Electronic Supporting Information (ESI)

Red to NIR-emissive anthracene-conjugated PMI dyes with dual functions: singlet-oxygen response and lipid-droplet imaging†

Rupam Roy,*[a#] Aasif Khan,[a#] Tanoy Dutta,[a] and Apurba Lal Koner*[a]

(a) Bionanotechnology Laboratory, Department of Chemistry, Indian Institute of Science Education and Research Bhopal, Bhopal By-pass Road, Bhauri, Bhopal 462066, Madhya Pradesh, India. E-mail: rupam16@iiserb.ac.in, akoner@iiserb.ac.in

[#] These authors contributed to this work equally.

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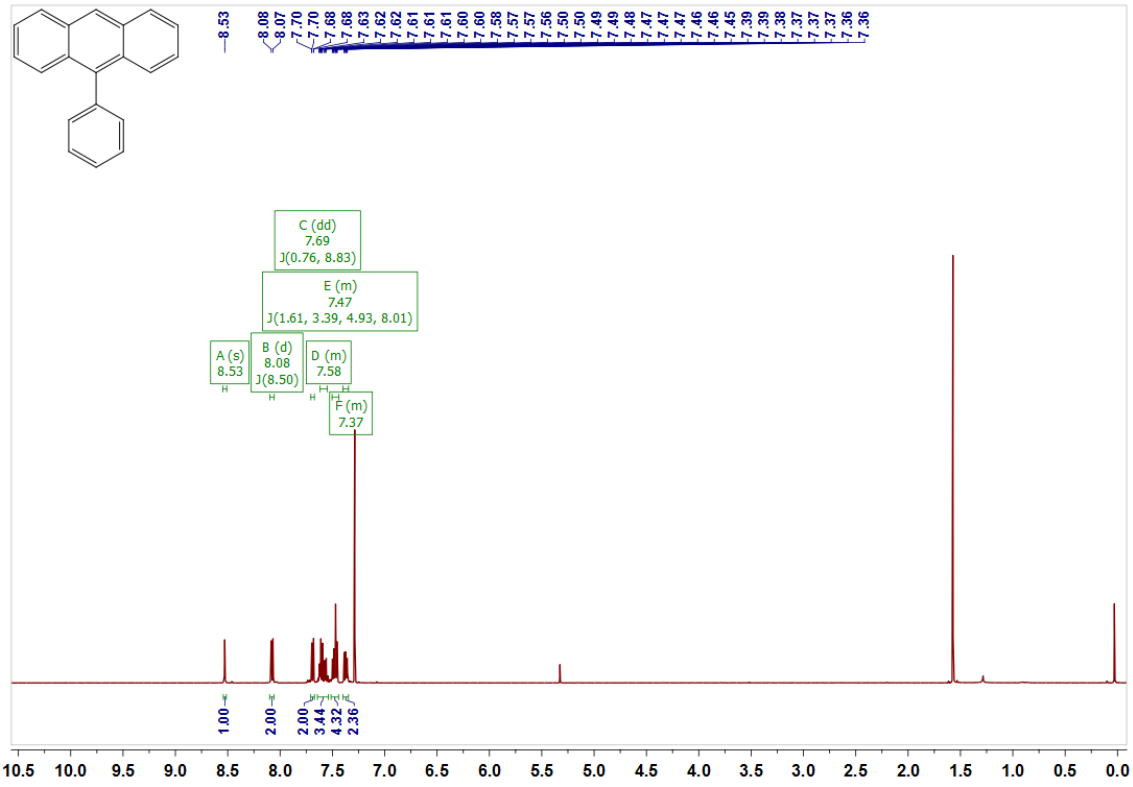


Fig. S1 ^{1}H NMR spectrum of 9-phenyl anthracene **(I)** recorded in $CDCl_3$ at 500 MHz.

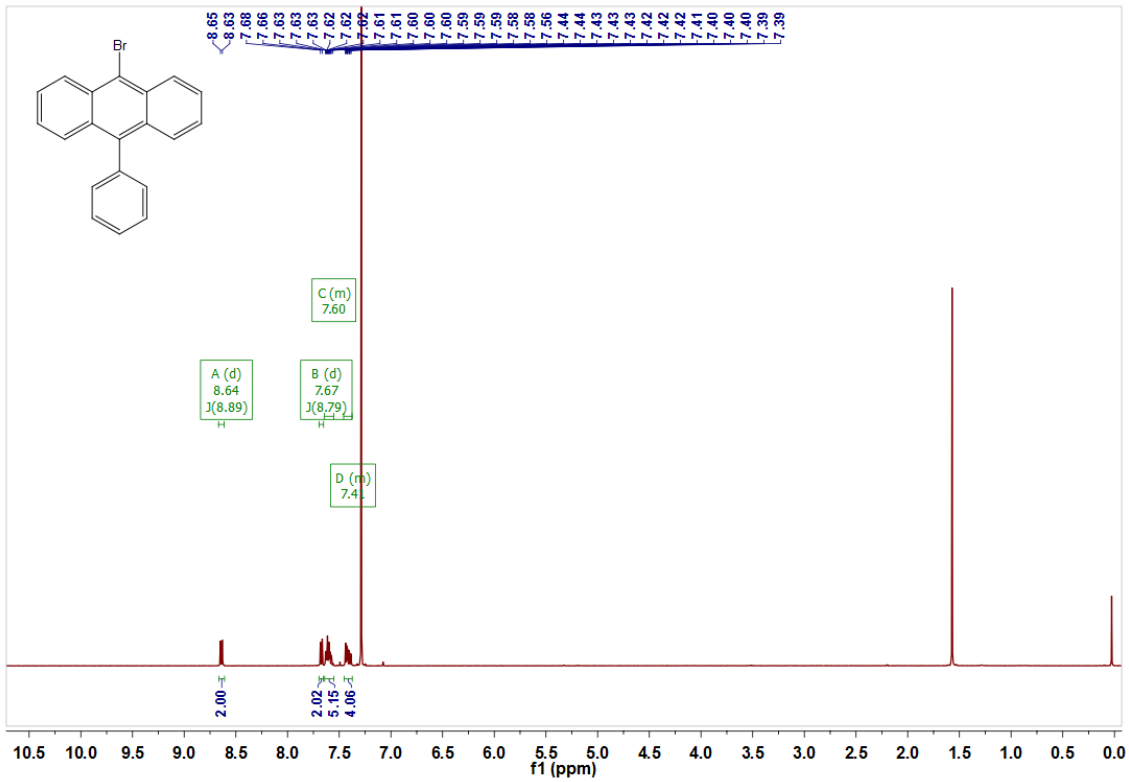


Fig. S2 ^{1}H NMR spectrum of 9-bromo-10-phenylanthracene **(II)** recorded in $CDCl_3$ at 500 MHz.

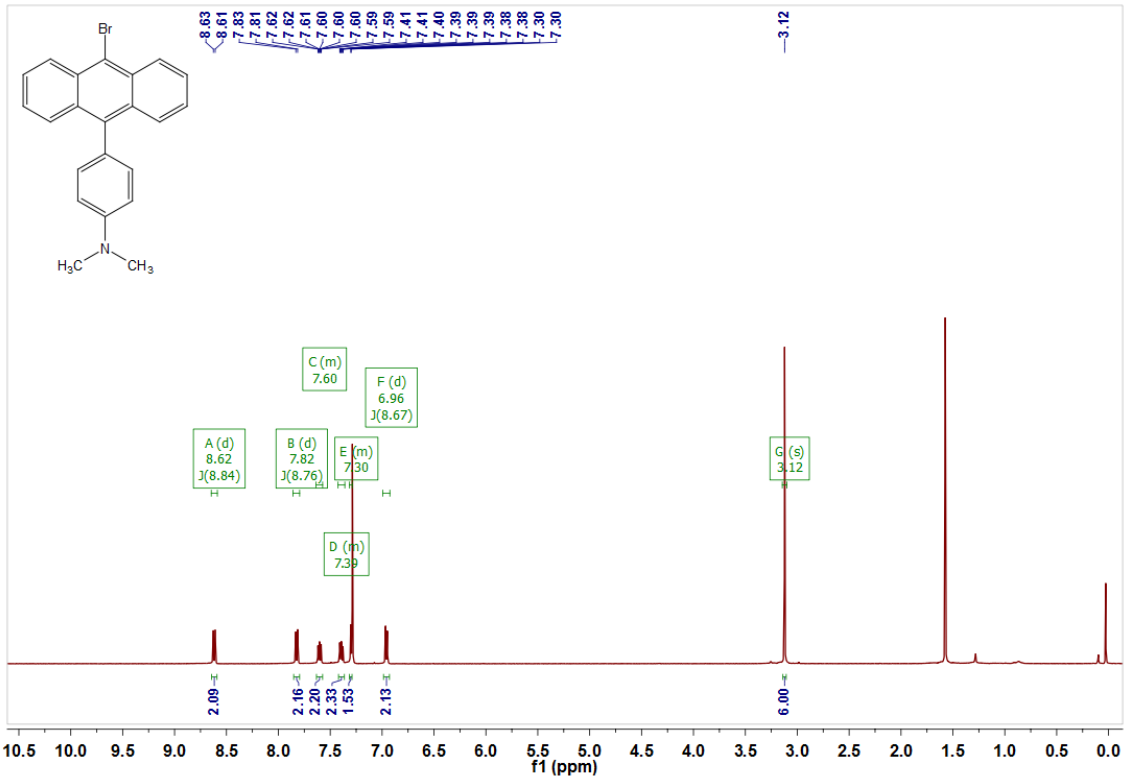


Fig. S3 ^{1}H NMR spectrum of 4-(10-bromoanthracene-9-yl)-*N*, *N*-dimethylaniline **(III)** recorded in $CDCl_3$ at 500 MHz.

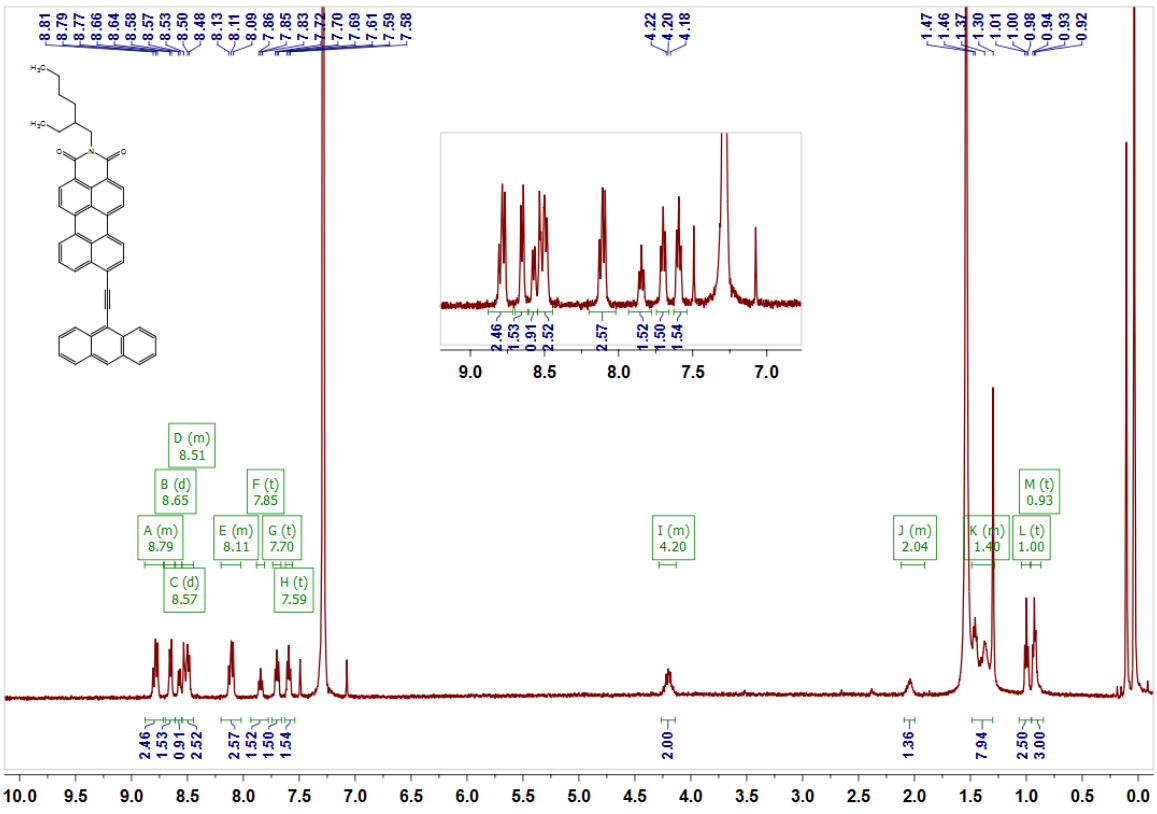


Fig. S4 ^{1}H NMR spectrum for compound **1** recorded in $CDCl_3$ at 500 MHz.

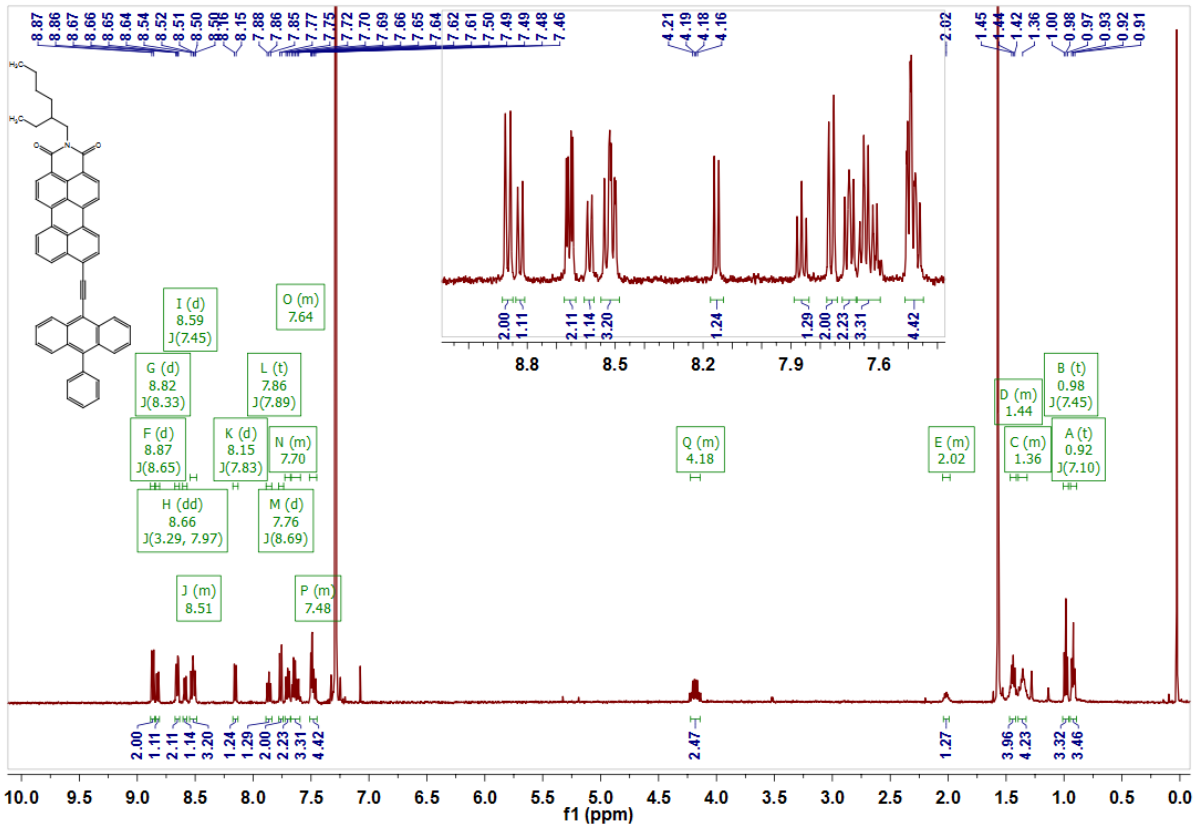


Fig. S5 ^{1}H NMR spectrum for compound **2** recorded in $CDCl_3$ at 500 MHz.

