**Supporting Information**

for

# Stimuli-Responsive Luminescent Supramolecular Assemblies and Co-assemblies by Orthogonal Dipole-Dipole Interaction and Halogen Bonding

*Akshoy Jamadar,[a] Ajeet Kumar Singh,[b] Lisa Roy*[b] and Anindita Das*[a]*

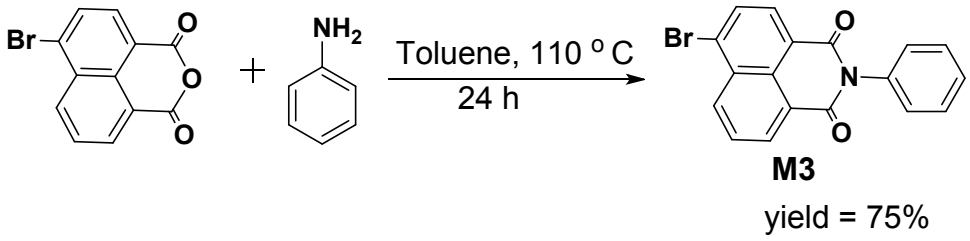
[a]School of Applied and Interdisciplinary Sciences,
Indian Association for the Cultivation of Science, Jadavpur, Kolkata-700032, India

[b]Institute of Chemical Technology, Mumbai-IOC Odisha Campus Bhubaneswar,
IIT Kharagpur Extension Centre, Bhubaneswar-751013, India

*Corresponding author's email: psuad2@iacs.res.in, l.roy@iocb.ictmumbai.edu.in*

**Materials and methods:** All reagents were obtained from commercial suppliers and used without further purification unless otherwise mentioned. 4-Bromo-1,8-naphthalic anhydride was purchased from TCI Co and iodopentafluorobenzene was purchased from Sigma-Aldrich. Solvents were dried properly following standard protocols before setting up the reactions. $^{1}H$, $^{13}C$ and $^{19}F$ NMR spectra were recorded on a Bruker 500 MHz and 400 MHz NMR spectrometer using $CDCl_3$ or $C_6D_{12}$ as solvent. Chemical shifts (δ) are in ppm unit with TMS as the internal standard. The coupling constant (*J*) is reported in hertz (Hz). HRMS measurements were done on XEVO G2-XS Q Tof and Micromass Q-Tof Micro machine. Column chromatography was carried out on silica gel (100-200 mesh). SCXRD were recorded in Bruker Apex-III D8 venture instrument with CMOS detector. WAXRD in thin films were measured in Rigaku SmartLab advance instrument using Cu-Kα tube (α = 0.15406 nm). For UV-Vis studies, spectroscopic grade solvents were used and spectra were recorded in a JASCO V-750 spectrophotometer. Fluorescence spectra were recorded in a FluoroMax-3 spectrophotometer from Horiba Jobin Yvon. FTIR spectra were obtained in a Perkin Elmer Spectrum 100 FT-IR Spectrometer. Transmission Electron Microscopy (TEM) was performed in JEOL-2010EX machine and JEOL-JEM-2100F machine operating at an accelerating voltage of 200 KV. Atomic force microscopy (AFM) images were taken in an Innova instrument from Bruker. Confocal laser scanning microscopy was performed in Carl Zeiss LSM888 machine.

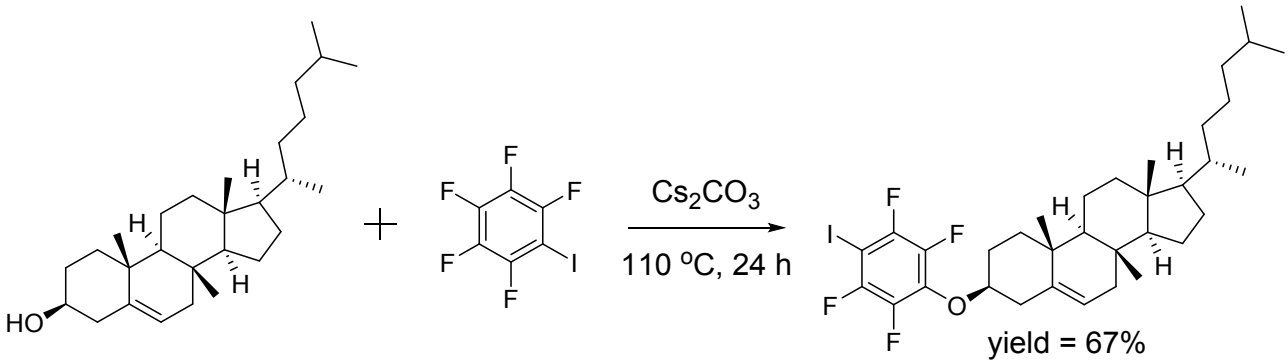
**Synthesis and characterization:** Synthetic protocols for **M1** and **M2** are reported by us elsewhere.[1] Synthesis of **M3** and **Chol-D** are outlined in **Scheme S1** and **Scheme S2**, respectively.




**Scheme S1**: Synthetic scheme for preparation of **M3**.

**Synthesis of 6-bromo-2-phenyl-1H-benzo[*de*]isoquinoline-1,3(2H)-dione (M3):[1]** Aniline (251.4 mg, 2.70 mmol) and 4-Bromo-1,8-naphthalic anhydride (500 mg, 1.80 mmol) were taken in 10 mL toluene and the reaction mixture was stirred at 110 °C for 24 h. The reaction was cooled to room temperature and the solvent was removed under reduced pressure to obtain a brown crude

which was purified by column chromatography using silica gel (100-200 mesh) as stationary phase and 1:9 (v/v) dichloromethane: hexane solvent mixture as eluent to obtain pure product as white solid (500 mg, yield 75%). M.P. = 208°C-210°C; $^{1}$H NMR (400 MHz, $CDCl_3$, TMS): $\delta$ (ppm) = 8.72 (d, $J$ = 8.0 Hz, 1H), 8.65 (d, $J$ = 8.5, 1H), 8.47 (d, $J$ = 7.9 Hz, 1H), 8.10 (d, $J$ = 7.9 Hz, 1H), 7.89 (dd, $J$ = 7.4 Hz, 1H), 7.56 (t, $J$ = 7.4 Hz, 2H), 7.49 (t, $J$ = 7.4 Hz, 1H), 7.32 (d, $J$ = 7.3 Hz, 2H). $^{13}$C-NMR (101 MHz, $CDCl_3$, ppm): $\delta$ 163.94, 135.27, 133.79, 132.59, 131.74, 131.38, 130.99, 130.83, 129.57, 128.99, 128.71, 128.35, 123.44, 122.56. HRMS (ESI): m/z calcd for $C_{18}H_{10}BrNO_2H$ [**M3**+ H]$^{+}$: 351.9973; experimentally found : 351.5632.




**Scheme S2**: Synthetic scheme for preparation of **Chol-D**.

**Synthesis of Cholesterol donor (Chol-D)[2]:** In a 10 mL sealed tube, cholesterol (387 mg, 2.0 mmol) available from commercial source, cesium carbonate (1.63 g, 5.0 mmol) and iodopentafluorobenzene (1.0 mL, 8.0 mmol) were taken and the reaction mixture was heated at 110 ºC for 24 hours. The reaction mixture was cooled and work up was done using water and dichloromethane. The organic extract was dried over $Na_2SO_4$ and the crude product was purified by column chromatography using a silica gel column (100-200 mesh). Initially the column was packed and eluted with hexane to remove the excess iodopentafluorobenzene. Then the desired product was eluted with 5:95 (v/v) dichloromethane : hexane solvent mixture and collected as a white solid (900 mg, yield = 67 %). M.P. = 120°C. $^{1}$H-NMR (400 MHz, $CDCl_3$, ppm): $\delta$ 5.38-5.37 (m, 1H), 4.14-3.94 (m, 1H), 2.55-2.40 (m, 2H), 2.03-1.78 (m, 6H), 1.53-0.85 (m, 34H), 0.68 (s, 3H). $^{13}$C-NMR (101 MHz, $CDCl_3$, ppm): $\delta$ 148.5-146.2 (m, 2H), 142.8-139.8 (m, 2H), 139.6, 137.2, 123.2, 84.9, 64.2, 56.9, 56.3, 50.2, 42.5, 39.9, 39.6, 39.7, 39.2, 37.1, 36.8, 36.3, 35.9, 32.1,

32.0, 28.7, 28.4, 28.2, 24.4, 23.9, 22.9, 22.7, 21.2, 19.4, 18.9, 12.0. $^{19}$F NMR (377 MHz, $CDCl_3$, ppm): $\delta$ -121.65 (d, $J$ = 18.5, 2F), -153.11 (d, $J$ = 18.5, 2F).

**Experimental procedures:**

**Solution preparation:**

**Solution preparation for M1, M2, M3** and **Chol-D:** Measured amount of **M1**, **M2**, **M3** and **Chol-D** were individually dissolved in a good solvent, dioxane to prepare 4.0 mM stock solutions. In each case, 100 μL of the stock solution was taken in a glass vial and diluted with fresh 100 μL dioxane. To this, 800 μL methylcyclohexane (MCH) was added to make a final concentration of 0.4 mM in 20% dioxane/MCH (v/v). The final solution was heated to break any preformed aggregate and allowed to equilibrate at room temperature for at least 1 h prior to experimental measurements. This technique was followed in all the reported self-assembly studies in solution.

**Preparation of 1:1 co-assembled solution:** From the prepared 4.0 mM stock solutions of **M1** and **M2** in dioxane, 100 μL of **M1** was mixed with 100 μL of **M2** in a glass vial. To this, 800 μL MCH was added to make the individual dye concentration = 0.4 mM in 20% dioxane/MCH. Finally, the solution was heated and allowed to stand at room temperature for at least 1 h to attend equilibrium, prior to any physical measurements. The same protocol was followed for 1:1 mixture of **M2**:**M3**, **M1**:**Chol-D** and **M2**:**Chol-D**. For the **M1**:**M2** co-assembly with varying fraction of **M1**, different solutions were prepared by mixing 100 μL of the stock solution of **M2** (4.0 mM) with a variable volume of the stock solution of **M1** (4.0 mM) in dioxane. The remaining volume was adjusted by addition of dioxane to reach a final volume of 200 μL. To this, 800 μL MCH was added to make the final **M2** concentration = 0.4 mM in 20% dioxane/MCH.

**UV-visible studies:** 0.4 mM solutions of **M1**, **M2** and **M3** were prepared as mentioned above. These solutions were transferred into 0.1 cm path length cuvette, and the UV−vis measurements were recorded at different temperature intervals. The same protocol was followed for **Chol-D** and all the co-assembled solutions.

**Quantum yield measurements:** Relative quantum yield (φ) measurement of **M1**, **M2** and **M3** in dioxane and their aggregates in 20% dioxane/MCH (v/v) mixture were carried in comparison to

an accepted standard, quinine sulphate in 0.1 M, $H_2SO_4$ [$\lambda_{ex}$ = 350 nm, 25 °C] using the following formula.[3]

$$\varphi = \varphi_R \frac{I\ OD\ \eta^2}{I_R OD_R \eta_R^2}$$

Where φ = the quantum yield of the sample, $\varphi_R$ = quantum yield of quinine sulphate under the above-mentioned conditions (0.577), I = integrated emission intensity of the sample, OD = optical density of the sample and $\eta$ = refractive index of the sample. The suffix"R" for all the above-described parameters stand for the reference, quinine sulphate.

**Single Crystal X-Ray Diffraction (SCXRD) studies:** The structure of **M2** and **M3** were analyzed using single crystal X-ray diffraction technique. Diffraction-quality crystals were obtained from dioxane. Single crystals for analysis were coated with Parabar oil prior to mounting under a nitrogen cold stream. Data were collected at 151K on a Bruker D8VENTURE Microfocus diffractometer equipped with PHOTON II Detector, with Mo Kα radiation (λ = 0.71073Å), controlled by the APEX3 (v2017.3-0) software package. Space group was assigned by systematic absences (determined by XPREP) and analysis of metric symmetry and was further checked by PLATON.[4] Structure was solved by direct method and refined against all data in the reported 2θ ranges by full-matrix least squares on F2 using the SHELXL program suite[5] in the OLEX2 interface.[6] The details of crystal data collection and refinement of compound **M2** and **M3** are summarized in Table **S1** and **S2**, respectively.

**Wide Angle X-Ray Diffraction (WAXRD) studies:** The self-assembled solutions of **M1**, **M2** and **M3** in 20% dioxane/MCH were drop casted on a glass slide (multiple times) to make a thin film and air dried for two days. The prepared films were placed under Rigaku SmartLab advance instrument using Cu-Kα tube. Same protocol was followed for different **M1**:**M2** co-assembled systems.

**FT-Raman studies:** Thin films were prepared from a solution of **M2, Chol-D** and their 1:1 mixture in 20% dioxane/MCH. FT-Raman spectra were recorded with a triple Raman spectrometer (Model: T64000, Make: J-Y HORIBA) equipped with 1800 grooves/mm gratings, TE cooled synapse CCD and with an open stage Olympus microscope with 50x objective. The sample were

excited with a 532 nm wavelength laser from DPSS (mod: YAG laser, make: spectra physics). The laser power was set to 6 mW. The software package Lab Spec 5.93 was used to record the Raman spectra. The Raman data were background corrected and in the end the spectra were vector normalized.

**FT-IR studies:** Spectra were recorded from solutions of **M1**, **M2** and their 1:1 mixture with **Chol-D** in 20% dioxane/MCH (Conc. = 0.4 mM).

**Diffusion-Ordered NMR Spectroscopy (DOSY):** Solutions of **M1**, **M2** and **M3** were prepared with 5 mM concentration of each in molecularly dissolved solvent $CDCl_3$ and in aggregated solvent 1:9 $CDCl_3$:$C_6D_{12}$ (v/v). For preparation of aggregated samples, 5 mM concentration of individuals were made in a good solvent ($CHCl_3$), then the solvent was completely removed by heating to get a thin film. To this, 10% of $CDCl_3$ was added followed by 90% $C_6D_{12}$ (v/v). The sample was heated to break any preformed aggregate and equilibrated at room temperature before taking the measurements. The data was recorded at 25 $^oC$ in Bruker 400 MHz instrument. A diffusion gradient duration ($\delta$) of 2 ms and diffusion time ($\Delta$) of 200 ms were used for the DOSY measurements. The diffusion coefficient values were obtained using TopSpin 2.1 software following a standard fitting procedure.

**Transmission Electron Microscopy (TEM) studies:** Solutions of **M1**, **M2** and **M3** were prepared in 20% dioxane/MCH at a concentration of 0.4 mM following similar protocol as discussed earlier. Sample solutions were drop casted on copper grids and were left open to air for 24 h for slow drying prior to imaging. Various co-assembled solutions were prepared following the same procedure.

For the acid-responsive disassembly studies, 5% (v/v) trifluoroacetic acid (TFA) was added to the aggregated solution of **M2**, **M1+Chol-D** and **M2+Chol-D** in 20% dioxane/MCH. These solutions were allowed to equilibrate for 1 h prior to drop casting on the copper grids. All the samples were left open to air for 24 h for slow drying before capturing the images.

**Atomic Force Microscopy (AFM) studies:** Solutions of **M2** in 20% dioxane/MCH(v/v) (Conc. = 0.4 mM) was spin-coated on Mica substrate and allowed to air dry for 24 h before capturing the AFM images.

**Confocal Laser Scanning Microscopy (CSLM) studies:** Solutions of **M1** and **M2** in 20% dioxane/MCH (Conc. of **M1** = **M2** = 0.4 mM) were drop casted on microscopic grade cover glass and allowed to dry in a desiccator for 24 h. The images were captured from a confocal laser scanning microscope (Carl Zeiss LSM880) at 10× magnification. For blue emission, 340 nm laser light was used and for green emission, 488 nm laser light was used. Similar procedure was followed for **M1** and **M2** co-assembled systems.

**Fluorescence microscopy studies:** Solution of **M3** in 20% dioxane/MCH (Conc. of **M3** = 0.4 mM) was drop casted on micro glass slide and allowed to dry in a desiccator for 24 h, and images were captured from a fluorescence microscope Olympus IX73 at 10X magnification.

**Additional figures:**

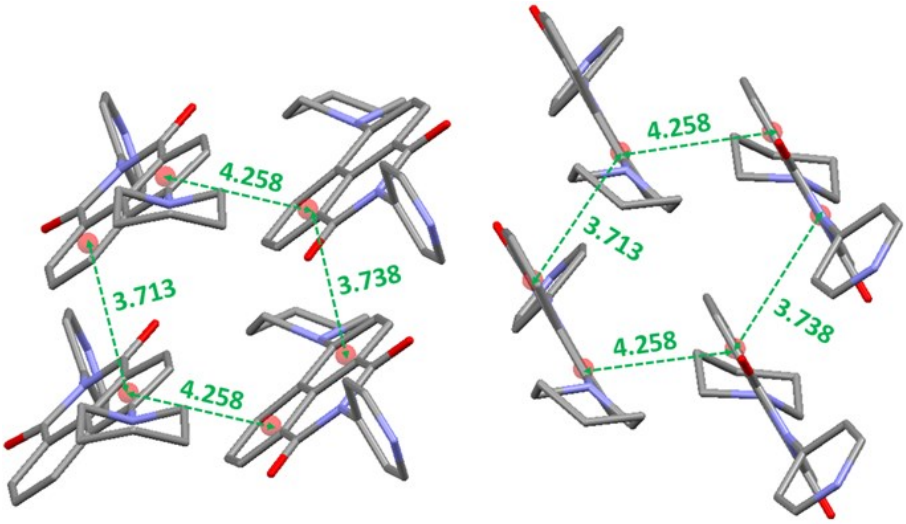



**Figure S1**. Single crystal structure of **M1** showing slipped head-to-head stacking (3.713, 3.738 Å) within the same column and antiparallel head-to-tail stacking (4.258 Å) between two adjacent columns.[1]

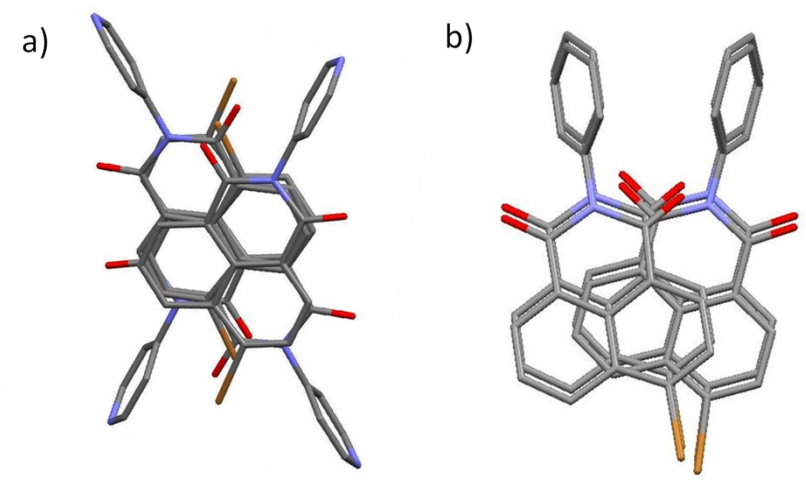



**Figure S2**. SCXRD packing diagram (Top view) of a) **M2** showing rotationally displaced alternate parallel and antiparallel units and b) **M3** showing rotationally displaced parallel units.

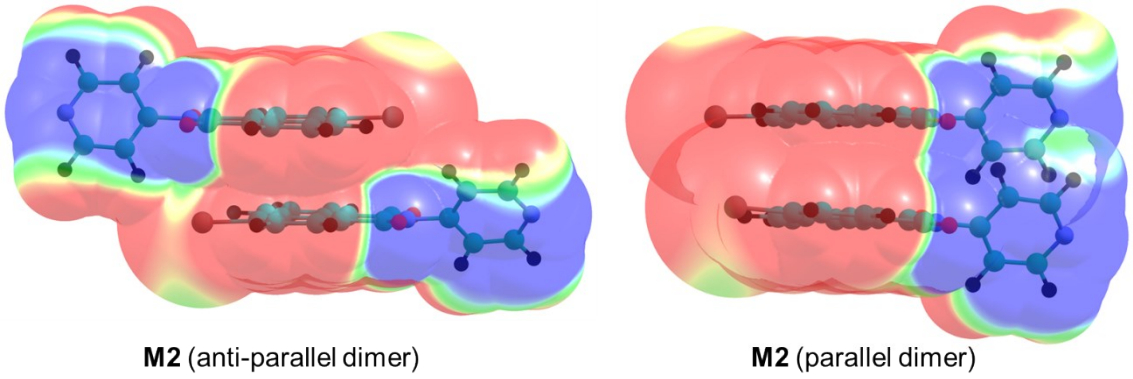



**Figure S3**. Molecular electrostatic potential (MEP) surface at B3LYP(D3BJ)/def2-TZVP level of theory for antiparallel and parallel dimer of **M2**. The color spectrum ranges from negative (blue) to positive (red) potential within ±0.01 au.

