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## **Supporting Information**



**Figure S1:** <sup>1</sup>H NMR spectrum of **1** in CDCl<sub>3</sub> at 25 °C.

**Figure S2:** <sup>13</sup>C NMR spectrum of **1** in CDCl<sub>3</sub> at 25 °C.







Figure S4: <sup>1</sup>H NMR spectrum of 2 in DMSO-d<sub>6</sub> at 25 °C.





Figure S5: <sup>13</sup>C NMR spectrum of 2 in DMSO-d<sub>6</sub> at 25 °C.



**Figure S7.** Solid state packing of **2**. View along a axis.

Figure S8. Solid state packing of 2. View along b axis.



Figure S9. Compounds 1 and 2 under UV-vis light



- 1 –in acetonitrile
- 2 in mixture of acetonitrile + methanol+ chloroform (1:1:1)

**Figure S10.** Absorption spectrum of GP-GR-53 at 5x10<sup>-6</sup> in mixture 1:1:1 of Acetonitrile, Methanol and Chloroform.





**Figure S11.** Emission spectrum of **2** at  $\lambda_{ex}$ = 360 nm excitation.



Figure S12. Concentration depended PL Spectra of compound 2 at  $\lambda_{ex}$ =358 nm.

Figure S13. Concentration depended PL Spectra of compound 1 at  $\lambda_{ex}$ =358 nm.







Figure S15. Emission spectrum of compound 2 at  $\lambda_{ex}$ =358 nm.









**Figure S17.** Emission spectra of **2** in solid state at room temperature with different excitations (red line,  $\lambda_{ex}$ =320 nm; filter used UV-35), (black line,  $\lambda_{ex}$ =330 nm; filter used UV-35), (blue line,  $\lambda_{ex}$ =397 nm; filter used L-42), spectra of **2** in solid state at room temperature. (Note: (black line,  $\lambda_{ex}$ =330 nm; filter used UV-35) peak at 660 is double excitation energy).





Figure S19. 3D fluorescence spectrum of 2 in DMSO.







Figure S21. 3D fluorescence spectrum of 2 in film mode.





**Figure S22.** Top:  $\pi \cdots \pi$  interaction in **1**. Bottom:  $\pi \cdots \pi$  interaction in **2**.



**Figure S23.** C-H·····Br and C-H·····Hhydrogen bonding interactions in **2**.

Table S1. Crystal data and structure refinement for 1.

Empirical formula	$C_{3.38}H_{3.63}N_{0.63}Se_{0.25}$
Formula weight	581.48
Temperature/K	293
Crystal system	orthorhombic
Space group	Pbca
a/Å	16.0791(3)
b/Å	11.5168(2)
c/Å	29.4333(6)
a/°	90
β/°	90
$\gamma/^{\circ}$	90
Volume/Å <sup>3</sup>	5450.48(19)
Z	8
$\rho_{calc}g/cm^3$	1.4171

3.568
2344.3
$0.08\times0.06\times0.06$
Cu Ka ( $\lambda$ = 1.54184)
6 to 141.74
-16 $\leq$ h $\leq$ 19, -13 $\leq$ k $\leq$ 13, - 35 $\leq$ l $\leq$ 26
14786
5164 [ $R_{int} = 0.0321$ , $R_{sigma} = 0.0332$ ]
5164/0/311
1.042
$R_1 = 0.0515, wR_2 = 0.1503$
$R_1 = 0.0712, wR_2 = 0.1786$
0.90/-1.15

