Supplementary Materials

Contents

1. Syntheses

1.1. General

All starting materials were obtained from commercial suppliers (Sigma-Aldrich, Fluka, Merck, Alfa Aesar, Reanal, Molar Chemicals, Fluorochem) and used without further purification.

Analytical thin-layer chromatography (TLC) was performed on silica gel 60 F254 precoated aluminum TLC plates or aluminum oxide 60 F254 precoated aluminum TLC plates from Merck. Flash column chromatography was performed on a *Teledyne ISCO COMBI Flash Nextgen 300+* automated flash chromatographer with silica gel (25–40 μm) from Zeochem, aluminum oxide (activated, neutral, Brockmann I) or RediSep®Rf C18 High Performance GOLD column. Microwave reactions were performed in an *AntonPaar Monowave 400* reactor using sealed tubes with fast heating and then maintaining a constant temperature.

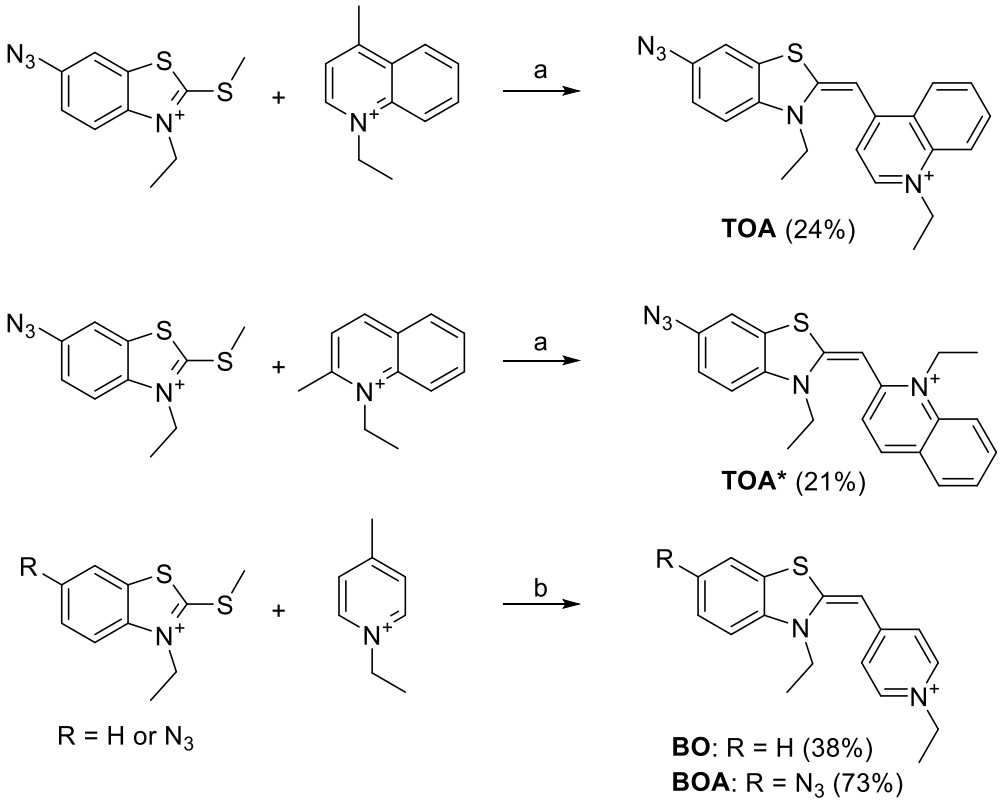
NMR spectra were recorded on a *Varian Inova* 500 MHz or a *Varian Inova* 300 MHz spectrometer. Chemical shifts (δ) are given in parts per million (ppm) using solvent signals as the reference for samples made in $CDCl_3$, CD_3OD, acetone-d6 or DMSO-d6; and using 1,4-dioxane as an internal reference for samples made in D_2O.

Analytical RP-HPLC-UV/Vis-MS experiments were performed on a *SHIMADZU LCMS-2020* system using a Phenomenex Kinetex EVO C18 column (50 × 2.10 mm I.D.) with 2.6 μm silica (100 Å pore size) as a stationary phase with a photodiode array UV/Vis (190–800 nm) and an ESI-MS detector. Linear gradient elution (0 min 0% B; 2.0 min 100% B; 2.5 min 100% B; 3.0 min 0% B; 4.0 min 0% B) with eluent A (95% water, 4.99 %MeCN, 0.1% HCOOH) and eluent B (95% MeCN, 4.99% water, 0.1% HCOOH) was used at a flow rate of 1.0 mL/min at 40°C. The samples were dissolved in the mixture of water and MeCN (1:1 V/V).

The exact masses were determined with an *Agilent 6230* time-of-flight mass spectrometer.

Every synthetic procedure with the involvement of azide group was carried out under light-free conditions and the products were stored in low-actinic glassware at –4 ^{0}C. Compounds TO, TO*, Cy1[1] and Cy1A[2] were synthesized as described in the literature.

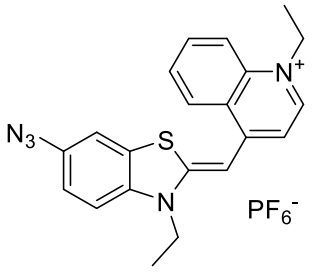
*1.2. Synthesis of **TOA**, **TOA***, **BO** and **BOA***



Scheme S1. a) Et_3N, EtOH, 75 °C, 60 min **b**) Et_3N, CH_2Cl_2, rt, 16 h.

General method for the synthesis of TOA and TOA*

N-Ethyl-2-methyl-quinolinium iodide [3] or *N*-ethyl-4-methyl-quinolinium iodide [4] (100 mg, 0.33 mmol, 1.0 equiv.) was dissolved in 10 mL ethanol and *N*-ethyl-6-azido-2-methylsulfanylbenzothiazolium sulfate [5] (110 mg, 0.37 mmol, 1.1 equiv.) and triethylamine (37 mg, 51 µL, 0.37 mmol, 1.1 equiv.) were added to the solution. The mixture was stirred at 75 °C for 60 min in N_2 atmosphere. After cooling, the solid was filtered and washed with cold ethanol. The salt was dissolved in acetonitrile, 300 mg (1.84 mmol, 5.5 equiv.) ammonium-hexafluorophosphate and water was added to the solution. The acetonitrile was removed, the product was filtered, washed with water, and dried *in vacuo*. The product was used without further purification.



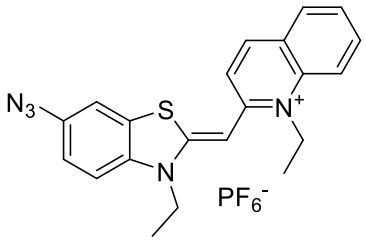
4-((6-Azido-3-ethyl-1,3-benzothiazol-2(3*H*)-ylidene)methyl)-1-ethylquinolin-1-ium hexafluorophosphate(V) (TOA).

Yield: 24% (41 mg, 0.079 mmol)

^{1}H NMR (500 MHz, DMSO-d6) δ 8.80 (d, J = 8.6 Hz, 1H), 8.69 (d, J = 7.1 Hz, 1H), 8.17 (d, J = 9.2 Hz, 1H), 8.01 (t, J = 7.3 Hz, 1H), 7.93 (d, J = 2.1 Hz, 1H), 7.82 – 7.74 (m, 2H) [contained in this multiplet: 7.79 (d, J = 8.9 Hz, 1H), 7.78 (t, J = 7.6 Hz, 1H)], 7.41 – 7.34 (m, 2H) [contained in this multiplet: 7.38 (d, J = 7.2 Hz, 1H), 7.36 (dd, J = 8.9, 2.3 Hz, 1H)], 6.93 (s, 1H), 4.71 – 4.63 (m, 4H), 1.48 (t, J = 7.1 Hz, 3H), 1.37 (t, J = 7.0 Hz, 3H).

^{13}C NMR (126 MHz, DMSO-d6) δ 158.7, 148.8, 144.0, 137.1, 136.9, 136.1, 133.3, 126.9, 125.9, 124.3, 119.7, 118.0, 113.8, 113.4, 108.3, 87.5, 49.5, 41.2, 14.7, 12.2.

HRMS: $[M]^+$: calcd for $[C_{21}H_{20}N_5S]^+$: m/z = 374.1434, found: 374.1432.



2-((6-Azido-3-ethyl-1,3-benzothiazol-2(3*H*)-ylidene)methyl)-1-ethylquinolin-1-ium hexafluorophosphate(V) (TOA*).

Yield: 21 % (40 mg, 0.071 mmol)

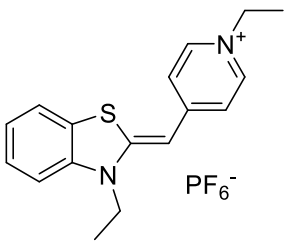
^{1}H NMR (500 MHz, DMSO-d6) δ 8.47 (d, J = 9.3 Hz, 1H), 8.13 (d, J = 8.9 Hz, 1H), 8.04 (d, J = 9.4 Hz, 2H), 7.93 (t, J = 7.4 Hz, 1H), 7.89 (d, J = 2.2 Hz, 1H), 7.80 (d, J = 8.9 Hz, 1H), 7.63 (t, J = 7.5 Hz, 1H), 7.35 (dd, J = 8.8, 2.2 Hz, 1H), 6.08 (s, 1H), 4.72 (q, J = 7.0 Hz, 2H), 4.56 (q, J = 7.0 Hz, 2H), 1.50 (t, J = 7.1 Hz, 3H), 1.38 (t, J = 7.1 Hz, 3H).

^{13}C NMR (126 MHz, DMSO-d6) δ 160.6, 152.1, 140.0, 138.6, 137.3, 136.4, 133.7, 129.7, 125.7, 125.4, 124.2, 119.5, 118.6, 116.9, 113.9, 113.3, 84.9, 44.0, 41.5, 12.1, 11.8.

HRMS: $[M]^+$: calcd for $[C_{21}H_{20}N_5S]^+$: m/z = 374.1434, found: 374.1443.

General method for BO and BOA

A mixture of *N*-ethyl-4-methylpyridinium iodide[6] (100 mg, 0.40 mmol, 1.0 equiv.), *N*-ethyl-2-methylsulfanylbenzothiazolium ethylsulfate[7] (148 mg, 0.44 mmol, 1.1 equiv.) or *N*-ethyl-6-azido-2-methylsulfanylbenzothiazolium sulfate[5] (132 mg, 0.44 mmol, 1.1 equiv.) and triethyl-amine (81 mg, 112 µL, 0.80 mmol, 2.0 equiv.) was stirred at rt overnight. Diethyl ether was added and the mixture was cooled to 0 °C. The solid was filtered and washed with cold ether. The salt was dissolved in acetonitrile, 326 mg (2.00 mmol, 5.0 equiv.) ammonium-hexafluorophosphate and water was added to the solution. The acetonitrile was removed, the product was filtered, washed with water and dried *in vacuo*. The product was used without further purification.



1-Ethyl-4-((3-ethyl-1,3-benzothiazol-2(3*H*)-ylidene)methyl)pyridin-1-ium hexafluorophosphate(V) (BO).

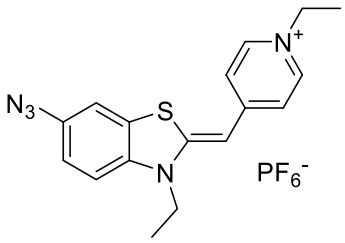
Yield: 38 % (66 mg, 0.152 mmol)

^{1}H NMR (500 MHz, DMSO-d6) δ 8.39 (d, J = 6.0 Hz, 2H), 7.92 (d, J = 7.8 Hz, 1H), 7.60 (d, J = 8.1 Hz, 1H), 7.53 (t, J = 7.7 Hz, 1H), 7.44 (d, J = 5.7 Hz, 2H), 7.31 (t, J = 7.5 Hz, 1H),

6.32 (s, 1H), 4.32 (q, *J* = 7.0 Hz, 2H), 4.26 (q, *J* = 7.3 Hz, 2H), 1.44 (t, *J* = 7.0 Hz, 3H), 1.31 (t, *J* = 6.5 Hz, 3H).

^{13}C NMR (126 MHz, DMSO-d6) δ 156.1, 150.5, 140.9, 139.5, 127.9, 123.50, 123.46, 122.6, 118.6, 111.7, 88.9, 53.0, 40.3, 16.0, 11.7.

HRMS: $[M]^+$: calcd for $[C_{17}H_{19}N_2S]^+$: m/z = 283.1264, found: 283.1270.



4-((6-Azido-3-ethyl-1,3-benzothiazol-2(3*H*)-ylidene)methyl)-1-ethylpyridin-1-ium hexafluorophosphate(V) (BOA).

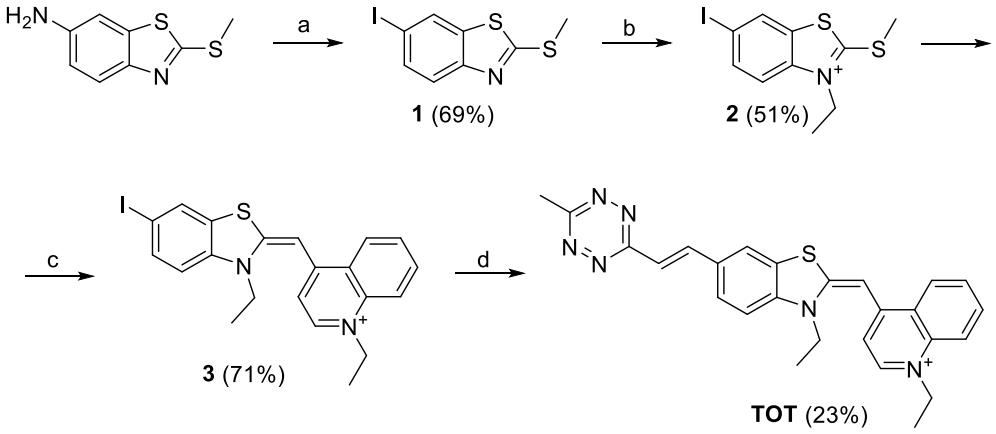
Yield: 73 % (138 mg, 0.94 mmol)

^{1}H NMR (500 MHz, DMSO-d6) δ 8.40 (d, *J* = 6.6 Hz, 2H), 7.80 (d, *J* = 1.8 Hz, 1H), 7.60 (d, *J* = 8.8 Hz, 1H), 7.41 (d, *J* = 6.5 Hz, 2H), 7.26 (dd, *J* = 8.3, 1.8 Hz, 1H), 6.30 (s, 1H), 4.30 (q, *J* = 6.6 Hz, 2H), 4.26 (q, *J* = 7.2 Hz, 2H), 1.44 (t, *J* = 7.0 Hz, 3H), 1.29 (t, *J* = 6.6 Hz, 3H).

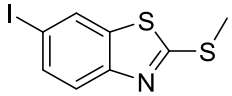
^{13}C NMR (126 MHz, DMSO-d6) δ 155.9, 150.5, 141.0, 137.2, 135.1, 125.4, 119.2, 118.7, 113.3, 112.7, 89.2, 53.1, 40.6, 16.0, 11.8.

HRMS: $[M]^+$: calcd for $[C_{17}H_{18}N_5S]^+$: m/z = 324.1278, found: 324.1279.

1.3. Synthesis of ***TOT***



Scheme S2. a) 1. $NaNO_2$, HCl, H_2O, 0 °C, 10 min, 2. KI, 40°C, 20 min, **b**) $(EtO)_2SO_2$, 100°C, 16 h, c) *N*-ethyl-4-methyl-quinolinium iodide, Et_3N, CH_2Cl_2, rt, 16 h, d) 2-(6-methyl-1,2,4,5-tetrazin-3-yl)ethyl methanesulfonate, $Pd_2(dba)_3$, QPhos, Cy_2NMe, DMF, 100 °C MW, 60 min.



6-Iodo-2-(methylsulfanyl)benzo[d]thiazole (1).

To a solution of 6-amino-2-(methylsulfanyl)benzothiazole[5] (1.96 g, 10 mmol, 1.0 equiv.) in 10 mL 20% aqueous HCl cooled to 0°C was added a solution of $NaNO_2$ (0.76 g, 11 mmol, 1.1 equiv.) in 4 mL water and the mixture was stirred for 10 min. A solution of KI (1.83 g, 11 mmol, 1.1 equiv.) dissolved in 3 mL water was added, the reaction mixture was let to warm up to rt, then it was stirred at 40 °C for 20 min. After cooling down the

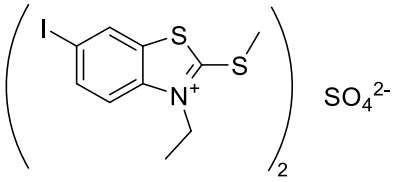
reaction mixture was extracted with CH_2Cl_2 (3 x 20 mL), the combined organic phase was washed with 5% aqueous $NaHSO_3$ solution and water, dried with $MgSO_4$, filtered and evaporated. The crude product was purified by flash column chromatography on silica using hexanes/EtOAc as eluent.

Yield: 69 % (2.12 g, 6.9 mmol)

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 (d, J = 1.7 Hz, 1H), 7.68 (dd, J = 8.5, 1.2 Hz, 1H), 7.58 (d, J = 8.5 Hz, 1H), 2.78 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 169.0, 152.8, 137.3, 135.3, 129.5, 122.9, 88.1, 16.1.

MS: $[M+H]^+$: calcd for $[C_8H_7INS_2]^+$: m/z = 308, found: 308.



3-Ethyl-6-iodo-2-(methylsulfanyl)-1,3-benzothiazolium sulfate (2).

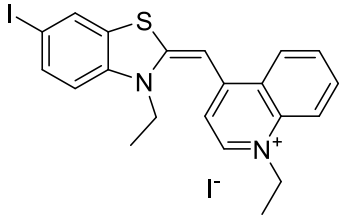
A mixture of **1** (924 mg, 3 mmol, 1.0 equiv.) and diethyl sulfate (1.54 g, 1.3 mL, 10 mmol, 3.3 equiv.) was stirred at 100 °C for 16 h. After cooling to rt acetone and diethyl ether was added and the mixture was stirred until the product solidified. The precipitate was filtered and washed with acetone. The product was used without further purification.

Yield: 51% (588 mg, 1.53 mmol)

^{1}H NMR (500 MHz, D_2O) δ 8.49 (d, J = 1.5 Hz, 1H), 8.14 (dd, J = 8.9, 1.5 Hz, 1H), 7.76 (d, J = 8.9 Hz, 1H), 4.62 (q, J = 7.4 Hz, 2H), 3.08 (s, 3H), 1.50 (t, J = 7.4 Hz, 3H).

^{13}C NMR (126 MHz, D_2O) δ 182.1, 141.7, 138.9, 132.2, 130.7, 116.8, 91.7, 46.6, 18.5, 12.0.

MS: $[M]^+$: calcd for $[C_{10}H_{11}INS_2]^+$: m/z = 336, found: 336.



1-Ethyl-4-((3-ethyl-6-iodo-1,3-benzothiazol-2(3*H*)-ylidene)methyl)quinolin-1-ium iodide (3).

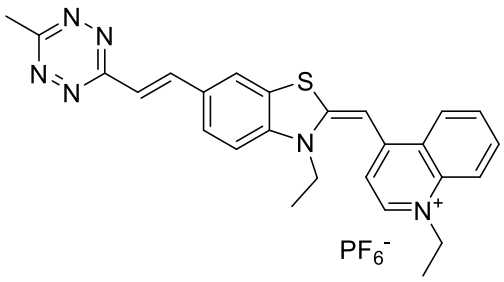
A mixture of *N*-ethyl-4-methylquinolinium iodide[4] (425 mg, 1.42 mmol, 1.0 equiv.), **2** (546 mg, 1.42 mmol, 1.0 equiv.) and triethyl-amine (315 mg, 433 µl, 3.13 mmol, 2.2 equiv.) was stirred at rt overnight. Diethyl ether was added and the mixture was cooled to 0 °C. The solid was filtered and washed with cold ether. The product was used without further purification.

Yield: 71% (592 mg, 1.01 mmol)

^{1}H NMR (500 MHz, DMSO-d6) δ 8.80 (d, J = 8.6 Hz, 1H), 8.72 (d, J = 7.1 Hz, 1H), 8.42 (d, J = 1.7 Hz, 1H), 8.19 (d, J = 8.8 Hz, 1H), 8.03 (t, J = 7.9 Hz, 1H), 7.90 (dd, J = 8.6, 1.8 Hz, 1H), 7.79 (t, J = 7.6 Hz, 1H), 7.56 (d, J = 8.7 Hz, 1H), 7.41 (d, J = 7.1 Hz, 1H), 6.92 (s, 1H), 4.67 (q, J = 7.2 Hz, 2H), 4.62 (q, J = 7.0 Hz, 2H), 1.49 (t, J = 7.1 Hz, 3H), 1.36 (t, J = 7.1 Hz, 3H).

^{13}C NMR (126 MHz, DMSO-d6) δ 158.4, 149.0, 144.2, 139.5, 136.8, 136.5, 133.4, 130.8, 127.0, 126.2, 125.9, 124.4, 118.0, 114.4, 108.7, 87.4, 49.6, 45.8, 14.7, 12.1.

HRMS: $[M]^+$: calcd for $[C_{21}H_{20}IN_2S]^+$: m/z = 459.0387, found: 459.0391.



1-Ethyl-4-((3-ethyl-6-(2-(6-methyl-1,2,4,5-tetrazin-3-yl)vinyl)-1,3-benzothiazol-2(3*H*)-ylidene)methyl)quinolin-1-ium hexafluorophosphate(V) (TOT).

In a dried microwave pressure tube with magnetic stir bar was dissolved **3** (58.6 mg, 0.1 mmol, 1.0 equiv.), 2-(6-methyl-1,2,4,5-tetrazin-3-yl)ethyl methanesulfonate[8] (65.6 mg, 0.3 mmol, 3.0 equiv.), *N,N*-dicyclohexylmethylamine (98 mg, 107 µL, 0.5 mmol, 5 equiv.), tris(dibenzylideneacetone)dipalladium(0) ($Pd_2(dba)_3$, 9.2 mg, 0.01 mmol, 0.1 equiv.) and 1,2,3,4,5-pentaphenyl-1′-(di-*tert*-butylphosphino)ferrocene (QPhos, 7.1 mg, 0.01 mmol, 0.1 equiv.) in 5 mL dimethylformamide. The mixture was heated in a microwave reactor at 100 °C for 60 min. The solvent was evaporated in vacuo and the crude product was purified by flash column chromatography on C18 silica using water/MeOH containing 0.1% TFA as eluent. Ammonium hexafluorophosphate was added to the product containing fraction and MeOH was removed. The precipitated product was collected by filtration, washed with water and dried.

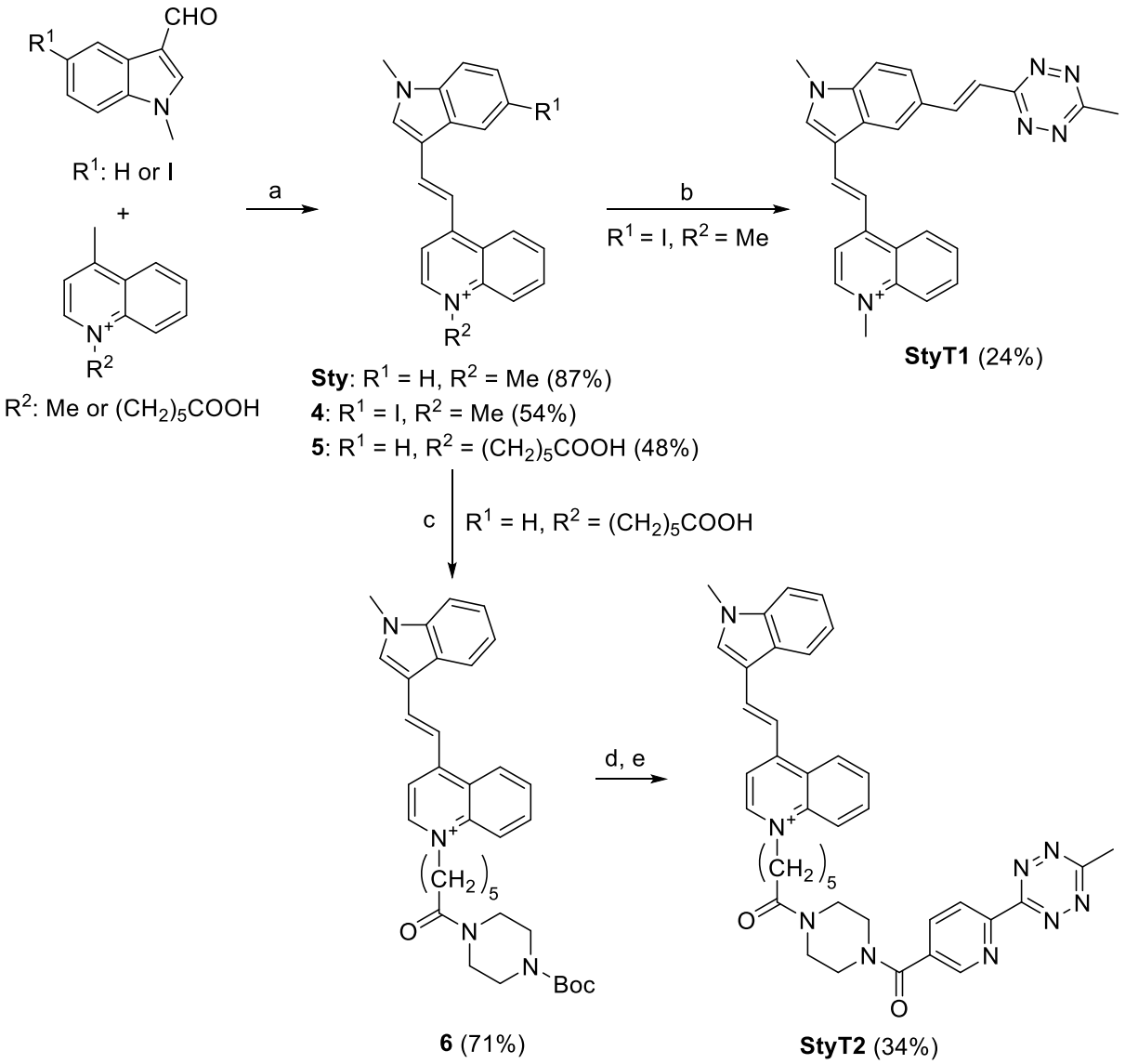
Yield: 23% (14 mg, 0,023 mmol)

^{1}H NMR (500 MHz, DMSO-d6) δ 8.82 (d, J = 8.5 Hz, 1H), 8.74 (d, J = 7.1 Hz, 1H), 8.54 (d, J = 1.6 Hz, 1H), 8.31 (d, J = 16.2 Hz, 1H), 8.20 (d, J = 8.8 Hz, 1H), 8.13 (dd, J = 8.6, 1.7 Hz, 1H), 8.03 (t, J = 7.7 Hz, 1H), 7.86 – 7.77 (m, 2H) [contained in this multiplet: 7.83 (d, J = 9.0 Hz, 1H), 7.80 (t, J = 7.7 Hz, 2H)], 7.69 (d, J = 16.2 Hz, 1H), 7.50 (d, J = 7.1 Hz, 1H), 6.99 (s, 1H), 4.74 – 4.65 (m, 4H), 2.96 (s, 3H), 1.51 (t, J = 7.2 Hz, 3H), 1.42 (t, J = 7.1 Hz, 3H).

^{13}C NMR (126 MHz, DMSO-d6) δ 166.0, 164.1, 158.4, 149.0, 144.3, 140.7, 138.2, 136.8, 133.4, 131.4, 128.8, 127.0, 125.9, 124.8, 124.5, 122.0, 120.9, 118.1, 112.8, 109.0, 88.0, 49.7, 41.2, 20.8, 14.7, 12.2.

HRMS: $[M]^+$: calcd for $[C_{26}H_{25}N_6S]^+$: m/z = 453.1856, found: 453.1857.

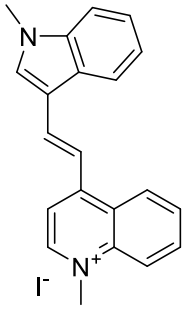
1.4. Synthesis of Styryl dyes



Scheme S3. a) piperidine, EtOH, Δ, 16 h for **Sty** and **4**, 60 min for **5**, b) 2-(6-methyl-1,2,4,5-tetrazin-3-yl)ethyl methanesulfonate, $Pd_2(dba)_3$, QPhos, Cy_2NMe, DMF, 100 °C MW, 60 min, c) Boc-piperazine, HATU, iPr_2NEt, CH_2Cl_2, rt, 30 min, d) TFA, CH_2Cl_2, rt, 20 min, e) 6-(6-methyl-1,2,4,5-tetrazin-3-yl)nicotinic acid, HOBt, HBTU, iPr_2NEt, MeCN, rt, 60 min.

General procedure for the synthesis of Sty and 4

A mixture of 1-methyl-1*H*-indole-3-carbaldehyde[9] (80 mg, 0.5 mmol, 1.0 equiv.) or 5-iodo-1-methyl-1*H*-indole-3-carbaldehyde[10] (143 mg, 0.5 mmol, 1.0 equiv.), *N*-methyl-4-methylquinolinium iodide[4] (200 mg, 0.7 mmol, 1.4 equiv.) and piperidine (128 mg, 148 µL, 1.5 mmol, 3.0 equiv.) in 8 mL EtOH was refluxed for 16 h. After cooling down the precipitate was filtered and washed with EtOH. The product was used without further purification.



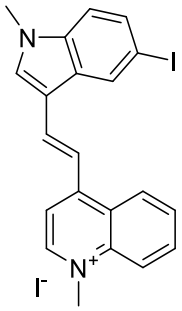
1-Methyl-4-(2-(1-methyl-1*H*-indol-3-yl)vinyl)quinolin-1-ium iodide (Sty).

Yield: 87% (186 mg, 0.44 mmol)

^{1}H NMR (500 MHz, DMSO-d6) δ 9.10 (d, J = 6.7 Hz, 1H), 8.96 (d, J = 8.5 Hz, 1H), 8.54 (d, J = 15.6 Hz, 1H), 8.43 (d, J = 6.7 Hz, 1H), 8.35 (d, J = 8.8 Hz, 1H), 8.32 (s, 1H), 8.28 (d, J = 7.5 Hz, 1H), 8.22 (t, J = 7.6 Hz, 1H), 8.04 – 7.98 (m, 2H), 7.62 (d, J = 7.5 Hz, 1H), 7.39 – 7.32 (m, 2H), 4.45 (s, 3H), 3.94 (s, 3H).

^{13}C NMR (75 MHz, DMSO-d6) δ 153.4, 146.6, 138.8, 137.9, 137.9, 136.1, 134.6, 128.5, 126.1, 125.9, 125.4, 123.2, 121.8, 120.4, 119.0, 113.6, 113.4, 112.6, 111.1, 43.9, 33.4.

HRMS: $[M]^{+}$: calcd for $[C_{21}H_{19}N_2]^{+}$: m/z = 299.1543, found: 299.1549.



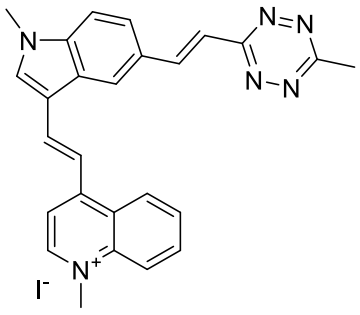
4-(2-(5-Iodo-1-methyl-1*H*-indol-3-yl)vinyl)-1-methylquinolin-1-ium iodide (4).

Yield: 54% (149 mg, 0.27 mmol)

^{1}H NMR (500 MHz, acetone-d6) δ 9.13 (d, J = 6.6 Hz, 1H), 8.95 (d, J = 8.6 Hz, 1H), 8.52 (d, J = 15.7 Hz, 1H), 8.49 (d, J = 1.6 Hz, 1H), 8.48 – 8.43 (m, 2H), 8.27 (ddd, J = 8.6, 6.9, 1.3 Hz, 1H), 8.22 (s, 1H), 8.13 (d, J = 15.7 Hz, 1H), 8.07 – 8.02 (m, 1H), 7.65 (dd, J = 8.5, 1.6 Hz, 1H), 7.44 (d, J = 8.6 Hz, 1H), 4.67 (s, 3H), 3.99 (s, 3H).

^{13}C NMR (75 MHz, acetone-d6) δ 155.5, 147.6, 140.2, 138.3, 137.9, 136.3, 135.8, 132.5, 129.7, 129.4, 127.1, 119.7, 115.0, 114.7, 114.1, 114.0, 111.9, 86.2, 72.8, 45.1, 34.0.

HRMS: $[M]^{+}$: calcd for $[C_{21}H_{18}IN_2]^{+}$: m/z = 425.0510, found: 425.0514.



1-Methyl-4-(2-(1-methyl-5-(2-(6-methyl-1,2,4,5-tetrazin-3-yl)vinyl)-1*H*-indol-3-yl)vinyl)quinolin-1-ium iodide (StyT1).

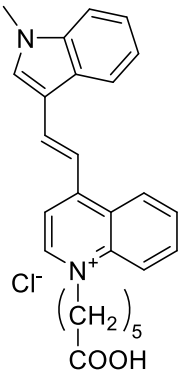
In a dried microwave pressure tube with magnetic stir bar was dissolved **4** (55.2 mg, 0.1 mmol, 1.0 equiv.), 2-(6-methyl-1,2,4,5-tetrazin-3-yl)ethyl methanesulfonate[8] (65.6 mg, 0.3 mmol, 3.0 equiv.), *N,N*-dicyclohexylmethylamine (98 mg, 107 µL, 0.5 mmol, 5 equiv.), tris(dibenzylideneacetone)dipalladium(0) ($Pd_2(dba)_3$, 9.2 mg, 0.01 mmol, 0.1 equiv.) and 1,2,3,4,5-pentaphenyl-1′-(di-*tert*-butylphosphino)ferrocene (QPhos, 7.1 mg, 0.01 mmol, 0.1 equiv.) in 5 mL dimethylformamide. The mixture was heated in a microwave reactor at 100 °C for 60 min. The solvent was evaporated in vacuo and the crude product was purified by flash chromatography on alumina using CH_2Cl_2/MeOH as eluent. Hexane was added to the fractions containing the product, the precipitate was filtered and washed with hexane.

Yield: 24% (13 mg, 0,024 mmol)

^{1}H NMR (500 MHz, DMSO-d6) δ 9.17 (d, *J* = 6.6 Hz, 1H), 9.03 (d, *J* = 8.5 Hz, 1H), 8.74 (s, 1H), 8.58 (d, *J* = 15.7 Hz, 1H), 8.52 (d, *J* = 16.3 Hz, 1H), 8.46 (d, *J* = 6.7 Hz, 1H), 8.43 – 8.35 (m, 2H), 8.24 (t, *J* = 7.9 Hz, 1H), 8.13 (d, *J* = 15.7 Hz, 1H), 8.05 (t, *J* = 7.7 Hz, 1H), 7.95 (d, *J* = 8.6 Hz, 1H), 7.74 – 7.68 (m, 2H), 4.48 (s, 3H), 3.98 (s, 3H), 2.97 (s, 3H).

^{13}C NMR (126 MHz, DMSO-d6) δ 165.8, 164.4, 153.6, 146.7, 141.1, 138.8, 138.6, 136.9, 136.2, 134.6, 128.8, 128.6, 126.4, 126.9, 125.5, 122.6, 121.5, 119.0, 118.8, 114.2, 113.8, 113.8, 111.7, 44.0, 33.5, 20.8.

HRMS: $[M]^+$: calcd for $[C_{26}H_{23}N_6]^+$: m/z = 419.1979, found: 419.1979.



1-(5-Carboxypentyl)-4-(2-(1-methyl-1*H*-indol-3-yl)vinyl)quinolin-1-ium chloride (5).

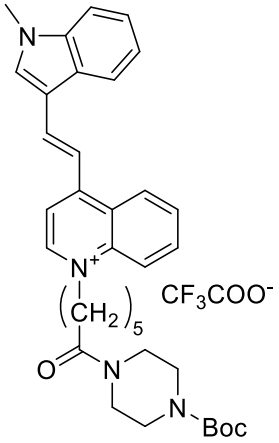
A mixture of 1-methyl-1*H*-indole-3-carbaldehyde[9] (80 mg, 0.5 mmol, 1.0 equiv.) *N*-(5-carboxypentyl)-4-methylquinolin-1-ium bromide[11] (237 mg, 0.7 mmol, 1.4 equiv.) and piperidine (128 mg, 148 µL, 1.5 mmol, 3.0 equiv.) in 8 mL EtOH was refluxed for 1 h. After cooling down to rt, the reaction mixture was diluted with water and acidifed to pH 5 using 2M aqueous HCl. The product was collected by filtration, washed with water and dried. The product was used without further purification.

Yield: 48% (105 mg, 0.24 mmol)

^{1}H NMR (500 MHz, CD_3OD) δ 8.72 (d, *J* = 6.4 Hz, 1H), 8.60 (d, *J* = 8.5 Hz, 1H), 8.23 – 8.14 (m, 2H), 8.12 – 8.03 (m, 2H), 7.96 (d, *J* = 7.7 Hz, 1H), 7.89 – 7.82 (m, 2H), 7.72 (d, *J* = 15.5 Hz, 1H), 7.41 (d, *J* = 8.0 Hz, 1H), 7.32 (t, *J* = 7.4 Hz, 1H), 7.27 (t, *J* = 7.4 Hz, 1H), 4.66 (t, *J* = 7.5 Hz, 2H), 3.81 (s, 3H), 2.27 (t, *J* = 7.1 Hz, 2H), 1.97 (p, *J* = 7.6 Hz, 2H), 1.68 (p, *J* = 7.3 Hz, 2H), 1.47 (p, *J* = 7.7 Hz, 2H).

^{13}C NMR (126 MHz, CD_3OD) δ 179.4, 162.3, 155.8, 146.3, 139.9, 139.7, 139.4, 137.8, 135.9, 129.7, 127.4, 127.2, 124.7, 123.3, 121.4, 119.4, 115.6, 114.3, 113.7, 111.7, 57.4, 36.4, 33.7, 30.3, 27.1, 26.0.

HRMS: $[M]^+$: calcd for $[C_{26}H_{27}N_2O_2]^+$: m/z = 399.2068, found: 399.2065.



1-(6-(4-(*Tert*-butoxycarbonyl)piperazin-1-yl)-6-oxohexyl)-4-(2-(1-methyl-1*H*-indol-3-yl)vinyl)quinolin-1-ium trifluoroacetate (6).

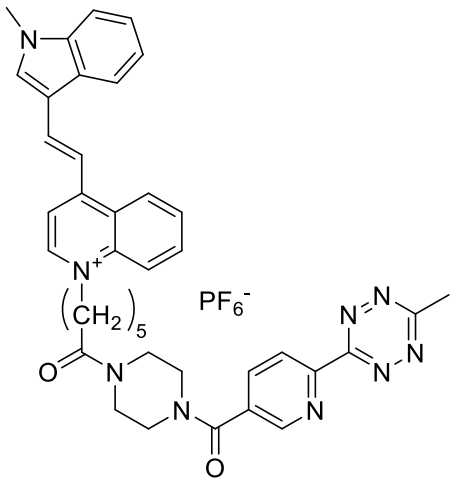
A solution of **5** (100 mg, 0.23 mmol, 1.0 equiv.), 1-Boc-piperazine (42.8 mg, 0.23 mmol, 1.0 equiv.), HATU (104.9 mg, 0.276 mmol, 1.2 equiv.) and iPr_2NEt (31.9 mg, 43 µL, 0.345 mmol, 1.5 equiv.) in 5 mL CH_2Cl_2 was stirred at rt for 30 min. The solvent was removed and the residue was purified by flash column chromatography on C18 silica using water/MeCN containing 0.1% TFA as eluent.

Yield: 71% (111 mg; 0.163 mmol)

1H NMR (500 MHz, CD_3OD) δ 8.86 (d, J = 6.8 Hz, 1H), 8.79 (d, J = 8.5 Hz, 1H), 8.38 (d, J = 15.5 Hz, 1H), 8.32 (d, J = 8.9 Hz, 1H), 8.21 (d, J = 6.7 Hz, 1H), 8.19 – 8.11 (m, 2H), 8.00 – 7.92 (m, 3H), 7.52 (dd, J = 6.9, 1.6 Hz, 1H), 7.41 – 7.33 (m, 2H), 4.83 (t, J = 7.5 Hz, 2H), 3.92 (s, 3H), 3.57 – 3.48 (m, 4H), 3.46 – 3.37 (m, 4H), 2.44 (t, J = 7.2 Hz, 2H), 2.06 (p, J = 7.8 Hz, 2H), 1.69 (p, J = 7.3 Hz, 3H), 1.51 (p, J = 7.9 Hz, 2H), 1.46 (s, 9H).

^{13}C NMR (126 MHz, CD_3OD) δ 172.4, 160.7 (q, J = 35 Hz), 154.8, 154.6, 145.0, 138.5, 138.4, 138.1, 136.5, 134.5, 128.3, 126.1, 125.9, 125.8, 123.3, 122.0, 120.0, 118.1, 114.3, 114.2 (q, J = 253 Hz), 112.9, 112.3, 110.3, 80.3, 56.0, 45.0, 41.2, 32.3, 32.1, 29.0, 27.2, 25.7, 24.2.

HRMS: $[M]^+$: calcd for $[C_{35}H_{43}N_4O_3]^+$: m/z = 567.3330, found: 567.3337.



1-(6-(4-(6-(6-Methyl-1,2,4,5-tetrazin-3-yl)nicotinoyl)piperazin-1-yl)-6-oxohexyl)-4-(2-(1-methyl-1*H*-indol-3-yl)vinyl)quinolin-1-ium hexafluorophosphate(V) (StyT2).

To a solution of **6** (100 mg, 0.15 mmol, 1.0 equiv.) in 2 mL CH_2Cl_2 was added 0.5 mL TFA, and it was stirred at rt for 20 min. The volatiles were removed and the residue was dissolved in 5 mL MeCN. 6-(6-Methyl-1,2,4,5-tetrazin-3-yl)nicotinic acid[12] (45.7 mg, 0.21 mmol, 1.4 equiv.), HOBt hydrate (24.0 mg, 0.15 mmol, 1.0 equiv.), HBTU (56.8 mg, 0.15

mmol, 1.0 equiv.) and iPr_2NEt (58 mg, 78 µL, 0.45 mmol, 3.0 equiv) were added and the mixture was stirred at rt for 1 h. The crude product was purified by flash column chromatography on C18 silica using water/MeCN containing 0.1% TFA as eluent. Ammonium hexafluorophosphate was added to the product containing fraction and MeCN was removed. The precipitated product was collected by filtration, washed with water and dried.

Yield: 34% (41 mg, 0.051 mmol)

^{1}H NMR (500 MHz, acetone-d6) δ 9.09 (d, J = 6.8 Hz, 1H), 8.93 (d, J = 8.4 Hz, 1H), 8.89 (d, J = 2.1 Hz, 1H), 8.58 (d, J = 8.0 Hz, 1H), 8.54 – 8.45 (m, 2H), 8.37 (d, J = 6.7 Hz, 1H), 8.26 – 8.17 (m, 2H), 8.16 – 8.11 (m, 2H), 8.07 (d, J = 15.6 Hz, 1H), 8.00 (t, J = 7.8 Hz, 1H), 7.57 (d, J = 7.9 Hz, 1H), 7.38 (t, J = 7.1 Hz, 1H), 7.33 (t, J = 7.5 Hz, 1H), 5.02 (t, J = 7.6 Hz, 2H), 3.98 (s, 3H), 3.80 – 3.53 (m, 8H), 3.09 (s, 3H), 2.50 – 2.39 (m, 2H), 2.17 (p, J = 7.5 Hz, 2H), 1.72 (p, J = 7.4 Hz, 2H), 1.58 (p, J = 7.7 Hz, 2H).

^{13}C NMR (126 MHz, acetone-d6) δ 171.7, 169.0, 167.6, 164.4, 155.7, 152.5, 149.7, 146.7, 139.6, 139.5, 139.3, 137.6, 137.2, 136.8, 135.8, 134.9, 129.6, 127.3, 127.0, 124.4, 124.3,

123.0, 121.4, 119.6, 115.2, 114.5, 113.7, 111.8, 57.4, 33.8, 33.0, 30.6, 30.2, 26.8, 25.0, 21.4.

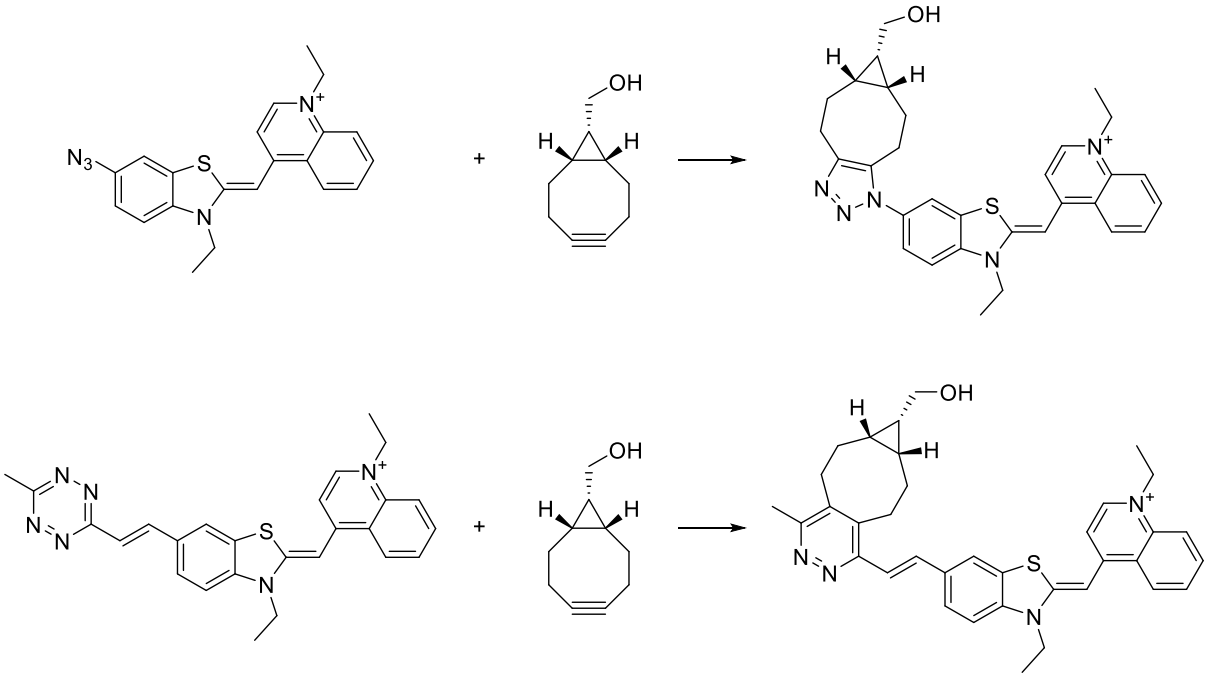
HRMS: $[M]^+$: calcd for $[C_{39}H_{40}N_9O_2]^+$: m/z = 666.3300, found: 666.3307.

2. Spectroscopic characterization

Photophysical measurements were performed on a *JASCO FP 8300* spectrofluorometer and a *JASCO v750* spectrophotometer. A stock solution in DMSO was prepared from the solid dyes (1 mM). Calf thymus DNA (Merck, 2618) was dissolved in TRIS (pH = 8.5) to give a stock solution of 2.0 mg/mL, which was diluted with PBS (pH = 7.4) to a concentration of 0.4 mg/mL. All spectroscopic measurements were conducted in PBS (pH=7.4) or 0.4 mg/mL DNA solution.

All of the dyes (1 mM) were reacted with (1*R*,8*S*,9*s*)-Bicyclo6.1.0non-4-yn-9-ylmethanol (BCN) in DMSO at room temperature (Scheme S4). The completion of the reaction was verified by HPLC-MS.

Absorbance and emission spectra were recorded using 0.5–2.5 µM concentration of the compounds in quartz cuvettes with 1 cm optical path length. Quantum yields were determined using Coumarin-153 (Φ_{EtOH} = 0.55)[13] as standard for **Cy1**, **Cy1A**, **BO**, **BOA**, **TO*** and **TOA***, and Rhodamine-6g (Φ_{EtOH} = 0.95)[14] as standard for **TO**, **TOA**, **TOT**, **Sty**, **StyT1** and **StyT2**.



Scheme S4. Representative reactions of azides and tetrazines with BCN using **TOA** and **TOT** as examples.

Table S1. Absorption maxima and molar extinction coefficients at the absorption maxima of the dyes in the presence or absence of BCN and DNA.

	$\lambda_{abs,PBS}$ (nm)	ε_{PBS}	+BCN $\lambda_{abs,PBS}$ (nm)	+BCN ε_{PBS}	$\lambda_{abs,DNA}$ (nm)	ε_{DNA}	+BCN $\lambda_{abs,DNA}$ (nm)	+BCN ε_{DNA}
Cy1	422	64600	–	–	428	69800	–	–
Cy1A	432	77200	425	79800	439	96000	430	87600
BO	455	61700	–	–	455	68500	–	–
BOA	454	73900	443	80200	465	79100	445	95300
TO*	483	45800	–	–	492	53600	–	–
TOA*	490	51400	481	52800	496	77400	484	67100
TO	502	56900	–	–	511	76300	–	–
TOA	511	47600	499	60200	519	84300	504	80000
TOT	500	19200	498	23500	529	52500	526	50000
Sty	483	27100	–	–	522	36700	–	–
StyT1	491	16100	490	9300	513	13100	517	15200
StyT2	500	7100	500	7200	518	9400	515	9100

Table S2. Emission maxima and fluorescence quantum yields of the dyes in the presence or absence of BCN and DNA.

	$\lambda_{em,PBS}$ (nm)	Φ_{PBS}	+BCN $\lambda_{em,PBS}$ (nm)	+BCN Φ_{PBS}	$\lambda_{em,DNA}$ (nm)	Φ_{DNA}	+BCN $\lambda_{em,DNA}$ (nm)	+BCN Φ_{DNA}
Cy1	475	0.0028	–	–	463	0.41	–	–
Cy1A	478	0.0014	478	0.0028	487	0.047	457	0.19
BO	474	0.00053	–	–	480	0.24	–	–
BOA	N.D.	N.D.	469	0.0010	489	0.017	471	0.094
TO*	547	0.00013	–	–	544	0.050	–	–
TOA*	570	0.00021	557	0.00046	555	0.030	533	0.16
TO	539	0.00029	–	–	530	0.30	–	–
TOA	565	0.00033	540	0.00061	542	0.083	528	0.53
TOT	N.D.	N.D.	601	0.0016	543	0.014	548	0.24
Sty	595	0.0031	–	–	588	0.19	–	–
StyT1	602	0.00093	601	0.0024	590	0.014	599	0.072
StyT2	598	0.014	596	0.013	583	0.15	584	0.15

3. Conversion of TOA and TOT in the cycloaddition reactions

10 mM stock solutions of **TOA**, **TOT** and BCN were prepared in DMSO. 5 μL of the dye solution was diluted with 100 μL MeCN and 890 μL 0.02M HEPES, then 5 μL of the BCN solution was added. The reaction was followed using LCMS.

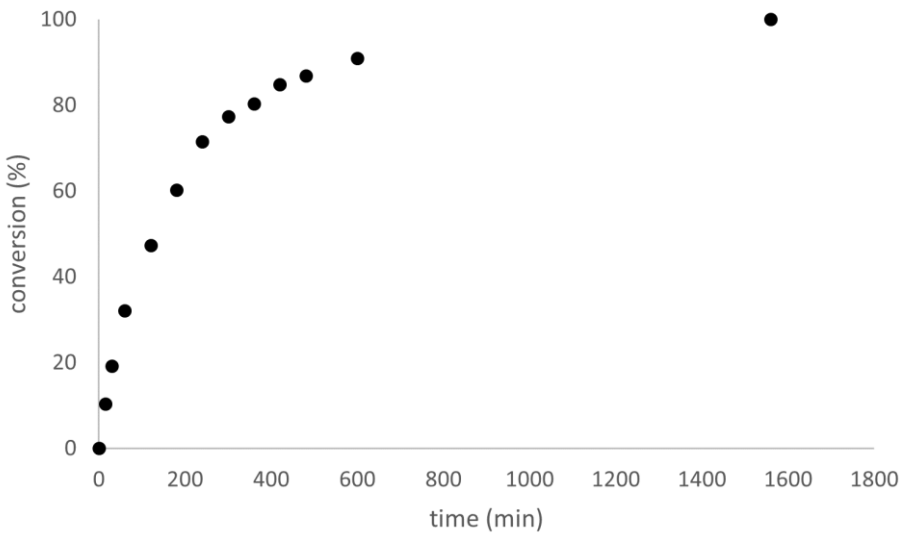


Figure S1. Conversion of the cycloaddition reaction of **TOA** and BCN as a function of time.

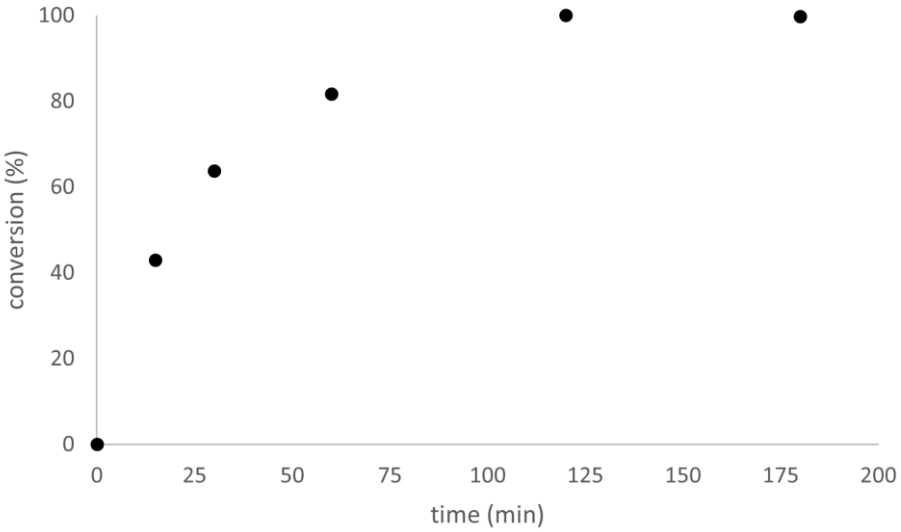


Figure S2. Conversion of the cycloaddition reaction of **TOT** and BCN as a function of time.

4. Cellular studies

4.1. Cell culture

HEK293T (ATCC; CRL-3216, Manassas, VA, USA) were maintained in Dulbecco's modified Eagle's medium (DMEM, Gibco 41965-039) supplemented with 10% FBS (Gibco 10500-064), 1% penicillin-streptomycin (Gibco 15140-122), 1% Glutamax (Gibco 35050-061) and 1% sodium pyruvate (Life Technologies, Gibco 11360-070). The cells were cultured at 37°C in a 5% CO_2 atmosphere and passaged - using trypsin (Gibco 25300-054) every 3-4 days until 20 passages.

4.2. Effect of dyes on cell viability

An MTT viability test was carried out to assess the toxicity of **TO** and **TOT** dyes on HEK293T cells. Cells were transferred into a 48-well plate (Thermo Fisher Scientific,

130187) (30,000 cells/well) and incubated for 48 h at 37 °C in a 5% CO_2 atmosphere. Cells were then treated with compounds **TO** and **TOT** in the concentration range of 1 µM-10 µM for 24 h incubation period at 37 °C in 5% CO_2 atmosphere. After the incubation period, supernatants were replaced with 0.5 mg/ml MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide) solution (in complete DMEM) and incubated for 120 min at 37 °C in the dark. The insoluble formazan crystals were dissolved in 250 µL DMSO. Absorbance was detected at 540 nm using a Biotek Synergy 2 Cytation 3 imaging plate reader with Gen5 software version 3.08 (Biotek Winooski, VT, USA). Viability was expressed as percentage (n=3) of the readings of untreated control cells.

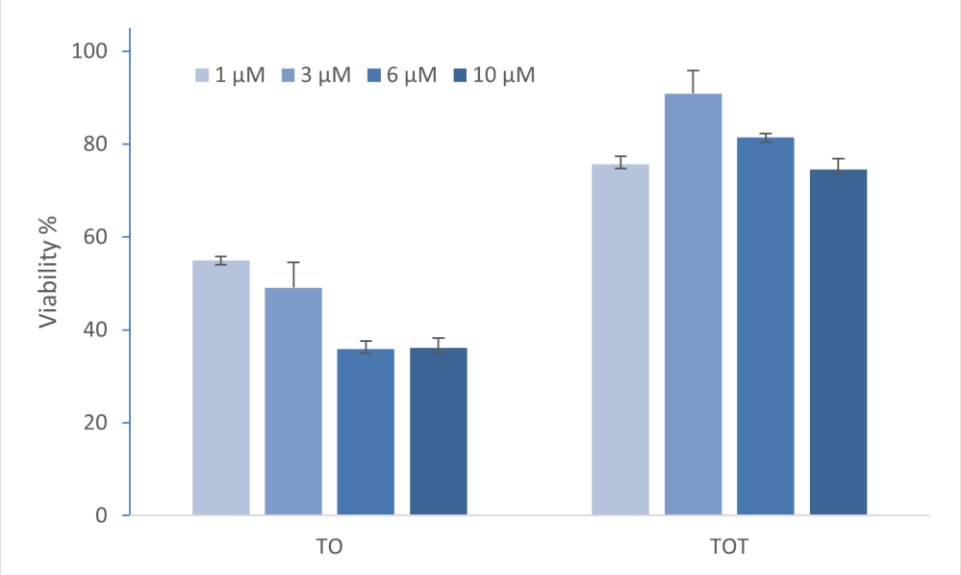


Figure S3. Viability of HEK293T cells upon treatment of **TO** and **TOT** in the percentage of untreated controls (n=3).

4.3. Live-cell labeling

HEK293T (40,000 cell/well) cells were transferred into µ-Slide 8 well plates (Ibidi 80827) and were incubated for 40 h at 37°C in a 5% CO_2 atmosphere. Ibidi plates were pretreated with 0.01 mg/mL Poly-L-lysine (Sigma P5899) for 4 hours at room temperature and washed afterwards.

Overexpression of DNA binding protein histone H2B and LaminA as well as Vimentin and TOMM20 in fusion with HaloTag self-labeling enzyme was achieved by transfection with 0.25 µg plasmids using Lipofectamine3000 (ThermoScientific L3000-008) transfection agent in OptiMEM medium (Gibco 31985-062) for four hours according to the manufacturer's protocol. Subsequently, the supernatant was replaced with complete DMEM medium for overnight. The day after transfection, the bioorthogonally reactive chemical reporter BCN in HaloTag substrate (HaloBCN) was administered to the cells before the fluorescent labeling step in the concentration of 3 µM in complete DMEM for 60 min at 37°C in the dark. After removing HaloBCN **TOT** or **SiR-tet**[15] (Figure S4) was added to the cells -in 6 µM or 3 µM, respectively- in media for 90 min at 37°C in the dark. Afterwards, a two-hour washing step – with complete culturing media – was interpolated followed by fixation (4% PFA for 10 min at 25°C) and quick washing – twice – with PBS prior to imaging.

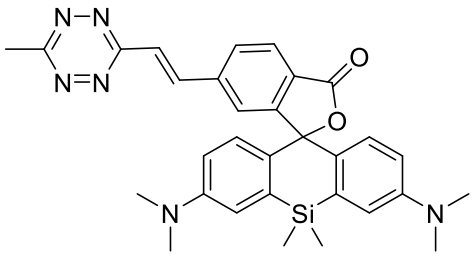


Figure S4. Structure of SiR-tet.

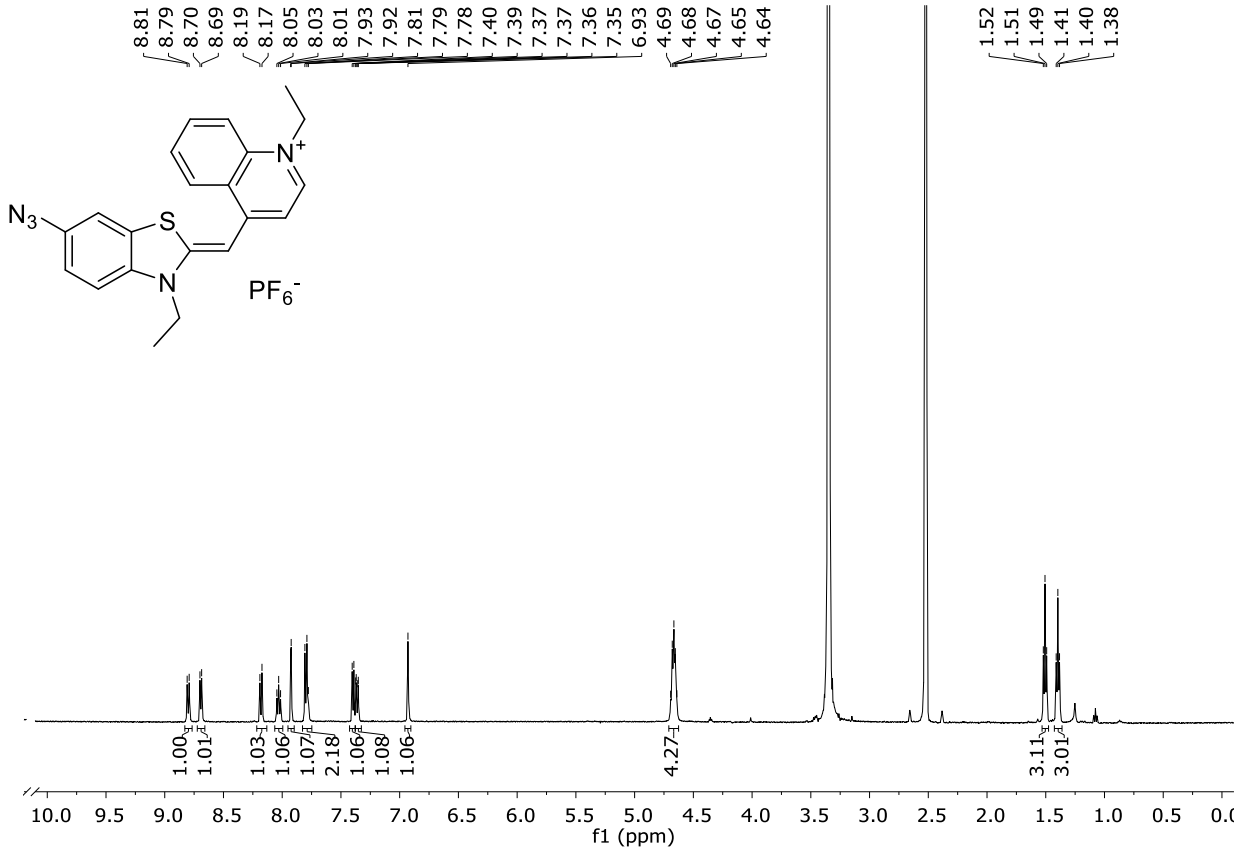
4.4. Construction of HaloTag plasmids

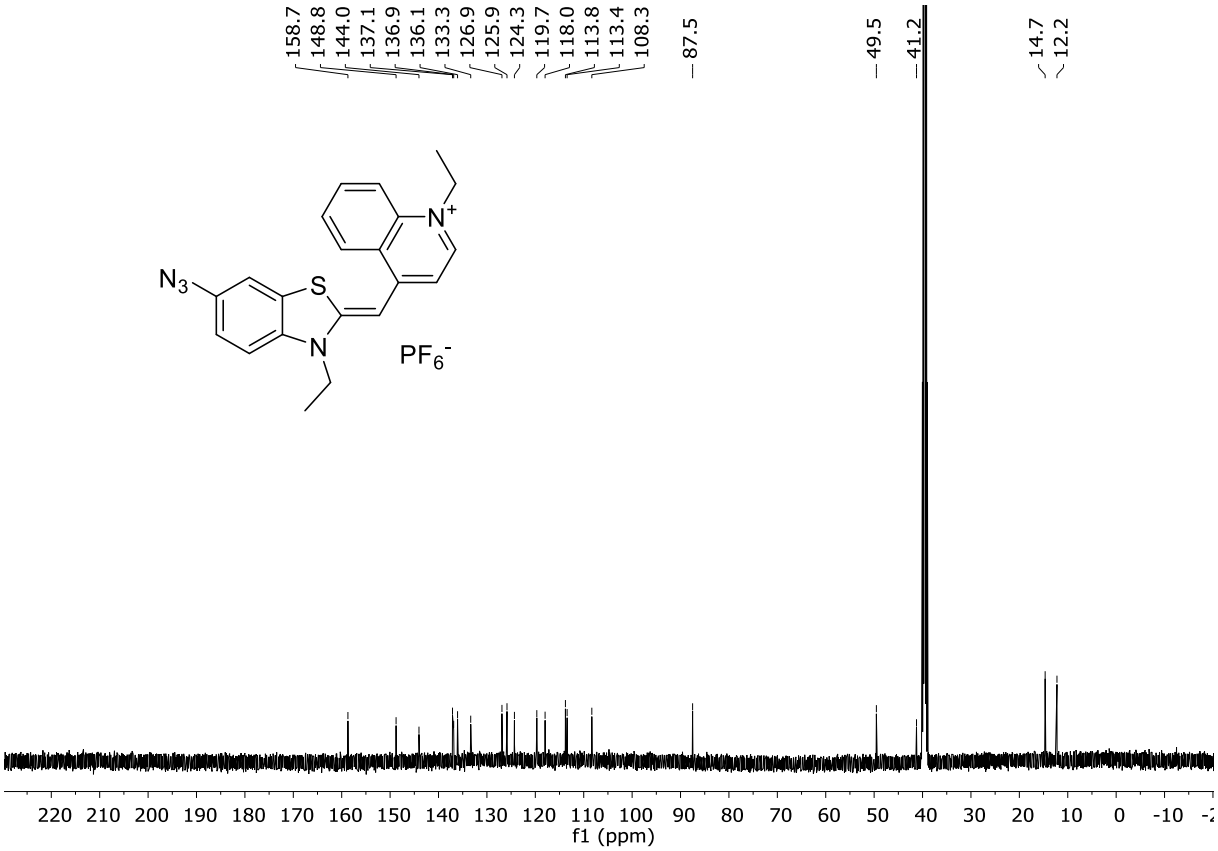
The construction of plasmids (Lamin-HaloTag, H2B-HaloTag, Vimentin-HaloTag and TOMM20-HaloTag) applied here was reported previously in Szatmari et al.[16]

4.5. Fluorescent confocal microscopy

Confocal images were acquired on a Leica TCS SP8 microscope using the 488 nm laser for excitation. The images were taken using a Leica HC PL APO 100x/1.40 oil immersion objective along with Leica HyD detector. Images were analyzed using Leica Application Suite X and ImageJ software (NIH).

5. NMR Spectra

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137.1
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136.1
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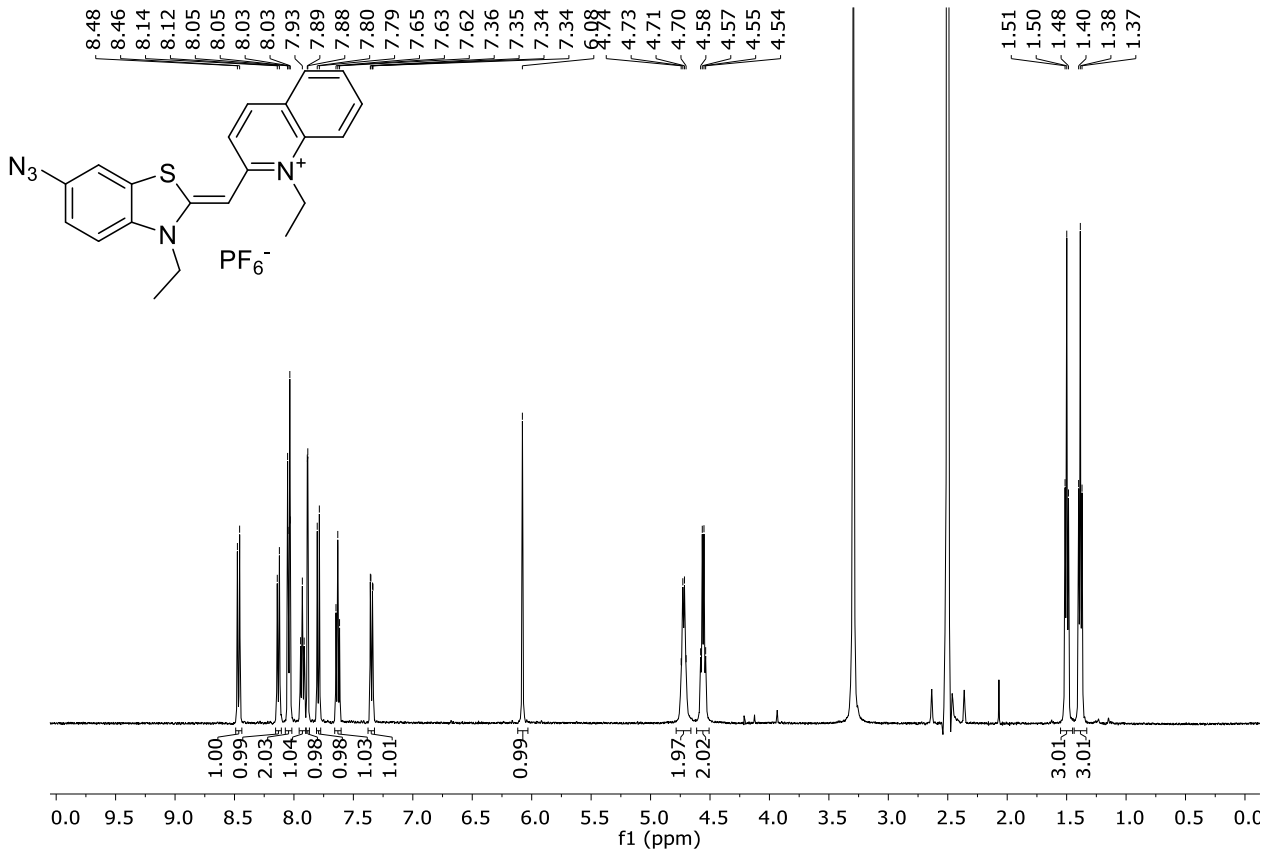
124.3
119.7
118.0
113.8
113.4
108.3
87.5
49.5
41.2
14.7
12.2
N3
S
N
N+
PF6-
f1 (ppm)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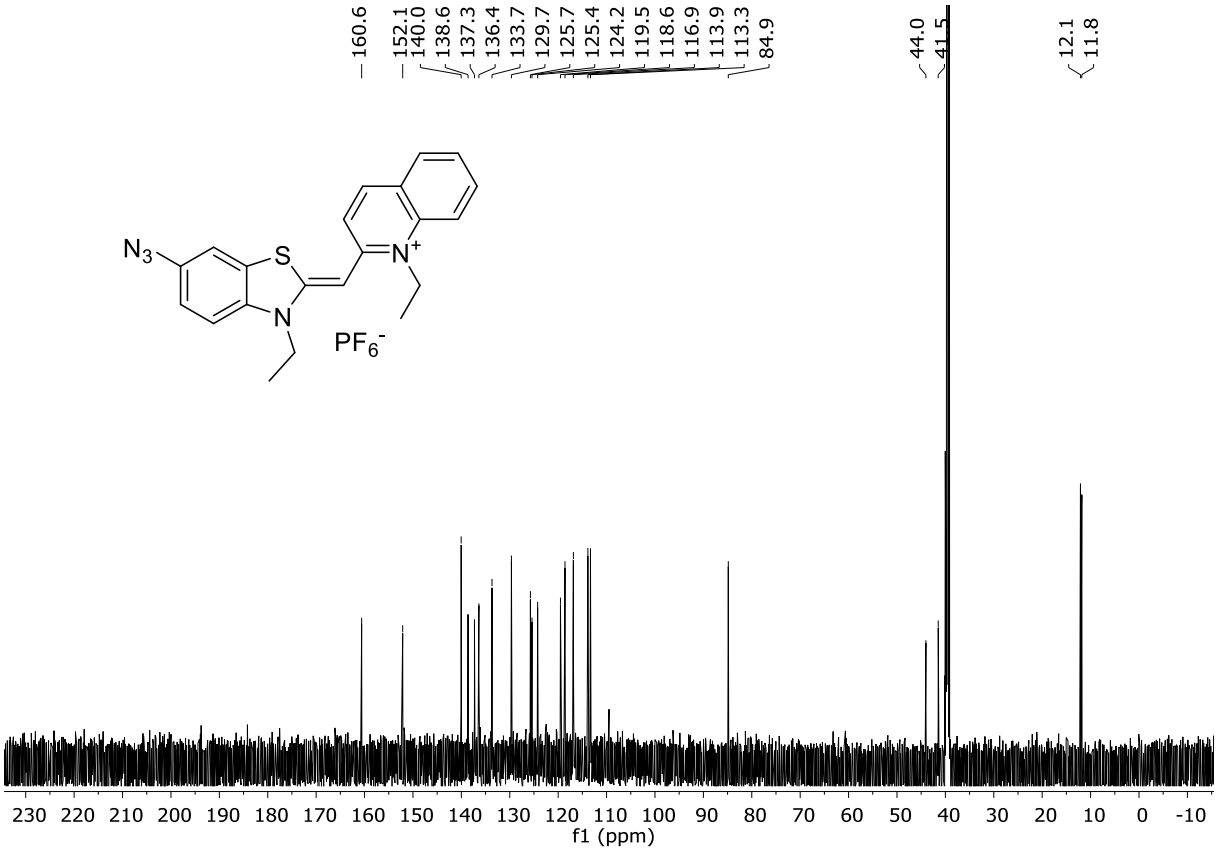
7.65
7.63
7.62
7.36
7.35
7.34
7.34
6.08
4.74
4.73
4.71
4.70
4.58
4.57
4.55
4.54
1.51
1.50
1.48
1.40
1.38
1.37
N3
S
N
N+
PF6-
1.00
0.99
2.03
1.04
0.98
0.98
1.03
1.01
0.99
1.97
2.02
3.01
3.01
f1 (ppm)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113.9
113.3
84.9
44.0
41.5
12.1
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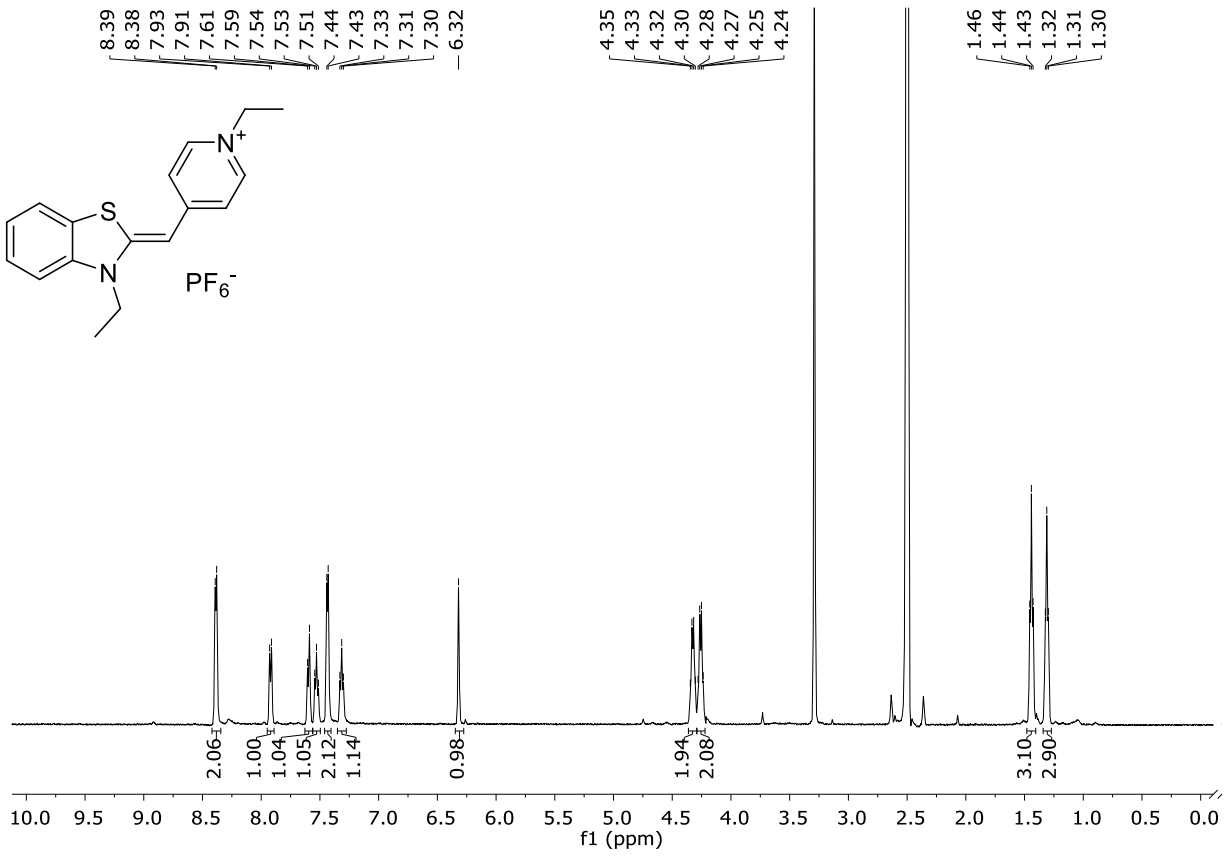
N+
N
PF6-
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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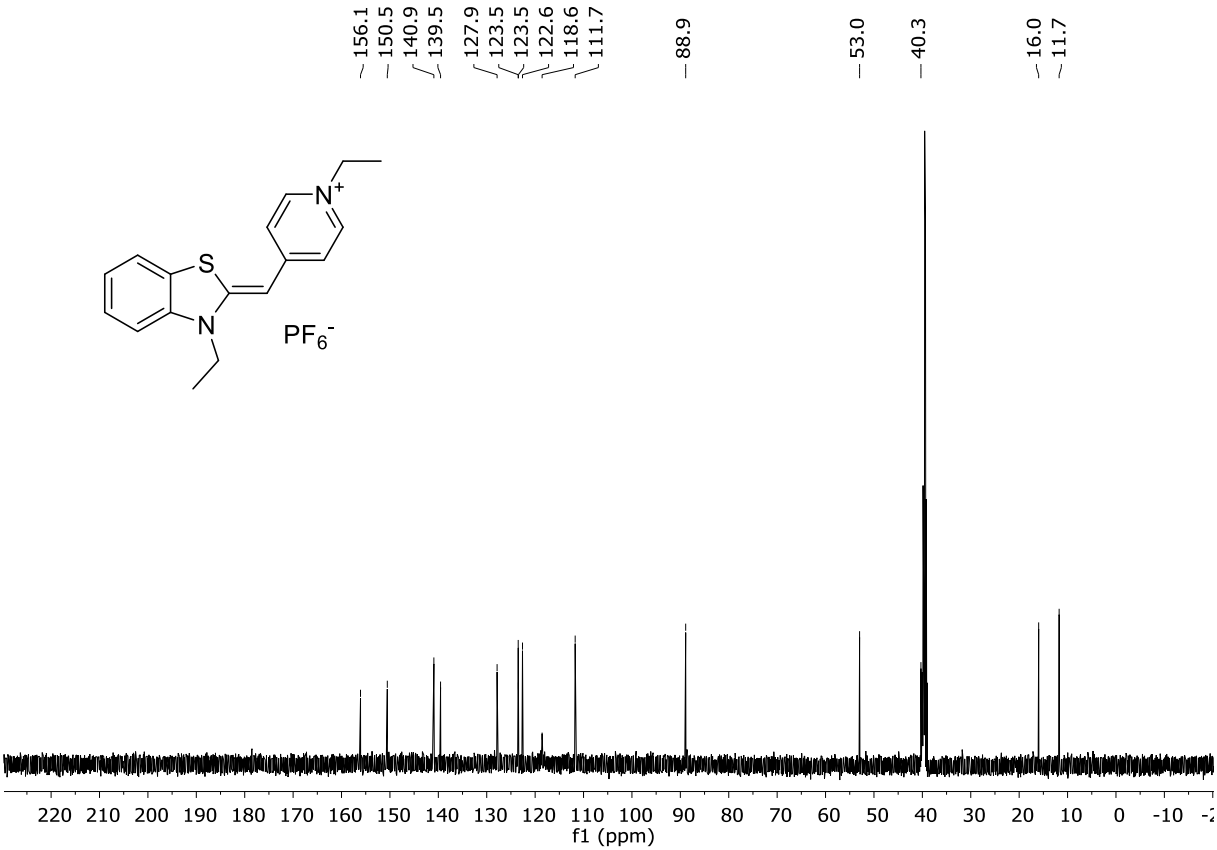
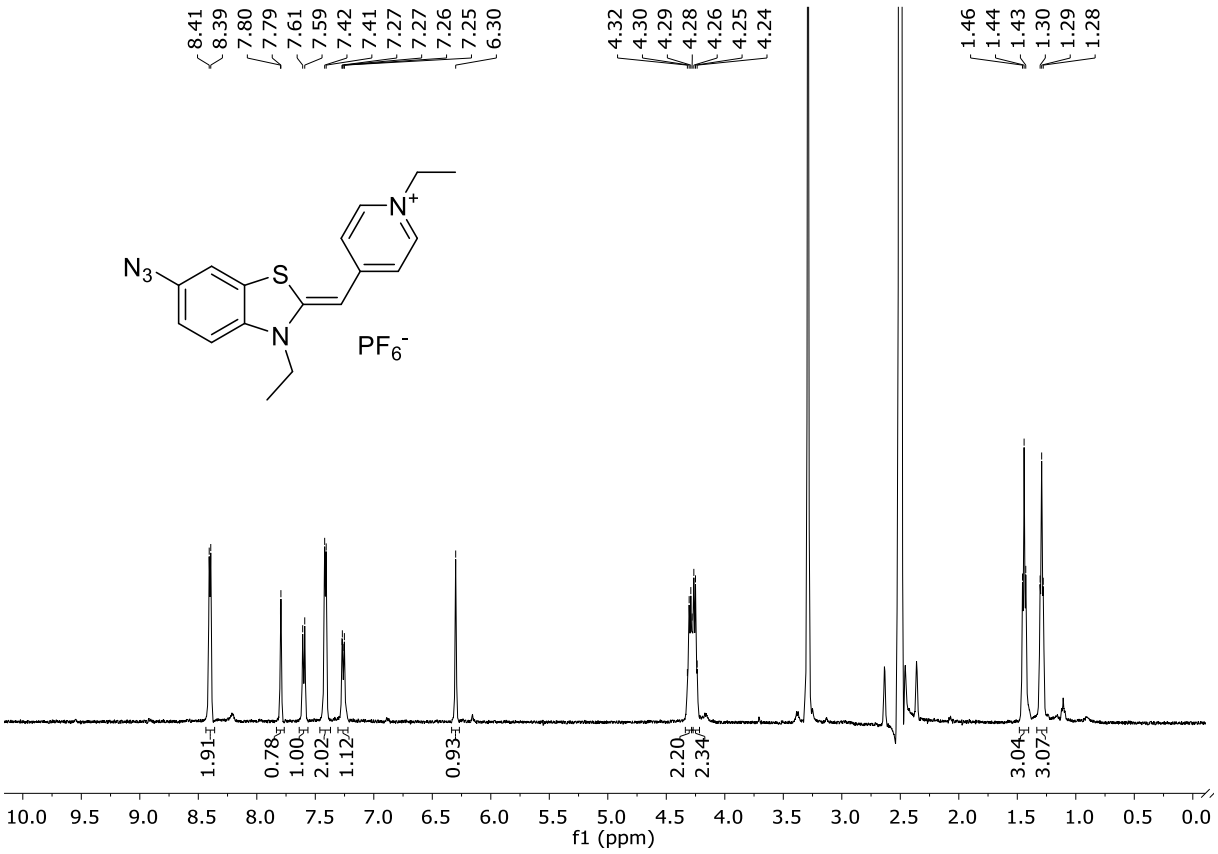
4.33
4.32
4.30
4.28
4.27
4.25
4.24
1.46
1.44
1.43
1.32
1.31
1.30
N+
S
N
PF6-
2.06
1.00
1.04
1.05
2.12
1.14
0.98
1.94
2.08
3.10
2.90
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


156.1
150.5
140.9
139.5
127.9
123.5
123.5
122.6
118.6
111.7
88.9
53.0
40.3
16.0
11.7
N+
S
N
PF6-
f1 (ppm)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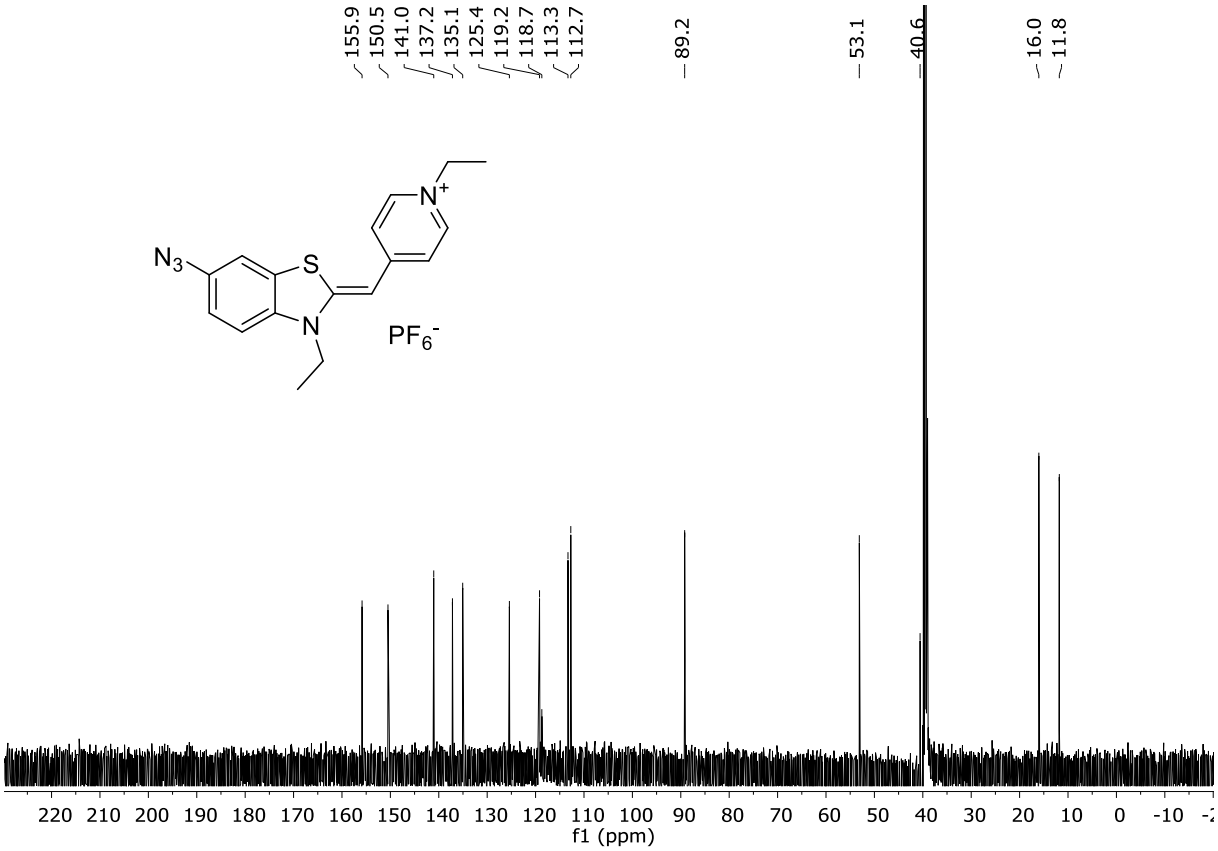
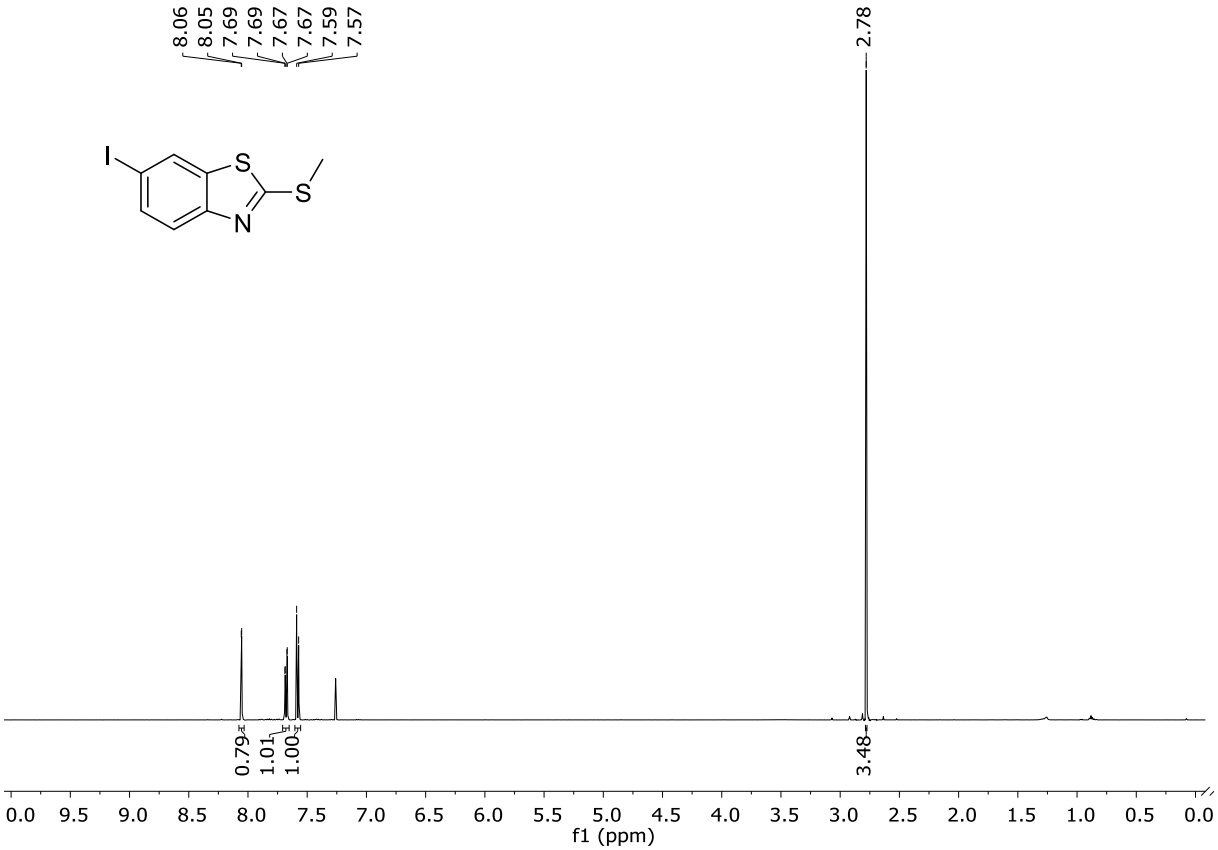
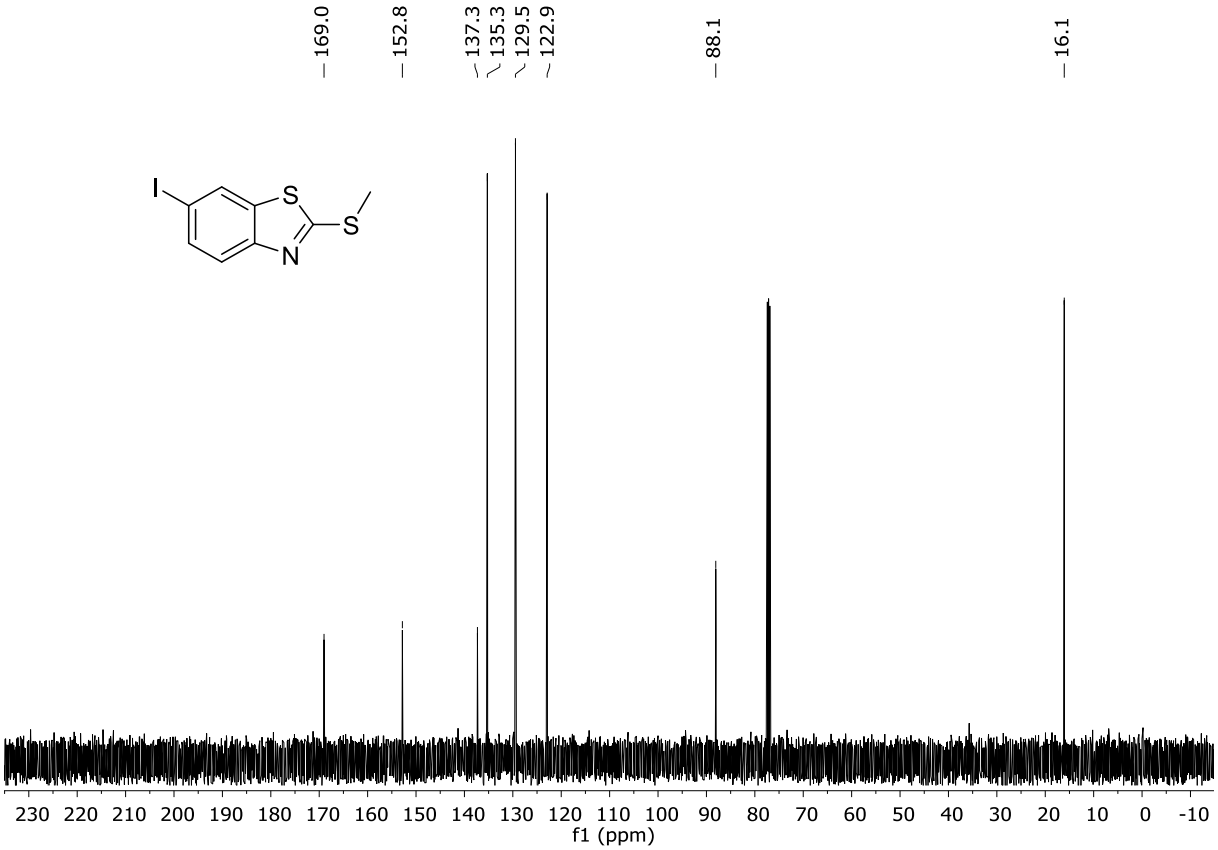
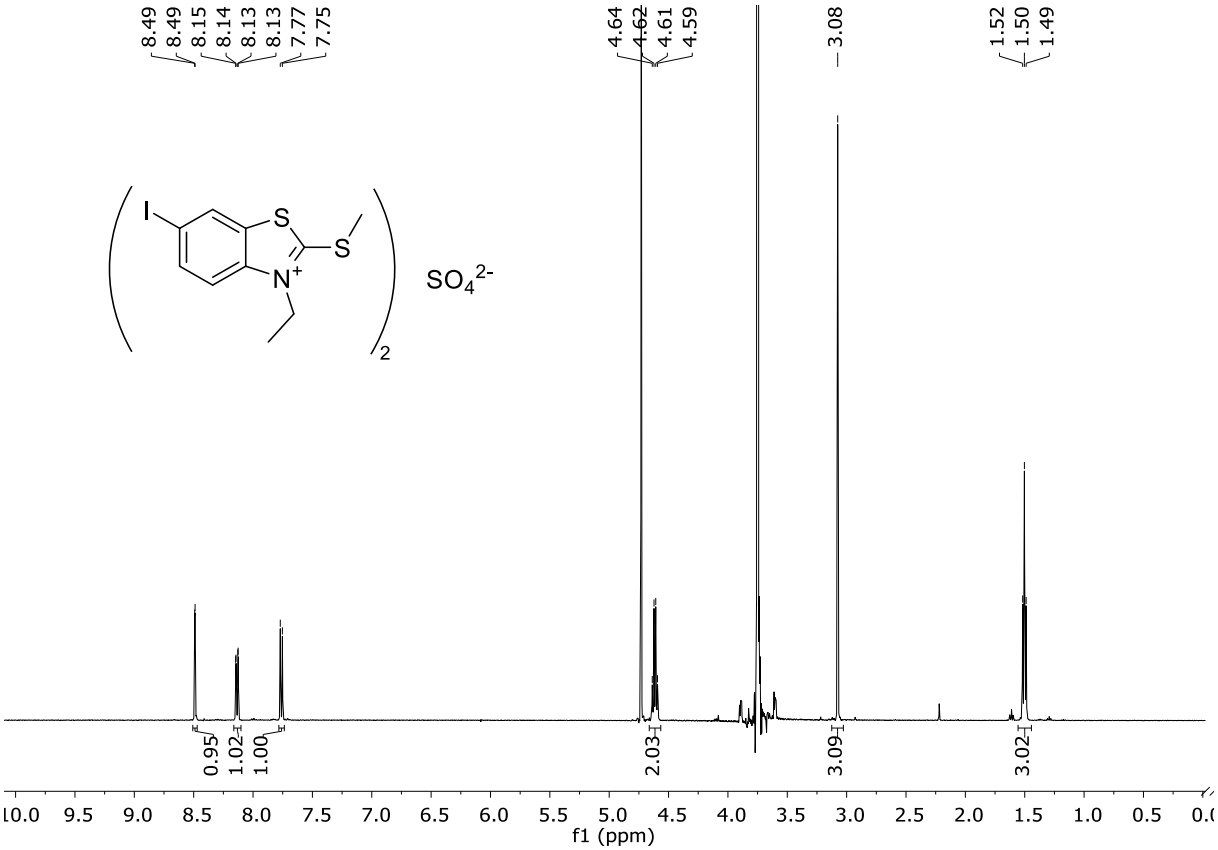
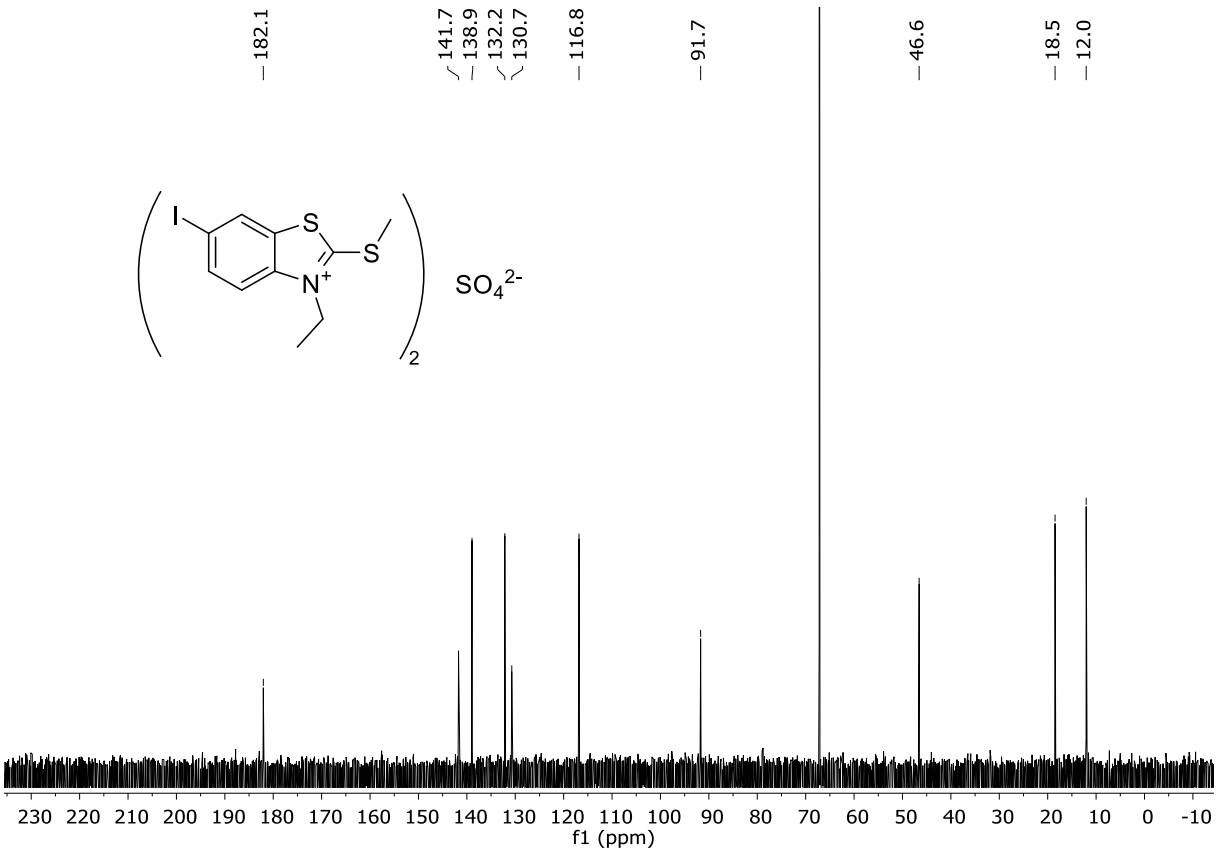
8.39
7.80
7.79
7.61
7.59
7.42
7.41
7.27
7.27
7.26
7.25
6.30
4.32
4.30
4.29
4.28
4.26
4.25
4.24
1.46
1.44
1.43
1.30
1.29
1.28
N3
N+
S
N
PF6-
1.91
0.78
1.00
2.02
1.12
0.93
2.20
2.34
3.04
3.07
f1 (ppm)

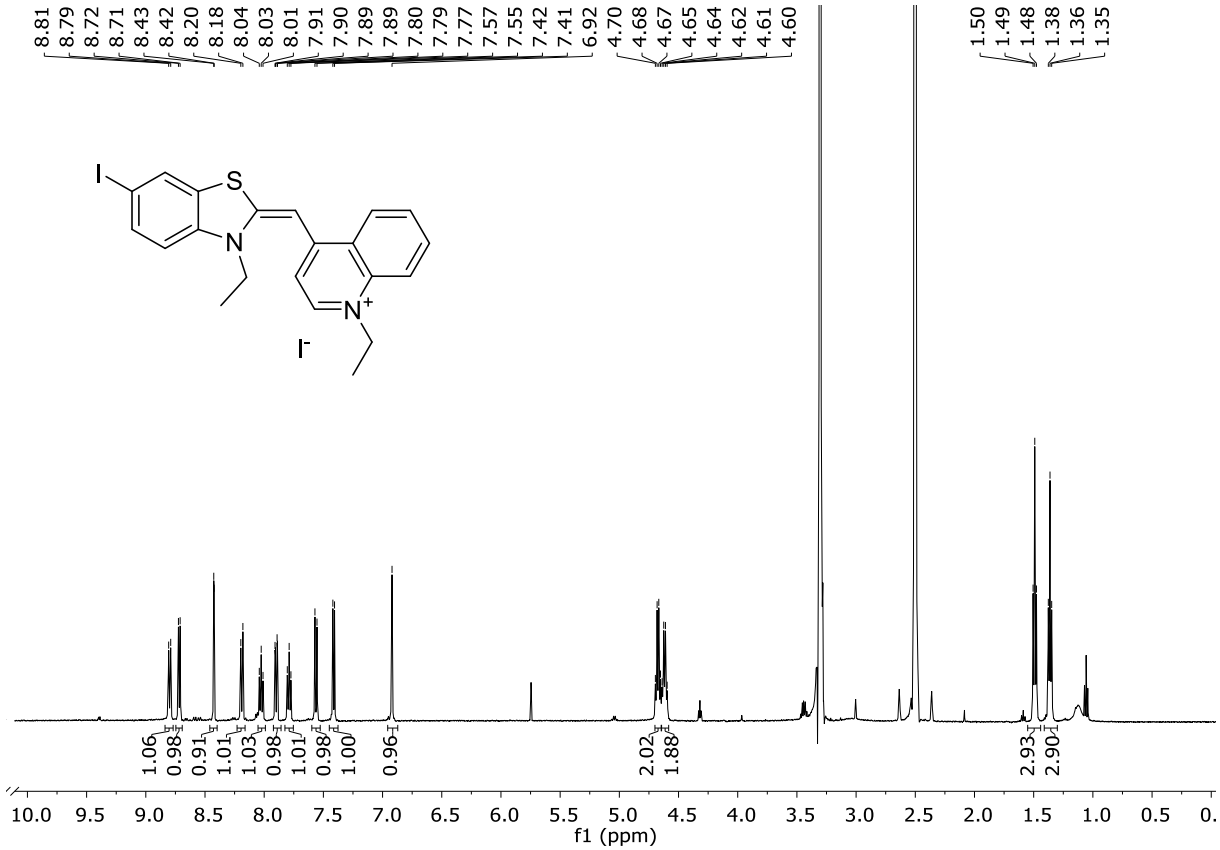

155.9
150.5
141.0
137.2
135.1
125.4
119.2
118.7
113.3
112.7
89.2
53.1
40.6
16.0
11.8
N3
S
N
N+
PF6-
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

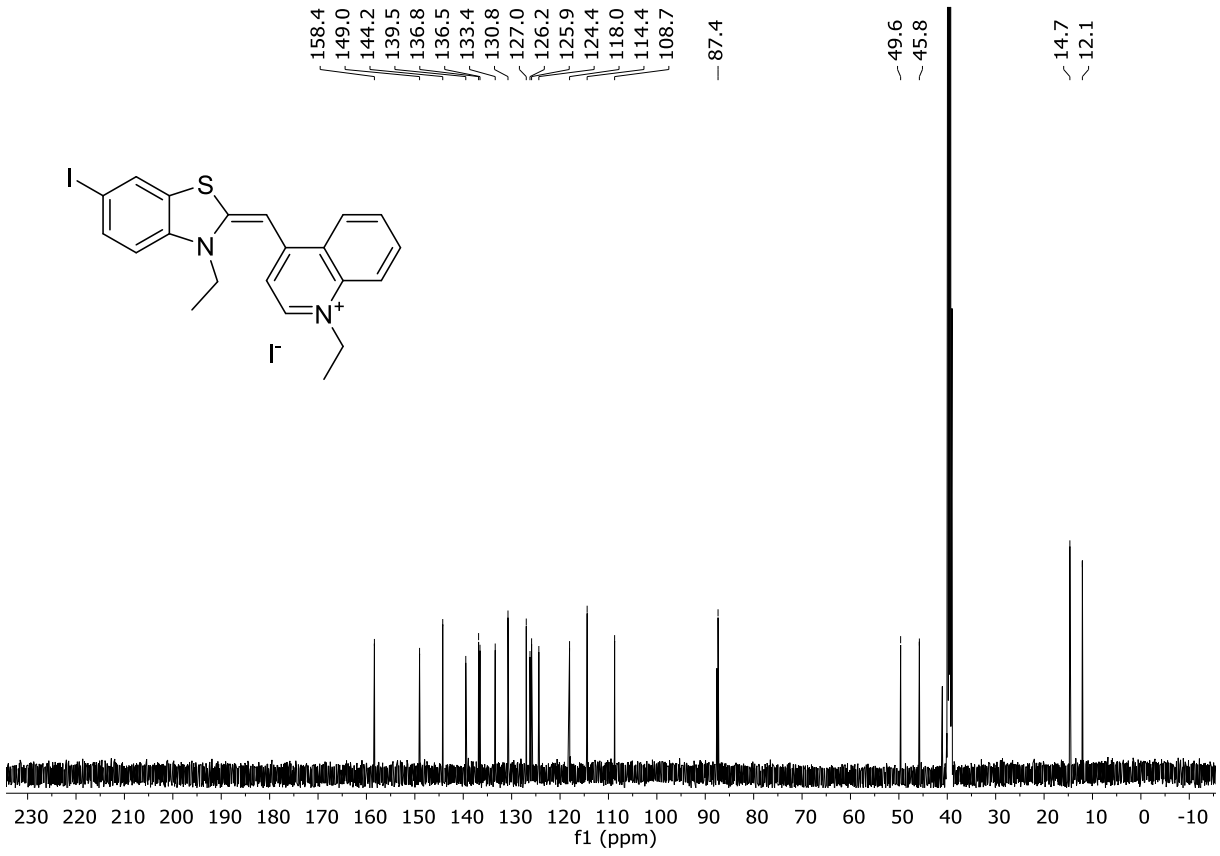

8.06
8.05
7.69
7.69
7.67
7.67
7.59
7.57
2.78
I
S
S
N
0.79
1.01
1.00
3.48
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

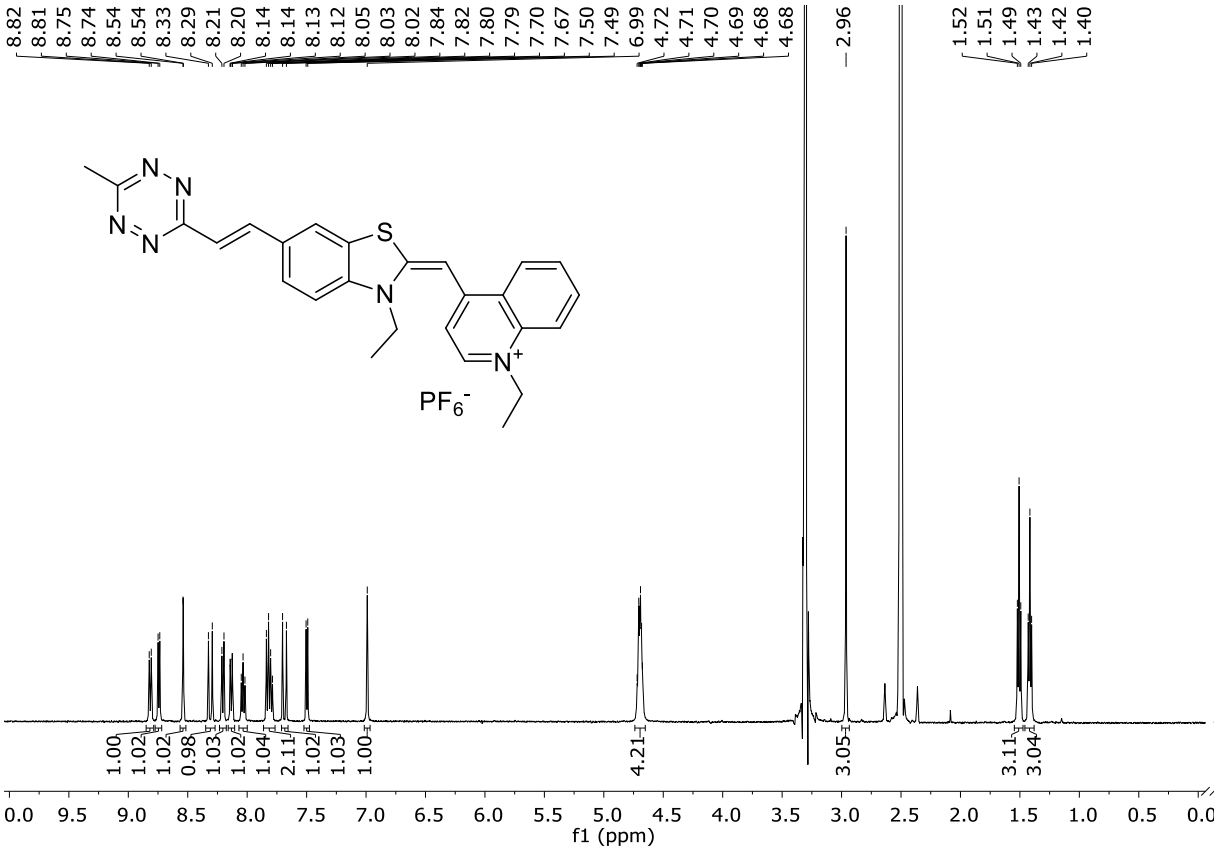

169.0
152.8
137.3
135.3
129.5
122.9
88.1
16.1
I
S
S
N
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

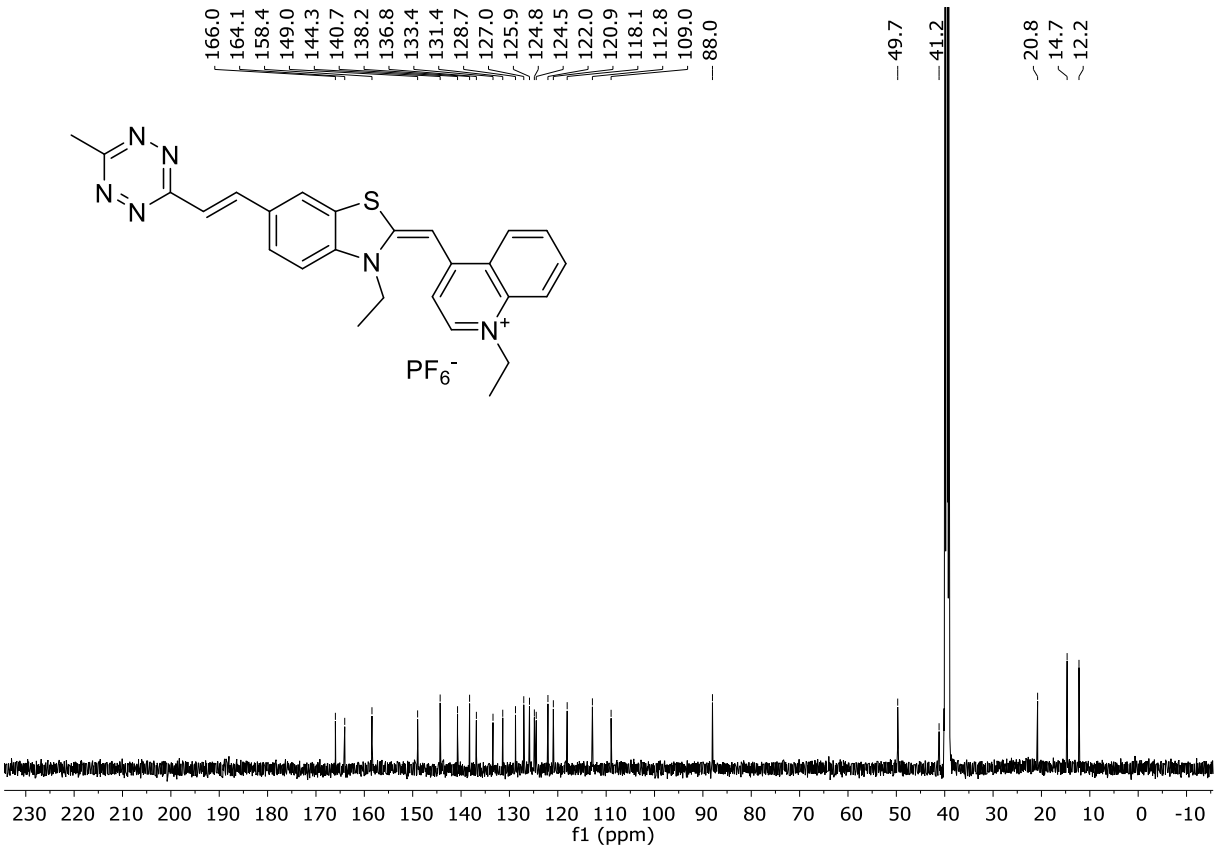

8.49
8.49
8.15
8.14
8.13
8.13
7.77
7.75
4.64
4.62
4.61
4.59
3.08
1.52
1.50
1.49
I
S
S
N+
SO4 2-
2
0.95
1.02
1.00
2.03
3.09
3.02
f1 (ppm)

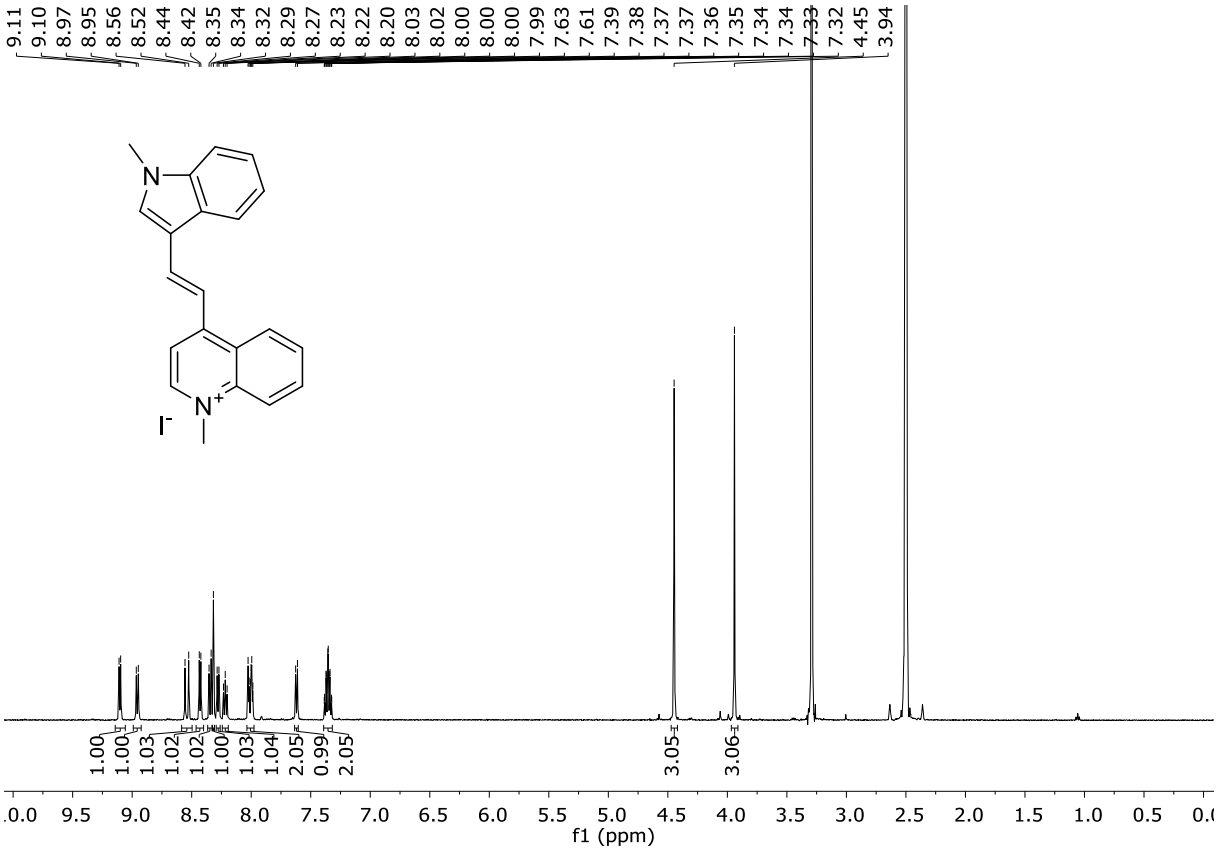

182.1
141.7
138.9
132.2
130.7
116.8
91.7
46.6
18.5
12.0
I
S
S
N+
SO4 2-
2
f1 (ppm)

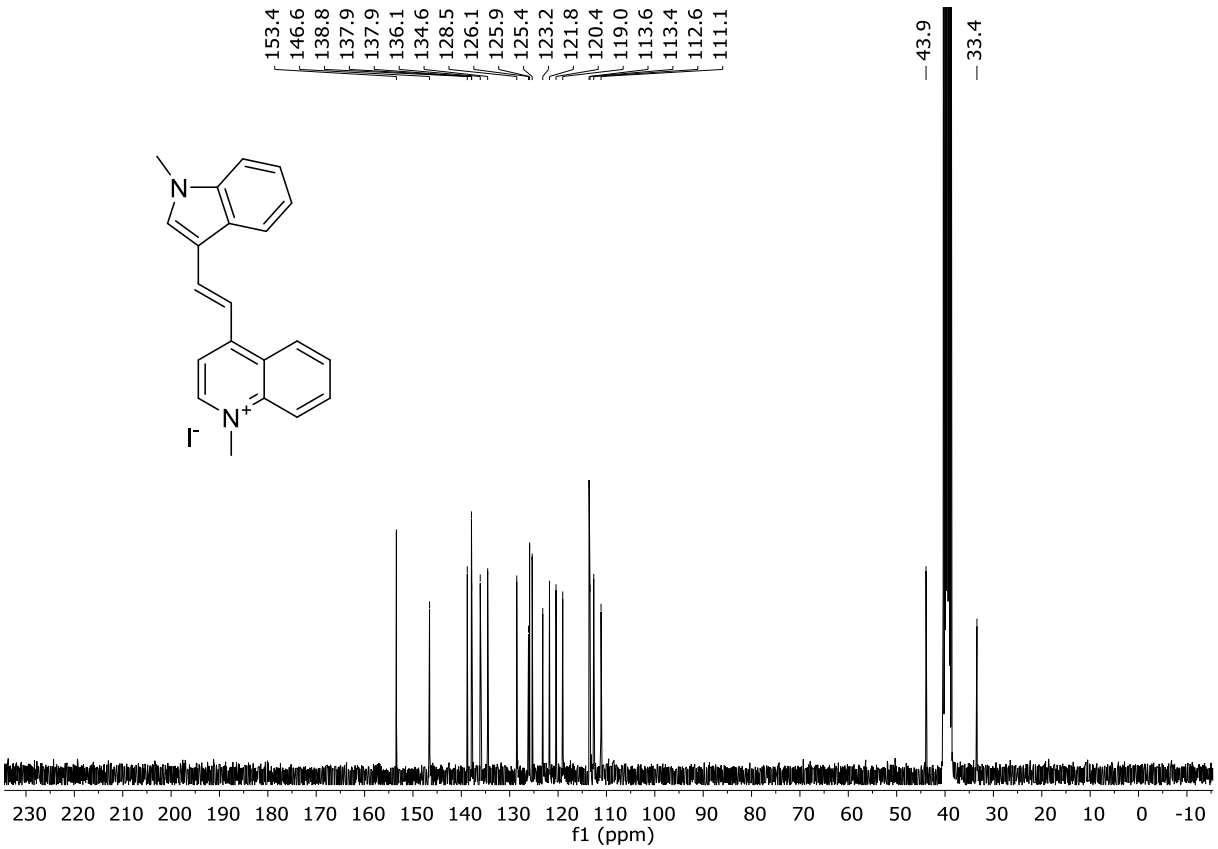

8.81
8.79
8.72
8.71
8.43
8.42
8.20
8.18
8.04
8.03
8.01
7.91
7.90
7.89
7.89
7.80
7.79
7.77
7.57
7.55
7.42
7.41
6.92
4.70
4.68
4.67
4.65
4.64
4.62
4.61
4.60
1.50
1.49
1.48
1.38
1.36
1.35
I
S
N
N+
I-
1.06
0.98
0.91
1.01
1.03
0.98
1.01
0.98
1.00
0.96
2.02
1.88
2.93
2.90
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
f1 (ppm)

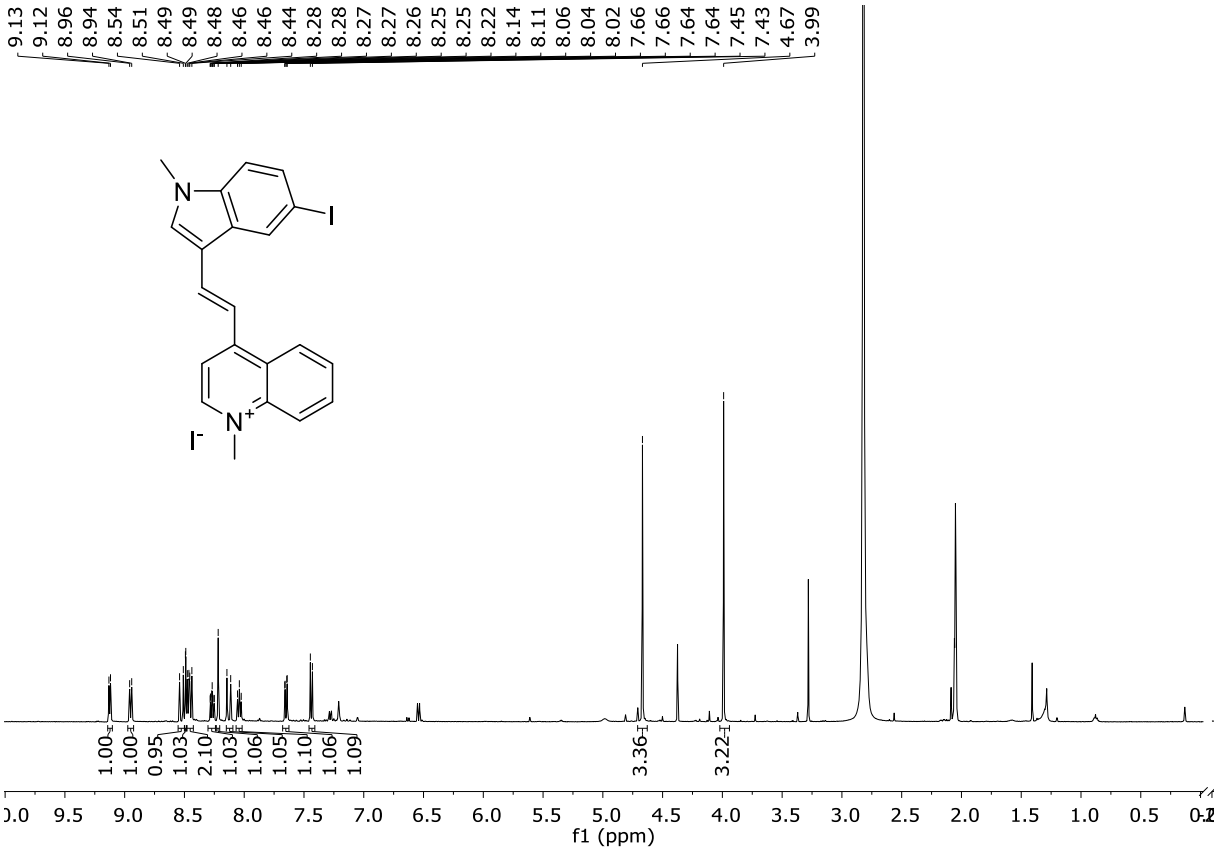

158.4
149.0
144.2
139.5
136.8
136.5
133.4
130.8
127.0
126.2
125.9
124.4
118.0
114.4
108.7
87.4
49.6
45.8
14.7
12.1
I
S
N
N+
I-
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

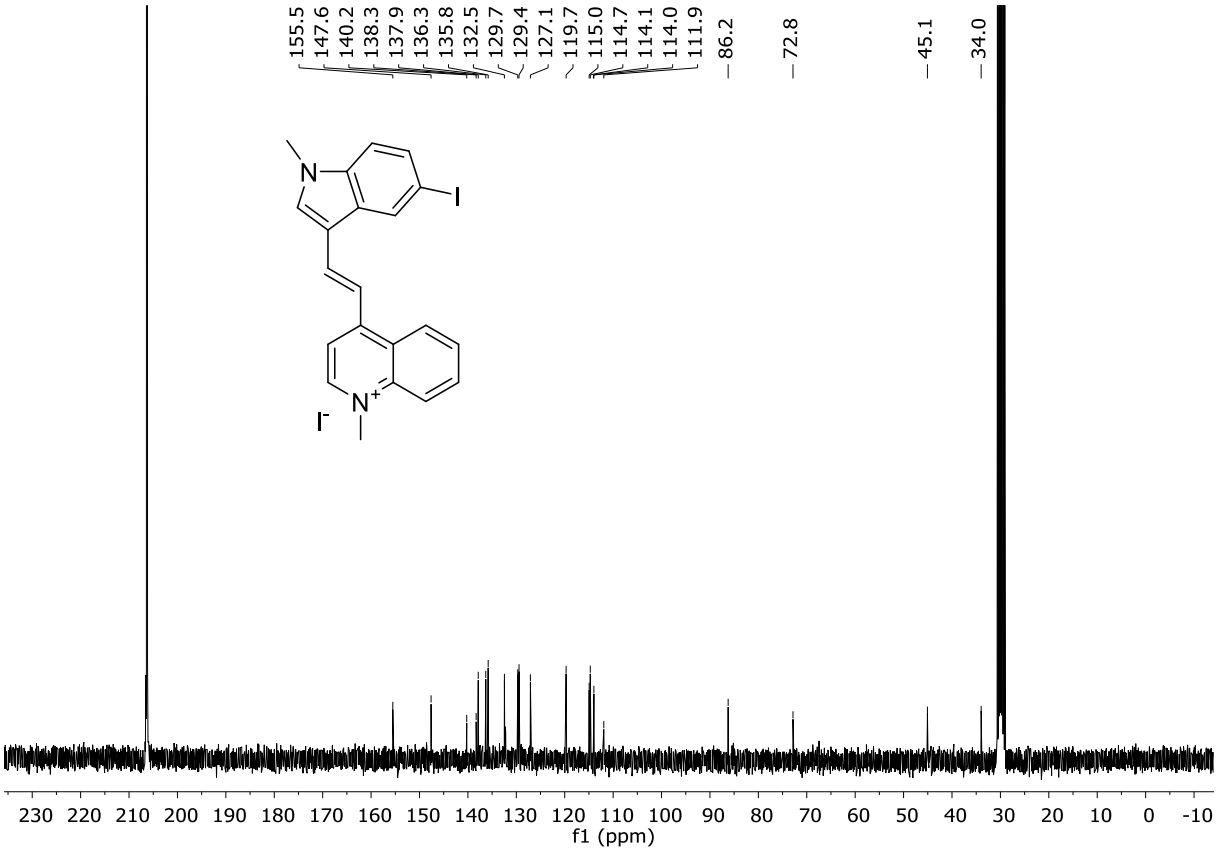

8.82
8.81
8.75
8.74
8.54
8.54
8.33
8.29
8.21
8.20
8.14
8.14
8.13
8.12
8.05
8.03
8.02
7.84
7.82
7.80
7.79
7.70
7.67
7.50
7.49
6.99
4.72
4.71
4.70
4.69
4.68
4.68
2.96
1.52
1.51
1.49
1.43
1.42
1.40
PF6-
1.00
1.02
1.02
0.98
1.03
1.02
1.04
2.11
1.02
1.03
1.00
4.21
3.05
3.11
3.04
f1 (ppm)

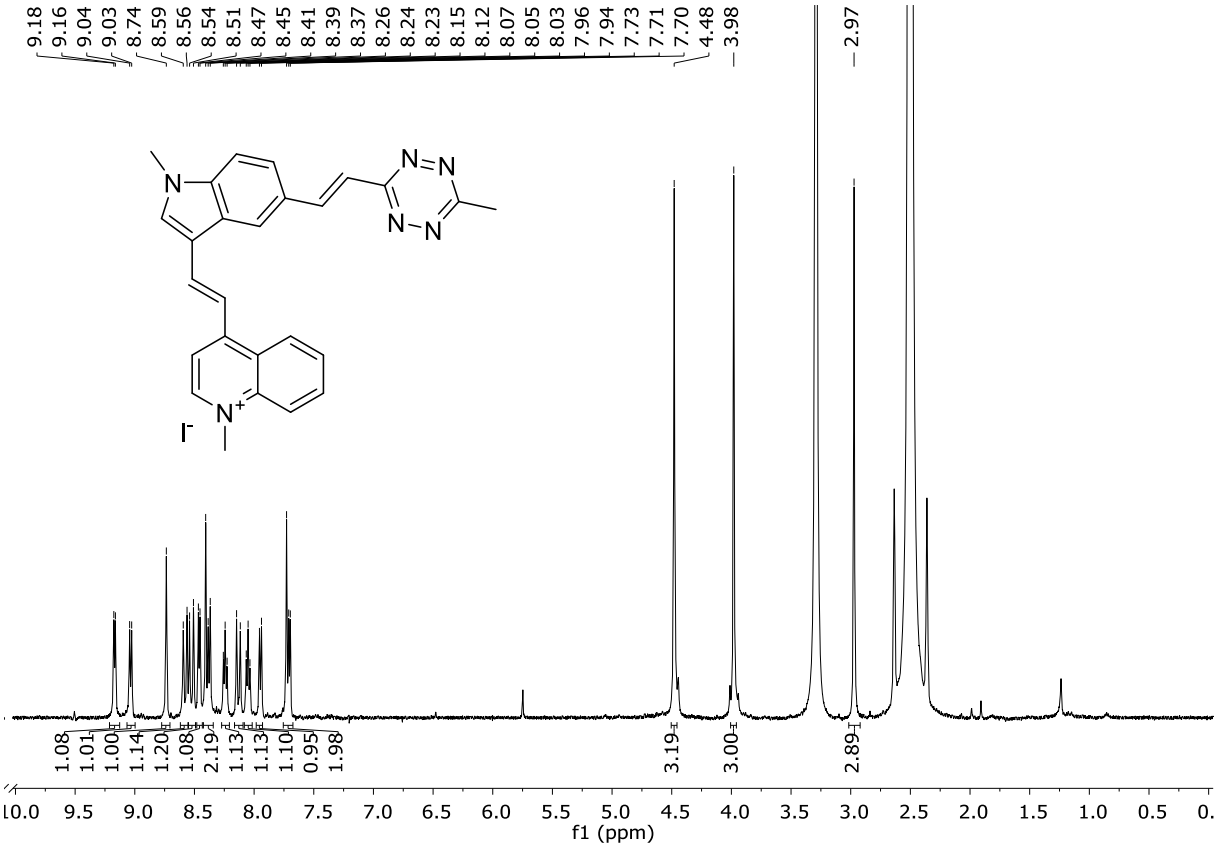

166.0
164.1
158.4
149.0
144.3
140.7
138.2
136.8
133.4
131.4
128.7
127.0
125.9
124.8
124.5
122.0
120.9
118.1
112.8
109.0
88.0
49.7
41.2
20.8
14.7
12.2
PF6-
f1 (ppm)

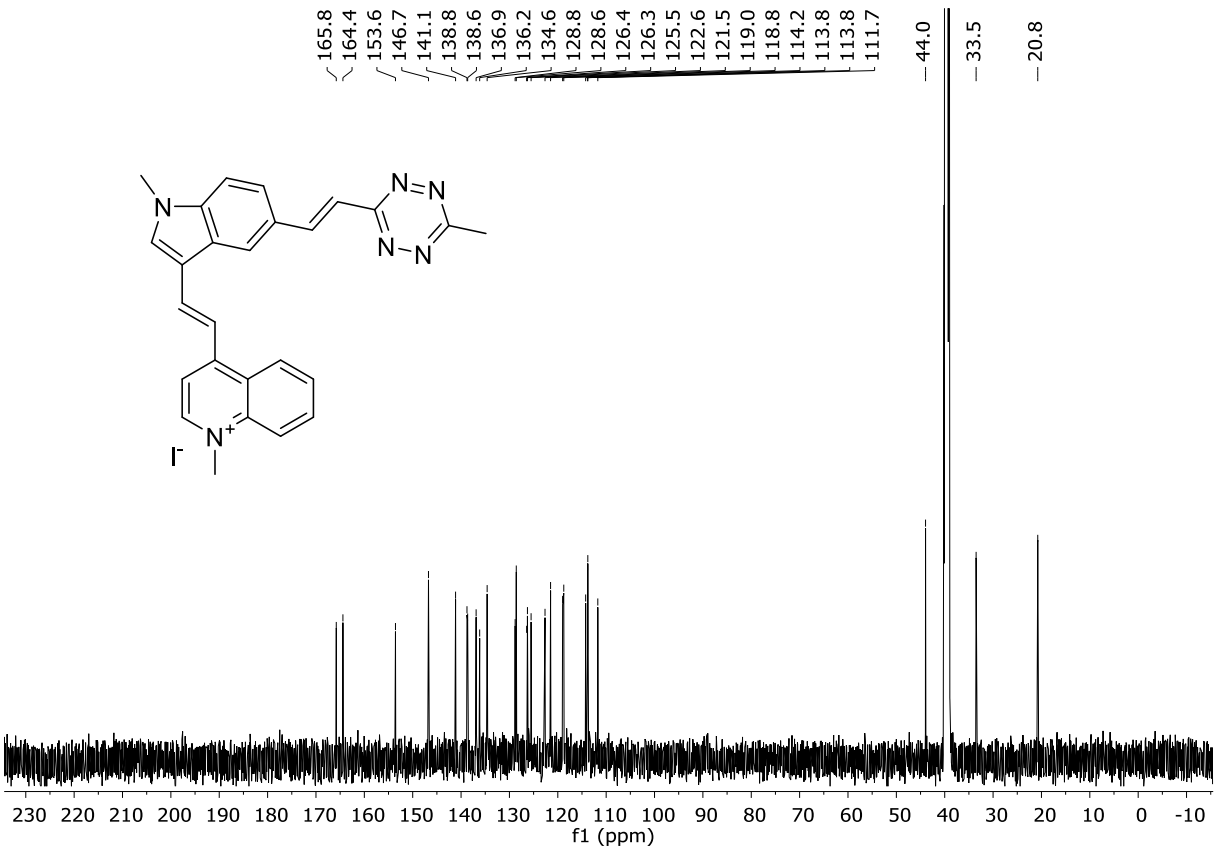

9.11
9.10
8.97
8.95
8.56
8.52
8.44
8.42
8.35
8.34
8.32
8.29
8.27
8.23
8.22
8.20
8.03
8.02
8.00
8.00
8.00
7.99
7.63
7.61
7.39
7.38
7.37
7.37
7.36
7.35
7.34
7.34
7.33
7.32
4.45
3.94
1.00
1.00
1.03
1.02
1.02
1.00
1.03
1.04
2.05
0.99
2.05
3.05
3.06
f1 (ppm)

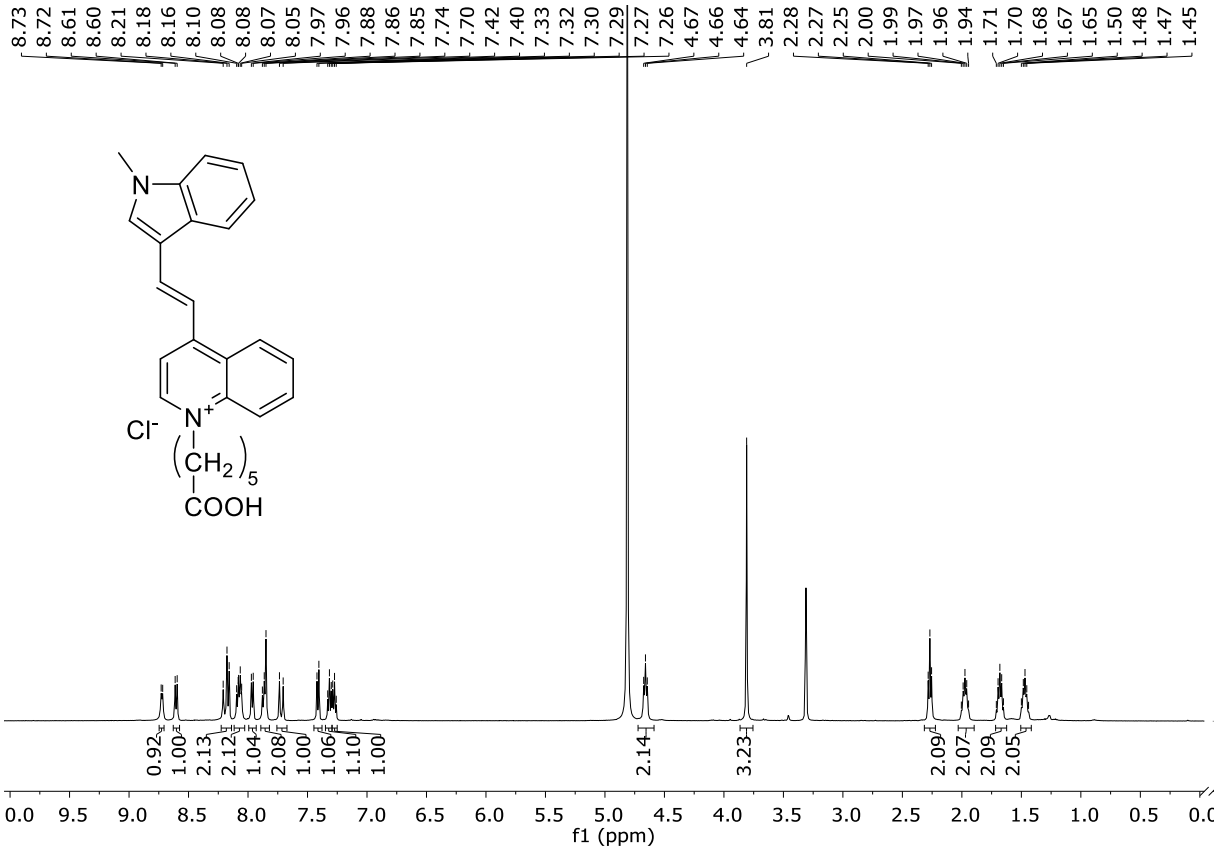

153.4
146.6
138.8
137.9
137.9
136.1
134.6
128.5
126.1
125.9
125.4
123.2
121.8
120.4
119.0
113.6
113.4
112.6
111.1
43.9
33.4
f1 (ppm)

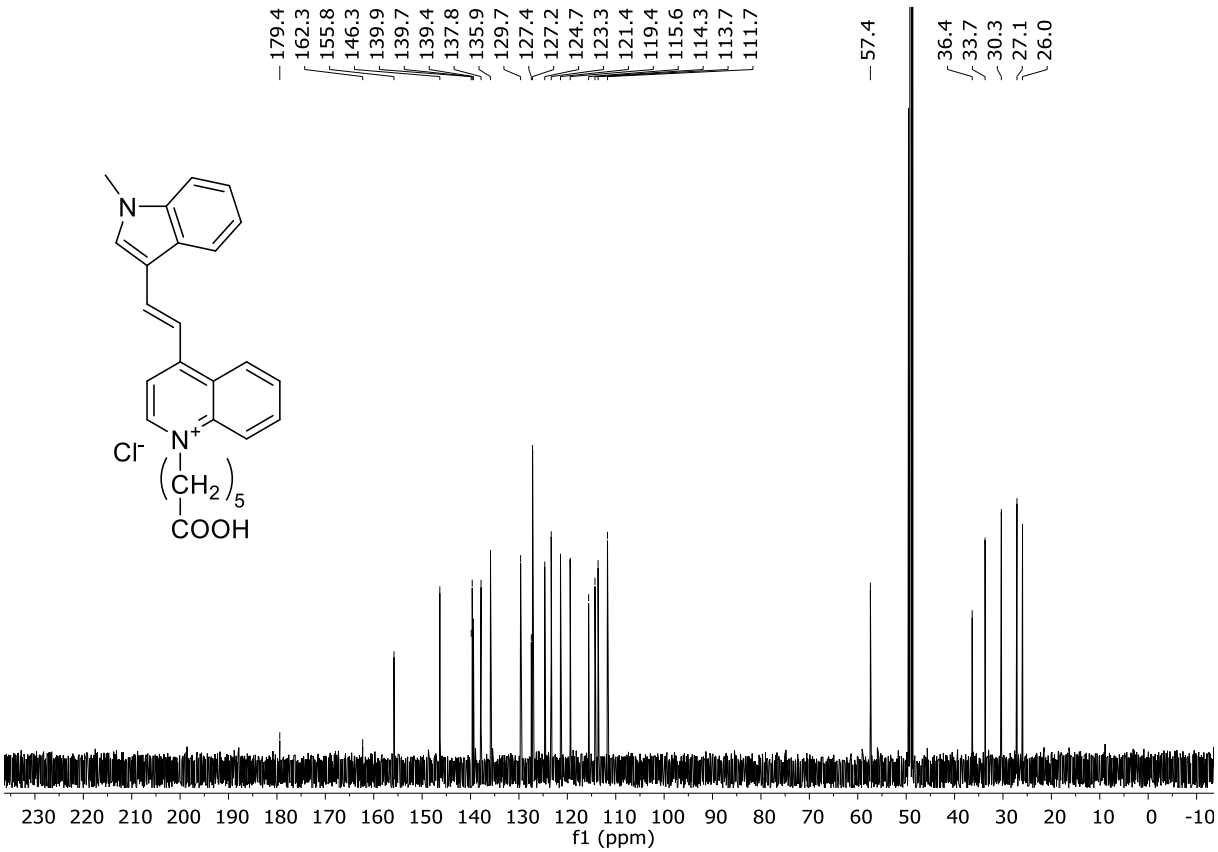

9.13
9.12
8.96
8.94
8.54
8.51
8.49
8.49
8.48
8.46
8.46
8.44
8.28
8.28
8.27
8.26
8.25
8.25
8.22
8.14
8.11
8.06
8.04
8.02
7.66
7.66
7.64
7.64
7.45
7.43
4.67
3.99
N
I
N+
I-
1.00
1.00
0.95
1.03
2.10
1.03
1.06
1.05
1.10
1.06
1.09
3.36
3.22
f1 (ppm)

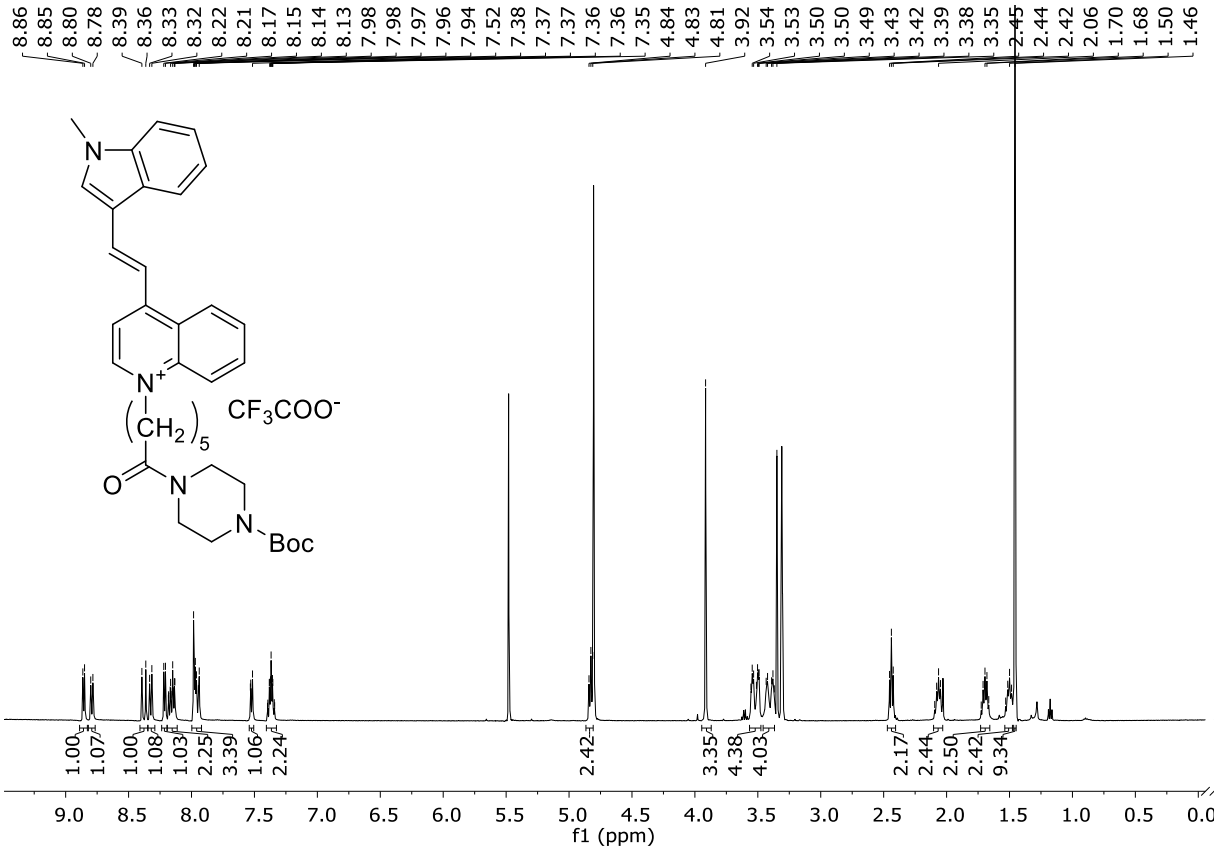

155.5
147.6
140.2
138.3
137.9
136.3
135.8
132.5
129.7
129.4
127.1
119.7
115.0
114.7
114.1
114.0
111.9
86.2
72.8
45.1
34.0
N
I
N+
I-
f1 (ppm)

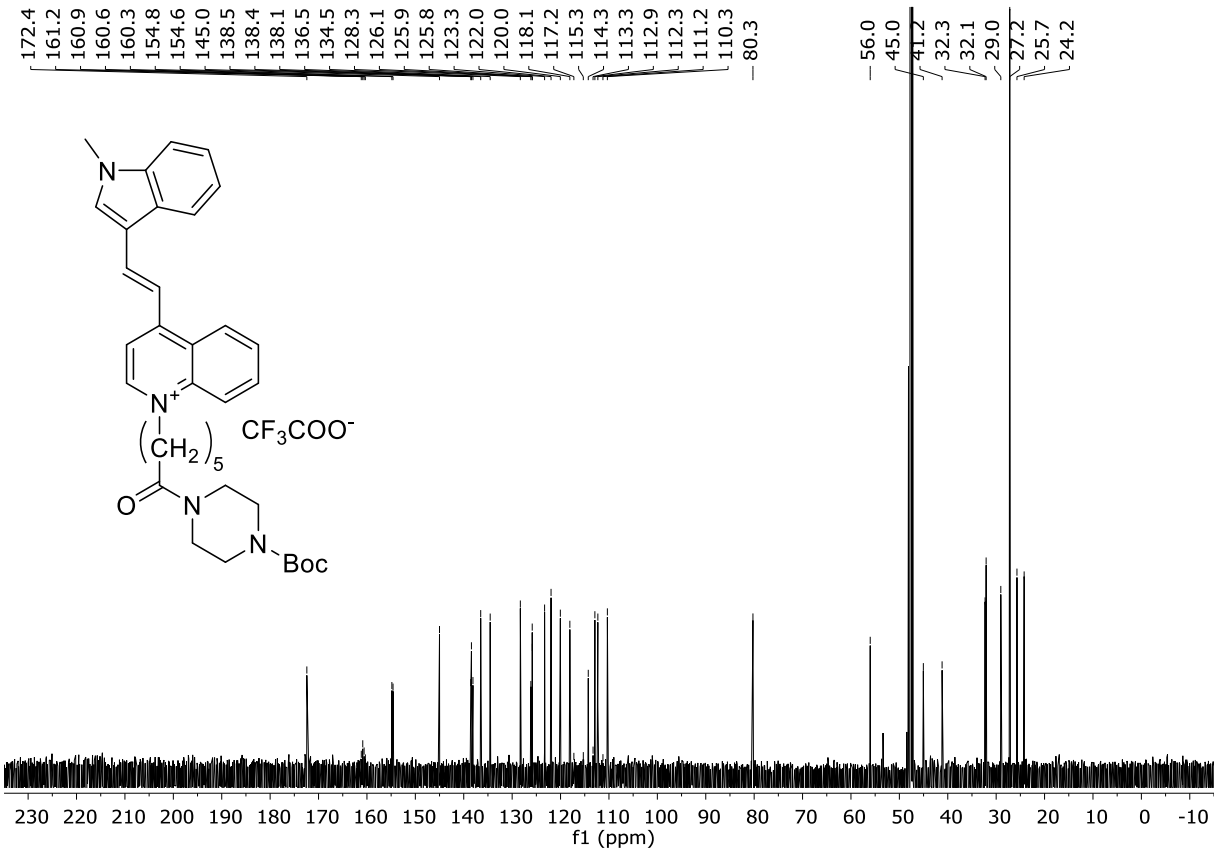

9.18
9.16
9.04
9.03
8.74
8.59
8.56
8.54
8.51
8.47
8.45
8.41
8.39
8.37
8.26
8.24
8.23
8.15
8.12
8.07
8.05
8.03
7.96
7.94
7.73
7.71
7.70
4.48
3.98
2.97
1.08
1.01
1.00
1.14
1.20
1.08
2.19
1.13
1.13
1.10
0.95
1.98
3.19
3.00
2.89
f1 (ppm)

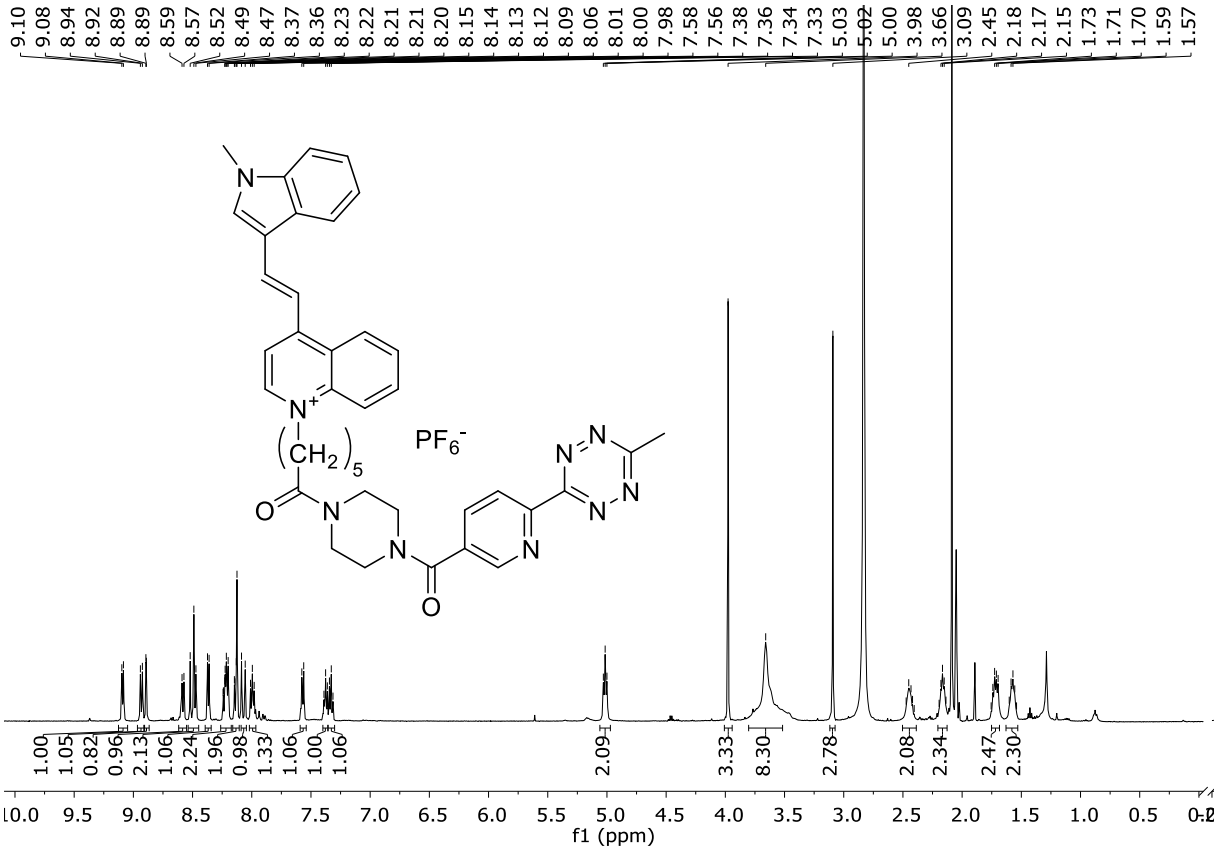

165.8
164.4
153.6
146.7
141.1
138.8
138.6
136.9
136.2
134.6
128.8
128.6
126.4
126.3
125.5
122.6
121.5
119.0
118.8
114.2
113.8
113.8
111.7
44.0
33.5
20.8
f1 (ppm)

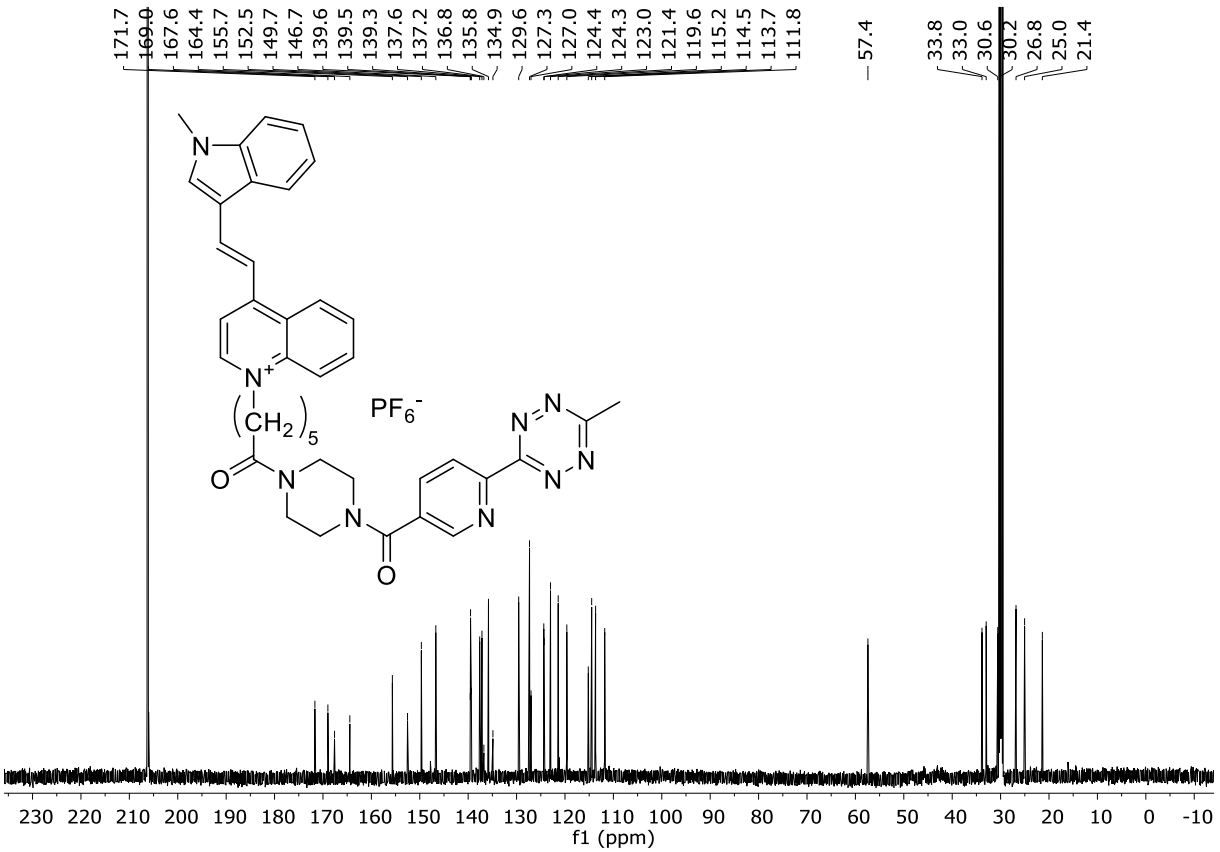

8.73 8.72 8.61 8.60 8.21 8.18 8.16 8.10 8.08 8.08 8.07 8.05 7.97 7.96 7.88 7.86 7.85 7.74 7.70 7.42 7.40 7.33 7.32 7.30 7.29 7.27 7.26 4.67 4.66 4.64 3.81 2.28 2.27 2.25 2.00 1.99 1.97 1.96 1.94 1.71 1.70 1.68 1.67 1.65 1.50 1.48 1.47 1.45
0.92 1.00 2.13 2.12 1.04 2.08 1.00 1.06 1.10 1.00 2.14 3.23 2.09 2.07 2.09 2.05
0.0 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)


179.4 162.3 155.8 146.3 139.9 139.7 139.4 137.8 135.9 129.7 127.4 127.2 124.7 123.3 121.4 119.4 115.6 114.3 113.7 111.7 57.4 36.4 33.7 30.3 27.1 26.0
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.86 8.85 8.80 8.78 8.39 8.36 8.33 8.32 8.22 8.21 8.17 8.15 8.14 8.13 7.98 7.98 7.97 7.96 7.94 7.52 7.38 7.37 7.37 7.36 7.36 7.35 4.84 4.83 4.81 3.92 3.54 3.53 3.50 3.50 3.49 3.43 3.42 3.39 3.38 3.35 2.45 2.44 2.42 2.06 1.70 1.68 1.50 1.46
CF3COO-
Boc
1.00 1.07 1.00 1.08 1.03 2.25 3.39 1.06 2.24 2.42 3.35 4.38 4.03 2.17 2.44 2.50 2.42 9.34
f1 (ppm)


172.4 161.2 160.9 160.6 160.3 154.8 154.6 145.0 138.5 138.4 138.1 136.5 134.5 128.3 126.1 125.9 125.8 123.3 122.0 120.0 118.1 117.2 115.3 114.3 113.3 112.9 112.3 111.2 110.3 80.3
56.0 45.0 41.2 32.3 32.1 29.0 27.2 25.7 24.2
CF3COO-
Boc
f1 (ppm)


9.10 9.08 8.94 8.92 8.89 8.89 8.59 8.57 8.52 8.49 8.47 8.37 8.36 8.23 8.22 8.21 8.21 8.20 8.15 8.14 8.13 8.12 8.09 8.06 8.01 8.00 7.98 7.58 7.56 7.38 7.36 7.34 7.33 5.03 5.02 5.00 3.98 3.66 3.09 2.45 2.18 2.17 2.15 1.73 1.71 1.70 1.59 1.57
PF6-
1.00 1.05 0.82 0.96 2.13 1.06 2.24 1.96 0.98 1.33 1.06 1.00 1.06 2.09 3.33 8.30 2.78 2.08 2.34 2.47 2.30
f1 (ppm)


171.7 169.0 167.6 164.4 155.7 152.5 149.7 146.7 139.6 139.5 139.3 137.6 137.2 136.8 135.8 134.9 129.6 127.3 127.0 124.4 124.3 123.0 121.4 119.6 115.2 114.5 113.7 111.8 57.4 33.8 33.0 30.6 30.2 26.8 25.0 21.4
PF6-
f1 (ppm)

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