Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

A Smart Molecular Probe for Selective recognition of Nitric Oxide in 100% aqueous solution with Cell Imaging application and DFT Studies

Ananya Dutta[a], Abu Saleh Musha Islam[a], Debjani Maiti[a], Mihir Saslmal[a], Chandradoy Pradhan[b] ,Mahammad Ali[a,c].

[a]Department of Chemistry Jadavpur University, Kolkata 700 032, India; Fax: 91-33-2414-6223, E-mail: m_ali2062@yahoo.com, mali@chemistry.jdvu.ac.in

[b]Molecular & Human Genetics Division, CSIR-Indian Institute of Chemical Biology, 4 Raja S.C. Mallick Road, Kolkata-700032, India.

[c]Vice-Chancellor, Aliah University, Il-A/27, Action Area II, Newtown, Action Area II, Kolkata, West Bengal 700160,

Supporting Information for Publication

No.	Content.	Figure.No.
1.	^{1}H NMR spectrum of (**HqEN$_{480}$**) in DMSO-d_6.	**Fig.S1**
2.	^{13}CNMR spectrum of **(HqEN$_{480}$)** in DMSO-d$_6$	**Fig. S1a**
3.	Mass spectrum of **(HqEN$_{480}$)** in MeCN.	**Fig.S2**
4.	IR spectrum of **(HqEN$_{480}$)** in solid state.	**Fig.S3**
6.	Mass spectrum of **(HqPA)** in MeOH.	**Fig. S4**
7.	^{1}H NMR spectrum of (**HqPA**) in $CDCl_3$.	**Fig. S5**
8.	Fluorescence titration of **(HqEN$_{480}$)** with NO in aqueous solution at λ_{ex}=350nm.	**Fig. S6**
9.	Fluorescence titration of **(HqPA)** with NO in aqueous solution at λ_{ex}=390nm.	**Fig. S7**
10.	Selectivity of HqPA towards NO over various ions.	**Fig. S8**
11.	^{1}H NMR spectrum of **(HqEN$_{480}$-NO)** in DMSO-d$_6$.	**Fig. S9**
12.	^{13}CNMR spectrum of **(HqEN$_{480}$-NO)** in DMSO-d$_6$.	**Fig. S9a**
13.	Mass spectrum of **(HqEN$_{480}$-NO)** in MeCN.	**Fig. S10**
14.	IR spectrum of **(HqEN$_{480}$-NO)** in solid state.	**Fig. S11**
15.	^{1}H NMR spectrum of **(HqPA-NO)** in DMSO-d$_6$.	**Fig. S12**
16.	LOD of **(HqEN$_{480}$-NO)** from fluorescence study.	**Fig. S13**
17.	LOD of **(HqEN$_{480}$-NO)** from UV-vis study.	**Fig. S13a**
18.	Fluorescence response towards NO over various amino acids at λ_{ex}=390nm.	**Fig. S14**
19.	UV-vis absorbtion spectra of **HqEN$_{480}$** towards various RONS and NO.	**Fig. S15**

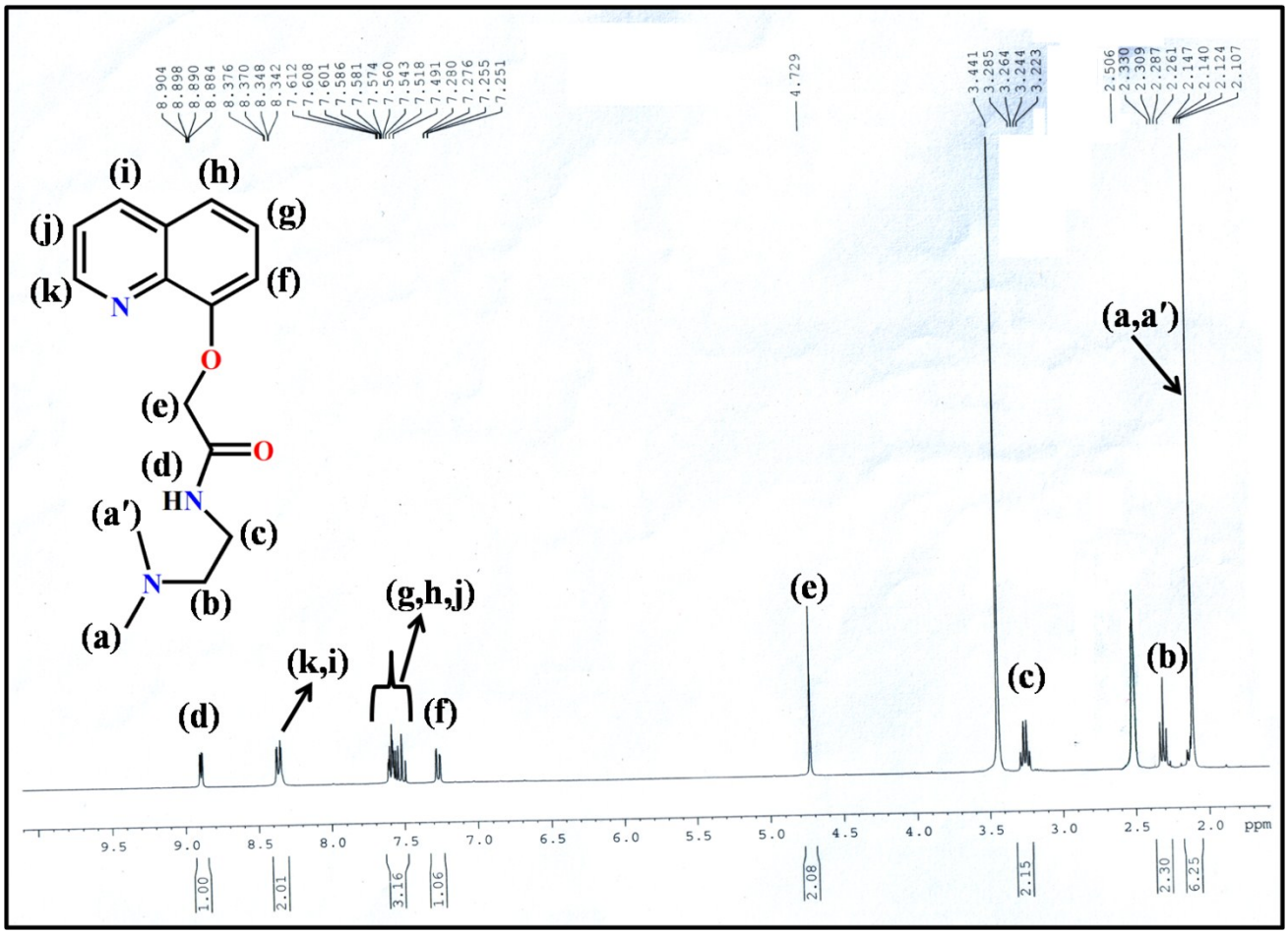

Fig.S1.[1]H NMR spectrum of spectrum of (**HqEN$_{480}$**) in DMSO-d_6.

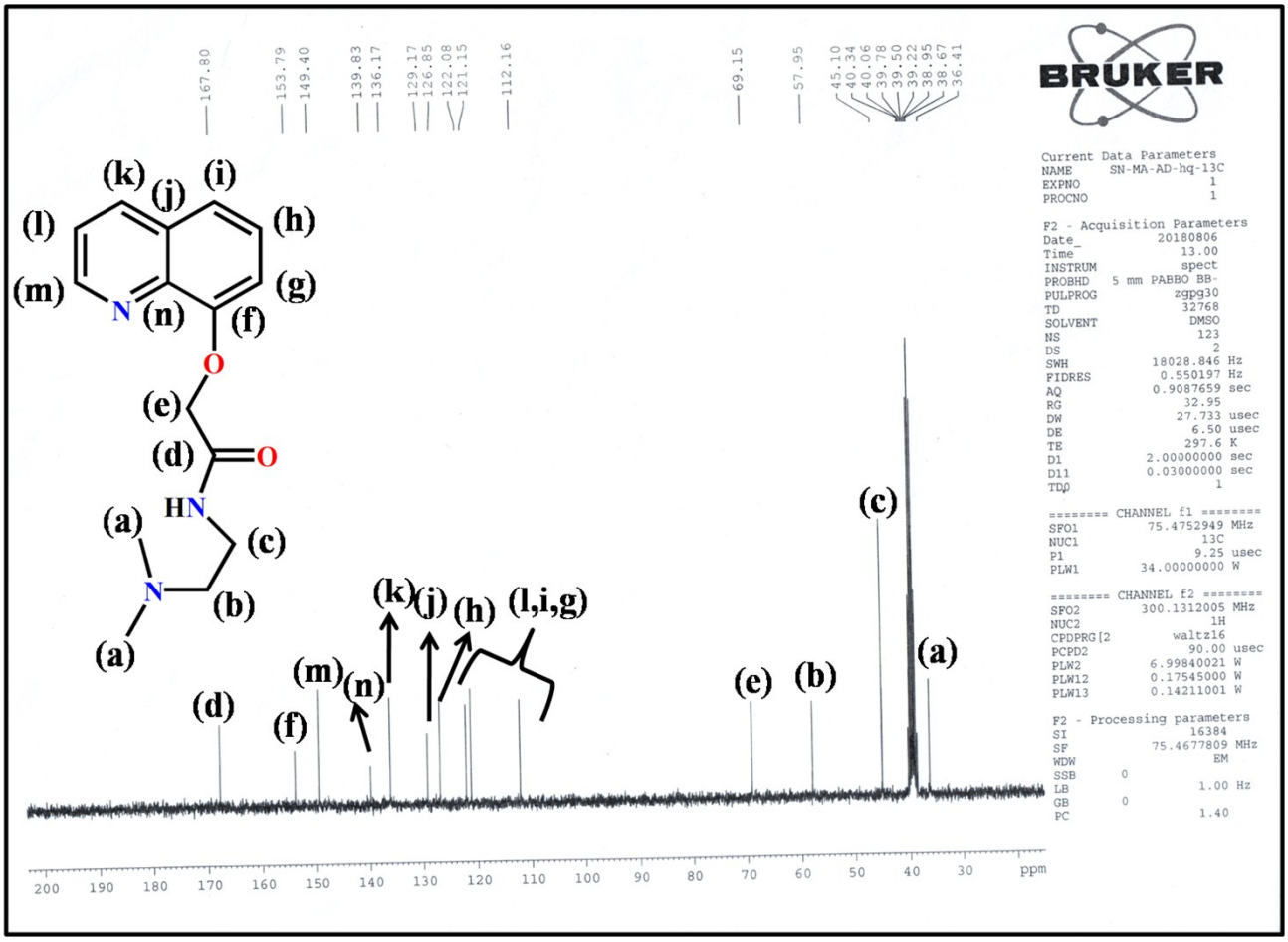

Fig. S1a. ^{13}C NMR spectrum of spectrum of (**HqEN$_{480}$**) in DMSO-d_6.

