Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supporting Information for

Supramolecularly cross-linked amphiphilic block copolymer assembly by the dipolar interaction of a merocyanine dye

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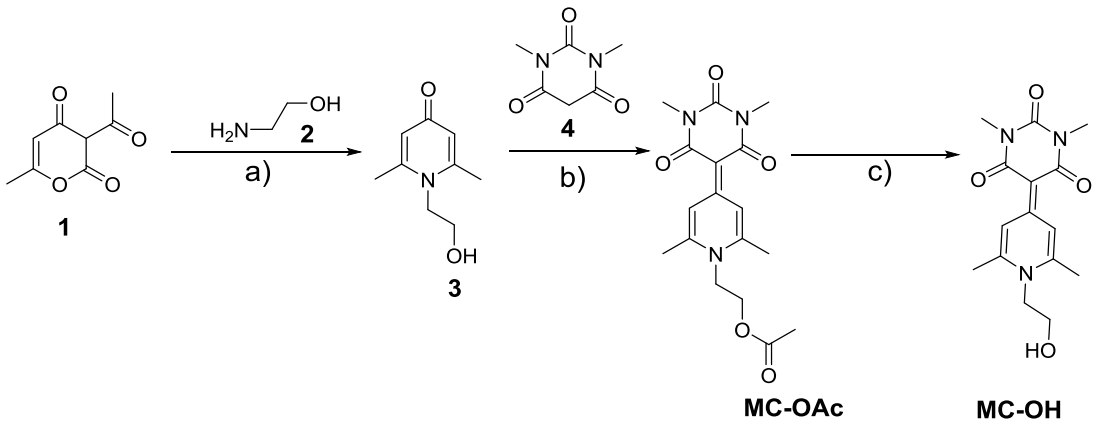
Materials and Methods: All Chemicals were purchased from commercial suppliers and no further purification was done unless otherwise mentioned. Acryloyl chloride was purchased from Alfa Aesar. Dried solvents for polymerization were purchased from Sigma-Aldrich. ^{1}H, ^{13}C and ^{19}F NMR spectra were measured on a Bruker 500 MHz, 400 MHz and 300 MHz NMR spectrometer using $CDCl_3$ and DMSO-D_6 as solvent. Chemical shifts (δ) are reported in ppm unit with TMS as the internal standard. The coupling constant (*J*) is reported in hertz (Hz). HRMS 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). Spectroscopic grade solvents were used for UV-Vis studies, and UV-Vis spectra were recorded in a JASCO V-750 spectrophotometer. Transmission Electron Microscopy (TEM) was performed in JEOL-2010EX machine operating at an accelerating voltage of 200KV. Fluorescence spectra were recorded in a FluoroMax-3 spectrophotometer, from Horiba Jobin Yvon. FTIR spectra were recorded in a Perkin Elmer Spectrum 100 FT-IR Spectrometer. Olympus IX73 model was used for fluorescence microscopy images. Number average molecular weight (Mn) and dispersity (Đ) of the polymers were measured by size exclusion chromatography (SEC) at 30°C using a Waters machine equipped with a 515 HPLC pump, Waters 2414 RI detector, and HSPgel HT 4.0/HSPgel HT 2.5 columns connected in a series. THF was used as an eluent. For size exclusion chromatography in DMF solvent, Acquity Advanced Polymer Chromatography system was used. Dynamic Light Scattering (DLS) measurements were recorded in Malvern instrument.

Synthesis and Characterization

Synthesis of MC-OH: MC-OH was synthesized by a reported procedure[1] following the synthetic route drawn in the Scheme S1.



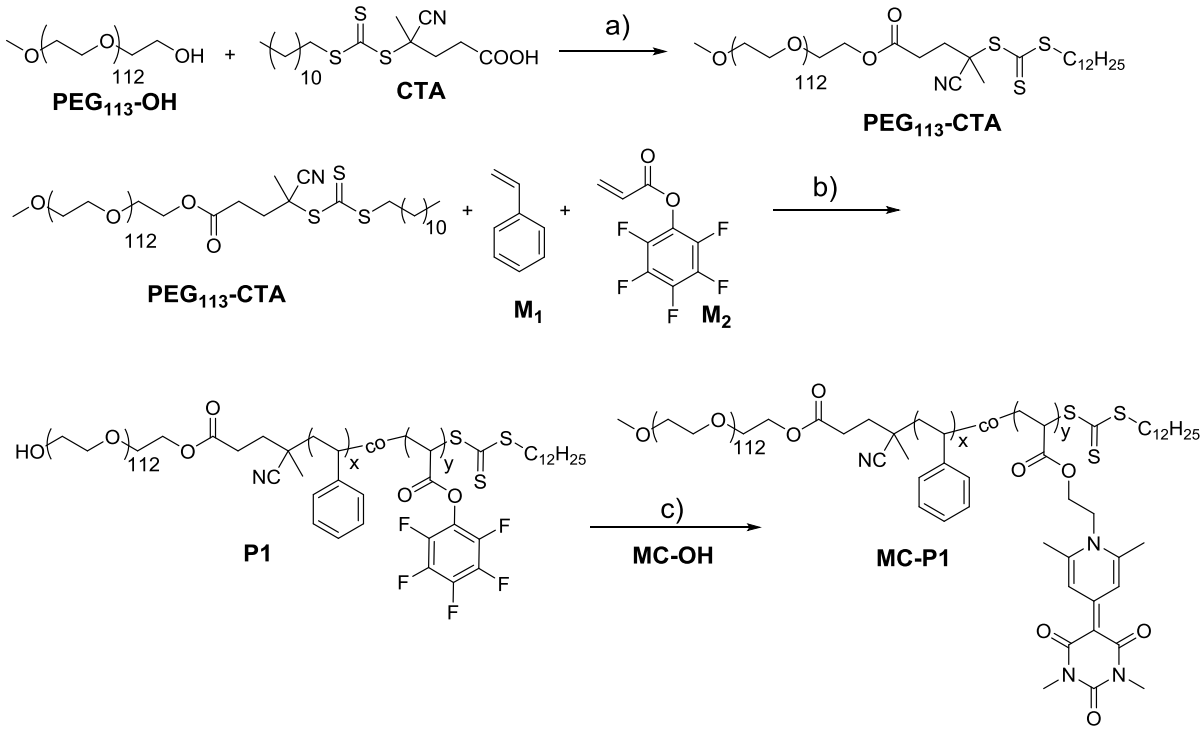
Reagents and Conditions: a) H_2O, 100 °C, 15 h, yield = 55%; b) AcOH, Ac_2O, 110 °C, 15 h, yield = 10%; c) K_2CO_3, MeOH, rt, 12 h, yield = 43%.

Scheme S1: Synthesis of MC-OH.

Synthesis of Compound 3: Dehydroacetic acid (**1**) (10.0 g, 59.47 mmol) and ethanolamine (**2)** (5.38 mL, 89.2 mmol) were taken in a round bottom flask with 150 mL of water and the mixture was refluxed for 15 h at 100 °C. After 15 h, the mixture was cooled to room temperature. Excess water was evaporated under reduced pressure and the brown crude obtained was further refluxed with 35 mL ethanol. The solution was initially cooled to room temperature and then kept in freezer overnight to obtain yellowish white crystals (5.5 g, 55%). M.P. = 116-118 °C; ^{1}H NMR (400 MHz, DMSO-d6, TMS): δ (ppm) = 5.92 (s, 2H), 5.07 (t, *J* = 5.3 Hz, 1H), 3.97-3.93 (m, 2H,), 3.60 (q, *J* = 5.7 Hz, 2H), 2.28 (s, 6H); ^{13}C NMR (100 MHz, DMSO-d6): δ (ppm) = 20.21, 48.39, 59.81, 117.57, 149.53, 177.26. HRMS (ESI): m /z calcd for $C_9H_{14}NO_2$ $[M + H]^+$:168.1019; found: 168.1018.