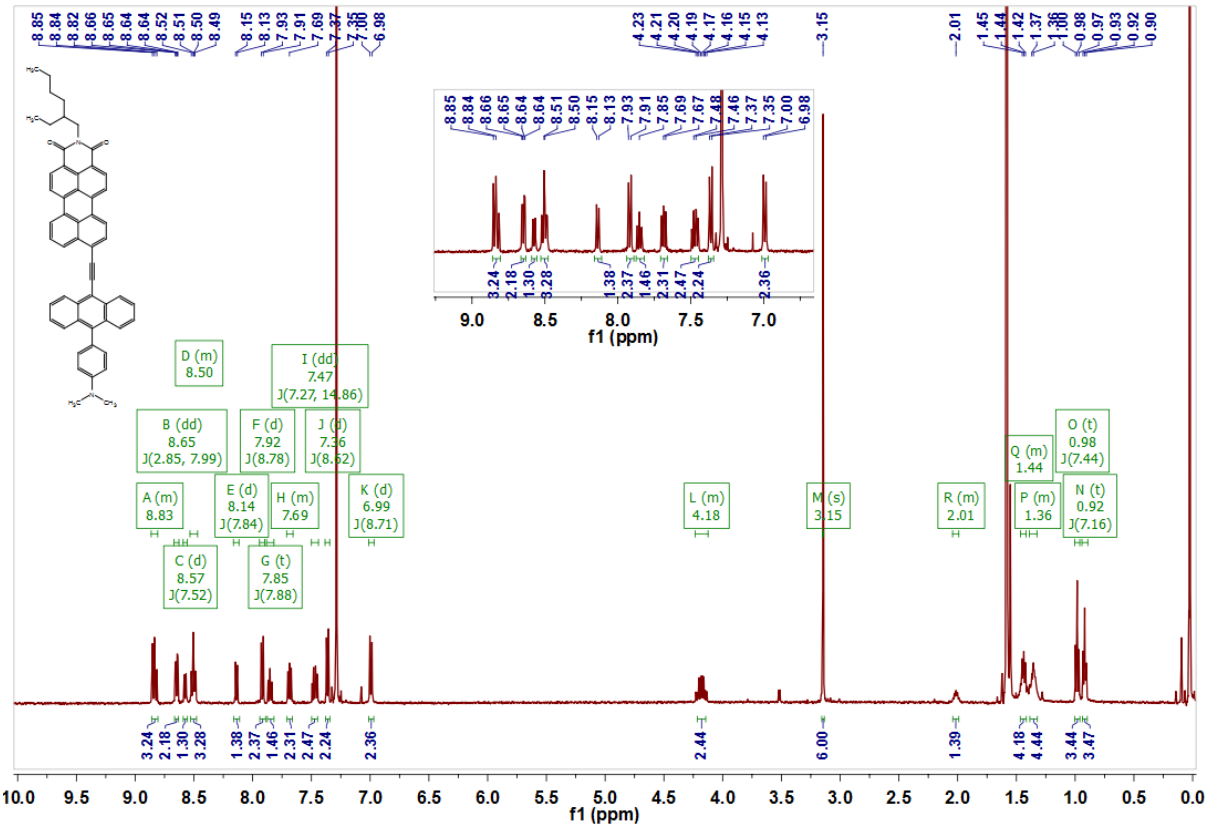


Fig. S6 ^{1}H NMR spectrum for compound **3** recorded in $CDCl_3$ at 500 MHz.

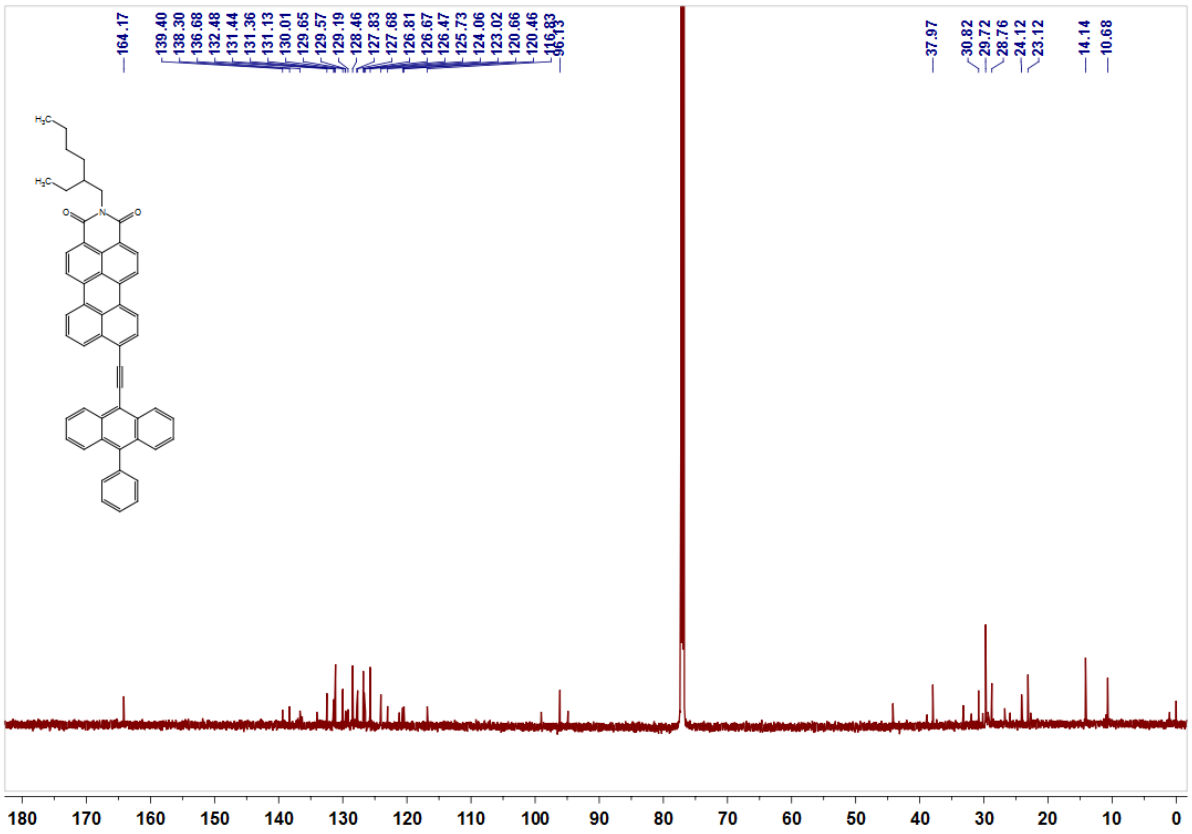


Fig. S7 ^{13}C NMR spectrum for compound **2** recorded in $CDCl_3$ at 175 MHz.

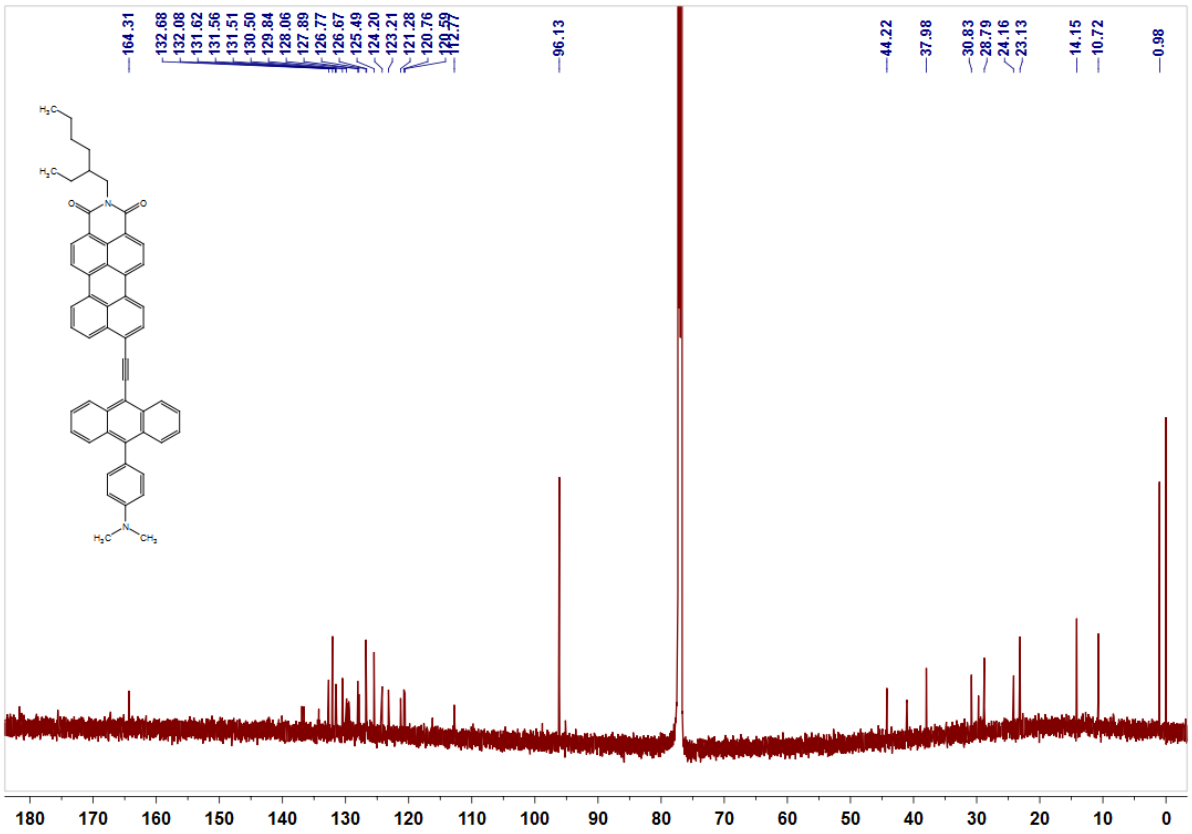


Fig. S8 ^{13}C NMR spectrum for compound **3** recorded in $CDCl_3$ at 175 MHz.

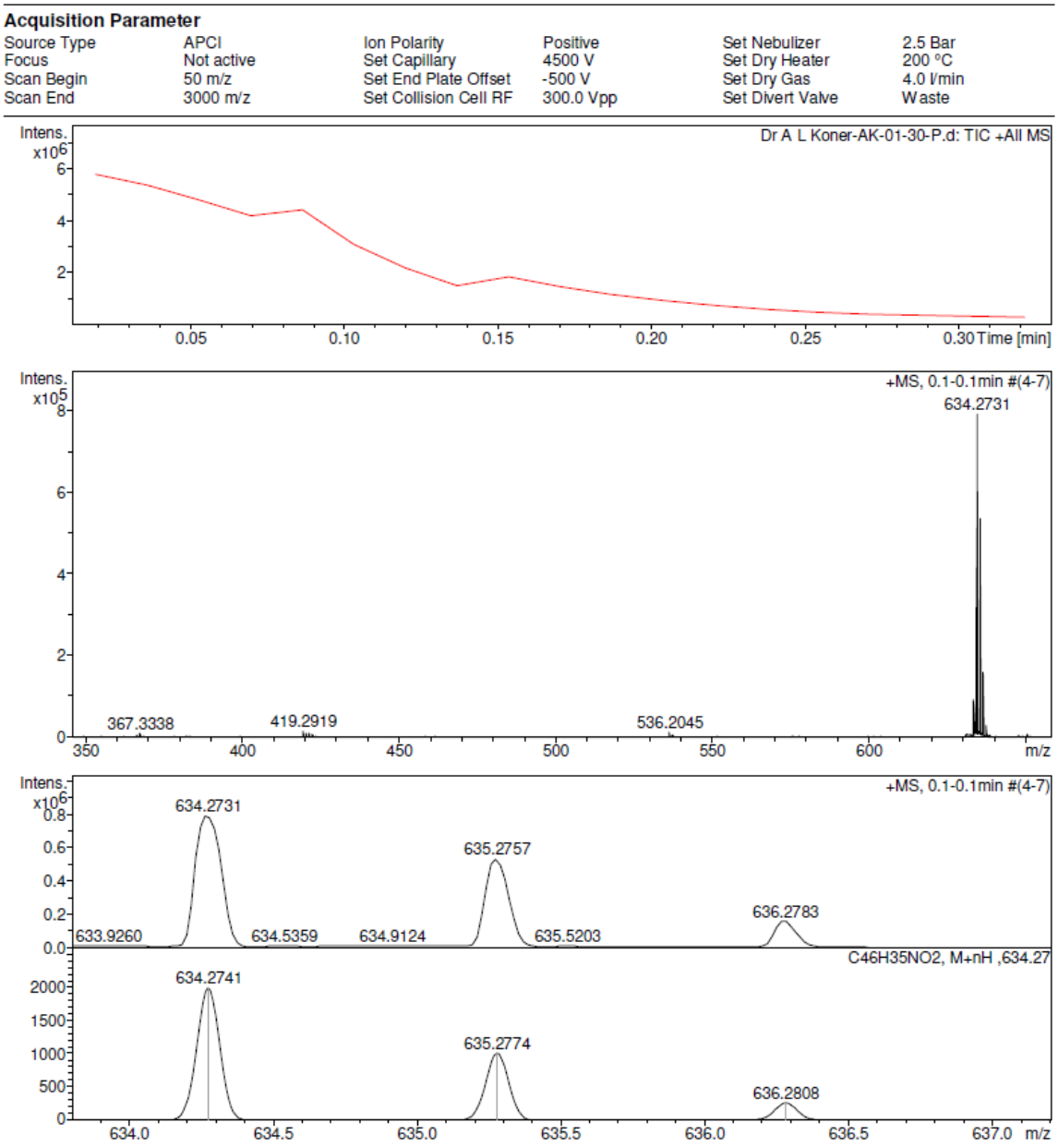


Fig. S9 APCI mass spectrum for compound **1**; **Calculated mass** – 633.2668 Da and **Obtained mass** – *m/z* 634.2731 Da $[M+H]^+$.

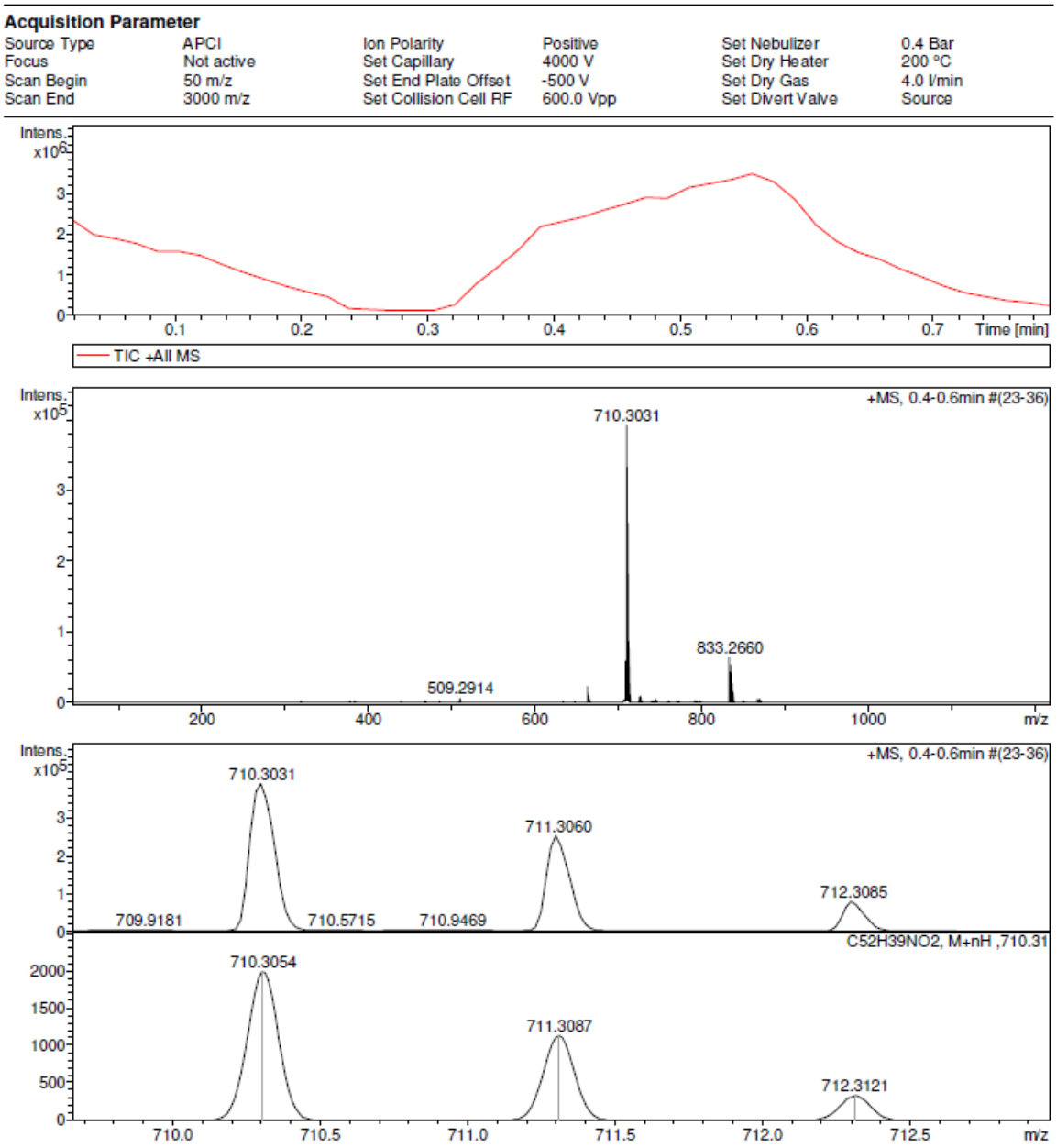


Fig. S10 APCI mass spectrum for compound **2**, **Calculated mass** – 709.2981 Da and **Obtained mass** – *m/z* 710.3031 Da $[M+H]^+$.

