Supporting Information for

Anion-Assisted Supramolecular Polymerization of Luminescent Organic π-Conjugated Chromophore in Moderately Polar Solvent: Tunable Nanostructures and Corresponding Effect on Electronic Property

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Materials and Methods: All the reagents were purchased from commercial source and used as such without further purification. ^{1}H NMR spectra were recorded on a Bruker DPX-300 MHz and 400 MHz NMR spectrometer and all the spectra were calibrated against TMS. UV-Vis spectra were recorded in a Labtronics LT-291 UV/Vis spectrophotometer. MASS spectra were recorded on using Qtof Micro YA263 mass spectrometer. TEM, SEM and AFM images were collected using a 200 KV Transmission Electron Microscope (MODEL: JEOL JEM 2100 HR with EELS),JEOL Scanning Microscope-JSM-6700F and Bruker Innova-S2 instrument in the tapping mode respectively. Fluorescence spectra were recorded on HORIBA scientific Fluoromax-4 fluorescence spectrophotometer. Cyclic voltammetry was recorded on CH Instrument (MODEL: CHI600E, Electrochemical Analyzer) and current - voltage measurements were recorded on Keithley 2611B source meter.

UV-visible spectroscopic studies: For fluoride variable experiment,Stock solutionof NMI-2(1.0 mM) was prepared in THF solvent and kept it to equilibrate at room temperature for 2h. Then, an aliquot (100 µl) was taken from stock solution and diluted to the final concentration at 0.1 mM. Then solutions were allowed to equilibrate at room temperature for 1 h before spectral measurements were carried out.

To prepare 1 Equivalent TBAF to NMI (NMI.1F), 0.1 microliter of 1(M) TBAF solution was added in 1ml of 0.1mM THF solution of NMI-2. Here the final concentration of both TBAF and NMI is 0.1 mM. Hence, the solution contains 1 equivalent NMI and 1 equivalent TBAF.

The ratio of NMI and TBAF = 1:1. Similarly, for 5 (NMI:TBAF = 1:5), 10 (NMI:TBAF = 1:10), 25 (NMI:TBAF= 1:25) and 50 (NMI:TBAF = 1:50) equivalents of TBAF the individual concentration was maintained accordingly.

For BF_3addition experiment,50equivof TBAF was added in THF solution of NMI-2 (0.1mM) and then the solution was equilibrated at room temperature for1h. Next, the spectra were recorded with the gradual addition of BF_3 to the NMI.50F^- solution. Exactly the similar procedure was followed for methanol addition experiment.

FT-IR Characterization: At first the sample was mixed with KBr to make a pellet, then it was placed in the chamber inside the instrument and spectrum was recorded at room temperature.

Job's plot to determine the binding ratio: At first nine sets of Sample solution **(**1 ml**)** containing NMI-2 and TBAF were prepared with varying the mole fraction of NMI-2 or TBAF from 0.1 to 0.9, but the final concentration of all the solution was maintained at 1mM. The solutions were allowed to equilibrate at room temperature for 1 h and then the UV-vis spectral data were recorded at room temperature**.**

Atomic Force Microscopic (AFM) Experiment: In a typical AFM experiment, 20µl of NMI.F^- adducts in variable ratio of NMI and F^-(concentration = 0.1mM) were placed on a microscopic cover glass and allowed to air dry overnight before the images were taken.

Time Correlated Single Photon Counting (TCSPC) experiment: In a typical experiment, 0.5mM solutions of NMI.F^-adducts in variable ratio of NMI and F^-were used for the measurement. Samples were excited at 420 nm and emissions were monitored at 515 nm for all the solution.

Measurement of Fluorescence quantum yield: Fluorescence quantum yield at room temperature was estimated at a single excitation wavelength(420nm) using quinine sulphate

in Sulfuric acid (0.1M) aqueous solution (Φ = 0.546) as the reference according to the equation:

$$\Phi_X = \Phi_{ST}[Grad_X/Grad_{ST}] [\eta^2_X/ \eta^2_{ST}].$$

Where the subscripts ST and X indicate standard and test, respectively, Φ is the fluorescence quantum yield, Grad is the gradient from the plot of integrated fluorescence intensity vs. absorbance and η the refractive index of the solvent.

In this method, the average quantum yields of NMI-2, NMI-2 with 0.5 equiv. TBAF and NMI-2 with 50 equiv. TBAF in THF were estimated to be 0.48, 0.44 and 0.15respectively.

Electrochemical measurements: Cyclic voltammetry of fluoride variable NMI-2 was performed in THF solvent (concentration = 1.0 mM) at a scan rate 100 mVs^{-1} using Tetra-n-butylammonium perchlorate as a supporting electrolyte. A three-electrode cell consisting of a glassy carbon working electrode, a platinum wire as the counter electrode and Ag/AgCl was used as pseudo reference electrode. Reference electrode was ferrocene/ferrocenium couple ($E_{Fc/Fc}^{+}$= 0.40V). The HOMO and LUMO energy levels were calculated using following equations.

E_{HOMO}= - (E_{Ox} onset –$E_{Fc/Fc}^{+}$onset) - 4.80 eV.

E_{LUMO}= - (E_{Red} onset - $E_{Fc/Fc}^{+}$onset) - 4.80 eV.

$E_{gap}=E_{LUMO}–E_{HOMO}$.

For Current – voltage measurements, fluoride variable NMI-2 solution (concentration = 1.0 mM) was spin coated on microscopic glass slide and kept under vacuum overnight. Silver paste was used at connection points. The conductivity(G) was measured using the following equation.

$$G=(1/R)[\ln 2/(\pi t)].$$

Where t is the film thickness measured by digital micrometer (average film thickness 42 micrometer).

Synthesis of the Napthalimide Derivative (NMI-2): The synthetic procedure of NMI-2 is outlined below:

Compound NMI-C1: At first, Compound A (0.632g, 1.15 mmol) (synthesis is followed from the previous report)[1] and 4-Nitro 1,8 Napthalic Anhydride (0.27g, 1.09 mmol) were taken in 35 ml dried Toluene in a round bottle flask and the solution was stirred at 100^0C for 24h under Argon atmosphere. Thenreaction was stopped and allowscooling until reaches to room temperatureand then the solution was evaporated to get the crude the product. Then it was purified by column chromatography using silica gel as stationary phase and 20%ethyl acetate in hexane as eluent to get the compound NMI-C1 as a light -yellow solid in 60% of yield.^{1}H-NMR (400 MHz, $CDCl_3$, TMS): δ (ppm) = 8.90 (d, 1H), 8.72 (d, 1H), 8.70 (d, 1H),8.40 (d, 1H), 7.98 (t, 1H), 6.90 (s, 2H), 3.5 (t, 4H), 3.95 (t, 6H), 1.74 (m, 6H), 1.34 (m,6H), 1.30 (m, 24H), 0.90 (t, 9H).

ESI-MS: m/z calculated for [C45H63N3O8Na] $(M+Na)^+$ =796.4615, Found-796.4511.

Compound NMI-2: At first, ethyl acetate was degassed and then Compound NMI-C1 (0.41g, 0.53mmol) was dissolved and Pd/C was added carefully to the solution. The reaction mixture was stirred under H_2 atmosphere at room temperature for 24h. Next, Pd/C was filtered off using celite 545 as filtering agent and then ethyl acetate was evaporated to get the brown color crude product. It was then washed with ethyl acetate to get the pure product as a yellow solid in 93% yield.^{1}H-NMR (300MHz, $CDCl_3$ TMS):δ (ppm) = 8.56 (d, 1H), 8.40 (d, 1H), 8.20 (d, 1H),7.50 (t, 1H), 7.05 (t, 2H), 6.8 (d, 1H), 4.00 (t, 6H), 3.5 (t, 4H), 1.74 (m, 6H), 1.34 (m ,6H), 1.30 (m, 24H), 0.90 (m, 9H).

ESI-MS: m/z calculated for $[C_{45}H_{65}N_3O_6Na](M+Na)^+$ = 766.4873, Found-766.5182.

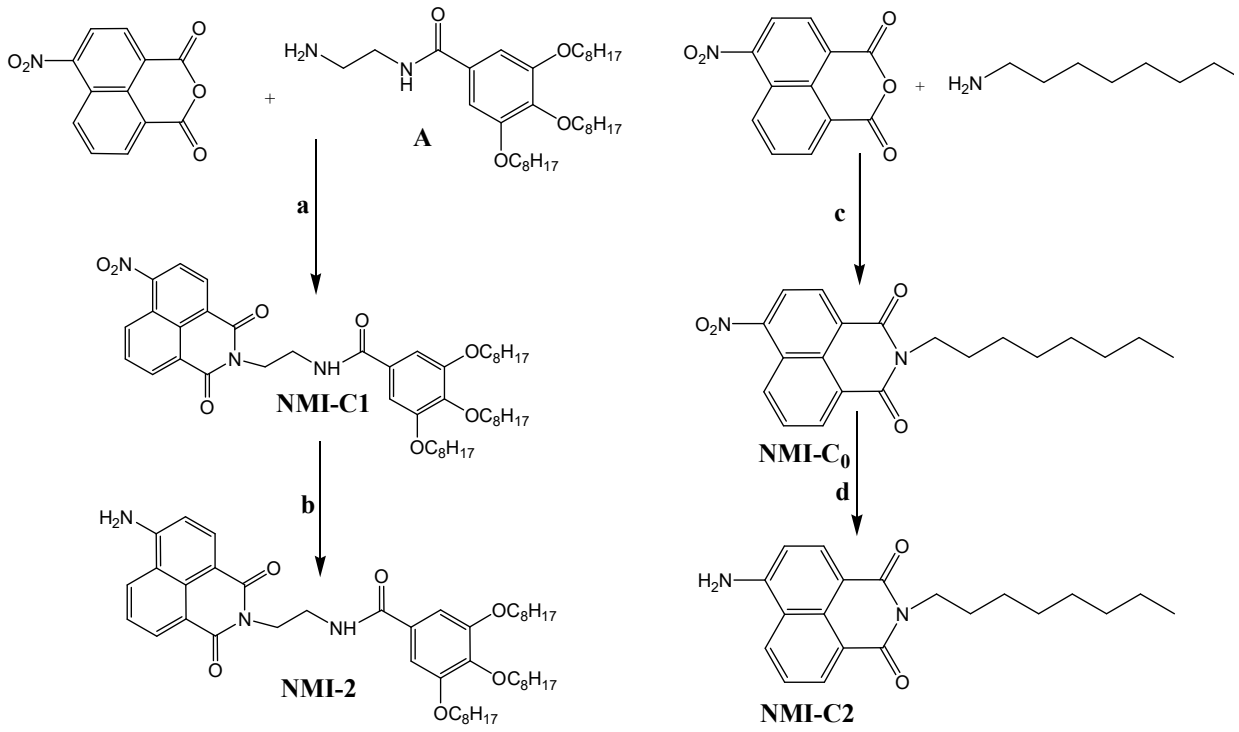
Synthesis of the Napthalimide Derivative (NMI-C2): The synthetic procedure of compound NMI-C is same as compound NMI-2 which is outlined below:

Compound NMI-C_0: 4-Nitro 1,8 NapthalicAnhydride(0.55g ,2.26 mmol) and n-Octyl amine (0.3g, 2.32 mmol) were takenin 30 ml of dried toluene and the solution was refluxed at 100^0C for 24h under Argon atmosphere. Then the reaction was stopped to allow cool and the solvent was evaporated to get the crude product. It was purified by column chromatography using silica gel as stationary phase and 20%ethyl acetate in hexane as eluentto get the compound as a light -yellow solid in 75% yield.^{1}H-NMR (300MHz, $CDCl_3$ TMS): δ (ppm) = 8.79 (d, 1H), 8.68 (d, 1H), 8.70 (d, 1H),8.36 (d, 1H), 7.95 (t, 1H), 4.11 (t, 2H), 1.30-1.65 (m, 12H), 0.90 (t, 3H).

ESI-MS: m/z calculated for $[C_{20}H_{22}N_2O_4](M+H)^+$ = 355.1580, Found-355.1572.

Compound NMI-C2: The compound NMI-C_0 (0.4g, 1.13 mmol) was dissolved in degassed ethyl acetate and then Pd/C was added carefully to this the solution. The reaction mixture was stirred under H_2 atmosphere at room temperature for 24h. Then Pd/C was filtered off using celite 545 as filtering agent. Then ethyl acetate was evaporated to get the pure product as yellow solid in 97% yield.^{1}H-NMR (300MHz, $CDCl_3$ TMS): δ (ppm) = 8.55 (d, 1H), 8.36 (d, 1H), 8.05 (d, 1H), 7.62 (t, 1H), 6.83 (d, 1H), 4.07 (t, 2H), 1.30-1.65 (m, 12H), 0.90 (t, 3H).

ESI-MS: m/z calculated for $[C_{20}H_{24}N_2O_2]$ $(M+H)^+$ = 325.1838, Found-325.9832.



Reagents and conditions: a) Toluene, 100^0C, 24h ,60%, b) Ethyl acetate, Pd/C, rt, 24h, 93%,

c) Toluene, 100^0C, 24h ,75%, d) Ethyl acetate, Pd/C, rt, 24h, 97%.

