

Supporting Information

Imidazole-based fluorescent probes: Concomitant effects of N1 substitution and lone pair on selective recognition of Picric Acid

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Experimental section

Materials:

All the reaction carried out under nitrogen atmosphere. Commercially available reagents (sigma aldrich) were used as purchased without any further purification. All the reaction were monitored by thin-layer chromatography (TLC) with silica gel 60 F₂₅₄ Aluminium plates (Merck). Column chromatography was carried out using silica gel (Sigma-Aldrich).

General information for Measurements:

^1H NMR and ^{13}C NMR spectra were measured using an AV 400 Avance-III 400 MHz FT-NMR spectrometer (Bruker Biospin International, Switzerland) with tetramethylsilane (TMS) as the internal standard reference. The absorption and photoluminescence (PL) excitation and emission spectra of the synthesized luminophores were measured using a SHIMADZU UV-2450 spectrophotometer and a HORIBAFLUOROMAX – 4P spectrophotometer, respectively. Thin film making with the help of spin coating instrument (Holmarc Spin coater, Model No. HO-TH-OSC) by stages were at 1000 rpm (60 sec). The prepared thin film were kept under UV drying for 10 sec to get excess solvent evaporation. The absolute fluorescence quantum yield was measured with

Edinburgh Spectrofluorometer, FS5 with Integrating Sphere SC-30. The electrochemical properties of the fluorophores were measured by using Cyclic voltammetry (CV) experiments were performed in dimethyl formamide (DMF) solution containing 0.1 M tert-butyl ammonium perchlorate (Bu_4NClO_4) using as the supporting electrolyte, and the scan rate was continued at 100 mV s^{-1} using an AUTOLAB 302N Modular potentiostat at room temperature. The working (glass-carbon rod), auxiliary (counter, Pt wire) and reference (Ag/AgCl wire) electrode were used for CV analysis. The CIE color chromaticity coordinates of the fluorophores were calculated from the emission spectral values by using MATLAB software.

Detection Measurement of Nitroaromatic compound:

For quantitative measurement, the emission measurements were performed in increasing the different concentrations of PA in THF ($1 \times 10^{-5} \text{ M}$). Subsequent addition of $0 \mu\text{L}$ to $120 \mu\text{L}$ in the respective fluorophores ($1 \times 10^{-5} \text{ M}$) of the solution. By subsequent addition of picric acid the absolute decreasing of the intensity was observed as compared to other nitroaromatics compound. We also check the response time within 10sec adding the concentration of PA the quenching of emission happens which results that even if with the low concentration of PA the fluorophores perfectly responses.

NMR Spectra of all luminophores:

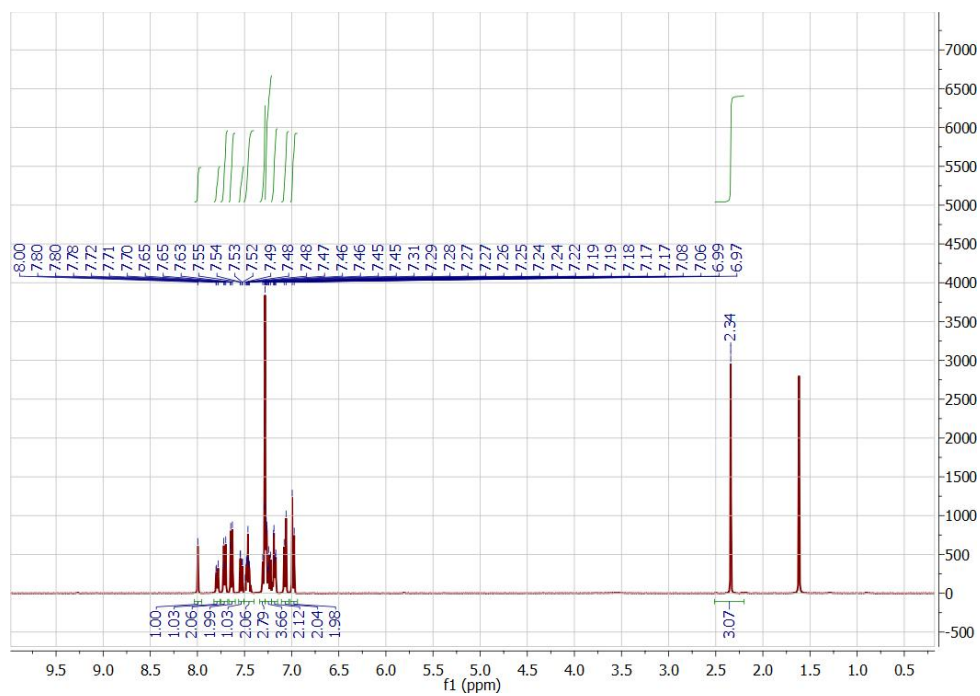


Fig. S12. ^1H NMR spectrum of 2-NTPI-2.

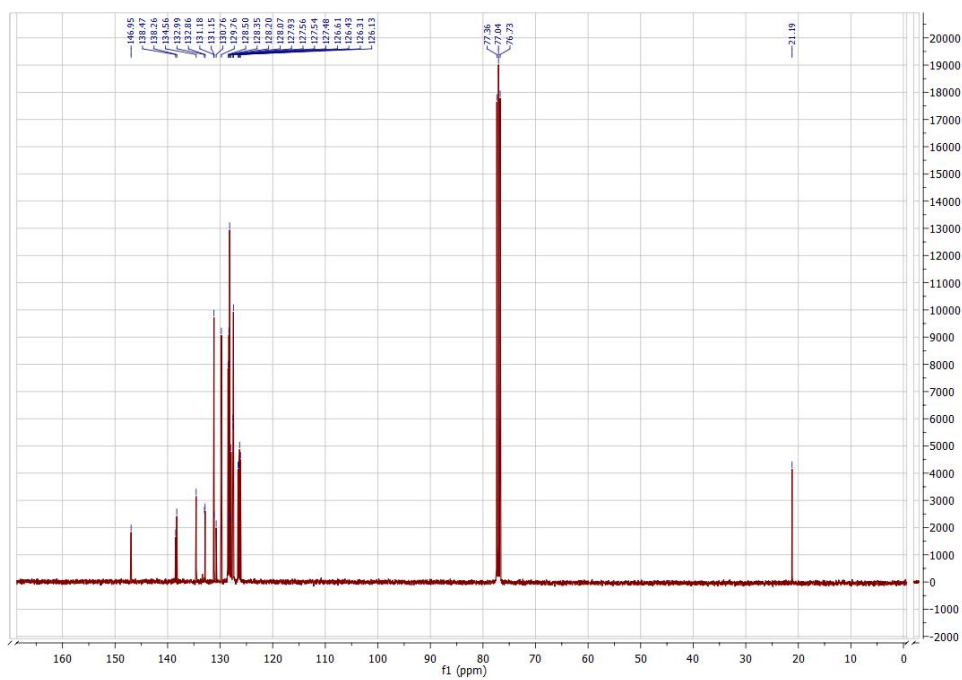


Fig. S12(i). ^{13}C NMR spectrum of 2-NTPI-2.

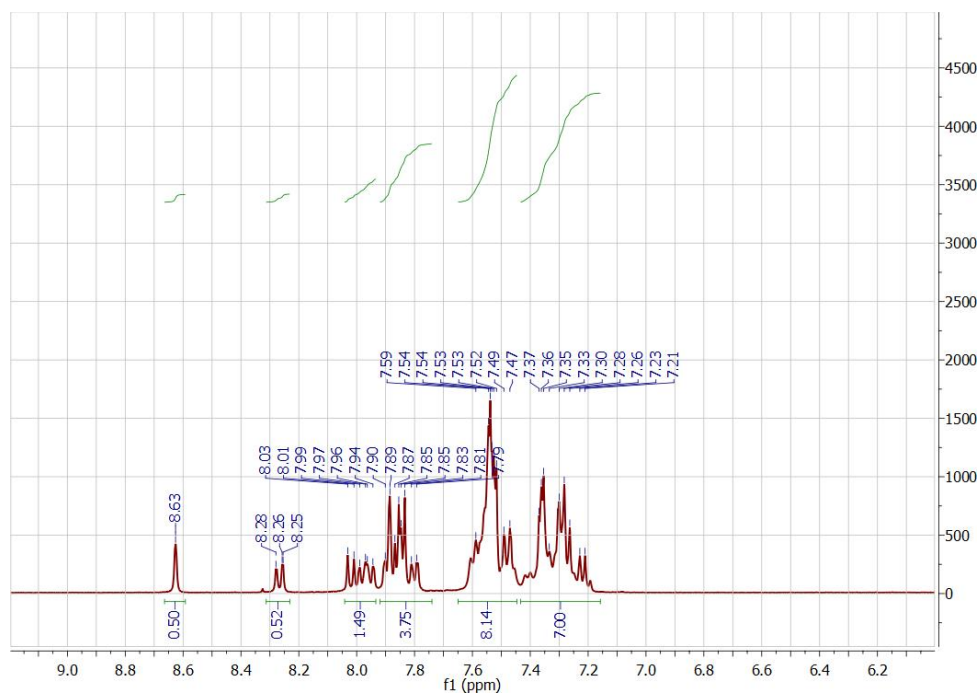


Fig. S13. ^1H NMR spectrum of 2-NTPI-3.

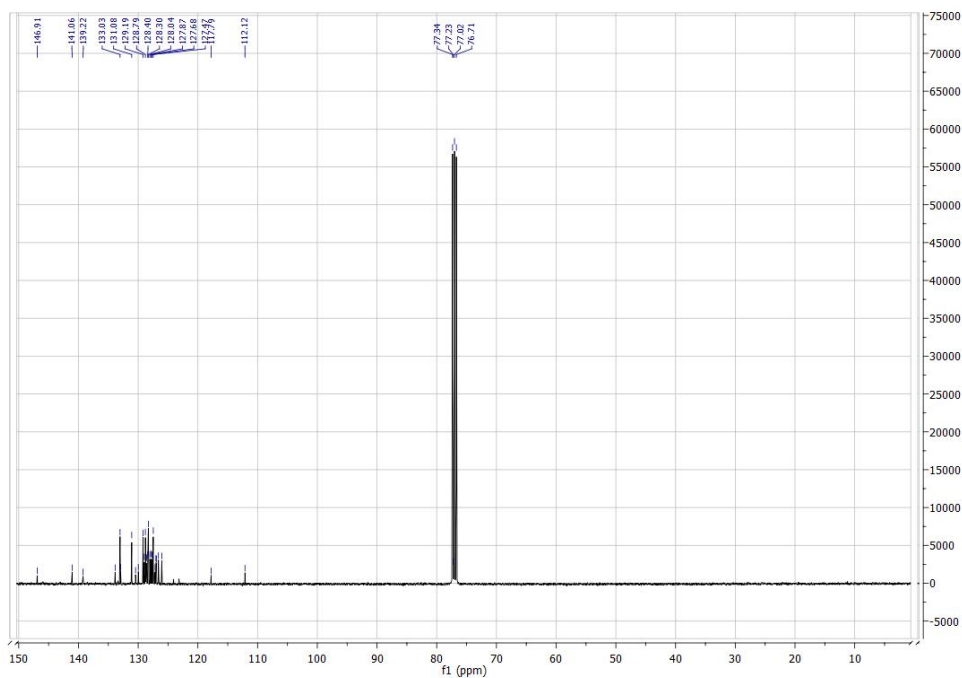


Fig. S13(i). ^{13}C NMR spectrum of 2-NTPI-3.

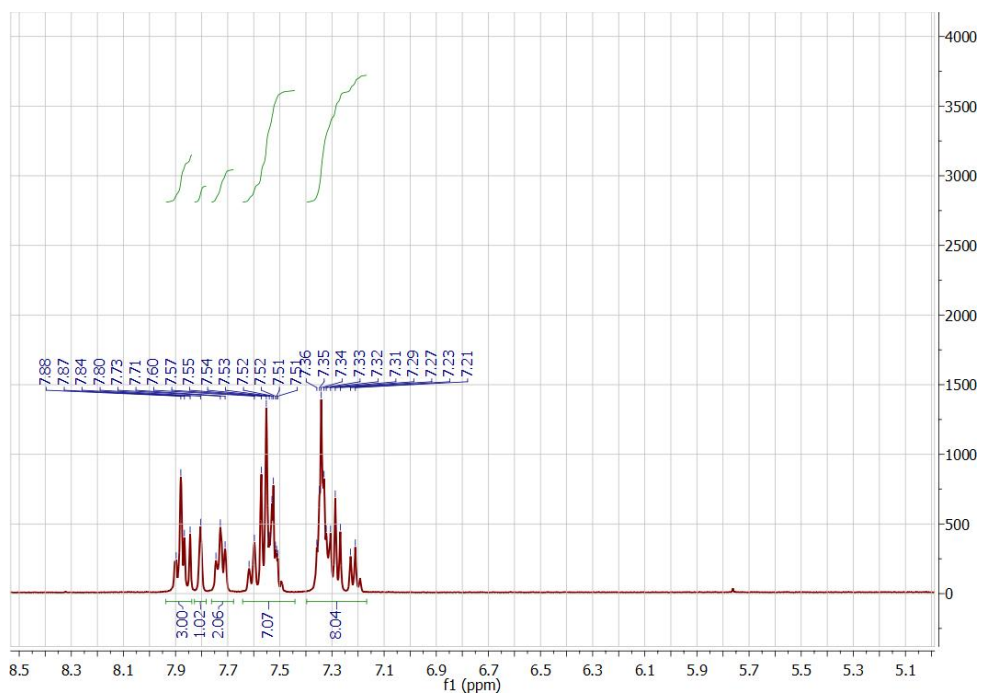


Fig. S14. ^1H NMR spectrum of 2-NTPI-4.

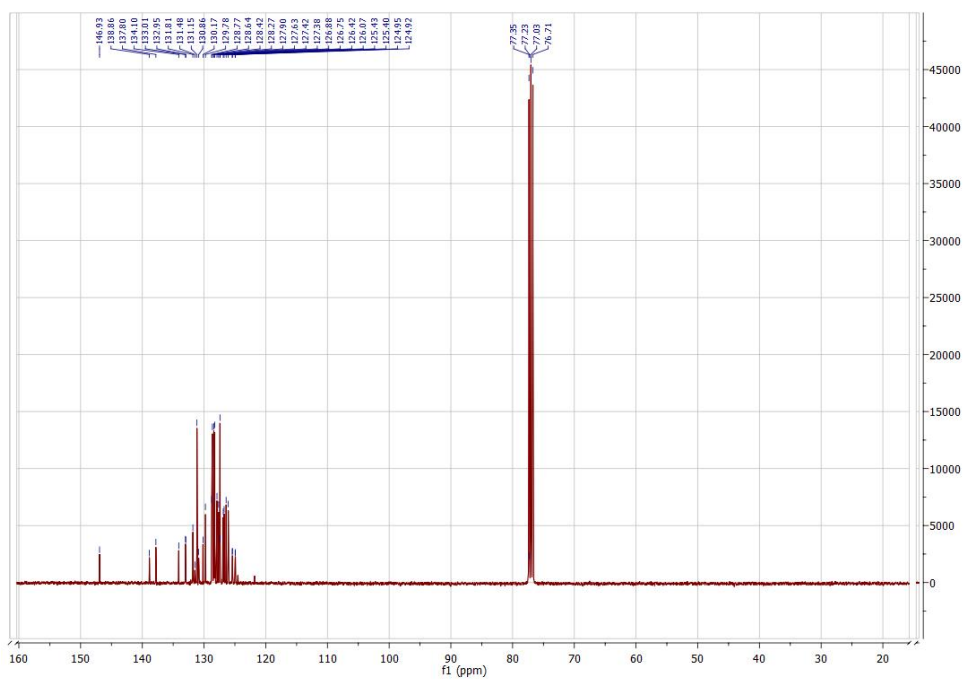


Fig. S14(i). ^{13}C NMR spectrum of 2-NTPI-4.

