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Support information

Design, Synthesis, and Bioimaging Applications of a New Class of Carborhodamines

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Contents

1. Experimental methods

1.1. Regents and solvents

All reagents and solvents were purchased from commercial suppliers and used without further purification unless otherwise stated.

1.2. Equipment and measurements

Thin-layer chromatography (TLC) was used to monitor the reactions and silica gel (200–300 mesh) was performed to column chromatography. Absorption spectra were obtained on Varian Cary 4000 spectrophotometer. Fluorescence spectra were obtained on a Hitachi F-7000 fluorescence spectrometer. The ^{1}H NMR and ^{13}C NMR spectra were measured on a Bruker spectrometer, and recorded at 600 and 150 MHz, respectively. High resolution mass spectra were obtained on a Thermo Scientific Q Exactive Mass spectrometer. The fluorescence imaging assays in cells were performed in a Zeiss LSM 880+ Airyscan Laser Scanning Confocal Microscope with a 60×oil–immersion objective lens.

*1.3 Chemical stability test of **MCR1-5***

We prepared test solution of **MCR1-5** (2 μM) containing 20 μM various ROS ($^1O_2$, H_2O_2, HOCl, TBHP, and •OH) by adding reagents as follows:

MCR1-5: 2 mM stock solution in DMSO diluted to 2 μM with PBS

$^1O_2$: generated in situ by mixing 20 μM NaOCl and 200 μM H_2O_2

H_2O_2: commercial 30% H_2O_2 solution diluted to 20 μM (Its concentration was determined by using an extinction coefficient of 43.6 $M^{-1}cm^{-1}$ at 240 nm.)

HOCl: commercial NaClO solution diluted to 20 μM（Its concentration was determined using an extinction coefficient of 350 $M^{-1}cm^{-1}$ at 293 nm.)

TBHP: commercial TBHP solution (70 % by weight in H_2O) diluted to 20 μM

•OH: generated in situ by mixing 20 μM Fe $(ClO_4)_2$ with 200 μM H_2O_2.

MCR1-5 solutions containing each ROS were kept in dark for 30 min and then corresponding fluorescence spectra of the samples were measured.

1.4 Photobleaching Assays.

The in vitro photobleaching assays were carried out in square cross section quartz cells (1 × 1 cm). The PBS solutions of the dyes (2 μM) were irradiated with a 620 nm LED light source (45 mW/cm^2) at room temperature for 30 min. The fluorescent intensities at the emission maxima of **MCR1 − 5** and **Cy5** were measured every one minute on a Hitachi F-7000 fluorescence spectrometer.

1.5 Cell Culture and Fluorescence Imaging.

The HeLa cells were kindly provided by Key Laboratory of Chemical Biology and Molecular Engineering of Ministry of Education (China). HeLa Cells were grown in DMEM medium supplemented with 10% FBS (fetal bovine serum) and 1% antibiotics at 37 °C in a humidified environment of 5% CO_2. Cells were plated on a glass-bottom cell culture dish (30 mm) and allowed to adhere for 12 h. For imaging experiments with **MCR1-5**, the cells were treated with the corresponding dye (1 μM) in DMEM medium for 15 min. After the cells were washed with PBS for three times, the fluorescence imaging assays were performed. For imaging experiments with the $^1O_2$ probe **MCR-DMA**, the living HeLa cells were cultivated with 5-ALA (150 μg/mL) in

DMEM medium for 4 h and washed three times with PBS, then treated with **MCR-DMA** (0.5 μM) for another 30 min. In the control experiment with $^1O_2$ scavenger NaN_3, the 5-ALA (150 μg/mL) treated cells were first cultivated with **MCR-DMA** (0.5 μM) for 30 min and then treated with NaN_3 (200 μM) for another 10 min. All the cells were washed three times with PBS before imaging, and the fluorescence imaging were then performed in a Zeiss LSM 880+ Airyscan Laser Scanning Confocal Microscope with a 60×oil–immersion objective lens. To evaluate the subcellular localization, HeLa cells were co-stained with the corresponding dye (**MCR1-5** or **MCR-DMA**, 0.5 μM) and MitoTracker Green FM (0.2 μM) or LysoTracker Green (0.2 μM) in the culture medium for 15 min at 37 °C. After the cells were washed three times with PBS, fluorescence imaging was performed. Emission was collected at 500−600 nm for LysoTracker Green and MitoTracker Green (excited at 488 nm), and at 650−750 nm for **MCR1-5** and **MCR-DMA** (excited at 633 nm).

1.6 Cytotoxicity Assays.

HeLa cells were seeded into a 96-well plate in DMEM medium supplemented with 10% FBS and 1% antibiotics at 37°C in a humidified environment of 5% CO_2. After 24 h of cell attachment, the cells were washed with PBS, followed by addition of increasing concentrations of the corresponding dye in DMEM medium. The final concentrations of the dyes were kept from 0 to 10 μM. The cells were then incubated at 37 °C in an atmosphere of 5% CO_2 and 95% air for 24 h, followed by MTT assays. Untreated assays with DMEM medium (n = 6) were also conducted under the same conditions.

*1.7 Selectivity Tests of **MCR-DMA**.*

The aqueous solutions of Na^+, K^+, Mg^{2+}, Fe^{3+}, Cu^{2+}, Zn^{2+} were prepared from their chloride salts and the aqueous solutions of Cl^-, Br^-, CO_3^{2-}, were prepared from their sodium salts. O_2^- was prepared by dissolving KO_2 to dry dimethyl sulfoxide. Hydroxyl radical (•OH) was generated in situ through the Fenton reaction of $Fe(ClO_4)_2$ and H_2O_2 (10 equiv) and its concentration was equal to the Fe(II) concentration. $^1O_2$ was generated in situ by photoirradiation of TMPyP4. NO was generated from a commercially available NO donor NOC-9 (dissolved in 0.1M NaOH solution). H_2O_2 solution was prepared by dilution of commercial H_2O_2 solution in deionized water, and its

concentration was determined by using an extinction coefficient of 43.6 $M^{-1}cm^{-1}$ at 240 nm. HClO solution was prepared by the dilution of commercial NaClO solution in deionized water, and its concentration was determined using an extinction coefficient of 350 $M^{-1}cm^{-1}$ at 293 nm. $ONOO^-$ was generated from a commercially available $ONOO^-$ donor SIN-1 (dissolved in 0.01 M NaOH solution). The aqueous solutions of Cys, GSH were freshly prepared by dissolving Cys and GSH in deionized water.

The test solution of **MCR-DMA** (5 μM) in 10 mM PBS buffer solution (pH 7.4) was prepared by placing 5 μL of the **MCR-DMA** stock solution (2 mM in DMSO) in 1.995 mL buffer solution containing various biological species. The resulting solutions were kept at ambient temperature for 15 min and then the fluorescence intensities were measured.

1.8 Determination of Quantum Yields

Fluorescence quantum yields of all samples were determined via the relative determination method and Cy5 (Φ = 0.27 in PBS) was selected as the standard.

The quantum yields were calculated using the following Equation:

$$\Phi_u = [(A_s F A_u \eta^2)/(A_u F A_s \eta_0^2)]\Phi_s$$

Where A_s and A_u are the absorbance of the reference and sample solution at the reference excitation wavelength, FA_s and FA_u are the corresponding integrated fluorescence intensity, and η and η_0 are the solvent refractive indexes of sample and reference, respectively. Absorbance of sample and reference at their respective excitation wavelengths was controlled to be lower than 0.05. Reported values are averages (n = 3).

2. Synthesis and characterization of the compounds

*2.1.Synthesis of compounds **2-4***

Synthesis of compound **2**: compound **1** [1] (1.43 g, 6.0 mmol) was dissolved in dry DMF (30 mL) under N_2 and then sodium hydride (0.72 g, 30 mmol) was added slowly. 30 minutes later, methyl iodide (1.86 mL, 30 mmol) was added dropwise. The reaction mixture was heated at 90 °C for 18 h and then quenched by the addition of water. The remaining solution was extracted with ethyl acetate for three times and the combined organic layer was dried over Na_2SO_4. The solvent was evaporated and the residue was purified by silica gel chromatography (CH_2Cl_2 / PE = 1 / 1) to yield **2** as a red solid (1.41 g, 80%). ^{1}H-NMR ($CDCl_3$, 600 MHz) δ (ppm): 8.16 (d, *J* = 8.4 Hz, 2H),

7.46 (d, J = 3.0 Hz, 2H), 6.97 (q, J = 3.0 Hz, 2H), 3.15 (s, 12H). ^{13}C-NMR ($CDCl_3$, 150 MHz): δ 185.3, 181.0, 153.1, 135.0, 129.2, 123.0, 115.9, 108.6, 40.3. HRMS: calculated for $C_{18}H_{19}N_2O_2$ $[M+H]^+$: 295.1441; found: 295.1442.

Synthesis of compound **3***:* compound **2** (1.00 g, 3.4 mmol) was dissolved in dry THF (100 mL) and then methyl magnesium bromide (1.0 M in THF, 10 mL) was added dropwise. The reaction mixture was stirred at room temperature for 30 min and quenched by the addition of water. The remaining solution was diluted with brine and then extracted with ethyl acetate for three times. The combined organic layer was dried over Na_2SO_4, filtered and evaporated. The residue was purified by silica gel chromatography (CH_2Cl_2 / EtOAc = 20 / 1) to yield **3** as a yellow solid (0.51g, 49%). ^{1}H-NMR ($CDCl_3$, 600 MHz) δ (ppm): 8.14 (d, J = 8.4 Hz, 2H), 7.10 (s, 2H), 6.75 (d, J = 8.4 Hz, 2H), 3.12 (s, 12H), 1.70 (s, 3H). ^{13}C-NMR ($CDCl_3$, 150 MHz): δ 180.8, 153.3, 150.8, 129.1, 119.5, 111.3, 106.8, 71.2, 40.2, 37.6. HRMS: calculated for $C_{19}H_{23}N_2O_2$ $[M+H]^+$: 311.1754; found: 311.1751.

Synthesis of compound **4***:* compound **3** (0.31 g, 1.0 mmol) and sodium hydride (0.072 g, 3.0 mmol) were dissolved in dry DMF (10 mL) and then methyl iodide (186 μL, 3.0 mmol) was added. The reaction mixture was stirred at room temperature for 6 h. It was subsequently quenched with saturated NH_4Cl, diluted with water, and extracted with ethyl acetate for three times. The combined organics were washed with brine, dried over Na_2SO_4, filtered and evaporated. The residue was purified by silica gel chromatography (CH_2Cl_2 / EtOAc = 50 / 1) to provide **4** as a yellow solid (0.26 g, 80%). ^{1}H-NMR ($CDCl_3$, 600 MHz) δ (ppm): 8.23 (d, J = 8.4 Hz, 2H), 6.94 (s, 2H), 6.81(d, J = 8.4 Hz, 2H), 3.14 (s, 12H), 2.98 (s, 3H), 1.71 (s, 3H). ^{13}C-NMR ($CDCl_3$, 150 MHz): δ 180.7, 153.3, 147.2, 129.2, 121.3, 111.6, 107.1, 76.2, 52.4, 40.2, 37.3. HRMS: calculated for $C_{20}H_{25}N_2O_2$ $[M+H]^+$: 325.1911; found: 325.1913.

*2.2. General Procedures for Synthesis of **MCRs***

Bromobenzene derivative (3.0 mmol) and anhydrous THF (10 mL) were added to a flame dried flask flushed with argon. The solution was cooled to −78 °C, and then *n*-BuLi (2.4 M, 1.2 mmol) was added. The resulting mixture was stirred for 1 h at the same temperature. Compound **4** (0.11 g, 0.33mmol) in anhydrous THF (10 mL) was slowly added to the mixture, and after that, the mixture was warmed to room temperature and then stirred for 2 h. The reaction was quenched by

addition of 2 N HCl until the solution color turned from yellow to bluish green. The mixture was extracted with CH_2Cl_2 and the organic layer was dried over Na_2SO_4 and then evaporated to dryness. The crude product was purified by silica column chromatography (CH_2Cl_2 / CH_3OH = 30 / 1) to afford desired products.

MCR-1: (70%, blue solid) ^{1}H-NMR ($CDCl_3$, 600 MHz) δ (ppm): 7.57 (m, 4H), 7.33 (m, 1H), 7.28 (m, 2H), 7.19 (d, *J* = 9.6 Hz, 2H), 6.79 (q, *J* = 2.4 Hz, 2H), 3.50 (s, 12H), 3.14 (s, 3H), 1.72 (s, 3H). ^{13}C-NMR ($CDCl_3$, 150 MHz): δ 162.4, 156.2, 151.7, 138.1, 134.9, 130.0, 129.4, 128.9, 128,4, 121.3, 113.6, 111.5, 79.9, 53.8, 41.7, 39.5. HRMS: calculated for $[M]^+$: 385.2274; found: 385.2271.

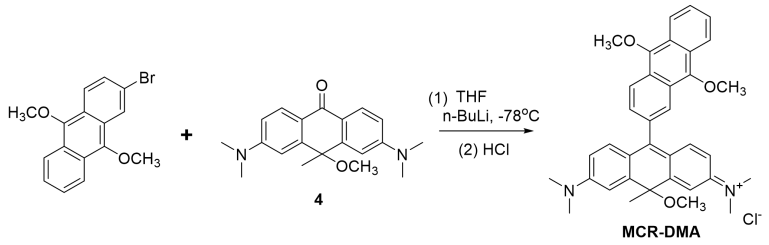
MCR-2: (80%, blue solid) ^{1}H-NMR ($CDCl_3$, 600 MHz) δ (ppm): 7.44 (s, 1H), 7.36 (d, *J* = 4.2 Hz, 2H), 7.21 (s, 2H), 7.13 (d, *J* = 7.8 Hz, 1H), 7.06 (d, *J* = 9.6 Hz, 2H), 6.76 (d, *J* = 9.0 Hz, 2H), 3.48 (s, 12H), 3.13 (s, 3H), 2.04 (s, 3H), 1.67 (s, 3H). ^{13}C-NMR ($CDCl_3$, 150 MHz): δ 162.2, 156.3, 151.6, 137.4, 135.4, 134.4, 130.4, 129.5, 129.4, 125.8, 121.2, 113.9, 111.1, 79.7, 53.8, 41.8, 39.6, 19.5. HRMS: calculated for $[M]^+$: 399.2431; found: 399.2428.

