

# Supporting Information

## “Click” Disaggregation-Induced Emission of a Fluorescent Dye

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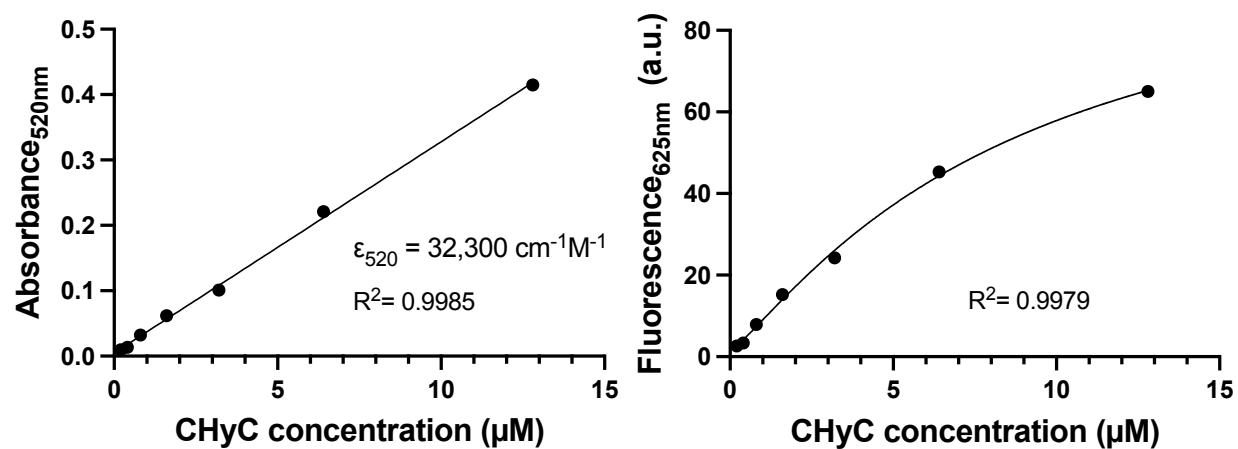
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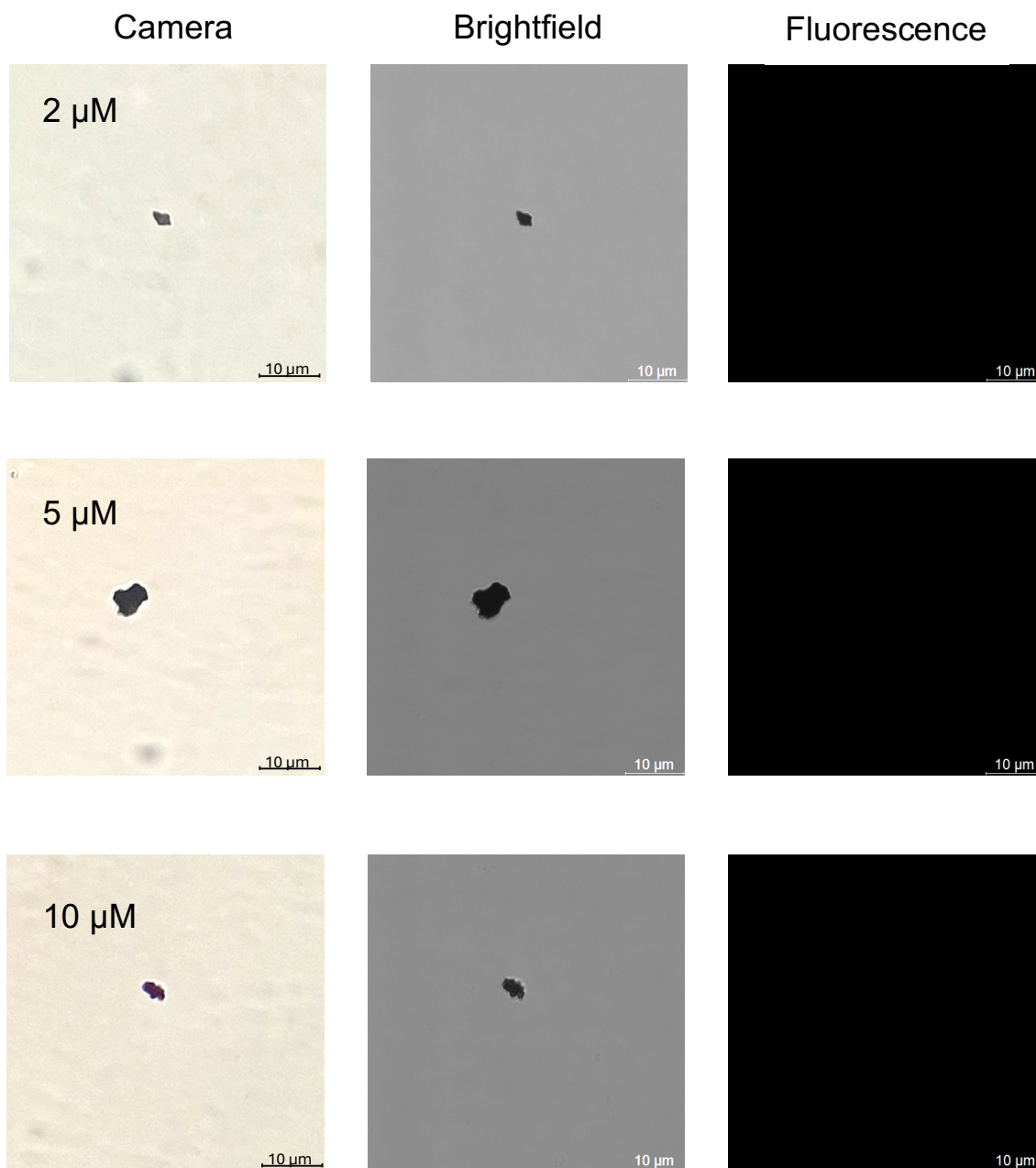
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## Supplemental Figures



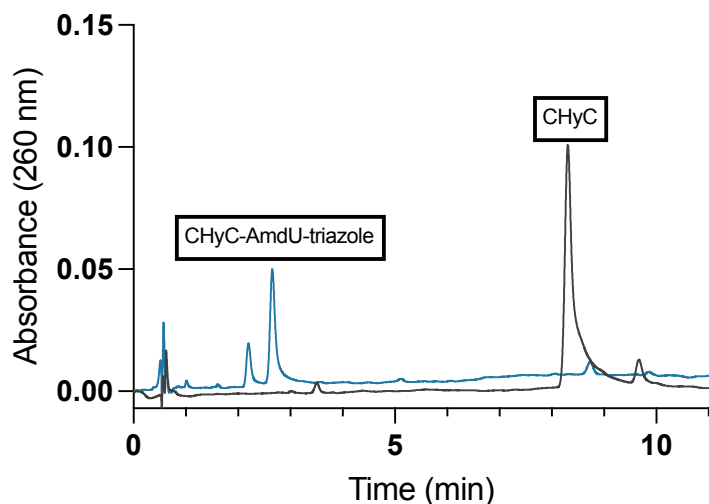
**Figure S1.** Absorbance value at 520 nm and fluorescence at 625 nm over a range of CHyC concentrations (0.2 – 12.4 μM) in PBS pH 7.4 (2% EtOH). Using the linear fit to the absorbance graph, the extinction coefficient was obtained assuming  $\epsilon = \frac{\text{slope}}{l}$  and path length ( $l = 1$ ). The fluorescence was fitted to a sigmoidal non-linear regression.



