Electronic Supplementary Information

Dimethyldioxirane (DMDO) as a valuable oxidant for the synthesis of polyfunctional aromatic imidazolium monomers bearing epoxides.

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I. General experimental and analytical data

All reagents were purchased from Sigma Aldrich, Alfa Aesar or TCI and were used without further purification and used as received. Solvents were used in RPE grade without further purification. Anhydrous solvents were obtained from a PURESOLV SPS400 apparatus developed by Innovative Technology Inc. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AvanceIII 400 MHz, 500 MHz or AvanceNEO 600 MHz spectrometer. Samples were dissolved in an appropriate deuterated solvent ($CDCl_3$, DMSO-d^6, acetone-d_6). The chemical shifts (δ) are expressed in ppm relative to internal tetramethylsilane for ^{1}H and ^{13}C nuclei, and coupling constants are indicated in Hz. Abbreviations for signal coupling are as follows: s=singlet; d=doublet; dd=doublet of doublets; t=triplet; q=quartet; quin=quintet; m=multiplet; br=broad signal. To assign the signals to the different proton and carbon atoms, as well as the relative stereochemistry of the cycloadducts, additional 2D NMR experiments (COSY, HSQC, HMBC) and NOESY experiments were performed. Mass spectra were obtained on a GC/MS Saturn 2000 spectrometer. High-resolution mass spectra (HRMS) were performed on Q-TOF Micro WATERS by electrospray ionization (ESI). Infrared (IR) spectra were recorded with a Perkin Elmer 16 PC FTIR ATR spectrometer, using the pure product (oil or solid). Thin Layer Chromatography (TLC) was run on pre-coated aluminum plates of silica gel 60 F-254 (Merck). Flash chromatography was performed on silica gel column (Merck silica gel, 40-63 mm) using air pressure.

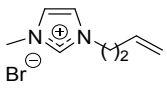
Preparation of Dimethyldioxirane. This reagent was prepared according to the procedure described by D. F. Taber.[1] Titration of different solutions prepared by this procedure afforded a DMDO concentration between 0.04 mol/L and 0.09 mol/L.[2]

In a 1 mL volumetric test tube, a 0.7 M (C_{sol}) solution of thioanisole in acetone-d_6 is prepared, to a total volume of 1 mL (0.08 mL of thioanisole + 0.92 mL of acetone-d_6). A 0.6 mL portion of this solution is transferred to a tube and chilled to ca. 10 °C in a dry ice/water bath. Upon reaching 10 °C, 3.0 mL of the obtained DMDO solution is added to the thioanisole solution. The resulting solution is stirred for 10 min and then a portion of the solution is added directly to an NMR tube.

II. Procedure for the synthesis of salts 1a-e (*N*-alkylation)

To a solution of 1-methylimidazole (1.0 equiv) or 1-arylimidazole (1.0 equiv) in CH_3CN was added halide alkylating agent (1.0 equiv). The mixture was refluxed at 80 °C and regularly monitored by ^{1}H NMR. After complete conversion of the starting material, the mixture was cooled to room temperature. Evaporation of volatile compounds under reduced pressure afforded the imidazolium salt which was directly engaged for the next step.

1-But-3-enyl-3-methylimidazolium bromide (1a)[3]



The title compound was prepared according to the general procedure with 1-methylimidazole (0.97 mL, 12.18 mmol) in CH_3CN (20 mL) and 4-bromo-butene (1.23 mL, 12.18 mmol). The product **1a** was obtained as a clear yellow oil (2.64 g, 100 %).

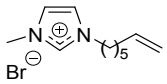
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.29 (s, 1H), 7.52-7.55 (m, 2H), 5.76 (ddt, *J* = 17.4, 10.0, 6.9 Hz, 1H), 5.04-5.08 (m, 2H), 4.43 (t, *J* = 6.9 Hz, 2H), 4.06 (s, 3H), 2.65 (q, *J* = 6.9 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.4, 132.2, 123.5, 122.3, 119.7, 49.2, 36.7, 34.4. IR (neat) cm^{-1} 3417, 3145, 3078, 1641, 1567, 1459, 1429, 1165, 928, 753. HRMS m/z (ESI): calcd. for $C_8H_{13}N_2$ $[M]^+$: 137.1079, found: 137.1078.

1-(6-Hepten-1-yl)-3-methylimidazolium bromide (1b)

[1] D. F. Taber, P. W. DeMatteo and R. A. Hassan, *Org. Synth.*, 2013, **90**, 350-357.

[2] H. Mikula, D. Svatunek, D. Lumpi, F. Glöcklhofer, C. Hametner and J. Fröhlich, *Org. Process Res. Dev.*, 2013, **7**, 313-316.

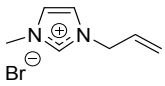
[3] (a) P. D. Pham, J. Vitz, C. Chamignon, A. Martel and S. Legoupy, *Eur. J. Org. Chem.*, 2009, 3249-3257. (b) J. Vitz, D. H. Mac and S. Legoupy, *Green Chem.*, 2007, **9**, 431-433.



The title compound was prepared according to the general procedure with 1-methylimidazole (0.97 mL, 12.18 mmol) in CH_3CN (20 mL) and 7-bromo-1-heptene (1.86 mL, 12.18 mmol). The product **1b** was obtained as a yellow oil (3.16 g, 100 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.33 (s, 1H), 7.42-7.55 (m, 2H), 5.70 (ddt, *J* = 17.0, 10.3, 6.7 Hz, 1H), 4.87-4.95 (m, 2H), 4.28 (t, *J* = 7.4 Hz, 2H), 4.07 (s, 3H), 1.96-2.01 (m, 2H), 1.84-1.92 (m, 2H), 1.30-1.42 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.2, 137.5, 123.7, 122.0, 115.0, 50.1, 36.8, 33.4, 30.2, 28.1, 25.6. IR (neat) cm^{-1} 3422, 3065, 2932, 2858, 1639, 1569, 1461, 1167, 997, 911. HRMS m/z (ESI): calcd. for $C_{11}H_{19}N_2$ $[M]^+$: 179.1548, found: 179.1548.

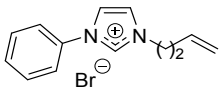
3-Methyl-1-(2-propen-1-yl)imidazolium bromide (1c)[4]



The title compound was prepared according to the general procedure with 1-methylimidazole (0.97 ml, 12.18 mmol) in CH_3CN (20 mL) and allyl bromide (1.05 ml, 6.09 mmol). The product **1c** was obtained as a yellow oil (2.63 g, 100 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.34 (s, 1H), 7.35-7.47 (m, 2H), 6.00 (ddt, *J* = 16.8, 10.3, 6.5 Hz, 1H), 5.45-5.50 (m, 2H), 5.00 (d, *J* = 6.4 Hz, 2H), 4.11 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.8, 129.8, 123.6, 122.9, 121.8, 52.3, 37.0. IR (neat) cm^{-1} 3403, 3146, 3087, 1646, 1573, 1449, 1424, 1163, 948, 754. HRMS m/z (ESI): calcd. for $C_7H_{11}N_2$ $[M]^+$: 123.0922, found: 123.0924.

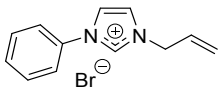
3-(3-Buten-1-yl)-1-phenylimidazolium bromide (1d)



The title compound was prepared according to the general procedure with 1-phenylimidazole (6.83 g, 47.4 mmol) in CH_3CN (45 mL) and 4-bromo-butene (4.78 mL, 47.4 mmol). The product **1d** was obtained as a yellow oil (12.62 g, 95 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 11.00 (s, 1H), 7.71-7.77 (m, 4H), 7.49-7.57 (m, 3H), 5.90 (ddt, *J* = 17.2, 10.0, 6.9 Hz, 1H), 5.07-5.11 (m, 2H), 4.72 (t, *J* = 6.8 Hz, 2H), 2.75 (q, *J* = 6.8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.1, 134.5, 132.6, 130.7, 130.4, 123.3, 121.9, 120.5, 119.8, 49.6, 34.6. IR (neat) cm^{-1} 3070, 1640, 1597, 1567, 1551, 1496, 1463, 1200, 1072, 999. HRMS m/z (ESI): calcd. for $C_{13}H_{15}N_2$ $[M]^+$: 199.1235, found: 199.1234.

1-Phenyl-3-(2-propen-1-yl)imidazolium bromide (1e)



The title compound was prepared according to the general procedure with 1-phenylimidazole (2.00 g, 13.87 mmol) in CH_3CN (20 mL) and allyl bromide (1.24 ml, 13.87 mmol). The product **1e** was obtained as a white solid (3.66 g, 99 %).

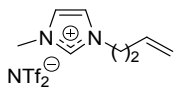
^{1}H NMR (400 MHz, $CDCl_3$) δ 11.01 (s, 1H), 7.68-7.83 (m, 3H), 7.45-7.66 (m, 4H), 6.10 (ddt, *J* = 17.1, 10.1, 6.6 Hz, 1H), 5.42-5.65 (m, 2H), 5.27 (d, *J* = 6.5 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.3, 134.6, 130.8, 130.5, 130.0, 123.2, 122.8, 122.0, 120.8, 52.6. IR (neat) cm^{-1} 3059, 2996, 1553, 1495, 1416, 1231, 1206, 1075, 1004, 929. Mp: 131.2 °C. HRMS m/z (ESI): calcd. for $C_{12}H_{13}N_2$ $[M]^+$: 185.1079, found: 185.1081.

[4] (a) J. R. Harjani, J. Farrell, M. T. Garcia, R. D. Singer and P. J. Scammells, *Green Chem.*, 2009, **11**, 821-829. (b) F. E. Hahn, B. Heidrich, T. Pape, A. Hepp, M. Martin, E. Sola and L. A. Oro, *Inorganica Chimica Acta*, 2006, **359**, 4840-4846.

III. Procedure for the synthesis of salts 2a-g (anion metathesis)

Protocol with $LiNTf_2$. To a solution of imidazolium bromide **1** (1.0 equiv) in H_2O was added $LiNTf_2$ (1.1 equiv). The solution was stirred at rt for 24 h and then extracted with dichloromethane. The organic layer was washed several times with water, dried over $MgSO_4$ and concentrated under reduced pressure. The imidazolium salt was pure enough to be used for the next step.

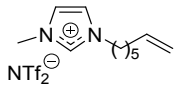
1-(3-Buten-1-yl)-3-methylimidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl] methane sulfonamide (2a)[5]



The title compound was prepared according to the general procedure with compound **1a** (2.60 g, 12.00 mmol) in H_2O (20 mL) and $LiNTf_2$ (3.79 g, 13.20 mmol). The product **2a** was obtained as a yellow oil (3.96 g, 79 %).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.05 (s, 1H), 7.73-7.79 (m, 2H), 5.80 (ddt, *J* = 17.1, 10.3, 6.9 Hz, 1H), 5.07-5.12 (m, 2H), 4.47 (t, *J* = 6.9 Hz, 2H), 4.07 (s, 3H), 2.72 (q, *J* = 6.9 Hz, 2H). ^{13}C NMR (100 MHz, acetone-d_6) δ 137.4, 134.1, 124.8, 123.5, 121.0 (q, J_{CF} = 322.4 Hz), 119.1, 49.8, 36.7, 34.9. ^{19}F NMR (376 MHz, acetone-d_6) δ -80.0. IR (neat) cm^{-1} 3158, 3122, 1568, 1464, 1432, 1347, 1330, 1178, 1133, 1052. HRMS m/z (ESI): calcd. for $C_8H_{13}N_2$ [M]$^+$: 137.1079, found: 137.1081.

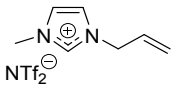
1-(6-Hepten-1-yl)-3-methylimidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methane sulfonamide (2b)



The title compound was prepared according to the general procedure with compound **1b** (1.00 g, 3.86 mmol) in H_2O (6 mL) and $LiNTf_2$ (1.22 g, 4.24 mmol). The product **2b** was obtained as a yellow oil (1.19 g, 67 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (s, 1H), 7.29-7.31 (m, 2H), 5.75 (ddt, *J* = 17.1, 10.3, 6.5 Hz, 1H), 4.92-5.01 (m, 2H), 4.15 (t, *J* = 7.4 Hz, 2H), 3.93 (s, 3H), 2.01-2.07 (m, 2H), 1.82-1.90 (m, 2H), 1.29-1.46 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.3, 136.2, 123.8, 122.3, 120.0 (q, J_{CF} = 322.4 Hz), 115.0, 50.3, 36.5, 33.4, 30.0, 28.1, 25.6. ^{19}F NMR (376 MHz, $CDCl_3$) δ -79.1. IR (neat) cm^{-1} 3157, 2934, 1641, 1574, 1463, 1348, 1330, 1179, 1133, 1052. HRMS m/z (ESI): calcd. for $C_{11}H_{19}N_2$ [M]$^+$: 179.1548, found: 179.1548.

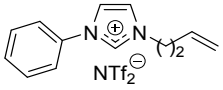
3-Methyl-1-(2-propen-1-yl)imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methane sulfonamide (2c)[6]



The title compound was prepared according to the general procedure with compound **1c** (2.63 g, 12.95 mmol) in H_2O (20 mL) and $LiNTf_2$ (4.09 g, 14.25 mmol). The product **2c** was obtained as a yellow oil (3.95 g, 76 %).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.05 (s, 1H), 7.74-7.76 (m, 2H), 6.14 (ddt, *J* = 17.1, 10.3, 6.1 Hz, 1H), 5.41-5.45 (m, 2H), 5.02 (d, *J* = 6.4 Hz, 2H), 4.09 (s, 3H). ^{13}C NMR (100 MHz, acetone-d_6) δ 137.6, 132.0, 125.0, 123.5, 121.5, 121.0 (q, J_{CF} = 322.4 Hz), 52.5, 36.8. ^{19}F NMR (376 MHz, acetone-d_6) δ -79.0. IR (neat) cm^{-1} 3158, 3123, 1575, 1426, 1347, 1330, 1177, 1132, 1051, 740. HRMS m/z (ESI): calcd. for $C_7H_{11}N_2$ [M]$^+$: 123.0922, found: 123.0922.

1-Phenyl-(3-buten-1-yl)imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methane sulfonamide (2d)



The title compound was prepared according to the general procedure with compound **1d** (12.62 g, 45.20 mmol) in H_2O (100 mL) and $LiNTf_2$ (14.27 g, 49.72 mmol). The product **2d** was obtained as yellow oil (18.15 g, 84 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.05 (s, 1H), 7.56-7.63 (m, 7H), 5.79 (ddt, *J* = 17.0, 10.1, 7.0 Hz, 1H), 5.07-5.15 (m, 2H), 4.40 (t, *J* = 6.8 Hz, 2H), 2.67 (q, *J* = 6.8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.4, 134.2, 132.1, 130.9, 130.8, 123.5, 122.2, 121.7, 120.1, 120.0 (q, J_{CF} = 322.4 Hz), 49.9, 34.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ -78.9. IR (neat) cm^{-1} 3147, 1554, 1497, 1347, 1329, 1177, 1132, 1052, 930, 761. HRMS m/z (ESI): calcd. for $C_{13}H_{15}N_2$ [M]$^+$: 199.1235, found: 199.1234.

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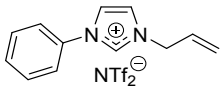
[5] M. H. G. Prechtl, J. D. Scholten and J. Dupont, *Journal of Molecular Catalysis A: Chemical*, 2009, **313**, 74-78.

[6] Z. Fei, D. Kuang, D. Zhao, C. Klein, W. H. Ang, S. M. Zakeeruddin, M. Grätzel and P. J. Dyson, *Inorg. Chem.*, 2006, **45**, 10407-10409.

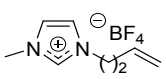
1-Phenyl-3-(2-propen-1-yl)imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methane sulfonamide (2e)



The title compound was prepared according to the general procedure with compound **1e** (3.21 g, 12.12 mmol) in H_2O (20 mL) and lithium bis(trifluoromethanesulfonyl)imide (3.83 g, 13.33 mmol). The product **2e** was obtained as a yellow oil (4.77 g, 85 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.03 (s, 1H), 7.45-7.68 (m, 7H), 5.97-6.11 (m, 1H), 5.48-5.59 (m, 2H), 4.91 (d, J = 6.5 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.4, 134.2, 130.9, 130.8, 129.1, 123.9, 123.2, 122.4, 122.0, 120.0 (q, J_{CF} = 322.4 Hz), 52.8. ^{19}F NMR (376 MHz, $CDCl_3$) δ -78.9. IR (neat) cm^{-1} 3147, 3107, 1554, 1497, 1347, 1329, 1177, 1132, 1051, 949. HRMS m/z (ESI): calcd. for $C_{12}H_{13}N_2$ $[M]^+$: 185.1079, found: 185.1083.

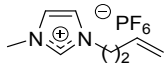
1-(3-Buten-1-yl)-3-methylimidazolium tetrafluoroborate (2f)[7]



To a solution of compound **1a** (500 mg, 2.30 mmol, 1.0 equiv) in dry acetone (4.6 mL) was added sodium tetrafluoroborate (455 mg, 4.14 mmol, 1.8 equiv). The reaction mixture was stirred at room temperature for 24 h. The precipitated solid sodium bromide was filtered off, and the filtrate was evaporated to afford a white solid-pale yellow oil. It was washed with diethyl ether and dried under reduced pressure. The product **2f** was isolated as a yellow oil (515 mg, 100 %).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.00 (s, 1H), 7.69-7.75 (m, 2H), 5.85 (ddt, J = 17.2, 10.2, 6.9 Hz, 1H), 5.04-5.12 (m, 2H), 4.43 (t, J = 6.9 Hz, 2H), 4.03 (s, 3H), 2.69 (q, J = 6.9 Hz, 2H). ^{13}C NMR (100 MHz, acetone-d_6) δ 137.6, 134.2, 124.7, 123.4, 119.0, 49.6, 36.5, 34.9. ^{19}F NMR (376 MHz, acetone-d_6) δ -152.2, -152.3. IR (neat) cm^{-1} 3634, 3163, 3122, 1643, 1575, 1169, 1032, 931, 847, 753. HRMS m/z (ESI): calcd. for $C_8H_{13}N_2$ $[M]^+$: 137.1079, found: 137.1078.

1-(3-Buten-1-yl)-3-methylimidazolium hexafluorophosphate (2g)



To a solution of compound **1a** (500 mg, 2.30 mmol, 1.0 equiv) in dry acetone (6.15 mL) was added potassium hexafluorophosphate (465 mg, 2.53 mmol, 1.1 equiv). The reaction mixture was stirred at room temperature for 30 h. The precipitated solid potassium bromide was filtered off, and the filtrate was evaporated to afford a pale yellow oil. It was washed with diethyl ether and dried under reduced pressure. The product **2g** was obtained as a yellow oil (641 mg, 99 %).

^{1}H NMR (400 MHz, acetone-d_6) δ 8.96 (s, 1H), 7.68-7.74 (m, 2H), 5.84 (ddt, J = 17.2, 10.3, 6.9 Hz, 1H), 5.06-5.12 (m, 2H), 4.44 (t, J = 6.9 Hz, 2H), 4.04 (s, 3H), 2.70 (q, J = 6.9 Hz, 2H). ^{13}C NMR (100 MHz, acetone-d_6) δ 137.4, 134.1, 124.7, 123.5, 119.1, 49.7, 36.6, 34.9. ^{19}F NMR (376 MHz, acetone-d_6) δ -71.5, -73.3. IR (neat) cm^{-1} 3172, 3126, 1644, 1575, 1465, 1431, 1168, 934, 814, 740. HRMS m/z (ESI): calcd. for $C_8H_{13}N_2$ $[M]^+$: 137.1079, found: 137.1080.

[7] (a) P. D. Pham, J. Vitz, C. Chamignon, A. Martel and S. Legoupy, *Eur. J. Org. Chem.*, 2009, 3249-3257. (b) J. Vitz, D. H. Mac and S. Legoupy, *Green Chem.*, 2007, **9**, 431-433.

IV. Procedure for the synthesis of salts 3a-g (epoxidation)

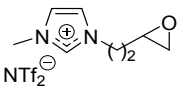
Procedure I: With mCPBA.

To a solution of corresponding alkene in CH_3CN, mCPBA was added and the reaction mixture was stirred at room temperature or 40 °C (^{1}H NMR monitoring). The reaction mixture was concentrated under reduced pressure and the crude product was washed with diethyl ether to extract the excess of mCPBA and 3-chlorobenzoic acid.

Procedure II: With DMDO.

To a solution of corresponding alkene in acetone (1.00 mL) was added freshly prepared DMDO. The reaction mixture was stirred at room temperature until the reaction is completed (^{1}H NMR monitoring). Two drops of DMS was added to quench the reaction mixture and neutralized the excess of DMDO. The crude was concentrated under reduced pressure.

1-[2-(Oxiran-2-yl)ethyl]-3-methylimidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl] methanesulfonamide (3a)

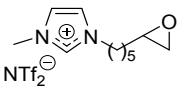


Procedure I. The title compound was prepared with compound **2a** (100 mg, 0.240 mmol, 1.0 equiv) in CH_2Cl_2 (11 mL) and mCPBA (151 mg, 0.672 mmol, 2.8 equiv). The reaction mixture was stirred at room temperature for 6 days. The crude product was concentrated under reduced pressure and washed with diethyl ether to afford a yellow oil (88 mg, 85 %).

Procedure II. The title compound was prepared with compound **2a** (100 mg, 0.240 mmol, 1.0 equiv) in $(CH_3)_2CO$ (1 mL) and freshly prepared DMDO (0.04 mol/L) (7.99 mL, 0.335 mmol, 1.4 equiv). The reaction mixture was stirred at room temperature for 6 h. The product **3a** was obtained as a yellow oil (103 mg, 99 %).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.11 (s, 1H), 7.75-7.83 (m, 2H), 4.57 (t, *J* = 6.9 Hz, 2H), 4.10 (s, 3H), 3.01-3.04 (m, 1H), 2.70-2.72 (m, 1H), 2.47-2.49 (m, 1H), 2.35-2.40 (m, 1H), 1.97-2.05 (m, 1H). ^{13}C NMR (100 MHz, acetone-d_6) δ 137.7, 124.9, 123.7, 121.0 (q, J_{CF} = 322.4 Hz), 49.6, 48.0, 46.5, 36.7, 33.7. ^{19}F NMR (376 MHz, acetone-d_6) δ -80.0. IR (neat) cm^{-1} 3159, 3122, 1575, 1348, 1330, 1177, 1132, 1051, 789, 740. HRMS m/z (ESI): calcd. for $C_8H_{13}N_2O$ $[M]^+$: 153.1028, found: 153.1029.

3-Methyl-1-[5-(oxiran-2-yl)pentyl]imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl] methanesulfonamide (3b)

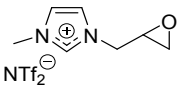


Procedure I. The title compound was prepared with compound **2b** (200 mg, 0.435 mmol, 1.0 equiv) in CH_3CN (6 mL) and mCPBA (195 mg, 0.871 mmol, 2.0 equiv). The reaction mixture was stirred at room temperature for 72 h. The crude product was concentrated under reduced pressure and pressure and washed with diethyl ether to afford a yellow oil (172 mg, 83 %).

Procedure II. The title compound was prepared with compound **2b** (100 mg, 0.218 mmol, 1.0 equiv) in $(CH_3)_2CO$ (1 mL) and freshly prepared DMDO (0.08 mol/L) (3.81 mL, 0.305 mmol, 1.4 equiv). The reaction mixture was stirred at room temperature for 2 h. The product **3b** was obtained as a yellow oil (92 mg, 89 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (s, 1H), 7.29-7.30 (m, 2H), 4.18 (t, *J* = 7.4 Hz, 2H), 3.94 (s, 3H), 2.87-2.90 (m, 1H), 2.72-2.74 (m, 1H), 2.44-2.46 (m, 1H), 1.85-1.93 (m, 2H), 1.36-1.55 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.4, 123.8, 122.4, 120.0 (q, J_{CF} = 322.4 Hz), 52.0, 50.2, 47.0, 36.5, 32.0, 29.9, 25.9, 25.4. ^{19}F NMR (376 MHz, $CDCl_3$) δ -79.0. IR (neat) cm^{-1} 3157, 3120, 2941, 1574, 1464, 1348, 1331, 1178, 1133, 1052. HRMS m/z (ESI): calcd. for $C_{11}H_{19}N_2O$ $[M]^+$: 195.1497, found: 195.1497.

1-[(Oxiran-2-yl)methyl]-3-methylimidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl] methanesulfonamide (3c)

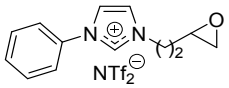


Procedure I. The title compound was prepared with compound **2c** (200 mg, 0.496 mmol, 1.0 equiv) in CH_3CN (6 mL) and mCPBA (556 mg, 2.48 mmol, 5.0 equiv). The reaction mixture was stirred at 40 °C for 30 days. The crude product was concentrated under reduced pressure and washed with diethyl ether to afford a yellow oil (116 mg, 56 %).

Procedure II. The title compound was prepared with compound **2c** (200 mg, 0.496 mmol, 1.0 equiv) in $(CH_3)_2CO$ (1.00 mL) and freshly prepared DMDO (0.07 mol/L) (17 mL, 1.19 mmol, 2.4 equiv). The reaction was stirred at room temperature for 12 h. The product **3c** was obtained as a yellow oil (200 mg, 96 %).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.06 (s, 1H), 7.78 (m, 2H), 4.90 (dd, *J* = 14.8, 2.6 Hz, 1H), 4.34 (dd, *J* = 14.8, 2.6 Hz, 1H), 4.12 (s, 3H), 3.47-3.51 (m, 1H), 2.92-2.95 (m, 1H), 2.70-2.72 (m, 1H). ^{13}C NMR (100 MHz, acetone-d_6) δ 138.0, 124.9, 124.1, 121.0 (q, J_{CF} = 322.4 Hz), 52.2, 50.3, 45.9, 36.9. ^{19}F NMR (376 MHz, acetone-d_6) δ -80.0. IR (neat) cm^{-1} 3161, 3123, 1578, 1567, 1347, 1329, 1173, 1132, 1051, 740. HRMS m/z (ESI): calcd. for $C_7H_{11}N_2O$ $[M]^+$: 139.0871, found: 139.0871.

3-[2-(Oxiran-2-yl)ethyl]-1-phenylimidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl] methanesulfonamide (3d)

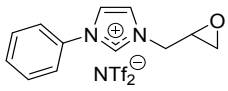


Procedure I. The title compound was prepared with compound **2d** (18.06 g, 37.67 mmol, 1.0 equiv) in CH_3CN (190 mL) and mCPBA (25.33 g, 113 mmol, 3.0 equiv). The reaction mixture was stirred at 40 °C for 24 h. The crude product was evaporated under reduced pressure and washed with diethyl ether to afford a brown oil (14.10 g, 76 %).

Procedure II. The title compound was prepared with compound **2d** (100 mg, 0.209 mmol, 1.00 equiv) in acetone (1 mL) and freshly prepared DMDO (0.087 mol/L) (5.76 mL, 0.50 mmol, 2.4 equiv). The reaction mixture was stirred at room temperature for 12 h. The product **3d** was obtained as a brown oil (89 mg, 87 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.08 (s, 1H), 7.50-7.63 (m, 7H), 4.51 (t, *J* = 6.8 Hz, 2H), 3.03-3.09 (m, 1H), 2.74-2.78 (m, 1H), 2.40-2.55 (m, 2H), 1.85-1.97 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.6, 134.5, 130.9, 130.8, 123.9, 122.4, 121.7, 120.0 (q, J_{CF} = 322.4 Hz), 49.4, 48.2, 46.5, 32.6. ^{19}F NMR (376 MHz, $CDCl_3$) δ -78.9. IR (neat) cm^{-1} 3149, 1728, 1554, 1497, 1347, 1328, 1178, 1132, 1051, 761. HRMS m/z (ESI): calcd. for $C_{13}H_{15}N_2O$ $[M]^+$: 215.1184, found: 215.1186.

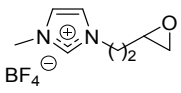
1-[(Oxiran-2-yl)methyl]-1-phenylimidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl] methanesulfonamide (3e)



Procedure II. The title compound was prepared with compound **2e** (100 mg, 0.215 mmol, 1.0 equiv) in acetone (1 mL) and freshly prepared DMDO (0.046 mol/L) (11 mL, 0.516 mmol, 2.4 equiv). The reaction mixture was stirred at room temperature for 12 h. The product **3e** was obtained as a yellow oil (103 mg, 100 %).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.64 (s, 1H), 8.24-8.29 (m, 1H), 8.00-8.05 (m, 1H), 7.82-7.87 (m, 2H), 7.63-7.74 (m, 3H), 4.97-5.05 (m, 1H), 4.42-4.51 (m, 1H), 3.56-3.63 (m, 1H), 2.78-2.86 (m, 2H). ^{13}C NMR (100 MHz, acetone-d_6) δ 136.6, 136.0, 131.3, 125.0, 123.4, 123.0, 120.0 (q, J_{CF} = 322.4 Hz), 52.8, 50.2, 46.0, 42.6. ^{19}F NMR (376 MHz, acetone-d_6) δ -79.9. IR (neat) cm^{-1} 3149, 1598, 1556, 1497, 1348, 1329, 1178, 1132, 1051, 913. HRMS m/z (ESI): calcd. for $C_{12}H_{13}N_2O$ $[M]^+$: 201.1028, found: 201.1027.

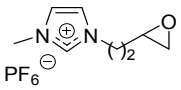
3-[2-(Oxiran-2-yl)ethyl]1-methylimidazolium tetrafluoroborate (3f)



Procedure II. The title compound was prepared with compound **2f** (100 mg, 0.4464 mmol, 1.0 equiv) in acetone (1.0 mL) and freshly prepared DMDO (0.07 mol/L) (8.93 mL, 0.625 mmol, 1.4 equiv). The reaction mixture was stirred at room temperature for 6 h. The product **3f** was obtained as a yellow oil (107 mg, 100 %).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.06 (s, 1H), 7.72-7.80 (m, 2H), 4.55 (t, *J* = 6.9 Hz, 2H), 4.07 (s, 3H), 3.01-3.05 (m, 1H), 2.69-2.71 (m, 1H), 2.47-2.49 (m, 1H), 2.29-2.37 (m, 1H), 1.98-2.09 (m, 1H). ^{13}C NMR (100 MHz, acetone-d_6) δ 137.9, 124.8, 123.6, 49.6, 47.9, 46.5, 36.7, 33.7. ^{19}F NMR (376 MHz, acetone-d_6) δ -152.2, -152.3. IR (neat) cm^{-1} 3165, 2935, 1635, 1576, 1463, 1430, 1290, 1168, 1014, 952. HRMS m/z (ESI): calcd. for $C_8H_{13}N_2O$ [M]$^+$: 153.1028, found: 153.1025.

1-[2-(Oxiran-2-yl)ethyl]-3-methylimidazolium hexafluorophosphate (3g)

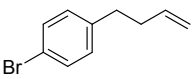


Procedure II. The title compound was prepared with compound **2g** (100 mg, 0.354 mmol, 1.00 equiv) in acetone (1.00 mL) and freshly prepared DMDO (0.06 mol/L) (8.27 mL, 0.496 mmol, 1.4 equiv). The reaction mixture was stirred at room temperature for 6 h. The product **3g** was obtained as a yellow oil (85 mg, 80 %).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.06 (s, 1H), 7.73-7.81 (m, 2H), 4.56 (t, *J* = 6.9 Hz, 2H), 4.08 (s, 3H), 3.00-3.05 (m, 1H), 2.70-2.72 (m, 1H), 2.47-2.49 (m, 1H), 2.31-2.39 (m, 1H), 1.96-2.10 (m, 1H). ^{13}C NMR (100 MHz, acetone-d_6) δ 137.7, 124.9, 123.7, 49.6, 47.9, 46.5, 36.7, 33.7. ^{19}F NMR (376 MHz, acetone-d_6) δ -71.6, -73.5. IR (neat) cm^{-1} 3171, 3125, 2971, 1576, 1464, 1429, 1168, 1024, 817, 749. HRMS m/z (ESI): calcd. for $C_8H_{13}N_2O$ [M]$^+$: 153.1028, found: 153.1029.

V. Preparation of the polyfunctional epoxidized salts

1-Bromo-4-(3-buten-1-yl)benzene (4a)

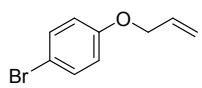


Under inert atmosphere, allylmagnesium bromide 1.0 M in diethyl ether (16 mL, 16.00 mmol, 2 equiv) was added dropwise to a solution of 4-bromobenzyl bromide (2.0 g, 8.0 mmol, 1.0 equiv) in dry THF (38 mL) cooled at 0 °C. The reaction was stirred for 2 h at 0 °C. A saturated aqueous NH_4Cl (60 mL) was added and the aqueous layer was extracted 3 times with CH_2Cl_2. The combined organic layers were dried over $MgSO_4$ and concentrated under reduced pressure. The product **4a** was obtained as clear yellow oil (1.64 g, 97 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, *J* = 8.3 Hz, 2H), 7.06 (d, *J* = 8.3 Hz, 2H), 5.80 (ddt, *J* = 17.2, 10.3, 6.6 Hz, 1H), 4.95-5.06 (m, 2H), 2.66 (t, *J* = 7.3 Hz, 2H), 2.35 (q, *J* = 7.3 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.9, 137.7, 131.5, 130.4, 119.7, 115.4, 35.4, 34.9. IR (neat) cm^{-1} 3078, 2929, 2857, 1641, 1488, 1403, 1072, 1011, 911, 801. HRMS m/z (ASAP): calcd. for $C_{10}H_{11}Br$ [M]$^+$: 210.0044, found: 210.0042.

Procedure for the synthesis of 4b-c. To a solution of 4-bromophenol (1.0 equiv) and K_2CO_3 (2.5 equiv) in CH_3CN was added alkylating agent (2.0 equiv), and the mixture was refluxed (80 °C). The reaction mixture was then cooled to 22 °C and the solvent was removed under reduced pressure. The residue was partitioned between CH_2Cl_2 and water and the aqueous layer was extracted with CH_2Cl_2. The combined organic extracts were washed with water, dried with $MgSO_4$ and concentrated *in vacuo*.

1-Bromo-4-(2-propen-1-yloxy)benzene (4b)[8]

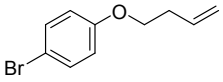


The title compound was prepared with 4-bromophenol (2.0 g, 11.56 mmol, 1.0 equiv)**,** K_2CO_3 (3.994 g, 28.90 mmol, 2.5 equiv) and allyl bromide (2 mL, 23.12 mmol, 2.0 equiv) in CH_3CN (30 mL). The mixture was refluxed (80 °C) for 72 h. The product **4b** was obtained as a yellow oil (2.31 g, 94 %).

[8] W. Kurosawa, H. Kobayashi, T. Kan and T. Fukuyama, *Tetrahedron*, 2004, **60**, 9615-9628.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 9.0 Hz, 2H), 6.80 (d, *J* = 9.0 Hz, 2H), 6.03 (ddt, *J* = 17.3, 10.4, 5.3 Hz, 1H), 5.40 (dd, *J* = 17.3, 1.4 Hz, 1H), 5.30 (dd, *J* = 10.4, 1.4 Hz, 1H), 4.51 (d, *J* = 5.2 Hz, 2H,). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.8, 133.0, 132.4, 118.0, 116.7, 113.1, 69.1. IR (neat) cm^{-1} 3084, 2918, 1590, 1486, 1284, 1238, 1226, 1171, 996, 818. HRMS m/z (ASAP): calcd. for C_9H_9BrO $[M]^+$: 211.9837, found: 211.9831.

1-Bromo-4-(3-buten-1-yloxy)benzene (4c)

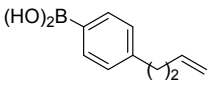


The title compound was prepared with 4-bromophenol (5.00 g, 28.90 mmol, 1.0 equiv)**,** K_2CO_3 (9.99 g, 72.25 mmol, 2.5 equiv) and 4-bromo-but-1-ene (15.60 g, 11.64 mL, 57.80 mmol, 2.0 equiv) in CH_3CN (140 mL). The mixture was stirred and refluxed for 72 h. The product **4c** was obtained as a yellow oil (6.28 g, 96 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 9.0 Hz, 2H), 6.78 (d, *J* = 9.0 Hz, 2H), 5.90 (ddt, *J* = 17.1, 10.3, 6.7 Hz, 1H), 5.11-5.20 (m, 2H), 3.98 (t, *J* = 6.7 Hz, 2H), 2.54 (q, *J* = 6.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.1, 134.3, 132.4, 117.3, 116.5, 112.9, 67.6, 33.7. IR (neat) cm^{-1} 3078, 2926, 1591, 1488, 1470, 1285, 1239, 1171, 1033, 1002. HRMS m/z (ASAP): calcd. for $C_{10}H_{11}BrO$ $[M]^+$: 225.9993, found: 225.9992.

Procedure for the synthesis of 5a-c. In a dry round-bottom flask purged with N_2, compound **4a**, **4b** or **4c** (1.0 equiv) was dissolved in dry THF and cooled to -78 °C. n-BuLi (1.2 equiv) was added dropwise and the reaction mixture was stirred for 1h. Triisopropyl borate (1.5 equiv) was added dropwise and the reaction mixture was allowed to slowly warm up to room temperature overnight. Water was slowly added followed by acidification with 1 M HCl and the reaction mixture was stirred for 1 h. The reaction mixture was extracted with diethyl ether and the combined organic layers were dried over $MgSO_4$. Evaporation of volatile compounds under reduced pressure afforded product **5a, 5b** or **5c**.

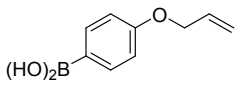
4-(3-Buten-1-yl)phenyl boronic acid (5a)



The title compound was prepared with compound **4a** (1.56 g, 7.39 mmol, 1.0 equiv), n-BuLi (3.55 mL, 8.87 mmol, 1.2 equiv) and triisopropyl borate (2.56 mL, 11.09 mmol, 1.5 equiv) in THF (13 mL). Water (5 mL) and 1 M HCl (12.65 mL) was added after reaction. The product **5a** was obtained as a white solid (1.26 g, 97 %) and used without purification.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 8.3 Hz, 2H), 7.33 (d, *J* = 8.3 Hz, 2H), 5.99 (ddt, *J* = 17.1, 10.1, 6.7 Hz, 1H), 5.11-4.98 (m, 2H), 2.81 (t, *J* = 7.3 Hz, 2H), 2.44 (q, *J* = 7.3 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.0, 138.0, 135.9, 133.7, 128.3, 115.3, 35.9, 35.4. IR (neat) cm^{-1} 3078, 2926, 2857, 1609, 1407, 1337, 1305, 1181, 1020, 910. Mp: 69.5 °C. HRMS m/z (ESI): calcd. for $C_{10}H_{12}BO_2$ $[M-H]^-$: 175.0930, found: 175.0928.

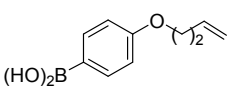
4-(2-Propen-1-yloxy)phenyl boronic acid (5b)



The title compound was prepared with compound **4b** (2.22 g, 10.41 mmol, 1.0 equiv), n-BuLi (5 mL, 12.49 mmol, 1.2 equiv) and triisopropyl borate (3.61 mL, 15.61 mmol, 1.5 equiv) in THF (15 mL). Water (5.3 mL) and 1 M HCl (15.76 mL) was added after reaction. The crude was purified by flash chromatography on silica gel with cyclohexane/ethyl acetate (7/3). The product **5b** was obtained as a white solid (1.13 g, 61 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 9.0 Hz, 2H), 7.03 (d, *J* = 9.0 Hz, 2H), 6.10 (ddt, *J* = 17.1, 10.6, 5.3 Hz, 1H), 5.50 (dd, *J* = 17.1, 1.2 Hz, 1H), 5.33 (dd, *J* = 10.6, 1.2 Hz, 1H), 4.64 (d, *J* = 5.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.4, 137.6, 135.4, 133.1, 118.1, 114.4, 68.8. IR (neat) cm^{-1} 2860, 1601, 1414, 1350, 1305, 1244, 1171, 1009, 832, 745. Mp: 105.8 °C. HRMS m/z (ESI): calcd. for $C_9H_{10}BO_3$ $[M-H]^-$: 177.0723, found: 177.0721.

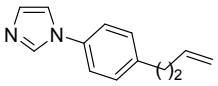
4-(3-Buten-1-yloxy)phenyl boronic acid (5c)



The title compound was prepared with compound **4c** (5.87 g, 25.86 mmol, 1.0 equiv), n-BuLi 2.5 M in hexane (12.41 mL, 31.03 mmol, 1.2 equiv) and triisopropyl borate (7.83 mL, 38.79 mmol, 1.5 equiv) in THF (39 mL). Water (13 mL) and 1 M HCl (39 mL) was added after reaction. The crude was purified by flash chromatography on silica gel with cyclohexane/ethyl acetate (6/ 4). The product **5c** was obtained as a white solid (3.08 g, 62 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 9.0 Hz, 2H), 7.01 (d, *J* = 9.0 Hz, 2H), 5.86-6.00 (m, 1H), 5.12-5.23 (m, 2H), 4.11 (t, *J* = 6.7 Hz, 2H), 2.59 (q, *J* = 6.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.7, 137.6, 135.4, 134.5, 117.3, 114.2, 67.2, 33.8. IR (neat) cm^{-1} 1603, 1353, 1245, 1172, 1028, 919, 835, 746, 688, 570. Mp: 118.5 °C. HRMS m/z (ESI): calcd. for $C_{10}H_{12}BO_3$ [M-H]$^-$: 191.0879, found: 191.0876.

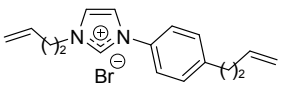
1-[4-(3-Buten-1-yl)phenyl]-1*H*-Imidazole (6)



Boronic acid **5a** (1.19 g, 6.76 mmol, 1.0 equiv), imidazole (552 mg, 8.11 mmol, 1.2 equiv) and copper iodide (51.50 mg, 0.270 mmol, 0.04 equiv) were mixed in methanol (36 mL). The mixture solution was refluxing 5 h with pumping air continuously. Then, the solvent was evaporated under reduced pressure and diethyl ether was added. The organic phase was filtered through celite and concentrated under reduced pressure. The crude was purified by flash chromatography on silica gel with 100 % ethyl acetate. The product **6** was obtained as a clear yellow oil (1.05 g, 78 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (s, 1H), 7.14-7.29 (m, 6H), 5.81 (ddt, *J* = 17.0, 10.4, 6.6 Hz, 1H), 4.94-5.06 (m, 2H), 2.69-2.76 (t, *J* = 7.3 Hz, 2H), 2.32-2.40 (q, *J* = 7.3 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.6, 137.6, 135.8, 135.5, 130.4, 130.0, 121.7, 118.5, 115.6, 35.4, 34.9. IR (neat) cm^{-1} 3116, 2925, 1640, 1521, 1488, 1303, 1245, 1056, 904, 810. HRMS m/z (ESI): calcd. for $C_{13}H_{15}N_2$ [M+H]$^+$: 199.1235, found: 199.1237.

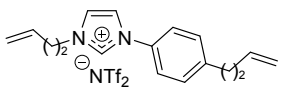
1-[4-(3-Buten-1-yl)phenyl]-3-(3-buten-1-yl)imidazolium bromide (7a)



The title compound was prepared according to the general procedure for *N*-alkylation (II) with a solution of compound **6** (1.05 g, 5.27 mmol, 1.0 equiv) in CH_3CN (35 mL) and 4-bromobutene (1.06 mL, 10.54 mmol, 2.0 equiv). The mixture was refluxed at 80 °C for 48 h. The product **7a** was obtained as a yellow oil (1.75 g, 100 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.94 (s, 1H), 7.63-7.72 (m, 4H), 7.34 (d, *J* = 8.3 Hz, 2H), 5.72-5.94 (m, 2H), 4.95-5.12 (m, 4H), 4.71 (t, *J* = 6.7 Hz, 2H), 2.73-2.77 (m, 4H), 2.35 (q, *J* = 7.3 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.7, 137.1, 136.1, 132.7, 132.5, 130.7, 123.2, 121.8, 120.4, 119.7, 115.8, 49.6, 35.1, 34.9, 34.7. IR (neat) cm^{-1} 3049, 2855, 1640, 1566, 1550, 1515, 1438, 1198, 1071, 914. HRMS m/z (ESI): calcd. for $C_{17}H_{21}N_2$ [M]$^+$: 253.1705, found: 253.1704.

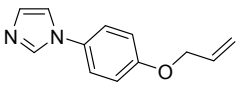
1-[4-(3-Buten-1-yl)phenyl]-3-(3-buten-1-yl)imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl) sulfonyl] methanesulfonamide (7b)



The title compound was prepared according to the general procedure for anion metathesis (III) with a solution of compound **7a** (3.21 g, 9.64 mmol, 1.0 equiv) in H_2O (80 mL) and lithium bis(trifluoromethanesulfonyl)imide (3.04 g, 10.60 mmol, 1.1 equiv). The solution was stirred at room temperature for 24 h and then extracted with CH_2Cl_2. The organic layer was washed three times with water. The product was dried over $MgSO_4$ and concentrated under reduced pressure. The product **7b** was obtained as a yellow oil (4.73 g, 92 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.09 (s, 1H), 7.36-7.60 (m, 6H), 5.74-5.88 (m, 2H), 4.97-5.20 (m, 4H), 4.43 (t, *J* = 6.7 Hz, 2H), 2.79 (t, *J* = 7.3 Hz, 2H), 2.68 (q, *J* = 6.7 Hz, 2H), 2.39 (q, *J* = 7.3 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.3, 137.1, 134.5, 132.3, 132.2, 130.8, 123.3, 122.2, 121.6, 120.1, 120.0 (q, J_{CF}=322.4 Hz), 115.9, 49.9, 35.1, 35.0, 34.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ -78.9. IR (neat) cm^{-1} 3145, 2931, 1553, 1348, 1329, 1179, 1133, 1053, 918, 838. HRMS m/z (ESI): calcd. for $C_{17}H_{21}N_2$ [M]$^+$: 253.1705, found: 253.1704.

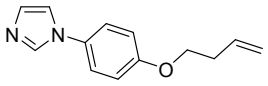
1-[4-(2-Propen-1-yloxy)phenyl]-1*H*-Imidazole (8)



Boronic acid **5b** (1.13 g, 6.35 mmol, 1.0 equiv), imidazole (519 mg, 7.62 mmol, 1.2 equiv) and copper iodide (48.36 mg, 0.254 mmol, 0.04 equiv) were mixed in methanol (35 mL). The mixture solution was refluxing 5 h with pumping air continuously. Then, the solvent was evaporated under reduced pressure and diethyl ether was added. The organic phase was filtered through celite and concentrated *in vacuo*. The crude was purified by flash chromatography on silica gel with 100 % ethyl acetate. The product **8** was obtained as a yellow oil (627 mg, 49 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (s, 1H), 7.29 (d, *J* = 9.0 Hz, 2H), 7.18-7.20 (m, 2H), 7.00 (d, *J* = 9.0 Hz, 2H), 6.06 (ddt, *J* = 17.3, 10.6, 5.2 Hz, 1H), 5.43 (dd, *J* = 17.3, 1.3 Hz 1H), 5.32 (dd, *J* = 10.6, 1.3 Hz, 1H), 4.56 (d, *J* = 5.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.1, 136.0, 132.9, 131.0, 130.2, 123.3, 118.9, 118.2, 115.9, 69.3. IR (neat) cm^{-1} 3115, 2866, 1516, 1300, 1239, 1178, 1056, 1018, 995, 827. HRMS m/z (ESI): calcd. for $C_{12}H_{13}N_2O$ $[M+H]^+$: 201.1028, found: 201.1032.

