

Electronic Supplementary Information (ESI)

Phenyl selenoxide functionalized TPA/TPE π -conjugated imidazo[1,2-a]pyridine: A fluorescent probe for the selective detection of water in organic solvents

Jerome Issac,^a R. Rameshbabu Priyadharsan,^b Kamalanathan Chidambaranathan,^a Subramanian Karthikeyan,^c Dohyun Moon,^{d*} Savarimuthu Philip Anthony,^{b*} Vedichi Madhu^{a*}

^a*Multifunctional Materials and Catalysis Laboratory, Division of Physical Sciences, Karunya Institute of Technology and Sciences, Coimbatore-641 114, Tamil Nadu, India. Tel: +914222614483; E-mail: madhu@karunya.edu; vmadhuu1@gmail.com.*

^b*School of Chemical & Biotechnology, SASTRA University, Thanjavur- 613401, Tamil Nadu, India. Tel: +914362264101; E-mail: philip@biotech.sastra.edu*

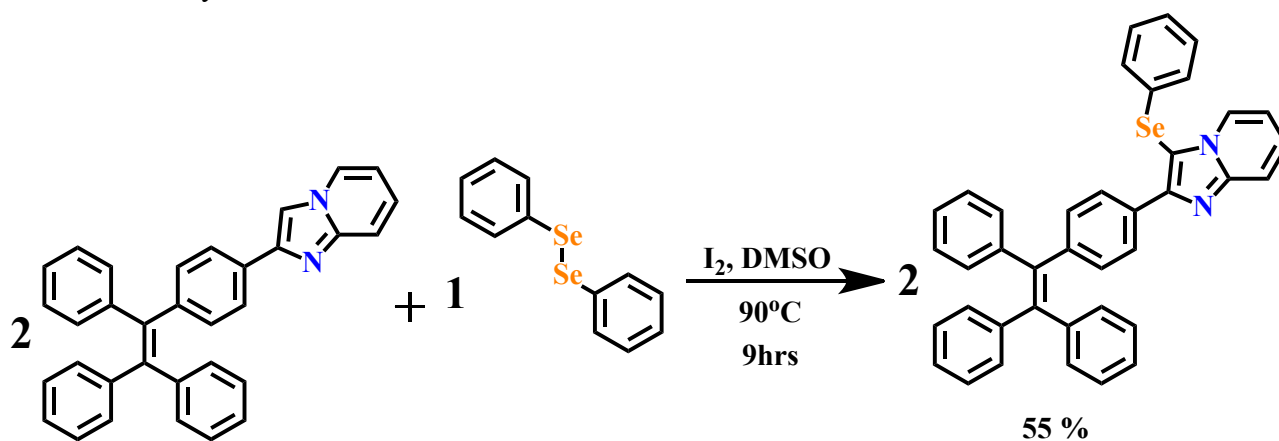
^c*PG and Research Department of Chemistry, KhadirMohideen College (affiliated to Bharathidasan University), Adirampattinam, Tamil Nadu, India.*

^d*Beamline Department, Pohang Accelerator Laboratory, 80 Jigokro-127 beongil, Nam-gu, Pohang, Gyeongbuk Korea; E-mail: dmoon@postech.ac.kr.*

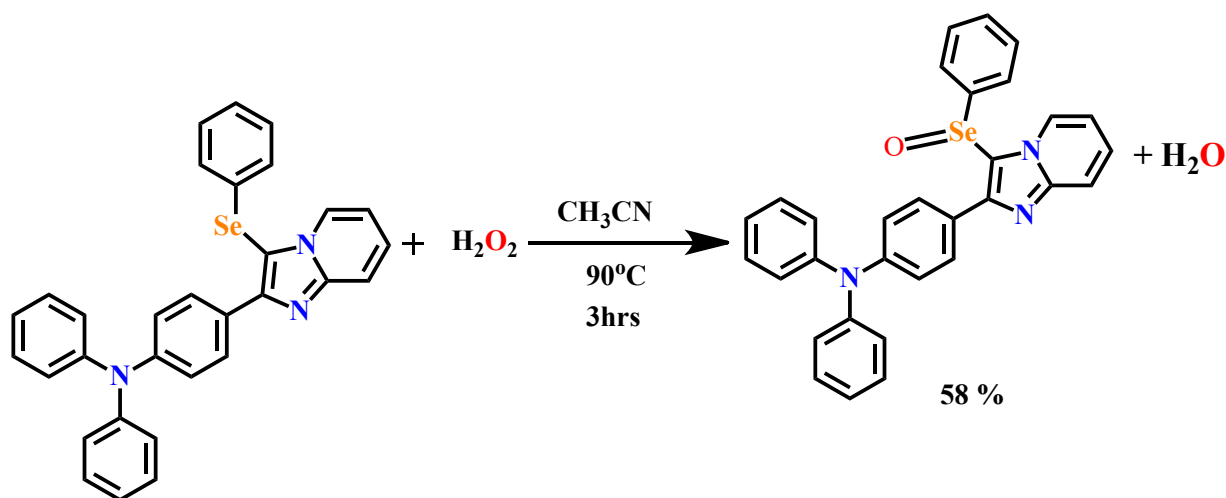
S.No.	Content	Page No.
1.	Experimental Section	3
2.	FT-IR Analysis	5
3.	NMR Analysis	7
4.	Mass Spectrometry (MS) Analysis	11
5.	Single Crystal X-ray Crystallography Studies	13
6.	Photophysical studies	14