MCR-3: (62%, blue solid) ^{1}H-NMR ($CDCl_3$, 600 MHz) δ (ppm): 7.33 (t, *J* = 7.8Hz, 1H), 7.23 (s, 2H), 7.19 (t, *J* = 4.8 Hz, 2H), 7.01 (d, *J* = 9.6 Hz, 2H), 6.75 (d, *J* = 9.6 Hz, 2H), 3.49 (s, 12H); 3.11 (s, 3H); 1.99 (s, 3H); 1.93 (s, 3H); 1.69 (s, 3H). ^{13}C-NMR ($CDCl_3$, 150 MHz): δ 163.1, 156.5, 151.6, 136.4, 135.9, 135.2, 134.3, 129.0, 127.7, 120.7, 114.1, 111.3, 79.6, 53.6, 41.7, 39.6, 19.7, 19.6. HRMS: calculated for $[M]^+$: 413.2587; found: 413.2584.

MCR-4: (60%, blue solid) ^{1}H-NMR ($CDCl_3$, 600 MHz) δ (ppm): 7.53 (q, *J* = 4.2Hz, 1H), 7.20 (s, 2H), 7.15-7.06 (m, 5H), 6.76-6.74 (dd, *J* = 2.4 Hz, 2H), 3.70 (s, 3H), 3.47 (s, 12H); 3.11 (s, 3H); 1.68 (s, 3H). ^{13}C-NMR ($CDCl_3$, 150 MHz): δ 160.8, 156.8, 156.5, 156.3, 156.2, 151.5, 151.4, 137.7, 137.6, 131.1, 131.0, 129.9, 123.8, 123.6, 121.8, 121.5, 120.5, 113.6, 111.3, 111.1, 111.0, 79.9, 55.9, 53.8, 41.7, 39.4. HRMS: calculated for $[M]^+$: 415.2380; found: 415.2377.

MCR-5: (50%, blue solid) ^{1}H-NMR ($CDCl_3$, 600 MHz) δ (ppm): 7.49 (t, *J* = 8.4 Hz, 1H), 7.18 (s, 2H), 7.16 (d, *J* = 8.4 Hz, 2H), 6.77 (d, *J* = 8.4 Hz, 2H), 6.73-6.69 (dd, *J* = 7.8 Hz, 2H), 3.68 (s, 3H), 3.66 (s, 3H), 3.45 (s, 12H), 3.14 (s, 3H), 1.68 (s, 3H). ^{13}C-NMR ($CDCl_3$, 150 MHz): δ 157.7, 157.4, 156.4, 151.8, 137.5, 131.6, 122.1, 113.6, 111.8, 110.5, 103.9, 79.9, 56.2, 53.8, 41.6, 39.3. HRMS: calculated for $[M]^+$: 445.2486; found: 445.2484.

*2.3. Synthesis of **MCR-DMA***



2-bromo-9,10-dimethoxyanthracene [2] (0.316 g, 1.0 mmol) and anhydrous THF (10 mL) were added to a flame dried flask flushed with argon. The solution was cooled to −78 °C, and then *n*-BuLi (2.4 M, 0.33 mmol) was added. The resulting mixture was stirred for 1 h at the same temperature. Compound **5** (0.11 g, 0.33mmol) in anhydrous THF (10 mL) was slowly added to the mixture, and after that, the mixture was warmed to room temperature and then stirred for 2 h. The reaction was quenched by addition of 2 N HCl until the solution color turned from yellow to bluish green. The mixture was extracted with CH_2Cl_2 and the organic layer was dried over Na_2SO_4 and then evaporated to dryness. The crude product was purified by silica column chromatography (CH_2Cl_2 / CH_3OH = 30 / 1) to afford **MCR-DMA** (65%, blue solid). ^{1}H-NMR ($CDCl_3$, 600 MHz) δ (ppm): 8.46 (t, *J* = 7.2 Hz, 1H), 8.37 (d, *J* = 7.2 Hz, 1H), 8.33 (d, *J* = 7.2 Hz, 1H), 8.23 (s, 1H), 7.59 (m, 2H), 7.36 (m, 3H), 7.28 (s, 2H), 6.80 (d, *J* = 8.4 Hz, 2H), 4.22 (s, 3H), 4.12 (s, 3H), 3.45 (s, 12H), 3.17-3.14 (d, 3H), 1.76-1.73 (d, 3H). ^{13}C-NMR ($CDCl_3$, 150 MHz): δ 163.9, 156.3, 152.1, 149.2, 148.8, 138.5, 126.2, 126.0, 124.1, 123.5, 121.5, 121.4, 113.5, 111.3, 79.5, 64.0, 63.6, 53.7, 41.5, 39.7. HRMS: calculated for $[M]^+$: 545.2799; found: 545.2793.

3. Reference:

[1] Huang, H. Synthesis, telomerase inhibition and cytotoxic studies on 2,7-disubstituted anthraquinone derivatives. US 20090253709A1.

[2] Seidel, N.; Hahn, T.; Simon, L.; Kortus, J.; Weber, E. Synthesis and properties of new 9,10-anthraquinone derived compounds for molecular electronics. *New Journal of Chemistry*. 2013, **37**, 601-610.

4. Supplementary Figures

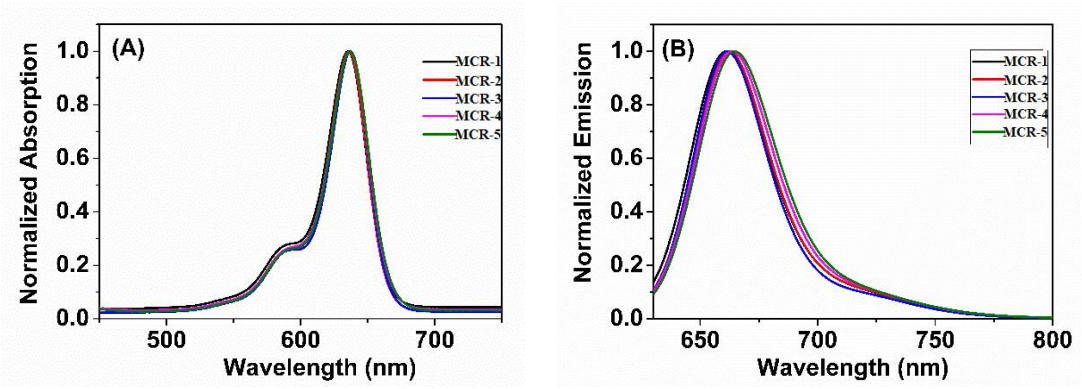


Figure S1. Normalized absorption (A) and emission (B) spectra of **MCR1−5** in EtOH at 25 °C. λ_{ex} = 620 nm; slits, 5/5 nm.

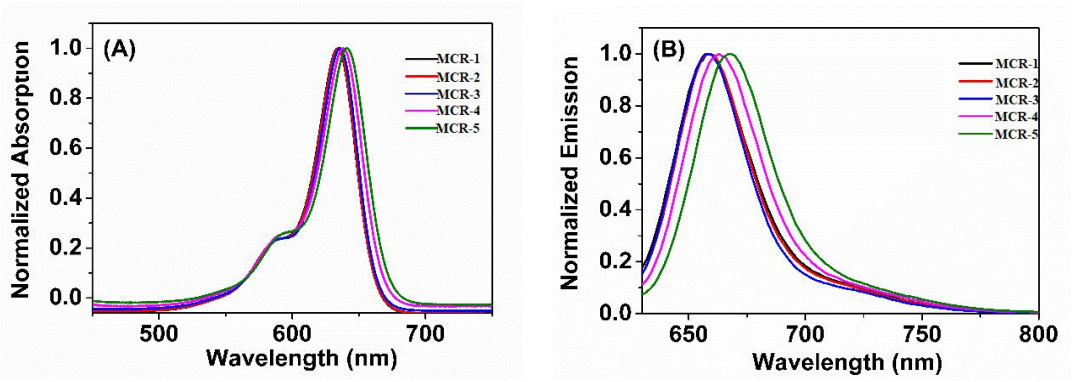


Figure S2. Normalized absorption (A) and emission (B) spectra of **MCR1−5** in PBS at 25 °C. λ_{ex} = 620 nm; slits, 5/5 nm.

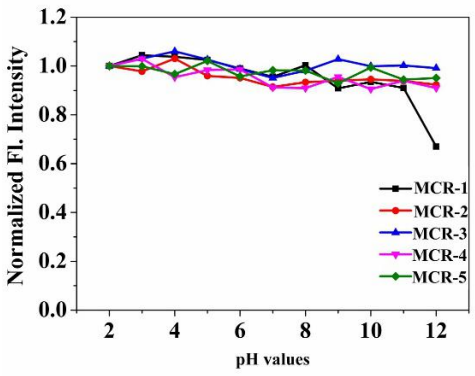


Figure S3. Normalized fluorescence intensities of **MCR1-5** at various pH values.

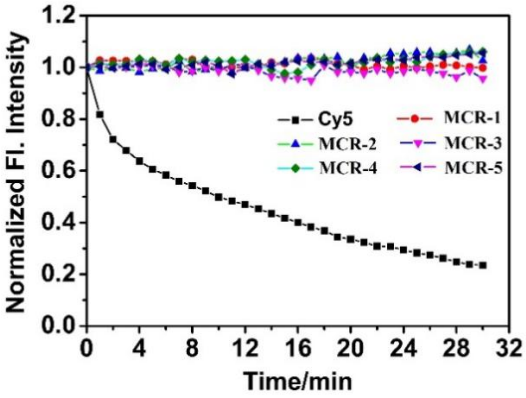


Figure S4. Normalized time-dependent fluorescence intensity changes of **MCR1-5** and Cy5 in PBS (10 mM, pH 7.4) with irradiation by a LED lamp (45 mW/cm^2) for 30 min.

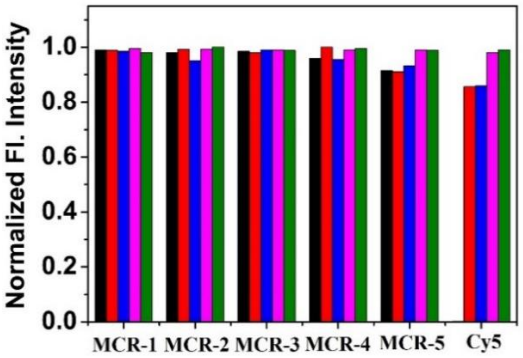


Figure S5. Normalized fluorescence intensity changes of **MCR1-5** and Cy5 in PBS toward common ROS. The solutions of **MCR1-5** (2 μM) were mixed with various ROS (20 μM) for 30 min (black: HClO, red: H_2O_2, blue: TBHP, pink: •OH, green: $^1O_2$).

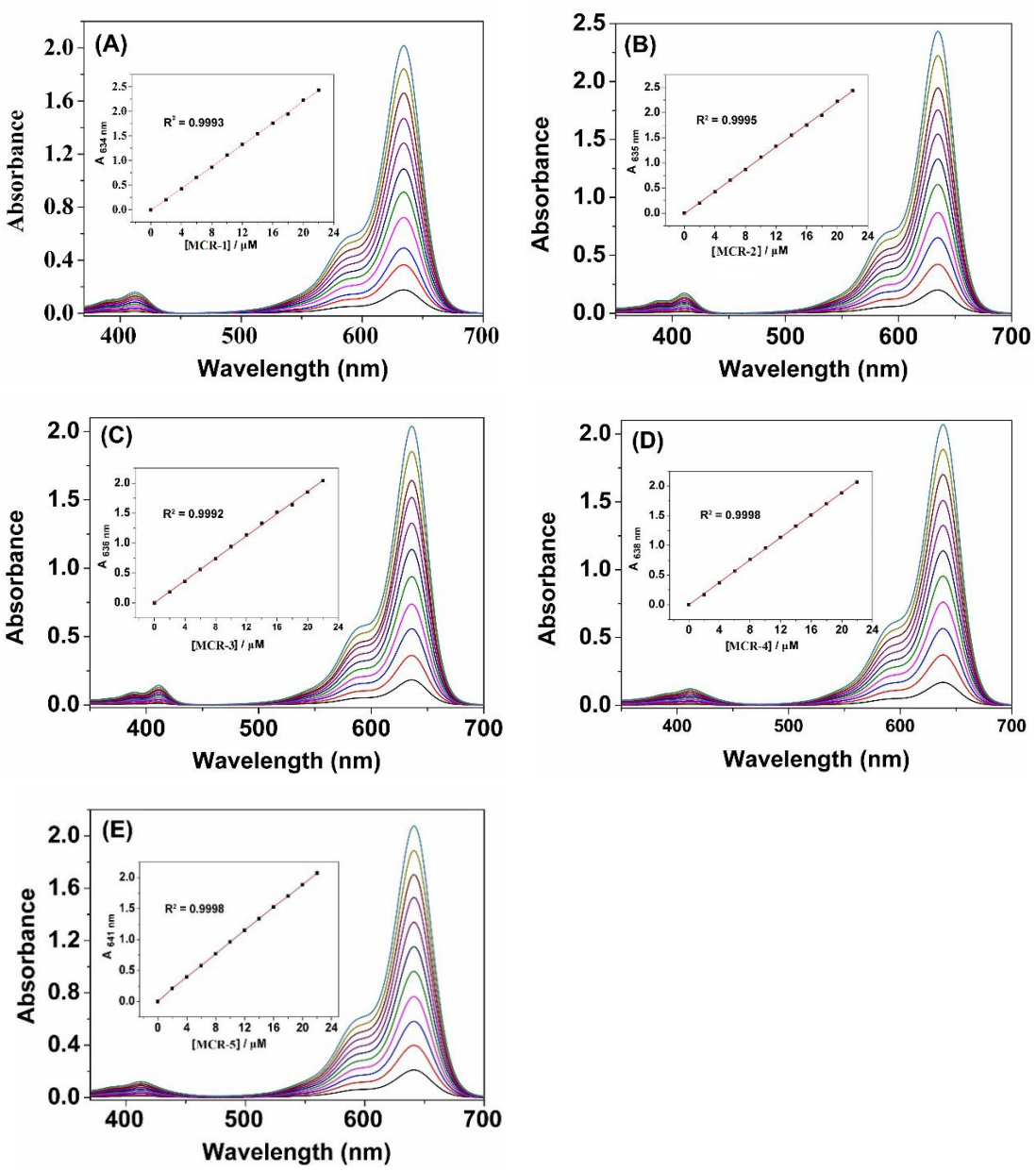


Figure S6. Solubility evaluation of **MCR1-5** in PBS (10 mM, pH = 7.4) by absorption spectra. (inset) Plots of absorption intensity vs dye concentrations.

