Supplementary Information

Bifunctional phase-transfer catalysts for fixation of CO_2 with epoxides under ambient pressure

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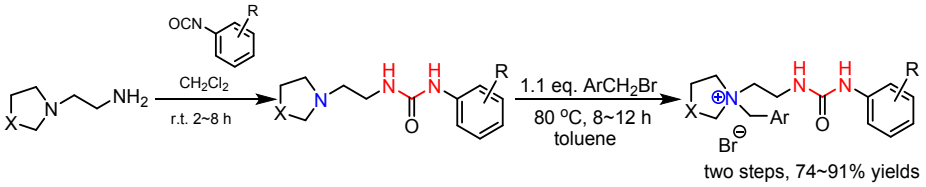
General

^{1}H NMR, ^{13}C NMR, ^{19}F and ^{31}P spectra were recorded at room temperature using 400 MHz *Bruker spectrometer*. The data are reported as follows: chemical shift δ in ppm (from internal tetramethylsilane on the δ scale in case of ^{1}H and $CDCl_3$ triplet in case of ^{13}C), multiplicity (br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz) and integration. High resolution mass spectra were obtained by peak matching on *BrukermaXis Spectrometer*. Melting points are reported uncorrected and measured on *Fukai-X-6* melting point apparatus. HPLC data were recorded on *Agilent 1260* with UV detector. Analytical thin layer chromatography was performed on 0.25 mm silica gel plates with UV-254 fluorescent indicator. Flash column chromatography was performed using indicated solvent system on 200~300 mesh silica gel (SiO_2). All air- and water-sensitive reactions were carried out under an inert atmosphere in glassware, which had been oven-dried as per standard procedure. Unless otherwise noted, all reagents were commercially obtained and used without further purification. Benzyl chloride and benzyl bromide were freshly distilled and used in following steps.

1. The synthesis of achiral phase-transfer catalysts (APTCs)

A. Synthesis of **APTCs** with a urea group



APTC-1: X = CH_2, R = 3,5-$(CF_3)_2$, Ar = Ph, 91% yield; **APTC-4**: X = CH_2O, R = 3,5-$(CF_3)_2$, Ar = Ph, 89% yield;
APTC-6: X = CH_2, R = 4-CH_3, Ar = Ph, 79% yield; **APTC-7**: X = CH_2, R = 3,5-$(CH_3)_2$, Ar = Ph, 74% yield;
APTC-8: X = CH_2, R = 3,5-$(CF_3)_2$, Ar = 4-$CF_3C_6H_4$, 83% yield; **APTC-9**: X = CH_2, R = 4-CH_3, Ar = 4-$CF_3C_6H_4$, 85% yield;
APTC-10: X = CH_2, R = 3,5-$(CH_3)_2$, Ar = 4-$CF_3C_6H_4$, 83% yield.

Typical procedure:

To 1.0 mmol of 2-(pyrrolidin-1-yl)ethan-1-amine (115 mg) in dry CH_2Cl_2 (4.0 mL) was added by 1.05 mmol of 3,5-bistrifluorometylphenylisocyanate (270 mg) in dry CH_2Cl_2 (1.0 mL) at room temperature (r.t.). The mixture was stirred for 8 h under inert atmosphere. When TLC indicates the complete consumption of starting materials, the reaction mixture was evaporated under reduced pressure to yield a light yellow glue which was purified by a flash column chromatography (petroether/ethyl acetate = 2/1, v/v) to give pure urea product as off-white powder (351 mg, 95% yield). To the above-prepared urea in dry toluene (4.0 mL) was added by 1.05 mmol of BnBr (180 mg) in dry toluene (1.0 mL) at room temperature (r.t.). The mixture was heated to 80 °C by an oil-bath and stirred for 12 h under inert atmosphere. The reaction mixture was cooled to r.t. and the precipitate was collected and washed by dry Et_2O for three to five times. This precipitate was dried under a reduced pressure to give **APTC-1** as a pale powder (490 mg, 91% yield in two steps) which was used directly without further purification.

APTC-4 and **APTC-6~10** was obtained by using the same procedure as **APTC-1**, respectively.

APTC-1: pale powder, 91% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.45 (s, 1H), 8.06 (s, 2H), 7.90 (t, J = 5.76 Hz, 1H), 7.57-7.48 (m, 4H), 7.45 (s, 1H), 4.75 (s, 2H), 4.02-3.98 (m, 2H), 3.86-3.73 (m, 4H), 3.62 (t, J = 5.72 Hz, 2H), 2.33 (m, 2H), 2.19 (m, 2H), 1.80 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 155.89, 141.16, 132.55, 131.98, 131.65, 131.19, 129.74, 126.90, 124.69, 121.98, 117.97, 115.13, 62.61, 61.43, 59.59, 58.41, 34.97, 21.30, 18.44; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -62.90; HRMS (ESI) *m/z* calcd. for $C_{22}H_{24}F_6N_3O^+$ $[M\text{-}Br]^+$: 460.1818, found 460.1829.

APTC-4: white powder, 89% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.52 (s, 1H), 8.03 (s, 2H), 7.61-7.44 (m, 6H), 7.28 (s, 1H), 5.08 (s, 2H), 4.13-4.00 (m, 7H), 3.88-3.85 (m, 2H), 3.54 (bs, 2H), 1.95 (bs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 155.75, 140.92, 133.31, 132.10, 131.76, 131.41, 129.70, 125.37, 124.64, 121.93, 117.99, 115.38, 66.34, 60.38, 56.81, 56.32, 33.97; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -62.91; HRMS (ESI) *m/z* calcd. for $C_{22}H_{24}F_6N_3O_2^+$ $[M\text{-}Br]^+$: 476.1767, found 476.1779.

APTC-6: white powder, 79% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.66 (bs, 1H), 7.53-7.39 (m, 8H), 7.00 (s, 2H), 4.75 (s, 2H), 3.87-3.46 (m, 8H), 2.24 (s, 3H), 2.11-2.06 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.37, 136.79, 132.67, 131.76, 130.85, 129.55, 129.30, 127.36, 118.98, 62.49, 61.30, 59.44, 34.99, 21.27, 20.73; HRMS (ESI) *m/z* calcd. for $C_{21}H_{28}N_3O^+$ $[M\text{-}Br]^+$: 338.2227, found 338.2234.

APTC-7: white powder, 74% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.76 (s, 1H), 8.37 (s, 1H), 7.57-7.49 (m, 3H), 7.47-7.43 (m, 2H), 7.15 (s, 2H), 6.64 (s, 1H), 4.54 (s, 2H), 3.95-3.94 (m, 2H), 3.61 (m, 4H), 3.47 (m, 2H), 2.27 (s, 6H), 2.25 (s, 2H), 2.11 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.73, 138.43, 132.36, 131.14, 129.75, 126.92, 116.95, 62.00, 61.31, 60.01, 34.92, 21.36, 21.10; HRMS (ESI) *m/z* calcd. for $C_{22}H_{30}N_3O^+$ $[M\text{-}Br]^+$: 352.2383, found 352.2392.

APTC-8: white powder, 83% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.58 (s, 1H), 8.03 (s, 2H), 7.81 (d, *J* = 7.76 Hz, 2H), 7.67 (d, *J* = 7.84 Hz, 2H), 7.53 (bs, 1H), 7.42 (s, 1H), 5.01 (s, 2H), 4.05 (d, *J* = 5.12 Hz, 2H), 3.87 (br, 2H), 3.74-3.71 (m, 2H), 3.66 (br, 2H), 2.27 (s, 2H), 2.15 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 155.83, 141.05, 133.29, 133.01, 131.86, 130.88, 129.35, 128.23, 126.49, 124.62, 121.91, 117.85, 115.25, 61.73, 61.45, 59.61, 35.11, 21.22; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -62.99, -63.26; HRMS (ESI) *m/z* calcd. for $C_{23}H_{23}F_9N_3O^+$ $[M\text{-}Br]^+$: 528.1692, found 528.1698.

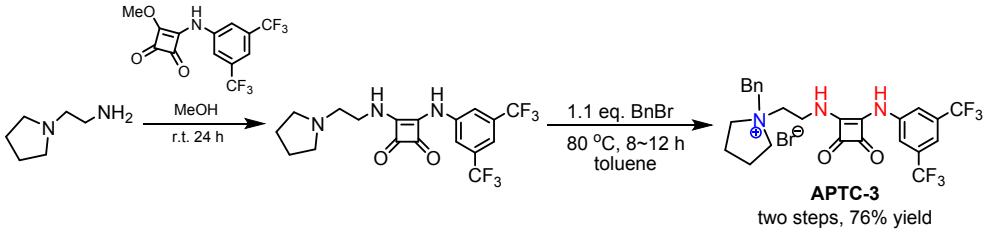
APTC-9: white powder, 85% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.69 (s, 1H), 7.76 (d, *J* = 7.0 Hz, 2H), 7.58 (d, *J* = 7.04 Hz, 2H), 7.36 (d, *J* = 6.72 Hz, 3H), 7.01 (d, J = 7.36 Hz, 2H), 4.99 (s, 1H), 3.95 (s, 2H), 3.76 (s, 2H), 3.71 (s, 2H), 3.53 (s, 1H), 2.25 (s, 3H), 2.12 (br, 2H), 2.07 (br, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.34, 136.62, 133.39, 132.91, 132.58, 132.05, 131.29, 129.38, 126.30, 124.72, 122.01, 118.95, 61.59, 61.34, 59.51, 35.15, 21.18, 20.67; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -63.08; HRMS (ESI) *m/z* calcd. for $C_{22}H_{27}F_3N_3O^+$ $[M\text{-}Br]^+$: 406.2101, found 406.2107.

APTC-10: white powder, 83% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.47 (s, 1H), 7.74 (s, 2H), 7.67 (s, 2H), 7.05 (m, 2H), 6.63 (s, 1H), 4.87 (s, 2H), 3.90~3.52 (dd, *J* = 1.96, 6.56 Hz, 8H), 2.23 (s, 6H), 2.11 (br, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.21, 138.87, 138.52, 133.26, 131.22, 126.44, 124.43, 116.57, 61.53, 59.42, 49.51, 49.30, 34.89, 21.34, 21.37; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -63.15; HRMS (ESI) *m/z* calcd. for $C_{23}H_{29}F_3N_3O^+$ $[M\text{-}Br]^+$: 420.2257, found 420.2264.

B. Synthesis of **APTCs** with a squaramide group (**APTC-3**)

Step 1: To a solution of 3-((3,5-bis(trifluoromethyl)phenyl)amino)-4-methoxycyclobut-3-ene-1,2-dione (1.0 mmol) in MeOH (3 mL) was added a solution of 2-morpholinoethan-1-amine (1.0 mmol) in MeOH (2 mL) at r.t.. The mixture was stirred for 24 h. The reaction mixture was filtered, and the precipitate was washed with cold MeOH (2×1.0 mL) to afford pure squaramide.

Step 2: To 0.5 mmol of squaramide in anhydrous toluene (2.0 mL) was added by 0.6 mmol of BnBr in anhydrous toluene (1.0 mL) at room temperature (r.t.). The mixture was stirred for 12 h under inert atmosphere (checked by TLC) at 80 °C. The precipitate was collected and washed by anhydrous Et_2O (3×1.0 mL) to afford pure phase-transfer catalysts.

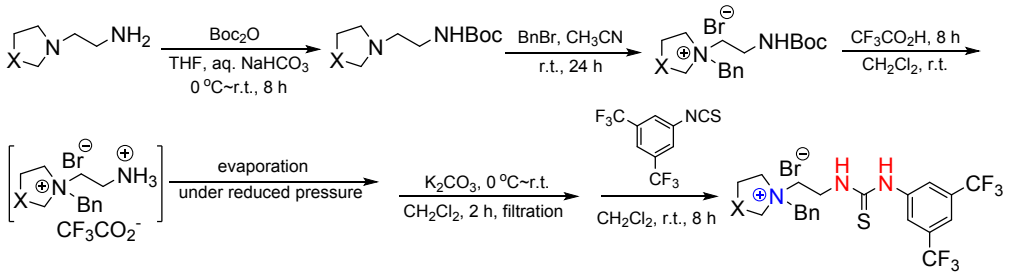


APTC-3: white powder, 76% yield; ^{1}H NMR (400 MHz, DMSO-d_6) δ: 10.84 (s, 1H), 8.27 (br, 1H), 8.12 (s, 2H), 7.69 (br, 1H), 7.64 (d, *J* = 5.08 Hz, 2H), 7.55 (m, 3H), 4.85, (s, 2H), 4.24 (s, 2H), 3.59 (s, 4H), 3.45 (s, 2H), 2.07 (s, 4H); ^{13}C NMR (100 MHz, DMSO-d_6) δ: 170.09, 163.94, 141.47, 133.18, 131.66, 130.86, 129.64, 128.80, 124.96, 122.25, 118.51, 115.51, 62.56, 61.43, 58.98, 38.53, 21.47; ^{19}F NMR (376 MHz, DMSO-d_6) δ: -61.73;

HRMS (ESI) *m/z* calcd. for $C_{25}H_{24}F_6N_3O_2^+$ [M-Br]$^+$: 512.1767, found 512.1777.

Synthesis of **APTCs** with a thiourea group (**APTC-2** and **APTC-5**)

APTC-2 and APTC-5 were synthesized according to the literature procedure.[1]

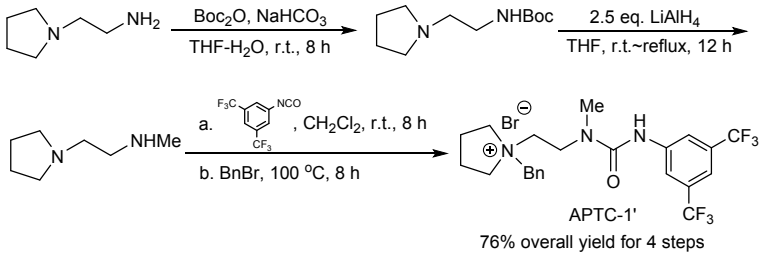


APTC-2: X = CH_2, 47% overall yields in 4 steps; **APTC-5**: X = CH_2O, 42% overall yields in 4 steps

APTC-2: light yellow powder, 47% yield for 4 steps; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.49 (s, 1H), 7.38-7.24 (m, 5H), 7.21 (s, 2H), 4.30 (s, 2H), 3.85-3.82 (m, 2H), 3.37-3.35 (m, 6H), 2.18-2.14 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 154.10, 150.74, 135.97, 132.80, 129.02, 128.66, 127.68, 124.79, 122.86, 122.08, 116.06, 55.26, 54.83, 39.09, 36.08, 23.35; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -62.80; HRMS (ESI) *m/z* calcd. for $C_{22}H_{24}F_6N_3S^+$ [M-Br]$^+$: 476.1590, found 476.1598.

APTC-5: light yellow powder, 42% yield for 4 steps; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.49 (s, 1H), 7.32-7.27 (m, 5H), 7.20 (s, 2H), 4.93 (s, 2H), 4.06 (s, 2H), 3.68 (t, J = 4.68 Hz, 4H), 2.56 (t, J = 6.52 Hz, 2H), 2.49 (br, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 151.11, 133.39, 132.93, 128.83, 128.60, 127.81, 124.85, 122.83, 122.14, 115.78, 66.78, 56.33, 53.10, 38.85, 35.78; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -64.22; HRMS (ESI) *m/z* calcd. for $C_{22}H_{24}F_6N_3OS^+$ [M-Br]$^+$: 492.1539, found 492.1543.

C. Synthesis of **APTC-1'(mono-NMe-APTC-1)**



76% overall yield for 4 steps

The free amino group (-NH_2) in 2-(pyrrolidin-1-yl)ethan-1-amine (330 mg) was protected by Boc_2O in the mixed solvent of THF-H_2O in the presence of $NaHCO_3$ to provide N-Boc-2-(pyrrolidin-1-yl)ethan-1-amine in quant. Yield which was directed reduced by 2.5 eq. $LiAlH_4$ in THF following by addition of 3,5-bistrifluorometylphenylisocyanate to give urea. To the above-prepared urea in dry toluene (4.0 mL) was added by 1.1 eq. of BnBr in dry toluene (1.0 mL) at room temperature (r.t.). The mixture was heated to 100 °C by an oil-bath and stirred for 8 h under inert atmosphere. The reaction mixture was cooled to r.t. and the precipitate was collected and washed by dry Et_2O for three to five times. This precipitate was dried under a reduced pressure to give **APTC-1'** as a white powder (76% overall yield for 4 steps) which was used directly without further purification.

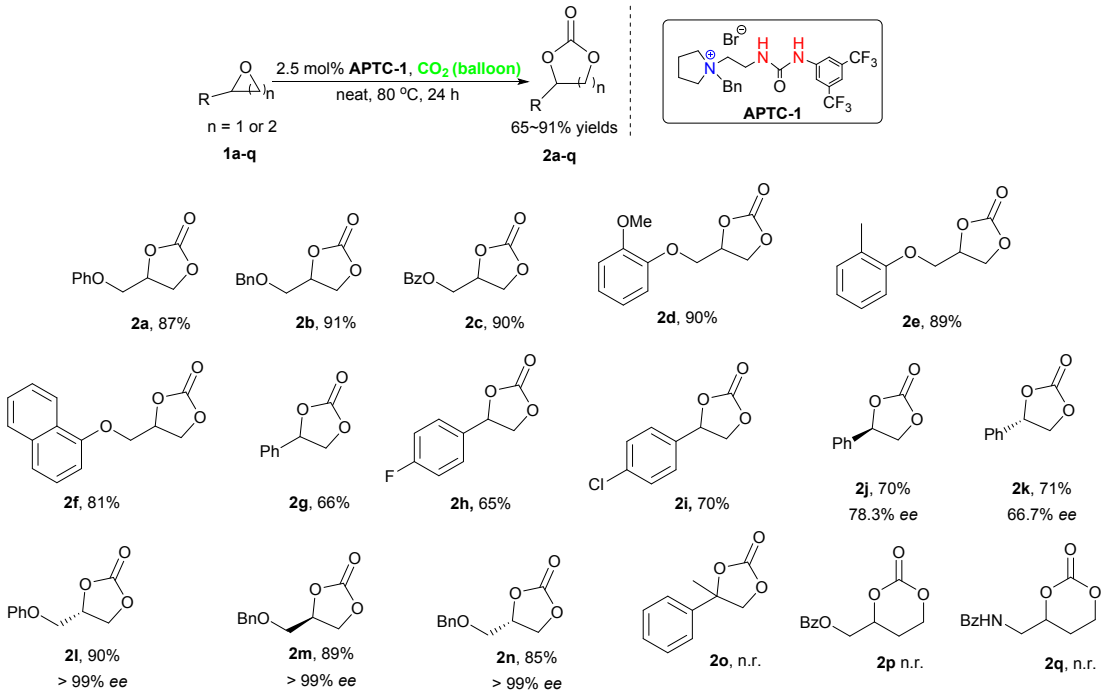
APTC-1': white powder, ^{1}H NMR (400 MHz, $CDCl_3$ plus one drop of MeOD) δ: 8.04 (s, 2H), 7.50-7.48 (m, 6H), 4.57 (s, 2H), 4.02 (t, J = 5.64 Hz, 2H), 3.88-3.84 (m, 2H), 3.74 (t, J = 5.76 Hz, 2H), 3.61-3.57 (m, 2H), 3.25 (s, 3H, N-Me), 2.34 (m, 2H), 2.07 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$ plus one drop of MeOD) δ: 156.18, 141.05, 132.50, 131.64, 131.12, 129.67, 127.07, 124.86, 121.95, 119.87, 116.03, 61.90, 61.00, 43.44, 35.86, 21.38; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -63.11.

2. The cycloaddition of CO_2 to epoxides by APTCs

Typical procedure:

A mixture of 0.5 mmol of epoxide **1a** and 2.5 mol% of **APTC-1** (6.8 mg) was heated at 80 °C for 24 h under CO_2 atmosphere (1atm, using a balloon). After cooled to room temperature, a small amount of CH_2Cl_2 was added to the mixture and it was purified by a flash column chromatography (petroether/ethyl acetate = 10/1 to 3/1, v/v) to give cyclic carbonate **2a** as off-white solid.

Table S1. **APTC-1** catalyzed cycloaddition of CO_2 to epoxides.



2a:[2] white powder, 87% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.32 (t, *J* = 8.36 Hz, 2H), 7.03 (t, *J* = 7.36 Hz, 1H), 6.92 (d, *J* = 7.96 Hz, 2H), 5.07-5.02 (m, 1H), 4.62 (t, *J* = 8.48 Hz, 1H), 4.54 (dd, *J* = 5.88, 2.52 Hz, 1H), 4.25 (dd, *J* = 6.76, 3.88 Hz, 1H), 4.14 (dd, *J* = 7.12, 3.52 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 157.78, 154.86, 129.71, 121.97, 114.61, 74.26, 66.87, 66.25; HRMS (ESI) *m/z* calcd. for $C_{10}H_{10}O_4Na^+$ $[M+Na]^+$: 217.0471, found 217.0473.

2b:[2] white powder, 91% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.41-7.33 (m, *5*H), 4.86-4.81 (m, 1H), 4.61(q, *J* = 10.08 Hz, 2H), 4.50 (t, *J* =8.36 Hz,1H), 4.40(dd, *J* = 6.04, 2.28 Hz, 1H), 3.73(dd, *J* = 7.12, 3.84 Hz, 1H), 3.63(dd, *J* = 7.28, 3.68 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 155.03, 137.11, 128.61, 128.11, 127.79, 75.06, 73.69, 68.84, 66.32; HRMS (ESI) *m/z* calcd. for $C_{11}H_{12}NaO_4^+$ $[M+Na]^+$: 231.0628, found 231.0631.

2c:[2] white powder, 90% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.05 (s, 1H), 8.03 (s, 1H), 7.62 (t, *J* = 7.40 Hz, 1H), 7.48 (t, *J* = 7.81 Hz, 2H), 5.10-5.06 (m, 1H), 4.67-4.59 (m, 2H), 4.53 (dd, *J* = 8.72, 3.88 Hz, 1H), 4.45 (dd, *J* = 5.64, 3.12 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.98, 154.53, 133.77, 129.80, 128.68, 73.94, 66.13, 63.66; HRMS (ESI) *m/z* calcd. for $C_{11}H_{10}NaO_5^+$ $[M+Na]^+$: 245.0420, found 245.0418.

2d:[2] white powder, 90% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.05-6.89 (m, 4H), 5.04-5.00 (m, 1H), 4.61 (d, *J* = 7.00 Hz, 2H), 4.22 (q, *J* = 4.44 Hz, 2H), 3.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 154.90, 150.36, 147.46, 123.41, 121.02, 116.59, 112.53, 74.58, 69.31, 66.37, 55.89; HRMS (ESI) *m/z* calcd. for $C_{11}H_{12}NaO_5^+$ $[M+Na]^+$: 247.0577, found 247.0589.

2e:[2] white powder, 89% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.18 (d, *J* = 4.60 Hz, 2H), 6.95 (t, *J* = 7.36 Hz, 1H), 6.80 (d, *J* = 8.44 Hz, 1H), 5.08-5.04 (m, 1H), 4.66-4.57 (m, 2H), 4.27 (dd, *J* = 7.56, 3.12 Hz, 1H), 4.13 (dd, *J* = 7.96, 2.72 Hz, 1H), 2.24 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 155.81, 154.92, 131.07, 127.07, 126.92, 121.64, 110.89, 74.34, 67.05, 66.27, 15.96; HRMS (ESI) *m/z* calcd. for $C_{11}H_{12}NaO_4^+$ $[M+Na]^+$: 231.0628, found 231.0624.

2f: [2] white powder, 81% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.14 (t, *J* = 5.24 Hz, 1H), 7.79 (t, *J* = 3.96 Hz, 1H), 7.52-7.47 (m, 3H), 7.35 (t, *J* = 7.60Hz, 1H), 6.77 (d, *J* = 7.60 Hz, 1H), 5.15 (m, 1H), 4.70-4.63 (m, 2H), 4.42 (dd,

J = 7.64, 3.08 Hz, 1H), 4.26 (d, *J* = 10.72 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 155.15, 153.37, 134.47, 127.53, 126.77, 125.84, 125.49, 125.19, 121.61, 121.47, 104.83, 74.39, 67.21, 66.40; HRMS (ESI) *m/z* calcd. for $C_{14}H_{12}NaO_4^+$ $[M+Na]^+$: 267.0628, found 267.0627.

2g:[2] white powder, 66% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.45-7.36 (m, 5H), 5.69 (t, *J* = 8.00 Hz, 1H), 4.81 (t, *J* = 8.40 Hz, 1H), 4.34 (dd, *J* = 7.84, 0.76 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 154.83, 135.81,129.76, 129.26, 125.89, 78.00, 71.18; HRMS (ESI) *m/z* calcd. for $C_9H_8NaO_3^+$ $[M+Na]^+$: 187.0366, found 187.0372.

2h:[2] white powder, 65% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.38 (t, *J* = 7.08 Hz, 2H), 7.15 (t, *J* = 8.08 Hz, 2H), 5.69 (t, *J* = 7.96 Hz, 1H), 4.82 (t, *J* = 8.68 Hz, 1H), 4.34 (t, *J* = 8.60 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 164.64, 162.16, 154.63, 131.58, 128.07, 127.99, 116.49, 116.27, 71.11; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -110.90; HRMS (ESI) *m/z* calcd. for $C_9H_7FNaO_3^+$ $[M+Na]^+$: 205.0271, found 205.0276.

2i:[2] white powder, 70% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.43 (d, *J* = 8.20 Hz, 2H), 7.32 (d, *J* = 8.16 Hz, 2H), 5.68 (t, *J* = 7.92 Hz, 1H), 4.82 (t, *J* = 8.40 Hz, 1H), 4.32 (t, *J* = 8.12 Hz, 1H); HRMS (ESI) *m/z* calcd. for $C_9H_7ClNaO_3$+ $[M+Na]^+$: 220.9976, found 220.9980.

2j: [2] white powder, 70% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.46 (br, 3H), 7.40 (br, 2H), 5.69 (t, *J* = 7.76 Hz, 1H), 4.82 (t, *J* = 8.24 Hz, 1H), 4.36 (t, *J* = 7.84 Hz, 1H), 2.19 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 154.77, 135.83, 129.74, 129.25, 125.85, 77.96, 71.14; HRMS (ESI) *m/z* calcd. for $C_9H_8NaO_3^+$ $[M+Na]^+$: 187.0366, found 187.0368; HPLC: Chiralpak OD-H (^{i}PrOH/*n*-Hexane) = 20:80, flow rate = 1.0 mL/min, 216 nm, *rac*-form: t_r = 12.051 and 14.617 min; *enan*-form: *R*-major t_r = 12.238 and *S*-minor t_r = 14.870 min, 78.3% *ee*.

2k:[2] white powder, 71% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.45 (br, 3H), 7.39 (br, 2H), 5.69 (t, *J* = 7.68 Hz, 1H), 4.82 (t, *J* = 8.28 Hz, 1H), 4.36 (t, *J* = 7.96 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 154.82, 135.85, 129.73, 129.24, 125.88, 77.99, 71.16; HRMS (ESI) *m/z* calcd. for $C_9H_8NaO_3^+$ $[M+Na]^+$: 187.0366, found 187.0368; HPLC: Chiralpak OD-H (^{i}PrOH/*n*-Hexane) = 20:80, flow rate = 1.0 mL/min, 216 nm, *rac*-form: t_r = 12.051 and 14.617 min; *enan*-form: *S*-major t_r = 15.007 and *R*-minor t_r = 14.876 min, 66.7% *ee*.

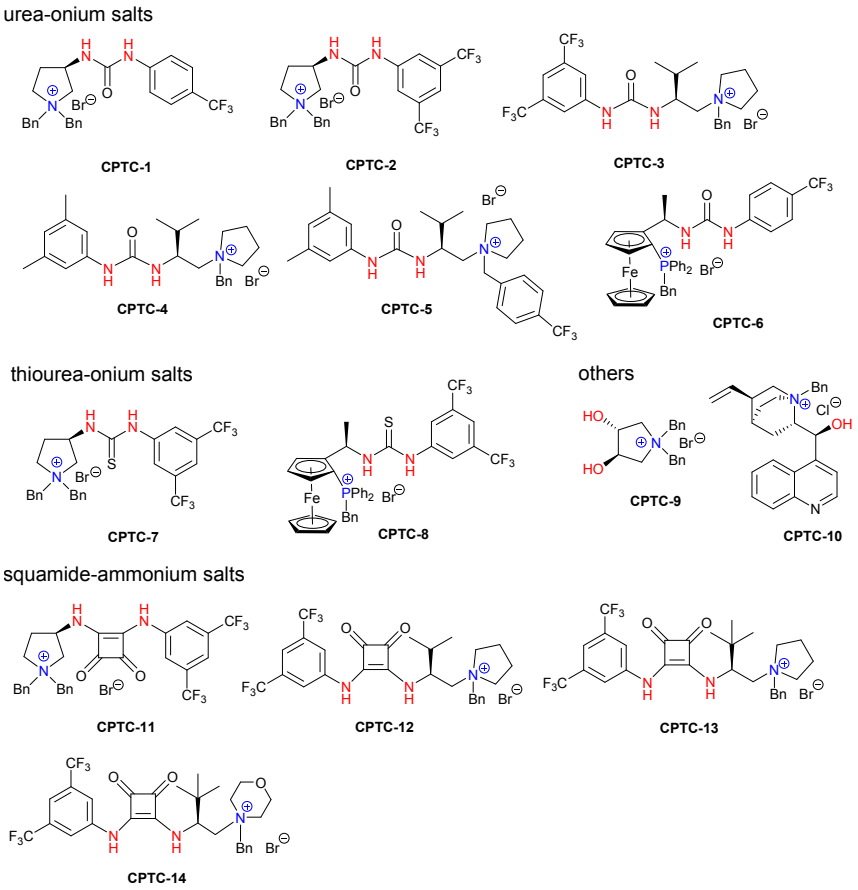
2l:[2] white powder, 90% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.33 (t, *J* = 7.96 Hz, 2H), 7.04 (t, *J* = 7.36 Hz, 1H), 6.93 (d, *J* = 8.00 Hz, 2H), 5.07-5.02 (m, 1H), 4.64 (t, *J* = 8.44 Hz, 1H), 4.56 (dd, *J* = 5.92, 2.48 Hz, 1H), 4.26 (dd, *J* = 6.44, 4.12 Hz, 1H), 4.16 (dd, *J* = 7.08, 3.52 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 157.76, 154.70, 129.71, 122.01, 114.61, 74.13, 66.86, 66.25; HRMS (ESI) *m/z* calcd. for $C_{10}H_{10}O_4Na^+$ $[M+Na]^+$: 217.0471, found 217.0468; HPLC: Chiralpak OD-H (^{i}PrOH/*n*-Hexane) = 20:80, flow rate = 1.0 mL/min, 216 nm, *rac*-form: t_r = 24.394 and 31.924 min; *S*-form: t_r = 31.441 min, >99% *ee*.

2m:[2] white powder, 85% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.40-7.28 (m, 5H), 4.84-4.79 (m, 1H), 4.60 (q, *J* = 9.52 Hz, 2H), 4.48 (t, *J* = 8.36 Hz, 1H), 4.39 (dd, *J* = 6.00, 2.24 Hz, 1H), 3.72 (dd, *J* = 7.32, 3.68 Hz, 1H), 3.62 (dd, *J* = 7.36, 3.64 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 155.07, 137.18, 128.59, 128.08, 127.76, 75.13, 73.65, 68.88, 66.30; HRMS (ESI) *m/z* calcd. for $C_{11}H_{12}NaO_4^+$ $[M+Na]^+$: 231.0628, found 231.0619; HPLC: Chiralpak OD-H (^{i}PrOH/*n*-Hexane) = 10:90, flow rate = 1.0 mL/min, 254 nm, *rac*-form: t_r = 35.168 and 49.587 min; *R*-form: t_r = 34.856 min, >99% *ee*.

2n:[2] white powder, 89% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.40-7.28 (m, 5H), 4.85-4.79 (m, 1H), 4.60 (q, *J* = 9.36 Hz, 1H), 4.48 (t, *J* = 8.36 Hz, 1H), 4.38 (dd, *J* = 6.00, 2.24 Hz, 1H), 3.72 (dd, *J* = 7.36, 3.64 Hz, 1H), 3.61 (dd, *J* = 7.36, 3.64 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 155.08, 137.19, 128.59, 128.07, 127.76, 75.14, 73.64, 68.89, 66.30; HRMS (ESI) *m/z* calcd. for $C_{11}H_{12}NaO_4^+$ $[M+Na]^+$: 231.0628, found 231.0624; HPLC: Chiralpak OD-H (^{i}PrOH/*n*-Hexane) = 10:90, flow rate = 1.0 mL/min, 254 nm, t_r = 35.168 and 49.587 min; *S*-form: t_r = 49.568 min, >99% *ee*.

3. The synthesis of chiral phase-transfer catalysts (CPTC-1~15)

CPTC-1, **CPTC-2**, **CPTC-6**, **CPTC-7~1**4 are known compounds, and the synthesis of them can be found in our previous report.[3] **CPTC-3~5** were prepared as the procedure of **APTC-1**.



CPTC-3: white powder, 87% yield for two steps; $[\alpha]^{20}_D$ -25° (c = 0.20, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.57 (s, 1H), 8.10 (s, 2H), 8.00-7.93 (m, 1H), 7.60-7.41(m, 5H), 4.82 (d, *J* = 13.44 Hz, 1H), 4.63 (m, 1H), 4.45 (d, *J* = 13.48 Hz, 1H), 4.24 (m, 1H), 3.83 (dd, *J* =11.44, 2.44 Hz, 1H), 3.73-3.61 (m, 3H), 3.30 (d, *J* = 13.56 Hz, 1H), 2.49 (m, 1H), 2.34 (m, 1H), 2.17 (m, 2H), 1.95-1.88 (m, 1H), 1.84 (s, 2H), 1.09 (d, *J* = 6.76 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 155.88, 141.26, 132.27, 131.97, 131.65, 131.31, 129.81, 126.94, 124.73, 122.02, 118.04, 115.09, 63.42, 61.92, 61.69, 61.58, 49.64, 32.87, 21.61, 20.42, 19.62, 17.37; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -62.86; HRMS (ESI) *m/z* calcd. for $C_{25}H_{34}BrF_6N_4O^+$ $[M+NH_4]^+$: 599.1815, found 599.1832.

CPTC-4: white powder, 79% yield for two steps; $[\alpha]^{20}_D$ -14° (c = 0.25, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.60 (s, 1H), 7.81 (d, *J* = 9.6 Hz, 1H), 7.55-7.50 (m, 4H), 7.22 (s, 2H), 6.64 (s, 1H), 4.87 (d, *J* = 13.52 Hz, 1H), 4.62 (t, *J* = 12.76 Hz, 1H), 4.43 (d, *J* = 13.44 Hz, 1H), 4.30-4.23 (m, 1H), 3.76 (t, *J* = 12.76 Hz, 1H), 3.62 (m, 2H), 3.27 (d, *J* = 13.72 Hz, 1H), 2.45 (s, 1H), 2.27 (s, 6H), 2.19 (s, 1H), 2.13 (m, 2H), 1.89 (t, *J* = 5.52 Hz, 1H), 1.85 (s, 1H), 1.7 (d, *J* = 6.56 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.26, 138.32, 132.45, 131.06, 129.65, 127.29, 124.05, 116.51, 63.41, 61.75, 49.57, 32.87, 21.63, 21.38, 20.50, 19.68, 17.52; HRMS (ESI) *m/z* calcd. for $C_{25}H_{36}BrN_3NaO^+$ $[M+Na]^+$: 499.1934, found 499.1966.

CPTC-5: white powder, 82% yield for two steps; $[\alpha]^{20}_D$ -32° (c = 0.20, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.78 (s, 1H), 7.68-7.65 (m, 5H), 7.19 (s, 2H), 6.65 (s, 1H), 5.03 (d, *J* = 13.04 Hz, 1H), 4.82 (d, *J* = 13.2 Hz, 1H), 4.51 (m, 1H), 4.22 (m, 1H), 3.91-3.85 (m, 2H), 3.56 (d, *J* = 7.28 Hz, 1H), 3.50-3.46 (m, 1H), 3.34 (d, *J* = 6.90 Hz, 1H), 2.36 (m, 1H), 2.26 (s, 6H), 2.20-2.14 (m, 1H), 2.08 (s, 2H), 1.92 (s, 2H), 1.09-1.06 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.31, 139.22, 136.48, 133.27, 126.46, 124.27,116.48, 63.41, 61.96, 61.21, 60.90, 49.82, 32.87, 21.40, 21.22, 20.62, 19.66, 17.65; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -63.12; HRMS (ESI) *m/z* calcd. for $C_{26}H_{35}BrF_3KN_3O^+$ $[M+K]^+$: 580.1547, found 580.1549.

4. The kinetic resolution of epoxides by CO_2 in the presence of CPTCs

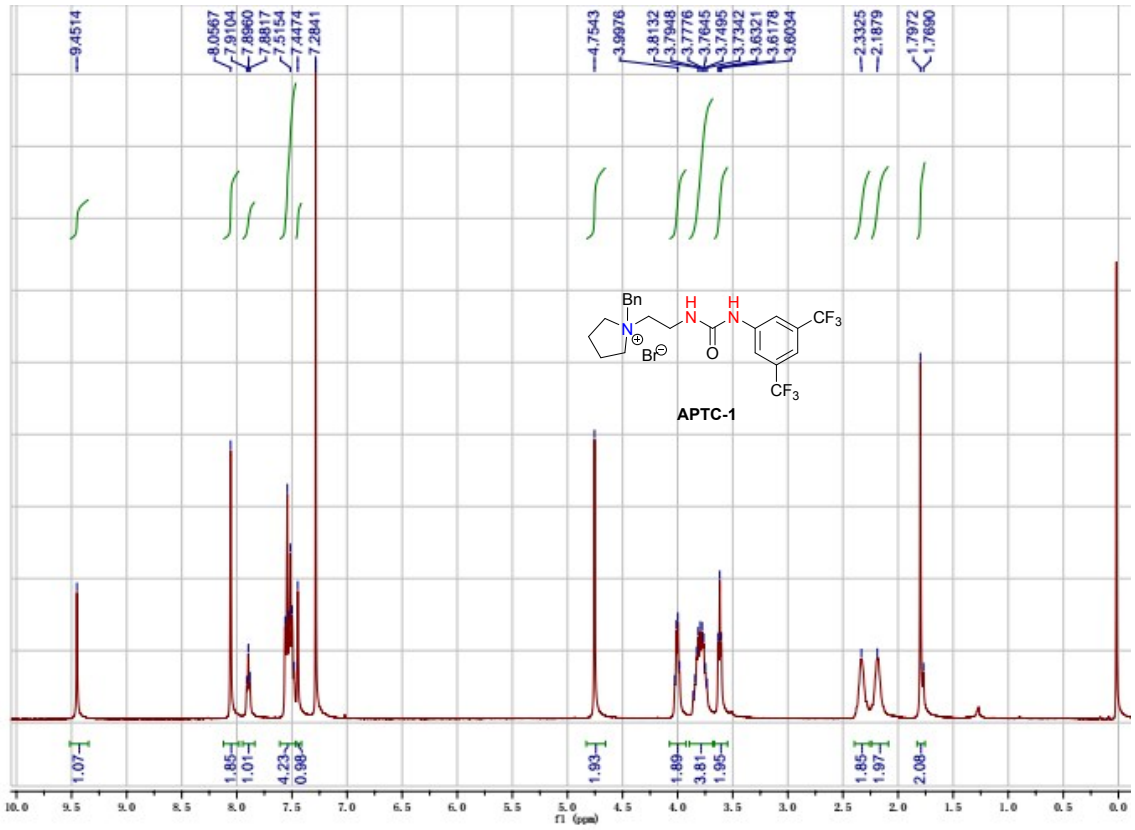
Typical procedure:

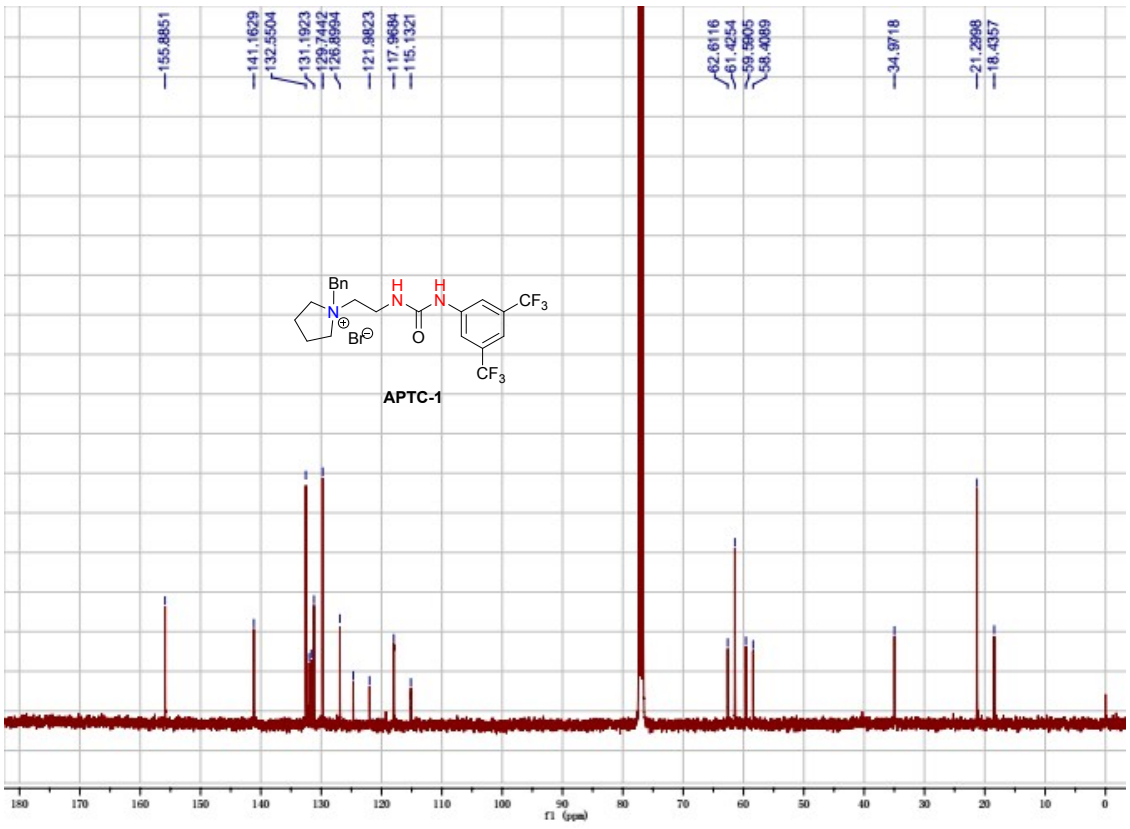
A mixture of 0.25 mmol of epoxide **1g** and 1.0 mol% of **CPTC-2** (1.5 mg) was heated at 60 °C for 24 h under CO_2 atmosphere (1atm, using a balloon). After cooled to room temperature, a small amount of CH_2Cl_2 was added to the mixture and it was purified by a flash column chromatography (petroether/ethyl acetate = 10/1 to 3/1, v/v) to give cyclic carbonate and epoxide respectively. The *ee* of products were determined by HPLC using a chiral column (Daicel Chiralpak AD-H or OD-H), and the absolute configurations of products were assigned according to literature report.[4]

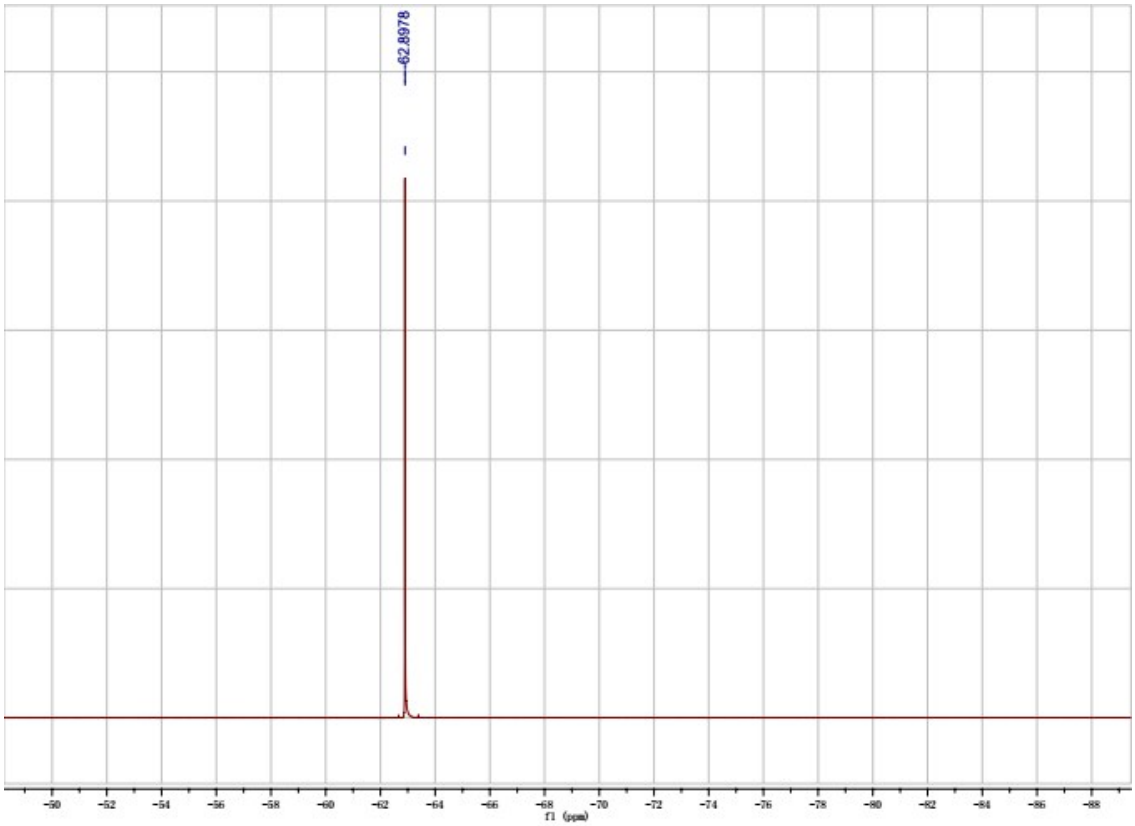
Notes and References

1. J. Novacek, M. Waser, *Eur. J. Org. Chem.*, 2014, 802.
2. (a) W. Clegg, R. W. Harrington, M. North, R. Pasquale, *Chem.–Eur. J.*, 2010, **16**, 6828; (b) L. Wu, H. Yang, H. Wang, J. Lu, *RSC Adv.*, 2015, **5**, 23189; (c) H. Büttner, J. Steinbauer, T. Werner, *ChemSusChem*, 2015, **8**, 2655.
3. J.-C. Zhu, D.-X. Cui, Y.-D. Li, J.-X. He, W.-P. Chen, P.-A. Wang, *Org. Biomol. Chem.*, 2018, **16**, 3012.
4. (a) Y. Toda, Y. Komiyama, A. Kikuchi, H. Suga, *ACS Catal.*, 2016, **6**, 6906; (b) S.-Y. Liu, N. Suematsu, K. Maruoka, S. Shirakawa, *Green Chem.*, 2016, **18**, 4611; (c) J. Qin, V. A. Larionov, K. Harms, E. Meggers, *ChemSusChem*, 2019, **12**, 320; (d) T. Ema, M. Yokoyama, S. Watanabe, S. Sasaki, H. Ota, K. Takaishi, *Org. Lett*., 2017, **19**, 4070; (e) K. Takaishi, T. Okuyama, S. Kadosaki, M. Uchiyama, T. Ema, *Org. Lett.* 2019, **21**, 1397.

