Supporting Information for

Luminescent property switching in 1D supramolecular polymerization of organic donor-π-acceptor chromophore

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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 and AFM images were collected using a 200 KV Transmission Electron Microscope (MODEL: JEOL JEM 2100 HR with EELS) and Bruker Innova-S2 instrument in the tapping mode respectively. Fluorescence spectra were recorded on HORIBA scientific Fluoromax-4 fluorescence spectrophotometer. Rheological experiments were performed with an AR-2000 advanced Rheometer (TA instruments) by cone and plate geometry in a peltier plate.

UV-visible spectroscopic studies: For UV/Vis spectroscopic studies, stock solutions of **NMI-2** and **NMI-C** were made in THF (1.0 mM). An aliquot (50 µl) was added to an appropriate amount of methylcyclohexane (MCH)/THF or Dodecane/THF mixture to adjust the desired solvent composition and final concentration at 0.1 mM. The solutions were allowed to equilibrate at room temperature for 1 h before spectral measurements. For methanol experiments a solution of a particular chromophore in MCH/ THF (95:5) and Dodecane/THF (95:5) was taken and gradually methanol was added and spectra were recorded. For variable-temperature experiments, a particular chromophore solution in

MCH/ THF (95:5) and Dodecane/THF (95:5) was heated from room temperature (25^{o}C) to 65^{o}C temperature and vice versa. The solution was allowed to equilibrate for 10 minutes at the desired temperature before each measurement.

Atomic Force Microscopic (AFM) Study: In a typical AFM experiment, 25 µl solution of **NMI-2** of each solvent compositions (MCH/THF), (concentration = 0.1mM) were placed on a microscopic cover glass and allowed to air dry overnight before the images were taken. For gel in dodecane and MCH, sample for the AFM measurements were prepared from dilute gel.

Determination of T_{gel} (gel to sol transition temperature): In a typical experiment, at first 2 wt% (w/v) solution of the NMI-2 in MCH or Dodecane was prepared in a screw-capped sample vial. The solvent was heated with a hot air gun and then allowed to cool to room temperature for 1h. After the formation of gel, it was put into the oil bath to calculate the T_{gel} value. Then wt% of the gel was varied by adding required amount of solvent and corresponding T_{gel} was measured. The process was continued until it reaches to the CGC (critical gelation concentration) value.

Enthalpy of Melting (ΔH_m) Calculation: T_{gel} of **NMI-2** gelator in a given solvent was determined by above-mentioned method at different gelator concentrations (wt%) and these data were used to determine the ΔH_m value using Schroeder-van Larr equation.

Rheological Measurements: In a typical experiment, 1.4 wt% gel was made in both methylcyclohexane (MCH) and Dodecane, then they were left overnight at room temperature before measurements were carried out. In the rheometer the cone diameter, cone angel and truncation were 40 mm, 4^{o} 0’ 22” and 121 µM respectively. Stress-

amplitude sweep measurement was carried out to measure gel strength. The runs were conducted at a constant oscillation frequency of 1Hz and temperature 25^{o}C.

Measurement of fluorescence quantum yield: Fluorescence quantum yield at room temperature was estimated at a single excitation wavelength (400 nm) using quinine sulfate in sulfuric acid (0.1 M) aqueous solution ($\Phi = 0.546$) as the reference according to the equation **S1**:

$$\Phi_X = \Phi_{ST}\left(\frac{Grad_X}{Grad_{ST}}\right)\left(\frac{\eta_X^2}{\eta_{ST}^2}\right) \longrightarrow S1$$

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. For 97: 3 MCH/ THF or dodecane/THF solution, the refractive index of the solvent was taken as that of the MCH or dodecane.

In this method, the average quantum yields of **NMI-2** were estimated to be 0.47, 0.1 and 0.03 for THF, dodecane/THF and MCH/THF (97:3) solution respectively.

Time Correlated Single Photon Counting (TCSPC) experiment: In a typical experiment, 0.1mM solutions of the **NMI-2** were used for the measurement. Samples were excited at 420 nm and emissions were monitored at 515 nm for all the solution.

Computational Studies: All calculations were carried out within the Gaussian 09 program package.[1] To reduce computational cost, the large hydrocarbon chains were replaced by methyl groups. Geometry optimizations were performed with Head-Gordon's ωB97x-D functional,[2] which takes into account long-range dispersion interactions like π-π stacking, H-bonding etc. in conjunction with Pople's triple-

ζ quality 6-311G(d,p) basis set on all atoms. Optimizations always employed the polar continuum model (CPCM) with the dielectric constant and other parameters of the respective solvents: MCH (ε=2.071, refractive index = 1.423) and THF (ε= 7.25, refractive index = 1.407). Excited state time-dependent DFT (TD-DFT) calculations were conducted on the optimized geometries, together with the hybrid exchange-correlation functional B3LYP [3] in MCH and THF (CPCM) solvent, with nstates=5 and root=1, and Pople basis 6-311G(d,p), as implemented in the software.

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

Compound NMI-1: At first, Compound A (0.712g, 1.30 mmol) (synthesis is followed from the our previous report)[4] and 4-Nitro 1,8 Napthalic Anhydride (0.3g , 1.23 mmol) were dissolved in 40 ml dried Toluene and the solution was refluxed at 100^0C for 24h under Argon atmosphere. Next, the reaction was stopped and the solution was evaporated to get the crude the product. The residue was purified by column chromatography using ethyl acetate in hexane (1:5) as the eluent to get the compound **NMI-1** as a light -yellow solid in 67% of yield.

^{1}H-NMR (300 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).

^{13}C-NMR (400 MHz, $CDCl_3$, TMS): δ (ppm) = 167.94, 165.21, 164.36, 153.44, 150.62, 140.89, 132.46, 129.93, 129.14, 126.60, 124.02, 122.69, 105.38, 73.29, 69.14, 39.91, 36.60, 31.84, 30.92, 29.12, 26.12, 22.12, 22.67, 14.00.

ESI-MS: m/z calculated for $[C_{45}H_{63}N_3O_8Na]$ $(M+Na)^+$ =796.4615, Found-796.4513.

Compound NMI-2: Compound **NMI-1** (0.45g, 0.58mmol) was dissolved in degassed ethyl acetate and then Pd/C was added 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 hexane to get the pure product as a yellow solid in 96% 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).

^{13}C-NMR (300 MHz, $CDCl_3$, TMS): δ (ppm) =167.5, 165.4, 157.5, 152.9, 144.9, 140.6, 139.1, 138.9, 135.7, 131.8, 129.2, 127.2, 124.6, 122.8, 119.7, 116.9, 112.2, 105.2, 69.0, 42.9, 39.2, 31.8, 29.4, 25.9, 22.7, 14.1.

ESI-MS: m/z calculated for $[C_{45}H_{65}N_3O_6Na]$ $(M+Na)^+$ = 766.4771, Found-766.4772.

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

Compound NMI-C_0: At first, n-Octyl amine (0.3g, 2.32 mmol) and 4-Nitro 1,8 Napthalic Anhydride (0.55g ,2.26 mmol) were dissolved in 25 ml of dried toluene and the solution was refluxed at 100^0C for 24h under Argon atmosphere. The solution was evaporated to get the crude product. The residue was purified by column chromatography using ethyl acetate in hexane (1:5) as the eluent to get the compound as a light -yellow solid in 71% 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).

^{13}C-NMR (300 MHz, $CDCl_3$, TMS): δ (ppm) = 164.6, 164.1, 149.2, 133.7, 131.4, 129.7, 126.8, 124.8, 123.1, 120.1, 112.0, 109.5, 40.2, 31.8, 29.1, 28.1, 27.1, 22.6, 14.1.

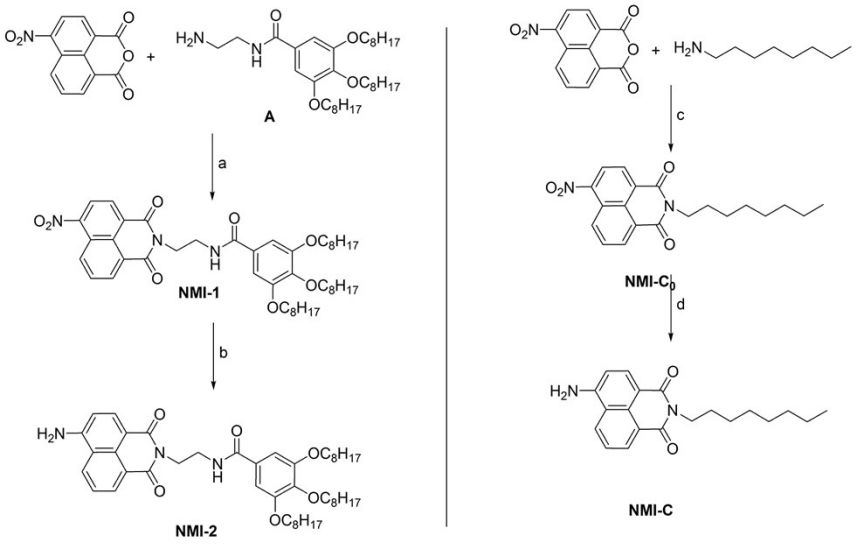
ESI-MS: m/z calculated for $[C_{20}H_{22}N_2O_4]$ $(M+H)^+$ = 355.1580, Found-355.1572.

Compound NMI-C: The compound **NMI-C_0** (0.4g, 1.13 mmol) was dissolved in degassed ethyl acetate and then Pd/C was added to the solution. The reaction mixture was stirred under H_2 atmosphere at Room temperature for 24h. The Pd/C was filtered off using celite 545 as filtering agent and then ethyl acetate was evaporated to get the pure product as yellow solid in 93% yield. The product was used for studies without any further purification.

^{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).

^{13}C-NMR (300 MHz, $CDCl_3$, TMS): δ (ppm) =164.6, 164.1, 149.2, 133.7, 131.4,129.7,126.8, 124.8,123.1,120.1,112.0,109.5,40.2,31.8,29.1,28.1,27.1,22.6,14.1.

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



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

Additional figures:

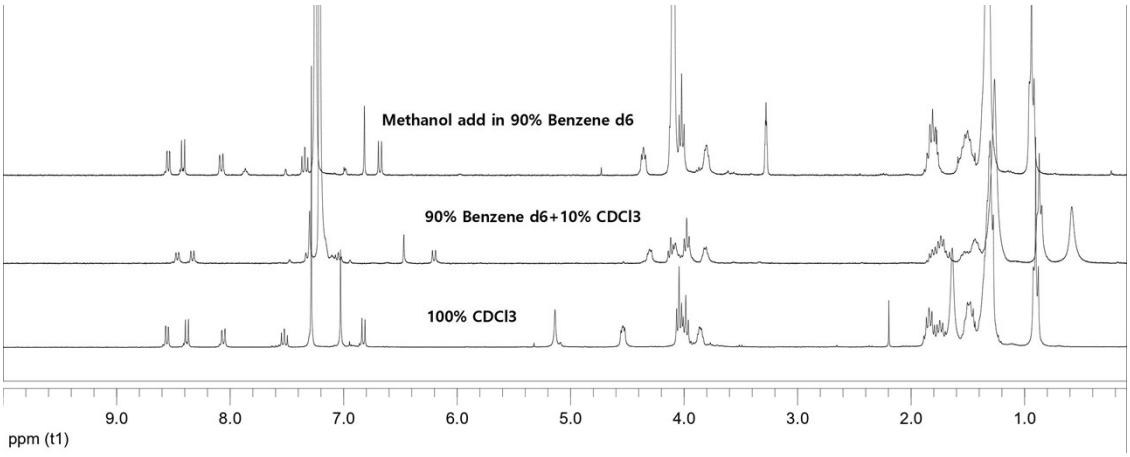


Figure S1: ^{1}H-NMR stack plot. ^{1}H-NMR spectrum of **NMI-2** in (Bottom) $CDCl_3$; (Middle) 90% benzene-d6 + 10% $CDCl_3$ (self-assembled form); (Top) after methanol addition to the self-assembled form.

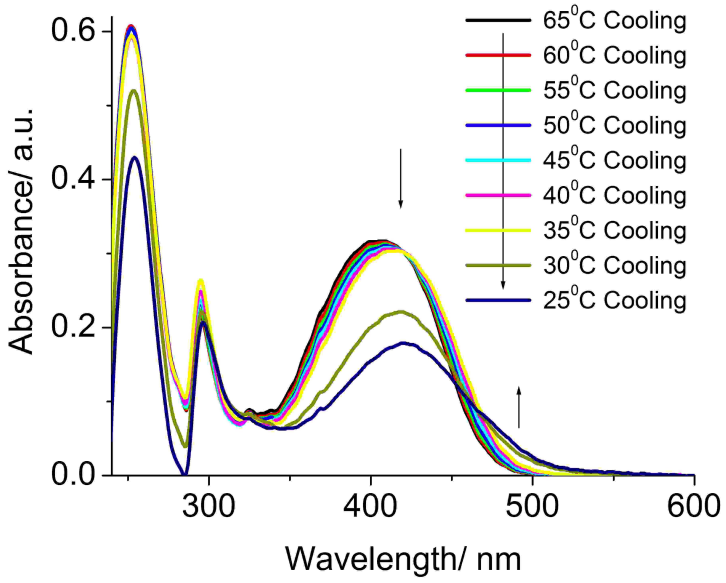


Figure S2: Variable temperature (cooling) UV/Vis spectra of **NMI-2** in dodecane.