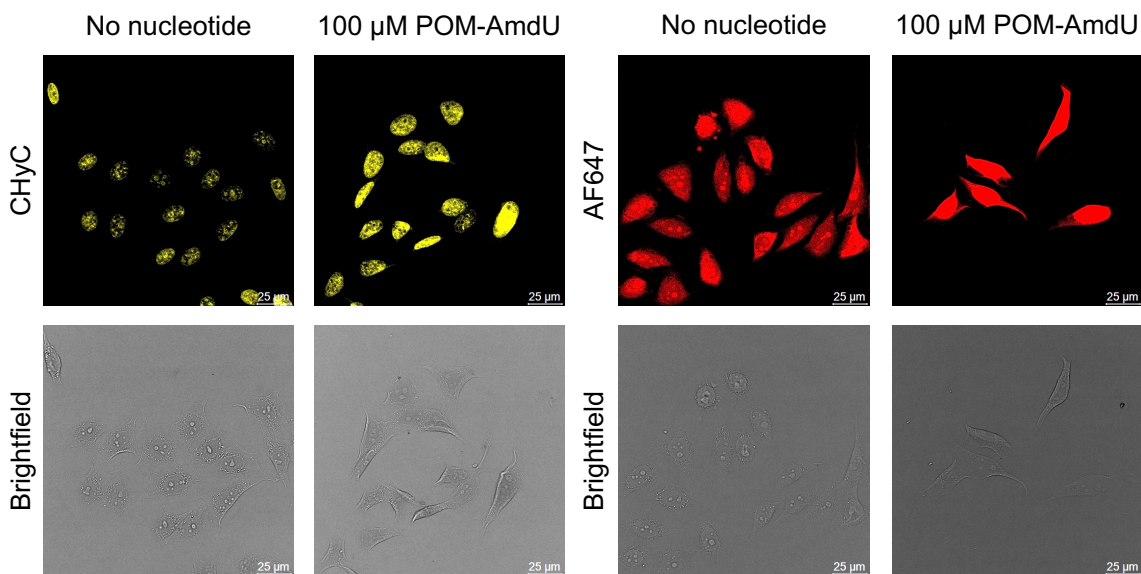
**Figure S2.** Colour camera image, brightfield, and fluorescence emission of CHyC aggregate at various concentrations. 2, 5, or 10 μM CHyC in PBS (pH 7.4) with 2 % ethanol was imaged using confocal microscopy. A HC PL APO 63x/1.40 OIL CS2 objective lens was used with a 3.4x zoom to closely observed the microparticle. Fluorescence emission was captured from 590 to 650 nm with an excitation of 561 nm.

**Table S1.** Photophysical properties of 2  $\mu\text{M}$  solution of CHyC in various solvents (0.5% DMSO).

Solvent	Quantum yield (% $\Phi_{546}$ )	Extinction coefficient ( $\epsilon_{546}$ ) $\text{cm}^{-1} \text{M}^{-1}$	Brightness ( $\Phi_{546} \times \epsilon_{546}$ ) $\text{cm}^{-1} \text{M}^{-1}$
Methanol	1.0%	50 750	531
PBS pH 7.4	0.9%	28 050	245
Acetonitrile	1.1%	41 700	469
DMSO	5.4%	41 900	2268



**Figure S3.** RP-HPLC trace of CuAAC reaction between CHyC and AmdU (blue) compared to unreacted CHyC (black). The gradient of ACN: 0.1 M aqueous triethylammonium acetate pH 7.0 (TEAA) was applied: 30:70 to 65:35 over 19 min with a flow rate of 3.0 mL/min and a column temperature of 50°C. Elution was monitored by UV absorption at 260 nm.



**Figure S4.** No-wash imaging of cells in staining solutions containing 10  $\mu\text{M}$  CHyC or the Cy5 derivative "AF647 alkyne". HeLa cells were pre-treated with 100  $\mu\text{M}$  of POM-AmdU for 17 hours followed by fixation, denaturation, and incubation with 10  $\mu\text{M}$  CHyC or AF647 in the presence of 1 mM  $\text{CuSO}_4$ , 2 mM THPTA, and 10 mM sodium ascorbate for 2 hours and directly imaged without removing the staining solutions. Negative controls received identical treatment but were not pre-incubated with POM-AmdU. CHyC fluorescence was captured from 590 to 650 nm with an excitation of 561 nm. AF647 was excited at 633 nm and fluorescence sampled from 650 to 700 nm.

## General Methods and Synthetic Procedures

Starting materials were obtained in the highest commercial grades and used without further purification. AmdU and POM-AmdU were synthesized in our lab.<sup>1-2</sup> Reactions sensitive to moisture and/or air were carried out under an atmosphere of argon in anhydrous solvents and oven-dried glassware. Analytical thin-layer chromatography was performed on pre-coated 250  $\mu\text{m}$  thick silica gel 60 F254 plates and visualized by ultraviolet light.

NMR spectra were recorded with a Bruker AVIII- 400 or AVIIHD 500 (400 MHz for  $^1\text{H}$ , 101 MHz for  $^{13}\text{C}$  or 500 MHz for  $^1\text{H}$ , 126 MHz for  $^{13}\text{C}$ ).  $^{13}\text{C}$  spectra were measured with broadband proton decoupled. Chemical shifts ( $\delta$ ) are given in parts per million (ppm) with residual solvent peaks used as internal standards:  $d_6$ -DMSO ( $\delta\text{H} = 2.50$  ppm),  $\text{CDCl}_3$  ( $\delta\text{H} = 7.26$  ppm),  $d_6$ -DMSO ( $\delta\text{C} = 40.5$  ppm), or  $\text{CDCl}_3$  ( $\delta\text{C} = 77.23$  ppm). Coupling constants (J) are given in hertz (Hz). The following abbreviations were used to describe multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, sext = sextet, m = multiplet, dd = doublet-doublet, ddd = doublet-doublet-doublet, dt = doublet-triplet, dq = doublet-quartet, br = broad. Mass spectra were recorded on an Advion expression CMS, and high-resolution mass spectra were obtained on a Bruker MaXis high-resolution QTOF or a Thermo QExactive high-resolution Orbitrap. Masses are given as m/z.

**Photophysical Properties.** DMSO stock solutions of the CHyC was prepared and stored at  $-20^\circ\text{C}$ . The samples were then thawed and diluted to an  $OD = 0.08 \pm 0.02$  at the most red-shifted absorbance maxima. All measurements were collected on a Molecular Devices SpectraMax M5 in a 1 cm path-length quartz cuvette. Quantum yields were calculated using the most red-shifted absorbance maxima of samples. Rhodamine 6G ( $\Phi_{R546} = 0.88$ ) in ethanol ( $n_R = 1.360$ ) was used as a fluorescent standard.<sup>3</sup> Quantum yields were calculated using the equation shown below:

$$\Phi = \Phi_R \frac{F A_R n^2}{F_R A n_R^2}$$

where  $\Phi_R$  is the quantum yield of the fluorescent standard,  $F$  and  $F_R$  are the integrated emissions of the sample and reference respectively.  $A$  and  $A_R$  are the optical densities of the sample and reference respectively (both  $0.08 \pm 0.02$ ).  $n$  and  $n_R$  are the refractive indexes of the sample and reference respectively.

**Monitoring CHyC CuAAC Reaction.** UV spectra were collected using a Molecular Devices SpectraMax M5 spectrophotometer. 1 mL solution of 100  $\mu\text{M}$  CHyC in PBS buffer (pH 7.4, 1.3% DMSO) had the following added to obtain the final concentrations of 1 mM  $\text{CuSO}_4$ , 2 mM Tris(benzyltriazolylmethyl)amine (THPTA), 1 mM 5-(Azidomethyl)-2'-deoxyuridine (AmdU), and 10 mM sodium ascorbate (added last). Fluorescence spectra were taken at time 0 min, 20 min, 40 min, and 60 min (excitation: 546 nm; emission: 570-750 nm). After an hour, the reaction mixture was loaded onto a Glen Gel-Pak™ 1.0 Desalting Column to remove salts prior to analysis by HPLC column chromatography on an analytical C-8 reverse-phase column (Dr Maisch ReproSil-Pur Basic-C8, 5  $\mu\text{m}$  150 x 4.6 mm) using a Waters Acquity HPLC with 2998 PDA and 2475 FDA detectors. The gradient of ACN: 0.1 M aqueous triethylammonium acetate pH 7.0 (TEAA) was applied: 30:70 to 65:35 over 19 min with a flow rate of 3.0 mL/min and a column temperature of  $50^\circ\text{C}$ . Elution was monitored by UV absorption at 260 nm.