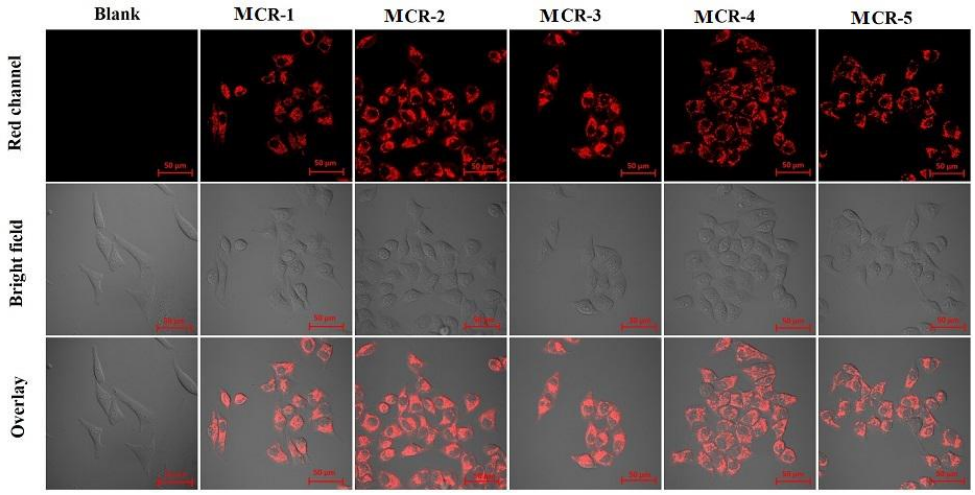


Figure S7. Fluorescence images of HeLa cells incubated with **MCR1-5** (1 μM) for 15 min at 37 °C. Excited at 633 nm and collected at 650-750 nm, scale bar 50 μm.

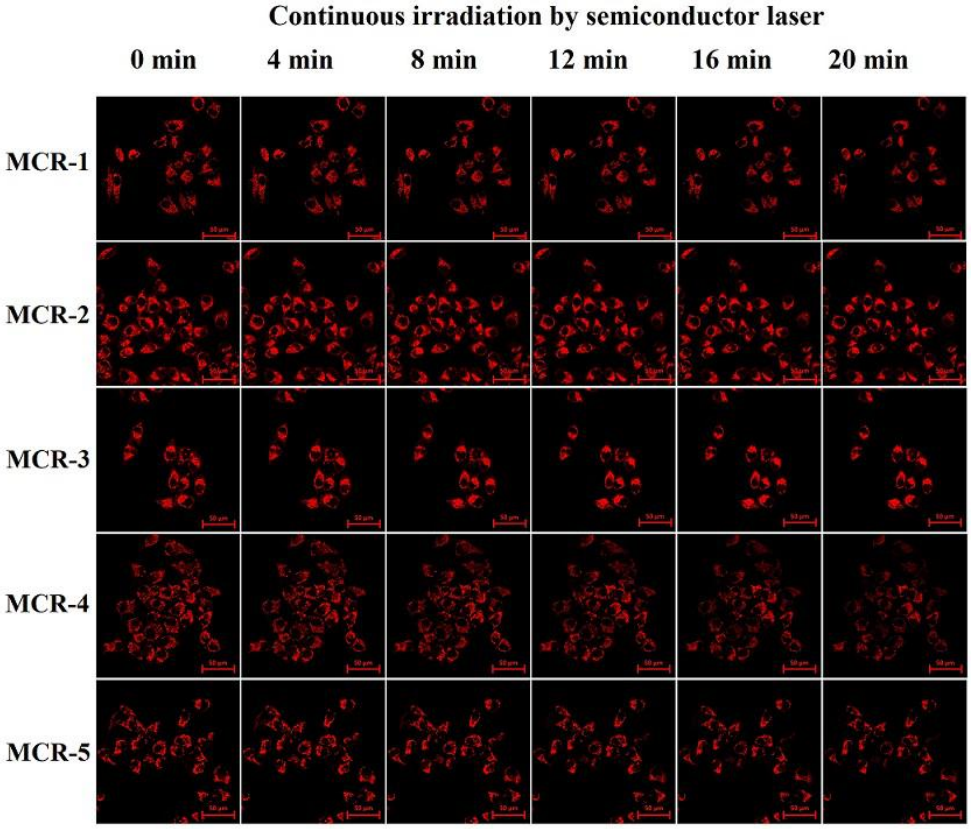


Figure S8. The intracellular photostability assays. Time-dependent confocal images of HeLa cells stained with **MCR1-5** (1 μM), respectively, under continuous irradiation by semiconductor laser (633 nm, 2% of laser power) for 20 min. Images were obtained at indicated time point. Scale bar: 50 μm.

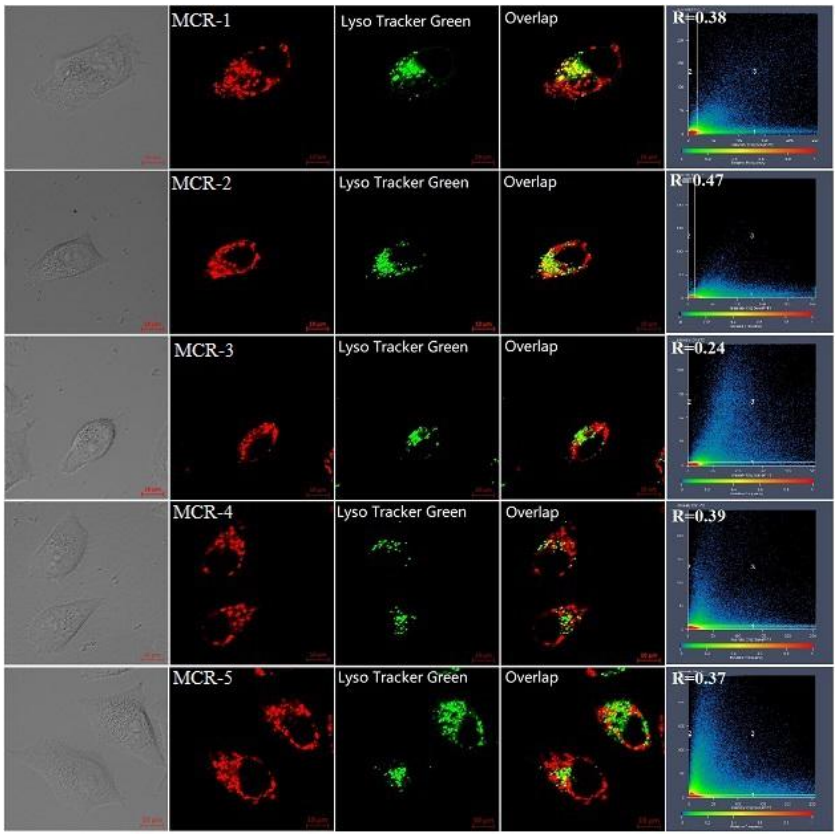


Figure S9. Fluorescence images of HeLa cells costained with **MCR**s (0.5 μM, 15 min) and Lyso Tracker Green (0.2 μM, 15 min) in PBS at 37 °C. For **MCR**s, emissions were collected at 650−750 nm (λ_{ex} = 633 nm); for Lyso Tracker Green, at 500−600 (λ_{ex} = 488 nm). Scale bar: 10 μm.

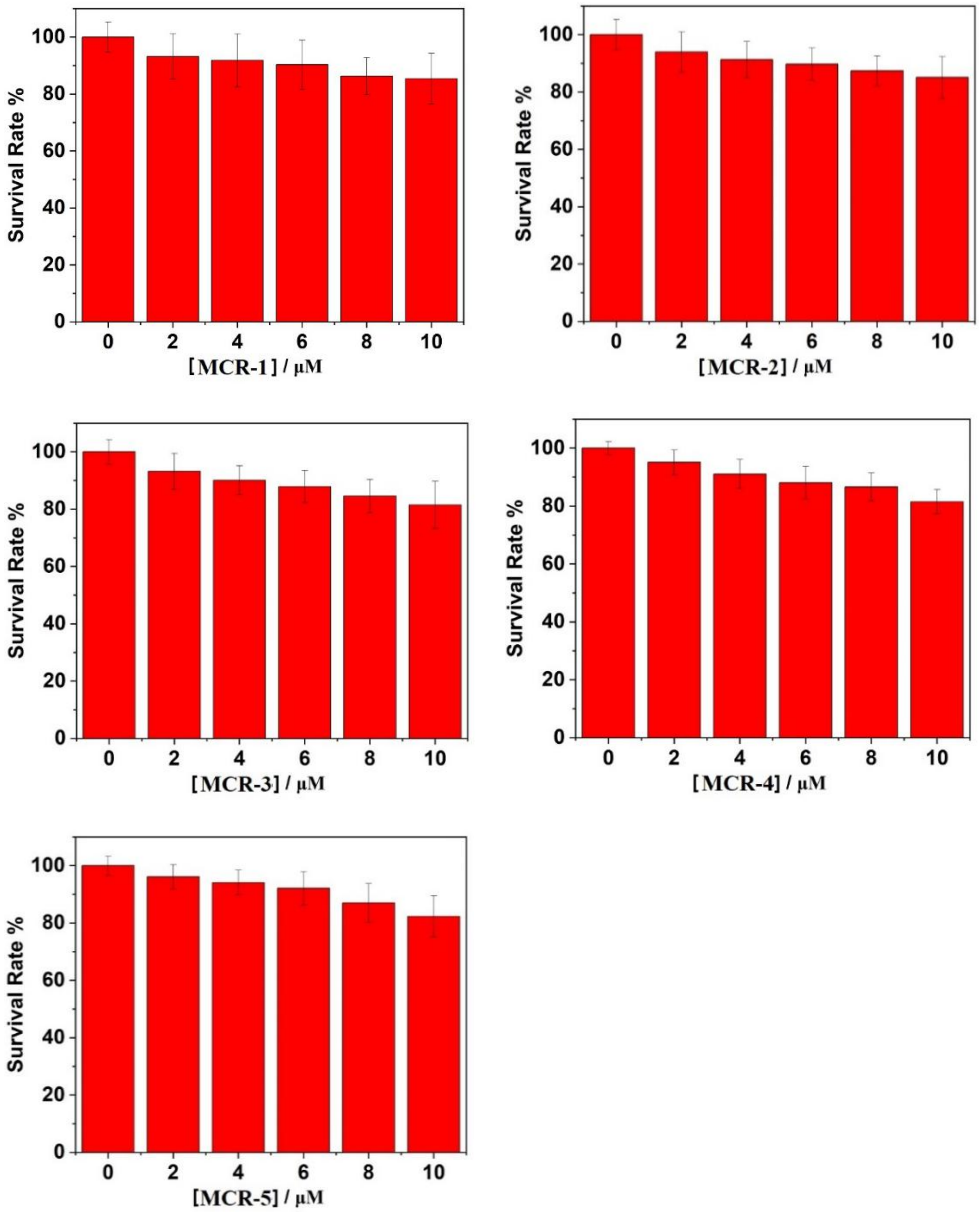


Figure S10. Percentage of viable HeLa cells after treatment with increasing concentrations of **MCR1-5** (0−10 μM) after 24 h, respectively.

Table S1. Photophysical Properties of MCR-DMA in Representative Solvents

Dyes	Solvents	$\lambda_{abs}/\lambda_{em}$	ε_{max} ($M^{-1}cm^{-1}10^5$)	Φ_f[a]	Stokes shift (nm)
MCR-DMA	CH_2Cl_2	640/667	1.42	0.007	27
	EtOH	639/666	1.12	0.004	27
	PBS	639/665	0.97	0.002	26

[a] Determined using Cy5 as standard (Φ_f = 0.27 in PBS at pH 7.4).

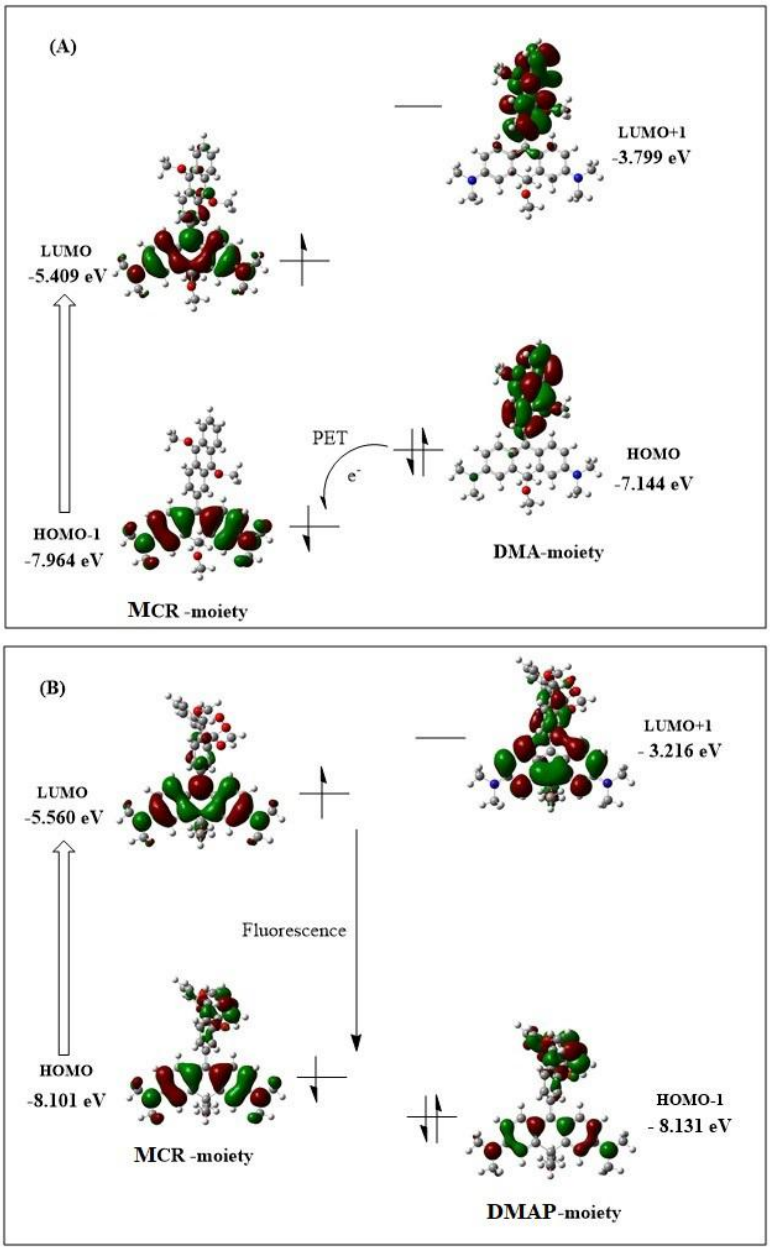


Figure S11. Frontier orbital energy representation of PET processes in **MCR-DMA** (A) and its oxidation products **MCR-DMAP** (B), respectively. All the quantum-chemical calculations were done with the Gaussian 09 suite. The geometry optimizations of **MCR-DMA** and its oxidation product **MCR-DMAP** were performed using density functional theory (DFT) with Becke's three-parameter hybrid exchange function with Lee-Yang-Parr gradient-corrected correlation functional (B3-LYP functional) and 6-31** basis set.

