

**Supporting Information**

**Novel 2-naphthyl substituted zinc naphthalocyanine: synthesis, optical,  
electrochemical and spectroelectrochemical properties**

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**Figure S1.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of dinitrile **2** in DMSO- $\text{d}_6$ : aromatic region (top), expanded fragment of aromatic region (bottom).

**Figure S2.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of dinitrile **2** in DMSO- $\text{d}_6$ : aromatic region (top), expanded fragment of aromatic region (bottom).

**Figure S3.** EI mass spectrum of compound **2**.

**Figure S4.** MALDI-TOF mass spectrum of complex **3**, isotopic pattern for the molecular ion (inset A) and simulated MS pattern of the molecular ion (inset B).

**Figure S5.** FT-IR spectra of zinc complex **3** in ZnSe (A) and compound **2** in KBr (B).

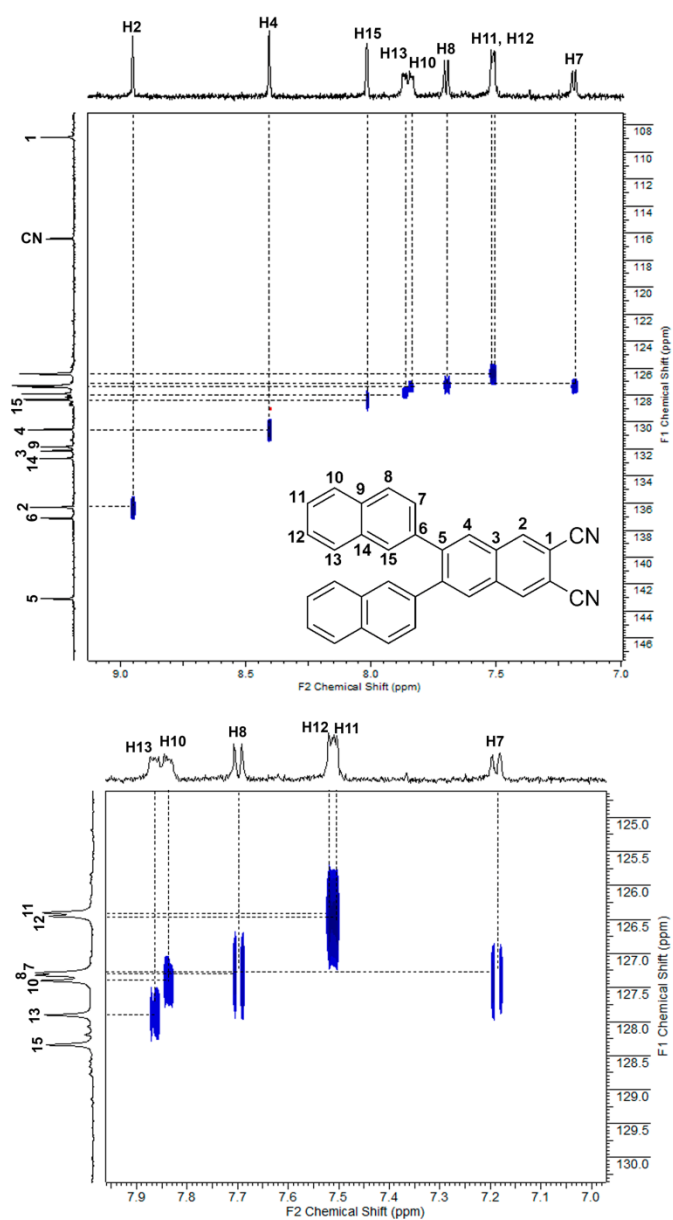
**Figure S6.** Thermogram (TG), derivative thermogravimetric curve (DTG) and differential scanning calorimetry (DSC) (A); results of evolved gas analysis by mass-spectrometry (B-G) for complex **3**.

**Figure S7.** UV-Vis spectra of the solution of **3** in *o*-DCB after addition of 1 vol % pyridine at various concentrations (green line -  $c=1.1\times 10^{-4}$ , blue line –  $c=6.9\times 10^{-6}$ , dashed lines – intermediate concentrations) (A). The molar extinction coefficient vs concentration plot (B).