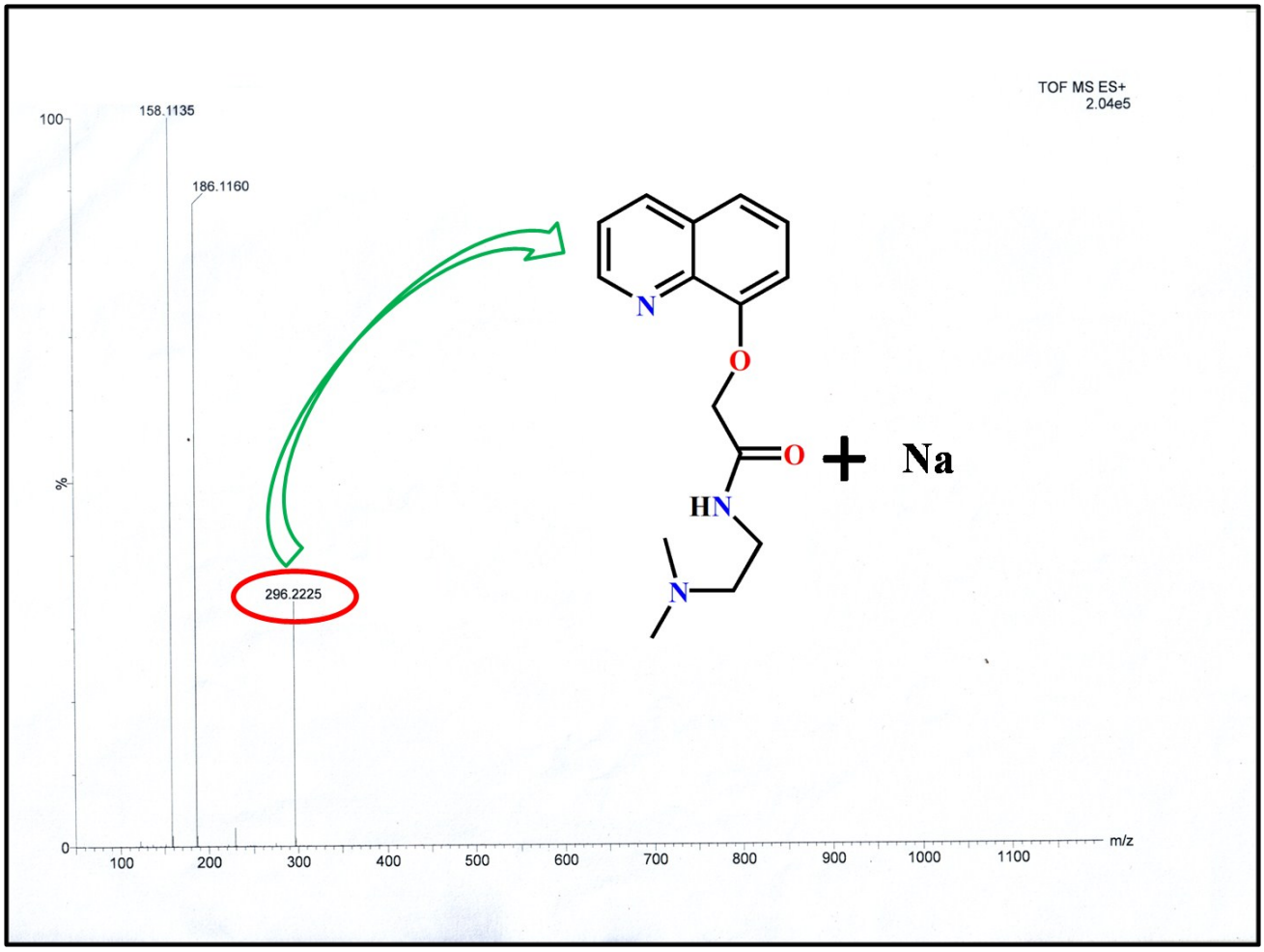

Fig. S2. Mass spectrum of **HqEN$_{480}$** in MeCN.

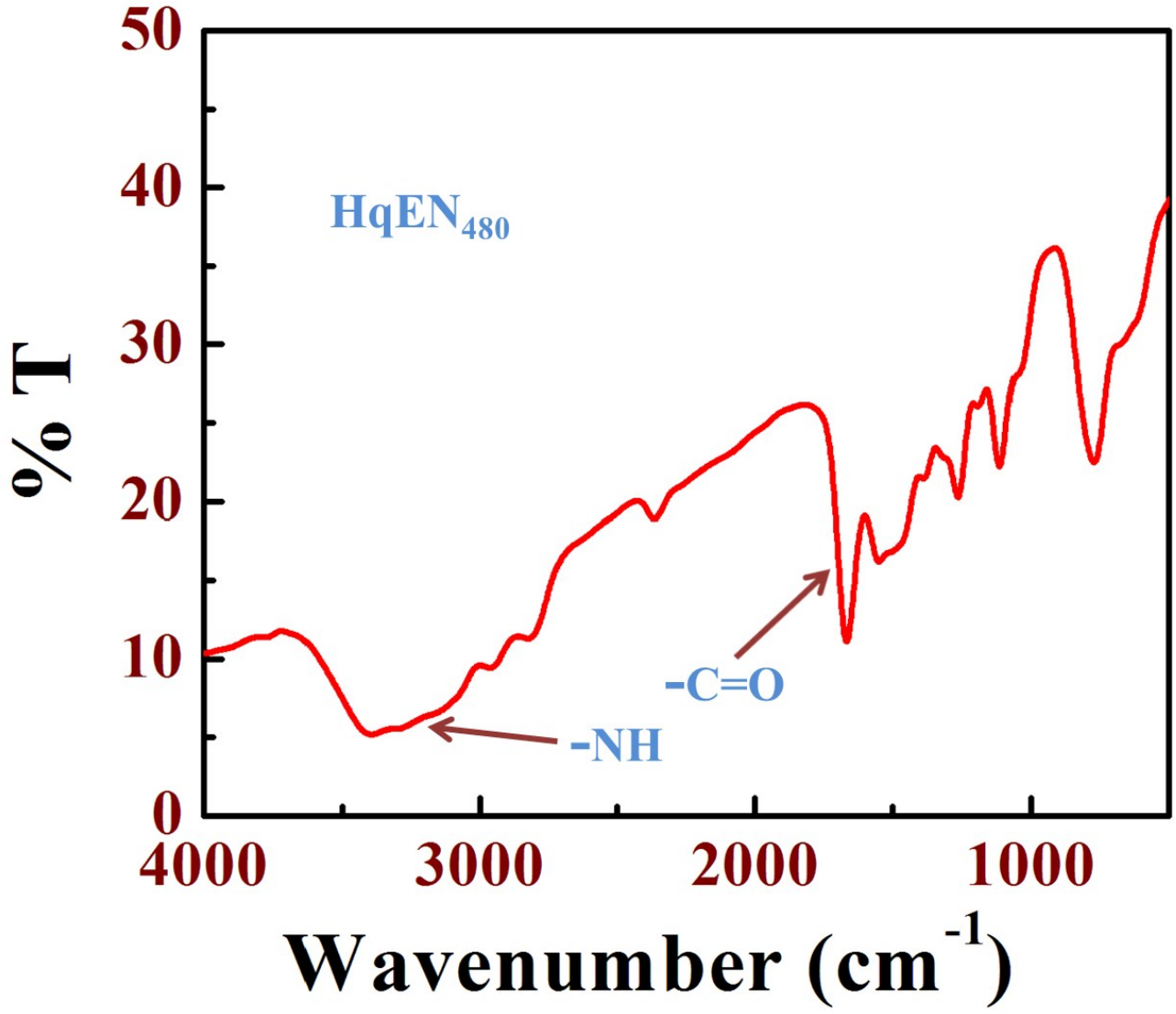

Fig. S3. IR spectrum of **$HqEN_{480}$** in solid state.

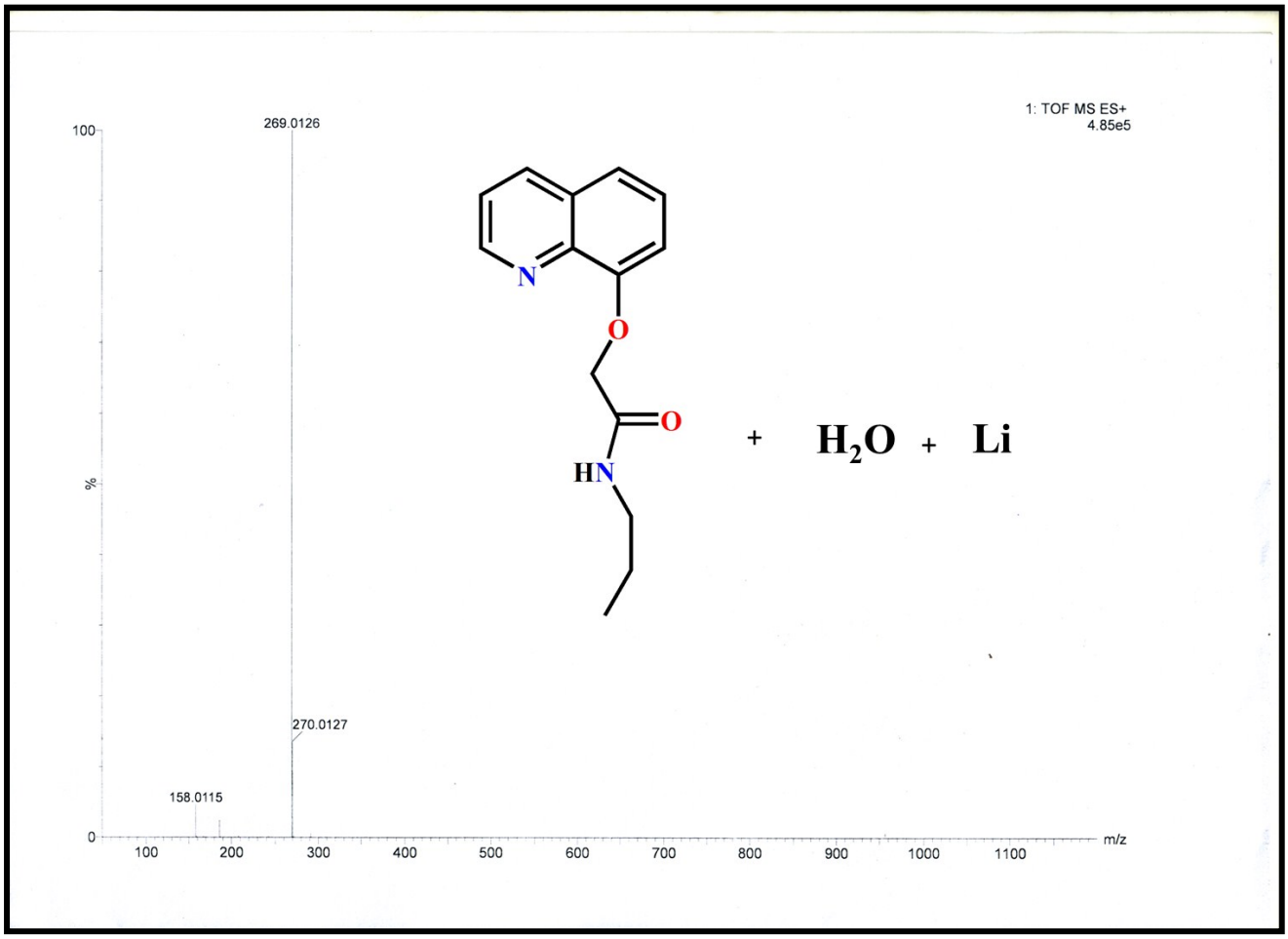

Fig. S4. Mass spectrum of **HqPA** in MeOH.