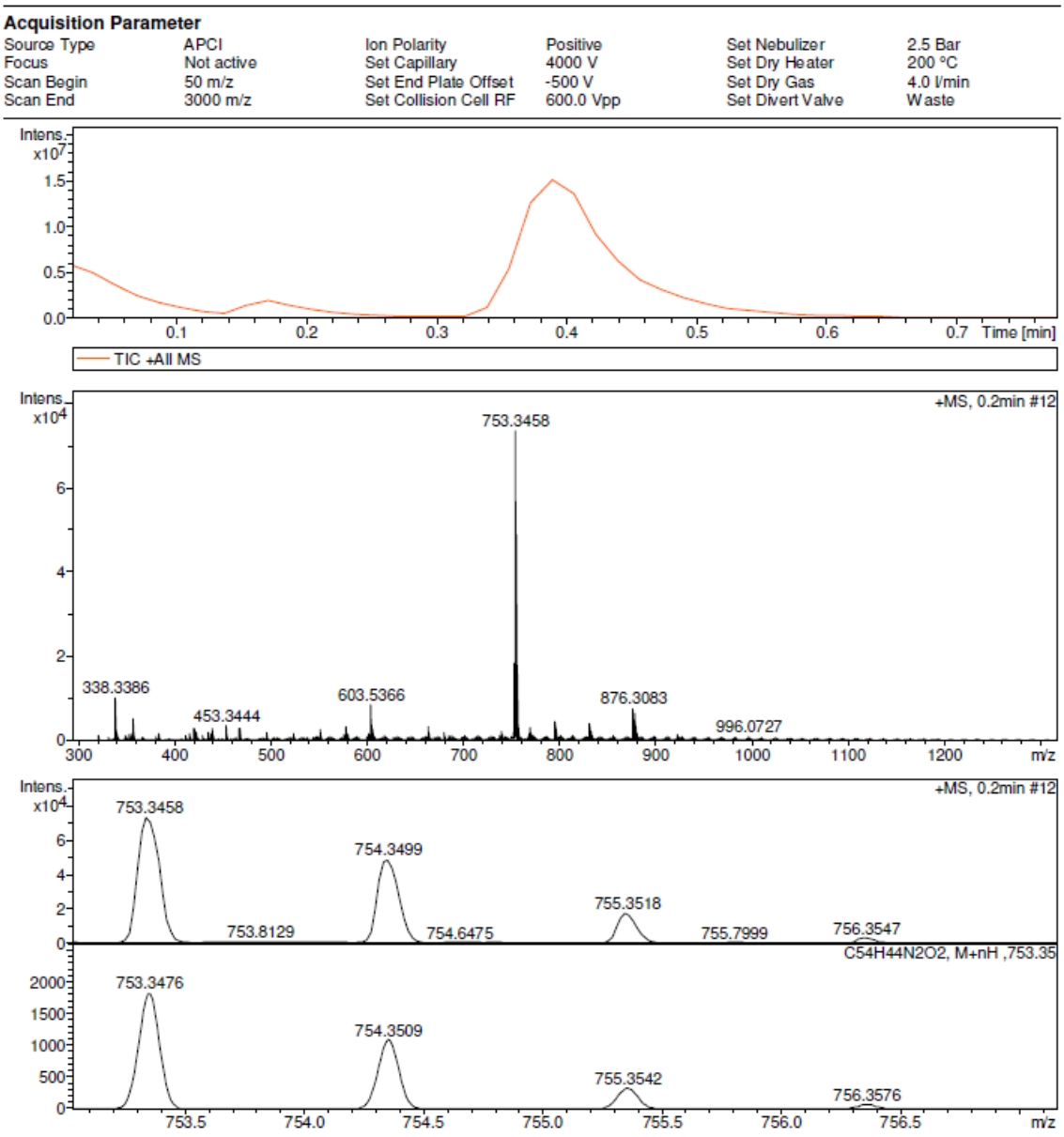


Fig. S11 APCI mass spectrum for compound **3**, **Calculated mass** – 752.3403 Da and **Obtained mass** – *m/z* 753.3486 Da $[M+H]^+$.

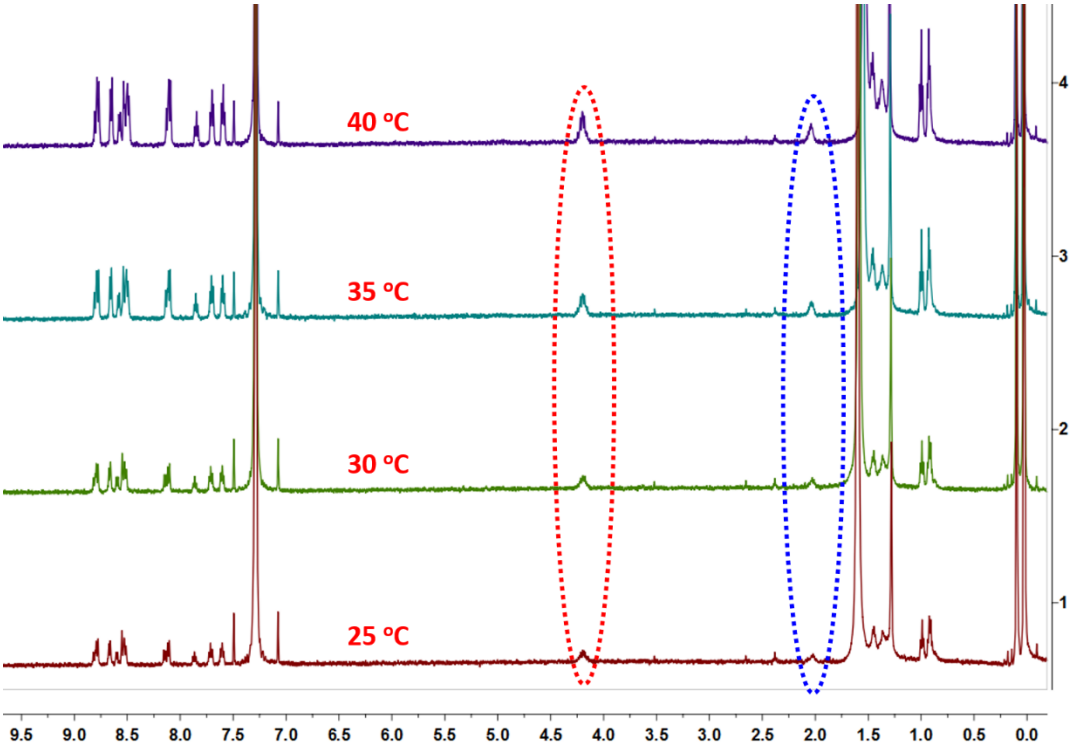


Fig. S12 Variable temperature (VT)-dependent ^{1}H NMR spectra of compound **1** in $CDCl_3$.

Note: To check the effect of aggregation in ^{1}H NMR spectra, we have carried out the variable temperature (VT)-dependent ^{1}H NMR study of probe **1** (PMI-Anth) (the most hydrophobic and planer molecule studied in this and prone to aggregation). This study demonstrates that while increasing temperature from 25 °C to 40 °C, the ^{1}H NMR peaks in the aromatic region become well-resolved with gaining a little high intensity. This spectral comparison manifests that there may be a possibility of aggregation for probe **1** at RT (25 °C) but at moderately high temperature, the peaks become sharp due to an increase in solubility of the compound in $CDCl_3$.

Optical purity plots:

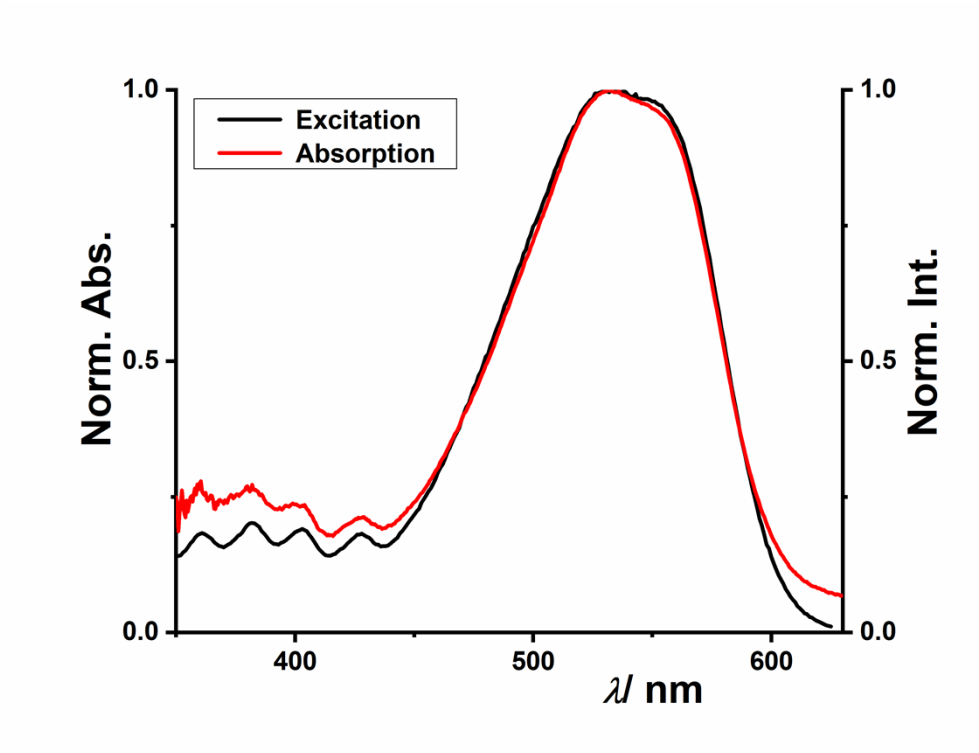


Fig. S13 Optical purity plot for compound **1** measured in $CHCl_3$.

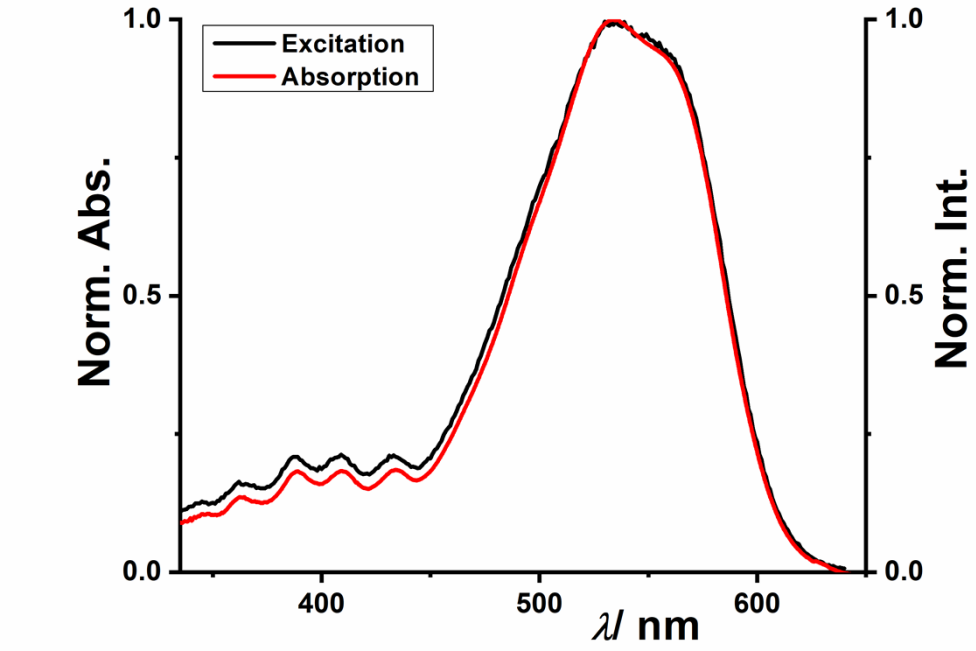


Fig. S14 Optical purity plot for compound **2** measured in $CHCl_3$.

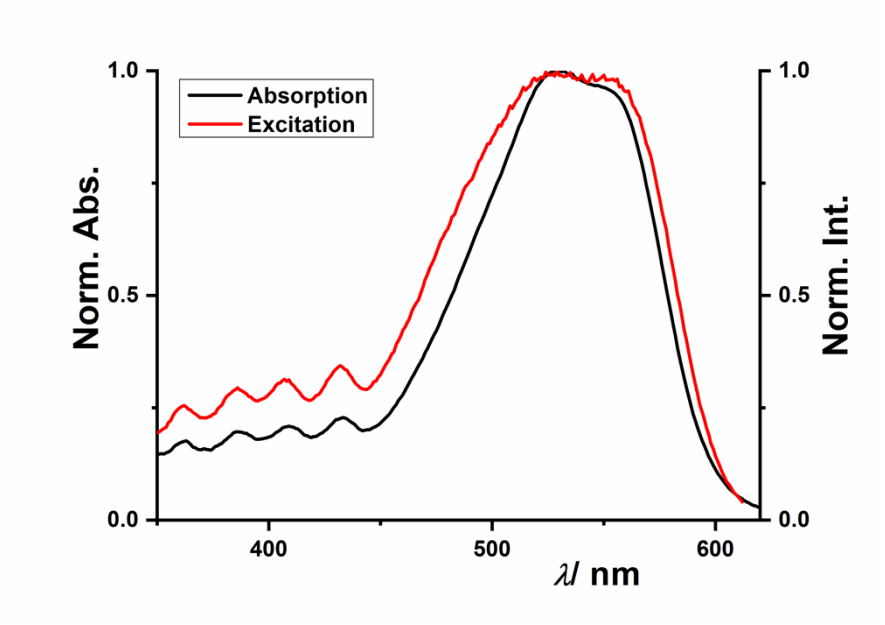


Fig. S15 Optical purity plot for compound **3** measured in $CHCl_3$.

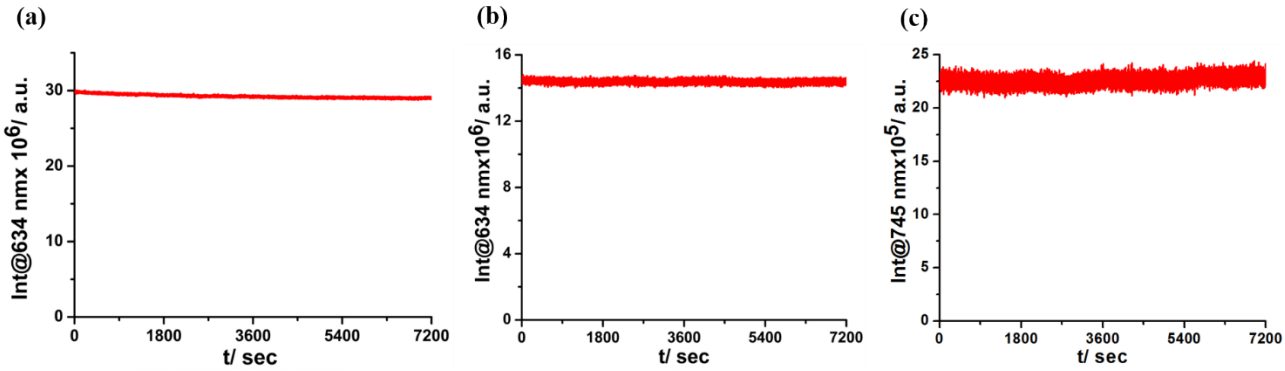


Fig. S16 Photostability plots for compound (a) **1**, (b) **2**, and (c) **3** in $CHCl_3$ at λ_{ex}= 533 nm using 70 lx intensity.

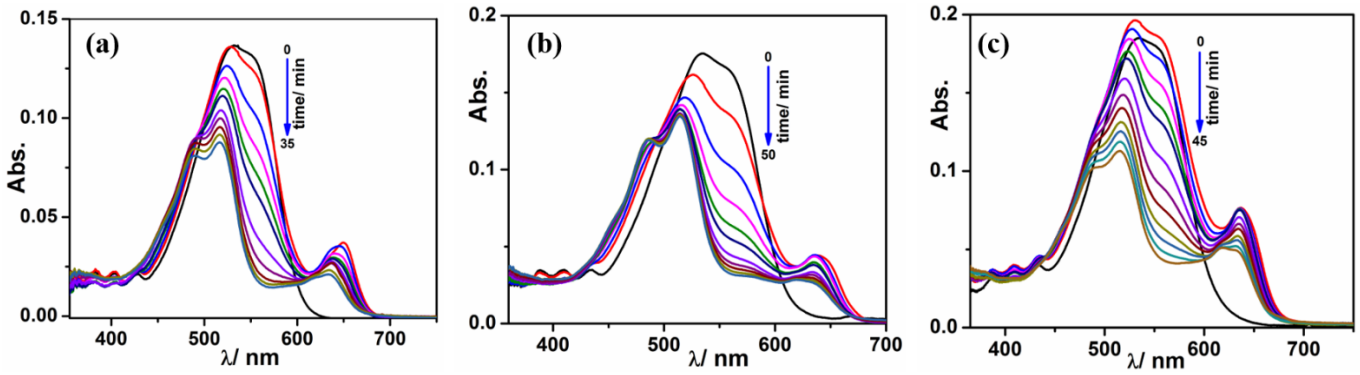


Fig. S17 Time-dependent UV-Vis. absorption spectra in $CDCl_3$ for (a) **1**, (b) **2**, and (c) **3** in absence (black color spectrum) and in presence of Methylene blue (MB) under visible light irradiation [[**1**/**2**/**3**] = 5 μM, MB: 2 μM].