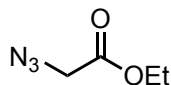
**Confocal Laser Scanning Microscopy (CLSM).** Confocal Laser Scanning Microscopy (CLSM) was performed on Leica Stellaris 5 LIAchroic (Leica Microsystems) equipped with a HC PL APO 63x/1.40 OIL CS2 (FWD: 0.14 mm). CHyC was excited at 561 nm and emission was sampled between 590 and 650 nm. AlexaFluor 647 alkyne (AF647) was excited at 633 nm and emission was sampled between 650 and 700 nm. Both cyanines were excited using 0.36% laser intensity and processed similarly to avoid discrepancies. Hoechst 33342 was excited at 405 nm, and emission was sampled between 410 and 480 nm. HyD detectors were used. Image analysis was performed using Leica LAS AF Lite 2.6.3 (Leica Microsystems). Images were processed in Image-J software. Colocalization between the two dyes was measured based on the Pearson correlation coefficient (PCC) using the JACoP and Colocalization Finder plugins.<sup>4-5</sup>

**Aggregate CLSM Imaging.** 400  $\mu\text{L}$  of a 2, 5, or 10  $\mu\text{M}$  CHyC in PBS buffer (pH 7.4, 2% ethanol) were imaged in a  $\mu$ -slide 8-well chambers (ibidi®, cat-#: 80826) along with a control consisting of only PBS buffer (pH 7.4, 2% ethanol). Each well was meticulously examined for aggregates on two separate occasions to ensure consistency of particle formation. HC PL APO 63x/1.40 OIL CS2 (FWD: 0.14 mm) objective lens was used along with a 3.4x zoom to obtain adequate visualization of the aggregates. The z-stacks were recorded with a step size of 1  $\mu\text{m}$  spanning 10  $\mu\text{m}$  for a total of 10 steps. CHyC aggregates were excited at 561 nm and emission was sampled between 590 and 650 nm. To obtain coloured images, an Apple iPhone 13 mini with a 26 mm focal length was used to capture aggregate appearance through the eyepiece.

**Eukaryotic Cell Culture.** Eukaryotic cells (HeLa) were cultivated at 37 °C, 5 % CO<sub>2</sub> in DMEM (Gibco) containing 4.5 g/l glucose, 10 % FBS (Gibco), 50,000 units Penicillin, and 50 mg Streptomycin per L (Sigma Aldrich), and 1% MEM non-essential amino acids (Sigma Aldrich) Cells were grown to confluency and passaged every 2 to 4 days using a Trypsin-EDTA solution (Sigma Aldrich). Cells were counted using an *Olympus Automated Cell Counter Model R1* for the determination of seeding density.

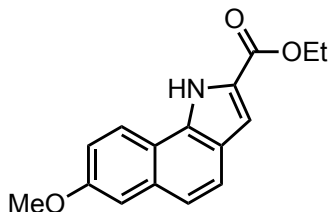
**General Cellular Labeling.** HeLa cells were seeded in DMEM media in  $\mu$ -slide 8-well chambers (ibidi®, cat-#: 80826) at densities of  $5.0 \times 10^4 - 5.5 \times 10^4$  cells per mL (10000 cells per well) and allowed to settle overnight. They were aspirated and incubated with or without 100  $\mu$ M of POM-AmdU. After incubating for 24 hours, cells were aspirated, washed with PBS, fixed using 4% PFA in PBS for 15 min at room temperature. The cells were aspirated and then PFA solution was quenched using 50 mM glycine:NH<sub>4</sub>Cl in PBS for 5 min at room temperature. The cells were washed with PBS, permeabilized with 0.2% TritonX100 in PBS for 15 min at 4°C and washed again with PBS. The denaturation is done by treating the cells with 2M HCl (aq.) for 30 min at room temperature. The cells are then washed with PBS, neutralized with a 0.1 M Na<sub>2</sub>B<sub>4</sub>O<sub>7</sub> · 10H<sub>2</sub>O. The cells were washed with PBS before incubation with 2 mM THPTA, 1 mM CuSO<sub>4</sub>, 10  $\mu$ M alkyne dye, and 10 mM sodium ascorbate (added last) for 2 hours at room temperature in the dark. Cells were washed with PBS three times and imaged using confocal microscopy. Cells can be left in PBS at 4°C for up to 1 month.

#### Ethyl 2-azidoacetate (1a)



Ethyl 2-bromoacetate (2.00 mL, 18.0 mmol, 1.0 eq) was dissolved in 72.0 mL of water:acetone (1:3, 0.25M). NaN<sub>3</sub> (2.34g, 36.1 mmol, 2.0 eq) was added and the solution was stirred for 30 minutes at room temperature. The reaction mixture was diluted with 50 mL of DCM and the organic phase was washed with water (2x25 mL) before being dried over MgSO<sub>4</sub> and concentrated under reduced pressure. The crude was dried on high vacuum to yield a clear oil in a 98% yield (2.29g, 17.7 mmol) which was passed onto the next step without further purification. Analytical data in accordance with literature values.<sup>6</sup>

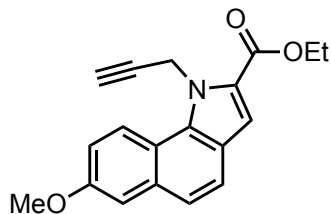
#### Ethyl 7-methoxy-1H-benzo[g]indole-2-carboxylate (2)



Procedure adapted from the literature.<sup>7</sup> Ethyl 2-azidoacetate (0.94 mL, 8.13 mmol, 1.5 eq), ethyl trifluoroacetate (0.97 mL, 8.13 mmol, 1.5 eq) and 6-methoxy-2-naphthaldehyde (1.01 g, 5.42 mmol, 1.0 eq) were added to a round bottom flask under argon. The mixture was dissolved in 34 mL of absolute ethanol and then the solution was cooled to 0°C and purged with argon. 20% NaOEt in EtOH was also cooled to 0°C and 4.61 mL (13.55 mmol, 2.5 eq) was added in one portion. The ice bath was removed, and after stirring overnight, the reaction was quenched with 4 mL of NH<sub>4</sub>Cl (aq. sat.). The ethanol-water was evaporated under reduced pressure and the orange oily solid was dissolved in 20 mL of EtOAc. The organic phase was washed with water (2x25 mL) and the organic phase was dried over MgSO<sub>4</sub> and concentrated under reduced pressure. The crude yellow oil was purified by silica gel column chromatography (0-8% EtOAc in hexanes) to give a yellow oil. This product was pushed forward to the Hemetsberger indolization. The ethyl (Z)-2-azido-3-(6-methoxynaphthalen-2-yl)acrylate (1.09 g, 3.67 mmol, 1.0 eq) was dissolved in 24 mL of 1,4-dioxane and heated to 110°C overnight. The crude product was purified by silica gel column chromatography (0-45% EtOAc in hexanes) to give a single regioisomeric indole as a light brown solid (900 mg, 3.34 mmol) in a 62% over two steps.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  9.86 (s, 1H), 8.11 (d, *J* = 8.9 Hz, 1H), 7.65 (d, *J* = 8.7 Hz, 1H), 7.43 (d, *J* = 8.7 Hz, 1H), 7.32 (d, *J* = 2.1 Hz, 1H), 7.28 (d, *J* = 2.5 Hz, 1H), 7.21 (dd, *J* = 8.9, 2.5 Hz, 1H), 4.46 (q, *J* = 7.1 Hz, 2H), 3.95 (s, 3H), 1.45 (t, *J* = 7.1 Hz, 3H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>)  $\delta$  162.22, 157.64, 133.49, 133.24, 125.28, 122.61, 122.14, 121.91, 121.46, 117.21, 116.57, 110.28, 108.53, 60.97, 55.42, 14.52. **HR-ESI-MS (m/z):** [M + Na]<sup>+</sup> calc. for C<sub>16</sub>H<sub>15</sub>NNaO<sub>3</sub>: 292.0944, found: 292.0949.

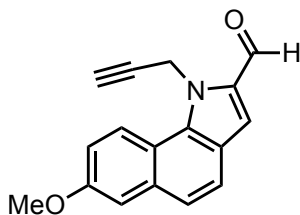
### Ethyl 7-methoxy-1-(prop-2-yn-1-yl)-1*H*-benzo[*g*]indole-2-carboxylate (3)



Sodium hydride 60% dispersion in mineral oil (17.8 mg, 0.44 mmol, 1.2 eq) was added to a round bottom flask under argon and dissolved in 2.2 mL DMF at 0°C. To this flask, ethyl 7-methoxy-1*H*-benzo[*g*]indole-2-carboxylate (100.8 mg, 0.37 mmol, 1.0 eq) in 0.37 mL of DMF was added dropwise, before stirring for 30 minutes at 0°C. 60  $\mu$ L of propargyl bromide, 80% in toluene (0.55 mmol, 1.5 eq), was added over the course of 15 minutes at 0°C. After the addition, the reaction was allowed to warm to room temperature and stirred overnight. The reaction was quenched with 2 mL of NH<sub>4</sub>Cl (aq. sat.) and extracted with 15 mL of EtOAc. The organic phase was washed with water (2x15 mL), dried over MgSO<sub>4</sub>, and concentrated under reduced pressure. The product was dried on high vacuum to yield a brown solid in a 83% yield (94.5 mg, 0.31 mmol) which was passed onto the next step without further purification.