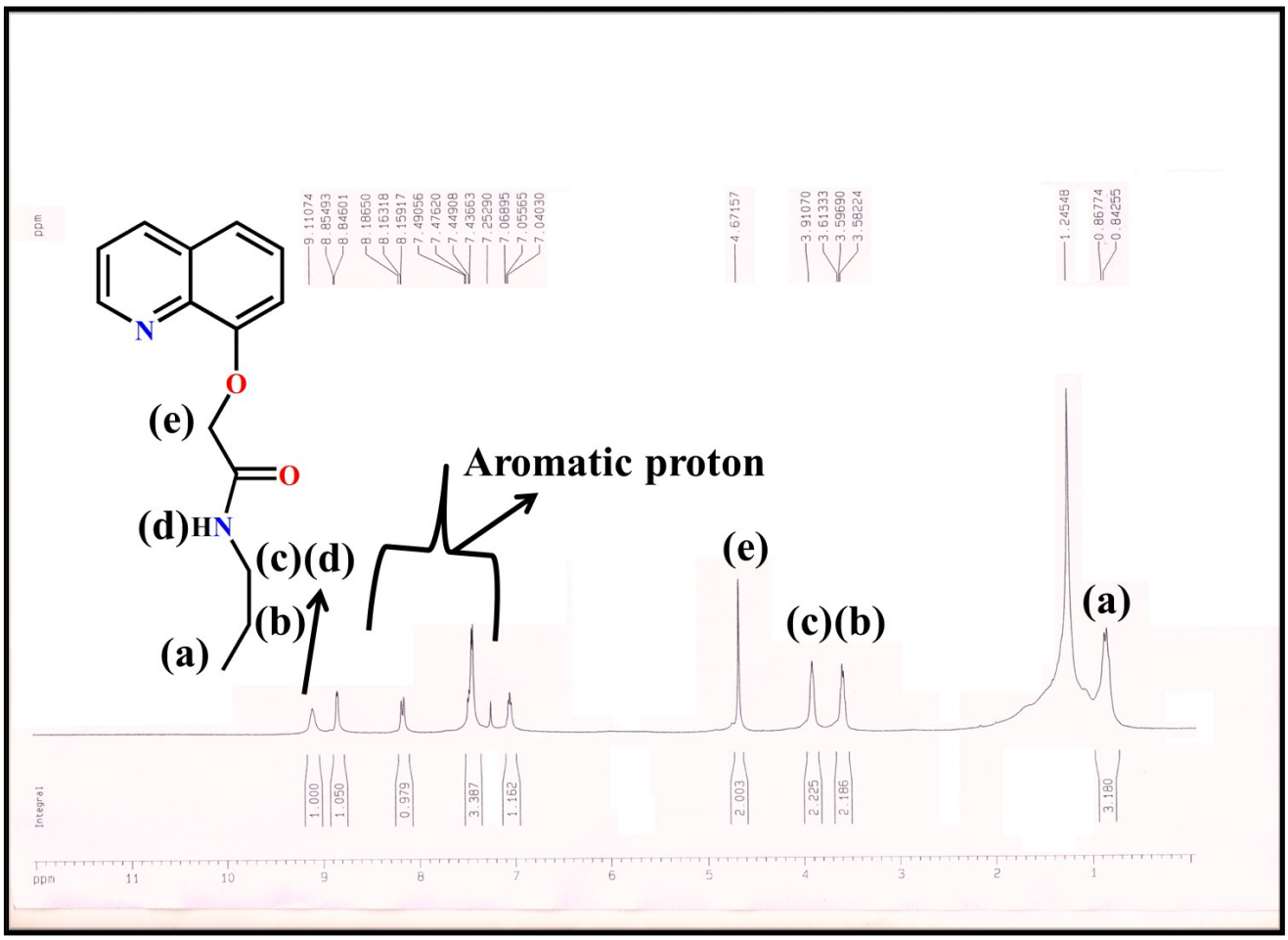

Fig. S5. ^{1}H NMR spectrum of **HqPA** in $CDCl_3$.

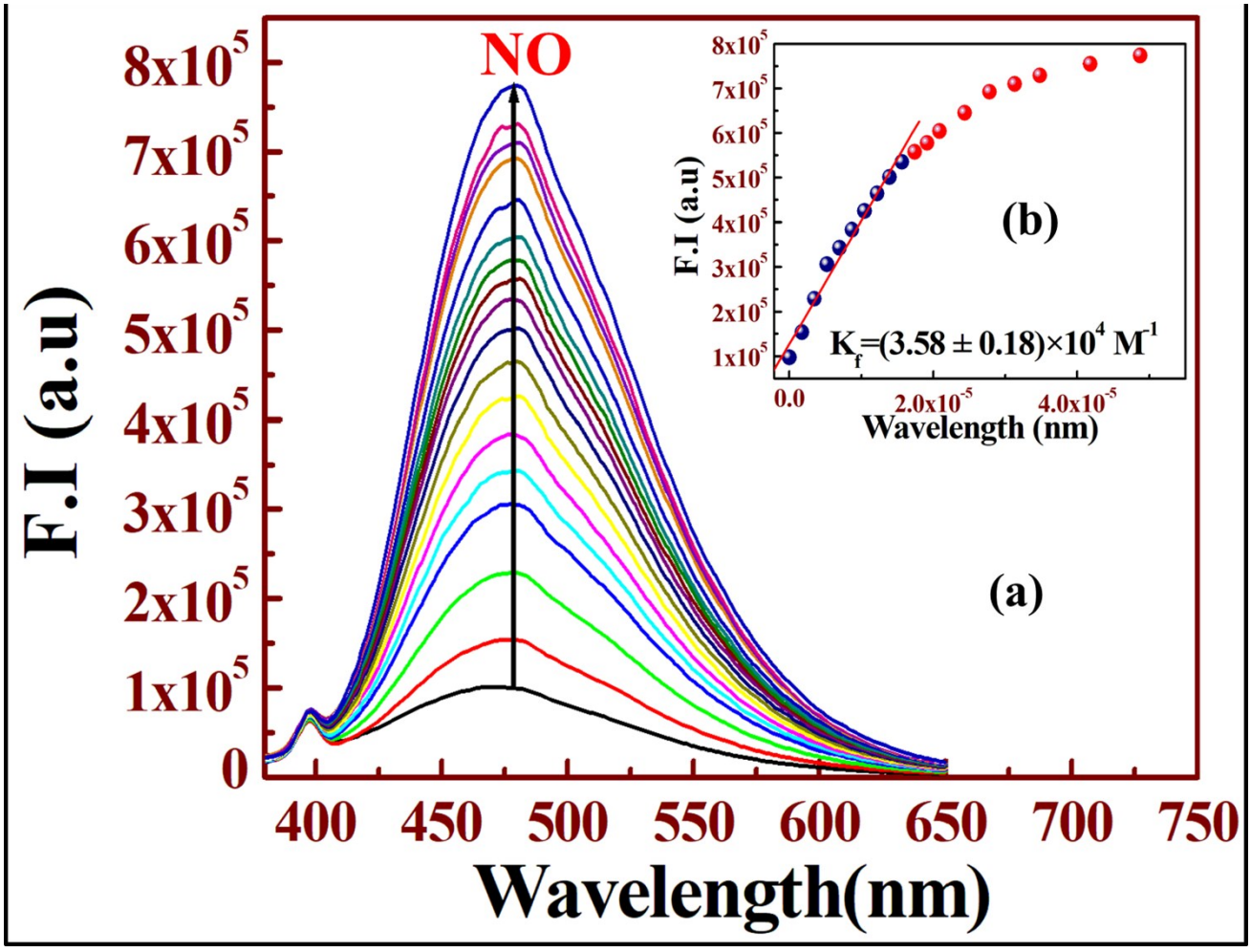

Fig. S6. Fluorescence titration of $HqEN_{480}$ with NO in aqueous HEPES buffer at λ_{ex}=350nm.

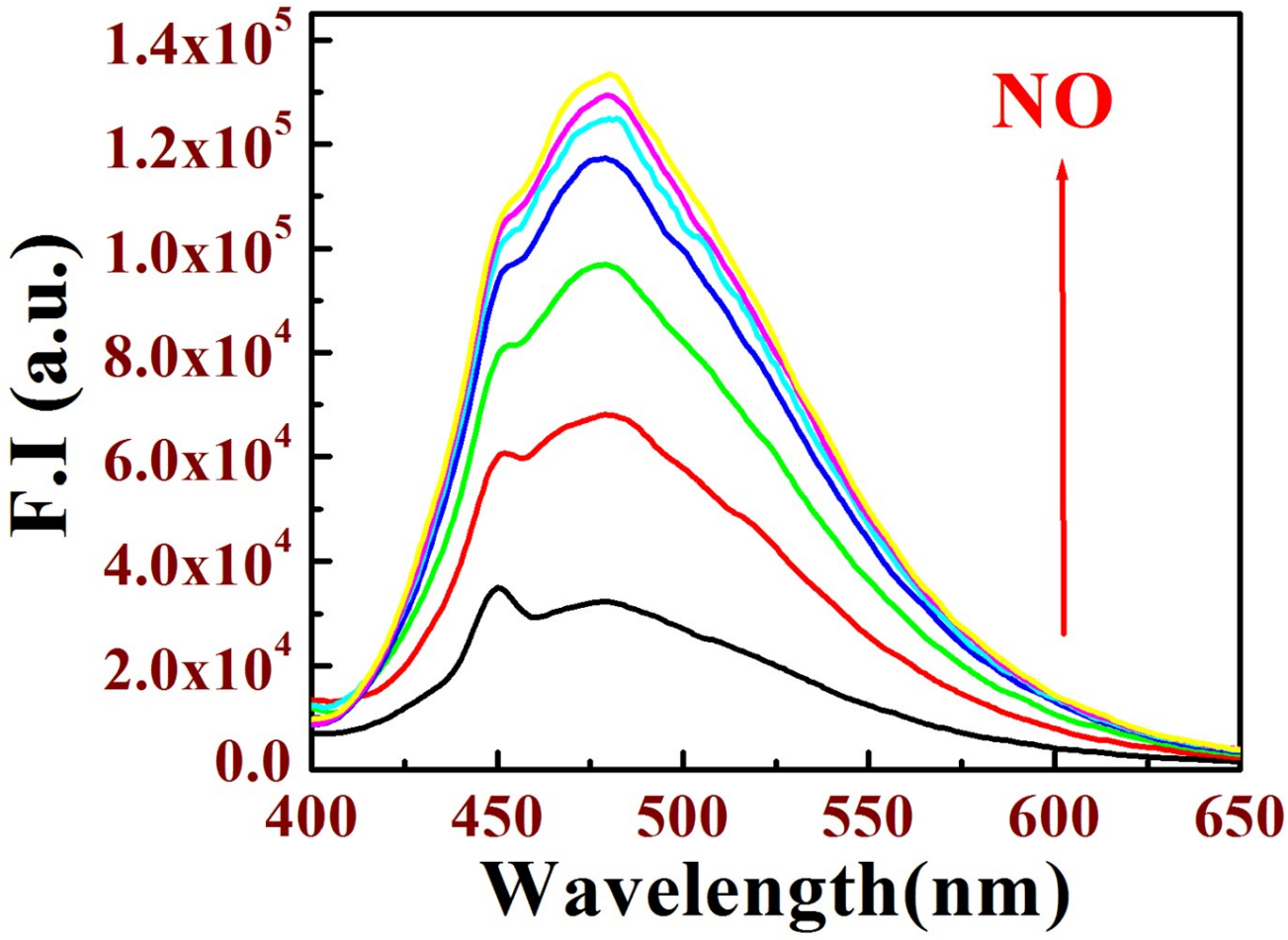

Fig. S7. Fluorescence titration of **(HqPA)** with NO in aqueous solution at λ_{ex}=390nm.