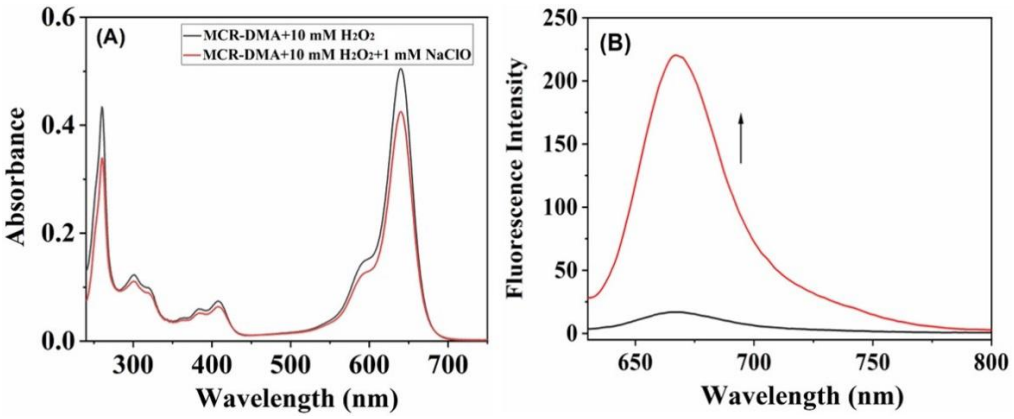


Figure S12. Absorbance (A) and fluorescence (B) changes of **MCR-DMA** in PBS solution in the presence of 10 mM H_2O_2 and 1 mM NaClO.

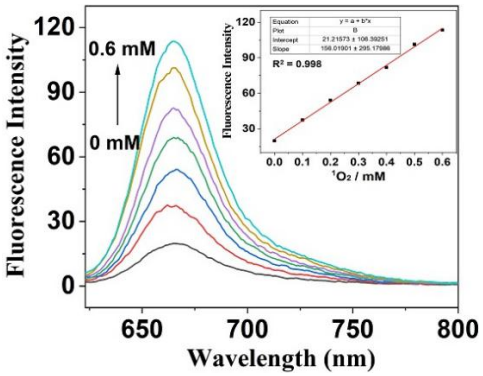


Figure S13. Fluorescence intensity changes of **MCR-DMA** (5 μM) in PBS to various dosage of $^1O_2$ (0 to 0.60 mM). Inset: The linear relationship between fluorescence intensity (F_{667} nm) and $^1O_2$ concentration. $^1O_2$ was generated *in situ* by adding NaClO to 10 equiv. of H_2O_2, and the concentration of $^1O_2$ was equal to the NaClO concentration.

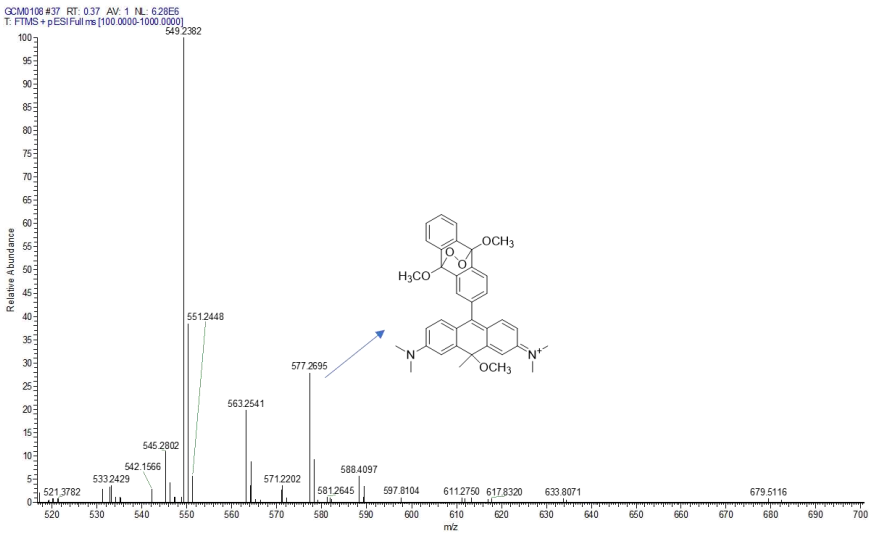


Figure S14. HRMS spectra of **MCR-DMA** in the presence of $^1O_2$.

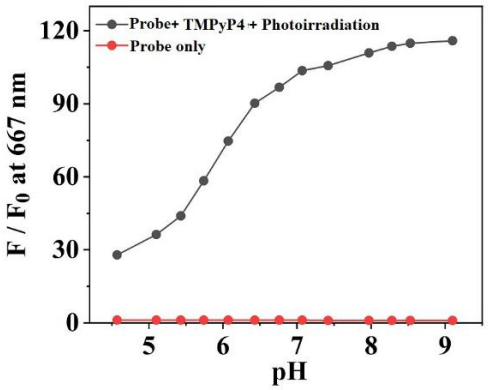


Figure S15. Fluorescence responses of **MCR-DMA** toward $^1O_2$ at different pH values.

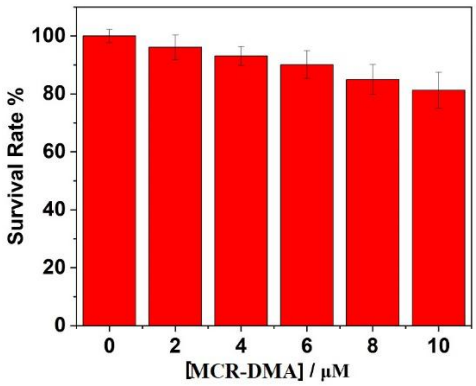


Figure S16. Percentage of viable HeLa cells after treatment with indicated concentrations of **MCR-DMA** after 24 hours.

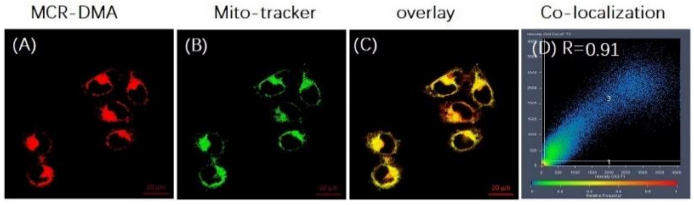


Figure S17. Fluorescence images of HeLa cells co-stained with **MCR-DMA** (0.5 μM) and Mito Tracker Green FM (0.2 μM). (A) **MCR-DMA** in red channel (The image was obtained at the higher excitation power in order to obtain the clear fluorescence image of **MCR-DMA** itself.). (B) Mito-Tracker Green in green channel. (C) Overlay of (A) and (B). (D) Colocalization scatter plots and Pearson's colocalization coefficients. For **MCR-DMA**, λ_{ex}: 633 nm, collect from 650−750 nm; for Mito Tracker green, λ_{ex}: 488 nm, collect from 500−600 nm. Scale bar: 20 μm.

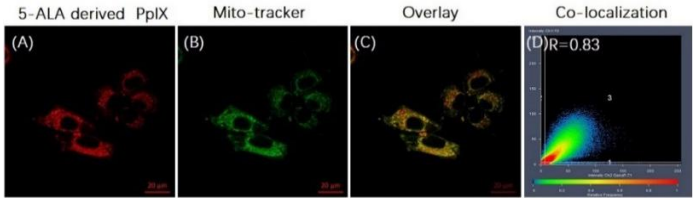
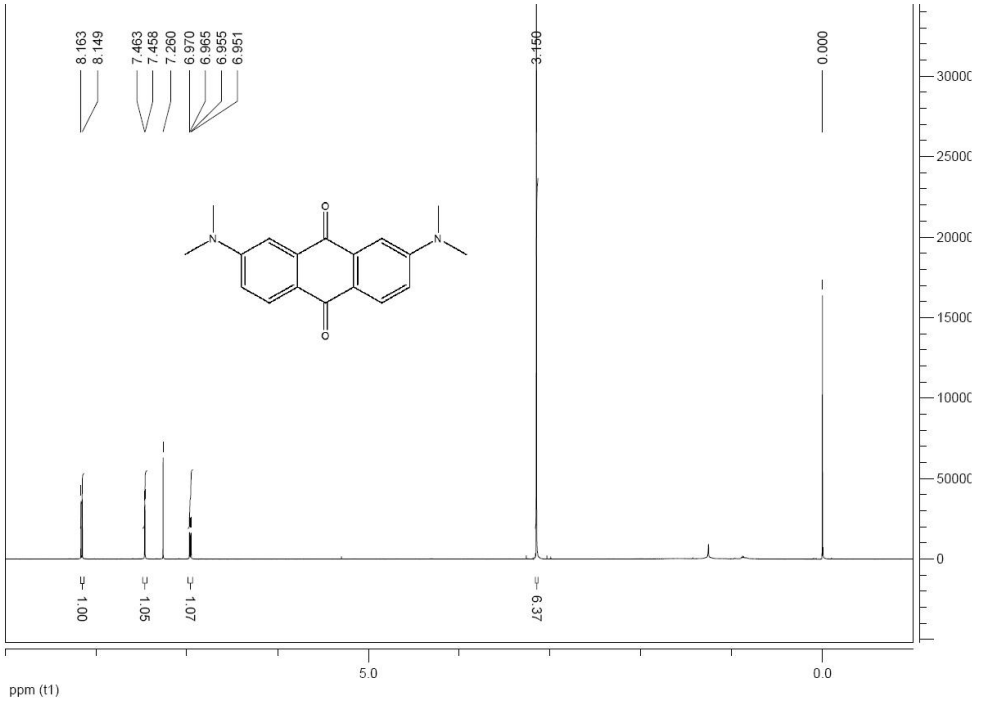
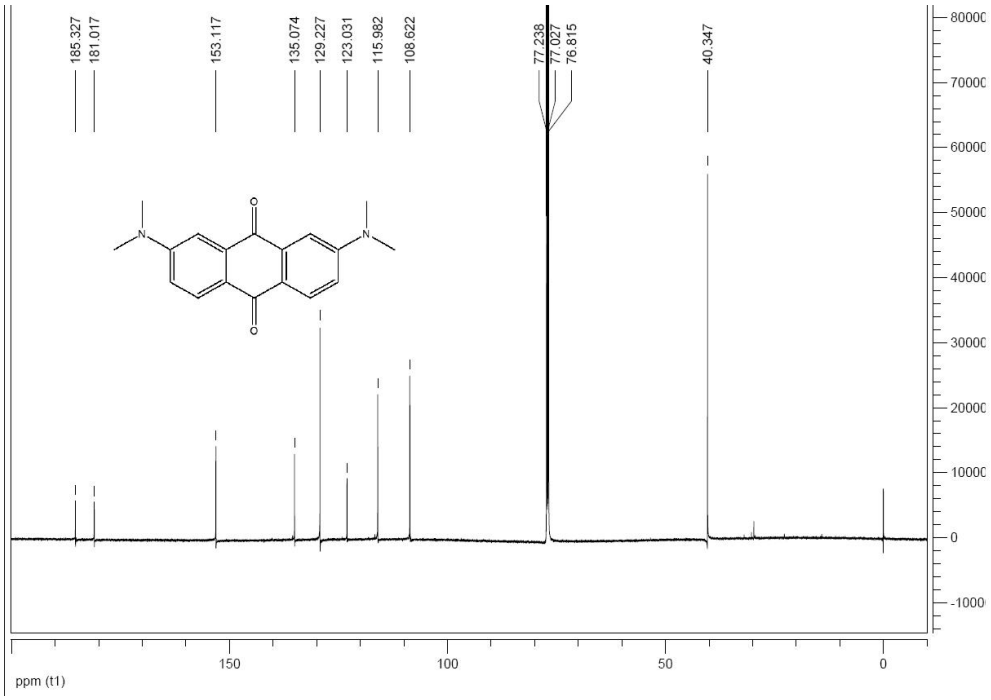


Figure S18. Fluorescence images of HeLa cells co-stained with **5-ALA** (150 μg/mL) and Mito Tracker Green FM (0.2 μM). (A) **5-ALA** derived **PpIX** in red channel. (B) Mito-Tracker Green in green channel. (C) Overlay of (A) and (B). (D) Colocalization scatter plots and Pearson's colocalization coefficients. For **5-ALA** derived **PpIX**, λ_{ex}: 405 nm, collect at 600−650 nm; for Mito Tracker green, λ_{ex}: 488 nm, collect at 500−600 nm. Scale bar: 20 μm.

