Supporting Information for

BINOL Derivatives with Aggression-induced Emission

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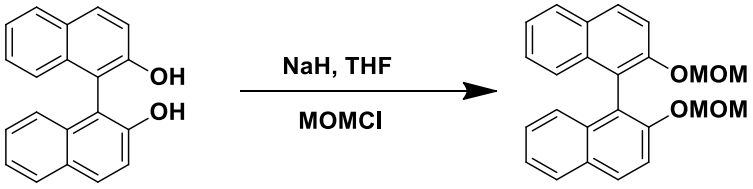
Contents

1. Experimental Section

1.1 General information

All chemicals and solvents were commercially available and were used without further purification. (S)-(-)-1,1'-bi-2-naphthol was purchased from xxx. Sodium hydride, n-butyllithium solution, acetophenone, Diethyl carbonate were purchased from Innochem. Chloromethyl methyl ether was purchased from Xiya Reagent. ^{1}H NMR, ^{13}C NMR spectra were measured on a Bruker AM400 NMR spectrometer. Proton Chemical shifts of NMR spectra were given in ppm relative to internals reference TMS (1H, 0.00 ppm). ESI-HRMS spectral data were recorded on a Finnigan LCQDECA mass spectrometer. Fluorescence emission spectra were obtained using Hitachi F-7000 spectrometer at 298 K. Absorption spectra were recorded on a Hitachi PharmaSpec UV-1900UV-Visible Spectrophotometer. The absolute fluorescence quantum yield was measured using a Hamamatsu quantum yield spectrometer C11347 Quantaurus_QY. The fluorescence lifetime was measured using a Hamamatsu Compact Fluorescence Lifetime Spectrometer C11367. Single crystal were grown from EtOAc/DCM via solute solution diffusion method. Single crystal X-ray diffraction intensity data were collected on a Agilent Technologies (Gemini). The ground-state geometries were optimized using the density function theory (DFT) method with B3LYP hybrid functional at the basis set level of 6-31G (d, p). All the calculations were performed using Gaussian 09 package. MTT method was used for testing the cell viability and described in the experimental section. HeLa cells were obtained from Shanghai Institute of Biochemistry and Cell Biochemistry and Cell Biology, Chinese Academy of Science. Confocal lasing scanning microscopic (CLSM) images of single-photo and two-photo excitation were obtained using LSM 780 (Zeiss) and Nikon A1R MP^{+}, respectively. Unless otherwise noted, materials were obtained from commercial suppliers and were used without further purification. All the solvents were dried according to the standard methods prior to use. All of the solvents were either HPLC or spectroscopic grade in the optical spectroscopic studies.

1.2 Reaction procedures

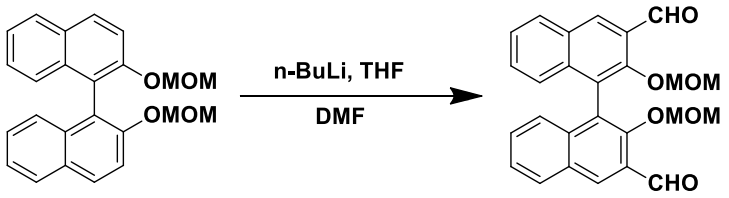


BIN-1 BIN-2

2,2′-Bis- (methoxymethoxy)-1,1′-binaphthyl (**BIN-2**)

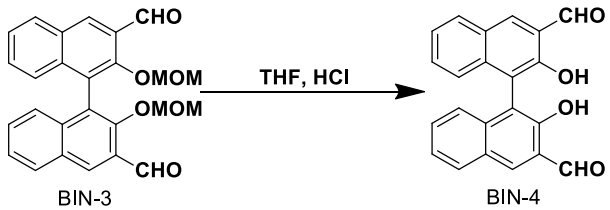
Under nitrogen, (S)-(-)-1,1'-bi-2-naphthol (5 g, 17.5 mmol) was added to a suspension of NaH (1.75 g, 43.75 mmol, 60% dispersion in mineral oil) in dry THF (100 mL) at 0 °C with stirring. The resulting solution was stirred at 0 °C for 1 h, and then methoxymethyl chloride (3.3 mL, 43.75 mmol) was slowly added. The mixture was allowed to warm to room temperature and stirred overnight to afford a creamlike mixture. Water was added to quench the reaction. The organic layer was separated, and the aqueous layer was extracted with ethyl acetate (30 mL × 3). The combined organic

extracts were washed with brine, and dried over Na_2SO_4. After removal of the solvent, the residue was purified by column chromatography on silica gel. Elution with hexane/ethyl acetate (5:1) gave compound BIN-2 as a white solid in 88% yield (8.26 g).^{1}H NMR (400 MHz, $CDCl_3$): δ (TMS, ppm) 7.97-7.90 (d, 2H), 7.89-7.83 (d, 2H), 7.60-7.53 (d, 2H), 7.37-7.30 (t, 2H), 7.26-7.17 (t, 2H), 7.17-7.11 (d, 2H), 5.10-5.05 (d, 2H), 4.99-4.93 (d, 2H), 3.15-3.10 (s, 6H).^{13}C NMR (100 MHz, $CDCl_3$): δ (TMS, ppm) 152.59, 133.97, 129.84, 129.36, 127.84, 126.27, 125.51, 124.04, 121.25, 117.24, 95.16, 55.81.



BIN-2 BIN-3

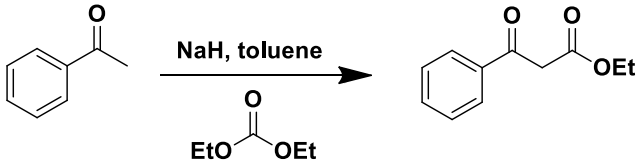
(S)-3,3′-Diformyl- 2,2′-bis(methoxymethoxy)-1,1′-binaphthyl (**BIN-3**)
Under nitrogen, n-butyllithium (2.5 M in hexane, 13.9 mL, 34.7 mmol) was added to a solution of BIN-2 (5 g, 13.37 mmol) in dry THF (100 mL) at room temperature. The mixture was stirred for 3 h, which produced a gray suspension. After the mixture was cooled to 0 °C, dry DMF (3.5 mL, 45 mmol) was added. The reaction mixture was allowed to warm to room temperature and stirred for 4 h. Saturated NH_4Cl (50 mL) was then added to quench the reaction. The organic layer was separated, and the aqueous phase was extracted with ethyl acetate (50 mL × 3). The combined organic phase was washed with water and brine and dried over Na_2SO_4. Concentration with a rotary evaporator and subsequent chromatography on silica gel eluted with hexane/ ethyl acetate (5:1) afforded BIN-3 as yellow crystals in 47% yield (2.9 g). ^{1}H NMR (400 MHz, $CDCl_3$): δ (TMS, ppm) 10.58-10.49 (s, 2H), 8.64-8.56 (s, 2H), 8.11-8.02 (d, 2H), 7.55-7.46 (t, 2H), 7.46-7.36 (t, 2H), 7.23-7.18 (d, 2H), 4.74-4.64 (dd, 4H), 2.87-2.83 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (TMS, ppm) 190.66, 154.03, 136.67, 132.29, 130.30, 130.05, 129.63, 128.83, 126.27, 126.08, 125.89, 100.62, 57.02.



BIN-3 BIN-4

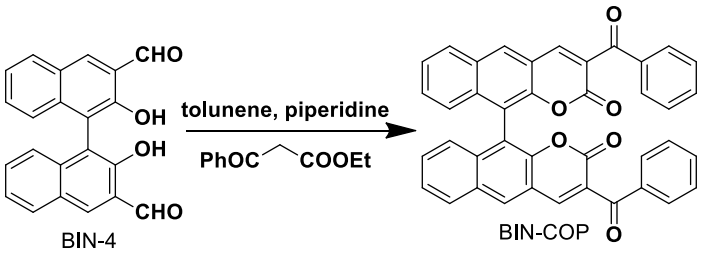
(S)-3,3′-Diformyl- 2,2′-dihydroxy-1,1′-binaphthyl (**BIN-4**)
After compound BIN-3 (2 g, 4.6 mmol) was dissolved in THF (100 mL) and HCl (12 N, 2 mL) were added successively, and the mixture was heated at reflux for about 2 h. The resulting yellow solution was concentrated with a rotary evaporator. Water (30 mL) was then added, and the solution was extracted with EtOAc (30 mL × 3). The combined extract was dried over Na_2SO_4. After removal of the solvent, the residue was purified by column chromatography on silica gel eluted with hexane/ ethyl acetate (4:1) to give BIN-4 as yellow needle crystals in 88% yield (1.32 g). ^{1}H NMR

(400 MHz, $CDCl_3$): δ (TMS, ppm) 10.62-10.57 (s, 2H), 10.22-10.18 (s, 2H), 8.38-8.34 (s, 2H), 8.03-7.97 (d, 2H), 7.47-7,37 (m, 4H), 7.24-7.17 (d, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (TMS, ppm) 196.99, 153.82, 138.72, 137,61, 130,89, 130.21, 127.83, 125.03, 124.71, 122.28, 116.67.



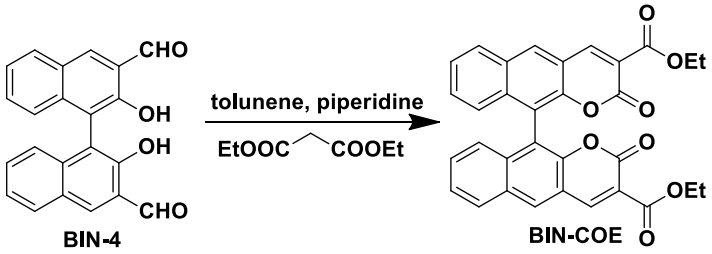
ethyl benzoylacetate

To a dried three-necked flask equipped with a dropping funnel, a condenser, and a magnetic stirrer was added NaH (280 mmol), diethyl carbonate (200 mmol), and toluene (100 mL). The mixture was heated to reflux. A solution of acetophenone (100 mmol) in toluene (50 mL) was added dropwise from the dropping funnel over 1-2 h. After the addition, the mixture was heated to reflux until the evolution of hydrogen ceased (15-20 min). When the reaction was cooled to room temperature, glacial acetic acid (30 mL) was added dropwise and a heavy, pasty solid appeared. Ice-water was added until the solid was dissolved completely. The toluene layer was separated, and the water layer was extracted with EtOAc (3×100 mL). The combined organic solution was washed with water (100 mL) and brine (100 mL), then dried over Na2SO4. After evaporation of the solvent, the mixture was distilled under reduced pressure or subjected chromatography to give the ethyl benzoylacetate in 80% yield.



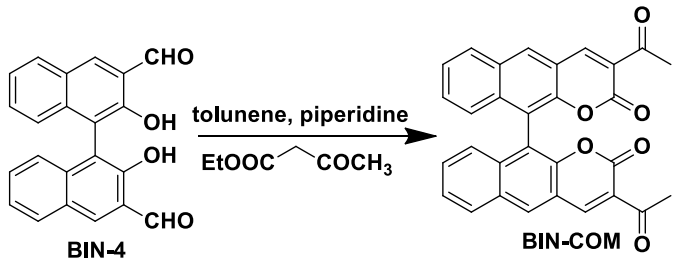
(S)-3,3'-dibenzoyl-2H,2'H-[10,10'-bibenzo[g]chromene]-2,2'-dione (**BIN-COP**)

After compound BIN-4 (300 mg, 0.87 mmol) and ethyl benzoylacetate (367 mg, 1.91 mmol) was added in tolunene (3 mL), the piperidine (0.25 mL) was dropped to the stirred solution. Then the mixture was heated at reflux for about 4 h. The mixture was filtrated, and the solid was washed with EtOH (5mL× 3). The residue was purified by column chromatography on silica gel eluted with hexane/ethyl acetate (2:1) to give BIN-Ph as yellow solid in 61% yield (440 mg), mp=262-263℃. ^1H NMR (400 MHz, $CDCl_3$): δ (TMS, ppm) 8.33-8.30 (s, 2H), 8.28-8.25 (s, 2H), 8.06-8.01 (d, 2H), 7.95-7.90 (d, 4H), 7.61-7.55 (t, 2H), 7.53-7.39 (m, 8H), 7.22-7.17 (d, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (TMS, ppm) 191.49, 158.06, 148.48, 145.31, 136.09, 134.94, 133.87, 131.42, 130.40, 129.79, 129.37, 128.62, 127.56, 126.33, 125.54, 118.15, 116.80. HRMS (ESI): *m/z*: Calcd for $C_{40}H_{22}O_6Na^+$: 621.1314 $[M+Na]^+$; Found: 621.1330.