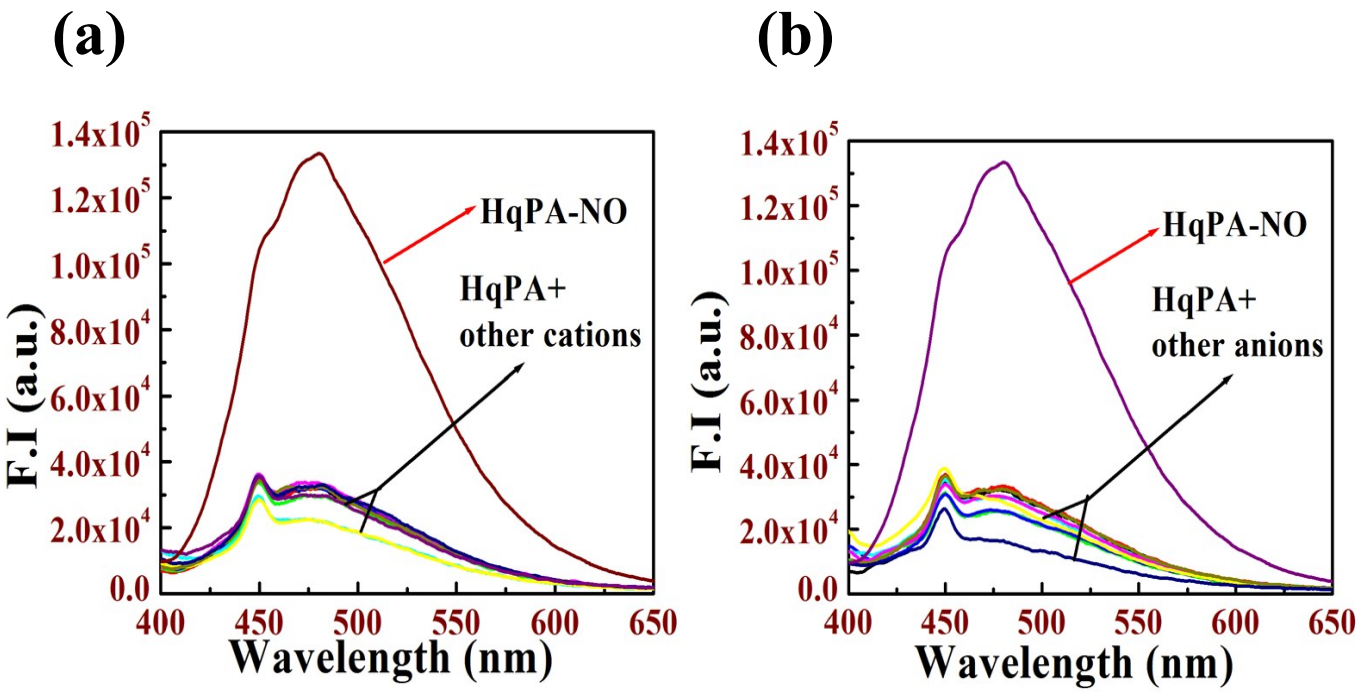

Fig. S8. Selectivity of HqPA towards NO over various ions(a) Cd^{2+}, Sm^{3+}, Na^{+}, Zn^{2+}, al^{3+}, Fe^{3+}, pb^{2+}, K^{+}, Eu^{2+}. (b) CH_3COO^{-}, NO_2^{-}, Cl^{-}, N_3^{-}, SCN^{-}, NO_3^{-}, PPi, S^{2-}. .

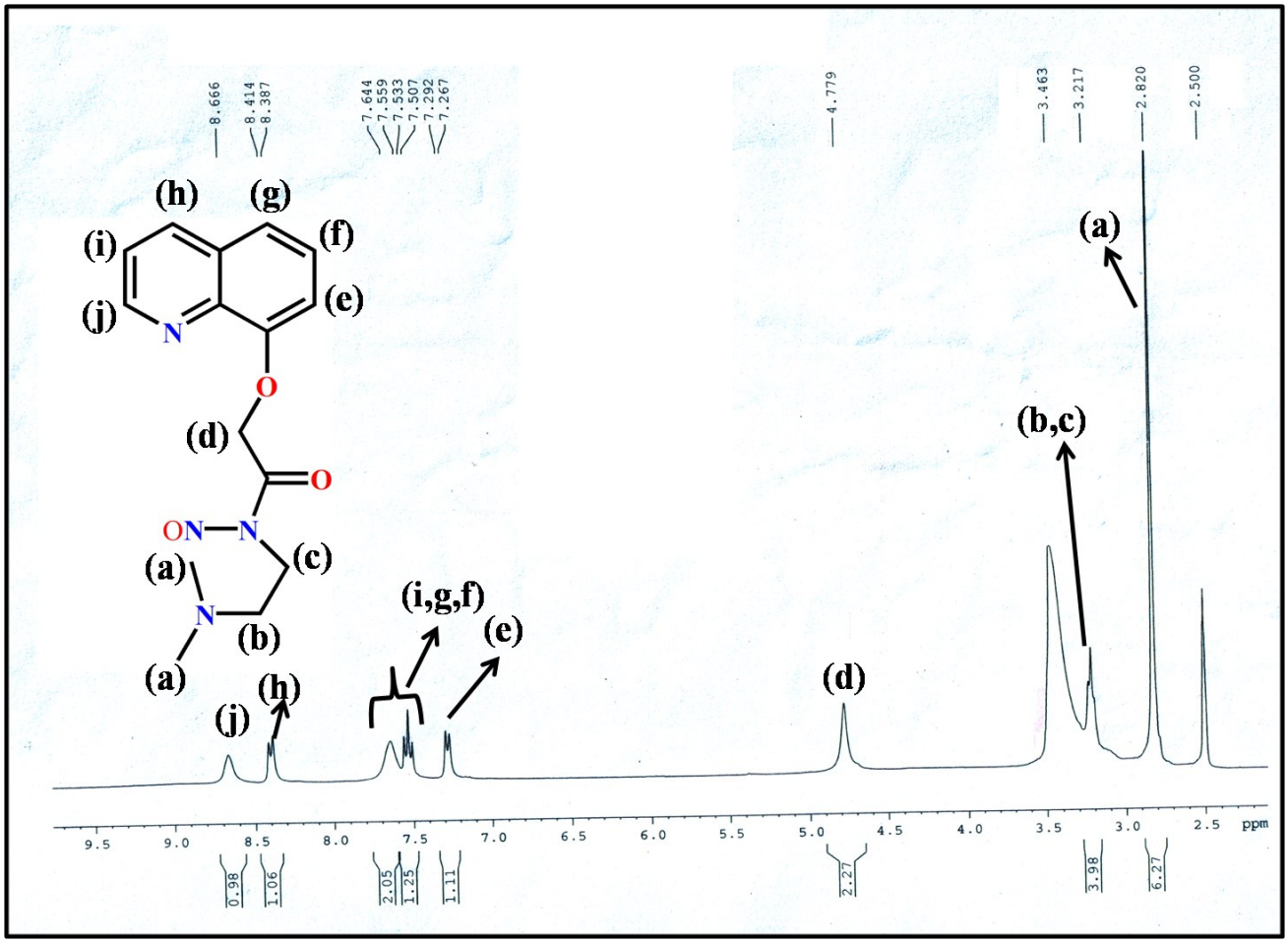

Fig.S9.[1]H NMR spectrum of **HqEN$_{480}$-NO** in DMSO-d_6.

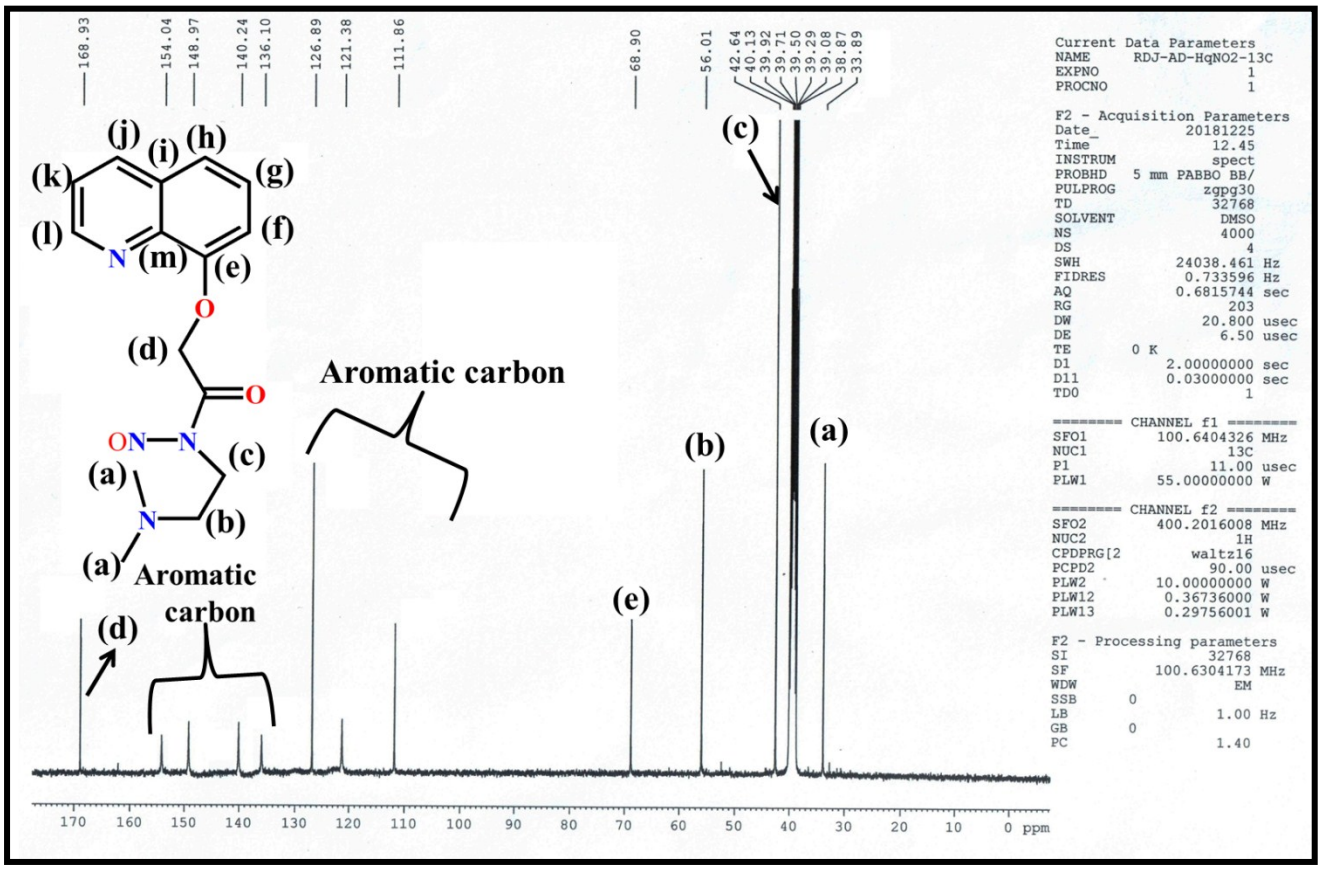

Fig.S9a. ^{13}C NMR spectrum of **HqEN$_{480}$-NO** in DMSO-d_6.