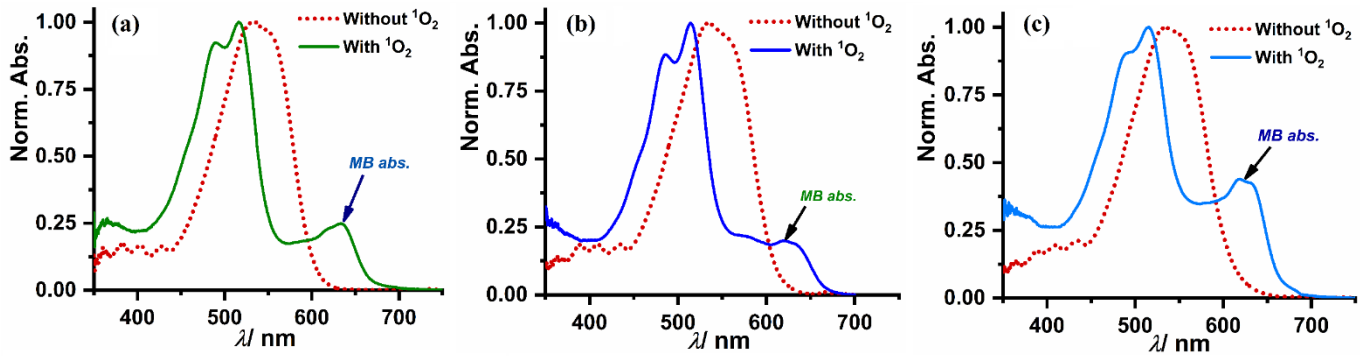
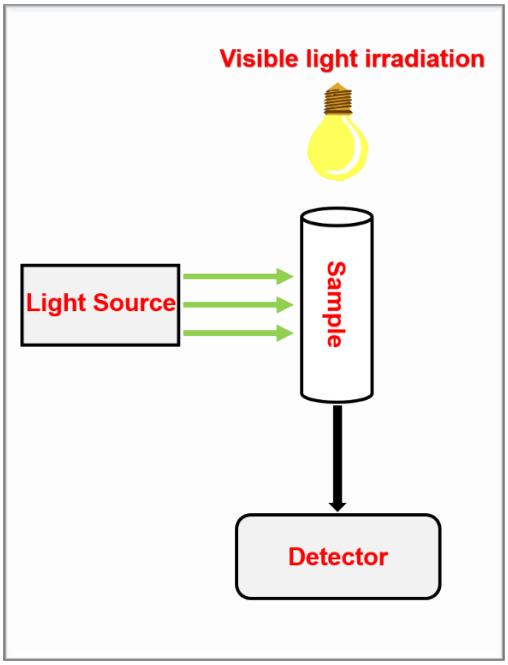


Fig. S18 Representation of initial (before reaction) and final (after reaction) absorption spectra for compound **1** (a), **2** (b), and **3** (c) respectively.



Scheme S1 Schematic diagram for $^1O_2$ reaction kinetics experiment.

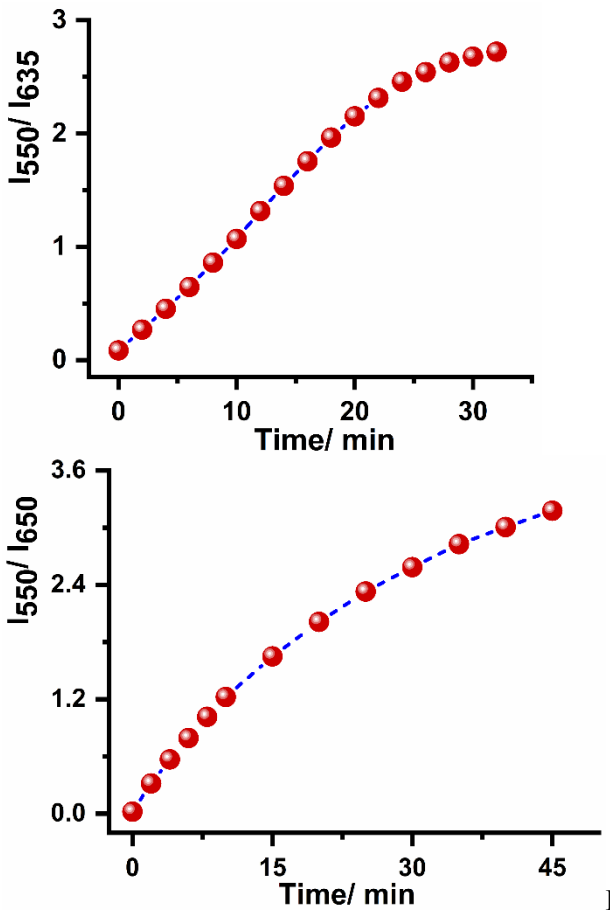


Fig. S19 Plots representing the change in fluorescence intensity ratio at two wavelengths with time on reaction with $^1O_2$ for **1** (left) and **2** (right) in $CDCl_3$.

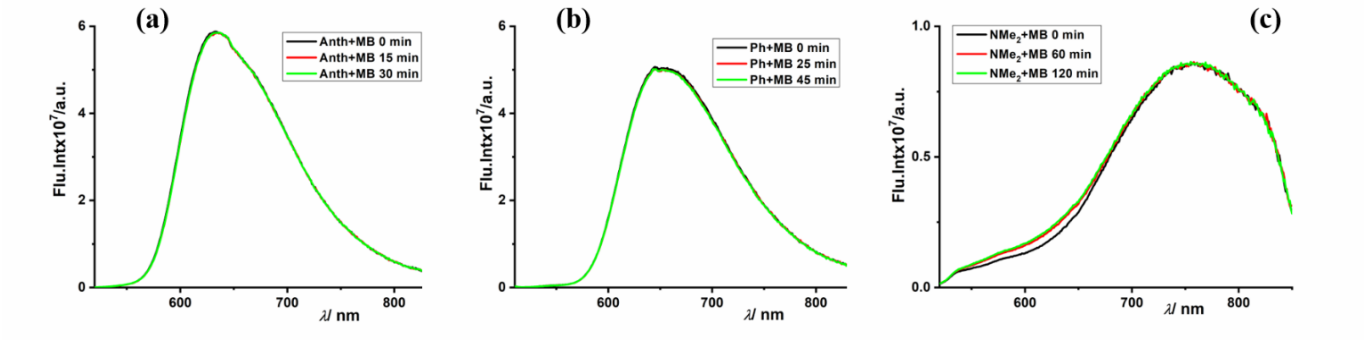


Fig. S20 Time-dependent emission spectra recorded in dark for (a) **1**, (b) **2** and (c) **3**. [**1**/**2**/**3**] = 5 μM and MB: 2 μM].

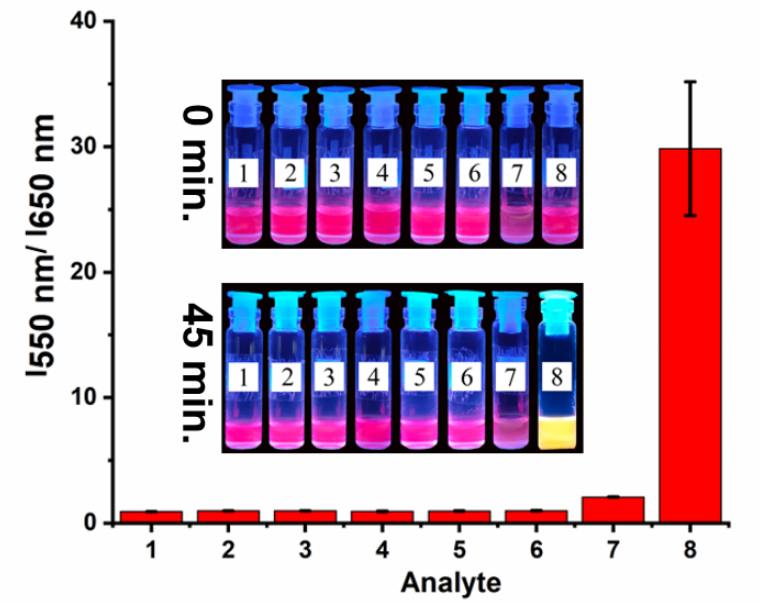


Fig. S21 Selectivity plot for probe **2** (1: Probe only; 2: H_2O_2; 3: ^tBuOOH; 4: Dicumyl peroxide; 5: KO_2; 6: NaOCl; 7: DDQ; 8: $^1O_2$) [Concentration: **1** (5 μM), 2-7 (1 mM), 8 (5 μM probe and 2 μM MB]; Inset pictures showing the color change under UV light on addition of the analyte at 0 min (top) and after 45 min (bottom).

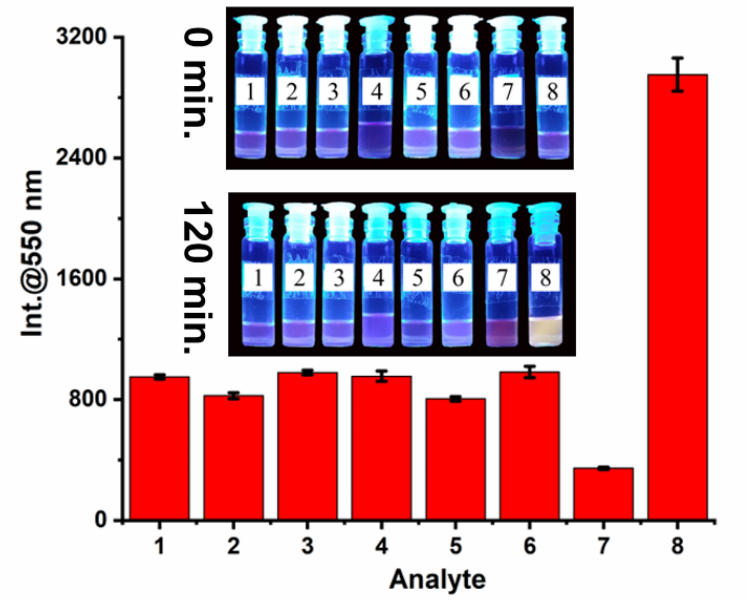


Fig. S22 Selectivity plot for probe **3** (1: Probe only; 2: H_2O_2; 3: ^tBuOOH; 4: Dicumyl peroxide; 5: KO_2; 6: NaOCl; 7: DDQ; 8: $^1O_2$) [Concentration: **1** (5 μM), 2-7 (1 mM), 8 (5 μM probe and 2 μM MB]; Inset pictures showing the color change under UV light on addition of the analyte at 0 min (top) and after 2 h (bottom).

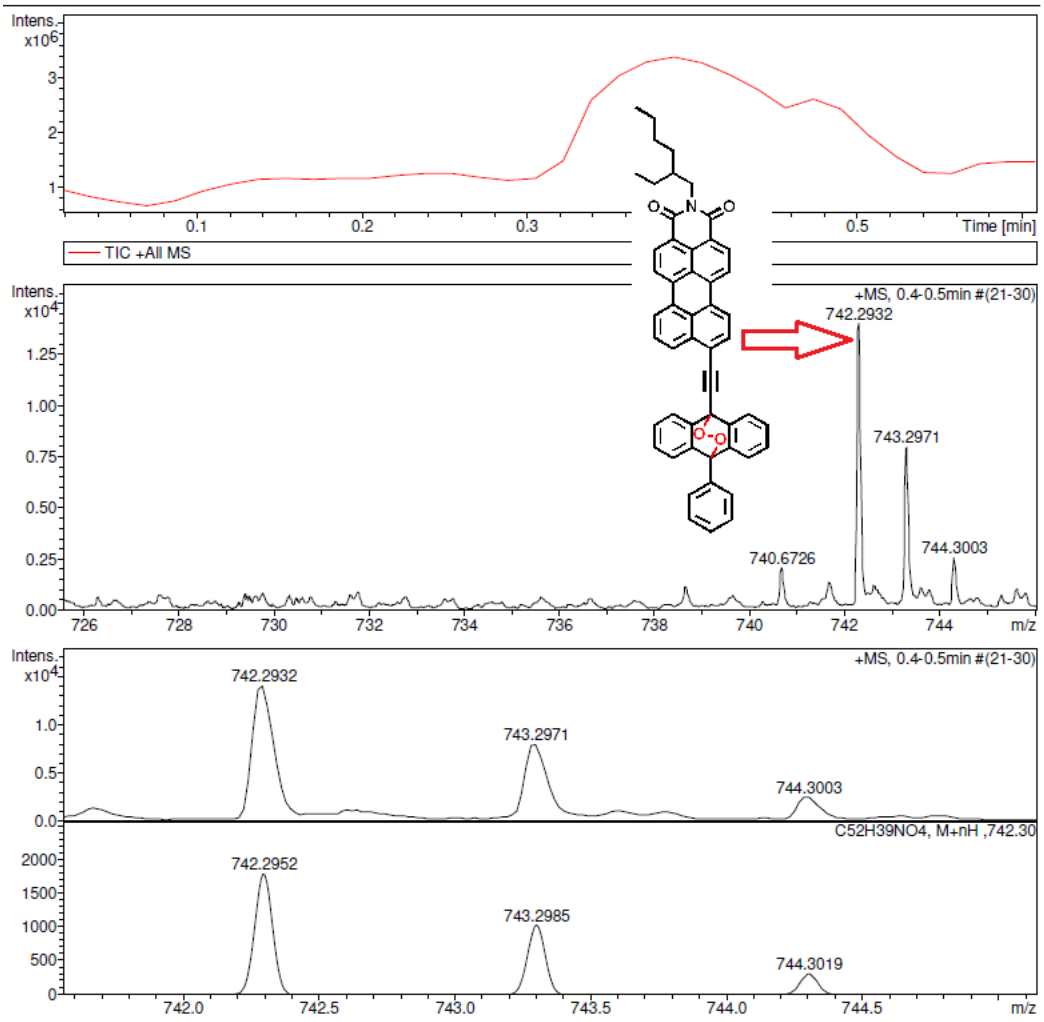


Fig. S23 APCI mass spectrum for endoperoxide corresponding to **2**. **Calculated mass** – 741.2879 Da and **Obtained mass** – *m/z* 742.2932 Da $[M+H]^+$.

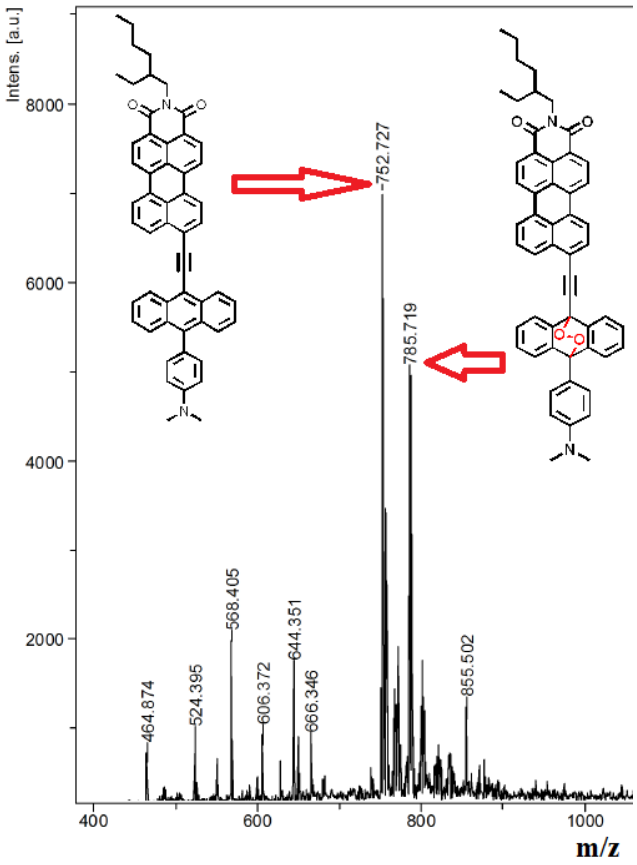


Fig. S24 MALDI mass spectrum for endoperoxide corresponding to **3**. **Calculated mass** – 784.330 Da and **Obtained mass** – *m/z* 785.719 Da $[M+H]^+$ (another peak at m/z 752.727 showing for the unreacted **3** during reaction with $^1O_2$ because compound **3** reacts slowly to $^1O_2$).

3. Density Functional Theory (DFT) Studies

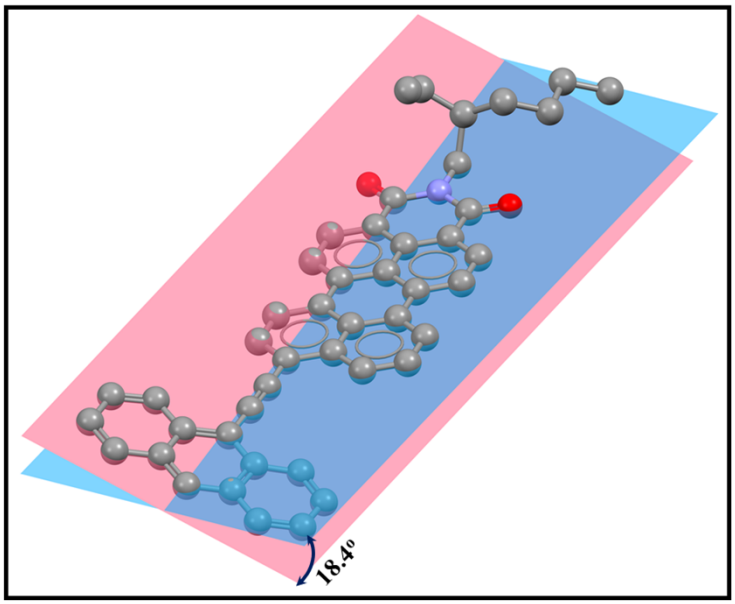


Fig. S25 Representation of PMI and anthracene planes and their corresponding dihedral angle in optimized geometry of **1**. PMI and anthracene planes are presented by blue and pink color.