Scheme 1: Schematic representation of the synthesis of **NMI-2 and NMI-C2.**

Additional Figures:

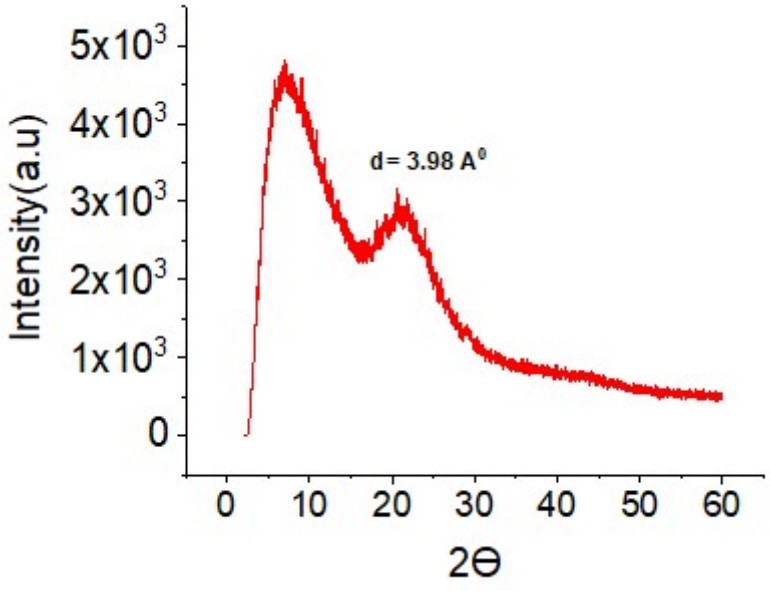
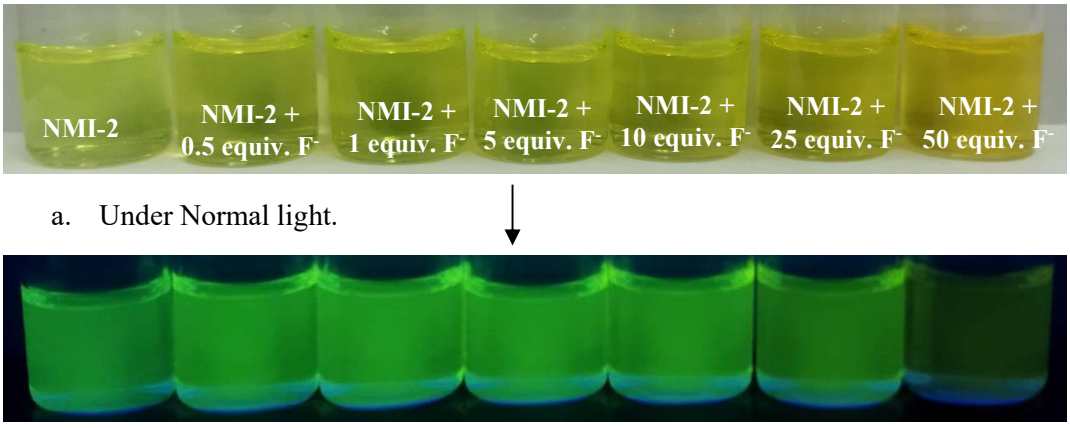


Figure S1: Powder X-RD plot of NMI-2 in presence of 0.5equiv. of F^- anion.



a. Under Normal light.

b. Under UV light.

Figure S2: Images of fluoride NMI.F^- adducts at variable NMI-2 and F^- ratio. a)Under normal light b) Under UV light.

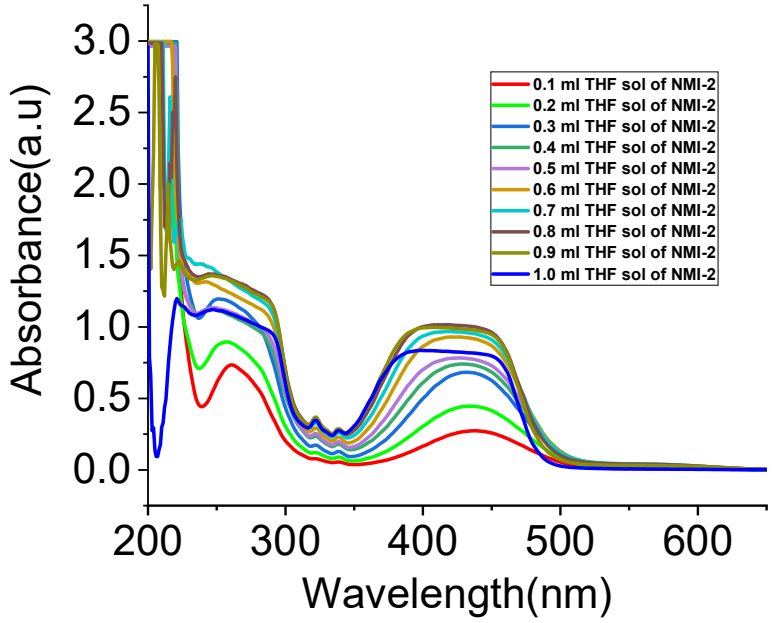


Figure S3:UV-vis spectra for Job's plot diagram to know the binding ratio of NMI and F^- anion and binding constant.

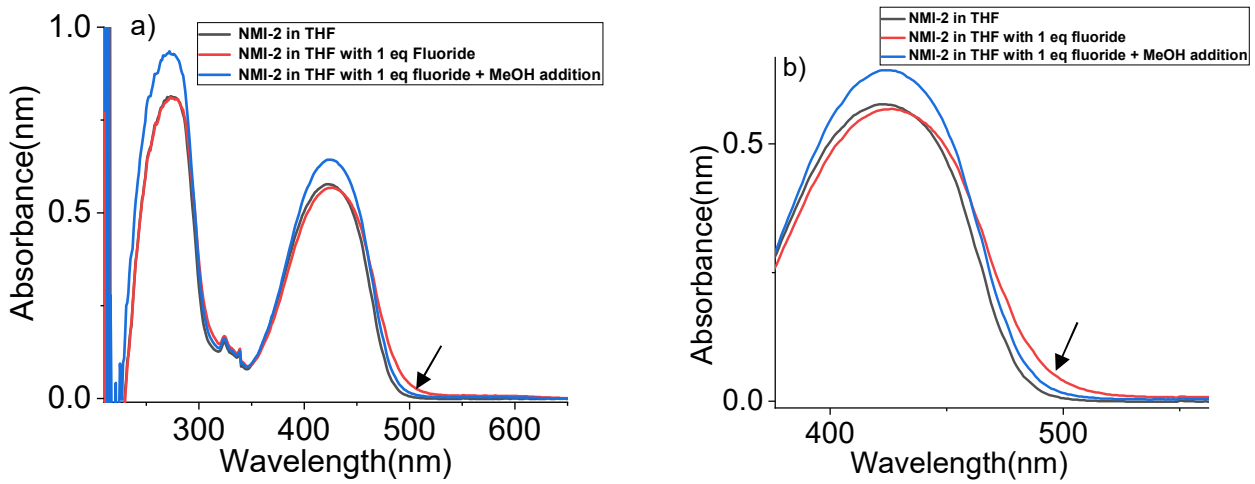


Figure S4: Methanol additions to NMI.1F- adduct, a) full spectrum b) zoomed spectrum.

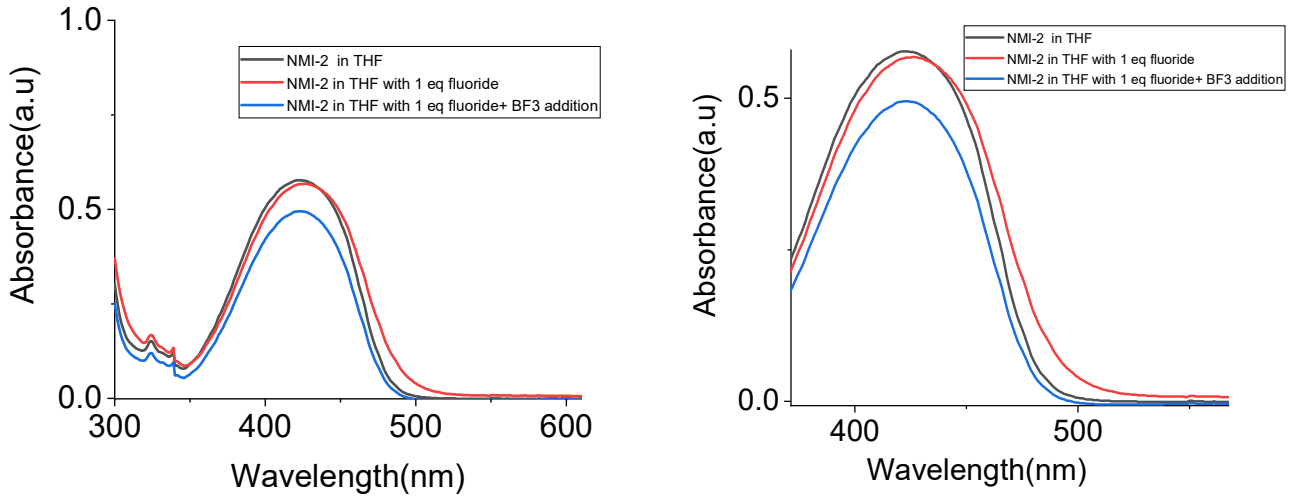


Figure S5: BF_3additions to NMI.1F^- adduct, a) Full spectrum b) Zoomed spectrum.

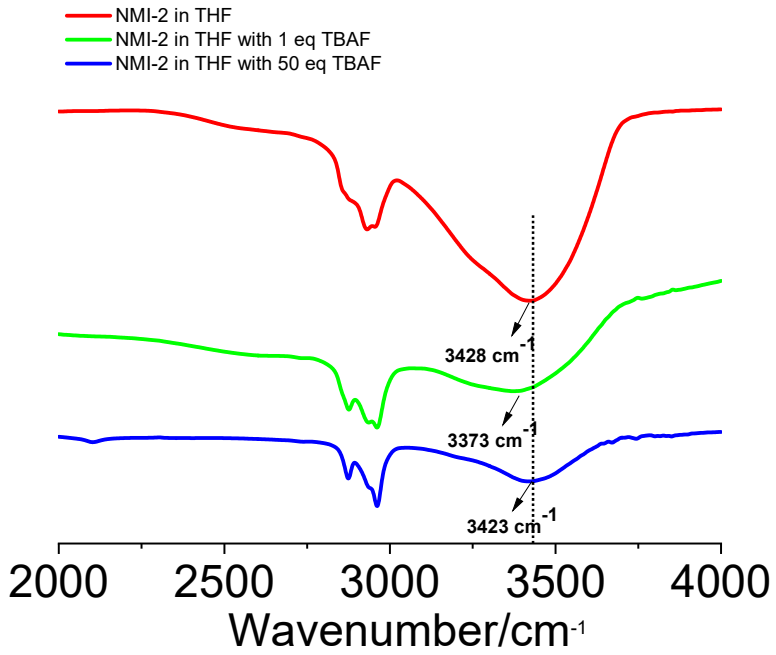


Figure S6: Combined IR plot of NMI-2 in THF, NMI.1F^- (NMI-2: F^- = 1:1) and NMI.50 F^- (NMI-2: F^- = 1:50) adducts.

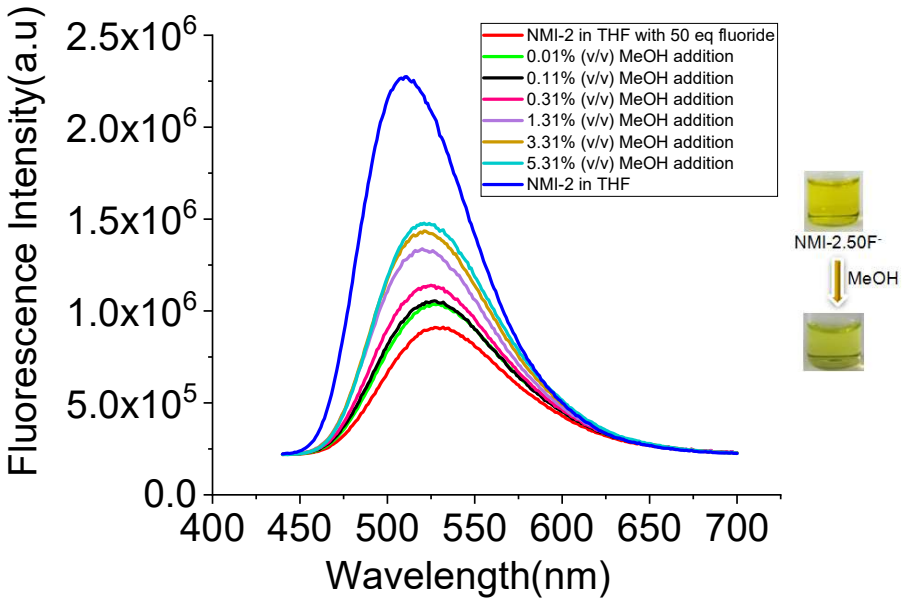


Figure S7: Monitoring emission spectra upon addition ofMeOH to NMI.50 F^-(NMI:F^- = 1:50) solution.

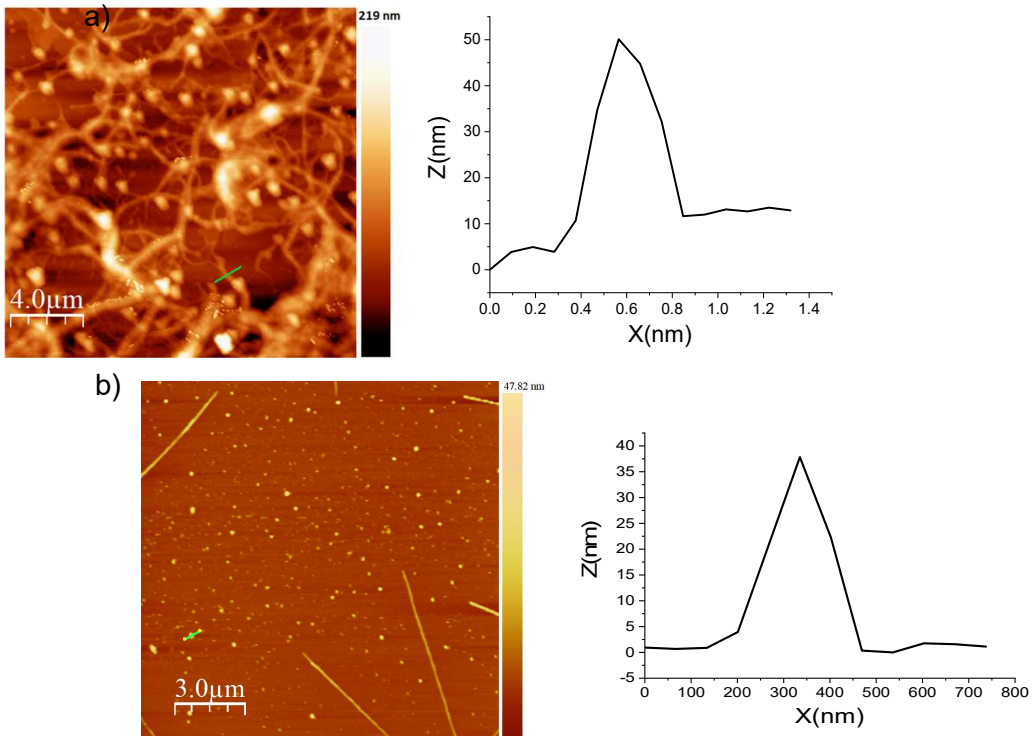


Figure S8:AFM images of a) NMI.0.5F^- (NMI: F^- = 1:0.5) b) NMI.50 F^- (NMI:F^- = 1:50) solution in THF. Figure a shows incomplete polymerization in presence of 0.5 equiv. of F^- and figure b shows completely depolymerized structure.