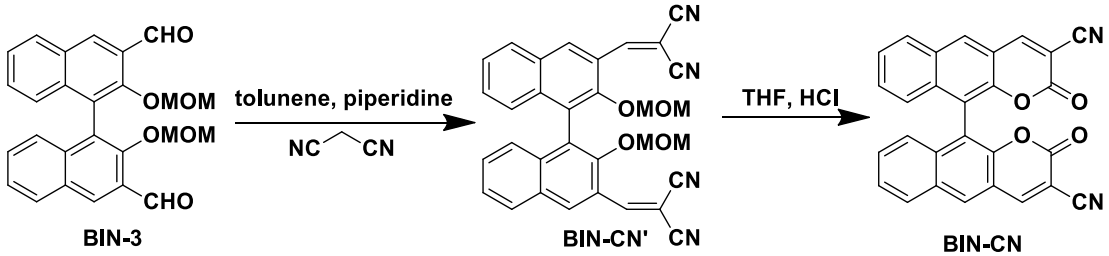
(S)-diethyl 2,2'-dioxo-2H,2'H-[10,10'-bibenzo[g]chromene]-3,3'-dicarboxylate (**BIN-COE**)

The preparation procedure was the same as that of BIN-COOE by using diethyl malonate (305 mg, 1.91 mmol) as the starting material. After workup, the crude product was purified by column chromatography on silica gel. Elution with hexane/ethyl acetate (4:1) gave BIN-COOE as a yellow crystal in 20% yield (232 mg) , mp=245-246℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ (TMS, ppm) 8.74-8.70 (s, 2H), 8.37-8.33 (s, 2H), 8.07-8.01 (d, 2H), 7.53-7.47 (t, 2H), 7.42-7.36 (t, 2H), 7.15-7.10 (d, 2H), 4.43-4.35 (q, 4H), 1.41-1.35 (t, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (TMS, ppm) 162.80, 156.27, 148.62, 148.58, 135.25, 132.07, 130.28, 129.92, 129.52, 126.15, 125,40, 118.94, 117.95, 116.36, 61.97, 40.91, 14.17. HRMS (ESI): *m/z*: Calcd for $C_{32}H_{22}O_8Na^+$: 557.1212 $[M+Na]^+$; Found: 557.1214.



(S)-3,3'-diacetyl-2H,2'H-[10,10'-bibenzo[g]chromene]-2,2'-dione (**BIN-COM**)

The preparation procedure was the same as that of BIN-COM by using diethyl malonate (305 mg, 1.91 mmol) as the starting material. After workup, the crude product was purified by column chromatography on silica gel. Elution with hexane/ethyl acetate (4:1) gave BIN-COM as a yellow crystal in 72% yield (297 mg), mp=247-248℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ (TMS, ppm) 8.73-8.71 (s, 2H), 8.42-8.39 (s, 2H), 8.09-8.05 (d, 2H), 7.55-7.49 (t, 2H), 7.44-7.38 (t, 2H), 7.16-7.12 (d, 2H), 2.67-2.64 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ (TMS, ppm) 195.29, 158.79, 148.73, 147.54, 135.33, 132.90, 130.40, 130.10, 129.58, 126.29, 125.51, 125.21, 118.26, 116.40, 30.54. HRMS (ESI): *m/z*: Calcd for $C_{32}H_{18}O_6Na^+$: 497.1001 $[M+Na]^+$; Found: 497.1000.



(S)-2,2'-((2,2'-bis(methoxymethoxy)-[1,1'-binaphthalene]-3,3'-diyl)bis(methanylyidene))dimalono
-nitrile (**BIN-CN'**)

The preparation procedure was the same as that of BIN-CN' by using malononitrile (126 mg, 1.91 mmol) as the starting material. After workup, the crude product was purified by column chromatography on silica gel. Elution with hexane/ethyl acetate (4:1) gave BIN-CN' as a yellow crystal in 84% yield (382 mg).

2,2'-dioxo-2H,2'H-[10,10'-bibenzo[g]chromene]-3,3'-dicarbonitrile (**BIN-CN**)

After compound BIN-CN' (300 mg, 0.57 mmol) was dissolved in THF (50 mL), the HCl (12N, 2 mL) was dropped to the stirred solution. Then the mixture was heated at reflux for about 1 h. Saturated $NaHCO_3$ (30 mL) was then added to adjust the pH. The organic layer was separated, and the aqueous phase was extracted with ethyl acetate (50 mL × 3). The combined organic phase was washed with water and brine and dried over Na_2SO_4. Concentration with a rotary evaporator and subsequent chromatography on silica gel eluted with DCM/ MeOH (100:1) afforded BIN-CN as yellow solid in 10% yield (27 mg) , mp=289-290℃. ^{1}H NMR (400 MHz, d_6-DMSO): δ (TMS, ppm) 9.22-9.20 (s, 2H), 8.75-8.72 (s, 2H), 8.31-8.26 (d, 2H), 7.65-7.59 (t, 2H), 7.56-7.49 (t, 2H), 7.20-7.15 (d, 2H). ^{13}C NMR (100 MHz, d_6-DMSO): δ (TMS, ppm) 156.92, 154.17, 147.86, 135.01, 133.53, 131.23, 130.52, 127.17, 125.72, 117.94, 116.24, 114.92, 103.06.HRMS (ESI): *m/z*: Calcd for $C_{28}H_{12}N_2O_4Na^+$: 463.0695 $[M+Na]^+$; Found: 463.0691.

1.2 Cell culture and imaging

Hela cells were cultured in Dulbecco's modified Eagle medium (DMEM) containing 10% fetal bovine serum and 1% Antibiotic–antimycotic at 37℃ in a 5% CO_2/95% air incubator. For fluorescence imaging, cells (4×10^3/well) were passed on a 6-well plate and incubated for 24 h. Before the staining experiment, cells were washed twice with physiological saline, incubated with 5 μM probe for 5 min at 37℃， then washed twice with physiological saline. The confocal fluorescent images were captured with an excitation light at 405 nm.

1.3 Cytotoxicity study

Toxicity toward HeLa cells was determined by MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-di-phenyltetrazolium bromide) reduction assay following literature procedures. About 10^4 cells per well were seeded in 96-well plates and cultured overnight for 70-80% cell confluence. The medium was replaced with 100 μL of fresh medium with different concentration of probes, to which 100 μL complexes at 200 μL. 24 hours later, 100 μL of 20% MTT solution in PBS was replaced with the old medium in each well for additional 0.5h incubation. The metabolic activity of the probes treated cells was expressed as a relative to untreated cell controls taken as 100% metabolic activity.

2. Absorption and FL spectra of BIN-CN, BIN-COM, BIN-COE, BIN-COP in different solution

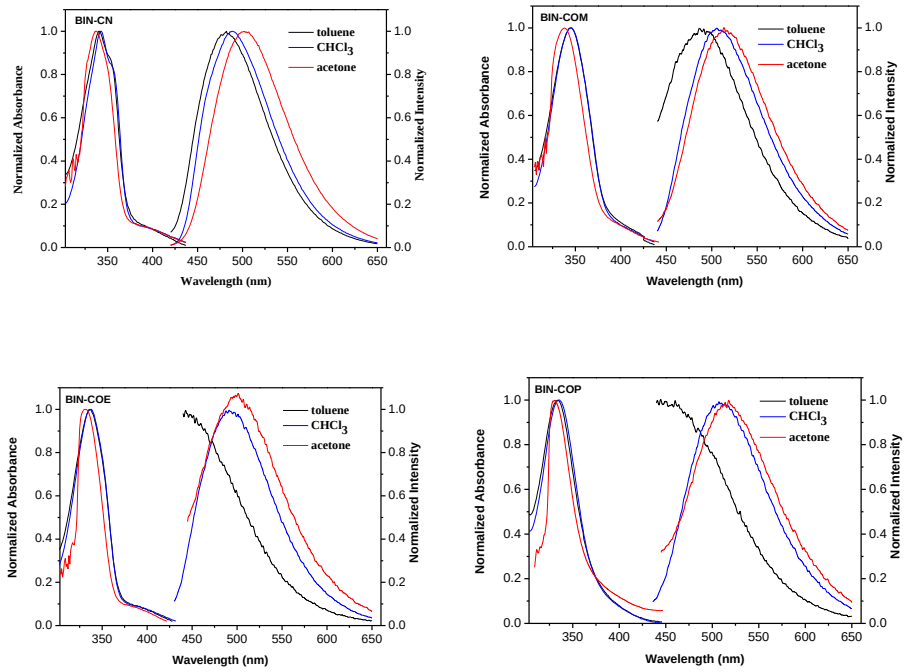


Fig. S1. Absorption and FL spectra (solutions were excited at their absorption maxima of the longest wavelength) of fluorophores BIN-CN, BIN-COM, BIN-COE, BIN-COP in different solution.

3. Photophysical data of BIN-CN, BIN-COM, BIN-COE, BIN-COP in different solvents

Table S1. Optical transitions of all the compounds in different solvents

	toluene			CHCl3			acetone		
Compound	λ_{ab} (nm)	λ_{em} (nm)	Stokes shift (nm)	λ_{ab} (nm)	λ_{em} (nm)	Stokes shift (nm)	λ_{ab} (nm)	λ_{em} (nm)	Stokes shift (nm)
BIN-CN	340	480	140	344	488	144	345	502	157
BIN-COM	341	490	149	348	508	160	348	513	165
BIN-COE	340	458	118	342	494	152	343	501	158
BIN-COP	338	470	132	339	509	170	342	518	176