NMR spectra copies of all new compounds



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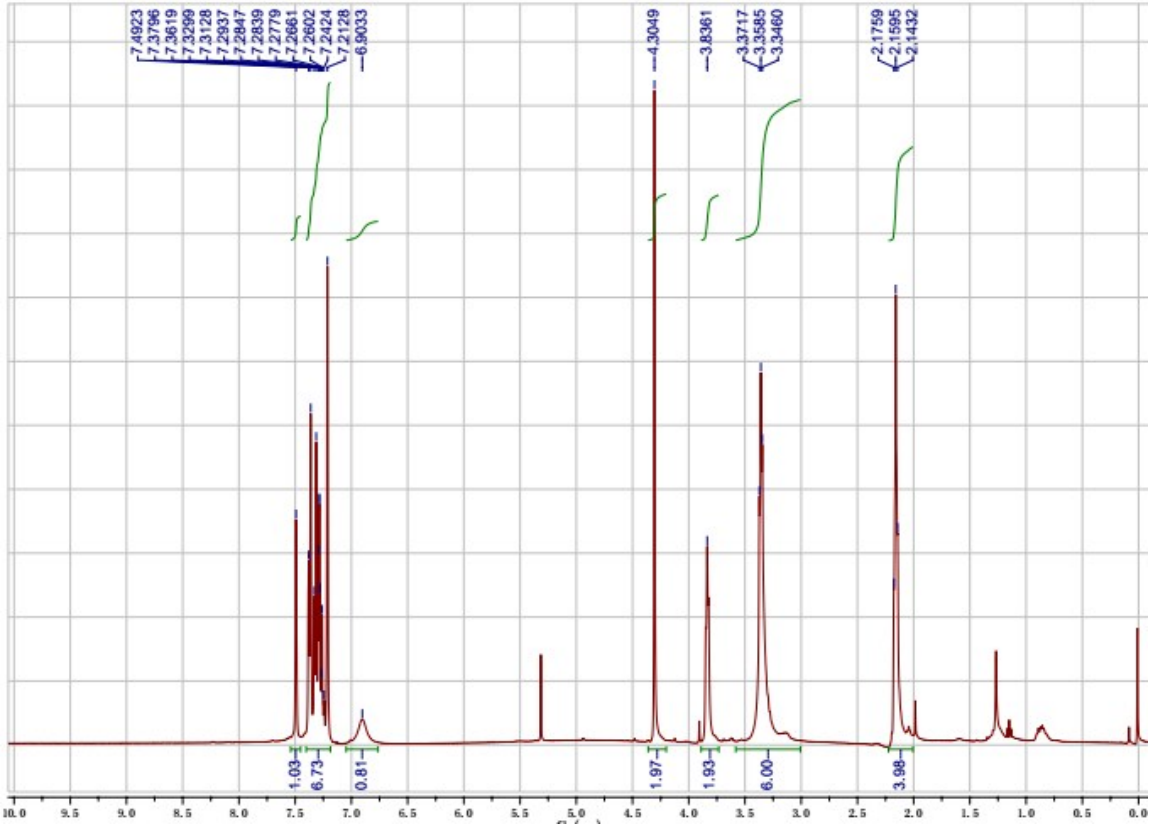
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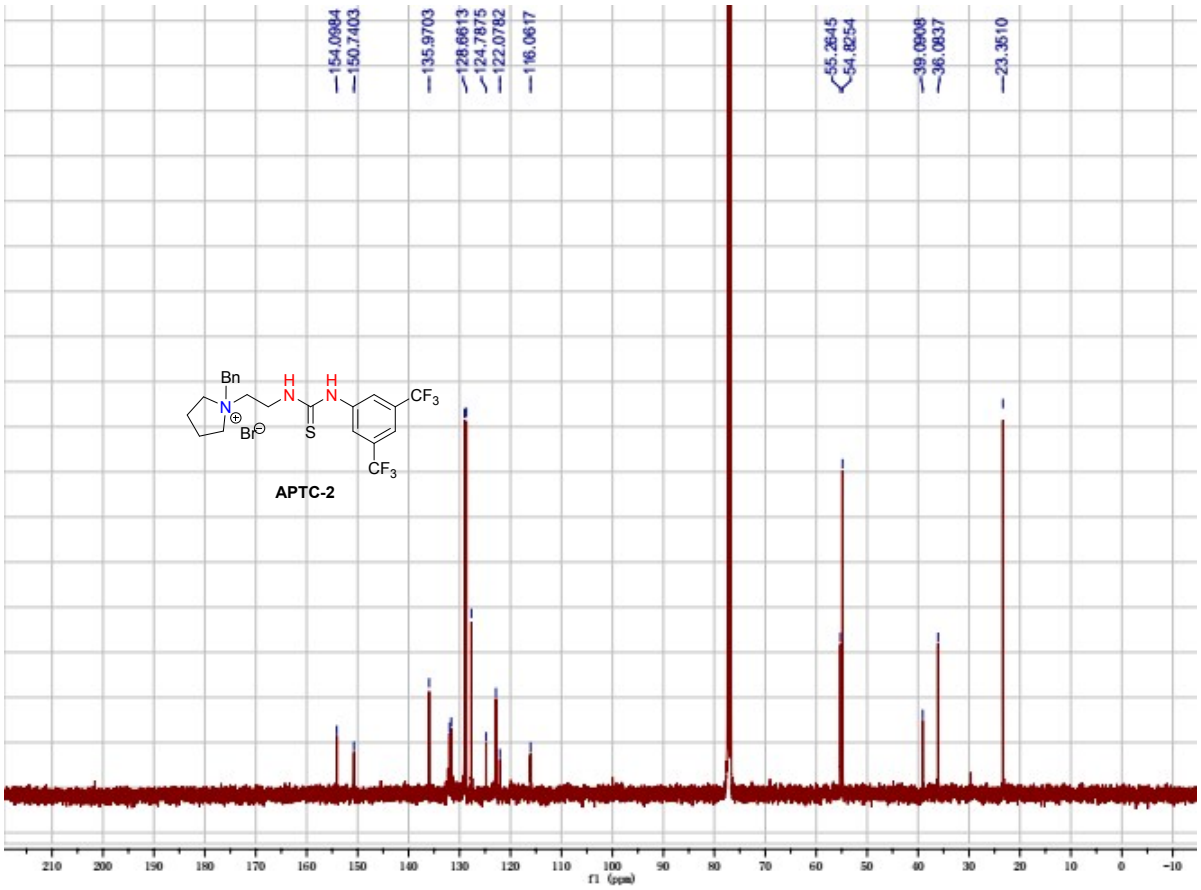
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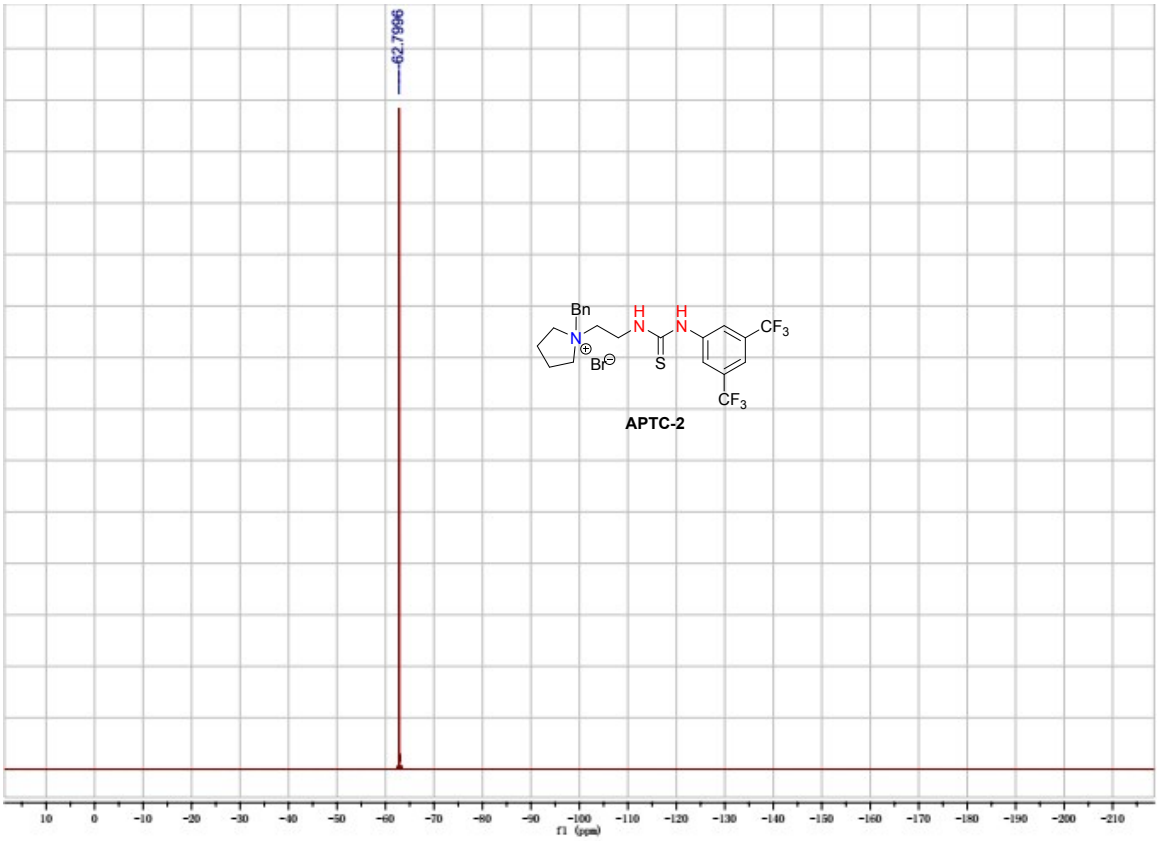
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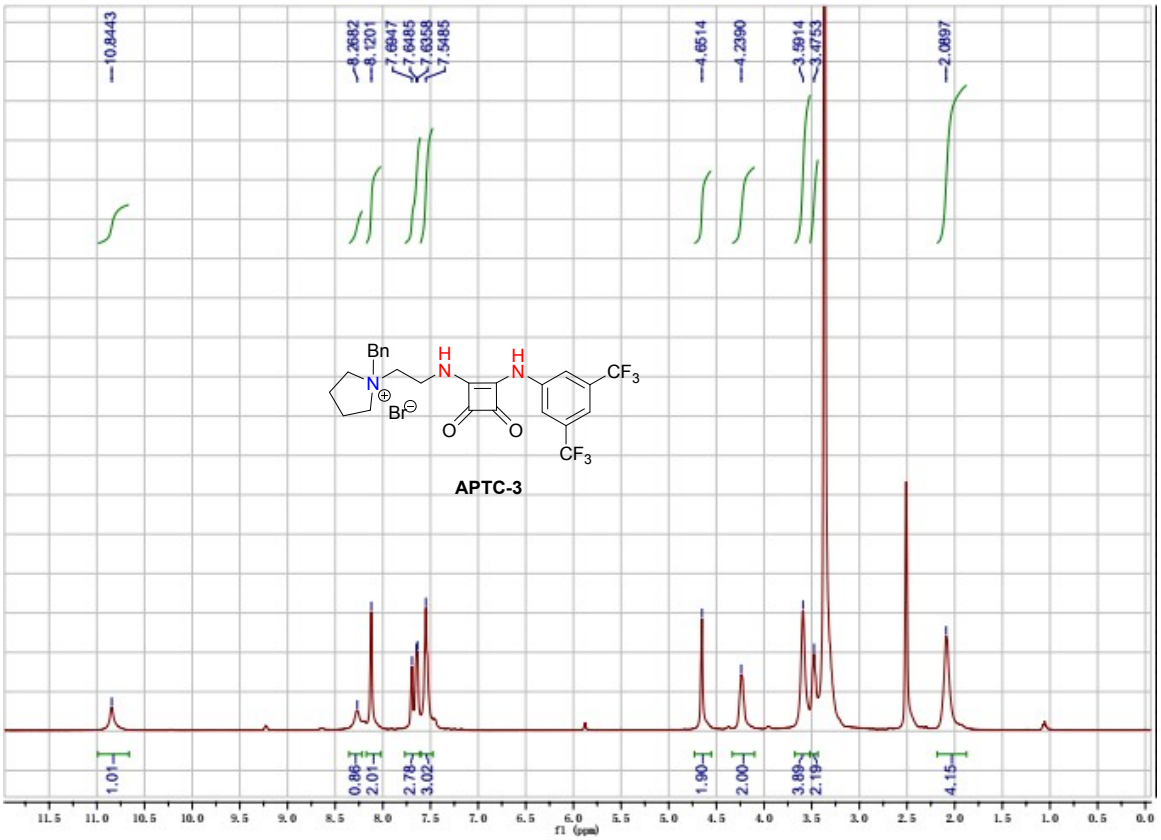
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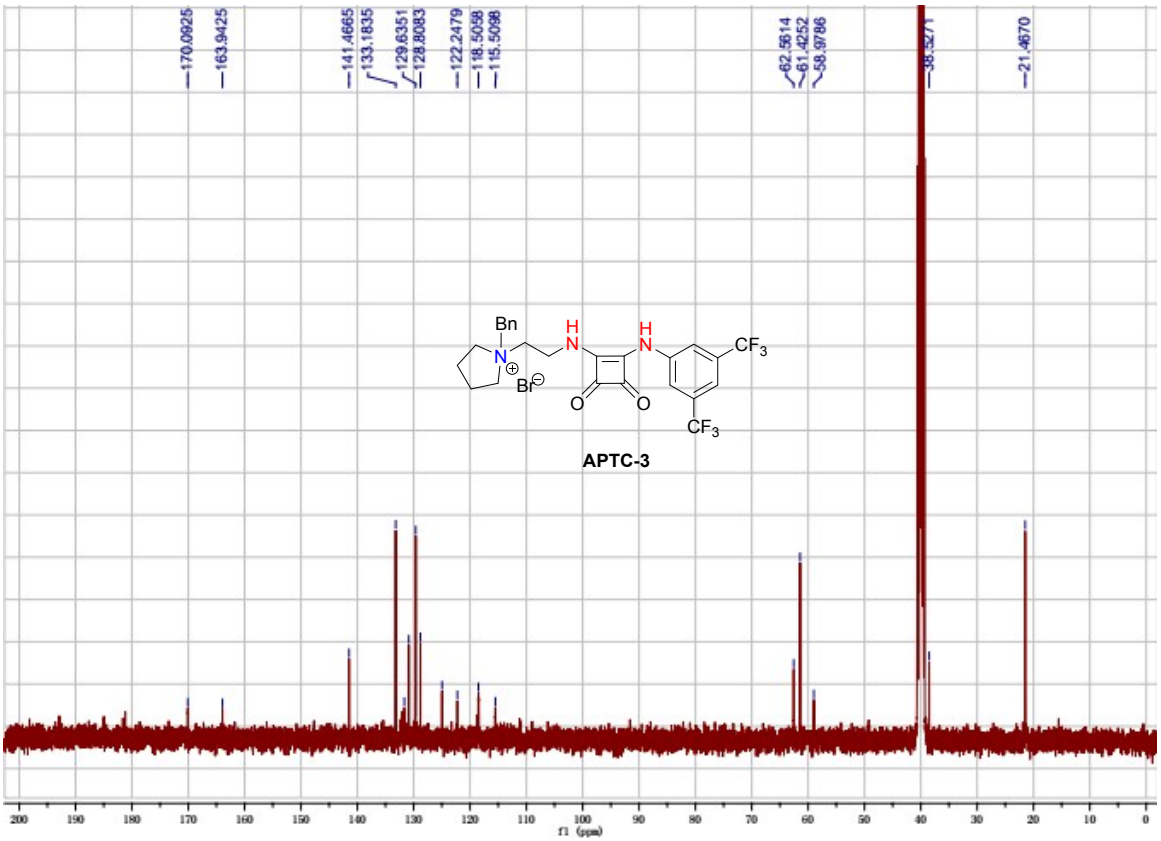
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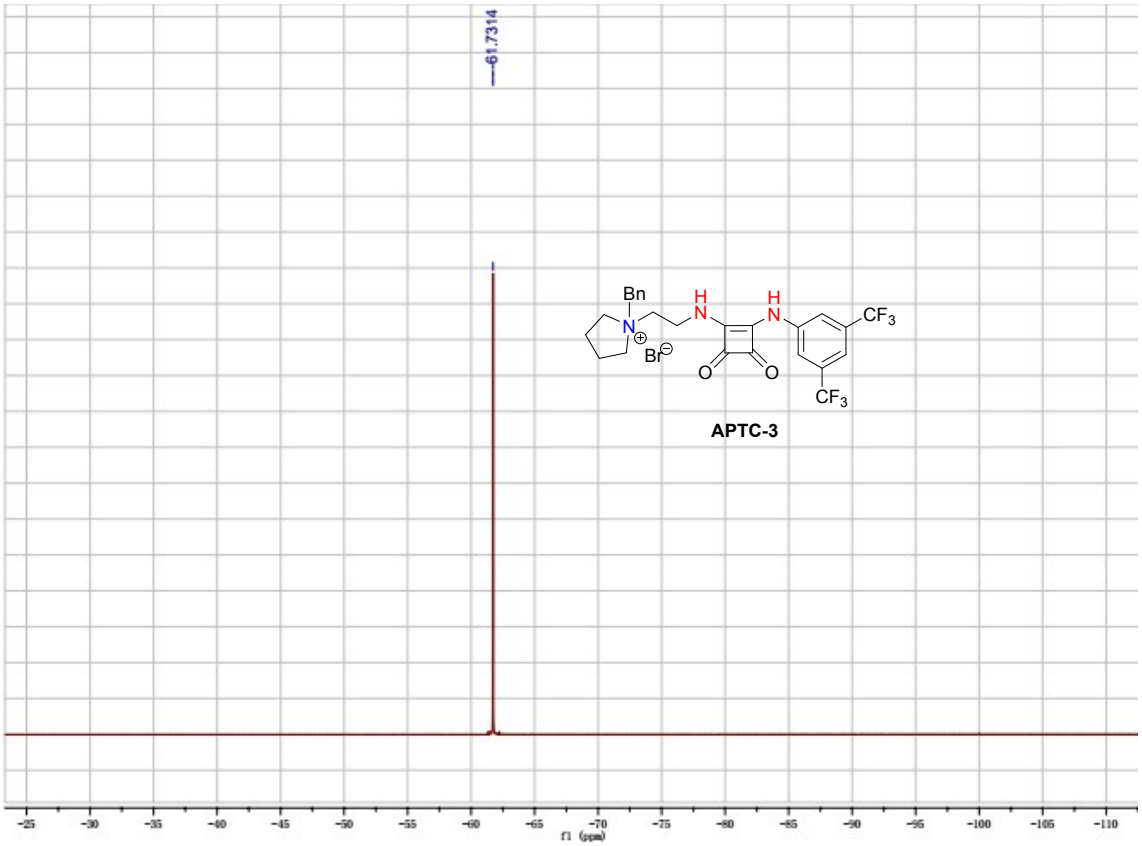
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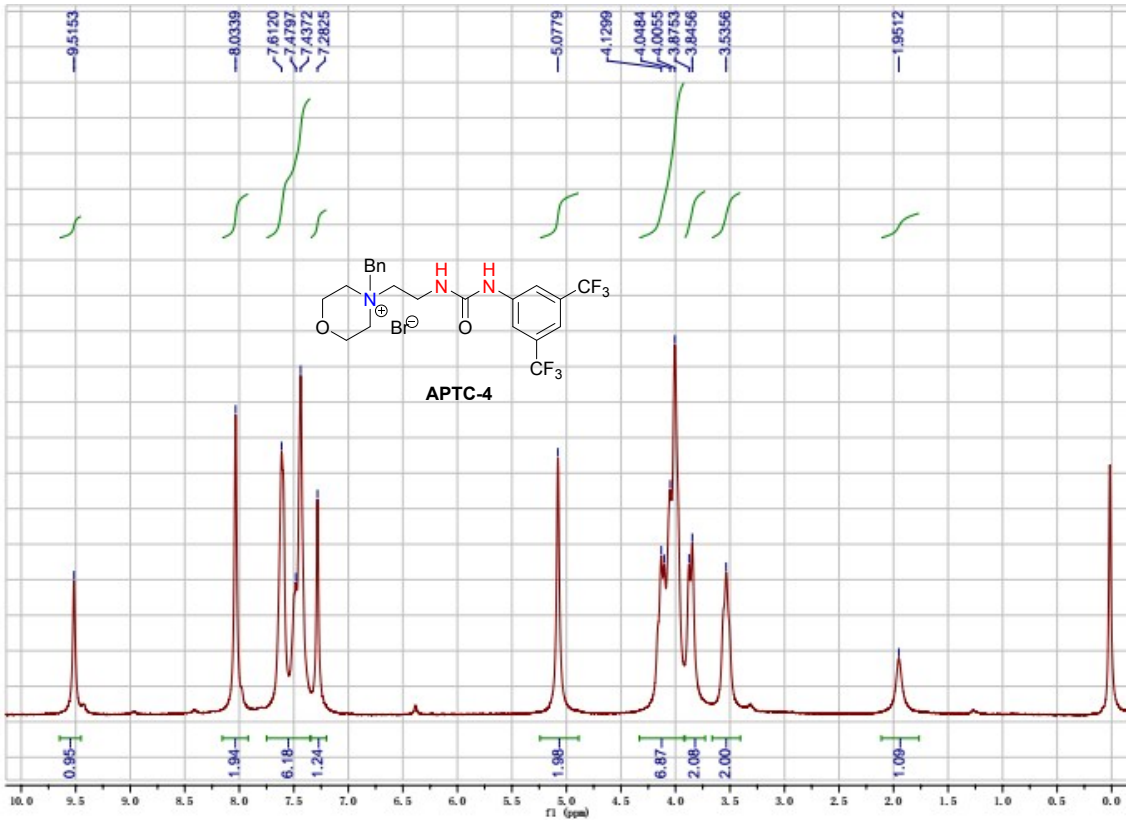
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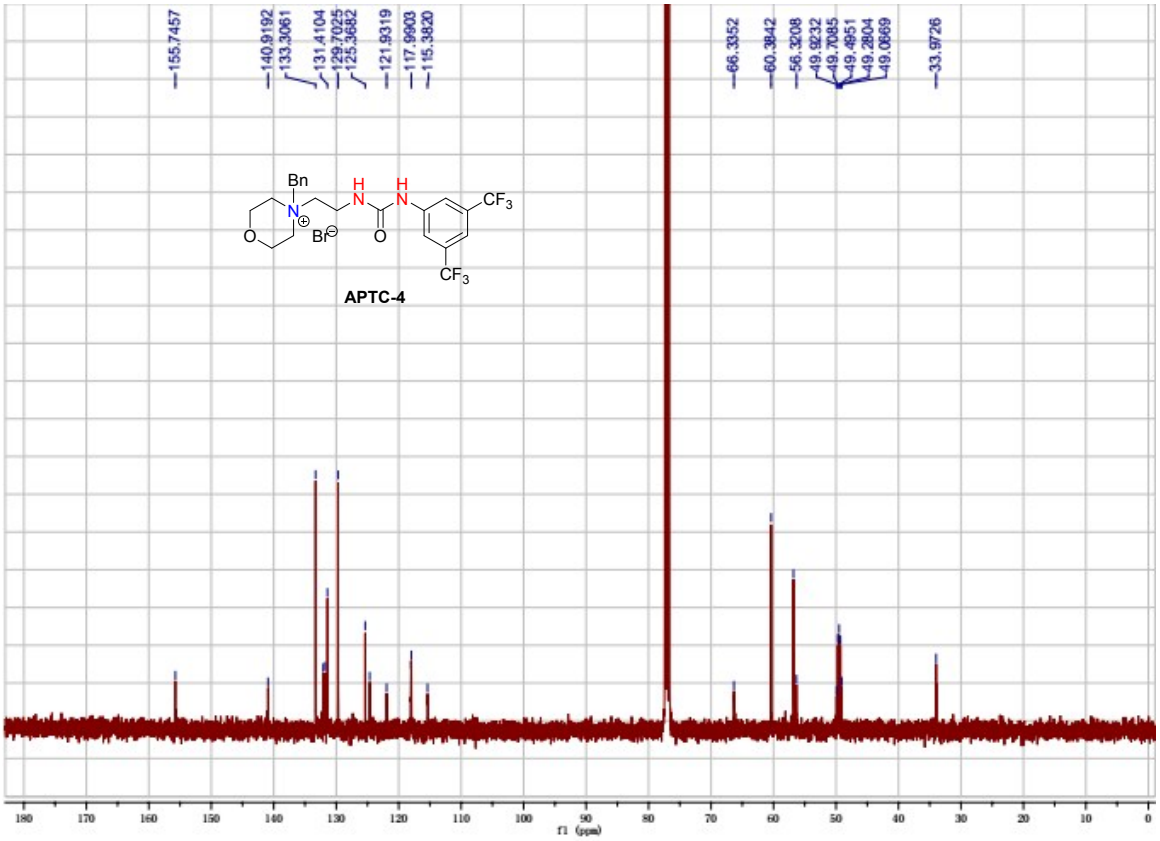
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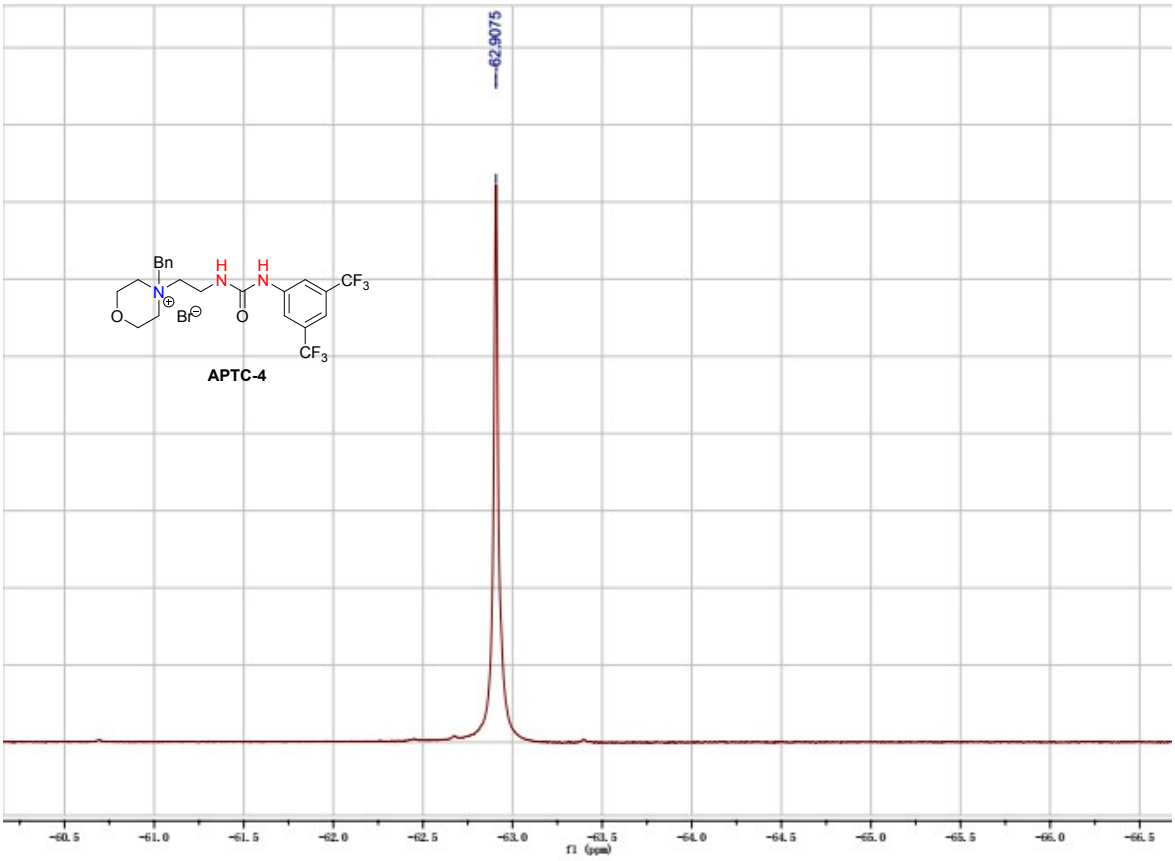
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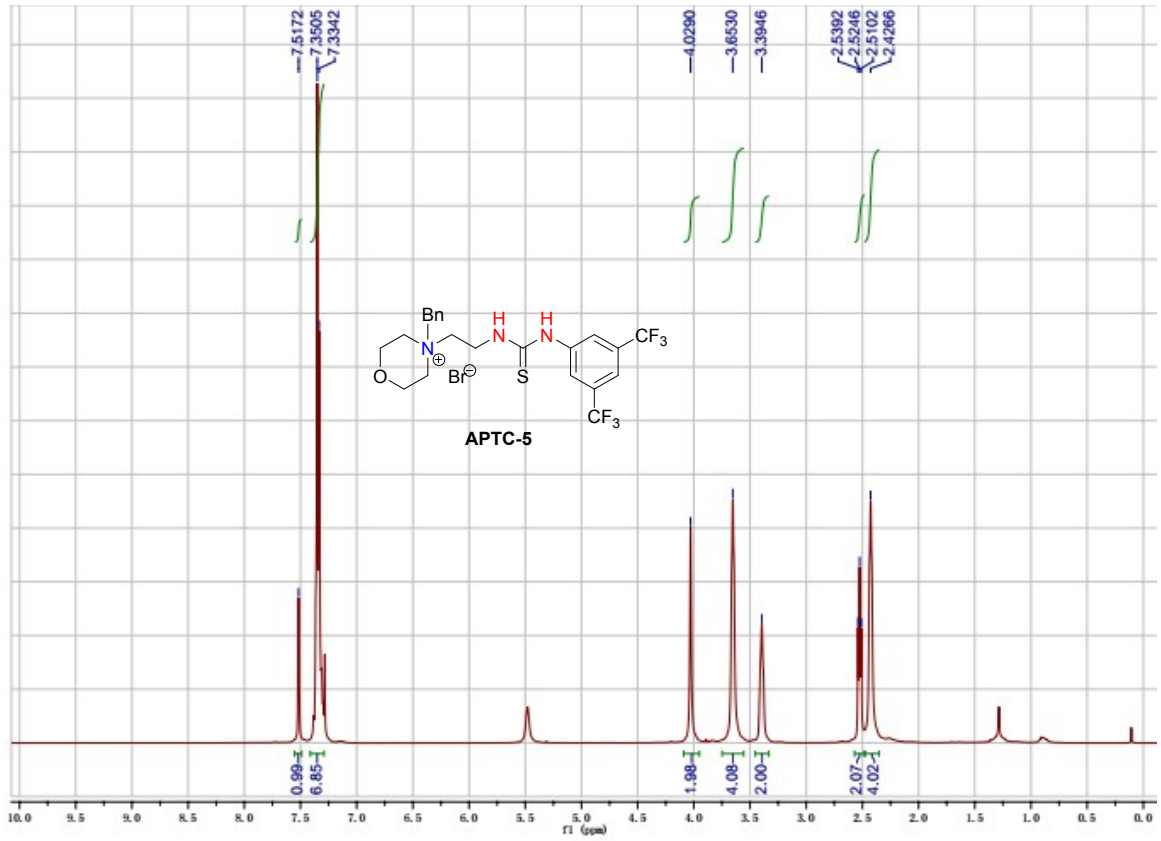
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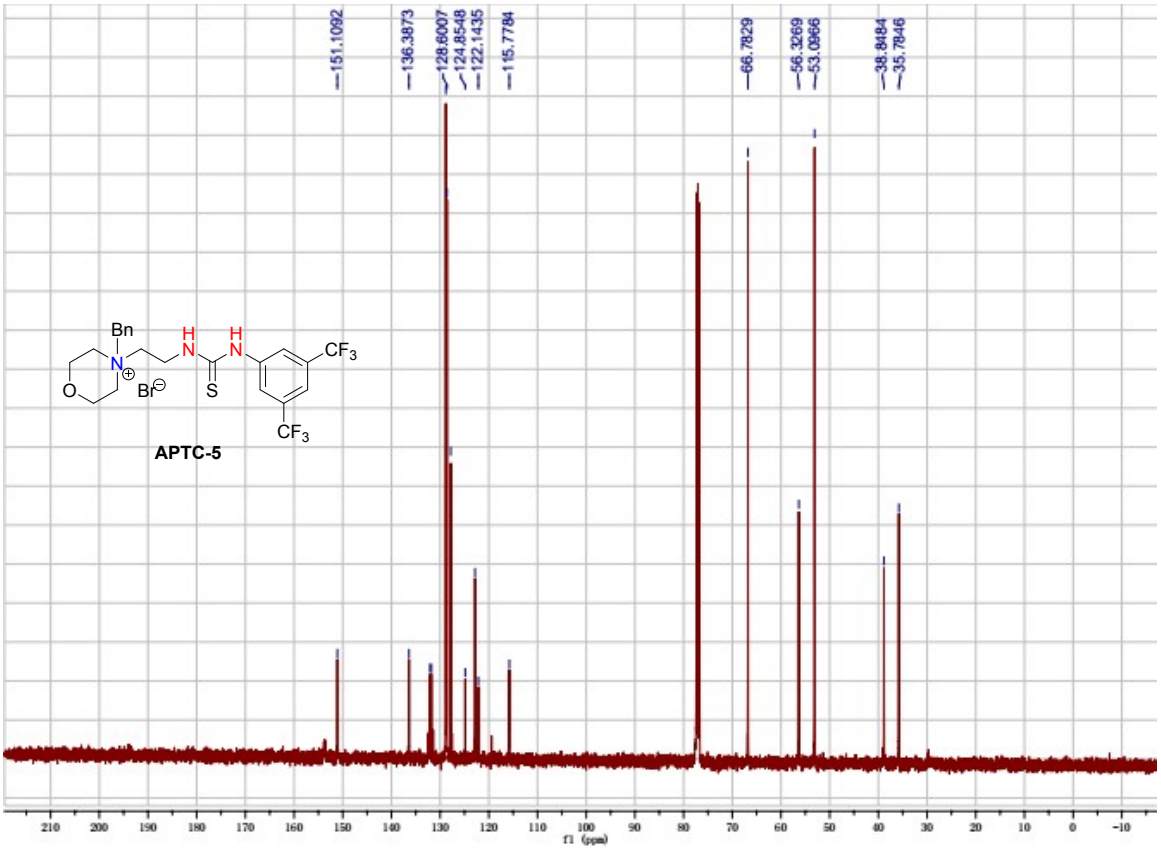
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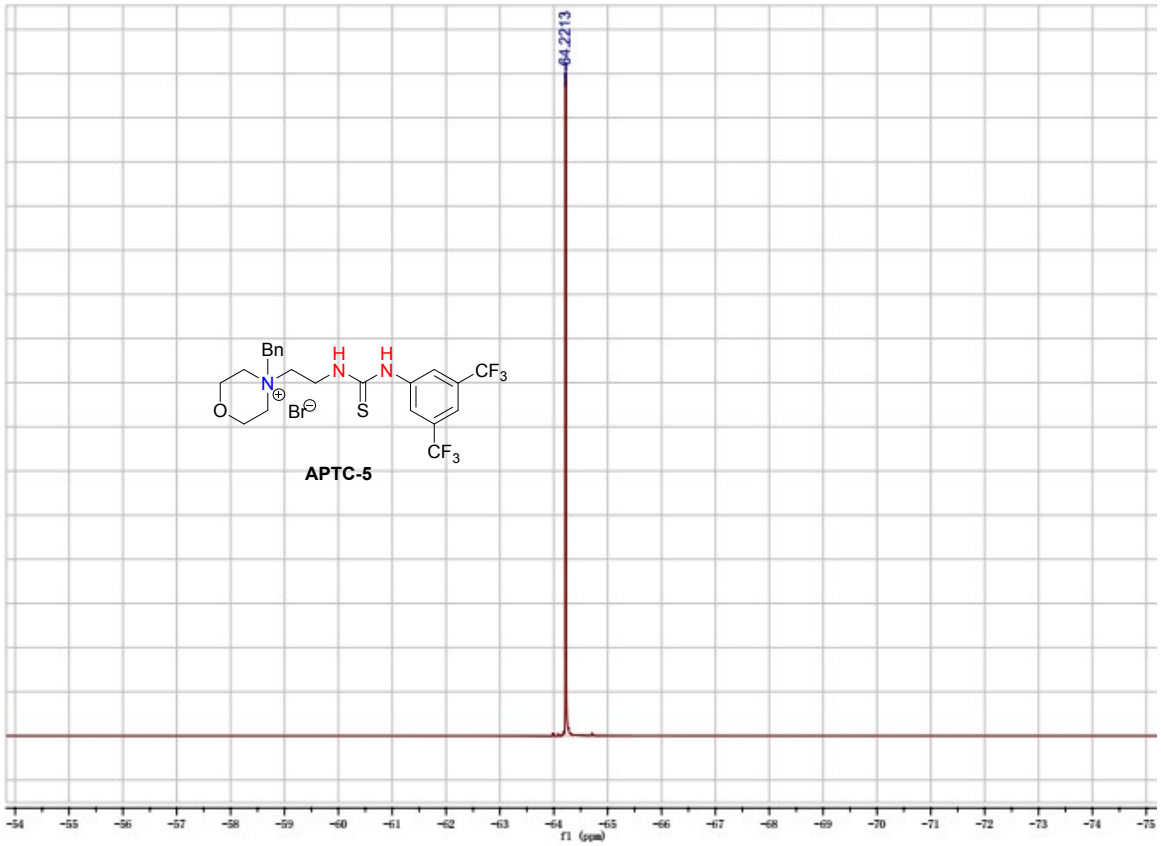
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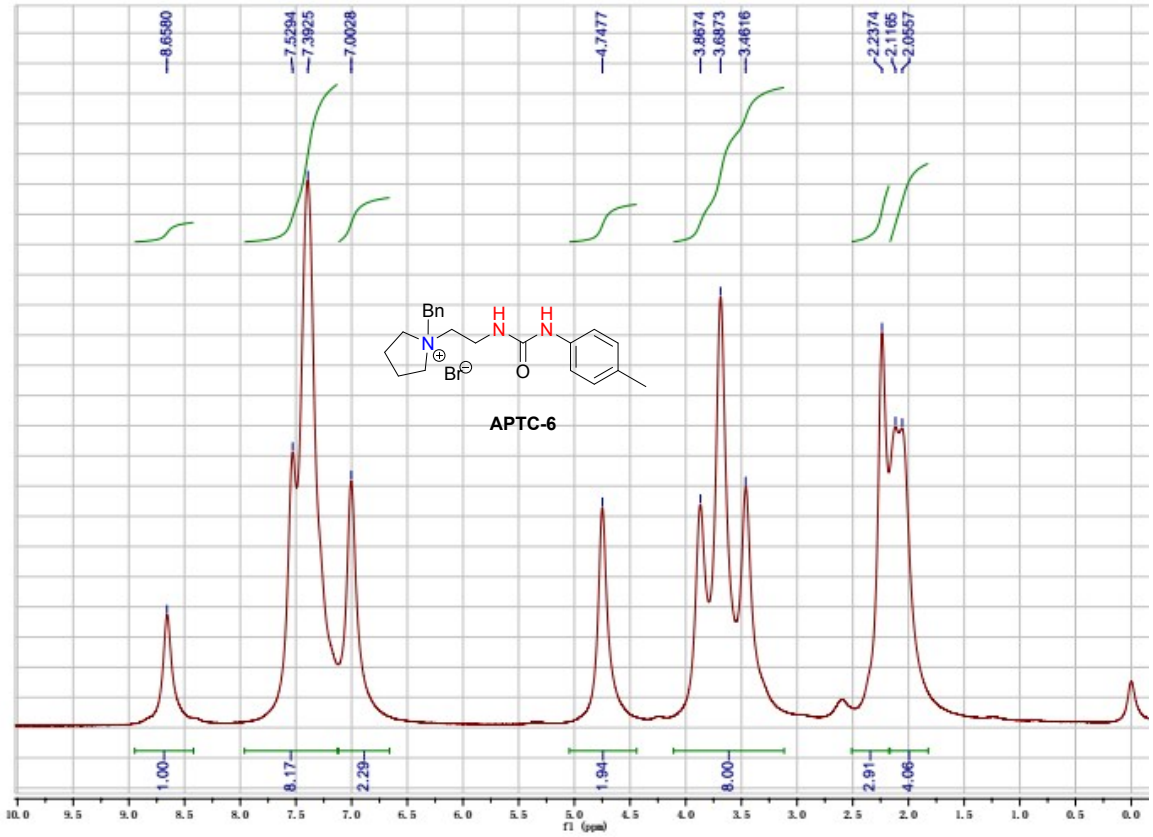
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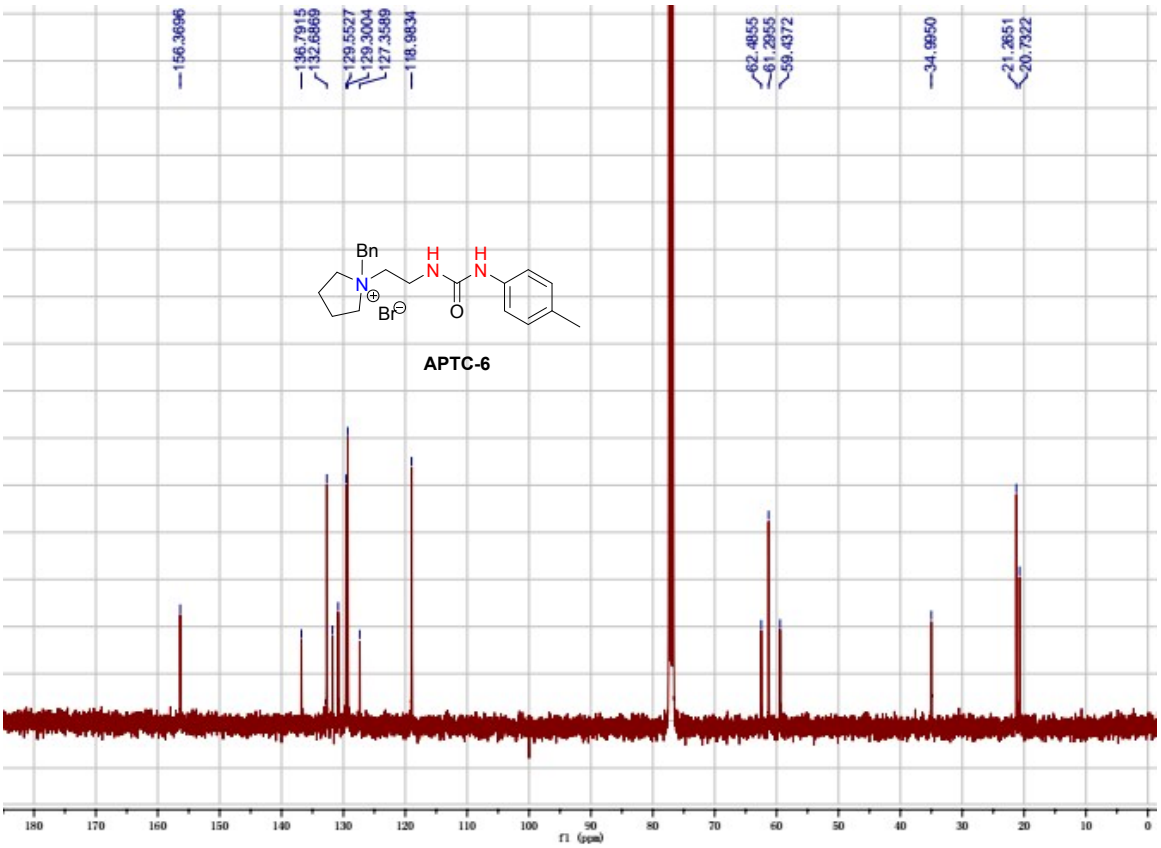
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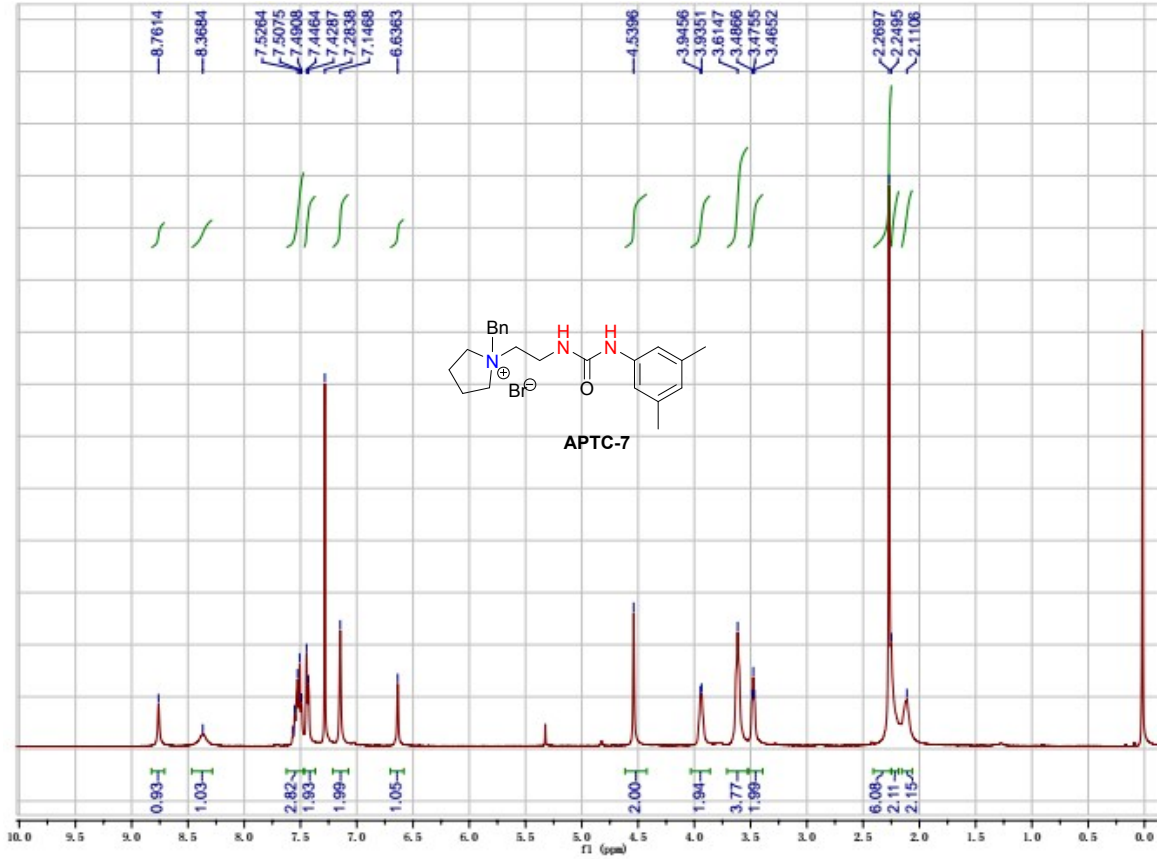
APTC-6
f1 (ppm)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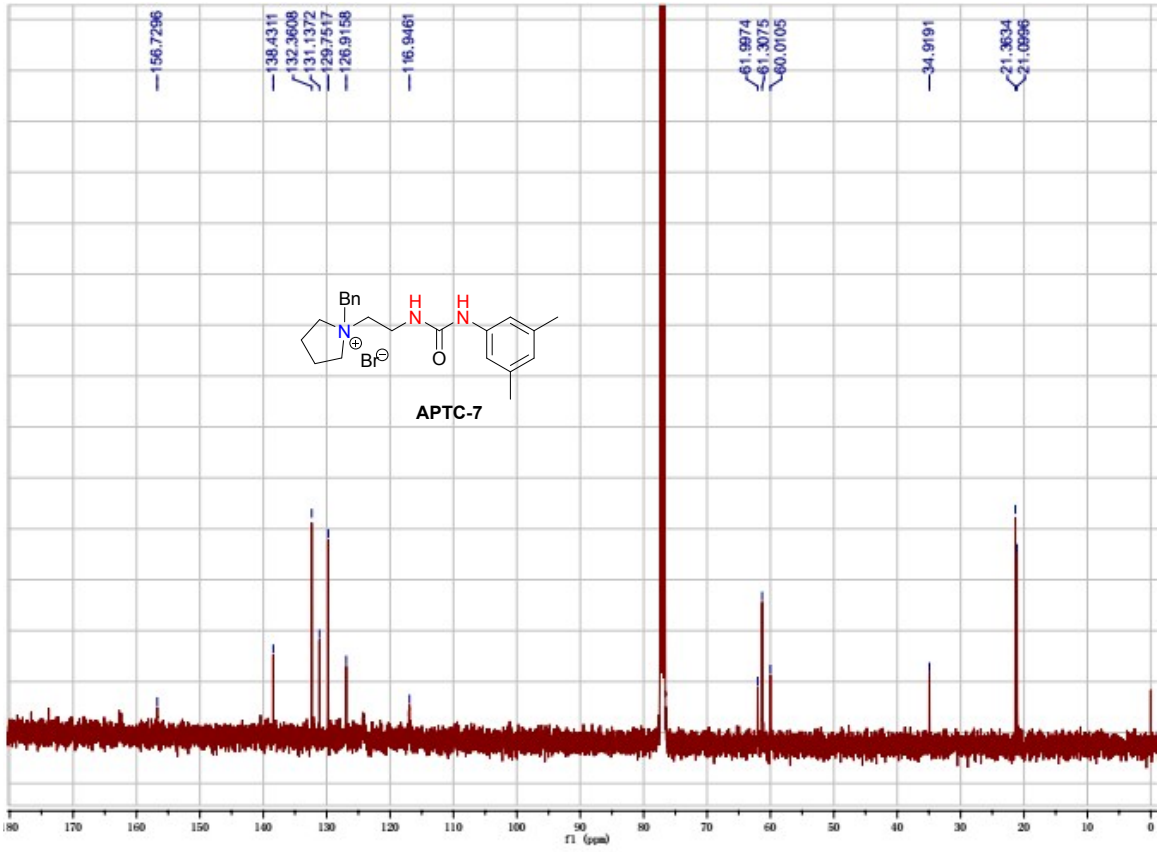
7.5264
7.5075
7.4908
7.4464
7.4287
7.2838
7.1468
6.6363
4.5396
3.9456
3.9351
3.6147
3.4866
3.4755
3.4652
2.2697
2.2495
2.1106
Bn
H
N
H
N
N
Br
O
APTC-7
0.93
1.03
2.82
1.93
1.99
1.05
2.00
1.94
3.77
1.99
6.08
2.11
2.15
f1 (ppm)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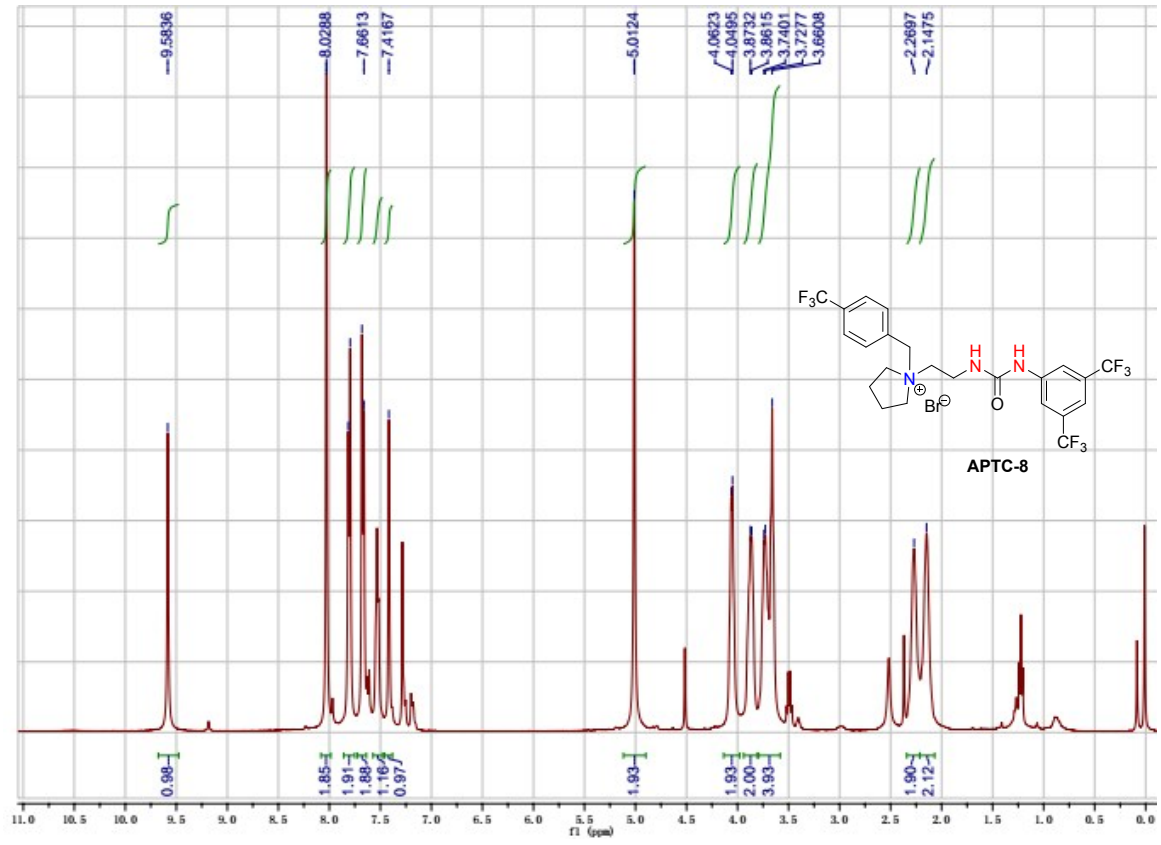
132.3608
131.1372
129.7517
126.9158
116.9461
61.9974
61.3075
60.0105
34.9191
21.3634
21.0996
Bn
N
H
N
H
N
O
Br
APTC-7
f1 (ppm)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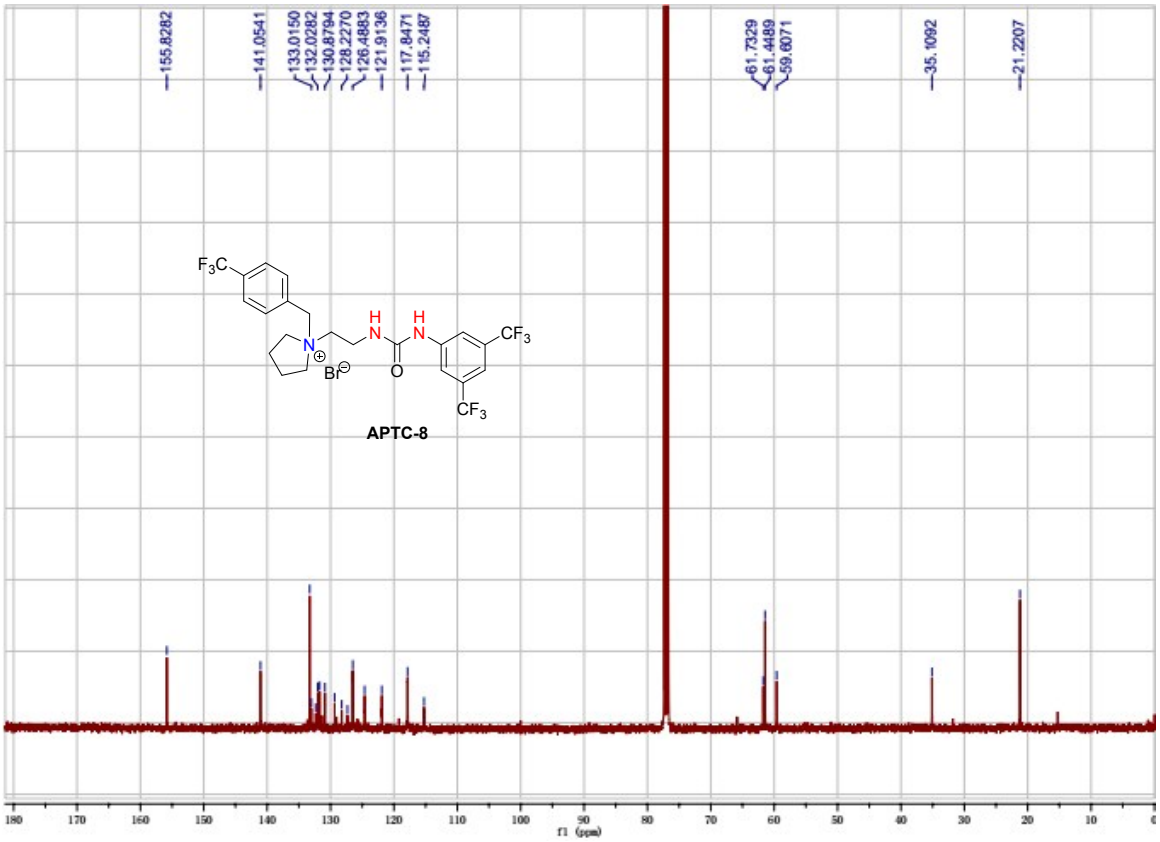
8.0288
7.6613
7.4167
5.0124
4.0623
4.0495
3.8732
3.8615
3.7401
3.7277
3.6608
2.2697
2.1475
0.98
1.85
1.91
1.88
1.16
0.97
1.93
1.93
2.00
3.93
1.90
2.12
F3C
CF3
CF3
APTC-8
f1 (ppm)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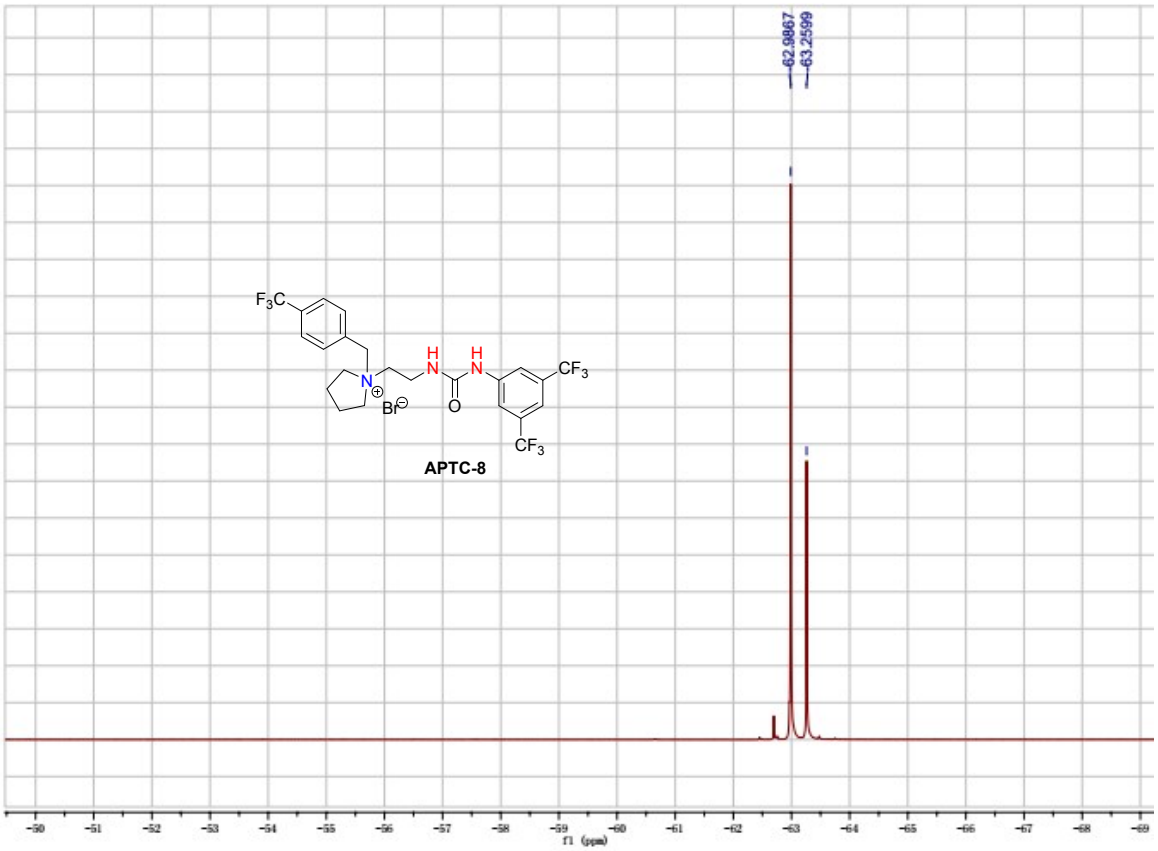
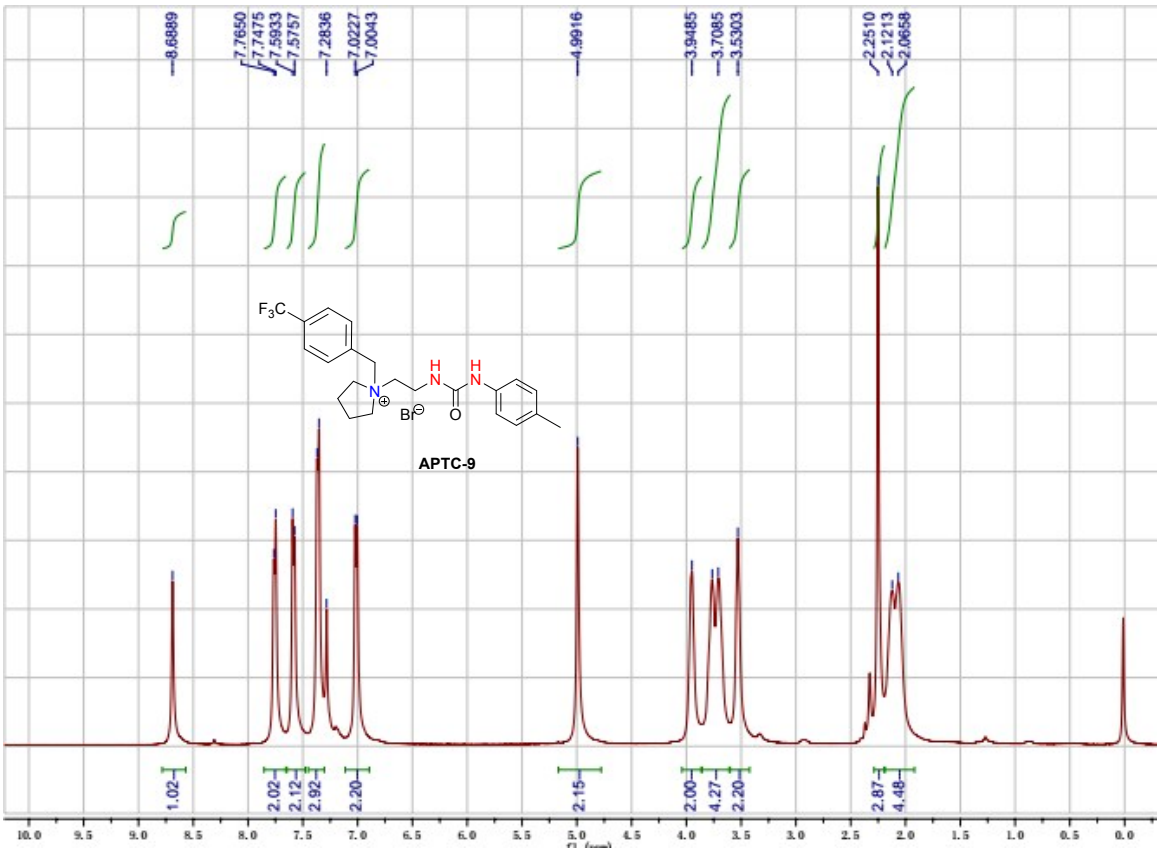
141.0541
133.0150
132.0282
130.8794
128.2270
126.4883
121.9136
117.8471
115.2487
61.7329
61.4489
59.6071
35.1092
21.2207
F3C
H
N
H
N
CF3
N
Br
O
CF3
APTC-8
f1 (ppm)