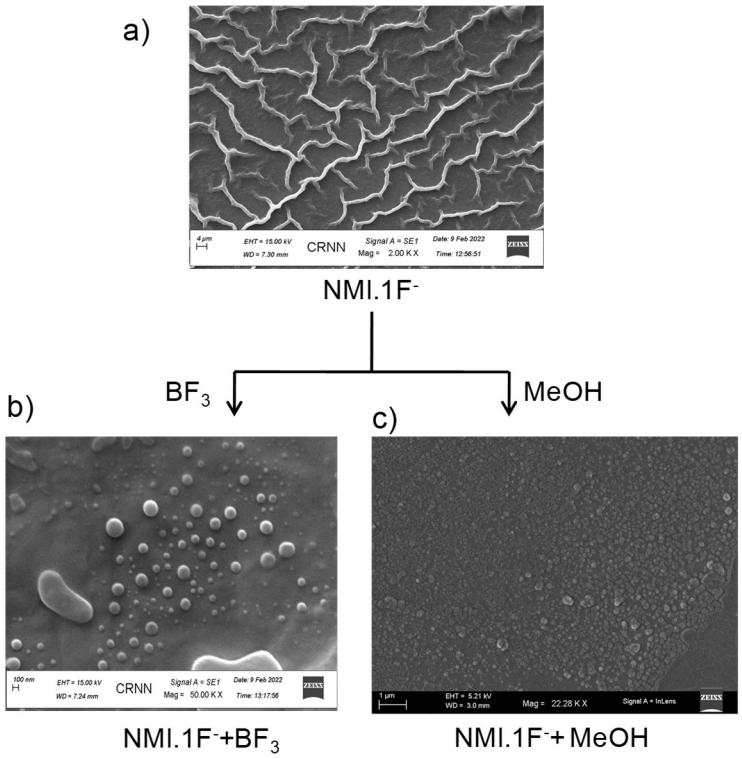


Figure S9:SEM images of a) NMI-2 upon addition of 1 equiv. of F^- anion; b) BF_3 addition to NMI.1F$^-$(NMI-2: F^- = 1:1) solution; c)MeOH addition to NMI.1F$^-$ solution. Nanofiber to nanoparticle transformation indicates depolymerization of supramolecular polymer upon addition of BF_3 or MeOH.

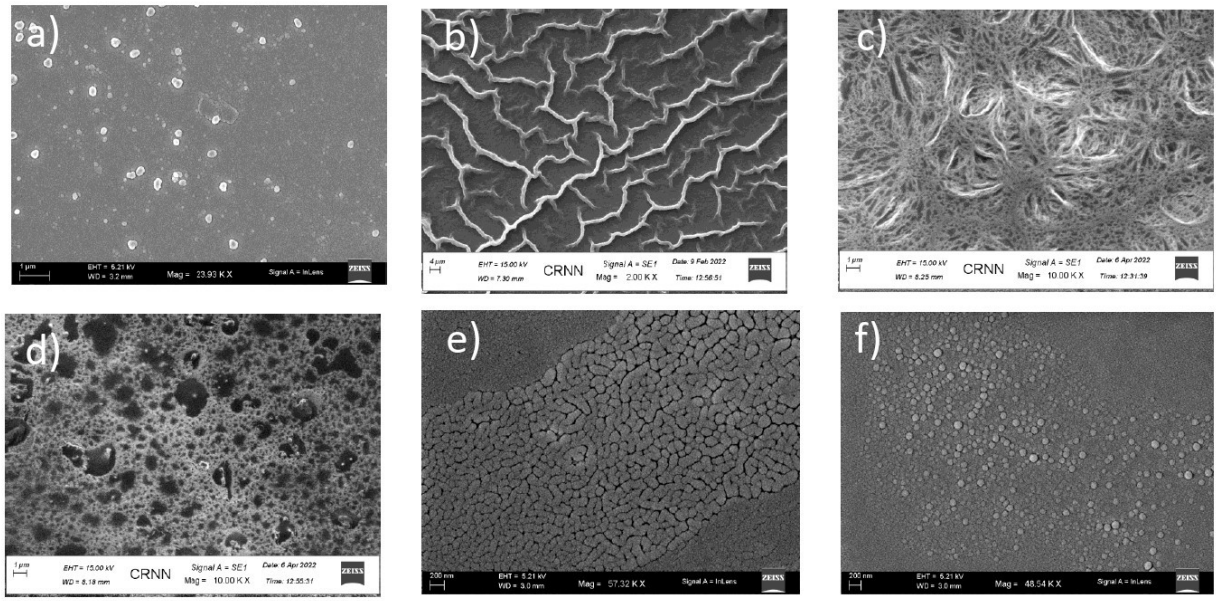


Figure S10: Morphology tuning by varying NMI-2 and F^- anion ratio in the solution. SEM images of a) NMI-2,b) NMI.1F^-(NMI-2: F^- = 1:1), c) NMI.5F^- (NMI-2: F^- = 1:5),d) NMI.10F^- (NMI-2: F^- = 1:10),e) NMI.25F^- (NMI-2: F^- = 1:25),and f) NMI.50F^- (NMI-2: F^- = 1:50) adduct.

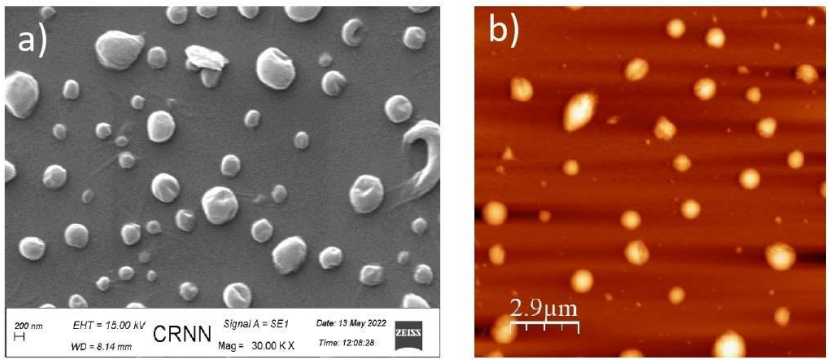


Figure S11:a) SEM image of NMI-C1 without F^- anion and b) AFM of NMI-C1 in presence of 1equiv. of F^- anion.

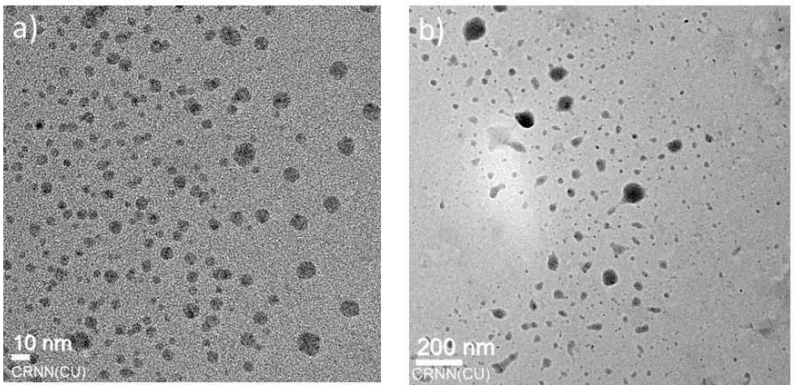


Figure S12:TEM image of NMI-C2; a) without F^- anion and b) with 1equiv. of F^- anion.

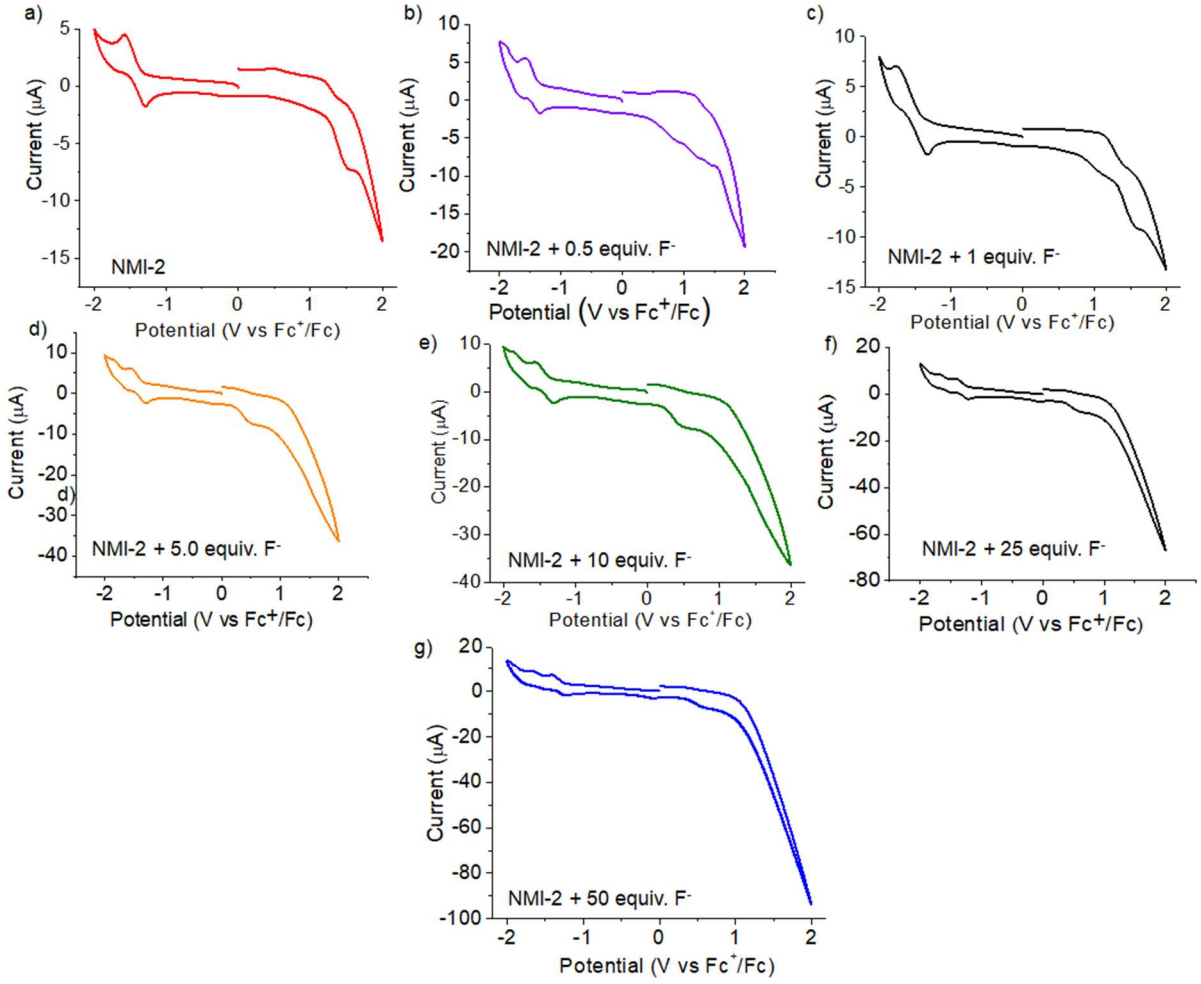


Figure S13: Cyclic Voltamogramsplot of NMI-2 in presence a) in absence and in presence of b) 0.5equiv, c) 1equiv. d) 5 equiv., e) 10 equiv., f) 25 equiv. and g) 50equiv. F^- anion. Solvent = THF, supporting electrolyte = TBAP (Tetrabutyl ammonium perchlorate). Potentials are internally referenced to the ferrocene/ferrocenium (Fc/Fc+) couple.

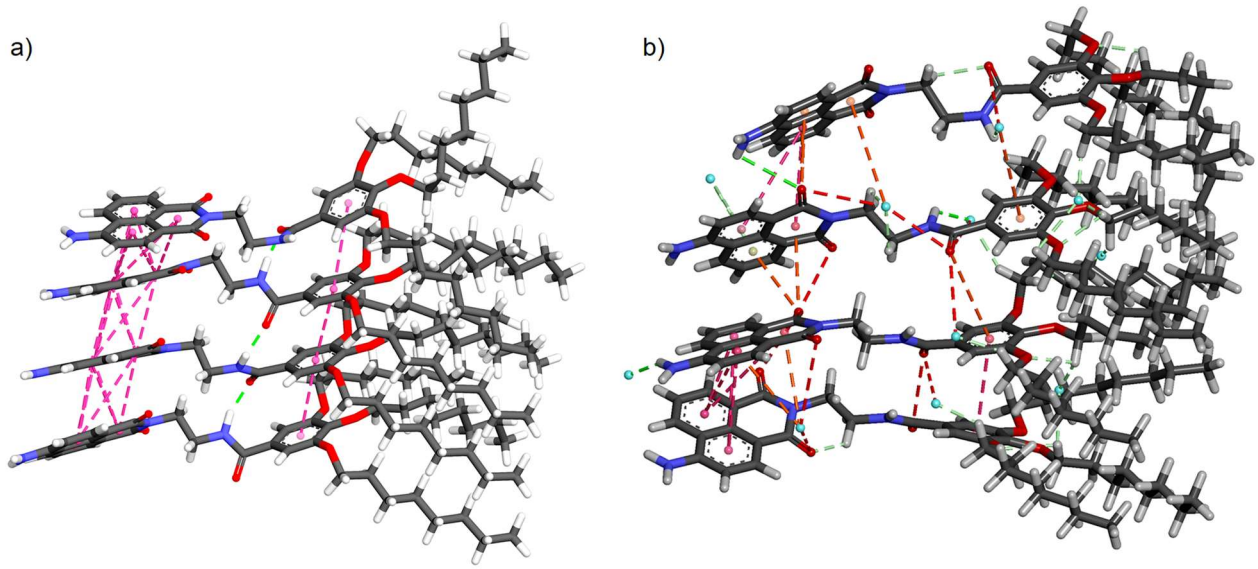
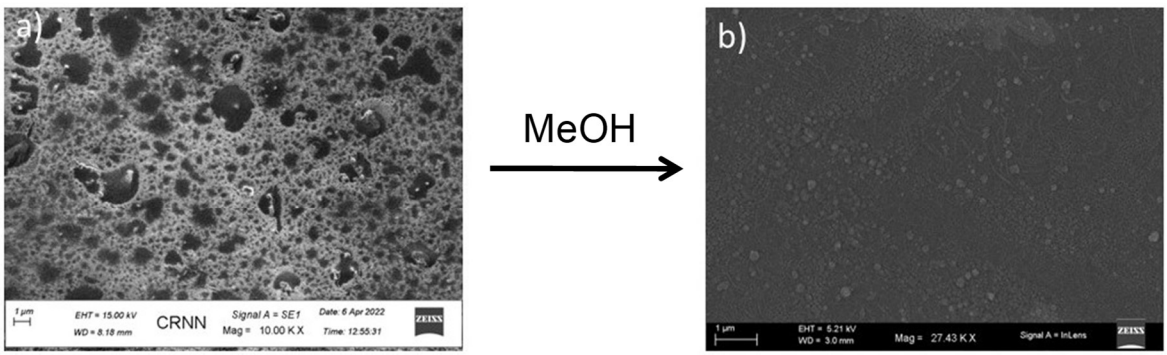


Figure S14: Computational tetramer of NMI-2 a) in absence of F^- anion and b) in presence of excess of F^- anion. Excess anions destroyed the ordered structure as shown in the picture. Pink and green dotted line indicates π-π stacking and H-bonding respectively. Light green point represents F^- anion.