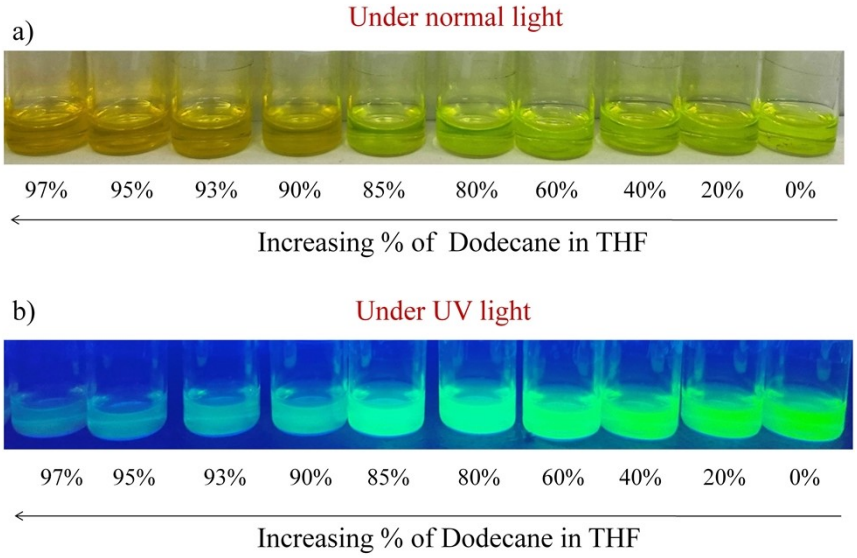


Figure S3: Images of samples with different solvent composition (dodecane/THF). (a) under normal light and (b) under UV light.

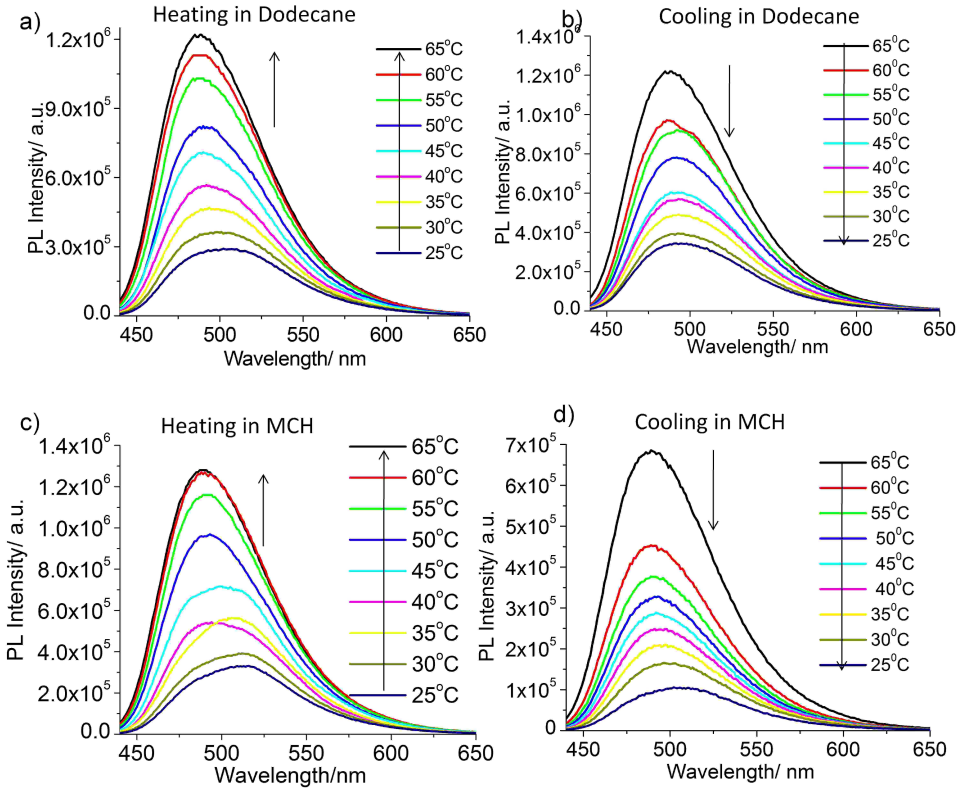


Figure S4: Variable temperature emission spectra of **NMI-2** in MCH/THF and dodecane/THF solvent composition. (a) heating, (b) cooling in dodecane/THF solvent mixture, (c) heating, (d) cooling in MCH/THF solvent mixture

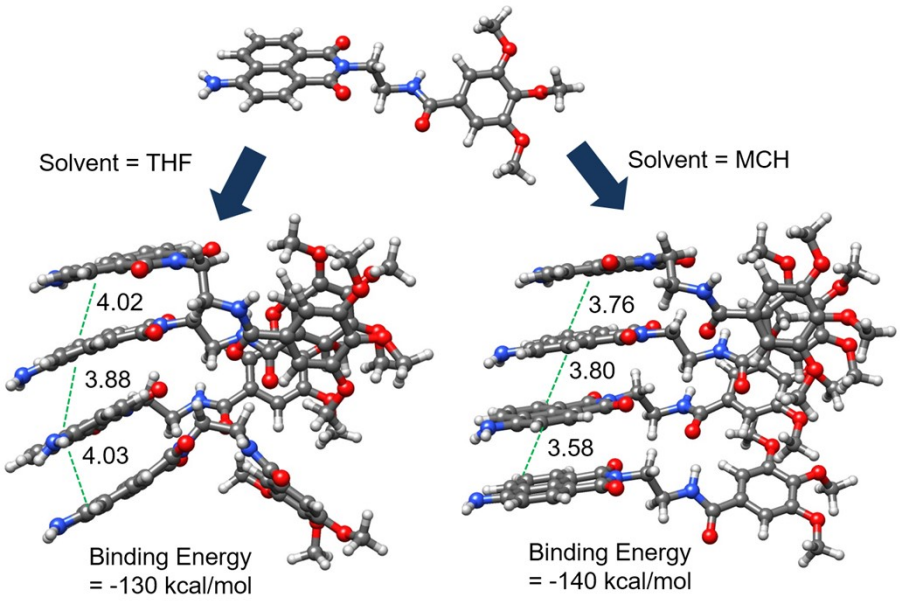


Figure S5. DFT optimized tetramer model of NMI-2 as observed in THF and MCH solvent with binding energies relative to the monomer in same solvent. Interplanar distances shown are in units of Å.

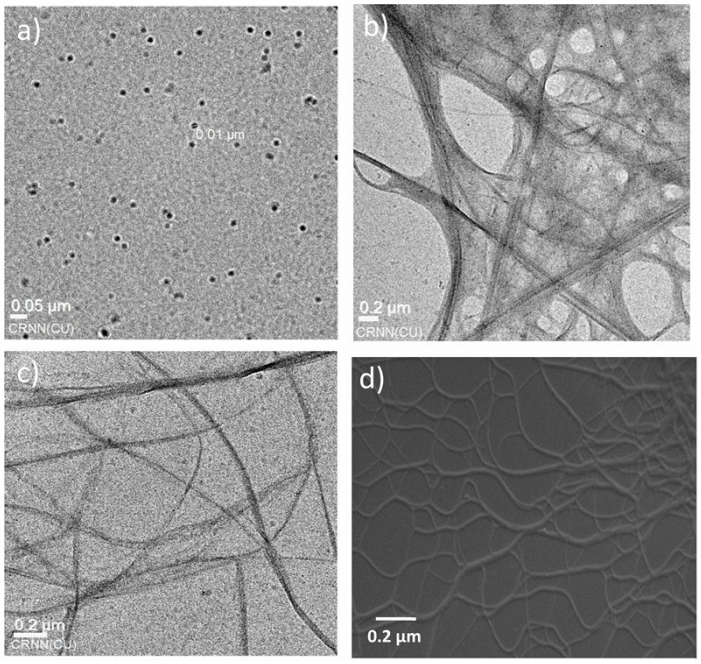


Figure S6: TEM images of NMI-2 in (a) THF; (b) dodecane; (c) MCH. (d) SEM images of NMI-2 in MCH. Concentration of NMI-2 solution = 0.1 mM. Temperature = 25°C.

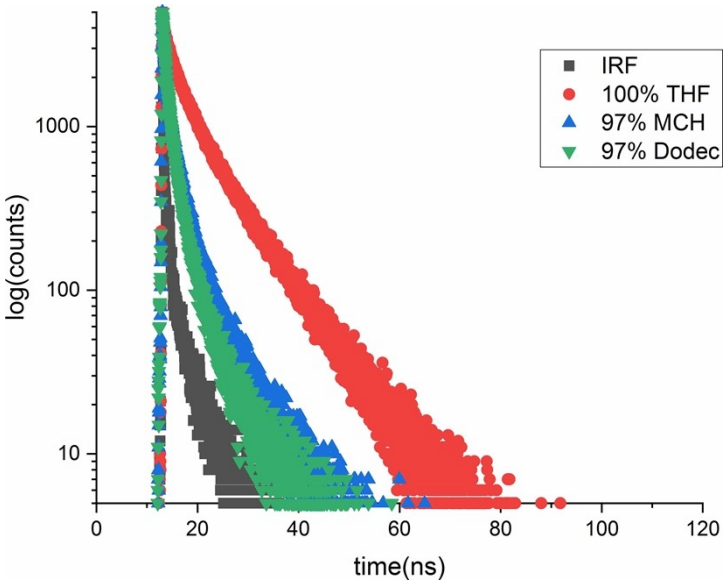


Figure S7: Time resolved fluorescence decay of **NMI-2** in THF, MCH/THF and dodecane/THF (97:3) as labeled in the plot**.** Emission was monitored at 515 nm). Concentration of **NMI-2** = 0.1mM, λ_{ex} = 420 nm.

Table S1. Fluorescence lifetime data for THF, MCH/THF or dodecane/THF (97:3) solution (emission monitored at 515 nm) of **NMI-2**

Sample	Component Lifetimes (ns)[a]			
	τ_1	τ_2	τ_3	τ_{avg}
NMI-2 (THF)	2.59 (32 %)	9.77 (13%)	0.41(55%)	2.31
NMI-2 (97:3) MCH/THF	1.81 (14 %)	9.85 (1 %)	0.26 (85 %)	0.54
NMI-2 (97:3) dodecane/THF	1.30 (2%)	12.99 (1%)	0.39 (79%)	0.61

[a] Values in parenthesis shows the decay contribution corresponding to each lifetime. Average lifetimes (τ_{avg}) were calculated using the following equation: $\tau_{avg} = a_1\tau_1 + a_2\tau_2 + a_3\tau_3$

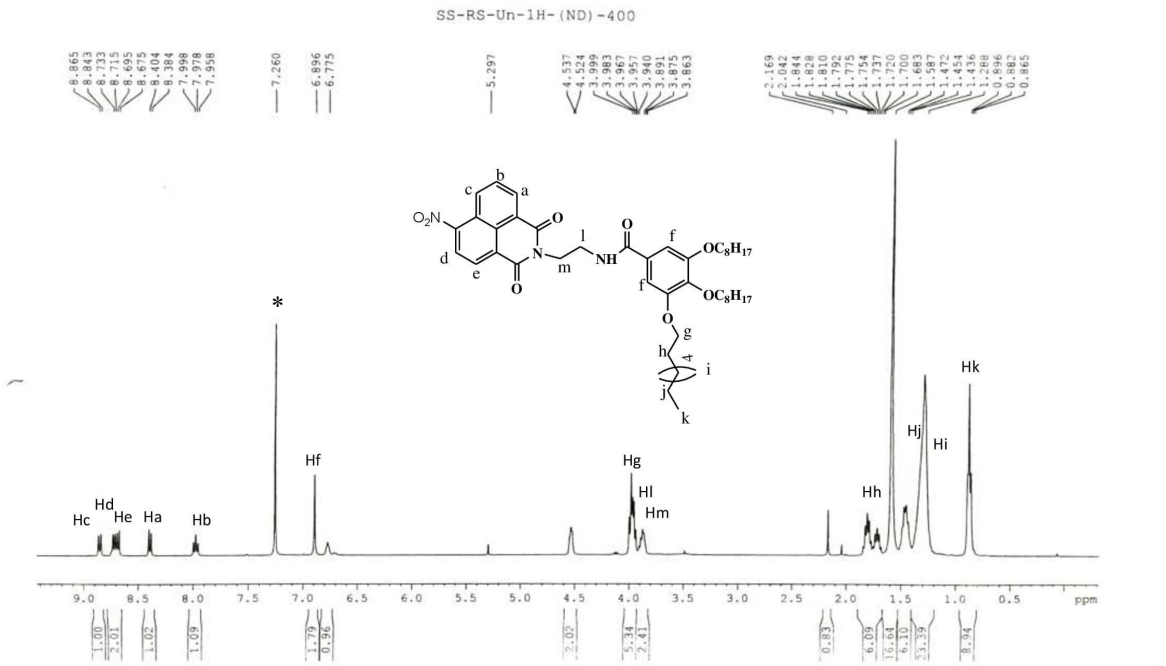


Figure S8: ^{1}H- NMR spectrum of Compound **NMI-1**. Solvent-$CDCl_3$* indicates solvent peak.