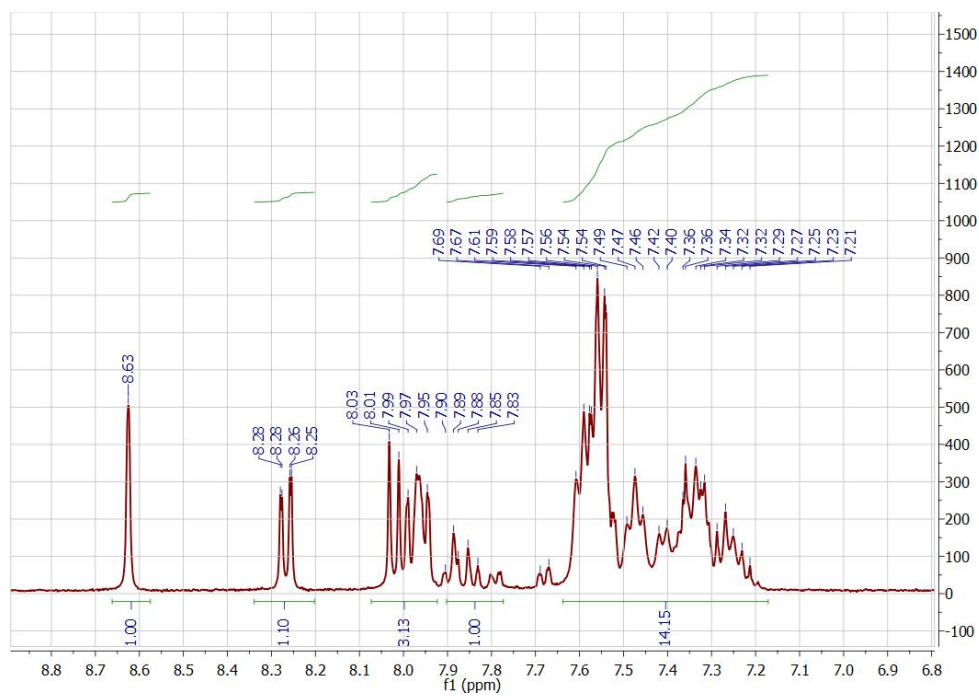


Fig. SI5. ^1H NMR spectrum of 2-NTPI-5.

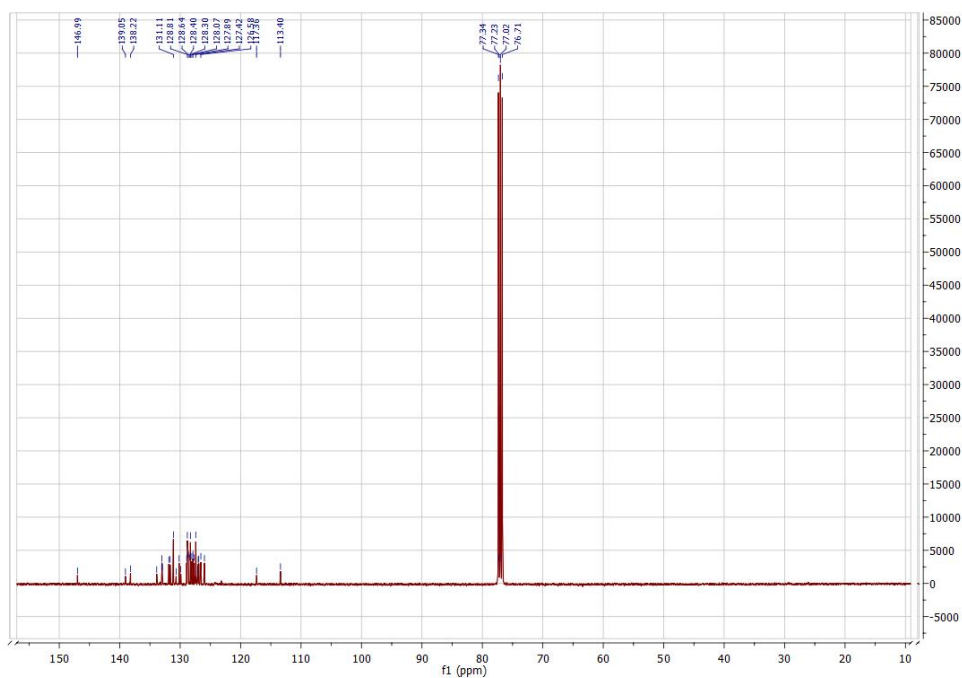


Fig. SI5(i). ^{13}C NMR spectrum of 2-NTPI-5.

Mass Spectra of all the luminophores.

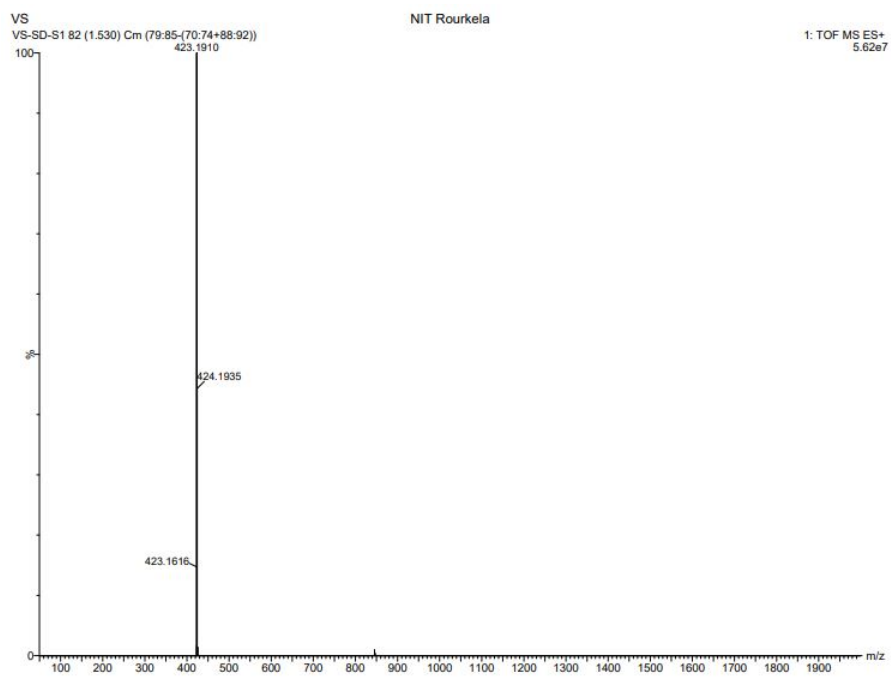


Fig. S16. Mass spectrum of the 2-NTPI-1.

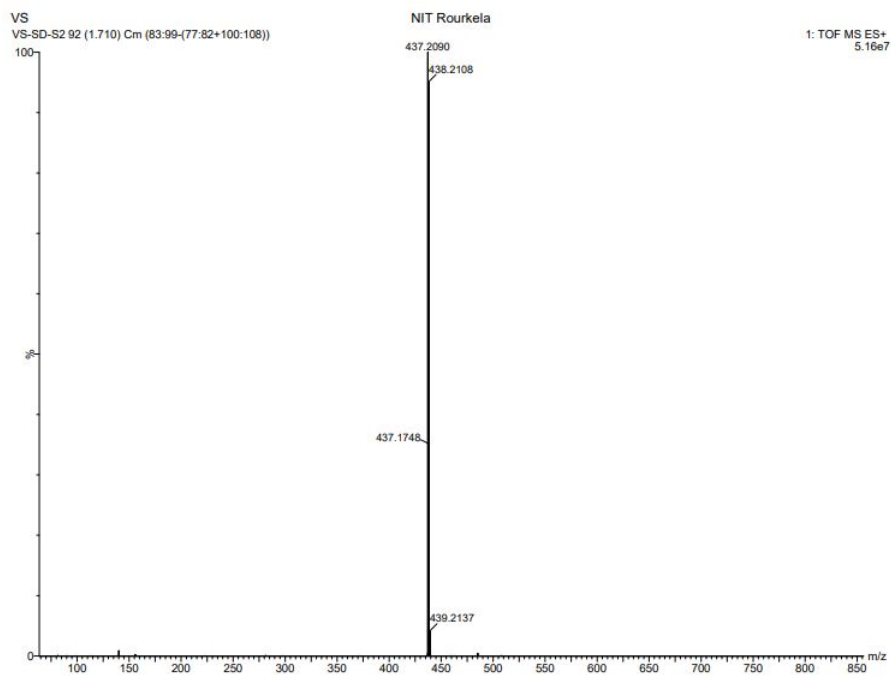


Fig. S17. Mass spectrum of the 2-NTPI-2.

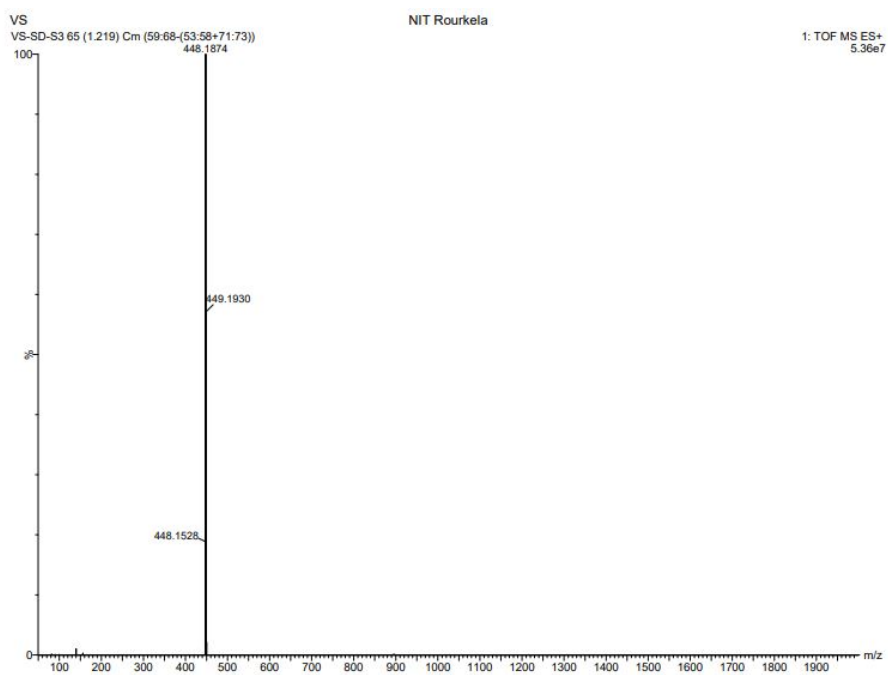


Fig. S18. Mass spectrum of the 2-NTPI-3

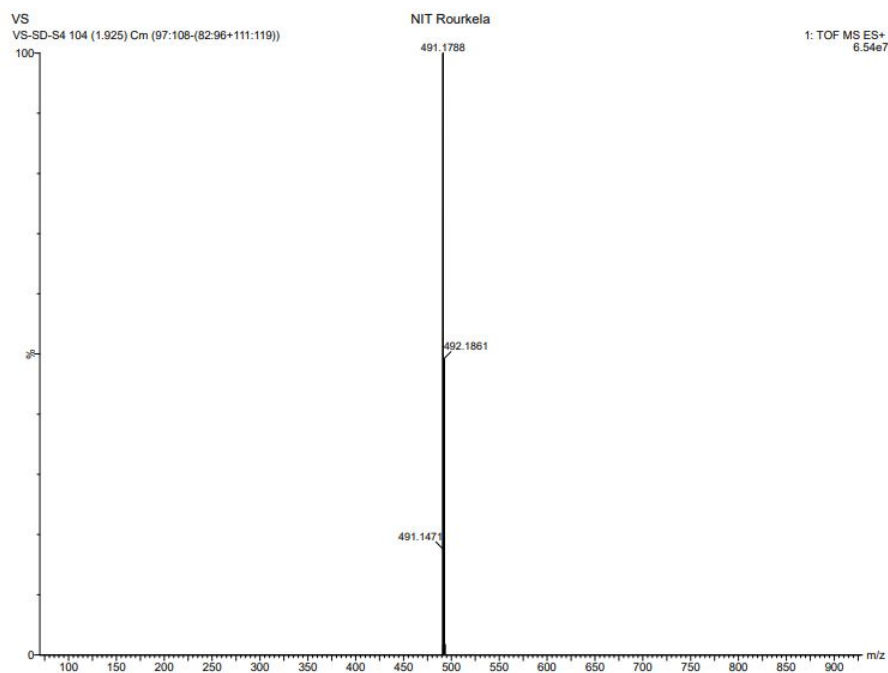


Fig. S19. Mass spectrum of the 2-NTPI-4

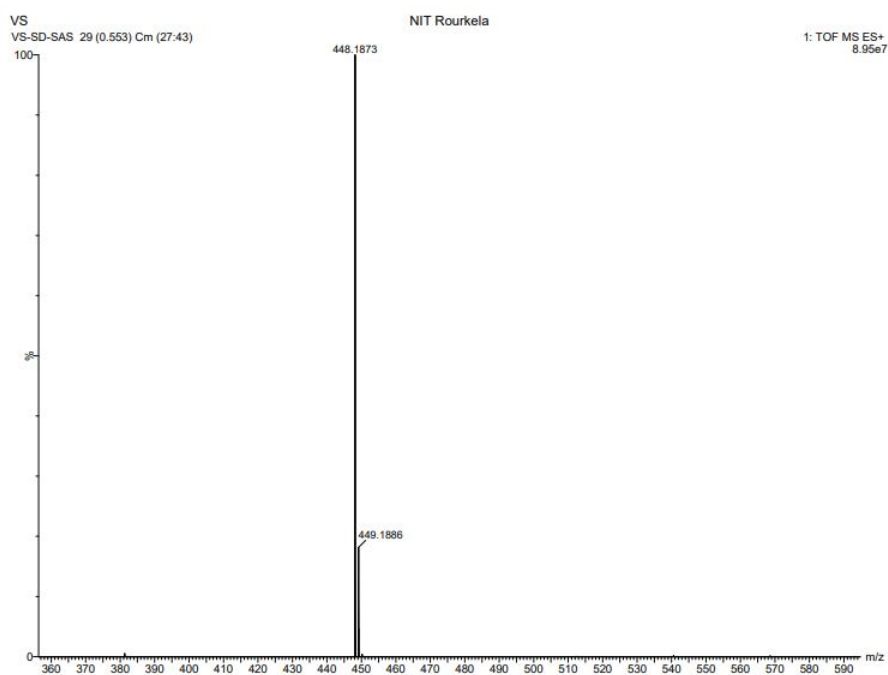


Fig. S110. Mass spectrum of the 2-NTPI-5

S13. ^1H -NMR spectra with PA (0, 0.5, 1.0 equiv) in CDCl_3 .

^1H NMR Spectra of all luminophores after the addition of PA :

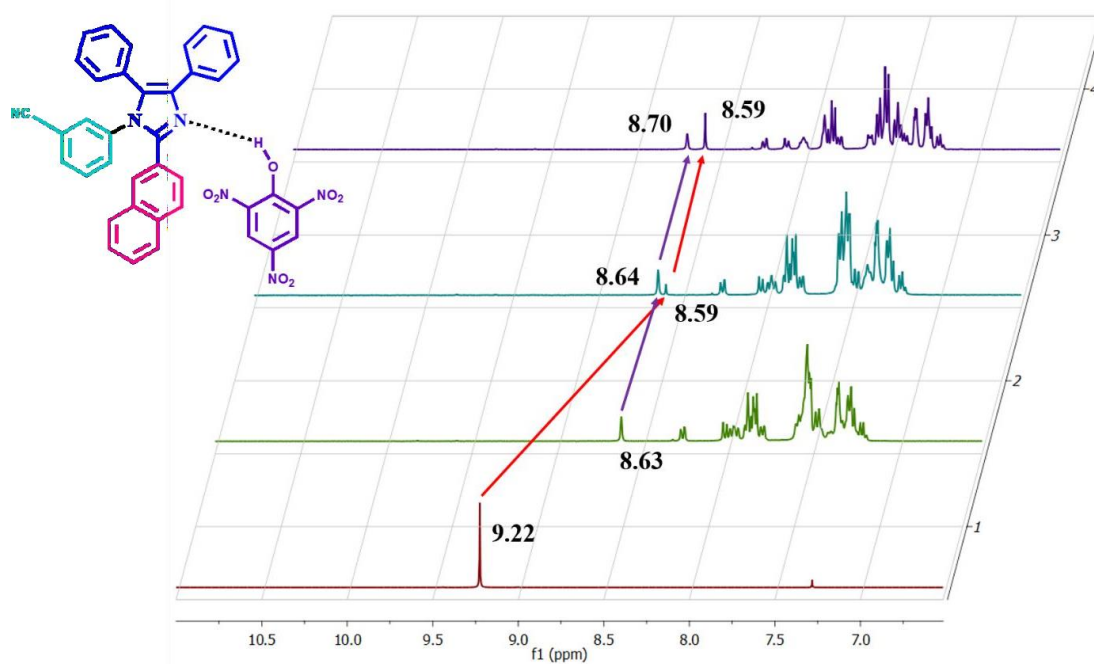


Fig. SI11 ^1H NMR spectrum of 2-NTPI-3 with PA (0, 0.5, 1.0 equiv) in CDCl_3 .