1. Experimental Section

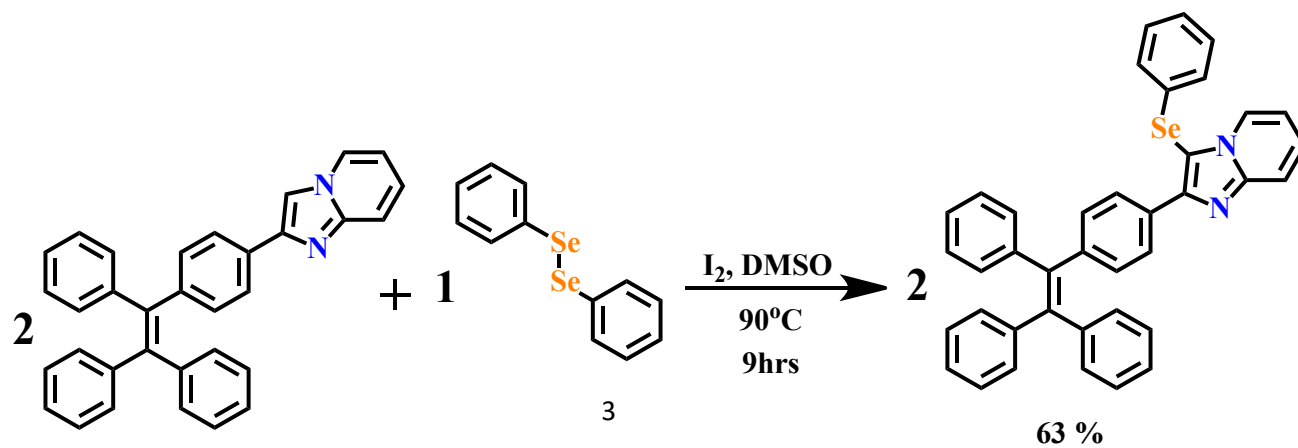
Scheme S1. Synthesis of Se-TPA



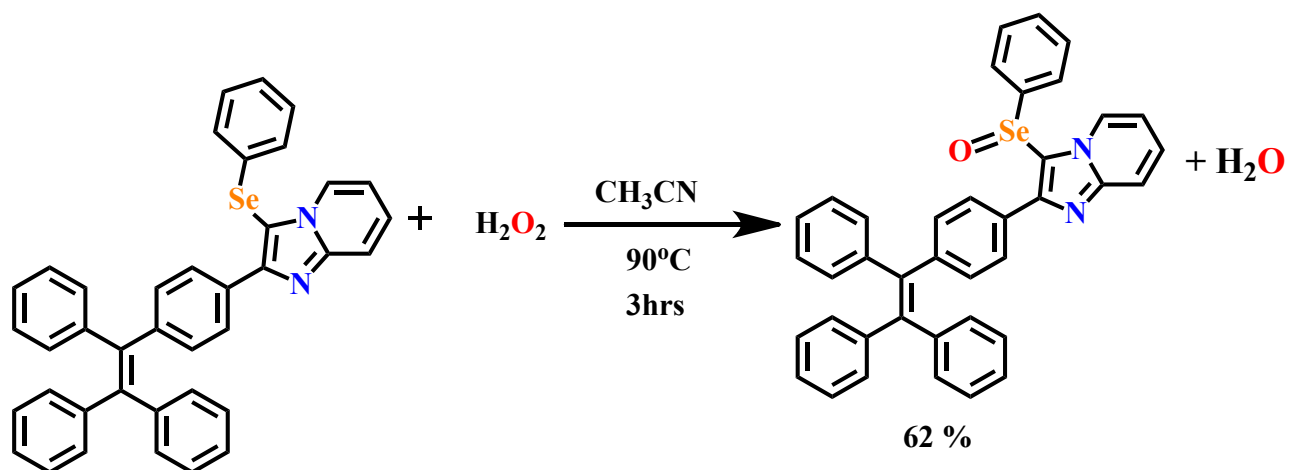
Scheme S2. Synthesis of SeO-TPA



Scheme S3. Synthesis of Se-TPE



Scheme S4. Synthesis of SeO-TPE



2. FT-IR Analysis

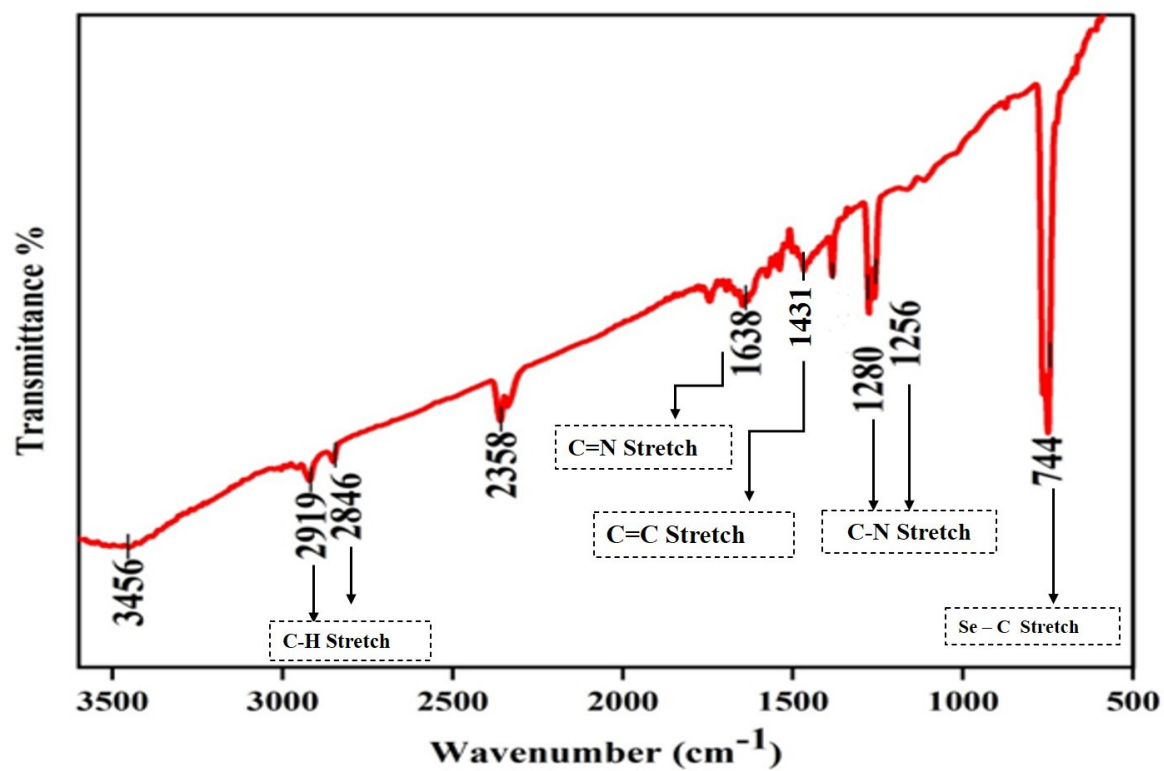


Fig. S1 FT-IR spectrum of Se-TPA.

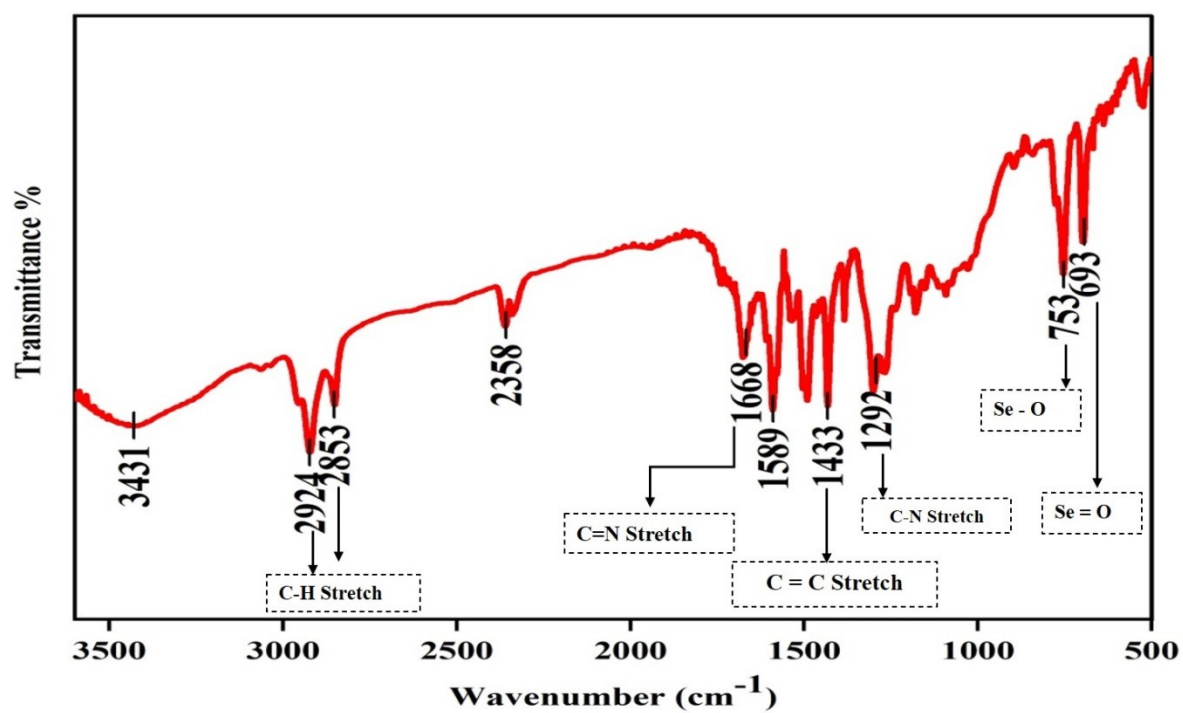


Fig. S2 FT-IR spectrum of SeO-TPA.

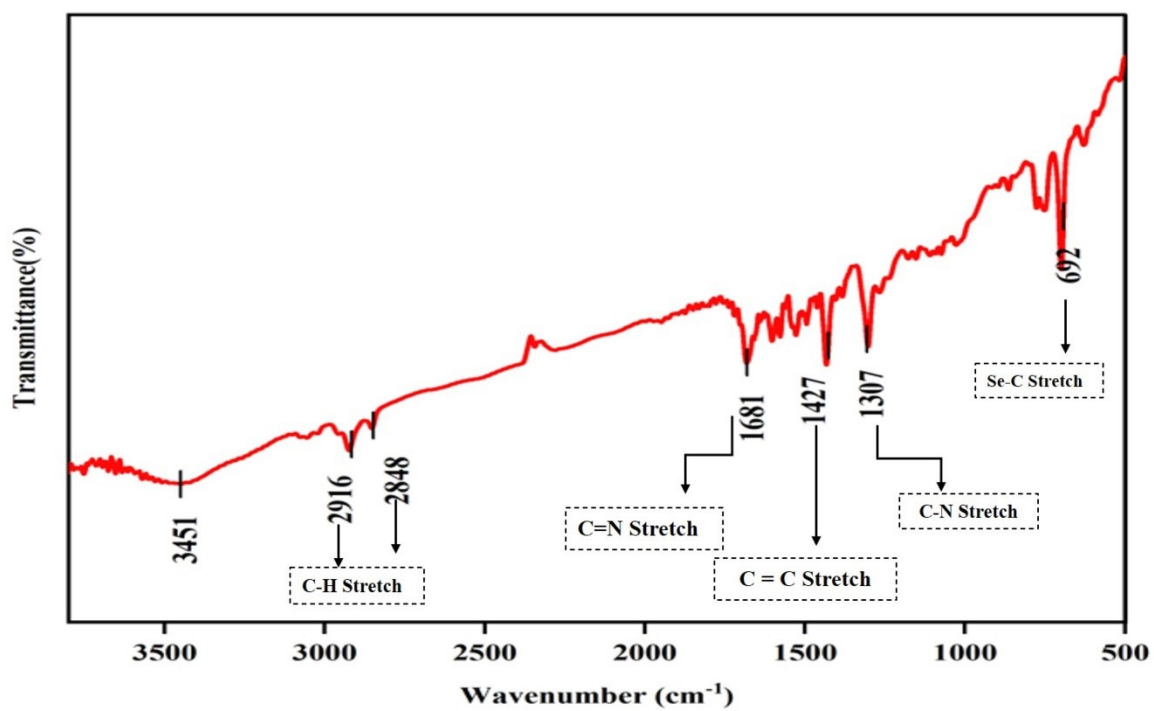


Fig. S3 FT-IR spectrum of Se-TPE.