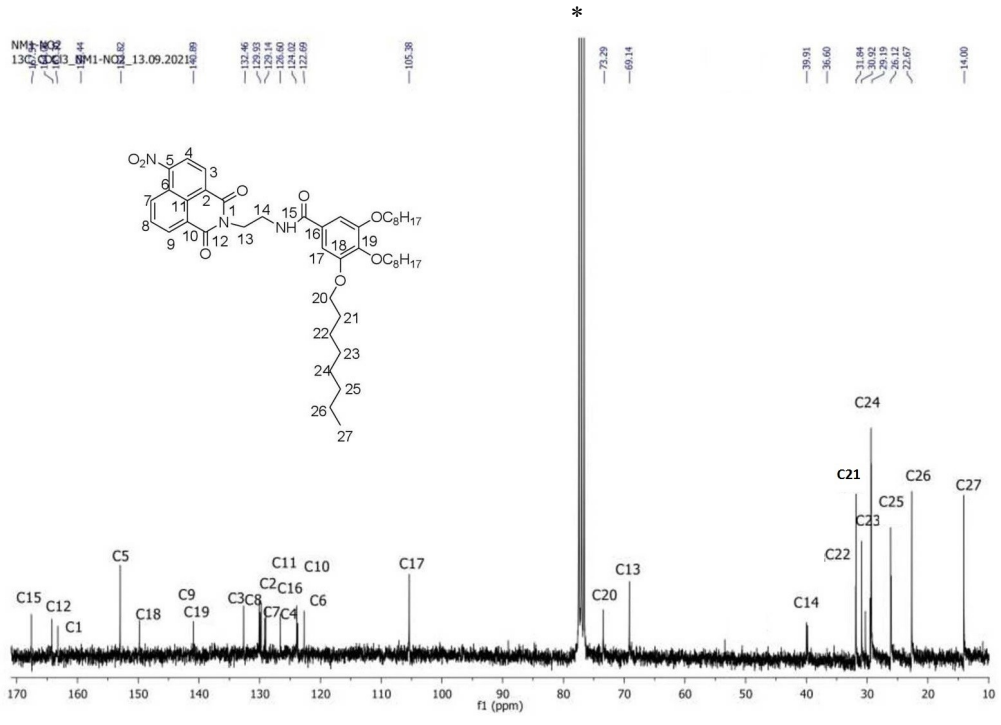


Figure S9: ^{13}C- NMR spectrum of Compound **NMI-1**. Solvent-$CDCl_3$* indicates solvent peak.

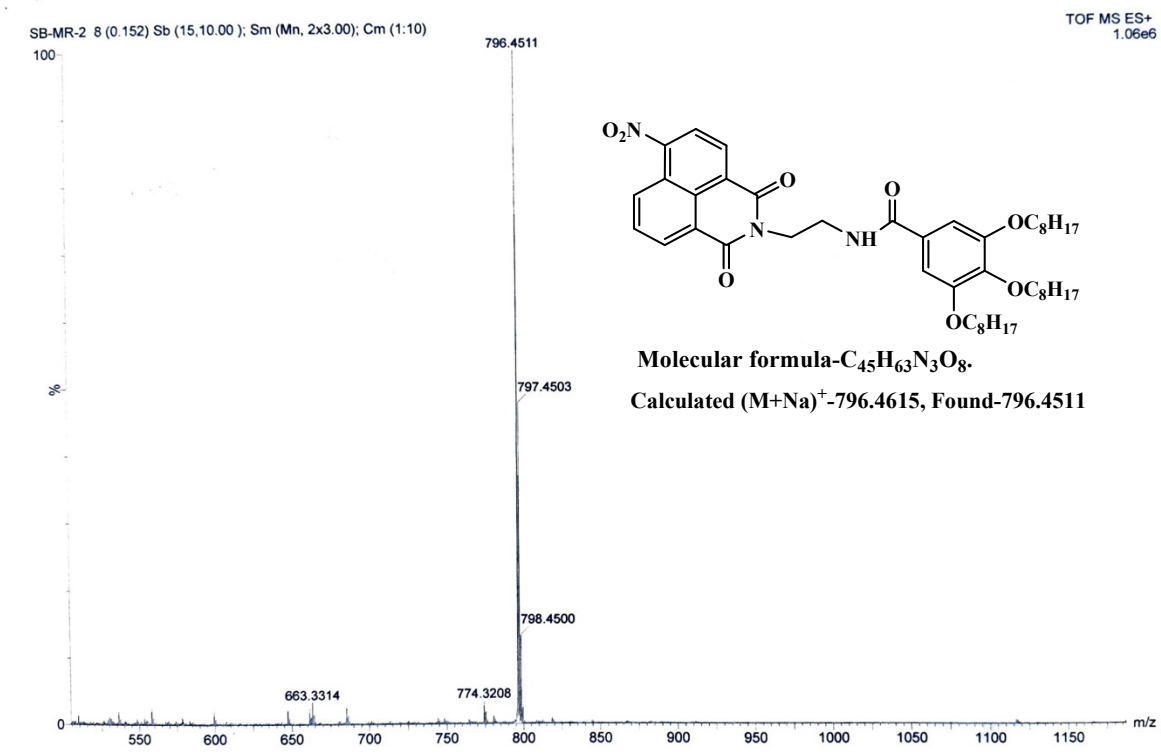


Figure S10: ESI-MS spectrum of Compound **NMI-1**.

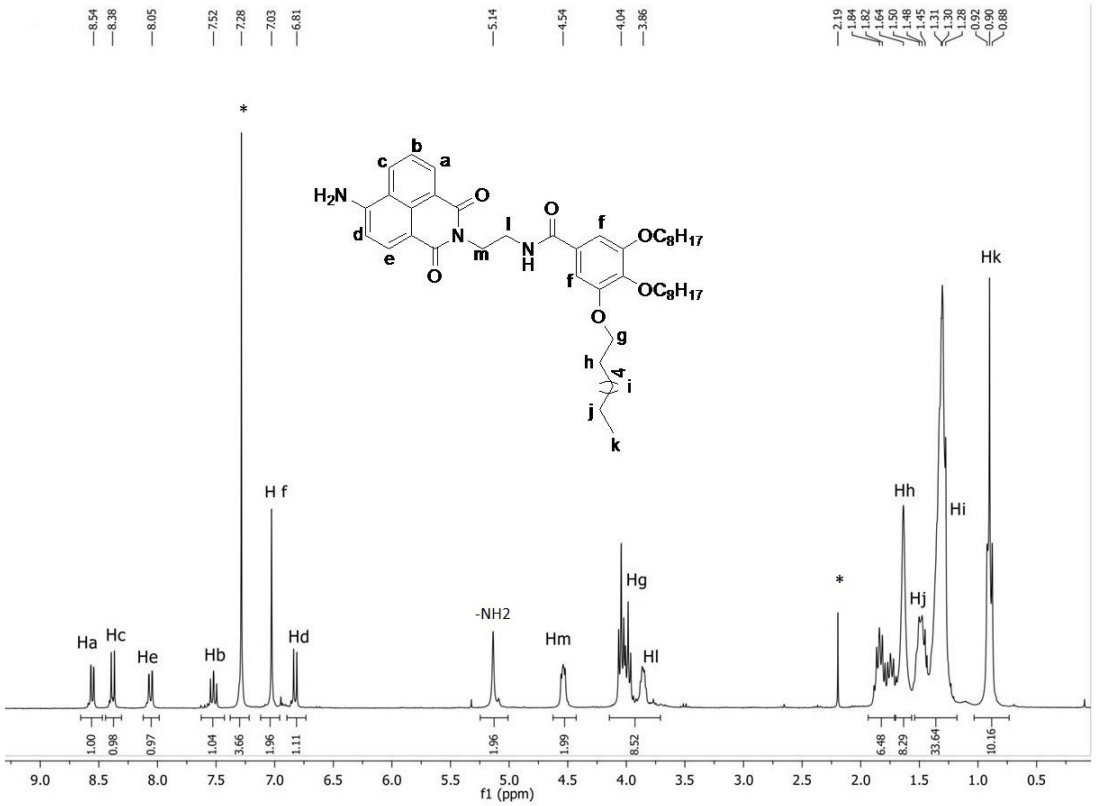


Figure S11: ^{1}H-NMR spectrum of **NMI-2**. Solvent = $CDCl_3$. * indicates solvent peak.

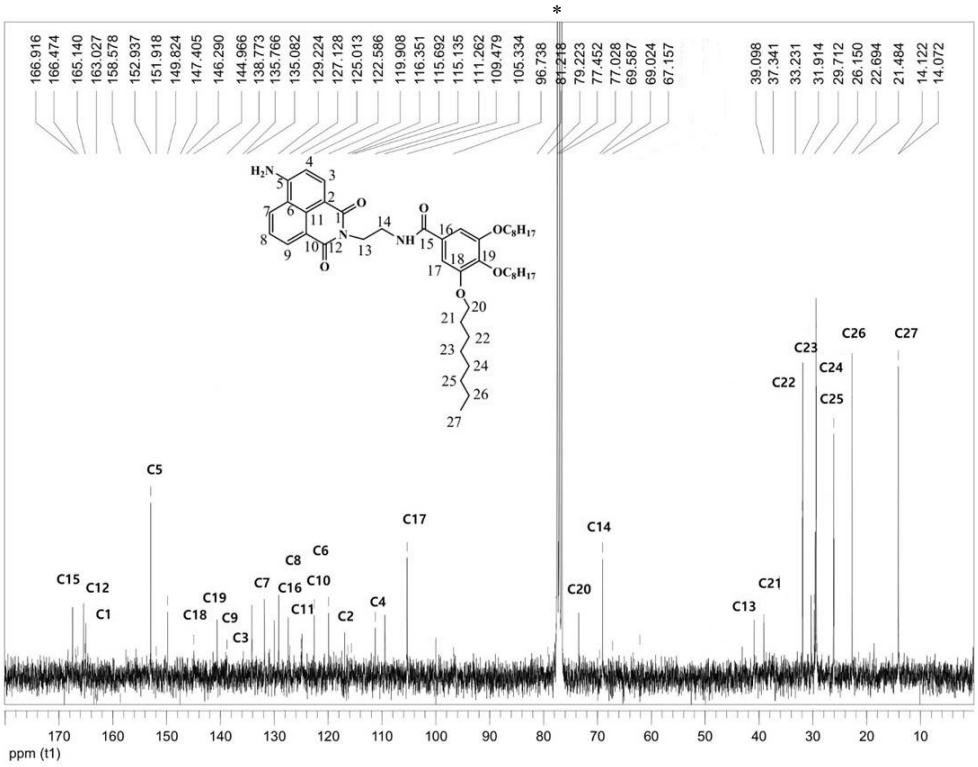


Figure S12: ^{13}C-NMR spectrum of **NMI-2**. Solvent = $CDCl_3$. * indicates solvent peak

