

## Supporting Information

# ***Oligo(p-phenyleneethynylene)* Derived Porous Luminescent Nanoscale Coordination Polymer of Gd<sup>III</sup>: Bimodal Imaging and Nitroaromatic Sensing**

Venkata M Suresh,<sup>†</sup> Snehajyoti Chatarjee,<sup>‡</sup> Rahul Modak,<sup>‡</sup> Vivek Tiwari,<sup>§</sup> Anant B Patel,<sup>§</sup>

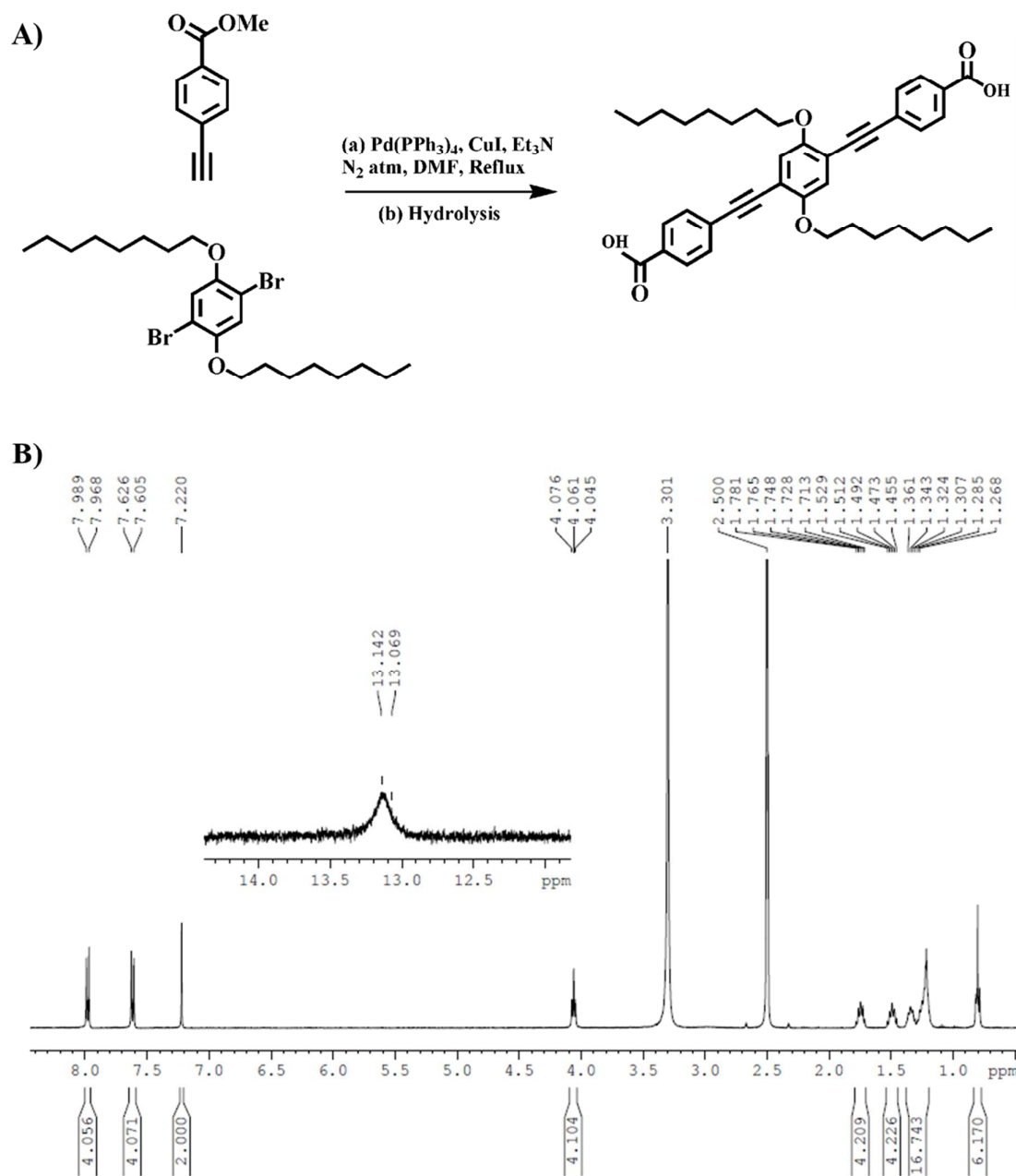
Tapas K Kundu,<sup>‡</sup> and Tapas Kumar Maji\*,<sup>†</sup>