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.62 (d, *J* = 9.2 Hz, 1H), 7.65 (d, *J* = 8.6 Hz, 1H), 7.48 (d, *J* = 8.6 Hz, 2H), 7.35 (d, *J* = 2.6 Hz, 1H), 7.32 (dd, *J* = 9.2, 2.6 Hz, 1H), 5.83 (s, 2H), 4.46 (q, *J* = 7.1 Hz, 2H), 3.99 (s, 3H), 2.47 (t, *J* = 2.3 Hz, 1H), 1.48 (t, *J* = 7.1 Hz, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  161.94, 157.10, 135.08, 134.51, 125.40, 123.88, 122.45, 122.30, 121.81, 117.35, 116.77, 113.07, 109.23, 79.42, 73.40, 60.60, 55.33, 37.40, 14.43. HR-ESI-MS (*m/z*): [M + Na]<sup>+</sup> calc. for C<sub>19</sub>H<sub>17</sub>NNaO<sub>3</sub>: 330.1101, found: 330.1104.

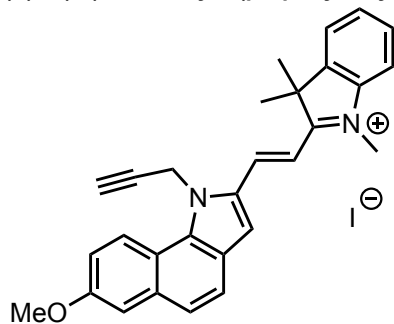
### 7-methoxy-1-(prop-2-yn-1-yl)-1*H*-benzo[*g*]indole-2-carbaldehyde (4)



Ethyl 7-methoxy-1-(prop-2-yn-1-yl)-1*H*-benzo[*g*]indole-2-carboxylate (76.1 mg, 0.25 mmol, 1.0 eq) was added to a round bottom flask under argon, dissolved in 1.7 mL of THF, and purged with argon. The reaction was cooled to -78°C and lithium aluminum hydride (28.2 mg, 0.74 mmol, 3.0 eq) was added in one portion. After warming to room temperature, the reaction was stirred overnight before being quenched with cold water and extracted with 10 mL of DCM. The organic phase was washed with water (2x15 mL), dried over MgSO<sub>4</sub>, and concentrated under reduced pressure. This crude product was dissolved in 5.0 mL of dry ACN followed by the addition of MnO<sub>2</sub> (113.0 mg, 1.30 mmol, 5.2 eq). After stirring overnight, the reaction mixture was filtered through a pad of celite and concentrated under reduced pressure. The product was dried on high vacuum to yield a brown solid in a 79% yield (51.9 mg, 0.20 mmol) which was passed onto the next step without further purification.

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  9.81 (s, 1H), 8.57 (d, *J* = 9.1 Hz, 1H), 7.62 (d, *J* = 8.7 Hz, 1H), 7.46 (d, *J* = 8.7 Hz, 1H), 7.33 (s, 1H), 7.31 (d, *J* = 2.6 Hz, 1H), 7.28 (dd, *J* = 9.1, 2.6 Hz, 2H), 5.86 (s, 2H), 3.96 (s, 3H), 2.39 (t, *J* = 2.4 Hz, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  181.47, 157.91, 136.28, 136.06, 133.21, 124.62, 123.21, 123.04, 121.91, 120.46, 117.10, 116.99, 109.47, 78.71, 73.81, 55.39, 37.32. HR-ESI-MS (*m/z*): [M + Na]<sup>+</sup> calc. for C<sub>17</sub>H<sub>13</sub>NNaO<sub>2</sub>: 286.0838, found: 286.0844.

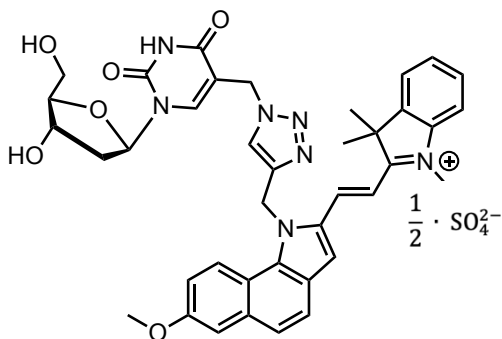
**(E)-2-(2-(7-methoxy-1-(prop-2-yn-1-yl)-1H-benzo[g]indol-2-yl)vinyl)-1,3,3-trimethyl-3H-indol-1-ium (CHyC, 5)**



7-methoxy-1-(prop-2-yn-1-yl)-1H-benzo[g]indole-2-carbaldehyde (11.3 mg, 43.1  $\mu\text{mol}$ , 1.0 eq) and 1,2,3,3-tetramethyl-3H-indol-1-ium iodide (15.6 mg, 51.7  $\mu\text{mol}$ , 1.2 eq) were added to a round bottom flask under argon, dissolved in 0.54 mL of EtOH, and heated to 70°C overnight. The reaction mixture was concentrated under reduced pressure. The crude product was purified by silica gel column chromatography (0-2% MeOH in DCM) to give a purple-black solid (21.3 mg, 39.0  $\mu\text{mol}$ ) in a 91% yield.

**$^1\text{H NMR}$**  (400 MHz, DMSO)  $\delta$  8.56 (d,  $J$  = 9.3 Hz, 1H), 8.32 (d,  $J$  = 15.6 Hz, 1H), 8.21 (s, 1H), 7.89 – 7.83 (m, 2H), 7.72 (d,  $J$  = 8.7 Hz, 1H), 7.68 – 7.60 (m, 3H), 7.59 – 7.55 (m, 2H), 7.37 (dd,  $J$  = 9.2, 2.7 Hz, 1H), 5.82 (s, 2H), 4.11 (s, 3H), 3.95 (s, 3H), 3.68 (t,  $J$  = 2.1 Hz, 1H), 1.85 (s, 6H).  **$^{13}\text{C NMR}$**  (101 MHz, DMSO)  $\delta$  180.19, 158.30, 143.61, 142.48, 138.89, 136.66, 136.04, 135.02, 129.40, 129.01, 125.14, 125.10, 124.21, 123.27, 121.91, 117.56, 116.49, 114.94, 113.55, 110.65, 110.62, 79.52, 77.72, 55.92, 51.86, 36.53, 34.36, 26.49. **HR-ESI-MS** ( $m/z$ ):  $[\text{M}]^+$  calc. for  $\text{C}_{29}\text{H}_{27}\text{N}_2\text{O}$ : 419.21179, found: 419.21092.

