Supporting Information

Asymmetric Trifluoromethylation of Aromatic Aldehydes by Cooperative Catalyst with (IPr)CuF and Quinidine-Derived Quaternary Ammonium Salt

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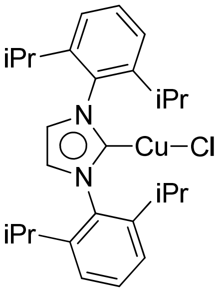
1. General information

All reactions were carried out under argon atmosphere using typical vacuum-line techniques unless otherwise noted. Solvents were transferred *via* syringe and were introduced into the reaction vessels through a rubber septum. The ^{1}H-NMR (400 MHz) spectra for solution in $CDCl_3$ and DMSO-d_6 were recorded on Bruker Avance 400 and Varian Mercury 400. Chemical shifts were reported downfield in ppm from tetramethylsilane ($CDCl_3$, $\delta = 7.26$; DMSO-d_6, $\delta = 2.50$). Spectra were reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz), integration and assignment. ^{13}C NMR spectra were collected on Bruker Avance 400 and a Varian Mercury 400 (100 MHz) with complete proton decoupling. Chemical shifts were reported in ppm from the tetramethylsilane ($CDCl_3$, $\delta = 77.0$; DMSO-d_6, $\delta = 39.5$). The IR spectra were recorded on Thermo Scientific Nicolet iS10 with KBr pellets. Elemental analyses were performed on an Elementar Vario MICRO CUBE instrument. Enantiomeric excesses were determined by HPLC on Shimadzu LC-20A apparatus with Chiralpak OJ-H, AS-H, OD-H and AD-H. Optical rotations were measured on a Krüss P8000 polarimeter. HRMS was recorded on Bruker Apex IV FTMS. All melting points were determined on a XT4A melting point apparatus without correction. Analytical thin layer chromatography (TLC) was performed using F254 pre-coated silica gel plate. Column chromatography was performed with silica gel (200–300 mesh). Petroleum ether (PE) used had a boiling point range of 60–90 ^{o}C.

2 Preparation of Catalysts

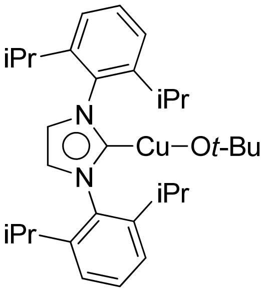
2.1 Typical procedure for (IPr)CuF preparation

[1,3-Bis(2,6-di-*iso*-propylphenyl)imidazol-2-ylidene] copper (I) chloride, (IPr)CuCl[1]



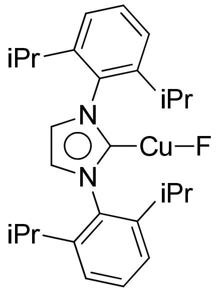
An oven-dried Schlenk flask containing 1,3-bis(2,6-di-*iso*-propylphenyl) imidazolium chloride (849.0 mg, 2.00 mmol), CuCl (198.0 mg, 2.00 mmol), NaO*t*-Bu (192.0 mg, 2.00 mmol) was evacuated and refilled with argon three times. THF (10 mL) were added to this Schlenk flask. The resulting suspension was stirred at room temperature for 4 h. Then, it was filtered through Celite in glovebox. The title compound was obtained as a white powder (788.6 mg, 81% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.48 (t, J = 8.0 Hz, 2H), 7.29 (d, J = 7.6 Hz, 4H), 7.11 (s, 2H), 2.53–2.60 (m, 4H), 1.30 (d, J =12 Hz, 12H), 1.22 (d, J = 6.8 Hz, 12H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 180.6, 145.6, 134.4, 130.6, 124.2, 123.2, 28.8, 24.9, 23.9; IR (KBr) 3160, 3137, 3070, 2968, 2926, 2869, 1963, 1577, 1469, 1456, 1405, 1383, 1327, 1114, 1104, 1212, 1058, 937, 946, 809, 765, 742, 699 cm^{-1}.

[1,3-Bis(2,6-di-*iso*-propylphenyl)imidazol-2-ylidene]copper(I) *tert*-butoxide, (IPr)Cu(O*t*-Bu)[2]



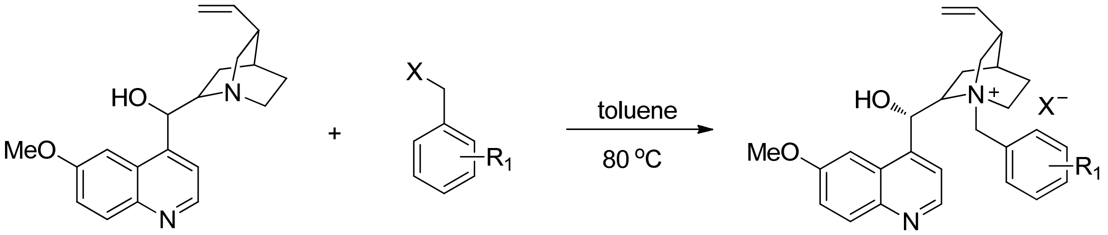
In a glovebox, a 30 mL round-bottom flask was charged with (IPr)CuCl (969.0 mg, 2.00 mmol) and NaOt-Bu (192.0 mg, 2.00 mmol). Anhydrous THF (12.0 mL) was added. The resulting opaque brown solution was stirred for 2.0 h. It was filtered through Celite in glovebox and concentrated *in vacuo* affording (IPr)Cu(O*t*-Bu) as an off-white powder (802.2 mg, 79% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.48 (t, J = 8.0 Hz, 2H), 7.29 (d, J = 7.6 Hz, 4H), 7.11 (s, 2H), 2.53–2.60 (m, 4H), 1.30 (d, J = 6.8 Hz, 12H), 1.26 (s, 9H), 1.22 (d, J = 6.8 Hz, 12H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 180.6, 145.6, 134.4, 130.6, 124.2, 123.2, 31.2, 28.8, 24.9, 23.9; IR (KBr) 3396, 3136, 3073, 2263, 2927, 2869, 1593, 1470, 1407, 1385, 1364, 1330, 1213, 1060, 935, 805, 758, 745 cm^{-1}.

[1,3-Bis(2,6-di-*iso*-propylphenyl)imidazol-2-ylidene]copper (I) fluoride, (IPr)CuF[3]



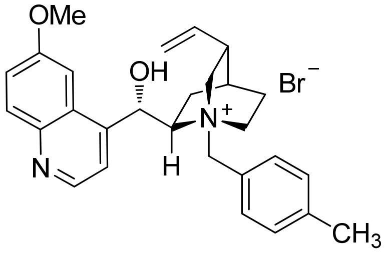
In glovebox, (IPr)CuO*t*-Bu (1043 mg, 2.00 mmol) and benzene (18 mL) were added to a 50 mL round-bottom flask equipped with a Teflon-coated stirbar. The flask was sealed with a rubber septum and took out from the glovebox. Triethylamine tris(hydrofluoride) (110.0 μL, 0.67 mmol) was added via a syringe. The resulting white suspension was stirred for 6 h at room temperature. The solvent was removed under reduced pressure. In the glovebox, the white solid was suspended in hexane (5 mL), filtered, and washed with hexane (5 mL) to afford (IPr)CuF as a white powder (801.0 mg, 85%). ^{1}H NMR (400 MHz, CDCl$_3$): δ 7.48 (t, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 7.6 Hz, 4H), 7.14 (s, 2H), 2.51–2.58 (m, 4H), 1.30 (d, *J* = 6.8 Hz, 12H), 1.22 (d, *J* = 6.8 Hz, 12H); ^{13}C NMR (100 MHz, CDCl$_3$): δ 180.5, 145.6, 134.6, 130.5, 124.2, 123.2, 28.8, 24.7, 24.0; IR (KBr) 3166, 3138, 3076, 3031, 1963, 2926, 2869, 1591, 1467, 1402, 1362, 1329, 1276, 1209, 1181, 1061, 944, 807, 766, 744, 699, 560, 542 cm^{-1}.

2.2 Typical procedure for ammonium bromides of cinchona alkaloids



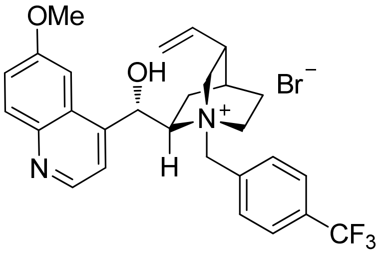
The ammonium bromides of cinchona alkaloids were synthesized following known procedures.[4] To a flame-dried flask equipped with a magnetic stirring bar and a condenser was added cinchona alkaloids (1 mmol), toluene (5 mL), and benzyl bromide derivatives (1.2 mmol, 1.2 equiv). The mixture was heated at 80 °C until a TLC analysis showing that the starting material was completely consumed. Cooled to room temperature and poured onto Et$_2$O (30 mL) with stirring, the resulting suspension was stirred for another 1 h. Then the precipitate was purified by flash chromatography.

