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Electronic Supplementary Information (ESI)

Sequential oxidation of sulfur annulated perylenediimide: An efficient strategy to generate ultra-stable radical anions and dianions †

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Chemicals

All the solvents and reagents were purchased from commercial sources and were used as received. Perylene-3,4,9,10-tetracarboxylic dianhydride, 2-ethylhexylamine, cerium (IV) ammonium nitrate (CAN), sulfur powder, N-methyl-2-pyrrolidone (NMP), sodium sulfate, *meta*-chloroperoxybenzoic acid (*m*CPBA) and tetrabutylammonium hexafluorophosphate ($TBAPF_6$) were purchased from Sigma. Imidazole and CrO_3 were purchased from Sisco Research Laboratories (SRL). Sodium nitrite was purchased from VETEC sigma, concentrated nitric acid and H_2O_2 were purchased from SDFCL. Triethylamine (TEA), diethylamine (DEA) and H_5IO_6 were purchased from Spectrochem. All the spectroscopic grade solvents like dichloromethane (DCM), chloroform and tetrahydrofuran (THF) used for UV-Vis. absorption and fluorescence spectroscopy were obtained from SRL. *N, N*-dimethylformamide (DMF) was purchased from Sigma. Thin Layer chromatography (TLC) analyses were carried out by using Merck TLC Silica gel 60 F_{254}. Column chromatography was performed on silica gel (230-400 mesh size), purchased from Rankem.

Experimental

Steady-state Measurements

The stock solutions of 1 mM concentration of compounds were made in dichloroethane (DCE) and diluted as required in the experiments. All steady-state absorption measurements were carried out using Shimadzu 1800 UV-spectrophotometer using 1 cm path length quartz cuvettes. All steady-state fluorescence measurements were carried out using HORIBA Jobin Yvon Fluorolog fluorimeter. Absolute fluorescence quantum yield measurement was also performed in integrating sphere using HORIBA Jobin Yvon Fluorolog fluorimeter. The data were plotted with the help of Origin 8.0 software. Fluorescence spectra were recorded using 1 cm path length quartz cuvette and keeping both excitation and emission slit at 2 nm. All the experiments were carried out at ambient temperature

(298 K) unless otherwise mentioned. In all the experiments related to light irradiation was performed by exposure visible light using a Luzchem photoreactor having cooled fluorescent lamp. The intensity of light used was ~960 lx (measured with a lux meter) and wavelength range lie between 400-700 nm.

Spectroscopic investigations of radical anions were done at 10 μM concentration of compounds in DMF. When other reducing agents were used, the same was done in 10 μM concentration of compounds in solvents with a certain concentration of reducing agent/ electron donating species.

Nuclear Magnetic Resonance Spectroscopy and Mass Spectrometry

^{1}H NMR spectra were recorded on Bruker 500 MHz spectrometer and ^{13}C NMR spectra were recorded on Bruker 700 MHz spectrometer in $CDCl_3$ solvent. Chemical shifts were reported in ppm scale with respect to tetramethylsilane (TMS) (δ = 0.00 ppm). The residual solvents' peaks were assigned as reported in literature.[1] The mass spectra for all the compounds were recorded using atmospheric pressure chemical ionization (APCI) in chloroform solvent.

Density Functional Theory (DFT) Calculations

The structures of the molecules were optimized by DFT using the B3LYP density functional with basis set 6-31G(d). Quantum chemical calculation was performed with the Gaussian 16 package.[2] Optimization and calculation of frontier orbital energies were carried out using DCM as solvent. Structures were visualized using Mercury 3.8 software.

Electron Paramagnetic Resonance Spectroscopy

The samples required for EPR spectroscopy were prepared in DMF and chloroform with and/ or without reducing agent *i.e.,* TEA at 30 μM concentration of compounds. The measurements were recorded at a temperature of 150 K. Modulation amplitude was set to 1. Time constant was set to

24. All the EPR spectra was measured in Microwave frequency of 9.4 GHz at the X-band on a Bruker BioSpin GmbH spectrometer. The Lande factor, *g* was calculated using:

$$g = \frac{h.v}{H_{\circ}.\beta}$$

$$\Rightarrow g = \frac{6716.1496}{H_{\circ}}$$

h being Planck's constant

v is the operating frequency (9.4 GHz for X-band)

$H_{\circ}$ is magnetic field (Gauss)

β is the Bohr Magneton

Time-resolved Fluorescence Lifetime Measurement

Time-resolved fluorescence experiments were performed using the time-correlated single-photon counting (TCSPC) technique. The fluorescence lifetime of time-resolved fluorescence measurement was carried out using time-correlated single-photon counting (TCSPC) setup from a Hamamatsu MCP photomultiplier (R-23809U-50). For **SAN-PDI** (460 nm) while for **1**, **2**, and **3** (509 nm) picosecond laser was used as an excitation source for the lifetime measurements and the photon count was set up to 10,000. The instrument response function (IRF) was measured using a dilute suspension of Ludox (Sigma Aldrich) before starting the measurement. The emission polarizer was fixed at a magic angle (54.7 ^{o}) with respect to the excitation polarizer. The decay was determined by using the deconvolution method supplied by EZ time software. The fitting parameter (chi-square value (χ^2)) is considered in the range from 0.9-1.2. Lifetime measurement by TCSPC was performed at room temperature (298 K) using a very dilute solution with O.D. less than 0.1

Electrochemical Measurements

Spectro-electrochemistry Experiment

Absorption spectra were taken using an HR 4000 spectrophotometer developed by Ocean Optics along with a 1 cm cuvette holder and a DT-MINI-2-GS UV-Vis.-NIR light source. A CH electrochemical analyzer was used to hold the samples at desired potentials. A Pt working electrode, Ag/AgCl as reference electrode, and a Pt counter electrode were also used in this measurement. Supporting electrolyte used was 0.1 M tetrabutylammonium hexafluorophosphate ($TBAPF_6$) in dry chloroform solvent.

Cyclic Voltammetry (CV) Experiment

Cyclic voltammetry experiments of **SAN-PDI**, **1**, **2**, and **3** were performed in dry chloroform solvent using a BioLogic SP-300 potentiostat (BioLogic, France) in a three-electrode setup at room temperature (25 ^{o}C). In this experiment, working, counter and reference electrodes were glassy carbon disc (3 mm in diameter), platinum wire, and standard calomel electrode (SCE) electrode, respectively.

Half-life ($t_{1/2}$) Calculations for Dianionic Species

(i) **For compound 1:**

Since absorbance at 693 nm decrease from 0.23 to 0.22 in = 170 days

Hence absorbance decreases per day = 0.01/170 = 5.8 x 10^{-5} per day

Since 5.8 x 10^{-5} decrease in absorbance takes = 1 day

Hence, decrease in absorbance to 0.115 (half of the absorbance) will take = 0.115/ 5.8 x 10^{-5} days = 1982 days = 5.4 years

(ii) **For compound 2:**

Since absorbance at 675 nm decrease from 0.093 to 0.091 in = 160 days

Hence absorbance decreases per day = 0.002/160 = 1.25 x 10^{-5} per day

Since 1.25 x 10^{-5} decrease in absorbance takes = 1 day

Hence, decrease in absorbance to 0.047 (half of the absorbance) will take = 0.047/ 1.25 x 10^{-5} days = 4177 days = 11.4 years

(iii) **For compound 3:**

Since absorbance at 725 nm decrease from 0.11998 to 0.11899 in = 155 days

Hence absorbance decreases per day = 0.001/155 = 6.45 x 10^{-6} per day

Since 6.45 x 10^{-6} decrease in absorbance takes = 1 day

Hence, decrease in absorbance to 0.06 (half of the absorbance) will take = 0.06/ 6.45 x 10^{-6} days = 93023 days = 25.4 years

Synthesis of Precursor Molecules (**1, 2**, and **3)**

Synthesis of SAN-PDI

As reported by Langhals *et al*,[3] the mixture of perylene-3,4,9,10-tetracarboxylic dianhydride (**PDA**) (500 mg, 1.27 mmol) and 2-ethylhexylamine (388 mg, 2.99 mmol) was heated at 140 °C in presence of imidazole (6.9 g) for 4 h. Before cooling it down, ethanol (25 mL) was added to dissolve imidazole followed by the addition of 2 M hydrochloric acid (10 mL). The reaction mixture was then allowed to cool down for 1 h. Thereafter, it was vacuum filtered and purified by column

chromatography using chloroform as mobile phase to obtain orange fluorescent crystalline product 2-ethylhexyl perylene diimide (**PDI**) in **87%** yield.

In the next step, to activate *bay* position of the perylene core, nitro groups were introduced at the said positions to get **1,6-** and **1,7-dinitro PDI,** as reported.[4] **PDI** (200 mg, 0.36 mmol), sodium nitrite (30 mg, 0.44 mmol) and concentrated nitric acid (1 mL, 24.5 mmol) were added in 40 mL of DCM. The mixture was stirred at room temperature for 4 h. The reaction was monitored with TLC. After completion, the reaction mixture was neutralized with 15% KOH (aqueous solution) and further extracted with DCM and dried over Na_2SO_4 to yield mono nitrated PDI derivative in **78%** yield. It was further nitrated using 2 equivalents cerium (IV) ammonium nitrate (CAN), and excess of conc. nitric acid (120 equivalents) in DCM solvent. The reaction mixture was stirred at room temperature for 48 h followed by neutralization using 15% KOH (aqueous solution). It was further extracted with DCM and dried over Na_2SO_4 to yield **35%** di-nitrated products (**1,7-Dinitro PDI** and **1,6-Dinitro PDI** in 3:1 ratio) after purifying by column chromatography using DCM as mobile phase.[4]

Without further purification/separation of dinitro products (**1,7-Dinitro PDI** and **1,6-Dinitro PDI**), **SAN-PDI** was synthesized. As reported by Tang and co-workers,[5] Sulfur powder (82 mg, 2.54 mmol) was dissolved in NMP (22 mL) at 70 °C under inert atmosphere for 30 minutes. After it dissolved, dinitro PDI derivative (200 mg, 0.25 mmol) was added to it. The temperature was raised to 190 °C and the reaction mixture was stirred for 4 h. After the completion observed from TLC and color change (dark red to dark green), 2 M HCl was added to the mixture and stirred for 5 minutes. The precipitate was filtered using vacuum filtration and purified with column chromatography using DCM as eluent to obtain **SAN-PDI** in **52%** yield. Other possible sulfur annulated products were not isolated. **SAN-PDI** was characterized using ^{1}H NMR, ^{13}C NMR and APCI-HRMS.

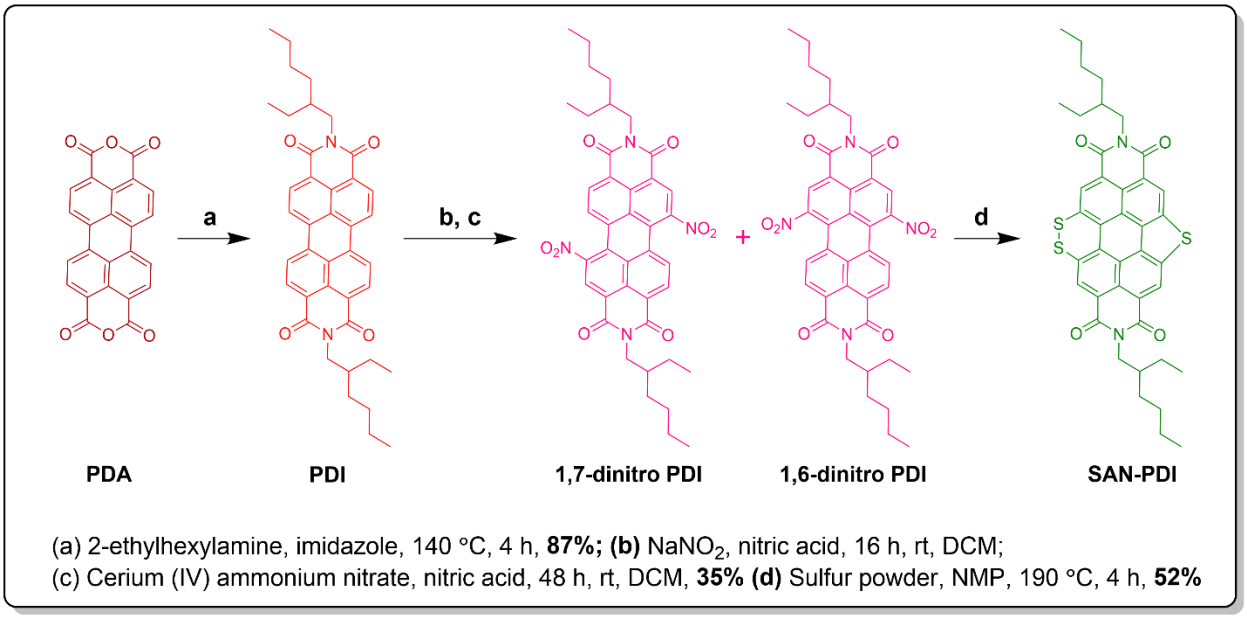
SAN-PDI:

^{1}H NMR (500 MHz, $CDCl_3$):

δ 9.12 (s, 2H), 8.53 (s, 2H), 4.24 – 4.11 (m, J = 13.2, 7.4 Hz, 4H), 2.01 – 1.91 (m, 2H), 1.47 – 1.28 (m, 16H), 0.96 (t, J = 7.4 Hz, 6H), 0.90 (t, J = 7.0 Hz, 6H)

^{13}C NMR (175 MHz, $CDCl_3$):

δ 163.73, 162.90, 139.21, 132.08, 130.73, 129.97, 128.22, 127.24, 125.11, 125.08, 123.70, 123.67, 123.00, 122.74, 122.63, 96.13, 44.70, 38.01, 30.74, 28.69, 24.06, 23.11, 14.14, 10.66



Scheme S1: Synthesis of **SAN-PDI**

Synthesis of 1, 2 and 3 (Scheme 2)

In an inert atmosphere, **SAN-PDI** (10 mg) was dissolved in 3 mL DCM. In the mixture, *m*CPBA (73 mg, 9 equivalents) was added. The reaction mixture was allowed to stir at room temperature for 2h. Quick color change from dark green to red was observed at the beginning. After completion of the reaction (from TLC), the mixture was extracted in DCM while side product benzoic acid was separated in water. DCM layer was dried under reduced pressure and the residue was purified

with column chromatography with DCM: Hexane (2:1) as mobile phase. Compound **1** was obtained as red powder in **40%** yield. With same procedure, **2O-SAN-PDI (2)** and **3O-SAN-PDI (3)** were synthesized using 50 equivalents *m*CPBA in 2 h and 12 h and isolated in **23%** and **35%** yield, respectively (see **Table S1**). All the isolated compounds **1**, **2**, and **3** were characterized using ^{1}H NMR, ^{13}C NMR and APCI-HRMS while compounds **4**, **5**, and **6** were not isolated but were characterized by APCI-HRMS in crude reaction mixture.

^{1}H NMR (500 MHz, $CDCl_3$) of 1:

δ 9.61 (s, 1H), 9.52 (s, 1H), 9.43 (s, 1H), 9.19 (s, J = 8.1 Hz, 1H), 4.36 – 4.26 (m, 4H), 2.06 (dd, J = 12.9, 6.3 Hz, 2H), 1.52 – 1.44 (m, 8H), 1.42 – 1.32 (m, 8H), 1.00 (t, J = 20.2, 10.1 Hz, 6H), 0.93 (t, J = 6.6 Hz, 6H)

^{13}C NMR (175 MHz, $CDCl_3$) of 1:

δ 163.70, 162.76, 140.11, 139.14, 139.14, 133.38, 130.41, 128.84, 128.71, 126.98, 125.76, 124.62, 124.12, 124.04, 123.88, 123.75, 123.06, 122.54, 122.40, 122.20, 96.13, 44.91, 38.05, 30.76, 28.69, 24.09, 23.10, 14.14, 10.66

^{1}H NMR (500 MHz, $CDCl_3$) of 2:

δ 9.59 (s, 1H), 9.45 (s, 1H), 9.33 (s, 1H), 8.77 (s, 1H), 4.38 – 4.22 (m, J = 11.8, 7.1 Hz, 4H), 2.11 – 1.99 (m, 2H), 1.52 – 1.32 (m, J = 20.7, 12.8, 6.0 Hz, 16H), 1.01 (t, J = 7.4 Hz, 6H), 0.93 (t, J = 6.8 Hz, 6H)

^{13}C NMR (125 MHz, CDCl3) of 2:

δ 163.23, 162.28, 150.91, 141.44, 139.90, 131.02, 130.14, 129.90, 129.14, 127.33, 126.98, 126.84, 126.63, 124.00, 123.48, 122.52, 122.30, 121.57, 120.44, 119.64, 114.67, 96.12, 45.07, 38.08, 30.76, 28.68, 24.09, 23.10, 14.12, 10.66.

^{1}H NMR (500 MHz, $CDCl_3$) of 3:

δ 9.09 (s, 1H), 9.00 (s, 1H), 8.90 (s, 1H), 8.59 (s, 1H), 4.26 – 4.12 (m, 4H), 1.99 – 1.88 (m, 2H), 1.44 – 1.26 (m, 16H), 0.95 (t, J = 7.4 Hz, 6H), 0.90 (t, J = 6.7 Hz, 6H)

^{13}C NMR (175 MHz, $CDCl_3$) of 3:

δ 161.91, 161.25, 153.04, 138.85, 137.89, 131.42, 130.89, 130.04, 129.20, 128.34, 127.89, 127.55, 127.52, 126.88, 126.52, 125.79, 125.71, 125.45, 124.00, 121.75, 120.85, 115.25, 45.21, 37.90, 30.64, 28.64, 23.98, 23.06, 14.12, 10.58

Table S1: Detail of reaction conditions for synthesis of compound **1**, **2**, **3**, **4**, **5**, and **6** at 298 K

Compound	Equivalents of *m*CPBA used	Time (h)	Yield (%)
1	9	2	40
2	50	2	23
3	50	12	35
4[a]	50	12	Not isolated
5[a]	50	48	Not isolated
6[a]	50	48	Not isolated

[a] Observed in APCI-HRMS in crude reaction mixture

Scheme S2: Structure elucidation of isolated compounds 1, 2, and 3

Structure determination for compounds **1**, **2** and **3** has been done based on the following:

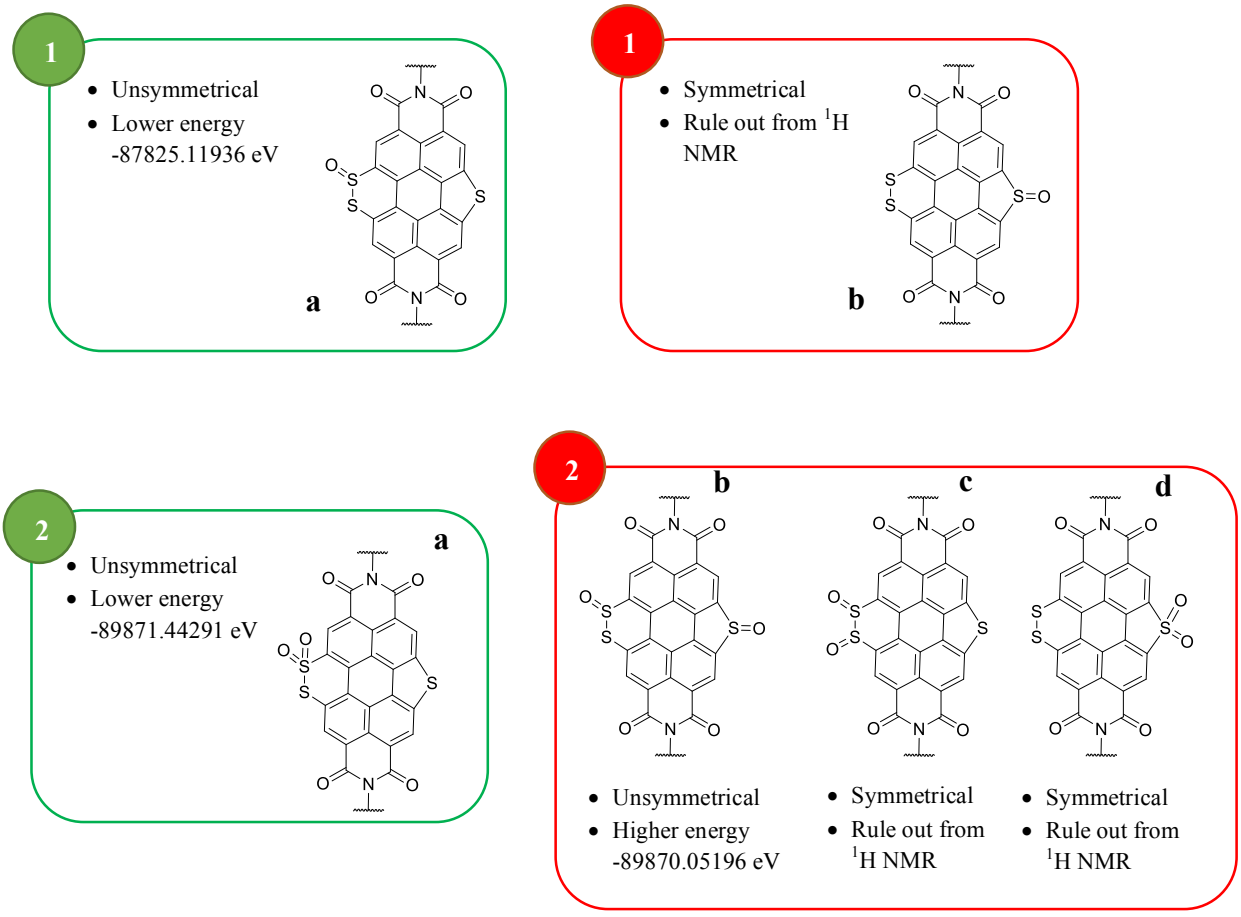
a. Mass spectrometry (APCI-HRMS) of compounds **1**, **2**, and **3** (after isolation) while **4**, **5**, and **6** (in reaction mixture) confirm the formation of all compounds

b. NMR spectrum of all isolated compounds **1**, **2**, and **3** have four singlet peaks in aromatic region, indicating all structures to be unsymmetrical in nature.

c. Potential energy of optimized structure from DFT calculations.