NMI.10F^-

Figure S15:SEM imageof NMI-2.10F^- (NMI-2: F^- = 1:10) adduct a) before and b) after methanol addition.

Table S1: Fluorescence lifetime data.

Sample	Component Lifetimes(ns)[a]		
	τ_1	τ_2	τ_{avg}
0 eqv fluoride in 100% THF	3.55(4.39%)	10.36(95.61%)	10.06
0.5 eqv fluoride in 100% THF	3.22(4.39%)	9.96(95.61%)	9.66
1 eqv fluoride in 100% THF	2.89(4.31%)	9.73(95.69%)	9.44
5 eqv fluoride in 100% THF	1.95(6.73%)	8.11(93.27%)	7.70
10 eqv fluoride in 100% THF	1.51(11.65%)	6.56(88.35%)	5.97
25 eqv fluoride in 100% THF	1.22(15.61%)	5.56(84.39%)	4.88
50 eqv fluoride in 100% THF	0.91(24.86%)	4.11(75.14%)	3.31

Values in parenthesis shows the decay contribution corresponding to each lifetime. Average lifetimes (τ_{avg}) were calculated using the following equation: $\tau_{avg} = a_1\tau_1 + a_2\tau_2$.

Table S2: HOMO-LUMO energy level from UV/Vis and CV experiments

System	Eg^{opt} [eV]	E_{ox} [V]	E_{red} [V]	E_{HOMO} [eV]	E_{LUMO} [eV]	E_g^{CV} [eV]	Conductivity ($S.cm^{-1}$)
$NMI.0F^-$	2.57	1.37	-1.43	-5.77	-2.97	2.80	$1.76x10^{-8}$
$NMI.0.5F^-$	2.53	1.31	-1.47	-5.71	-2.93	2.78	$1.29x10^{-6}$
$NMI.1F^-$	2.52	1.18	-1.55	-5.58	-2.86	2.72	$1.36x10^{-6}$
$NMI.5F^-$	2.44	0.55	-1.58	-4.95	-2.82	2.13	$6.69x10^{-6}$
$NMI.10F^-$	2.38	0.46	-1.58	-4.86	-2.82	2.04	$1.45x10^{-4}$
$NMI.25F^-$	2.37	0.58	-1.31	-4.98	-3.09	1.89	$6.7x10^{-5}$
$NMI.50F^-$	2.32	0.57	-1.31	-4.97	-3.09	1.88	$1.6x10^{-5}$

$NMI.0F^-$ (NMI: F- = 1:0), $NMI.0.5F^-$ (NMI: F- = 1:0.5), $NMI.1F^-$ (NMI: F^- = 1:1), $NMI.5F^-$ (NMI: F- = 1:5), $NMI.10F^-$ (NMI: F- = 1:10), $NMI.25F^-$ (NMI: F- = 1:25),$NMI.50F^-$ (NMI: F^- = 1:50).

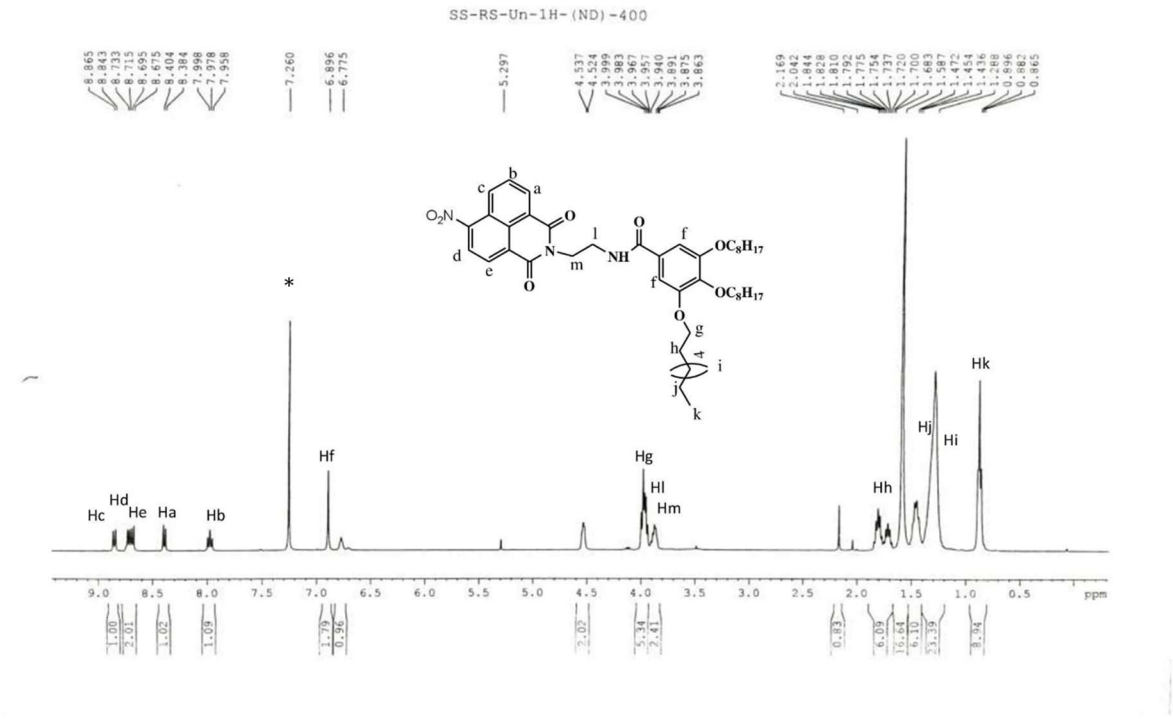


Figure S16: ^{1}H- NMR spectrum of Compound **NMI-C1**. Solvent-$CDCl_3$*indicatessolventpeak.

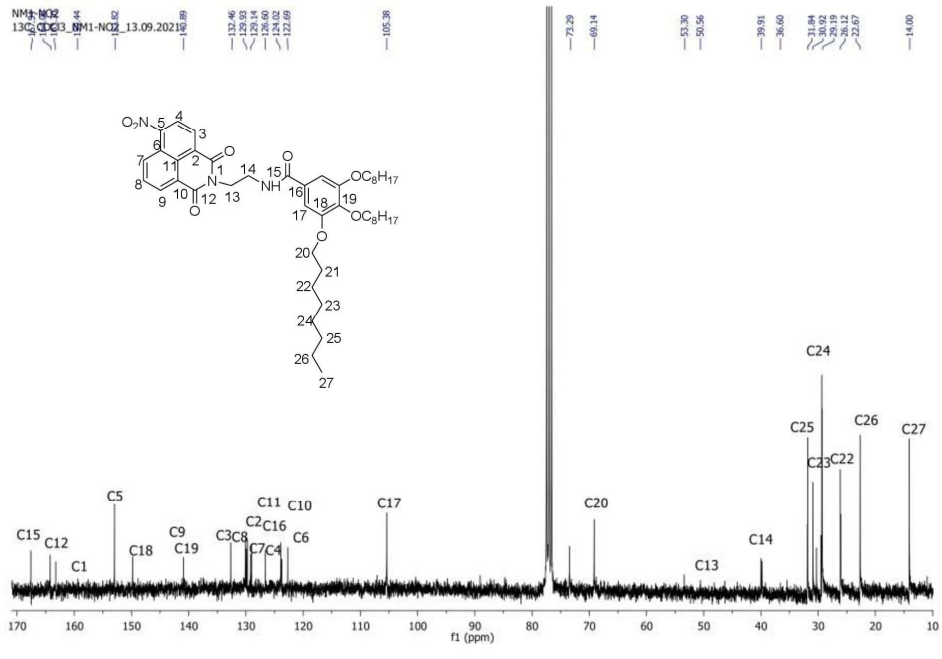


Figure S17: ^{13}C- NMR spectrum of Compound **NMI-C1**. Solvent-$CDCl_3$.*indicatessolventpeak

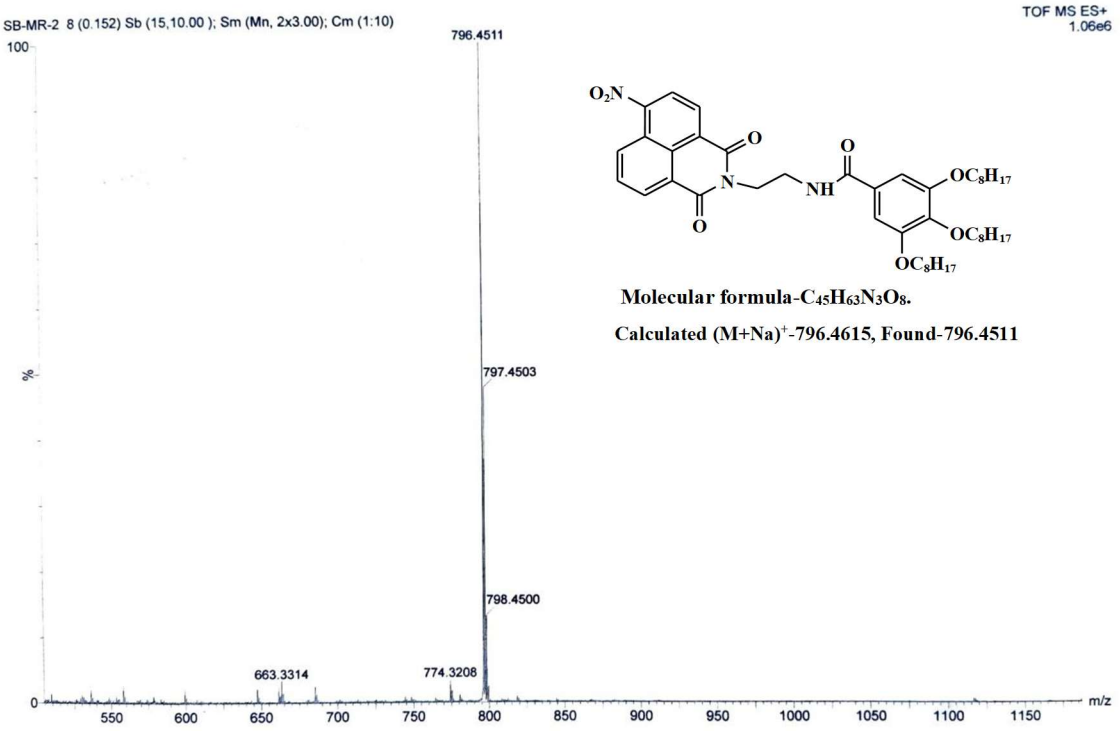


Figure S18: ESI-MS spectrum of Compound **NMI-C1**.