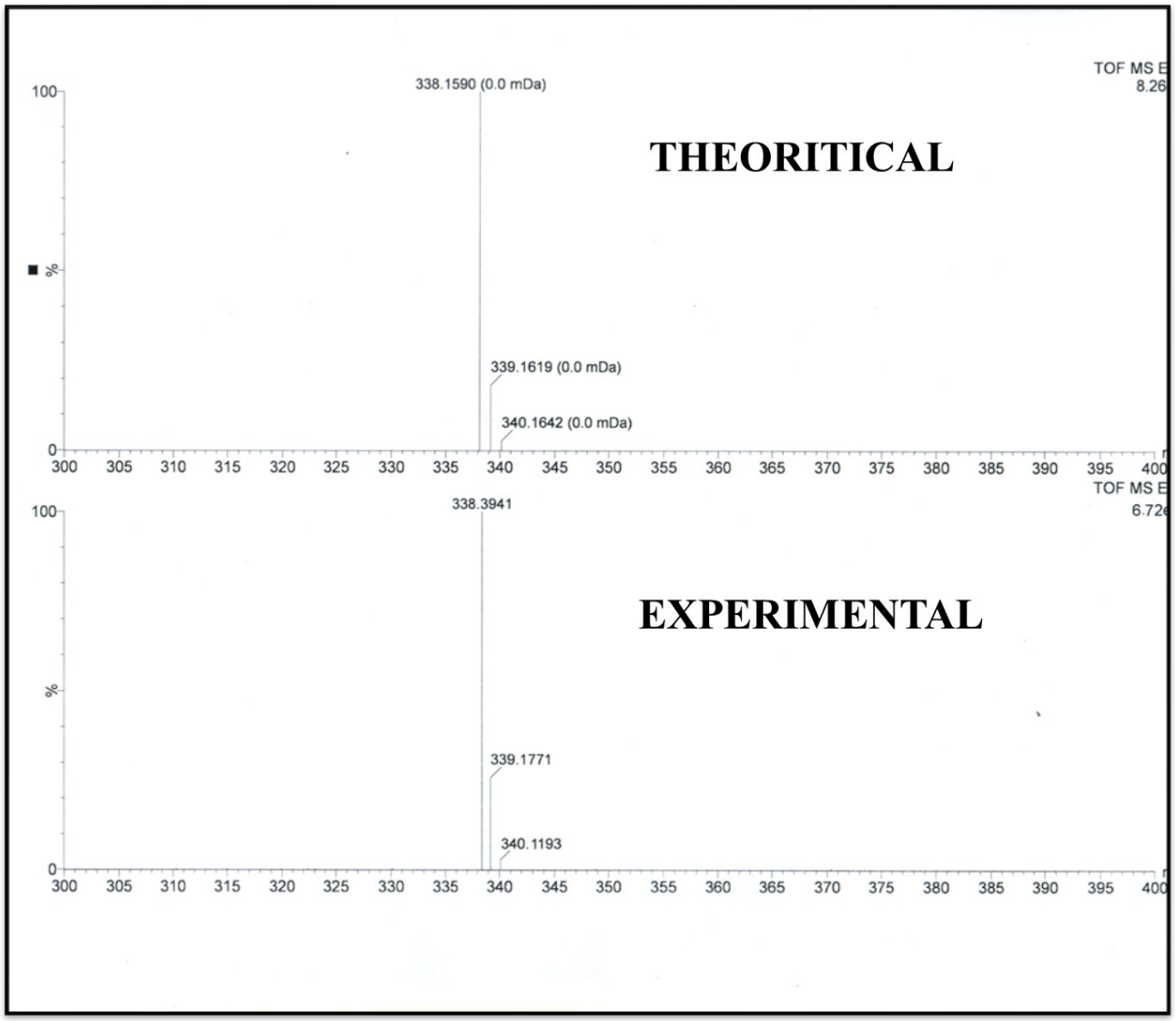

Fig. S10. Mass spectrum of **HqEN$_{480}$-NO** in MeCN**.**

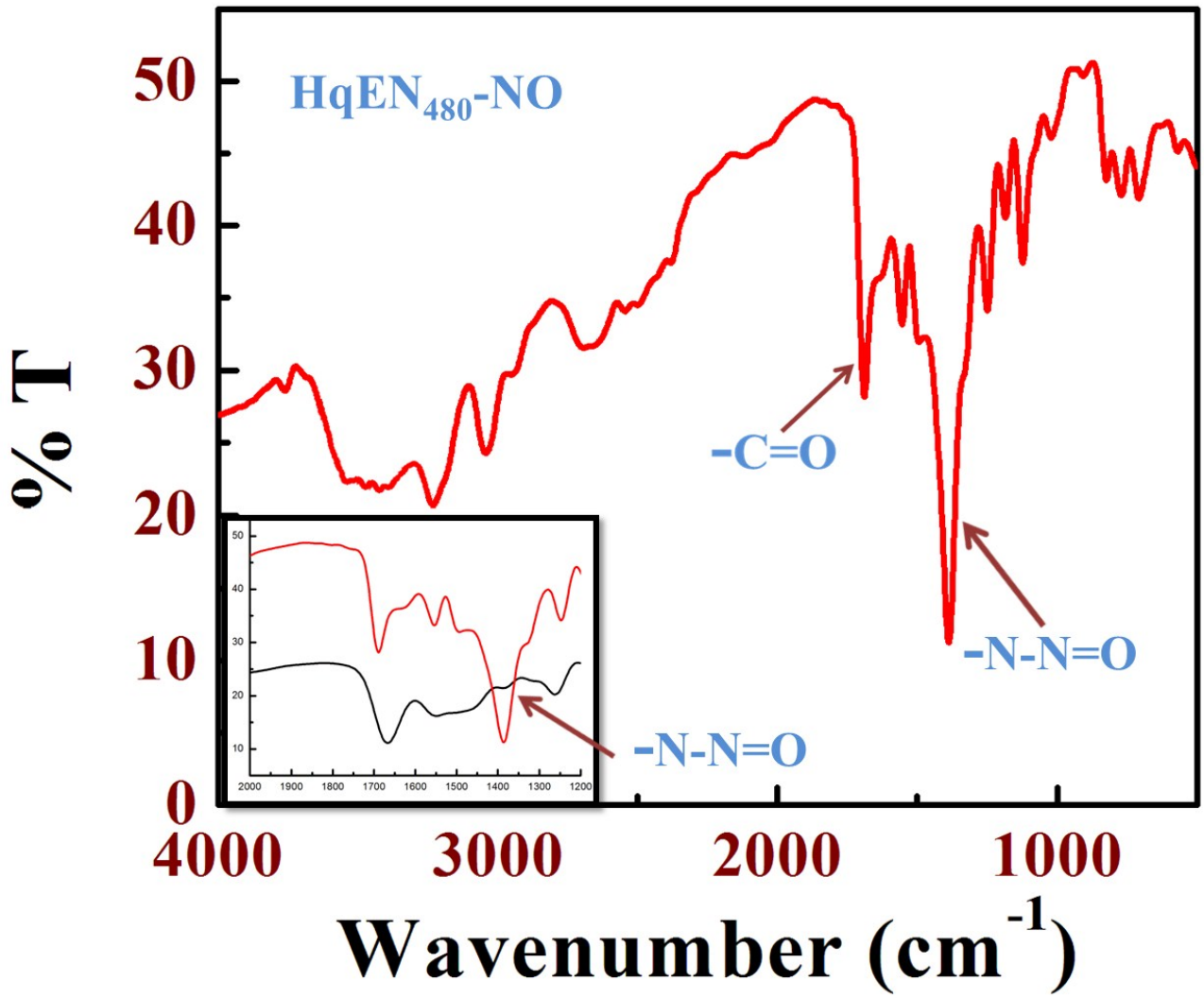

Fig. S11. IR spectrum of **($HqEN_{480}$-NO)** in solid state.