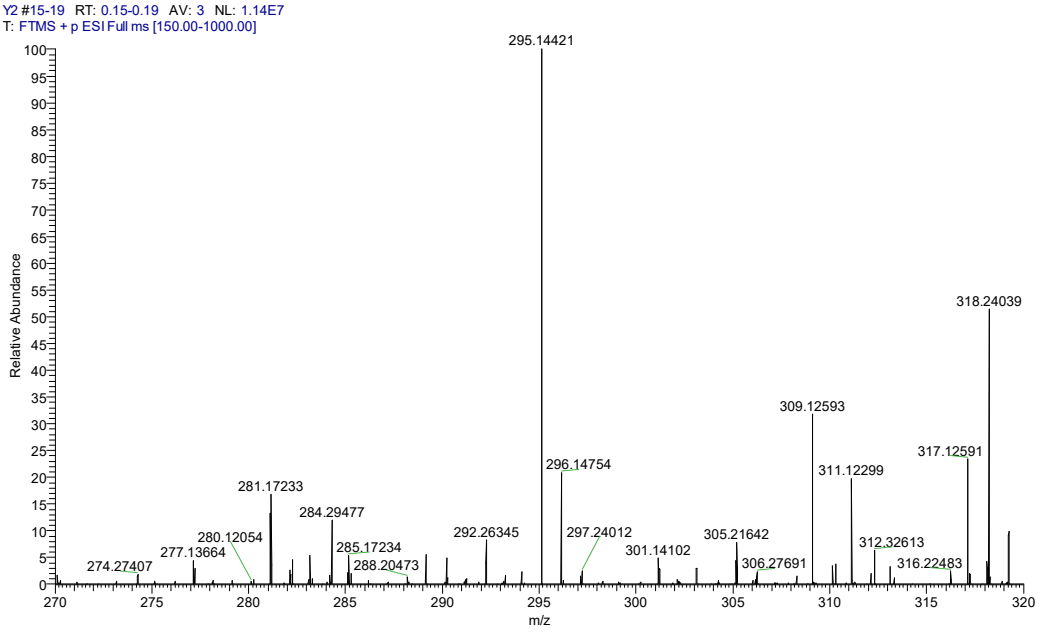
5. ^{1}H NMR ,^{13}C NMR and HRMS spectra



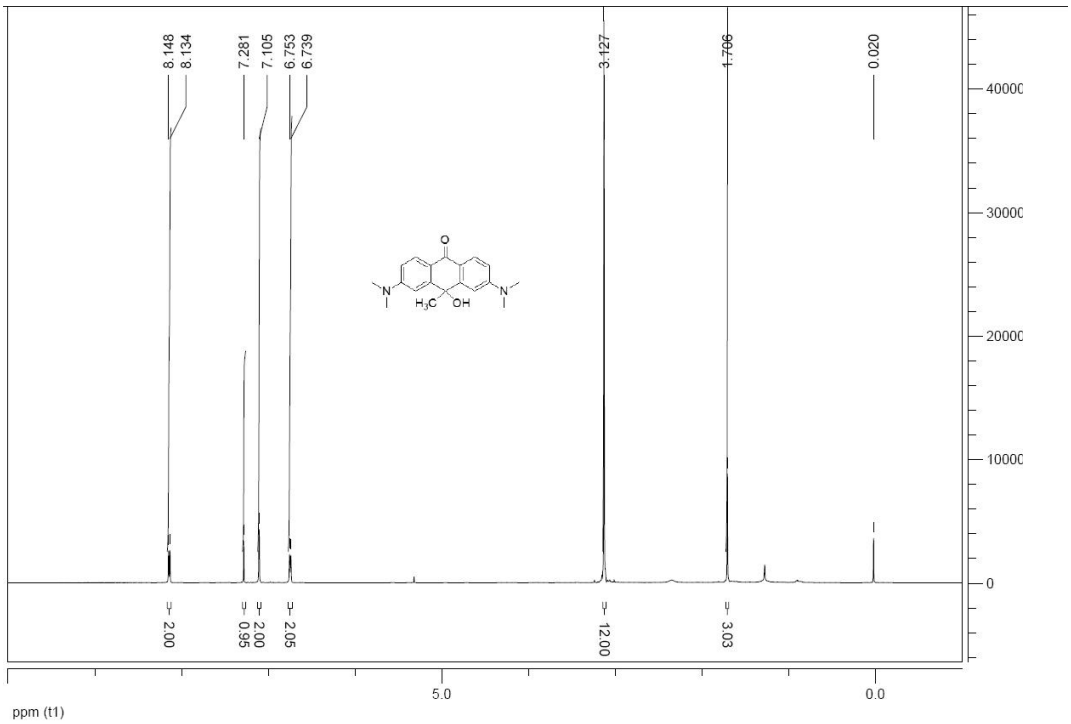
^{1}H NMR spectra of compound **2**.



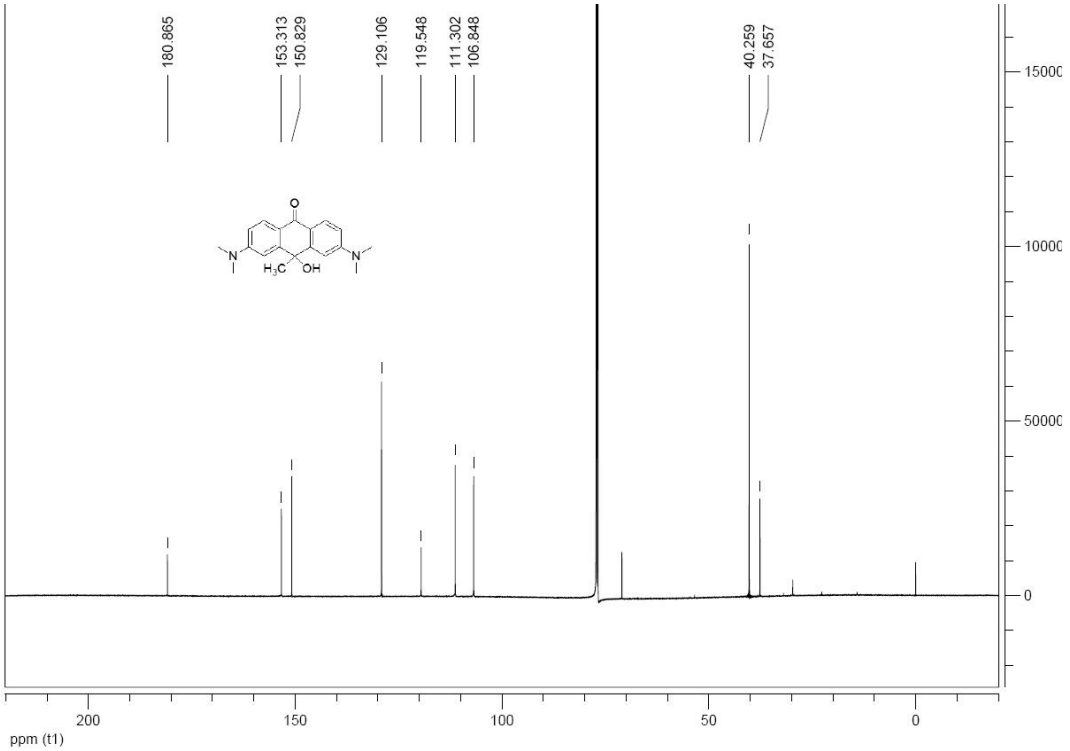
^{13}C NMR spectra of compound **2**.



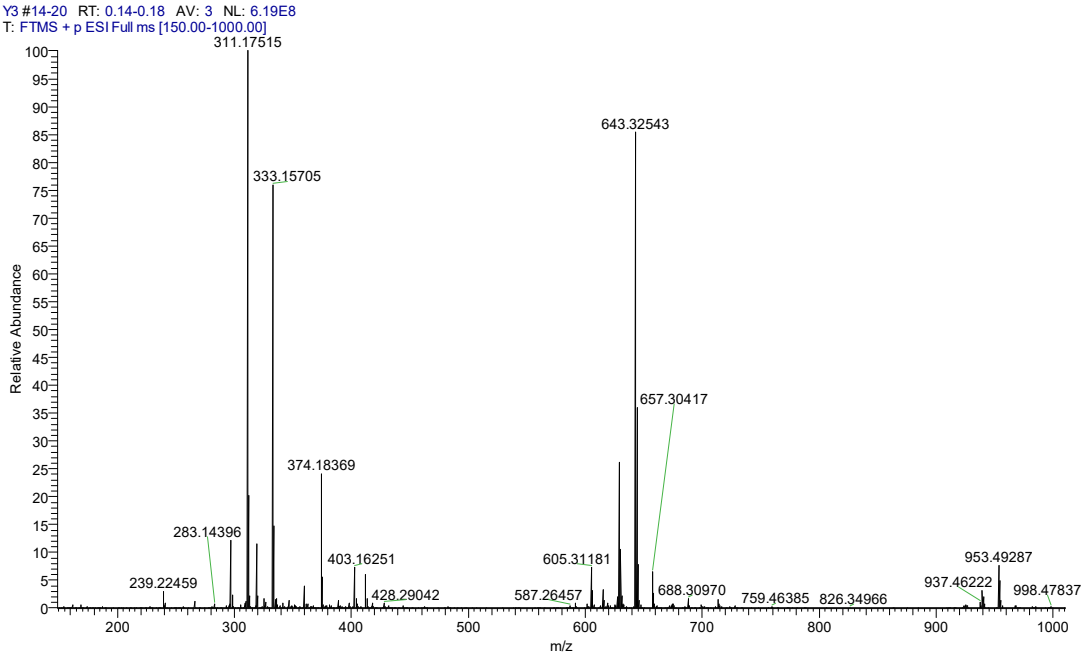
HRMS spectra of compound **2**.



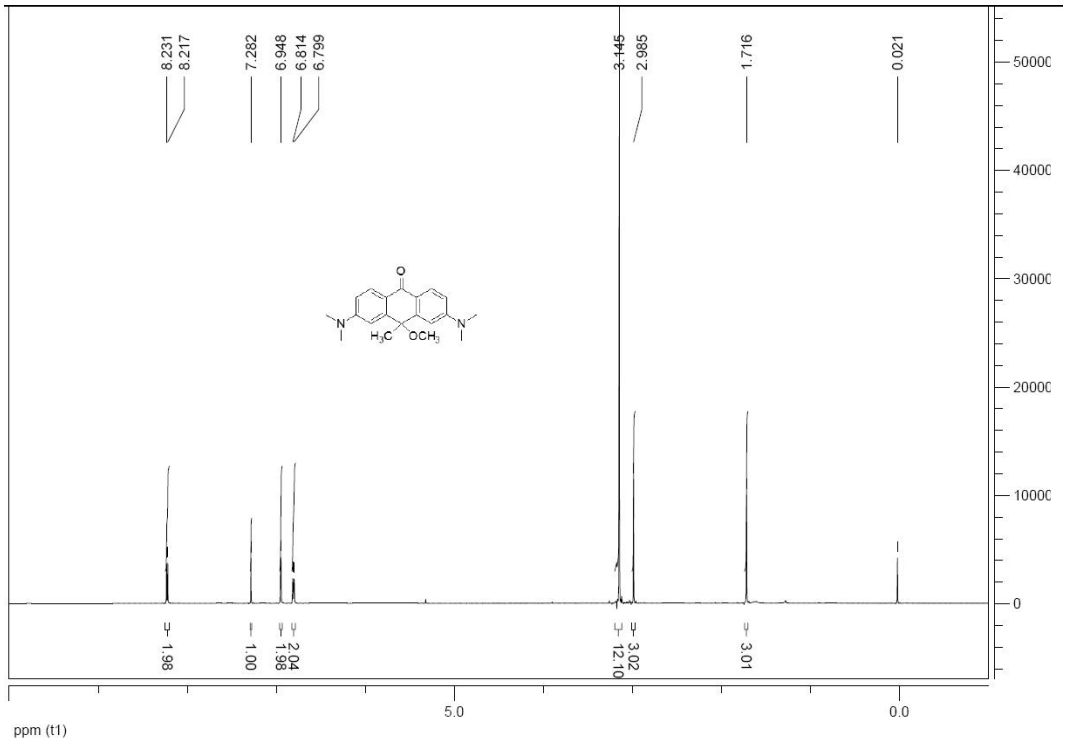
^{1}H NMR spectra of compound **3**.



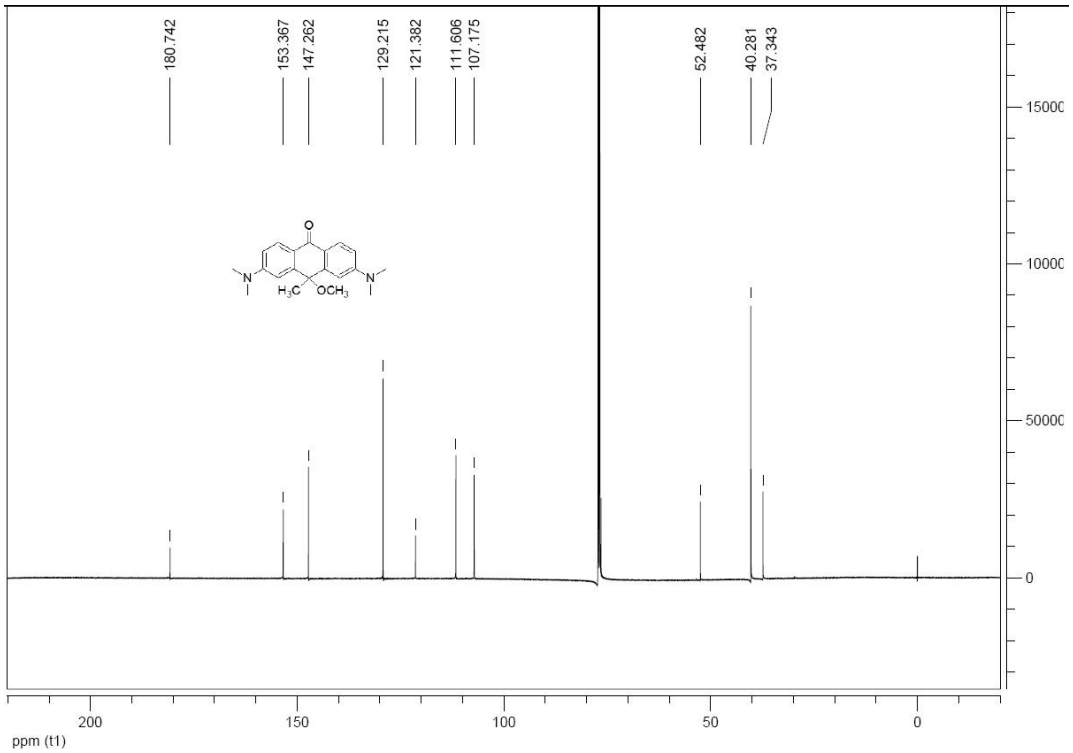
^{13}C NMR spectra of compound **3**



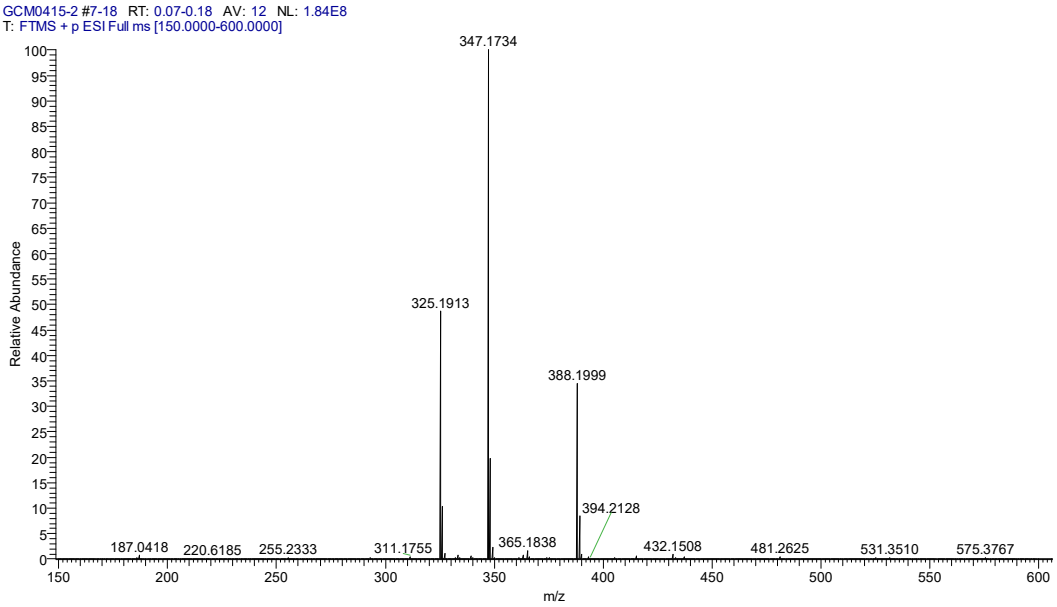
HRMS spectra of compound **3**.