**CHyC-triazole-AmdU 6**

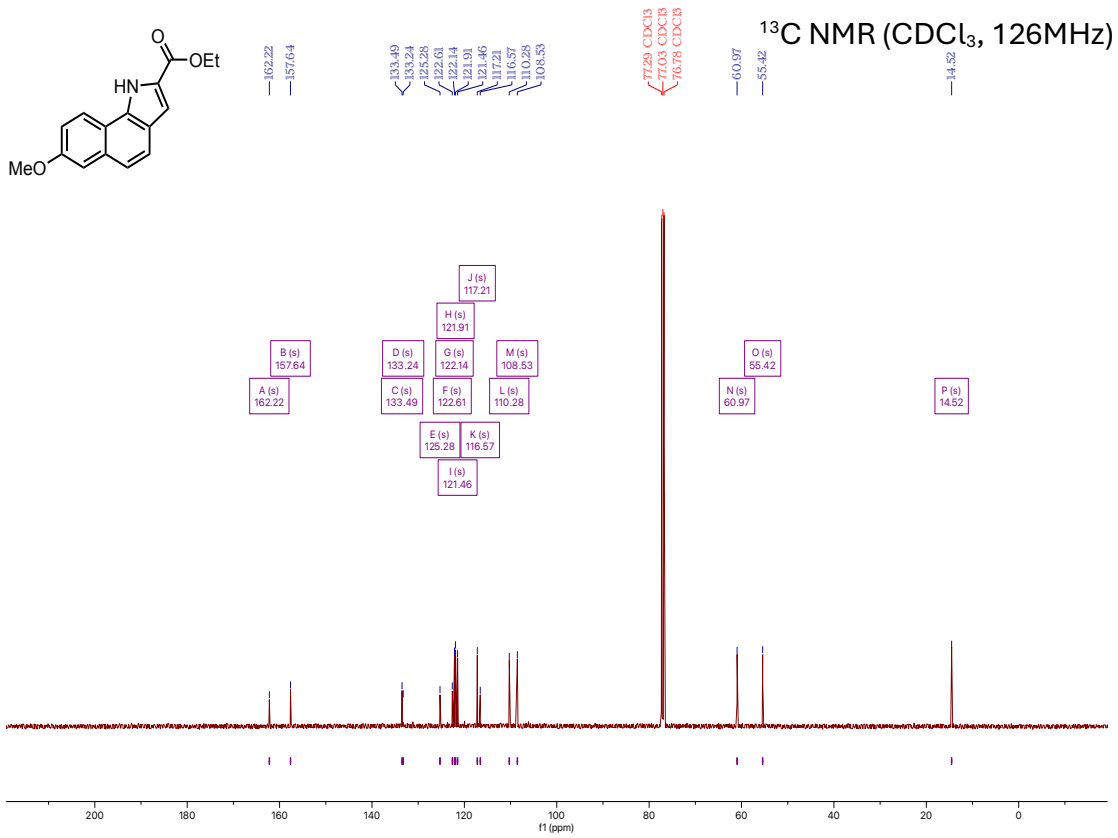
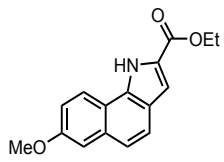
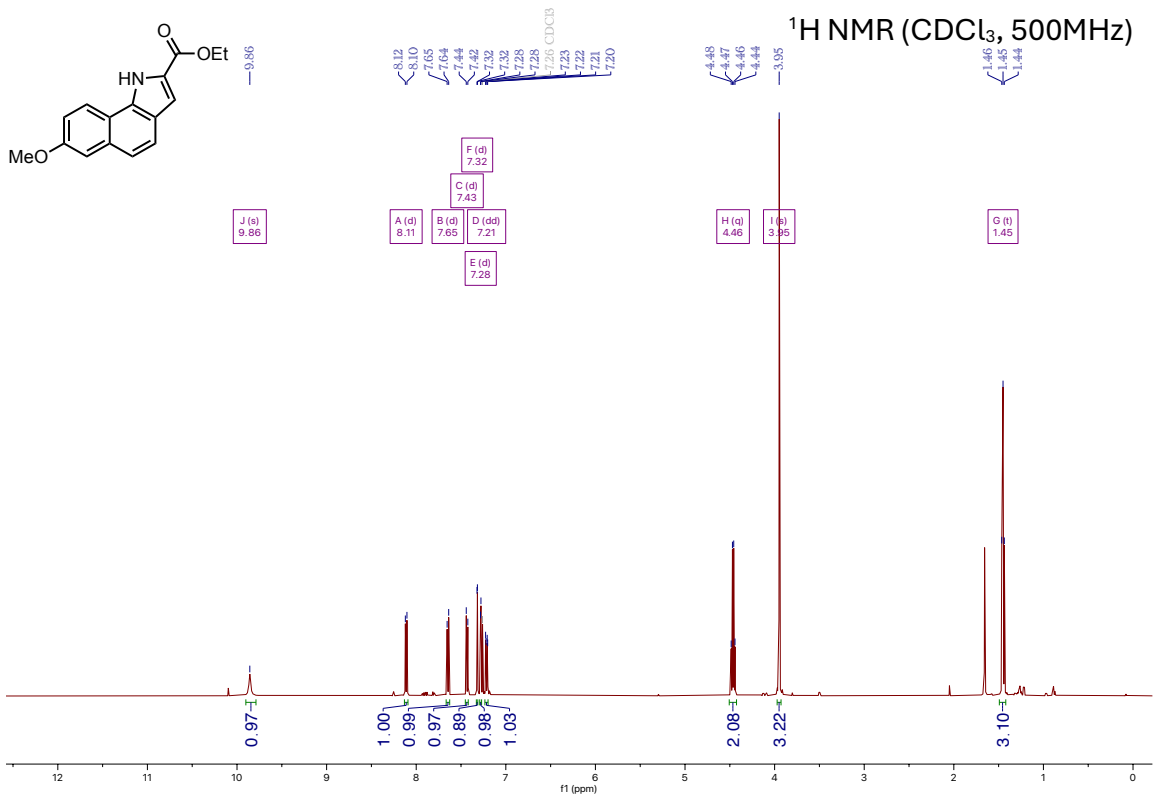
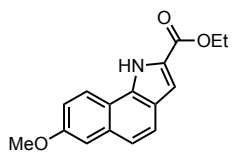


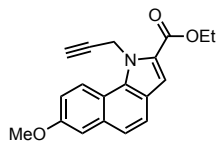
CHyC (15.00 mg, 27.45  $\mu\text{mol}$ , 1.0 eq), copper sulfate (4.38 mg, 27.4  $\mu\text{mol}$ , 1.0 eq) and THPTA (23.85 mg, 54.90  $\mu\text{mol}$ , 2.0 eq) were added to a round bottom flask and dissolved in 2.50 mL of water with 0.5 mL of DCM. 5-(azidomethyl)-2'-deoxyuridine (11.66 mg, 41.17  $\mu\text{mol}$ , 1.5 eq) and sodium ascorbate (54.38 mg, 274.5  $\mu\text{mol}$ , 10.0 eq) were added and the reaction was stirred for 3 days. The reaction mixture was concentrated under reduced pressure. The crude product was purified by silica gel column chromatography (0-10% MeOH in DCM) to give a purple-black solid (14.20 mg, 18.91  $\mu\text{mol}$ ) in a 69% yield.

**$^1\text{H NMR}$**  (500 MHz, MeOD)  $\delta$  8.54 (d,  $J$  = 15.4 Hz, 1H), 8.40 (d,  $J$  = 9.2 Hz, 1H), 8.28 (s, 1H), 8.09 (s, 1H), 7.99 (s, 1H), 7.69 (q,  $J$  = 1.0 Hz, 2H), 7.68 (t,  $J$  = 1.2 Hz, 3H), 7.63 (d,  $J$  = 8.8 Hz, 1H), 7.60 (td,  $J$  = 7.8, 1.3 Hz, 1H), 7.55 (td,  $J$  = 7.4, 1.0 Hz, 1H), 7.50 (d,  $J$  = 8.8 Hz, 1H), 7.47 (d,  $J$  = 15.5 Hz, 1H), 7.43 (d,  $J$  = 2.7 Hz, 1H), 7.25 (dd,  $J$  = 9.2, 2.7 Hz, 1H), 6.19 (t,  $J$  = 6.6 Hz, 1H), 6.14 (s, 2H), 5.25 (d,  $J$  = 2.3 Hz, 2H), 4.35 (dt,  $J$  = 6.5, 3.4 Hz, 1H), 4.03 (s, 3H), 3.95 (s, 3H), 3.90 (q,  $J$  = 3.4 Hz, 1H), 3.74 (dd,  $J$  = 12.1, 3.2 Hz, 1H), 3.68 (dd,  $J$  = 12.1, 3.7 Hz, 1H), 2.26 (ddd,  $J$  = 13.6, 6.1, 3.5 Hz, 1H), 2.15 (dt,  $J$  = 13.7, 6.5 Hz, 1H), 1.77 (s, 6H).  **$^{13}\text{C NMR}$**  (126 MHz, MeOD)  $\delta$  180.24, 162.08, 161.79, 158.69, 142.89, 141.99, 141.54, 140.31, 140.24, 137.77, 136.64, 135.19, 135.16, 128.97, 128.41, 125.68, 124.03, 123.95, 123.36, 122.39, 121.17, 116.91, 116.28, 113.66, 113.51, 110.04, 107.91, 87.72, 85.49, 70.64, 61.29, 54.58, 51.48, 41.64, 40.12, 32.40, 25.77, 22.33. **HR-ESI-MS** ( $m/z$ ):  $[\text{M}]^+$  calc. for  $\text{C}_{39}\text{H}_{40}\text{N}_7\text{O}_6$ : 702.3035, found: 702.3048.

