Synthesis and Spectral Properties of 6'-Triazolyl-Dihydroxanthene-Hemicyanine Fused Near-Infrared Dyes

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Supporting Information

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1. General

Chemicals, reagents and solvents were purchased from commercial vendors and used without further purification. Triethylamine, dichloromethane (DCM), dimethylformamide (DMF), ethyl acetate (EtOAc), petroleum ether (PE, b.p.60-90 ^{o}C), acetonitrile (MeCN), methanol (MeOH) and ethanol (EtOH) used in this work were reagent grade and purchased from Concord Technology, China. Thin-layer chromatography (TLC) was carried on pre-coated glass plates with 0.2 mm silica gel (local vendor, China) and visualized under UV (254 nm) and/or potassium permanganate ($KMnO_4$) stain. Flash-column chromatography was performed using regular silica gel 60 (200-300 mesh, 50-74 μm) provided by commercial vendors in China with specified eluents. Solvents used for photophysical characterizations: chloroform ($CHCl_3$, for spectroscopy, #167730010), dimethylsulfoxide (DMSO, for spectrometry, #D5293) and absolute EtOH (99% # E/0600DF/17) were provided by Acros, TCI and Fisher respectively. Bovine serum albumine (BSA, standard grade, lyophilized, #1000-70) was purchased from H2B. Formic acid (puriss p.a., ACS reagent, reag. Ph. Eur., ⩾98%, #33015) was purchased from Sigma-Aldrich. The HPLC-gradient grade MeCN was obtained from Carlo Erba or VWR. All aq. mobile phase and buffers used in this work (aq. formic acid and phosphate buffered saline) and aq. mobile-phases for HPLC were prepared using ultrapure water produced by an ELGA PURELAB Ultra system (purified to 18.2 MΩ.cm).

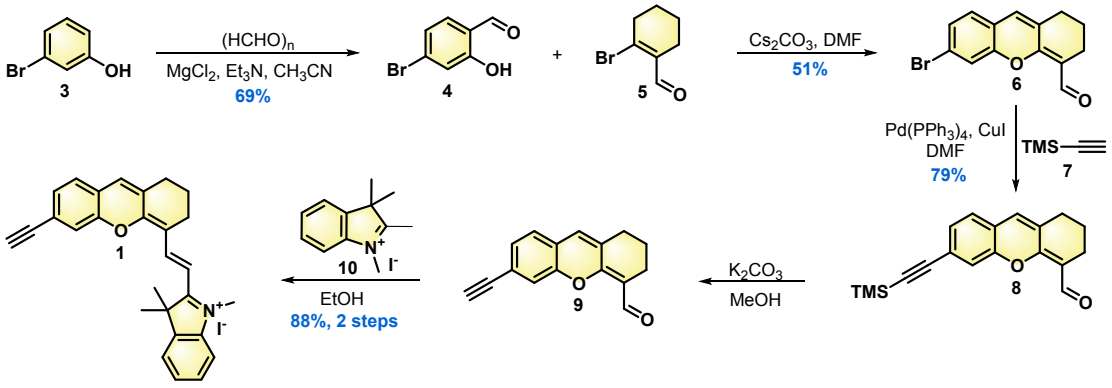
2. Instruments and methods

^{1}H, ^{13}C and ^{19}F NMR spectra were recorded on Brüker Avance 400 MHz or 600 MHz spectrometers. Chemical shifts (δ) are reported in parts per million (ppm) and residual non-deuterated solvent peaks were used as internal reference (proton δ = 7.26 and carbon δ = 77.16 for $CDCl_3$ and proton δ = 2.50 and carbon δ = 39.52 for DMSO-d_6).[1] ^{1}H NMR coupling constants (J) are reported in Hertz (Hz). The following abbreviations were used in reporting multiplicities: s (singlet), d (doublet), t (triplet), m (multiplet), dd (doublet of doublets), ddd (doublet of doublet of doublets). HPLC-MS analyses were performed on a Thermo-Dionex Ultimate 3000 instrument (pump + autosampler at 20 °C + column oven at 25 °C) equipped with a diode array detector (Thermo-Dionex DAD 3000-RS) and a MSQ Plus single quadrupole mass spectrometer. Low-resolution mass spectra (LRMS) were recorded on a Thermo Scientific MSQ Plus single quadrupole equipped with an electrospray ionization (ESI) source (HPLC-MS coupling). High-resolution mass spectra (HRMS) were recorded on micrOTOF-QII equipped with an ESI analytical source. UV-visible spectra were obtained either on a Varian Cary 50 scan (single-beam) or an Agilent technologies 60 (single-beam) spectrophotometer (software Cary WinUV) by using rectangular quartz cells (Hellma, 100-QS, 45 × 12.5 × 12.5 mm, pathlength: 10 mm, chamber volume: 3.5 mL), at 25 °C (using a temperature control system combined with water circulation). Fluorescence spectra (emission/excitation spectra) were recorded with an HORIBA Jobin Yvon

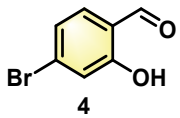
Fluorolog spectrofluorometer (FluorEssence software) at 25 °C (using a temperature control system combined with water circulation), with standard fluorometer cells (Labbox, LB Q, light path: 10 mm, width:10 mm, chamber volume: 3.5 mL). The absorption and fluorescence emission spectra were recorded with dye solutions of concentrations in the range of 10^{-5}-10^{-6} M. The emission spectra were recorded in the range of 635-850 nm after excitation at 620 nm (shutter: Auto Open, integration time = 0.1 s, 1 nm step, HV(S1) = 950 V, excitation slit = 5 nm and emission slit = 5 nm). The excitation spectra were recorded in the range of 400-750 nm after emission at 760 nm (excitation slit = 5 nm for spectra recorded in $CHCl_3$ and 12 nm for spectra recorded in EtOH or PBS + 5% BSA and emission slit = 5 nm). All excitation/emission spectra are corrected. High-performance liquid chromatography analyses, the following chromatographic systems were used for the analytical experiments: *System A*: RP-HPLC (Phenomenex Kinetex C_{18} column, 2.6 µm, 2.1 × 50 mm) with MeCN (+ 0.1% FA) and 0.1% aq. formic acid (aq. FA, pH 2.5) as eluents [5% MeCN (0.1 min) followed by a linear gradient from 5% to 100% (5 min) of MeCN, then 100% MeCN (4 min)] at a flow rate of 0.5 mL min^{-1}. UV-visible detection was achieved at four distinct wavelengths 220, 260, 600 and 650 nm (+ diode array detection in the range 220-800 nm). Low resolution ESI-MS detection in the positive/negative mode (full scan, 100-1500 a.m.u., peaking format: centroid, needle voltage: 3.0 kV, probe temperature: 350 °C, cone voltage: 75 V, detector voltage: 1153 V and scan time: 1 s). *System B*: system A with the following gradient [5% MeCN (0.1 min), followed by a linear gradient from 5% to 50% (2.5 min) and 50% to 100% (5 min) of MeCN].

3. Synthesized compounds

3.1 Preparation of alkynyl-based DHX-hemicyanine fused dyes 1

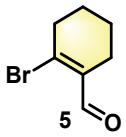


Scheme S1. Synthetic route towards alkynyl-based DHX-hemicyanine fused dye **1**.

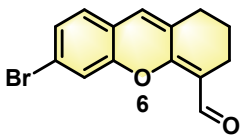


4-Bromo-2-hydroxybenzaldehyde (4). To 3-bromophenol **3** (1.0 g, 5.8 mmol) in dry

CH_3CN (30 mL) at room temperature were added $MgCl_2$ powder (0.8 g, 8.9 mmol) and TEA (3.2 mL, 22.9 mmol) and the solution was stirred for 20 min. Paraformaldehyde (1.2 g, 41.6 mmol) was added and the mixture was refluxed at 100 °C for 18 h. Deionised water was added and the mixture was acidified with aq. 1.0 M HCl to pH 2. The solution was extracted with Et_2O (2 × 50 mL) and the combined organic layers were washed with brine (2 × 50 mL) and dried over anhydrous Na_2SO_4, filtered and concentrated in vacuo. Purification by flash-column chromatography on silica gel (eluent: 10% EtOAc in hexanes) afforded 4-bromo-2-hydroxybenzaldehyde **4** as a white solid (0.8 g, yield 69%). R_f (hexanes-EtOAc 9:1 (v/v)): 0.6; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.11 (s, 1 H), 9.86 (s, 1 H), 7.41 (d, J = 8.2 Hz, 1 H), 7.22-7.13 (m, 2 H) ppm. The spectral data matched with those reported in the literature.[2]

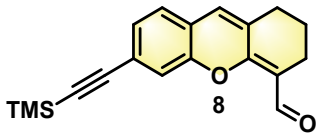


6-Bromocyclohex-1-ene-1-carbaldehyde (5). To a mixture of DMF (23.5 mL, 306.0 mmol) and $CHCl_3$ (100 mL) at 0 °C was added PBr_3 (24.2 mL, 255.0 mmol) portion wise under an atmosphere of N_2. After 1.5 h, cyclohexanone (10.5 mL, 102.0 mmol) was added and the mixture was stirred at room temperature overnight. The resulting solution was poured onto ice and then solid $NaHCO_3$ was slowly added until pH ~ 7. The aq. layer was extracted with DCM and the organic layer was washed with deionised water. The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The yellow mixture was purified by flash-column chromatography on silica gel (eluent: 100% PE) and 6-bromocyclohex-1-ene-1-carbaldehyde **5** was obtained as a pale yellow liquid (13.6 g, yield 72%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 10.01 (s, 1 H), 2.74 (m, 2 H), 2.26 (m, 2 H), 1.75 (m, 2 H), 1.68 (m, 2 H) ppm. The spectral data matched with those reported in the literature.[2]

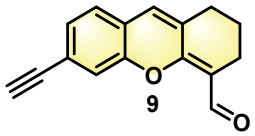


6-Bromo-2,3-dihydro-1*H*-xanthene-4-carbaldehyde (6). To Cs_2CO_3 (1.2 g, 3.7 mmol) and benzaldehyde **2** (0.3 g, 1.3 mmol) was added DMF (10 mL). 6-Bromocyclohex-1-ene-1-carbaldehyde **3** (0.5 g, 2.6 mmol) in DMF (1 mL) was added slowly and the resulting reaction mixture was stirred at room temperature for 48 h. The mixture was then filtered, washed with deionised water (20 mL) and extracted with EtOAc (3 × 50 mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. Purification by flash-column chromatography on silica gel (eluent: 20% EtOAc in hexanes) afforded 6-bromo-2,3-dihydro-1*H*-xanthene-4-carbaldehyde **6** as a yellow solid (0.2 g, yield 51%). R_f (hexanes-EtOAc 4:1 (v/v)): 0.5; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 10.32 (s, 1 H), 7.30-7.27 (m, 1 H), 7.20 (dd, J = 8.1 Hz, J = 1.9 Hz, 1 H), 7.01 (d, J = 8.2 Hz, 1 H), 6.62 (s,

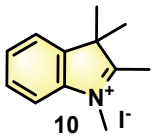
1 H), 2.57 (t, J = 6.6 Hz, J = 1.5 Hz, 2 H), 2.44 (t, J = 6.1 Hz, 2 H), 1.73 (p, J = 6.2 Hz, 2 H) ppm. The spectral data matched with those reported in the literature.[2]



6-((Trimethylsilyl)ethynyl)-2,3-dihydro-1*H*-xanthene-4-carbaldehyde (8). $Pd(PPh_3)_4$ (67.5 mg, 8.3 mmol%) and CuI (23.6 mg, 0.1 mmol) were degassed in a flame-dried round bottom flask. TEA (1.2 mL, 8.3 mmol) in dry DMF (10 mL) was added with aryl bromide **6** (1.2 g, 4.1 mmol). The solution was degassed again then trimethylsilylacetylene **7** was added (1.8 mL, 12.4 mmol). The reaction mixture was heated to 85 °C for 24 h. After being cooled to room temperature, the reaction mixture was concentrated under vacuum and the resulting residue was purified by flash-column chromatography on silica gel (eluent: 1% EtOAc in PE) affording pure TMS-protected terminal alkyne **8** as a orange solid (1.0 g, yield 79%). m.p 155-157 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 10.30 (s, 1 H), 7.17 (s, 1 H), 7.13 (dd, J = 7.8 Hz, J = 1.2 Hz, 1 H), 7.05 (d, J = 7.8 Hz, 1 H), 6.62 (s, 1 H), 2.58 (ddd, J = 7.5 Hz, J = 5.8 Hz, J = 1.6 Hz, 2 H), 2.43 (t, J = 6.0 Hz, 2 H), 1.71 (m, J = 6.1 Hz, 2 H), 0.25 (s, 9 H); ^{13}C NMR (101 MHz, $CDCl_3$): δ = 188.0, 159.9, 151.7, 130.8, 127.6, 126.5, 126.1, 124.6, 121.6, 118.6, 113.8, 104.0, 96.9, 30.3, 21.6, 20.4, 0.0 ppm; HRMS (ESI+): *m/z* 331.1141 $[M + Na]^+$, calcd for $C_{19}H_{20}O_2SiNa^+$ 331.1125.

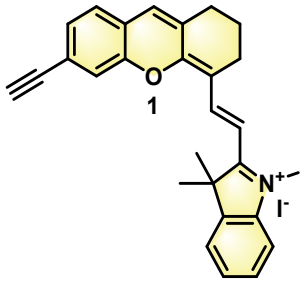


6-Ethynyl-2,3-dihydro-1*H*-xanthene-4-carbaldehyde (9). TMS-protected terminal alkyne **8** (1.0 g, 3.3 mmol) was dissolved in dry MeOH (30 mL) and treated with anhydrous K_2CO_3 (1.8 g, 13.2 mmol). The mixture was stirred at room temperature for 5 h. The solvent was removed, and the residue was taken up in 100 mL of DCM and washed with 100 mL of deionised water. The organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. This compound was used in the next step without further purification, and the yield was assumed to be quantitative. m.p 198-200 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 10.26 (s, 1 H), 7.36 (d, J = 7.9 Hz, 1 H), 7.34 (s, 1 H), 7.24 (dd, J = 7.8 Hz, J = 1.5 Hz, 1 H), 7.01 (s, 1 H), 4.37 (s, 1 H), 2.59 (ddd, J = 7.0 Hz, J = 5.3 Hz, J = 1.6 Hz, 2 H), 2.30 (t, J = 6.0 Hz, 2 H), 1.63 (m, J = 6.1 Hz, 2 H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ = 188.1, 159.8, 151.7, 131.1, 127.7, 126.6, 125.9, 123.6, 122.0, 118.9, 113.9, 82.8, 79.3, 30.3, 21.6, 20.4 ppm; HRMS (ESI+): *m/z* 237.0910 $[M + H]^+$, calcd for $C_{16}H_{13}O_2^+$ 237.0910.



10

1,2,3,3-tetramethyl-3*H*-indol-1-ium iodide 10. To 2,3,3-trimethyl-3*H*-indole (32 mL, 200.0 mmol) in CH_3CN (200 mL) was added iodomethane (14 mL, 228.0 mmol) portion-wise and the solution was refluxed overnight. The precipitate was filtered and washed with Et_2O and dried in vacuo to afford 1,2,3,3-tetramethyl-3*H*-indol-1-ium iodide **7** as a light pink solid (56.5 g, 94%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.91 (m, 1H), 7.82 (m, 1H), 7.62 (m, 2H), 3.97 (s, 3H), 2.76 (s, 3H), 1.53 (s, 3H). The spectral data matched with the reference.[2]



1

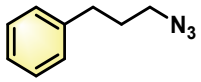
Alkynyl-based DHX-hemicyanine fused dye (1). To aldehyde **9** (236 mg, 1.0 mmol) in EtOH (2 mL) was added 1,2,3,3-tetramethyl-3*H*-indol-1-ium iodide **7** (301 mg, 1.0 mmol) and the solution was refluxed at 80 °C for 4 h. The reaction mixture was concentrated and the crude product was purified by flash-column chromatography on silica gel (eluent: 1% MeOH in DCM) to afford DHX **1** as a dark blue solid (345 mg, yield 88%). m.p >300 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.56 (d, J = 15.3 Hz, 1 H), 7.80-7.73 (m, 2 H), 7.62 (s, 1 H), 7.58 (m, 1 H), 7.52 (m, 2 H), 7.39-7.33 (m, 2 H), 6.68 (d, J = 15.4 Hz, 1 H), 4.52 (s, 1 H), 3.95 (s, 3 H), 2.72 (t, J = 6.0 Hz, 2 H), 2.67 (t, J = 6.0 Hz, 2 H), 1.83 (p, J = 5.9 Hz, 2 H), 1.77 (s, 6 H) ppm; ^{13}C NMR (101 MHz, DMSO-d_6): δ = 179.0, 158.0, 151.8, 145.1, 142.4, 142.1, 131.1, 129.8, 128.8, 128.4, 127.8, 127.6, 123.8, 122.6, 122.2, 118.6, 114.3, 113.8, 107.2, 83.8, 82.6, 50.8, 33.2, 28.7, 26.9, 23.5, 19.7 ppm; HRMS (ESI+): *m/z* 392.2019 $[M]^{+\bullet}$, calcd for $C_{28}H_{26}NO^+$ 392.2009; HPLC (system B): t_R = 5.2 min (purity 96% at 260 nm and 99% at 600 nm); LRMS (ESI+, recorded during RP-HPLC analysis): *m/z* 392.3 $[M]^{+\bullet}$ (100), calcd for $C_{28}H_{26}NO^+$ 392.2; UV-vis (recorded during the HPLC analysis): λ_{max} = 559 and 592 nm (broad band).

3.2. Preparation of organic azides 11a-11o

Procedure A: general method for preparing azide 11a-11d.

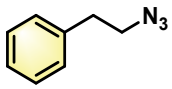
A solution of alkyl bromide (5.0 mmol) and NaN_3 (6.5 mmol) in DMF (10 mL) was heated at 80 °C overnight. The reaction mixture was cooled, diluted with EtOAc, washed with deionised water and brine, dried over anhydrous Na_2SO_4 and concentrated

under reduced pressure, to afford the corresponding alkyl azide which was used without further purification.



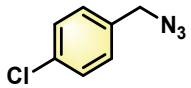
11a

1-(3-Azidopropyl)benzene (11a). Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.30 (m, 5 H), 3.31 (t, *J* = 6.8 Hz, 2 H), 2.75 (t, *J* = 7.9 Hz, 2 H), 1.95 (m, 2 H) ppm. The spectral data matched with those reported in the literature.[3]



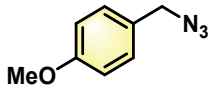
11b

1-(2-Azidoethyl)benzene (11b). Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): *δ* = 7.41 (m, 2 H), 7.32 (m, 3 H), 3.55 (t, *J* = 7.1 Hz, 2 H), 2.97 (t, *J* = 7.1 Hz, 2 H) ppm. The spectral data matched with those reported in the literature.[3]



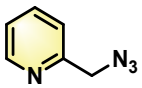
11c

1-(Azidomethyl)-4-bromobenzene (11c). Colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$): *δ* = 7.53-7.49 (m, 2 H), 7.21-7.19 (m, 2 H), 4.30 (s, 2 H) ppm. The spectral data matched with those reported in the literature.[4]



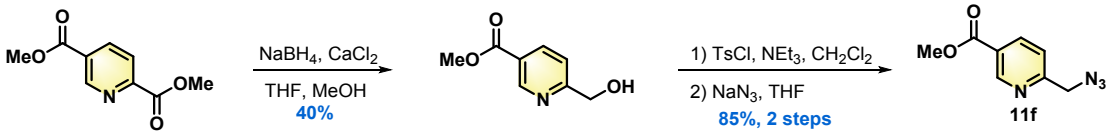
11d

4-Methoxybenzyl azide (11d). Colourless oil; ^{1}H NMR (600 MHz, $CDCl_3$): *δ* = 7.24 (dd, *J* = 8.7 Hz, *J* = 2.1 Hz, 2 H), 6.90 (dd, *J* = 8.7 Hz, *J* = 2.1 Hz, 2 H), 4.27 (s, 2 H), 3.82 (s, 3 H) ppm. The spectral data matched with those reported in the literature.[5]



11e

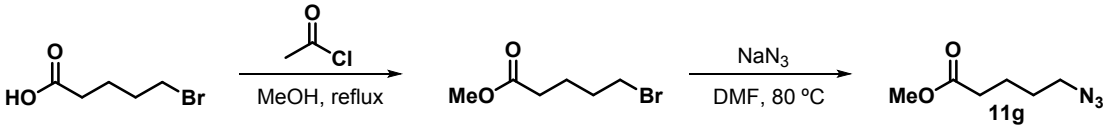
2-(Azidomethyl)pyridine (11e). NaN_3 (11.8 g, 181.6 mmol) and 2-chloromethylpyridine hydrochloride (5.7 g, 45.1 mmol) were added to 200 mL of deionised water. The resulting reaction mixture was heated to 50 °C for 24 h. Thereafter, reaction was neutralised with solid $NaHCO_3$ (11.8 g, 140.5 mmol) and extracted with DCM (3 × 30 mL). The combined organic layers were dried over anhydrous $MgSO_4$ and evaporated under reduced pressure, to give the desired 2-(azidomethyl)pyridine **11e** as a yellow oil (4.6 g, yield 75%). ^{1}H NMR (400 MHz, $CDCl_3$): *δ* = 8.64 (d, *J* = 4.2 Hz, 1 H), 7.77 (t, *J* = 7.6 Hz, 1 H), 7.36 (d, *J* = 7.6 Hz, 1 H), 7.28 (t, *J* = 4.2 Hz, 1 H), 4.42 (s, 2 H) ppm. The spectral data matched with those reported in the literature.[6]



Scheme S2 Synthetic route towards organic azide **11f**.

Methyl 5-(azidomethyl)nicotinate (11f). $NaBH_4$ (265 mg, 7.0 mmol) was added in portions to a slurry of 2,5-pyridinedicarboxylic acid dimethyl ester (544 mg, 2.8 mmol) and $CaCl_2$ (1.2 g, 11.2 mmol) in a mixture of dry THF (5 mL) and dry MeOH (10 mL). The reaction was stirred at 0 °C for 3 h. Excess of $NaBH_4$ was then quenched by adding 10 mL of ice-cold water. After extraction with $CHCl_3$ (3 × 20 mL), the combined organic layers were dried over anhydrous $MgSO_4$ and finally concentrated under reduced pressure to provide intermediate benzyl alcohol as a white solid (187 mg, yield 40%). R_f (EtOAc-hexanes 1:1 (v/v)): 0.3; ^{1}H NMR (600 MHz, $CDCl_3$): δ = 9.16, (d, *J* = 2.0 Hz, 1 H), 8.29 (dd, *J* = 2.0 Hz, *J* = 8.5 Hz, 1 H), 7.36 (d, *J* = 8.5 Hz, 1 H), 4.83 (s, 2 H), 3.96 (s, 3 H) ppm. The spectral data matched with those reported in the literature.[6]

To a solution of 6-(hydroxymethyl)nicotinic acid methyl ester (16.7 mg, 0.1 mmol) in DCM (2 mL) was added tosyl chloride (TsCl, 25.6 mg, 0.1 mmol) and TEA (62 µL, 0.4 mmol). The resulting reaction mixture was stirred for 2 h. Thereafter, DCM was removed under reduced pressure and the resulting residue was dissolved in THF (1 mL), and NaN_3 (58 mg, 0.9 mmol) was added. The reaction mixture was stirred at room temperature for 24 h, then diluted with EtOAc and deionised water. The aq. layer was further extracted with EtOAc thrice. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The resulting residue was purified by flash-column chromatography over silica gel (eluent: EtOAc-hexanes 4:1 (v/v)) to afford alkyl azide **11f** as a light yellow solid (16 mg, overall yield 85%). R_f (EtOAc-hexanes 1:1 (v/v): 0.8); ^{1}H NMR (600 MHz, $CDCl_3$): *δ* = 9.18 (d, *J* = 2.0 Hz, 1 H), 8.32 (dd, *J* = 8.5 Hz, *J* = 2.0 Hz, 1 H), 7.44 (d, *J* = 8.5 Hz, 1 H), 4.56 (s, 2 H), 3.95 (s, 3 H) ppm. The spectral data matched with those reported in the literature.[6]



Scheme S3. Synthetic route towards organic azide **11g**.

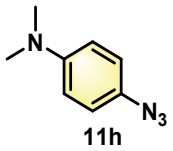
Methyl 5-azidopentanoate (11g). 5-Bromovaleric acid (3.0 g ,16.6 mmol) was dissolved in MeOH (50 mL) and acetyl chloride (1.3 g, 16.6 mmol) was added. The resulting reaction mixture was refluxed for 5 h. Thereafter, solvent was removed under reduced pressure, affording intermediate δ-bromo ester as a yellowish solid (3.5 g, yield

99%). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 3.67 (s, 3 H), 3.41 (t, J = 6.3 Hz, 2 H), 2.35 (t, J = 7.4 Hz, 2 H), 1.65-1.67 (m, 2 H), 1.56-1.59 (m, 2 H).

A solution of methyl 5-bromovalerate (3.4 g, 16.4 mmol) and NaN_3 (1.6 g, 24.6 mmol) in DMF (35 mL) was heated at 80 ^{o}C overnight. The reaction mixture was cooled top room temperature, diluted with EtOAc, washed with deionised water and brine, dried over anhydrous Na_2SO_4 and finally concentrated under reduced pressure, to afford pure methyl 5-azidopentanoate **11g** as a pale yellow oil (2.6 g, yield 95%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.67 (s, 3 H), 3.39 (t, J = 7.0 Hz, 2 H), 2.38 (m, 2 H), 1.91-1.60 (m, 4 H) ppm. The spectral data matched with those reported in the literature.[7]

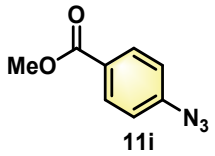
Procedure B: general method for preparing azide 11h-11m.

Aniline (5.0 mmol) was dissolved in aq. 2.0 M HCl (10 mL). The solution was cooled to 0 ^{o}C and aq. solution of $NaNO_2$ (6.0 mmol) in 1.5 mL deionised water was slowly added. The mixture was stirred for 30 min followed by the addition of NaN_3 (7.5 mmol) in deionised water (1.5 mL). After 3 h of stirring, the resulting solution was extracted with EtOAc (3 × 50 mL). The combined organic layers were washed with brine (20 mL), dried over anhydrous Na_2SO_4, and finally concentrated under reduced pressure to provide the corresponding pure organic azide.



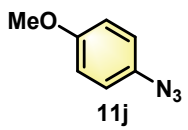
11h

5-Azido-*N*,*N*-dimethylaniline (11h). Brown crystalline solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 6.91 (d, J =7.8 Hz, 2 H), 6.71 (d, J = 8.4 Hz, 2 H), 2.93 (s, 6 H) ppm. The spectral data matched with those reported in the literature.[8]



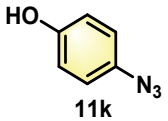
11i

Methyl 4-azidobenzoate (11i). Pale yellow soild; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.05-8.01 (m, 2 H), 7.09-7.04 (m, 2 H), 3.91 (s, 3 H) ppm. The spectral data matched with those reported in the literature.[9]



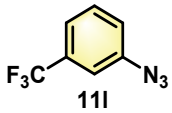
11j

1-Azido-4-methoxybenzene (11j). Brown solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 6.96-6.92 (m, 2 H), 6.90-6.86 (m, 2 H), 3.78 (s, 3 H) ppm. The spectral data matched with those reported in the literature.[9]



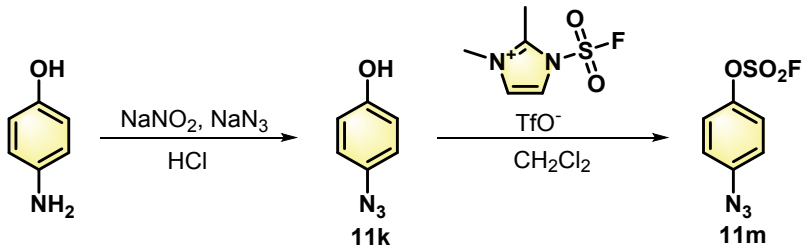
11k

4-Azidophenol (11k). Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 6.95-6.87 (m, 2 H), 6.86-6.79 (m, 2 H), 5.13 (brs, 1 H) ppm. The spectral data matched with those reported in the literature.[9]



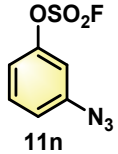
11l

1-Azido-3-trifluoromethylbenzene (11l). Orange oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.48-7.44 (m, 1 H), 7.39-7.37 (m, 1 H), 7.24 (s, 1 H), 7.20-7.18 (m, 1 H) ppm. The spectral data matched with those reported in the literature.[10]



Scheme S4. Synthetic route towards organic azide **11m**.

4-Azidophenyl fluorosulfate (11m). 4-Azidophenol **11k** (5.0 mmol), prepared according to procedure A described above, was dissolved in DCM (5 mL). TEA (1.2 mL, 8.0 mmol) was added, followed by 1-(fluorosulfonyl)-2,3- dimethyl-1*H*-imidazol-3-ium trifluoromethanesulfonate (2.1 g, 6.5 mmol). The resulting reaction mixture was stirred at room temperature for 2 h. Therafter, volatiles were removed under reduced pressure, and the resulting crude product was purified by flash-column chromatography over silica gel (eluent: 100% PE) to provide compound **11m** as a pale yellow liquid (1.0 g, yield 92%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.35-7.30 (m, 2 H), 7.12-7.07 (m, 2 H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ = 146.6, 140.8, 122.5, 120.7 ppm; ^{19}F NMR (377 MHz, $CDCl_3$): δ = 37.2 (s, 1 F) ppm; HRMS (ESI-): *m/z* 213.9928 $[M - H]^-$, calcd for $C_6H_4N_3O_4S^-$ 213.9928. *Please note: hydrolysis of fluorosulfate moiety was occurred during the ionisation process.*

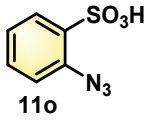


11n

4-Azidophenyl fluorosulfate (11n). The same procedure as that devised for **11m** was used. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.45 (t, J = 8.2 Hz, 1 H), 7.15-7.11 (m, 1 H), 7.09 (ddd, J = 8.1 Hz, J = 2.1 Hz, J = 1.0 Hz, 1 H), 6.99 (td, J = 2.2 Hz, J = 1.0 Hz, 1 H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): δ = 150.7, 142.6, 131.4, 119.2, 117.1, 112.1

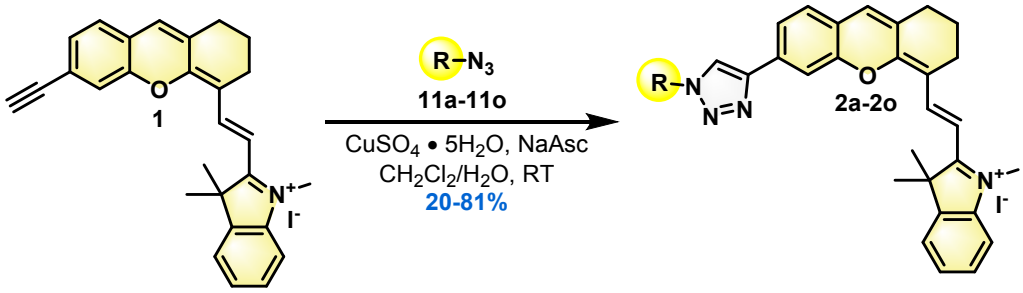
ppm; ^{19}F NMR (377 MHz, $CDCl_3$): δ = 38.0 (s, 1 F) ppm; HRMS (ESI-): *m/z* 213.9927 [M - H]$^-$, calcd for $C_6H_4N_3O_4S^-$ 213.9928. *Please note: hydrolysis of fluorosulfate moiety was occurred during the ionisation process.*

2-Azidophenyl (11o).



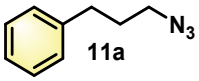
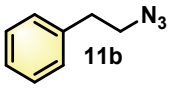
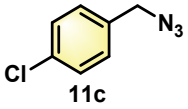
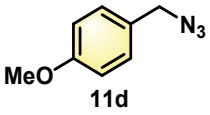
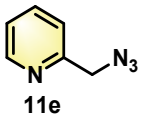
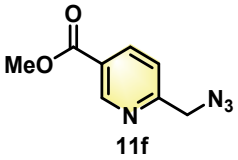
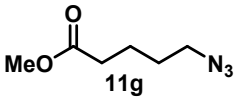
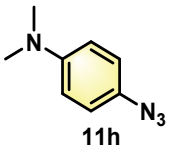
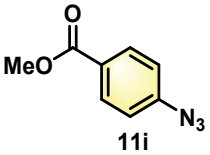
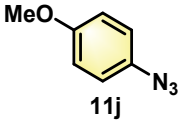
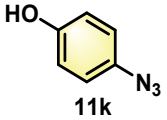
2-Azidobenzenesulfonic acid (11o). Prepared according to procedure B. Pink solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.2 Hz, 1H), 7.37 (t, *J* = 8.0 Hz, 1H), 7.17-7.15 (m, 2H), 2.51 (s, 1H). The spectral data matched with those reported in the literature.[11]

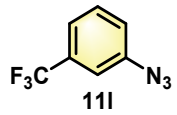
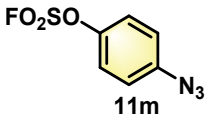
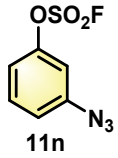
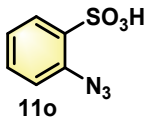
3.3 General procedure for the CuAAC reaction

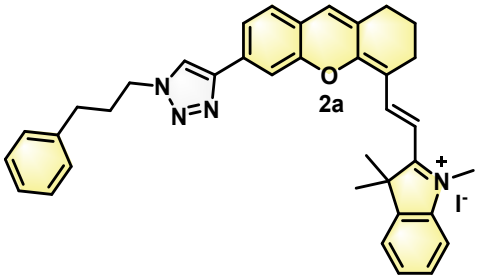


General procedure for the synthesis of tetrazole-based DHX-hemicyanine fused dyes 2a-2o. To a mixture of alkynyl-based DHX-hemicyanine fused dye **1** (784 mg, 2.0 mmol, 1.0 equiv.) and the corresponding organic azide (2.6 mmol, 1.3 equiv.) in deionised water and CH_2Cl_2 (1:1 (v/v), 100 mL), sodium ascorbate (79.2 mg, 0.4 mmol, 0.2 equiv.) was added, followed by the addition of $CuSO_4$ • 5 H_2O (25 mg, 0.1 mmol, 0.05 equiv.). The heterogeneous mixture was stirred vigorously at room temperature overnight. Thereafter, the reaction mixture was concentrated under reduced pressure and directly purified by flash-column chromatography on silica gel (eluent: 1% MeOH in DCM) to afford the corresponding triazole **2a-2o** as a dark blue solid.

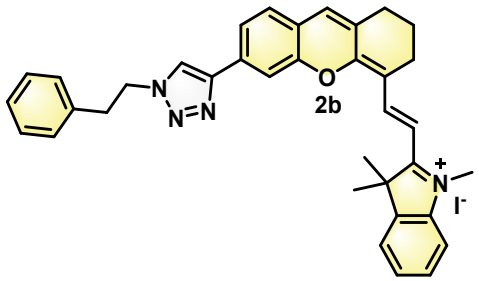
Table S1. Triazole-based DHX-hemicyanine fused dyes synthesised through CuAAc reaction from alkynyl-based DHX **1** and the corresponding organic azides (structures of starting materials and reaction yields).

Organic azide	Product	Yield
 11a	**2a**	50%
 11b	**2b**	52%
 11c	**2c**	74%
 11d	**2d**	36%
 11e	**2e**	81%
 11f	**2f**	61%
 11g	**2g**	67%
 11h	**2h**	36%
 11i	**2i**	22%
 11j	**2j**	80%
 11k	**2k**	41%

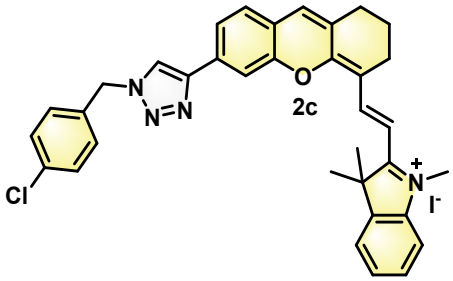
 11l	**2l**	43%
 11m	**2m**	48%
 11n	**2n**	20%
 11o	**2o**	14%


2a

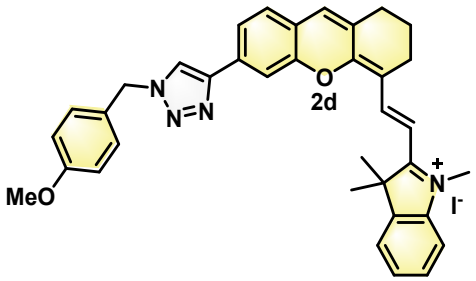
2a: 51 mg, 50% yield; dark blue solid; m.p 80-82 ^{o}C; ^{1}H NMR (600 MHz, DMSO-d_6): δ = 8.85 (s, 1 H), 8.59 (d, J = 15.2 Hz, 1 H), 7.85 (s, 1 H), 7.77 (m, 2 H), 7.72 (d, J = 8.0 Hz, 1 H), 7.61 (d, J = 8.0 Hz, 1 H), 7.56 (td, J = 7.7 Hz, J = 1.2 Hz, 1 H), 7.51-7.48 (m, 1 H), 7.41 (s, 1 H), 7.31 (t, J = 7.6 Hz, 2 H), 7.26-7.23 (m, 2 H), 7.21 (td, J = 7.2 Hz, J = 1.4 Hz, 1 H), 6.59 (d, J = 15.2 Hz, 1 H), 4.45 (t, J = 7.1 Hz, 2 H), 3.91 (s, 3 H), 2.72 (t, J = 6.2 Hz, 2 H), 2.66-2.61 (m, 4 H), 2.23-2.17 (m, 2 H), 1.87-1.81 (m, 2 H), 1.80 (s, 6 H) ppm; ^{13}C NMR (151 MHz, DMSO-d_6): δ = 178.4, 159.0, 152.6, 145.0, 144.9, 142.2, 142.2, 140.7, 133.7, 131.0, 129.8, 128.8, 128.4, 128.3, 128.2, 127.5, 126.0, 122.7, 122.6, 122.2, 121.1, 114.1, 113.6, 111.2, 106.2, 50.6, 49.2, 33.0, 31.9, 31.3, 28.7, 27.0, 23.5, 19.8 ppm; HRMS (ESI+): *m/z* 553.2972 $[M]^{+\bullet}$, calcd for $C_{37}H_{37}N_4O^+$ 553.2962; HPLC (system A): t_R = 5.3 min (purity 95% at 260 nm and 99% at 600 nm); LRMS (ESI+, recorded during RP-HPLC analysis): *m/z* 553.3 (100) and 554.3 (30) $[M]^{+\bullet}$, calcd for $C_{37}H_{37}N_4O^+$ 553.3; UV-vis (recorded during the HPLC analysis): λ_{max} = 571, 601 and 647 nm (broad band).



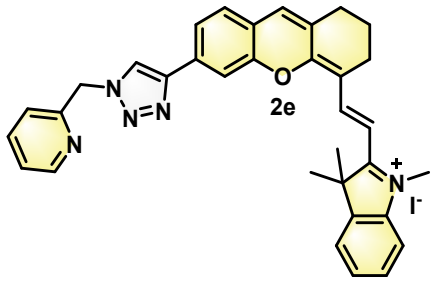
2b: 52 mg, 52% yield; dark blue solid; m.p 88-90 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.77 (s, 1 H), 8.61 (d, J = 15.2 Hz, 1 H), 7.84 (s, 1 H), 7.82-7.70 (m, 3 H), 7.64-7.48 (m, 3 H), 7.42 (s, 1 H), 7.33-7.19 (m, 5 H), 6.62 (d, J = 15.3 Hz, 1 H), 4.71 (t, J = 7.3 Hz, 2 H), 3.92 (s, 3 H), 3.25 (t, J = 7.3 Hz, 2 H), 2.78-2.70 (m, 2 H), 2.67 (t, J = 5.9 Hz, 2 H), 1.88-1.83 (m, 2 H), 1.81 (s, 6 H) ppm; ^{13}C NMR (101 MHz, DMSO-d_6): δ = 178.5, 159.0, 152.7, 145.0, 144.8, 142.2, 142.2, 137.5, 133.6, 131.0, 129.9, 128.8, 128.7, 128.4, 128.2, 127.6, 126.6, 122.8, 122.6, 122.1, 121.1, 114.2, 113.6, 111.3, 106.3, 50.8, 50.6, 35.5, 33.0, 28.7, 27.1, 23.5, 19.8 ppm; HRMS (ESI+): *m/z* 539.2802 $[M]^{+\bullet}$, calcd for $C_{36}H_{35}N_4O^+$ 539.2805; HPLC (system A): t_R = 5.2 min (purity 96% at 260 nm and 99% at 600 nm); LRMS (ESI+, recorded during RP-HPLC analysis): *m/z* 539.1 (100) and 540.2 (45) $[M]^{+\bullet}$, calcd for $C_{36}H_{35}N_4O^+$ 539.3; UV-vis (recorded during the HPLC analysis): λ_{max} = 569, 601 and 648 nm (broad band).



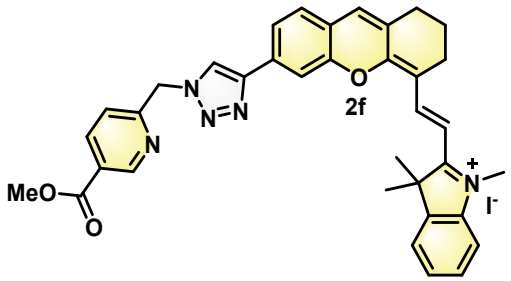
2c: 76 mg, 74% yield; dark blue solid; m.p 202-204 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.90 (s, 1 H), 8.62-8.57 (m, 1 H), 8.57-8.53 (m, 1 H), 7.88 (s, 1 H), 7.87-7.84 (m, 1 H), 7.79 (m, 2 H), 7.72 (d, J = 8.0 Hz, 1 H), 7.62-7.46 (m, 3 H), 7.43-7.35 (m, 3 H), 6.60 (d, J = 15.3 Hz, 1 H), 5.82 (s, 2 H), 3.91 (s, 3 H), 2.72 (t, J = 6.0 Hz, 2 H), 2.64 (t, J = 6.0 Hz, 2 H), 1.85-1.81 (m, 2 H), 1.80 (s, 6 H) ppm; ^{13}C NMR (101 MHz, DMSO-d_6): δ = 178.5, 159.0, 154.7, 152.6, 149.5, 145.1, 144.9, 142.2, 142.2, 137.4, 133.5, 131.0, 129.9, 128.8, 128.2, 127.5, 123.8, 123.4, 122.6, 122.3, 122.2, 121.2, 114.1, 113.6, 111.4, 106.2, 54.7, 50.6, 33.0, 28.7, 27.0, 23.5, 19.8 ppm; HRMS (ESI+): *m/z* 559.2254 $[M]^{+\bullet}$, calcd for $C_{35}H_{32}ClN_4O^+$ 559.2259; HPLC (system A): t_R = 5.3 min (purity 97% at 260 nm and 99% at 600 nm); LRMS (ESI+, recorded during RP-HPLC analysis): *m/z* 559.3 (100), 560.4 (40) and 561.4 (30) $[M]^{+\bullet}$, calcd for $C_{35}H_{32}ClN_4O^+$ 559.2; UV-vis (recorded during the HPLC analysis): λ_{max} = 568, 601 and 647 nm (broad band).



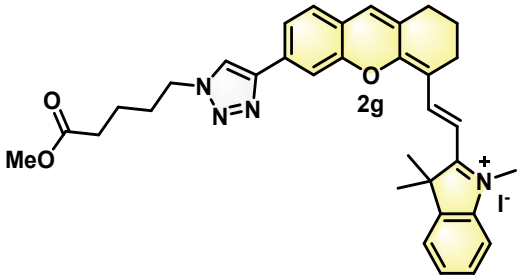
2d: 37 mg, 36% yield; dark blue solid; m.p 189-191 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 9.05 (dd, J = 2.2, J = 1.0 Hz, 1 H), 8.92 (s, 1 H), 8.61 (d, J = 15.2 Hz, 1 H), 8.36 (dd, J = 8.2 Hz, J = 2.2 Hz, 1 H), 7.89 (s, 1 H), 7.79 (m, 2 H), 7.74-7.70 (m, 1 H), 7.63-7.47 (m, 4 H), 7.42 (s, 1 H), 6.62 (d, J = 15.2 Hz, 1 H), 5.95 (s, 2 H), 3.92 (s, 3 H), 3.88 (s, 3 H), 2.73 (t, J = 5.9 Hz, 2 H), 2.69-2.62 (m, 2 H), 1.88-1.81 (m, 2 H), 1.80 (s, 6 H) ppm; ^{13}C NMR (101 MHz, DMSO-d_6): δ = 178.5, 159.2, 159.0, 152.7, 145.3, 144.9, 142.2, 142.2, 133.5, 131.0, 129.9, 129.6, 128.8, 128.2, 127.7, 127.6, 126.5, 122.7, 122.6, 122.2, 121.2, 114.2, 114.2, 113.6, 111.3, 106.2, 55.2, 52.7, 50.6, 32.9, 28.7, 27.0, 23.5, 19.8 ppm; HRMS (ESI+): *m/z* 555.2778 $[M]^{+\bullet}$, calcd for $C_{36}H_{35}N_4O_2^+$ 555.2755; HPLC (system A): t_R = 5.1 min (purity 96% at 260 nm and 98% at 600 nm); LRMS (ESI+, recorded during RP-HPLC analysis): *m/z* 555.0 (100) and 556.5 (55) $[M]^{+\bullet}$, calcd for $C_{36}H_{35}N_4O_2^+$ 555.3; UV-vis (recorded during the HPLC analysis): λ_{max} = 568, 601 and 647 nm (broad band).



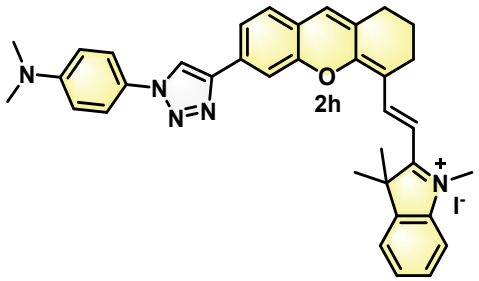
2e: 79 mg, 81% yield; dark blue solid; m.p 226-228 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.87 (s, 1 H), 8.59 (d, J = 15.2 Hz, 1 H), 7.86 (s, 1 H), 7.80-7.70 (m, 3 H), 7.63-7.53 (m, 2 H), 7.53-7.45 (m, 3 H), 7.43-7.36 (m, 3 H), 6.61 (d, J = 15.2 Hz, 1 H), 5.72 (s, 2 H), 3.92 (s, 3 H), 2.72 (t, J = 6.0 Hz, 2 H), 2.65 (t, J = 6.1 Hz, 2 H), 1.87-1.81 (m, 2 H), 1.79 (s, 6 H) ppm; ^{13}C NMR (101 MHz, DMSO-d_6): δ = 178.5, 158.9, 152.6, 145.3, 144.9, 142.2, 142.2, 134.8, 133.4, 132.9, 131.0, 130.0, 129.8, 128.8, 128.2, 127.6, 123.0, 122.6, 122.2, 121.2, 114.2, 113.6, 111.4, 106.3, 52.3, 50.6, 33.0, 28.7, 27.0, 23.5, 19.8 ppm; HRMS (ESI+): *m/z* 526.2605 $[M]^{+\bullet}$, calcd for $C_{34}H_{32}N_5O^+$ 526.2601; HPLC (system A): t_R = 4.7 min (purity 98% at 260 nm and 99% at 600 nm); LRMS (ESI+, recorded during RP-HPLC analysis): *m/z* 526.3 (100) and 527.4 (35) $[M]^{+\bullet}$, calcd for $C_{34}H_{32}N_5O^+$ 526.2; UV-vis (recorded during the HPLC analysis): λ_{max} = 567, 601 and 646 nm (broad band). **Note**: we found that dye **2e** was contaminated by a small quantity of 3,4-dihydroxy-2-oxobutanoic acid coming from the CuAAC reaction and which we estimated to be 1.4% by integration by ^{1}H NMR analysis.



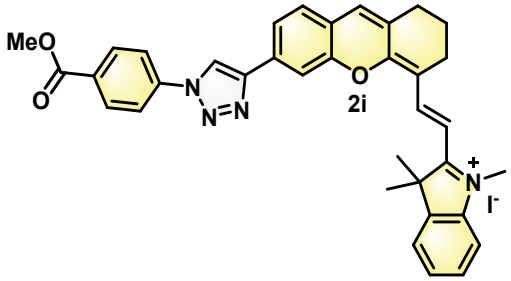
2f: 65 mg, 61% yield; dark blue solid; m.p 125-127 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 9.05 (dd, J = 2.2 Hz, J = 1.0 Hz, 1 H), 8.92 (s, 1 H), 8.61 (d, J = 15.2 Hz, 1 H), 8.36 (dd, J = 8.2 Hz, J = 2.2 Hz, 1H), 7.89 (s, 1 H), 7.79 (m, 2 H), 7.74-7.70 (m, 1 H), 7.63-7.47 (m, 4 H), 7.42 (s, 1 H), 6.62 (d, J = 15.2 Hz, 1 H), 5.95 (s, 2 H), 3.92 (s, 3 H), 3.88 (s, 3 H), 2.73 (t, J = 5.9 Hz, 2 H), 2.69-2.62 (m, 2 H), 1.88-1.81 (m, 2 H), 1.80 (s, 6 H) ppm; ^{13}C NMR (101 MHz, DMSO-d_6): δ = 178.5, 164.8, 159.2, 159.0, 152.7, 149.9, 145.2, 145.0, 142.2, 142.2, 138.2, 133.4, 131.0, 130.0, 128.8, 128.2, 127.5, 125.0, 124.0, 122.6, 122.2, 121.2, 114.2, 113.6, 111.4, 106.3, 54.3, 52.5, 50.6, 33.0, 28.7, 27.0, 23.5, 19.8 ppm; HRMS (ESI+): *m/z* 584.2673 $[M]^{+\bullet}$, calcd for $C_{36}H_{34}N_5O_3^+$ 584.2656; HPLC (system A): t_R = 4.8 min (purity 97% at 260 nm and 100% at 600 nm); LRMS (ESI+, recorded during RP-HPLC analysis): *m/z* 584.4 (100) and 585.4 (40) $[M]^{+\bullet}$, calcd for $C_{36}H_{34}N_5O_3^+$ 584.2; UV-vis (recorded during the HPLC analysis): λ_{max} = 570, 601 and 646 nm (broad band). **Note**: we found that dye **2f** was contaminated by a small quantity of 3,4-dihydroxy-2-oxobutanoic acid coming from the CuAAC reaction and which we estimated to be 2.4% by integration by ^{1}H NMR analysis.



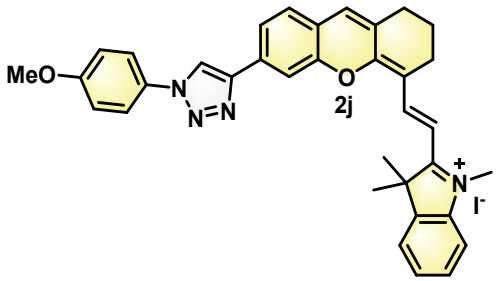
2g: 68 mg, 67% yield; dark blue solid; m.p 84-86 °C; ^{1}H NMR (400 MHz, CD_3OD): δ = 8.73 (d, J = 15.2 Hz, 1 H), 8.65 (s, 1 H), 7.85 (s, 1 H), 7.71 (m, 2 H), 7.63-7.47 (m, 4 H), 7.27 (s, 1 H), 6.55 (d, J = 15.2 Hz, 1 H), 4.49 (t, J = 7.0 Hz, 2 H), 3.90 (s, 3 H), 3.66 (s, 3 H), 2.76 (t, J = 6.0 Hz, 2 H), 2.67 (t, J = 6.1 Hz, 2 H), 2.42 (t, J = 7.3 Hz, 2 H), 2.06-1.96 (m, 2 H), 1.95-1.88 (m, 2 H), 1.85 (s, 6 H), 1.69-1.63 (m, 2H) ppm; ^{13}C NMR (101 MHz, CD_3OD): δ = 180.4, 175.3, 165.2, 161.2, 154.4, 147.2, 147.1, 143.6, 143.5, 135.0, 132.7, 131.6, 130.2, 129.4, 128.9, 123.7, 123.6, 123.0, 116.0, 114.3, 112.9, 106.7, 52.3, 52.1, 51.2, 33.9, 33.4, 30.6, 30.3, 28.2, 24.9, 22.9, 21.4 ppm; HRMS (ESI+): *m/z* 549.2874 $[M]^{+\bullet}$, calcd for $C_{34}H_{37}N_4O_3^+$ 549.2860; HPLC (system A): t_R = 4.9 min (purity 97% at 260 nm and 99% at 600 nm); LRMS (ESI+, recorded during RP-HPLC analysis): *m/z* 549.4 (100) and 550.5 (25) $[M]^{+\bullet}$, calcd for $C_{34}H_{37}N_4O_3^+$ 549.3; UV-vis (recorded during the HPLC analysis): λ_{max} = 569, 601 and 647 nm (broad band).



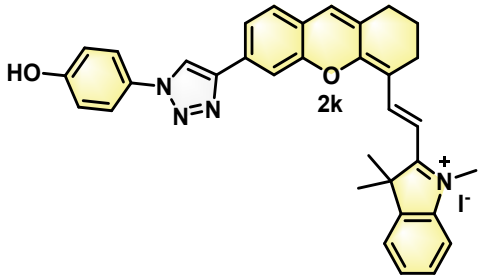
2h: 37 mg, 36% yield; dark blue solid; m.p 191-193 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.30 (s, 1 H), 8.65 (d, J = 15.5 Hz, 1 H), 7.95 (s, 1 H), 7.86-7.78 (m, 2 H), 7.74-7.65 (m, 4 H), 7.57-7.49 (m, 2 H), 7.44 (s, 1 H), 6.90 (d, J = 8.6 Hz, 2 H), 6.66 (d, J = 15.3 Hz, 1 H), 3.93 (s, 3 H), 3.00 (s, 6 H), 2.80 – 2.73 (m, 2 H), 2.73 – 2.67 (m, 2 H), 1.93 – 1.85 (m, 2 H), 1.81 (s, 6 H); ^{13}C NMR (101 MHz, DMSO-d_6): δ = 178.4, 159.0, 152.6, 150.4, 145.4, 144.9, 142.2, 142.1, 133.4, 131.0, 129.9, 128.8, 128.2, 127.5, 125.8, 122.6, 122.2, 121.3, 121.2, 120.4, 114.2, 113.6, 112.2, 111.3, 106.2, 50.6, 32.9, 28.7, 27.1, 23.5, 19.8 ppm; HRMS (ESI+): *m/z* 554.2912 $[M]^{+\bullet}$, calcd for $C_{36}H_{36}N_5O^+$ $[M]^{+\bullet}$ 554.2914; HPLC (system A): t_R = 5.4 min (purity 82% at 260 nm and 85% at 600 nm); LRMS (ESI+, recorded during RP-HPLC analysis): *m/z* 554.2 $[M]^{+\bullet}$ (100), calcd for $C_{36}H_{36}N_5O^+$ 554.3; UV-vis (recorded during the HPLC analysis): λ_{max} = 572, 604 and 650 nm (broad band).



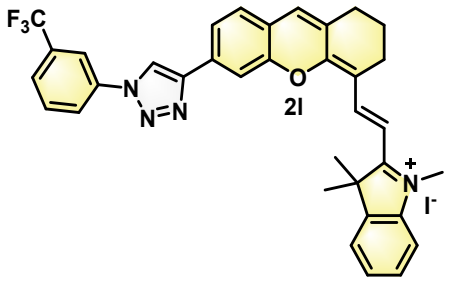
2i: 23 mg, 22% yield; dark blue solid; m.p 176-178 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 9.63 (s, 1 H), 8.61 (d, J = 15.2 Hz, 1 H), 8.48 (s, 1 H), 8.30-8.22 (m, 1 H), 8.10 (d, J = 7.8 Hz, 1 H), 7.93 (s, 1 H), 7.83 (dt, J = 13.9 Hz, J = 7.7 Hz, 3 H), 7.72 (d, J = 7.9 Hz, 1 H), 7.65 (d, J = 8.0 Hz, 1 H), 7.54 (m, 2 H), 7.42 (s, 1 H), 6.63 (d, J = 15.2 Hz, 1 H), 3.94 (s, 3 H), 3.92 (s, 3 H), 2.75 (t, J = 6.0 Hz, 2 H), 2.67 (t, J = 5.7 Hz, 2 H), 1.90-1.85 (m, 2 H), 1.82 (s, 6 H) ppm; ^{13}C NMR (101 MHz, DMSO-d_6): δ = 178.5, 165.2, 158.8, 152.6, 146.1, 144.9, 142.2, 142.1, 136.6, 132.8, 131.3, 130.8, 130.7, 130.1, 129.2, 128.8, 128.2, 127.6, 124.4, 122.6, 122.3, 121.5, 121.1, 120.0, 114.2, 113.6, 111.5, 106.4, 52.6, 50.7, 33.0, 28.7, 27.1, 23.5, 19.8 ppm; HRMS (ESI+): *m/z* 569.2550 $[M]^{+\bullet}$, calcd for $C_{36}H_{33}N_4O_3^+$ 569.2547; HPLC (system A): t_R = 5.3 min (purity 94% at 260 nm and 96% at 600 nm); LRMS (ESI+, recorded during RP-HPLC analysis): *m/z* 569.4 (100) and 570.4 (30) $[M]^{+\bullet}$, calcd for $C_{36}H_{33}N_4O_3^+$ 569.2; UV-vis (recorded during the HPLC analysis): λ_{max} = 568, 601 and 646 nm (broad band).



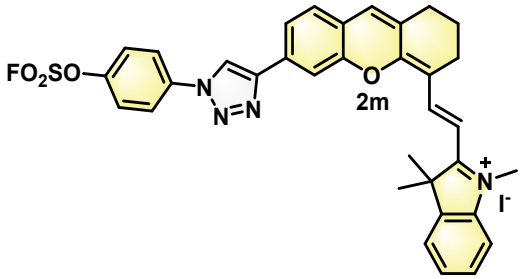
2j: 80 mg, 80% yield; dark blue solid; m.p 225-227 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 9.37 (s, 1 H), 8.61-8.51 (m, 1 H), 7.88-7.86 (m, 1 H), 7.85 (s, 1 H), 7.84-7.76 (m, 3 H), 7.73-7.68 (m, 1 H), 7.62 (m, 1 H), 7.59-7.46 (m, 2 H), 7.40 (s, 1 H), 7.21-7.14 (m, 2 H), 6.58 (d, J = 15.2 Hz, 1 H), 3.89 (s, 3 H), 3.85 (s, 3 H), 2.73 (t, J = 6.1 Hz, 2 H), 2.64 (m, 2 H),1.89-1.84 (m, 2 H), 1.80 (s, 6 H) ppm; ^{13}C NMR (101 MHz, DMSO-d_6): δ = 178.4, 159.4, 158.9, 152.6, 145.7, 144.9, 142.2, 142.1, 133.1, 130.9, 130.0, 129.8, 128.8, 128.2, 127.6, 122.6, 122.2, 121.7, 121.4, 120.8, 114.9, 114.2, 113.6, 111.4, 106.3, 55.6, 50.6, 33.0, 28.7, 27.1, 23.5, 19.8 ppm; HRMS (ESI+): *m/z* 541.2603 $[M]^{+\bullet}$, calcd for $C_{35}H_{33}N_4O_2^+$ 541.2598; HPLC (system A): t_R = 5.3 min (purity 98% at 260 nm and 99% at 600 nm); LRMS (ESI+, recorded during RP-HPLC analysis): *m/z* 541.3 (100) and 542.5 (30) $[M]^{+\bullet}$, calcd for $C_{35}H_{33}N_4O_2^+$ 541.2; UV-vis (recorded during the HPLC analysis): λ_{max} = 570, 602 and 648 nm (broad band). **Note**: we found that dye **2j** was contaminated by a small quantity of 3,4-dihydroxy-2-oxobutanoic acid coming from the CuAAC reaction and which we estimated to be 1.6% by integration by ^{1}H NMR analysis.



2k: 40 mg, 41% yield; dark blue solid; m.p 227-229 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 10.06 (s, 1 H), 9.32 (s, 1 H), 8.58 (d, J = 15.2 Hz, 1 H), 7.88 (s, 1 H), 7.85-7.76 (m, 2 H), 7.74-7.68 (m, 3 H), 7.65-7.47 (m, 3 H), 7.40 (s, 1 H), 7.02-6.96 (m, 2 H), 6.59 (d, J = 15.3 Hz, 1 H), 3.90 (s, 3 H), 2.73 (t, J = 6.0 Hz, 2 H), 2.63 (m, 2 H), 1.87-1.81 (m, 2 H), 1.81 (s, 6 H) ppm; ^{13}C NMR (101 MHz, DMSO-d_6): δ = 178.5, 158.9, 158.0, 152.6, 145.6, 144.9, 142.2, 142.2, 133.2, 131.0, 130.0, 128.8, 128.5, 128.2, 127.6, 122.6, 122.2, 121.9, 121.3, 120.8, 116.1, 114.2, 113.6, 111.4, 106.3, 50.6, 33.0, 28.7, 27.1, 23.5, 19.8 ppm; HRMS (ESI+): *m/z* 527.2437 $[M]^{+\bullet}$, calcd for $C_{34}H_{31}N_4O_2^+$ 527.2442; HPLC (system A): t_R = 4.9 min (purity 97% at 260 nm and 99% at 600 nm); HPLC (system B): t_R = 5.1 min (purity 96% at 260 nm and 99% at 600 nm); LRMS (ESI+, recorded during RP-HPLC analysis): *m/z* 527.2 (100) and 528.4 (40) $[M]^{+\bullet}$, calcd for $C_{34}H_{31}N_4O_2^+$ 527.2; LRMS (ESI-, recorded during RP-HPLC analysis): *m/z* 525.2 (100) $[M^+ - 2H]^-$ and 571.2 (60) $[M^+ - 2H + FA]^-$, calcd for $C_{34}H_{29}N_4O_2^-$ 525.2; UV-vis (recorded during the HPLC analysis): λ_{max} = 569, 602 and 647 nm (broad band).

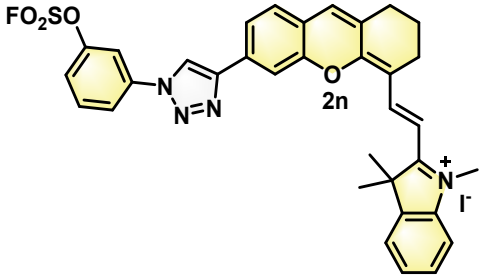


2l: 45 mg, 43% yield; dark blue solid; m.p 63-65 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 9.64 (s, 1 H), 8.58 (d, J = 15.3 Hz, 1 H), 8.35-8.27 (m, 2 H), 7.94-7.90 (m, 2 H), 7.89 (s, 1 H), 7.80 (ddd, J = 7.1 Hz, J = 5.9 Hz, J = 1.4 Hz, 2 H), 7.73-7.69 (m, 1 H), 7.65 (d, J = 8.1 Hz, 1 H), 7.53 (m, 2 H), 7.40 (s, 1 H), 6.60 (d, J = 15.3 Hz, 1 H), 3.91 (s, 3 H), 2.74 (t, J = 5.9 Hz, 2 H), 2.65 (t, J = 6.0 Hz, 2 H), 1.89-1.84 (m, 2 H), 1.81 (s, 6 H) ppm; ^{13}C NMR (101 MHz, DMSO-d_6): δ = 178.6, 158.8, 152.6, 146.1, 144.9, 142.3, 142.1, 136.9, 132.7, 131.5, 130.7, 130.6 (q, J = 32.8 Hz), 130.4, 130.2, 128.8, 128.3, 127.6, 125.5 (q, J = 3.6 Hz), 124.0, 123.6 (q, J = 273.7 Hz), 122.6, 122.3, 121.6, 121.3, 116.6, 116.6 (q, J = 3.9 Hz), 114.2, 113.6, 111.5, 106.5, 50.7, 33.0, 28.7, 27.0, 23.6, 19.8 ppm; ^{19}F NMR (376 MHz, DMSO-d_6): δ = -61.2 (s, 3 F); HRMS (ESI+): *m/z* 579.2363 $[M]^{+\bullet}$, calcd for $C_{35}H_{30}F_3N_4O^+$ 579.2366; HPLC (system A): t_R = 5.5 min (purity 98% at 260 nm and 100% at 600 nm); LRMS (ESI+, recorded during RP-HPLC analysis): *m/z* 579.4 (100) and 580.5 (35) $[M]^{+\bullet}$, calcd for $C_{35}H_{30}F_3N_4O^+$ 579.2; UV-vis (recorded during the HPLC analysis): λ_{max} = 568, 601 and 645 nm (broad band). **Note**: we found that dye **2l** was contaminated by a small quantity of 3,4-dihydroxy-2-oxobutanoic acid coming from the CuAAC reaction and which we estimated to be 2.8% by integration by ^{1}H NMR analysis.

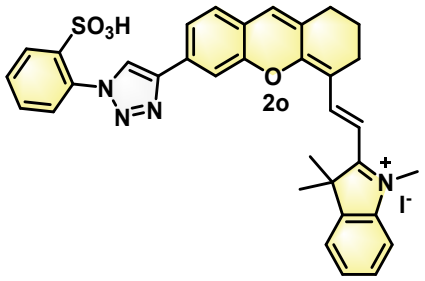


2m: 53 mg, 48% yield; dark blue solid; m.p 173-175 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 9.54 (s, 1 H), 8.57 (d, J = 15.3 Hz, 1 H), 8.20-8.13 (m, 2 H), 7.9-7.90 (m, 2 H), 7.86 (s, 1 H), 7.79 (m, 2 H), 7.71 (d, J = 7.8 Hz, 1 H), 7.64 (d, J = 8.0 Hz, 1 H), 7.59-7.47 (m, 2 H), 7.40 (s, 1 H), 6.59 (d, J = 15.1 Hz, 1 H), 3.90 (s, 3 H), 2.73 (t, J = 5.8 Hz, 2 H), 2.63 (t, J = 6.1 Hz, 2 H), 1.88-1.82 (m, 2 H), 1.81 (s, 6 H) ppm; ^{13}C NMR (101 MHz, DMSO-d_6): δ = 178.5, 158.7, 152.6, 148.9, 146.1, 144.9, 142.2, 142.1, 136.5, 132.4, 130.7, 130.22, 128.8, 128.3, 127.6, 123.1, 122.6, 122.3, 121.6, 121.3, 114.2, 113.6, 111.5, 106.4, 50.7, 33.0, 28.7, 27.0, 23.5, 19.8 ppm; ^{19}F NMR (377 MHz, DMSO-d_6): δ = 39.1 (s, 1 F); HRMS (ESI+): *m/z* 609.1977 $[M]^{+\bullet}$, calcd for $C_{34}H_{30}FN_4O_4S^+$ 609.1966; HPLC (system A): t_R = 5.4 min (purity 96% at 260 nm and 98% at 600 nm); LRMS (ESI+, recorded during RP-HPLC analysis): *m/z* 609.4 (100) and 610.3 (30) $[M]^{+\bullet}$, calcd for $C_{34}H_{30}FN_4O_4S^+$ 609.2; LRMS (ESI-, recorded during

RP-HPLC analysis): *m/z* 653.3 (90) $[M^+ - 2H + FA]^-$, calcd for $C_{34}H_{29}FN_4O_4S^-$ 607.2; UV-vis (recorded during the HPLC analysis): λ_{max} = 567, 601 and 645 nm (broad band).



2n: 22 mg, 20% yield; dark blue solid; m.p 223-225 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 9.54 (s, 1 H), 8.58 (d, *J* = 15.2 Hz, 1 H), 8.26 (t, *J* = 2.2 Hz, 1 H), 8.14 (m, 1 H), 7.88 (d, *J* = 8.4 Hz, 1 H), 7.87 (s, 1 H), 7.83-7.75 (m, 3 H), 7.73-7.69 (m, 1 H), 7.64 (d, *J* = 8.0 Hz, 1 H), 7.53 (m, 2 H), 7.39 (s, 1 H), 6.60 (d, *J* = 15.2 Hz, 1 H), 3.90 (s, 3 H), 2.73 (t, *J* = 6.0 Hz, 2 H), 2.64 (t, *J* = 6.1 Hz, 2 H), 1.89-1.82 (m, 2 H), 1.81 (s, 6 H) ppm; ^{13}C NMR (101 MHz, DMSO-d_6): δ = 178.6, 158.7, 152.6, 149.8, 146.2, 144.9, 142.2, 142.1, 137.7, 132.5, 132.5, 130.7, 130.3, 128.8, 128.3, 127.6, 122.6, 122.3, 121.6, 121.4, 121.2, 120.5, 114.2, 113.6, 113.2, 111.5, 106.5, 50.7, 33.0, 28.7, 27.0, 23.5, 19.8 ppm; ^{19}F NMR (377 MHz, CD_3OD): δ = 36.6 (s, 1 F) ppm; HRMS (ESI+): *m/z* 609.1983 $[M]^{+\bullet}$, calcd for $C_{34}H_{30}FN_4O_4S^+$ 609.1966; HPLC (system A): t_R = 5.4 min (purity 97% at 260 nm and 99% at 600 nm); LRMS (ESI+, recorded during RP-HPLC analysis): *m/z* 609.4 (100) and 610.3 (40) $[M]^{+\bullet}$, calcd for $C_{34}H_{30}FN_4O_4S^+$ 609.2; LRMS (ESI-, recorded during RP-HPLC analysis): *m/z* 653.4 (100) $[M^+ - 2H + FA]^-$, calcd for $C_{34}H_{29}FN_4O_4S^-$ 607.2; UV-vis (recorded during the HPLC analysis): λ_{max} = 568, 601 and 645 nm (broad band).



2o: 15 mg, 14% yield; m.p. 235-237 °C; ^{1}H NMR (600 MHz, DMSO-d_6) δ 9.23 (s, 1H), 8.65 (d, *J* = 14.9 Hz, 1H), 8.07-7.99 (m, 1H), 7.91 (s, 1H), 7.90 (s, 1H), 7.83-7.78 (m, 3H), 7.71 (d, *J* = 8.1 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.61-7.58 (m, 2H), 7.55 (d, *J* = 7.9 Hz, 2H), 7.46 (s, 1H), 6.64 (d, *J* = 15.2 Hz, 1H), 3.92 (s, 3H), 2.71-2.66 (m, 2H), 2.64 (t, *J* = 5.9 Hz, 2H), 1.89-1.83 (m, 2H), 1.81 (s, 6H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 178.6, 158.8, 152.7, 149.0, 146.2, 145.0, 142.3, 142.2, 136.5, 132.7, 130.8, 130.3, 128.9, 128.4, 127.7, 123.2, 122.7, 122.4, 121.6, 121.3, 114.3, 113.7, 111.6, 106.5, 50.8, 33.0, 28.8, 27.1, 23.6, 19.8; HPLC (system A): t_R = 4.7 min (purity 95% at 260 nm and 97% at 600 nm); LRMS (ESI+, recorded during RP-HPLC analysis): *m/z* 563.2 (60),

591.4 (100) $[M]^{+\bullet}$ and 1181.7 (15) $[2M^{+} - H]^{+\bullet}$, calcd for $C_{34}H_{31}N_4O_4S^{+}$ 591.7; LRMS (ESI-, recorded during RP-HPLC analysis): *m/z* 589.3 (100) $[M^{+} - 2H]^{-}$, calcd for $C_{34}H_{29}N_4O_4S^{-}$ 589.78; UV-vis (recorded during the HPLC analysis): λ_{max} = 569, 602 and 649 nm (broad band); HRMS (ESI+): *m/z* 591.2055 $[M]^{+\bullet}$, calcd for $C_{34}H_{31}N_4O_4S^{+}$ 591.2060.

4. References

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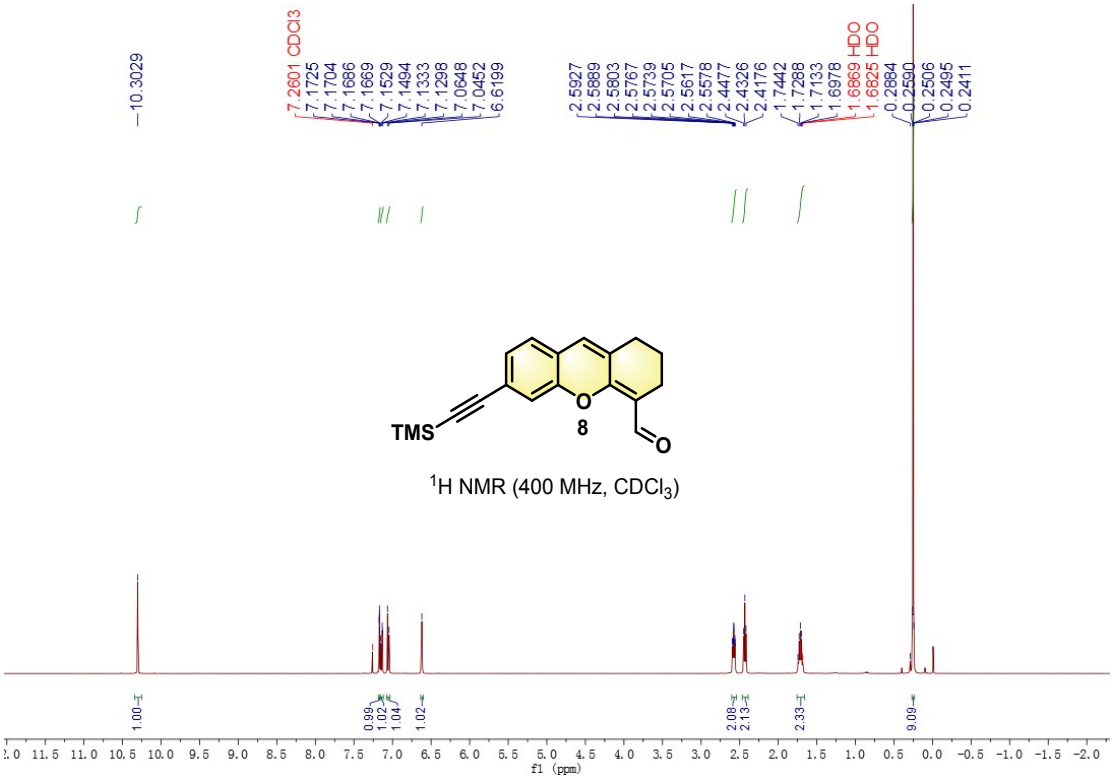
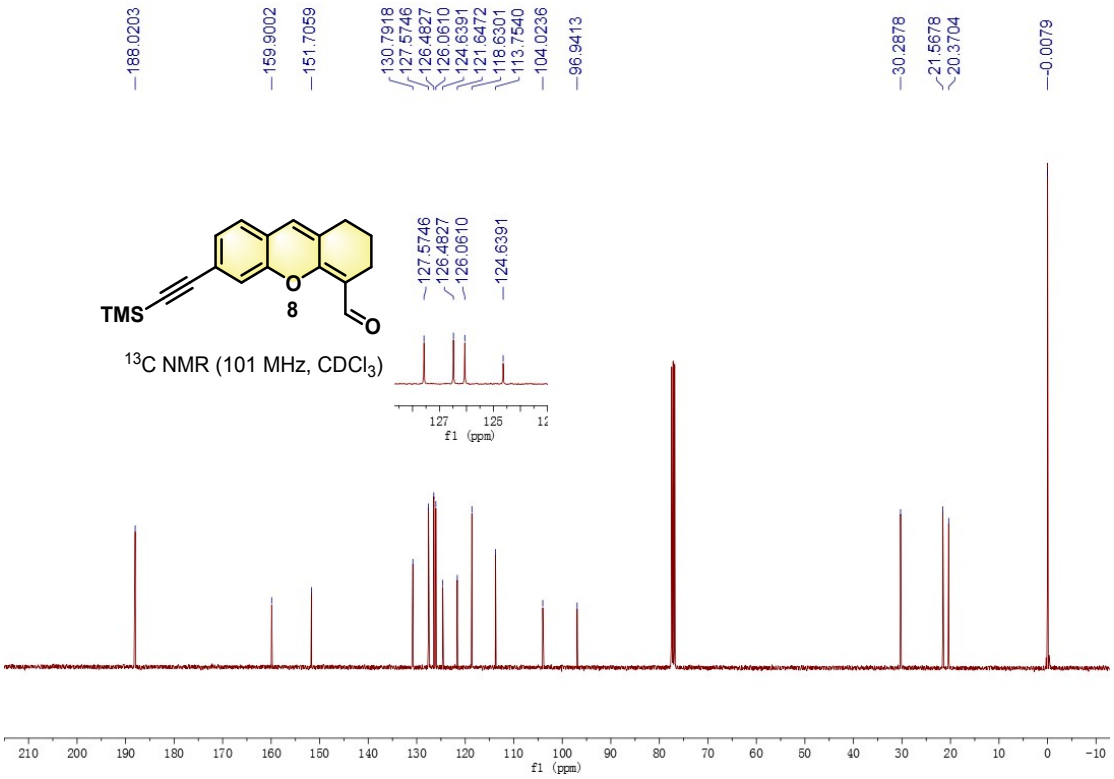
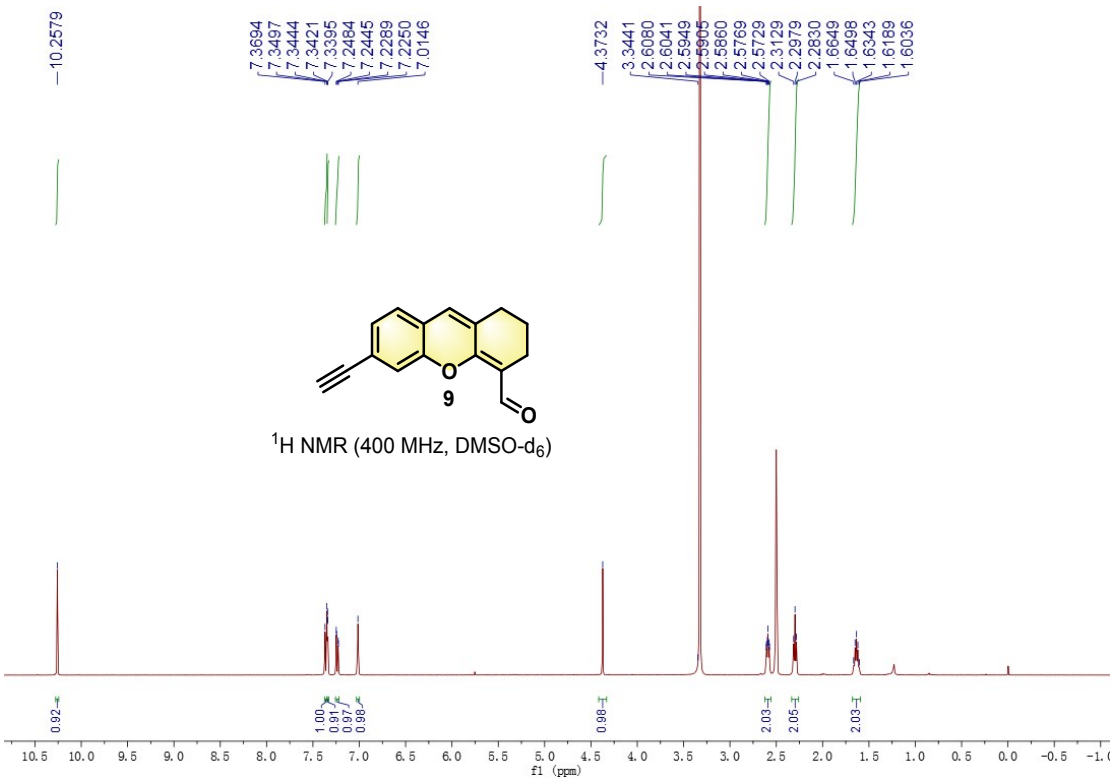
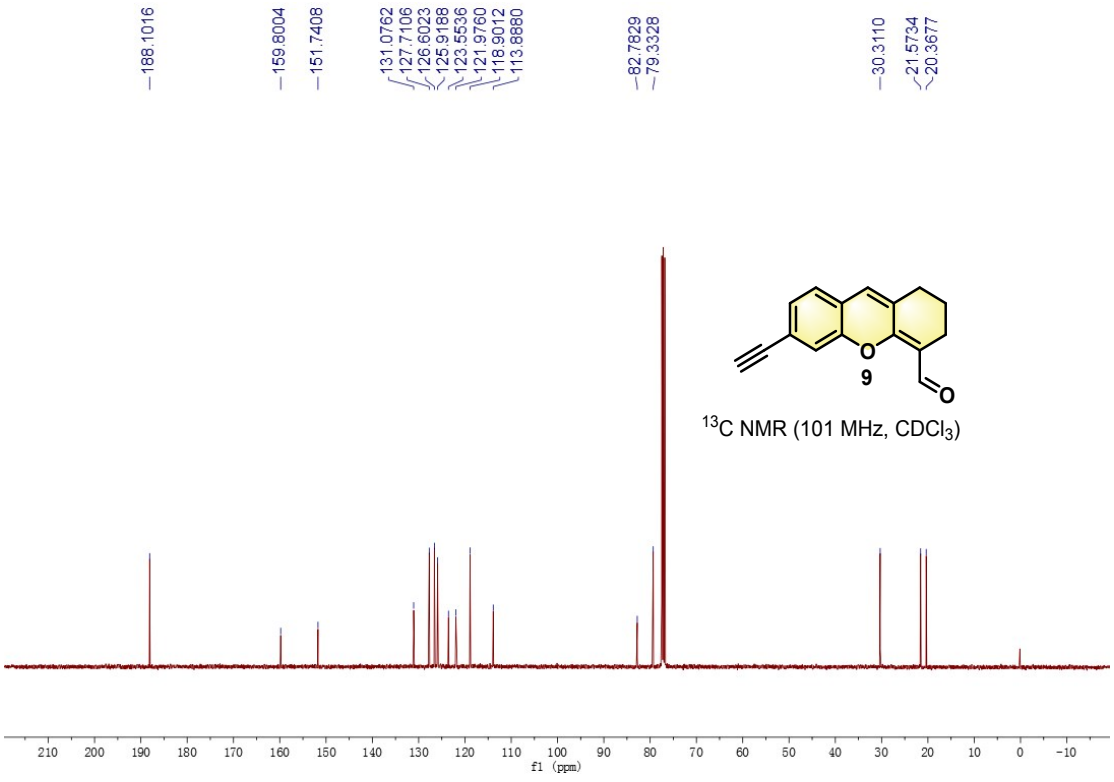
5. ^{1}H, ^{19}F and ^{13}C NMR spectra of synthesised compounds


10.3029
7.2601 CDCl3
7.1725
7.1704
7.1686
7.1669
7.1529
7.1494
7.1333
7.1298
7.0648
7.0452
6.6199
2.5927
2.5889
2.5803
2.5767
2.5739
2.5705
2.5617
2.5578
2.4477
2.4326
2.4176
1.7442
1.7288
1.7133
1.6978
1.6869 HDO
1.6825 HDO
0.2884
0.2590
0.2506
0.2495
0.2411
TMS
O
8
O
1H NMR (400 MHz, CDCl3)
1.00
0.99
1.02
1.04
1.02
2.08
2.13
2.33
9.09
f1 (ppm)

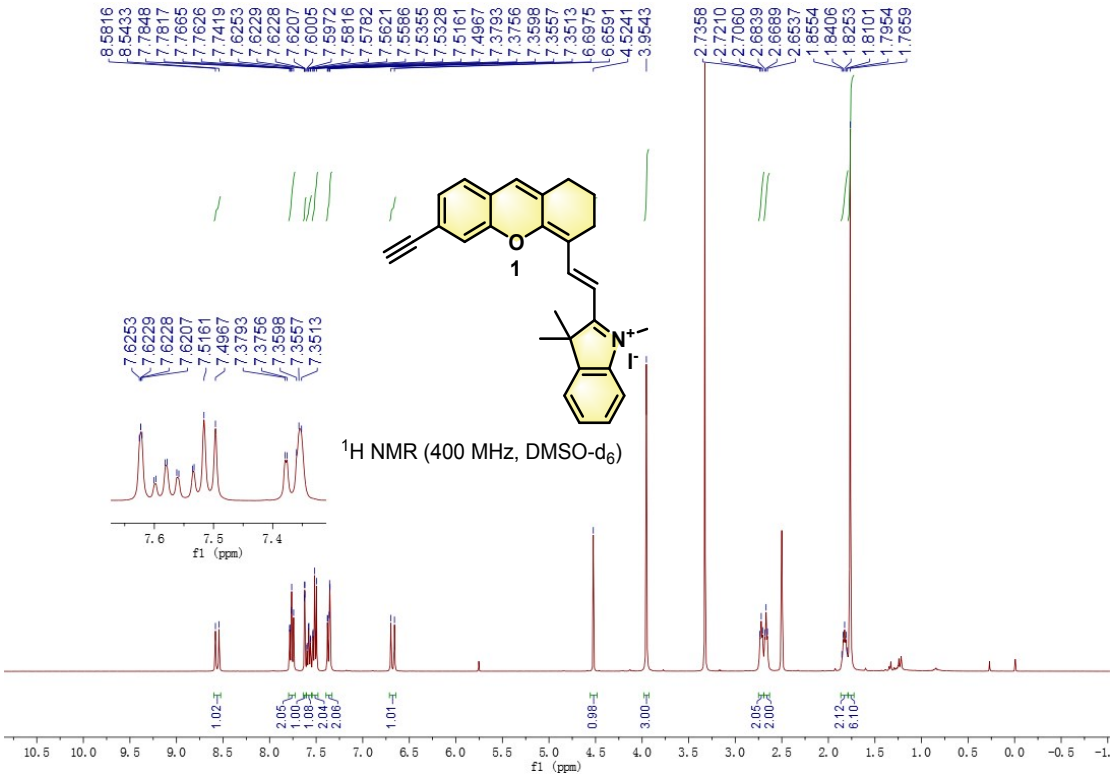

188.0203
159.9002
151.7059
130.7918
127.5746
126.4827
126.0610
124.6391
121.6472
118.6301
113.7540
104.0236
96.9413
30.2878
21.5678
20.3704
0.0079
TMS
O
8
O
13C NMR (101 MHz, CDCl3)
127.5746
126.4827
126.0610
124.6391
f1 (ppm)
f1 (ppm)

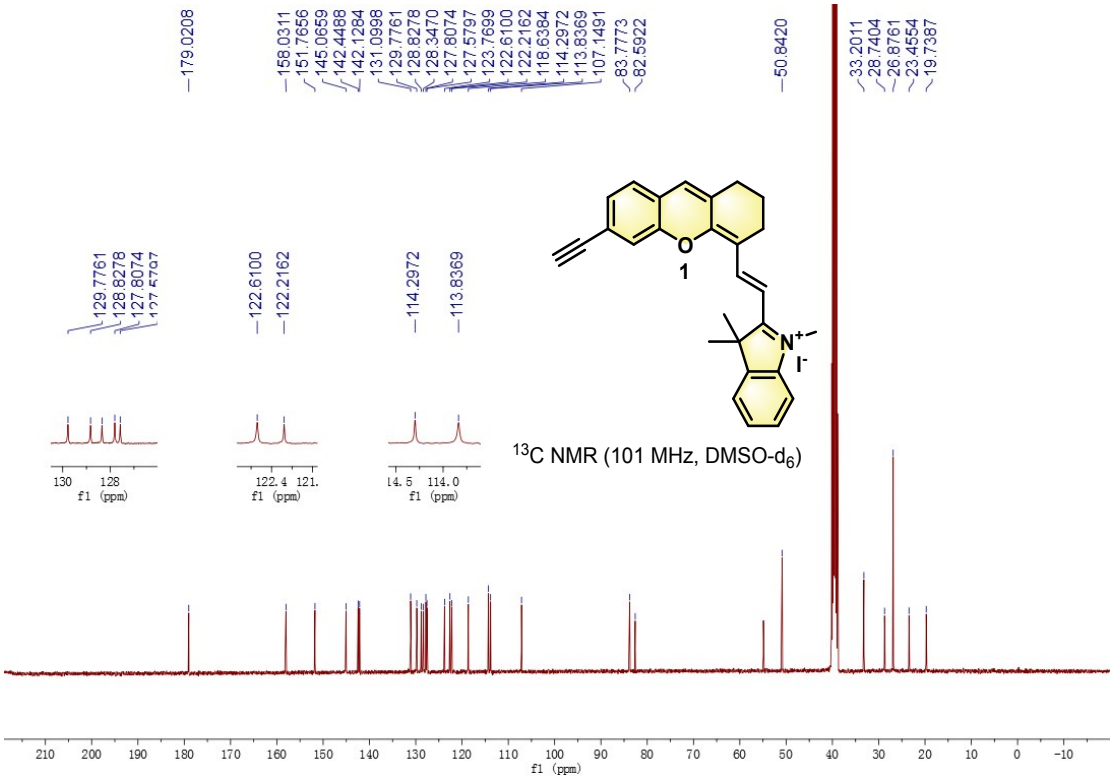


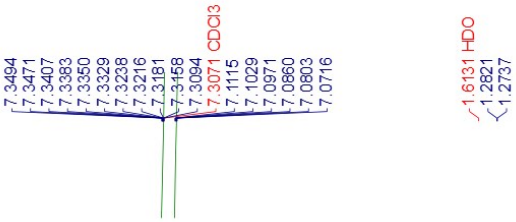
^{1}H NMR (400 MHz, DMSO-d_6)

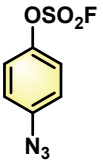


^{13}C NMR (101 MHz, $CDCl_3$)


8.5816
8.5433
7.7848
7.7817
7.7665
7.7626
7.7419
7.6253
7.6229
7.6228
7.6207
7.6005
7.5972
7.5816
7.5782
7.5621
7.5586
7.5355
7.5328
7.5161
7.4967
7.3793
7.3756
7.3598
7.3557
7.3513
6.6975
6.6591
4.5241
3.9543
2.7358
2.7210
2.7060
2.6839
2.6689
2.6537
1.8554
1.8406
1.8253
1.8101
1.7954
1.7659
O
1
N+
I-
1H NMR (400 MHz, DMSO-d6)
f1 (ppm)

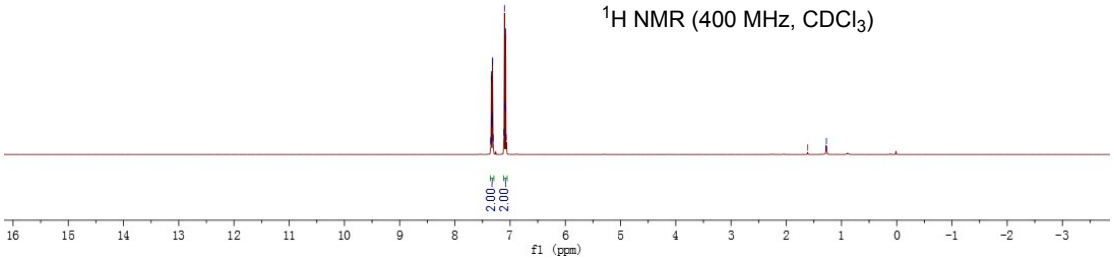

179.0208
158.0311
151.7656
145.0659
142.4488
142.1284
131.0998
129.7761
128.8278
128.3470
127.8074
127.5797
123.7699
122.6100
122.2162
118.6384
114.2972
113.8369
107.1491
83.7773
82.5922
50.8420
33.2011
28.7404
26.8761
23.4554
19.7387
O
1
N+
I-
13C NMR (101 MHz, DMSO-d6)
f1 (ppm)

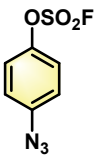




11m

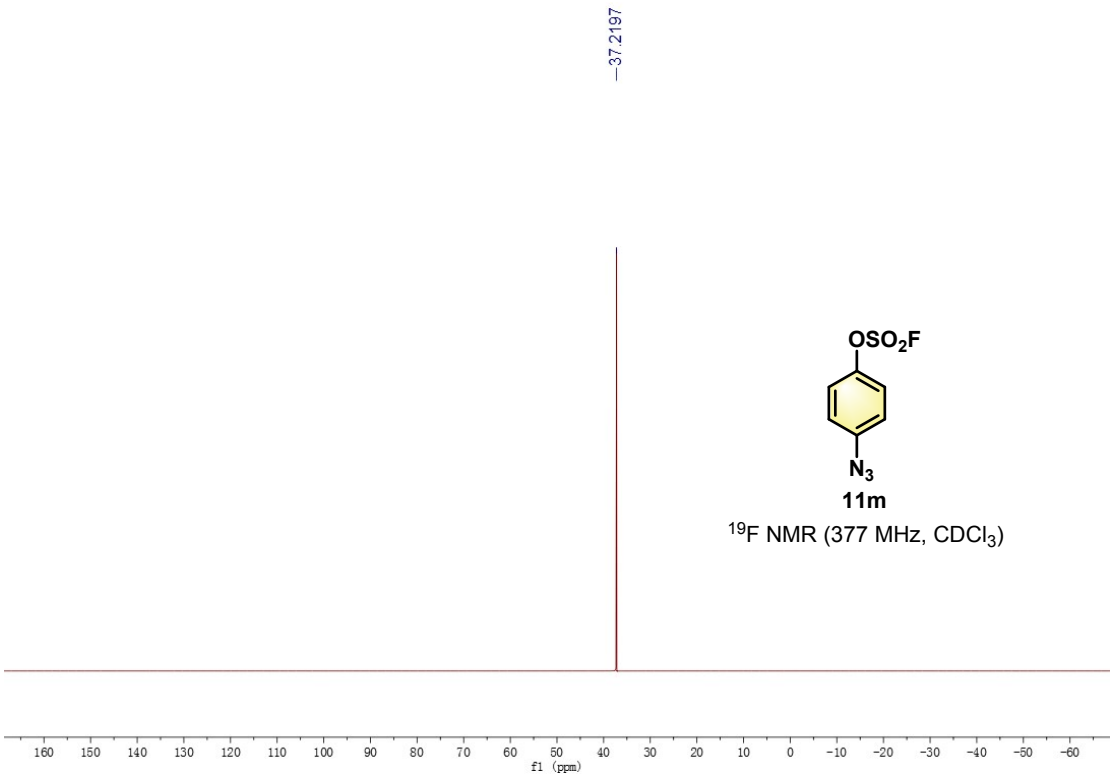
^{1}H NMR (400 MHz, $CDCl_3$)





11m

^{13}C NMR (101 MHz, $CDCl_3$)

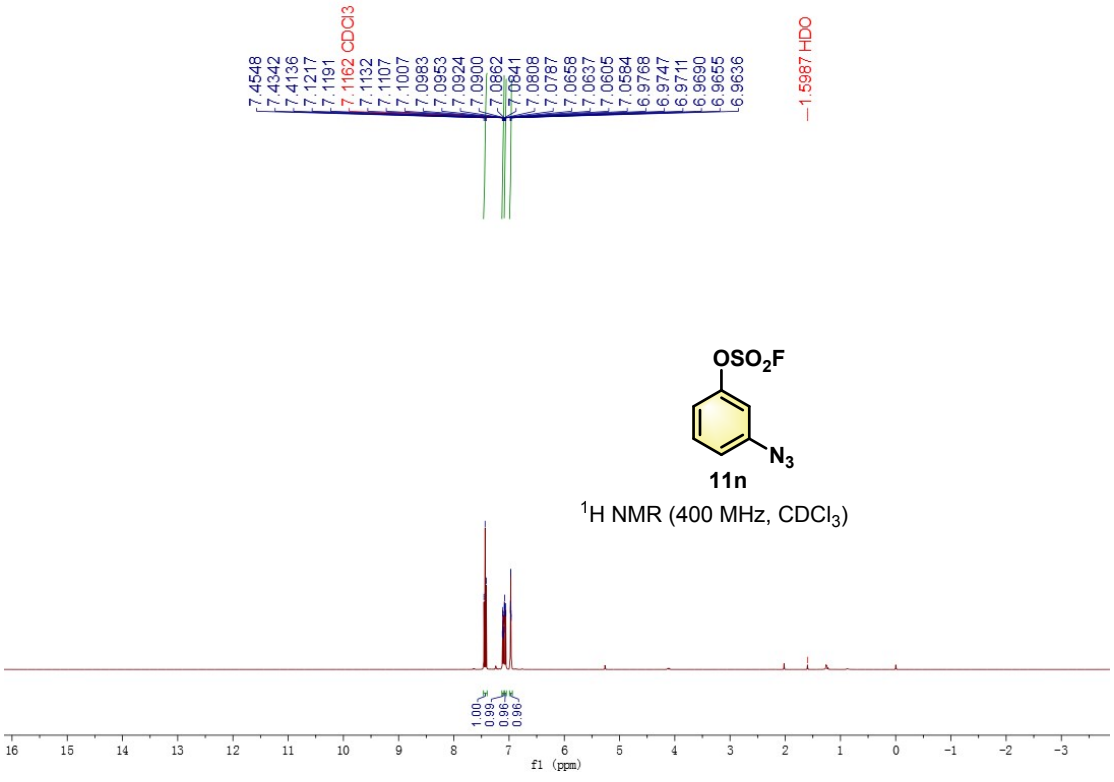


OSO_2F

N_3

11m

^{19}F NMR (377 MHz, $CDCl_3$)

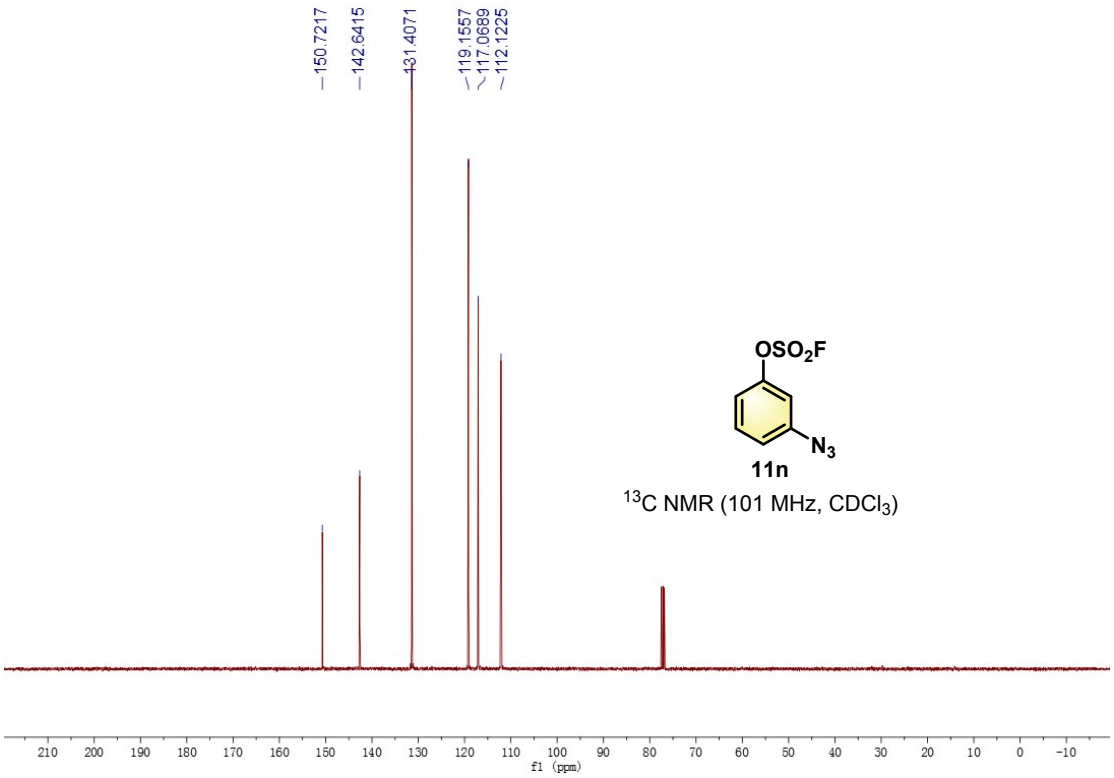


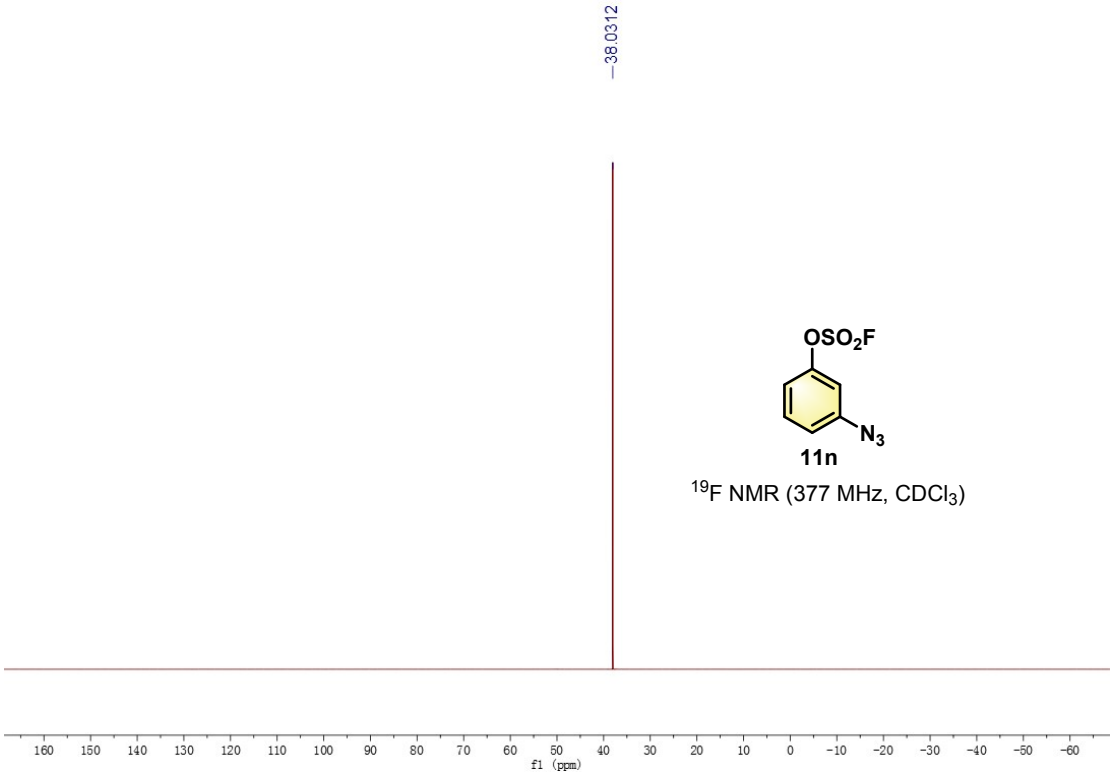
OSO_2F

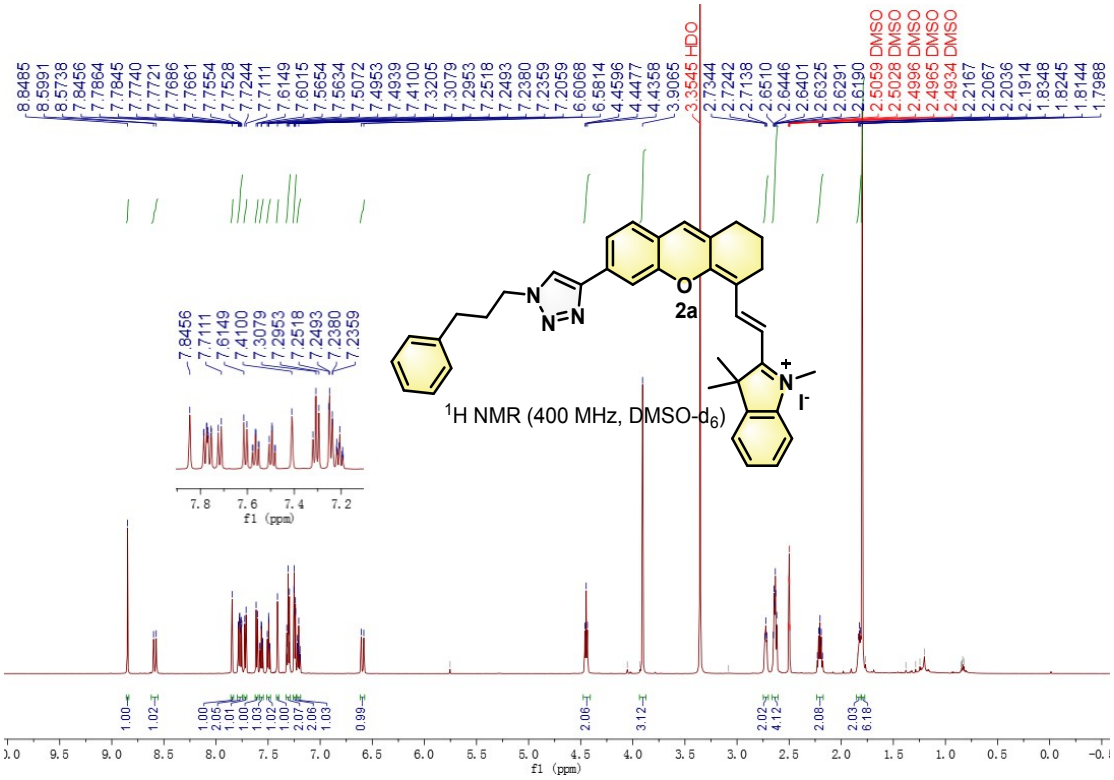
N_3

11n

^{1}H NMR (400 MHz, $CDCl_3$)


150.7217
142.6415
131.4071
119.1557
117.0689
112.1225
OSO2F
N3
11n
13C NMR (101 MHz, CDCl3)
f1 (ppm)


38.0312
OSO2F
N3
11n
19F NMR (377 MHz, CDCl3)
f1 (ppm)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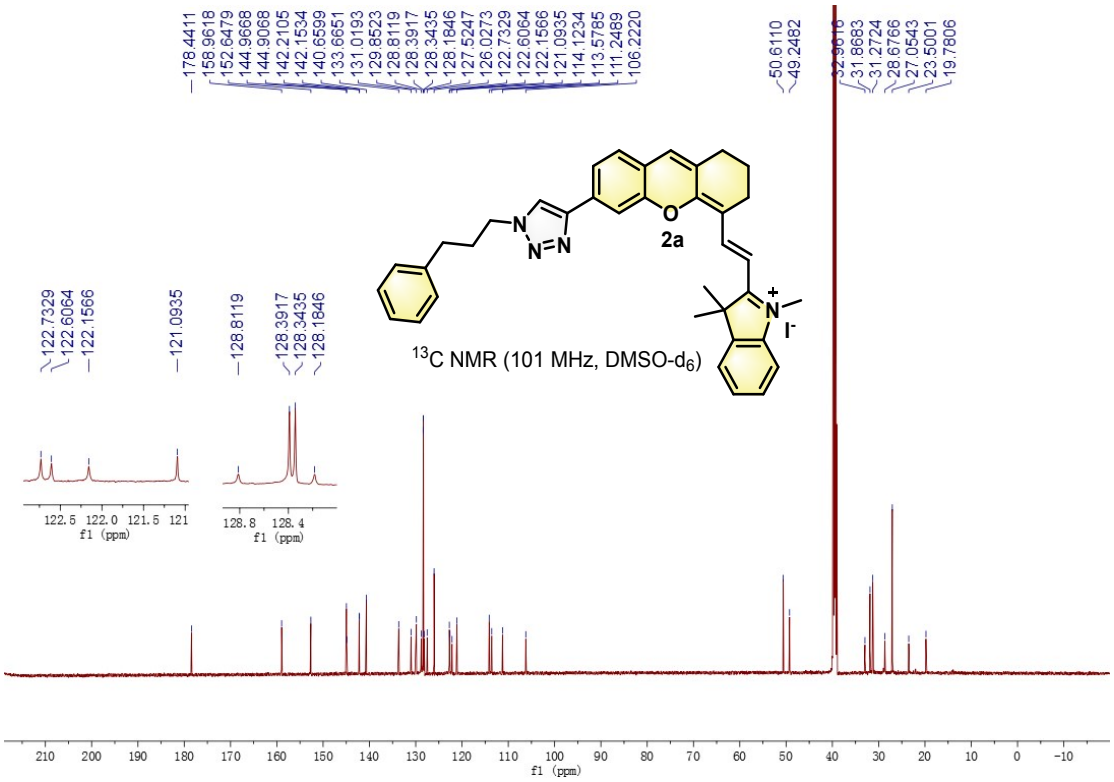
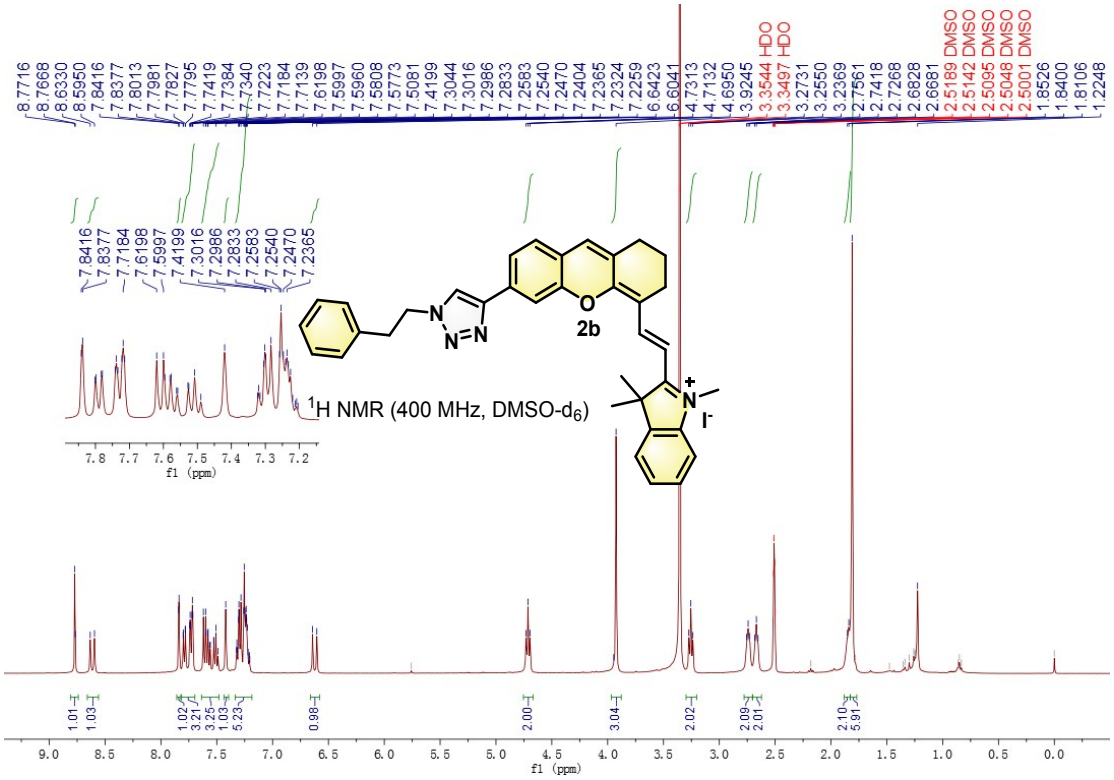
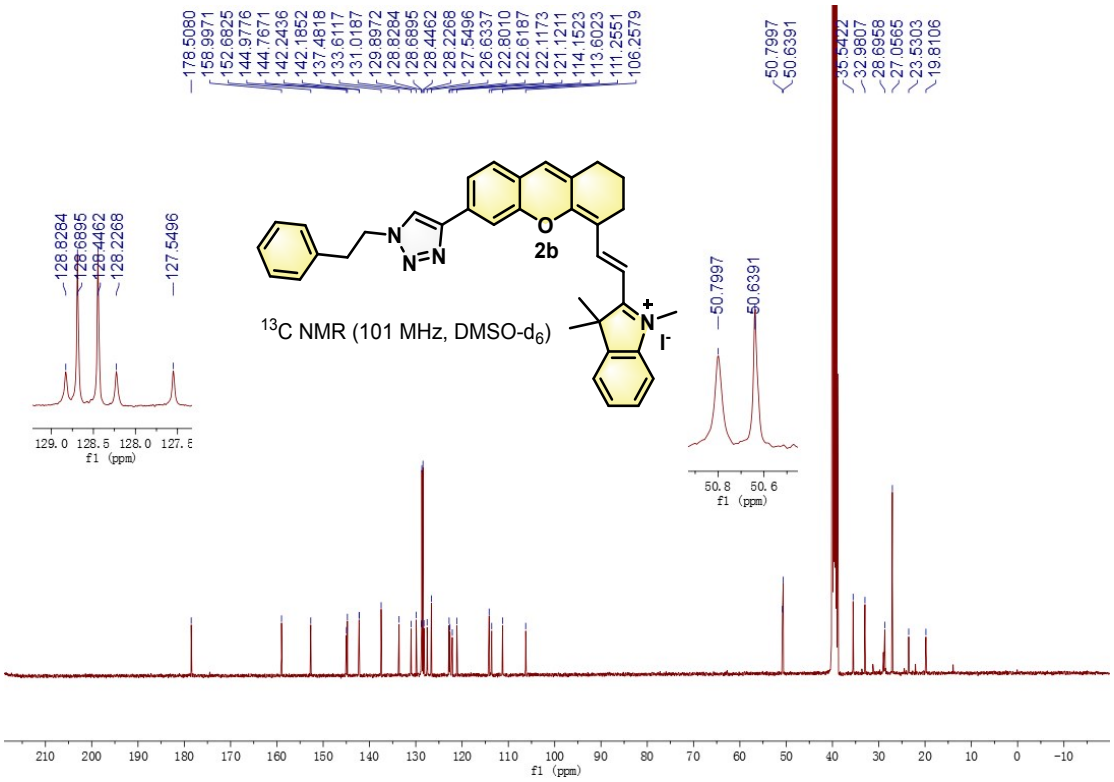
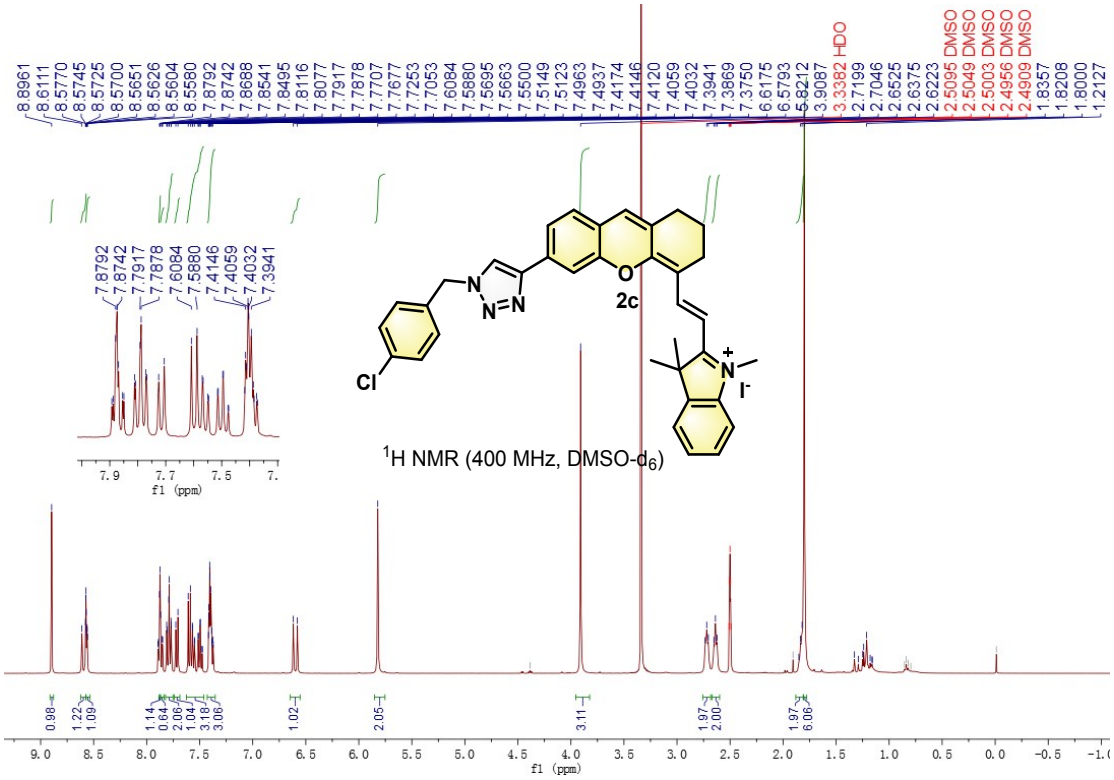
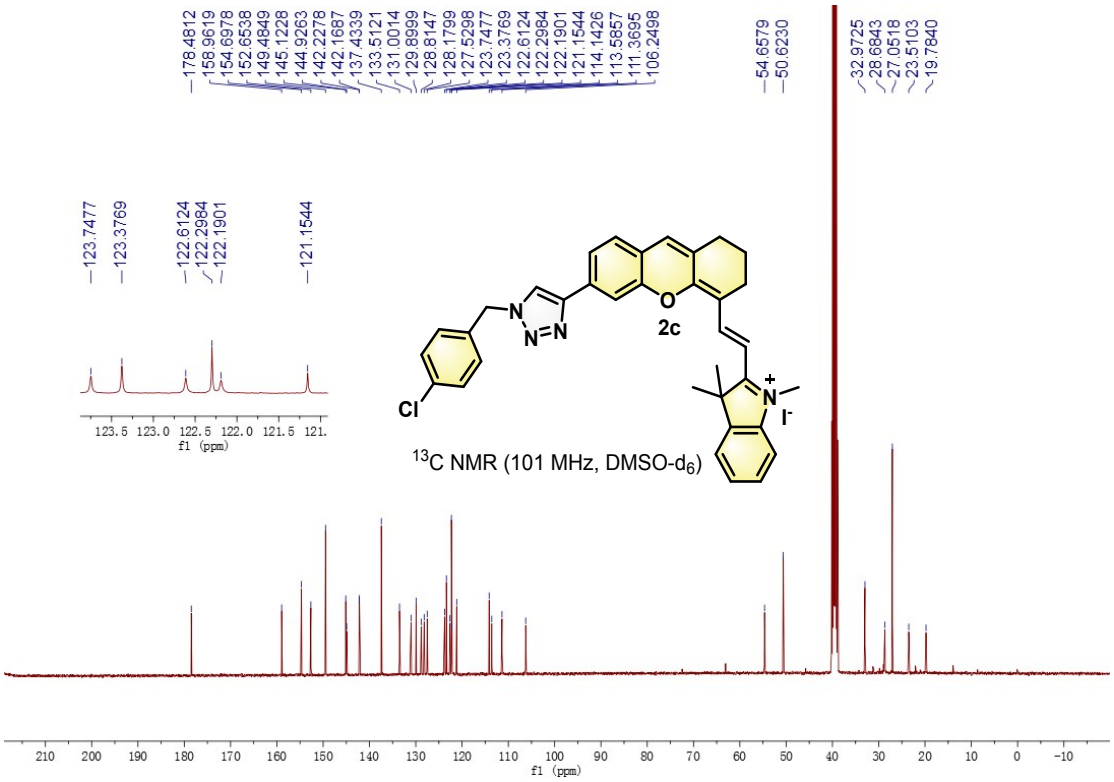
^{1}H NMR (400 MHz, DMSO-d$_6$)
f1 (ppm)

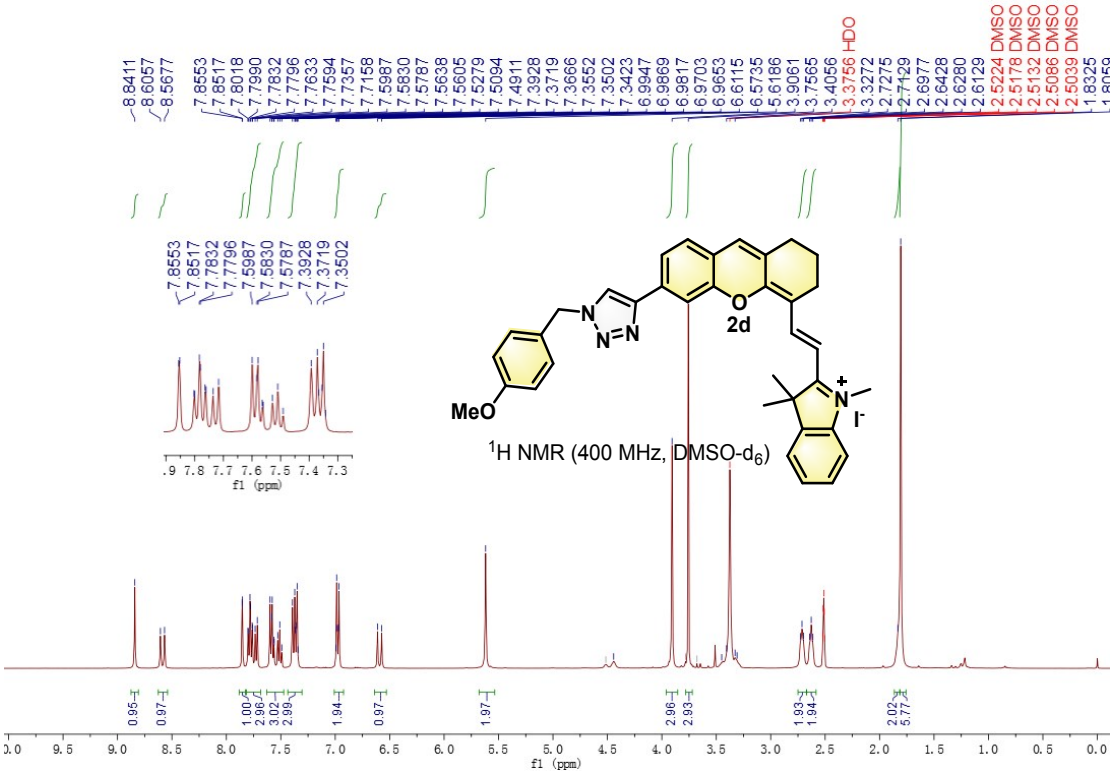

2a
^{13}C NMR (101 MHz, DMSO-d$_6$)
f1 (ppm)

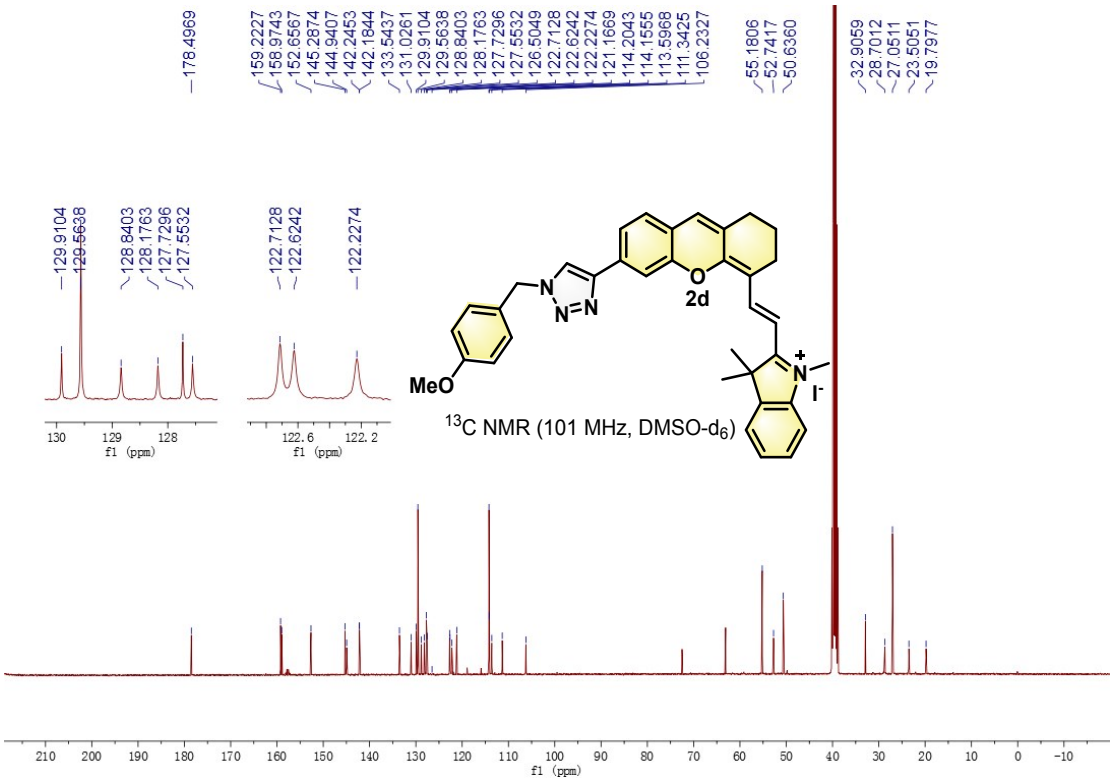

2b
^{1}H NMR (400 MHz, DMSO-d$_6$)

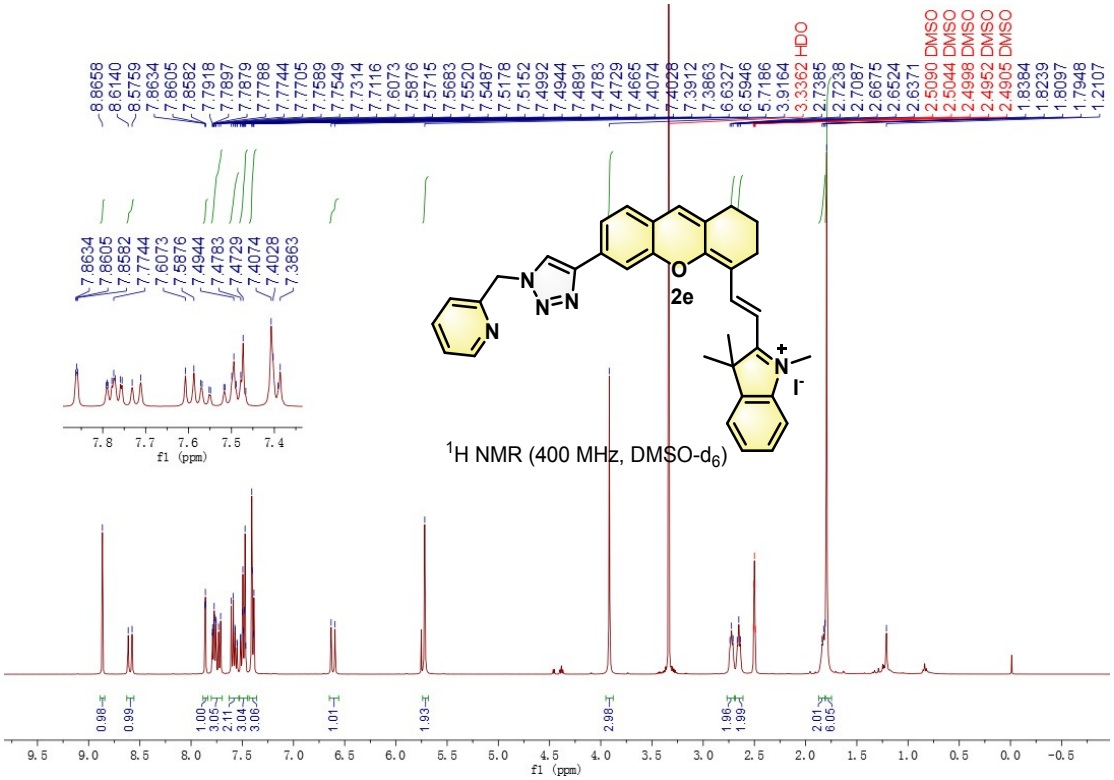

2b
^{13}C NMR (101 MHz, DMSO-d$_6$)

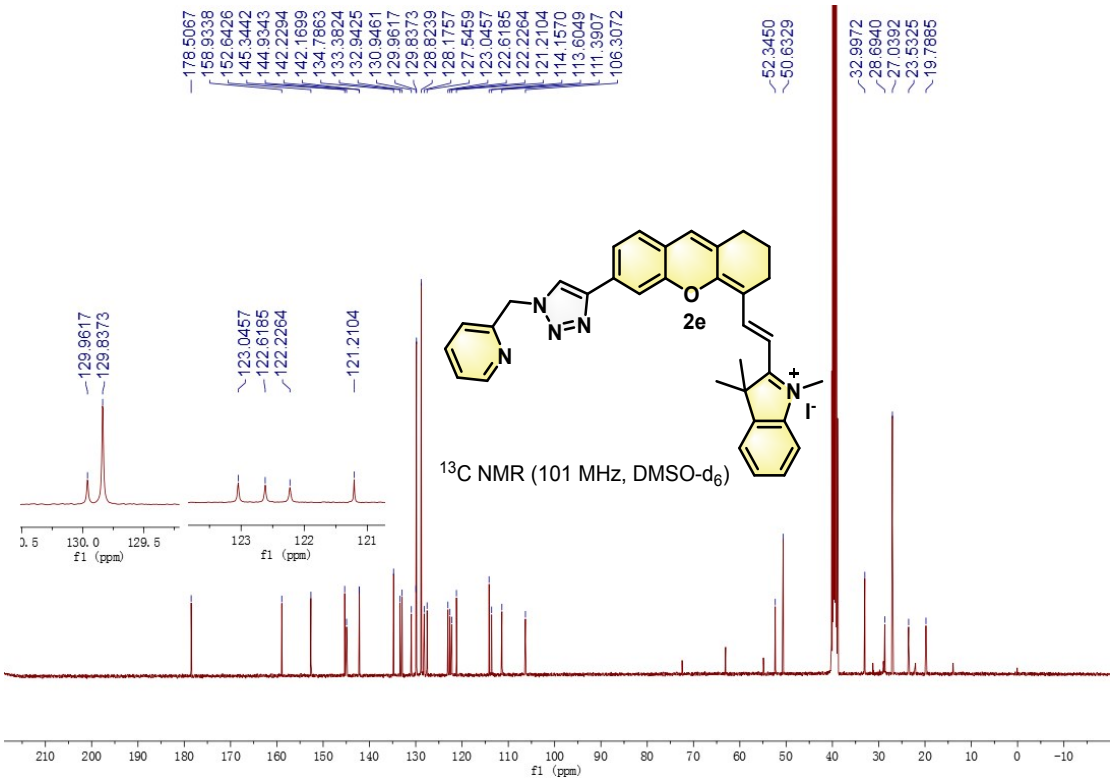

2c
Cl
I-
1H NMR (400 MHz, DMSO-d6)
f1 (ppm)

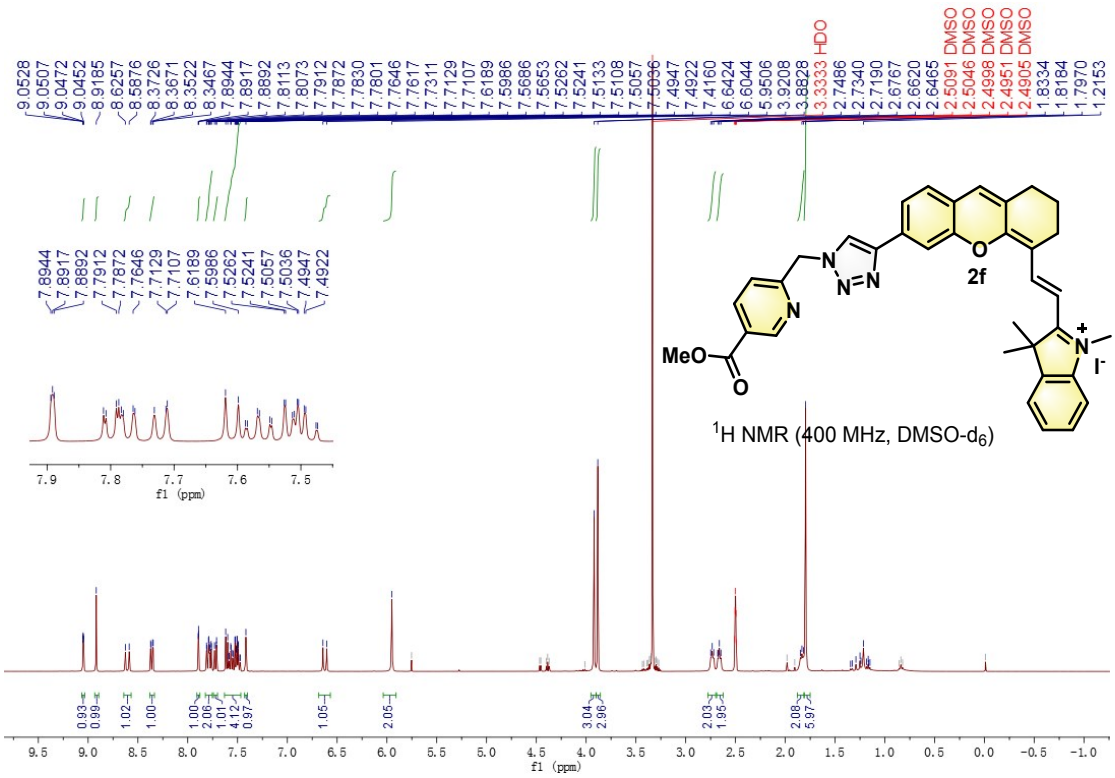

2c
Cl
I-
13C NMR (101 MHz, DMSO-d6)
f1 (ppm)

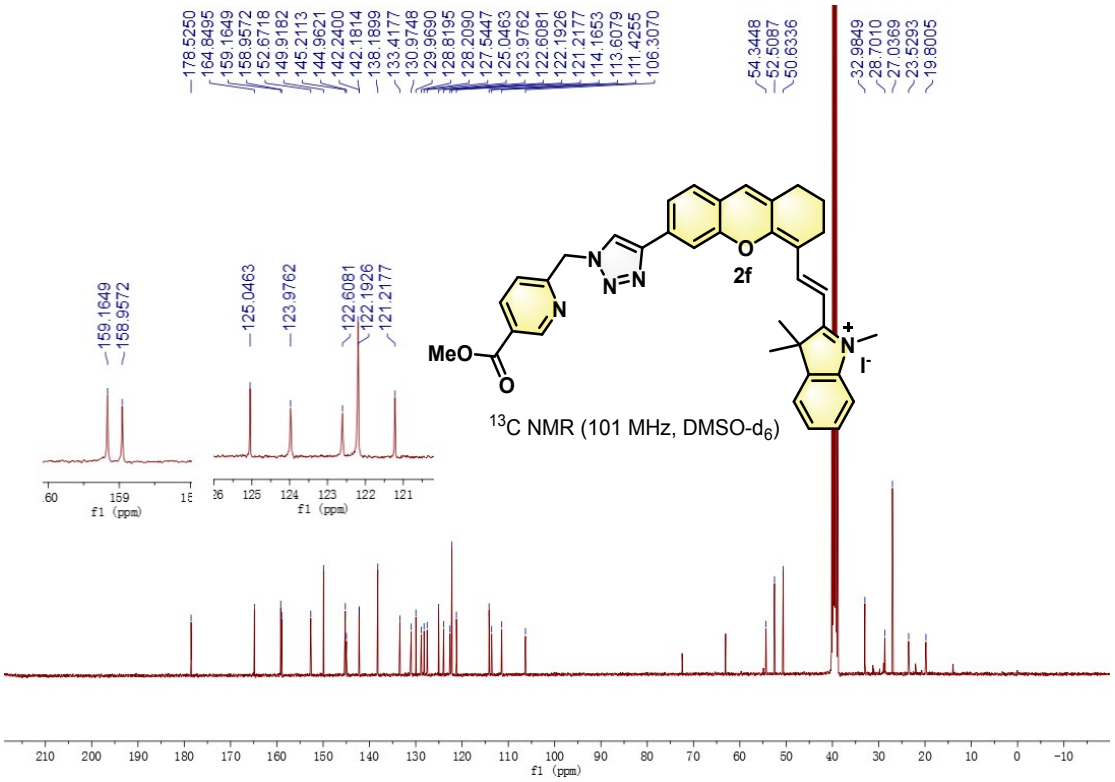

2d
MeO
^{1}H NMR (400 MHz, DMSO-d$_6$)

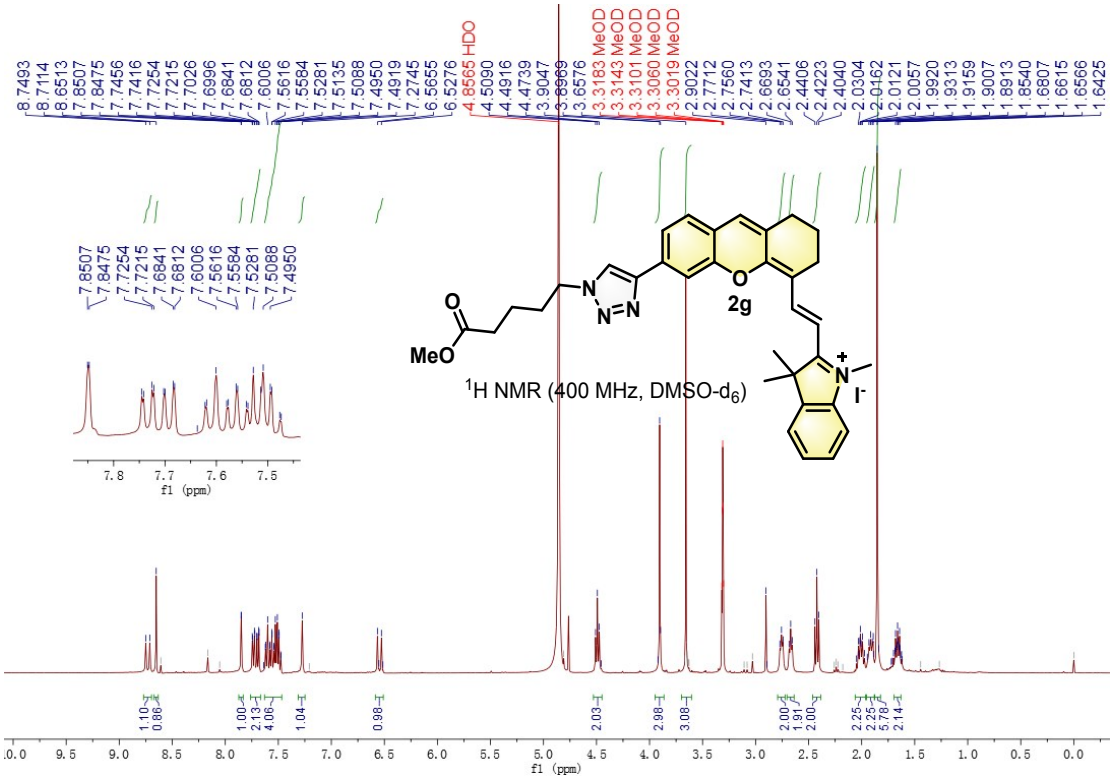

2d
MeO
^{13}C NMR (101 MHz, DMSO-d$_6$)

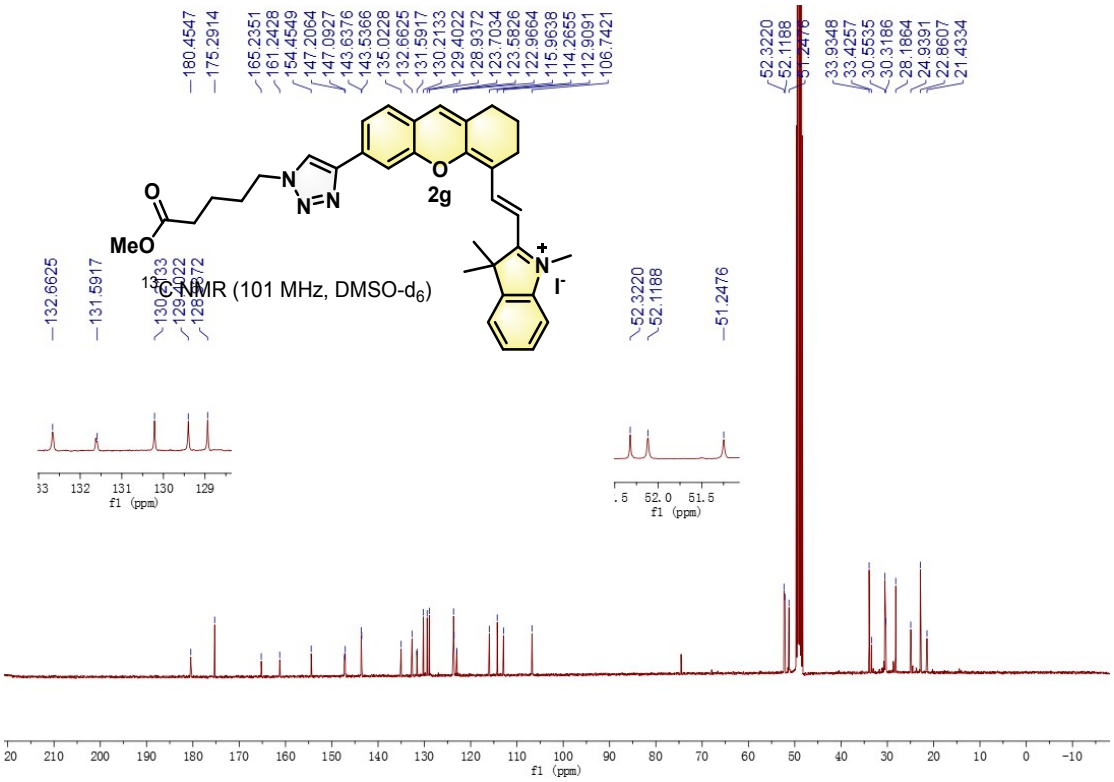

2e
^{1}H NMR (400 MHz, DMSO-d$_6$)

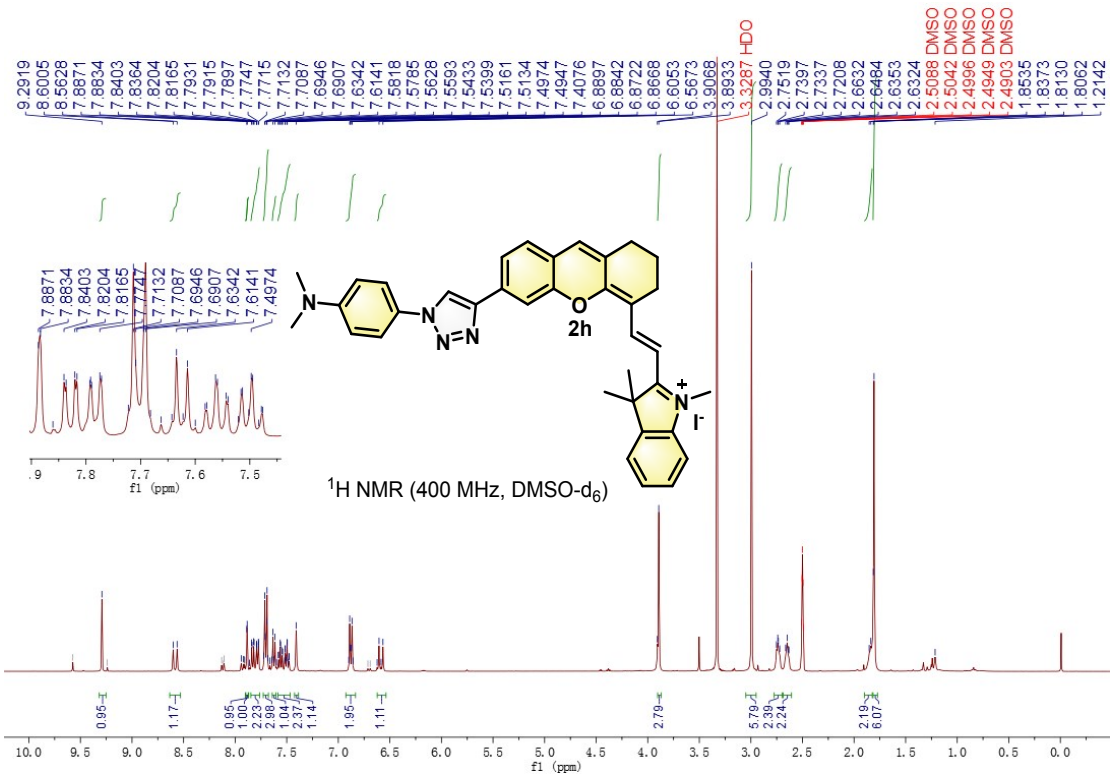

2e
^{13}C NMR (101 MHz, DMSO-d$_6$)

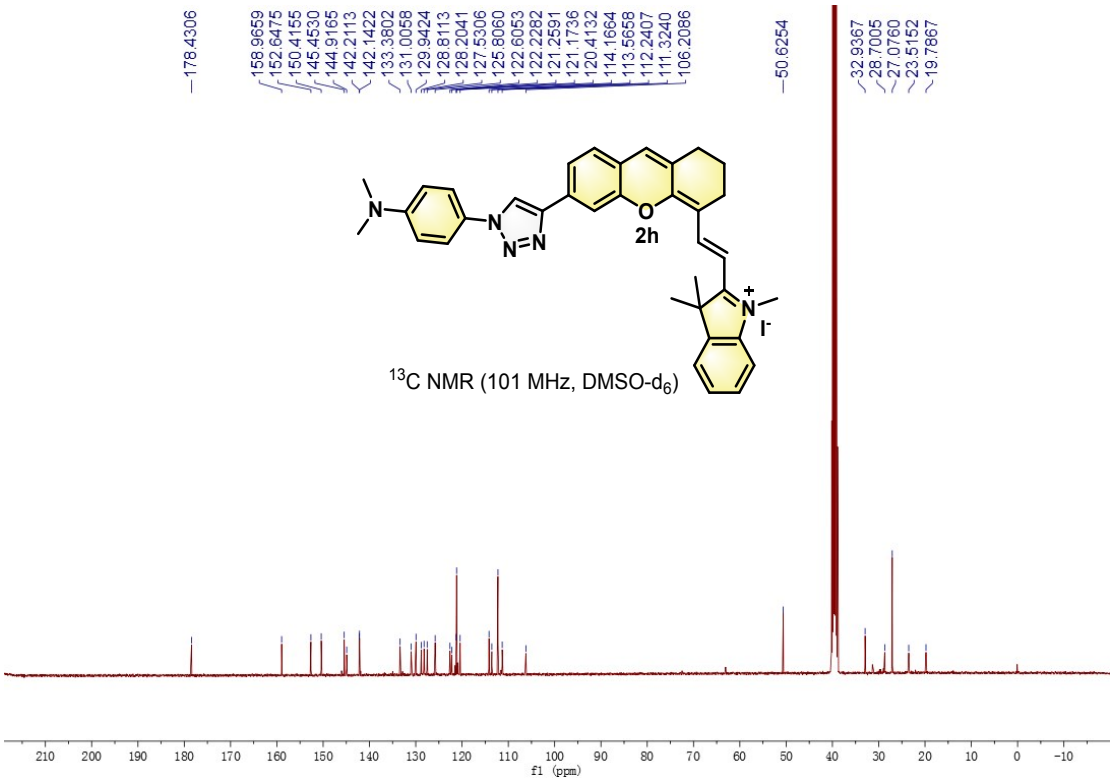

2f
MeO
O
N
N=N
O
N
I-
^{1}H NMR (400 MHz, DMSO-d$_6$)
f1 (ppm)

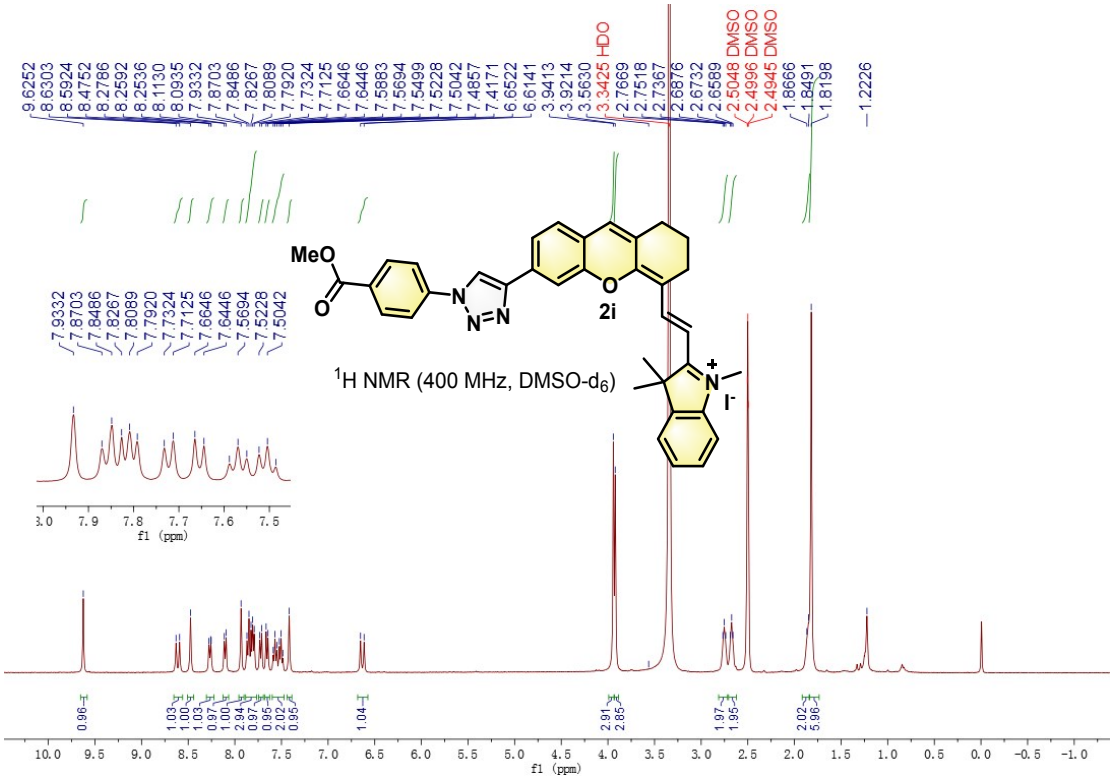

2f
MeO
O
N
N=N
O
N
I-
^{13}C NMR (101 MHz, DMSO-d$_6$)
f1 (ppm)

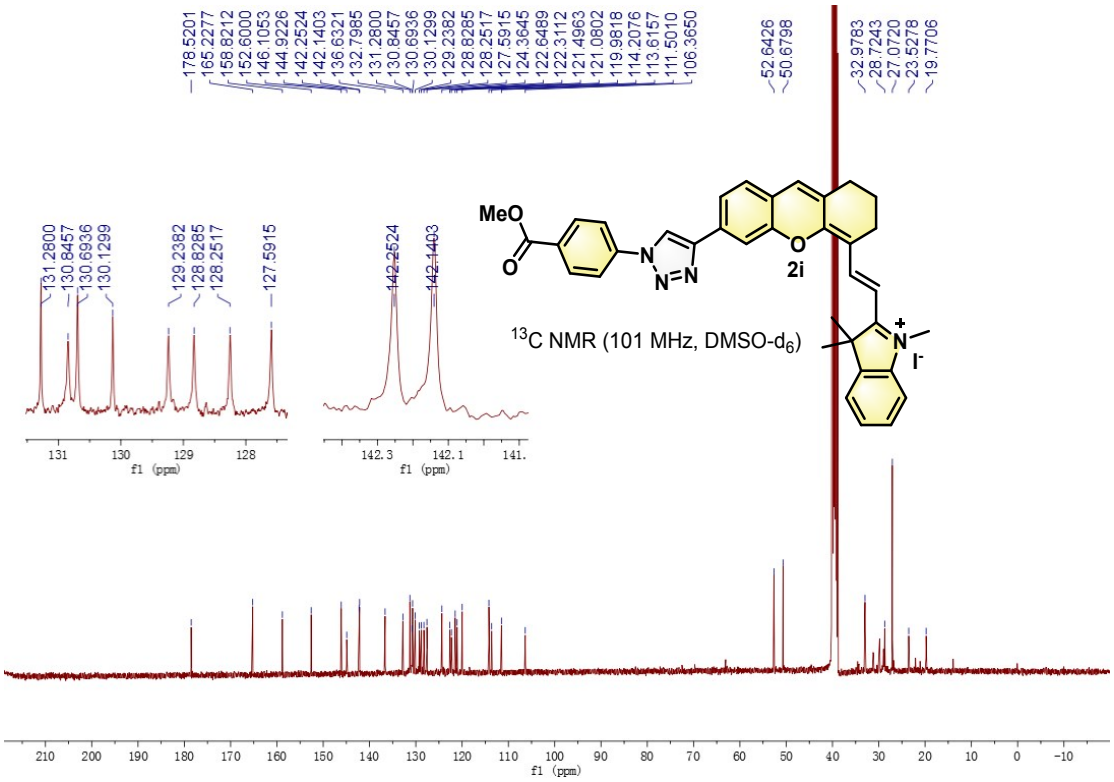

2g
MeO
I-
1H NMR (400 MHz, DMSO-d6)
f1 (ppm)

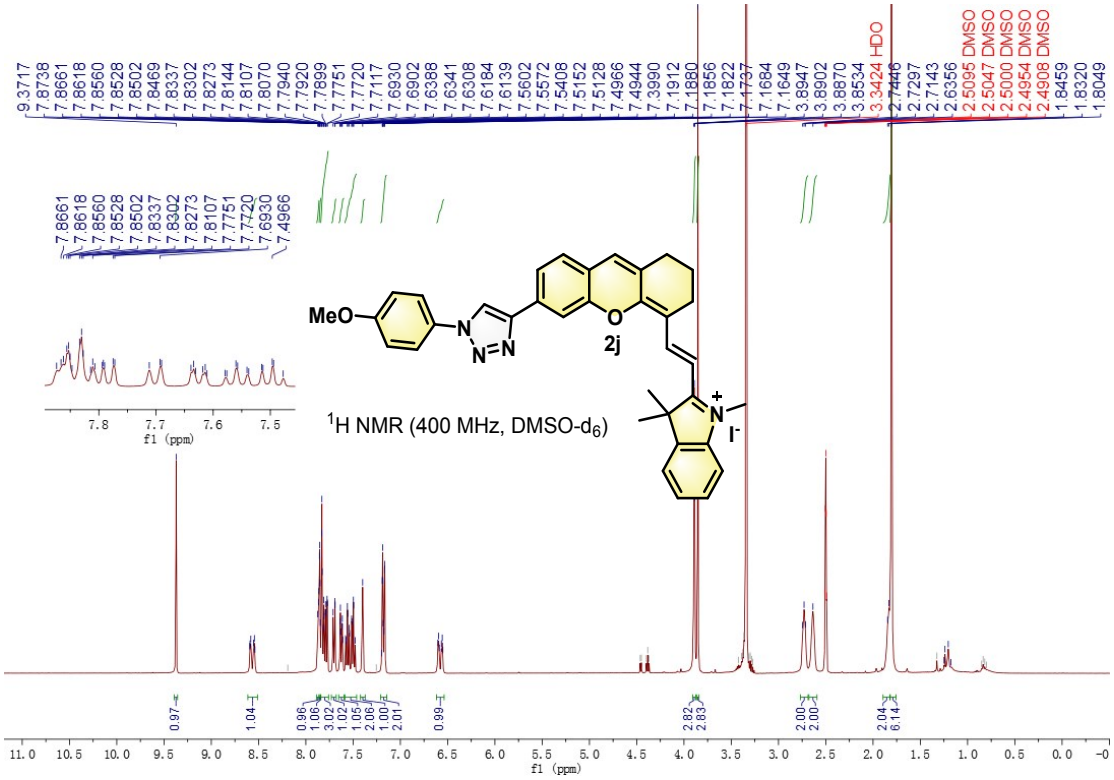

2g
MeO
I-
13C NMR (101 MHz, DMSO-d6)
f1 (ppm)

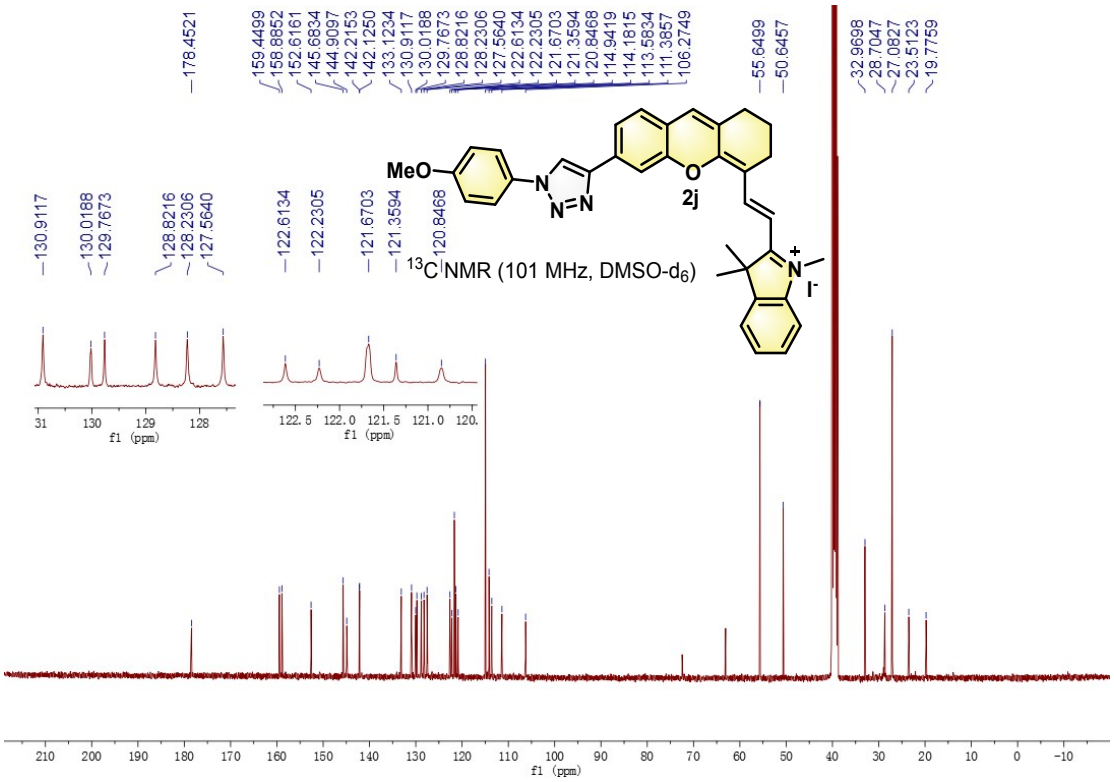

2h
^{1}H NMR (400 MHz, DMSO-d$_6$)

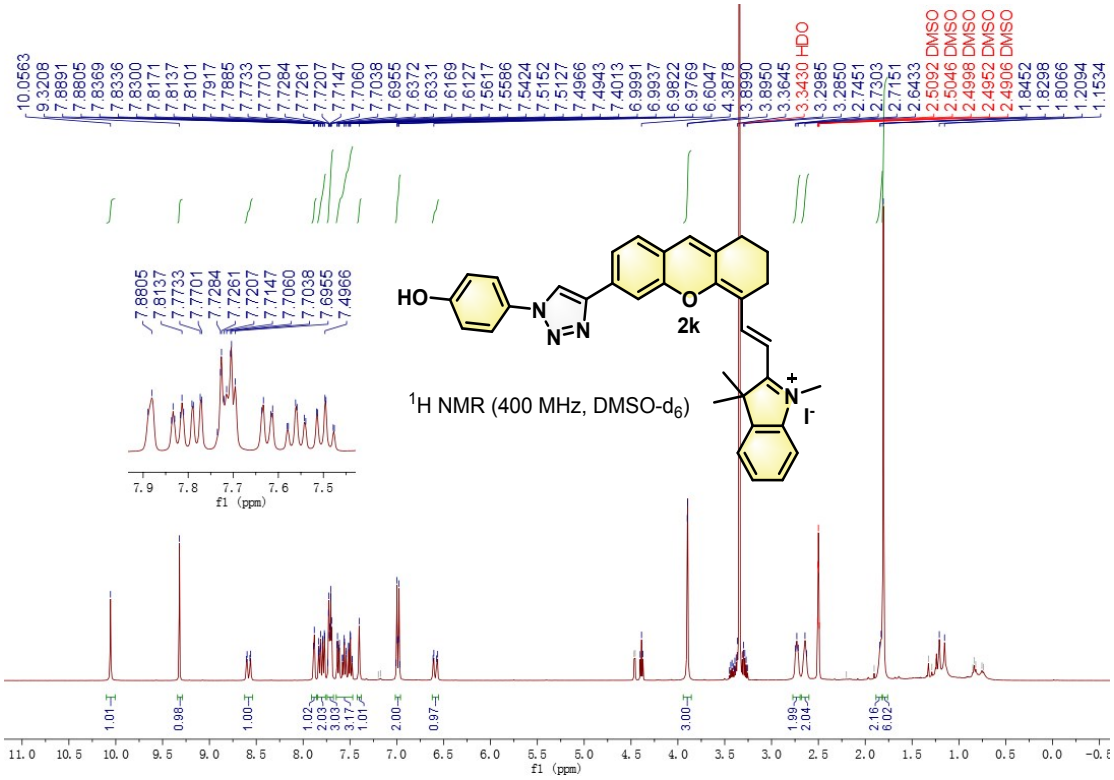

2h
^{13}C NMR (101 MHz, DMSO-d$_6$)

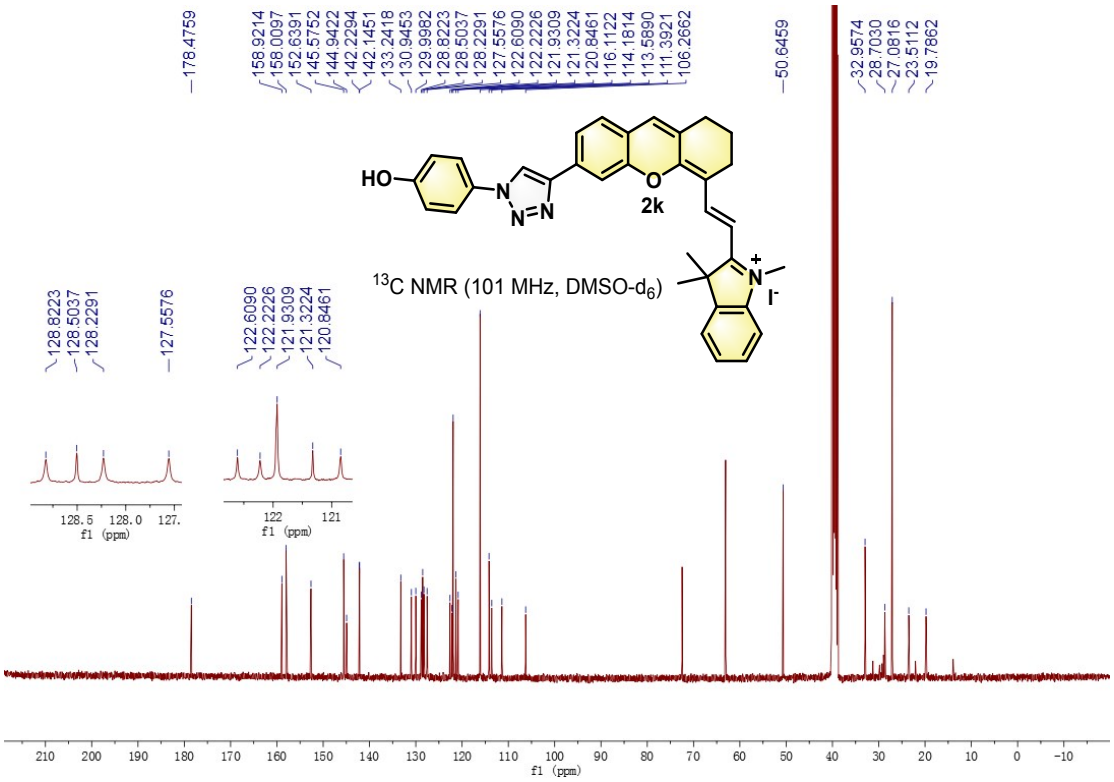

MeO
O
N
N=N
O
2i
I-
1H NMR (400 MHz, DMSO-d6)
f1 (ppm)

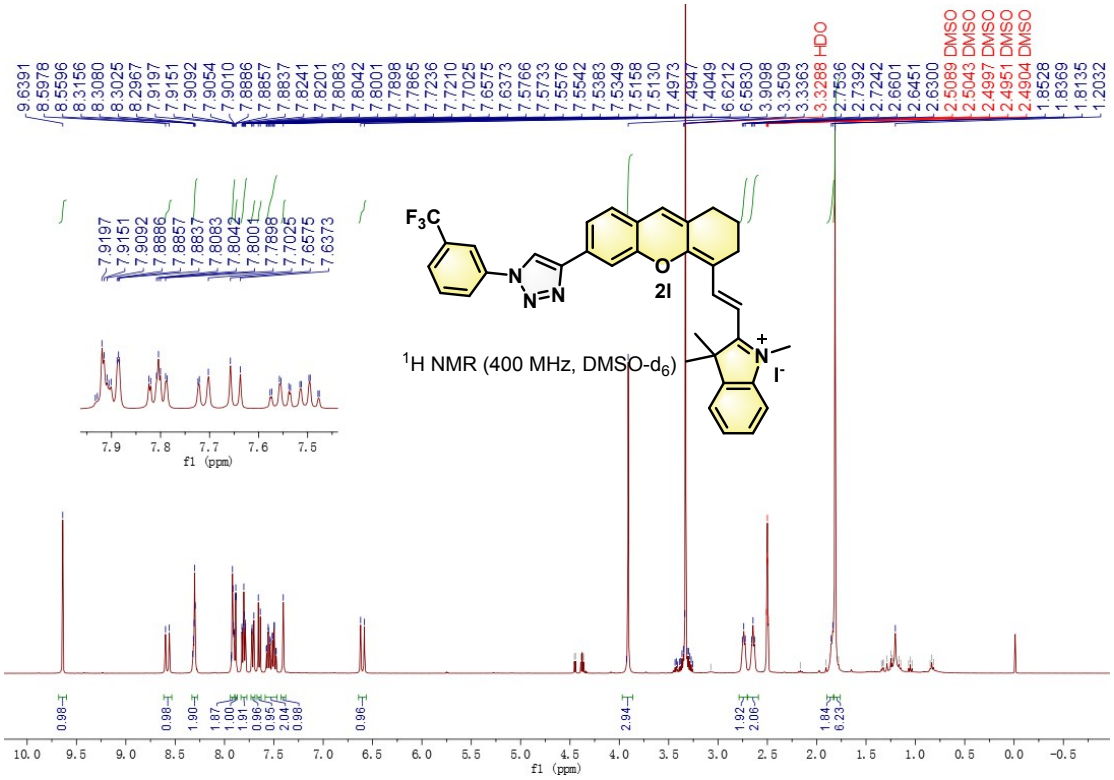

MeO
O
N
N=N
O
2i
I-
13C NMR (101 MHz, DMSO-d6)
f1 (ppm)

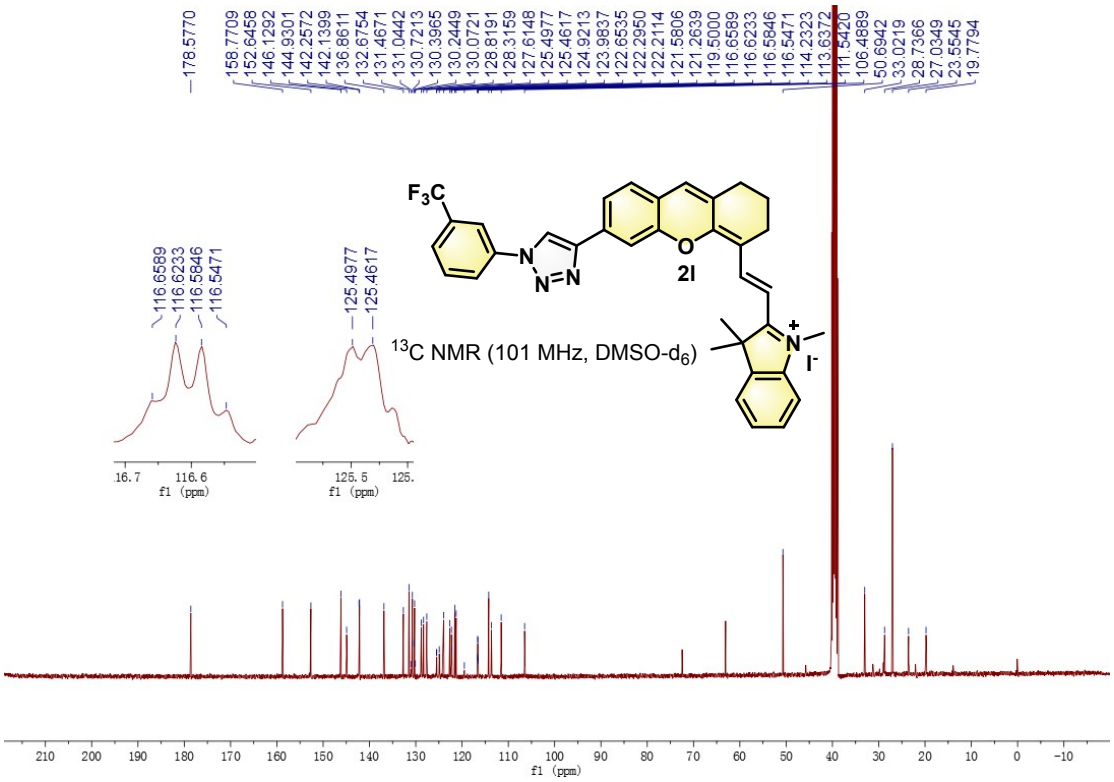

MeO
2j
^{1}H NMR (400 MHz, DMSO-d$_6$)

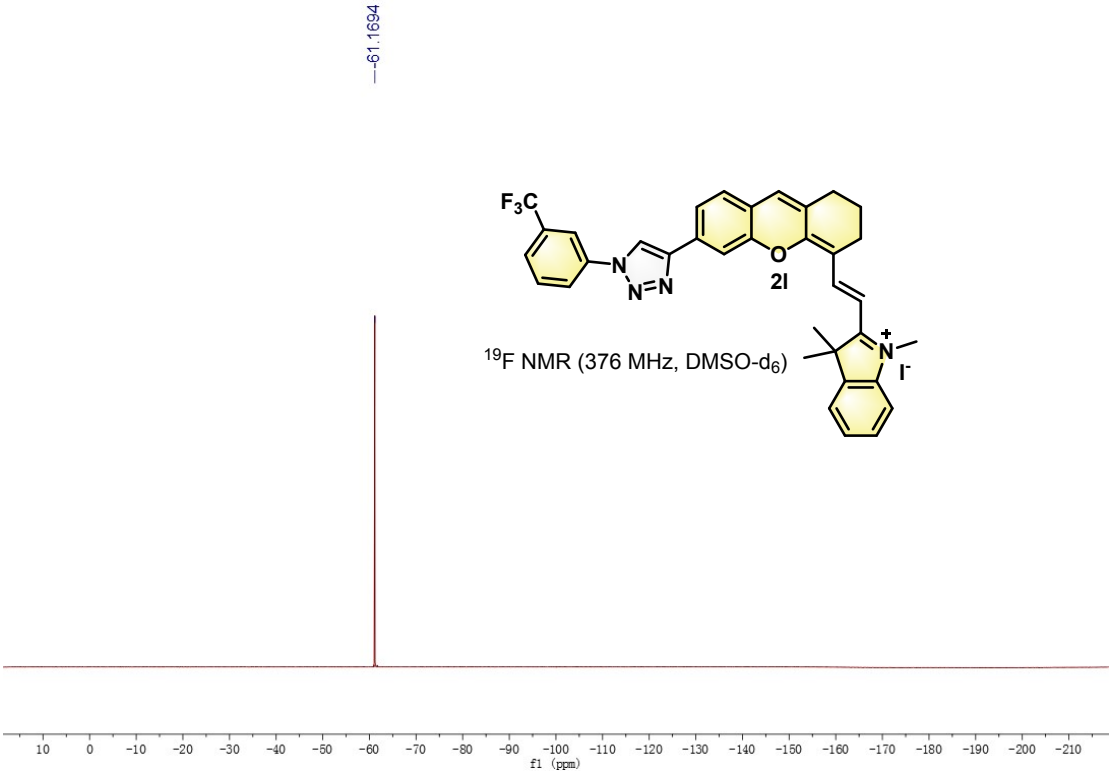

MeO
2j
^{13}C NMR (101 MHz, DMSO-d$_6$)

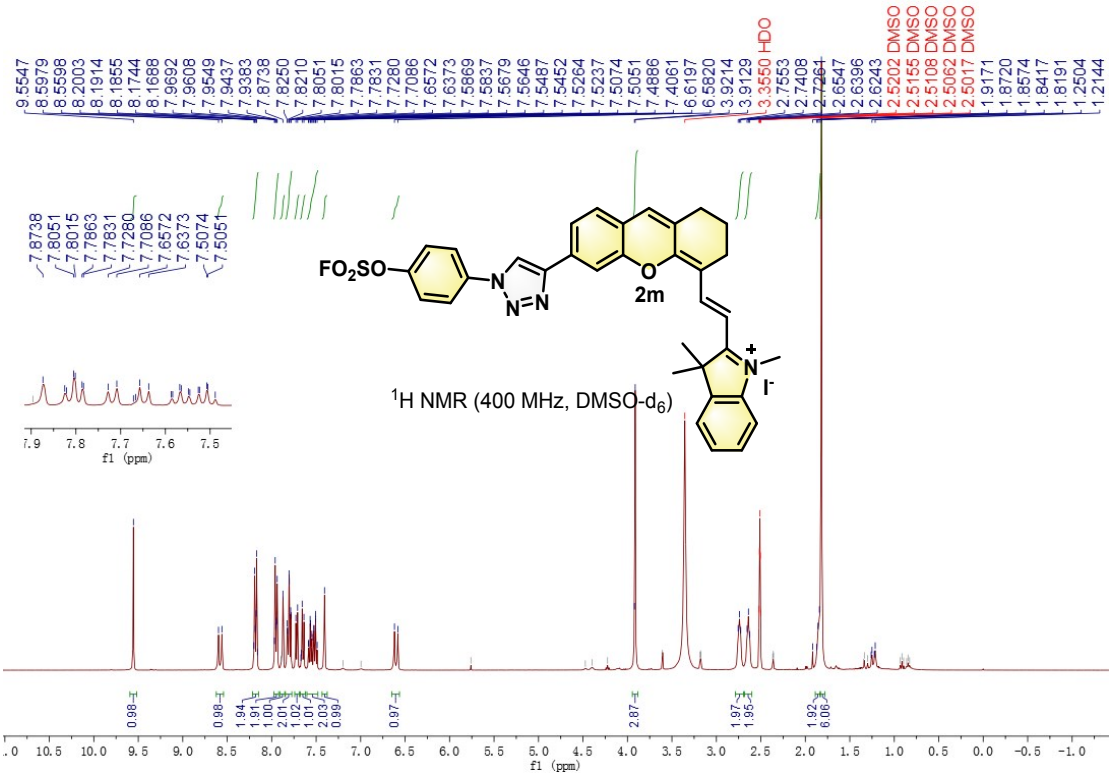

HO
N
N=N
O
2k
I-
1H NMR (400 MHz, DMSO-d6)
f1 (ppm)

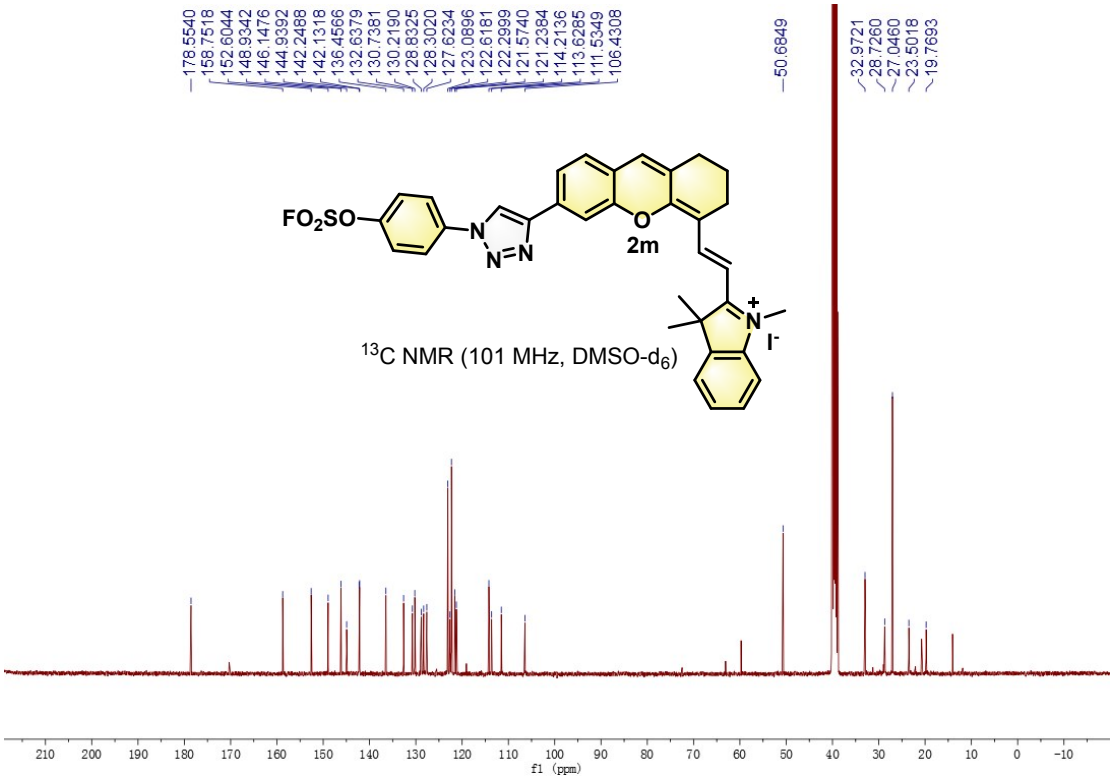

HO
N
N=N
O
2k
I-
13C NMR (101 MHz, DMSO-d6)
f1 (ppm)

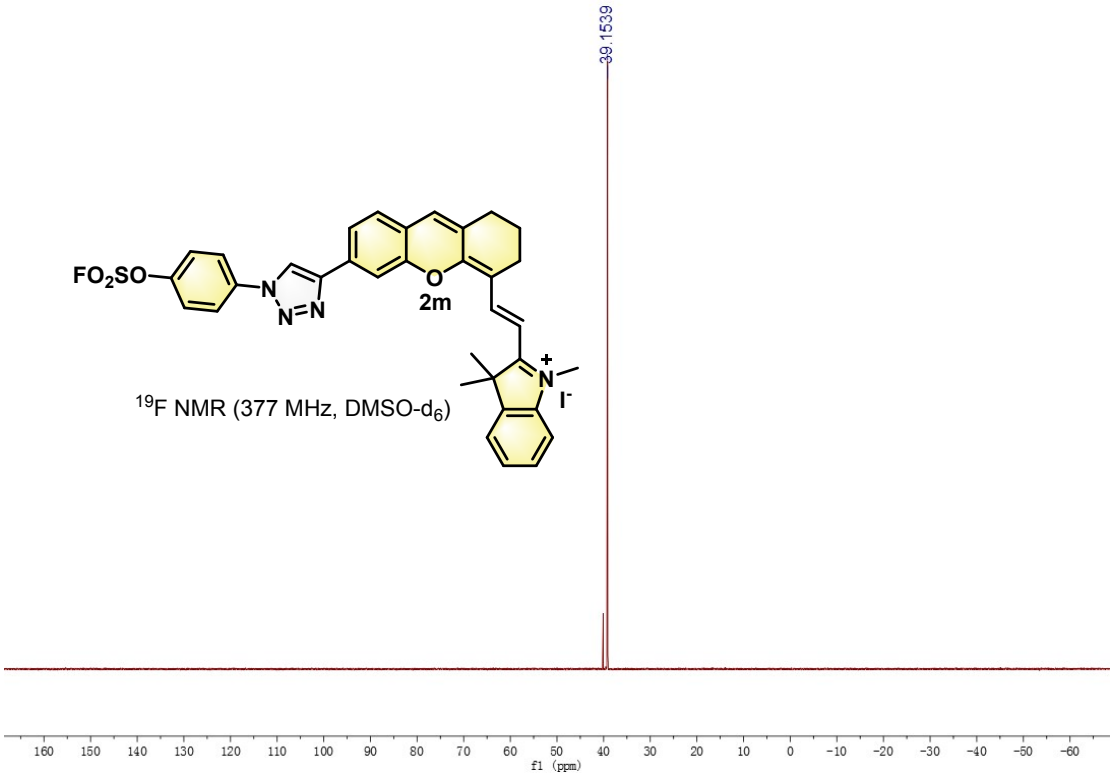

2I
^{1}H NMR (400 MHz, DMSO-d$_6$)
f1 (ppm)

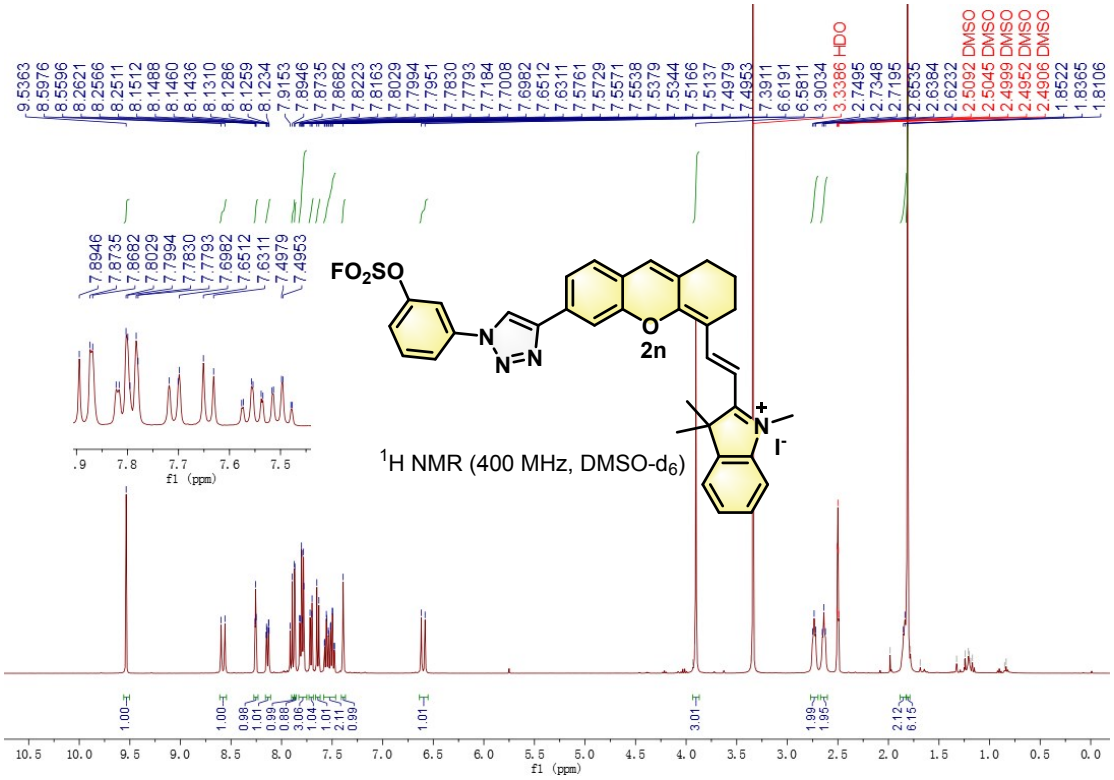

2I
^{13}C NMR (101 MHz, DMSO-d$_6$)
f1 (ppm)

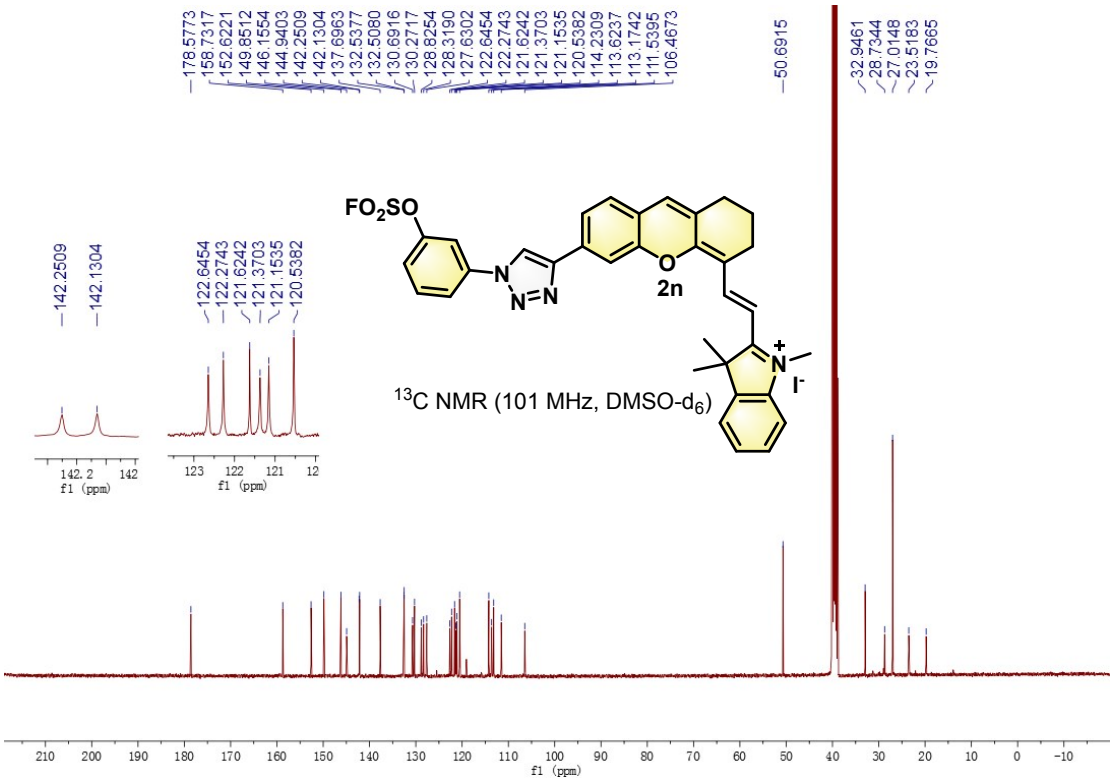

-61.1694
F3C
N
N=N
O
2l
N+
I-
19F NMR (376 MHz, DMSO-d6)
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

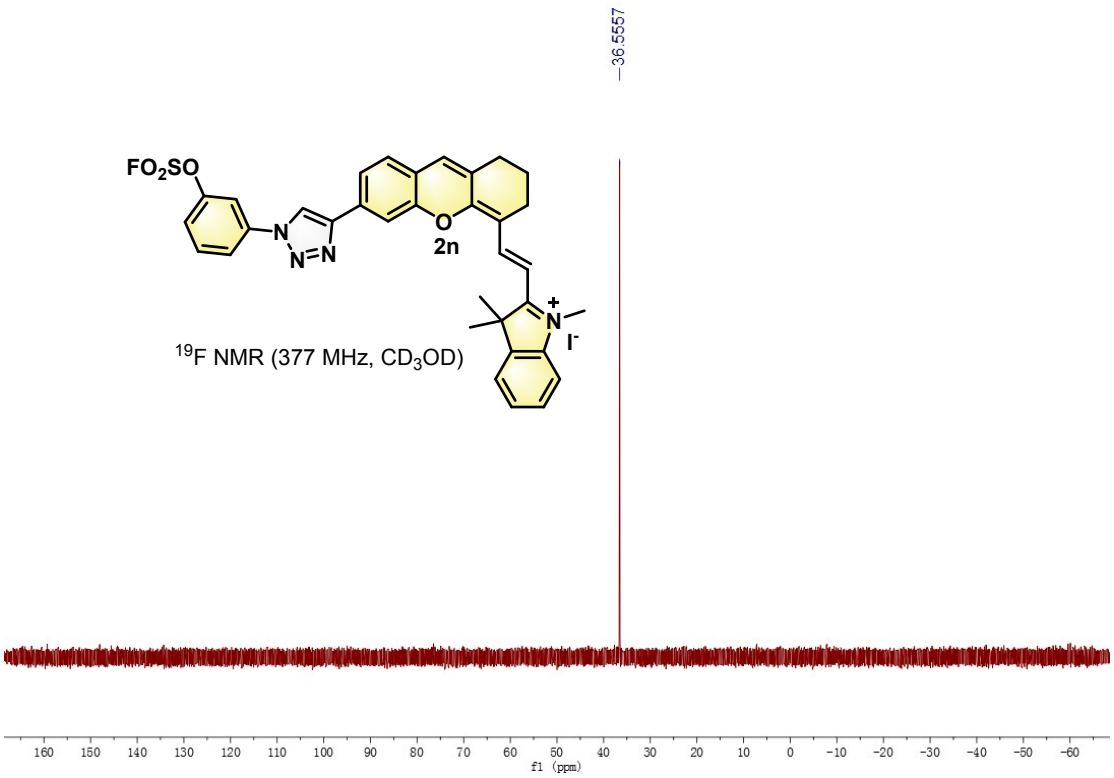

9.5547 8.5979 8.5598 8.2003 8.1914 8.1855 8.1744 8.1688 7.9692 7.9608 7.9549 7.9437 7.9383 7.8738 7.8250 7.8210 7.8051 7.8015 7.7863 7.7831 7.7280 7.7086 7.6572 7.6373 7.5869 7.5837 7.5679 7.5646 7.5487 7.5452 7.5264 7.5237 7.5074 7.5051 7.4886 7.4061 6.6197 6.5820 3.9214 3.9129 3.3550 HDO 2.7553 2.7408 2.7261 2.6547 2.6396 2.6243 2.5202 DMSO 2.5155 DMSO 2.5108 DMSO 2.5062 DMSO 2.5017 DMSO 1.9171 1.8720 1.8574 1.8417 1.8191 1.2504 1.2144
7.8738 7.8051 7.8015 7.7863 7.7831 7.7280 7.7086 7.6572 7.6373 7.5074 7.5051
FO2SO
N
N=N
O
2m
N+
I-
1H NMR (400 MHz, DMSO-d6)
0.98 0.98 1.94 1.91 1.00 2.01 1.02 1.01 2.03 0.99 0.97 2.87 1.97 1.95 1.92 6.06
f1 (ppm)

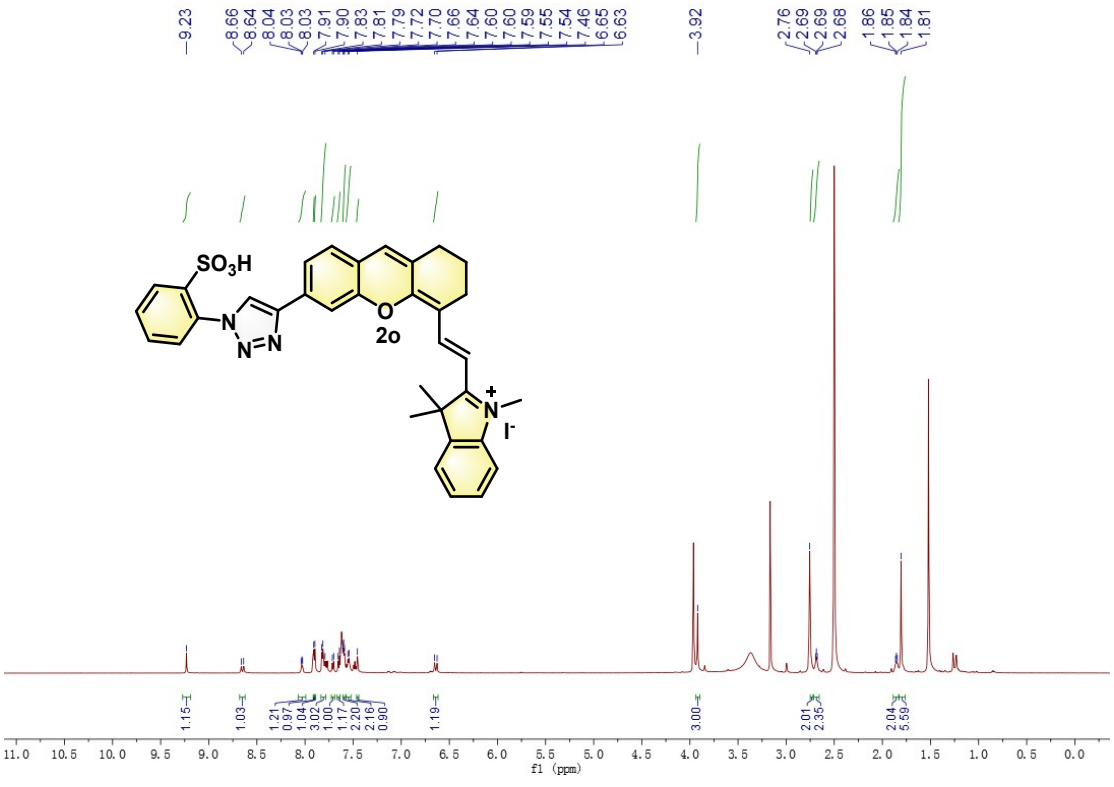

178.5540
158.7518
152.6044
148.9342
146.1476
144.9392
142.2488
142.1318
136.4566
132.6379
130.7381
130.2190
128.8325
128.3020
127.6234
123.0896
122.6181
122.2999
121.5740
121.2384
114.2136
113.6285
111.5349
106.4308
50.6849
32.9721
28.7260
27.0460
23.5018
19.7693
FO2SO
N
N=N
O
2m
N+
I-
13C NMR (101 MHz, DMSO-d6)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

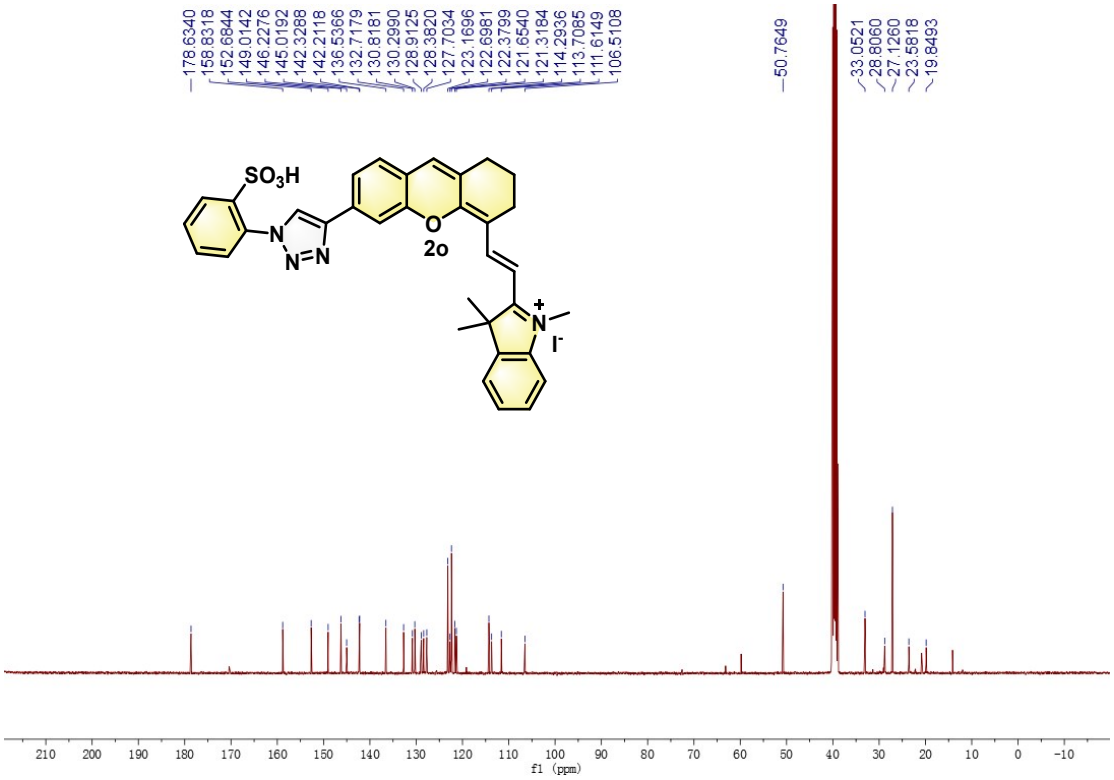

39.1539
FO2SO
N
N=N
O
2m
N+
I-
19F NMR (377 MHz, DMSO-d6)
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60
f1 (ppm)


FO2SO
2n
1H NMR (400 MHz, DMSO-d6)


FO2SO
2n
13C NMR (101 MHz, DMSO-d6)


-36.5557
FO2SO
N
N=N
O
2n
N+
I-
19F NMR (377 MHz, CD3OD)
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60
f1 (ppm)

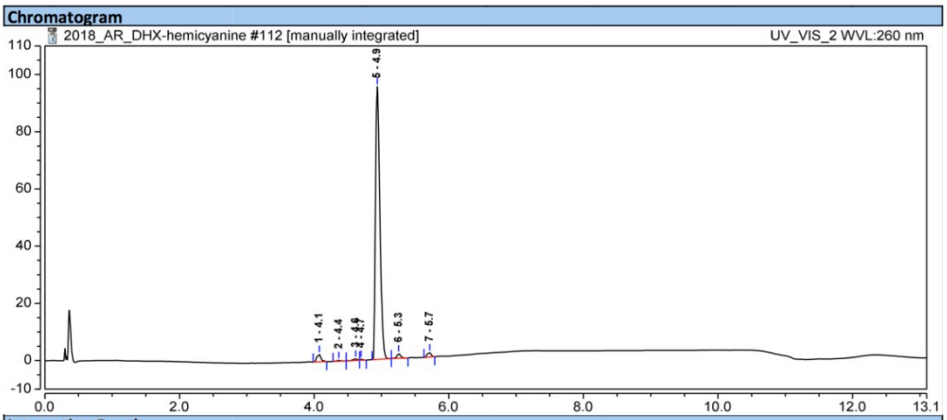

9.23
8.66
8.64
8.04
8.03
8.03
7.91
7.90
7.83
7.81
7.79
7.72
7.70
7.66
7.64
7.60
7.60
7.59
7.55
7.54
7.46
6.65
6.63
3.92
2.76
2.69
2.69
2.68
1.86
1.85
1.84
1.81
SO3H
N
N=N
O
2o
N+
I-
1.15
1.03
1.21
0.97
1.04
3.02
1.00
1.17
2.20
2.16
0.90
1.19
3.00
2.01
2.35
2.04
5.59
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 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)



6. RP-HPLC analyses of triazole-based DHX-hemicyanine fused dyes

<u>Please note:</u> RP-HPLC analyses were performed before re-numbering that we decided to do during the drafting of manuscript. That explains why the injection name "Trz-DHX-2x-QC" displayed on each e-copy of RP-HPLC elution profile is different from the molecule ID "2x" used in manuscript.

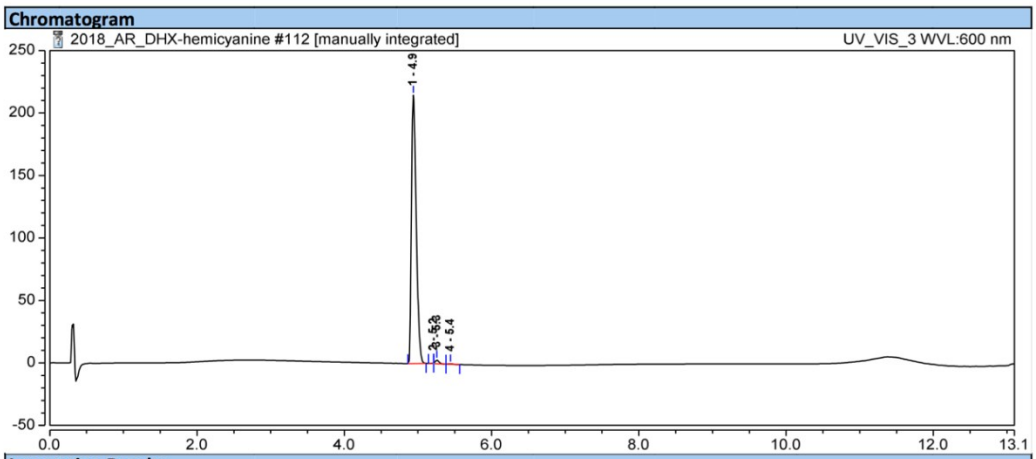
*RP-HPLC elution profile of alkynyl-based DHX-hemicyanine fused dye **1** (system A, 260 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.1	0.186	2.624	2.42	2.57	n.a.
2		4.4	0.017	0.282	0.22	0.28	n.a.
3		4.6	0.042	0.546	0.55	0.53	n.a.
4		4.7	0.015	0.328	0.20	0.32	n.a.
5		4.9	7.240	95.334	93.95	93.26	n.a.
6		5.3	0.098	1.595	1.27	1.56	n.a.
7		5.7	0.108	1.518	1.40	1.48	n.a.
Total:			**7.707**	**102.227**	**100.00**	**100.00**	

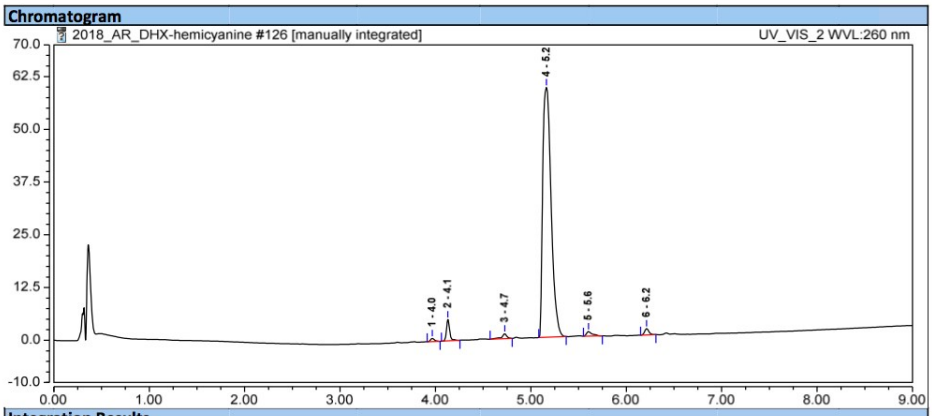
*RP-HPLC elution profile of of alkynyl-based DHX-hemicyanine fused dye **1** (system A, 600 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.9	16.251	214.697	98.69	98.25	n.a.
2		5.2	0.014	0.397	0.08	0.18	n.a.
3		5.3	0.176	3.045	1.07	1.39	n.a.
4		5.4	0.026	0.384	0.16	0.18	n.a.
Total:			**16.467**	**218.524**	**100.00**	**100.00**	

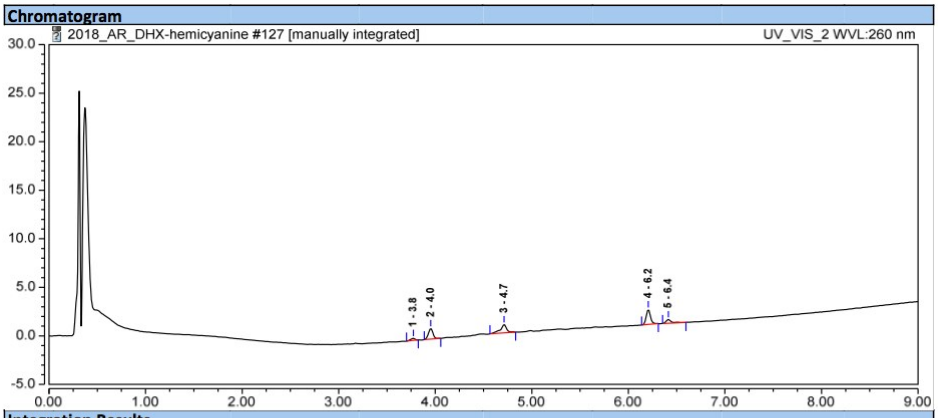
*RP-HPLC elution profile of alkynyl-based DHX-hemicyanine fused dye **1** (system B, 260 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.0	0.037	0.788	0.57	1.15	n.a.
2		4.1	0.194	5.063	3.02	7.36	n.a.
3		4.7	0.072	1.163	1.12	1.69	n.a.
4		5.2	5.978	59.173	92.96	86.03	n.a.
5		5.6	0.074	1.067	1.15	1.55	n.a.
6		6.2	0.076	1.526	1.18	2.22	n.a.
Total:			**6.431**	**68.780**	**100.00**	**100.00**	

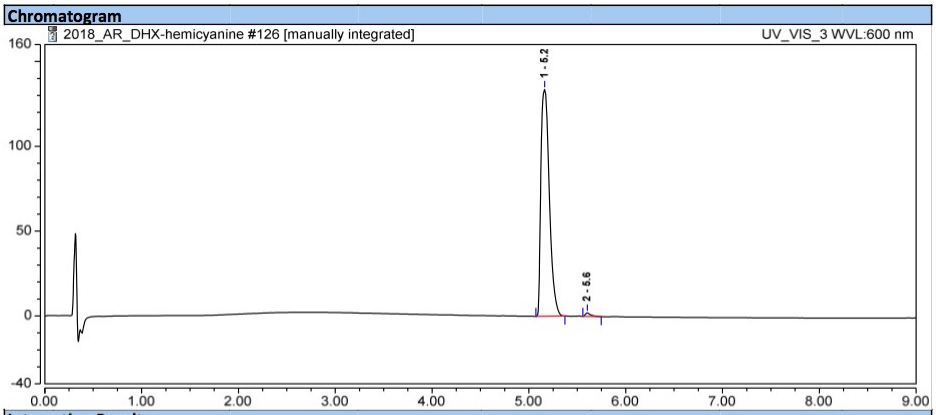
RP-HPLC elution profile of a blank sample (system B, 260 nm)



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		3.8	0.011	0.210	4.69	5.14	n.a.
2		4.0	0.061	1.101	25.41	26.92	n.a.
3		4.7	0.065	0.860	26.92	21.04	n.a.
4		6.2	0.079	1.537	32.73	37.59	n.a.
5		6.4	0.025	0.381	10.25	9.32	n.a.
Total:			**0.240**	**4.089**	**100.00**	**100.00**	

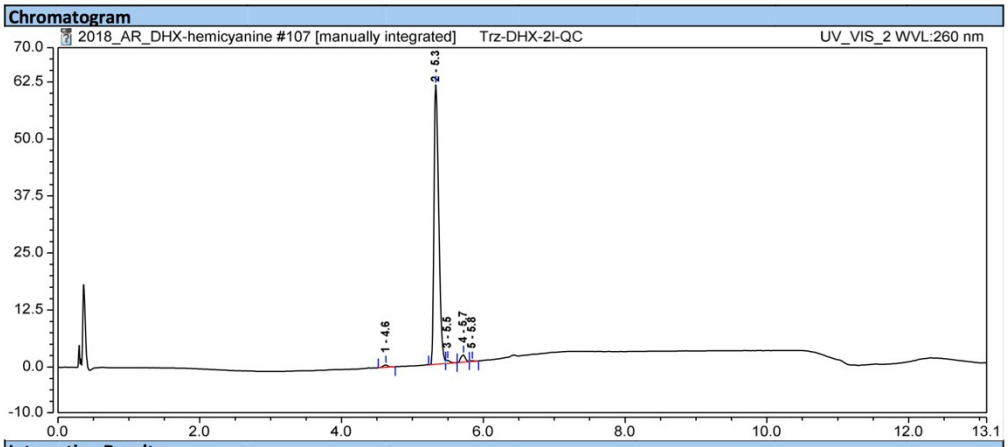
*RP-HPLC elution profile of alkynyl-based DHX-hemicyanine fused dye **1** (system B, 600 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.2	13.463	133.588	99.03	98.47	n.a.
2		5.6	0.132	2.082	0.97	1.53	n.a.
Total:			**13.595**	**135.670**	**100.00**	**100.00**	

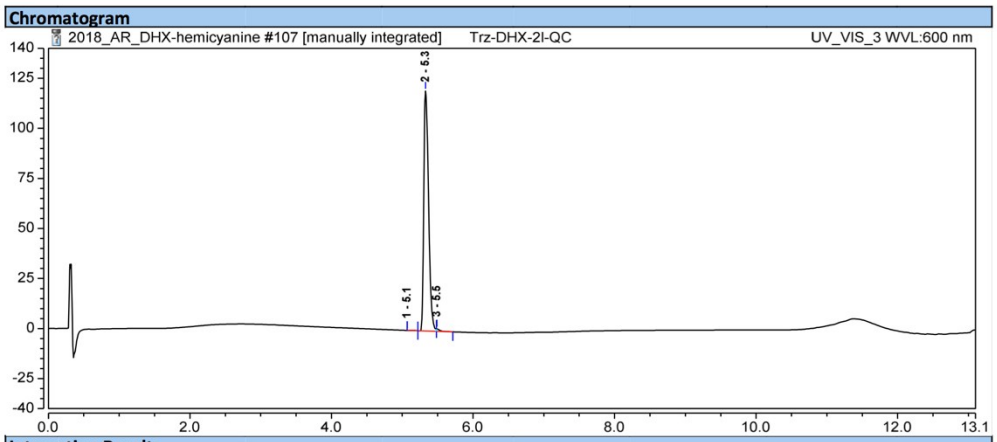
*RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye **2a** (260 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.6	0.040	0.511	0.81	0.80	n.a.
2		5.3	4.750	61.201	95.57	95.35	n.a.
3		5.5	0.044	0.676	0.89	1.05	n.a.
4		5.7	0.122	1.622	2.46	2.53	n.a.
5		5.8	0.013	0.177	0.26	0.28	n.a.
Total:			**4.970**	**64.187**	**100.00**	**100.00**	

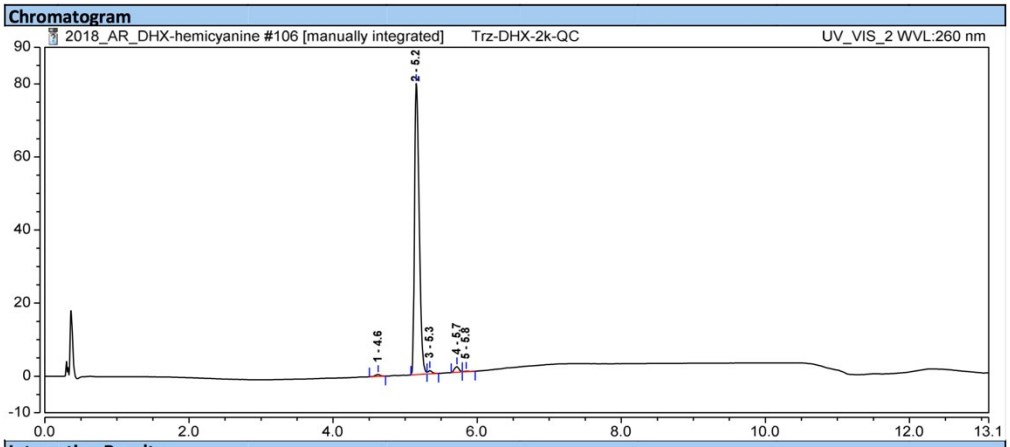
RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2a*** *(600 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.1	0.004	0.000	0.05	0.00	n.a.
2		5.3	9.310	119.905	99.22	99.00	n.a.
3		5.5	0.069	1.213	0.74	1.00	n.a.
Total:			**9.383**	**121.118**	**100.00**	**100.00**	

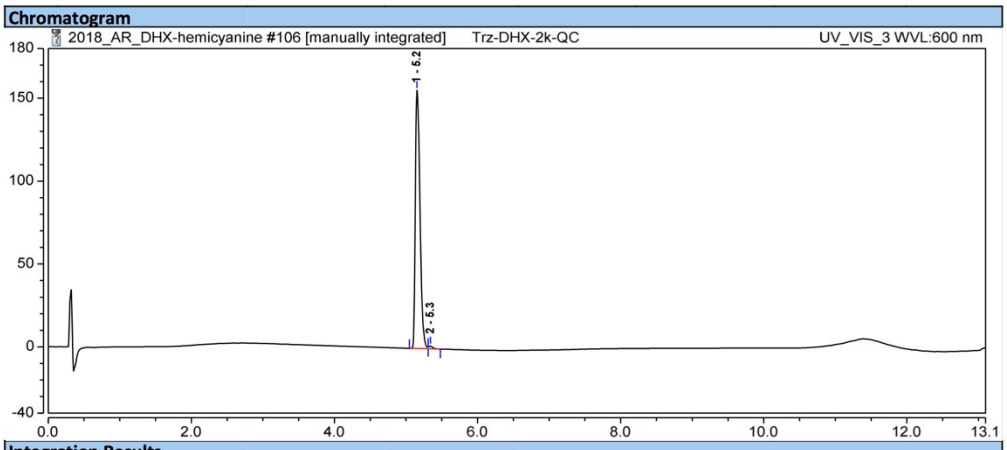
RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2b*** *(260 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.6	0.042	0.534	0.68	0.64	n.a.
2		5.2	5.978	79.692	96.29	96.14	n.a.
3		5.3	0.061	0.953	0.98	1.15	n.a.
4		5.7	0.114	1.561	1.84	1.88	n.a.
5		5.8	0.013	0.151	0.21	0.18	n.a.
Total:			**6.208**	**82.891**	**100.00**	**100.00**	

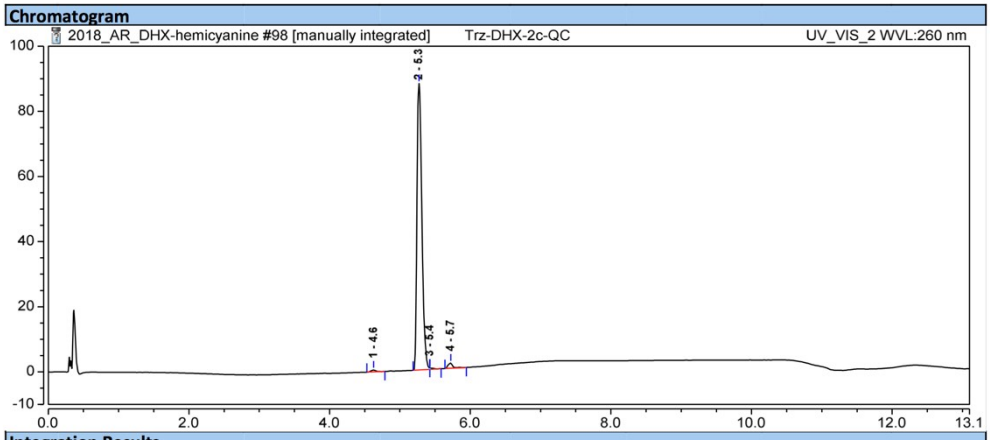
RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2b*** *(600 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.2	11.669	155.732	99.14	98.94	n.a.
2		5.3	0.101	1.665	0.86	1.06	n.a.
Total:			**11.770**	**157.397**	**100.00**	**100.00**	

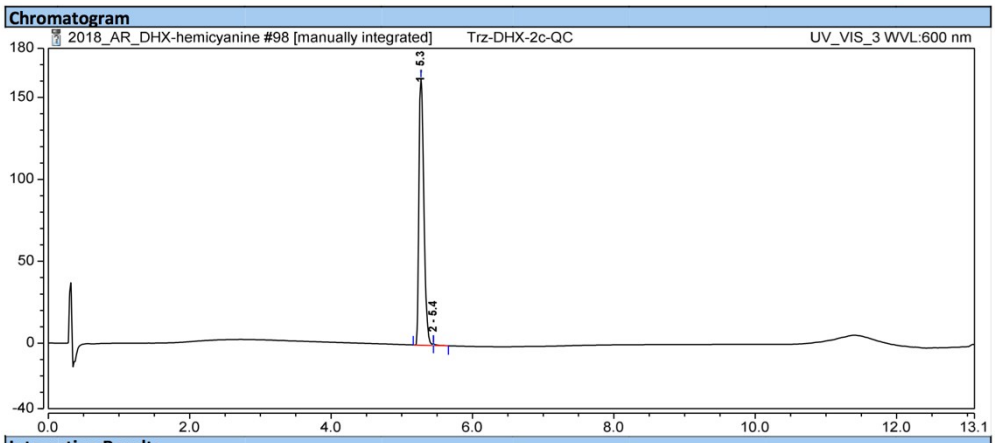
RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2c*** *(260 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.6	0.047	0.559	0.65	0.62	n.a.
2		5.3	7.078	88.001	97.35	97.24	n.a.
3		5.4	0.020	0.365	0.27	0.40	n.a.
4		5.7	0.126	1.577	1.73	1.74	n.a.
Total:			**7.270**	**90.502**	**100.00**	**100.00**	

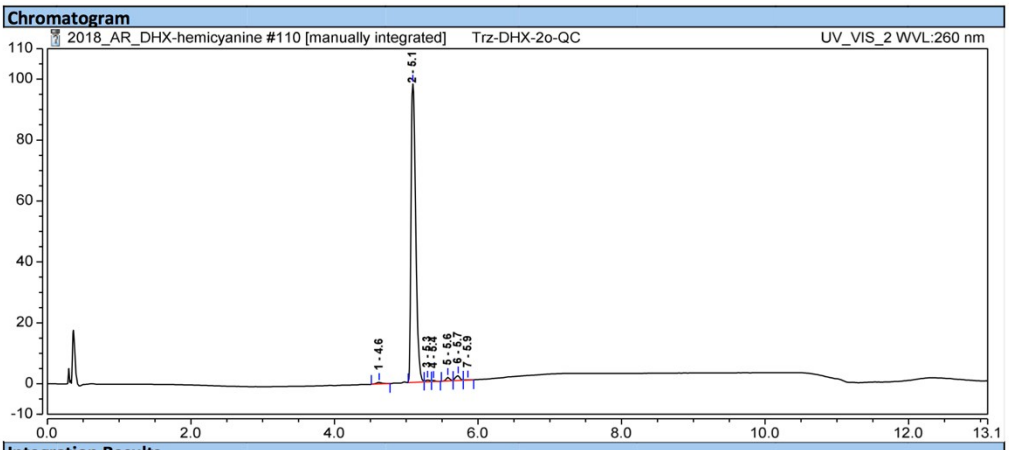
RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2c*** *(600 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.3	13.046	162.126	99.69	99.56	n.a.
2		5.4	0.041	0.715	0.31	0.44	n.a.
Total:			**13.087**	**162.841**	**100.00**	**100.00**	

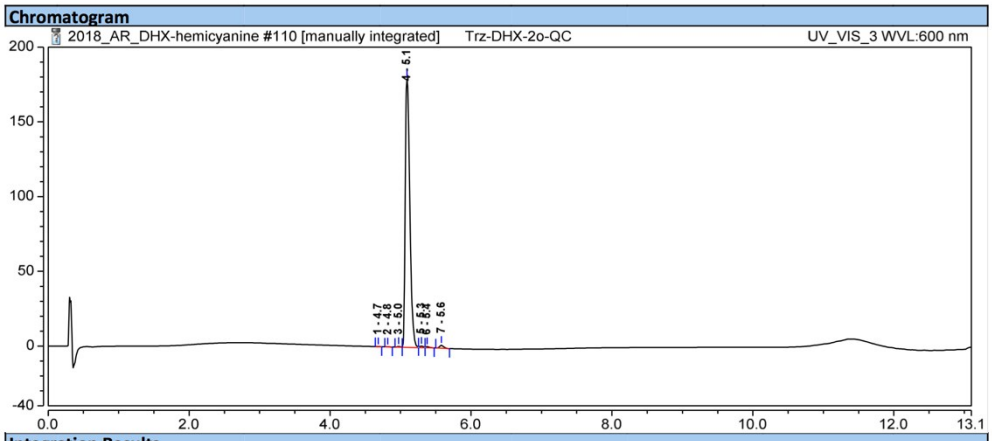
RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2d*** *(260 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.6	0.048	0.530	0.64	0.52	n.a.
2		5.1	7.298	97.948	95.96	95.69	n.a.
3		5.3	0.042	0.605	0.55	0.59	n.a.
4		5.4	0.021	0.391	0.28	0.38	n.a.
5		5.6	0.071	1.179	0.93	1.15	n.a.
6		5.7	0.115	1.601	1.51	1.56	n.a.
7		5.9	0.010	0.109	0.13	0.11	n.a.
Total:			**7.606**	**102.364**	**100.00**	**100.00**	

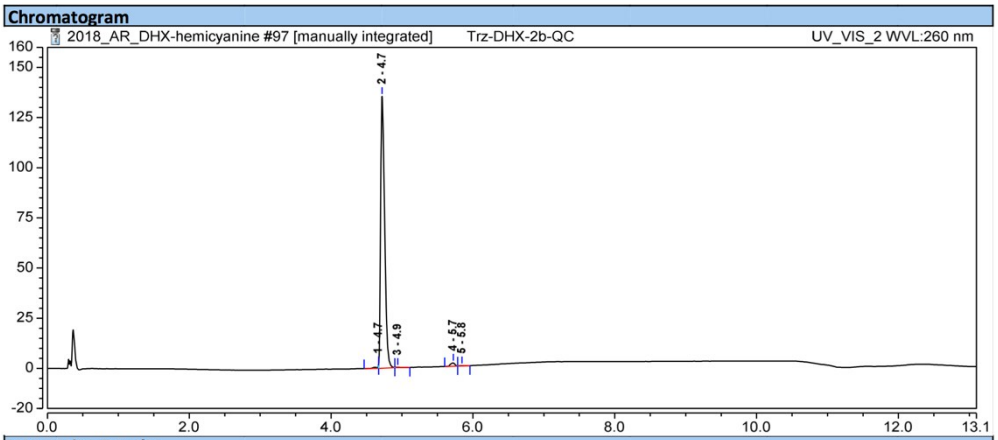
RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2d*** *(600 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.7	0.006	0.143	0.05	0.08	n.a.
2		4.8	0.007	0.161	0.05	0.09	n.a.
3		5.0	0.026	0.537	0.19	0.29	n.a.
4		5.1	13.371	179.452	97.86	97.37	n.a.
5		5.3	0.074	1.122	0.54	0.61	n.a.
6		5.4	0.049	0.803	0.36	0.44	n.a.
7		5.6	0.130	2.078	0.95	1.13	n.a.
Total:			**13.664**	**184.296**	**100.00**	**100.00**	

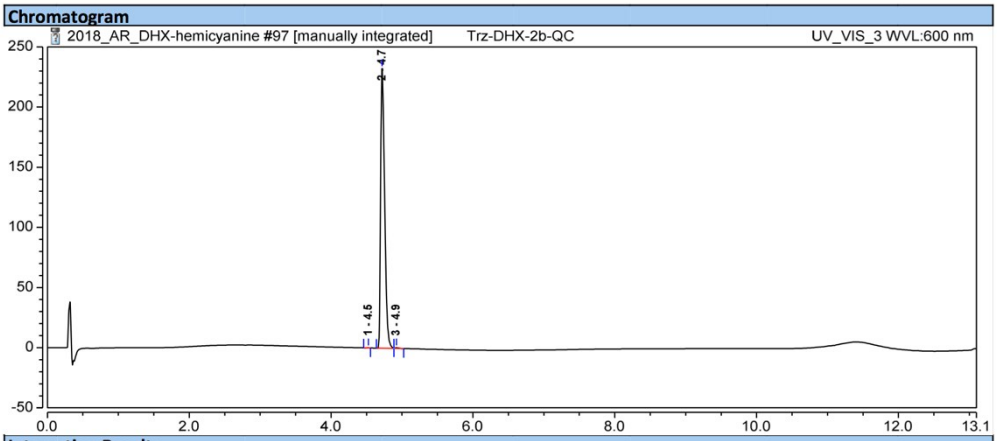
RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2e*** *(260 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.7	0.048	1.296	0.53	0.93	n.a.
2		4.7	8.922	135.487	97.83	97.61	n.a.
3		4.9	0.022	0.272	0.24	0.20	n.a.
4		5.7	0.115	1.617	1.26	1.16	n.a.
5		5.8	0.013	0.138	0.14	0.10	n.a.
Total:			**9.120**	**138.810**	**100.00**	**100.00**	

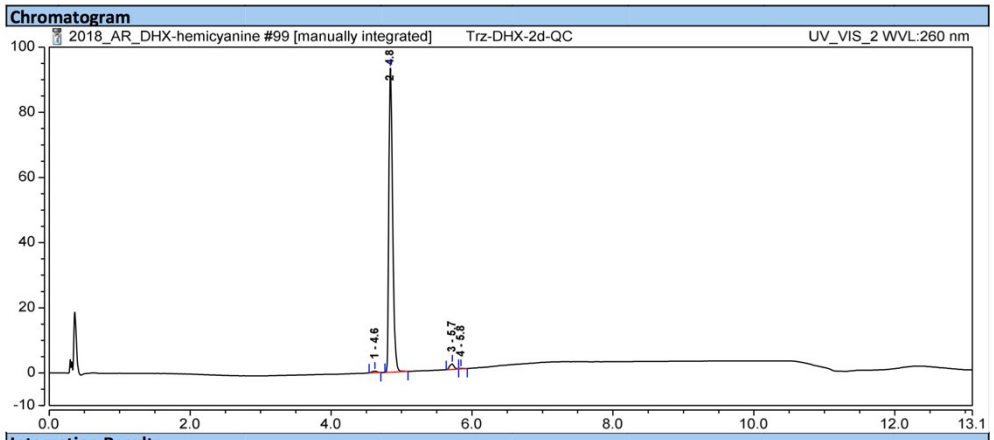
RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2e*** *(600 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.5	0.002	0.092	0.02	0.04	n.a.
2		4.7	15.284	232.469	99.70	99.71	n.a.
3		4.9	0.043	0.590	0.28	0.25	n.a.
Total:			**15.329**	**233.152**	**100.00**	**100.00**	

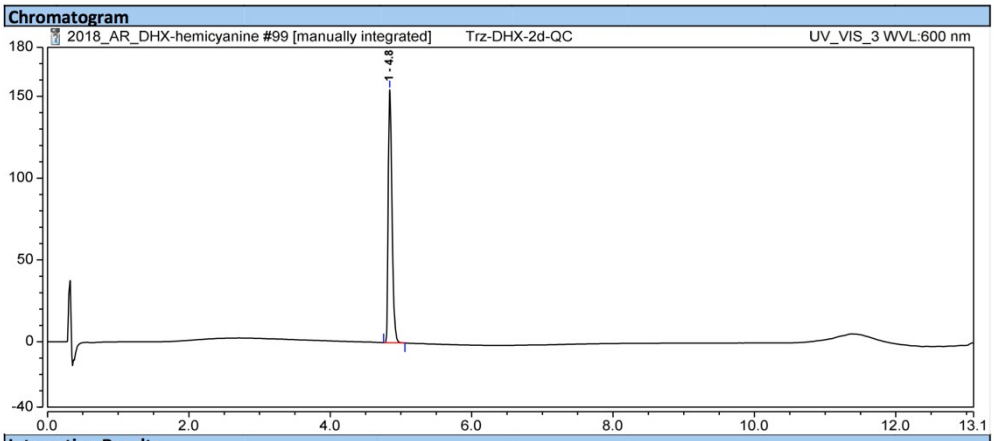
RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2f*** *(260 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.6	0.040	0.510	0.68	0.53	n.a.
2		4.8	5.728	93.313	97.04	97.56	n.a.
3		5.7	0.124	1.670	2.10	1.75	n.a.
4		5.8	0.010	0.150	0.17	0.16	n.a.
Total:			**5.903**	**95.643**	**100.00**	**100.00**	

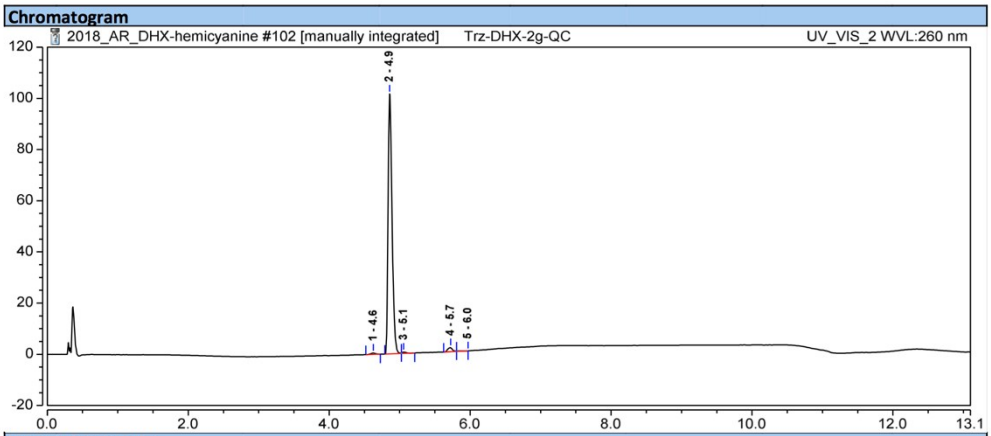
RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2f*** *(600 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.8	9.466	154.633	100.00	100.00	n.a.
Total:			**9.466**	**154.633**	**100.00**	**100.00**	

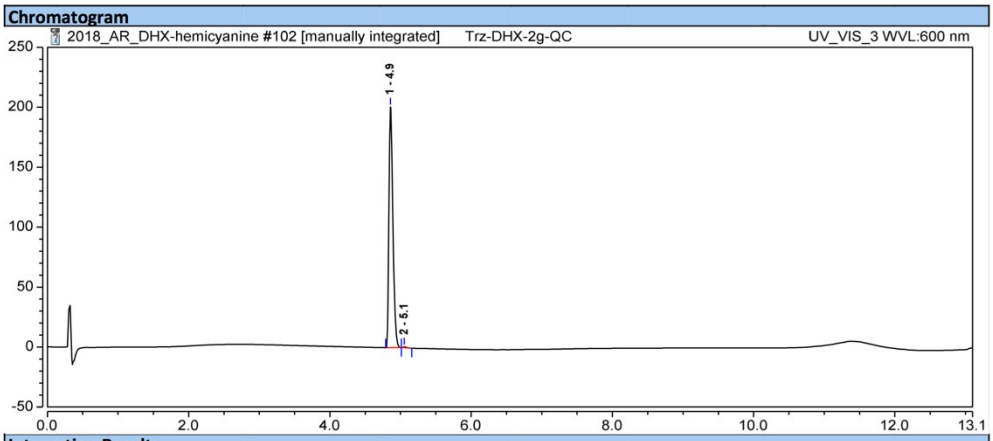
RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2g*** *(260 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.6	0.039	0.497	0.57	0.48	n.a.
2		4.9	6.624	101.587	96.99	97.45	n.a.
3		5.1	0.033	0.548	0.49	0.53	n.a.
4		5.7	0.121	1.615	1.78	1.55	n.a.
5		6.0	0.011	0.000	0.17	0.00	n.a.
Total:			**6.829**	**104.247**	**100.00**	**100.00**	

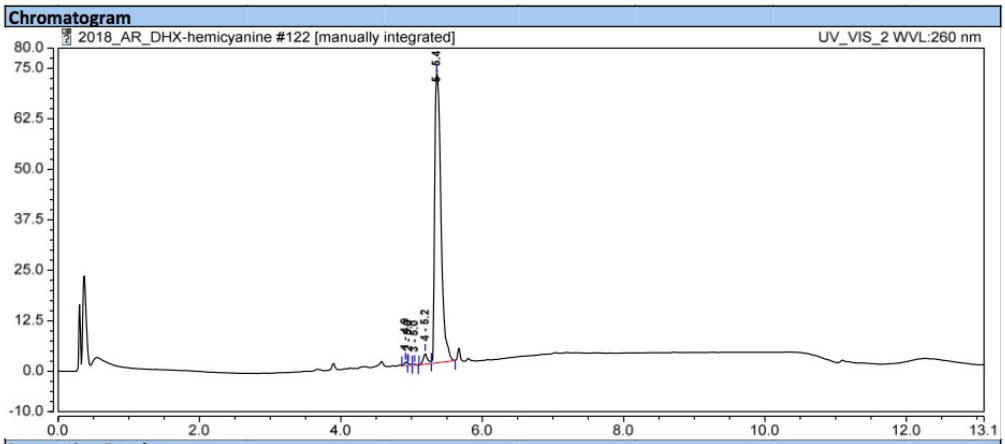
RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2g*** *(600 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.9	13.035	200.801	99.69	99.63	n.a.
2		5.1	0.041	0.749	0.31	0.37	n.a.
Total:			**13.076**	**201.550**	**100.00**	**100.00**	

RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2h*** *(260 nm)*

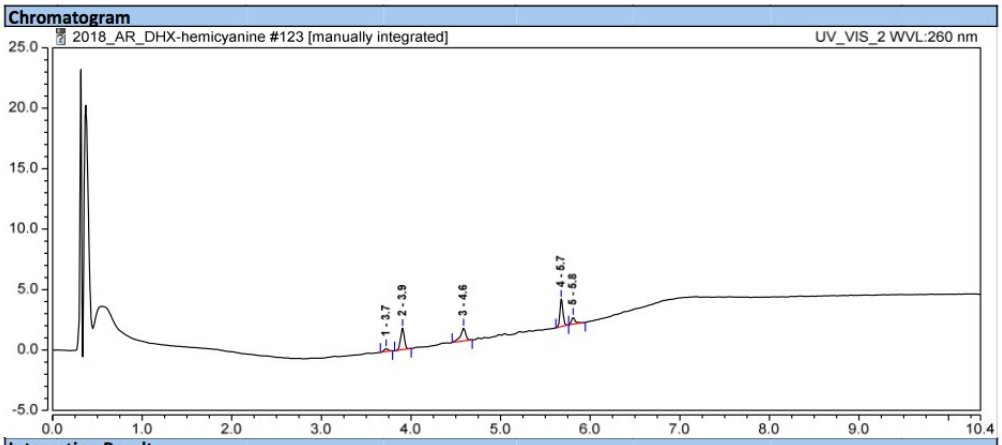


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.9	0.037	0.878	0.49	1.16	n.a.
2		5.0	0.020	0.485	0.27	0.64	n.a.
3		5.0	0.012	0.251	0.16	0.33	n.a.
4		5.2	0.184	2.718	2.45	3.58	n.a.
5		5.4	7.239	71.679	96.62	94.30	n.a.
Total:			**7.492**	**76.012**	**100.00**	**100.00**	

<u>Please note:</u> non-integrated peaks at t_R = 3.9, 4.6, 5.7 and 5.8 min were found in blank sample (vide infra).

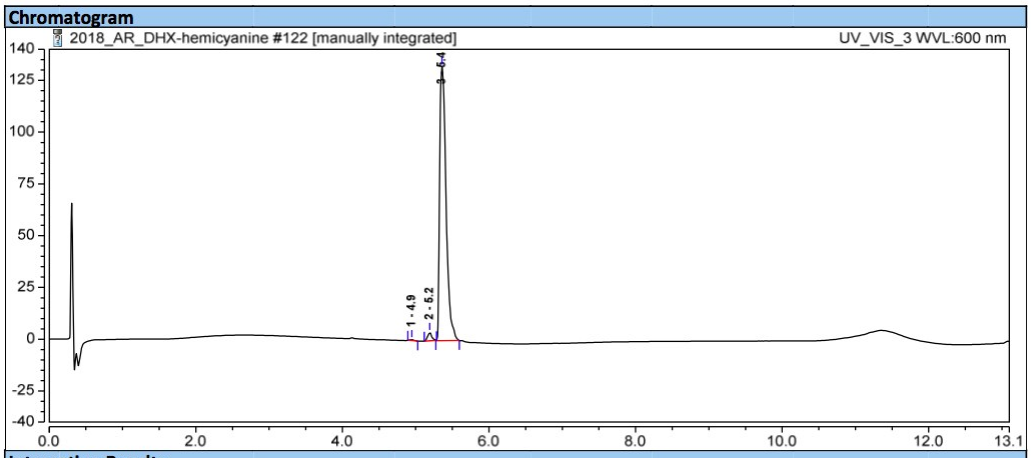
RP-HPLC elution profile of a blank sample (260 nm)



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		3.7	0.013	0.252	4.62	4.24	n.a.
2		3.9	0.083	1.760	29.31	29.67	n.a.
3		4.6	0.072	1.070	25.49	18.03	n.a.
4		5.7	0.087	2.266	30.63	38.20	n.a.
5		5.8	0.028	0.585	9.95	9.86	n.a.
Total:			**0.283**	**5.932**	**100.00**	**100.00**	

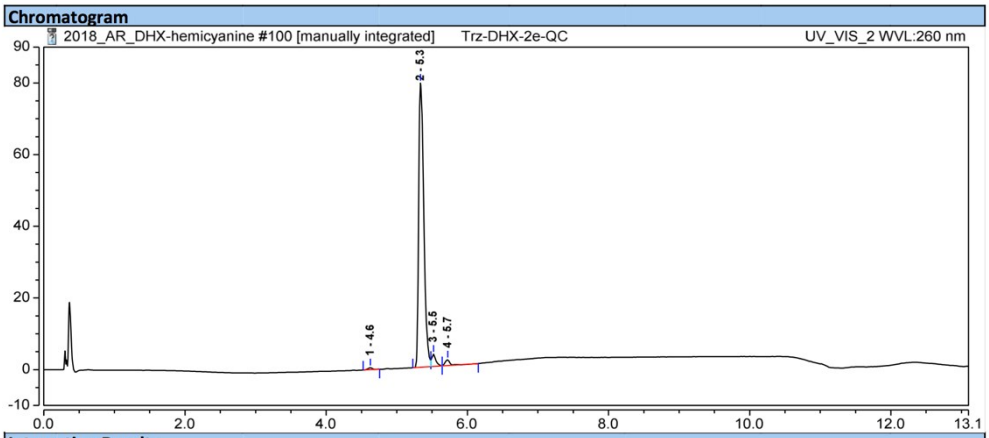
*RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye **2h** (600 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.9	0.026	0.474	0.19	0.35	n.a.
2		5.2	0.253	4.111	1.87	3.01	n.a.
3		5.4	13.251	132.231	97.94	96.65	n.a.
Total:			**13.530**	**136.817**	**100.00**	**100.00**	

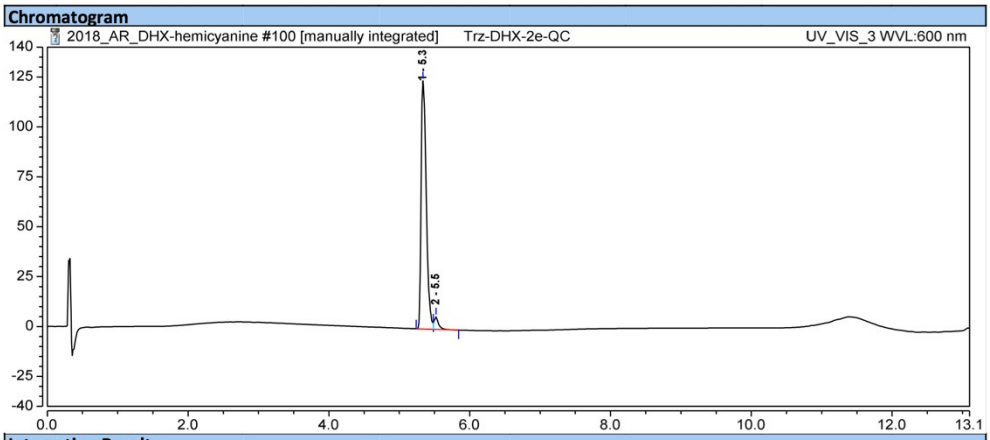
RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2i*** *(260 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.6	0.044	0.546	0.62	0.64	n.a.
2		5.3	6.674	79.287	94.40	93.46	n.a.
3		5.5	0.233	3.406	3.29	4.01	n.a.
4		5.7	0.119	1.601	1.69	1.89	n.a.
Total:			**7.069**	**84.840**	**100.00**	**100.00**	

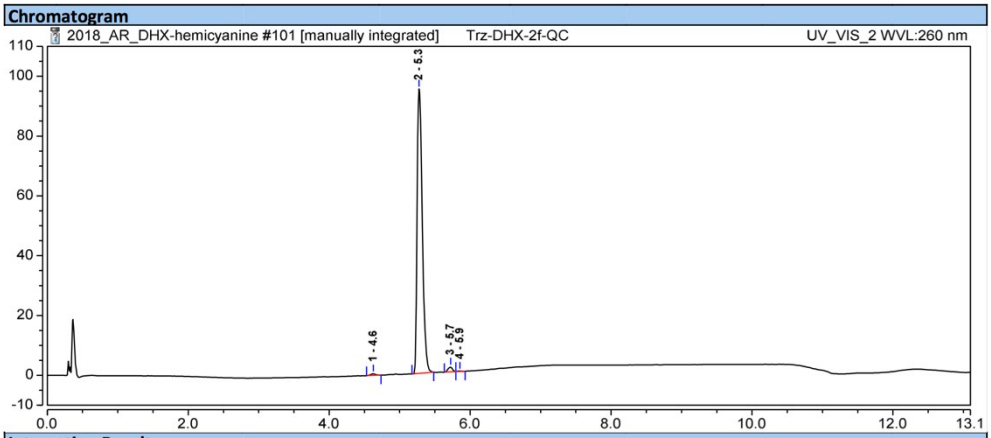
RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2i*** *(600 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.3	10.472	124.314	95.84	95.20	n.a.
2		5.5	0.454	6.272	4.16	4.80	n.a.
Total:			**10.926**	**130.586**	**100.00**	**100.00**	

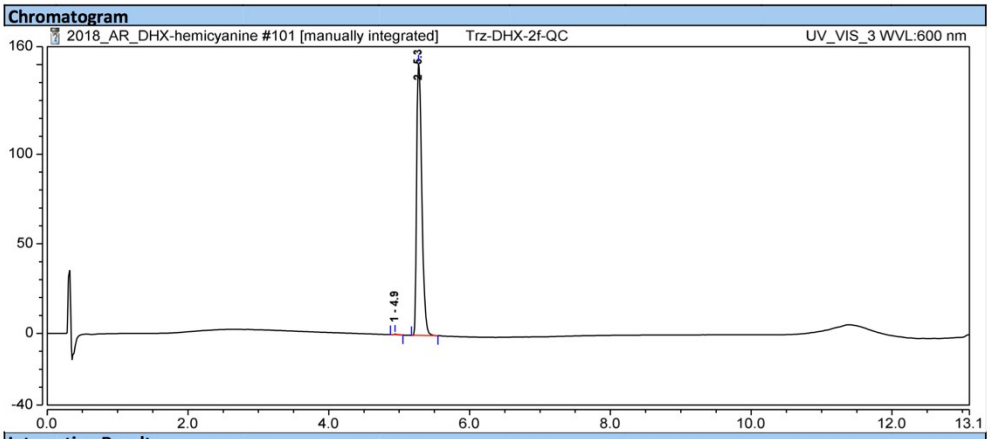
RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2j*** *(260 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.6	0.045	0.549	0.55	0.56	n.a.
2		5.3	8.055	95.149	97.83	97.61	n.a.
3		5.7	0.120	1.645	1.46	1.69	n.a.
4		5.9	0.013	0.134	0.16	0.14	n.a.
Total:			**8.233**	**97.476**	**100.00**	**100.00**	

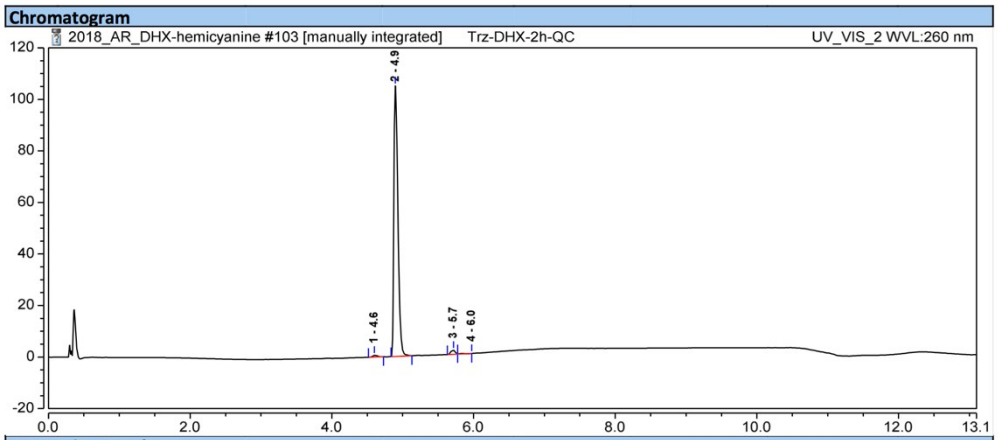
RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2j*** *(600 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.9	0.018	0.375	0.14	0.25	n.a.
2		5.3	12.846	151.557	99.86	99.75	n.a.
Total:			**12.864**	**151.933**	**100.00**	**100.00**	

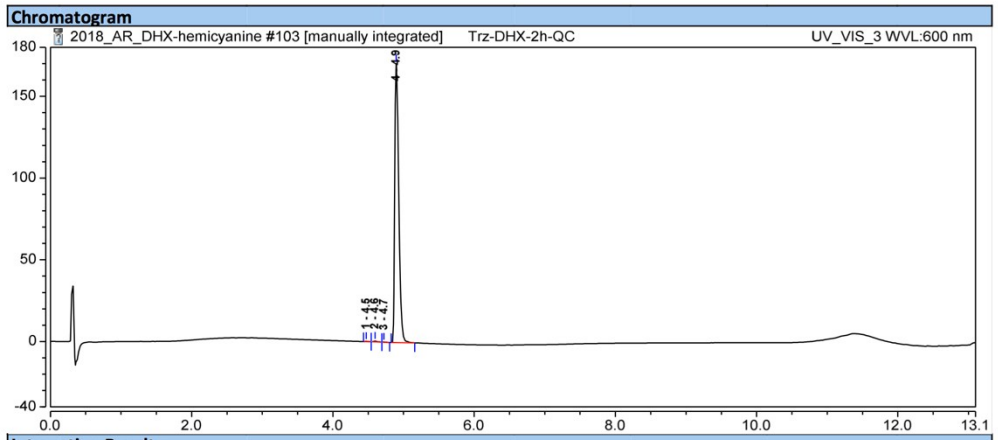
RP-HPLC elution profile triazole-based DHX-hemicyanine fused dye ***2k*** *(system A, 260 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.6	0.052	0.699	0.74	0.65	n.a.
2		4.9	6.876	105.007	97.37	97.86	n.a.
3		5.7	0.117	1.595	1.65	1.49	n.a.
4		6.0	0.016	0.000	0.23	0.00	n.a.
Total:			**7.062**	**107.301**	**100.00**	**100.00**	

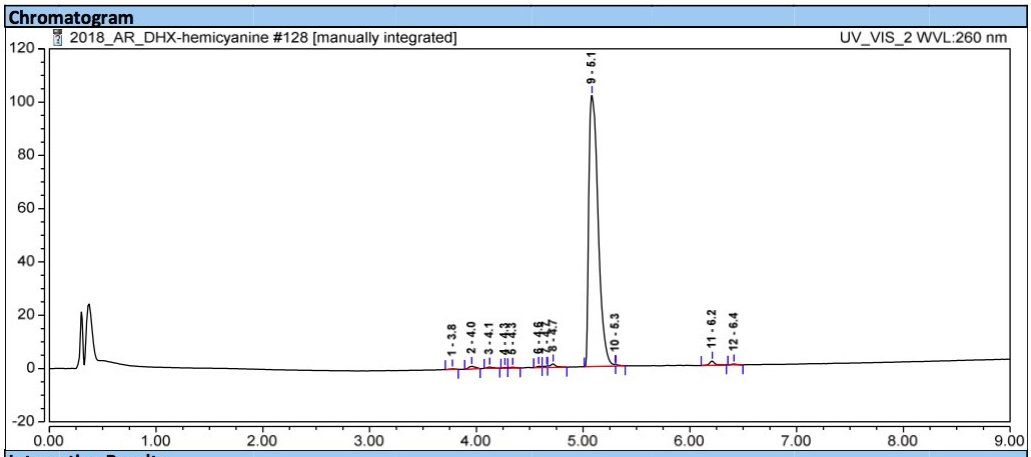
RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2k*** *(system A, 600 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.5	0.010	0.193	0.09	0.11	n.a.
2		4.6	0.031	0.523	0.28	0.30	n.a.
3		4.7	0.004	0.078	0.03	0.05	n.a.
4		4.9	11.166	170.676	99.60	99.54	n.a.
Total:			**11.211**	**171.469**	**100.00**	**100.00**	

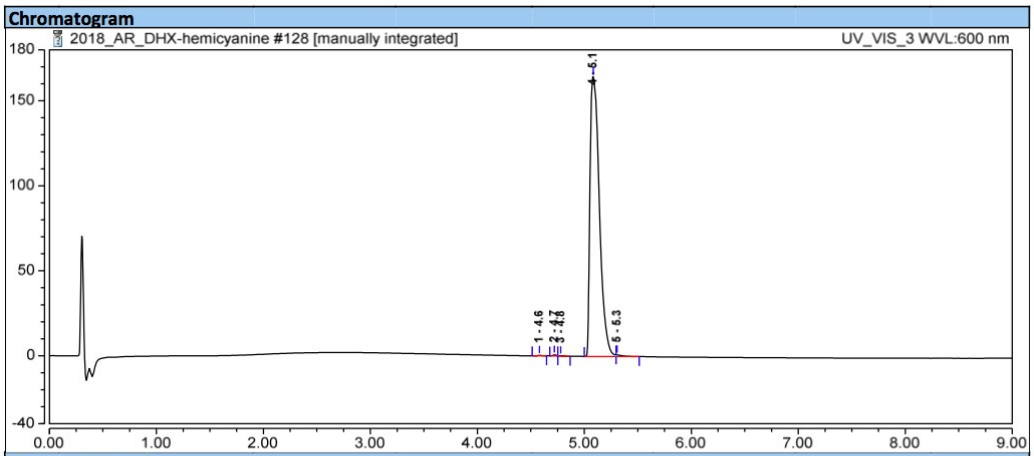
RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2k*** *(system B, 260 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		3.8	0.014	0.221	0.13	0.20	n.a.
2		4.0	0.071	1.009	0.66	0.93	n.a.
3		4.1	0.030	0.528	0.29	0.49	n.a.
4		4.3	0.009	0.226	0.08	0.21	n.a.
5		4.3	0.021	0.326	0.20	0.30	n.a.
6		4.6	0.022	0.457	0.21	0.42	n.a.
7		4.7	0.021	0.464	0.19	0.43	n.a.
8		4.7	0.081	1.256	0.76	1.16	n.a.
9		5.1	10.236	101.696	96.27	93.59	n.a.
10		5.3	0.021	0.531	0.20	0.49	n.a.
11		6.2	0.088	1.570	0.82	1.45	n.a.
12		6.4	0.020	0.372	0.18	0.34	n.a.
Total:			**10.633**	**108.656**	**100.00**	**100.00**	

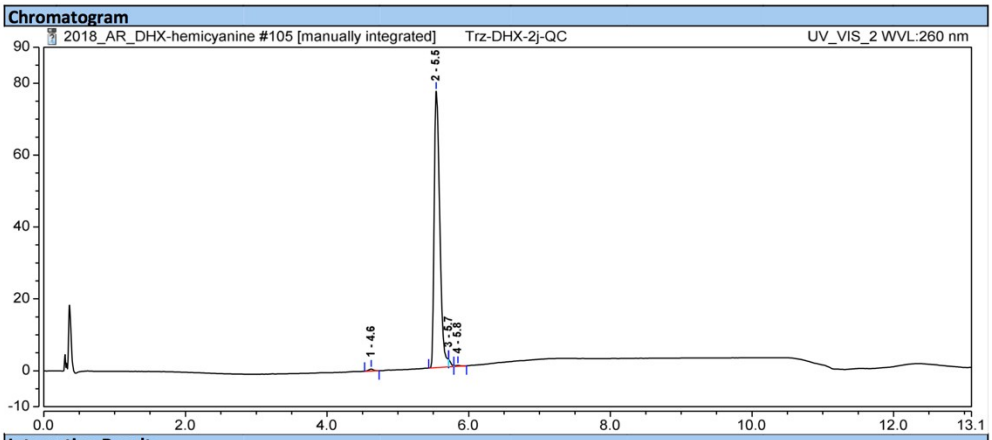
RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2k*** *(system B, 600 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.6	0.014	0.365	0.09	0.22	n.a.
2		4.7	0.022	0.608	0.13	0.36	n.a.
3		4.8	0.010	0.241	0.06	0.14	n.a.
4		5.1	16.560	164.601	99.35	98.69	n.a.
5		5.3	0.063	0.966	0.38	0.58	n.a.
Total:			**16.669**	**166.781**	**100.00**	**100.00**	

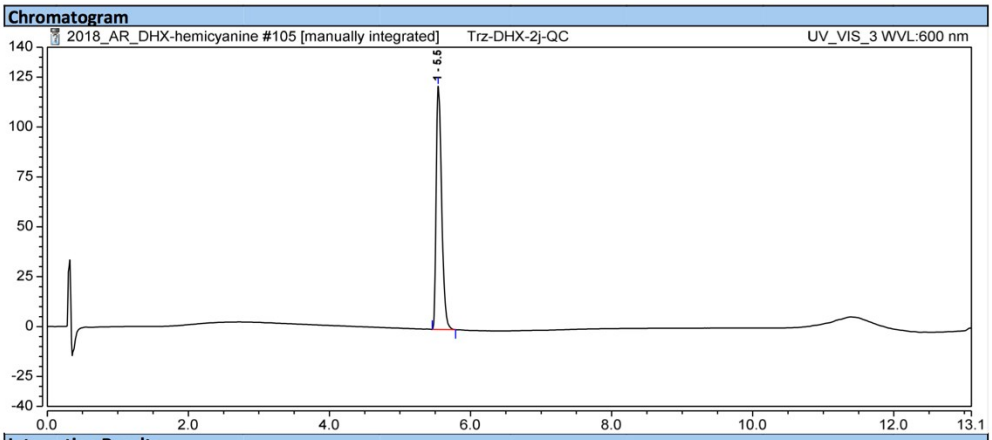
*RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye **2l** (260 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.6	0.041	0.538	0.58	0.67	n.a.
2		5.5	7.025	76.854	98.14	96.41	n.a.
3		5.7	0.071	2.090	0.99	2.62	n.a.
4		5.8	0.021	0.237	0.30	0.30	n.a.
Total:			**7.158**	**79.719**	**100.00**	**100.00**	

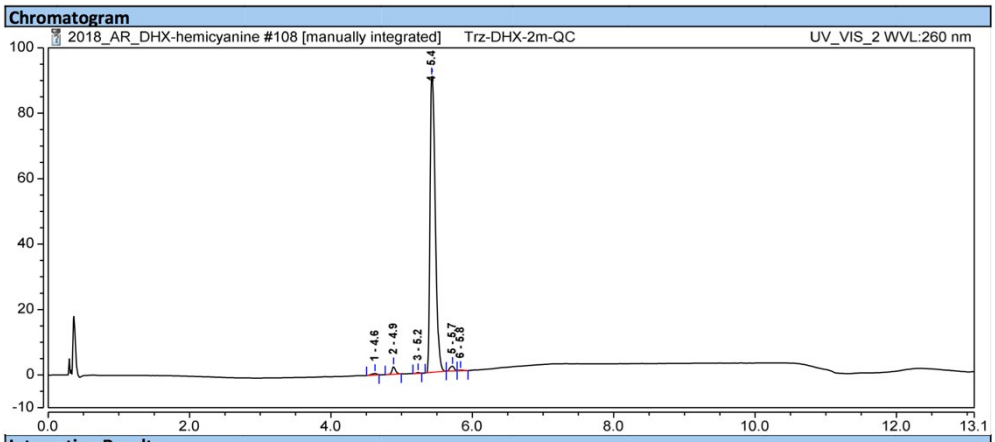
*RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye **2l** (600 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.5	11.053	121.856	100.00	100.00	n.a.
Total:			**11.053**	**121.856**	**100.00**	**100.00**	

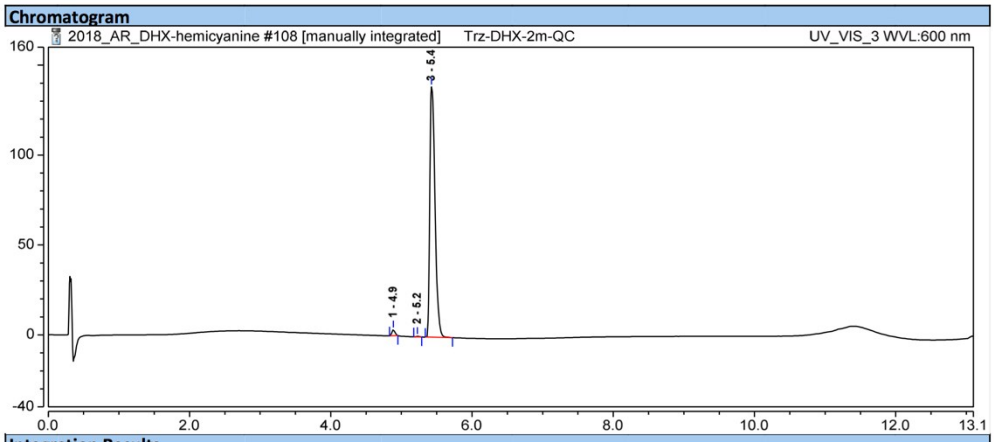
RP-HPLC elution profile triazole-based DHX-hemicyanine fused dye ***2m*** *(260 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.6	0.037	0.464	0.46	0.49	n.a.
2		4.9	0.136	2.401	1.71	2.52	n.a.
3		5.2	0.013	0.265	0.17	0.28	n.a.
4		5.4	7.691	90.367	96.15	94.92	n.a.
5		5.7	0.107	1.526	1.33	1.60	n.a.
6		5.8	0.014	0.179	0.17	0.19	n.a.
Total:			**7.998**	**95.203**	**100.00**	**100.00**	

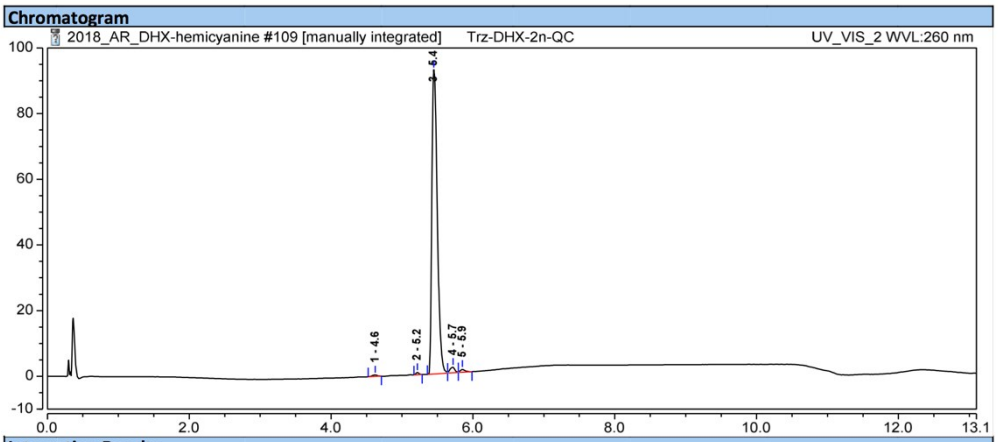
RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2m*** *(600 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.9	0.170	3.398	1.41	2.38	n.a.
2		5.2	0.018	0.386	0.15	0.27	n.a.
3		5.4	11.877	139.184	98.44	97.35	n.a.
Total:			**12.066**	**142.968**	**100.00**	**100.00**	

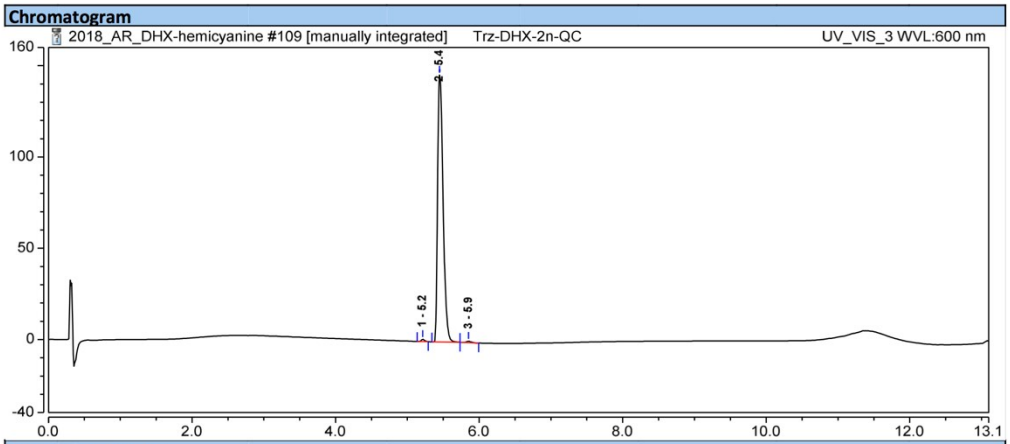
RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2n*** *(260 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.6	0.041	0.495	0.49	0.51	n.a.
2		5.2	0.033	0.674	0.40	0.70	n.a.
3		5.4	8.177	92.662	96.68	96.10	n.a.
4		5.7	0.137	1.706	1.61	1.77	n.a.
5		5.9	0.069	0.885	0.82	0.92	n.a.
Total:			**8.458**	**96.421**	**100.00**	**100.00**	

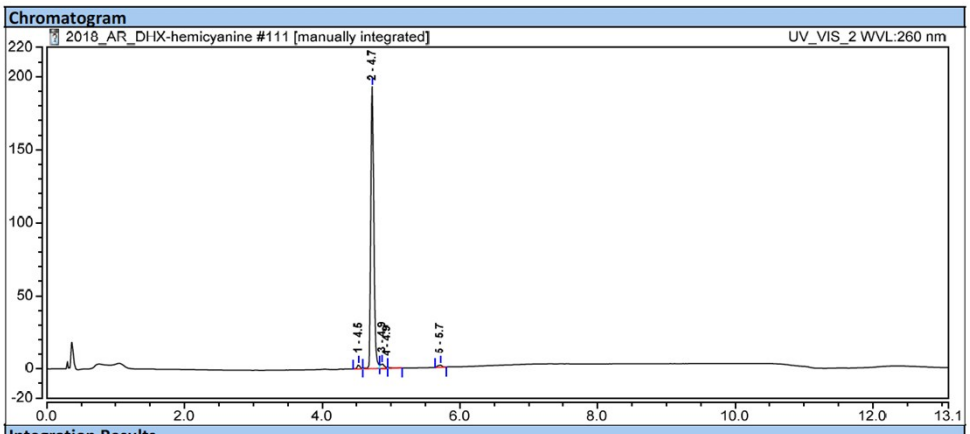
RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2n*** *(600 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.2	0.064	1.262	0.49	0.85	n.a.
2		5.4	12.888	146.164	99.05	98.57	n.a.
3		5.9	0.060	0.858	0.46	0.58	n.a.
Total:			**13.012**	**148.283**	**100.00**	**100.00**	

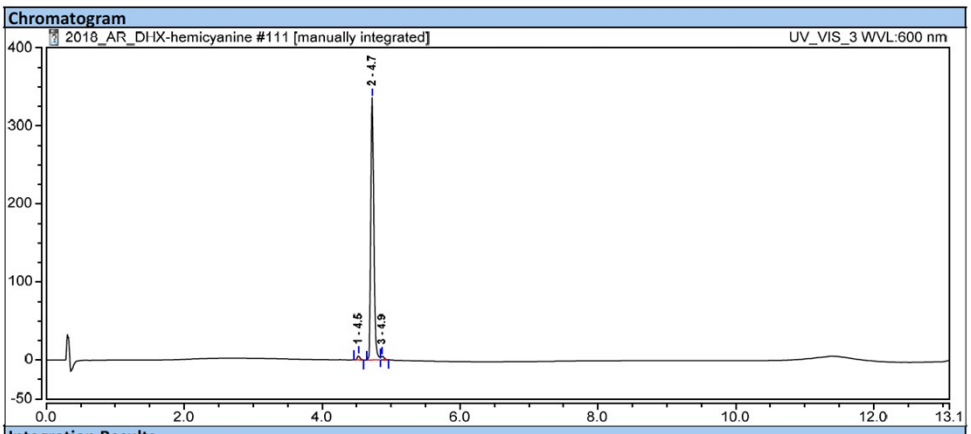
RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2o*** *(260 nm)*



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.5	0.136	2.884	1.33	1.43	n.a.
2		4.7	9.789	193.089	95.19	96.01	n.a.
3		4.9	0.216	3.165	2.10	1.57	n.a.
4		4.9	0.037	0.472	0.36	0.23	n.a.
5		5.7	0.105	1.503	1.02	0.75	n.a.
Total:			**10.283**	**201.113**	**100.00**	**100.00**	

RP-HPLC elution profile of triazole-based DHX-hemicyanine fused dye ***2o*** *(600 nm)*

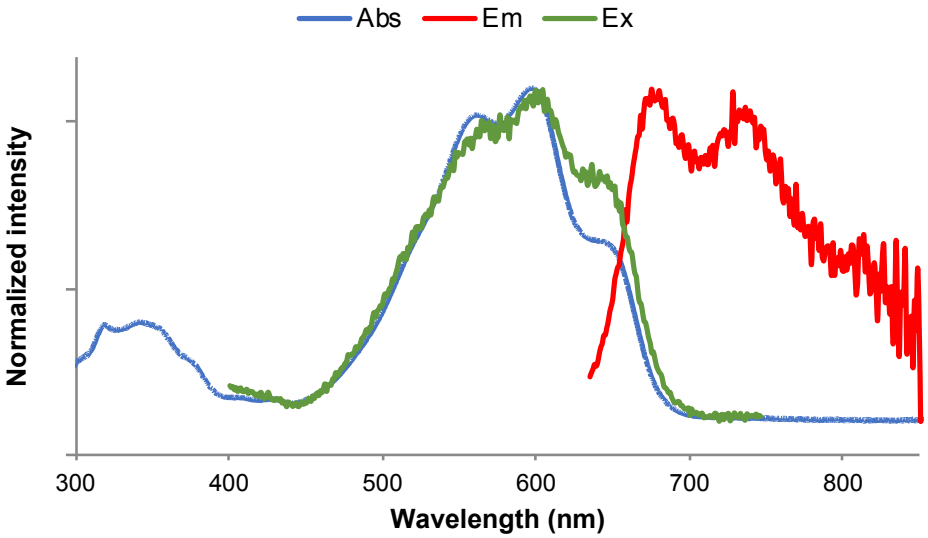


Integration Results

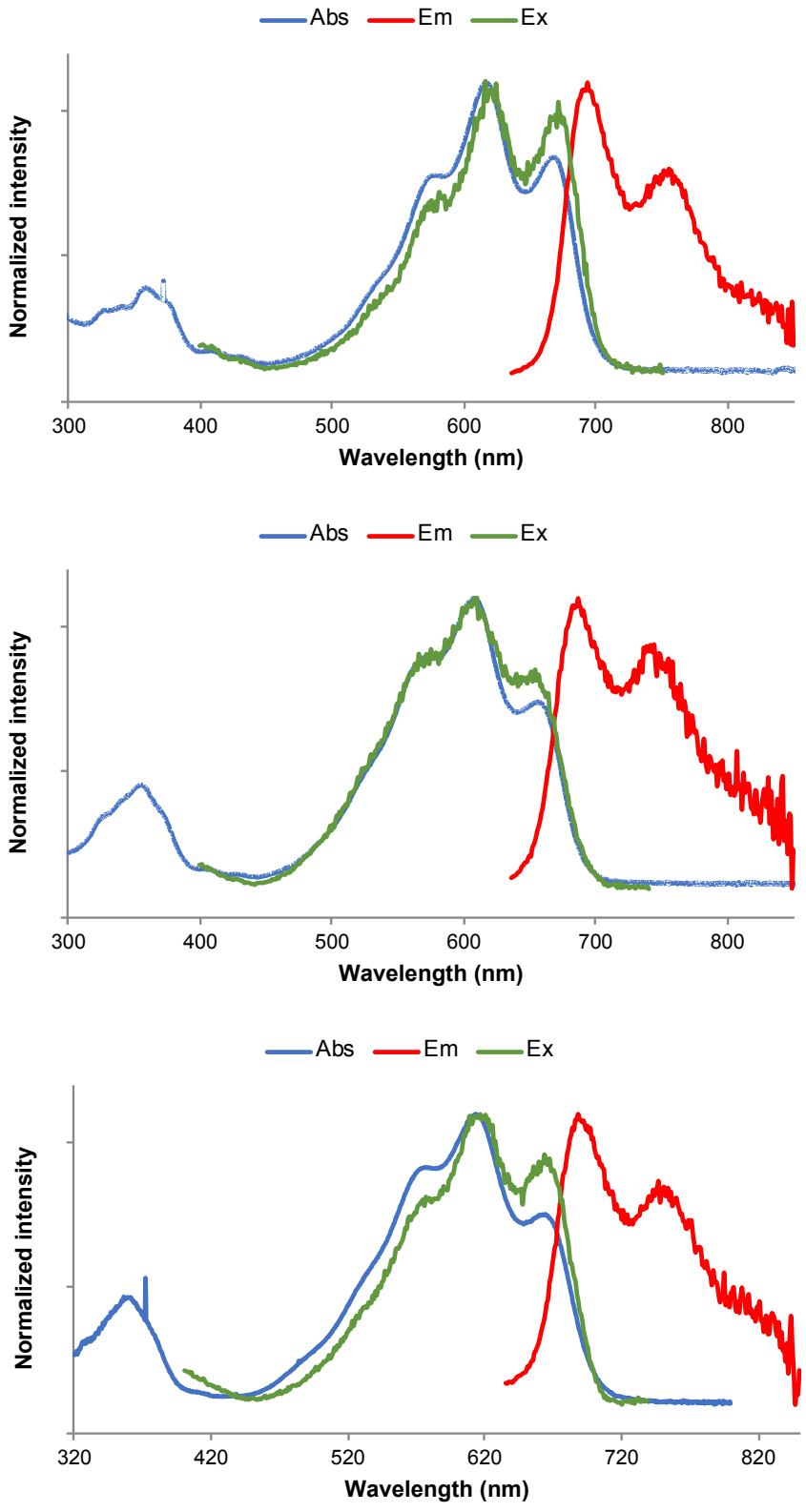
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.5	0.228	5.391	1.31	1.56	n.a.
2		4.7	16.956	336.175	97.24	97.12	n.a.
3		4.9	0.253	4.571	1.45	1.32	n.a.
Total:			**17.437**	**346.137**	**100.00**	**100.00**	

7. Photophysical data of DHX-hemicyanine fused dyes (alkyne and triazole derivatives)

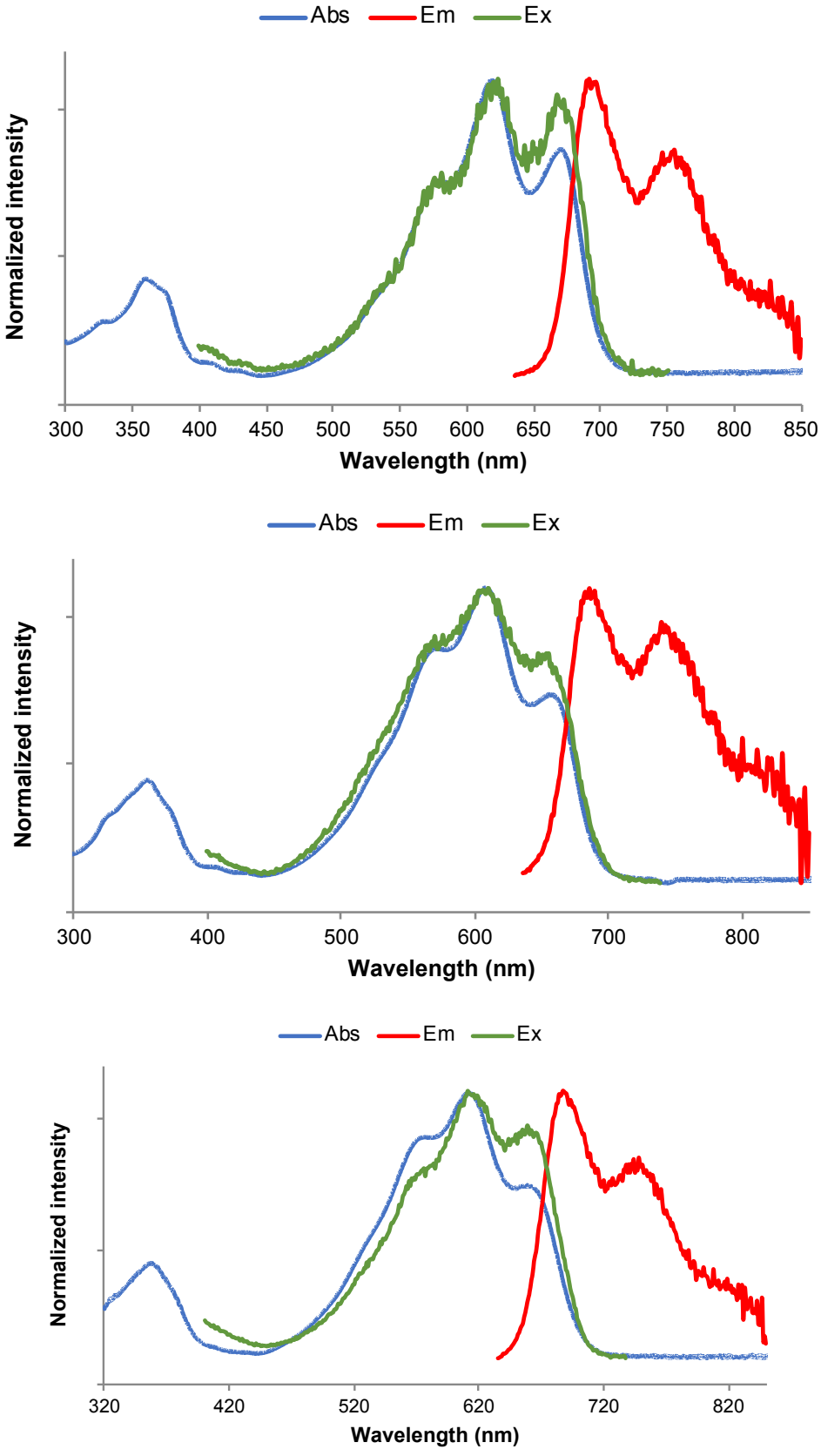
*Normalised absorption, excitation (Em at 760 nm), emission (Ex at 620 nm) spectra of alkynyl-based DHX-hemicyanine fused dye **1** in EtOH*



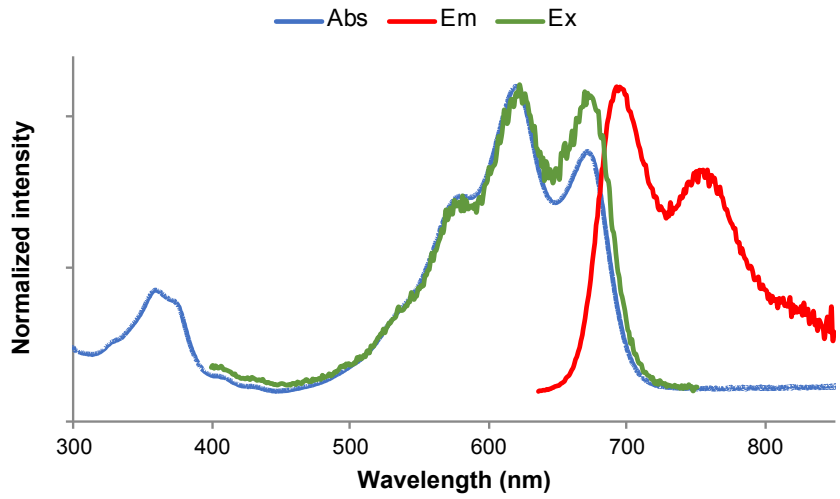
Normalised absorption, excitation (Em at 760 nm), emission (Ex at 620 nm) spectra of triazole-based DHX-hemicyanine fused dye ***2a*** *in $CHCl_3$ (top), EtOH (middle) and PBS + 5% BSA (bottom)*

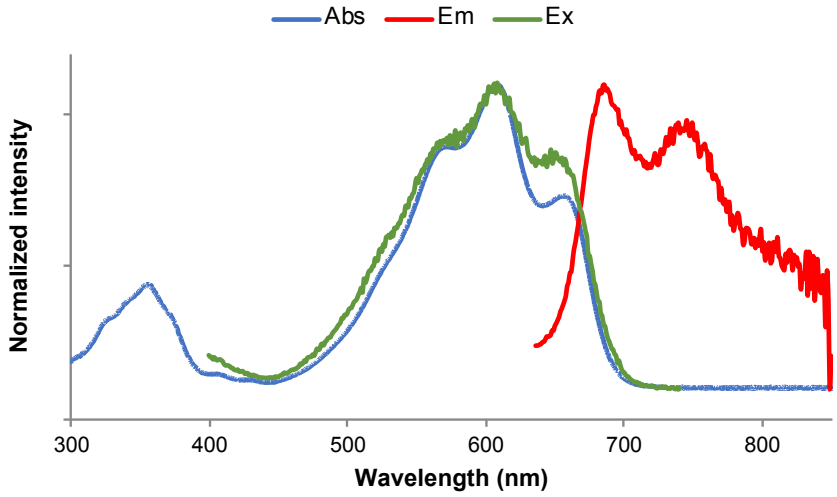


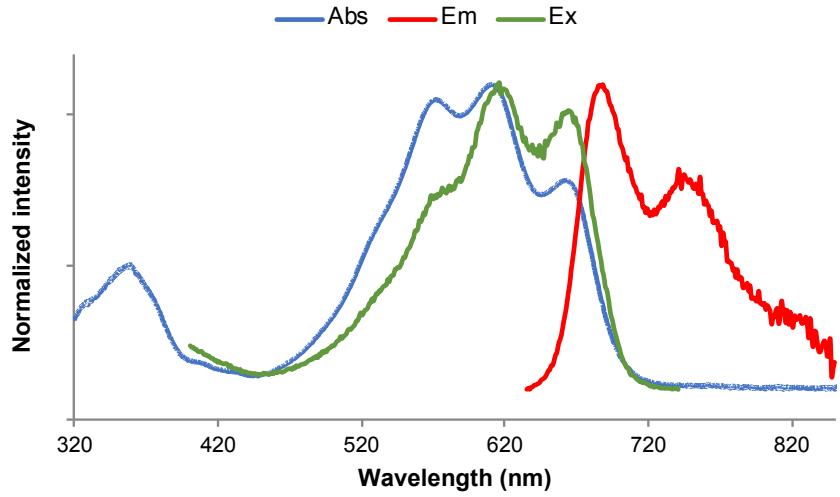
Normalised absorption, excitation (Em at 760 nm), emission (Ex at 620 nm) spectra of triazole-based DHX-hemicyanine fused dye ***2b*** *in* $CHCl_3$ *(top), EtOH (middle) and PBS + 5% BSA (bottom)*



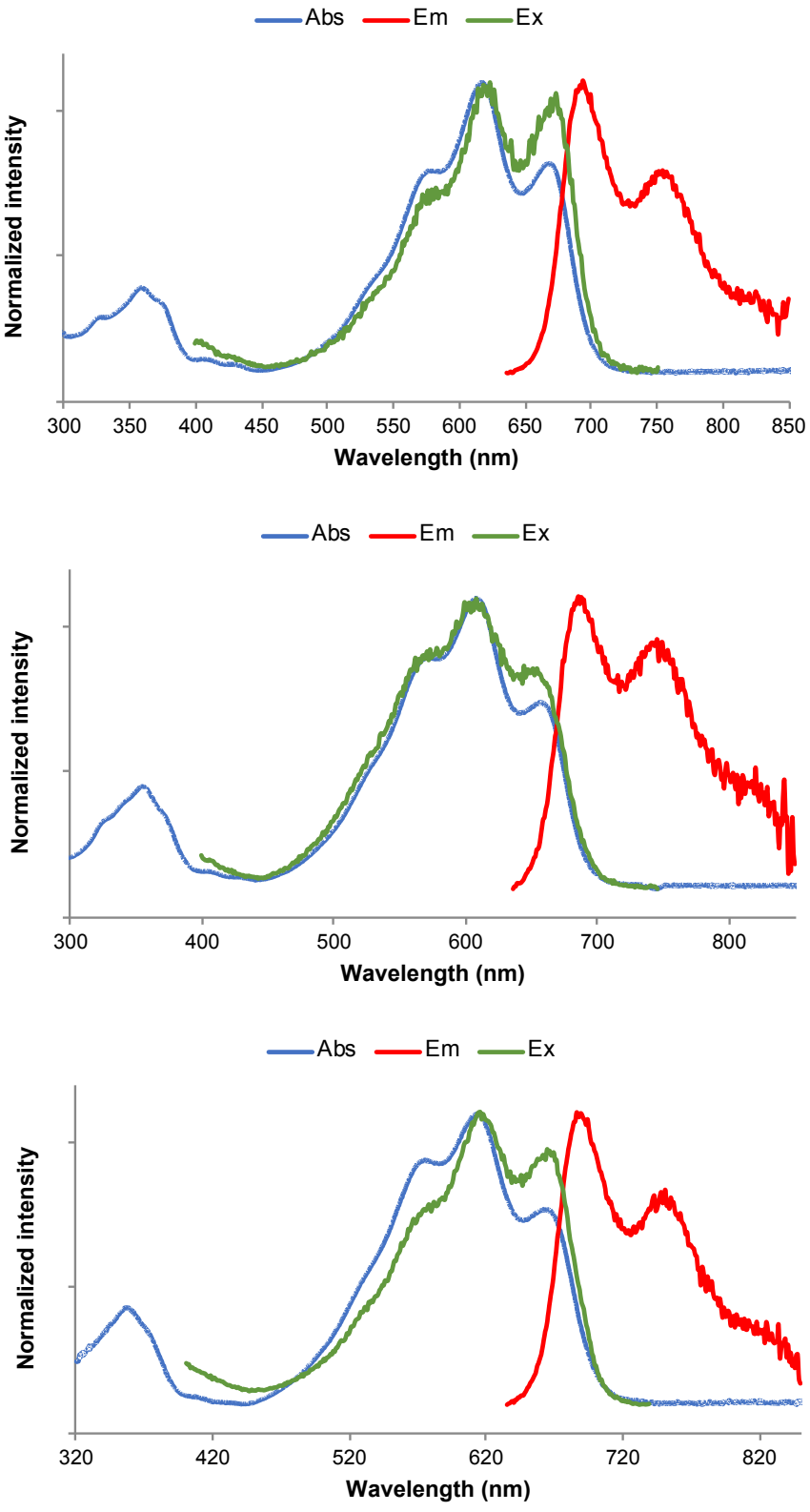
Normalised absorption, excitation (Em at 760 nm), emission (Ex at 620 nm) spectra of triazole-based DHX-hemicyanine fused dye ***2c*** *in $CHCl_3$ (top), EtOH (middle) and PBS + 5% BSA (bottom)*



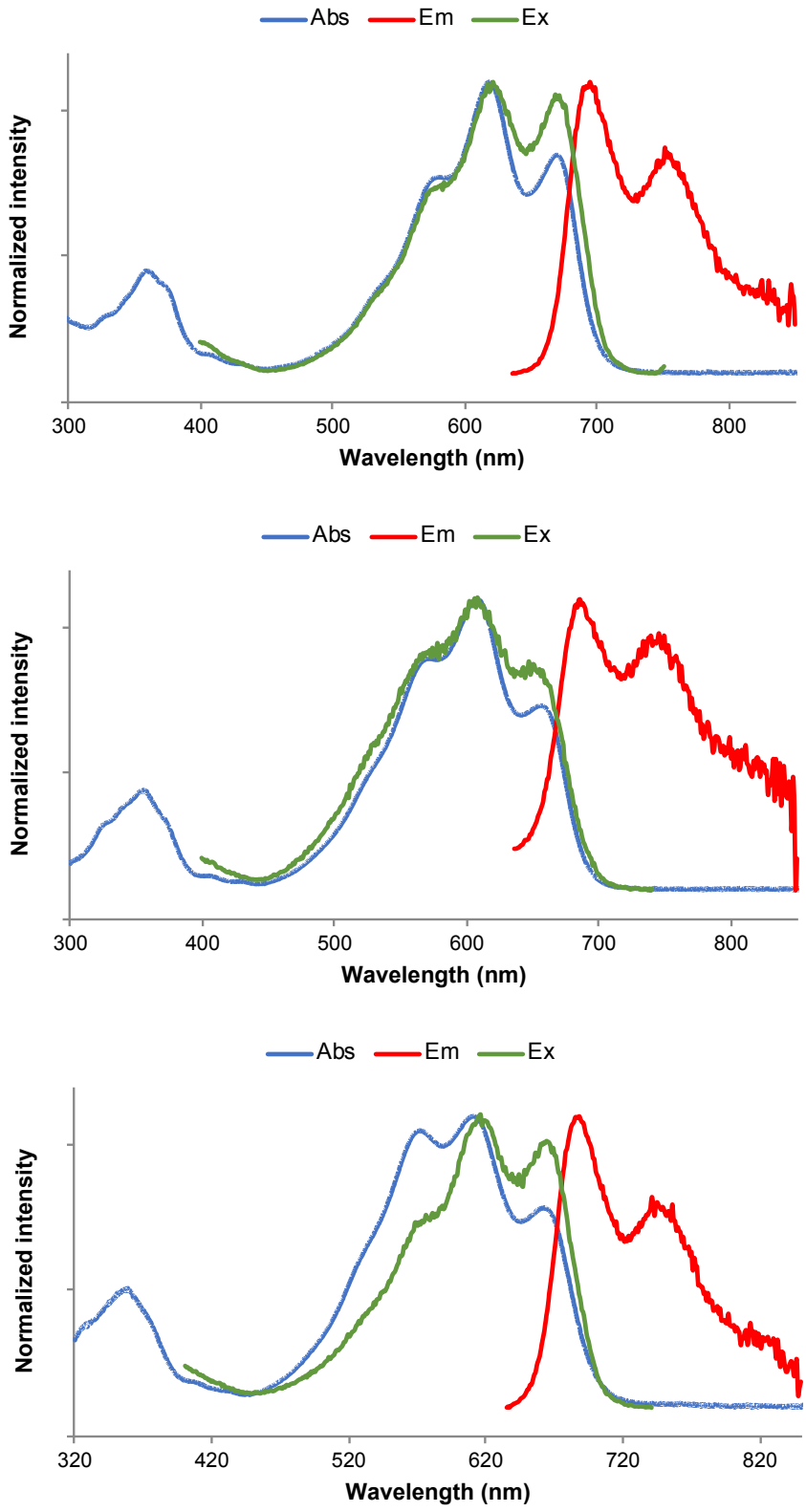




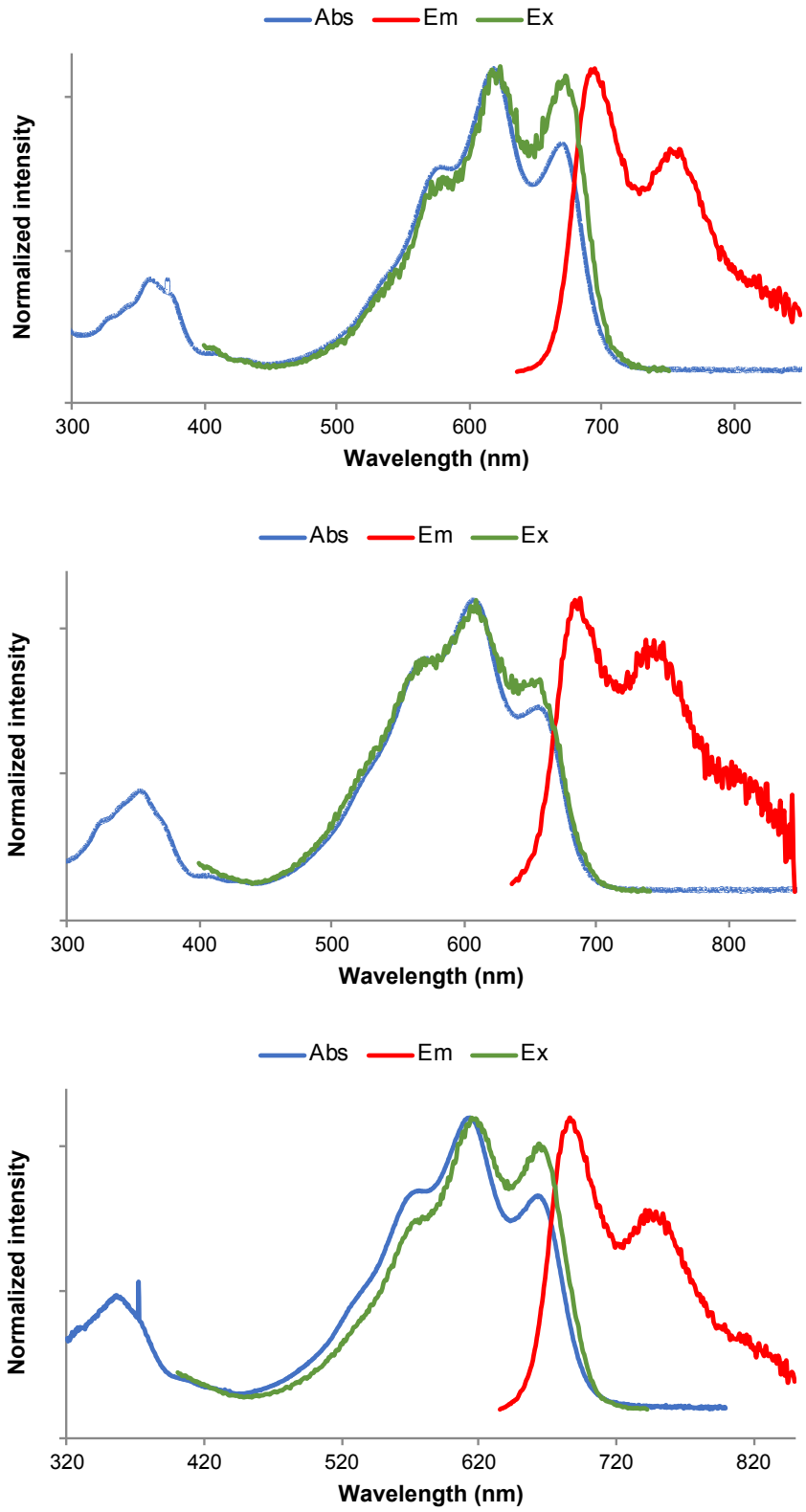
Normalised absorption, excitation (Em at 760 nm), emission (Ex at 620 nm) spectra of triazole-based DHX-hemicyanine fused dye ***2d*** *in* $CHCl_3$ *(top), EtOH (middle) and PBS + 5% BSA (bottom)*



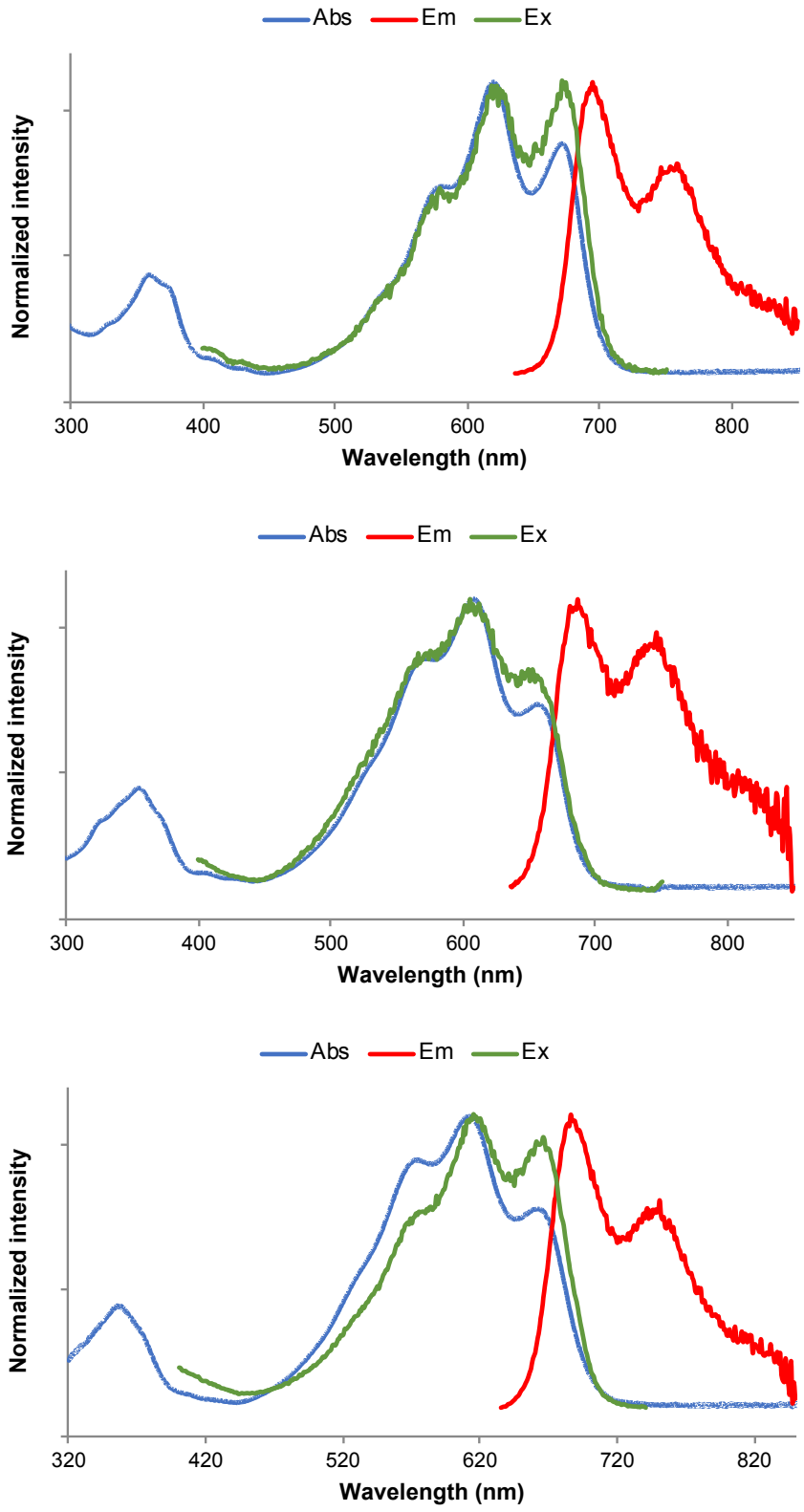
Normalised absorption, excitation (Em at 760 nm), emission (Ex at 620 nm) spectra of triazole-based DHX-hemicyanine fused dye ***2e*** *in $CHCl_3$ (top), EtOH (middle) and PBS + 5% BSA (bottom)*



Normalised absorption, excitation (Em at 760 nm), emission (Ex at 620 nm) spectra of triazole-based DHX-hemicyanine fused dye ***2f*** *in $CHCl_3$ (top), EtOH (middle) and PBS + 5% BSA (bottom)*

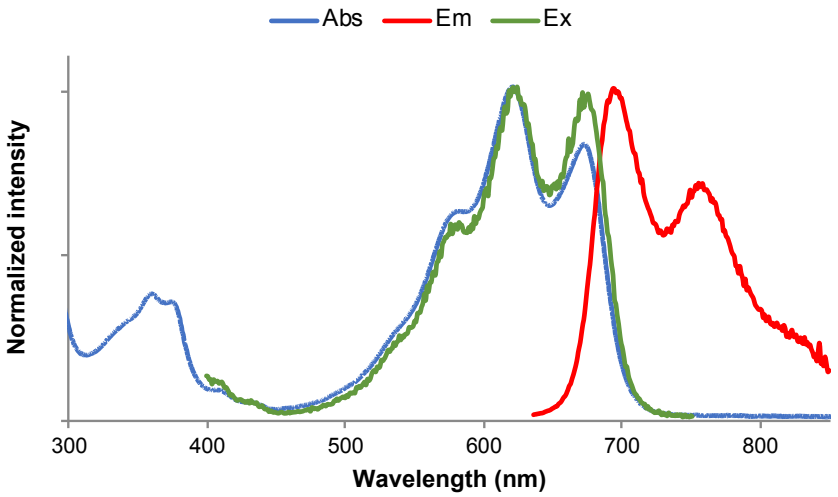


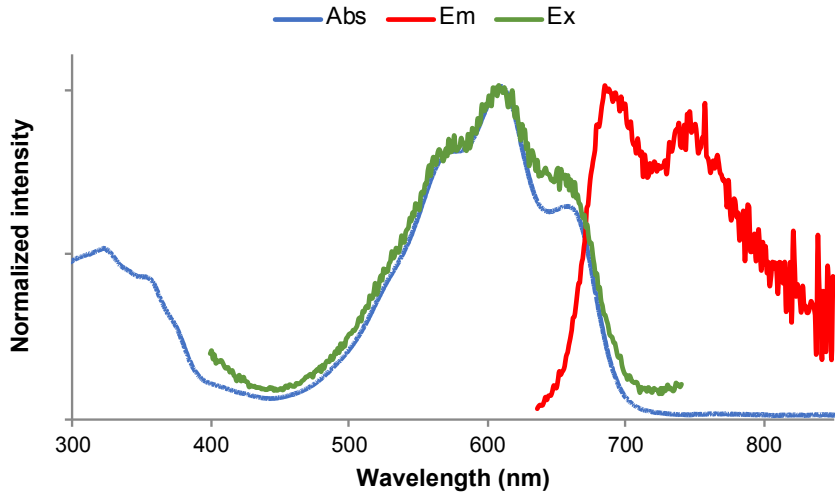
Normalised absorption, excitation (Em at 760 nm), emission (Ex at 620 nm) spectra of triazole-based DHX-hemicyanine fused dye ***2g*** *in $CHCl_3$ (top), EtOH (middle) and PBS + 5% BSA (bottom)*

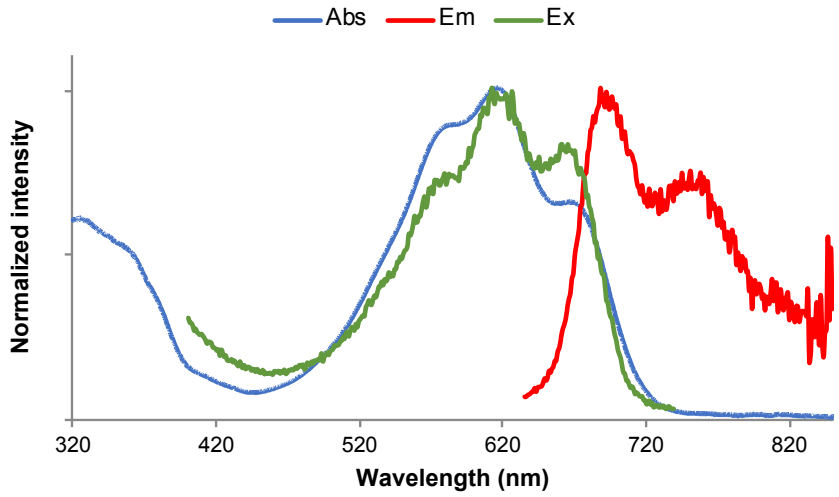


Normalised absorption, excitation (Em at 760 nm), emission (Ex at 620 nm) spectra of

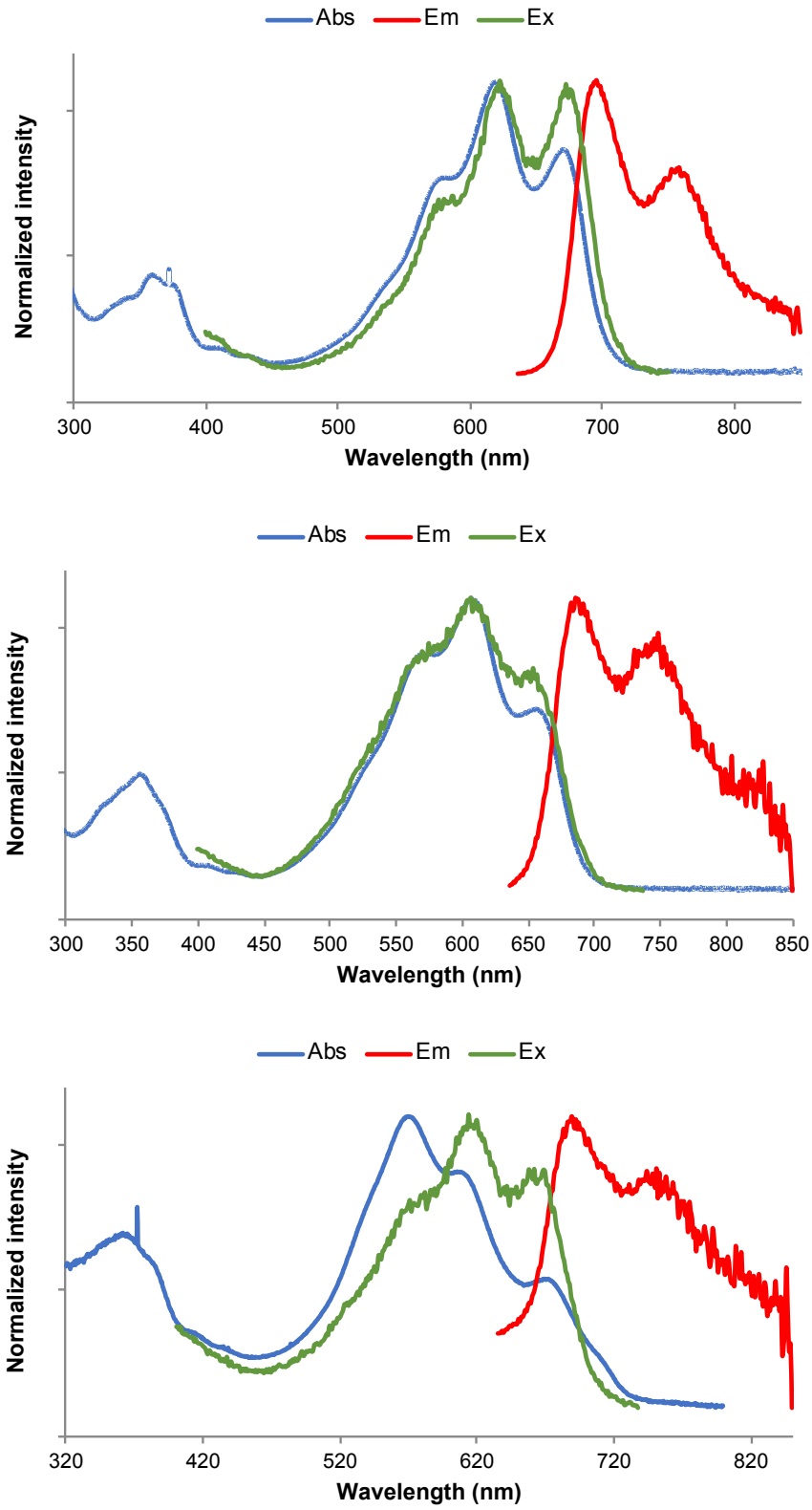
triazole-based DHX-hemicyanine fused dye ***2h*** *in* $CHCl_3$ *(top), EtOH (middle) and PBS + 5% BSA (bottom)*



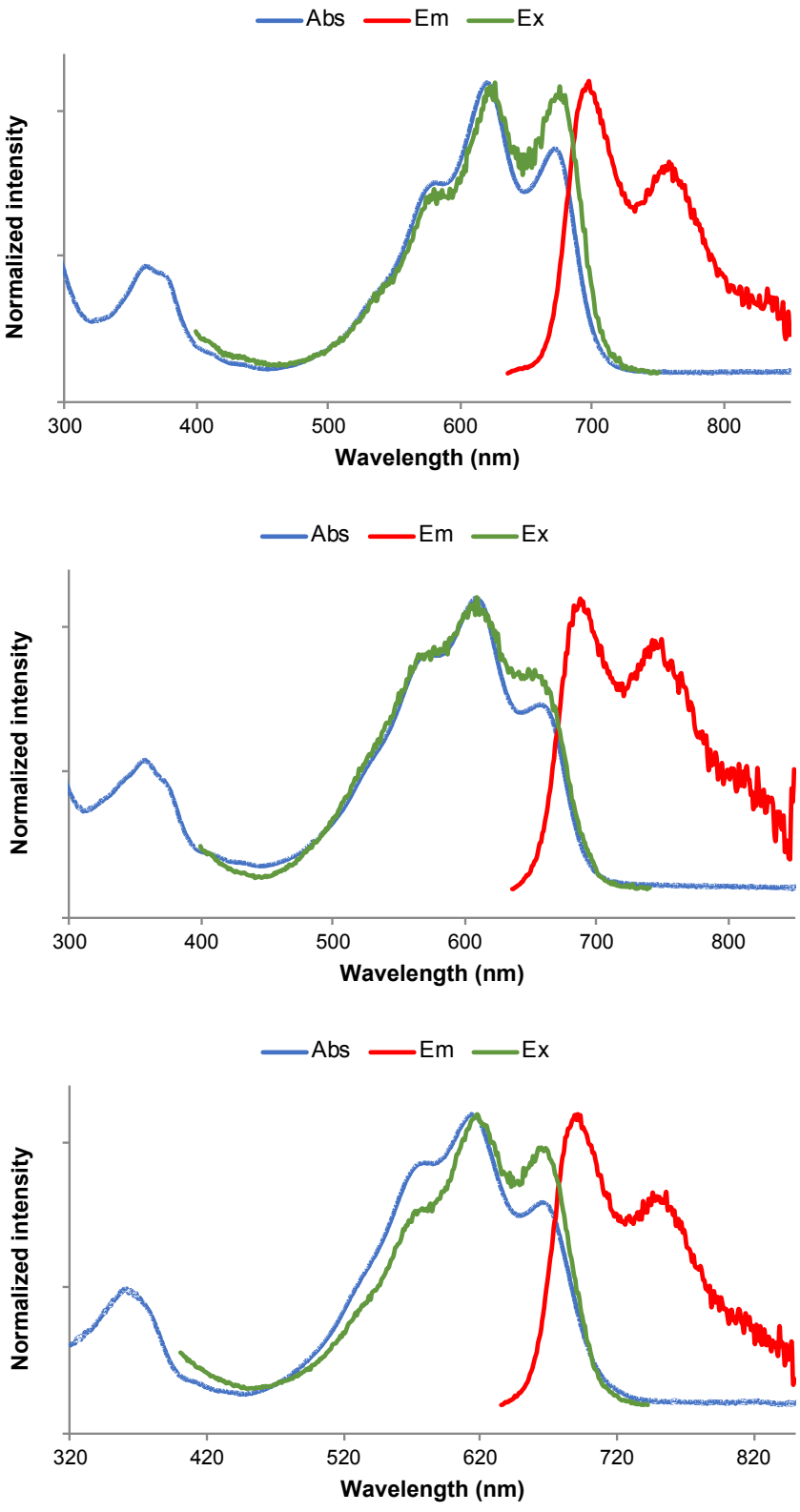




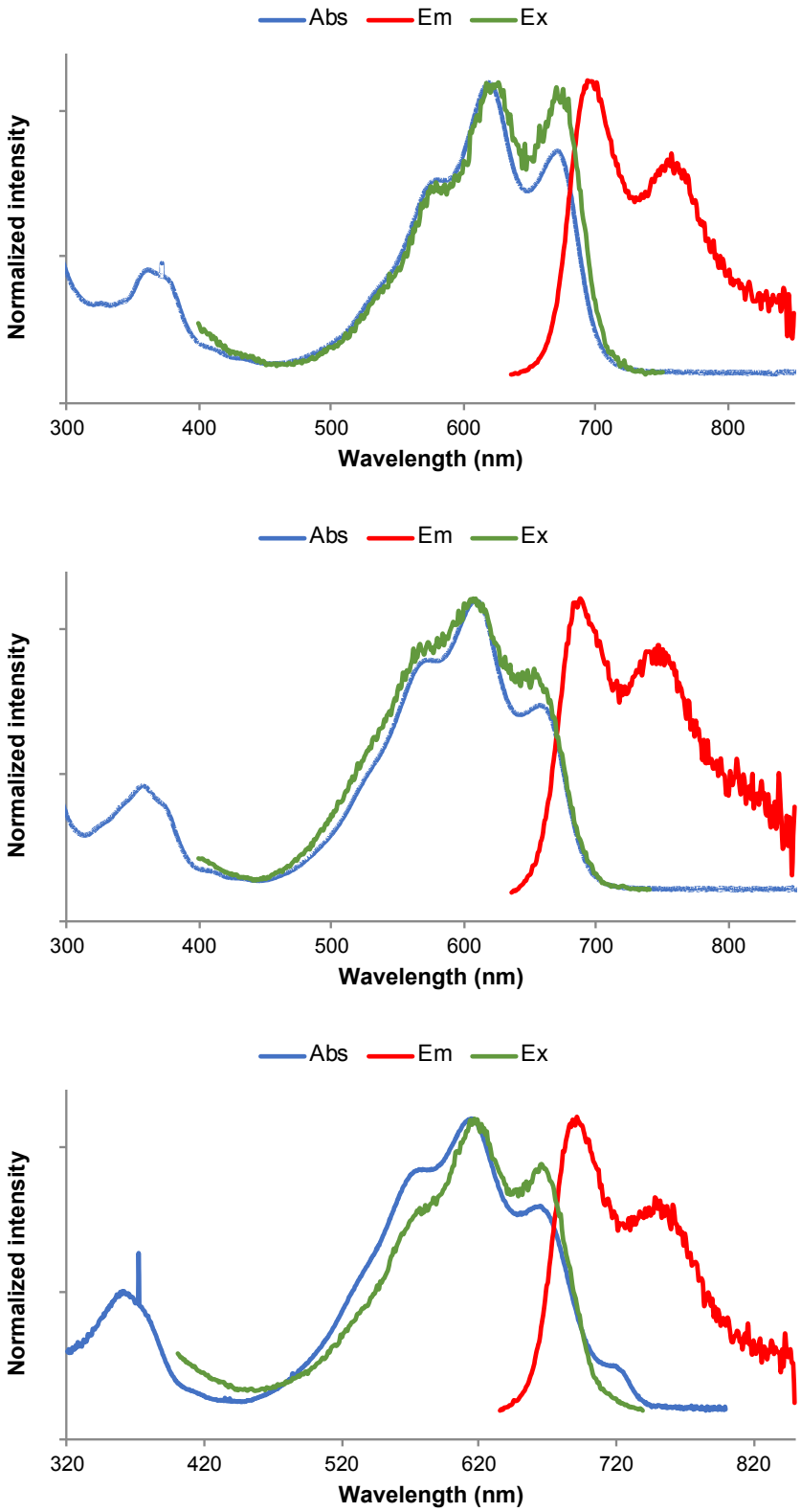
Normalised absorption, excitation (Em at 760 nm), emission (Ex at 620 nm) spectra of triazole-based DHX-hemicyanine fused dye ***2i*** *in* $CHCl_3$ *(top), EtOH (middle) and PBS + 5% BSA (bottom)*



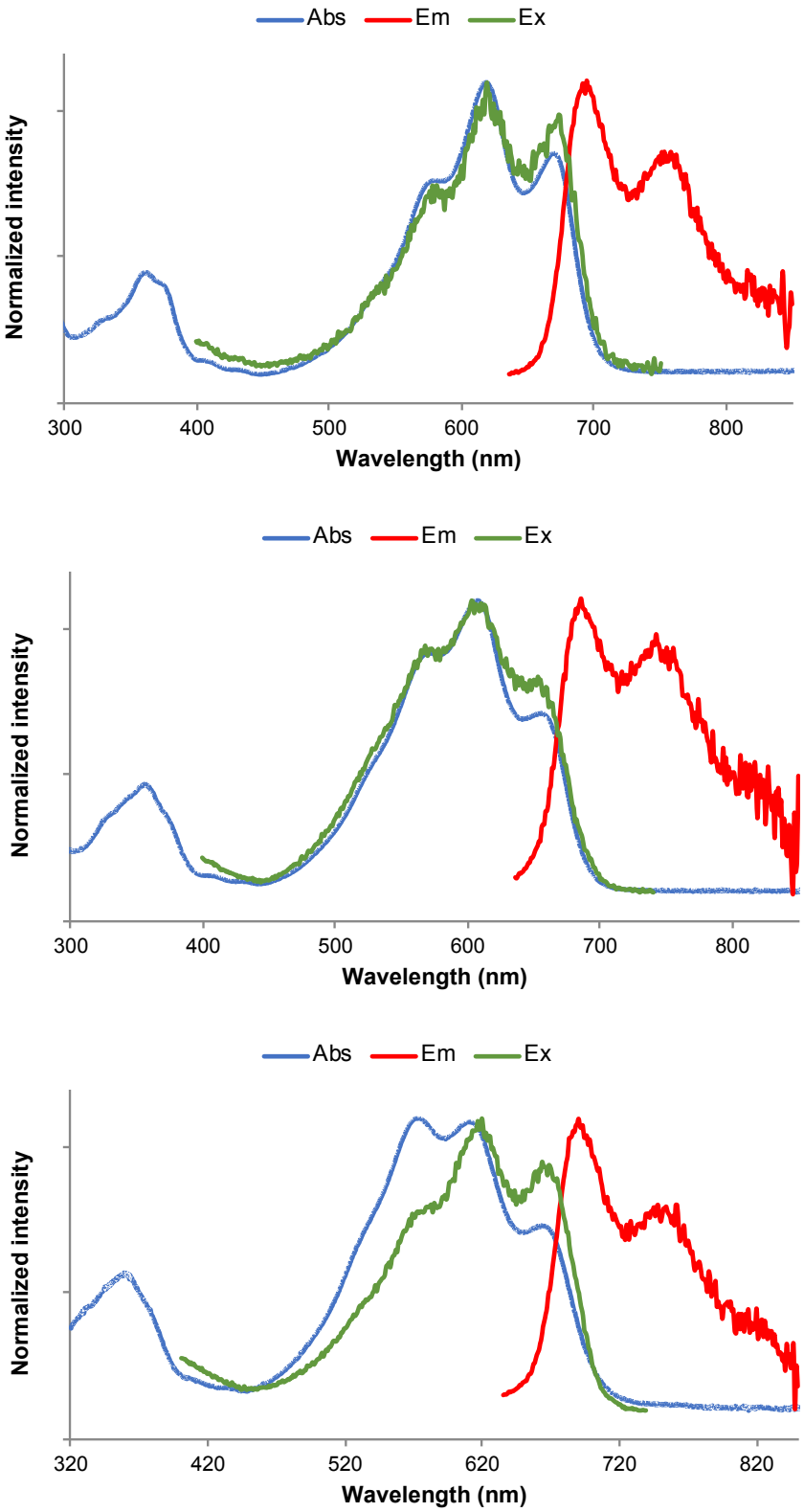
Normalised absorption, excitation (Em at 760 nm), emission (Ex at 620 nm) spectra of triazole-based DHX-hemicyanine fused dye ***2j*** *in $CHCl_3$ (top), EtOH (middle) and PBS + 5% BSA (bottom)*



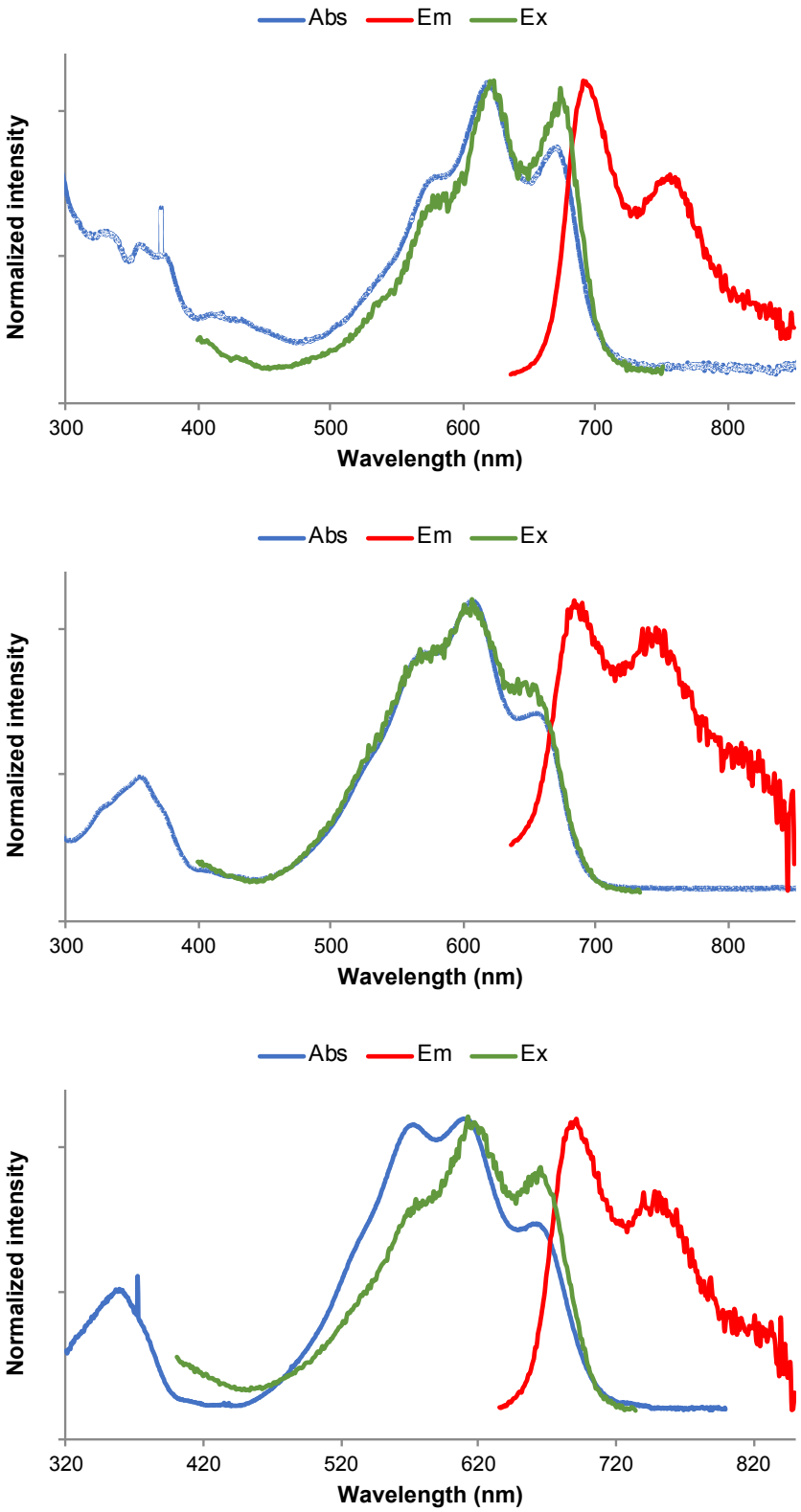
Normalised absorption, excitation (Em at 760 nm), emission (Ex at 620 nm) spectra of triazole-based DHX-hemicyanine fused dye ***2k*** *in $CHCl_3$ (top), EtOH (middle) and PBS + 5% BSA (bottom)*



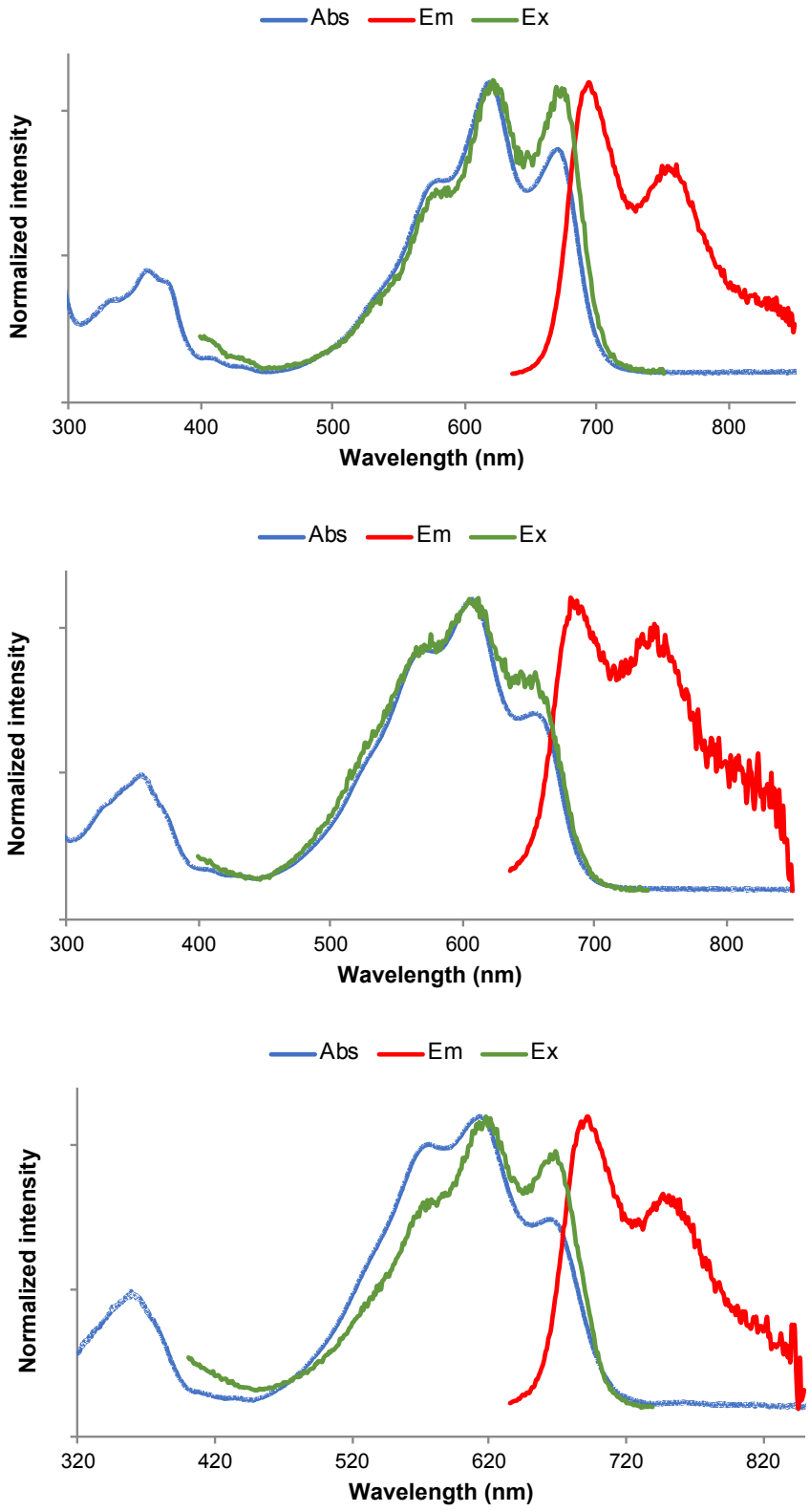
*Normalised absorption, excitation (Em at 760 nm), emission (Ex at 620 nm) spectra of triazole-based DHX-hemicyanine fused dye **2l** in $CHCl_3$ (top), EtOH (middle) and PBS + 5% BSA (bottom)*



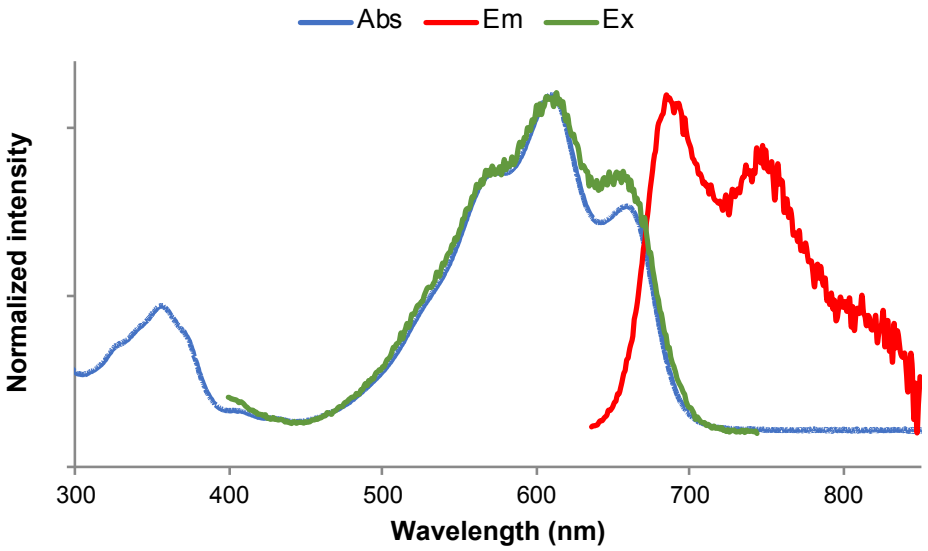
Normalised absorption, excitation (Em at 760 nm), emission (Ex at 620 nm) spectra of triazole-based DHX-hemicyanine fused dye ***2m*** *in* $CHCl_3$ *(top), EtOH (middle) and PBS + 5% BSA (bottom)*



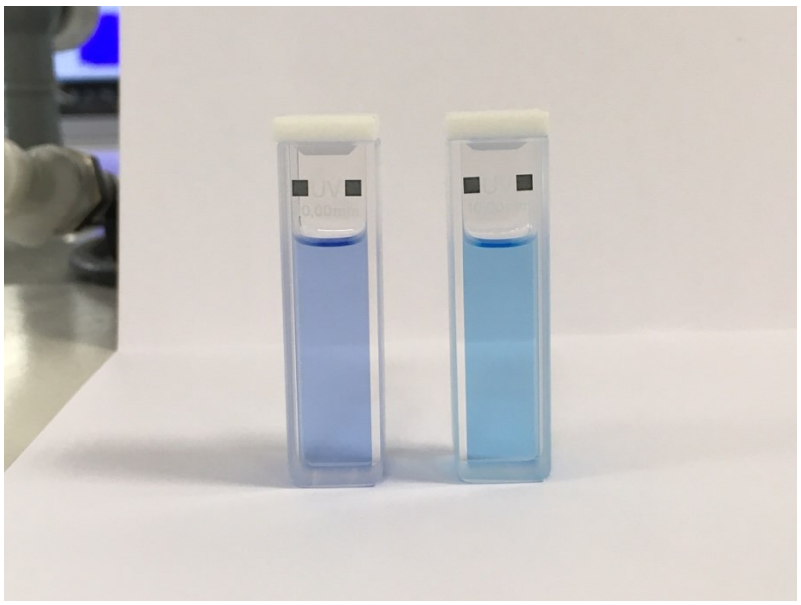
Normalised absorption, excitation (Em at 760 nm), emission (Ex at 620 nm) spectra of triazole-based DHX-hemicyanine fused dye ***2n*** *in* $CHCl_3$ *(top), EtOH (middle) and PBS + 5% BSA (bottom)*



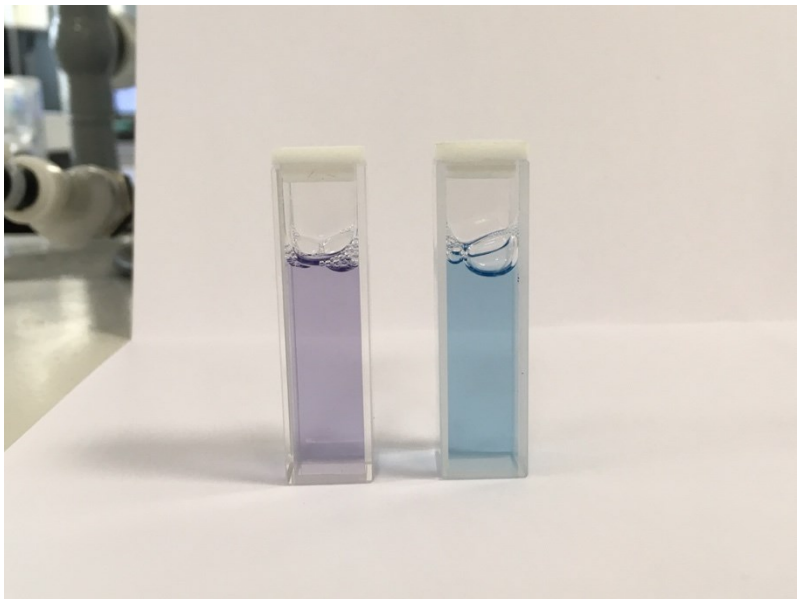
Normalised absorption, excitation (Em at 760 nm), emission (Ex at 620 nm) spectra of triazole-based DHX-hemicyanine fused dye ***2o*** *in EtOH*



Picture of $CHCl_3$ *solutions (concentration: 5.0 μM) of DHX-hemicyanine fused dyes: alkyne* ***1*** *(left) and triazole derivative* ***2o*** *(right)*

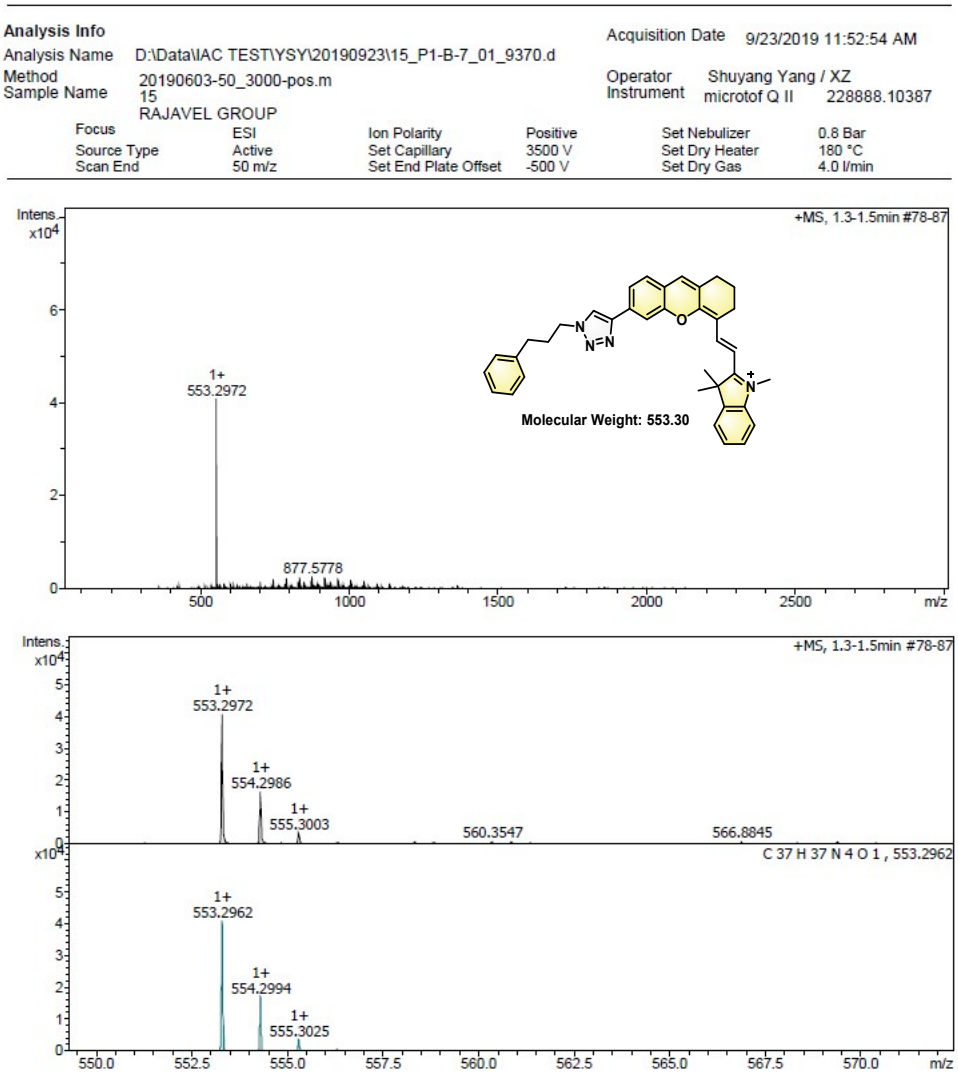


*Picture of PBS + 5% BSA solutions (concentration: 5.0 μM) of DHX-hemicyanine fused dyes: alkyne **1** (left) and triazole derivative **2o** (right)*



8. HRMS data of DHX-hemicyanine fused dyes (alkyne and triazole derivatives)

Triazole-based DHX-hemicyanine fused dye 2a



Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
553.297200	1	C37H37N4O	80.10	553.296188	1.0	1.8	9.5	21.5	even	ok	M

Calibration Info:

Date: 9/25/2019 4:23:22 PM
Polarity: Positive
Calibration spectrum: +MS, 4.6-4.7min #274-278: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290	622.0290	26078	0.097
922.0098	922.0095	63479	-0.366
1221.9906	1221.9910	86996	0.326
1521.9715	1521.9718	80159	0.210
1821.9523	1821.9517	61558	-0.362
2121.9332	2121.9332	39070	0.041
2421.9140	2421.9141	6401	0.055
2721.8948			

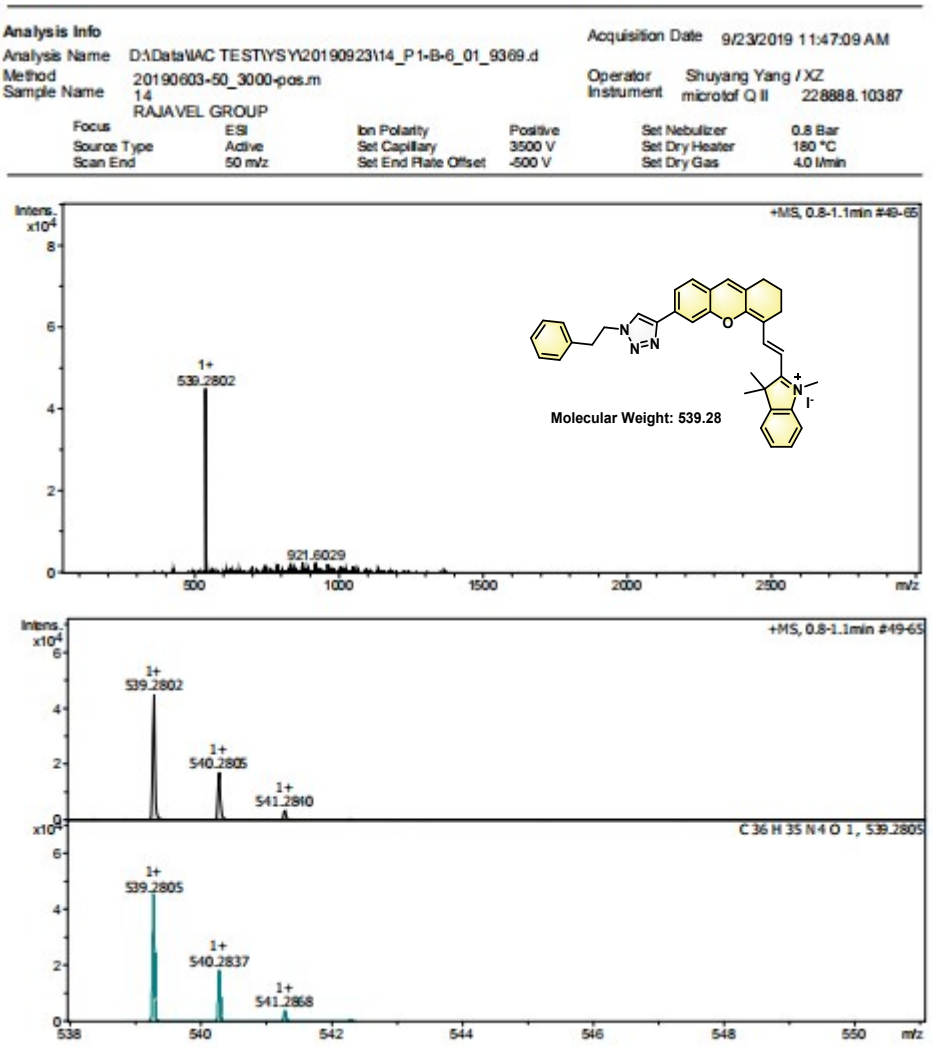
Standard deviation: 0.394

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	553.2972	14683	1729.3	100.0	0.0377
2	554.2986	12900	692.4	40.1	0.0430
3	555.3003	11924	140.8	8.2	0.0466
4	613.4204	12288	33.1	2.2	0.0499
5	657.4491	11435	38.1	2.7	0.0575
6	701.4750	12249	51.3	3.8	0.0573
7	745.5021	14241	66.9	5.2	0.0523
8	746.5052	12770	26.7	2.1	0.0585
9	785.5056	9518	27.8	2.3	0.0825
10	789.5264	12708	66.7	5.5	0.0621
11	790.5288	14568	35.0	2.9	0.0543
12	829.5276	12611	43.1	3.7	0.0658
13	831.5024	12395	25.6	2.2	0.0671
14	833.5533	13364	72.7	6.2	0.0624
15	834.5573	13861	37.7	3.2	0.0602
16	872.6228	12994	24.6	2.2	0.0672
17	873.5543	11245	50.8	4.5	0.0777
18	874.5534	12527	28.9	2.6	0.0698
19	875.5314	12326	32.1	2.8	0.0710
20	877.5778	13014	73.6	6.5	0.0674
21	878.5823	12677	34.9	3.1	0.0693
22	893.5522	14163	26.9	2.4	0.0631
23	897.5357	12660	25.1	2.3	0.0709
24	917.5760	13493	66.6	6.0	0.0680
25	918.5788	11569	28.5	2.6	0.0794
26	919.5573	11271	26.1	2.4	0.0816
27	921.6041	12926	62.7	5.7	0.0713
28	922.6062	13127	33.8	3.1	0.0703
29	937.5769	12747	23.0	2.1	0.0736
30	961.6011	12677	60.4	5.6	0.0759
31	962.6024	13625	35.0	3.3	0.0706
32	963.5901	12360	23.3	2.2	0.0780
33	965.6291	13186	49.0	4.6	0.0732
34	966.6290	12987	26.0	2.4	0.0744
35	1005.6267	13589	51.9	5.0	0.0740
36	1006.6295	13455	28.0	2.7	0.0748
37	1009.6518	12958	32.7	3.1	0.0779
38	1049.6535	13547	42.2	4.1	0.0775
39	1053.6786	13898	21.5	2.1	0.0758
40	1093.6812	13105	29.9	3.0	0.0835

#	m/z	Res.	S/N	I %	FWHM
1	553.2962	14683		100.0	0.0377
2	554.2994	14709		41.9	0.0377
3	555.3025	14736		8.8	0.0377
4	556.3056	14762		1.2	0.0377

Triazole-based DHX-hemicyanine fused dye 2b



Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
539.280163	1	C36H35N4O	100.00	539.280538	-0.4	-0.7	13.2	21.5	even	ok	M

Calibration Info:

Date: 9/25/2019 4:19:47 PM
Polarity: Positive
Calibration spectrum: +MS, 4.6-4.7min #272-278: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290	622.0290	24386	0.008
922.0098	922.0097	60434	-0.105
1221.9906	1221.9909	82075	0.225
1521.9715	1521.9717	76151	0.128
1821.9523	1821.9508	54660	-0.810
2121.9332	2121.9349	33875	0.814
2421.9140	2421.9134	4682	-0.260
2721.8948			

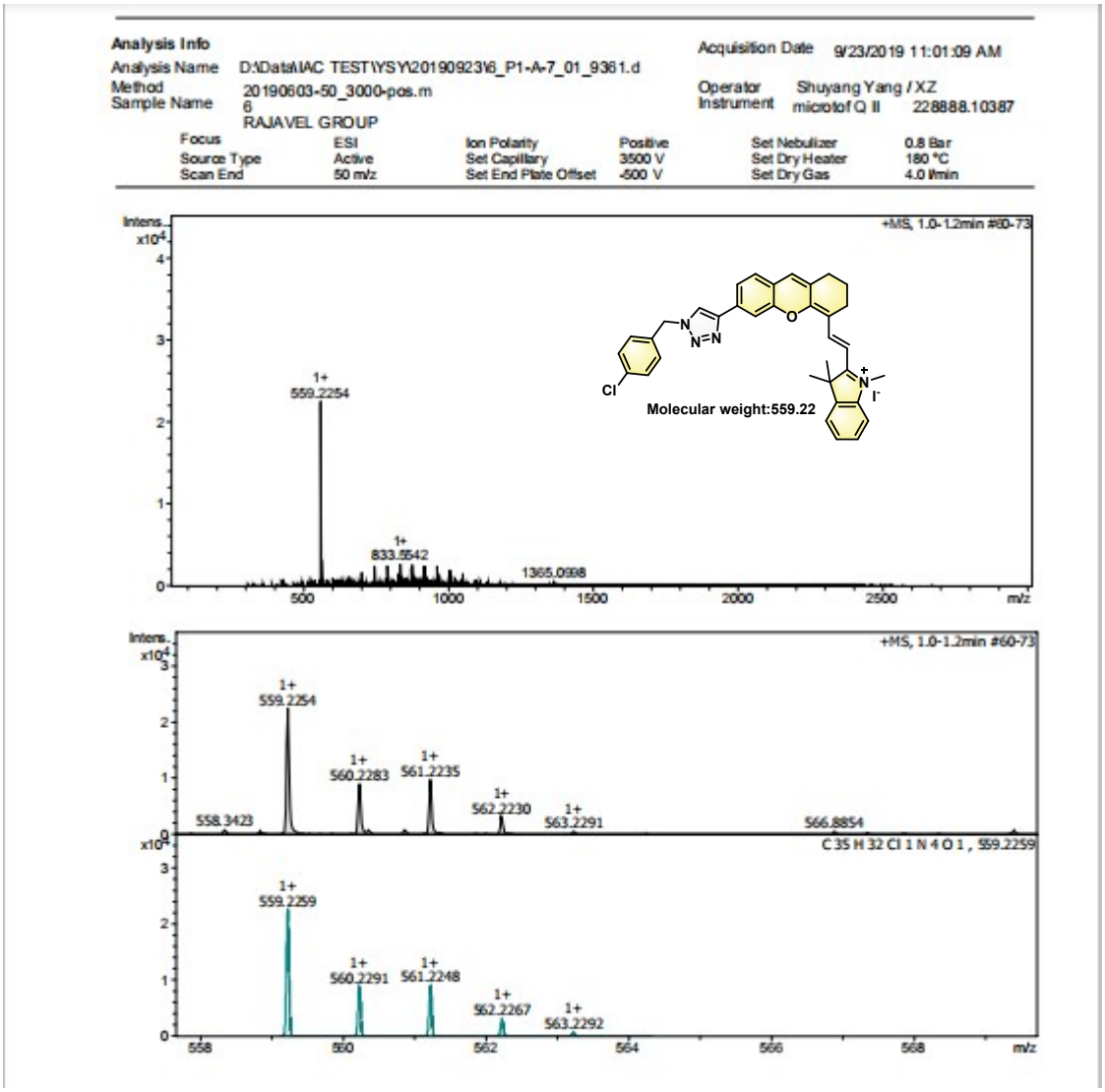
Standard deviation: 0.728

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	430.9094	14346	72.6	2.0	0.0300
2	539.2802	15535	2511.5	100.0	0.0347
3	540.2805	13678	959.5	38.2	0.0395
4	541.2840	12768	195.2	7.8	0.0424
5	613.4210	13000	39.5	1.9	0.0472
6	657.4499	11644	40.5	2.1	0.0565
7	701.4742	13835	56.9	3.2	0.0507
8	745.5016	13837	69.0	4.1	0.0539
9	746.5047	13175	30.9	1.9	0.0567
10	785.5056	10199	29.1	1.8	0.0770
11	789.5264	12708	74.1	4.7	0.0621
12	790.5291	13876	35.8	2.3	0.0570
13	829.5292	12677	40.8	2.7	0.0654
14	833.5538	12703	77.0	5.1	0.0656
15	834.5566	14040	40.8	2.7	0.0594
16	849.5247	12763	32.8	2.2	0.0666
17	873.5529	12251	52.7	3.6	0.0713
18	874.5520	13634	27.3	1.9	0.0641
19	877.5764	13135	81.2	5.5	0.0668
20	878.5823	13257	38.3	2.6	0.0663
21	893.5523	12540	36.6	2.5	0.0713
22	917.5788	13125	62.1	4.4	0.0699
23	918.5782	9142	33.0	2.3	0.1005
24	921.6029	14602	79.5	5.6	0.0631
25	922.6067	14737	42.0	3.0	0.0626
26	937.5791	12047	35.2	2.5	0.0778
27	961.6024	13136	64.0	4.7	0.0732
28	962.6042	12302	30.9	2.2	0.0782
29	965.6301	13826	58.5	4.3	0.0698
30	966.6323	12924	33.4	2.4	0.0748
31	981.6041	13202	30.8	2.3	0.0744
32	1005.6293	13042	52.5	4.0	0.0771
33	1006.6298	13354	32.2	2.4	0.0754
34	1009.6557	12959	43.6	3.3	0.0779
35	1010.6585	13468	24.5	1.8	0.0750
36	1025.6317	12545	23.0	1.7	0.0818
37	1049.6543	13232	48.4	3.7	0.0793
38	1050.6559	13348	27.7	2.1	0.0787
39	1053.6817	13363	30.6	2.4	0.0788
40	1093.6769	12704	33.7	2.6	0.0861

#	m/z	Res.	S/N	I %	FWHM
1	539.2805	15535		100.0	0.0347
2	540.2837	15563		40.8	0.0347
3	541.2868	15592		8.3	0.0347
4	542.2899	15621		1.1	0.0347

Triazole-based DHX-hemicyanine fused dye 2c



Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
559.225361	1	C35H32ClN4O	99.46	559.225916	-0.6	-1.0	15.5	21.5	even	ok	M

Calibration Info:

Date: 9/25/2019 10:20:47 AM
Polarity: Positive
Calibration spectrum: +MS, 4.6-4.7min #272-279: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290	622.0289	23619	-0.027
922.0098	922.0099	58266	0.125
1221.9906	1221.9904	77212	-0.233
1521.9715	1521.9719	77408	0.292
1821.9523	1821.9517	50859	-0.325
2121.9332	2121.9337	32493	0.244
2421.9140	2421.9138	4307	-0.075
2721.8948			

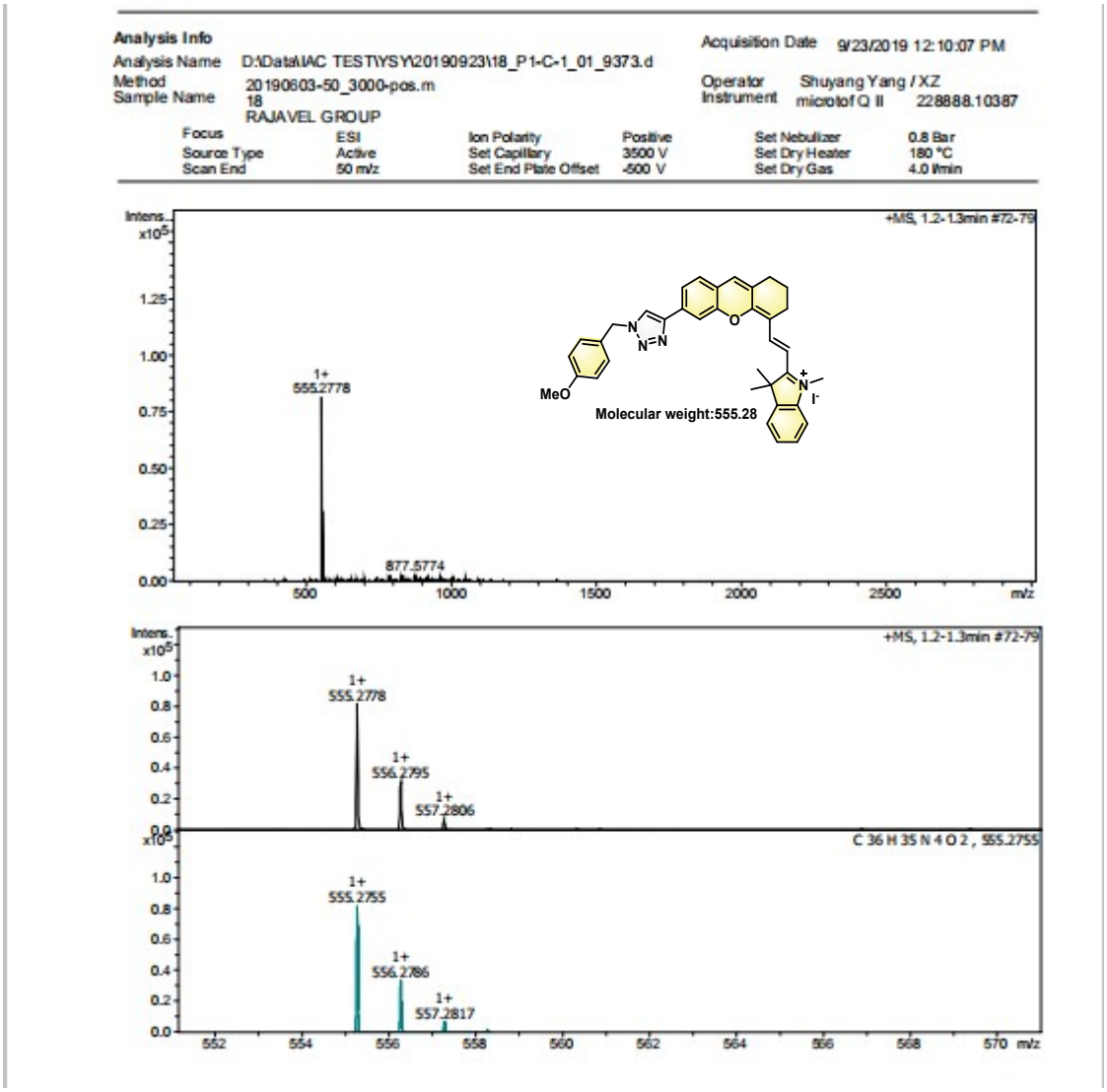
Standard deviation: 0.344

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	559.2254	13389	884.4	100.0	0.0418
2	560.2283	13250	353.6	40.0	0.0423
3	561.2235	14229	380.9	43.3	0.0394
4	562.2230	13510	125.4	14.3	0.0416
5	602.3668	13911	32.4	4.1	0.0433
6	657.4499	12598	35.2	5.0	0.0522
7	701.4771	13583	49.4	7.6	0.0516
8	745.5031	15042	66.0	10.7	0.0496
9	746.5053	14353	26.9	4.4	0.0520
10	785.5057	8781	26.4	4.4	0.0895
11	789.5286	13042	66.9	11.3	0.0605
12	790.5304	14268	31.3	5.3	0.0554
13	828.5994	14450	23.7	4.1	0.0573
14	829.5293	12340	40.0	7.0	0.0672
15	831.5011	11632	24.8	4.3	0.0715
16	833.5542	13137	68.8	12.1	0.0635
17	834.5561	13327	35.2	6.2	0.0626
18	853.5110	13392	26.7	4.8	0.0637
19	873.5533	13457	53.5	9.7	0.0649
20	874.5516	12595	26.6	4.8	0.0694
21	875.5302	11803	29.7	5.4	0.0742
22	876.0247	14833	24.0	4.3	0.0591
23	877.5773	12780	65.4	11.8	0.0687
24	878.5846	13020	32.4	5.9	0.0675
25	897.5390	12027	22.7	4.1	0.0746
26	916.6519	14052	22.3	4.1	0.0652
27	917.5789	12782	58.7	10.8	0.0718
28	918.5825	11392	27.8	5.1	0.0806
29	919.5600	10845	26.3	4.8	0.0848
30	921.6042	13732	59.1	10.8	0.0671
31	922.6071	13464	28.8	5.3	0.0685
32	961.6030	13107	58.6	10.9	0.0734
33	962.6051	13435	32.1	6.0	0.0716
34	963.5909	11428	21.9	4.1	0.0843
35	965.6290	12582	37.5	7.0	0.0767
36	966.6319	14227	24.6	4.6	0.0679
37	1005.6297	13185	46.7	8.8	0.0763
38	1006.6293	12590	25.6	4.8	0.0800
39	1009.6549	13291	26.3	5.0	0.0760
40	1049.6527	13830	37.5	7.1	0.0759

#	m/z	Res.	S/N	I %	FWHM
1	559.2259	13389		100.0	0.0418
2	560.2291	13413		39.7	0.0418
3	561.2248	13437		39.9	0.0418
4	562.2267	13461		13.7	0.0418

Triazole-based DHX-hemicyanine fused dye 2d



Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
555.277836	1	C36H35N4O2	44.03	555.275453	2.4	4.3	13.0	21.5	even	ok	M

Calibration Info:

Date: 9/25/2019 4:42:53 PM
Polarity: Positive
Calibration spectrum: +MS, 4.6-4.6min #272-276: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290	622.0290	23437	0.080
922.0098	922.0095	62023	-0.366
1221.9906	1221.9912	107098	0.482
1521.9715	1521.9716	103490	0.083
1821.9523	1821.9511	75823	-0.665
2121.9332	2121.9342	56879	0.507
2421.9140	2421.9137	12791	-0.121
2721.8948			

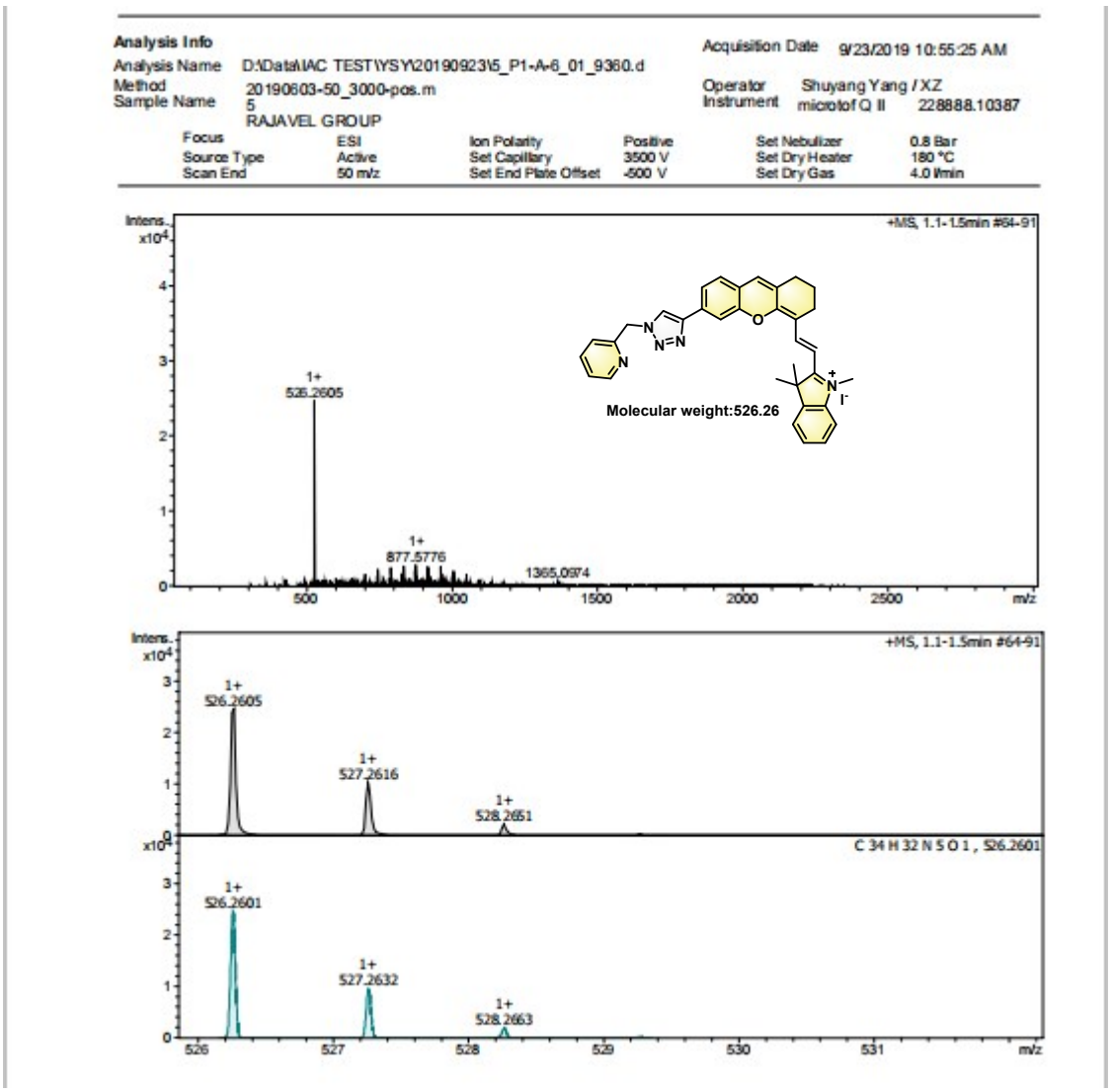
Standard deviation: 0.629

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	555.2778	15981	2947.0	100.0	0.0347
2	556.2795	14165	1129.0	38.4	0.0393
3	557.2806	12655	238.0	8.1	0.0440
4	602.3664	14887	30.5	1.1	0.0405
5	609.1953	12716	37.3	1.4	0.0479
6	613.4207	11996	32.8	1.2	0.0514
7	657.4491	13098	35.8	1.5	0.0502
8	675.3316	12487	36.9	1.5	0.0541
9	701.4769	12365	41.6	1.8	0.0567
10	745.5023	15052	59.0	2.7	0.0495
11	746.5038	15779	27.1	1.2	0.0473
12	785.5033	14568	29.2	1.4	0.0539
13	789.5276	13671	66.7	3.2	0.0578
14	790.5312	14077	31.4	1.5	0.0562
15	828.5984	13860	23.6	1.2	0.0598
16	829.5297	13679	37.7	1.8	0.0606
17	831.5073	11191	23.7	1.2	0.0743
18	833.5541	12690	66.0	3.2	0.0657
19	834.5579	12600	31.7	1.6	0.0662
20	873.5552	11743	47.0	2.4	0.0744
21	874.5536	13200	26.8	1.4	0.0663
22	875.5333	15914	29.2	1.5	0.0550
23	877.5774	15283	69.5	3.5	0.0574
24	878.5833	14289	36.8	1.9	0.0615
25	893.5527	16965	22.8	1.2	0.0527
26	897.5371	13200	22.4	1.1	0.0680
27	917.5786	10959	46.8	2.4	0.0837
28	918.5823	11024	26.8	1.4	0.0833
29	919.5626	10849	23.8	1.2	0.0848
30	921.6048	13145	55.5	2.9	0.0701
31	922.6086	13374	29.9	1.5	0.0690
32	961.6015	14921	53.8	2.8	0.0644
33	962.6037	13328	27.2	1.4	0.0722
34	965.6299	13576	39.5	2.1	0.0711
35	966.6300	14419	22.8	1.2	0.0670
36	1005.6304	12605	43.6	2.3	0.0798
37	1006.6296	14791	26.7	1.4	0.0681
38	1009.6549	14616	29.3	1.6	0.0691
39	1049.6524	14364	35.6	1.9	0.0731
40	1093.6851	12643	21.5	1.2	0.0865

#	m/z	Res.	S/N	I %	FWHM
1	555.2755	15981		100.0	0.0347
2	556.2786	16010		40.8	0.0347
3	557.2817	16039		8.5	0.0347
4	558.2846	16068		1.2	0.0347

Triazole-based DHX-hemicyanine fused dye 2e



Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
526.260471	1	C34H32N5O	100.00	526.260137	-0.3	-0.6	14.4	21.5	even	ok	M

Calibration Info:

Date:	9/25/2019 10:24:08 AM
Polarity:	Positive
Calibration spectrum:	+MS, 4.6-4.7min #273-277: Scan
Reference mass list:	ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode:	Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290	622.0290	30644	-0.011
922.0098	922.0098	75322	0.022
1221.9906	1221.9906	106342	-0.021
1521.9715	1521.9717	98841	0.176
1821.9523	1821.9515	65053	-0.461
2121.9332	2121.9341	44150	0.433
2421.9140	2421.9137	6136	-0.139
2721.8948			

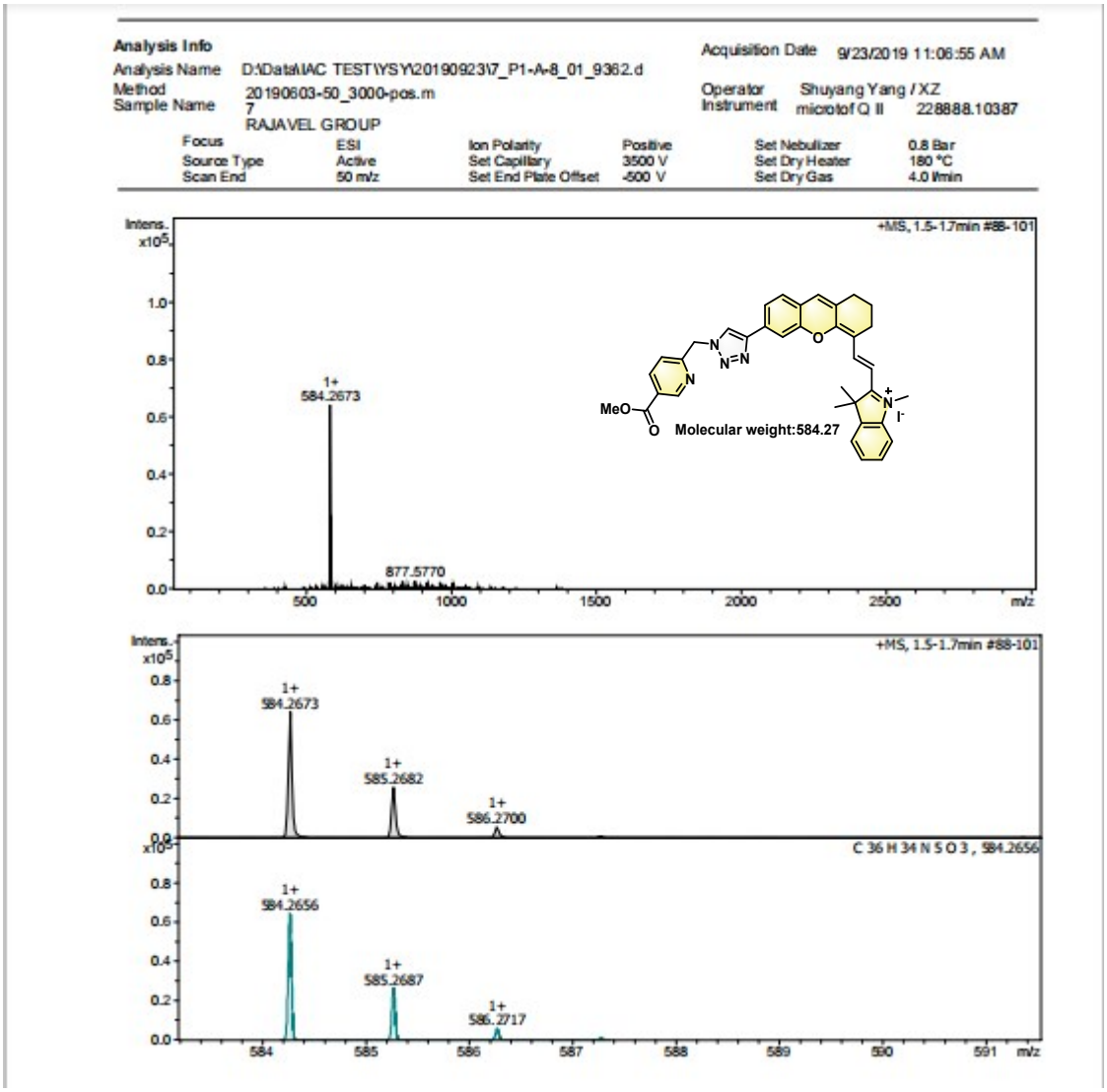
Standard deviation: 0.404

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	526.2605	13516	1375.4	100.0	0.0389
2	527.2616	12426	572.2	41.7	0.0424
3	528.2651	13188	118.7	8.7	0.0401
4	538.3436	14460	50.8	3.8	0.0372
5	602.3669	15605	47.8	4.3	0.0386
6	613.4211	12383	42.3	3.9	0.0495
7	657.4496	12425	45.7	4.7	0.0529
8	701.4757	13175	60.0	6.5	0.0532
9	745.5017	14167	81.2	9.3	0.0526
10	746.5037	14164	35.6	4.1	0.0527
11	785.5042	12318	35.3	4.2	0.0638
12	789.5272	13278	86.2	10.4	0.0595
13	790.5297	13838	40.9	4.9	0.0580
14	829.5271	12787	55.0	6.9	0.0649
15	831.5036	11076	32.0	4.0	0.0751
16	833.5546	12699	88.4	11.1	0.0656
17	834.5567	13845	47.0	5.9	0.0603
18	853.5108	14641	35.5	4.5	0.0583
19	872.6231	15063	31.8	4.1	0.0579
20	873.5521	12513	66.7	8.5	0.0698
21	874.5526	12822	36.7	4.7	0.0693
22	875.5324	12442	40.5	5.2	0.0704
23	876.0245	14032	29.4	3.8	0.0624
24	877.5776	13169	91.0	11.7	0.0666
25	878.5823	13430	43.5	5.6	0.0654
26	897.5349	13003	32.9	4.3	0.0690
27	917.5769	13013	80.1	10.5	0.0705
28	918.5797	12166	38.1	5.0	0.0755
29	919.5589	10204	33.1	4.4	0.0901
30	921.6030	13341	74.3	9.8	0.0691
31	922.6063	14616	41.4	5.5	0.0631
32	961.6015	13695	78.6	10.6	0.0702
33	962.6029	12205	37.5	5.1	0.0789
34	963.5888	13155	32.1	4.3	0.0732
35	965.6277	13024	50.7	6.9	0.0741
36	966.6312	13409	30.4	4.1	0.0721
37	1005.6288	13609	62.1	8.6	0.0739
38	1006.6292	13575	34.8	4.8	0.0742
39	1009.6537	13534	34.4	4.7	0.0746
40	1049.6530	12612	47.1	6.6	0.0832

#	m/z	Res.	S/N	I %	FWHM
1	526.2601	13516		100.0	0.0389
2	527.2632	13542		39.0	0.0389
3	528.2663	13567		7.6	0.0389
4	529.2693	13593		1.0	0.0389

Triazole-based DHX-hemicyanine fused dye 2f



Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
584.267335	1	C39H34N5O3	51.68	584.265616	1.7	2.9	5.5	22.5	even	ok	M

Calibration Info:

Date: 9/25/2019 10:35:49 AM
Polarity: Positive
Calibration spectrum: +MS, 4.6-4.7min #273-277: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290	622.0289	29697	-0.113
922.0098	922.0102	73417	0.410
1221.9906	1221.9901	99026	-0.410
1521.9715	1521.9717	97595	0.121
1821.9523	1821.9517	65759	-0.334
2121.9332	2121.9344	43926	0.570
2421.9140	2421.9134	6844	-0.244
2721.8948			

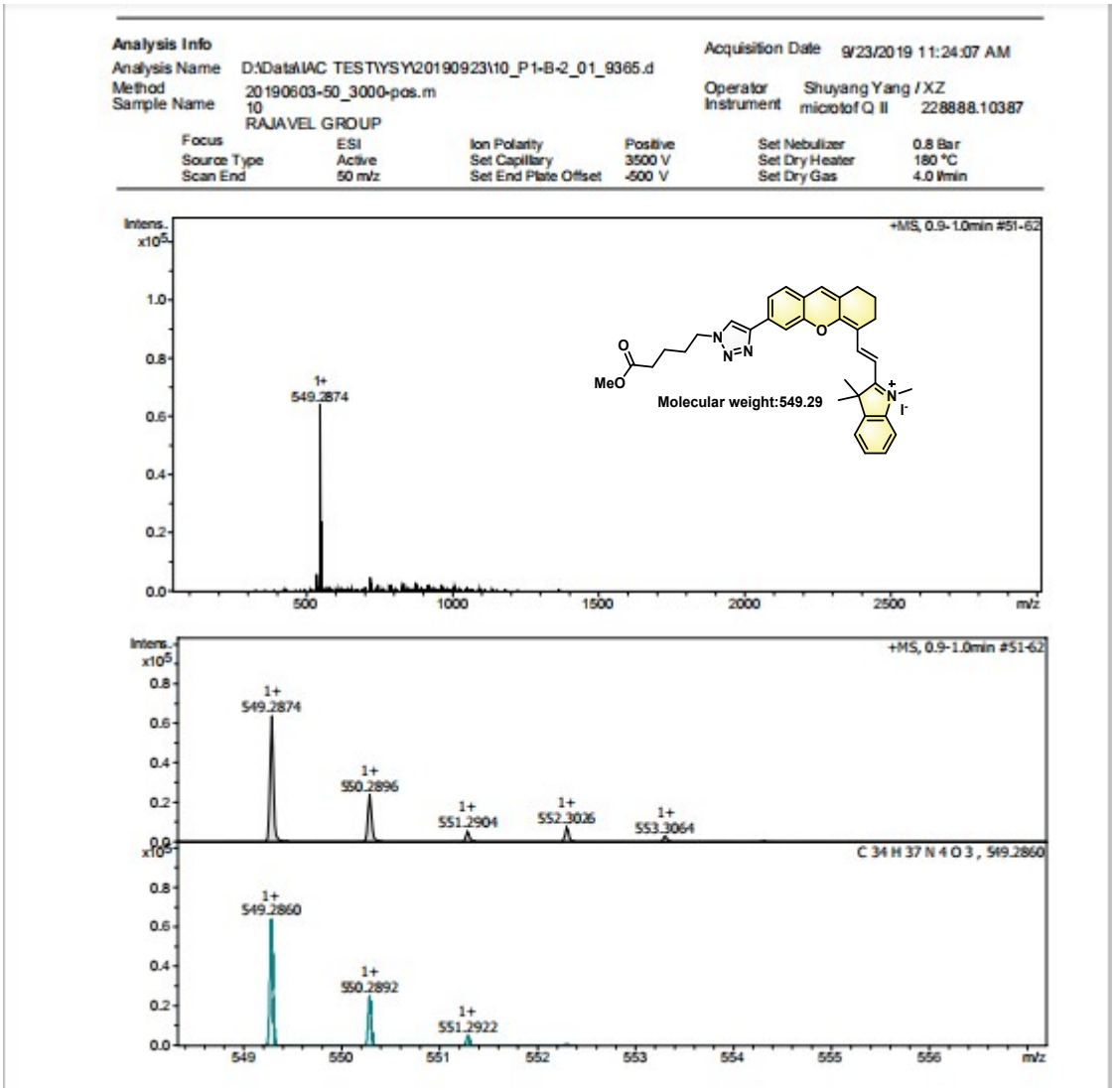
Standard deviation: 0.558

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	584.2673	16090	2779.7	100.0	0.0363
2	585.2682	14073	1115.3	40.2	0.0416
3	586.2700	13468	236.8	8.5	0.0435
4	602.3654	16850	43.5	1.6	0.0357
5	613.4202	14678	42.5	1.6	0.0418
6	657.4487	12543	45.0	1.9	0.0524
7	701.4763	13238	56.9	2.5	0.0530
8	745.5030	14039	77.5	3.7	0.0531
9	746.5045	14044	32.1	1.5	0.0532
10	785.5029	11104	32.9	1.6	0.0707
11	789.5264	13422	79.8	4.0	0.0588
12	790.5298	13258	39.4	2.0	0.0596
13	828.5966	15477	28.4	1.5	0.0535
14	829.5266	13409	50.0	2.6	0.0619
15	831.5016	12872	32.7	1.7	0.0646
16	833.5536	13343	83.9	4.4	0.0625
17	834.5552	13959	44.3	2.3	0.0598
18	853.5094	14762	33.2	1.7	0.0578
19	872.6218	14373	28.5	1.5	0.0607
20	873.5520	13853	68.5	3.7	0.0631
21	874.5529	11793	29.7	1.6	0.0742
22	875.5308	10796	31.2	1.7	0.0811
23	876.0254	16144	28.1	1.5	0.0543
24	877.5770	13422	85.5	4.6	0.0654
25	878.5840	13036	41.2	2.2	0.0674
26	897.5375	13216	28.6	1.6	0.0679
27	917.5783	12396	69.7	3.8	0.0740
28	918.5801	11327	32.5	1.8	0.0811
29	919.5591	11439	31.8	1.7	0.0804
30	921.6030	13620	69.0	3.8	0.0677
31	922.6050	14212	38.0	2.1	0.0649
32	961.6010	14421	71.8	4.0	0.0667
33	962.6024	13113	33.9	1.9	0.0734
34	963.5891	12747	26.1	1.5	0.0756
35	965.6278	13231	48.7	2.7	0.0730
36	966.6297	14519	26.4	1.5	0.0666
37	1005.6280	13858	55.4	3.2	0.0726
38	1006.6302	12084	26.9	1.5	0.0834
39	1009.6548	12849	30.3	1.7	0.0786
40	1049.6523	15476	44.6	2.6	0.0678

#	m/z	Res.	S/N	I %	FWHM
1	584.2656	16090		100.0	0.0363
2	585.2687	16118		41.3	0.0363
3	586.2717	16146		8.9	0.0363
4	587.2746	16173		1.3	0.0363

Triazole-based DHX-hemicyanine fused dye 2g



Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
549.287409	1	C34H37N4O3	49.54	549.286017	1.4	2.5	55.2	18.5	even	ok	M

Calibration Info:

Date: 9/25/2019 11:00:11 AM
Polarity: Positive
Calibration spectrum: +MS, 4.6-4.7min #273-277: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290	622.0289	28355	-0.061
922.0098	922.0099	71603	0.150
1221.9906	1221.9906	97729	-0.012
1521.9715	1521.9716	87493	0.085
1821.9523	1821.9509	62855	-0.785
2121.9332	2121.9352	42031	0.980
2421.9140	2421.9131	5726	-0.357
2721.8948			

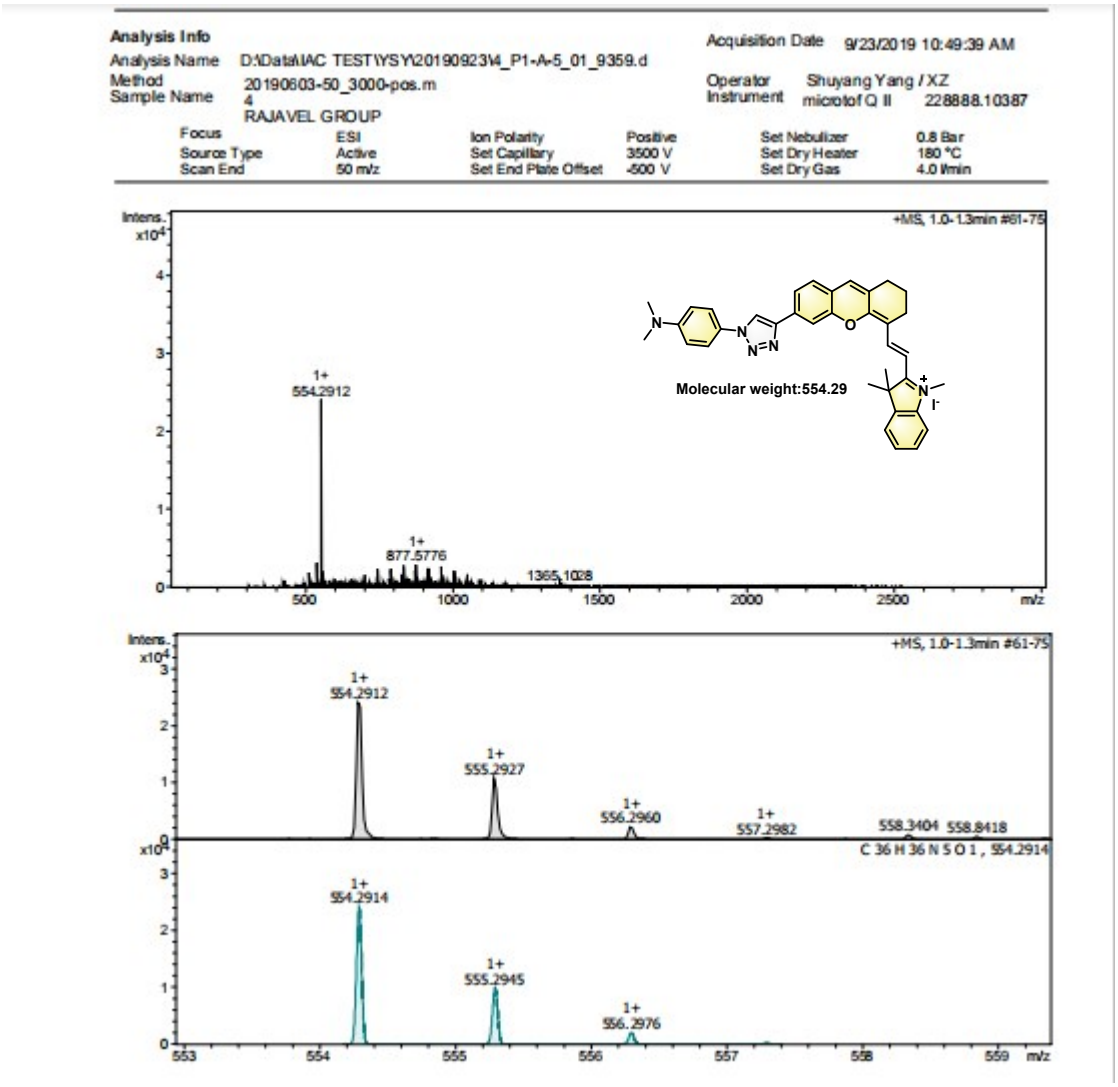
Standard deviation: 0.793

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	535.2681	13353	223.8	9.2	0.0401
2	536.2764	10962	81.5	3.4	0.0489
3	549.2874	15853	2352.1	100.0	0.0346
4	550.2896	13658	883.7	37.7	0.0403
5	551.2904	13622	199.6	8.5	0.0405
6	552.3026	14123	283.4	12.1	0.0391
7	553.3064	13073	101.6	4.3	0.0423
8	613.4187	12506	29.5	1.4	0.0490
9	657.4495	11414	31.7	1.7	0.0576
10	701.4763	12138	41.4	2.3	0.0578
11	720.3871	14076	132.8	7.6	0.0512
12	721.3928	11849	79.3	4.6	0.0609
13	722.3975	11273	28.9	1.7	0.0641
14	723.4056	11920	38.2	2.2	0.0607
15	745.5018	15524	61.6	3.6	0.0480
16	746.5061	14283	26.0	1.5	0.0523
17	785.5051	12154	25.2	1.5	0.0646
18	789.5267	13529	63.7	3.9	0.0584
19	790.5284	14096	29.9	1.8	0.0561
20	828.5985	15658	23.0	1.5	0.0529
21	829.5289	12579	34.1	2.1	0.0659
22	833.5537	12804	64.3	4.1	0.0651
23	834.5566	12951	32.7	2.1	0.0644
24	872.6214	13942	23.5	1.5	0.0626
25	873.5555	8381	41.6	2.7	0.1042
26	875.5324	11108	23.7	1.5	0.0788
27	877.5776	13349	64.8	4.2	0.0657
28	878.5823	13570	31.2	2.0	0.0647
29	917.5797	13419	51.5	3.4	0.0684
30	918.5789	12918	27.6	1.8	0.0711
31	921.6031	13874	54.8	3.6	0.0664
32	922.6070	17009	33.8	2.2	0.0542
33	961.6024	12751	49.8	3.3	0.0754
34	962.6034	11005	22.5	1.5	0.0875
35	965.6310	13184	39.3	2.6	0.0732
36	1005.6297	13654	43.3	2.9	0.0736
37	1006.6290	13481	24.8	1.7	0.0747
38	1009.6539	13836	28.4	1.9	0.0730
39	1049.6549	12419	33.1	2.2	0.0845
40	1093.6779	11070	20.5	1.4	0.0988

#	m/z	Res.	S/N	I %	FWHM
1	549.2860	15853		100.0	0.0346
2	550.2892	15882		38.8	0.0346
3	551.2922	15911		7.9	0.0346
4	552.2955	15940		1.1	0.0346

Triazole-based DHX-hemicyanine fused dye 2h



Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
554.291232	1	C36H36N5O	100.00	554.291437	0.2	0.4	18.3	21.5	even	ok	M

Calibration Info:

Date: 9/24/2019 4:56:39 PM
Polarity: Positive
Calibration spectrum: +MS, 4.6-4.7min #272-280: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290	622.0289	21308	-0.091
922.0098	922.0101	52188	0.328
1221.9906	1221.9902	71478	-0.320
1521.9715	1521.9716	70121	0.102
1821.9523	1821.9517	46504	-0.316
2121.9332	2121.9342	31318	0.511
2421.9140	2421.9135	3991	-0.214
2721.8948			

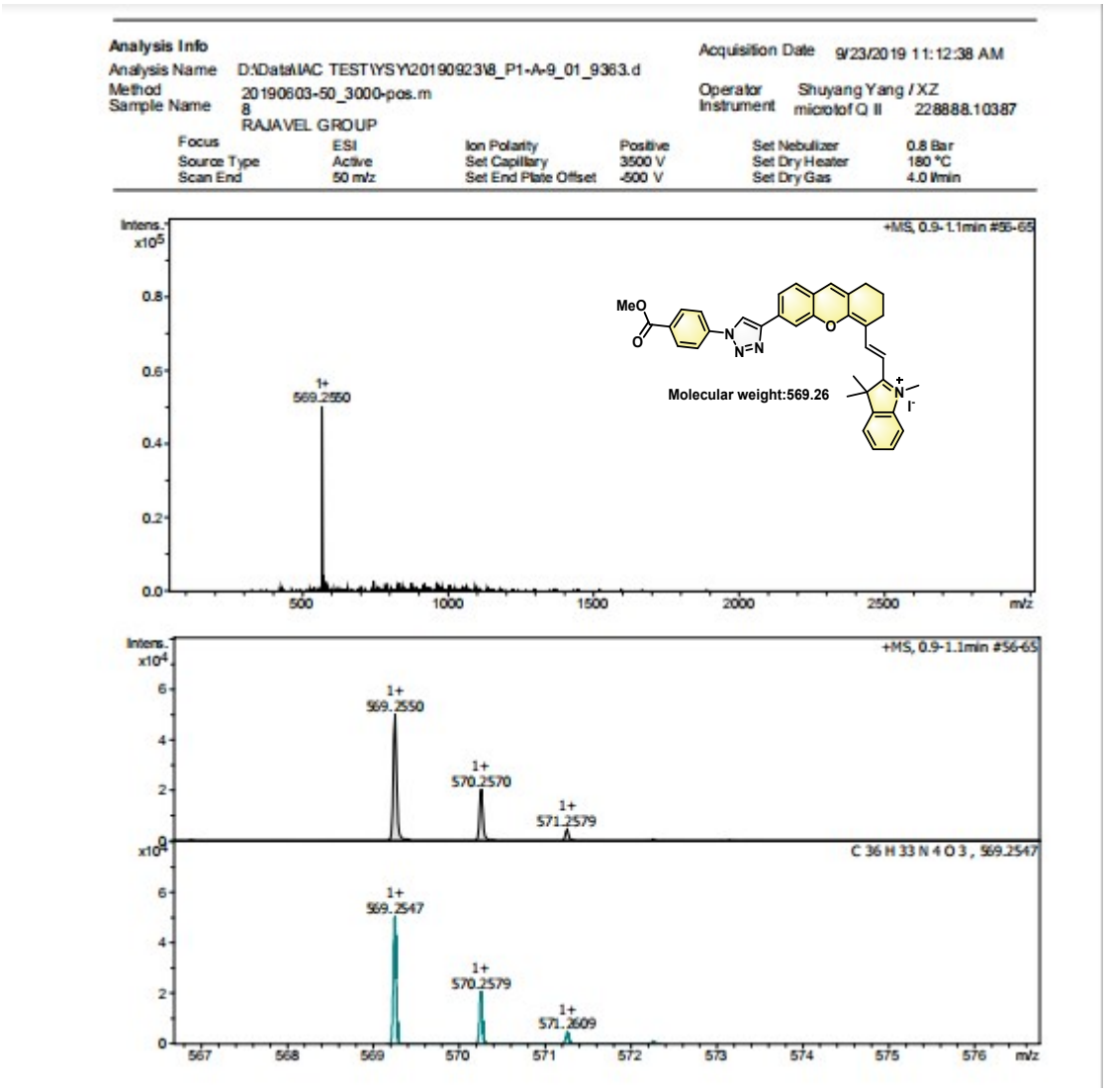
Standard deviation: 0.480

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	430.9107	13662	58.1	4.0	0.0315
2	511.2599	13018	88.9	7.9	0.0393
3	539.2673	12180	74.3	7.2	0.0443
4	540.2717	13546	135.3	13.2	0.0399
5	541.2775	12459	46.6	4.5	0.0434
6	554.2912	12873	993.4	100.0	0.0431
7	555.2927	13733	444.2	44.8	0.0404
8	556.2960	12460	90.4	9.1	0.0446
9	602.3652	14825	36.5	4.2	0.0406
10	657.4494	11586	35.2	4.5	0.0567
11	701.4755	12458	48.6	6.7	0.0563
12	745.5030	14245	66.8	9.7	0.0523
13	746.5043	13386	28.5	4.1	0.0558
14	785.5046	10215	30.1	4.5	0.0769
15	789.5292	12868	66.5	10.0	0.0614
16	790.5309	13322	33.4	5.1	0.0593
17	829.5295	12249	46.5	7.3	0.0677
18	831.5050	13324	30.0	4.7	0.0624
19	833.5554	13450	74.0	11.6	0.0620
20	834.5568	12283	33.3	5.2	0.0679
21	853.5109	12920	28.5	4.5	0.0661
22	873.5536	12958	54.9	8.8	0.0674
23	874.5542	12352	27.8	4.5	0.0708
24	875.5327	11431	31.9	5.1	0.0766
25	877.5776	14161	75.8	12.2	0.0620
26	878.5836	13524	36.4	5.9	0.0650
27	917.5795	12918	64.7	10.5	0.0710
28	918.5812	11140	30.0	4.9	0.0825
29	919.5813	11132	27.0	4.4	0.0826
30	921.6049	12548	58.1	9.5	0.0734
31	922.6060	15154	34.7	5.6	0.0609
32	961.6029	13916	68.0	11.3	0.0691
33	962.6039	13382	32.9	5.4	0.0719
34	963.5912	12244	23.9	4.0	0.0787
35	965.6304	13062	41.1	6.8	0.0739
36	1005.6318	13674	51.9	8.8	0.0735
37	1006.6290	13683	29.5	5.0	0.0736
38	1009.6545	13280	28.2	4.8	0.0760
39	1049.6553	14219	41.0	7.0	0.0738
40	1093.6798	11710	24.5	4.2	0.0934

#	m/z	Res.	S/N	I %	FWHM
1	554.2914	12873		100.0	0.0431
2	555.2945	12896		41.2	0.0431
3	556.2976	12920		8.5	0.0431
4	557.3007	12943		1.2	0.0431

Triazole-based DHX-hemicyanine fused dye 2i



Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
569.255034	1	C36H33N4O3	100.00	569.254717	0.3	0.6	1.5	22.5	even	ok	M

Calibration Info:

Date:	9/25/2019 10:57:59 AM
Polarity:	Positive
Calibration spectrum:	+MS, 4.6-4.7min #273-277: Scan
Reference mass list:	ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode:	Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290	622.0290	29247	-0.001
922.0098	922.0098	74970	-0.003
1221.9906	1221.9906	99646	-0.042
1521.9715	1521.9719	91966	0.263
1821.9523	1821.9514	64734	-0.497
2121.9332	2121.9340	42327	0.394
2421.9140	2421.9137	5962	-0.113
2721.8948			

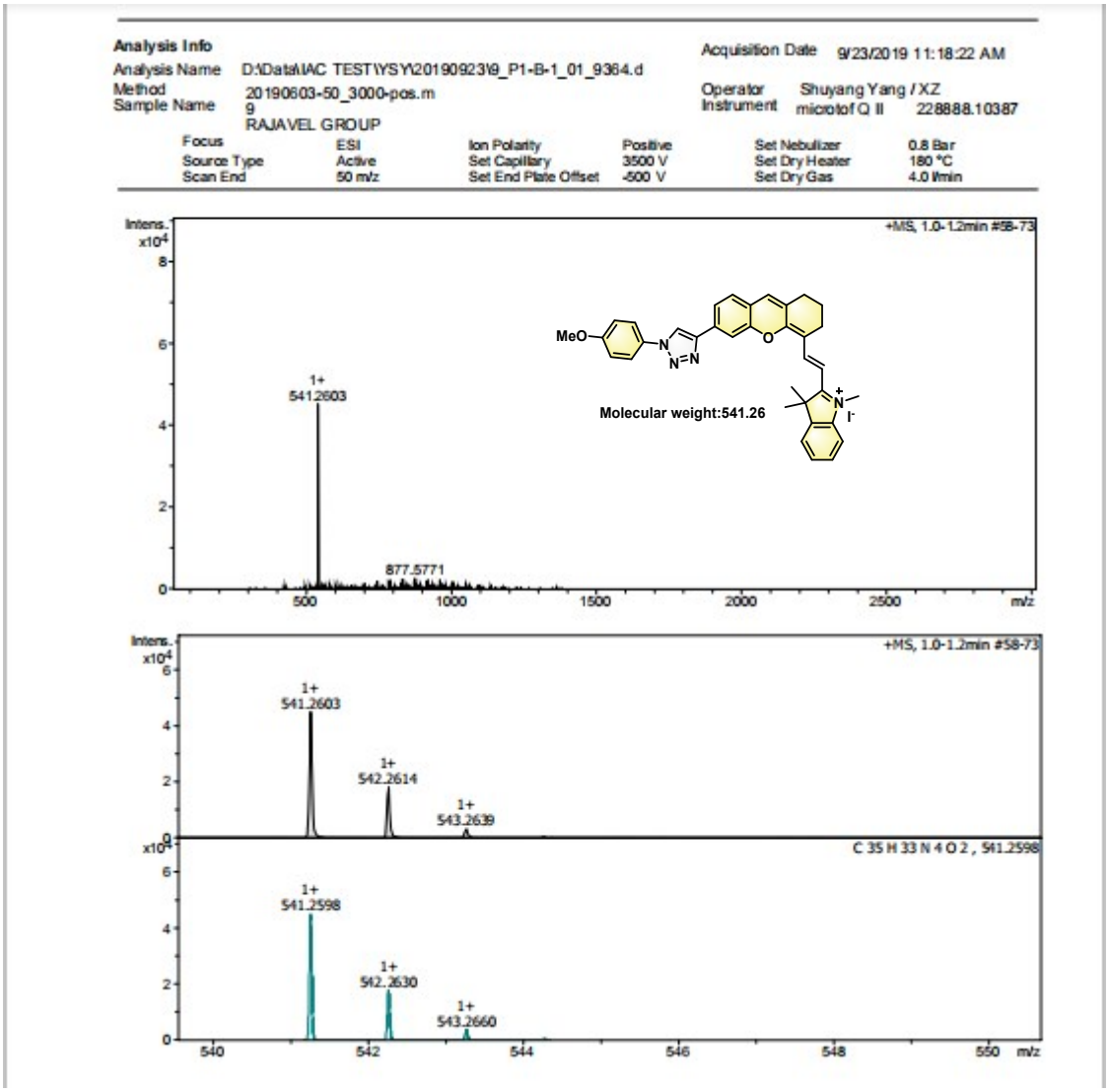
Standard deviation: 0.420

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	430.9089	18579	48.0	1.8	0.0232
2	541.2447	11688	45.9	2.2	0.0463
3	569.2550	15205	1912.3	100.0	0.0374
4	570.2570	13368	776.4	40.6	0.0427
5	571.2579	13491	169.2	8.9	0.0423
6	584.2635	12033	98.5	5.3	0.0486
7	585.2657	14491	50.8	2.7	0.0404
8	613.4208	13607	28.8	1.6	0.0451
9	657.4492	14132	33.0	2.0	0.0465
10	701.4762	14823	43.4	2.9	0.0473
11	745.5024	14761	56.8	3.9	0.0505
12	746.3047	15084	78.8	5.5	0.0495
13	747.3074	15315	44.8	3.1	0.0488
14	789.5270	13163	60.2	4.4	0.0600
15	790.5301	13758	26.7	1.9	0.0575
16	829.5309	12165	27.2	2.1	0.0682
17	833.5548	13221	60.7	4.6	0.0630
18	834.5572	15802	35.6	2.7	0.0528
19	849.5270	13027	27.1	2.1	0.0652
20	873.5556	12941	38.0	3.0	0.0675
21	877.5776	13278	61.8	4.8	0.0661
22	878.5815	12831	30.5	2.4	0.0685
23	893.5522	12660	29.1	2.3	0.0706
24	917.5804	12203	44.0	3.5	0.0752
25	918.5801	10754	22.2	1.8	0.0854
26	921.6045	12581	53.8	4.3	0.0733
27	922.6087	13452	30.9	2.5	0.0686
28	937.5781	14737	30.2	2.5	0.0636
29	961.6019	16305	52.2	4.3	0.0590
30	962.6062	13249	23.9	2.0	0.0727
31	965.6295	13772	45.5	3.8	0.0701
32	966.6315	12400	25.0	2.1	0.0780
33	981.6055	11835	24.3	2.0	0.0829
34	1005.6312	14409	41.9	3.6	0.0698
35	1006.6325	14671	23.3	2.0	0.0686
36	1009.6564	14238	35.0	3.0	0.0709
37	1025.6316	11522	19.0	1.6	0.0890
38	1049.6562	14118	36.0	3.1	0.0743
39	1053.6825	13545	26.9	2.3	0.0778
40	1093.6805	12552	23.0	2.0	0.0871

#	m/z	Res.	S/N	I %	FWHM
1	569.2547	15205		100.0	0.0374
2	570.2579	15232		40.9	0.0374
3	571.2609	15259		8.8	0.0374
4	572.2638	15286		1.3	0.0374

Triazole-based DHX-hemicyanine fused dye 2j



Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
541.260340	1	C35H33N4O2	100.00	541.259803	0.5	1.0	6.0	21.5	even	ok	M

Calibration Info:

Date: 9/25/2019 10:58:59 AM
Polarity: Positive
Calibration spectrum: +MS, 4.6-4.6min #273-276: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290	622.0290	28911	0.061
922.0098	922.0096	73650	-0.258
1221.9906	1221.9910	101567	0.262
1521.9715	1521.9719	92334	0.262
1821.9523	1821.9511	64064	-0.679
2121.9332	2121.9341	43296	0.452
2421.9140	2421.9137	6242	-0.099
2721.8948			

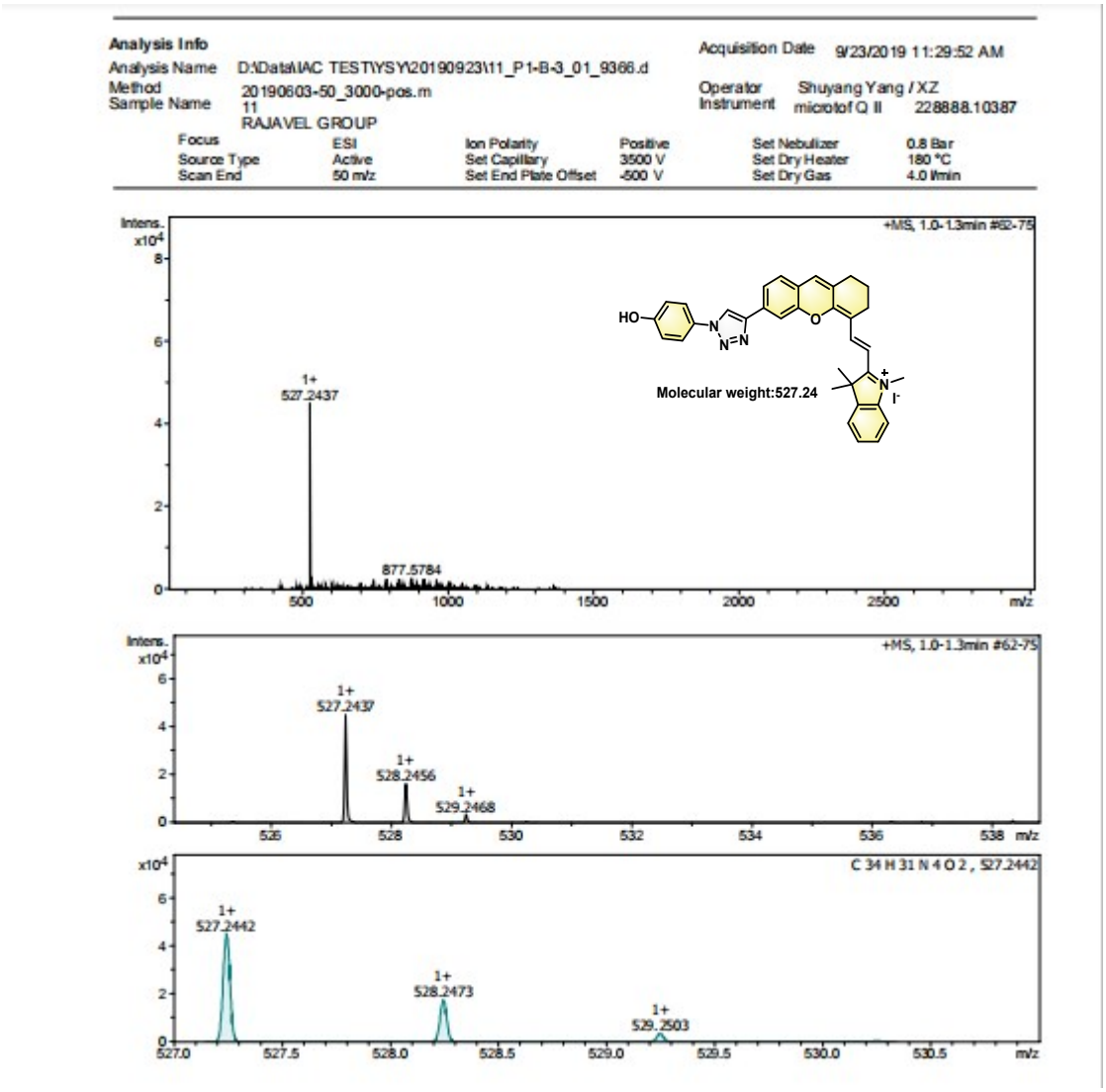
Standard deviation: 0.565

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	513.2505	14316	50.6	2.2	0.0359
2	541.2603	15042	2112.3	100.0	0.0360
3	542.2614	14208	854.0	40.4	0.0382
4	543.2639	11926	150.1	7.1	0.0456
5	602.3671	17981	36.3	2.0	0.0335
6	613.4203	12290	33.4	1.9	0.0499
7	657.4483	12814	37.3	2.3	0.0513
8	701.4770	13266	51.7	3.5	0.0529
9	745.5025	13625	65.5	4.6	0.0547
10	746.5046	13616	28.4	2.0	0.0548
11	785.5072	11755	28.2	2.1	0.0668
12	789.5270	13501	73.0	5.4	0.0585
13	790.5284	14139	35.1	2.6	0.0559
14	828.5985	12876	25.9	2.0	0.0644
15	829.5272	12567	41.2	3.1	0.0660
16	833.5554	12889	75.3	5.8	0.0647
17	834.5557	12774	34.1	2.6	0.0653
18	873.5536	13726	54.3	4.3	0.0636
19	874.5531	12714	27.8	2.2	0.0688
20	875.5339	11147	24.4	1.9	0.0785
21	877.5771	13415	75.5	6.0	0.0654
22	878.5822	13572	37.0	2.9	0.0647
23	893.5518	12960	25.0	2.0	0.0689
24	916.6490	13342	23.5	1.9	0.0692
25	917.5793	12511	59.7	4.8	0.0733
26	918.5812	11782	29.9	2.4	0.0780
27	919.5607	11267	26.3	2.1	0.0816
28	921.6030	13181	62.9	5.1	0.0699
29	922.6072	13256	32.5	2.6	0.0696
30	961.6020	14548	65.7	5.4	0.0661
31	962.6057	11833	30.5	2.5	0.0814
32	965.6304	13206	49.0	4.0	0.0731
33	966.6319	14140	29.3	2.4	0.0684
34	1005.6289	13504	53.1	4.5	0.0745
35	1006.6288	12283	28.7	2.4	0.0820
36	1009.6541	13817	35.5	3.0	0.0731
37	1049.6531	13370	42.9	3.7	0.0785
38	1050.6582	11677	22.9	1.9	0.0900
39	1053.6811	13702	23.2	2.0	0.0769
40	1093.6788	12570	26.6	2.3	0.0870

#	m/z	Res.	S/N	I %	FWHM
1	541.2598	15042		100.0	0.0360
2	542.2630	15070		39.7	0.0360
3	543.2660	15097		8.1	0.0360
4	544.2689	15125		1.1	0.0360

Triazole-based DHX-hemicyanine fused dye 2k



Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
527.243687	1	C34H31N4O2	100.00	527.244153	0.5	0.9	11.4	21.5	even	ok	M

Calibration Info:

Date: 9/25/2019 12:57:21 PM
Polarity: Positive
Calibration spectrum: +MS, 4.6-4.6min #274-276: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290	622.0289	28472	-0.138
922.0098	922.0102	74152	0.477
1221.9906	1221.9902	101386	-0.396
1521.9715	1521.9715	95438	-0.010
1821.9523	1821.9517	66975	-0.325
2121.9332	2121.9346	43865	0.706
2421.9140	2421.9132	7167	-0.313
2721.8948			

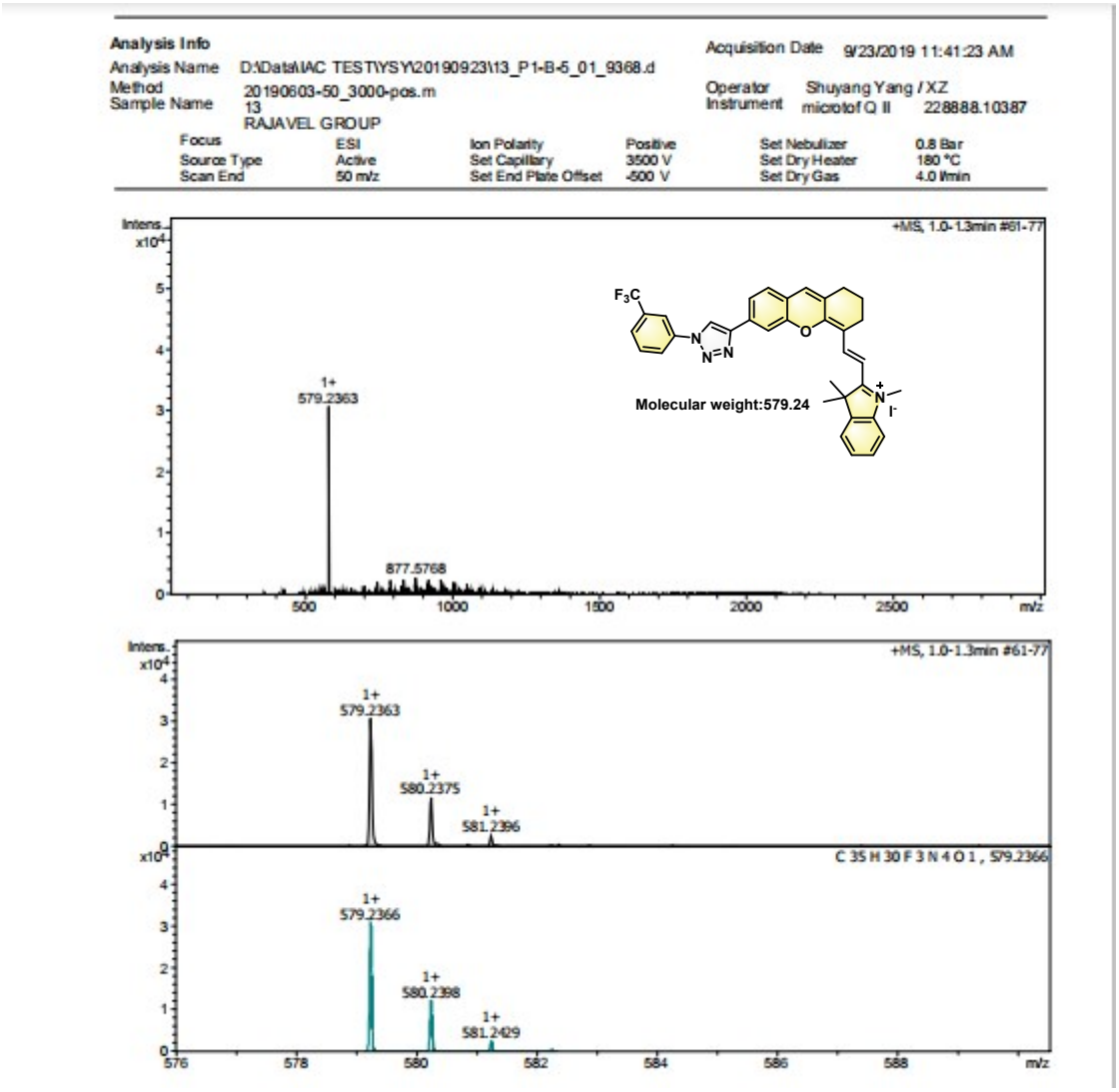
Standard deviation: 0.633

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	484.2120	13432	44.4	2.0	0.0360
2	527.3437	15037	1971.7	100.0	0.0351
3	528.3456	13574	717.1	36.4	0.0389
4	529.3468	13232	141.7	7.2	0.0400
5	613.4198	12642	33.8	2.1	0.0485
6	657.4486	12663	38.6	2.6	0.0519
7	701.4761	13629	50.6	3.7	0.0515
8	745.5027	14407	67.7	5.2	0.0517
9	746.5059	13884	27.9	2.1	0.0538
10	785.5083	10264	31.5	2.5	0.0765
11	789.5273	13319	70.0	5.6	0.0593
12	790.5299	12548	31.3	2.5	0.0630
13	828.5989	14370	25.4	2.1	0.0577
14	829.5279	13077	42.5	3.5	0.0634
15	833.5541	12147	69.3	5.7	0.0686
16	834.5580	12899	35.3	2.9	0.0647
17	853.5109	14717	25.7	2.2	0.0580
18	872.6213	13894	26.0	2.2	0.0628
19	873.5529	13082	51.5	4.4	0.0670
20	874.5538	12731	26.4	2.2	0.0687
21	875.5324	16046	32.9	2.8	0.0546
22	877.5784	13237	73.6	6.3	0.0663
23	878.5844	12940	33.0	2.8	0.0679
24	916.6483	14575	22.3	1.9	0.0629
25	917.5784	12153	59.1	5.2	0.0755
26	918.5801	11817	30.0	2.6	0.0777
27	919.5590	11369	26.6	2.3	0.0809
28	921.6030	13916	64.5	5.6	0.0662
29	922.6065	13479	32.8	2.9	0.0684
30	961.6018	13179	60.7	5.4	0.0730
31	962.6030	12615	29.8	2.7	0.0763
32	963.5896	12883	22.7	2.0	0.0748
33	965.6287	13413	44.9	4.0	0.0720
34	966.6295	14317	26.3	2.3	0.0675
35	1005.6283	13404	47.5	4.3	0.0750
36	1006.6311	13336	28.1	2.5	0.0755
37	1009.6543	14158	31.9	2.9	0.0713
38	1049.6547	12384	35.9	3.3	0.0848
39	1050.6571	14249	23.3	2.1	0.0737
40	1093.6797	12978	25.5	2.3	0.0843

#	m/z	Res.	S/N	I %	FWHM
1	527.2442	15037		100.0	0.0351
2	528.2473	15086		38.6	0.0351
3	529.2503	15094		7.6	0.0351
4	530.2538	15123		1.0	0.0351

Triazole-based DHX-hemicyanine fused dye 2l



Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
579.236305	1	C35H30F3N4O	100.00	579.236623	0.3	0.5	9.5	21.5	even	ok	M

Calibration Info:

Date: 9/25/2019 1:06:04 PM
Polarity: Positive
Calibration spectrum: +MS, 4.6-4.7min #272-277: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290	622.0290	25017	-0.013
922.0098	922.0099	64876	0.068
1221.9906	1221.9904	86483	-0.168
1521.9715	1521.9719	77379	0.300
1821.9523	1821.9516	57174	-0.373
2121.9332	2121.9337	36688	0.259
2421.9140	2421.9138	5296	-0.072
2721.8948			

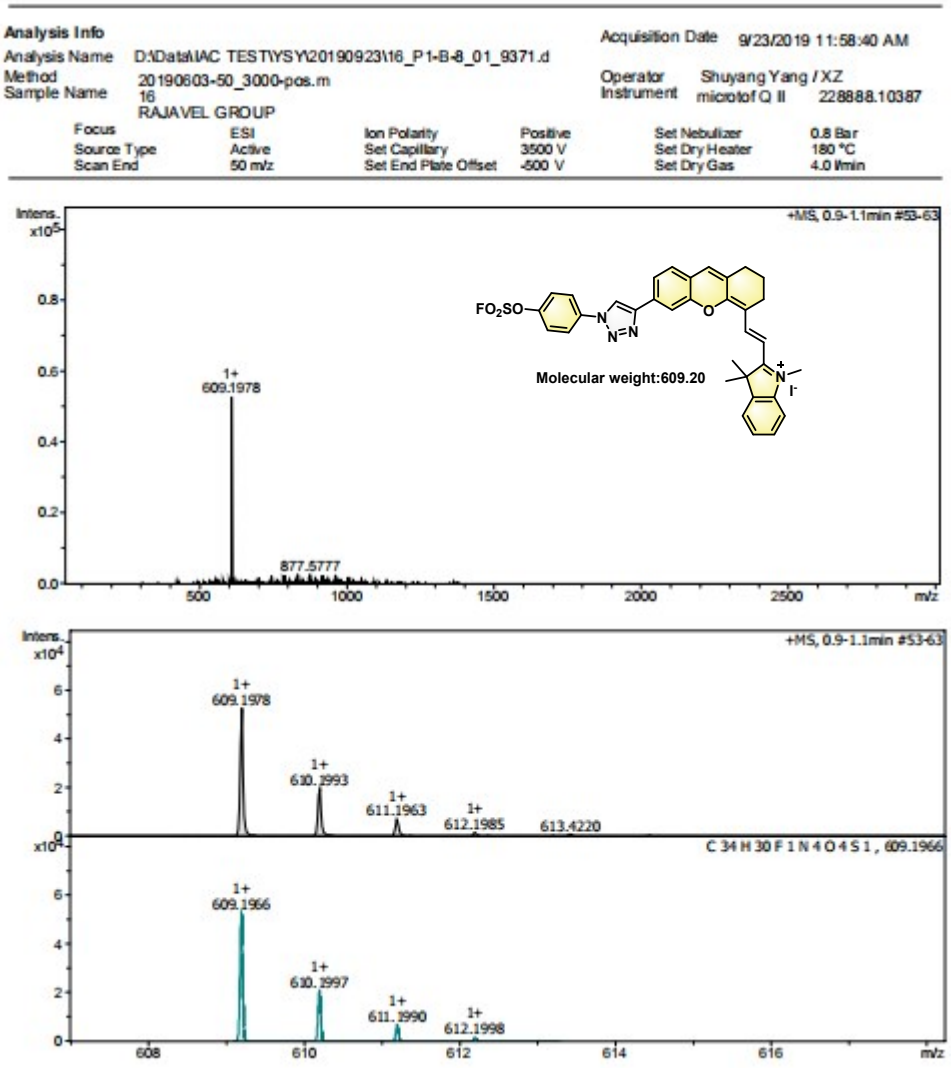
Standard deviation: 0.348

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	430.9081	13818	63.5	2.8	0.0312
2	579.2363	14627	1472.3	100.0	0.0396
3	580.2375	13073	556.5	37.8	0.0444
4	581.2396	13735	122.1	8.3	0.0423
5	657.4505	11460	42.8	3.5	0.0574
6	701.4753	13313	52.9	4.6	0.0527
7	745.5030	14215	70.8	6.5	0.0524
8	746.5055	14341	30.4	2.8	0.0521
9	785.5060	9880	28.9	2.8	0.0795
10	789.5257	13334	79.9	7.7	0.0592
11	790.5294	13848	35.5	3.4	0.0571
12	829.5263	13188	46.1	4.6	0.0629
13	833.5544	12536	81.5	8.2	0.0665
14	834.5574	12227	37.1	3.7	0.0683
15	849.5251	13598	33.8	3.4	0.0625
16	873.5535	12194	52.5	5.4	0.0716
17	874.5537	11725	28.5	2.9	0.0746
18	875.5333	11707	27.6	2.8	0.0748
19	877.5768	13662	84.9	8.8	0.0642
20	878.5827	13074	39.4	4.1	0.0672
21	893.5530	12825	35.8	3.8	0.0697
22	917.5785	11766	59.0	6.3	0.0780
23	918.5819	11483	30.3	3.2	0.0800
24	919.5612	12022	27.0	2.9	0.0765
25	921.6031	13735	75.0	8.0	0.0671
26	922.6066	15078	43.0	4.6	0.0612
27	937.5773	14018	34.9	3.8	0.0669
28	961.6017	14667	71.6	7.8	0.0656
29	962.6040	12086	31.5	3.5	0.0798
30	965.6299	13918	59.5	6.5	0.0694
31	966.6312	13906	34.7	3.8	0.0695
32	981.6042	14615	31.3	3.5	0.0672
33	1005.6296	13084	57.2	6.5	0.0769
34	1006.6319	13148	33.7	3.8	0.0766
35	1009.6553	13773	44.6	5.0	0.0733
36	1025.6335	13420	24.4	2.8	0.0764
37	1049.6536	13764	49.9	5.7	0.0763
38	1050.6581	12589	26.9	3.1	0.0835
39	1053.6801	12475	28.2	3.3	0.0845
40	1093.6794	11456	30.9	3.6	0.0955

#	m/z	Res.	S/N	I %	FWHM
1	579.2366	14627		100.0	0.0396
2	580.2398	14652		39.7	0.0396
3	581.2429	14677		7.9	0.0396
4	582.2460	14703		1.0	0.0396

Triazole-based DHX-hemicyanine fused dye 2m



Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
609.197770	1	C34H30FN4O4S	68.97	609.196631	-1.1	-1.9	12.2	21.5	even	ok	M

Calibration Info:

Date:	9/25/2019 4:37:23 PM
Polarity:	Positive
Calibration spectrum:	+MS, 4.6-4.7min #275-277: Scan
Reference mass list:	ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode:	Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290	622.0290	27078	0.057
922.0098	922.0096	66156	-0.257
1221.9906	1221.9910	89012	0.329
1521.9715	1521.9716	89297	0.073
1821.9523	1821.9515	65495	-0.466
2121.9332	2121.9339	41446	0.344
2421.9140	2421.9138	6272	-0.079
2721.8948			

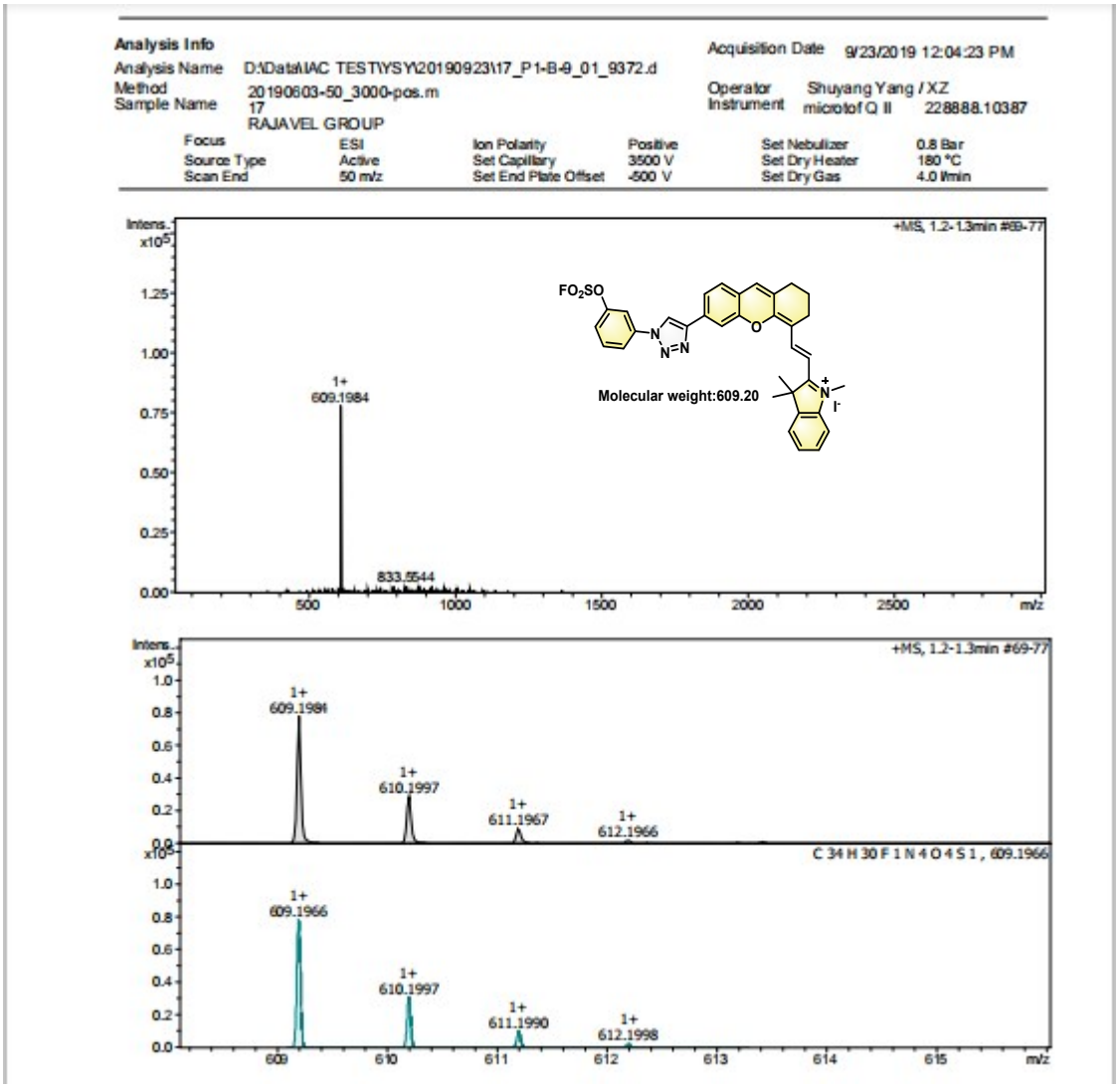
Standard deviation: 0.436

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	553.2945	12591	54.0	2.4	0.0439
2	581.1894	12517	37.3	1.7	0.0464
3	602.3661	17698	35.7	1.8	0.0340
4	609.1978	15495	2005.2	100.0	0.0393
5	610.1993	13469	736.9	36.8	0.0453
6	611.1963	13609	255.1	12.8	0.0449
7	612.1985	12080	59.4	3.0	0.0509
8	613.4220	10421	33.8	1.7	0.0589
9	657.4503	13858	43.1	2.3	0.0474
10	701.4749	14547	53.8	3.2	0.0482
11	745.5017	14657	69.2	4.3	0.0509
12	746.5043	14395	28.4	1.8	0.0519
13	785.5044	11826	28.5	1.8	0.0664
14	789.5264	13667	72.9	4.7	0.0578
15	790.5305	14463	36.0	2.3	0.0547
16	829.5278	12473	43.8	2.9	0.0665
17	833.5532	13445	77.3	5.2	0.0620
18	834.5552	12737	35.6	2.4	0.0655
19	853.5088	13943	24.8	1.7	0.0612
20	872.6226	13764	25.6	1.8	0.0634
21	873.5532	12422	52.5	3.6	0.0703
22	874.5526	11234	24.9	1.7	0.0778
23	875.5340	11199	27.8	1.9	0.0782
24	877.5777	14037	78.2	5.4	0.0625
25	878.5835	13357	37.7	2.6	0.0658
26	893.5541	12865	24.5	1.7	0.0695
27	917.5782	11816	57.8	4.1	0.0777
28	918.5791	8985	32.0	2.3	0.1022
29	919.5587	10794	24.4	1.7	0.0852
30	921.6027	13071	62.5	4.4	0.0705
31	922.6059	17528	38.5	2.7	0.0526
32	961.6022	13460	60.3	4.4	0.0714
33	962.6040	11448	29.9	2.2	0.0841
34	963.5937	12650	23.9	1.7	0.0762
35	965.6304	12754	41.0	3.0	0.0757
36	966.6297	13776	24.4	1.8	0.0702
37	1005.6285	13625	53.0	3.9	0.0738
38	1006.6284	13345	30.2	2.2	0.0754
39	1009.6540	12734	31.0	2.3	0.0793
40	1049.6548	13869	39.8	3.0	0.0757

#	m/z	Res.	S/N	I %	FWHM
1	609.1966	15495		100.0	0.0393
2	610.1997	15520		39.5	0.0393
3	611.1990	15546		12.9	0.0393
4	612.1998	15571		3.0	0.0393

Triazole-based DHX-hemicyanine fused dye 2n



Evaluation Spectra / Validation Formula:

Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule	Adduct
609.198365	1	C34H30FN4O4S	51.48	609.196631	-1.7	-2.8	13.2	21.5	even	ok	M

Calibration Info:

Date: 9/25/2019 4:41:44 PM
Polarity: Positive
Calibration spectrum: +MS, 4.6-4.6min #273-276: Scan
Reference mass list: ESI: Tuning Mix ES-TOF (ESI) (pos)
Calibration mode: Enhanced Quadratic

Reference m/z	Resulting m/z	Intensity	Error [ppm]
118.0863			
322.0481			
622.0290	622.0289	27286	-0.032
922.0098	922.0099	73568	0.097
1221.9906	1221.9905	96887	-0.085
1521.9715	1521.9717	89604	0.160
1821.9523	1821.9515	63100	-0.468
2121.9332	2121.9342	40297	0.503
2421.9140	2421.9136	6747	-0.175
2721.8948			

Standard deviation: 0.445

Mass List:

#	m/z	Res.	S/N	I %	FWHM
1	581.1879	13100	64.7	2.3	0.0444
2	609.1984	16292	2657.0	100.0	0.0374
3	610.1997	14264	977.0	36.9	0.0428
4	611.1967	12868	309.9	11.7	0.0475
5	612.1966	11232	66.3	2.5	0.0545
6	613.4209	12255	35.4	1.3	0.0501
7	657.4507	12947	40.0	1.6	0.0508
8	701.4759	13747	48.6	2.1	0.0510
9	735.0894	13218	31.8	1.4	0.0556
10	745.5026	14826	59.2	2.7	0.0503
11	746.5042	15501	29.7	1.4	0.0482
12	785.5072	12545	28.6	1.4	0.0626
13	789.5269	13040	67.6	3.2	0.0605
14	790.5295	13277	29.6	1.4	0.0595
15	829.5292	12359	39.0	1.9	0.0671
16	833.5544	14046	71.2	3.5	0.0593
17	834.5569	12666	34.3	1.7	0.0659
18	853.5124	12952	24.3	1.2	0.0659
19	873.5502	13699	52.8	2.7	0.0638
20	874.5543	12371	24.1	1.2	0.0707
21	875.5314	12094	28.7	1.5	0.0724
22	877.5770	12866	69.0	3.5	0.0682
23	878.5824	14014	35.1	1.8	0.0627
24	916.6482	14736	23.0	1.2	0.0622
25	917.5780	12655	59.2	3.1	0.0725
26	918.5803	11668	27.6	1.4	0.0787
27	919.5595	11667	25.8	1.3	0.0788
28	921.6040	12727	52.8	2.8	0.0724
29	922.6083	13837	30.7	1.6	0.0667
30	937.5782	15225	21.9	1.2	0.0616
31	961.6018	13407	55.4	2.9	0.0717
32	962.6038	11359	25.8	1.4	0.0847
33	963.5935	13004	23.3	1.2	0.0741
34	965.6300	13299	39.3	2.1	0.0726
35	966.6284	14409	23.9	1.3	0.0671
36	1005.6278	13219	44.5	2.4	0.0761
37	1006.6297	13431	25.1	1.3	0.0749
38	1009.6534	13104	27.6	1.5	0.0771
39	1049.6522	13110	34.9	1.9	0.0801
40	1053.6783	14638	21.1	1.2	0.0720

#	m/z	Res.	S/N	I %	FWHM
1	609.1966	16292		100.0	0.0374
2	610.1997	16319		39.5	0.0374
3	611.1990	16345		12.9	0.0374
4	612.1998	16372		3.0	0.0374

Triazole-based DHX-hemicyanine fused dye 2o