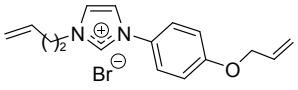
1-[4-(3-buten-1-yloxy)phenyl]-1*H*-Imidazole (9)



Boronic acid **5c** (1.26 g, 6.57 mmol, 1.0 equiv), imidazole (537 mg, 7.89 mmol, 1.2 equiv) and copper iodide (50 mg, 0.26 mmol, 0.04 equiv) were solubilized in methanol (40 mL). The mixture solution was refluxing 5 h at 60 °C with pumping air continuously. Then, the solvent was evaporated under reduced pressure and diethyl ether was added. The organic phase was filtered through celite and concentrated *in vacuo*. The crude was purified by flash chromatography on silica gel with 100 % ethyl acetate. The product **9** was obtained as a pale yellow solid (868 mg, 62 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (s, 1H), 7.29 (d, *J* = 9.0 Hz, 2H), 7.18-7.20 (m, 2H), 6.98 (d, *J* = 9.0 Hz, 2H), 5.91 (ddt, *J* = 17.1, 10.2, 6.8 Hz, 1H), 5.12-5.21 (m, 2H), 4.05 (t, *J* = 6.7 Hz, 2H), 2.57 (q, *J* = 6.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.4, 136.0, 134.3, 130.9, 130.2, 123.3, 118.9, 117.4, 115.7, 67.8, 33.7. IR (neat) cm^{-1} 3100, 2925, 1517, 1302, 1260, 1242, 1177, 1058, 913, 832. Mp: 50.8 °C. HRMS m/z (ESI): calcd. for $C_{13}H_{15}N_2O$ $[M+H]^+$: 215.1184, found: 215.1190.

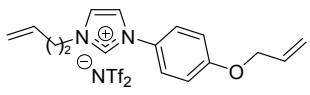
3-(But-3-en-1-yl)-1-[4-(2-propen-1-yloxy)phenyl]imidazolium bromide (10a)



The title compound was prepared according to the general procedure for *N*-alkylation (II) with a solution of compound **8** (598 mg, 2.98 mmol, 1.0 equiv) in CH_3CN (20 mL) and 4-bromobutene (0.60 mL, 5.97 mmol, 2.0 equiv). The mixture was refluxed at 80 °C for 48 h. The product **10a** was obtained as a yellow oil (987 mg, 99 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.87 (s, 1H), 7.58-7.69 (m, 4H), 7.03 (d, *J* = 9.0 Hz, 2H), 6.01 (ddt, *J* = 17.2, 10.6, 5.3 Hz, 1H), 5.88 (ddt, *J* = 17.3, 9.9, 7.0 Hz, 1H), 5.41 (dd, *J* = 17.2, 1.2 Hz, 1H), 5.31 (dd, *J* = 10.6, 1.2 Hz, 1H), 5.06-5.12 (m, 2H), 4.69 (t, *J* = 6.7 Hz, 2H), 4.56 (d, *J* = 5.2 Hz, 2H), 2.74 (q, *J* = 6.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 136.1, 132.7, 132.4, 127.6, 123.4, 122.9, 120.6, 119.7, 118.5, 116.5, 69.4, 49.6, 34.6. IR (neat) cm^{-1} 3062, 1552, 1510, 1417, 1251, 1185, 1073, 994, 924, 831. HRMS m/z (ESI): calcd. for $C_{16}H_{19}N_2O$ $[M]^+$: 255.1497, found: 255.1496.

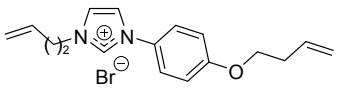
3-(3-Buten-1-yl)-1-[4-(2-propen-1-yloxy)phenyl]imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (10b)



The title compound was prepared according to the general procedure for anion metathesis (III) with a solution of compound **10a** (935 mg, 2.79 mmol, 1.0 equiv) in H_2O (40 mL) and lithium bis(trifluoromethanesulfonyl)imide (881 mg, 3.07 mmol, 1.1 equiv). The solution was stirred at room temperature for 24 h and then extracted with dichloromethane. The organic layer was washed three times with water. The product is dried with $MgSO_4$ and then concentrated *in vacuo*. The product was obtained (1.24 g, 83 %) as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.02 (s, 1H), 7.44-7.53 (m, 4H), 7.06 (d, *J* = 9.0 Hz, 2H), 6.04 (ddt, *J* = 17.1, 10.5, 5.2 Hz, 1H), 5.79 (ddt, *J* = 17.1, 10.2, 6.9 Hz, 1H), 5.43 (dd, *J* = 17.1, 1.1 Hz, 1H), 5.33 (dd, *J* = 10.5, 1.1 Hz 1H), 5.07-5.18 (m, 2H), 4.59 (d, *J* = 5.2 Hz, 2H), 4.40 (t, *J* = 6.7 Hz, 2H), 2.67 (q, *J* = 6.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.3, 134.4, 132.3, 132.2, 127.4, 123.9, 123.1, 121.9, 120.1, 120.0 (q, J_{CF} = 322.4 Hz), 118.6, 116.6, 69.4, 49.9, 34.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ -78.9. IR (neat) cm^{-1} 3147, 2925, 1554, 1512, 1348, 1178, 1133, 1052, 929, 831. HRMS m/z (ESI): calcd. for $C_{16}H_{19}N_2O$ $[M]^+$: 255.1497, found: 255.1499.

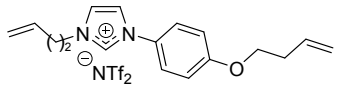
3-(3-Buten-1-yl)-1-[4-(3-buten-1-yloxy)phenyl]imidazolium bromide (11a)



The title compound was prepared according to the general procedure for *N*-alkylation (II) with a solution of compound **9** (4.78 g, 22.32 mmol, 1.0 equiv) in CH_3CN (100 mL) and 4-bromo-but-1-ene (6.03 g, 4.5 mL, 44.63 mmol, 2.0 equiv). The mixture was refluxed at 80 °C for 48 h. It was then cooled to 22 °C and the solvent was removed *in vacuo*. The product (7.64 g, 98 %) was obtained as a yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.79 (s, 1H), 7.63-7.69 (m, 4H), 7.00 (d, *J* = 9.0 Hz, 2H), 5.81-5.91 (m, 2H), 5.06-5.18 (m, 4H), 4.67 (t, *J* = 6.7 Hz, 2H), 4.01 (t, *J* = 6.7 Hz, 2H), 2.73 (q, *J* = 6.7 Hz, 2H), 2.53 (q, *J* = 6.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.2, 135.9, 134.0, 132.7, 127.5, 123.4, 123.1, 120.7, 119.7, 117.6, 116.2, 67.9, 49.6, 34.6, 33.5. IR (neat) cm^{-1} 3072, 2980, 1552, 1512, 1250, 1185, 1073, 995, 918, 832. HRMS m/z (ESI): calcd. for $C_{17}H_{21}N_2O$ $[M]^+$: 269.1654, found: 269.1653.

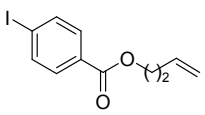
3-(3-Buten-1-yl)-1-[4-(3-buten-1-yloxy)phenyl]imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl) sulfonyl]methanesulfonamide (11b)



The title compound was prepared according to the general procedure for anion metathesis (III) with a solution of compound **11a** (7.64 g, 21.89 mmol, 1.0 equiv) in H_2O (350 mL) was added lithium bis(trifluoromethanesulfonyl)imide (6.91 g, 24.08 mmol, 1.1 equiv). The solution was stirred at room temperature for 24 h and then extracted with dichloromethane. The organic layer was washed several times with water. The product is dried with $MgSO_4$ and then concentrated under reduced pressure. The product **11b** was obtained as a yellow oil (11.0 g, 91 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.97 (s, 1H), 7.44-7.52 (m, 4H), 7.04 (d, *J* = 9.0 Hz, 2H), 5.74-5.94 (m, 2H), 5.08-5.21 (m, 4H), 4.39 (t, *J* = 6.7 Hz, 2H), 4.06 (t, *J* = 6.7 Hz, 2H), 2.67 (q, *J* = 6.7 Hz, 2H), 2.57 (q, *J* = 6.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 134.3, 134.0, 132.2, 127.3, 123.8, 123.1, 121.9, 120.1, 120.0 (q, J_{CF} = 322.4 Hz), 117.6, 116.3, 68.0, 49.9, 34.3, 33.5. ^{19}F NMR (376 MHz, $CDCl_3$) δ -78.9. IR (neat) cm^{-1} 3146, 2930, 1554, 1513, 1348, 1178, 1133, 1052, 925, 832. HRMS m/z (ESI): calcd. for $C_{17}H_{21}N_2O$ $[M]^+$: 269.1654, found: 269.1656.

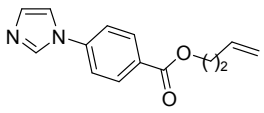
3-Butenyl 4-iodobenzoate (12)



To a sealed tube under argon was placed iron (III) acetylacetonate (337 mg, 0.954 mmol, 0.1 equiv), Na_2CO_3 (101 mg, 0.954 mmol, 0.1 equiv), methyl 4-iodobenzoate (2.50 g, 9.54 mmol, 1.0 equiv) and molecular sieves 4 Å in heptane (60 mL). 3-buten-1-ol (2.43 mL, 28.62 mmol, 3 equiv) was added and the reaction mixture was stirred at 80 °C for 72 h. The crude was filtered on celite, washed with ethyl acetate and concentrated under reduced pressure. The product was purified by flash chromatography on silica gel with cyclohexane/ethyl acetate (9/1). The product **12** was obtained as a clear yellow oil (2.47 g, 86 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72-7.82 (m, 4H), 5.85 (ddt, *J* = 17.1, 10.3, 6.8 Hz, 1H), 5.08-5.21 (m, 2H), 4.36 (t, *J* = 6.7 Hz, 2H), 2.52 (q, *J* = 6.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.2, 137.9, 134.0, 131.2, 130.0, 117.6, 100.8, 64.3, 33.3. IR (neat) cm^{-1} 3079, 2957, 1717, 1586, 1393, 1263, 1176, 1100, 1007, 916. HRMS m/z (ASAP): calcd. for $C_{11}H_{12}IO_2$ $[M+H]^+$: 302.9882, found: 302.9885.

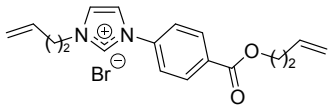
1-[4-(3-Buten-1-yloxy)carbonyl]phenyl-1*H*-imidazole (13)



A sealed tube with a magnetic stirring bar was charged with CuI (61.90 mg, 0.325 mmol, 0.2 equiv), K_3PO_4 (690 mg, 3.25 mmol, 2.0 equiv), imidazole (132.756 mg, 1.95 mmol, 1.2 equiv), compound **12** (491 mg, 1.625 mmol, 1.0 equiv) and *N,N'*-dimethylethylenediamine (0.041 mL, 0.325 mmol, 0.2 equiv) in DMF (3 mL) under argon. The reaction was stirred at 40 °C for 40 h then diluted with 2-3 mL of ethyl acetate, filtered through a plug of silica gel, and washed with 10-20 mL of ethyl acetate. The filtrate was concentrated under reduced pressure. The crude was purified by flash chromatography on silica gel with 100 % ethyl acetate. The product **13** was obtained as a pale green solid (394 mg, 100 %).

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.46 (br, 1H), 8.06 (d, *J* = 8.7 Hz, 2H), 7.91 (br, 1H), 7,85 (d, *J* = 8.7 Hz, 2H), 7.20 (br, 1H), 5.89 (ddt, *J* = 17.1, 10.3, 6.6 Hz, 1H), 5.18 (dd, *J* = 17.1, 1.8 Hz, 1H), 5.10 (dd, *J* = 10.3, 1.8 Hz, 1H), 4.35 (t, *J* = 6.6 Hz, 2H), 2.40-2.50 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.4, 140.9, 136.3, 135.1, 131.4, 130.9, 128.2, 120.4, 118.5, 117.8, 64.2, 33.2. IR (neat) cm^{-1} 3122, 2978, 1708, 1609, 1525, 1263, 1192, 1125, 1062, 925. Mp: 46.8 °C. HRMS m/z (ESI): calcd. for $C_{14}H_{15}N_2O_2$ $[M+H]^+$: 243.1134, found: 243.1137.

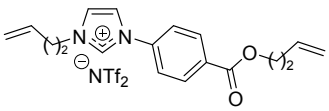
3-(3-Buten-1-yl)-1-{4-[(3-buten-1-yloxy)carbonyl]phenyl}imidazolium bromide (14a)



The title compound was prepared according to the general procedure for *N*-alkylation (II) with compound **13** (674.3 mg, 2.78 mmol, 1.0 equiv) in CH_3CN (30 ml) and 4-bromo-but-1-ene (0.56 ml, 5.57 mmol, 2.0 equiv). The mixture was refluxed for 72 h. It was cooled to 22 °C and the solvent was removed under reduced pressure. The product **14a** was obtained as a yellow oil (1.05 g, 100 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 11.37 (s, 1H), 8.24 (d, *J* = 8.7 Hz, 2H), 7.94 (d, *J* = 8.7 Hz, 2H), 7.70-7.73 (m, 1H), 7.55-7.58 (m, 1H), 5.79-5.96 (m, 2H), 5.09-5.22 (m, 4H), 4.72 (t, *J* = 6.7 Hz, 2H), 4.40 (t, *J* = 6.7 Hz, 2H), 2.78 (q, *J* = 6.7 Hz, 2H), 2.53 (q, *J* = 6.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.9, 137.5, 137.1, 133.8, 132.5, 132.3, 132.2, 123.2, 121.8, 120.1, 120.0, 117.9, 64.8, 50.0, 34.6, 33.2. IR (neat) cm^{-1} 3063, 2980, 1715, 1609, 1549, 1279, 1222, 1112, 1070, 919. HRMS m/z (ESI): calcd. for $C_{18}H_{21}N_2O_2$ $[M]^+$: 297.1603, found: 297.1605.

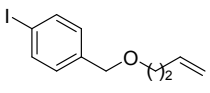
3-(3-Buten-1-yl)-1-{4-[(3-buten-1-yloxy)carbonyl]phenyl}imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (14b)



The title compound was prepared according to the general procedure for anion metathesis (III) with a solution of compound **14a** (1.04 g, 2.766 mmol, 1.0 equiv) in H_2O (50 mL) and lithium bis(trifluoromethanesulfonyl)imide (874 mg, 3.043 mmol, 1.1 equiv). The solution was stirred at room temperature for 24 h and then extracted with dichloromethane. The organic layer was washed three times with water. The product is dried over $MgSO_4$ and then concentrated under reduced pressure. The product **14b** was obtained as a yellow oil (1.23 g, 77 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.24 (d, *J* = 8.7 Hz, 2H), 7.64-7.71 (m, 3H), 7.54-7.58 (m, 1H), 5.74-5.92 (m, 2H), 5.08-5.22 (m, 4H), 4.38-4.47 (m, 4H), 2.51-2.73 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.9, 137.5, 134.7, 133.8, 132.7, 132.1, 132.0, 123.8, 122.2, 121.5, 120.3, 120.0 (q, J_{CF} = 322.4 Hz), 117.8, 64.9, 50.1, 34.2, 33.2. ^{19}F NMR (376 MHz, $CDCl_3$) δ -78.9. IR (neat) cm^{-1} 3144, 2984, 1717, 1552, 1348, 1281, 1179, 1133, 1053, 924. HRMS m/z (ESI): calcd. for $C_{18}H_{21}N_2O_2$ $[M]^+$: 297.1603, found: 297.1605.

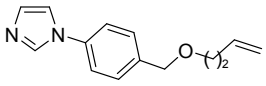
1-[(3-Buten-1-yloxy)methyl]-4-iodobenzene (15)



To a solution of 4-iodobenzylalcohol (1.00 g, 4.27 mmol, 1.0 equiv) in CH_2Cl_2 (20 mL) was added triethylamine (0.89 mL, 6.41 mmol, 1.5 equiv) at room temperature. Then, methanesulfonyl chloride (0.36 mL, 4.70 mmol, 1.1 equiv) was added at -10 °C. After 1.5 h at -10 °C, the reaction was quenched with water (13 mL) and the organic layer was successively washed with a 1 M HCl solution (11 mL), a saturated bicarbonate solution (11 mL) and brine (11 mL). After drying over $MgSO_4$, filtration and evaporation under reduced pressure, 4-iodobenzyl mesylate was obtained (981 mg, 74 %). But-3-ene-1-ol (0.26 mL, 3.02 mmol, 1.0 equiv) was added dropwise to a stirred suspension of NaH (181 mg, 4.53 mmol, 1.5 equiv) in dry THF (15 mL) at 0 °C. The mixture was stirred at 22 °C for 30 min. A solution of 4-iodobenzyl mesylate (942 mg, 3.02 mmol, 1.0 equiv) in THF (6 mL) was added dropwise to the mixture at 0 °C. After 30 min, the mixture was heated under reflux (60 °C) for 12 h. After cooling, water was slowly added at 0 °C. The mixture was concentrated under reduced pressure and extracted with dichloromethane (2 x 20 mL). The combined organic extracts were washed with water (2 x 20 mL), dried over anhydrous $MgSO_4$, and concentrated under reduced pressure. The product **15** was obtained as a yellow oil (736 mg, 85 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.2 Hz, 2H), 7.09 (d, *J* = 8.2 Hz, 2H), 5.83 (ddt, *J* = 17.1, 10.4, 6.7 Hz, 1H), 4.98-5.16 (m, 2H), 4.46 (s, 2H), 3.51 (t, *J* = 6.7 Hz, 2H), 2.37 (q, *J* = 6.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.3, 137.6, 135.3, 129.6, 116.6, 93.1, 72.3, 69.9, 34.3. IR (neat) cm^{-1} 3386, 3077, 2924, 1706, 1586, 1484, 1393, 1270, 1103, 1008. HRMS m/z (ASAP): calcd. for $C_{11}H_{14}IO$ $[M+H]^+$: 289.0089, found: 289.0089.

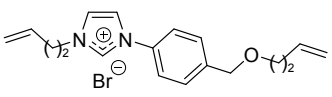
1-[(3-Buten-1-oxy)methyl]phenyl-1*H*-imidazole (16)



A sealed tube was charged with CuI (86 mg, 0.45 mmol, 0.2 equiv), K_3PO_4 (947 mg, 4.46 mmol, 2.0 equiv), imidazole (212 mg, 3.12 mmol, 1.4 equiv), compound **15** (642 mg, 2.23 mmol, 1.0 equiv) and N,N'-dimethylethylenediamine (0.05 mL, 0.45 mmol, 0.2 equiv) in DMF (4 mL) under argon. After 40 h at 40 °C, the reaction mixture was diluted with 2-3 mL of ethyl acetate, filtered through a plug of silica gel, and washed with 10-20 mL of ethyl acetate. The filtrate was concentrated under reduced pressure. The crude was purified by flash chromatography on silica gel with 100 % ethyl acetate. The product **16** was obtained as a clear yellow oil (509 mg, 100 %).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 (s, 1H), 7.46 (d, *J* = 8.2 Hz, 2H), 7.37 (d, *J* = 8.2 Hz, 2H), 7.26-7.29 (m, 1H), 7.20-7.23 (m, 1H), 5.85 (ddt, *J* = 17.1, 10.3, 6.7 Hz, 1H), 5.03-5.16 (m, 2H), 4.56 (s, 2H), 3.56 (t, *J* = 6.7 Hz, 2H), 2.40 (q, *J* = 6.7 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.3, 136.7, 135.6, 135.2, 130.2, 129.2, 121.6, 118.5, 116.7, 72.2, 70.0, 34.3. IR (neat) cm^{-1} 3392, 3118, 2860, 1716, 1611, 1524, 1488, 1304, 1100, 1058. HRMS m/z (ESI): calcd. for $C_{14}H_{17}N_2O$ $[M+H]^+$: 229.1341, found: 229.1344.

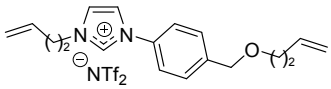
3-(3-Buten-1-yl)-1-{4-[(3-buten-1-yloxy)methyl]phenyl}imidazolium bromide (17a)



The title compound was prepared according to the general procedure for *N*-alkylation (II) with compound **16** (170 mg, 0.75 mmol, 1.0 equiv) in CH_3CN (5 ml) and 4-bromo-but-1-ene (0.16 ml, 1.50 mmol, 2.0 equiv). The mixture was refluxed for 72 h. It was cooled to 22 °C and the solvent was removed under reduced pressure. The product **17a** was obtained as a yellow oil (254 mg, 94 %).

^{1}H NMR (500 MHz, $CDCl_3$) δ 11.14 (s, 1H), 7.73 (d, *J* = 8.2 Hz, 2H), 7.49-7.58 (m, 4H), 5.79-5.96 (m, 2H), 5.03-5.16 (m, 4H), 4.73 (t, *J* = 6.7 Hz, 2H), 4.57 (s, 2H), 3.56 (t, *J* = 6.7 Hz, 2H), 2.76 (q, *J* = 6.7 Hz, 2H), 2.39 (q, *J* = 6.7 Hz, 2H).^{13}C NMR (126 MHz, $CDCl_3$) δ 141.6, 135.1, 133.6, 132.6, 129.5, 122.8, 121.9, 120.1, 119.9, 116.8, 71.8, 70.2, 49.8, 34.7, 34.3, 27.0. IR (neat) cm^{-1} 3423, 3075, 2862, 1718, 1640, 1567, 1552, 1200, 1099, 1073. HRMS m/z (ESI): calcd. for $C_{18}H_{23}N_2O$ $[M]^+$: 283.1810, found: 283.1809.

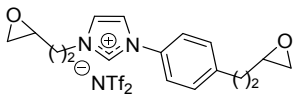
3-(3-Buten-1-yl)-1-{4-[(3-buten-1-yloxy)methyl]phenyl}imidazolium bromide (17b)



The title compound was prepared according to the general procedure for anion metathesis (III) with a solution of compound **17a** (197 mg, 0.54 mmol, 1.0 equiv) in H_2O (15 mL) and lithium bis(trifluoromethanesulfonyl)imide (171 mg, 0.60 mmol, 1.1 equiv). The solution was stirred at room temperature for 24 h and then extracted with CH_2Cl_2. The organic layer was washed three times with water. The product was dried over $MgSO_4$ and concentrated under reduced pressure. The product **17b** was obtained as a yellow oil (238 mg, 78 %).

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.10 (s, 1H), 7.50-7.60 (m, 6H), 5.75-5.90 (m, 2H), 5.04-5.19 (m, 4H), 4.59 (s, 2H), 4.42 (t, *J* = 6.7 Hz, 2H), 3.57 (t, *J* = 6.7 Hz, 2H), 2.68 (q, *J* = 6.7 Hz, 2H), 2.40 (q, *J* = 6.7 Hz, 2H).^{13}C NMR (126 MHz, $CDCl_3$) δ 142.1, 135.1, 134.5, 133.4, 132.1, 129.5, 123.4, 122.3, 121.6, 120.2, 120.0 (q, J_{CF} = 322.4 Hz), 116.8, 71.7, 70.3, 50.0, 34.3 (2C). ^{19}F NMR (471 MHz, $CDCl_3$) δ -78.9. IR (neat) cm^{-1} 3146, 2918, 1718, 1642, 1553, 1462, 1350, 1191, 1135, 1056. HRMS m/z (ESI): calcd. for $C_{18}H_{23}N_2O$ $[M]^+$: 283.1810, found: 283.1811.

3-[2-(Oxiran-2-yl)ethyl]-1-{4-[2-(oxiran-2-yl)ethyl]phenyl}imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (18)

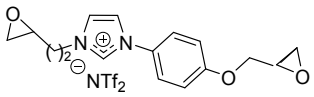


Procedure I. The title compound was prepared according to the general procedure for epoxidation (IV) with a solution of compound **7b** (1.35 g, 2.54 mmol, 1.0 equiv) in CH_3CN (32 mL) and mCPBA (2.27 g, 10.14 mmol, 4.0 equiv). The reaction mixture was stirred at 40 °C for 24 h. The product **18** was obtained as a yellow oil (1.27 g, 89 %).

Procedure II. The title compound was prepared according to the general procedure for epoxidation (IV) with a solution of compound **7b** (100 mg, 0.187 mmol, 1.00 eq.) in acetone (1.00 mL) and freshly prepared DMDO (0.046 mol/L) (11.41 mL, 0.525 mmol, 2.8 equiv). The reaction mixture was stirred at room temperature for 12h. The product **18** was obtained as a yellow oil (106 mg, 100 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.03 (s, 1H), 7.58-7.64 (m, 2H), 7.36-7.50 (m, 4H), 4.49 (t, *J* = 6.7 Hz, 2H), 3.00-3.08 (m, 1H), 2.71-2.96 (m, 5H), 2.37-2.53 (m, 3H), 1.72-1.96 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.6, 134.4, 132.5, 130.6, 123.8, 122.3, 121.7, 120.0 (q, J_{CF} = 322.4 Hz), 51.6, 49.3, 48.0, 47.2, 46.4, 33.9, 32.6, 31.9. ^{19}F NMR (376 MHz, $CDCl_3$) δ -78.9. IR (neat) cm^{-1} 3146, 2932, 1555, 1459, 1348, 1329, 1178, 1133, 1052, 915. HRMS m/z (ESI): calcd. for $C_{17}H_{21}N_2O_2$ $[M]^+$: 285.1603, found: 285.1602.

3-[2-(Oxiran-2-yl)ethyl]-1-{4-[(oxiran-2-yl)methoxy]phenyl}imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (19)

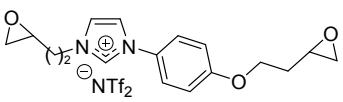


Procedure I. The title compound was prepared according to the general procedure for epoxidation (IV) with a solution of compound **10b** (100 mg, 0.1867 mmol, 1.0 equiv) in CH_3CN (4 mL) and mCPBA (167 mg, 0.7470 mmol, 4 equiv). The reaction mixture was stirred at 40 °C for 5 d. The product **19** was obtained as a yellow oil (69 mg, 65 %).

Procedure II. The title compound was prepared according to the general procedure for epoxidation (IV) with a solution of compound **10b** (200 mg, 0.37 mmol, 1.00 equiv) in acetone (1.00 mL) and freshly prepared DMDO (0.08 mol/L) (13.07 mL, 1.05 mmol, 2.8 equiv). The reaction mixture was stirred at room temperature for 12 h. The product **19** was obtained as a yellow oil (212 mg, 100 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.05 (s, 1H), 7.44-7.56 (m, 4H), 7.08 (d, *J* = 9.0 Hz, 2H), 4.52 (t, *J* = 6.7 Hz, 2H), 4.33-4.38 (m, 1H), 3.90-3.97 (m, 1H), 3.35-3.41 (m, 1H), 3.04-3.10 (m, 1H), 2.91-2.96 (m, 1H), 2.76-2.83 (m, 2H), 2.46-2.57 (m, 2H), 1.82-1.94 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.2, 134.8, 124.1, 124.0, 123.5, 121.9, 120.0 (q, J_{CF} = 322.4 Hz), 116.5, 69.5, 50.0, 49.4, 48.2, 46.6, 44.6, 32.6. ^{19}F NMR (376 MHz, $CDCl_3$) δ -78.9. IR (neat) cm^{-1} 3148, 2934, 1556, 1513, 1348, 1329, 1178, 1132, 1052, 915. HRMS m/z (ESI): calcd. for $C_{16}H_{19}N_2O_3$ $[M]^+$: 287.1396, found: 287.1398.

3-[2-(Oxiran-2-yl)ethyl]-1-{4-[(2-oxiran-2-yl)ethoxy]phenyl}imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (20)

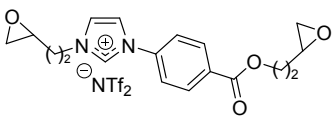


Procedure I. The title compound was prepared according to the general procedure for epoxidation (IV) with a solution of compound **11b** (3.51 g, 6.39 mmol, 1.0 equiv) in CH_3CN (80 mL) and mCPBA (5.73 g, 25.55 mmol, 4 equiv). The reaction mixture was stirred at 40 °C for 24 h. The product was obtained as yellow oil (3.32 g, 89 %).

Procedure II. The title compound was prepared according to the general procedure for epoxidation (IV) with a solution of compound **11b** (100 mg, 0.18 mmol, 1.0 equiv) in acetone (1.00 mL) and freshly prepared DMDO (0.087 mol/L) (5.86 mL, 0.510 mmol, 2.8 equiv). The reaction mixture was stirred at room temperature for 12 h. The product was obtained as a yellow oil (98 mg, 92 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.02 (s, 1H), 7.45-7.57 (m, 4H), 7.05 (d, *J* = 9.0 Hz, 2H), 4.50 (t, *J* = 6.7 Hz, 2H), 4.13-4.20 (m, 2H), 3.04-3.17 (m, 2H), 2.77-2.85 (m, 2H), 2.43-2.60 (m, 3H), 2.12-2.21 (m, 1H), 1.84-1.96 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.5, 134.6, 127.5, 124.0, 123.6, 122.0, 120.0 (q, J_{CF} = 322.4 Hz), 116.2, 65.5, 49.6, 49.4, 48.1, 47.2, 46.5, 32.6, 32.4. ^{19}F NMR (376 MHz, $CDCl_3$) δ -78.9. IR (neat) cm^{-1} 3147, 2933, 1556, 1514, 1348, 1330, 1178, 1132, 1052, 831. HRMS m/z (ESI): calcd. for $C_{17}H_{21}N_2O_3$ $[M]^+$: 301.1552, found: 301.1554.

3-[2-(Oxiran-2-yl)ethyl]-1-{4-[((2-oxiran-2-yl)ethoxy)carbonyl]phenyl}imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (21)

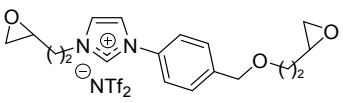


Procedure I. The title compound was prepared according to the general procedure for epoxidation (IV) with a solution of compound **14b** (1.13 g, 1.95 mmol, 1.0 equiv) in CH_3CN (30 mL) and mCPBA (2.19 g, 9.75 mmol, 5.0 equiv). The reaction mixture was stirred at 40 °C for 24 h. The product **21** was obtained as a yellow oil (1.05 g, 88 %).

Procedure II. The title compound was prepared according to the general procedure for epoxidation (IV) with a solution of compound **14b** (100 mg, 0.173 mmol, 1.0 equiv) in acetone (1.00 mL) and freshly prepared DMDO (0.08 mol/L) (6.06 mL, 0.4848 mmol, 2.8 equiv). The reaction mixture was stirred at room temperature for 5 h. The product **21** was obtained as a yellow oil (97 mg, 92 %).

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.33 (s, 1H), 8.27 (d, *J* = 8.7 Hz, 2H), 7.69 (d, *J* = 8.7 Hz, 2H), 7.63-7.65 (m, 1H), 7.59-7.61 (m, 1H), 4.50-4.62 (m, 4H), 3.07-3.14 (m, 2H), 2.81-2.86 (m, 2H), 2.55-2.60 (m, 3H), 2.11-2.20 (m, 1H), 1.85-1.97 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.8, 137.6, 135.5, 132.6, 132.2, 124.0, 122.4, 121.3, 120.0 (q, J_{CF} = 322.4 Hz), 63.0, 49.7, 49.5, 48.6, 47.0, 46.6, 32.5, 32.0. ^{19}F NMR (376 MHz, $CDCl_3$) δ -78.9. IR (neat) cm^{-1} 3145, 2965, 1717, 1553, 1348, 1281, 1179, 1132, 1052, 857. HRMS m/z (ESI): calcd. for $C_{18}H_{21}N_2O_4$ $[M]^+$: 329.1501, found: 329.1501.

3-[2-(Oxiran-2-yl)ethyl]-1-{4-[((2-oxiran-2-yl)ethoxy)methyl]phenyl}imidazolium 1,1,1-trifluoro-*N*-[(trifluoromethyl)sulfonyl]methanesulfonamide (22)



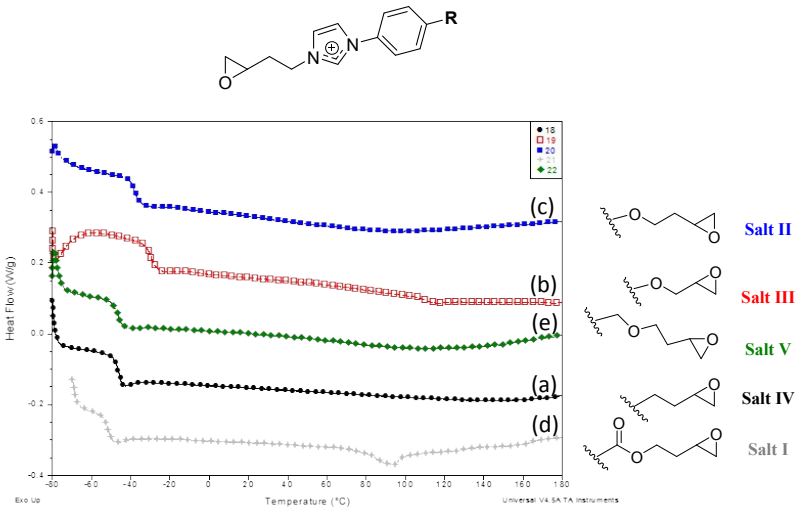
Procedure I. The title compound was prepared according to the general procedure for epoxidation (IV) with a solution of compound **17b** (501 mg, 0.89 mmol, 1.0 equiv) in CH_3CN (15 mL) and mCPBA (795 mg, 3.55 mmol, 4.0 equiv). The reaction mixture was stirred at 40 °C for 24 h. The product **22** was obtained as a yellow oil (404 mg, 76 %).

Procedure II. The title compound was prepared according to the general procedure for epoxidation (IV) with a solution of compound **17b** (100 mg, 0.177 mmol, 1.0 equiv) in acetone (1.00 mL) and freshly prepared DMDO (0.04 mol/L) (11.8 mL, 0.497 mmol, 2.8 equiv). The reaction mixture was stirred at room temperature for 12 h. The product **22** was obtained as a yellow oil (96 mg, 92 %).

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.17 (s, 1H), 7.52-7.59 (m, 6H), 4.61 (s, 2H), 4.56 (t, *J* = 6.7 Hz, 2H), 3.63-3.72 (m, 2H), 3.04-3.13 (m, 2H), 2.77-2.84 (m, 2H), 2.50-2.59 (m, 3H), 1.73-2.02 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.0, 135.0, 133.5, 129.5, 123.7, 122.4, 121.6, 120.0 (q, J_{CF} = 322.4 Hz), 71.9, 67.8, 50.1, 49.5, 48.3, 47.2, 46.6, 33.0, 32.6. ^{19}F NMR (376 MHz, $CDCl_3$) δ -78.9. IR (neat) cm^{-1} 3543, 3147, 2930, 1724, 1555, 1515, 1348, 1194, 1139, 1055. HRMS m/z (ESI): calcd. for $C_{18}H_{23}N_2O_3$ $[M]^+$: 315.1709, found: 315.1707.

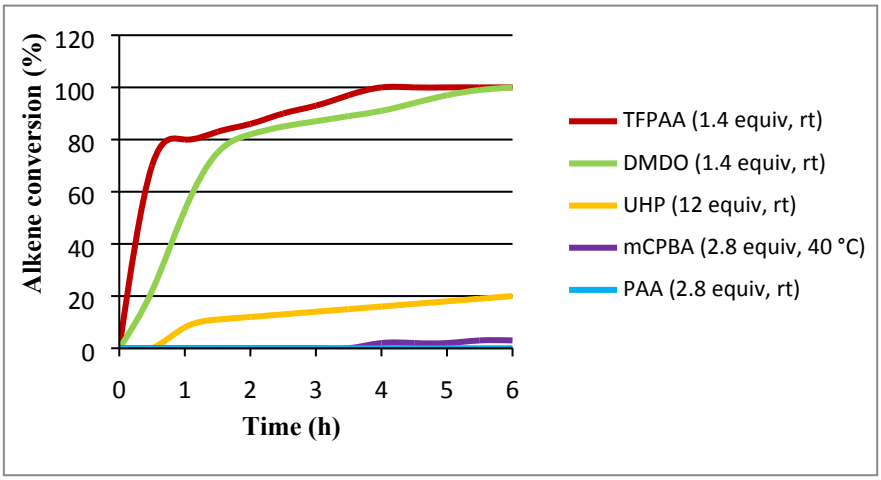
VI. DSC thermograms of epoxy monomers

Protocol: A rate of 10 K.min^{-1} under nitrogen flow of 50 mL.min^{-1}

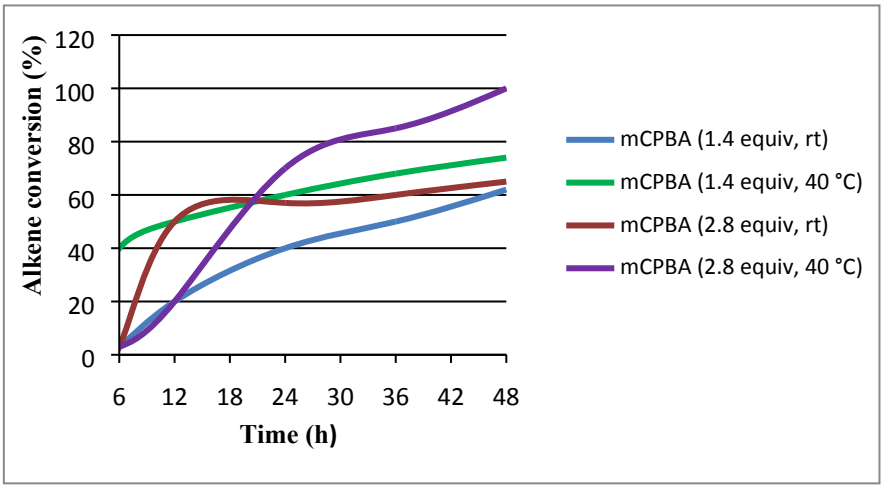


VII. Chemical kinetics of the epoxidation of 2a

Evolution of the reaction with different oxidazing agent (monitoring by ^{1}H NMR):

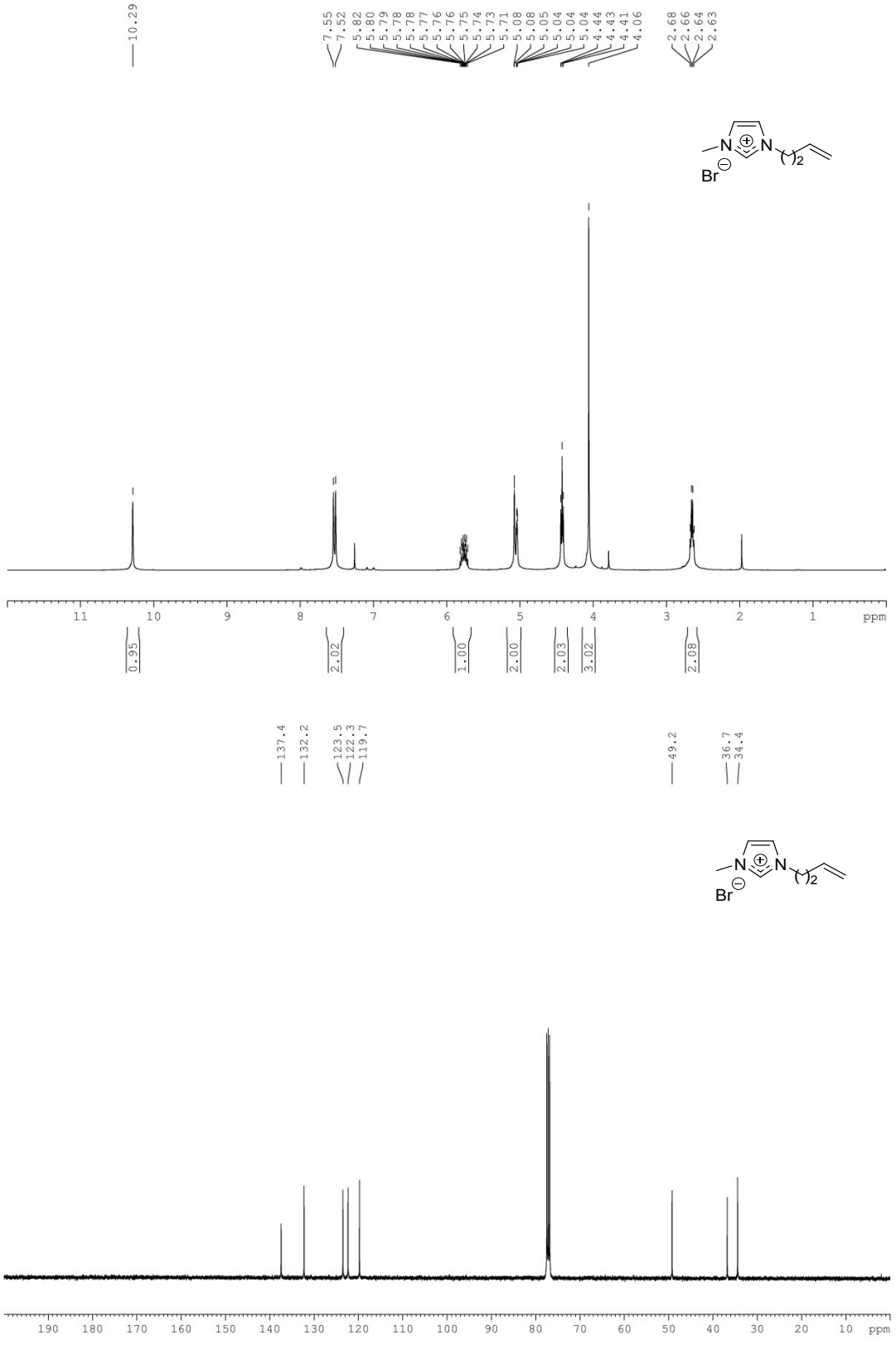


*Optimization of the epoxidation of **2a** with mCPBA (monitoring by ^{1}H NMR):*

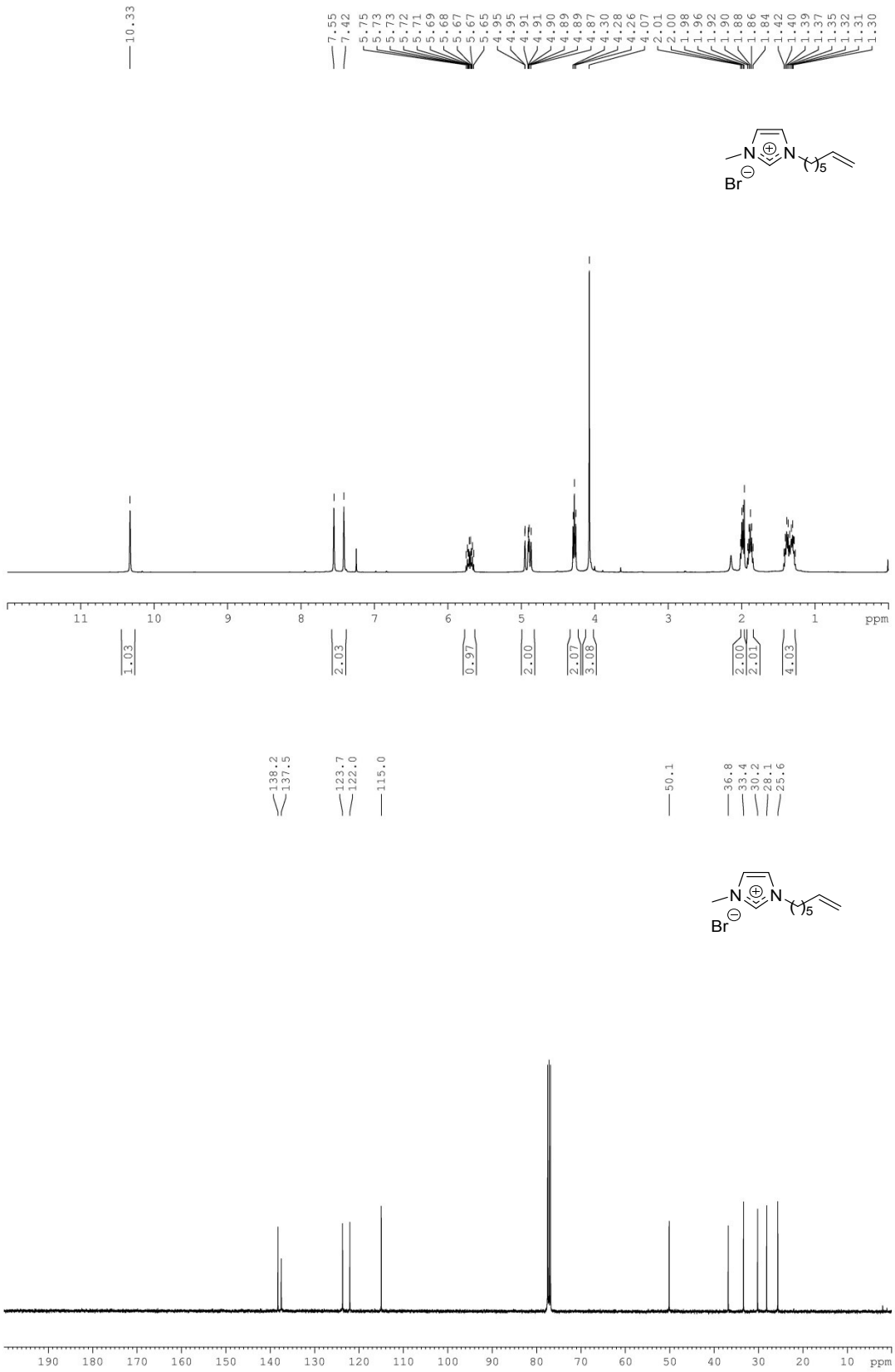


VIII. NMR spectrum

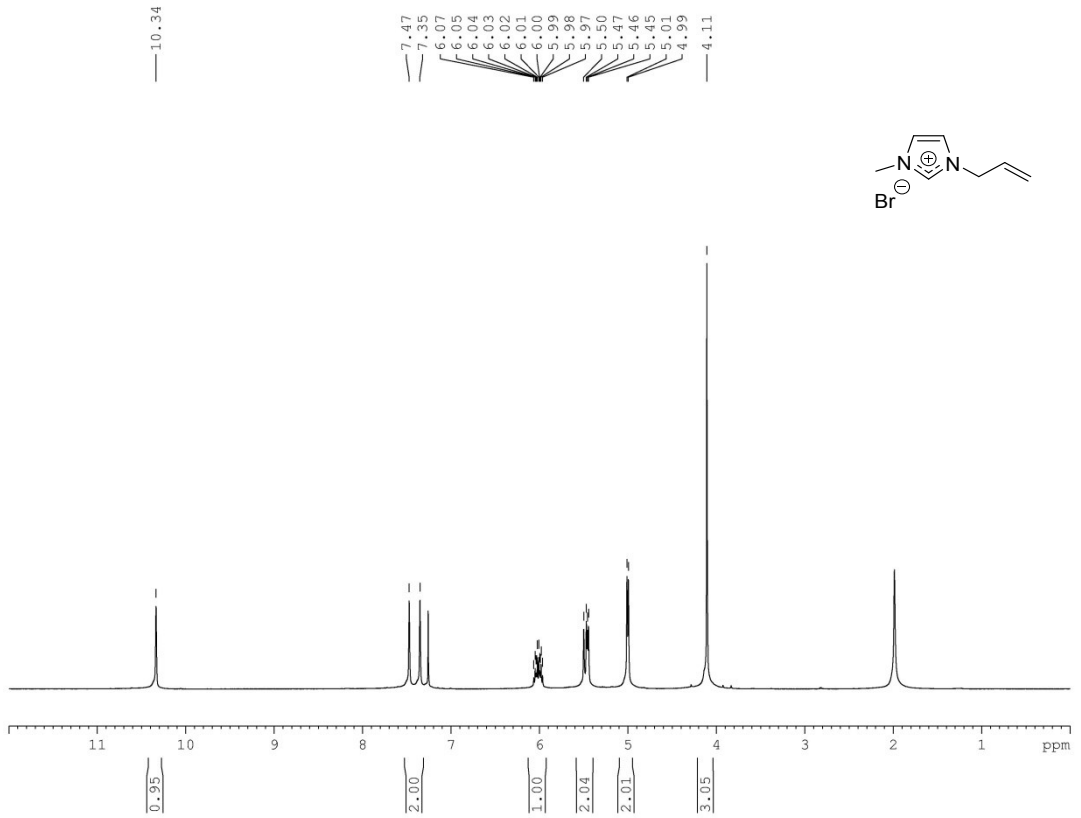
Compound 1a:

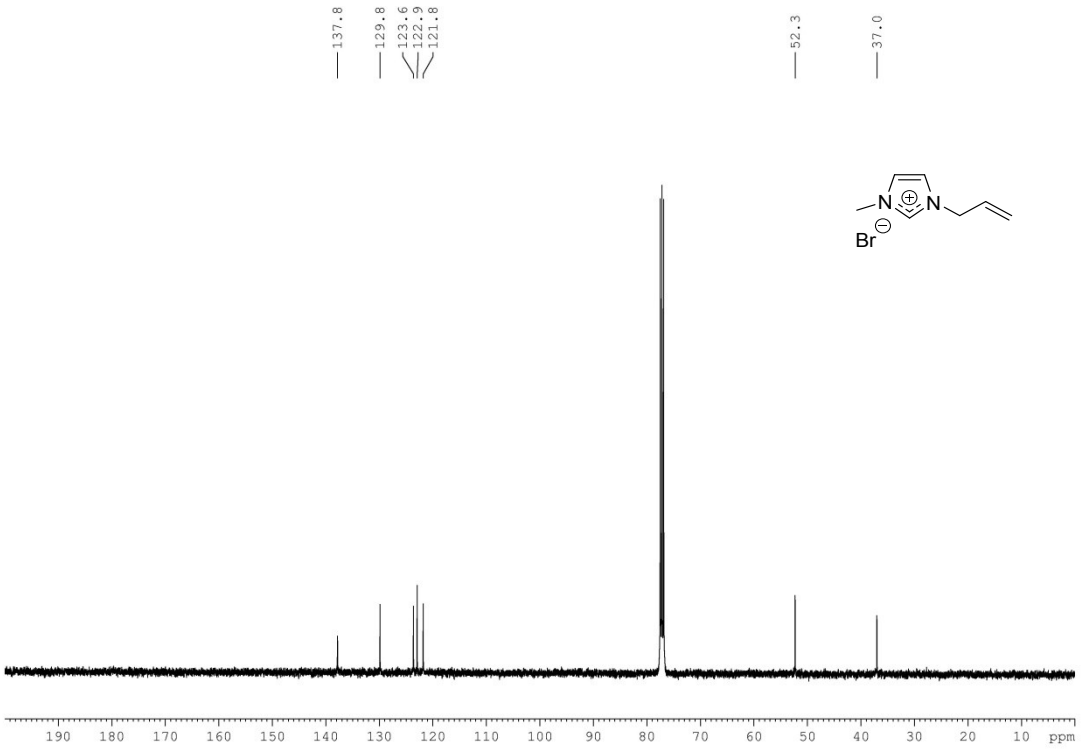


Compound 1b:

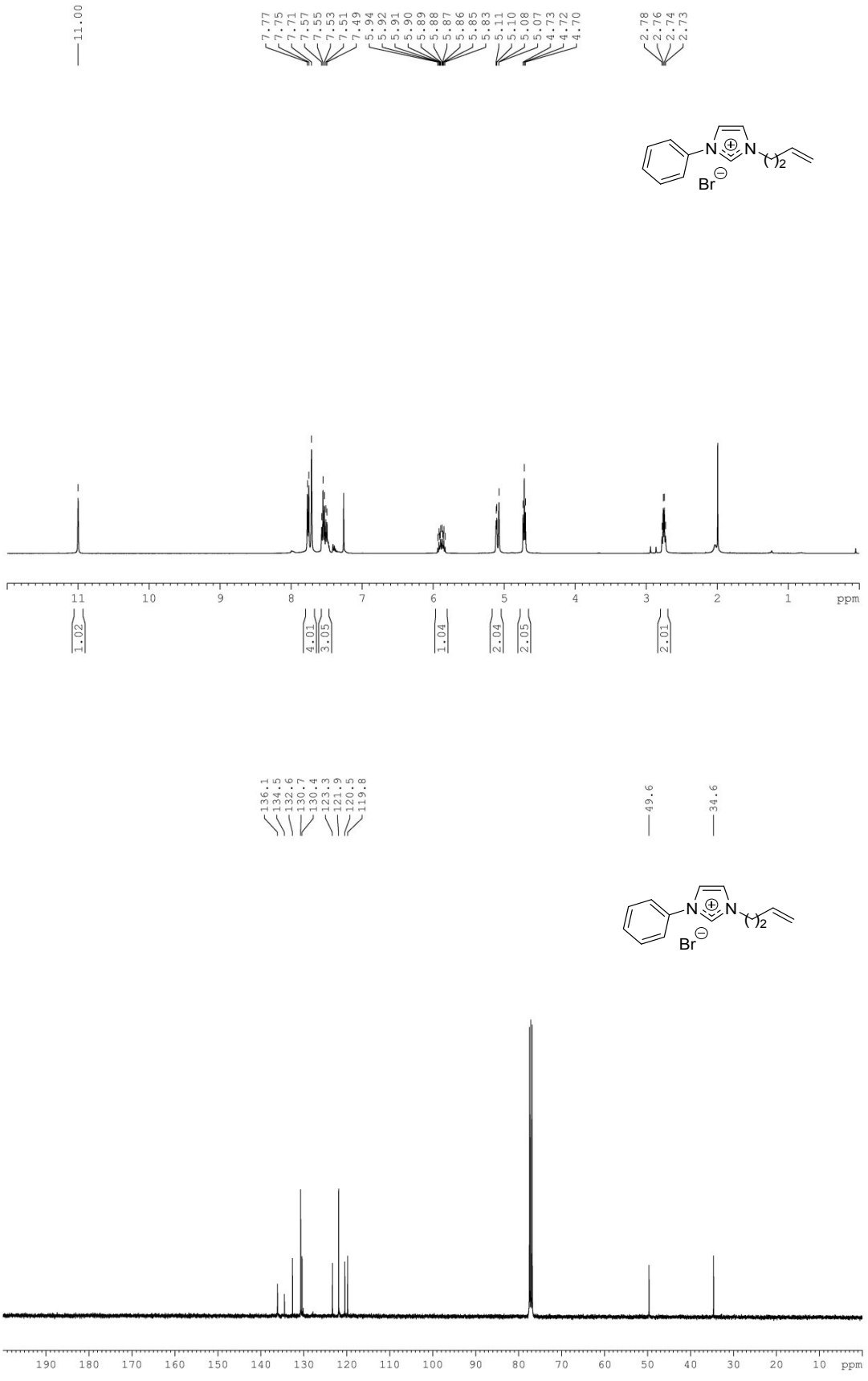

10.33
7.55
7.42
5.75
5.73
5.73
5.72
5.71
5.69
5.68
5.67
5.67
5.65
4.95
4.91
4.91
4.90
4.89
4.89
4.87
4.30
4.28
4.26
4.07
2.01
2.00
1.98
1.96
1.92
1.90
1.88
1.86
1.84
1.42
1.40
1.39
1.37
1.35
1.32
1.31
1.30
Br
5
11
10
9
8
7
6
5
4
3
2
1
ppm
1.03
2.03
0.97
2.00
2.07
3.08
2.00
2.01
4.03
138.2
137.5
123.7
122.0
115.0
50.1
36.8
33.4
30.2
28.1
25.6
Br
5
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

Compound 1c:

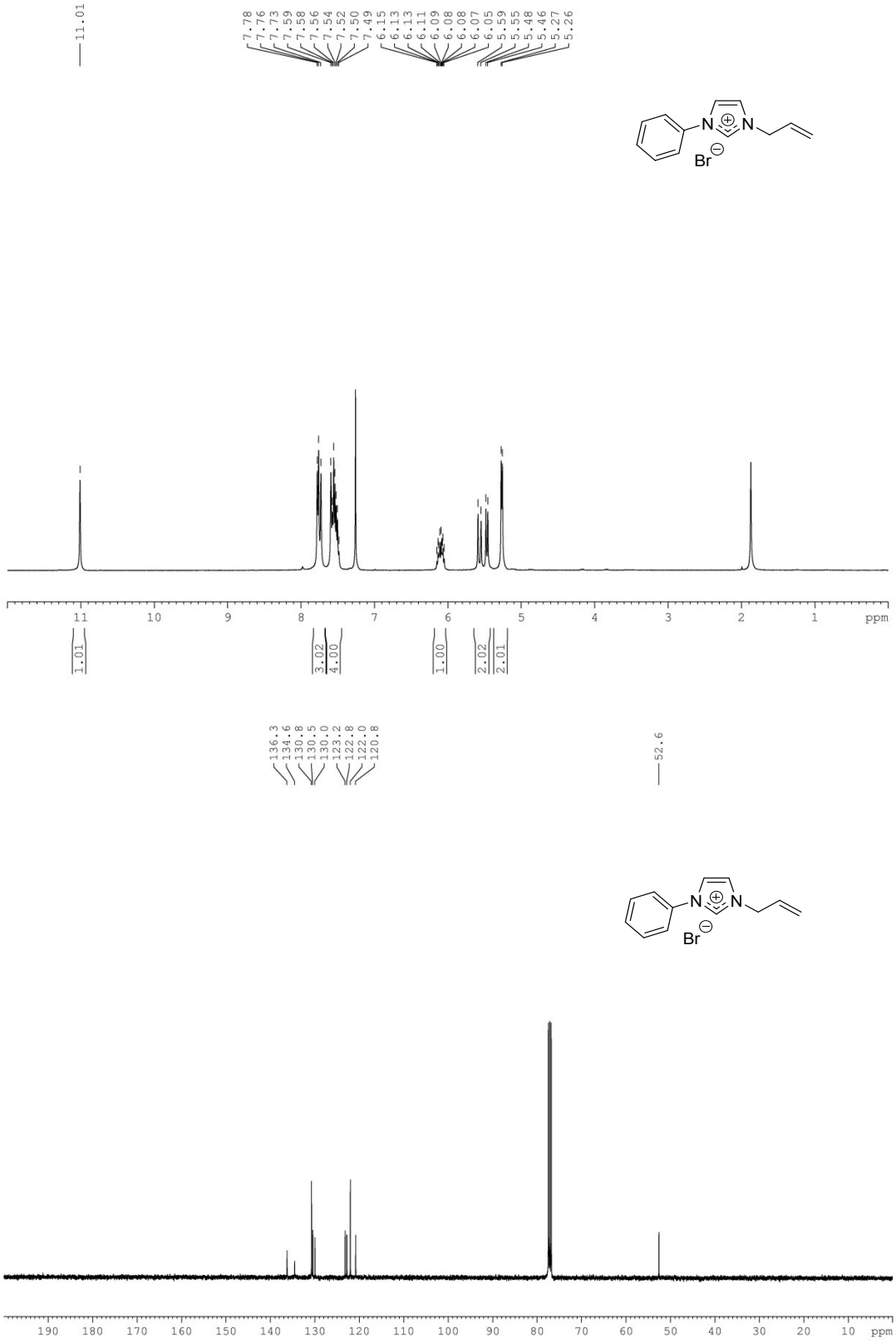

10.34
7.47
7.35
6.07
6.05
6.04
6.03
6.02
6.01
6.00
5.99
5.98
5.97
5.50
5.47
5.46
5.45
5.01
4.99
4.11
Br
11
10
9
8
7
6
5
4
3
2
1
ppm
0.95
2.00
1.00
2.04
2.01
3.05


137.8
129.8
123.6
122.9
121.8
52.3
37.0
Br
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

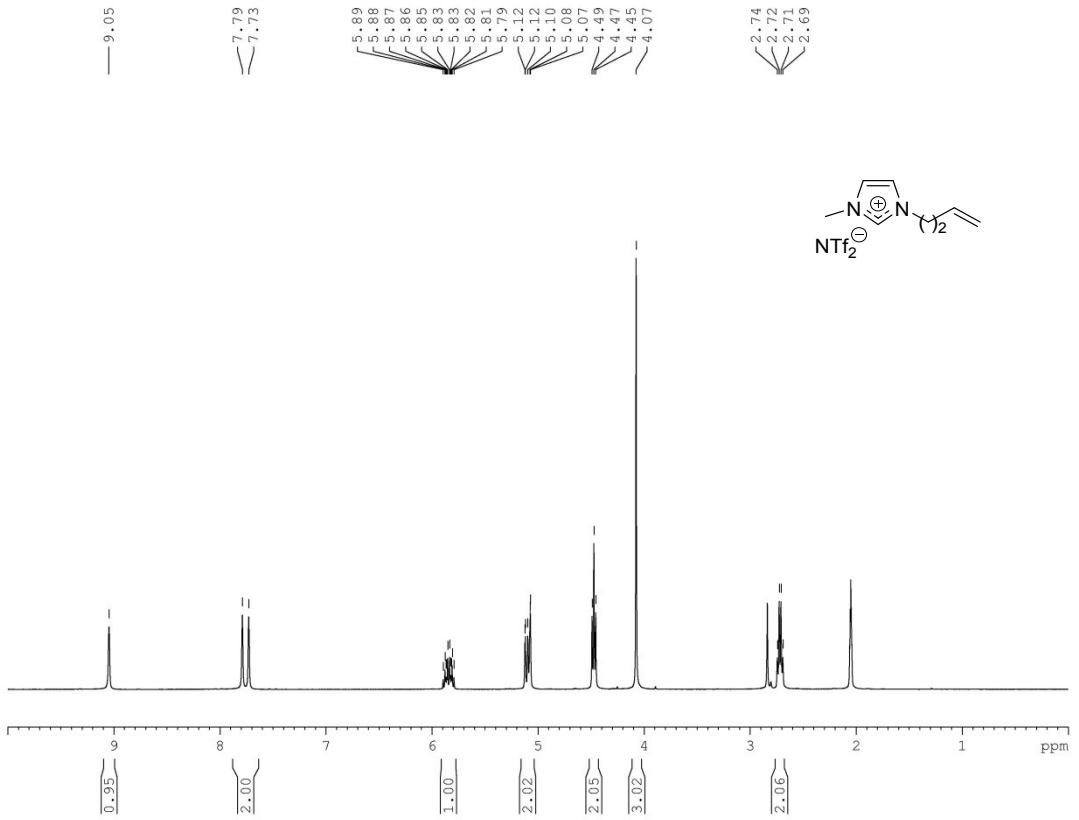
Compound 1d:

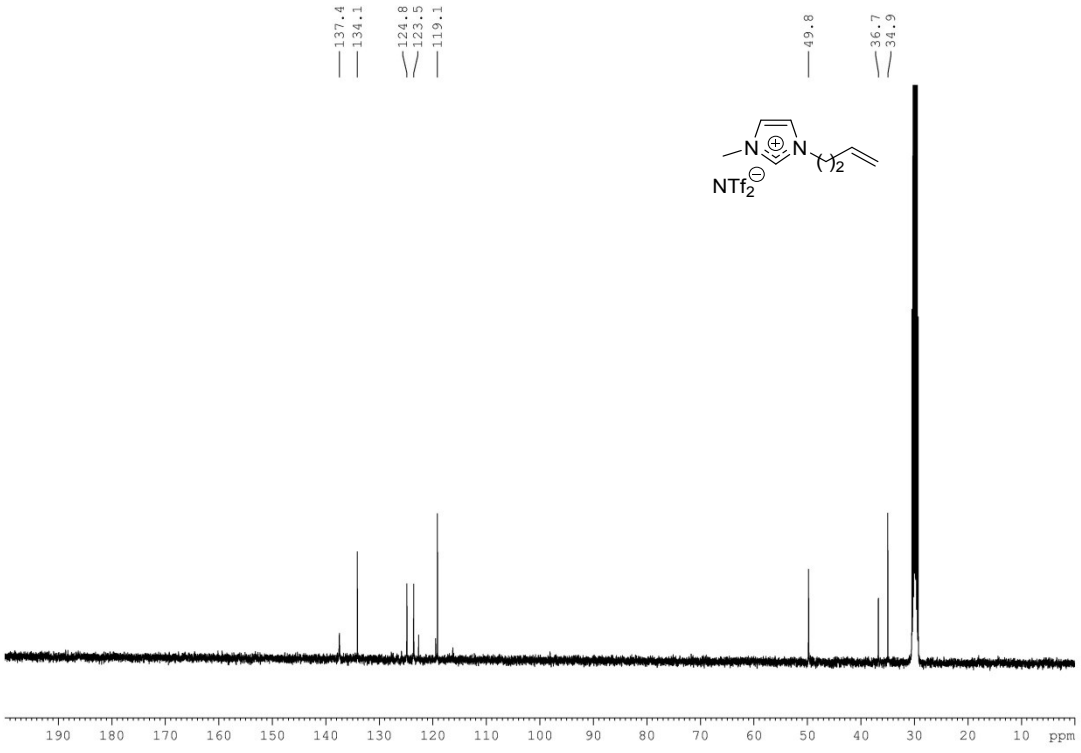

11.00
7.77
7.75
7.71
7.57
7.55
7.53
7.51
7.49
5.94
5.92
5.91
5.90
5.89
5.88
5.87
5.86
5.85
5.83
5.11
5.10
5.08
5.07
4.73
4.72
4.70
2.78
2.76
2.74
2.73
N
N
Br
11
10
9
8
7
6
5
4
3
2
1
ppm
1.02
4.01
3.05
1.04
2.04
2.05
2.01
136.1
134.5
132.6
130.7
130.4
123.3
121.9
120.5
119.8
49.6
34.6
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

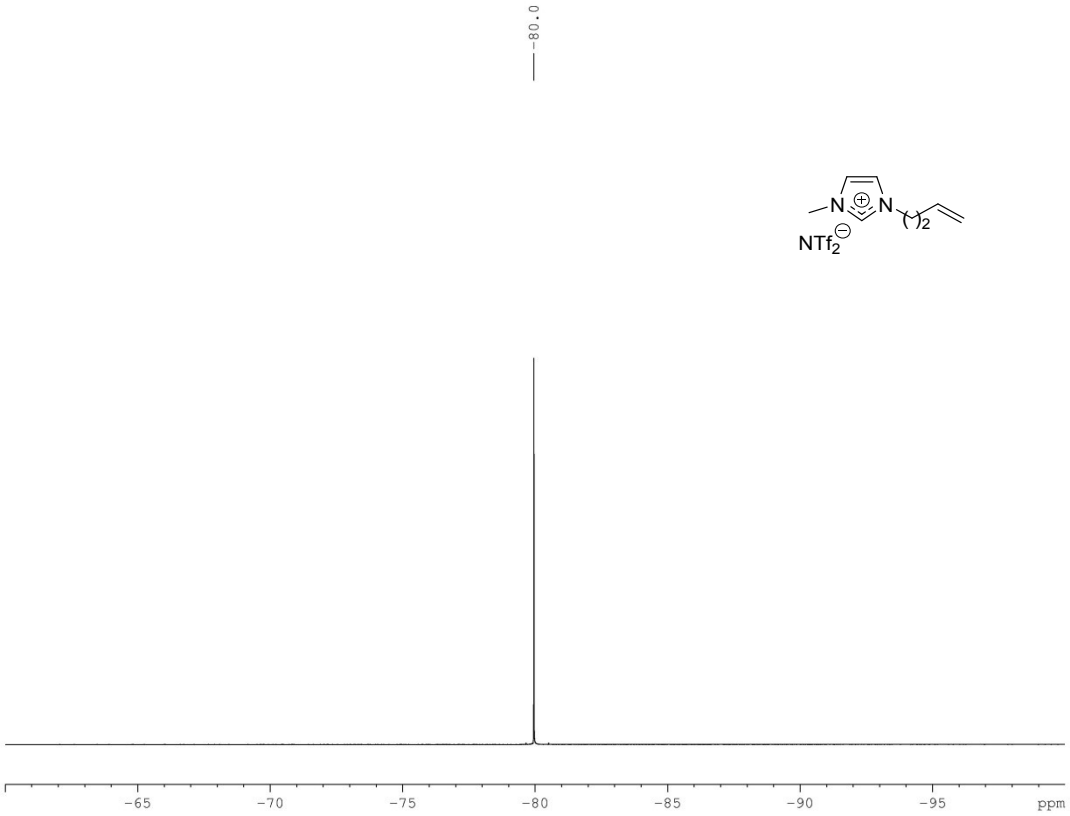
Compound 1e:


11.01
7.78
7.76
7.73
7.59
7.58
7.56
7.54
7.52
7.50
7.49
6.15
6.13
6.13
6.11
6.09
6.08
6.08
6.07
6.05
5.59
5.55
5.48
5.46
5.27
5.26
Br
11
10
9
8
7
6
5
4
3
2
1
ppm
1.01
3.02
4.00
1.00
2.02
2.01
136.3
134.6
130.8
130.5
130.0
123.2
122.8
122.0
120.8
52.6
Br
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

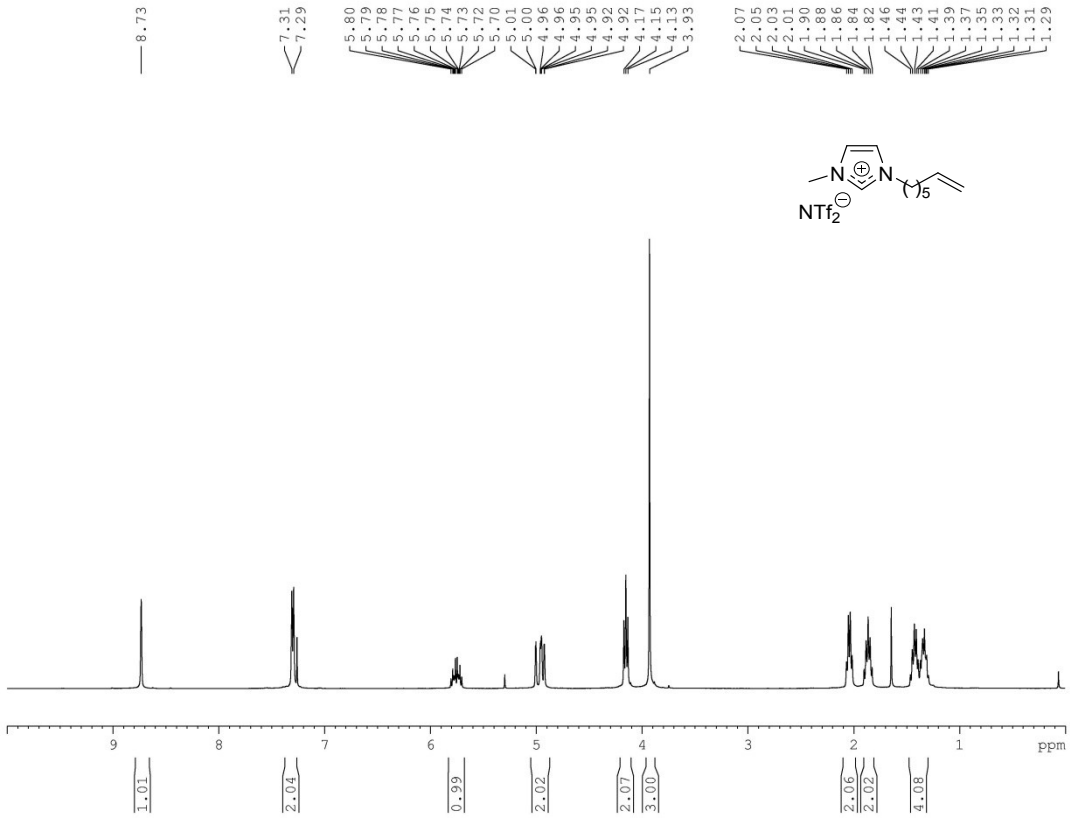
Compound 2a:

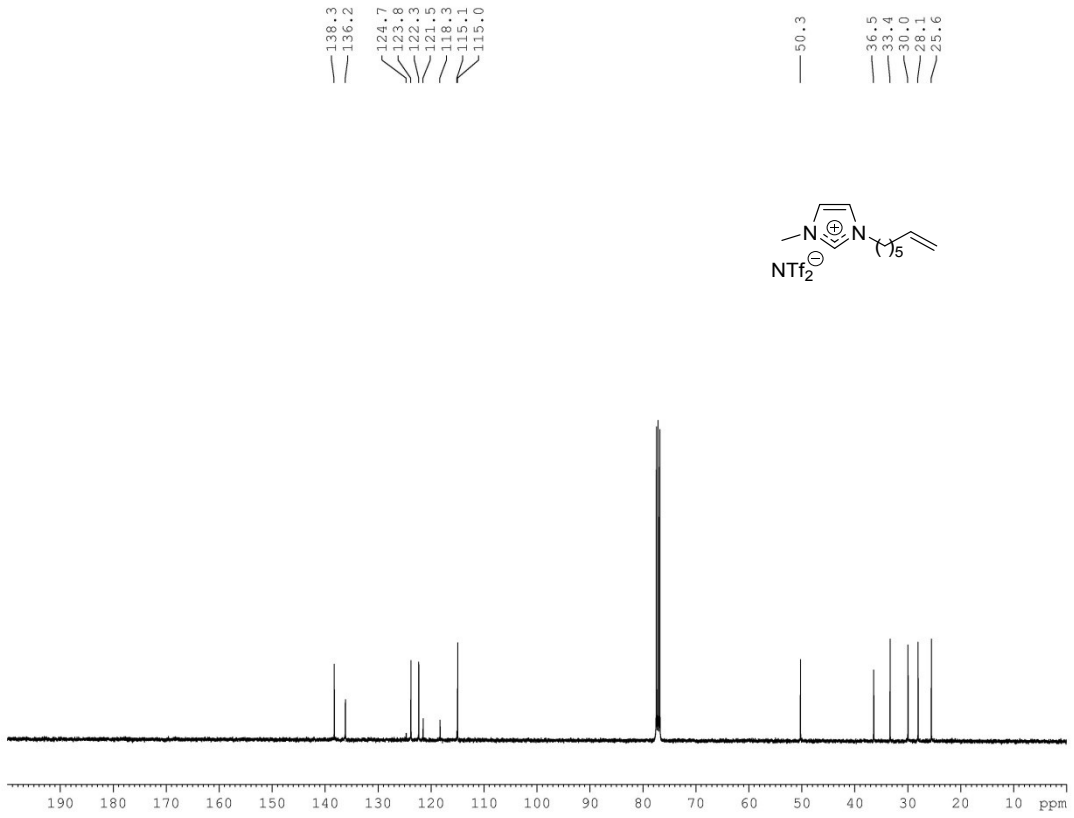

9.05
7.79
7.73
5.89
5.88
5.87
5.86
5.85
5.83
5.83
5.82
5.81
5.79
5.12
5.12
5.10
5.08
5.07
4.49
4.47
4.45
4.07
2.74
2.72
2.71
2.69
NTf2
9
8
7
6
5
4
3
2
1
ppm
0.95
2.00
1.00
2.02
2.05
3.02
2.06

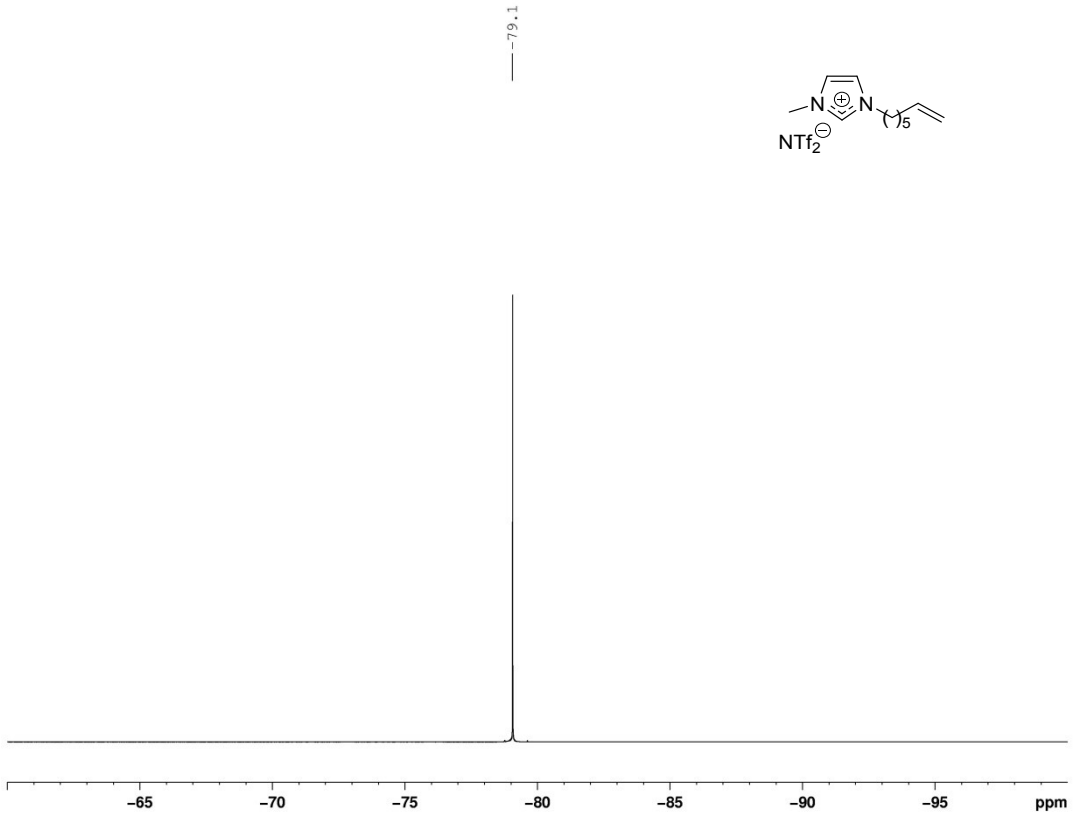

137.4
134.1
124.8
123.5
119.1
49.8
36.7
34.9
NTf2
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


-80.0
NTf2
-65
-70
-75
-80
-85
-90
-95
ppm

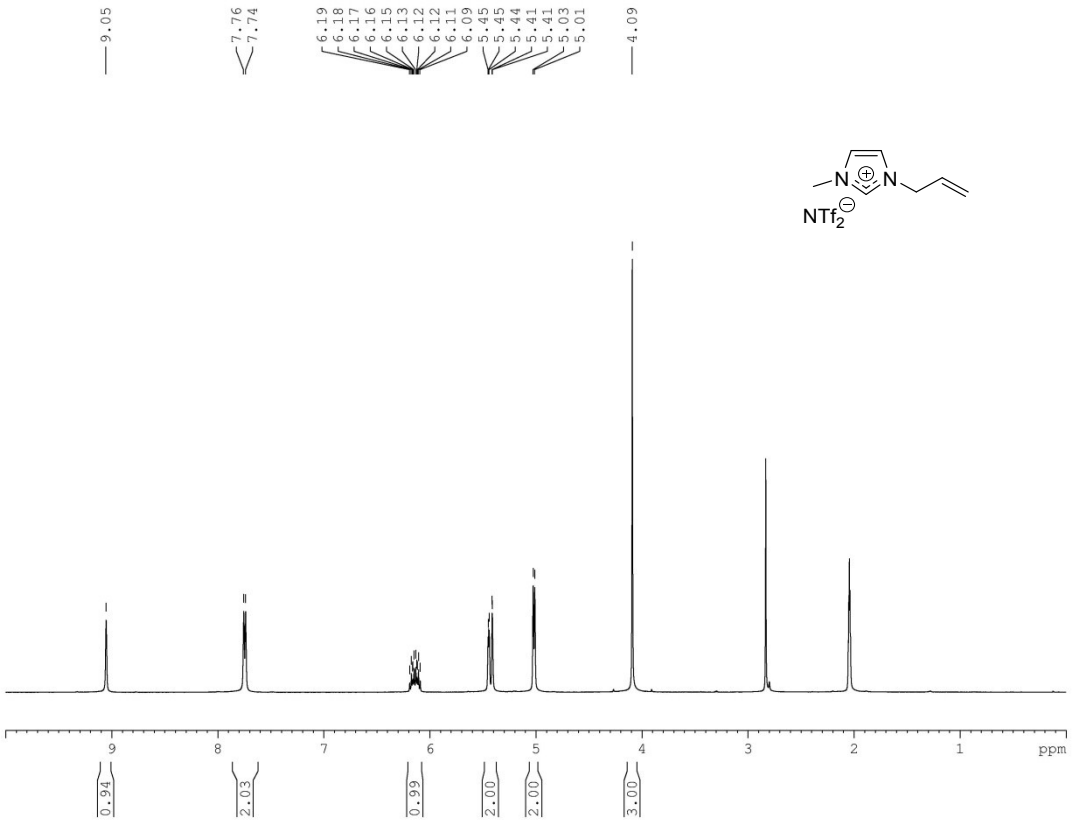
Compound 2b:

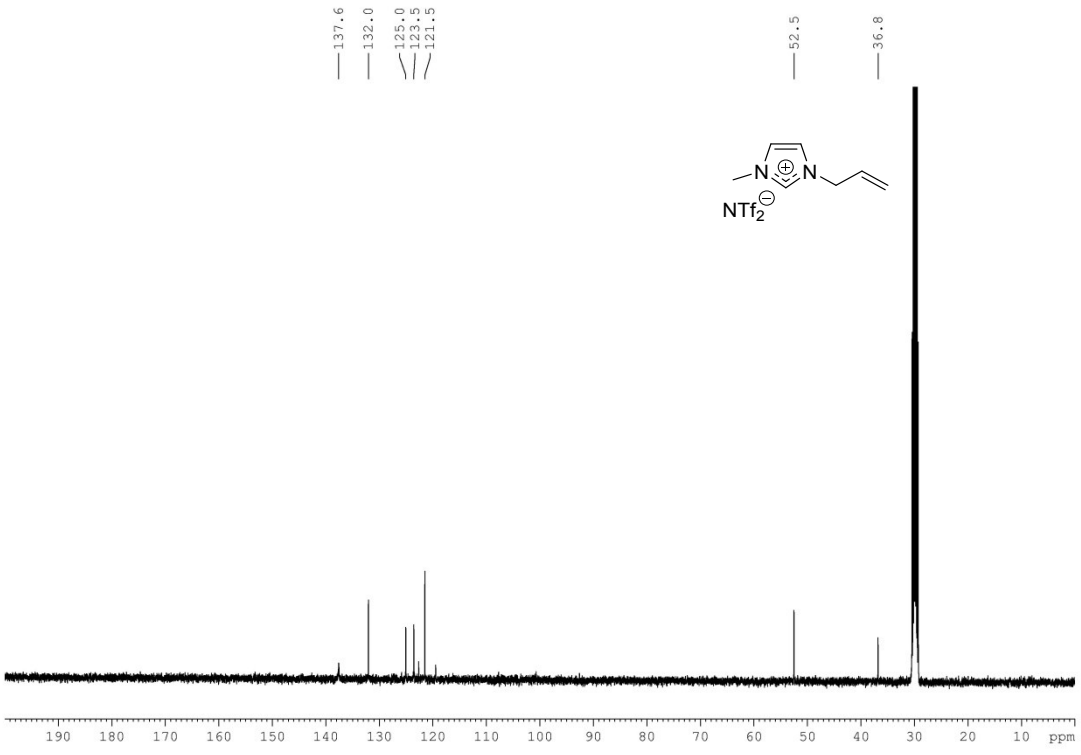

8.73
7.31
7.29
5.80
5.79
5.78
5.77
5.76
5.75
5.74
5.73
5.72
5.70
5.01
5.00
4.96
4.95
4.95
4.92
4.92
4.17
4.15
4.13
3.93
2.07
2.05
2.03
2.01
1.90
1.88
1.86
1.84
1.82
1.46
1.44
1.43
1.41
1.39
1.37
1.35
1.33
1.32
1.31
1.29
NTf2
9
8
7
6
5
4
3
2
1
ppm
1.01
2.04
0.99
2.02
2.07
3.00
2.06
2.02
4.08

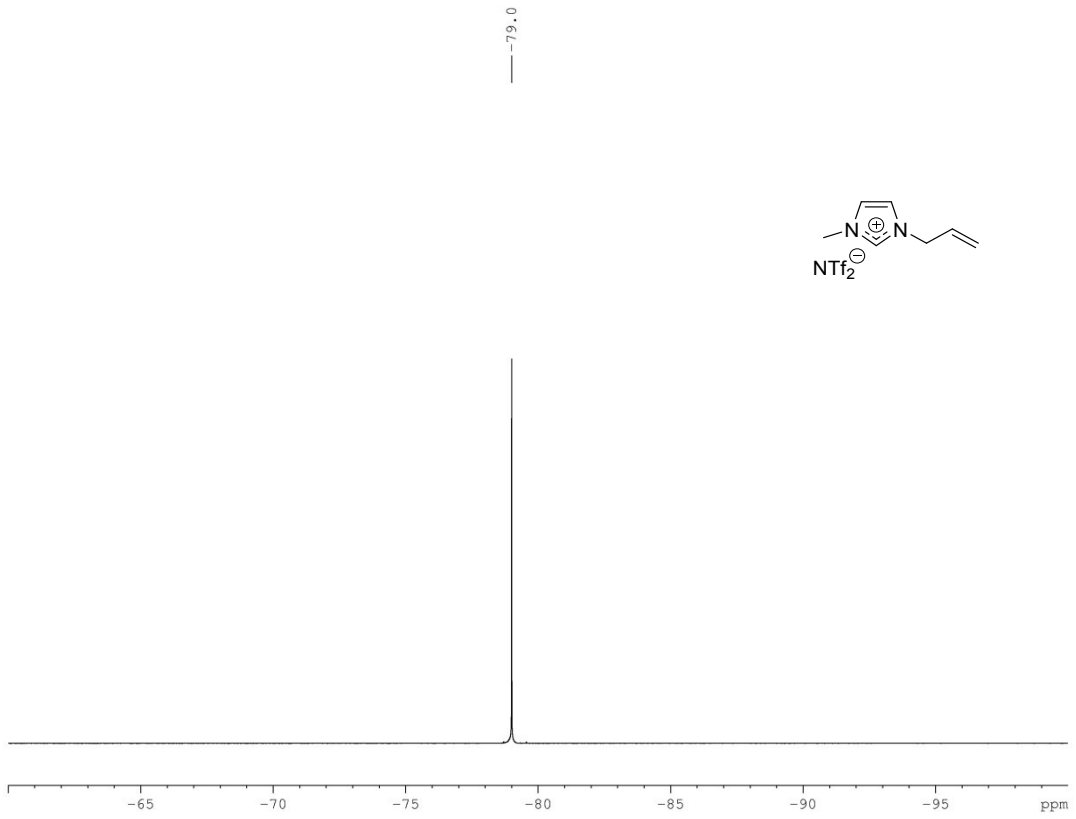

138.3
136.2
124.7
123.8
122.3
121.5
118.3
115.1
115.0
50.3
36.5
33.4
30.0
28.1
25.6
N
N
5
NTf2
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


-79.1
N
N
5
NTf2
-65 -70 -75 -80 -85 -90 -95 ppm

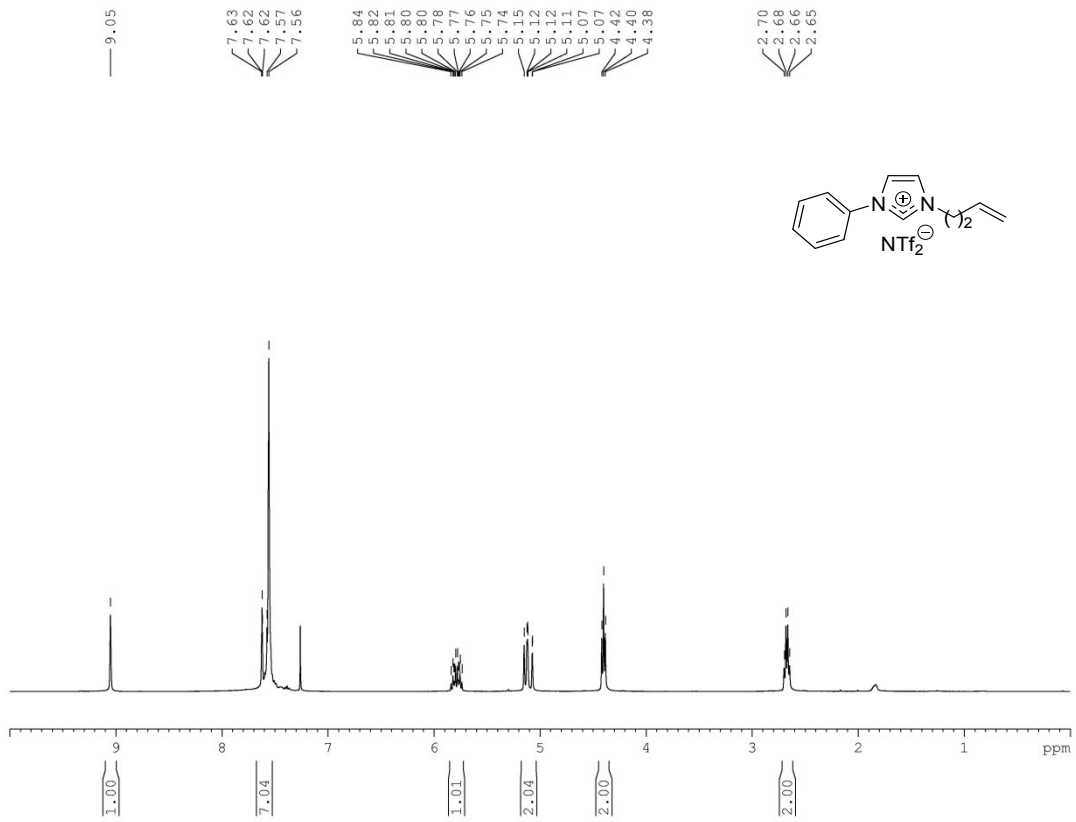
Compound 2c:

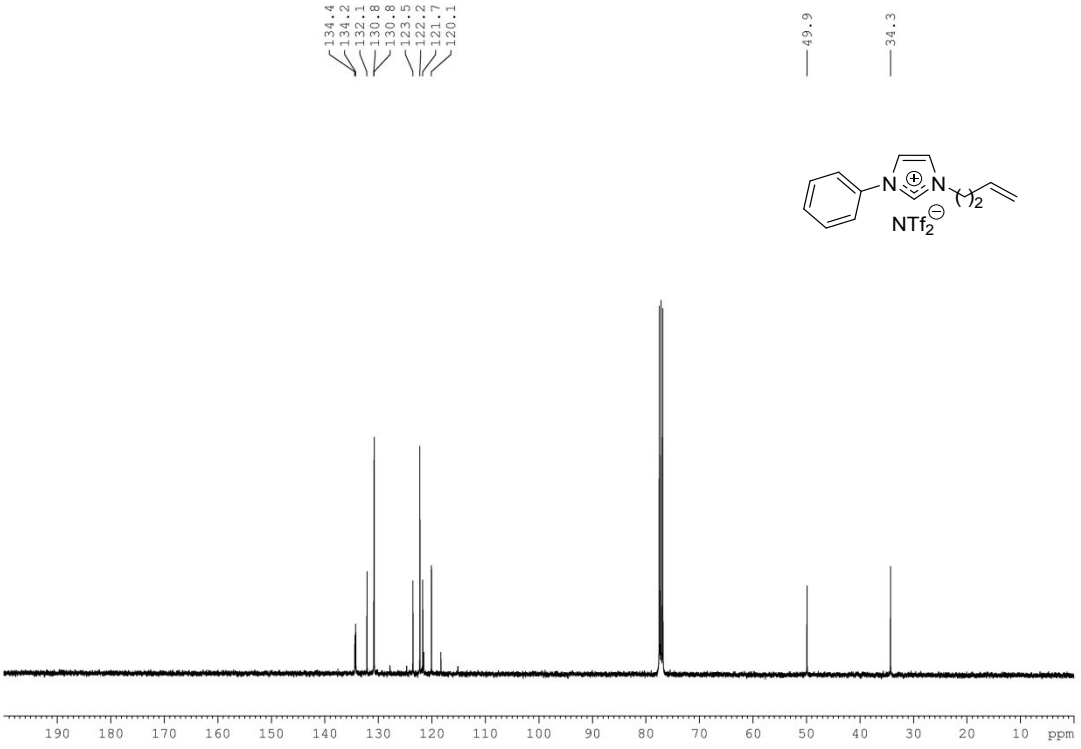

9.05
7.76
7.74
6.19
6.18
6.17
6.16
6.15
6.13
6.12
6.12
6.11
6.09
5.45
5.45
5.44
5.41
5.41
5.03
5.01
4.09
NTf2
9
8
7
6
5
4
3
2
1
ppm
0.94
2.03
0.99
2.00
2.00
3.00

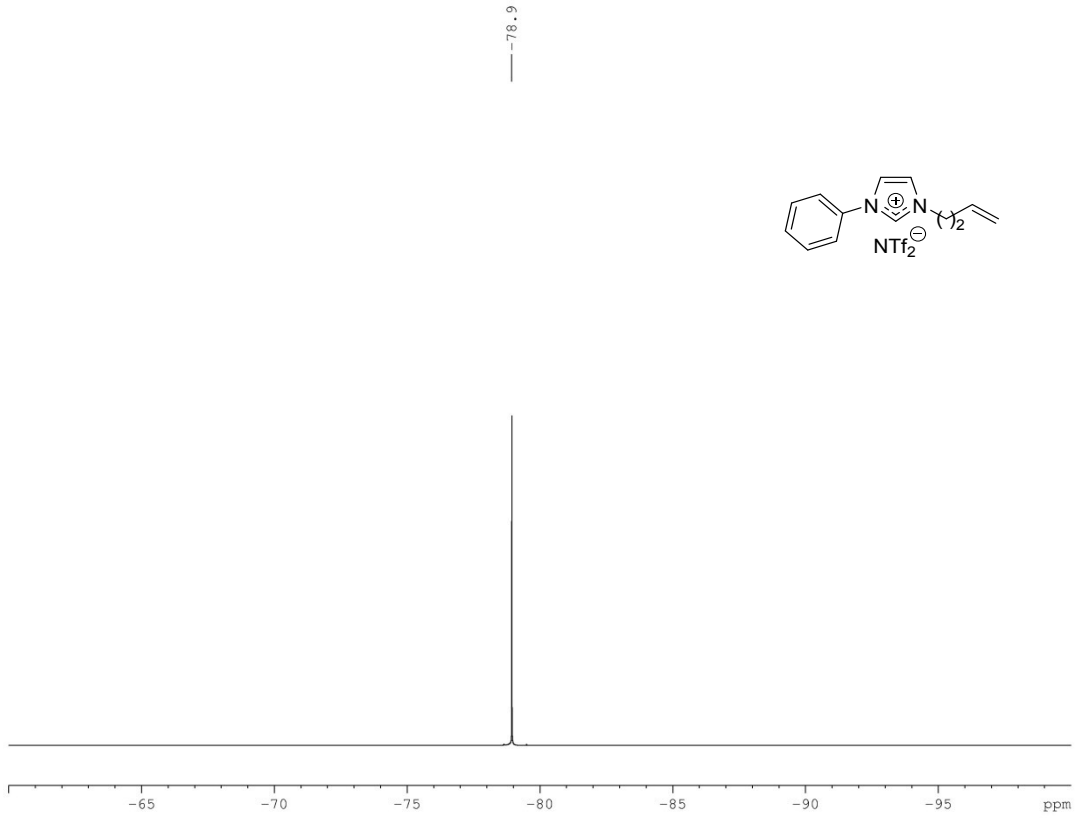

137.6
132.0
125.0
123.5
121.5
52.5
36.8
NTf2
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