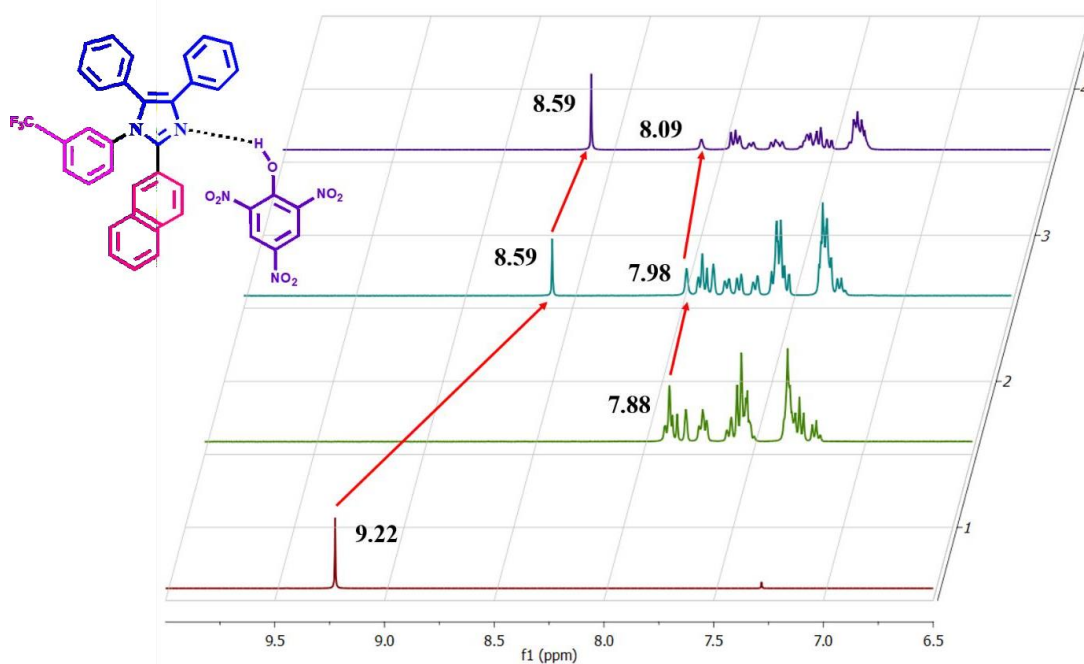


Fig. SI12 ^1H NMR spectrum of 2-NTPI-4 with PA (0, 0.5, 1.0 equiv) in CDCl_3 .

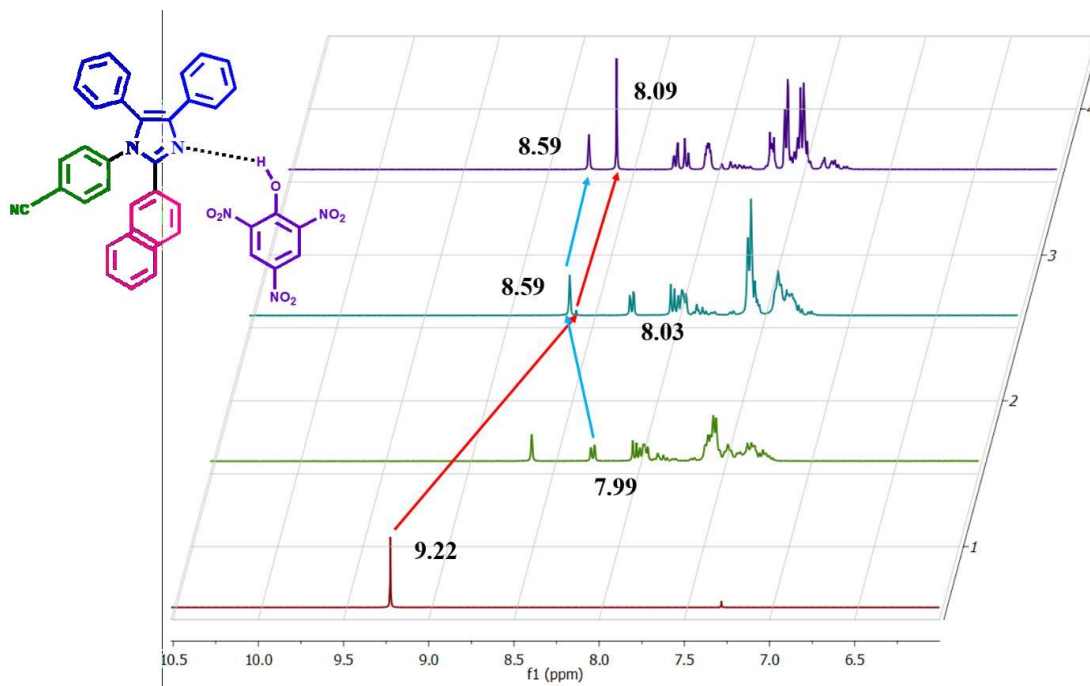


Fig. SI13 ^1H NMR spectrum of 2-NTPI-5 with PA (0, 0.5, 1.0 equiv) in CDCl_3 .

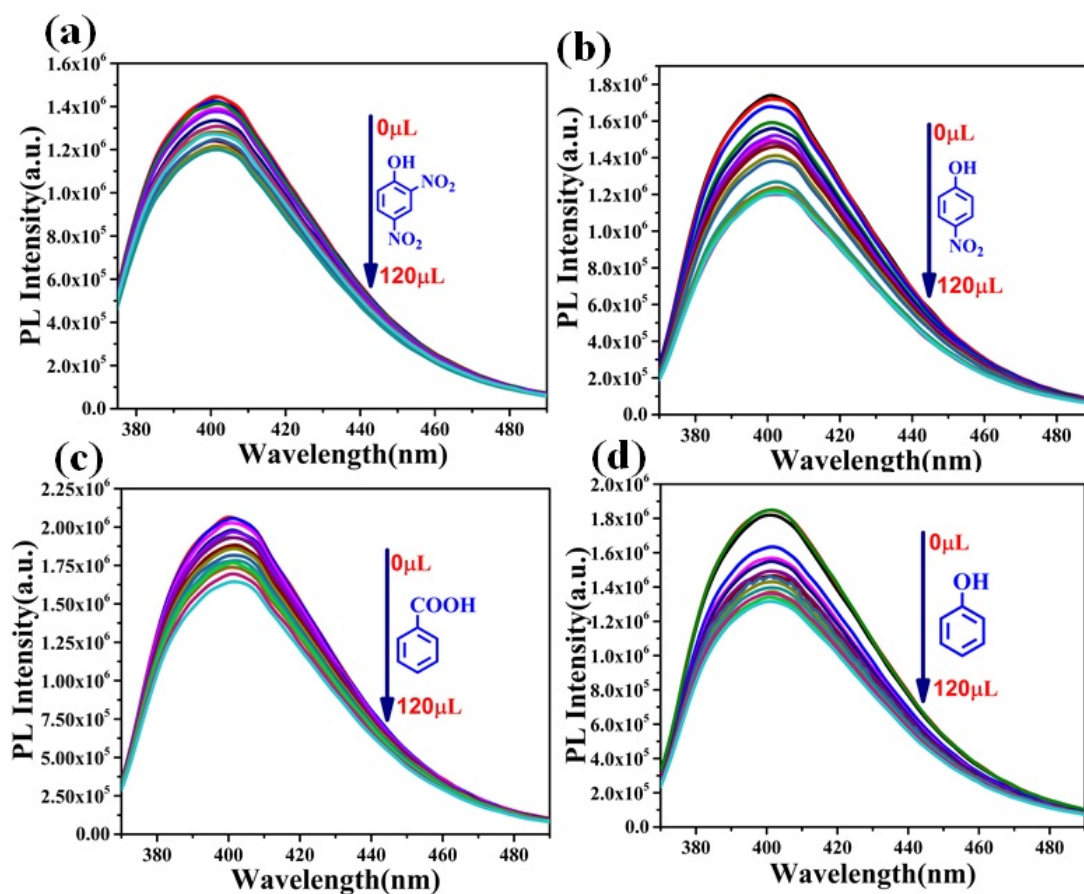


Fig. SI14. Change in the fluorescence of 2-NTPI-3 upon the addition of different quenchers excited at 341nm in THF solvent (1×10^{-5} M).

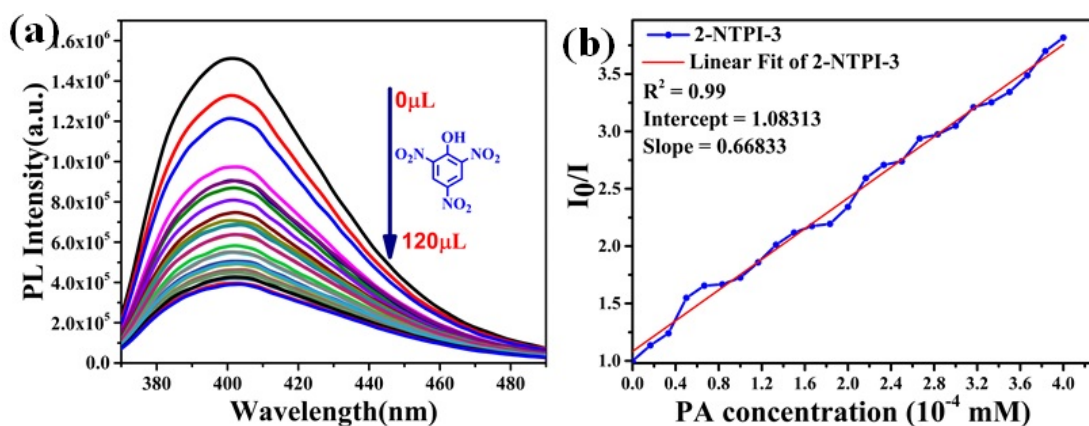


Fig. SI15. (a) Change in the fluorescence of 2-NTPI-3 upon the addition of PA excited at 341 nm in THF solvent (1×10^{-5} M). (b) Stern–Volmer plots of 2-NTPI-3 using PA as a quencher. Inset: Stern–Volmer plots at lower concentration region of PA.

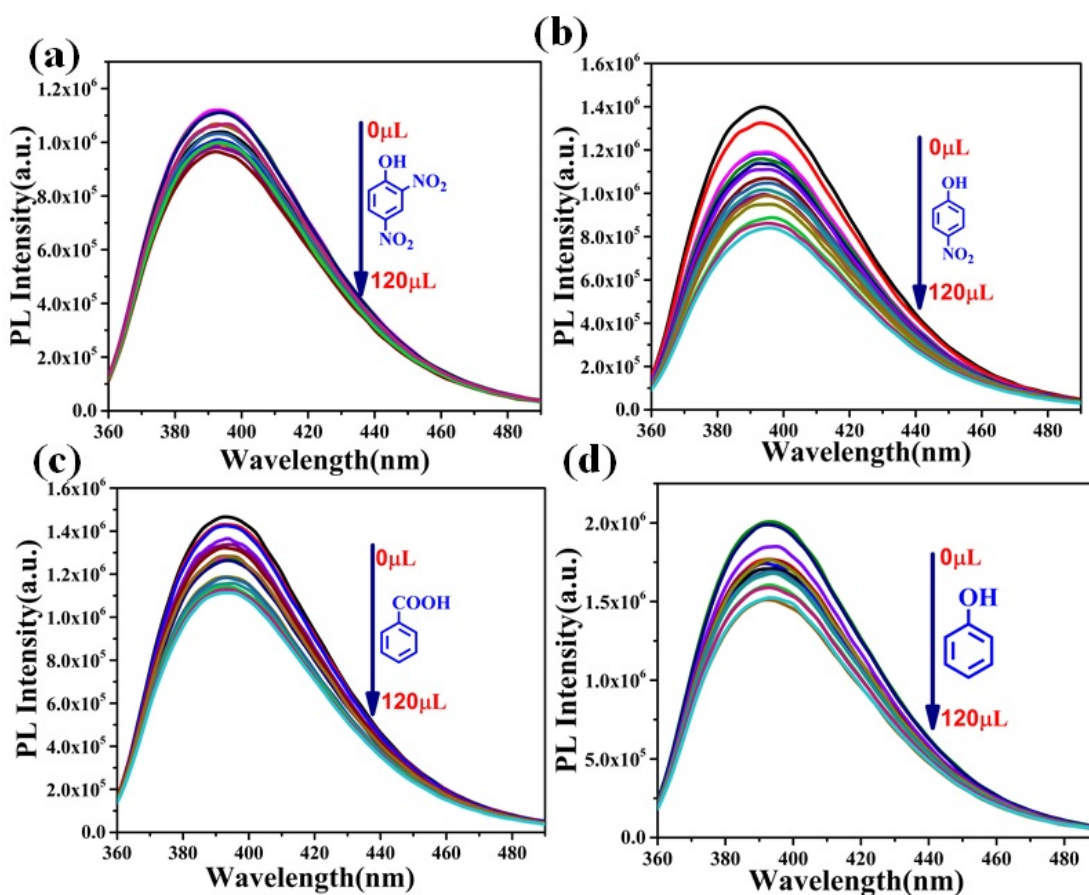


Fig. SI16. Change in the fluorescence of 2-NTPI-3 upon the addition of different quenchers excited at 337 nm in THF solvent (1×10^{-5} M).

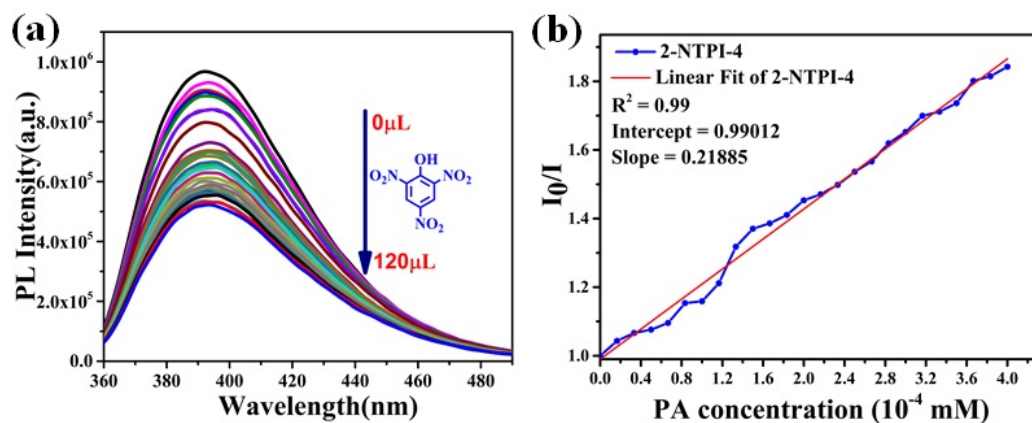


Fig. SI17. (a) Change in the fluorescence of 2-NTPI-4 upon the addition of PA excited at 337 nm in THF solvent (1×10^{-5} M). (b) Stern–Volmer plots of 2-NTPI-4 using PA as a quencher. Inset: Stern–Volmer plots at lower concentration region of PA.

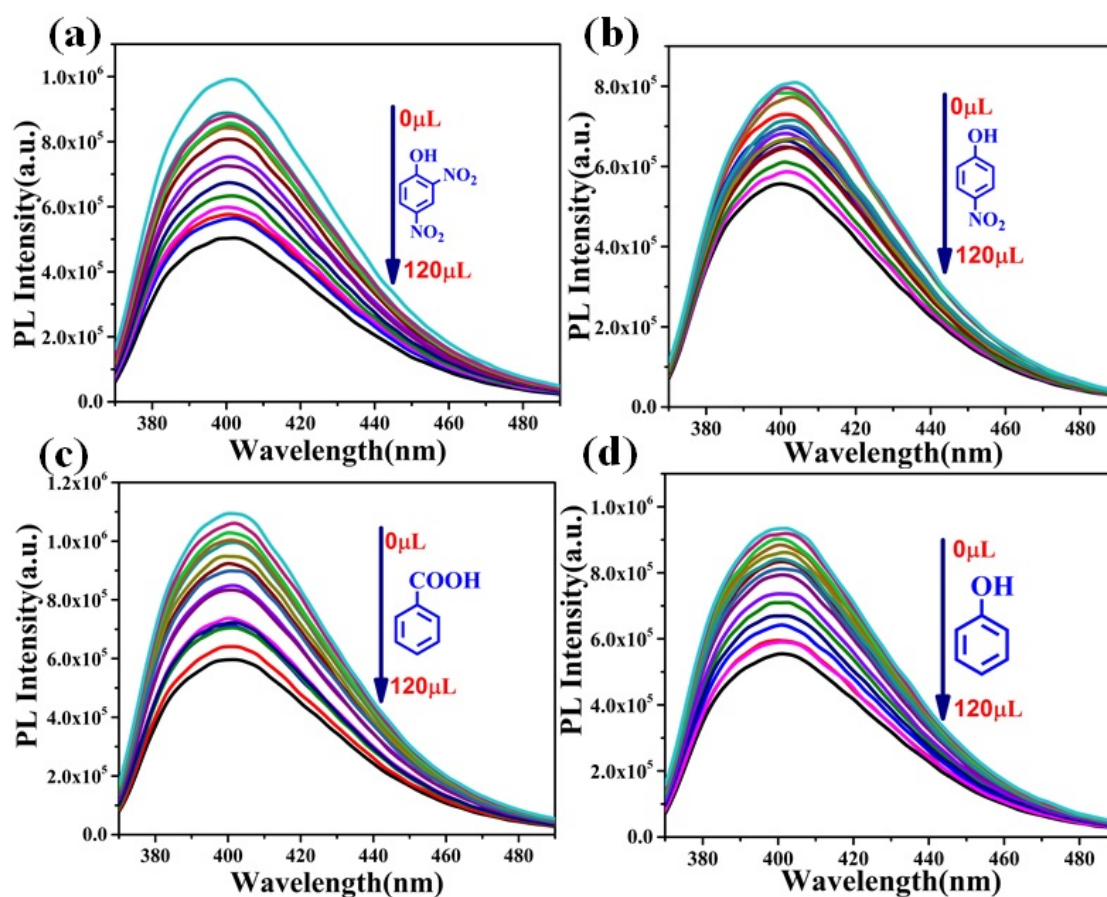


Fig. SI18. Change in the fluorescence of 2-NTPI-5 upon the addition of different quenchers excited at 335 nm in THF solvent (1×10^{-5} M).