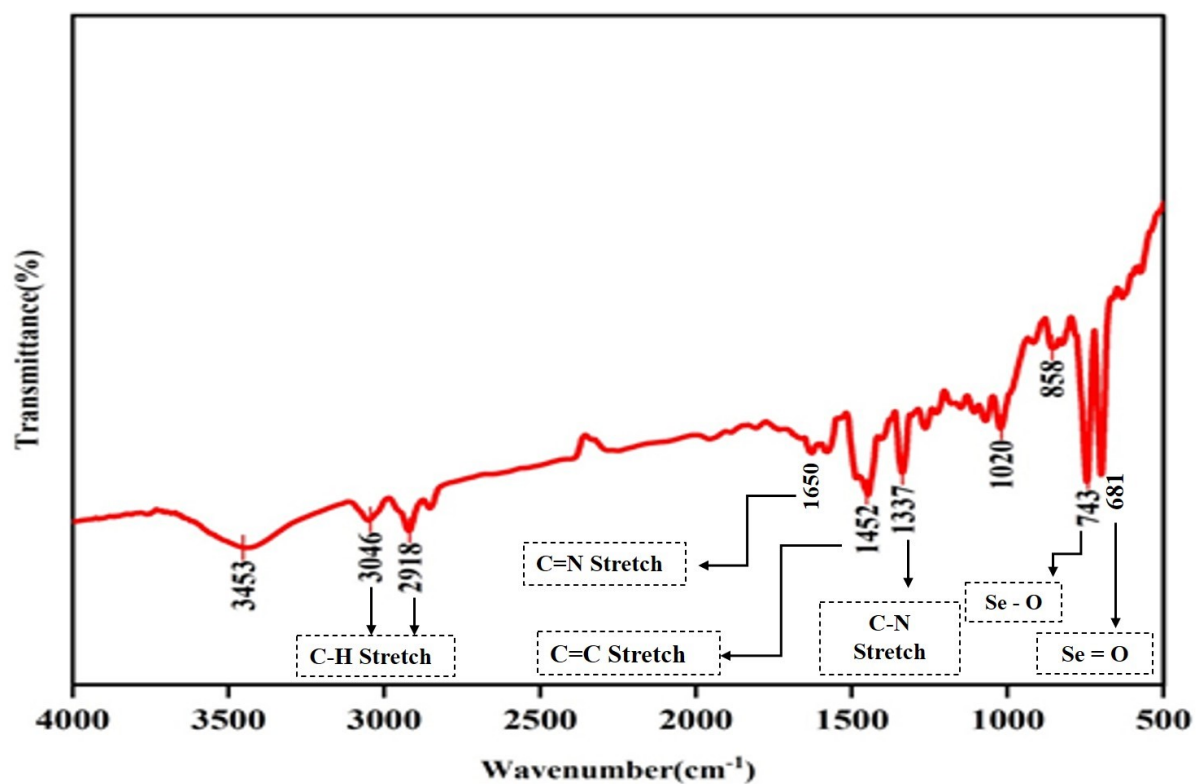


Fig. S4 FT-IR spectrum of SeO-TPE.

3. NMR Analysis

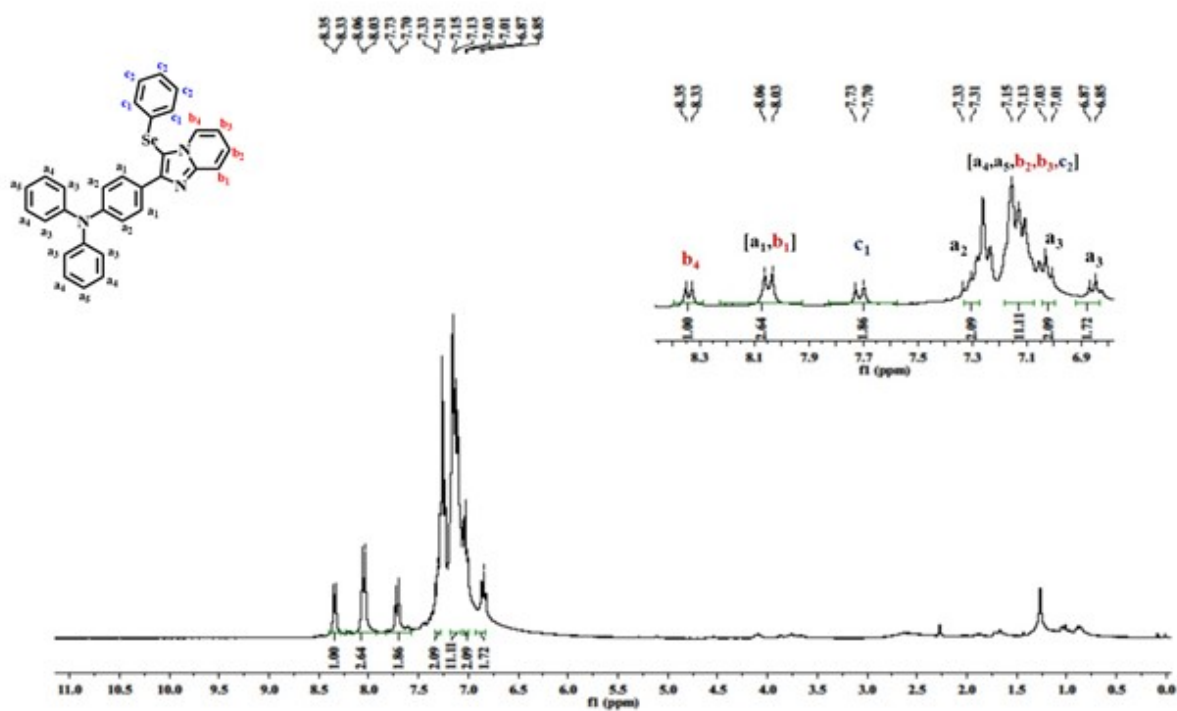


Fig. S5 ^1H NMR spectrum of Se-TPA.

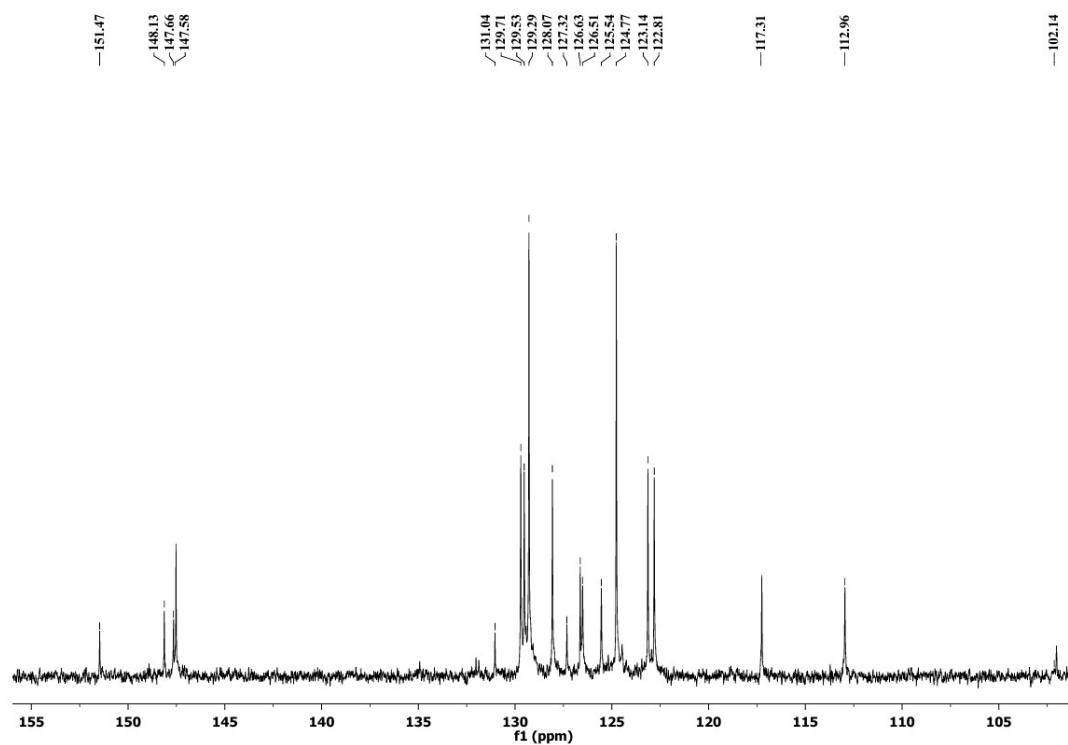


Fig. S6 ^{13}C NMR spectrum of Se-TPA.