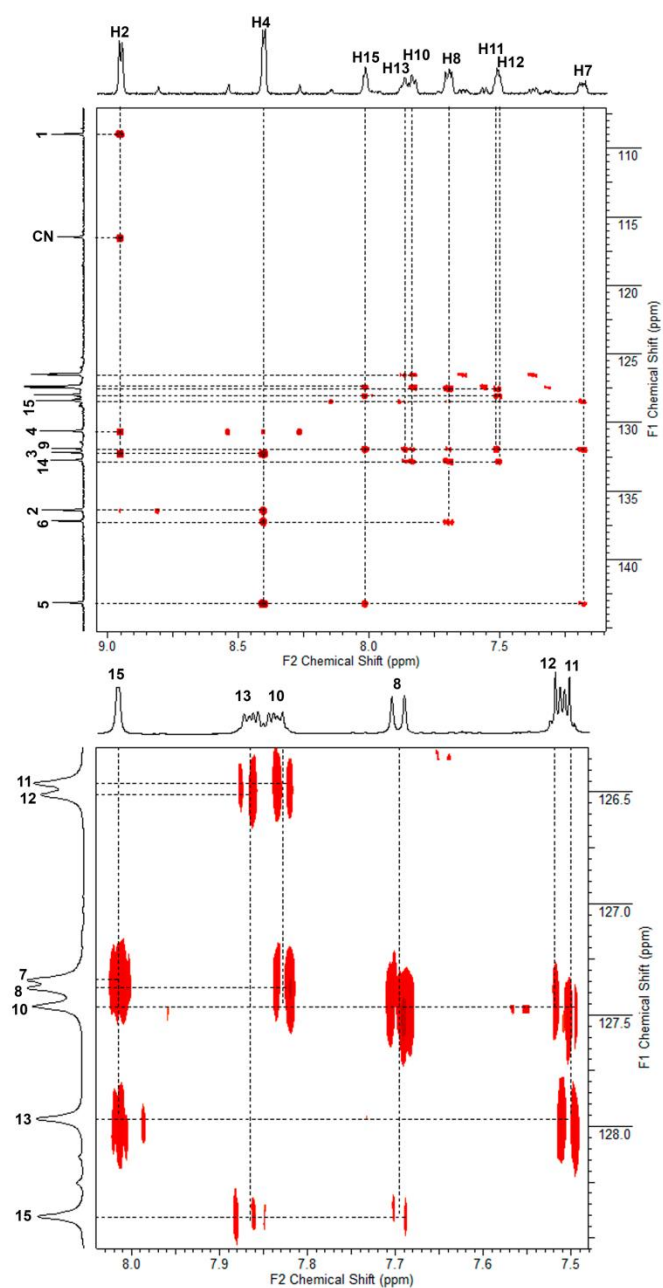
**Figure S8.** UV-Vis (solid lines) and fluorescence (dash lines,  $\lambda_{\text{ex}} = 695 \text{ nm}$ ), spectra of solution of compound **3** diluted from  $c=2.0\times 10^{-5} \text{ M}$  to  $c=1.25\times 10^{-6} \text{ M}$  in *o*-DCB after the addition of 1 vol% pyridine (A). Fluorescence quantum yield at various concentrations for the solution of compound **3** in *o*-DCB after the addition of 1 vol% pyridine (B).

**Figure S9.** UV-Vis (solid lines) and fluorescence (dash lines,  $\lambda_{\text{ex}} = 695 \text{ nm}$ ), spectra of solution of compound **3** diluted from  $c=2.0\times 10^{-5} \text{ M}$  to  $c=0.625\times 10^{-6} \text{ M}$  in *o*-DCB after addition of 0.12 M of  $\text{NBu}_4\text{F}$  (A). Fluorescence quantum yield at various concentrations for the solution of compound **3** in *o*-DCB after addition of 0.12 M of  $\text{NBu}_4\text{F}$ ,  $\lambda_{\text{ex}} = 695 \text{ nm}$  (B).