Synthesis of MC-OAc: Compound (**3)** (5.50 g, 32.9 mmol) and 1, 3-Dimethylbarbituric acid (**4**) (6.16 g, 39.48 mmol) were taken together in a round bottom flask. To that acetic acid (10 mL) and acetic anhydride (70 mL) were added and the reaction mixture was heated at 112 °C under argon atmosphere. After 15 h, the reaction was stopped and the mixture was cooled to room temperature and excess acetic acid was evaporated under rotary evaporator to obtain a brown solid. The crude was purified by column chromatography using silica gel (100-200 mesh) as a stationary phase and 2-4% MeOH in $CHCl_3$ as eluent to obtain the desired product as light brown solid (1.1 gm, 10 %). M.P. = 251 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ (ppm) = 9.04 (s, 2H), 4.40-4.31 (m, 4H), 3.36 (s, 6H), 2.63 (s, 6H), 2.08 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$,): δ (ppm) = 25.57, 29.78, 47.42, 61.44, 90.05, 121.69, 148.02, 152.29, 156.19, 164.61, 170.51. HRMS (ESI): m/z calcd for $C_{17}H_{21}N_3O_5Na$ $[M+Na]^+$: 370.1379; found: 370.1378.

Synthesis of MC-OH: MC-OAc (0.90 g, 2.6 mmol) and K_2CO_3 (0.72 g, 5.2 mmol) were taken in a round bottom flask with 45 mL methanol and the mixture was stirred at room temperature for 12 h. Excess methanol was removed under rotary evaporator and the crude was dissolved in CH_2Cl_2 and filtered. The residue was washed multiple times with CH_2Cl_2. The desired product was obtained as light yellow solid by removing the organic CH_2Cl_2 phase (330 mg, 43 %). M.P. = 295 °C; ^{1}H NMR (400 MHz, DMSO-d6, TMS): δ (ppm) = 8.83 (s, 2H), 4.34 (t, *J* = 5.4 Hz, 2H), 3.79-3.73 (m, 2H), 3.16 (s, 6H), 2.63 (s, 6H); ^{13}C NMR (100 MHz, DMSO-d6): δ (ppm) = 21.88, 27.83, 52.19, 59.85, 87.51, 120.90, 150.35, 152.08, 154.58, 163.38. HRMS (ESI): m/z calculated for $C_{15}H_{20}N_3O_4$ $[M+H]^+$: 306.1448; found: 306.1445.



Reagents and conditions: a) dry DCM, DMAP, EDC.HCL, 0°C-rt, 48 h, yield = 45%; b) AIBN, dioxane, 100 °C, 8 h, yield = 50%; c) DMF, DMAP, 120°C, 60 h, yield = 73%.

Scheme 2: Synthesis of P1 and MC-P1.

Synthesis of PEG_{113}-CTA:[2] Commercial available **PEG_{113}-OH** (0.31g, 0.062 mmol) was taken in a round bottom flask with 4-Cyano-4-[(dodecylsulfanylthiocarbonyl)sulfanyl]pentanoic acid (**CTA**) (0.05g, 0.124 mmol) in dry CH_2Cl_2. A mixture of 4-Dimethylaminopyridine (DMAP) (0.024g, 0.012 mmol) and *N*-(3-Dimethylaminopropyl)-*N′*-ethylcarbodiimide hydrochloride (EDC.HCL) (0.02g, 0.124 mmol) in dry CH_2Cl_2 was added dropwise to the reaction mixture for 1 h in ice cold condition and then the mixture was stirred for 48 h at rt. The product was precipitated from diethyl ether and the process was repeated thrice for purification. After drying under vacuum for 5 h, the desired product was obtained as pale yellowish power (Yield = 150 mg, 45%).^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ (ppm) = 4.5-4.1 (m, 4H), 3.84-3.47 (m, 113H), 3.39 (s, 3H), 1.52-1.11 (m, 22H), 0.89 (m, 3H).

Synthesis of P1: PEG_{113}-CTA (200 mg, 0.0371 mmol), Styrene (**M1**) (464 mg, 4.455 mmol) and pentafluorophenyl acrylate (**M2**) (265 mg, 1.114 mmol) were taken along with dry 1, 4-dioxane (6 mL) in a glass vial equipped with a septum and an inlet/outlet gas tube. **M1:M2** feed ratio was maintained at 8:2. The above solution was degassed for 15 min. To this a solution of azobisisobutyronitrile (AIBN) (0.60 mg, 0.0037 mmol) in degassed 1,4-dioxane

was added and the reaction vial was immersed in a preheated oil bath at 100 °C for 8 h. The reaction was quenched by exposing to air. The solution was diluted with CH_2Cl_2 and purified by precipitating from hexane to afford a white solid. The process was repeated thrice to obtain a pure polymer which was dried under vacuum at 40 °C for 48 h (Yield = 456 mg, 50 %). ^{1}H NMR of **P1** (400 MHz, $CDCl_3$, TMS): δ (ppm) = 7.22-6.88 (bs, 3H), 6.85-6.29 (bs, 2H), 3.64 (s, 4H), 3.33 (s, 3H), 2.53-1.15 (multiple bs, 6H), 0.86 (m, 3H). FTIR shows characteristic peak for PFP-ester carbonyl stretching at 1783 cm^{-1}. From the crude ^{1}H NMR and ^{19}F NMR, **M1** and **M2** conversion were calculated to be 32% and 62%, from which the degree of polymerization (DP) for **M1** and **M2** were estimated to be 38 and 19, respectively. Molar mass calculated from ^{1}H NMR = 13,800 g/ mol; GPC (PS standard, THF): Mn = 3760 g/mol, Đ =1.18 for **P1** and Mn =1470 g/mol, Đ =1.23 for **PEG_{113}-CTA.** The values obtained were under estimated; GPC (PMMA standard, DMF): Mn = 24800 g/mol, Đ =1.07 for **P1** and Mn =19020 g/mol, Đ =1.23 for **PEG_{113}-CTA.** The values obtained were over estimated.

Synthesis of MC-P1: The transesterification of **P1** with **MC-OH** was performed following literature procedure as follows:[1]

P1 (60 mg, 0.013 mmol of PFP-ester, 1.0 equiv) and DMAP (4.64 mg, 0.003 mM, 0.2 equiv) were taken with 2.0 mL dry DMF and added with **MC-OH** (7.7 mg, 0.025 mM, 2.0 equiv). The mixture was stirred at 120 °C for 60 h. The formation of the product was monitored by FTIR measurements. The conversion was quantitative as no PFP-ester carbonyl peak at 1783 cm^{-1} was seen after the reaction. The mixture was dissolved in CH_2Cl_2 and purified by precipitation from hexane. The precipitation method was repeated thrice to obtain solid brown polymer **MC-P1** (yield = 50 mg, 73%). ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ (ppm) = δ 8.97 (s, 2H), 7.07 (bs, 3H), 6.58 (bs, 2H), 3.64 (s, 4H), 3.36 (s, 3H), 2.08-1.15 (multiple bs, 6H); By comparing the integrals of aromatic protons of MC and styrene with methylene proton signals of PEG_{113} in **MC-P1**, the degree of polymerization (DP) of **M1** and **M2** were estimated to be 45 and 18, respectively, which was comparable with the value obtained from the crude ^{1}H NMR data of **P1** (**M1:M2**:: 38:19). Molar mass from ^{1}H NMR of **MC-P1**: 15,500 g / mol. GPC (PS standard, THF): Mn = 1577 g/ mol, Đ =1.6 which was under estimated.

Synthesis of P2: The **PEG_{113}-CTA** (100 mg, 0.02 mmol) and Styrene (**M1**) (312 mg, 3.0 mmol) were taken along with dry 1, 4-dioxane (200 µL) in a glass vial equipped with a septum and an inlet/outlet gas tube. The above solution was degassed for 15 min. To this a

solution of AIBN (0.82 mg, 0.005 mmol) in degassed 1,4-dioxane was added and the reaction vial was immersed in a preheated oil bath at 72 °C for 22 h. The solution was diluted with CH_2Cl_2 and purified by precipitating from cold diethyl ether to afford off white solid. The process was repeated thrice to obtain a pure polymer which was dried under vacuum at 40 °C for 4 h (Yield = 70 mg, 16 %). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ (ppm) = 7.26-6.87 (bs, 3H), 6.72-6.33 (bs, 2H), 3.66 (s, 4H), 3.38 (s, 3H), 1.97-1.21 (multiple bs, 6H). Molar mass calculated from ^{1}H NMR = 10,080 g/ mol; GPC (PS standard, THF): Mn = 2155 g/mol, Đ =1.15. This value was under estimated.

Experimental procedures:

Sample preparation in water: Measured amount (1.0 mg) of polymer **MC-P1** was taken in a glass vial and dissolved in 100 µL THF. To this 1.0 mL water was added dropwise and the THF was evaporated by gently heating the solution. The aqueous solution was further heated to 90 °C to break any pre-aggregated structure and then cooled to room temperature to obtain a clear solution. The final **MC-P1** concentration becomes 1.0 mg / mL in water. The solution was allowed to equilibrate at room temperature for 1.0 h before any physical studies were performed.