62.9867
63.2599
F3C
H
N
H
N
CF3
N
Br
O
CF3
APTC-8
f1 (ppm)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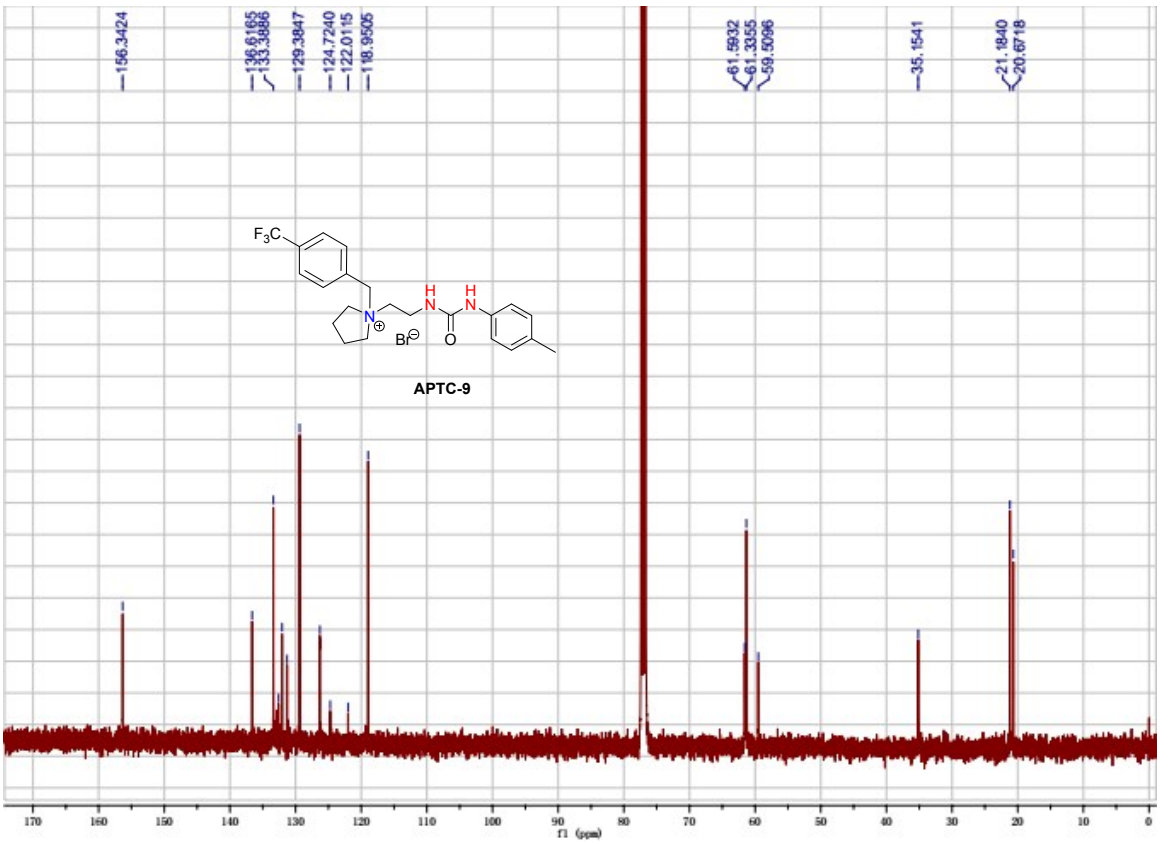
7.7650
7.7475
7.5933
7.5757
7.2836
7.0227
7.0043
4.9916
3.9485
3.7085
3.5303
2.2510
2.1213
2.0658
F3C
Br
APTC-9
1.02
2.02
2.12
2.92
2.20
2.15
2.00
4.27
2.20
2.87
4.48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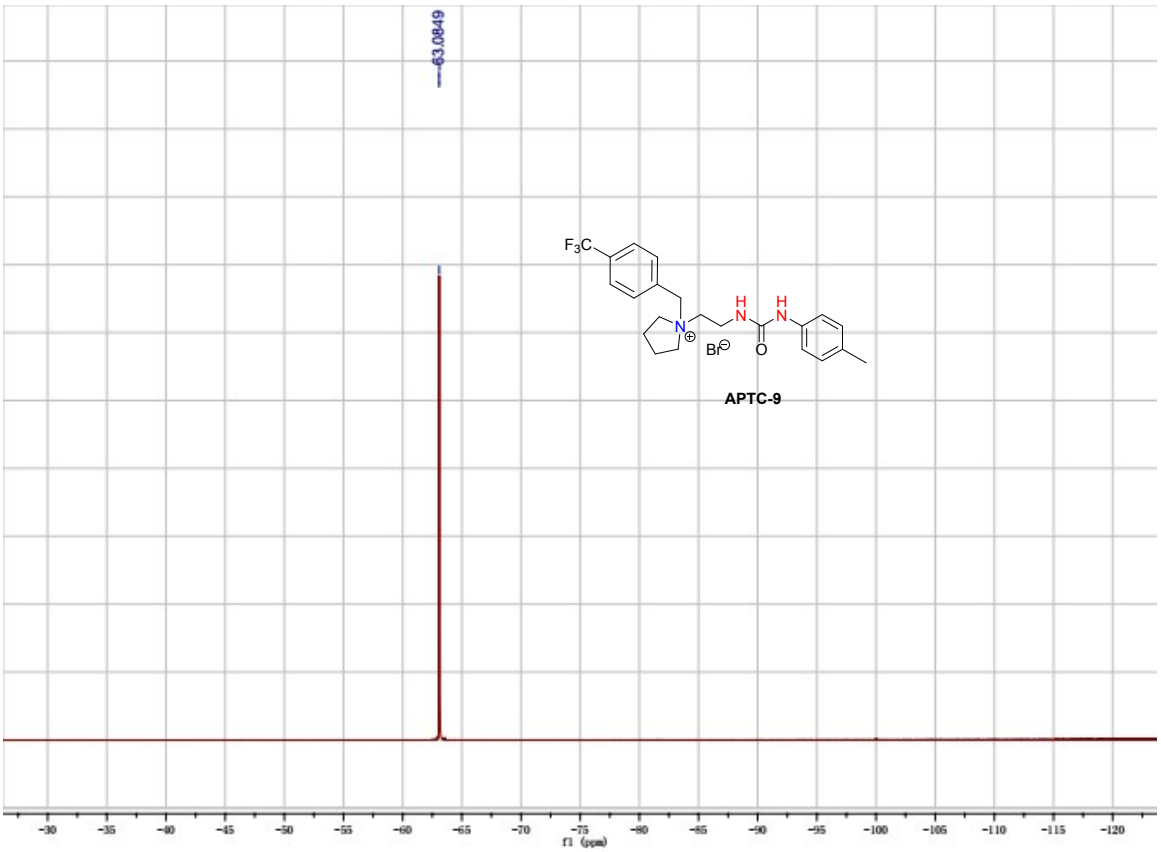
133.3886
129.3847
124.7240
122.0115
118.9505
61.5932
61.3355
59.5096
35.1541
21.1840
20.6718
F3C
Br
APTC-9


-63.0849
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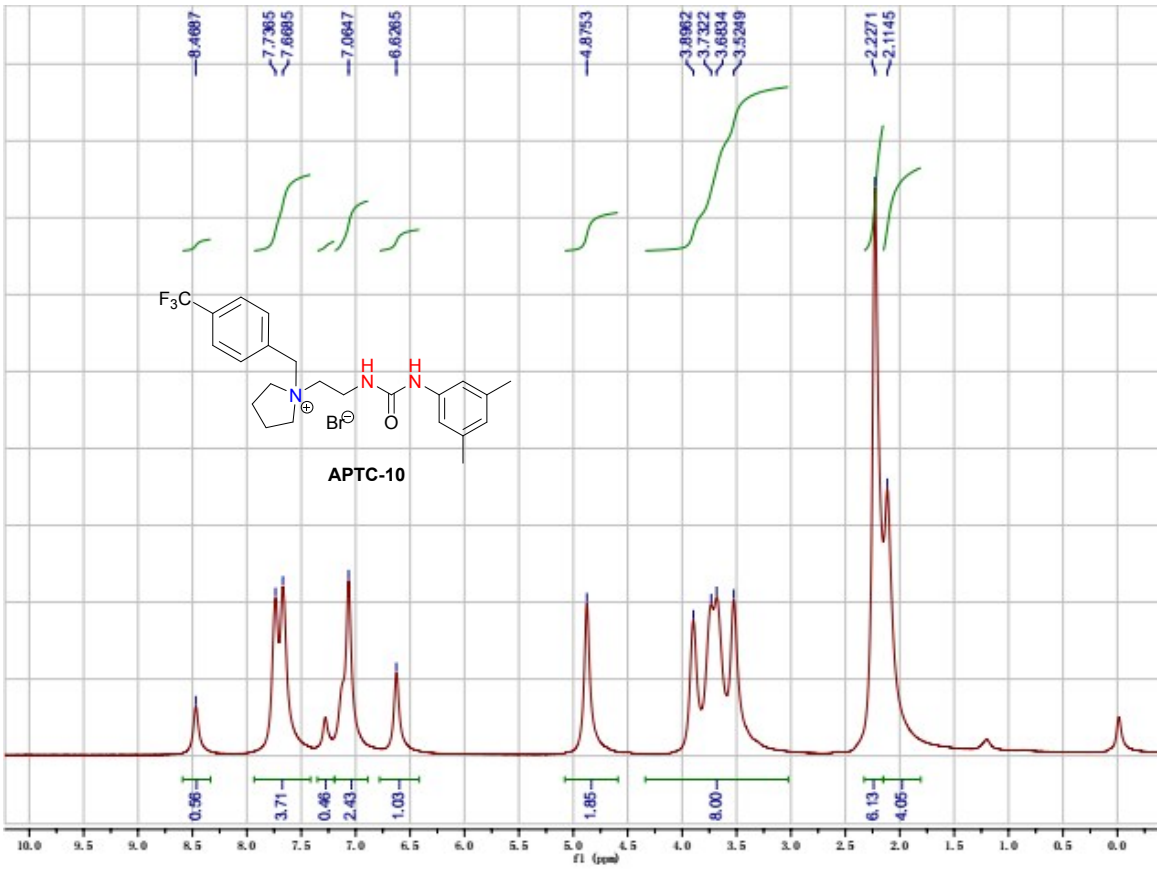
Br
APTC-9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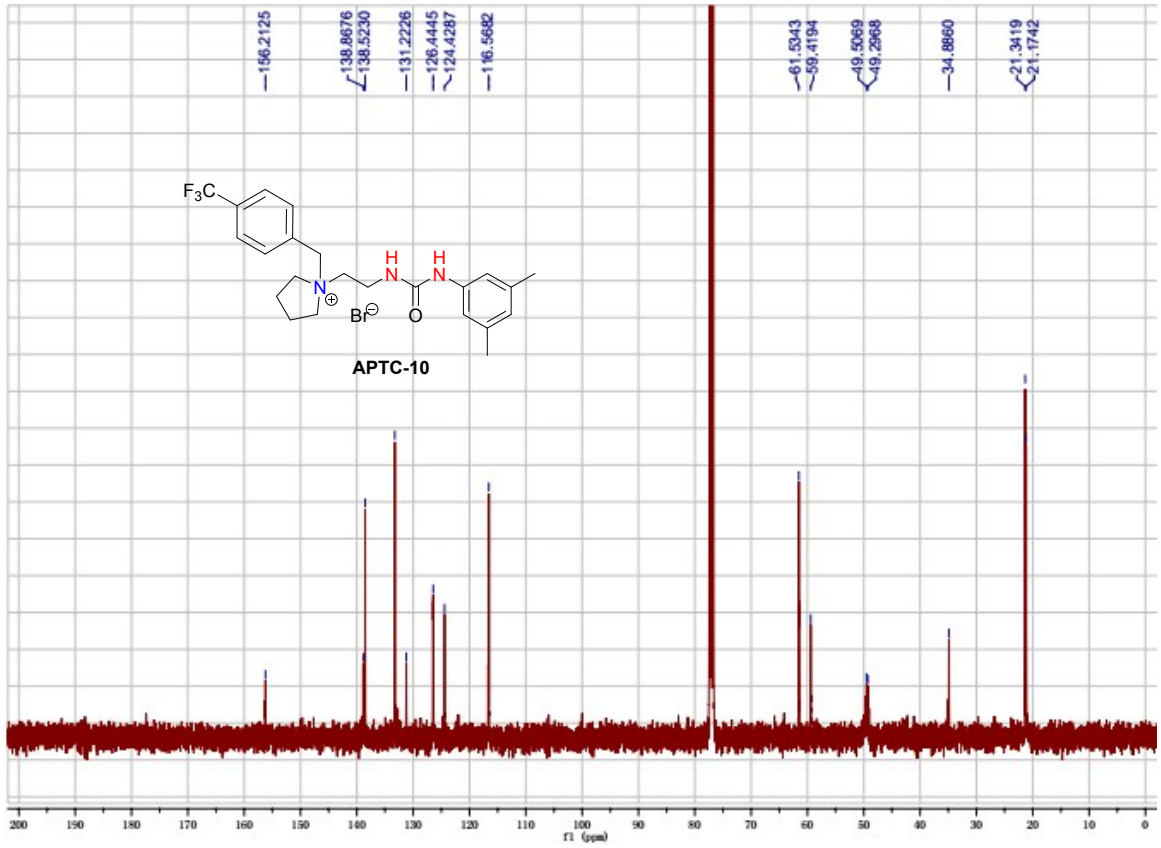
7.7365
7.6685
7.0647
6.6285
4.8753
3.8982
3.7322
3.6834
3.5249
2.2271
2.1145
F3C
Br
APTC-10
0.56
3.71
0.46
2.43
1.03
1.85
8.00
6.13
4.05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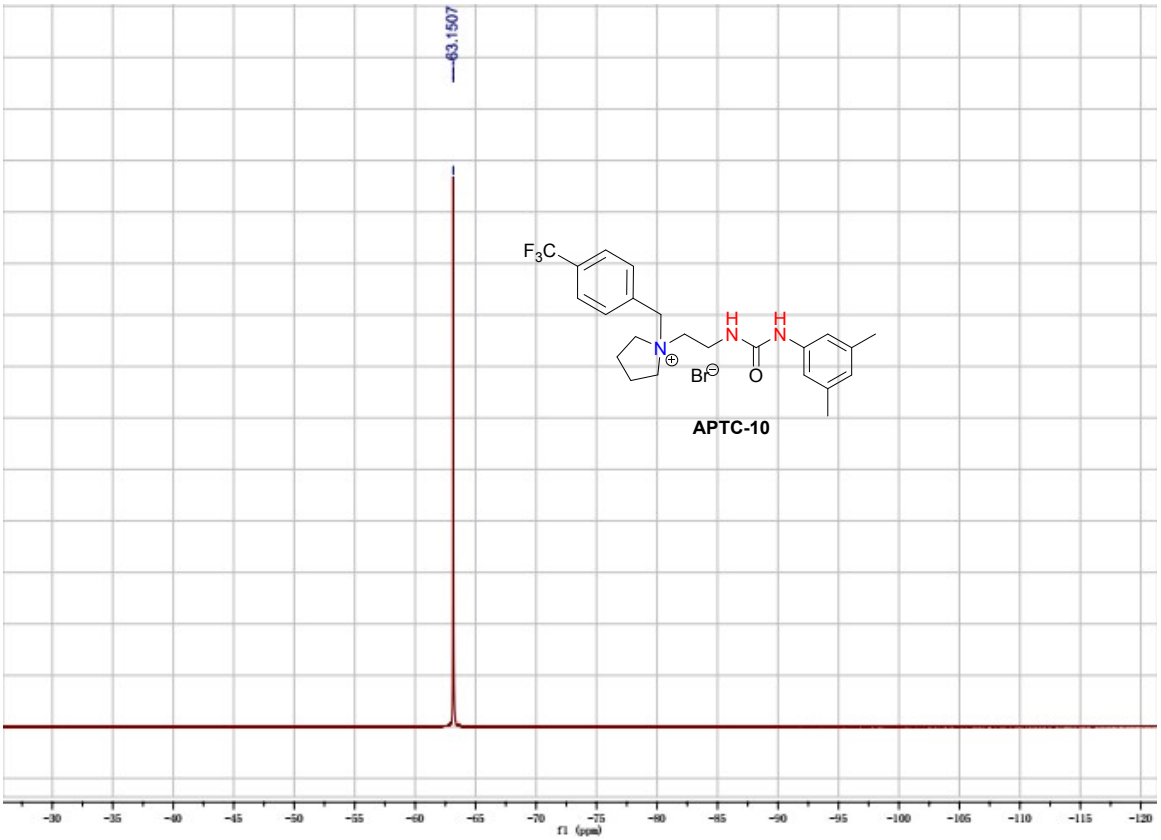
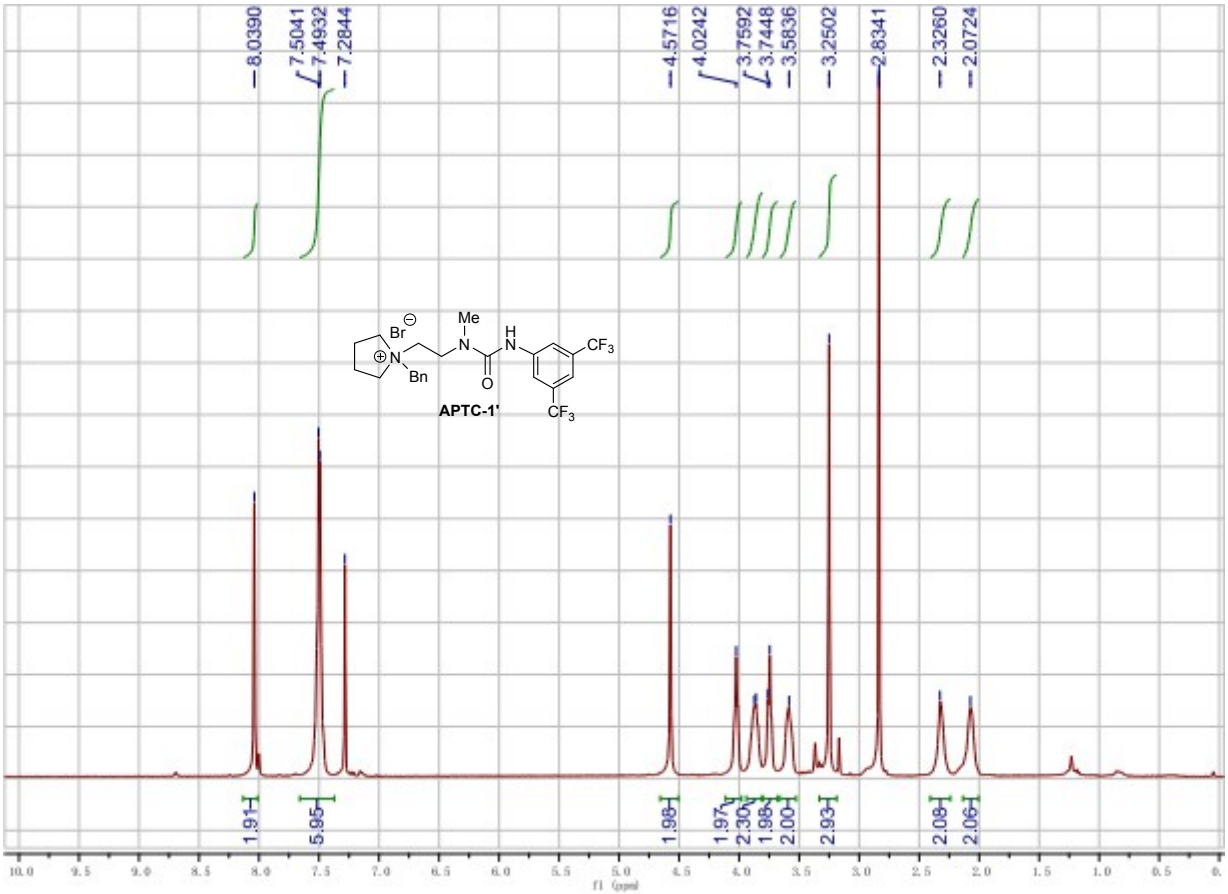
138.8676
138.5230
131.2226
126.4445
124.4287
116.5682
61.5343
59.4194
49.5069
49.2968
34.8860
21.3419
21.1742
F3C
H
N
H
N
N
Br
O
APTC-10
f1 (ppm)


63.1507
F3C
H
N
H
N
N
Br
O
APTC-10
f1 (ppm)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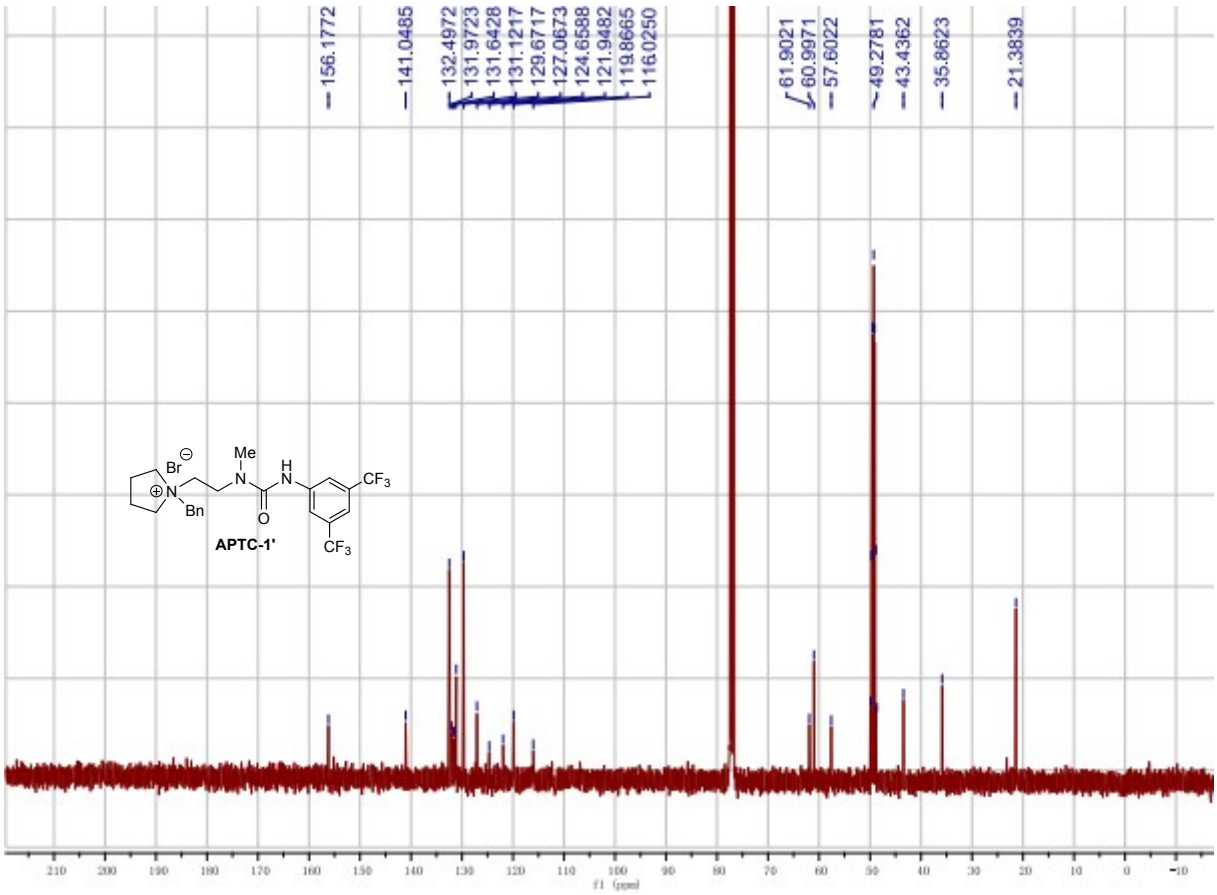
7.5041
7.4932
7.2844
4.5716
4.0242
3.7592
3.7448
3.5836
3.2502
2.8341
2.3260
2.0724
Me
Br
N
H
N
CF3
Bn
O
APTC-1'
CF3
1.91
5.95
1.98
1.97
2.30
1.98
2.00
2.93
2.08
2.06
f1 (ppm)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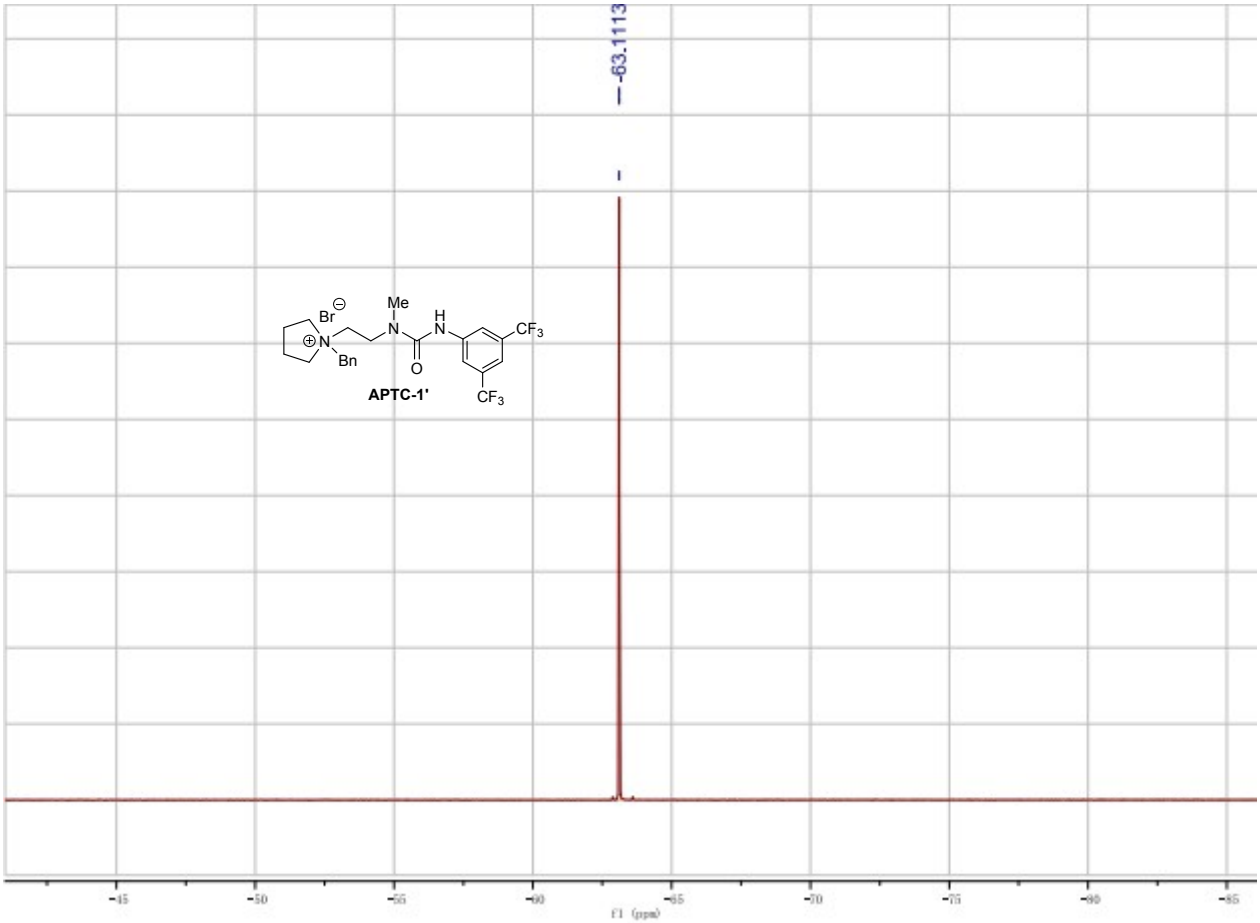
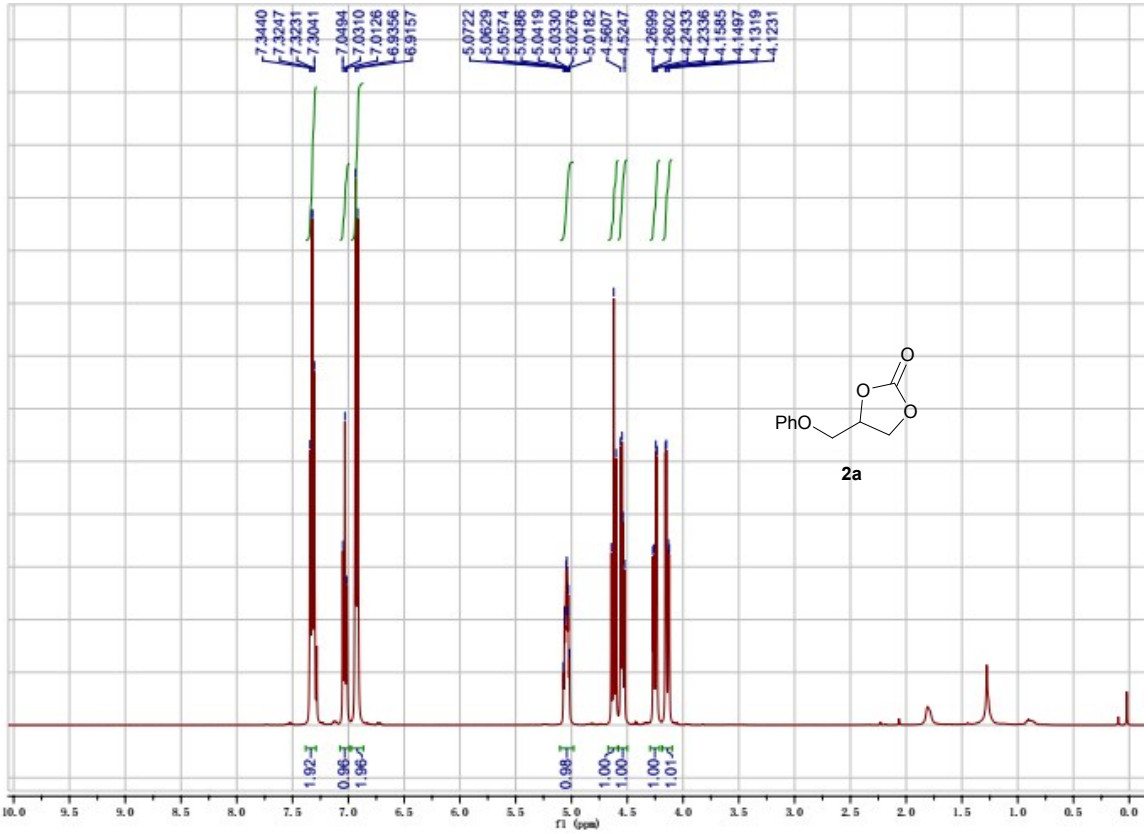
141.0485
132.4972
131.9723
131.6428
131.1217
129.6717
127.0673
124.6588
121.9482
119.8665
116.0250
61.9021
60.9971
57.6022
49.2781
43.4362
35.8623
21.3839
Me
Br
N
H
N
CF3
Bn
O
APTC-1'
CF3
f1 (ppm)