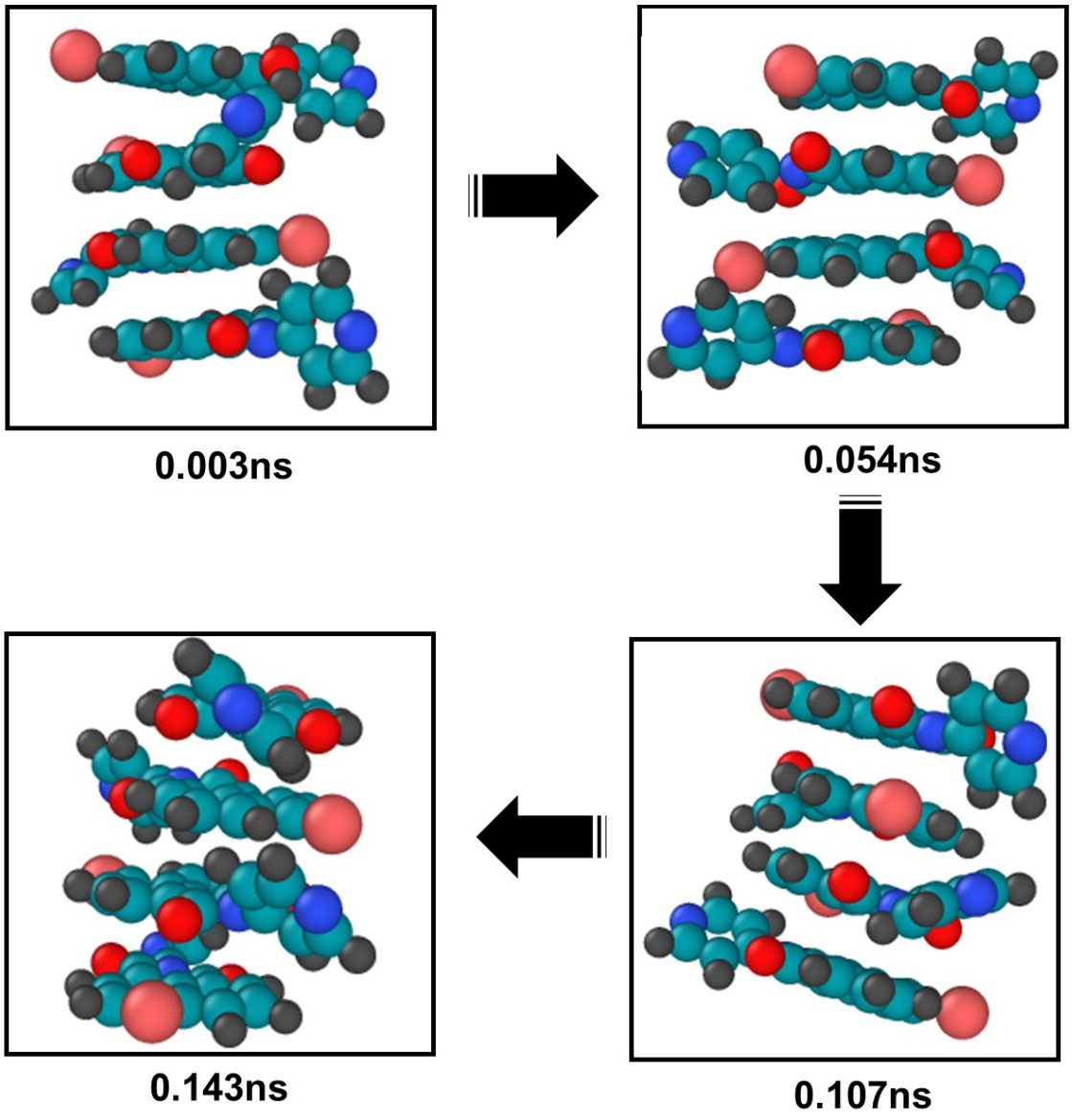



**Figure S4**. Snapshots of the molecular dynamic simulation of **M2** at successive time-intervals at the semi-empirical SCC-DFTB level of theory with the DFTB+ program package. The tetramer consists of both parallel and antiparallel motifs at the end of simulation.

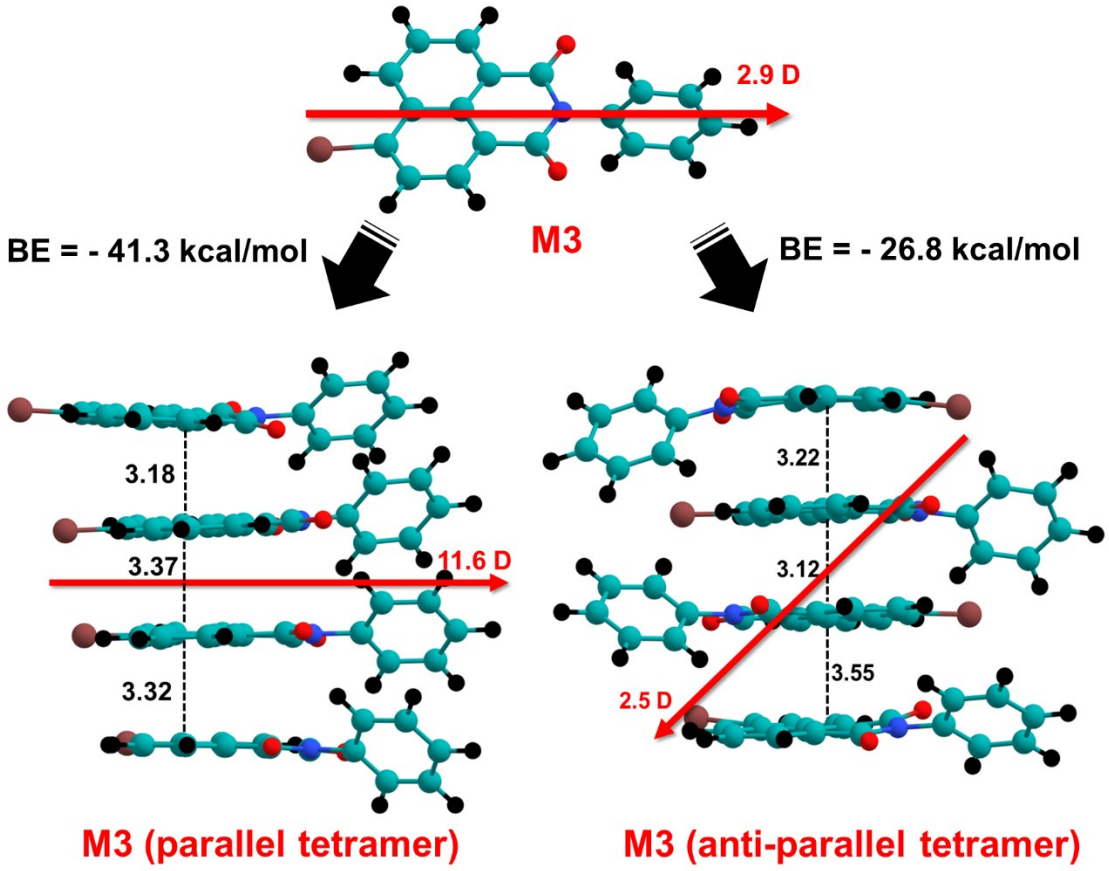



**Figure S5**. Optimized geometry of parallel and antiparallel stacking of **M3** at semi-empirical tight-binding SCC-DFTB method. Binding energies and dipole moments are calculated at B3LYP(D3BJ)/CPCM=MCH/def2-TZVP level of theory. Color coding: C(teal), O(red), Br(brown), H(black) and N(blue). Bond distances shown are in units of Å.

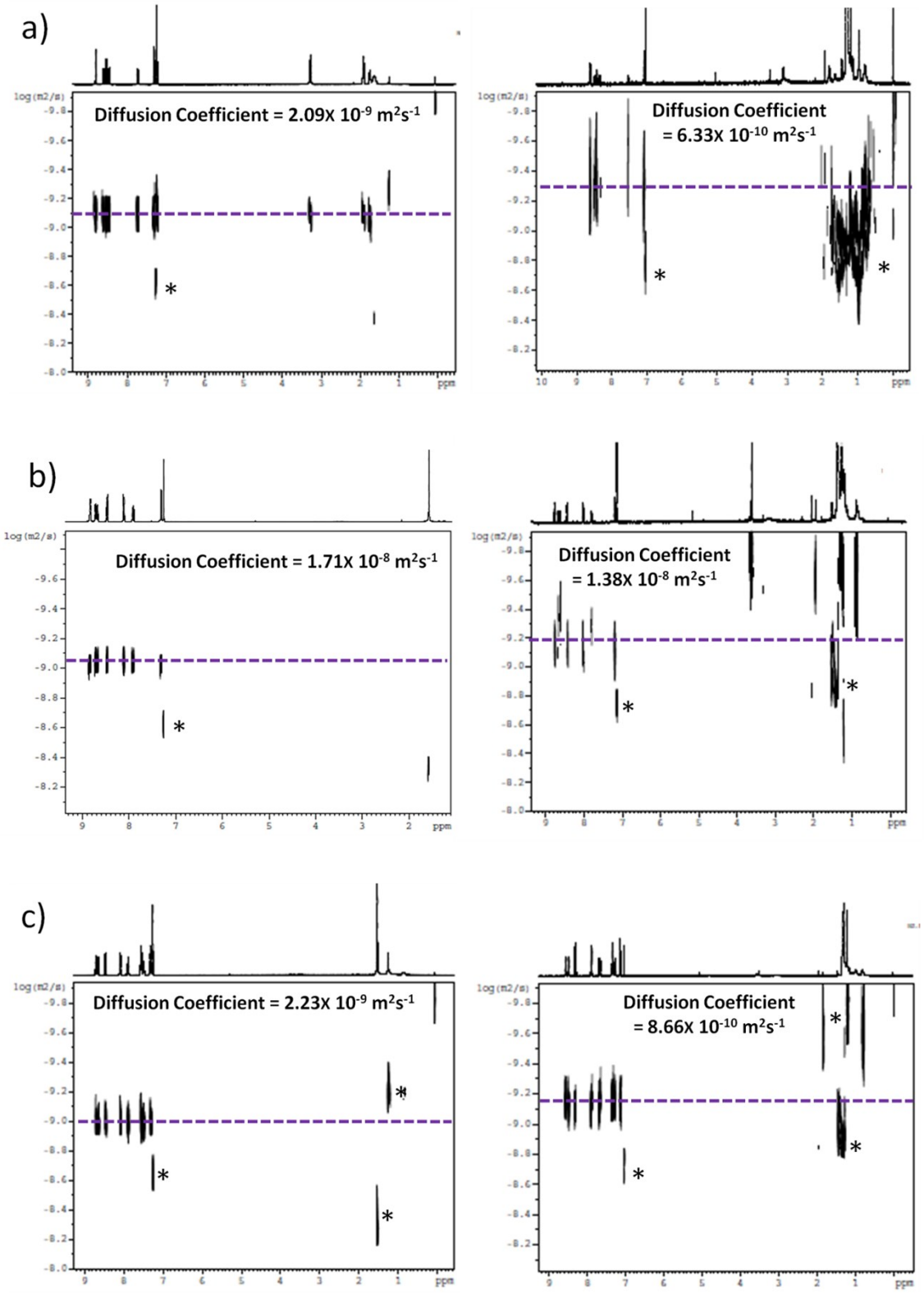



**Figure S6**. DOSY data of a) **M1**, b) **M2** and c) **M3** in $CDCl_3$ (left) and 10% $CDCl_3/C_6D_{12}$ (v/v) (right).

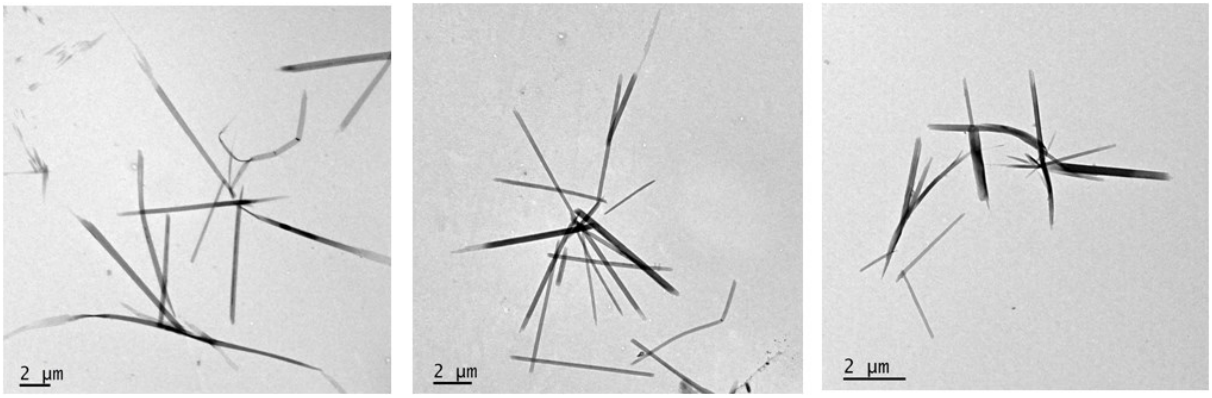



**Figure S7**. TEM images from a solution of **M2** in 20% dioxane/MCH; Conc. of **M2** = 0.4 mM.

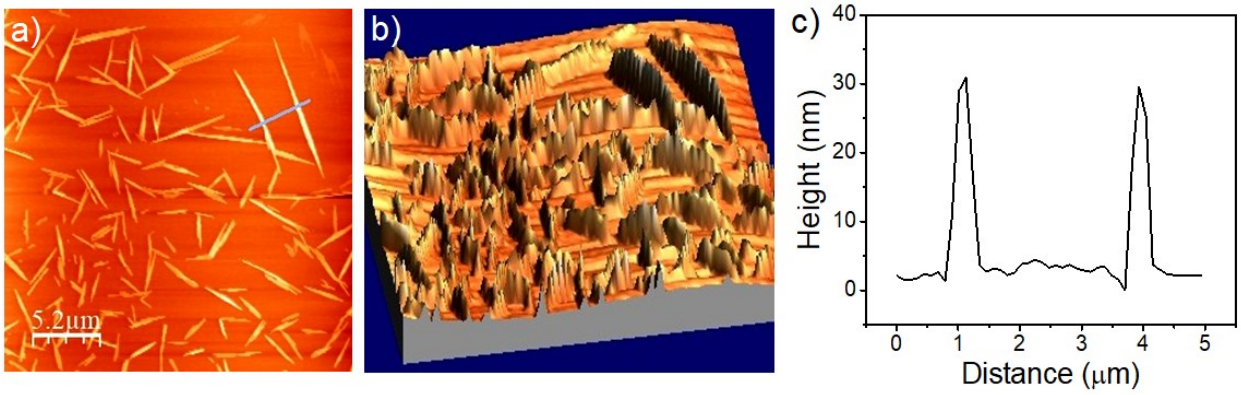



**Figure S8**. a) AFM images from a solution of **M2** in 20% dioxane/MCH, b) 3D view and c) AFM height profile of highlighted rods. Conc. of **M2** = 0.4 mM.

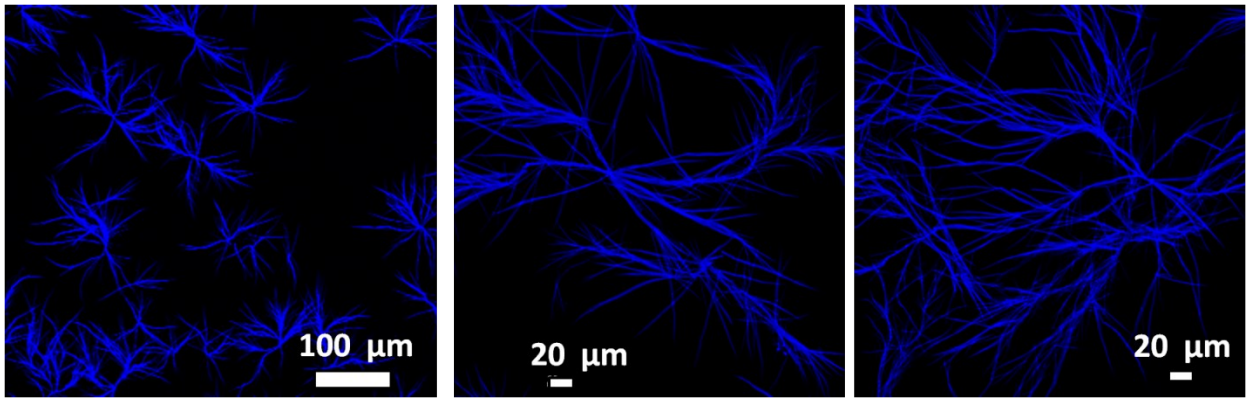



**Figure S9**. a) CLSM images from a solution of **M2** in 20% dioxane/MCH; Conc. of **M2** = 0.4 mM.

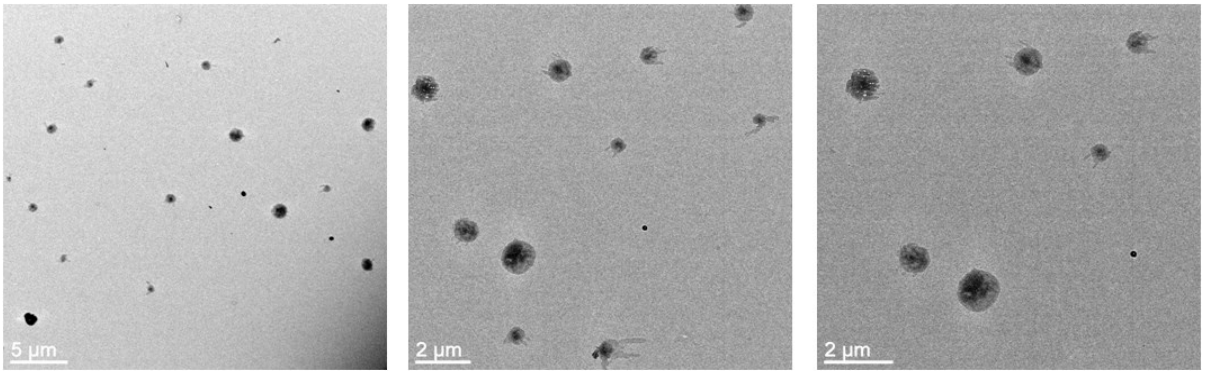



**Figure S10**. TEM images from a solution of **M1** in 20% dioxane/MCH; Conc. of **M1** = 0.4 mM.

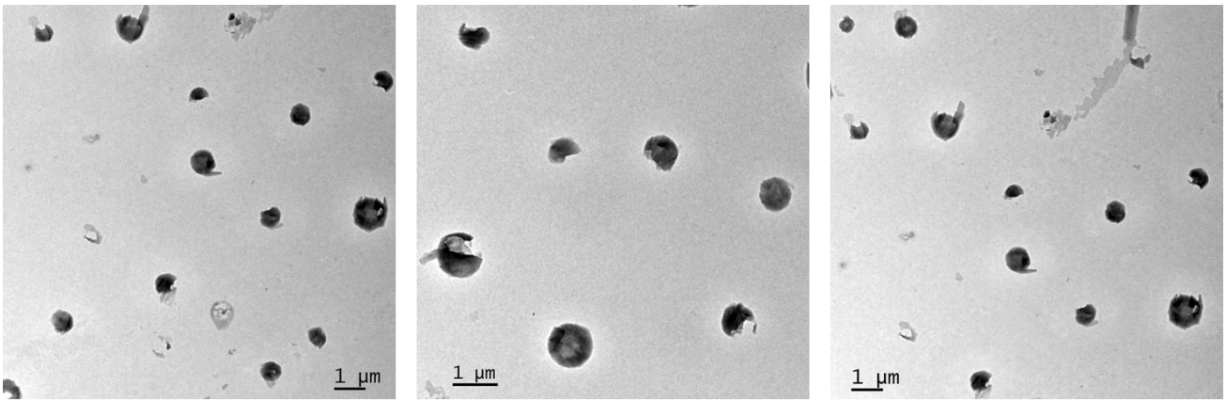



**Figure S11**. TEM images from a solution of **M3** in 20% dioxane/MCH; Conc. of **M3** = 0.4 mM.

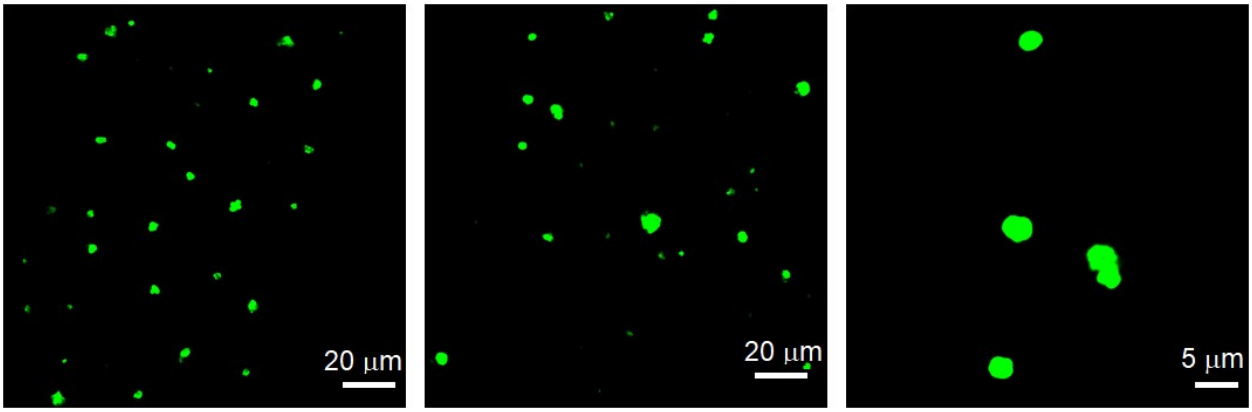



**Figure S12**. CLSM images from a solution of **M1** in 20% dioxane/MCH; Conc. of **M1** = 0.4 mM.

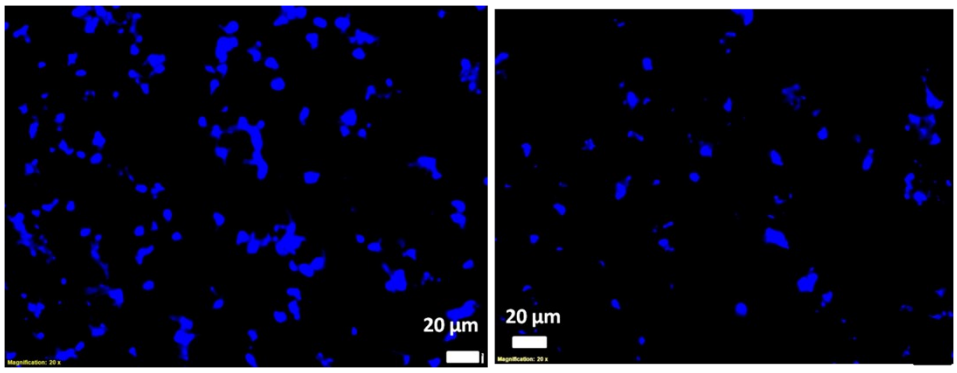



**Figure S13**. Fluorescence microscopy images of **M3** in 20% dioxane/MCH; Conc. = 0.4 mM.

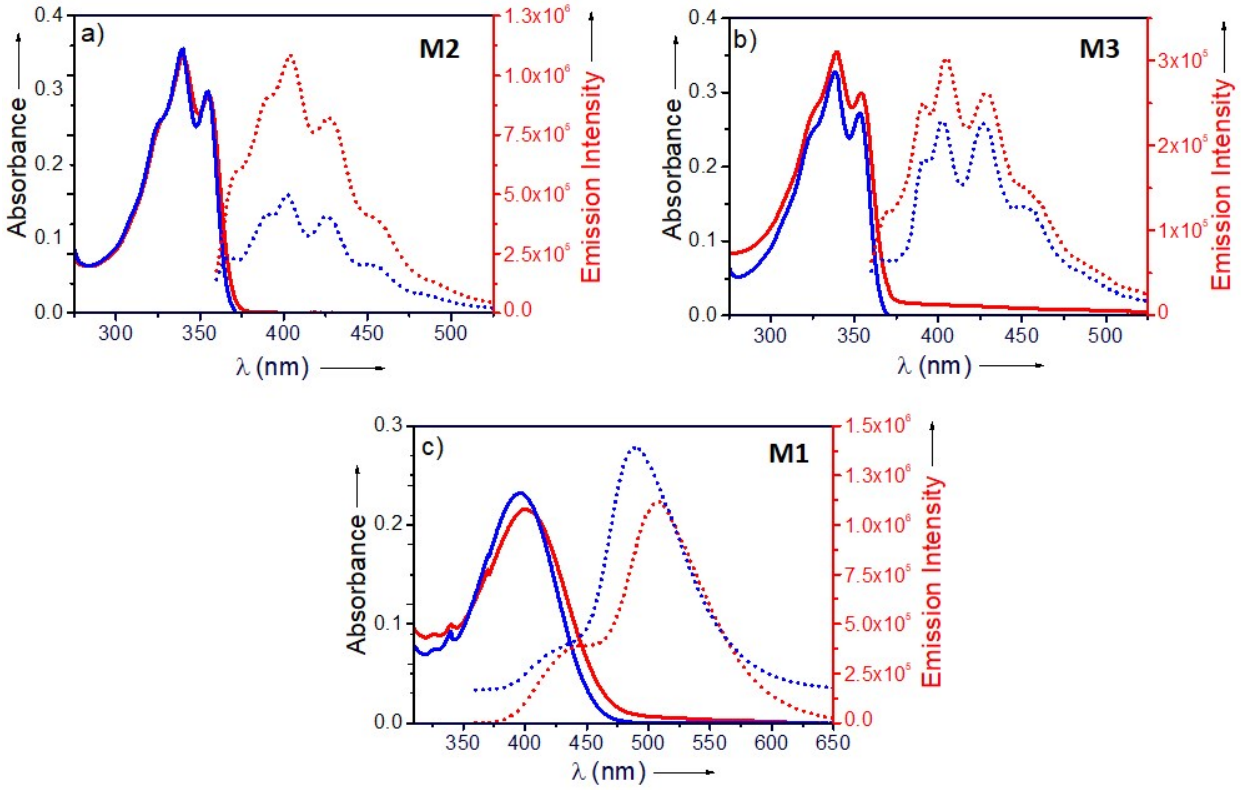



**Figure S14**. UV-visible absorption (solid lines) and emission (dotted lines) spectra of a) **M2**, b) **M3** and c) **M1** in dioxane (red lines) and 20% dioxane/MCH (blue lines). Conc. of **M1** = **M2** = **M3** = 0.02 mM, $\lambda_{ex}$ = 350 nm, excitation and emission slit = 2 nm for **M1** and 5 nm for **M2** and **M3**. Path length = 10 mm. The quantum yield calculated from these spectral data are reported in **Table S3**.