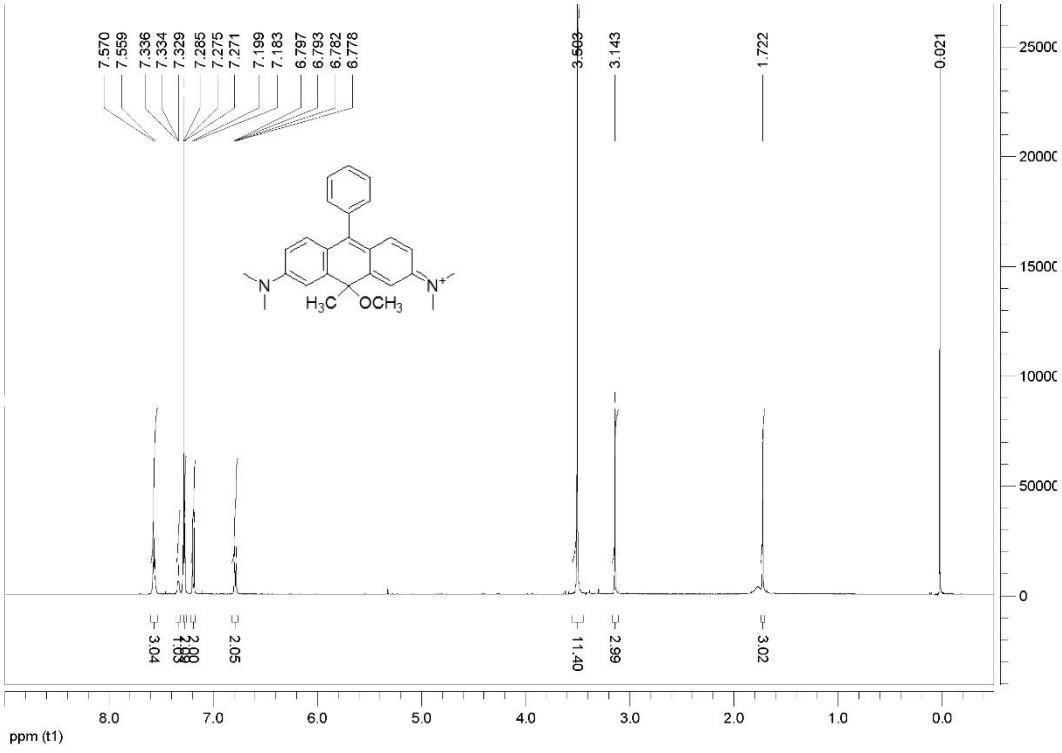
^{1}H NMR spectra of compound **4**.



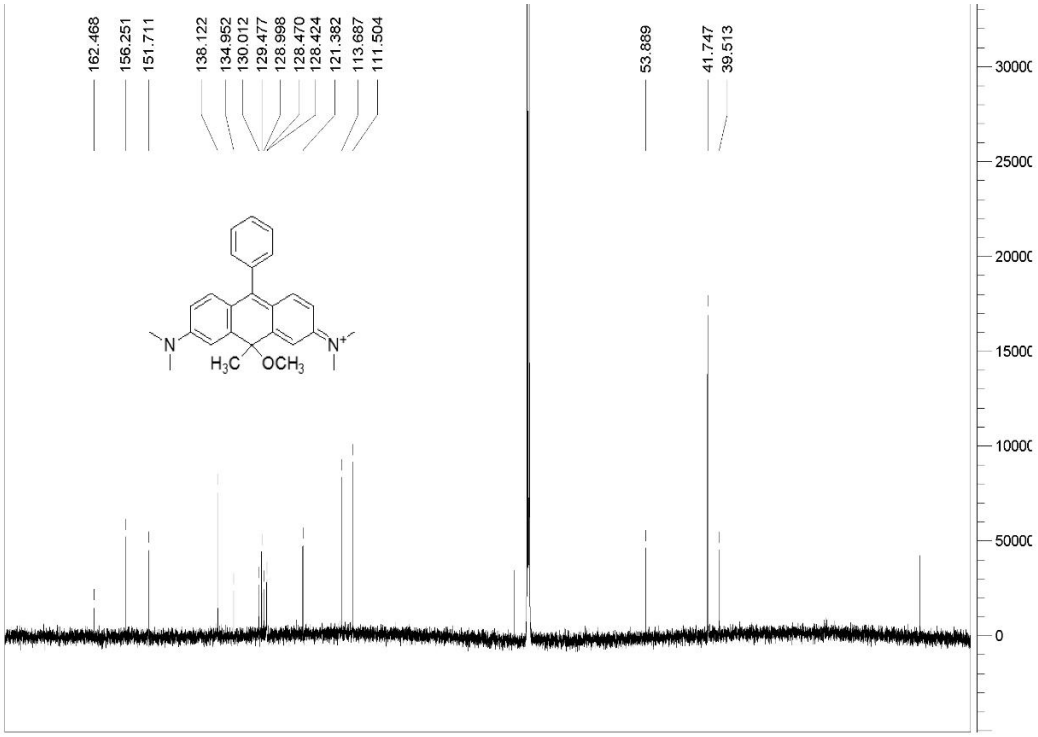
^{13}C NMR spectra of compound **4**



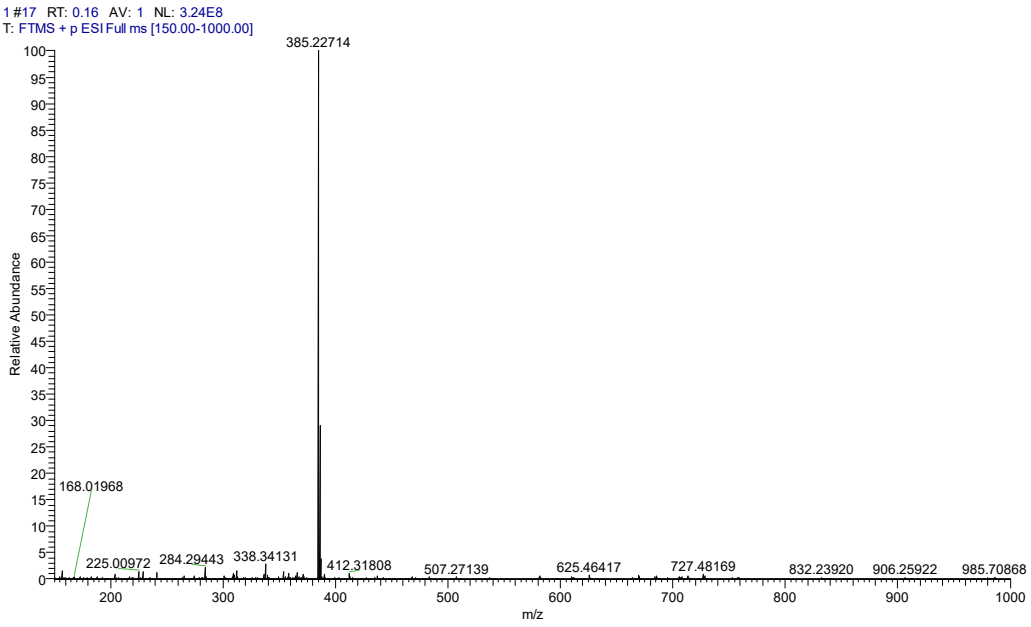
HRMS spectra of compound **4**.



^{1}H NMR spectra of **MCR-1**



^{13}C NMR spectra of **MCR-1**



HRMS spectra of **MCR-1**

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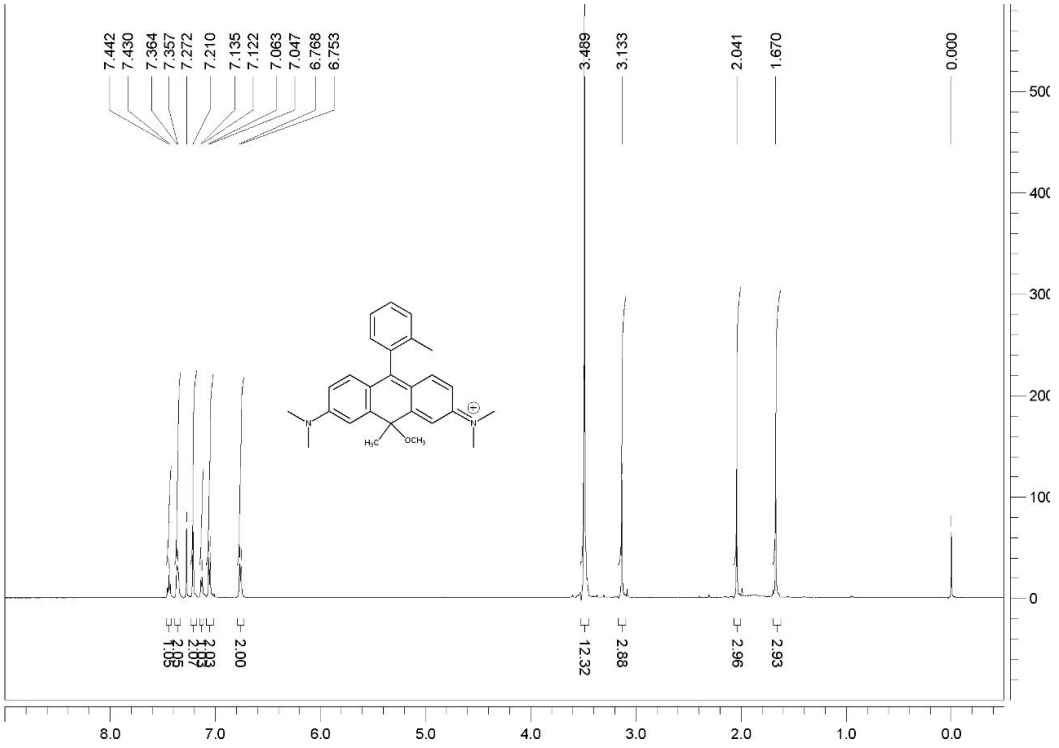
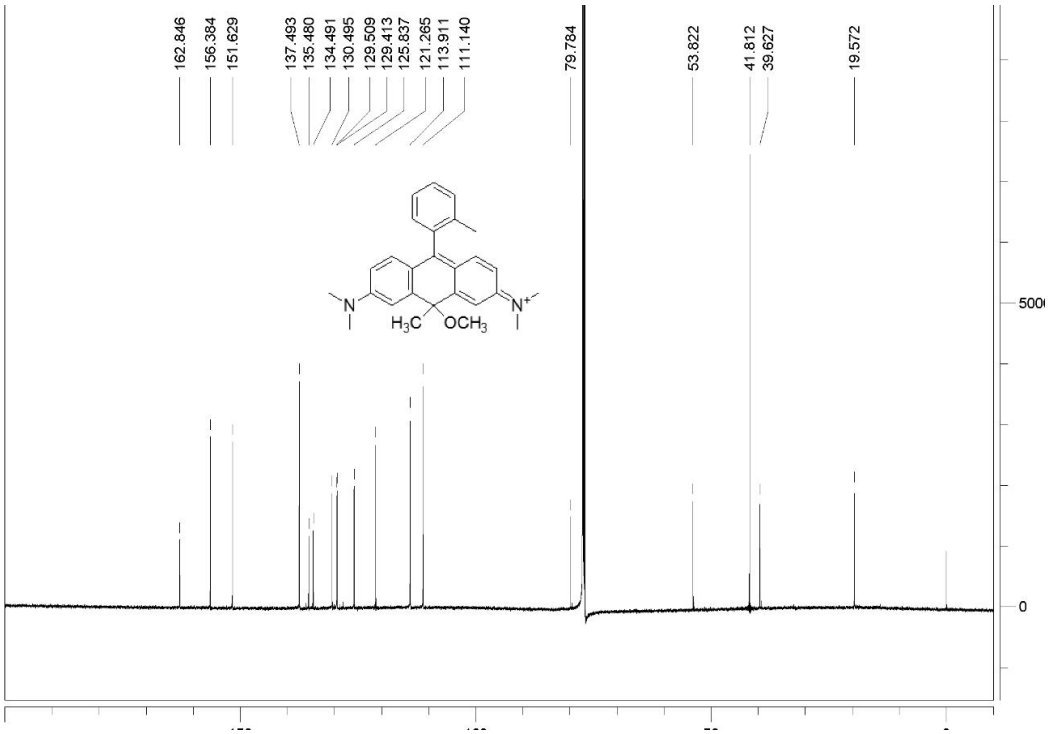
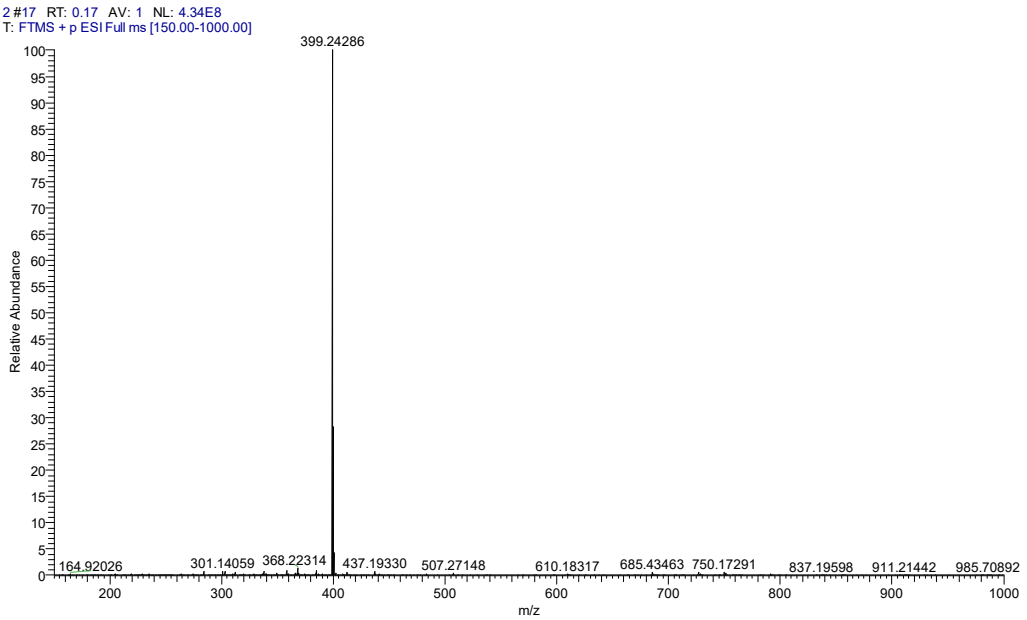


