## Supporting Information for:

# Detection of Zinc Ions under Aqueous Conditions using Chirality Assisted Solid-state Fluorescence of a Bipyridyl based Fluorophore

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### Contents

Synthetic details, characterization data and spectral changes of **1a**. Solid-state quantum yield calculation for **1a**.

#### **Experimental Section**

All solvents were purified and dried by standard methods prior to use. Melting point was determined with a Mel-Temp-II melting point apparatus and is uncorrected. NMR spectra were recorded on 300 MHz Bruker Avance DPX spectrometer. FT-IR spectrum was recorded on a Nicolet Impact 400D infrared spectrophotometer. High-resolution mass spectra were recorded on a JEOL JM AX 505 HA mass spectrometer. Electronic absorption spectra were recorded on a Shimadzu UV-3101 PC NIR scanning spectrophotometer and the emission spectra were measured on a SPEX-Fluorolog F112X spectrofluorimeter.

# **Method of preparation of 1a.** [(5,5'-bis((E)-2-(1-((S)-3,7-dimethyloctyl)-1H-pyrrol-2-yl)vinyl)-2,2'-bipyridine)]

A suspension of sodium hydride (12 mmol) in dry THF was added slowly to a solution of the *tetraethyl 2,2'-bipyridine-5,5'-diylbis(methylene)diphosphonate* (2 mmol) and the respective (*S*)-*1-(3,7-dimethyloctyl)-1H-pyrrole-2-carbaldehyde* (4 mmol) in THF. After refluxing for 12 h, the fluorescent reaction mixture obtained was cooled followed by the removal of THF under reduced pressure to give a pasty residue. The residue was suspended in water and extracted with dichloromethane. The organic layer was washed with brine, dried over  $Na_2SO_4$  and concentrated to give the crude product, which was further purified by column chromatography over basic alumina using ethyl acetate-petroleum ether as eluent. Yields, melting points, and spectral details of each product are given below. Yield 41%; mp. 82 <sup>o</sup>C; IR (KBr)  $v_{max}$  2925, 2853, 1699, 1626, 1467, 1209, 1045, 950, 850, 727 cm<sup>-1</sup>; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz)  $\delta$  0.83 (m, 12H, CH<sub>3</sub>), 1.12 (m, 16H, CH<sub>2</sub>), 1.71 (m, 2H, CH), 3.97 (m, 4H, NCH<sub>2</sub>), 6.17 (t, 2H, aromatic), 6.57 (d, 2H, aromatic), 6.71 (s, 2H, aromatic), 6.85 (d, 2H, vinylic, *J* = 16.08 Hz), 7.05 (d, 2H, vinylic, *J* = 16.02 Hz), 7.84 (m, 2H, aromatic), 8.34 (d, 2H, aromatic), 8.70 (s, 2H, aromatic); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz)  $\delta$  10.63, 13.98, 22.94, 23.86, 28.56, 29.65, 30.54, 41.27, 50.88, 107.34, 108.37, 119.16, 120.70, 121.20, 1124.08, 130.96, 132.58, 133.53, 147.36, 153.87; HRMS-FAB: [M+H]<sup>+</sup>:Calculated for C<sub>42</sub>H<sub>58</sub>N<sub>4</sub>: 619.47, Obtained: 619.76.

### Method of preparation of dipstick probe and PMMA film

Thermoplastic or glass supports were cut into small units having 10cm length and 4mm radius. This can be prepared in variable length depending upon the nature of the samples to be analyzed. To 10mg of **1a** dissolved in 15ml chloroform, 2gm of finely powdered alumina was added and allow 10 minutes for the solvent to evaporate off at room temperature. **1a** containing finely powdered alumina is yellow in color and having a greenish yellow fluorescence. The fine powdered alumina slurry was bound to one end of the above mentioned thermoplastic support up to 5cm from the bottom of the stick, such that the end with **1a** can be dipped into sample solution for detection purpose. The dipstick probe can be used as such for detection purposes.

**1a** dissolved in chloroform was added to a viscous solution of PMMA in chloroform, and drop casted over glass slides. The film after solvent evaporation was kept in vacuum oven for 12 hours and used as such for quantum yield measurements.



Figure S1. <sup>1</sup>H NMR Spectrum of 1a in CDCl<sub>3</sub>.



Figure S2. High resolution mass spectrum of 1a.

### **Fluorescence Quantum Yield in Solution**

Fluorescence quantum yield was determined in spectroscopic grade CH<sub>3</sub>CN using optically matching solutions of quinine sulfate ( $\Phi_{\rm f} = 0.546$  in 1N H<sub>2</sub>SO<sub>4</sub>) as standard at an excitation wavelength of 360 nm. The quantum yield is calculated using equation **1**.

where,  $A_s$  and  $A_r$  are the absorbance of the sample and reference solutions, respectively at the same excitation wavelength,  $F_s$  and  $F_r$  are the corresponding relative integrated fluorescence intensities and  $\eta$  is the refractive index of the solvents.<sup>1</sup>

### Fluorescence Quantum Yield in Solid-state

Solid state quantum yield was calculated by Horiba Jobin Yvon Quantum Yield Calculator using equation  $2^{2}$ 

 $\Phi_{f \text{ (solid state)}} = E_i(\lambda) - (1 - A)E_0(\lambda)/L_e(\lambda)A....(2)$ 

{ *A* (*film absorbance*) =  $L_0(\lambda)-L_i(\lambda)/L_0(\lambda)$  }

where  $E_i(\lambda)$  and  $E_0(\lambda)$  are respectively, the integrated luminescence as a result of the direct excitation of the film and as secondary excitation.  $L_0(\lambda)$  and  $L_i(\lambda)$  are integrated excitations when the excited light directly hits the sphere, and when the film is directly excited.  $L_e(\lambda)$  is the integrated excitation profile for an empty sphere.



Figure S3. (a) Magnification of excitation lines. Red solid line gives  $L_0$  parameter (integrated excitation when the light directly hits the sphere in the absence of sample film). Dashed line gives  $L_i$  parameter (integrated excitation when the sample film is directly excited). (b) Photoluminescence of 1a in PMMA matrix. The fluorescence quantum yield of the emission in the film state is calculated as described above.<sup>1</sup>



**Figure S4**. Changes in the (a) absorption and (b) emission spectra of **1a** (6  $\mu$ M) upon addition of Zn<sup>2+</sup> (0–6  $\mu$ M) in acetonitrile.



Figure S5. Absorption spectra of 1a and 1a- $Zn^{2+}$  complex in the solid state.

## **References:**

- (1) "Physical Constants of Organic Compounds" in CRC hand book of Chemistry and Physics, 88<sup>th</sup> (CD-Rom Version 2008), David R. Lide, ed., CRC Press/Taylor and Francis, Boca Raton, FL.
- (2) L.-O. Pålsson, A. P. Monkman, Adv. Mater. 2002, 14, 757-758.