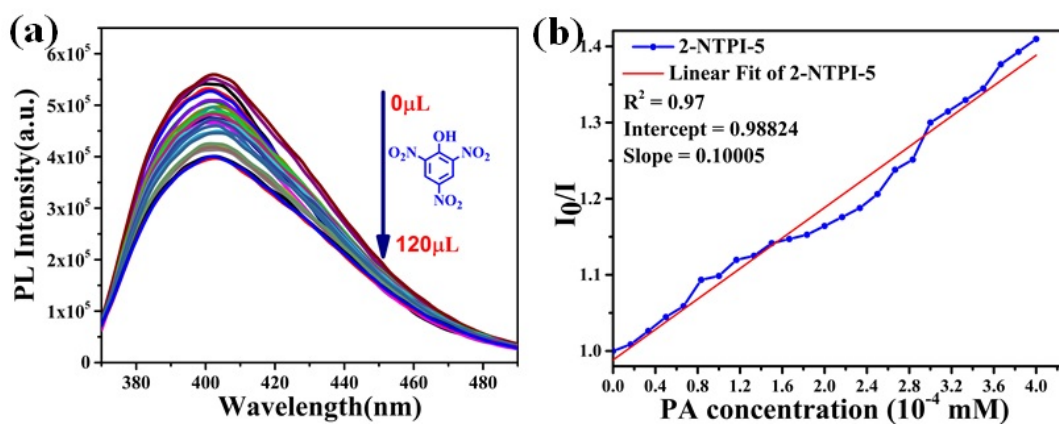


Fig. SI19. (a) Change in the fluorescence of 2-NTPI-5 upon the addition of PA excited at 335 nm in THF solvent (1×10^{-5} M). (b) Stern–Volmer plots of 2-NTPI-5 using PA as a quencher. Inset: Stern–Volmer plots at lower concentration region of PA.

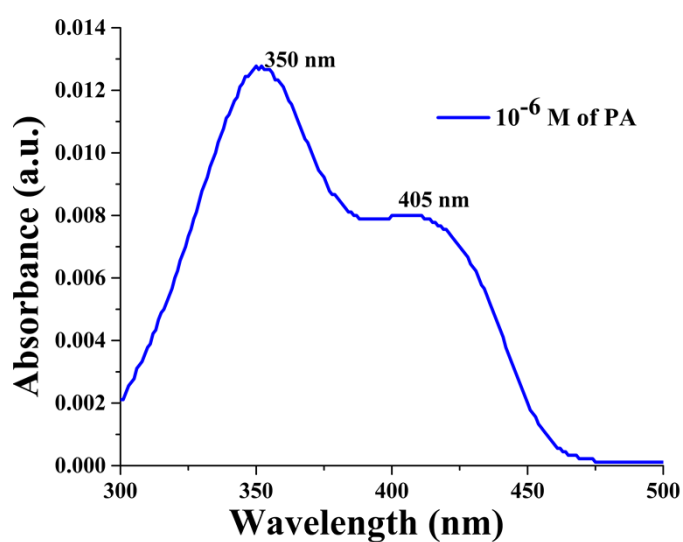


Fig. SI20. The absorbance spectra of picric acid in THF solution (10^{-6} M).

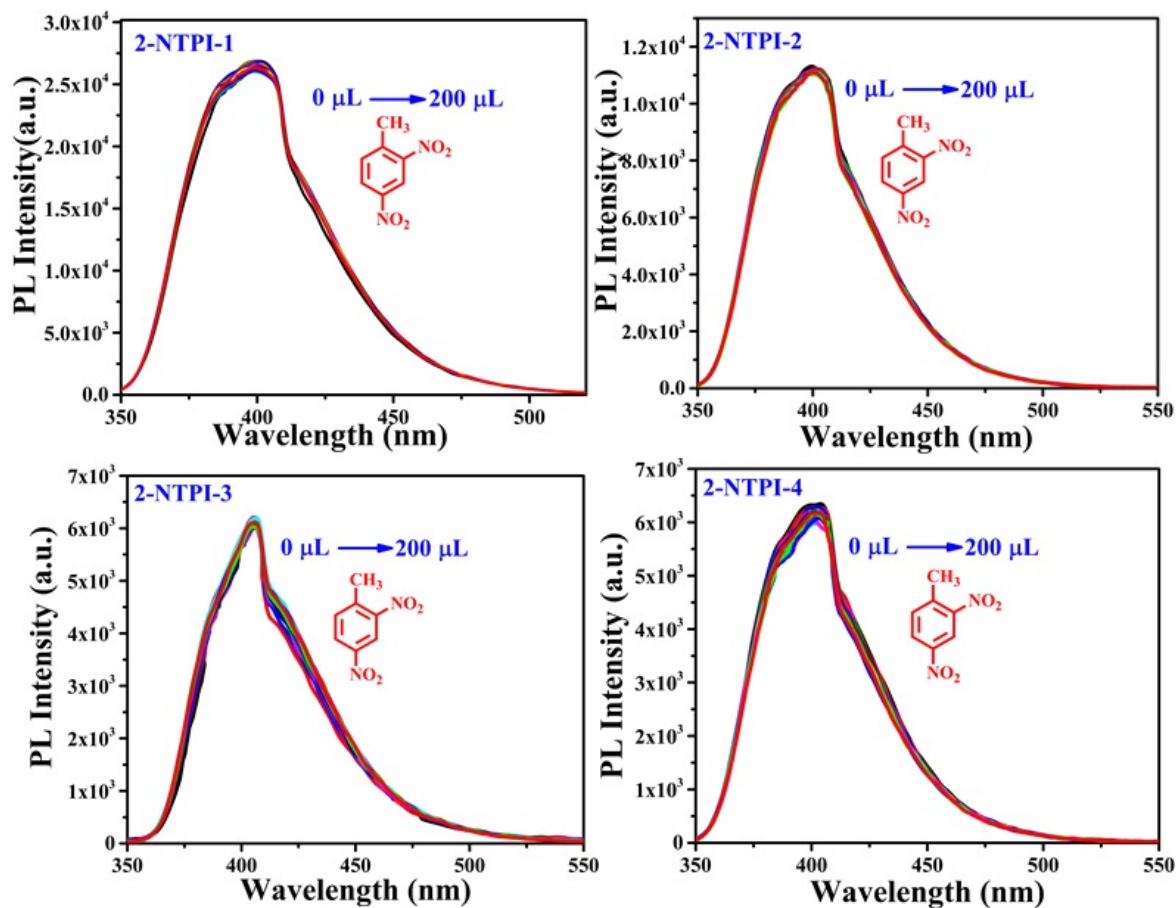
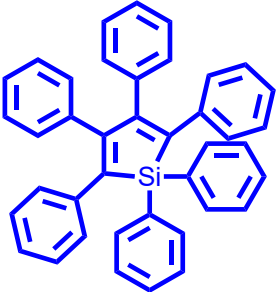
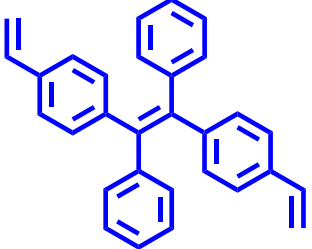
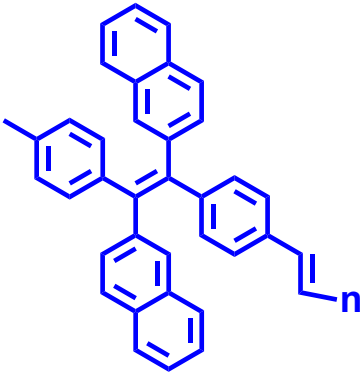
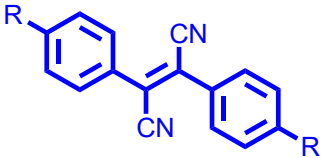
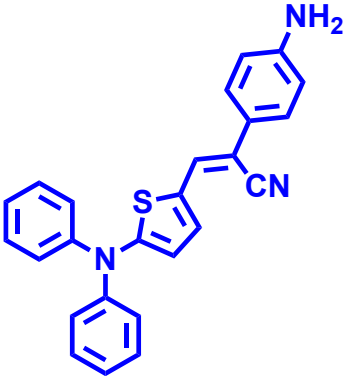
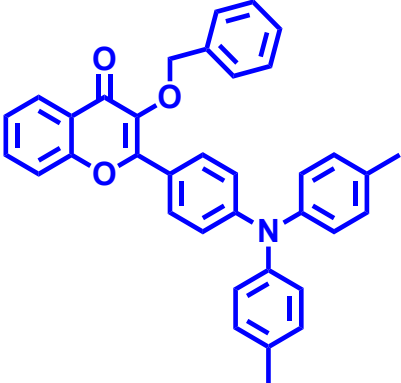
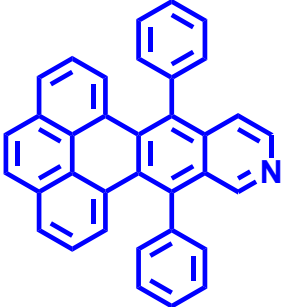
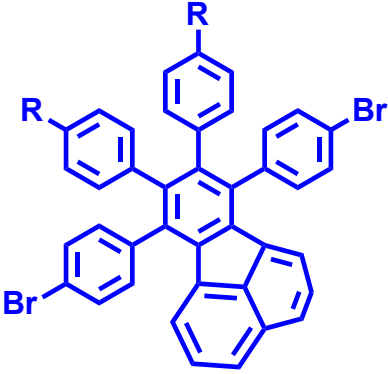
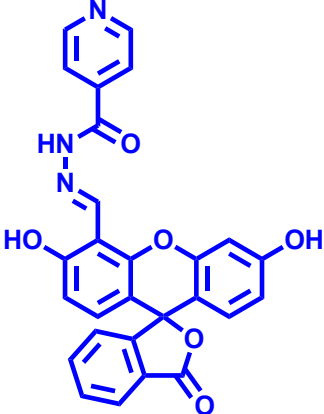


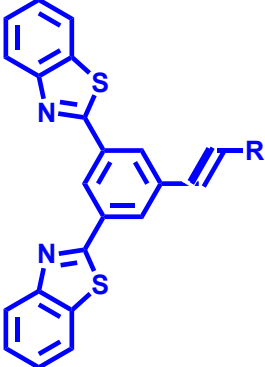
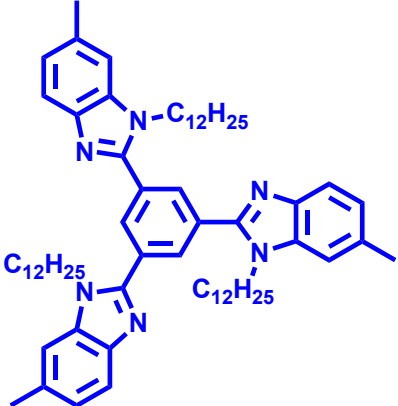
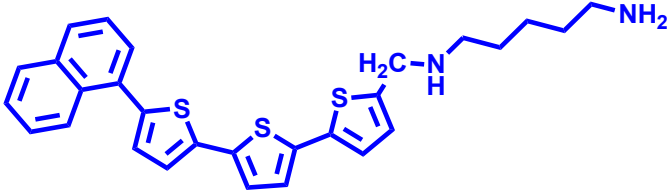
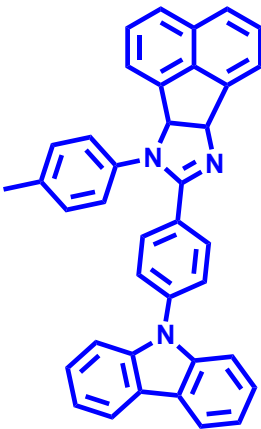
Fig. SI21. (a) Change in the fluorescence of 2-NTPI-1, 2-NTPI-2, 2-NTPI-3 and 2-NTPI-4 upon the addition of DNT excited at 325 nm in THF solvent (1×10^{-5} M).

Table ST1: The Comparison of our luminophores with other reported PA sensors.

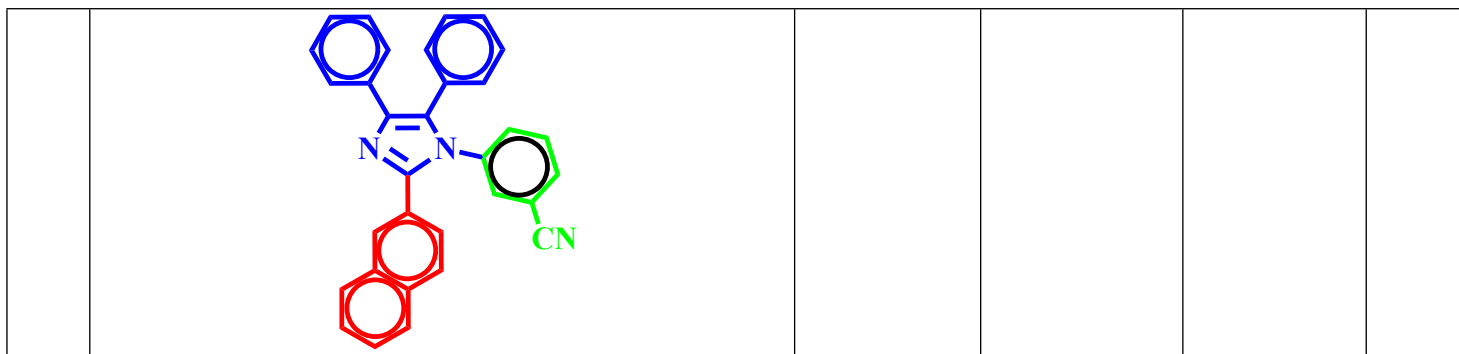
S. No	Sensor	Solvent	Quenching constant (M ⁻¹)	Detection limit (M)	Ref.
1	Hexaphenylsilole 	THF/Water	-	4.81 ppb	1
2	Tetraphenylethene 	Water	2.7×10^5	0.4 ppm	2

3	Polymers based on di (naphthalen-2-yl)- 1,2-diphenylethene 	H ₂ O/THF (9/1)	4.70×10^4	1.81×10^{-6}	3
4	Triazine-COF	THF	8.71×10^4	10.7 ppm	4
5	poly(silylenevinylene)	THF	8.491×10^3	1.0 ppm	5
6	Diphenylfumaronitriles 	H ₂ O/THF (8/2)	5.60×10^4	1.80×10^{-10}	6
7	Imidazole derivatives	H ₂ O/DMF (9/1)	1.30×10^4	3.55×10^{-6}	7
8	Thiophene aromatic amine derivatives 	THF	-	5.70×10^{-6}	8
9	3-(Benzyloxy)-2-(4- (di-p-tolylamino)phenyl)- 4H-chromen-4-one	Water	1.93×10^4	3.70×10^{-9}	9

					
10	[P(dimethylacrylamide-co-Benzophenone acrylamide-co-glycidyl methacrylate)]	Water	7.75×10^4	5.60×10^{-7}	10
11	9,14-diphenylpyreno [4,5-g]isoquinoline	MeCN	-	2.42×10^{-6}	11
					
12	7,10-bis(4-bromophenyl)-8,9-bis(4-(2-(2-(2-methoxyethoxy) ethoxy)ethoxy)phenyl)-fluoranthene	EtOH	5.60×10^5	2.6 ppb	12
					
13	Fluorescein derivatives	EtOH	2.50×10^5	1.10×10^{-7}	13
					
14	1,3-Bis(benzo[d]thiazol-	H ₂ O/THF	1.54×10^5	29.1 ppb	14

	2-yl)benzene derivatives 	(9/1)			
15	1,3,5-tri(1H-benzo[d]imidazol-2-yl)benzene derivative 	THF	1.15×10^5	50 ppb	15
16	tetraphenylethylene	THF	5.7×10^4	1.45 ppb	16
17	Terthiophene 	THF/water	5.7×10^3	70 ppb	17
18	AC-2 	THF	2.5×10^3	450 ppb	18
19	2-NTPI-1	THF	0.47×10^4	195ppb	This work

20	<p style="text-align: center;">2-NTPI-2</p>	THF	1.88×10^4	446ppb	This work
21	<p style="text-align: center;">2-NTPI-3</p>	THF	2.19×10^4	202ppb	This work
22	<p style="text-align: center;">2-NTPI-4</p>	THF	0.64×10^4	297ppb	This work
23	<p style="text-align: center;">2-NTPI-5</p>	THF	0.34×10^4	401ppb	This work



SI5 DFT analysis of luminophores with and without PA.