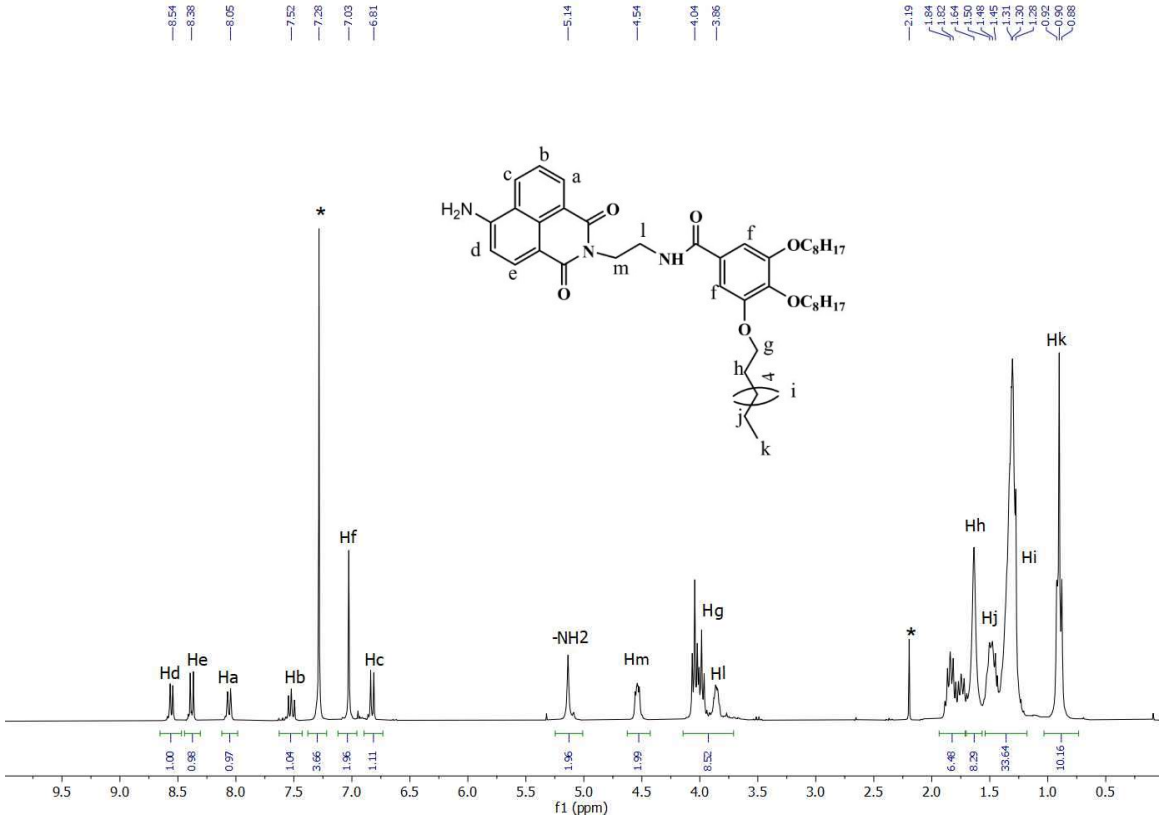


Figure S19: ^{1}H- NMR spectrum of Compound **NMI-2**. Solvent-$CDCl_3$*indicatessolventpeak

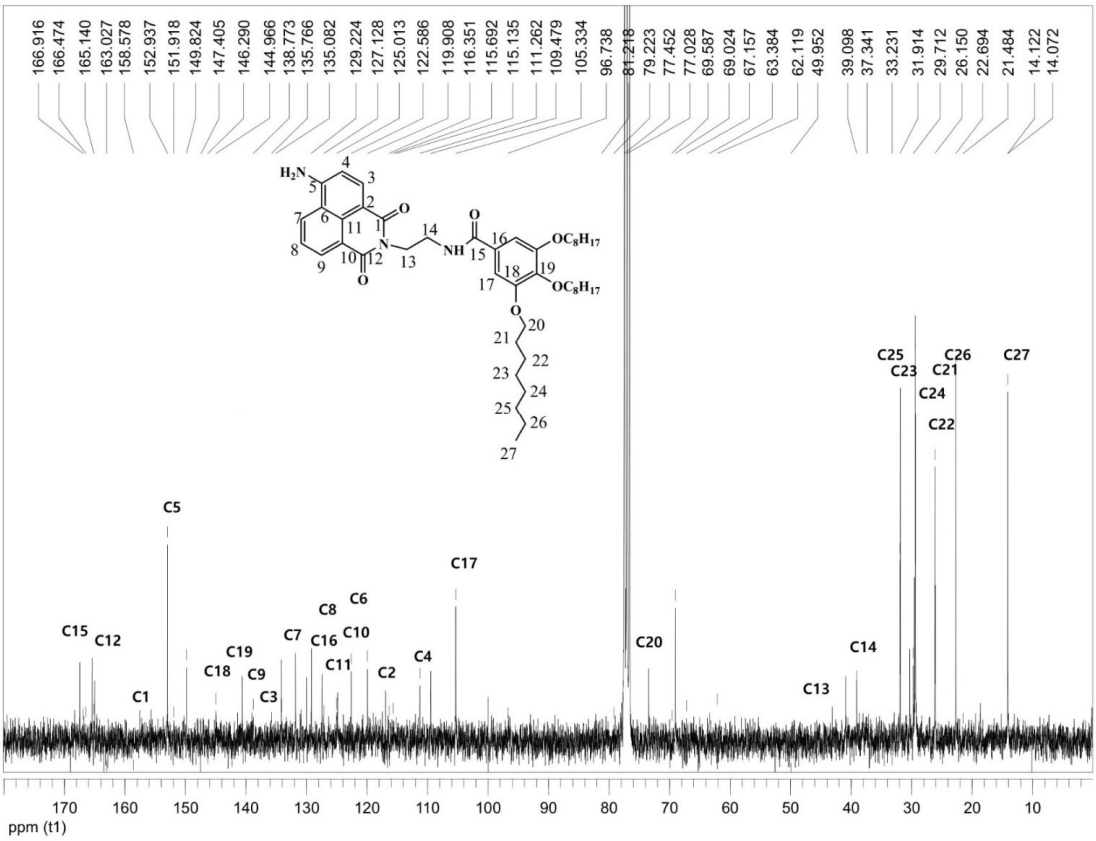
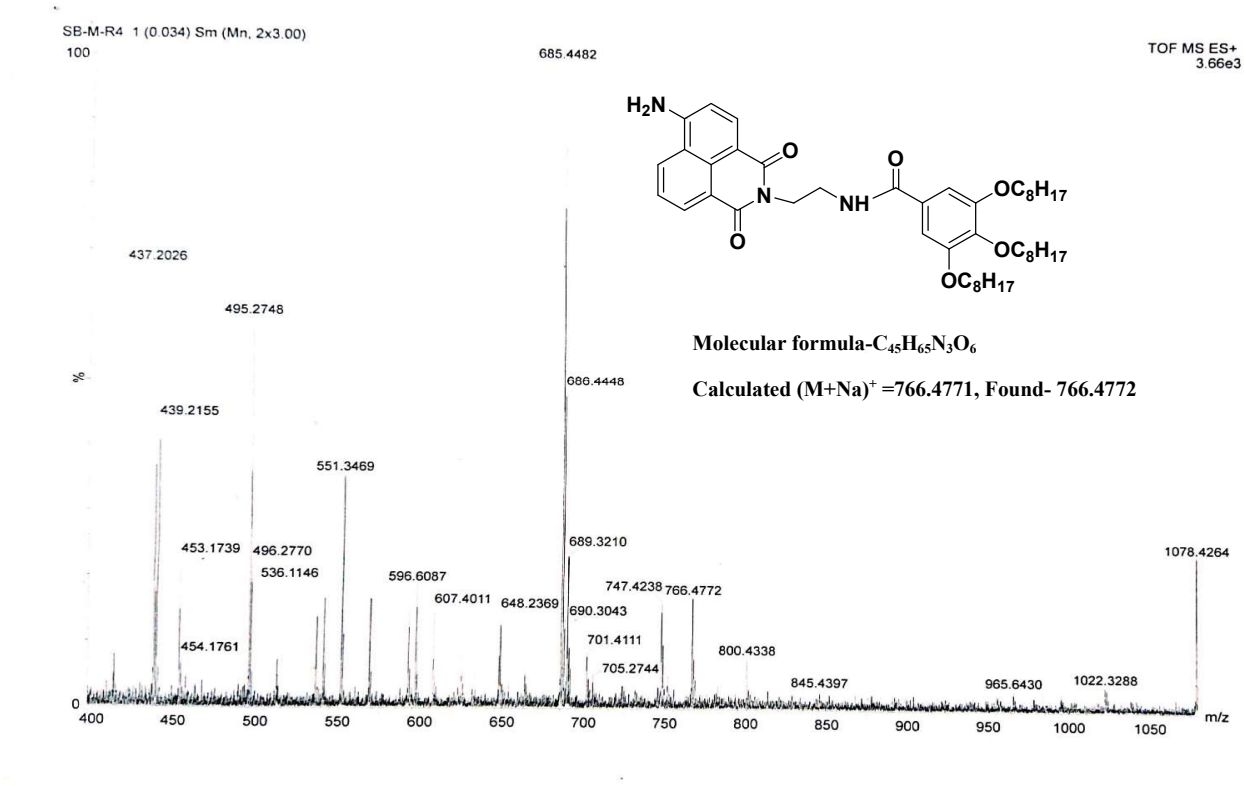


Figure S20: ^{13}C- NMR spectrum of Compound **NMI-2**. Solvent-$CDCl_3$.



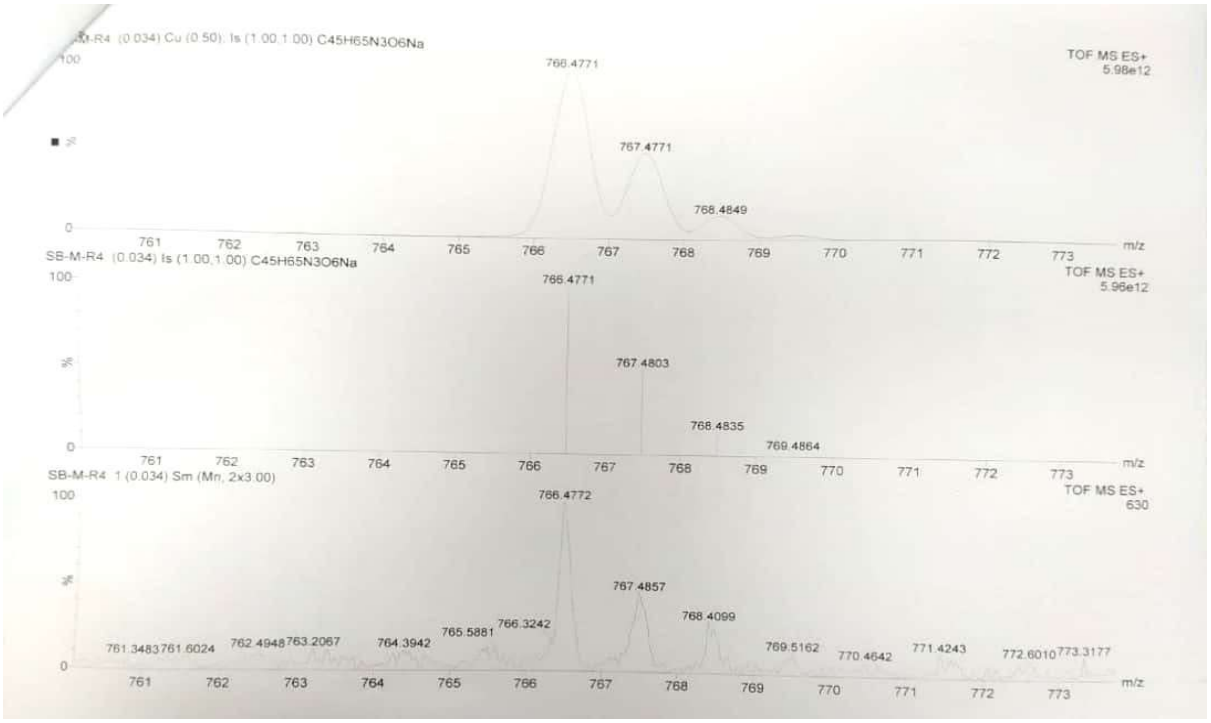
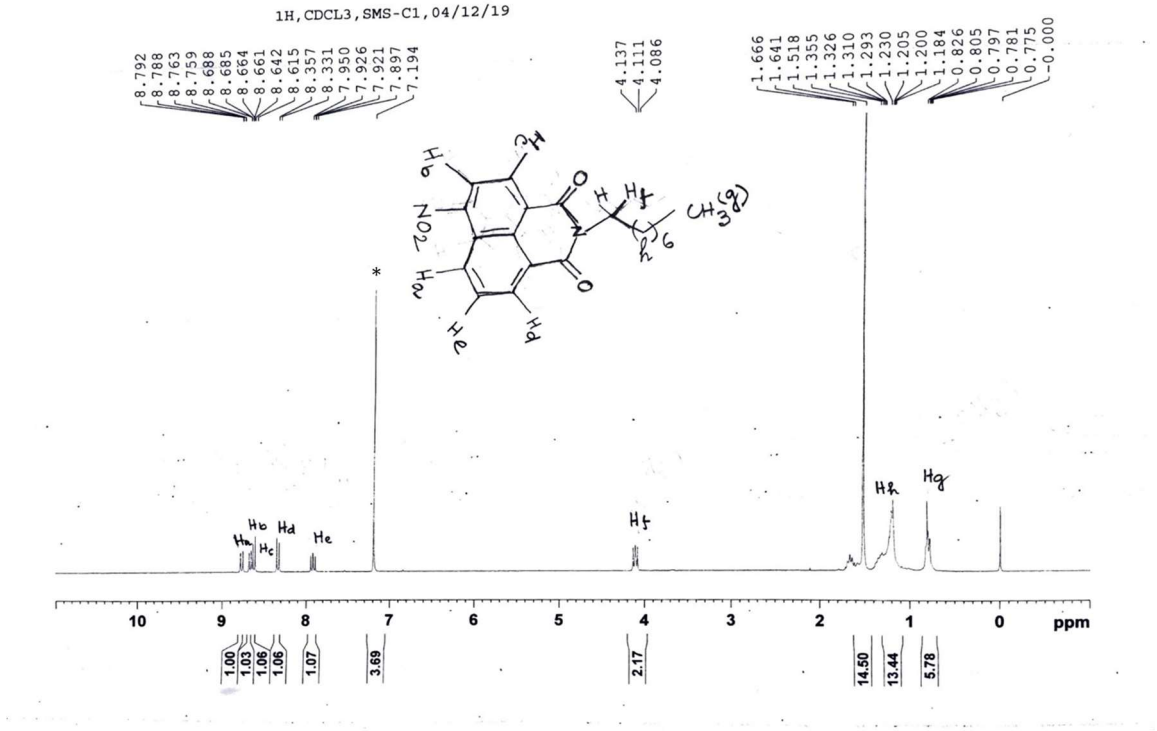
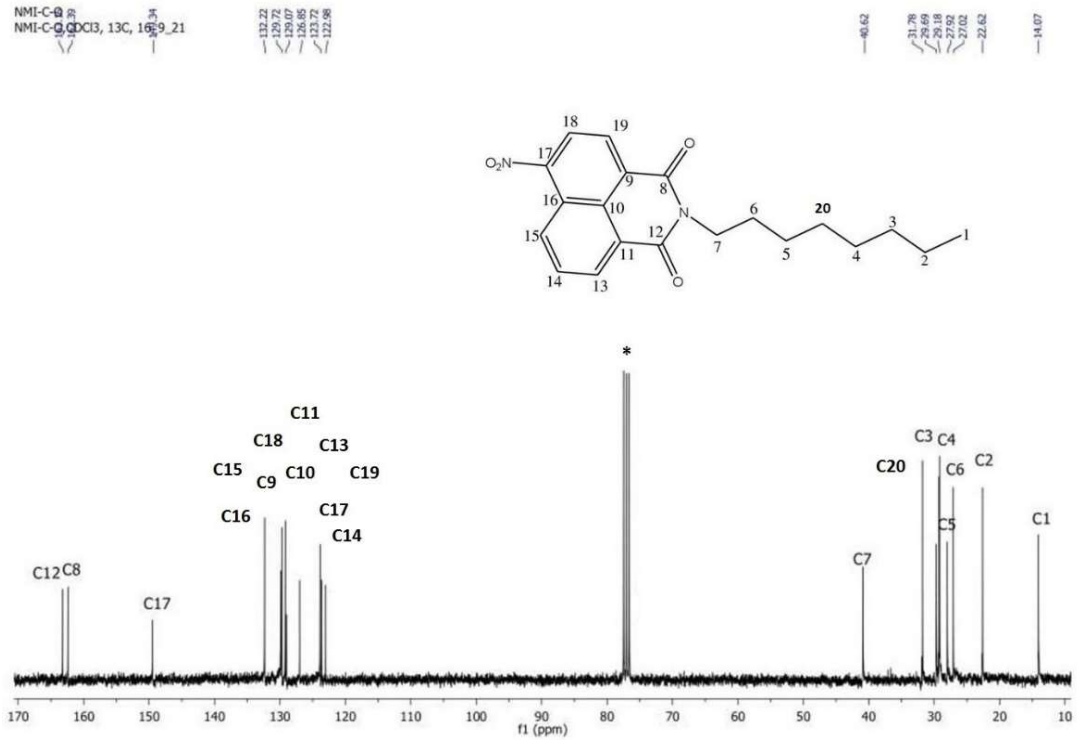