***N*-(4-Methylbenzyl)quinidinium Bromide (3a)**



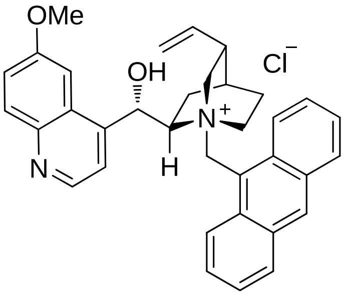
Prepared according to the general procedure, quinidine (324.4 mg, 1.0 mmol) and 4-methylbenzyl bromide (221.1 mg, 1.2 mmol, 1.2 equiv) were stirred for 12 h. The resulting precipitate was purified by flash chromatography (MeOH/EtOAc = 1/10, V/V) to give a white solid (407.5 mg, 80% yield). $[\alpha]_D^{28}$ = +154.3 (*c* 0.35, CH_3OH); m.p. 240 °C (decomp.); ^{1}H NMR (400 MHz, DMSO–d_6): δ 8.81 (d, *J* = 4.4 Hz, 1H), 8.02 (d, *J* = 5.2 Hz, 1H), 7.77 (d, *J* = 4.4 Hz, 1H), 7.60 (t, *J* = 3.8 Hz, 2H), 7.50 (dd, *J* = 9.2, 2.0 Hz, 1H), 7.44 (s, 1H), 7.38 (d, *J* = 7.6 Hz, 2H), 6.84 (s, 1H), 6.53 (s, 1H), 6.03 (ddd, *J* = 17.6, 10.0, 7.2 Hz, 1H), 5.25 (s, 1H), 5.22 (d, *J* = 6.0 Hz, 1H), 5.00 (d, *J* = 12.8 Hz, 1H), 4.72 (d, *J* = 12.8 Hz, 1H), 4.23–4.19 (m, 1H), 4.07 (s, 3H), 3.96–3.94 (m, 1H), 3.85 (t, *J* = 9.2 Hz, 1H), 3.48 (t, *J* = 11.4 Hz, 1H), 2.90 (q, *J* = 9.6 Hz, 1H), 2.66 (q, *J* = 8.4 Hz, 1H), 2.39 (s, 4H), 1.89 (s, 1H), 1.76 (t, *J* = 8.8 Hz, 2H), 1.12–1.05 (m, 1H); ^{13}C NMR (100 MHz, DMSO–d_6): δ157.9, 147.9, 144.2, 144.0, 140.4, 137.7, 134.0, 131.9, 130.1, 125.9, 125.2, 121.9, 120.8, 117.5, 102.8, 67.7, 65.1, 63.6, 56.4, 56.1, 54.2, 37.2, 26.9, 23.6, 21.4, 21.1; IR (KBr) 3406, 3054, 1620, 1585, 1508, 1467, 1417, 1353, 1255, 1239, 1227, 1125, 1037, 1002, 928, 931, 816 cm^{-1}. HRMS calcd for $[C_{28}H_{33}N_2O_2]^+$: 429.2536, found 429.2540.

***N*-(4-Trifluoromethylbenzyl)quinidinium Bromide (3b)**[5]



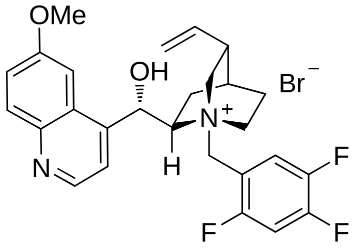
Prepared according to the general procedure, quinidine (324.4 mg, 1.0 mmol) and 4-trifluoromethylbenzyl bromide (286.8 mg, 1.2 mmol, 1.2 equiv) were stirred for 12 h. The resulting precipitate was purified by flash chromatography (MeOH/EtOAc = 1/10, v/v) to give a white solid (490.1 mg, 87% yield). $[\alpha]_D^{28}$ = +184.2 (*c* 0.15, CH_3OH); m.p. 218 °C (decomp.); ^{1}H NMR (400 MHz, DMSO–d_6): δ 8.82 (d, *J* = 4.4 Hz, 1H), 8.02 (d, *J* = 9.2 Hz, 1H), 7.97 (dd, *J* = 10.4, 9.2 Hz, 4H), 7.77 (d, *J* = 4.4 Hz, 1H), 7.51 (dd, *J* = 9.2, 2.4 Hz, 1H), 7.44 (d, *J* = 2.4 Hz, 1H), 6.84 (d, *J* = 3.6 Hz, 1H), 6.52 (s, 1H), 6.03 (ddd, *J* = 17.4, 10.5, 6.9 Hz, 1H), 5.25 (s, 1H), 5.10 (d, *J* = 8.4 Hz, 2H), 4.85 (d, *J* = 12.8 Hz, 1H), 4.28–4.22 (m, 1H), 4.06 (s, 3H), 4.02–4.00 (m, 1H), 3.86 (t, *J* = 9.4 Hz, 1H), 3.50 (t, *J* = 11.4 Hz, 1H), 3.00–2.90 (m, 1H), 2.69–2.63 (m, 1H), 2.40 (t, *J* = 11.4 Hz, 1H), 1.91 (s, 1H), 1.79–1.75 (m, 2H), 1.15–1.07 (m, 1H); ^{13}C NMR (100 MHz, DMSO–d_6): δ158.0, 147.9, 144.2, 143.8, 137.7, 135.1, 133.0, 131.9, 130.9 (q, *J* = 31.8 Hz), 126.4, 126.3, 125.9, 123.1, 121.7, 120.8, 117.5, 103.0, 68.1, 65.2, 62.9, 56.5, 56.2, 54.5, 37.2, 26.8, 23.6, 21.1; IR (KBr) 3398, 3209, 2954, 1621, 1589, 1509, 1373, 1427, 1325, 1227, 1241, 1170, 1125, 1068, 1021, 1003, 934, 864, 832 cm^{-1}.

***N*-(9-Anthracenylmethyl)quinidinium Chloride (3c)**[6]



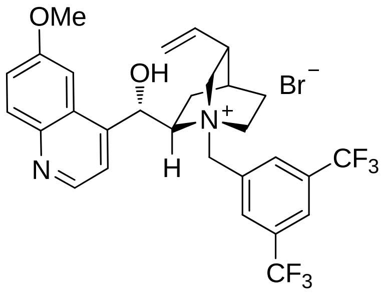
Prepared according to the general procedure, quinidine (324.4 mg, 1.0 mmol) and 9-anthracenylmethyl chloride (272.1 mg, 1.2 mmol, equiv) were stirred for 12 h. The resulting precipitate was purified by flash chromatography (MeOH/EtOAc = 1/10, V/V) to give a light yellow solid (457.5 mg, 80% yield). $[\alpha]_D^{28}$ = +390.0 (*c* 0.12, CH_3OH); m.p. 161 °C (decomp.) (lit.[6] m.p. 160 °C, decomp.); ^1H NMR (400 MHz, DMSO–d_6): δ 8.98 (s, 1H), 8.86 (d, *J* = 4.4 Hz, 1H), 8.79 (d, *J* = 9.2 Hz, 1H), 8.70 (d, *J* = 9.2 Hz, 1H), 8.28 (dd, *J* = 8.2, 3.0 Hz, 2H), 8.05 (d, *J* = 9.2 Hz, 1H), 7.90 (d, *J* = 4.4 Hz, 1H), 7.82–7.74 (m, 3H), 7.69–7.64 (m, 3H), 7.53 (dd, *J* = 7.6, 2.4 Hz, 1H), 6.98 (s, 1H), 6.33 (d, *J* = 14.4 Hz, 1H), 6.03 (ddd, *J* = 17.2, 10.2, 7.2 Hz, 1H), 5.88 (d, *J* = 14.0 Hz, 1H), 5.18 (d, *J* = 10.4 Hz, 1H), 5.08 (d, *J* = 17.2 Hz, 1H), 4.46 (t, *J* = 9.2 Hz, 2H), 4.21 (s, 4H), 3.18 (t, *J* = 11.2 Hz, 1H), 2.62–2.54 (m, 1H), 2.46–2.35 (m,2H), 1.78 (s, 1H), 1.69 (d, *J* = 8.4 Hz, 1H), 1.56–1.53 (m, 1H), 1.10–1.04 (m, 1H); ^{13}C NMR (100 MHz, DMSO–d_6): δ157.9, 147.9, 144.3, 137.9, 133.5, 133.3, 132.5, 131.8, 131.7, 131.6, 130.2, 128.3, 128.0, 126.1, 126.0, 125.3, 125.0, 122.3, 121.0, 119.3, 117.5, 103.2, 67.9, 65.7, 56.5, 56.1, 55.8, 55.6, 37.7, 26.1, 24.2, 21.6; IR (KBr) 3394, 3183, 1621, 1508, 1458, 1473, 1431, 1258, 1362, 1240, 1227, 1029, 922, 864, 744 cm^{-1}.