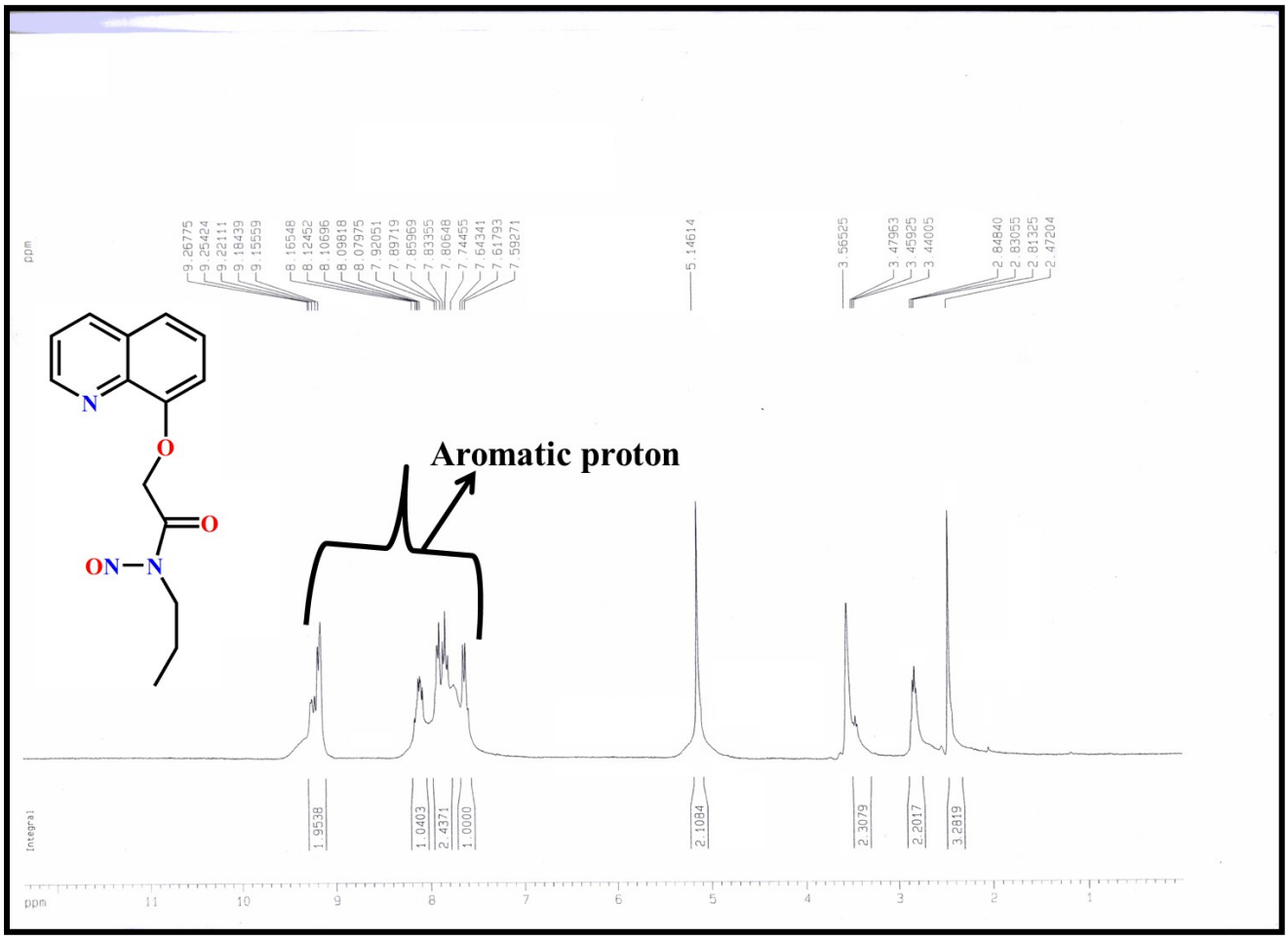

Fig. S12. ^{1}H NMR spectrum of **HqPA-NO** in DMSO-d_6.

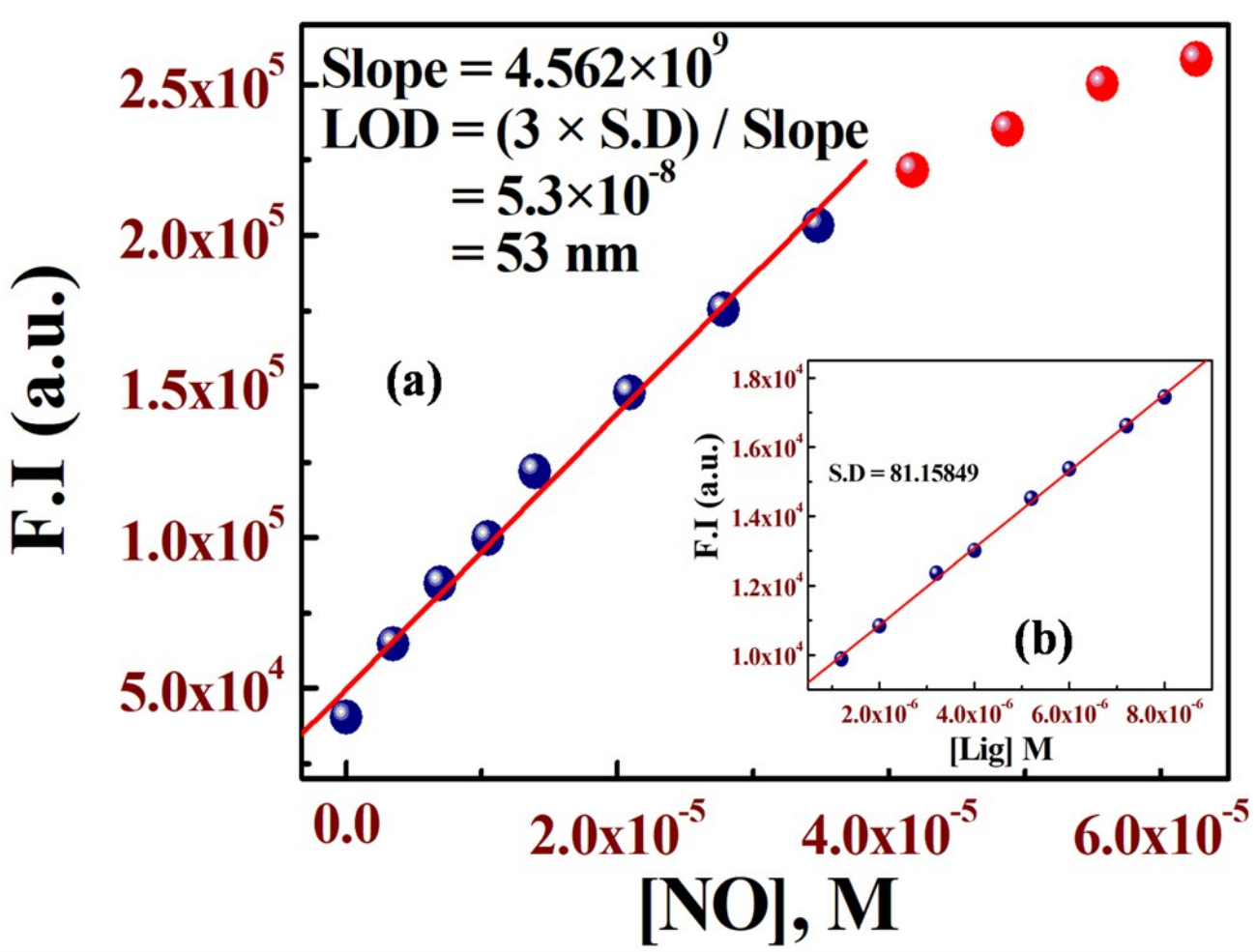

Fig. S13. LOD of ($HqEN_{480}$-NO) from fluorescence study.