-79.0
NTf2
-65
-70
-75
-80
-85
-90
-95
ppm

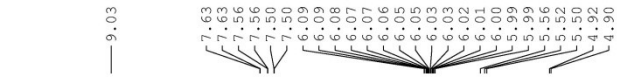
Compound 2d:

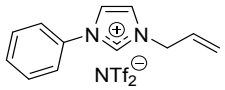

9.05
7.63
7.62
7.62
7.57
7.56
5.84
5.82
5.81
5.80
5.80
5.78
5.77
5.76
5.75
5.74
5.15
5.12
5.12
5.11
5.07
5.07
4.42
4.40
4.38
2.70
2.68
2.66
2.65
NTf2
9
8
7
6
5
4
3
2
1
ppm
1.00
7.04
1.01
2.04
2.00
2.00

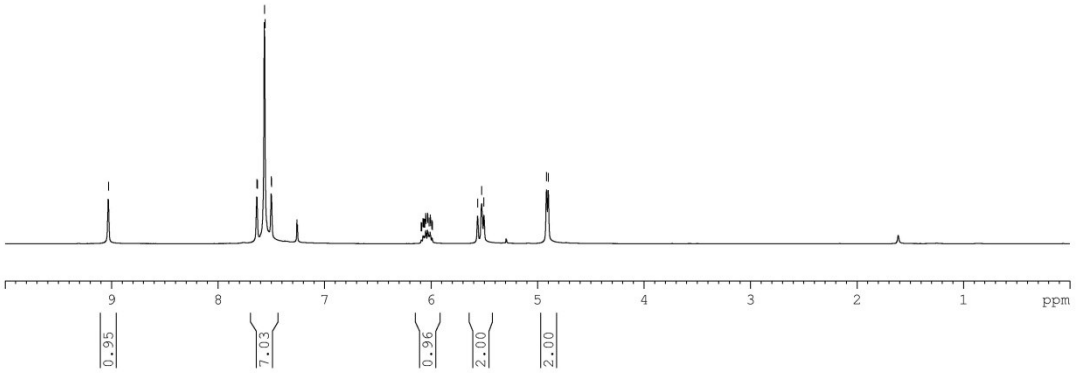

134.4
134.2
132.1
130.8
130.8
123.5
122.2
121.7
120.1
49.9
34.3
N
N
()2
NTf2
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

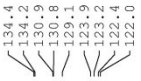

-78.9
N
N
()2
NTf2
-65 -70 -75 -80 -85 -90 -95 ppm

Compound 2e:

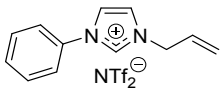

9.03
7.63
7.63
7.56
7.56
7.50
7.50
6.09
6.09
6.08
6.07
6.07
6.06
6.05
6.05
6.03
6.03
6.02
6.01
6.00
5.99
5.99
5.56
5.52
5.50
4.92
4.90

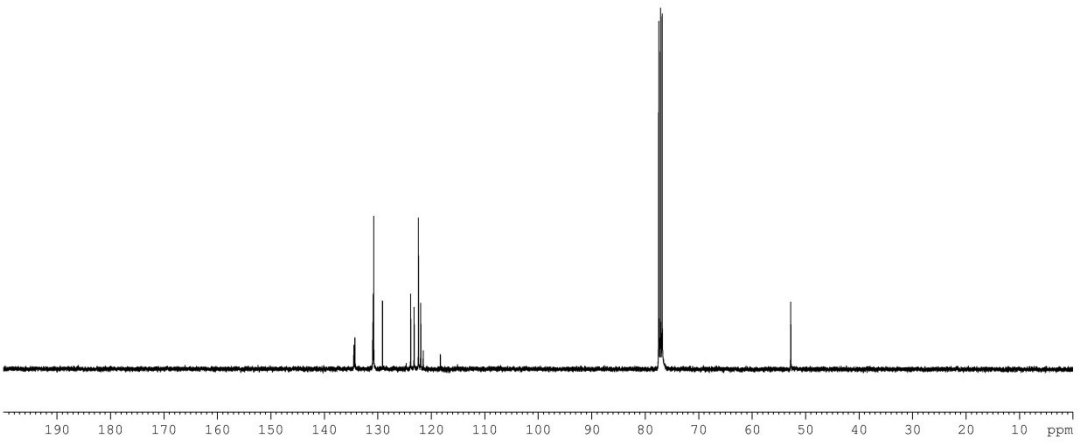

N
N
NTf2

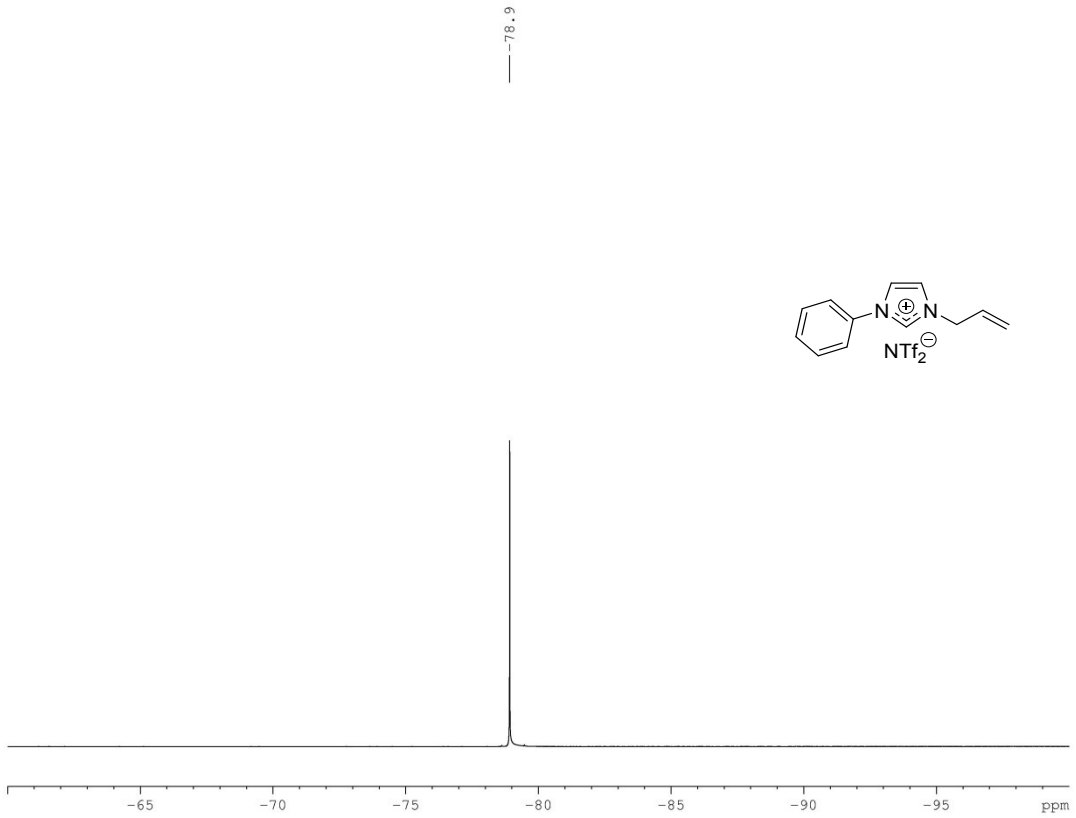

9
8
7
6
5
4
3
2
1
ppm
0.95
7.03
0.96
2.00
2.00


134.4
134.2
130.9
130.8
129.1
123.9
123.2
122.4
122.0

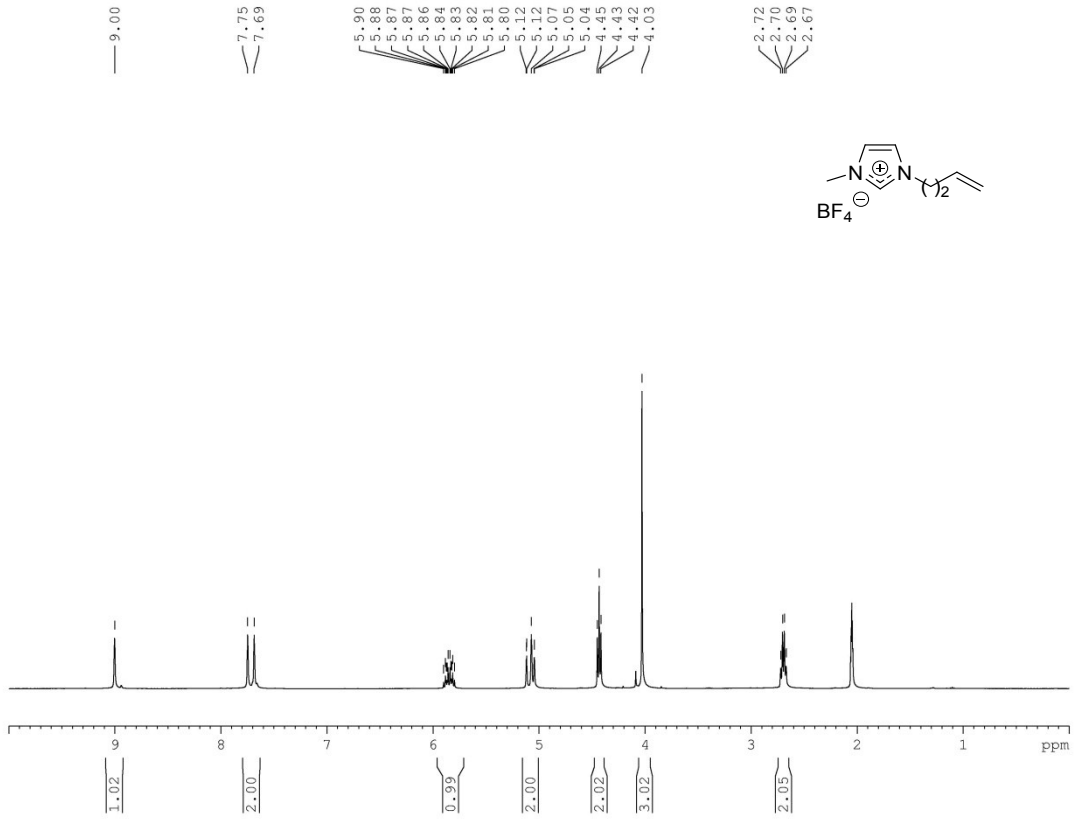

52.8

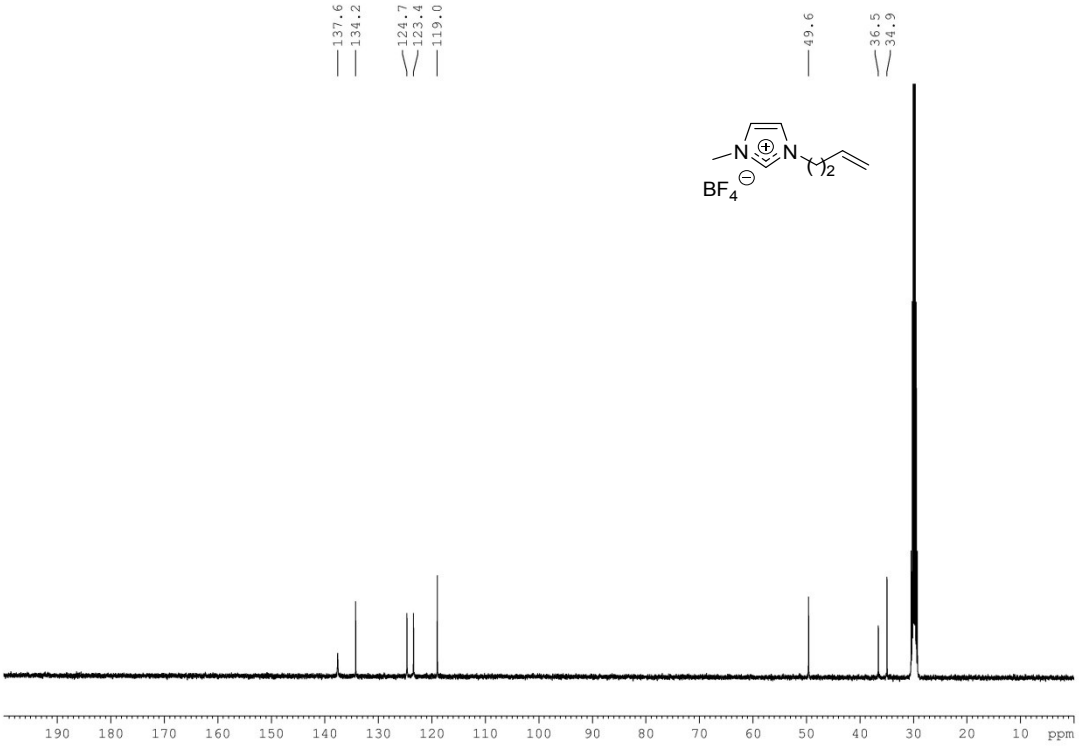

N
N
NTf2

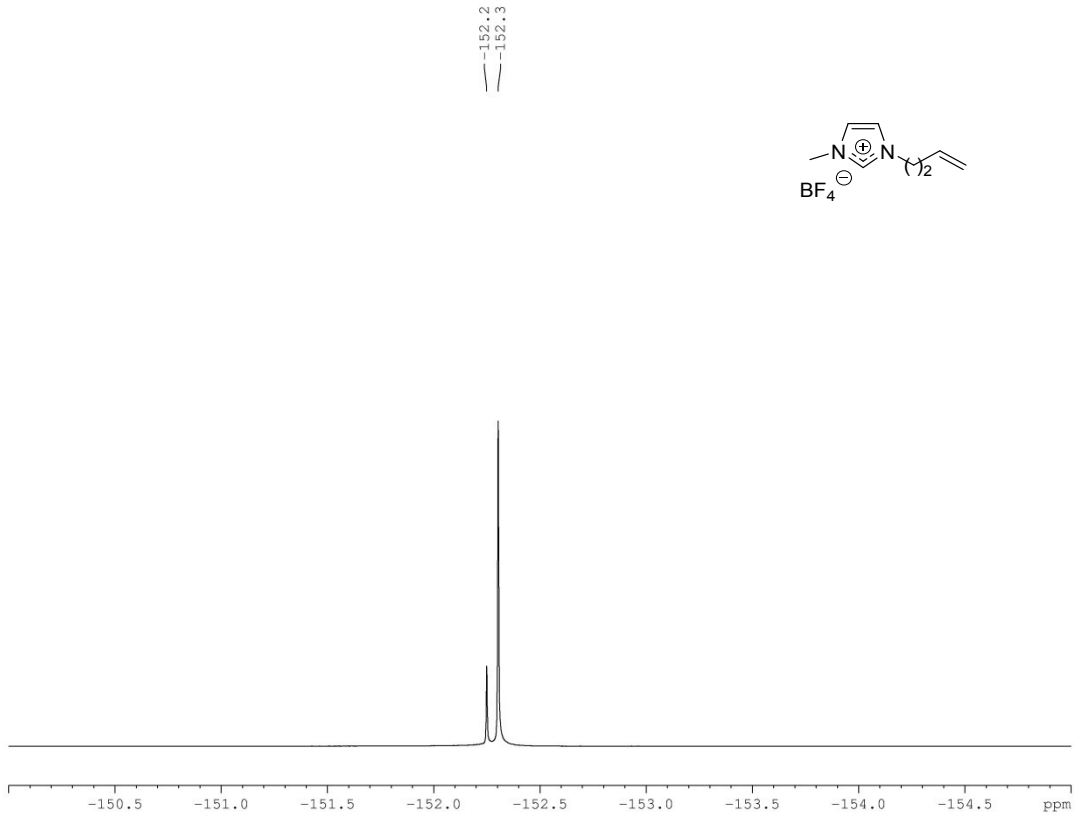

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


-78.9
NTf2
-65
-70
-75
-80
-85
-90
-95
ppm

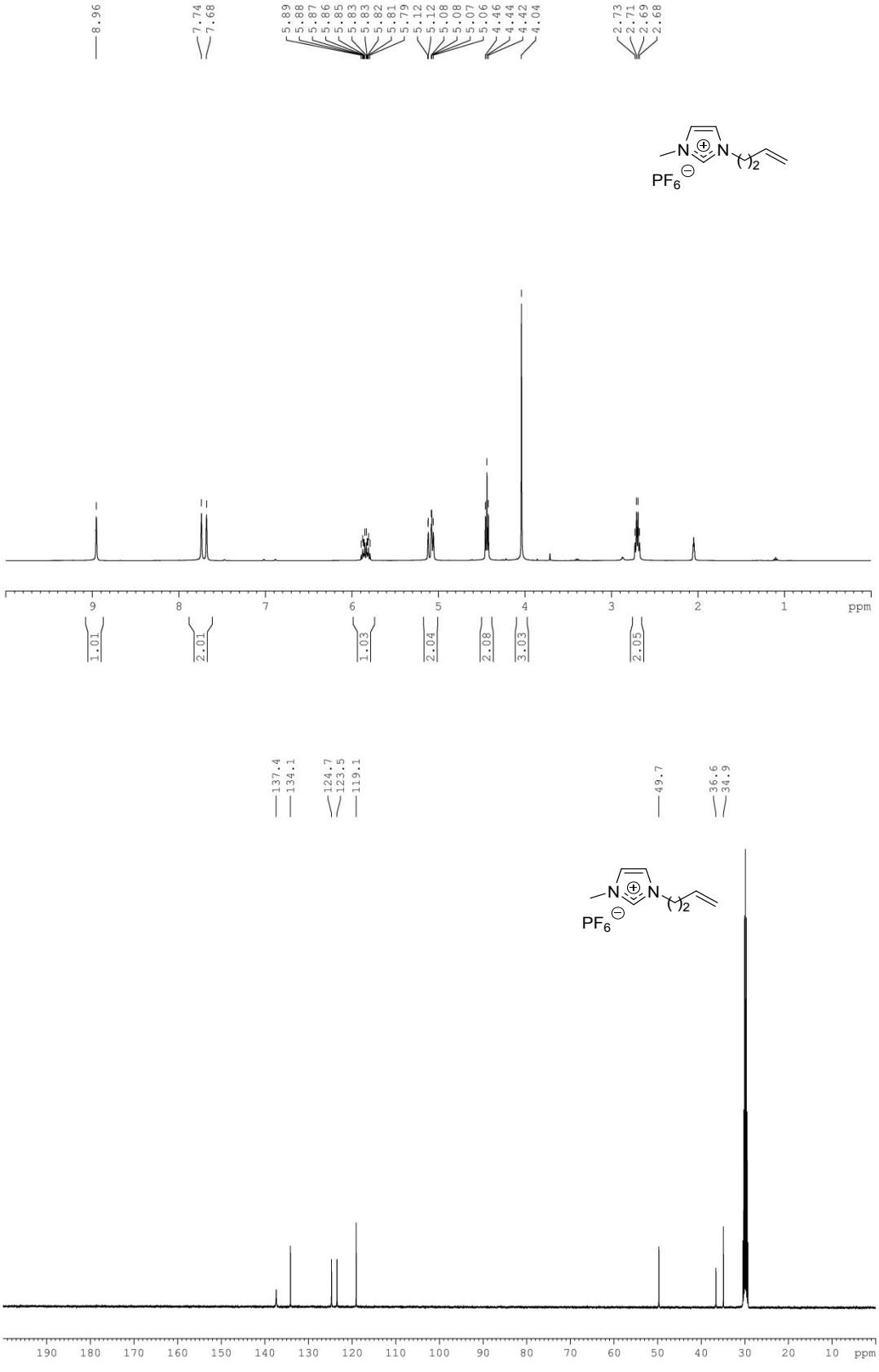
Compound 2f:

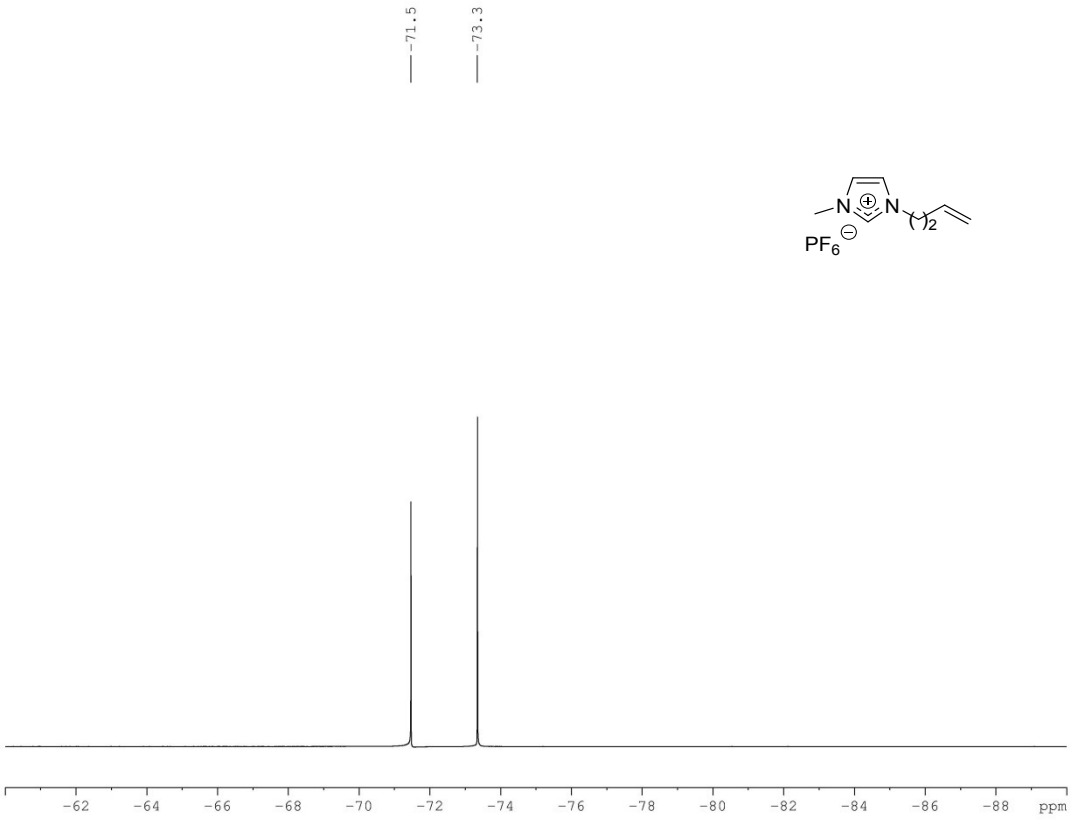

9.00
7.75
7.69
5.90
5.88
5.87
5.87
5.86
5.84
5.83
5.82
5.81
5.80
5.12
5.07
5.05
5.04
4.45
4.43
4.42
4.03
2.72
2.70
2.69
2.67
BF4
2
9
8
7
6
5
4
3
2
1
ppm
1.02
2.00
0.99
2.00
2.02
3.02
2.05


137.6
134.2
124.7
123.4
119.0
49.6
36.5
34.9
BF4
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

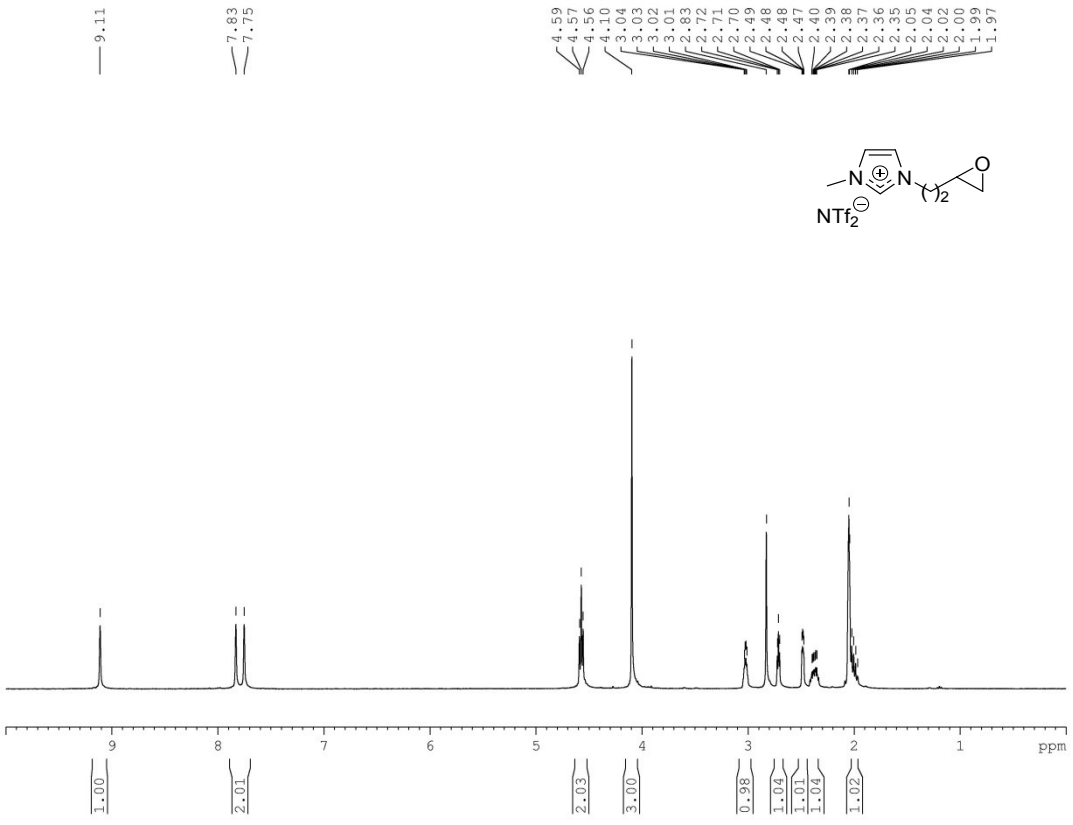

-152.2
-152.3
BF4
-150.5 -151.0 -151.5 -152.0 -152.5 -153.0 -153.5 -154.0 -154.5 ppm

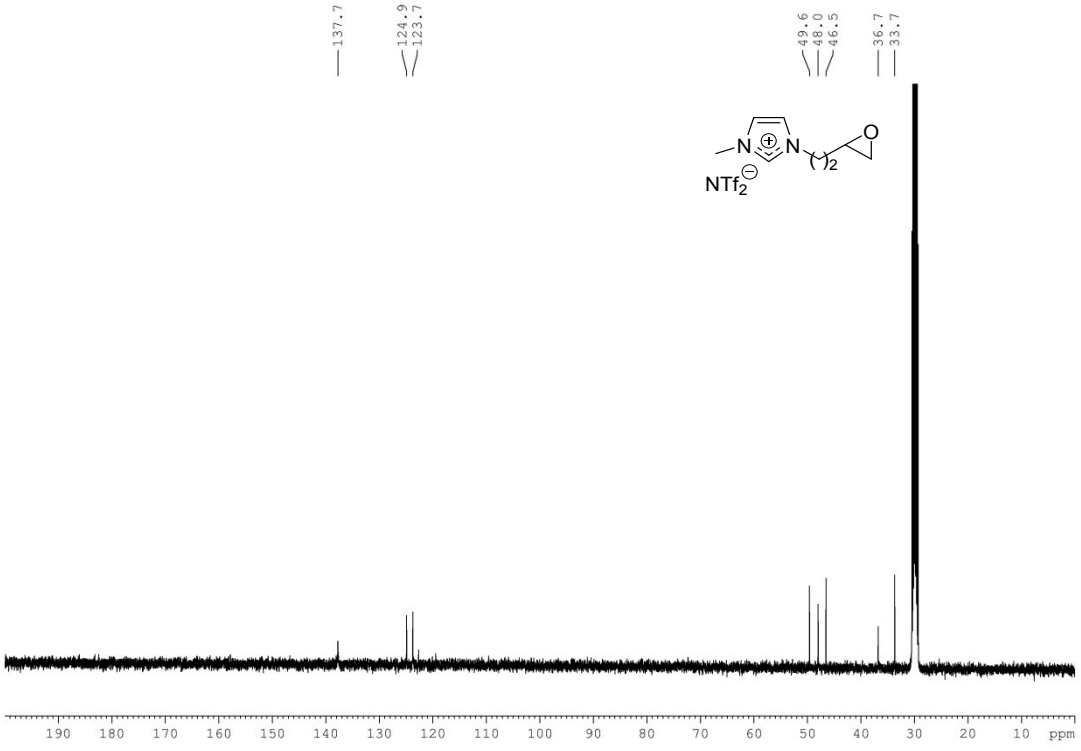
Compound 2g:

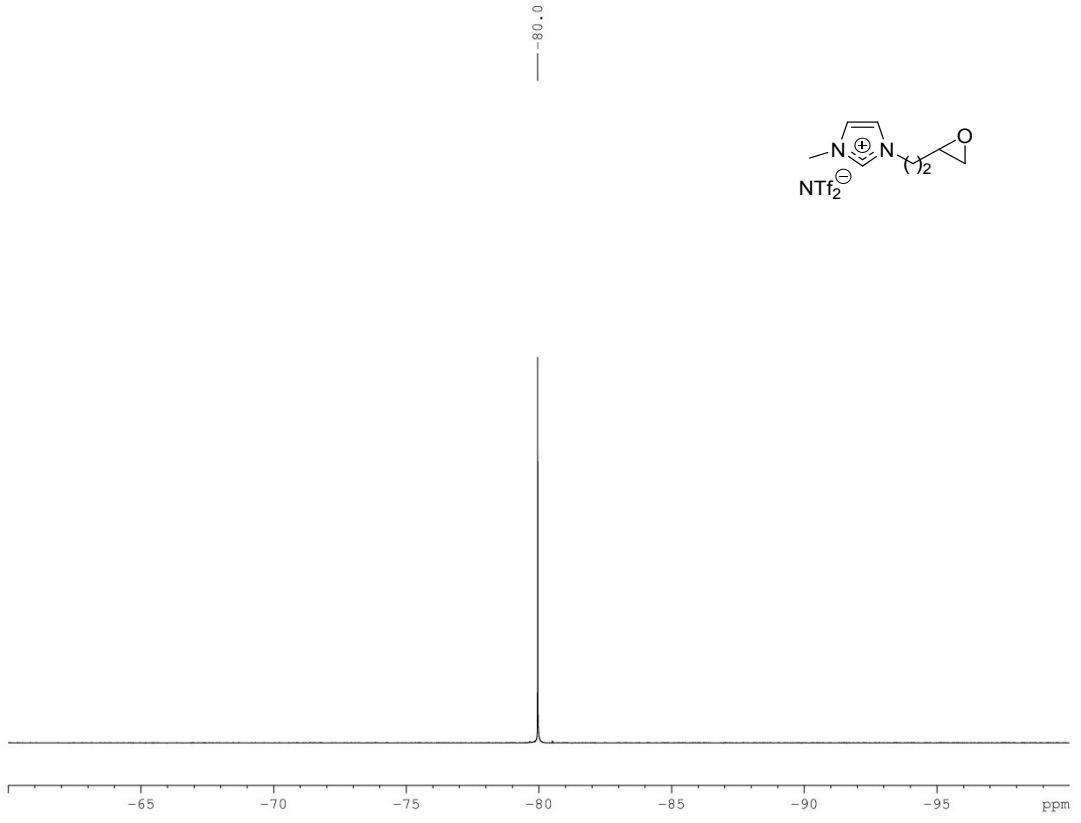

8.96
7.74
7.68
5.89
5.88
5.87
5.86
5.85
5.83
5.83
5.82
5.81
5.79
5.12
5.12
5.08
5.08
5.07
5.06
4.46
4.44
4.42
4.04
2.73
2.71
2.69
2.68
PF6
ppm
1.01
2.01
1.03
2.04
2.08
3.03
2.05
137.4
134.1
124.7
123.5
119.1
49.7
36.6
34.9
PF6
ppm


-71.5
-73.3
PF6
-62
-64
-66
-68
-70
-72
-74
-76
-78
-80
-82
-84
-86
-88
ppm

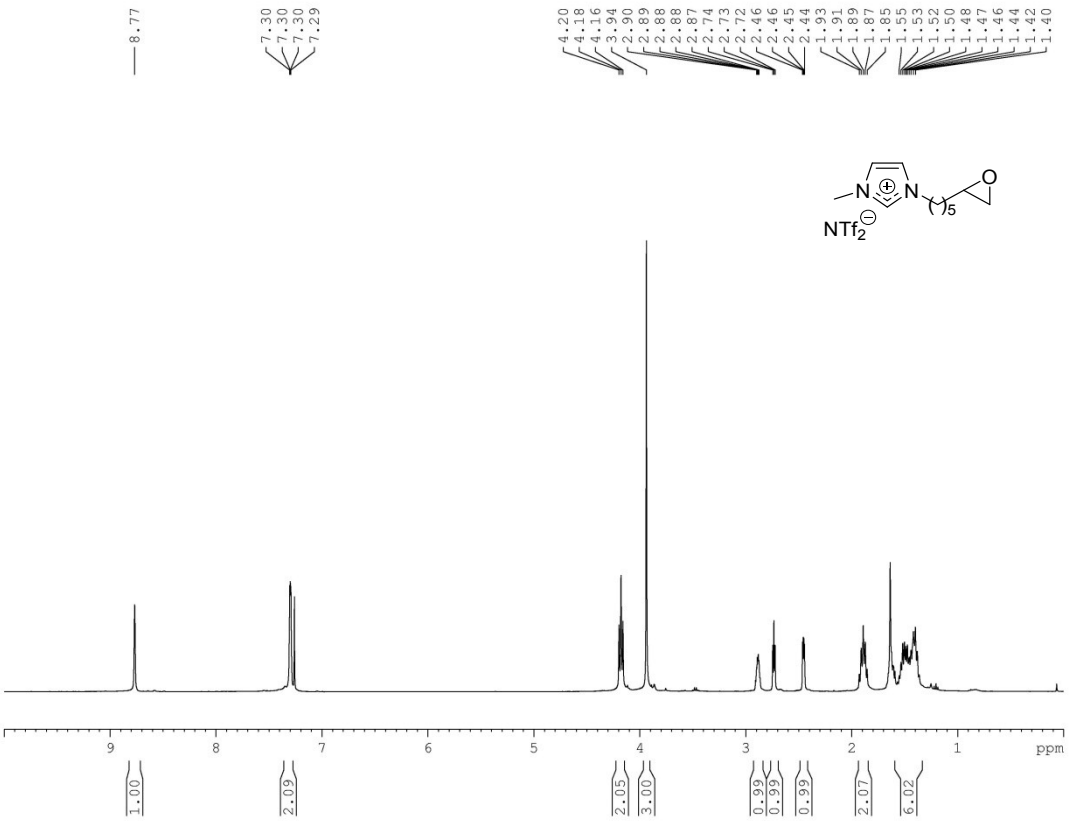
Compound 3a:

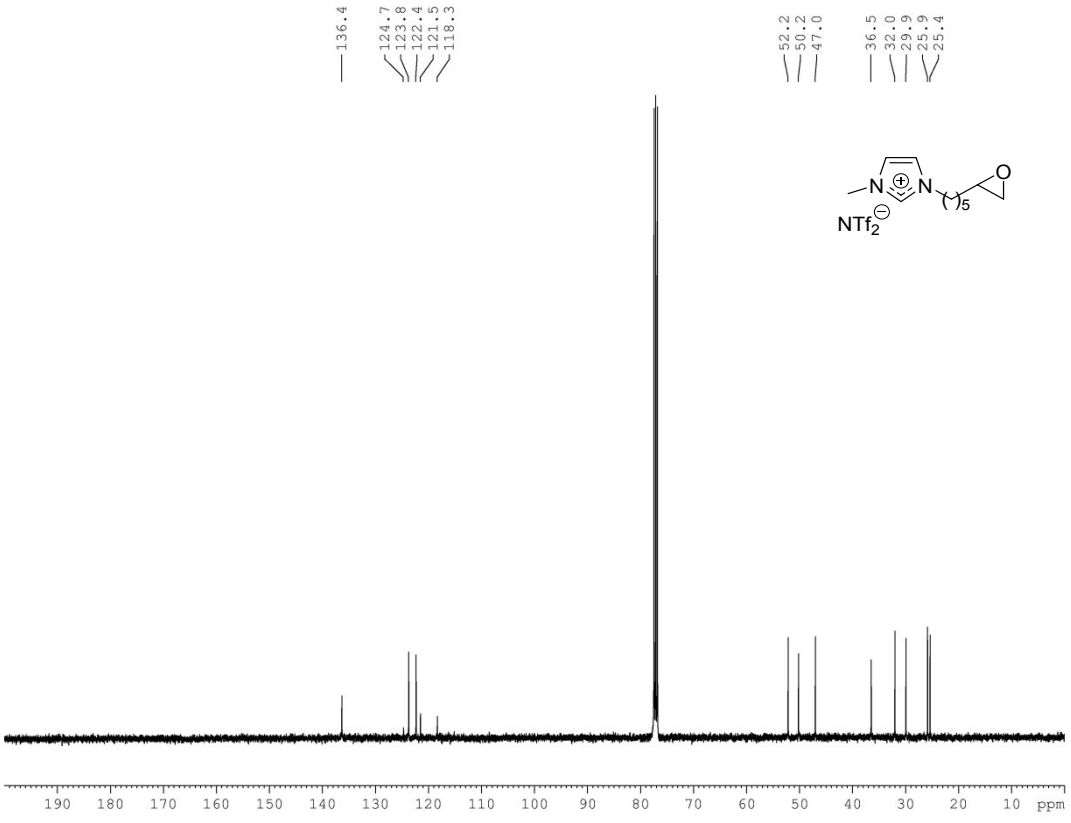

9.11
7.83
7.75
4.59
4.57
4.56
4.10
3.04
3.03
3.02
3.01
2.83
2.72
2.71
2.70
2.49
2.48
2.47
2.40
2.39
2.38
2.37
2.36
2.35
2.05
2.04
2.02
2.00
1.99
1.97
NTf2
9
8
7
6
5
4
3
2
1
ppm
1.00
2.01
2.03
3.00
0.98
1.04
1.01
1.04
1.02

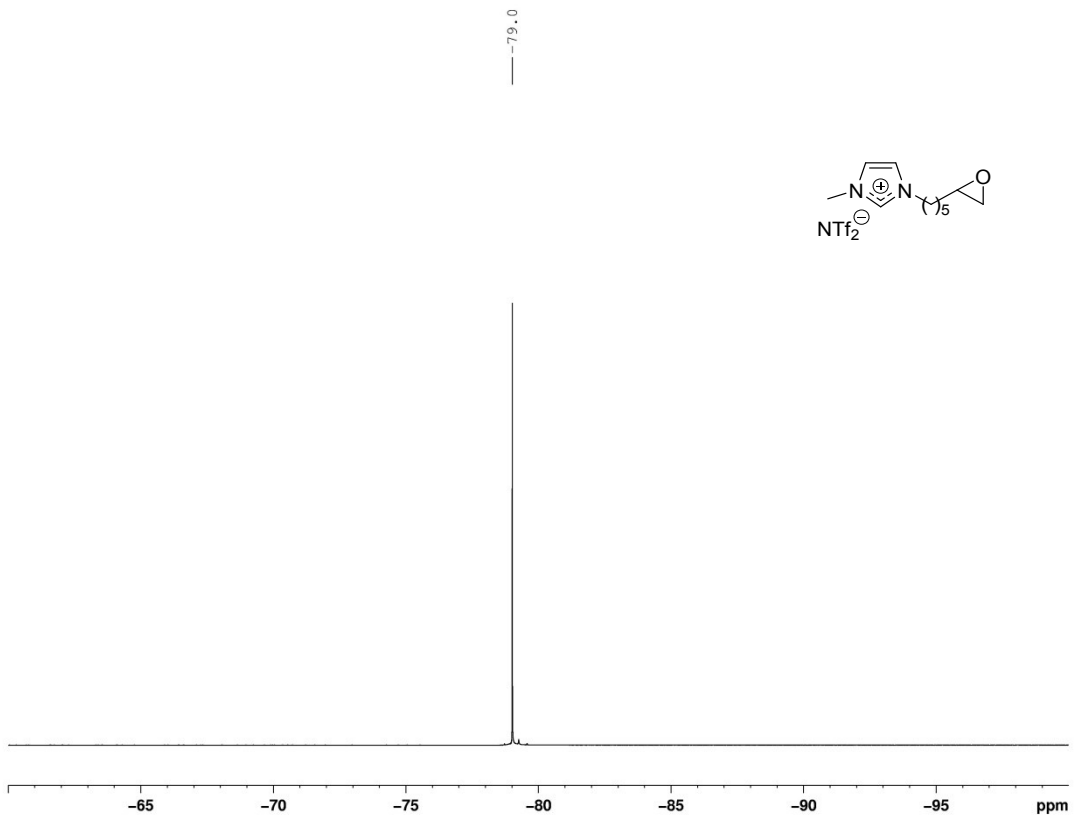

137.7
124.9
123.7
49.6
48.0
46.5
36.7
33.7
N
N
O
2
NTf2
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


80.0
N
N
O
2
NTf2
-65 -70 -75 -80 -85 -90 -95 ppm

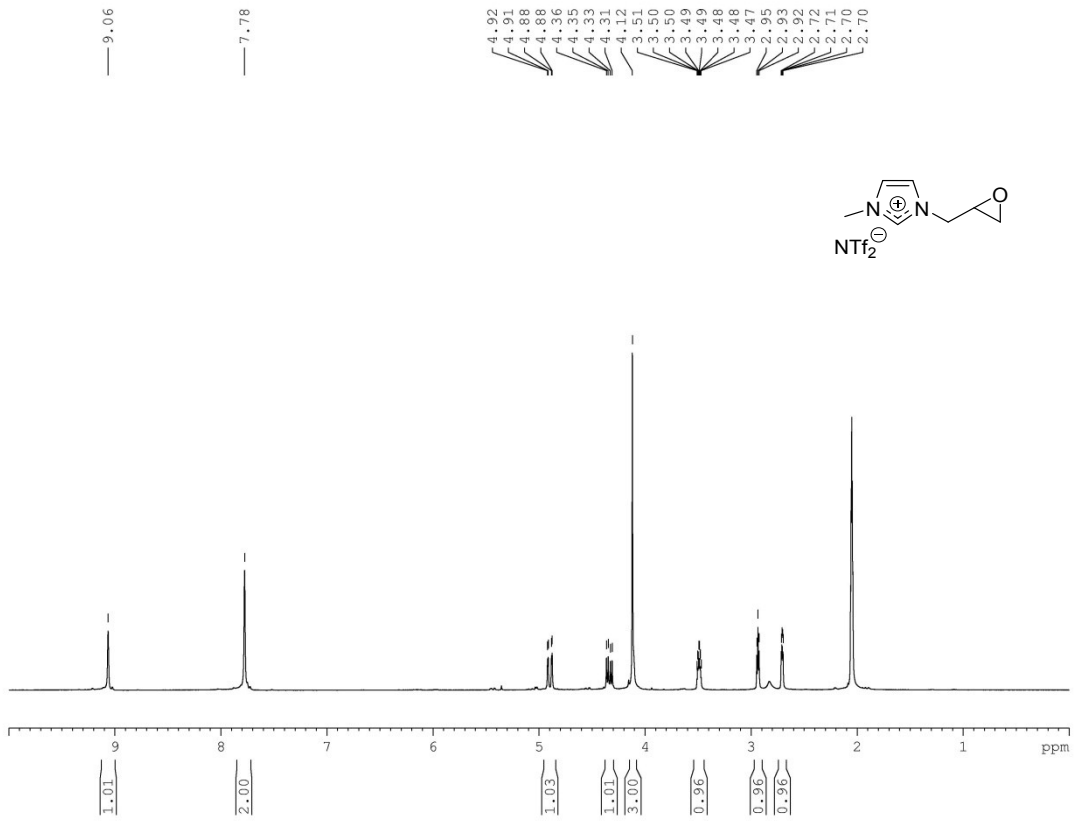
Compound 3b:

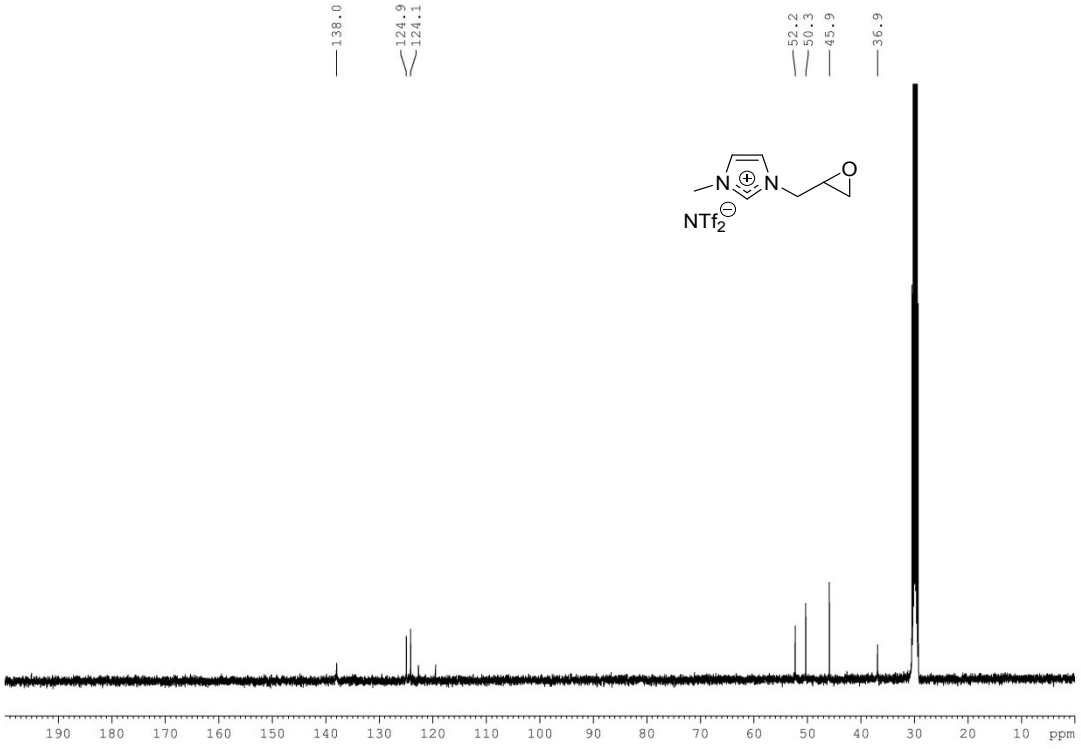

8.77
7.30
7.30
7.30
7.29
4.20
4.18
4.16
3.94
2.90
2.89
2.88
2.88
2.87
2.74
2.73
2.72
2.46
2.46
2.45
2.44
1.93
1.91
1.89
1.87
1.85
1.55
1.53
1.52
1.50
1.48
1.47
1.46
1.44
1.42
1.40
NTf2
9
8
7
6
5
4
3
2
1
ppm
1.00
2.09
2.05
3.00
0.99
0.99
0.99
2.07
6.02