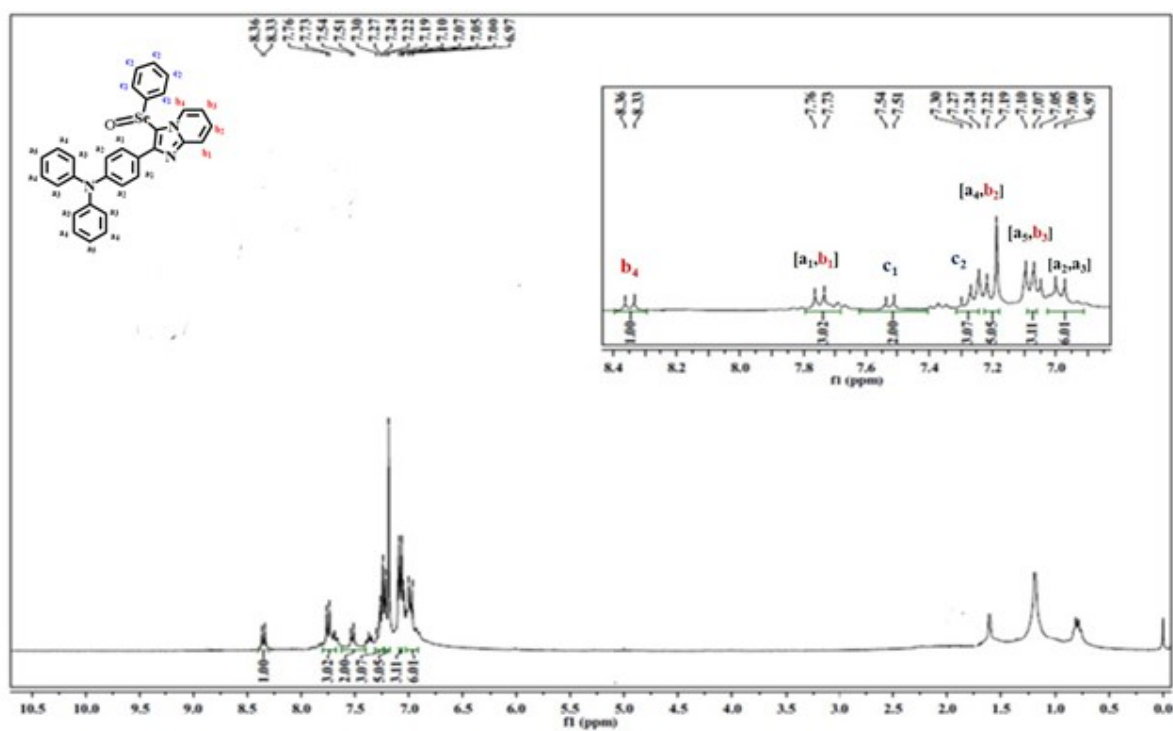


Fig. S7 ^1H NMR spectrum of SeO-TPA.

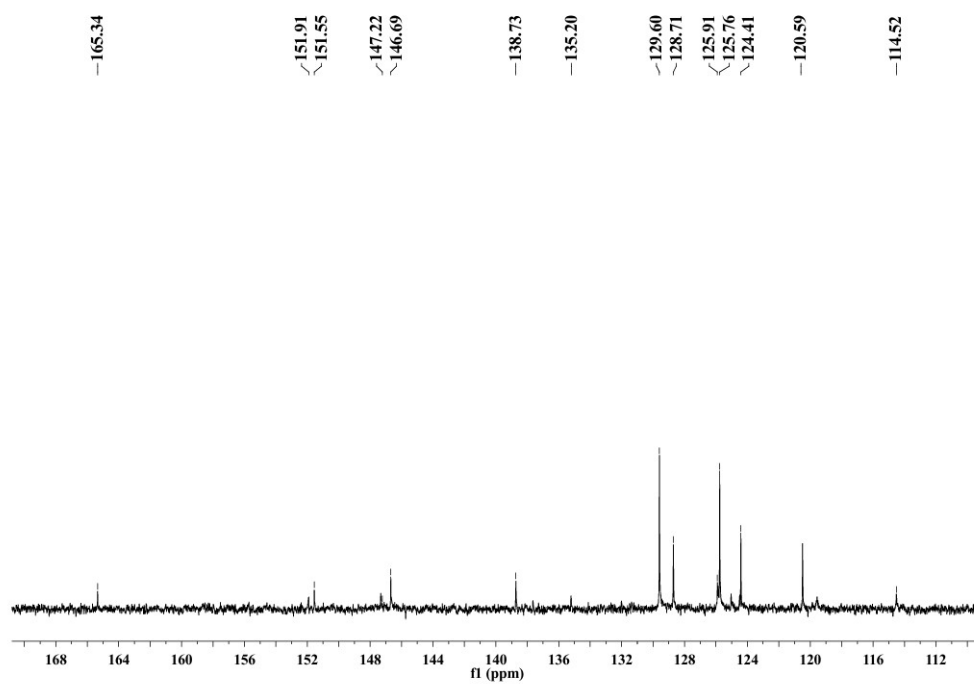


Fig. S8 ^{13}C NMR spectrum of SeO-TPA.

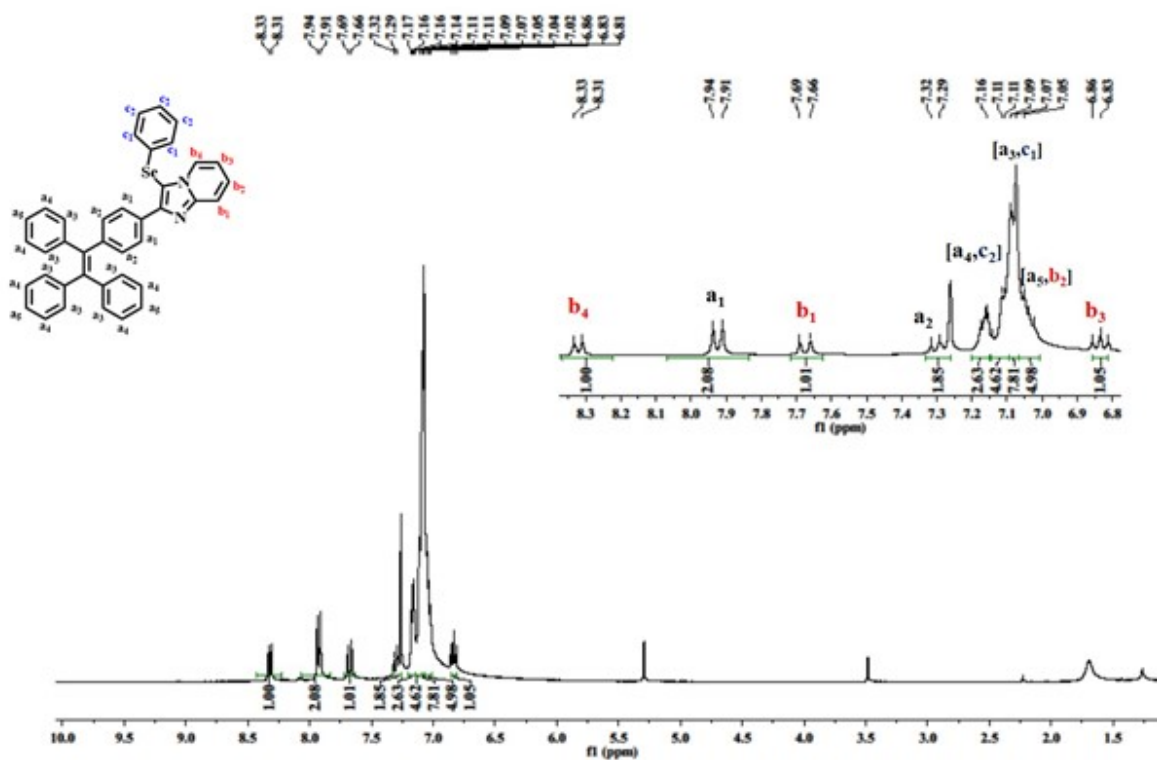


Fig. S9 ^1H NMR spectrum of Se-TPE.

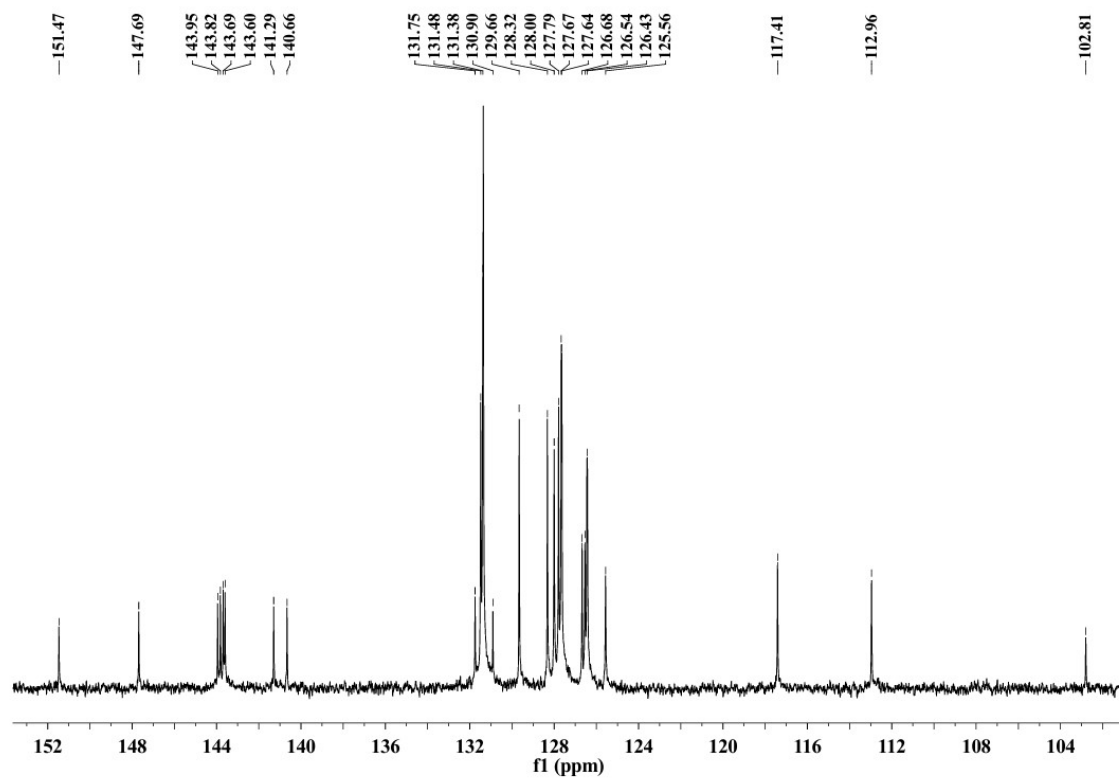


Fig. S10 ^{13}C NMR spectrum of Se-TPE.