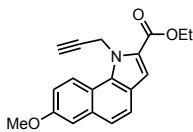
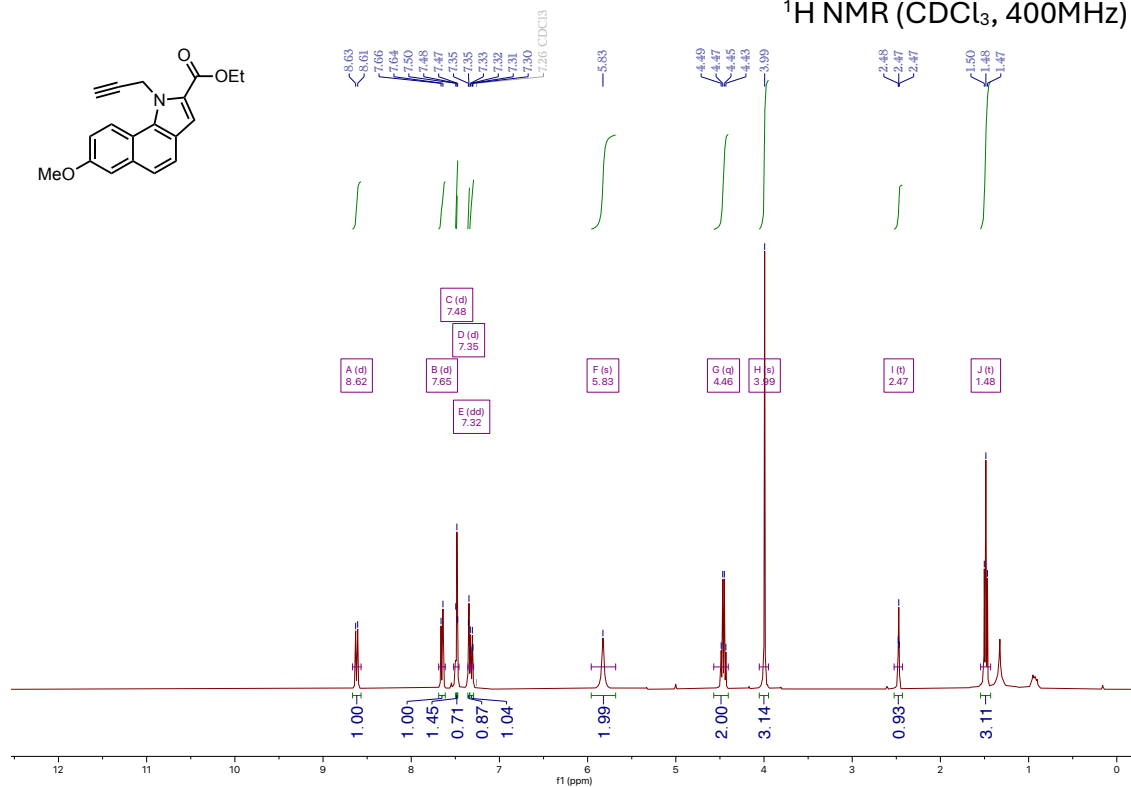