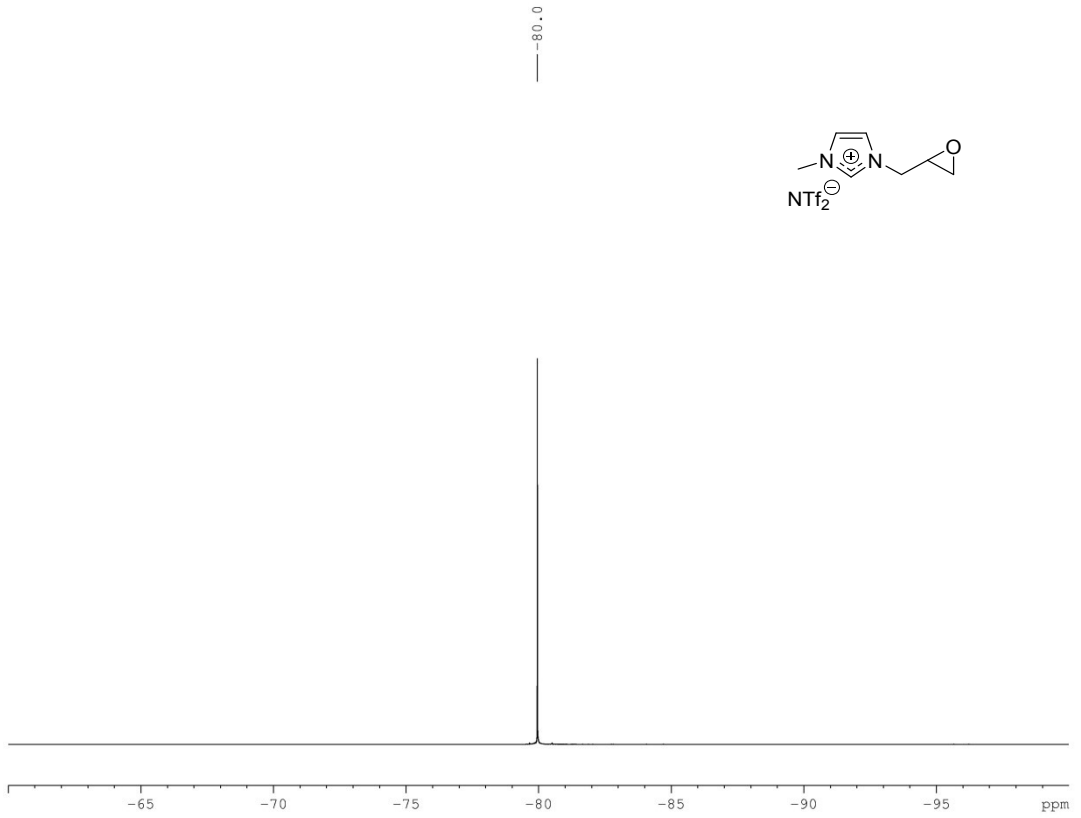

136.4
124.7
123.8
122.4
121.5
118.3
52.2
50.2
47.0
36.5
32.0
29.9
25.9
25.4
NTf2
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


-79.0
NTf2
−65
−70
−75
−80
−85
−90
−95
ppm

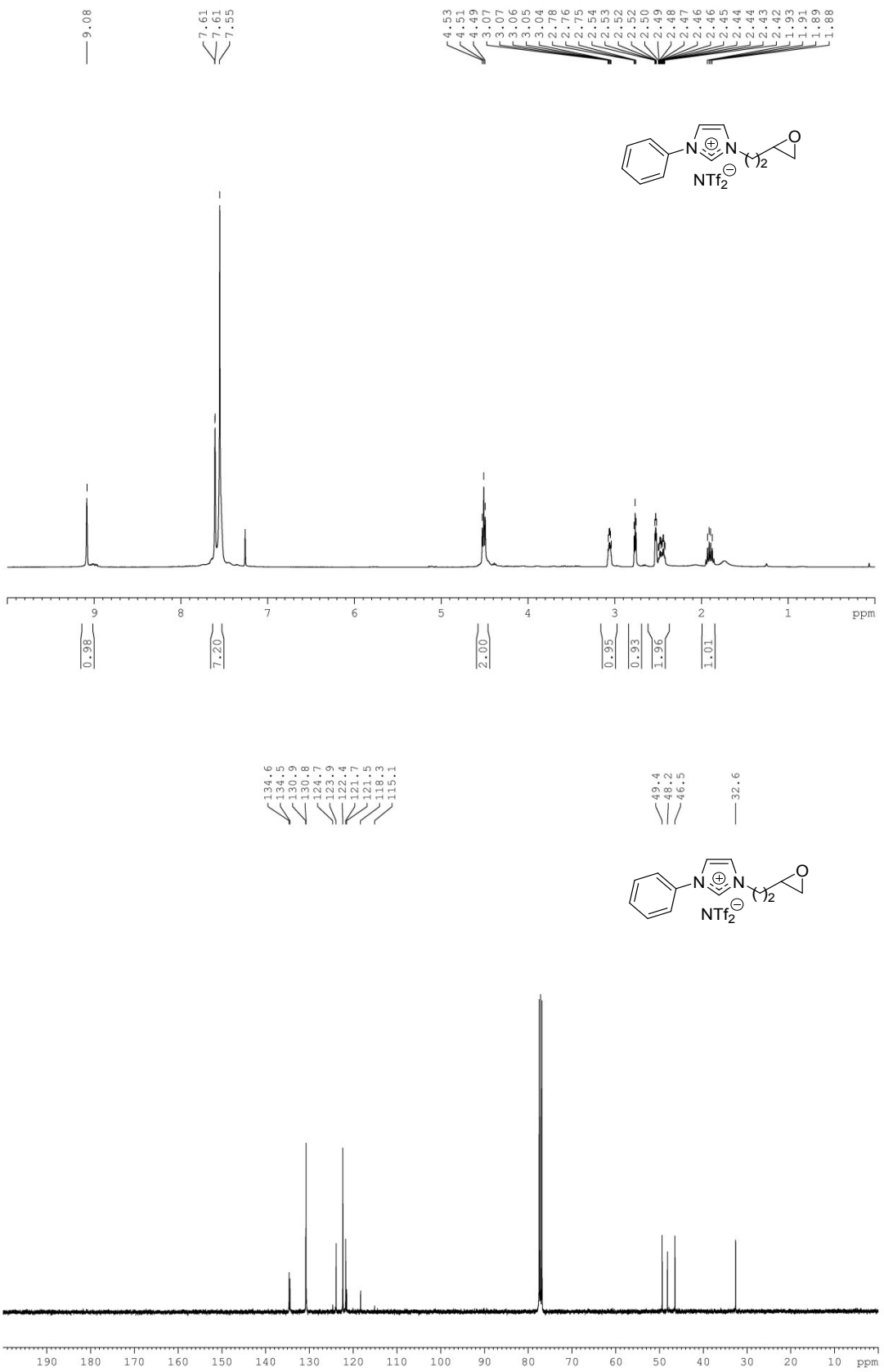
Compound 3c:

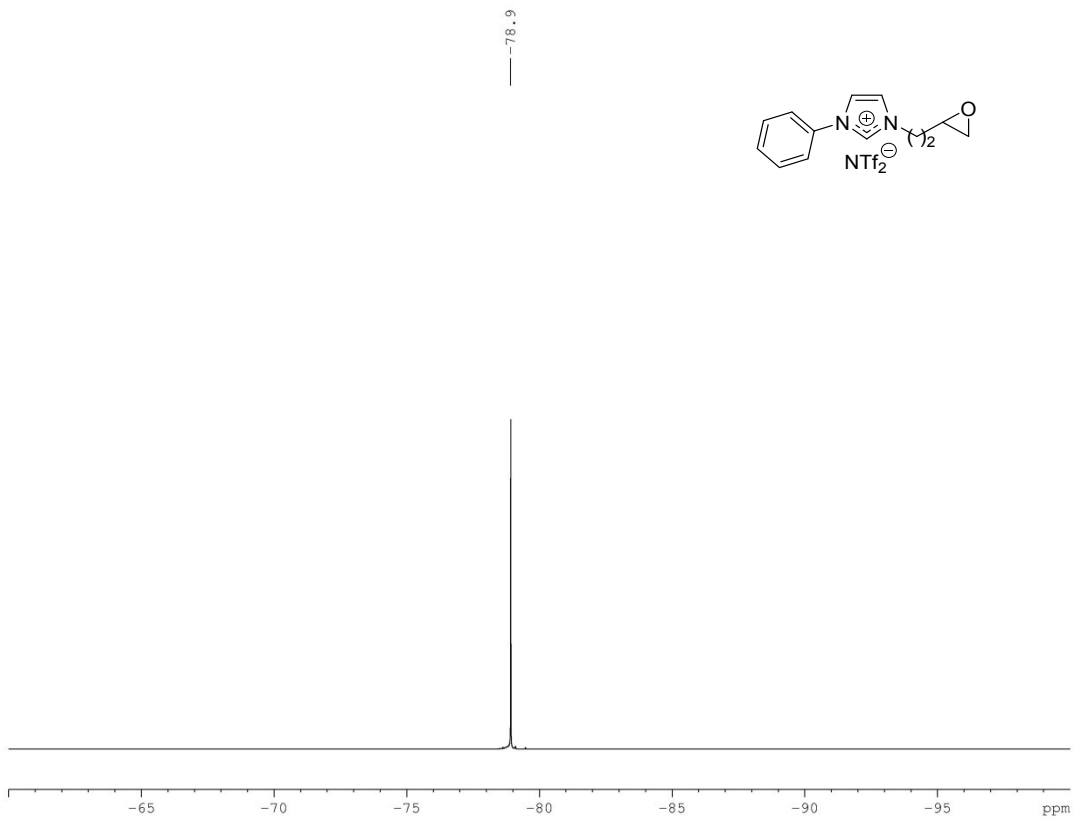

9.06
7.78
4.92
4.91
4.88
4.36
4.35
4.33
4.31
4.12
3.51
3.50
3.49
3.48
3.47
2.95
2.93
2.92
2.72
2.71
2.70
2.70
NTf2
9
8
7
6
5
4
3
2
1
ppm
1.01
2.00
1.03
1.01
3.00
0.96
0.96
0.96


138.0
124.9
124.1
52.2
50.3
45.9
36.9
N
N
O
NTf2
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

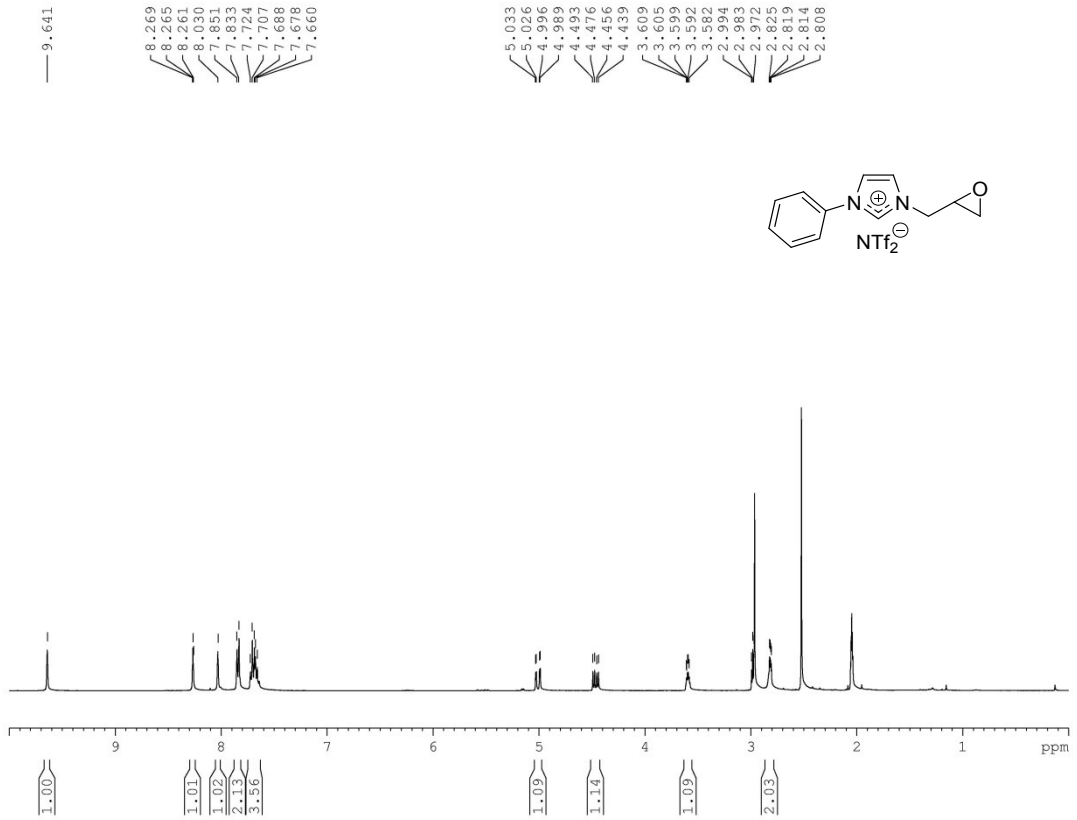

-80.0
N
N
O
NTf2
-65 -70 -75 -80 -85 -90 -95 ppm

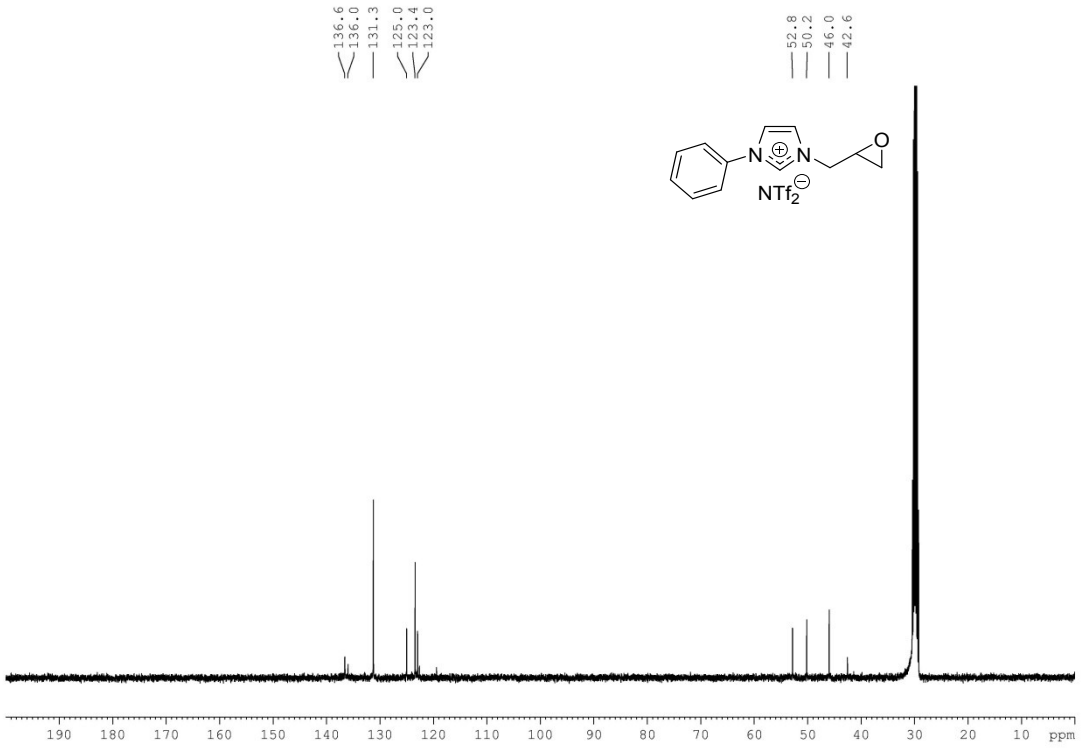
Compound 3d:

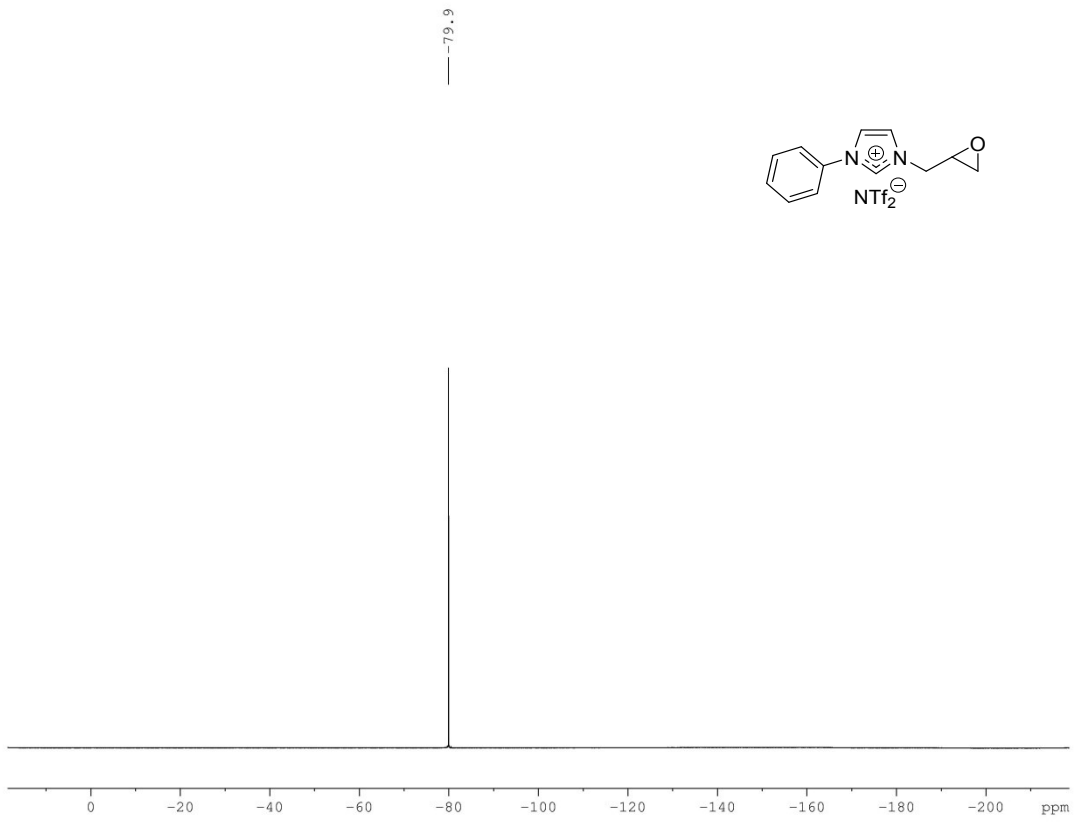

9.08
7.61
7.61
7.55
4.53
4.51
4.49
3.07
3.07
3.06
3.05
3.04
2.78
2.76
2.75
2.54
2.53
2.52
2.52
2.50
2.49
2.48
2.47
2.46
2.46
2.45
2.44
2.44
2.43
2.42
1.93
1.91
1.89
1.88
NTf2
ppm
0.98
7.20
2.00
0.95
0.93
1.96
1.01
134.6
134.5
130.9
130.8
124.7
123.9
122.4
121.7
121.5
118.3
115.1
49.4
48.2
46.5
32.6
NTf2
ppm


-78.9
NTf2
-65
-70
-75
-80
-85
-90
-95
ppm

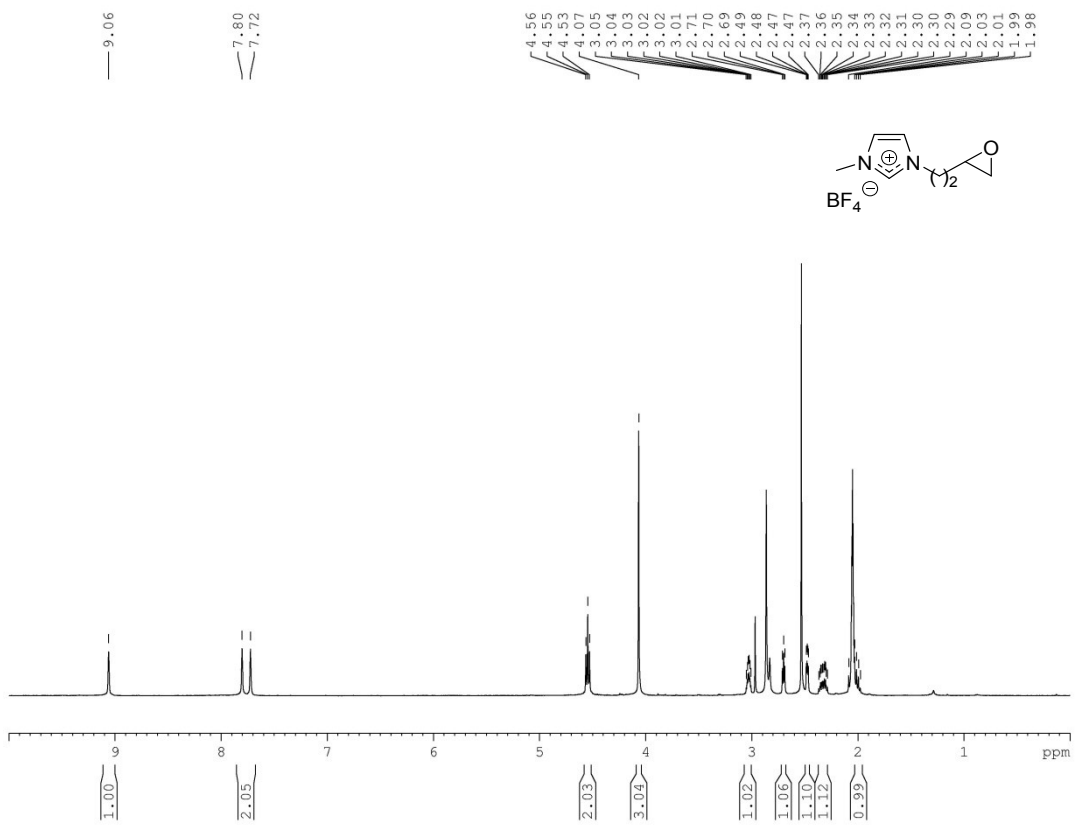
Compound 3e:

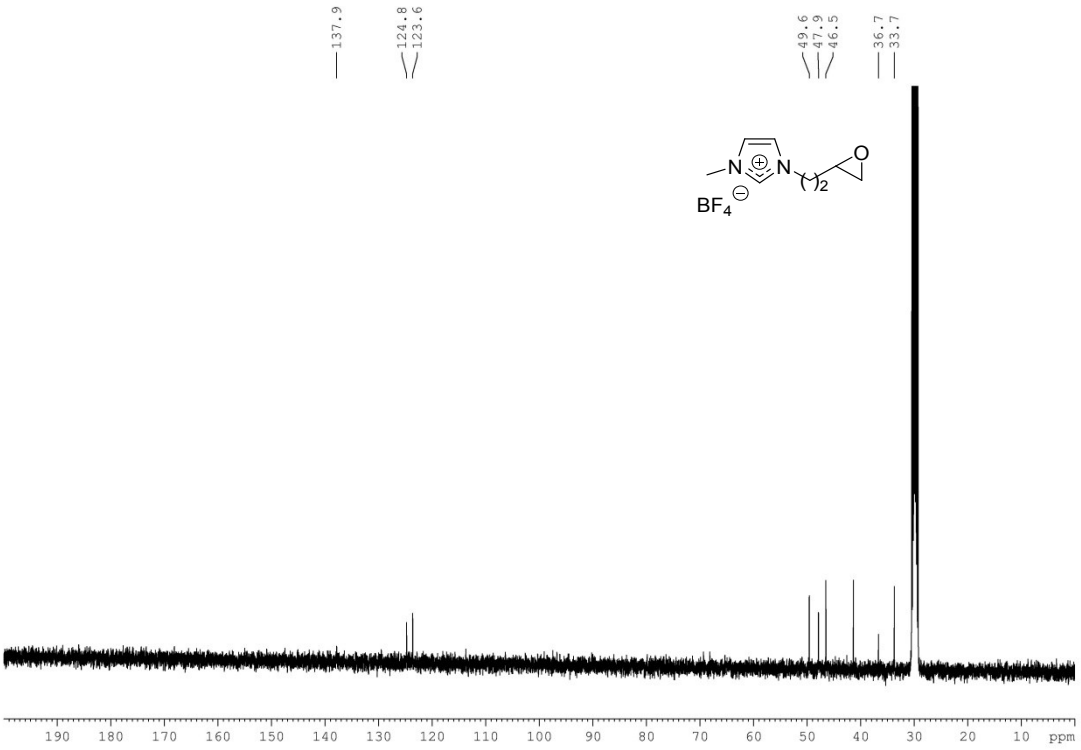

9.641
8.269
8.265
8.261
8.030
7.851
7.833
7.724
7.707
7.688
7.678
7.660
5.033
5.026
4.996
4.989
4.493
4.476
4.456
4.439
3.609
3.605
3.599
3.592
3.582
2.994
2.983
2.972
2.825
2.819
2.814
2.808
NTf2
9
8
7
6
5
4
3
2
1
ppm
1.00
1.01
1.02
2.13
3.56
1.09
1.14
1.09
2.03

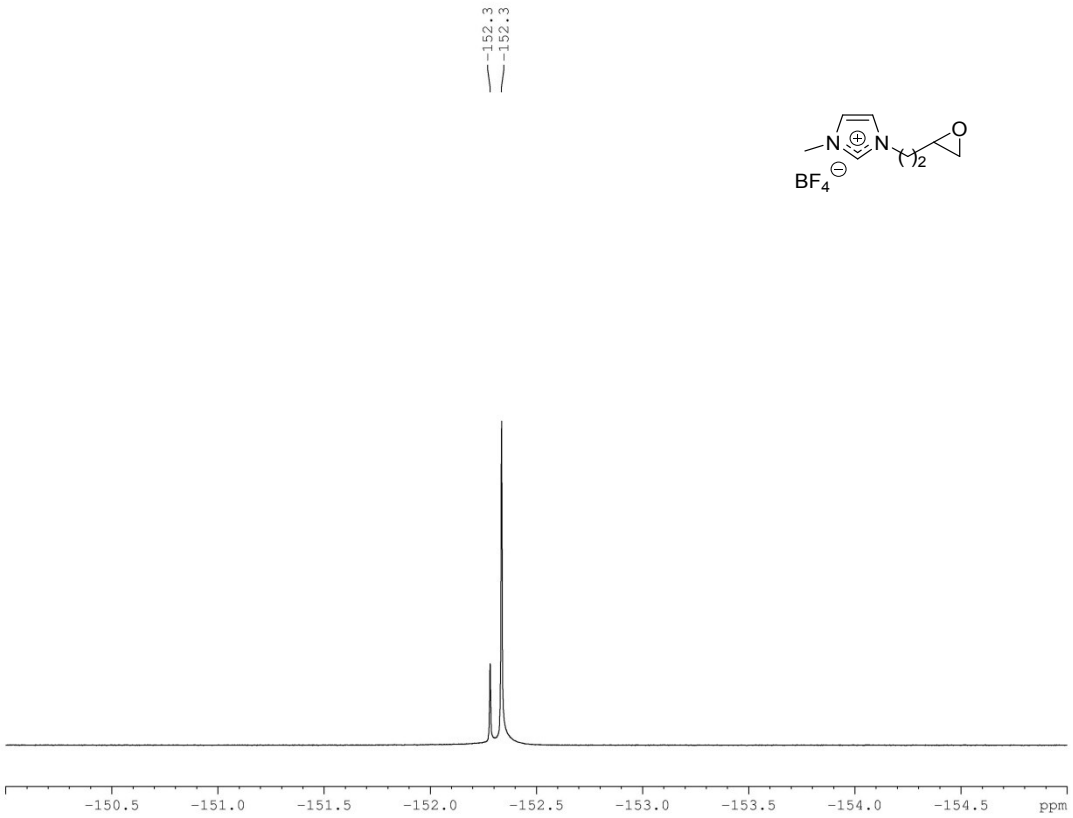

136.6
136.0
131.3
125.0
123.4
123.0
52.8
50.2
46.0
42.6
N
N
O
NTf2
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


-79.9
N
N
O
NTf2
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 ppm

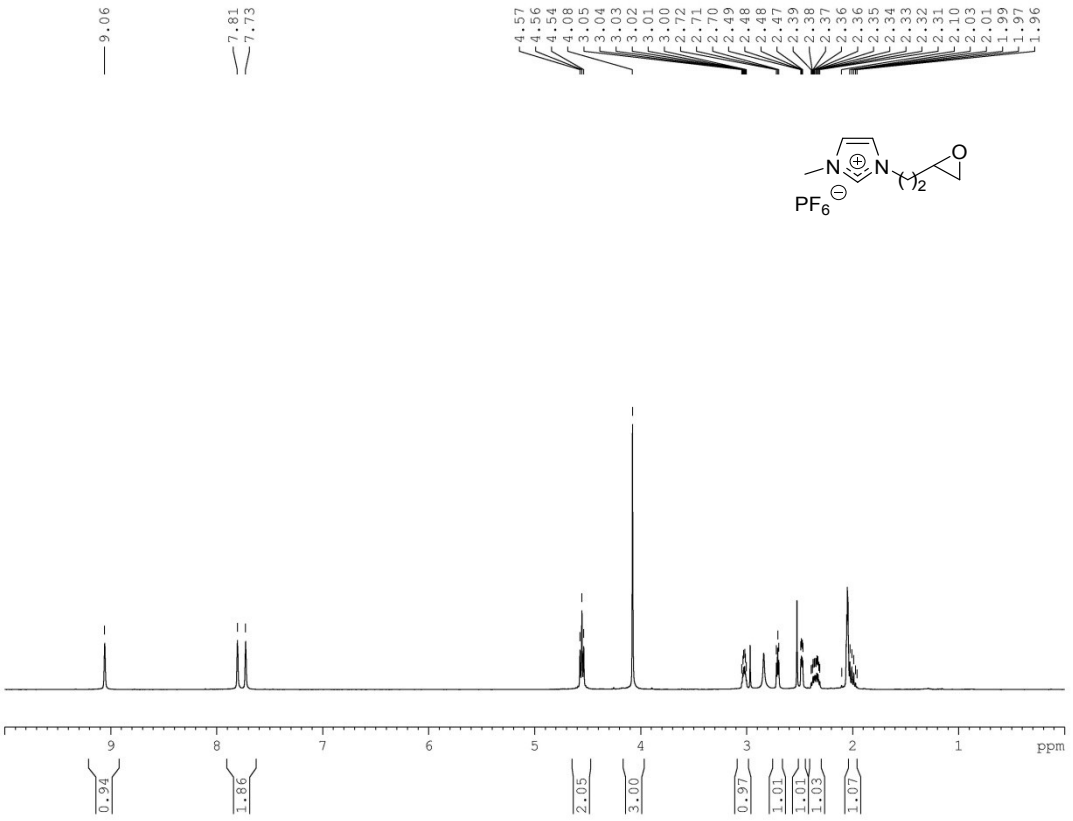
Compound 3f:

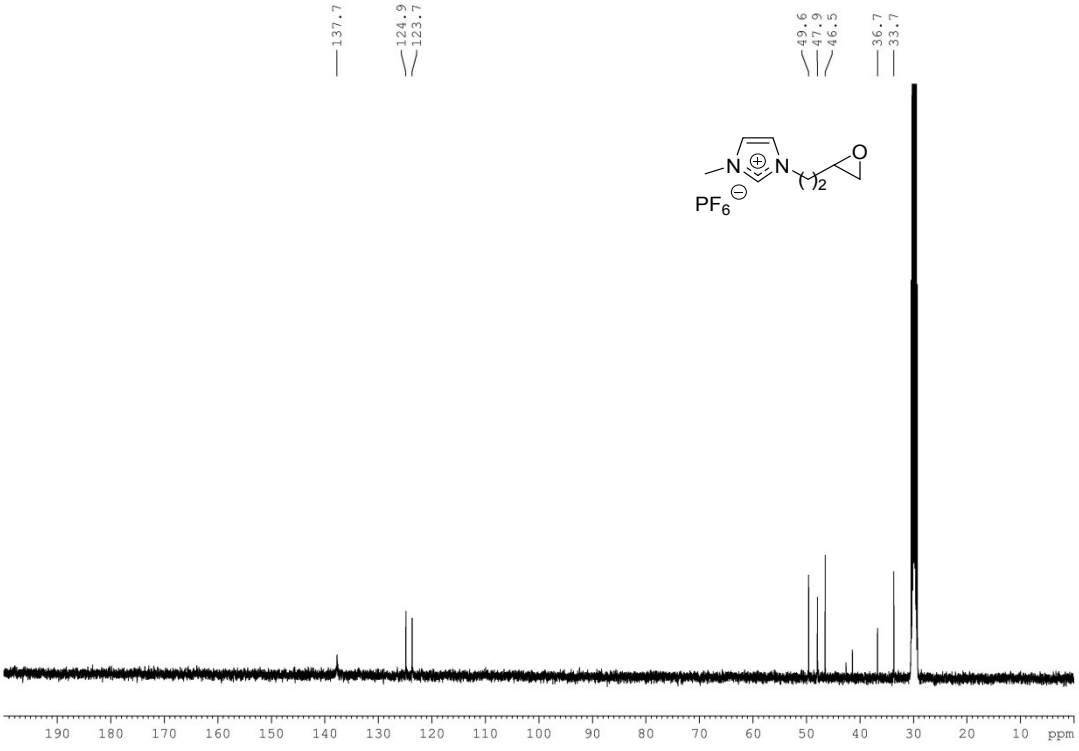

9.06
7.80
7.72
4.56
4.55
4.53
4.07
3.05
3.04
3.03
3.02
3.02
3.01
2.71
2.70
2.69
2.49
2.48
2.47
2.37
2.36
2.35
2.34
2.33
2.32
2.31
2.30
2.30
2.29
2.09
2.03
2.01
1.99
1.98
N
N
O
)2
BF4
9
8
7
6
5
4
3
2
1
ppm
1.00
2.05
2.03
3.04
1.02
1.06
1.10
1.12
0.99

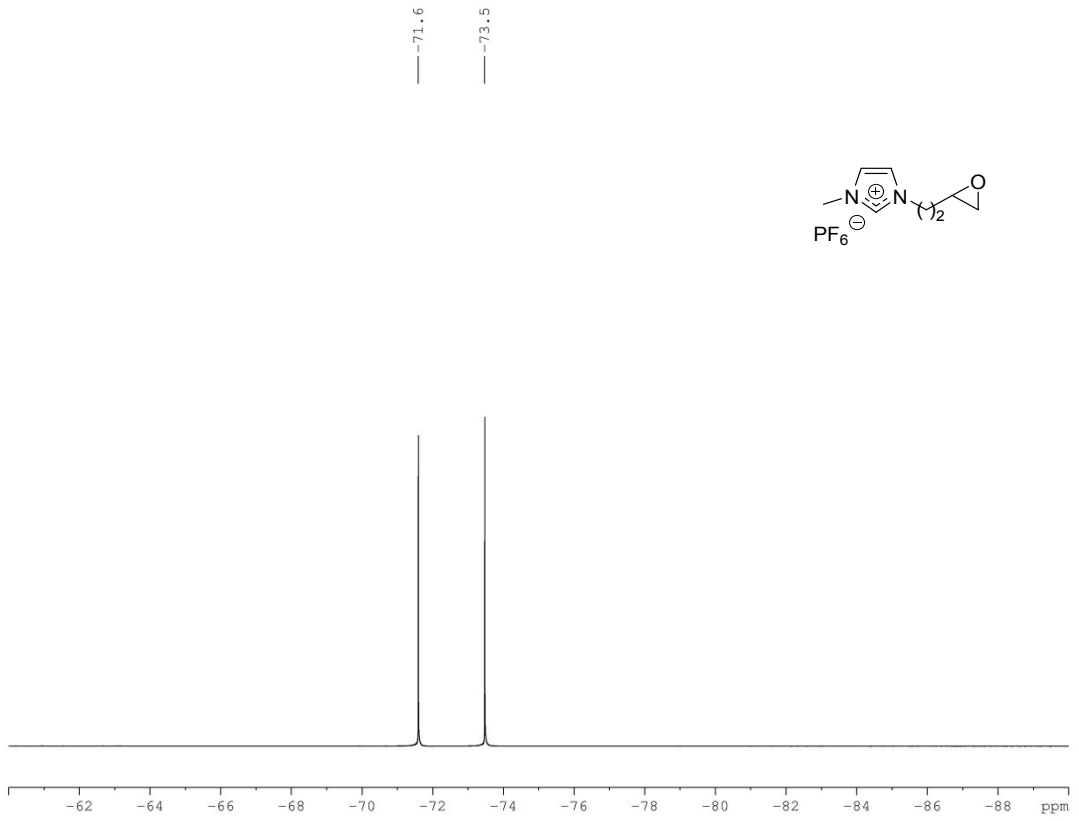

137.9
124.8
123.6
49.6
47.9
46.5
36.7
33.7
N
N
O
)2
BF4
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


-152.3
-152.3
BF4
-150.5
-151.0
-151.5
-152.0
-152.5
-153.0
-153.5
-154.0
-154.5
ppm

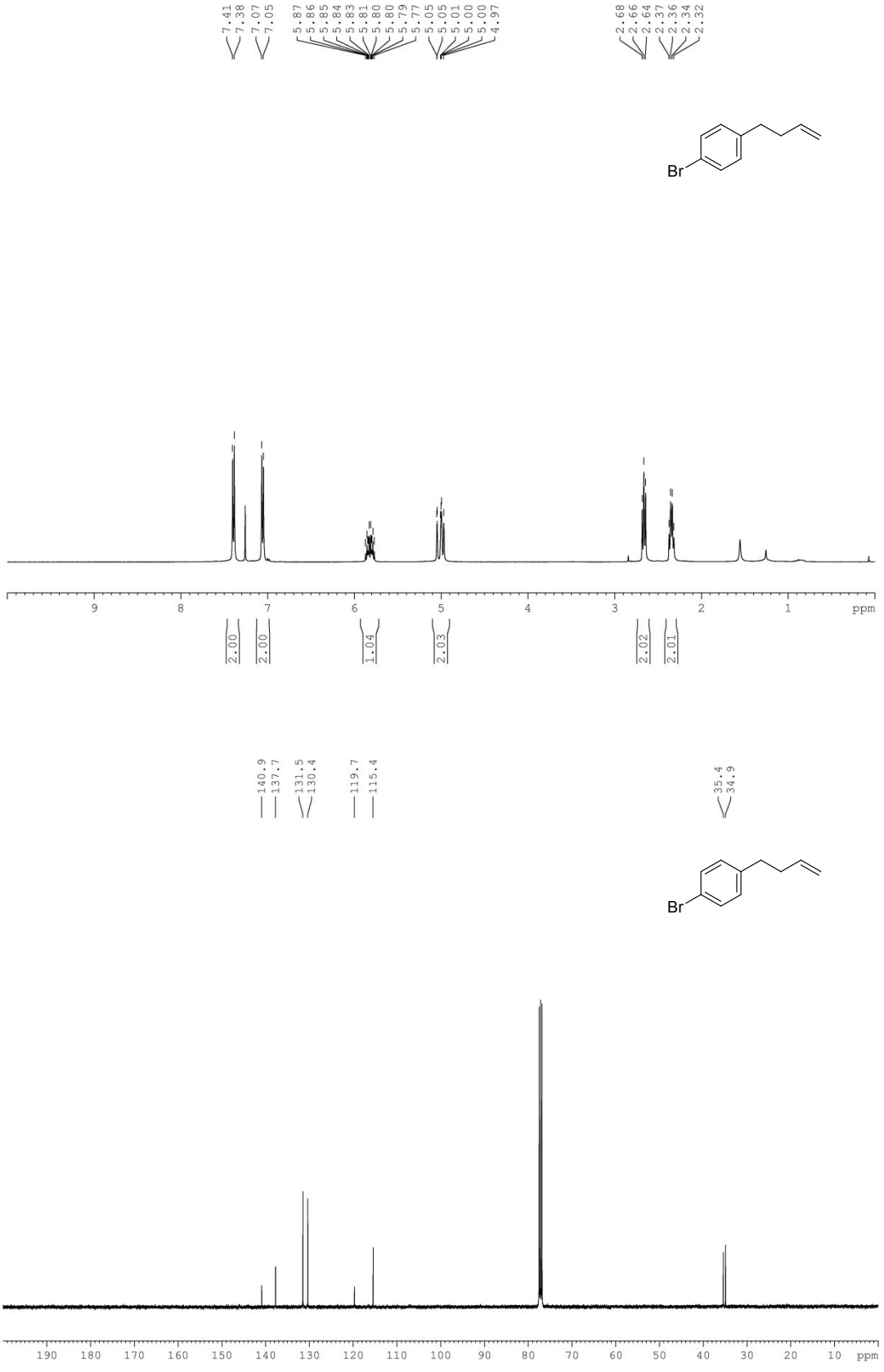
Compound 3g:


9.06
7.81
7.73
4.57
4.56
4.54
4.08
3.05
3.04
3.03
3.02
3.01
3.00
2.72
2.71
2.70
2.49
2.48
2.48
2.47
2.39
2.38
2.37
2.36
2.36
2.35
2.34
2.33
2.32
2.31
2.10
2.03
2.01
1.99
1.97
1.96
PF6
9
8
7
6
5
4
3
2
1
ppm
0.94
1.86
2.05
3.00
0.97
1.01
1.01
1.03
1.07

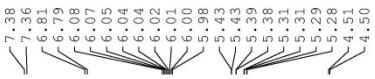

137.7
124.9
123.7
49.6
47.9
46.5
36.7
33.7
N
N
O
PF6
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

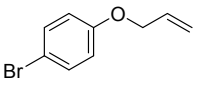

-71.6
-73.5
N
N
O
PF6
-62 -64 -66 -68 -70 -72 -74 -76 -78 -80 -82 -84 -86 -88 ppm

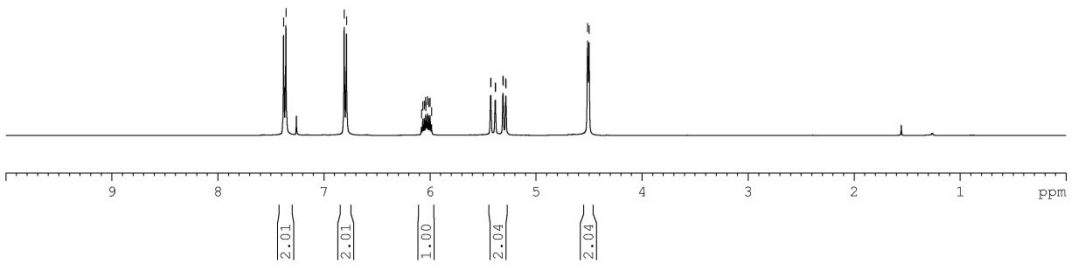
Compound 4a:


7.41
7.38
7.07
7.05
5.87
5.86
5.85
5.84
5.83
5.81
5.80
5.80
5.79
5.77
5.05
5.05
5.01
5.00
5.00
4.97
2.68
2.66
2.64
2.37
2.36
2.34
2.32
Br
9
8
7
6
5
4
3
2
1
ppm
2.00
2.00
1.04
2.03
2.02
2.01
140.9
137.7
131.5
130.4
119.7
115.4
35.4
34.9
Br
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

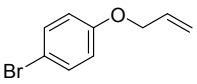
Compound 4b:

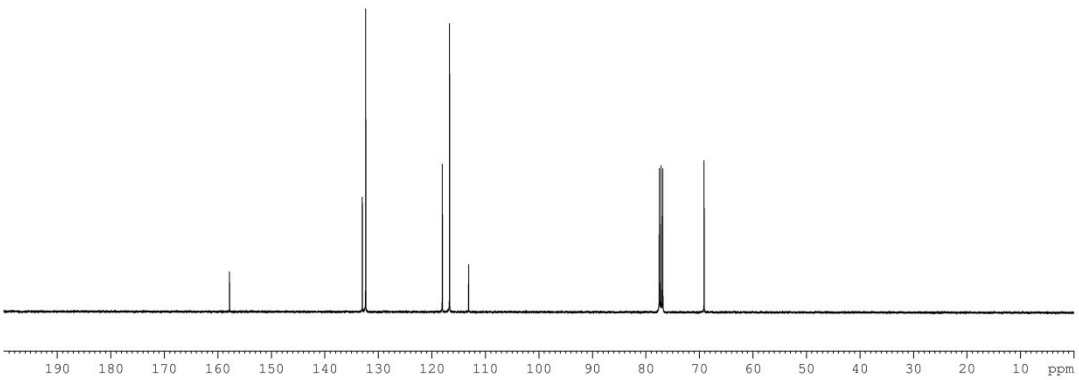

7.38
7.36
6.81
6.79
6.08
6.07
6.05
6.04
6.04
6.02
6.01
6.00
5.98
5.43
5.39
5.38
5.31
5.31
5.29
5.28
4.51
4.50