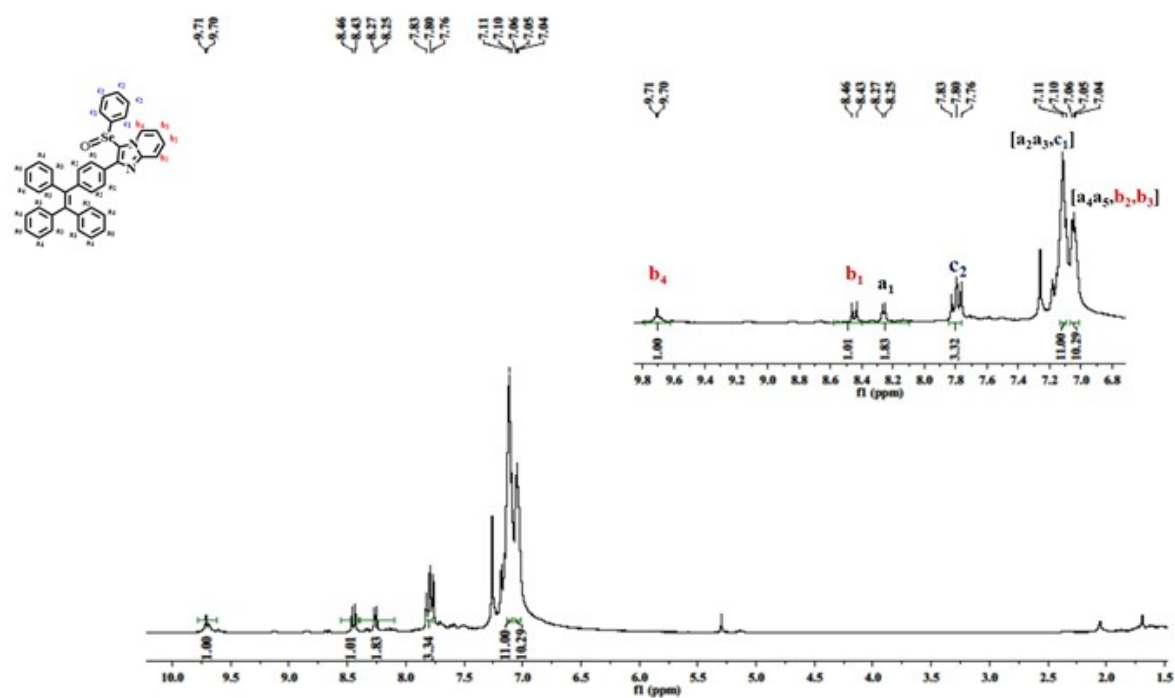


Fig. S11 ^1H NMR spectrum of SeO-TPE.

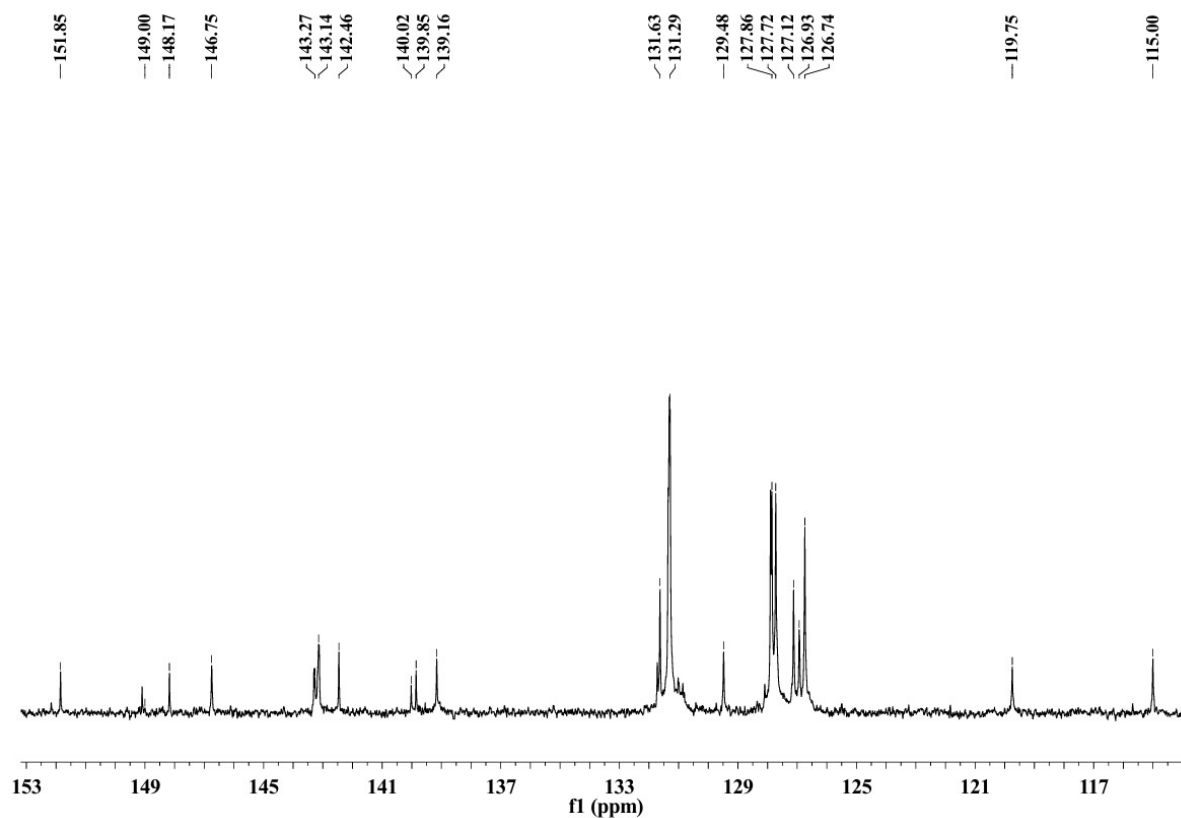


Fig. S12 ^{13}C NMR spectrum of SeO-TPE.

4. Mass Spectrometry (MS) Analysis

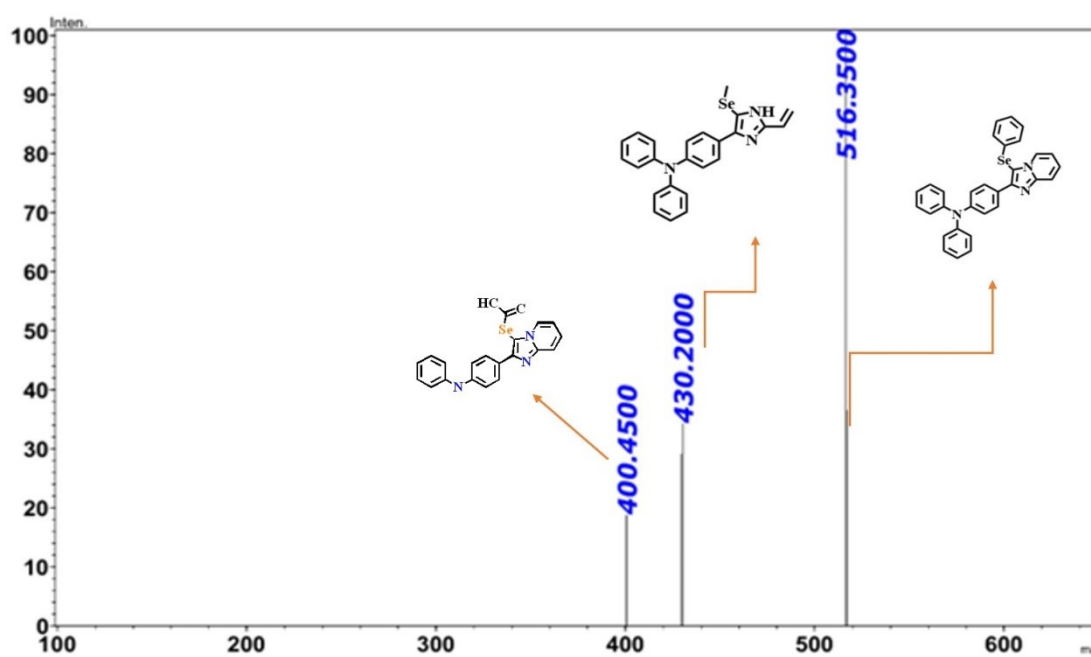


Fig. S13 Mass spectrum of Se-TPA.