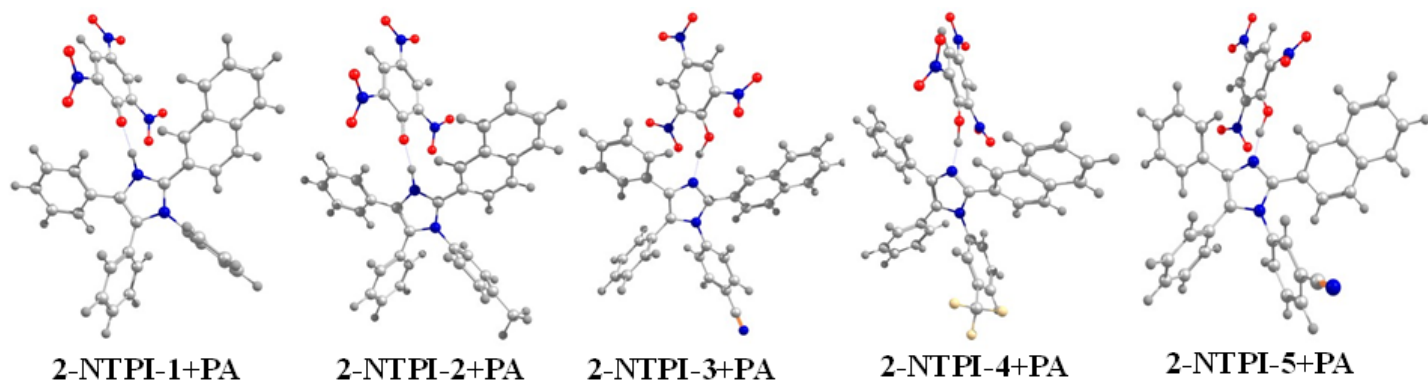


Fig. SI22 Optimized geometry of luminophores interacted with PA obtained from DFT using Gaussian 09 program.

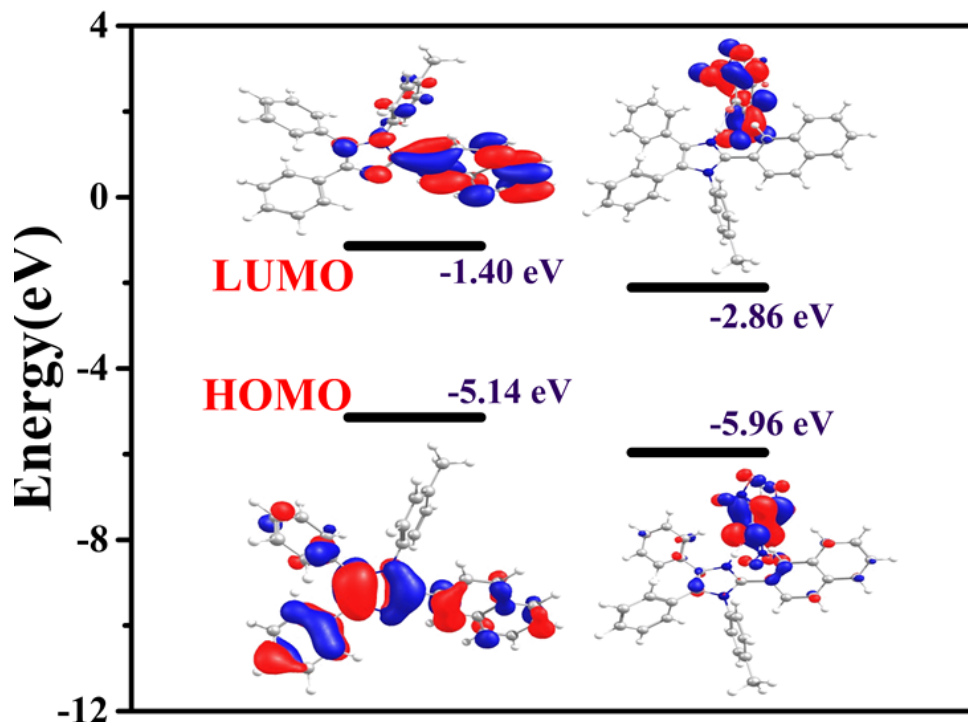


Fig. SI23 Frontier molecular orbitals of 2-NTPI-2 and 2-NTPI-2+ PA obtained from DFT using Gaussian 09 program.

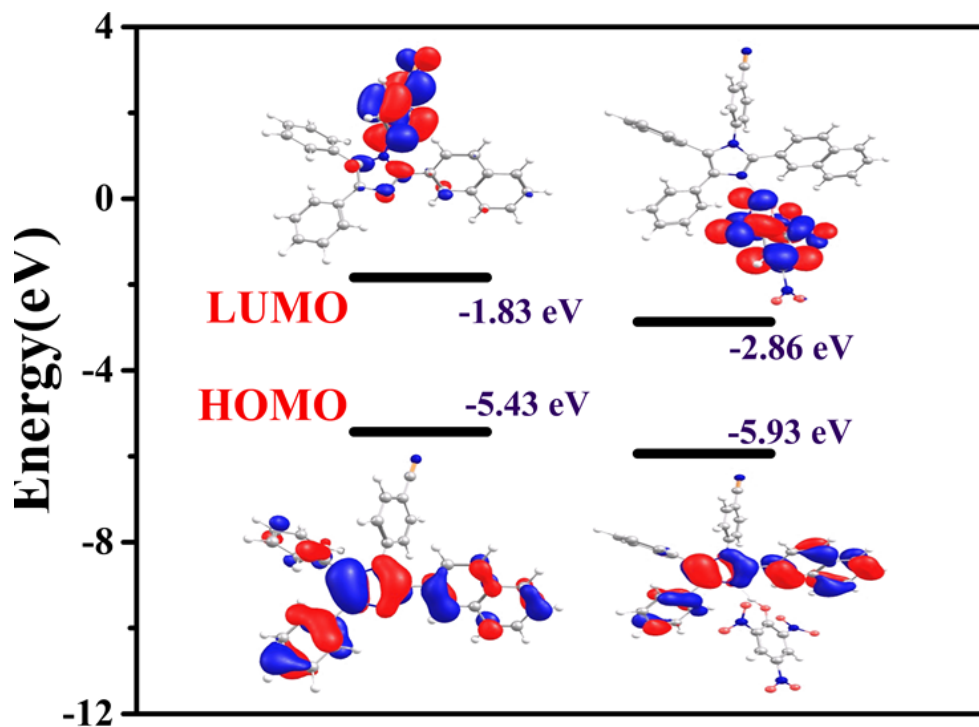


Fig. SI24 Frontier molecular orbitals of 2-NTPI-3 and 2-NTPI-3+ PA obtained from DFT using Gaussian 09 program.

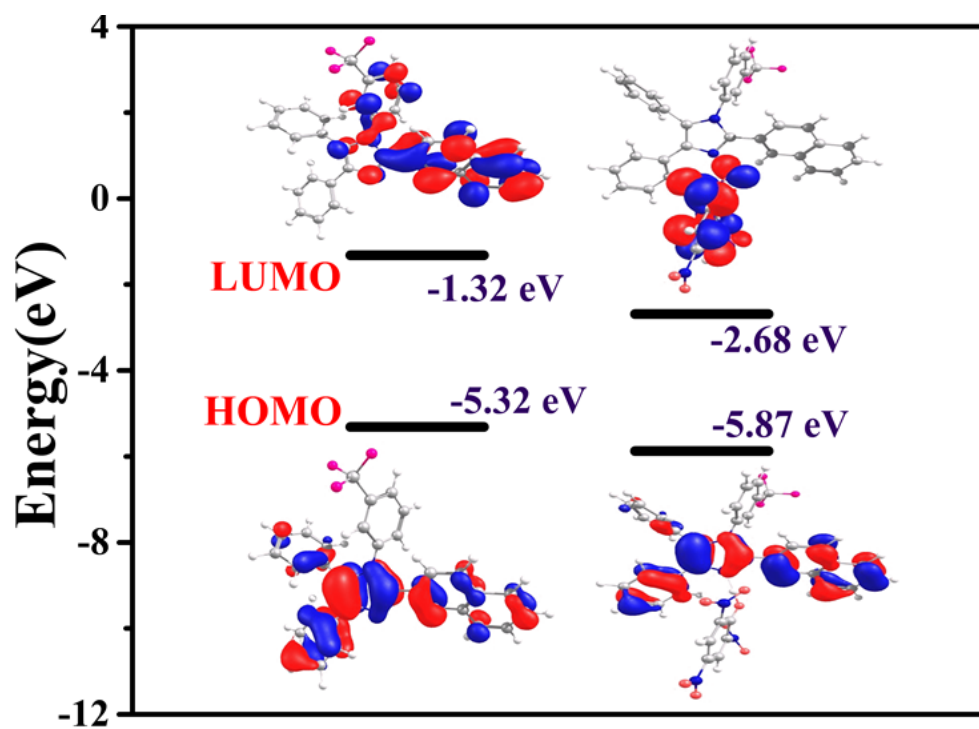


Fig. SI25 Frontier molecular orbitals of 2-NTPI-4 and 2-NTPI-4+PA obtained from DFT using Gaussian 09 program.

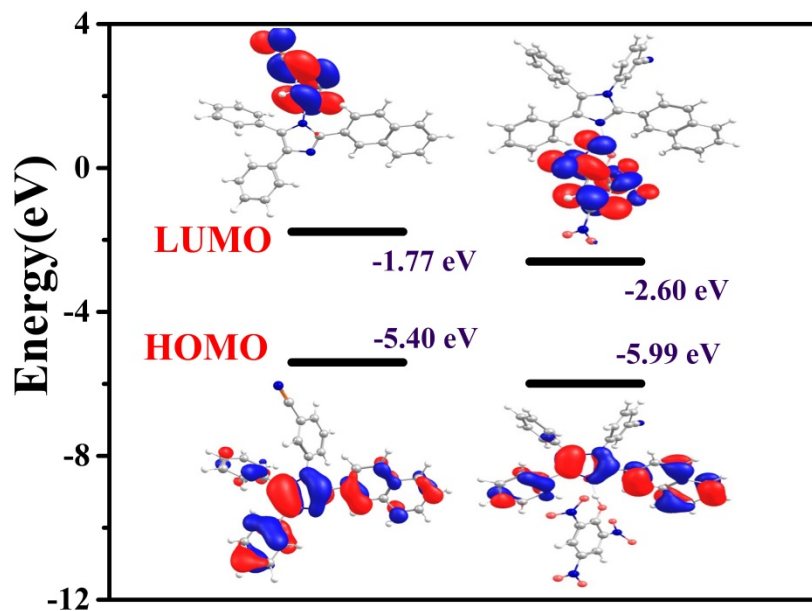


Fig. SI26 Frontier molecular orbitals of 2-NTPI-5 and 2-NTPI-5+ PA obtained from DFT using Gaussian 09 program.

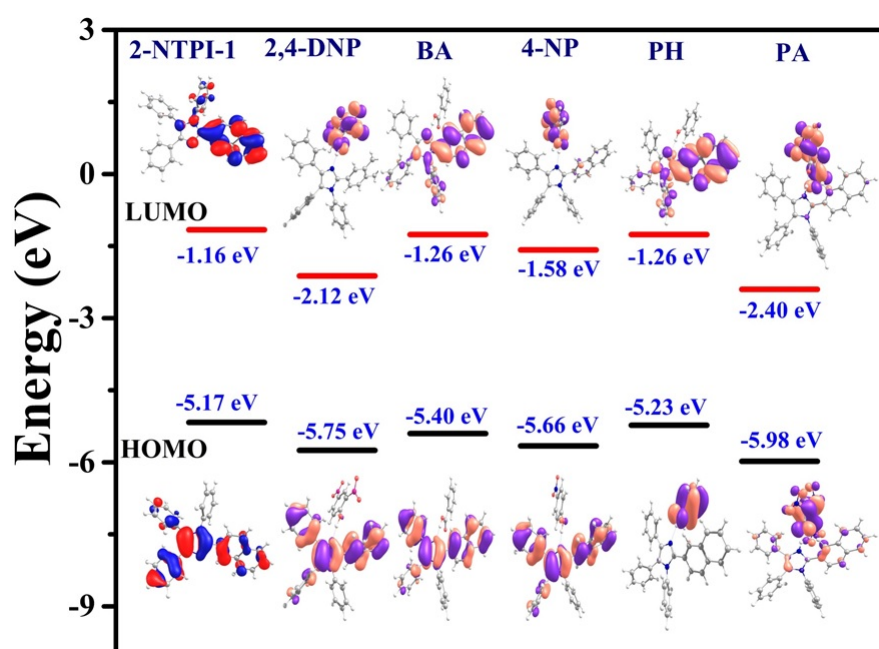


Fig. SI27 Frontier molecular orbitals of 2-NTPI-1 and different quenchers obtained from DFT.

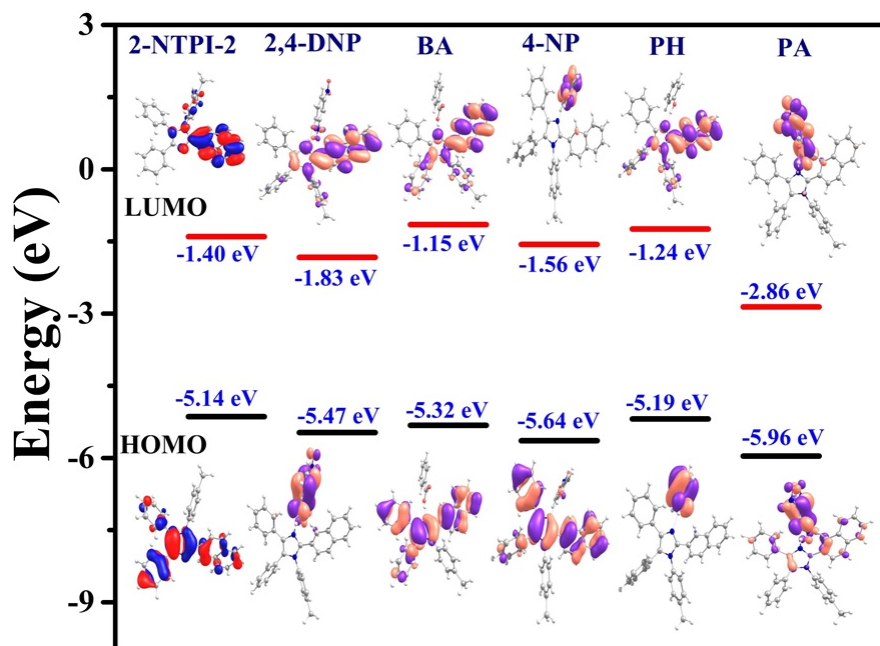


Fig. SI28 Frontier molecular orbitals of 2-NTPI-2 and different quenchers obtained from DFT.