4. Fluorescence spectra of BIN-CN, BIN-COM, BIN-COE, BIN-COP in THF/water mixtures

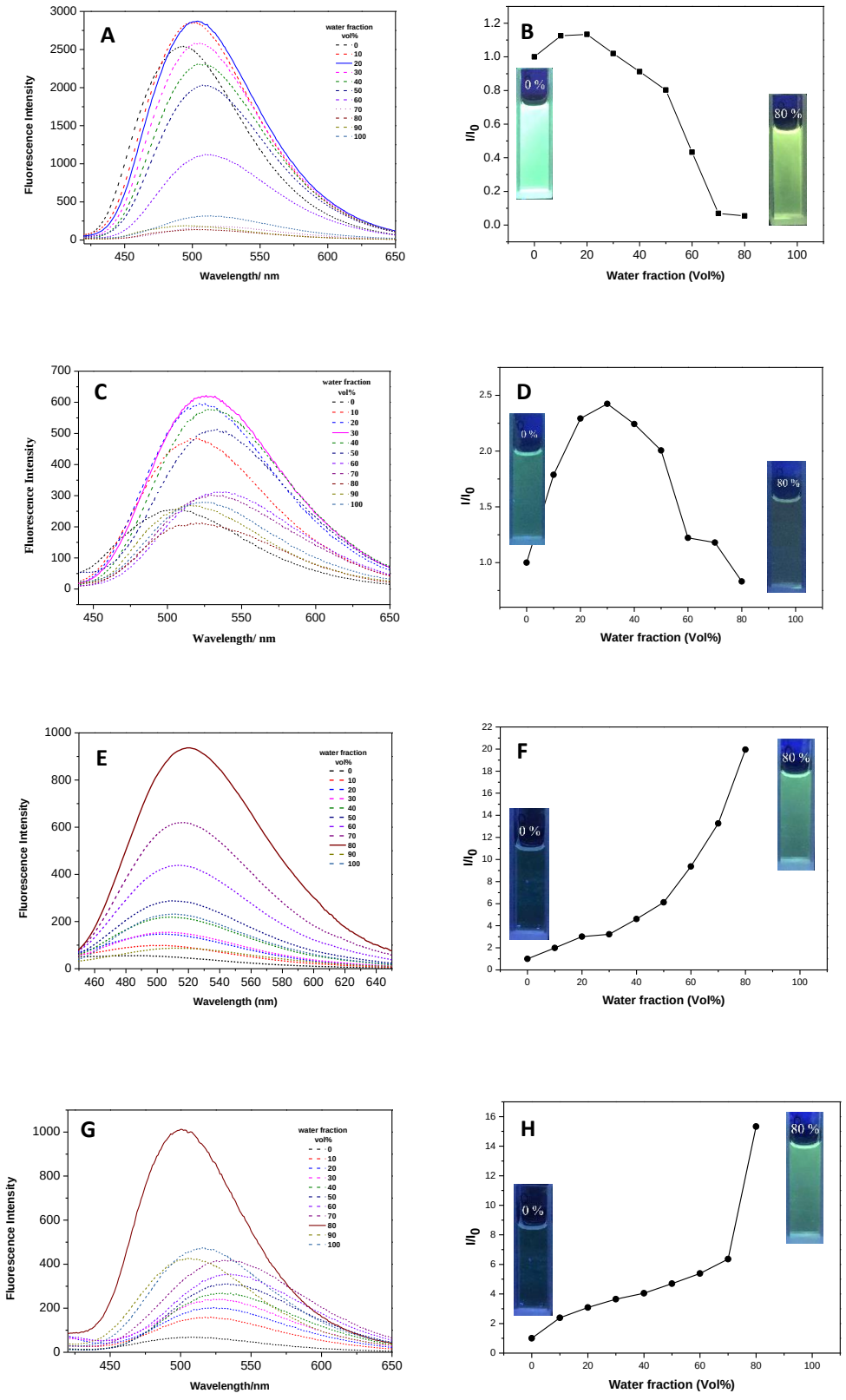


Fig. S2. Fluorescence spectra of all the compounds in THF/water mixtures and

dependence of the I/I_0 ratios of all the compounds on the solvent composition of the THF/water mixture. BIN-CN: (A) and (B); BIN-COM: (C) and (D); BIN-COE: (E) and (F); BIN-COP: (G) and (H). Concentration: 10 μM, λ_{ex} = 340 nm.

5. Solid fluorescence spectra of BIN-CN, BIN-COM, BIN-COE, BIN-COP

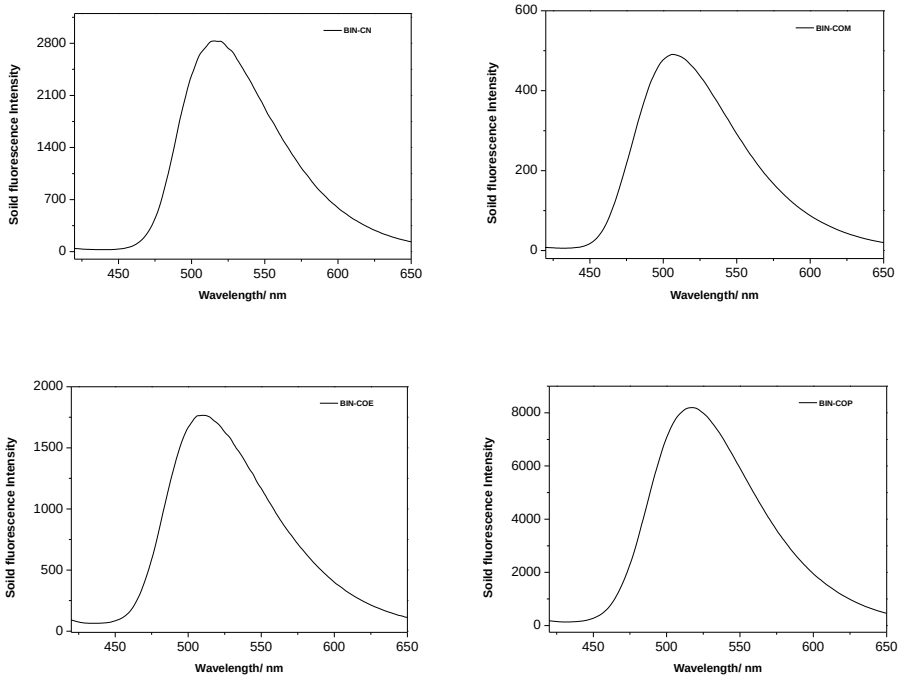


Fig. S2. Solid fluorescence spectra of all the compounds, λ_{ex} = 340 nm.

6. Fluorescent lifetime and quantum yield of BIN-CN, BIN-COM, BIN-COE, BIN-COP in solution and in solid

Table S2. Fluorescent lifetime of all the compounds in DMSO and in solid.

Compd.	Lifetime in soluetion (ns)	Lifetime in solid state (ns)
BIN-CN	τ_1=2.01 (6.8%) τ_2=4.08 (93.2%)	τ_1=1.52 (38%) τ_2=0.17 (53%) τ_3=3.57 (9%)
BIN-COM	τ_1=6.50 (49%) τ_2=1.93 (43%) τ_3=4.80 (7%)	τ_1=0.23 (47%) τ_2=1.68 (50%) τ_3=4.76 (3%)
BIN-COE	τ_1=1.49 (17%) τ_2=3.08 (83%)	τ_1=0.17 (78%) τ_2=0.74 (21%) τ_3=4.19 (1%)
BIN-COP	τ_1=2.08 (25%) τ_2=4.03 (70%) τ_3=6.08 (5%)	τ_1=1.23 (27%) τ_2=3.93 (8%) τ_3=0.17 (65%)

Table S3. Quantum yield of all the compounds in DMSO and in solid.

Compd.	Quantum yield in soluetion (%)	Quantum yield in solid state (%)
BIN-CN	1.9	1.45
BIN-COM	0.99	0.98
BIN-COE	0.54	0.01
BIN-COP	0.58	0.97

Table S4. The rate constants for radiative (k_r) and nonradiative decay (k_{nr}) were calculated from the Φ and τ values according to the formulae $k_r = \Phi_F/\tau$ and $k_{nr} = (1-\Phi_F)/\tau$.

Compound	Solution		Solid state	
	k_r (s^{-1})	k_{nr} (s^{-1})	k_r (s^{-1})	k_{nr} (s^{-1})
BIN-CN	4.82×10^6	2.49×10^8	1.46×10^7	9.95×10^7
BIN-COM	2.28×10^6	2.27×10^8	8.90×10^6	9.00×10^8
BIN-COE	1.92×10^6	3.54×10^8	3.00×10^5	3.03×10^9
BIN-COP	1.59×10^6	2.72×10^8	1.27×10^7	1.30×10^7

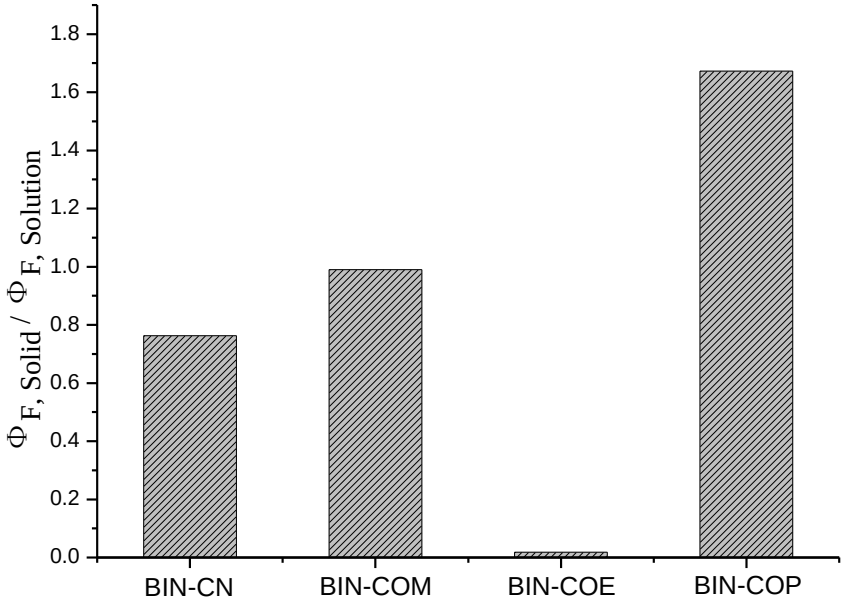


Fig. S4 The ratio of the quantum yields for the solid and solution states of all the compounds.

7. Theoretical Calculation of BIN-COE and BIN-COP Based on the Single Crystal

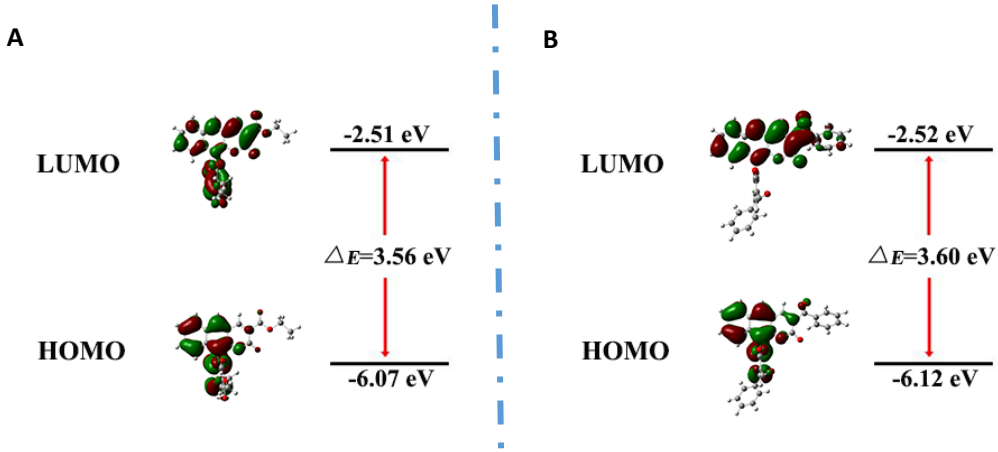


Fig. S5 Molecular orbital amplitude plots of HOMO and LUMO levels of A) BIN-COE and B) BIN-COP calculated at the B3LYP/6-31G (d, p) level of theory.

8. Views of the molecular stacking structures in single crystals of BIN-COE and BIN-COP

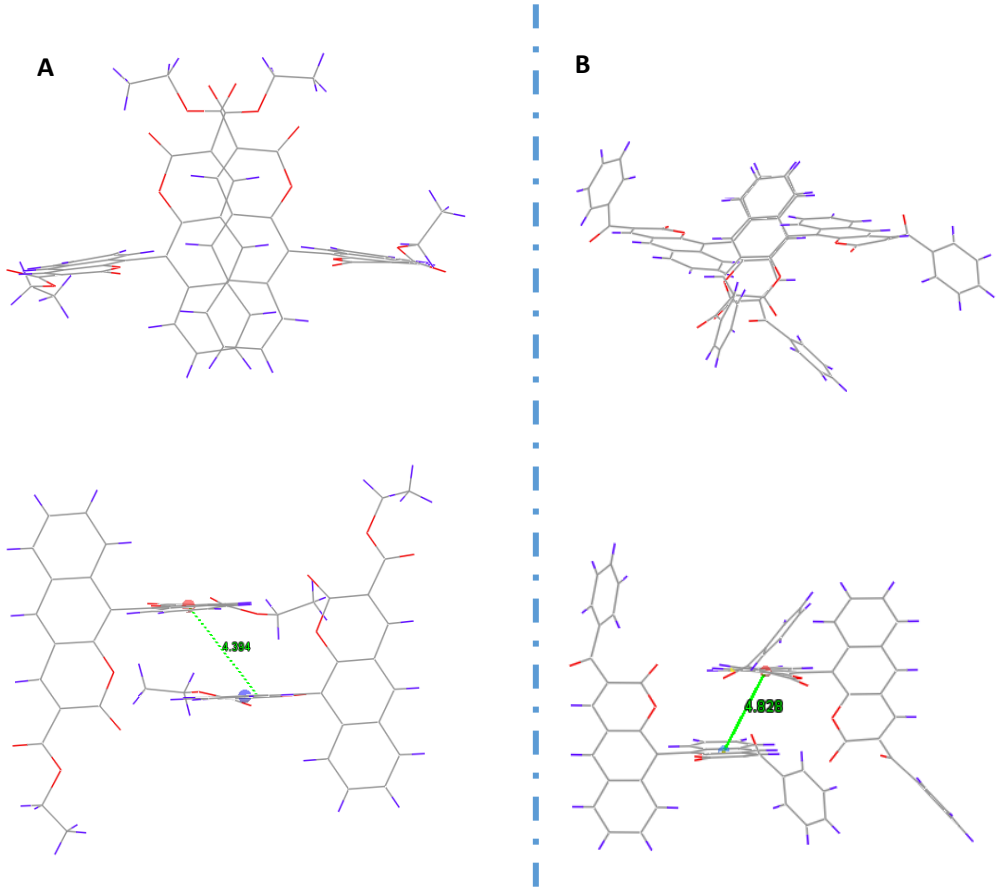


Fig. S6 Side and top view of crystal packing mode of A) BIN-COE and B) BIN-COP. Carbon, hydrogen, and oxygen atoms are shown in gray, blue, and red, respectively.