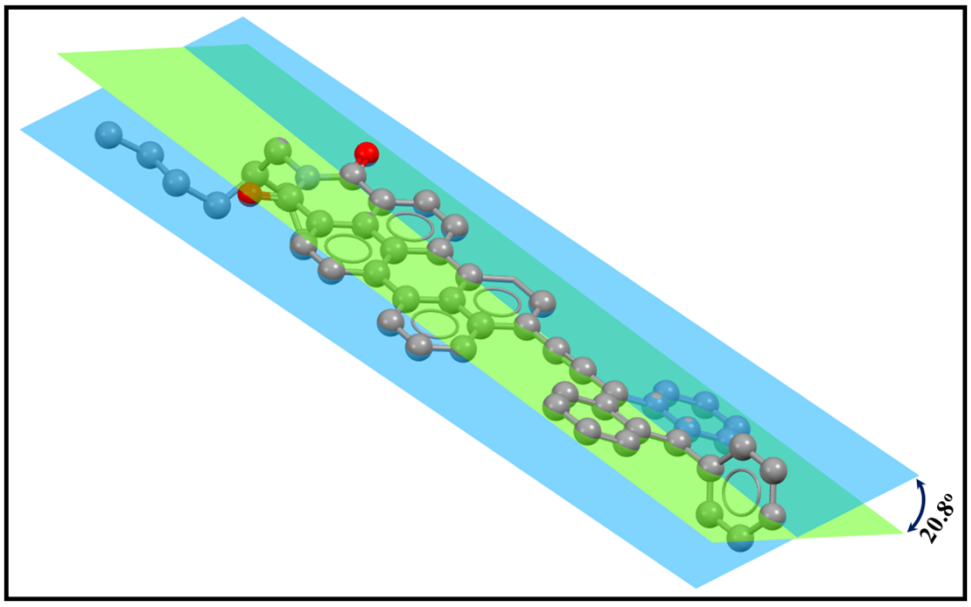


Fig. S26 Representation of PMI and anthracene planes and their corresponding dihedral angle in optimized geometry of **2**. PMI and anthracene planes are presented by blue and light green color.

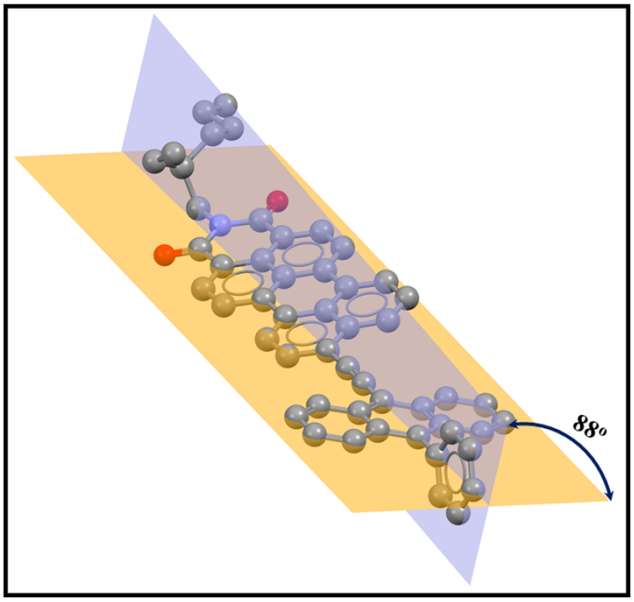


Fig. S27 Representation of Phenyl and anthracene planes and their corresponding dihedral angle in optimized geometry of **2**. Phenyl and anthracene planes are presented by violet and light orange color.

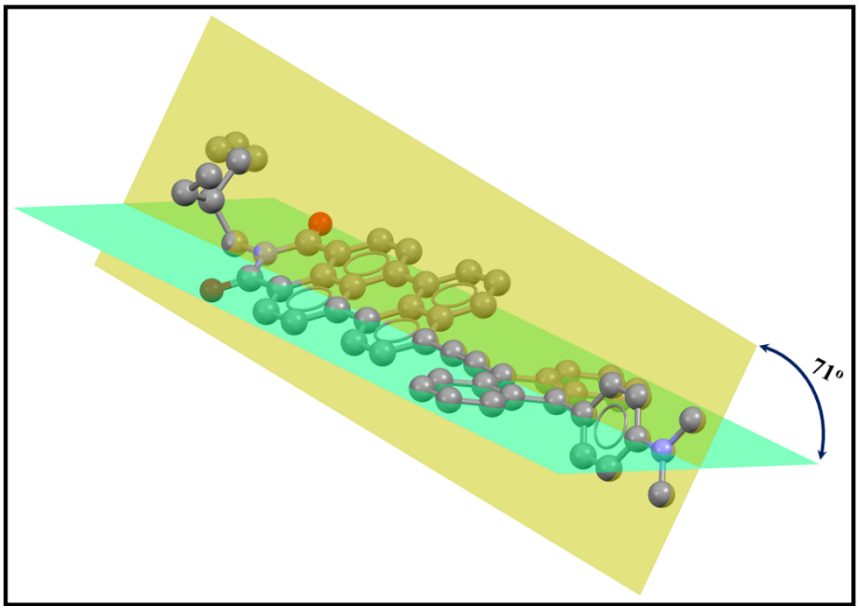


Fig. S28 Representation of N, N-dimethyl Phenyl and anthracene planes and their corresponding dihedral angle in optimized geometry of **3**. N, N-PhNMe$_2$ and anthracene planes are presented by yellow and cyan color.

DFT Calculation Data:

Symbolic Z-matrix for the optimized configuration of compound **1**

Symbolic Z-matrix:
Charge = 0 and Multiplicity = 1

C	0.52213	2.83395	0.32404
C	-0.02312	1.5862	0.01944
C	0.85909	0.46824	-0.1608
C	2.27573	0.6663	-0.02979
C	2.76994	1.95582	0.28723
C	1.90726	3.01819	0.45978
H	-0.11855	3.68991	0.46688
C	0.34713	-0.83592	-0.46453
C	3.17133	-0.44757	-0.2145
H	2.29251	3.99825	0.70251
C	2.63261	-1.70288	-0.50222
C	1.25387	-1.88745	-0.62245
H	3.29538	-2.54462	-0.64026
H	0.90216	-2.88199	-0.84771
C	-1.10062	-1.03508	-0.59783
C	-1.47522	1.38948	-0.11682
C	-1.97996	0.08262	-0.41634
C	-2.38914	2.44002	0.03535
C	-1.66011	-2.28452	-0.89891
C	-3.91299	-1.39553	-0.8439
C	-3.39332	-0.11073	-0.54393
C	-4.27958	0.98266	-0.37576
C	-3.76479	2.24214	-0.09364
H	-4.44721	3.07035	0.02708
C	-3.0387	-2.46189	-1.02084
H	-3.443	-3.43592	-1.25314
C	-5.72889	0.79734	-0.50729
C	-5.35863	-1.60578	-0.97317
N	-6.20264	-0.50591	-0.73214
O	-6.53611	1.75723	-0.42333
O	-5.84723	-2.7232	-1.28055
C	-7.67259	-0.7104	-0.88282
H	-8.06228	0.19223	-1.3453
H	-7.78155	-1.53502	-1.58132
C	-8.49148	-1.03544	0.3949
H	-9.46998	-1.31029	-0.01883
C	-8.72284	0.16846	1.34065
H	-9.16985	-0.21335	2.26648
H	-7.76187	0.60322	1.62184
C	-9.63347	1.28453	0.78922
H	-9.57477	2.14094	1.47105
H	-9.24498	1.6409	-0.16858
C	-11.11394	0.89053	0.63549
H	-11.20948	0.05254	-0.06188

H	-11.49051	0.53122	1.5999
C	-11.99165	2.05243	0.14453
H	-11.65541	2.41246	-0.83143
H	-13.03639	1.74933	0.04608
H	-11.95263	2.89512	0.83994
C	-8.01123	-2.29574	1.16869
H	-7.75636	-3.07328	0.44561
H	-8.86933	-2.66948	1.73763
C	-6.83943	-2.10856	2.14971
H	-5.93595	-1.74726	1.65952
H	-7.08872	-1.40253	2.9438
H	-6.59528	-3.0615	2.6251
H	-1.02689	-3.14495	-1.04407
H	-2.04285	3.43645	0.25776
H	3.83482	2.09468	0.40084
C	4.57837	-0.29181	-0.11198
C	5.79039	-0.20169	-0.03272
C	7.2047	-0.12573	0.07017
C	7.96204	-1.31891	0.26935
C	7.86238	1.13678	-0.01908
C	7.35289	-2.60925	0.36157
C	9.39867	-1.23361	0.38944
C	9.29965	1.19715	0.10859
C	8.10952	-3.73954	0.55554
H	6.27835	-2.68507	0.27653
C	10.1512	-2.43628	0.59157
C	10.02702	0.01646	0.30961
C	9.52759	-3.65489	0.67238
H	11.22731	-2.36019	0.6794
H	7.62813	-4.70576	0.62168
H	10.10528	-4.55606	0.82511
C	7.15385	2.35873	-0.23951
H	6.08017	2.32407	-0.35388
C	9.95134	2.47064	0.02363
H	11.02856	2.50383	0.12342
C	7.81504	3.56047	-0.31803
H	7.25849	4.47225	-0.4868
C	9.23266	3.62028	-0.18196
H	9.73497	4.57569	-0.24538
H	11.10465	0.07153	0.4041

Table S1: Calculated energy of Kohn-Sham molecular orbitals (MO) of compound **1** by DFT using B3LYP/ 6-311G as basis-set

Molecular Orbitals (MOs)	Energy/ Hartree	Energy/ eV
LUMO+4	-0.04319	-1.175
LUMO+3	-0.05411	-1.472
LUMO+2	-0.05738	-1.561

LUMO+1	-0.08826	-2.401
LUMO	-0.12127	-3.299
HOMO	-0.20120	-5.475
HOMO-1	-0.22059	-6.002
HOMO-2	-0.26014	-7.079
HOMO-3	-0.26535	-7.220
HOMO-4	-0.27118	-7.379

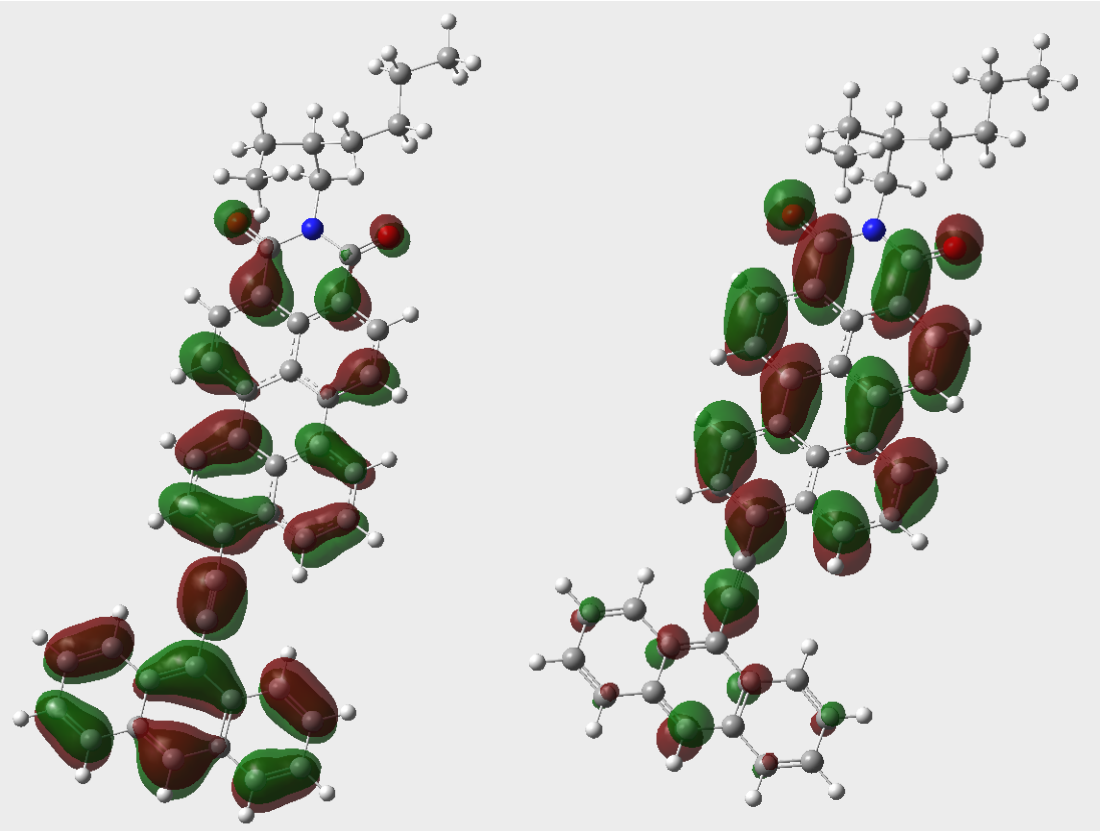


Fig. S29 Representation of HOMO and LUMO electronic distributions for compound **1**.

Symbolic Z-matrix for the optimized configuration of compound **2**

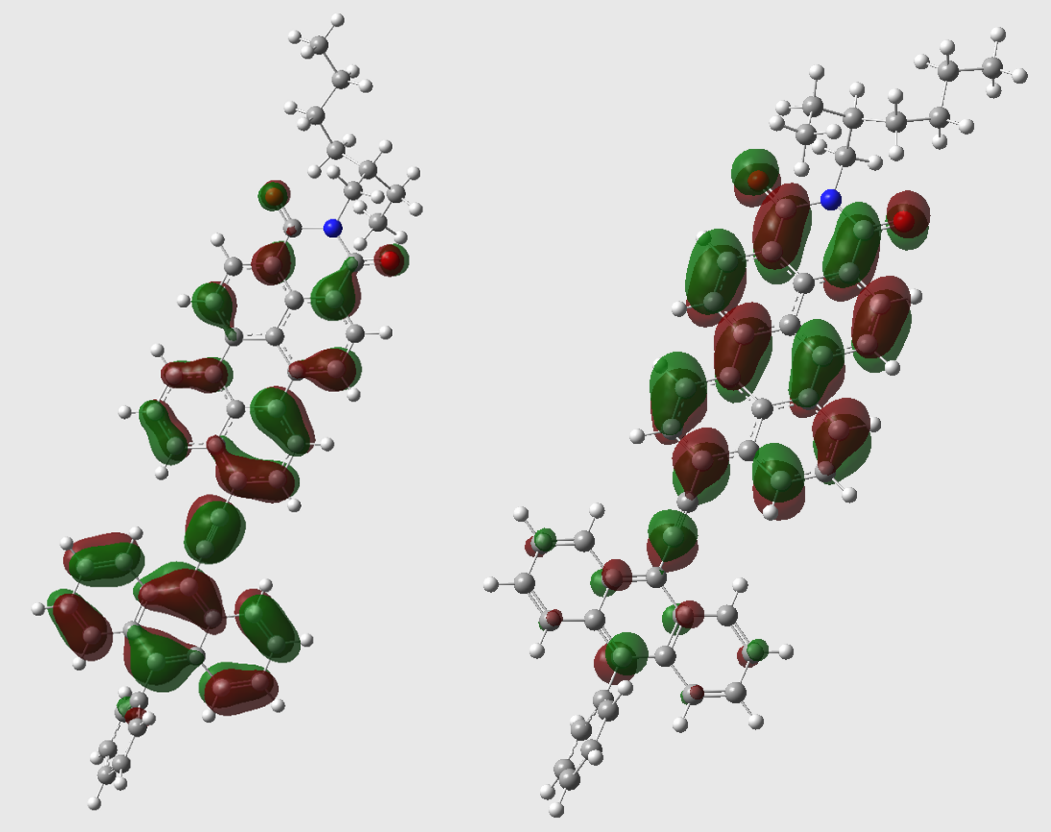
Symbolic Z-matrix:
Charge =0 and Multiplicity = 1

C	0.85369	-2.8128	0.30688
C	1.40909	-1.57095	-0.00327
C	0.53492	-0.4507	-0.20699
C	-0.88432	-0.64044	-0.09259
C	-1.38907	-1.92424	0.23125
C	-0.53401	-2.98891	0.4261
H	1.48818	-3.67031	0.46693
C	1.05739	0.84763	-0.51771
C	-1.77162	0.47606	-0.2999
H	-0.92731	-3.96448	0.67393
C	-1.22284	1.72596	-0.59168
C	0.15831	1.90234	-0.6964
H	-1.87947	2.56967	-0.74603
H	0.518	2.89291	-0.92653
C	2.50769	1.03767	-0.63655
C	2.86385	-1.38276	-0.12216
C	3.37895	-0.08219	-0.43114
C	3.77045	-2.43568	0.05516
C	3.07718	2.28029	-0.94673
C	5.32459	1.38056	-0.85447
C	4.79473	0.10246	-0.54395
C	5.67324	-0.99304	-0.35083
C	5.14862	-2.24617	-0.05877
H	5.82526	-3.07606	0.0813
C	4.45802	2.449	-1.0551
H	4.87	3.41788	-1.29533
C	7.125	-0.81658	-0.46677
C	6.77272	1.58161	-0.9704
N	7.60816	0.48105	-0.70397
O	7.92617	-1.77918	-0.3594
O	7.27056	2.69184	-1.28865
C	9.0809	0.67573	-0.83991
H	9.47109	-0.2357	-1.28435
H	9.20285	1.48927	-1.54917
C	9.88635	1.01559	0.44246
H	10.8721	1.2757	0.03641
C	10.09671	-0.17383	1.41113
H	10.53672	0.22008	2.33526
H	9.12901	-0.59579	1.68896
C	11.00457	-1.30624	0.88929
H	10.92993	-2.15117	1.58377
H	10.62539	-1.67464	-0.06766
C	12.4902	-0.92695	0.74865
H	12.60168	-0.10073	0.03971
H	12.8574	-0.5558	1.71221
C	13.36416	-2.10369	0.28719