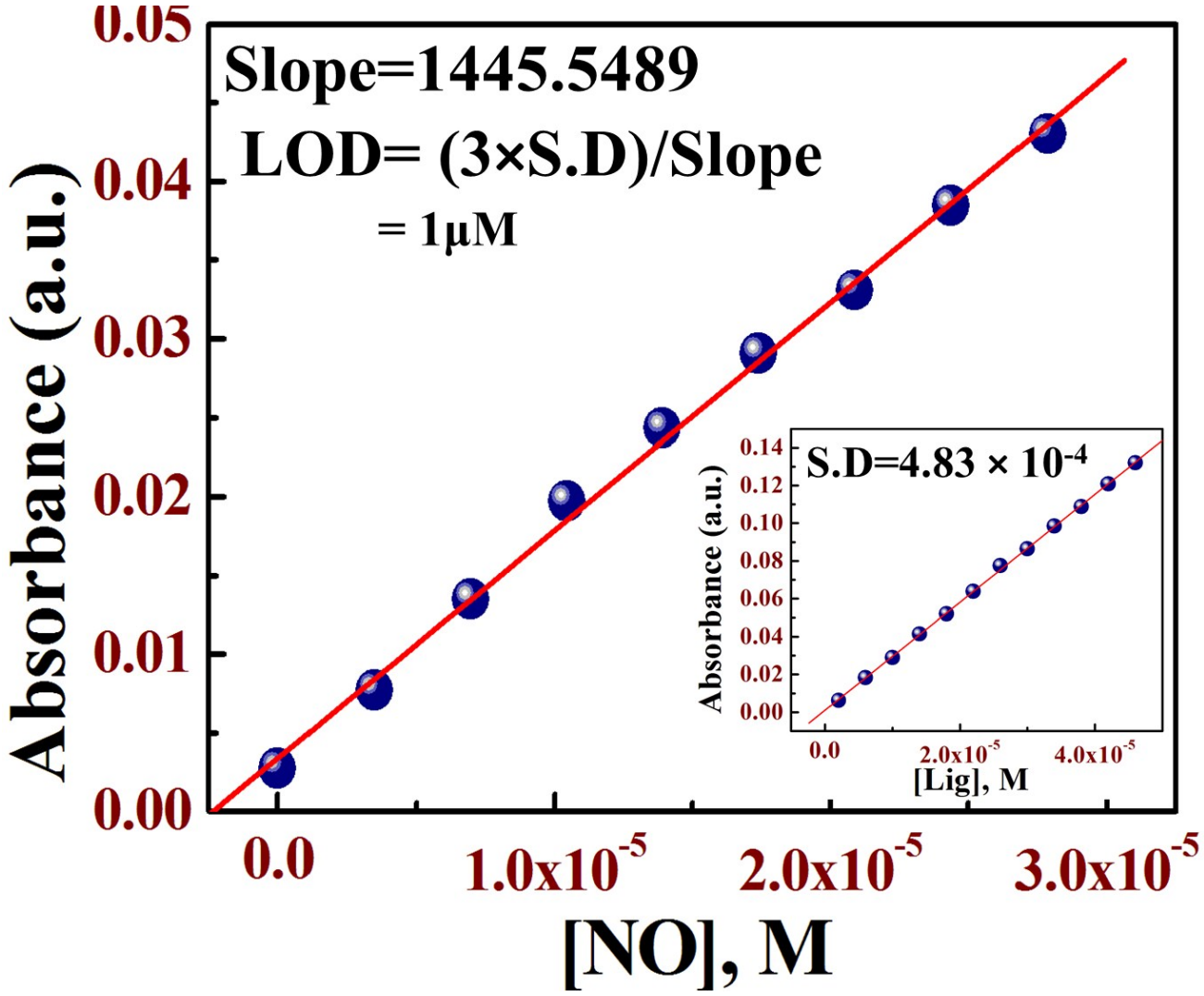

Fig. S13a. LOD of **($HqEN_{480}$-NO)** from UV-vis study**.**

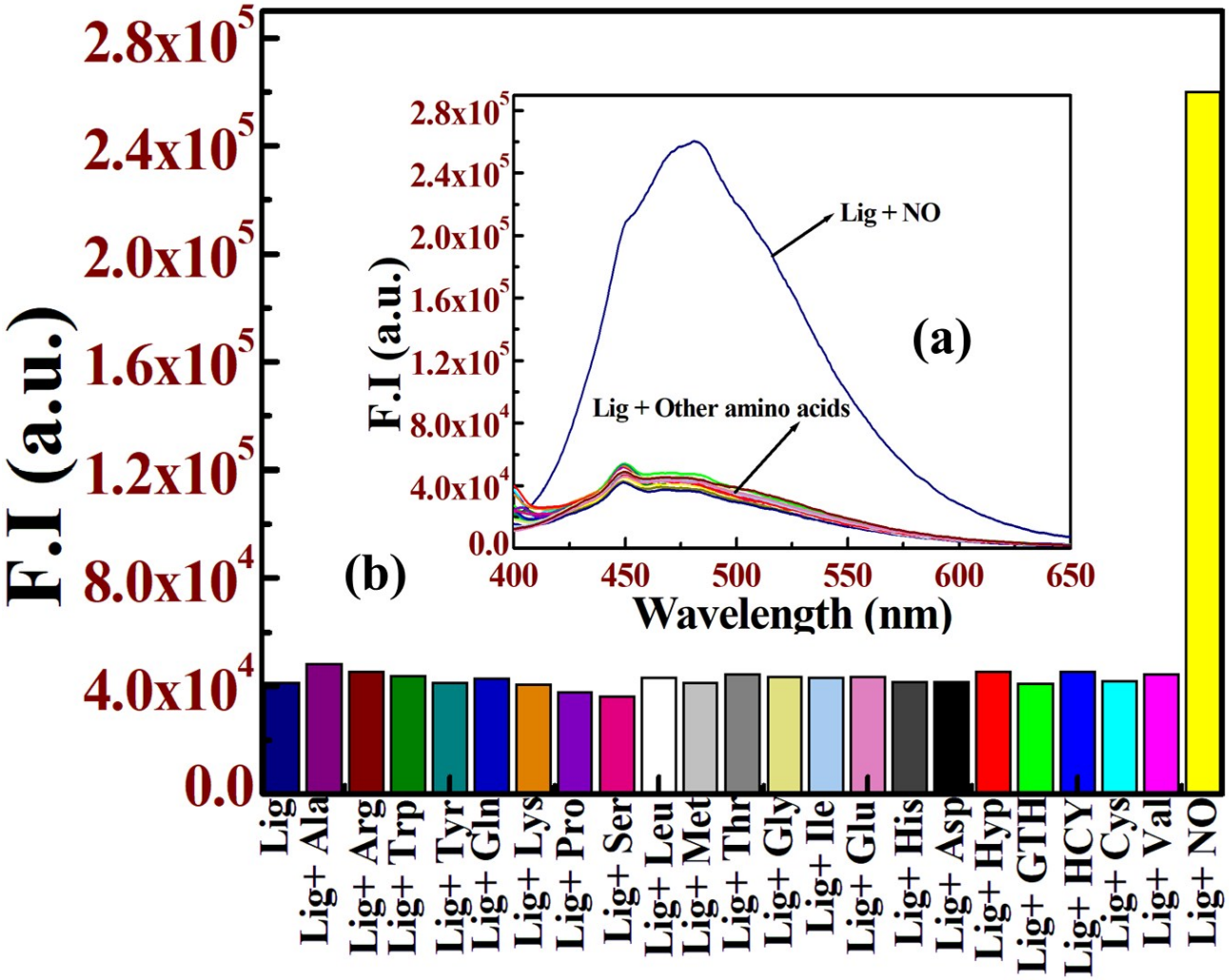

Fig. S14. Fluorescence response of $HqEN_{480}$ towards various aminoacids in aqueous HEPES buffer at λ_{ex}=390nm.

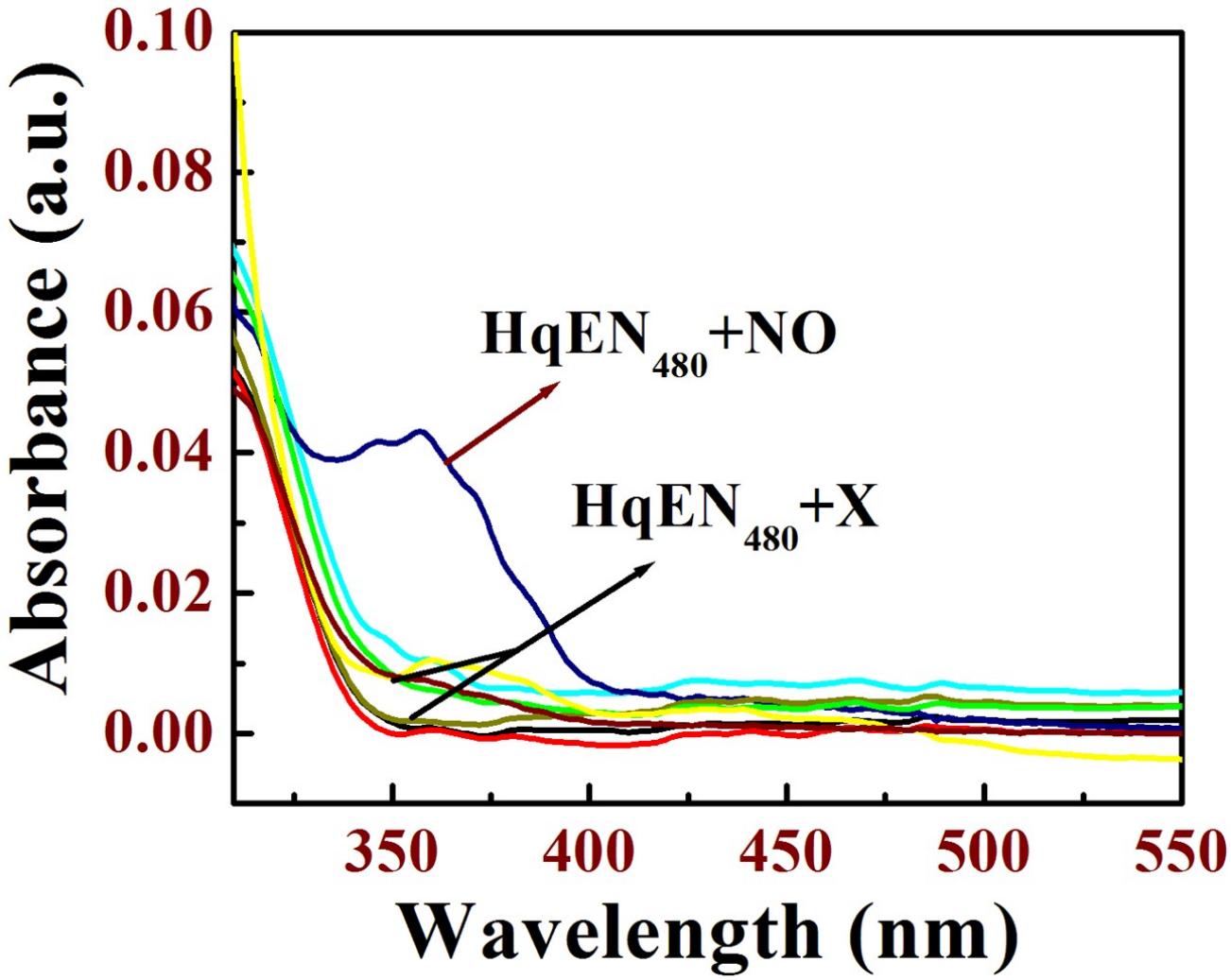

Fig. S15. UV-vis absorbtion spectra of **$HqEN_{480}$** towards various RONS (X=H_2O_2, ,DHA,TEMPO,KO_2,$ONOO^-$,AA and NO).

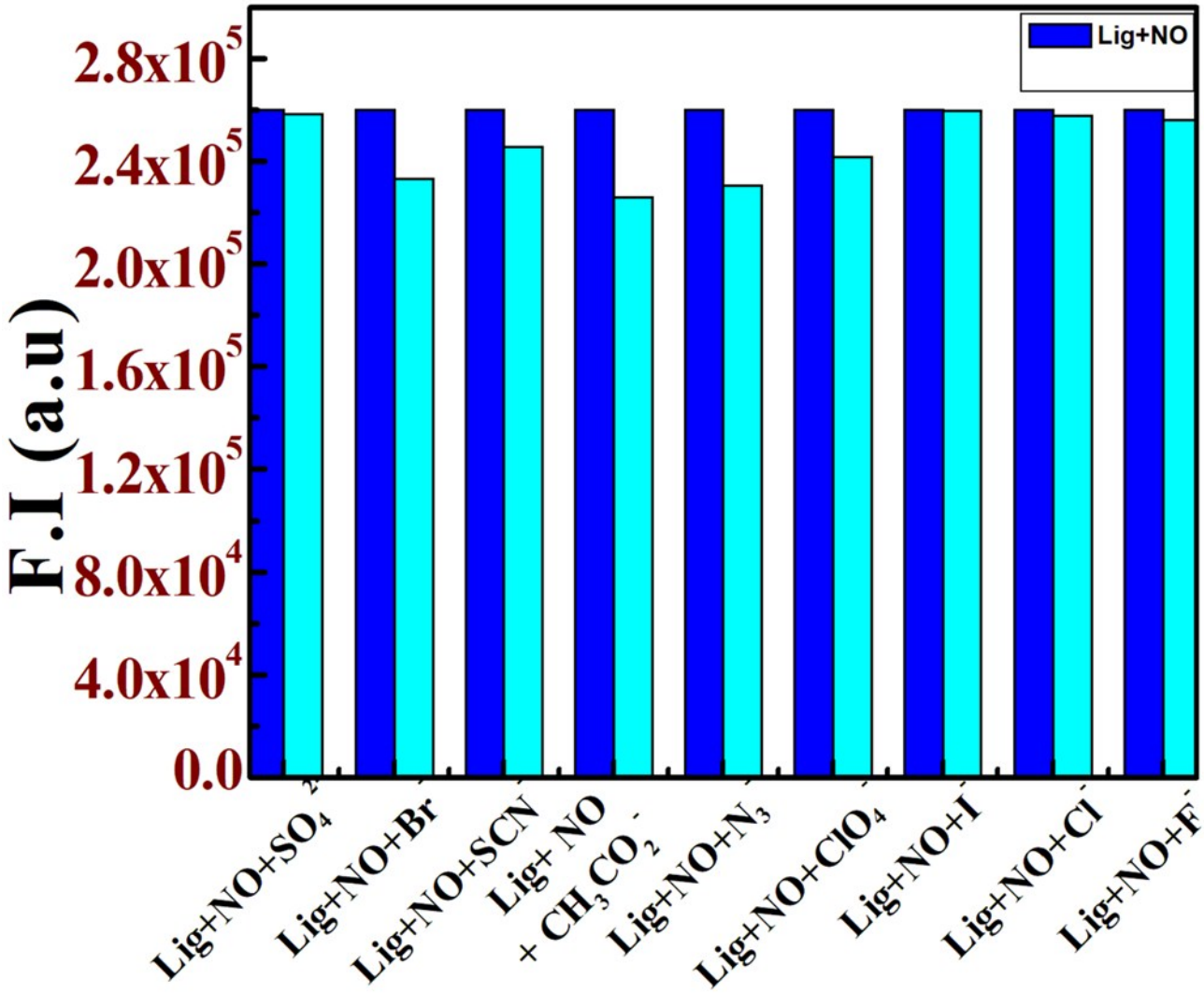

Fig. S16. Bar plot of Competitive study of ions over NO at λ_{ex}=390nm.