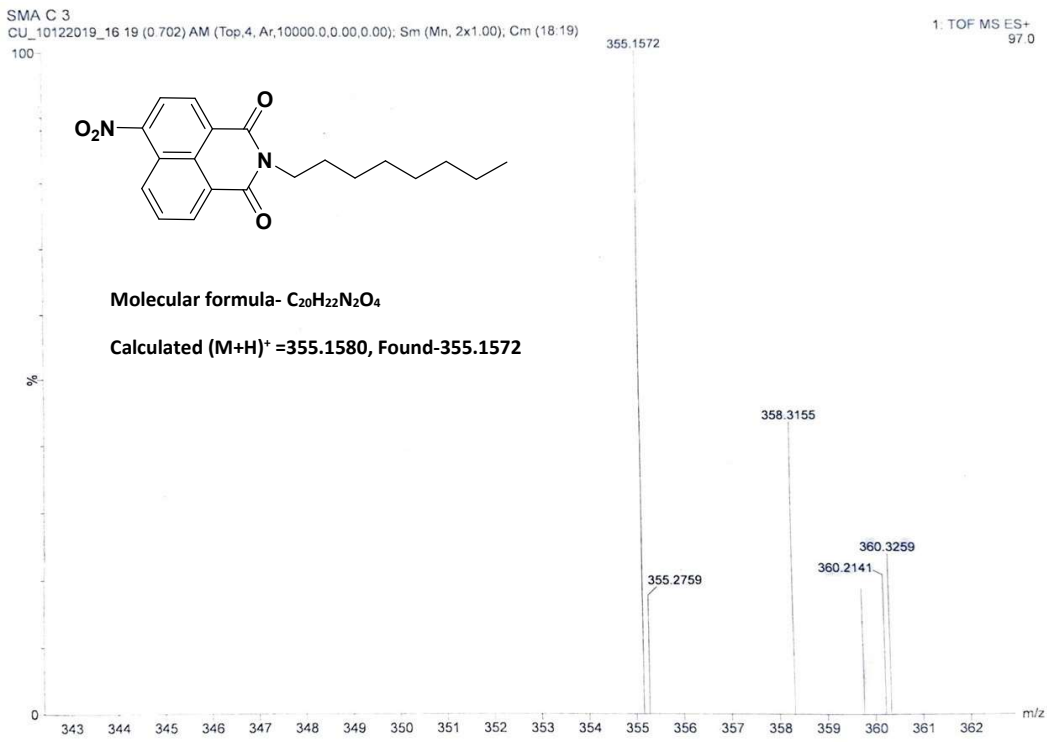
Figure S21: ESI-MS spectrum of Compound **NMI-2**.



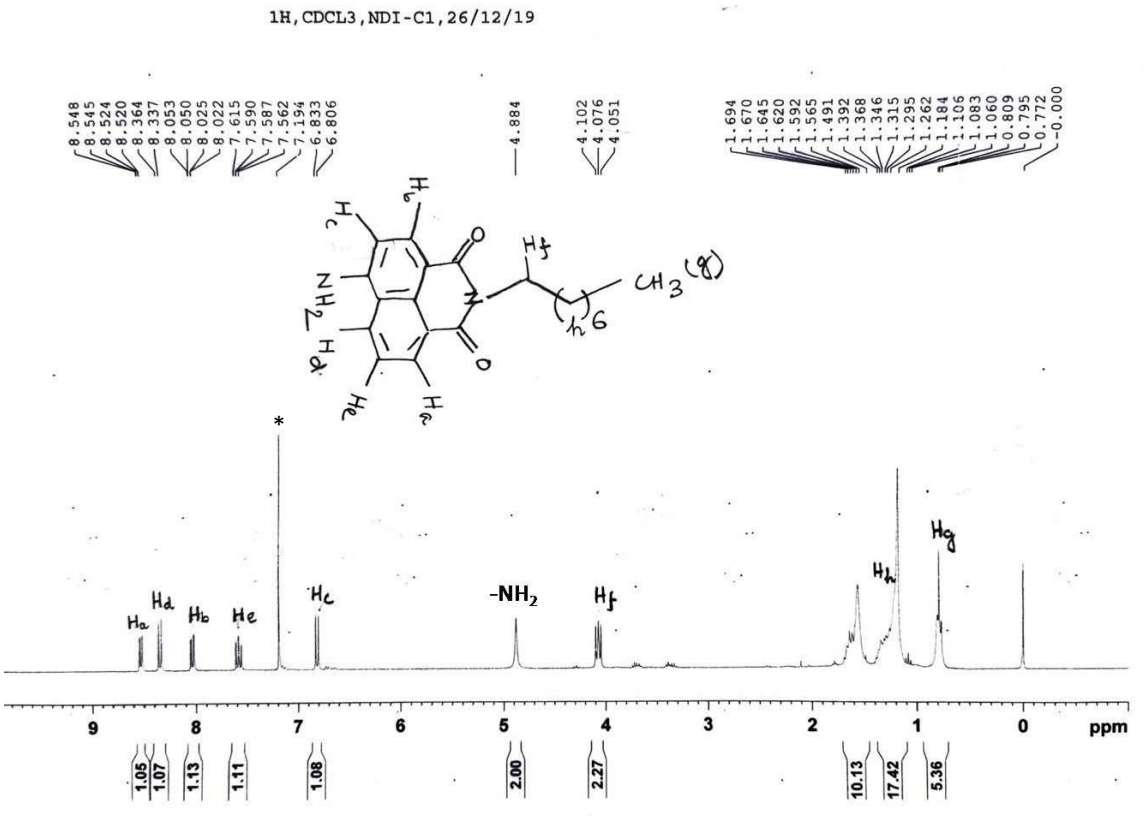
FigureS22: ^{1}H-NMRspectrumofCompound**NMI-C$_0$**.Solvent-$CDCl_3$.*indicatessolventpeak



FigureS23: ^{13}C-NMRspectrumofCompound**NMI-C$_0$**.Solvent-$CDCl_3$.*indicatessolventpeak



FigureS24:ESI-MSspectrumof**NMI-C$_0$**



FigureS25:^{1}H-NMRspectrumofCompound**NMI-C2**.Solvent-$CDCl_3$.*indicatessolventpeak.

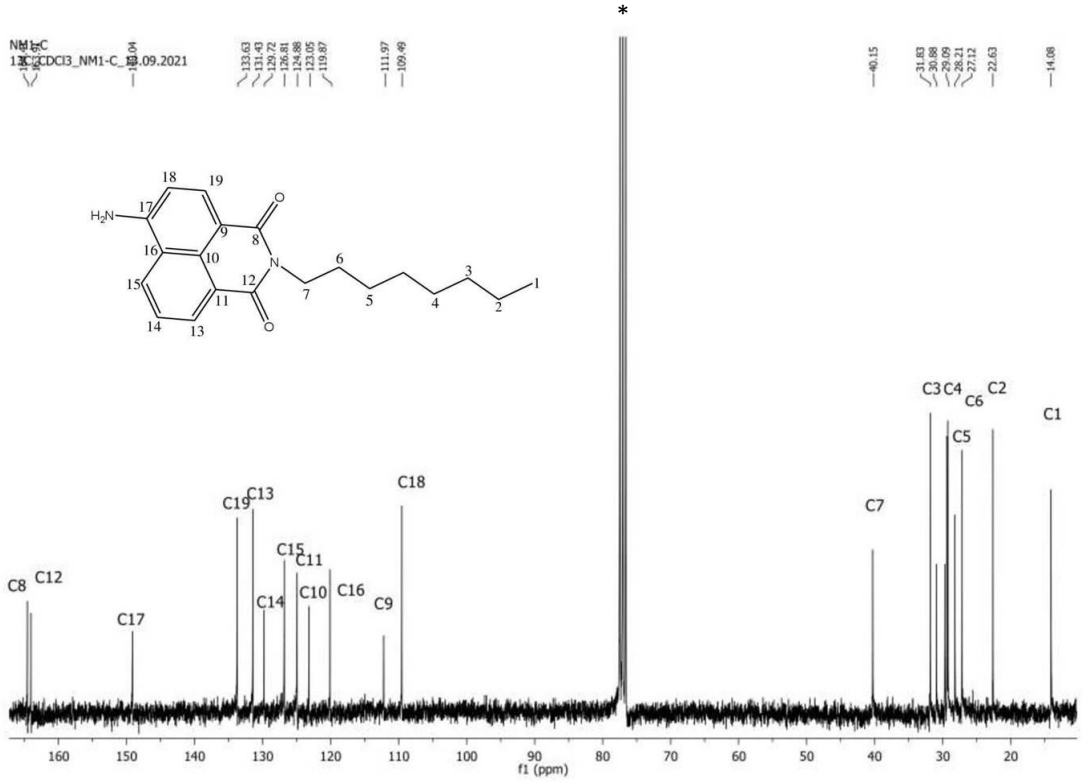
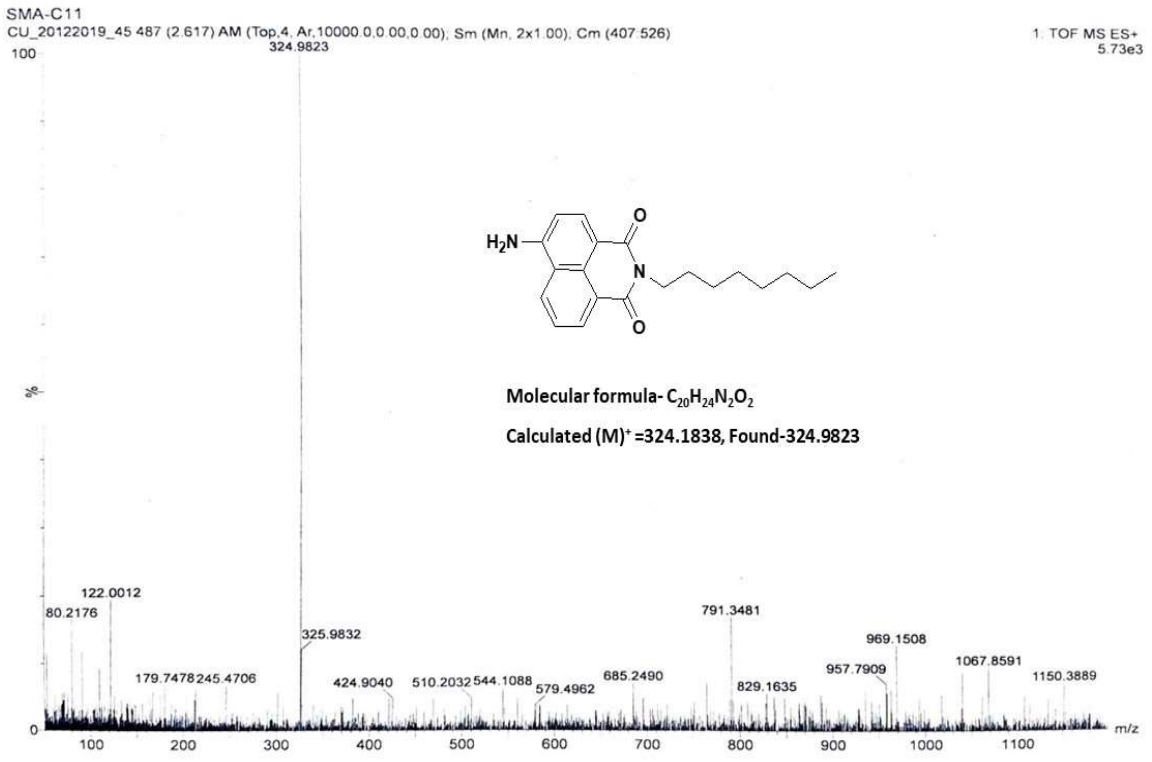


Figure S26: ^{13}C-NMR spectrum of Compound **NMI-C2**. Solvent-$CDCl_3$. * indicates solvent peak