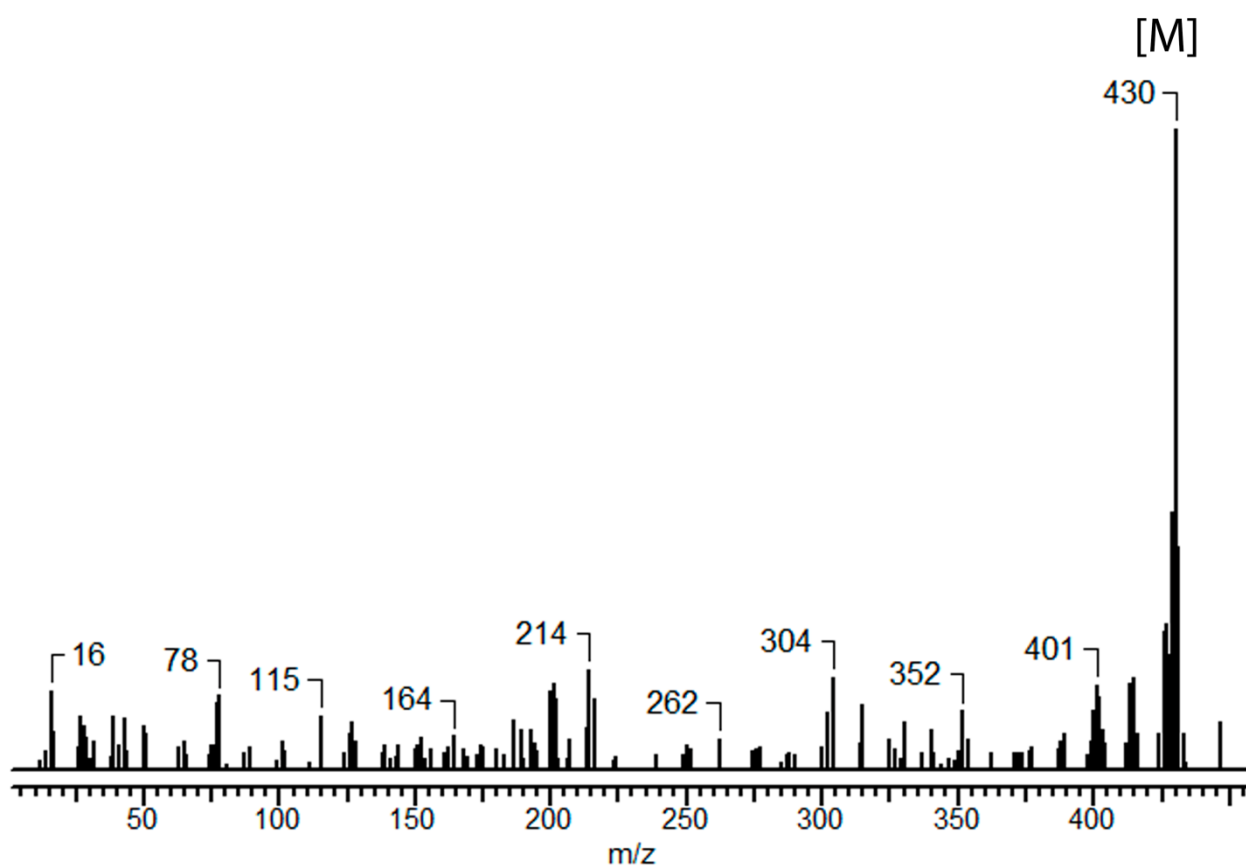
**Figure S10.** EPR spectra of freshly prepared solution of compound **3** in *o*-DCB ( $c=3\times 10^{-5} \text{ M}$ ) (black line) and solution after 7 days storage (blue line).