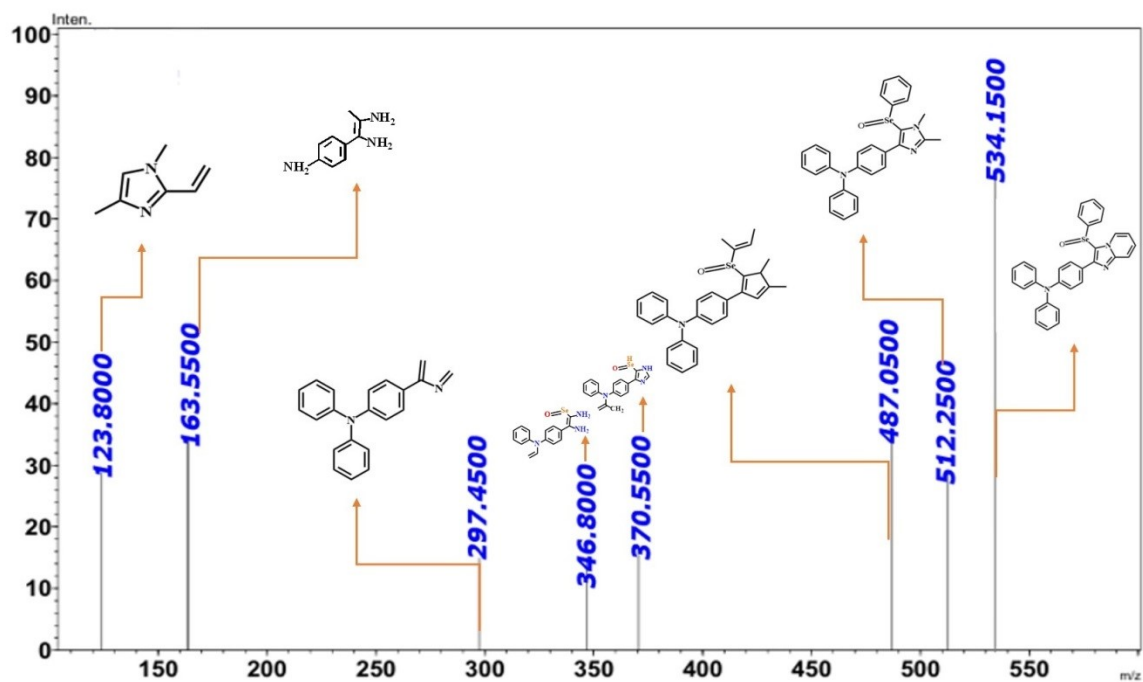


Fig. S14 Mass spectrum of SeO-TPA

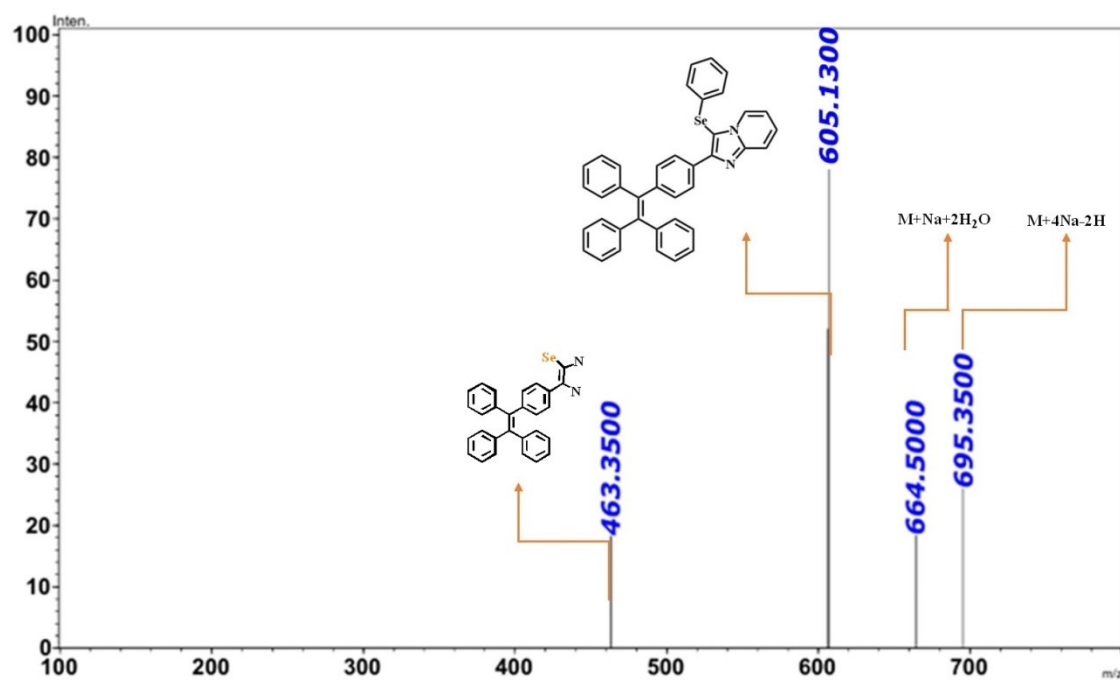


Fig. S15 Mass spectrum of Se-TPE.

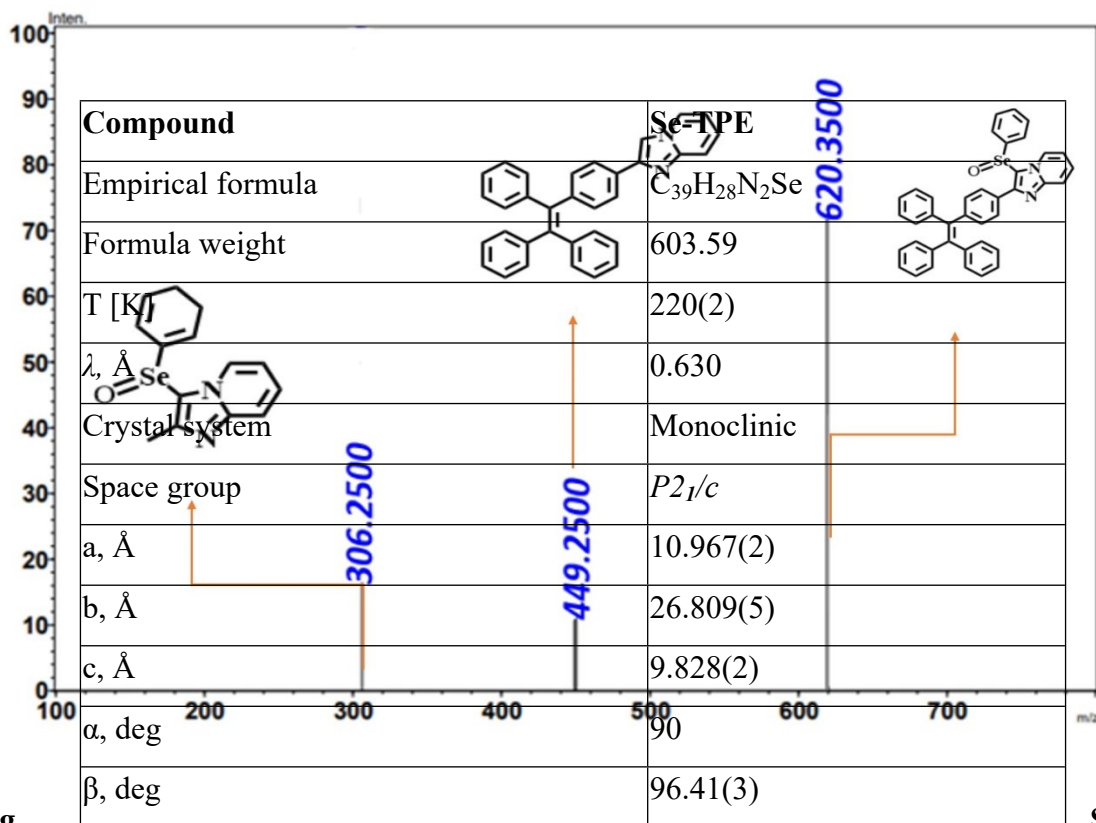


Fig.

S16

Mass spectrum of SeO-TPE.

5. Single Crystal X-ray Crystallography Studies

Table	γ , deg	90	S1.
	Volume ($\text{\AA}^3$)	2871.5(10)	
	Z	4	
	d_{calc} (mg/cm ³)	1.396	
	μ (mm ⁻¹)	0.974	
	F(000)	1240	
	Crystal size/mm ³	0.128 x 0.097 x 0.084	
	2 θ range for data collection/ $^\circ$	1.656 to 25.000	
	Reflections collected	26897	
	Data/restraints/parameters	7258 / 0 / 379	
	Goodness-of-fit on F^2	1.052	
	R [$I > 2\sigma(I)$]	$R_1 = 0.0402$ $wR_2 = 0.1056$	
	R [all data]	$R_1 = 0.0488$ $wR_2 = 0.1107$	
	Largest diff. Peak/hole [$e \text{\AA}^{-3}$]	0.815 / -0.806	
	CCDC number	2491312	