(Green Rectangle: Isolated; Red Rectangle: Not Isolated)

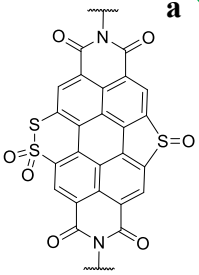
(2-ethylhexylamine as imide substituent)



3

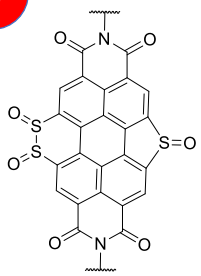
- Unsymmetrical
- Lower energy -91916.34 eV
- More likely to be formed from **2**

a



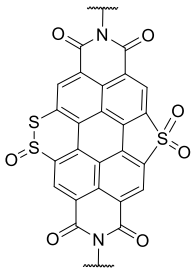
3

b



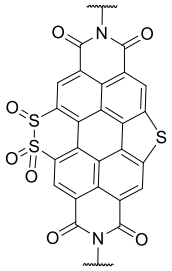
- Symmetrical
- Rule out from ^{1}H NMR

c



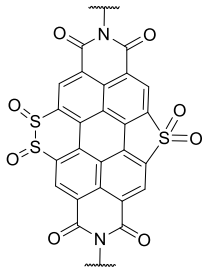
- Unsymmetrical
- Slightly lower energy -91916.51 eV, but unlikely be formed from **2**

d

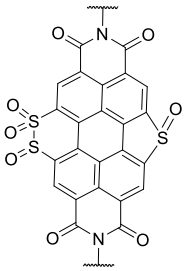


- Unsymmetrical
- Slightly lower energy -91916.78 eV but very unlikely to be formed due to possibility of S-S bond breaking

4



a



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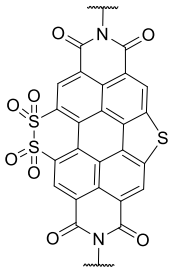
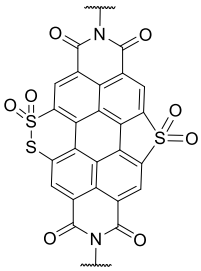
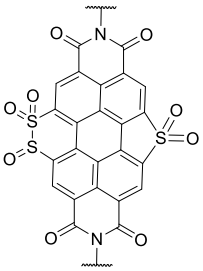


c

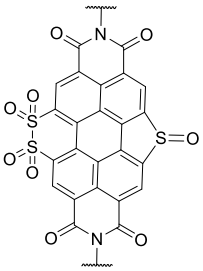


d

5

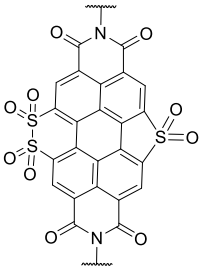


a



b

6



a

Table S2: Optimized energy from DFT of all the possible isomers of compounds **1**, **2**, **3**, **4**, **5**, and **6**

Compound	Isomer	Optimized energy (eV)
1O-SAN-PDI (1)	a	**-87825.11936**
	b	-87824.30502
2O-SAN-PDI (2)	a	**-89871.44291**
	b	-89870.05196
	c	-89870.47792
	d	-89870.76664
3O-SAN-PDI (3)	a	**-91916.34705**
	b	-91915.37417
	c	-91916.51241
	d	-91916.77614
4O-SAN-PDI (4)	a	-93961.81433
	b	-93961.65042
	c	-93963.02961
	d	-93962.79396
5O-SAN-PDI (5)	a	-96008.07964
	b	-96007.87445
6O-SAN-PDI (6)	a	-98054.28723

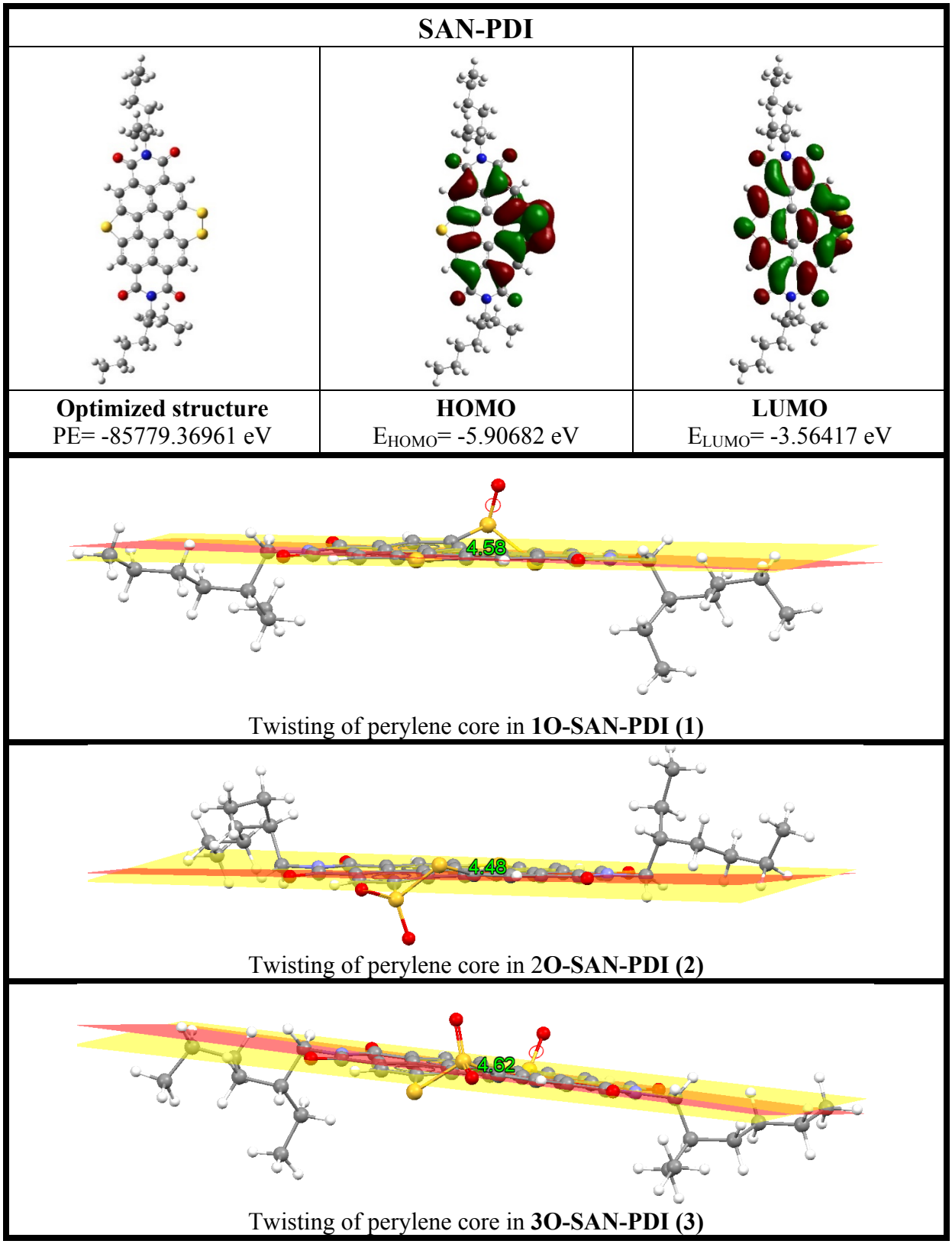


Fig. S1: Showing the twisting of perylene core of **1**, **2**, and **3** upon oxidation of **SAN-PDI**

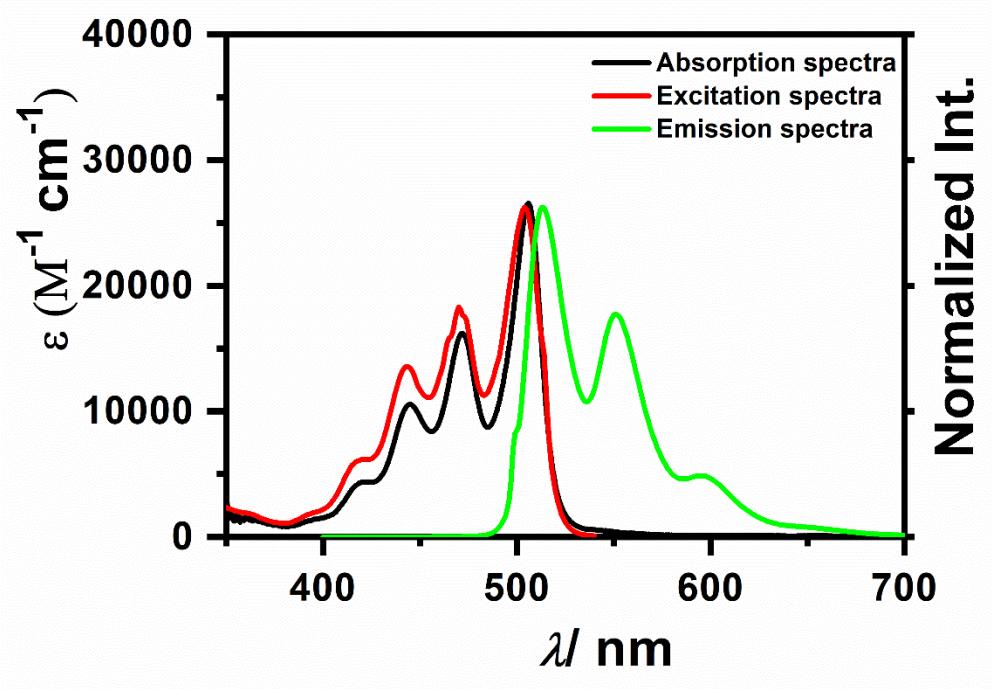


Fig. S2: Absorption, excitation, and emission spectra of **2** in DCM solvent

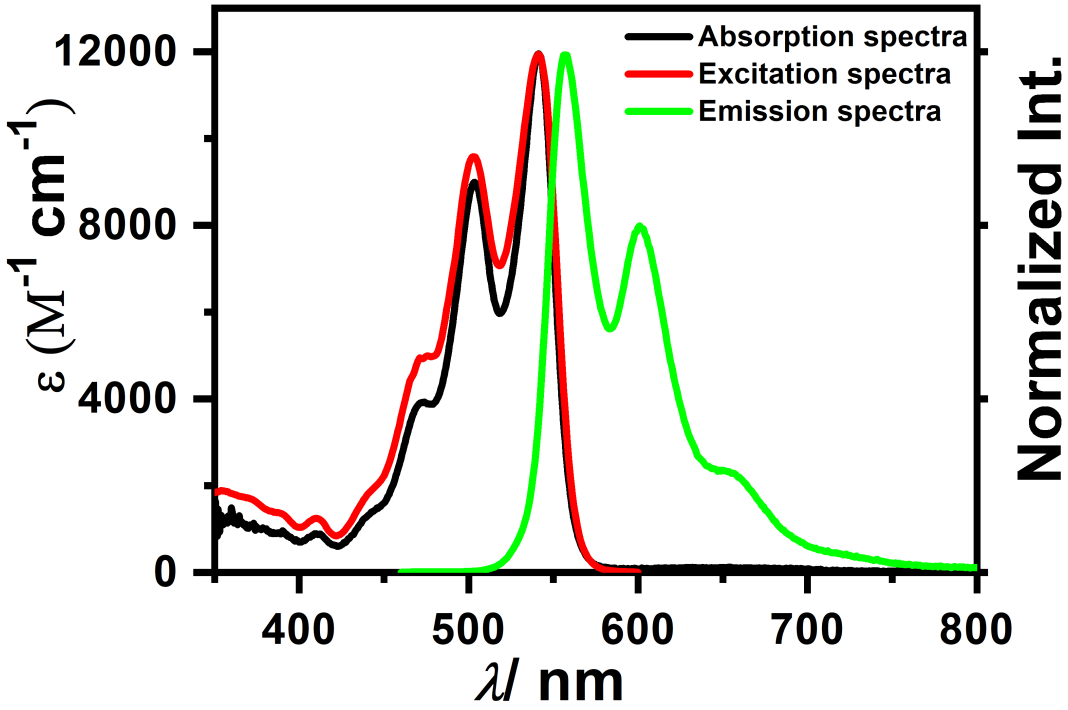


Fig. S3: Absorption, excitation, and emission spectra of **3** in DCM solvent

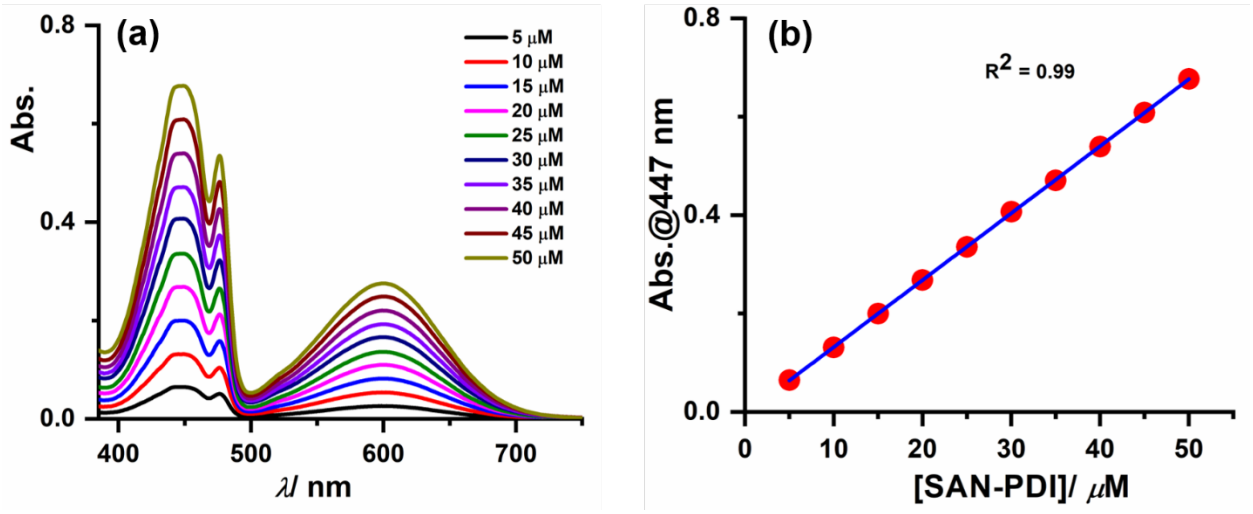


Fig. S4: Concentration-dependent UV-Vis. absorption spectra (a) and respective Abs. *vs* concentration plot (b) for **SAN-PDI** in DCM solvent

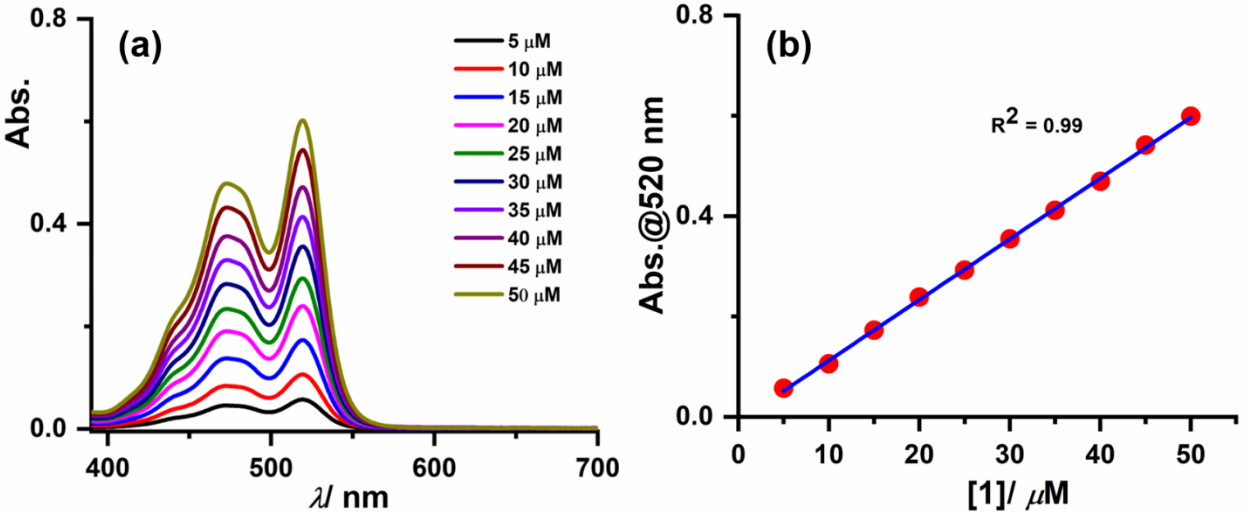


Fig. S5: Concentration-dependent UV-Vis. absorption spectra (a) and respective Abs. *vs* concentration plot (b) for **1** in DCM solvent

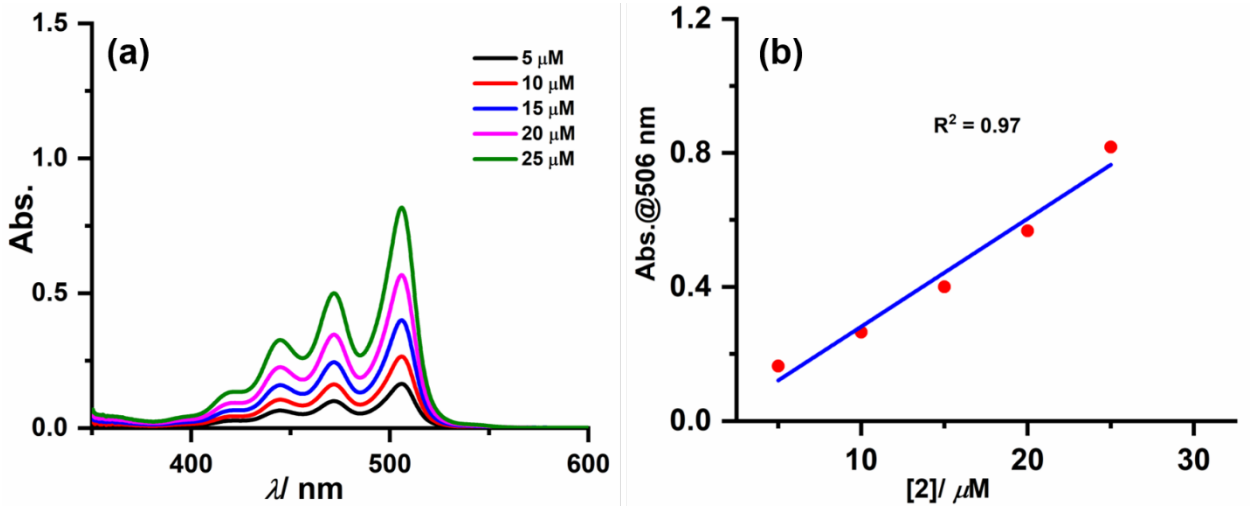


Fig. S6: Concentration-dependent UV-Vis. absorption spectra (a) and respective Abs. *vs* concentration plot (b) for **2** in DCM solvent

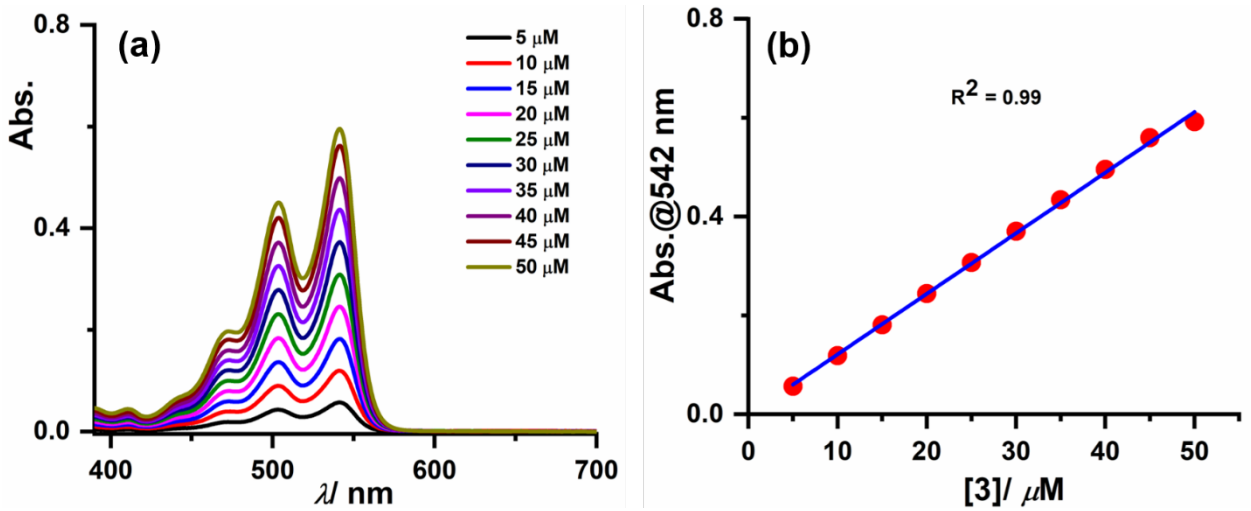


Fig. S7: Concentration-dependent UV-Vis. absorption spectra (a) and respective Abs. *vs* concentration plot (b) for **3** in DCM solvent

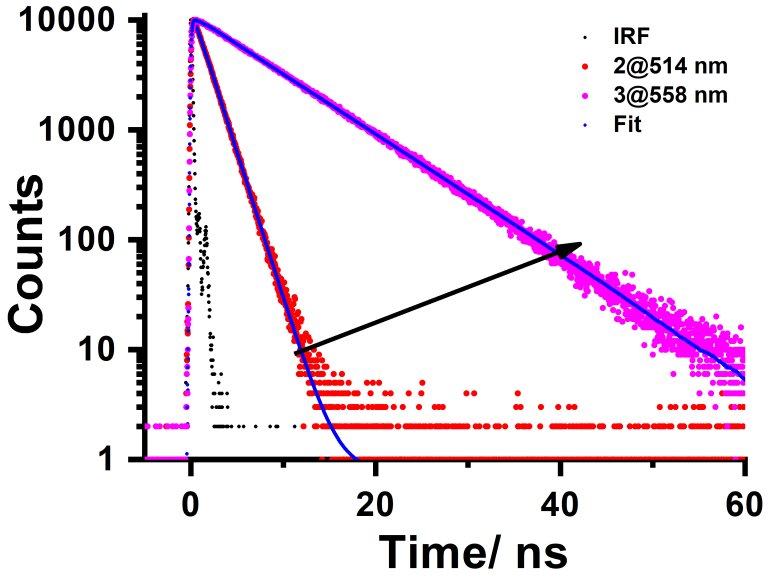


Fig. S8: Fluorescent lifetime plot for **2** and **3** in DCM solvent

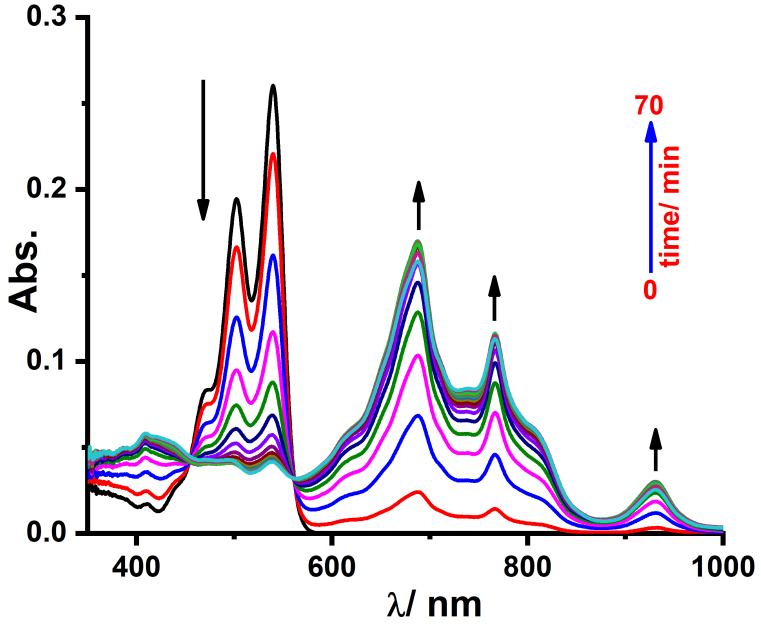


Fig. S9: Generation of $\mathbf{3}^{\bullet-}$ from **3** using 100 μM diethylamine (DEA) in THF