H	13.03693	-2.4764	-0.68705
H	14.41255	-1.81081	0.19703
H	13.30943	-2.93482	0.99533
C	9.40663	2.29258	1.18855
H	9.16888	3.05983	0.44878
H	10.26	2.66862	1.76307
C	8.21957	2.13261	2.15572
H	7.32037	1.76888	1.65955
H	8.45168	1.43992	2.96665
H	7.97602	3.09617	2.60955
H	2.4502	3.14203	-1.1101
H	3.41638	-3.42748	0.28583
H	-2.45592	-2.05699	0.3326
C	-3.18093	0.3281	-0.2157
C	-4.39433	0.24433	-0.15323
C	-5.81046	0.17353	-0.06952
C	-6.56531	1.35999	0.15646
C	-6.47471	-1.07813	-0.20466
C	-5.93648	2.63737	0.29312
C	-8.0045	1.28424	0.25923
C	-7.91399	-1.14118	-0.09559
C	-6.67189	3.77514	0.51392
H	-4.86007	2.69399	0.21999
C	-8.7321	2.49957	0.49224
C	-8.66253	0.03721	0.13639
C	-8.09001	3.70523	0.61515
H	-9.80765	2.44997	0.57084
H	-6.17505	4.73057	0.61324
H	-8.65882	4.60809	0.79039
C	-5.75551	-2.28831	-0.45617
H	-4.68118	-2.2388	-0.55579
C	-8.54832	-2.42168	-0.23273
H	-9.62336	-2.47635	-0.15068
C	-6.40272	-3.49204	-0.58284
H	-5.83749	-4.39386	-0.77434
C	-7.81974	-3.55992	-0.46657
H	-8.3195	-4.51356	-0.56739
C	-10.1558	-0.03601	0.25261
C	-10.76401	-0.27177	1.49649
C	-10.97063	0.12849	-0.87957
C	-12.15594	-0.34144	1.60567
H	-10.14614	-0.4002	2.37544
C	-12.36265	0.05861	-0.77008
H	-10.51304	0.31025	-1.84312
C	-12.95863	-0.1765	0.4727
H	-12.61006	-0.52361	2.57051
H	-12.97722	0.187	-1.65105
H	-14.03558	-0.23044	0.55729

Table S2: Calculated energy of Kohn-Sham molecular orbitals (MO) of compound **2** by DFT using B3LYP/ 6-311G as basis-set

Molecular Orbitals (MOs)	Energy/ Hartree	Energy/ eV
LUMO+4	-0.04323	-1.176
LUMO+3	-0.05415	-1.473
LUMO+2	-0.05766	-1.569
LUMO+1	-0.08895	-2.420
LUMO	-0.12160	-3.308
HOMO	-0.20102	-5.470
HOMO-1	-0.22019	-5.991
HOMO-2	-0.25978	-7.069
HOMO-3	-0.26307	-7.158
HOMO-4	-0.26515	-7.215



E_{HOMO} = -5.470 eV E_{LUMO} = -3.308 eV

Fig. S30 Representation of HOMO and LUMO electronic distributions for compound **2**.

Symbolic Z-matrix for the optimized configuration of compound **3**

Symbolic Z-matrix:
Charge =0 Multiplicity = 1

C	1.74049	-2.78748	0.32416
C	2.30552	-1.54976	0.0144
C	1.43979	-0.42366	-0.1931
C	0.01894	-0.60339	-0.08264
C	-0.49577	-1.88325	0.2411
C	0.35132	-2.95375	0.4396
H	2.36855	-3.64925	0.48678
C	1.97221	0.87064	-0.50356
C	-0.8603	0.51921	-0.29274
H	-0.04949	-3.92623	0.68762
C	-0.30149	1.76615	-0.57894
C	1.08102	1.93256	-0.68051
H	-0.95181	2.61474	-0.73342
H	1.44843	2.92096	-0.90789
C	3.42353	1.04909	-0.62457
C	3.76182	-1.37192	-0.1008
C	4.28658	-0.07641	-0.41469
C	4.66081	-2.43031	0.0836
C	4.00226	2.28574	-0.94221
C	6.24298	1.36958	-0.84636
C	5.70376	0.09726	-0.52835
C	6.5742	-1.00355	-0.3289
C	6.04032	-2.25121	-0.0298
H	6.71092	-3.08507	0.11565
C	5.3841	2.44334	-1.05268
H	5.80317	3.40758	-1.29923
C	8.02713	-0.83843	-0.44564
C	7.69223	1.55899	-0.96499
N	8.51971	0.45397	-0.6918
O	8.82136	-1.80615	-0.33169
O	8.19829	2.66331	-1.29115
C	9.99378	0.63683	-0.82967
H	10.37711	-0.28079	-1.26731
H	10.12154	1.44408	-1.54506
C	10.802	0.98039	0.44998
H	11.78963	1.23011	0.04197
C	11.00357	-0.20321	1.42754
H	11.44661	0.19432	2.34868
H	10.03278	-0.61596	1.70849
C	11.90312	-1.34618	0.91437
H	11.82251	-2.18506	1.61549
H	11.52105	-1.71932	-0.03959
C	13.39146	-0.97894	0.7704
H	13.50894	-0.1603	0.05368
H	13.76126	-0.6014	1.73048
C	14.25691	-2.16635	0.32031

H	13.92673	-2.5463	-0.65013
H	15.30732	-1.88184	0.22705
H	14.19647	-2.99003	1.03665
C	10.33176	2.26654	1.18632
H	10.10044	3.02998	0.44059
H	11.18772	2.64024	1.75852
C	9.14294	2.12324	2.15383
H	8.2413	1.76246	1.66
H	9.3692	1.43526	2.9704
H	8.90647	3.0922	2.59985
H	3.38155	3.15105	-1.11059
H	4.2994	-3.41828	0.31927
H	-1.5639	-2.00807	0.34001
C	-2.27068	0.37862	-0.21944
C	-3.48516	0.29774	-0.17079
C	-4.9019	0.2258	-0.10784
C	-5.65925	1.40072	0.1645
C	-5.566	-1.01643	-0.31291
C	-5.02778	2.66709	0.37383
C	-7.0994	1.32164	0.25157
C	-7.00767	-1.0804	-0.24156
C	-5.75975	3.79136	0.66408
H	-3.95113	2.72488	0.30392
C	-7.82029	2.51948	0.57802
C	-7.76489	0.08505	0.04596
C	-7.17624	3.71459	0.77534
H	-8.89365	2.46363	0.67375
H	-5.26065	4.73842	0.8182
H	-7.74261	4.60213	1.0225
C	-4.84116	-2.21278	-0.61119
H	-3.76407	-2.16097	-0.67406
C	-7.63849	-2.34438	-0.49721
H	-8.71601	-2.39541	-0.47212
C	-5.48562	-3.40435	-0.83183
H	-4.91585	-4.29552	-1.05728
C	-6.90594	-3.46977	-0.77851
H	-7.40611	-4.40932	-0.96991
C	-9.25491	0.01052	0.12824
C	-9.89819	-0.64007	1.19543
C	-10.07197	0.58519	-0.86064
C	-11.28591	-0.71458	1.28101
H	-9.30294	-1.09098	1.97948
C	-11.46098	0.5146	-0.79795
H	-9.61353	1.09028	-1.70146
C	-12.11207	-0.13861	0.28087
H	-11.72613	-1.21829	2.12762
H	-12.03838	0.96529	-1.59012
N	-13.49379	-0.21065	0.35417
C	-14.13881	-0.90016	1.47459
H	-15.21596	-0.85781	1.34434

H	-13.84611	-1.95314	1.52633
H	-13.89574	-0.43391	2.43428
C	-14.32136	0.40007	-0.68939
H	-14.13314	-0.0446	-1.67144
H	-15.3684	0.24619	-0.44665
H	-14.14754	1.47751	-0.76713

Table S3: Calculated energy of Kohn-Sham molecular orbitals (MO) of compound **3** by DFT using B3LYP/ 6-311G as basis-set

Molecular Orbitals (MOs)	Energy/ Hartree	Energy/ eV
LUMO+4	-0.04298	-1.169
LUMO+3	-0.05396	-1.468
LUMO+2	-0.05733	-1.560
LUMO+1	-0.08728	-2.375
LUMO	-0.12115	-3.297
HOMO	-0.19249	-5.238
HOMO-1	-0.20326	-5.531
HOMO-2	-0.21945	-5.971
HOMO-3	-0.25787	-7.017
HOMO-4	-0.26141	-7.113

Table S4: Summarization of theoretical data obtained from DFT calculations

Compound	**E_{HOMO}/ eV**	**E_{LUMO}/ eV**	**$\Delta E_{HOMO-LUMO}$ / eV**	**μ_g/ D**	**DA (PMI-Anth)**	**DA (Anth-R)**
1	-5.475	-3.299	2.176	11.09	18.4°	-
2	-5.470	-3.308	2.162	11.44	20.8°	88°
3	-5.238	-3.297	1.941	15.64	24.3°	71°

DA (PMI-Anth): dihedral angle between PMI and anthracene planes

DA (Anth-R): dihedral angle between anthracene and phenyl (**2**)/ N, N-dimethyl phenyl (**3**)

Symbolic Z-matrix for the optimized configuration of **1-Ep**

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

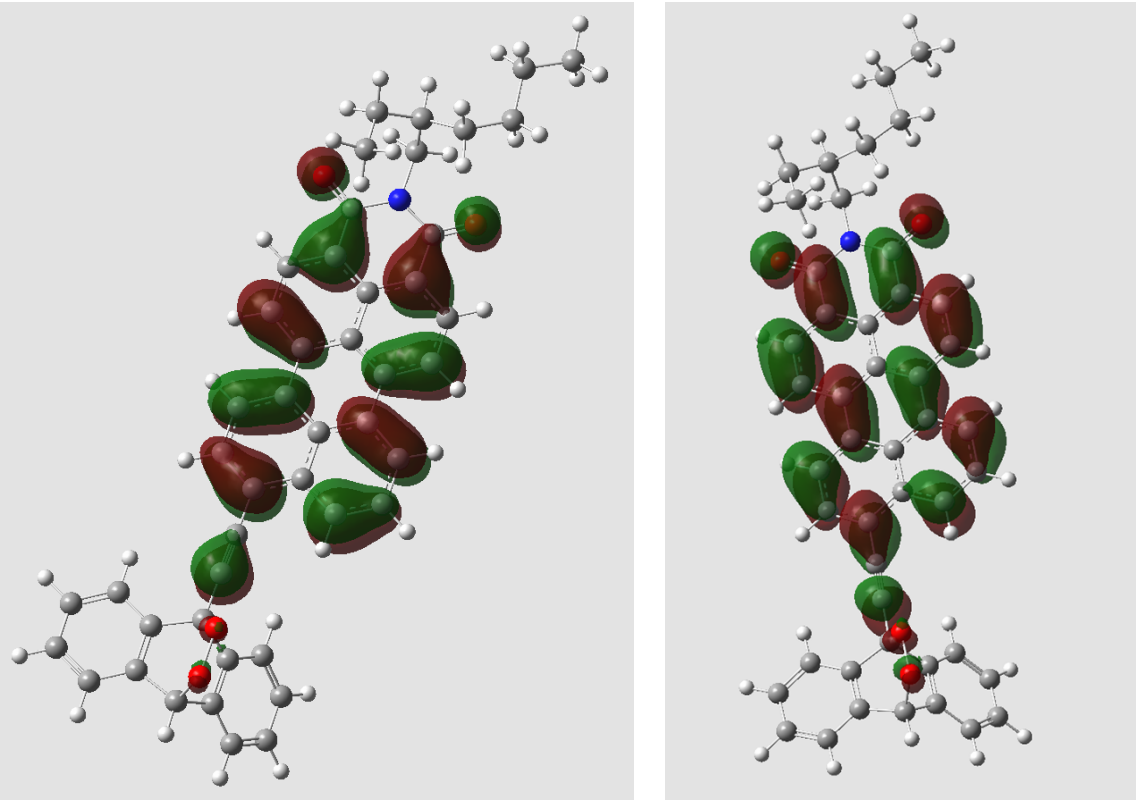
C	-0.13464	-2.80309	0.46982
C	0.41092	-1.56468	0.13267
C	-0.47002	-0.44716	-0.05499
C	-1.88425	-0.63552	0.10894
C	-2.38158	-1.91824	0.45356
C	-1.51922	-2.97944	0.62912

H	0.50425	-3.65945	0.61778
C	0.03939	0.84778	-0.40122
C	-2.77104	0.48171	-0.07457
H	-1.9036	-3.95467	0.89177
C	-2.24069	1.7251	-0.40574
C	-0.86257	1.89983	-0.56647
H	-2.90325	2.56721	-0.54182
H	-0.51173	2.88649	-0.82395
C	1.48799	1.03663	-0.56859
C	1.86173	-1.37644	-0.03203
C	2.36526	-0.07931	-0.37364
C	2.77444	-2.42479	0.1327
C	2.04448	2.27421	-0.9133
C	4.29475	1.38005	-0.87227
C	3.77647	0.10537	-0.53035
C	4.66232	-0.98618	-0.34914
C	4.14922	-2.23532	-0.0249
H	4.83071	-3.06253	0.10687
C	3.42254	2.44403	-1.06345
H	3.82557	3.41016	-1.32825
C	6.11055	-0.80898	-0.51011
C	5.74076	1.5826	-1.02814
N	6.58491	0.48741	-0.77147
O	6.91497	-1.76951	-0.41867
O	6.22577	2.69034	-1.37055
C	8.05382	0.68442	-0.94353
H	8.43591	-0.22967	-1.38948
H	8.15736	1.49233	-1.66207
C	8.8865	1.03636	0.31808
H	9.86324	1.29254	-0.11146
C	9.11702	-0.14411	1.29311
H	9.57405	0.25863	2.20502
H	8.15529	-0.56438	1.59348
C	10.01609	-1.28032	0.76434
H	9.9557	-2.11888	1.46783
H	9.61926	-1.65797	-0.18182
C	11.49828	-0.90084	0.59174
H	11.59511	-0.08053	-0.12616
H	11.88365	-0.52124	1.54484
C	12.36449	-2.08058	0.12342
H	12.01943	-2.4615	-0.84147
H	13.4107	-1.78754	0.0112
H	12.32394	-2.90597	0.83918
C	8.42273	2.32035	1.06242
H	8.16923	3.08125	0.32126
H	9.2885	2.70127	1.61468
C	7.2574	2.16962	2.05706
H	6.34625	1.80517	1.58382
H	7.50612	1.48149	2.86691
H	7.0265	3.1367	2.50995

H	1.41195	3.13286	-1.07097
H	2.42936	-3.41366	0.38823
H	-3.4459	-2.05231	0.57966
C	-4.17922	0.33011	0.07615
C	-5.37798	0.2159	0.20403
C	-6.80614	0.07266	0.3785
C	-7.63748	1.3315	0.20172
C	-7.4618	-1.09856	-0.33295
C	-7.18166	2.57823	-0.21632
C	-8.9851	1.14609	0.55728
C	-8.81145	-1.26456	0.02437
C	-8.0895	3.64348	-0.2963
H	-6.14345	2.72183	-0.48143
C	-9.88184	2.20959	0.49776
C	-9.28041	-0.24988	1.02821
C	-9.42953	3.46129	0.05791
H	-10.91596	2.0693	0.78272
C	-6.85173	-1.98103	-1.21966
H	-5.81188	-1.85692	-1.488
C	-9.55565	-2.31626	-0.50336
H	-10.59094	-2.4495	-0.21932
C	-7.60699	-3.02806	-1.76639
H	-7.14559	-3.71064	-2.4665
C	-8.94882	-3.19494	-1.41155
H	-9.52224	-4.00648	-1.83768
O	-6.94509	-0.27235	1.90267
O	-8.42291	-0.46417	2.26973
H	-7.74783	4.61247	-0.63292
H	-10.12124	4.28988	-0.00522
H	-10.29179	-0.40386	1.39443

Table S5: Calculated energy of Kohn-Sham molecular orbitals (MO) of **1-Ep** by DFT using B3LYP/ 6-311G as basis-set

Molecular Orbitals (MOs)	Energy/ Hartree	Energy/ eV
LUMO+4	-0.04510	-1.227
LUMO+3	-0.05405	-1.470
LUMO+2	-0.05553	-1.511
LUMO+1	-0.07457	-2.029
LUMO	-0.12316	-3.351
HOMO	-0.21578	-5.871
HOMO-1	-0.25491	-6.936
HOMO-2	-0.25546	-6.951
HOMO-3	-0.26974	-7.340
HOMO-4	-0.27268	-7.420



E_{HOMO} = -5.871 eV E_{LUMO} = -3.351 eV

Fig. S31 Representation of HOMO and LUMO electronic distributions for compound **1-EP**.