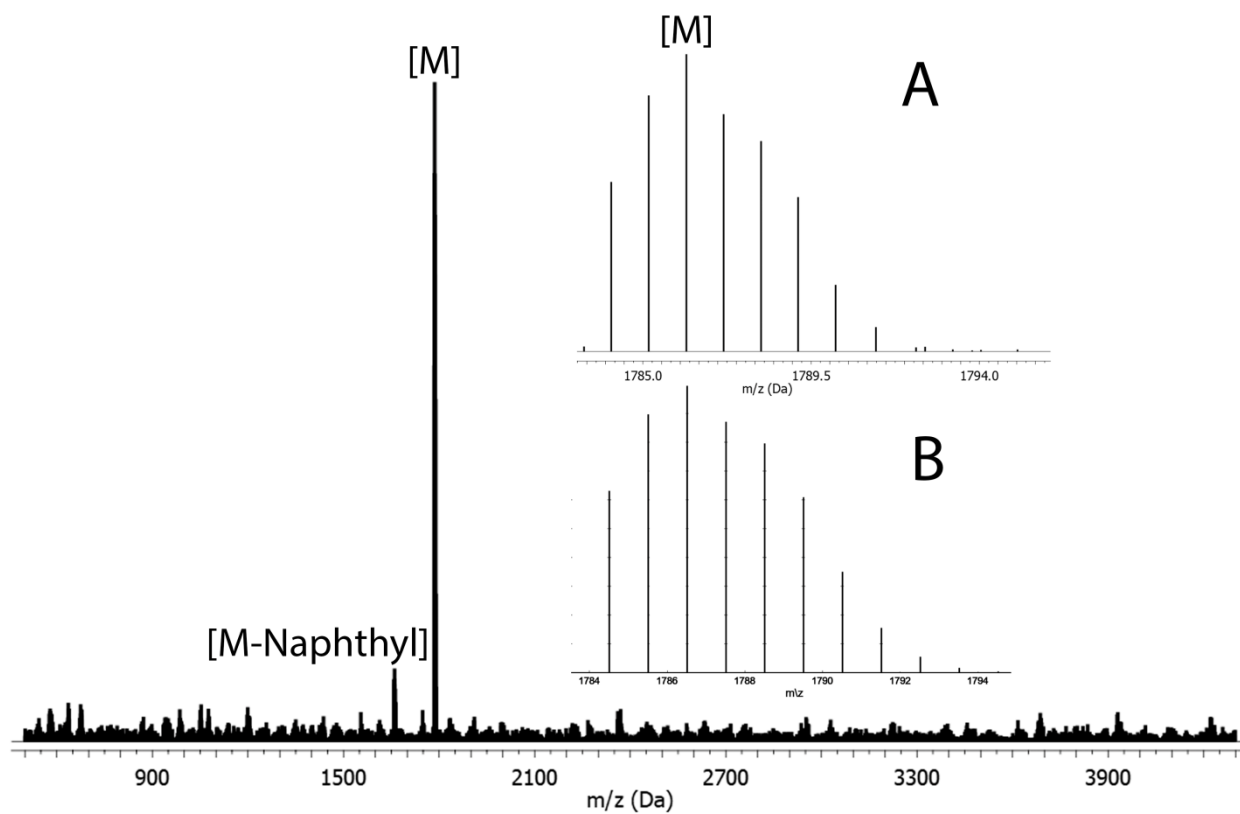
**Figure S1.**  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of dinitrile **2** in  $\text{DMSO-d}_6$ : aromatic region (top), expanded fragment of aromatic region (bottom).



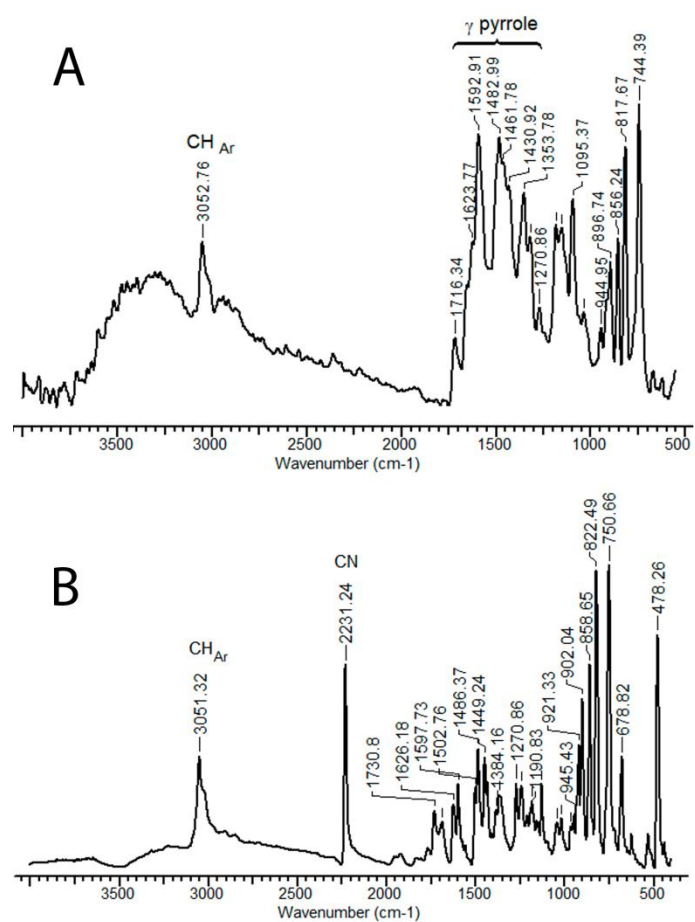
**Figure S2.**  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of dinitrile **2** in  $\text{DMSO-d}_6$ : aromatic region (top), expanded fragment of aromatic region (bottom).