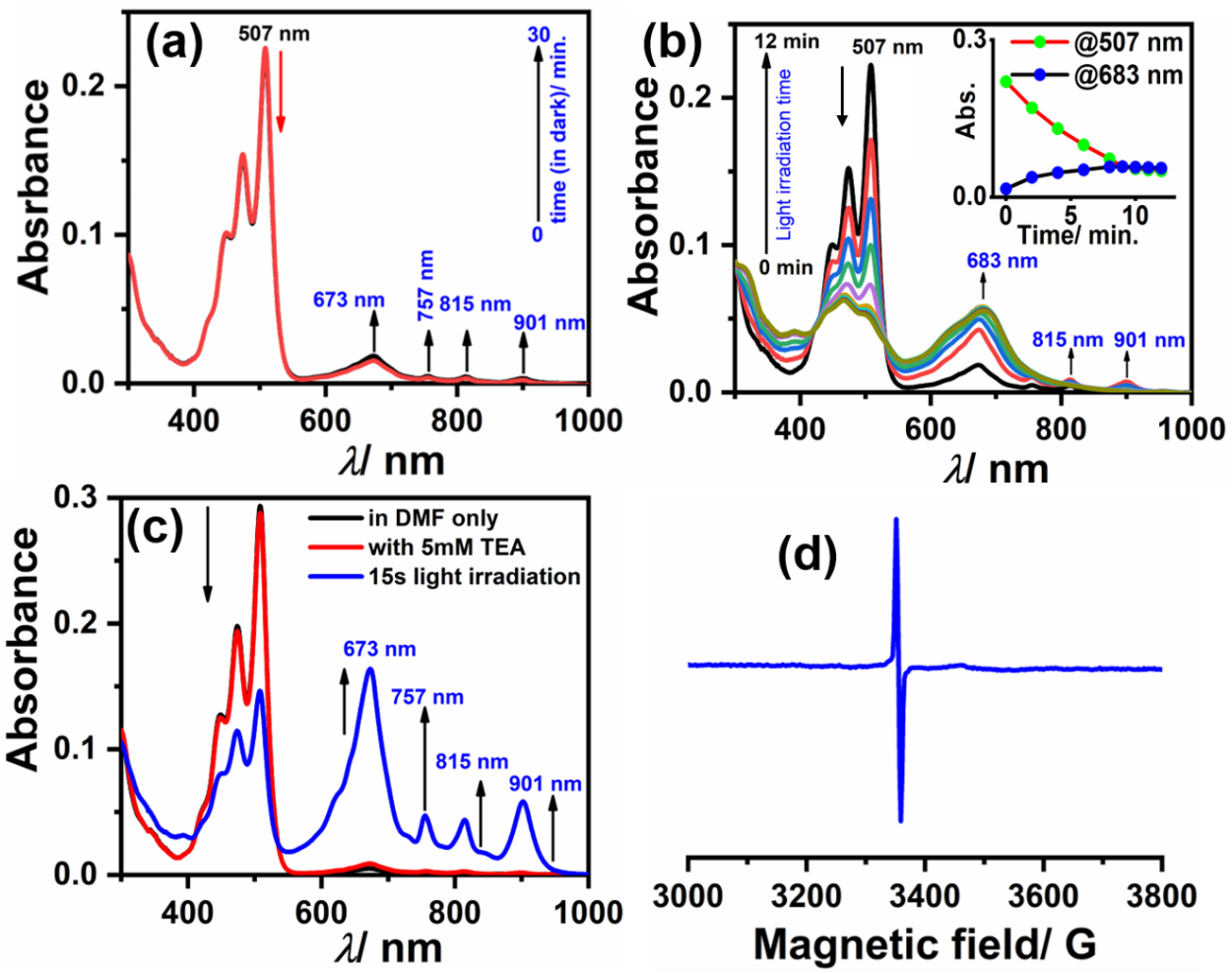


Fig. S10: Radical anion generation monitored using UV-Vis.-NIR absorption spectroscopy, electronic absorption spectra for **2** (10 μM) in DMF only (a) in dark (b) upon visible light irradiation (c) with the addition of external TEA and visible light irradiation for just 15 seconds (d) confirmation of radical anion by EPR spectrum

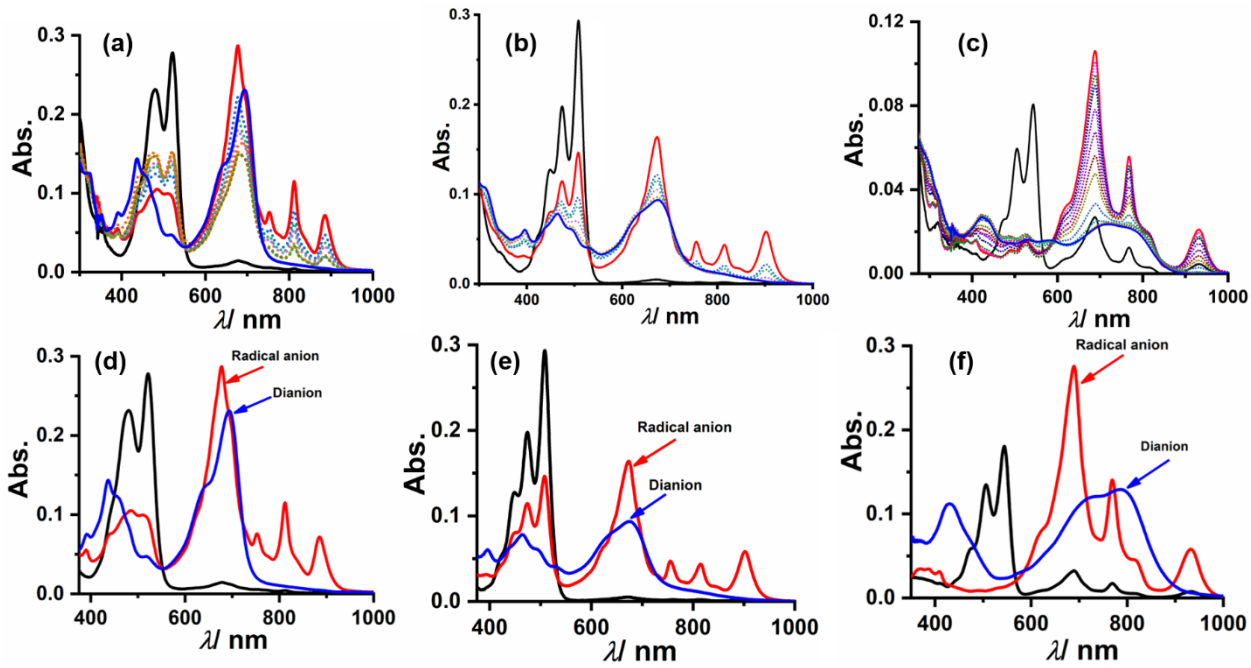


Fig. S11: UV-Vis.-NIR absorption spectra in DMF at 0 min (black), radical anion (red), dianion (blue), and spectral change over time (dotted) of **1** (a & d), **2** (b & e), and **3** (c & f)

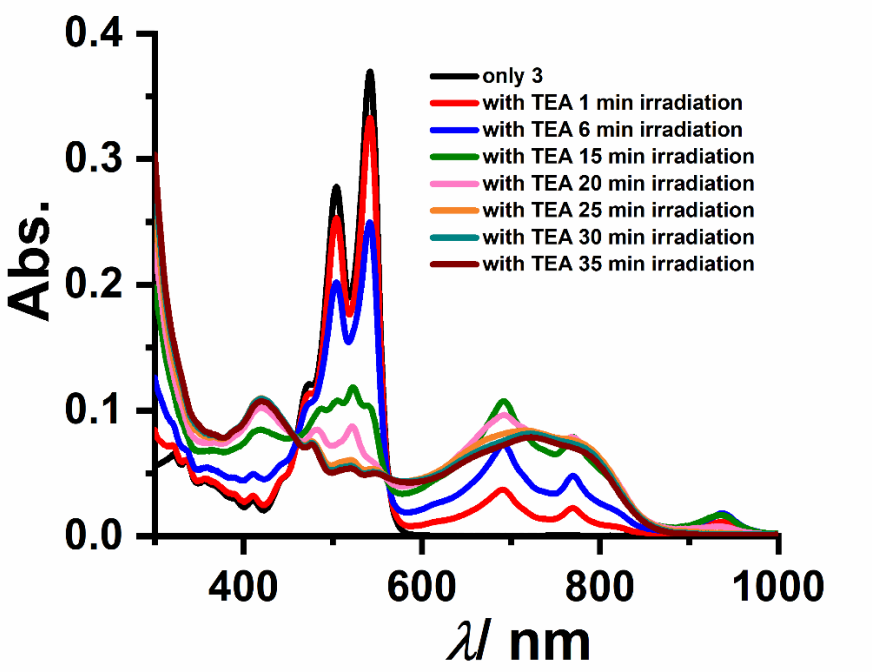


Fig. S12: Radical anion and dianion formation of **3** using TEA and visible light irradiation in chloroform solvent monitored by UV-Vis.-NIR absorption spectroscopy

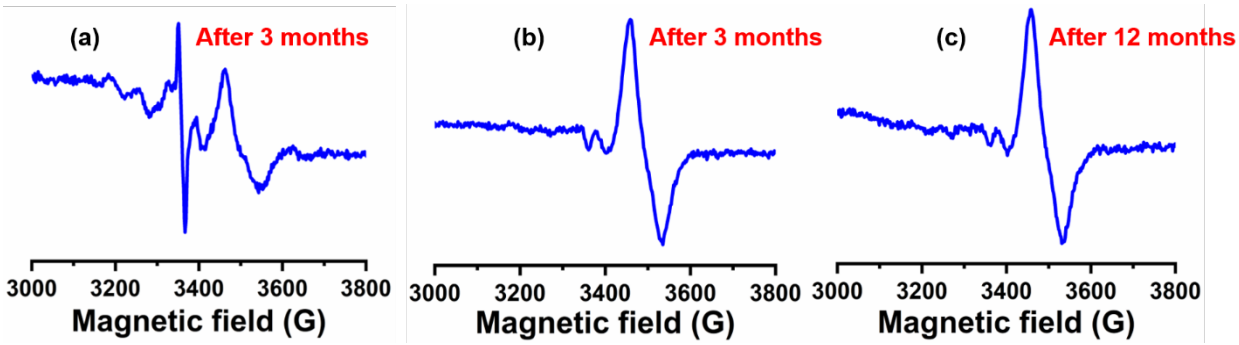


Fig. S13: EPR spectra in DMF solution of **1** (a), **2** (b), and **3** (c)

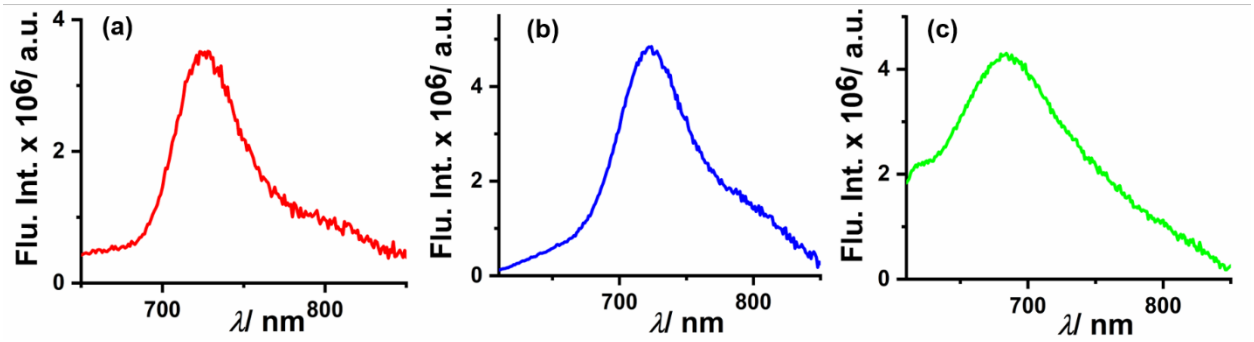


Fig. S14: Fluorescence emission spectra of dianions upon excitation at 600 nm wavelength (a) **1**, (b) **2**, and (c) **3**

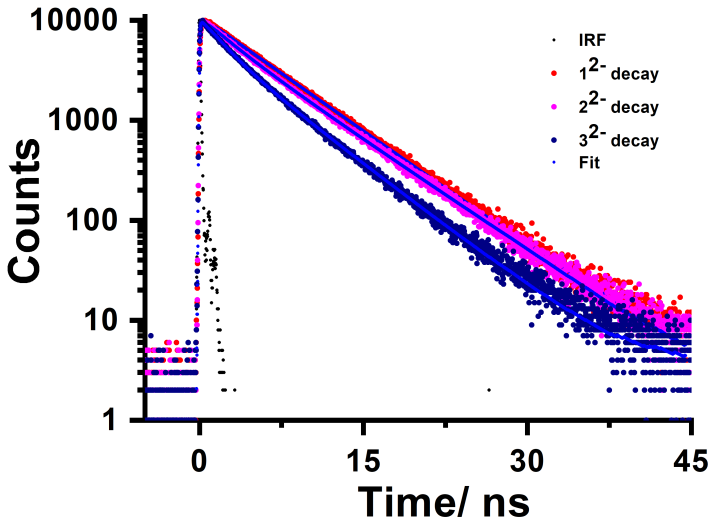


Fig. S15: Fluorescence lifetime decay plot for dianions corresponding to **1**, **2**, and **3**. [λ_{ex} = 633 nm]

Table S3: Summary of photophysical and redox properties.

Compound	Φ_F [%]	τ_{avg}[c] (ns)	E_{LUMO} [eV][d]
SAN-PDI	–[nd]	–[nd]	-4.02
1	12[a]	–[nd]	-4.1
1^{2-}	24[b]	5.4	–
2	25[a]	1.6	-4.16
2^{2-}	16[b]	5.7	–
3	83[a]	8.0	-4.55
3^{2-}	4[b]	4.9	–

[a] Absolute quantum yields were determined using integrating sphere system, [b] Fluorescence quantum yield of dianions were determined relative to 2-(2-ethylhexyl)-8-((10-phenylanthracen-9-yl)ethynyl)-1H-benzo[10,5]anthra[2,1,9-def]isoquinoline-1,3(2H)-dione (λ_{ex} = 600 nm).[6] [c] Fluorescence lifetime measurement of dianions were performed using time-correlated single-photon counting (TCSPC) setup [λ_{ex} = 633 nm]. [d] Calculated according the known literature procedure using the formula [LUMO = -(E_{red}^{onset} + 4.4) eV][7] [nd]: not determined due to low quantum yield and short lifetime.

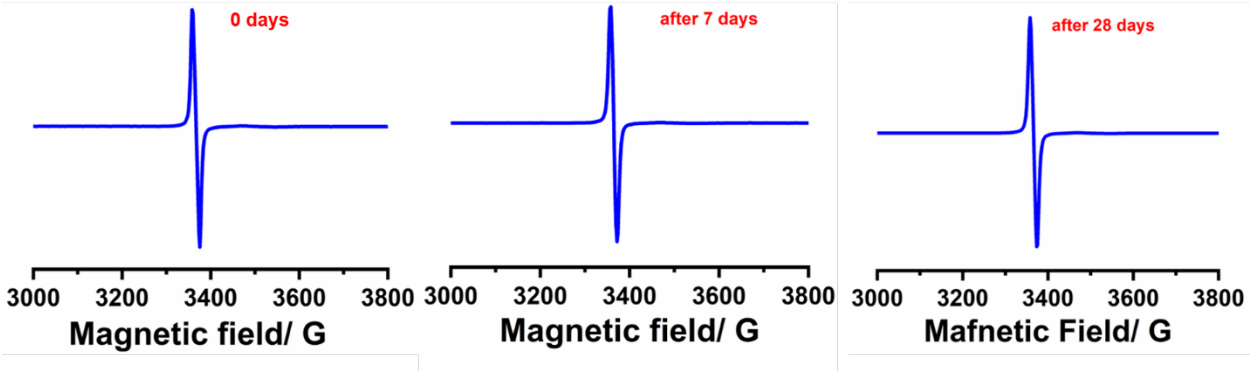


Fig. S16: EPR at different days showing stability of radical anion generated in solid-state thin film of **3**

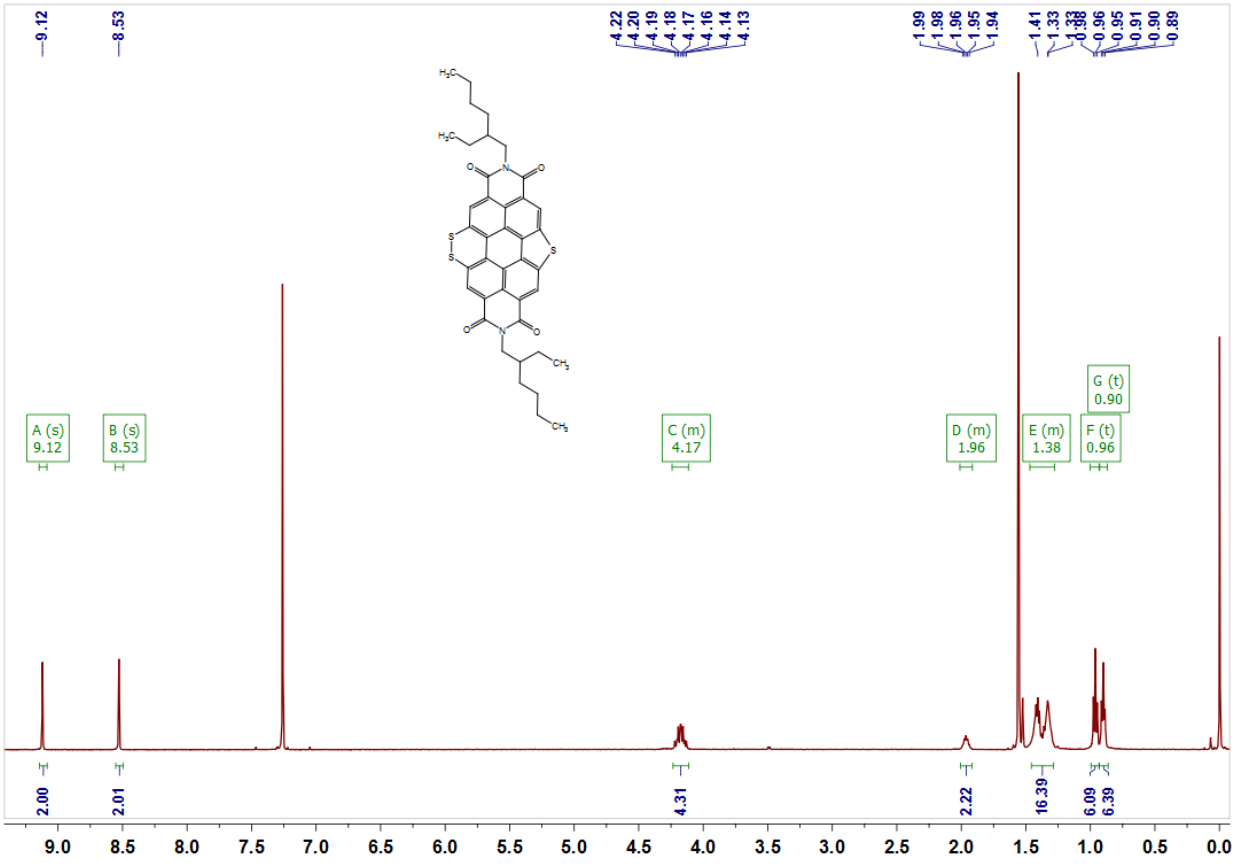


Fig. S17: ^{1}H NMR of **SAN-PDI** recorded in $CDCl_3$ at 500 MHz.

