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Supporting Information

Novel 2-naphthyl substituted zinc naphthalocyanine: synthesis, optical,

electrochemical and spectroelectrochemical properties

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Figure S1. ¹H-¹³C HSQC spectrum of dinitrile **2** in DMSO-d₆: aromatic region (top), expanded fragment of aromatic region (bottom).

Figure S2. ¹H-¹³C HMBC spectrum of dinitrile **2** in DMSO-d₆: 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 1vol % pyridine at various

concentrations (green line - c=1.1×10⁻⁴, blue line – c=6.9×10⁻⁶, dashed lines – intermediate

concentrations) (A). The molar extinction coefficient vs concentration plot (B).

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

Figure S9. UV-Vis (solid lines) and fluorescence (dash lines, $\lambda_{ex} = 695$ nm), spectra of solution of compound **3** diluted from c=2.0×10⁻⁵ M to c=0.625×10⁻⁶ M in *o*-DCB after addition of 0.12 M of NBu₄F (**A**). Fluorescence quantum yield at various concentrations for the solution of compound **3** in *o*-DCB after addition of 0.12 M of NBu₄F, $\lambda_{ex} = 695$ nm (**B**).

Figure S10. EPR spectra of freshly prepared solution of compound **3** in *o*-DCB ($c=3\times10^{-5}$ M) (black line) and solution after 7 days storage (blue line).



Figure S1. ¹H-¹³C HSQC spectrum of dinitrile **2** in DMSO-d₆: aromatic region (top), expanded fragment of aromatic region (bottom).



Figure S2. ¹H-¹³C HMBC spectrum of dinitrile **2** in DMSO-d₆: aromatic region (top), expanded fragment of aromatic region (bottom).



Figure S3. El 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 1vol % pyridine at various concentrations (green line - $c=1.1\times10^{-4}$, blue line - $c=6.9\times10^{-6}$, dashed lines - intermediate concentrations) (A). The molar extinction coefficient of *Q* band vs concentration plot (B).



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



Figure S9. UV-Vis (solid lines) and fluorescence (dash lines, $\lambda_{ex} = 695$ nm), spectra of solution of compound **3** diluted from c=2.0×10⁻⁵ M to c=0.625×10⁻⁶ M in *o*-DCB after addition of 0.12 M of NBu₄F (**A**). Fluorescence quantum yield at various concentrations for the solution of compound **3** in *o*-DCB after addition of 0.12 M of NBu₄F, $\lambda_{ex} = 695$ nm (**B**).



Figure S10. EPR spectra of freshly prepared solution of compound **3** in *o*-DCB ($c=3\times10^{-5}$ M) (black line) and solution after 7 days storage (blue line).