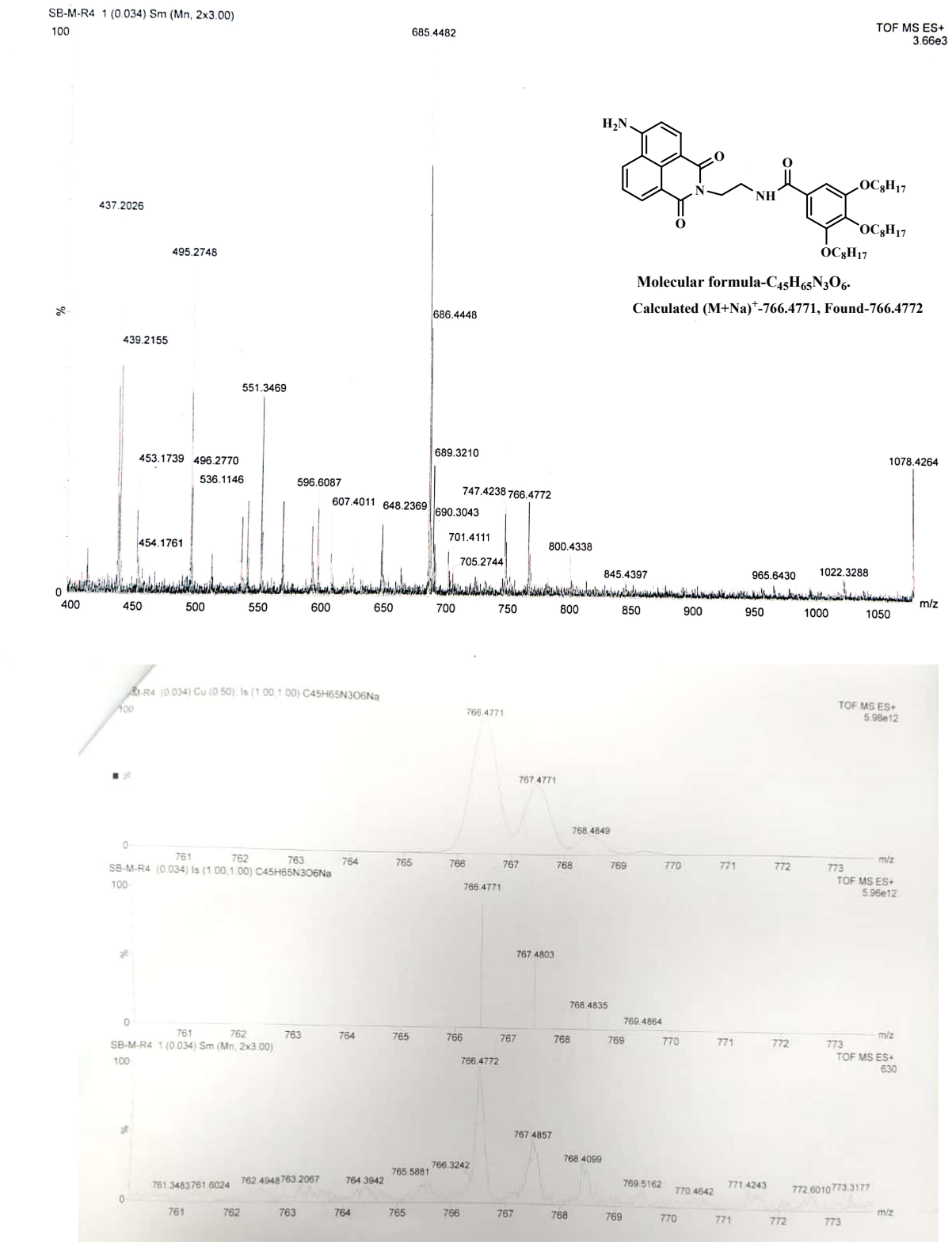


Figure S13: ESI-MS spectra of **NMI-2**

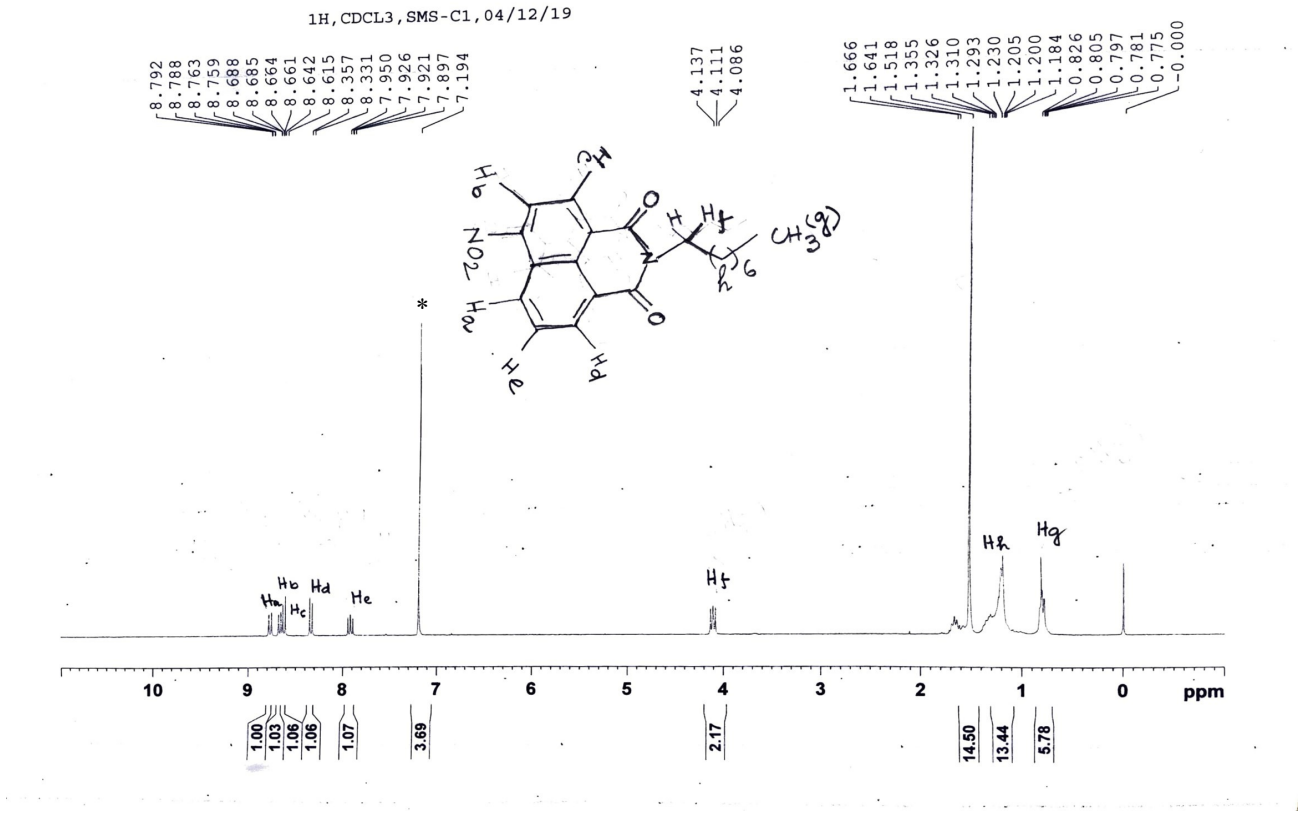


Figure S14: ^{1}H- NMR spectrum of Compound **NMI-C$_0$**. Solvent-CDCl$_3$. * indicates solvent peak

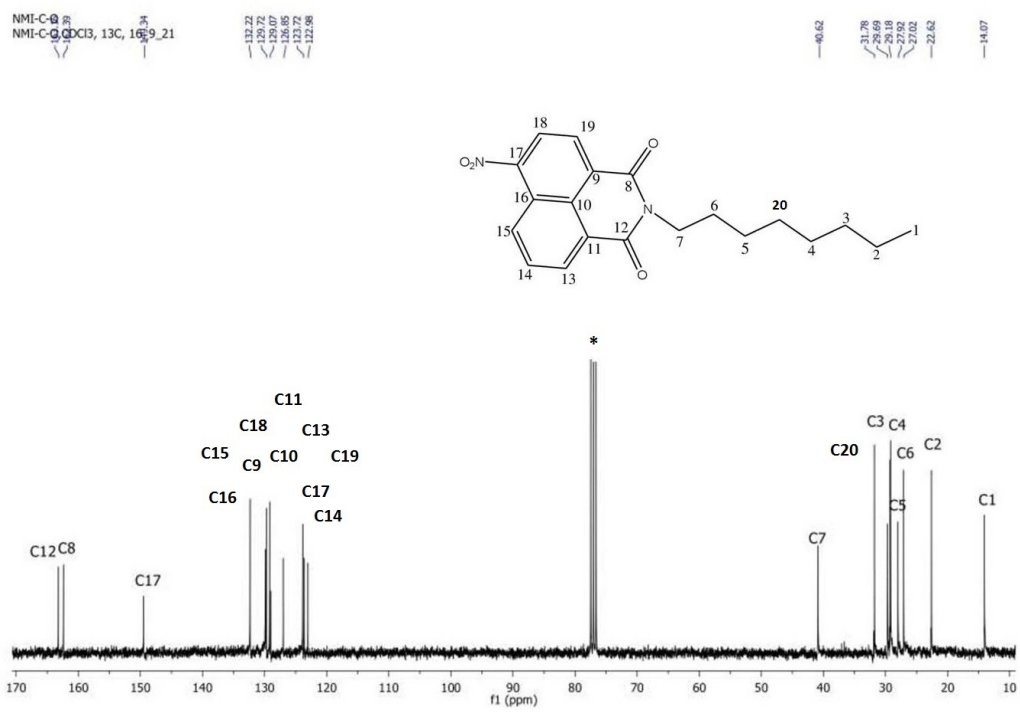
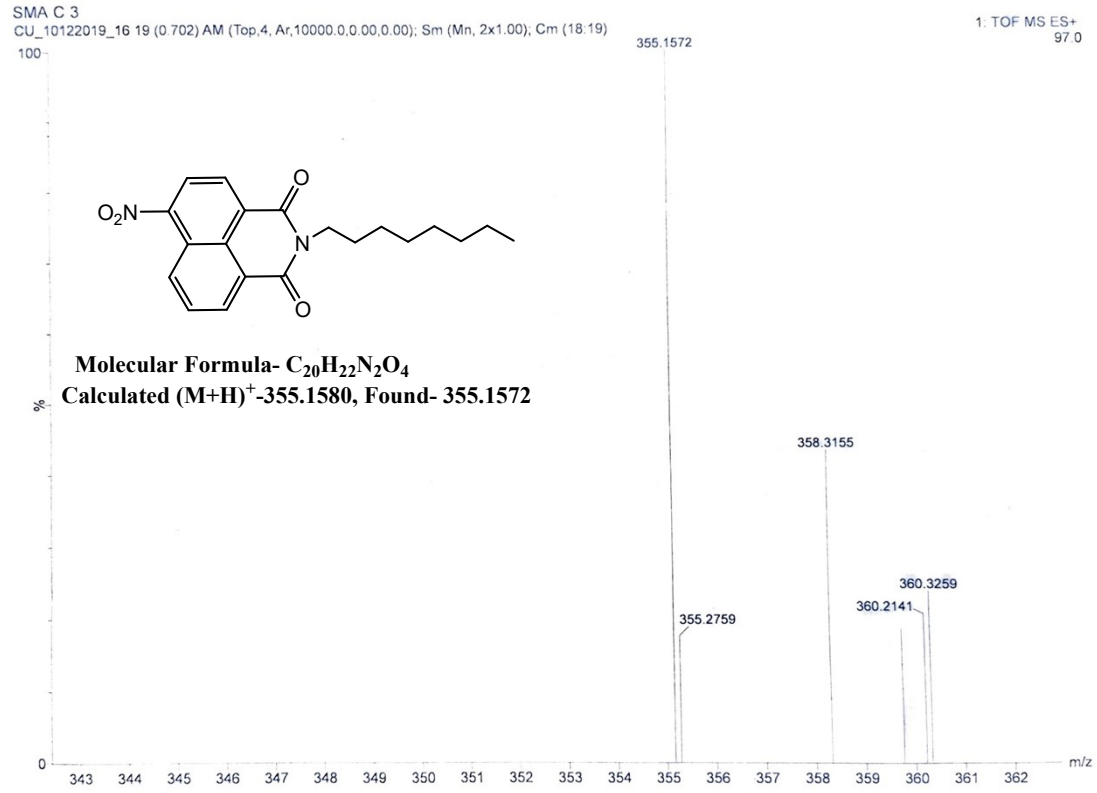


Figure S15: ^{13}C- NMR spectrum of Compound **NMI-C$_0$**. Solvent-CDCl$_3$. * indicates solvent peak.



. Figure S16: ESI-MS spectrum of **NMI-C0**

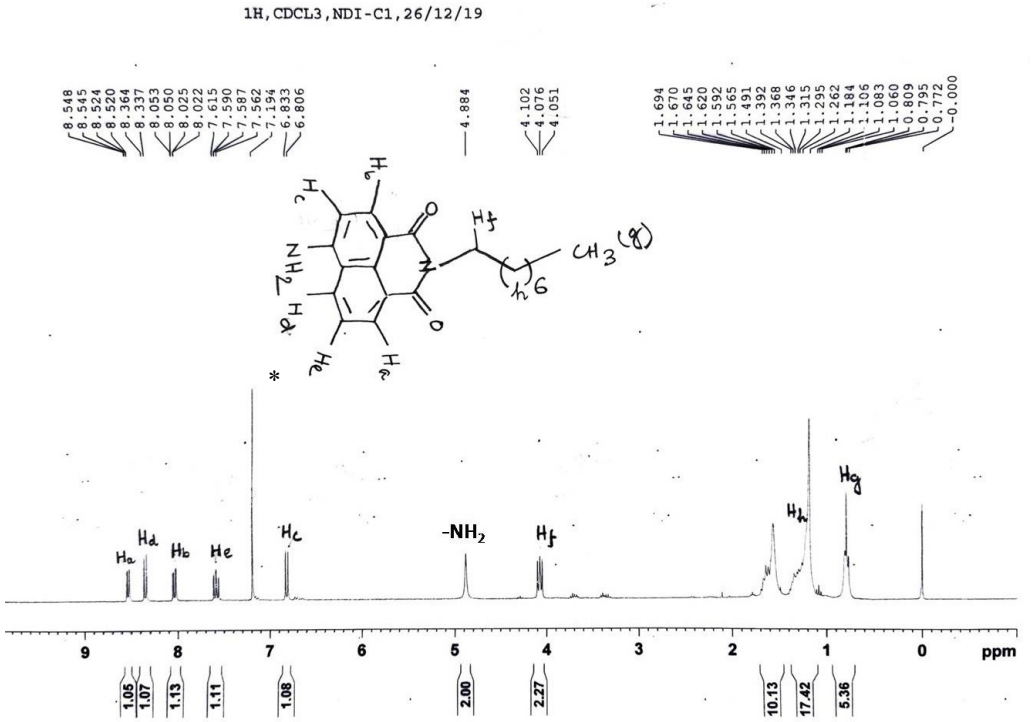


Figure S17: ^{1}H- NMR spectrum of Compound **NMI-C**. Solvent-$CDCl_3$. * indicates solvent peak.