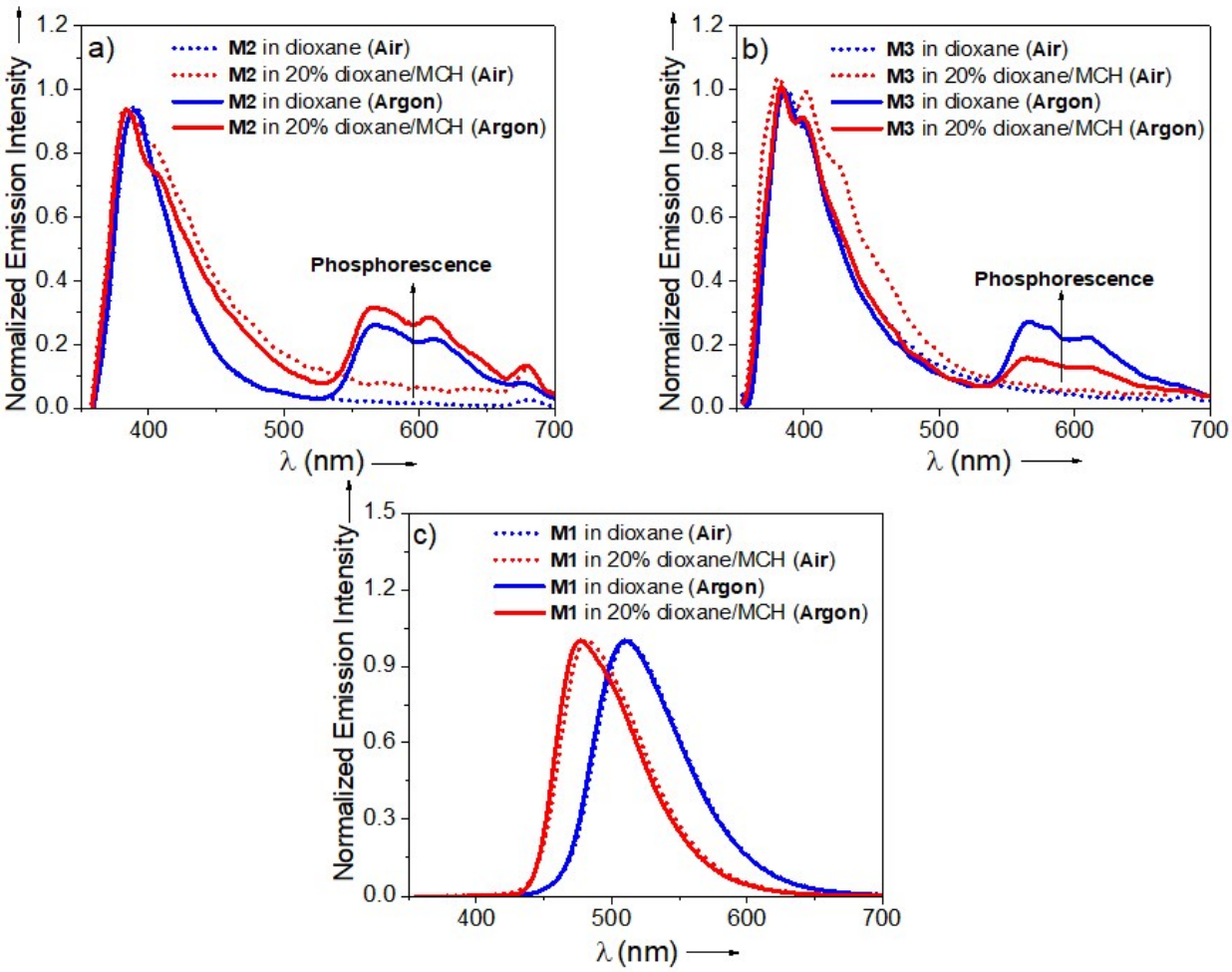



**Figure S15**. Steady state emission spectra of a) **M2**, b) **M3** and c) **M1** in solution at room temperature under air and air-free condition. Conc. of **M1** = **M2** = **M3** = 0.4 mM, $\lambda_{ex}$ = 340 nm, excitation and emission slit = 2 nm for **M1** and 5 nm for **M2** and **M3**. Path length = 10 mm.

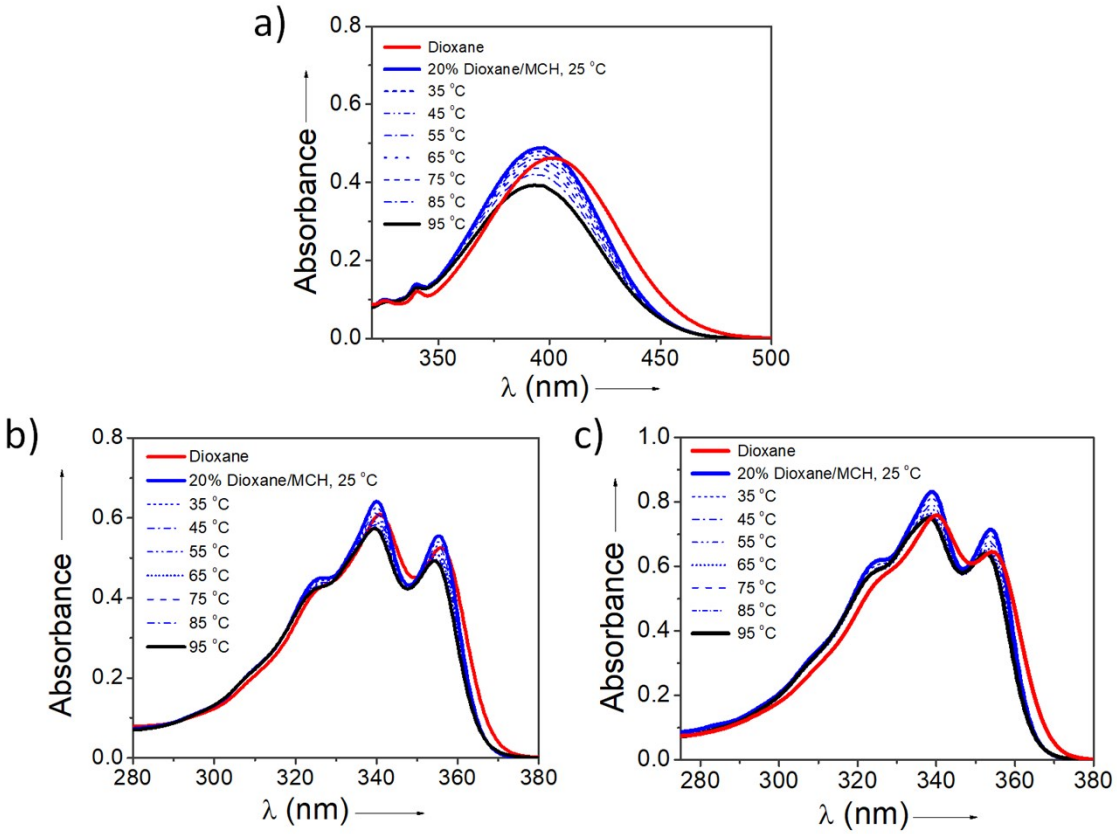



**Figure S16**. Solvent and temperature dependent UV-visible absorption spectra of a) **M1**, b) **M2** and c) **M3**. Conc. = 0.4 mM, path length = 1.0 mm.

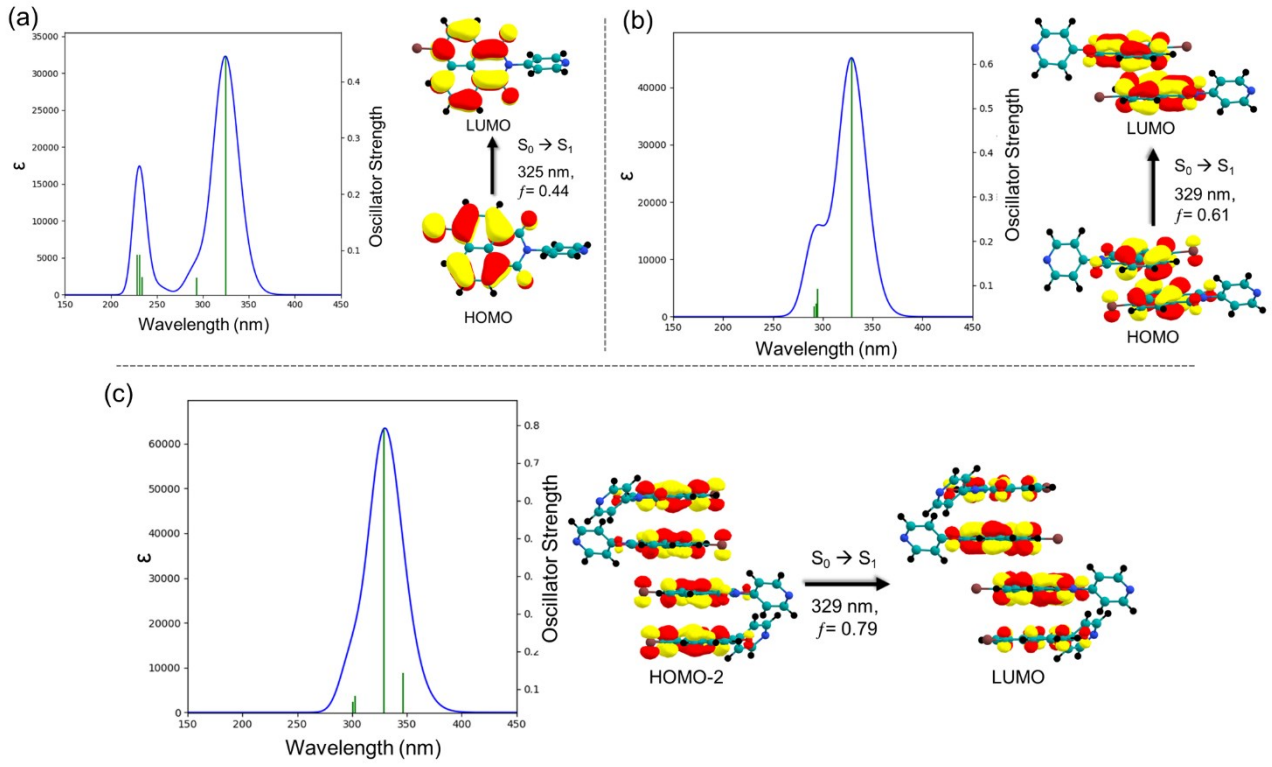



**Figure S17**. TD-DFT calculations in MCH solvent showing theoretical UV-data for a) monomer b) dimer and c) tetramer of **M2**.

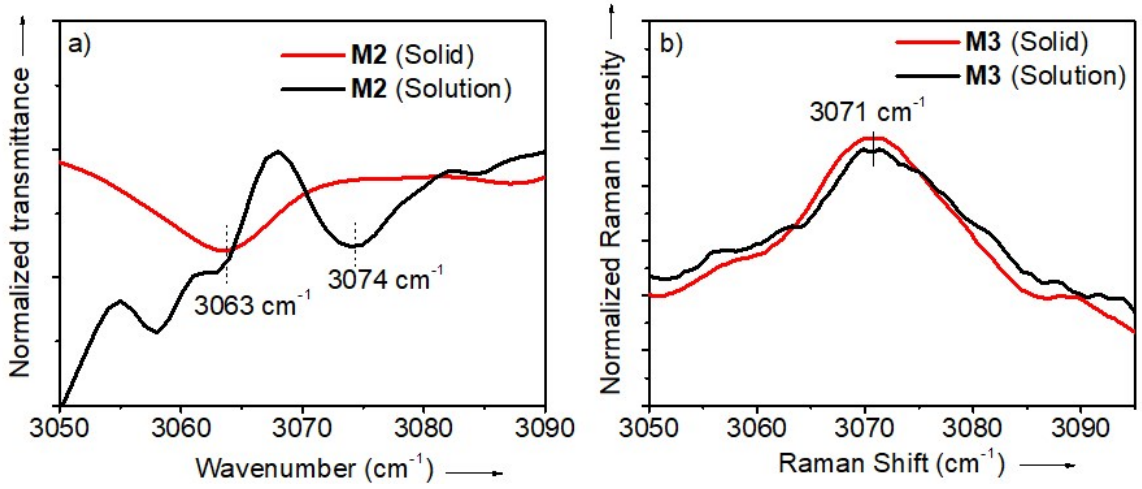



**Figure S18**. a) FTIR spectra of **M2** and b) Raman spectra of **M3** corresponding to the aromatic C-H stretching mode in solid and solution. Conc. = 0.4 mM, 20% dioxane/MCH.

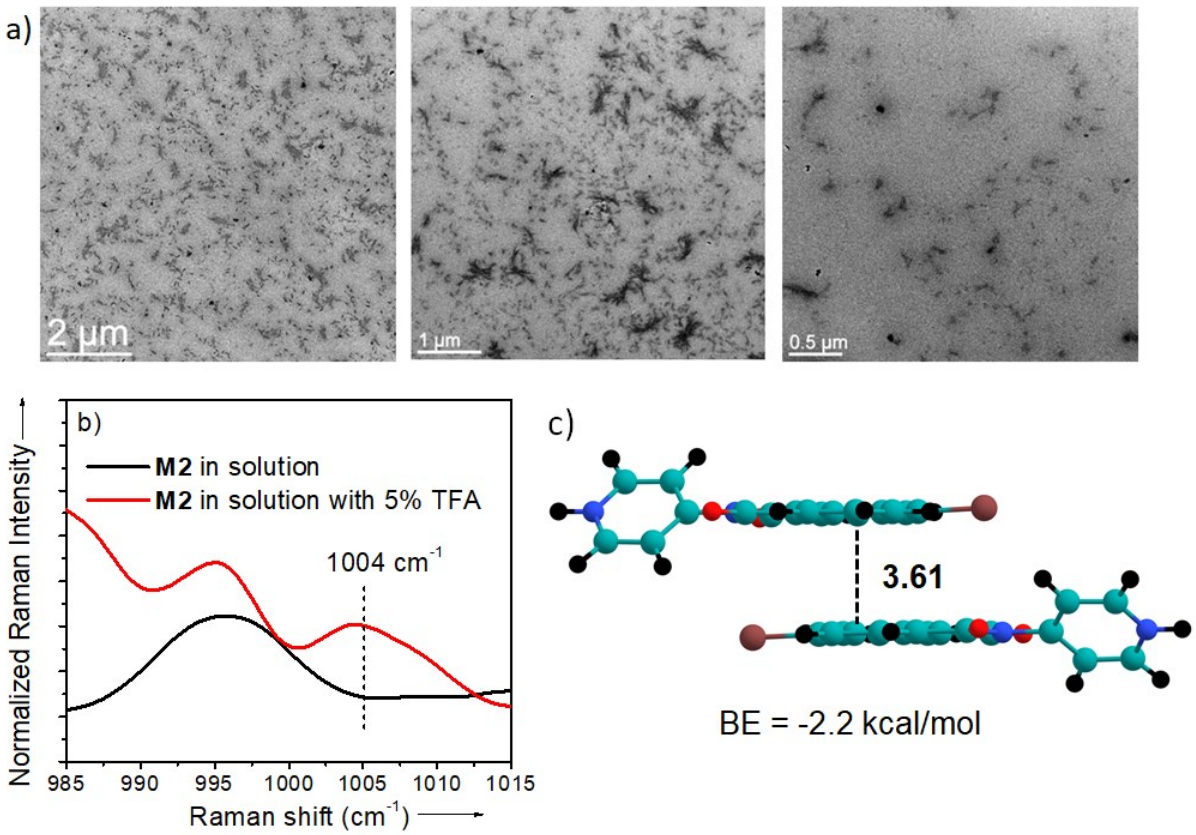



**Figure S19**. a) TEM images from a solution of **M2** in 20% dioxane/MCH with 5% trifluoroacetic acid (TFA) from different sections of the copper grid. b) Raman spectra showing pyridyl ring breathing mode for **M2** in 20% dioxane/MCH in presence and absence of TFA. Conc. of **M2** = 0.4 mM. c) DFT calculation on antiparallel dimer of protonated **M2** showing reduction of stability on protonation of pyridine (BE = -2.2 kcal/mol). Bond distances shown are in units of Å.

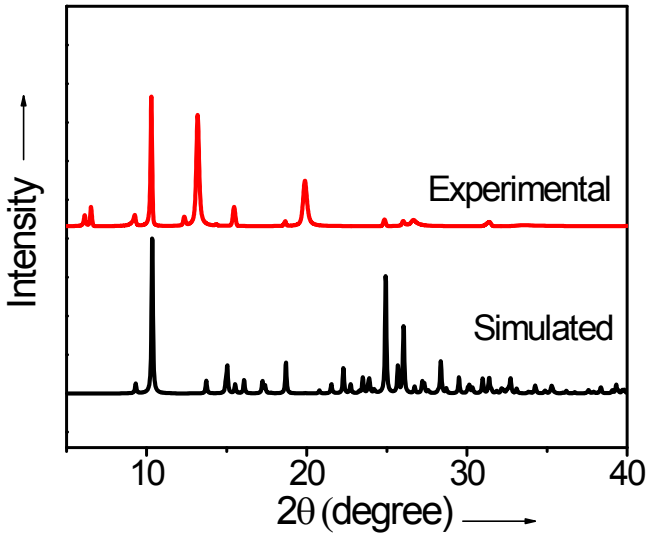



**Figure S20**. Comparison between the WAXRD pattern obtained from simulated single crystal XRD data and thin film of **M2** in 20% dioxane/MCH.

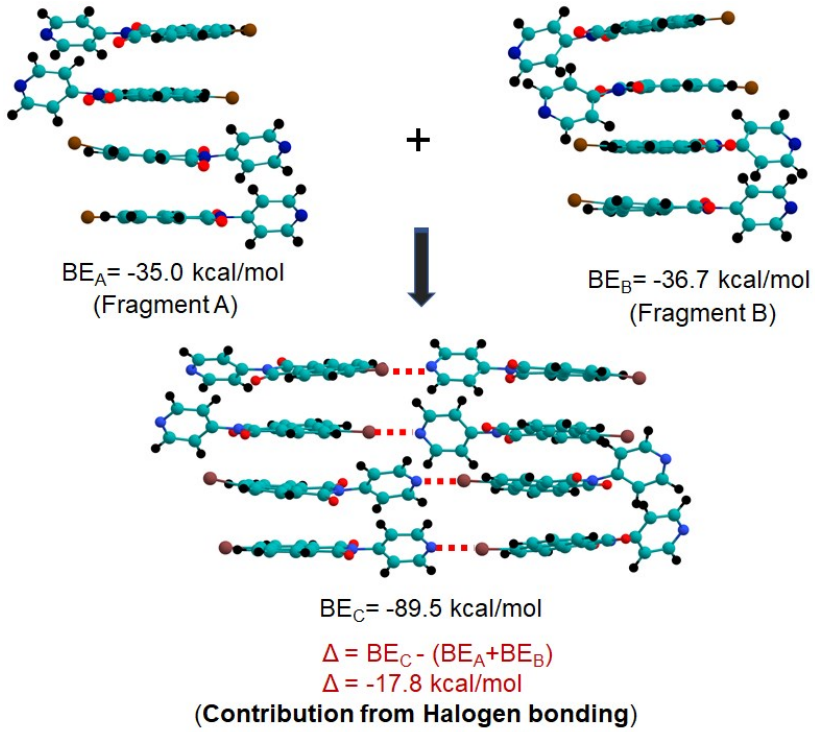



**Figure S21**. Energy decomposition analysis showing contribution from the halogen bonds in the oligomer model of **M2**.