Sample preparation in toluene: Measured amount (1.0 mg) of polymer **MC-P1** was taken in a glass vial. To this 1.0 mL toluene was added and the solution was heated to 90 $^\circ$C to break any pre-aggregated structure and cooled to room temperature to obtain a clear solution. The final concentration becomes 1.0 mg/ mL in toluene. The solution was allowed to equilibrate at room temperature for 1.0 h before any physical studies were done.

UV-Vis studies: Solvent-dependant UV-Vis absorption spectroscopic experiments were performed using a quartz cuvette of 1.0 mm path length at 25 °C. For variable temperature UV-Vis studies, two separate solutions of **MC-P1** (1.0 mg/ mL) in water and toluene were heated from 25°C to 90 °C at an interval of 10 °C. Before taking the measurements, each time sample was allowed to stand for 5.0 min after the desired temperature was reached.

Photoluminescence studies: Samples were prepared in the same way as discussed earlier. The emission intensity for **MC-P1** solutions were recorded in a quartz cuvette of 10 mm path length. The excitation wavelength (λ_{ex}) was maintained at = 372 nm. Excitation and emission band width = 3 nm each.

Dynamic light scattering studies: Experiments were carried out with a solution of **MC-P1** (1.0 mg/ mL) in water and toluene separately. The solutions were prepared following the procedure described earlier. Samples were equilibrated for 4.0 h before taking the reading. For variable temperature studies, the solution was heated from 25 ^{o}C to higher temperatures and the spectral measurements were carried out at different temperatures.

Transmission Electron Microscopy (TEM) studies: 0.5 mg/mL solution of **MC-P1** in water and toluene separately were drop casted on copper grids and slowly air dried for 48 h prior to imaging.

Dye encapsulation studies: A stock solution of Nile red in THF (1×10^{-4} M) was freshly prepared. 10 µL of stock solution was taken in a vial. To this, 1.0 mL solution of **MC-P1** (1 mg/ mL) in water was added dropwise (final dye concentration = 1×10^{-6} M) and trace amount of THF was removed by slowly heating the solution. The solution was sonicated for 15 min and allowed to equilibrate for 2.0 h at room temperature before taking the photoluminescence spectra.

Similar procedure was followed for encapsulating Rodamine B (stock = 1×10^{-4} M in THF) in **MC-P1** aggregates in toluene. Final concentration of **MC-P1** = 1.0 mg/ mL and Rodamine B = 1×10^{-6} M in toluene.

Fluorescence microscopy (FM): Nile red and Rodamine B encapsulated solutions of **MC-P1** (0.5 mg/mL) in water and toluene, respectively were drop-casted on glass slides and air dried overnight before FM images were captured. For fluorescence microscopy images of **MC-P1** aggregates in water and toluene, **MC-P1** concentration was kept at 1.0 mg / mL. The samples were drop-casted on glass slides and air dried overnight before FM images were captured.

CMC Determination: For determination of CMC of **MC-P1** in water, 10 µL stock solution of Nile red in THF (1×10^{-4} M) was transferred to 10 different vials. To these, different measured quantity of a stock solution of **MC-P1** in THF (1.0 mg/ mL) was added and the solvent was removed by heating to obtain a thin film. To this, water was added dropwise and the final volume was adjusted to 1.0 mL. All the solutions were sonicated for 10 min and then allowed to equilibrate for 2.0 h prior to measuring the spectra. All the resulting solutions had same Nile red concentration (1×10^{-6} M) but varying concentrations of polymer (1.0 - 0.0 mg/mL). The emission spectra were recorded for each solution at an excitation wavelength (λ_{ex}) = 530 nm. Both excitation and emission band width were kept at 3.0 nm.

For determination of CMC of **MC-P1** in toluene by UV-Vis spectroscopy, 1.0 mg/ mL solution of **MC-P1** in toluene was prepared. The solution was diluted stepwise (from 1.0 mg/ mL to 0.008 mg/mL) with measured quantity of toluene and in each step the UV-Vis spectra of **MC-P1** were recorded in a quartz cuvette of 1.0 mm path length.

Förster Resonance Energy Transfer (FRET) Studies: Stock solutions of the donor dye DiO (3,3´-di-octadecyloxacarbocyanine perchlorate) and the acceptor dye DiI (1,10-dioctadecyl-3,3,30,30-tetramethylindocarbocyanine perchlorate) were prepared in THF (1×10^{-4} M). 10 µL each of DiO and DiI stock solutions were taken in two separate vials and THF was removed. To these two vials, measured quantity (0.6 mg in 30 µL THF) of **MC-P1** was added followed by dropwise addition of 600 µL water to make the final polymer concentration 1.0 mg/ mL. Finally THF was removed by slowly heating the solution. Both the solutions were sonicated for 30 min in a water bath at room temperature and allowed to equilibrate for 2.0 h and filtered to remove any non-encapsulated dye. Final dye concentration = 1.6×10^{-6} M.

- **Kinetic Study:** 500 µL each of individual DiO and DiI loaded **MC-P1** (1.0 mg/mL) solutions were mixed in 1:1 ratio and emission spectra were recorded to monitor FRET with time.
- **Dilution Experiment with THF:** 5.0 µL of each DiO and DiI stock solutions (1×10^{-4} M) in THF were taken in a single vial. To this, measured quantity (0.6 mg in 30 µL THF) of **MC-P1** was added followed by dropwise addition of 600 µL water. Finally the THF was removed by slowly heating the solution. The final concentration of **MC-P1** = 1.0 mg /mL in water and coencapsulated DiO and DiI concentration = 0.8×10^{-6} M each. The solution was equilibrated for 30 min before taking the measurements. To this solution, measured volume of THF was added stepwise and the emission spectra were recorded to monitor FRET.
- **Dilution Experiment with water:** Similar procedure was followed for the sample preparation as done for dilution experiment with THF. Final **MC-P1** concentration = 1.0 mg / mL and coencapsulated DiO and DiI concentration = 0.8×10^{-6} M.

Additional Figures:

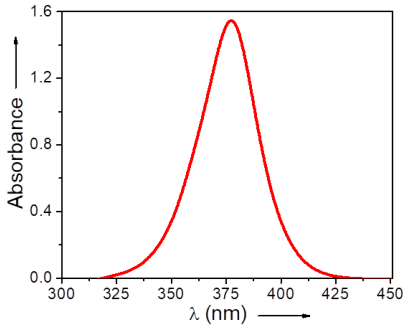


Figure S1: UV-Vis absorption spectrum of **MCOH** in THF showing λ_{max} = 378 nm (Conc. = 0.5 mg / mL). Path length = 1.0 mm.

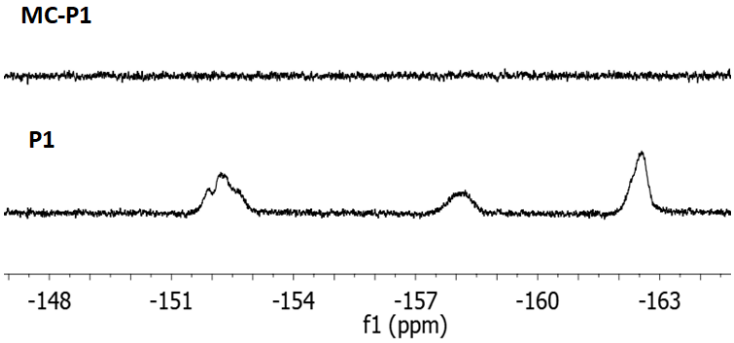


Figure S2: ^{19}F NMR spectrum of **P1** and **MC-P1** in $CDCl_3$.