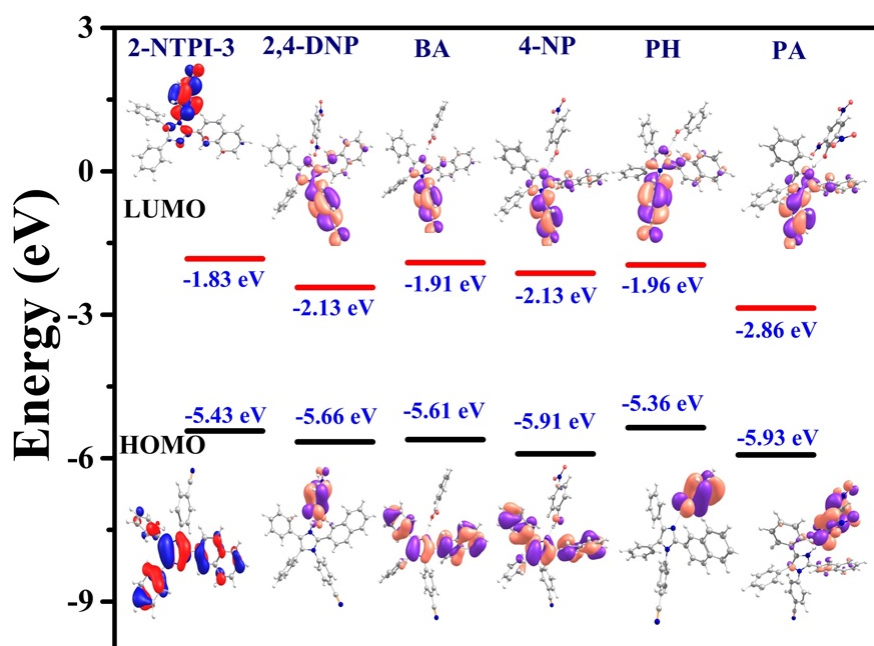


Fig. SI29 Frontier molecular orbitals of 2-NTPI-3 and different quenchers obtained from DFT.

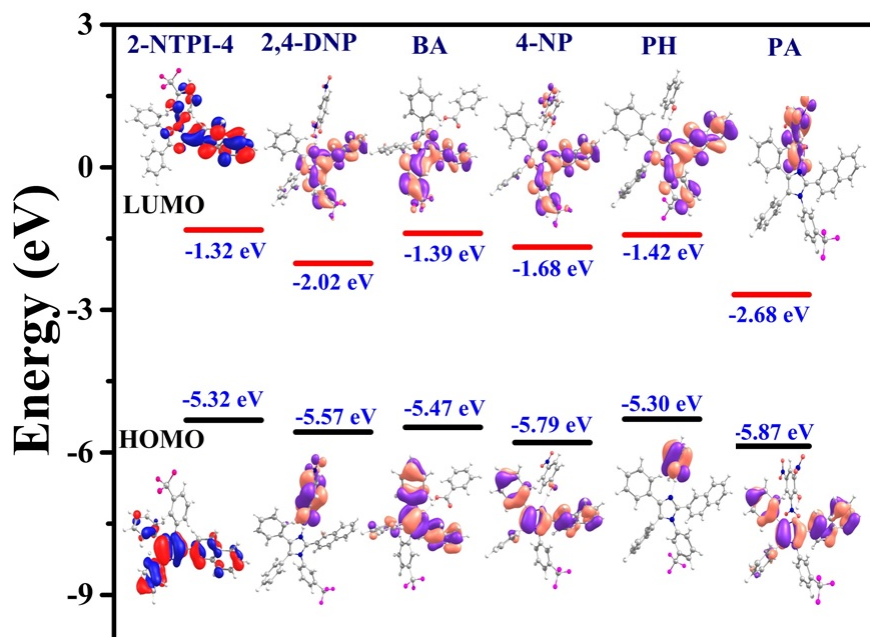


Fig. SI30 Frontier molecular orbitals of 2-NTPI-4 and different quenchers obtained from DFT.

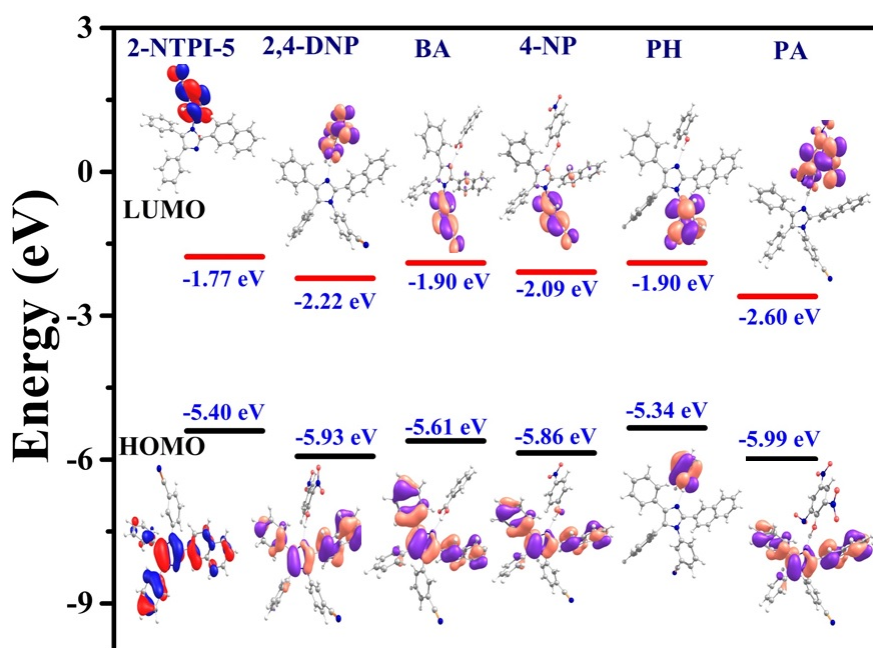


Fig. SI31 Frontier molecular orbitals of 2-NTPI-5 and different quenchers obtained from DFT.

SI6. Lifetime of the respective luminophores in presence and absence of PA.

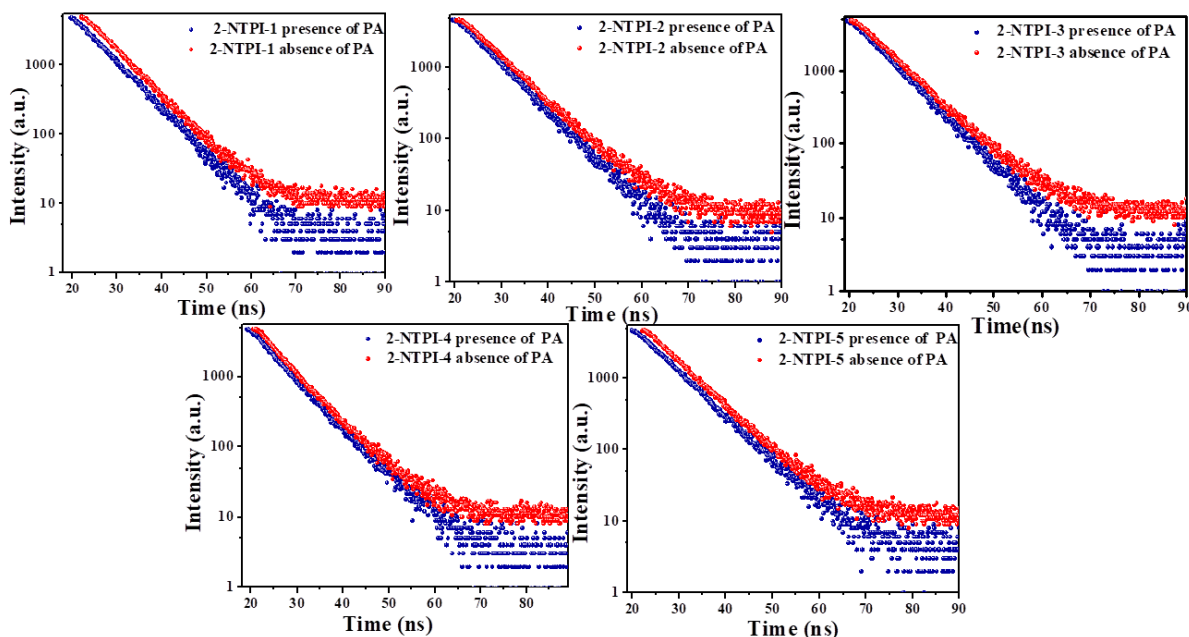


Fig. SI32 Lifetime of all the luminophores in the absence and presence of PA.

The fluorescence lifetime of the luminophores were estimated by using the time-correlated single-photon counting technique and the decay curves are shown in **Fig. SI32** (supporting information). The decay curve was fitted into the bi-exponential function and the average lifetime of the fluorophores is calculated by equation (1).⁵

$$I(t) = A_1 \exp\left(-\frac{t}{\tau_1}\right) + A_2 \exp\left(-\frac{t}{\tau_2}\right) + I_0 \dots\dots\dots(1)$$

In the above equation, I_0 and $I(t)$ at time 0 and t , denotes the intensities, A_1 and A_2 represent as constants, τ_1 and τ_2 represent as constant the fast and slow decay. The average lifetime (τ_{avg}) value can be predictable from the subsequent double exponential equation (2):

$$\tau_{avg} = \frac{A_1 \tau_1^2 + A_2 \tau_2^2}{A_1 \tau_1 + A_2 \tau_2} \dots\dots\dots(2)$$

Table ST2: Lifetime of the respective luminophores in nanosecond range

Compound	Lifetime without PA (s)	Lifetime with PA (s)
2-NTPI-1	4.77 x 10 ⁻⁹	3.98 x 10 ⁻⁹
2-NTPI-2	5.12 x 10 ⁻⁹	4.69 x 10 ⁻⁹
2-NTPI-3	5.14 x 10 ⁻⁹	4.76 x 10 ⁻⁹

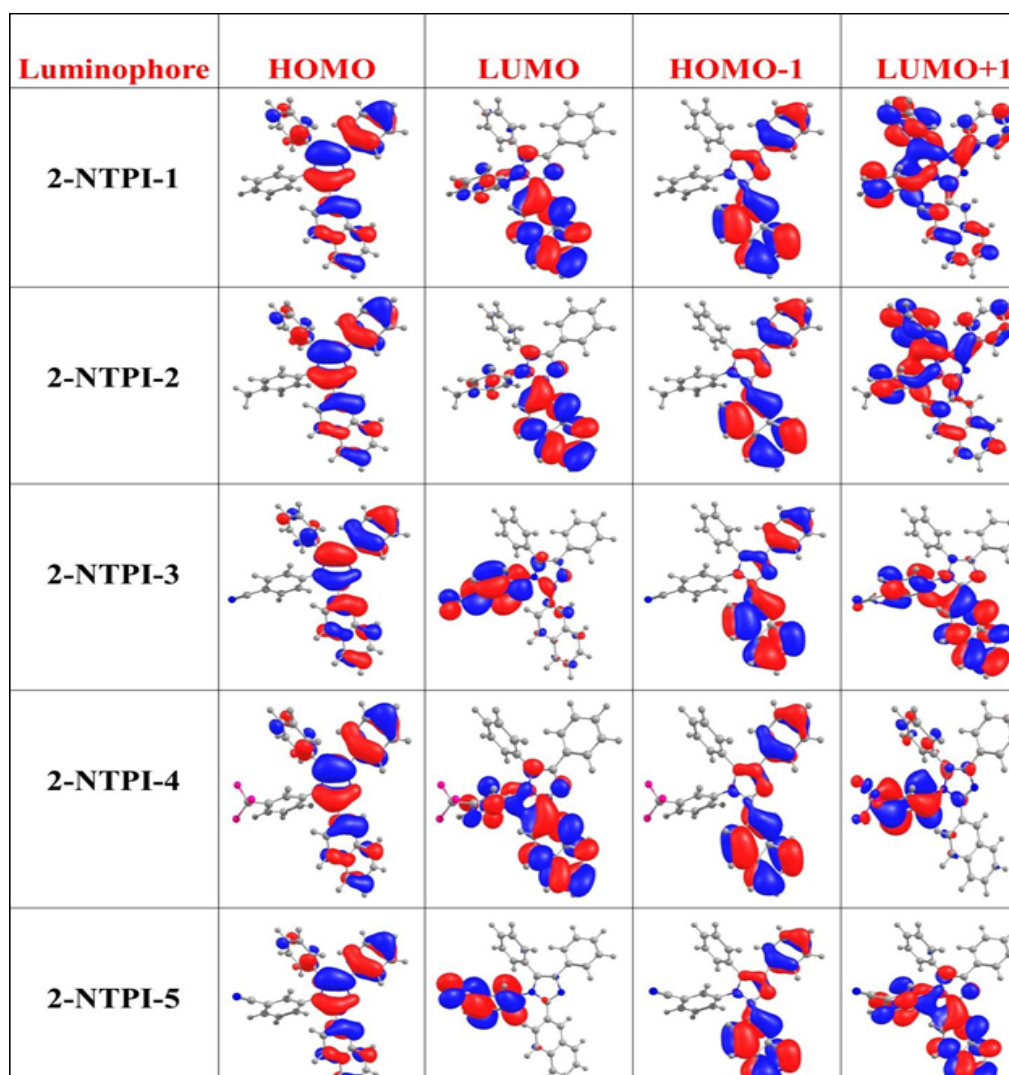
2-NTPI-4	4.30 x 10 ⁻⁹	3.92 x 10 ⁻⁹
2-NTPI-5	5.05 x 10 ⁻⁹	4.90x 10 ⁻⁹

Table ST3: Computed Vertical Transitions and Their Oscillator Strengths and Configurations

Compound	State	<i>f</i>	λ_{\max} nm	Energy (eV)	Configuration
2-NTPI- 1	Triplet	0	485.34	2.5546	HOMO → LUMO+3 (10.25%) HOMO-1 → LUMO (41.01%) HOMO-1 → LUMO+2(11.88%) HOMO →LUMO (50.56%)
	S1	0.222	348.98	3.5528	HOMO → LUMO (68.84%)
	S2	0.1199	325.05	3.8143	HOMO → LUMO (68.01%)
	S3	0.665	313.63	3.9533	HOMO → LUMO+2 (68.79 %)
2-NTPI -2	Triplet	0	485.87	2.551	HOMO-1 → LUMO+1 (10.4%) HOMO-1→LUMO(41.2%) HOMO → LUMO (50.6%)
	S1	0.223	349.31	3.549	HOMO → LUMO (68.84%)
	S2	0.167	323.76	3.8295	HOMO → LUMO+1 (68.18%)
	2-NTPI -3	Triplet	0	485.1	2.5558
S1		0.015	358.01	3.463	HOMO → LUMO+1 (70.23%)
S2		0.164	354.10	3.5014	HOMO → LUMO (67.97%)
2-NTPI -4		Triplet	0	485.11	2.555

	S1	0.0154	358.01	3.463	HOMO → LUMO+1 (70.23%)
	S2	0.164	354.10	3.5014	HOMO → LUMO (67.97%)
2-NTPI-5	Triplet	0	484.25	2.5604	HOMO-1→LUMO+1 (36.49%) HOMO→LUMO+1(47.32%) HOMO-1→ LUMO+2 (21.68%) HOMO-1→ LUMO+3 (12.41%) HOMO → LUMO+2 (16.7%)
	S1	0.004		3.0803	HOMO-1→ LUMO (50.13%)
	S2	0.0694		3.4691	HOMO → LUMO+2 (47.07%)
	S3	0.2249		3.7847	HOMO-1→LUMO (50.73%) HOMO→LUMO+2 (47.07)

Table ST4: FMO orbitals of the luminophores



2-NTPI-1

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symmetry c1

C	1.6073430	0.0436310	-0.0171230
C	1.3594600	-1.3229910	-0.0523110
C	-2.0510890	-0.2172130	-0.2232660
C	-2.8474020	-1.2058970	0.3328010
C	-2.6756700	0.8638950	-0.9117030
C	-4.2600870	-1.1559330	0.2473870
H	-2.3708130	-2.0402270	0.8372240
C	-4.0445130	0.9367380	-1.0086630
H	-2.0667790	1.6261590	-1.3827500
C	-4.8794830	-0.0572780	-0.4328440
H	-4.5060310	1.7622090	-1.5443640
C	-0.5892480	-0.3757760	-0.1334180
C	0.0871520	2.0521080	0.0363420
C	0.5459410	2.9147860	-0.9635210
C	-0.6203810	2.5546090	1.1323630
C	0.2927850	4.2825020	-0.8636080
H	1.0975370	2.5112860	-1.8055970
C	-0.8789960	3.9223020	1.2186780
H	-0.9667760	1.8728060	1.9018100
C	-0.4220890	4.7884090	0.2237830
H	0.6517540	4.9516910	-1.6395210
H	-1.4337030	4.3101530	2.0675580
H	-0.6212400	5.8532660	0.2959240
N	0.3441370	0.6465650	-0.0573300
N	0.0060610	-1.5526170	-0.1301870
C	-6.2961880	-0.0075520	-0.5130200
H	-6.7622690	0.8265570	-1.0313220
C	-7.0684700	-0.9966790	0.0532980
H	-8.1513330	-0.9480420	-0.0145940
C	-6.4574630	-2.0835610	0.7268240
H	-7.0779780	-2.8577470	1.1685340
C	-5.0868900	-2.1609150	0.8211940
H	-4.6149790	-2.9938190	1.3355320
C	2.8665860	0.8128890	0.0191170
C	3.8354080	0.6142360	-0.9798400
C	3.1354350	1.7410910	1.0392530
C	5.0373570	1.3193380	-0.9559970
H	3.6380200	-0.1013980	-1.7716090
C	4.3354910	2.4506180	1.0569920
H	3.8868990	-1.4551000	1.0482780
C	5.2906240	2.2422310	0.0607670
H	5.7745020	1.1511340	-1.7357560
H	4.5262910	3.1629060	1.8544520
H	6.2261140	2.7936510	0.0773290
C	2.2934920	-2.4634940	-0.0061610
C	1.8873980	-3.6937740	-0.5520340
C	3.5629050	-2.3832080	0.5911910
C	2.7317880	-4.8008050	-0.5210970
H	0.8994070	-3.7628260	-0.9937770
C	4.4065510	-3.4927330	0.6168880
C	3.9983860	-4.7052810	0.0590080
H	2.4000780	-5.7413200	-0.9523150