9. Crystallographic data of BIN-COE and BIN-COP

Crystal data and structure refinements of BIN-COE:

Identification code	BIN-COE
Empirical formula	$C_{32}H_{22}O_8$
Formula weight	534.49
Temperature/K	129.9(4)
Crystal system	triclinic
Space group	P1
a/Å	12.7039(6)
b/Å	13.6838(11)
c/Å	20.0466(13)
α/°	71.882(7)
β/°	78.624(5)
γ/°	75.444(6)
Volume/Å^3	3178.8(4)
Z	4
ρ_{calc}g/cm^3	1.117
μ/mm^{-1}	0.081
F(000)	1112.0
Crystal size/mm^3	0.3 × 0.25 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.036 to 52.744
Index ranges	$-15 \leq h \leq 15$, $-14 \leq k \leq 17$, $-25 \leq l \leq 25$
Reflections collected	25698
Independent reflections	17982 [R_{int} = 0.0263, R_{sigma} = 0.0502]
Data/restraints/parameters	17982/4/1431
Goodness-of-fit on F^2	0.911
Final R indexes [I>=2σ (I)]	R_1 = 0.0564, wR_2 = 0.1454
Final R indexes [all data]	R_1 = 0.0840, wR_2 = 0.1626
Largest diff. peak/hole / e Å^{-3}	0.42/-0.31
Flack parameter	-0.4(5)
CCDC number	1588883

Crystal data and structure refinements of BIN-COP:

Empirical formula	$C_{40}H_{22}O_6$
Formula weight	598.14
Temperature/K	293.7(4)
Crystal system	orthorhombic

Space group	$P2_12_12_1$
a/Å	11.7124(4)
b/Å	22.5365(7)
c/Å	24.3520(7)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	6427.9(4)
Z	4
ρ_{calc}g/cm^3	1.347
μ/mm^{-1}	0.756
F(000)	2712.0
Crystal size/mm^3	0.5 × 0.2 × 0.2
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.508 to 145.584
Index ranges	-14 ≤ h ≤ 14, -27 ≤ k ≤ 27, -18 ≤ l ≤ 29
Reflections collected	20075
Independent reflections	11300 [R_{int} = 0.0244, R_{sigma} = 0.0335]
Data/restraints/parameters	11300/0/897
Goodness-of-fit on F^2	1.022
Final R indexes [I>=2σ (I)]	R_1 = 0.0512, wR_2 = 0.1374
Final R indexes [all data]	R_1 = 0.0615, wR_2 = 0.1481
Largest diff. peak/hole / e Å^{-3}	0.19/-0.26
Flack parameter	0.18(10)
CCDC number	1588882

10. Circular dichroism (CD) spectra of all compounds

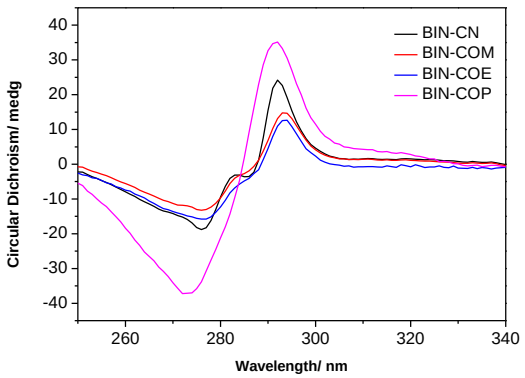


Figure S7 CD spectra of BIN-CN, BIN-COM, BIN-COE and BIN-COP.

10. Single-photo CLSM images of Hela cells incubated with BIN-CN, BIN-COM,BIN-COE and BIN-COP

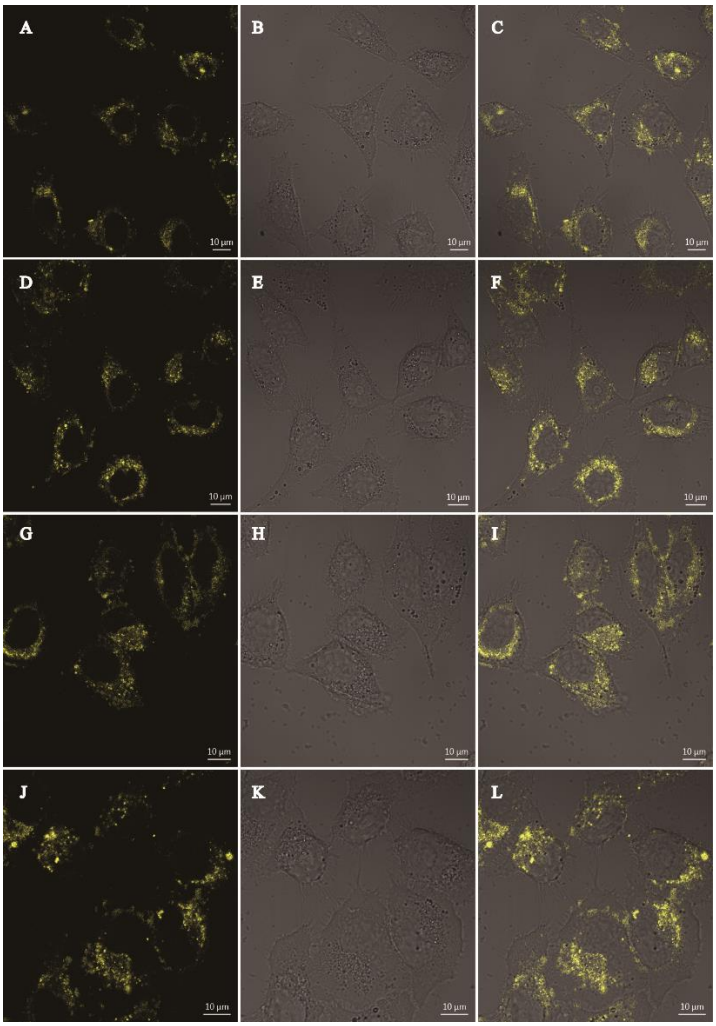


Fig. S8. Bright field and fluorescent images of Hela cells stained with (A-C) BIN-CN, (D-E) BIN-COM, (G-I) BIN-COE, (J-L) BIN-COP. Concentration 5 μM. Excitation wavelength: 405 nm.

11. Cytotoxicity of BIN-COP on Hela cells evaluated by MTT assay

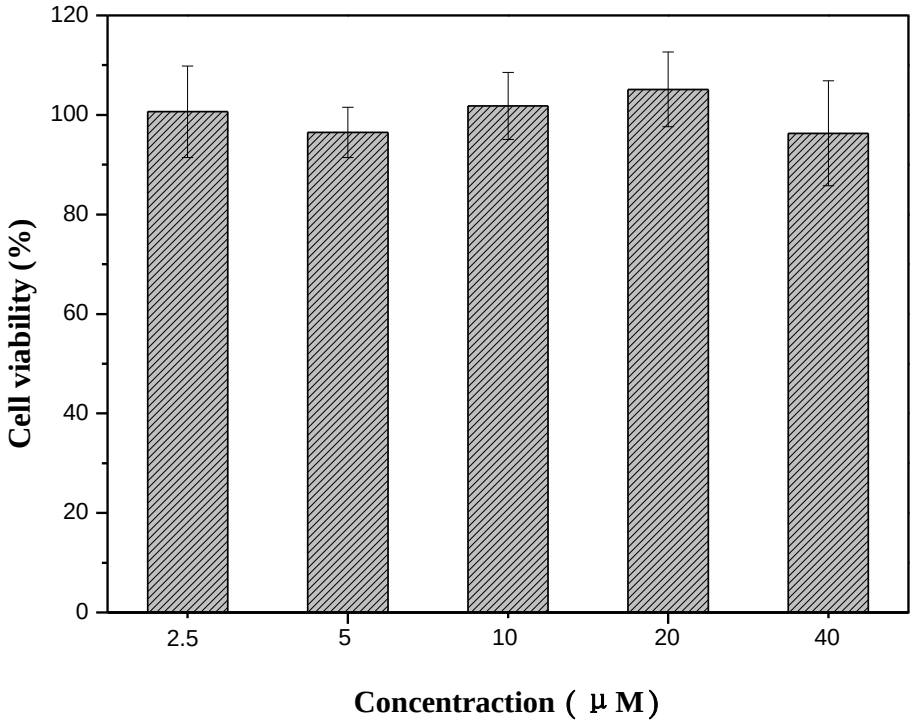


Fig. S9. Cell viabilities of Hela cells after incubation with different concentrations of BIN-COP (0, 2.5, 5, 10, 20, 40 μM) for 24 h.