-63.1113
Br
Me
N
H
N
CF3
N
Bn
O
CF3
APTC-1'
f1 (ppm)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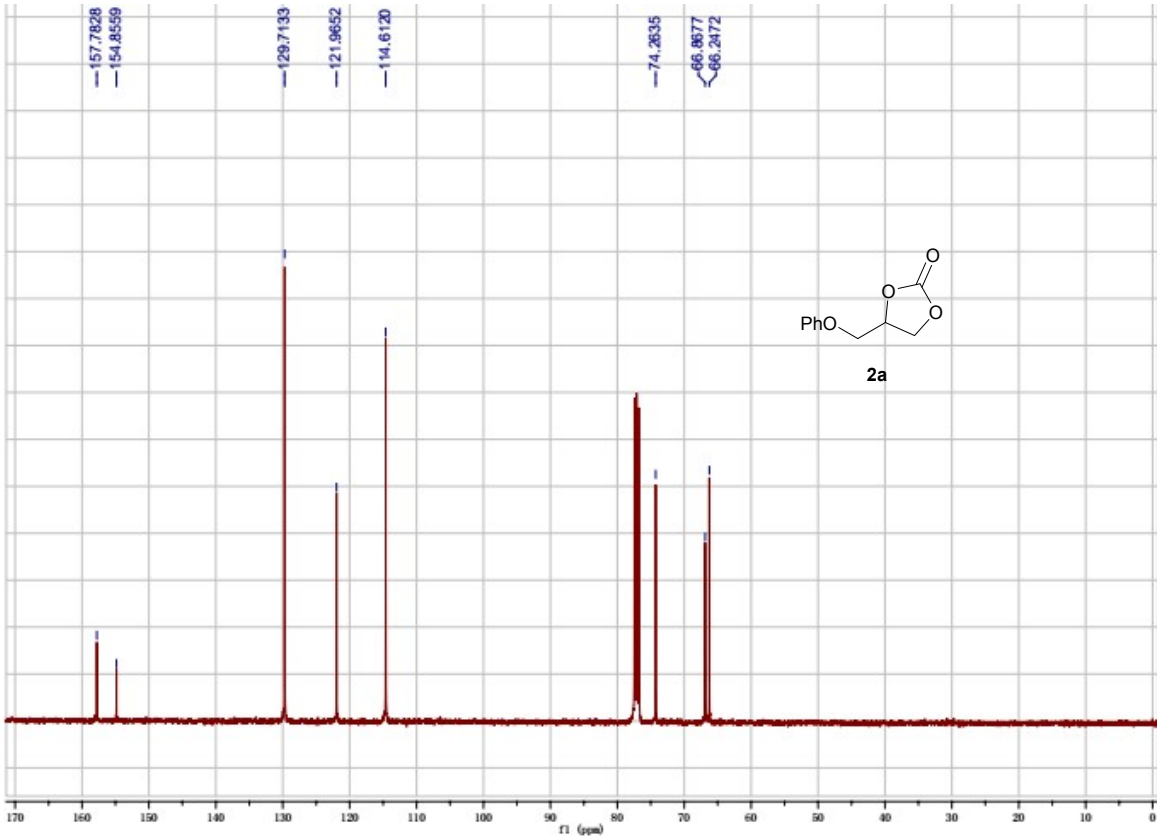
7.3231
7.3041
7.0494
7.0310
7.0126
6.9356
6.9157
5.0722
5.0629
5.0574
5.0486
5.0419
5.0330
5.0276
5.0182
4.5607
4.5247
4.2699
4.2602
4.2433
4.2336
4.1585
4.1497
4.1319
4.1231
1.92
0.96
1.96
0.98
1.00
1.00
1.00
1.01
f1 (ppm)
O
O
O
O
PhO
2a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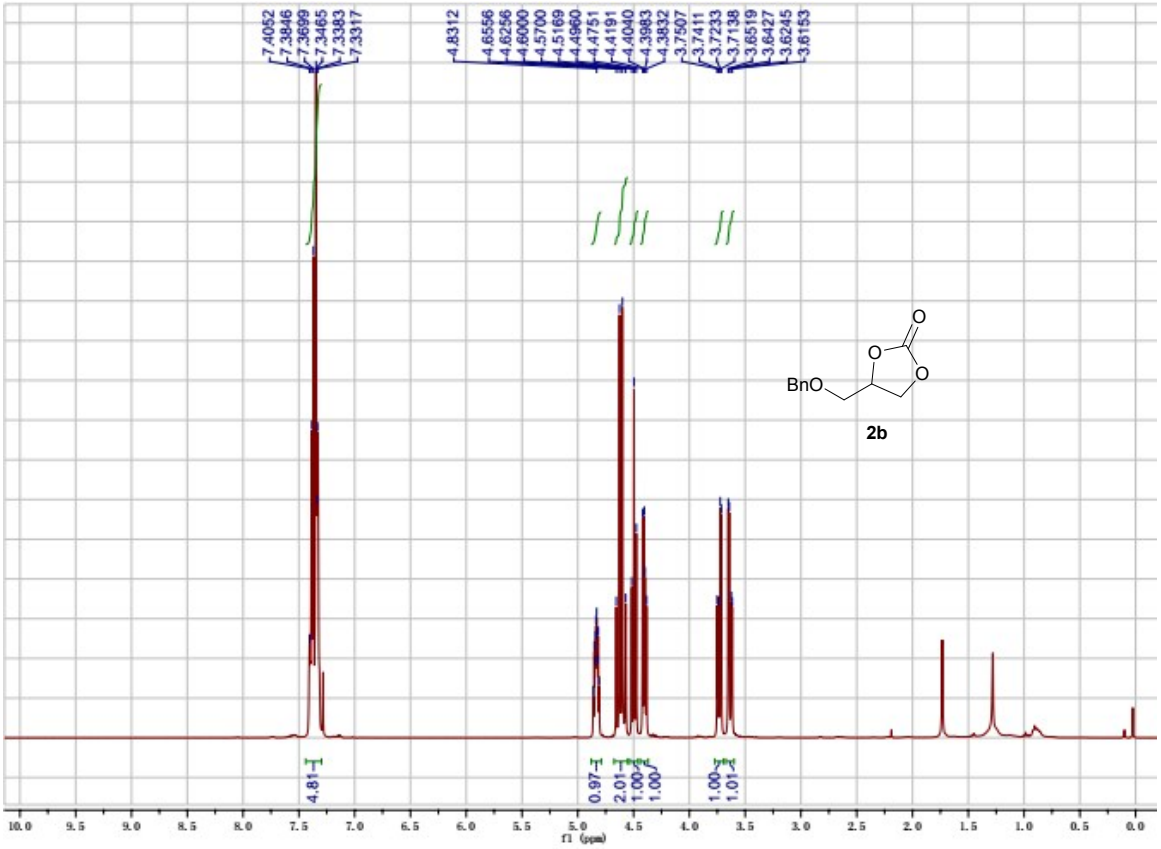
154.8559
129.7133
121.9652
114.6120
74.2635
66.8677
66.2472
PhO
O
O
O
2a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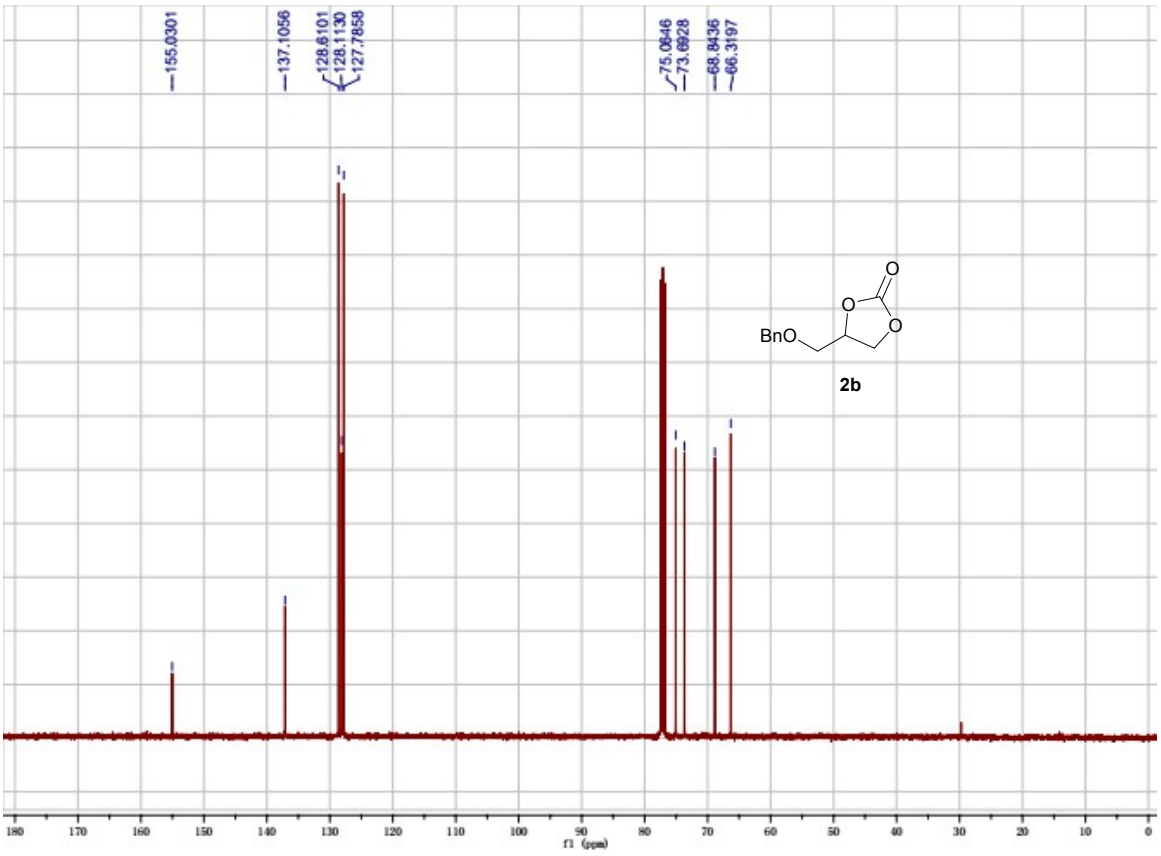
7.3465
7.3383
7.3317
4.8312
4.6556
4.6256
4.6000
4.5700
4.5169
4.4960
4.4751
4.4191
4.4040
4.3983
4.3832
3.7507
3.7411
3.7233
3.7138
3.6519
3.6427
3.6245
3.6153
4.81
0.97
2.01
1.00
1.00
1.00
1.01
BnO
O
O
O
2b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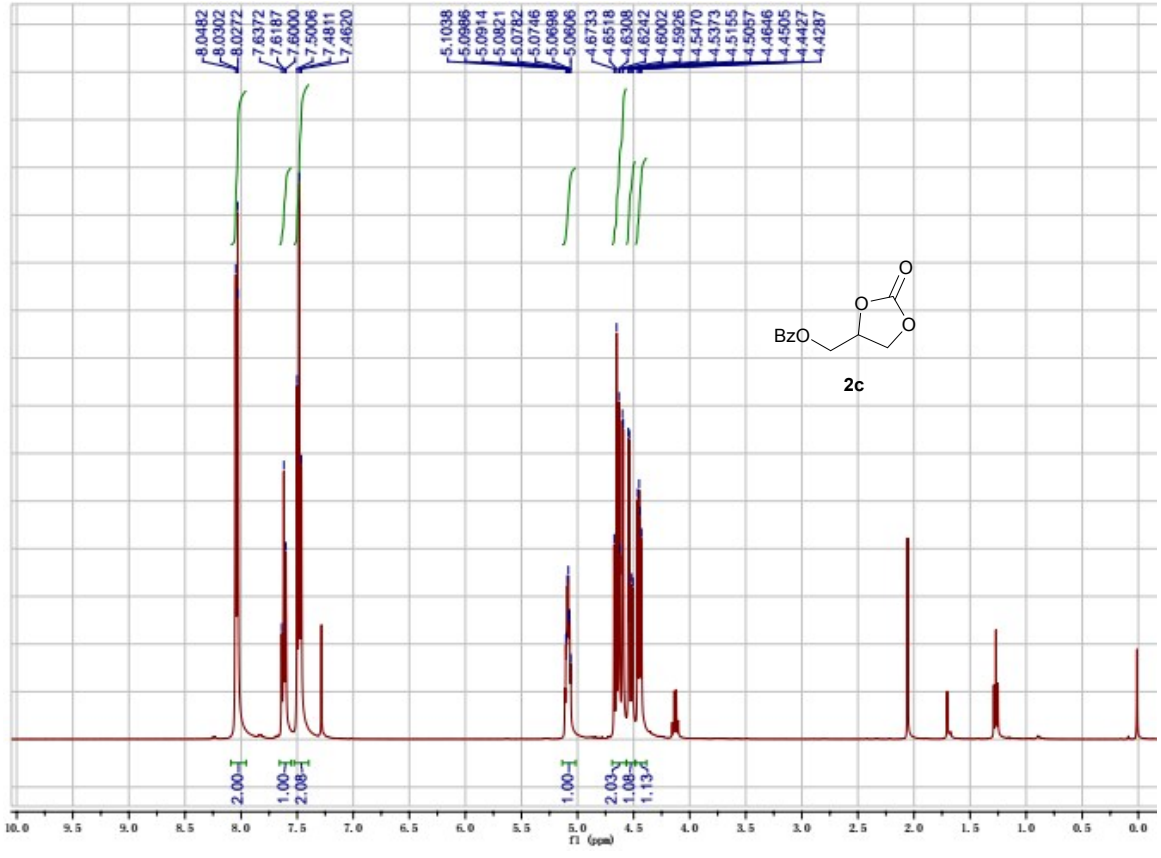
127.7858
75.0646
73.6928
68.8436
66.3197
BnO
O
O
O
2b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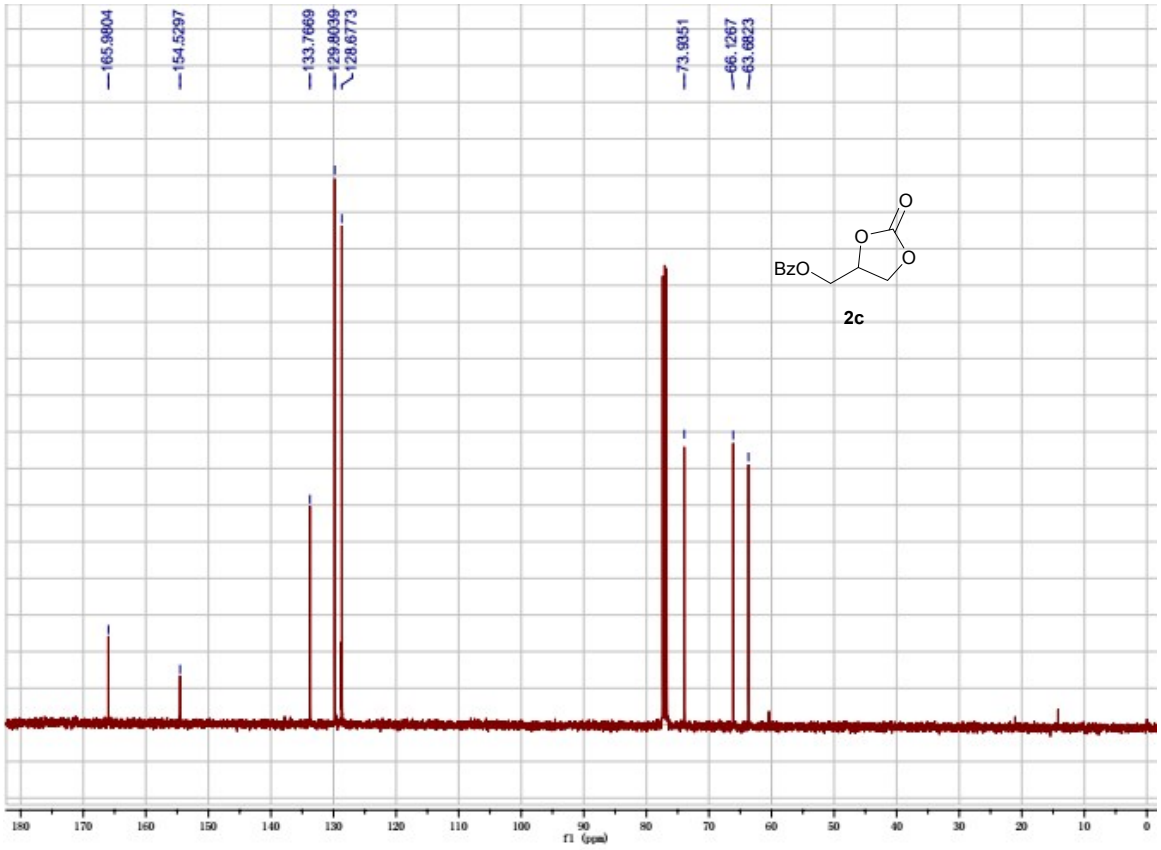
8.0302
8.0272
7.6372
7.6187
7.6000
7.5006
7.4811
7.4620
5.1038
5.0986
5.0914
5.0821
5.0782
5.0746
5.0698
5.0606
4.6733
4.6518
4.6308
4.6242
4.6002
4.5926
4.5470
4.5373
4.5155
4.5057
4.4646
4.4505
4.4427
4.4287
2.00
1.00
2.08
1.00
2.03
1.08
1.13
BzO
O
O
O
2c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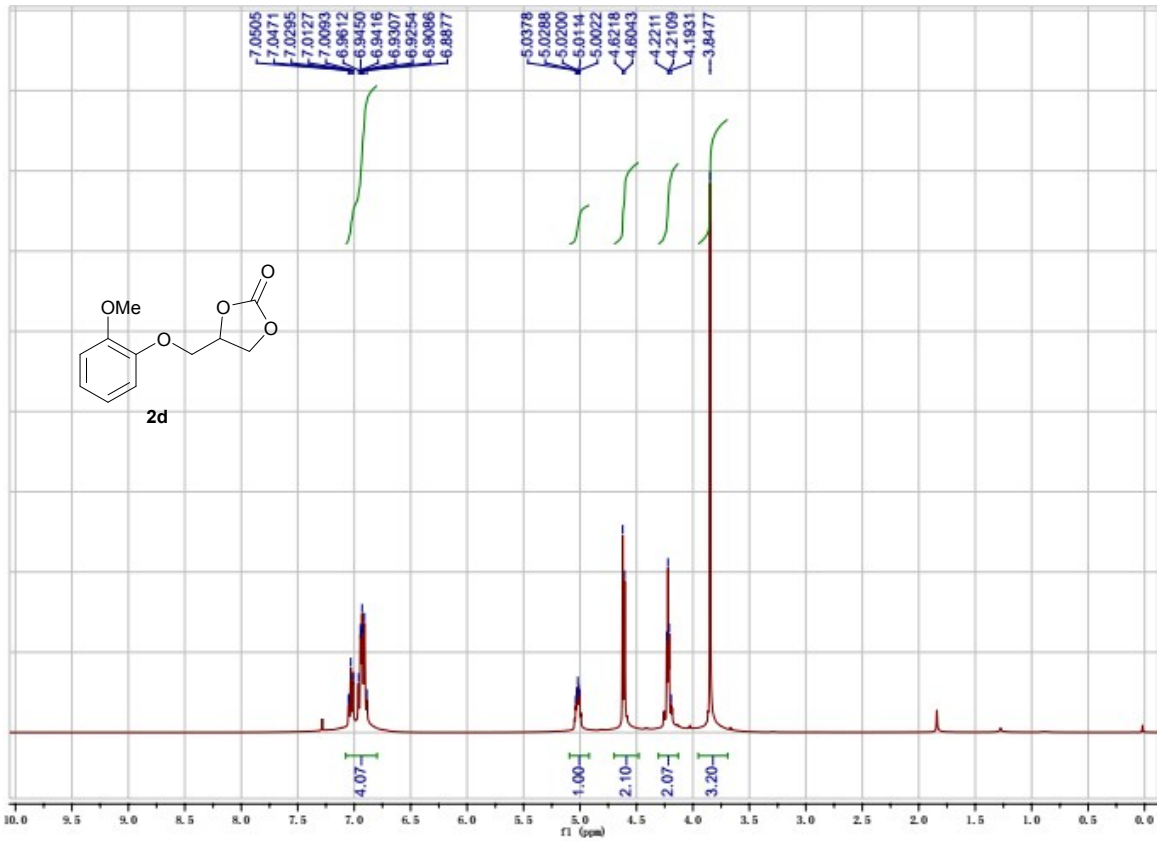
129.8039
128.6773
73.9351
66.1267
63.6823
BzO
O
O
O
2c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7.0295
7.0127
7.0093
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6.9450
6.9416
6.9307
6.9254
6.9086
6.8877
5.0378
5.0288
5.0200
5.0114
5.0022
4.6218
4.6043
4.2211
4.2109
4.1931
3.8477
OMe
O
O
O
O
2d
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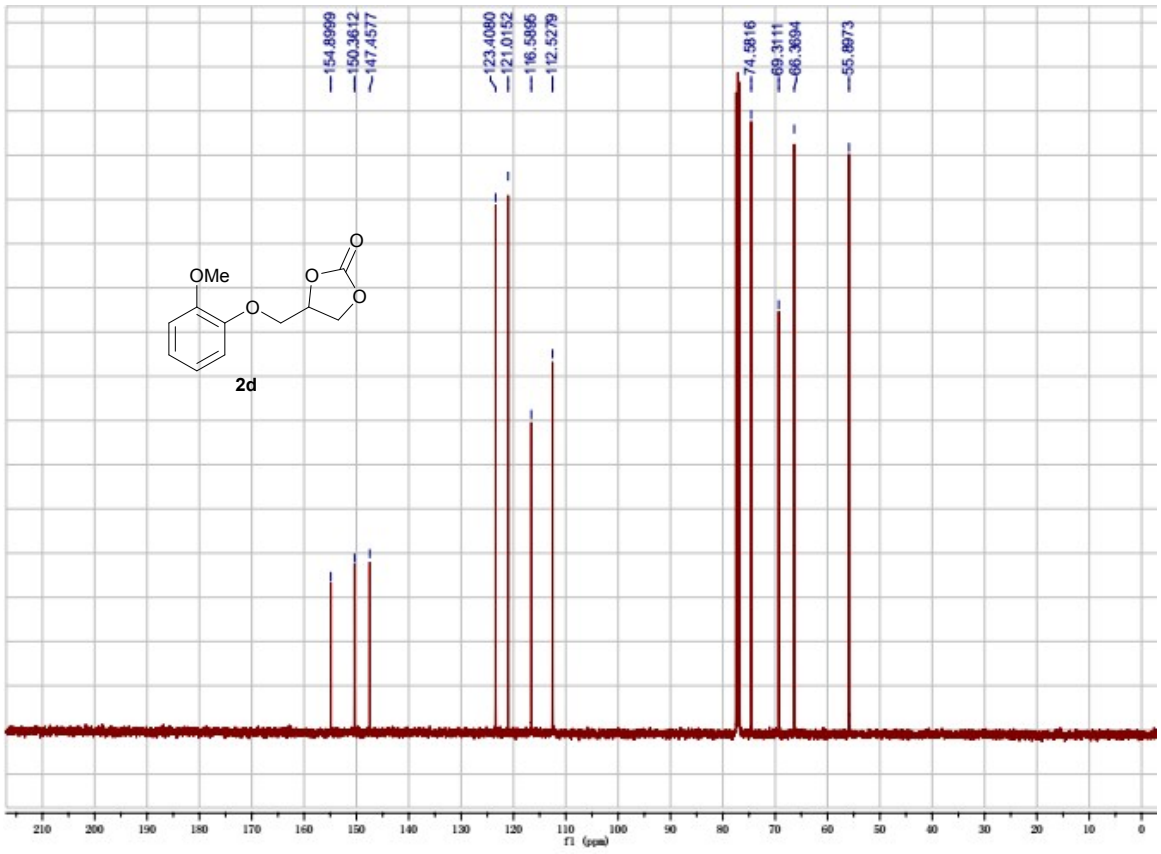
1.00
2.10
2.07
3.20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121.0152
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112.5279
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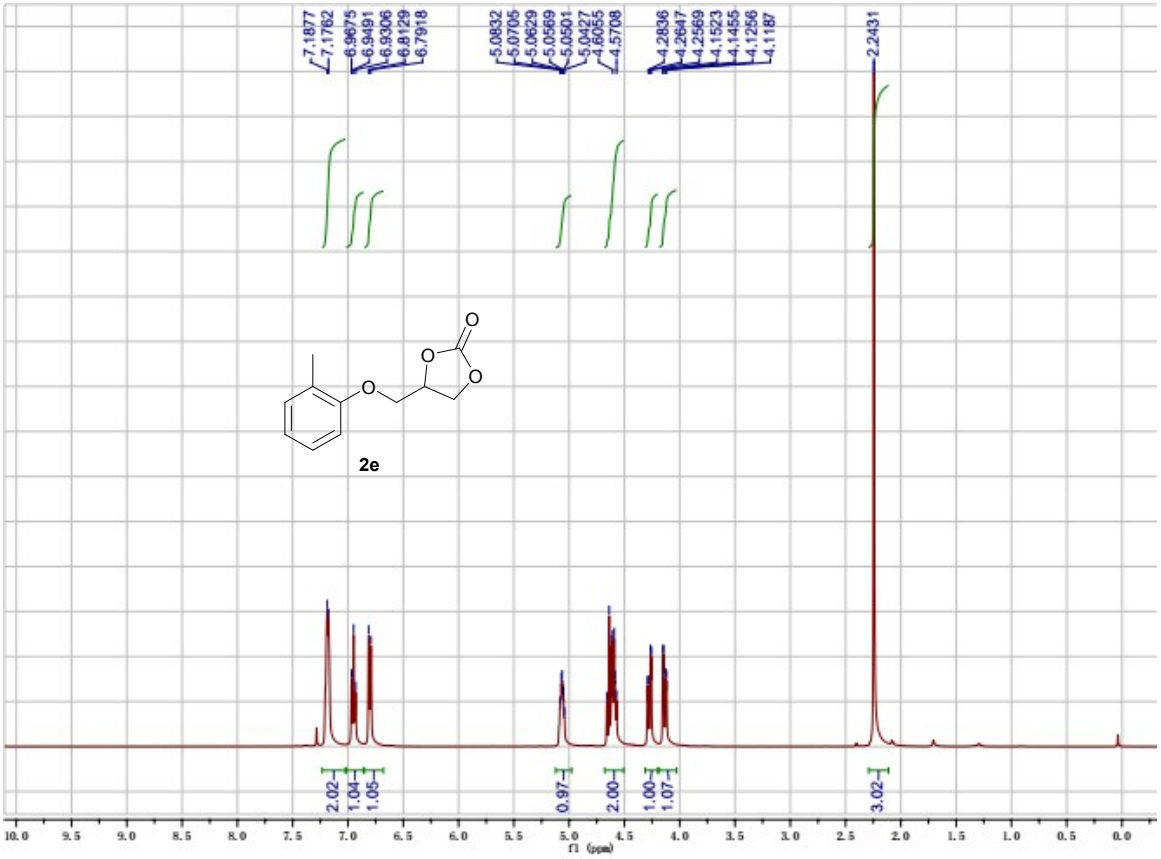
69.3111
66.3694
55.8973
OMe
O
O
O
O
2d
f1 (ppm)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6.9306
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6.7918
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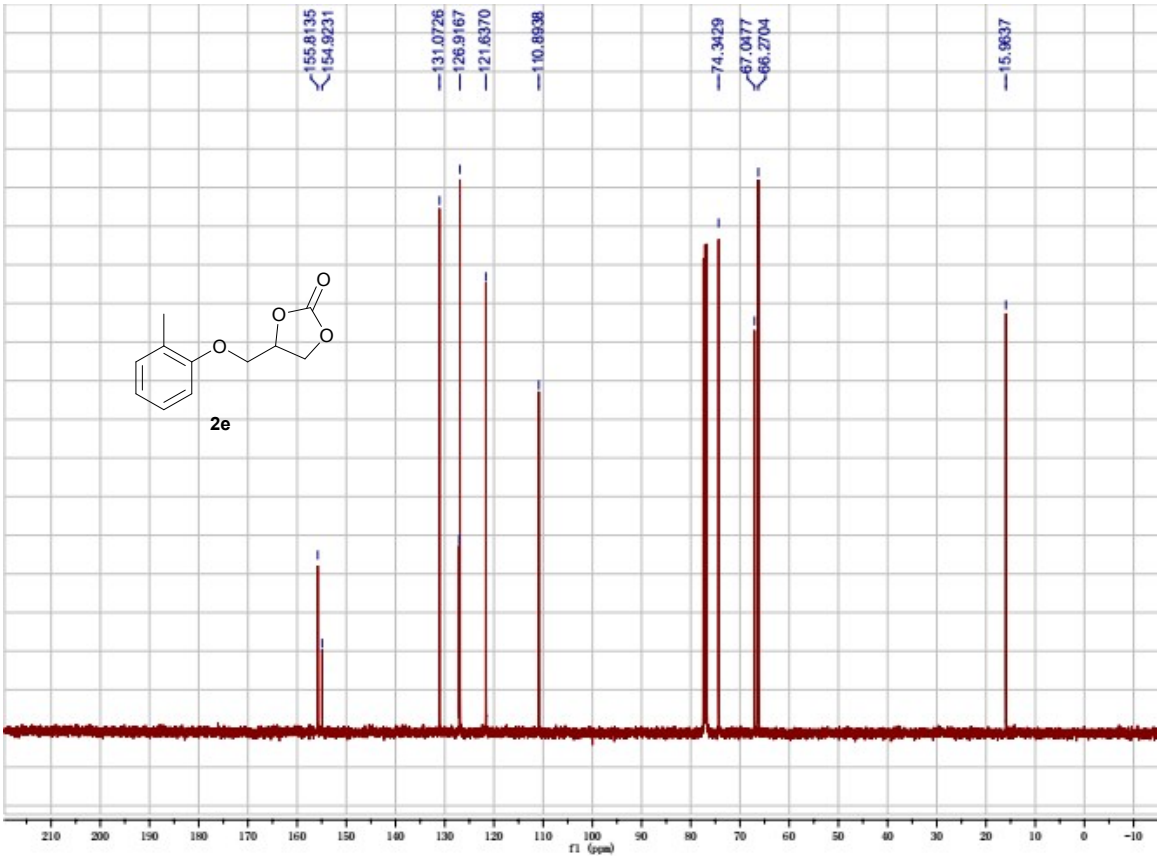
5.0705
5.0629
5.0569
5.0501
5.0427
4.6055
4.5708
4.2836
4.2647
4.2569
4.1523
4.1455
4.1256
4.1187
2.2431
2.02
1.04
1.05
0.97
2.00
1.00
1.07
3.02
O
O
O
O
2e
f1 (ppm)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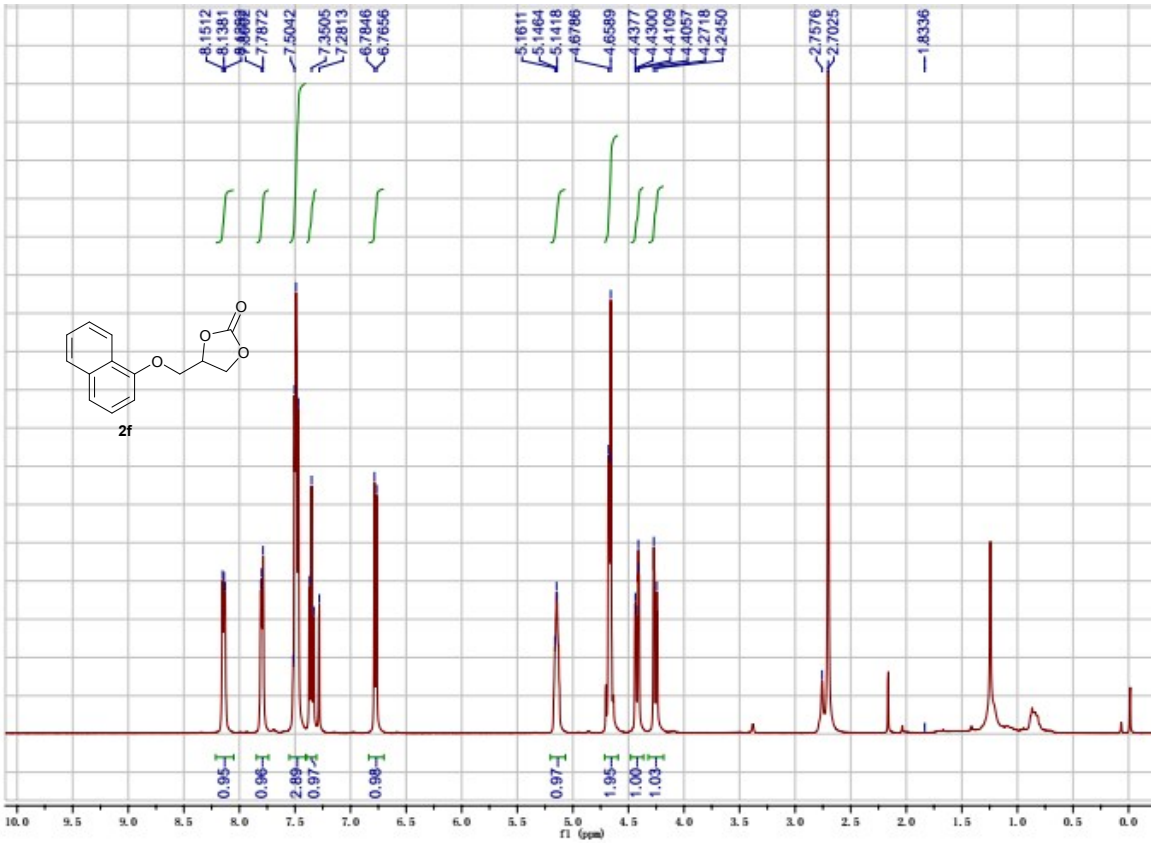
66.2704
15.9637
2e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5.1418
4.6786
4.6589
4.4377
4.4300
4.4109
4.4057
4.2718
4.2450
2.7576
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0.96
2.89
0.97
0.98
0.97
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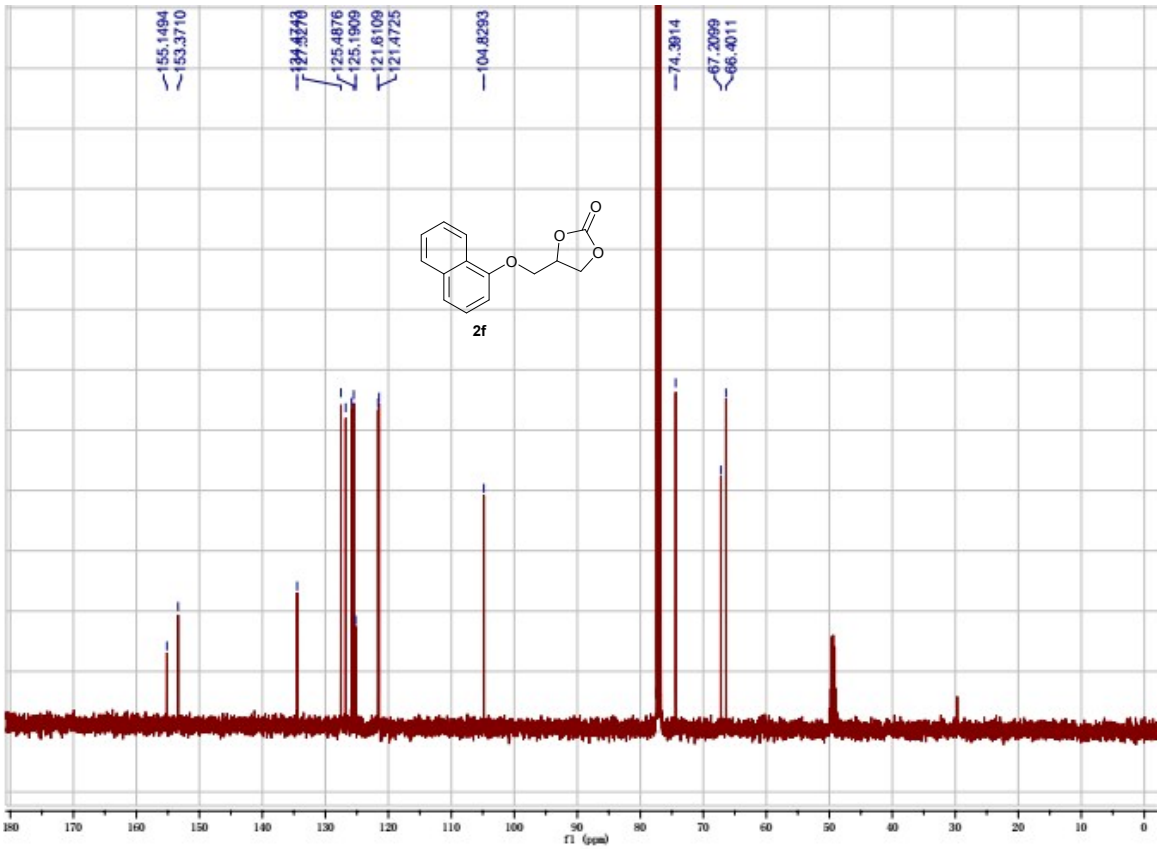
1.03
2f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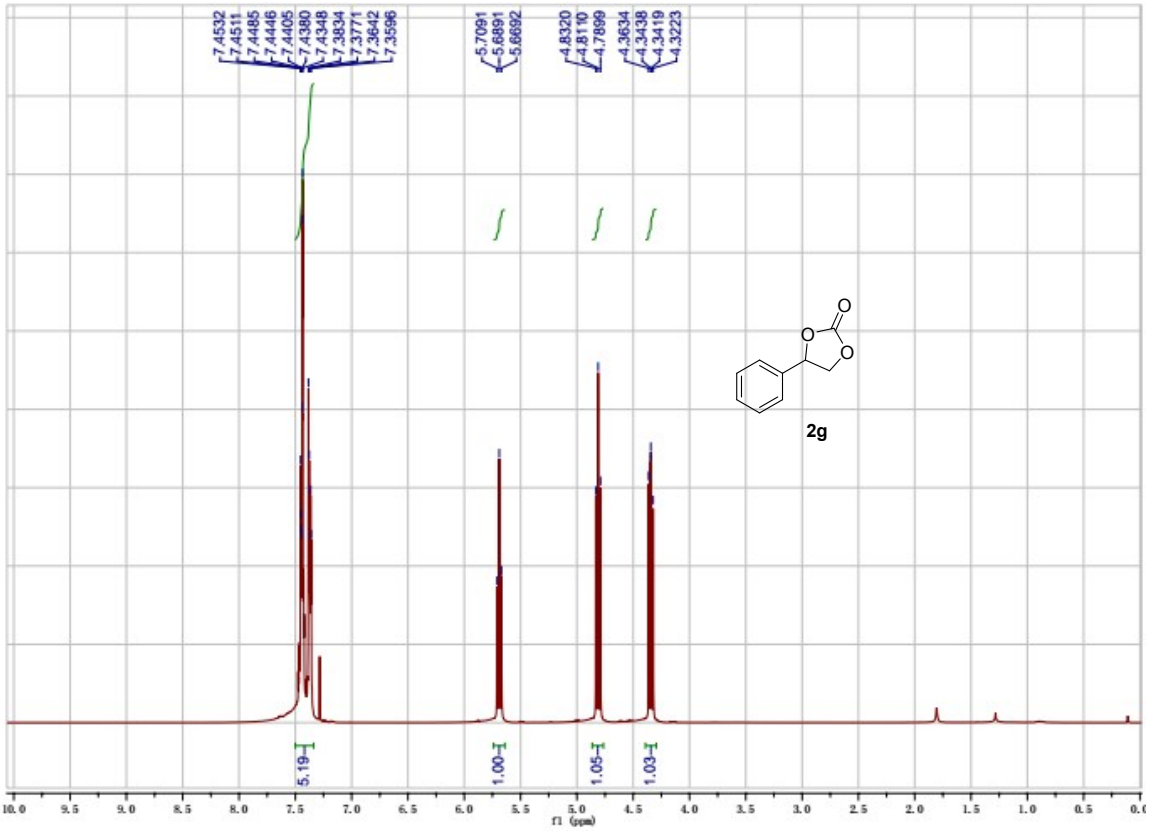
67.2099
66.4011
2f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7.4380
7.4348
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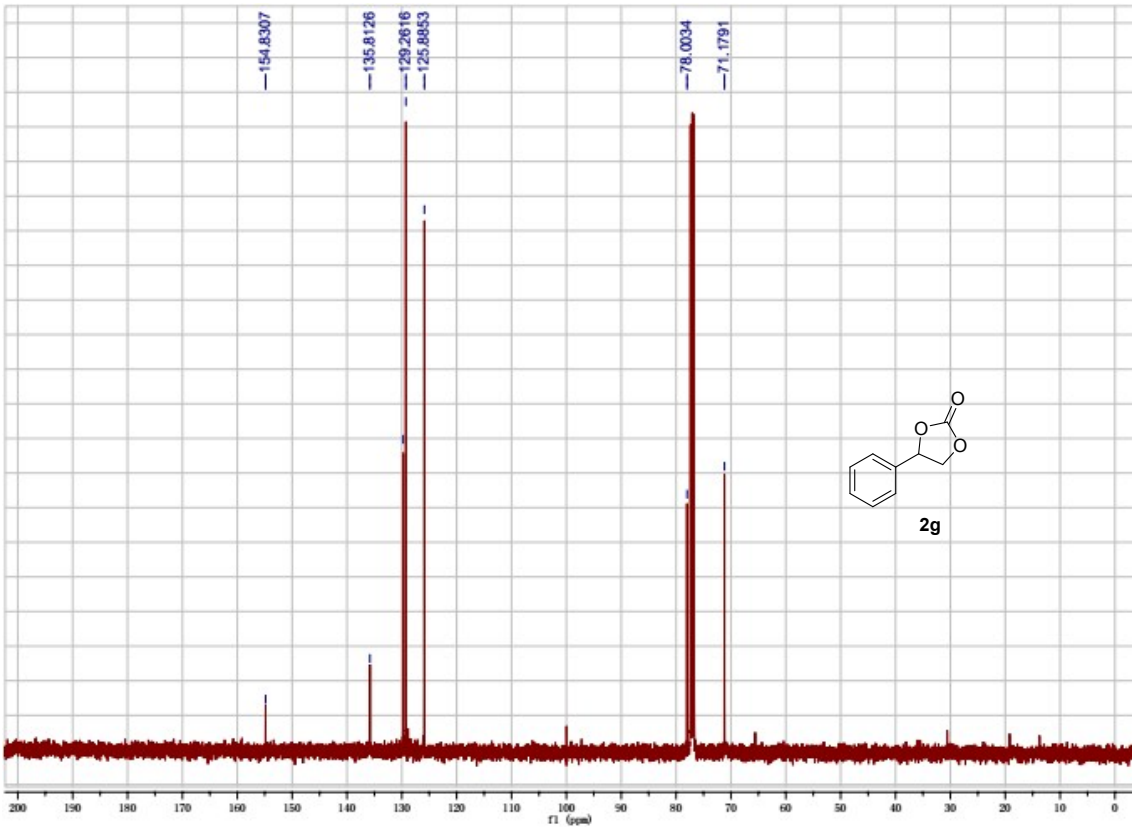
7.3771
7.3642
7.3596
5.7091
5.6891
5.6692
4.8320
4.8110
4.7899
4.3634
4.3438
4.3419
4.3223
5.19
1.00
1.05
1.03
2g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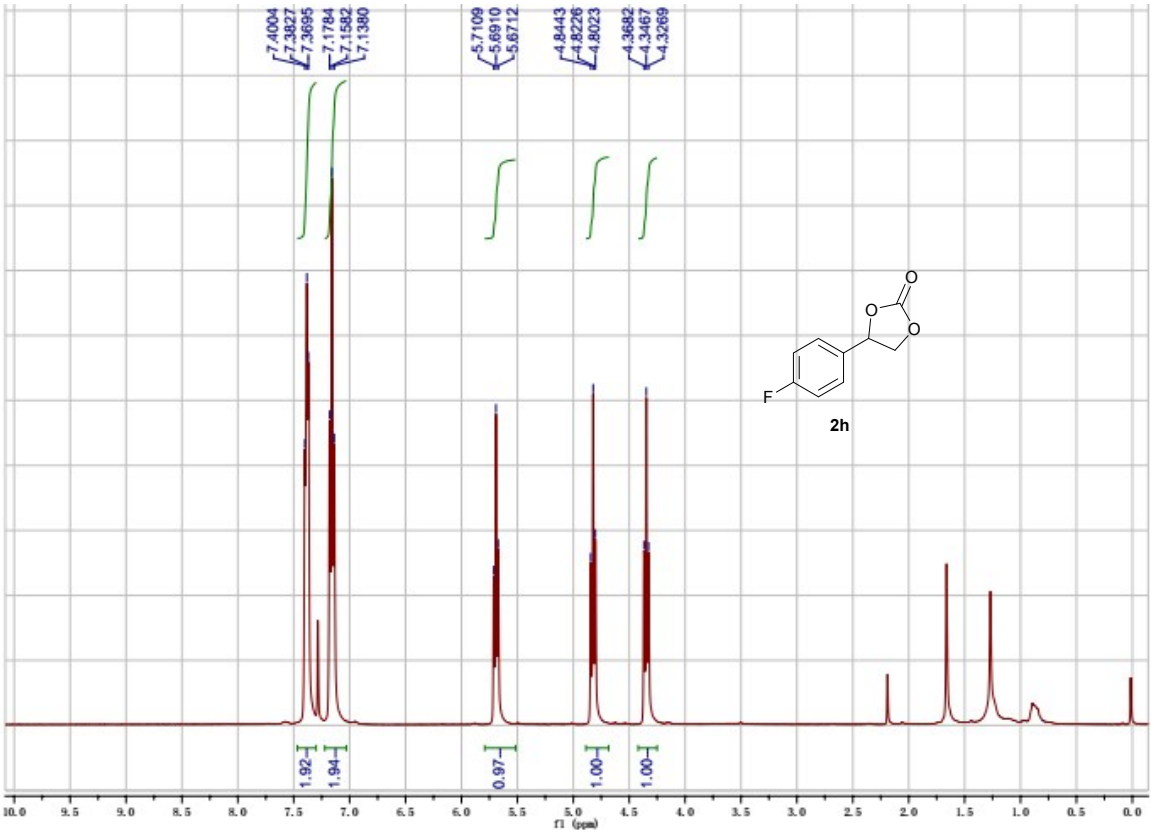
O
O
O
2g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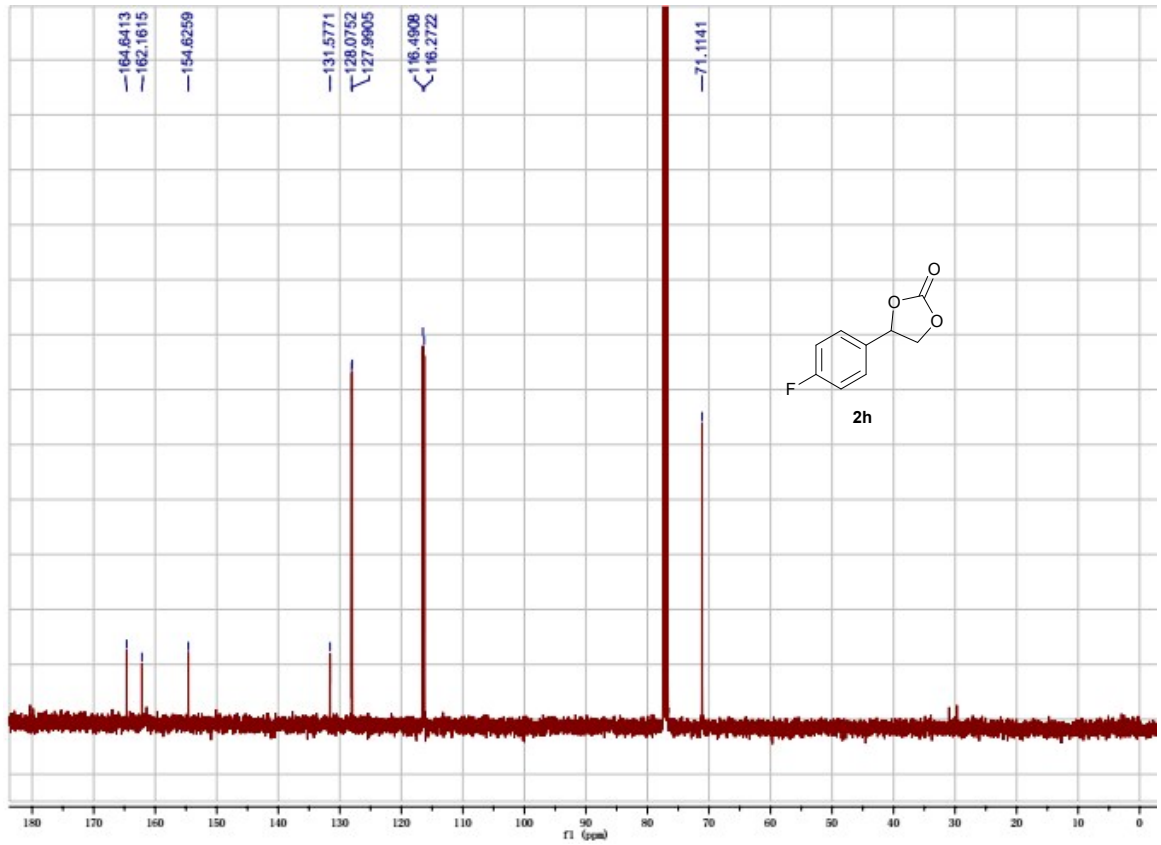
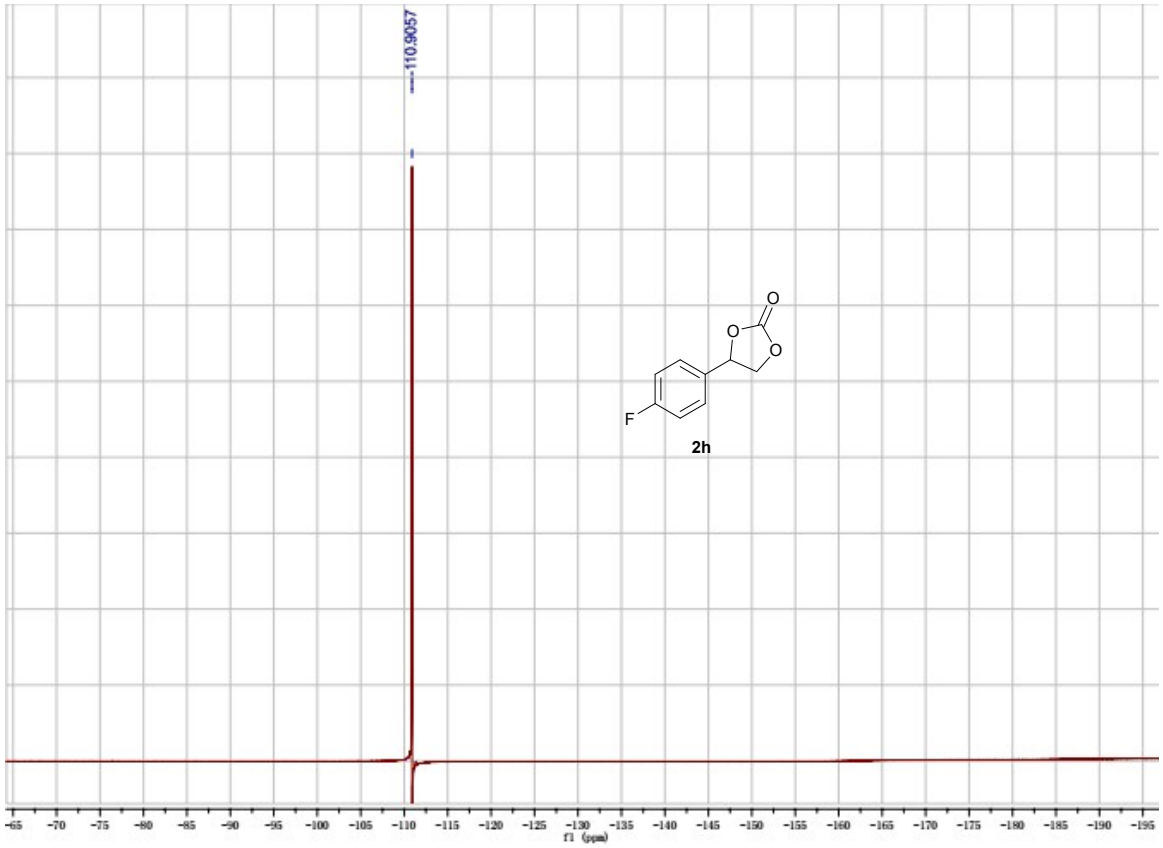
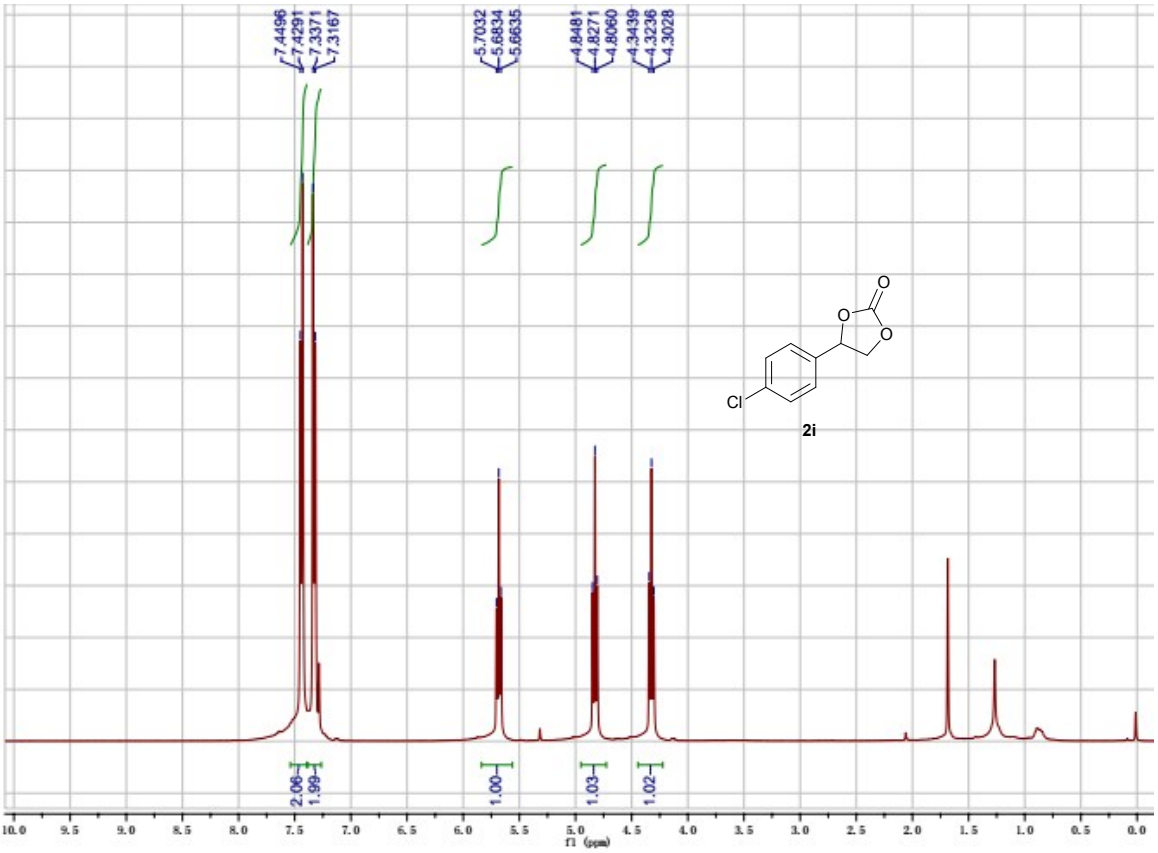
7.1784
7.1582
7.1380
5.7109
5.6910
5.6712
4.8443
4.8226
4.8023
4.3682
4.3467
4.3269
1.92
1.94
0.97
1.00
1.00
O
O
O
F
2h