<sup>†</sup>Molecular Materials Laboratory, Chemistry and Physics of Materials Unit, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Jakkur, Bangalore, India-560064

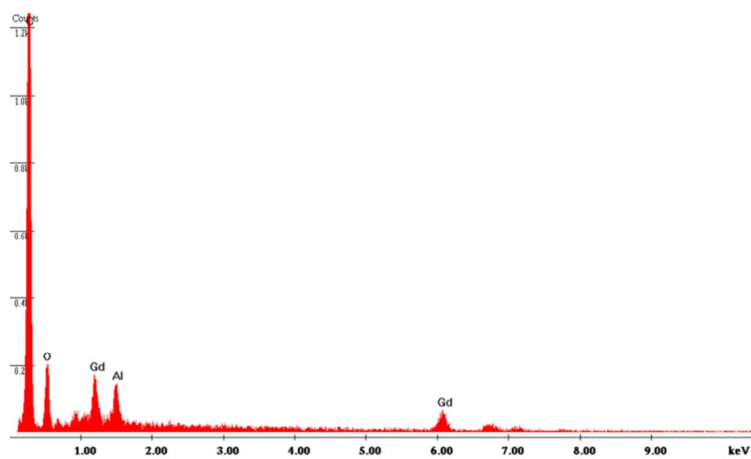
<sup>‡</sup>Transcription and Disease Laboratory, Molecular Biology and Genetics Unit, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Jakkur, Bangalore, India-560064

<sup>§</sup>NMR Microimaging and Spectroscopy, Centre for Cellular & Molecular Biology, Uppal Road, Hyderabad, India-500007

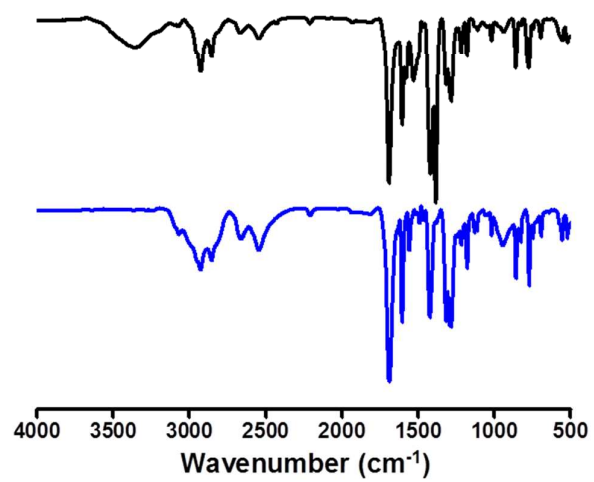
\*Corresponding Author Tel: +91-80-22082826; e-mail address: tmaji@jncasr.ac.in



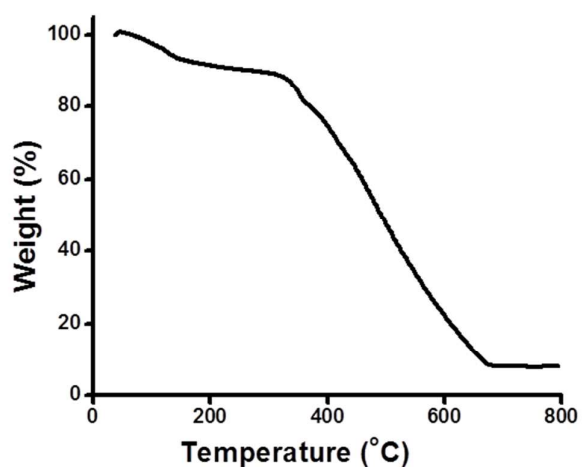
**Figure S1.** A) Synthetic scheme of OPEA ligand and B)  $^1\text{H}$  NMR spectra of OPEA in  $\text{dms-}d_6$ .