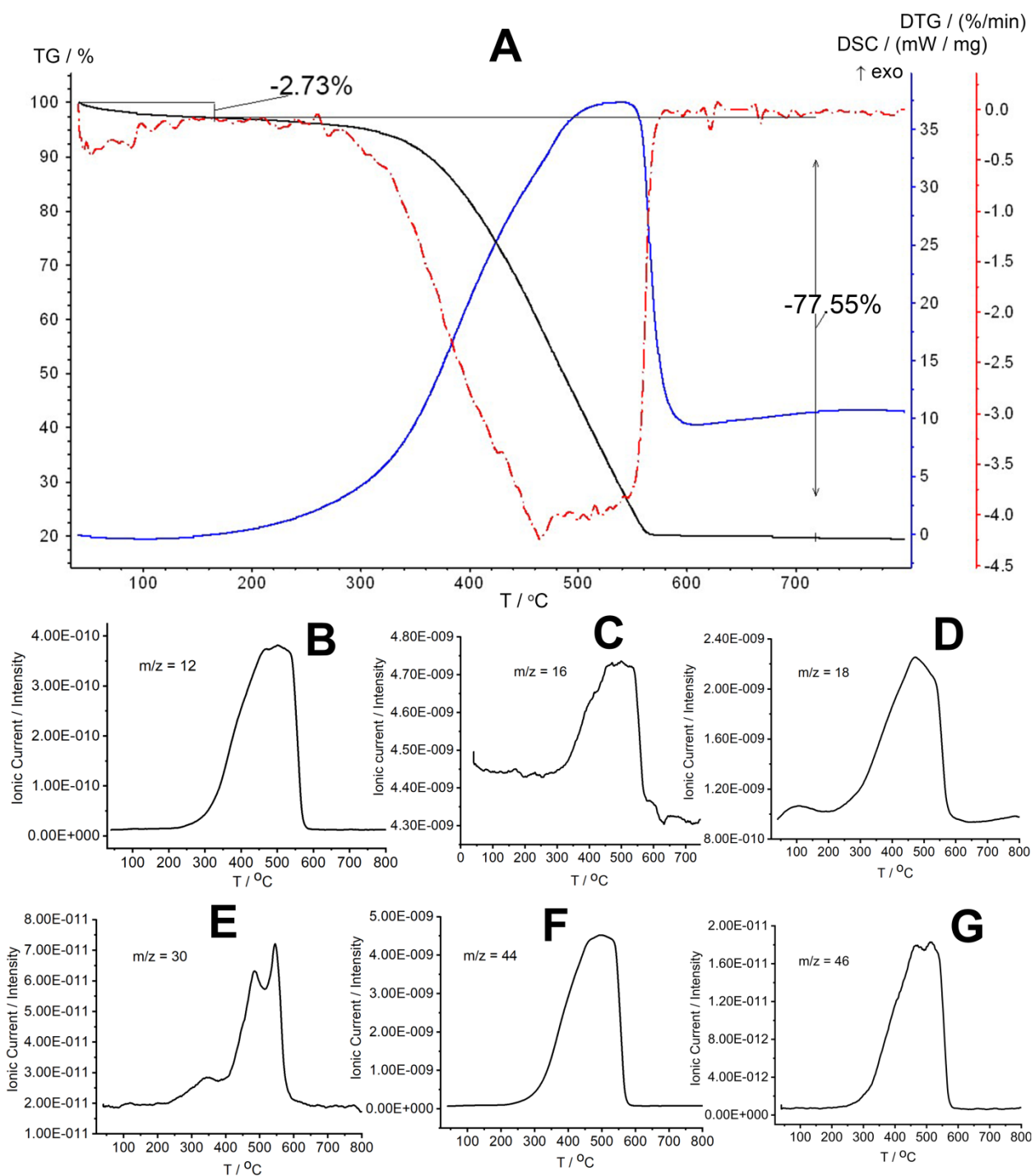
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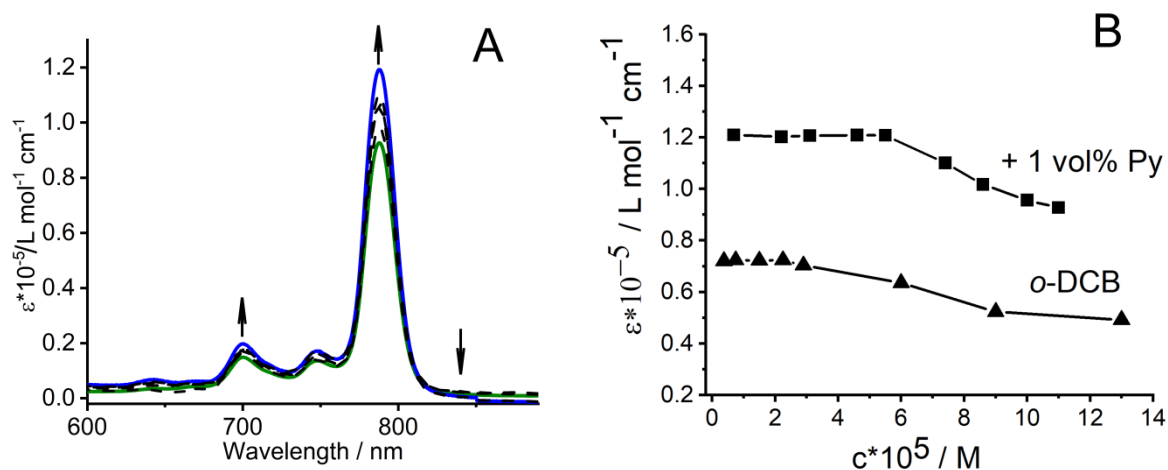