Symbolic Z-matrix for the optimized configuration of **2-Ep**

Symbolic Z-matrix:
Charge =0 and Multiplicity = 1

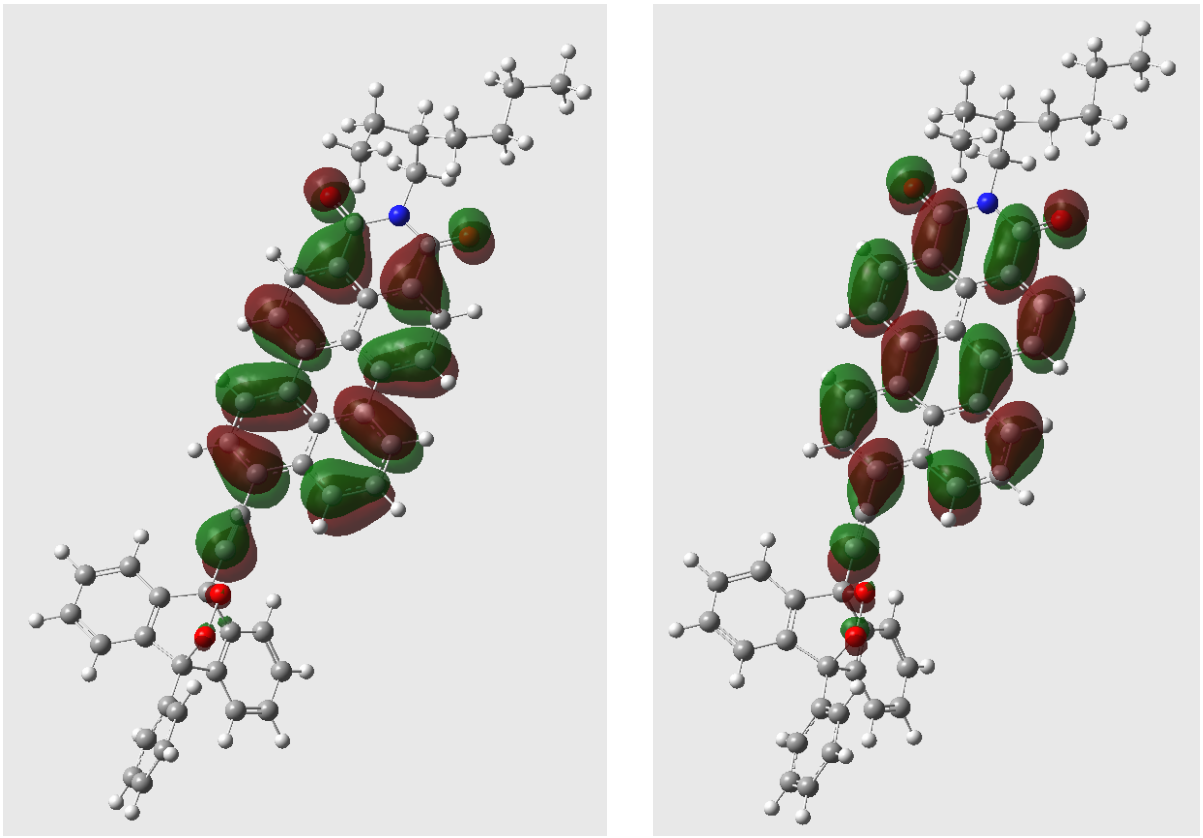
C	1.03441	-2.73487	0.29471
C	1.61827	-1.50023	0.01241
C	0.76855	-0.35974	-0.18106
C	-0.65452	-0.52185	-0.07812
C	-1.1916	-1.80215	0.21155
C	-0.35882	-2.88567	0.39346
H	1.6492	-3.60834	0.44495
C	1.31758	0.93211	-0.47403
C	-1.51007	0.61869	-0.26625
H	-0.77336	-3.8589	0.61425
C	-0.94178	1.85953	-0.53816
C	0.44496	2.0083	-0.64122
H	-1.58092	2.71939	-0.6754
H	0.82603	2.99389	-0.85634
C	2.77468	1.09191	-0.58892
C	3.07795	-1.33926	-0.09106
C	3.62063	-0.04695	-0.388
C	3.96208	-2.40956	0.08781
C	3.36881	2.323	-0.8912
C	5.59638	1.37761	-0.79744
C	5.03993	0.10931	-0.49428

C	5.89572	-1.00417	-0.30212
C	5.34528	-2.24699	-0.01716
H	6.00413	-3.09086	0.12377
C	4.75424	2.46432	-0.99552
H	5.18654	3.42548	-1.23051
C	7.35199	-0.85638	-0.41231
C	7.05029	1.54912	-0.91032
N	7.86225	0.43156	-0.64625
O	8.13241	-1.83487	-0.30375
O	7.5693	2.64988	-1.22437
C	9.33905	0.59613	-0.78142
H	9.71041	-0.32265	-1.22679
H	9.47772	1.40761	-1.48994
C	10.15057	0.91786	0.50175
H	11.13983	1.16482	0.09612
C	10.34359	-0.27953	1.46416
H	10.79165	0.10272	2.3893
H	9.36988	-0.68756	1.74184
C	11.23226	-1.4236	0.93474
H	11.14623	-2.27032	1.62566
H	10.84485	-1.78172	-0.02287
C	12.72329	-1.06729	0.79116
H	12.84598	-0.2419	0.08314
H	13.09846	-0.70339	1.7544
C	13.57776	-2.25684	0.32609
H	13.24226	-2.62363	-0.6476
H	14.63024	-1.97992	0.23331
H	13.51229	-3.0877	1.03363
C	9.691	2.19836	1.25453
H	9.46485	2.97309	0.51892
H	10.55051	2.55819	1.83019
C	8.50248	2.05189	2.22201
H	7.59737	1.70349	1.72551
H	8.72502	1.35248	3.02981
H	8.27365	3.01702	2.68007
H	2.76043	3.19826	-1.0526
H	3.58743	-3.39511	0.31253
H	-2.26273	-1.91664	0.29097
C	-2.92624	0.48966	-0.18538
C	-4.13126	0.38882	-0.12376
C	-5.56854	0.2501	-0.03917
C	-6.37503	1.52913	-0.09209
C	-6.19559	-0.81238	-0.9159
C	-5.86363	2.80572	-0.30892
C	-7.74289	1.33458	0.17251
C	-7.56311	-1.01326	-0.6558
C	-6.72925	3.90563	-0.27449
H	-4.80904	2.94385	-0.50202
C	-8.59467	2.43698	0.23672
C	-8.11285	-0.11787	0.44738

C	-8.08608	3.72106	0.00094
H	-9.64156	2.30663	0.46514
C	-5.52643	-1.58643	-1.86015
H	-4.47364	-1.42731	-2.04635
C	-8.25378	-2.01397	-1.33886
H	-9.29713	-2.19716	-1.13157
C	-6.23228	-2.56883	-2.5652
H	-5.72381	-3.16496	-3.3101
C	-7.58725	-2.78258	-2.30217
H	-8.1283	-3.54786	-2.84127
C	-9.55478	-0.36963	0.84712
C	-9.89357	-0.84498	2.12156
C	-10.57892	-0.12147	-0.08323
C	-11.23265	-1.06829	2.45842
H	-9.11803	-1.03952	2.84559
C	-11.91463	-0.34549	0.25711
H	-10.33679	0.24571	-1.07124
C	-12.24614	-0.82012	1.53015
H	-11.47888	-1.43534	3.44557
H	-12.6911	-0.14974	-0.46974
H	-13.28067	-0.99341	1.79329
O	-5.78738	-0.27853	1.41837
O	-7.27345	-0.49121	1.68514
H	-6.34274	4.89889	-0.45563
H	-8.75107	4.57279	0.03706

Table S6: Calculated energy of Kohn-Sham molecular orbitals (MO) of **2-Ep** by DFT using B3LYP/ 6-311G as basis-set

Molecular Orbitals (MOs)	Energy/ Hartree	Energy/ eV
LUMO+4	-0.04511	-1.227
LUMO+3	-0.05466	-1.487
LUMO+2	-0.05557	-1.512
LUMO+1	-0.07405	-2.015
LUMO	-0.12308	-3.349
HOMO	-0.21578	-5.871
HOMO-1	-0.25604	-6.967
HOMO-2	-0.25687	-6.989
HOMO-3	-0.26620	-7.243
HOMO-4	-0.26732	-7.274



E_{HOMO} = -5.871 eV E_{LUMO} = -3.349 eV

Fig. S32 Representation of HOMO and LUMO electronic distributions for compound **2-EP**.

Symbolic Z-matrix for the optimized configuration of **3-Ep**

Symbolic Z-matrix:
Charge = 0 and Multiplicity = 1

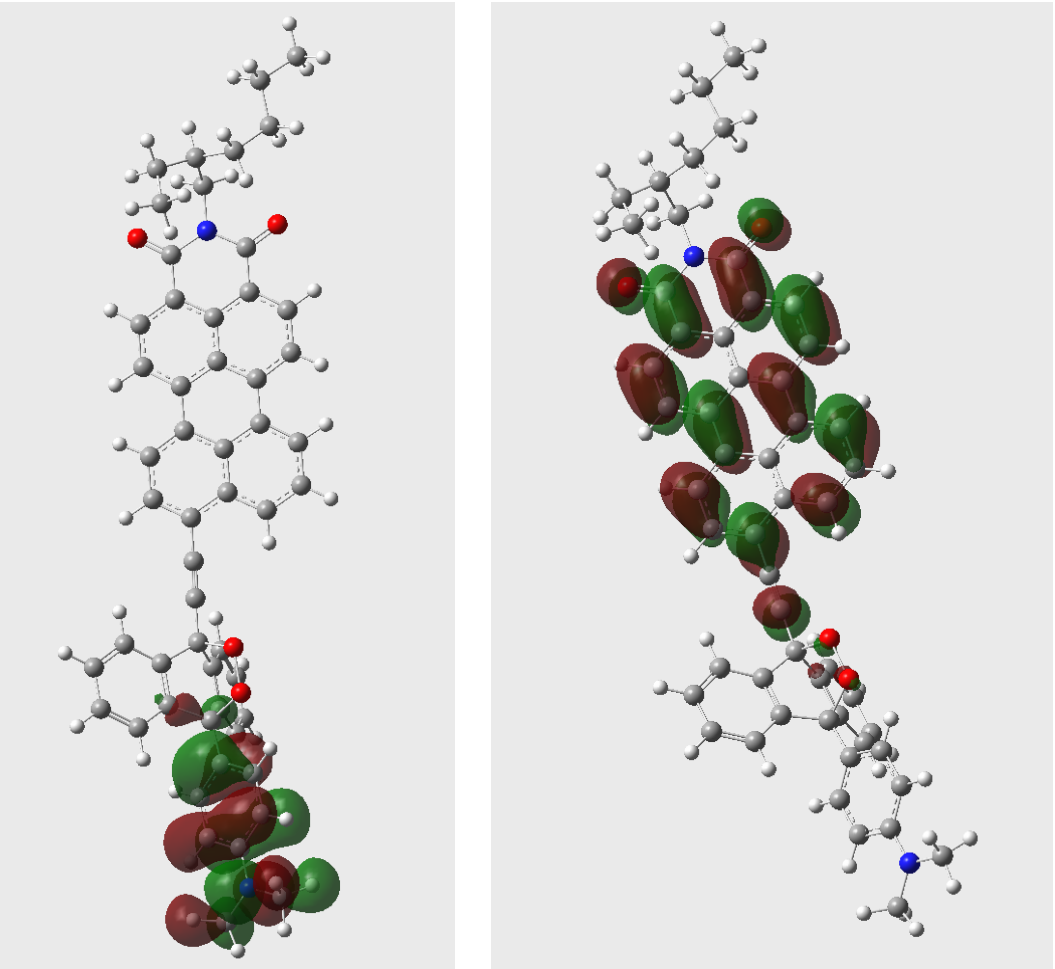
C	1.74049	-2.78748	0.32416
C	2.30552	-1.54976	0.0144
C	1.43979	-0.42366	-0.1931
C	0.01894	-0.60339	-0.08264
C	-0.49577	-1.88325	0.2411
C	0.35132	-2.95375	0.4396
H	2.36855	-3.64925	0.48678
C	1.97221	0.87064	-0.50356
C	-0.8603	0.51921	-0.29274
H	-0.04949	-3.92623	0.68762
C	-0.30149	1.76615	-0.57894
C	1.08102	1.93256	-0.68051
H	-0.95181	2.61474	-0.73342
H	1.44843	2.92096	-0.90789
C	3.42353	1.04909	-0.62457
C	3.76182	-1.37192	-0.1008
C	4.28658	-0.07641	-0.41469
C	4.66081	-2.43031	0.0836
C	4.00226	2.28574	-0.94221

C	6.24298	1.36958	-0.84636
C	5.70376	0.09726	-0.52835
C	6.5742	-1.00355	-0.3289
C	6.04032	-2.25121	-0.0298
H	6.71092	-3.08507	0.11565
C	5.3841	2.44334	-1.05268
H	5.80317	3.40758	-1.29923
C	8.02713	-0.83843	-0.44564
C	7.69223	1.55899	-0.96499
N	8.51971	0.45397	-0.6918
O	8.82136	-1.80615	-0.33169
O	8.19829	2.66331	-1.29115
C	9.99378	0.63683	-0.82967
H	10.37711	-0.28079	-1.26731
H	10.12154	1.44408	-1.54506
C	10.802	0.98039	0.44998
H	11.78963	1.23011	0.04197
C	11.00357	-0.20321	1.42754
H	11.44661	0.19432	2.34868
H	10.03278	-0.61596	1.70849
C	11.90312	-1.34618	0.91437
H	11.82251	-2.18506	1.61549
H	11.52105	-1.71932	-0.03959
C	13.39146	-0.97894	0.7704
H	13.50894	-0.1603	0.05368
H	13.76126	-0.6014	1.73048
C	14.25691	-2.16635	0.32031
H	13.92673	-2.5463	-0.65013
H	15.30732	-1.88184	0.22705
H	14.19647	-2.99003	1.03665
C	10.33176	2.26654	1.18632
H	10.10044	3.02998	0.44059
H	11.18772	2.64024	1.75852
C	9.14294	2.12324	2.15383
H	8.2413	1.76246	1.66
H	9.3692	1.43526	2.9704
H	8.90647	3.0922	2.59985
H	3.38155	3.15105	-1.11059
H	4.2994	-3.41828	0.31927
H	-1.5639	-2.00807	0.34001
C	-2.27068	0.37862	-0.21944
C	-3.48516	0.29774	-0.17079
C	-4.9019	0.2258	-0.10784
C	-5.65925	1.40072	0.1645
C	-5.566	-1.01643	-0.31291
C	-5.02778	2.66709	0.37383
C	-7.0994	1.32164	0.25157
C	-7.00767	-1.0804	-0.24156
C	-5.75975	3.79136	0.66408
H	-3.95113	2.72488	0.30392

C	-7.82029	2.51948	0.57802
C	-7.76489	0.08505	0.04596
C	-7.17624	3.71459	0.77534
H	-8.89365	2.46363	0.67375
H	-5.26065	4.73842	0.8182
H	-7.74261	4.60213	1.0225
C	-4.84116	-2.21278	-0.61119
H	-3.76407	-2.16097	-0.67406
C	-7.63849	-2.34438	-0.49721
H	-8.71601	-2.39541	-0.47212
C	-5.48562	-3.40435	-0.83183
H	-4.91585	-4.29552	-1.05728
C	-6.90594	-3.46977	-0.77851
H	-7.40611	-4.40932	-0.96991
C	-9.25491	0.01052	0.12824
C	-9.89819	-0.64007	1.19543
C	-10.07197	0.58519	-0.86064
C	-11.28591	-0.71458	1.28101
H	-9.30294	-1.09098	1.97948
C	-11.46098	0.5146	-0.79795
H	-9.61353	1.09028	-1.70146
C	-12.11207	-0.13861	0.28087
H	-11.72613	-1.21829	2.12762
H	-12.03838	0.96529	-1.59012
N	-13.49379	-0.21065	0.35417
C	-14.13881	-0.90016	1.47459
H	-15.21596	-0.85781	1.34434
H	-13.84611	-1.95314	1.52633
H	-13.89574	-0.43391	2.43428
C	-14.32136	0.40007	-0.68939
H	-14.13314	-0.0446	-1.67144
H	-15.3684	0.24619	-0.44665
H	-14.14754	1.47751	-0.76713

Table S7: Calculated energy of Kohn-Sham molecular orbitals (MO) of **3-Ep** by DFT using B3LYP/ 6-311G as basis-set

Molecular Orbitals (MOs)	Energy/ Hartree	Energy/ eV
LUMO+4	-0.04485	-1.220
LUMO+3	-0.05510	-1.499
LUMO+2	-0.05775	-1.571
LUMO+1	-0.07034	-1.914
LUMO	-0.12215	-3.324
HOMO	-0.19772	-5.380
HOMO-1	-0.21513	-5.854
HOMO-2	-0.25469	-6.930
HOMO-3	-0.25547	-6.951
HOMO-4	-0.26201	-7.129



E_{HOMO} = -5.380 eV E_{LUMO} = -3.324 eV

Fig. S33 Representation of HOMO and LUMO electronic distributions for compound **3-EP**.