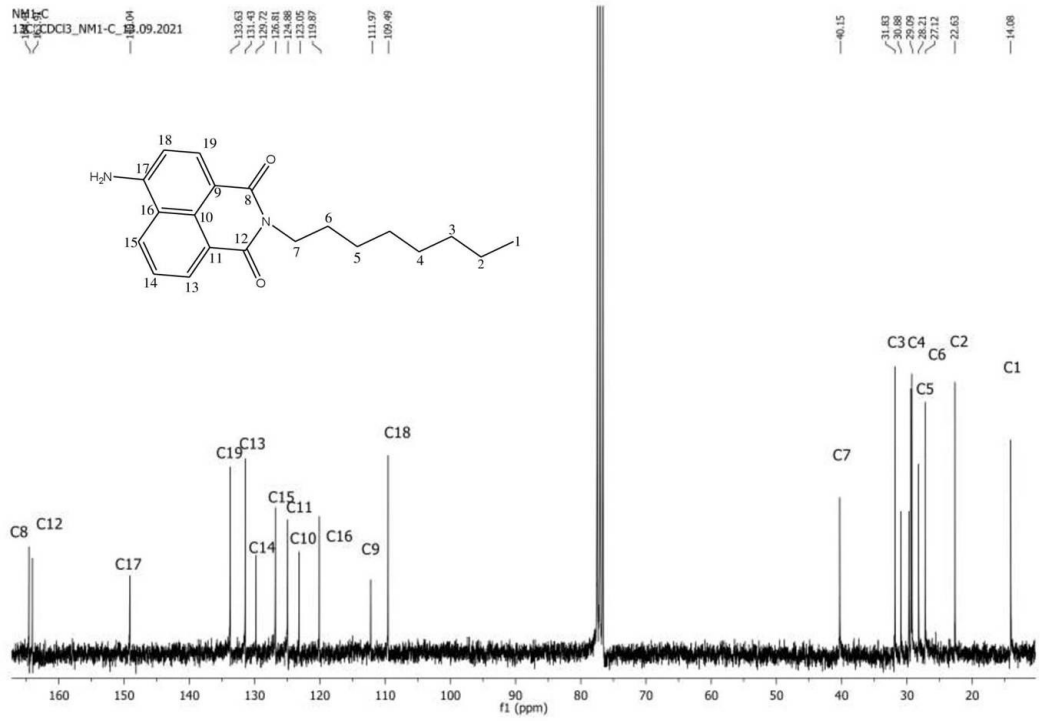


Figure S18: ^{13}C- NMR spectrum of Compound **NMI-C**. Solvent-$CDCl_3$. * indicates solvent peak.

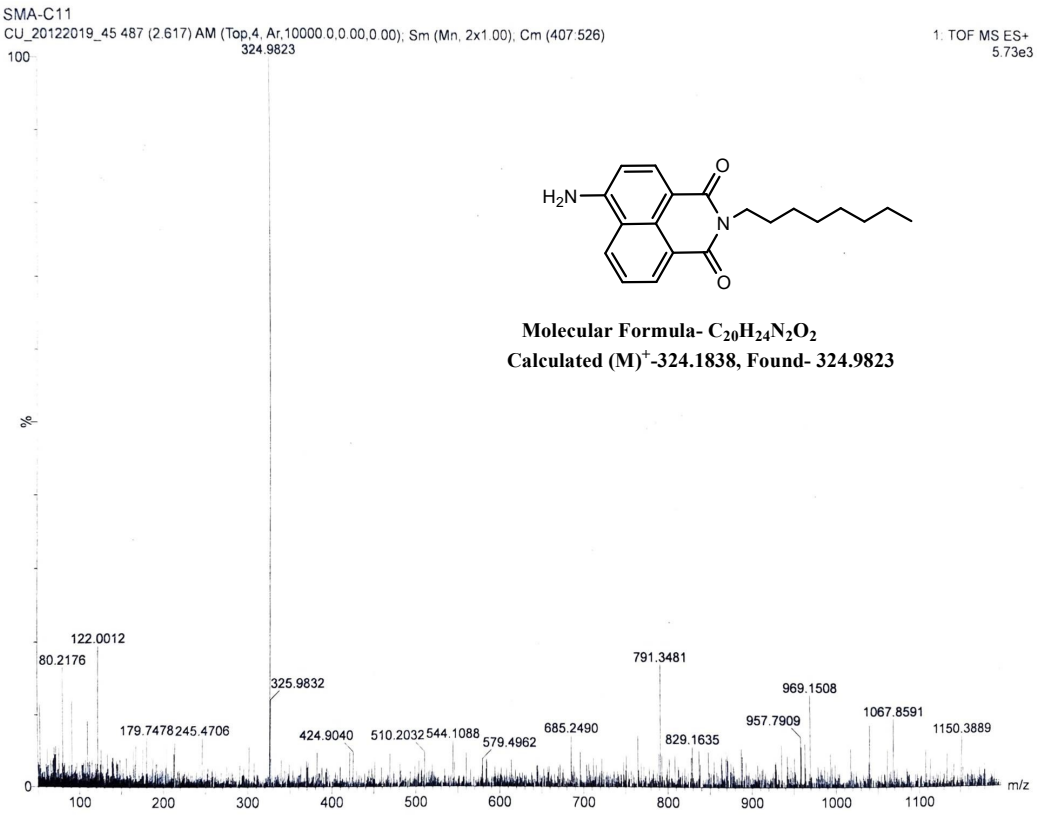
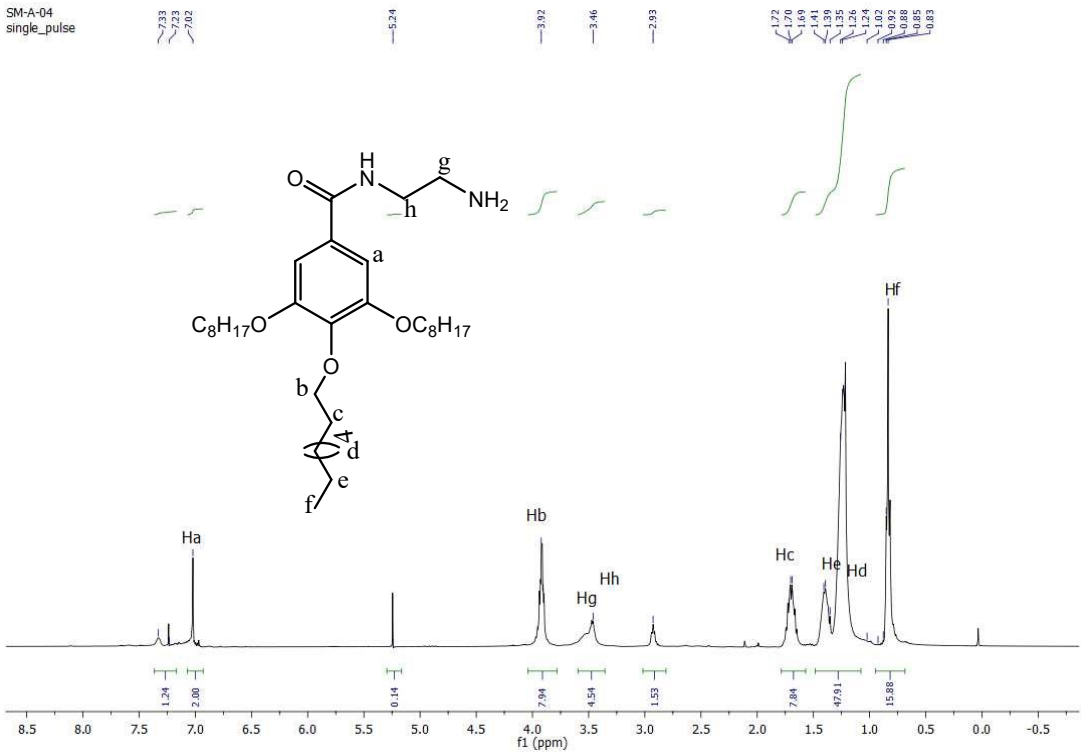


Figure S19: ESI-MS spectrum of **NMI-C**



FigureS20:[1]H-NMR spectrum of **compound-A** ((N-aminoethyl)-3,4,5-tris(octyloxy) benzamide). Solvent-$CDCl_3$.

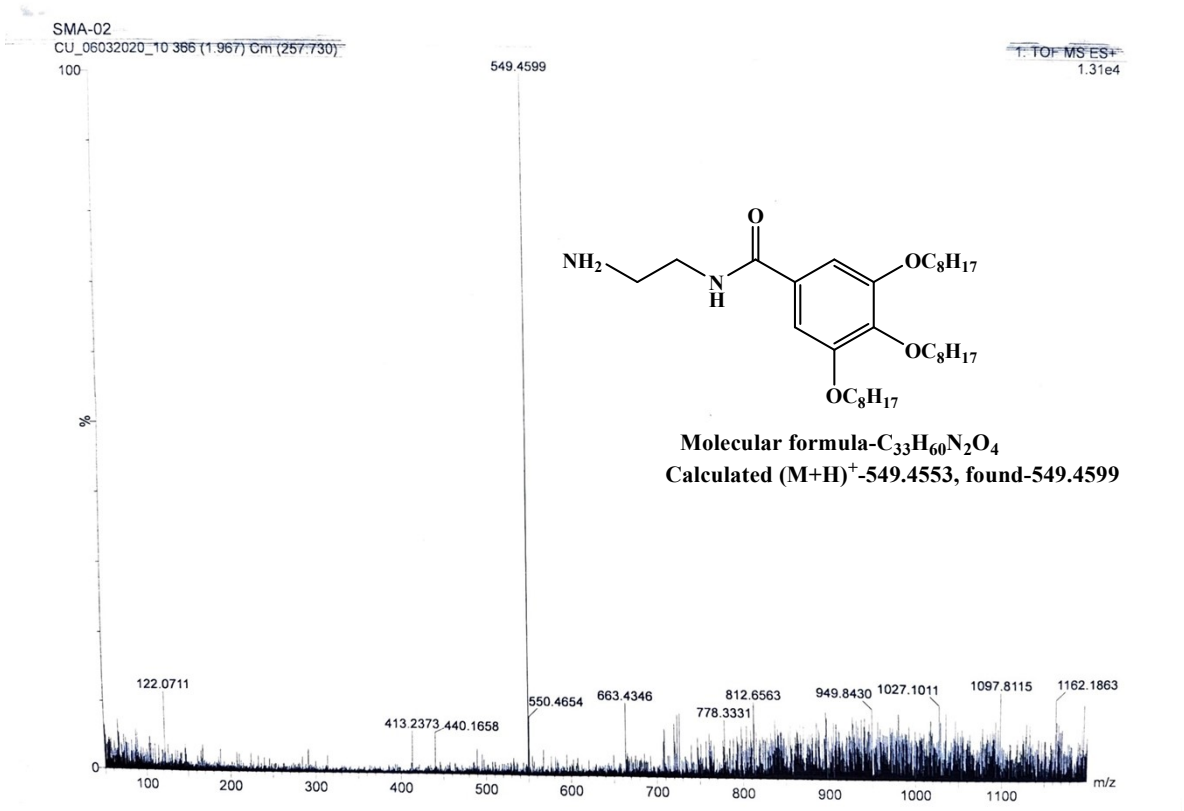


Figure S21: ESI-MS spectrum of Compound **-A.**

XYZ Coordinates (For DFT Optimization)

Monomer (THF)

C	-6.607062000	-0.012722000	-0.131803000
C	-7.248605000	-1.227191000	0.310868000
C	-5.194439000	0.115643000	0.034341000
C	-6.470117000	-2.220737000	0.915058000
C	-4.441556000	-0.919560000	0.638765000
H	-6.950607000	-3.131507000	1.253879000
C	-5.097243000	-2.065384000	1.072881000
H	-4.513772000	-2.852155000	1.535048000
N	-8.597256000	-1.393634000	0.186197000
H	-9.109936000	-0.853802000	-0.491349000
H	-8.974217000	-2.312729000	0.358817000
C	-7.315959000	1.061981000	-0.715794000
C	-4.549200000	1.295699000	-0.413197000
C	-6.666569000	2.204449000	-1.139705000
C	-5.276487000	2.319271000	-0.994140000
C	-2.992684000	-0.798963000	0.808346000
N	-2.398887000	0.399165000	0.355551000
C	-3.083899000	1.447570000	-0.264192000
O	-2.294891000	-1.669397000	1.312782000
O	-2.480362000	2.437246000	-0.657330000
C	-0.945429000	0.545985000	0.523984000
H	-0.654764000	-0.027030000	1.401207000
H	-0.738662000	1.601939000	0.687265000
C	-0.179043000	0.040416000	-0.709361000
H	-0.341119000	-1.029102000	-0.835309000
H	-0.534783000	0.559112000	-1.602309000
N	1.252998000	0.252327000	-0.570221000
H	1.612276000	1.176057000	-0.752480000
C	2.139273000	-0.764314000	-0.377500000
O	1.793813000	-1.941841000	-0.317565000
C	3.585211000	-0.366191000	-0.258245000
C	4.533818000	-1.333177000	-0.592911000
C	3.982359000	0.897343000	0.189709000
H	4.186829000	-2.305227000	-0.909976000
H	3.247000000	1.622805000	0.506507000
C	5.893614000	-1.030935000	-0.508282000
C	5.344516000	1.198356000	0.289897000
C	6.305840000	0.242436000	-0.078827000
H	-8.392297000	1.011542000	-0.826184000
H	-7.231570000	3.015178000	-1.582691000
H	-4.753896000	3.207441000	-1.325976000
O	6.897021000	-1.893245000	-0.821694000
O	7.635567000	0.569147000	-0.045561000
O	5.841150000	2.382587000	0.735938000
C	4.920399000	3.409166000	1.105566000
H	4.289189000	3.096371000	1.942969000
H	4.291010000	3.701916000	0.259726000
C	8.331519000	0.141854000	1.137223000
H	8.305977000	-0.946721000	1.231320000
H	9.362745000	0.473338000	1.020478000
C	6.547119000	-3.202577000	-1.274328000
H	7.491073000	-3.707841000	-1.467858000
H	5.989198000	-3.751715000	-0.510225000
H	5.531982000	4.255510000	1.411308000
H	7.898905000	0.604256000	2.029260000
H	5.960808000	-3.159134000	-2.196788000