164.6413
162.1615
154.6259
131.5771
128.0752
127.9905
116.4908
116.2722
71.1141
O
O
O
F
2h


110.9057
O
O
O
F
2h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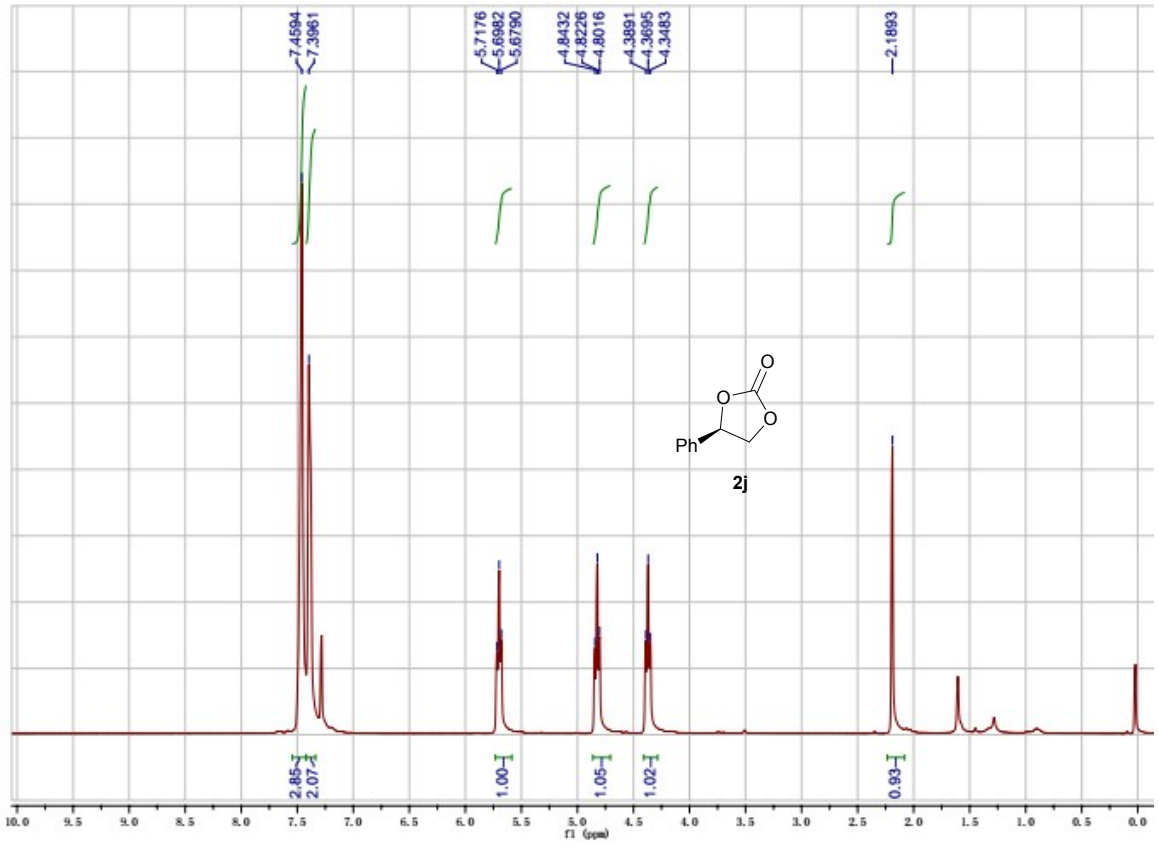
7.4291
7.3371
7.3167
5.7032
5.6834
5.6635
4.8481
4.8271
4.8060
4.3439
4.3236
4.3028
O
O
O
Cl
2i
2.06
1.99
1.00
1.03
1.02
f1 (ppm)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5.7176
5.6982
5.6790
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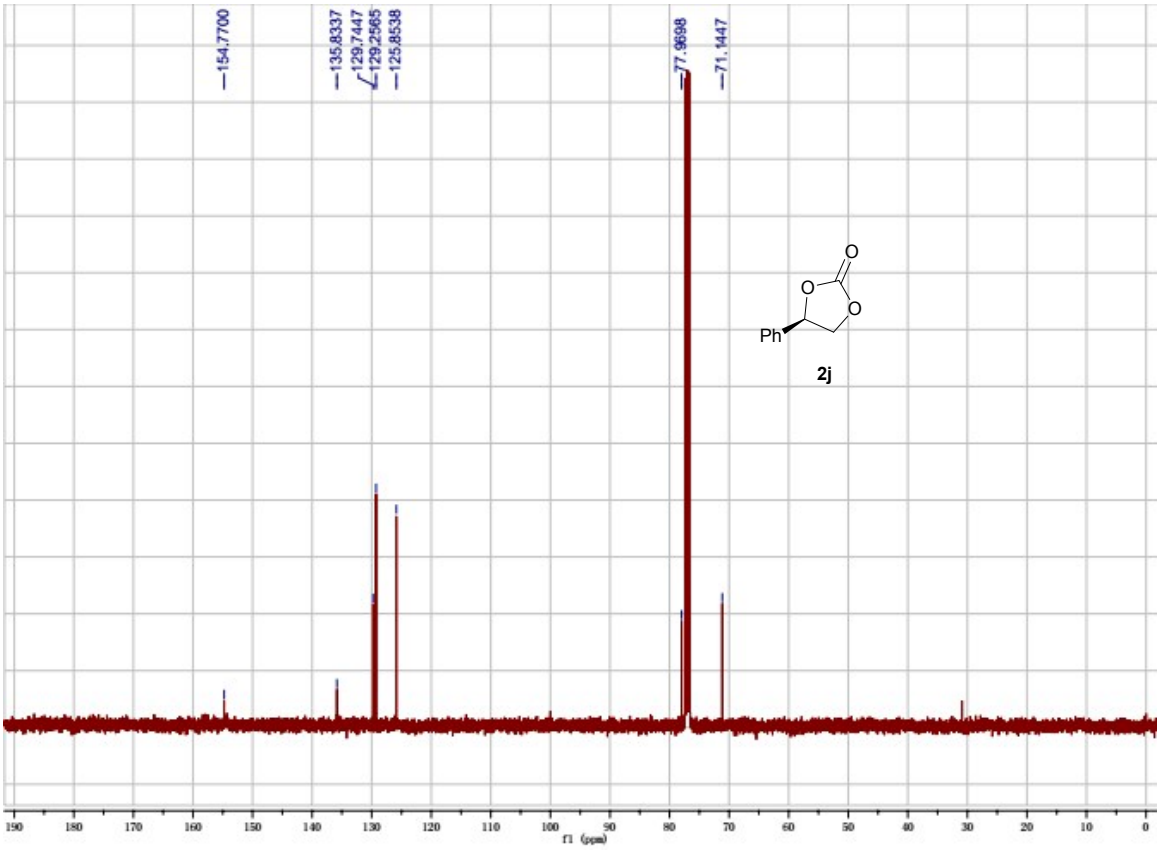
4.8226
4.8016
4.3891
4.3695
4.3483
2.1893
O
O
O
Ph
2j
2.85
2.07
1.00
1.05
1.02
0.93
f1 (ppm)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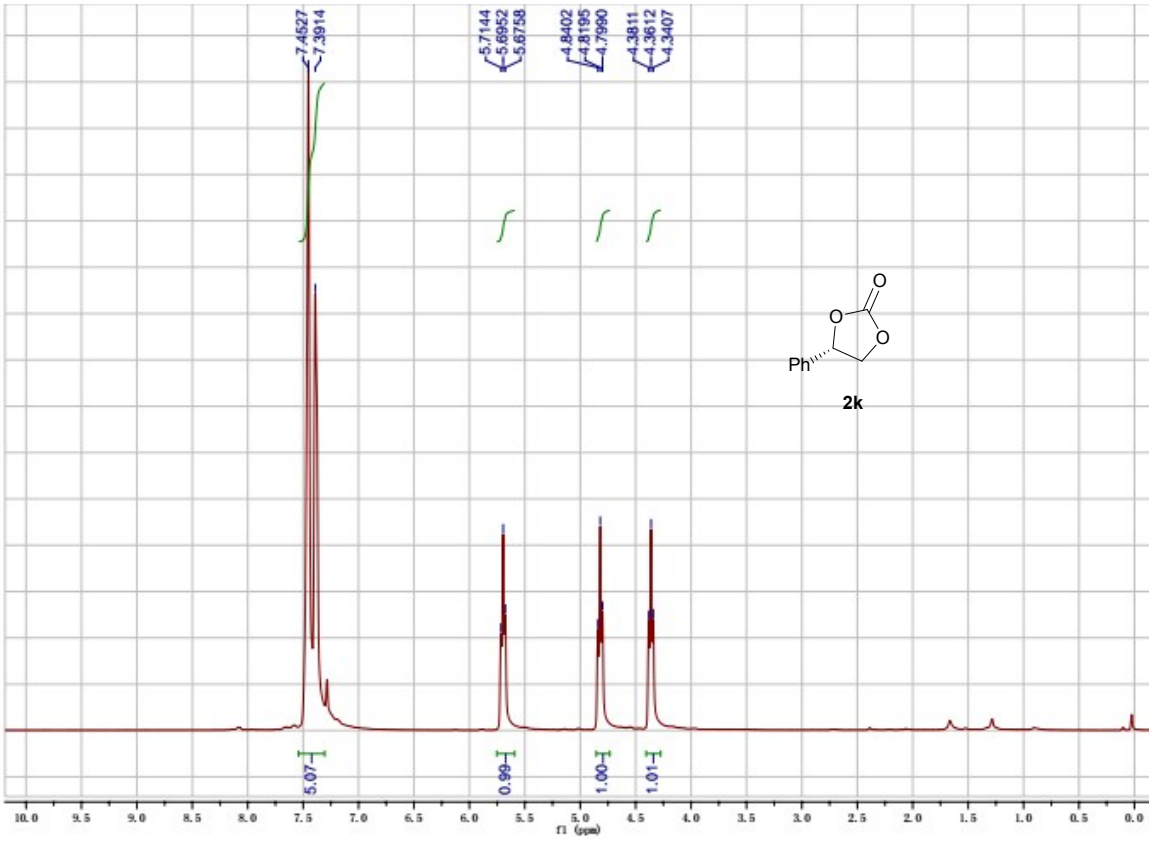
O
O
O
Ph
2j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5.6758
4.8402
4.8195
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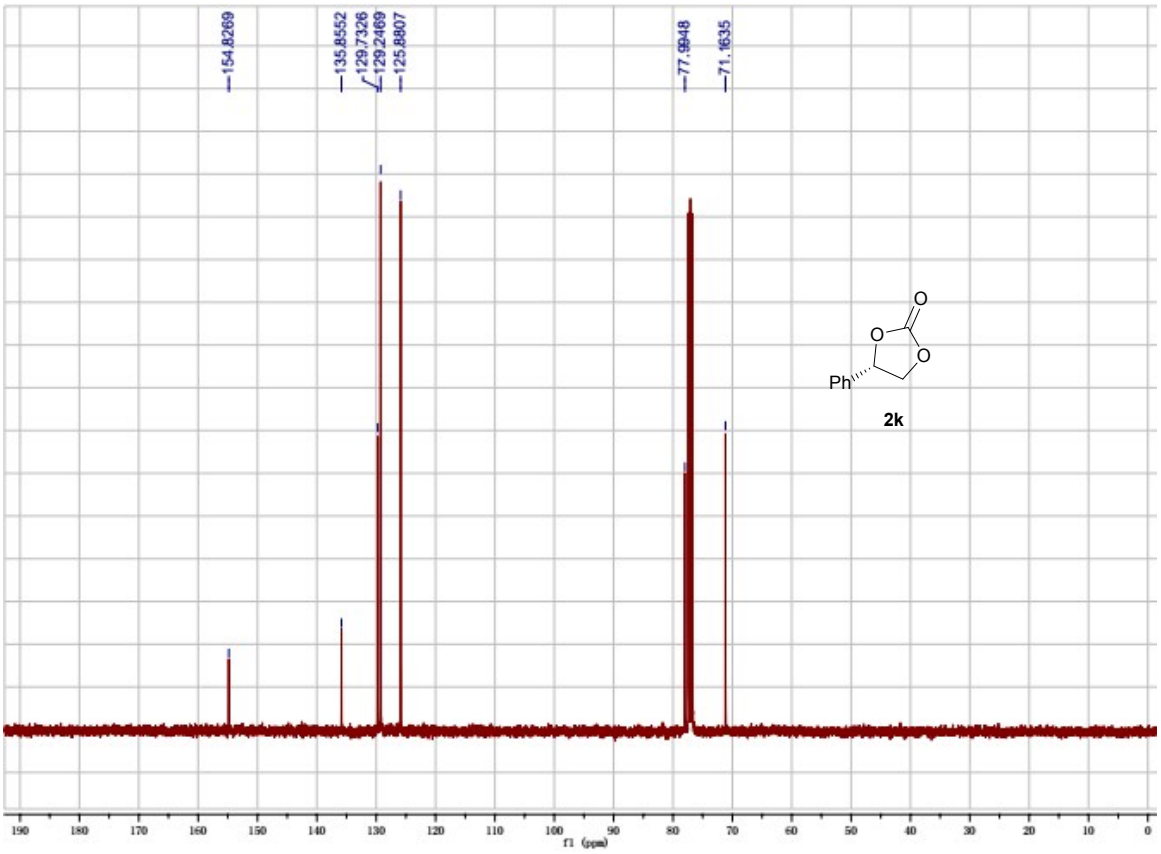
4.3612
4.3407
5.07
0.99
1.00
1.01
O
O
O
Ph
2k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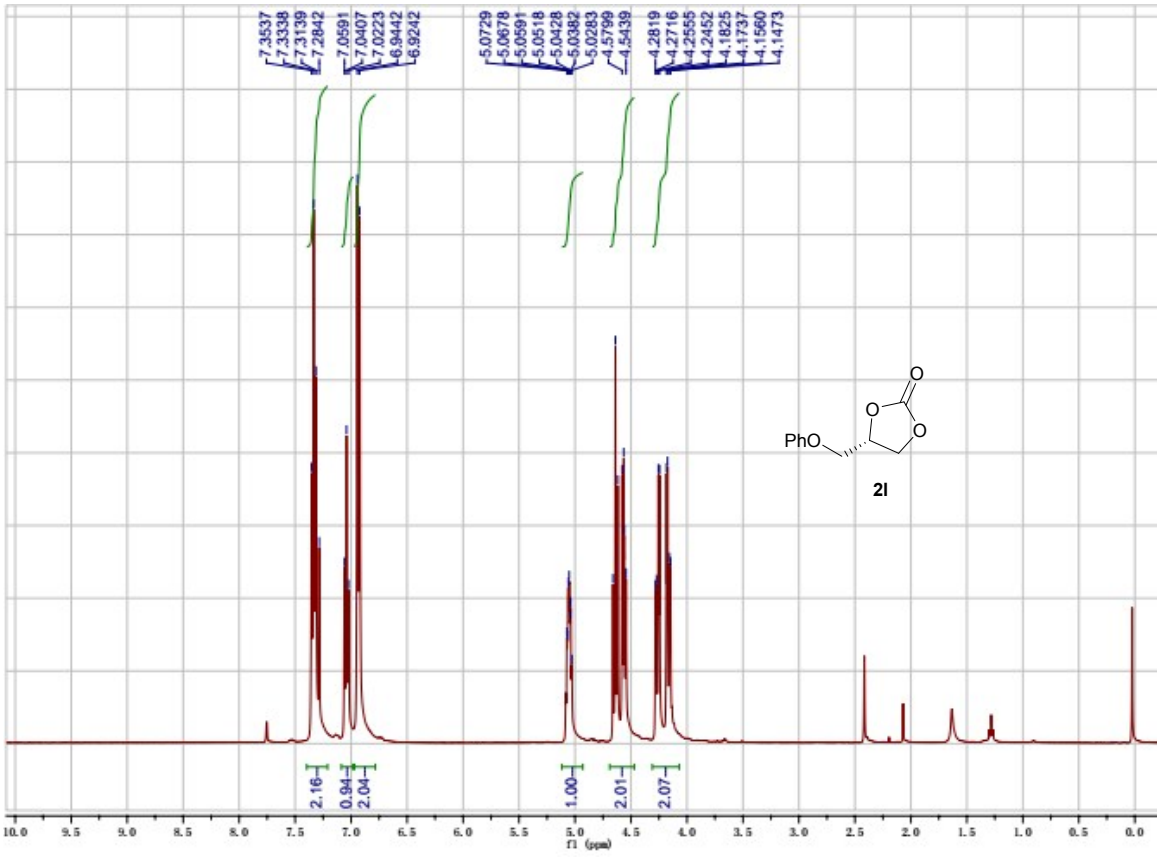
2k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7.0407
7.0223
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6.9242
5.0729
5.0678
5.0591
5.0518
5.0428
5.0382
5.0283
4.5799
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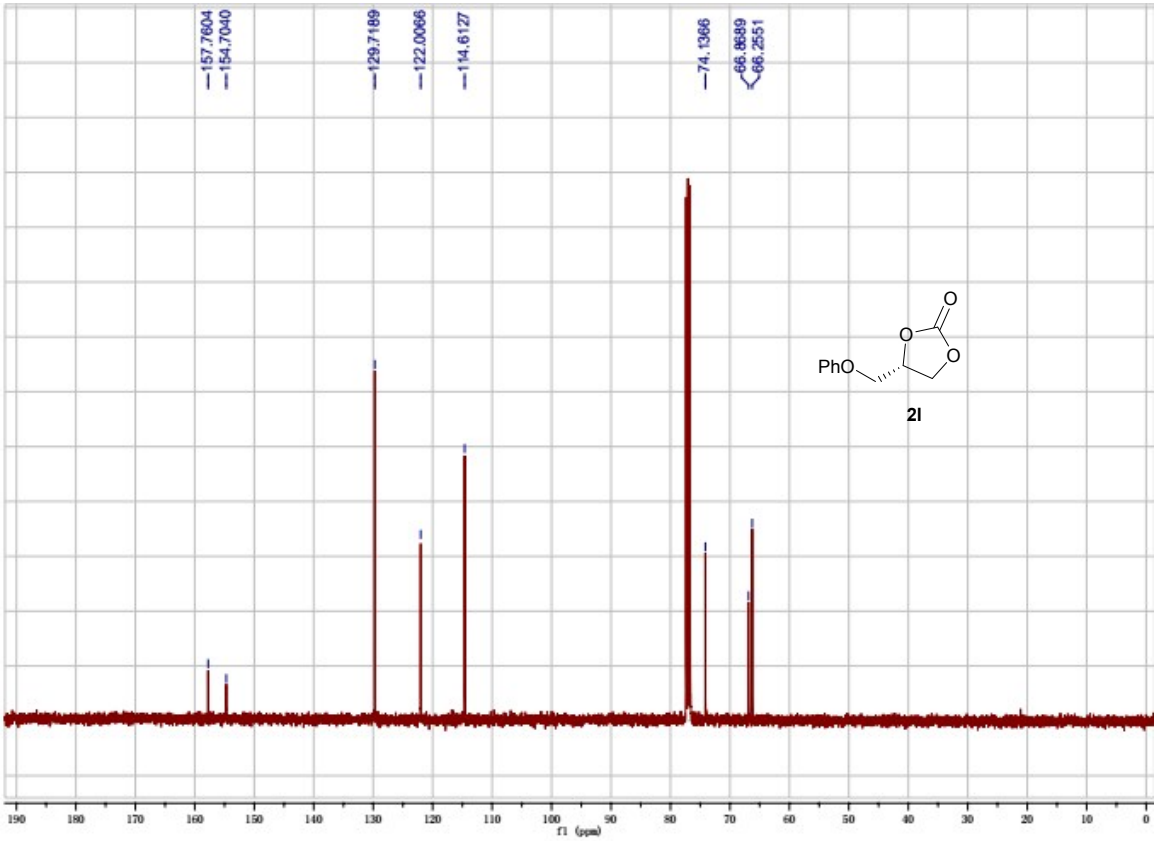
4.2452
4.1825
4.1737
4.1560
4.1473
PhO
2l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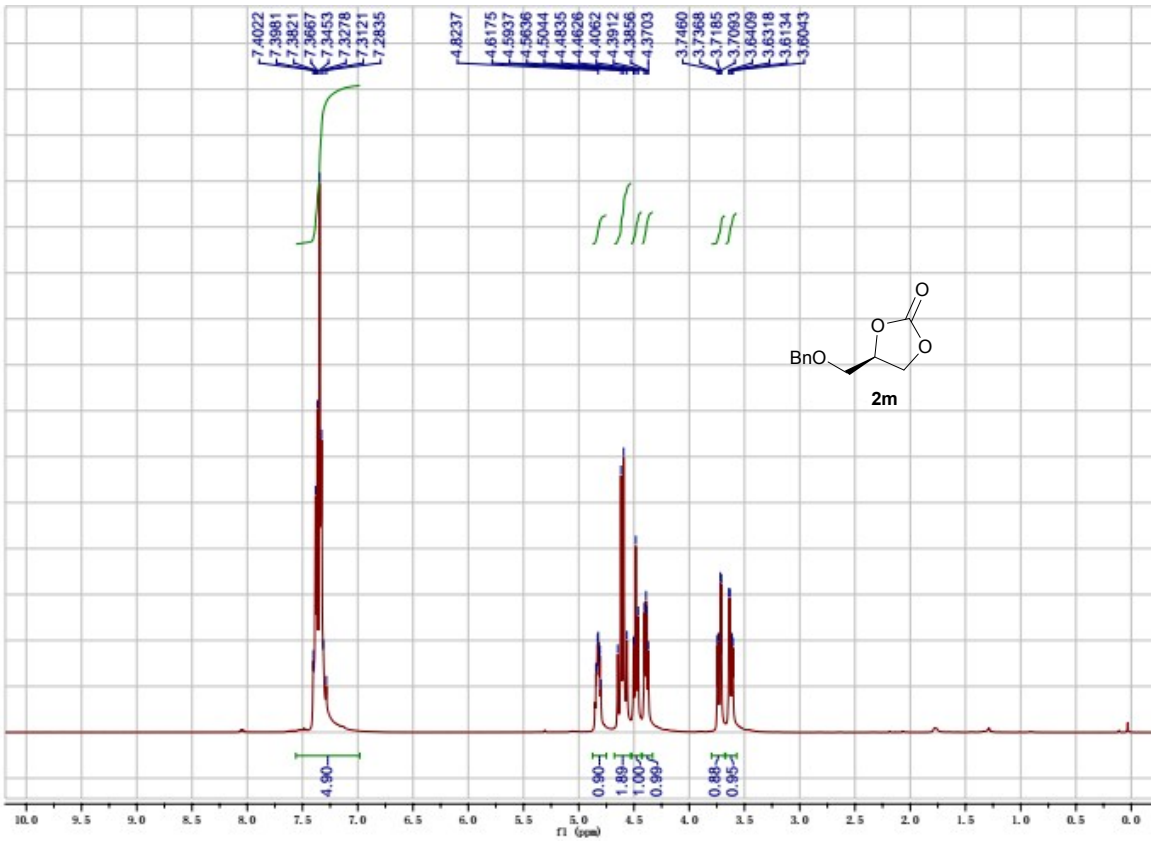
PhO
2l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4.5937
4.5636
4.5044
4.4835
4.4626
4.4062
4.3912
4.3856
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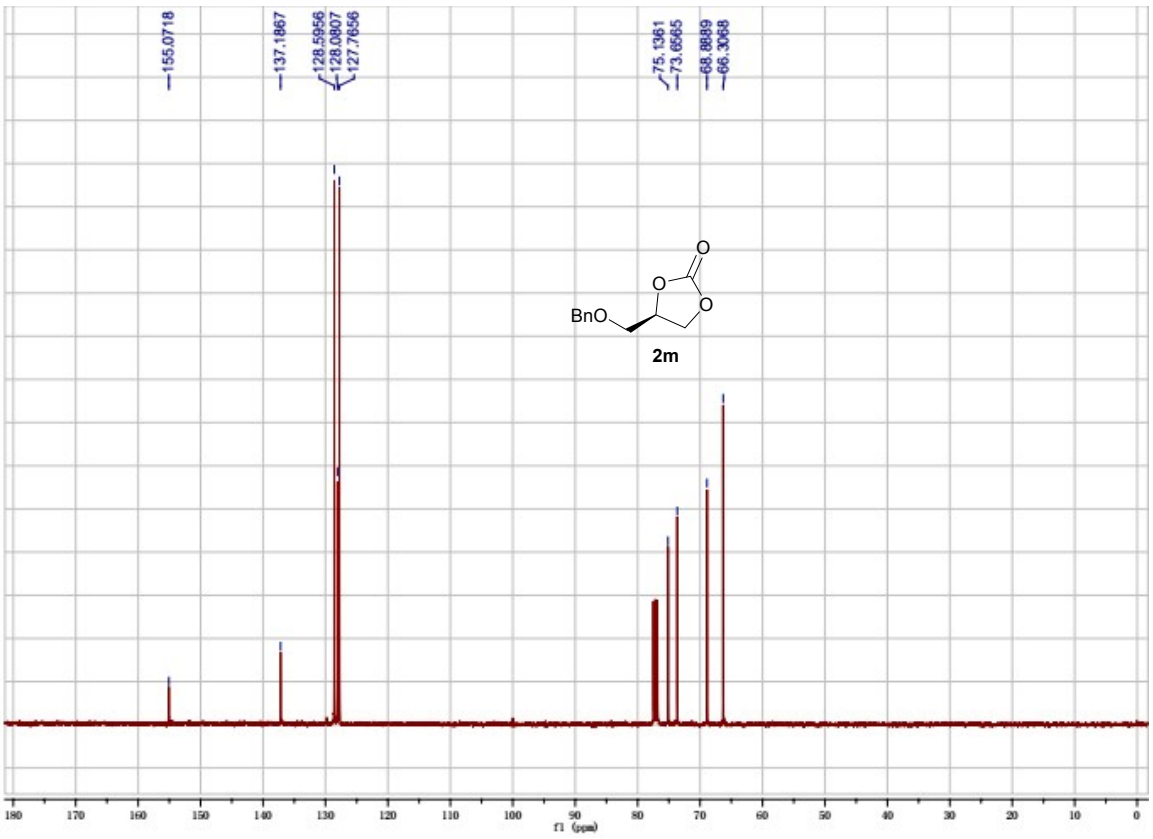
BnO
2m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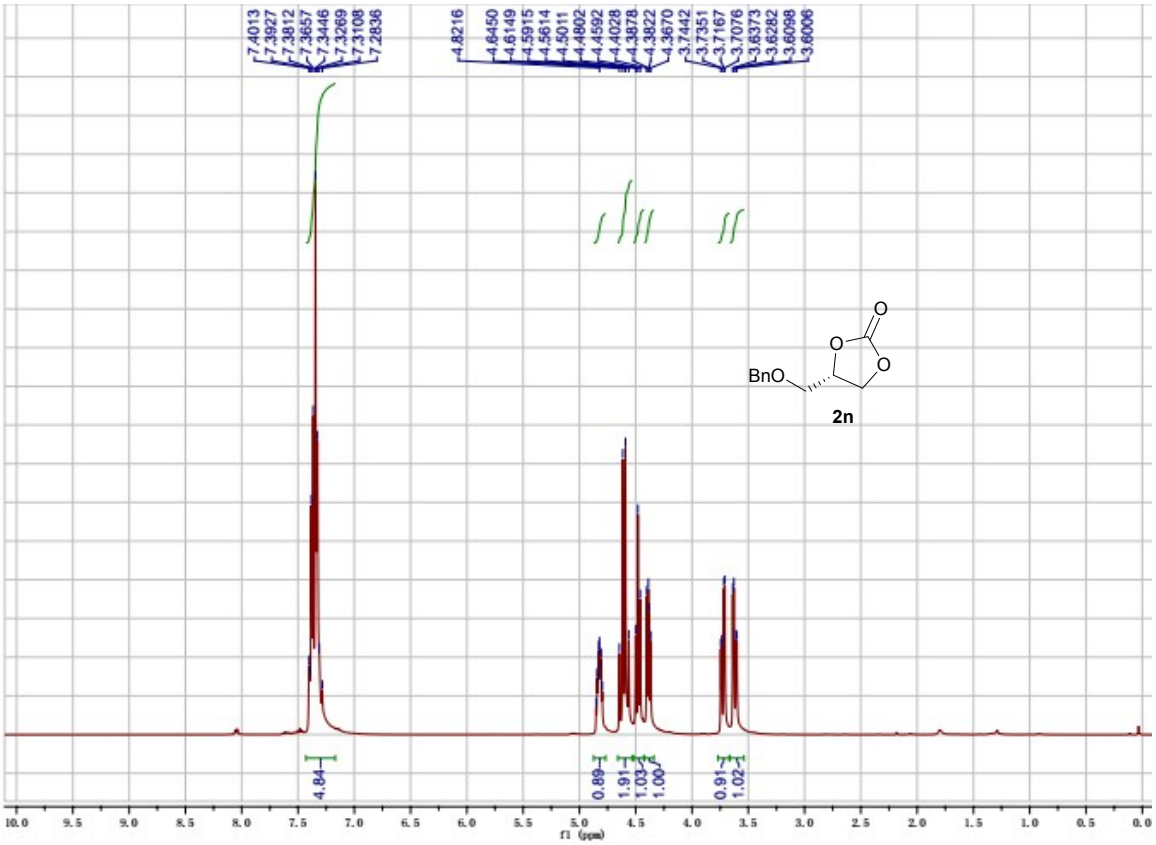
O
O
O
2m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7.3446
7.3269
7.3108
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4.6450
4.6149
4.5915
4.5614
4.5011
4.4802
4.4592
4.4028
4.3878
4.3822
4.3670
3.7442
3.7351
3.7167
3.7076
3.6373
3.6282
3.6098
3.6006
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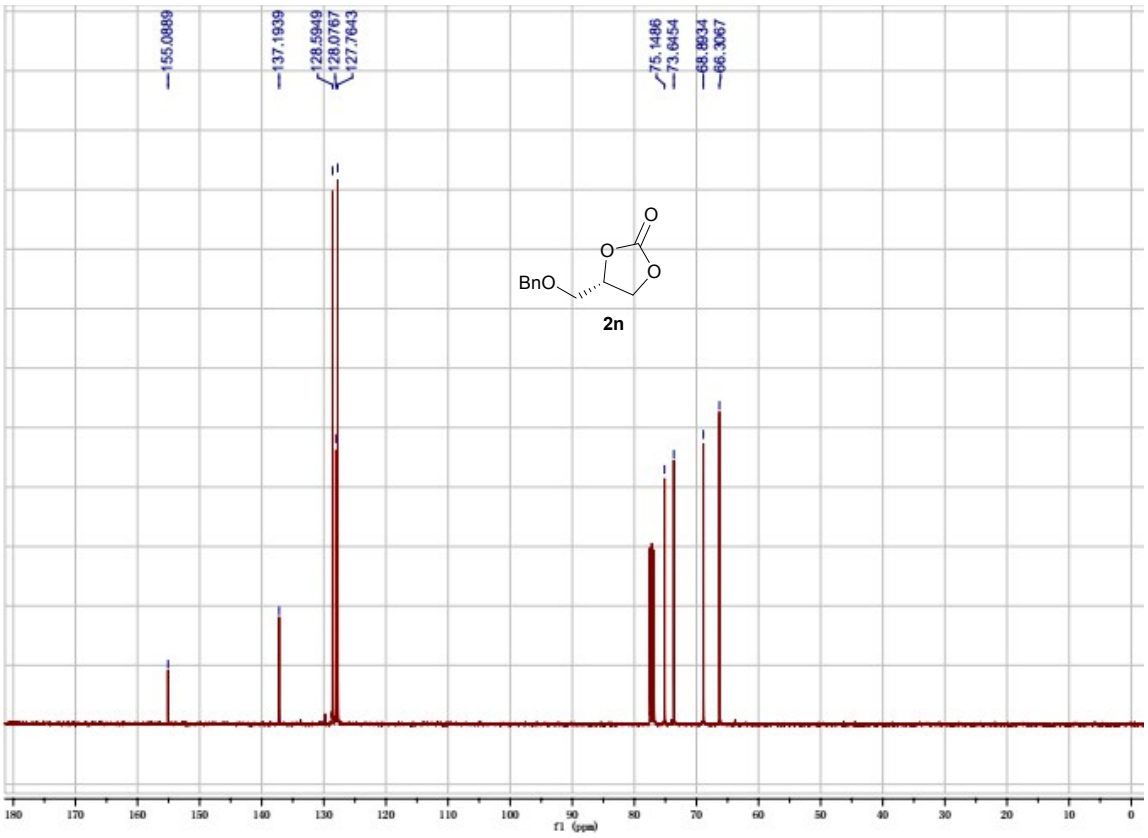
1.03
1.00
0.91
1.02
BnO
O
O
O
2n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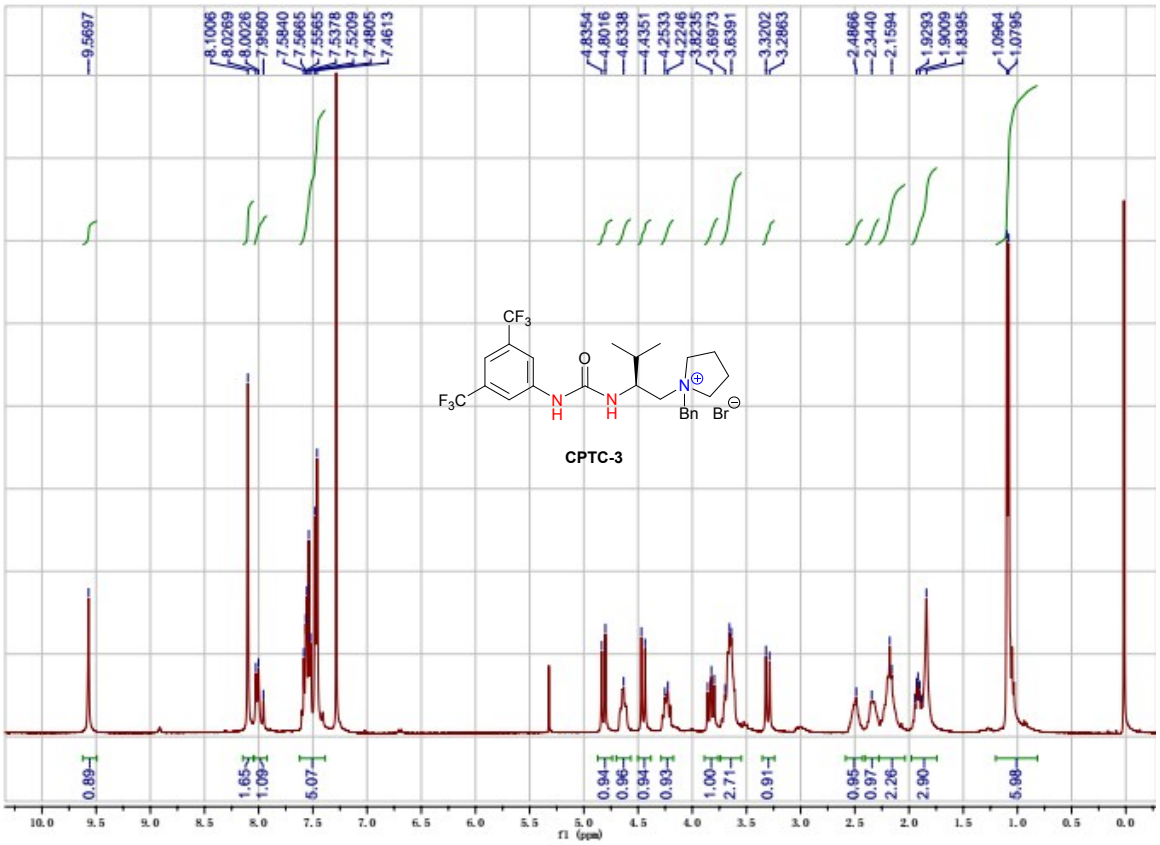
73.6454
68.8934
66.3067
BnO
O
O
O
2n
f1 (ppm)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8.0026
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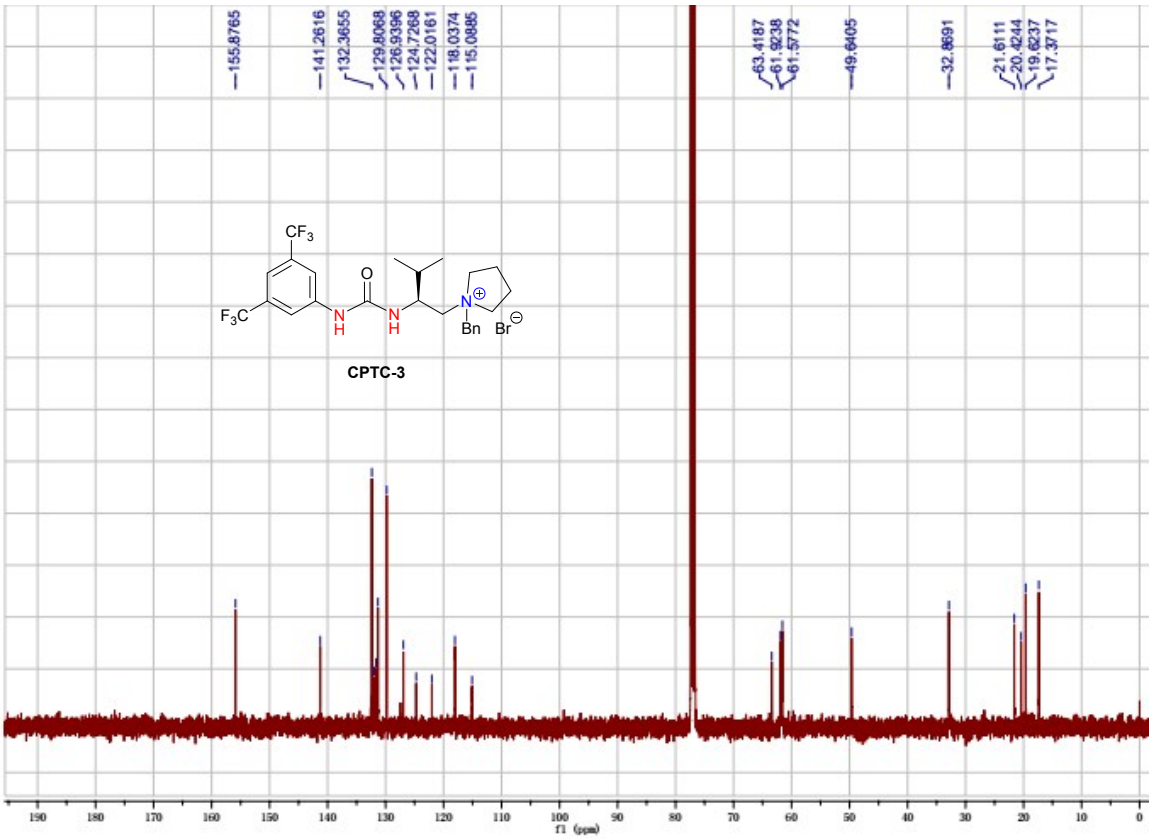
7.4805
7.4613
4.8354
4.8016
4.6338
4.4351
4.2533
4.2246
3.8235
3.6973
3.6391
3.3202
3.2863
2.4866
2.3440
2.1594
1.9293
1.9009
1.8395
1.0964
1.0795
CF3
F3C
N
H
O
N
H
N
Bn
Br
CPTC-3
0.89
1.65
1.09
5.07
0.94
0.96
0.94
0.93
1.00
2.71
0.91
0.95
0.97
2.26
2.90
5.98
f1 (ppm)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122.0161
118.0374
115.0885
63.4187
61.9238
61.5772
49.6405
32.8691
21.6111
20.4244
19.6237
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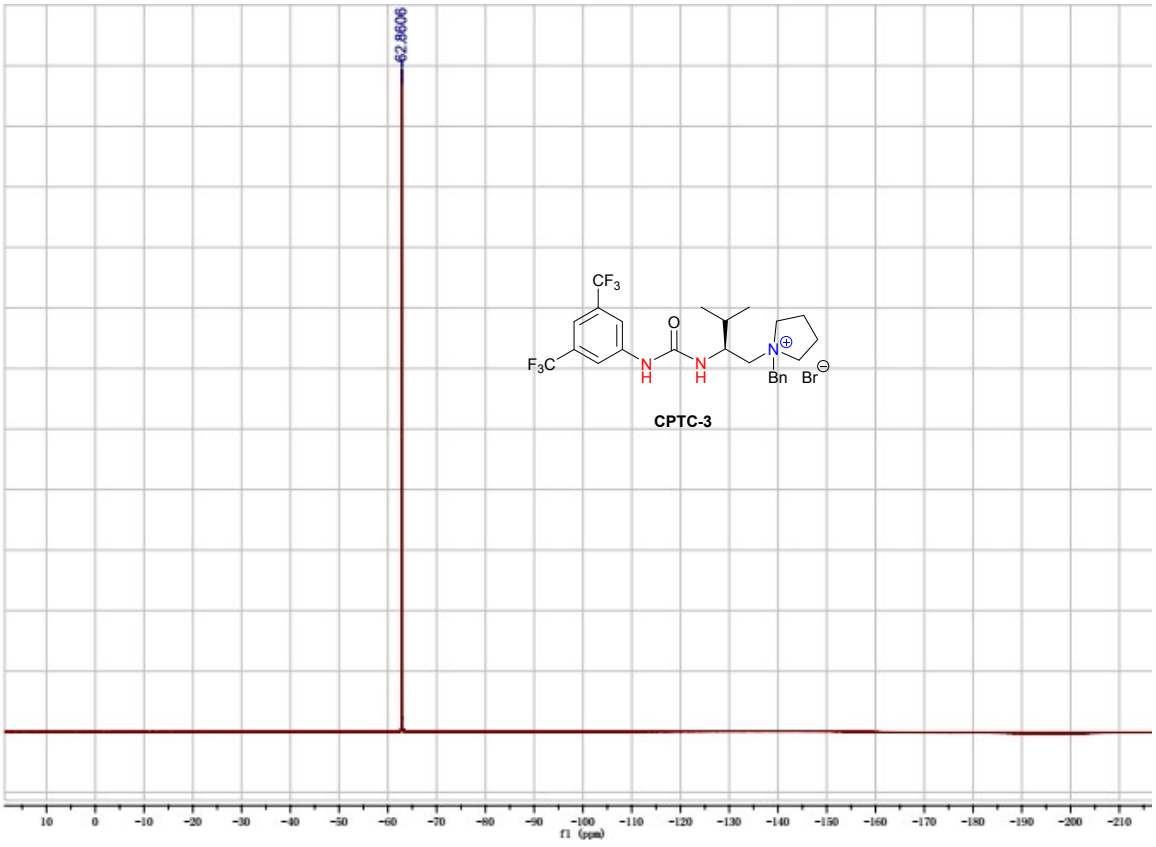
CF3
F3C
O
N
H
N
H
N
Bn
Br
CPTC-3
f1 (ppm)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H
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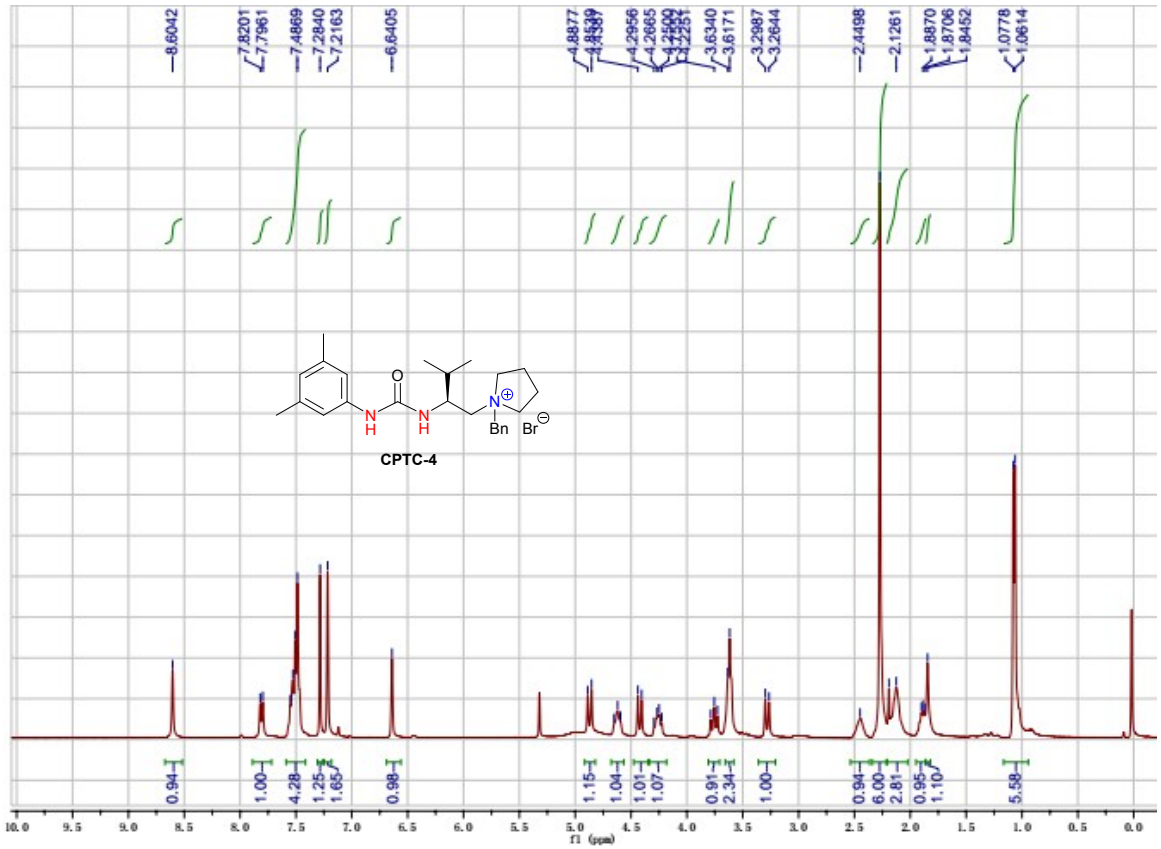
H
N
Bn
Br
CPTC-3
f1 (ppm)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7.2163
6.6405
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4.8387
4.2956
4.2665
4.2509
4.2251
3.6340
3.6171
3.2987
3.2644
2.4498
2.1261
1.8870
1.8706
1.8452
1.0778
1.0614
0.94
1.00
4.28
1.25
1.65
0.98
1.15
1.04
1.01
1.07
0.91
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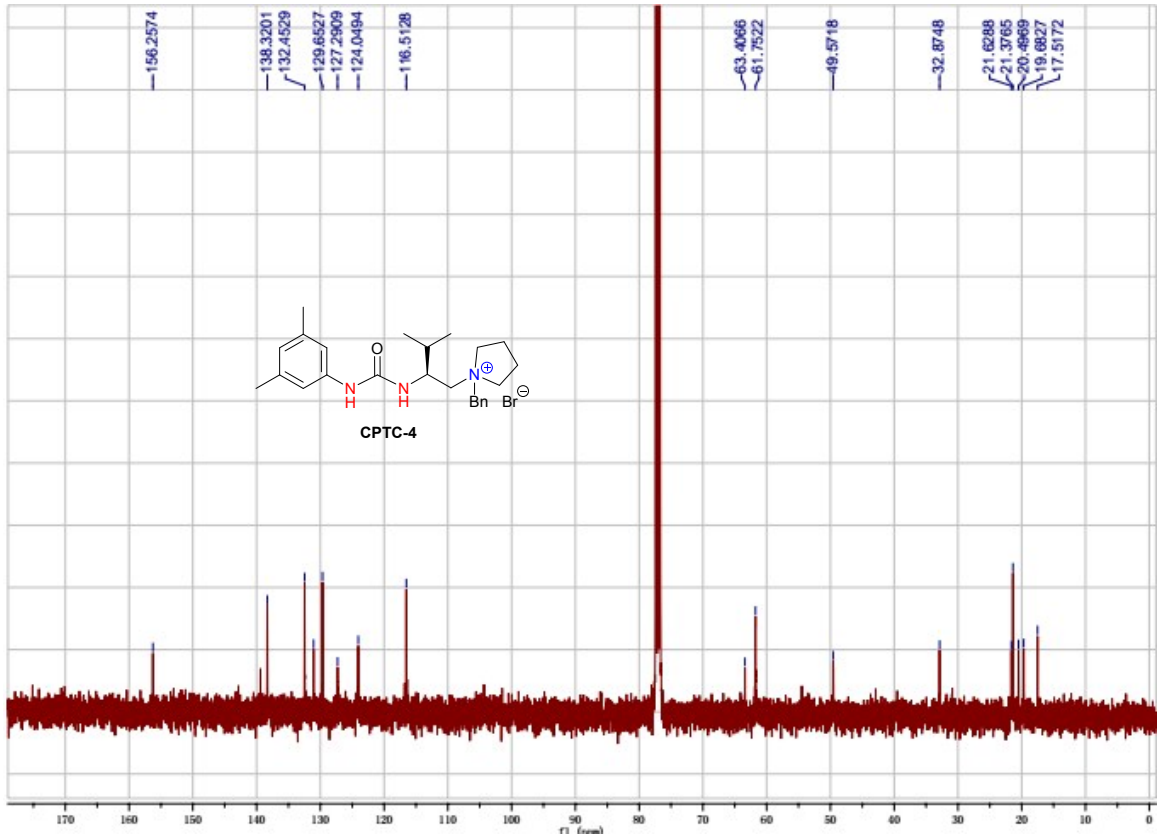
1.00
0.94
6.00
2.81
0.95
1.10
5.58
f1 (ppm)