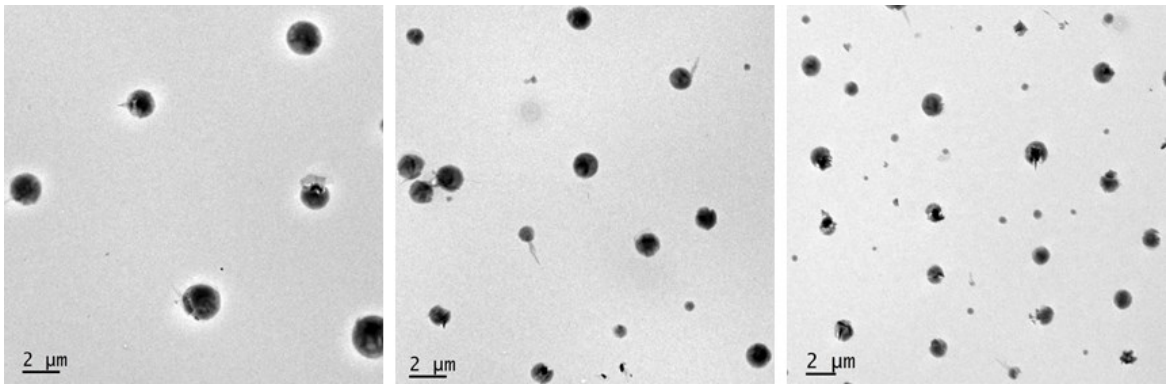



**Figure S22**. TEM images from a 1:1 mixture of **M1** and **M2** in 20% dioxane/MCH. Conc. of **M1** = **M2** = 0.4 mM.

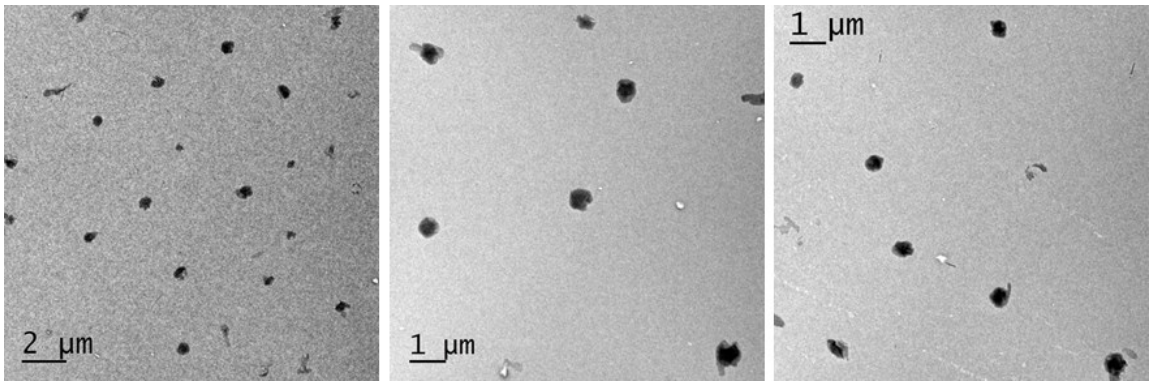



**Figure S23**. TEM images from a 1:1 mixture of **M2** and **M3** in 20% dioxane/MCH. Conc. of **M2** = **M3** = 0.4 mM.

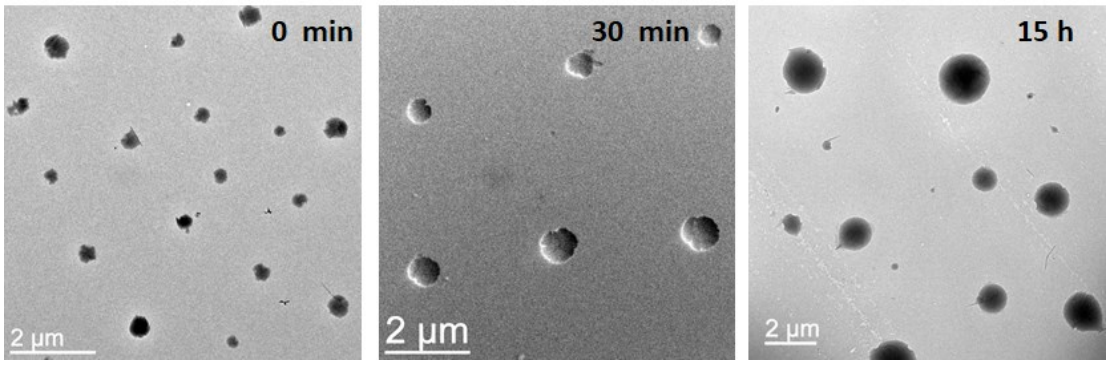



**Figure S24**. TEM images from a 1:1 mixture of **M1** and **M2** in 20% dioxane/MCH captured at different time interval. Conc. of **M1** = **M2** = 0.4 mM.

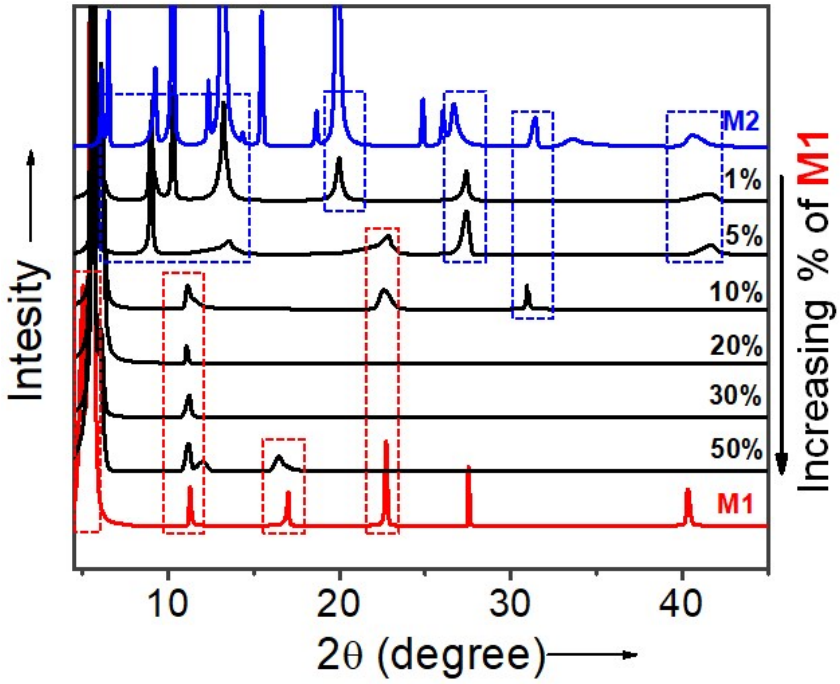



**Figure S25**. WAXRD data from thin films of **M1**, **M2** and their co-assemblies with varying **M1** fractions (1%, 5%, 10%, 20%, 30% and 50%) taken from 20% dioxane/MCH solvent mixture.

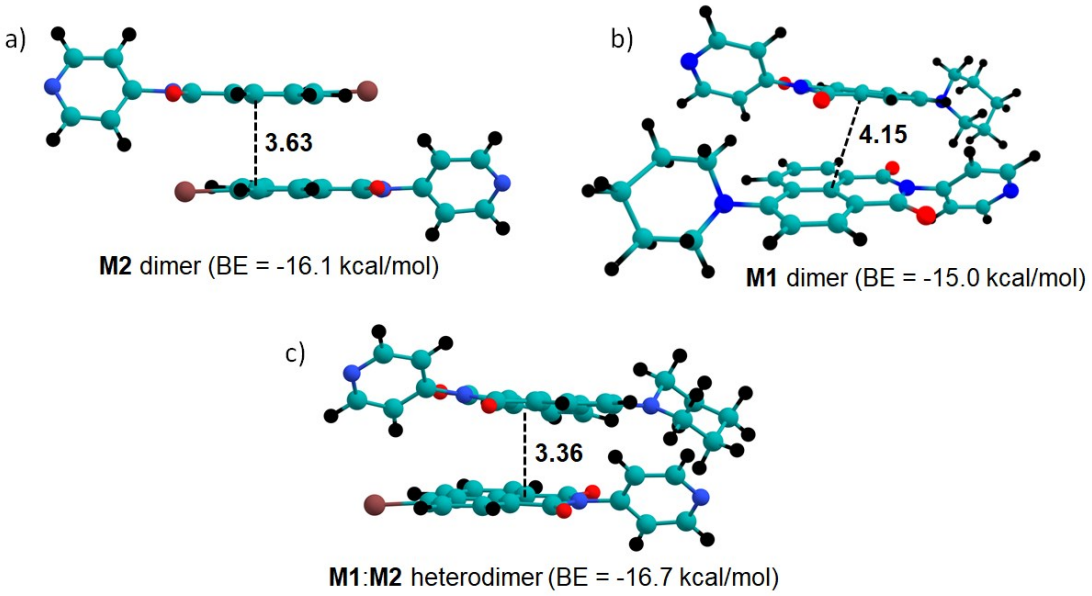
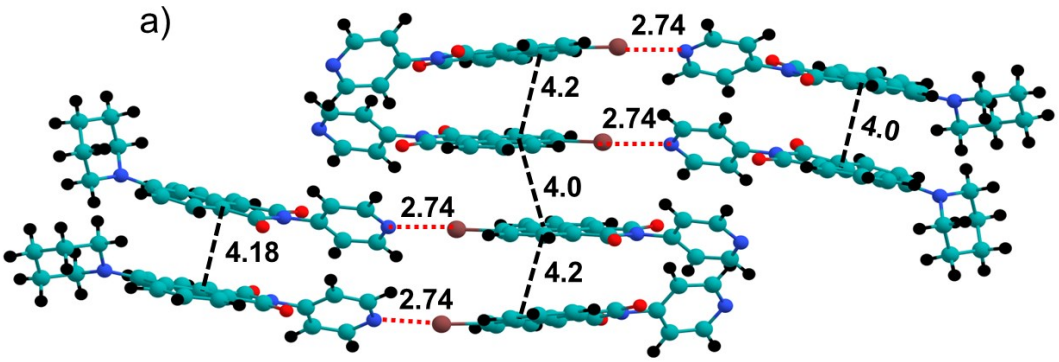
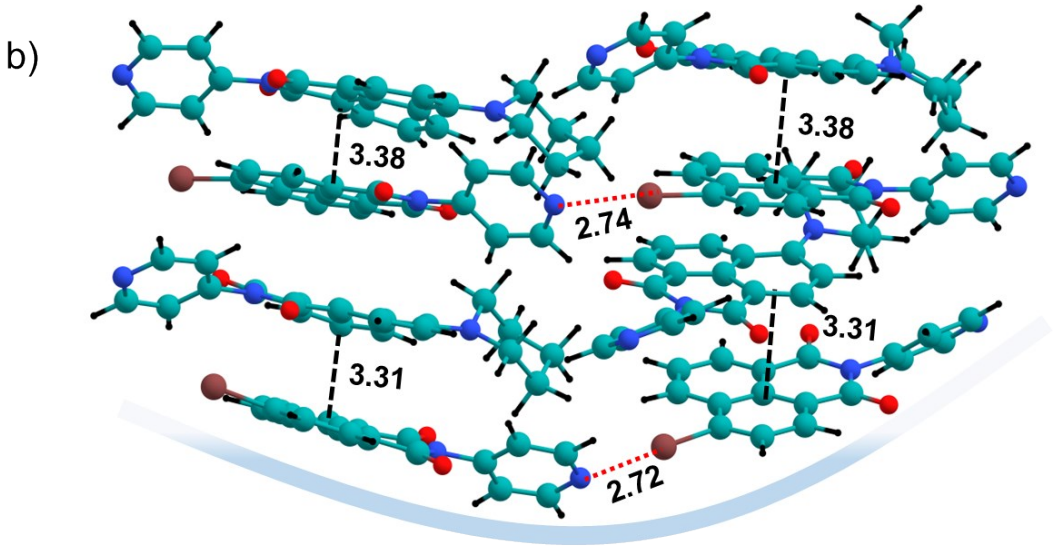



**Figure S26**. DFT calculation on the antiparallel homodimer of a) **M2** and b) **M1** and heterodimer c) **M1**:**M2**, showing comparable binding energy (BE) in the heterodimer. Bond distances shown are in units of Å.




**M1+M2** co-assembly (Model A)

BE = -77.0 kcal/mol




**M1+M2** co-assembly (Model B)

BE = -93.6 kcal/mol

**Figure S27**. DFT calculation for the **M1**+**M2** co-assembly: a) **M2** tetramer unit interacting with **M1** monomers on both sides by halogen bonding (Model A). b) Possible lateral interaction between two hetero-tetramers of **M1** and **M2** by halogen bonding (Model B) that leads to adoption of spherical geometry. Bond distances shown are in units of Å; Red dotted lines indicate halogen bonds.

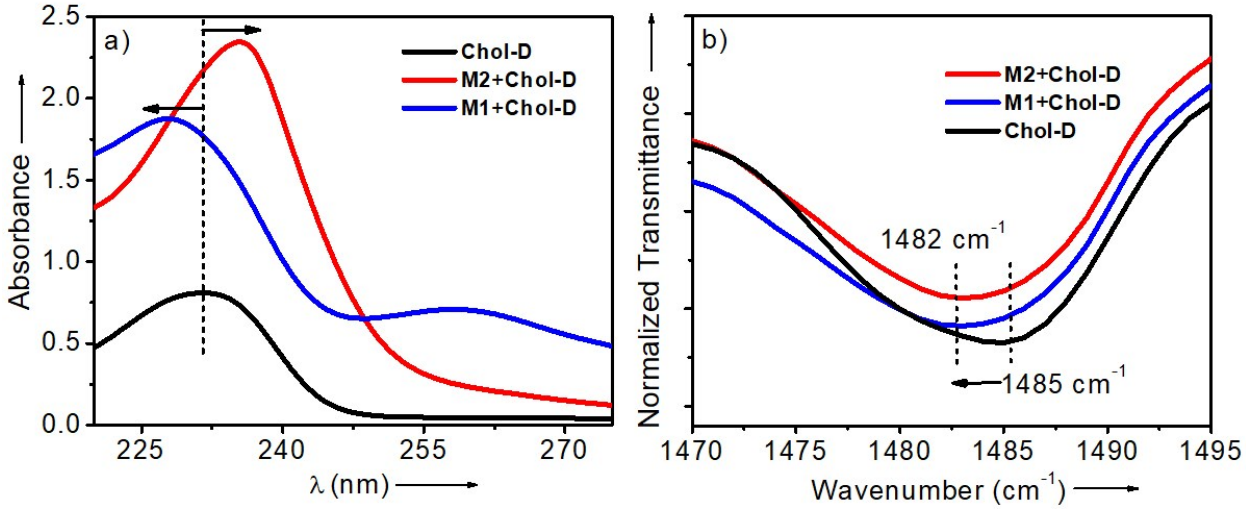



**Figure S28**. Selected region from a) UV-Visible absorption spectra and b) FTIR spectra of **Chol-D** and its 1:1 complex with **M1** and **M2** in 20% dioxane/MCH. Conc. of the individual components = 0.4 mM. Path length = 1.0 mm.

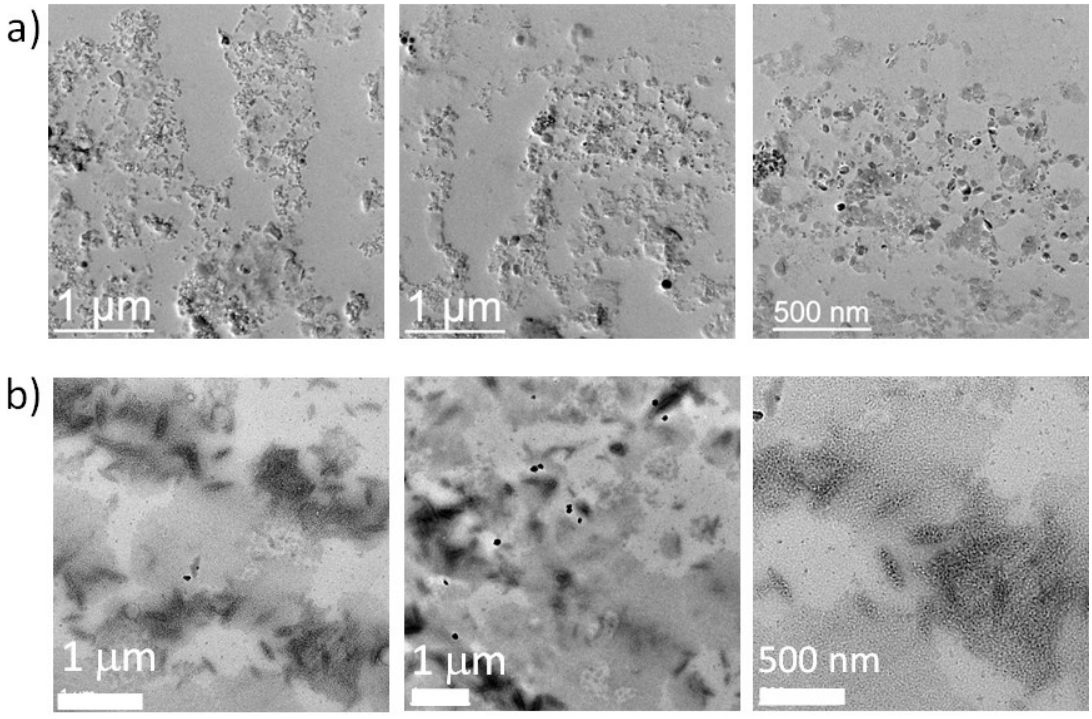



**Figure S29**. TEM images captured from different sections of the copper grid showing disassembly of a) **M1+Chol-D** and b) **M2+Chol-D** in presence of 5% TFA. Solvent = 20% dioxane/MCH; Conc. = 0.4 mM.

**X-Ray structure determinations:**

**Table S1**

| Compound | **M2** |
|---|---|
| Empirical formula | $C_{17}H_9BrN_2O_2$ |
| FW | 353.17 |
| T, K | 299(2) |
| Crystal system | Monoclinic |
| Space group | C2/c |
| a, Å | 20.906(9) |
| b, Å | 11.404(4) |
| c, Å | 14.412(5) |
| α, deg | 90.00° |
| β, deg | 125.210°(11) |
| γ, deg | 90.00° |
| V, $Å^3$ | 2807.3(18) |
| Z, ρ, Mg $m^{-3}$ | 8, 1.671 |
| μ, $mm^{-1}$ | 2.937 |
| F(000) | 1408 |
| Refln. collected | 11648 |
| Ind. Reflen | 2823 |
| Data/restn./param | 2823 / 0 / 199 |
| GOF on $F^2$ | 1.075 |
| Final R indices [I>2σ(I)] | 0.1056, 0.2986 |

**Table S2**

| Compound | **M3** |
|---|---|
| Empirical formula | $C_{18}H_{10}BrNO_2$ |
| FW | 348.92 |
| T, K | 100 |
| Crystal system | Monoclinic |
| Space group | P21/c |
| a, Å | 6.929(11) |
| b, Å | 16.018(9) |
| c, Å | 24.94(3) |
| α, deg | 90.00° |
| β, deg | 94.66(8) |
| γ, deg | 90.00° |
| V, $Å^3$ | 2759(5) |
| Z, ρ, Mg $m^{-3}$ | 8, 1.680 |
| μ, $mm^{-1}$ | 2.985 |
| F(000) | 1394 |
| Refln. collected | 19655 |
| Ind. Reflen | 5159 |
| Data/restn./param | 5159 / 0 / 371 |
| GOF on $F^2$ | 1.037 |
| Final R indices [I>2σ(I)] | 0.1260, 0.3163 |

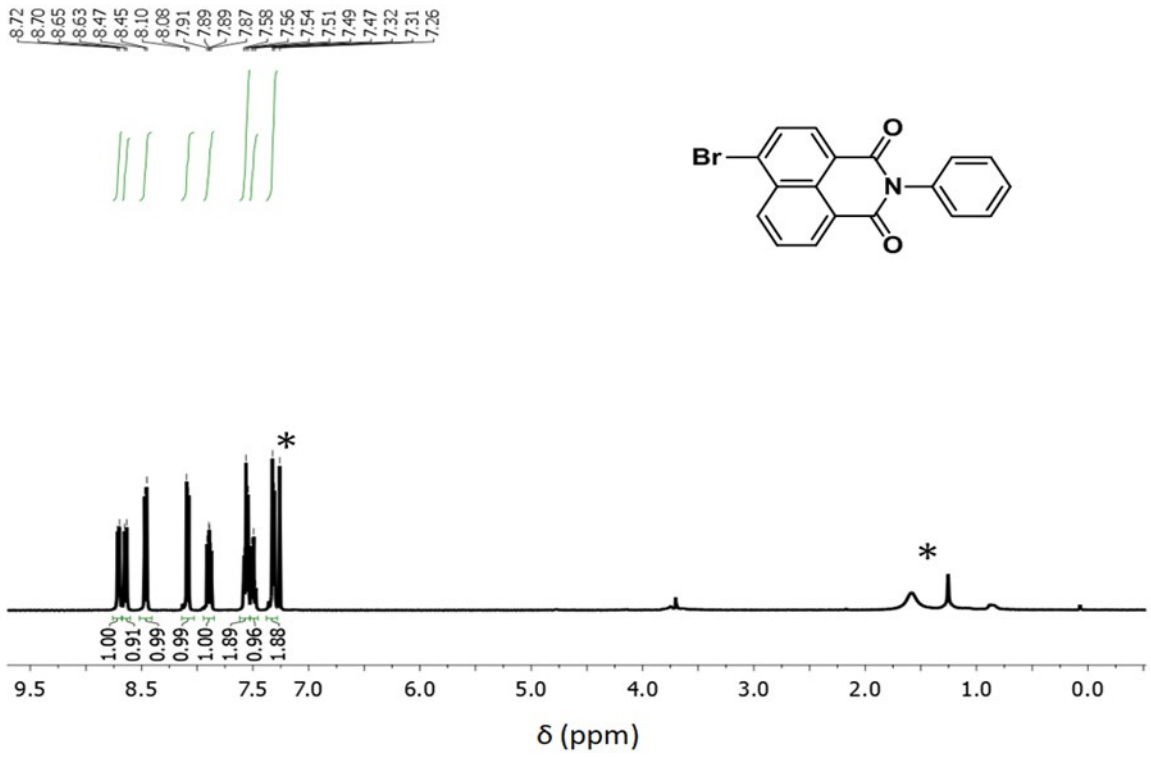
**Table S3**

Emission quantum yield (φ) of **M1**, **M2** and **M3** in dioxane and 20% dioxane/MCH (v/v) recorded against a standard quinine sulphate solution in 0.1M $H_2SO_4$.