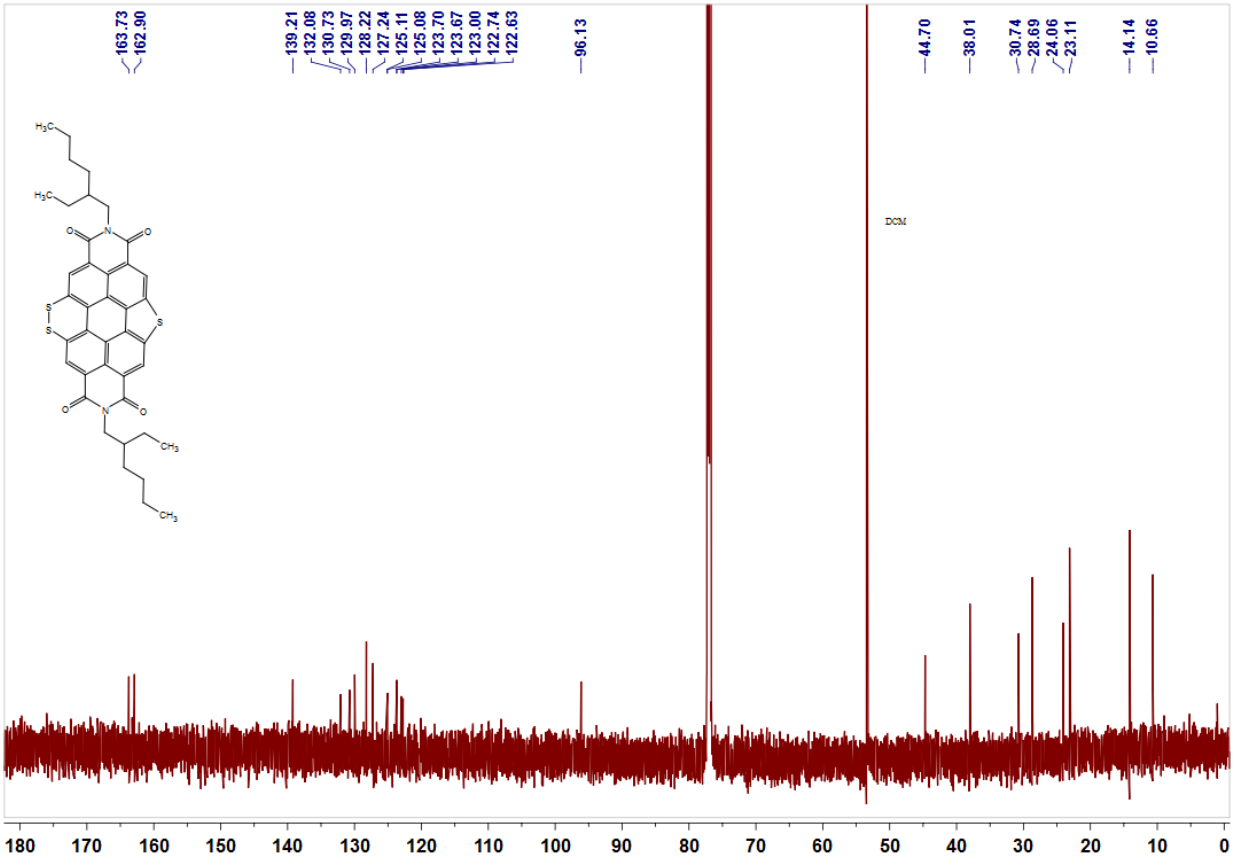


Fig. S18: ^{13}C NMR of **SAN-PDI** recorded in $CDCl_3$ at 175 MHz.

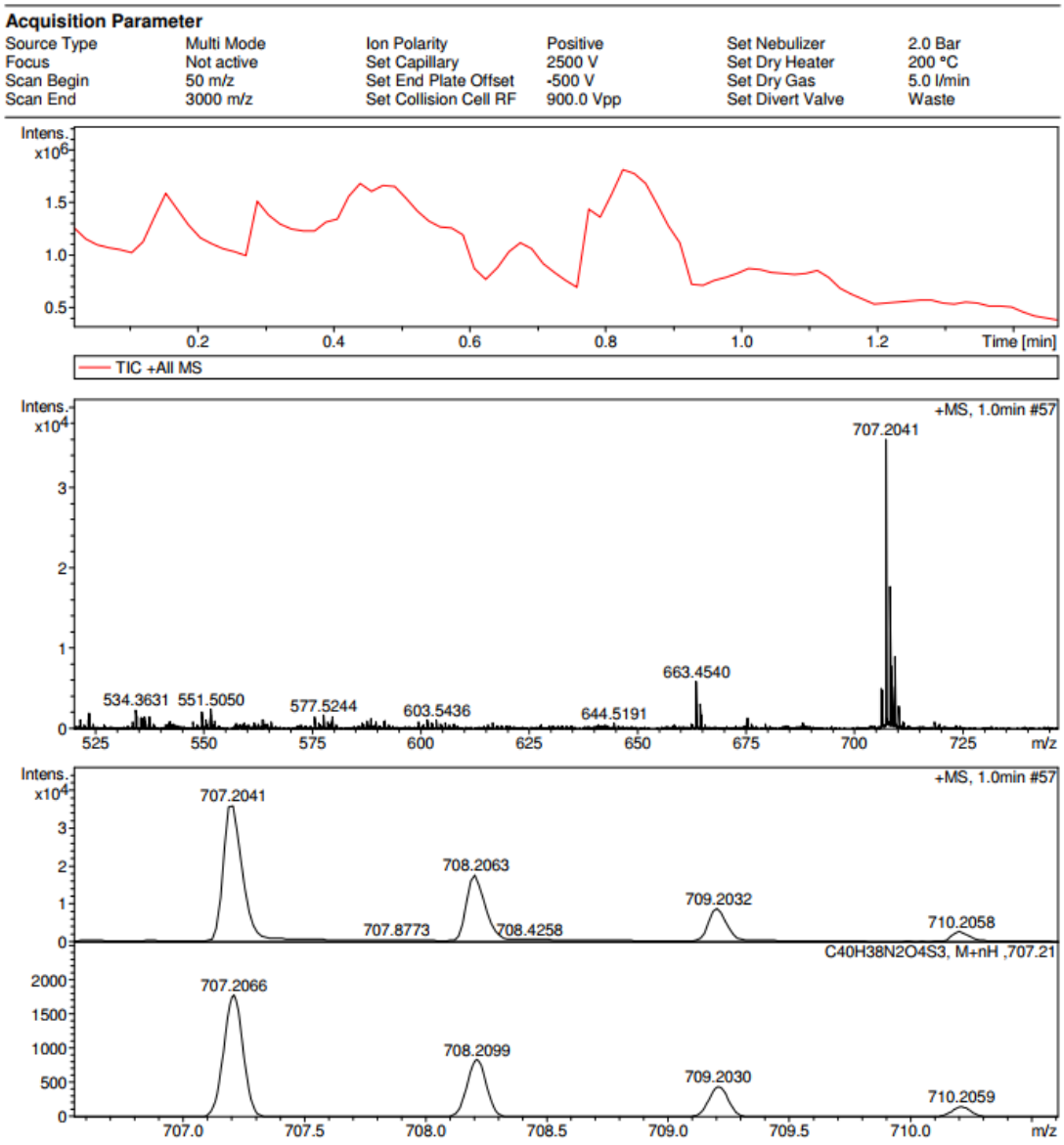


Fig. S19: APCI-HRMS of **SAN-PDI**; **Calculated mass** – 706.1994 Da and **Obtained mass** – *m/z* 707.2041 Da $[M+H]^+$

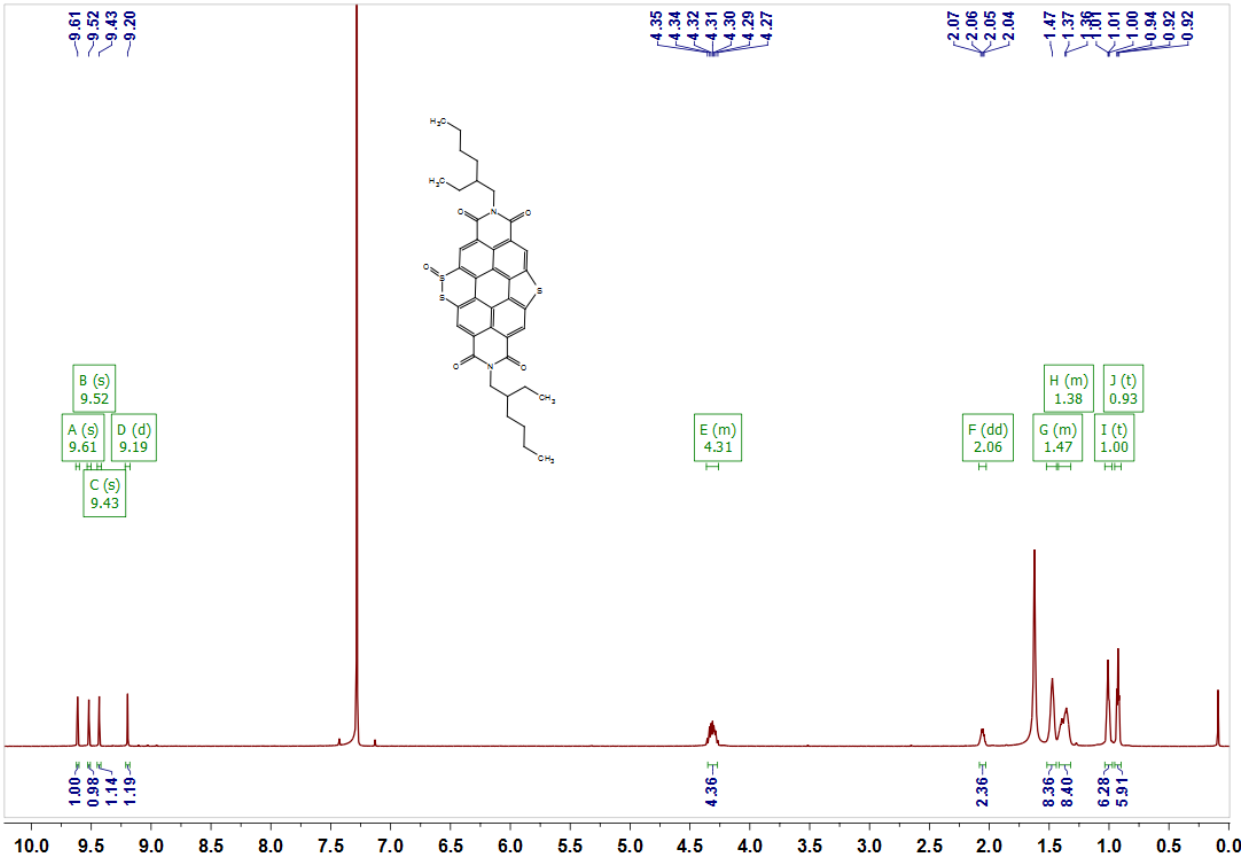


Fig. S20: ^{1}H NMR of **1** recorded in $CDCl_3$ at 500 MHz.

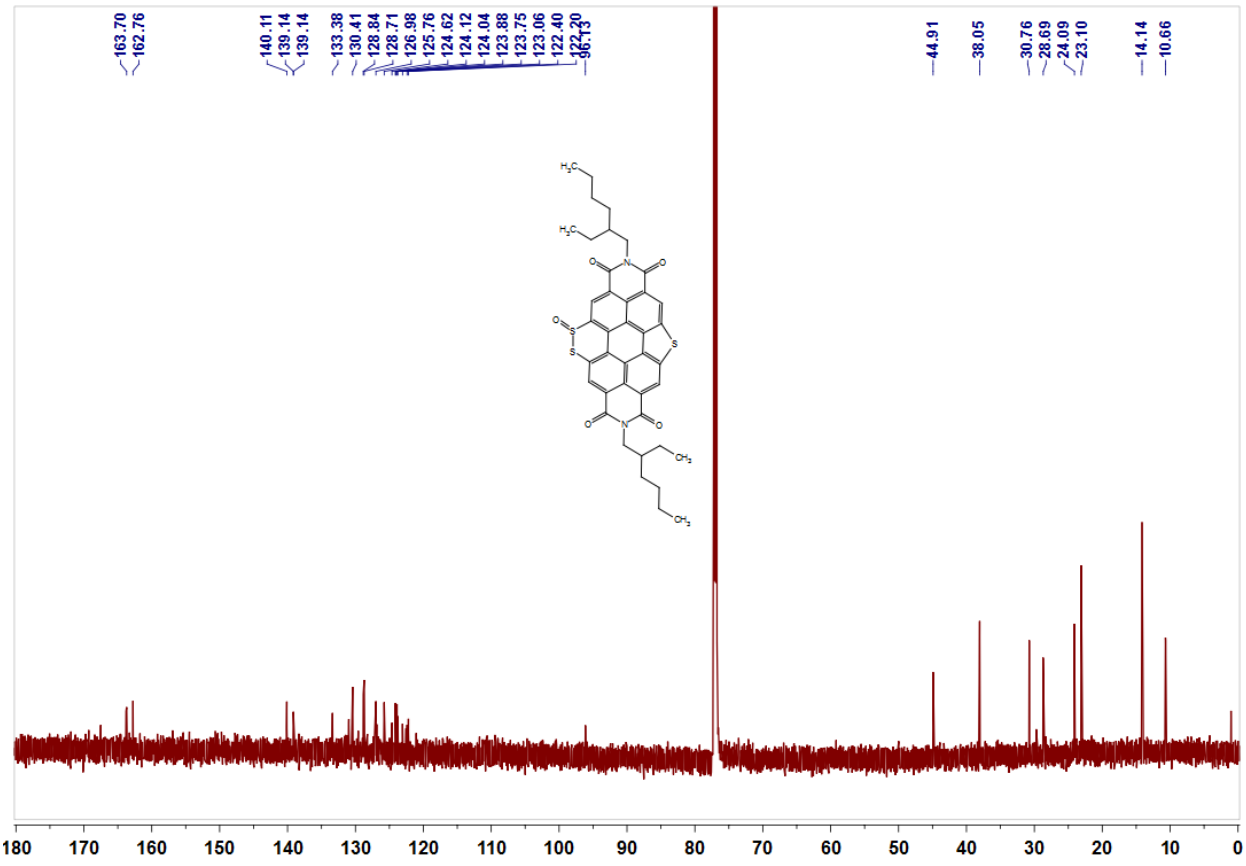


Fig. S21: ^{13}C NMR of **1** recorded in $CDCl_3$ at 175 MHz.

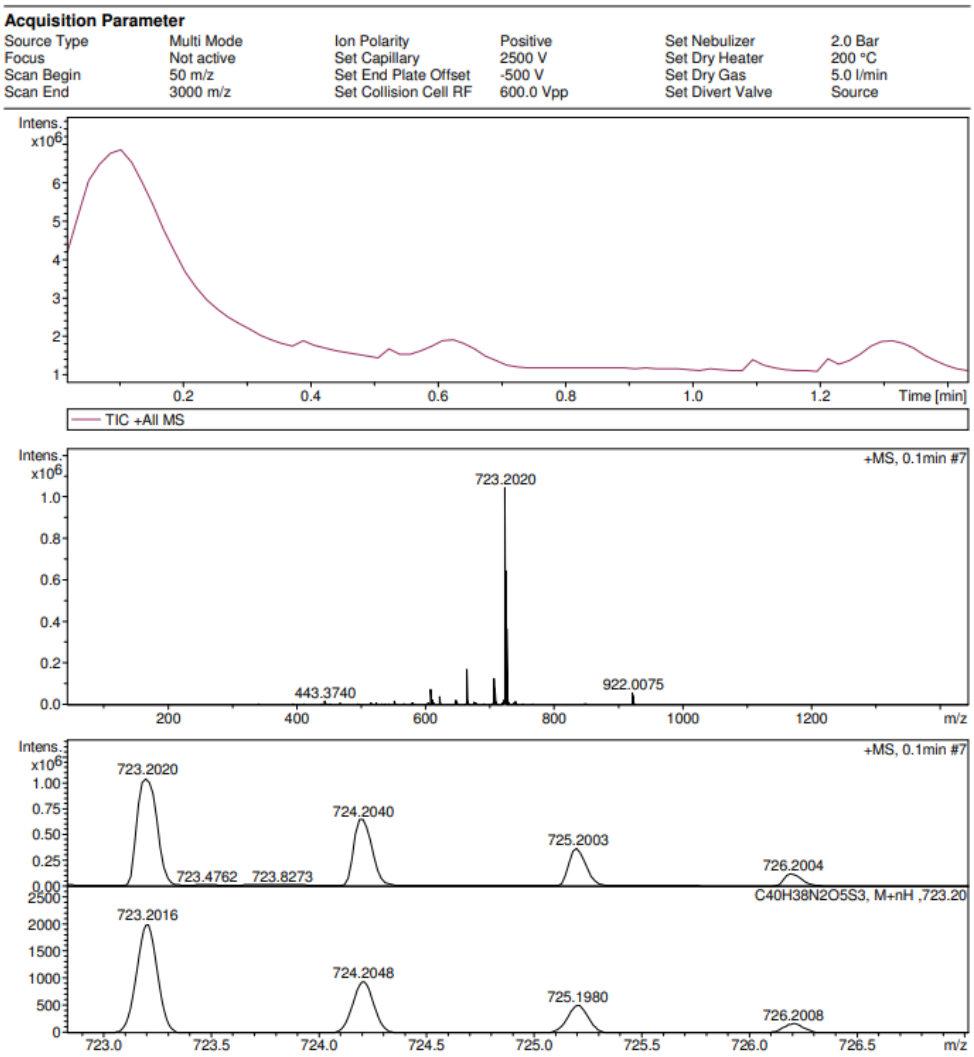


Fig. S22: APCI-HRMS of **1**; **Calculated mass** – 722.1943 Da and **Obtained mass** – *m/z* 723.2020 Da $[M+H]^+$

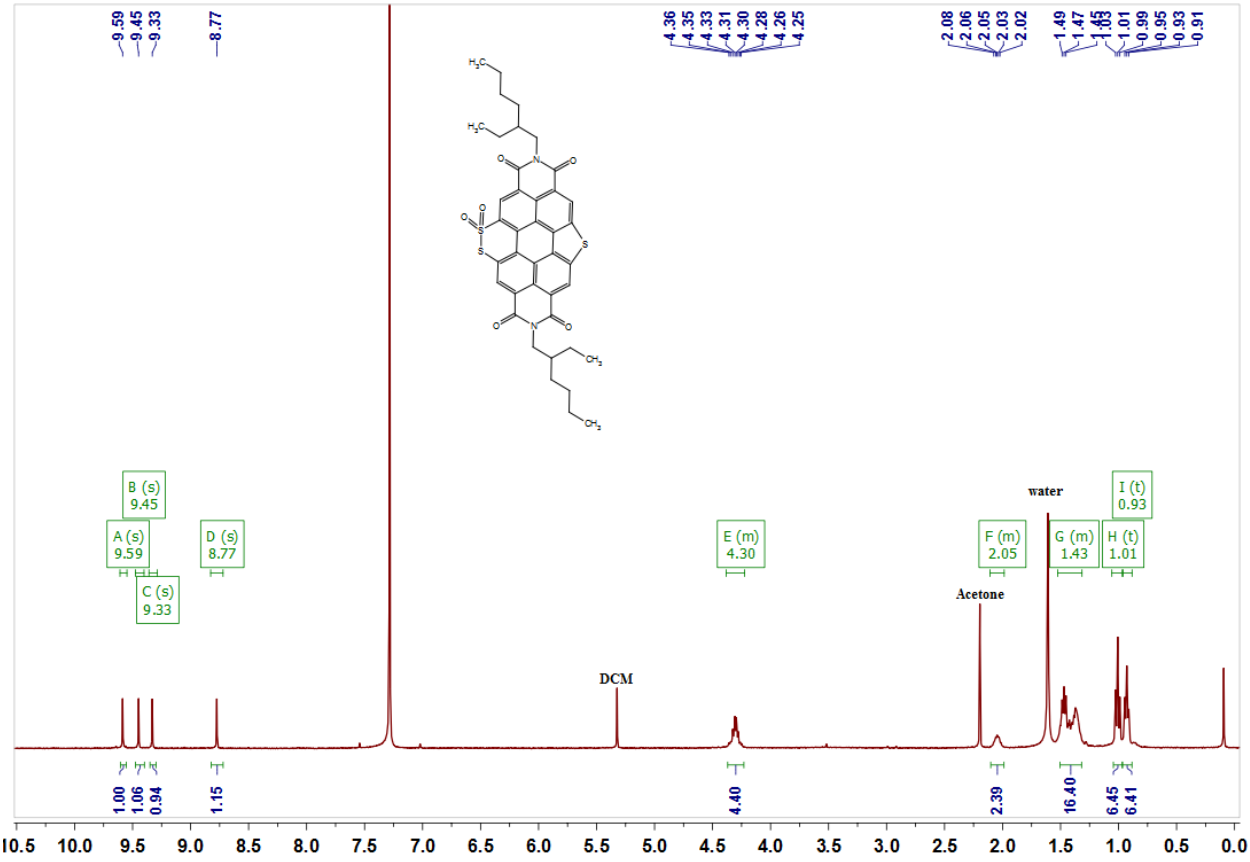


Fig. S23: ^{1}H NMR of **2** recorded in $CDCl_3$ at 500 MHz.

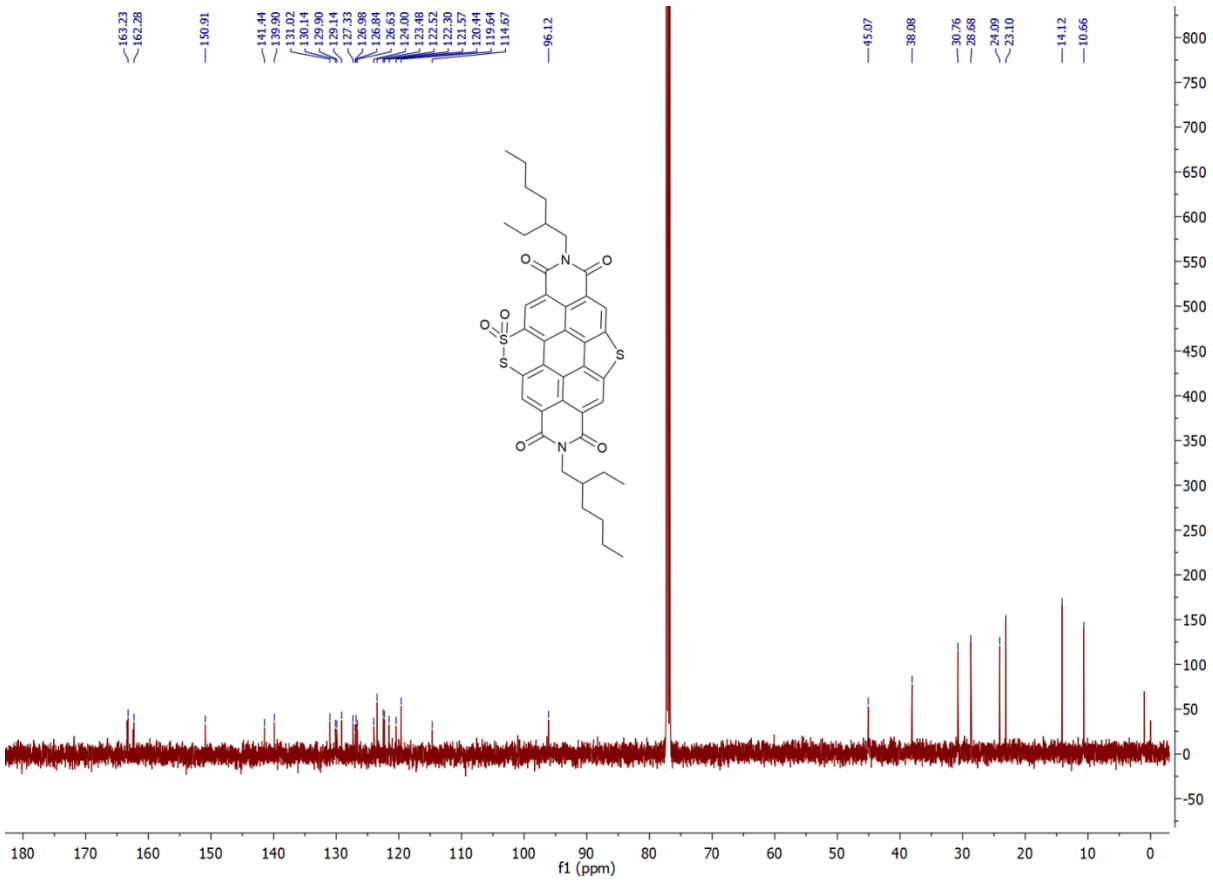


Fig. S24: ^{13}C NMR of **2** recorded in $CDCl_3$ at 125 MHz.