N-(2,4,5-Trifluorobenzyl)quinidinium Bromide (3d)



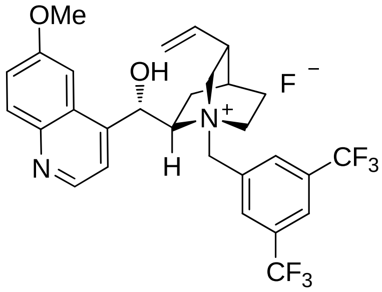
Prepared according to the general procedure, quinidine (324.4 mg, 1.0 mmol) and 2,4,5-trifluorobenzyl bromide (158.8 μL, 1.2 mmol, 1.2 equiv) were stirred for 12 h. The resulting precipitate was purified by flash chromatography (MeOH/EtOAc = 1/10, V/V) to give a white solid (379.1 mg, 69% yield). $[\alpha]_D^{28}$ = +194.8 (*c* 0.19, CH_3OH); m.p. 182–185 °C (decomp.); ^1H NMR (400 MHz, DMSO–d_6): δ 8.82 (d, *J* = 4.4 Hz, 1H), 8.16–8.10 (m, 1H), 8.02 (d, *J* = 9.2 Hz, 1H), 7.91–7.85 (m, 1H), 7.76 (d, *J* = 4.4 Hz, 1H), 7.50 (dd, *J* = 9.6, 2.8 Hz, 1H), 7.40 (d, *J* = 2.4 Hz, 1H), 6.84 (d, *J* = 2.8 Hz, 1H), 6.50 (s, 1H), 6.03 (ddd, *J* = 17.2, 10.4, 6.8 Hz, 1H), 5.26–5.21 (m, 2H), 5.01 (d, *J* = 12.8 Hz, 1H), 4.77 (d, *J* = 13.6 Hz, 1H), 4.23–4.18 (m, 1H), 4.06 (s, 3H), 3.94–3.82 (m, 2H), 3.49 (t, *J* = 11.4 Hz, 1H), 3.22–3.15 (m, 1H), 2.67–2.60 (m, 1H), 2.36 (t, *J* = 11.8 Hz, 1H), 1.90 (s, 1H), 1.84–1.75 (m, 2H), 1.10–1.05 (m, 1H); ^{13}C NMR (100 MHz, DMSO–d_6): δ 158.0 (ddd, *J* = 244.1, 9.9, 2.3 Hz), 157.9, 151.5 (dt, *J* = 251.2, 13.6 Hz), 147.9, 146.7 (ddd, *J* = 241.8, 12.6, 2.4 Hz), 144.2, 143.7, 137.7, 131.9, 125.9, 123.8 (dd, *J* = 19.1, 2.7 Hz), 122.0, 120.7, 117.6, 112.8 (dt, *J* = 17.0, 5.6 Hz), 107.5 (dd, *J* = 29.5, 21.4 Hz), 102.7, 68.0, 65.3, 56.4, 56.1, 56.0, 54.7, 37.5, 26.6, 23.7, 21.0; IR (KBr) 3394, 3198, 3006, 1621, 1520, 1473, 1469, 1431, 1338, 1259, 1241, 1226, 1205, 1158, 1113, 1026, 851, 828, 719 cm^{-1}; HRMS calcd for $[C_{27}H_{28}F_3N_2O_2]^+$: 469.2097, found 469.2098.

N-(3,5-Ditrifluoromethylbenzyl)quinidinium Bromide (3e)[7]



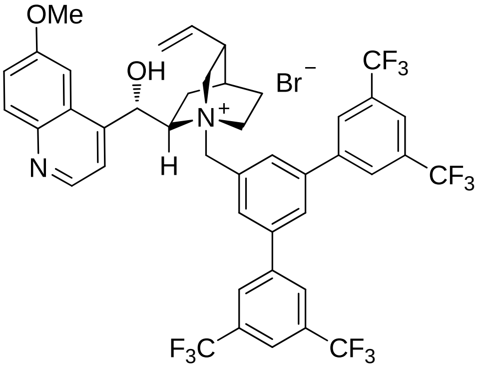
Prepared according to the general procedure, quinidine (324.4 mg, 1.0 mmol) and 3,5-ditrifluoromethylbenzyl bromide (368.4 mg, 1.2 mmol, 1.2 equiv) were stirred for 12 h. The resulting precipitate was purified by flash chromatography (MeOH/EtOAc = 1/10, V/V) to give a white solid (536.7 mg, 85% yield). $[\alpha]_D^{28}$ = +176.1 (c 0.19, CH_3OH); m.p. 177 °C (decomp.); ^{1}H NMR (400 MHz, DMSO–d_6): δ 8.82 (d, J = 4.8 Hz, 1H), 8.56 (s, 2H), 8.38 (s, 1H), 8.04 (d, J = 9.2 Hz, 1H), 7.77 (d, J = 4.4 Hz, 1H), 7.53 (dd, J = 7.2, 2.4 Hz 1H), 7.44 (d, J = 2.4 Hz, 1H), 6.78 (d, J = 3.2 Hz, 1H), 6.48 (s, 1H), 6.04 (ddd, J = 17.4, 10.2, 7.2 Hz, 1H), 5.28 (d, J = 2.8 Hz, 1H), 5.22 (d, J = 12.4 Hz, 2H), 5.01 (d, J = 12.8 Hz, 1H), 4.34 (t, J = 10.0 Hz, 1H), 4.10–4.13 (m, 1H), 4.06 (s, 3H), 3.80 (m, t, J = 9.4 Hz, 1H), 3.48 (t, J = 11.4 Hz, 1H), 3.04 (q, J = 9.6 Hz, 1H), 2.62 (q, J =8.4 Hz, 1H), 2.42 (t, J = 11.6 Hz, 1H), 1.91 (s, 1H), 1.85–1.72 (m, 2H), 1.20–1.13 (m, 1H); ^{13}C NMR (100 MHz, DMSO–d_6): δ 158.1, 147.9, 144.2, 143.7, 137.8, 135.1, 132.0, 131.7, 131.3 (q, J = 33.1 Hz), 130.1, 126.0, 125.0, 124.6 (q, J = 4.1 Hz), 123.7 (q, J = 271.3 Hz), 121.5, 120.9, 117.6, 103.1, 68.4, 65.2, 61.8, 56.3, 56.2, 54.7, 37.4, 26.9, 23.6, 21.1; IR (KBr) 3394, 3201, 2954, 2664, 1622, 1509, 1473, 1432, 1374, 1281, 1214, 1226, 1178, 1135, 1027, 1005, 866, 905, 843, 828, 709, 682 cm^{-1}.

N-(3,5-Ditrifluoromethylbenzyl)quinidinium Fluoride (3f)[8]