FigureS27: ESI-MS spectrum of **NMI-C2.**

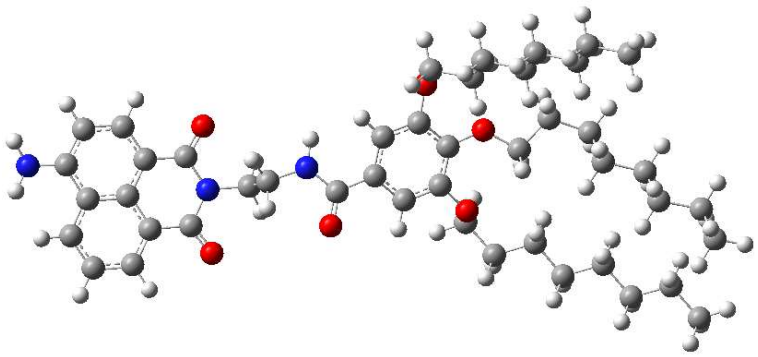
Computational

The compound NMI-2 and its assembly in the presence of F- ion with different amount was investigated using DFT method.[2,3] Gaussian 09W D1 revision[4]using the ωB97XD functional and 6-311G(d,p)basis set to optimize the geometry of the molecule. The 6-31G (d,p) basis set has been employed for the molecular electrostatic potential map (MEP) generation. HOMO, LUMO, and MEP were visualized using GaussView 5 software.[5]

NCI Plot

NCIPLOT Version 4.0 was utilized for the calculations of NCI Plot of interactions between **2** and amino acids present in the vicinity of the molecule using standard procedure.[6]

Coordinates of the energy minimized compound



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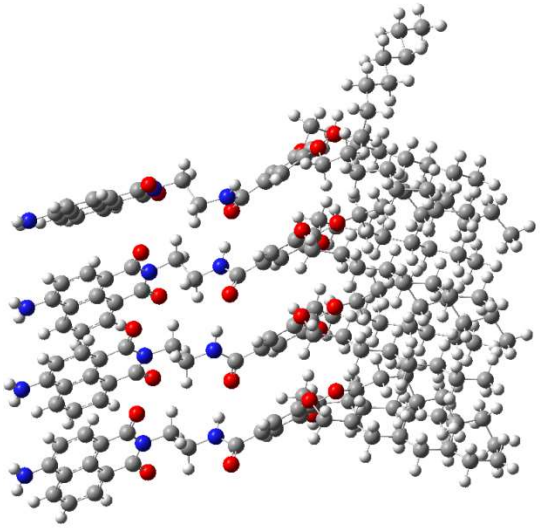

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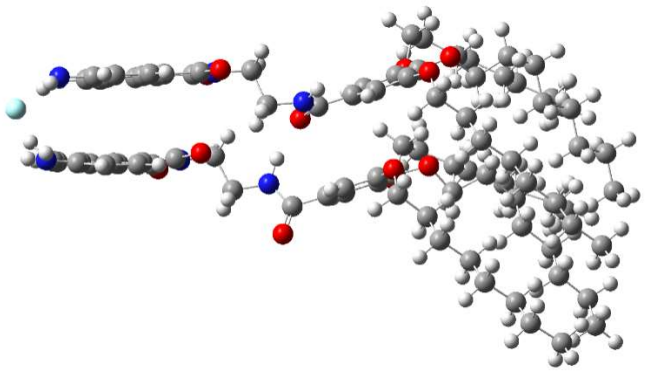

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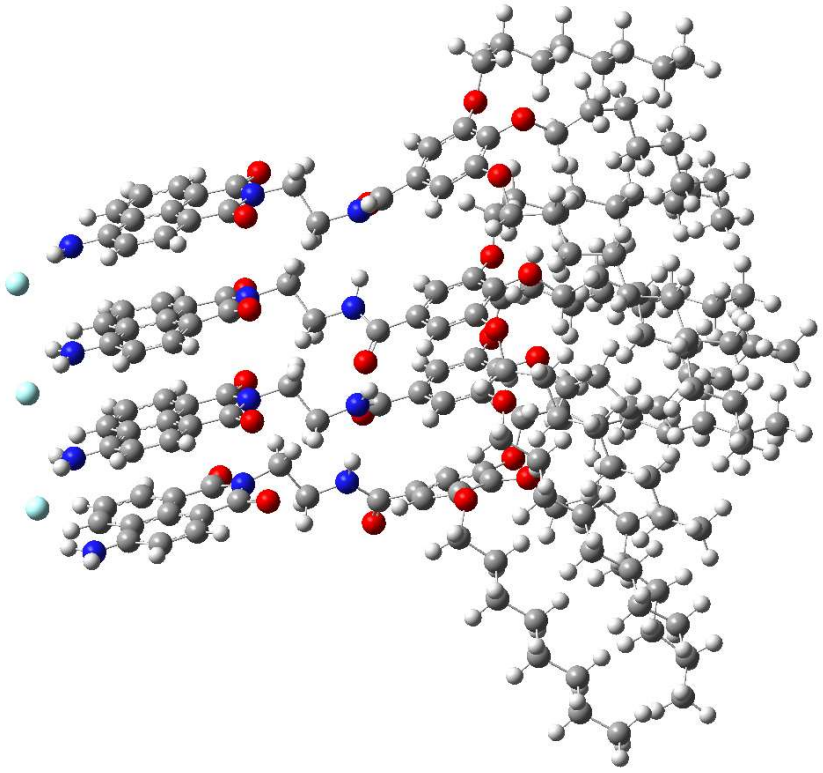

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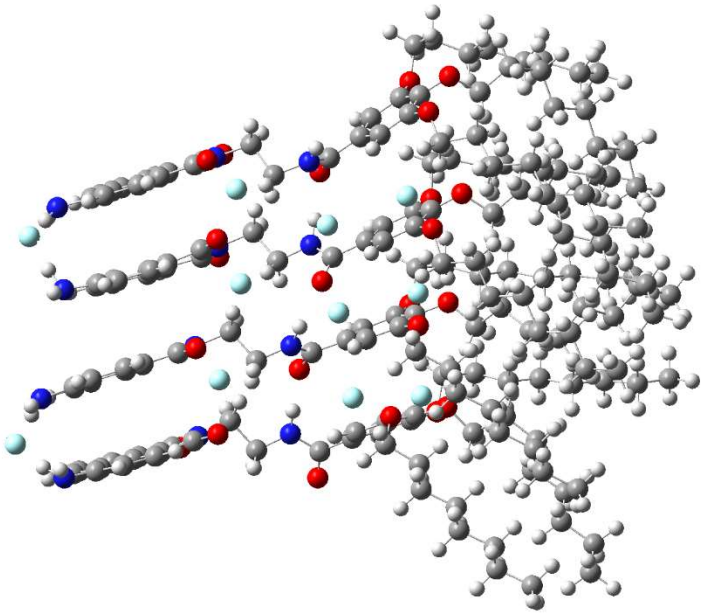

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H	1.51600000	-4.70100000	5.72400000
H	2.67500000	-3.39100000	6.02500000
H	0.80000000	-1.82100000	6.45400000
H	-0.36800000	-3.12600000	6.16500000
H	0.54200000	-4.39800000	8.07400000
H	1.78200000	-3.16200000	8.33700000
H	-0.02400000	-1.47400000	8.77100000
H	-1.23900000	-2.74900000	8.56600000
H	-0.74400000	-2.36800000	10.96100000
H	0.97400000	-2.71200000	10.67800000
H	-0.23800000	-4.00000000	10.47700000
H	-1.97200000	-2.31000000	0.94700000
H	-0.82000000	-3.12800000	2.03200000
H	-0.43200000	-1.01900000	3.23500000
H	-1.54700000	-0.16600000	2.16200000
H	-2.34600000	-2.48000000	3.99100000
H	-2.49400000	-0.77200000	4.42200000
H	-3.91000000	-2.12400000	2.07200000
H	-4.00100000	-0.39800000	2.47600000
H	-4.88800000	-2.70900000	4.26300000
H	-4.94200000	-0.99200000	4.71300000
H	-6.47600000	-0.53100000	2.82300000
H	-6.41700000	-2.24000000	2.34400000
H	-7.39800000	-2.89100000	4.53100000
H	-7.43300000	-1.18800000	5.03100000
H	-9.65100000	-1.93600000	4.20700000
H	-8.93500000	-2.35600000	2.63700000
H	-8.98300000	-0.65900000	3.17200000
H	-1.75500000	0.20100000	-2.98100000
H	-1.70800000	-1.54300000	-3.36300000
H	-2.72100000	-2.10800000	-1.23600000
H	-2.49900000	-0.46000000	-0.62400000
H	-4.10900000	0.37800000	-2.34600000
H	-4.39200000	-1.29400000	-2.87000000
H	-5.24000000	-1.87800000	-0.62100000
H	-4.87500000	-0.24300000	-0.03800000
H	-6.46200000	0.70600000	-1.70700000
H	-6.85600000	-0.93500000	-2.25600000
H	-7.70500000	-1.49700000	0.00700000

H	-7.27600000	0.12700000	0.57800000
H	-8.83500000	1.12300000	-1.09900000
H	-9.27900000	-0.50600000	-1.64200000
H	-10.95600000	0.37800000	-0.06100000
H	-9.70000000	0.62000000	1.16900000
H	-10.13200000	-1.02700000	0.64400000
F	4.17300000	-4.22200000	-15.38100000
C	3.71200000	-0.13700000	-13.03800000
C	4.32700000	-1.34600000	-13.31500000
C	4.89700000	-2.13700000	-12.27100000
C	4.78600000	-1.66900000	-10.93700000
C	4.11200000	-0.45000000	-10.66100000
C	3.59900000	0.30200000	-11.71600000
C	5.58000000	-3.35300000	-12.51300000
C	6.14800000	-4.06200000	-11.47800000
C	6.04200000	-3.59400000	-10.15900000
C	5.36200000	-2.41600000	-9.87800000
C	5.23500000	-1.92900000	-8.50900000
N	4.57700000	-0.72600000	-8.24500000
C	3.98000000	-0.00500000	-9.28400000
O	3.35600000	1.00300000	-8.95700000
O	5.68700000	-2.53600000	-7.54400000
N	4.37700000	-1.76600000	-14.62600000
C	4.55200000	-0.17600000	-6.85500000
C	3.18400000	-0.48800000	-6.22500000
N	3.26600000	-0.08400000	-4.80400000
C	3.32800000	-0.97000000	-3.76100000
C	3.23300000	-0.47100000	-2.38900000
O	3.46100000	-2.15600000	-4.03600000
C	3.97700000	-1.06800000	-1.35900000
C	3.90300000	-0.56700000	-0.06300000
C	3.06600000	0.51400000	0.23800000
C	2.30300000	1.09300000	-0.78400000
C	2.39000000	0.60900000	-2.08600000
O	1.47800000	2.16800000	-0.50000000
O	2.99800000	0.99800000	1.53500000
O	4.67100000	-1.17200000	0.91000000
C	5.75600000	-0.40800000	1.48600000
C	6.02500000	-1.01600000	2.86600000
C	4.95300000	-0.59700000	3.88400000
C	5.26500000	-1.18800000	5.26400000
C	4.27300000	-0.68400000	6.31900000
C	4.57900000	-1.34100000	7.67200000
C	3.67300000	-0.77700000	8.77100000
C	3.95700000	-1.45600000	10.11400000
C	1.78200000	0.79300000	2.27900000
C	1.54000000	2.11100000	3.02100000
C	0.17500000	2.14400000	3.73100000
C	0.11100000	1.32400000	5.03000000
C	0.78400000	2.06200000	6.19400000
C	0.55400000	1.33000000	7.51900000
C	1.18100000	2.11300000	8.67800000
C	0.88900000	1.43400000	10.02000000
C	0.19800000	2.42200000	-1.12700000
C	-0.82000000	2.15700000	-0.02100000
C	-2.22800000	2.64000000	-0.38600000

C	-3.17300000	2.37600000	0.79300000
C	-4.58600000	2.89100000	0.49800000
C	-5.51100000	2.59600000	1.68500000
C	-6.93000000	3.10700000	1.41000000
C	-7.85400000	2.77500000	2.58600000
H	5.65100000	-3.72000000	-13.50900000
H	3.82700000	-1.26900000	-15.33100000
H	4.42900000	-2.82300000	-14.83200000
H	3.32900000	0.45500000	-13.83000000
H	3.12000000	1.22900000	-11.52000000
H	6.66900000	-4.96500000	-11.67700000
H	6.49600000	-4.14800000	-9.37600000
H	5.31300000	-0.64400000	-6.24600000
H	4.67300000	0.89900000	-6.88600000
H	2.39900000	0.07200000	-6.73600000
H	2.97400000	-1.55100000	-6.31500000
H	3.37700000	0.92400000	-4.56600000
H	4.60300000	-1.89600000	-1.56900000
H	1.83100000	1.06400000	-2.85900000
H	6.64100000	-0.49800000	0.85600000
H	5.48300000	0.64000000	1.59200000
H	6.06100000	-2.10300000	2.78200000
H	6.99500000	-0.65800000	3.21200000
H	4.92600000	0.49200000	3.94800000
H	3.97700000	-0.95000000	3.54800000
H	5.21700000	-2.27600000	5.20800000
H	6.27400000	-0.89800000	5.56100000
H	4.35800000	0.40000000	6.40900000
H	3.25400000	-0.93000000	6.01500000
H	4.42500000	-2.41900000	7.59300000
H	5.62100000	-1.15800000	7.93800000
H	3.84200000	0.29600000	8.86900000
H	2.63100000	-0.94500000	8.50100000
H	3.30200000	-1.03900000	10.88000000
H	4.99400000	-1.28900000	10.40700000
H	3.77400000	-2.52900000	10.03700000
H	1.90600000	-0.03100000	2.97900000
H	0.95400000	0.58200000	1.60300000
H	2.34800000	2.27900000	3.73200000
H	1.56500000	2.91300000	2.28500000
H	-0.08300000	3.18000000	3.95300000
H	-0.58600000	1.77100000	3.04600000
H	-0.94000000	1.16700000	5.28000000
H	0.57900000	0.34900000	4.89200000
H	1.85600000	2.15400000	6.00900000
H	0.35000000	3.05700000	6.27000000
H	-0.51900000	1.22500000	7.69400000
H	1.00100000	0.33800000	7.46400000
H	2.26000000	2.17600000	8.53100000
H	0.77300000	3.12600000	8.70100000
H	1.36200000	1.99700000	10.82600000
H	1.28100000	0.41700000	10.02300000
H	-0.18700000	1.40200000	10.19500000
H	0.14800000	3.46200000	-1.44900000
H	0.01100000	1.75700000	-1.96900000
H	-0.83500000	1.08600000	0.18200000