Table S8: Thermodynamic feasibility of $^1O_2$ reaction for compounds **1-3**

Compound	E_{Comp}/ eV	E_{EP}/ eV	E_{EP} - E_{Comp}/ eV	ΔE^a/ eV
1	-53856.8745	-57947.1918	-4090.3173	-2.201
2	-60143.9423	-64234.2161	-4090.2738	-2.158
3	-63789.1956	-67879.4776	-4090.282	-2.166

ΔE^a is calculated by following this equation: $\Delta E^a = E_{EP} - E_{Comp} - E(^1O_2)$; $E(^1O_2)$ = -4088.1158 eV

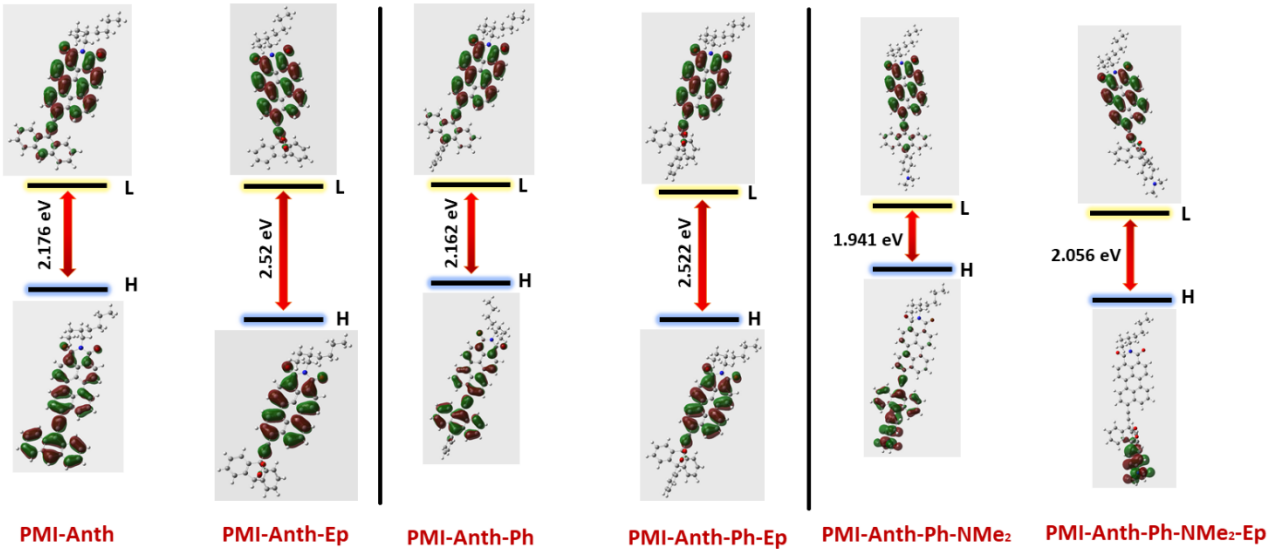


Fig. S34 Orbital picture and the band gap of compound **1-3** and their corresponding endoperoxides.

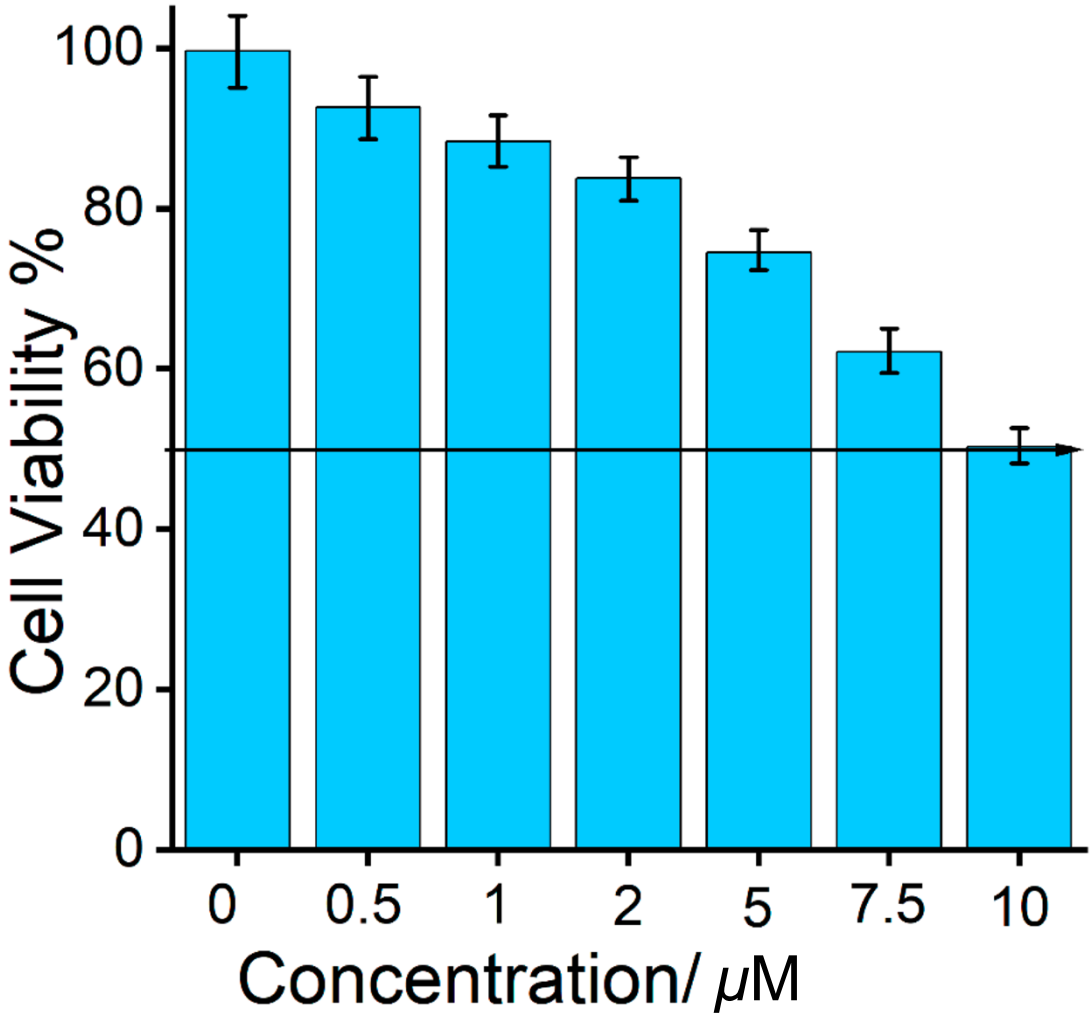


Fig. S35 MTT assay showing cell viability in the presence of compound **2** (0–10 μM).

Spectral scanning experiment:

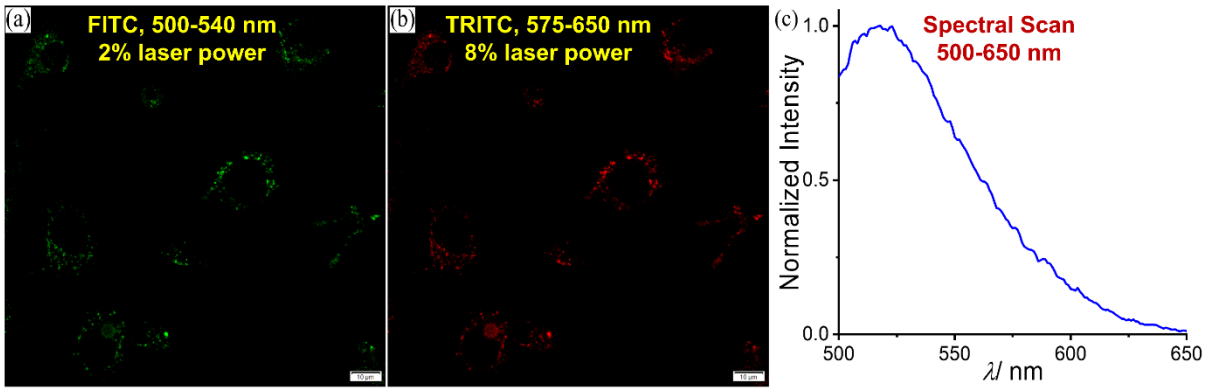


Fig. S36 CLSM images of live HepG2 cells stained with 2 μM **2** in (a) FITC, and (b) TRITC channel; (c) spectral scanning performed in lambda mode in the live cells shows the emission profile of the compound **2**.

Note: The probe of interest has emissions both in the green and red channels. Hence, we have performed a spectral scanning experiment in live cells stained with compound **2**. It is evident from the intensity profile in **Fig S36** that the probe gives maximum emission in the green channel. This fact could be supported by the laser power required to image the individual channels 2% for the green channel while 8% for the red channel, suggesting a much weaker red emission of the probe inside cells. Now, the colocalization experiment was performed using the commercially available tracker LipidSpot 610 which was excited by a 594 nm laser with only 0.5% laser power in a sequential scanning mode. The low laser power was only enough to excite LipidSpot 610 while the sequential scanning ensured zero crosstalk between imaging channels.

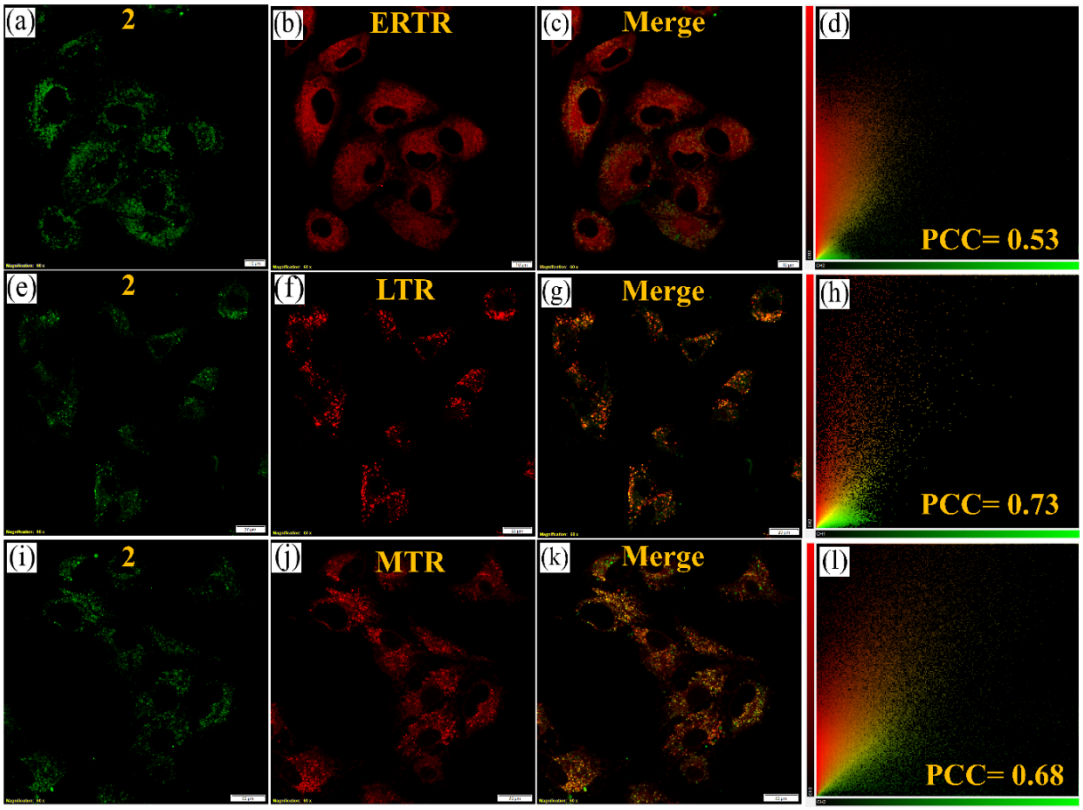


Fig. S37 Confocal live-cell co-localization experiments in HepG2 cells. (a), (e), and (i) show FITC channel images stained with 2 μM **2**; (b), (f) and (j) show the TRITC channel images stained with 0.3 μM ER-Tracker Red 0.3 μM LysoTracker Red, and 0.3 μM MitoTracker Red; (c), (g), and (k) show the corresponding merge images, (d), (h), and (l) show the scatter plot to get the respective Pearson's correlation coefficients. (a-c: scale bar: 10 μm, e-g and i-k: scale bar: 20 μm).

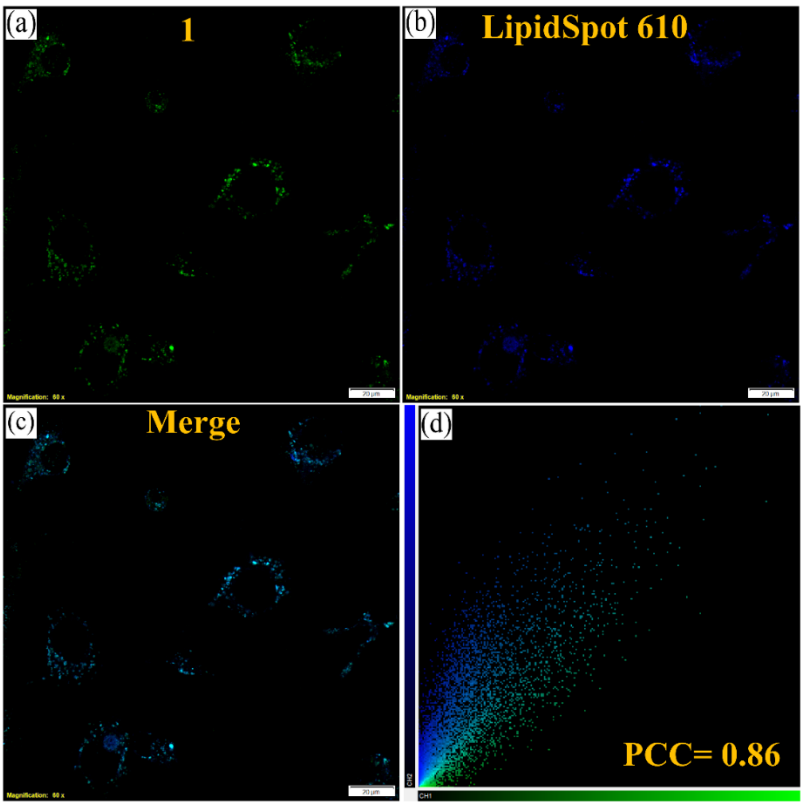


Fig. S38 CLSM images of HepG2 cells stained with (a) 2 μM **1**, (b) 0.5 μM of LipidSpot 610, (c) merge image of (a) and (b), (d) scatter plot showing Pearson's correlation coefficient of 0.86 ± 0.02.

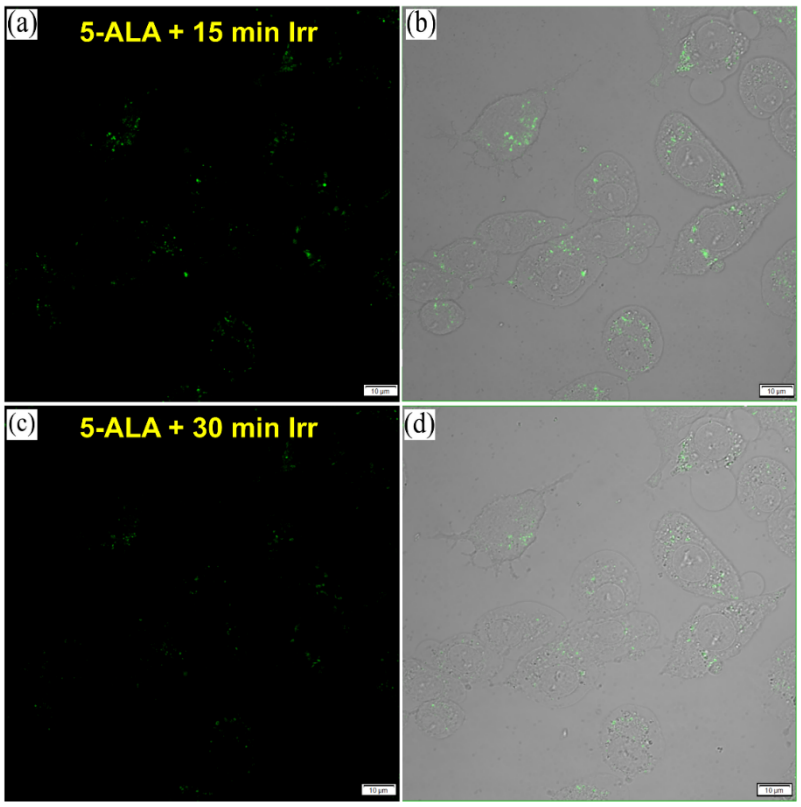


Fig. S39 CLSM images of live HepG2 cells treated with 1 mM 5-ALA for 4 h and stained with 2 μM **2**. (a) and (c) show FITC channel images at different irradiation time; (b) and (d) are the corresponding merge images with DIC.

Note: In order to detect singlet oxygen at the cellular level, 5-aminolevulinic acid (5-ALA) was used as the photosensitizer as it is known to cause the accumulation of protoporphyrin IX in the mitochondria of cancer cells which generates singlet oxygen upon light irradiation. However, in our case, the probe of interest is localizing in the lipid droplets while the 5-ALA induced $^1O_2$ generation occurs in mitochondria. Hence, we could not get a conclusive result as can be seen in **Fig. S39**. The experiment was performed by treating the live HepG2 cells with 1 mM 5-ALA and staining with 2 μM probe **2**. From the confocal microscopy images, no changes in fluorescence signal could be observed.