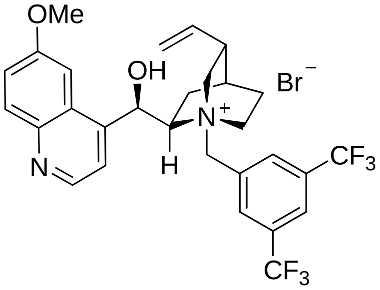
The column of Amberlyst A-26 (OH^- form, 500 mg) was washed with methanol. A solution of the *N*-(3,5-ditrifluoromethylbenzyl)quinidinium bromide (126.2 mg, 0.2 mmol) in methanol (5 mL) was slowly passed through the column and the column then washed with methanol. The eluent was neutralized until pH = 7 with HF and the solvents were removed *in vacuo*. The residue was coevaporated with toluene three times and dried under vaccum overnight and the chiral ammonium fluoride was used without further purification. $[\alpha]_D^{28}$ = +127.2 (c 0.14, CH_3OH); m.p. 190 °C (decomp.); ^{1}H NMR (400 MHz, DMSO–d_6): δ 8.83 (d, J = 4.4 Hz, 1H), 8.53 (s, 2H), 8.38 (s,1H), 8.05 (d, J = 9.2 Hz, 1H), 7.78 (d, J = 4.4 Hz, 1H), 7.55 (dd, J = 9.2, 2.4 Hz, 1H), 7.44 (d, J = 2.4 Hz, 1H), 6.75 (d, J = 2.8 Hz, 1H), 6.46 (s, 1H), 6.05 (ddd, J = 17.6, 10.4, 7.2 Hz, 1H), 5.24–5.29 (m, 2H), 5.14 (d, J = 12.8 Hz, 1H), 4.97 (d, J = 12.8 Hz, 1H), 4.32 (t, J = 9.2 Hz, 1H), 4.05 (s, 3H), 4.03 (t, J = 12.0, 1H), 3.78 (t, J = 10.0 Hz, 1H), 3.49 (t, J= 11.4, 1H), 3.13–2.99 (m, 1H), 2.62 (q, J = 2.4 Hz, 1H), 2.43 (t, J = 11.4 Hz, 1H), 1.92 (s, 1H), 1.83–1.76 (m, 2H), 1.46–1.20 (m, 1H); ^{13}C NMR (100 MHz, DMSO–d_6): δ158.1, 147.9, 144.1, 143.8, 137.7, 135.1, 132.0, 131.7, 131.3 (q, J = 33.1 Hz), 126.0, 124.7 (q, J = 1.9 Hz), 123.7 (q, J = 271.8 Hz), 121.4, 120.9, 117.6, 103.2, 68.5, 65.3, 61.9, 56.2, 54.8, 46.3, 44.7, 37.4, 26.9, 23.6, 21.0; IR (KBr) 3462, 2950, 1622, 1601, 1497, 1463, 1427, 1375, 1280, 1245, 1181, 1135, 1083, 903, 845, 748, 683, 483 cm^{-1}; HRMS calcd for $[C_{29}H_{29}F_6N_2O_2]^+$: 551.2127, found 551.2135.

***N*-(3,3'',5,5''-tetrakis(trifluoromethyl)-1,1':3',1''-terbenzyl)quinidinium Bromide (3g)**[7]



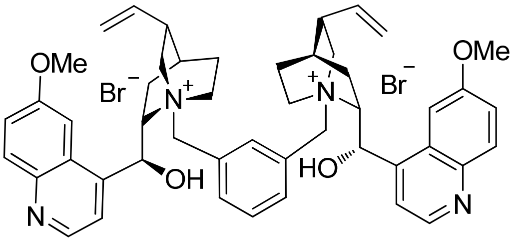
Prepared according to the general procedure, quinidine (324.4 mg, 1.0 mmol) and 3,3",5,5"-tetrakis(trifluoromethyl)-1,1':3',1"-terbenzyl bromide (714.0 mg, 1.2 mmol, 1.2equiv) were stirred for 12 h. The resulting precipitate was purified by flash chromatography (MeOH/EtOAc = 1/10, V/V) to give a white solid (919.4 mg, 71% yield). $[\alpha]_D^{28}$ = +129.5 (*c* 0.14, CH_3OH); m.p. 186 °C (decomp.); ^1H NMR (400 MHz, $CDCl_3$): δ 8.39 (d, *J* = 4.4 Hz, 1H), 8.29 (s, 2H), 8.00 (s, 4H), 7.84 (s, 2H), 7.69 (d, *J* = 6.0 Hz, 2H), 7.60 (s, 1H), 7.42 (s, 1H), 6.94 (d, *J* = 8.8 Hz, 1H), 6.71 (d, *J* = 5.6 Hz, 1H), 6.44 (s, 1H), 6.00 (s, 2H), 5.88 (ddd, *J* = 17.0, 10.2, 7.0 Hz, 1H), 5.23–5.17 (m, 2H), 4.66 (t, *J* = 10.0 Hz, 1H), 4.36 (t, *J* = 10.0 Hz, 1H),4.10 (t, *J* = 9.0 Hz, 1H), 3.77 (s, 3H), 3.34 (t, *J*= 11.2, 1H), 2.98 (q, *J* = 10.0 Hz, 1H), 2.28–2.43(m, 2H), 1.82 (s, 1H), 1.78 (d, *J*= 8.4 Hz, 2H), 0.90–0.83 (m, 1H); ^{13}C NMR (100 MHz, DMSO–d_6): δ 157.8, 147.0, 143.9, 142.1, 139.8, 135.1, 133.1, 132.5 (q, *J* = 33.4 Hz), 131.5, 130.2, 127.3, 127.2, 127.1, 126.0, 123.1 (q, *J* = 272.0 Hz), 122.1 (q, *J* = 3.4 Hz), 120.4, 120.1, 118.4, 102.8, 68.2, 66.8, 61.5, 56.9, 56.3, 54.5, 38.1, 27.1, 24.0, 21.7; IR (KBr) 3402, 3196, 2946, 1711, 1621, 1509, 1432, 1280, 1239, 1226, 1176, 1134, 1029, 1002, 900, 885, 844, 827, 718, 704, 683, 640 cm^{-1}.

***N*-(3,5-Ditrifluoromethylbenzyl)quininium Bromide (4)**[9]



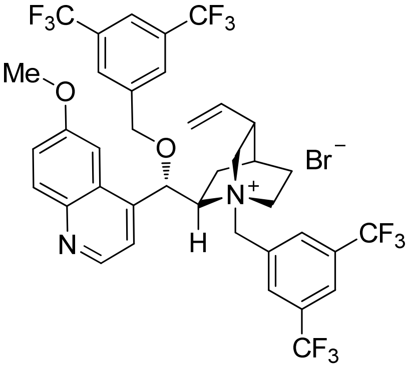
Prepared according to the general procedure, quinine (324.4 mg, 1.0 mmol) and 3,5-ditrifluoromethylbenzyl bromide (368.4 mg, 1.2 mmol, 1.2 equiv) were stirred for 12 h. The resulting precipitate was purified by flash chromatography (MeOH/EtOAc = 1/10, V/V) to give a white solid (372.3 mg, 59% yield). $[\alpha]_D^{28}$ = –164.5 (*c* 0.15, CH_3OH); m.p. 192 °C (decomp.); ^1H NMR (400 MHz, DMSO–d_6): δ 8.82 (d, *J* = 4.4 Hz, 1H), 8.52 (s, 2H), 8.37 (s,1H), 8.04 (d, *J* = 9.2 Hz, 1H), 7.76 (d, *J* = 4.4 Hz, 1H), 7.52 (dd, *J* = 9.2, 2.4 Hz, 1H), 7.40 (d, *J* = 2.8 Hz, 1H), 6.71 (d, *J* = 4.4 Hz, 1H), 6.56 (d, *J* = 4.4 Hz, 1H), 5.77 (ddd, *J* = 17.4, 10.5, 6.8 Hz, 1H), 5.67 (d, *J* = 12.4 Hz, 1H), 5.15 (d, *J* = 17.2 Hz, 1H), 5.03 (d, *J* = 4.4 Hz, 1H), 5.00 (d, *J* = 6.0 Hz, 1H), 4.41 (t, *J* = 11.2 Hz, 1H), 4.04 (s, 3H), 3.83 (dd, *J* = 16.8, 10.0 Hz, 2H), 3.47 (t, *J*= 11.4, 1H), 3.30–3.23 (m, 1H), 2.67–2.65 (m,1H), 2.28–2.24 (m, 1H), 2.19–2.12 (m, 1H), 2.03–1.99 (m, 1H), 1.82 (t, *J* = 10 Hz, 1H),1.47–1.53 (m,1 Hz); ^{13}C NMR (100 MHz, DMSO–d$_6$): δ158.1, 147.9, 144.2, 144.0, 138.5, 135.0, 132.0, 131.7, 131.3 (q, *J* = 33.0 Hz), 125.9, 124.7 (q, *J* = 3.4 Hz), 123.6 (q, *J* = 272.0 Hz), 121.8, 120.8, 117.2, 102.5, 69.1, 64.1, 61.8, 59.7, 56.3, 51.2, 37.7, 26.6, 24.7, 21.0; IR (KBr) 3406, 3218, 2983, 1706, 1622, 1509, 1473, 1432, 1374, 1280, 1241, 1226, 1178, 1137, 1028, 904, 843, 827, 683 cm^{-1}.