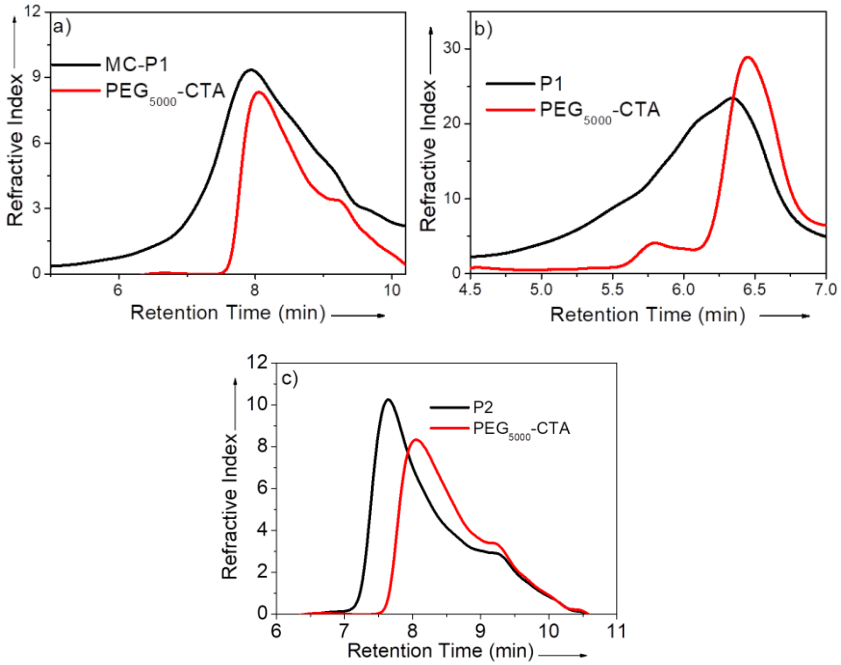


Figure S3: a) GPC chromatogram in THF and b) in DMF. No signal for **MC-P1** was observed in DMF GPC chromatogram. c) GPC chromatogram of **P2** in THF.

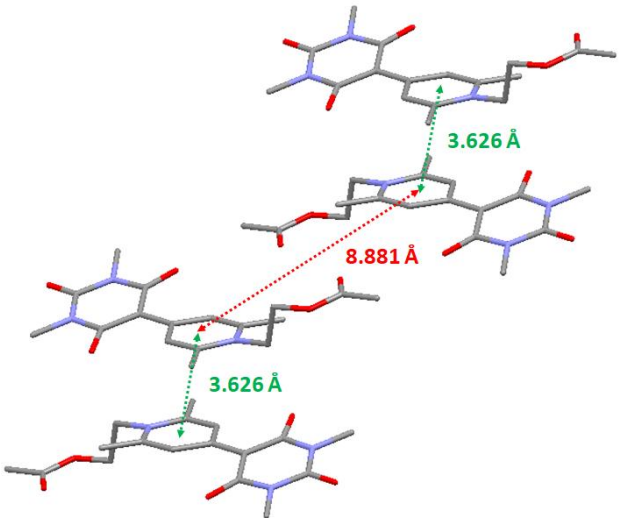


Figure S4: Single crystal structure of **MC-OAc** from CH_2Cl_2. Two anti-parallel dimers are far from π-stacking distance (8.881 Å) for extended stacking.

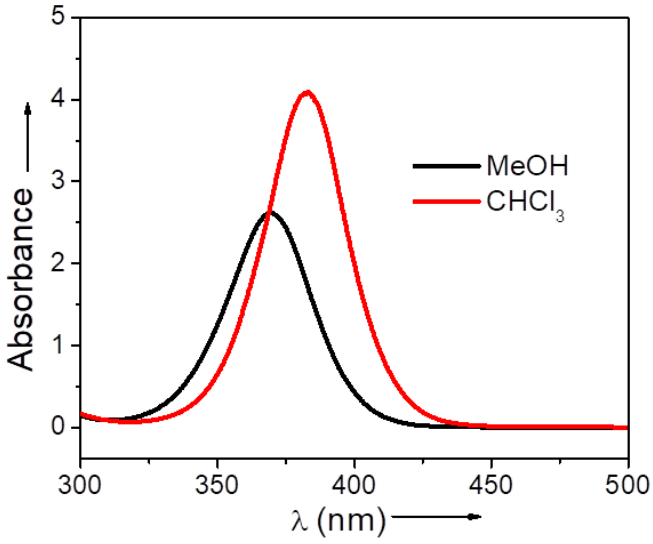
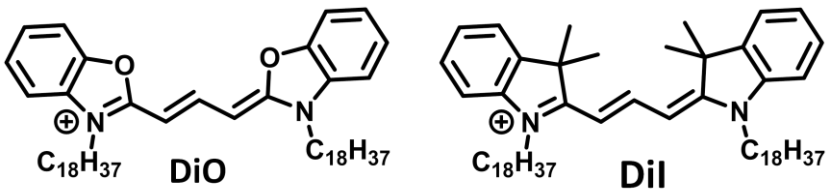


Figure S5: Solvent-dependent UV-Vis absorption spectra of **MC-OAc** (Conc. = 0.5 mg / mL, path length = 1.0 mm).



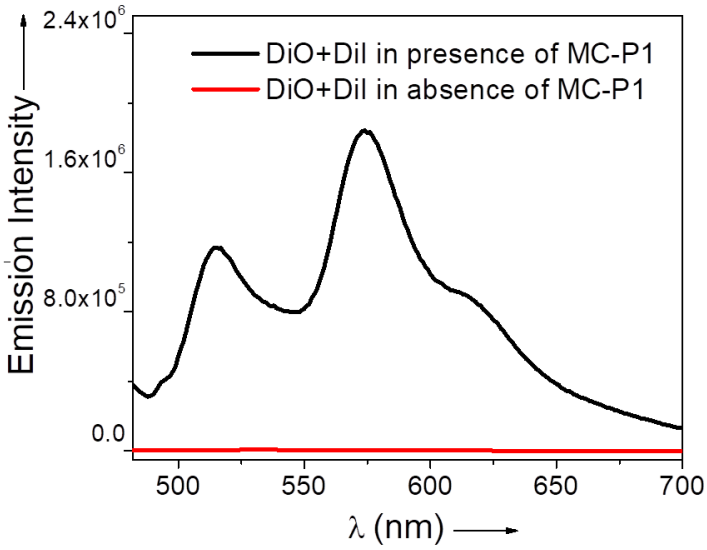


Figure S6: Structure of DiO and DiI dyes (Top); Emission intensity from an aqueous solution of DiO+DiI coencapsulated in **MC-P1** micelle and in absence of **MC-P1** micelle (Bottom). Dye Conc. = 0.8 x10^{-6} M, λ_{ex} = 450 nm.

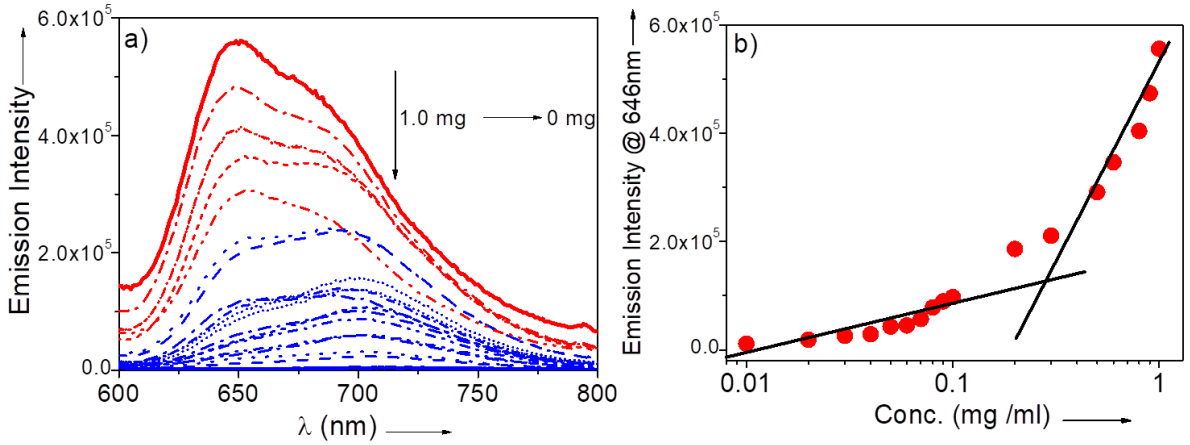


Figure S7: a) Concentration-dependent emission spectra of Nile red (Conc. = 1 × 10^{-6} M, λ_{ex} = 530 nm) loaded **P2** in water; b) Nile red emission vs. **P2** concentration plot; CMC = 0.29 mg/mL ≈ 2.9 x 10^{-5} M.