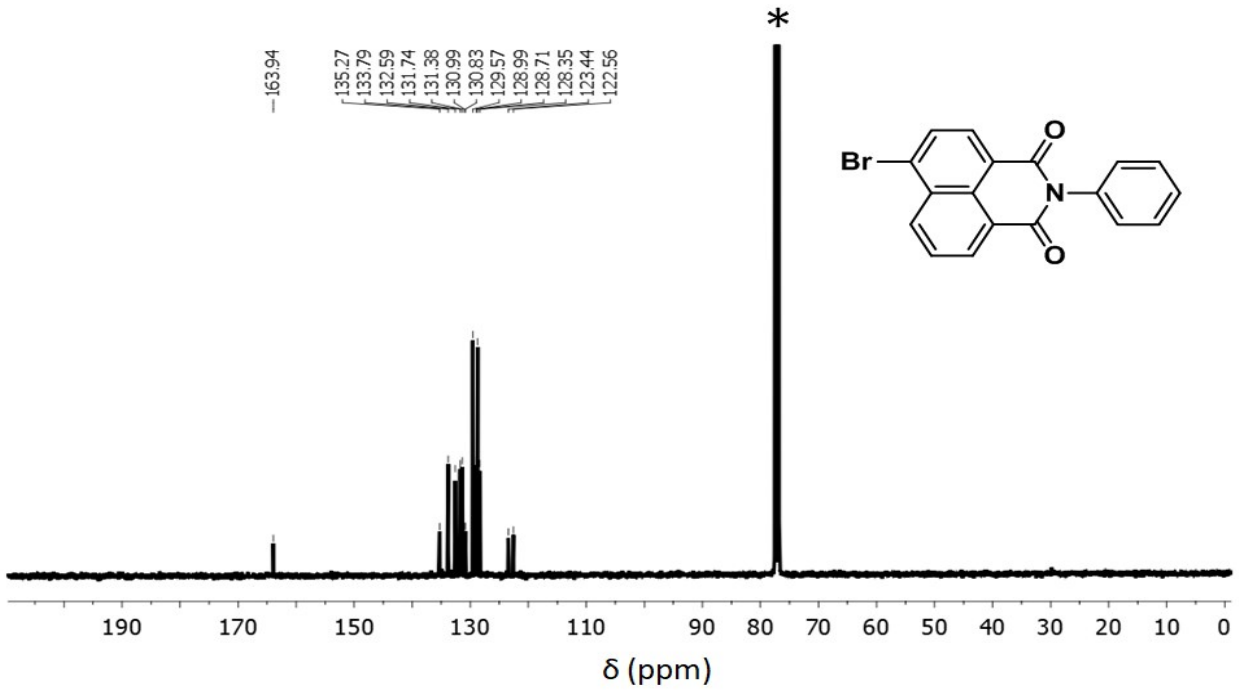
| Solvent | **M1** | **M2** | **M3** |
|---|---|---|---|
| Dioxane | 0.516 | 0.0038 | 0.0011 |
| Dioxane/MCH (1:4) | 0.734 | 0.0014 | 0.0009 |

**NMR and HRMS spectra:**

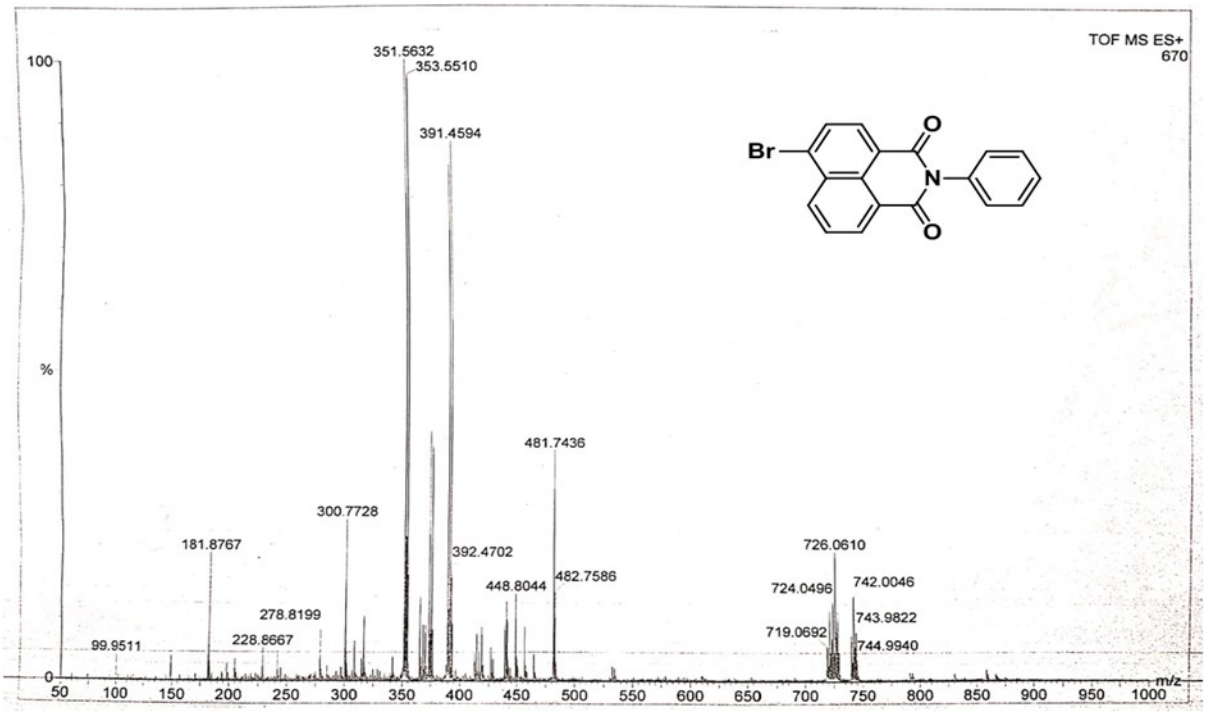
$^1$H NMR spectrum of **M3** in $CDCl_3$



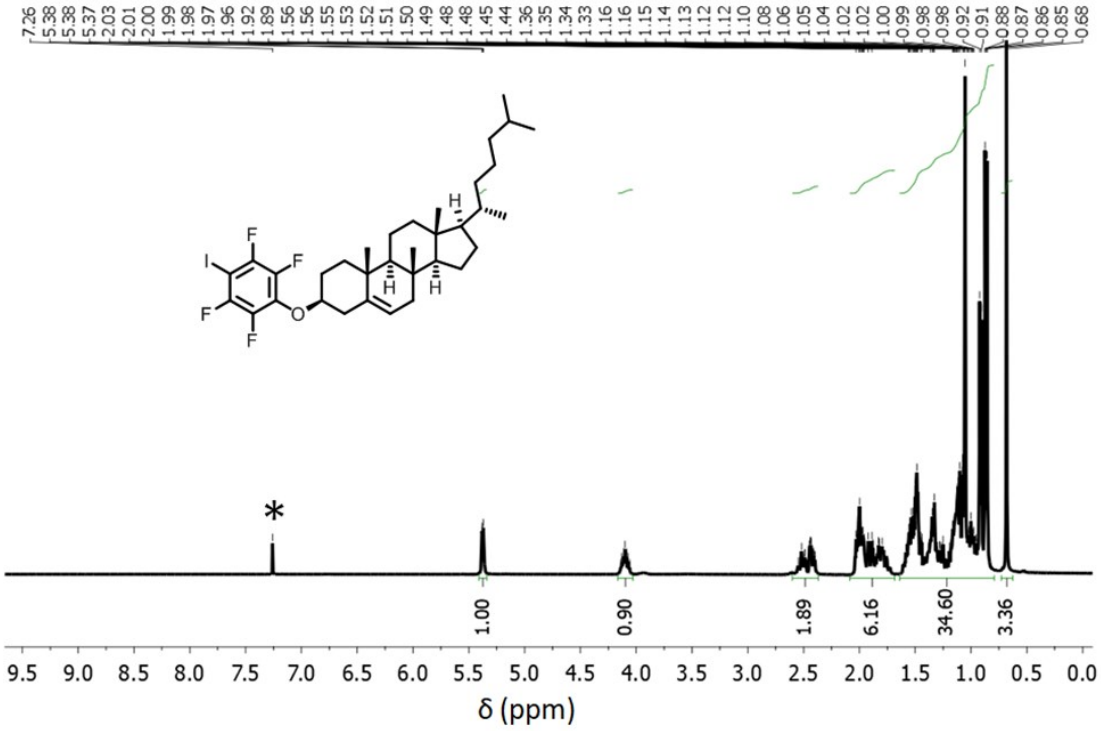
$^{13}C$ NMR spectrum of **M3** in $CDCl_3$



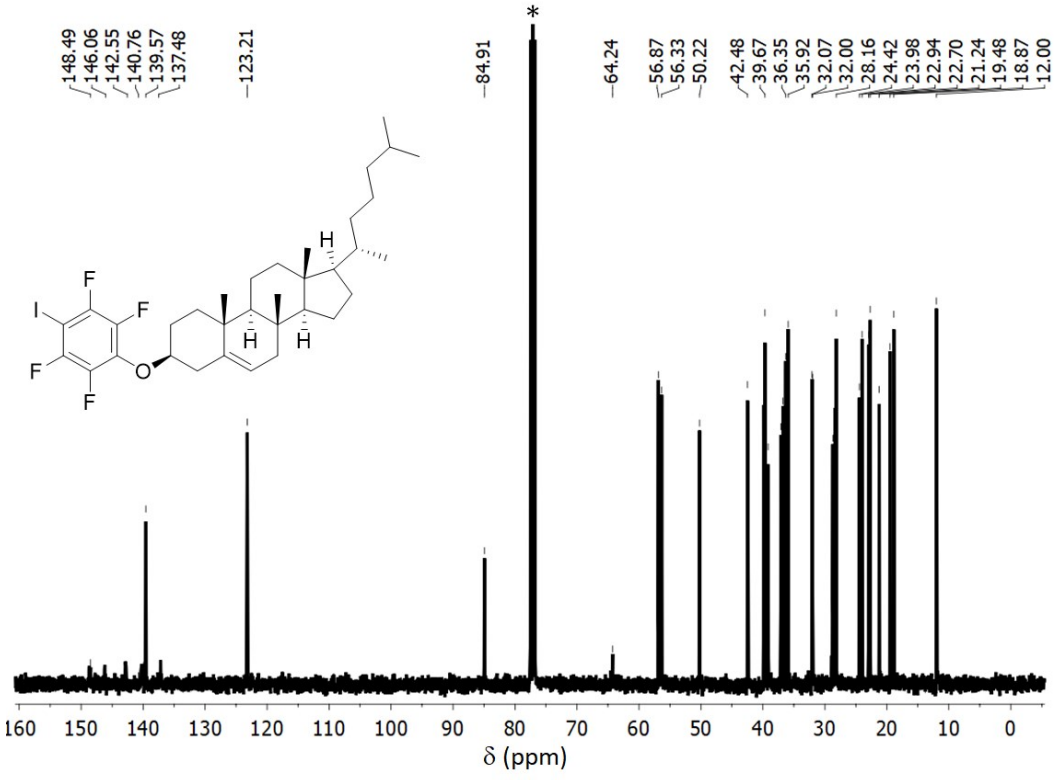

HRMS data of **M3**



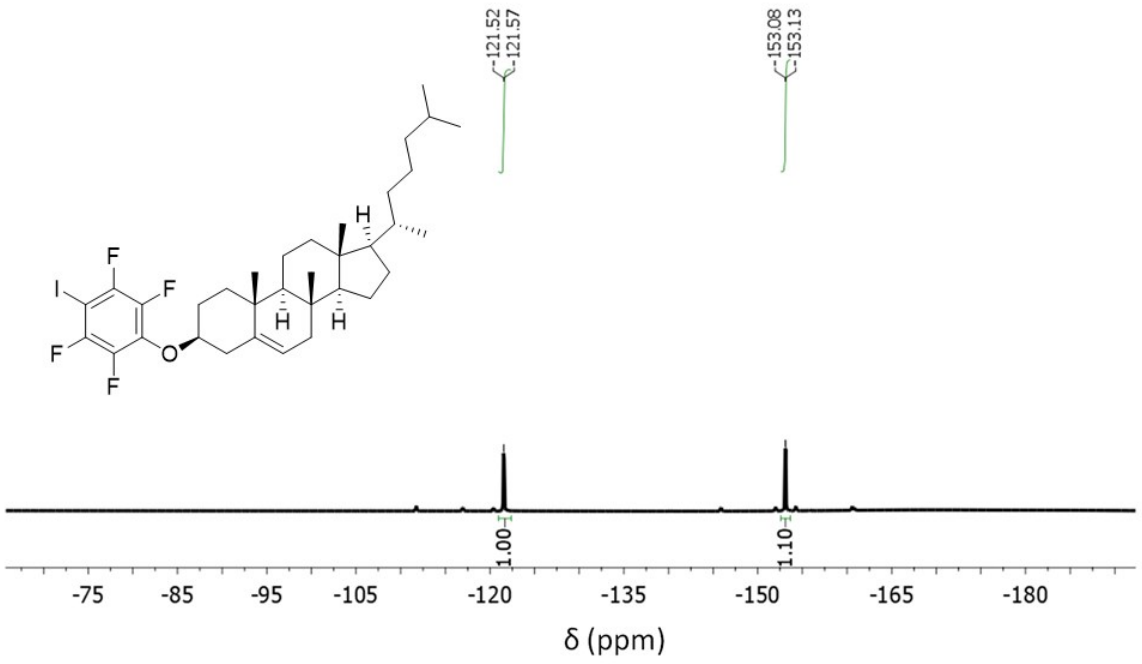
$^{1}$H NMR spectrum of **Chol-D** in $CDCl_3$




$^{13}$C NMR spectrum of **Chol-D** in $CDCl_3$



$^{19}F$ NMR spectrum of **Chol-D** in $CDCl_3$




**Computational studies:**

All DFT calculations were performed within the ORCA 4.2.1 program package.[7] We selected the hybrid B3LYP functional[8] together with the semi-empirical D3BJ dispersion correction,[9] in conjunction to triple-ζ quality def2-TZVP basis set for optimization of monomers and dimers and with the def2-SD effective core potential for bromine.[10] The density-fitting resolution of identity (RI) and chain of sphere (COSX) approximations were utilized to resolve the problem of Hartree-Fock exchange computational time in hybrid DFT together with the auxiliary Coulomb-fitting basis set def2/J.[11] For optimization of the tetramers and higher-ordered aggregates, the semi-empirical SCC-DFTB level of theory was used as implemented in DFTB+ program package.[12] Final single point energy calculations were carried out in methylcyclohexane (MCH) solvent employing the polar continuum model (CPCM)[13] together with the def2-TZVP basis set. Excited state time-dependent DFT (TD-DFT) calculations were conducted with the DFT/SCC-DFTB optimized geometries, together with the long-range corrected hybrid exchange-correlation functional CAM-B3LYP in MCH (CPCM) solvent, with n states =10 and root =1, as implemented

in the Gaussian 09 software.[14] In order to reduce the computational cost associated with the excited state calculations, mixed Pople basis set (6-31++G(d,p) on C, N, O; 6-31G on H, LANL2DZ basis and LANL2 pseudo potential on Br) was employed for all the TDDFT calculations.

## XYZ coordinates

**M2 monomer**

| | | | |
|---|---|---|---|
| Br | -1.288146000 | 2.264736000 | 2.267666000 |
| O | -1.737759000 | -2.036885000 | -4.135013000 |
| O | 0.971921000 | 1.649298000 | -4.212079000 |
| N | -0.336056000 | -0.229497000 | -4.167018000 |
| N | 1.100831000 | -1.330250000 | -7.997003000 |
| C | 0.029824000 | 2.619705000 | -0.212550000 |
| C | 0.373247000 | 2.320314000 | -1.545336000 |
| C | -0.197707000 | 1.236979000 | -2.193144000 |
| C | -1.147520000 | 0.425520000 | -1.521348000 |
| C | -1.533447000 | 0.725761000 | -0.173696000 |
| C | -0.893053000 | 1.835968000 | 0.456800000 |
| C | -2.518180000 | -0.090592000 | 0.444130000 |
| C | -3.081738000 | -1.157501000 | -0.229713000 |
| C | -2.675923000 | -1.469984000 | -1.543697000 |
| C | -1.723635000 | -0.691727000 | -2.181886000 |
| C | -1.297607000 | -1.065482000 | -3.556578000 |
| C | 0.205935000 | 0.942479000 | -3.591076000 |
| C | 1.282076000 | -2.118904000 | -6.935264000 |
| C | 0.827345000 | -1.804181000 | -5.651984000 |
| C | 0.136770000 | -0.604773000 | -5.472776000 |
| C | -0.065580000 | 0.225729000 | -6.573911000 |
| C | 0.441968000 | -0.184557000 | -7.810098000 |
| H | 0.496732000 | 3.464463000 | 0.295034000 |
| H | 1.097128000 | 2.932134000 | -2.086348000 |
| H | -2.831739000 | 0.141638000 | 1.462308000 |
| H | -3.840507000 | -1.770072000 | 0.261662000 |
| H | -3.098306000 | -2.320593000 | -2.081063000 |
| H | 1.823227000 | -3.056781000 | -7.106597000 |
| H | 1.003729000 | -2.479819000 | -4.814383000 |
| H | -0.591776000 | 1.174565000 | -6.469633000 |
| H | 0.303005000 | 0.452307000 | -8.691303000 |

**M2 dimer (parallel stacking)**

| | | | |
|---|---|---|---|
| Br | 5.041650000 | 8.720614000 | 11.187072000 |
| Br | 3.385888000 | 8.644453000 | 6.541317000 |
| O | 5.790637000 | 1.926978000 | 12.053352000 |
| O | 2.152434000 | 1.830399000 | 9.284558000 |
| O | 2.675908000 | 1.848434000 | 5.647543000 |
| O | 6.334047000 | 1.760862000 | 8.388400000 |
| N | 3.881425000 | -2.369669000 | 10.929018000 |
| N | 4.547566000 | -2.442297000 | 6.827712000 |
| N | 3.950759000 | 1.856403000 | 10.696001000 |
| N | 4.515935000 | 1.784733000 | 7.003798000 |
| C | 2.831354000 | -0.239216000 | 11.316425000 |
| C | 2.854733000 | -1.635254000 | 11.363575000 |
| C | 4.936728000 | -1.725977000 | 10.424971000 |
| C | 5.021737000 | -0.334614000 | 10.323383000 |
| C | 3.938411000 | 0.416287000 | 10.776202000 |
| C | 5.973959000 | 6.143334000 | 11.897585000 |
| C | 5.966057000 | 4.735316000 | 11.940818000 |
| C | 4.970371000 | 2.536182000 | 11.403443000 |
| C | 3.513329000 | -1.783112000 | 7.355556000 |
| C | 5.566546000 | -1.723884000 | 6.350496000 |
| C | 3.443548000 | -0.389940000 | 7.438804000 |
| C | 5.603437000 | -0.327350000 | 6.376017000 |
| C | 4.518539000 | 0.343923000 | 6.940072000 |
| C | 4.957688000 | 6.821085000 | 11.248359000 |
| C | 2.802992000 | 6.769467000 | 9.941379000 |
| C | 3.882931000 | 6.133078000 | 10.608712000 |
| C | 1.881877000 | 4.620569000 | 9.301617000 |
| C | 1.826577000 | 6.028976000 | 9.302124000 |
| C | 3.917627000 | 4.700968000 | 10.637273000 |
| C | 4.958751000 | 4.018934000 | 11.316474000 |
| C | 2.908629000 | 3.965518000 | 9.963845000 |
| C | 2.947755000 | 2.481352000 | 9.937217000 |
| C | 3.480207000 | 6.745387000 | 6.472963000 |
| C | 5.631851000 | 6.700607000 | 7.785051000 |
| C | 4.558152000 | 6.060695000 | 7.110797000 |
| C | 2.468942000 | 6.064601000 | 5.819220000 |
| C | 2.485239000 | 4.656791000 | 5.769632000 |
| C | 6.569811000 | 4.554555000 | 8.408887000 |
| C | 6.613705000 | 5.963395000 | 8.419449000 |
| C | 4.533997000 | 4.628428000 | 7.072879000 |
| C | 3.497327000 | 3.943437000 | 6.389578000 |
| C | 5.549476000 | 3.895880000 | 7.740253000 |
| C | 3.492996000 | 2.460762000 | 6.298390000 |
| C | 5.524482000 | 2.410847000 | 7.752822000 |
| H | 6.752778000 | 4.185404000 | 12.460111000 |
| H | 6.780929000 | 6.700379000 | 12.374647000 |
| H | 1.999420000 | -2.181709000 | 11.777701000 |
| H | 1.968754000 | 0.320083000 | 11.680598000 |
| H | 5.762426000 | -2.346608000 | 10.060764000 |
| H | 5.889058000 | 0.148220000 | 9.878153000 |
| H | 2.695509000 | -2.392161000 | 7.755253000 |
| H | 6.404216000 | -2.284150000 | 5.919136000 |
| H | 2.597259000 | 0.112807000 | 7.902774000 |
| H | 6.458599000 | 0.220249000 | 5.978016000 |
| H | 2.758954000 | 7.858509000 | 9.928083000 |
| H | 1.130660000 | 4.019630000 | 8.787572000 |
| H | 1.013445000 | 6.541147000 | 8.784523000 |
| H | 5.666595000 | 7.789923000 | 7.807666000 |
| H | 1.659045000 | 6.618965000 | 5.344053000 |
| H | 1.701636000 | 4.104385000 | 5.248282000 |
| H | 7.324059000 | 3.956769000 | 8.922366000 |
| H | 7.421620000 | 6.478072000 | 8.942692000 |