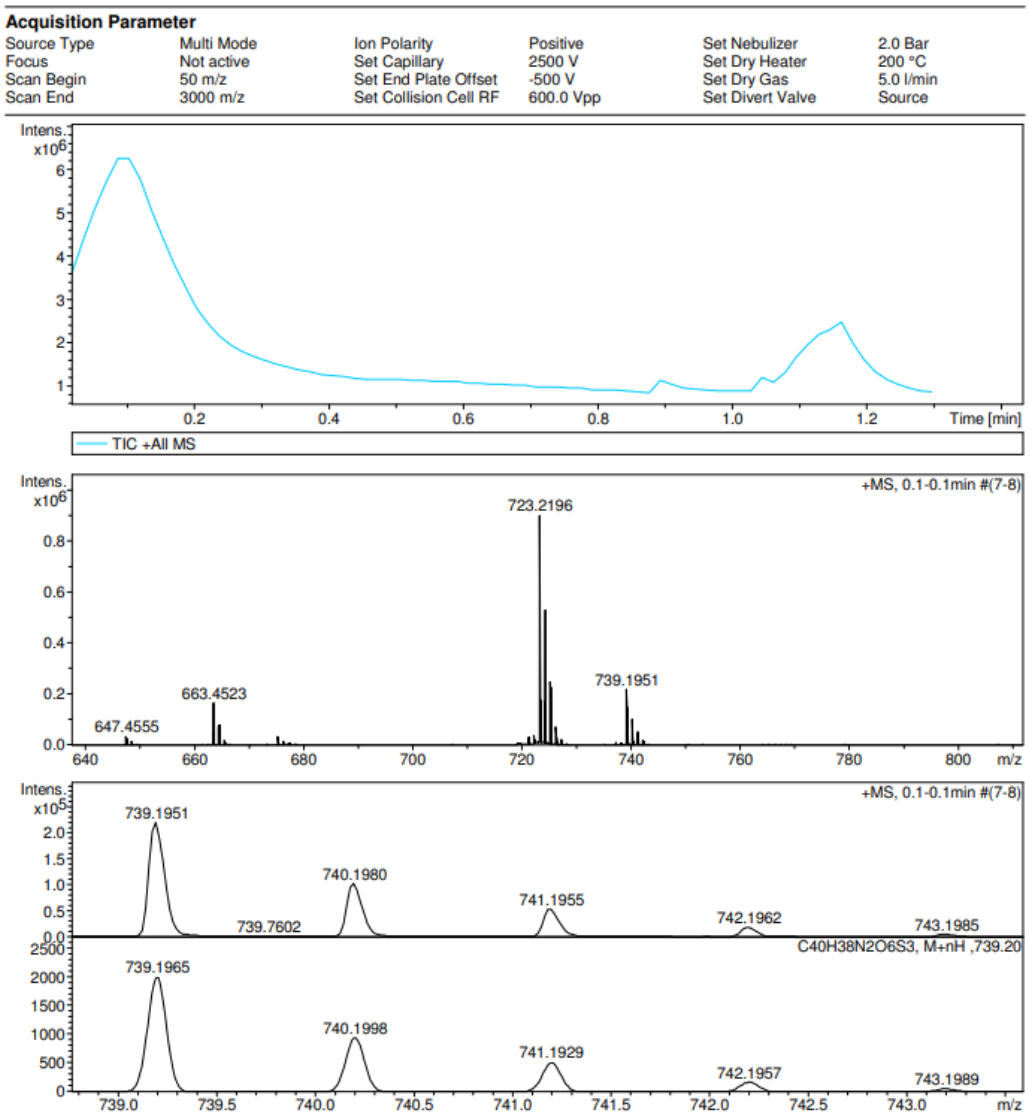


Fig. S25: APCI-HRMS of **2**; **Calculated mass** – 738.1892 Da and **Obtained mass** – *m/z* 739.1951 Da $[M+H]^+$

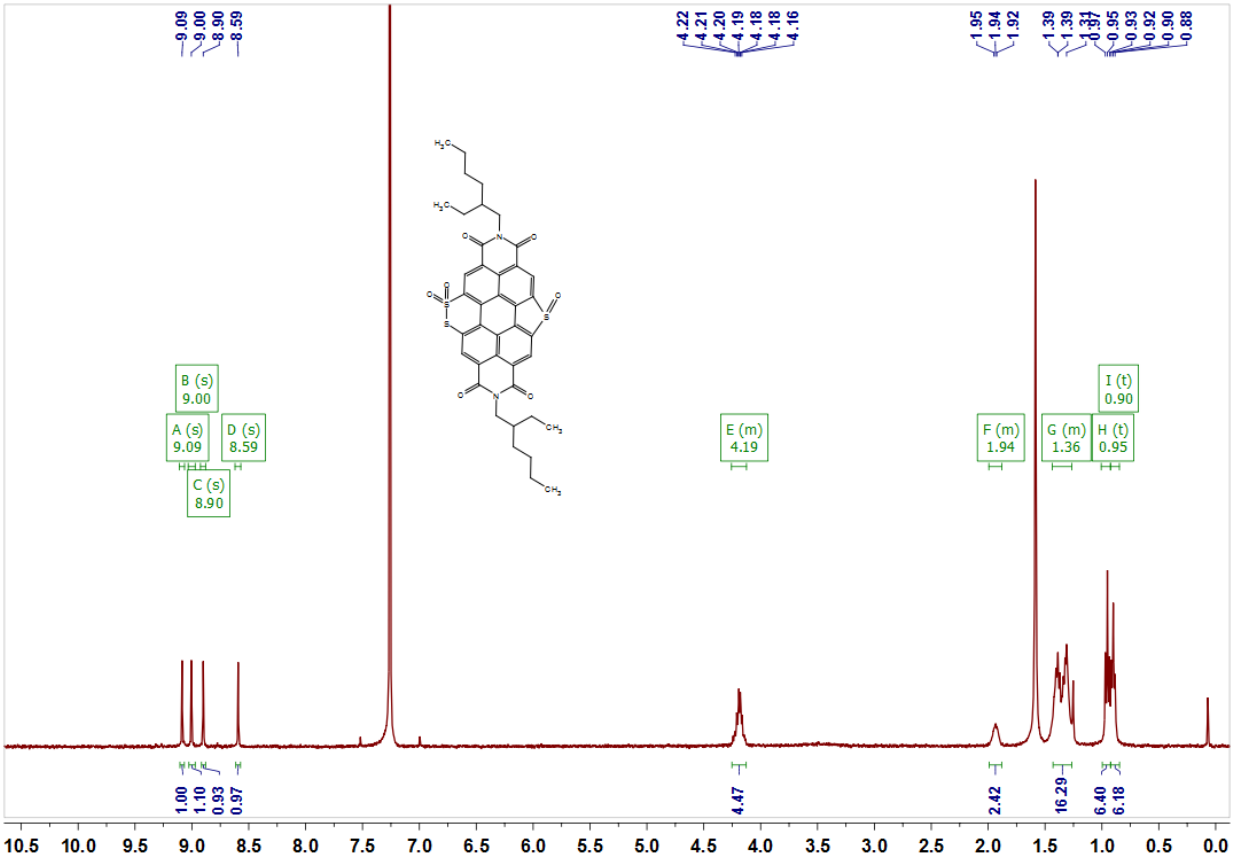


Fig. S26: ^{1}H NMR of **3** recorded in $CDCl_3$ at 500 MHz.

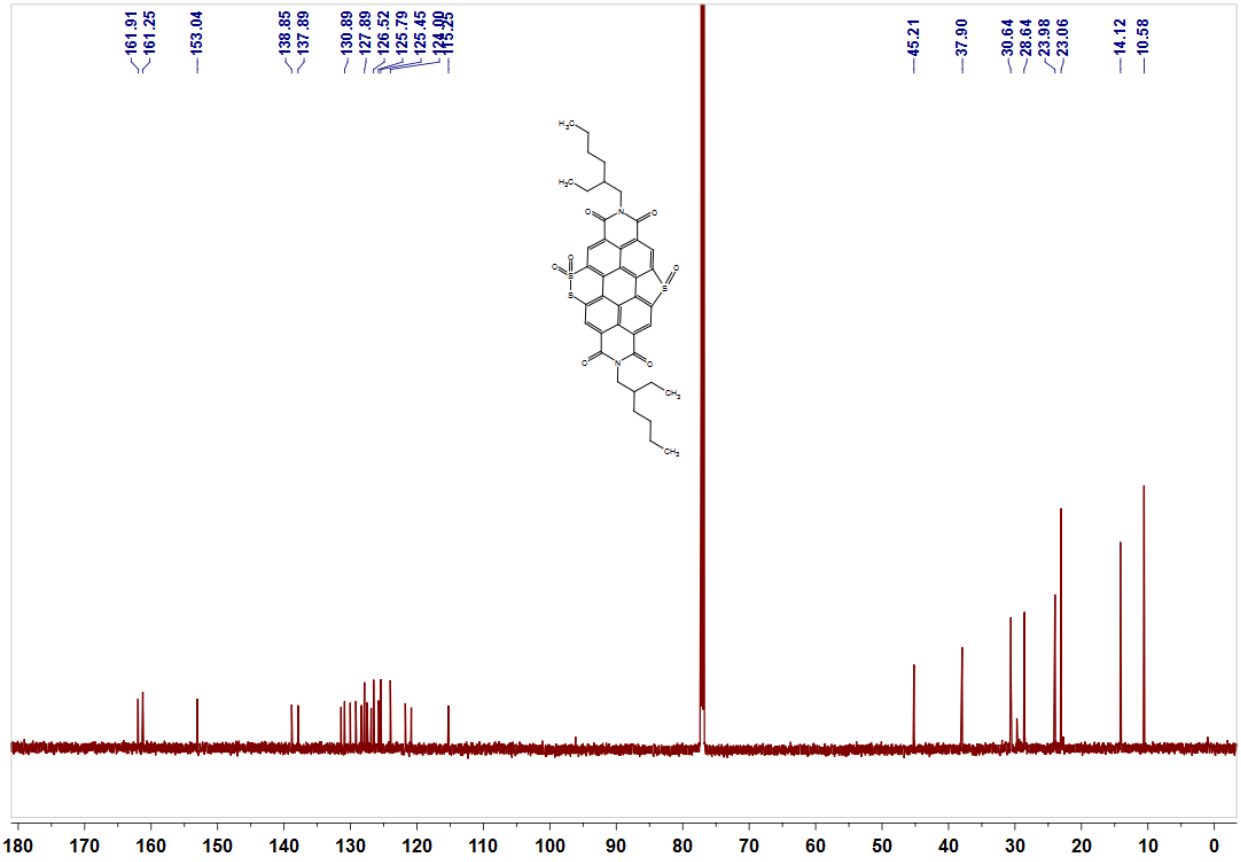


Fig. S27: ^{13}C NMR of **3** recorded in $CDCl_3$ at 175 MHz.

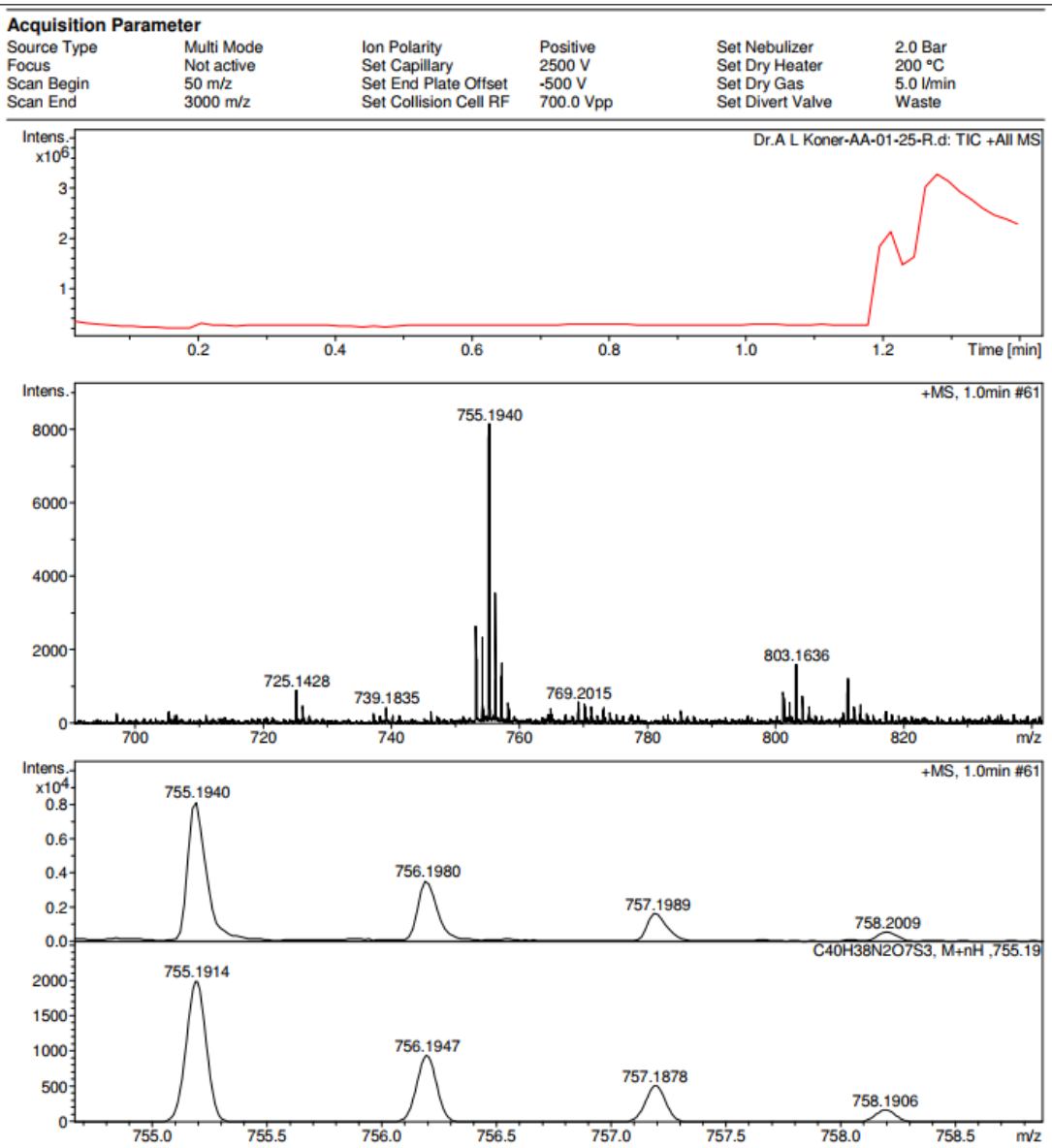


Fig. S28: APCI-HRMS of **3**; **Calculated mass** – 754.1841 Da and **Obtained mass** – *m/z* 755.1940 Da $[M+H]^+$

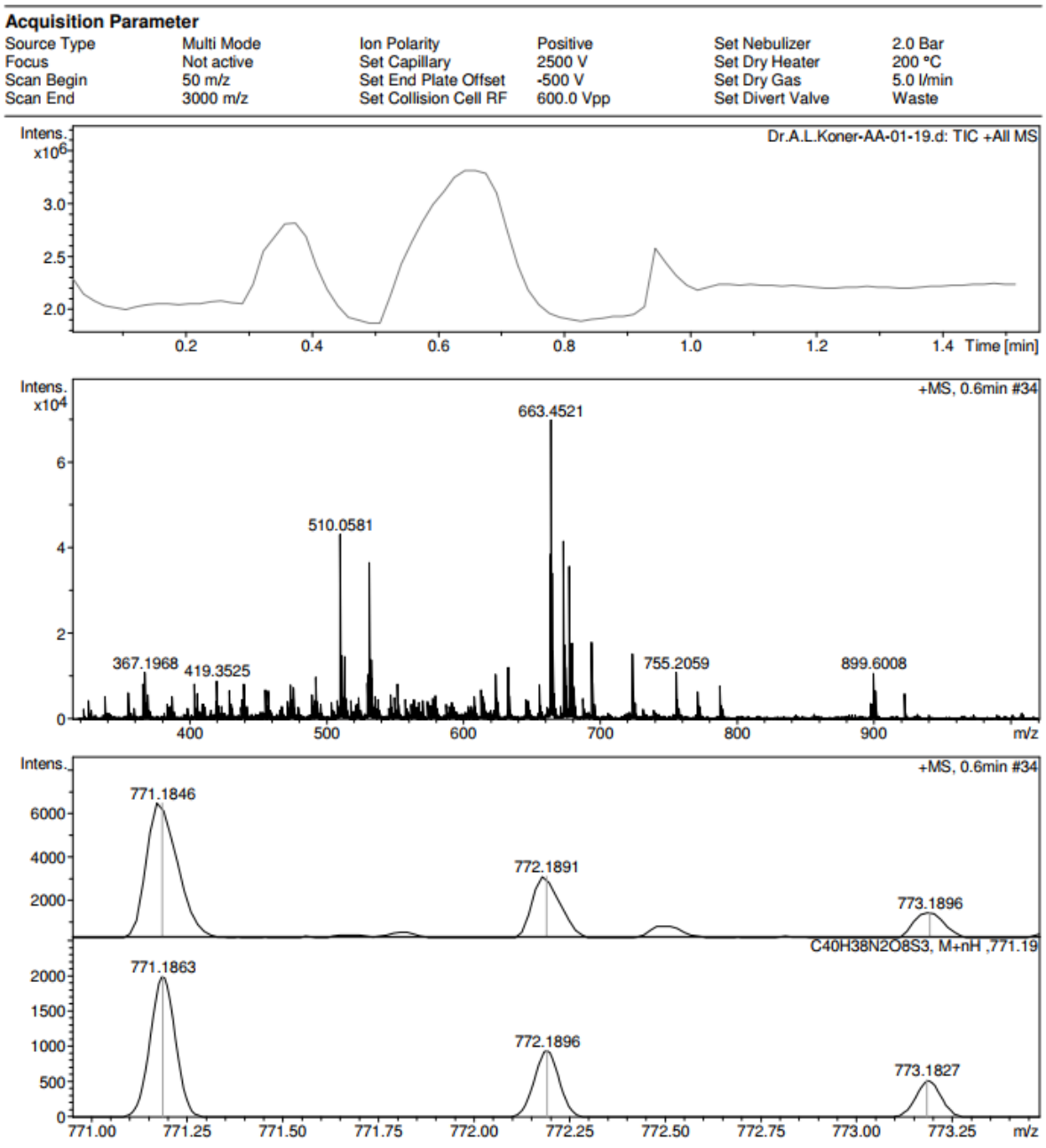


Fig. S29: APCI-HRMS of **4**; **Calculated mass** – 770.1790 Da and **Obtained mass** – *m/z* 771.1846 Da $[M+H]^+$

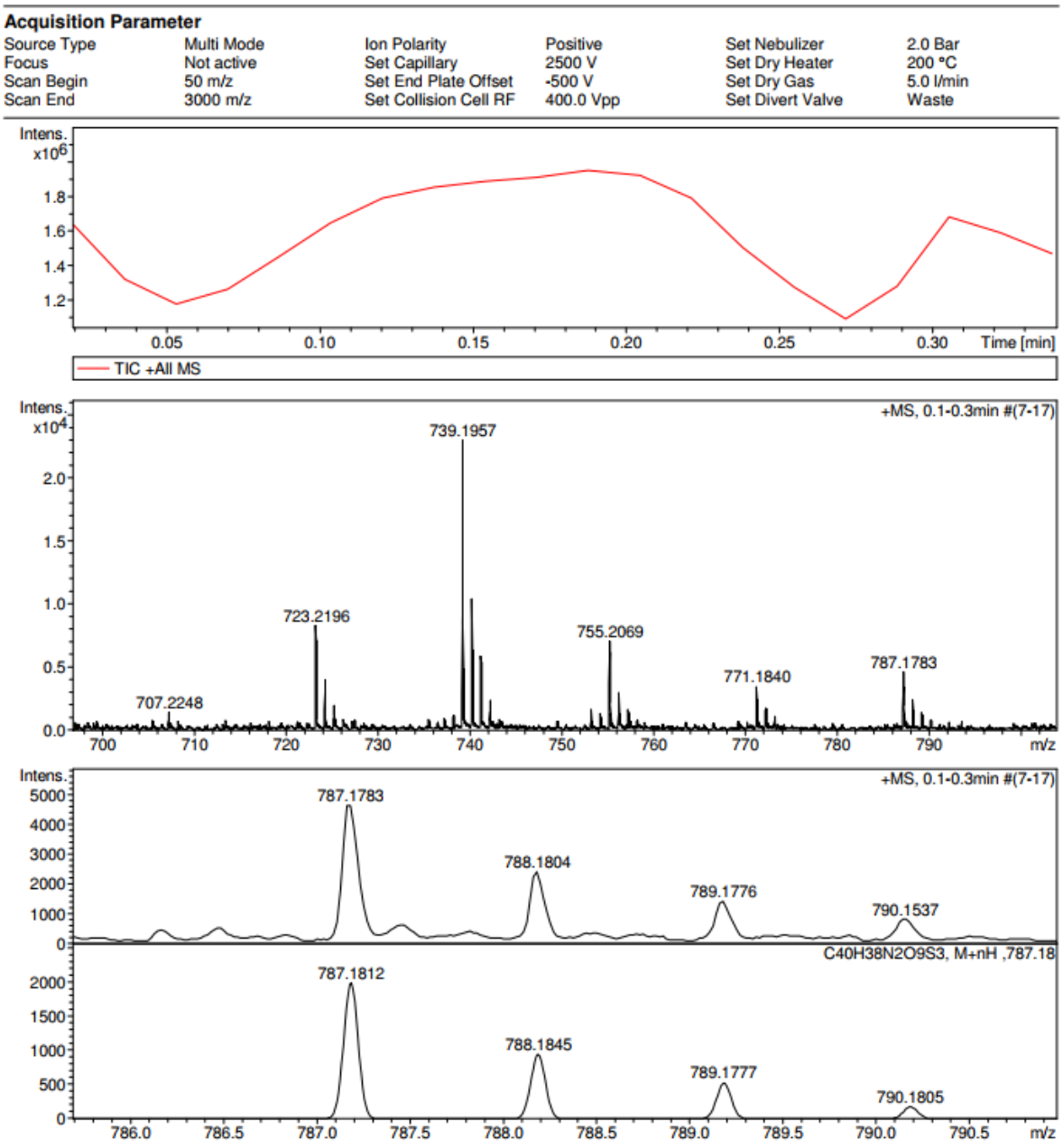


Fig. S30: APCI-HRMS of **5**; **Calculated mass** – 786.1739 Da and **Obtained mass** – *m/z* 787.1783 Da $[M+H]^+$