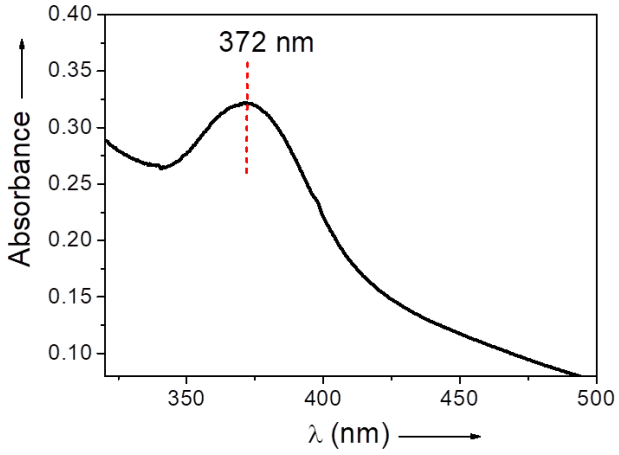


Figure S8: UV-Vis absorption spectrum of **MC-P1** in water below CMC (Conc. = 0.013 mg / mL); λ_{max} = 372 nm, Path length = 1.0 mm.

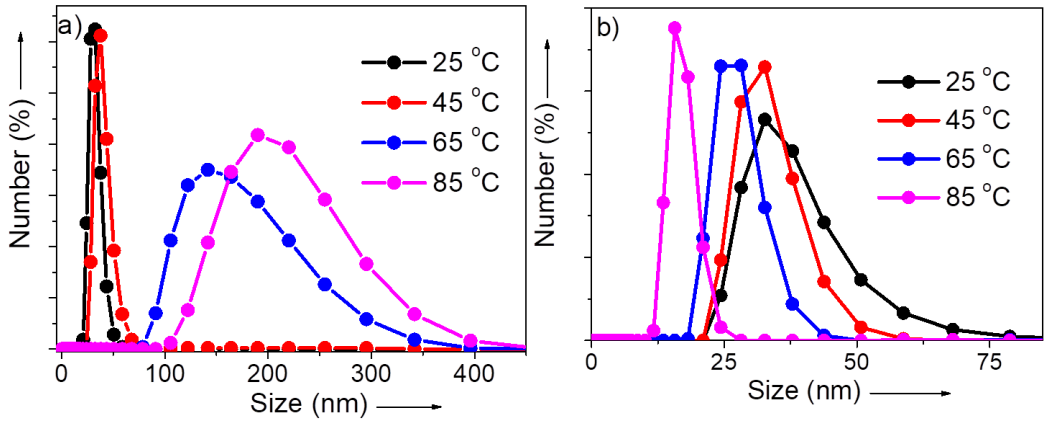


Figure S9: Variable-temperature DLS of a) **P1** and b) **P2** (Conc. = 1.0 mg /mL).

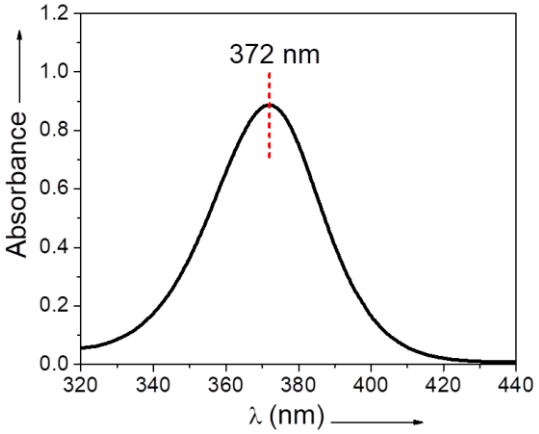


Figure S10: UV-Vis absorption spectrum of **MC-P1** in water with 62% THF (Conc. = 1.0 mg / mL); λ_{max} = 372 nm, Path length = 1.0 mm.

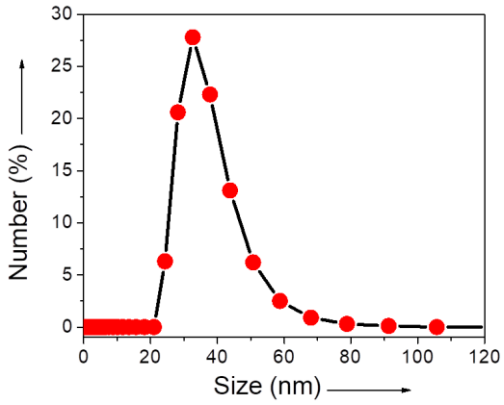


Figure S11: DLS data of **MC-P1** in Toluene at 25 ° C (Conc. = 1.0 mg / mL).

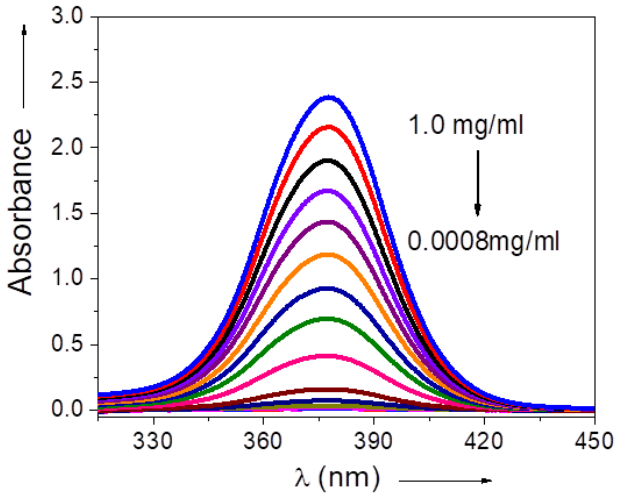


Figure S12: Concentration-dependent UV-Vis absorption spectra of **MC-P1** in toluene; Path length = 1.0 mm.

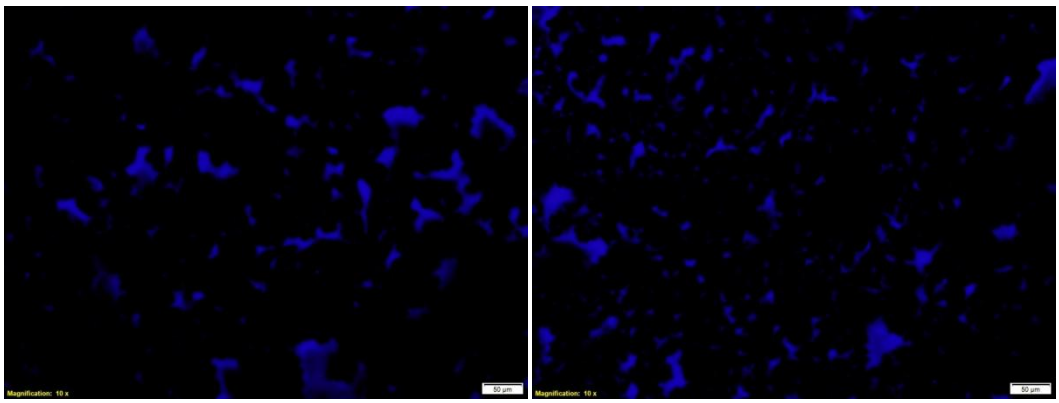


Figure S13: Fluorescence microscopy image from an aggregated solution of **MC-P1** in toluene (Conc. = 1.0 mg / mL).

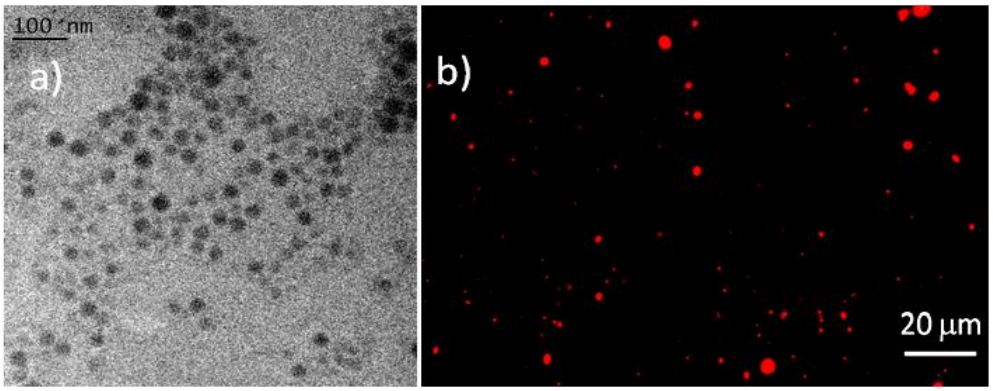


Figure S14: a) TEM image from an aqueous solution of **P1;** b) Nile red loaded aqueous solution of **P1** under fluorescence microscope. Conc. of **P1** = 1.0 mg / mL, Nile red = 1 × 10^{-6} M.