CPTC-4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127.2909
124.0494
116.5128
63.4066
61.7522
49.5718
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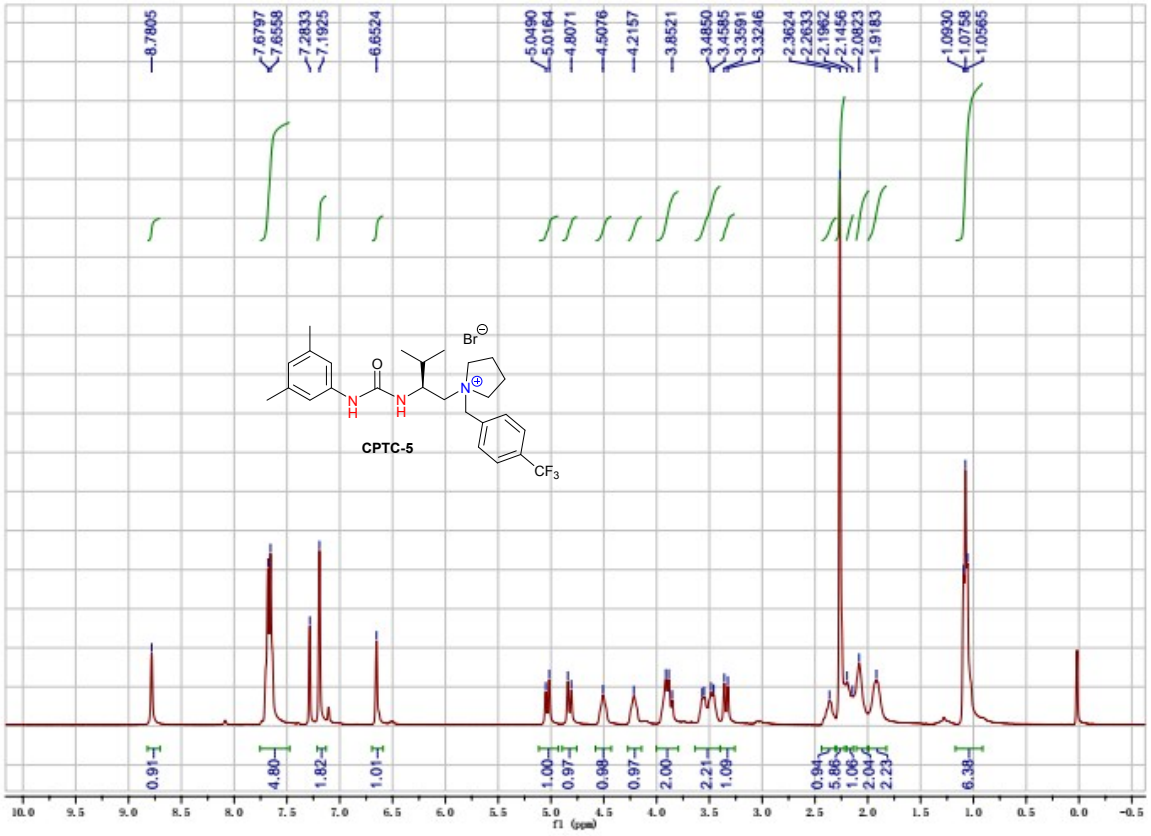
21.6288
21.3765
20.4969
19.6827
17.5172

CPTC-4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7.6558
7.2833
7.1925
6.6524
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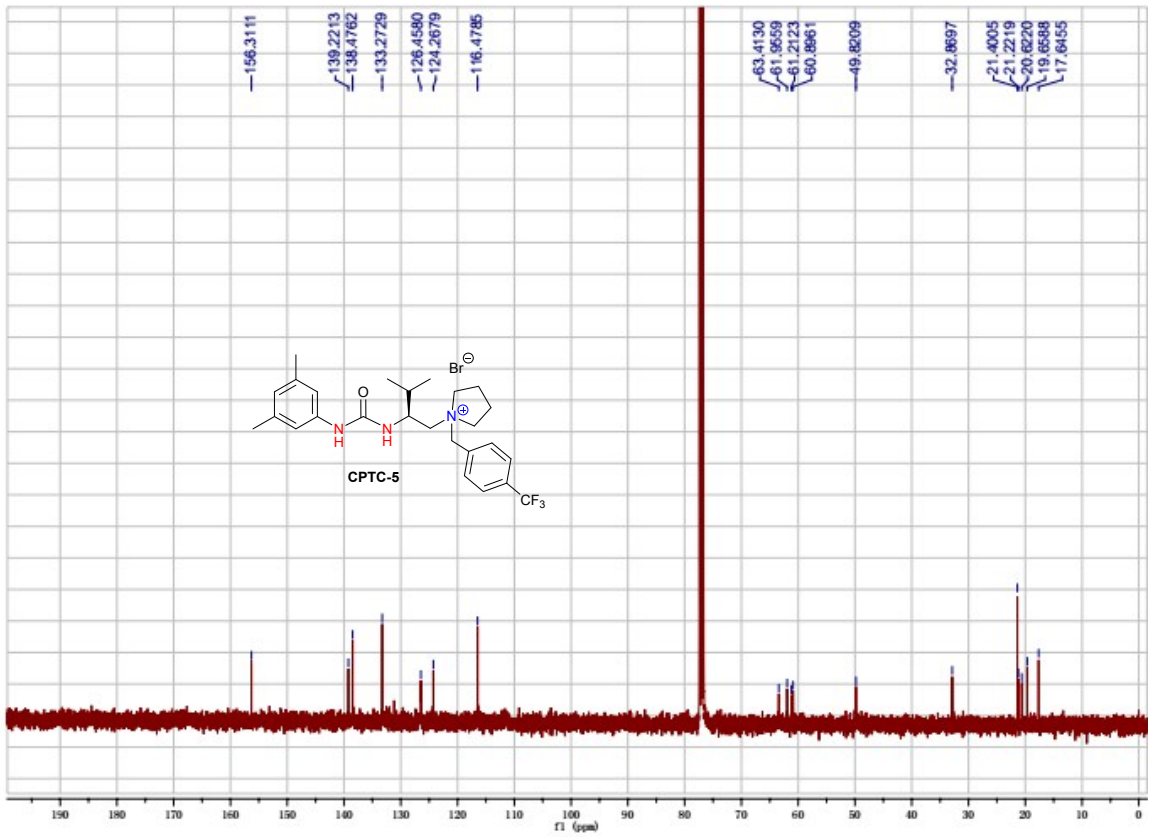
4.8071
4.5076
4.2157
3.8521
3.4850
3.4585
3.3591
3.3246
2.3624
2.2633
2.1962
2.1456
2.0823
1.9183
1.0930
1.0758
1.0565
Br
CPTC-5
CF3
0.91
4.80
1.82
1.01
1.00
0.97
0.98
0.97
2.00
2.21
1.09
0.94
5.86
1.06
2.04
2.23
6.38
f1 (ppm)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116.4785
63.4130
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60.8961
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32.8697
21.4005
21.2219
20.8220
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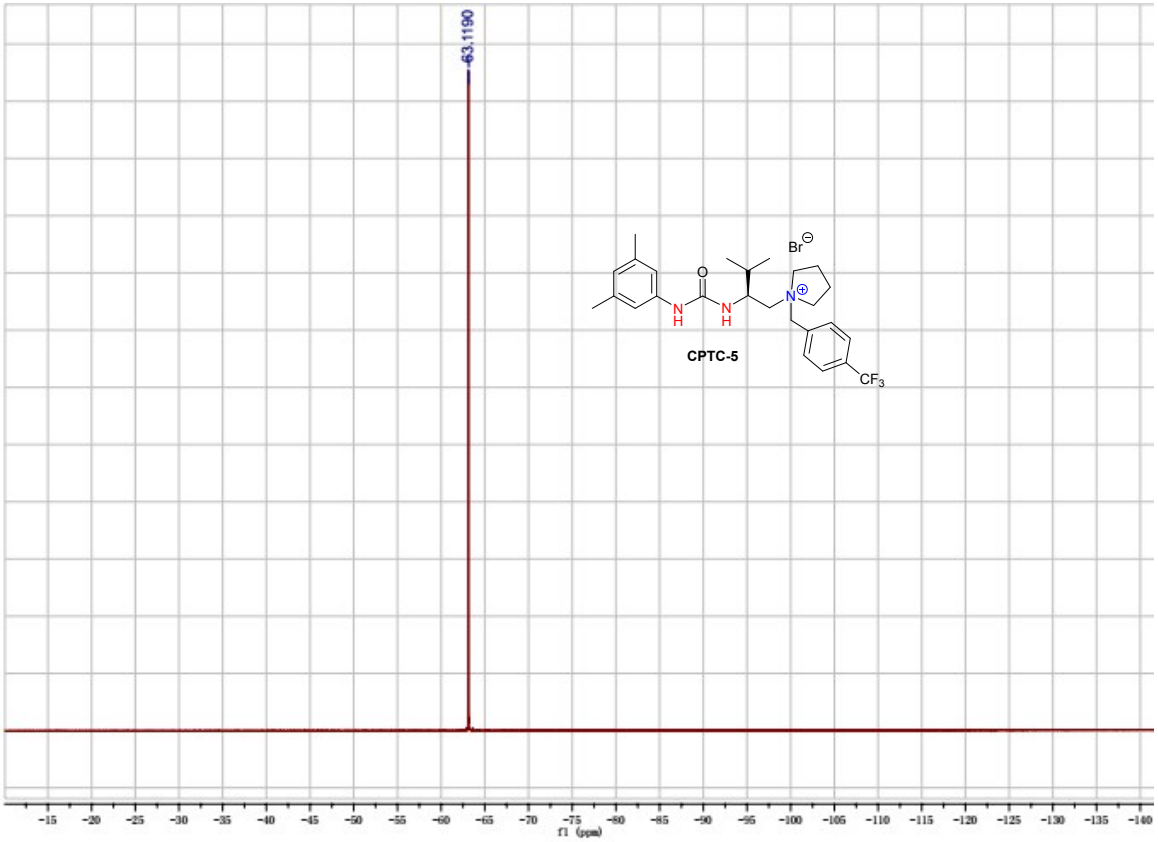
17.6455
Br
CPTC-5
CF3
f1 (ppm)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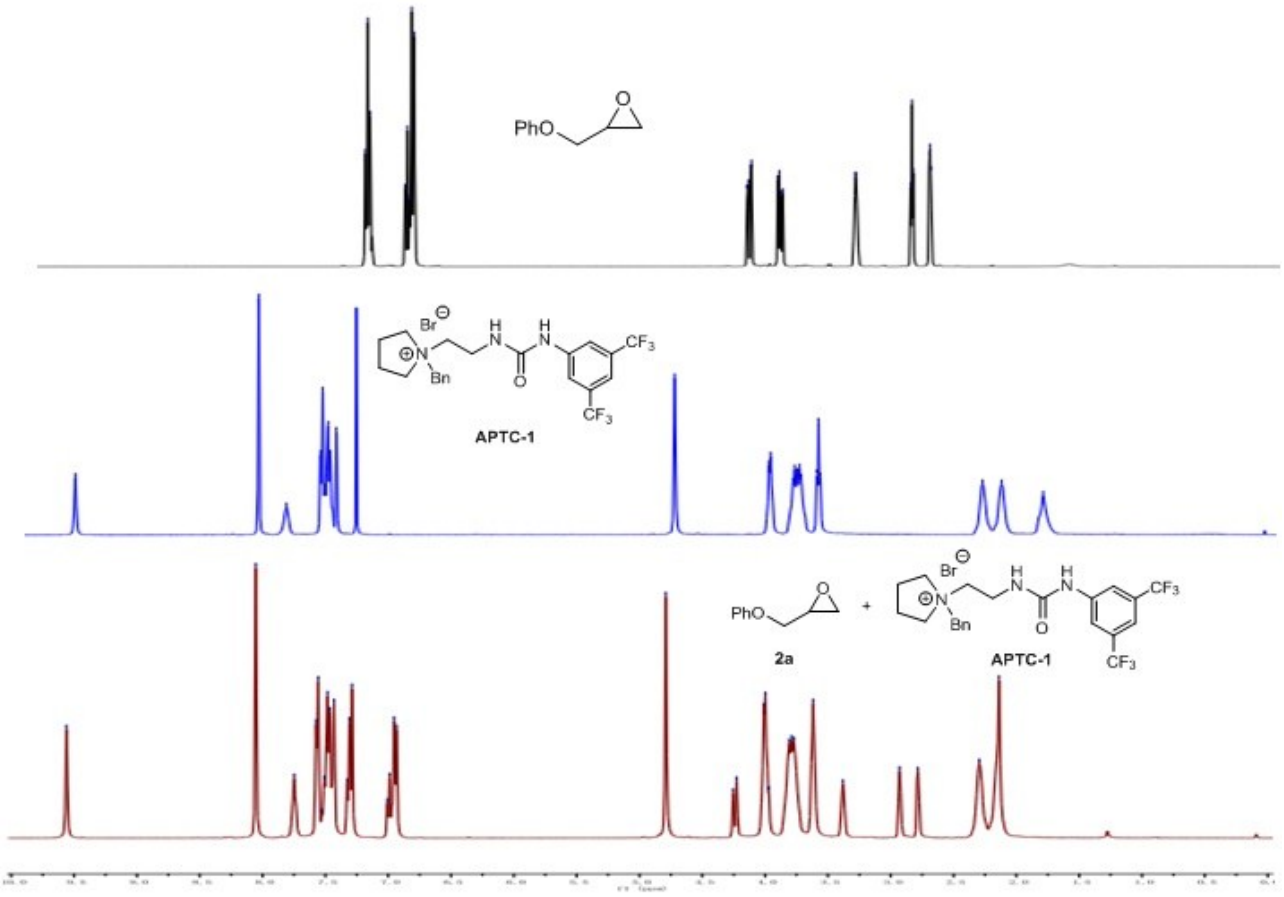
CPTC-5


PhO
APTC-1
2a
APTC-1

HRMS copies of all new compounds

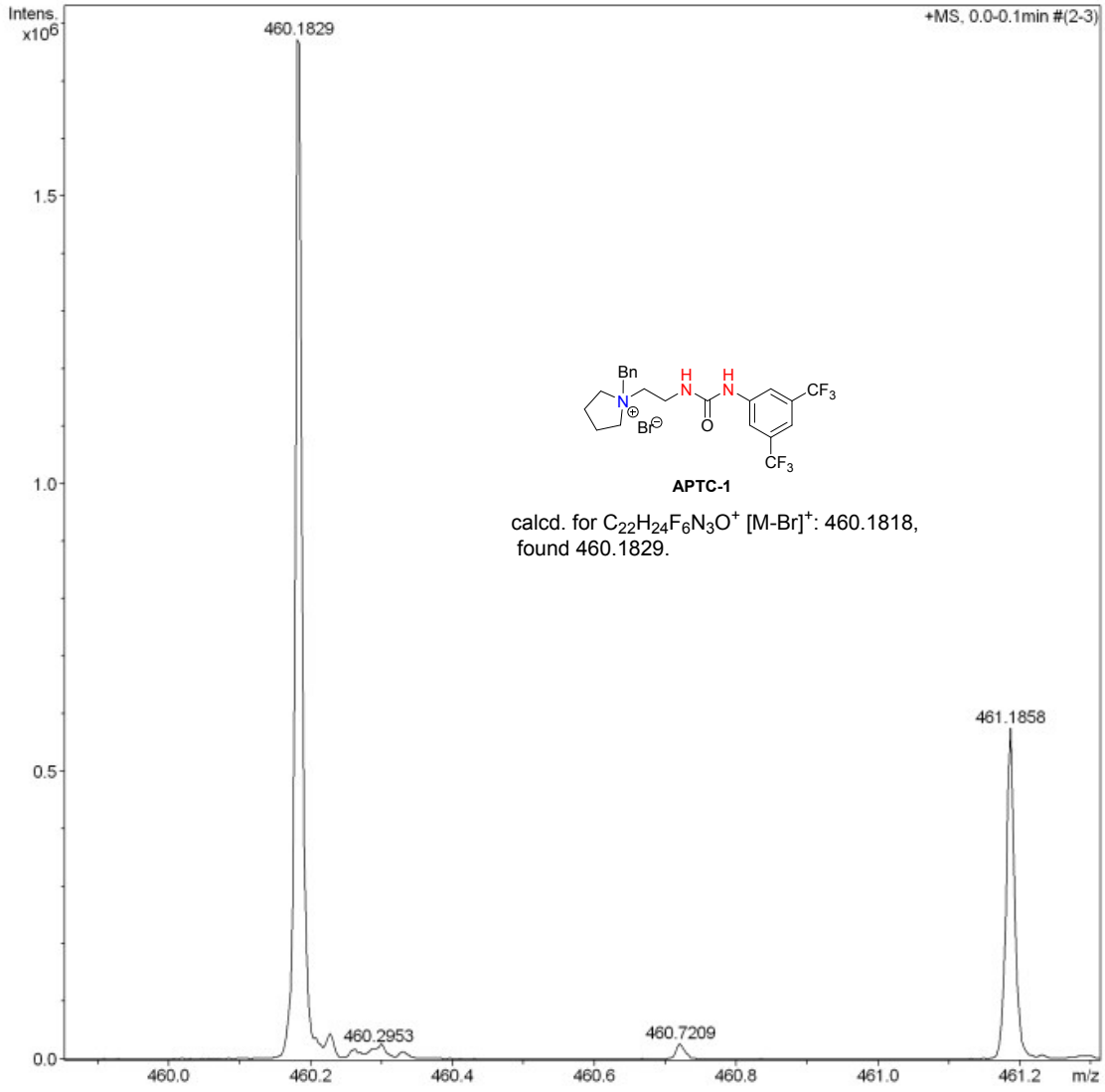
Display Report

Analysis Info

Analysis Name	D:\Data\FAN\data\2017\0911\lay-36.d	Acquisition Date	9/11/2017 12:15:17 PM
Method	pos_low-20151116.m	Operator	Fan
Sample Name	liuaiyun	Instrument	maXis 10103
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



APTC-1

calcd. for $C_{22}H_{24}F_6N_3O^+$ $[M\text{-}Br]^+$: 460.1818, found 460.1829.

Bruker Compass DataAnalysis 4.0 printed: 9/11/2017 12:16:29 PM Page 1 of 1

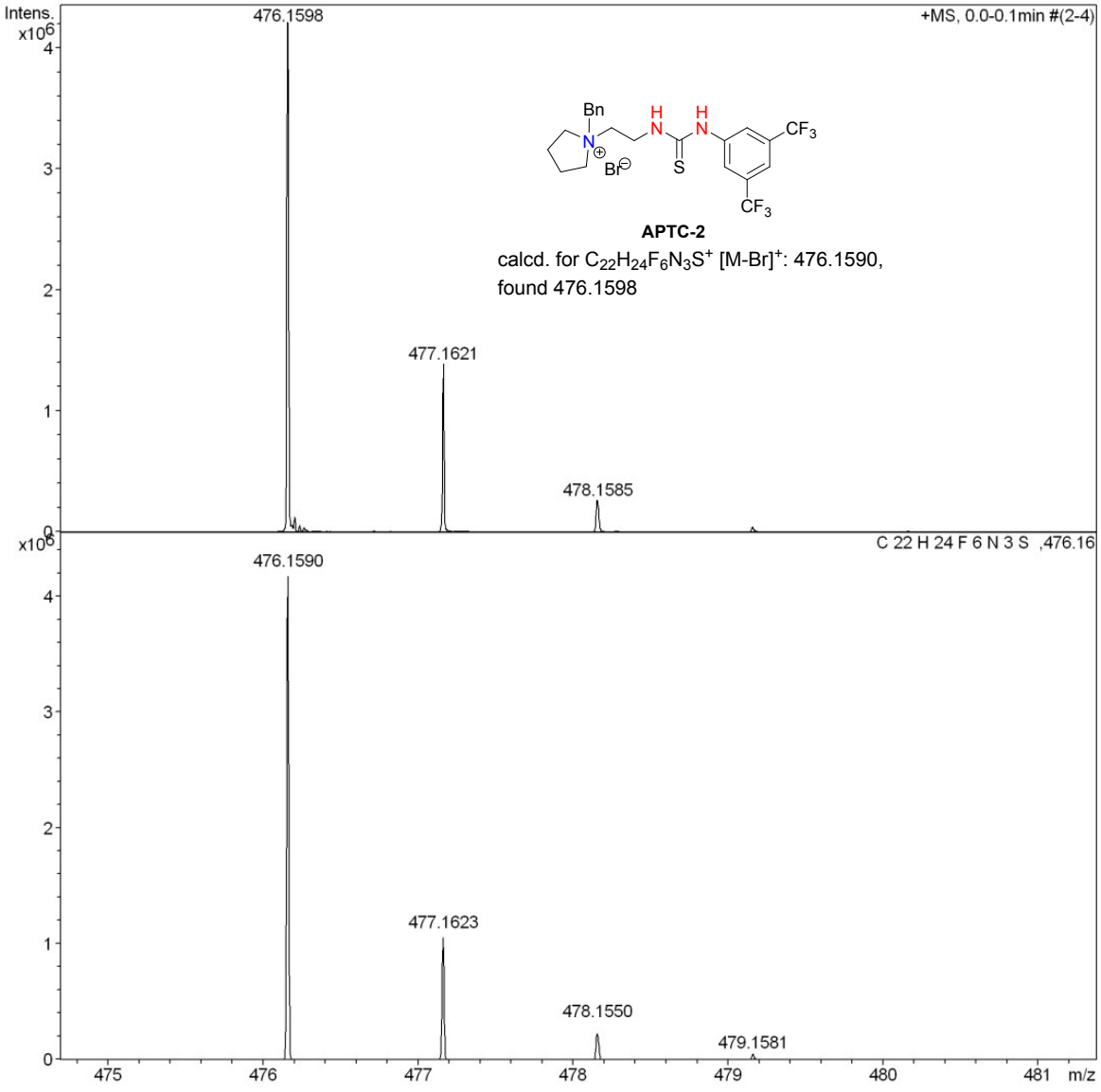
Display Report

nalysis Info

nalysis Name	D:\Data\2018\0622\c-1.d	Acquisition Date	6/22/2018 9:41:12 AM
ethod	pos_low-20151116.m	Operator	Fan
ample Name	liuaiyun	Instrument	maXis 10103
omment			

cquisition Parameter

ource Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
ocus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
can Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
can End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



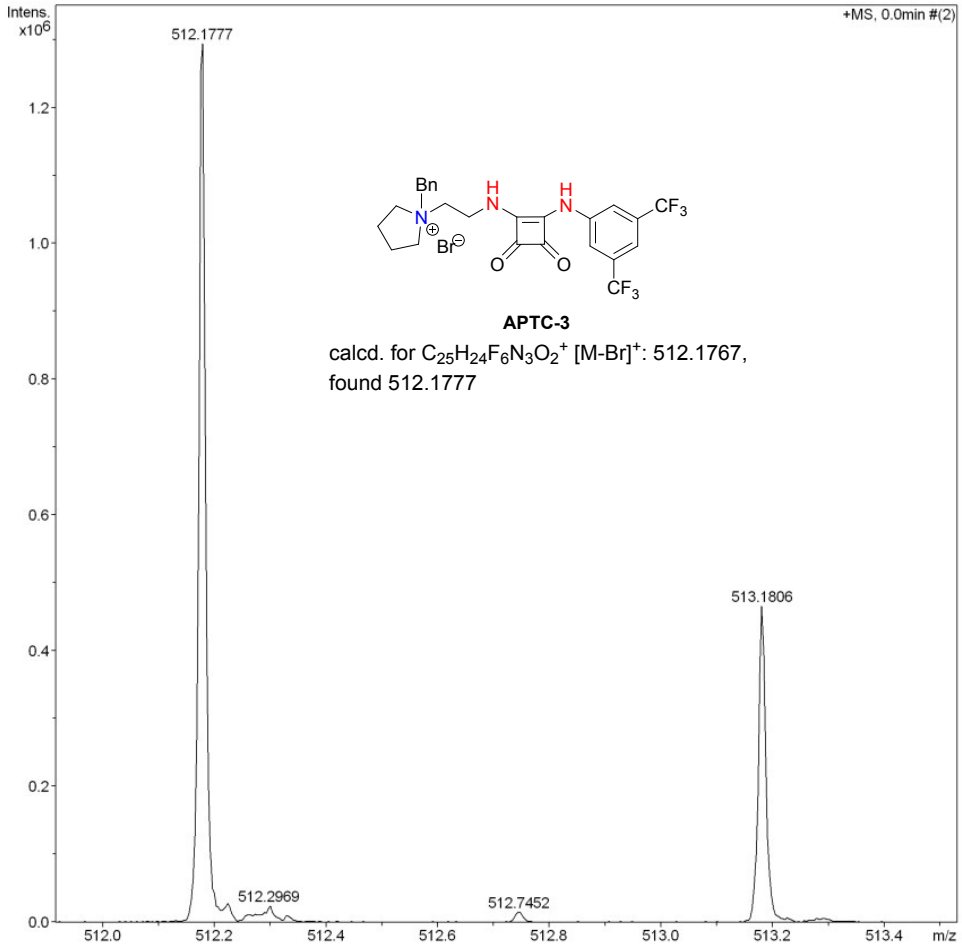
Display Report

Analysis Info

Analysis Name	D:\Data\FAN\data\2017\0911\lay-38.d	Acquisition Date	9/11/2017 12:18:44 PM
Method	pos_low-20151116.m	Operator	Fan
Sample Name	liuaiyun	Instrument	maXis 10103
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



APTC-3

calcd. for $C_{25}H_{24}F_6N_3O_2^+$ [M-Br]$^+$: 512.1767,
found 512.1777

Bruker Compass DataAnalysis 4.0 printed: 9/11/2017 12:19:54 PM Page 1 of 1

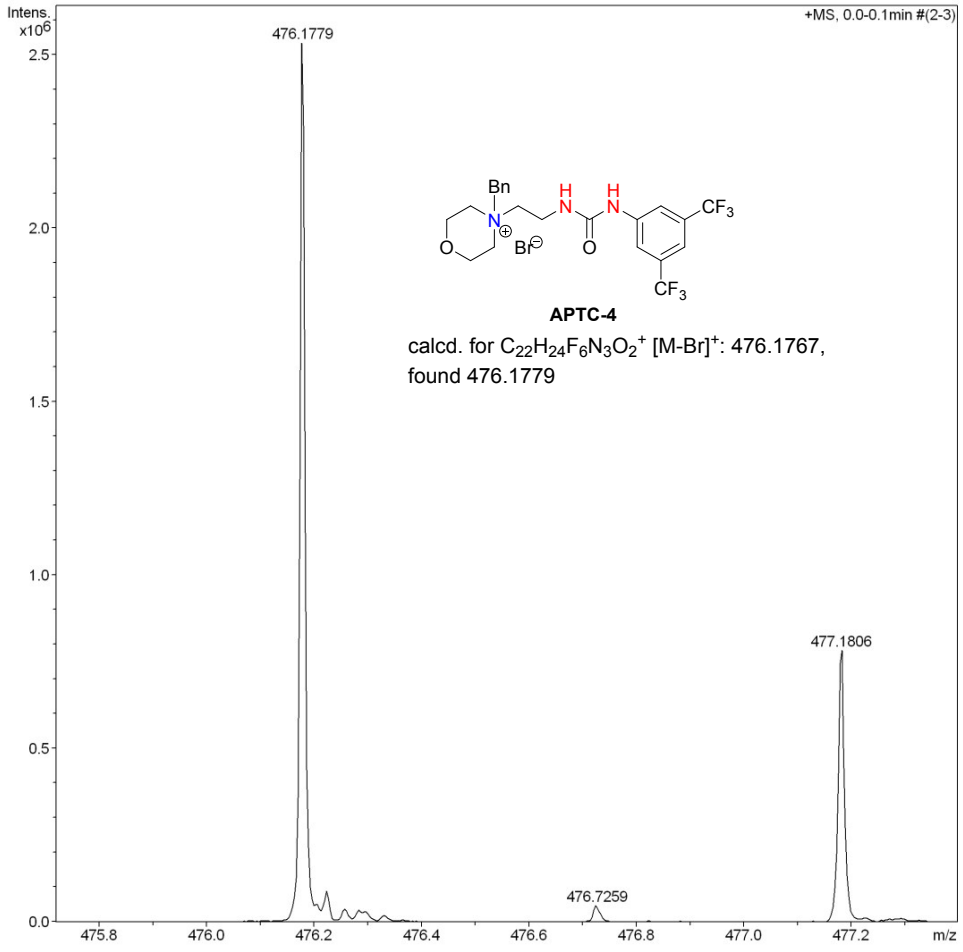
Display Report

Analysis Info

Analysis Name	D:\Data\FAN\data\2017\0911\lay-40.d	Acquisition Date	9/11/2017 12:25:44 PM
Method	pos_low-20151116.m	Operator	Fan
Sample Name	liuaiyun	Instrument	maXis 10103
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



APTC-4

calcd. for $C_{22}H_{24}F_6N_3O_2^+$ $[M\text{-}Br]^+$: 476.1767,
found 476.1779

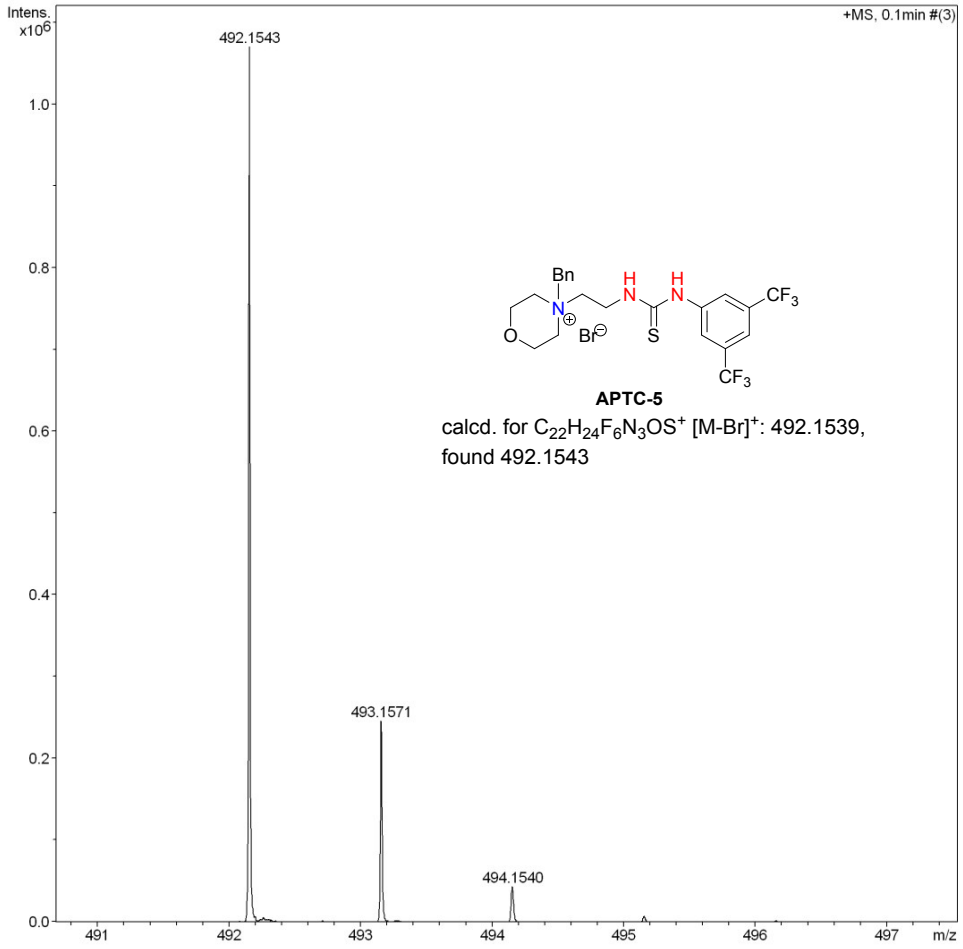
Display Report

Analysis Info

Analysis Name	D:\Data\2018\0622\c-2.d	Acquisition Date	6/22/2018 9:44:05 AM
Method	pos_low-20151116.m	Operator	Fan
Sample Name	liuaiyun	Instrument	maXis 10103
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



APTC-5

calcd. for $C_{22}H_{24}F_6N_3OS^+$ $[M\text{-}Br]^+$: 492.1539, found 492.1543

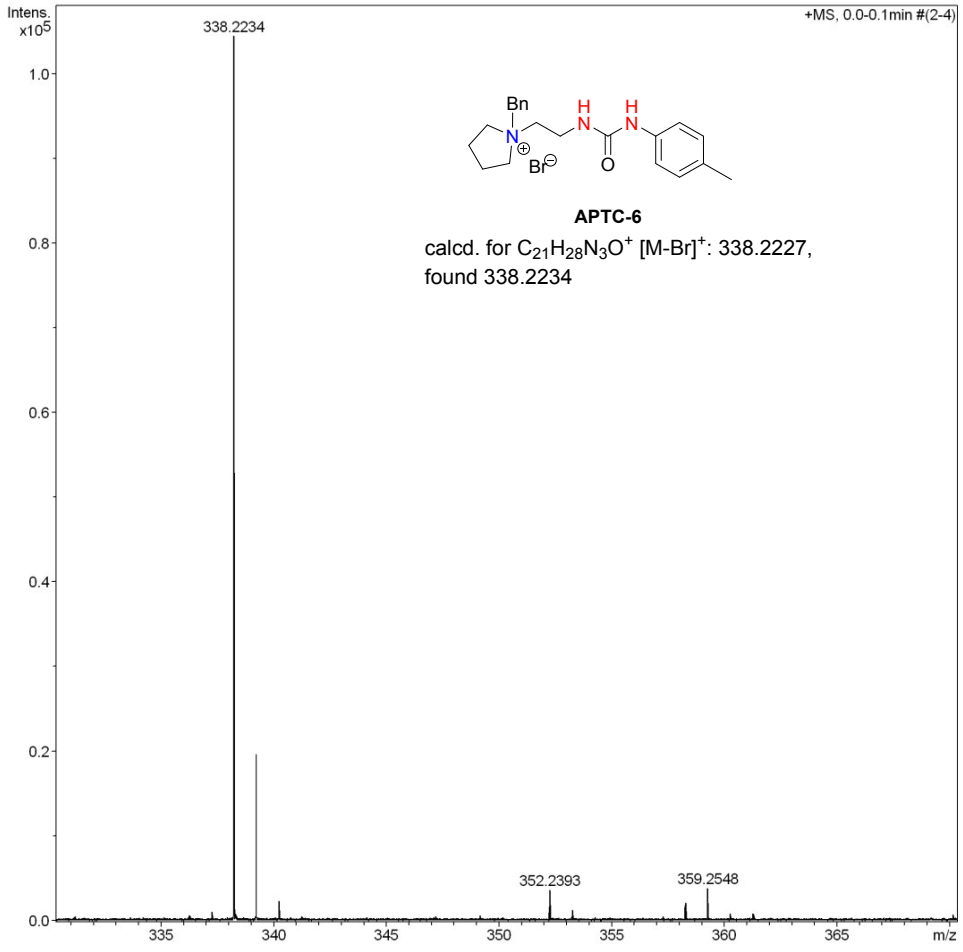
Display Report

Analysis Info

Analysis Name	D:\Data\2018\0622\c-6.d	Acquisition Date	6/22/2018 9:59:39 AM
Method	pos_low-20151116.m	Operator	Fan
Sample Name	liuaiyun	Instrument	maXis 10103
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



APTC-6

calcd. for $C_{21}H_{28}N_3O^+$ $[M\text{-}Br]^+$: 338.2227,
found 338.2234

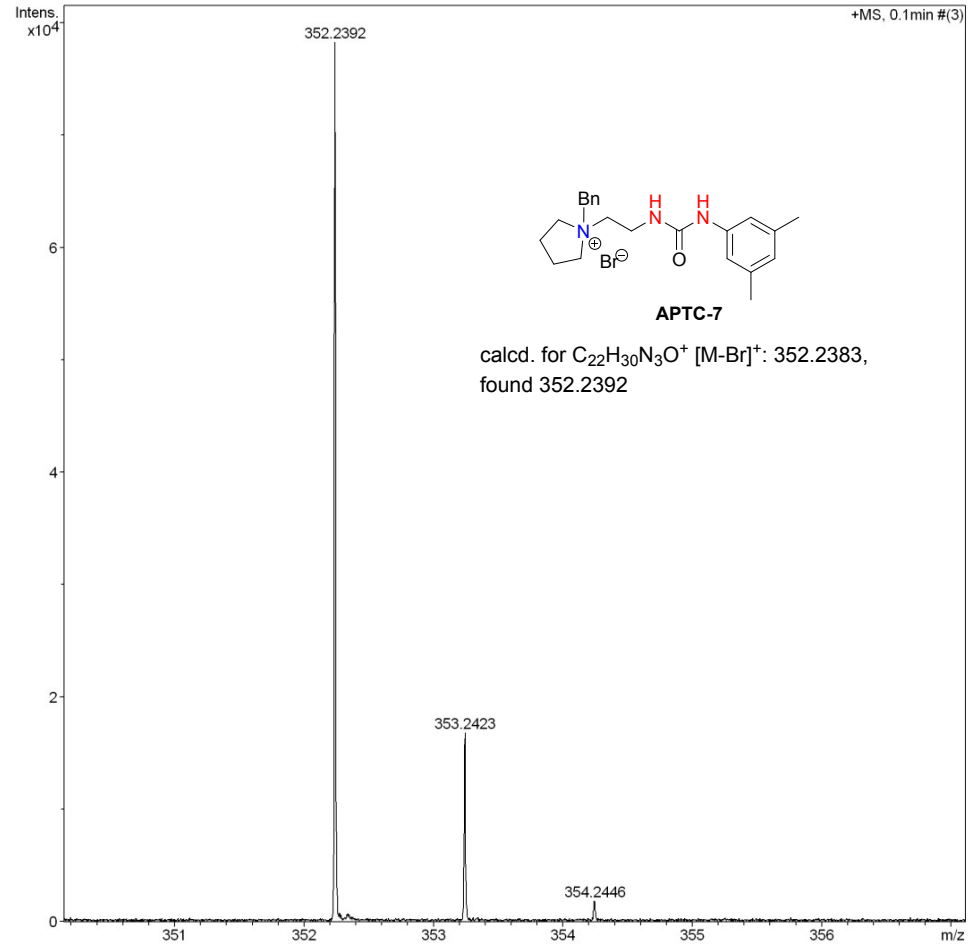
Display Report

Analysis Info

Analysis Name	D:\Data\2018\0622\c-4.d	Acquisition Date	6/22/2018 9:50:20 AM
Method	pos_low-20151116.m	Operator	Fan
Sample Name	liuaiyun	Instrument	maXis 10103
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



APTC-7

calcd. for $C_{22}H_{30}N_3O^+$ [M-Br]$^+$: 352.2383, found 352.2392

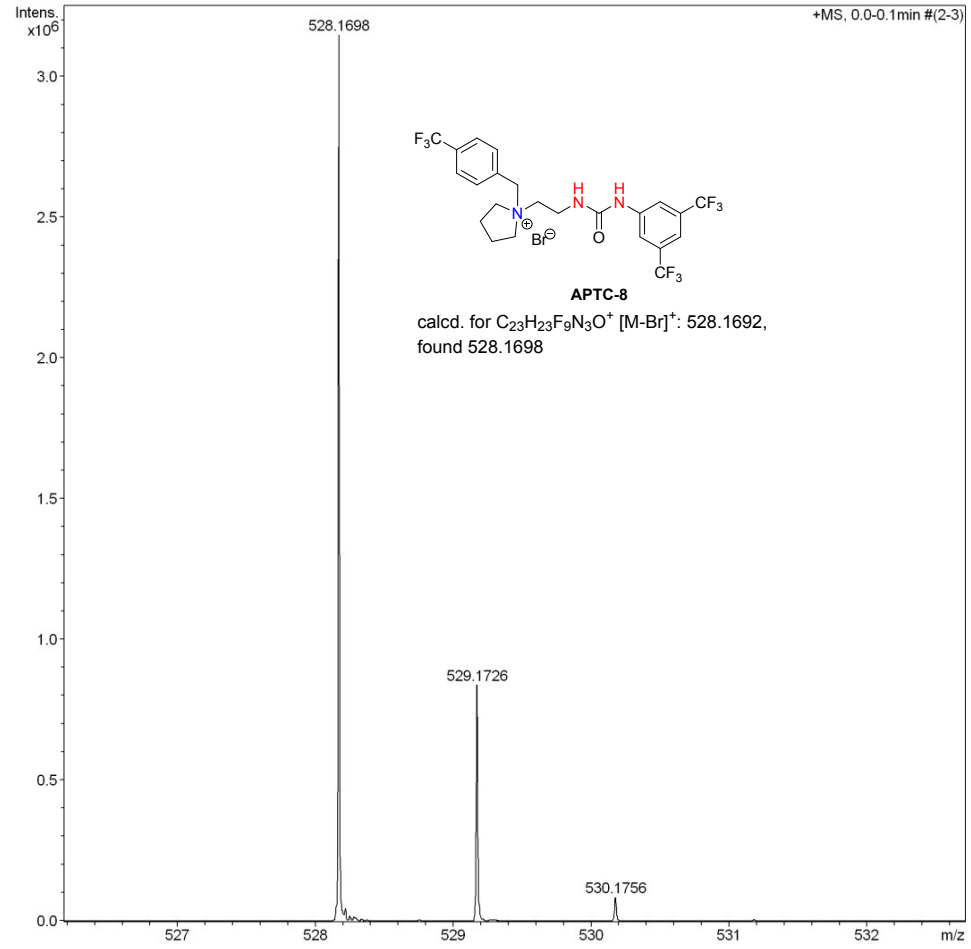
Display Report

Analysis Info

Analysis Name	D:\Data\2018\0622\c-3.d	Acquisition Date	6/22/2018 9:46:29 AM
Method	pos_low-20151116.m	Operator	Fan
Sample Name	liuaiyun	Instrument	maXis 10103
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



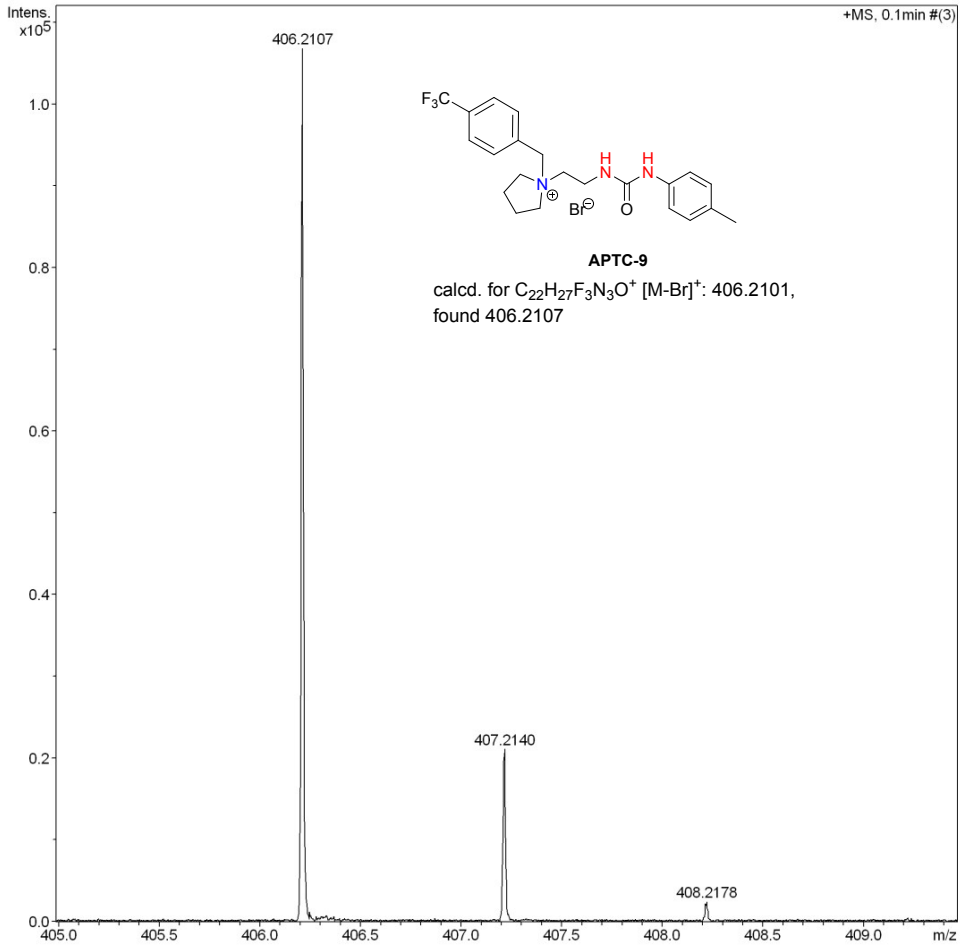
Display Report

Analysis Info

Analysis Name	D:\Data\2018\0622\c-7.d	Acquisition Date	6/22/2018 10:02:09 AM
Method	pos_low-20151116.m	Operator	Fan
Sample Name	liuaiyun	Instrument	maXis 10103
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



APTC-9

calcd. for $C_{22}H_{27}F_3N_3O^+$ $[M-Br]^+$: 406.2101, found 406.2107

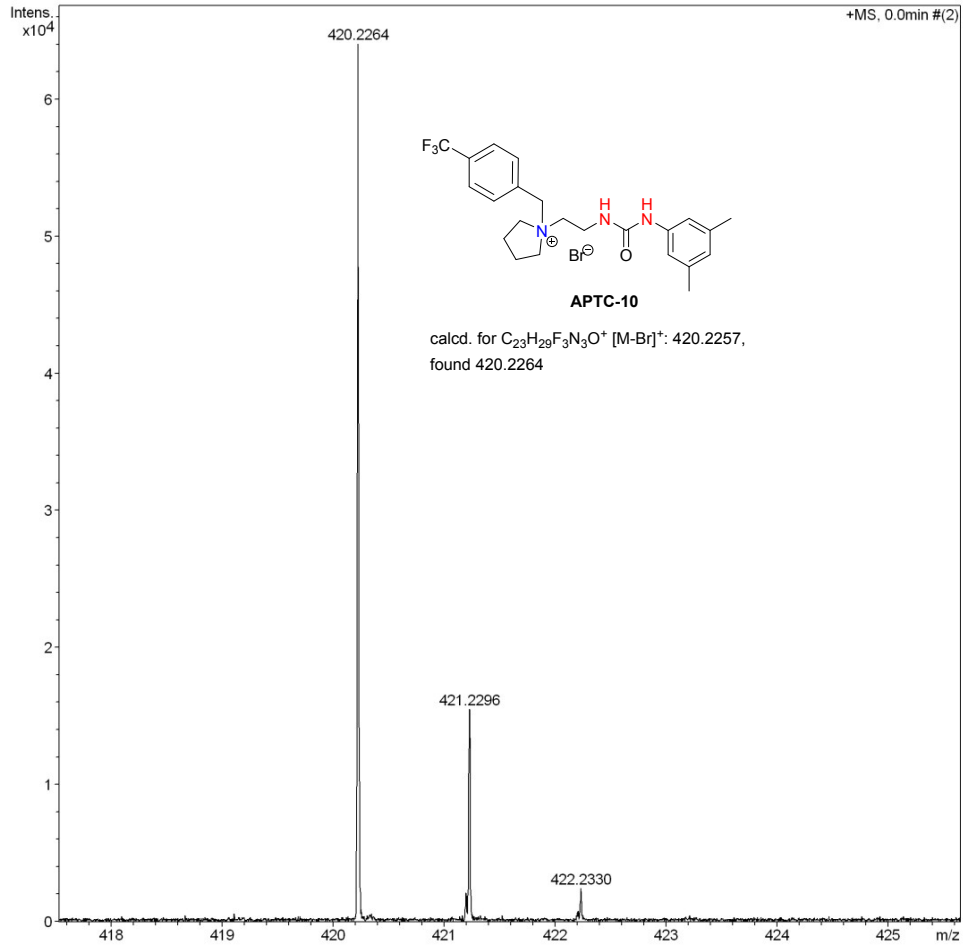
Display Report

Analysis Info

Analysis Name	D:\Data\2018\0622\c-5.d	Acquisition Date	6/22/2018 9:57:01 AM
Method	pos_low-20151116.m	Operator	Fan
Sample Name	liuaiyun	Instrument	maXis 10103
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