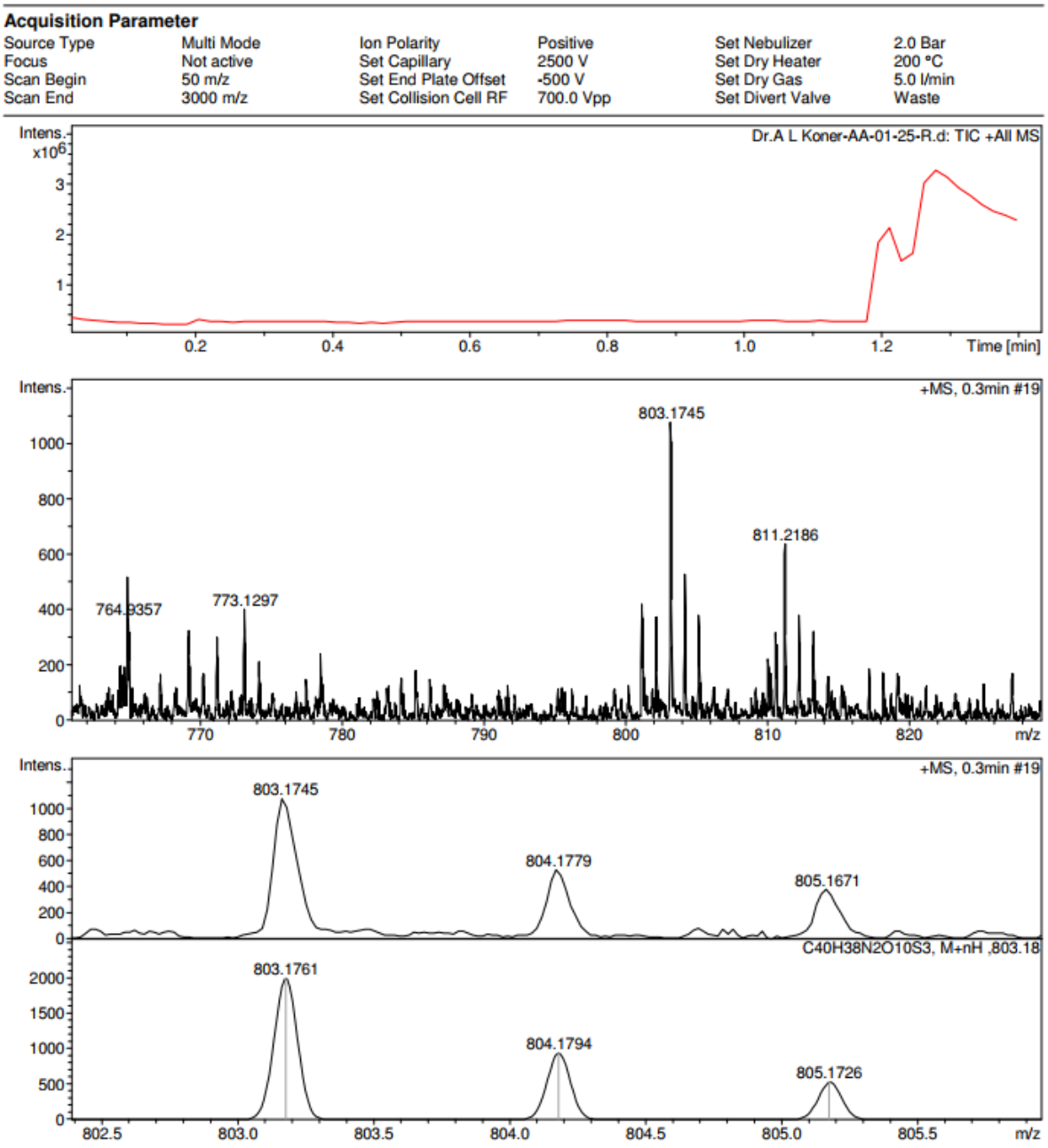


Fig. S31: APCI-MS of **6**; **Calculated mass** – 802.1689 Da and **Obtained mass** – *m/z* 803.1745 Da $[M+H]^+$

Co-ordinates for all optimized molecules from DFT calculation

SAN-PDI

C	1.406	-2.159	-0.470
C	0.788	-0.909	-0.439
C	1.473	0.313	-0.365
C	2.885	0.244	-0.356
C	3.529	-1.030	-0.364
C	2.813	-2.224	-0.418
C	3.612	1.448	-0.375
H	3.356	-3.162	-0.433
C	2.929	2.659	-0.445
C	1.522	2.714	-0.474
H	3.506	3.577	-0.490
C	-0.608	-0.953	-0.534
C	-1.375	0.221	-0.502
C	-1.138	-2.240	-0.621
C	-2.779	0.056	-0.523
C	-2.537	-2.396	-0.685
C	-3.335	-1.255	-0.633
H	-3.014	-3.367	-0.761
C	0.744	1.543	-0.385
C	-2.988	2.447	-0.235
C	-0.733	1.491	-0.375
C	-1.589	2.596	-0.192
H	-3.627	3.316	-0.118
C	-3.586	1.202	-0.408
C	5.011	-1.076	-0.334
C	5.093	1.419	-0.353
N	5.697	0.152	-0.292

O	5.634	-2.133	-0.344
O	5.764	2.445	-0.386
C	7.175	0.081	-0.267
H	7.460	-0.688	-0.986
H	7.538	1.045	-0.624
C	7.762	-0.254	1.121
H	7.251	-1.159	1.473
C	7.506	0.844	2.178
H	6.427	1.036	2.242
H	7.793	0.432	3.155
C	8.241	2.174	1.965
H	9.328	2.040	1.947
H	7.938	2.656	1.030
H	8.011	2.869	2.781
C	9.264	-0.595	0.989
H	9.717	-0.549	1.990
H	9.771	0.178	0.394
C	9.563	-1.976	0.387
H	9.071	-2.749	0.996
H	9.127	-2.060	-0.618
C	11.065	-2.281	0.301
H	11.507	-2.204	1.305
H	11.556	-1.510	-0.309
C	11.367	-3.664	-0.285
H	12.446	-3.851	-0.333
H	10.917	-4.459	0.323
H	10.966	-3.759	-1.302
C	-5.061	1.071	-0.443
C	-4.810	-1.404	-0.677

N	-5.578	-0.229	-0.558
O	-5.809	2.040	-0.375
O	-5.351	-2.497	-0.806
C	-7.051	-0.354	-0.616
H	-7.255	-1.312	-1.091
H	-7.408	0.448	-1.266
C	-7.746	-0.251	0.759
H	-7.402	0.687	1.216
C	-9.274	-0.101	0.562
H	-9.720	0.153	1.531
H	-9.452	0.772	-0.084
C	-10.006	-1.314	-0.036
H	-9.545	-1.588	-0.995
H	-9.885	-2.186	0.621
C	-11.508	-1.077	-0.276
H	-11.911	-1.933	-0.833
H	-11.636	-0.201	-0.928
C	-12.335	-0.886	1.002
H	-12.032	0.009	1.558
H	-13.400	-0.780	0.767
H	-12.226	-1.747	1.673
C	-7.345	-1.402	1.704
H	-7.641	-2.364	1.267
H	-6.250	-1.429	1.774
C	-7.918	-1.279	3.121
H	-7.656	-0.312	3.571
H	-9.010	-1.366	3.133
H	-7.519	-2.066	3.770
S	0.177	-3.434	-0.602

S	0.773	4.291	-0.862
S	-0.949	4.181	0.331

1O-SAN-PDI (1) structure a

C	1.386	-2.213	-0.654
C	0.769	-0.966	-0.546
C	1.454	0.246	-0.383
C	2.865	0.174	-0.342
C	3.508	-1.096	-0.435
C	2.790	-2.282	-0.591
C	3.598	1.372	-0.231
H	3.334	-3.217	-0.665
C	2.917	2.583	-0.223
C	1.511	2.643	-0.272
H	3.499	3.499	-0.185
C	-0.627	-1.004	-0.628
C	-1.391	0.163	-0.498
C	-1.160	-2.283	-0.791
C	-2.793	0.002	-0.510
C	-2.559	-2.434	-0.843
C	-3.353	-1.296	-0.700
H	-3.040	-3.396	-0.976
C	0.724	1.477	-0.313
C	-2.997	2.369	-0.067
C	-0.743	1.424	-0.293
C	-1.591	2.518	-0.033
H	-3.633	3.231	0.106
C	-3.596	1.141	-0.305
C	4.989	-1.150	-0.376

C	5.077	1.336	-0.170
N	5.676	0.067	-0.208
O	5.609	-2.203	-0.466
O	5.748	2.360	-0.090
C	7.154	-0.012	-0.149
H	7.457	-0.707	-0.933
H	7.526	0.981	-0.399
C	7.701	-0.485	1.215
H	7.187	-1.424	1.456
C	7.405	0.497	2.371
H	6.323	0.676	2.421
H	7.666	-0.013	3.309
C	8.135	1.846	2.319
H	9.223	1.720	2.323
H	7.858	2.419	1.429
H	7.872	2.451	3.195
C	9.209	-0.804	1.094
H	9.630	-0.863	2.108
H	9.728	0.031	0.602
C	9.537	-2.111	0.357
H	9.029	-2.946	0.862
H	9.136	-2.087	-0.666
C	11.043	-2.401	0.291
H	11.450	-2.430	1.311
H	11.549	-1.567	-0.215
C	11.373	-3.712	-0.430
H	12.455	-3.890	-0.460
H	10.908	-4.568	0.074
H	11.008	-3.698	-1.464

C	-5.073	1.014	-0.327
C	-4.830	-1.440	-0.729
N	-5.594	-0.275	-0.520
O	-5.816	1.978	-0.184
O	-5.374	-2.521	-0.922
C	-7.068	-0.394	-0.563
H	-7.281	-1.320	-1.096
H	-7.434	0.449	-1.153
C	-7.741	-0.381	0.827
H	-7.395	0.529	1.336
C	-9.273	-0.230	0.664
H	-9.704	-0.035	1.652
H	-9.466	0.676	0.071
C	-10.008	-1.413	0.010
H	-9.559	-1.633	-0.967
H	-9.875	-2.319	0.618
C	-11.514	-1.170	-0.197
H	-11.921	-1.998	-0.792
H	-11.653	-0.262	-0.802
C	-12.324	-1.048	1.100
H	-12.016	-0.183	1.697
H	-13.393	-0.934	0.884
H	-12.204	-1.943	1.724
C	-7.317	-1.586	1.692
H	-7.610	-2.522	1.200
H	-6.221	-1.607	1.746
C	-7.871	-1.557	3.122
H	-7.612	-0.619	3.628
H	-8.962	-1.654	3.142

H	-7.457	-2.380	3.715
S	0.154	-3.477	-0.861
S	0.879	4.312	-0.601
S	-0.986	4.099	0.488
O	0.629	4.391	-2.081

1O-SAN-PDI (1) structure b

C	1.425	-2.063	-0.508
C	0.795	-0.831	-0.473
C	1.471	0.394	-0.395
C	2.886	0.329	-0.375
C	3.539	-0.934	-0.381
C	2.823	-2.132	-0.457
C	3.611	1.539	-0.388
H	3.365	-3.071	-0.482
C	2.926	2.743	-0.465
C	1.515	2.795	-0.502
H	3.499	3.663	-0.504
C	-0.621	-0.875	-0.575
C	-1.381	0.302	-0.541
C	-1.165	-2.144	-0.666
C	-2.788	0.141	-0.547
C	-2.554	-2.304	-0.733
C	-3.353	-1.159	-0.658
H	-3.030	-3.275	-0.818
C	0.742	1.625	-0.418
C	-2.991	2.528	-0.233
C	-0.737	1.574	-0.406
C	-1.586	2.674	-0.202

H	-3.626	3.398	-0.102
C	-3.593	1.291	-0.412
C	5.021	-0.974	-0.334
C	5.094	1.518	-0.352
N	5.703	0.255	-0.286
O	5.644	-2.029	-0.339
O	5.757	2.549	-0.379
C	7.182	0.190	-0.246
H	7.476	-0.575	-0.965
H	7.543	1.156	-0.596
C	7.755	-0.147	1.148
H	7.247	-1.057	1.491
C	7.481	0.945	2.206
H	6.400	1.129	2.260
H	7.761	0.531	3.184
C	8.209	2.281	2.006
H	9.297	2.154	1.998
H	7.912	2.765	1.070
H	7.965	2.971	2.823
C	9.261	-0.478	1.030
H	9.702	-0.436	2.036
H	9.770	0.302	0.446
C	9.575	-1.854	0.421
H	9.079	-2.633	1.018
H	9.153	-1.932	-0.590
C	11.079	-2.150	0.354
H	11.508	-2.078	1.364
H	11.575	-1.371	-0.243
C	11.397	-3.526	-0.240

H	12.477	-3.707	-0.274
H	10.942	-4.328	0.356
H	11.010	-3.615	-1.263
C	-5.070	1.167	-0.433
C	-4.830	-1.304	-0.682
N	-5.594	-0.128	-0.552
O	-5.810	2.141	-0.352
O	-5.372	-2.396	-0.811
C	-7.069	-0.248	-0.598
H	-7.279	-1.203	-1.077
H	-7.427	0.559	-1.240
C	-7.751	-0.151	0.784
H	-7.400	0.782	1.244
C	-9.280	0.006	0.599
H	-9.717	0.254	1.574
H	-9.459	0.885	-0.038
C	-10.021	-1.199	-0.003
H	-9.569	-1.467	-0.967
H	-9.899	-2.077	0.646
C	-11.524	-0.954	-0.228
H	-11.935	-1.805	-0.789
H	-11.654	-0.073	-0.872
C	-12.340	-0.771	1.058
H	-12.029	0.117	1.619
H	-13.407	-0.659	0.833
H	-12.230	-1.639	1.721
C	-7.347	-1.311	1.717
H	-7.650	-2.269	1.276
H	-6.252	-1.343	1.779

C	-7.909	-1.195	3.139
H	-7.640	-0.234	3.594
H	-9.001	-1.278	3.159
H	-7.508	-1.989	3.780
S	0.184	-3.393	-0.819
S	0.766	4.375	-0.876
S	-0.945	4.257	0.326
O	0.149	-4.427	0.286

2O-SAN-PDI (2) structure a

C	1.352	-2.324	-0.651
C	0.741	-1.074	-0.547
C	1.432	0.134	-0.390
C	2.844	0.061	-0.353
C	3.481	-1.213	-0.440
C	2.758	-2.396	-0.589
C	3.581	1.256	-0.247
H	3.298	-3.334	-0.658
C	2.911	2.474	-0.246
C	1.509	2.521	-0.302
H	3.484	3.394	-0.206
C	-0.655	-1.103	-0.629
C	-1.414	0.067	-0.501
C	-1.193	-2.381	-0.787
C	-2.818	-0.089	-0.510
C	-2.594	-2.526	-0.838
C	-3.383	-1.386	-0.698
H	-3.078	-3.487	-0.968
C	0.708	1.364	-0.328

C	-3.014	2.279	-0.067
C	-0.763	1.326	-0.299
C	-1.611	2.422	-0.038
H	-3.649	3.142	0.107
C	-3.617	1.051	-0.306
C	4.962	-1.273	-0.380
C	5.062	1.213	-0.181
N	5.654	-0.059	-0.214
O	5.576	-2.330	-0.466
O	5.735	2.234	-0.102
C	7.132	-0.145	-0.152
H	7.433	-0.843	-0.933
H	7.509	0.845	-0.404
C	7.674	-0.616	1.215
H	7.154	-1.551	1.459
C	7.382	0.372	2.367
H	6.301	0.558	2.415
H	7.638	-0.136	3.307
C	8.120	1.716	2.311
H	9.208	1.584	2.317
H	7.848	2.288	1.418
H	7.860	2.327	3.183
C	9.180	-0.945	1.098
H	9.598	-1.004	2.112
H	9.706	-0.115	0.604
C	9.501	-2.256	0.365
H	8.986	-3.087	0.869
H	9.104	-2.231	-0.660
C	11.005	-2.556	0.304

H	11.409	-2.587	1.326
H	11.519	-1.727	-0.202
C	11.329	-3.871	-0.413
H	12.409	-4.057	-0.440
H	10.856	-4.723	0.090
H	10.967	-3.857	-1.449
C	-5.095	0.929	-0.327
C	-4.861	-1.524	-0.725
N	-5.621	-0.357	-0.517
O	-5.832	1.898	-0.185
O	-5.409	-2.604	-0.916
C	-7.096	-0.470	-0.560
H	-7.313	-1.395	-1.092
H	-7.458	0.373	-1.152
C	-7.768	-0.452	0.830
H	-7.418	0.457	1.338
C	-9.299	-0.293	0.667
H	-9.729	-0.095	1.655
H	-9.488	0.615	0.074
C	-10.041	-1.471	0.014
H	-9.593	-1.694	-0.964
H	-9.912	-2.378	0.621
C	-11.545	-1.221	-0.192
H	-11.957	-2.047	-0.788
H	-11.680	-0.313	-0.797
C	-12.354	-1.095	1.105
H	-12.042	-0.231	1.702
H	-13.423	-0.976	0.890
H	-12.238	-1.990	1.729

C	-7.351	-1.658	1.696
H	-7.649	-2.593	1.204
H	-6.255	-1.685	1.750
C	-7.905	-1.625	3.125
H	-7.641	-0.688	3.631
H	-8.996	-1.717	3.146
H	-7.495	-2.450	3.719
S	0.114	-3.581	-0.852
S	0.774	4.117	-0.627
S	-1.008	4.001	0.526
O	0.427	4.171	-2.053
O	1.589	5.180	-0.028

2O-SAN-PDI (2) structure b

C	1.409	-2.145	-0.507
C	0.778	-0.914	-0.453
C	1.453	0.308	-0.335
C	2.868	0.245	-0.303
C	3.522	-1.015	-0.347
C	2.804	-2.213	-0.438
C	3.597	1.454	-0.247
H	3.348	-3.151	-0.465
C	2.911	2.656	-0.288
C	1.500	2.709	-0.333
H	3.488	3.576	-0.291
C	-0.638	-0.956	-0.536
C	-1.395	0.218	-0.449
C	-1.183	-2.225	-0.644
C	-2.800	0.058	-0.461

C	-2.572	-2.383	-0.684
C	-3.368	-1.235	-0.602
H	-3.050	-3.353	-0.768
C	0.720	1.542	-0.316
C	-3.004	2.439	-0.102
C	-0.749	1.487	-0.292
C	-1.592	2.589	-0.075
H	-3.637	3.309	0.037
C	-3.605	1.210	-0.299
C	5.003	-1.058	-0.299
C	5.078	1.432	-0.193
N	5.685	0.167	-0.185
O	5.626	-2.112	-0.350
O	5.739	2.463	-0.158
C	7.164	0.099	-0.135
H	7.464	-0.630	-0.889
H	7.529	1.081	-0.434
C	7.725	-0.307	1.245
H	7.210	-1.231	1.538
C	7.445	0.733	2.353
H	6.363	0.918	2.406
H	7.715	0.271	3.312
C	8.178	2.075	2.224
H	9.266	1.945	2.220
H	7.891	2.604	1.310
H	7.929	2.724	3.071
C	9.230	-0.638	1.123
H	9.663	-0.643	2.134
H	9.746	0.167	0.580

C	9.544	-1.985	0.455
H	9.042	-2.789	1.012
H	9.128	-2.016	-0.562
C	11.048	-2.282	0.383
H	11.471	-2.256	1.398
H	11.550	-1.479	-0.176
C	11.365	-3.632	-0.269
H	12.446	-3.814	-0.305
H	10.906	-4.458	0.288
H	10.985	-3.674	-1.297
C	-5.083	1.088	-0.323
C	-4.846	-1.375	-0.638
N	-5.608	-0.202	-0.474
O	-5.820	2.061	-0.215
O	-5.388	-2.461	-0.796
C	-7.084	-0.318	-0.525
H	-7.295	-1.260	-1.028
H	-7.440	0.505	-1.147
C	-7.767	-0.255	0.858
H	-7.416	0.667	1.341
C	-9.296	-0.095	0.677
H	-9.733	0.131	1.657
H	-9.475	0.797	0.059
C	-10.036	-1.287	0.049
H	-9.582	-1.536	-0.919
H	-9.915	-2.179	0.681
C	-11.538	-1.038	-0.174
H	-11.948	-1.877	-0.752
H	-11.667	-0.144	-0.801

C	-12.357	-0.879	1.114
H	-12.046	-0.001	1.692
H	-13.423	-0.762	0.889
H	-12.248	-1.759	1.760
C	-7.362	-1.436	1.764
H	-7.661	-2.384	1.298
H	-6.267	-1.467	1.826
C	-7.926	-1.357	3.187
H	-7.660	-0.406	3.667
H	-9.018	-1.443	3.203
H	-7.524	-2.166	3.809
S	0.150	-3.496	-0.505
S	0.867	4.362	-0.734
S	-0.997	4.194	0.363
O	0.620	4.375	-2.215
O	0.242	-4.380	-1.730

2O-SAN-PDI (2) structure c

C	1.454	-2.341	-0.477
C	0.828	-1.099	-0.396
C	1.504	0.126	-0.295
C	2.917	0.074	-0.298
C	3.572	-1.195	-0.348
C	2.864	-2.392	-0.438
C	3.634	1.283	-0.293
H	3.416	-3.324	-0.490
C	2.937	2.489	-0.355
C	1.533	2.529	-0.346
H	3.507	3.410	-0.418