Crystal data and structural refinement for compound **Se-TPE**

5. Photophysical studies

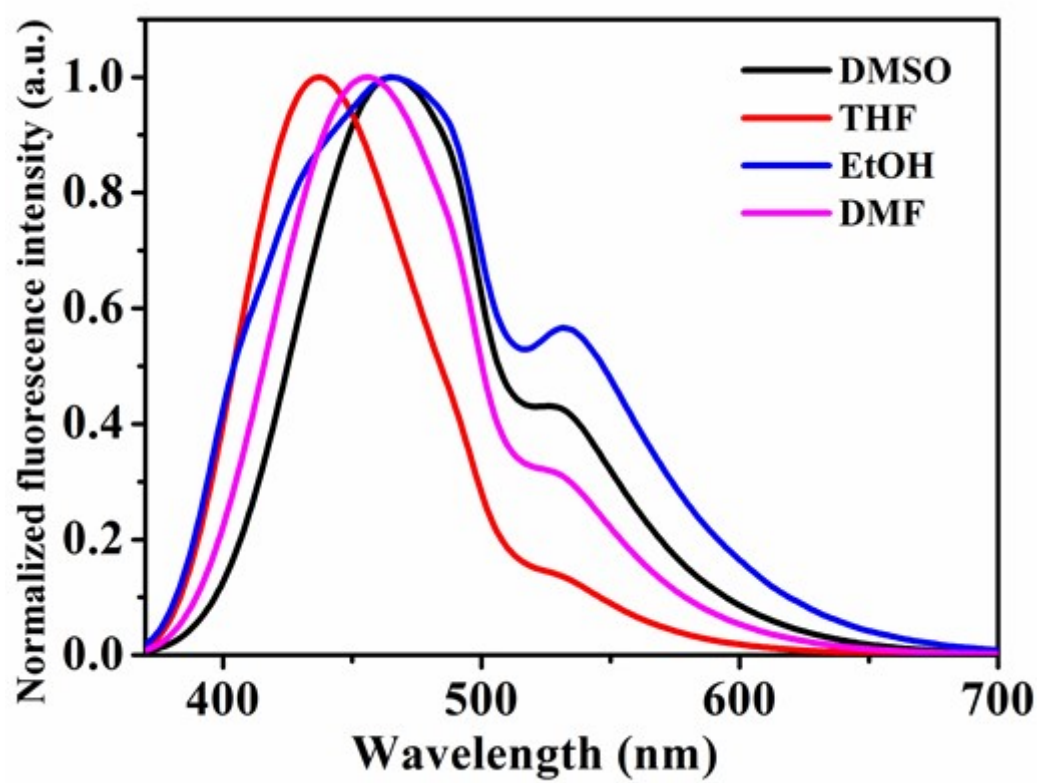


Fig. S17 Normalized emission spectra of **SeO-TPA** in different solvents (1×10^{-5} M) .

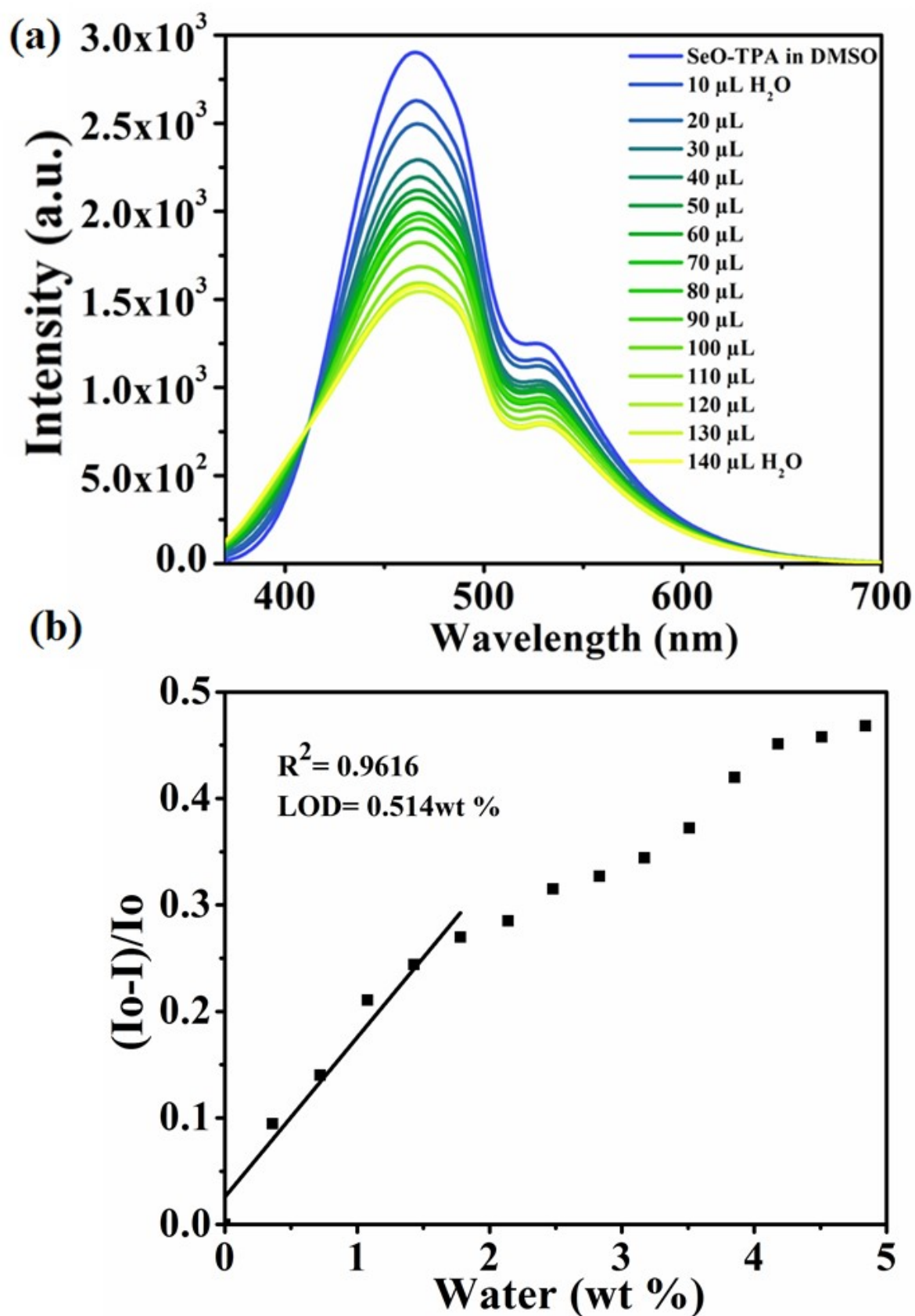


Fig. S18 (a) The effect of water addition on SeO-TPA (10^{-5} M) emission in DMSO. (b) The limit of water detection in DMSO.

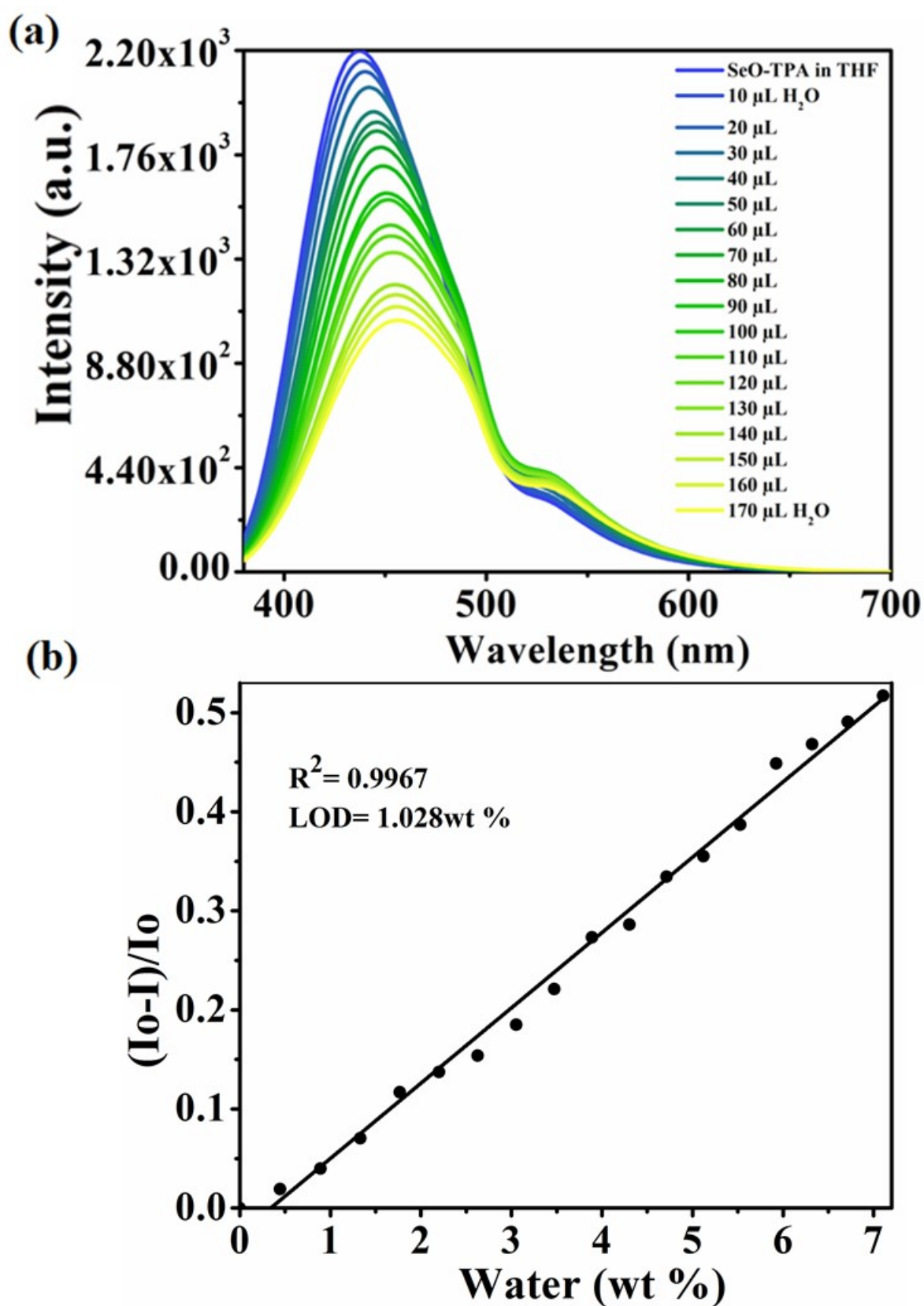


Fig. S19 (a) The effect of water addition on SeO-TPA (10^{-5} M) emission in THF. (b) The limit of water detection in THF.