# NMR Spectra

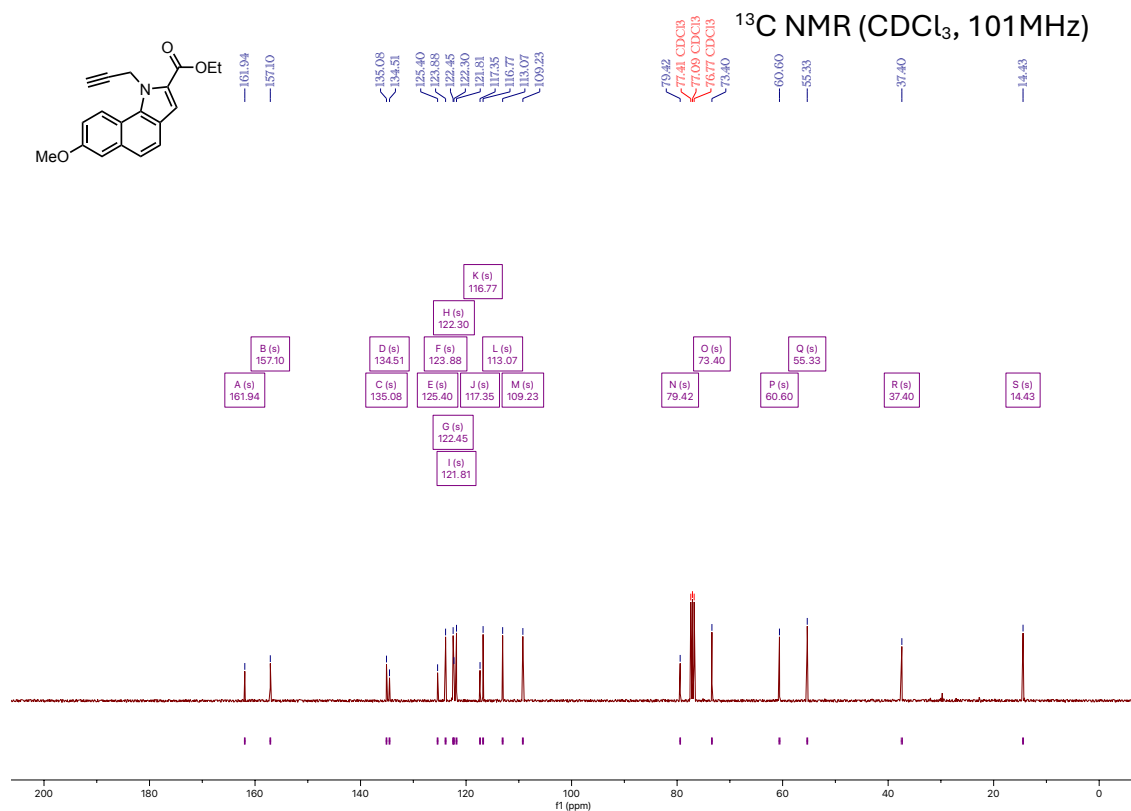


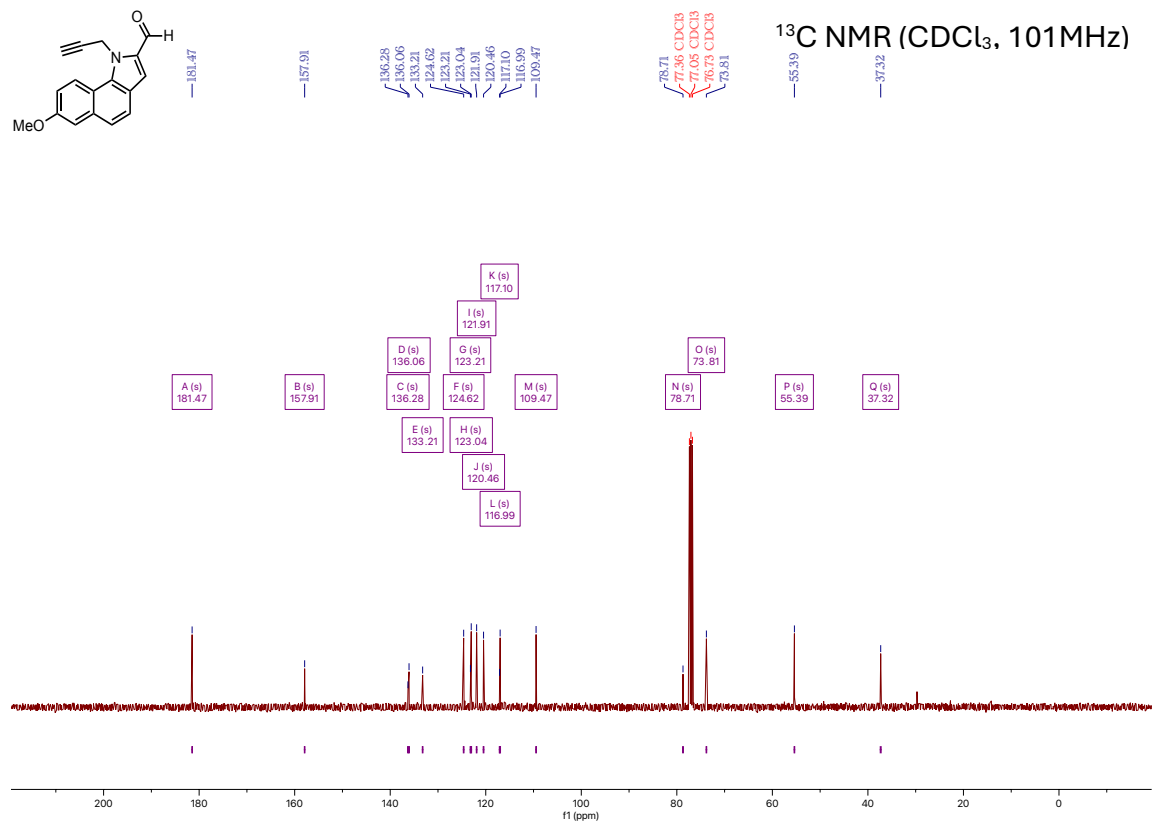
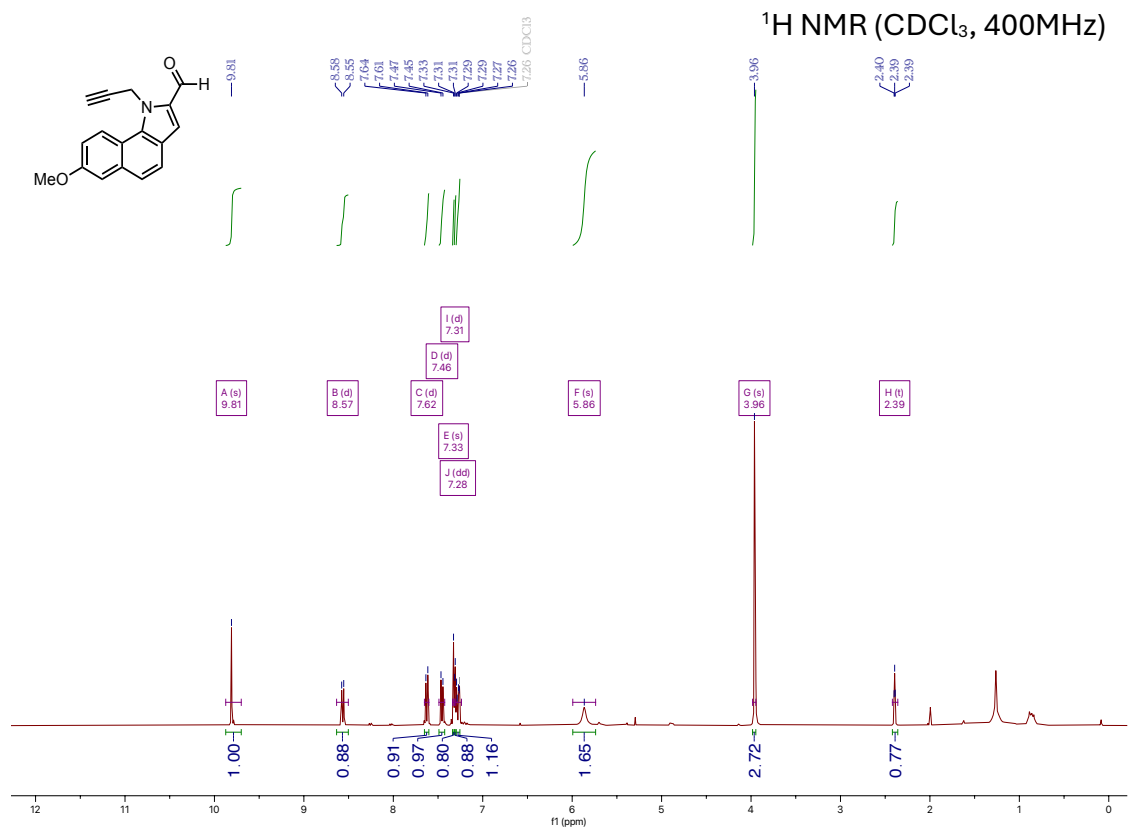


<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400MHz)

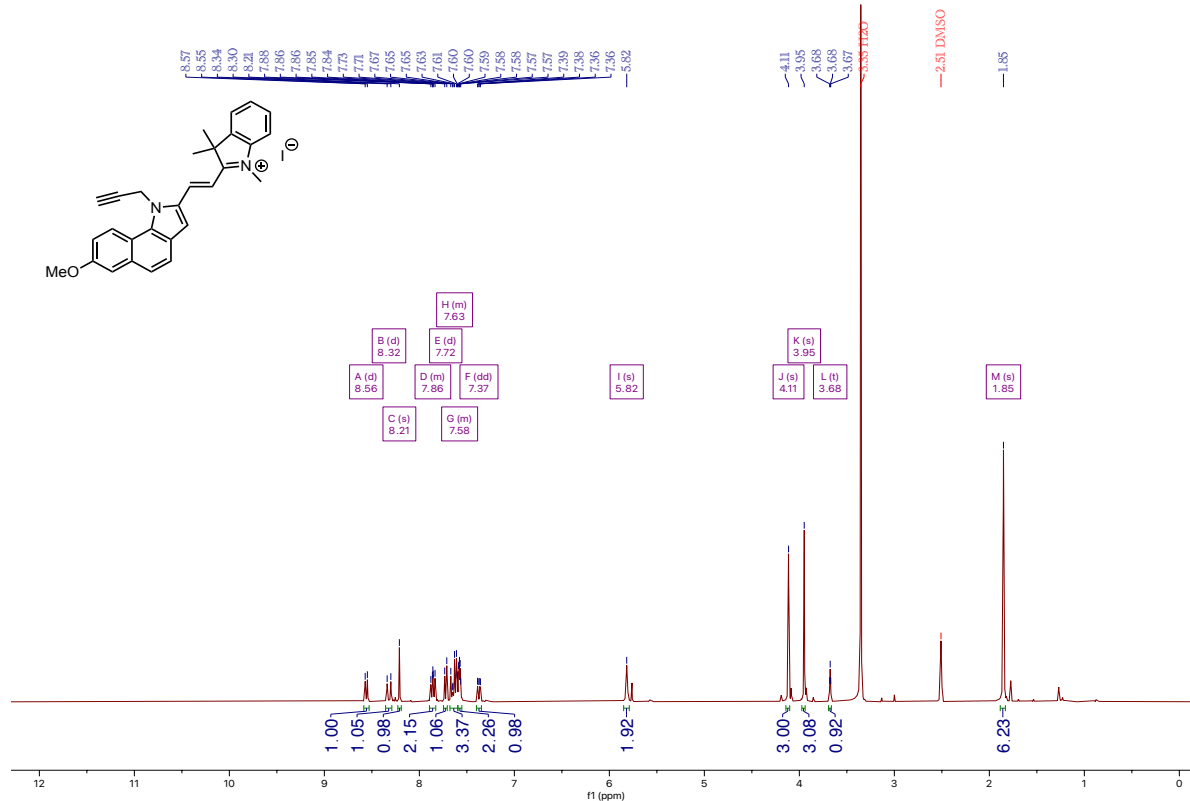


<sup>13</sup>C NMR (CDCl<sub>3</sub>, 101MHz)

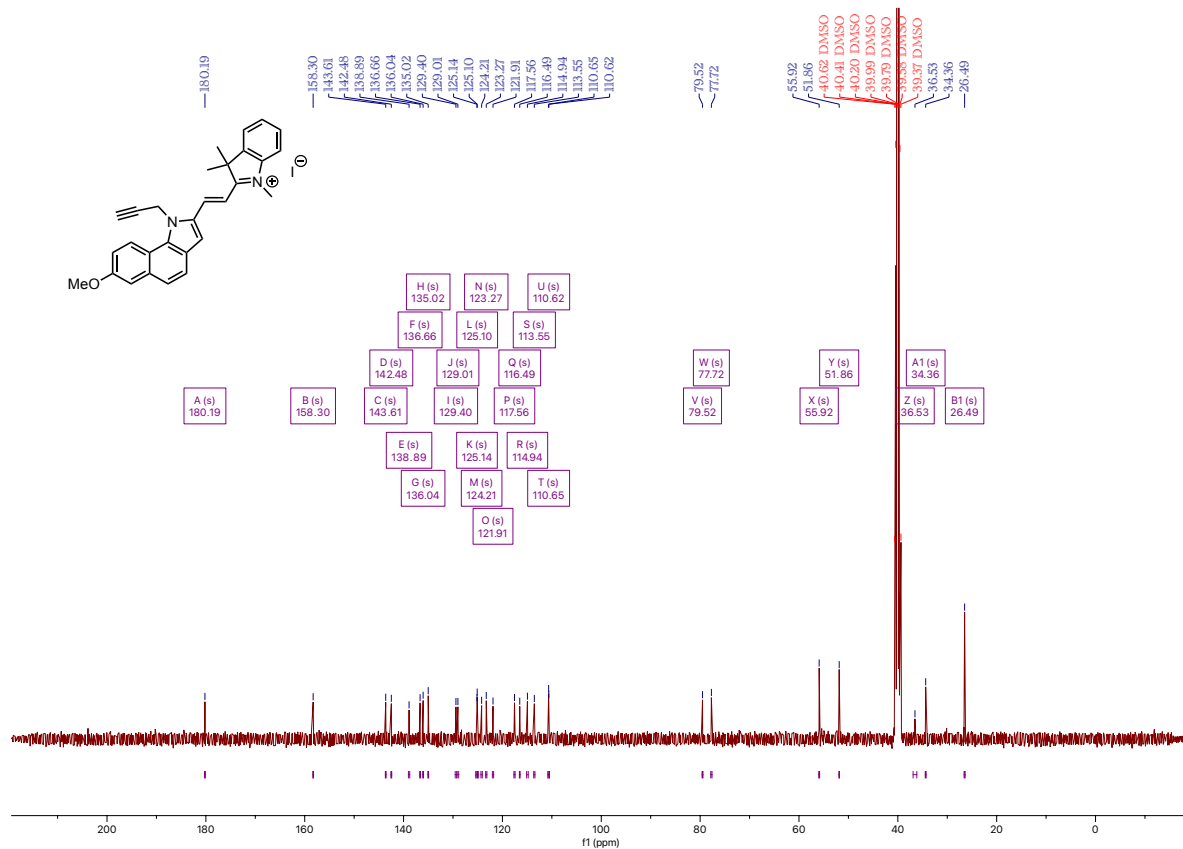


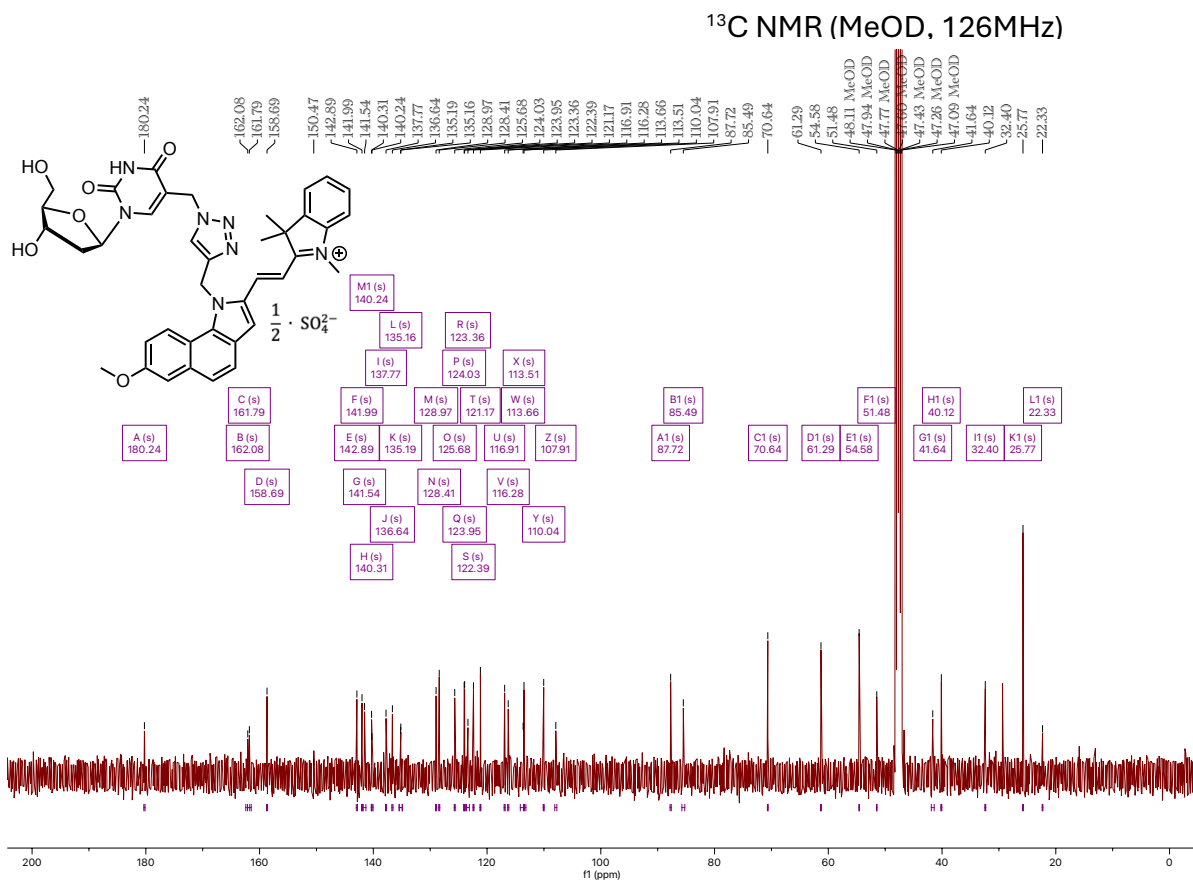
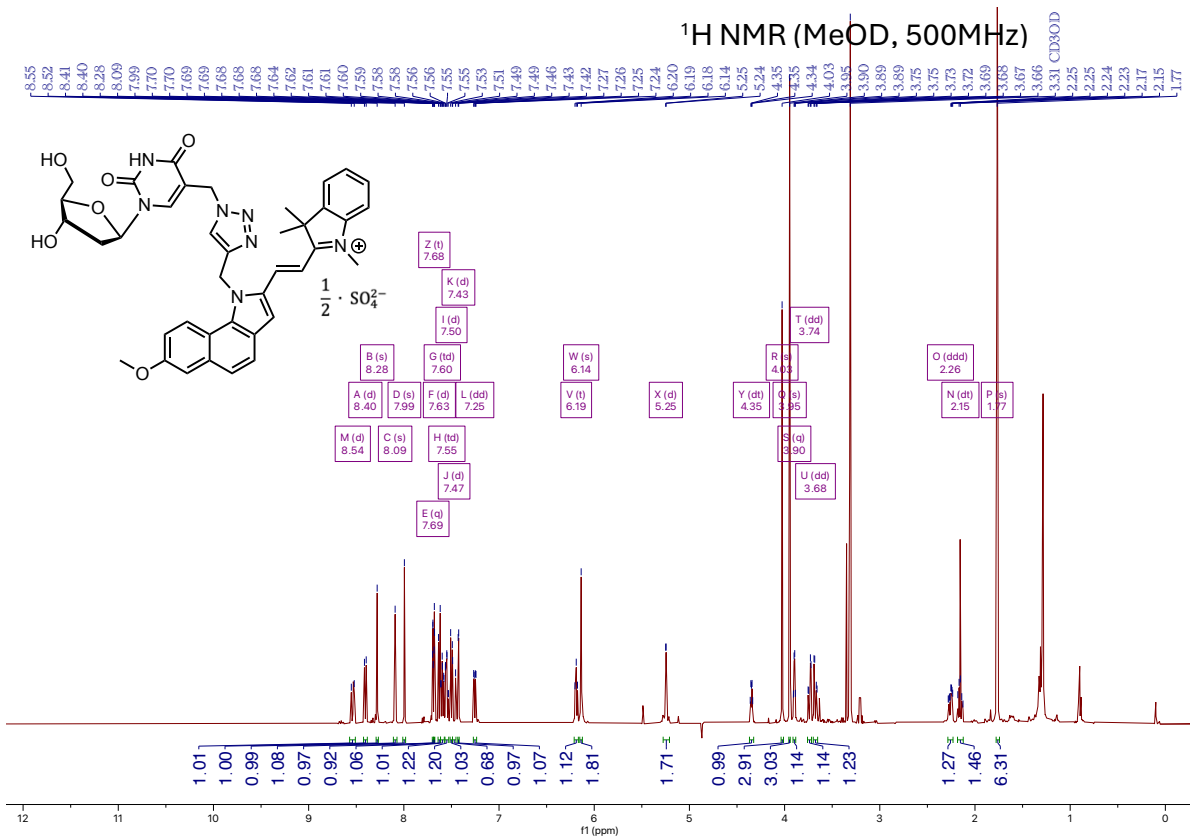


<sup>1</sup>H NMR (DMSO, 400MHz)



<sup>13</sup>C NMR (DMSO, 101MHz)





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