**Figure S5.** FT-IR spectra of zinc complex **3** in ZnSe (A) and compound **2** in KBr (B).

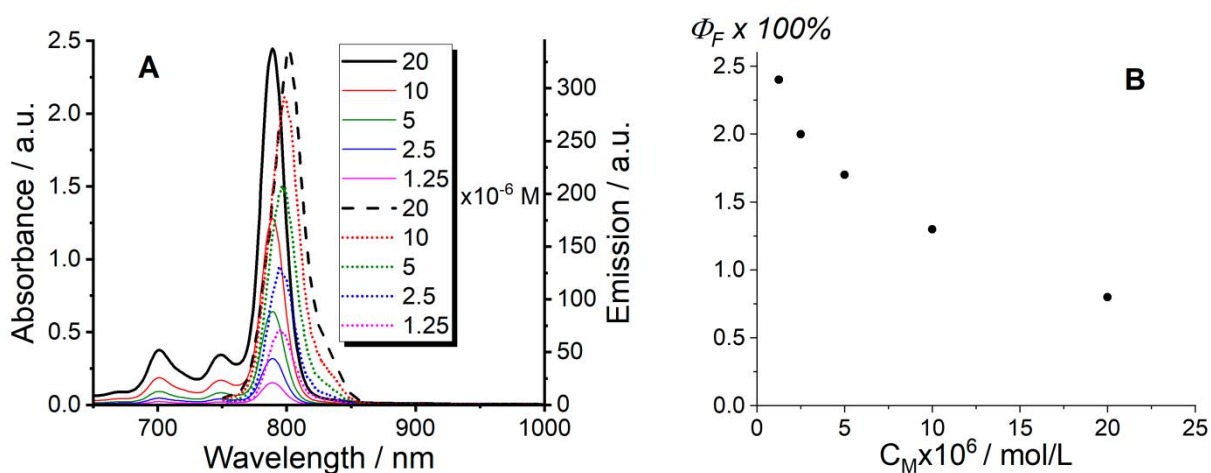


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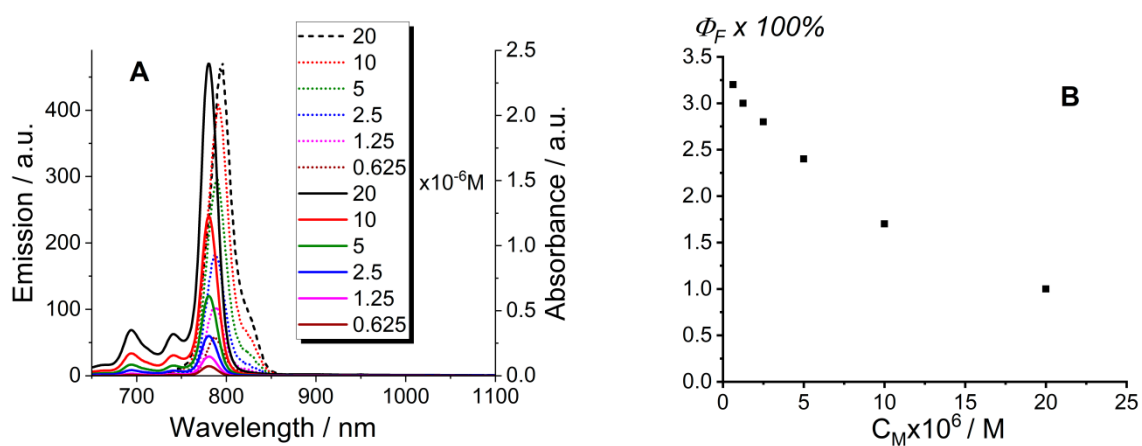




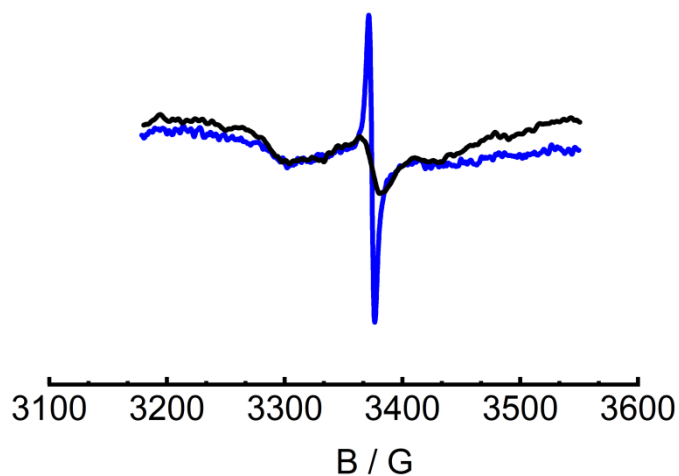
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**Figure S8.** UV-Vis (solid lines) and fluorescence (dash lines,  $\lambda_{\text{ex}} = 695$  nm), spectra of solution of compound **3** diluted from  $c = 2.0 \times 10^{-5}$  M to  $c = 1.25 \times 10^{-6}$  M in *o*-DCB after the addition of 1 vol% pyridine (A). Fluorescence quantum yield at various concentrations for the solution of compound **3** in *o*-DCB after the addition of 1 vol% pyridine (B).



**Figure S9.** UV-Vis (solid lines) and fluorescence (dash lines,  $\lambda_{\text{ex}} = 695 \text{ nm}$ ), spectra of solution of compound **3** diluted from  $c=2.0 \times 10^{-5} \text{ M}$  to  $c=0.625 \times 10^{-6} \text{ M}$  in *o*-DCB after addition of 0.12 M of NBu<sub>4</sub>F (A). Fluorescence quantum yield at various concentrations for the solution of compound **3** in *o*-DCB after addition of 0.12 M of NBu<sub>4</sub>F,  $\lambda_{\text{ex}} = 695 \text{ nm}$  (B).



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