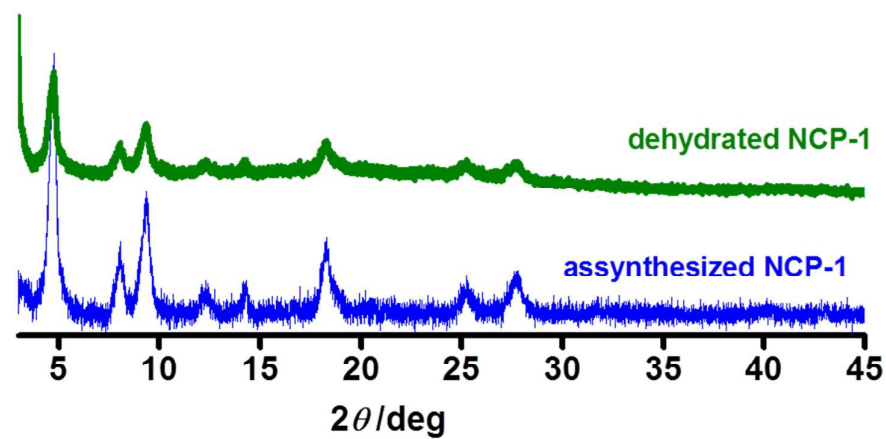
**Figure S2.** Energy dispersive X-ray analysis (EDAX) of NCP-1.



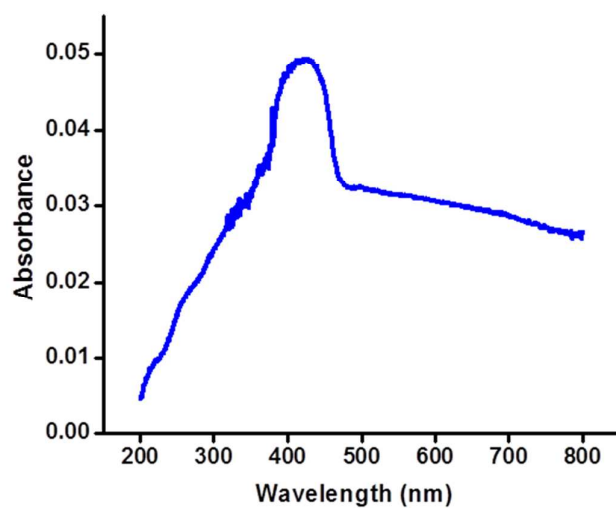
**Figure S3.** FTIR spectra of OPEA (blue) and NCP-1 (black).



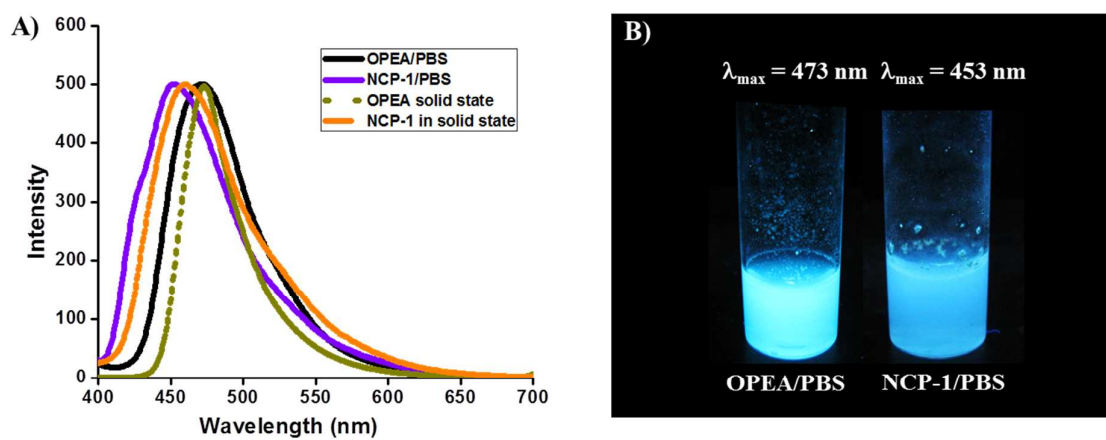
**Figure S4.** TGA curve of NCP-1 in the temperature range of 30-800 °C with a heating rate of 5 °C/min.