1,3-Bis(quinidinium-*N*-methylene)benzene Dibromide (5)[7]



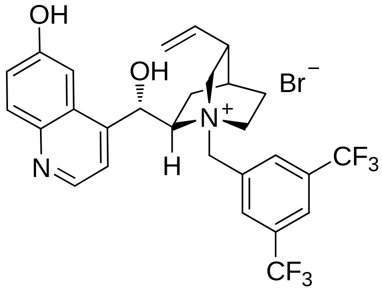
A mixture of quinidine (324.4 mg, 1.0 mmol) with α,α'-dibromo-*m*-xylene (132.0 mg, 0.5 mmol) in a mixture of ethanol (1 mL), DMF (1.2 mL), and chloroform (0.4 mL) was stirred at 100 °C for 8 h. After cooling the reaction mixture to room temperature, the reaction mixture was diluted with methanol (40 mL) and then added to ether (200 mL) dropwise with stirring. The solid precipitated was filtered. The resulting precipitate was purified by flash chromatography (MeOH/EtOAc = 1/10, V/V) to give a white solid (456.4 mg, 75% yield). $[\alpha]_D^{28}$ = +197.2 (*c* 0.14, CH_3OH); m.p. 218 °C (decomp.); ^{1}H NMR (400 MHz, DMSO–d$_6$): δ 8.82 (d, *J* = 4.0 Hz, 2H), 8.07 (s, 1H), 8.03 (d, *J* = 8.8 Hz, 2H), 7.90 (d, *J* = 7.6 Hz, 2H), 7.78 (d, *J* = 4.4 Hz, 2H), 7.74 (d, *J* = 7.6 Hz, 1H), 7.52 (d, *J* = 2.0 Hz, 1H), 7.50 (d, *J* = 2.0 Hz, 1H), 7.44 (d, *J* = 2.0 Hz, 2H), 6.83 (d, *J* = 3.2 Hz, 2H), 6.56 (s, 2H), 6.03 (ddd, *J* = 16.8, 10.4, 6.8 Hz, 2H), 5.22–5.12 (m, 6H), 4.82 (d, *J* = 12.4 Hz, 2H), 4.24–4.19 (m, 2H), 4.09–3.99 (m, 8H), 3.85–3.80 (m, 2H), 3.53–3.47 (m, 2H), 3.27–3.22 (m, 2H), 2.77–2.70 (m, 2H), 2.42 (t, *J* = 11.4 Hz, 2H), 1.91 (s, 2H), 1.76–1.74 (m, 4H), 1.16–1.12 (m, 2H); ^{13}C NMR (100 MHz, DMSO–d$_6$): δ158.0, 147.9, 144.2, 143.9, 139.2, 137.7, 135.7, 131.9, 130.2, 129.0, 125.9, 121.8, 120.9, 117.5, 102.8, 68.0, 65.1, 63.3, 56.2, 54.1, 37.3, 26.9, 23.5, 21.1; IR (KBr) 3386, 2951, 2361, 1621, 1590, 1509, 1473, 1459, 1431, 1358, 1241, 1227, 1207, 1026, 1001, 934, 866, 828, 717, 855 cm^{-1}.

***N*-(3,5-Ditrifluoromethyl)benzyl-O(9)-3,5-ditrifluoromethylbenzyl)quinidinium Bromide (6)**



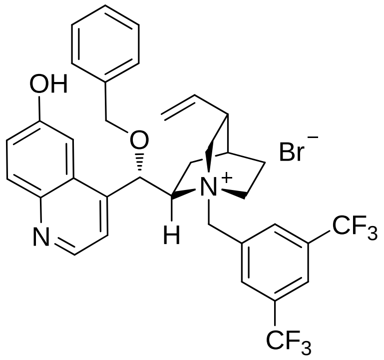
To a suspension of *N*-(3,5-ditrifluoromethylbenzyl)quinidinium bromide (632.5 mg, 1.0 mmol) in dichloromethane (3 mL) was added 3,5-ditrifluoromethylbenzyl bromide (920.0 μL, 5.0 mmol) and 50% aqueous KOH (560.0 μL, 5.0 mmol). The resulting mixture was stirred vigorously at room temperature for 4 h. The mixture was diluted with water (5 mL) and extracted with dichloromethane (3 x 20 mL). The combined organic extracts were dried over Na_2SO_4, filtered and concentrated *in vacuo*. The crude solid was purified by flash chromatography (MeOH/EtOAc = 1/10, V/V) to give a white solid (540.3 mg, 63% yield). $[\alpha]_D^{28}$ = +78.1 (*c* 0.31, CH_2Cl_2); m.p. 150 °C (decomp.); ^1H NMR (400 MHz, DMSO–d_6): δ 8.80 (d, *J* = 2.8 Hz, 1H), 8.53 (s, 2H), 8.39 (s, 1H), 8.27 (s, 2H), 8.09 (s, 1H), 8.04 (d, *J* = 9.2 Hz, 1H), 7.75 (d, *J* = 1.2 Hz, 1H), 7.56–7.48 (m, 2H), 6.57 (s, 1H), 6.01–5.96 (m, 1H), 5.19–5.02 (m, 5H), 4.68 (d, *J* = 12.0 Hz, 1H), 4.07 (s, 4H), 3.86–3.83 (m, 1H), 3.58–3.52 (m, 1H), 3.00–2.93 (m, 1H), 2.64 (d, *J* = 9.2 Hz, 2H), 1.98 (s, 1H), 1.81–1.74 (m, 2H),1.45–1.42 (m, 1H), 0.86–0.74 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 184.6, 158.8, 146.7,146.6, 146.5, 145.0, 141.3, 139.4, 137.8, 137.7, 134.9, 134.5, 134.4, 134.3, 132.5 (q, *J* = 33.0 Hz), 131.6, 130.2, 128.2 (q, *J* = 33.0 Hz), 124.6, 124.5, 124.4, 123.1 (q, *J* = 271.7 Hz), 122.7 (q, *J* = 271.9 Hz), 122.3 (q, *J* = 2.8 Hz), 118.2, 101.7, 73.1, 69.4, 67.5,61.5, 61.4, 56.1, 55.1, 37.7, 26.9, 23.6, 21.9, 11.0; IR (KBr) 3420, 2961, 1622, 1508, 1475, 1433, 1372, 1280, 1241, 1227, 1177, 1135, 1030, 902, 843, 828, 707, 683 cm^{-1}; HRMS calcd for $[C_{38}H_{33}F_{12}N_2O_2]^+$: 777.2344, found 777.2331.

N-(3,5-Ditrifluoromethyl)benzyl)-6´-hydroxyquinidinium Bromide (7)



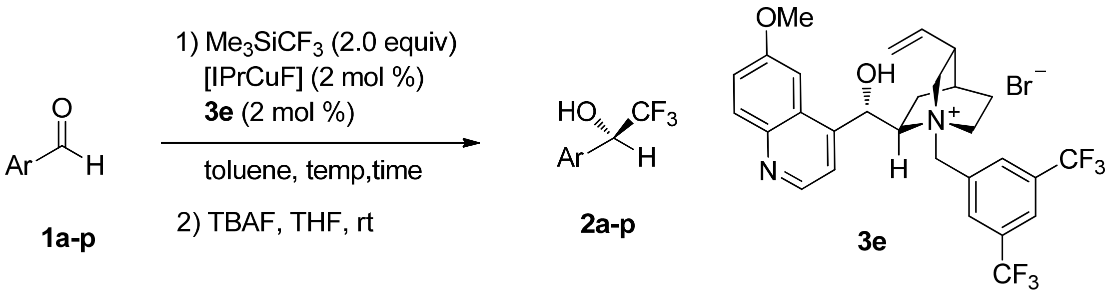
Ethanethiol (2.30 mL, 30.8 mmol) was added under argon atmosphere to a stirred suspension of sodium hydride (370.0 mg, 15.4 mmol) in dry DMF (15 ml). Quinidine (500 mg, 1.5mmol) in dry DMF (7.5 mL) was added dropwise and the reaction mixture was stirred at 110 °C for 13 h. The solvent and excess ethanethiol were removed under reduced pressure. Then the 3,5-ditrifluoromethylbenzyl bromide (675.4 mg, 2.2 mmol) was added in THF (9 mL). The reaction mixture was refluxed and monitored by TLC analysis. The solvent was removed under reduced pressure and the residue was purified by flash chromatography (MeOH/EtOAc = 1/20, V/V). The product was obtained as pale white solid (481.6 mg, 52 %). $[\alpha]_D^{28}$ = +182.3 (*c* 0.16, CH_3OH); m.p. 258 °C (decomp.); ^1H NMR (400 MHz, DMSO–d_6): δ 10.06 (s, 1H), 8.75 (d, *J* = 4.4 Hz, 1H), 8.63 (s, 2H), 8.37 (s, 1H), 7.95 (d, *J* = 8.8 Hz, 1H), 7.70 (d, *J* = 4.4 Hz, 1H), 7.67 (d, *J* = 2.4 Hz, 1H), 7.38 (dd, *J* = 9.0, 2.2 Hz, 1H), 6.68 (d, *J* = 3.6 Hz, 1H), 6.32 (s, 1H), 6.02 (ddd, *J* = 17.4, 10.5, 6.9 Hz, 1H), 5.38 (d, *J* = 12.4 Hz, 1H), 5.26–5.19 (m, 3H), 4.32 (t, *J* = 9.6 Hz, 1H), 4.13 (t, *J* = 9.6 Hz, 1H), 3.92 (t, *J* = 9.6 Hz, 1H), 3.49 (t, *J* = 11.2 Hz, 1H), 3.12–3.05 (m, 1H), 2.65–2.59 (m, 1H), 2.33 (t, *J* = 11.6 Hz, 1H), 1.89 (s, 1H), 1.83–1.78 (m, 2H), 1.17–1.09 (m, 1H); ^{13}C NMR (100 MHz, DMSO–d_6): δ156.5, 147.2, 143.4, 143.1, 137.7, 135.2, 131.9, 131.7, 131.2 (q, *J* = 33.0 Hz), 126.1, 124.6 (q, *J* = 3.2 Hz), 123.7 (q, *J* = 271.8 Hz), 122.2, 120.4, 117.6, 105.1, 68.2, 65.3, 60.9, 56.3, 54.7, 37.3, 26.9, 23.6, 21.0; IR (KBr) 3369, 3234, 1622, 1531, 1469, 1217, 1181, 1135, 1003, 927, 905, 864, 842, 736, 709, 683 cm^{-1}; HRMS calcd for $[C_{28}H_{27}F_6N_2O_2]^+$: 537.1971, found 537.1959.