**M2 dimer (antiparallel stacking)**

| | | | |
|---|---|---|---|
| Br | 0.975200000 | -0.850205000 | 1.178804000 |
| Br | 0.546185000 | -0.977040000 | -6.222527000 |
| O | -2.532618000 | -2.849547000 | -4.400394000 |
| O | 1.358016000 | -5.079265000 | -5.282964000 |
| O | 0.600611000 | 3.114906000 | 0.322835000 |
| O | 4.373420000 | 0.759527000 | -0.785535000 |
| N | -0.613983000 | -4.024465000 | -4.813825000 |
| N | -2.400159000 | -5.725655000 | -8.257322000 |
| N | 4.338473000 | 3.257994000 | 3.393753000 |
| N | 2.509789000 | 1.964714000 | -0.211049000 |
| C | 0.314039000 | -1.549973000 | -0.460160000 |
| C | -0.982124000 | -1.231945000 | -0.821992000 |
| C | -1.529510000 | -1.753956000 | -2.008842000 |
| C | 0.553476000 | -2.911384000 | -2.473965000 |
| C | 1.139609000 | -2.380003000 | -1.278064000 |
| C | 2.488659000 | -2.710002000 | -0.982919000 |
| C | 3.214836000 | -3.538932000 | -1.817135000 |

| | | | |
|---|---|---|---|
| C | 2.630443000 | -4.073684000 | -2.984092000 |
| C | 1.321467000 | -3.762217000 | -3.311873000 |
| C | -0.782206000 | -2.589051000 | -2.822671000 |
| C | -1.405164000 | -3.136883000 | -4.053422000 |
| C | 0.731783000 | -4.348970000 | -4.543694000 |
| C | -1.214251000 | -4.602571000 | -5.985913000 |
| C | -2.288146000 | -5.483690000 | -5.864441000 |
| C | -2.843713000 | -6.015520000 | -7.031899000 |
| C | -1.366637000 | -4.886637000 | -8.358549000 |
| C | -0.734846000 | -4.298313000 | -7.259698000 |
| C | 3.757127000 | 1.492942000 | 1.860627000 |
| C | 4.342320000 | 1.972931000 | 3.033942000 |
| C | 3.750054000 | 4.123173000 | 2.565280000 |
| C | 3.144076000 | 3.759108000 | 1.359240000 |
| C | 3.140969000 | 2.408510000 | 1.002527000 |
| C | 3.237474000 | 1.094858000 | -1.055046000 |
| C | 3.231287000 | -0.220839000 | -3.144254000 |
| C | 2.546176000 | 0.614130000 | -2.276902000 |
| C | 1.207377000 | 0.982174000 | -2.555893000 |
| C | 0.509556000 | 1.836088000 | -1.663726000 |
| C | 1.172192000 | 2.370087000 | -0.444750000 |
| C | -0.804418000 | 2.192487000 | -1.921191000 |
| C | -1.459280000 | 1.701779000 | -3.070582000 |
| C | -0.800913000 | 0.870155000 | -3.956703000 |
| C | 0.550437000 | 0.495582000 | -3.733291000 |
| C | 1.311944000 | -0.339193000 | -4.605279000 |
| C | 2.614686000 | -0.700705000 | -4.314579000 |
| H | -1.580808000 | -0.582925000 | -0.182268000 |
| H | -2.551435000 | -1.513139000 | -2.304594000 |
| H | 2.953022000 | -2.287598000 | -0.091580000 |
| H | 4.247806000 | -3.788248000 | -1.564823000 |
| H | 3.188566000 | -4.734864000 | -3.649381000 |
| H | -2.688149000 | -5.748523000 | -4.884611000 |
| H | -3.689637000 | -6.709720000 | -6.965675000 |
| H | -1.009426000 | -4.661645000 | -9.370669000 |
| H | 0.121048000 | -3.637214000 | -7.392539000 |
| H | 4.837458000 | 1.271976000 | 3.715505000 |
| H | 3.804212000 | 0.434456000 | 1.613649000 |
| H | 3.755105000 | 5.175329000 | 2.873490000 |
| H | 2.675450000 | 4.511443000 | 0.726842000 |
| H | 4.257658000 | -0.497639000 | -2.901311000 |
| H | -1.311130000 | 2.853509000 | -1.216046000 |
| H | -2.495728000 | 1.985635000 | -3.266323000 |
| H | -1.319956000 | 0.480389000 | -4.832883000 |
| H | 3.162903000 | -1.352645000 | -4.995421000 |

**M2 tetramer**

| | | | |
|---|---|---|---|
| Br | 1.905892000 | 8.394653000 | 9.338464000 |
| Br | 6.025348000 | 8.478226000 | 7.919275000 |
| Br | 10.686786000 | 3.017944000 | 2.439647000 |
| Br | 6.567317000 | 2.934398000 | 3.858801000 |
| O | 5.762270000 | 3.467161000 | 12.251075000 |
| O | 6.830445000 | 7.945440000 | -0.473007000 |
| O | 2.829705000 | 0.742738000 | 9.979823000 |
| O | 2.434791000 | 3.240087000 | 5.211210000 |
| O | 5.503129000 | 0.768227000 | 7.592187000 |
| O | 9.762997000 | 10.669859000 | 1.798266000 |
| O | 10.157870000 | 8.172532000 | 6.566880000 |
| O | 7.089551000 | 10.644396000 | 4.185882000 |
| N | 6.375375000 | -1.353382000 | 12.597315000 |
| N | 6.217357000 | 12.765984000 | -0.819263000 |
| N | 10.486195000 | 13.034122000 | 6.740024000 |
| N | 2.106475000 | -1.621503000 | 5.038061000 |
| N | 4.303812000 | 2.071142000 | 11.145919000 |
| N | 3.959919000 | 1.968971000 | 6.377476000 |
| N | 8.288897000 | 9.341457000 | 0.632160000 |
| N | 8.632751000 | 9.443650000 | 5.400603000 |
| C | 5.331517000 | 0.788494000 | 12.997019000 |
| C | 6.016344000 | -0.352685000 | 13.424468000 |
| C | 6.056720000 | -1.231487000 | 11.293715000 |
| C | 5.381336000 | -0.126860000 | 10.765998000 |
| C | 5.008439000 | 0.903595000 | 11.638705000 |
| C | 3.798478000 | 6.961325000 | 10.871270000 |
| C | 4.452167000 | 5.823123000 | 11.376261000 |
| C | 4.766126000 | 3.352681000 | 11.534576000 |
| C | 6.536001000 | 12.644091000 | 0.484340000 |
| C | 6.576392000 | 11.765283000 | -1.646410000 |
| C | 7.261212000 | 10.624103000 | -1.218953000 |
| C | 7.211377000 | 11.539464000 | 1.012066000 |
| C | 7.584278000 | 10.509005000 | 0.139364000 |
| C | 8.140534000 | 5.589476000 | 0.401824000 |
| C | 7.826583000 | 8.059919000 | 0.243501000 |
| C | 9.561301000 | 10.852827000 | 7.212238000 |
| C | 10.173932000 | 12.047480000 | 7.602036000 |
| C | 10.193794000 | 12.843770000 | 5.438405000 |
| C | 9.589564000 | 11.682600000 | 4.946924000 |
| C | 9.264178000 | 10.667745000 | 5.855906000 |
| C | 2.398883000 | -1.431152000 | 6.339679000 |
| C | 2.418731000 | -0.634859000 | 4.176049000 |
| C | 3.003113000 | -0.269982000 | 6.831158000 |
| C | 3.031362000 | 0.559794000 | 4.565845000 |
| C | 3.328492000 | 0.744876000 | 5.922176000 |
| C | 2.725485000 | 6.831366000 | 10.007310000 |
| C | 1.155467000 | 5.339928000 | 8.737406000 |
| C | 2.252649000 | 5.545242000 | 9.615420000 |
| C | 1.416356000 | 2.938510000 | 8.898049000 |
| C | 0.746535000 | 4.067496000 | 8.388434000 |
| C | 2.928932000 | 4.394456000 | 10.133622000 |
| C | 4.035922000 | 4.545801000 | 11.016809000 |
| C | 2.497520000 | 3.088888000 | 9.759405000 |
| C | 3.199356000 | 1.879356000 | 10.282771000 |
| C | 5.260460000 | 6.848518000 | 7.351737000 |
| C | 6.890779000 | 5.494984000 | 8.698056000 |
| C | 5.794062000 | 5.606186000 | 7.802478000 |
| C | 4.179459000 | 6.887155000 | 6.488657000 |
| C | 3.586729000 | 5.696717000 | 6.031279000 |
| C | 6.764224000 | 3.078333000 | 8.626191000 |
| C | 7.362609000 | 4.261002000 | 9.101899000 |
| C | 5.184235000 | 4.401217000 | 7.326336000 |
| C | 4.075090000 | 4.458215000 | 6.434017000 |
| C | 5.686608000 | 3.136101000 | 7.749071000 |
| C | 3.422475000 | 3.207334000 | 5.947340000 |
| C | 5.064335000 | 1.870271000 | 7.257530000 |
| C | 9.867202000 | 4.581232000 | 1.770791000 |
| C | 11.437214000 | 6.072668000 | 3.040705000 |
| C | 10.340039000 | 5.867355000 | 2.162683000 |
| C | 8.794216000 | 4.451274000 | 0.906823000 |
| C | 11.176332000 | 8.474086000 | 2.880056000 |
| C | 11.846146000 | 7.345099000 | 3.389678000 |
| C | 9.663762000 | 7.018141000 | 1.644473000 |
| C | 8.556779000 | 6.866797000 | 0.761277000 |
| C | 10.095174000 | 8.323710000 | 2.018691000 |
| C | 9.393346000 | 9.533242000 | 1.495317000 |
| C | 7.332206000 | 4.564104000 | 4.426341000 |
| C | 5.701896000 | 5.917640000 | 3.080012000 |
| C | 6.798608000 | 5.806437000 | 3.975596000 |
| C | 8.413203000 | 4.525466000 | 5.289427000 |
| C | 9.005932000 | 5.715903000 | 5.746806000 |
| C | 5.828456000 | 8.334291000 | 3.151875000 |
| C | 5.230071000 | 7.151623000 | 2.676166000 |
| C | 7.408436000 | 7.011405000 | 4.451740000 |
| C | 8.517576000 | 6.954406000 | 5.344064000 |
| C | 6.906068000 | 8.276522000 | 4.029000000 |
| C | 9.170191000 | 8.205286000 | 5.830744000 |
| C | 7.528340000 | 9.542351000 | 4.520543000 |
| H | 5.297019000 | 5.929888000 | 12.053118000 |
| H | 4.144774000 | 7.947119000 | 11.168971000 |
| H | 6.280857000 | -0.461730000 | 14.482759000 |
| H | 5.058537000 | 1.566586000 | 13.703536000 |

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| H | 6.357227000 | -2.050093000 | 10.629875000 |
| H | 5.163639000 | -0.067402000 | 9.702568000 |
| H | 6.235490000 | 13.462700000 | 1.148175000 |
| H | 6.311888000 | 11.874327000 | -2.704704000 |
| H | 7.534195000 | 9.846009000 | -1.925465000 |
| H | 7.429063000 | 11.480008000 | 2.075498000 |
| H | 7.295687000 | 5.482712000 | -0.275040000 |
| H | 8.447920000 | 3.465479000 | 0.609120000 |
| H | 9.324738000 | 10.087362000 | 7.945269000 |
| H | 10.417509000 | 12.212568000 | 8.658121000 |
| H | 10.456804000 | 13.651820000 | 4.746526000 |
| H | 9.390386000 | 11.568443000 | 3.884202000 |
| H | 2.135879000 | -2.239203000 | 7.031559000 |
| H | 2.175148000 | -0.799946000 | 3.119965000 |
| H | 3.202297000 | -0.155826000 | 7.893879000 |
| H | 3.267919000 | 1.325261000 | 3.832814000 |
| H | 0.635824000 | 6.210113000 | 8.340403000 |
| H | 1.097908000 | 1.934684000 | 8.625254000 |
| H | -0.094091000 | 3.933430000 | 7.712605000 |
| H | 7.356086000 | 6.406593000 | 9.068313000 |
| H | 3.783488000 | 7.840553000 | 6.150388000 |
| H | 2.736612000 | 5.731443000 | 5.353422000 |
| H | 7.133822000 | 2.104501000 | 8.940204000 |
| H | 8.197371000 | 4.199265000 | 9.795082000 |
| H | 11.956851000 | 5.202482000 | 3.437715000 |
| H | 11.494780000 | 9.477912000 | 3.152852000 |
| H | 12.686767000 | 7.479164000 | 4.065514000 |
| H | 5.236589000 | 5.006032000 | 2.709754000 |
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| H | 9.856046000 | 5.681177000 | 6.424668000 |
| H | 5.458862000 | 9.308124000 | 2.837859000 |
| H | 4.395313000 | 7.213361000 | 1.982978000 |

**M2 oligomer**

| | | | |
|---|---|---|---|
| Br | 3.963087000 | -2.064134000 | 10.294580000 |
| Br | 4.439672000 | -3.507898000 | 6.366789000 |
| Br | 9.576250000 | -11.643576000 | 3.713992000 |
| Br | 8.137503000 | -11.790628000 | 7.549348000 |
| Br | 5.174429000 | 11.673555000 | 8.579087000 |
| Br | 5.170399000 | 10.250982000 | 4.527575000 |
| Br | 10.085479000 | 2.024211000 | 1.922772000 |
| Br | 8.289647000 | 1.640466000 | 5.412206000 |
| O | -0.259516000 | -8.151783000 | 8.074915000 |
| O | 3.672851000 | -8.964702000 | 10.322846000 |
| O | 2.843386000 | -11.050638000 | 6.142303000 |
| O | 6.312799000 | -9.713472000 | 8.812641000 |
| O | 8.731490000 | -4.991283000 | 2.167448000 |
| O | 12.547687000 | -4.570402000 | 4.703747000 |
| O | 9.814738000 | -5.213863000 | 6.337275000 |
| O | 5.792883000 | -5.338696000 | 4.120874000 |
| O | 5.787743000 | 5.295412000 | 11.144338000 |
| O | 7.136453000 | 7.426411000 | -1.198487000 |
| O | 2.896361000 | 4.375775000 | 7.699889000 |
| O | 3.418953000 | 3.608154000 | 3.845829000 |
| O | 6.354597000 | 3.170299000 | 7.357786000 |
| O | 10.074877000 | 9.766430000 | 1.451180000 |
| O | 10.462439000 | 8.101856000 | 6.565468000 |
| O | 7.444495000 | 8.979213000 | 3.207182000 |
| N | 1.650474000 | -8.609449000 | 9.283581000 |
| N | 0.949800000 | -12.812500000 | 9.304396000 |
| N | 4.433931000 | -10.386790000 | 7.672215000 |
| N | 4.899289000 | -14.321683000 | 9.209884000 |
| N | 10.500699000 | -0.546763000 | 2.837207000 |
| N | 7.724311000 | -1.000839000 | 5.280484000 |
| N | 10.621174000 | -4.732752000 | 3.455619000 |
| N | 7.769216000 | -5.224577000 | 5.297168000 |
| N | 4.280169000 | 0.671445000 | 10.379563000 |
| N | 6.835087000 | 12.280064000 | -1.176020000 |
| N | 8.940507000 | 12.734737000 | 5.823837000 |
| N | 4.309264000 | -0.841554000 | 5.730961000 |
| N | 4.247920000 | 4.811382000 | 9.505504000 |
| N | 4.846339000 | 3.356658000 | 5.631670000 |
| N | 8.564389000 | 8.628146000 | 0.146218000 |
| N | 8.944307000 | 8.581048000 | 4.906289000 |
| C | 4.411744000 | -4.825509000 | 10.791321000 |
| C | 4.164352000 | -6.205964000 | 10.715979000 |
| C | 3.066316000 | -6.691702000 | 10.012745000 |
| C | 2.208553000 | -5.777455000 | 9.341630000 |
| C | 2.476427000 | -4.372868000 | 9.385325000 |
| C | 3.592976000 | -3.915522000 | 10.146906000 |
| C | 1.622548000 | -3.510055000 | 8.648487000 |
| C | 0.559141000 | -4.006667000 | 7.918605000 |
| C | 0.282851000 | -5.386827000 | 7.907082000 |
| C | 1.091147000 | -6.272022000 | 8.610738000 |
| C | 0.762119000 | -7.725540000 | 8.614508000 |
| C | 2.837048000 | -8.153132000 | 9.909851000 |
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| C | 1.664696000 | -10.798296000 | 10.430333000 |
| C | 1.377525000 | -10.029313000 | 9.292225000 |
| C | 0.841992000 | -10.678989000 | 8.172790000 |
| C | 0.652487000 | -12.062726000 | 8.226234000 |
| C | 5.685405000 | -5.630992000 | 7.777058000 |
| C | 5.899486000 | -6.958516000 | 8.185981000 |
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| C | 3.992820000 | -7.665569000 | 6.863652000 |
| C | 3.756236000 | -6.312278000 | 6.466573000 |
| C | 4.640025000 | -5.296404000 | 6.932593000 |
| C | 2.654820000 | -6.045971000 | 5.613344000 |
| C | 1.835343000 | -7.062349000 | 5.161676000 |
| C | 2.096478000 | -8.397532000 | 5.519648000 |
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| C | 3.448874000 | -10.127033000 | 6.692158000 |
| C | 5.321023000 | -9.389925000 | 8.147421000 |
| C | 4.900178000 | -13.242635000 | 10.018190000 |
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| C | 4.591154000 | -11.729693000 | 8.176188000 |
| C | 4.590720000 | -12.841624000 | 7.323475000 |
| C | 4.741039000 | -14.111688000 | 7.889368000 |
| C | 10.748794000 | -1.049897000 | 4.061328000 |
| C | 10.303245000 | -1.399388000 | 1.816898000 |
| C | 10.346480000 | -2.784061000 | 1.971799000 |
| C | 10.804546000 | -2.422396000 | 4.313987000 |
| C | 10.595470000 | -3.309974000 | 3.248096000 |
| C | 8.696588000 | -7.794212000 | 2.446782000 |
| C | 9.623727000 | -5.520562000 | 2.837881000 |
| C | 8.077095000 | -3.072270000 | 6.434990000 |
| C | 8.042542000 | -1.680417000 | 6.395101000 |
| C | 7.425403000 | -1.682907000 | 4.161199000 |
| C | 7.423555000 | -3.078158000 | 4.107152000 |
| C | 7.761421000 | -3.787667000 | 5.268331000 |
| C | 9.635991000 | -9.774333000 | 3.474340000 |
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| C | 8.693675000 | -9.183850000 | 2.651496000 |
| C | 12.544356000 | -7.329733000 | 5.388205000 |
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| C | 10.636160000 | -7.579624000 | 3.900319000 |
| C | 9.657231000 | -6.990045000 | 3.051506000 |
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| C | 11.645852000 | -5.287038000 | 4.278547000 |
| C | 8.398844000 | -10.034349000 | 6.944054000 |
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| C | 9.420216000 | -9.282939000 | 7.498659000 |
| C | 9.572002000 | -7.927667000 | 7.170478000 |
| C | 5.702590000 | -8.177329000 | 4.225317000 |
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| C | 8.677077000 | -7.304079000 | 6.305129000 |

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| C | 6.697892000 | -7.423918000 | 4.839086000 |
| C | 8.814916000 | -5.863149000 | 6.008414000 |
| C | 6.702324000 | -5.942306000 | 4.691240000 |
| C | 3.068755000 | 2.691573000 | 9.907714000 |
| C | 3.121980000 | 1.324475000 | 10.177941000 |
| C | 5.432805000 | 1.364647000 | 10.332856000 |
| C | 5.477565000 | 2.735626000 | 10.072171000 |
| C | 4.271578000 | 3.410514000 | 9.838201000 |
| C | 5.904104000 | 9.403319000 | 10.088730000 |
| C | 5.888940000 | 8.051053000 | 10.470550000 |
| C | 5.077928000 | 5.708883000 | 10.228247000 |
| C | 7.034924000 | 12.033885000 | 0.134080000 |
| C | 7.202731000 | 11.325925000 | -2.053204000 |
| C | 7.781355000 | 10.112426000 | -1.671379000 |
| C | 7.597985000 | 10.850248000 | 0.616196000 |
| C | 7.982499000 | 9.870422000 | -0.307148000 |
| C | 8.156956000 | 4.926044000 | -0.341009000 |
| C | 8.054714000 | 7.414878000 | -0.375478000 |
| C | 8.874293000 | 10.430592000 | 6.544022000 |
| C | 8.852959000 | 11.804787000 | 6.794665000 |
| C | 9.081702000 | 12.301524000 | 4.555897000 |
| C | 9.120644000 | 10.949126000 | 4.202761000 |
| C | 8.999512000 | 9.992628000 | 5.216831000 |
| C | 4.272195000 | -0.111421000 | 6.859422000 |
| C | 4.498397000 | -0.210398000 | 4.558096000 |
| C | 4.425168000 | 1.273123000 | 6.861409000 |
| C | 4.670867000 | 1.173186000 | 4.464457000 |
| C | 4.641062000 | 1.931659000 | 5.644241000 |
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| C | 3.715620000 | 6.436432000 | 3.787897000 |
| C | 6.839537000 | 5.941834000 | 7.484990000 |
| C | 7.079267000 | 7.328951000 | 7.474334000 |
| C | 5.258036000 | 6.203919000 | 5.647051000 |
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| C | 5.730690000 | 3.906555000 | 6.582913000 |
| C | 9.573115000 | 3.696871000 | 1.202787000 |
| C | 11.060052000 | 4.983645000 | 2.753280000 |
| C | 10.100028000 | 4.920475000 | 1.710104000 |
| C | 8.632078000 | 3.716011000 | 0.187680000 |
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| C | 11.531114000 | 6.196290000 | 3.220869000 |
| C | 9.622415000 | 6.151291000 | 1.158026000 |
| C | 8.631870000 | 6.143716000 | 0.135698000 |
| C | 10.113086000 | 7.393514000 | 1.654110000 |
| C | 9.602528000 | 8.680232000 | 1.101445000 |
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| C | 9.667597000 | 3.937857000 | 6.344240000 |
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| C | 6.928770000 | 6.250836000 | 2.761811000 |
| C | 6.634704000 | 4.880398000 | 2.645514000 |
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| C | 9.386913000 | 6.224182000 | 5.571999000 |
| C | 7.832490000 | 6.696727000 | 3.722573000 |
| C | 9.661083000 | 7.672902000 | 5.733697000 |
| C | 8.064355000 | 8.151642000 | 3.894351000 |
| H | 5.267453000 | -4.473836000 | 11.361509000 |
| H | 4.826378000 | -6.914398000 | 11.208515000 |
| H | 1.825024000 | -2.440884000 | 8.660885000 |
| H | -0.075031000 | -3.327313000 | 7.354063000 |
| H | -0.563240000 | -5.780551000 | 7.348609000 |
| H | 1.676721000 | -12.790501000 | 11.261720000 |
| H | 2.059672000 | -10.338438000 | 11.330172000 |
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| H | 0.253371000 | -12.584805000 | 7.350303000 |
| H | 6.357825000 | -4.855760000 | 8.137866000 |
| H | 6.721894000 | -7.203479000 | 8.854447000 |
| H | 2.468317000 | -5.015782000 | 5.318091000 |
| H | 0.990890000 | -6.834879000 | 4.516019000 |
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| H | 5.024060000 | -13.426294000 | 11.091823000 |
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| H | 4.740319000 | -14.995558000 | 7.240861000 |
| H | 10.900574000 | -0.329080000 | 4.868911000 |
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| H | 10.190542000 | -3.435438000 | 1.118928000 |
| H | 10.989730000 | -2.795745000 | 5.315546000 |
| H | 7.948285000 | -7.327930000 | 1.810397000 |
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| H | 11.595109000 | -10.601499000 | 5.205723000 |
| H | 13.277608000 | -6.687525000 | 5.869727000 |
| H | 13.262930000 | -9.149696000 | 6.309880000 |
| H | 6.400498000 | -11.255653000 | 5.516458000 |
| H | 10.095518000 | -9.730898000 | 8.221457000 |
| H | 10.371765000 | -7.337491000 | 7.611365000 |
| H | 4.982070000 | -7.673083000 | 3.585894000 |
| H | 4.845628000 | -10.144067000 | 3.949524000 |
| H | 6.559827000 | 7.690512000 | 11.246493000 |
| H | 6.601406000 | 10.081760000 | 10.571349000 |
| H | 2.206322000 | 0.729157000 | 10.226381000 |
| H | 2.116232000 | 3.182227000 | 9.736819000 |
| H | 6.354007000 | 0.798992000 | 10.494740000 |
| H | 6.427549000 | 3.254597000 | 10.015457000 |
| H | 6.726407000 | 12.814319000 | 0.839594000 |
| H | 7.033970000 | 11.535394000 | -3.115941000 |
| H | 8.065081000 | 9.375158000 | -2.415790000 |
| H | 7.719402000 | 10.682202000 | 1.681669000 |
| H | 7.397980000 | 4.928783000 | -1.120030000 |
| H | 8.234066000 | 2.780987000 | -0.197986000 |
| H | 8.800952000 | 9.720146000 | 7.362499000 |
| H | 8.753378000 | 12.165734000 | 7.825078000 |
| H | 9.167233000 | 13.066060000 | 3.775943000 |
| H | 9.260680000 | 10.648125000 | 3.167688000 |
| H | 4.114230000 | -0.655706000 | 7.795392000 |
| H | 4.523304000 | -0.835552000 | 3.660820000 |
| H | 4.376622000 | 1.832396000 | 7.787719000 |
| H | 4.834762000 | 1.644628000 | 3.500845000 |
| H | 3.161728000 | 10.458762000 | 7.205411000 |
| H | 1.850033000 | 6.395904000 | 6.612088000 |
| H | 1.697899000 | 8.830243000 | 6.057245000 |
| H | 6.600074000 | 9.217244000 | 6.568565000 |
| H | 3.456098000 | 8.427133000 | 3.009645000 |
| H | 3.036304000 | 5.981361000 | 3.071006000 |
| H | 7.363030000 | 5.291321000 | 8.181882000 |
| H | 7.789077000 | 7.759214000 | 8.176286000 |
| H | 11.417968000 | 4.052702000 | 3.188376000 |
| H | 11.427604000 | 8.361122000 | 3.037723000 |
| H | 12.263527000 | 6.222063000 | 4.023746000 |
| H | 6.987730000 | 2.905504000 | 3.408941000 |
| H | 10.129708000 | 3.246335000 | 7.043431000 |

| | | | |
|---|---|---|---|
| H | 10.692109000 | 5.661258000 | 7.171230000 |
| H | 6.448279000 | 6.980095000 | 2.113399000 |
| H | 5.931270000 | 4.544254000 | 1.888521000 |