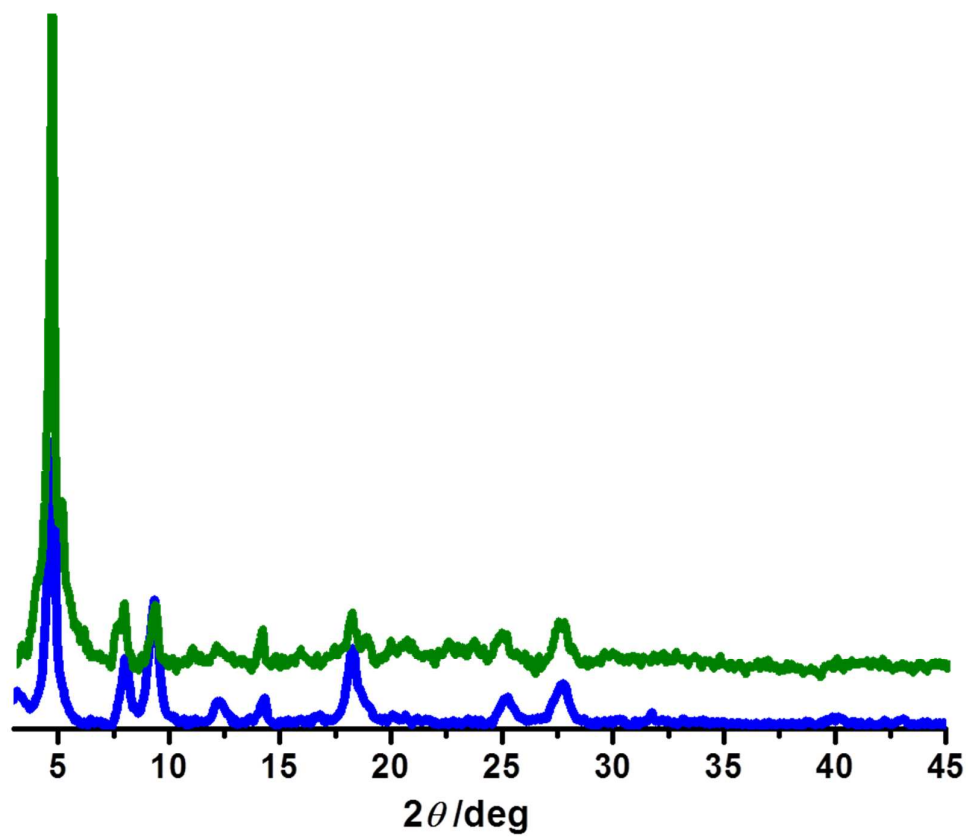
**Figure S5.** PXRD patterns of assynthesized NCP-1 (blue) and dehydrated NCP-1 (green) showing the stability of compound on removal of guest molecules.



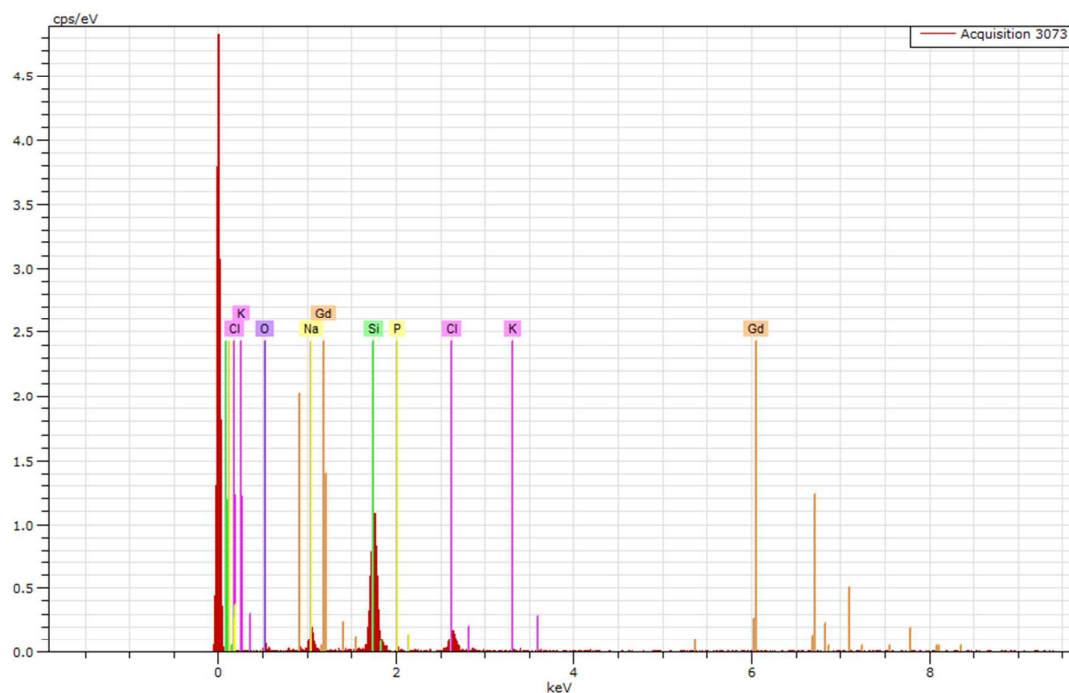
**Figure S6.** Solid state absorbance spectra of NCP-1.