N-(3,5-Ditrifluoromethyl)benzyl)-9-O-benzyl-6’-hydroxyquinidinium Bromide (8)



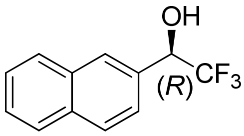
Sodium hydride (96.0 mg, 4.0 mmol) was added to a solution of quinidine (324.4 mg, 1.0 mmol) in dry DMF (5 mL). Benzyl chloride (173 μl, 1.5 mmol) was added dropwise. The reaction mixture was stirred at room temperature for 20 h and quenched by water. The aqueous phase was extracted with ethyl acetate. The organic layer was washed with brine, dried over Na_2SO_4, concentrated *in vacuo* to afford yellowish oil, which was used without purification. Ethanethiol (434.0 μL, 5.8 mmol) was added to a stirred suspension of sodium hydride (139.3 mg, 5.8 mmol) in dry DMF (3 mL). The yellowish oil (300 mg) in dry DMF (3 mL) was added dropwise and the reaction mixture was stirred at 110 °C for 15 h. The solvent and excess ethanethiol were removed under reduced pressure. The crude product was added the 3,5-ditrifluoromethylbenzyl bromide (336.2 mg, 1.1 mmol) in THF (6 mL). The reaction mixture was refluxed and monitored by TLC analysis. The solvent was removed under reduced pressure and the residue was purified by flash chromatography (MeOH/EtOAc = 1/20, V/V). The product was obtained as pale white solid (240.9 mg, 46 %). $[\alpha]_D^{28}$ = +68.9 (*c* 0.33, CH_3OH); m.p. 246 °C (decomp.); ^1H NMR (400 MHz, $CDCl_3$): δ 9.26 (s, 1 H), 8.83 (d, *J* = 3.6 Hz, 1H), 8.27 (s, 1H), 8.05 (d, *J* = 9.2 Hz, 2H), 7.97 (s,1H), 7.72–7.70 (m, 1H), 7.58–7.39 (m, 7H), 6.34 (d, *J* = 12.0 Hz, 1H), 6.05 (s, 1H), 5.93 (ddd, *J* = 17.0, 10.0, 7.2 Hz, 1H), 5.37 (d, *J* = 10.4 Hz, 1H), 5.24–5.13 (m, 2H), 5.07 (d, *J* = 12.4 Hz, 1H), 4.53 (t, *J* = 9.4 Hz, 1H), 4.33–4.29 (m, 2H), 4.16–4.11 (m, 1H), 3.75 (d, *J* = 12.0 Hz, 1H), 3.06 (t, *J* = 11.4 Hz, 1H), 2.75–2.67 (m, 1H), 2.51–2.36 (m, 2H), 2.02 (s, 1H), 1.95 (t, *J* = 10.4 Hz, 1H), 1.17–1.12 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.7, 157.4, 146.4, 144.1, 136.7, 135.8, 134.9, 134.0, 132.6 (q, *J* = 34.3 Hz), 132.3, 131.9, 130.9, 129.9, 129.8, 129.5, 129.4, 128.9, 125.9, 123.8, 122.7 (q, *J* = 272.4 Hz), 118.7, 104.8, 73.5, 72.0, 66.5, 59.4, 56.1, 54.4, 37.7, 27.0, 23.5, 21.7; IR (KBr) 3419, 3113, 2958, 2921, 2357, 1727, 1618, 1465, 1371, 1277, 1237, 1221, 1186, 1143, 1026, 903, 752, 706, 682 cm^{-1}; HRMS calcd for $[C_{35}H_{33}F_6N_2O_2]^+$: 627.2440, found 627.2434.

3 General procedure for the enantioselective trifluoromethylation reaction of aldehydes



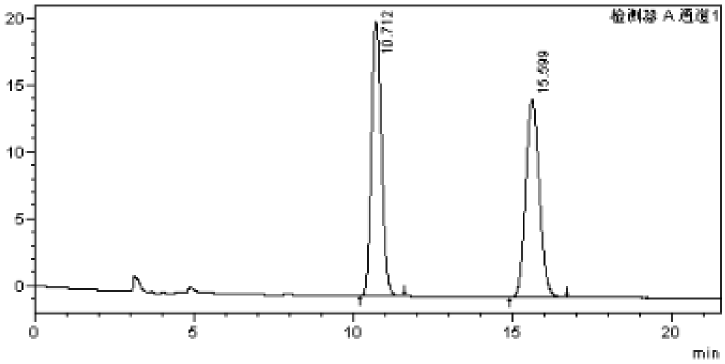
To a stirred solution of (IPr)CuF (1.9 mg, 0.004 mmol, 2 mol%) and *N*-(3,5-ditrifluoromethyl-benzyl)quinidinium bromide (**3e**) (2.6 mg, 0.004 mmol, 2 mol%) in toluene (0.6 mL) was added aryl aldehydes (**1a–p** 0.2 mmol) at –78 °C under argon atmosphere. Then this mixture was kept at –78 ^{o}C for 10 min. After that, Me_3SiCF_3 (60 µL, 0.4 mmol, 2 equiv) was added dropwise. After stirring for 1–2 h at –78 °C, the reaction was quenched with water. Aqueous layer was extracted with EtOAc (15 mL x 3), and the combined organic layers was washed with brine, dried over Na_2SO_4 and concentrated under reduced pressure. Then the crude product trimethylsilyl ether was treated with *n*-Bu_4NF (0.2 mL, 1 M in THF, 0.2 mmol) in THF (2.0 mL) at room temperature until all protected intermediate converted to final product. The resulting mixture was concentrated under reduced pressure, and purified by column chromatography on silica gel (PE/EtOAc = 20/1, V/V) to give trifluoromethylated alcohols **2a-p**.

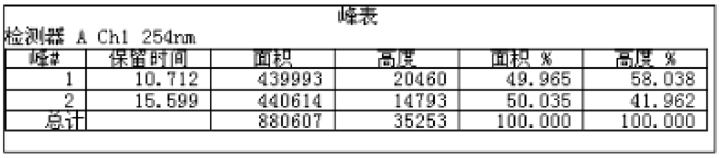
4. Analytical and spectral characterization data for the trifluoromethyl alcohols (2a-p)



2,2,2-trifluoro-1-(naphthalen-2-yl)ethanol (2a)[10]

The reaction of **1a** (31.2 mg, 0.20 mmol), Me_3SiCF_3 (60.0 µL, 0.40 mmol), (IPr)CuF (1.9 mg, 0.004 mmol, 2 mol%), quaternary ammonium salts (**3e)** (2.6 mg, 0.004 mmol, 2 mol%) for 1 h gave **2a** as a white solid (40.7 mg, 90%) by flash chromatography (PE/EtOAc = 20/1). m.p. 76–78 °C; $[\alpha]_D^{25}$ = –24.7 (*c* 0.21, CH_2Cl_2) [lit.[10] $[\alpha]_D^{20}$ = –23.7 (*c* 0.16, CH_2Cl_2, 71% ee)]; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96–7.86 (m, 4H), 7.59–7.51 (m, 3H), 5.19 (m, 1H), 2.77 (d, *J* = 4.4 Hz, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 133.8, 132.9, 131.3, 128.5, 128.3, 127.8, 127.4, 126.9, 126.6, 124.4 (q, *J*= 281.2 Hz), 124.3, 73.0 (q, *J* = 31.9 Hz) ppm; IR (KBr) 3374, 3062, 1602, 1507, 1341, 1247, 1262, 1193, 1124, 1085, 822, 792, 763, 752, 702, 486 cm^{-1}. The ee was determined by HPLC on Chiralpak OJ-H (*n*-hexane/*i*-PrOH = 80/20, 1.0 mL/min, 254 nm), t_R(major) = 10.7 min, t_S(minor) = 15.4 min, 75% ee.