C	-0.567	-1.150	-0.486
C	-1.339	0.016	-0.404
C	-1.091	-2.434	-0.627
C	-2.742	-0.142	-0.451
C	-2.492	-2.587	-0.705
C	-3.293	-1.450	-0.617
H	-2.967	-3.554	-0.822
C	0.768	1.349	-0.270
C	-2.956	2.236	-0.055
C	-0.703	1.279	-0.223
C	-1.560	2.365	0.015
H	-3.581	3.106	0.112
C	-3.551	1.001	-0.309
C	5.055	-1.229	-0.330
C	5.116	1.266	-0.283
N	5.730	0.003	-0.261
C	7.210	-0.055	-0.245
H	7.496	-0.805	-0.983
H	7.562	0.919	-0.582
C	7.806	-0.416	1.133
H	7.301	-1.331	1.469
C	7.552	0.659	2.214
H	6.472	0.845	2.288
H	7.847	0.228	3.180
C	8.280	1.996	2.024
H	9.367	1.866	1.996
H	7.969	2.496	1.101
H	8.052	2.672	2.856
C	9.309	-0.748	0.984

H	9.768	-0.716	1.983
H	9.808	0.038	0.399
C	9.610	-2.117	0.356
H	9.127	-2.902	0.956
H	9.165	-2.186	-0.646
C	11.112	-2.412	0.253
H	11.563	-2.348	1.254
H	11.594	-1.629	-0.349
C	11.416	-3.785	-0.357
H	12.496	-3.965	-0.417
H	10.976	-4.591	0.243
H	11.007	-3.866	-1.372
C	-5.025	0.869	-0.376
C	-4.769	-1.598	-0.684
N	-5.538	-0.428	-0.539
C	-7.011	-0.551	-0.619
H	-7.208	-1.496	-1.123
H	-7.360	0.269	-1.250
C	-7.722	-0.488	0.750
H	-7.392	0.441	1.234
C	-9.249	-0.345	0.539
H	-9.708	-0.116	1.508
H	-9.427	0.539	-0.091
C	-9.965	-1.552	-0.092
H	-9.490	-1.804	-1.050
H	-9.845	-2.436	0.549
C	-11.465	-1.321	-0.344
H	-11.856	-2.170	-0.922
H	-11.592	-0.434	-0.982

C	-12.308	-1.160	0.927
H	-12.018	-0.274	1.503
H	-13.372	-1.057	0.682
H	-12.201	-2.033	1.583
C	-7.322	-1.658	1.671
H	-7.602	-2.612	1.206
H	-6.228	-1.676	1.756
C	-7.915	-1.576	3.083
H	-7.670	-0.619	3.561
H	-9.006	-1.674	3.078
H	-7.517	-2.376	3.718
S	0.232	-3.618	-0.656
S	0.805	4.137	-0.822
S	-0.915	3.899	0.726
O	0.256	3.973	-2.219
O	-1.929	4.988	0.473
O	-5.773	1.836	-0.290
O	-5.305	-2.687	-0.855
O	5.685	-2.280	-0.371
O	5.774	2.300	-0.294

2O-SAN-PDI (2) structure d

C	1.442	-2.003	-0.373
C	0.795	-0.783	-0.382
C	1.468	0.446	-0.340
C	2.883	0.387	-0.332
C	3.545	-0.869	-0.300
C	2.837	-2.073	-0.319
C	3.606	1.599	-0.394

H	3.379	-3.012	-0.307
C	2.917	2.795	-0.507
C	1.504	2.842	-0.534
H	3.487	3.716	-0.584
C	-0.629	-0.831	-0.486
C	-1.387	0.348	-0.489
C	-1.189	-2.093	-0.540
C	-2.795	0.189	-0.505
C	-2.575	-2.260	-0.603
C	-3.367	-1.109	-0.582
H	-3.049	-3.233	-0.652
C	0.736	1.675	-0.402
C	-2.998	2.584	-0.265
C	-0.744	1.623	-0.389
C	-1.592	2.729	-0.227
H	-3.631	3.460	-0.168
C	-3.601	1.346	-0.413
C	5.029	-0.902	-0.272
C	5.090	1.586	-0.372
N	5.706	0.329	-0.271
C	7.186	0.271	-0.248
H	7.473	-0.516	-0.946
H	7.539	1.226	-0.635
C	7.778	-0.018	1.148
H	7.279	-0.919	1.526
C	7.511	1.107	2.173
H	6.430	1.287	2.235
H	7.806	0.726	3.161
C	8.229	2.439	1.920

H	9.318	2.318	1.904
H	7.919	2.890	0.972
H	7.990	3.154	2.716
C	9.284	-0.345	1.021
H	9.736	-0.270	2.020
H	9.782	0.419	0.408
C	9.598	-1.737	0.452
H	9.112	-2.500	1.077
H	9.167	-1.849	-0.552
C	11.103	-2.029	0.378
H	11.541	-1.925	1.381
H	11.589	-1.266	-0.247
C	11.421	-3.421	-0.176
H	12.502	-3.599	-0.216
H	10.976	-4.206	0.448
H	11.025	-3.543	-1.192
C	-5.078	1.226	-0.448
C	-4.846	-1.250	-0.621
N	-5.606	-0.070	-0.533
C	-7.081	-0.186	-0.590
H	-7.291	-1.155	-1.042
H	-7.430	0.602	-1.261
C	-7.776	-0.044	0.781
H	-7.426	0.901	1.216
C	-9.303	0.113	0.577
H	-9.748	0.393	1.539
H	-9.473	0.972	-0.089
C	-10.044	-1.107	0.006
H	-9.585	-1.406	-0.946

H	-9.929	-1.966	0.683
C	-11.544	-0.865	-0.238
H	-11.953	-1.730	-0.777
H	-11.665	-0.003	-0.910
C	-12.369	-0.640	1.035
H	-12.060	0.264	1.571
H	-13.434	-0.531	0.797
H	-12.267	-1.487	1.724
C	-7.386	-1.176	1.754
H	-7.689	-2.146	1.339
H	-6.292	-1.210	1.827
C	-7.961	-1.014	3.166
H	-7.693	-0.039	3.594
H	-9.054	-1.093	3.178
H	-7.569	-1.789	3.834
S	0.171	-3.314	-0.478
S	0.754	4.407	-0.960
S	-0.954	4.328	0.250
O	-5.814	2.205	-0.404
O	-5.385	-2.344	-0.722
O	5.654	-1.956	-0.249
O	5.746	2.619	-0.439
O	0.278	-4.037	-1.754
O	0.118	-4.085	0.774

3O-SAN-PDI (3) structure a

C	1.420	-2.453	-0.539
C	0.802	-1.204	-0.526
C	1.484	0.019	-0.470

C	2.896	-0.044	-0.430
C	3.542	-1.318	-0.419
C	2.829	-2.512	-0.475
C	3.622	1.159	-0.423
H	3.375	-3.450	-0.473
C	2.940	2.369	-0.529
C	1.540	2.411	-0.597
H	3.508	3.293	-0.576
C	-0.594	-1.252	-0.607
C	-1.362	-0.082	-0.561
C	-1.122	-2.540	-0.674
C	-2.768	-0.243	-0.563
C	-2.524	-2.695	-0.718
C	-3.323	-1.555	-0.663
H	-3.001	-3.666	-0.781
C	0.754	1.247	-0.504
C	-2.983	2.145	-0.258
C	-0.720	1.189	-0.446
C	-1.587	2.278	-0.247
H	-3.612	3.018	-0.121
C	-3.578	0.900	-0.441
C	5.025	-1.362	-0.359
C	5.104	1.133	-0.359
N	5.707	-0.133	-0.293
C	7.186	-0.202	-0.235
H	7.487	-0.963	-0.956
H	7.554	0.766	-0.574
C	7.741	-0.550	1.163
H	7.225	-1.461	1.494

C	7.458	0.536	2.225
H	6.377	0.724	2.267
H	7.725	0.114	3.204
C	8.194	1.871	2.044
H	9.282	1.739	2.050
H	7.912	2.362	1.107
H	7.942	2.555	2.862
C	9.247	-0.886	1.061
H	9.676	-0.852	2.073
H	9.766	-0.103	0.489
C	9.564	-2.258	0.447
H	9.058	-3.040	1.033
H	9.154	-2.328	-0.570
C	11.068	-2.559	0.395
H	11.484	-2.496	1.411
H	11.573	-1.778	-0.190
C	11.387	-3.933	-0.203
H	12.467	-4.118	-0.226
H	10.923	-4.737	0.382
H	11.013	-4.014	-1.231
C	-5.054	0.766	-0.468
C	-4.800	-1.708	-0.690
N	-5.569	-0.535	-0.571
C	-7.044	-0.663	-0.615
H	-7.249	-1.625	-1.081
H	-7.407	0.134	-1.267
C	-7.725	-0.551	0.766
H	-7.378	0.390	1.214
C	-9.255	-0.405	0.582

H	-9.692	-0.147	1.554
H	-9.440	0.463	-0.067
C	-9.990	-1.623	-0.001
H	-9.539	-1.903	-0.962
H	-9.861	-2.492	0.660
C	-11.495	-1.390	-0.226
H	-11.902	-2.251	-0.774
H	-11.631	-0.519	-0.883
C	-12.309	-1.193	1.058
H	-12.002	-0.295	1.606
H	-13.377	-1.091	0.834
H	-12.192	-2.051	1.734
C	-7.313	-1.696	1.715
H	-7.610	-2.661	1.287
H	-6.217	-1.720	1.775
C	-7.873	-1.564	3.136
H	-7.609	-0.595	3.578
H	-8.964	-1.654	3.159
H	-7.466	-2.347	3.786
S	0.194	-3.730	-0.651
S	0.855	4.020	-1.113
S	-0.934	3.868	0.299
O	-5.798	1.737	-0.403
O	-5.336	-2.803	-0.807
O	5.647	-2.417	-0.362
O	5.769	2.162	-0.367
O	-1.898	4.916	-0.079
O	1.781	5.089	-0.606
O	-0.473	3.750	1.695

3O-SAN-PDI (3) structure b

C	1.477	-2.113	-0.251
C	0.823	-0.895	-0.303
C	1.488	0.335	-0.341
C	2.902	0.283	-0.359
C	3.572	-0.964	-0.282
C	2.871	-2.174	-0.227
C	3.617	1.498	-0.491
H	3.420	-3.107	-0.184
C	2.923	2.682	-0.634
C	1.502	2.726	-0.631
H	3.486	3.601	-0.753
C	-0.601	-0.955	-0.379
C	-1.363	0.219	-0.440
C	-1.156	-2.221	-0.380
C	-2.770	0.057	-0.484
C	-2.539	-2.393	-0.448
C	-3.336	-1.245	-0.501
H	-3.012	-3.368	-0.457
C	0.747	1.559	-0.441
C	-2.987	2.458	-0.404
C	-0.722	1.503	-0.407
C	-1.583	2.608	-0.348
H	-3.628	3.334	-0.369
C	-3.583	1.213	-0.496
C	5.057	-0.988	-0.285
C	5.103	1.493	-0.500
N	5.727	0.245	-0.355

C	7.208	0.195	-0.357
H	7.487	-0.626	-1.018
H	7.548	1.131	-0.799
C	7.826	-0.018	1.042
H	7.336	-0.898	1.477
C	7.575	1.160	2.010
H	6.494	1.343	2.080
H	7.886	0.832	3.012
C	8.287	2.477	1.675
H	9.376	2.355	1.649
H	7.962	2.876	0.709
H	8.061	3.233	2.435
C	9.330	-0.349	0.907
H	9.800	-0.216	1.891
H	9.814	0.380	0.242
C	9.637	-1.771	0.412
H	9.165	-2.498	1.089
H	9.188	-1.940	-0.576
C	11.141	-2.063	0.327
H	11.598	-1.899	1.314
H	11.614	-1.338	-0.351
C	11.453	-3.486	-0.149
H	12.534	-3.663	-0.198
H	11.023	-4.233	0.529
H	11.039	-3.669	-1.148
C	-5.058	1.085	-0.565
C	-4.813	-1.395	-0.566
N	-5.580	-0.216	-0.575
C	-7.053	-0.342	-0.665

H	-7.246	-1.340	-1.055
H	-7.383	0.397	-1.398
C	-7.787	-0.109	0.673
H	-7.450	0.865	1.052
C	-9.307	0.030	0.415
H	-9.780	0.375	1.342
H	-9.458	0.839	-0.315
C	-10.030	-1.230	-0.090
H	-9.540	-1.598	-1.001
H	-9.940	-2.036	0.652
C	-11.521	-1.007	-0.401
H	-11.914	-1.912	-0.885
H	-11.618	-0.200	-1.141
C	-12.387	-0.685	0.822
H	-12.094	0.258	1.297
H	-13.443	-0.597	0.543
H	-12.309	-1.477	1.579
C	-7.424	-1.170	1.731
H	-7.717	-2.167	1.377
H	-6.332	-1.199	1.836
C	-8.036	-0.912	3.113
H	-7.777	0.089	3.480
H	-9.128	-0.989	3.101
H	-7.664	-1.640	3.843
S	0.210	-3.434	-0.274
S	0.788	4.299	-0.999
S	-1.069	4.285	0.124
O	-5.795	2.063	-0.611
O	-5.346	-2.496	-0.609

O	5.687	-2.037	-0.226
O	5.750	2.524	-0.630
O	0.304	-4.216	-1.515
O	0.175	-4.142	1.014
O	-0.801	4.245	1.600

3O-SAN-PDI (3) structure c

C	1.475	-2.246	-0.503
C	0.835	-1.024	-0.424
C	1.503	0.205	-0.325
C	2.918	0.159	-0.317
C	3.583	-1.098	-0.361
C	2.876	-2.299	-0.468
C	3.632	1.375	-0.311
H	3.428	-3.230	-0.528
C	2.932	2.573	-0.383
C	1.522	2.608	-0.380
H	3.497	3.498	-0.444
C	-0.581	-1.076	-0.520
C	-1.346	0.094	-0.440
C	-1.120	-2.341	-0.660
C	-2.752	-0.061	-0.470
C	-2.511	-2.497	-0.742
C	-3.313	-1.357	-0.634
H	-2.985	-3.464	-0.868
C	0.766	1.430	-0.305
C	-2.959	2.313	-0.056
C	-0.708	1.357	-0.253
C	-1.557	2.438	0.004

H	-3.578	3.187	0.121
C	-3.558	1.088	-0.313
C	5.067	-1.125	-0.326
C	5.116	1.368	-0.289
N	5.736	0.110	-0.256
C	7.217	0.059	-0.226
H	7.513	-0.692	-0.959
H	7.567	1.033	-0.563
C	7.800	-0.295	1.159
H	7.297	-1.211	1.494
C	7.531	0.783	2.233
H	6.449	0.963	2.297
H	7.819	0.356	3.204
C	8.253	2.123	2.045
H	9.342	1.999	2.028
H	7.950	2.618	1.117
H	8.014	2.801	2.872
C	9.306	-0.621	1.026
H	9.755	-0.584	2.029
H	9.807	0.165	0.444
C	9.618	-1.991	0.406
H	9.132	-2.776	1.003
H	9.185	-2.065	-0.601
C	11.123	-2.281	0.319
H	11.563	-2.212	1.324
H	11.608	-1.498	-0.280
C	11.438	-3.654	-0.283
H	12.519	-3.831	-0.331
H	10.994	-4.460	0.315

H	11.040	-3.740	-1.302
C	-5.036	0.964	-0.367
C	-4.791	-1.500	-0.683
N	-5.556	-0.329	-0.529
C	-7.030	-0.447	-0.598
H	-7.234	-1.390	-1.103
H	-7.381	0.375	-1.225
C	-7.730	-0.385	0.777
H	-7.391	0.541	1.262
C	-9.258	-0.234	0.577
H	-9.708	-0.006	1.550
H	-9.435	0.654	-0.047
C	-9.984	-1.434	-0.053
H	-9.518	-1.685	-1.015
H	-9.865	-2.321	0.584
C	-11.485	-1.194	-0.294
H	-11.884	-2.038	-0.872
H	-11.612	-0.304	-0.928
C	-12.318	-1.033	0.984
H	-12.019	-0.151	1.561
H	-13.383	-0.924	0.746
H	-12.211	-1.909	1.636
C	-7.329	-1.561	1.691
H	-7.618	-2.512	1.225
H	-6.235	-1.585	1.767
C	-7.911	-1.481	3.107
H	-7.657	-0.527	3.586
H	-9.003	-1.573	3.110
H	-7.512	-2.285	3.736

S	0.241	-3.575	-0.867
S	0.790	4.221	-0.847
S	-0.906	3.968	0.722
O	-5.776	1.935	-0.272
O	-5.328	-2.588	-0.850
O	5.698	-2.174	-0.357
O	5.765	2.407	-0.298
O	0.215	-4.655	0.190
O	0.243	4.058	-2.243
O	-1.930	5.053	0.500

3O-SAN-PDI (3) structure d

C	1.501	-2.270	-0.377
C	0.857	-1.045	-0.379
C	1.521	0.189	-0.375
C	2.934	0.140	-0.383
C	3.602	-1.113	-0.348
C	2.900	-2.322	-0.357
C	3.647	1.357	-0.466
H	3.453	-3.255	-0.356
C	2.952	2.548	-0.574
C	1.535	2.588	-0.578
H	3.516	3.470	-0.658
C	-0.558	-1.110	-0.456
C	-1.329	0.059	-0.475
C	-1.092	-2.385	-0.502
C	-2.735	-0.107	-0.508
C	-2.479	-2.555	-0.576
C	-3.289	-1.414	-0.566

H	-2.948	-3.532	-0.628
C	0.777	1.413	-0.435
C	-2.971	2.292	-0.345
C	-0.694	1.340	-0.397
C	-1.569	2.429	-0.285
H	-3.604	3.170	-0.281
C	-3.555	1.043	-0.475
C	5.087	-1.135	-0.334
C	5.133	1.353	-0.463
N	5.756	0.102	-0.356
C	7.237	0.053	-0.345
H	7.523	-0.744	-1.032
H	7.580	1.004	-0.752
C	7.843	-0.207	1.051
H	7.348	-1.101	1.452
C	7.584	0.939	2.055
H	6.503	1.121	2.122
H	7.887	0.578	3.048
C	8.301	2.265	1.769
H	9.389	2.143	1.747
H	7.984	2.696	0.814
H	8.068	2.997	2.552
C	9.347	-0.536	0.917
H	9.809	-0.436	1.910
H	9.838	0.214	0.281
C	9.657	-1.941	0.379
H	9.178	-2.689	1.028
H	9.215	-2.077	-0.618
C	11.161	-2.233	0.296

H	11.610	-2.102	1.291
H	11.640	-1.487	-0.354
C	11.475	-3.639	-0.225
H	12.555	-3.817	-0.272
H	11.038	-4.408	0.425
H	11.068	-3.788	-1.233
C	-5.030	0.905	-0.541
C	-4.765	-1.573	-0.619
N	-5.540	-0.399	-0.587
C	-7.013	-0.534	-0.668
H	-7.202	-1.522	-1.086
H	-7.356	0.223	-1.376
C	-7.737	-0.347	0.682
H	-7.407	0.620	1.086
C	-9.261	-0.219	0.443
H	-9.728	0.095	1.383
H	-9.428	0.609	-0.263
C	-9.974	-1.473	-0.090
H	-9.491	-1.808	-1.017
H	-9.866	-2.298	0.627
C	-11.471	-1.260	-0.378
H	-11.858	-2.154	-0.884
H	-11.587	-0.432	-1.092
C	-12.327	-0.985	0.865
H	-12.040	-0.053	1.364
H	-13.388	-0.902	0.600
H	-12.230	-1.798	1.596
C	-7.351	-1.433	1.707
H	-7.635	-2.422	1.328

H	-6.258	-1.451	1.802
C	-7.954	-1.221	3.101
H	-7.705	-0.227	3.494
H	-9.046	-1.311	3.096
H	-7.566	-1.963	3.808
S	0.270	-3.627	-0.622
S	0.822	4.179	-0.938
S	-0.950	4.027	0.224
O	-5.774	1.878	-0.554
O	-5.292	-2.676	-0.689
O	5.720	-2.183	-0.305
O	5.778	2.390	-0.550
O	-1.848	5.087	-0.246
O	-0.593	3.937	1.644
O	0.259	-4.618	0.521

4O-SAN-PDI (4) structure a

C	1.493	-2.188	-0.355
C	0.837	-0.976	-0.316
C	1.501	0.258	-0.255
C	2.917	0.217	-0.264
C	3.590	-1.034	-0.274
C	2.891	-2.243	-0.321
C	3.627	1.436	-0.311
H	3.444	-3.176	-0.346
C	2.921	2.627	-0.418
C	1.511	2.657	-0.401
H	3.482	3.550	-0.519
C	-0.589	-1.033	-0.410

C	-1.352	0.140	-0.363
C	-1.143	-2.292	-0.514
C	-2.758	-0.011	-0.403
C	-2.530	-2.455	-0.590
C	-3.326	-1.306	-0.535
H	-3.004	-3.425	-0.680
C	0.760	1.481	-0.272
C	-2.964	2.374	-0.059
C	-0.714	1.408	-0.213
C	-1.561	2.497	0.008
H	-3.581	3.255	0.087
C	-3.564	1.145	-0.287
C	5.076	-1.054	-0.262
C	5.111	1.437	-0.310
N	5.739	0.185	-0.243
C	7.221	0.141	-0.235
H	7.509	-0.629	-0.951
H	7.560	1.107	-0.606
C	7.828	-0.170	1.150
H	7.341	-1.083	1.515
C	7.559	0.932	2.200
H	6.476	1.101	2.274
H	7.865	0.534	3.177
C	8.263	2.276	1.968
H	9.352	2.165	1.942
H	7.942	2.743	1.032
H	8.024	2.973	2.781
C	9.335	-0.480	1.004
H	9.795	-0.420	2.001

H	9.821	0.302	0.403
C	9.658	-1.857	0.404
H	9.182	-2.637	1.016
H	9.221	-1.950	-0.600
C	11.165	-2.133	0.315
H	11.609	-2.046	1.317
H	11.640	-1.353	-0.298
C	11.491	-3.510	-0.271
H	12.574	-3.677	-0.321
H	11.058	-4.312	0.340
H	11.090	-3.614	-1.286
C	-5.041	1.026	-0.358
C	-4.805	-1.445	-0.603
N	-5.566	-0.268	-0.494
C	-7.040	-0.381	-0.588
H	-7.239	-1.335	-1.074
H	-7.373	0.428	-1.242
C	-7.766	-0.281	0.771
H	-7.428	0.653	1.241
C	-9.288	-0.121	0.537
H	-9.755	0.130	1.496
H	-9.445	0.756	-0.109
C	-10.011	-1.327	-0.085
H	-9.529	-1.600	-1.033
H	-9.911	-2.204	0.571
C	-11.506	-1.081	-0.359
H	-11.900	-1.933	-0.929
H	-11.613	-0.202	-1.010
C	-12.362	-0.891	0.900