**Figure S7.** A) Fluorescence spectra; OPEA in solid state (dark yellow), OPEA in PBS (black), NCP-1 in solid state (orange) and NCP-1 in PBS buffer (violet). Excitation wavelength is 390 nm in all cases. B) Images of OPEA and NCP-1 dispersed in PBS buffer under UV light.



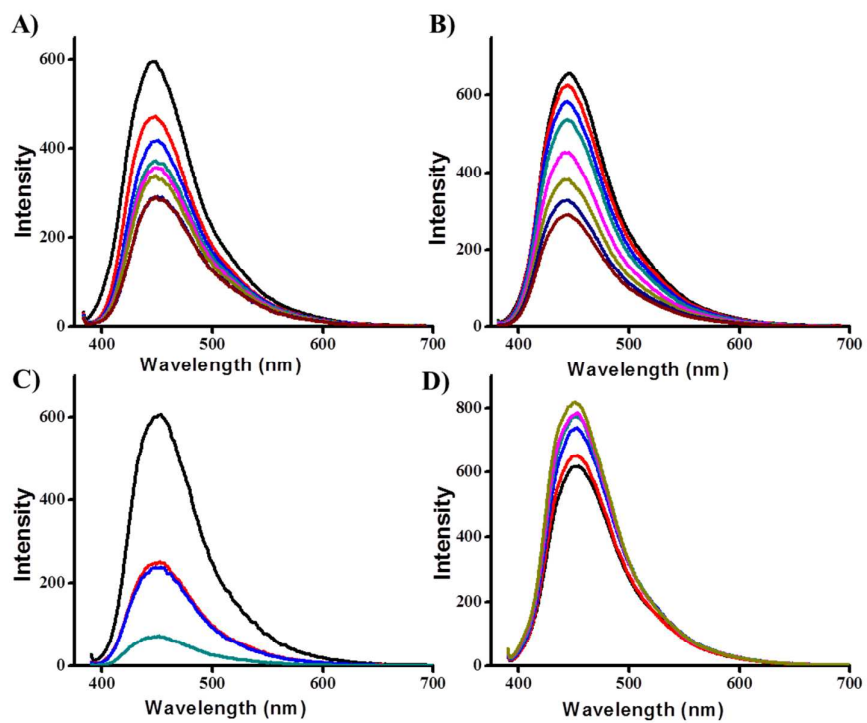
**Figure S8.** Powder X-ray diffraction pattern of assynthesized NCP-1 (blue) and NCP-1 incubated in PBS (green).



Spectrum: Acquisition 3073

El	AN	Series	unn. C [wt.%]	norm. C [wt.%]	Atom. C [at.%]	Error [wt.%]
Si	14	K-series	55.31	61.41	58.14	2.8
Cl	17	K-series	14.70	16.32	12.24	1.0
Na	11	K-series	10.04	11.15	12.90	1.1
O	8	K-series	8.14	9.04	15.03	5.9
P	15	K-series	1.37	1.53	1.31	0.3
K	19	K-series	0.50	0.56	0.38	0.2
Gd	64	L-series	0.00	0.00	0.00	0.0
Total:			90.07	100.00	100.00	

**Figure S9.** EDAX analysis of decant obtained from **NCP-1** incubated in PBS showing no leaching of  $\text{Gd}^{\text{III}}$  ions into the solution suggesting stability of **NCP-1** under physiological conditions.



**Figure S10.** Fluorescence behaviour of **NCP-1** in presence of A) nitromethane ( $1 \times 10^{-3}$  M), B) *o*-nitrophenol ( $3 \times 10^{-3}$  M), C) nitrobenzene ( $1 \times 10^{-4}$  M) and D) toluene. Black curves represent fluorescence intensity of **NCP-1** before analyte addition.