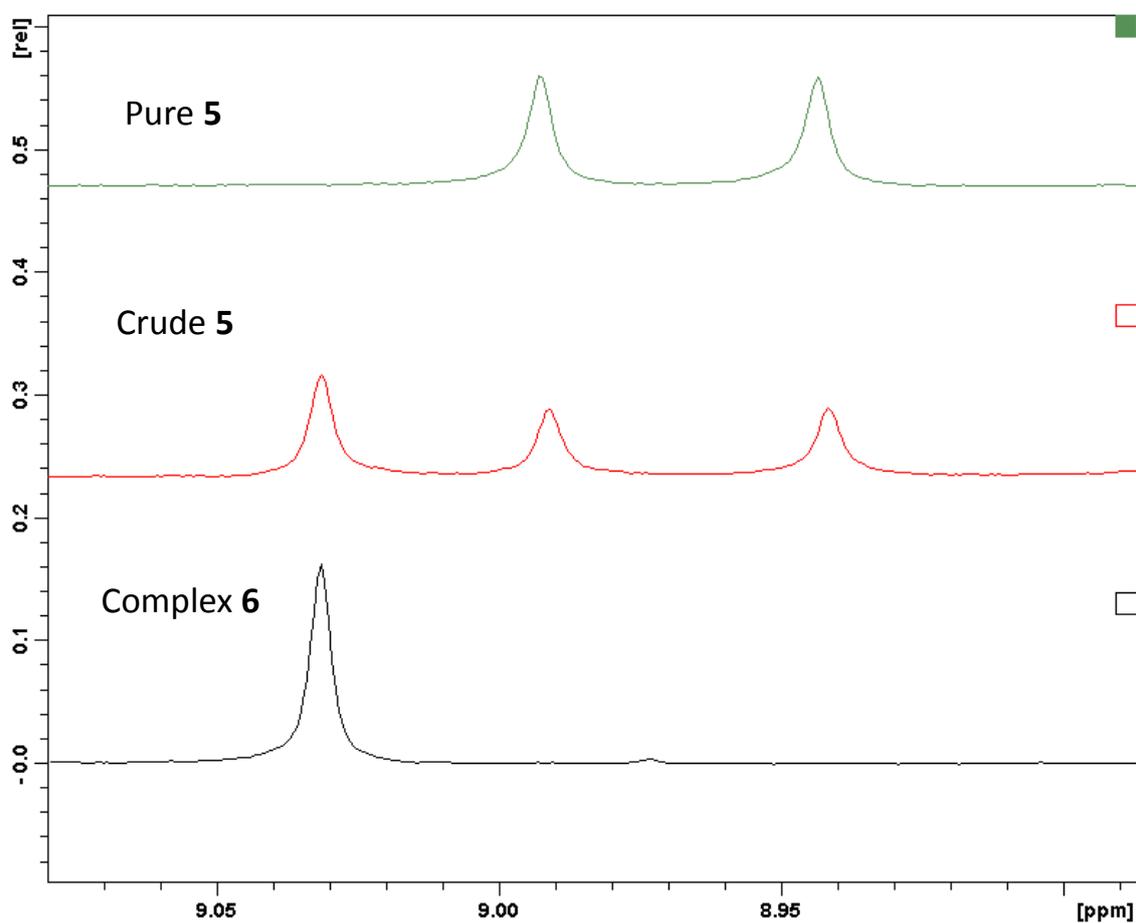


Comparison of the  $^1\text{H}/^{13}\text{C}$  NMR spectra for crude **5**, pure **5** and complex **1**:

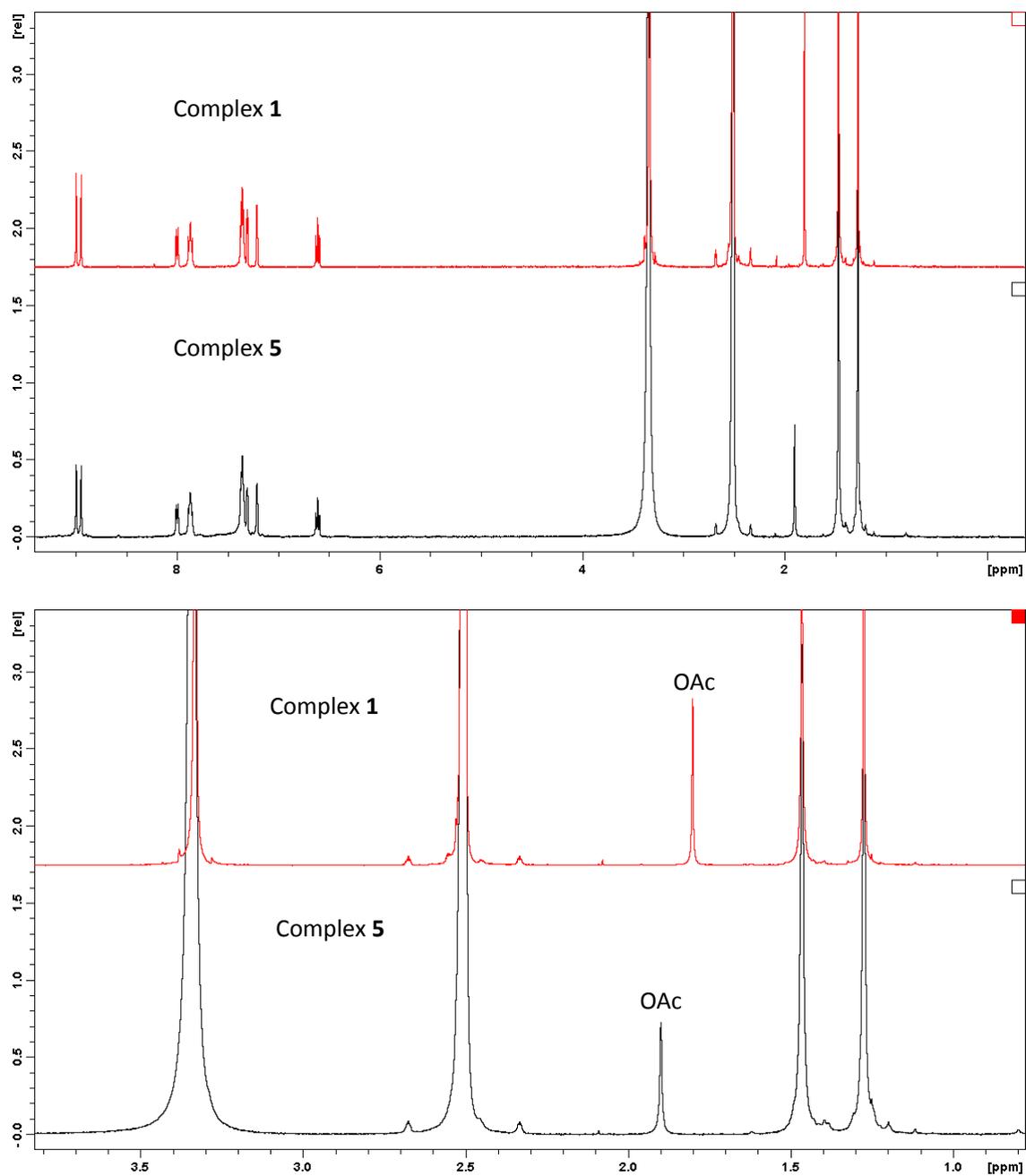


Solvent:  $\text{DMSO-}d_6$ , 400 MHz, r.t.

### IMINE REGION ( $\text{CH}=\text{N}$ ):



Full comparison between complex **1** and **5**; below an expansion is shown for the region where the OAc fragments resonate:



Comparison between complex **1** and **5**;  $^{13}\text{C}$  region of the OAc fragments (DMSO- $d_6$ ):