H	-12.067	-0.001	1.467
H	-13.421	-0.778	0.640
H	-12.274	-1.756	1.569
C	-7.394	-1.439	1.718
H	-7.681	-2.398	1.267
H	-6.301	-1.472	1.818
C	-8.003	-1.324	3.120
H	-7.751	-0.361	3.584
H	-9.096	-1.407	3.103
H	-7.624	-2.117	3.774
S	0.228	-3.508	-0.498
S	0.770	4.250	-0.925
S	-0.908	4.050	0.672
O	-5.776	2.003	-0.299
O	-5.341	-2.536	-0.747
O	5.709	-2.102	-0.268
O	5.753	2.479	-0.363
O	0.337	-4.184	-1.798
O	0.213	4.028	-2.308
O	-1.939	5.123	0.428
O	0.185	-4.316	0.729

4O-SAN-PDI (4) structure b

C	1.438	-2.363	-0.600
C	0.807	-1.134	-0.583
C	1.482	0.092	-0.522
C	2.895	0.034	-0.468
C	3.551	-1.228	-0.456
C	2.838	-2.427	-0.538

C	3.619	1.244	-0.450
H	3.382	-3.365	-0.548
C	2.937	2.447	-0.562
C	1.532	2.484	-0.644
H	3.499	3.374	-0.598
C	-0.609	-1.181	-0.665
C	-1.371	-0.005	-0.614
C	-1.155	-2.449	-0.737
C	-2.778	-0.161	-0.593
C	-2.547	-2.605	-0.777
C	-3.345	-1.462	-0.692
H	-3.025	-3.576	-0.847
C	0.753	1.322	-0.556
C	-2.983	2.223	-0.261
C	-0.725	1.265	-0.492
C	-1.580	2.351	-0.267
H	-3.604	3.099	-0.107
C	-3.584	0.988	-0.448
C	5.033	-1.266	-0.372
C	5.102	1.225	-0.363
N	5.710	-0.037	-0.287
C	7.188	-0.099	-0.193
H	7.511	-0.847	-0.918
H	7.558	0.875	-0.509
C	7.710	-0.466	1.213
H	7.212	-1.399	1.505
C	7.361	0.584	2.292
H	6.274	0.738	2.305
H	7.608	0.143	3.268

C	8.061	1.944	2.170
H	9.151	1.845	2.214
H	7.799	2.450	1.235
H	7.758	2.600	2.994
C	9.227	-0.753	1.152
H	9.616	-0.751	2.180
H	9.742	0.069	0.634
C	9.611	-2.087	0.493
H	9.094	-2.908	1.012
H	9.259	-2.117	-0.548
C	11.123	-2.350	0.509
H	11.482	-2.328	1.548
H	11.638	-1.528	-0.009
C	11.510	-3.684	-0.138
H	12.594	-3.842	-0.110
H	11.036	-4.527	0.380
H	11.194	-3.721	-1.188
C	-5.063	0.863	-0.456
C	-4.824	-1.607	-0.691
N	-5.586	-0.432	-0.558
C	-7.063	-0.553	-0.582
H	-7.279	-1.512	-1.051
H	-7.429	0.249	-1.227
C	-7.724	-0.444	0.808
H	-7.365	0.491	1.258
C	-9.255	-0.285	0.645
H	-9.678	-0.030	1.624
H	-9.442	0.590	0.005
C	-10.008	-1.492	0.061

H	-9.571	-1.767	-0.908
H	-9.877	-2.367	0.713
C	-11.513	-1.245	-0.143
H	-11.934	-2.098	-0.693
H	-11.651	-0.368	-0.791
C	-12.310	-1.053	1.154
H	-11.988	-0.162	1.705
H	-13.379	-0.940	0.943
H	-12.191	-1.917	1.820
C	-7.309	-1.598	1.744
H	-7.620	-2.559	1.314
H	-6.214	-1.633	1.791
C	-7.850	-1.472	3.173
H	-7.573	-0.508	3.618
H	-8.942	-1.552	3.209
H	-7.442	-2.262	3.813
S	0.196	-3.697	-0.906
S	0.845	4.098	-1.150
S	-0.921	3.940	0.290
O	-5.797	1.840	-0.376
O	-5.363	-2.701	-0.804
O	5.655	-2.321	-0.374
O	5.758	2.259	-0.359
O	-1.893	4.985	-0.070
O	1.786	5.159	-0.659
O	-0.449	3.804	1.679
O	0.170	-4.737	0.191

4O-SAN-PDI (4) structure c

C	1.420	-2.511	-0.516
C	0.802	-1.262	-0.459
C	1.484	-0.041	-0.377
C	2.898	-0.107	-0.363
C	3.544	-1.381	-0.392
C	2.829	-2.573	-0.470
C	3.632	1.090	-0.342
H	3.373	-3.510	-0.501
C	2.957	2.305	-0.397
C	1.556	2.346	-0.434
H	3.528	3.227	-0.419
C	-0.593	-1.308	-0.537
C	-1.363	-0.140	-0.466
C	-1.118	-2.595	-0.647
C	-2.769	-0.307	-0.495
C	-2.519	-2.754	-0.708
C	-3.320	-1.618	-0.633
H	-2.993	-3.724	-0.803
C	0.753	1.188	-0.372
C	-3.003	2.073	-0.166
C	-0.724	1.130	-0.315
C	-1.609	2.210	-0.115
H	-3.640	2.941	-0.034
C	-3.588	0.828	-0.373
C	5.027	-1.431	-0.355
C	5.116	1.059	-0.303
N	5.716	-0.207	-0.274
O	5.644	-2.489	-0.389

O	5.780	2.088	-0.299
C	7.196	-0.282	-0.238
H	7.484	-1.031	-0.976
H	7.563	0.690	-0.565
C	7.768	-0.656	1.146
H	7.249	-1.568	1.471
C	7.510	0.416	2.229
H	6.431	0.613	2.289
H	7.787	-0.023	3.197
C	8.255	1.747	2.056
H	9.341	1.606	2.044
H	7.964	2.255	1.131
H	8.021	2.422	2.888
C	9.269	-1.003	1.017
H	9.713	-0.986	2.022
H	9.786	-0.217	0.447
C	9.565	-2.370	0.381
H	9.062	-3.155	0.965
H	9.138	-2.424	-0.630
C	11.065	-2.682	0.301
H	11.499	-2.634	1.310
H	11.567	-1.898	-0.284
C	11.364	-4.051	-0.319
H	12.442	-4.244	-0.362
H	10.903	-4.858	0.264
H	10.972	-4.117	-1.341
C	-5.064	0.691	-0.425
C	-4.797	-1.775	-0.684
N	-5.573	-0.608	-0.556

O	-5.809	1.660	-0.353
O	-5.326	-2.870	-0.828
C	-7.047	-0.740	-0.623
H	-7.243	-1.695	-1.107
H	-7.403	0.065	-1.268
C	-7.747	-0.652	0.751
H	-7.411	0.285	1.216
C	-9.275	-0.511	0.548
H	-9.726	-0.267	1.517
H	-9.456	0.365	-0.092
C	-9.996	-1.725	-0.060
H	-9.530	-1.991	-1.018
H	-9.872	-2.601	0.592
C	-11.499	-1.497	-0.303
H	-11.894	-2.353	-0.866
H	-11.630	-0.619	-0.951
C	-12.331	-1.319	0.973
H	-12.036	-0.426	1.535
H	-13.396	-1.219	0.736
H	-12.219	-2.184	1.640
C	-7.341	-1.807	1.688
H	-7.626	-2.768	1.242
H	-6.246	-1.826	1.764
C	-7.921	-1.700	3.103
H	-7.670	-0.735	3.563
H	-9.013	-1.796	3.109
H	-7.519	-2.490	3.748
S	0.196	-3.783	-0.662
S	0.834	3.951	-0.799

S	-1.004	3.804	0.454
O	-1.945	4.857	0.053
O	0.365	3.976	-2.192
O	1.696	5.010	-0.262
O	-0.531	3.687	1.841

4O-SAN-PDI (4) structure d

C	1.519	-2.199	-0.257
C	0.858	-0.987	-0.293
C	1.517	0.249	-0.321
C	2.931	0.205	-0.345
C	3.608	-1.040	-0.283
C	2.914	-2.253	-0.238
C	3.640	1.422	-0.470
H	3.469	-3.184	-0.207
C	2.940	2.606	-0.604
C	1.521	2.642	-0.593
H	3.500	3.528	-0.719
C	-0.566	-1.057	-0.369
C	-1.336	0.112	-0.415
C	-1.114	-2.324	-0.384
C	-2.742	-0.053	-0.459
C	-2.498	-2.501	-0.453
C	-3.302	-1.357	-0.491
H	-2.966	-3.479	-0.473
C	0.769	1.470	-0.409
C	-2.978	2.349	-0.352
C	-0.701	1.395	-0.366
C	-1.576	2.486	-0.285

H	-3.610	3.230	-0.314
C	-3.562	1.099	-0.459
C	5.095	-1.056	-0.290
C	5.126	1.426	-0.484
N	5.758	0.182	-0.352
O	5.729	-2.102	-0.243
O	5.764	2.463	-0.607
C	7.239	0.140	-0.359
H	7.520	-0.675	-1.027
H	7.573	1.080	-0.795
C	7.862	-0.080	1.037
H	7.374	-0.964	1.469
C	7.612	1.092	2.012
H	6.531	1.274	2.086
H	7.926	0.760	3.011
C	8.321	2.412	1.681
H	9.410	2.291	1.651
H	7.994	2.816	0.719
H	8.096	3.164	2.446
C	9.365	-0.409	0.895
H	9.839	-0.279	1.879
H	9.847	0.323	0.231
C	9.672	-1.829	0.395
H	9.204	-2.558	1.072
H	9.218	-1.996	-0.591
C	11.176	-2.119	0.303
H	11.637	-1.957	1.288
H	11.645	-1.392	-0.376
C	11.487	-3.541	-0.178

H	12.568	-3.717	-0.233
H	11.061	-4.290	0.500
H	11.069	-3.722	-1.176
C	-5.037	0.964	-0.539
C	-4.778	-1.514	-0.560
N	-5.551	-0.340	-0.562
O	-5.777	1.938	-0.581
O	-5.304	-2.619	-0.612
C	-7.023	-0.473	-0.660
H	-7.210	-1.469	-1.058
H	-7.354	0.270	-1.389
C	-7.764	-0.253	0.677
H	-7.434	0.720	1.065
C	-9.284	-0.120	0.413
H	-9.762	0.216	1.341
H	-9.436	0.694	-0.311
C	-9.998	-1.380	-0.103
H	-9.502	-1.740	-1.015
H	-9.907	-2.191	0.633
C	-11.488	-1.162	-0.420
H	-11.875	-2.066	-0.911
H	-11.586	-0.351	-1.155
C	-12.362	-0.852	0.802
H	-12.075	0.089	1.284
H	-13.417	-0.767	0.518
H	-12.283	-1.648	1.554
C	-7.399	-1.320	1.729
H	-7.685	-2.316	1.366
H	-6.308	-1.344	1.838

C	-8.018	-1.076	3.110
H	-7.767	-0.076	3.485
H	-9.111	-1.159	3.092
H	-7.645	-1.807	3.836
S	0.260	-3.530	-0.294
S	0.807	4.221	-0.988
S	-0.959	4.097	0.186
O	-1.861	5.143	-0.303
O	-0.593	4.036	1.606
O	0.359	-4.295	-1.544
O	0.231	-4.251	0.986

5O-SAN-PDI (5) structure a

C	1.459	-2.297	-0.458
C	0.809	-1.081	-0.479
C	1.479	0.150	-0.450
C	2.894	0.100	-0.408
C	3.559	-1.155	-0.362
C	2.855	-2.360	-0.390
C	3.614	1.314	-0.436
H	3.400	-3.297	-0.364
C	2.925	2.508	-0.579
C	1.518	2.536	-0.652
H	3.482	3.437	-0.650
C	-0.616	-1.133	-0.567
C	-1.376	0.045	-0.547
C	-1.176	-2.392	-0.610
C	-2.785	-0.107	-0.541
C	-2.565	-2.555	-0.647

C	-3.358	-1.406	-0.614
H	-3.042	-3.528	-0.687
C	0.746	1.376	-0.521
C	-2.990	2.285	-0.270
C	-0.732	1.319	-0.456
C	-1.587	2.410	-0.267
H	-3.610	3.166	-0.146
C	-3.591	1.048	-0.435
C	5.044	-1.183	-0.297
C	5.098	1.306	-0.368
N	5.715	0.051	-0.265
O	5.668	-2.235	-0.271
O	5.747	2.343	-0.403
C	7.195	-0.002	-0.201
H	7.504	-0.779	-0.901
H	7.554	0.959	-0.566
C	7.749	-0.308	1.207
H	7.245	-1.217	1.559
C	7.448	0.801	2.240
H	6.364	0.975	2.275
H	7.717	0.408	3.230
C	8.165	2.141	2.026
H	9.255	2.025	2.041
H	7.881	2.604	1.076
H	7.900	2.843	2.825
C	9.260	-0.626	1.118
H	9.684	-0.562	2.130
H	9.770	0.150	0.529
C	9.597	-2.008	0.538

H	9.098	-2.782	1.139
H	9.194	-2.108	-0.479
C	11.105	-2.290	0.502
H	11.515	-2.198	1.518
H	11.604	-1.516	-0.099
C	11.446	-3.673	-0.063
H	12.529	-3.844	-0.075
H	10.989	-4.470	0.538
H	11.079	-3.783	-1.091
C	-5.071	0.927	-0.459
C	-4.838	-1.547	-0.633
N	-5.598	-0.369	-0.536
O	-5.801	1.908	-0.411
O	-5.375	-2.643	-0.727
C	-7.075	-0.485	-0.575
H	-7.289	-1.454	-1.023
H	-7.431	0.302	-1.243
C	-7.751	-0.341	0.805
H	-7.395	0.605	1.235
C	-9.280	-0.184	0.621
H	-9.712	0.096	1.589
H	-9.458	0.675	-0.043
C	-10.028	-1.405	0.060
H	-9.583	-1.703	-0.898
H	-9.905	-2.263	0.735
C	-11.532	-1.162	-0.163
H	-11.948	-2.027	-0.696
H	-11.663	-0.300	-0.833
C	-12.339	-0.938	1.122

H	-12.023	-0.034	1.654
H	-13.407	-0.830	0.899
H	-12.227	-1.786	1.809
C	-7.349	-1.472	1.774
H	-7.656	-2.443	1.364
H	-6.253	-1.506	1.834
C	-7.906	-1.309	3.193
H	-7.633	-0.334	3.617
H	-8.998	-1.388	3.219
H	-7.505	-2.084	3.857
S	0.188	-3.615	-0.554
S	0.825	4.133	-1.209
S	-0.929	4.015	0.250
O	-1.906	5.047	-0.133
O	-0.452	3.911	1.639
O	0.291	-4.334	-1.831
O	0.140	-4.379	0.699
O	1.772	5.209	-0.764

5O-SAN-PDI (5) structure b

C	1.444	-2.414	-0.559
C	0.810	-1.187	-0.502
C	1.485	0.039	-0.417
C	2.900	-0.021	-0.390
C	3.557	-1.283	-0.415
C	2.843	-2.479	-0.515
C	3.632	1.184	-0.362
H	3.388	-3.416	-0.558
C	2.953	2.391	-0.425

C	1.547	2.425	-0.471
H	3.518	3.316	-0.440
C	-0.605	-1.234	-0.582
C	-1.370	-0.061	-0.508
C	-1.146	-2.501	-0.694
C	-2.778	-0.226	-0.517
C	-2.537	-2.664	-0.753
C	-3.339	-1.526	-0.651
H	-3.009	-3.634	-0.855
C	0.752	1.269	-0.413
C	-3.006	2.151	-0.165
C	-0.729	1.210	-0.349
C	-1.605	2.284	-0.126
H	-3.637	3.021	-0.021
C	-3.595	0.915	-0.374
C	5.041	-1.326	-0.356
C	5.117	1.162	-0.305
N	5.723	-0.100	-0.267
O	5.658	-2.382	-0.383
O	5.771	2.196	-0.294
C	7.203	-0.168	-0.210
H	7.504	-0.915	-0.944
H	7.570	0.806	-0.532
C	7.756	-0.540	1.183
H	7.238	-1.455	1.499
C	7.475	0.530	2.262
H	6.394	0.719	2.308
H	7.741	0.091	3.234
C	8.213	1.865	2.102

H	9.301	1.731	2.106
H	7.934	2.372	1.173
H	7.962	2.537	2.930
C	9.261	-0.879	1.076
H	9.689	-0.861	2.088
H	9.782	-0.089	0.516
C	9.574	-2.242	0.441
H	9.064	-3.031	1.013
H	9.165	-2.295	-0.578
C	11.077	-2.547	0.387
H	11.492	-2.501	1.404
H	11.586	-1.760	-0.187
C	11.392	-3.913	-0.231
H	12.472	-4.102	-0.256
H	10.925	-4.724	0.341
H	11.019	-3.978	-1.261
C	-5.074	0.784	-0.410
C	-4.818	-1.679	-0.678
N	-5.590	-0.510	-0.540
O	-5.811	1.758	-0.327
O	-5.348	-2.773	-0.816
C	-7.065	-0.637	-0.593
H	-7.268	-1.591	-1.078
H	-7.424	0.171	-1.233
C	-7.751	-0.550	0.787
H	-7.407	0.382	1.254
C	-9.280	-0.400	0.599
H	-9.721	-0.159	1.573
H	-9.462	0.480	-0.036

C	-10.014	-1.607	-0.010
H	-9.557	-1.870	-0.973
H	-9.889	-2.487	0.637
C	-11.517	-1.369	-0.239
H	-11.922	-2.219	-0.804
H	-11.648	-0.487	-0.882
C	-12.338	-1.192	1.044
H	-12.032	-0.303	1.608
H	-13.404	-1.084	0.815
H	-12.225	-2.060	1.706
C	-7.344	-1.712	1.716
H	-7.639	-2.670	1.269
H	-6.249	-1.738	1.782
C	-7.911	-1.608	3.137
H	-7.650	-0.647	3.598
H	-9.003	-1.697	3.152
H	-7.508	-2.402	3.774
S	0.206	-3.740	-0.902
S	0.823	4.037	-0.822
S	-1.000	3.880	0.449
O	-1.950	4.927	0.058
O	-0.516	3.753	1.830
O	1.694	5.087	-0.284
O	0.345	4.067	-2.211
O	0.185	-4.816	0.158

6O-SAN-PDI (6) structure a

C	1.461	-2.353	-0.418
C	0.811	-1.137	-0.397

C	1.481	0.093	-0.344
C	2.898	0.039	-0.331
C	3.563	-1.216	-0.325
C	2.857	-2.419	-0.371
C	3.626	1.248	-0.348
H	3.402	-3.357	-0.379
C	2.943	2.448	-0.441
C	1.536	2.476	-0.478
H	3.505	3.375	-0.490
C	-0.614	-1.187	-0.482
C	-1.376	-0.012	-0.439
C	-1.170	-2.447	-0.563
C	-2.785	-0.171	-0.462
C	-2.558	-2.615	-0.620
C	-3.354	-1.470	-0.571
H	-3.029	-3.589	-0.691
C	0.746	1.322	-0.376
C	-3.012	2.213	-0.172
C	-0.736	1.263	-0.311
C	-1.610	2.343	-0.124
H	-3.641	3.088	-0.058
C	-3.601	0.975	-0.358
C	5.049	-1.251	-0.288
C	5.113	1.235	-0.307
N	5.727	-0.022	-0.243
O	5.668	-2.307	-0.295
O	5.761	2.272	-0.331
C	7.208	-0.082	-0.209
H	7.500	-0.846	-0.930

H	7.564	0.885	-0.562
C	7.787	-0.417	1.183
H	7.280	-1.327	1.530
C	7.516	0.678	2.240
H	6.435	0.861	2.299
H	7.801	0.265	3.217
C	8.242	2.014	2.034
H	9.331	1.887	2.025
H	7.945	2.496	1.097
H	8.000	2.705	2.849
C	9.292	-0.747	1.058
H	9.736	-0.704	2.062
H	9.798	0.033	0.472
C	9.604	-2.123	0.449
H	9.109	-2.902	1.047
H	9.179	-2.201	-0.561
C	11.108	-2.419	0.377
H	11.539	-2.347	1.386
H	11.602	-1.640	-0.221
C	11.423	-3.795	-0.217
H	12.503	-3.976	-0.255
H	10.971	-4.597	0.379
H	11.034	-3.884	-1.239
C	-5.081	0.850	-0.411
C	-4.834	-1.618	-0.618
N	-5.602	-0.445	-0.517
O	-5.813	1.829	-0.360
O	-5.362	-2.714	-0.737
C	-7.077	-0.567	-0.586

H	-7.278	-1.531	-1.052
H	-7.424	0.228	-1.249
C	-7.780	-0.446	0.783
H	-7.438	0.496	1.232
C	-9.306	-0.294	0.572
H	-9.758	-0.029	1.534
H	-9.477	0.572	-0.085
C	-10.037	-1.512	-0.019
H	-9.571	-1.796	-0.972
H	-9.921	-2.378	0.648
C	-11.537	-1.274	-0.268
H	-11.938	-2.135	-0.820
H	-11.659	-0.405	-0.930
C	-12.370	-1.070	1.003
H	-12.068	-0.171	1.552
H	-13.434	-0.964	0.761
H	-12.267	-1.925	1.683
C	-7.389	-1.587	1.744
H	-7.682	-2.554	1.314
H	-6.295	-1.615	1.826
C	-7.976	-1.448	3.154
H	-7.718	-0.478	3.596
H	-9.068	-1.535	3.156
H	-7.583	-2.229	3.815
S	0.193	-3.669	-0.540
S	0.809	4.077	-0.880
S	-1.006	3.957	0.405
O	-1.960	4.989	-0.010
O	-0.516	3.867	1.787

O	1.683	5.142	-0.381
O	0.325	4.059	-2.267
O	0.291	-4.356	-1.835
O	0.151	-4.462	0.695

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