12. Two-photo CLSM images of Hela cells incubated with BIN-CN, BIN-COM,BIN-COE and BIN-COP

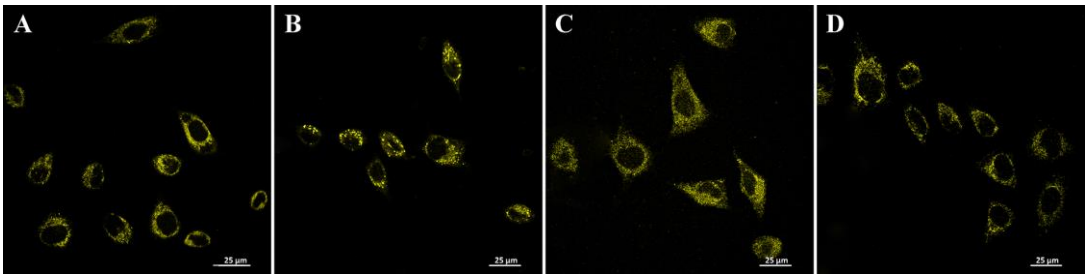
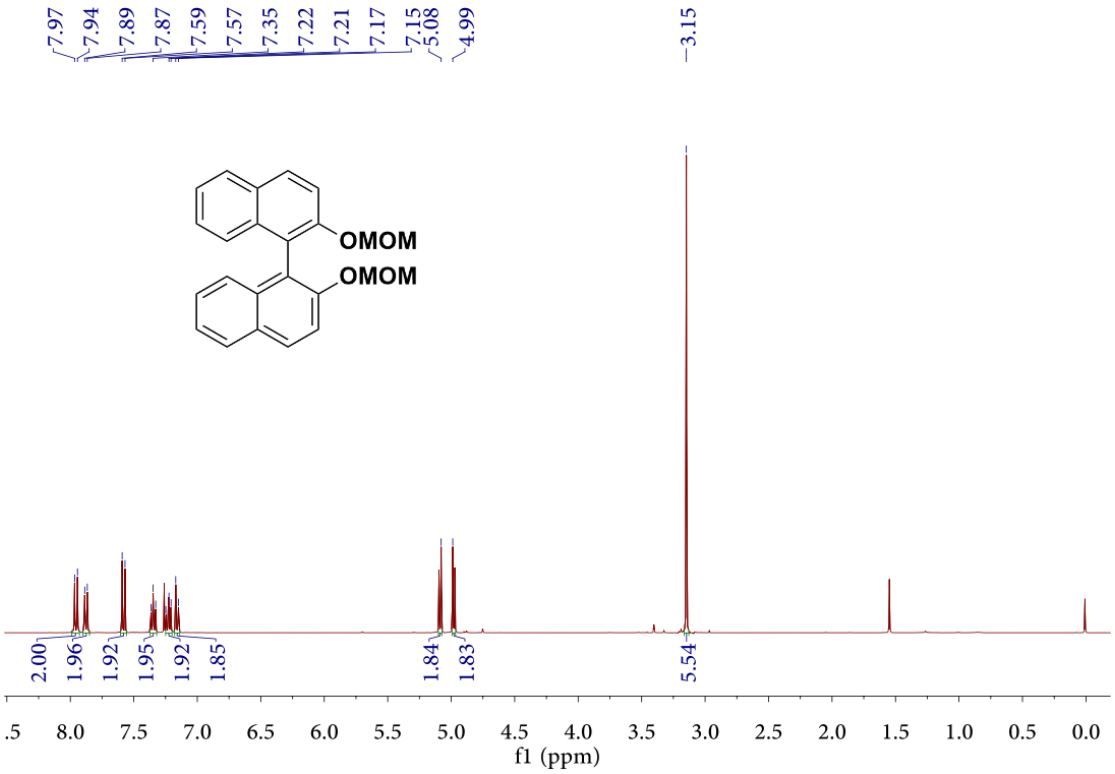
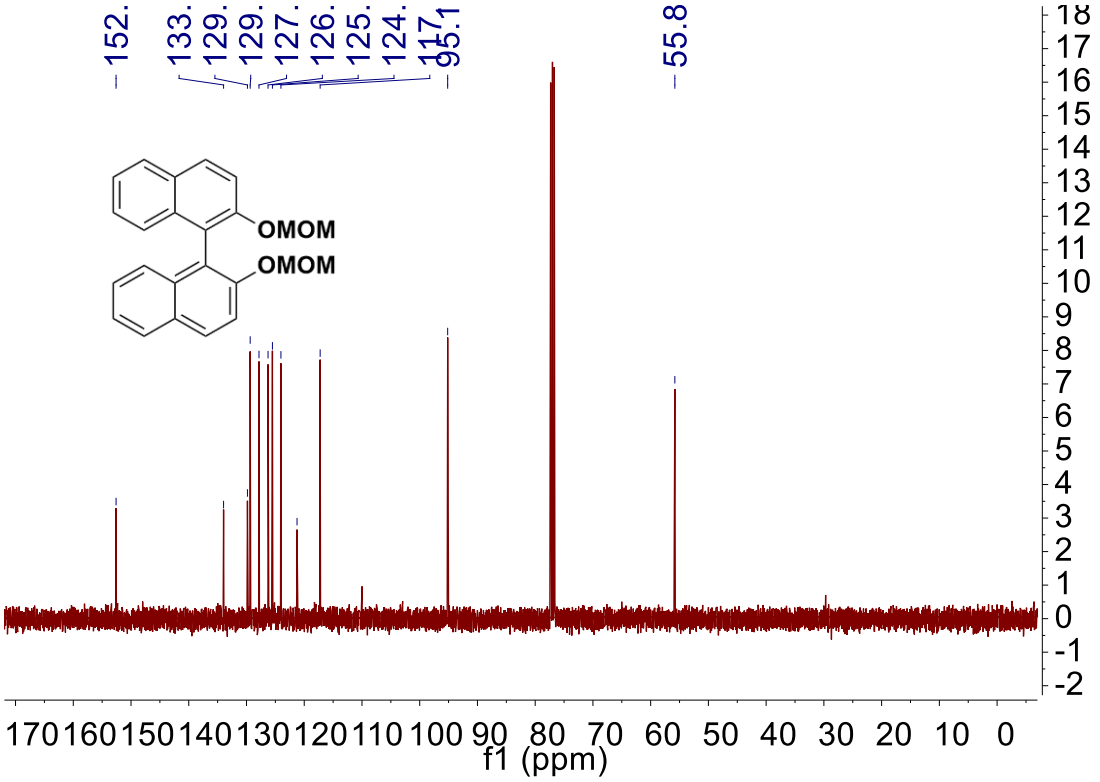


Fig. S10. Two-photo confocal fluorescent images of Hela cells stained with A) BIN-CN, B) BIN-COM, C) BIN-COE, D) BIN-COP. Concentration 5 μM. Excitation wavelength: 730 nm.

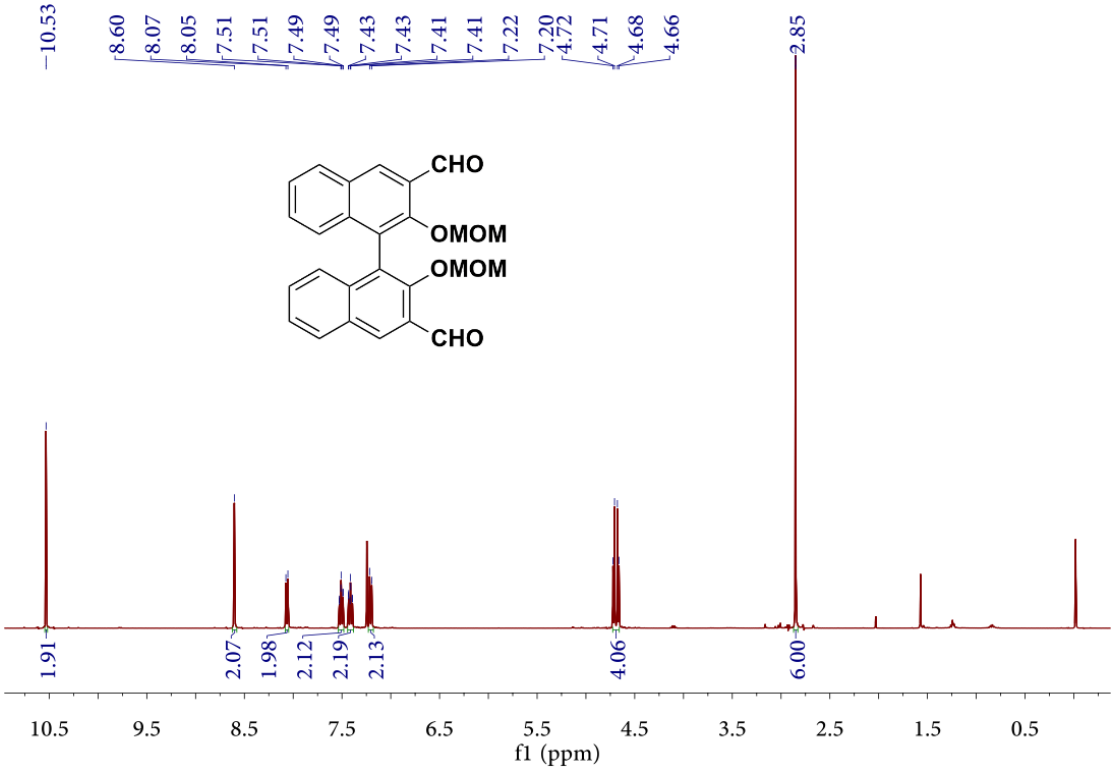
11. NMR Data

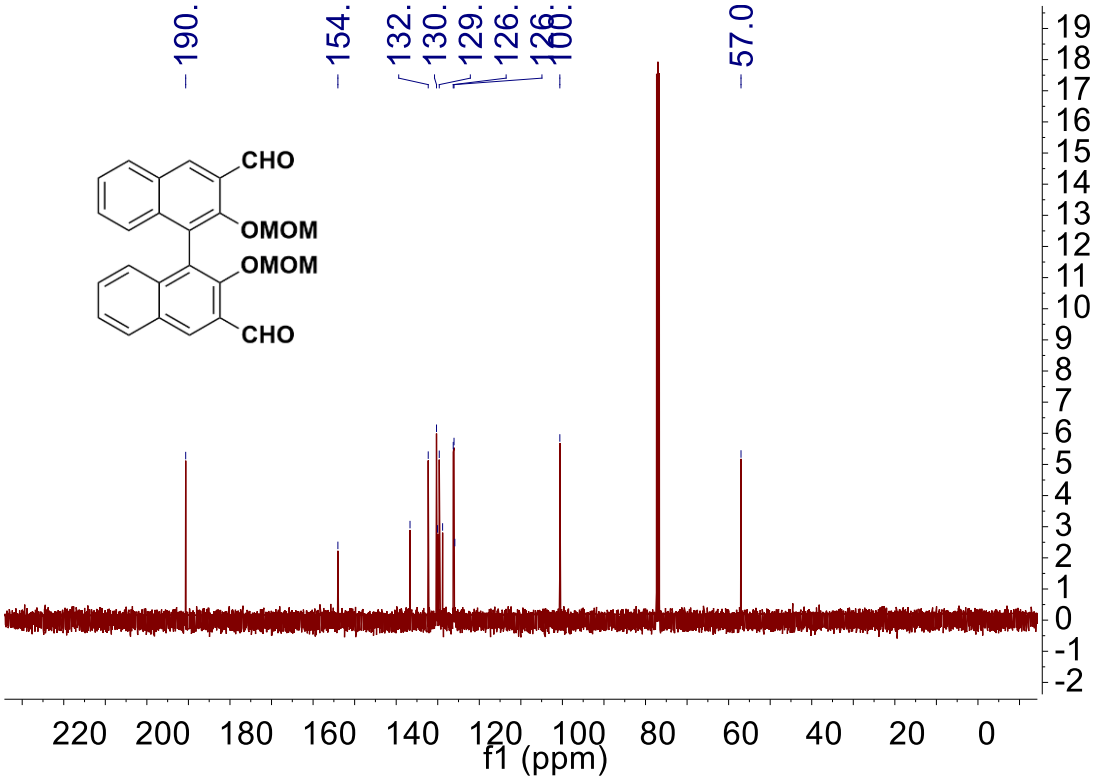
BIN-2:



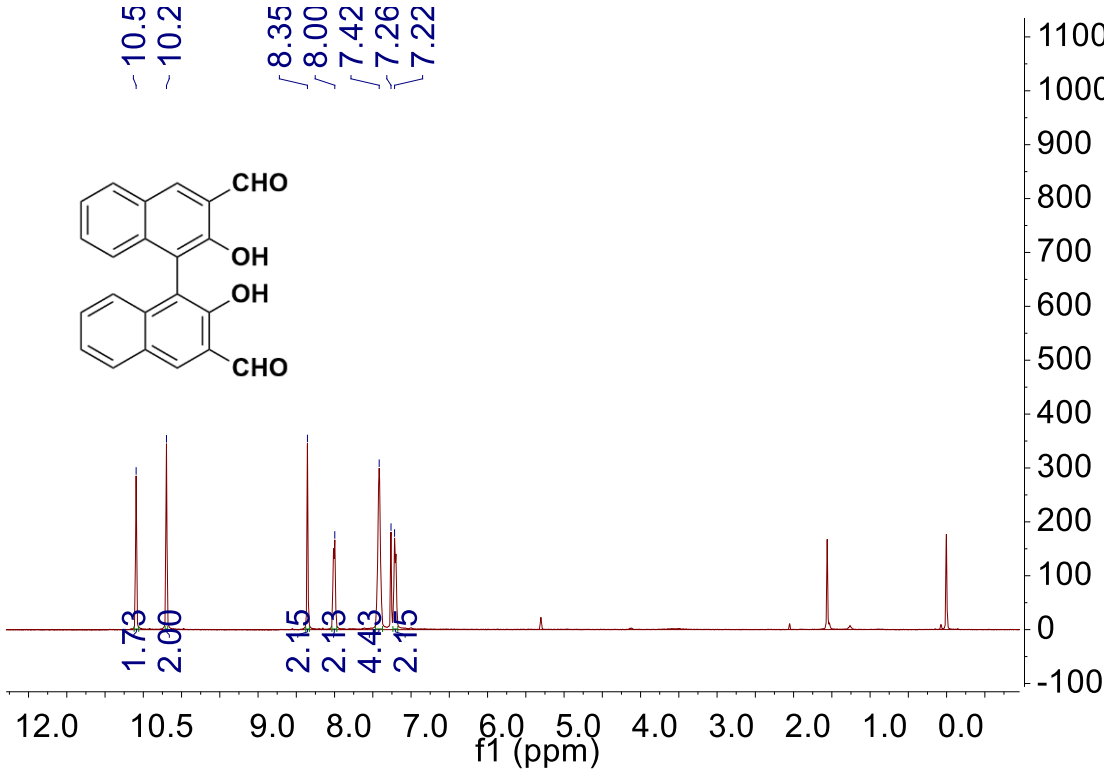


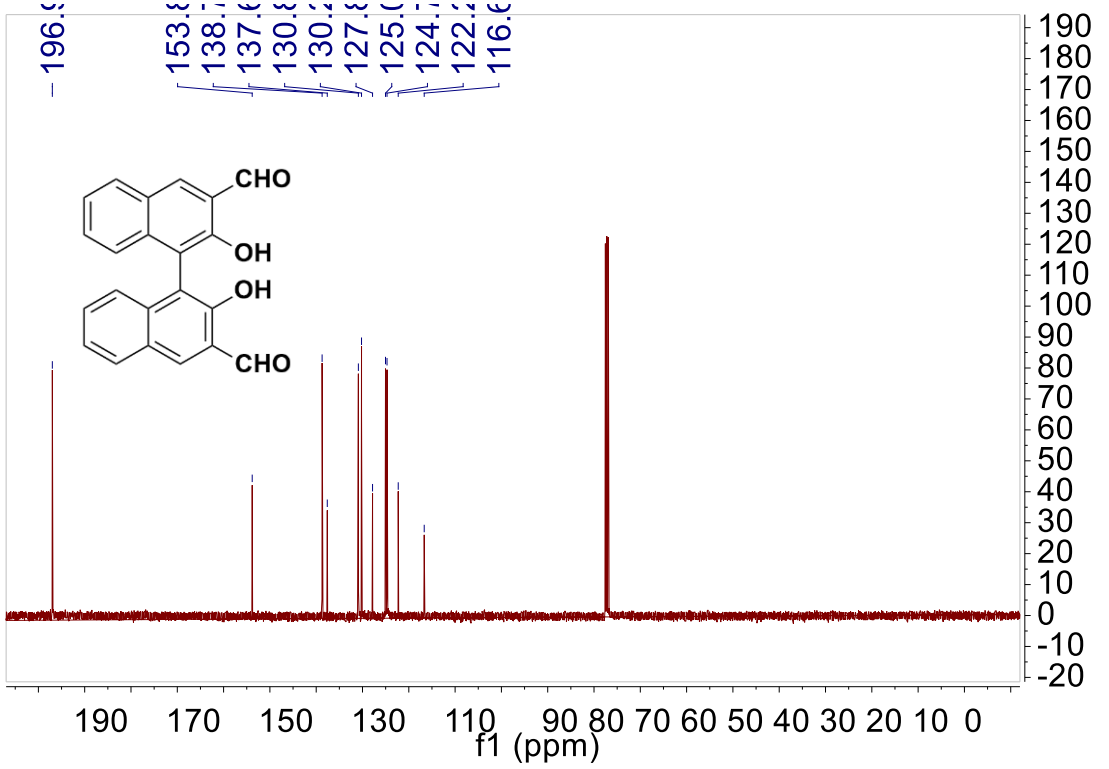
BIN-3:


10.53
8.60
8.07
8.05
7.51
7.51
7.49
7.49
7.43
7.43
7.41
7.41
7.22
7.20
4.72
4.71
4.68
4.66
2.85
CHO
OMOM
OMOM
CHO
1.91
2.07
1.98
2.12
2.19
2.13
4.06
6.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

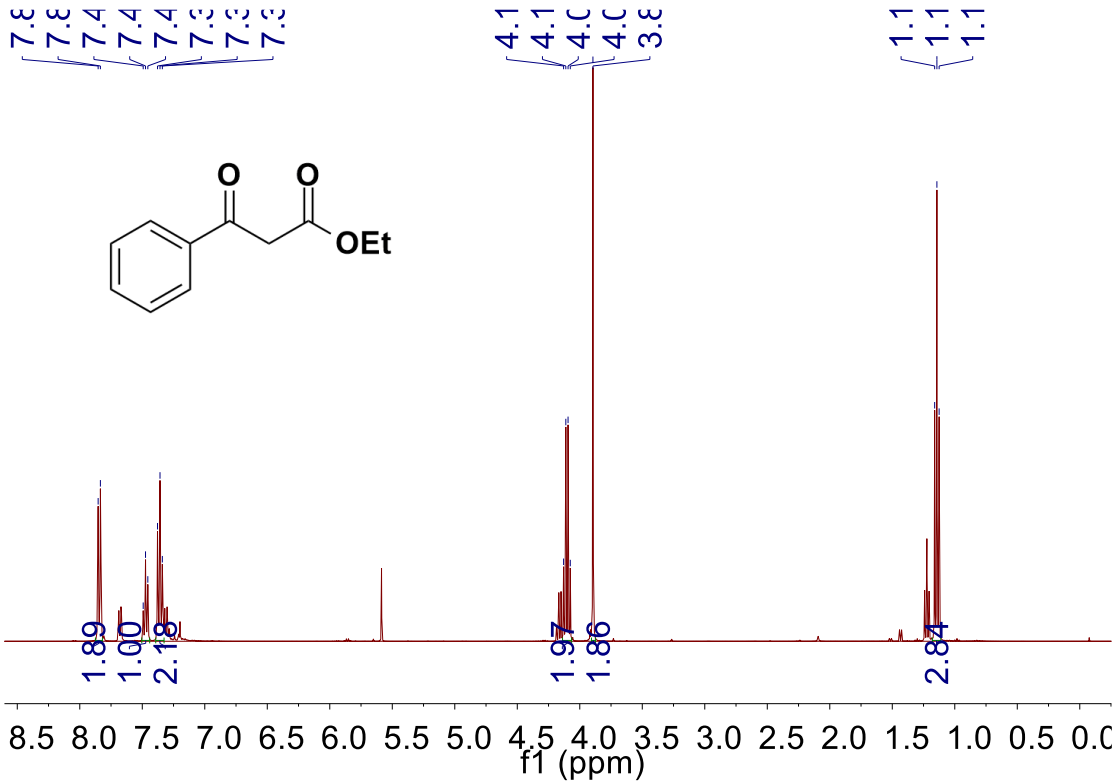

190.
154.
132.
130.
129.
126.
126.
100.
57.0
CHO
OMOM
OMOM
CHO
19
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
220
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

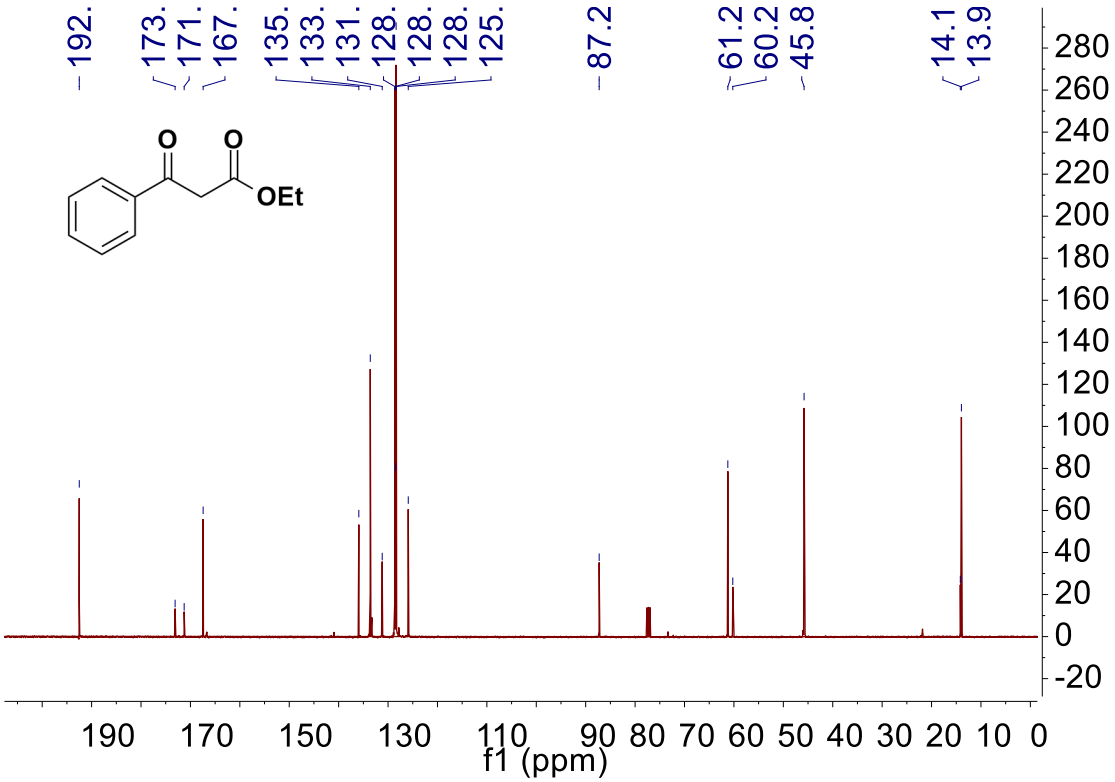
BIN-4:


10.5
10.2
8.35
8.00
7.42
7.26
7.22
CHO
OH
OH
CHO
1.73
2.00
2.15
2.13
4.43
2.15
f1 (ppm)

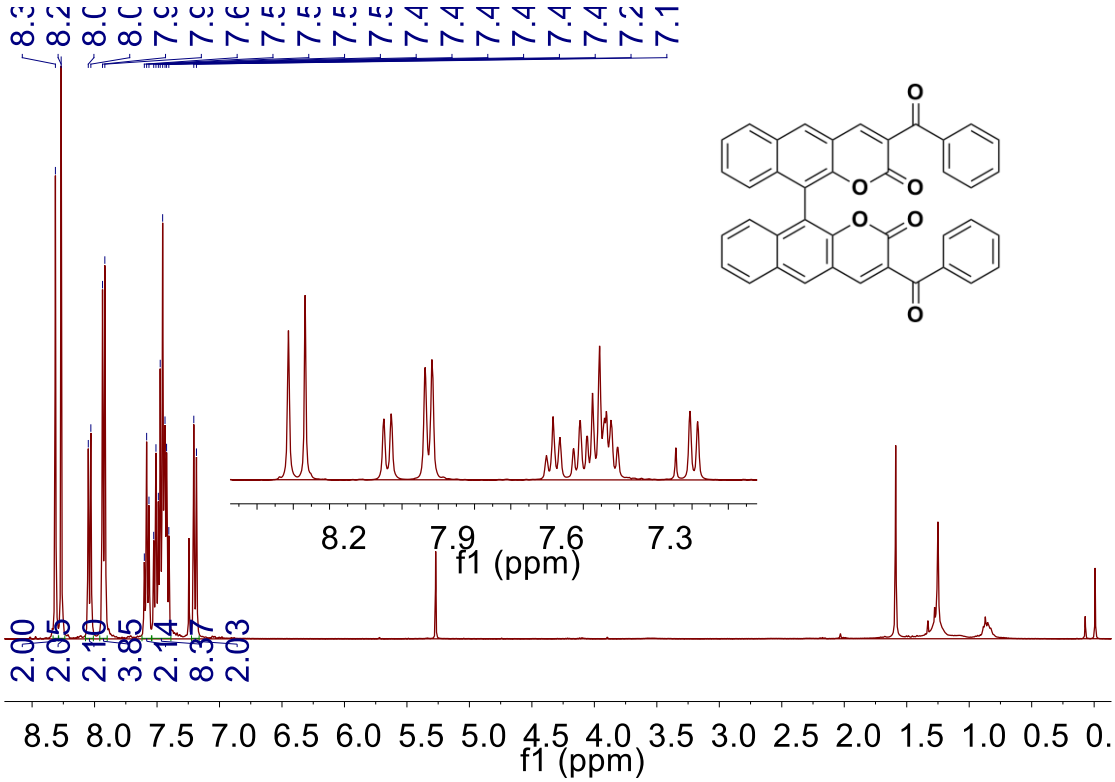

196.
153.
138.
137.
130.
130.
127.
125.
124.
122.
116.
CHO
OH
OH
CHO
f1 (ppm)