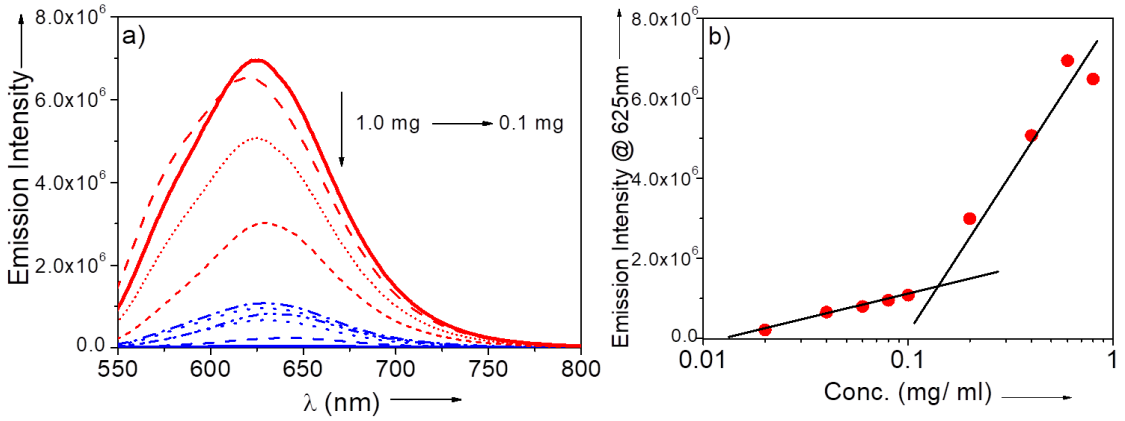


Figure S15: a) Concentration-dependent emission spectra of Nile red (Conc. = 1 × 10^{-6} M, λ_{ex} = 530 nm) loaded **P1** in water; b) Nile red emission vs. **P1** concentration plot; CMC = 0.14 mg/mL ≈ 1.0 x 10^{-5} M.

X-ray Structure Determination:

The molecular structure of **MC-OAc** was determined by single crystal X-ray structure determination. Diffraction-quality crystals were obtained by slow evaporation from a concentrated solution in CH_2Cl_2. Single crystal for **MC-OAc** was coated with Parabar oil and was mounted under a nitrogen cold stream. Data collection was performed at 100 K on a Bruker D8VENTURE Microfocus diffractometer equipped with PHOTON II Detector and Mo Kα radiation (λ = 0.71073 Å), controlled by the APEX3 (v2017.3-0) software package. Space group was assigned by systematic absences (determined by XPREP) and analysis of metric symmetry was further checked by PLATON.[3,4] Structure was solved by direct method and refined against all data in the reported 2θ ranges by full-matrix least squares on F^2 using

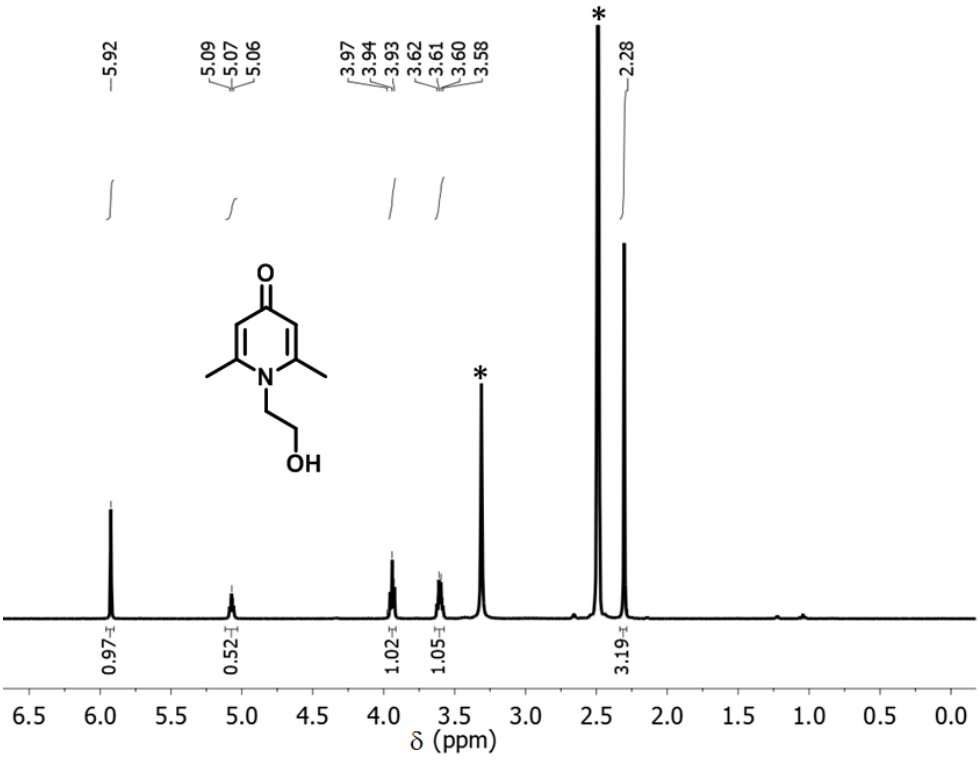
the SHELXL program suite[5] in the WinGX[6] interface. Non-hydrogen atoms were refined anisotropically, and hydrogen atoms were fixed at calculated positions and refined using a riding model. The details of crystal data collection and refinement of complexes are summarized in Table S1.

Table S1: Crystallographic Data for **MC-OAc**

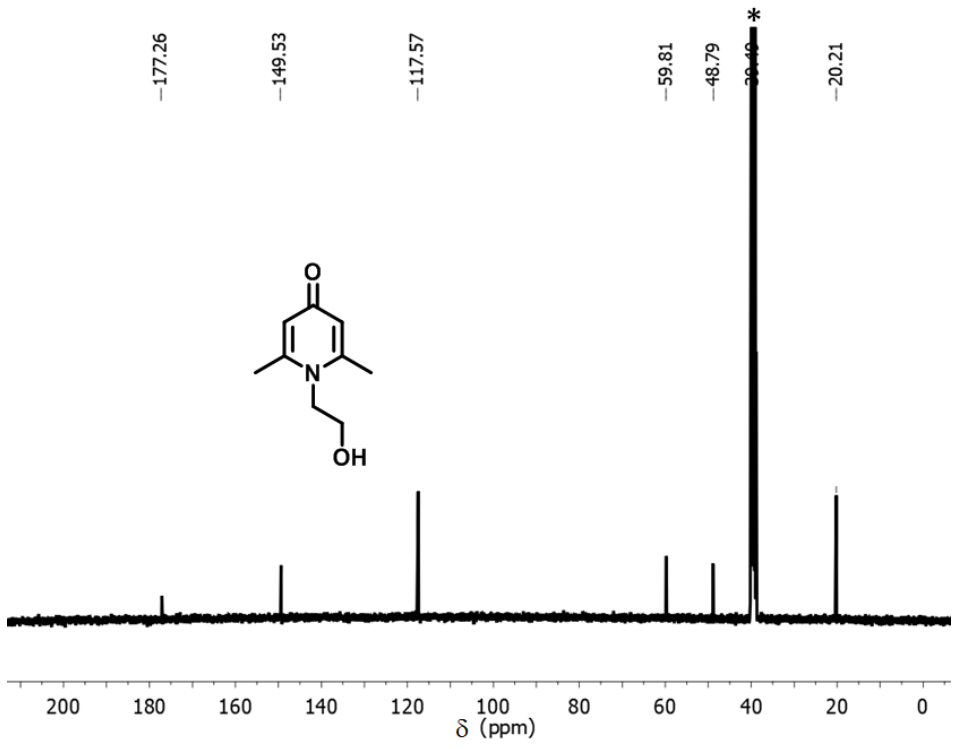
Compound	**MC-OAc**
Empirical formula	$C_{18}\ H_{23}\ Cl_2\ N_3\ O_5$
FW	432.29
T, K	119(2)
Crystal system	Monoclinic
Space group	$P2_1/c$
a, Å	11.6895(10)
b, Å	23.580(2)
c, Å	7.2918(7)
α, deg	90.00°
β, deg	94.989°(3)
γ, deg	90.00°
V, $Å^3$	2002.3(3)
Z, ρ, Mg m^{-3}	4, 1.434
μ, mm^{-1}	0.359
F(000)	904
Refln. collected	17289
Ind. Reflen	2907
Data/restn./param	2907 / 0 / 259
GOF on F^2	1.046
Final R indices [I>2σ(I)]	0.0684, 0.1682