Empirical formula	$C_{27}H_{29}N_5ZnSe_2Br_2$
Formula weight	1613 37
Temperature/K	203
Crystal system	monoclinic
Space group	P2 / n
	$\Gamma 2_1/\Pi$ 11 5441(0)
d/A	11.3441(9) 14.0004(12)
$\mathbf{D}/\mathbf{A}$	14.9994(13)
C/A	18.5505(18)
$\alpha/\circ$	90
β/ <sup>o</sup>	105.613(9)
$\gamma/3$	90
Volume/A <sup>3</sup>	3093.6(5)
Z	2
$\rho_{calc}g/cm^3$	1.7319
$\mu/\text{mm}^{-1}$	7.008
F(000)	1560.6
Crystal size/mm <sup>3</sup>	$0.21\times0.19\times0.15$
Radiation	Cu K $\alpha$ ( $\lambda$ = 1.54184)
20 range for data collection/°	7.7 to 145.46
Tu day nan aas	$-14 \le h \le 13, -18 \le k \le 17, -$
Index ranges	$22 \le l \le 18$
Reflections collected	12465
Independent reflections	$5798 [R_{int} = 0.0396, R_{sigma} = 0.05221$
	0.0533]
Data/restraints/parameters	5/98/0/338
Goodness-of-fit on $F^2$	1.038
Final K indexes $[1 \ge 2\sigma(1)]$	$R_1 = 0.0524, WR_2 = 0.1272$
Final R indexes [all data]	$R_1 = 0.0815, wR_2 = 0.1676$
Largest diff. peak/hole / e Å <sup>-3</sup>	0.99/-1.01

 Table S2. Crystal data and structure refinement for 2.\*

\* Symmetry code: 2-X,-Y,-Z

## Materials and methods

The solvents were purchased from commercial sources and freshly distilled under argon atmosphere prior to use. Unless otherwise stated, the chemicals were purchased from commercial sources. L was synthesized as reported.<sup>1</sup> Elemental analyses were performed by the Euro EA-300 elemental analyser. NMR spectra were recorded on Bruker Ultra shield 400 spectrometer at 25 °C. Chemical shifts are given relative to TMS and were referenced to the solvent resonances as internal standards. Thermogravimetric analysis (TGA) was performed using a TASDT Q600, Tzero-press. The UV-vis spectra were measured on a T90+ UV-visible spectrophotometer. Photoluminescent excitation spectra were recorded by a HORIBA JOBIN YVON Fluoromax 4P spectrofluorometer. The steady state and time resolved photoluminescence properties of 2 using fluorescence spectrometer from Edinburgh Instruments (FLS 1000) was investigated. For steady state luminescence measurement, the sample was exited using 360 nm collimated beam from the excitation monochromator of the spectrometer, which is pumped using a 450 W Xe2 continuous xenon lamp. The emission spectrum after passing through emission monochromator is scanned and detected in high-gain red sensitive photomultiplier (PMT) detector with spectral coverage from 200 nm to  $\sim 870$  nm. The luminescence lifetime was measured using standard time-correlated single photon counting (TCSPC) technique using picosecond pulsed diode laser of wavelength 405 nm from Edinburgh Instruments (EPL-405) with repetition rate 200 KHz. The decay is fitted using reconvolution fit analysis using the IRF to extract the life-time parameters from the whole time resolved measurement. FT-IR measurements were carried out on a Bruker Alpha-P Fourier transform spectrometer.

The crystal structures of **1** and **2** were measured on an Oxford Supernova diffractometer. Single crystals were mounted on a Goniometer KM4/Xcalibur equipped with Sapphire2 (large Be window) detector (CuK $\alpha$  radiation source,  $\lambda = 1.5418$  Å). Crystals of **1** were isolated from its CHCl<sub>3</sub> solution at room temperature over a period of 48 h, while **2** were obtained from mixture of acetonitrile, methanol and chloroform (2:1:0.5) solution of **2** at room temperature over a period of 48 h. The suitable single crystals for X-ray structural analysis were mounted at room temperature (293 K) in inert oil under an argon atmosphere. Using Olex2, the structure was solved with the ShelXS structure solution program using Direct Methods and refined with the

olex2.refine refinement package using Gauss-Newton minimization.<sup>2-4</sup> Absorption corrections were performed on the basis of multi-scans. Non-hydrogen atoms were anisotropically refined. Hydrogen atoms were included in the refinement in calculated positions riding on their carrier atoms. No restraint has been made for any of the compounds.

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