**M3 monomer**

| | | | |
|---|---|---|---|
| Br | -1.140630000 | 2.057494000 | 2.325734000 |
| O | -2.035761000 | -1.664521000 | -4.363627000 |
| O | 1.071149000 | 1.628642000 | -4.161795000 |
| N | -0.356196000 | -0.142048000 | -4.198736000 |
| C | 1.086846000 | -1.400253000 | -7.954576000 |
| C | 0.182836000 | 2.463006000 | -0.121642000 |
| C | 0.504366000 | 2.216361000 | -1.471724000 |
| C | -0.144399000 | 1.223588000 | -2.170225000 |
| C | -1.152867000 | 0.448303000 | -1.542405000 |
| C | -1.500954000 | 0.683851000 | -0.183737000 |
| C | -0.783220000 | 1.709623000 | 0.507900000 |
| C | -2.530837000 | -0.109664000 | 0.394125000 |
| C | -3.167531000 | -1.087394000 | -0.334334000 |
| C | -2.810991000 | -1.323295000 | -1.679146000 |
| C | -1.824709000 | -0.566898000 | -2.273081000 |
| C | -1.453328000 | -0.852522000 | -3.687529000 |
| C | 0.253450000 | 0.958409000 | -3.580165000 |
| C | 1.627223000 | -1.930573000 | -6.783073000 |
| C | 1.152319000 | -1.499697000 | -5.546005000 |
| C | 0.139654000 | -0.545096000 | -5.487395000 |
| C | -0.400259000 | -0.006741000 | -6.650750000 |
| C | 0.076951000 | -0.437106000 | -7.887436000 |
| H | 1.461654000 | -1.748232000 | -8.921584000 |
| H | 0.711709000 | 3.241910000 | 0.429052000 |
| H | 1.273825000 | 2.800262000 | -1.980668000 |
| H | -2.823388000 | 0.072704000 | 1.429854000 |
| H | -3.950097000 | -1.689345000 | 0.131772000 |
| H | -3.305378000 | -2.095727000 | -2.271388000 |
| H | 2.418214000 | -2.682337000 | -6.833309000 |
| H | 1.560777000 | -1.907364000 | -4.618356000 |
| H | -1.193874000 | 0.738861000 | -6.573988000 |
| H | -0.350640000 | -0.015957000 | -8.800932000 |

**M3 dimer**

| | | | |
|---|---|---|---|
| Br | 1.051764000 | 9.516010000 | 0.194828000 |
| Br | 4.663986000 | 11.317308000 | 1.665945000 |
| O | -1.030955000 | 7.982525000 | 7.477550000 |
| O | 2.311155000 | 5.946471000 | 6.711310000 |
| O | 0.541624000 | 12.167794000 | 6.537729000 |
| O | 3.368365000 | 10.098769000 | 8.307790000 |
| N | 2.855086000 | 8.010891000 | 7.531700000 |
| N | -0.268592000 | 10.083783000 | 7.019166000 |
| C | 3.542423000 | 9.790561000 | 5.971668000 |
| C | 0.146675000 | 9.315380000 | 4.309333000 |
| C | -1.351161000 | 11.211005000 | 10.954569000 |
| C | -0.005064000 | 11.031641000 | 10.627833000 |
| C | -2.333627000 | 11.041511000 | 9.974128000 |
| C | 0.368974000 | 10.671509000 | 9.330374000 |
| C | -1.967752000 | 10.686053000 | 8.675036000 |
| C | -0.619183000 | 10.493858000 | 8.362914000 |
| C | 1.253822000 | 6.859080000 | 10.712221000 |
| C | 2.371553000 | 6.738207000 | 11.540468000 |
| C | 0.785014000 | 9.928920000 | 2.034244000 |
| C | 3.646398000 | 7.015448000 | 11.036726000 |
| C | 1.399000000 | 7.266202000 | 9.383489000 |
| C | 0.001037000 | 7.594374000 | 2.573576000 |
| C | 1.070451000 | 11.213365000 | 2.456277000 |
| C | 3.330228000 | 7.053011000 | 2.761195000 |
| C | 0.906372000 | 11.563669000 | 3.810758000 |
| C | 4.204143000 | 10.661944000 | 3.393120000 |
| C | 0.312774000 | 8.930046000 | 2.938849000 |
| C | -0.442733000 | 6.684105000 | 3.514078000 |
| C | 3.734570000 | 8.349403000 | 2.510769000 |
| C | 0.268207000 | 11.052220000 | 6.146735000 |
| C | 3.799499000 | 7.420150000 | 9.710398000 |
| C | -0.575401000 | 8.760559000 | 6.660216000 |
| C | 4.255315000 | 11.543114000 | 4.457798000 |
| C | 3.807450000 | 9.301642000 | 3.561716000 |
| C | 2.976775000 | 6.647304000 | 4.065141000 |
| C | 2.673517000 | 7.551778000 | 8.893089000 |
| C | 2.694347000 | 7.075662000 | 6.487498000 |
| C | -0.608612000 | 7.066818000 | 4.860189000 |
| C | 3.041904000 | 7.544867000 | 5.116726000 |
| C | 3.256566000 | 9.346910000 | 7.357523000 |
| C | 3.928898000 | 11.102115000 | 5.754096000 |
| C | 3.462516000 | 8.881566000 | 4.887819000 |
| C | 0.453166000 | 10.634517000 | 4.730515000 |
| C | -0.327826000 | 8.365709000 | 5.250597000 |
| H | -1.638305000 | 11.490998000 | 11.971473000 |
| H | 0.767867000 | 11.170011000 | 11.387064000 |
| H | -3.387651000 | 11.187431000 | 10.223558000 |
| H | 1.419446000 | 10.531237000 | 9.078540000 |
| H | -2.725749000 | 10.543833000 | 7.901959000 |
| H | 0.256448000 | 6.636820000 | 11.099432000 |
| H | 2.250735000 | 6.416740000 | 12.578180000 |
| H | 4.525549000 | 6.911913000 | 11.676971000 |
| H | 0.523730000 | 7.364779000 | 8.744387000 |
| H | 0.122822000 | 7.291574000 | 1.533271000 |
| H | 1.435556000 | 11.951592000 | 1.742540000 |
| H | 3.275761000 | 6.335705000 | 1.940005000 |
| H | 1.134522000 | 12.572111000 | 4.158629000 |
| H | -0.676888000 | 5.661573000 | 3.209761000 |
| H | 3.999058000 | 8.658518000 | 1.499805000 |
| H | 4.788842000 | 7.646649000 | 9.308561000 |
| H | 4.560124000 | 12.576948000 | 4.292044000 |
| H | 2.648957000 | 5.628495000 | 4.277031000 |
| H | -0.962073000 | 6.362123000 | 5.613769000 |
| H | 3.974648000 | 11.781665000 | 6.605935000 |

**M3 tetramer (parallel stacking)**

| | | | |
|---|---|---|---|
| Br | 3.177503000 | 5.238390000 | 2.914429000 |
| Br | -0.165426000 | 6.120073000 | 0.745197000 |
| Br | 6.648932000 | 7.231916000 | 1.979564000 |
| Br | 10.170510000 | 9.303255000 | 1.868284000 |
| O | 3.723752000 | 11.328320000 | 6.083818000 |
| O | 0.488497000 | 12.110212000 | 4.093667000 |
| O | 2.924059000 | 8.722934000 | 9.798637000 |
| O | 0.446295000 | 9.324457000 | 7.750197000 |
| O | 7.012702000 | 11.580674000 | 7.309571000 |
| O | 6.104102000 | 7.724023000 | 9.665551000 |
| O | 10.286063000 | 11.189663000 | 8.487489000 |
| O | 9.426385000 | 6.709328000 | 9.117595000 |
| N | 0.389261000 | 10.757821000 | 5.955408000 |
| N | 3.259728000 | 10.080558000 | 7.966043000 |
| N | 6.541727000 | 9.686538000 | 8.538307000 |
| N | 9.845386000 | 8.957738000 | 8.852345000 |
| C | 3.381289000 | 9.010350000 | 5.721262000 |
| C | 0.125412000 | 8.302480000 | 5.627652000 |
| C | 0.347380000 | 9.774292000 | 3.669252000 |
| C | 0.155203000 | 8.473773000 | 4.214925000 |
| C | 3.180619000 | 7.725384000 | 6.298495000 |
| C | 3.479305000 | 9.130963000 | 4.339790000 |
| C | 3.476289000 | 10.226353000 | 6.582819000 |
| C | 3.029517000 | 7.606470000 | 7.708077000 |
| C | -0.053940000 | 7.035208000 | 6.168590000 |
| C | 3.042377000 | 8.818643000 | 8.577817000 |
| C | 3.222466000 | 11.261754000 | 8.812472000 |
| C | 2.852417000 | 6.353669000 | 8.280048000 |
| C | 3.123655000 | 6.560422000 | 5.470945000 |

| | | | |
|---|---|---|---|
| C | 3.398002000 | 7.995666000 | 3.512723000 |
| C | 0.320117000 | 9.473512000 | 6.529500000 |
| C | 4.188044000 | 12.269965000 | 8.677914000 |
| C | 0.425889000 | 10.971713000 | 4.556807000 |
| C | 2.942924000 | 5.300950000 | 6.100106000 |
| C | -0.214674000 | 5.918428000 | 5.326497000 |
| C | 0.002157000 | 7.340136000 | 3.354913000 |
| C | 3.239910000 | 6.735984000 | 4.062716000 |
| C | 0.410452000 | 9.931042000 | 2.289785000 |
| C | 2.816500000 | 5.200771000 | 7.471852000 |
| C | 0.274139000 | 8.823993000 | 1.434036000 |
| C | -0.189747000 | 6.065942000 | 3.952538000 |
| C | 2.217430000 | 11.372275000 | 9.784403000 |
| C | 4.156927000 | 13.368631000 | 9.536161000 |
| C | 0.060590000 | 7.557564000 | 1.947751000 |
| C | 3.174959000 | 13.470015000 | 10.521695000 |
| C | 2.203019000 | 12.475090000 | 10.636642000 |
| C | 0.411704000 | 11.910102000 | 6.840497000 |
| C | 1.325560000 | 12.950840000 | 6.628258000 |
| C | -0.501635000 | 11.976215000 | 7.902811000 |
| C | 1.328052000 | 14.046587000 | 7.490646000 |
| C | -0.489766000 | 13.080011000 | 8.754154000 |
| C | 0.424677000 | 14.114943000 | 8.551462000 |
| C | 6.659459000 | 8.151324000 | 3.629592000 |
| C | 6.507546000 | 7.435326000 | 4.851393000 |
| C | 6.344316000 | 6.027564000 | 4.931424000 |
| C | 6.184703000 | 5.395580000 | 6.149904000 |
| C | 6.172577000 | 6.139223000 | 7.345256000 |
| C | 6.336600000 | 7.518562000 | 7.315146000 |
| C | 6.518642000 | 8.183458000 | 6.070420000 |
| C | 6.811247000 | 9.526449000 | 3.625189000 |
| C | 6.847193000 | 10.246680000 | 4.832586000 |
| C | 6.711768000 | 9.592716000 | 6.051220000 |
| C | 6.776734000 | 10.371889000 | 7.321376000 |
| C | 5.547931000 | 10.201468000 | 10.748313000 |
| C | 5.549333000 | 10.929859000 | 11.936807000 |
| C | 6.529298000 | 11.893372000 | 12.176275000 |
| C | 7.512708000 | 12.131979000 | 11.216462000 |
| C | 7.523446000 | 11.415991000 | 10.020114000 |
| C | 6.538655000 | 10.445040000 | 9.785013000 |
| C | 6.306992000 | 8.291876000 | 8.591419000 |
| C | 10.102620000 | 9.490420000 | 3.746465000 |
| C | 9.909850000 | 8.350929000 | 4.579626000 |
| C | 9.746476000 | 7.028563000 | 4.089437000 |
| C | 9.537219000 | 5.969942000 | 4.952253000 |
| C | 9.487370000 | 6.179349000 | 6.344060000 |
| C | 9.658158000 | 7.453389000 | 6.870934000 |
| C | 9.873043000 | 8.555601000 | 5.995437000 |
| C | 10.236641000 | 10.755230000 | 4.290029000 |
| C | 10.217451000 | 10.940796000 | 5.682996000 |
| C | 10.050947000 | 9.858255000 | 6.538282000 |
| C | 10.079097000 | 10.071693000 | 8.011264000 |
| C | 10.825474000 | 9.959687000 | 10.886902000 |
| C | 10.772564000 | 10.220030000 | 12.256018000 |
| C | 9.739298000 | 9.697202000 | 13.034159000 |
| C | 8.762513000 | 8.896252000 | 12.441543000 |
| C | 8.800995000 | 8.628019000 | 11.074161000 |
| C | 9.827915000 | 9.174770000 | 10.290734000 |
| C | 9.622214000 | 7.653928000 | 8.352164000 |
| H | 3.623189000 | 10.118717000 | 3.908248000 |
| H | -0.059036000 | 6.922544000 | 7.250103000 |
| H | 2.743050000 | 6.283133000 | 9.359211000 |
| H | 3.461924000 | 8.118659000 | 2.435576000 |
| H | 4.967767000 | 12.197645000 | 7.926935000 |
| H | 2.903019000 | 4.409209000 | 5.477608000 |
| H | -0.356014000 | 4.932786000 | 5.762999000 |
| H | 0.556961000 | 10.928074000 | 1.881304000 |
| H | 2.680929000 | 4.225008000 | 7.932184000 |
| H | 0.323126000 | 8.975759000 | 0.359594000 |
| H | -0.318101000 | 5.200827000 | 3.305380000 |
| H | 1.450284000 | 10.609165000 | 9.862390000 |
| H | 4.915190000 | 14.141949000 | 9.440186000 |
| H | 3.161624000 | 14.325583000 | 11.193568000 |
| H | 1.424448000 | 12.559440000 | 11.391941000 |
| H | 2.039688000 | 12.894350000 | 5.814211000 |
| H | -1.211447000 | 11.169737000 | 8.062929000 |
| H | 2.048177000 | 14.846780000 | 7.338175000 |
| H | -1.194362000 | 13.128680000 | 9.581397000 |
| H | 0.436752000 | 14.969384000 | 9.224229000 |
| H | 6.350516000 | 5.449394000 | 4.009718000 |
| H | 6.061470000 | 4.315944000 | 6.187006000 |
| H | 6.037753000 | 5.650213000 | 8.306629000 |
| H | 6.911247000 | 10.061461000 | 2.685286000 |
| H | 6.979203000 | 11.325510000 | 4.829197000 |
| H | 4.769835000 | 9.464843000 | 10.572214000 |
| H | 4.773917000 | 10.744384000 | 12.676302000 |
| H | 6.526023000 | 12.456687000 | 13.107066000 |
| H | 8.284028000 | 12.876564000 | 11.398457000 |
| H | 8.303186000 | 11.606850000 | 9.290138000 |
| H | 9.789247000 | 6.861067000 | 3.015331000 |
| H | 9.408443000 | 4.965827000 | 4.555340000 |
| H | 9.316965000 | 5.349420000 | 7.025762000 |
| H | 10.369583000 | 11.616483000 | 3.641698000 |
| H | 10.334607000 | 11.933093000 | 6.110912000 |
| H | 11.632974000 | 10.368637000 | 10.287724000 |
| H | 11.542201000 | 10.836893000 | 12.714878000 |
| H | 9.697674000 | 9.911630000 | 14.099752000 |
| H | 7.954638000 | 8.486850000 | 13.042983000 |
| H | 8.025172000 | 8.016816000 | 10.623427000 |

**M3 tetramer (antiparallel stacking)**

| | | | |
|---|---|---|---|
| Br | 3.619968000 | 9.633095000 | 10.916437000 |
| Br | 1.038125000 | 9.977158000 | 2.079321000 |
| Br | 6.367199000 | 12.133715000 | 2.817282000 |
| Br | -1.492298000 | 6.567835000 | 10.386652000 |
| O | 5.001385000 | 6.072851000 | 5.189375000 |
| O | -0.386743000 | 12.535512000 | 8.315728000 |
| O | 4.132479000 | 10.150502000 | 3.230994000 |
| O | 0.878090000 | 8.316177000 | 9.627592000 |
| O | 5.989909000 | 11.288834000 | 9.610087000 |
| O | 8.381752000 | 7.477132000 | 8.636804000 |
| O | -0.639983000 | 4.560198000 | 3.849139000 |
| O | -1.683544000 | 8.975125000 | 3.089989000 |
| N | 0.314189000 | 10.457604000 | 9.005919000 |
| N | 4.619652000 | 8.102984000 | 4.167868000 |
| N | 7.234665000 | 9.397785000 | 9.184009000 |
| N | -1.129112000 | 6.768846000 | 3.432099000 |
| C | 4.500485000 | 7.876782000 | 6.649021000 |
| C | 0.928185000 | 8.768660000 | 7.289109000 |
| C | 0.261185000 | 11.034060000 | 6.588430000 |
| C | 0.720614000 | 9.728950000 | 6.257216000 |
| C | 4.081892000 | 9.231030000 | 6.767491000 |
| C | 4.596672000 | 7.092075000 | 7.795671000 |
| C | 4.741820000 | 7.270546000 | 5.315121000 |
| C | 3.927156000 | 10.023298000 | 5.594661000 |
| C | 1.375732000 | 7.491664000 | 6.965747000 |
| C | 4.223745000 | 9.452027000 | 4.254178000 |
| C | 4.885770000 | 7.521658000 | 2.866274000 |
| C | 3.486213000 | 11.338044000 | 5.704225000 |
| C | 3.786931000 | 9.787078000 | 8.052442000 |
| C | 4.305930000 | 7.628847000 | 9.059236000 |
| C | 0.697964000 | 9.135761000 | 8.712437000 |
| C | 4.052388000 | 7.809380000 | 1.775348000 |
| C | 0.033055000 | 11.419905000 | 8.001715000 |
| C | 3.356109000 | 11.137113000 | 8.114966000 |
| C | 1.630965000 | 7.144317000 | 5.625242000 |
| C | 0.977048000 | 9.381788000 | 4.892952000 |
| C | 3.929305000 | 8.953231000 | 9.199962000 |
| C | 0.051695000 | 11.963575000 | 5.573553000 |