O
Br

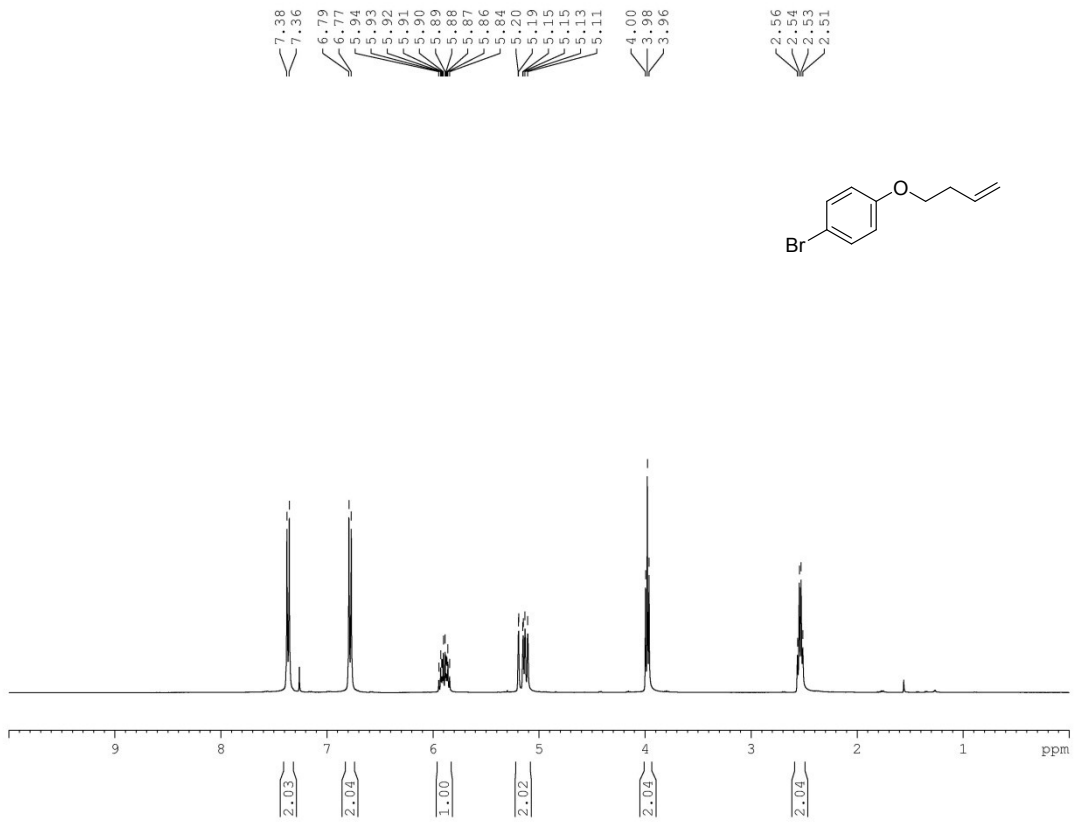

9
8
7
6
5
4
3
2
1
ppm
2.01
2.01
1.00
2.04
2.04

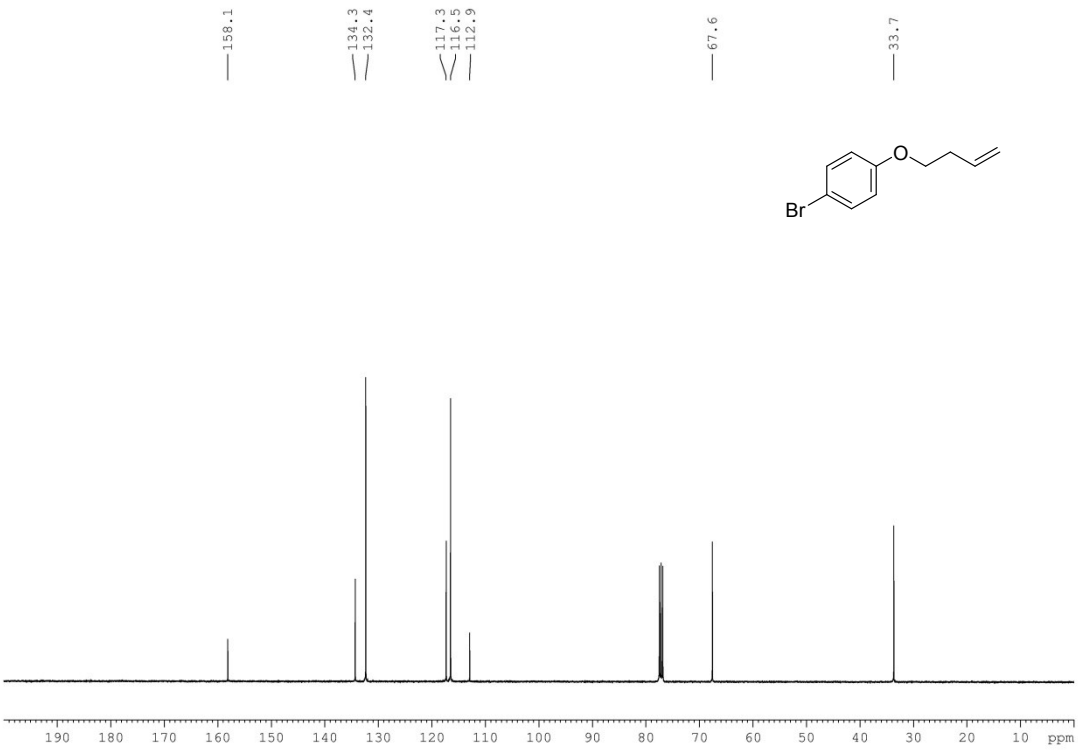

157.8
133.0
132.4
118.0
116.7
113.1
69.1


O
Br

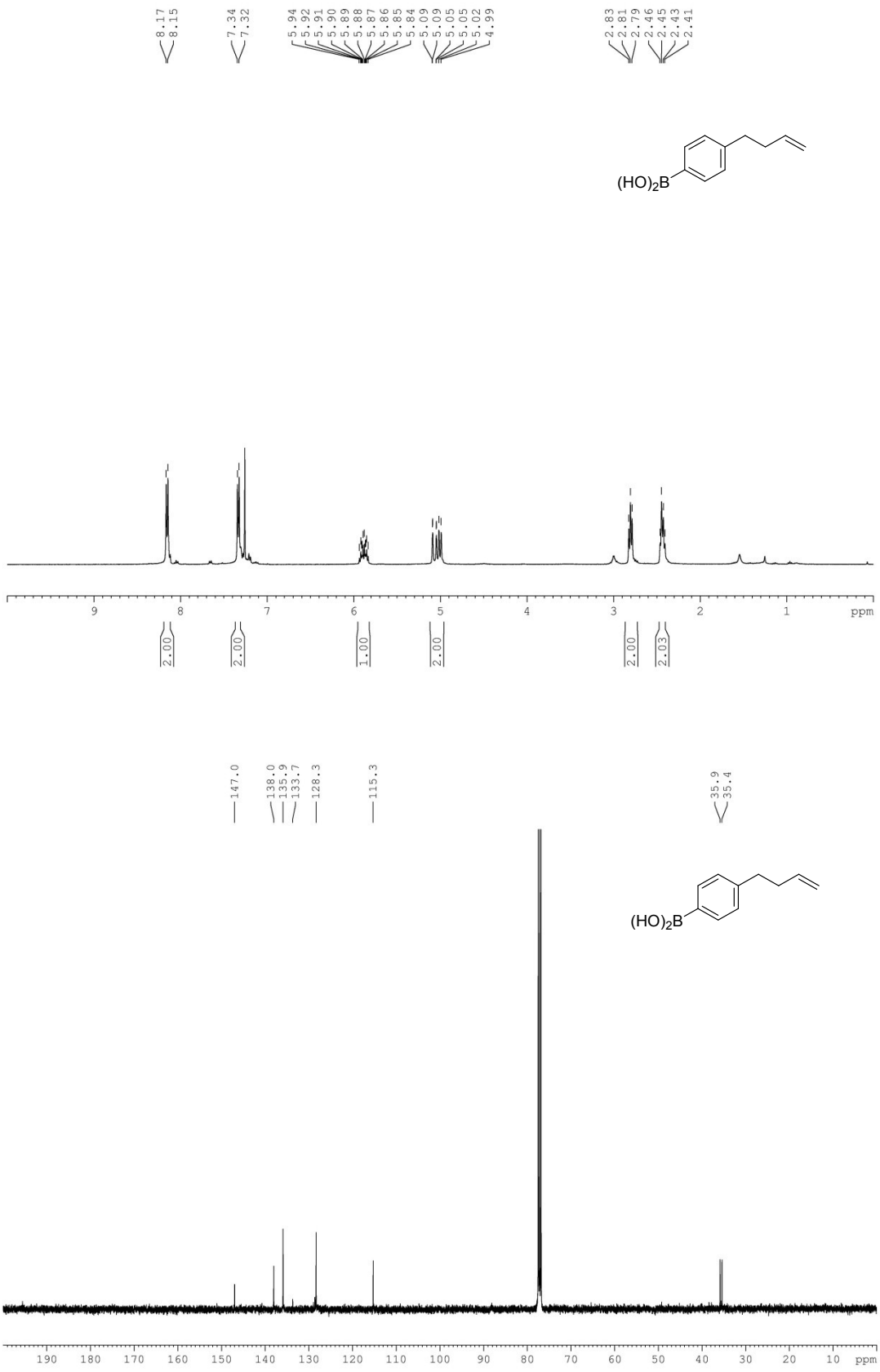

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

Compound 4c:

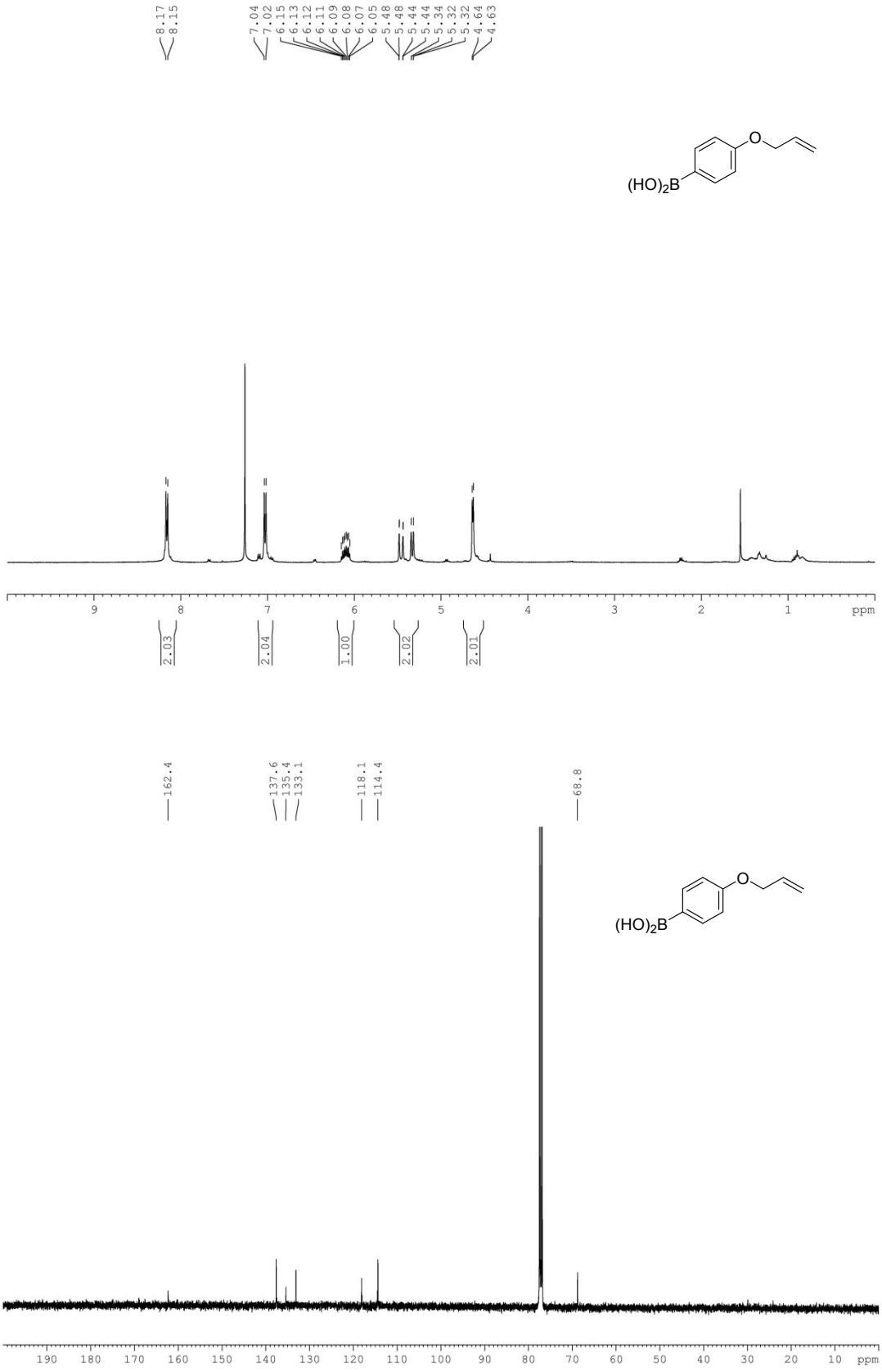

7.38
7.36
6.79
6.77
5.94
5.93
5.92
5.91
5.90
5.89
5.88
5.87
5.86
5.84
5.20
5.19
5.15
5.15
5.13
5.11
4.00
3.98
3.96
2.56
2.54
2.53
2.51
O
Br
9
8
7
6
5
4
3
2
1
ppm
2.03
2.04
1.00
2.02
2.04
2.04


158.1
134.3
132.4
117.3
116.5
112.9
67.6
33.7
O
Br
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

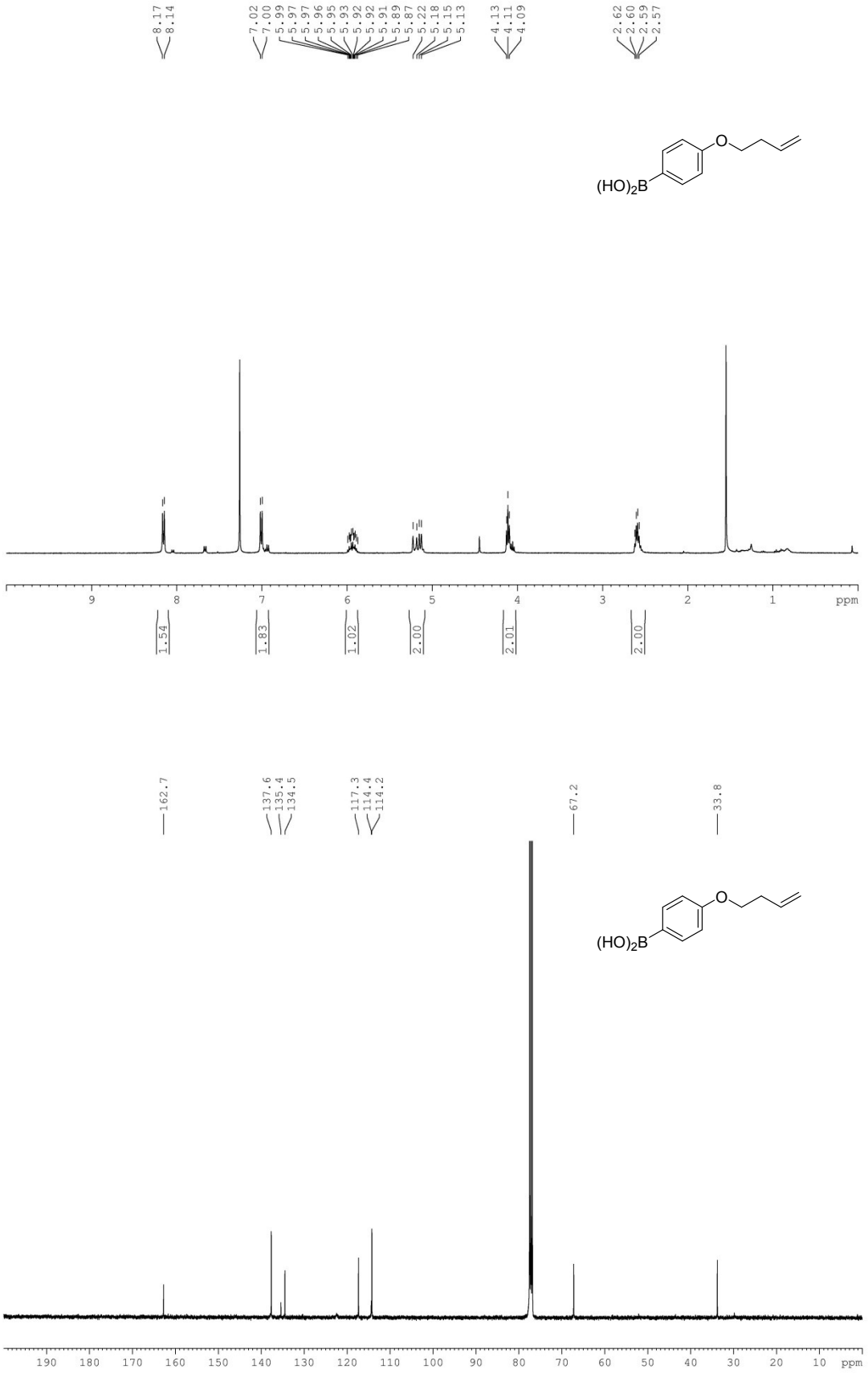
Compound 5a:


8.17
8.15
7.34
7.32
5.94
5.92
5.91
5.90
5.89
5.88
5.87
5.86
5.85
5.84
5.09
5.09
5.05
5.05
5.02
4.99
2.83
2.81
2.79
2.46
2.45
2.43
2.41
(HO)2B
9
8
7
6
5
4
3
2
1
ppm
2.00
2.00
1.00
2.00
2.00
2.03
147.0
138.0
135.9
133.7
128.3
115.3
35.9
35.4
(HO)2B
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

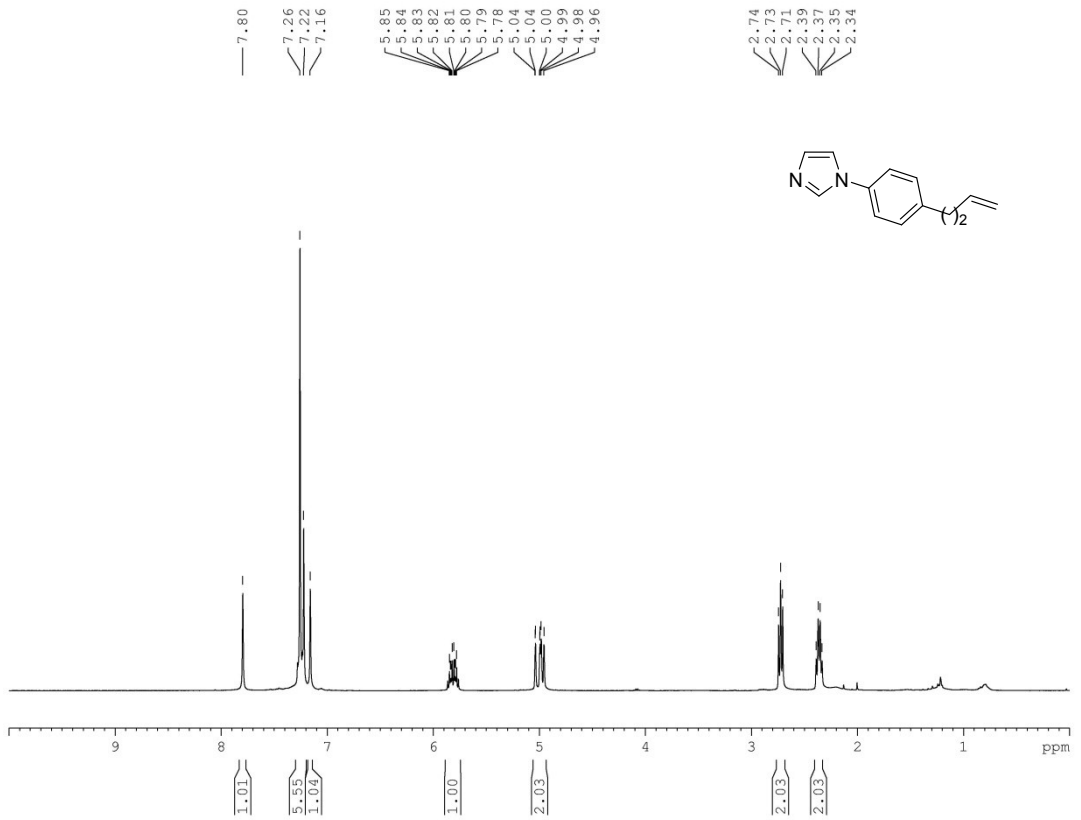
Compound 5b:

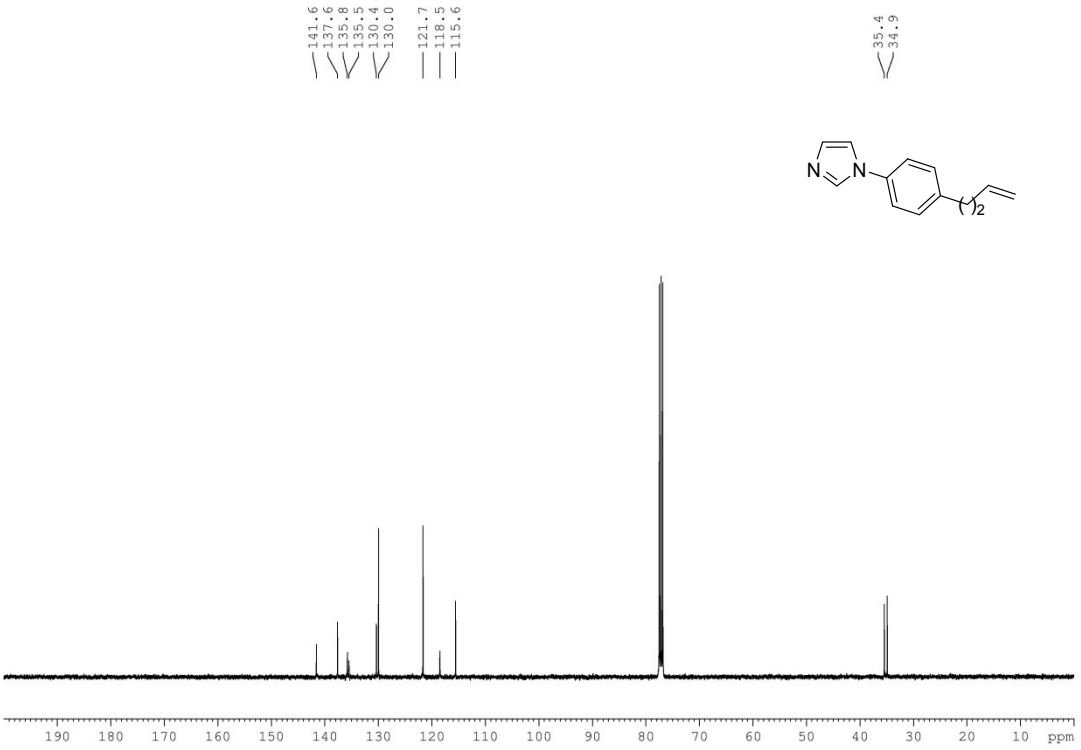

8.17
8.15
7.04
7.02
6.15
6.13
6.12
6.11
6.09
6.08
6.07
6.05
5.48
5.48
5.44
5.44
5.34
5.32
4.64
4.63
O
(HO)2B
9
8
7
6
5
4
3
2
1
ppm
2.03
2.04
1.00
2.02
2.01
162.4
137.6
135.4
133.1
118.1
114.4
68.8
O
(HO)2B
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

Compound 5c:

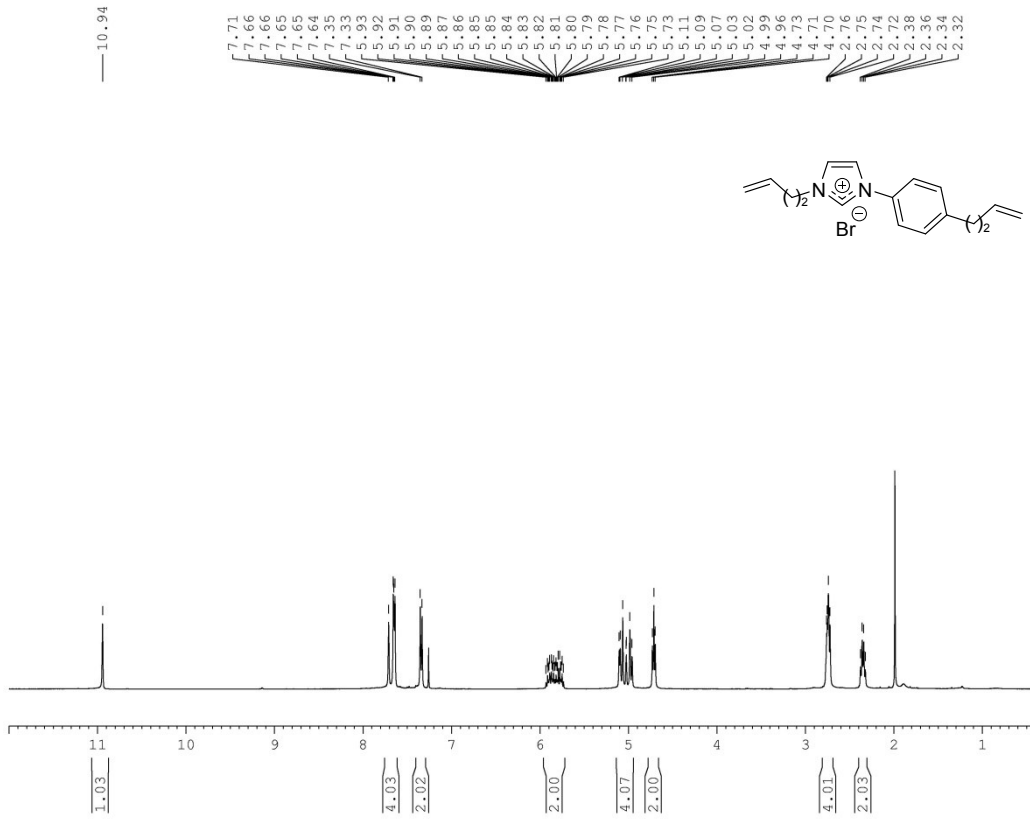

8.17
8.14
7.02
7.00
5.99
5.97
5.97
5.96
5.95
5.93
5.92
5.92
5.91
5.89
5.87
5.22
5.18
5.15
5.13
4.13
4.11
4.09
2.62
2.60
2.59
2.57
O
(HO)2B
9
8
7
6
5
4
3
2
1
ppm
1.54
1.83
1.02
2.00
2.01
2.00
162.7
137.6
135.4
134.5
117.3
114.4
114.2
67.2
33.8
O
(HO)2B
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

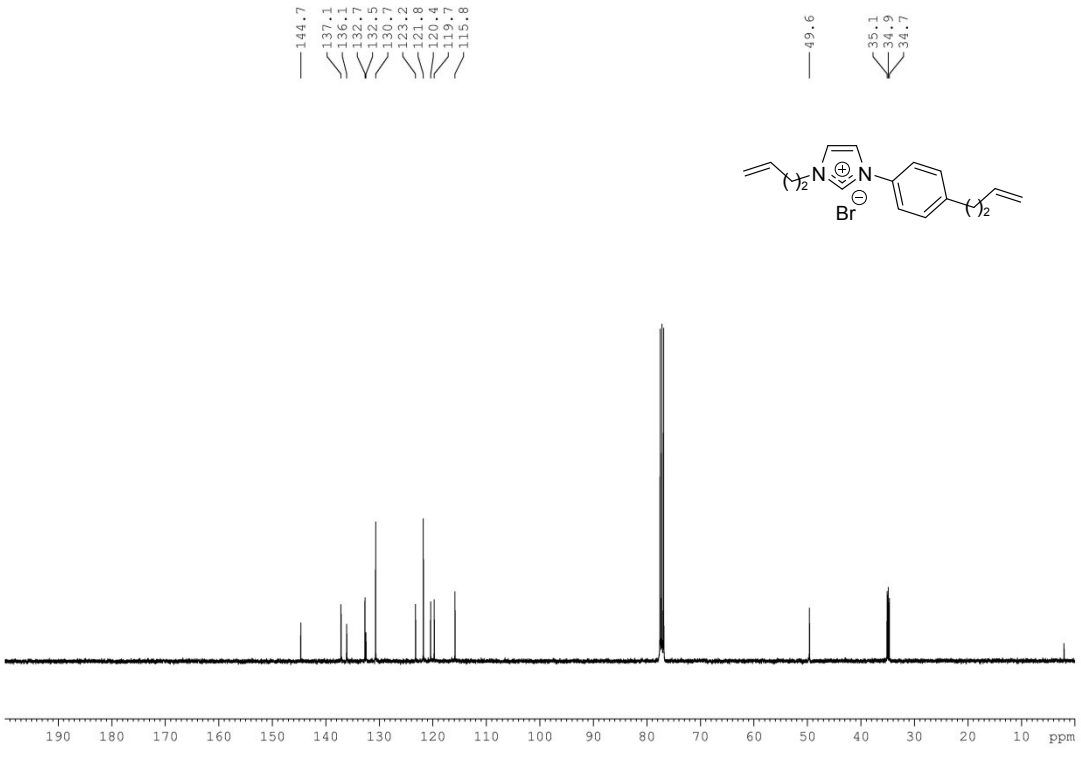
Compound 6:


7.80
7.26
7.22
7.16
5.85
5.84
5.83
5.82
5.81
5.80
5.79
5.78
5.04
5.00
4.99
4.98
4.96
2.74
2.73
2.71
2.39
2.37
2.35
2.34
N
N
2
9
8
7
6
5
4
3
2
1
ppm
1.01
5.55
1.04
1.00
2.03
2.03
2.03

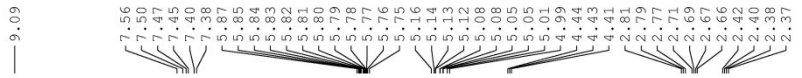

141.6
137.6
135.8
135.5
130.4
130.0
121.7
118.5
115.6
35.4
34.9
N
N
2
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

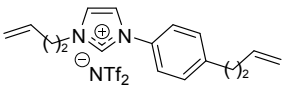
Compound 7a:

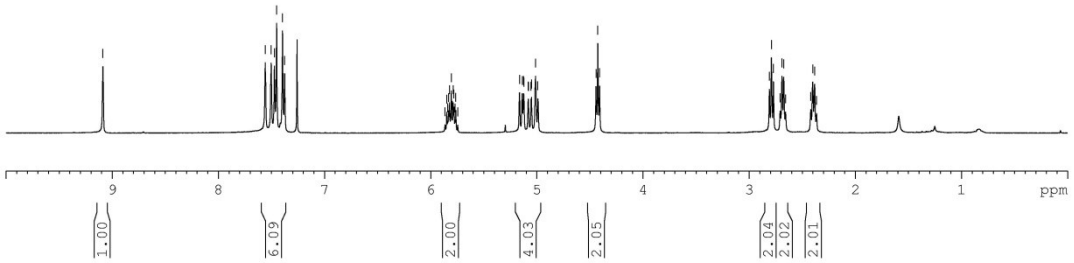

10.94
7.71
7.66
7.66
7.65
7.65
7.64
7.35
7.33
5.93
5.92
5.91
5.90
5.89
5.87
5.86
5.85
5.85
5.84
5.83
5.82
5.81
5.80
5.79
5.78
5.77
5.76
5.75
5.73
5.11
5.09
5.07
5.03
5.02
4.99
4.96
4.73
4.71
4.70
2.76
2.75
2.74
2.72
2.38
2.36
2.34
2.32
Br
11
10
9
8
7
6
5
4
3
2
1
ppm
1.03
4.03
2.02
2.00
4.07
2.00
4.01
2.03

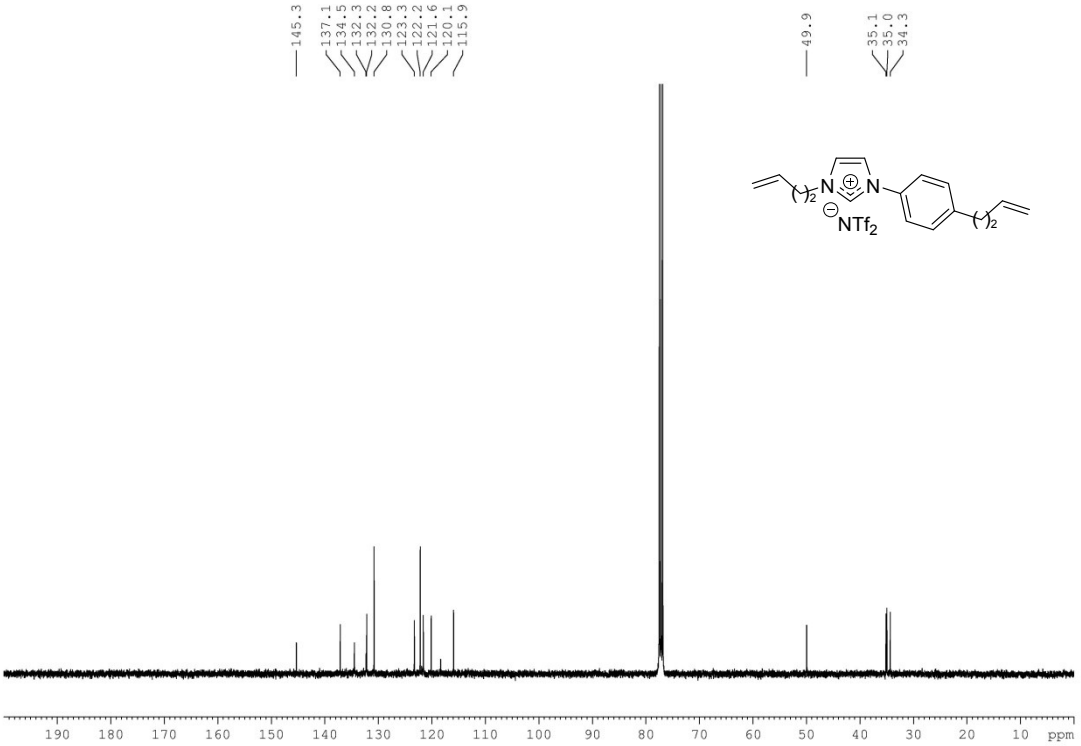

144.7
137.1
136.1
132.7
132.5
130.7
123.2
121.8
120.4
119.7
115.8
49.6
35.1
34.9
34.7
Br
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

Compound 7b:

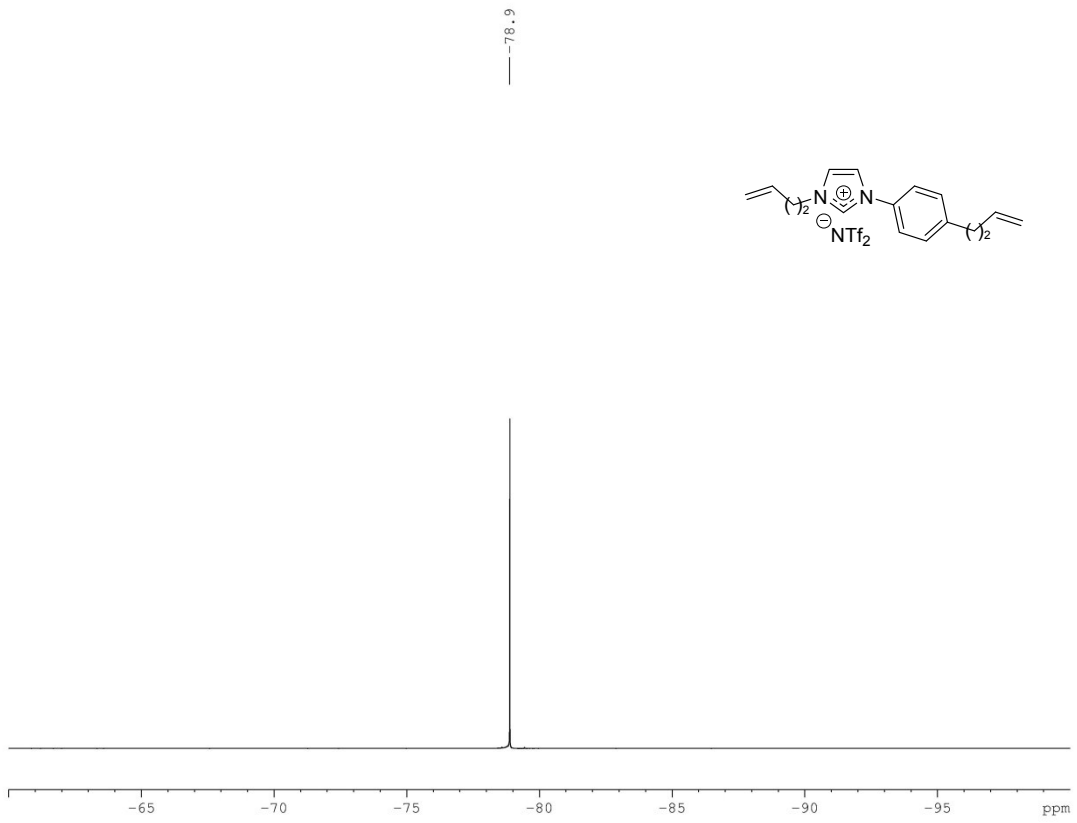

9.09
7.56
7.50
7.47
7.45
7.40
7.38
5.87
5.85
5.84
5.83
5.82
5.81
5.80
5.79
5.78
5.77
5.76
5.75
5.16
5.14
5.13
5.12
5.08
5.08
5.05
5.05
5.01
4.99
4.44
4.43
4.41
2.81
2.79
2.77
2.71
2.69
2.67
2.66
2.42
2.40
2.38
2.37


N
N
NTf2

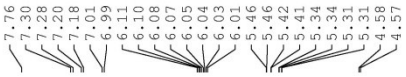

9
8
7
6
5
4
3
2
1
ppm
1.00
6.09
2.00
4.03
2.05
2.04
2.02
2.01

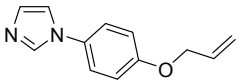

145.3
137.1
134.5
132.3
132.2
130.8
123.3
122.2
121.6
120.1
115.9
49.9
35.1
35.0
34.3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

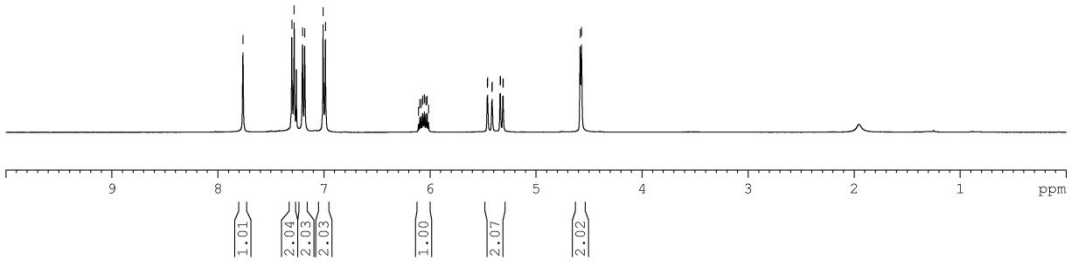
N
N
NTf2


-78.9
N
N
NTf2
-65
-70
-75
-80
-85
-90
-95
ppm

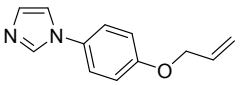
Compound 8:

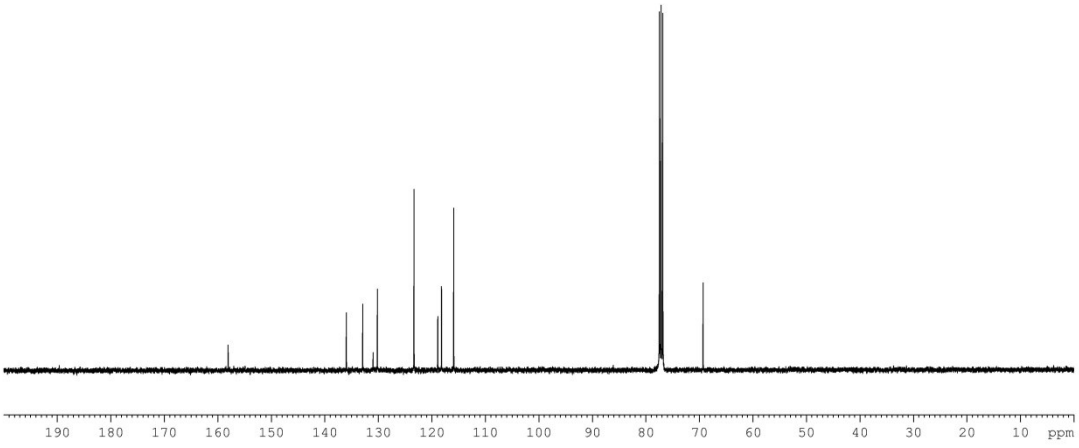

7.76
7.30
7.28
7.20
7.18
7.01
6.99
6.11
6.10
6.08
6.07
6.05
6.04
6.03
6.01
5.46
5.42
5.41
5.34
5.31
5.31
4.58
4.57



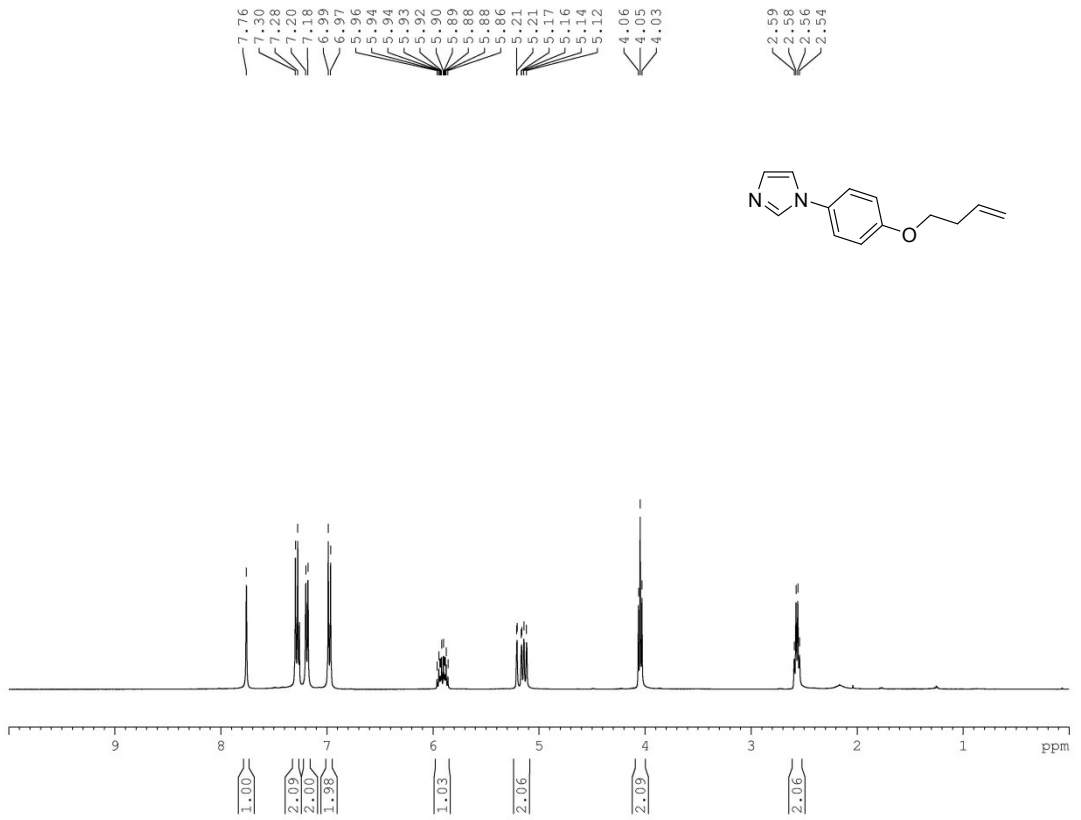

9
8
7
6
5
4
3
2
1
ppm
1.01
2.04
2.03
2.03
1.00
2.07
2.02

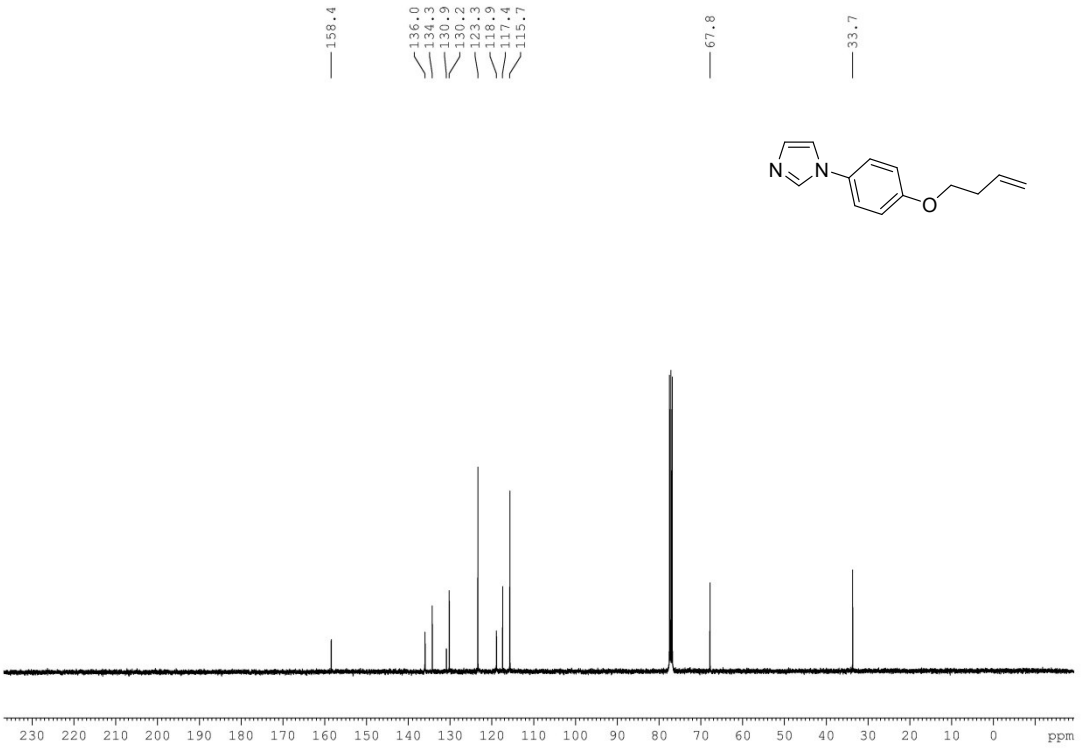

158.1
136.0
132.9
131.0
130.2
123.3
118.9
118.2
115.9
69.3



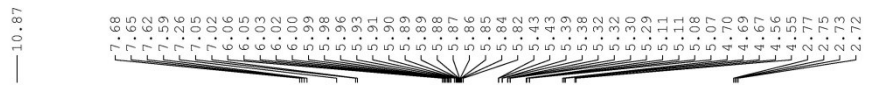

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

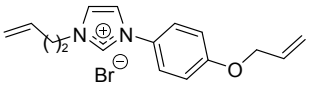
Compound 9:

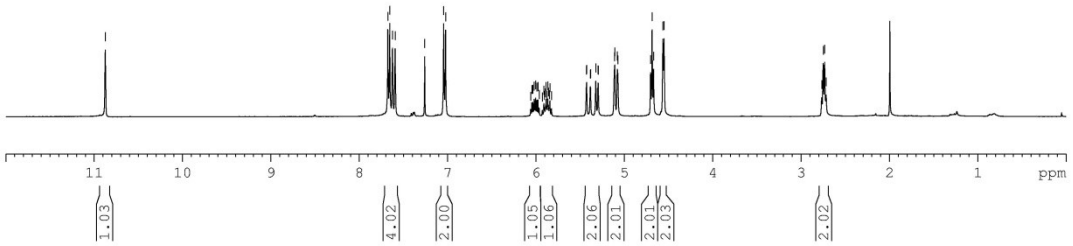

7.76
7.30
7.28
7.20
7.18
6.99
6.97
5.96
5.94
5.94
5.93
5.92
5.90
5.89
5.88
5.88
5.86
5.21
5.21
5.17
5.16
5.14
5.12
4.06
4.05
4.03
2.59
2.58
2.56
2.54
N
N
O
9
8
7
6
5
4
3
2
1
ppm
1.00
2.09
2.00
1.98
1.03
2.06
2.09
2.06

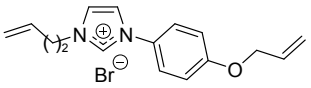

158.4
136.0
134.3
130.9
130.2
123.3
118.9
117.4
115.7
67.8
33.7
N
N
O
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

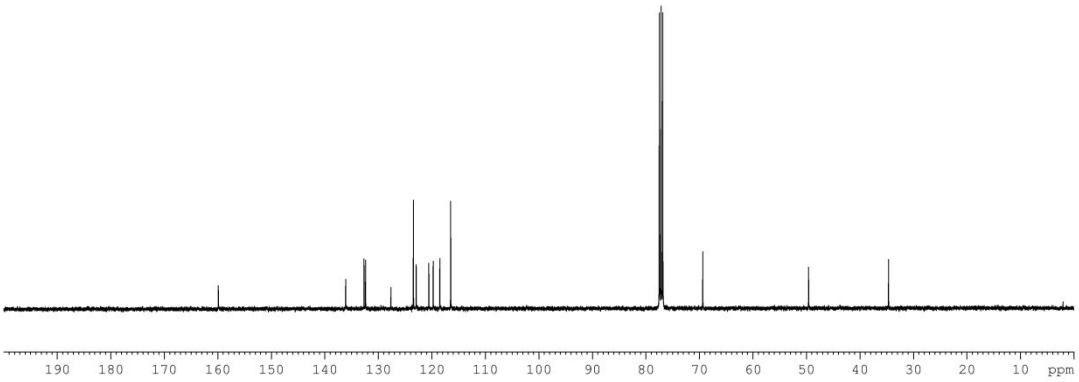
Compound 10a:



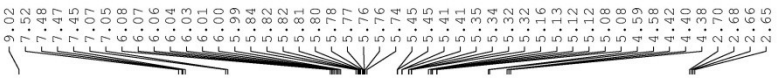


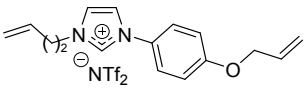


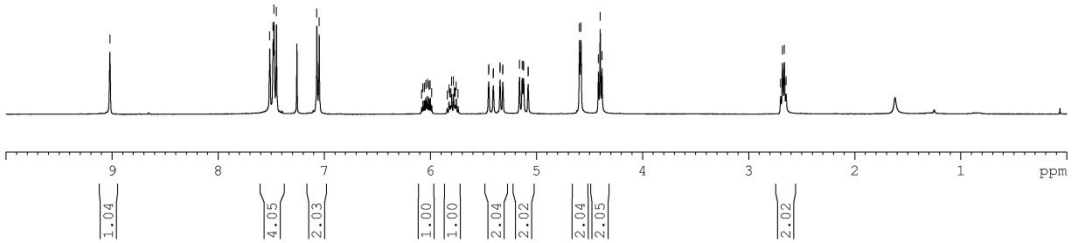


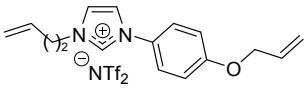


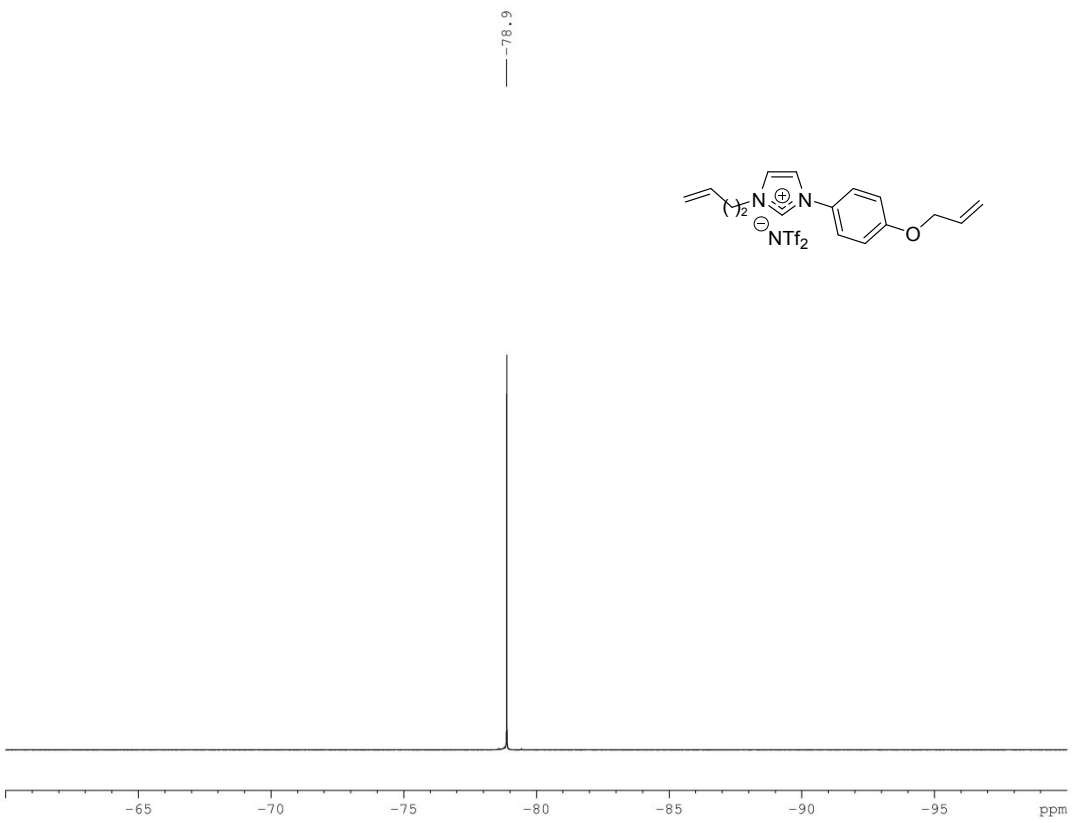
Compound 10b:



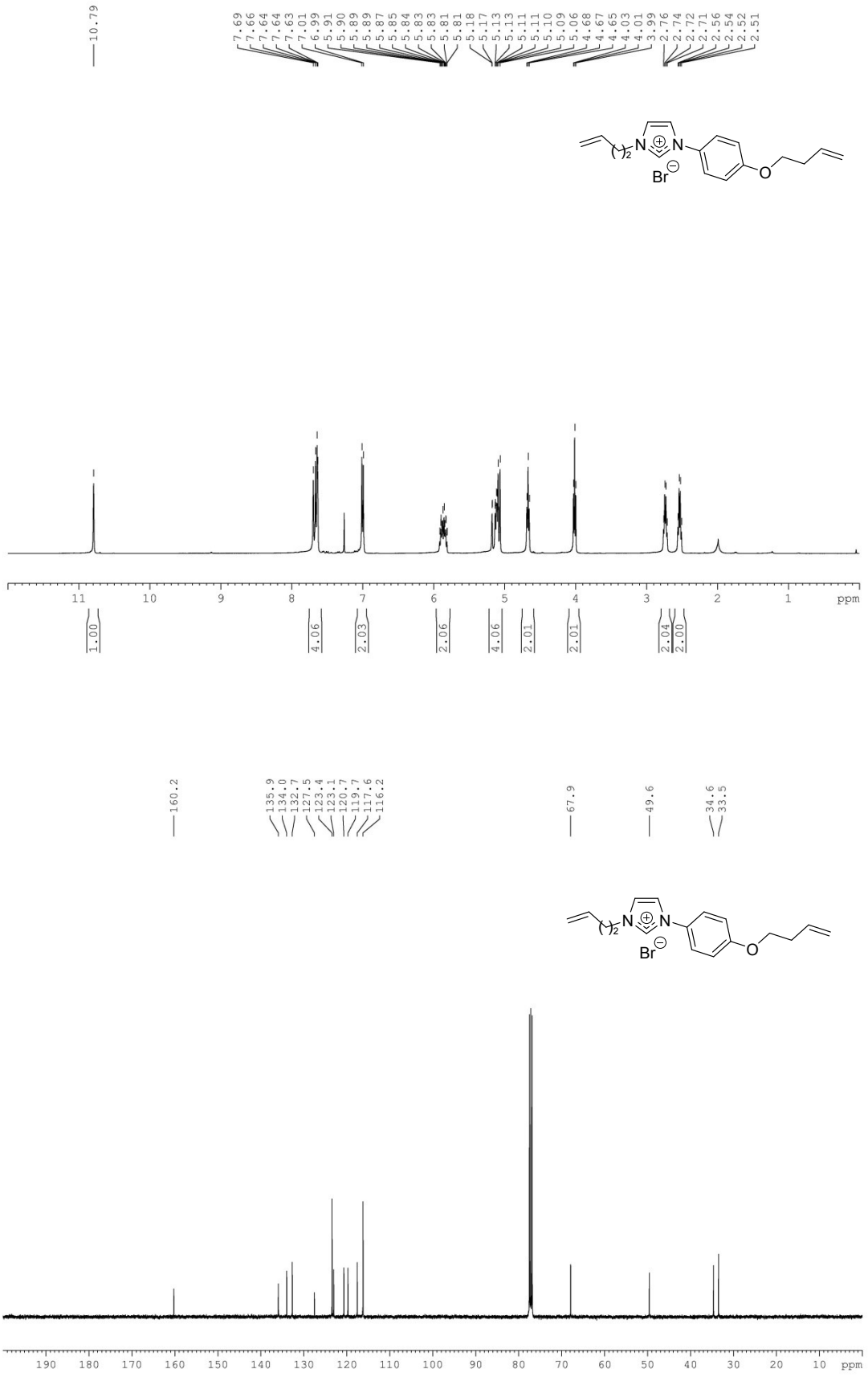




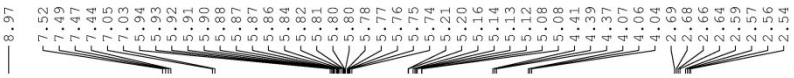


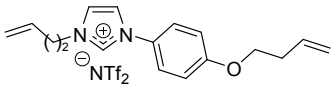

-78.9
N
N
NTf2
O
-65
-70
-75
-80
-85
-90
-95
ppm

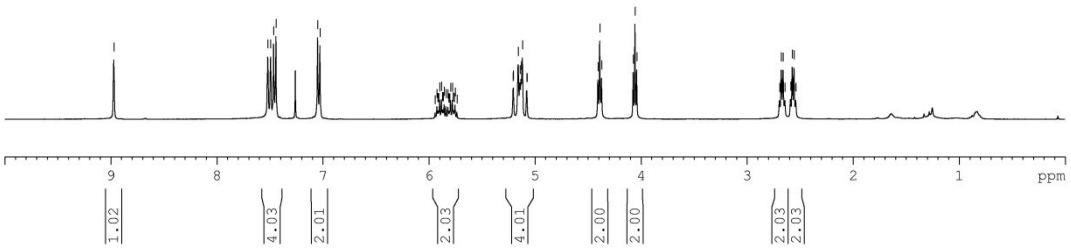
Compound 11a:

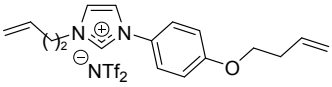


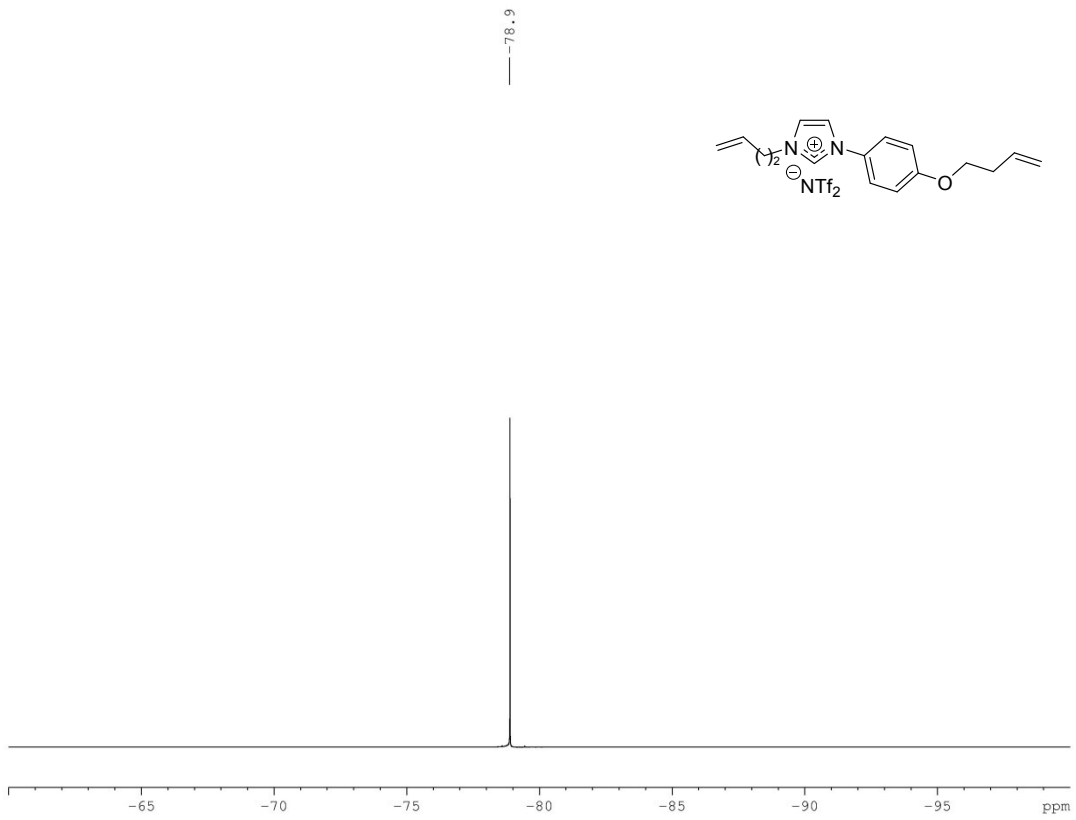
Compound 11b:



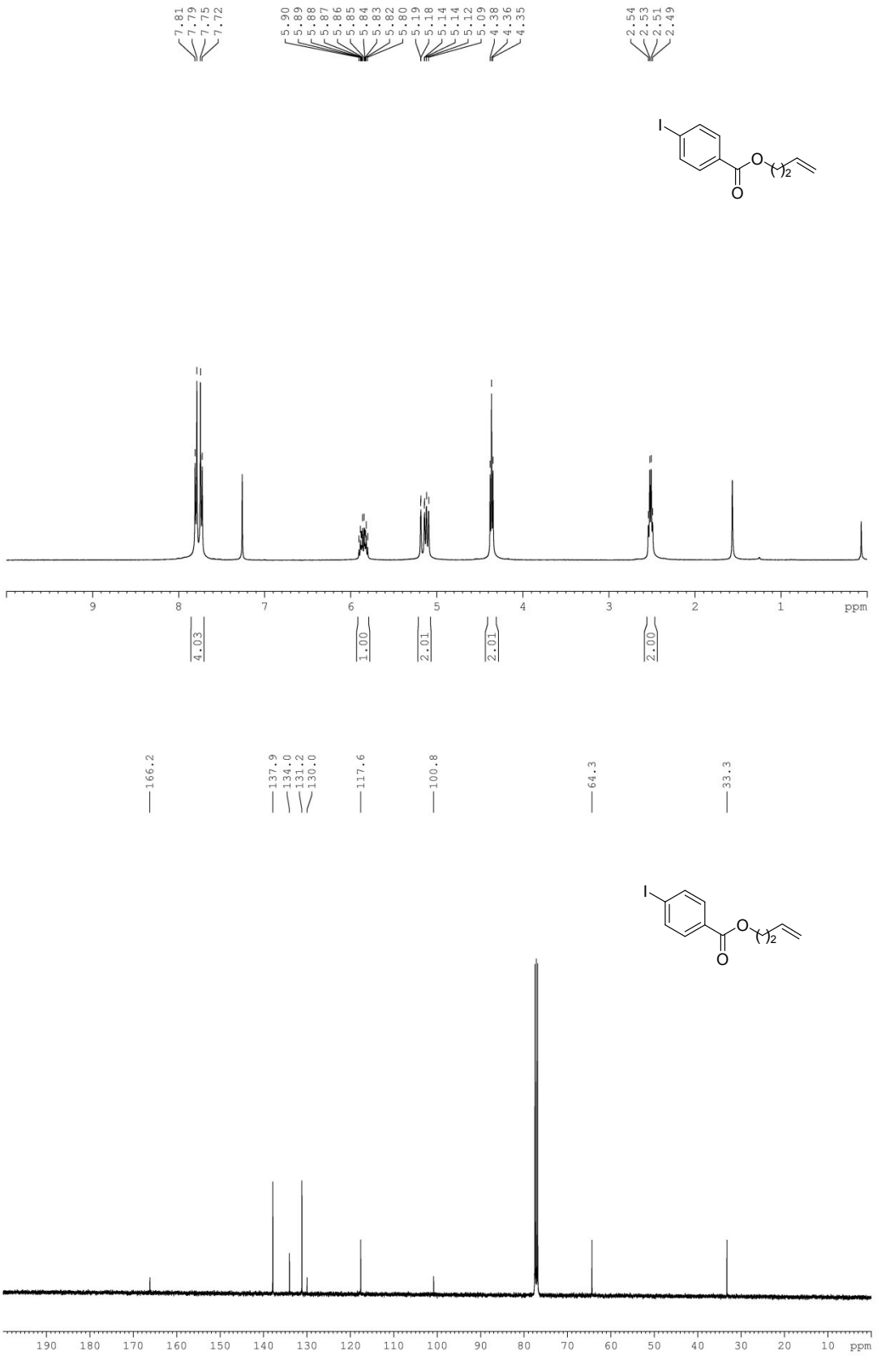




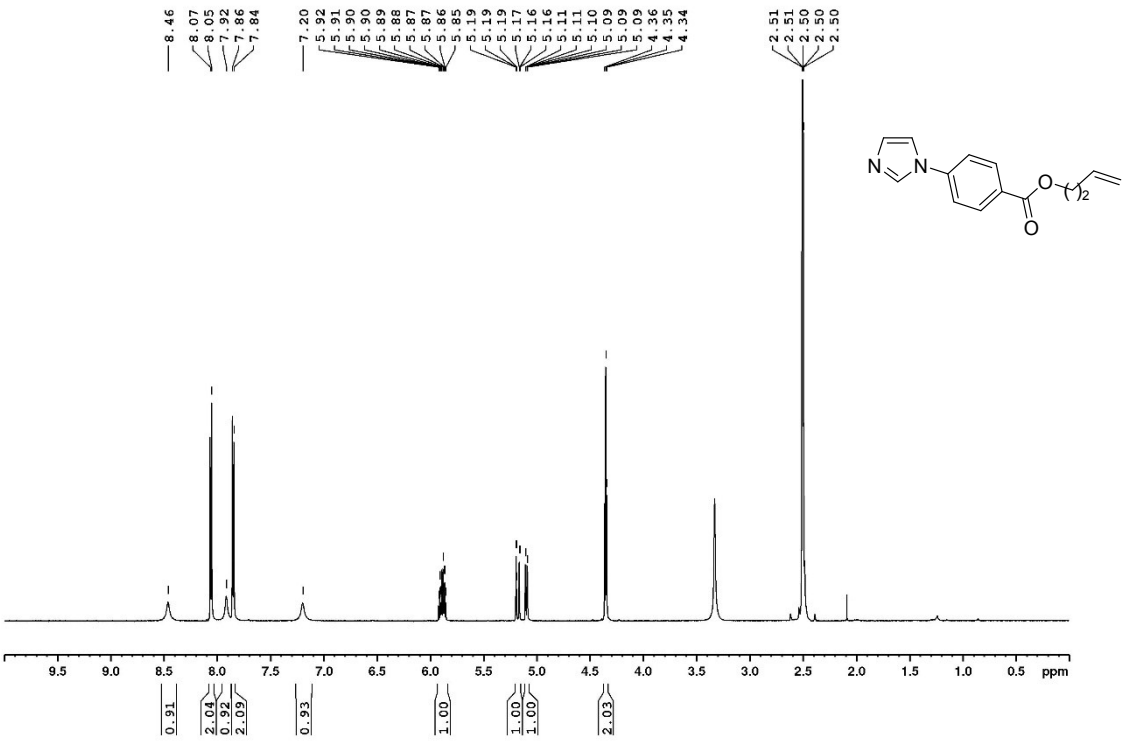


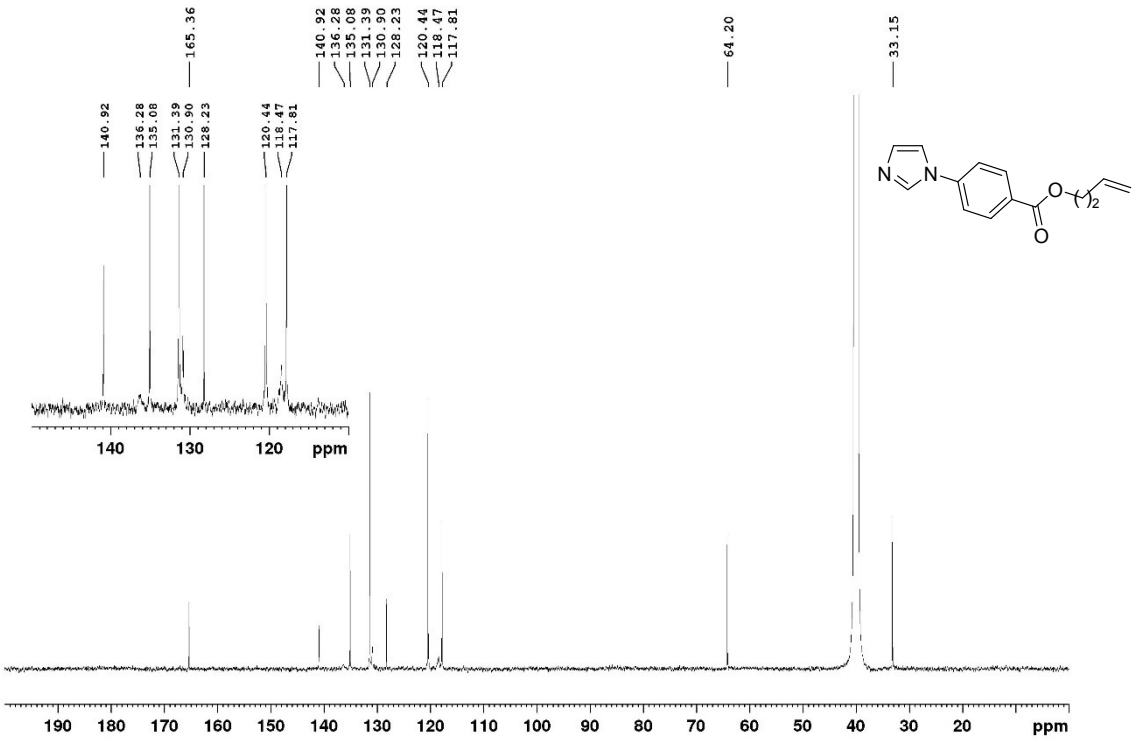

-78.9
N
N
NTf2
O
-65
-70
-75
-80
-85
-90
-95
ppm

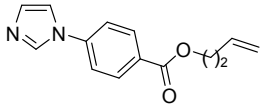
Compound 12:

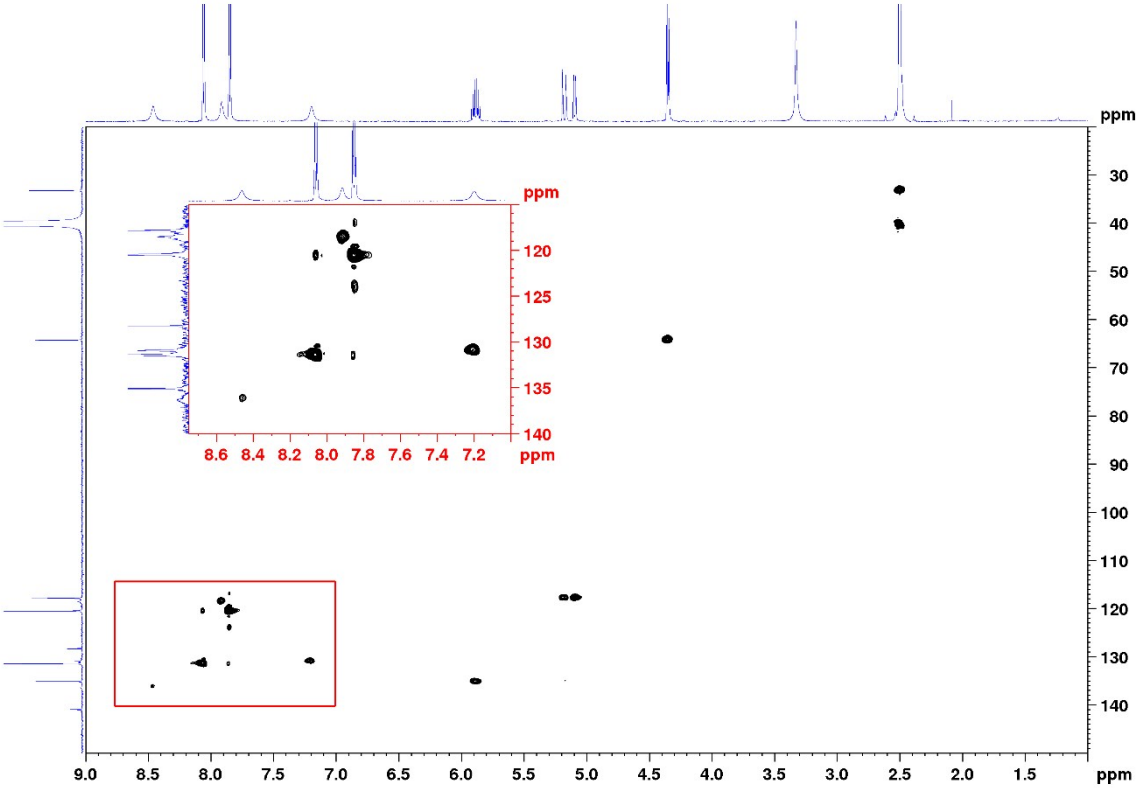

7.81
7.79
7.75
7.72
5.90
5.89
5.88
5.87
5.86
5.85
5.84
5.83
5.82
5.80
5.19
5.18
5.14
5.14
5.12
5.09
4.38
4.36
4.35
2.54
2.53
2.51
2.49
I
O
O
2
9
8
7
6
5
4
3
2
1
ppm
4.03
1.00
2.01
2.01
2.00
166.2
137.9
134.0
131.2
130.0
117.6
100.8
64.3
33.3
I
O
O
2
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

Compound 13:

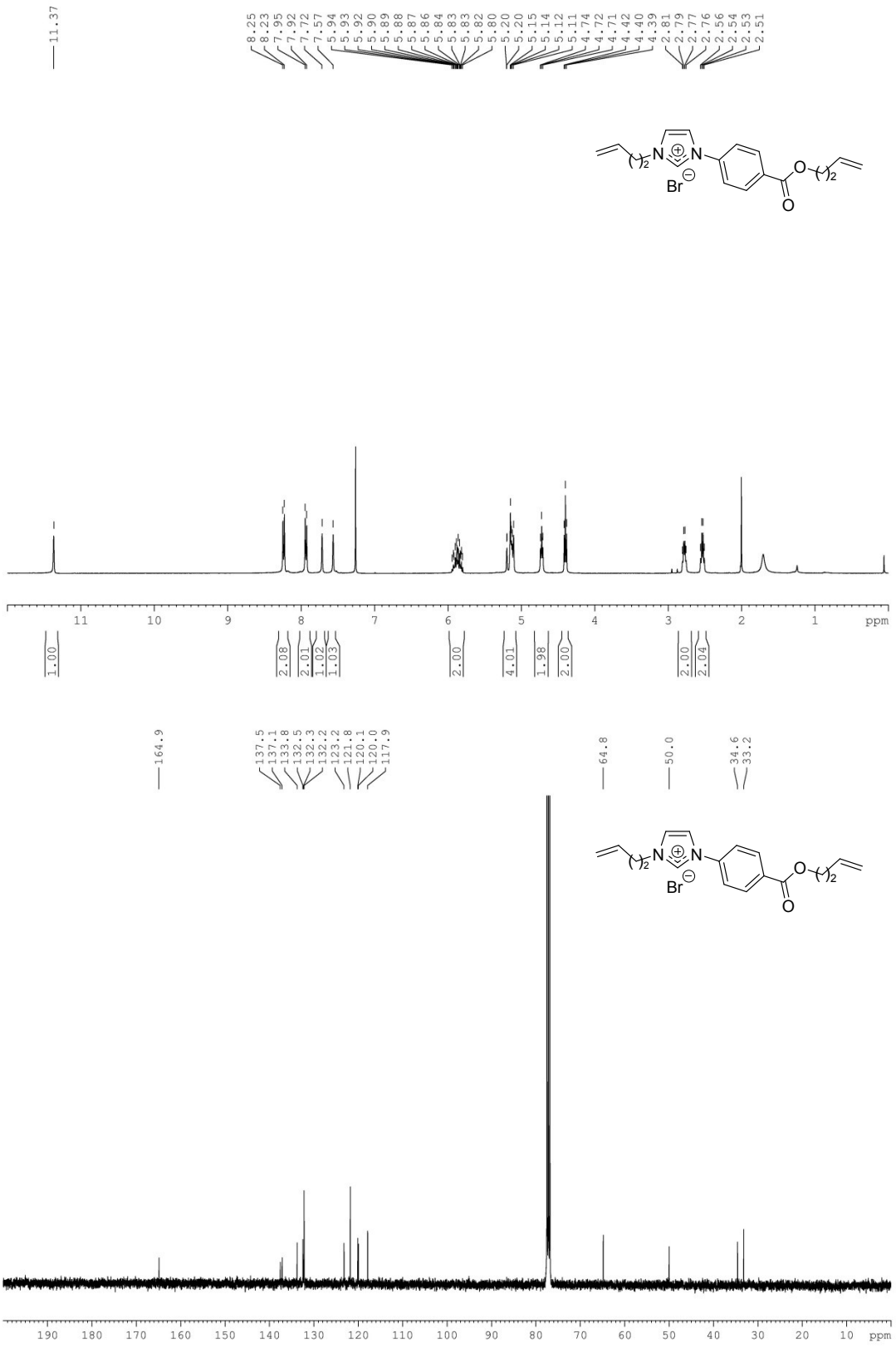

8.46
8.07
8.05
7.92
7.86
7.84
7.20
5.92
5.91
5.90
5.90
5.89
5.88
5.87
5.87
5.86
5.85
5.19
5.19
5.19
5.17
5.16
5.16
5.11
5.11
5.10
5.09
5.09
5.09
4.36
4.35
4.34
2.51
2.51
2.50
2.50
2.50
N
N
O
O
2
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.91
2.04
0.92
2.09
0.93
1.00
1.00
1.00
2.03


165.36
140.92
136.28
135.08
131.39
130.90
128.23
120.44
118.47
117.81
64.20
33.15
N
N
O
O
2
140 130 120 ppm
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

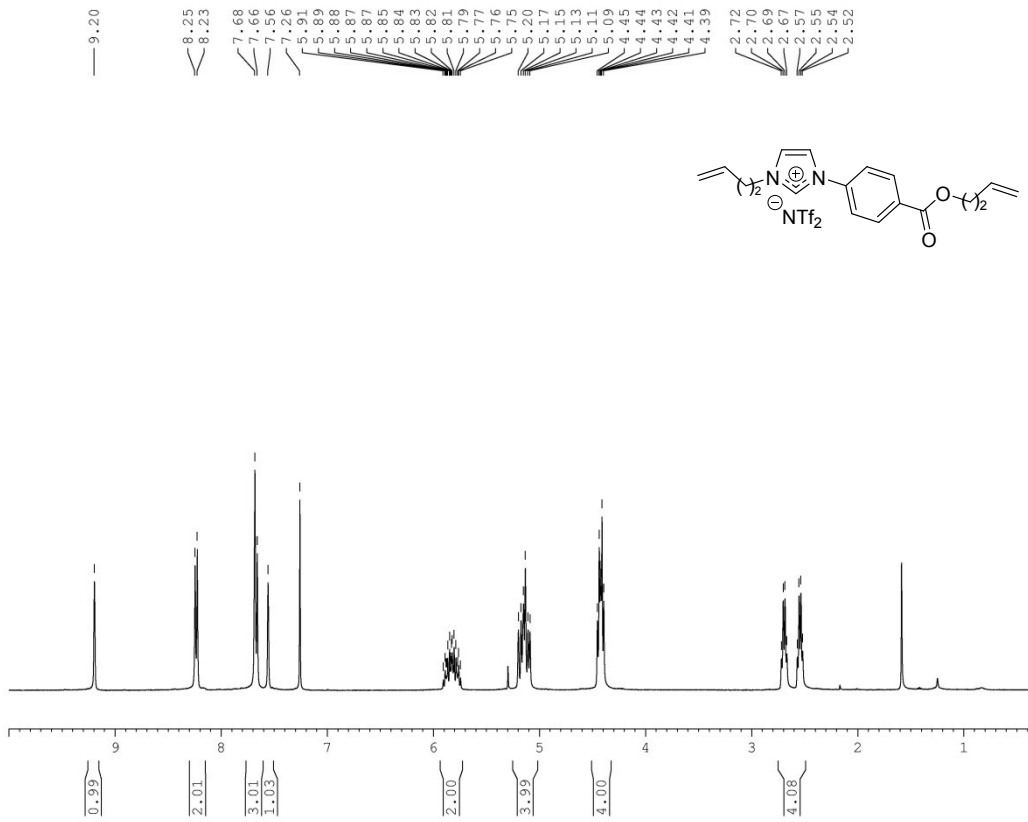

N
N
O
O
2

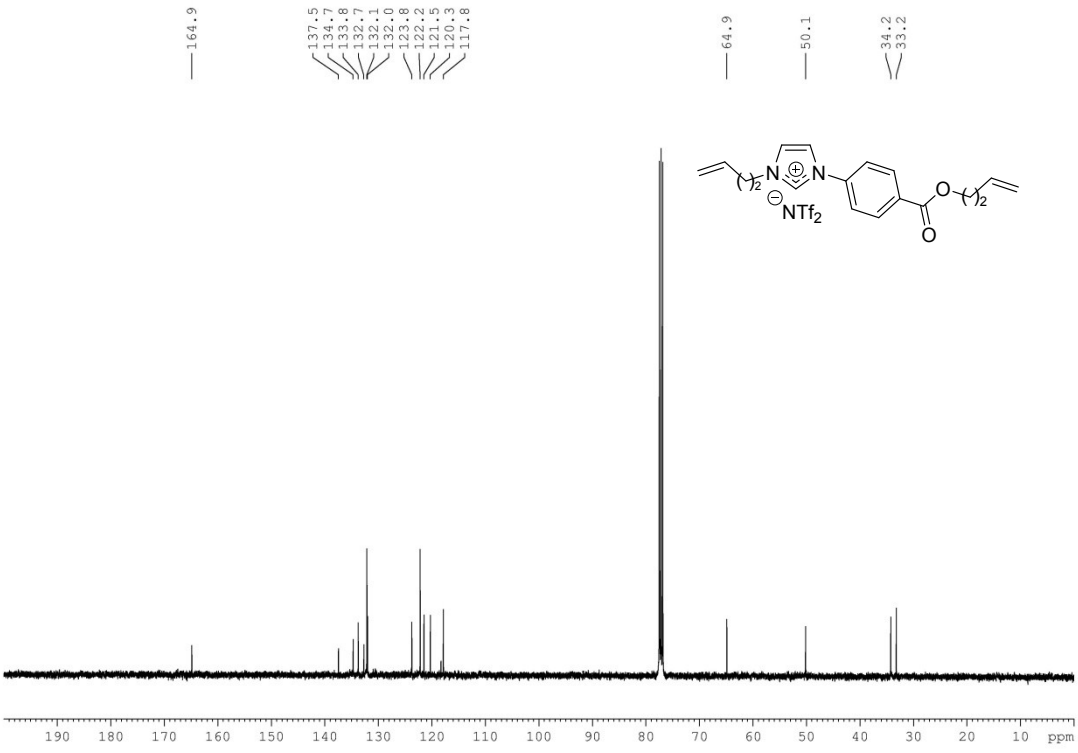

ppm
30
40
50
60
70
80
90
100
110
120
130
140
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
ppm
120
125
130
135
140
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
ppm

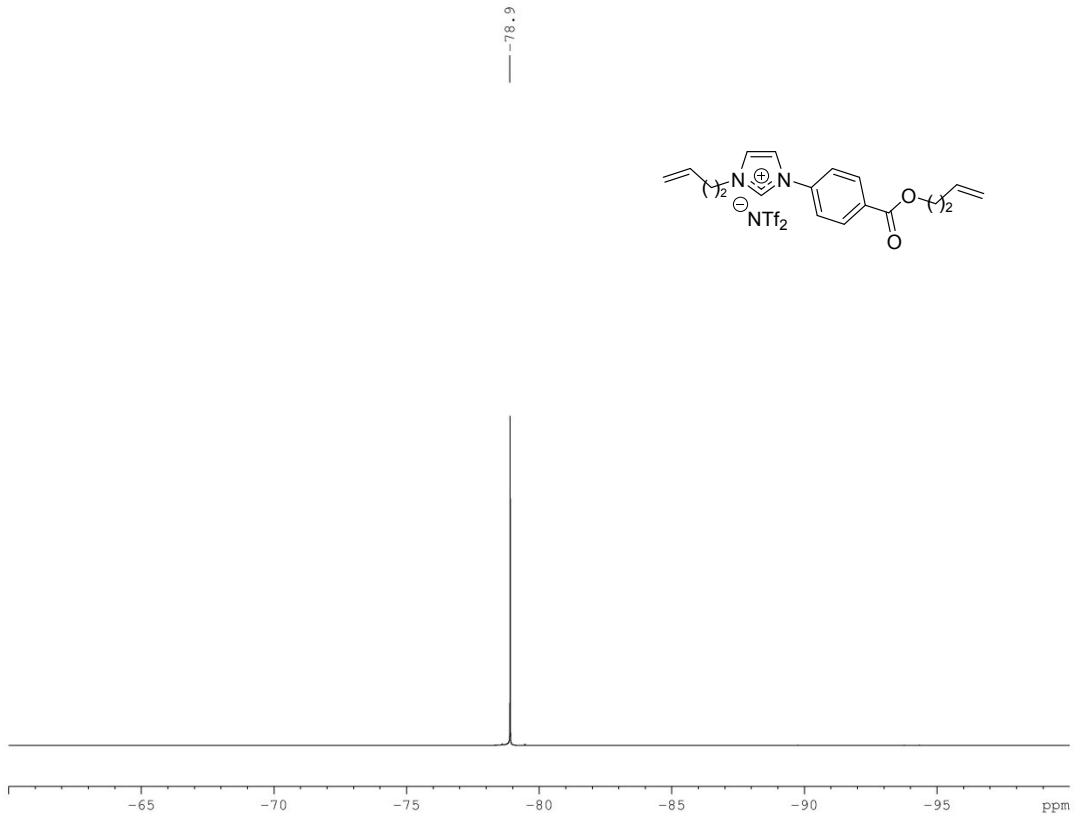
Compound 14a:



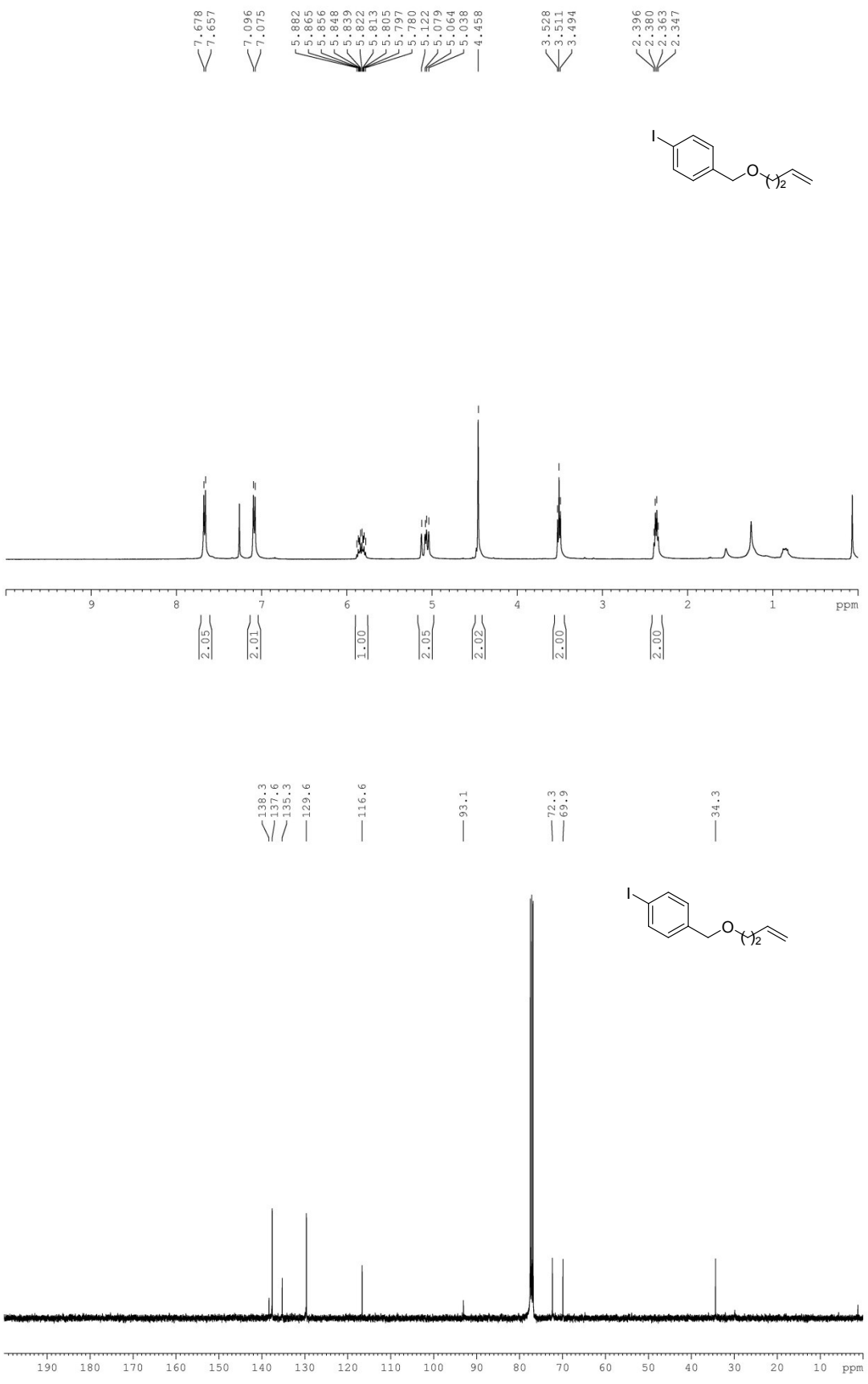
Compound 14b:



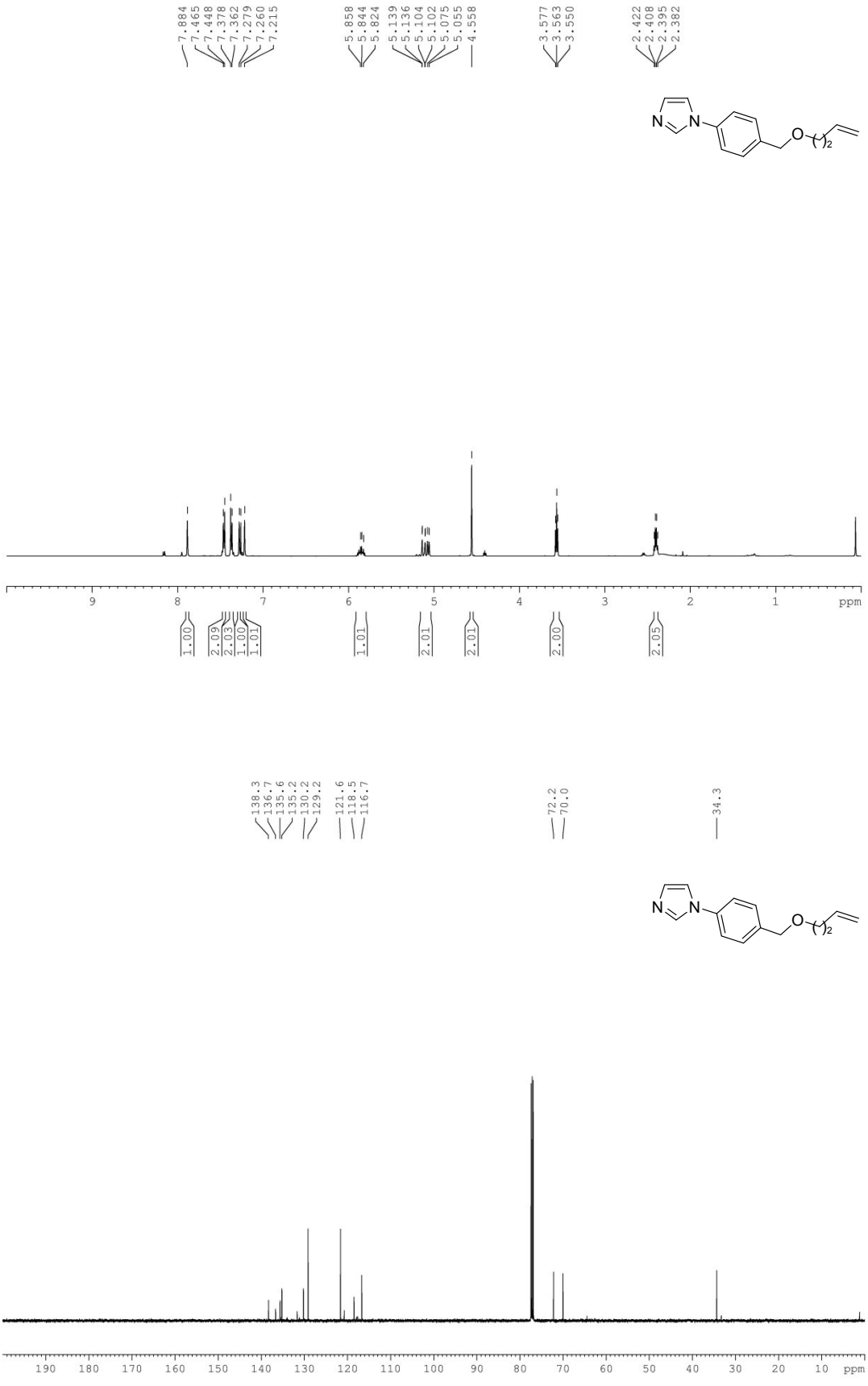



-78.9
NTf2
O
O
-65
-70
-75
-80
-85
-90
-95
ppm

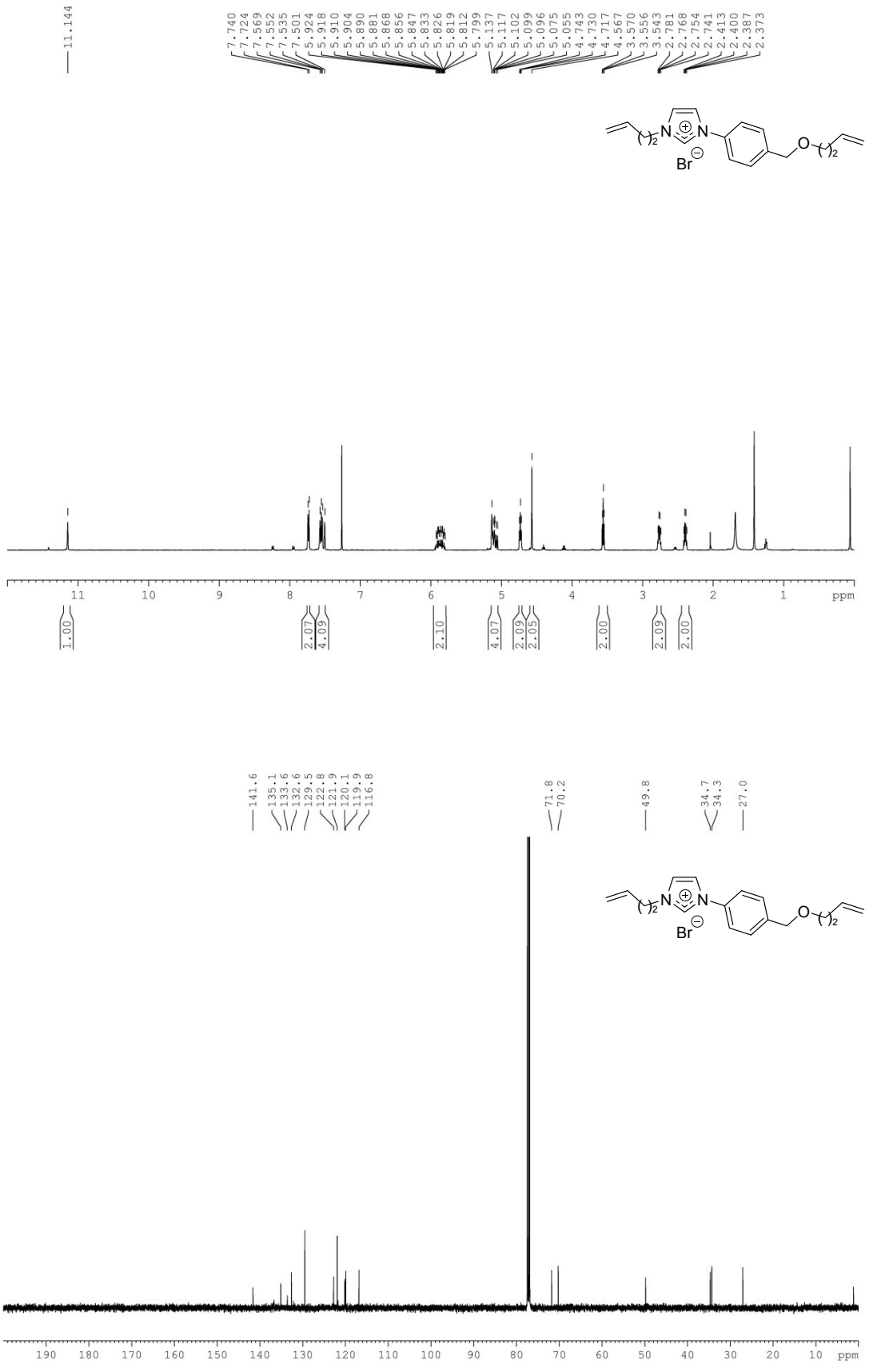
Compound 15:


7.678
7.657
7.096
7.075
5.882
5.865
5.856
5.848
5.839
5.822
5.813
5.805
5.797
5.780
5.122
5.079
5.064
5.038
4.458
3.528
3.511
3.494
2.396
2.380
2.363
2.347
I
O
2
9
8
7
6
5
4
3
2
1
ppm
2.05
2.01
1.00
2.05
2.02
2.00
2.00
138.3
137.6
135.3
129.6
116.6
93.1
72.3
69.9
34.3
I
O
2
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

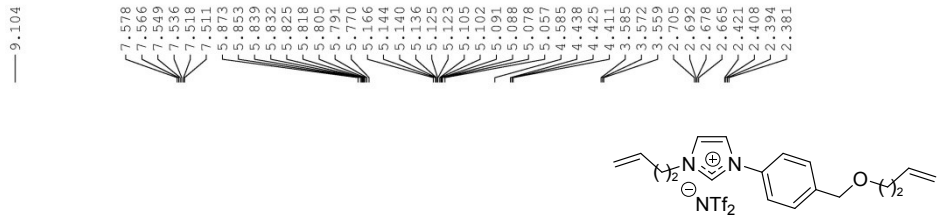
Compound 16:

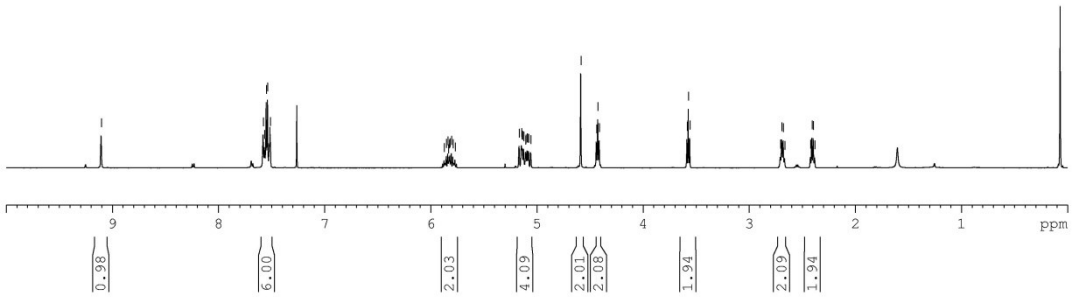

7.884
7.465
7.448
7.378
7.362
7.279
7.260
7.215
5.858
5.844
5.824
5.139
5.136
5.104
5.102
5.075
5.055
4.558
3.577
3.563
3.550
2.422
2.408
2.395
2.382
ppm
1.00
2.09
2.03
1.00
1.01
1.01
2.01
2.01
2.00
2.05
138.3
136.7
135.6
135.2
130.2
129.2
121.6
118.5
116.7
72.2
70.0
34.3
ppm

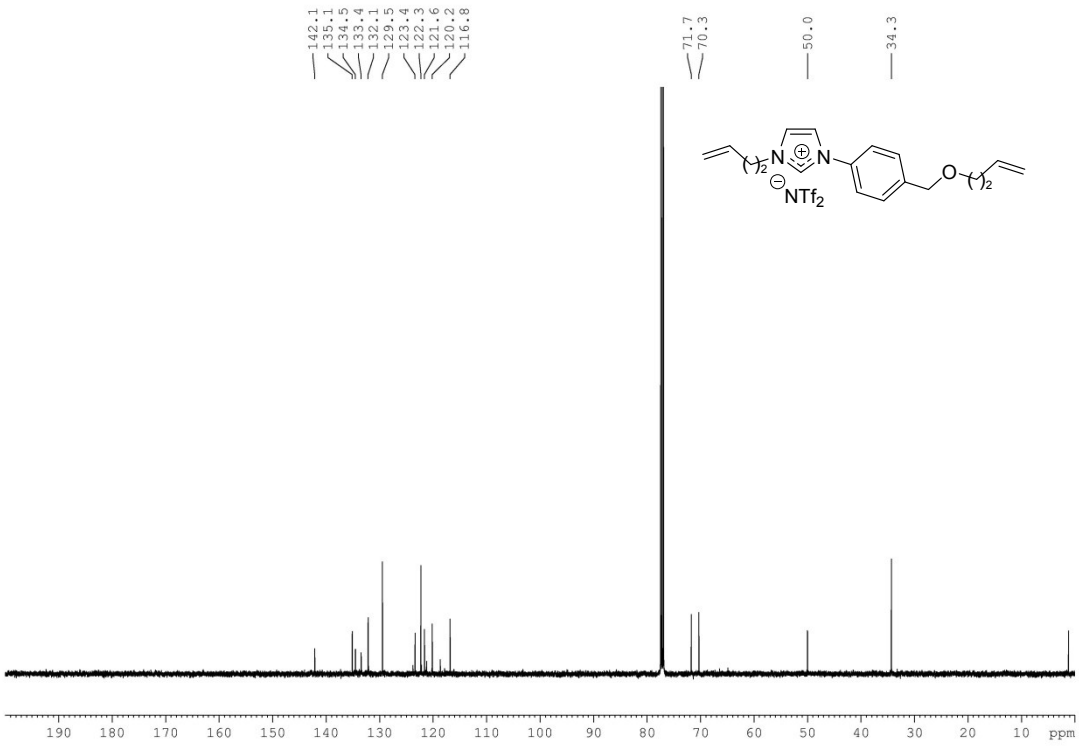
Compound 17a:

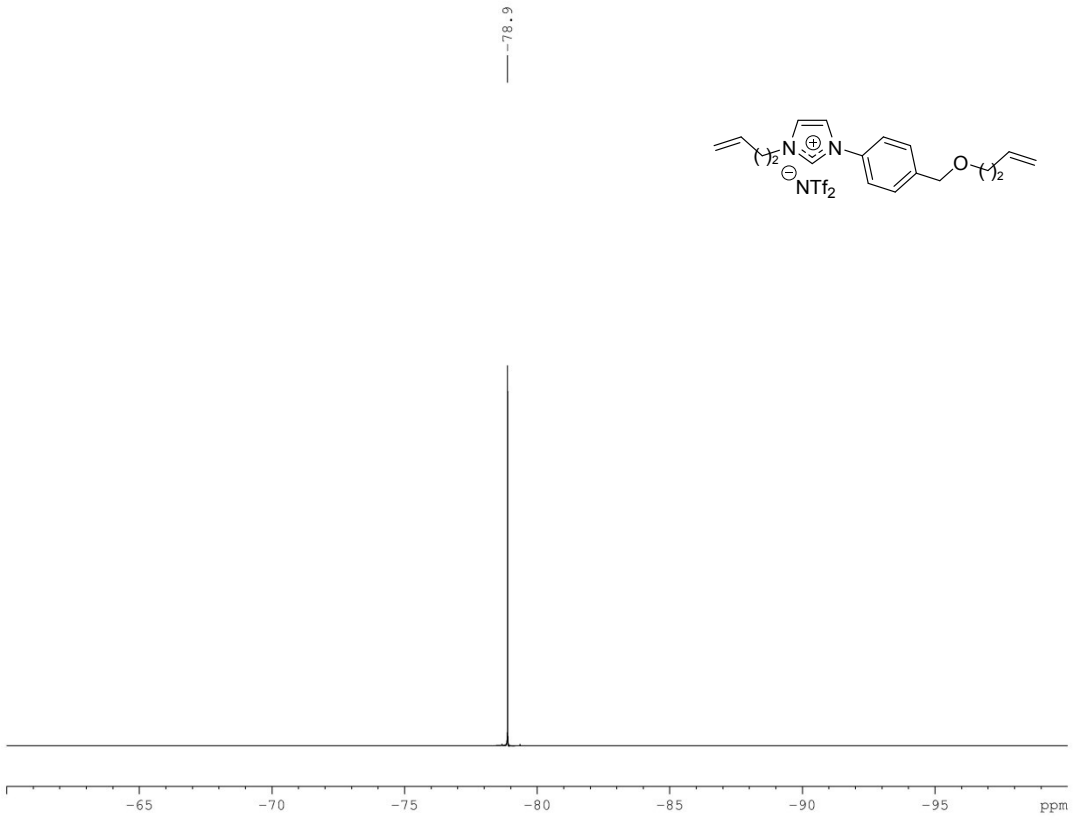


Compound 17b:

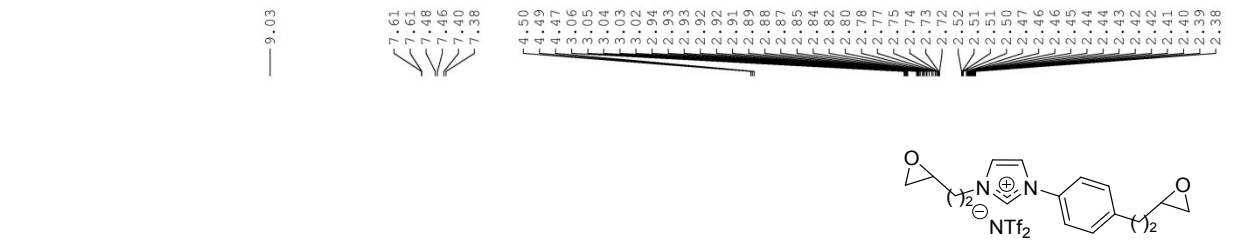


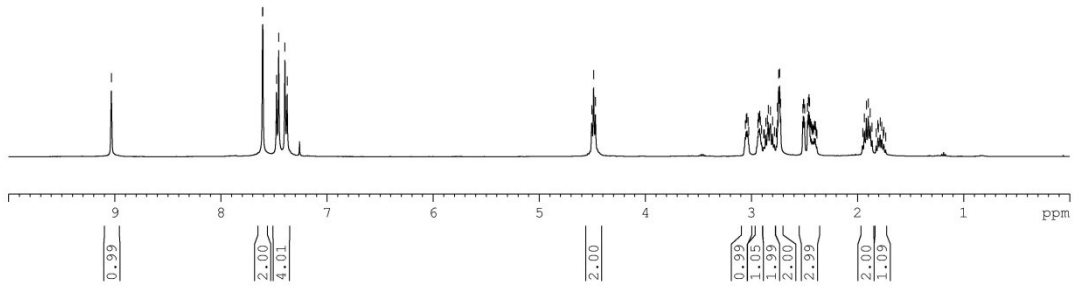


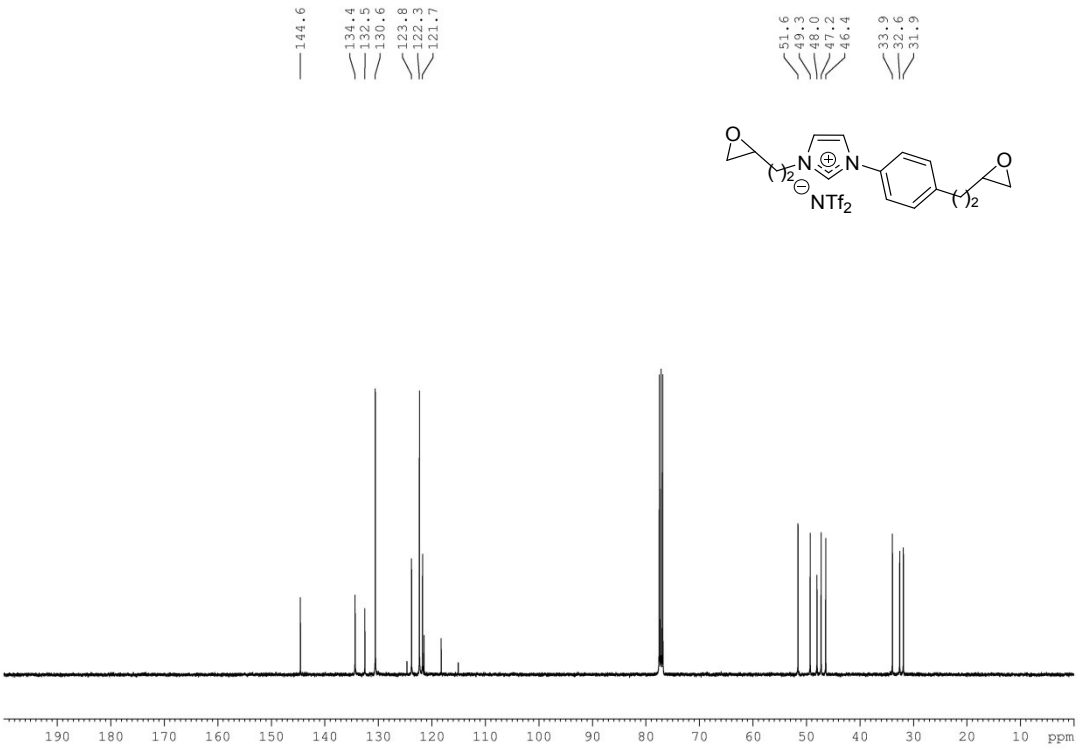


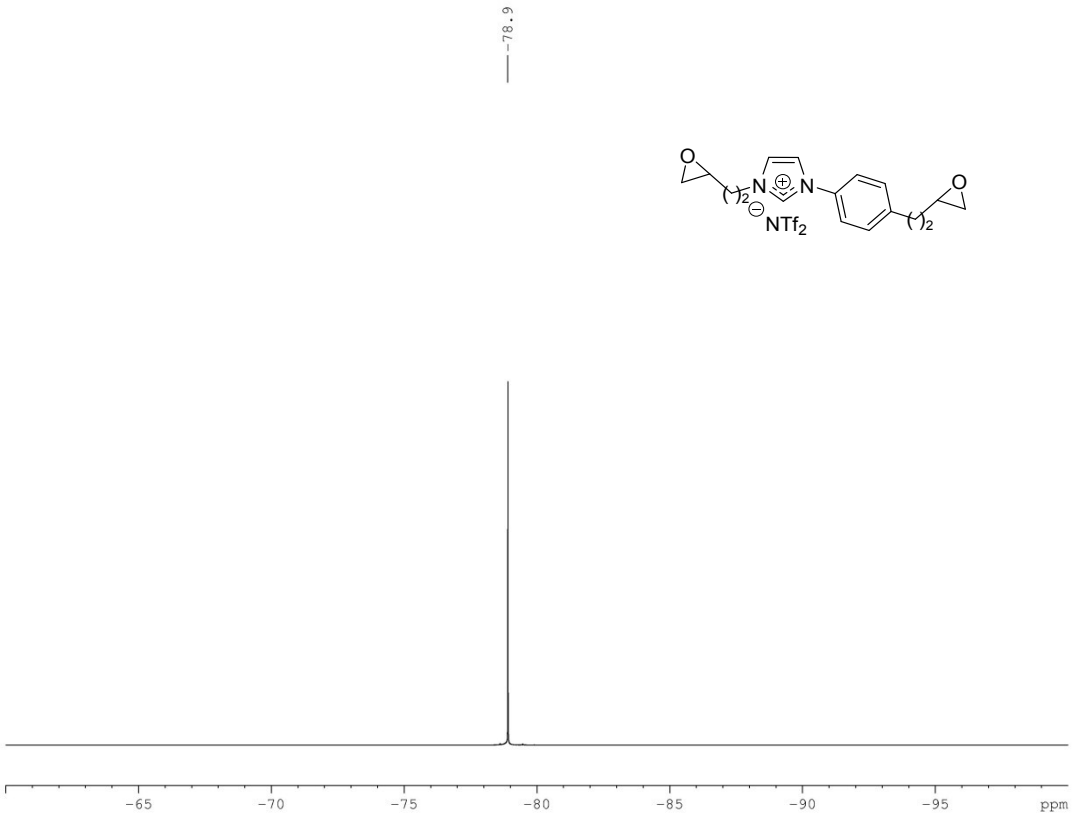

-78.9
N
N
O
NTf2
-65
-70
-75
-80
-85
-90
-95
ppm

Compound 18:

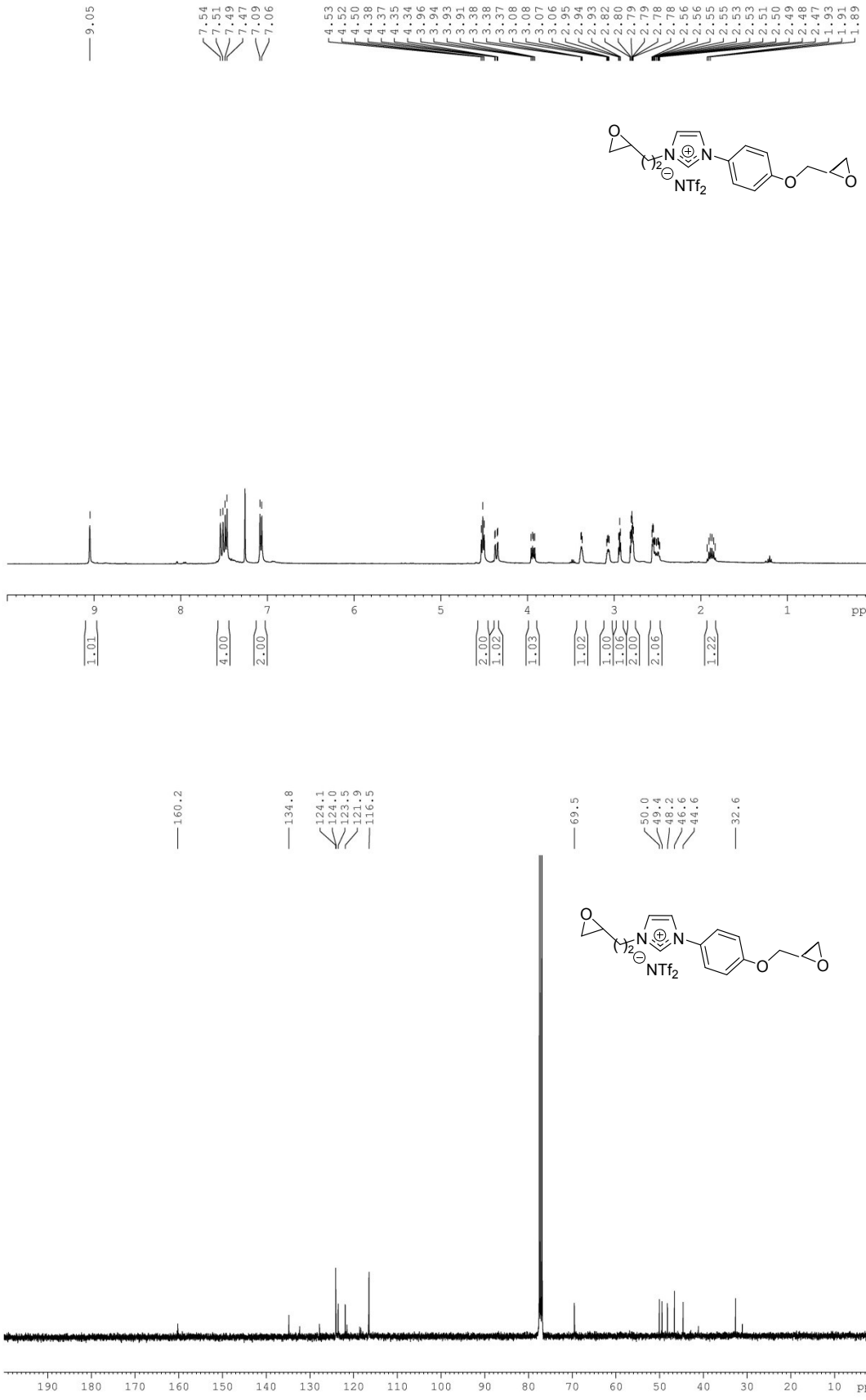

9.03
7.61
7.61
7.48
7.46
7.40
7.38
4.50
4.49
4.47
3.06
3.05
3.04
3.03
3.02
2.94
2.93
2.93
2.92
2.92
2.91
2.89
2.88
2.87
2.85
2.84
2.82
2.80
2.78
2.77
2.75
2.74
2.73
2.72
2.52
2.51
2.51
2.50
2.47
2.46
2.46
2.45
2.44
2.44
2.43
2.42
2.42
2.41
2.40
2.39
2.38
O
N
N
NTf2
O

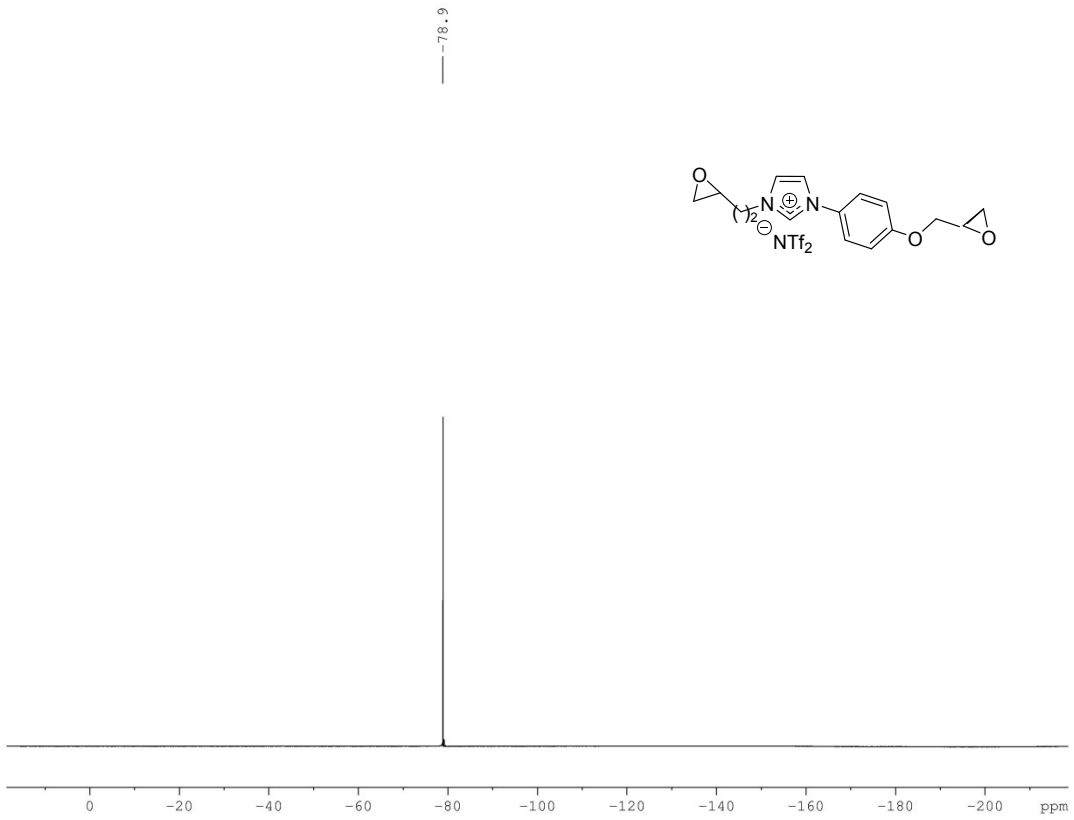

9
8
7
6
5
4
3
2
1
ppm
0.99
2.00
4.01
2.00
0.99
1.05
1.99
2.00
2.99
2.00
1.09


144.6
134.4
132.5
130.6
123.8
122.3
121.7
51.6
49.3
48.0
47.2
46.4
33.9
32.6
31.9
O
N
N
NTf2
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

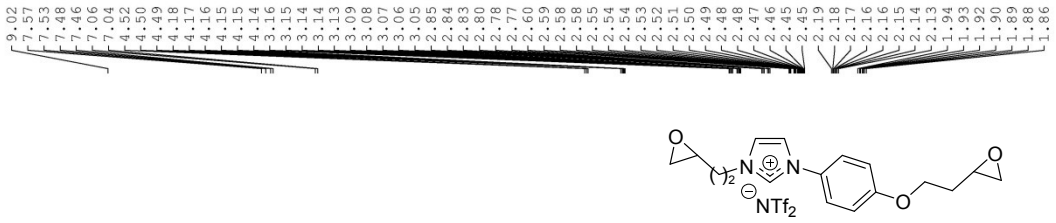

-78.9
O
N
N
NTf2
O
-65
-70
-75
-80
-85
-90
-95
ppm

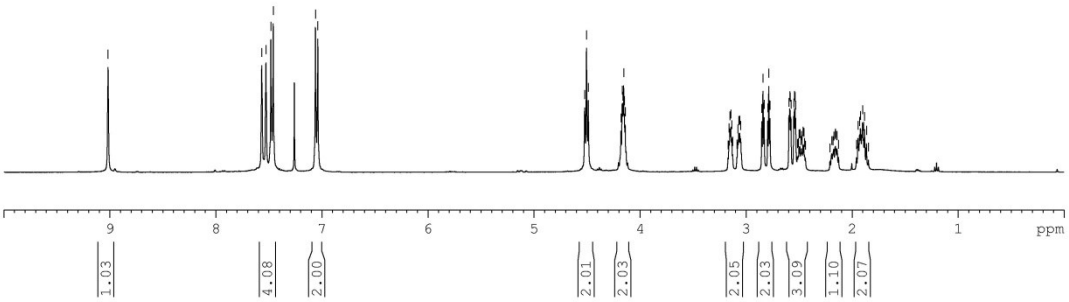
Compound 19:


9.05
7.54
7.51
7.49
7.47
7.09
7.06
4.53
4.52
4.50
4.38
4.37
4.35
4.34
3.96
3.94
3.93
3.91
3.38
3.37
3.08
3.08
3.07
3.06
2.95
2.94
2.93
2.82
2.80
2.79
2.79
2.78
2.56
2.56
2.55
2.55
2.53
2.53
2.51
2.50
2.49
2.48
2.47
1.93
1.91
1.89
NTf2
ppm
1.01
4.00
2.00
2.00
1.02
1.03
1.02
1.00
1.06
2.00
2.06
1.22
160.2
134.8
124.1
124.0
123.5
121.9
116.5
69.5
50.0
49.4
48.2
46.6
44.6
32.6
NTf2
ppm

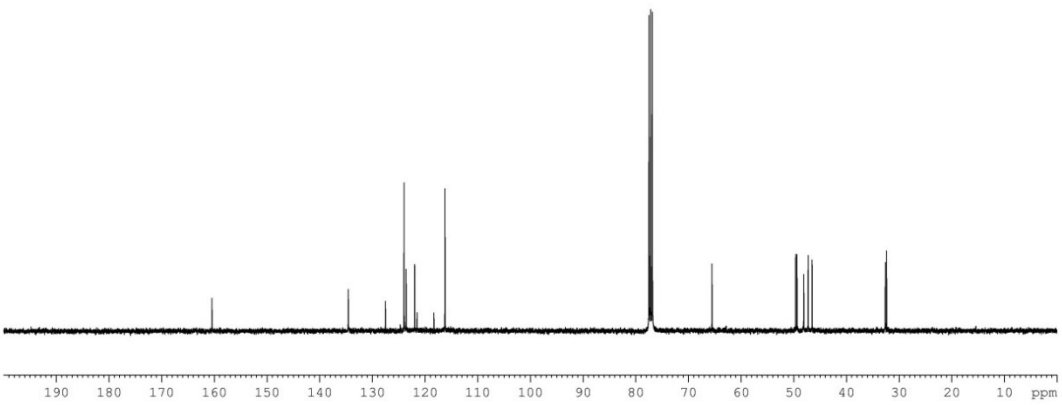

-78.9
O
N
N
NTf2
O
O
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

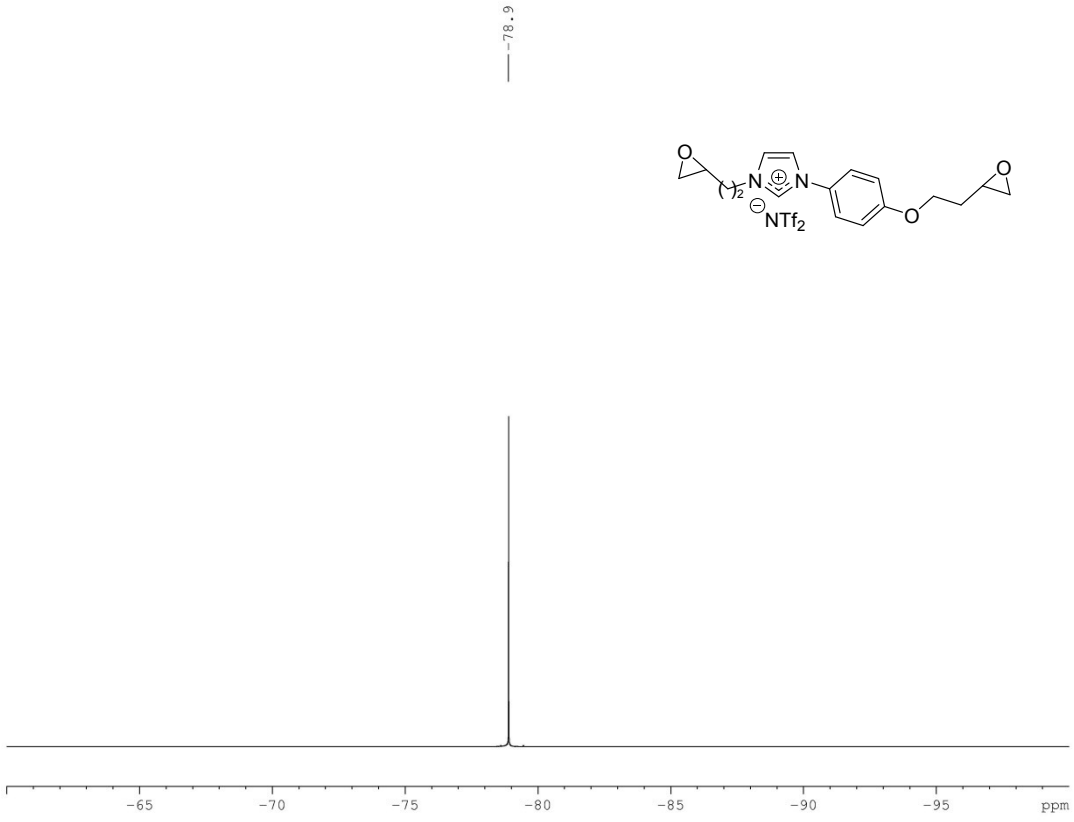
Compound 20:


9.02
7.57
7.53
7.48
7.46
7.06
7.04
4.52
4.50
4.49
4.18
4.17
4.16
4.15
4.15
4.14
4.14
3.16
3.15
3.14
3.14
3.13
3.09
3.08
3.07
3.06
3.05
2.85
2.84
2.83
2.80
2.78
2.77
2.60
2.59
2.58
2.58
2.55
2.54
2.54
2.53
2.52
2.51
2.50
2.49
2.48
2.48
2.47
2.46
2.45
2.45
2.19
2.18
2.17
2.16
2.16
2.15
2.14
2.13
1.94
1.93
1.92
1.90
1.89
1.88
1.86
O
N
N
NTf2
O
O

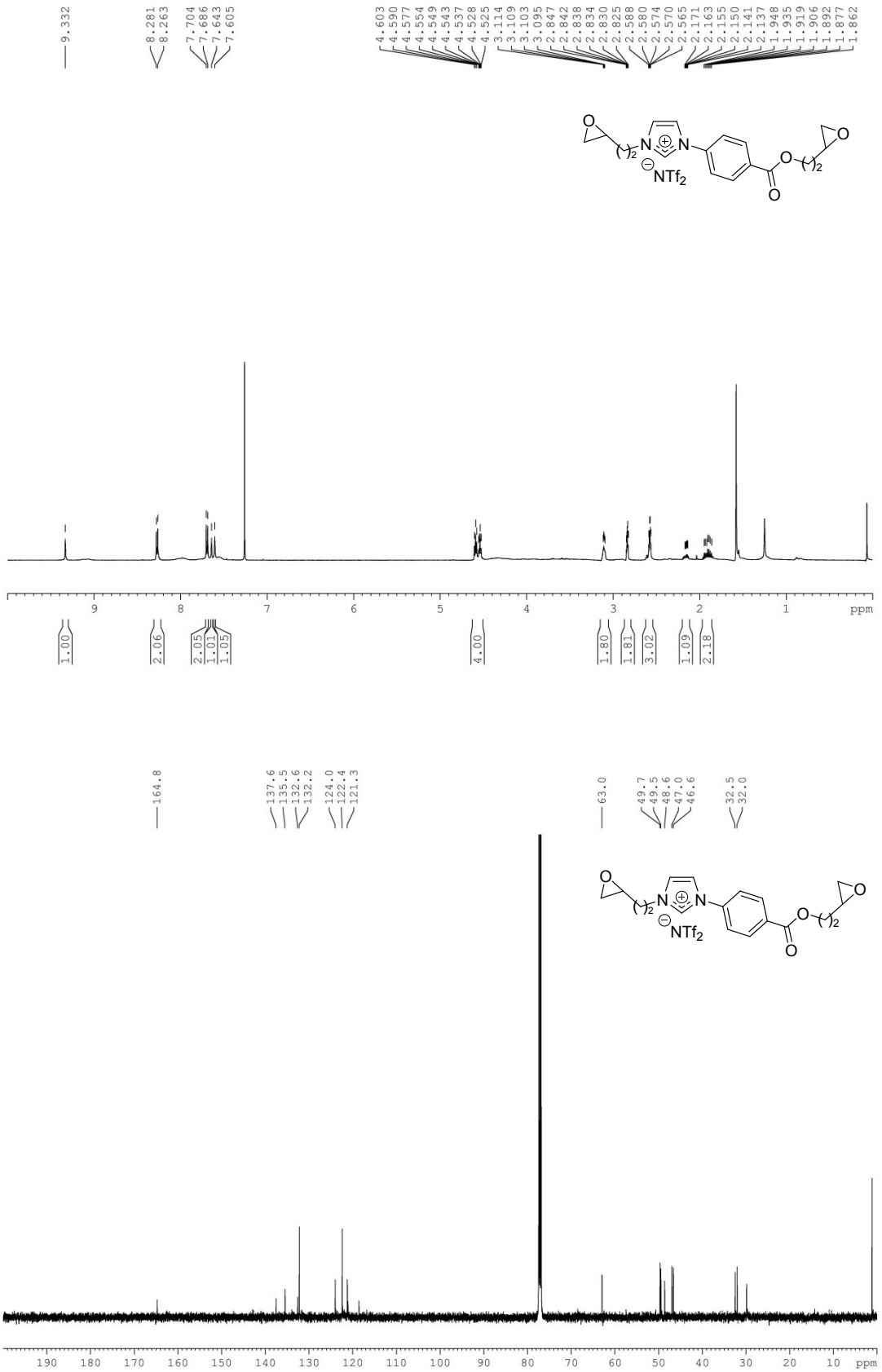

9
8
7
6
5
4
3
2
1
ppm
1.03
4.08
2.00
2.01
2.03
2.05
2.03
3.09
1.10
2.07

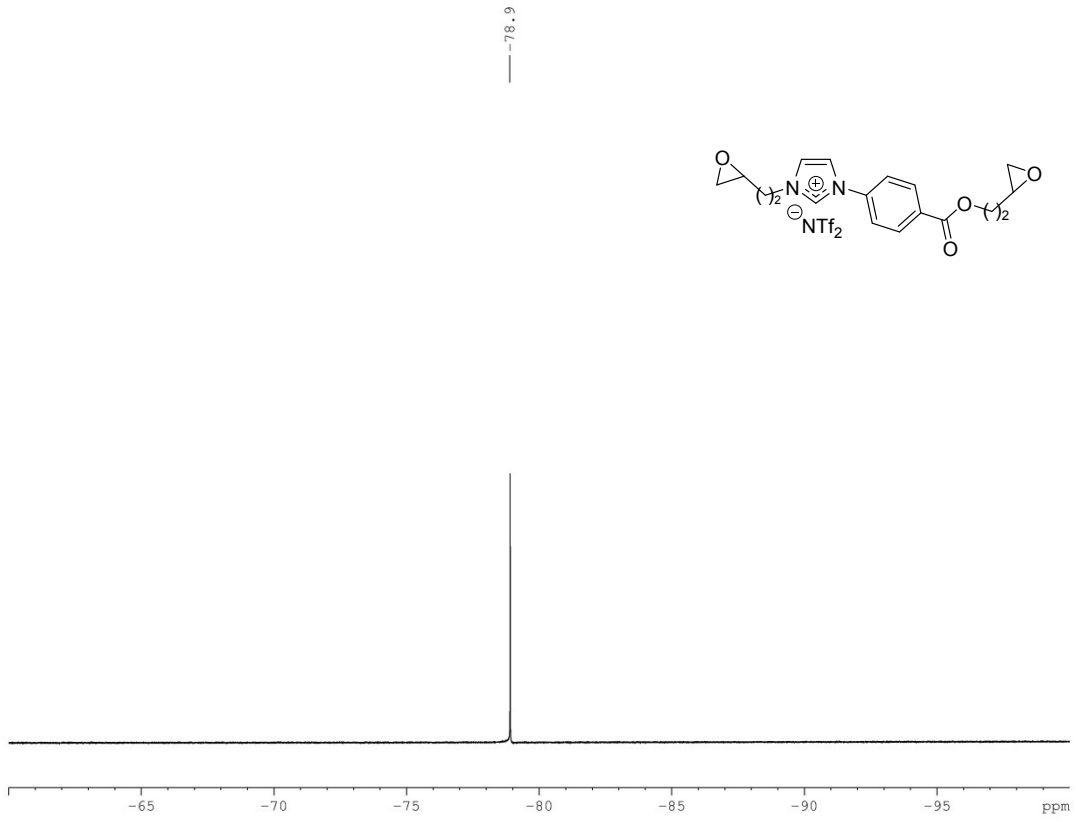

160.5
134.6
127.5
124.0
123.6
122.0
116.2
65.5
49.6
49.4
48.1
47.2
46.5
32.6
32.4
O
N
N
NTf2
O
O


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

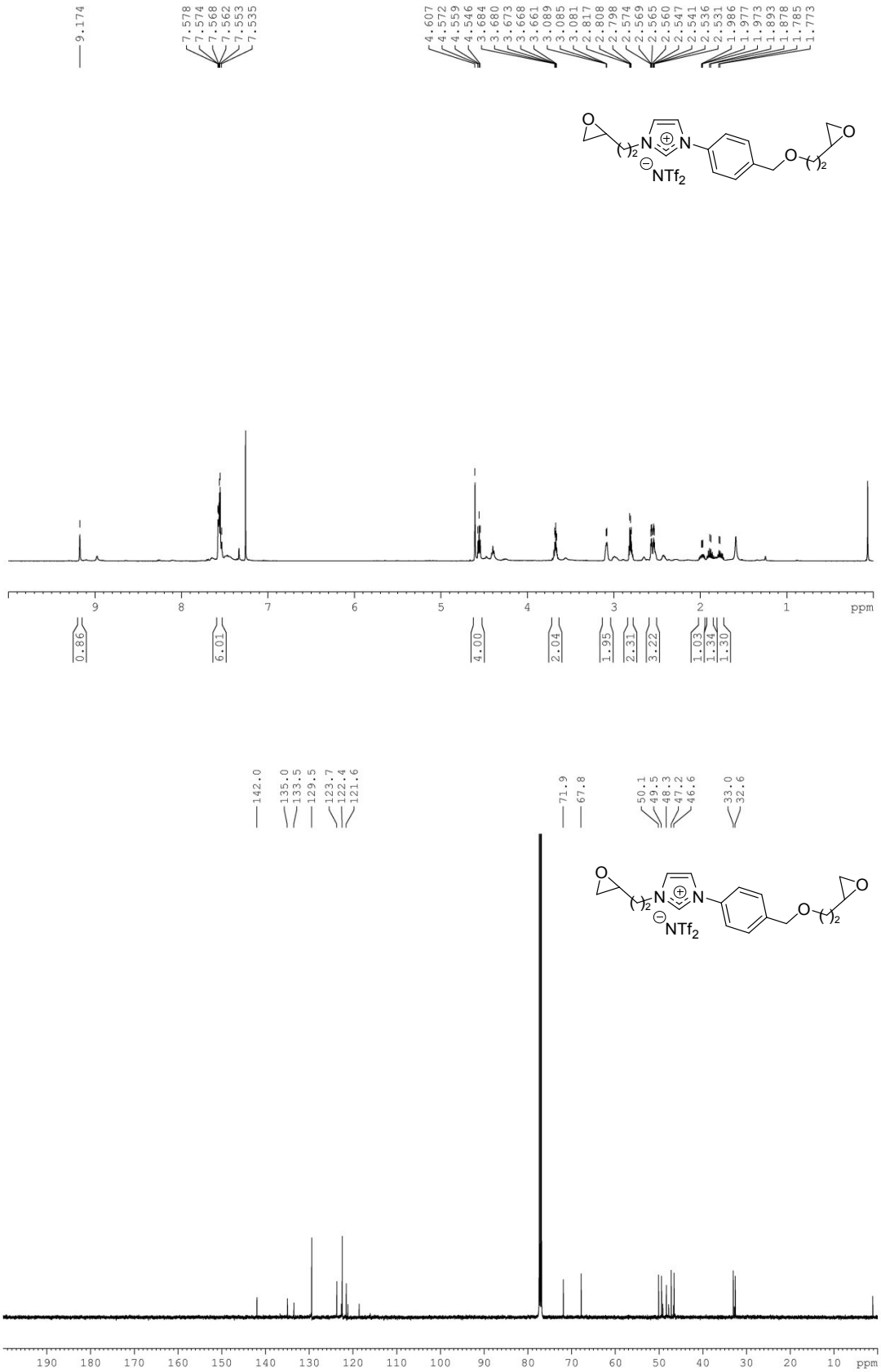

-78.9
O
N
N
NTf2
O
O
-65
-70
-75
-80
-85
-90
-95
ppm

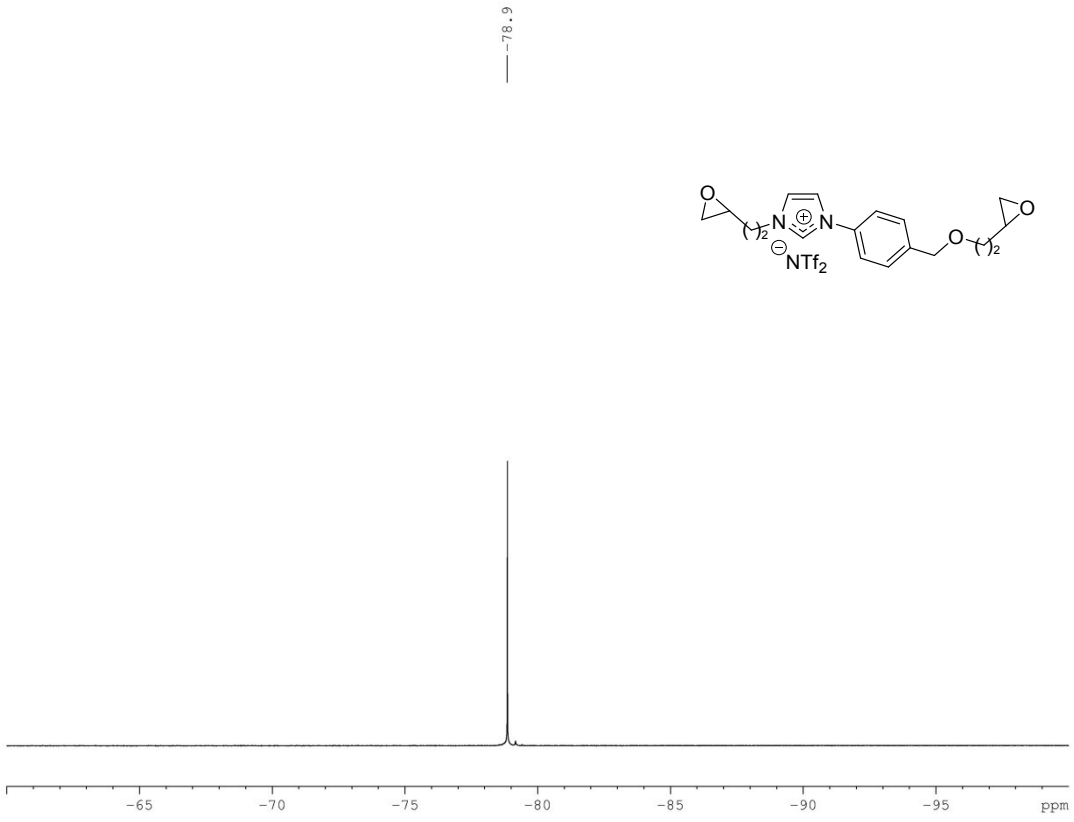
Compound 21:


9.332
8.281
8.263
7.704
7.686
7.643
7.605
4.603
4.590
4.577
4.554
4.549
4.543
4.537
4.528
4.525
3.114
3.109
3.103
3.095
2.847
2.842
2.838
2.834
2.830
2.825
2.588
2.580
2.574
2.570
2.565
2.171
2.163
2.155
2.150
2.141
2.137
1.948
1.935
1.919
1.906
1.892
1.877
1.862
NTf2
ppm
1.00
2.06
2.05
1.01
1.05
4.00
1.80
1.81
3.02
1.09
2.18
164.8
137.6
135.5
132.6
132.2
124.0
122.4
121.3
63.0
49.7
49.5
48.6
47.0
46.6
32.5
32.0
NTf2
ppm


-78.9
O
N
N
NTf2
O
O
O
-65
-70
-75
-80
-85
-90
-95
ppm

Compound 22:


9.174
7.578
7.574
7.568
7.562
7.553
7.535
4.607
4.572
4.559
4.546
3.684
3.680
3.673
3.668
3.661
3.089
3.085
3.081
2.817
2.808
2.798
2.574
2.569
2.565
2.560
2.547
2.541
2.536
2.531
1.986
1.977
1.973
1.893
1.878
1.785
1.773
NTf2
ppm
0.86
6.01
4.00
2.04
1.95
2.31
3.22
1.03
1.34
1.30
142.0
135.0
133.5
129.5
123.7
122.4
121.6
71.9
67.8
50.1
49.5
48.3
47.2
46.6
33.0
32.6
NTf2
ppm


-78.9
O
N
N
NTf2
O
O
-65
-70
-75
-80
-85
-90
-95
ppm