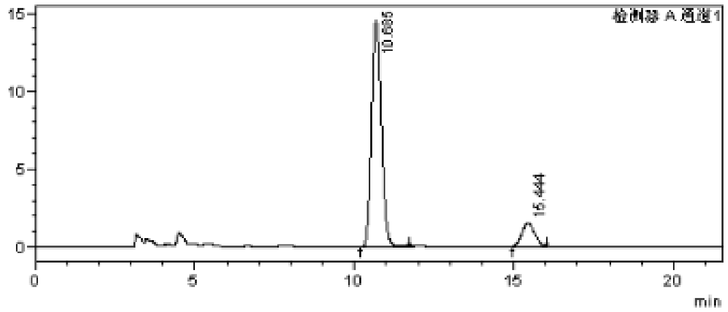




峰表

检测器 A Ch1 254nm

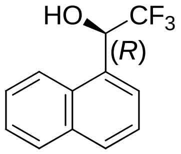
峰#	保留时间	面积	高度	面积 %	高度 %
1	10.712	439993	20460	49.965	58.038
2	15.599	440614	14793	50.035	41.962
总计		880607	35253	100.000	100.000



峰表

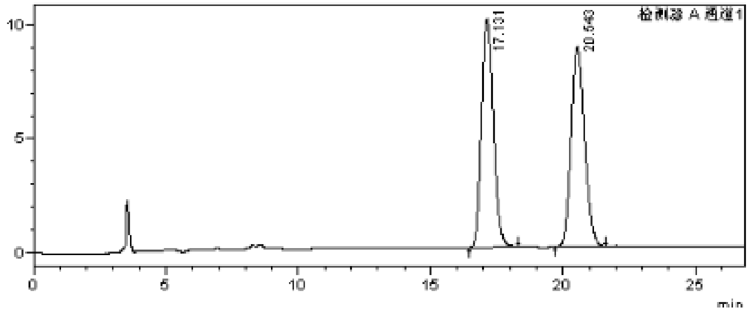
检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	10.685	306172	14562	87.619	90.601
2	15.444	43265	1511	12.381	9.399
总计		349437	16073	100.000	100.000



2,2,2-trifluoro-1-(naphthalen-1-yl)ethanol (2b)[11]

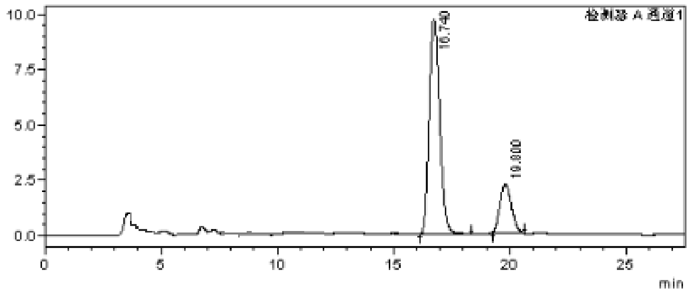
The reaction of **1b** (27.2 µL, 0.20 mmol), Me_3SiCF_3 (60.0 µL, 0.40 mmol), (IPr)CuF (1.9 mg, 0.004 mmol, 2 mol%), quaternary ammonium salts (**3e)** (2.6 mg, 0.004 mmol, 2 mol%) for 2 h gave **2b** as a colorless oil (39.8 mg, 88%) by flash chromatography (PE/EtOAc = 20/1). $[\alpha]_D^{25} = -14.6$ (*c* 0.47, CH_2Cl_2); ^1H NMR (400 MHz, $CDCl_3$): δ 8.06 (d, $J = 8.4$ Hz, 1 H), 7.93–7.91 (m, 2H), 7.84 (d, $J = 7.2$ Hz, 1H), 7.60–7.53 (m, 3H), 5.90 (m, 1H), 2.78 (d, $J = 4.0$ Hz, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 131.1, 130.3, 129.1, 126.1, 125.8, 125.2, 124.7 (q, $J = 281.7$ Hz), 122.8, 69.0 (q, $J = 32.0$ Hz) ppm; IR (KBr) 3421, 3046, 2927, 2847, 1515, 1399, 1355, 1264, 1167, 1126, 1093, 1030, 877, 781, 698, 632, 538 cm^{-1}. The ee was determined by HPLC on Chiralpak AS-H (*n*-hexane/*i*-PrOH = 98/2, 1.0 mL/min, 254 nm), t_R(major) = 16.7 min, t_S(minor) = 19.8 min, 60% ee.

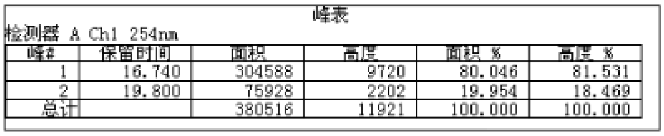


峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	17.131	311583	10021	50.034	53.360
2	20.543	311155	8759	49.966	46.640
总计		622738	18779	100.000	100.000

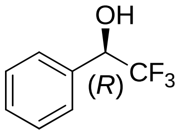




峰表

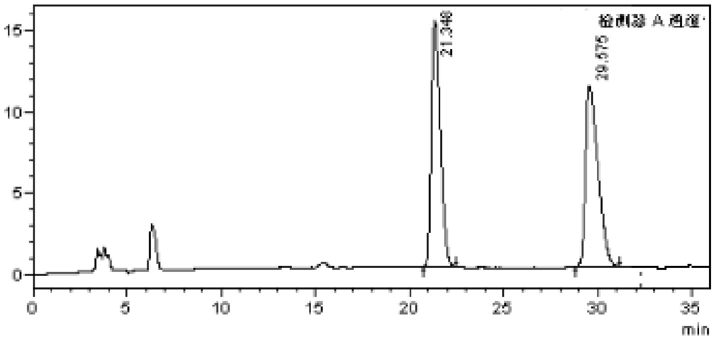
检测器 A Ch1 254nm

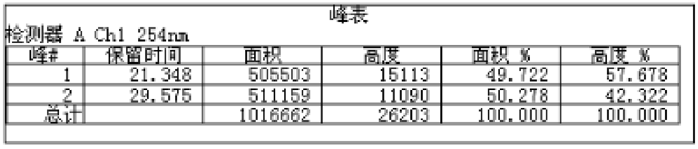
峰#	保留时间	面积	高度	面积 %	高度 %
1	16.740	304588	9720	80.046	81.531
2	19.800	75928	2202	19.954	18.469
总计		380516	11921	100.000	100.000



2,2,2-trifluoro-1-phenylethanol (2c)[10]

The reaction of **1c** (20.3 μL, 0.20 mmol), Me_3SiCF_3 (60.0 μL, 0.40 mmol), (IPr)CuF (1.9 mg, 0.004 mmol, 2 mol%), quaternary ammonium salts (**3e)** (2.6 mg, 0.004 mmol, 2 mol%) at –20°C for 2 h gave **2c** as a colorless oil (28.1 mg, 88%) by flash chromatography (PE/EtOAc = 20/1). $[\alpha]_D^{25}$= –13.1 (*c* 0.28, CH_2Cl_2) [lit.[10] $[\alpha]_D^{20}$ = –12.5 (*c* 0.40, CH_2Cl_2, 56% ee)]; ^1H NMR (400 MHz, $CDCl_3$): δ7.48–7.47 (m, 2H), 7.42–7.40 (m, 3H), 5.10 (q, *J* = 6.6 Hz, 1H), 2.73 (s, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 134.0, 129.6, 128.7, 127.5, 124.3 (q, *J*= 281.0 Hz), 72.9 (q, *J*= 32.0 Hz) ppm; IR (KBr) 3410, 2927, 2851, 2360, 2342, 1457, 1206, 1171, 1127, 1093, 1063, 1029, 860, 760, 705, 633 cm^{-1}. The ee was determined by HPLC on Chiralpak OJ-H (*n*-hexane/*i*-PrOH = 95/5, 1.0 mL/min, 254 nm), t_R(major) = 21.3 min, t_S (minor) = 29.4 min, 60% ee.