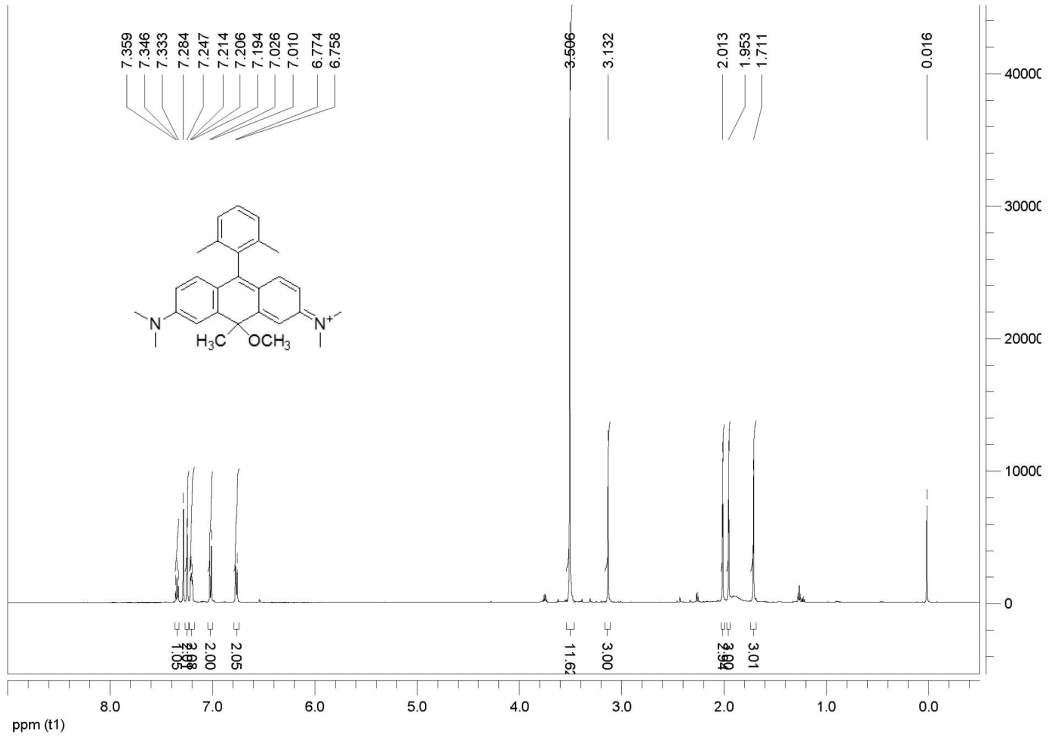
^{1}H NMR spectra of **MCR-2**



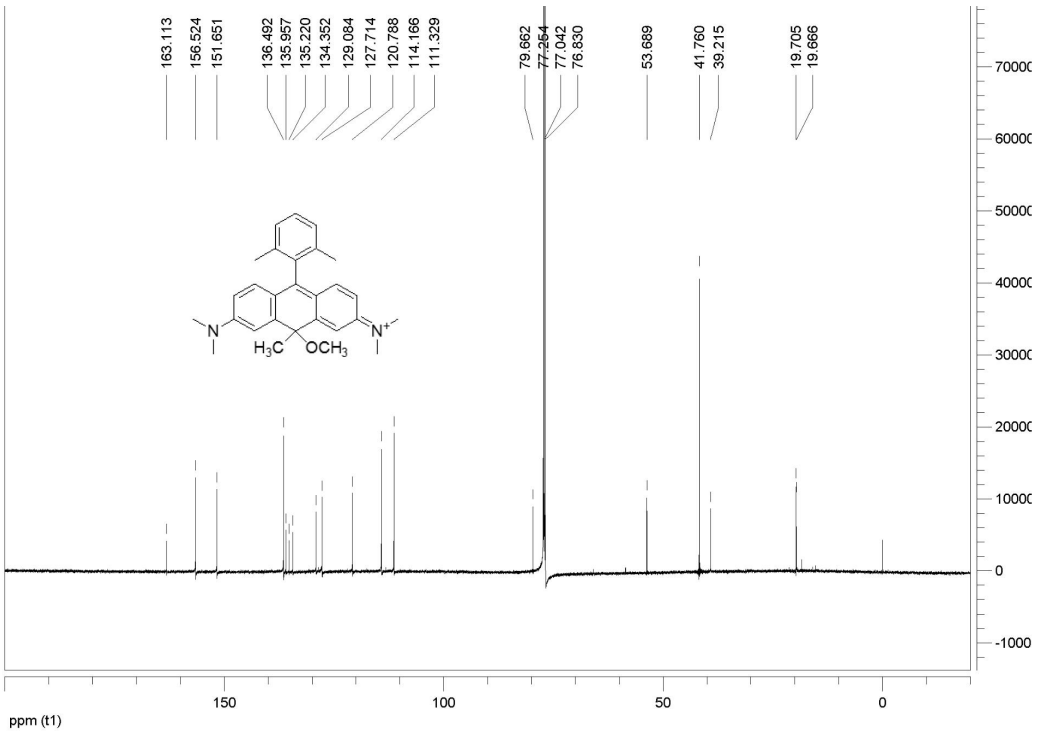
^{13}C NMR spectra of **MCR-2**



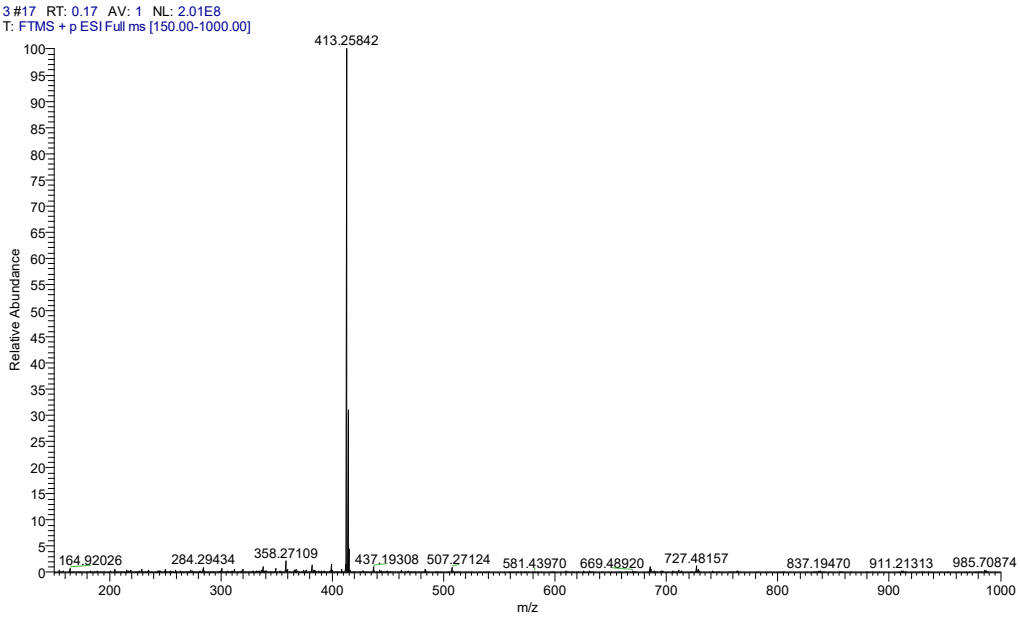
HRMS spectra of **MCR-2**



^{1}H NMR spectra of **MCR-3**



^{13}C NMR spectra of **MCR-3**



HRMS spectra of **MCR-3**

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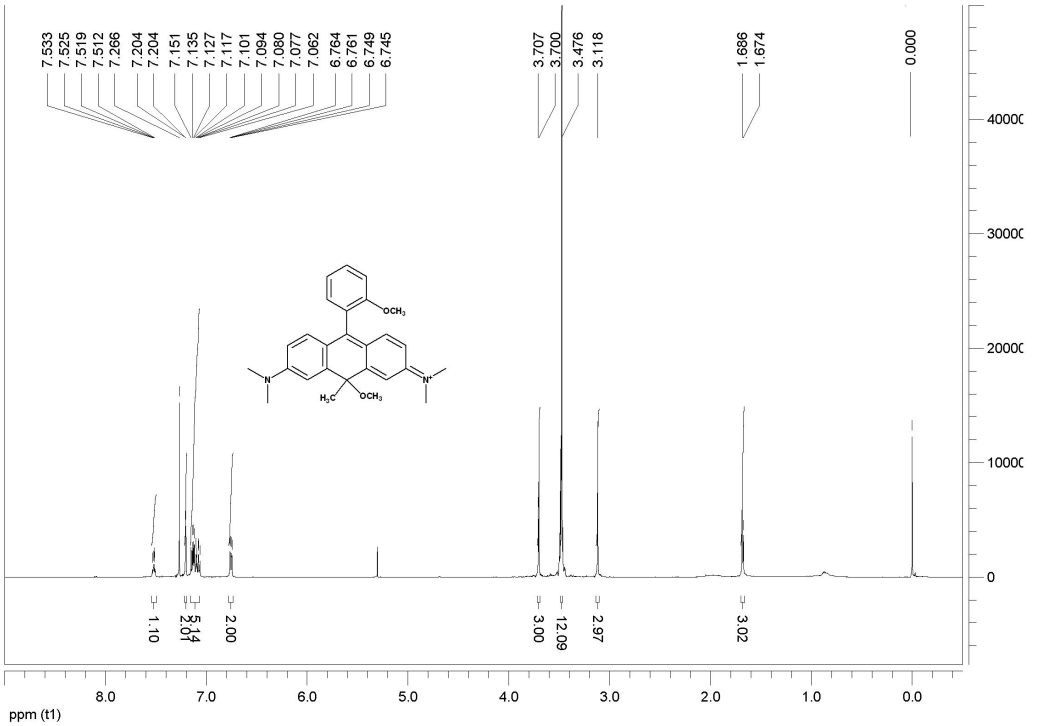
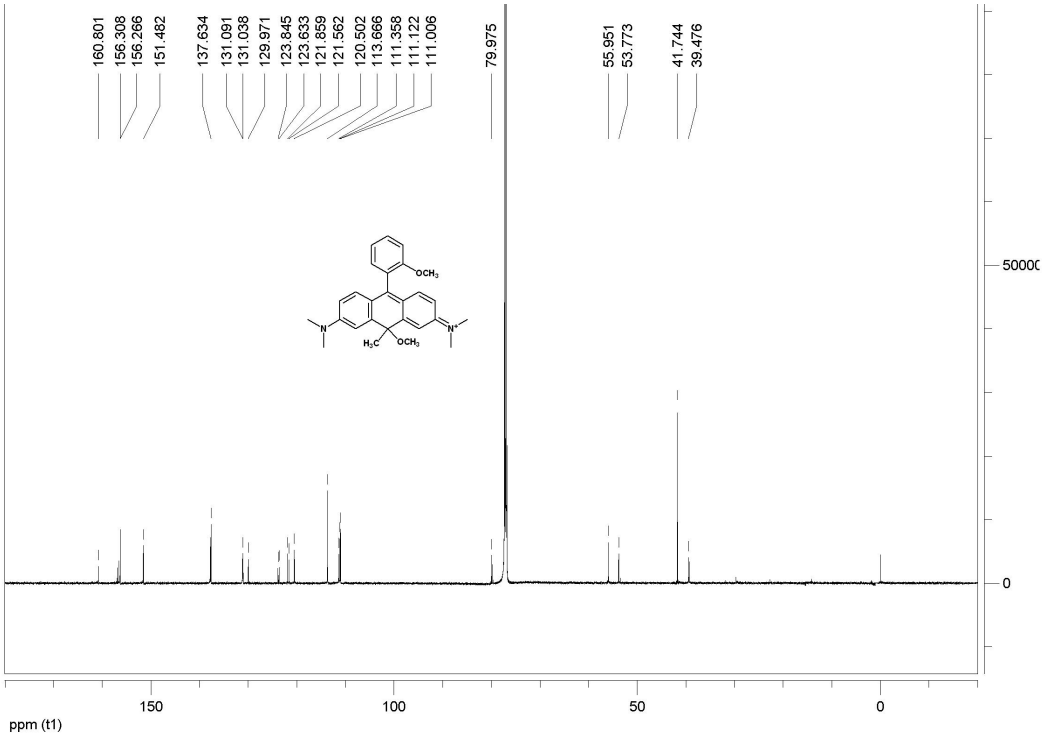
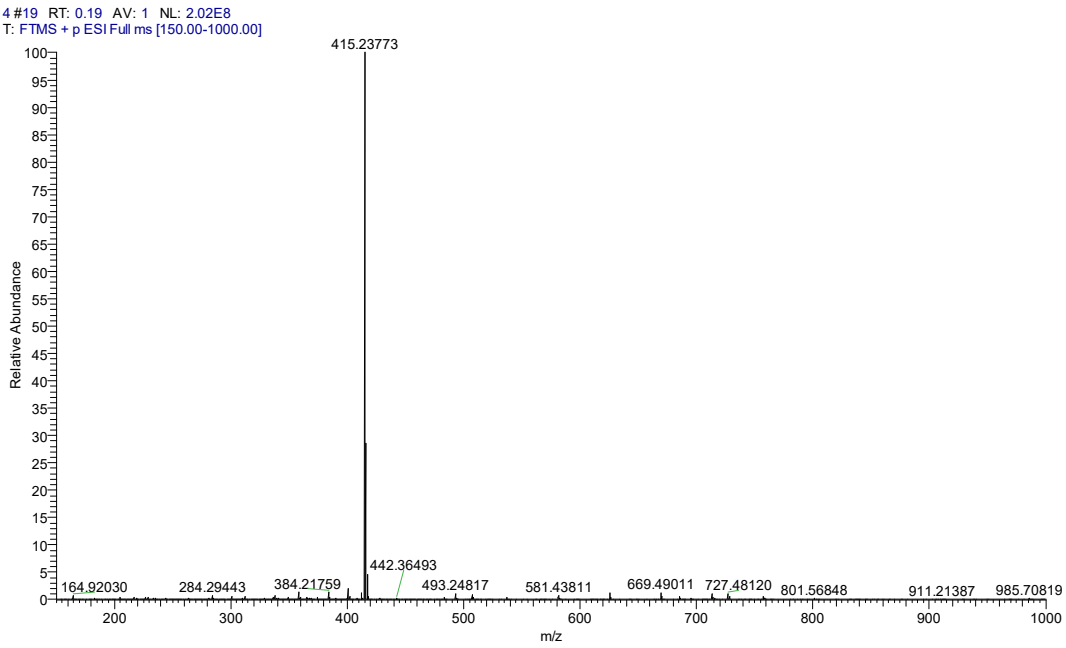