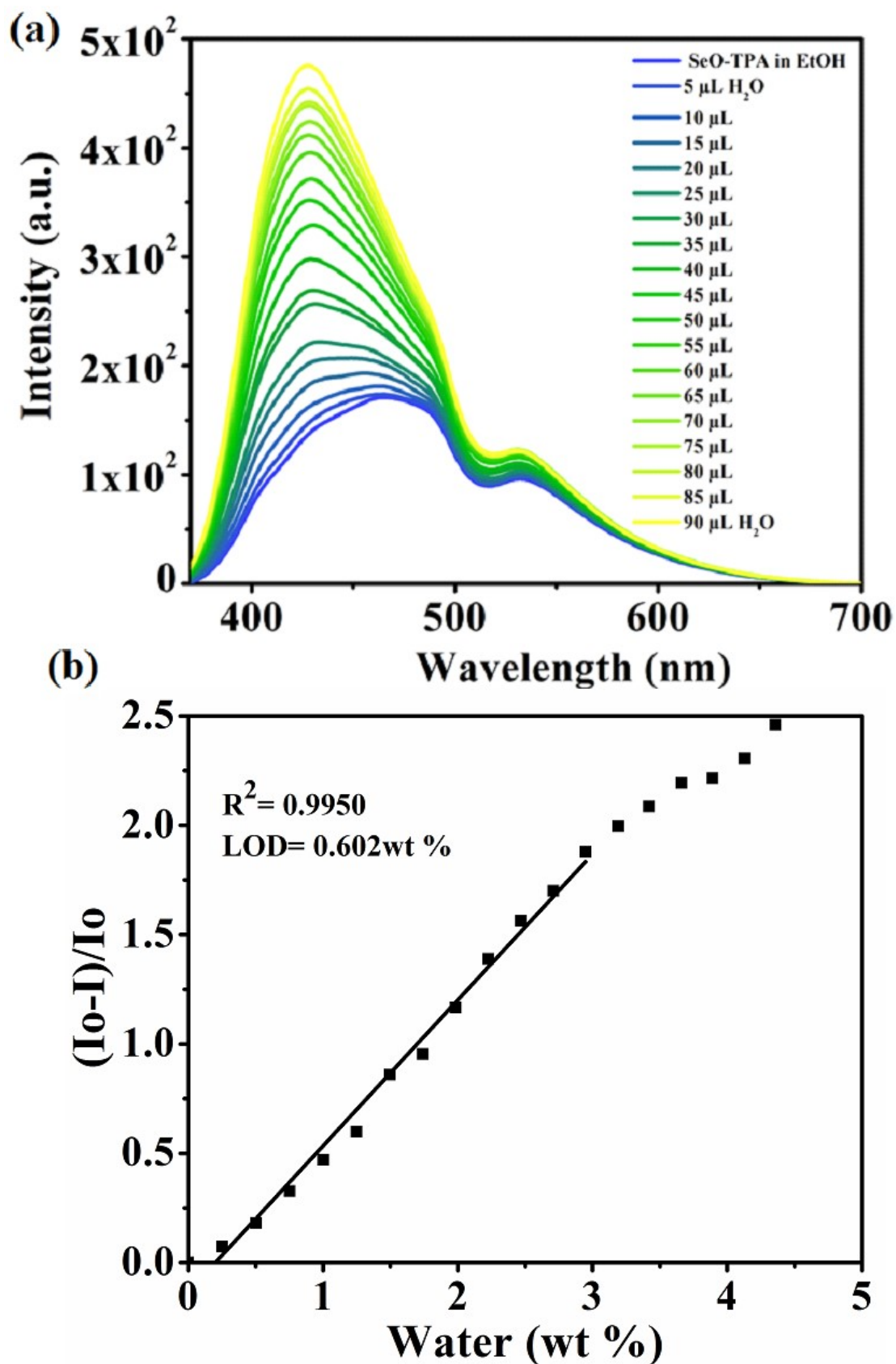


Fig. S20 (a) The effect of water addition on SeO-TPA (10^{-5} M) emission in Ethanol. (b) The limit of water detection in Ethanol.

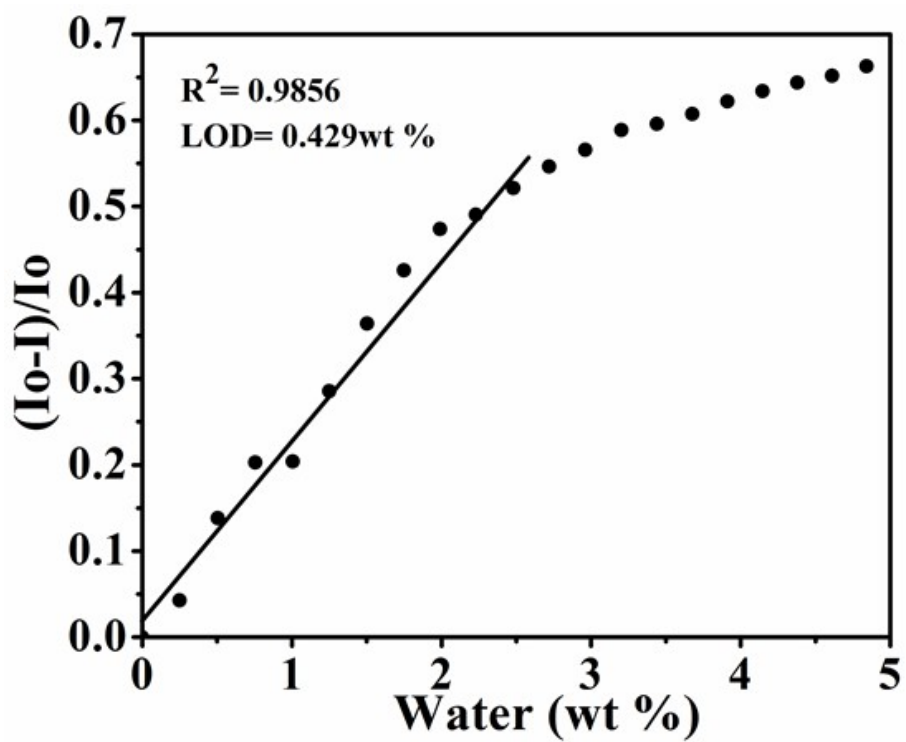


Fig. S21 The limit of water detection plot in CH_3CN .

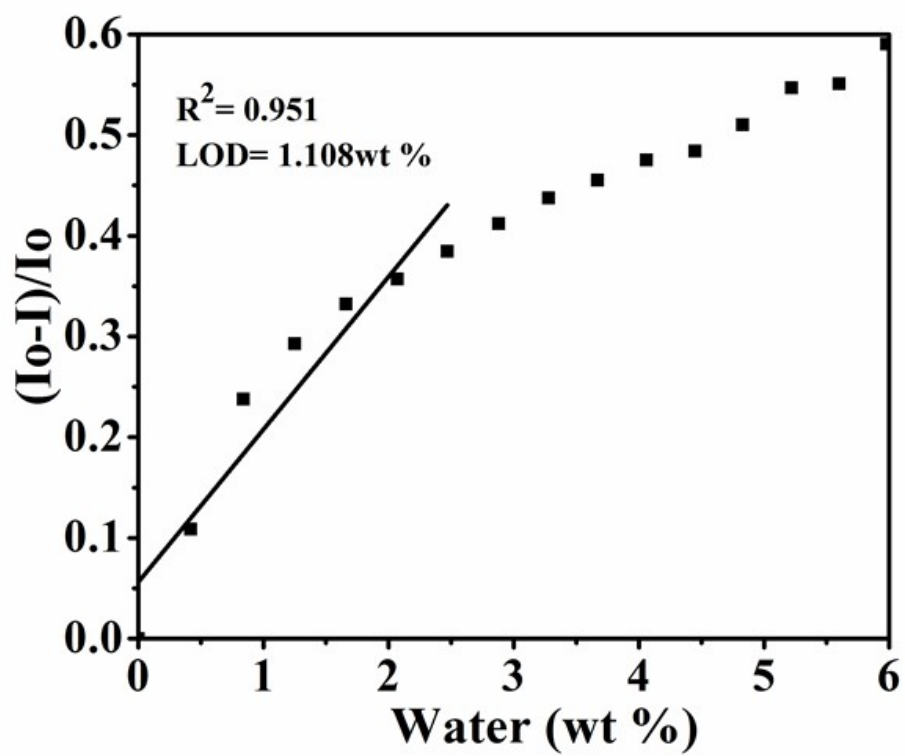


Fig. S22 The limit of water detection plot in DMF .