Monomer (MCH)

C	-6.618067000	0.017677000	-0.169704000
C	-7.287846000	-1.169179000	0.297050000
C	-5.206935000	0.125767000	0.019424000
C	-6.544468000	-2.151874000	0.952494000
C	-4.487266000	-0.900131000	0.676959000
H	-7.048089000	-3.043000000	1.310587000
C	-5.170211000	-2.015519000	1.138485000

H	-4.608601000	-2.793343000	1.641167000
N	-8.644791000	-1.312064000	0.144558000
H	-9.098957000	-0.828278000	-0.613134000
H	-9.027765000	-2.226816000	0.327883000
C	-7.295740000	1.088021000	-0.798709000
C	-4.529850000	1.276153000	-0.456570000
C	-6.615673000	2.201447000	-1.248380000
C	-5.224850000	2.292754000	-1.084619000
C	-3.036039000	-0.799906000	0.875786000
N	-2.410526000	0.367516000	0.386024000
C	-3.062313000	1.404926000	-0.286287000
O	-2.372088000	-1.660494000	1.431435000
O	-2.434808000	2.366309000	-0.705516000
C	-0.957676000	0.494156000	0.576448000
H	-0.692863000	-0.055962000	1.476386000
H	-0.738464000	1.552380000	0.709130000
C	-0.177593000	-0.061078000	-0.626162000
H	-0.317479000	-1.138724000	-0.699164000
H	-0.540416000	0.405788000	-1.545605000
N	1.249269000	0.181568000	-0.486259000
H	1.586974000	1.113735000	-0.665673000
C	2.165571000	-0.824731000	-0.358344000
O	1.850476000	-2.008418000	-0.346438000
C	3.602902000	-0.393596000	-0.245258000
C	4.568695000	-1.332179000	-0.607734000
C	3.978879000	0.869332000	0.222654000
H	4.235379000	-2.305649000	-0.935536000
H	3.231546000	1.570035000	0.566376000
C	5.922123000	-1.002089000	-0.531599000
C	5.334892000	1.198293000	0.312697000
C	6.313113000	0.272247000	-0.085920000
H	-8.372283000	1.056733000	-0.917478000
H	-7.156284000	3.010109000	-1.724896000
H	-4.675997000	3.157148000	-1.436555000
O	6.940407000	-1.839012000	-0.867649000
O	7.633237000	0.630486000	-0.065869000
O	5.811568000	2.384207000	0.778661000
C	4.875844000	3.384525000	1.167385000
H	4.254693000	3.050091000	2.004980000
H	4.234150000	3.678344000	0.330218000
C	8.363292000	0.184427000	1.085864000
H	8.367934000	-0.907095000	1.145951000
H	9.383130000	0.546099000	0.958006000
C	6.611641000	-3.142203000	-1.344952000
H	7.563268000	-3.625543000	-1.557582000
H	6.069726000	-3.719490000	-0.589440000
H	5.472184000	4.239185000	1.481073000
H	7.939437000	0.607949000	2.001661000
H	6.016209000	-3.090909000	-2.261644000

Dimer (THF)

C	-6.176802000	1.554997000	1.155185000
C	-6.376482000	0.276904000	1.818189000
C	-4.850459000	2.058271000	1.086291000
C	-5.282148000	-0.347177000	2.491363000
C	-3.782783000	1.367324000	1.711416000
H	-5.457860000	-1.276657000	3.015669000
C	-4.021066000	0.194308000	2.437072000
H	-3.189604000	-0.294294000	2.925081000
N	-7.546999000	-0.343336000	1.804539000
H	-8.338866000	-0.002859000	1.279058000
H	-7.650092000	-1.255213000	2.229276000
C	-7.211575000	2.300702000	0.575679000
C	-4.589865000	3.260302000	0.399339000
C	-6.941878000	3.501919000	-0.069606000
C	-5.633217000	3.976933000	-0.170206000
C	-2.387513000	1.861164000	1.599963000

N	-2.177433000	3.008476000	0.836017000
C	-3.195827000	3.755861000	0.237912000
O	-1.468287000	1.273898000	2.141071000
O	-2.939392000	4.759580000	-0.400282000
C	-0.781706000	3.424836000	0.599928000
H	-0.186348000	3.016478000	1.411743000
H	-0.745387000	4.512062000	0.632194000
C	-0.269928000	2.887321000	-0.751368000
H	-0.537159000	1.836542000	-0.858131000
H	-0.732380000	3.441476000	-1.569847000
N	1.176764000	3.000527000	-0.858456000
H	1.572312000	3.885356000	-1.136870000
C	2.006563000	1.931822000	-0.744082000
O	1.585969000	0.788301000	-0.550099000
C	3.474907000	2.210921000	-0.865907000
C	4.272054000	1.211431000	-1.425050000
C	4.040275000	3.394346000	-0.381533000
H	3.803851000	0.302651000	-1.771883000
H	3.419284000	4.141123000	0.092060000
C	5.652818000	1.395107000	-1.509250000
C	5.427231000	3.569182000	-0.441296000
C	6.237300000	2.573737000	-1.012498000
H	-8.238933000	1.964051000	0.626327000
H	-7.754839000	4.066890000	-0.506300000
H	-5.413574000	4.898428000	-0.692520000
O	6.519535000	0.496923000	-2.042594000
O	7.589932000	2.762295000	-1.104203000
O	6.087295000	4.658028000	0.034373000
C	5.322891000	5.719028000	0.607103000
H	4.773488000	5.382573000	1.491702000
H	4.624282000	6.143259000	-0.120470000
C	8.346242000	2.140158000	-0.049621000
H	8.125102000	1.071795000	0.011206000
H	9.396410000	2.283302000	-0.301133000
C	5.987565000	-0.692520000	-2.633013000
H	6.847835000	-1.237719000	-3.015634000
H	5.468611000	-1.306551000	-1.892968000
H	6.046354000	6.477566000	0.898632000
H	8.131421000	2.618861000	0.910405000
H	5.310251000	-0.452045000	-3.457706000
H	-9.039079000	-2.557423000	-2.081392000
N	-8.850276000	-2.758428000	-1.106893000
H	-9.321793000	-3.611876000	-0.836585000
C	-7.484987000	-2.755016000	-0.777244000
C	-6.979329000	-3.671505000	0.158440000
H	-7.651087000	-4.412782000	0.581236000
C	-5.644101000	-3.659926000	0.528558000
H	-5.256886000	-4.381308000	1.236013000
C	-4.757275000	-2.717425000	-0.028580000
C	-3.356783000	-2.731872000	0.357893000
O	-2.874380000	-3.559565000	1.147376000
N	-2.546265000	-1.728098000	-0.196011000
C	-2.983984000	-0.734817000	-1.101029000
O	-2.171363000	0.127982000	-1.493496000
C	-4.365442000	-0.781527000	-1.507912000
C	-5.241377000	-1.764900000	-0.964129000
C	-6.624588000	-1.771697000	-1.350731000
C	-7.081161000	-0.792776000	-2.276732000
H	-8.126218000	-0.753195000	-2.555534000
C	-6.193985000	0.146207000	-2.812784000
H	-6.563100000	0.877168000	-3.525018000
C	-4.859540000	0.165193000	-2.443275000

H	-4.171435000	0.892119000	-2.853459000
C	-1.137590000	-1.682382000	0.216469000
H	-0.861518000	-0.641259000	0.368185000
H	-1.059115000	-2.225375000	1.155180000
C	-0.202756000	-2.313712000	-0.825690000
H	-0.359655000	-1.830825000	-1.793318000
H	-0.404086000	-3.378977000	-0.928238000
N	1.190617000	-2.164986000	-0.424125000
H	1.559622000	-1.219695000	-0.401990000
C	2.022168000	-3.222212000	-0.247822000
O	1.678413000	-4.390793000	-0.432731000
C	3.430839000	-2.896192000	0.180009000
C	3.744387000	-1.751253000	0.916302000
H	2.967205000	-1.060016000	1.206174000
C	5.070863000	-1.511402000	1.288282000
C	6.084230000	-2.402347000	0.900919000
C	5.753483000	-3.565110000	0.183913000
C	4.425937000	-3.811259000	-0.170165000
H	4.137467000	-4.700887000	-0.709970000
O	6.799158000	-4.380395000	-0.121492000
H	5.859029000	-6.242238000	-0.277408000
C	6.527472000	-5.584116000	-0.840523000
H	7.491460000	-6.071849000	-0.970830000
H	6.091022000	-5.372062000	-1.821054000
O	7.396772000	-2.123270000	1.186870000
C	7.840598000	-2.586002000	2.472585000
H	7.270923000	-2.108924000	3.274610000
H	7.748290000	-3.673462000	2.545283000
H	8.890024000	-2.304630000	2.554257000
O	5.485764000	-0.438716000	2.016232000
C	4.495884000	0.462578000	2.516758000
H	3.793552000	-0.051928000	3.179736000
H	5.043448000	1.214459000	3.081458000
H	3.950253000	0.944233000	1.701947000

Dimer (MCH)

C	-5.972223000	1.320853000	1.428875000
C	-6.172241000	-0.081056000	1.760582000
C	-4.645531000	1.826175000	1.512786000
C	-5.110682000	-0.823180000	2.367492000
C	-3.595801000	1.021408000	2.025210000
H	-5.292125000	-1.851779000	2.654739000
C	-3.853950000	-0.276052000	2.494378000
H	-3.034256000	-0.853471000	2.902897000
N	-7.310115000	-0.709318000	1.480748000
H	-8.005376000	-0.293120000	0.876194000
H	-7.350319000	-1.720926000	1.544016000
C	-6.994467000	2.176673000	0.993656000
C	-4.364020000	3.140068000	1.084688000
C	-6.707873000	3.489736000	0.625143000
C	-5.393818000	3.966759000	0.649032000
C	-2.194718000	1.516466000	2.040305000
N	-1.957621000	2.773802000	1.483320000
C	-2.959441000	3.634494000	1.028442000
O	-1.293367000	0.833346000	2.504304000
O	-2.686330000	4.739504000	0.582223000
C	-0.553899000	3.171450000	1.258629000
H	0.056986000	2.597778000	1.952504000
H	-0.465108000	4.235518000	1.478298000
C	-0.142897000	2.859227000	-0.194277000
H	-0.400286000	1.826077000	-0.435075000
H	-0.689195000	3.511569000	-0.878885000

N	1.282500000	3.058292000	-0.407002000
H	1.588159000	3.917818000	-0.837081000
C	2.180159000	2.037336000	-0.309280000
O	1.836958000	0.900834000	0.040942000
C	3.598942000	2.370851000	-0.660206000
C	4.392578000	1.339837000	-1.171786000
C	4.119993000	3.660882000	-0.489359000
H	3.962213000	0.353324000	-1.275392000
H	3.517660000	4.436871000	-0.034685000
C	5.713845000	1.603889000	-1.546631000
C	5.449679000	3.920392000	-0.841537000
C	6.248422000	2.897550000	-1.386299000
H	-8.023929000	1.837618000	0.952801000
H	-7.511682000	4.139714000	0.298768000
H	-5.154013000	4.972590000	0.324857000
O	6.561734000	0.687400000	-2.083324000
O	7.520508000	3.191579000	-1.797207000
O	6.067043000	5.125147000	-0.691656000
C	5.307074000	6.208142000	-0.171805000
H	4.957543000	6.005310000	0.848161000
H	4.444745000	6.438849000	-0.809450000
C	8.564271000	2.712582000	-0.937495000
H	8.541826000	1.621806000	-0.858454000
H	9.503369000	3.026323000	-1.396891000
C	6.083811000	-0.644689000	-2.273068000
H	6.916638000	-1.196285000	-2.709512000
H	5.797912000	-1.108181000	-1.323283000
H	5.981260000	7.065081000	-0.155814000
H	8.482141000	3.158407000	0.060611000
H	5.232071000	-0.666507000	-2.962399000
H	-9.051886000	-1.823155000	-2.680190000
N	-8.918028000	-2.205817000	-1.749233000
H	-9.412815000	-3.088939000	-1.686970000
C	-7.553763000	-2.336863000	-1.405946000
C	-7.109572000	-3.447259000	-0.666186000
H	-7.819425000	-4.236536000	-0.426277000
C	-5.781433000	-3.567274000	-0.274194000
H	-5.432133000	-4.434679000	0.273722000
C	-4.846798000	-2.565954000	-0.612284000
C	-3.461609000	-2.708545000	-0.187408000
O	-3.044253000	-3.687320000	0.453513000
N	-2.597251000	-1.642539000	-0.509664000
C	-2.986304000	-0.451241000	-1.158478000
O	-2.156759000	0.478863000	-1.278162000
C	-4.349554000	-0.372331000	-1.631149000
C	-5.270583000	-1.420456000	-1.339645000
C	-6.644441000	-1.290090000	-1.748191000
C	-7.041362000	-0.115501000	-2.447283000
H	-8.078352000	0.023201000	-2.732720000
C	-6.106251000	0.885310000	-2.746209000
H	-6.430157000	1.766076000	-3.295009000
C	-4.783332000	0.773780000	-2.348140000
H	-4.056066000	1.545883000	-2.569056000
C	-1.201187000	-1.733253000	-0.060758000
H	-0.937065000	-0.803086000	0.444455000
H	-1.149980000	-2.560189000	0.645481000
C	-0.216321000	-1.974794000	-1.217232000
H	-0.335431000	-1.187740000	-1.966195000
H	-0.400626000	-2.944042000	-1.682829000
N	1.154385000	-1.976110000	-0.725281000
H	1.542928000	-1.083960000	-0.438634000
C	1.899719000	-3.112209000	-0.648167000