^{1}H NMR spectra of **MCR-4**



^{13}C NMR spectra of **MCR-4**



HRMS spectra of **MCR-4**

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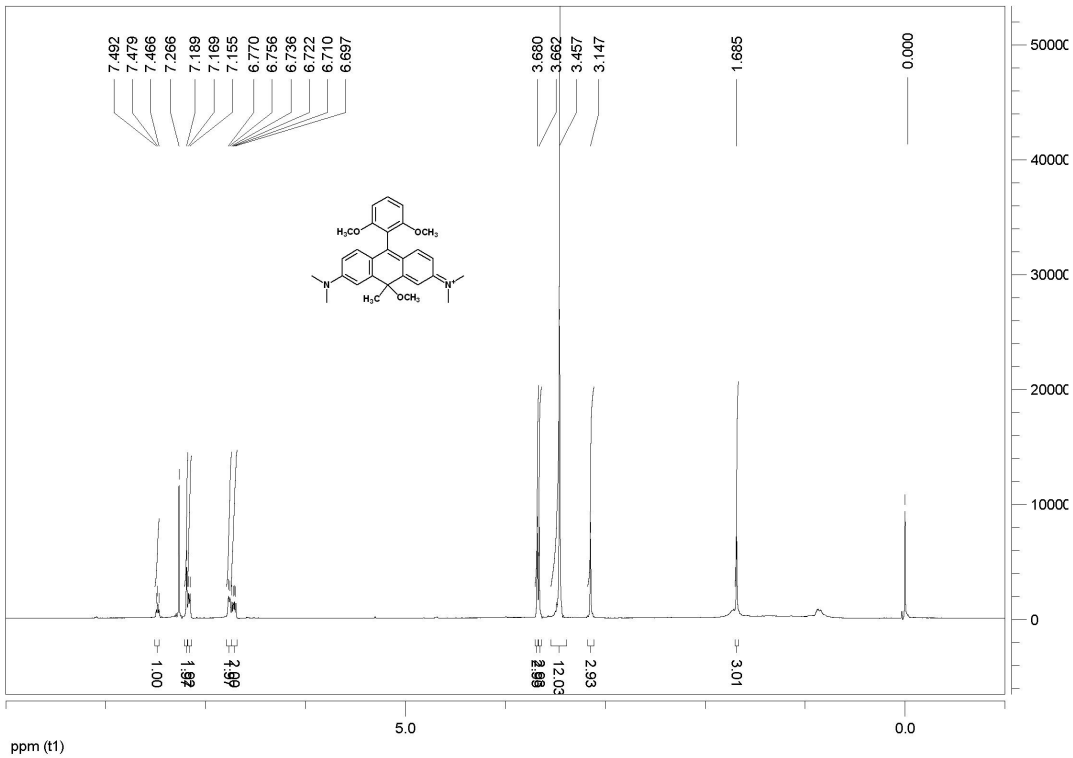
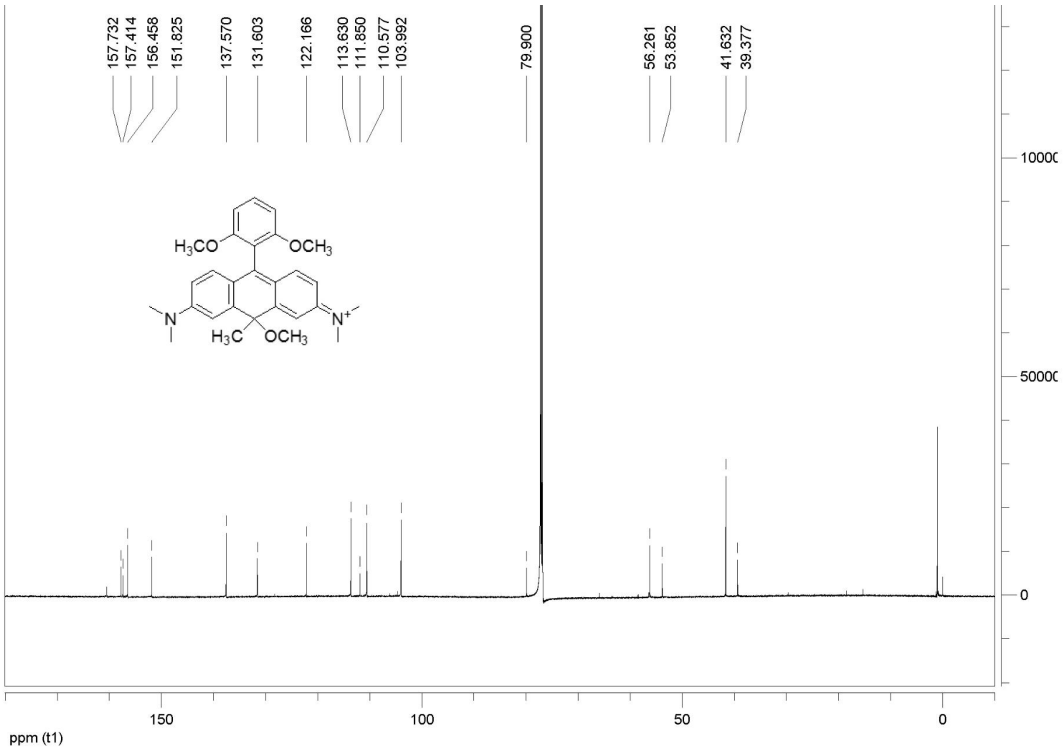
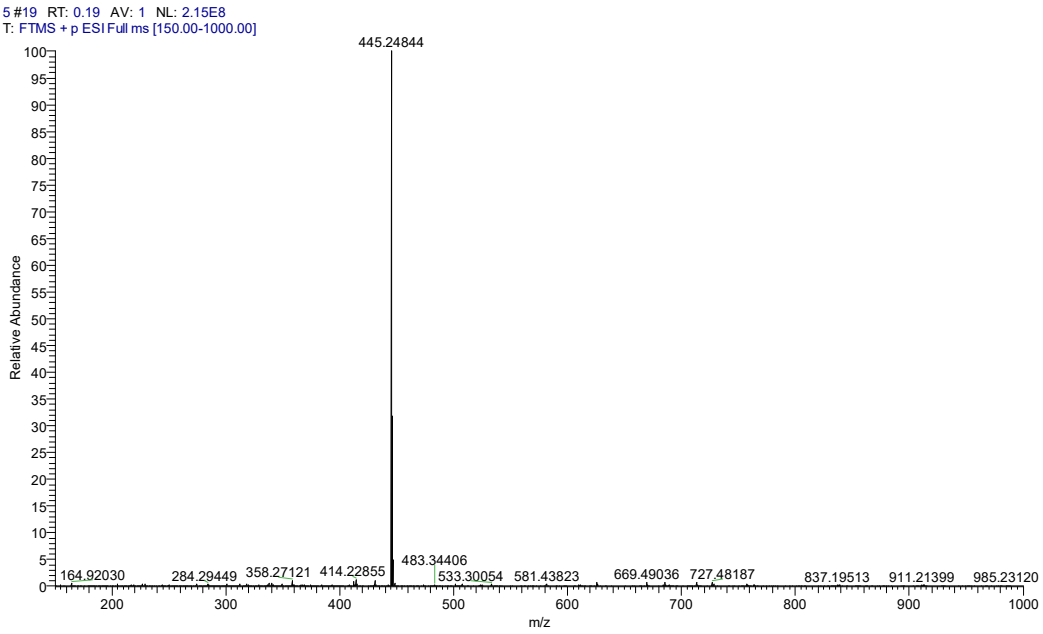


^{1}H NMR spectra of **MCR-5**



^{13}C NMR spectra of **MCR-5**



HRMS spectra of **MCR-5**

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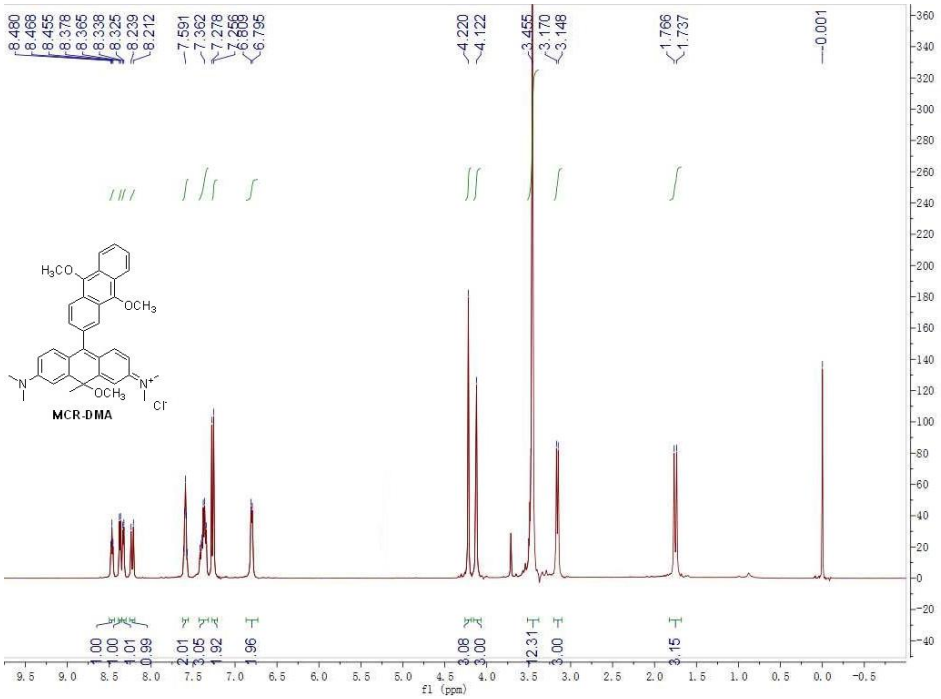
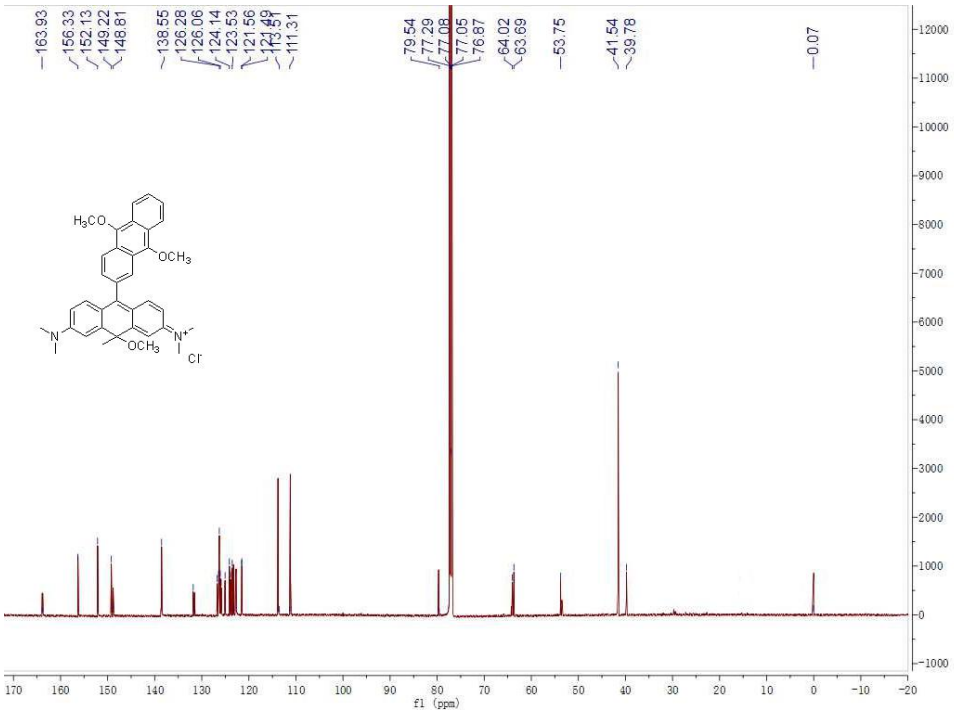
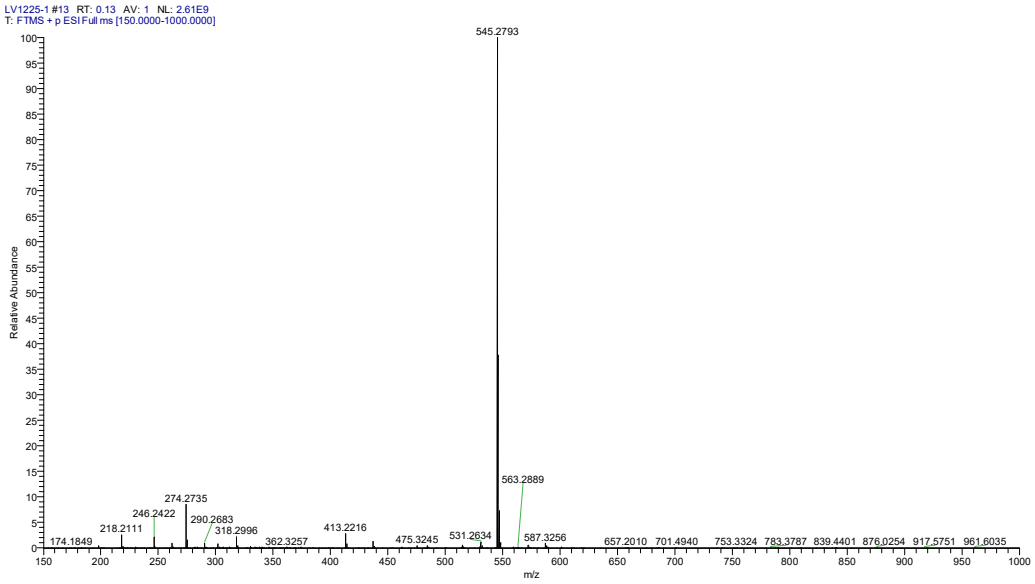


^{1}H NMR spectra of **MCR-DMA**



^{13}C NMR spectra of **MCR-DMA**



HRMS spectra of **MCR-DMA**