NMR & HRMS Spectra

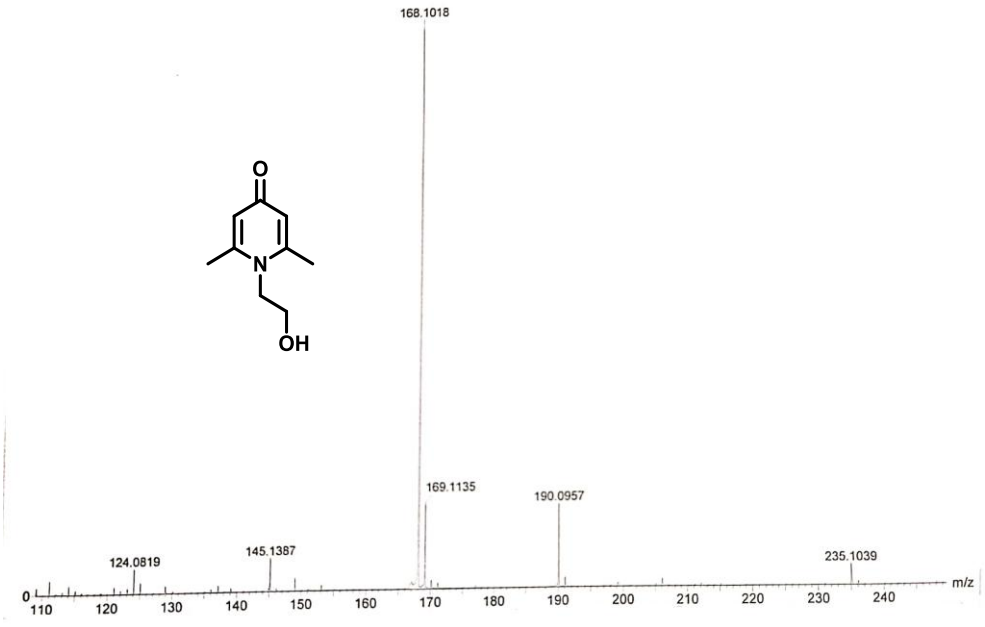
^{1}H NMR spectrum of Compound-3; (*) denotes residual solvent peak from DMSO-d6.



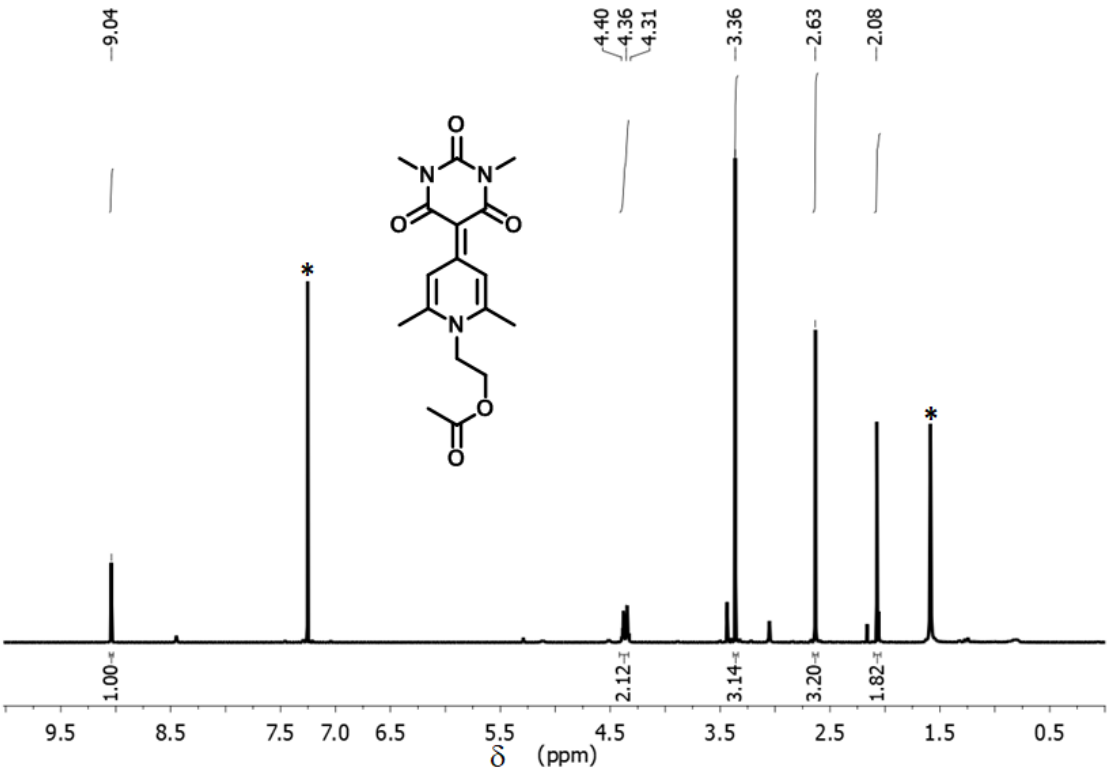
^{13}C NMR spectrum of Compound-3; (*) denotes residual solvent peak from DMSO-d6.



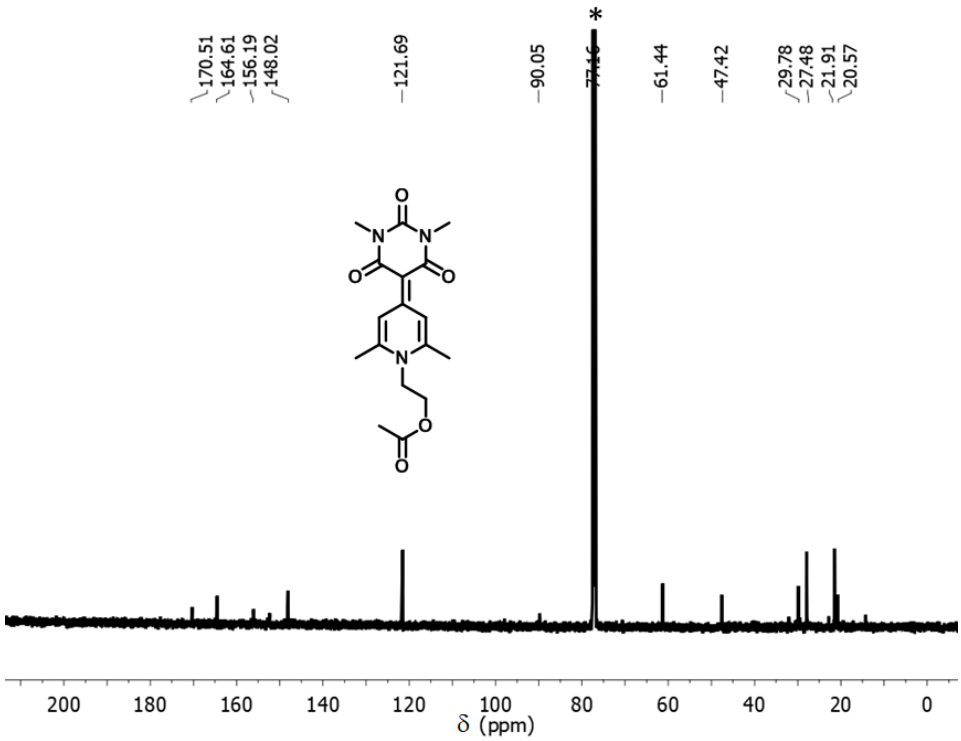
HRMS Spectrum of Compound-3.



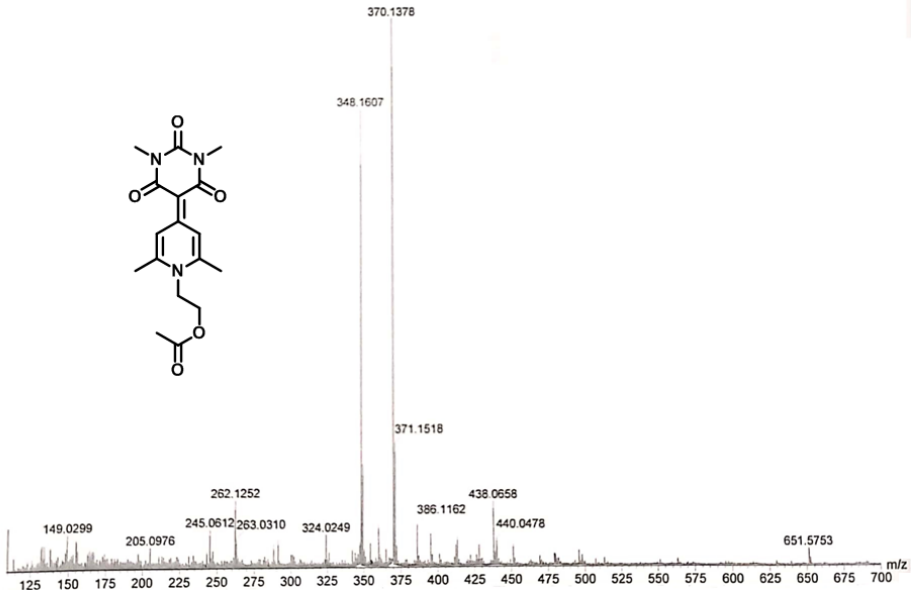
^{1}H NMR spectrum of MC-OAc; (*) denotes residual solvent peak for $CDCl_3$.