O	1.515676000	-4.198857000	-1.091268000
C	3.252635000	-2.990108000	0.008324000
C	3.567356000	-1.968253000	0.912077000
H	2.835435000	-1.212851000	1.162359000
C	4.832318000	-1.943234000	1.513777000
C	5.785200000	-2.928515000	1.198094000
C	5.449407000	-3.960418000	0.301100000
C	4.184025000	-3.990098000	-0.289610000
H	3.882660000	-4.776703000	-0.968164000
O	6.430451000	-4.883195000	0.081733000
H	5.304393000	-6.567778000	-0.439324000
C	6.142055000	-5.960690000	-0.802404000
H	7.045386000	-6.571175000	-0.832889000
H	5.912327000	-5.601953000	-1.812729000
O	7.044470000	-2.862479000	1.742573000
C	7.216733000	-3.650406000	2.925195000
H	6.538322000	-3.319514000	3.720175000
H	7.050506000	-4.713360000	2.718355000
H	8.249559000	-3.501834000	3.247283000
O	5.234904000	-1.012606000	2.424981000
C	4.299607000	-0.008242000	2.807396000
H	3.425573000	-0.444364000	3.306744000
H	4.829701000	0.638122000	3.508276000
H	3.963000000	0.579403000	1.946837000

Tetramer (THF)

C	0.875221000	1.178085000	-8.298300000
C	-0.271624000	0.320932000	-8.531716000
C	1.612357000	1.028115000	-7.073717000
C	-0.703184000	-0.534461000	-7.492802000
C	1.206111000	0.079368000	-6.094493000
H	-1.589320000	-1.164511000	-7.658849000
C	0.031317000	-0.658719000	-6.309318000
H	-0.279946000	-1.378480000	-5.538079000
N	-0.934543000	0.358192000	-9.723040000
H	-0.471682000	0.737388000	-10.549672000
H	-1.626081000	-0.367616000	-9.913721000
C	1.309851000	2.148607000	-9.239526000
C	2.775695000	1.825218000	-6.858889000
C	2.426817000	2.946449000	-8.992260000
C	3.164700000	2.779188000	-7.802863000
C	2.037176000	-0.177504000	-4.913997000
N	3.237802000	0.566668000	-4.805274000
C	3.637119000	1.594372000	-5.673813000
O	1.764732000	-1.011698000	-4.041145000
O	4.678496000	2.235251000	-5.474857000
C	4.153064000	0.185915000	-3.722405000
H	3.592660000	0.201813000	-2.768322000
H	4.931242000	0.969134000	-3.700889000
C	4.813575000	-1.195856000	-3.962121000
H	4.262669000	-1.979649000	-3.402762000
H	4.759704000	-1.464259000	-5.035733000
N	6.218851000	-1.188761000	-3.600992000
H	6.473680000	-0.920479000	-2.649462000
C	7.217895000	-1.529823000	-4.477119000
O	6.980180000	-2.020544000	-5.593941000
C	8.618951000	-1.227126000	-4.028384000
C	9.672312000	-1.742478000	-4.801882000
C	8.892686000	-0.344220000	-2.963387000
H	9.422959000	-2.390957000	-5.648046000
H	8.080582000	0.086703000	-2.366996000
C	10.998076000	-1.338632000	-4.561883000

C	10.217627000	0.032580000	-2.688577000
C	11.283926000	-0.436083000	-3.502020000
H	0.755553000	2.293288000	-10.178331000
H	2.745554000	3.689813000	-9.736429000
H	4.068435000	3.371287000	-7.604056000
O	12.059596000	-1.725748000	-5.314861000
O	12.516357000	0.085324000	-3.254505000
O	10.574334000	0.879030000	-1.678543000
C	9.532713000	1.462335000	-0.892610000
H	8.945875000	0.662250000	-0.384137000
H	8.833859000	2.019984000	-1.555470000
C	13.676705000	-0.764694000	-3.182347000
H	13.960761000	-1.108017000	-4.197790000
H	14.473146000	-0.091480000	-2.805559000
C	11.830201000	-2.592196000	-6.447388000
H	11.422807000	-3.567893000	-6.098337000
H	11.079657000	-2.123644000	-7.119397000
N	-0.679163000	-4.032146000	-11.121369000
H	-0.585584000	-4.025381000	-12.137382000
H	-1.046501000	-4.903637000	-10.737185000
C	0.207038000	-3.323914000	-10.362513000
C	0.392429000	-3.628827000	-8.996812000
H	-0.199050000	-4.440509000	-8.548379000
C	1.369525000	-2.976023000	-8.240101000
H	1.546920000	-3.262560000	-7.194473000
C	2.182560000	-1.980176000	-8.797125000
C	1.941285000	-1.561803000	-10.133173000
C	0.947498000	-2.216785000	-10.937700000
C	0.726581000	-1.751209000	-12.258966000
C	1.450969000	-0.674321000	-12.775093000
H	1.252129000	-0.319699000	-13.796664000
H	-0.045061000	-2.218969000	-12.888284000
C	2.447420000	-0.053305000	-11.994018000
C	2.708698000	-0.503787000	-10.697042000
H	3.051078000	0.775030000	-12.391386000
C	3.842910000	0.077180000	-9.939302000
C	3.316831000	-1.453846000	-8.040128000
O	3.643013000	-1.878273000	-6.923992000
N	4.069574000	-0.429094000	-8.657549000
O	4.595150000	0.937560000	-10.417870000
C	5.254623000	0.054057000	-7.964015000
H	5.126412000	-0.167763000	-6.892501000
H	5.293127000	1.149605000	-8.113841000
C	6.570153000	-0.562757000	-8.448656000
H	6.620981000	-0.550807000	-9.556298000
H	6.662715000	-1.608638000	-8.107243000
N	7.617131000	0.229763000	-7.843518000
H	7.382057000	1.189059000	-7.582895000
C	8.890663000	-0.177579000	-7.590993000
O	9.367141000	-1.234069000	-8.037472000
C	9.648530000	0.788923000	-6.728062000
C	8.946766000	1.559144000	-5.780405000
H	7.885890000	1.358224000	-5.595340000
C	9.623979000	2.539682000	-5.038488000
C	11.031056000	0.946962000	-6.899312000
H	11.546403000	0.321477000	-7.634852000
C	11.718183000	1.924739000	-6.151435000
O	11.651012000	3.781819000	-4.601248000
O	13.053460000	2.156103000	-6.246564000
C	13.814650000	1.268963000	-7.080453000
H	13.642527000	0.222411000	-6.738044000
C	11.008248000	2.763418000	-5.251484000

O	9.023212000	3.324328000	-4.097478000
C	7.624476000	3.113102000	-3.863346000
H	7.046609000	3.242870000	-4.804758000
H	7.458652000	2.063156000	-3.528819000
C	11.964017000	3.537892000	-3.207972000
H	11.756086000	4.486328000	-2.666426000
H	11.290346000	2.754950000	-2.808804000
H	13.457738000	1.348988000	-8.128096000
C	5.078763000	-1.918414000	-12.672262000
H	4.622940000	-1.582325000	-13.618937000
H	4.996791000	-1.114917000	-11.921383000
N	4.275031000	-3.049823000	-12.197127000
C	3.474460000	-3.748614000	-13.110486000
O	3.454162000	-3.437740000	-14.307826000
C	4.379456000	-3.344264000	-10.817309000
O	5.117340000	-2.648235000	-10.111186000
C	3.588115000	-4.462489000	-10.309038000
C	2.748709000	-5.209700000	-11.176586000
C	2.670750000	-4.871258000	-12.559493000
C	1.834152000	-5.592487000	-13.416998000
H	1.796216000	-5.302983000	-14.477263000
C	3.628283000	-4.786783000	-8.945237000
H	4.253124000	-4.173951000	-8.281721000
C	2.884576000	-5.850169000	-8.430441000
H	2.945787000	-6.093250000	-7.360113000
C	2.063903000	-6.639918000	-9.264375000
C	1.972823000	-6.310054000	-10.672907000
C	1.137715000	-7.018877000	-11.574336000
C	1.067400000	-6.669247000	-12.924405000
H	0.408814000	-7.230759000	-13.603012000
H	0.521470000	-7.855955000	-11.213716000
N	1.326385000	-7.665030000	-8.738377000
H	1.575961000	-7.972704000	-7.796667000
H	1.034467000	-8.429640000	-9.350119000
H	6.800690000	-2.499192000	-13.899735000
C	6.571921000	-2.270999000	-12.836422000
H	6.825037000	-3.167273000	-12.237166000
N	7.437968000	-1.203862000	-12.357204000
H	7.347164000	-0.263576000	-12.748607000
C	8.428881000	-1.442228000	-11.455760000
O	8.664990000	-2.590112000	-11.034308000
C	9.280200000	-0.288501000	-11.032011000
C	10.642237000	-0.578312000	-10.817556000
H	10.997633000	-1.603549000	-10.975545000
C	11.503948000	0.424171000	-10.361230000
O	12.835160000	0.240770000	-10.141116000
C	13.406410000	-1.047937000	-10.420700000
H	12.886073000	-1.829572000	-9.824044000
C	10.998771000	1.723913000	-10.070203000
C	9.619131000	1.987581000	-10.244882000
C	8.766612000	0.986762000	-10.758353000
H	7.695453000	1.213211000	-10.859703000
O	9.061493000	3.201785000	-9.961541000
C	9.381064000	3.841475000	-8.700292000
H	10.277495000	4.481944000	-8.822355000
H	9.623556000	3.062612000	-7.948854000
O	11.831064000	2.691181000	-9.567973000
C	12.768417000	3.259819000	-10.509558000
H	13.372103000	2.447491000	-10.969993000
H	13.448273000	3.878491000	-9.889318000
H	13.259292000	-1.300859000	-11.495338000
N	6.632747000	-5.641941000	-8.859750000

C	6.175408000	-6.600566000	-7.929508000
O	6.357957000	-6.416104000	-6.718373000
O	7.083033000	-4.979804000	-11.012494000
C	6.533671000	-5.781046000	-10.255079000
C	5.685075000	-6.888006000	-10.760976000
C	5.379153000	-6.937420000	-12.123203000
H	5.814343000	-6.174248000	-12.784534000
H	4.248126000	-7.949949000	-13.685741000
C	4.505164000	-7.927586000	-12.617074000
C	3.950849000	-8.868213000	-11.748889000
H	3.257863000	-9.616783000	-12.160227000
C	4.257232000	-8.860326000	-10.361043000
C	5.144045000	-7.846802000	-9.859439000
C	5.442945000	-7.756018000	-8.470228000
C	4.915529000	-8.720439000	-7.600226000
H	5.151955000	-8.641662000	-6.528690000
C	4.071408000	-9.737985000	-8.064035000
H	3.652782000	-10.469914000	-7.356604000
C	3.692399000	-9.812381000	-9.423660000
N	2.767568000	-10.728910000	-9.834860000
H	2.662677000	-10.945207000	-10.826019000
H	2.504457000	-11.479269000	-9.194437000
C	7.108615000	-4.354810000	-8.319620000
H	6.948263000	-3.608168000	-9.117066000
H	6.455365000	-4.102479000	-7.463011000
C	8.548693000	-4.307357000	-7.820691000
H	8.775047000	-5.149832000	-7.141662000
H	8.633298000	-3.358839000	-7.246840000
N	9.516774000	-4.312828000	-8.898394000
H	9.340476000	-3.640001000	-9.664261000
C	10.696423000	-4.974150000	-8.800879000
O	11.013994000	-5.658776000	-7.804359000
C	11.645385000	-4.829483000	-9.964927000
C	11.269517000	-4.245219000	-11.188190000
H	10.235656000	-3.921014000	-11.348054000
C	12.218502000	-4.104464000	-12.219289000
C	13.549952000	-4.548846000	-12.019729000
C	13.909855000	-5.161084000	-10.791061000
C	12.955897000	-5.305636000	-9.769961000
H	13.190738000	-5.769953000	-8.804664000
O	11.972595000	-3.541969000	-13.435225000
C	10.643245000	-3.111149000	-13.789346000
H	10.801484000	-2.231153000	-14.444101000
H	10.091605000	-2.770908000	-12.892048000
O	14.482899000	-4.319847000	-12.998665000
C	14.942124000	-5.489739000	-13.711634000
H	15.771204000	-5.124277000	-14.351552000
H	15.364881000	-6.224081000	-12.991431000
O	15.212875000	-5.545497000	-10.682943000
C	15.662531000	-6.049039000	-9.420396000
H	15.131758000	-6.998399000	-9.178851000
H	15.413846000	-5.318352000	-8.616695000
H	14.144843141	-5.961125954	-14.267095584
H	10.080391813	-3.908495003	-14.251769660
H	16.728466175	-6.212407623	-9.479496729
H	14.457308552	-1.013239370	-10.174106595
H	12.270800371	3.815014022	-11.290926145
H	8.535644215	4.434111302	-8.383357306
H	14.861473453	1.528094868	-7.022046389
H	12.989401879	3.219160512	-3.092230524
H	7.301935654	3.825299129	-3.118266826
H	12.763567858	-2.745915164	-6.968537428