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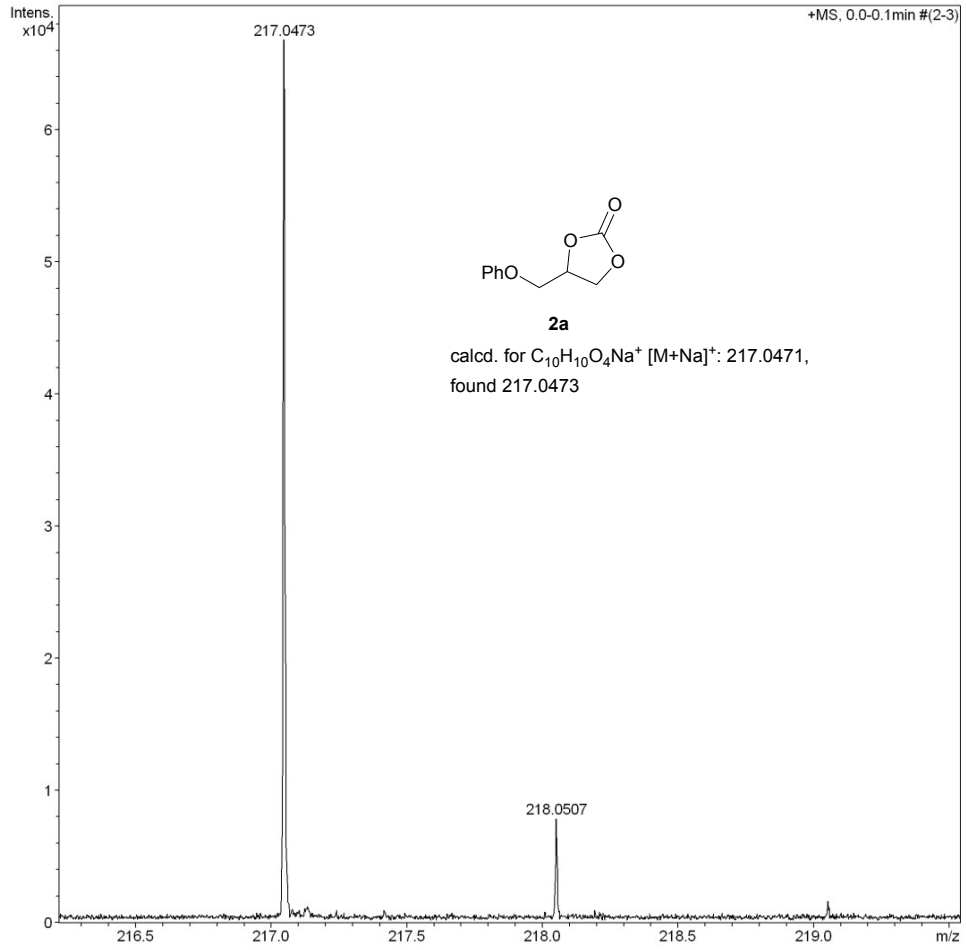
Display Report

Analysis Info

Analysis Name	D:\Data\2018\0112\lay-13.d	Acquisition Date	1/12/2018 10:32:19 AM
Method	pos_low-20151116.m	Operator	Fan
Sample Name	liuaiyun	Instrument	maXis 10103
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



2a

calcd. for $C_{10}H_{10}O_4Na^+$ $[M+Na]^+$: 217.0471,
found 217.0473

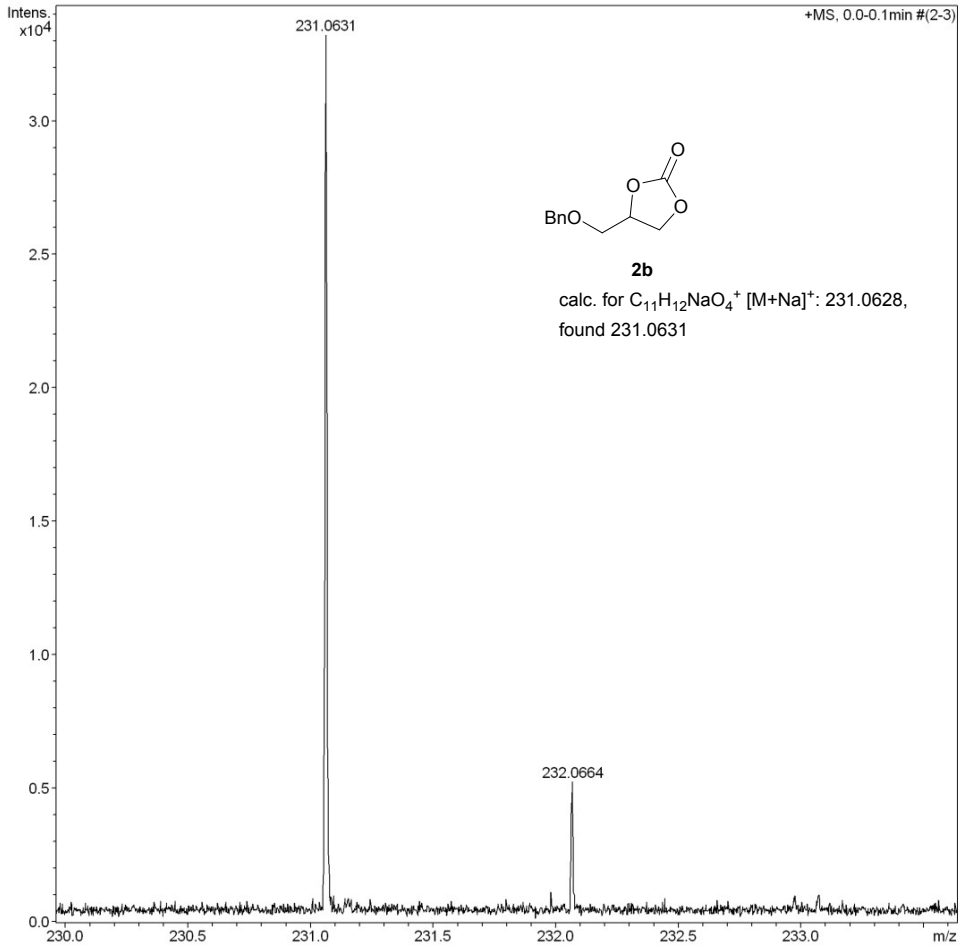
Display Report

Analysis Info

Analysis Name	D:\Data\2018\0112\lay-14.d	Acquisition Date	1/12/2018 10:39:49 AM
Method	pos_low-20151116.m	Operator	Fan
Sample Name	liuaiyun	Instrument	maXis 10103
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



2b

calc. for $C_{11}H_{12}NaO_4^+$ $[M+Na]^+$: 231.0628,
found 231.0631

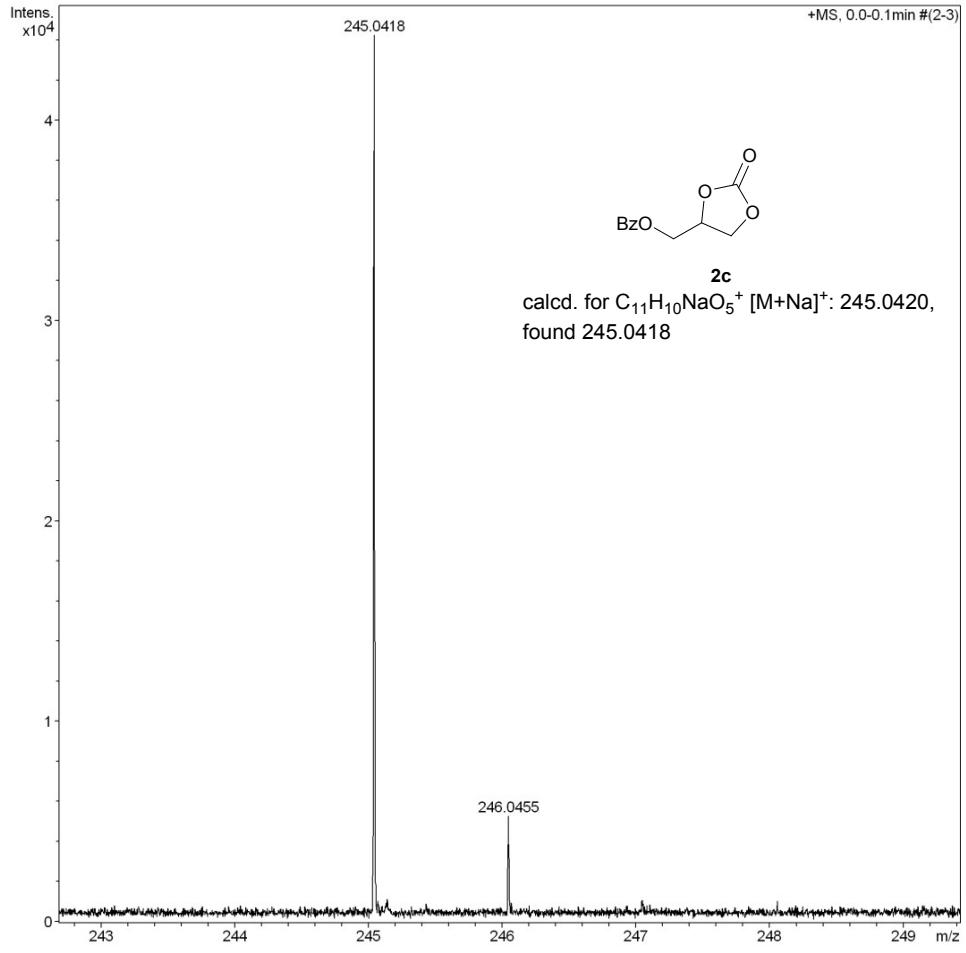
Display Report

Analysis Info

Analysis Name	D:\Data\2018\0112\lay-19.d	Acquisition Date	1/12/2018 10:55:53 AM
Method	pos_low-20151116.m	Operator	Fan
Sample Name	liuaiyun	Instrument	maXis 10103
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



2c

calcd. for $C_{11}H_{10}NaO_5^+$ $[M+Na]^+$: 245.0420, found 245.0418

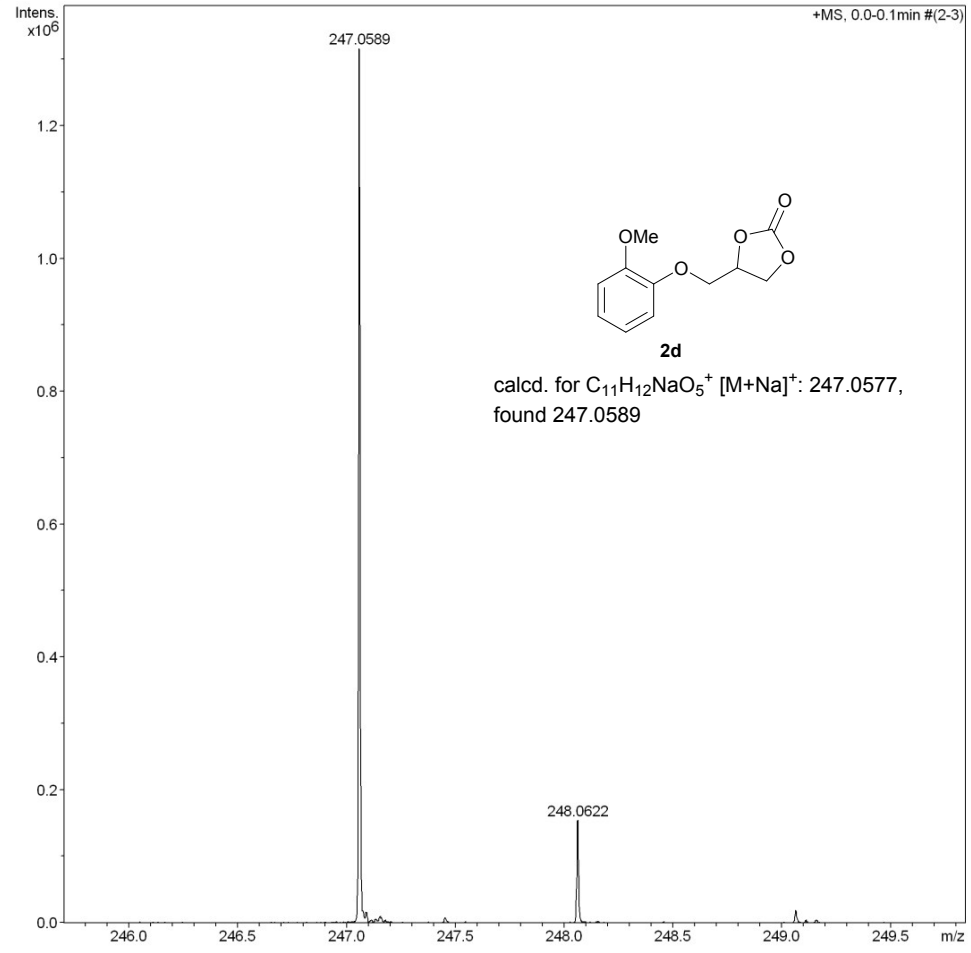
Display Report

Analysis Info

Analysis Name	D:\Data\2018\0112\lay-11.d	Acquisition Date	1/12/2018 10:09:37 AM
Method	pos_low-20151116.m	Operator	Fan
Sample Name	liuaiyun	Instrument	maXis 10103
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



2d

calcd. for $C_{11}H_{12}NaO_5^+$ [M+Na]$^+$: 247.0577, found 247.0589

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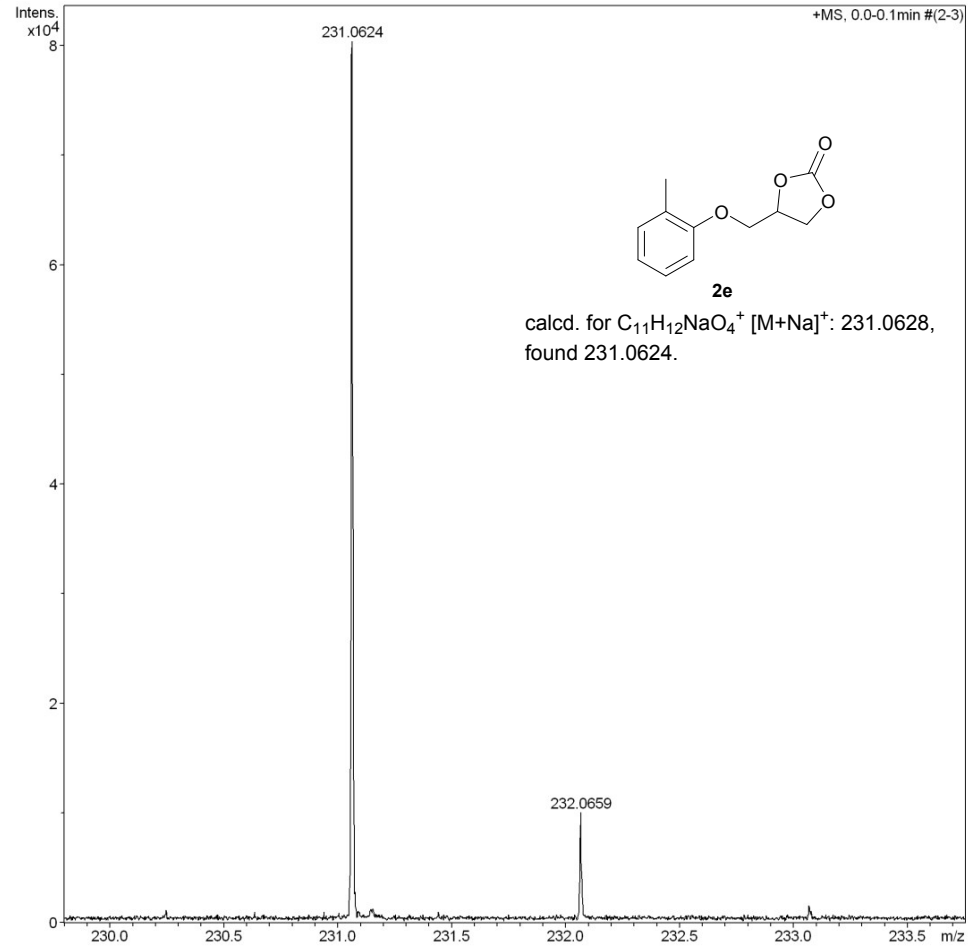
Display Report

Analysis Info

Analysis Name	D:\Data\2018\0112\lay-18.d	Acquisition Date	1/12/2018 10:52:43 AM
Method	pos_low-20151116.m	Operator	Fan
Sample Name	liuaiyun	Instrument	maXis 10103
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



2e

calcd. for $C_{11}H_{12}NaO_4^+$ $[M+Na]^+$: 231.0628, found 231.0624.

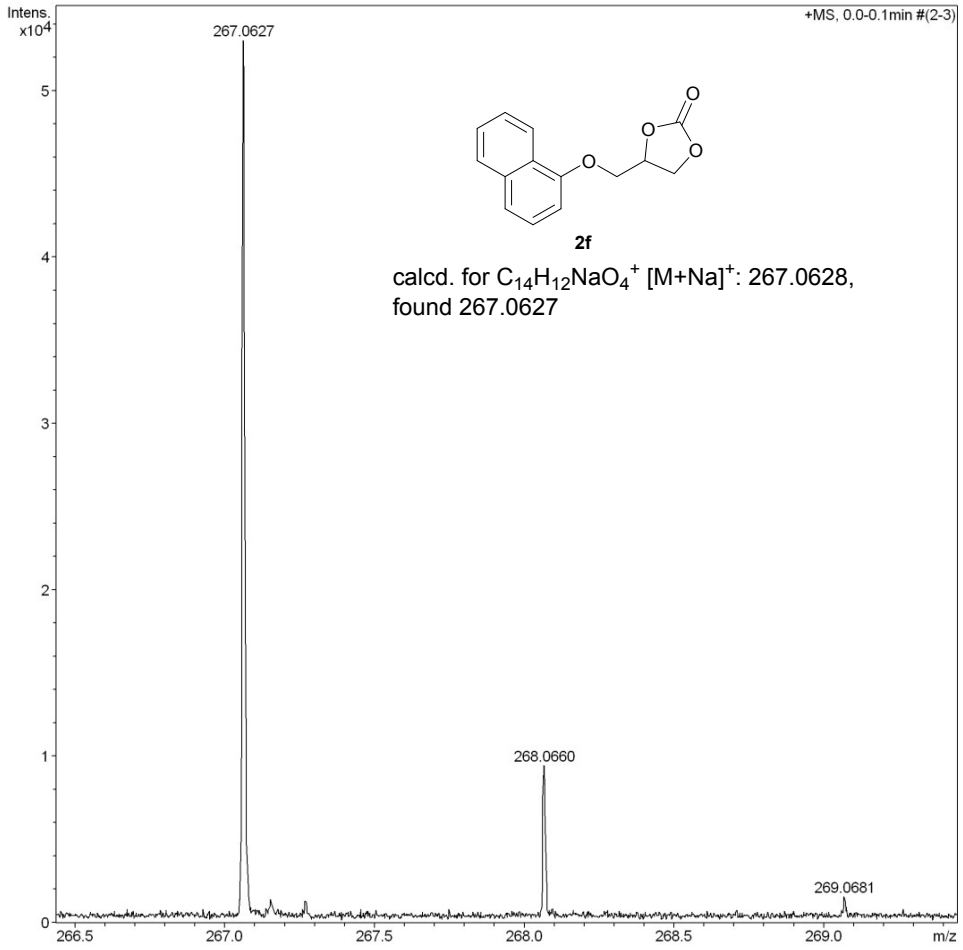
Display Report

Analysis Info

Analysis Name	D:\Data\2018\0112\lay-12.d	Acquisition Date	1/12/2018 10:24:29 AM
Method	pos_low-20151116.m	Operator	Fan
Sample Name	liuaiyun	Instrument	maXis 10103
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



2f

calcd. for $C_{14}H_{12}NaO_4^+$ $[M+Na]^+$: 267.0628, found 267.0627

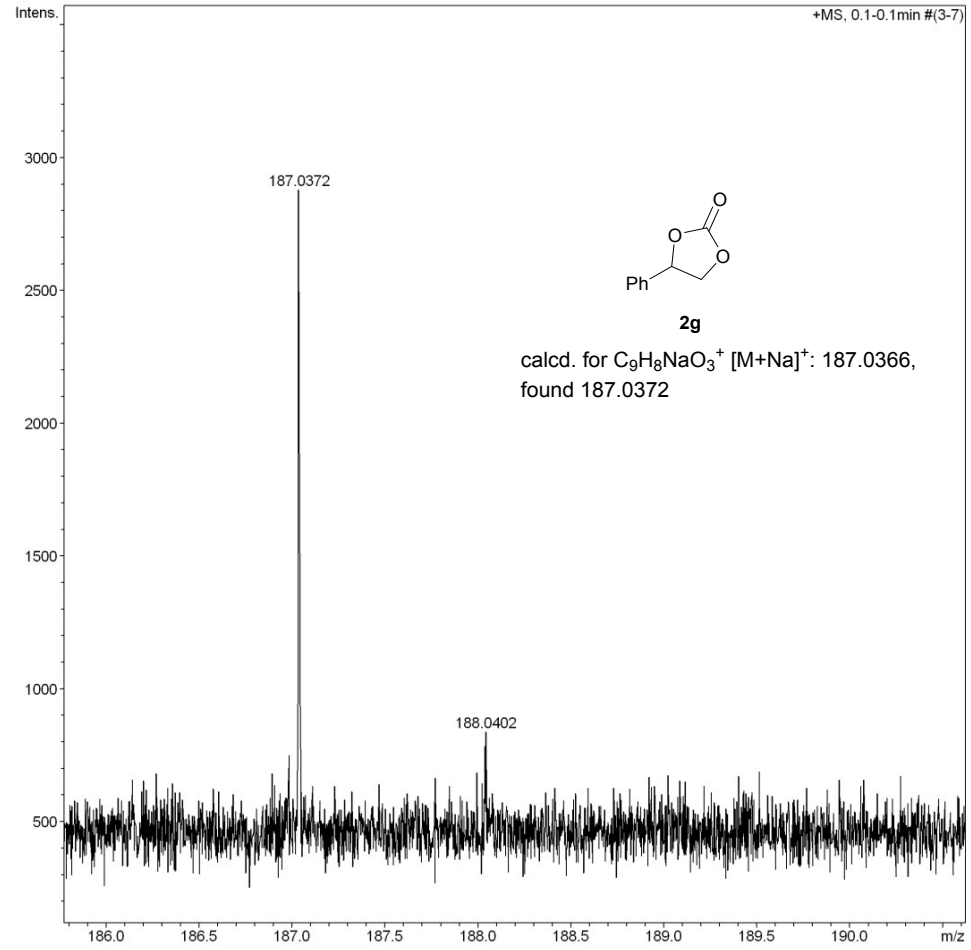
Display Report

Analysis Info

Analysis Name	D:\Data\2018\0112\lay-6.d	Acquisition Date	1/12/2018 9:18:16 AM
Method	pos_low-20151116.m	Operator	Fan
Sample Name	liuaiyun	Instrument	maXis 10103
Comment	tianxinwei		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



2g

calcd. for $C_9H_8NaO_3^+$ $[M+Na]^+$: 187.0366, found 187.0372

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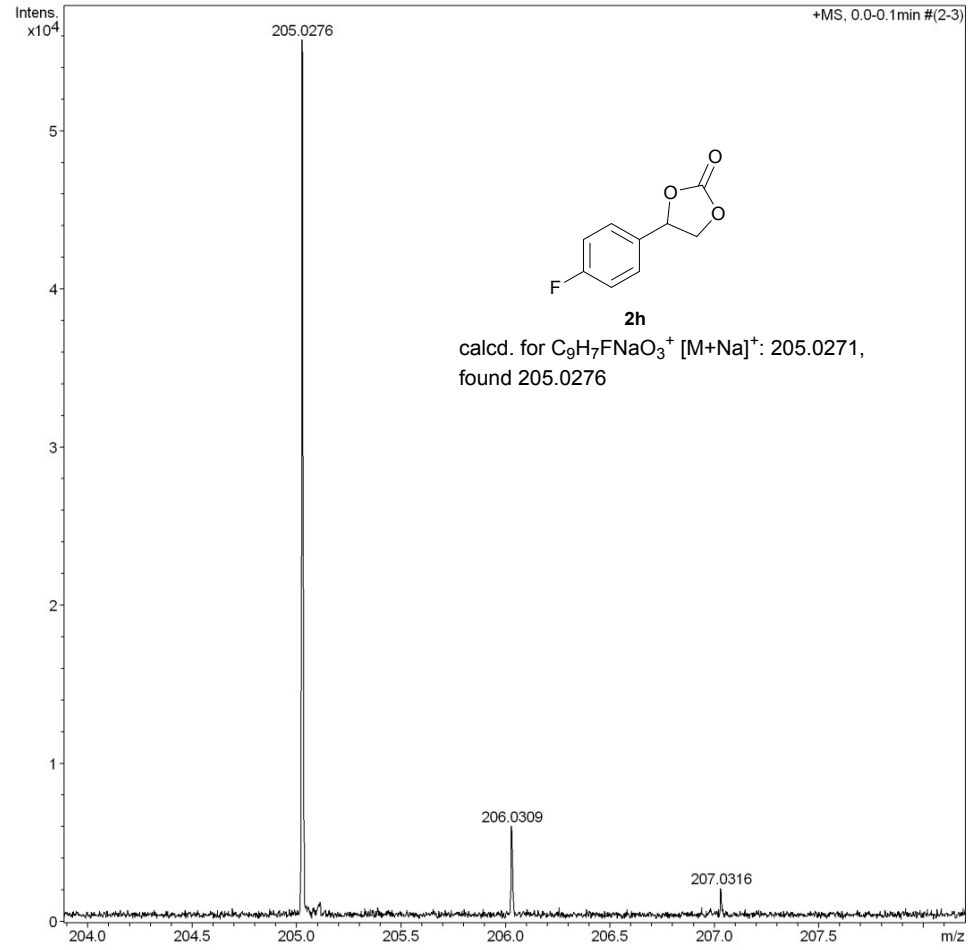
Display Report

Analysis Info

Analysis Name	D:\Data\2018\0112\lay-7.d	Acquisition Date	1/12/2018 9:31:47 AM
Method	pos_low-20151116.m	Operator	Fan
Sample Name	liuaiyun	Instrument	maXis 10103
Comment	tianxinwei		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



2h

calcd. for $C_9H_7FNaO_3^+$ $[M+Na]^+$: 205.0271,
found 205.0276

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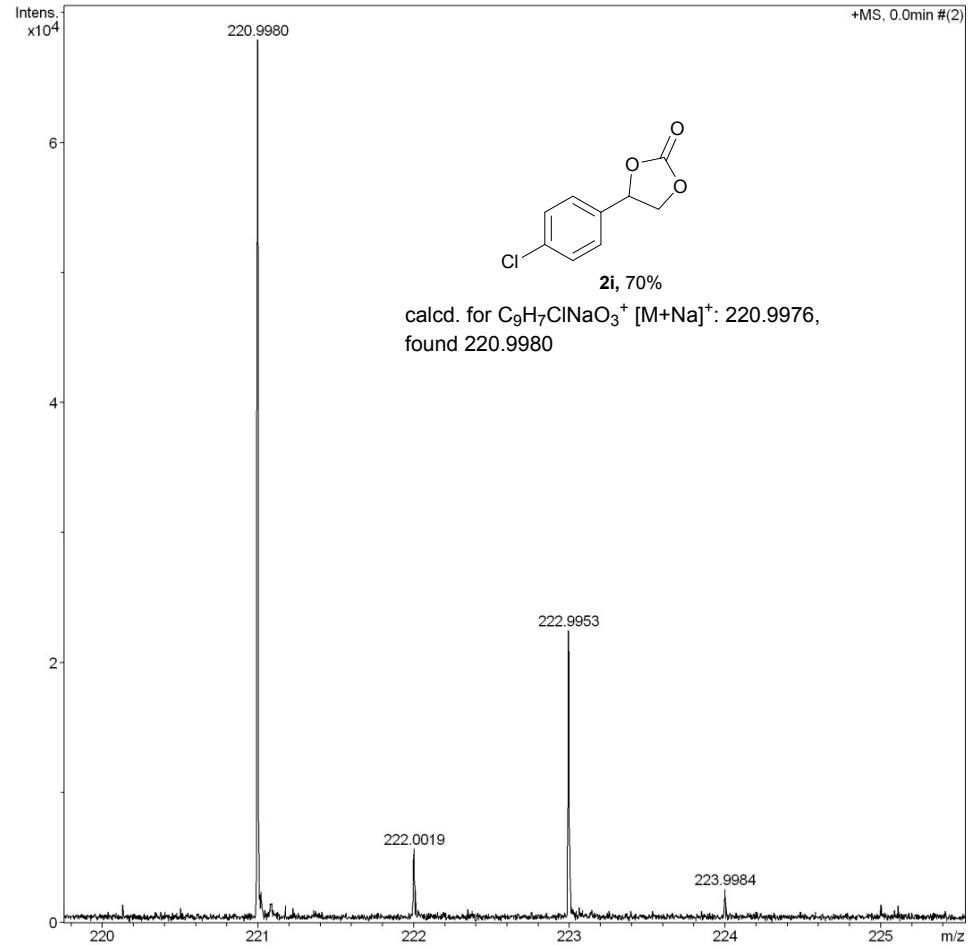
Display Report

Analysis Info

Analysis Name	D:\Data\2018\0112\lay-8.d	Acquisition Date	1/12/2018 9:35:39 AM
Method	pos_low-20151116.m	Operator	Fan
Sample Name	liuaiyun	Instrument	maXis 10103
Comment	tianxinwei		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



2i, 70%

calcd. for $C_9H_7ClNaO_3^+$ $[M+Na]^+$: 220.9976, found 220.9980

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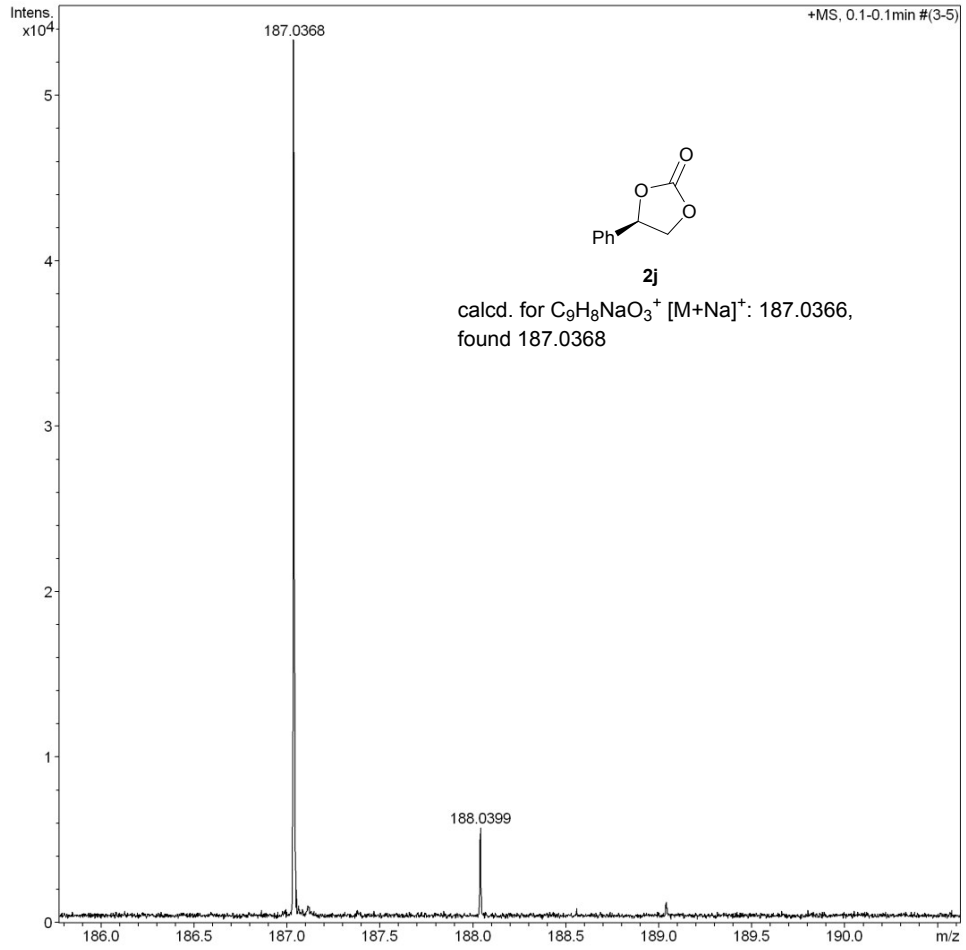
Display Report

Analysis Info

Analysis Name	D:\Data\2018\0112\lay-9.d	Acquisition Date	1/12/2018 9:23:37 AM
Method	pos_low-20151116.m	Operator	Fan
Sample Name	liuaiyun	Instrument	maXis 10103
Comment	tianxinwei		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



2j

calcd. for $C_9H_8NaO_3^+$ $[M+Na]^+$: 187.0366, found 187.0368

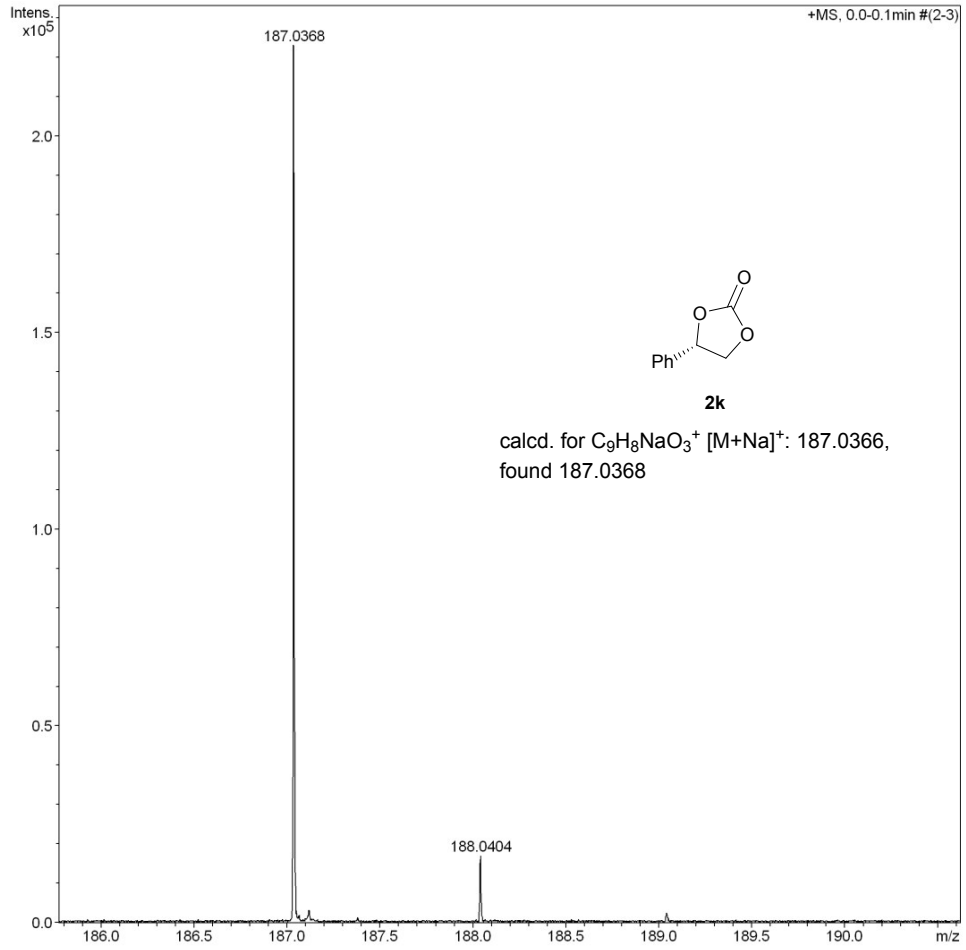
Display Report

Analysis Info

Analysis Name	D:\Data\2018\0112\lay-10.d	Acquisition Date	1/12/2018 9:27:44 AM
Method	pos_low-20151116.m	Operator	Fan
Sample Name	liuaiyun	Instrument	maXis 10103
Comment	tianxinwei		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



2k

calcd. for $C_9H_8NaO_3^+$ $[M+Na]^+$: 187.0366,
found 187.0368

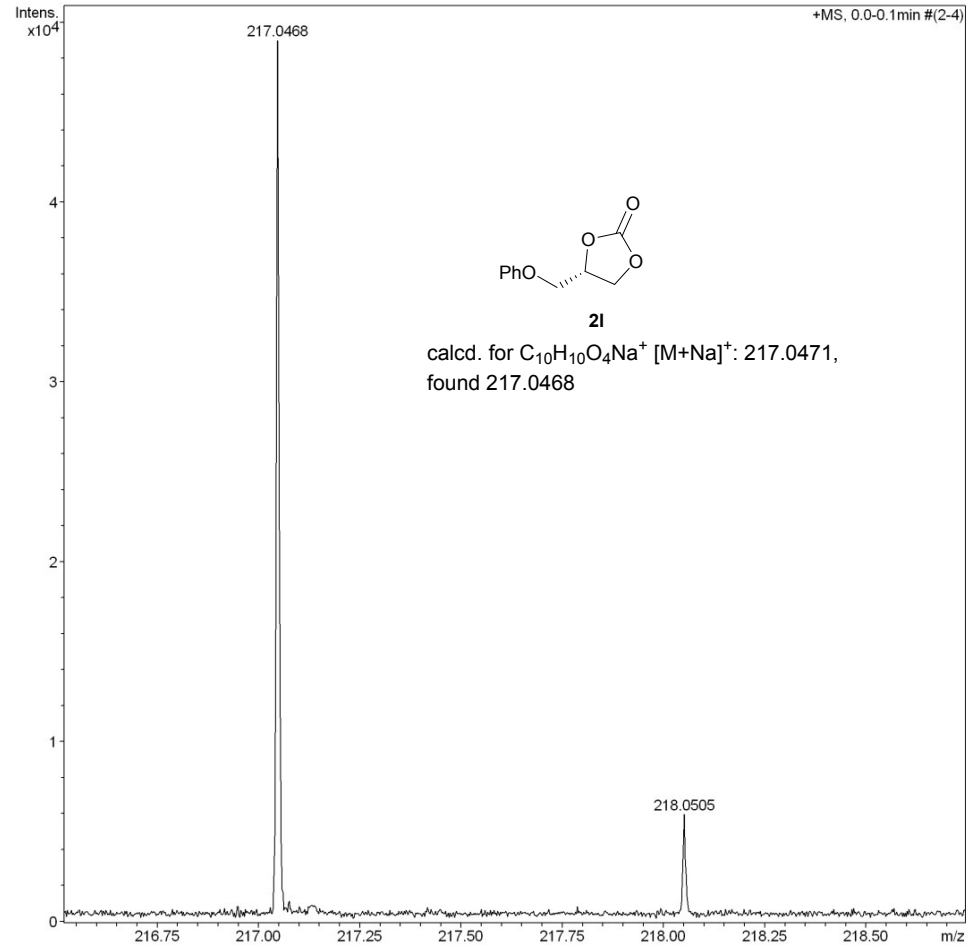
Display Report

Analysis Info

Analysis Name	D:\Data\2018\0112\lay-15.d	Acquisition Date	1/12/2018 10:43:15 AM
Method	pos_low-20151116.m	Operator	Fan
Sample Name	liuaiyun	Instrument	maXis 10103
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



2l

calcd. for $C_{10}H_{10}O_4Na^+$ $[M+Na]^+$: 217.0471,
found 217.0468

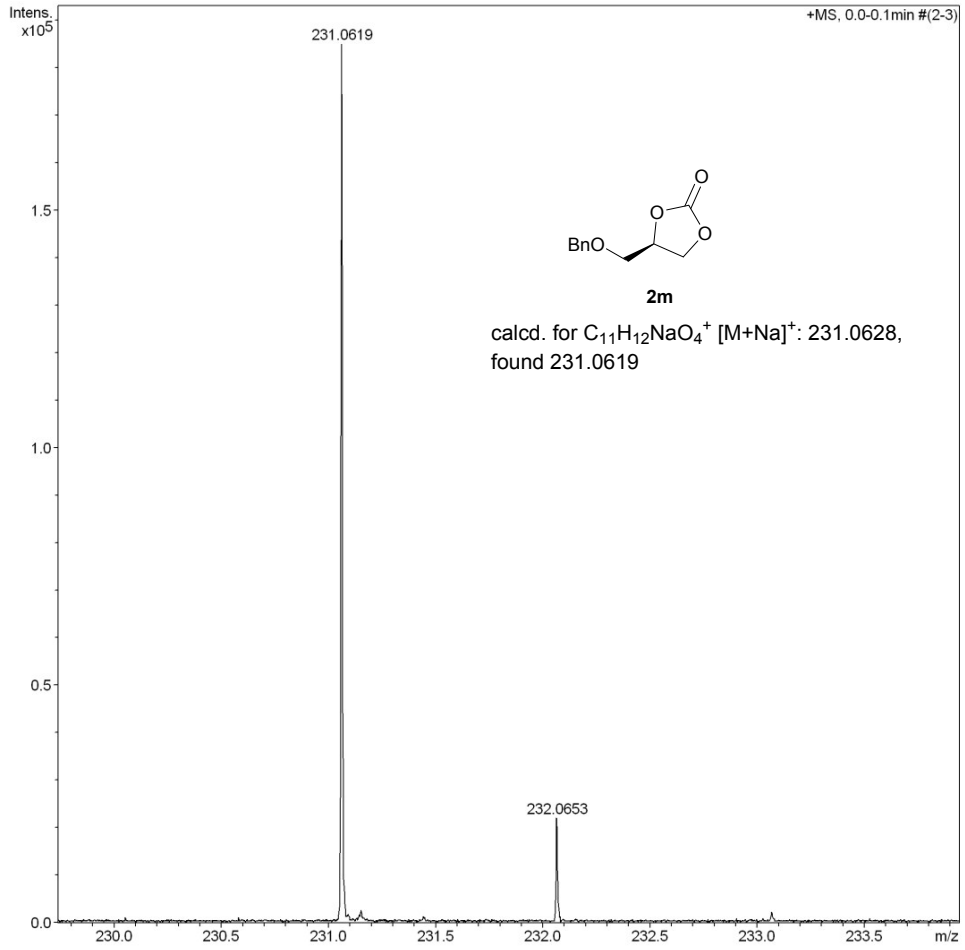
Display Report

Analysis Info

Analysis Name	D:\Data\2018\0112\lay-16.d	Acquisition Date	1/12/2018 10:46:19 AM
Method	pos_low-20151116.m	Operator	Fan
Sample Name	liuaiyun	Instrument	maXis 10103
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



2m

calcd. for $C_{11}H_{12}NaO_4^+$ $[M+Na]^+$: 231.0628, found 231.0619

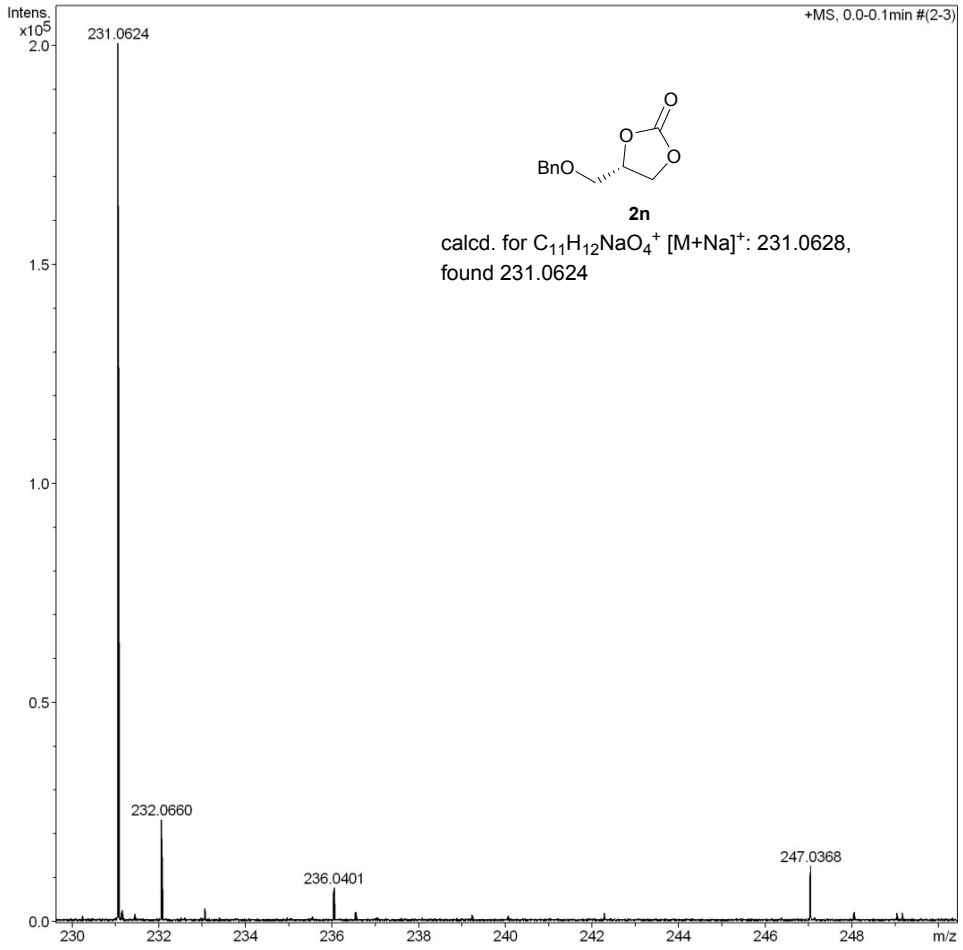
Display Report

Analysis Info

Analysis Name	D:\Data\2018\0112\lay-18-1.d	Acquisition Date	1/12/2018 11:12:42 AM
Method	pos_low-20151116.m	Operator	Fan
Sample Name	liuaiyun	Instrument	maXis 10103
Comment			

Acquisition Parameter

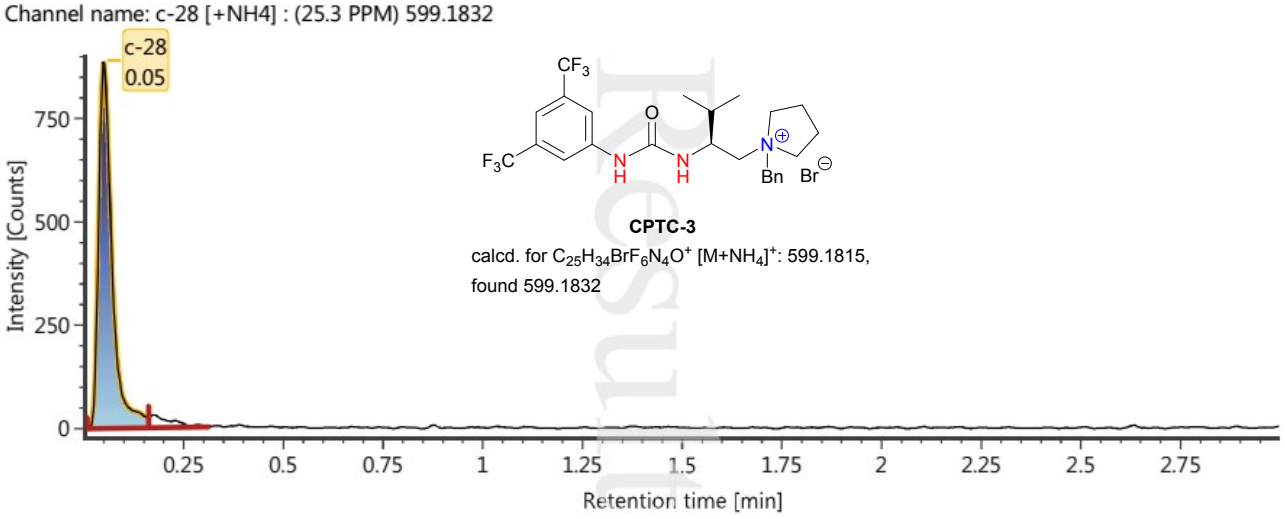
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



2n

calcd. for $C_{11}H_{12}NaO_4^+$ $[M+Na]^+$: 231.0628,
found 231.0624

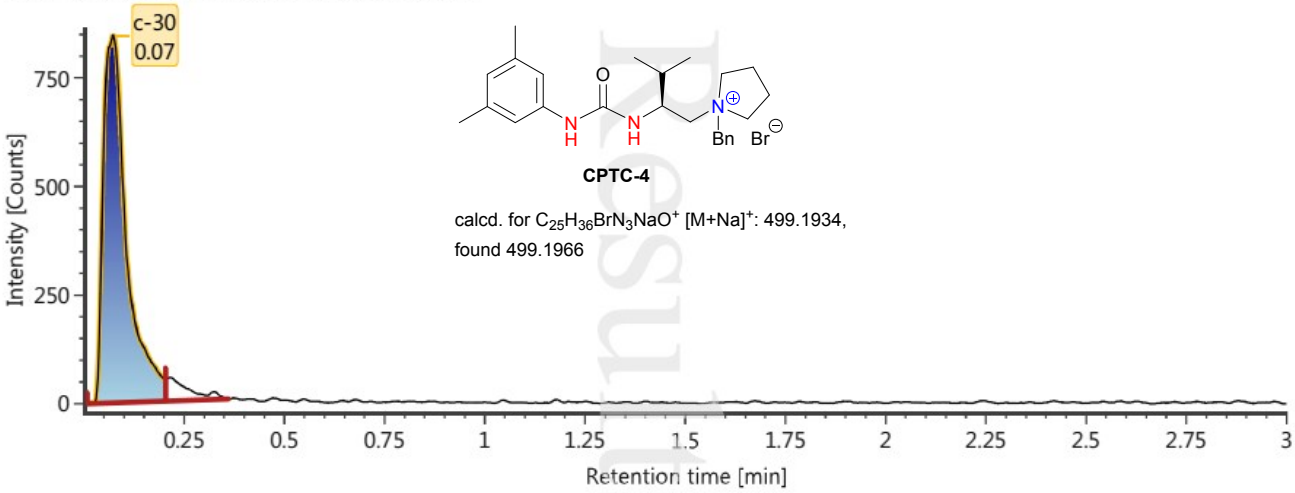
Item name: c16
Channel name: c-28 [+NH4] : (25.3 PPM) 599.1832



CPTC-3

calcd. for $C_{25}H_{34}BrF_6N_4O^+$ [M+NH$_4$]$^+$: 599.1815,
found 599.1832

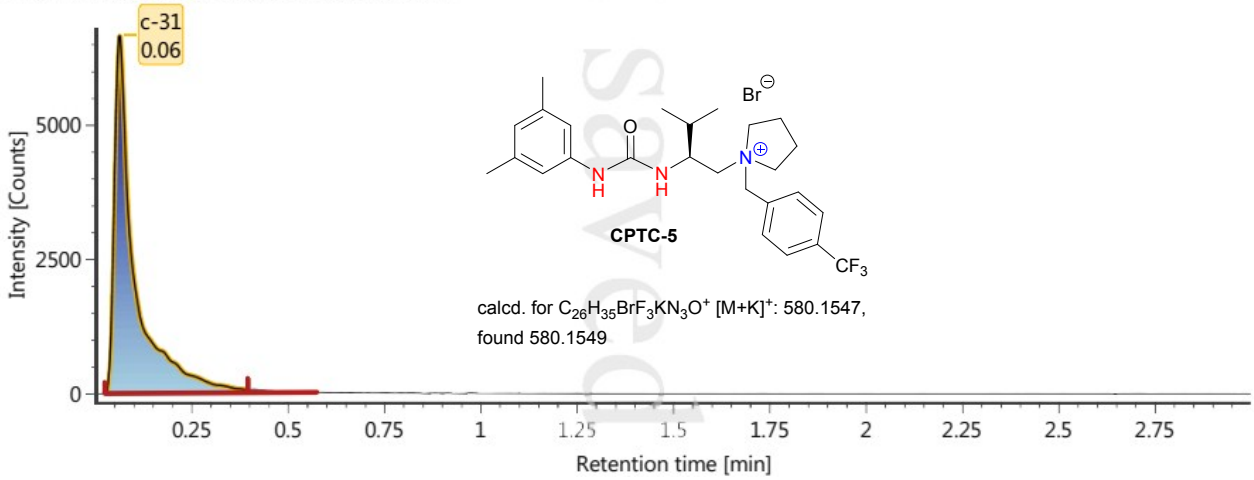
Item name: c22
Channel name: c-30 [+Na] : (25.3 PPM) 496.1966



CPTC-4

calcd. for $C_{25}H_{36}BrN_3NaO^+$ [M+Na]$^+$: 499.1934,
found 499.1966

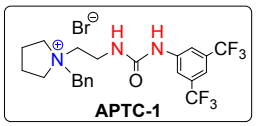
Item name: c26
Channel name: c-31 [+K] : (25.3 PPM) 580.1549



CPTC-5

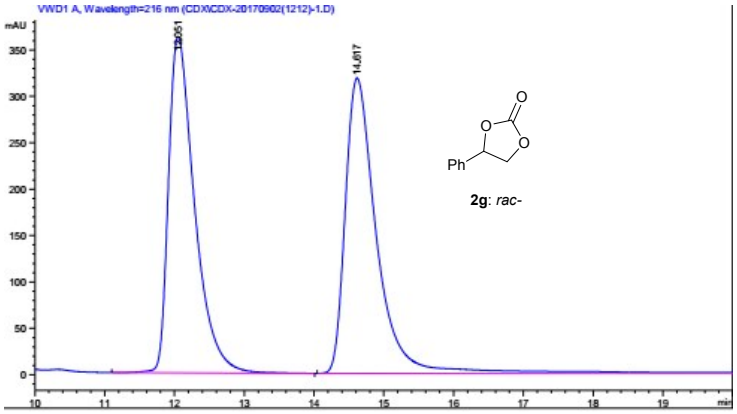
calcd. for $C_{26}H_{35}BrF_3KN_3O^+$ [M+K]$^+$: 580.1547,
found 580.1549

HPLC copies of cyclic carbonates from APTC-1 catalyzed fixation of CO_2 with chiral epoxides



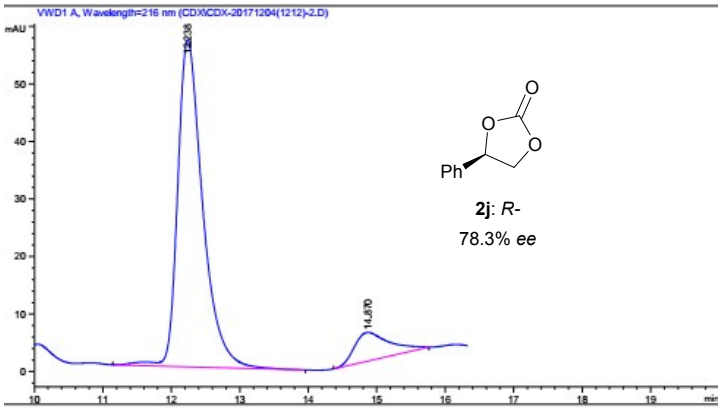
APTC-1

HPLC: Chiralpak OD-H (*i*PrOH/*n*-Hexane) = 20:80, flow rate = 1.0 mL/min, 216 nm.