H	5.3833980	-3.4107920	1.0854510
H	4.6577800	-5.5681640	0.0821140
H	2.4019470	1.9022240	1.8223440

2-NTPI-2

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symmetry c1

C	1.6382750	-0.1314220	-0.0271050
C	1.4335120	-1.5055980	-0.0484810
C	-2.0096480	-0.5088290	-0.2294790
C	-2.7735390	-1.5229720	0.3265690
C	-2.6694910	0.5515790	-0.9172730
C	-4.1870820	-1.5188490	0.2417380
H	-2.2697790	-2.3414410	0.8305480
C	-4.0400590	0.5801640	-1.0132620
H	-2.0858600	1.3332330	-1.3882180
C	-4.8421720	-0.4404320	-0.4374650
H	-4.5284710	1.3903270	-1.5485480
C	-0.5434830	-0.6201790	-0.1395370
C	0.0569700	1.8291170	0.0062100
C	0.4735760	2.6980620	-1.0050650
C	-0.6486120	2.3280500	1.1042430
C	0.1797500	4.0572410	-0.9136700
H	1.0298340	2.3084710	-1.8508310
C	-0.9445820	3.6874140	1.1774370
H	-0.9631350	1.6499420	1.8906610
C	-0.5379960	4.5754900	0.1724420
H	0.5131240	4.7260600	-1.7026100
H	-1.4956950	4.0649960	2.0346290
N	0.3573250	0.4311610	-0.0738350
N	0.0882210	-1.7782350	-0.1238800
C	-6.2597870	-0.4365720	-0.5168050
H	-6.7529510	0.3822800	-1.0344350
C	-6.9993280	-1.4506050	0.0491600
H	-8.0832460	-1.4370950	-0.0182060
C	-6.3530510	-2.5176490	0.7215360
H	-6.9479360	-3.3118710	1.1629620
C	-4.9806410	-2.5505520	0.8151730
H	-4.4815770	-3.3679780	1.3287120
C	2.8721390	0.6783520	-0.0019010
C	3.8435870	0.5020380	-1.0024000
C	3.1149060	1.6230850	1.0096970
C	5.0226040	1.2451960	-0.9889360
H	3.6664830	-0.2261900	-1.7874780
C	4.2917410	2.3706160	1.0169280
H	3.9599800	-1.5463460	1.0578480
C	5.2496920	2.1843800	0.0189420
H	5.7621360	1.0937430	-1.7698900
H	4.4626340	3.0952140	1.8078280
H	6.1671990	2.7654400	0.0275290
C	2.4025520	-2.6158080	0.0106760
C	2.0366220	-3.8644760	-0.5215980
C	3.6668240	-2.4894170	0.6107240
C	2.9146540	-4.9444420	-0.4738880

H	1.0527910	-3.9695120	-0.9655440
C	4.5438740	-3.5720850	0.6546700
C	4.1751710	-4.8033280	0.1102900
H	2.6137930	-5.8999460	-0.8946970
H	5.5156510	-3.4543060	1.1261110
H	4.8601710	-5.6455590	0.1470390
H	2.3792610	1.7670490	1.7944330
C	-0.8847900	6.0432300	0.2473220
H	-0.1602350	6.6543900	-0.2982410
H	-1.8718350	6.2389320	-0.1897920
H	-0.9142980	6.3948920	1.2828570

2-NTPI-3

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symmetry c1

C	1.6731730	-0.1915290	-0.0343020
C	1.5301160	-1.5717470	-0.0421880
C	-1.9571280	-0.7342350	-0.2427240
C	-2.6894510	-1.7439590	0.3605640
C	-2.6443500	0.2624650	-0.9956340
C	-4.1014890	-1.7946480	0.2616750
H	-2.1634670	-2.5156970	0.9134140
C	-4.0137270	0.2376850	-1.1063480
H	-2.0816250	1.0344240	-1.5075600
C	-4.7853290	-0.7781180	-0.4818670
H	-4.5242250	0.9981090	-1.6913290
C	-0.4887450	-0.7833730	-0.1375730
C	-0.0015950	1.6882140	-0.0065440
C	0.4594000	2.5912080	-0.9718190
C	-0.8190570	2.1327990	1.0393070
C	0.1039080	3.9327610	-0.8936570
H	1.0942610	2.2380480	-1.7759720
C	-1.1855800	3.4715230	1.1146440
H	-1.1651590	1.4258670	1.7847940
C	-0.7241040	4.3813740	0.1488770
H	0.4585570	4.6362670	-1.6387380
H	-1.8212140	3.8197400	1.9212340
N	0.3641260	0.3121810	-0.0815780
N	0.1967960	-1.9070390	-0.1152410
C	-6.2011730	-0.8282660	-0.5751980
H	-6.7165440	-0.0566370	-1.1411530
C	-6.9110620	-1.8358810	0.0380490
H	-7.9938480	-1.8642820	-0.0402810
C	-6.2362260	-2.8417730	0.7735660
H	-6.8085070	-3.6314350	1.2513200
C	-4.8647430	-2.8214660	0.8825630
H	-4.3437540	-3.5919420	1.4444900
C	2.8682200	0.6750710	-0.0078170
C	3.8335720	0.5635150	-1.0233550
C	3.0776760	1.6113420	1.0190000
C	4.9747210	1.3637900	-1.0102870
H	3.6824990	-0.1591000	-1.8190290
C	4.2161780	2.4162400	1.0255590
H	4.0605410	-1.4834280	1.0519410

C	5.1680930	2.2951300	0.0117970
H	5.7109060	1.2630330	-1.8023480
H	4.3623490	3.1337210	1.8276040
H	6.0556130	2.9207970	0.0195770
C	2.5493030	-2.6356190	0.0241810
C	2.2388930	-3.9045130	-0.4948900
C	3.8095140	-2.4431720	0.6148830
C	3.1677790	-4.9409020	-0.4436870
H	1.2589300	-4.0604560	-0.9322820
C	4.7370480	-3.4826200	0.6627100
C	4.4235280	-4.7345290	0.1310850
H	2.9103890	-5.9132400	-0.8543310
H	5.7049290	-3.3148720	1.1267030
H	5.1479390	-5.5428730	0.1704720
H	2.3484460	1.7017660	1.8181170
C	-1.0954690	5.7640350	0.2277270
N	-1.3964040	6.8859110	0.2916150

2-NTPI-4

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symmetry c1

C	-1.2678630	1.0239180	0.1555130
C	-0.7066080	2.2700930	-0.0880860
C	2.3351800	0.3619230	-0.1411050
C	3.3699880	1.1870530	0.2696300
C	2.6485030	-0.9166030	-0.6886570
C	4.7234770	0.7809850	0.1757560
H	3.1317580	2.1695450	0.6642910
C	3.9532970	-1.3358000	-0.7897250
H	1.8534340	-1.5569030	-1.0523060
C	5.0279510	-0.5132330	-0.3588430
H	4.1776950	-2.3090950	-1.2181600
C	0.9596670	0.8817300	-0.0542380
C	-0.2585140	-1.2566360	0.5054310
C	-0.9910630	-2.1215410	-0.3116640
C	0.4036090	-1.7469880	1.6346980
C	-1.0535790	-3.4777640	0.0073190
H	-1.5007040	-1.7391080	-1.1873470
C	0.3448730	-3.1071540	1.9369010
H	0.9655850	-1.0631250	2.2613740
C	-0.3834650	-3.9766780	1.1280640
H	0.8681080	-3.4873700	2.8082710
N	-0.1845200	0.1344200	0.1882570
N	0.6582690	2.1534220	-0.2199090
C	6.3854680	-0.9200640	-0.4462570
H	6.6129210	-1.9016490	-0.8539890
C	7.3979310	-0.0878110	-0.0246570
H	8.4326810	-0.4095950	-0.0968030
C	7.0983950	1.1923540	0.5041250
H	7.9066190	1.8395290	0.8317400
C	5.7929780	1.6161910	0.6015270
H	5.5598430	2.5979920	1.0047710
C	-2.6689810	0.5899610	0.3247640
C	-3.6031910	0.8336980	-0.6966690

C	-3.1038630	-0.0586860	1.4929660
C	-4.9329630	0.4420290	-0.5519440
H	-3.2770170	1.3357290	-1.6019860
C	-4.4330990	-0.4557170	1.6324260
H	-3.0891090	3.1477410	0.9896060
C	-5.3515810	-0.2066550	0.6113800
H	-5.6411400	0.6383820	-1.3515300
H	-4.7521150	-0.9557040	2.5422100
H	-6.3867120	-0.5157540	0.7216640
C	-1.3416500	3.5965160	-0.1989520
C	-0.6762870	4.6095880	-0.9110310
C	-2.5715000	3.9020490	0.4080820
C	-1.2330360	5.8807430	-1.0285440
H	0.2826670	4.3810470	-1.3628120
C	-3.1263980	5.1750040	0.2864780
C	-2.4633480	6.1693750	-0.4344330
H	-0.7046730	6.6486520	-1.5867310
H	-4.0767360	5.3921950	0.7660770
H	-2.8977770	7.1606380	-0.5266600
H	-2.3975890	-0.2447480	2.2959950
H	-0.4285730	-5.0357350	1.3570310
C	-1.8827210	-4.4127900	-0.8340050
F	-3.0962500	-4.6346130	-0.2798560
F	-1.2871940	-5.6197520	-0.9653800
F	-2.0948950	-3.9258690	-2.0748360

2-NTPI-5

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symmetry c1

C	1.5339530	-0.3602360	0.0803370
C	1.2050370	-1.6989120	-0.0793740
C	-2.1320210	-0.3737440	-0.1903380
C	-3.0020000	-1.3356650	0.2973780
C	-2.6689030	0.7871190	-0.8202370
C	-4.4065360	-1.1810810	0.2006500
H	-2.5921100	-2.2299430	0.7557680
C	-4.0276970	0.9622550	-0.9267620
H	-2.0005950	1.5287080	-1.2422300
C	-4.9374940	-0.0028940	-0.4187300
H	-4.4230550	1.8468820	-1.4189690
C	-0.6854280	-0.6345500	-0.0958810
C	0.1316610	1.7172690	0.3156730
C	0.7062540	2.6468780	-0.5518330
C	-0.6105530	2.1492120	1.4206530
C	0.5340020	4.0176270	-0.3073160
H	1.2832800	2.3118940	-1.4051440
C	-0.7891700	3.5132140	1.6500160
H	-1.0449760	1.4136700	2.0886720
C	-0.2196830	4.4528760	0.7952330
H	-1.3701680	3.8430000	2.5049910
N	0.3071530	0.3203950	0.0811880
N	-0.1600370	-1.8380400	-0.1923880
C	-6.3459520	0.1518840	-0.5097130
H	-6.7452310	1.0455940	-0.9821990

C	-7.1931580	-0.8117860	-0.0107070
H	-8.2688240	-0.6827580	-0.0861710
C	-6.6695590	-1.9771180	0.6024590
H	-7.3491170	-2.7300000	0.9906810
C	-5.3093350	-2.1572410	0.7052940
H	-4.9043610	-3.0504770	1.1732470
C	2.8340130	0.3301210	0.2005180
C	3.7800670	0.2228570	-0.8332880
C	3.1598410	1.0938530	1.3341850
C	5.0156080	0.8605600	-0.7347090
H	3.5383700	-0.3671020	-1.7117290
C	4.3938590	1.7361580	1.4274680
H	3.7202750	-2.0617530	0.9924550
C	5.3251240	1.6217390	0.3939810
H	5.7344360	0.7678210	-1.5433810
H	4.6298120	2.3219710	2.3109870
H	6.2858920	2.1222780	0.4678760
C	2.0693630	-2.8928650	-0.1263700
C	1.5913770	-4.0517070	-0.7624740
C	3.3418960	-2.9316900	0.4680660
C	2.3698750	-5.2051320	-0.8187900
H	0.6015460	-4.0297110	-1.2048140
C	4.1187050	-4.0875270	0.4078620
C	3.6395500	-5.2282860	-0.2380320
H	1.9839650	-6.0891530	-1.3187320
H	5.0986270	-4.0983020	0.8767790
H	4.2466170	-6.1278580	-0.2827470
H	2.4452840	1.1760960	2.1474140
H	-0.3493520	5.5149740	0.9708030
C	1.1241850	4.9782500	-1.1949790
N	1.5983710	5.7612930	-1.9123680

2-NTPI-1 + PA

symmetry c1

C	-4.7629230	-2.1946860	-1.0436750
C	-4.2794170	-1.5982420	0.1310920
C	-5.0586780	-1.6596460	1.2967380
C	-6.2989650	-2.2964720	1.2837740
C	-6.7733850	-2.8825580	0.1090910
C	-6.0020050	-2.8332930	-1.0530930
H	-4.1600100	-2.1589780	-1.9455040
H	-4.6822290	-1.2264810	2.2179050
H	-6.8906180	-2.3413750	2.1930520
H	-7.7382550	-3.3804940	0.1013060
H	-6.3639030	-3.2919470	-1.9681460
C	-2.9550320	-0.9405660	0.1202240
C	-1.6931200	-1.4727980	-0.0389890
C	-1.2393900	-2.8667710	-0.1511780
C	-0.0927430	-3.1743030	-0.9029090
C	-1.9389740	-3.9043320	0.4890210
C	0.3378970	-4.4948030	-1.0127750
H	0.4768010	-2.3943540	-1.3954160
C	-1.5043690	-5.2216050	0.3686210
H	-2.8115590	-3.6785430	1.0915480

C	-0.3659520	-5.5218610	-0.3830060
H	1.2289100	-4.7076280	-1.5947120
H	-2.0505090	-6.0136890	0.8722330
H	-0.0276330	-6.5500830	-0.4710250
C	-0.8444620	2.0769020	-0.0338480
C	0.2582930	2.2503680	-0.8576960
C	-1.3179420	3.1716800	0.7474070
C	0.9151160	3.5014910	-0.9439760
H	0.6432410	1.4199280	-1.44005000
C	-0.6954540	4.3927050	0.6769130
H	-2.1573570	3.0351660	1.4172260
C	0.4285070	4.6020570	-0.1668820
H	-1.0547980	5.2180590	1.2850340
C	-1.4726780	0.7548100	0.0268100
C	-3.8789860	1.4059140	0.1454540
C	-4.5554780	1.7197500	1.3251470
C	-4.2432650	1.9896540	-1.0682410
C	-5.6077670	2.6342710	1.2861400
H	-4.2492900	1.2629830	2.2601240
C	-5.2944400	2.9057740	-1.0969580
H	-3.7050600	1.7297590	-1.9736440
C	-5.9770570	3.2271170	0.0773180
H	-6.1353250	2.8844540	2.2010000
H	-5.5792610	3.3655460	-2.0378340
H	-6.7955220	3.9396160	0.0509570
N	-2.7938700	0.4567920	0.1689890
N	-0.8170290	-0.4033660	-0.0932580
C	2.8848790	-0.7100720	-0.1354740
C	3.9969840	-1.2393180	-0.9150080
C	5.2980480	-1.2918590	-0.4644200
C	5.5902380	-0.8687990	0.8341790
C	4.5890090	-0.3808950	1.6656340
C	3.2821180	-0.3117390	1.2094050
H	6.0842510	-1.6650810	-1.1073860
H	4.8255000	-0.0526210	2.6687130
O	1.7404070	-0.5585620	-0.6352640
H	0.2437480	-0.4699040	-0.1175270
N	2.3045160	0.2062690	2.1562900
N	3.7621610	-1.7465350	-2.2672470
N	6.9558110	-0.9471520	1.3235870
O	2.7206560	0.8199270	3.1433640
O	4.6777810	-1.6226670	-3.0860410
O	7.8167700	-1.3871840	0.5559100
O	7.1785180	-0.5686750	2.4770170
O	2.6885680	-2.2973790	-2.5167780
O	1.1033330	-0.0026460	1.9491070
C	1.0898350	5.8539290	-0.2605400
H	0.7225370	6.6875710	0.3317040
C	2.1821390	6.0093500	-1.0845480
H	2.6824130	6.9710790	-1.1468520
C	2.0451880	3.6943470	-1.7849170
H	2.4131160	2.8550890	-2.3681860
C	2.6645760	4.9209150	-1.8527250
H	3.5293870	5.0588670	-2.4942380