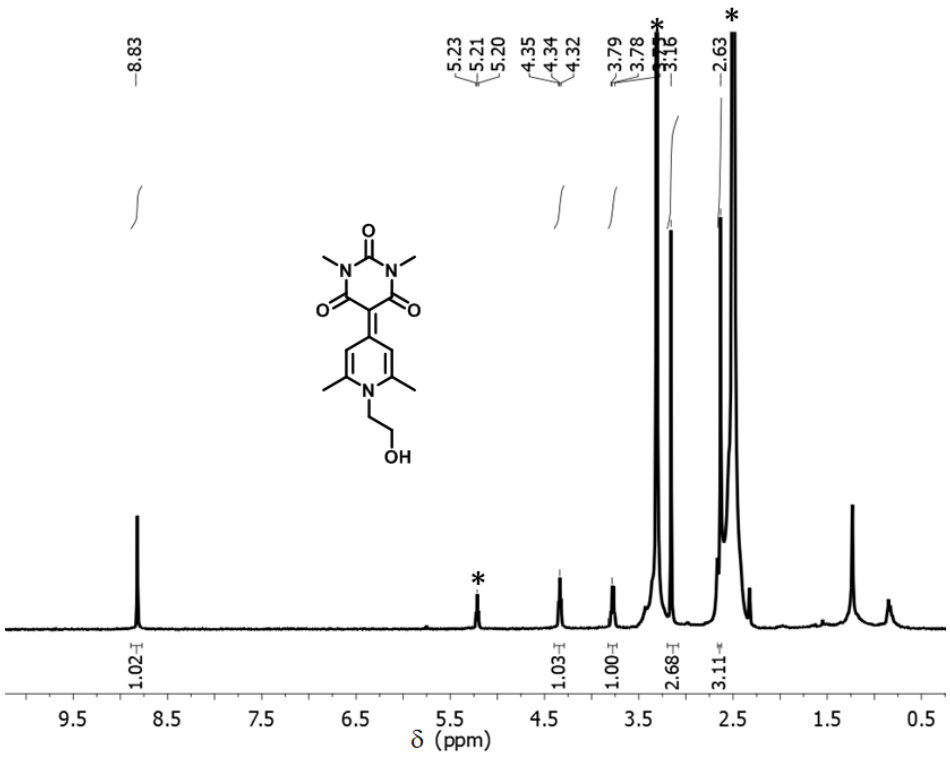
^{13}C NMR spectrum of MC-OAC; (*) denotes residual solvent peak for $CDCl_3$.



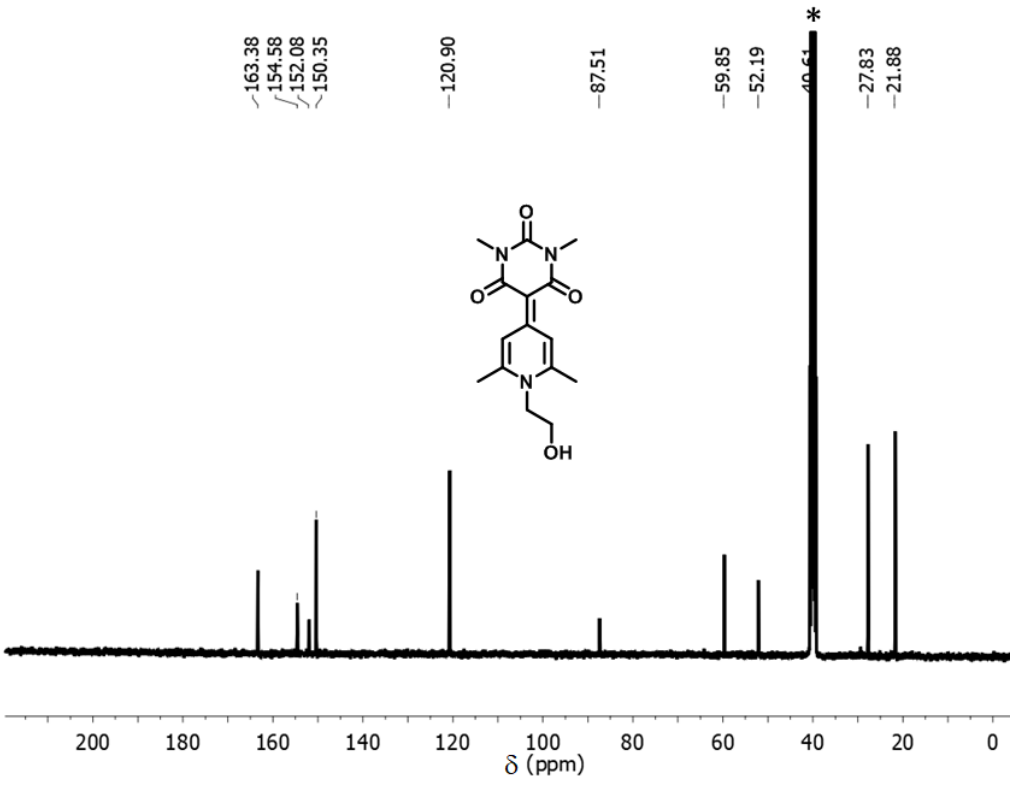
HRMS Spectrum of MC-OAc.



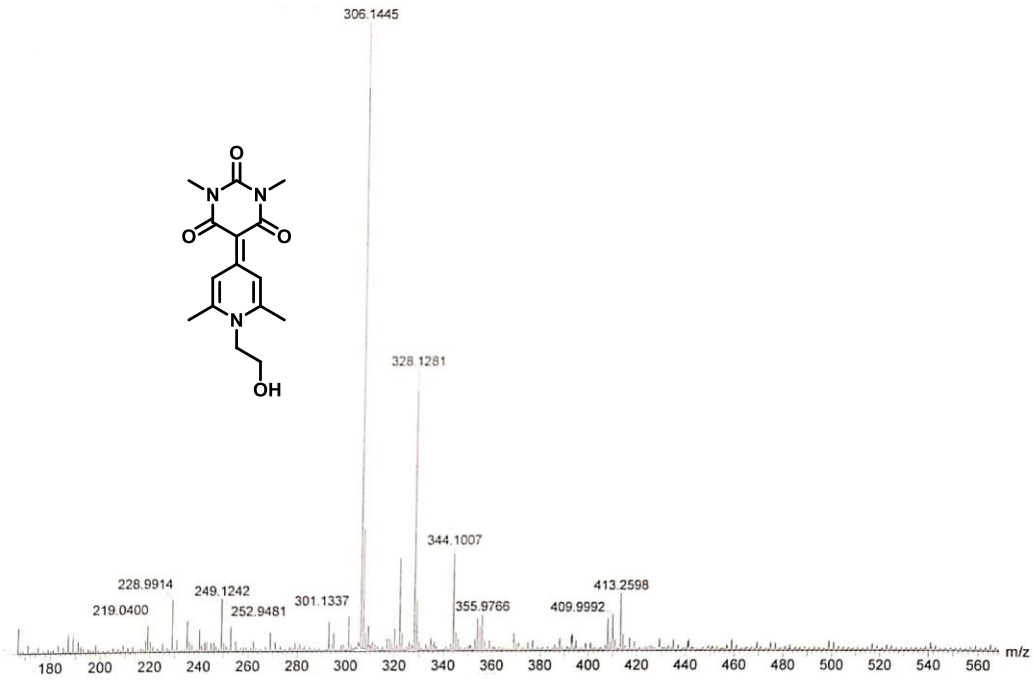
^{1}H NMR spectrum of MC-OH; (*) denotes residual solvent peak for DMSO-d6.



^{13}C NMR spectrum of MC-OH; (*) denotes residual solvent peak from DMSO-d6.



HRMS Spectrum of MC-OH.



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