2g: *rac-*

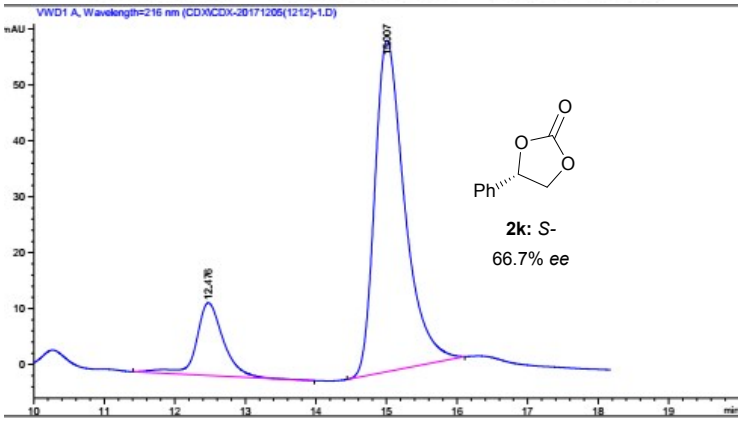
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.051	BB	0.3933	9417.72656	362.22098	48.5185
2	14.617	BB	0.4705	9992.86523	318.05972	51.4815



2j: *R-*

78.3% *ee*

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.238	BB	0.3835	1443.82312	56.80726	89.1300
2	14.870	BB	0.5134	176.08395	4.98111	10.8700

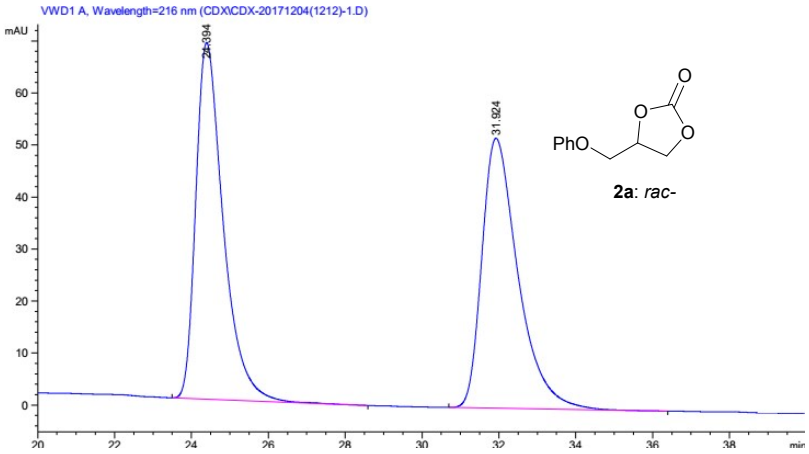


2k: *S-*

66.7% *ee*

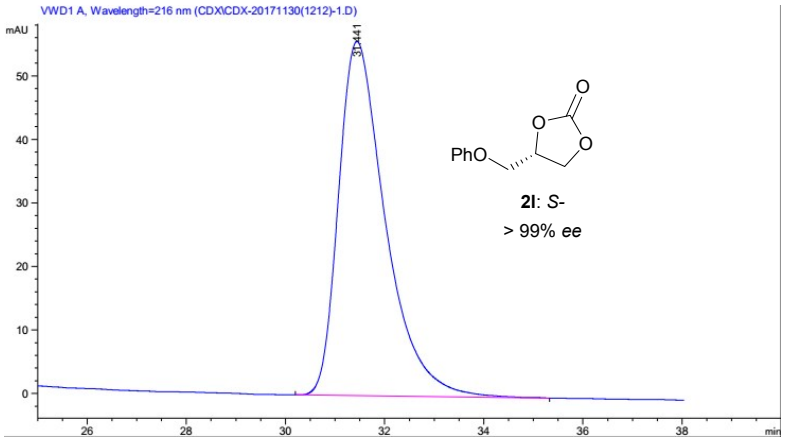
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.476	BB	0.3953	346.71918	12.99544	16.6301
2	15.007	BB	0.4434	1738.17468	59.22198	83.3699

HPLC: Chiralpak OD-H (^{i}PrOH/*n*-Hexane) = 20:80, flow rate = 1.0 mL/min, 216 nm.



2a: *rac*-

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	24.394	BB	0.7514	3404.42065	68.55317	50.0249
2	31.924	BB	0.9925	3401.02856	51.90422	49.9751

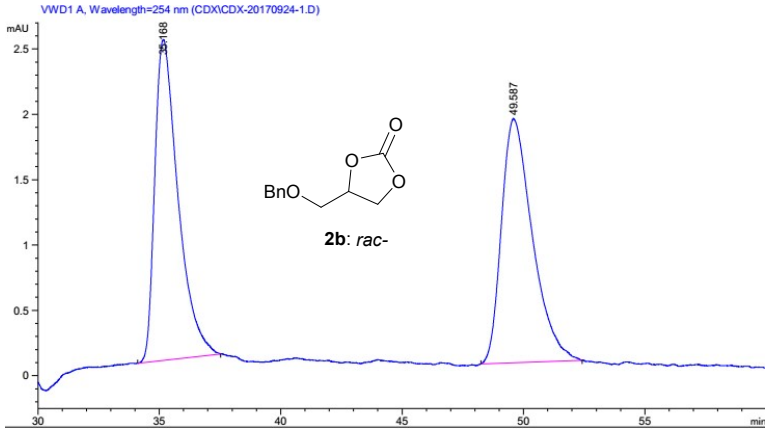


2l: *S*-

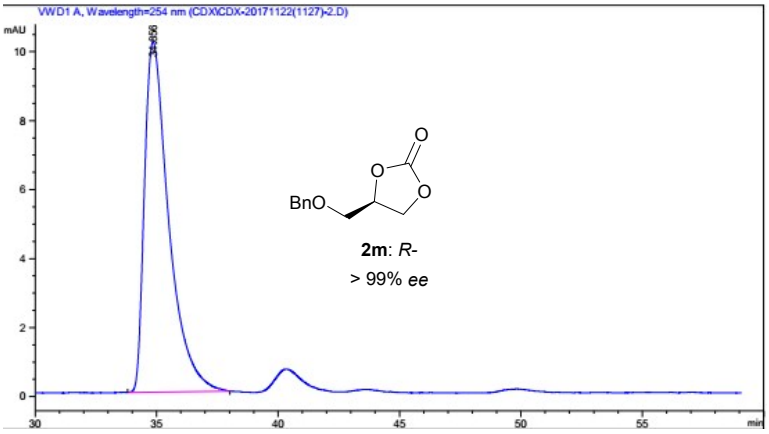
> 99% *ee*

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	31.441	BB	0.9922	3660.85938	55.74454	100.0000

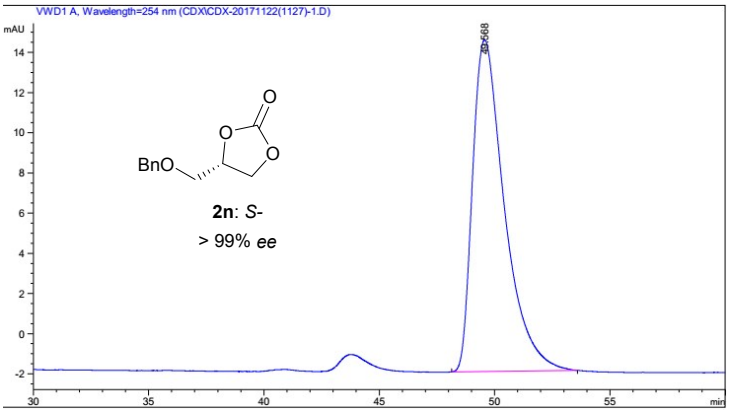
HPLC: Chiralpak OD-H (^{i}PrOH/*n*-Hexane) = 10:90, flow rate = 1.0 mL/min, 254 nm.



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	35.168	BB	0.9103	163.96121	2.45464	49.7817
2	49.587	BB	1.0470	165.39894	1.86982	50.2183

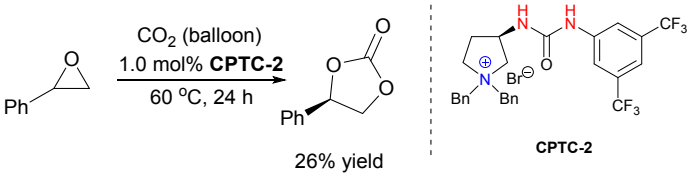


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	34.856	BB	1.0227	706.71167	10.15786	100.0000



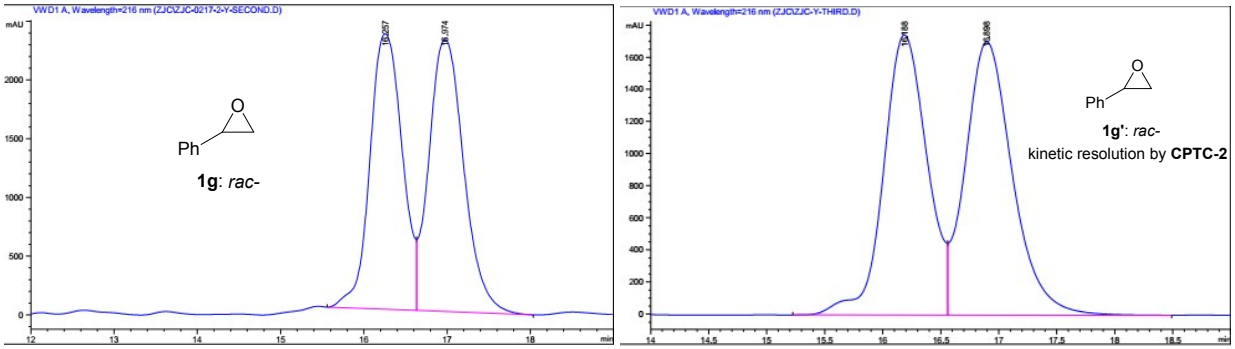
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	49.568	BB	1.3892	1586.49561	16.50781	100.0000

HPLC copies of producs from the kinetic resolution of *rac*-epoxides by CO_2 with CPTCs



For epoxide **1g** and **1g'**:

HPLC: Chiralpak AD-H (^{i}PrOH/*n*-Hexane) = 0.2:99.8, flow rate = 0.3 mL/min, 216 nm.

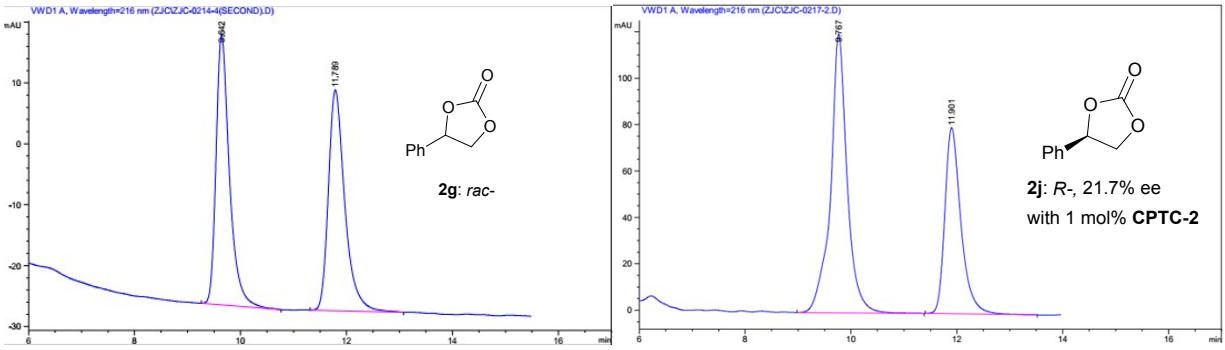


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.257	BV	0.4216	6.34322e4	2344.84497	48.4172
2	16.974	VB	0.4492	6.75794e4	2317.21606	51.5828

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	16.188	BV	0.4004	4.55240e4	1744.77588	48.5556
2	16.898	VB	0.4296	4.82324e4	1702.31604	51.4444

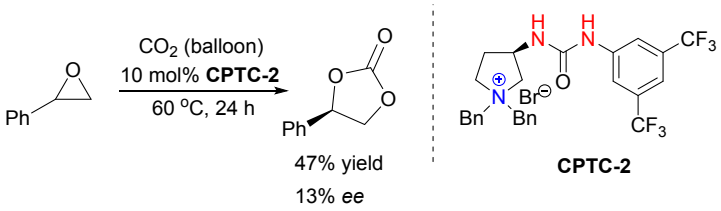
For cyclic carbonate **2g** and **2j**:

HPLC: Chiralpak OD-H (^{i}PrOH/*n*-Hexane) = 20:80, flow rate = 1.0 mL/min, 216 nm.



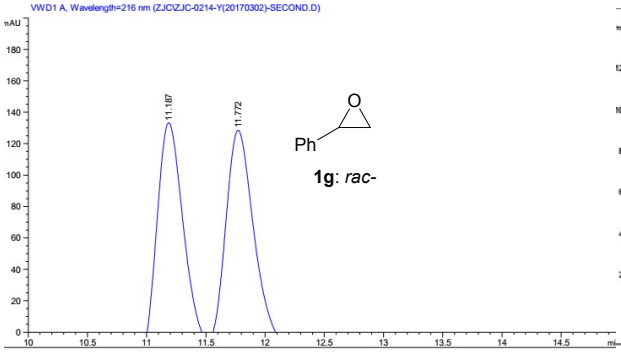
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.642	BB	0.2658	782.31256	44.35572	50.1434
2	11.789	BB	0.3237	777.83801	36.19916	49.8566

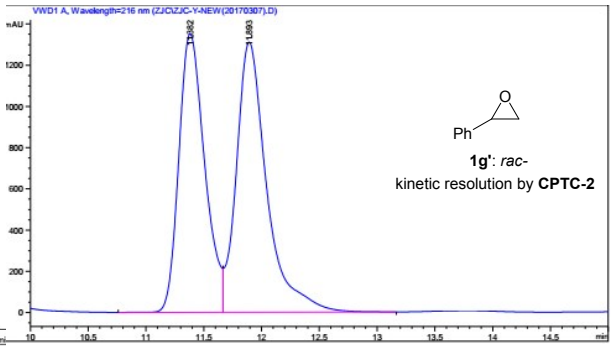
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.767	BB	0.3147	2619.81592	120.01179	60.8269
2	11.901	BB	0.3178	1687.18921	80.07686	39.1731



For epoxide **1g** and **1g'**:

HPLC: Chiralpak AD-H (*i*PrOH/*n*-Hexane) = 1:99, flow rate = 0.3 mL/min, 216 nm.



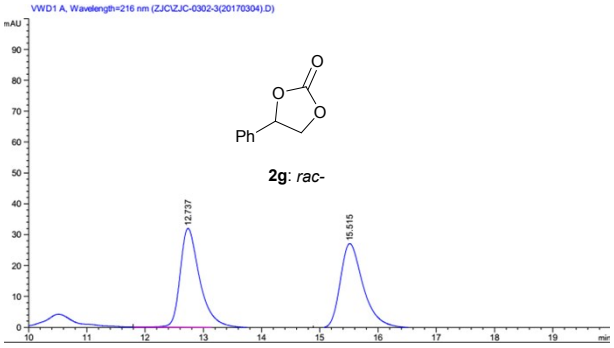


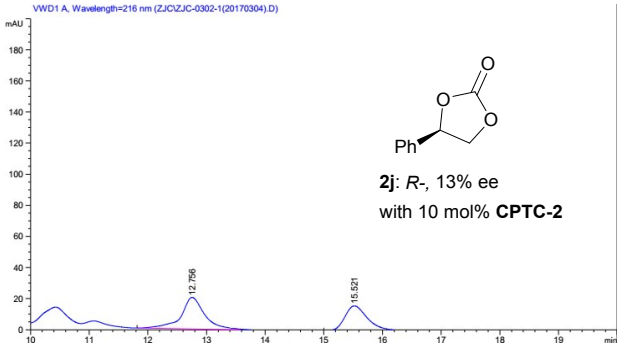
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.187	VV	0.2553	2617.95630	156.37517	46.4802
2	11.772	VB	0.2925	3014.45386	151.88600	53.5198

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.382	BV	0.2381	2.09822e4	1351.58093	46.7616
2	11.893	VB	0.2717	2.38884e4	1310.44312	53.2384

For cyclic carbonate **2g** and **2j**:

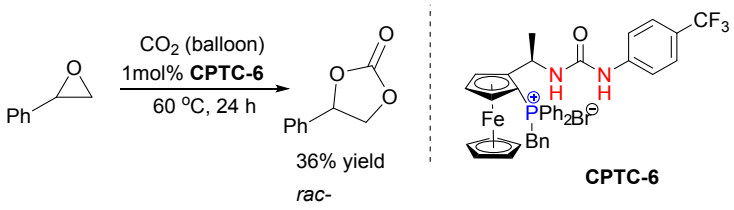
HPLC: Chiralpak OD-H (*i*PrOH/*n*-Hexane) = 20:80, flow rate = 1.0 mL/min, 216 nm.



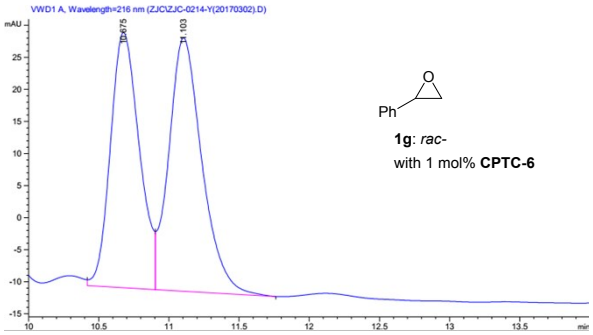


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.737	BB	0.3502	750.52100	32.05175	49.5643
2	15.515	BB	0.4183	763.71655	27.47141	50.4357

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.756	BB	0.4068	574.36926	20.32117	56.4960
2	15.521	BB	0.4160	442.28592	16.07409	43.5040

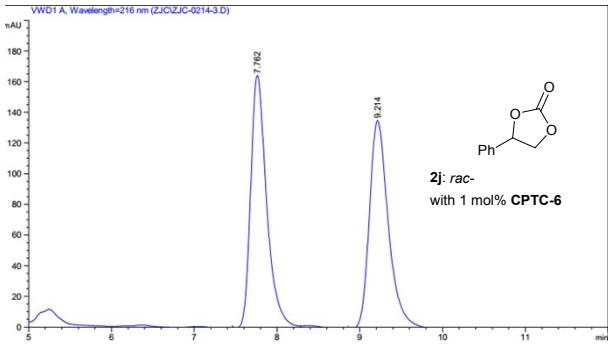


For epoxide: HPLC: Chiralpak AD-H (*i*PrOH/*n*-Hexane) = 1:99, flow rate = 0.3 mL/min, 216 nm.
For cyclic carbonate HPLC: Chiralpak OD-H (*i*PrOH/*n*-Hexane) = 20:80, flow rate = 1.0 mL/min, 216 nm.



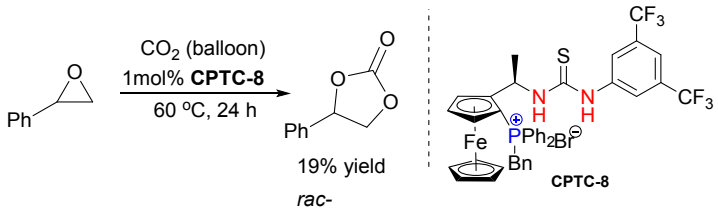
1g: *rac*-
with 1 mol% **CPTC-6**

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.675	VV	0.2191	570.01056	39.80342	46.7801
2	11.103	VB	0.2454	648.47870	39.52533	53.2199

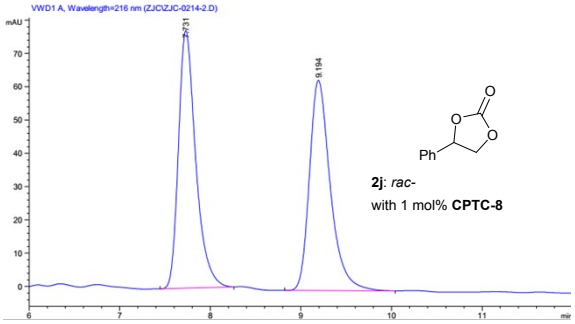


2j: *rac*-
with 1 mol% **CPTC-6**

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.762	BV	0.2032	2221.07690	164.86708	50.4380
2	9.214	BB	0.2434	2182.50293	135.90697	49.5620

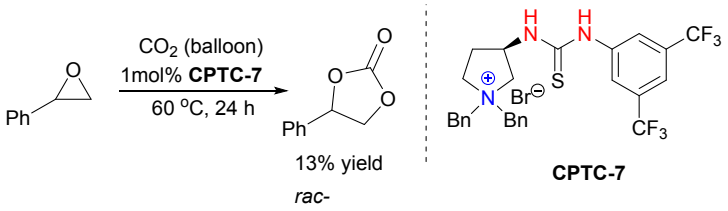


For cyclic carbonate HPLC: Chiralpak OD-H (*i*PrOH/*n*-Hexane) = 20:80, flow rate = 1.0 mL/min, 216 nm.

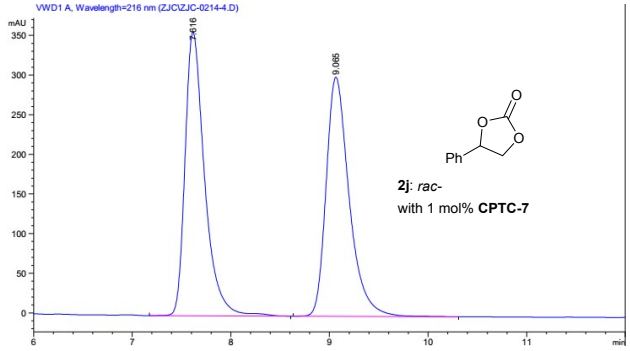


2j: *rac*-
with 1 mol% **CPTC-8**

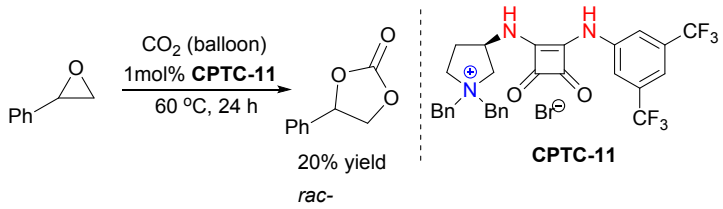
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.731	BB	0.2000	1021.64734	77.38027	50.2722
2	9.194	BB	0.2426	1010.58240	63.17895	49.7278



For cyclic carbonate HPLC: Chiralpak OD-H (*i*PrOH/*n*-Hexane) = 20:80, flow rate = 1.0 mL/min, 216 nm.

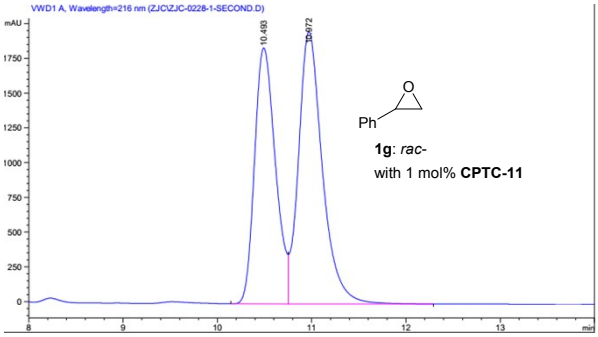


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.616	BB	0.2090	4936.02148	357.78143	50.1905
2	9.065	BB	0.2465	4898.54834	301.57758	49.8095

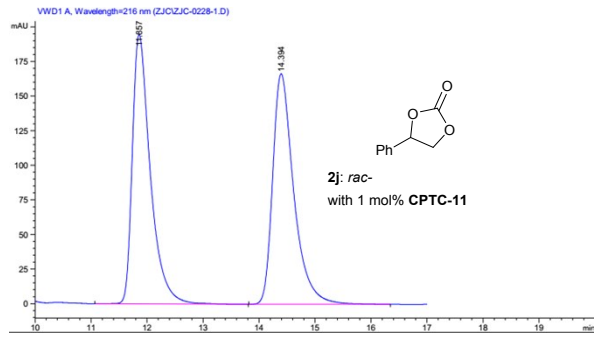


For epoxide: HPLC: Chiralpak AD-H (*i*PrOH/*n*-Hexane) = 1:99, flow rate = 0.3 mL/min, 216 nm.

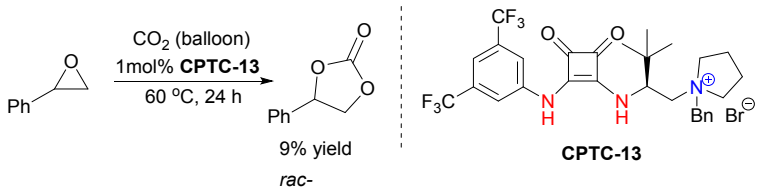
For cyclic carbonate HPLC: Chiralpak OD-H (*i*PrOH/*n*-Hexane) = 20:80, flow rate = 1.0 mL/min, 216 nm.



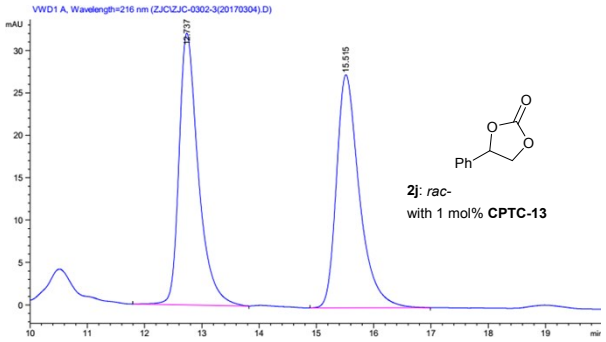
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	10.493	BV	0.2373	2.83036e4	1841.87341	45.0686
2	10.972	VV	0.2654	3.44975e4	1958.98682	54.9314



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	11.857	BB	0.3340	4339.14697	194.71982	49.8935
2	14.394	BB	0.3942	4357.66602	166.58583	50.1065

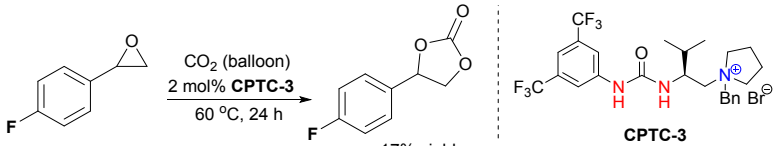


For cyclic carbonate HPLC: Chiralpak OD-H (*i*PrOH/*n*-Hexane) = 20:80, flow rate = 1.0 mL/min, 216 nm.

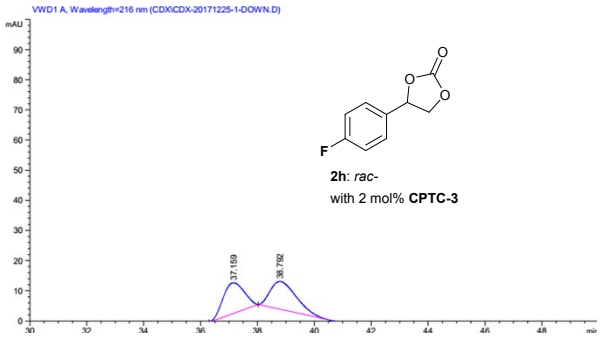


2j: *rac-*
with 1 mol% **CPTC-13**

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	12.737	BB	0.3502	750.52100	32.05175	49.5643
2	15.515	BB	0.4183	763.71655	27.47141	50.4357

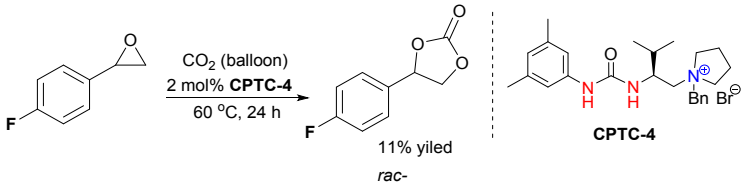


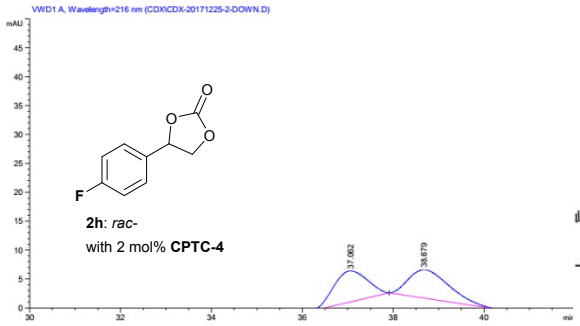
For cyclic carbonate HPLC: Chiralpak OD-H (*i*PrOH/*n*-Hexane) = 5:95, flow rate = 1.0 mL/min, 216 nm.



2h: *rac-*
with 2 mol% **CPTC-3**

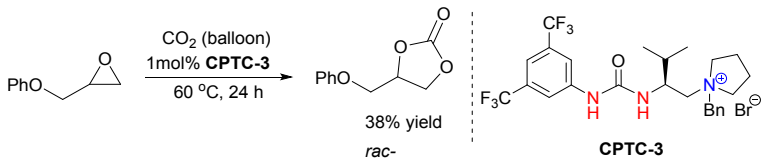
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	37.159	BB	0.8318	523.35345	10.14657	46.9283
2	38.792	BB	1.0030	591.86615	9.19462	53.0717





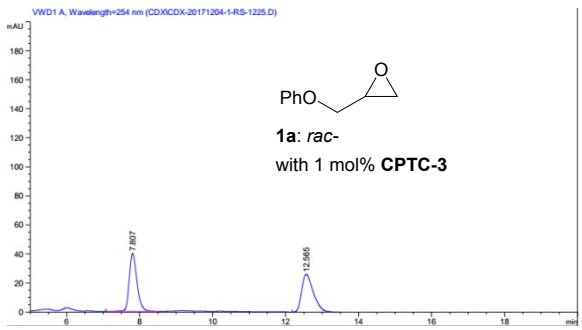
2h: *rac-*
with 2 mol% **CPTC-4**

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	37.062	BB	0.7920	276.72958	5.36279	47.4542
2	38.679	BB	0.9166	306.42126	4.89281	52.5458

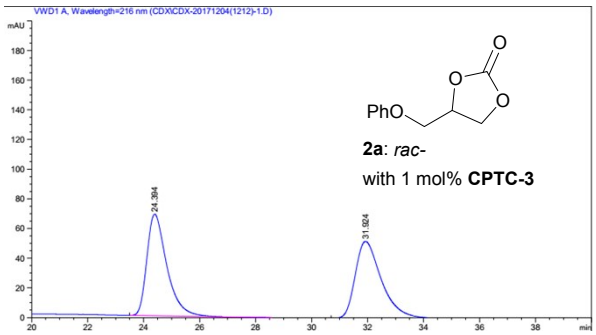


For epoxide: HPLC: Chiralpak OD-H (*i*PrOH/*n*-Hexane) = 10:90, flow rate = 1.0 mL/min, 254 nm.

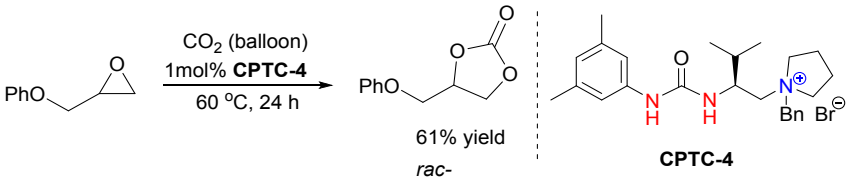
For cyclic carbonate HPLC: Chiralpak OD-H (*i*PrOH/*n*-Hexane) = 20:80, flow rate = 1.0 mL/min, 216 nm.



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.807	BB	0.2257	588.83411	40.00146	50.3882
2	12.565	BB	0.3397	579.76080	26.04378	49.6118

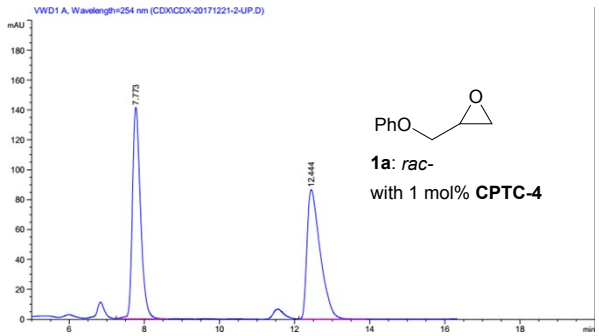


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	24.394	BB	0.7514	3404.42065	68.55317	50.0249
2	31.924	BB	0.9925	3401.02856	51.90422	49.9751

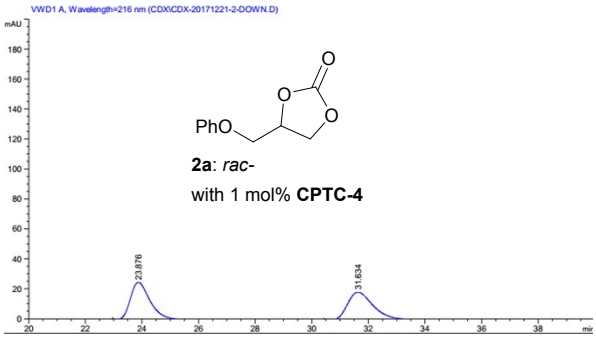


For epoxide: HPLC: Chiralpak OD-H (*i*PrOH/*n*-Hexane) = 10:90, flow rate = 1.0 mL/min, 254 nm.

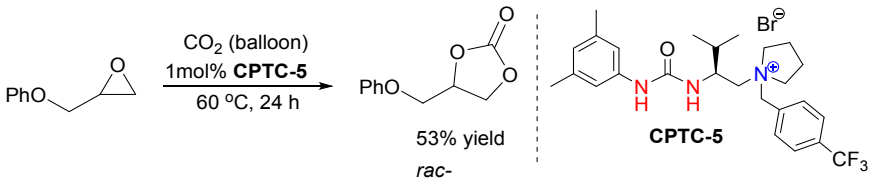
For cyclic carbonate HPLC: Chiralpak OD-H (*i*PrOH/*n*-Hexane) = 20:80, flow rate = 1.0 mL/min, 216 nm.



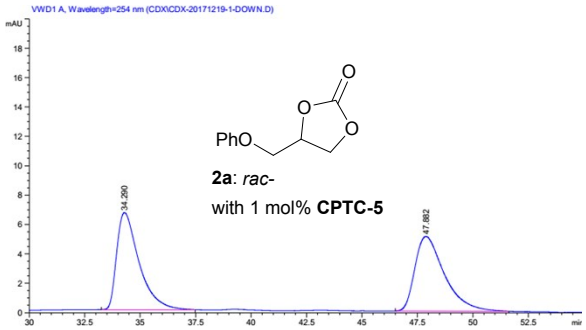
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.773	BB	0.2291	2110.14453	141.39114	49.9726
2	12.444	VB	0.3667	2112.45459	86.57761	50.0274



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	23.876	BB	0.7476	1239.18457	25.20487	49.9077
2	31.634	BB	0.9819	1243.77051	18.94522	50.0923

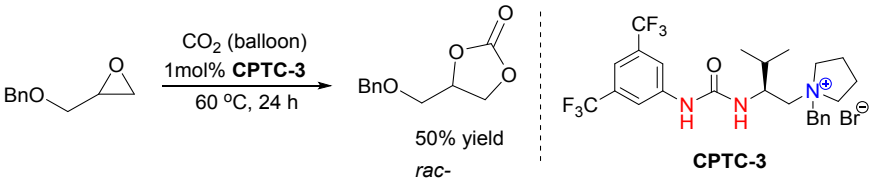


For cyclic carbonate HPLC: Chiralpak OD-H (*i*PrOH/*n*-Hexane) = 20:80, flow rate = 1.0 mL/min, 216 nm



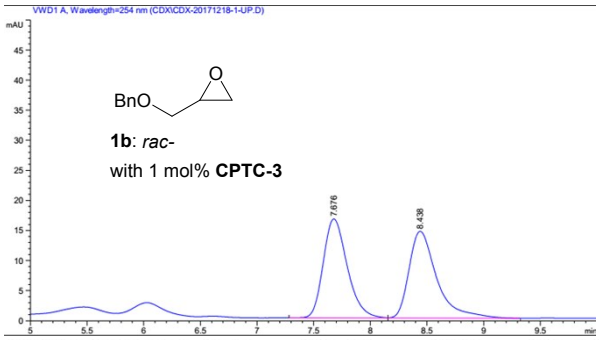
2a: *rac*-
with 1 mol% **CPTC-5**

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	34.290	BB	1.0139	463.19806	6.60680	49.7412
2	47.882	BB	1.2592	468.01828	5.07810	50.2588



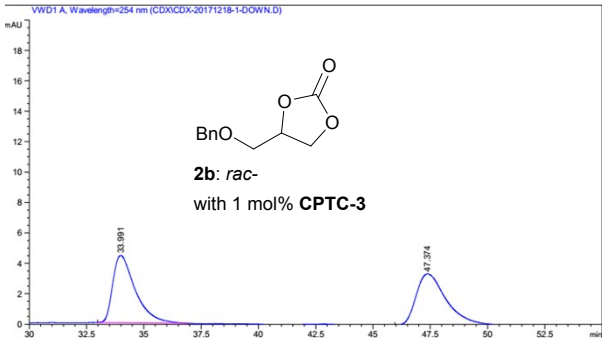
For epoxide: HPLC: Chiralpak OD-H (*i*PrOH/*n*-Hexane) = 10:90, flow rate = 1.0 mL/min, 254 nm.

For cyclic carbonate HPLC: Chiralpak OD-H (*i*PrOH/*n*-Hexane) = 10:90, flow rate = 1.0 mL/min, 216 nm.



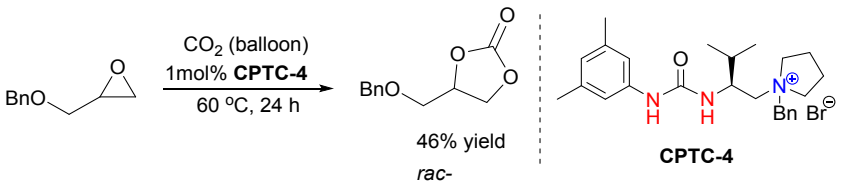
1b: *rac*-
with 1 mol% **CPTC-3**

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.676	BV	0.2265	241.78091	16.44549	49.6439
2	8.438	VB	0.2564	245.24913	14.42469	50.3561



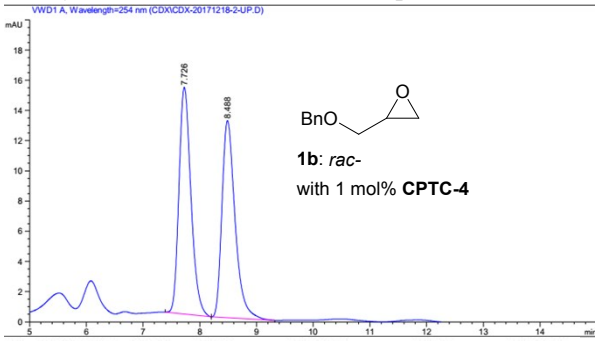
2b: *rac*-
with 1 mol% **CPTC-3**

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	33.991	BB	0.9526	301.92841	4.42728	49.7397
2	47.374	BB	1.0915	305.08881	3.36265	50.2603

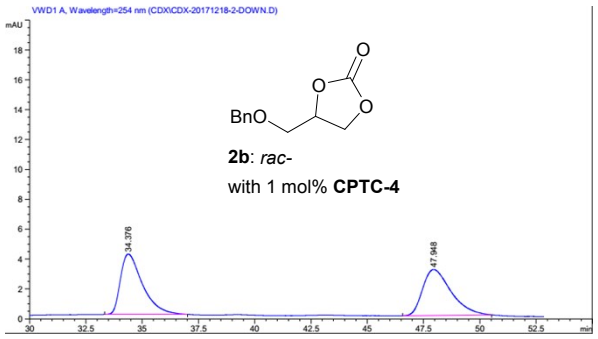


For epoxide: HPLC: Chiralpak OD-H (*i*PrOH/*n*-Hexane) = 10:90, flow rate = 1.0 mL/min, 254 nm.

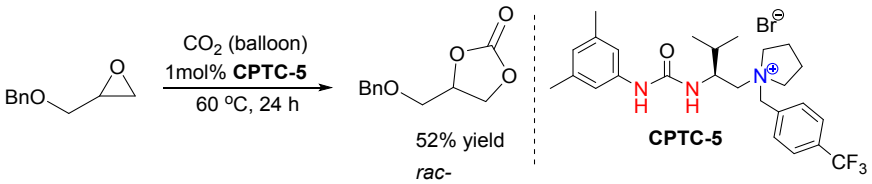
For cyclic carbonate HPLC: Chiralpak OD-H (*i*PrOH/*n*-Hexane) = 10:90, flow rate = 1.0 mL/min, 216 nm.



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.726	BB	0.2262	220.44572	15.02495	51.2174
2	8.488	BB	0.2456	209.96577	13.05670	48.7826

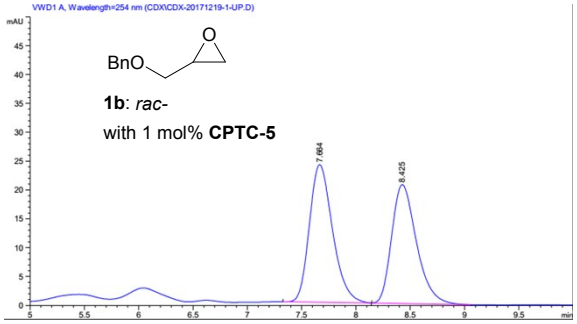


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	34.376	BB	0.9524	276.01184	4.03819	50.5048
2	47.948	BB	1.0547	270.49384	3.08276	49.4952

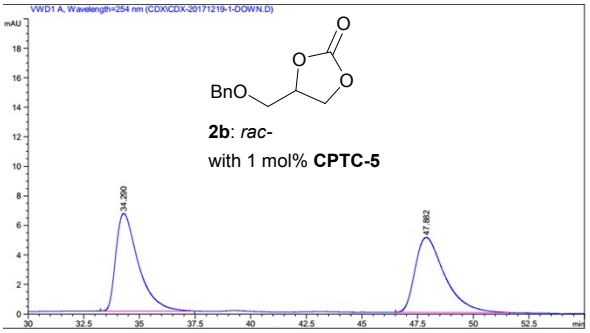


For epoxide: HPLC: Chiralpak OD-H (*i*PrOH/*n*-Hexane) = 10:90, flow rate = 1.0 mL/min, 254 nm.

For cyclic carbonate HPLC: Chiralpak OD-H (*i*PrOH/*n*-Hexane) = 10:90, flow rate = 1.0 mL/min, 216 nm.



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	7.664	BB	0.2291	353.63394	23.83842	51.9892
2	8.425	BB	0.2440	326.57248	20.59390	48.0108



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	34.290	BB	1.0139	463.19806	6.60680	49.7412
2	47.882	BB	1.2592	468.01828	5.07810	50.2588