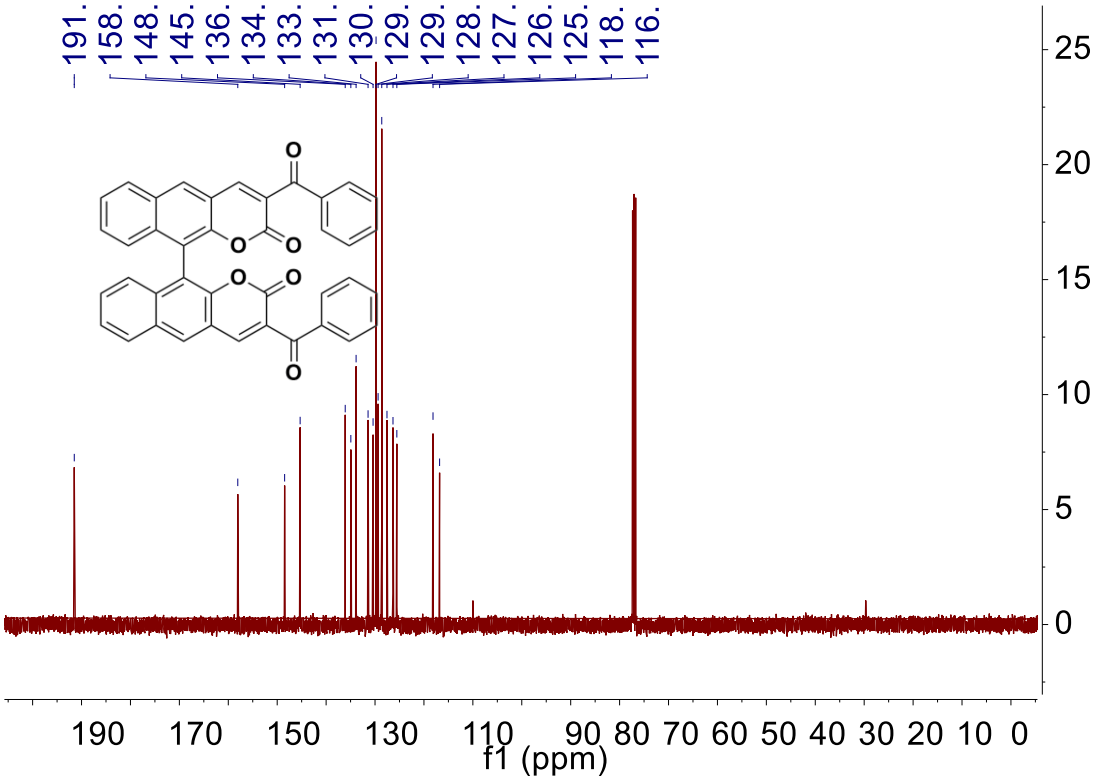
ethyl benzoylacetate：



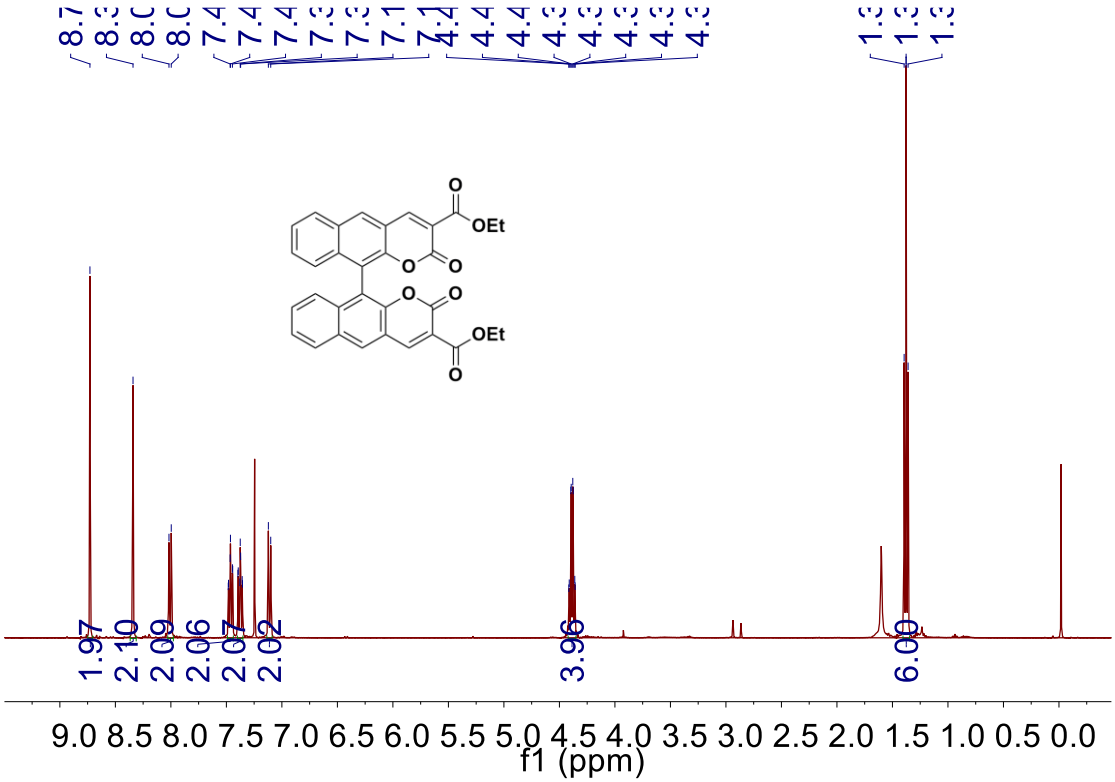


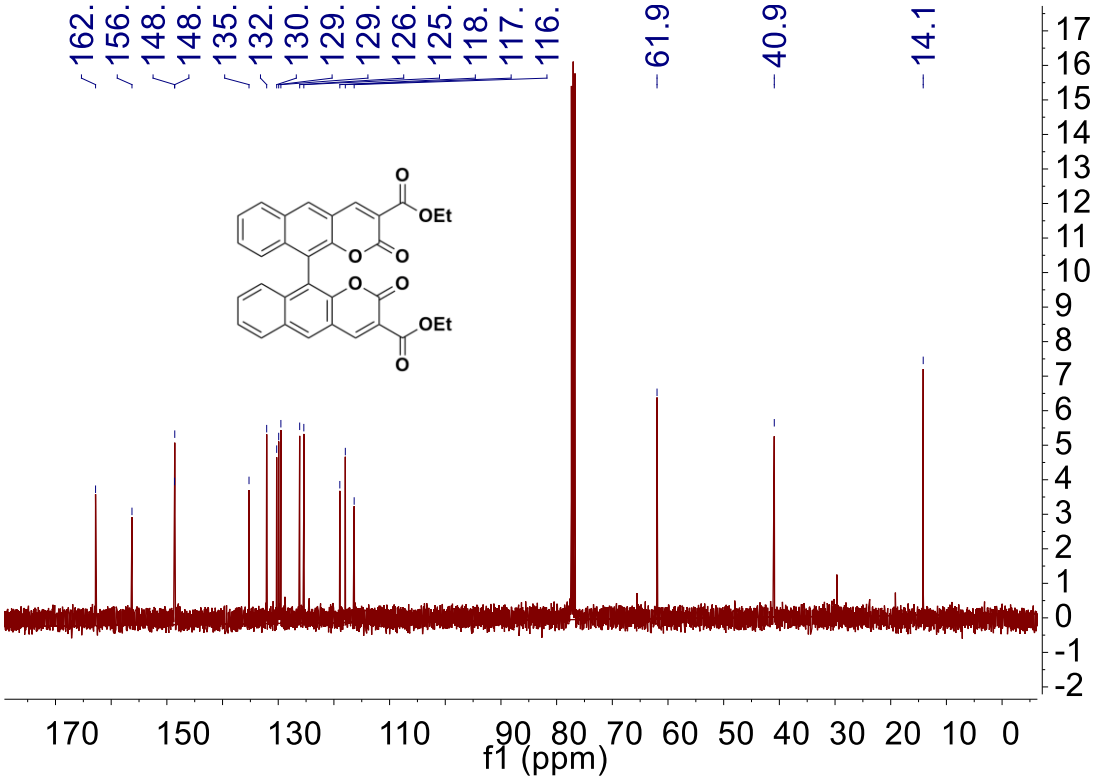
BIN-COP:


8.2
7.9
7.6
7.3
f1 (ppm)
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
f1 (ppm)