H	13.510929461	-1.636857850	-2.567327741
H	9.981916207	2.121828654	-0.164815661

Tetramer (MCH)

C	0.905178000	0.812760000	-8.064586000
C	-0.283419000	-0.014316000	-8.074553000
C	1.760198000	0.778429000	-6.910556000
C	-0.588157000	-0.787192000	-6.935288000
C	1.409863000	-0.003432000	-5.773875000
H	-1.485233000	-1.423973000	-6.950324000
C	0.238175000	-0.770427000	-5.805957000
H	-0.007109000	-1.378164000	-4.922936000
N	-1.122892000	-0.017317000	-9.160496000
H	-0.725190000	0.217535000	-10.070967000
H	-1.805907000	-0.775238000	-9.203865000
C	1.276151000	1.642323000	-9.157465000
C	2.968811000	1.537882000	-6.911784000
C	2.457824000	2.379616000	-9.137407000
C	3.313524000	2.318321000	-8.016751000
C	2.250198000	0.001313000	-4.569904000
N	3.431985000	0.777939000	-4.624899000
C	3.872909000	1.517252000	-5.734350000
O	1.956487000	-0.577115000	-3.519101000
O	4.946782000	2.130286000	-5.711798000
C	4.247862000	0.803081000	-3.407662000
H	3.607821000	1.155877000	-2.574971000
H	5.041287000	1.546970000	-3.600183000
C	4.898186000	-0.559677000	-3.064043000
H	4.332429000	-1.068886000	-2.261456000
H	4.880765000	-1.217588000	-3.955624000
N	6.289548000	-0.408535000	-2.678784000
H	6.520083000	-0.017256000	-1.764301000
C	7.307746000	-0.667054000	-3.558376000
O	7.113675000	-1.209458000	-4.655719000
C	8.679753000	-0.234219000	-3.143853000
C	9.759631000	-0.968190000	-3.653841000
C	8.891505000	0.958665000	-2.424977000
H	9.545114000	-1.841672000	-4.280373000
H	8.036994000	1.538898000	-2.055115000
C	11.073238000	-0.507732000	-3.465177000
C	10.204214000	1.437036000	-2.253964000
C	11.304963000	0.716978000	-2.786027000
H	0.625053000	1.711155000	-10.041184000
H	2.732150000	3.001650000	-10.001285000
H	4.258206000	2.879045000	-7.986645000
O	12.171384000	-1.151291000	-3.941544000
O	12.548769000	1.271186000	-2.692924000
O	10.515604000	2.601435000	-1.613707000
C	9.442753000	3.442474000	-1.193376000
H	8.842710000	2.930773000	-0.403906000
H	8.762484000	3.641067000	-2.051987000
C	13.540322000	0.568685000	-1.923898000
H	13.710159000	-0.439604000	-2.358400000
H	14.466438000	1.162502000	-2.062110000
C	11.970688000	-2.446836000	-4.537612000
H	11.486306000	-3.111995000	-3.785067000
H	11.284993000	-2.357392000	-5.409274000
N	-1.127617000	-4.280144000	-9.447229000
H	-1.181929000	-4.316379000	-10.467740000
H	-1.446739000	-5.153199000	-9.019952000
C	0.022933000	-3.743074000	-8.907652000
C	0.449211000	-4.114770000	-7.618735000

H	-0.133836000	-4.864466000	-7.063070000
C	1.613689000	-3.578891000	-7.053845000
H	1.947846000	-3.888521000	-6.053196000
C	2.397408000	-2.653261000	-7.750355000
C	1.978983000	-2.223096000	-9.037720000
C	0.784972000	-2.755266000	-9.637254000
C	0.402943000	-2.278613000	-10.919877000
C	1.153817000	-1.310760000	-11.585018000
H	0.845118000	-0.964440000	-12.581669000
H	-0.504075000	-2.668029000	-11.405374000
C	2.328260000	-0.794988000	-10.994333000
C	2.747498000	-1.255539000	-9.746759000
H	2.936323000	-0.033778000	-11.502352000
C	4.009902000	-0.731578000	-9.167437000
C	3.628835000	-2.130449000	-7.133859000
O	3.990921000	-2.433521000	-5.995439000
N	4.395481000	-1.236481000	-7.920297000
O	4.711376000	0.101693000	-9.752679000
C	5.658154000	-0.738772000	-7.372623000
H	5.671375000	-0.928132000	-6.286164000
H	5.679268000	0.352806000	-7.553205000
C	6.910475000	-1.365639000	-8.018932000
H	6.779046000	-1.416083000	-9.119911000
H	7.110740000	-2.387650000	-7.648932000
N	8.034162000	-0.521715000	-7.686484000
H	7.906114000	0.478950000	-7.850755000
C	9.168120000	-0.872509000	-7.008859000
O	9.553996000	-2.041250000	-6.854457000
C	9.904787000	0.332438000	-6.492604000
C	9.169673000	1.407648000	-5.954494000
H	8.089346000	1.298779000	-5.802961000
C	9.838889000	2.583153000	-5.577233000
C	11.301280000	0.390746000	-6.579187000
H	11.844177000	-0.465692000	-6.990288000
C	11.978271000	1.566218000	-6.195828000
O	11.878602000	3.883707000	-5.526608000
O	13.328140000	1.712267000	-6.257646000
C	14.090833000	0.520353000	-6.492160000
H	13.814294000	-0.229344000	-5.717605000
C	11.243380000	2.694572000	-5.749597000
O	9.213023000	3.684084000	-5.065447000
C	7.808348000	3.581867000	-4.807543000
H	7.252797000	3.327344000	-5.735506000
H	7.624743000	2.750656000	-4.089085000
C	12.046121000	4.283476000	-4.148780000
H	11.759969000	5.356683000	-4.086791000
H	11.356558000	3.708243000	-3.501093000
H	13.831371000	0.098998000	-7.485540000
C	5.258711000	-2.557460000	-11.480471000
H	4.777138000	-1.590161000	-11.714975000
H	5.702138000	-2.504541000	-10.471565000
N	4.223629000	-3.582568000	-11.381172000
C	3.309905000	-3.682230000	-12.434507000
O	3.434546000	-2.976047000	-13.439164000
C	4.182553000	-4.341814000	-10.184787000
O	5.032607000	-4.175482000	-9.306933000
C	3.068732000	-5.291775000	-10.050261000
C	2.073020000	-5.400808000	-11.060147000
C	2.171801000	-4.619681000	-12.246488000
C	1.180198000	-4.687883000	-13.225830000
H	1.293437000	-4.061857000	-14.122645000
C	2.950381000	-6.054954000	-8.884799000

H	3.726622000	-5.949833000	-8.113562000
C	1.870266000	-6.929385000	-8.700986000
H	1.807701000	-7.533080000	-7.784011000
C	0.866136000	-7.063954000	-9.674077000
C	0.947796000	-6.274568000	-10.882960000
C	-0.054497000	-6.301521000	-11.889592000
C	0.054591000	-5.519156000	-13.040008000
H	-0.733641000	-5.556841000	-13.806420000
H	-0.944615000	-6.935154000	-11.758174000
N	-0.222400000	-7.888811000	-9.455577000
H	-0.099683000	-8.557882000	-8.691685000
H	-0.613510000	-8.352628000	-10.279674000
H	6.079526000	-2.605593000	-13.516473000
C	6.394525000	-2.827817000	-12.480851000
H	6.701633000	-3.887950000	-12.427806000
N	7.528353000	-1.986479000	-12.122160000
H	7.527782000	-1.008328000	-12.416941000
C	8.376302000	-2.364056000	-11.117621000
O	8.371957000	-3.534582000	-10.685496000
C	9.351821000	-1.357906000	-10.619481000
C	10.497273000	-1.876391000	-9.990495000
H	10.544163000	-2.956417000	-9.824207000
C	11.538437000	-1.023590000	-9.610125000
O	12.708127000	-1.447963000	-9.058341000
C	12.868636000	-2.843771000	-8.761690000
H	12.251377000	-3.093388000	-7.869245000
C	11.408889000	0.379636000	-9.797437000
C	10.188944000	0.901079000	-10.304307000
C	9.180007000	0.032248000	-10.751183000
H	8.257066000	0.479785000	-11.147982000
O	9.980607000	2.248278000	-10.391087000
C	10.170239000	3.008935000	-9.168574000
H	11.101585000	3.604100000	-9.255603000
H	10.301031000	2.306735000	-8.322052000
O	12.386686000	1.259718000	-9.441342000
C	13.687921000	1.119880000	-10.056074000
H	14.196297000	0.212269000	-9.668061000
H	14.241886000	2.012196000	-9.700710000
H	12.503550000	-3.458598000	-9.609841000
N	5.978314000	-7.177118000	-10.737488000
C	5.546818000	-8.117060000	-9.768640000
O	6.203408000	-8.309158000	-8.744128000
O	5.685446000	-5.970769000	-12.667814000
C	5.280294000	-6.858811000	-11.909017000
C	4.045189000	-7.631021000	-12.196100000
C	3.354504000	-7.385658000	-13.384370000
H	3.759642000	-6.635777000	-14.078092000
H	1.614034000	-7.878242000	-14.596028000
C	2.161087000	-8.082969000	-13.664786000
C	1.657797000	-9.008721000	-12.752482000
H	0.707305000	-9.512294000	-12.985608000
C	2.334384000	-9.283054000	-11.533001000
C	3.560608000	-8.584725000	-11.258359000
C	4.280888000	-8.821650000	-10.054722000
C	3.772016000	-9.736023000	-9.126764000
H	4.342157000	-9.908540000	-8.202079000
C	2.566254000	-10.416144000	-9.361740000
H	2.187316000	-11.130130000	-8.614006000
C	1.833530000	-10.216429000	-10.547726000
N	0.626590000	-10.854598000	-10.745671000
H	0.317437000	-10.998351000	-11.708566000
H	0.427356000	-11.651589000	-10.137742000

C	7.228906000	-6.446006000	-10.491386000
H	7.043833000	-5.372064000	-10.673836000
H	7.477186000	-6.578521000	-9.424720000
C	8.361540000	-6.957440000	-11.397205000
H	7.961723000	-7.111846000	-12.424101000
H	8.751660000	-7.934844000	-11.047658000
N	9.458217000	-6.004498000	-11.431494000
H	9.227483000	-5.016792000	-11.228875000
C	10.741761000	-6.393837000	-11.674869000
O	11.080060000	-7.585034000	-11.774100000
C	11.756022000	-5.282969000	-11.818915000
C	11.411322000	-3.992351000	-12.261004000
H	10.370712000	-3.767531000	-12.521655000
C	12.409504000	-3.007024000	-12.408416000
C	13.754189000	-3.310400000	-12.077158000
C	14.094538000	-4.627276000	-11.667936000
C	13.099351000	-5.612361000	-11.552517000
H	13.324659000	-6.645416000	-11.259912000
O	12.199401000	-1.734718000	-12.841549000
C	10.985748000	-1.355761000	-13.504398000
H	10.830861000	-0.296452000	-13.219009000
H	10.118493000	-1.921977000	-13.111488000
O	14.699111000	-2.319248000	-12.117425000
C	15.657533000	-2.404804000	-13.190715000
H	16.428518000	-1.646362000	-12.944685000
H	16.147161000	-3.403088000	-13.177422000
O	15.414612000	-4.830399000	-11.391061000
C	15.857636000	-6.166591000	-11.138433000
H	15.609062000	-6.815113000	-12.010081000
H	15.327766000	-6.584468000	-10.252787000
H	16.923484594	-6.142364297	-10.965864632
H	15.194094666	-2.252549080	-14.154272652
H	11.061153083	-1.534383053	-14.566851875
H	13.914230162	-3.047185112	-8.583489138
H	13.631408176	1.037358872	-11.131432807
H	9.316032113	3.649870667	-9.007539637
H	15.145148598	0.751543733	-6.455153730
H	13.063232464	4.111476865	-3.828935402
H	7.475719195	4.532666673	-4.418007303
H	12.921818761	-2.847057560	-4.856317158
H	13.246677844	0.454140195	-0.890915620
H	9.862427603	4.362548147	-0.814249647

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