| | | | |
|---|---|---|---|
| C | 3.201817000 | 11.891792000 | 6.967259000 |
| C | 0.297001000 | 11.629597000 | 4.233539000 |
| C | 1.442928000 | 8.070450000 | 4.615310000 |
| C | 5.979807000 | 6.659439000 | 2.694351000 |
| C | 4.329799000 | 7.258613000 | 0.524602000 |
| C | 0.752010000 | 10.368962000 | 3.888952000 |
| C | 5.420729000 | 6.406507000 | 0.352119000 |
| C | 6.238597000 | 6.105076000 | 1.441816000 |
| C | 0.234139000 | 10.881106000 | 10.390923000 |
| C | -0.436829000 | 10.097437000 | 11.338828000 |
| C | 0.855498000 | 12.077968000 | 10.781355000 |
| C | -0.468158000 | 10.504670000 | 12.672772000 |
| C | 0.810062000 | 12.476774000 | 12.116097000 |
| C | 0.154094000 | 11.690105000 | 13.064626000 |
| C | 6.619830000 | 11.701146000 | 4.627226000 |
| C | 7.161169000 | 10.435907000 | 4.999181000 |
| C | 7.655019000 | 9.488055000 | 4.066394000 |
| C | 8.193800000 | 8.287046000 | 4.486945000 |
| C | 8.233154000 | 7.960935000 | 5.855392000 |
| C | 7.746258000 | 8.852270000 | 6.804631000 |
| C | 7.218274000 | 10.107431000 | 6.390792000 |
| C | 6.232432000 | 12.610172000 | 5.595765000 |
| C | 6.276412000 | 12.271722000 | 6.959499000 |
| C | 6.734413000 | 11.023247000 | 7.367943000 |
| C | 6.630915000 | 10.614672000 | 8.793324000 |
| C | 6.894357000 | 7.705092000 | 10.957541000 |
| C | 6.810686000 | 7.370611000 | 12.308757000 |
| C | 7.017892000 | 8.339168000 | 13.291524000 |
| C | 7.328451000 | 9.647628000 | 12.918625000 |
| C | 7.420735000 | 9.995039000 | 11.571680000 |
| C | 7.189686000 | 9.025436000 | 10.583084000 |
| C | 7.822360000 | 8.504361000 | 8.252155000 |
| C | -1.466075000 | 6.299192000 | 8.526886000 |
| C | -1.850293000 | 7.343882000 | 7.636265000 |
| C | -2.331099000 | 8.608897000 | 8.064758000 |
| C | -2.635383000 | 9.604659000 | 7.155601000 |
| C | -2.441141000 | 9.394821000 | 5.776846000 |
| C | -1.973434000 | 8.171643000 | 5.309091000 |
| C | -1.698995000 | 7.120282000 | 6.230554000 |
| C | -1.027635000 | 5.080830000 | 8.038667000 |
| C | -0.917059000 | 4.859027000 | 6.656629000 |
| C | -1.224466000 | 5.867923000 | 5.749584000 |
| C | -0.984775000 | 5.653547000 | 4.297988000 |
| C | -1.319425000 | 7.209116000 | 1.004344000 |
| C | -0.764154000 | 7.173229000 | -0.275072000 |
| C | 0.485633000 | 6.590011000 | -0.487885000 |
| C | 1.181538000 | 6.028758000 | 0.584189000 |
| C | 0.645740000 | 6.070274000 | 1.870014000 |
| C | -0.607667000 | 6.666607000 | 2.084172000 |
| C | -1.620894000 | 8.016603000 | 3.870142000 |
| H | 4.896265000 | 6.051828000 | 7.693462000 |
| H | 1.530006000 | 6.770936000 | 7.764867000 |
| H | 3.361657000 | 11.926873000 | 4.798677000 |
| H | 4.377697000 | 6.990308000 | 9.934321000 |
| H | 3.188020000 | 8.459588000 | 1.895395000 |
| H | 3.150482000 | 11.570023000 | 9.091504000 |
| H | 1.986275000 | 6.145815000 | 5.384784000 |
| H | -0.301552000 | 12.956927000 | 5.840317000 |
| H | 2.861192000 | 12.921700000 | 7.037280000 |
| H | 0.121053000 | 12.373191000 | 3.462054000 |
| H | 1.650816000 | 7.802503000 | 3.580770000 |
| H | 6.623272000 | 6.418769000 | 3.533911000 |
| H | 3.684264000 | 7.496195000 | -0.317903000 |
| H | 5.630431000 | 5.976607000 | -0.624392000 |
| H | 7.087583000 | 5.436730000 | 1.317275000 |
| H | -0.925371000 | 9.173477000 | 11.039027000 |
| H | 1.375055000 | 12.686985000 | 10.047199000 |
| H | -0.983499000 | 9.891252000 | 13.408257000 |
| H | 1.296326000 | 13.401592000 | 12.417217000 |
| H | 0.127261000 | 12.001492000 | 14.106115000 |
| H | 7.613386000 | 9.731347000 | 3.006891000 |
| H | 8.594586000 | 7.588621000 | 3.756855000 |
| H | 8.646489000 | 7.012706000 | 6.189988000 |
| H | 5.838833000 | 13.580424000 | 5.305976000 |
| H | 5.919253000 | 12.972241000 | 7.710592000 |
| H | 6.729197000 | 6.944991000 | 10.201193000 |
| H | 6.575668000 | 6.347566000 | 12.593382000 |
| H | 6.943267000 | 8.074133000 | 14.343416000 |
| H | 7.500906000 | 10.404259000 | 13.680569000 |
| H | 7.665979000 | 11.014374000 | 11.290816000 |
| H | -2.451863000 | 8.785701000 | 9.132062000 |
| H | -2.998276000 | 10.566991000 | 7.507095000 |
| H | -2.627263000 | 10.193185000 | 5.062440000 |
| H | -0.741388000 | 4.290122000 | 8.726021000 |
| H | -0.555806000 | 3.905936000 | 6.277809000 |
| H | -2.293065000 | 7.661333000 | 1.162818000 |
| H | -1.312521000 | 7.603184000 | -1.109972000 |
| H | 0.913962000 | 6.566713000 | -1.487175000 |
| H | 2.152515000 | 5.566289000 | 0.423632000 |
| H | 1.198546000 | 5.642286000 | 2.701144000 |

**M1+M2 heterodimer**

| | | | |
|---|---|---|---|
| Br | 18.541377000 | 3.250858000 | 2.844782000 |
| O | 24.488482000 | 0.094911000 | 4.269694000 |
| O | 24.955174000 | 3.625665000 | 7.144819000 |
| O | 18.699647000 | 4.179225000 | 8.341620000 |
| O | 20.549945000 | 0.308083000 | 6.749787000 |
| N | 28.422005000 | 0.286780000 | 7.142513000 |
| N | 15.842409000 | 1.037066000 | 5.927858000 |
| N | 25.405539000 | 2.269963000 | 10.470114000 |
| N | 24.733130000 | 1.839107000 | 5.730703000 |
| N | 19.552403000 | 2.167921000 | 7.648650000 |
| C | 27.859853000 | 2.365348000 | 10.333888000 |
| C | 27.927456000 | 2.980904000 | 11.734346000 |
| C | 26.606735000 | 1.505177000 | 10.147057000 |
| C | 26.619301000 | 3.711076000 | 12.059877000 |
| C | 28.323810000 | 1.537659000 | 6.686151000 |
| C | 27.319235000 | -0.466646000 | 7.100617000 |
| C | 26.084907000 | -0.011400000 | 6.632078000 |
| C | 16.522477000 | 0.215698000 | 6.733057000 |
| C | 16.378835000 | 2.233887000 | 5.685729000 |
| C | 25.423911000 | 2.784103000 | 11.841909000 |
| C | 27.141678000 | 2.095274000 | 6.191141000 |
| C | 17.595662000 | 2.666761000 | 6.220651000 |
| C | 20.470882000 | 4.575834000 | 5.069741000 |
| C | 17.745938000 | 0.541526000 | 7.319003000 |
| C | 20.666968000 | 1.396558000 | 3.043367000 |
| C | 21.230527000 | 5.242671000 | 6.010807000 |
| C | 25.988931000 | 1.307350000 | 6.177483000 |
| C | 22.352899000 | 5.320936000 | 10.099227000 |
| C | 20.188201000 | 2.598008000 | 3.534238000 |
| C | 23.380199000 | 4.392381000 | 10.155174000 |
| C | 24.011811000 | 1.097795000 | 4.758803000 |
| C | 24.281741000 | 3.045436000 | 6.315353000 |
| C | 22.482619000 | 4.734170000 | 6.411269000 |
| C | 24.029360000 | 0.847256000 | 9.078655000 |
| C | 21.914436000 | 0.906613000 | 3.470962000 |
| C | 24.233015000 | 2.047922000 | 9.775640000 |
| C | 21.104169000 | 4.966100000 | 9.558110000 |
| C | 19.637784000 | 3.405829000 | 8.325118000 |
| C | 22.874599000 | 0.617956000 | 8.325894000 |
| C | 23.202342000 | 3.063570000 | 9.695881000 |
| C | 18.299908000 | 1.798110000 | 7.053759000 |
| C | 22.191822000 | 2.838330000 | 4.912581000 |
| C | 20.928238000 | 3.710874000 | 8.993628000 |
| C | 22.679712000 | 1.620704000 | 4.378745000 |
| C | 20.637941000 | 1.261338000 | 7.502060000 |
| C | 21.977400000 | 2.755906000 | 9.022409000 |
| C | 22.962464000 | 3.554344000 | 5.866537000 |

| | | | |
|---|---|---|---|
| C | 21.836481000 | 1.541749000 | 8.303939000 |
| C | 20.920259000 | 3.355544000 | 4.498462000 |
| H | 20.273803000 | 5.673294000 | 9.520770000 |
| H | 22.520849000 | 6.335977000 | 10.466508000 |
| H | 22.305705000 | -0.034568000 | 3.081790000 |
| H | 20.078559000 | 0.833399000 | 2.318536000 |
| H | 27.413923000 | -1.493272000 | 7.473592000 |
| H | 25.218915000 | -0.670335000 | 6.623197000 |
| H | 28.744876000 | 1.744366000 | 10.120437000 |
| H | 27.836082000 | 3.167466000 | 9.576502000 |
| H | 28.786089000 | 3.666152000 | 11.822664000 |
| H | 28.088217000 | 2.181583000 | 12.480652000 |
| H | 26.550599000 | 1.170015000 | 9.107074000 |
| H | 26.672335000 | 0.597221000 | 10.783770000 |
| H | 26.621410000 | 4.077997000 | 13.099710000 |
| H | 26.512544000 | 4.592718000 | 11.402894000 |
| H | 29.235998000 | 2.144495000 | 6.714324000 |
| H | 16.070616000 | -0.762746000 | 6.934083000 |
| H | 15.815304000 | 2.901721000 | 5.024066000 |
| H | 25.503246000 | 1.921813000 | 12.537660000 |
| H | 24.475379000 | 3.281398000 | 12.071082000 |
| H | 27.120350000 | 3.125700000 | 5.839358000 |
| H | 17.975430000 | 3.660501000 | 6.001019000 |
| H | 19.508319000 | 4.981652000 | 4.758500000 |
| H | 18.259831000 | -0.173167000 | 7.960533000 |
| H | 20.847779000 | 6.159948000 | 6.462577000 |
| H | 24.355888000 | 4.702518000 | 10.523776000 |
| H | 23.083902000 | 5.244508000 | 7.164537000 |
| H | 24.781568000 | 0.064625000 | 9.135870000 |
| H | 22.751008000 | -0.309972000 | 7.763457000 |

**M2+M1 co-assembly (Model A)**

| | | | |
|---|---|---|---|
| Br | 2.862747000 | 9.217984000 | 11.494830000 |
| Br | 4.887930000 | 8.840515000 | 7.611475000 |
| Br | 9.608189000 | 2.980980000 | 0.950657000 |
| Br | 7.583205000 | 3.358164000 | 4.834091000 |
| O | 3.951743000 | 16.497324000 | 11.026110000 |
| O | 8.519577000 | -4.298461000 | 1.419330000 |
| O | 0.609974000 | 15.361121000 | 8.066897000 |
| O | 4.939491000 | 16.280766000 | 7.878832000 |
| O | 8.115970000 | 14.631653000 | 10.772918000 |
| O | 11.861483000 | -3.162087000 | 4.378322000 |
| O | 7.532006000 | -4.082043000 | 4.566673000 |
| O | 4.355280000 | -2.433139000 | 1.672741000 |
| O | 4.996226000 | 2.956451000 | 13.537600000 |
| O | 7.474569000 | 9.242519000 | -1.091945000 |
| O | 2.754489000 | 1.680264000 | 9.724976000 |
| O | 2.446174000 | 2.924638000 | 4.981893000 |
| O | 5.572326000 | 1.116682000 | 7.833409000 |
| O | 9.716671000 | 10.518711000 | 2.720463000 |
| O | 10.025103000 | 9.274004000 | 7.463623000 |
| O | 6.898886000 | 11.082006000 | 4.612206000 |
| N | 9.645800000 | -10.126348000 | 3.966098000 |
| N | 4.143457000 | -9.490840000 | 3.523087000 |
| N | 2.826205000 | 22.325213000 | 8.479047000 |
| N | 8.328467000 | 21.689293000 | 8.922432000 |
| N | 2.464174000 | 11.851620000 | 10.842708000 |
| N | 10.006848000 | 0.347343000 | 1.602723000 |
| N | 7.012837000 | 0.771887000 | 4.145027000 |
| N | 5.458287000 | 11.426794000 | 8.300559000 |
| N | 2.286730000 | 15.883456000 | 9.555462000 |
| N | 6.570652000 | 15.401405000 | 9.246076000 |
| N | 10.184658000 | -3.684509000 | 2.889864000 |
| N | 5.900720000 | -3.202793000 | 3.199509000 |
| N | 4.986609000 | -1.767697000 | 12.367214000 |
| N | 7.484266000 | 13.966663000 | 0.078470000 |
| N | 9.696917000 | 14.144009000 | 7.132712000 |
| N | 2.774342000 | -1.945369000 | 5.312920000 |
| N | 3.871465000 | 2.278667000 | 11.646656000 |
| N | 3.968275000 | 1.983475000 | 6.431102000 |
| N | 8.599495000 | 9.920301000 | 0.798903000 |
| N | 8.502960000 | 10.215189000 | 6.014473000 |
| C | 9.741711000 | -12.538791000 | 3.453292000 |
| C | 9.504322000 | -12.874487000 | 4.924488000 |
| C | 9.983267000 | -11.734370000 | 5.822403000 |
| C | 9.352402000 | -10.412280000 | 5.385984000 |
| C | 9.143532000 | -11.179315000 | 3.072487000 |
| C | 4.490350000 | -11.029553000 | 5.469084000 |
| C | 2.977911000 | -11.196843000 | 5.606900000 |
| C | 2.250263000 | -9.965000000 | 5.073574000 |
| C | 2.676566000 | -9.618934000 | 3.634194000 |
| C | 4.852662000 | -10.680607000 | 4.018170000 |
| C | 2.489033000 | 23.933193000 | 6.622652000 |
| C | 2.968008000 | 25.073302000 | 7.520562000 |
| C | 2.730468000 | 24.737685000 | 8.991752000 |
| C | 3.328494000 | 23.378169000 | 9.372658000 |
| C | 3.119743000 | 22.611064000 | 7.059173000 |
| C | 10.221773000 | 22.163247000 | 7.372019000 |
| C | 9.494256000 | 23.395140000 | 6.838628000 |
| C | 7.981797000 | 23.227987000 | 6.976380000 |
| C | 7.619390000 | 22.879111000 | 8.427286000 |
| C | 9.795374000 | 21.817256000 | 8.811389000 |
| C | 2.438893000 | 14.199680000 | 11.357288000 |
| C | 2.494662000 | 12.857728000 | 11.734867000 |
| C | 2.386444000 | 12.151094000 | 9.533160000 |
| C | 2.334140000 | 13.463211000 | 9.062420000 |
| C | 2.358663000 | 14.515709000 | 9.990813000 |
| C | 3.627459000 | 20.599943000 | 10.021906000 |
| C | 3.701212000 | 19.259311000 | 10.421977000 |
| C | 3.126163000 | 16.848371000 | 10.175862000 |
| C | 10.084686000 | 0.047845000 | 2.912259000 |
| C | 9.976364000 | -0.658747000 | 0.710543000 |
| C | 10.032248000 | -2.000703000 | 1.088089000 |
| C | 10.137110000 | -1.264280000 | 3.382966000 |
| C | 10.112595000 | -2.316757000 | 2.454551000 |
| C | 8.770379000 | -7.060449000 | 2.023350000 |
| C | 9.345253000 | -4.649471000 | 2.269500000 |
| C | 6.534527000 | -1.476937000 | 4.840552000 |
| C | 6.878033000 | -0.153109000 | 5.114405000 |
| C | 6.823118000 | 0.403381000 | 2.865031000 |
| C | 6.478402000 | -0.898599000 | 2.498814000 |
| C | 6.317147000 | -1.861274000 | 3.507569000 |
| C | 5.647985000 | 11.795299000 | 9.580557000 |
| C | 5.593184000 | 12.351772000 | 7.331177000 |
| C | 5.992776000 | 13.097260000 | 9.946775000 |
| C | 5.936772000 | 13.675579000 | 7.605029000 |
| C | 6.154135000 | 14.059914000 | 8.938016000 |
| C | 2.843028000 | 20.990113000 | 8.925555000 |
| C | 0.990617000 | 20.332628000 | 7.342873000 |
| C | 1.990068000 | 20.002840000 | 8.297656000 |
| C | 0.351232000 | 18.007164000 | 7.128474000 |
| C | 0.193560000 | 19.357107000 | 6.769945000 |
| C | 2.091990000 | 18.637590000 | 8.713775000 |
| C | 2.977292000 | 18.264929000 | 9.766689000 |
| C | 1.276292000 | 17.643479000 | 8.101430000 |
| C | 1.359253000 | 16.220843000 | 8.534908000 |
| C | 7.714031000 | 20.432286000 | 8.898647000 |
| C | 9.118642000 | 19.569280000 | 10.815143000 |
| C | 8.184932000 | 19.367101000 | 9.763352000 |
| C | 6.594099000 | 20.184149000 | 8.084418000 |
| C | 6.025273000 | 18.908720000 | 7.997561000 |
| C | 9.076814000 | 17.215669000 | 11.381502000 |
| C | 9.549596000 | 18.519586000 | 11.608163000 |
| C | 7.621625000 | 18.059608000 | 9.617258000 |
| C | 6.544333000 | 17.829653000 | 8.713125000 |
| C | 8.107331000 | 16.981726000 | 10.412156000 |
| C | 5.950378000 | 16.482169000 | 8.563840000 |

| | | | |
|---|---|---|---|
| C | 7.611262000 | 15.594639000 | 10.190477000 |
| C | 9.628827000 | -8.791234000 | 3.519641000 |
| C | 11.481309000 | -8.133650000 | 5.102201000 |
| C | 10.481754000 | -7.803911000 | 4.147508000 |
| C | 8.844275000 | -8.401089000 | 2.423368000 |
| C | 12.120516000 | -5.808141000 | 5.316632000 |
| C | 12.278329000 | -7.158083000 | 5.675101000 |
| C | 10.379685000 | -6.438655000 | 3.731446000 |
| C | 9.494269000 | -6.066031000 | 2.678615000 |
| C | 11.195350000 | -5.444499000 | 4.343762000 |
| C | 11.112239000 | -4.021855000 | 3.910338000 |
| C | 4.757783000 | -8.233778000 | 3.546877000 |
| C | 3.353013000 | -7.370848000 | 1.630463000 |
| C | 4.286753000 | -7.168613000 | 2.682217000 |
| C | 5.877729000 | -7.985564000 | 4.361064000 |
| C | 6.446447000 | -6.710088000 | 4.447926000 |
| C | 3.394617000 | -5.017222000 | 1.064154000 |
| C | 2.921935000 | -6.321174000 | 0.837485000 |
| C | 4.849954000 | -5.861075000 | 2.828316000 |
| C | 5.927265000 | -5.631049000 | 3.732409000 |
| C | 4.364122000 | -4.783217000 | 2.033463000 |
| C | 6.521111000 | -4.283518000 | 3.881699000 |
| C | 4.860087000 | -3.396095000 | 2.255146000 |
| C | 4.096313000 | 0.334807000 | 13.158979000 |
| C | 4.479984000 | -0.995294000 | 13.348332000 |
| C | 5.131006000 | -1.209293000 | 11.148847000 |
| C | 4.785504000 | 0.113874000 | 10.859404000 |
| C | 4.252920000 | 0.903747000 | 11.887355000 |
| C | 4.007648000 | 7.034997000 | 12.905719000 |
| C | 4.345297000 | 5.694505000 | 13.155353000 |
| C | 4.302782000 | 3.270687000 | 12.567802000 |
| C | 7.339983000 | 13.408251000 | 1.296846000 |
| C | 7.990807000 | 13.194270000 | -0.902700000 |
| C | 8.374502000 | 11.864170000 | -0.713391000 |
| C | 7.685519000 | 12.085084000 | 1.586249000 |
| C | 8.218014000 | 11.295221000 | 0.558243000 |
| C | 8.125521000 | 6.504464000 | -0.709749000 |
| C | 8.168095000 | 8.928283000 | -0.122205000 |
| C | 9.073734000 | 11.891187000 | 7.747319000 |
| C | 9.467072000 | 13.194839000 | 8.063329000 |
| C | 9.553284000 | 13.795032000 | 5.837743000 |
| C | 9.170349000 | 12.517953000 | 5.421338000 |
| C | 8.916959000 | 11.545517000 | 6.398632000 |
| C | 2.917948000 | -1.596364000 | 6.607885000 |
| C | 3.004205000 | -0.996219000 | 4.382288000 |
| C | 3.300874000 | -0.319275000 | 7.024270000 |
| C | 3.397535000 | 0.307441000 | 4.698277000 |
| C | 3.554284000 | 0.653140000 | 6.046960000 |
| C | 3.233281000 | 7.388622000 | 11.814911000 |
| C | 1.930924000 | 6.659772000 | 9.802213000 |
| C | 2.753562000 | 6.381426000 | 10.925444000 |
| C | 1.869007000 | 4.315086000 | 9.202423000 |
| C | 1.490441000 | 5.650128000 | 8.967638000 |
| C | 3.116704000 | 5.019030000 | 11.172706000 |
| C | 3.918364000 | 4.682288000 | 12.300677000 |
| C | 2.678304000 | 3.992469000 | 10.286944000 |
| C | 3.090463000 | 2.577321000 | 10.505133000 |
| C | 4.461267000 | 7.068756000 | 7.094168000 |
| C | 6.074460000 | 6.064607000 | 8.727057000 |
| C | 5.095374000 | 5.946624000 | 7.705691000 |
| C | 3.515503000 | 6.871676000 | 6.103164000 |
| C | 3.155772000 | 5.580152000 | 5.685179000 |
| C | 6.312212000 | 3.657454000 | 8.847639000 |
| C | 6.668572000 | 4.947654000 | 9.283798000 |
| C | 4.729853000 | 4.631903000 | 7.272426000 |
| C | 3.748358000 | 4.457237000 | 6.255194000 |
| C | 5.349998000 | 3.489099000 | 7.856935000 |
| C | 3.332233000 | 3.096301000 | 5.822056000 |
| C | 4.985688000 | 2.117582000 | 7.402340000 |
| C | 9.237633000 | 4.810342000 | 0.630609000 |
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| C | 9.315463000 | 6.618500000 | 6.760341000 |
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| C | 7.741342000 | 7.566774000 | 5.173146000 |
| C | 8.722870000 | 7.741424000 | 6.190350000 |
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| H | 6.133245000 | 13.351740000 | 10.991674000 |
| H | 6.056092000 | 14.386228000 | 6.793695000 |
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| H | 3.035328000 | 7.728149000 | 5.636120000 |
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| H | 6.783099000 | 2.776313000 | 9.279012000 |
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| H | 11.616002000 | 6.312851000 | 4.328488000 |
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**M2+M1 co-assembly (Model B)**

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| O | -6.952112000 | 2.677349000 | -22.470241000 |
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