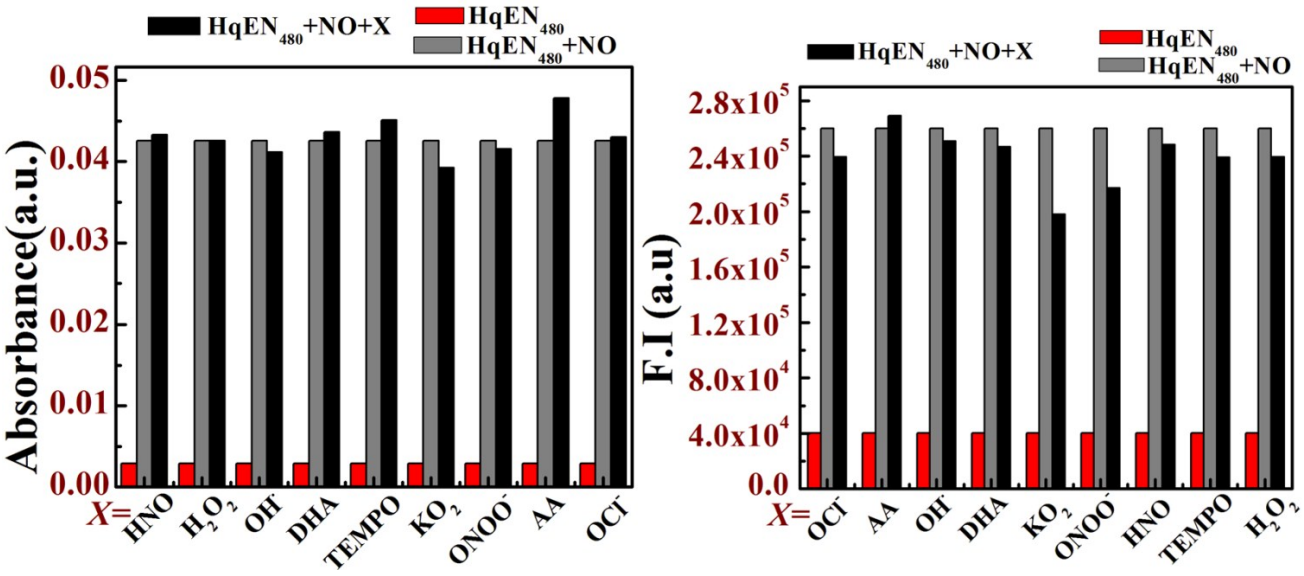

Fig. S17. Bar plot of Competitive study of reactive species over NO from fluorescence at λ_{ex}=390nm and UV-vis absorbtion method .

Table S1. List of some selected bond lengths of **$HqEN_{480}$** in the ground state calculated at B3LYP Levels.

Bond Lengths (Å)			
O17-C18	1.450	C21-N23	1.351
C18-C21	1.522	N23-C25	1.459
C21-O22	1.255	C25-C28	1.532
Bond Angles (º)			
O17-C18-C21	108.92	O22-C21-N23	124.97
C18-C21-O22	118.72	C21-N23-C25	122.24
C18-C21-N23	116.30	N23-C25-C28	109.87

Table S2. Some selected geometrical parameters for **[$HqEN_{480}$-NO]** in the ground state calculated at B3LYP Levels.

Bond Lengths (Å)			
C10-O17	1.385	C21-O22	1.238
O17-C18	1.453	N23-N39	1.385
C18-C21	1.517	N39-O40	1.246
C21-N23	1.404	N23-C24	1.473
	Bond Angles (º)		
C10-O17-C18	118.56	C21-N23-C24	121.78
O17-C18-C21	105.62	N23-N39-O40	114.22
C18-C21-N23	116.94	C21-N23-N39	116.47
C18-C21-O22	122.09		

Table S3. Vertical excitation energies and oscillator strengths (f_{cal}) of some low-lying excited singlet states obtained from TDDFT// B3LYP/6-31G calculations of **$HqEN_{480}$**.

Electronic transition	**Composition**	**Excitation Energy**	**Oscillator strength (*f*)**	**CI**	**λ_{exp} (nm)**
$S_0 \rightarrow S_2$	HOMO –1→ LUMO	4.0372 eV (307.10 nm)	0.1045	0.69360	314

Table S4. Vertical excitation energies and oscillator strengths (f_{cal}) of some low-lying excited singlets obtained from TDDFT// B3LYP/6-31G calculations of **[$HqEN_{480}$-NO].**

Electronic transition	**Composition**	**Excitation Energy**	**Oscillator strength (*f*)**	**CI**	**λ_{exp} (nm)**
$S_0 \rightarrow S_8$	HOMO → LUMO + 2	4.0721 eV (304.47 nm)	0.0814	0.50961	355
	HOMO – 1 → LUMO + 1			0.47473	

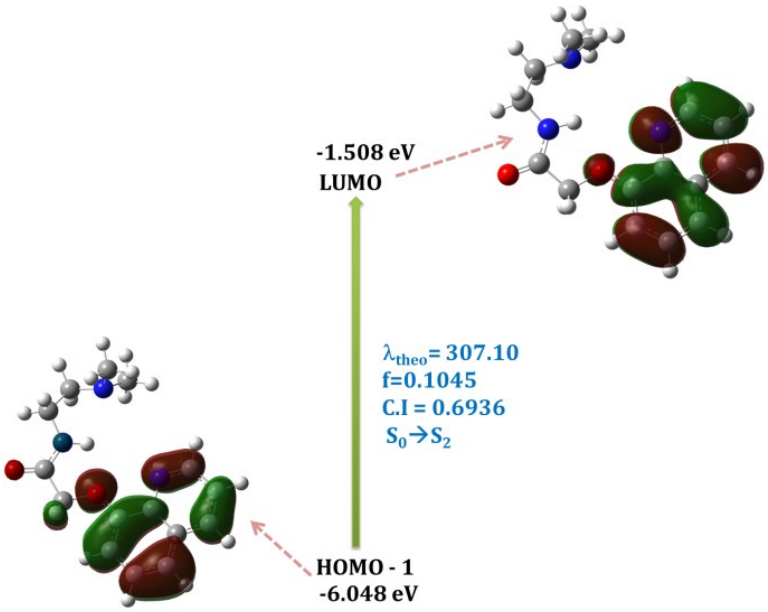

Fig. S18. Frontier molecular orbitals involved in the UV-Vis absorption of **HqEN$_{480}$.**

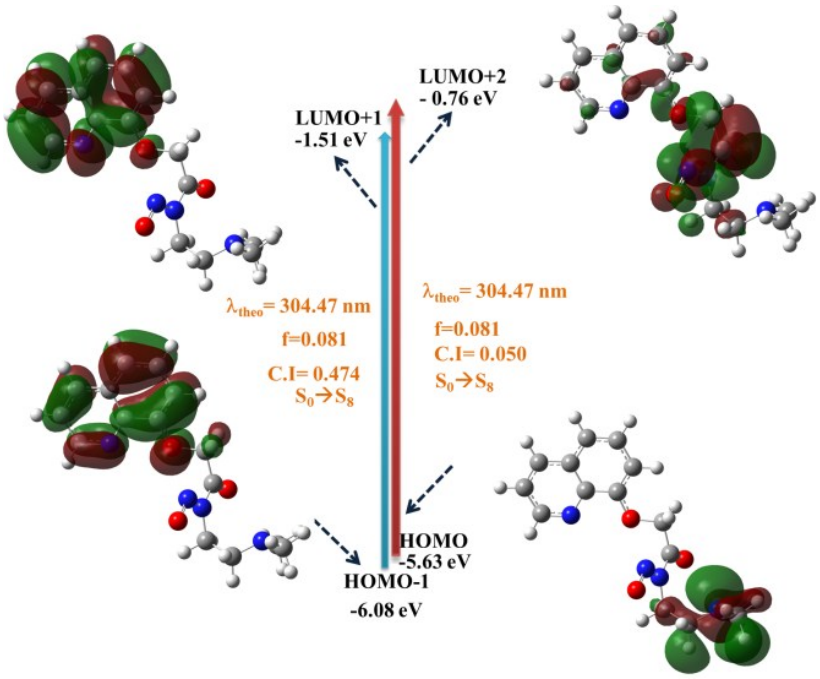

Fig. S19. Frontier molecular orbitals involved in the UV-Vis absorption of **[HqEN$_{480}$-NO]**.

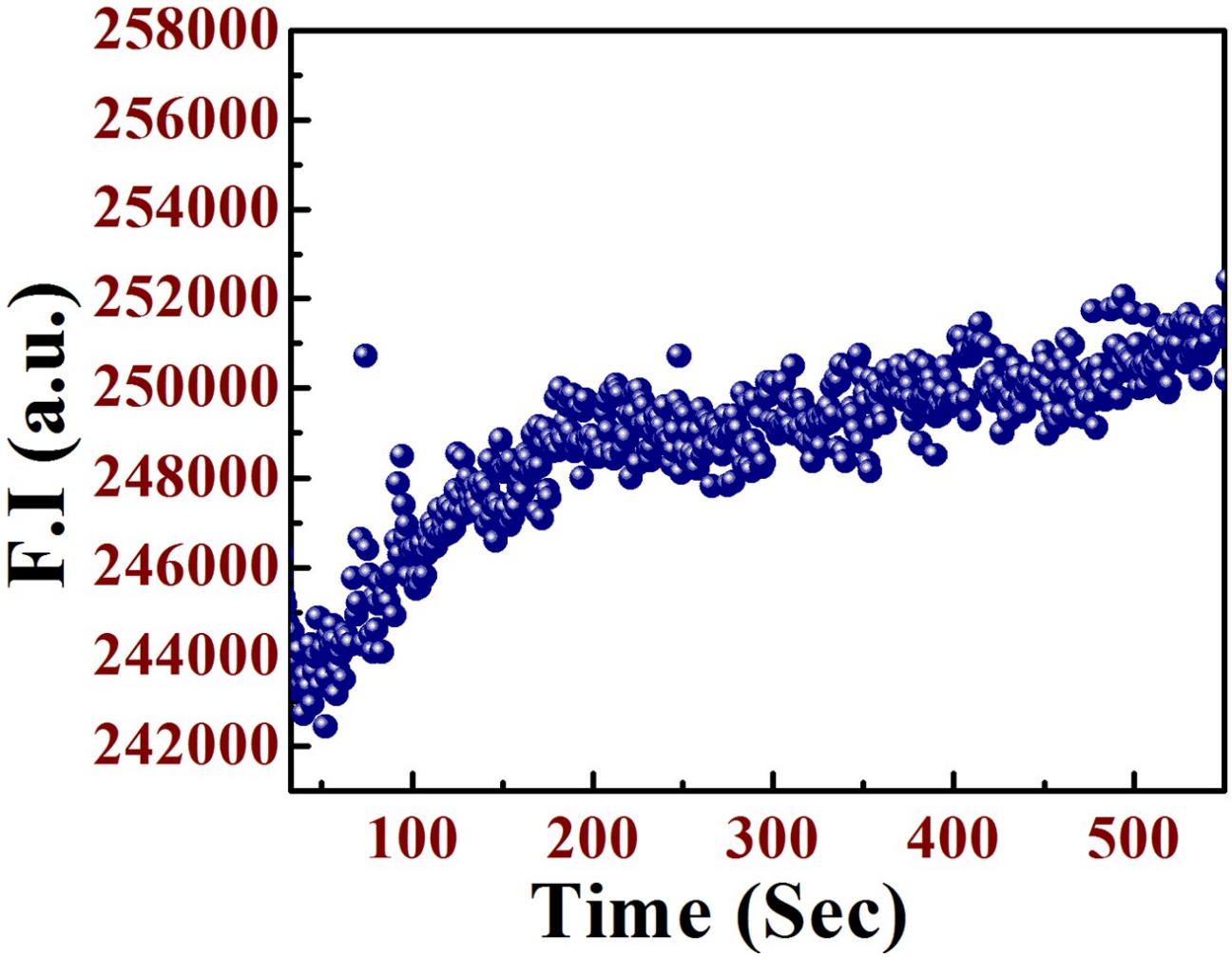

Fig. S20. The response time of the probe towards NO.