2-NTPI-2 + PA

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symmetry c1

C	-4.3024180	-2.7862360	-1.0340520
C	-3.9100170	-2.0976440	0.1245240
C	-4.7024970	-2.2000390	1.2782980
C	-5.8674450	-2.9659850	1.2690680
C	-6.2516740	-3.6432780	0.1106460
C	-5.4653360	-3.5546790	-1.0391740
H	-3.6885920	-2.7185840	-1.9266020
H	-4.3941150	-1.6958100	2.1882450
H	-6.4697030	-3.0404690	2.1694210
H	-7.1574340	-4.2421140	0.1059640
H	-5.7567370	-4.0832120	-1.9416390
C	-2.6639470	-1.3028570	0.1108780
C	-1.3534110	-1.6999100	-0.0516470
C	-0.7541510	-3.0377920	-0.1654800
C	0.4161280	-3.2209000	-0.9214080
C	-1.3345980	-4.1436680	0.4793980
C	0.9866370	-4.4873370	-1.0312340
H	0.8963920	-2.3846290	-1.4167950
C	-0.7604400	-5.4064360	0.3591070
H	-2.2238770	-4.0123260	1.0855170
C	0.4004900	-5.5833610	-0.3971740
H	1.8931090	-4.6036170	-1.6165850
H	-1.2153250	-6.2518880	0.8666540
H	0.8476530	-6.5691440	-0.4851080
C	-0.8784210	1.9180770	-0.0329390
C	0.1998650	2.2065590	-0.8569590
C	-1.4589890	2.9554130	0.7543000
C	0.7273270	3.5178960	-0.9366860
H	0.6659230	1.4224510	-1.4441690
C	-0.9626090	4.2332360	0.6903630
H	-2.2802160	2.7315130	1.4230220
C	0.1336060	4.5594980	-0.1527960
H	-1.4026910	5.0149030	1.3031800
C	-1.3669140	0.5380120	0.0235750
C	-3.8278010	0.9344160	0.1458360
C	-4.5210180	1.1992270	1.3265600
C	-4.2708840	1.4621030	-1.0667560
C	-5.6619270	1.9984620	1.2873530
H	-4.1592910	0.7980770	2.2674740
C	-5.4112000	2.2616400	-1.0901080
H	-3.7222450	1.2528140	-1.9791740
C	-6.1282860	2.5398090	0.0817520
H	-6.1954010	2.2074780	2.2102320
H	-5.7487000	2.6760810	-2.0358540
N	-2.6496050	0.1033850	0.1663810
N	-0.5940560	-0.5448670	-0.1027960
C	3.1195260	-0.4955020	-0.1421620
C	4.2750000	-0.9138210	-0.9265290
C	5.5740570	-0.8695010	-0.4694840
C	5.8250280	-0.4521470	0.8395690
C	4.7837600	-0.0646720	1.6747960
C	3.4774580	-0.0929530	1.2126000

H	6.3910500	-1.1630130	-1.1153670
H	4.9887100	0.2610540	2.6856270
O	1.9679450	-0.4318570	-0.6441240
H	0.4673650	-0.5016420	-0.1260200
N	2.4571800	0.3253270	2.1638860
N	4.0887490	-1.4080870	-2.2910290
N	7.1902190	-0.4298380	1.3354390
O	2.8187440	0.9485550	3.1664100
O	4.9942690	-1.1899150	-3.1013570
O	8.0872070	-0.7843330	0.5646720
O	7.3768820	-0.0571900	2.4971640
O	3.0657340	-2.0403680	-2.5596000
O	1.2772130	0.0274020	1.9443190
C	0.6659110	5.8719260	-0.2393760
H	0.2175030	6.6609890	0.3580870
C	1.7360020	6.1411760	-1.0631750
H	2.1371320	7.1486300	-1.1200120
C	1.8313770	3.8282180	-1.7770810
H	2.2813730	3.0333710	-2.3650190
C	2.3243960	5.1111570	-1.8380270
H	3.1702510	5.3388970	-2.4792520
C	-7.3809790	3.3806780	0.0407380
H	-8.2564980	2.7657270	-0.2005050
H	-7.5734930	3.8598760	1.0043810
H	-7.3131380	4.1621180	-0.7214400

2-NTPI-3 + PA

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symmetry c1

C	-3.9183060	-2.8974720	-1.4336670
C	-3.2666750	-2.6490180	-0.2167370
C	-3.6236720	-3.4052680	0.9108480
C	-4.6106600	-4.3869000	0.8229150
C	-5.2548140	-4.6232220	-0.3927850
C	-4.9063790	-3.8781750	-1.5202540
H	-3.6408580	-2.3245220	-2.3131260
H	-3.1158080	-3.2258060	1.8544270
H	-4.8740980	-4.9676240	1.7018150
H	-6.0225890	-5.3879480	-0.4618890
H	-5.4007400	-4.0624900	-2.4692350
C	-2.2148330	-1.6082630	-0.1307090
C	-0.8506680	-1.6605400	-0.3343630
C	0.0118560	-2.7970610	-0.7018640
C	1.0987970	-2.5807470	-1.5679040
C	-0.2154050	-4.0953370	-0.2194280
C	1.9322250	-3.6343110	-1.9381130
H	1.2773370	-1.5842980	-1.9594380
C	0.6173790	-5.1471640	-0.5968730
H	-1.0358970	-4.2801750	0.4638860
C	1.6940900	-4.9224270	-1.4555980
H	2.7642110	-3.4496450	-2.6114750
H	0.4303920	-6.1436450	-0.2079390
H	2.3438240	-5.7431590	-1.7441030
C	-1.1664700	1.8994520	0.2228810

C	-0.2200480	2.5693290	-0.5363950
C	-1.9210080	2.6234120	1.1923220
C	0.0150790	3.9556700	-0.3652600
H	0.3690460	2.0296600	-1.2689600
C	-1.7243490	3.9719140	1.3637580
H	-2.6406370	2.1030110	1.8141310
C	-0.7608220	4.6808940	0.5962120
H	-2.3010960	4.5125350	2.1093570
C	-1.3250610	0.4489460	0.0339340
C	-3.8260480	0.2977310	0.1821790
C	-4.6681200	-0.0544010	1.2411960
C	-4.2664290	1.1789780	-0.8105420
C	-5.9529070	0.4734580	1.3083430
H	-4.3144100	-0.7338770	2.0072630
C	-5.5462280	1.7169160	-0.7410190
H	-3.6043120	1.4407090	-1.6280870
C	-6.3986030	1.3642490	0.3183050
H	-6.6120230	0.2054850	2.1264920
H	-5.8932170	2.4030200	-1.5055190
N	-2.5083810	-0.2539870	0.1006220
N	-0.3277890	-0.3870840	-0.2166490
C	3.2560150	0.1065800	0.0492930
C	4.3646050	0.8010710	-0.5342020
C	5.6834470	0.4976360	-0.2575540
C	5.9631840	-0.5678800	0.5945000
C	4.9426840	-1.2846970	1.2006700
C	3.6196490	-0.9390070	0.9551320
H	6.4837650	1.0738420	-0.7027790
H	5.1658610	-2.0990190	1.8768240
O	2.0622910	0.4966750	-0.2767220
H	1.1672510	-0.0140230	-0.0597480
N	2.6112100	-1.6700010	1.7270090
N	4.1345670	1.9112110	-1.4750830
N	7.3554530	-0.9236490	0.8688270
O	2.9409880	-2.7407630	2.2317010
O	4.9295500	2.8495140	-1.4230710
O	8.2298480	-0.2612190	0.3102260
O	7.5623380	-1.8620300	1.6376220
O	3.1990890	1.8260840	-2.2669200
O	1.5026430	-1.1484840	1.8566200
C	-0.5296420	6.0721490	0.7557360
H	-1.1193020	6.6225150	1.4840340
C	0.4294860	6.7135580	0.0041040
H	0.5997440	7.7780380	0.1355350
C	1.0041990	4.6440980	-1.1207340
H	1.6089550	4.0833570	-1.8284740
C	1.2054470	5.9932080	-0.9376910
H	1.9665420	6.5110920	-1.5132810
C	-7.7218780	1.9126750	0.3892890
N	-8.7951480	2.3570160	0.4474320

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symmetry c1

C	-2.5346220	-3.7915090	-1.1227590
C	-2.1836350	-3.1698430	0.0860950
C	-2.5595060	-3.7788040	1.2940590
C	-3.2779110	-4.9739800	1.2920530
C	-3.6254860	-5.5805280	0.0839520
C	-3.2489460	-4.9887120	-1.1227730
H	-2.2398110	-3.3314360	-2.0605550
H	-2.2667610	-3.3263190	2.2361320
H	-3.5580110	-5.4354630	2.2342660
H	-4.1827580	-6.5124870	0.0832960
H	-3.5126190	-5.4577450	-2.0658610
C	-1.4068600	-1.9119670	0.0605790
C	-0.1240910	-1.6488780	-0.3802940
C	0.9095480	-2.5743610	-0.8776540
C	1.8169110	-2.1457500	-1.8622380
C	1.0199750	-3.8841330	-0.3809680
C	2.8059360	-3.0063720	-2.3349610
H	1.7547540	-1.1382230	-2.2572160
C	2.0056420	-4.7427320	-0.8632780
H	0.3424160	-4.2248550	0.3940530
C	2.9025230	-4.3083500	-1.8412810
H	3.4981220	-2.6522580	-3.0929490
H	2.0796870	-5.7503590	-0.4648940
H	3.6727000	-4.9783690	-2.2118400
C	-1.1376590	1.7412290	0.3646530
C	-0.5243670	2.5910580	-0.5423100
C	-1.8535040	2.2972710	1.4641410
C	-0.6031270	3.9983370	-0.4032340
H	0.0298030	2.1785040	-1.3791360
C	-1.9487140	3.6583890	1.6179270
H	-2.3059490	1.6422780	2.1984540
C	-1.3372550	4.5498780	0.6962520
H	-2.4893170	4.0707940	2.4654640
C	-0.9897200	0.2912410	0.1763630
C	-3.3207330	-0.4339570	0.7599640
C	-3.7789020	-0.6994210	2.0515970
C	-4.1919200	0.0460680	-0.2179980
C	-5.1210210	-0.4856620	2.3653350
H	-3.0837690	-1.0583060	2.8025700
C	-5.5311510	0.2615110	0.1069520
H	-3.8285860	0.2432460	-1.2195500
C	-5.9994760	-0.0067340	1.3958980
H	-5.4803580	-0.6935530	3.3677720
N	-1.9442650	-0.6667290	0.4222920
N	0.1073830	-0.2893540	-0.2930390
C	3.4788800	0.5648870	-0.1465960
C	4.6670850	0.7338030	-0.9230840
C	5.9390490	0.5097130	-0.4335160
C	6.0819660	0.0278910	0.8657470
C	4.9749290	-0.1855730	1.6742090
C	3.7065010	0.1034920	1.1879190
H	6.8068140	0.6867120	-1.0552900
H	5.0930180	-0.553120	2.6846910
O	2.3346540	0.8583480	-0.6885350
H	1.4259850	0.3852470	-0.3710900

N	2.6078160	-0.0305210	2.1507910
N	4.5754660	1.1440950	-2.3346050
N	7.4193170	-0.2493280	1.3873770
O	2.7650310	-0.8111010	3.0891020
O	5.4300710	1.9334330	-2.7363490
O	8.3741720	-0.0470860	0.6367000
O	7.5055980	-0.6676760	2.5418970
O	3.6934030	0.6472890	-3.0292480
O	1.6113400	0.6726930	1.9867160
C	-1.4200430	5.9606530	0.8289860
H	-1.9762650	6.3769330	1.6646080
C	-0.8050260	6.7888210	-0.0828670
H	-0.8740620	7.8667690	0.0287990
C	0.0203330	4.8806970	-1.3273730
H	0.5790660	4.4592340	-2.1584080
C	-0.0779990	6.2440360	-1.1701810
H	0.4037680	6.9093980	-1.8801790
H	-7.0455050	0.1537280	1.6327520
C	-6.4779500	0.8288260	-0.9199110
F	-6.6356760	2.1616260	-0.7616760
F	-7.7050420	0.2729410	-0.8173730
F	-6.0386680	0.6245540	-2.1792040

2-NTPI-5 +PA

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symmetry c1

C	3.8427490	-3.0567200	1.2954410
C	3.3313950	-2.6596100	0.0507580
C	3.8156610	-3.2819470	-1.1109750
C	4.7946880	-4.2717660	-1.0295580
C	5.2997700	-4.6552580	0.2140880
C	4.8201710	-4.0483940	1.3757000
H	3.4658650	-2.5873450	2.1987860
H	3.4057490	-3.0018440	-2.0770440
H	5.1566600	-4.7483520	-1.9356680
H	6.0601040	-5.4278940	0.2776570
H	5.2060140	-4.3466920	2.3457750
C	2.2827270	-1.6167240	-0.0197970
C	0.9337770	-1.6596620	0.2677730
C	0.0987840	-2.7896510	0.7089520
C	-0.9553340	-2.5594240	1.6106220
C	0.3248620	-4.0989520	0.2558850
C	-1.7597770	-3.6115370	2.0442070
H	-1.1316220	-1.5536040	1.9786800
C	-0.4789070	-5.1485220	0.6964300
H	1.1206620	-4.2923740	-0.4544730
C	-1.5238480	-4.9104810	1.5905270
H	-2.5669420	-3.4169890	2.7444350
H	-0.2949250	-6.1540040	0.3298600
H	-2.1510730	-5.7298030	1.9286070
C	1.2123400	1.8759040	-0.4418480
C	0.2999580	2.5636540	0.3432840
C	1.9239170	2.5790070	-1.4580070
C	0.0568250	3.9457180	0.1523310

H	-0.2546810	2.0418650	1.1144430
C	1.7200950	3.9237960	-1.6491480
H	2.6159110	2.0461010	-2.0997330
C	0.7903400	4.6498950	-0.8567120
H	2.2645840	4.4481890	-2.4298030
C	1.3801650	0.4311240	-0.2235910
C	3.8713530	0.2745270	-0.4912940
C	4.6148270	0.0088560	-1.6443530
C	4.4014440	1.0660640	0.5261320
C	5.8978210	0.5396970	-1.7797570
H	4.1833230	-0.6008850	-2.4295780
C	5.6887560	1.6042300	0.3802870
H	3.8217050	1.2670680	1.4194110
C	6.4397400	1.3374860	-0.7761580
H	6.4740950	0.3332120	-2.6754640
N	2.5569950	-0.2762970	-0.3368250
N	0.4015620	-0.3933910	0.1247330
C	-3.1850780	0.0756820	0.0025710
C	-4.2734260	0.7865000	0.6057660
C	-5.6009600	0.4753040	0.3854400
C	-5.9105520	-0.6137860	-0.4255630
C	-4.9117950	-1.3473030	-1.0479090
C	-3.5811770	-0.9947900	-0.8604780
H	-6.3851520	1.0641990	0.8425470
H	-5.1585210	-2.1804880	-1.6921430
O	-1.9812690	0.4717860	0.2758040
H	-1.0837060	-0.0365500	0.0363600
N	-2.6014560	-1.7471160	-1.6483000
N	-4.0116210	1.9244230	1.5041990
N	-7.3112180	-0.9766900	-0.6394360
O	-2.9455720	-2.8360000	-2.1025230
O	-4.8128280	2.8578690	1.4565710
O	-8.1656940	-0.2983450	-0.0690530
O	-7.5451950	-1.9366030	-1.3733060
O	-3.0447530	1.8666740	2.2598490
O	-1.5025110	-1.2252330	-1.8423070
C	0.5521900	6.0375020	-1.0357880
H	1.1103380	6.5720980	-1.7998010
C	-0.3741970	6.6951520	-0.2576500
H	-0.5500210	7.7567880	-0.4039090
C	-0.8989180	4.6506340	0.9351000
H	-1.4712340	4.1059530	1.6812970
C	-1.1086140	5.9954790	0.7318350
H	-1.8438620	6.5260940	1.3289840
H	7.4350110	1.7558010	-0.8767920
C	6.2418480	2.4209640	1.4222430
N	6.6961050	3.0808400	2.2651390

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