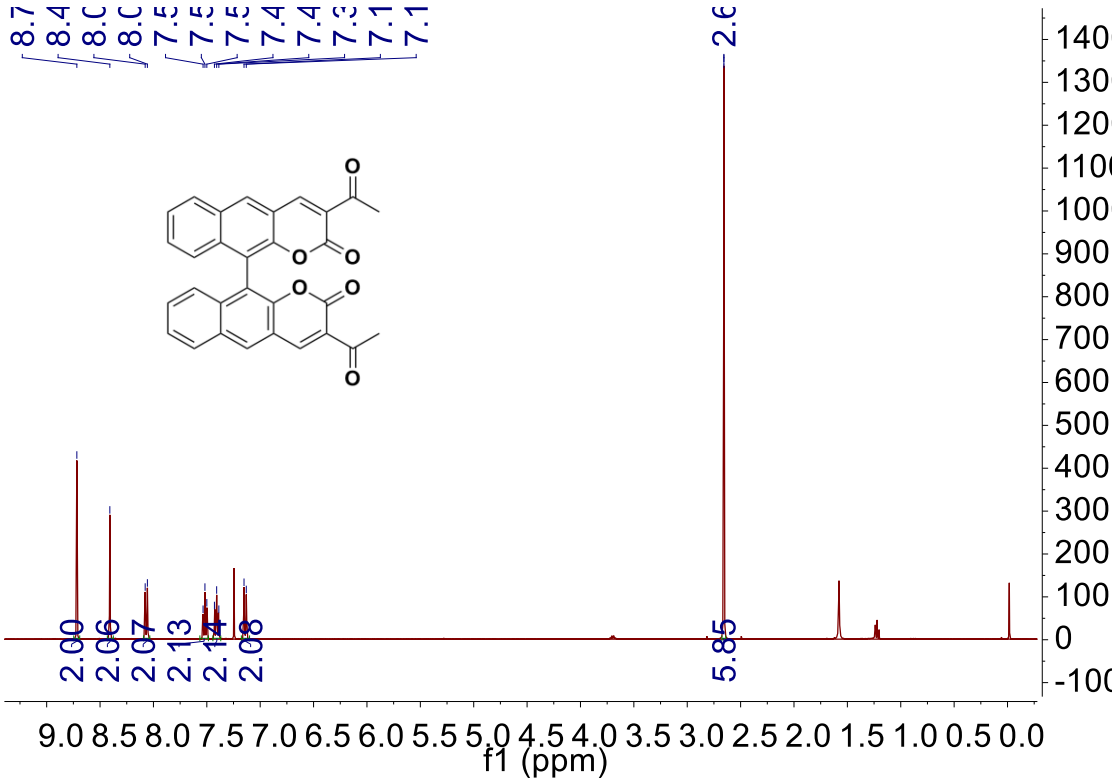

25
20
15
10
5
0
190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

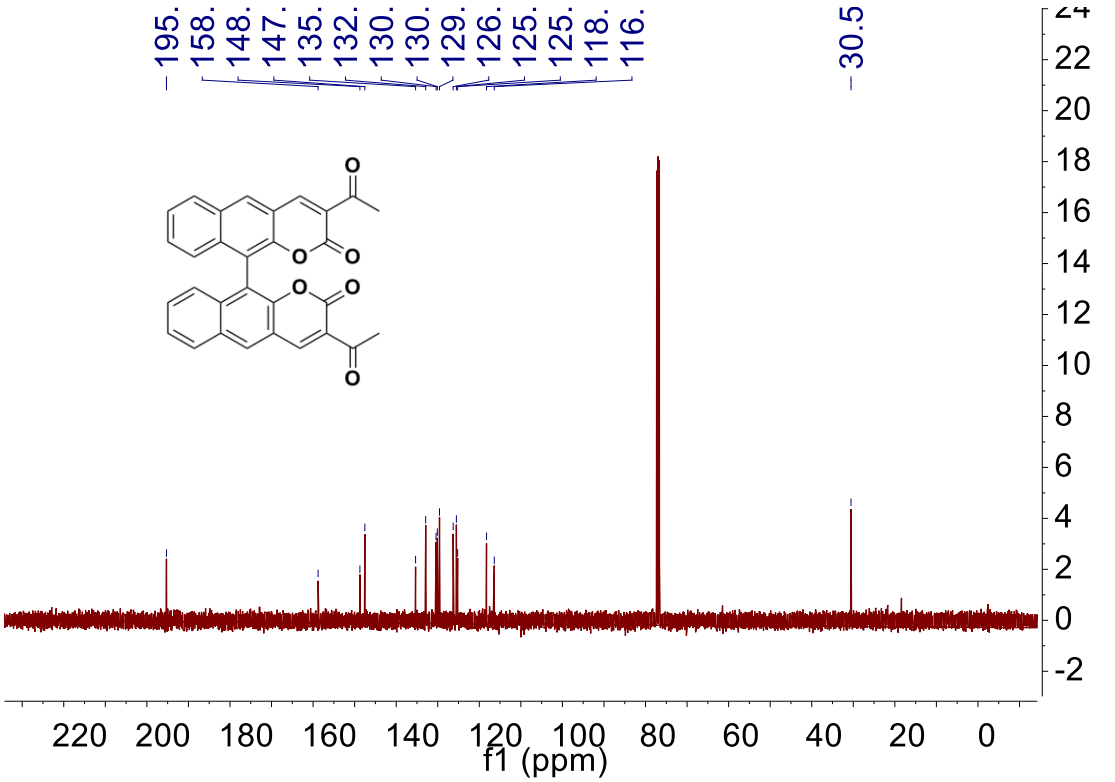
BIN-COE:


8.7
8.3
8.0
8.0
7.4
7.4
7.4
7.3
7.3
7.1
7.1
4.4
4.4
4.4
4.3
4.3
4.3
4.3
4.3
1.3
1.3
1.3
OEt
OEt
1.97
2.10
2.09
2.06
2.07
2.02
3.96
6.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

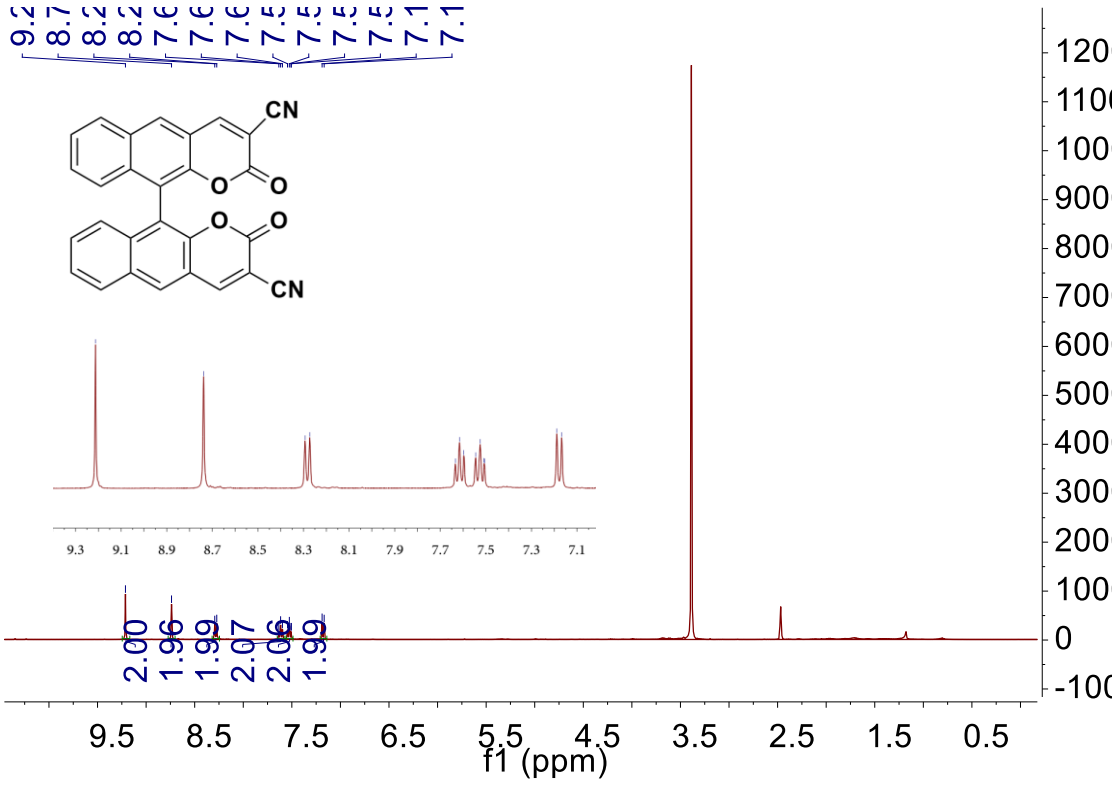

162.
156.
148.
148.
135.
132.
130.
129.
129.
126.
125.
118.
117.
116.
61.9
40.9
14.1
OEt
OEt
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

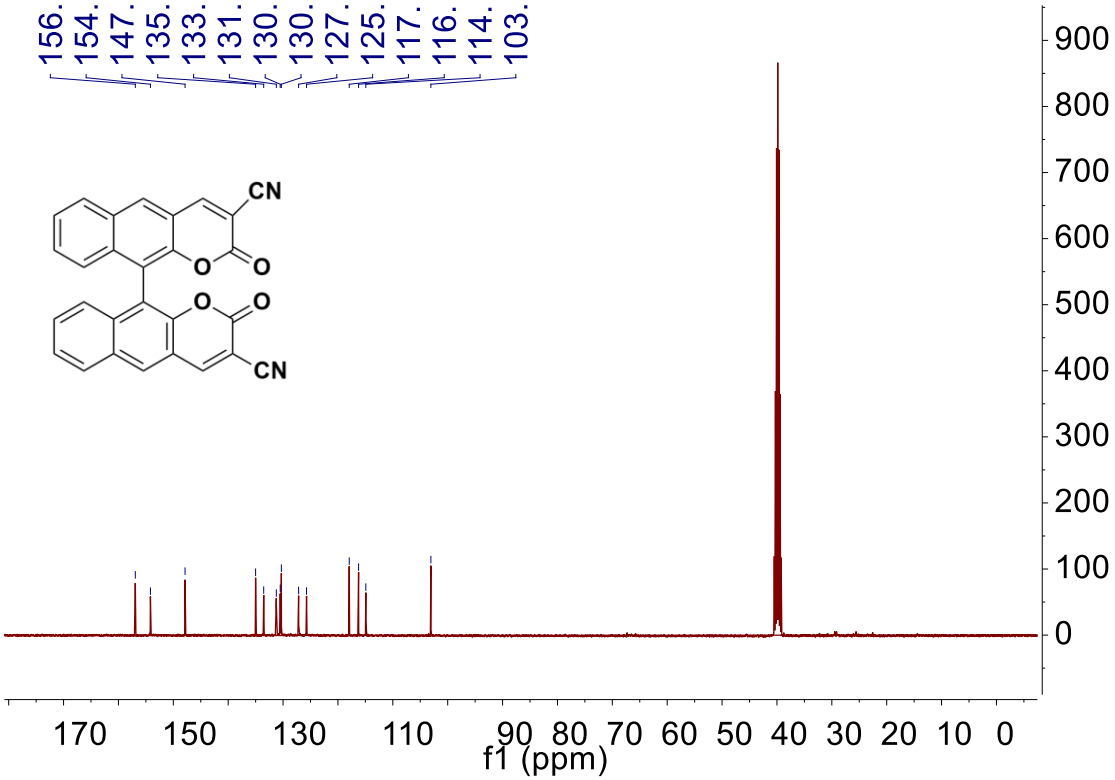
BIN-COM:


8.7
8.4
8.0
8.0
7.4
7.4
7.1
7.1
2.6
2.00
2.06
2.07
2.13
2.14
2.08
5.85
f1 (ppm)


195.
158.
148.
147.
135.
132.
130.
130.
129.
126.
125.
125.
118.
116.
30.5
f1 (ppm)

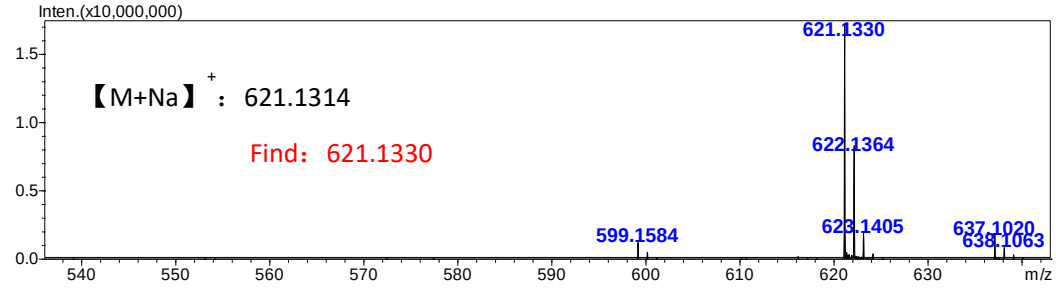
BIN-CN:



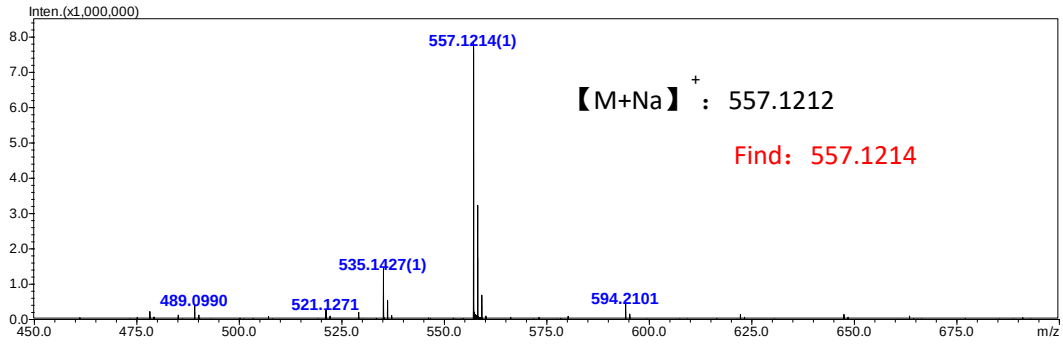


12. ESI-MS Data

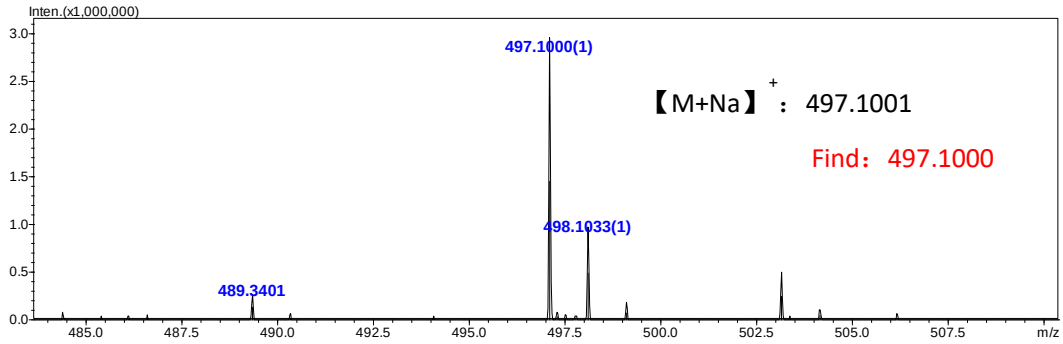
BIN-COP:



BIN-COE:



BIN-COM:



BIN-CN: