Supplementary Information

Facile one-pot synthesis of novel imidates as multifunctional organic fluorescent materials

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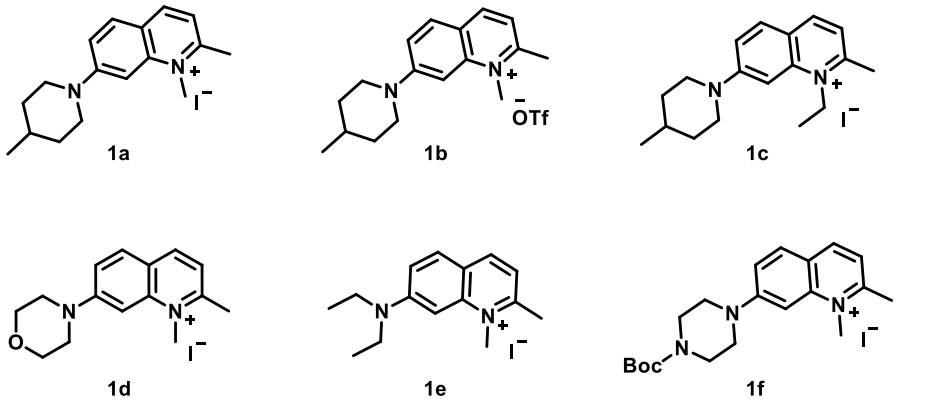
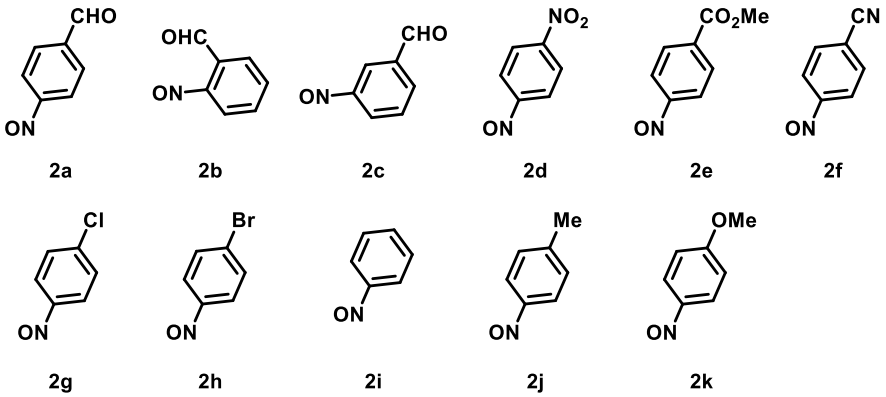
General remarks

Proton (^{1}H) and carbon (^{13}C) NMR spectra were determined by Bruker Avance III HD 400 MHz spectrometer. High resolution mass spectrometry was obtained with a Bruker Impact II mass instrument under the conditions of electrospray ionization (ESI) in positive mode. Melting points were determined on a XD-4 digital micro melting point apparatus. IR spectra were obtained using IR spectrophotometer VERTEX 70 FT-IR (Bruker Optics). UV-vis absorption spectra were obtained by a U-4100 spectrophotometer (Hitachi) and fluorescence spectra were measured on a LS-55 fluorescence spectrophotometer (PerkinElmer). The absolute fluorescence quantum yield was measured on an Edinburgh Instruments FLS920 Fluorescence Spectrometer. For single-crystal X-ray diffraction, intensity data and cell parameters were recorded at 293 K on a Bruker Apex II single crystal diffractometer employing Cu K_{α} (λ = 1.54184 Å) and a CCD area detector. Thin-layer chromatography (TLC) was conducted on silica gel $60F_{254}$ plates (Merck KGaA) and column chromatography was carried out over silica gel (200-300 mesh). Unless otherwise stated, all reagents and solvents were purchased from commercial provider. Twice-distilled water was used throughout all experiments.

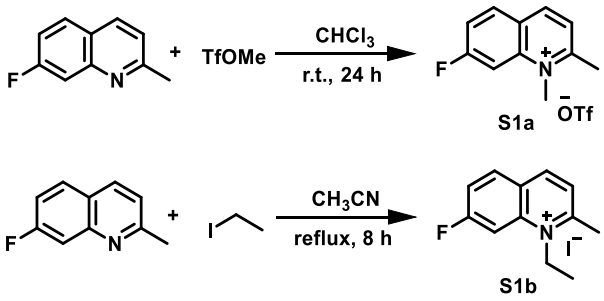
Photophysical Characterization of the Compounds. The stock solutions of compound **4a**, **4j**, **4k**, **4m**, **4n**, **4p**, **4q**, **4u**, **4ad** and **4al** (4×10^{-3} M) in dimethyl sulfoxide were prepared. The diluted solutions (2×10^{-5} M) in dimethyl sulfoxide, acetonitrile, ethyl alcohol, acetone, tetrahydrofuran and dichloromethane, respectively, were used for fluorescence measurements. Test solutions (4×10^{-5} M) in dimethyl sulfoxide, acetonitrile, ethyl alcohol, acetone, tetrahydrofuran and dichloromethane, respectively, were made for UV−vis spectra.





Materials and Methods. Quinolinium salt substrates **1a** and **1e** were prepared according to literature procedures[1, 2]. **1b**, **1c**, **1d** and **1f** were synthesized by the following method. Nitrosoarene substrates **2a-c, 2e-h** and **2k** were prepared according to literature procedures[3]. **2d**, **2i** and **2j** were synthesized by the following method.

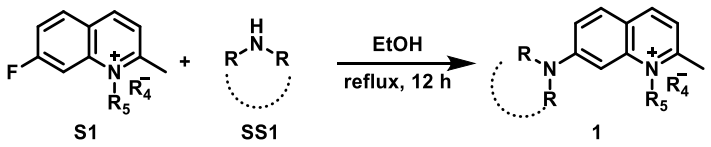
General procedure for the synthesis of quinolinium salts



7-Fluoro-2-methylquinoline (1.61 g, 10 mmol) and methyl trifluoromethanesulfonate (4.14 mL, 40 mmol) were added to 20 mL of chloroform. The mixture was stirred at room temperature for 24 h. Afterward, the solvent was removed under reduced pressure, and 20 mL of ether was added to precipitate the desired product **S1a** as a yellow solid. The resulting crude residue was used directly for

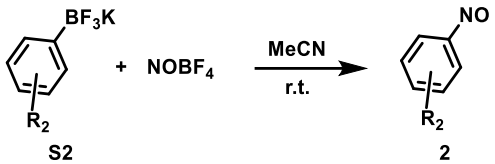
the next step.

A 100 mL pressure tubing was charged with 7-fluoro-2-methylquinoline (1.61 g, 10 mmol), iodoethane (7.80 g, 50 mmol) and acetonitrile (20 mL). After the reaction was carried out at 85 °C for 8 h, the generated yellow solid was collected by filtration and washed with acetonitrile (10 mL) to obtain **S1b**. The resulting crude residues were used directly for the next step.



Compound **S1** (10 mmol) and **SS1** (22 mmol) were added into EtOH (40 mL). The mixture was refluxed for 12 h. Then, the mixture solution was concentrated under reduced pressure. The residue was recrystallized with Et_2O/DCM to obtain compound **1**.

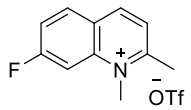
General procedure for preparations of nitrosoarenes



Compound **2** was synthesized according to the reported method[3]. Potassium organotrifluoroborate **S2** (10 mmol) was dissolved in CH_3CN (100 mL) and $NOBF_4$ (1.2 g, 10.3 mmol) was added. The reaction was stirred open to air at room temperature until the reaction became homogeneous. The reaction mixture changed from a white slurry to a green or black solution. The crude mixture was added H_2O (100 mL) and CH_2Cl_2 (100 mL). The layers were separated, and the aqueous layer was extracted with DCM. The combined organic layers were dried over Na_2SO_4, filtered, and concentrated under reduced pressure.

Analysis data of starting materials

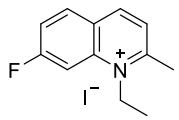
1. 7-fluoro-1,2-dimethylquinolin-1-ium trifluoromethanesulfonate (S1a)



S1a

Yellow solid, m.p. = 142-144 °C; R_f = 0.2 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 3083.50, 1606.56, 1522.07, 1440.95, 1388.57, 1266.90, 1151.99, 1030.32, 866.40, 634.89, 513.22. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.11 (d, J = 8.4 Hz, 1H), 8.56 – 8.50 (m, 2H), 8.10 (d, J = 8.5 Hz, 1H), 8.00-7.93 (m, 1H), 4.40 (s, 3H), 3.07 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 166.9, 164.4, 162.6, 145.8, 141.3 (d, J_{C-F} = 50.7 Hz), 134.1 (d, J_{C-F} = 43.3 Hz), 125.0 (d, J_{C-F} = 9.0 Hz), 122.7, 119.6 (d, J_{C-F} = 99.4 Hz), 105.8 (d, J_{C-F} = 111.4 Hz), 105.7, 40.5, 23.5. ^{19}F NMR (376 MHz, DMSO-d_6): δ -77.76 (s), -98.67 (s). HRMS (ESI) m/z calcd for $[C_{11}H_{11}FN]^+$ [M-OTf]$^+$: 176.0870, found 176.0873.

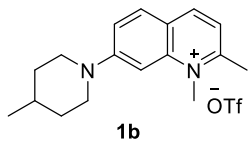
2. 1-ethyl-7-fluoro-2-methylquinolin-1-ium iodide (S1b)



S1b

Yellow solid, m.p. = 210-212 °C; R_f = 0.2 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 3447.42, 3031.71, 1603.78, 1526.04, 1353.68, 1218.49, 1140.76, 870.38. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.14 (d, J = 8.4 Hz, 1H), 8.60 – 8.53 (m, 2H), 8.13 (d, J = 8.5 Hz, 1H), 8.02-7.95 (m, 1H), 4.97 (q, J = 7.2 Hz, 2H), 3.12 (s, 3H), 1.51 (t, J = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 167.3, 164.7, 161.9, 146.0, 140.1 (d, J_{C-F} = 51 Hz), 134.4 (d, J_{C-F} = 44 Hz), 125.5 (d, J_{C-F} = 9.0 Hz), 119.7 (d, J_{C-F} = 99.6 Hz), 105.6 (d, J_{C-F} = 112.0 Hz), 48.1, 22.9, 13.7. ^{19}F NMR (376 MHz, DMSO-d_6): δ -98.51 (s). HRMS (ESI) m/z calcd for $[C_{12}H_{13}FN]^+$ [M-I]$^+$: 190.1027, found 190.1033.

3. 1,2-dimethyl-7-(4-methylpiperidin-1-yl)quinolin-1-ium trifluoromethane-sulfonate (1b)

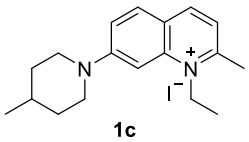


1b

Yellow solid, m.p. = 195-197 °C; R_f = 0.2 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2924.65, 1631.91, 1579.52, 1268.59, 1228.03, 1151.99, 1028.63, 842.74, 634.89. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.60 (d, J = 7.9 Hz, 1H), 8.03 (d, J = 9.6 Hz, 1H), 7.71 (d, J = 9.2 Hz, 1H), 7.51 (d, J = 8.0 Hz, 1H), 7.16 (s, 1H), 4.30 (d, J = 13.3 Hz, 2H), 4.18 (s, 3H), 3.11 (t, J = 12.5 Hz, 2H), 2.90 (s, 3H), 1.84 – 1.71 (m, 3H), 1.26 – 1.12 (m, 2H), 0.95 (d, J = 6.2 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 157.8, 154.7, 143.4, 143.0, 132.1, 122.8,

121.6, 119.6, 119.0 (d, $J_{C\text{-}F}$ = 77.6 Hz), 96.3, 47.7, 39.0, 33.8, 30.7, 23.0, 22.0. ^{19}F NMR (376 MHz, DMSO-d_6): δ -77.74 (s). HRMS (ESI) m/z calcd for $[C_{17}H_{23}N_2]^+$ [M-OTf]$^+$: 255.1856, found 255.1864.

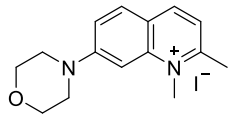
4. 1-ethyl-2-methyl-7-(4-methylpiperidin-1-yl)quinolin-1-ium iodide (1c)



1c

Yellow solid, m.p. = 270-272 °C; R_f = 0.2 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2929.57, 1629.47, 1572.39, 1518.48, 1407.50, 1313.96, 1226.75, 1134.80, 1082.48, 958.81, 855.75. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.63 (d, J = 8.0 Hz, 1H), 8.06 (d, J = 9.4 Hz, 1H), 7.73 (dd, J = 9.4, 2.1 Hz, 1H), 7.54 (d, J = 8.1 Hz, 1H), 7.17 (d, J = 2.3 Hz, 1H), 4.81 (q, J = 7.2 Hz, 2H), 4.31 (d, J = 13.4 Hz, 2H), 3.13 (t, J = 12.8 Hz, 2H), 2.94 (s, 3H), 1.83 – 1.73 (m, 3H), 1.46 (t, J = 7.1 Hz, 3H), 1.25 – 1.13 (m, 2H), 0.95 (d, J = 6.2 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 157.3, 154.9, 143.7, 141.8, 132.3, 122.0, 119.4, 119.3, 96.0, 47.8, 46.0, 33.8, 30.8, 22.3, 22.0, 13.0. HRMS (ESI) m/z calcd for $[C_{18}H_{25}N_2]^+$ [M-I]$^+$: 269.2012, found 269.2013.

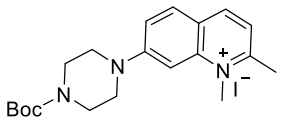
5. 1,2-dimethyl-7-morpholinoquinolin-1-ium iodide (1d)



1d

Yellow solid, m.p. = 145-147 °C; R_f = 0.2 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 3532.45, 2948.68, 1630.57, 1569.81, 1234.34, 1118.11, 859.25, 608.30. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.70 (d, J = 8.1 Hz, 1H), 8.12 (d, J = 9.3 Hz, 1H), 7.74 (dd, J = 9.3, 2.2 Hz, 1H), 7.62 (d, J = 8.1 Hz, 1H), 7.25 (d, J = 2.3 Hz, 1H), 4.23 (s, 3H), 3.80 (dd, J = 5.9, 3.9 Hz, 4H), 3.66 (dd, J = 5.8, 4.0 Hz, 4H), 2.94 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 158.5, 155.2, 143.9, 142.6, 132.0, 122.0, 119.8, 118.8, 97.1, 66.3, 47.3, 39.3, 23.2. HRMS (ESI) m/z calcd for $[C_{15}H_{19}N_2O]^+$ [M-I]$^+$: 243.1492, found 243.1492.

6. 7-(4-(tert-butoxycarbonyl)piperazin-1-yl)-1,2-dimethylquinolin-1-ium iodide (1f)

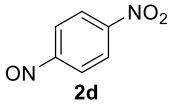


1f

Yellow solid, m.p. = 207-209 °C; R_f = 0.2 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2976.15, 1682.87, 1628.98, 1521.21, 1421.13, 1349.28, 1226.11, 1164.53, 816.74. ^{1}H NMR (400

MHz, DMSO-d_6) δ 8.69 (d, J = 8.1 Hz, 1H), 8.11 (d, J = 9.3 Hz, 1H), 7.71 (dd, J = 9.3, 2.2 Hz, 1H), 7.60 (d, J = 8.1 Hz, 1H), 7.22 (d, J = 2.2 Hz, 1H), 4.23 (s, 3H), 3.72 (dd, J = 6.8, 3.9 Hz, 4H), 3.54 (dd, J = 6.7, 3.8 Hz, 4H), 2.94 (s, 3H), 1.44 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 158.4, 154.6, 154.3, 143.8, 142.7, 132.0, 121.9, 119.6, 119.0, 97.0, 79.7, 46.7, 40.1, 39.3, 28.5, 23.2. HRMS (ESI) m/z calcd for $[C_{20}H_{28}N_3O_2]^+$ [M-I]$^+$: 342.2176, found 342.2179.

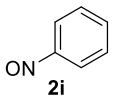
7. 1-nitro-4-nitrosobenzene (2d)



2d

Yellow solid, m.p. = 111-113 °C; R_f = 0.3 (CH_2Cl_2/PE =1:1); IR (KBr, cm^{-1}): 3109.58, 1613.58, 1528.91, 1346.72, 1259.47, 1102.94, 856.60. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.57 (s, 1H), 8.55 (s, 1H), 8.20 (s, 1H), 8.17 (s, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 163.7, 151.1, 126.3, 122.1. HRMS (ESI) m/z calcd for $[C_6H_5N_2O_3]^+$ [M+H]$^+$: 153.0295, found 153.0293.

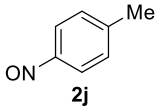
8. nitrosobenzene (2i)



2i

Yellow solid, m.p. = 56-58 °C; R_f = 0.5 (CH_2Cl_2/PE =1:1); IR (KBr, cm^{-1}): 3059.92, 1481.36, 1391.70, 1190.64, 948.83, 772.23, 690.72. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.97 (d, J = 1.2 Hz, 1H), 7.95 (d, J = 1.5 Hz, 1H), 7.92 – 7.87 (m, 1H), 7.77 (dd, J = 8.3, 7.2 Hz, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 166.6, 137.2, 130.3, 121.2. HRMS (ESI) m/z calcd for $[C_6H_6NO]^+$ [M+H]$^+$: 108.0444, found 108.0459.

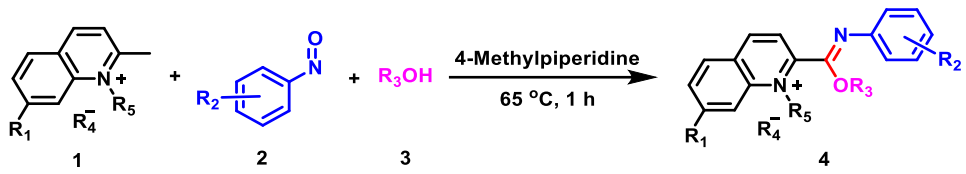
9. 1-methyl-4-nitrosobenzene (2j)



2j

Yellow solid, m.p. = 55-57 °C; R_f = 0.2 (CH_2Cl_2/PE =1:1); IR (KBr, cm^{-1}): 3055.70, 1924.08, 1598.19, 1495.55, 1251.77, 1013.13, 823.25, 756.53. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.81 (d, J = 8.3 Hz, 2H), 7.49 (d, J = 8.1 Hz, 2H), 2.39 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 166.2, 148.5, 130.5, 121.5, 21.9. HRMS (ESI) m/z calcd for $[C_7H_8NO]^+$ [M+H]$^+$: 122.0601, found 122.0607.

General procedure for the synthesis of imidates

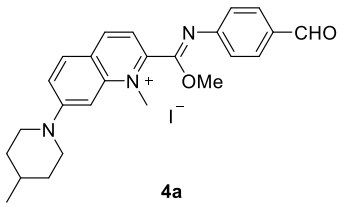


1 2 3 4

Compound **1** (0.5 mmol) was dissolved in alcohol **3** (20 mL) and 4-methylpiperidine (59 μL, 0.5 mmol) was added to the mixture at 65 °C under air, and stirred for 5 min. Then compound **2** (1.1 mmol) was added to the mixture and stirred at 65 °C for 1 h. After the solvent was removed *in vacuum*, the crude product was purified by flash chromatography on silica gel (CH_2Cl_2/CH_3OH = 80/1) to obtain desired product **4** as a solid.

Analysis data of imidate products

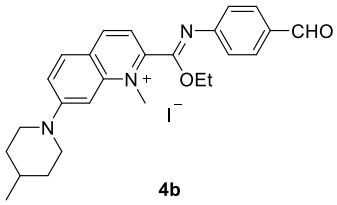
1. (*Z*)-2-(((4-formylphenyl)imino)(methoxy)methyl)-1-methyl-7-(4-methylpiperidin-1-yl)quinolin-1-ium iodide (4a)



4a

246 mg, 93% yield; Orange solid, m.p. = 164-166 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 3006.79, 1672.83, 1625.28, 1559.25, 1501.13, 1276.60, 1223.77, 1149.81, 816.98. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.82 (s, 1H), 8.65 (d, *J* = 7.9 Hz, 1H), 8.03 (d, *J* = 9.6 Hz, 1H), 7.82 (dd, *J* = 9.6, 2.2 Hz, 1H), 7.74 (d, *J* = 8.4 Hz, 2H), 7.54 (d, *J* = 7.9 Hz, 1H), 7.09 (d, *J* = 8.4 Hz, 2H), 7.03 (d, *J* = 2.2 Hz, 1H), 4.36 (d, *J* = 14.2 Hz, 2H), 4.27 (s, 3H), 4.18 (s, 3H), 3.18 (t, *J* = 12.8 Hz, 2H), 1.91-1.69 (m, 3H), 1.25-1.12 (m, 2H), 0.94 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 192.3, 155.2, 153.9, 151.2, 145.4, 143.7, 142.8, 132.9, 132.5, 131.3, 123.7, 122.0, 121.2, 116.5, 95.2, 65.4, 56.4, 47.8, 42.1, 34.0, 30.7, 21.9, 15.7. HRMS (ESI) m/z calcd for $[C_{25}H_{28}N_3O_2]^+$ $[M-I]^+$: 402.2176, found 402.2183.

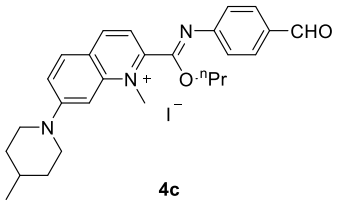
2. (*Z*)-2-(ethoxy((4-formylphenyl)imino)methyl)-1-methyl-7-(4-methylpiperidin-1-yl)quinolin-1-ium iodide (4b)



4b

277 mg, 84% yield; Orange solid, m.p. = 128-130 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 3426.79, 2919.62, 1667.55, 1625.28, 1553.96, 1495.85, 1353.21, 1273.96, 1223.77, 1144.53, 822.26, 748.30. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.81 (s, 1H), 8.63 (d, *J* = 7.9 Hz, 1H), 8.01 (d, *J* = 9.5 Hz, 1H), 7.81 (dd, *J* = 9.5, 2.2 Hz, 1H), 7.73 (d, *J* = 8.4 Hz, 2H), 7.52 (d, *J* = 7.9 Hz, 1H), 7.08 (d, *J* = 8.4 Hz, 2H), 7.02 (d, *J* = 2.2 Hz, 1H), 4.62 (q, *J* = 7.1 Hz, 2H), 4.35 (d, *J* = 13.3 Hz, 2H), 4.26 (s, 3H), 3.17 (t, *J* = 11.8 Hz, 2H), 1.84-1.74 (m, 3H), 1.46 (t, *J* = 7.1 Hz, 3H), 1.20-1.10 (m, 2H), 0.94 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 192.3, 155.2, 153.4, 151.3, 145.6, 143.8, 142.8, 132.9, 132.5, 131.3, 123.7, 122.1, 121.2, 116.4, 95.2, 65.3, 47.8, 41.9, 34.0, 30.7, 21.9, 14.3. HRMS (ESI) m/z calcd for $[C_{26}H_{30}N_3O_2]^+$ $[M-I]^+$: 416.2333, found 416.2337.

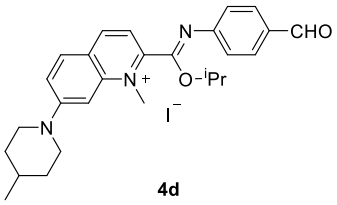
3. (*Z*)-2-(((4-formylphenyl)imino)(propoxy)methyl)-1-methyl-7-(4-methylpiperidin-1-yl)quinolin-1-ium iodide (4c)



4c

223 mg, 80% yield; Orange solid, m.p. = 194-196 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 3004.15, 1659.62, 1625.28, 1559.25, 1498.49, 1303.02, 1236.98, 1128.68, 814.34, 750.94. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.82 (s, 1H), 8.63 (d, *J* = 7.9 Hz, 1H), 8.02 (d, *J* = 9.4 Hz, 1H), 7.82 (dd, *J* = 9.5, 2.2 Hz, 1H), 7.74 (d, *J* = 8.3 Hz, 2H), 7.51 (d, *J* = 7.8 Hz, 1H), 7.09 (d, *J* = 8.1 Hz, 2H), 7.03 (d, *J* = 2.2 Hz, 1H), 4.53 (t, *J* = 6.5 Hz, 2H), 4.35 (d, *J* = 13.6 Hz, 2H), 4.28 (s, 3H), 3.18 (t, *J* = 12.3 Hz, 2H), 1.91-1.83 (m, 2H), 1.82-1.73 (m, 3H), 1.25-1.11 (m, 2H), 1.04 (t, *J* = 7.4 Hz, 3H), 0.94 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 192.3, 155.2, 153.6, 151.4, 145.5, 143.8, 142.8, 132.9, 132.5, 131.3, 123.7, 122.1, 121.2, 116.4, 95.2, 70.8, 47.9, 42.0, 34.0, 30.7, 21.9, 21.7, 10.9. HRMS (ESI) m/z calcd for $[C_{27}H_{32}N_3O_2]^+$ $[M]^+$: 430.2489, found 430.2503.

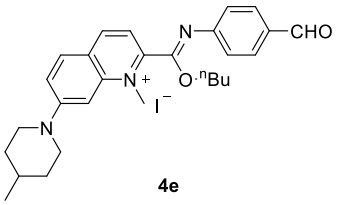
4. (*Z*)-2-(((4-formylphenyl)imino)(isopropoxy)methyl)-1-methyl-7-(4-methylpiperidin-1-yl)quinolin-1-ium iodide (4d)



4d

206 mg, 74% yield; Orange solid, m.p. = 182-184 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2924.83, 1667.47, 1628.98, 1562.26, 1503.25, 1305.66, 1226.11, 1154.26, 1095.25, 964.38, 820.68. ^1H NMR (400 MHz, DMSO-d_6) δ 9.81 (s, 1H), 8.64 (d, *J* = 7.9 Hz, 1H), 8.01 (d, *J* = 9.6 Hz, 1H), 7.81 (dd, *J* = 9.5, 2.1 Hz, 1H), 7.73 (d, *J* = 8.4 Hz, 2H), 7.51 (d, *J* = 7.9 Hz, 1H), 7.11 (d, *J* = 8.4 Hz, 2H), 7.02 (d, *J* = 2.2 Hz, 1H), 4.35 (d, *J* = 13.7 Hz, 2H), 4.27 (s, 3H), 3.18 (t, *J* = 12.5 Hz, 2H), 1.83-1.75 (m, 4H), 1.50 (d, *J* = 6.0 Hz, 6H), 1.24-1.14 (m, 2H), 0.94 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 192.3, 155.2, 152.7, 151.4, 145.7, 143.8, 142.8, 132.8, 132.5, 131.3, 123.6, 122.1, 121.2, 120.6, 116.4, 95.2, 73.0, 65.4, 47.8, 41.8, 34.0, 30.7, 21.9. HRMS (ESI) m/z calcd for $[C_{27}H_{32}N_3O_2]^+$ $[M-I]^+$: 430.2489, found 430.2506.

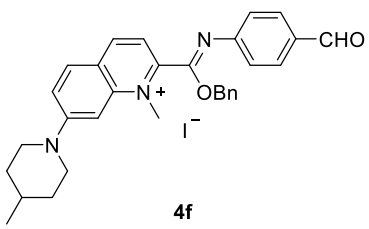
5. (*Z*)-2-(butoxy((4-formylphenyl)imino)methyl)-1-methyl-7-(4-methylpiperidin-1-yl)quinolin-1-ium iodide (4e)



4e

246 mg, 86% yield; Orange solid, m.p. = 212-214 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2945.36, 1664.91, 1626.42, 1562.26, 1500.68, 1356.98, 1308.23, 1236.38, 1154.26, 948.98, 820.68. ^1H NMR (400 MHz, DMSO-d_6) δ 9.82 (s, 1H), 8.63 (d, *J* = 7.9 Hz, 1H), 8.02 (d, *J* = 9.5 Hz, 1H), 7.82 (dd, *J* = 9.6, 2.2 Hz, 1H), 7.74 (d, *J* = 8.3 Hz, 2H), 7.50 (d, *J* = 7.9 Hz, 1H), 7.09 (d, *J* = 8.1 Hz, 2H), 7.03 (d, *J* = 2.2 Hz, 1H), 4.57 (t, *J* = 6.4 Hz, 2H), 4.36 (d, *J* = 13.6 Hz, 2H), 4.28 (s, 3H), 3.18 (t, *J* = 12.6 Hz, 2H), 1.87-1.80 (m, 3H), 1.80-1.73 (m, 2H), 1.56-1.43 (m, 2H), 1.26-1.11 (m, 2H), 0.99 (d, *J* = 7.4 Hz, 3H), 1.01-0.92 (m, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 191.2, 154.1, 152.5, 150.3, 144.4, 142.7, 141.8, 131.8, 131.4, 130.2, 122.6, 121.0, 120.1, 115.3, 94.1, 68.0, 46.8, 40.9, 32.9, 29.6, 29.2, 20.8, 18.2, 13.1. HRMS (ESI) m/z calcd for $[C_{28}H_{34}N_3O_2]^+$ $[M-I]^+$: 444.2646, found 444.2666.

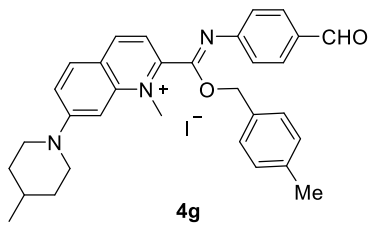
6. (*Z*)-2-((benzyloxy)((4-formylphenyl)imino)methyl)-1-methyl-7-(4-methyl-piperidin-1-yl)quinolin-1-ium iodide (4f)



4f

184 mg, 61% yield; Orange solid, m.p. = 145-147 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 3011.02, 1677.32, 1629.77, 1594.11, 1560.83, 1503.77, 1358.75, 1306.45, 1273.17, 1223.25, 1151.92, 959.36, 840.75, 750.94. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.84 (s, 1H), 8.64 (d, *J* = 7.9 Hz, 1H), 8.02 (d, *J* = 9.6 Hz, 1H), 7.81 (dd, *J* = 9.4, 2.1 Hz, 1H), 7.77 (d, *J* = 8.4 Hz, 2H), 7.64 – 7.59 (m, 2H), 7.55 (d, *J* = 7.9 Hz, 1H), 7.49 – 7.40 (m, 3H), 7.12 (d, *J* = 8.4 Hz, 2H), 7.02 (d, *J* = 2.2 Hz, 1H), 5.65 (s, 2H), 4.35 (d, *J* = 13.8 Hz, 2H), 4.29 (s, 3H), 3.18 (t, *J* = 12.4 Hz, 2H), 1.83-1.75 (m, 3H), 1.22-1.10 (m, 2H), 0.93 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 192.3, 155.1, 153.2, 151.1, 145.2, 143.8, 142.9, 135.4, 133.0, 132.5, 131.4, 129.4, 129.1, 123.8, 122.1, 121.2, 116.5, 95.2, 95.2, 70.8, 47.9, 42.0, 34.0, 30.7, 21.9. HRMS (ESI) m/z calcd for $[C_{31}H_{32}N_3O_2]^+$ [M-I]$^+$: 478.2489, found 478.2499.

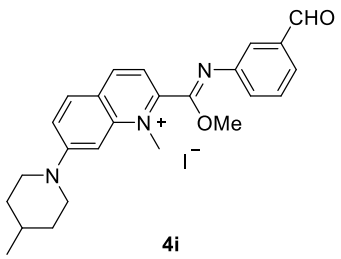
7. (*Z*)-2-(((4-formylphenyl)imino)((4-methylbenzyl)oxy)methyl)-1-methyl-7-(4-methylpiperidin-1-yl)quinolin-1-ium iodide (4g)



4g

203 mg, 74% yield; Orange solid, m.p. = 139-141 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2924.83, 1685.43, 1628.98, 1580.23, 1503.25, 1351.85, 1303.09, 1223.55, 1154.26, 966.94, 854.04. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.83 (s, 1H), 8.62 (d, *J* = 7.9 Hz, 1H), 8.01 (d, *J* = 9.6 Hz, 1H), 7.83 – 7.78 (m, 1H), 7.76 (d, *J* = 8.5 Hz, 2H), 7.55 – 7.50 (m, 2H), 7.49 (s, 1H), 7.26 (d, *J* = 7.8 Hz, 2H), 7.11 (d, *J* = 8.4 Hz, 2H), 7.01 (s, 1H), 5.59 (s, 2H), 4.35 (d, *J* = 13.8 Hz, 2H), 4.26 (s, 3H), 3.17 (t, *J* = 12.3 Hz, 2H), 2.34 (s, 3H), 1.83-1.75 (m, 3H), 1.20-1.12 (m, 2H), 0.93 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 192.3, 155.1, 153.2, 151.2, 145.2, 143.8, 142.9, 138.6, 133.0, 132.5, 132.4, 131.4, 129.8, 129.6, 123.7, 122.1, 121.2, 116.5, 95.2, 70.7, 47.8, 42.0, 34.0, 30.7, 21.9, 21.3. HRMS (ESI) m/z calcd for $[C_{32}H_{34}N_3O_2]^+$ [M-I]$^+$: 492.2646, found 492.2631.

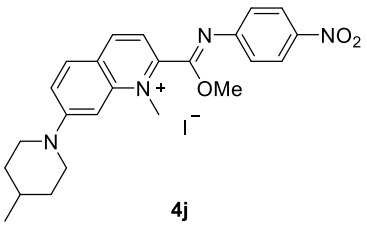
8. (*Z*)-2-(((3-formylphenyl)imino)(methoxy)methyl)-1-methyl-7-(4-methylpiperidin-1-yl)quinolin-1-ium iodide (4i)



4i

194 mg, 73% yield; Orange solid, m.p. = 152-154 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 3006.94, 2935.09, 1682.87, 1626.42, 1562.26, 1508.38, 1310.79, 1231.25, 956.68, 818.11, 684.68. ^1H NMR (400 MHz, DMSO-d_6) δ 9.89 (s, 1H), 8.65 (d, *J* = 7.9 Hz, 1H), 8.02 (d, *J* = 9.5 Hz, 1H), 7.82 (dd, *J* = 9.4, 2.2 Hz, 1H), 7.57 (d, *J* = 7.9 Hz, 1H), 7.54 (d, *J* = 7.5 Hz, 1H),7.45 – 7.37 (m, 2H), 7.17 (d, *J* = 7.8 Hz, 1H), 7.01 (d, *J* = 2.3 Hz, 1H), 4.35 (d, *J* = 13.2 Hz, 2H), 4.24 (s, 3H), 4.17 (s, 3H), 3.17 (t, *J* = 12.5 Hz, 2H), 1.85-1.72 (m, 3H), 1.28-1.11 (m, 2H), 0.94 (d, *J* = 5.9 Hz, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 193.2, 155.2, 154.4, 146.4, 145.6, 143.7, 142.8, 137.5, 132.5, 130.6, 127.2, 126.1, 123.6, 121.8, 121.2, 116.6, 95.1, 65.4, 56.2, 47.8, 42.0, 34.0, 30.6, 21.9, 15.6. HRMS (ESI) m/z calcd for $[C_{25}H_{28}N_3O_2]^+$ $[M-I]^+$: 402.2176, found 402.2170.

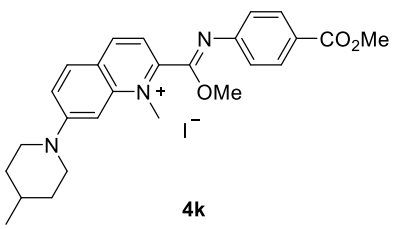
9. (*Z*)-2-(methoxy((4-nitrophenyl)imino)methyl)-1-methyl-7-(4-methylpiperidin-1-yl)quinolin-1-ium iodide (4j)



4j

227 mg, 83% yield; Orange solid, m.p. = 160-162 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 3006.79, 1678.11, 1627.92, 1556.60, 1503.77, 1329.43, 1276.60, 1229.06, 851.32, 753.58. ^1H NMR (400 MHz, DMSO-d_6) δ 8.67 (d, *J* = 7.9 Hz, 1H), 8.08 (d, *J* = 9.0 Hz, 2H), 8.04 (d, *J* = 9.6 Hz, 1H), 7.83 (dd, *J* = 9.6, 2.2 Hz, 1H), 7.57 (d, *J* = 7.8 Hz, 1H), 7.14 (d, *J* = 8.9 Hz, 2H), 7.03 (d, *J* = 2.3 Hz, 1H), 4.37 (d, *J* = 13.4 Hz, 2H), 4.26 (s, 3H), 4.18 (s, 3H), 3.23 – 3.13 (m, 2H), 1.84-1.75 (m, 3H), 1.24-1.12 (m, 2H), 0.94 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 155.2, 154.2, 151.9, 145.0, 144.3, 143.8, 142.9, 132.5, 125.5, 123.8, 122.4, 121.3, 116.4, 95.2, 65.4, 56.6, 47.8, 42.0, 34.0, 30.7, 21.9, 15.6. HRMS (ESI) m/z calcd for $[C_{24}H_{27}N_4O_3]^+$ $[M-I]^+$: 419.2078, found 419.2076.

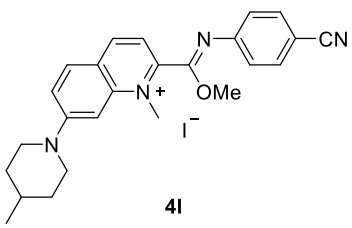
10. (*Z*)-2-(methoxy((4-(methoxycarbonyl)phenyl)imino)methyl)-1-methyl-7-(4-methylpiperidin-1-yl)quinolin-1-ium iodide (4k)



4k

245 mg, 88% yield; Orange solid, m.p. = 186-188 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2947.92, 1716.23, 1670.04, 1628.98, 1559.70, 1505.81, 1426.26, 1359.55, 1310.79, 1280.00, 1228.68, 1164.53, 1102.94, 956.68, 854.04. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.65 (d, J = 7.9 Hz, 1H), 8.03 (d, J = 9.5 Hz, 1H), 7.82 (dd, J = 9.6, 2.2 Hz, 1H), 7.77 (d, J = 8.5 Hz, 2H), 7.53 (d, J = 7.9 Hz, 1H), 7.04-7.00 (m, 2H), 7.00 (d, J = 1.9 Hz, 1H), 4.36 (d, J = 13.1 Hz, 2H), 4.25 (s, 3H), 4.16 (s, 3H), 3.75 (s, 3H), 3.18 (t, J = 12.3 Hz, 2H), 1.86-1.72 (m, 3H), 1.25-1.12 (m, 2H), 0.94 (d, J = 5.9 Hz, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 166.1, 155.2, 154.0, 150.1, 145.5, 143.7, 142.8, 132.5, 130.9, 125.9, 123.7, 121.6, 121.2, 116.5, 95.2, 56.3, 52.5, 47.8, 42.0, 34.0, 30.6, 21.9. HRMS (ESI) m/z calcd for $[C_{26}H_{30}N_3O_3]^+$ $[M\text{-}I]^+$: 432.2282, found 432.2286.

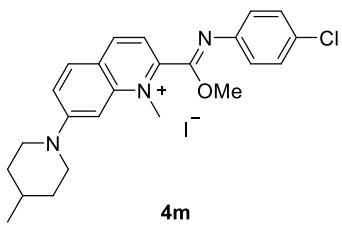
11. (*Z*)-2-(((4-cyanophenyl)imino)(methoxy)methyl)-1-methyl-7-(4-methylpiperidin-1-yl)quinolin-1-ium iodide (4l)



4l

224 mg, 85% yield; Orange solid, m.p. = 160-162 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 3432.55, 2927.39, 2222.12, 1674.30, 1630.02, 1561.13, 1507.01, 1279.03, 1229.82, 1172.42, 957.55, 855.86. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.65 (d, J = 7.8 Hz, 1H), 8.02 (d, J = 9.6 Hz, 1H), 7.82 (dd, J = 9.6, 2.2 Hz, 1H), 7.67 (d, J = 8.5 Hz, 2H), 7.53 (d, J = 7.9 Hz, 1H), 7.06 (d, J = 8.5 Hz, 2H), 7.01 (d, J = 2.2 Hz, 1H), 4.35 (d, J = 13.6 Hz, 2H), 4.22 (s, 3H), 4.15 (s, 3H), 3.18 (t, J = 12.3 Hz, 2H), 1.86-1.71 (m, 3H), 1.24–1.11 (m, 2H), 0.94 (d, J = 6.0 Hz, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 155.2, 154.2, 150.0, 145.2, 143.8, 142.9, 134.0, 132.6, 123.8, 122.5, 121.3, 119.1, 116.5, 107.2, 95.1, 56.4, 47.8, 42.0, 34.0, 30.7, 21.9; HRMS (ESI) m/z calcd for $[C_{25}H_{27}N_4O]^+$ $[M\text{-}I]^+$: 399.2179, found 399.2170.

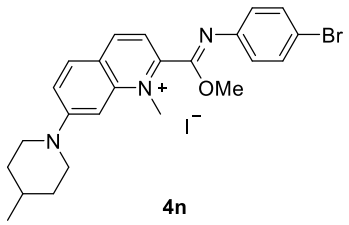
12. (*Z*)-2-(((4-chlorophenyl)imino)(methoxy)methyl)-1-methyl-7-(4-methylpiperidin-1-yl)quinolin-1-ium iodide (4m)



4m

210 mg, 78% yield; Orange solid, m.p. = 180-182 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2927.40, 1670.04, 1628.98, 1564.83, 1505.81, 1310.79, 1228.68, 1169.66, 961.81, 838.64. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.66 (d, *J* = 7.9 Hz, 1H), 8.04 (d, *J* = 9.4 Hz, 1H), 7.83 (d, *J* = 9.6 Hz, 1H), 7.51 (d, *J* = 7.9 Hz, 1H), 7.24 (d, *J* = 8.2 Hz, 2H), 7.03 (s, 1H), 6.89 (d, *J* = 8.1 Hz, 2H), 4.36 (d, *J* = 13.6 Hz, 2H), 4.22 (s, 3H), 4.13 (s, 3H), 3.18 (t, *J* = 12.8 Hz, 2H), 1.88-1.70 (m, 3H), 1.28-1.11 (m, 2H), 0.94 (d, *J* = 5.9 Hz, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 155.2, 154.1, 145.8, 144.5, 143.8, 142.8, 132.5, 129.6, 128.9, 123.6, 123.2, 121.2, 116.6, 95.2, 56.1, 47.8, 41.9, 34.0, 30.7, 21.9. HRMS (ESI) m/z calcd for $[C_{24}H_{27}ClN_3O]^+$ $[M\text{-}I]^+$: 408.1837, found 408.1839.

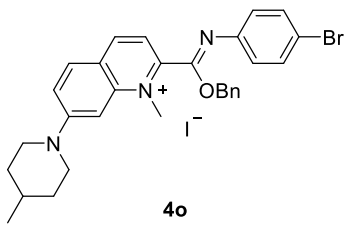
13. (*Z*)-2-(((4-bromophenyl)imino)(methoxy)methyl)-1-methyl-7-(4-methylpiperidin-1-yl)quinolin-1-ium iodide (4n)



4n

240 mg, 83% yield; Orange solid, m.p. = 157-159 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2945.36, 1670.04, 1631.55, 1559.70, 1505.81, 1362.11, 1313.36, 1228.68, 1172.23, 959.25, 859.17. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.67 (d, *J* = 7.9 Hz, 1H), 8.04 (d, *J* = 9.5 Hz, 1H), 7.83 (dd, *J* = 9.6, 2.2 Hz, 1H), 7.51 (d, *J* = 7.9 Hz, 1H), 7.36 (d, *J* = 8.5 Hz, 2H), 7.03 (d, *J* = 2.2 Hz, 1H), 6.83 (d, *J* = 8.2 Hz, 2H), 4.36 (d, *J* = 13.4 Hz, 2H), 4.22 (s, 3H), 4.13 (s, 3H), 3.25 – 3.12 (m, 2H), 1.88-1.71 (m, 3H), 1.27-1.11 (m, 2H), 0.94 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 155.2, 154.0, 145.8, 144.9, 143.7, 142.8, 132.5, 132.5, 124.1, 123.6, 121.2, 117.1, 116.6, 95.2, 56.1, 47.8, 41.9, 34.0, 30.7, 21.9. HRMS (ESI) m/z calcd for $[C_{24}H_{27}BrN_3O]^+$ $[M\text{-}I]^+$: 452.1332, found 452.1349.

14. (*Z*)-2-((benzyloxy)((4-bromophenyl)imino)methyl)-1-methyl-7-(4-methylpiperidin-1-yl)quinolin-1-ium iodide (4o)

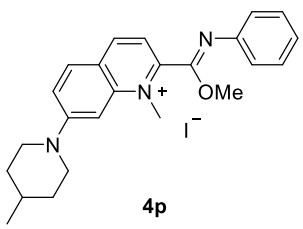


4o

192 mg, 59% yield; Orange solid, m.p. = 137-139 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2922.26, 2852.98, 1672.60, 1626.42, 1559.70, 1505.81, 1305.66, 1223.55. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.82 (d, *J* =

8.1 Hz, 1H), 8.15 (d, *J* = 9.5 Hz, 1H), 7.87 – 7.78 (m, 2H), 7.42 – 7.39 (m, 6H), 7.17 (s, 1H), 6.87 (d, *J* = 8.9 Hz, 2H), 6.45 (d, *J* = 8.3 Hz, 1H), 4.83-4.58 (m, 2H), 4.37 (d, *J* = 13.4 Hz, 2H), 4.23 (s, 3H), 3.18 (t, *J* = 11.7 Hz, 2H), 1.86-1.73 (m, 3H), 1.27-1.12 (m, 2H), 0.95 (d, *J* = 6.1 Hz, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 155.0, 154.6, 145.1, 144.2, 144.0, 137.5, 132.3, 132.2, 128.8, 128.5, 128.4, 123.1, 120.4, 116.3, 115.2, 110.3, 95.6, 82.7, 69.8, 47.9, 39.5, 33.9, 30.7, 22.0. HRMS (ESI) m/z calcd for $[C_{30}H_{31}BrN_3O]^+$ $[M\text{-}I]^+$: 528.1645, found 528.1638.

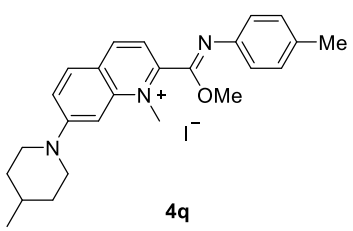
15. (*Z*)-2-(methoxy(phenylimino)methyl)-1-methyl-7-(4-methylpiperidin-1-yl)quinolin-1-ium iodide (4p)



4p

153 mg, 61% yield; Orange solid, m.p. = 162-164 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 3009.43, 2924.91, 1670.19, 1627.92, 1561.89, 1506.42, 1361.13, 1313.58, 1273.96, 1223.77, 1155.09, 853.96, 750.94. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.64 (d, *J* = 7.9 Hz, 1H), 8.03 (d, *J* = 9.5 Hz, 1H), 7.82 (dd, *J* = 9.6, 2.2 Hz, 1H), 7.49 (d, *J* = 7.9 Hz, 1H), 7.18 (t, *J* = 7.8 Hz, 2H), 7.02 (d, *J* = 2.3 Hz, 1H), 7.00-6.94 (m, 1H), 6.87-6.85 (m, 1H), 6.84 (s, 1H), 4.35 (d, *J* = 13.4 Hz, 2H), 4.22 (s, 3H), 4.13 (s, 3H), 3.17 (t, *J* = 11.7 Hz, 2H), 1.85-1.74 (m, 3H), 1.24-1.11 (m, 2H), 0.94 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 155.1, 153.7, 146.3, 145.5, 143.7, 142.7, 132.5, 129.6, 124.8, 123.5, 121.3, 121.1, 116.7, 95.2, 65.4, 55.9, 47.8, 42.0, 34.0, 30.7, 21.9, 15.7. HRMS (ESI) m/z calcd for $[C_{24}H_{28}N_3O]^+$ $[M\text{-}I]^+$: 374.2227, found 374.2239.

16. (*Z*)-2-(methoxy(p-tolylimino)methyl)-1-methyl-7-(4-methylpiperidin-1-yl)quinolin-1-ium iodide (4q)

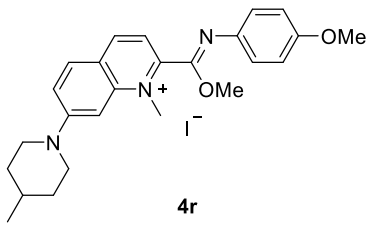


4q

196 mg, 76% yield; Orange solid, m.p. = 162-164 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 3014.72, 2924.91, 1667.55, 1622.64, 1561.89, 1506.42, 1358.49, 1276.60, 1226.42, 1157.74, 956.98, 859.25. 748.30. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.65 (d, *J* = 7.9 Hz, 1H), 8.04 (d, *J* = 9.5 Hz, 1H), 7.82 (dd, *J* = 9.6, 2.1 Hz, 1H), 7.48 (d, *J* = 7.9 Hz, 1H), 7.05

(d, *J* = 1.9 Hz, 1H), 6.98 (d, *J* = 7.8 Hz, 2H), 6.73 (d, *J* = 7.8 Hz, 2H), 4.35 (d, *J* = 13.5 Hz, 2H), 4.22 (s, 3H), 4.11 (s, 3H), 3.17 (t, *J* = 12.3 Hz, 2H), 2.14 (s, 3H), 1.88-1.70 (m, 3H), 1.24-1.11 (m, 2H), 0.94 (d, J = 6.0 Hz, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 155.1, 153.5, 146.5, 143.7, 142.9, 142.7, 133.8, 132.5, 130.1, 123.5, 121.2, 121.1, 116.7, 95.2, 65.4, 55.9, 47.8, 41.9, 34.0, 30.7, 21.9, 20.8, 15.7. HRMS (ESI) m/z calcd for $[C_{25}H_{30}BrN_3O]^+$ $[M\text{-}I]^+$: 388.2383, found 388.2400.

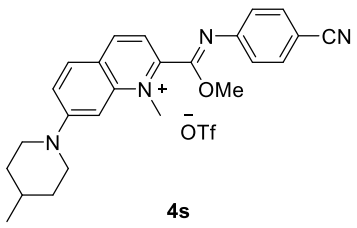
17. (*Z*)-2-(methoxy((4-methoxyphenyl)imino)methyl)-1-methyl-7-(4-methylpiperidin-1-yl)quinolin-1-ium iodide (4r)



4r

163 mg, 61% yield; Orange solid, m.p. = 155-157 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2919.70, 1667.47, 1623.85, 1559.70, 1503.25, 1459.62, 1362.11, 1310.79, 1223.55, 1169.66, 1020.83, 825.81. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.65 (d, *J* = 7.9 Hz, 1H), 8.04 (d, *J* = 9.5 Hz, 1H), 7.82 (dd, *J* = 9.5, 2.2 Hz, 1H), 7.47 (d, *J* = 7.9 Hz, 1H), 7.03 (d, *J* = 2.2 Hz, 1H), 6.81 – 6.68 (m, 4H), 4.35 (d, *J* = 13.5 Hz, 2H), 4.19 (s, 3H), 4.10 (s, 3H), 3.61 (s, 3H), 3.17 (t, *J* = 12.5 Hz, 2H), 1.85-1.74 (m, 3H), 1.21-1.13 (m, 2H), 0.94 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 156.5, 155.1, 153.5, 146.8, 143.8, 142.7, 138.3, 132.5, 125.2, 123.5, 122.5, 121.1, 116.7, 115.2, 114.8, 95.3, 55.8, 55.5, 47.8, 41.8, 34.0, 30.7, 21.9. HRMS (ESI) m/z calcd for $[C_{25}H_{30}N_3O_2]^+$ $[M\text{-}I]^+$: 404.2333, found 404.2333.

18. (*Z*)-2-(((4-cyanophenyl)imino)(methoxy)methyl)-1-methyl-7-(4-methylpiperidin-1-yl)quinolin-1-ium trifluoromethanesulfonate (4s)

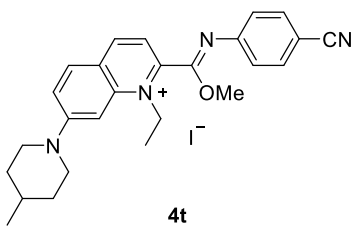


4s

183 mg, 67% yield; Orange solid, m.p. = 151-153 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 3599.90, 2951.04, 2225.65, 1681.16, 1630.72, 1564.61, 1508.95, 1228.88, 1152.34, 1027.09, 867.05, 637.42. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.64 (d, *J* = 7.8 Hz, 1H), 8.02 (d, *J* = 9.5 Hz, 1H), 7.82 (dd, *J* = 9.5, 2.2 Hz, 1H), 7.66 (d, *J* = 8.5 Hz, 2H), 7.52 (d, *J* = 7.8 Hz, 1H), 7.05 (d, *J* = 8.5 Hz, 2H), 7.01 (s, 1H), 4.35 (d, *J* = 13.6 Hz, 2H), 4.22 (s,

3H), 4.15 (s, 3H), 3.17 (t, *J* = 12.3 Hz, 2H), 1.84-1.74 (m, 3H), 1.25 –1.13 (m, 2H), 0.94 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 155.2, 154.1, 150.0, 145.2, 143.8, 142.9, 134.0, 132.5, 123.8, 122.4, 121.2, 119.1, 116.5, 107.3, 95.1, 56.4, 47.8, 41.9, 34.0, 30.7, 21.9; ^{19}F NMR (376 MHz, DMSO-d_6): δ -77.76 (s), -77.75 (s). HRMS (ESI) m/z calcd for $[C_{25}H_{27}N_4O]^+$ [M-OTf]$^+$: 399.2179, found 399.2179.

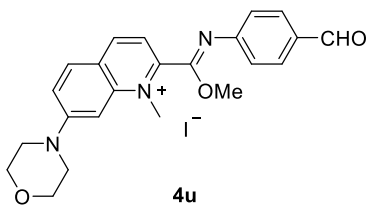
19. (*Z*)-2-(((4-cyanophenyl)imino)(methoxy)methyl)-1-ethyl-7-(4-methylpiperidin-1-yl)quinolin-1-ium iodide (4t)



4t

250 mg, 93% yield; Orange solid, m.p. = 166-168 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 3427.63, 2925.75, 2222.12, 1674.30, 1628.38, 1562.77, 1507.01, 1365.95, 1293.79, 1228.18, 1169.14, 955.91, 846.02. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.64 (d, *J* = 7.9 Hz, 1H), 8.03 (d, *J* = 9.5 Hz, 1H), 7.82 (dd, *J* = 9.7, 2.1 Hz, 1H), 7.67 (d, *J* = 8.5 Hz, 2H), 7.52 (d, *J* = 7.8 Hz, 1H), 7.07 (d, *J* = 8.4 Hz, 2H), 7.04 (d, *J* = 2.1 Hz, 1H). 5.14-4.52 (m, 2H), 4.36 (d, *J* = 13.5 Hz, 2H), 4.16 (s, 3H), 3.18 (t, *J* = 12.4 Hz, 2H), 1.84-1.75 (m, 3H), 1.50 (t, *J* = 6.9 Hz, 3H), 1.24-1.10 (m, 2H), 0.93 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 155.3, 154.1, 150.0, 144.7, 144.0, 141.5, 133.9, 132.9, 124.3, 122.5, 121.3, 119.1, 116.9, 107.2, 94.9, 56.3, 49.6, 47.9, 34.0, 30.7, 21.9, 14.0. HRMS (ESI) m/z calcd for $[C_{26}H_{29}N_4O]^+$ [M-I]$^+$: 413.2336, found 413.2343.

20. (*Z*)-2-(((4-formylphenyl)imino)(methoxy)methyl)-1-methyl-7-morpholinoquinolin-1-ium iodid*e* (4u)

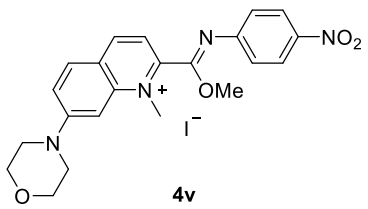


4u

176 mg, 68% yield; Orange solid, m.p. = 181-183 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2985.66, 2848.30, 1672.83, 1627.92, 1564.53, 1493.21, 1355.85, 1273.96, 1110.19, 1057.36, 951.70, 816.98, 753.58. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.81 (s, 1H), 8.74 (d, *J* = 7.9 Hz, 1H), 8.10 (d, *J* = 9.5 Hz, 1H), 7.83 (dd, *J* = 9.5, 2.2 Hz, 1H), 7.73 (d, *J* = 8.4 Hz, 2H), 7.65 (d, *J* = 7.9 Hz, 1H), 7.11 (d, *J* = 2.2 Hz, 1H), 7.08 (d, *J* = 8.3 Hz, 2H), 4.30 (s, 3H), 4.18 (s, 3H), 3.78 (dd, *J* = 5.9, 3.6 Hz, 4H), 3.73 (dd, *J* = 5.9, 3.3 Hz, 4H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 192.3, 155.7, 153.8, 151.1, 145.9, 144.4, 142.5, 132.9, 132.4, 131.3, 124.0, 122.0,

120.9, 117.2, 95.9, 66.2, 56.4, 47.2, 42.2. HRMS (ESI) m/z calcd for $[C_{23}H_{24}N_3O_3]^+$ $[M\text{-}I]^+$: 390.1813, found 390.1832.

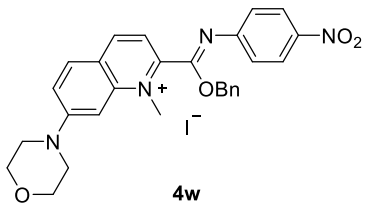
21. (*Z*)-2-(methoxy((4-nitrophenyl)imino)methyl)-1-methyl-7-morpholinoquinolin-1-ium iodide (4v)



4v

161 mg, 60% yield; Orange solid, m.p. = 181-183 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2978.72, 1664.91, 1631.55, 1562.26, 1505.81, 1336.45, 1236.38, 1169.66, 1108.08, 1033.66, 856.60. ^1H NMR (400 MHz, DMSO-d_6) δ 8.75 (d, *J* = 7.9 Hz, 1H), 8.10 (d, *J* = 9.5 Hz, 1H), 8.06 (d, *J* = 8.9 Hz, 2H), 7.83 (dd, *J* = 9.4, 2.2 Hz, 1H), 7.67 (d, *J* = 7.9 Hz, 1H), 7.12 (d, *J* = 8.9 Hz, 2H), 7.10 (d, *J* = 2.0 Hz, 1H), 4.28 (s, 3H), 4.18 (s, 3H), 3.79 – 3.76 (m, 4H), 3.75-3.70 (m, 4H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 154.6, 153.0, 150.7, 144.4, 143.4, 143.2, 141.5, 131.4, 124.4, 123.0, 121.3, 119.9, 116.1, 94.8, 65.2, 55.5, 46.2, 41.1. HRMS (ESI) m/z calcd for $[C_{22}H_{23}N_4O_4]^+$ $[M\text{-}I]^+$: 407.1714, found 407.1705.

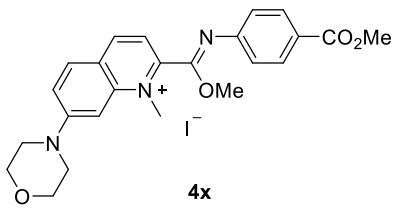
22. (*Z*)-2-((benzyloxy)((4-nitrophenyl)imino)methyl)-1-methyl-7-morpholinoquinolin-1-iumiodi*e* (4w)



4w

227 mg, 74% yield; Orange solid, m.p. = 130-132 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 1672.60, 1628.98, 1559.70, 1508.38, 1339.02, 1236.38, 1108.08, 851.47. ^1H NMR (400 MHz, DMSO-d_6) δ 8.75 (d, *J* = 7.9 Hz, 1H), 8.12-8.07 (m, 3H), 7.83 (dd, *J* = 9.5, 2.2 Hz, 1H), 7.69 (d, *J* = 7.9 Hz, 1H), 7.64 – 7.59 (m, 2H), 7.49 – 7.42 (m, 3H), 7.16 (d, *J* = 8.9 Hz, 2H), 7.10 (d, *J* = 2.1 Hz, 1H), 5.82 – 5.50 (m, 2H), 4.32 (s, 3H), 3.79-3.75 (m, 4H), 3.75-3.71 (m, 4H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 155.6, 153.4, 151.7, 145.2, 144.5, 144.4, 142.7, 135.3, 132.4, 129.4, 129.2, 129.1, 125.5, 124.2, 122.5, 121.0, 117.2, 95.9, 71.1, 66.2, 47.3, 42.2. HRMS (ESI) m/z calcd for $[C_{28}H_{27}N_4O_4]^+$ $[M\text{-}I]^+$: 483.2027, found 483.2013.

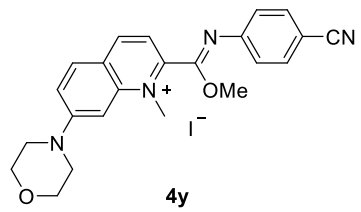
23. (*Z*)-2-(methoxy((4-(methoxycarbonyl)phenyl)imino)methyl)-1-methyl-7-morpholinoquinolin-1-ium iodide (4x)



4x

246 mg, 90% yield; Orange solid, m.p. = 207-209 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 3012.08, 2850.42, 1700.83, 1667.47, 1628.98, 1559.70, 1500.68, 1436.53, 1277.43, 1231.25, 1102.94, 951.55, 859.17, 771.92. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.73 (d, *J* = 7.9 Hz, 1H), 8.09 (d, *J* = 9.5 Hz, 1H), 7.83 (dd, *J* = 9.5, 2.2 Hz, 1H), 7.76 (d, *J* = 8.5 Hz, 2H), 7.62 (d, *J* = 7.9 Hz, 1H), 7.09 (d, *J* = 2.2 Hz, 1H), 6.99 (d, *J* = 8.5 Hz, 2H), 4.27 (s, 3H), 4.16 (s, 3H), 3.80-3.76 (m, 4H), 3.75 (s, 3H), 3.74-3.68 (m, 4H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 165.6, 155.2, 153.4, 149.6, 145.5, 144.0, 142.0, 131.9, 130.4, 125.5, 123.5, 121.2, 120.4, 116.8, 95.4, 65.8, 55.9, 54.9, 52.0, 46.7, 41.7, 13.2; HRMS (ESI) m/z calcd for $[C_{24}H_{26}N_3O_4]^+$ $[M\text{-}I]^+$: 420.1918, found 420.1909.

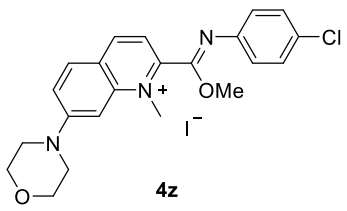
24. (*Z*)-2-(((4-cyanophenyl)imino)(methoxy)methyl)-1-methyl-7-morpholinoquinolin-1-ium iodide (4y)



4y

185 mg, 72% yield; Orange solid, m.p. = 199-201 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 3476.14, 2218.89, 1676.44, 1629.13, 1563.22, 1504.08, 1360.44, 1316.50, 1235.39, 1108.65, 951.49, 853.48. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.75 (d, *J* = 7.9 Hz, 1H), 8.10 (d, *J* = 9.5 Hz, 1H), 7.84 (dd, *J* = 9.5, 2.2 Hz, 1H), 7.66 (d, *J* = 8.4 Hz, 2H), 7.63 (s, 1 H), 7.10 (d, *J* = 2.2 Hz, 1H), 7.06 (d, *J* = 8.5 Hz, 2H), 4.27 (s, 3H), 4.16 (s, 3H), 3.81 – 3.76 (m, 4H), 3.75-3.69 (m, 4H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 155.7, 154.0, 149.9, 145.6, 144.5, 142.5, 134.0, 132.4, 124.1, 122.5, 121.0, 119.1, 117.2, 107.3, 95.9, 66.2, 56.5, 47.3, 42.2. HRMS (ESI) m/z calcd for $[C_{23}H_{23}N_4O_2]^+$ $[M\text{-}I]^+$: 387.1816, found 387.1807.

25. (*Z*)-2-(((4-chlorophenyl)imino)(methoxy)methyl)-1-methyl-7-morpholinoquinolin-1-ium iodide (4z)

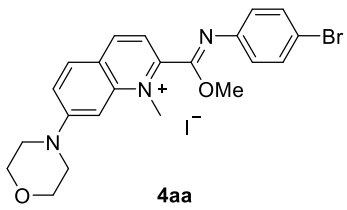


4z

183 mg, 70% yield; Orange solid, m.p. = 155-157 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2965.89, 2852.98, 1675.17, 1628.98, 1564.83, 1500.68, 1315.92, 1236.38, 1177.36, 846.34. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.75 (d, *J* = 8.0 Hz, 1H), 8.11 (d, *J* = 9.4 Hz, 1H), 7.84 (dd, *J* = 9.5, 2.2 Hz, 1H), 7.62

(d, *J* = 7.9 Hz, 1H), 7.23 (d, *J* = 8.6 Hz, 2H), 7.11 (d, *J* = 2.2 Hz, 1H), 6.88 (d, *J* = 8.3 Hz, 2H), 4.24 (s, 3H), 4.13 (s, 3H), 3.82-3.76 (m, 4H), 3.75-3.68 (m, 4H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 155.7, 146.3, 144.4, 144.4, 142.4, 132.4, 129.6, 129.0, 123.90, 123.89, 123.2, 120.9, 117.3, 95.9, 66.2, 56.2, 47.2, 42.1. HRMS (ESI) m/z calcd for $[C_{22}H_{23}ClN_3O_2]^+$ $[M\text{-}I]^+$: 396.1473, found 396.1466.

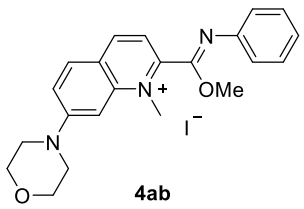
26. (*Z*)-2-(((4-bromophenyl)imino)(methoxy)methyl)-1-methyl-7-morpholinoquinolin-1-ium iodide (4aa)



4aa

207 mg, 73% yield; Orange solid, m.p. = 187-189 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2965.89, 2850.42, 1677.74, 1628.98, 1564.83, 1498.11, 1359.55, 1315.92, 1233.81, 1177.36, 1059.32, 846.34. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.75 (d, *J* = 8.0 Hz, 1H), 8.11 (d, *J* = 9.4 Hz, 1H), 7.84 (dd, *J* = 9.5, 2.2 Hz, 1H), 7.62 (d, *J* = 7.9 Hz, 1H), 7.23 (d, *J* = 8.6 Hz, 2H), 7.11 (d, *J* = 2.2 Hz, 1H), 6.88 (d, *J* = 8.3 Hz, 2H), 4.24 (s, 3H), 4.13 (s, 3H), 3.83-3.76 (m, 4H), 3.75-3.68 (m, 4H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 155.7, 146.3, 144.44, 144.41, 142.4, 132.4, 129.6, 129.0, 123.90, 123.89, 123.2, 120.9, 117.3, 95.9, 66.2, 56.2, 47.2, 42.1. HRMS (ESI) m/z calcd for $[C_{22}H_{23}BrN_3O_2]^+$ $[M\text{-}I]^+$: 440.0968, found 440.0982.

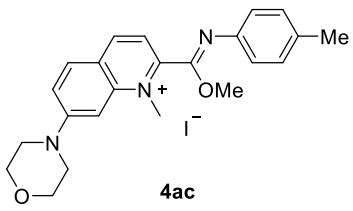
27. (*Z*)-2-(methoxy(phenylimino)methyl)-1-methyl-7-morpholinoquinolin-1-ium iodide (4ab)



4ab

165 mg, 67% yield; Orange solid, m.p. = 151-153 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 1682.87, 1626.42, 1567.40, 1500.68, 1313.36, 1233.81, 1108.08. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.74 (d, *J* = 8.0 Hz, 1H), 8.10 (d, *J* = 9.5 Hz, 1H), 7.83 (dd, *J* = 9.5, 2.2 Hz, 1H), 7.60 (d, *J* = 7.9 Hz, 1H), 7.17 (t, *J* = 7.8 Hz, 2H), 7.10 (d, *J* = 2.2 Hz, 1H), 6.96 (t, *J* = 7.4 Hz, 1H), 6.84 (d, *J* = 7.6 Hz, 2H), 4.26 (s, 3H), 4.14 (s, 3H), 3.81-3.75 (m, 4H), 3.74-3.67 (m, 4H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 155.6, 153.6, 146.7, 145.4, 144.4, 142.3, 132.4, 129.6, 124.9, 123.8, 121.3, 120.8, 117.4, 95.9, 66.2, 56.0, 47.2, 42.1. HRMS (ESI) m/z calcd for $[C_{22}H_{24}N_3O_2]^+$ $[M\text{-}I]^+$: 362.1863, found 362.1869.

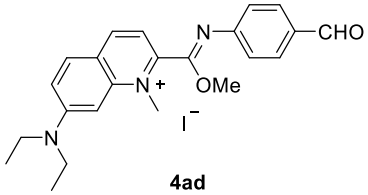
28. (*Z*)-2-(methoxy(p-tolylimino)methyl)-1-methyl-7-morpholinoquinolin-1-ium iodide (4ac)



4ac

128 mg, 51% yield; Orange solid, m.p. = 150-152 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 1672.60, 1631.55, 1564.83, 1500.68, 1310.79, 1233.81, 1108.08. ^1H NMR (400 MHz, DMSO-d_6) δ 8.74 (d, *J* = 8.0 Hz, 1H), 8.11 (d, *J* = 9.5 Hz, 1H), 7.83 (dd, *J* = 9.4, 2.2 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.11 (d, *J* = 2.2 Hz, 1H), 6.97 (d, *J* = 8.0 Hz, 2H), 6.72 (d, *J* = 8.2 Hz, 2H), 4.25 (s, 3H), 4.12 (s, 3H), 3.81 – 3.76 (m, 4H), 3.75-3.67 (m, 4H), 2.13 (s, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 155.6, 153.4, 147.0, 144.4, 142.8, 142.3, 133.8, 132.4, 130.1, 123.8, 121.2, 120.8, 117.4, 96.0, 66.2, 55.9, 47.2, 42.1, 20.8. HRMS (ESI) m/z calcd for $[C_{23}H_{26}N_3O_2]^+$ $[M-I]^+$: 376.2020, found 376.2033.

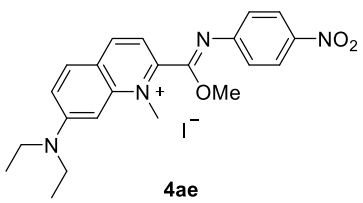
29. (*Z*)-7-(diethylamino)-2-(((4-formylphenyl)imino)(methoxy)methyl)-1-methylquinolin-1-ium iodide (4ad)



4ad

163 mg, 61% yield; Orange solid, m.p. = 134-136 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 3635.62, 2971.02, 1680.30, 1628.98, 1559.70, 1510.94, 1354.42, 1315.92, 1262.04, 1159.40, 1049.06, 820.68. ^1H NMR (400 MHz, DMSO-d_6) δ 9.82 (s, 1H), 8.63 (d, *J* = 7.8 Hz, 1H), 8.02 (d, *J* = 9.5 Hz, 1H), 7.74 (d, *J* = 8.4 Hz, 2H), 7.61 (dd, *J* = 9.5, 2.2 Hz, 1H), 7.48 (d, *J* = 7.9 Hz, 1H), 7.08 (d, *J* = 8.3 Hz, 2H), 6.76 (d, *J* = 2.2 Hz, 1H), 4.26 (s, 3H), 4.17 (s, 3H), 3.68 (q, *J* = 7.0 Hz, 4H), 1.22 (t, *J* = 7.0 Hz, 6H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 192.3, 154.0, 153.8, 151.3, 145.2, 143.7, 142.6, 132.9, 132.6, 131.3, 123.4, 122.0, 120.4, 115.9, 93.4, 56.3, 45.4, 41.8, 12.5. HRMS (ESI) m/z calcd for $[C_{23}H_{26}N_3O_2]^+$ $[M-I]^+$: 376.2020, found 376.2033.

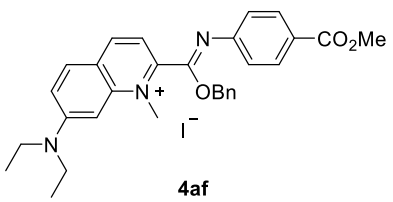
30. (*Z*)-7-(diethylamino)-2-(methoxy((4-nitrophenyl)imino)methyl)-1-methylquinolin-1-ium iodide (4ae)



4ae

192 mg, 74% yield; Orange solid, m.p. = 139-141 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2973.58, 1672.60, 1628.98, 1557.13, 1510.94, 1336.45, 1313.36, 1259.47, 1167.09, 1102.94, 854.04. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.65 (d, J = 7.9 Hz, 1H), 8.08 (d, J = 9.0 Hz, 2H), 8.03 (d, J = 9.5 Hz, 1H), 7.63 (dd, J = 9.5, 2.2 Hz, 1H), 7.52 (d, J = 7.8 Hz, 1H), 7.13 (d, J = 9.0 Hz, 2H), 6.76 (d, J = 2.1 Hz, 1H), 4.25 (s, 3H), 4.18 (s, 3H), 3.69 (q, J = 7.0 Hz, 4H), 1.22 (t, J = 7.0 Hz, 6H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 153.2, 152.7, 150.9, 143.7, 143.2, 142.7, 141.7, 131.6, 124.4, 122.4, 121.3, 119.4, 114.8, 92.3, 55.5, 44.3, 40.7, 11.5. HRMS (ESI) m/z calcd for $[C_{22}H_{25}N_4O_3]^+$ $[M-I]^+$: 393.1921, found 393.1913.

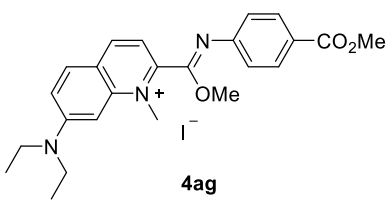
31. (*Z*)-2-((benzyloxy)((4-(methoxycarbonyl)phenyl)imino)methyl)-7-(diethylamino)-1-methylquinolin-1-ium iodide (4af)



4af

215 mg, 71% yield; Orange solid, m.p. = 112-114 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2976.15, 1716.23, 1631.55, 1559.70, 1510.94, 1274.87, 1164.53, 1100.38. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.62 (d, J = 7.8 Hz, 1H), 8.02 (d, J = 9.5 Hz, 1H), 7.80 (d, J = 8.6 Hz, 2H), 7.64-7.58 (m, 3H), 7.48 (s, 1H), 7.46 (s, 1H), 7.45 – 7.41 (m, 2H), 7.05 – 7.00 (m, 2H), 6.76 (d, J = 2.2 Hz, 1H), 5.62 (s, 2H), 4.27 (s, 3H), 3.76 (s, 3H), 3.68 (q, J = 7.2 Hz, 4H), 1.21 (t, J = 7.0 Hz, 6H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 166.1, 153.7, 153.3, 150.1, 145.1, 143.7, 142.7, 135.5, 132.6, 130.9, 129.4, 129.1, 129.1, 126.0, 123.4, 121.7, 120.4, 116.0, 93.4, 70.7, 52.5, 45.4, 41.8, 12.5. HRMS (ESI) m/z calcd for $[C_{30}H_{32}N_3O_3]^+$ $[M-I]^+$: 482.2438, found 482.2421.

32. (*Z*)-7-(diethylamino)-2-(methoxy((4-(methoxycarbonyl)phenyl)imino)methyl)-1-methylquinolin-1-ium iodide (4ag)

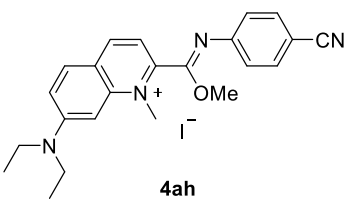


4ag

155 mg, 58% yield; Orange solid, m.p. = 147-149 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2976.15, 1713.66, 1631.55, 1559.70, 1510.94, 1313.36, 1274.87, 1167.09, 1097.81. ^{1}H NMR (400

MHz, DMSO-d_6) δ 8.62 (d, J = 7.9 Hz, 1H), 8.02 (d, J = 9.5 Hz, 1H), 7.77 (d, J = 8.6 Hz, 2H), 7.61 (dd, J = 9.5, 2.2 Hz, 1H), 7.46 (d, J = 7.9 Hz, 1H), 6.99 (d, J = 8.5 Hz, 2H), 6.75 (d, J = 2.2 Hz, 1H), 4.23 (s, 3H), 4.15 (s, 3H), 3.75 (s, 3H), 3.68 (q, J = 6.9 Hz, 4H), 1.22 (t, J = 7.0 Hz, 6H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 166.1, 154.1, 153.7, 150.2, 145.3, 143.7, 142.6, 132.6, 130.9, 125.9, 123.3, 121.7, 120.4, 115.9, 93.4, 56.3, 52.5, 45.4, 41.8, 12.5. HRMS (ESI) m/z calcd for $[C_{24}H_{28}N_3O_3]^+$ $[M\text{-}I]^+$: 406.2125, found 406.2105.

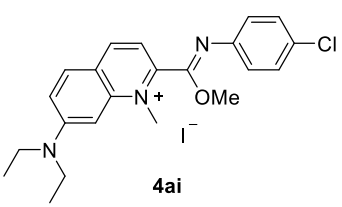
33. (*Z*)-2-(((4-cyanophenyl)imino)(methoxy)methyl)-7-(diethylamino)-1-methylquinolin-1-ium iodide (4ah)



4ah

188 mg, 75% yield; Orange solid, m.p. = 151-153 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 3425.45, 2974.25, 2223.96, 1671.37, 1632.50, 1559.84, 1512.52, 1309.74, 1264.12, 1164.41, 858.55. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.66 (d, J = 7.8 Hz, 1H), 8.05 (d, J = 9.6 Hz, 1H), 7.68 (d, J = 8.6 Hz, 2H), 7.64 (dd, J = 9.5, 2.2 Hz, 1H), 7.50 (d, J = 7.9 Hz, 1H), 7.08 (d, J = 8.5 Hz, 2H), 6.77 (d, J = 2.2 Hz, 1H), 4.25 (s, 3H), 4.16 (s, 3H), 3.70 (q, J = 7.1 Hz, 4H), 1.23 (t, J = 7.0 Hz, 6H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 154.2, 153.8, 150.0, 144.9, 143.7, 142.7, 134.0, 132.7, 123.5, 122.5, 120.5, 119.1, 115.9, 107.2, 93.4, 56.4, 45.4, 41.9, 12.5. HRMS (ESI) m/z calcd for $[C_{23}H_{25}N_4O]^+$ $[M\text{-}I]^+$: 373.2023, found 373.2023.

34. (*Z*)-2-(((4-chlorophenyl)imino)(methoxy)methyl)-7-(diethylamino)-1-methylquinolin-1-ium iodide (4al)

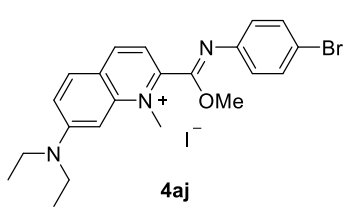


4ai

187 mg, 71% yield; Orange solid, m.p. = 118-120 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2971.02, 2924.83, 1672.60, 1628.98, 1562.26, 1508.38, 1310.79, 1264.60, 1156.83, 1074.72, 833.51. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.66 (d, J = 7.9 Hz, 1H), 8.05 (d, J = 9.5 Hz, 1H), 7.63 (dd, J = 9.5, 2.2 Hz, 1H), 7.46 (d, J = 7.8 Hz, 1H), 7.24 (d, J = 8.6 Hz, 2H), 6.89 (d, J = 8.6 Hz, 2H), 6.77 (d, J = 2.2 Hz, 1H), 4.22 (s, 3H), 4.13 (s, 3H), 3.69 (q, J = 7.2 Hz, 4H), 1.22 (t, J = 7.0 Hz, 6H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 154.2, 153.8, 145.6, 144.6, 143.7, 142.7, 132.7, 129.6, 129.0, 123.3, 123.2, 120.4, 116.0, 93.4, 56.1, 45.4, 41.8, 12.5.

HRMS (ESI) m/z calcd for $[C_{22}H_{25}ClN_3O]^+$ $[M-I]^+$: 382.1681, found 382.1665.

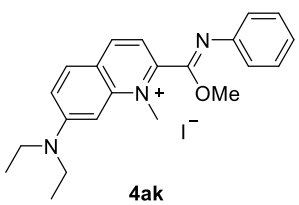
35. (*Z*)-2-(((4-bromophenyl)imino)(methoxy)methyl)-7-(diethylamino)-1-methylquinolin-1-ium iodide (4aj)



4aj

224 mg, 81% yield; Orange solid, m.p. = 142-144 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2976.15, 1670.04, 1628.98, 1562.26, 1513.51, 1349.28, 1313.36, 1259.47, 1167.09, 1072.15, 854.04. ^1H NMR (400 MHz, DMSO-d_6) δ 8.65 (d, *J* = 7.9 Hz, 1H), 8.05 (d, *J* = 9.5 Hz, 1H), 7.63 (dd, *J* = 9.5, 2.2 Hz, 1H), 7.45 (d, *J* = 7.9 Hz, 1H), 7.36 (d, *J* = 8.6 Hz, 2H), 6.83 (d, *J* = 8.5 Hz, 2H), 6.77 (d, *J* = 2.2 Hz, 1H), 4.22 (s, 3H), 4.13 (s, 3H), 3.69 (q, *J* = 7.4 Hz, 4H), 1.22 (t, *J* = 7.0 Hz, 6H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 154.1, 153.7, 145.6, 145.0, 143.7, 142.6, 132.6, 132.5, 123.6, 123.3, 120.4, 117.1, 116.0, 93.4, 56.1, 45.4, 41.8, 12.5. HRMS (ESI) m/z calcd for $[C_{22}H_{25}BrN_3O]^+$ $[M-I]^+$: 426.1176, found 426.1170.

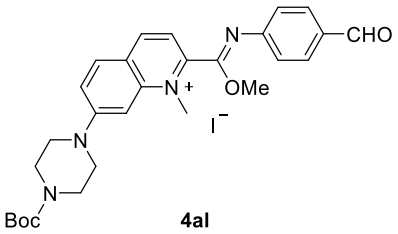
36. (*Z*)-7-(diethylamino)-2-(methoxy(phenylimino)methyl)-1-methylquinolin-1-ium iodide (4ak)



4ak

156 mg, 66% yield; Orange solid, m.p. = 172-174 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2968.45, 2927.40, 1672.60, 1631.55, 1559.70, 1513.51, 1349.28, 1313.92, 1262.04, 1167.09, 1051.62, 851.47. ^1H NMR (400 MHz, DMSO-d_6) δ 8.62 (d, *J* = 7.9 Hz, 1H), 8.03 (d, *J* = 9.5 Hz, 1H), 7.61 (dd, *J* = 9.5, 2.1 Hz, 1H), 7.43 (d, *J* = 7.8 Hz, 1H), 7.26 – 7.11 (m, 2H), 6.98 (d, *J* = 7.6 Hz, 1H), 6.90 – 6.81 (m, 2H), 6.76 (d, *J* = 2.4 Hz, 1H), 4.22 (s, 3H), 4.13 (s, 3H), 3.68 (q, *J* = 7.2 Hz, 4H), 1.21 (t, *J* = 6.9 Hz, 6H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 153.7, 146.1, 145.6, 143.6, 142.5, 132.6, 130.1, 129.6, 124.8, 123.2, 121.3, 120.3, 116.1, 93.4, 55.9, 45.4, 41.8, 12.5. HRMS (ESI) m/z calcd for $[C_{22}H_{26}N_3O]^+$ $[M-I]^+$: 348.2070, found 348.2080.

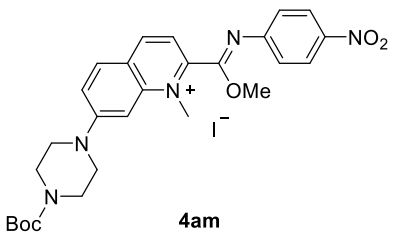
37. (*Z*)-7-(4-(tert-butoxycarbonyl)piperazin-1-yl)-2-(((4-formylphenyl)imino)(methoxy)methyl)-1-methylquinolin-1-ium iodide (4al)



4al

239 mg, 78% yield; Orange solid, m.p. = 158-160 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2978.72, 1688.00, 1631.55, 1562.26, 1408.30, 1315.92, 1226.11, 1161.96, 1077.28, 856.60. ^1H NMR (400 MHz, DMSO-d_6) δ 9.80 (s, 1H), 8.72 (d, *J* = 7.9 Hz, 1H), 8.08 (d, *J* = 9.5 Hz, 1H), 7.79 (dd, *J* = 9.6, 2.1 Hz, 1H), 7.73 (d, *J* = 8.4 Hz, 2H), 7.63 (d, *J* = 7.9 Hz, 1H), 7.12 – 7.04 (m, 3H), 4.28 (s, 3H), 4.17 (s, 3H), 3.78 (dd, *J* = 7.0, 3.9 Hz, 4H), 3.53 (dd, *J* = 6.3, 4.2 Hz, 4H), 1.44 (s, 9H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 192.3, 155.3, 154.3, 153.8, 151.1, 145.8, 144.4, 142.5, 132.9, 132.5, 131.3, 123.9, 122.0, 121.0, 117.1, 95.7, 79.8, 56.5, 56.4, 46.6, 42.2, 28.5. HRMS (ESI) m/z calcd for $[C_{28}H_{33}N_4O_4]^+$ $[M-I]^+$: 489.2496, found 489.2491.

38. (*Z*)-7-(4-(tert-butoxycarbonyl)piperazin-1-yl)-2-(methoxy((4-nitrophenyl)imino)methyl)-1-methylquinolin-1-ium iodide (4am)

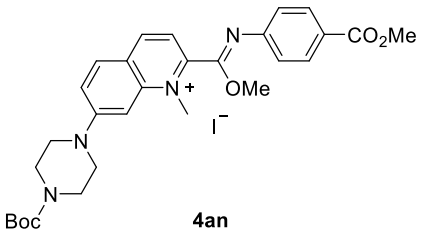


4am

241 mg, 76% yield; Orange solid, m.p. = 152-154 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2973.58, 1682.87, 1628.98, 1559.70, 1508.38, 1408.30, 1336.45, 1228.68, 1169.66, 846.34. ^1H NMR (400 MHz, DMSO-d_6) δ 8.73 (d, *J* = 8.0 Hz, 1H), 8.09 (d, *J* = 9.6 Hz, 1H), 8.06 (d, *J* = 9.0 Hz, 2H), 7.80 (dd, *J* = 9.5, 2.2 Hz, 1H), 7.65 (d, *J* = 7.9 Hz, 1H), 7.12 (d, *J* = 8.9 Hz, 2H), 7.05 (d, *J* = 2.2 Hz, 1H), 4.27 (s, 3H), 4.18 (s, 3H), 3.83-3.75 (m, 4H), 3.56 – 3.48 (m, 4H), 1.43 (s, 9H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 155.3, 154.3, 154.1, 151.8, 145.4, 144.5, 144.3, 142.6, 132.5, 125.5, 124.0, 122.4, 121.1, 117.0, 95.8, 79.8, 56.6, 55.4, 46.6, 42.2, 28.5. HRMS (ESI) m/z calcd for $[C_{27}H_{32}N_5O_5]^+$ $[M-I]^+$: 506.2398, found 506.2391.

39. (*Z*)-7-(4-(tert-butoxycarbonyl)piperazin-1-yl)-2-(methoxy((4-(methoxycarbonyl)phenyl)imino)methyl)-1-methylquinolin-1-ium iodide (4an)

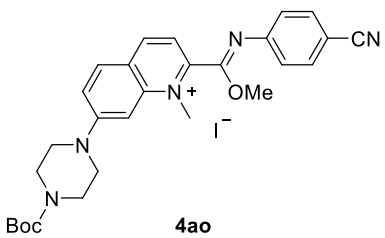
262 mg, 81% yield; Orange solid, m.p. = 143-145 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 3427.77, 2971.02, 1685.43, 1628.98, 1559.70, 1498.11, 1408.30,



4an

1359.55, 1274.87, 1223.55, 1164.53, 1113.21, 856.60, 774.49. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.72 (d, J = 8.0 Hz, 1H), 8.09 (d, J = 9.5 Hz, 1H), 7.80 (dd, J = 9.5, 2.2 Hz, 1H), 7.76 (d, J = 8.5 Hz, 2H), 7.61 (d, J = 7.9 Hz, 1H), 7.06 (d, J = 2.2 Hz, 1H), 6.99 (d, J = 8.6 Hz, 2H), 4.27 (s, 3H), 4.17 (s, 3H), 3.82 – 3.76 (m, 4H), 3.75 (s, 3H), 3.58-3.49 (m, 4H), 1.44 (s, 9H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 166.1, 155.3, 154.3, 153.9, 150.0, 145.9, 144.4, 142.5, 132.5, 130.9, 125.9, 123.8, 121.6, 121.0, 117.1, 95.8, 79.8, 56.5, 56.4, 52.5, 46.6, 42.2, 28.5. HRMS (ESI) m/z calcd for $[C_{29}H_{35}N_4O_5]^+$ $[M-I]^+$: 519.2602, found 519.2604.

40. (*Z*)-7-(4-(tert-butoxycarbonyl)piperazin-1-yl)-2-(((4-cyanophenyl)imino)(methoxy)methyl)-1-methylquinolin-1-ium iodide (4ao)

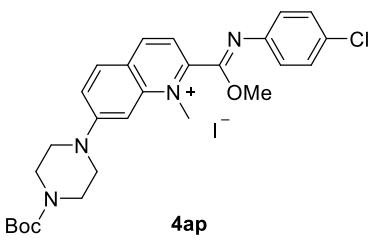


4ao

215 mg, 70% yield; Orange solid, m.p. = 162-164 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 3443.89, 2924.40, 2223.43, 1685.64, 1629.03, 1562.43, 1410.91, 1316.00, 1224.43, 1166.15, 856.46. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.73 (d, J = 8.0 Hz, 1H), 8.10 (d, J = 9.6 Hz, 1H), 7.80 (dd, J = 9.5, 2.2 Hz, 1H), 7.66 (d, J = 8.5 Hz, 2H), 7.62 (d, J = 7.9 Hz, 1H), 7.09 – 7.02 (m, 3H), 4.26 (s, 3H), 4.16 (s, 3H), 3.83-3.75 (m, 4H), 3.56 – 3.50 (m, 4H), 1.43 (s, 9H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 155.3, 154.3, 154.0, 149.9, 145.5, 144.4, 142.5, 134.0, 132.5, 123.9, 122.4, 121.1, 119.1, 117.0, 107.3, 95.7, 79.8, 56.5, 46.6, 42.2, 39.7, 28.5. HRMS (ESI) m/z calcd for $[C_{28}H_{32}N_5O_3]^+$ $[M-I]^+$: 486.2500, found 486.2486.

41. (*Z*)-7-(4-(tert-butoxycarbonyl)piperazin-1-yl)-2-(((4-chlorophenyl)imino)(methoxy)methyl)-1-methylquinolin-1-ium iodide (4ap)

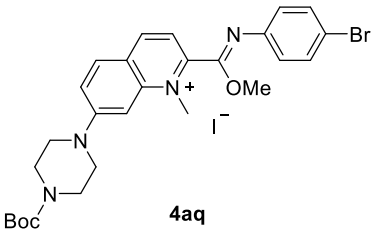
186 mg, 60% yield; Orange solid, m.p. = 170-172 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2922.26, 1680.30, 1628.98, 1562.26, 1498.11, 1413.43, 1310.79, 1223.55, 1164.53, 833.51. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.74 (d, J = 8.0 Hz, 1H),



4ap

8.10 (d, *J* = 9.5 Hz, 1H), 7.80 (dd, *J* = 9.4, 2.1 Hz, 1H), 7.60 (d, *J* = 7.9 Hz, 1H), 7.22 (d, *J* = 8.6 Hz, 2H), 7.06 (d, *J* = 2.2 Hz, 1H), 6.88 (d, *J* = 8.6 Hz, 2H), 4.24 (s, 3H), 4.13 (s, 3H), 3.84-3.74 (m, 4H), 3.57 – 3.50 (m, 4H), 1.43 (s, 9H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 155.2, 154.3, 154.0, 146.2, 144.43, 144.37, 142.5, 132.5, 129.6, 129.0, 123.8, 123.2, 121.0, 117.2, 95.8, 79.8, 56.2, 46.6, 42.1, 39.7, 28.5. HRMS (ESI) m/z calcd for $[C_{27}H_{32}ClN_4O_3]^+$ $[M-I]^+$: 495.2157, found 495.2166.

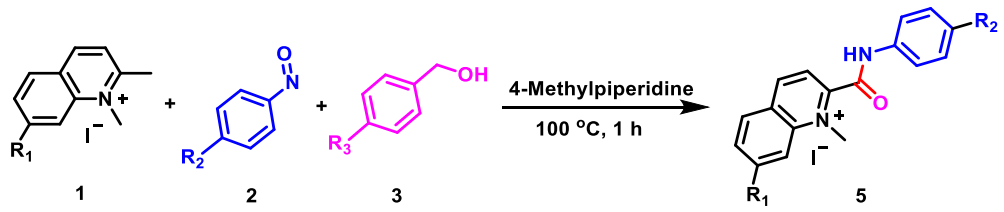
42. (*Z*)-2-(((4-bromophenyl)imino)(methoxy)methyl)-7-(4-(tert-butoxycarbonyl)piperazin-1-yl)-1-methylquinolin-1-ium iodide (4aq)



4aq

204 mg, 61% yield; Orange solid, m.p. = 148-150 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2947.92, 1716.23, 1628.98, 1505.81, 1313.36, 1274.87, 1223.55, 1172.23, 1108.08, 956.68, 851.47, 764.23. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.74 (d, *J* = 8.0 Hz, 1H), 8.11 (d, *J* = 9.5 Hz, 1H), 7.80 (dd, *J* = 9.5, 2.2 Hz, 1H), 7.60 (d, *J* = 7.9 Hz, 1H), 7.35 (d, *J* = 8.6 Hz, 2H), 7.06 (d, *J* = 2.3 Hz, 1H), 6.82 (d, *J* = 8.6 Hz, 2H), 4.24 (s, 3H), 4.13 (s, 3H), 3.85-3.74 (m, 4H), 3.57 – 3.48 (m, 4H), 1.43 (s, 9H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 155.2, 154.3, 153.9, 149.0, 146.2, 144.8, 144.4, 142.4, 132.5, 132.5, 123.8, 123.6, 121.0, 117.2, 95.8, 79.8, 56.2, 46.6, 42.1, 39.7, 28.5. HRMS (ESI) m/z calcd for $[C_{27}H_{32}BrN_4O_3]^+$ $[M-I]^+$: 539.1652, found 539.1659.

General procedure for the synthesis of amides



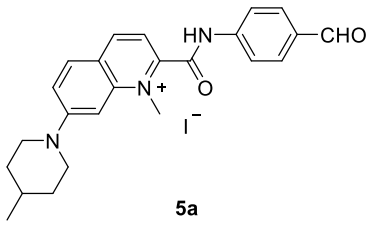
1 2 3 5

Compound **1** (0.5 mmol, 1.0 equiv) was dissolved in solvent **3** (20 mL) and 4-methylpiperidine (59 μL, 1.0 equiv) was added to the mixture at 100 °C, then the mixture was stirred at 100 °C for 5 min. Compound **2** was added to the mixture and

stirred at 100 °C for 1 h. After the solvent was removed *in vacuum*, the crude product was purified by flash chromatography (CH_2Cl_2/CH_3OH = 80/1) to obtain desired product **5** as a red solid.

Analysis data of imidate products

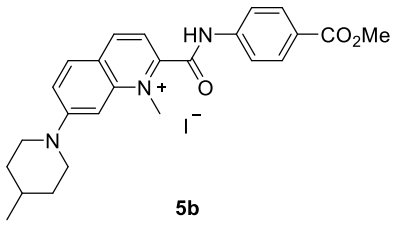
1. 2-((4-formylphenyl)carbamoyl)-1-methyl-7-(4-methylpiperidin-1-yl)quinolin-1-ium iodide (5a)



5a

205 mg, 80%, 111 mg, 43%, 145 mg, 56% yield; Orange solid, m.p. = 201-203 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2984.87, 2915.92, 2846.98, 1682.08, 1629.77, 1591.74, 1534.68, 1501.40, 1358.75, 1318.34, 1261.28, 1220.87, 1163.81, 966.49. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.65 (s, 1H), 9.98 (s, 1H), 8.88 (d, *J* = 7.9 Hz, 1H), 8.17 (d, *J* = 9.5 Hz, 1H), 8.02 (d, *J* = 8.6 Hz, 2H), 7.96 (d, *J* = 8.6 Hz, 2H), 7.89 (dd, *J* = 9.6, 2.2 Hz, 1H), 7.80 (d, *J* = 7.9 Hz, 1H), 7.15 (d, *J* = 2.2 Hz, 1H), 4.40 (d, *J* = 13.6 Hz, 2H), 4.28 (s, 3H), 3.21 (t, *J* = 12.4 Hz, 2H), 1.88-1.73 (m, 3H), 1.27-1.14 (m, 2H), 0.95 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 192.3, 160.7, 155.3, 149.2, 144.5, 143.3, 142.8, 133.3, 132.5, 131.4, 123.8, 121.0, 120.6, 115.2, 95.2, 47.9, 41.49, 34.0, 30.7, 22.0. HRMS (ESI) m/z calcd for $[C_{24}H_{26}N_3O_2]^+$ $[M-I]^+$: 388.2020, found 388.2036.

2. 2-((4-(methoxycarbonyl)phenyl)carbamoyl)-1-methyl-7-(4-methylpiperidin-1-yl)quinolin-1-ium iodide (5b)

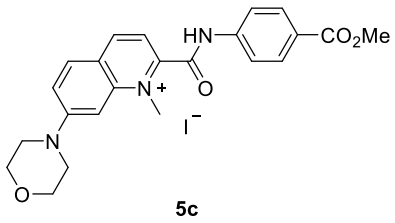


5b

179 mg, 66% yield; Orange solid, m.p. = 159-161 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2947.92, 1716.23, 1628.98, 1508.38, 1405.74, 1280.00, 1226.11, 1108.08, 959.25, 848.91, 764.23. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.60 (s, 1H), 8.88 (d, *J* = 7.9 Hz, 1H), 8.17 (d, *J* = 9.6 Hz, 1H), 8.06 (d, *J* = 8.7 Hz, 2H), 7.93-7.85 (m, 3H), 7.80 (d, *J* = 7.9 Hz, 1H), 7.15 (d, *J* = 2.2 Hz, 1H), 4.40 (d, *J* = 13.5 Hz, 2H), 4.28 (s, 3H), 3.86 (s, 3H), 3.20 (t, *J* = 11.7 Hz, 2H), 1.86-1.76 (m, 3H), 1.27-1.13 (m, 2H), 0.95 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 166.1, 160.6, 155.4, 149.3,

144.6, 142.8, 142.3, 132.5, 131.0, 126.3, 123.8, 121.0, 120.3, 115.2, 95.3, 52.6, 47.9, 41.4, 34.0, 30.7, 22.0. HRMS (ESI) m/z calcd for $[C_{25}H_{28}N_3O_3]^+$ $[M-I]^+$: 418.2126, found 418.2113.

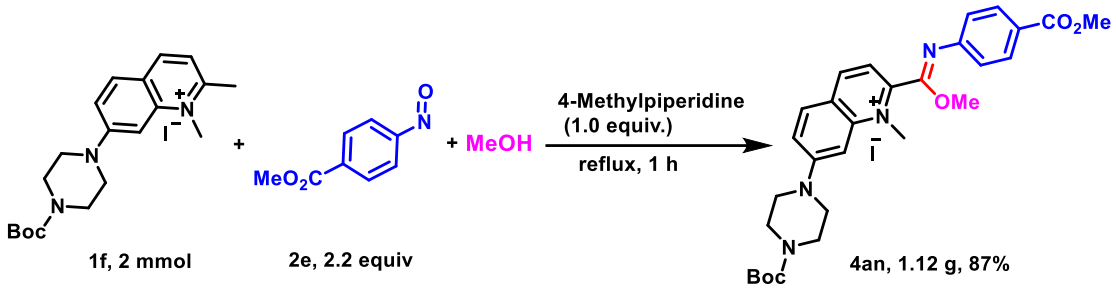
3. 2-((4-(methoxycarbonyl)phenyl)carbamoyl)-1-methyl-7-morpholinoquinolin-1-ium iodide (5c)



5c

174 mg, 65% yield; Orange solid, m.p. = 152-154 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2965.89, 1711.09, 1628.98, 1539.17, 1405.74, 1280.00, 1233.81, 1110.64, 856.60, 764.23. ^1H NMR (400 MHz, DMSO-d_6) δ 11.64 (s, 1H), 8.98 (d, J = 7.9 Hz, 1H), 8.25 (d, J = 9.5 Hz, 1H), 8.07 (d, J = 8.8 Hz, 2H), 7.95 – 7.85 (m, 4H), 7.24 (d, J = 2.2 Hz, 1H), 4.33 (s, 3H), 3.87 (s, 3H), 3.84 – 3.79 (m, 4H), 3.78-3.75 (m, 4H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 166.1, 160.5, 155.8, 149.7, 145.2, 142.4, 142.2, 132.4, 131.0, 126.4, 124.1, 120.7, 120.4, 115.9, 96.0, 66.2, 52.6, 47.3, 41.6. HRMS (ESI) m/z calcd for $[C_{23}H_{24}N_3O_4]^+$ $[M-I]^+$: 406.1762, found 406.1747.

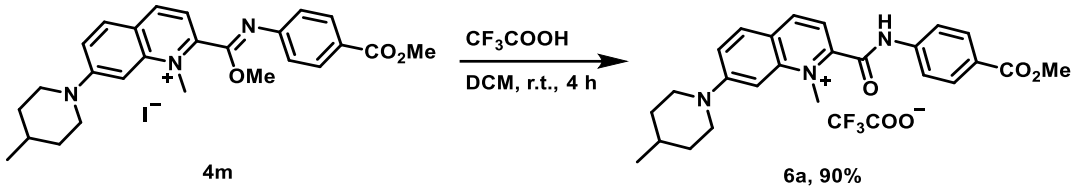
Experimental procedure for large scale reaction



1f, 2 mmol 2e, 2.2 equiv 4an, 1.12 g, 87%

Compound **1f** (939 mg, 2 mmol) was dissolved in MeOH (80 mL) and 4-methylpiperidine (0.24 mL) was added to the mixture at 65 °C under air and stirred for 5 min. Then compound **2e** (727 mg, 4.4 mmol) was added to the mixture and stirred at 65 °C for 1 h. After the solvent was removed *in vacuum*, the crude product was purified by flash chromatography on silica gel (CH_2Cl_2/CH_3OH = 80/1) to obtain desired product **4an** (1.12 g, 87%) as a red solid.

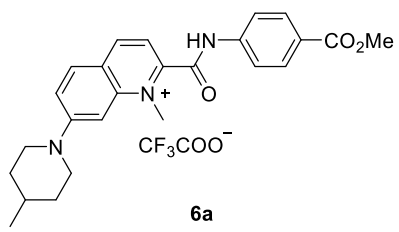
Synthetic applications of the imidate



To the solution of imidate **4m** (560 mg, 1 mmol) in CH_2Cl_2 (4.0 mL), trifluoroacetic acid (2 mL) was added. The mixture was stirred at 30 °C for 4 h. The reaction mixture was separated by by flash chromatography on silica gel (CH_2Cl_2/MeOH = 80/1) to obtain amide product **6a** (0.49 g, 92%).

Analysis data of starting materials and synthetic applications

1. **2-((4-(methoxycarbonyl)phenyl)carbamoyl)-1-methyl-7-(4-methylpiperidin-1-yl)quinolin-1-ium 2,2,2-trifluoroacetate (6a)**



6a

490 mg, 92% yield; Orange solid, m.p. = 147-149 °C; R_f = 0.3 (CH_2Cl_2:CH_3OH = 10:1); IR (KBr, cm^{-1}): 2953.06, 1682.87, 1600.75, 1503.25, 1408.30, 1323.62, 1228.68, 1200.45, 1177.36, 954.11, 764.23, 710.34. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.87 (s, 1H), 8.87 (d, *J* = 7.9 Hz, 1H), 8.16 (d, *J* = 9.5 Hz, 1H), 8.06 (d, *J* = 8.8 Hz, 2H), 7.94-7.85 (m, 3H), 7.78 (d, *J* = 7.9 Hz, 1H), 7.15 (d, *J* = 2.2 Hz, 1H), 4.40 (d, *J* = 13.6 Hz, 2H), 4.28 (s, 3H), 3.87 (s, 3H), 3.20 (t, *J* = 12.2 Hz, 2H), 1.88-1.70 (m, 3H), 1.28-1.14 (m, 2H), 0.96 (d, *J* = 6.0 Hz, 3H). ^{13}C NMR (101 MHz, DMSO) δ 166.1, 160.7, 155.3, 149.4, 144.5, 142.7, 142.4, 132.5, 130.9, 126.2, 123.8, 120.9, 120.3, 115.2, 95.3, 52.6, 47.8, 41.4, 33.9, 30.7, 21.9; HRMS (ESI) m/z calcd for $[C_{25}H_{28}N_3O_3]^+$ $[M\text{-}CF_3COO]^+$: 418.2126, found 418.2130.

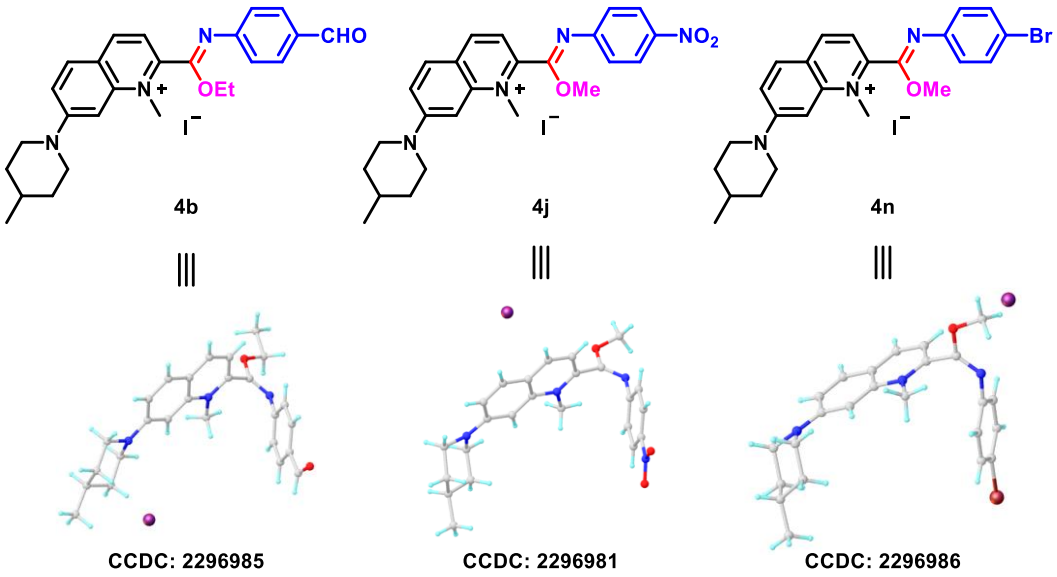


Fig. S1. X-ray single crystal diffraction diagram of **4b**, **4j** and **4n.**

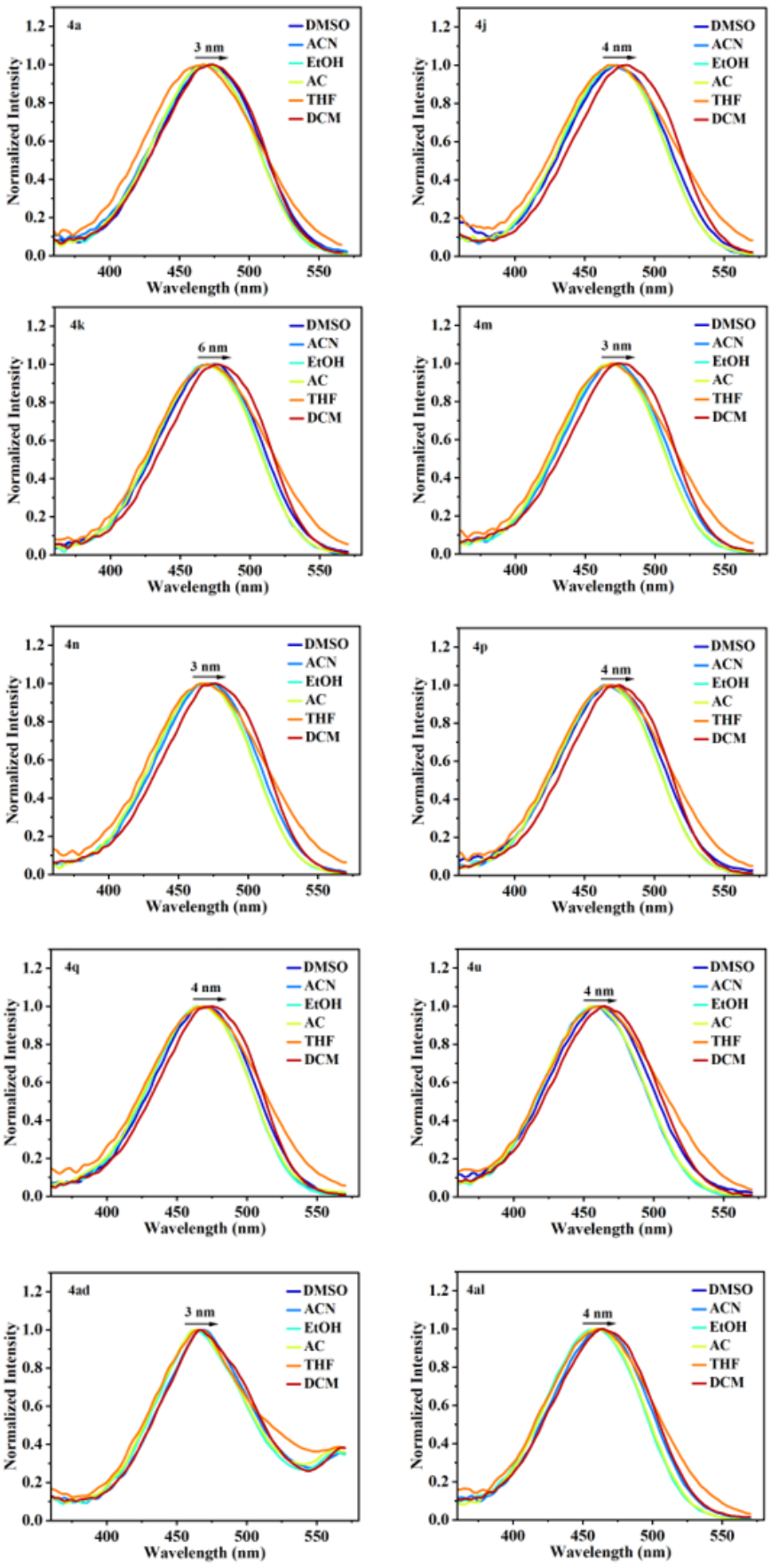


Fig. S2. Normalized UV-vis spectra of imidates **4a**, **4j**, **4k**, **4m**, **4n**, **4p**, **4q**, **4u**, **4ad** and

4al in different solvents (4×10^{-5} M).

References

1 Y. S. Chen, B. Z. Zhou, F. T. Liu, J. Y. Miao, B. X. Zhao, Z. M. Lin, A quinoline-salt-based fluorescent probe for precise monitoring of pH changes on mitochondria and water, Sens. Actuators B Chem., 2022, **373**, 132732.

2 F. T. Liu, N. Li, Y. S. Chen, H. Y. Yu, J. Y. Miao, B. X. Zhao, A quinoline-coumarin near-infrared ratiometric fluorescent probe for detection of sulfur dioxide derivatives, Anal. Chim. Acta, 2022, **1211**, 339908.

3 G. A. Molander, L. N. Cavalcanti, Nitrosation of aryl and heteroaryltrifluoroborates with nitrosonium tetrafluoroborate, J. Org. Chem., 2012, **77**, 4402.

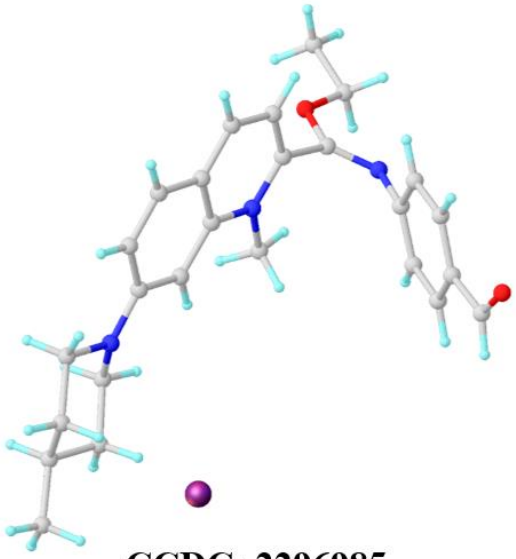
X-Ray Crystal Structure Data

Single crystal was chosen under an optical microscope and quickly coated with high vacuum grease (Dow Corning Corporation) to prevent decomposition. Intensity data and cell parameters were recorded at 173 K on a Bruker Apex II single crystal diffractometer, employing a Mo K_α radiation (λ = 0.71073 Å) and a CCD area detector. The raw frame data were processed using SAINT and SADABS to yield the reflection data file.[1] The structure was solved using the charge-flipping algorithm, as implemented in the program *SUPERFLIP*[2] and refined by full-matrix least-squares techniques against F_o^2 using the SHELXL program[3] through the OLEX2 interface.[4] Hydrogen atoms at carbon were placed in calculated positions and refined isotropically by using a riding model. Appropriate restraints or constraints were applied to the geometry and the atomic displacement parameters of the atoms in the cluster. All structures were examined using the Addsym subroutine of PLATON[5] to ensure that no additional symmetry could be applied to the models. **CCDC: 2296985 (4b), CCDC: 2296983 (4f), CCDC: 2296993 (4i), CCDC: 2296981 (4j), CCDC: 2296986 (4n), CCDC: 2296988 (4x), CCDC: 2296989 (4ae), CCDC: 2296987 (5a), CCDC: 2296990 (6a)** contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre.

References

1. *APEX3*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA, 2015.
2. Palatinus, L. & Chapuis, G. *SUPERFLIP* - a computer program for the solution of crystal structures by charge flipping in arbitrary dimensions. *J. Appl. Crystallogr.* **40**, 786 (2007).
3. Sheldrick, G.M. Crystal structure refinement with *SHELXL*. *Acta. Crystallogr. C* **71**, 3 (2015).
4. Dolomanov, O.V., Bourhis, L.J., Gildea, R. J., Howard, J.A.K. & Puschmann, H. *OLEX2*: a complete structure solution, refinement and analysis program. *J. Appl. Crystallogr.* **42**, 339 (2009).
5. Spek, A.L. Structure validation in chemical crystallography. *Acta. Crystallogr. Sect. D.* **65**, 148 (2009).

Crystal data and structure refinement for 4b (Thermal ellipsoids at the 30% probability level)

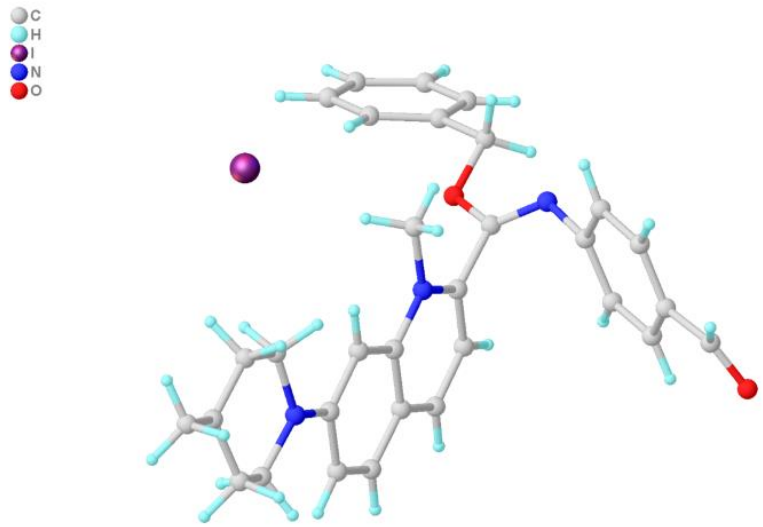


CCDC: 2296985

Table S2 Crystal data and structure refinement for 4b	
Empirical formula	$C_{27}H_{32}Cl_2I_{0.75}N_3O_2$
Formula weight	596.63
Temperature [K]	173.0
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	10.255(3)
b [Å]	10.808(3)
c [Å]	14.297(4)
α [°]	96.753(11)
β [°]	104.167(10)
γ [°]	112.127(10)
Volume [Å^3]	1383.9(6)
Z	2
ρ_{calc} [gcm^{-3}]	1.432
μ [mm^{-1}]	8.899
F(000)	610
Crystal size [mm^3]	0.08×0.06×0.05
Crystal colour	clear orangish orange
Crystal shape	block
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	6.56 to 130.45 (0.85 Å)

Index ranges	$-9 \le h \le 12$ $-12 \le k \le 12$ $-16 \le l \le 15$
Reflections collected	15832
Independent reflections	4637 $R_{int} = 0.0623$ $R_{sigma} = 0.0715$
Completeness to $\theta = 65.224°$	98.0 %
Data / Restraints / Parameters	4637/0/320
Goodness-of-fit on F^2	1.162
Final R indexes [$I \ge 2\sigma(I)$]	$R_1 = 0.0557$ w$R_2 = 0.1961$
Final R indexes [all data]	$R_1 = 0.0855$ w$R_2 = 0.2058$
Largest peak/hole [eÅ^{-3}]	1.33/-0.79
Extinction coefficient	0.0054(8)

Crystal data and structure refinement for 4f (Thermal ellipsoids at the 30% probability level)



CCDC: 2296983

Table S3 Crystal data and structure refinement for 4f	
Empirical formula	$C_{31}H_{31}IN_3O_2$
Formula weight	604.49
Temperature [K]	173.0
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)

a [Å]	10.7042(19)
b [Å]	10.8570(19)
c [Å]	13.812(2)
α [°]	99.501(8)
β [°]	101.662(7)
γ [°]	116.135(7)
Volume [Å^3]	1351.1(4)
Z	2
ρ_{calc} [gcm^{-3}]	1.486
μ [mm^{-1}]	9.568
F(000)	614
Crystal size [mm^3]	0.12×0.11×0.1
Crystal colour	clear light orange
Crystal shape	block
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	6.83 to 136.80 (0.83 Å)
Index ranges	−12 ≤ h ≤ 12 −13 ≤ k ≤ 13 −16 ≤ l ≤ 16
Reflections collected	22264
Independent reflections	4909 R_{int} = 0.0398 R_{sigma} = 0.0302
Completeness to θ = 67.679°	99.3 %
Data / Restraints / Parameters	4909/24/336
Goodness-of-fit on F^2	1.059
Final R indexes [I≥2σ(I)]	R_1 = 0.0384 wR_2 = 0.1019
Final R indexes [all data]	R_1 = 0.0395 wR_2 = 0.1028
Largest peak/hole [eÅ^{-3}]	1.39/-0.90

Crystal data and structure refinement for 4i (Thermal ellipsoids at the 30% probability level)

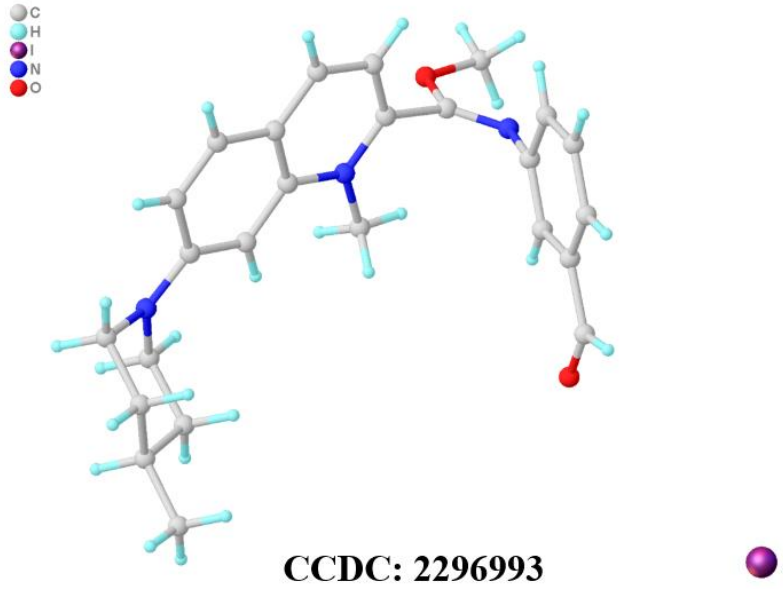
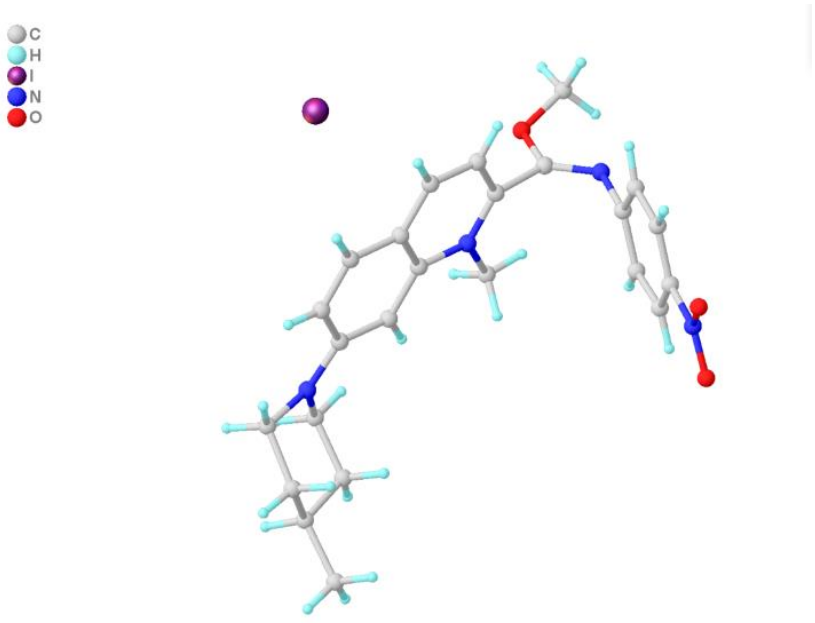


Table S4 Crystal data and structure refinement for 4i	
Empirical formula	$C_{26}H_{30}Cl_2IN_3O_2$
Formula weight	614.33
Temperature [K]	173.0
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	10.524(2)
b [Å]	11.177(2)
c [Å]	12.717(3)
α [°]	92.557(10)
β [°]	95.922(10)
γ [°]	113.297(10)
Volume [Å^3]	1360.6(5)
Z	2
ρ_{calc} [gcm^{-3}]	1.500
μ [mm^{-1}]	11.269
F(000)	620
Crystal size [mm^3]	0.2×0.2×0.02
Crystal colour	clear light white
Crystal shape	block
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	7.02 to 136.50 (0.83 Å)
Index ranges	−12 ≤ h ≤ 5 −10 ≤ k ≤ 13 −15 ≤ l ≤ 15
Reflections collected	14488

Independent reflections	4916 R_{int} = 0.0498 R_{sigma} = 0.0470
Completeness to θ = 68.25°	98.4 %
Data / Restraints / Parameters	4916/0/310
Goodness-of-fit on F^2	1.059
Final R indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0470 wR_2 = 0.1274
Final R indexes [all data]	R_1 = 0.0530 wR_2 = 0.1334
Largest peak/hole [eÅ^{-3}]	3.00/-0.92

Crystal data and structure refinement for 4j (Thermal ellipsoids at the 30% probability level)

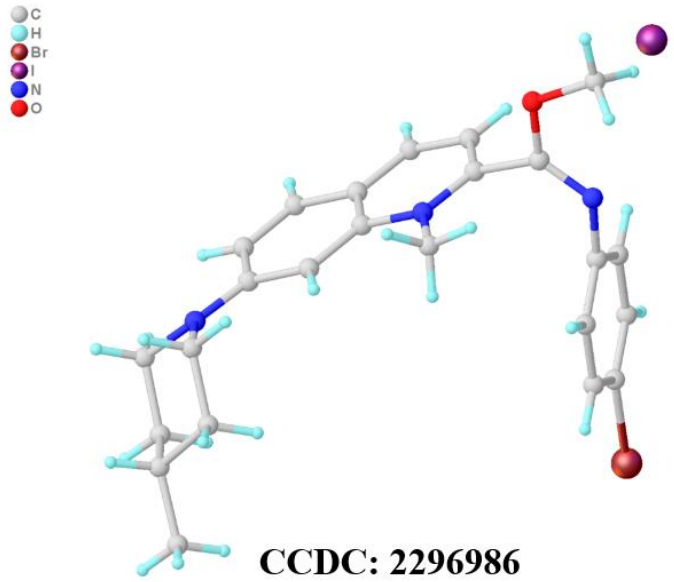


CCDC: 2296981

Table S5 Crystal data and structure refinement for 4j	
Empirical formula	$C_{30}H_{41}IN_4O_3$
Formula weight	632.57
Temperature [K]	173.0
Crystal system	monoclinic
Space group (number)	$P2_1/n$ (14)
a [Å]	17.078(5)
b [Å]	10.396(2)
c [Å]	17.758(5)

α [°]	90
β [°]	108.958(10)
γ [°]	90
Volume [Å^3]	2981.8(13)
Z	4
ρ_{calc} [gcm^{-3}]	1.409
μ [mm^{-1}]	8.723
F(000)	1304
Crystal size [mm^3]	0.08×0.06×0.05
Crystal colour	clear orangish orange
Crystal shape	block
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	8.74 to 130.17 (0.85 Å)
Index ranges	−20 ≤ h ≤ 14 −12 ≤ k ≤ 10 −17 ≤ l ≤ 20
Reflections collected	14070
Independent reflections	5016 R_{int} = 0.0524 R_{sigma} = 0.0590
Completeness to θ = 65.084°	98.6 %
Data / Restraints / Parameters	5016/47/349
Goodness-of-fit on F^2	1.093
Final R indexes [I≥2σ(I)]	R_1 = 0.0782 wR_2 = 0.2233
Final R indexes [all data]	R_1 = 0.1007 wR_2 = 0.2485
Largest peak/hole [eÅ^{-3}]	1.74/-2.37
Extinction coefficient	0.0026(3)

Crystal data and structure refinement for 4n (Thermal ellipsoids at the 30% probability level)

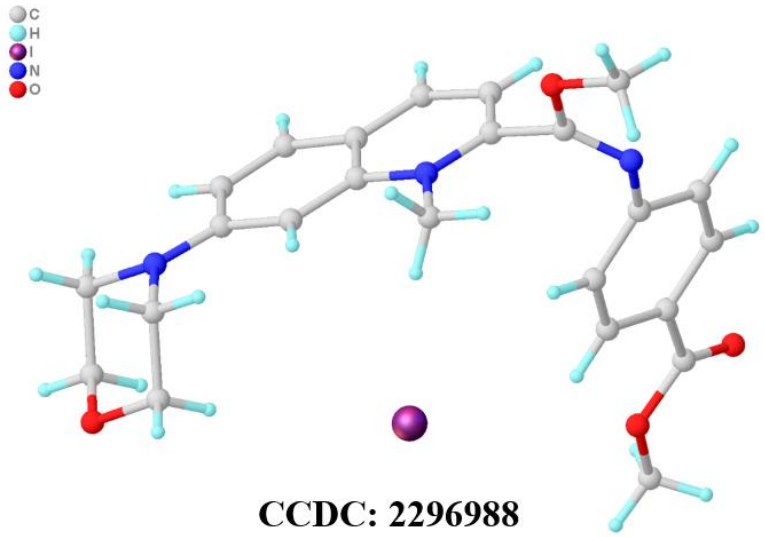


CCDC: 2296986

Table S6 Crystal data and structure refinement for 4n	
Empirical formula	$C_{25}H_{29}BrCl_2IN_3O$
Formula weight	665.22
Temperature [K]	173.0
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	10.3459(11)
b [Å]	11.5121(12)
c [Å]	12.6578(13)
α [°]	84.402(6)
β [°]	78.754(5)
γ [°]	70.128(5)
Volume [Å^3]	1389.8(3)
Z	2
ρ_{calc} [gcm^{-3}]	1.590
μ [mm^{-1}]	12.674
F(000)	660
Crystal size [mm^3]	0.006×0.004×0.002
Crystal colour	clear light yellow
Crystal shape	block
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	7.12 to 134.46 (0.84 Å)
Index ranges	−11 ≤ h ≤ 12 −13 ≤ k ≤ 13 −14 ≤ l ≤ 15
Reflections collected	18569
Independent reflections	4883

	R_{int} = 0.0473 R_{sigma} = 0.0402
Completeness to θ = 67.228°	98.0 %
Data / Restraints / Parameters	4883/144/320
Goodness-of-fit on F^2	1.047
Final R indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0376 wR_2 = 0.0962
Final R indexes [all data]	R_1 = 0.0432 wR_2 = 0.0998
Largest peak/hole [eÅ^{-3}]	1.26/-1.01
Extinction coefficient	0.00117(14)

Crystal data and structure refinement for 4x (Thermal ellipsoids at the 30% probability level)

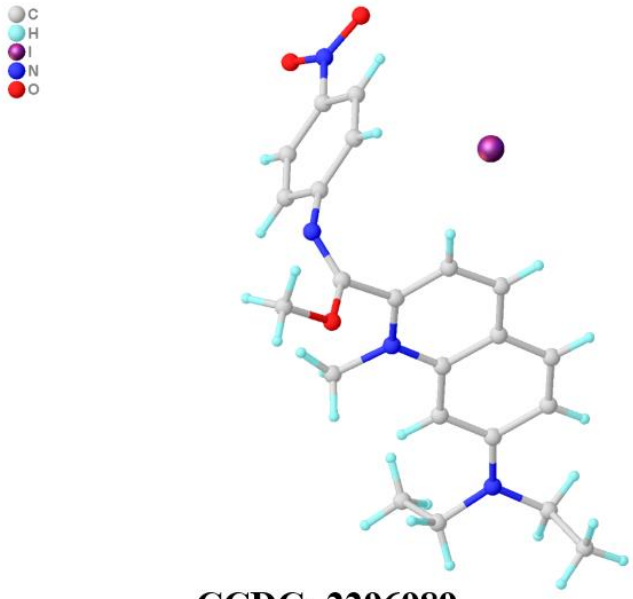


CCDC: 2296988

Table S7 Crystal data and structure refinement for 4x	
Empirical formula	$C_{24}H_{26}IN_3O_4$
Formula weight	547.38
Temperature [K]	173
Crystal system	monoclinic
Space group (number)	$P2_1/n$ (14)
a [Å]	9.9857(4)
b [Å]	16.0279(7)
c [Å]	14.3669(7)
α [°]	90
β [°]	92.359(2)
γ [°]	90
Volume [Å^3]	2297.47(18)

Z	4
ρ_{calc} [gcm^{-3}]	1.583
μ [mm^{-1}]	11.249
F(000)	1104
Crystal size [mm^3]	0.03×0.02×0.02
Crystal colour	clear light red
Crystal shape	block
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	8.27 to 136.48 (0.83 Å)
Index ranges	$-3 \leq h \leq 11$ $-19 \leq k \leq 19$ $-17 \leq l \leq 17$
Reflections collected	13306
Independent reflections	4109 R_{int} = 0.0384 R_{sigma} = 0.0364
Completeness to θ = 67.679°	98.1 %
Data / Restraints / Parameters	4109/0/292
Goodness-of-fit on F^2	1.033
Final R indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0272 wR_2 = 0.0677
Final R indexes [all data]	R_1 = 0.0290 wR_2 = 0.0687
Largest peak/hole [eÅ^{-3}]	0.72/-1.04

Crystal data and structure refinement for 4ae (Thermal ellipsoids at the 30% probability level)

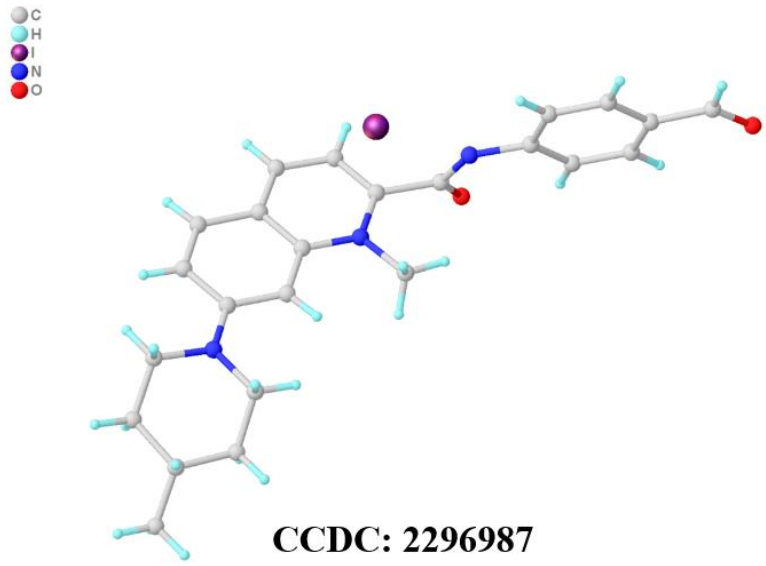


CCDC: 2296989

Table S8 Crystal data and structure refinement for 4ae	
Empirical formula	$C_{22.50}H_{26}ClIN_4O_3$
Formula weight	562.82
Temperature [K]	173.0
Crystal system	monoclinic
Space group (number)	$P2_1/c$ (14)
a [Å]	25.754(2)
b [Å]	13.9662(13)
c [Å]	14.3475(14)
α [°]	90
β [°]	103.041(4)
γ [°]	90
Volume [Å^3]	5027.4(8)
Z	8
ρ_{calc} [gcm^{-3}]	1.487
μ [mm^{-1}]	11.232
F(000)	2264
Crystal size [mm^3]	0.04×0.03×0.02
Crystal colour	clear light yellow
Crystal shape	block
Radiation	CuK_α (λ=1.54184 Å)
2θ range [°]	3.52 to 133.10 (0.84 Å)
Index ranges	−30 ≤ h ≤ 30 −15 ≤ k ≤ 16 −14 ≤ l ≤ 16
Reflections collected	53456
Independent reflections	8811

	R_{int} = 0.0513 R_{sigma} = 0.0351
Completeness to θ = 66.549°	99.3 %
Data / Restraints / Parameters	8811/50/596
Goodness-of-fit on F^2	1.049
Final R indexes [I≥2σ(I)]	R_1 = 0.0503 wR_2 = 0.1377
Final R indexes [all data]	R_1 = 0.0528 wR_2 = 0.1396
Largest peak/hole [eÅ^{-3}]	1.71/-1.08
Extinction coefficient	0.00065(5)

Crystal data and structure refinement for 5a (Thermal ellipsoids at the 30% probability level)



CCDC: 2296987

Table S9 Crystal data and structure refinement for 5a	
Empirical formula	$C_{50}H_{54}Cl_4I_2N_6O_4$
Formula weight	1198.59
Temperature [K]	173.0
Crystal system	monoclinic
Space group (number)	$P2_1/c$ (14)
a [Å]	29.663(3)
b [Å]	11.5826(12)
c [Å]	14.9235(16)
α [°]	90
β [°]	99.262(4)
γ [°]	90

Volume [Å^3]	5060.5(9)
Z	4
ρ_{calc} [gcm^{-3}]	1.573
μ [mm^{-1}]	12.105
F(000)	2408
Crystal size [mm^3]	0.06×0.06×0.05
Crystal colour	clear reddish red
Crystal shape	block
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	3.02 to 133.67 (0.84 Å)
Index ranges	−35 ≤ h ≤ 35 −13 ≤ k ≤ 13 −17 ≤ l ≤ 17
Reflections collected	42965
Independent reflections	8878 R_{int} = 0.0532 R_{sigma} = 0.0417
Completeness to θ = 66.836°	98.9 %
Data / Restraints / Parameters	8878/210/600
Goodness-of-fit on F^2	1.035
Final R indexes [I≥2σ(I)]	R_1 = 0.0610 wR_2 = 0.1615
Final R indexes [all data]	R_1 = 0.0800 wR_2 = 0.1751
Largest peak/hole [eÅ^{-3}]	1.66/-1.87
Extinction coefficient	0.00026(5)

Crystal data and structure refinement for 6a (Thermal ellipsoids at the 30% probability level)

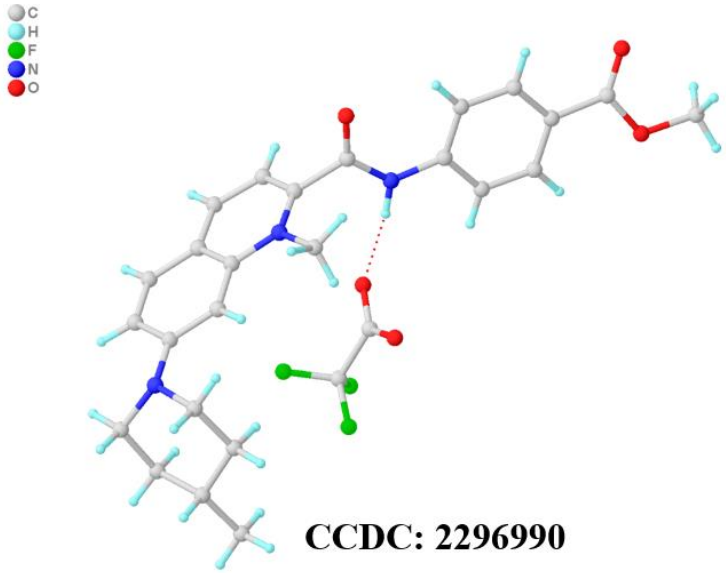
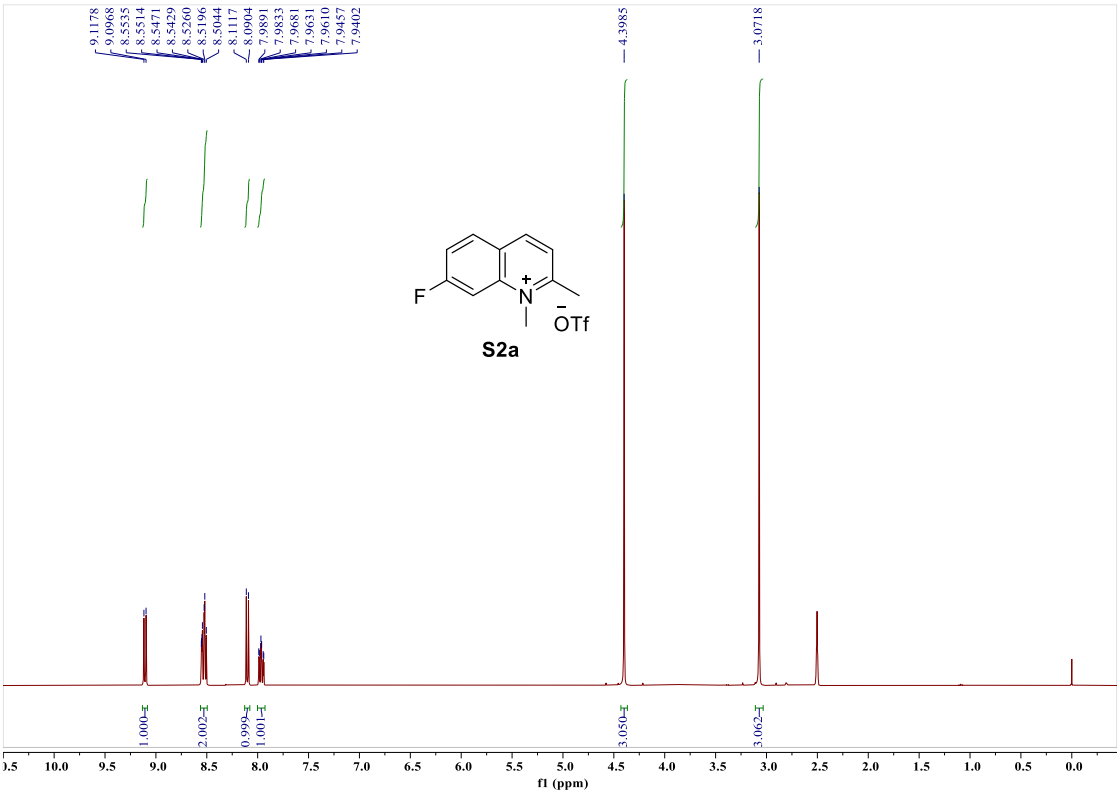
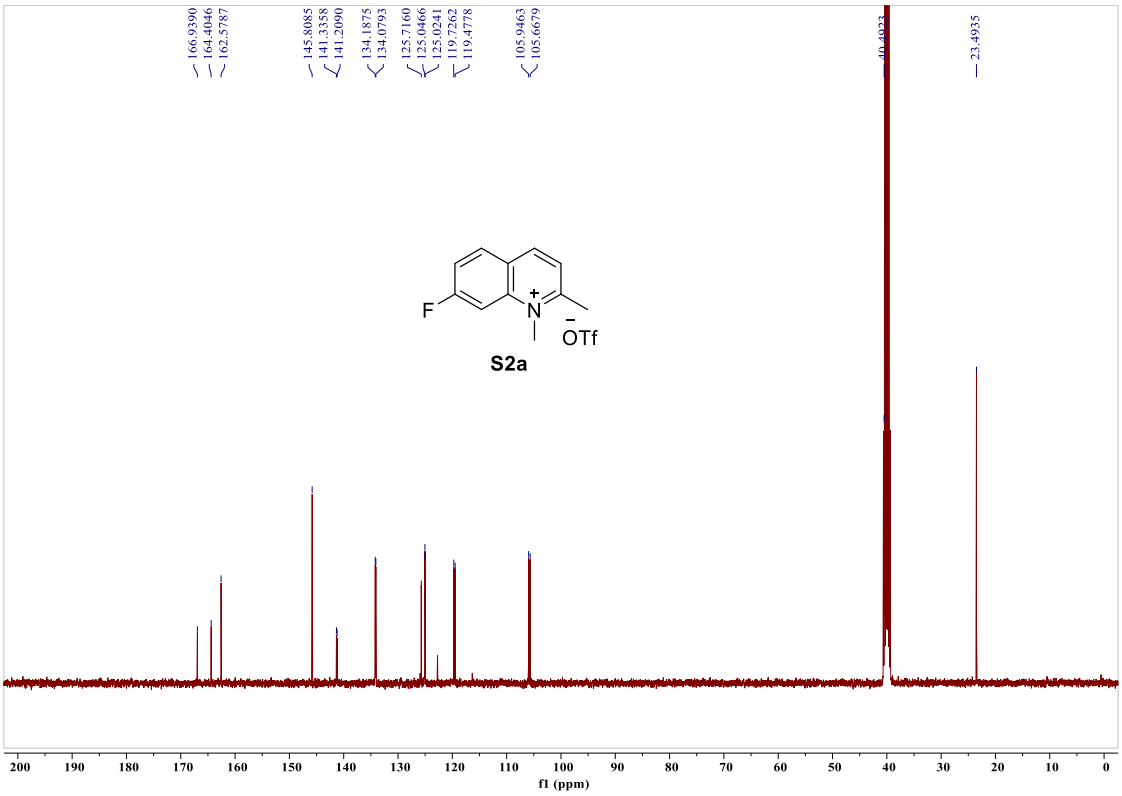


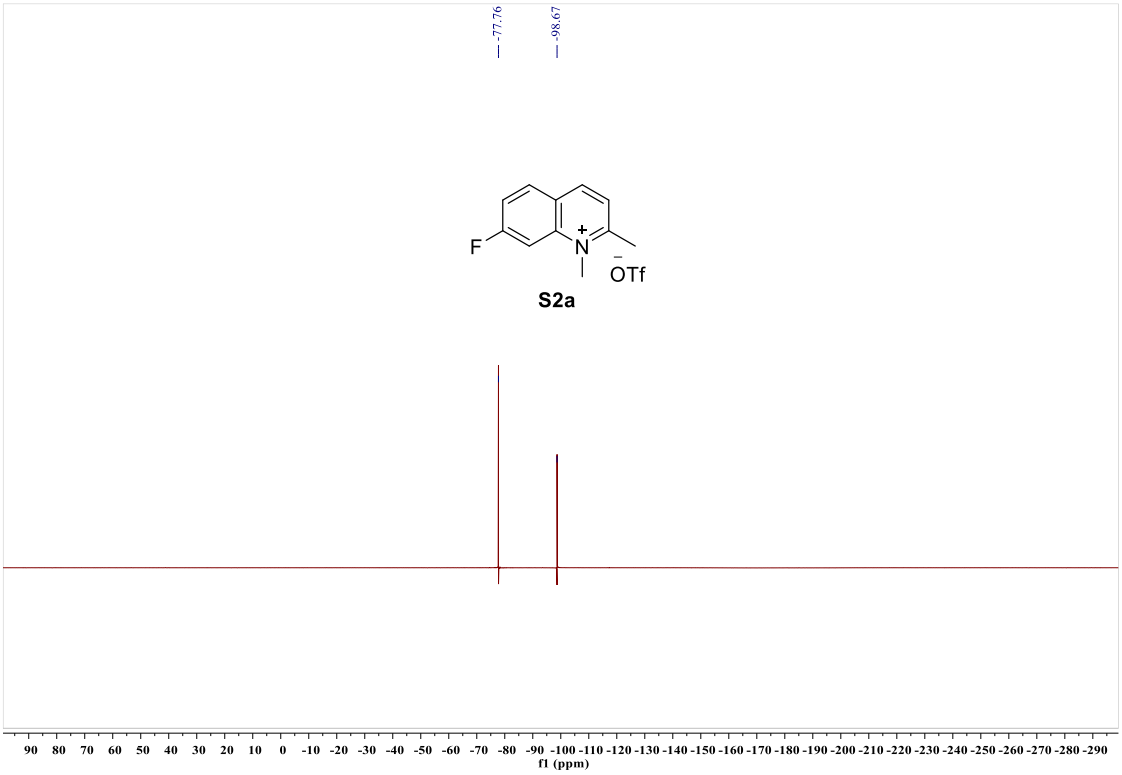
Table S10 Crystal data and structure refinement for 6a	
Empirical formula	$C_{26}H_{28}F_3N_4O_5$
Formula weight	533.52
Temperature [K]	173.0
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	9.1709(4)
b [Å]	10.3735(5)
c [Å]	14.4305(7)
α [°]	109.198(3)
β [°]	90.551(3)
γ [°]	104.138(3)
Volume [Å^3]	1251.14(10)
Z	2
ρ_{calc} [gcm^{-3}]	1.416
μ [mm^{-1}]	0.969
F(000)	558
Crystal size [mm^3]	0.04×0.03×0.02
Crystal colour	orange
Crystal shape	needle
Radiation	CuK_α (λ=1.54178 Å)
2θ range [°]	6.52 to 136.97 (0.83 Å)
Index ranges	−11 ≤ h ≤ 4 −11 ≤ k ≤ 12 −16 ≤ l ≤ 17
Reflections collected	13934
Independent reflections	4562

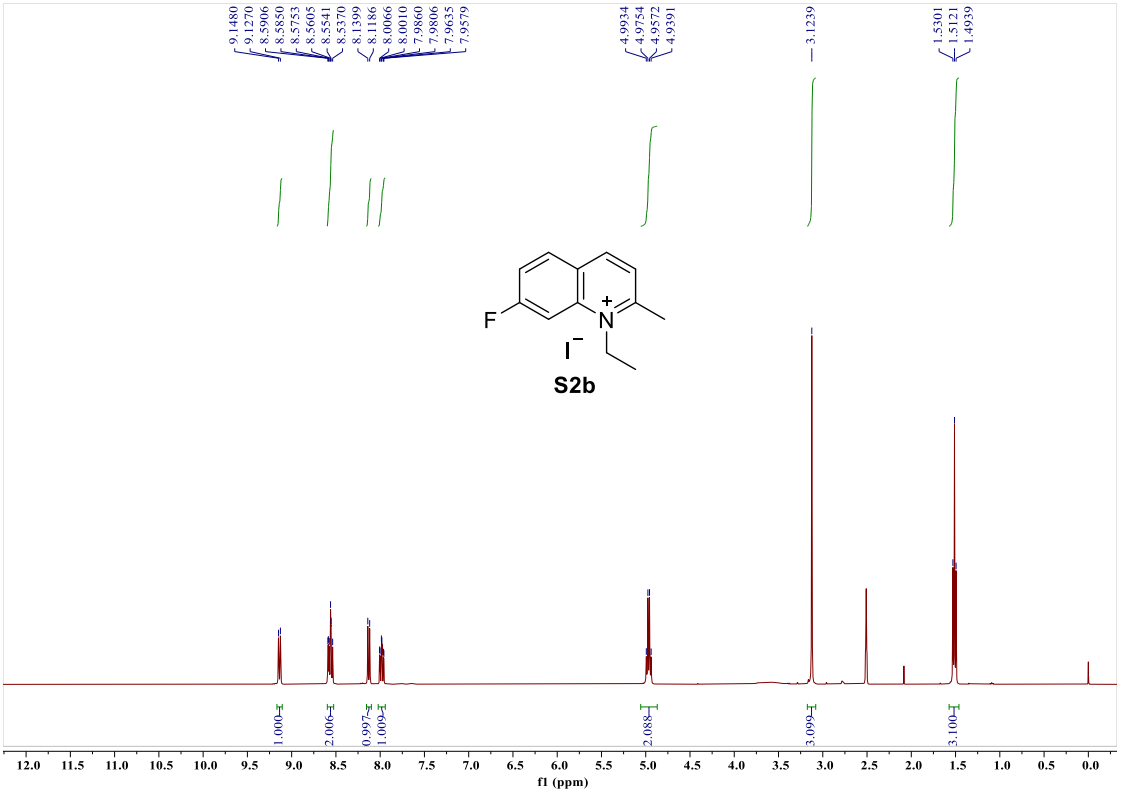
	R_{int} = 0.0431 R_{sigma} = 0.0370
Completeness to θ = 67.679°	99.3 %
Data / Restraints / Parameters	4562/0/357
Goodness-of-fit on F^2	0.926
Final R indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0398 wR_2 = 0.1114
Final R indexes [all data]	R_1 = 0.0544 wR_2 = 0.1209
Largest peak/hole [eÅ^{-3}]	0.35/-0.26

NMR spectrum for the starting materials






-77.76
-98.67
F
N
OTf
S2a
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -250 -260 -270 -280 -290
f1 (ppm)


9.1480
9.1270
8.5906
8.5850
8.5753
8.5605
8.5541
8.5370
8.1399
8.1186
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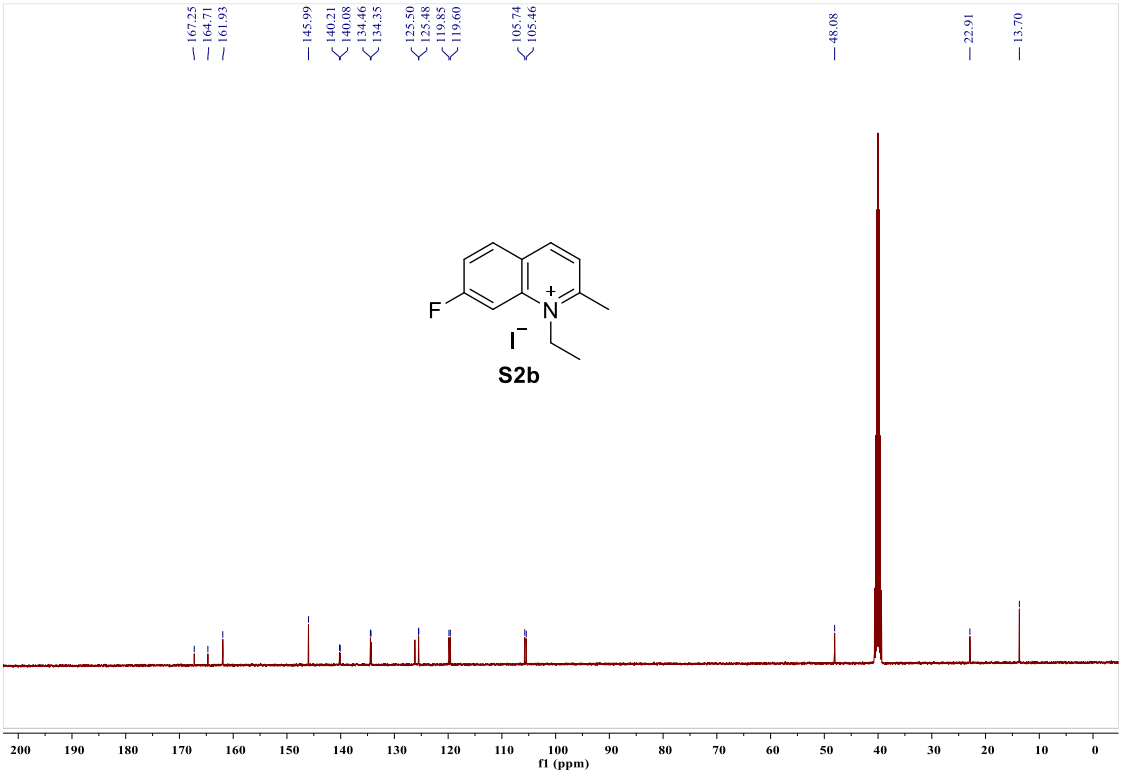
8.0010
7.9860
7.9806
7.9635
7.9579
4.9934
4.9754
4.9572
4.9391
3.1239
1.5301
1.5121
1.4939
F
N
I
S2b
1.000
2.006
0.997
1.009
2.088
3.099
3.100
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


167.25
164.71
161.93
145.99
140.21
140.08
134.46
134.35
125.50
125.48
119.85
119.60
105.74
105.46
48.08
22.91
13.70
F
N
I
S2b
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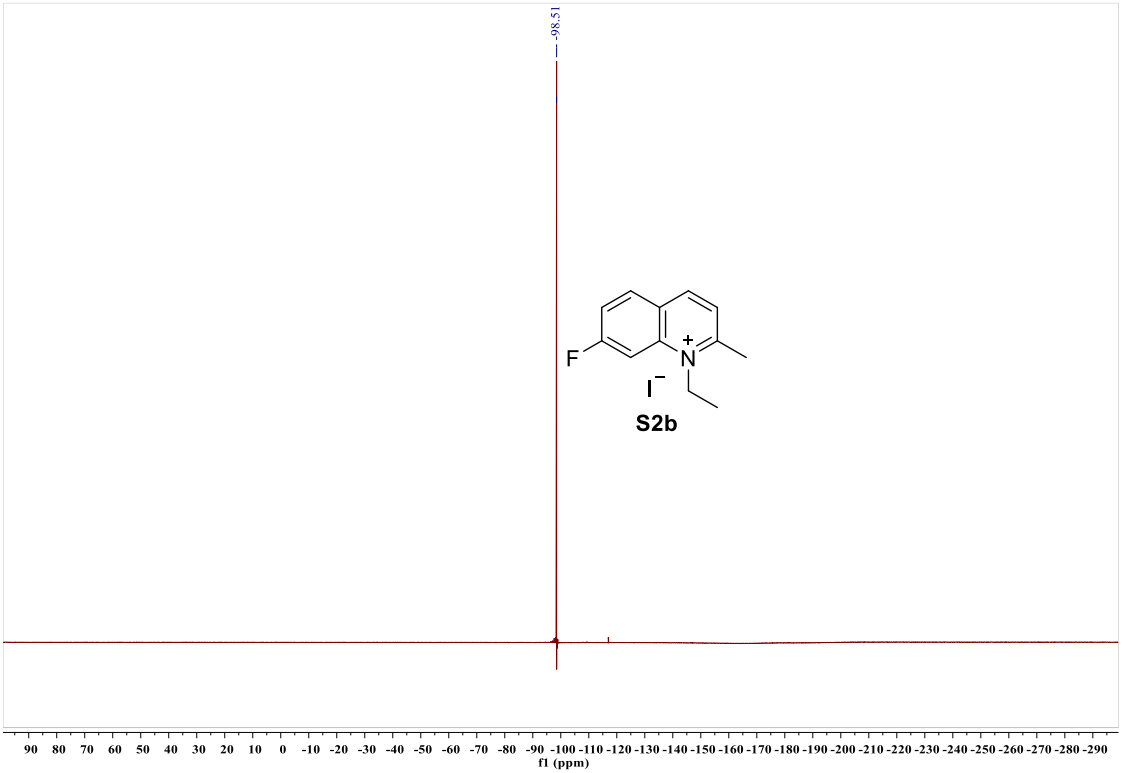
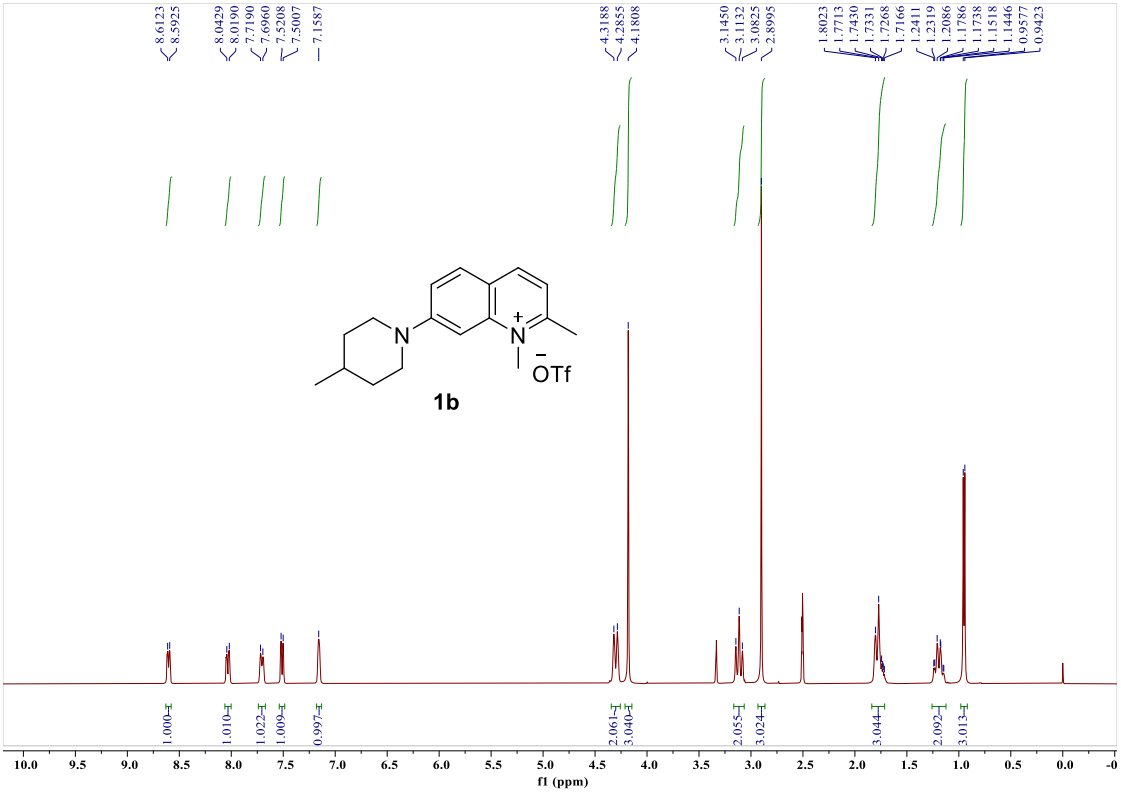
f1 (ppm)


-98.51
F
N
I
S2b
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -250 -260 -270 -280 -290
f1 (ppm)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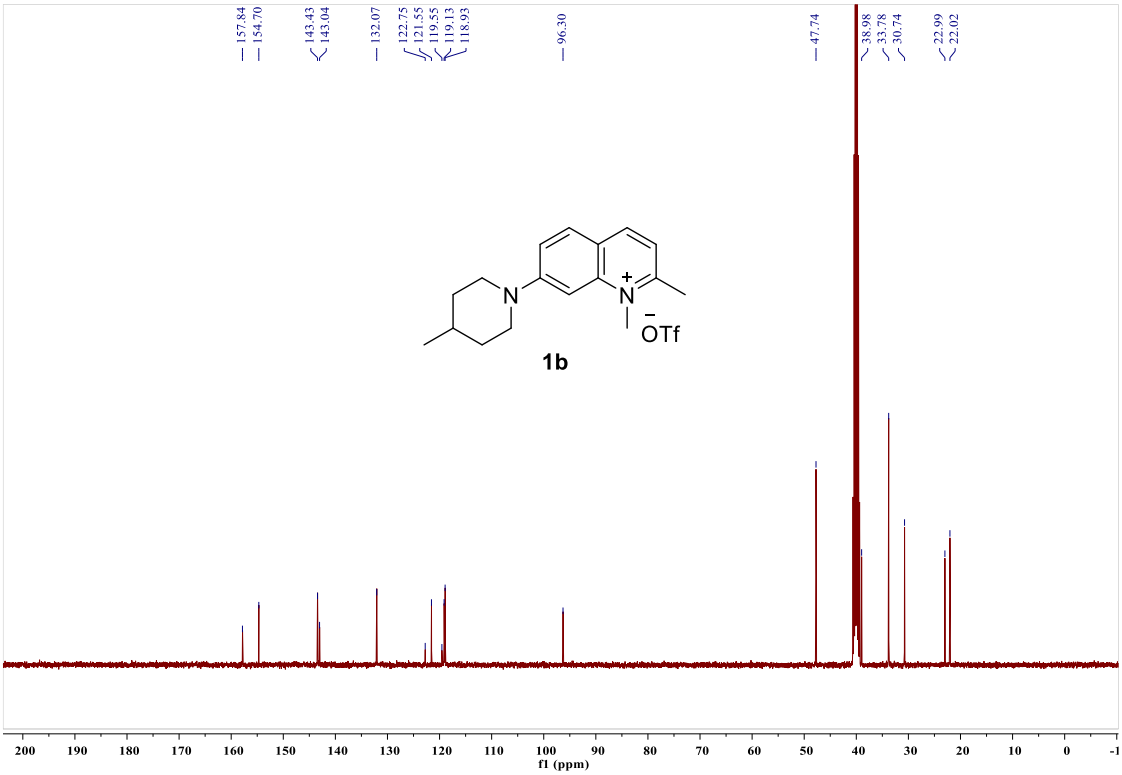
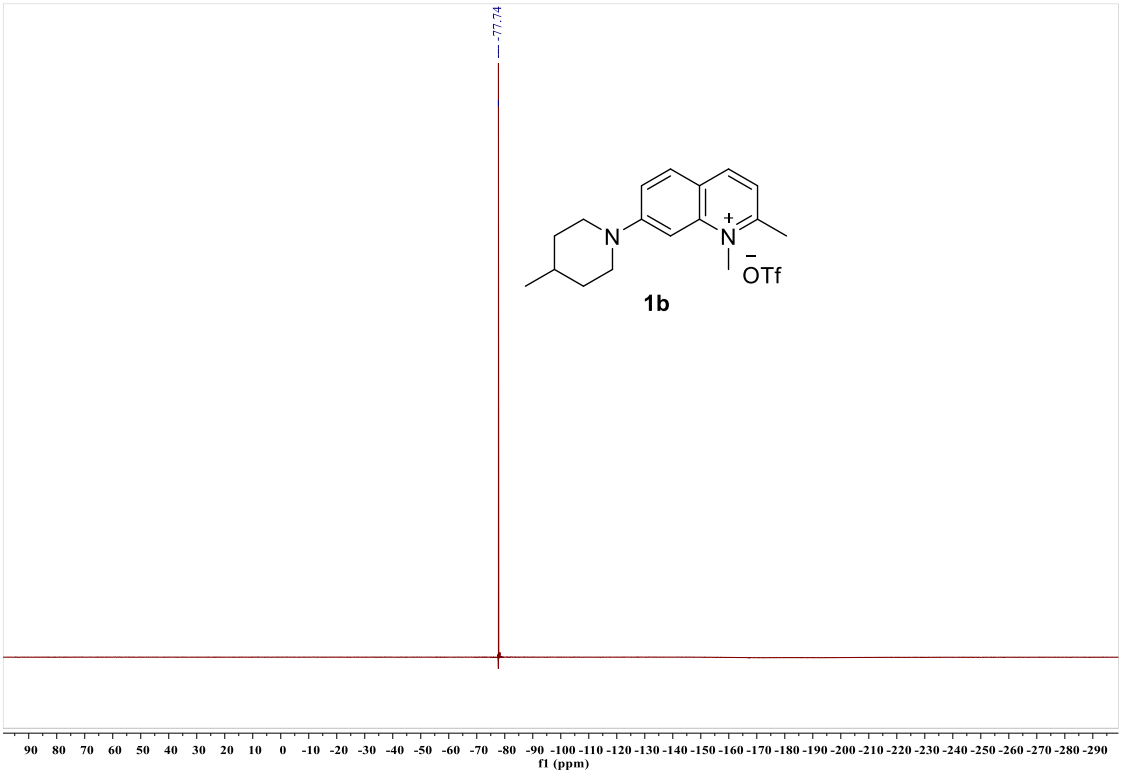
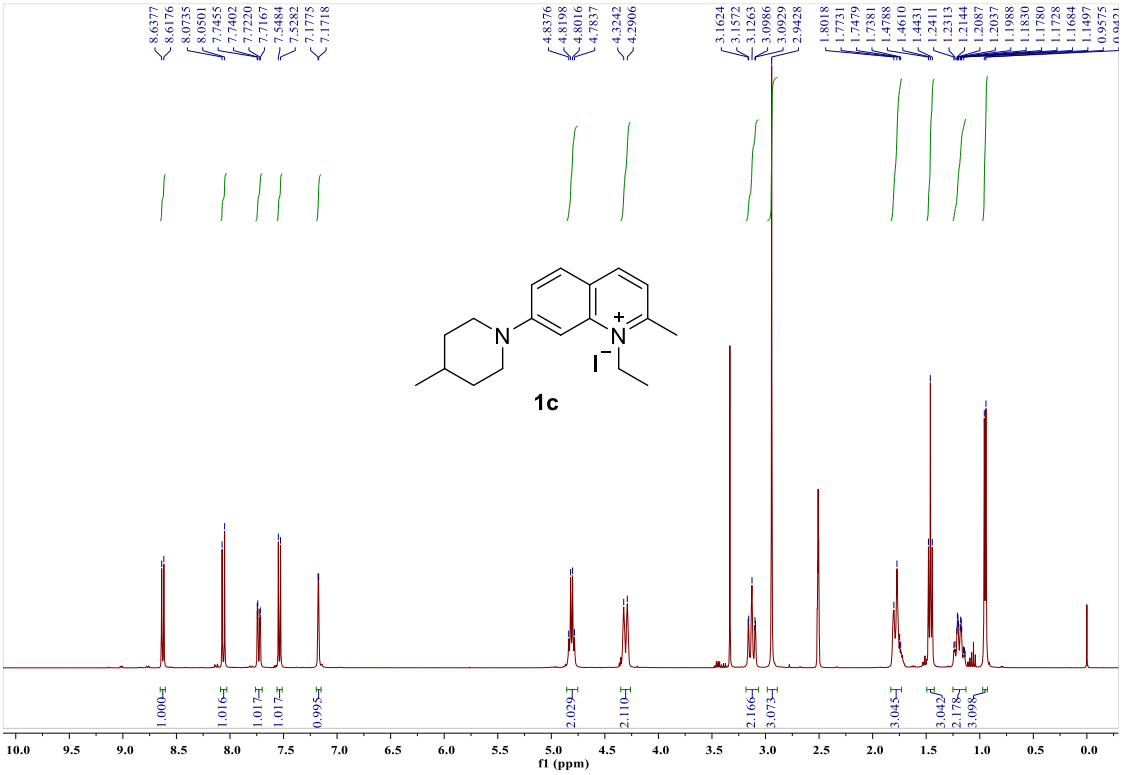
7.5208
7.5007
7.1587
4.3188
4.2855
4.1808
3.1450
3.1132
3.0825
2.8995
1.8023
1.7713
1.7430
1.7331
1.7268
1.7166
1.2411
1.2319
1.2086
1.1786
1.1738
1.1518
1.1446
0.9577
0.9423
1.000
1.010
1.022
1.009
0.997
2.061
3.040
2.055
3.024
3.044
2.092
3.013
N
N
OTf
1b
f1 (ppm)


157.84
154.70
143.43
143.04
132.07
122.75
121.55
119.55
119.13
118.93
96.30
47.74
38.98
33.78
30.74
22.99
22.02
N
N
OTf
1b
f1 (ppm)


-77.74
N
N
OTf
1b
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -250 -260 -270 -280 -290
f1 (ppm)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8.6176
8.0735
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7.7220
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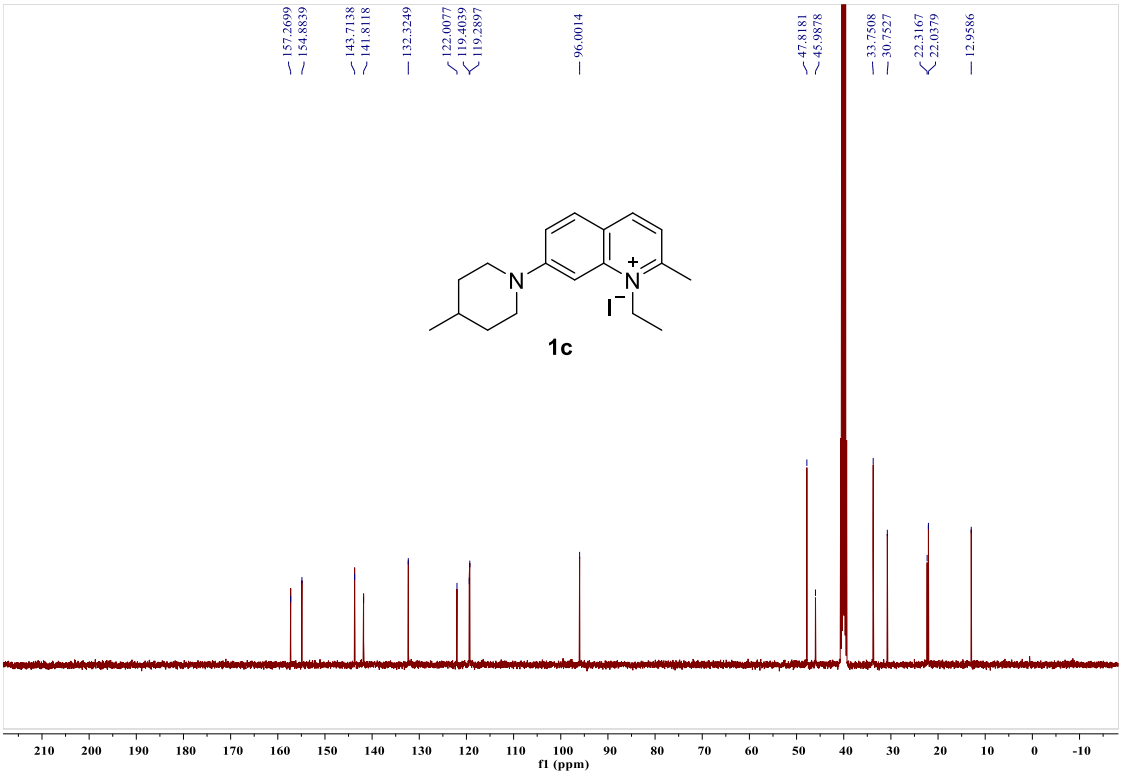
7.5484
7.5282
7.1775
7.1718
4.8376
4.8198
4.8016
4.7837
4.3242
4.2906
3.1624
3.1572
3.1263
3.0986
3.0929
2.9428
1.8018
1.7731
1.7479
1.7381
1.4788
1.4610
1.4431
1.2411
1.2313
1.2144
1.2087
1.2037
1.1988
1.1830
1.1780
1.1728
1.1684
1.1497
0.9575
0.9431
1.000
1.016
1.017
1.017
0.995
2.029
2.110
2.166
3.073
3.045
3.042
2.178
3.098
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)
N
N
I⁻
1c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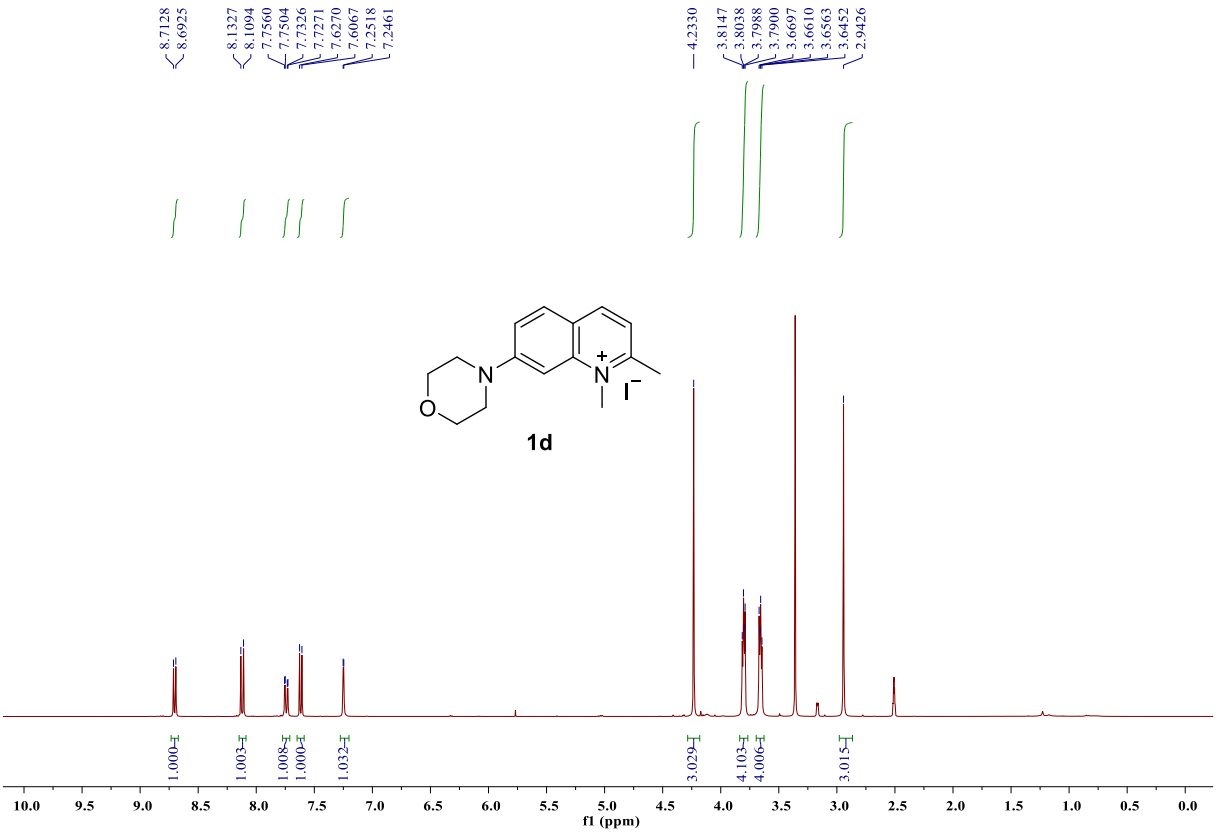
154.8839
143.7138
141.8118
132.3249
122.0077
119.4039
119.2897
96.0014
47.8181
45.9878
33.7508
30.7527
22.3167
22.0379
12.9586
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)
N
N
I⁻
1c


8.7128
8.6925
8.1327
8.1094
7.7560
7.7504
7.7326
7.7271
7.6270
7.6067
7.2518
7.2461
4.2330
3.8147
3.8038
3.7988
3.7900
3.6697
3.6610
3.6563
3.6452
2.9426
1d
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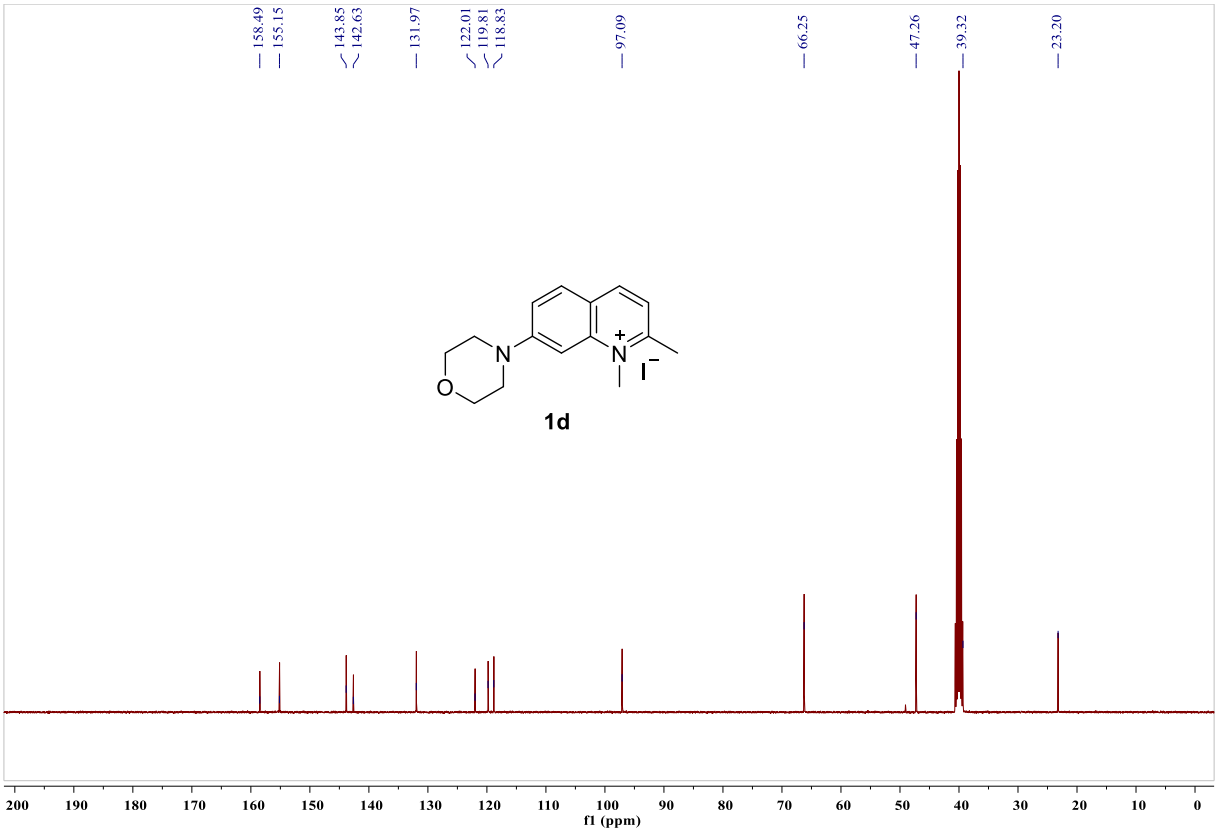
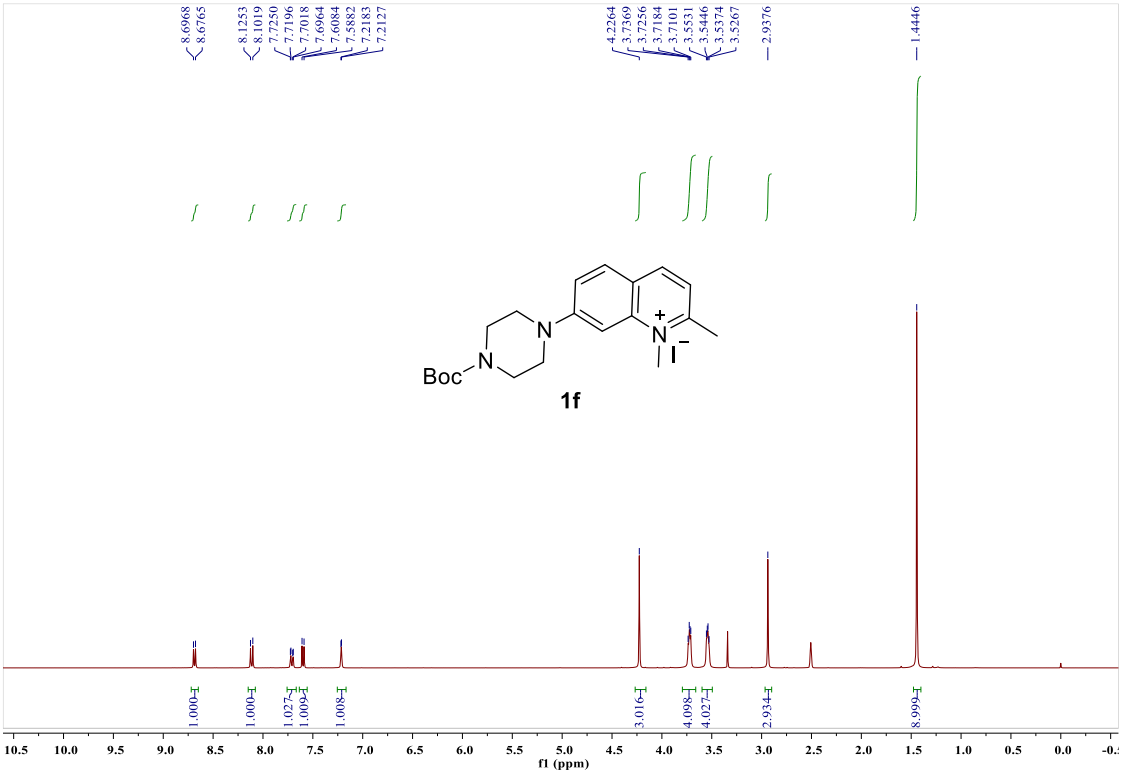
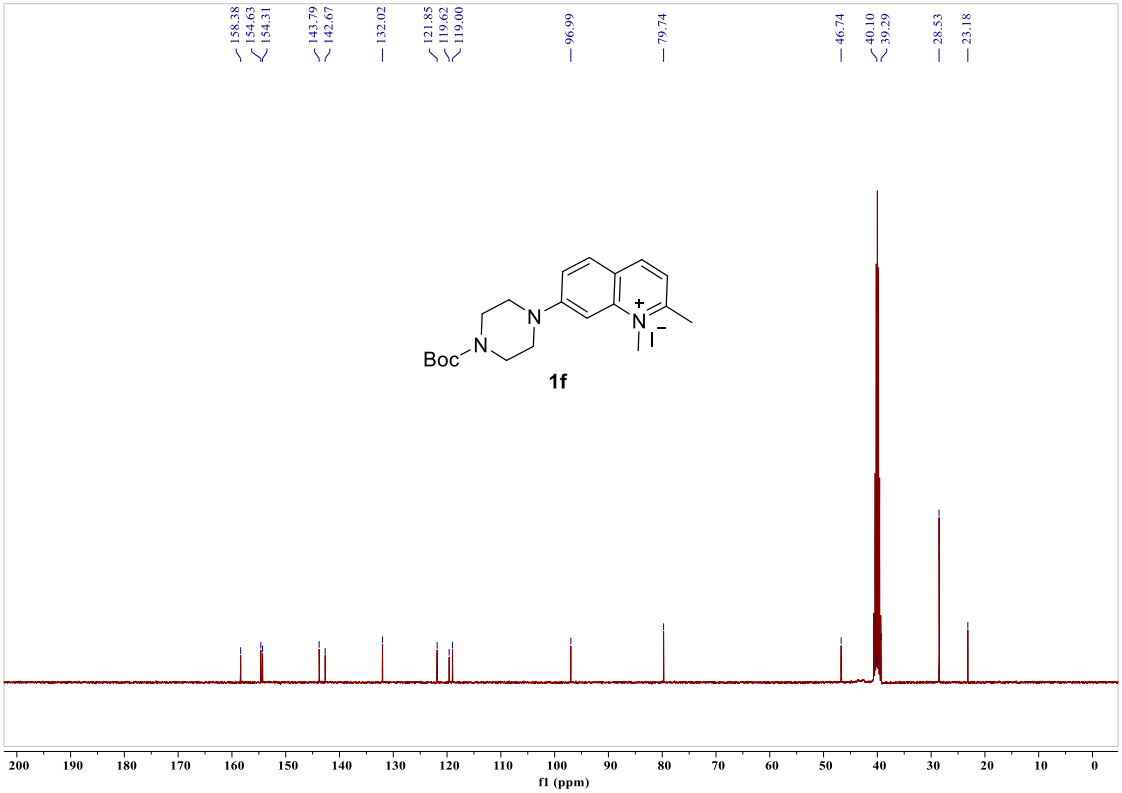
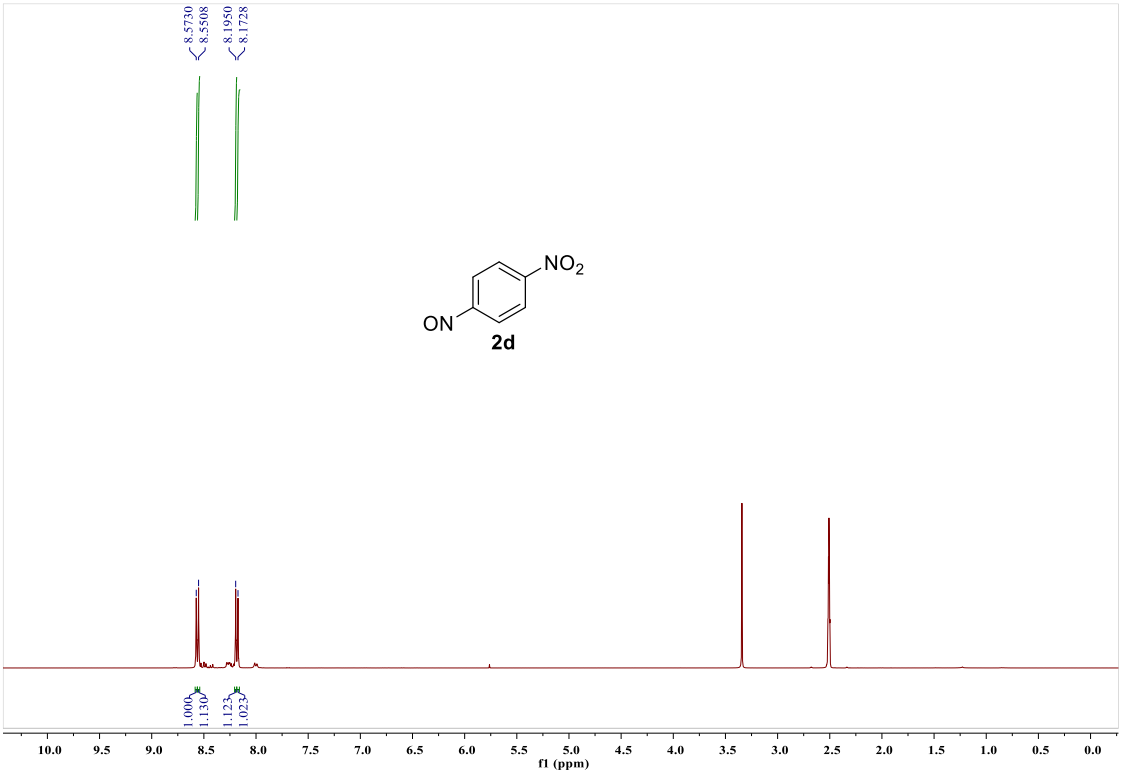
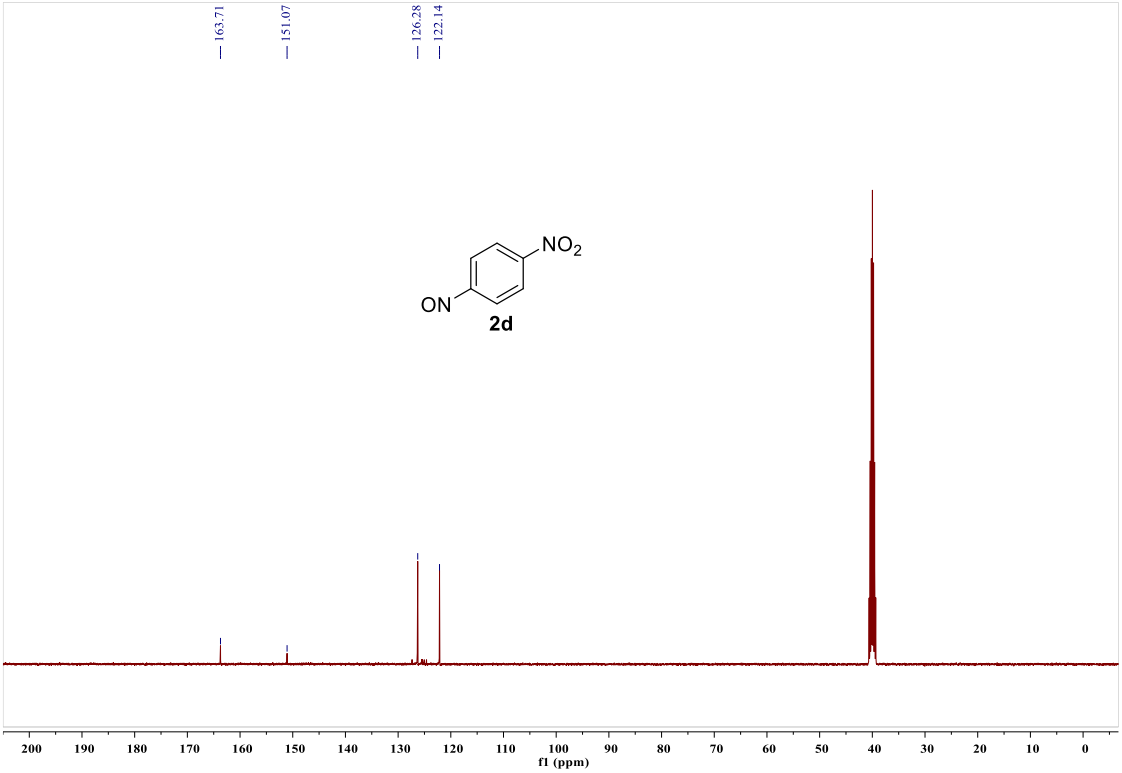
1.003
1.008
1.000
1.032
3.029
4.103
4.006
3.015
f1 (ppm)

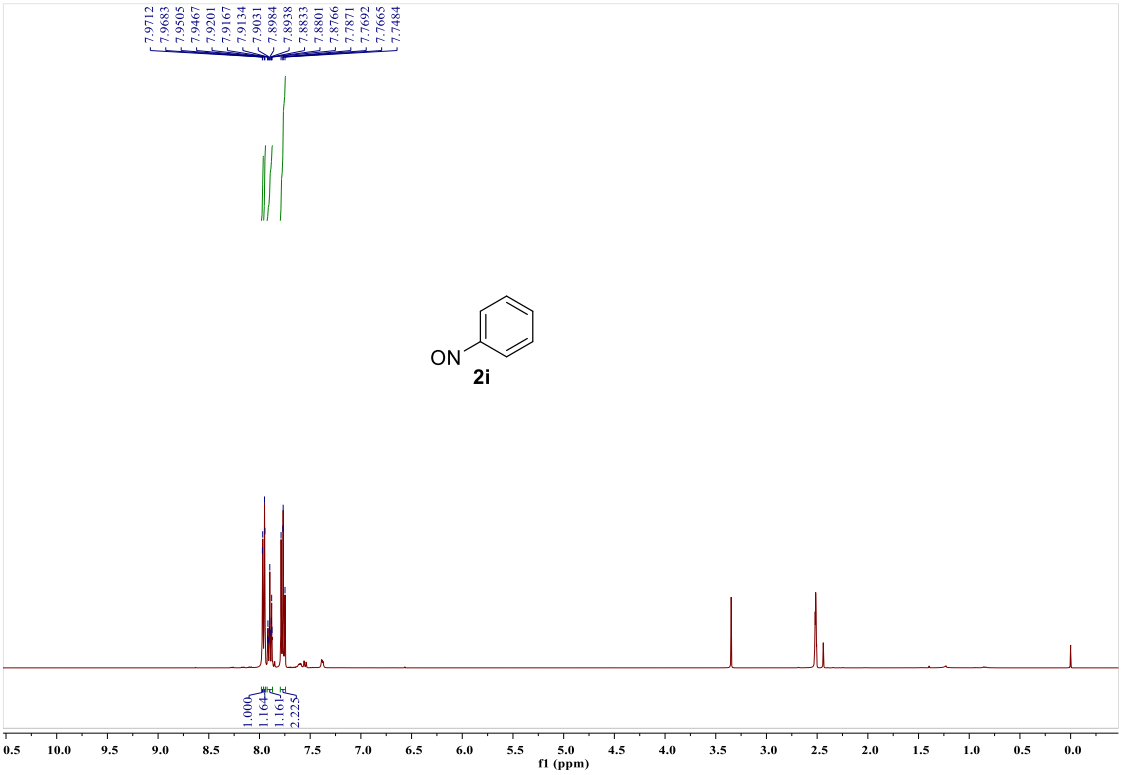

158.49
155.15
143.85
142.63
131.97
122.01
119.81
118.83
97.09
66.25
47.26
39.32
23.20
1d
f1 (ppm)

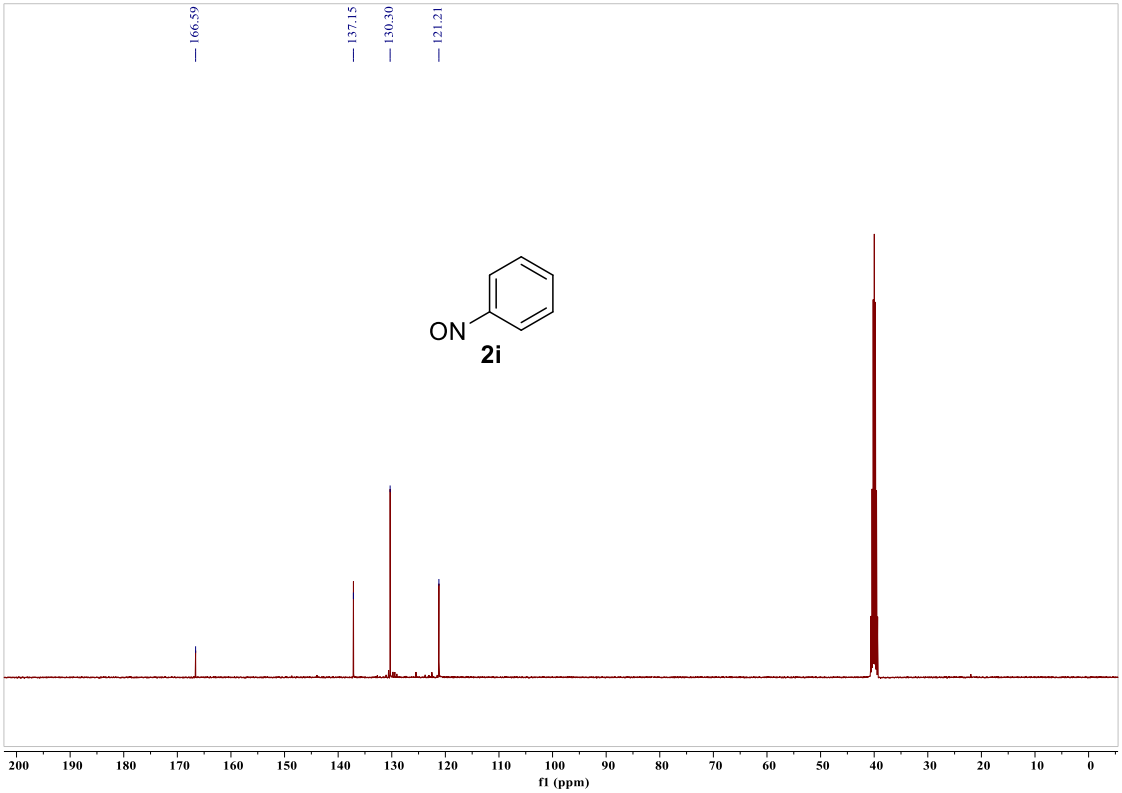

8.6968
8.6765
8.1253
8.1019
7.7250
7.7196
7.7018
7.6964
7.6084
7.5882
7.2183
7.2127
4.2264
3.7369
3.7256
3.7184
3.7101
3.5531
3.5446
3.5374
3.5267
2.9376
1.4446
1.000
1.000
1.027
1.009
1.008
3.016
4.098
4.027
2.934
8.999
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
Boc
N
N
I
1f

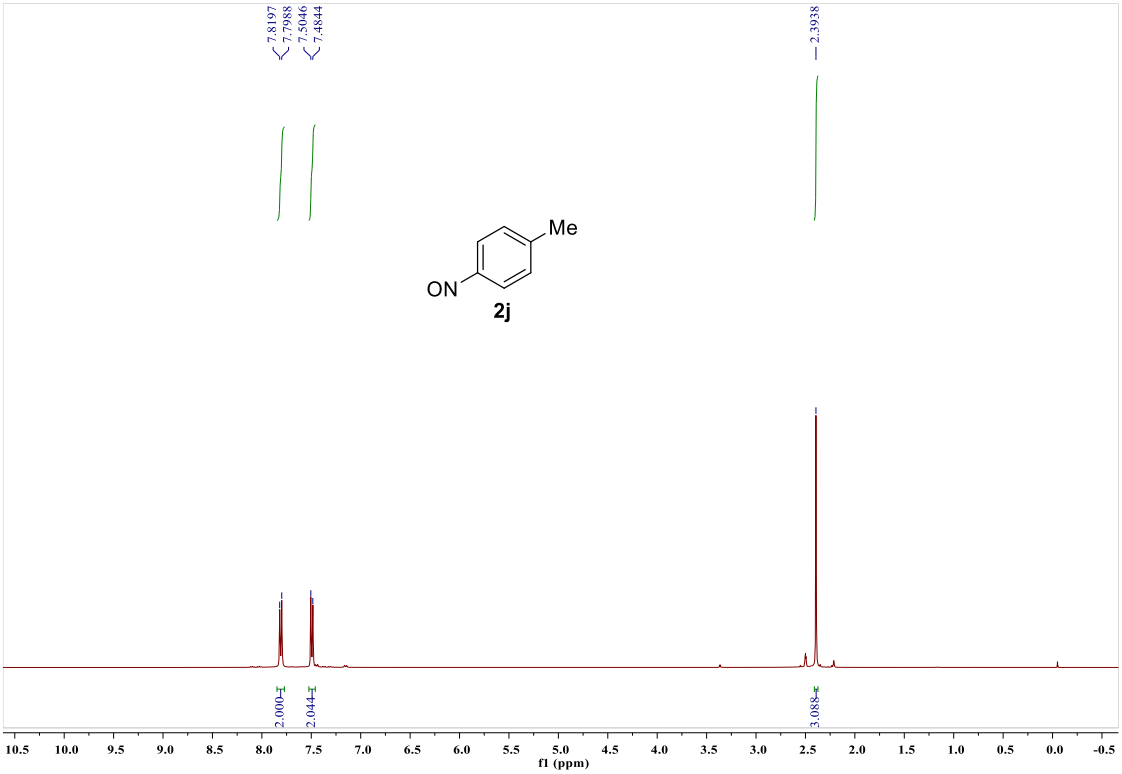

158.38
154.63
154.31
143.79
142.67
132.02
121.85
119.62
119.00
96.99
79.74
46.74
40.10
39.29
28.53
23.18
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
Boc
N
N
I
1f

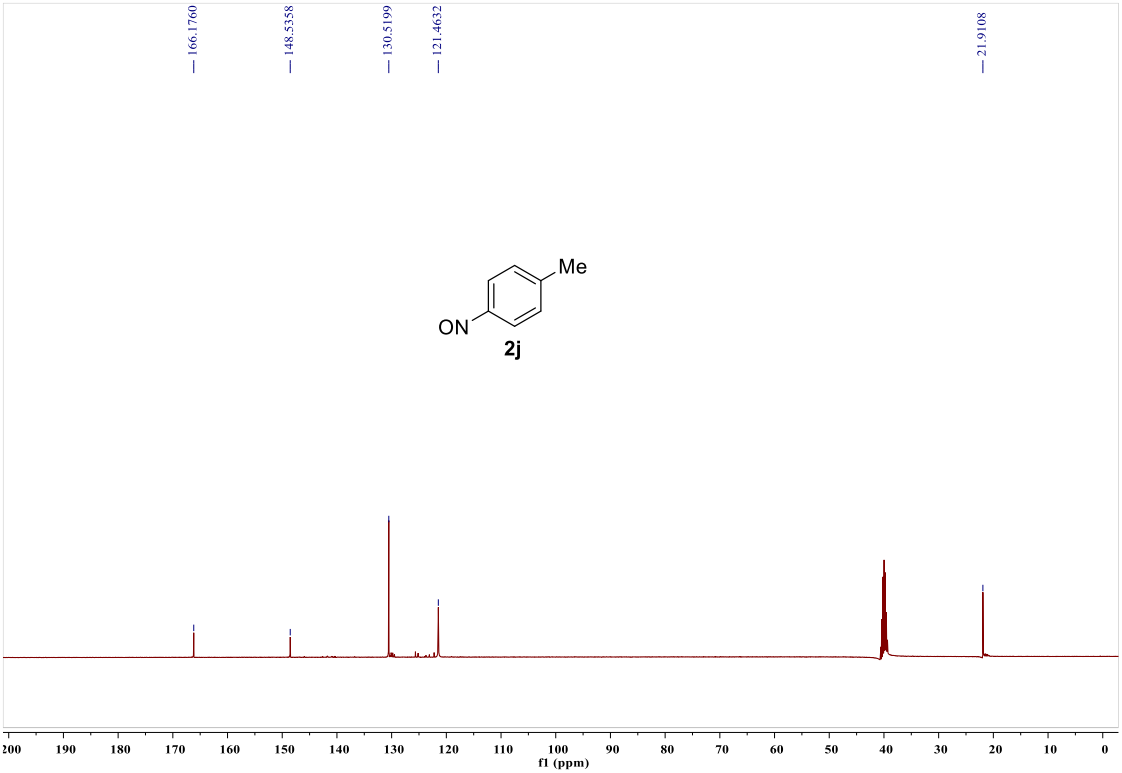

8.5730
8.5508
8.1950
8.1728
NO2
ON
2d
1.000
1.130
1.123
1.023
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


163.71
151.07
126.28
122.14
NO2
ON
2d
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

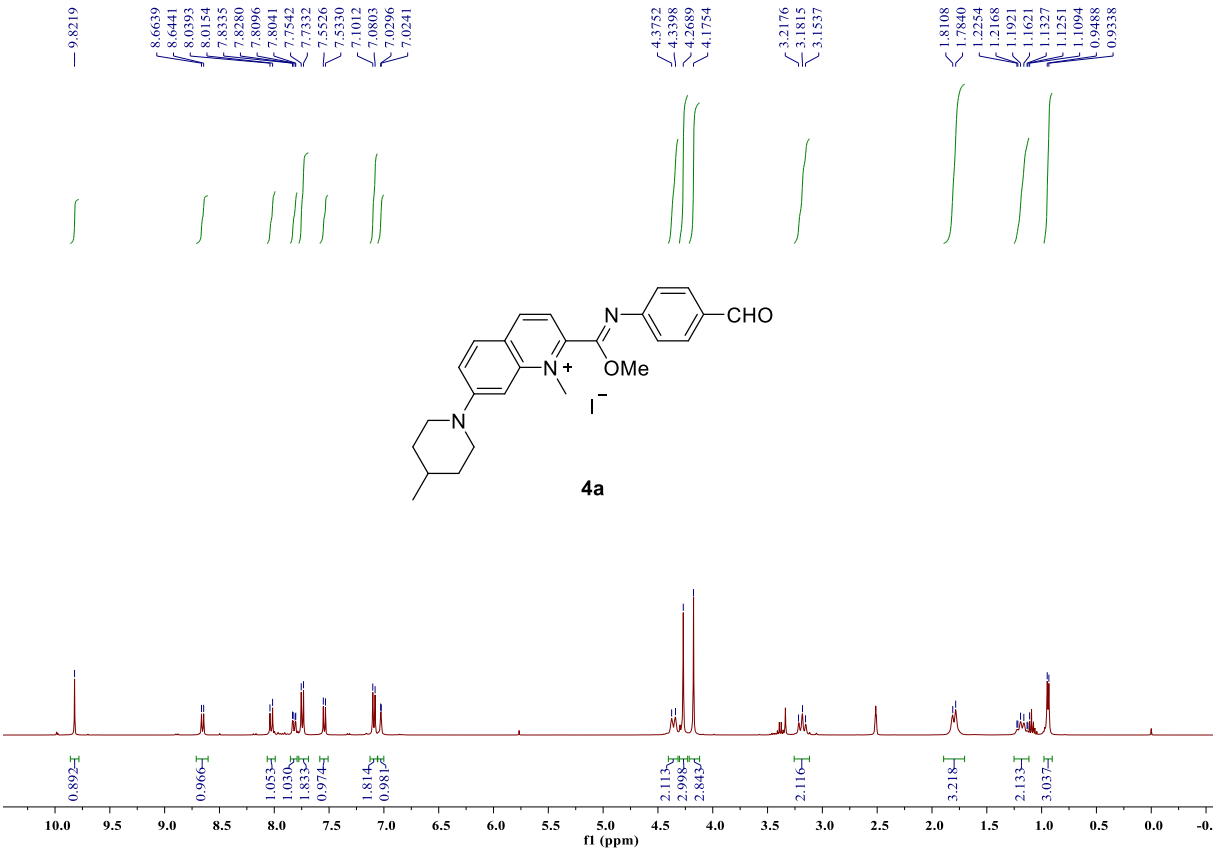

7.9712
7.9683
7.9505
7.9467
7.9201
7.9167
7.9134
7.9031
7.8984
7.8938
7.8833
7.8801
7.8766
7.7871
7.7692
7.7665
7.7484
ON
2i
1.000
1.164
1.161
2.225
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

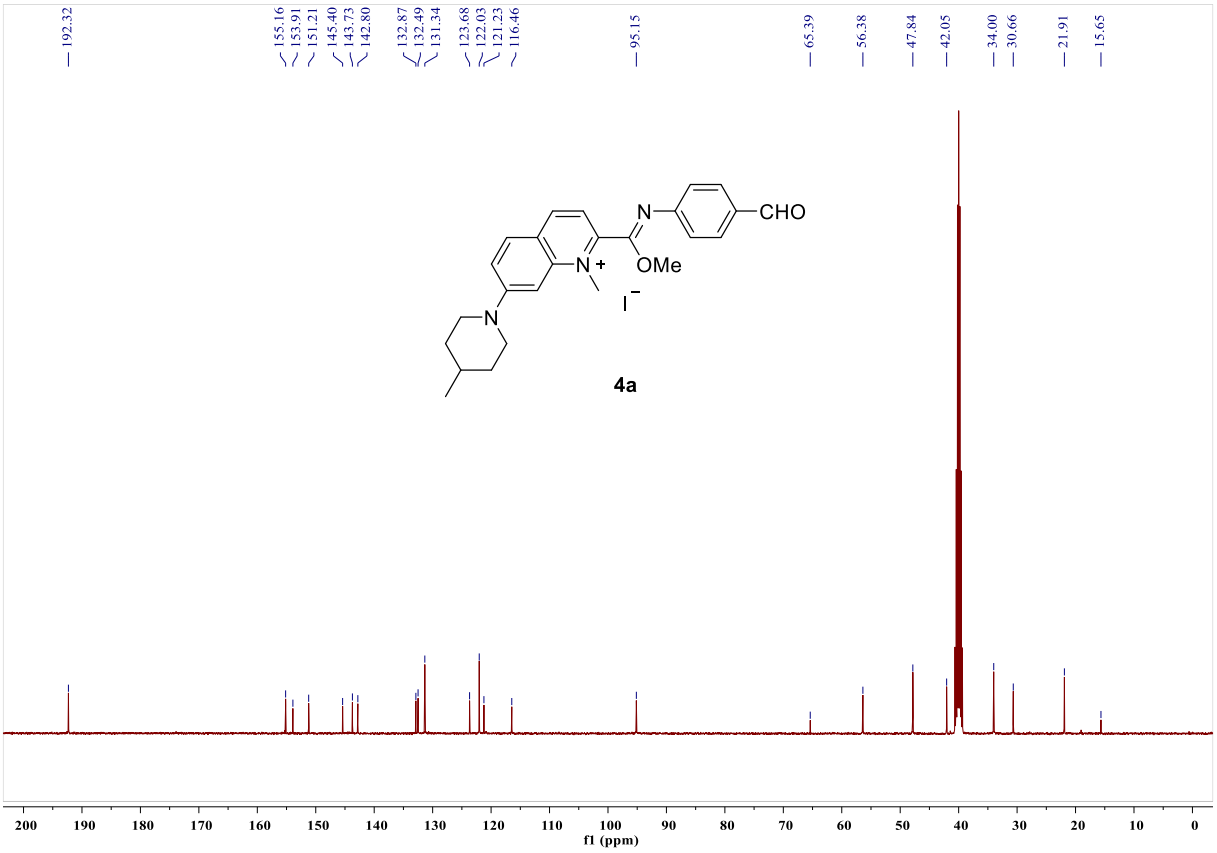

166.59
137.15
130.30
121.21
ON
2i
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

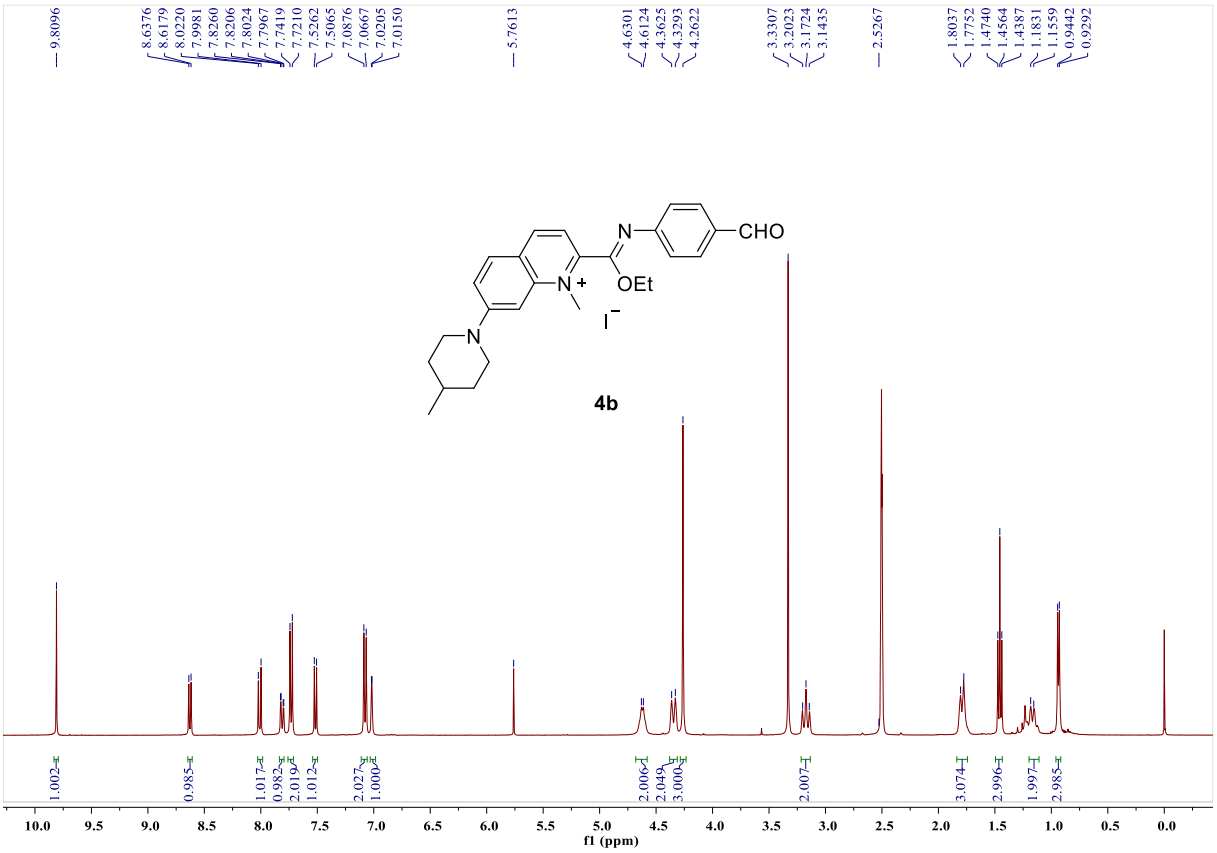

7.8197
7.7988
7.5046
7.4844
2.3938
Me
ON
2j
2.000
2.044
3.088
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


166.1760
148.5358
130.5199
121.4632
21.9108
Me
ON
2j
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

NMR spectrum for the products and synthetic application product






9.8096
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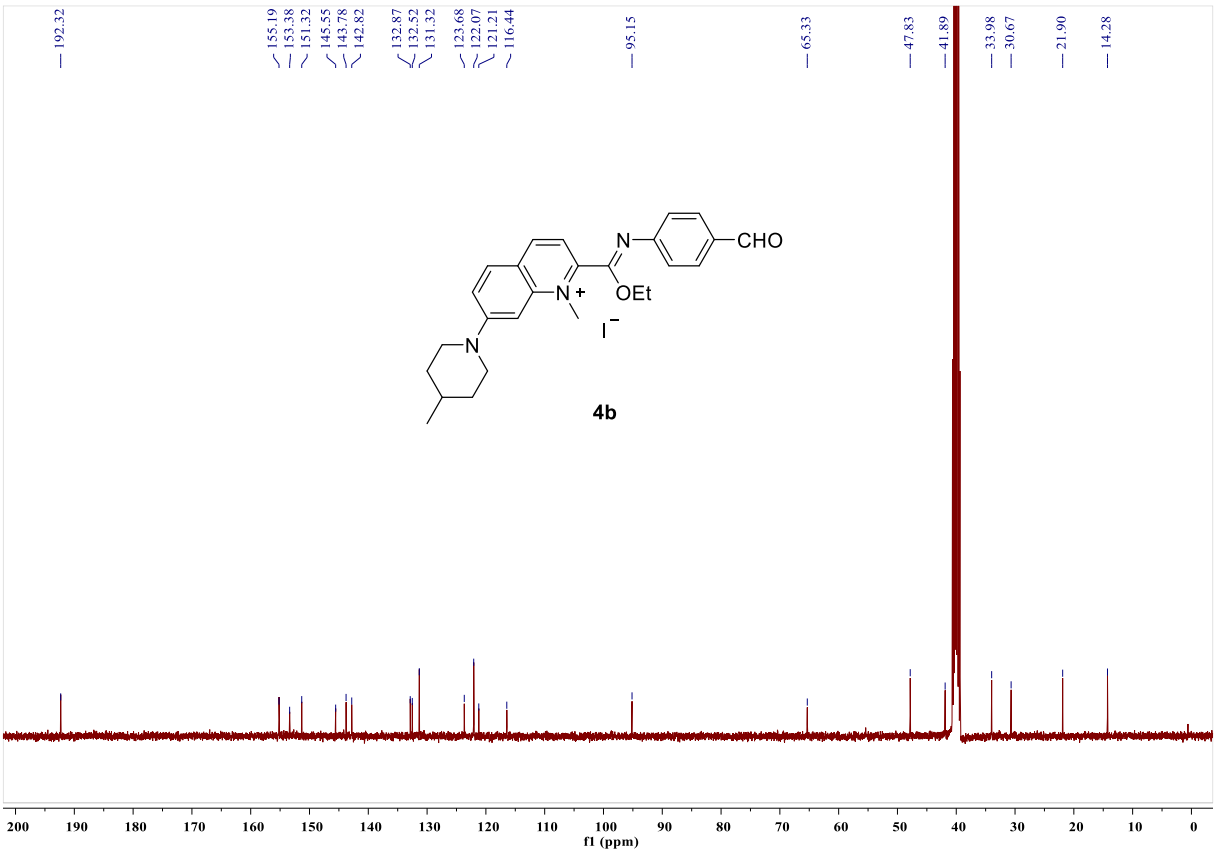
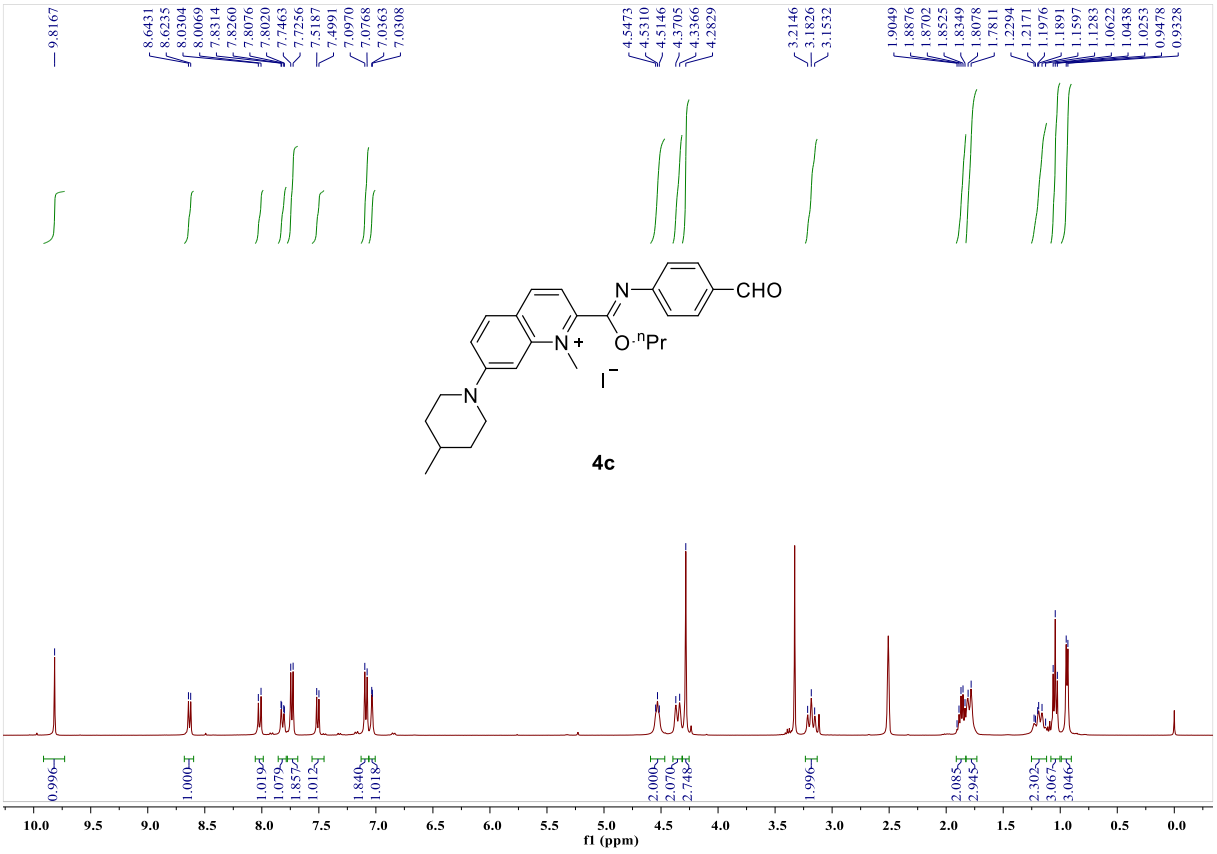
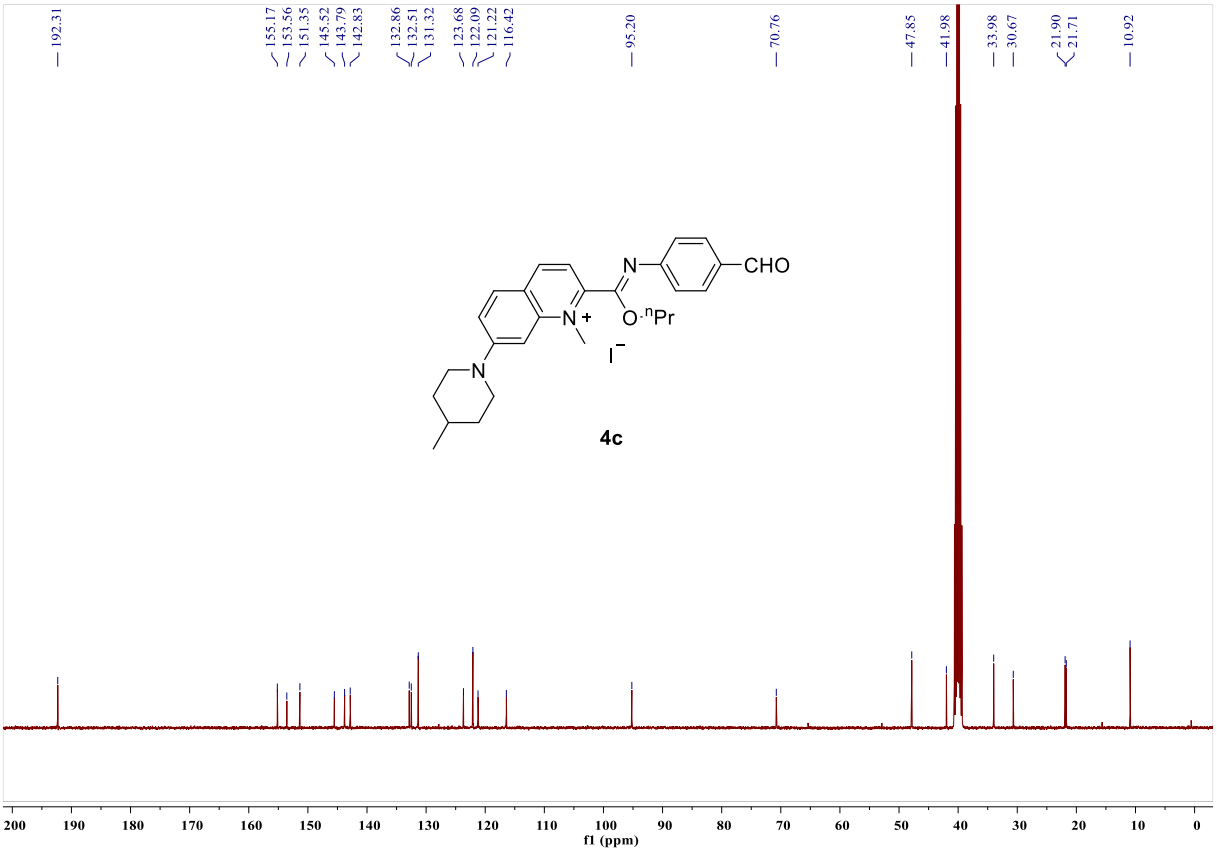
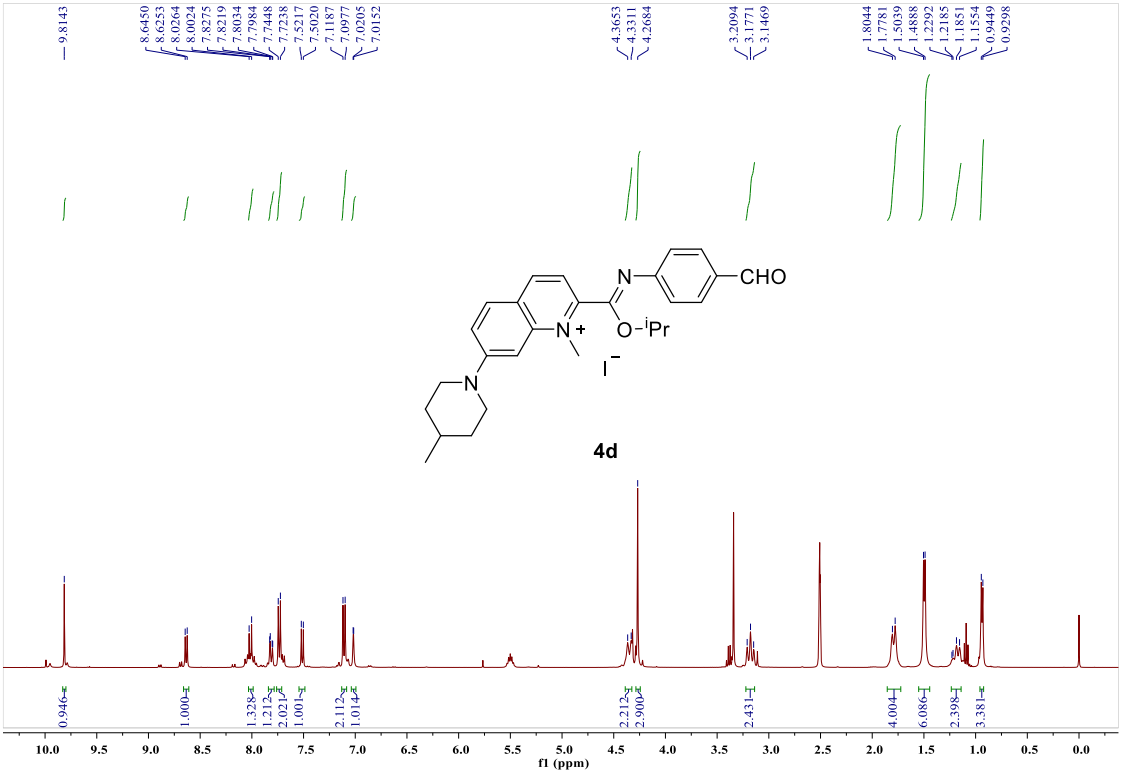
8.6179
8.0220
7.9981
7.8260
7.8206
7.8024
7.7967
7.7419
7.7210
7.5262
7.5065
7.0876
7.0667
7.0205
7.0150
5.7613
4.6301
4.6124
4.3625
4.3293
4.2622
3.3307
3.2023
3.1724
3.1435
2.5267
1.8037
1.7752
1.4740
1.4564
1.4387
1.1831
1.1559
0.9442
0.9292
1.002
0.985
1.017
0.982
2.019
1.012
2.027
1.000
2.006
2.049
3.000
2.007
3.074
2.996
1.997
2.985
f1 (ppm)
N
CHO
OEt
N+
I−
N
4b


192.32
155.19
153.38
151.32
145.55
143.78
142.82
132.87
132.52
131.32
123.68
122.07
121.21
116.44
95.15
65.33
47.83
41.89
33.98
30.67
21.90
14.28
f1 (ppm)
N
CHO
OEt
N+
I−
N
4b


9.8167
8.6431
8.6235
8.0304
8.0069
7.8314
7.8260
7.8076
7.8020
7.7463
7.7256
7.5187
7.4991
7.0970
7.0768
7.0363
7.0308
4.5473
4.5310
4.5146
4.3705
4.3366
4.2829
3.2146
3.1826
3.1532
1.9049
1.8876
1.8702
1.8525
1.8349
1.8078
1.7811
1.2294
1.2171
1.1976
1.1891
1.1597
1.1283
1.0622
1.0438
1.0253
0.9478
0.9328
CHO
N
N+
O
nPr
I−
N
4c
0.996
1.000
1.019
1.079
1.857
1.012
1.840
1.018
2.000
2.070
2.748
1.996
2.085
2.945
2.302
3.067
3.046
f1 (ppm)


192.31
155.17
153.56
151.35
145.52
143.79
142.83
132.86
132.51
131.32
123.68
122.09
121.22
116.42
95.20
70.76
47.85
41.98
33.98
30.67
21.90
21.71
10.92
CHO
N
N+
O
nPr
I−
N
4c
f1 (ppm)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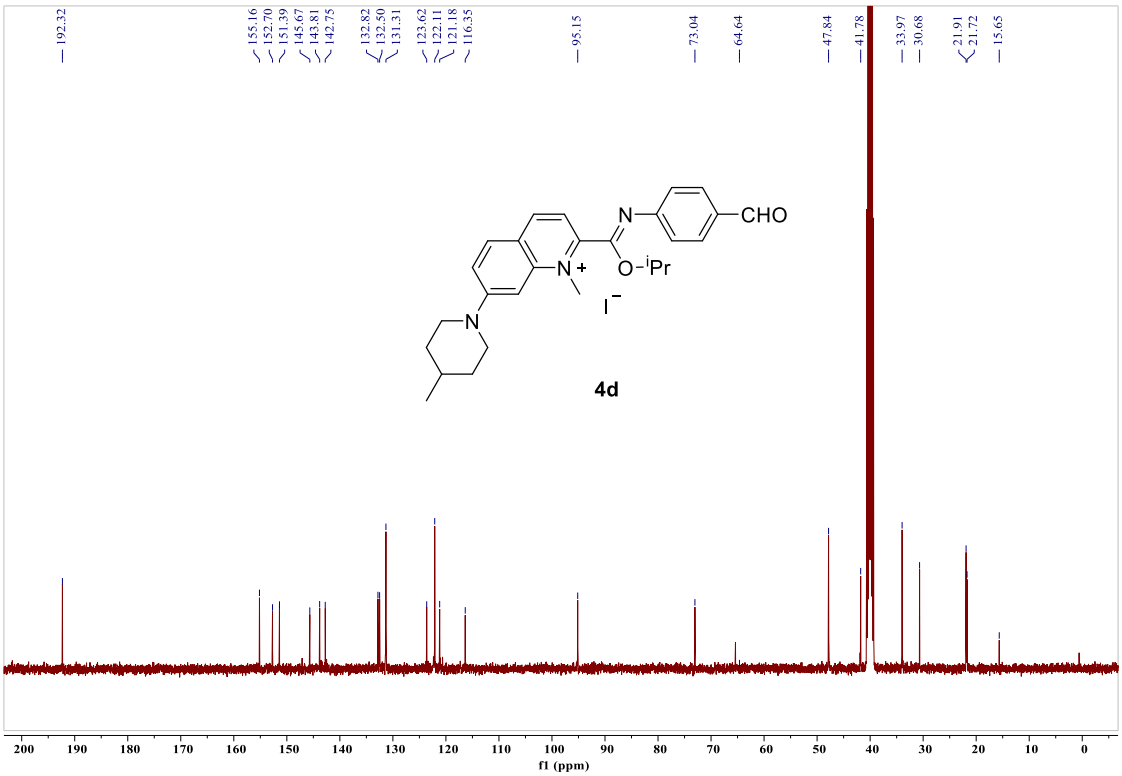
8.6253
8.0264
8.0024
7.8275
7.8219
7.8034
7.7984
7.7448
7.7238
7.5217
7.5020
7.1187
7.0977
7.0205
7.0152
4.3653
4.3311
4.2684
3.2094
3.1771
3.1469
1.8044
1.7781
1.5039
1.4888
1.2292
1.2185
1.1851
1.1554
0.9449
0.9298
N
CHO
N+
O-iPr
I−
N
4d
0.946
1.000
1.328
1.212
2.021
1.001
2.112
1.014
2.212
2.900
2.431
4.004
6.086
2.398
3.381
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)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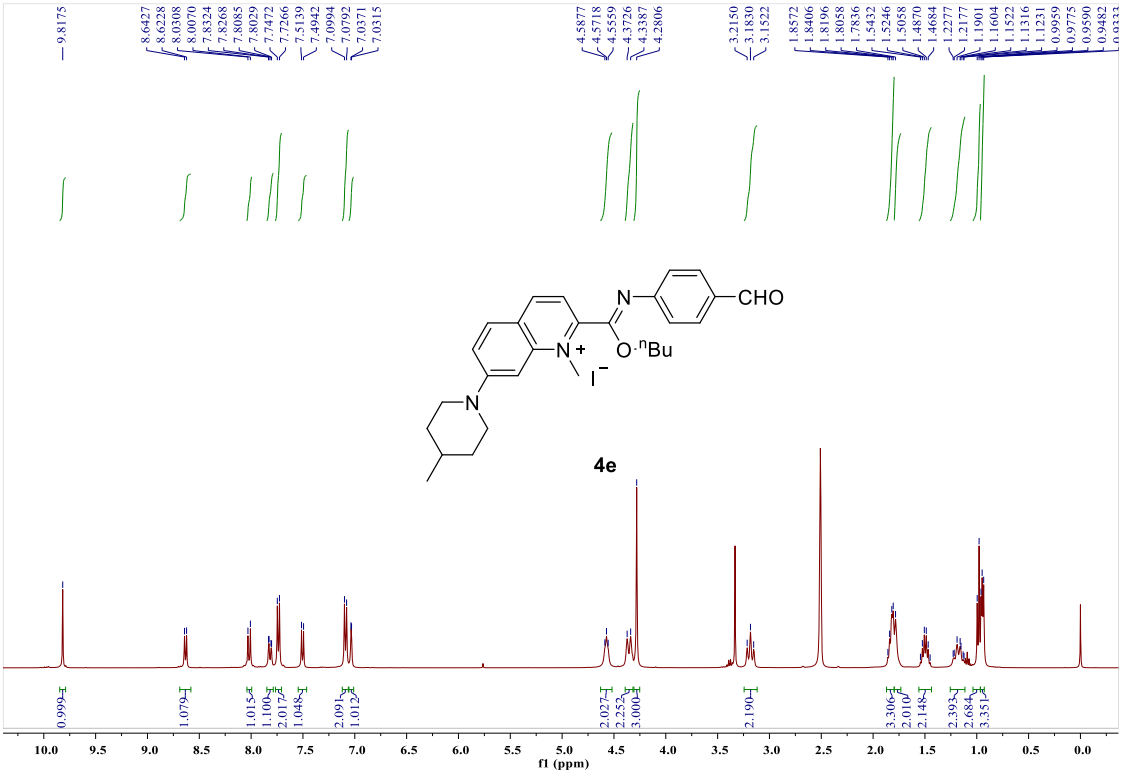
152.70
151.39
145.67
143.81
142.75
132.82
132.50
131.31
123.62
122.11
121.18
116.35
95.15
73.04
64.64
47.84
41.78
33.97
30.68
21.91
21.72
15.65
N
CHO
N+
O-iPr
I−
N
4d
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.6228
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8.0070
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7.8268
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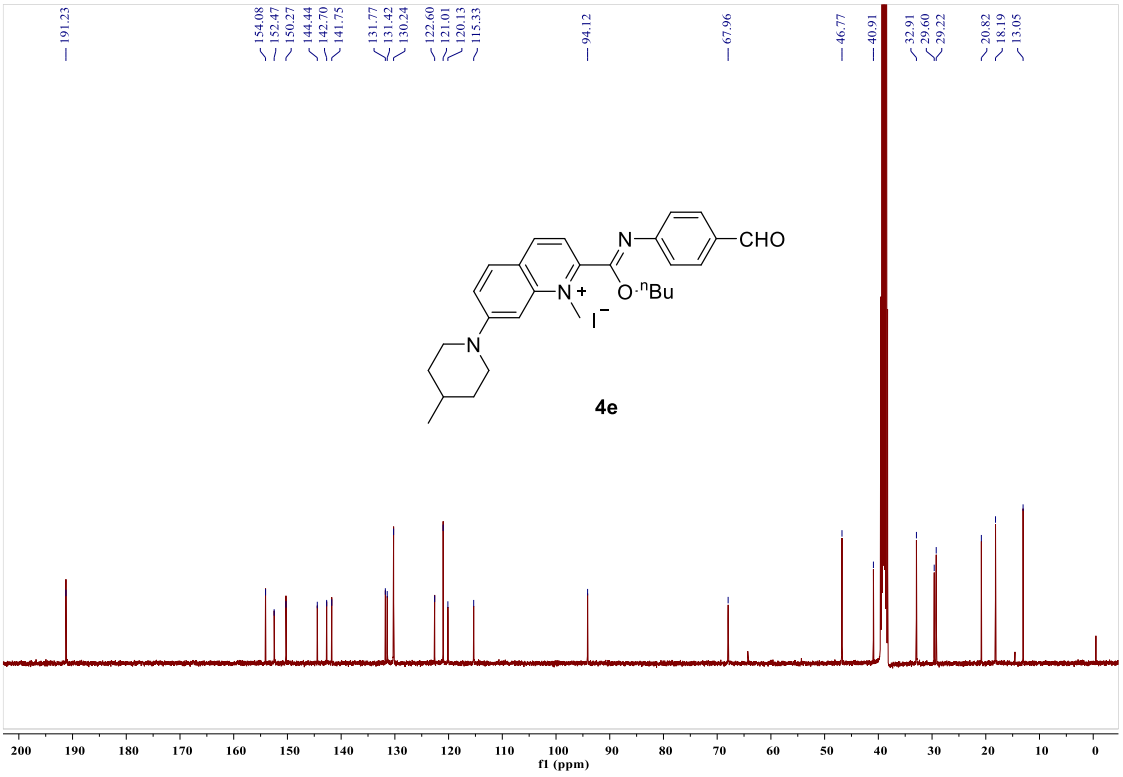
7.8029
7.7472
7.7266
7.5139
7.4942
7.0994
7.0792
7.0371
7.0315
4.5877
4.5718
4.5559
4.3726
4.3387
4.2806
3.2150
3.1830
3.1522
1.8572
1.8406
1.8196
1.8058
1.7836
1.5432
1.5246
1.5058
1.4870
1.4684
1.2277
1.2177
1.1901
1.1604
1.1522
1.1316
1.1231
0.9959
0.9775
0.9590
0.9482
N
CHO
N+
O
nBu
I−
N
4e
0.999
1.079
1.015
1.100
2.017
1.048
2.091
1.012
2.027
2.252
3.000
2.190
3.306
2.010
2.148
2.393
2.684
3.351
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)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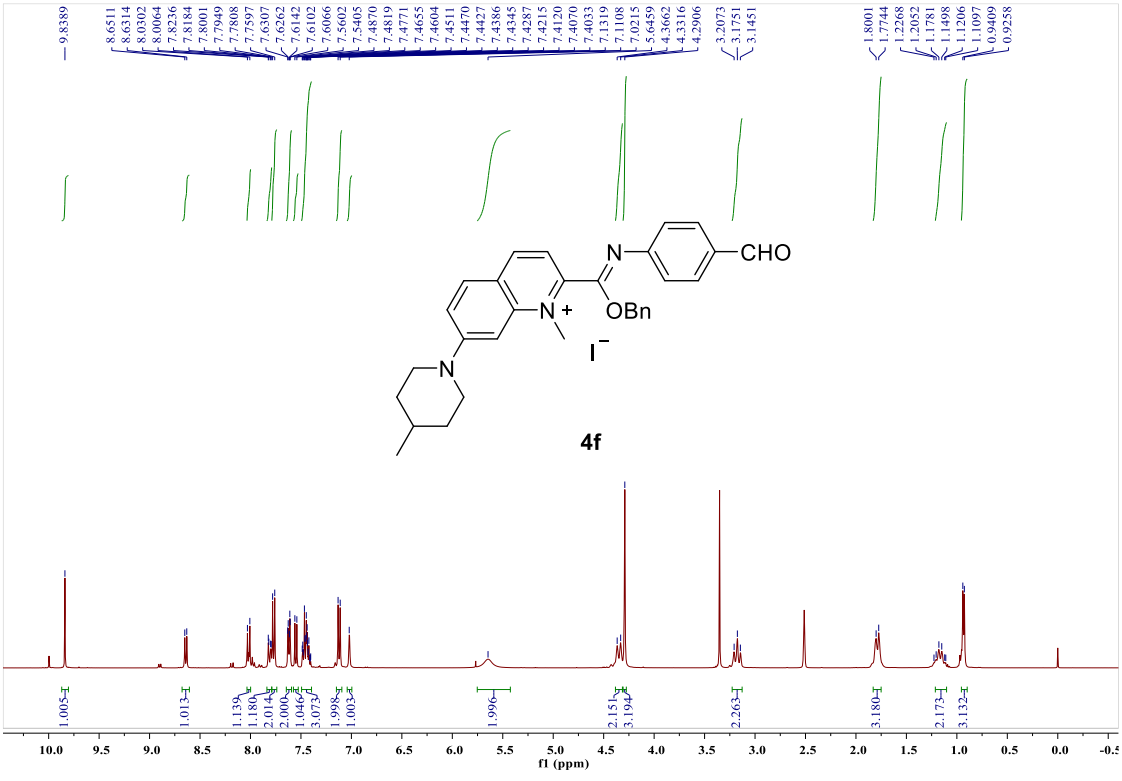
154.08
152.47
150.27
144.44
142.70
141.75
131.77
131.42
130.24
122.60
121.01
120.13
115.33
94.12
67.96
46.77
40.91
32.91
29.60
29.22
20.82
18.19
13.05
N
CHO
N+
O
nBu
I−
N
4e
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.0302
8.0064
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7.7597
7.6307
7.6262
7.6142
7.6102
7.6066
7.5602
7.5405
7.4870
7.4819
7.4771
7.4655
7.4604
7.4511
7.4470
7.4427
7.4386
7.4345
7.4287
7.4215
7.4120
7.4070
7.4033
7.1319
7.1108
7.0215
5.6459
4.3662
4.3316
4.2906
3.2073
3.1751
3.1451
1.8001
1.7744
1.2268
1.2052
1.1781
1.1498
1.1206
1.1097
0.9409
0.9258
CHO
N
N+
OBn
I−
N
4f
1.005
1.013
1.139
1.180
2.014
2.000
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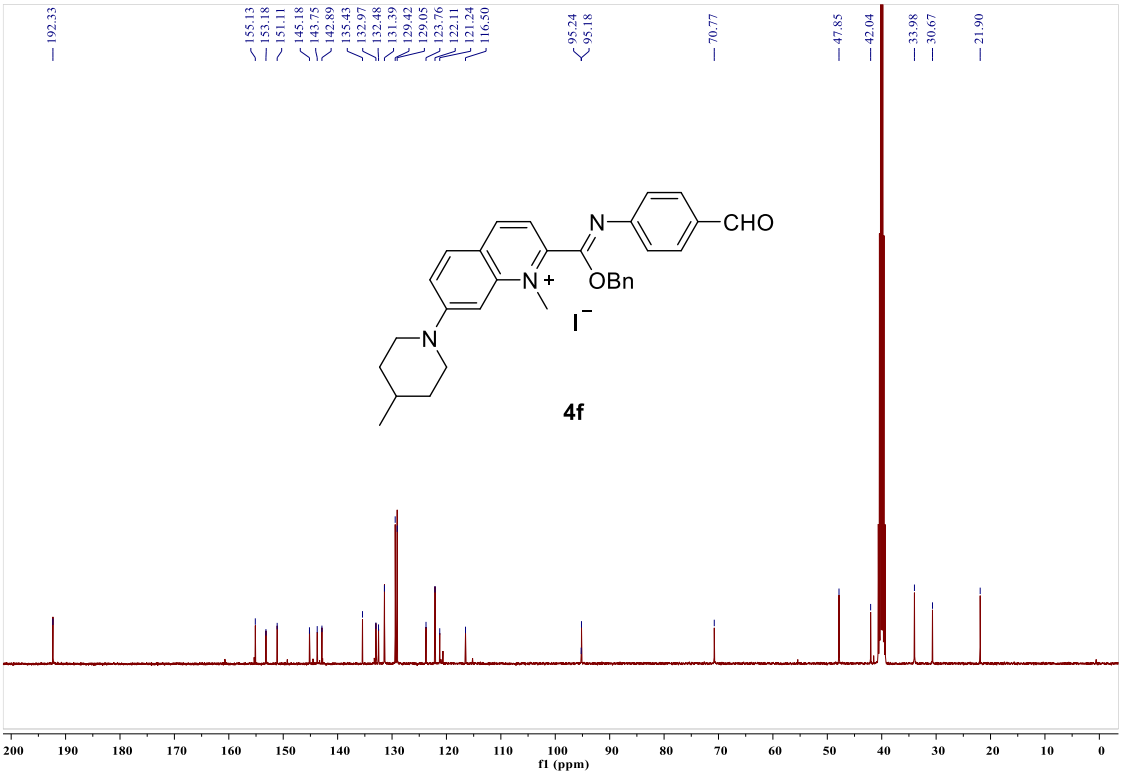
1.003
1.996
2.151
3.194
2.263
3.180
2.173
3.132
f1 (ppm)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142.89
135.43
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132.48
131.39
129.42
129.05
123.76
122.11
121.24
116.50
95.24
95.18
70.77
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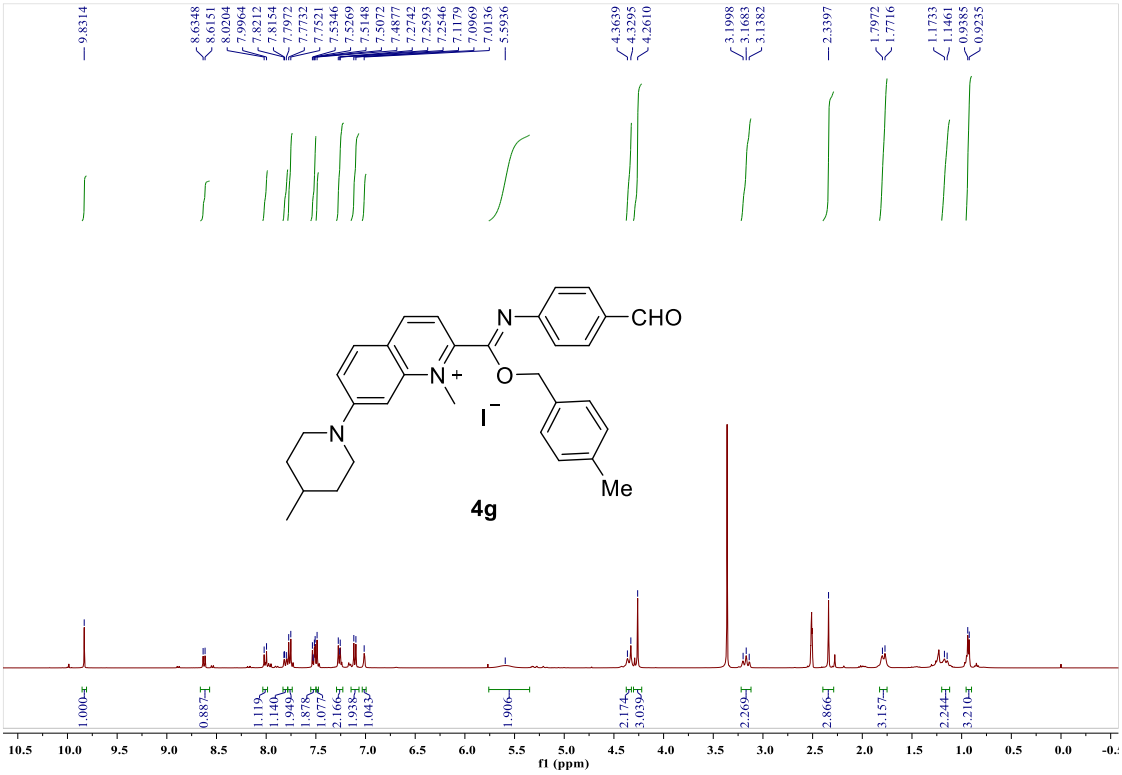
33.98
30.67
21.90
CHO
N
N+
OBn
I−
N
4f
f1 (ppm)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7.7521
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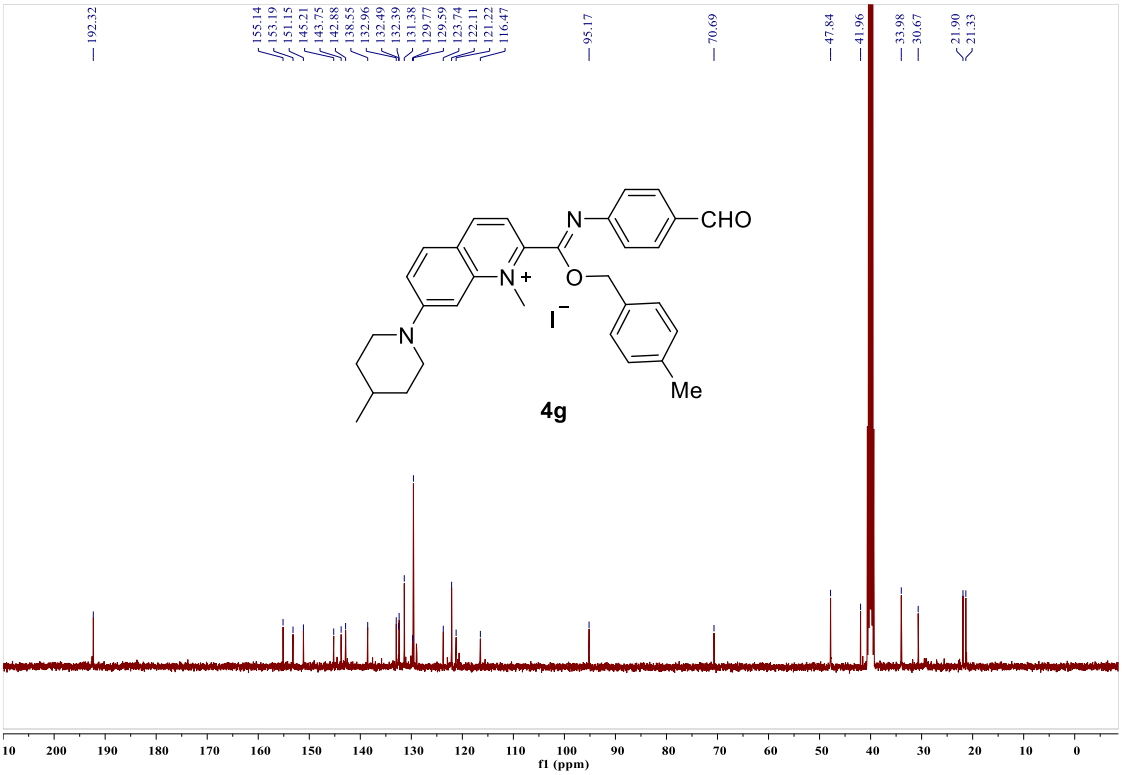
7.5269
7.5148
7.5072
7.4877
7.2742
7.2593
7.2546
7.1179
7.0969
7.0136
5.5936
4.3639
4.3295
4.2610
3.1998
3.1683
3.1382
2.3397
1.7972
1.7716
1.1733
1.1461
0.9385
0.9235
N
CHO
N+
O
I−
N
Me
4g
1.000
0.887
1.119
1.140
1.949
1.878
1.077
2.166
1.938
1.043
1.906
2.174
3.039
2.269
2.866
3.157
2.244
3.210
10.5 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)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142.88
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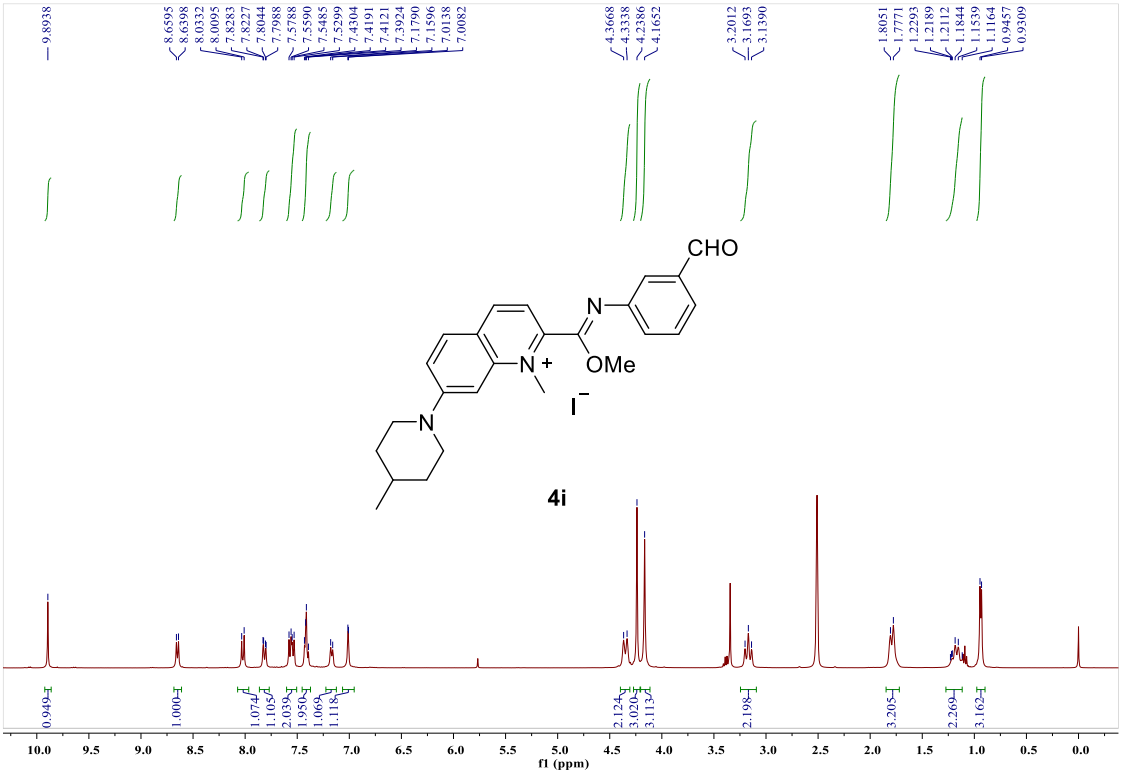
132.96
132.49
132.39
131.38
129.77
129.59
123.74
122.11
121.22
116.47
95.17
70.69
47.84
41.96
33.98
30.67
21.90
21.33
N
CHO
N+
O
I−
N
Me
4g
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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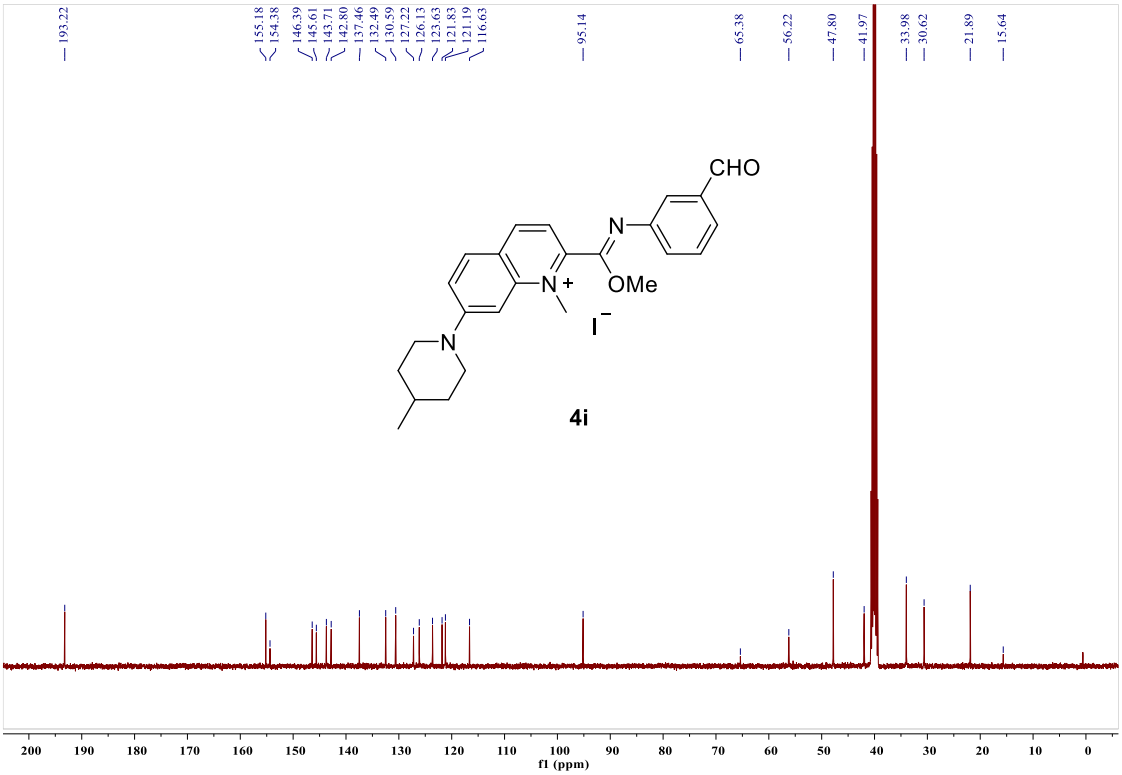
7.5590
7.5485
7.5299
7.4304
7.4191
7.4121
7.3924
7.1790
7.1596
7.0138
7.0082
4.3668
4.3338
4.2386
4.1652
3.2012
3.1693
3.1390
1.8051
1.7771
1.2293
1.2189
1.2112
1.1844
1.1539
1.1164
0.9457
0.9309
CHO
N
N+
OMe
I−
N
4i
0.949
1.000
1.074
1.105
2.039
1.950
1.069
1.118
2.124
3.020
3.113
2.198
3.205
2.269
3.162
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)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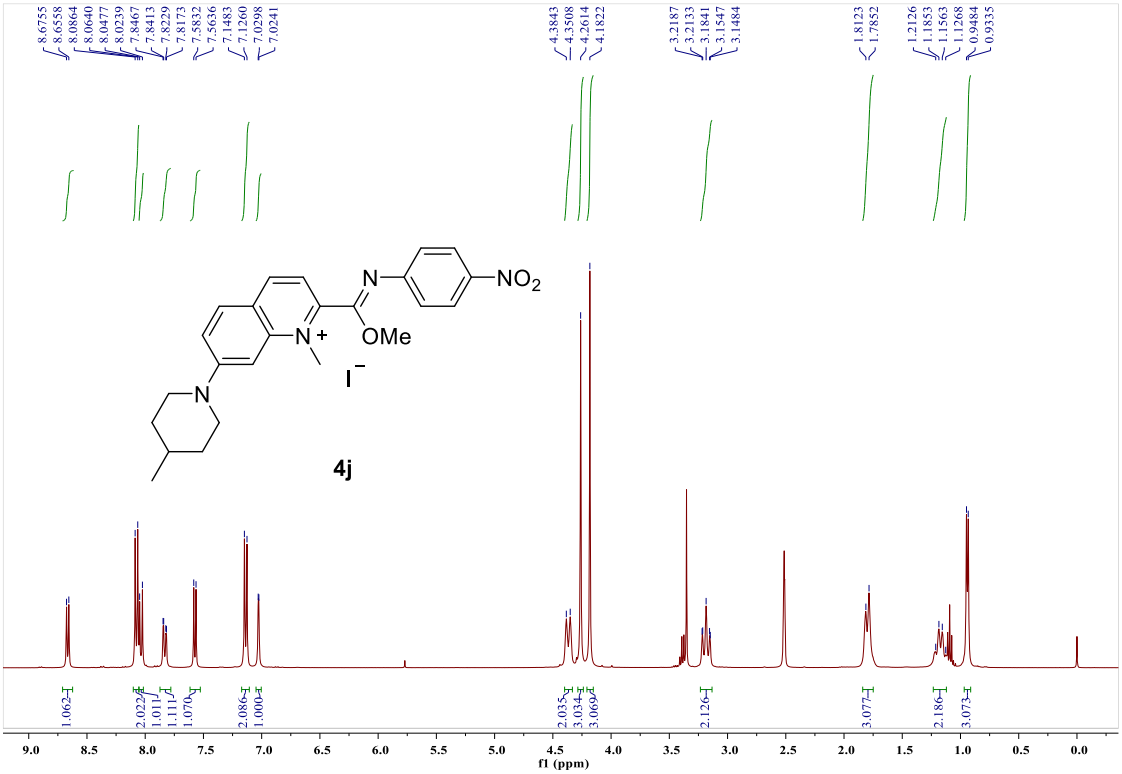
127.22
126.13
123.63
121.83
121.19
116.63
95.14
65.38
56.22
47.80
41.97
33.98
30.62
21.89
15.64
CHO
N
N+
OMe
I−
N
4i
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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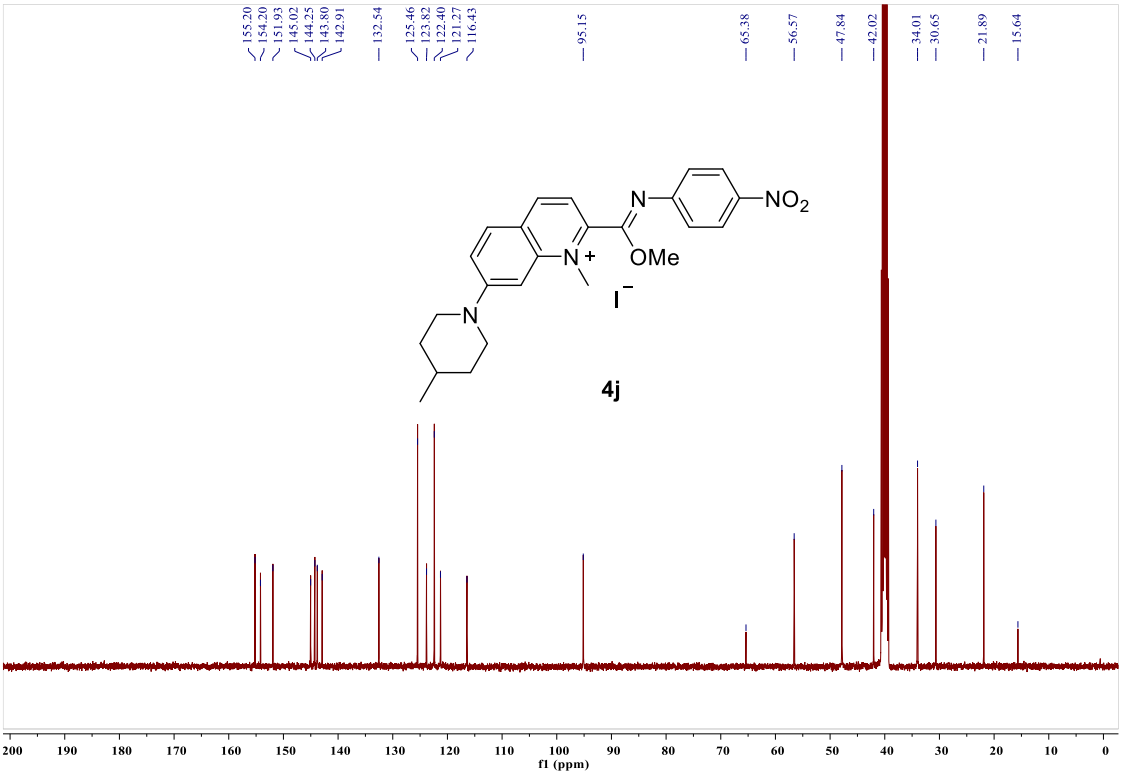
7.8467
7.8413
7.8229
7.8173
7.5832
7.5636
7.1483
7.1260
7.0298
7.0241
4.3843
4.3508
4.2614
4.1822
3.2187
3.2133
3.1841
3.1547
3.1484
1.8123
1.7852
1.2126
1.1853
1.1563
1.1268
0.9484
0.9335
N
NO2
N+
OMe
I−
N
4j
1.062
2.022
1.011
1.111
1.070
2.086
1.000
2.035
3.034
3.069
2.126
3.077
2.186
3.073
9.0 8.5 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)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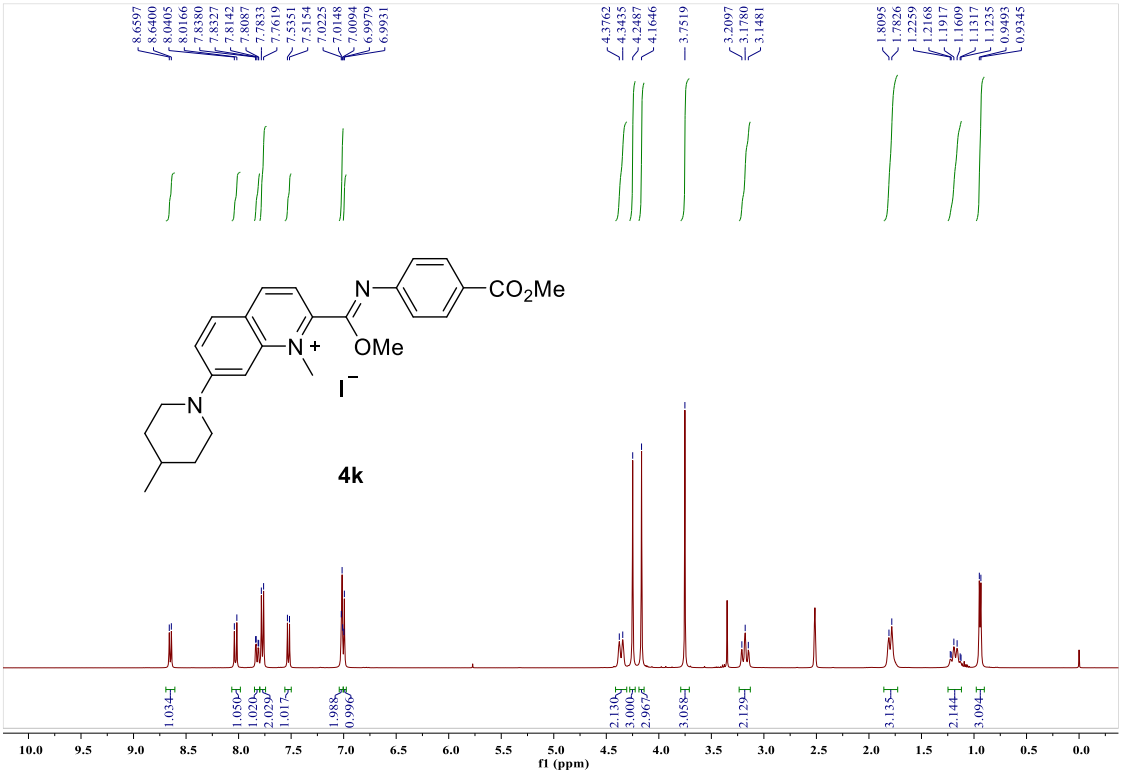
142.91
132.54
125.46
123.82
122.40
121.27
116.43
95.15
65.38
56.57
47.84
42.02
34.01
30.65
21.89
15.64
N
NO2
N+
OMe
I−
N
4j
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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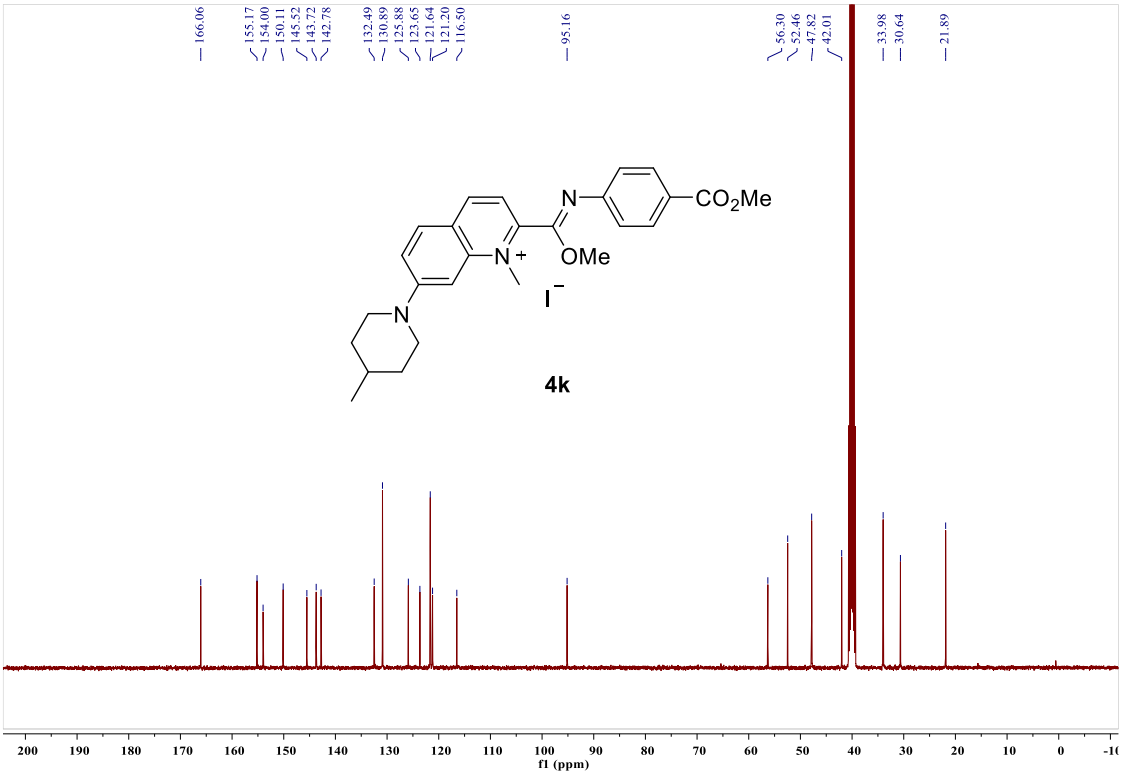
7.5154
7.0225
7.0148
7.0094
6.9979
6.9931
4.3762
4.3435
4.2487
4.1646
3.7519
3.2097
3.1780
3.1481
1.8095
1.7826
1.2259
1.2168
1.1917
1.1609
1.1317
1.1235
0.9493
0.9345
N
CO2Me
N+
OMe
I−
N
4k
1.034
1.050
1.020
2.029
1.017
1.988
0.996
2.130
3.000
2.967
3.058
2.129
3.133
2.144
3.094
10.0 9.5 9.0 8.5 8.0 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)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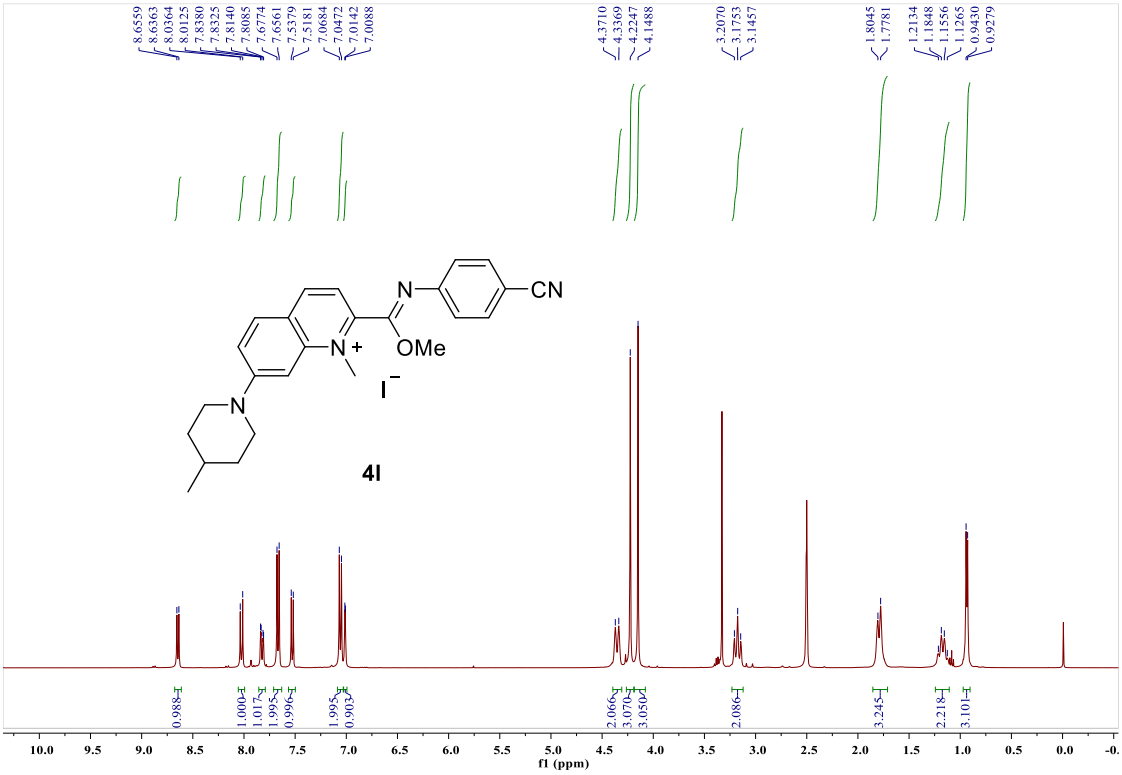
125.88
123.65
121.64
121.20
116.50
95.16
56.30
52.46
47.82
42.01
33.98
30.64
21.89
N
CO2Me
N+
OMe
I−
N
4k
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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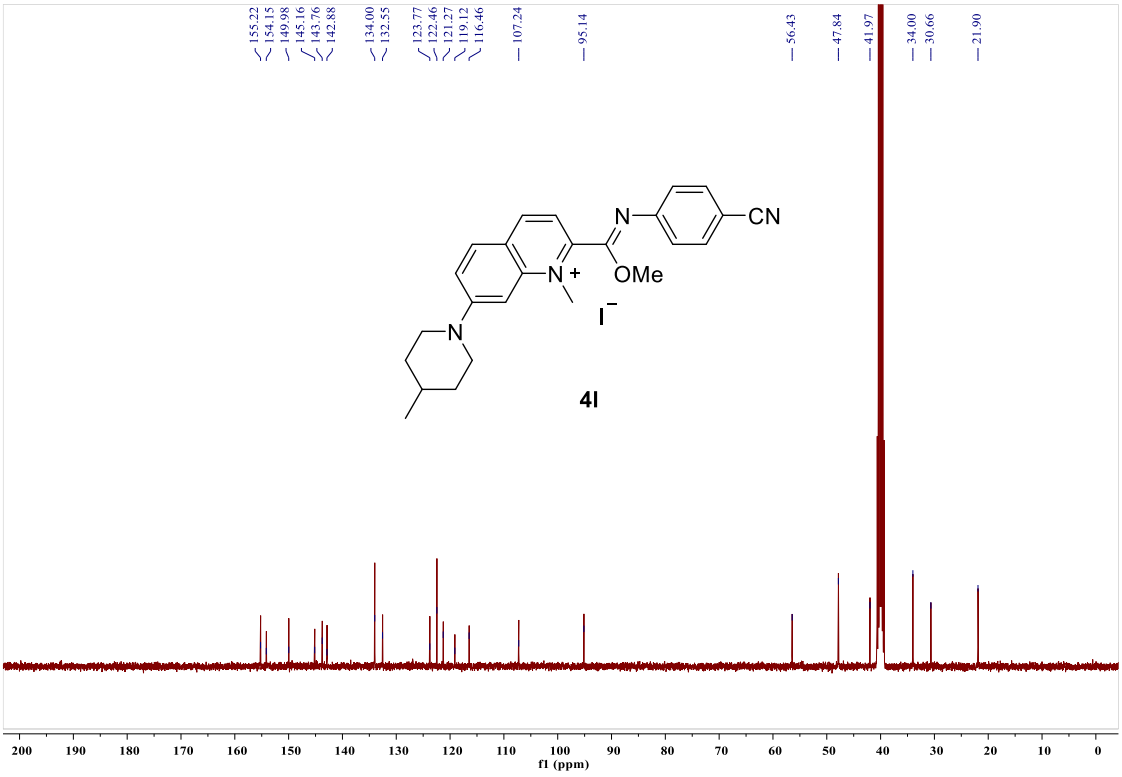
7.0684
7.0472
7.0142
7.0088
4.3710
4.3369
4.2247
4.1488
3.2070
3.1753
3.1457
1.8045
1.7781
1.2134
1.1848
1.1556
1.1265
0.9430
0.9279
N
CN
N+
OMe
I−
N
4l
0.988
1.000
1.017
1.995
0.996
1.995
0.903
2.066
3.070
3.050
2.086
3.245
2.218
3.101
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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121.27
119.12
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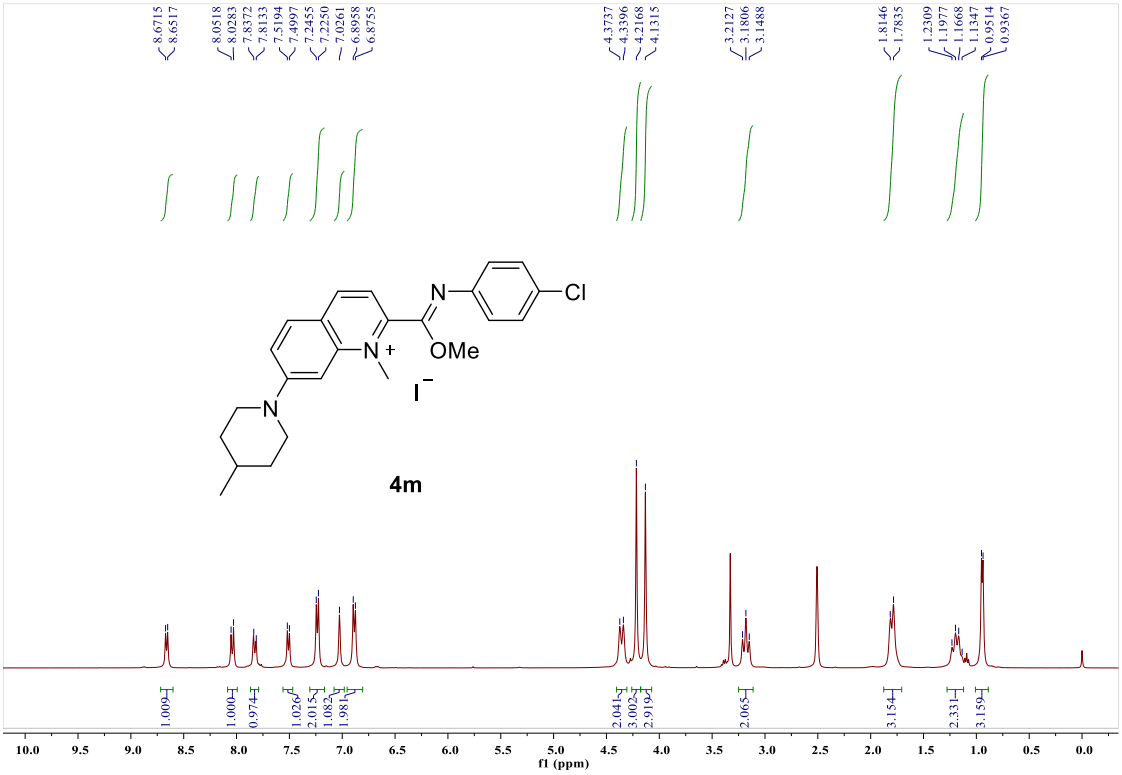
107.24
95.14
56.43
47.84
41.97
34.00
30.66
21.90
N
CN
N+
OMe
I−
N
4l
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.0261
6.8958
6.8755
4.3737
4.3396
4.2168
4.1315
3.2127
3.1806
3.1488
1.8146
1.7835
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1.1977
1.1668
1.1347
0.9514
0.9367
N
Cl
N+
OMe
I−
N
4m
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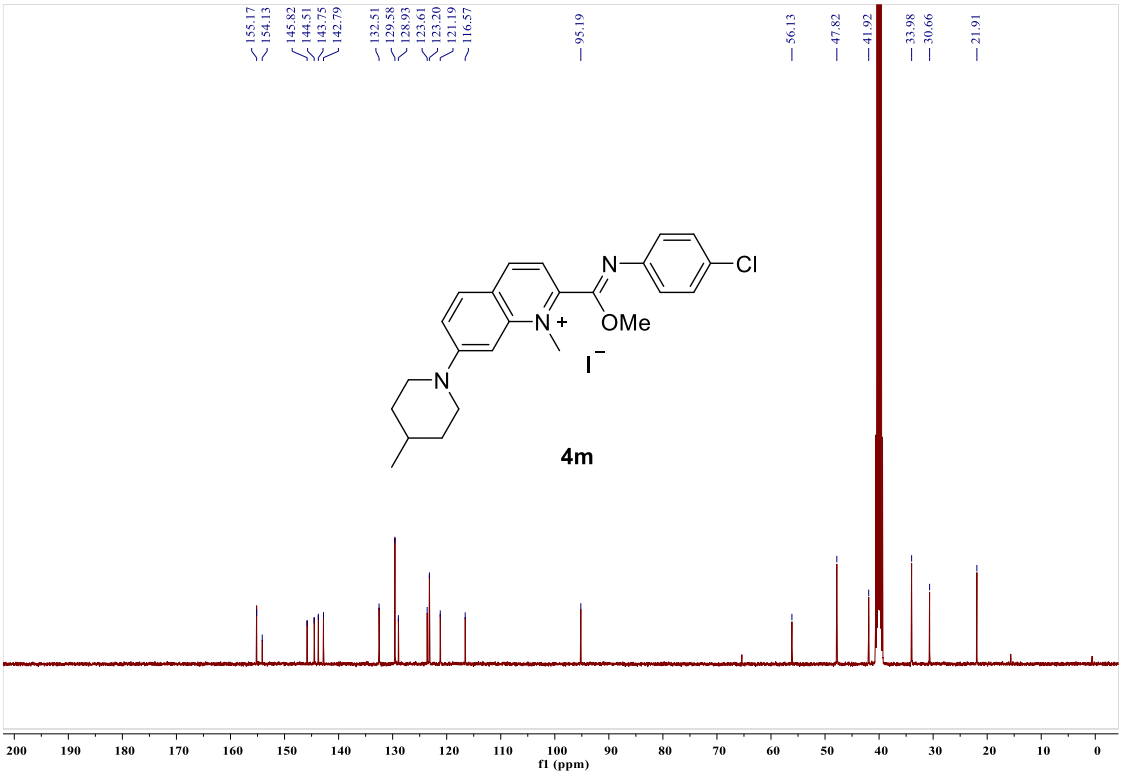
1.000
0.974
1.026
2.015
1.082
1.981
2.041
3.002
2.919
2.065
3.154
2.331
3.159
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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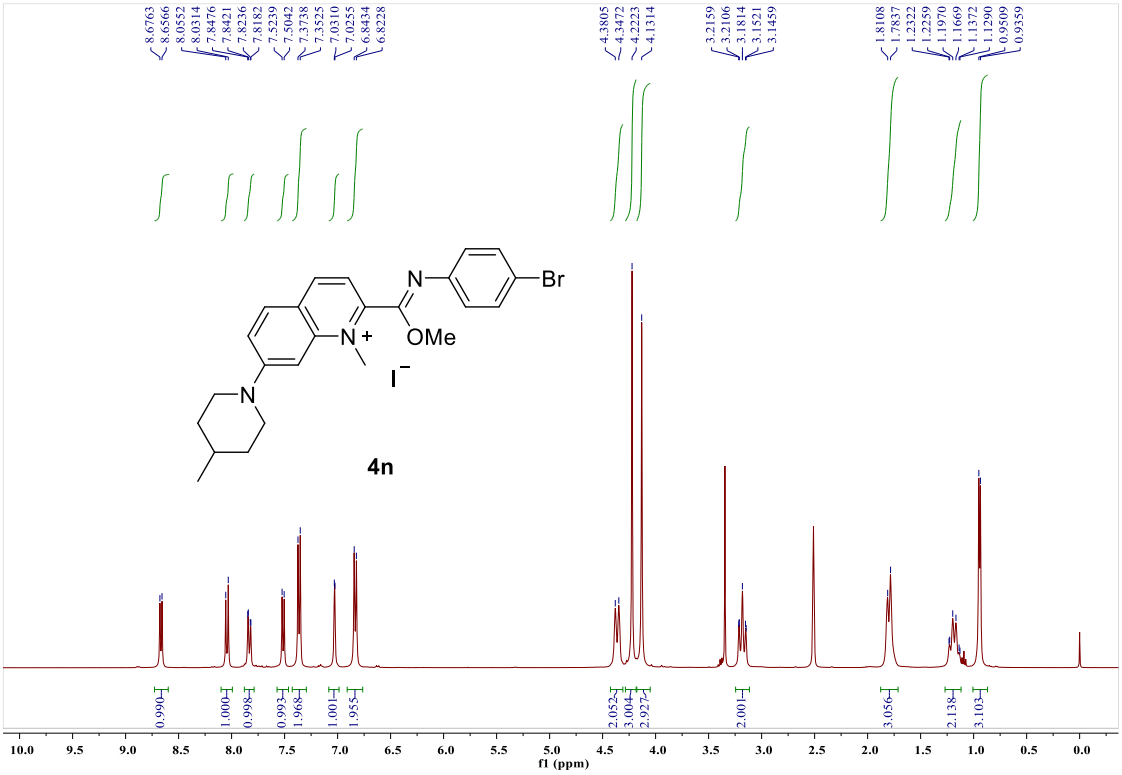
123.61
123.20
121.19
116.57
95.19
56.13
47.82
41.92
33.98
30.66
21.91
N
Cl
N+
OMe
I−
N
4m
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.3738
7.3525
7.0310
7.0255
6.8434
6.8228
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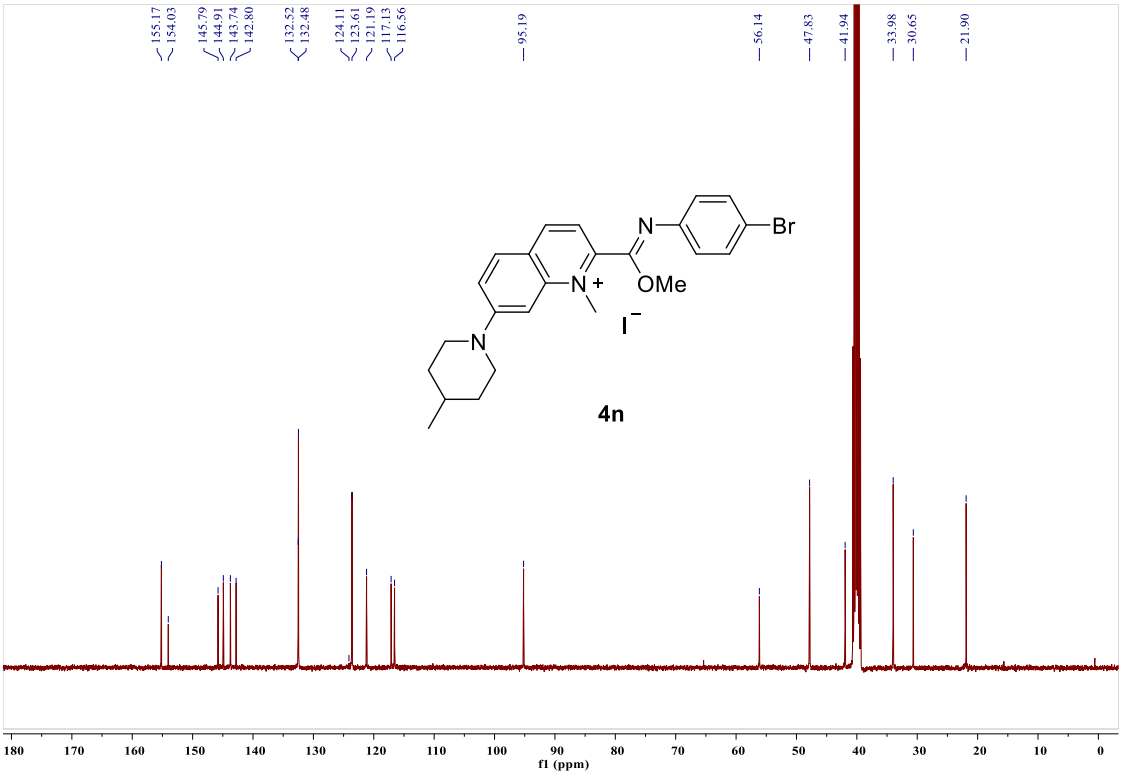
4.3472
4.2223
4.1314
3.2159
3.2106
3.1814
3.1521
3.1459
1.8108
1.7837
1.2322
1.2259
1.1970
1.1669
1.1372
1.1290
0.9509
0.9359
N
Br
N+
OMe
I−
N
4n
0.990
1.000
0.998
0.993
1.968
1.001
1.955
2.052
3.004
2.927
2.001
3.056
2.138
3.103
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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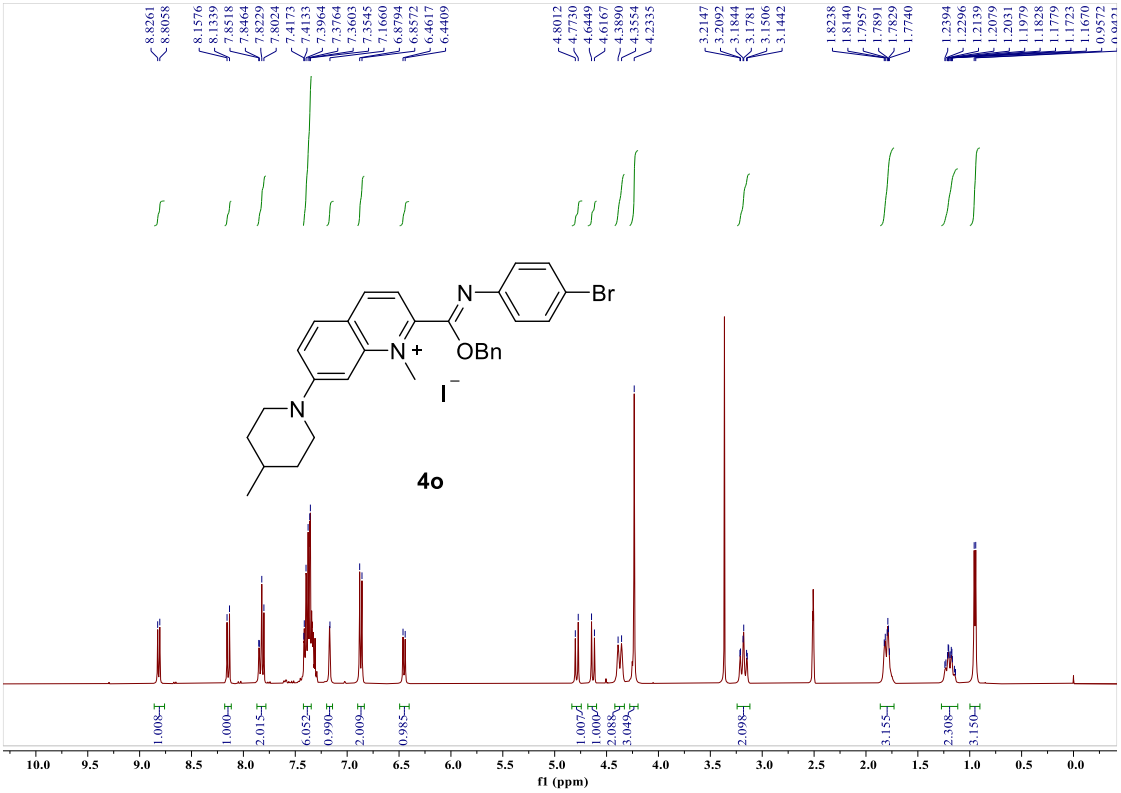
123.61
121.19
117.13
116.56
95.19
56.14
47.83
41.94
33.98
30.65
21.90
N
Br
N+
OMe
I−
N
4n
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.3545
7.1660
6.8794
6.8572
6.4617
6.4409
4.8012
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4.6449
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4.3890
4.3554
4.2335
3.2147
3.2092
3.1844
3.1781
3.1506
3.1442
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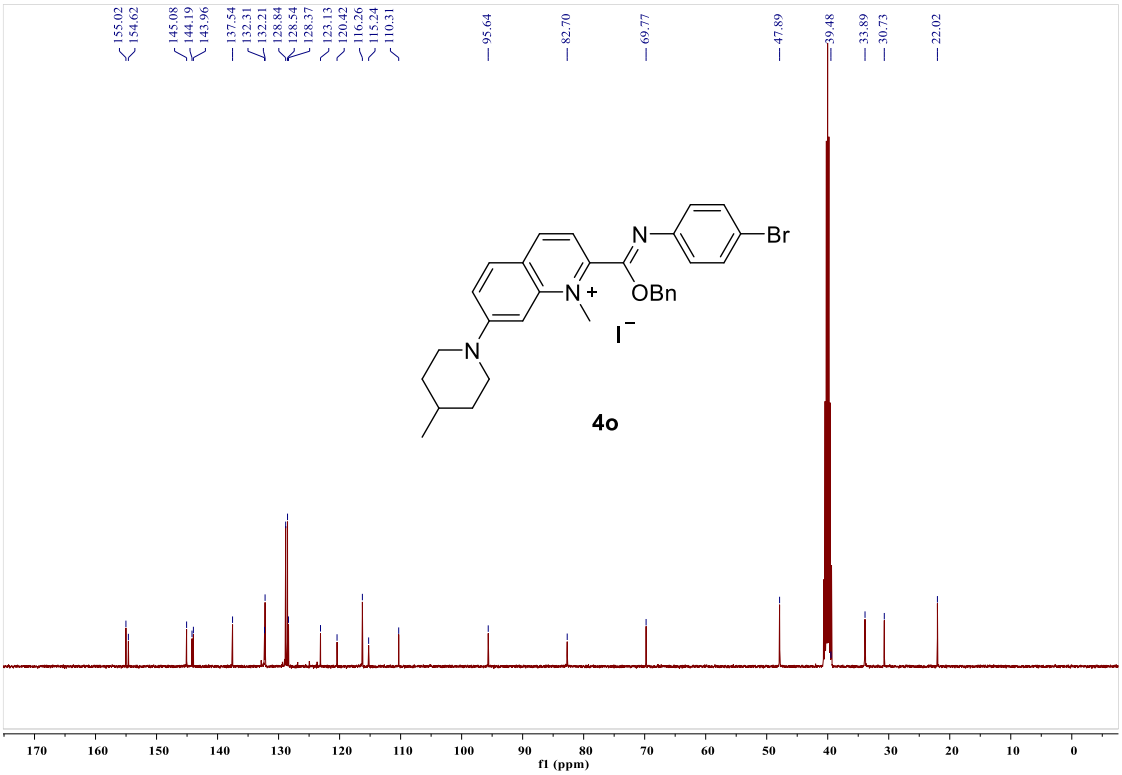
1.8140
1.7957
1.7891
1.7829
1.7740
1.2394
1.2296
1.2139
1.2079
1.2031
1.1979
1.1828
1.1779
1.1723
1.1670
0.9572
N
Br
N+
OBn
I−
N
4o
1.008
1.000
2.015
6.052
0.990
2.009
0.985
1.007
1.000
2.088
3.049
2.098
3.155
2.308
3.150
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.54
128.37
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116.26
115.24
110.31
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82.70
69.77
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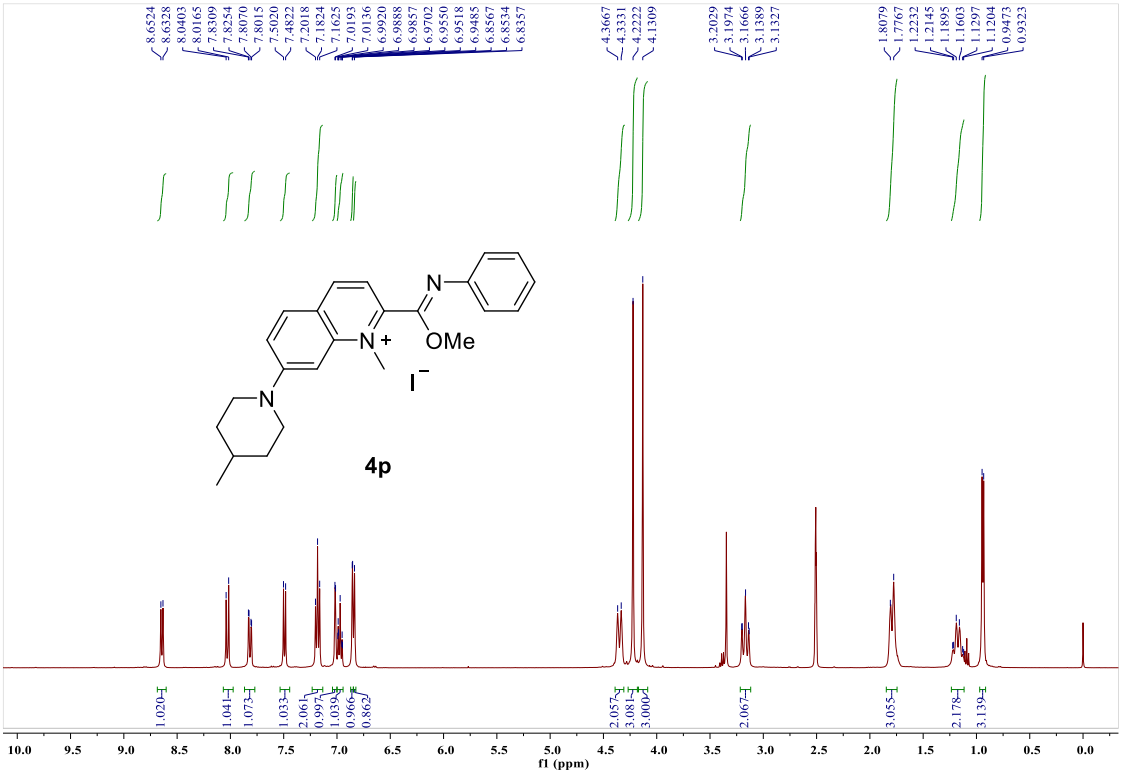
39.48
33.89
30.73
22.02
N
Br
N+
OBn
I−
N
4o
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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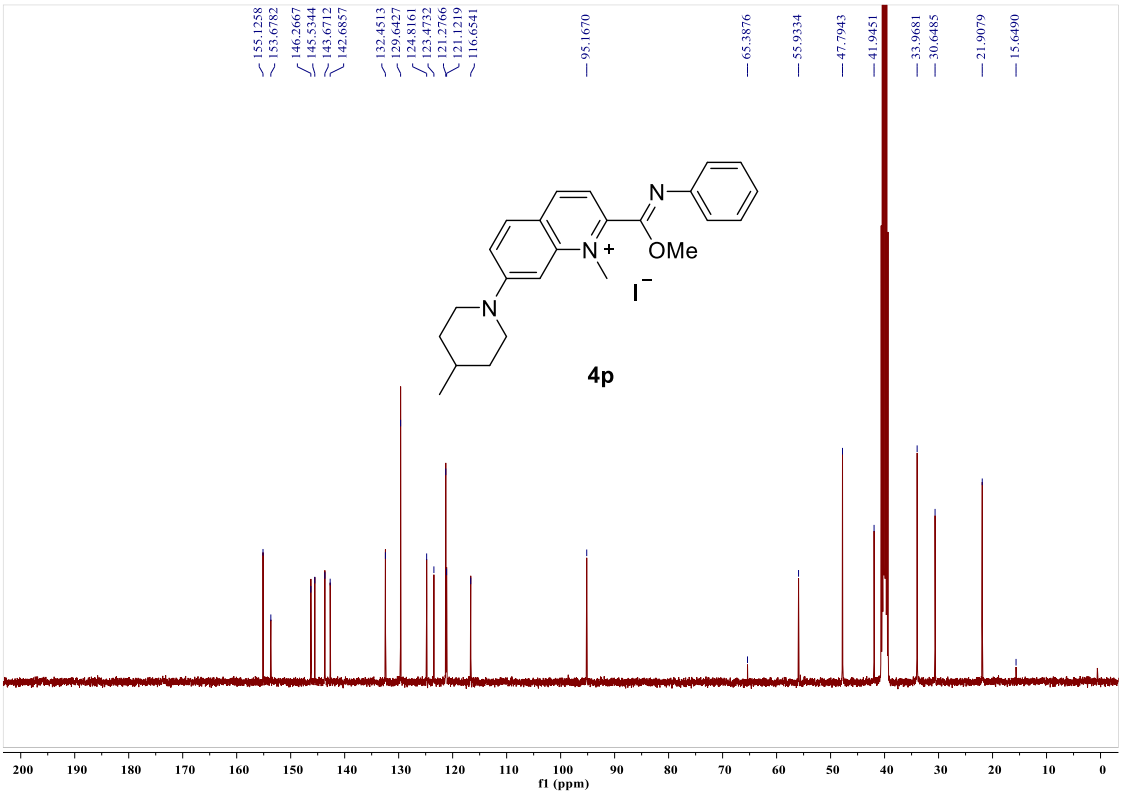
7.1824
7.1625
7.0193
7.0136
6.9920
6.9888
6.9857
6.9702
6.9550
6.9518
6.9485
6.8567
6.8534
6.8357
4.3667
4.3331
4.2222
4.1309
3.2029
3.1974
3.1666
3.1389
3.1327
1.8079
1.7767
1.2232
1.2145
1.1895
1.1603
1.1297
1.1204
0.9473
0.9323
N
N+
OMe
I−
N
4p
1.020
1.041
1.073
1.033
2.061
0.997
1.039
0.966
0.862
2.057
3.081
3.000
2.067
3.055
2.178
3.139
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)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116.6541
95.1670
65.3876
55.9334
47.7943
41.9451
33.9681
30.6485
21.9079
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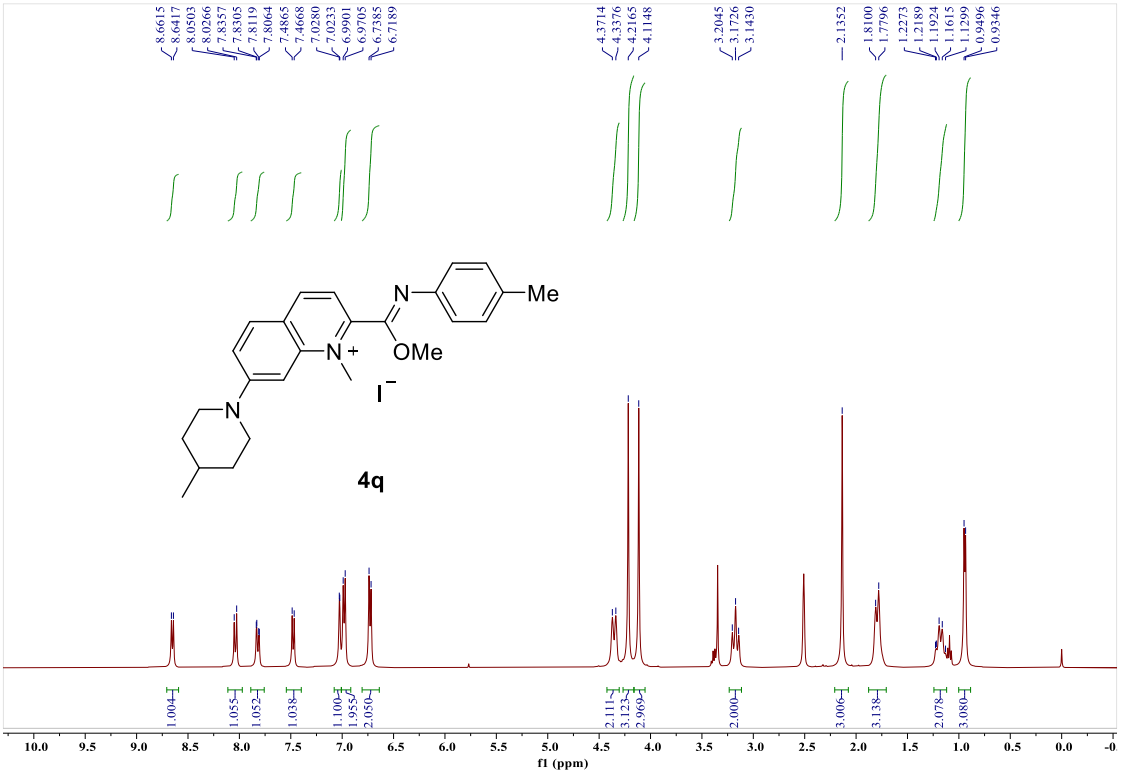
N
N+
OMe
I−
N
4p
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.0233
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6.9705
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6.7189
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4.3376
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4.1148
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3.1726
3.1430
2.1352
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1.7796
1.2273
1.2189
1.1924
1.1615
1.1299
0.9496
0.9346
N
Me
N+
OMe
I−
N
4q
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1.055
1.052
1.038
1.100
1.955
2.050
2.111
3.123
2.969
2.000
3.006
3.138
2.078
3.080
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
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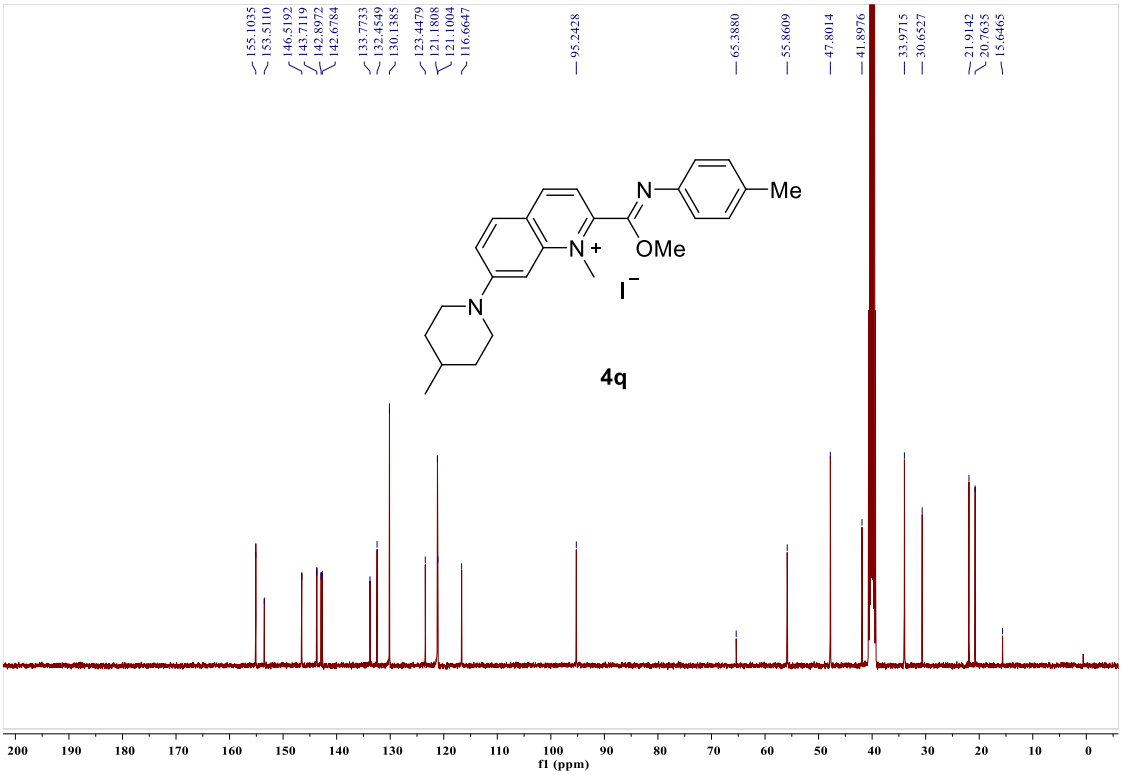
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41.8976
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30.6527
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20.7635
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N+
OMe
I−
N
4q
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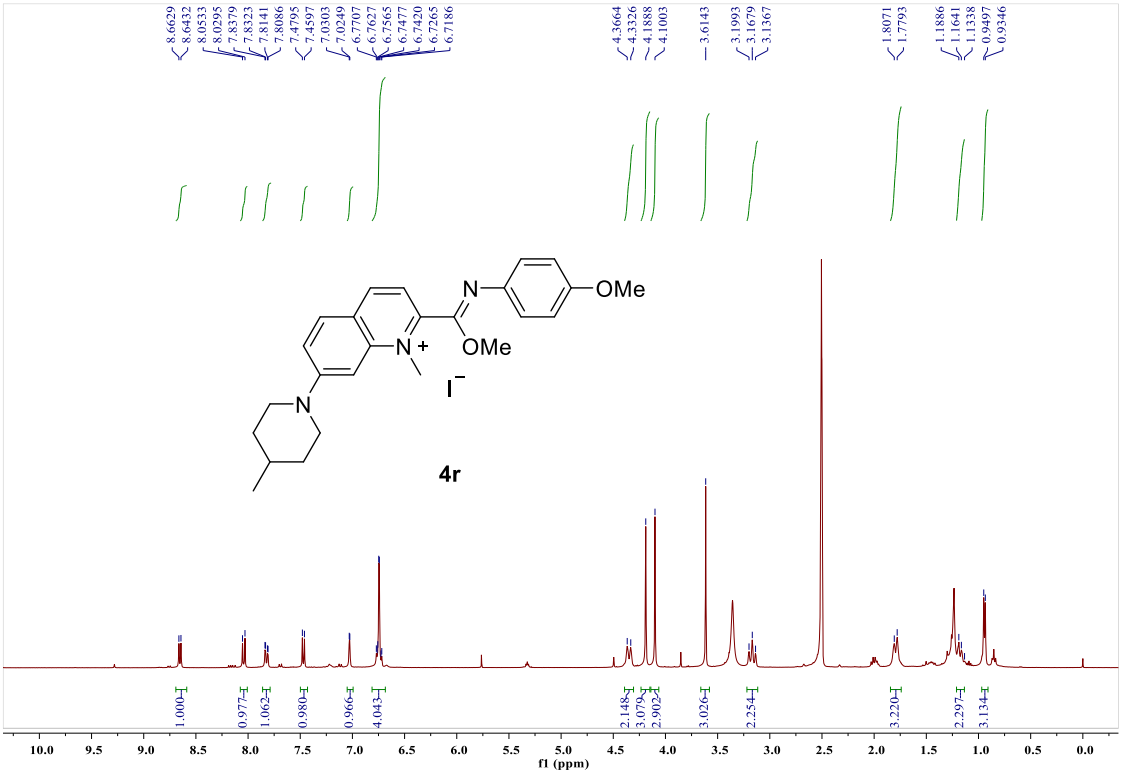
f1 (ppm)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7.0249
6.7707
6.7627
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6.7420
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6.7186
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4.3326
4.1888
4.1003
3.6143
3.1993
3.1679
3.1367
1.8071
1.7793
1.1886
1.1641
1.1338
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N
OMe
N+
OMe
I−
N
4r
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1.062
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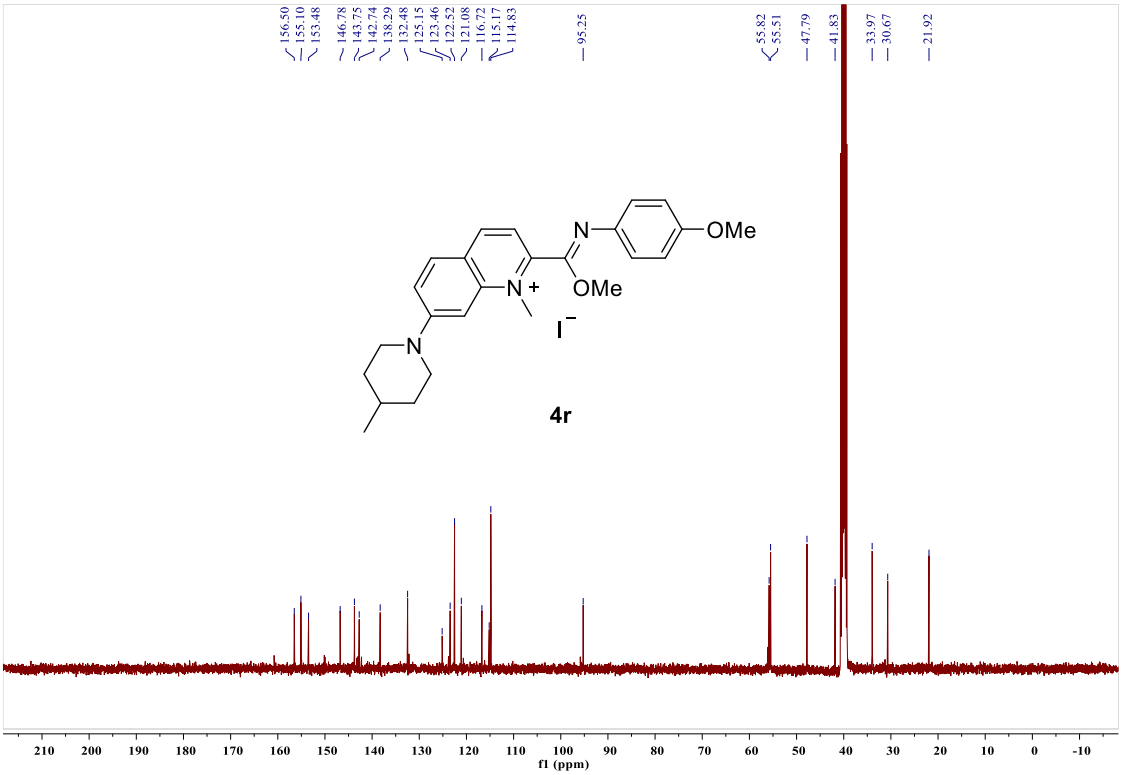
f1 (ppm)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114.83
95.25
55.82
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21.92
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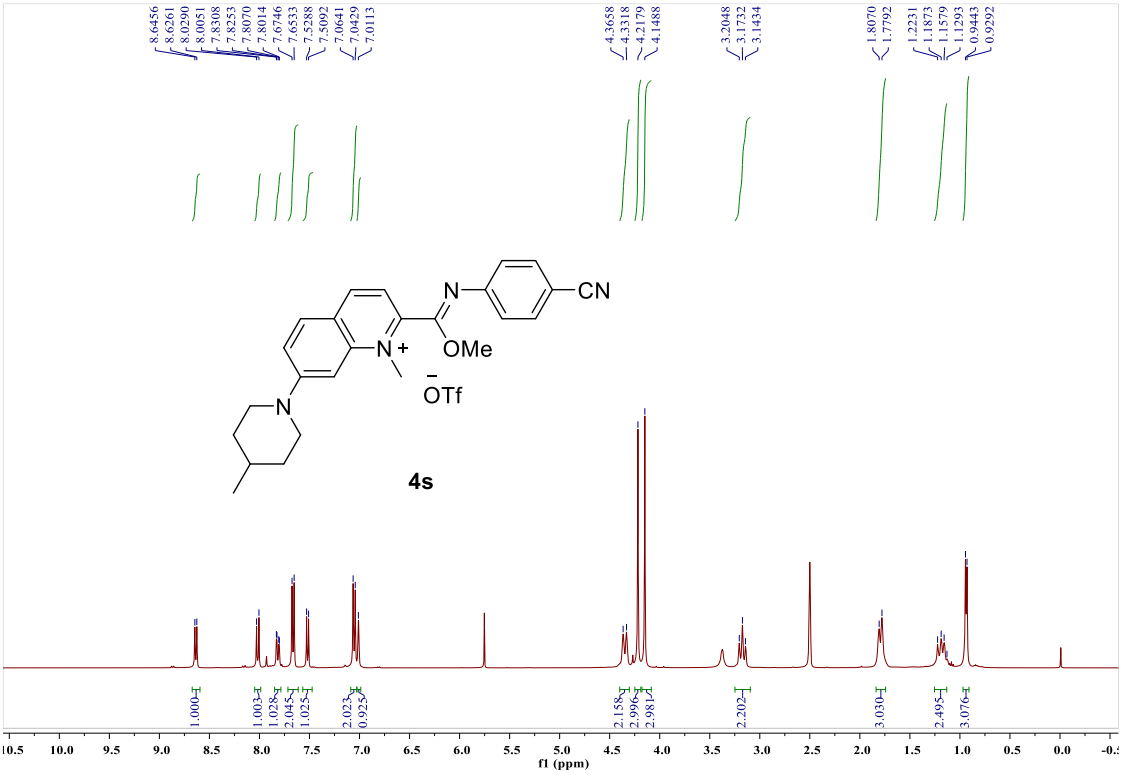
OMe
N+
OMe
I−
N
4r
f1 (ppm)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4.1488
3.2048
3.1732
3.1434
1.8070
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1.2231
1.1873
1.1579
1.1293
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0.9292
N
CN
N+
OMe
OTf
N
4s
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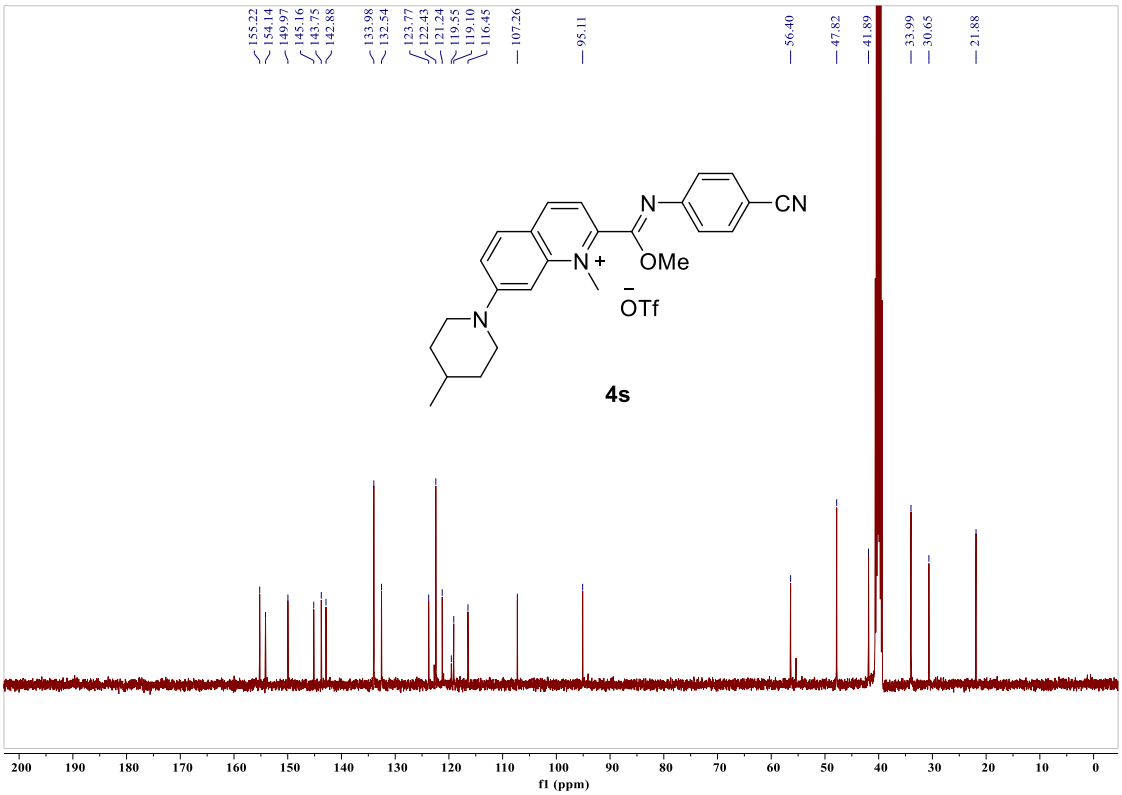
f1 (ppm)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121.24
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116.45
107.26
95.11
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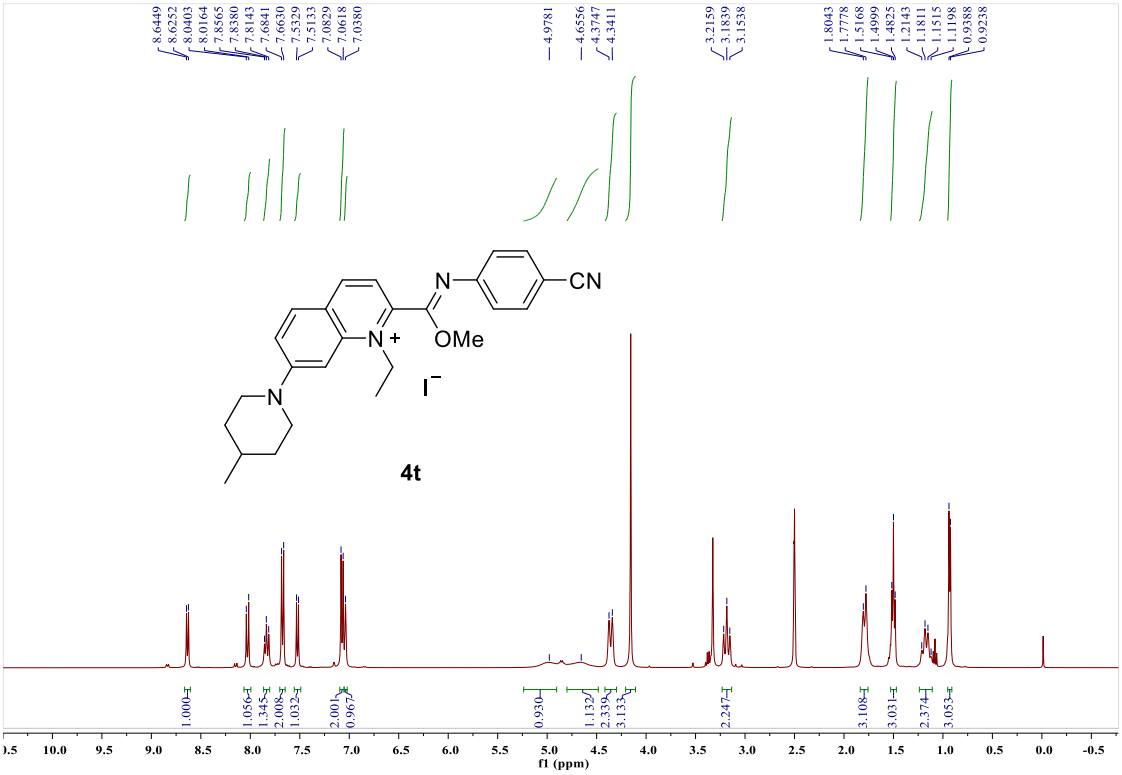
33.99
30.65
21.88
N
CN
N+
OMe
OTf
N
4s
f1 (ppm)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7.0618
7.0380
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4.3411
3.2159
3.1839
3.1538
1.8043
1.7778
1.5168
1.4999
1.4825
1.2143
1.1811
1.1515
1.1198
0.9388
0.9238
N
CN
N+
OMe
I−
N
4t
1.000
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1.345
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1.032
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2.247
3.108
3.031
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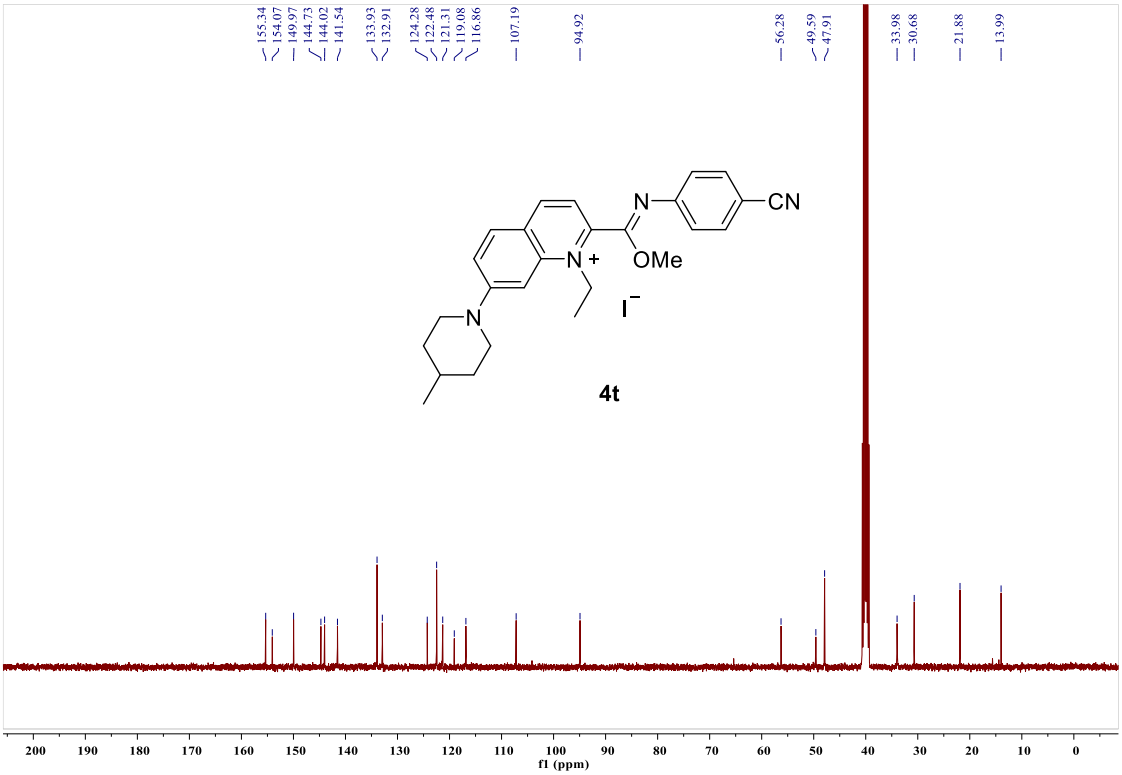
3.053
f1 (ppm)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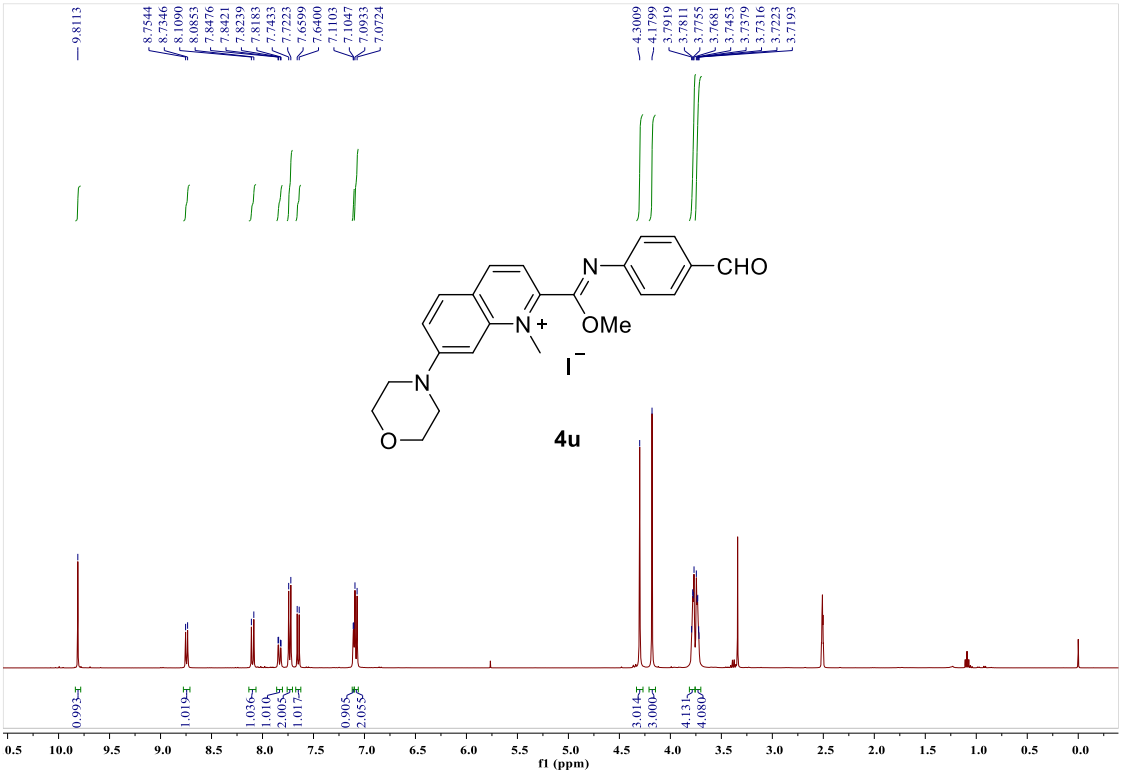
144.02
141.54
133.93
132.91
124.28
122.48
121.31
119.08
116.86
107.19
94.92
56.28
49.59
47.91
33.98
30.68
21.88
13.99
N
CN
N+
OMe
I−
N
4t
f1 (ppm)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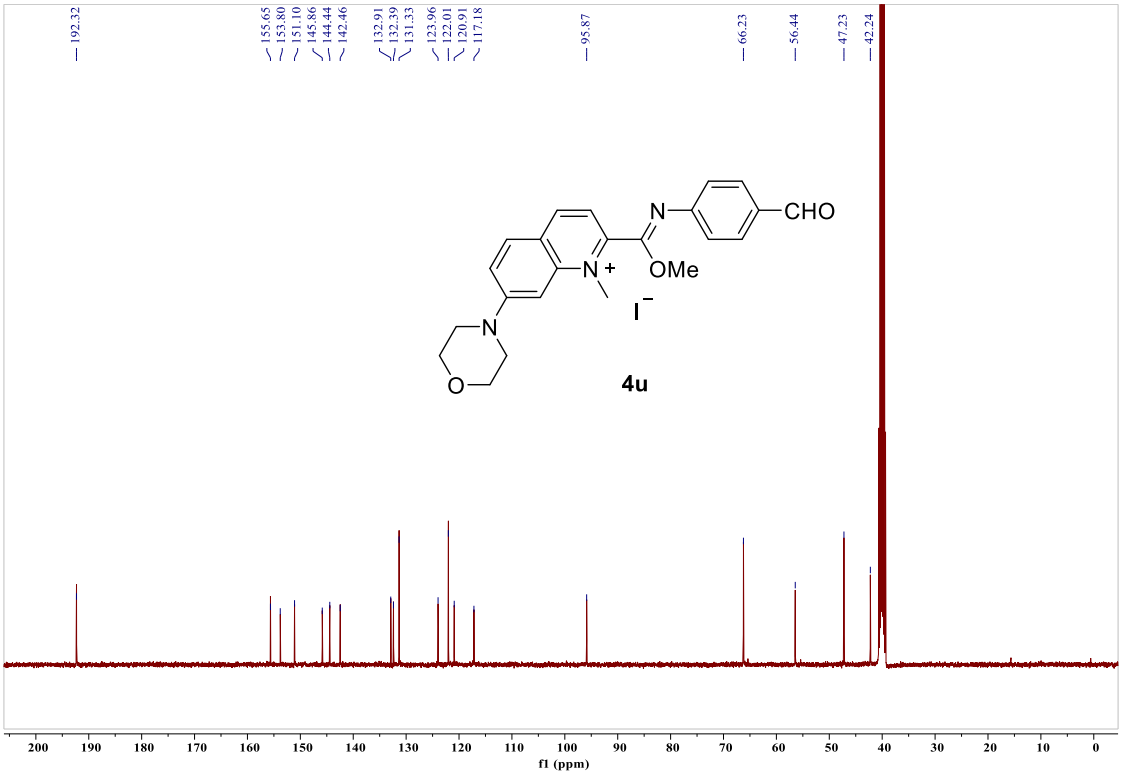
7.6599
7.6400
7.1103
7.1047
7.0933
7.0724
4.3009
4.1799
3.7919
3.7811
3.7755
3.7681
3.7453
3.7379
3.7316
3.7223
3.7193
N
CHO
N+
OMe
I−
N
O
4u
0.993
1.019
1.036
1.010
2.005
1.017
0.905
2.055
3.014
3.000
4.131
4.080
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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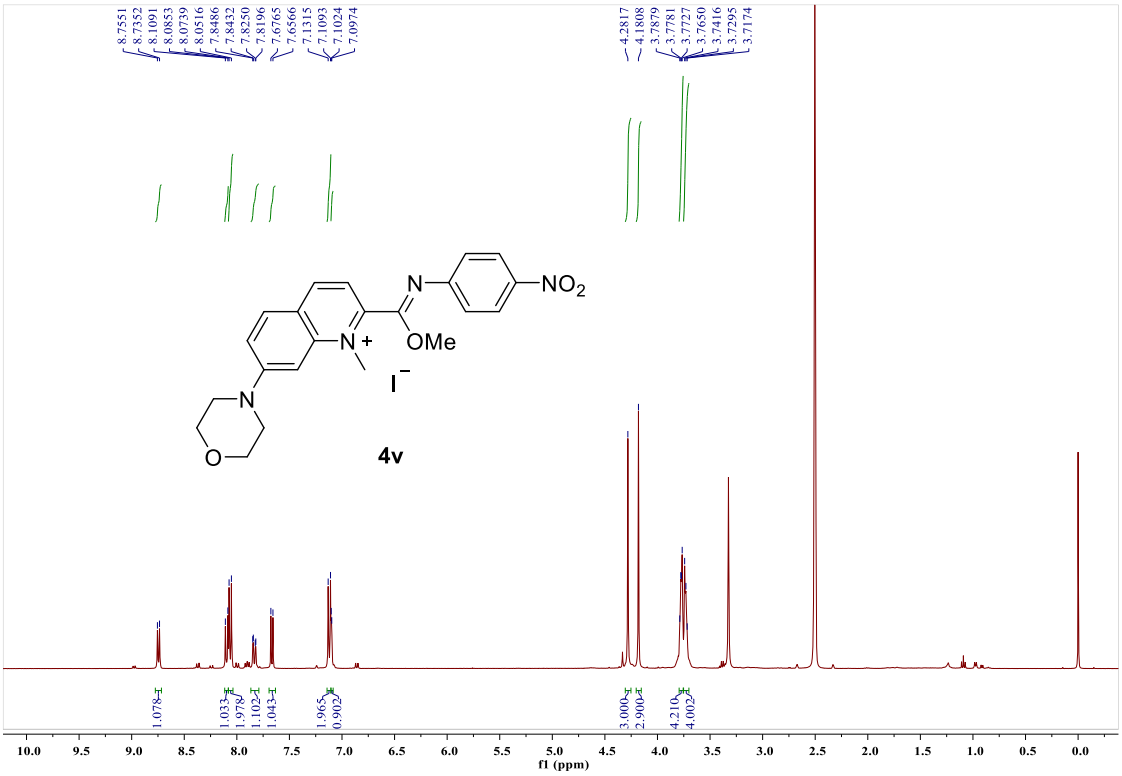
144.44
142.46
132.91
132.39
131.33
123.96
122.01
120.91
117.18
95.87
66.23
56.44
47.23
42.24
N
CHO
N+
OMe
I−
N
O
4u
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.1315
7.1093
7.1024
7.0974
4.2817
4.1808
3.7879
3.7781
3.7727
3.7650
3.7416
3.7295
3.7174
N
NO2
N+
OMe
I−
N
O
4v
1.078
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1.102
1.043
1.965
0.902
3.000
2.900
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4.002
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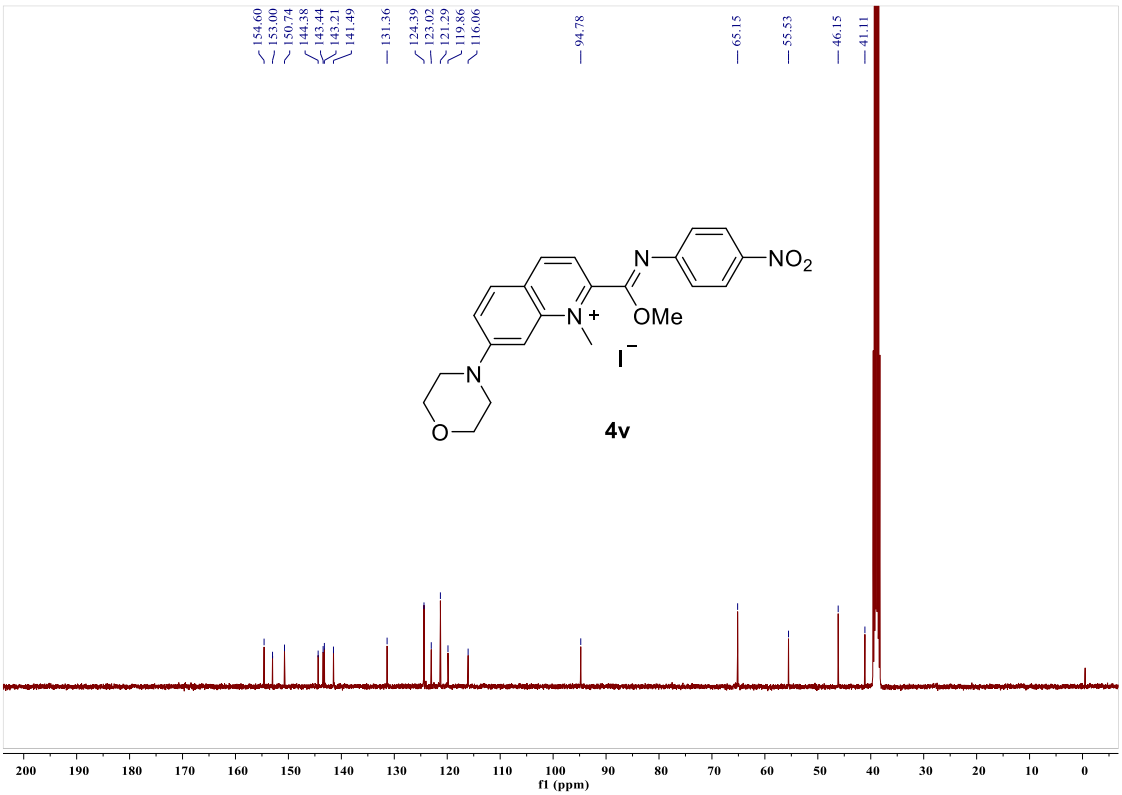
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141.49
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124.39
123.02
121.29
119.86
116.06
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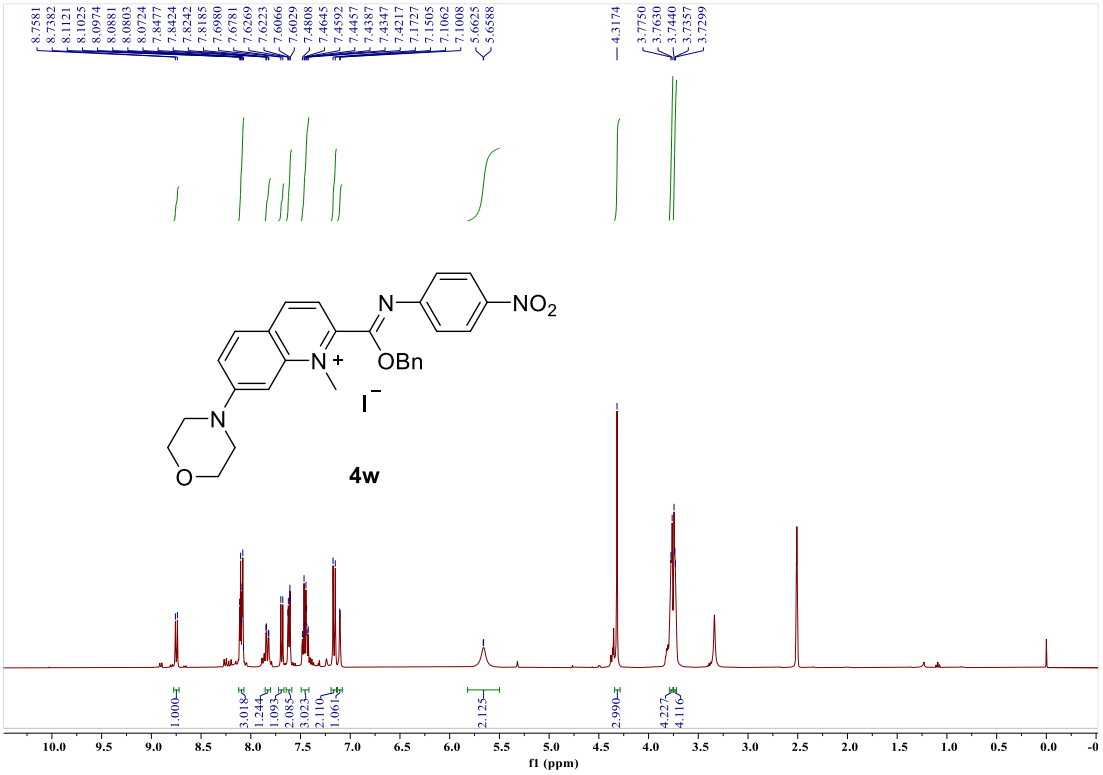
65.15
55.53
46.15
41.11
N
NO2
N+
OMe
I−
N
O
4v
f1 (ppm)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7.8185
7.6980
7.6781
7.6269
7.6223
7.6066
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7.4457
7.4387
7.4347
7.4217
7.1727
7.1505
7.1062
7.1008
5.6625
5.6588
4.3174
3.7750
3.7630
3.7440
3.7357
3.7299
N
NO2
N+
OBn
I−
N
O
4w
1.000
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3.023
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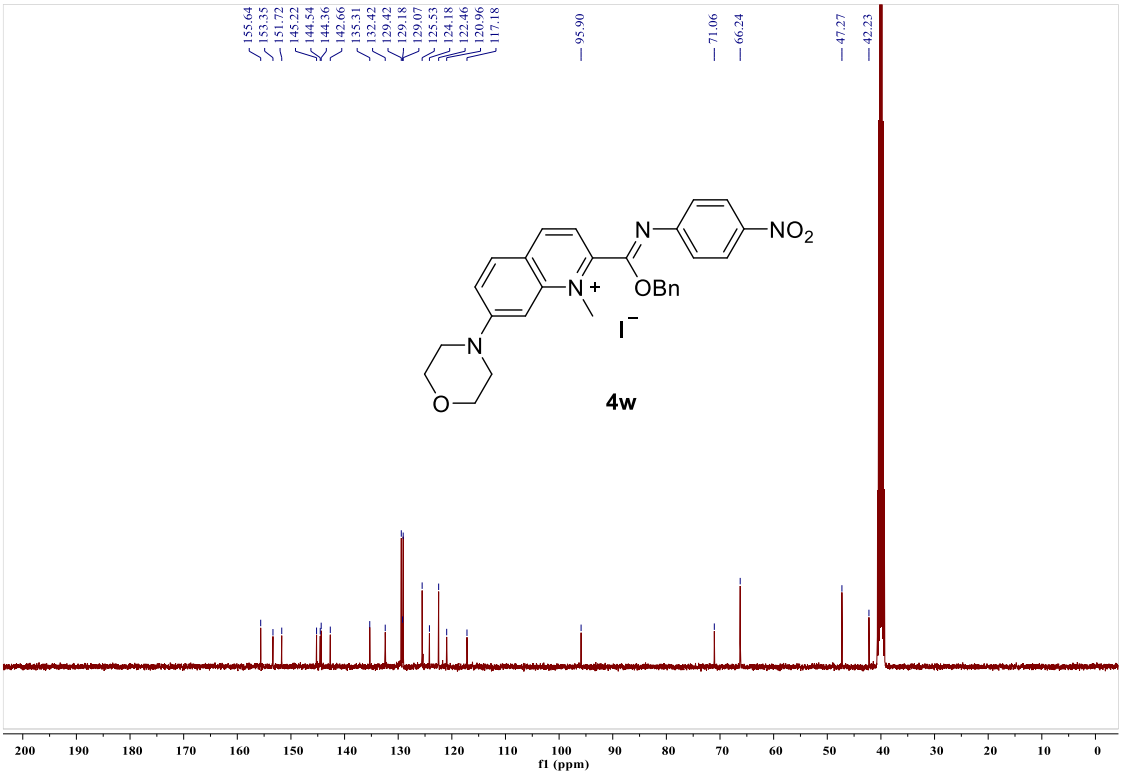
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129.18
129.07
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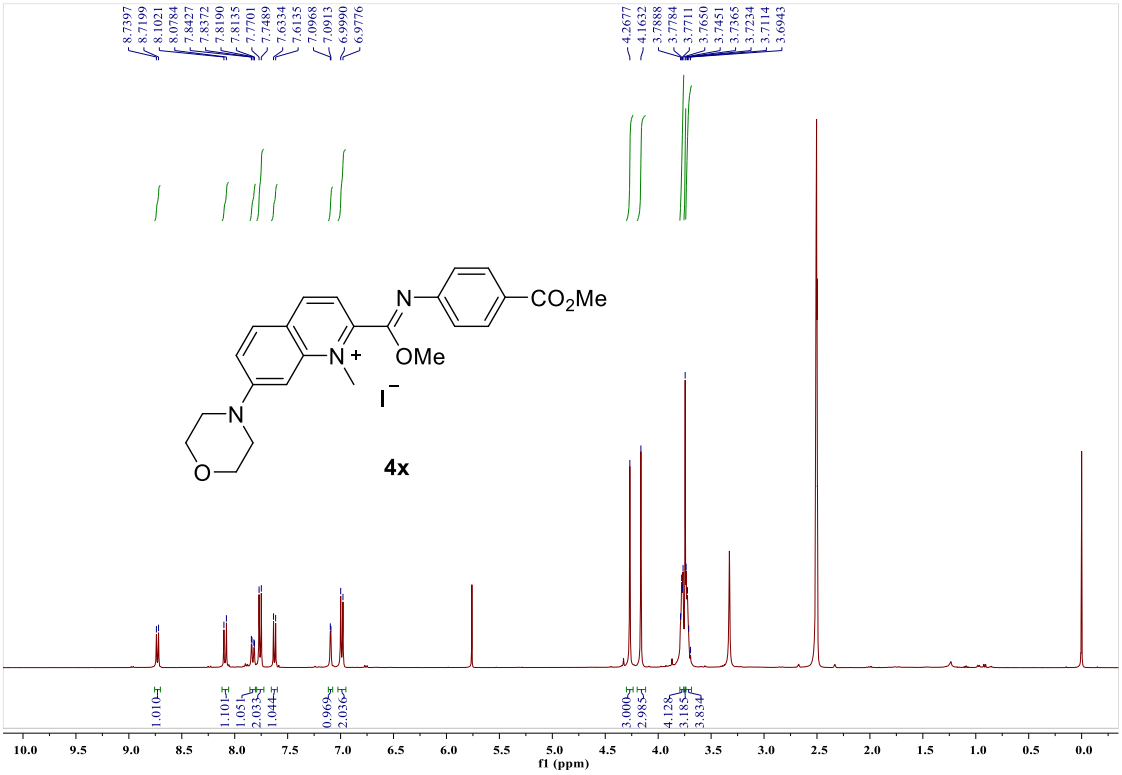
124.18
122.46
120.96
117.18
95.90
71.06
66.24
47.27
42.23
N
NO2
N+
OBn
I−
N
O
4w
f1 (ppm)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7.6135
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6.9776
4.2677
4.1632
3.7888
3.7784
3.7711
3.7650
3.7451
3.7365
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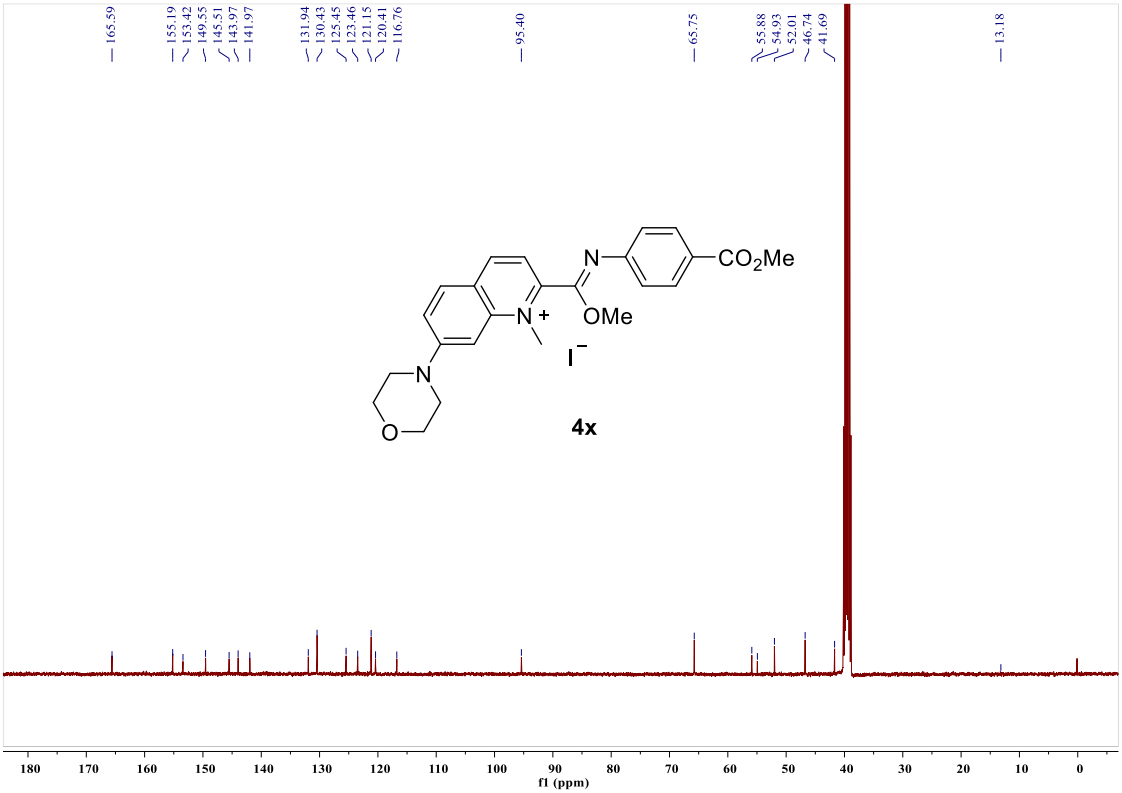
3.6943
N
CO2Me
N+
OMe
I−
N
O
4x
1.010
1.101
1.051
2.033
1.044
0.969
2.036
3.000
2.985
4.128
3.185
3.834
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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116.76
95.40
65.75
55.88
54.93
52.01
46.74
41.69
13.18
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CO2Me
N+
OMe
I−
N
O
4x
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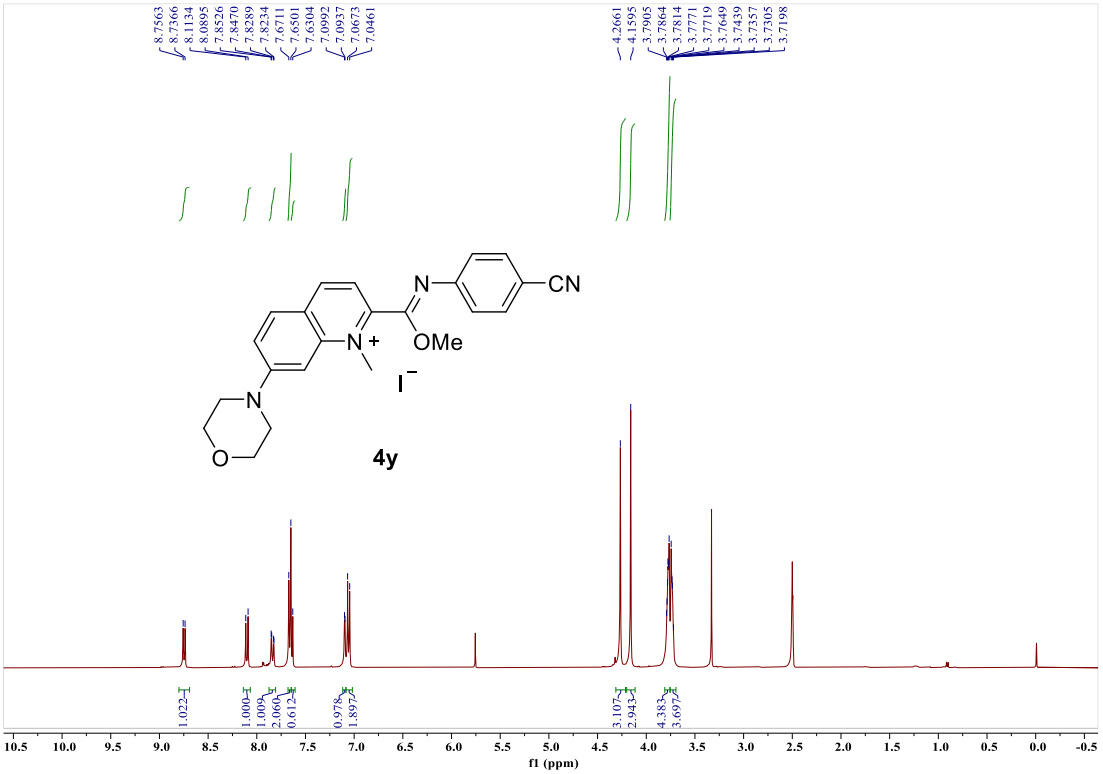
f1 (ppm)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3.7719
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CN
N+
OMe
I−
N
O
4y
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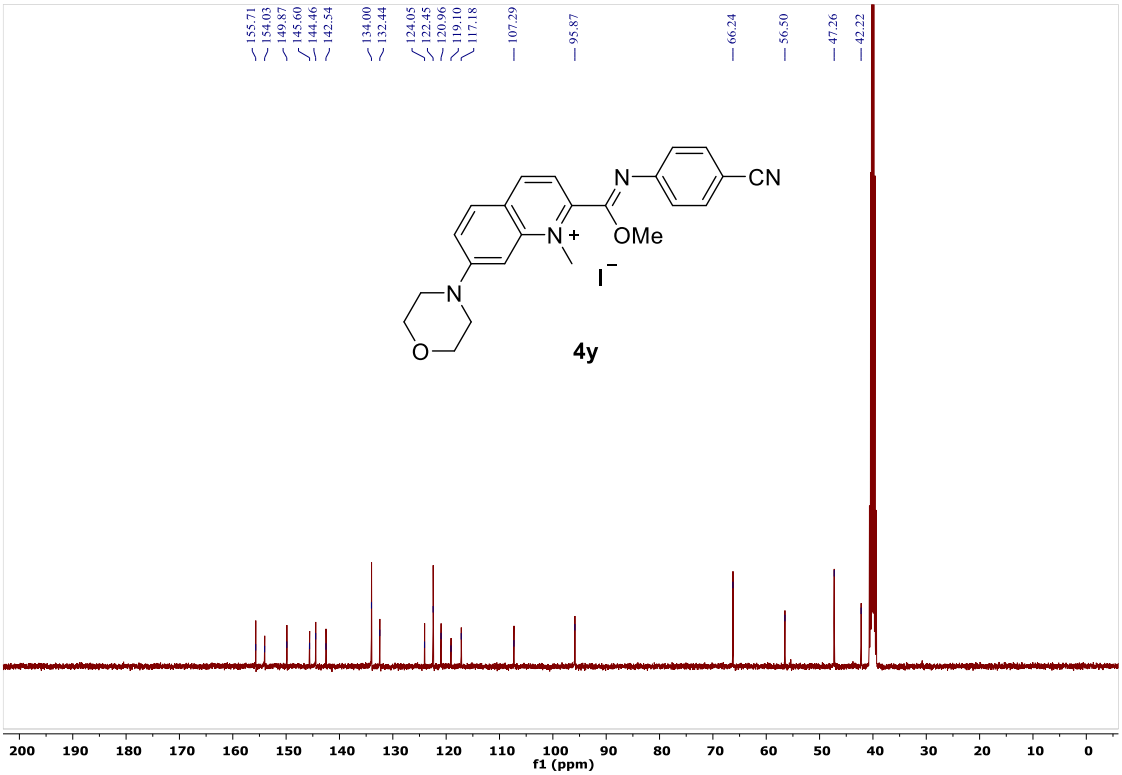
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117.18
107.29
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47.26
42.22
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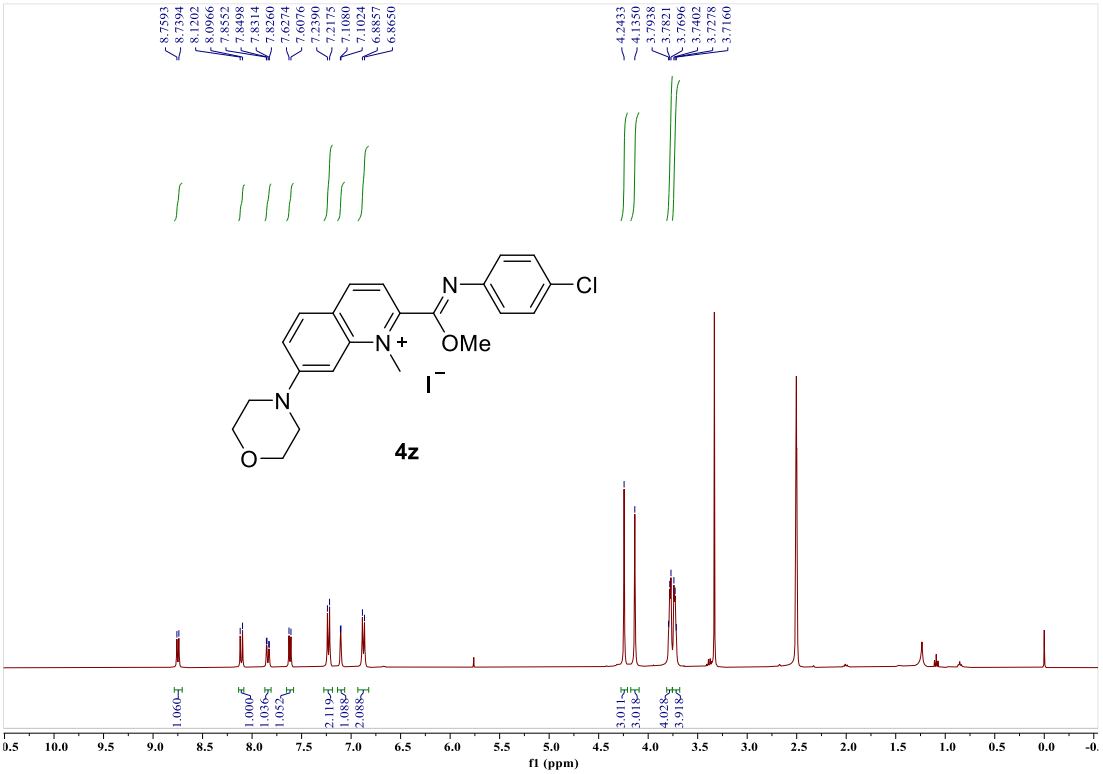
CN
N+
OMe
I−
N
O
4y
f1 (ppm)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7.2175
7.1080
7.1024
6.8857
6.8650
4.2433
4.1350
3.7938
3.7821
3.7696
3.7402
3.7278
3.7160
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Cl
N+
OMe
I−
N
O
4z
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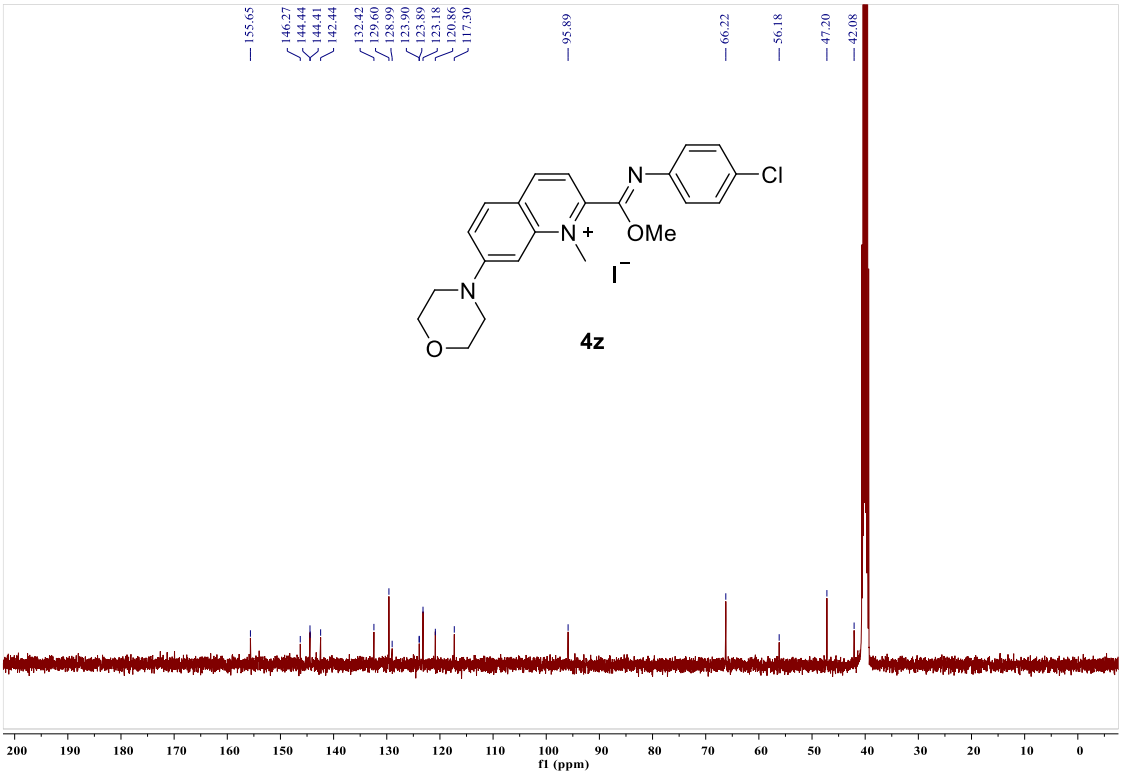
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123.18
120.86
117.30
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66.22
56.18
47.20
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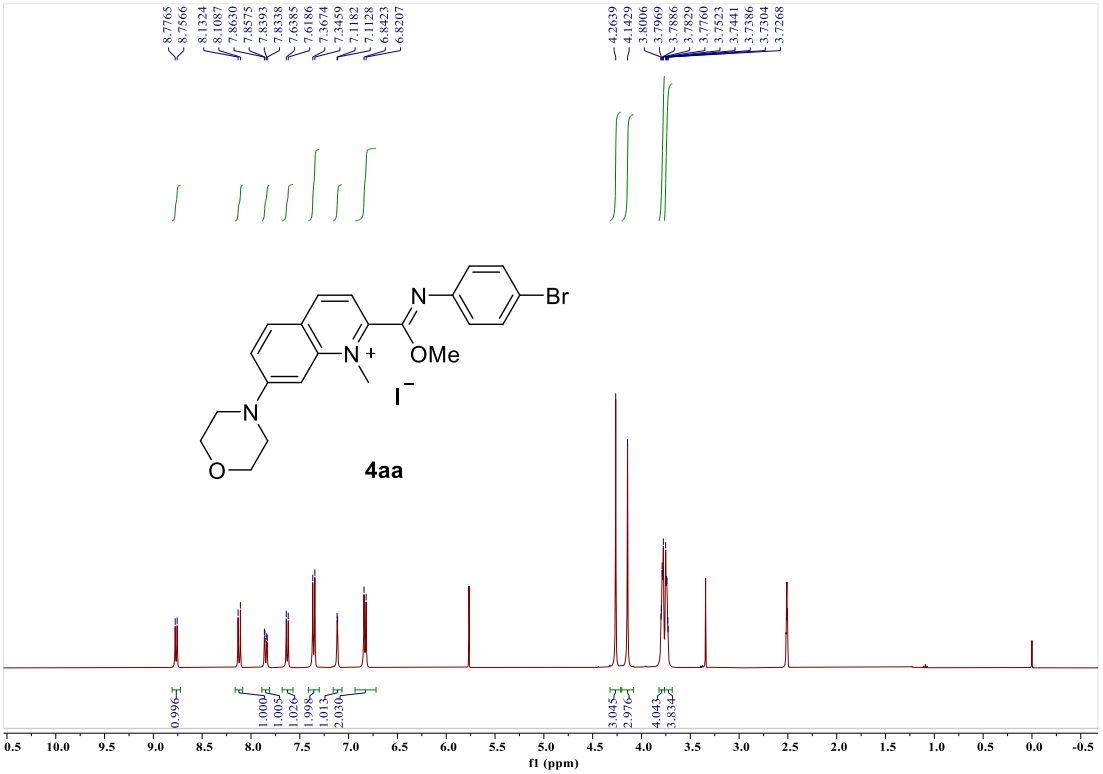
Cl
N+
OMe
I−
N
O
4z
f1 (ppm)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7.1182
7.1128
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4.1429
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3.7969
3.7886
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3.7760
3.7523
3.7441
3.7386
3.7304
3.7268
N
Br
N+
OMe
I−
N
O
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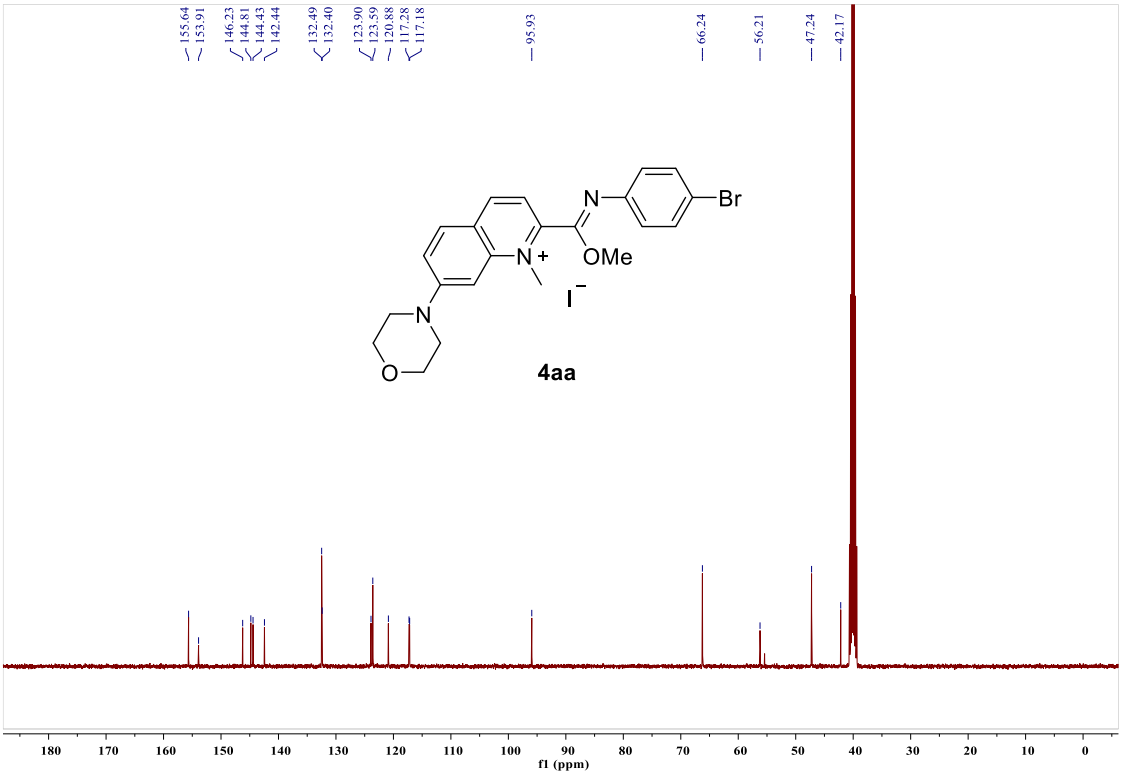
f1 (ppm)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117.28
117.18
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56.21
47.24
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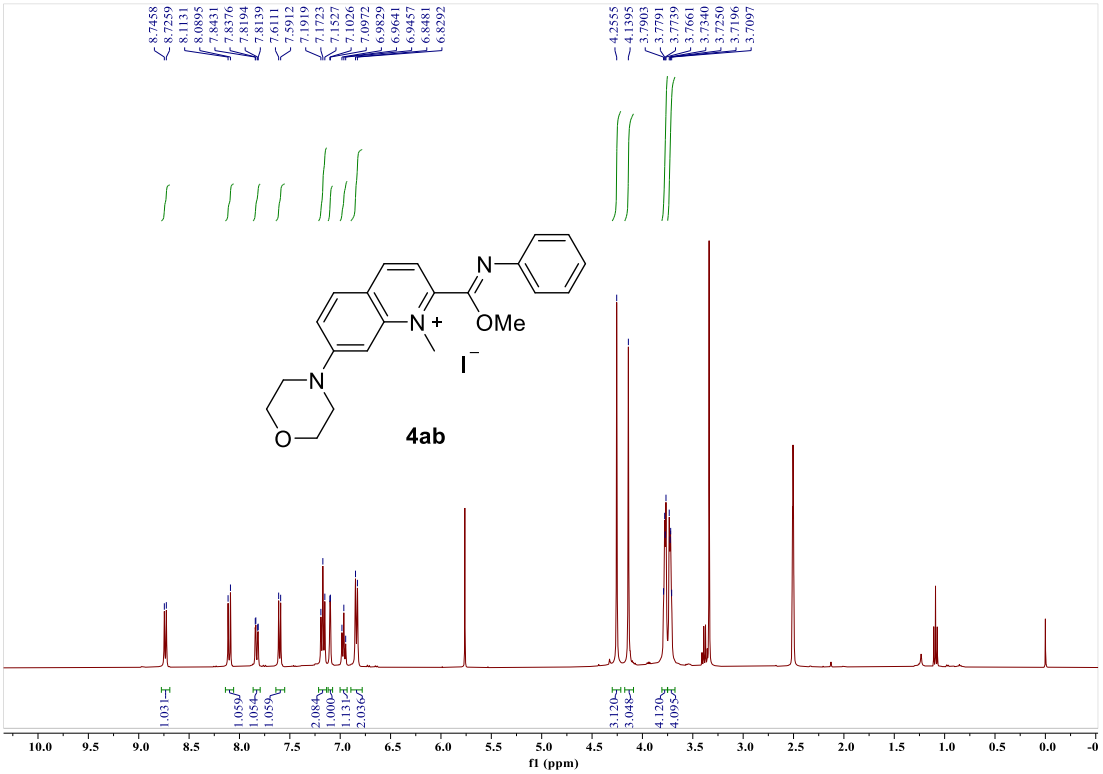
Br
N+
OMe
I−
N
O
4aa
f1 (ppm)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N
N+
OMe
I−
N
O
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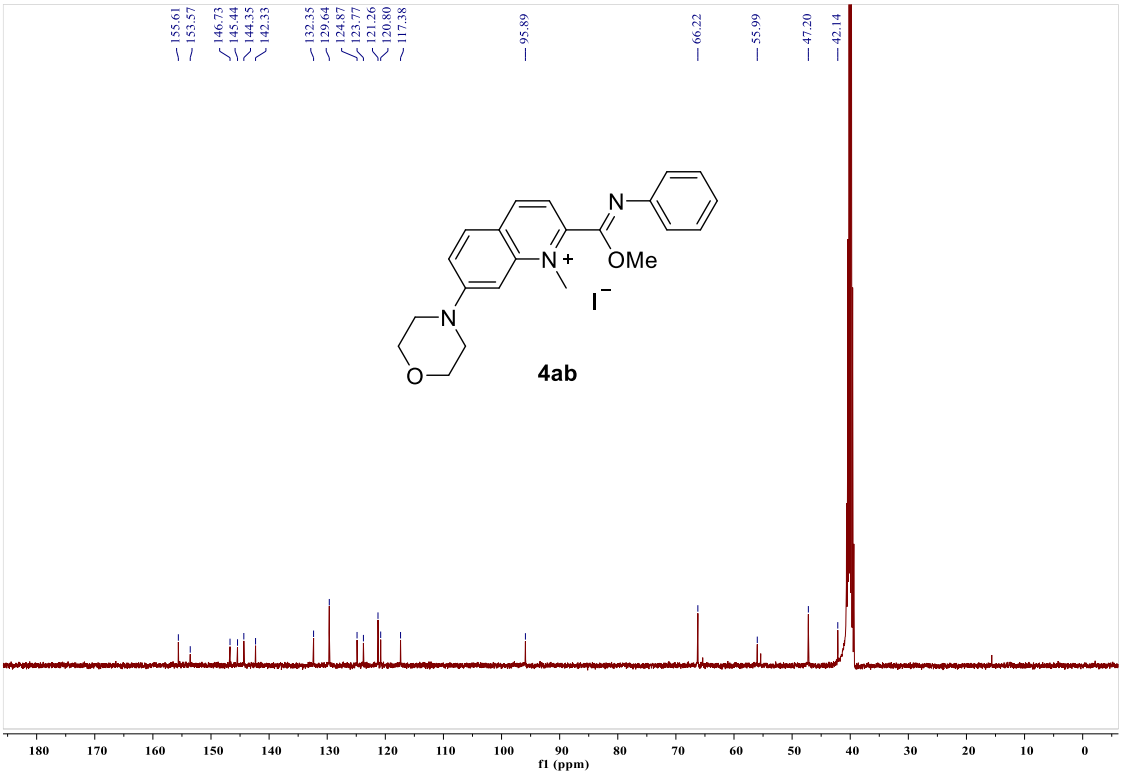
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47.20
42.14
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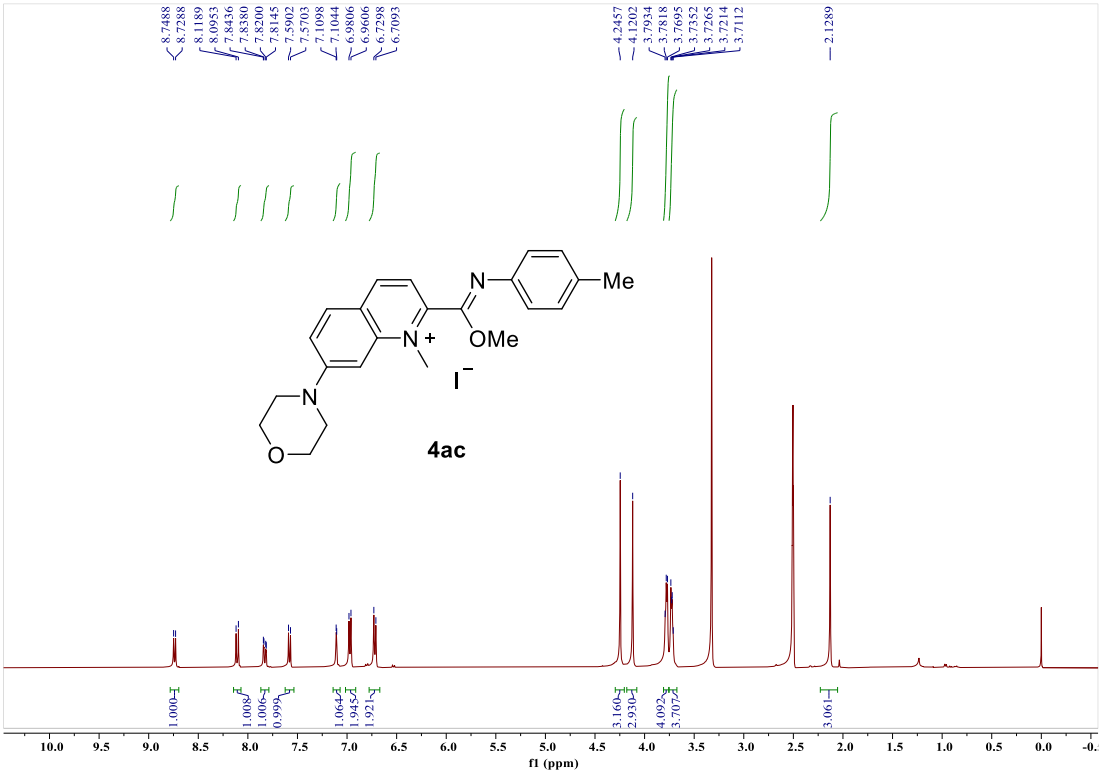
N+
OMe
I−
N
O
4ab
f1 (ppm)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7.5703
7.1098
7.1044
6.9806
6.9606
6.7298
6.7093
4.2457
4.1202
3.7934
3.7818
3.7695
3.7352
3.7265
3.7214
3.7112
2.1289
N
Me
N+
OMe
I−
N
O
4ac
1.000
1.008
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1.921
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2.930
4.092
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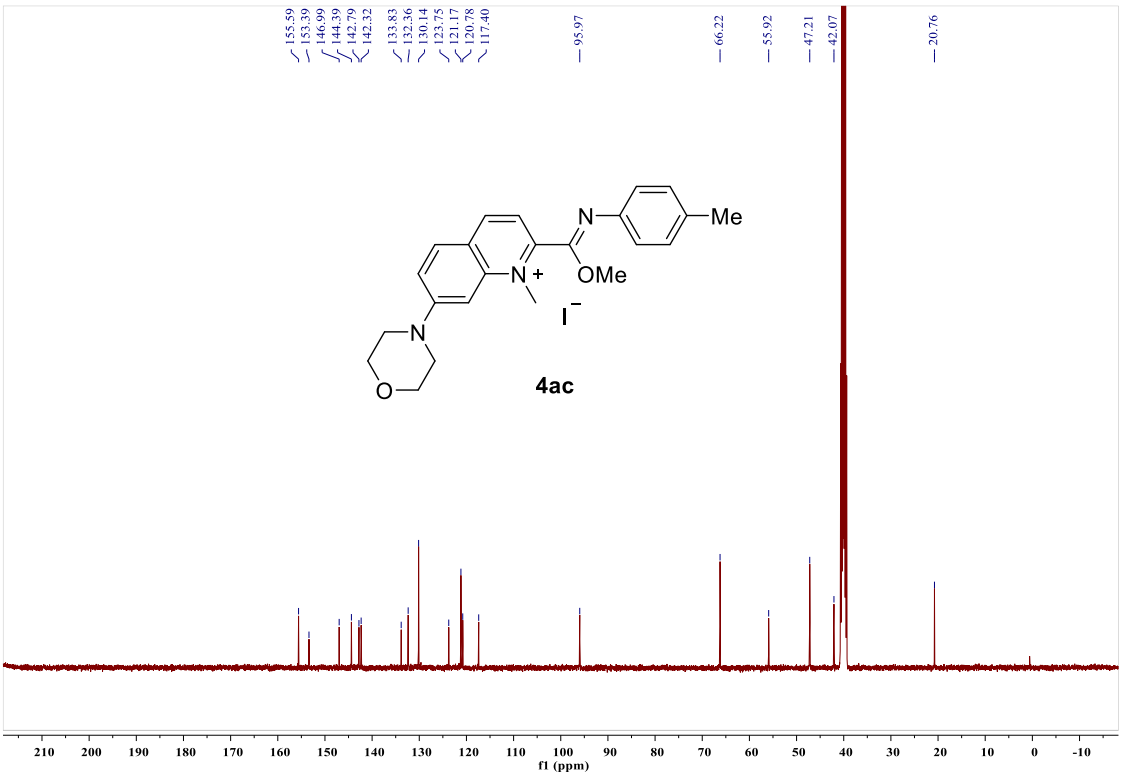
f1 (ppm)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132.36
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123.75
121.17
120.78
117.40
95.97
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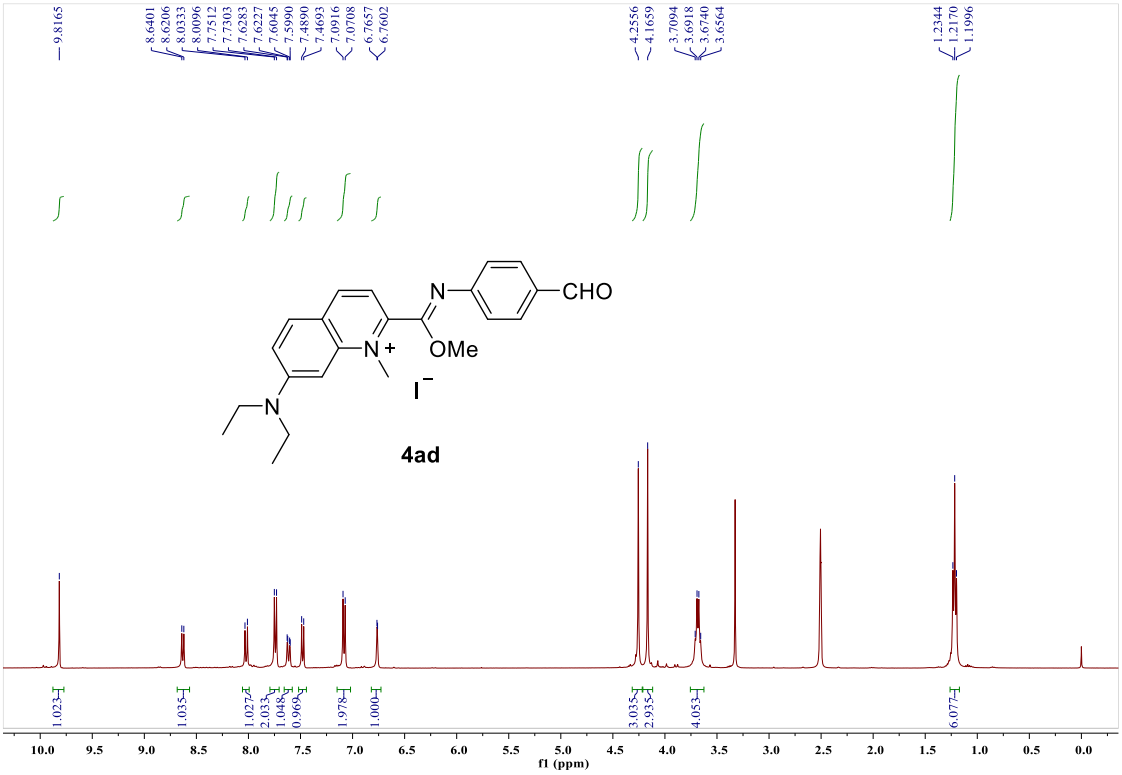
47.21
42.07
20.76
N
Me
N+
OMe
I−
N
O
4ac
f1 (ppm)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7.4890
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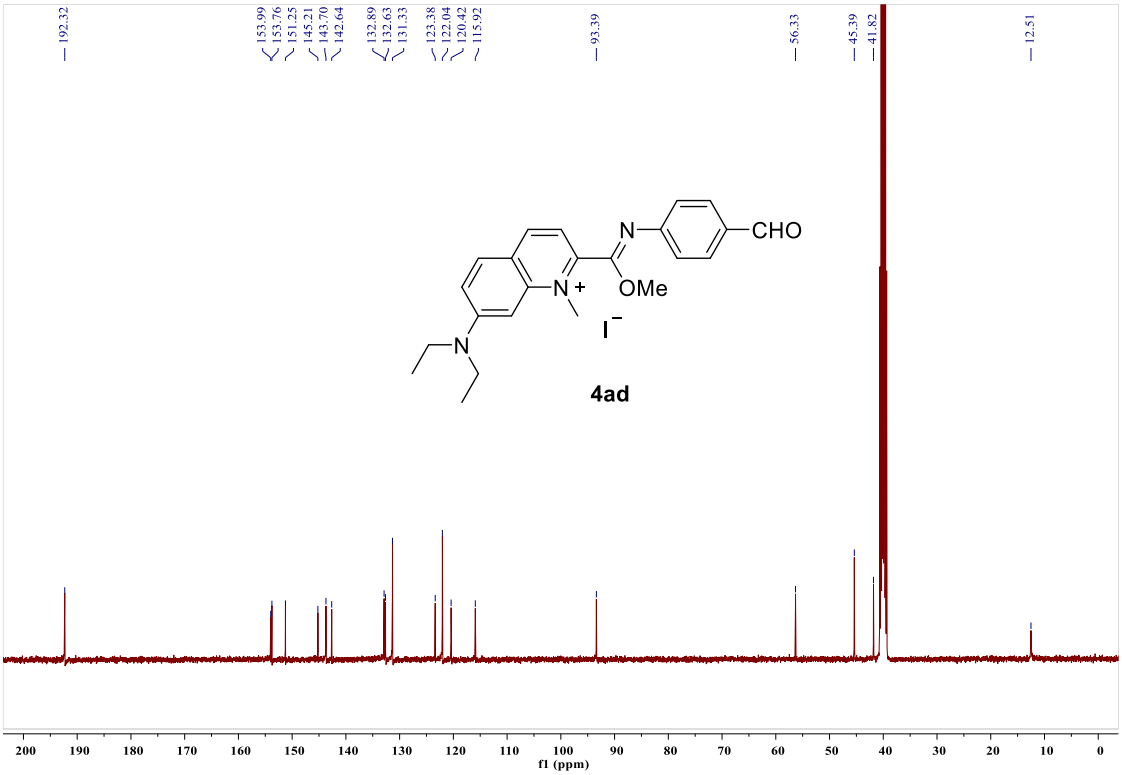
7.0916
7.0708
6.7657
6.7602
4.2556
4.1659
3.7094
3.6918
3.6740
3.6564
1.2344
1.2170
1.1996
N
CHO
N+
OMe
I−
N
4ad
1.023
1.035
1.027
2.033
1.048
0.969
1.978
1.000
3.035
2.935
4.053
6.077
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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151.25
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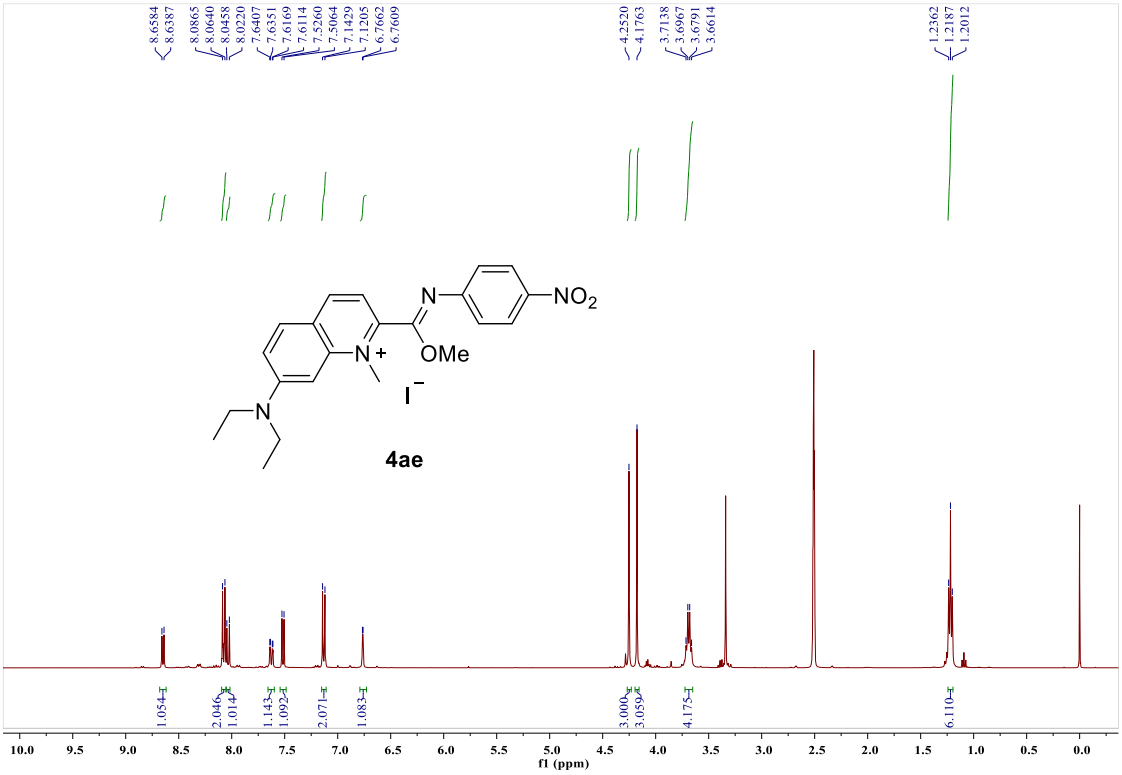
143.70
142.64
132.89
132.63
131.33
123.38
122.04
120.42
115.92
93.39
56.33
45.39
41.82
12.51
N
CHO
N+
OMe
I−
N
4ad
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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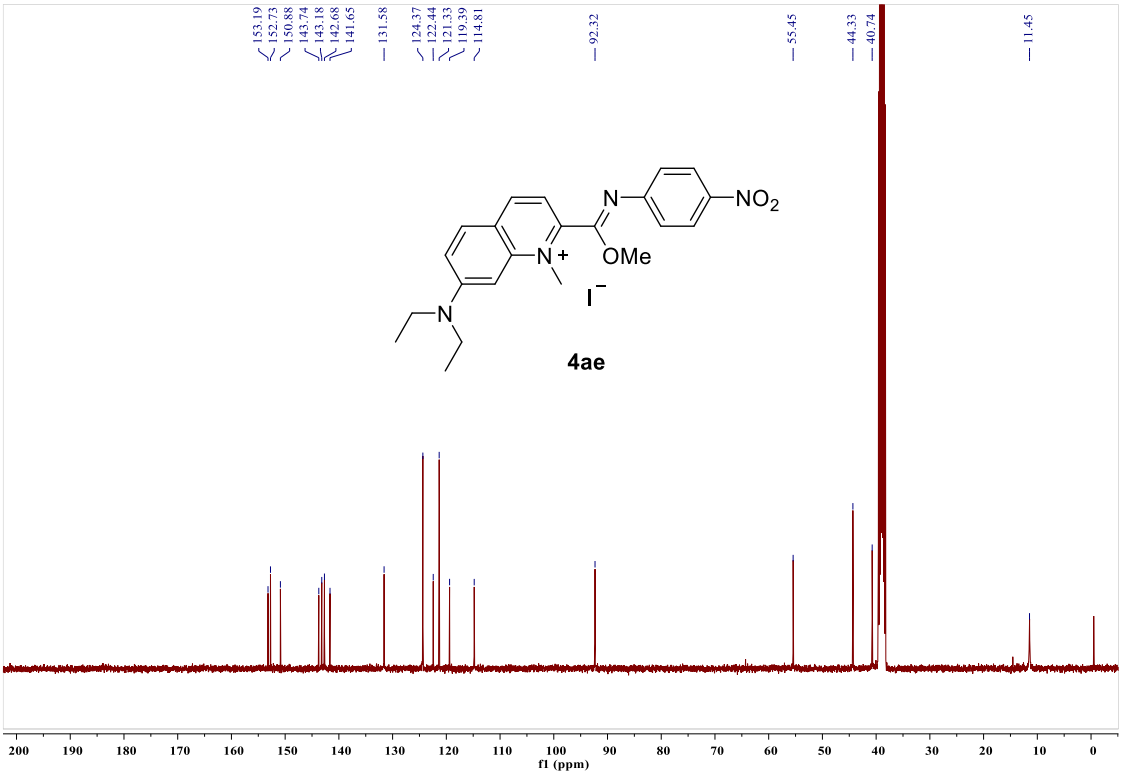
7.5064
7.1429
7.1205
6.7662
6.7609
4.2520
4.1763
3.7138
3.6967
3.6791
3.6614
1.2362
1.2187
1.2012
N
NO2
N+
OMe
I−
N
4ae
1.054
2.046
1.014
1.143
1.092
2.071
1.083
3.000
3.059
4.175
6.110
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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131.58
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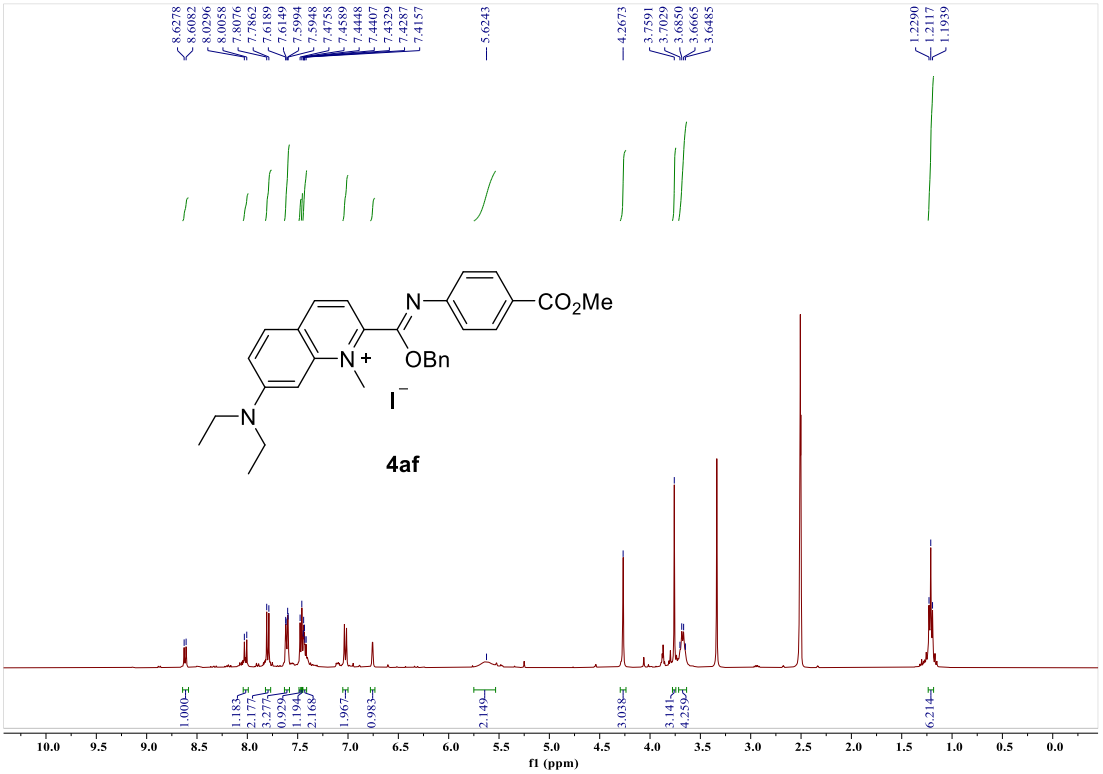
122.44
121.33
119.39
114.81
92.32
55.45
44.33
40.74
11.45
N
NO2
N+
OMe
I−
N
4ae
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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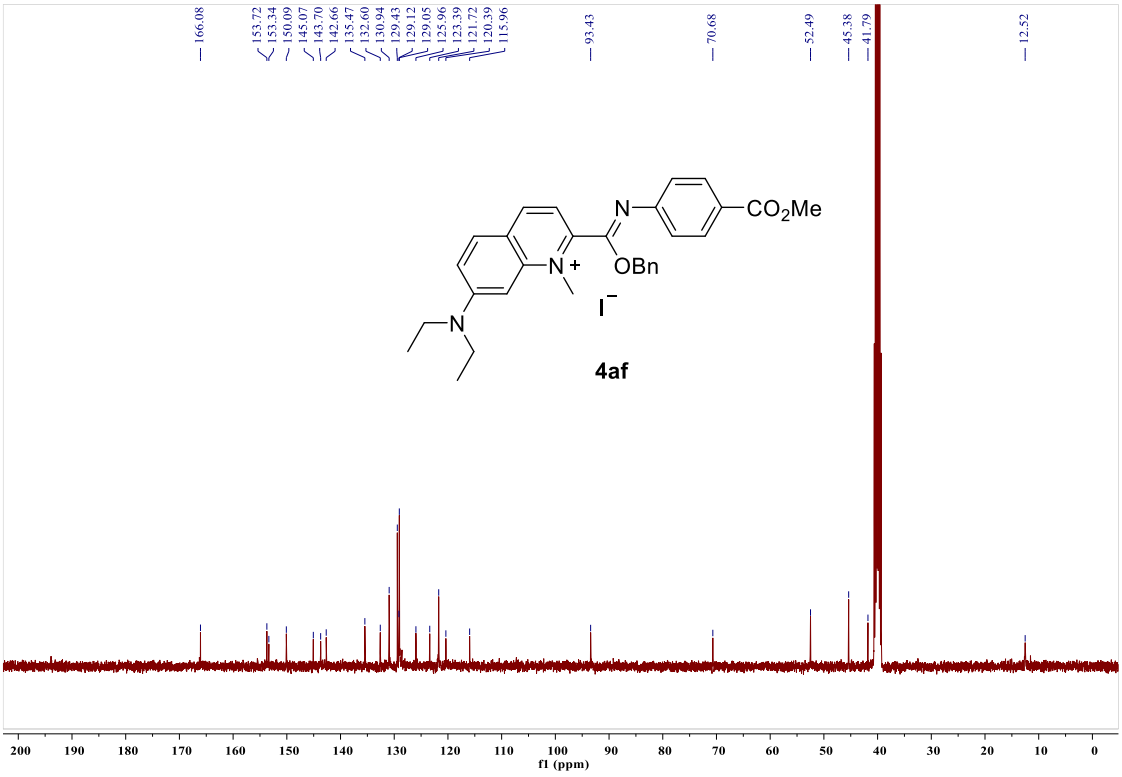
7.4589
7.4448
7.4407
7.4329
7.4287
7.4157
5.6243
4.2673
3.7591
3.7029
3.6850
3.6665
3.6485
1.2290
1.2117
1.1939
N
CO2Me
N+
OBn
I−
N
4af
1.000
1.183
2.177
3.277
0.929
1.194
2.168
1.967
0.983
2.149
3.038
3.141
4.259
6.214
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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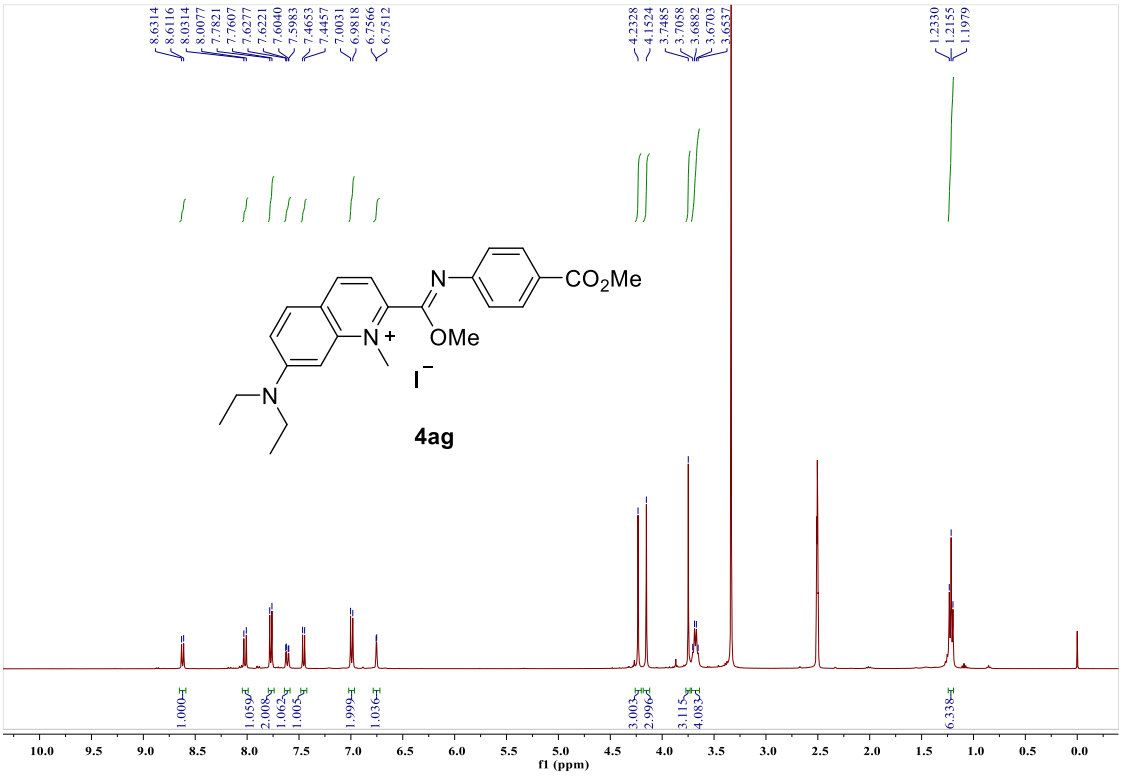
135.47
132.60
130.94
129.43
129.12
129.05
125.96
123.39
121.72
120.39
115.96
93.43
70.68
52.49
45.38
41.79
12.52
N
CO2Me
N+
OBn
I−
N
4af
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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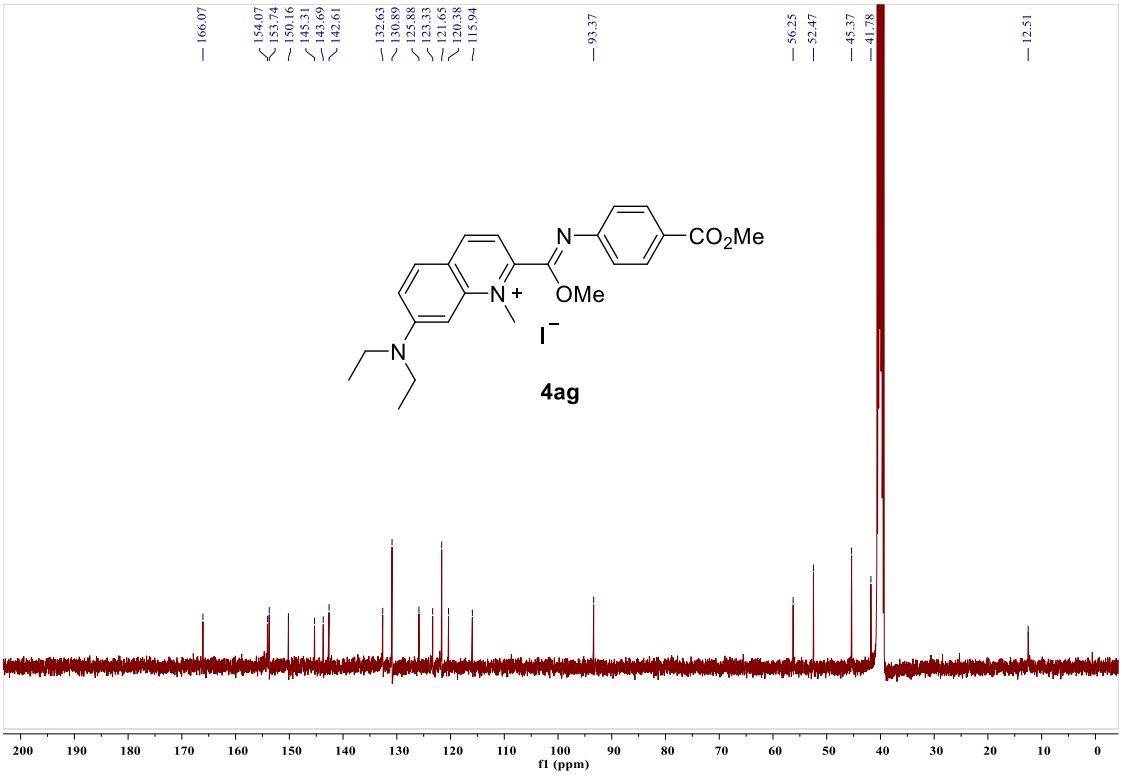
7.4457
7.0031
6.9818
6.7566
6.7512
4.2328
4.1524
3.7485
3.7058
3.6882
3.6703
3.6537
1.2330
1.2155
1.1979
N
CO2Me
N+
OMe
I−
N
4ag
1.000
1.059
2.008
1.062
1.005
1.999
1.036
3.003
2.996
3.115
4.083
6.338
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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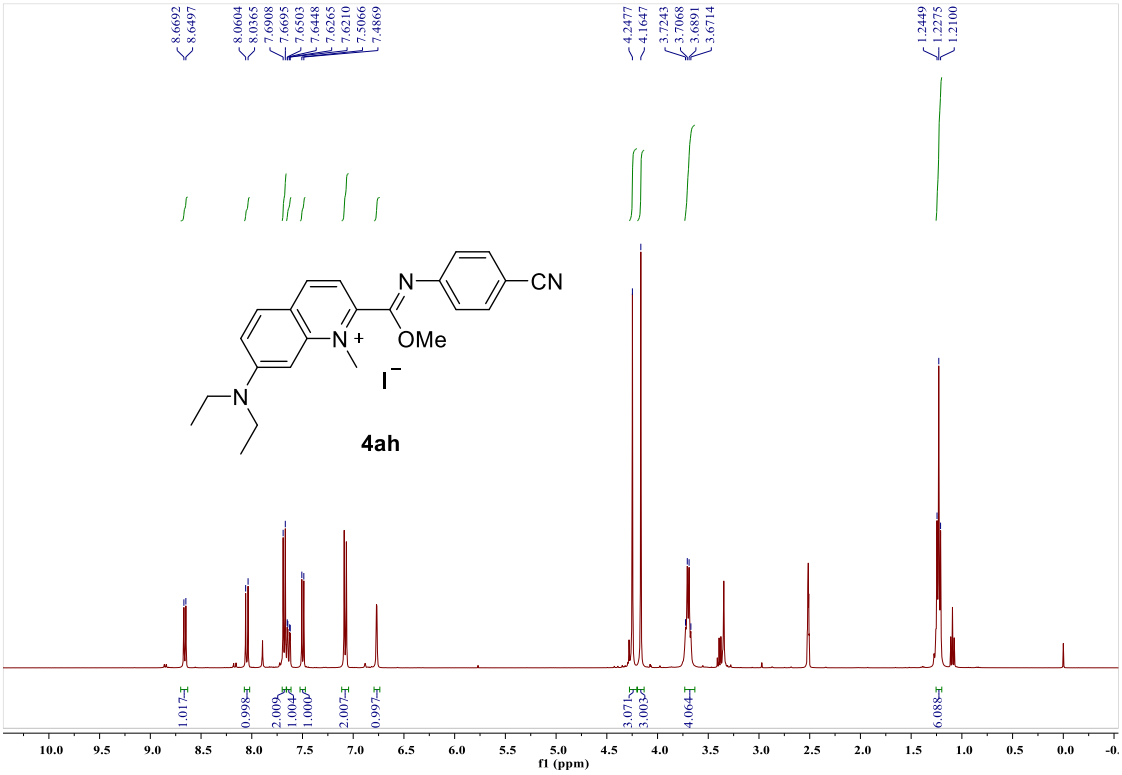
130.89
125.88
123.33
121.65
120.38
115.94
93.37
56.25
52.47
45.37
41.78
12.51
N
CO2Me
N+
OMe
I−
N
4ag
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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4.2477
4.1647
3.7243
3.7068
3.6891
3.6714
1.2449
1.2275
1.2100
N
CN
N+
OMe
I−
N
4ah
1.017
0.998
2.009
1.004
1.000
2.007
0.997
3.071
3.003
4.064
6.088
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
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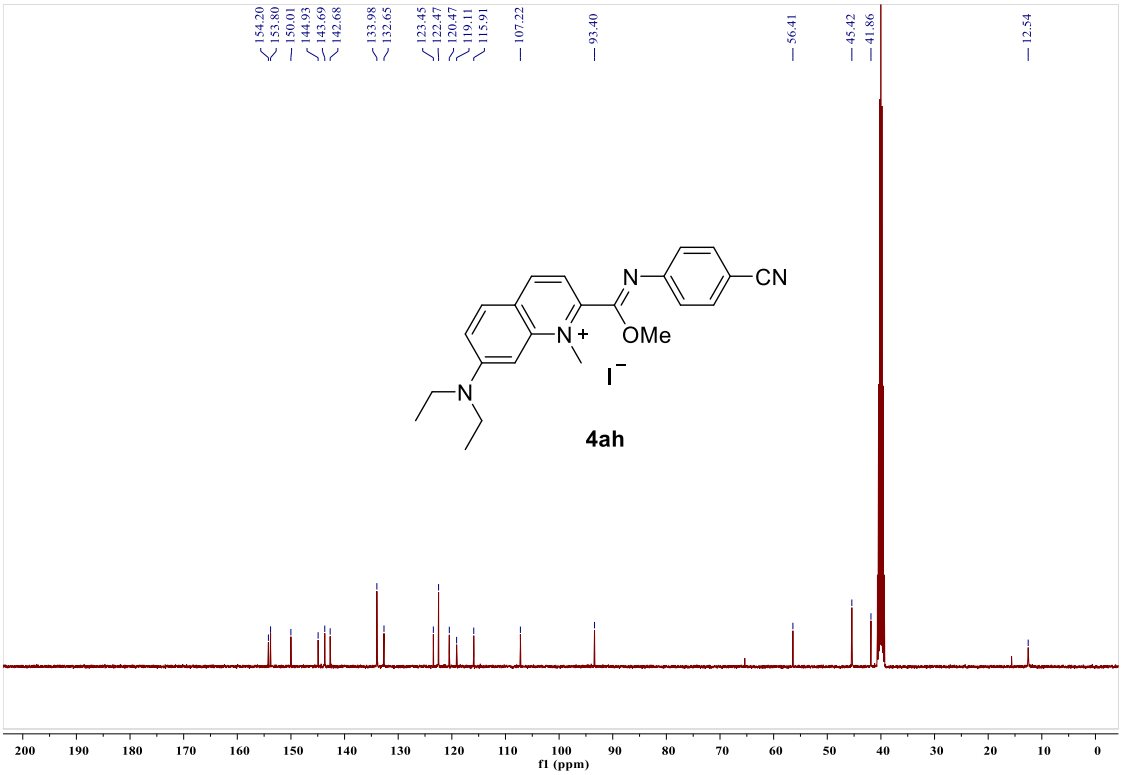
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120.47
119.11
115.91
107.22
93.40
56.41
45.42
41.86
12.54
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CN
N+
OMe
I−
N
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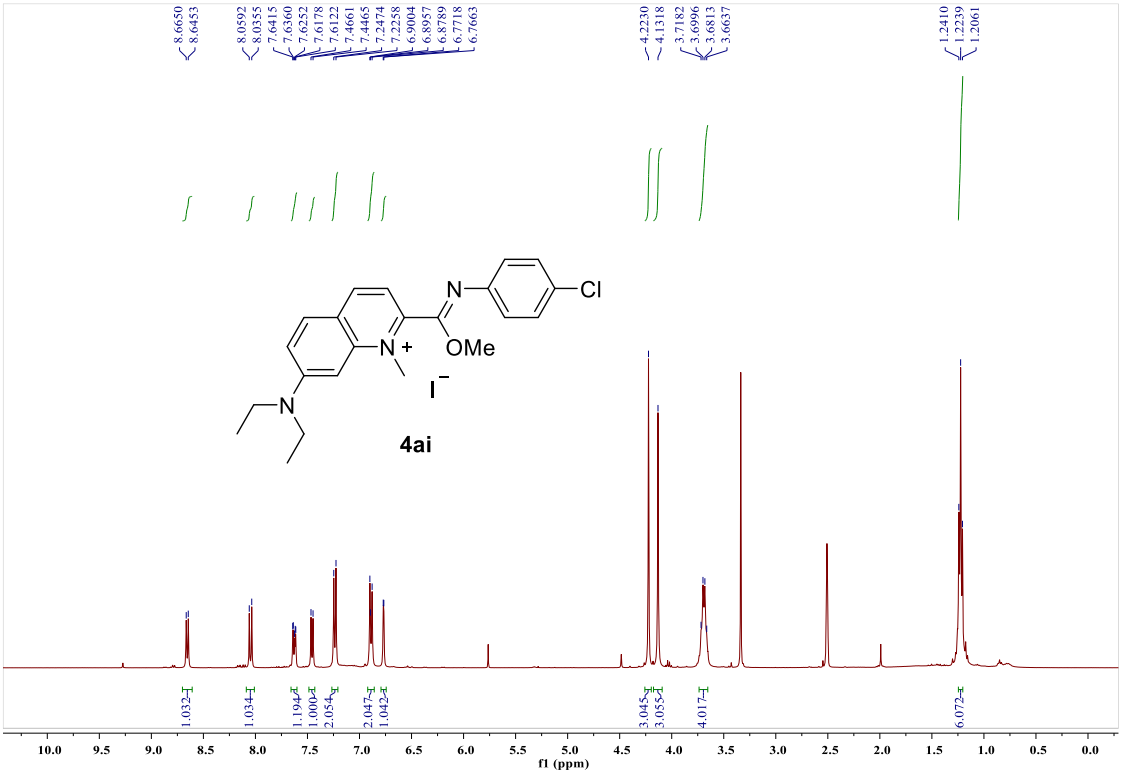
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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Cl
N+
OMe
I−
N
4ai
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1.034
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1.000
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2.047
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3.055
4.017
6.072
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
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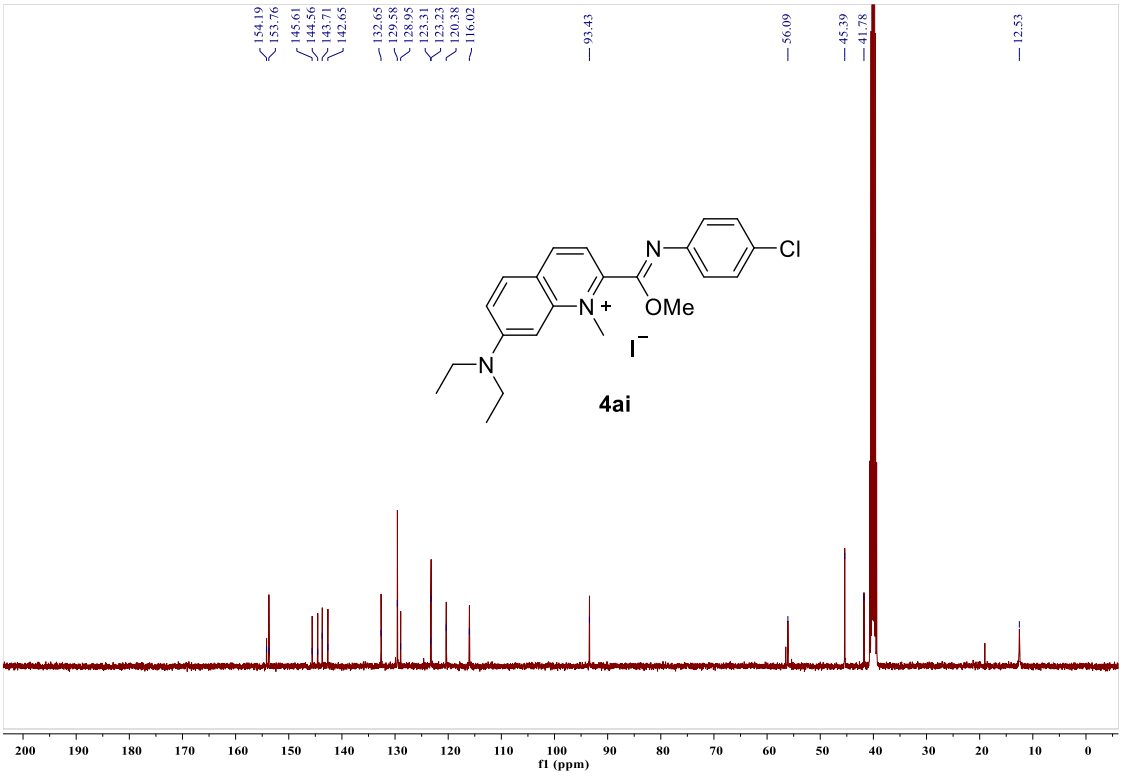
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120.38
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93.43
56.09
45.39
41.78
12.53
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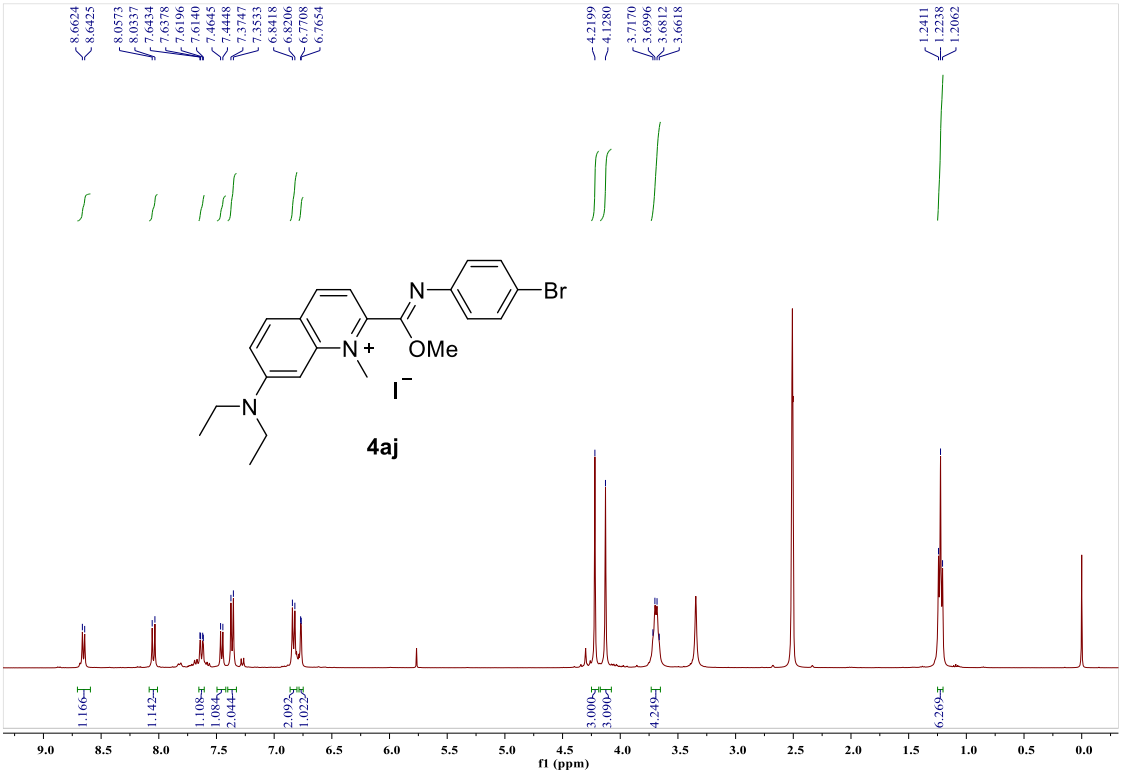
Cl
N+
OMe
I−
N
4ai
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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4.1280
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3.6996
3.6812
3.6618
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1.2238
1.2062
N
Br
N+
OMe
I−
N
4aj
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2.092
1.022
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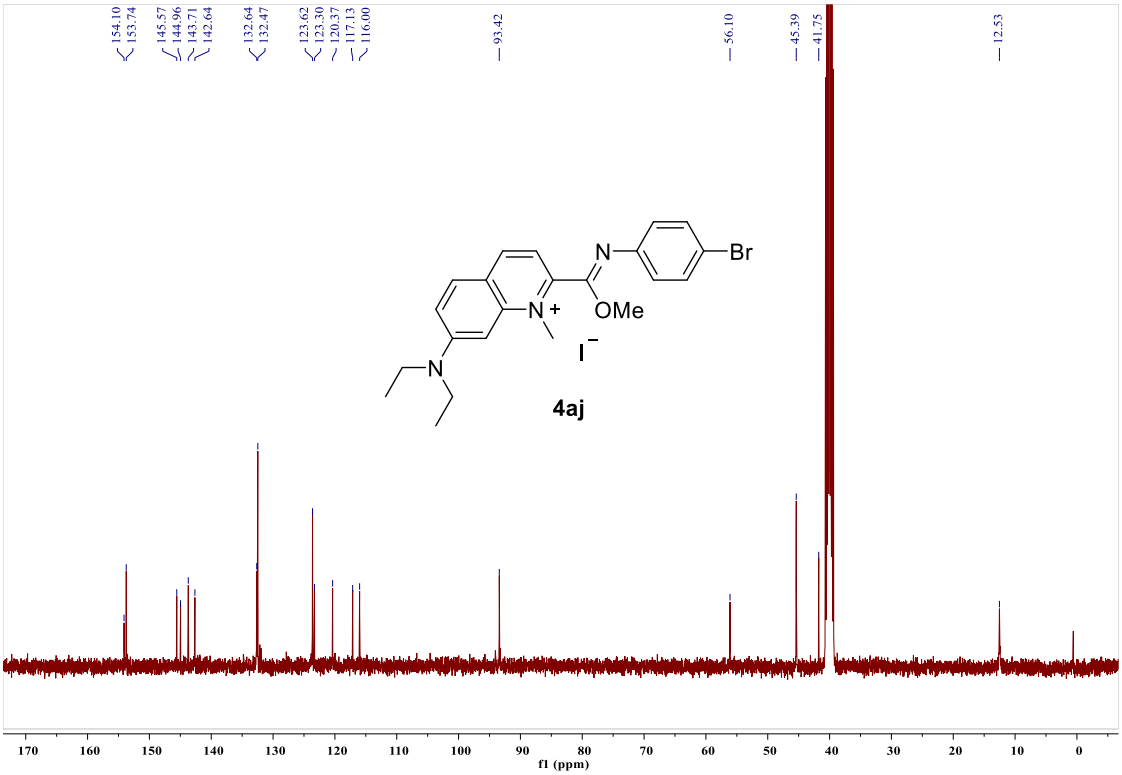
f1 (ppm)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116.00
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56.10
45.39
41.75
12.53
N
Br
N+
OMe
I−
N
4aj
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120
110
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90
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70
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50
40
30
20
10
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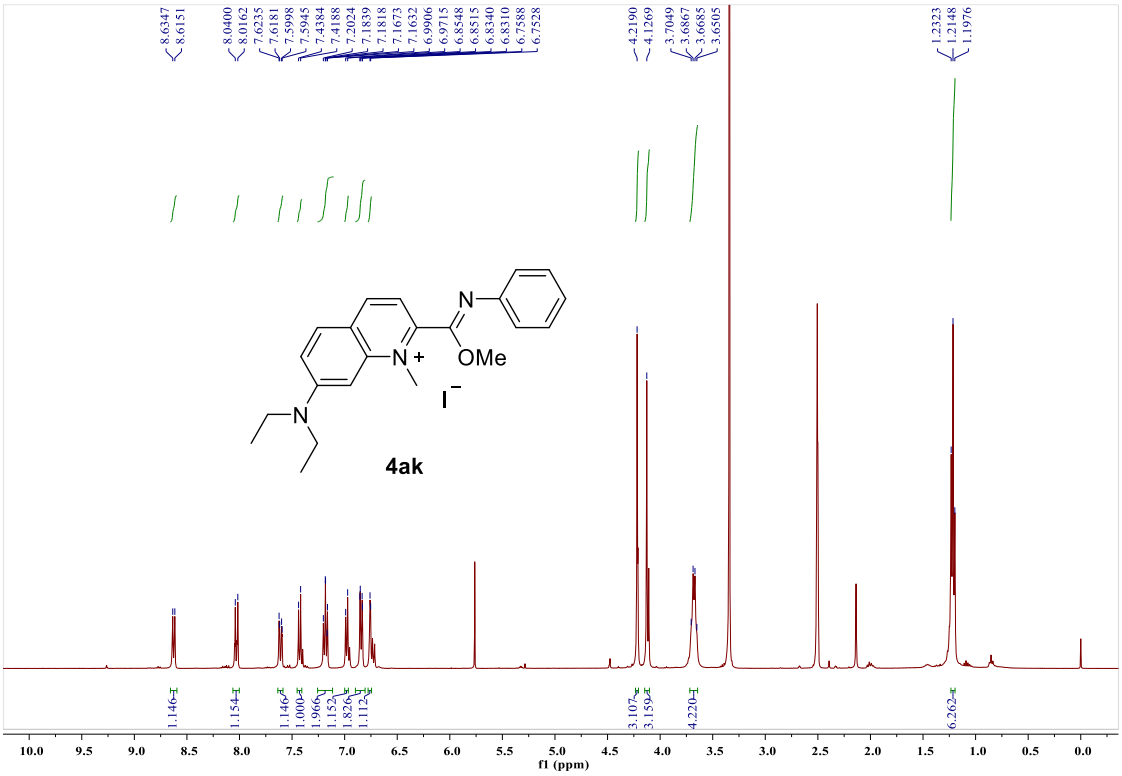
f1 (ppm)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N
N+
OMe
I−
N
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7.0
6.5
6.0
5.5
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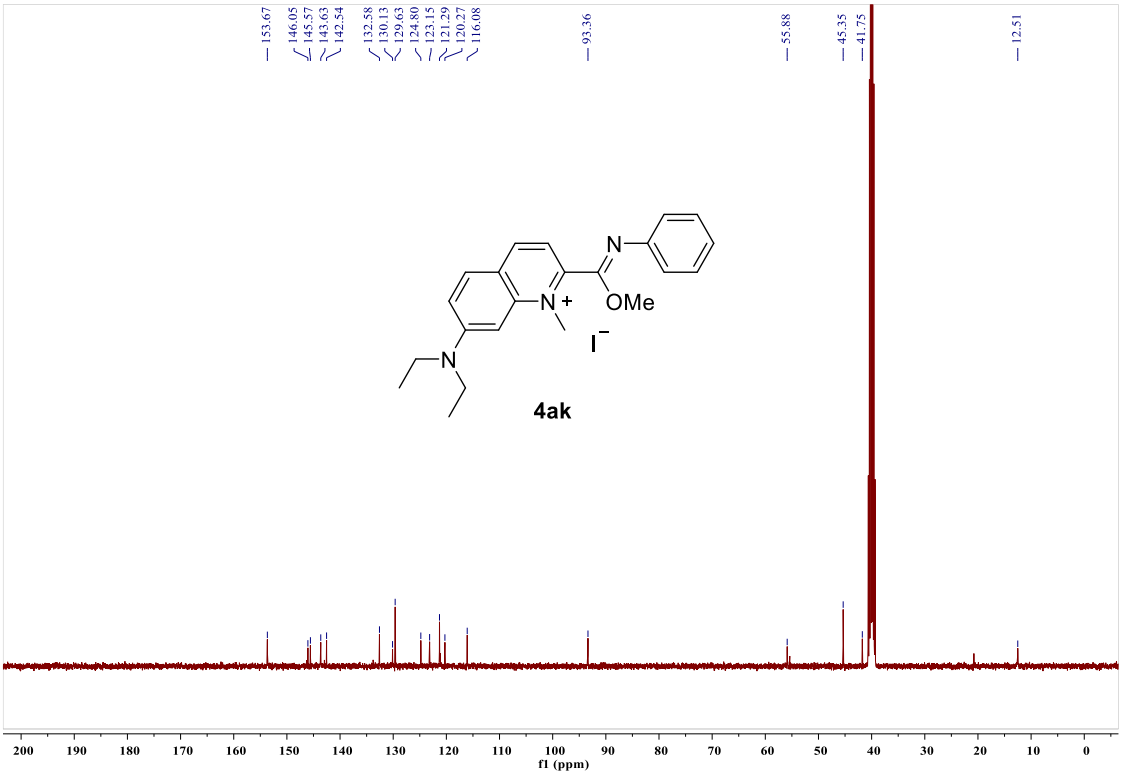
f1 (ppm)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93.36
55.88
45.35
41.75
12.51
N
N+
OMe
I−
N
4ak
200
190
180
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50
40
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10
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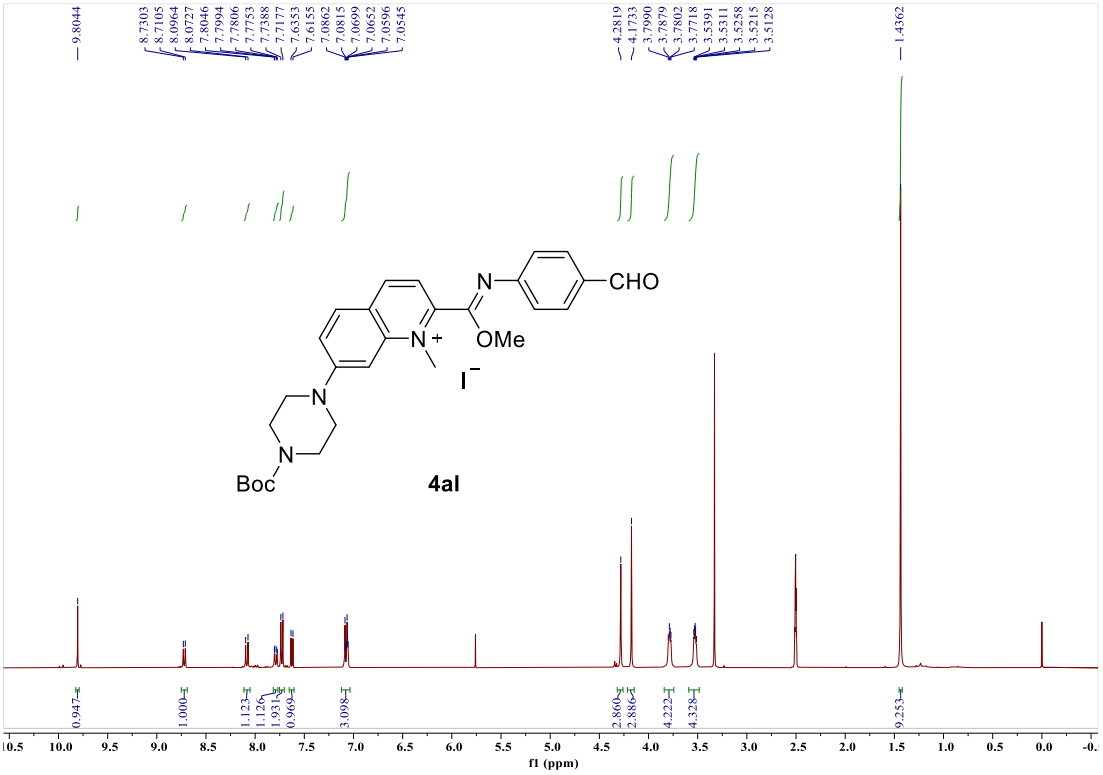
f1 (ppm)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7.0596
7.0545
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3.5311
3.5258
3.5215
3.5128
1.4362
CHO
N
N+
OMe
I−
N
N
Boc
4al
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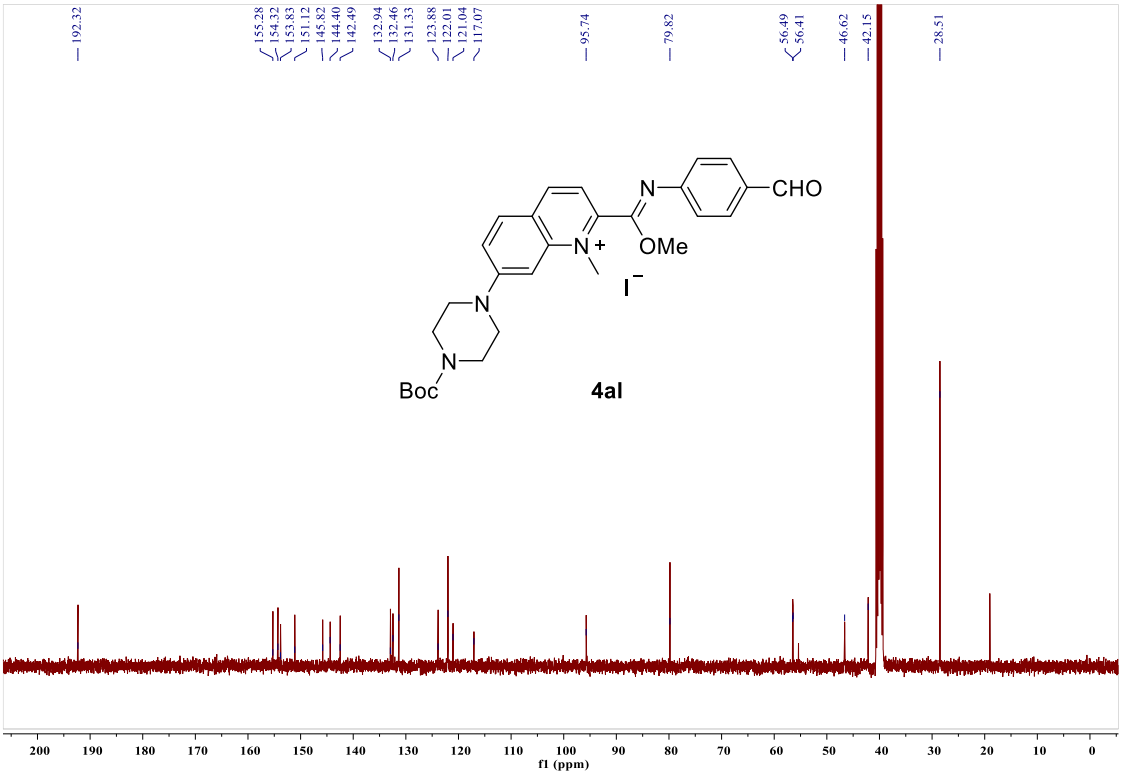
f1 (ppm)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131.33
123.88
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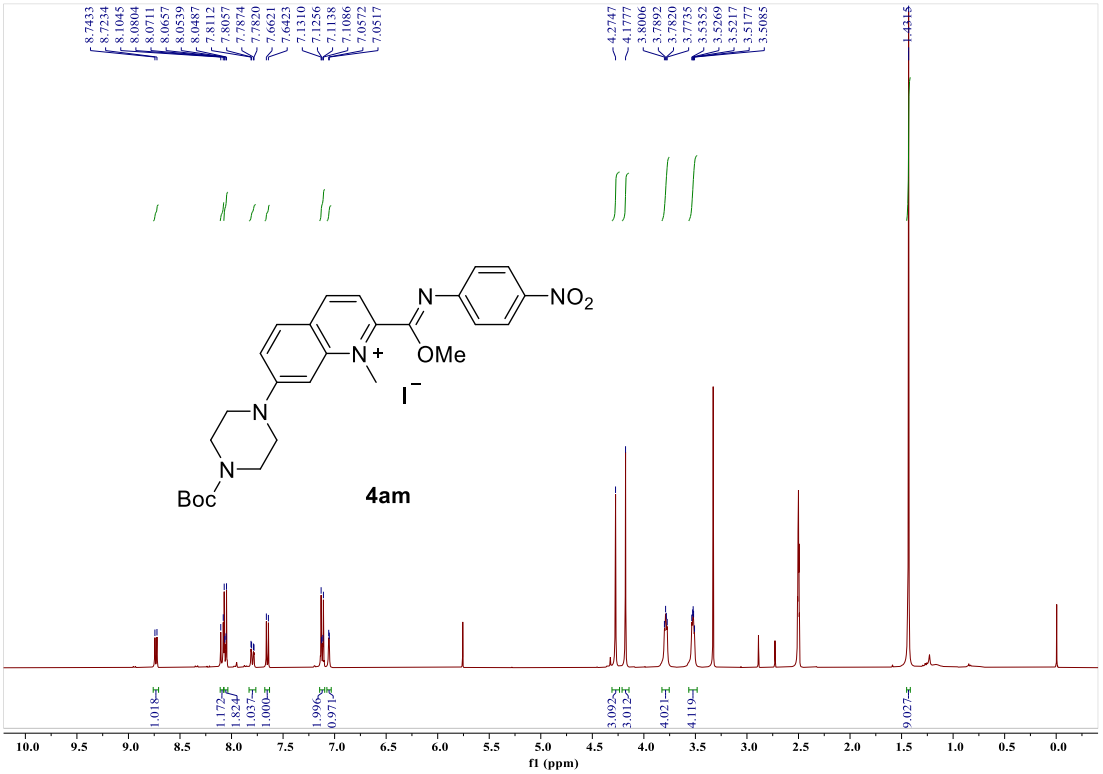
117.07
95.74
79.82
56.49
56.41
46.62
42.15
28.51
CHO
N
N+
OMe
I−
N
N
Boc
4al
f1 (ppm)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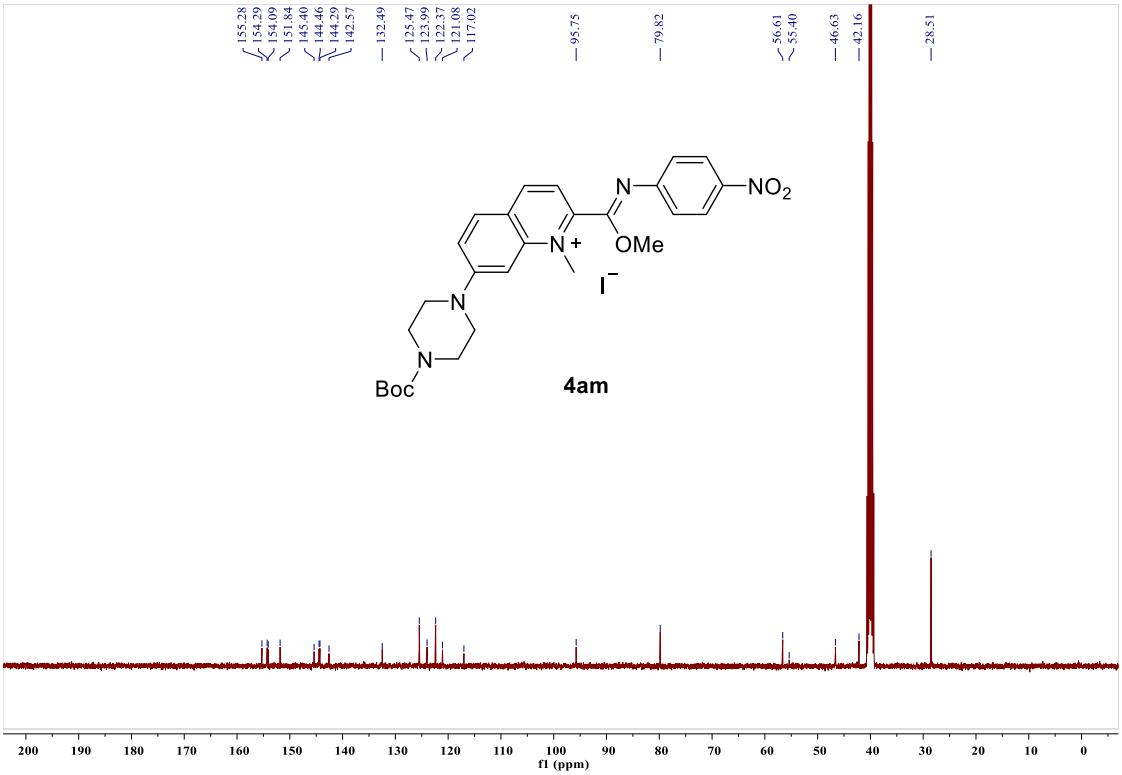
NO2
N+
OMe
I−
N
N
Boc
4am
f1 (ppm)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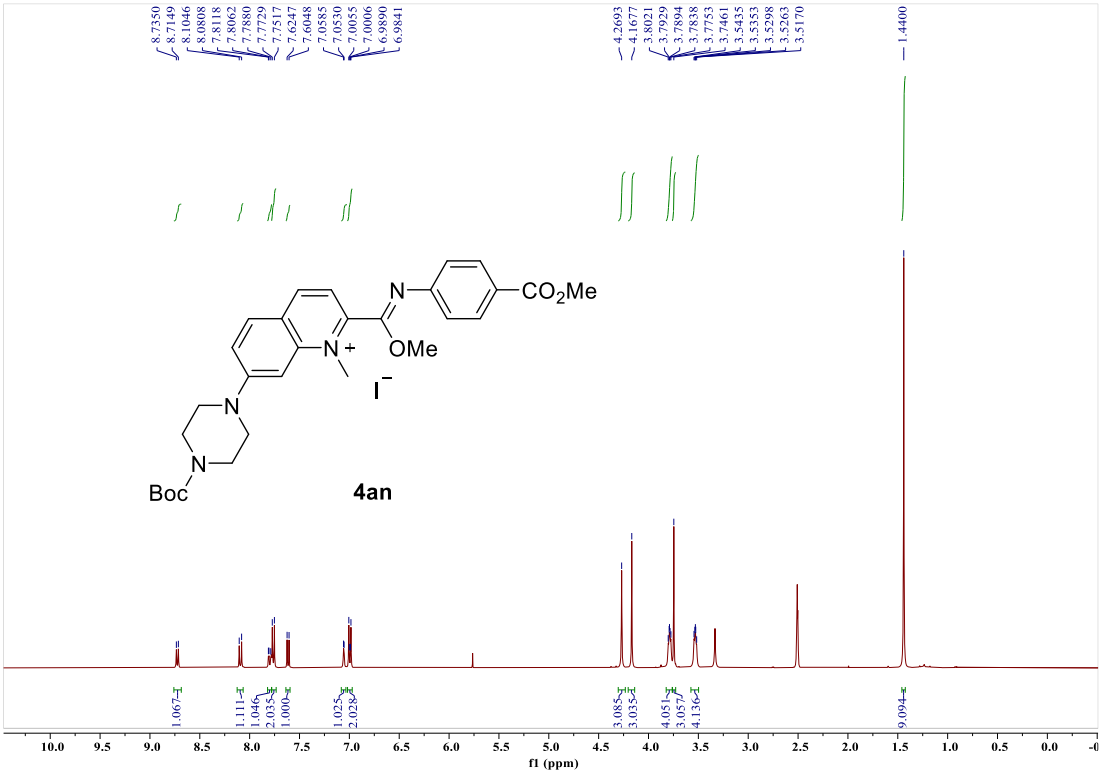
79.82
56.61
55.40
46.63
42.16
28.51
N
NO2
N+
OMe
I−
N
N
Boc
4am
f1 (ppm)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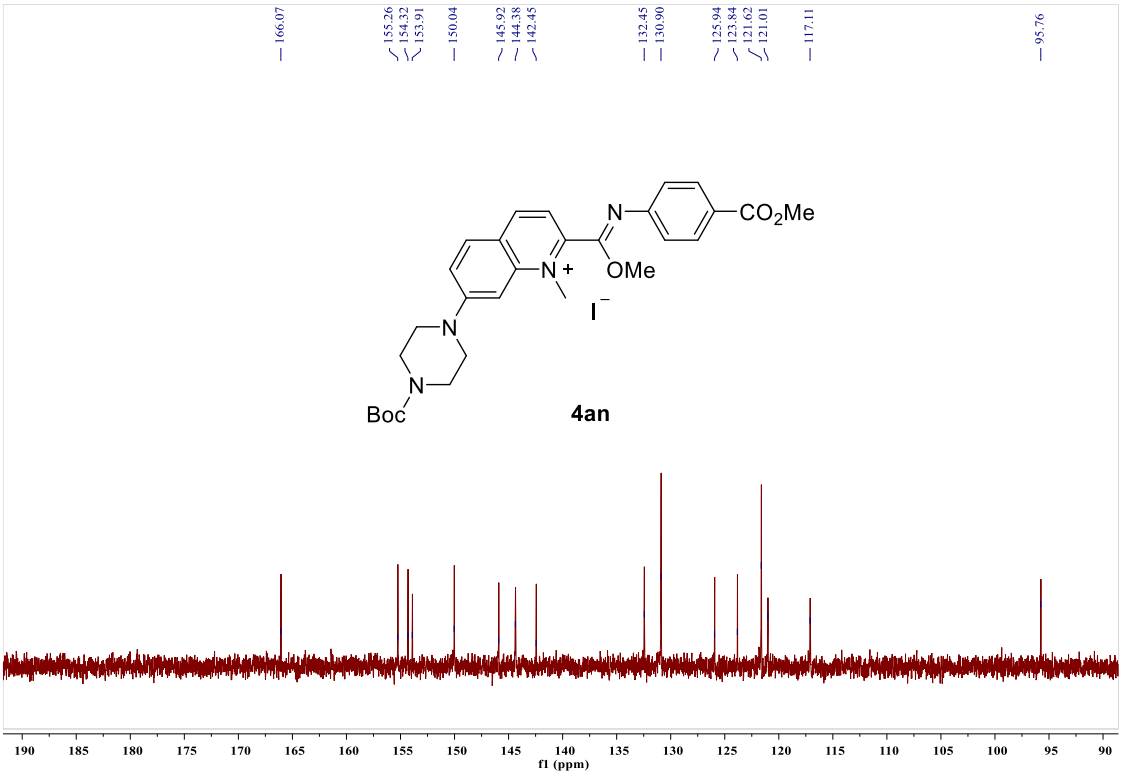
8.0808
8.0118
7.8062
7.7880
7.7729
7.7517
7.6247
7.6048
7.0585
7.0530
7.0055
7.0006
6.9890
6.9841
4.2693
4.1677
3.8021
3.7929
3.7894
3.7838
3.7753
3.7461
3.5435
3.5353
3.5298
3.5263
3.5170
1.4400
CO2Me
N
N+
OMe
I−
N
N
Boc
4an
1.067
1.111
1.046
2.035
1.000
1.025
2.028
3.085
3.035
4.051
3.057
4.136
9.094
f1 (ppm)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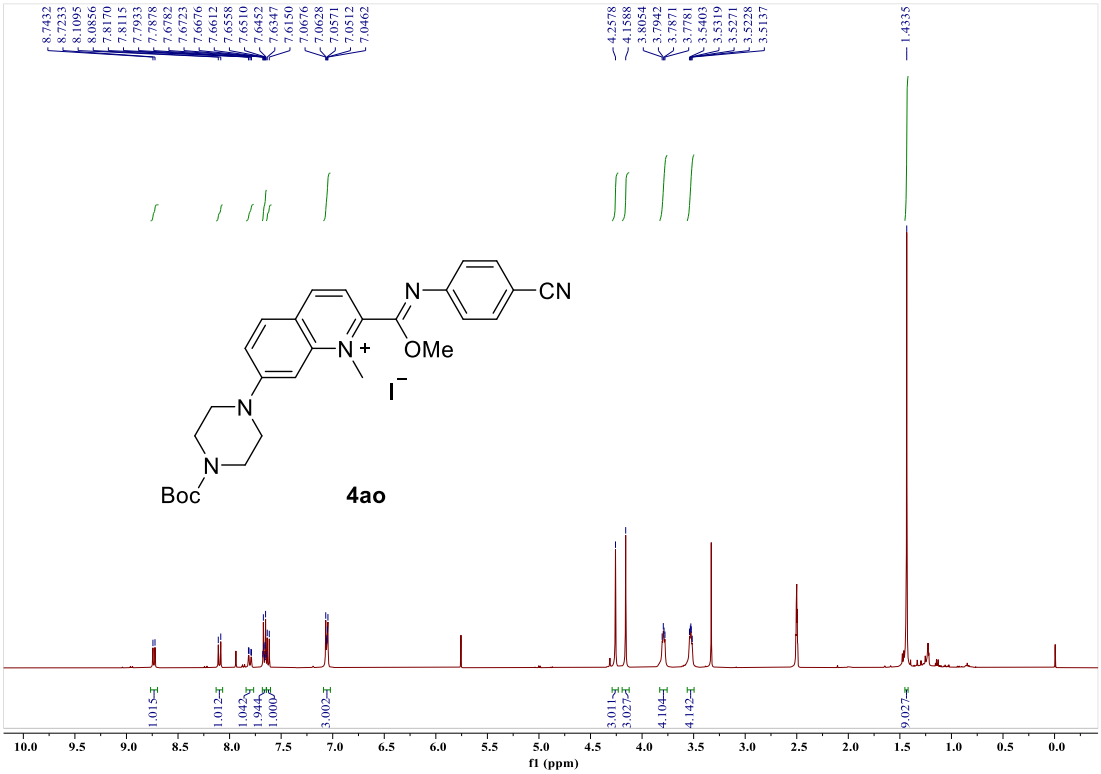
154.32
153.91
150.04
145.92
144.38
142.45
132.45
130.90
125.94
123.84
121.62
121.01
117.11
95.76
CO2Me
N
N+
OMe
I−
N
N
Boc
4an
f1 (ppm)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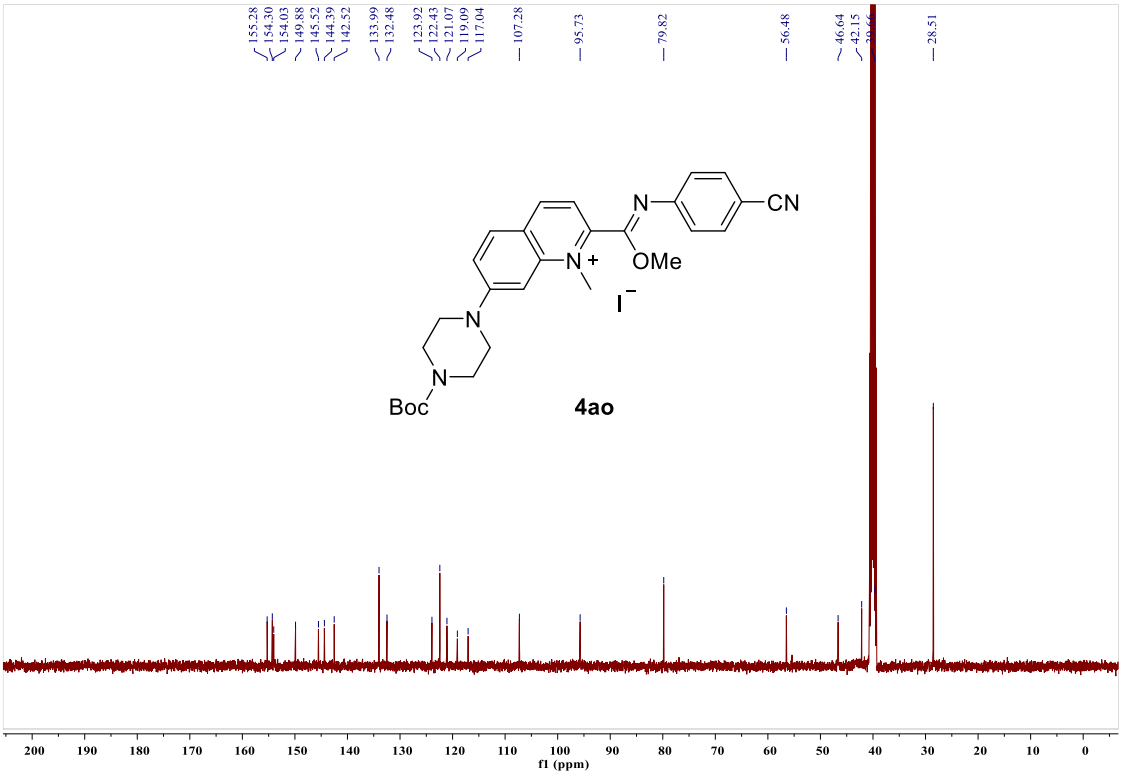
8.1095
8.0856
7.8170
7.8115
7.7933
7.7878
7.6782
7.6723
7.6676
7.6612
7.6558
7.6510
7.6452
7.6347
7.6150
7.0676
7.0628
7.0571
7.0512
7.0462
4.2578
4.1588
3.8054
3.7942
3.7871
3.7781
3.5403
3.5319
3.5271
3.5228
3.5137
1.4335
N
CN
N+
OMe
I−
N
N
Boc
4ao
1.015
1.012
1.042
1.944
1.000
3.002
3.011
3.027
4.104
4.142
9.027
f1 (ppm)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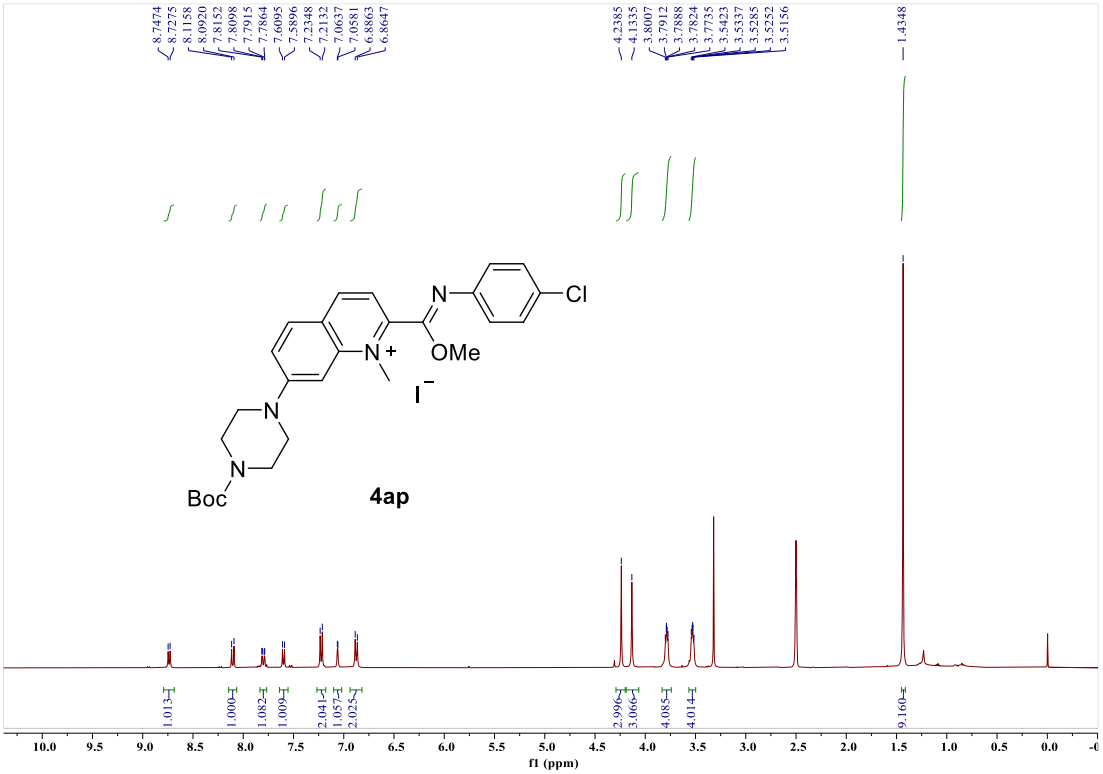
154.30
154.03
149.88
145.52
144.39
142.52
133.99
132.48
123.92
122.43
121.07
119.09
117.04
107.28
95.73
79.82
56.48
46.64
42.15
28.51
N
CN
N+
OMe
I−
N
N
Boc
4ao
f1 (ppm)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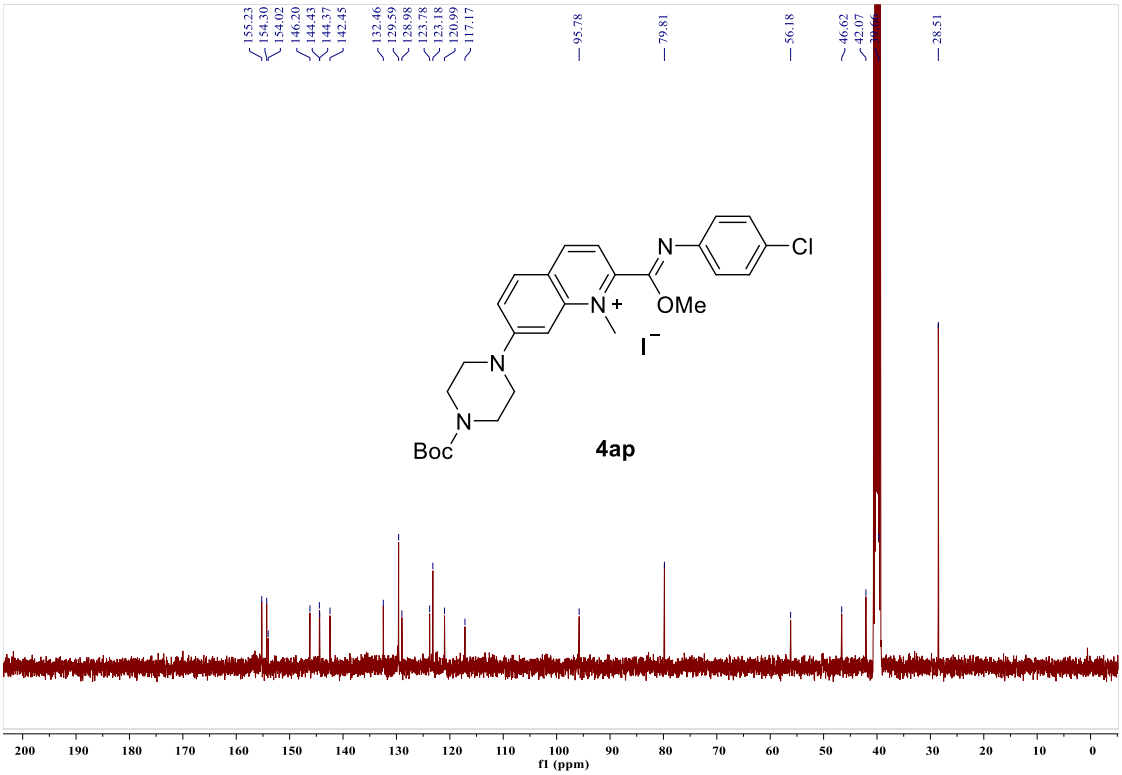
8.1158
8.0920
7.8152
7.8098
7.7915
7.7864
7.6095
7.5896
7.2348
7.2132
7.0637
7.0581
6.8863
6.8647
4.2385
4.1335
3.8007
3.7912
3.7888
3.7824
3.7735
3.5423
3.5337
3.5285
3.5252
3.5156
1.4348
N
Cl
N+
OMe
I−
N
N
Boc
4ap
1.013
1.000
1.082
1.009
2.041
1.057
2.025
2.996
3.066
4.085
4.014
9.160
f1 (ppm)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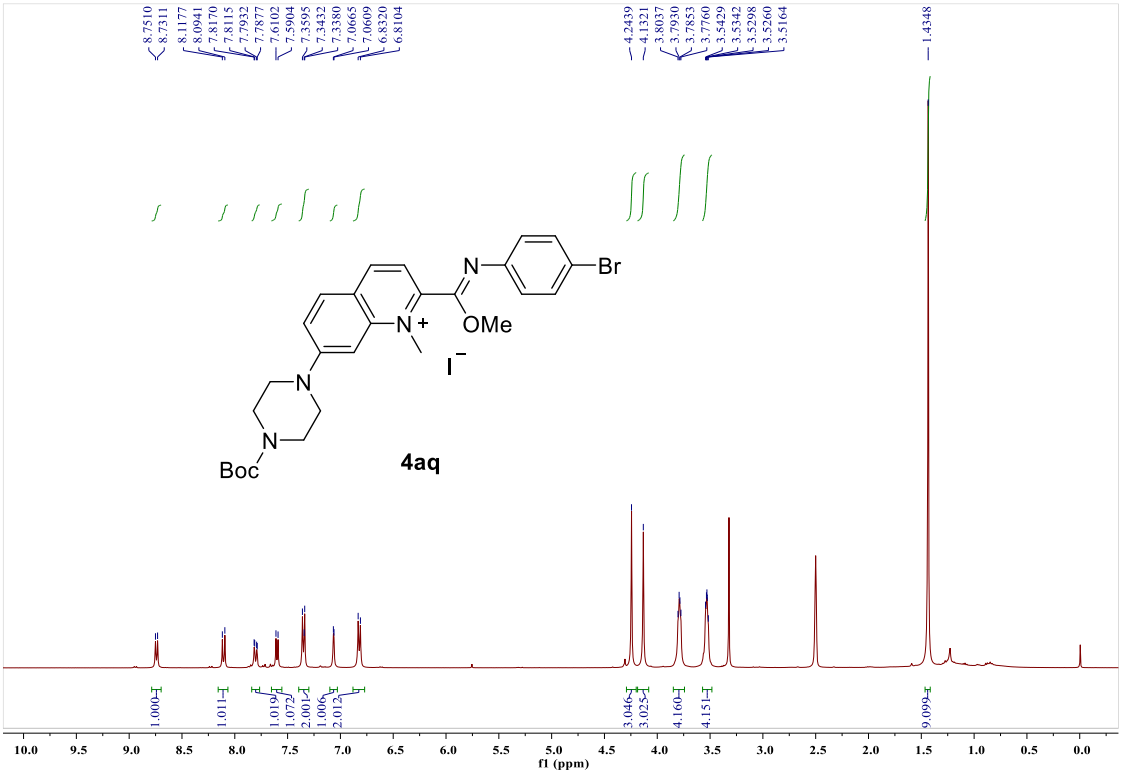
154.30
154.02
146.20
144.43
144.37
142.45
132.46
129.59
128.98
123.78
123.18
120.99
117.17
95.78
79.81
56.18
46.62
42.07
28.51
N
Cl
N+
OMe
I−
N
N
Boc
4ap
f1 (ppm)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8.1177
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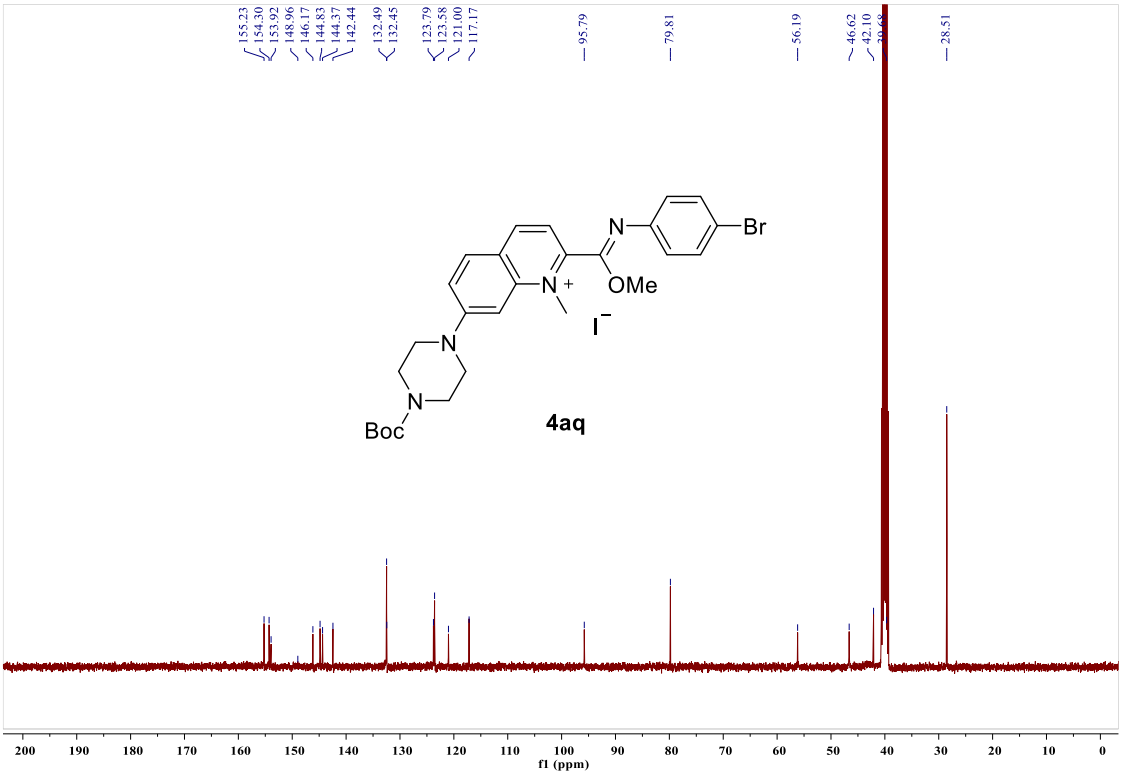
7.7877
7.6102
7.5904
7.3595
7.3432
7.3380
7.0665
7.0609
6.8320
6.8104
4.2439
4.1321
3.8037
3.7930
3.7853
3.7760
3.5429
3.5342
3.5298
3.5260
3.5164
1.4348
N
Br
N+
OMe
I−
N
N
Boc
4aq
1.000
1.011
1.019
1.072
2.001
1.006
2.012
3.046
3.025
4.160
4.151
9.099
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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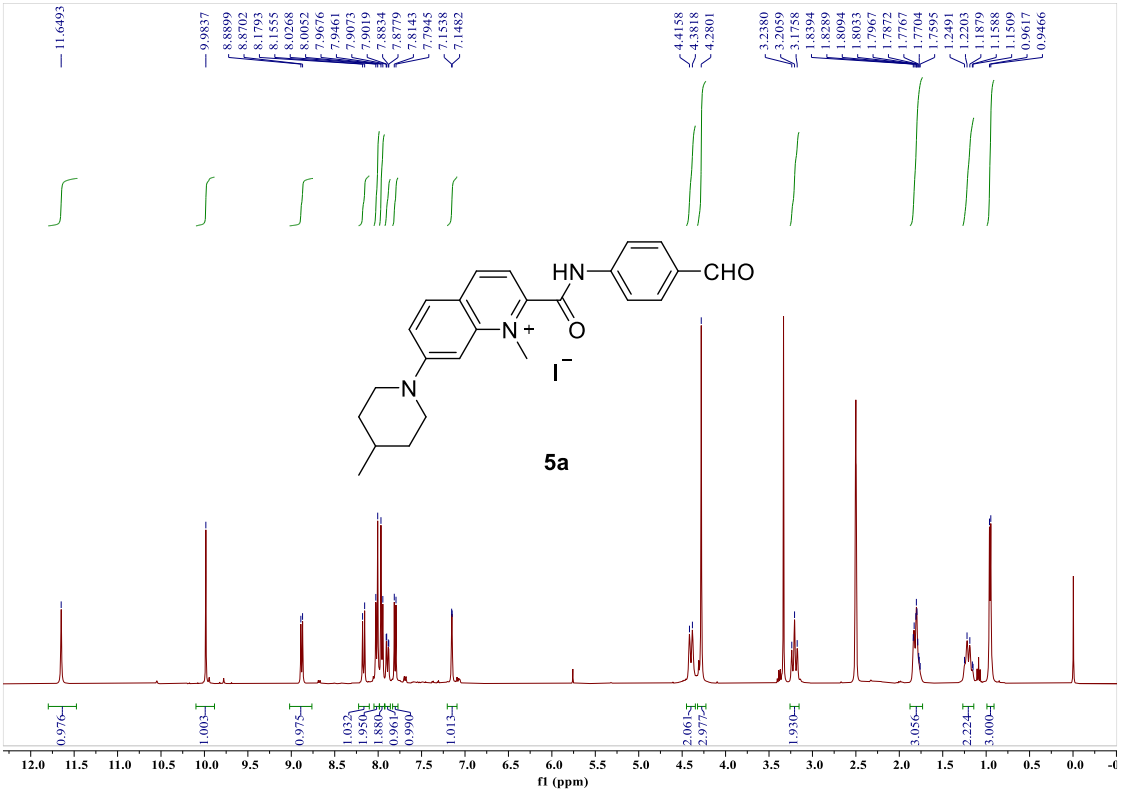
154.30
153.92
148.96
146.17
144.83
144.37
142.44
132.49
132.45
123.79
123.58
121.00
117.17
95.79
79.81
56.19
46.62
42.10
28.51
N
Br
N+
OMe
I−
N
N
Boc
4aq
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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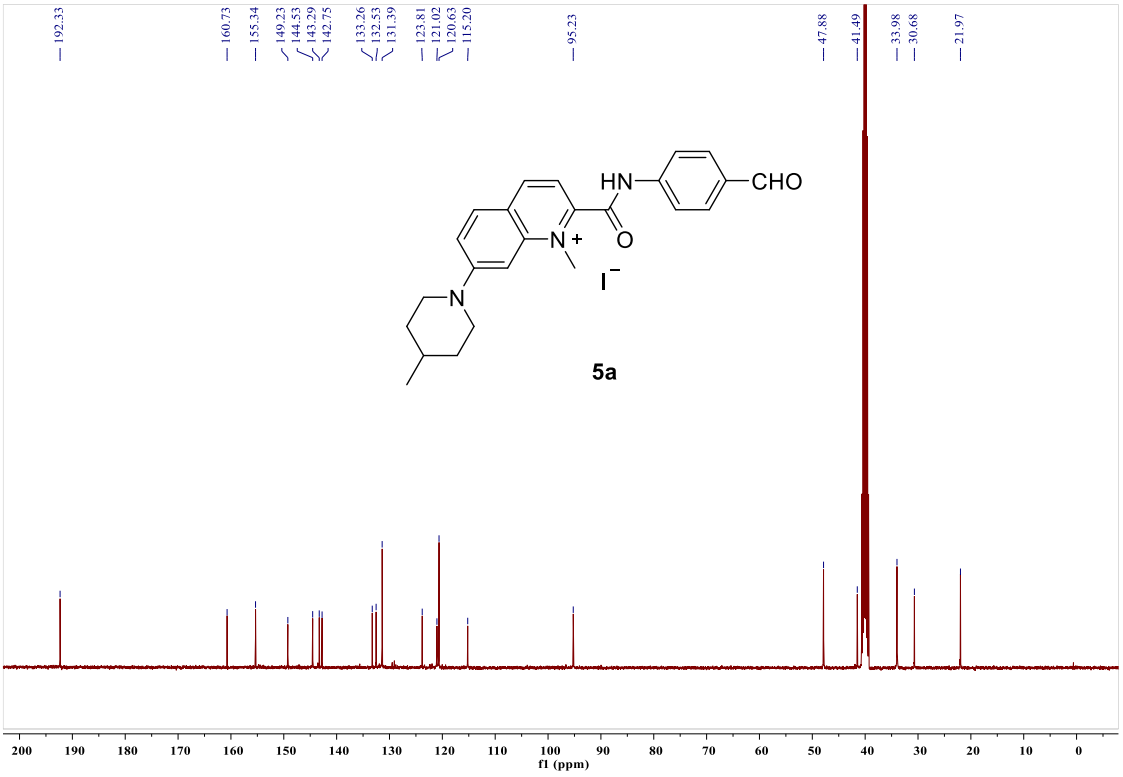
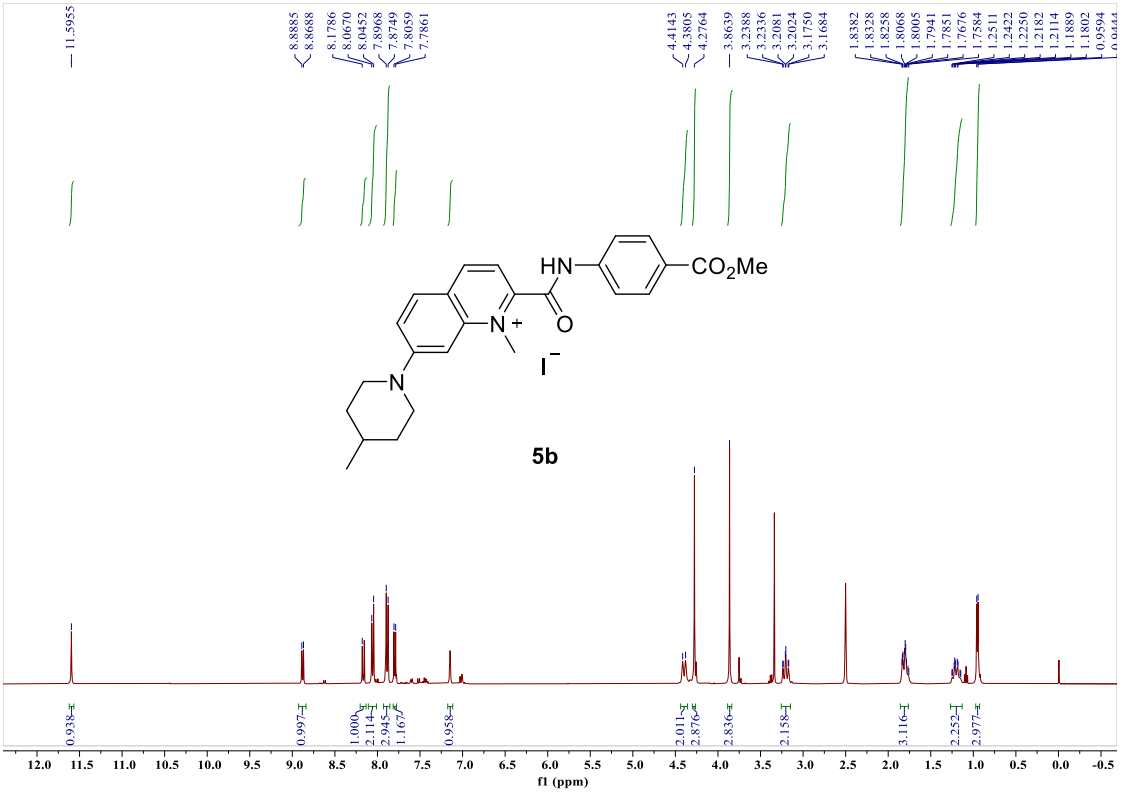
CHO
N+
O
I−
N
5a
f1 (ppm)


HN
CHO
N+
O
I−
N
5a
f1 (ppm)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8.1786
8.0670
8.0452
7.8968
7.8749
7.8059
7.7861
4.4143
4.3805
4.2764
3.8639
3.2388
3.2336
3.2081
3.2024
3.1750
3.1684
1.8382
1.8328
1.8258
1.8068
1.8005
1.7941
1.7851
1.7676
1.7584
1.2511
1.2422
1.2250
1.2182
1.2114
1.1889
1.1802
0.9594
HN
CO2Me
N+
O
I−
N
5b
0.938
0.997
1.000
2.114
2.945
1.167
0.958
2.011
2.876
2.836
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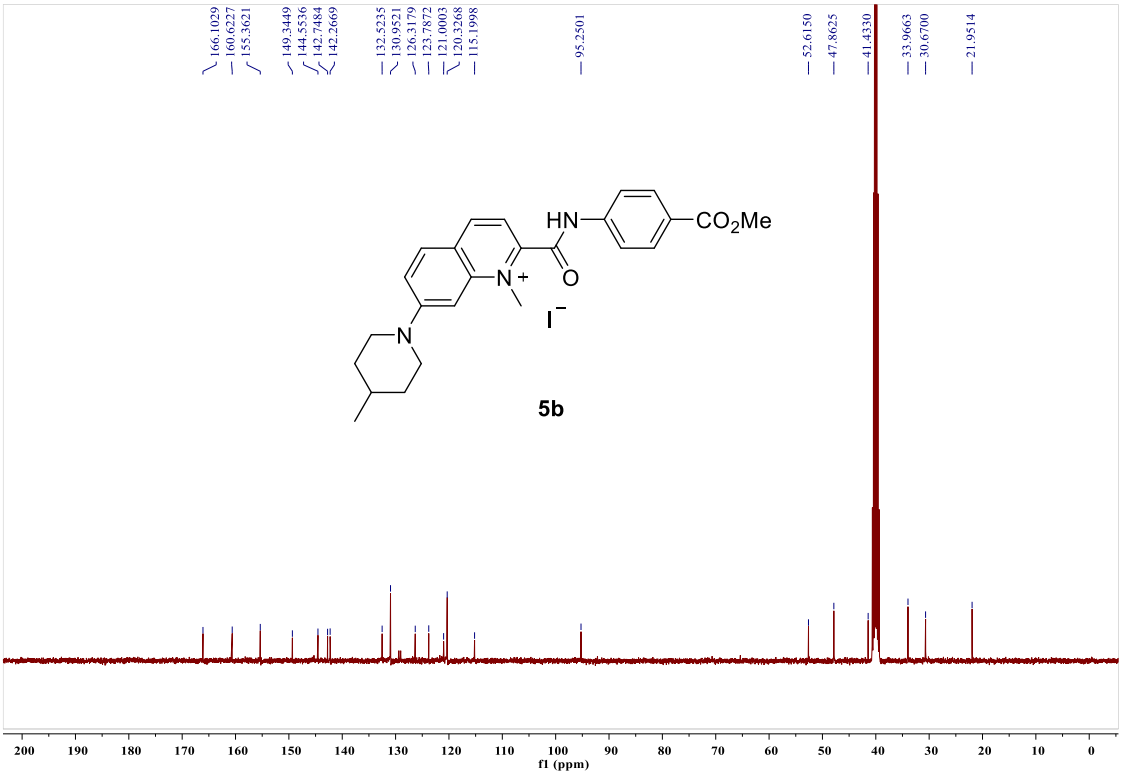
3.116
2.252
2.977
f1 (ppm)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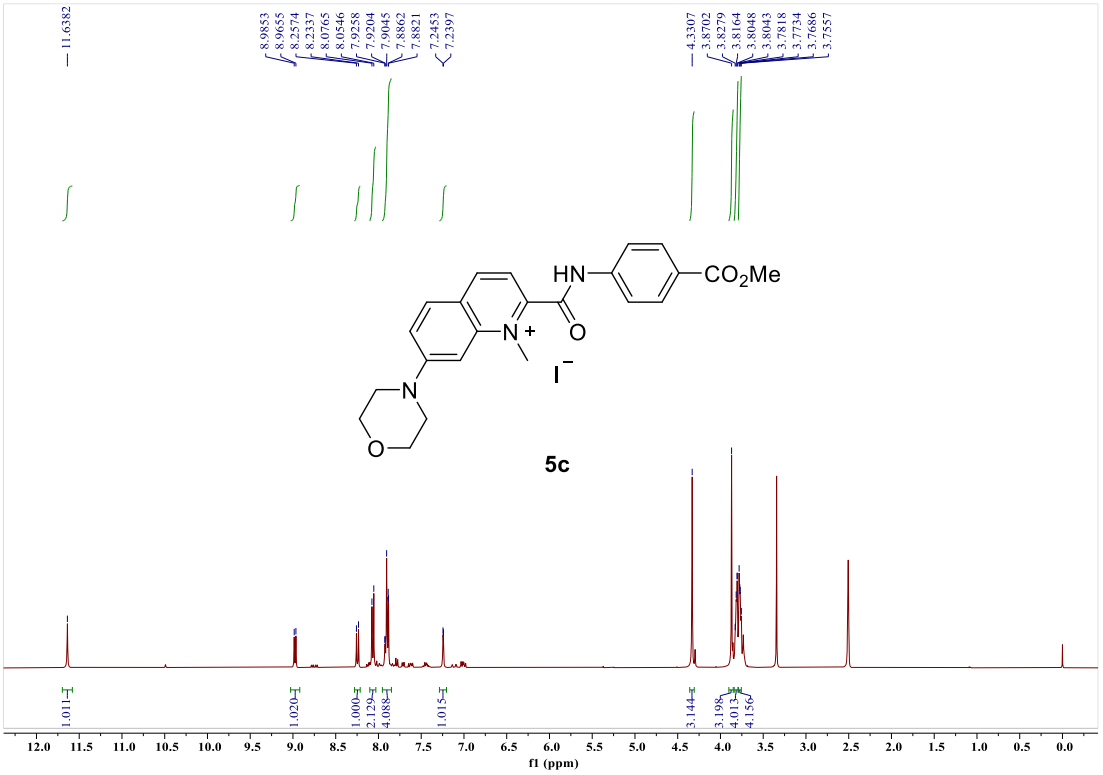
144.5536
142.7484
142.2669
132.5235
130.9521
126.3179
123.7872
121.0003
120.3268
115.1998
95.2501
52.6150
47.8625
41.4330
33.9663
30.6700
21.9514
HN
CO2Me
N+
O
I−
N
5b
f1 (ppm)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8.9655
8.2574
8.2337
8.0765
8.0546
7.9258
7.9204
7.9045
7.8862
7.8821
7.2453
7.2397
4.3307
3.8702
3.8279
3.8164
3.8048
3.8043
3.7818
3.7734
3.7686
3.7557
HN
CO2Me
N+
O
I−
N
O
5c
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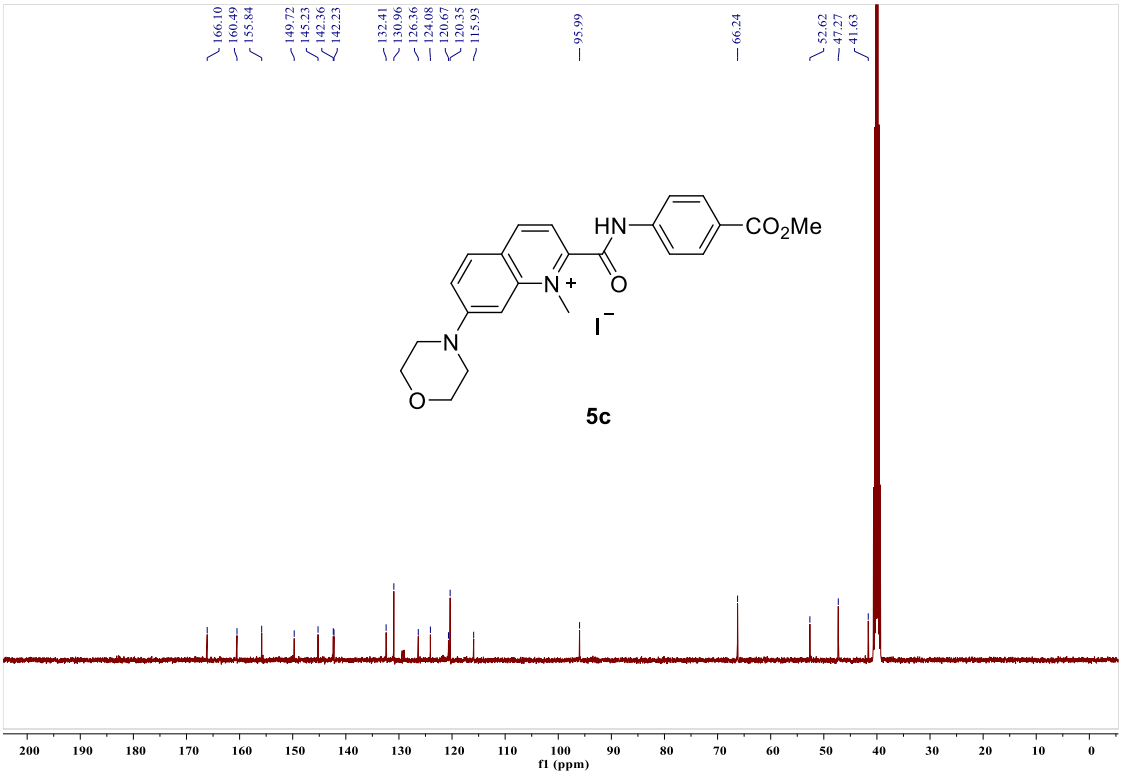
1.020
1.000
2.129
4.088
1.015
3.144
3.198
4.013
4.156
f1 (ppm)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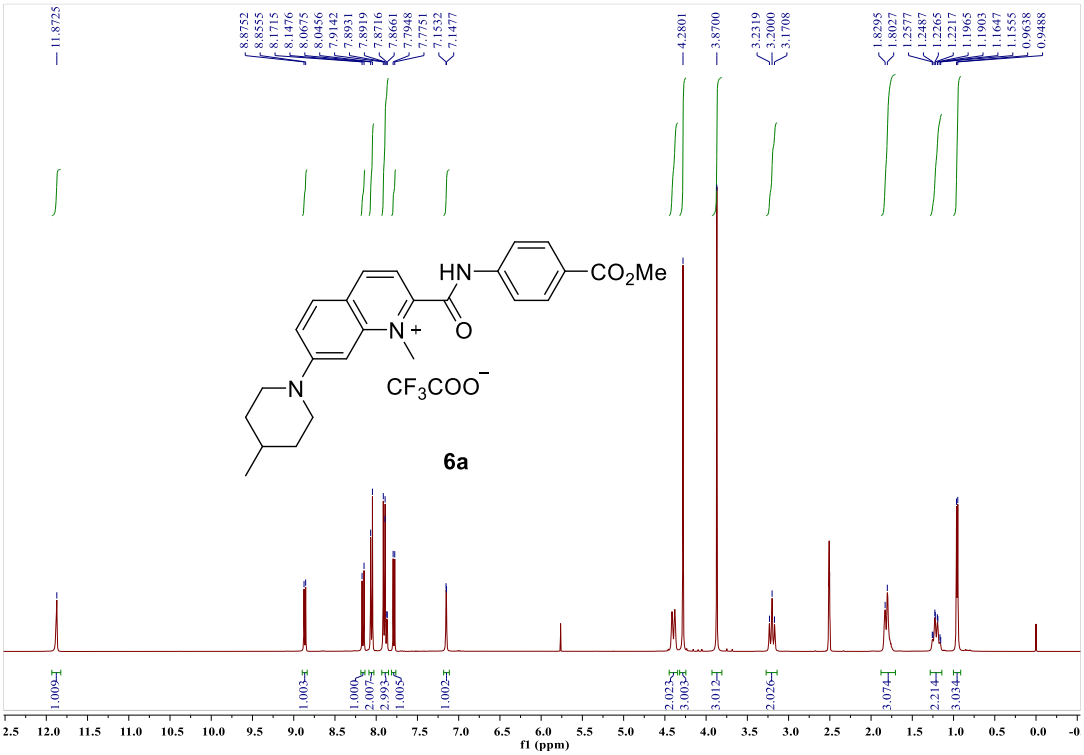
160.49
155.84
149.72
145.23
142.36
142.23
132.41
130.96
126.36
124.08
120.67
120.35
115.93
95.99
66.24
52.62
47.27
41.63
HN
CO2Me
N+
O
I−
N
O
5c
f1 (ppm)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8.1715
8.1476
8.0675
8.0456
7.9142
7.8931
7.8919
7.8716
7.8661
7.7948
7.7751
7.1532
7.1477
4.2801
3.8700
3.2319
3.2000
3.1708
1.8295
1.8027
1.2577
1.2487
1.2265
1.2217
1.1965
1.1903
1.1647
1.1555
0.9638
0.9488
HN
CO2Me
O
N+
N
CF3COO−
6a
1.009
1.003
1.000
2.007
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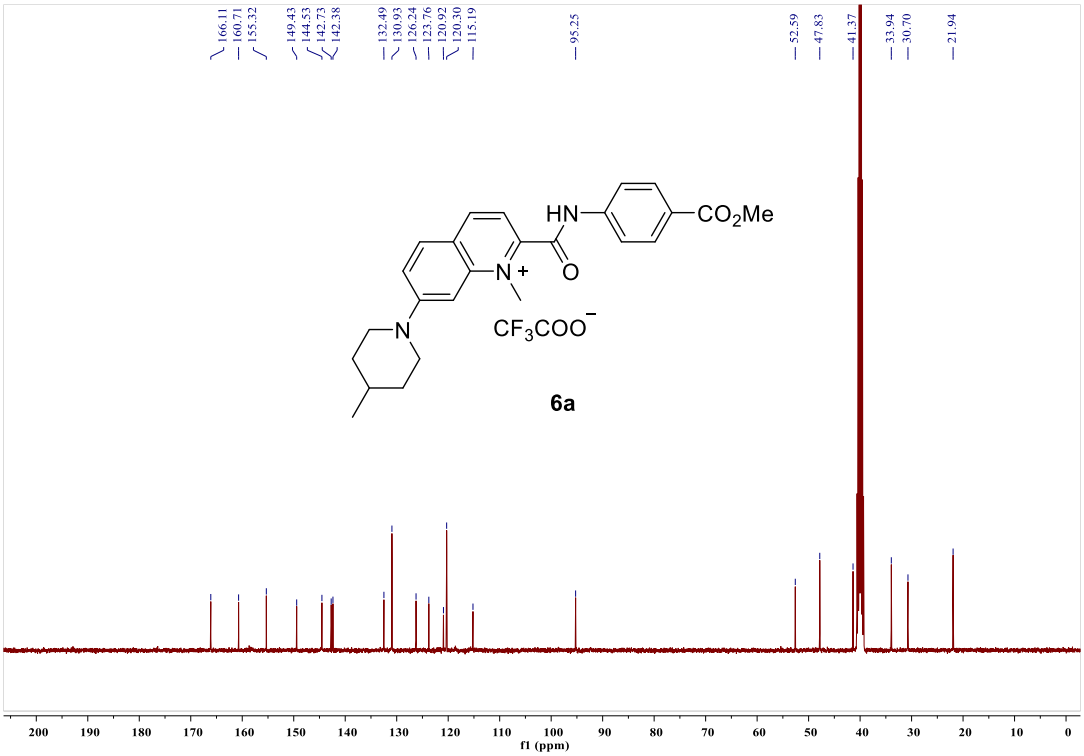
1.005
1.002
2.023
3.003
3.012
2.026
3.074
2.214
3.034
f1 (ppm)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144.53
142.73
142.38
132.49
130.93
126.24
123.76
120.92
120.30
115.19
95.25
52.59
47.83
41.37
33.94
30.70
21.94
HN
CO2Me
O
N+
N
CF3COO−
6a
f1 (ppm)