H	-0.49500000	2.67500000	0.87800000
H	-2.20400000	3.71100000	-0.59800000
H	-2.58400000	2.11000000	-1.27000000
H	-3.21300000	1.30400000	0.98500000
H	-2.79000000	2.87400000	1.68500000
H	-4.55300000	3.96800000	0.32300000
H	-4.97400000	2.40000000	-0.39600000
H	-5.54300000	1.52000000	1.85700000
H	-5.12000000	3.08100000	2.58100000
H	-6.90700000	4.18900000	1.26400000
H	-7.32000000	2.64100000	0.50400000
H	-8.86000000	3.13600000	2.37200000
H	-7.49000000	3.25700000	3.49400000
H	-7.89000000	1.69600000	2.74000000
C	6.99100000	1.30900000	-10.95200000
C	7.75200000	0.20000000	-11.27800000
C	8.31800000	-0.63500000	-10.26900000
C	8.16200000	-0.24600000	-8.91900000
C	7.49600000	0.96600000	-8.60500000
C	6.87600000	1.69600000	-9.61600000
C	9.00500000	-1.83800000	-10.56000000
C	9.48300000	-2.64000000	-9.54700000
C	9.30700000	-2.26200000	-8.20700000
C	8.66800000	-1.07200000	-7.88300000
C	8.50800000	-0.64700000	-6.49700000
N	7.99400000	0.62100000	-6.21100000
C	7.50000000	1.43500000	-7.23600000
O	7.09100000	2.54900000	-6.91400000
O	8.81900000	-1.34700000	-5.53800000
N	7.99500000	-0.05800000	-12.59900000
C	7.98500000	1.12300000	-4.80800000
C	6.53400000	0.99900000	-4.31700000
N	6.41400000	1.79500000	-3.09700000
C	5.25100000	2.40900000	-2.72800000
C	5.20500000	3.08700000	-1.43200000
O	4.30100000	2.35500000	-3.51000000
C	6.00600000	2.64800000	-0.36200000
C	5.95200000	3.29500000	0.86700000
C	5.12800000	4.40800000	1.04500000
C	4.28900000	4.81200000	0.00200000
C	4.33600000	4.17000000	-1.23300000
O	3.36000000	5.81100000	0.20600000
O	5.13700000	5.09400000	2.23400000
O	6.68600000	2.77400000	1.91100000
C	7.90900000	3.40900000	2.31400000
C	8.48600000	2.52900000	3.42700000
C	7.68000000	2.61700000	4.73100000
C	8.28300000	1.66800000	5.77400000
C	7.54100000	1.76700000	7.11200000
C	8.10700000	0.74300000	8.10400000
C	7.41400000	0.85400000	9.46800000
C	7.92000000	-0.23400000	10.41900000
C	4.18800000	4.71300000	3.24200000
C	4.25500000	5.86400000	4.24300000
C	3.36200000	5.70200000	5.47900000
C	1.86800000	5.80800000	5.14600000

C	1.05400000	5.86600000	6.44500000
C	-0.44900000	5.93300000	6.14800000
C	-1.25600000	5.85000000	7.44900000
C	-2.75400000	6.00100000	7.16600000
C	1.99000000	5.35400000	0.17700000
C	1.20400000	6.27400000	1.11100000
C	-0.20100000	5.69800000	1.32400000
C	-1.05300000	6.59000000	2.23100000
C	-2.41300000	5.92300000	2.47300000
C	-3.32300000	6.81800000	3.32200000
C	-4.66800000	6.12200000	3.56600000
C	-5.59200000	7.01100000	4.40300000
H	9.14500000	-2.12000000	-11.57500000
H	7.53900000	0.55900000	-13.27800000
H	9.04500000	-0.08500000	-12.84000000
H	6.53900000	1.88200000	-11.71900000
H	6.33000000	2.57500000	-9.37800000
H	9.98400000	-3.54900000	-9.77700000
H	9.67400000	-2.89600000	-7.43900000
H	8.62600000	0.53900000	-4.16200000
H	8.27600000	2.16200000	-4.79600000
H	5.85900000	1.39800000	-5.07200000
H	6.29200000	-0.04900000	-4.12400000
H	7.28000000	2.14600000	-2.64300000
H	6.64100000	1.81000000	-0.47800000
H	3.70600000	4.49000000	-2.02100000
H	8.60100000	3.42000000	1.47600000
H	7.72200000	4.42200000	2.67300000
H	8.51200000	1.49600000	3.07700000
H	9.51100000	2.85000000	3.61800000
H	7.70600000	3.64100000	5.10500000
H	6.64200000	2.33500000	4.54000000
H	8.22100000	0.64400000	5.40200000
H	9.33400000	1.91800000	5.93000000
H	7.66000000	2.77300000	7.51600000
H	6.47800000	1.57200000	6.95700000
H	7.96100000	-0.26200000	7.70400000
H	9.17800000	0.91300000	8.23100000
H	7.62000000	1.83100000	9.90500000
H	6.33600000	0.74700000	9.34300000
H	7.42000000	-0.13700000	11.38400000
H	8.99600000	-0.13200000	10.56700000
H	7.70500000	-1.22100000	10.00700000
H	3.19000000	4.62900000	2.81400000
H	4.48900000	3.77200000	3.70500000
H	5.28500000	5.94800000	4.57300000
H	3.99500000	6.78700000	3.72900000
H	3.56700000	4.74300000	5.95800000
H	3.61800000	6.49900000	6.17900000
H	1.56100000	4.94400000	4.55600000
H	1.68500000	6.71600000	4.57100000
H	1.27400000	4.98600000	7.05000000
H	1.34300000	6.75200000	7.01400000
H	-0.67000000	6.87300000	5.64300000
H	-0.73600000	5.10800000	5.49300000
H	-1.07700000	4.88500000	7.92700000

H	-0.94000000	6.64300000	8.13000000
H	-3.31300000	5.89900000	8.09700000
H	-3.08500000	5.23100000	6.46800000
H	-2.95400000	6.98500000	6.74200000
H	1.59300000	5.40100000	-0.83800000
H	1.93900000	4.33200000	0.55100000
H	1.71600000	6.33000000	2.07100000
H	1.14400000	7.27100000	0.67300000
H	-0.69800000	5.58700000	0.35900000
H	-0.10900000	4.71600000	1.79000000
H	-0.54600000	6.73200000	3.18600000
H	-1.19800000	7.56300000	1.75600000
H	-2.89800000	5.72800000	1.51400000
H	-2.26200000	4.97300000	2.98900000
H	-2.84100000	7.02300000	4.27800000
H	-3.49100000	7.76300000	2.80300000
H	-5.14900000	5.90800000	2.60900000
H	-4.50400000	5.18000000	4.09300000
H	-6.54200000	6.50000000	4.56400000
H	-5.77900000	7.95200000	3.88300000
H	-5.13400000	7.22100000	5.37100000
F	10.41600000	0.43200000	-13.20700000
C	8.86400000	4.55600000	-11.32500000
C	9.62400000	3.40100000	-11.39900000
C	10.14500000	2.78600000	-10.21800000
C	9.89700000	3.41400000	-8.97100000
C	9.13700000	4.61200000	-8.91000000
C	8.62100000	5.15500000	-10.08600000
C	10.88100000	1.57600000	-10.23900000
C	11.35200000	1.01600000	-9.07400000
C	11.11700000	1.64600000	-7.84300000
C	10.40400000	2.83600000	-7.77900000
C	10.15600000	3.49500000	-6.50300000
N	9.43200000	4.69000000	-6.45300000
C	8.92200000	5.25800000	-7.62500000
O	8.31900000	6.32500000	-7.50200000
O	10.56300000	3.03900000	-5.43800000
N	9.87100000	2.87300000	-12.64600000
C	9.22200000	5.38300000	-5.14900000
C	7.76500000	5.13600000	-4.70000000
N	7.66100000	5.70800000	-3.34400000
C	8.07300000	5.03400000	-2.22400000
C	8.25100000	5.77300000	-0.97400000
O	8.31500000	3.83500000	-2.33400000
C	9.25900000	5.37200000	-0.08400000
C	9.45400000	6.04600000	1.11500000
C	8.65600000	7.15000000	1.44300000
C	7.65400000	7.55500000	0.55800000
C	7.44300000	6.87400000	-0.64000000
O	6.86100000	8.63300000	0.89100000
O	8.80500000	7.81700000	2.64100000
O	10.41300000	5.53400000	1.96500000
C	11.52100000	6.31900000	2.46600000
C	12.15600000	5.46700000	3.57500000
C	11.23400000	5.37400000	4.80100000
C	11.81800000	4.50400000	5.91900000

C	10.87100000	4.52800000	7.12800000
C	11.34500000	3.57400000	8.23000000
C	10.40300000	3.65400000	9.43800000
C	10.83800000	2.67200000	10.53000000
C	8.19300000	7.21600000	3.79600000
C	8.38000000	8.22500000	4.93700000
C	8.31300000	7.60200000	6.34400000
C	7.07600000	6.72600000	6.57700000
C	7.05900000	6.14700000	7.99700000
C	5.84500000	5.22500000	8.17200000
C	5.85600000	4.55400000	9.55000000
C	4.69700000	3.55900000	9.66800000
C	5.42600000	8.51100000	0.85400000
C	4.93400000	9.24700000	2.10300000
C	3.40100000	9.22700000	2.15700000
C	2.87300000	9.68800000	3.52200000
C	1.33900000	9.64000000	3.53800000
C	0.79500000	9.87500000	4.95200000
C	-0.73900000	9.85700000	4.94700000
C	-1.28500000	9.97400000	6.37200000
H	11.05900000	1.08900000	-11.16700000
H	9.24500000	3.11600000	-13.41800000
H	10.18700000	1.84500000	-12.73300000
H	8.47300000	4.98500000	-12.21100000
H	8.04000000	6.04100000	-10.04400000
H	11.89000000	0.10200000	-9.10900000
H	11.49000000	1.20100000	-6.95400000
H	9.88500000	4.98900000	-4.39000000
H	9.36800000	6.44700000	-5.27500000
H	7.07000000	5.63200000	-5.37900000
H	7.53800000	4.07100000	-4.69000000
H	7.53600000	6.72700000	-3.27000000
H	9.87100000	4.54000000	-0.32100000
H	6.66500000	7.18300000	-1.28700000
H	12.24000000	6.48900000	1.66400000
H	11.18500000	7.27500000	2.86700000
H	12.36000000	4.46800000	3.18700000
H	13.09900000	5.92700000	3.87300000
H	11.05800000	6.38100000	5.18000000
H	10.28300000	4.93800000	4.49700000
H	11.93000000	3.48000000	5.55900000
H	12.79700000	4.88800000	6.21500000
H	10.82900000	5.54200000	7.52800000
H	9.86800000	4.23500000	6.81000000
H	11.35600000	2.55300000	7.84400000
H	12.35600000	3.84600000	8.53900000
H	10.41300000	4.66800000	9.84300000
H	9.38600000	3.41400000	9.12600000
H	10.14800000	2.73400000	11.37300000
H	11.84300000	2.91800000	10.87500000
H	10.83000000	1.65300000	10.14200000
H	8.69000000	6.27700000	4.02700000
H	7.13300000	7.03900000	3.61200000
H	9.35600000	8.70200000	4.82800000
H	7.61900000	8.99900000	4.83900000
H	9.20400000	6.99500000	6.50000000

H	8.32600000	8.40800000	7.08000000
H	6.17400000	7.32000000	6.41400000
H	7.09300000	5.89300000	5.87500000
H	7.97400000	5.57600000	8.16400000
H	7.01100000	6.95900000	8.72600000
H	4.92900000	5.80900000	8.06800000
H	5.86100000	4.45600000	7.39700000
H	6.80000000	4.02600000	9.69200000
H	5.76300000	5.31500000	10.32800000
H	4.72200000	3.08400000	10.65000000
H	4.78700000	2.78900000	8.90200000
H	3.74500000	4.07900000	9.55000000
H	5.02900000	8.97200000	-0.05100000
H	5.13400000	7.46100000	0.90900000
H	5.34500000	8.74900000	2.98200000
H	5.28900000	10.27900000	2.08500000
H	3.00300000	9.86900000	1.36900000
H	3.06200000	8.20800000	1.97600000
H	3.26500000	9.03100000	4.30000000
H	3.20900000	10.70800000	3.72200000
H	0.94800000	10.40300000	2.86200000
H	1.00400000	8.66300000	3.18900000
H	1.16500000	9.09000000	5.61500000
H	1.14600000	10.84100000	5.32300000
H	-1.11100000	10.69200000	4.34800000
H	-1.09600000	8.92700000	4.50300000
H	-2.37600000	9.95600000	6.34800000
H	-0.95600000	10.91100000	6.82300000
H	-0.93200000	9.13900000	6.97900000
H	4.91900000	-3.86100000	-16.00900000
H	9.52100000	0.58300000	-12.69900000
F	0.76624600	-0.79668100	-3.02748000
F	5.33460000	4.59245000	-3.27227000
F	3.21183000	1.58658000	-3.09681000
F	5.53414000	1.49607000	-6.32415000
F	3.20099000	-1.29047000	-7.64330000
F	8.18856000	4.06544000	-5.93417000
F	4.15041000	7.26088000	-0.81002600
F	2.07880000	3.51861000	-0.50707200
F	0.01121590	-0.52637500	-0.47066300

References

1.M. R. Molla, A. Das and S.Ghosh,*Chem. Eur. J*. 2010, **16**, 10084-10093.

2.M.Muthukkumar, T. Bhuvaneswari, G. Venkatesh, C. Kamal, P. Vennila, S. J.Armaković,Y. S.Mary andC.YPanicker,*J. Mol. Liq.*2018, **272**, 481–495.

3.G.Venkatesh, M.Govindaraju, C.Kamal, P.Vennila and S.Kaya, *RSC Adv.*2017, **7**, 1401–1412.

4. Gaussian 09, Revision D.01; Gaussian, Inc.: Wallingford, CT, **2009**.

5. GaussView, Version 5; Gaussian, Inc.: Wallingford, CT, **2009**.

6.J.Contreras-García, E. R.Johnson, S. Keinan, R.Chaudret, J. P.Piquemal, D. N.Beratan, W.Yang,*J. Chem. Theory Comput.*2011, **7**, 625–632.