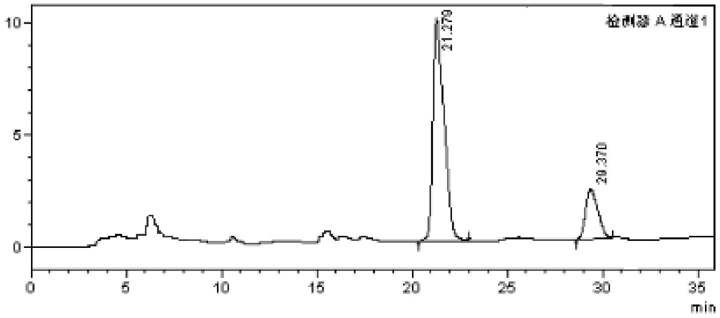




峰表

检测器 A Ch1 254nm

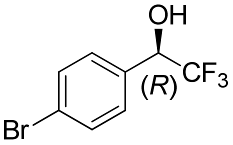
峰#	保留时间	面积	高度	面积 %	高度 %
1	21.348	505503	15113	49.722	57.678
2	29.575	511159	11090	50.278	42.322
总计		1016662	26203	100.000	100.000



峰表

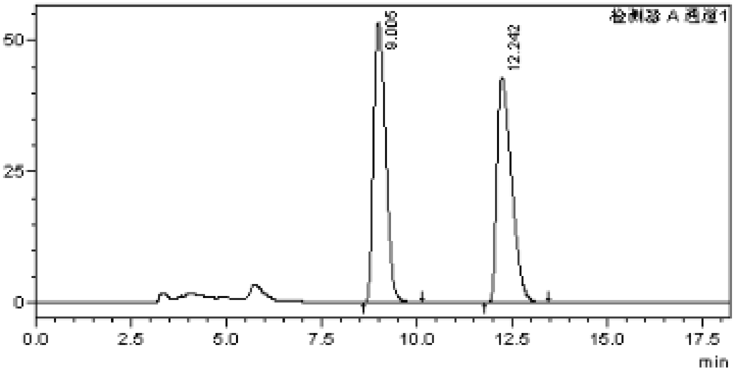
检测器 A Ch1 254nm

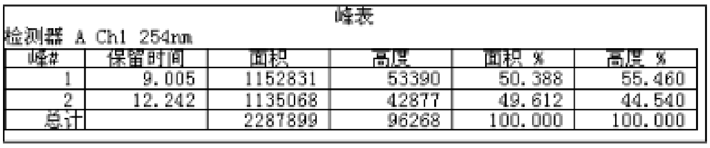
峰#	保留时间	面积	高度	面积 %	高度 %
1	21.279	405034	9921	80.161	81.733
2	29.370	100243	2217	19.839	18.267
总计		505277	12139	100.000	100.000



1-(4-bromophenyl)-2,2,2-trifluoroethanol (2d)[11]

The reaction of **1d** (37.0 mg, 0.20 mmol), Me_3SiCF_3 (60.0 μL, 0.40 mmol, 2 equiv), (IPr)CuF (1.9 mg, 0.004 mmol, 2 mol%), quaternary ammonium salts (**3e)** (2.6 mg, 0.004 mmol, 2 mol%) for 2 h gave **2d** as a colorless oil (41.3 mg, 81%) by flash chromatography (PE/EtOAc = 20/1). $[\alpha]_D^{25}$= –11.5 (*c* 0.24, CH_2Cl_2); ^1H NMR (400 MHz, $CDCl_3$): δ 7.55–7.52 (m, 2H), 7.34 (d, *J* = 8.4 Hz, 2H), 4.97 (q, *J* = 6.4 Hz, 1H), 2.98 (s, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 132.8, 131.9, 129.1, 124.0 (q, *J*= 281.1 Hz), 123.8, 72.2 (q, *J*= 32.1 Hz) ppm; IR (KBr) 3420, 2921, 2353, 1596, 1491, 1406, 1356, 1267, 1097, 1012, 871, 847, 807, 726, 667, 586 cm^{-1}. The ee was determined by HPLC on Chiralpak OD-H (*n*-hexane/*i*-PrOH = 95/5, 1.0 mL/min, 254 nm), t_R(major) = 9.1 min, t_S(minor) = 12.6 min, 57% ee.

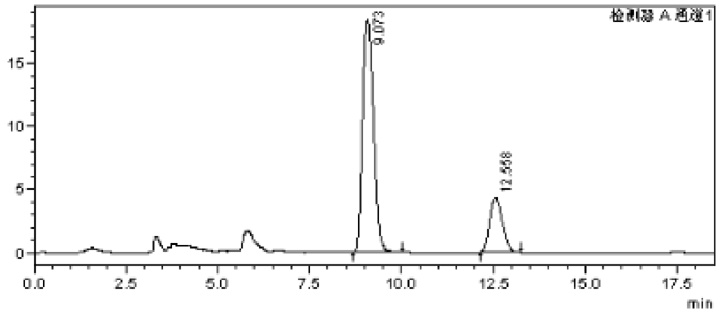


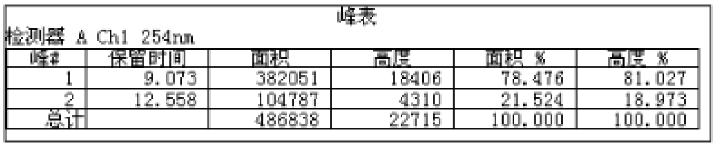


峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	9.005	1152831	53390	50.388	55.460
2	12.242	1135068	42877	49.612	44.540
总计		2287899	96268	100.000	100.000

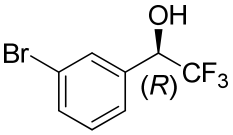




峰表

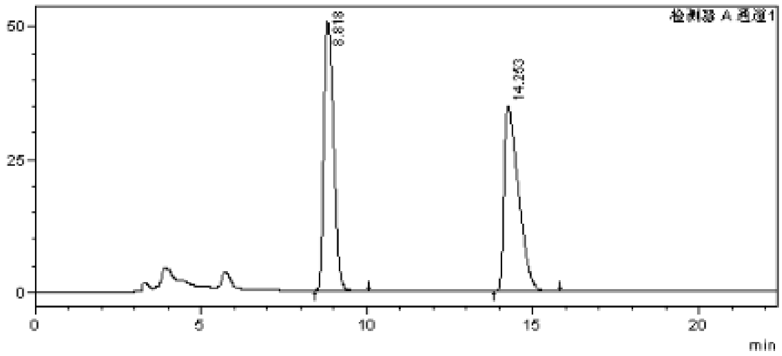
检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	9.073	382051	18406	78.476	81.027
2	12.558	104787	4310	21.524	18.973
总计		486838	22715	100.000	100.000



1-(3-bromophenyl)-2,2,2-trifluoroethanol (2e)[12]

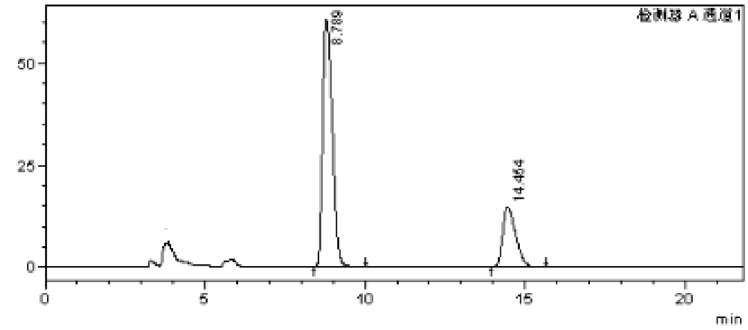
The reaction of **1e** (23.4 μL, 0.20 mmol), Me_3SiCF_3 (60.0 μL, 0.40 mmol), (IPr)CuF (1.9 mg, 0.004 mmol, 2 mol%), quaternary ammonium salts (**3e)** (2.6 mg, 0.004 mmol, 2 mol%) for 2 h gave **2e** as a colorless oil (41.7 mg, 82%) by flash chromatography (PE/EtOAc = 20/1). $[\alpha]_D^{25}$= –7.3 (*c* 0.11, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.64 (s, 1H), 7.55–7.52 (m, 1H), 7.40–7.38 (d, *J* = 7.6 Hz, 1H), 7.27 (t, *J* = 7.8 Hz, 1H), 5.00–4.95 (m, 1H), 3.01 (d, *J* = 4.4 Hz, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 136.3, 130.3, 124.0 (q, *J*=281.1 Hz), 123.2, 116.7, 114.7, 114.5, 72.2 (q, *J*= 32.1 Hz) ppm; IR (KBr) 3409, 3062, 2925, 1574, 1430, 1355, 1255, 1178, 1100, 1076, 997, 838, 784, 677, 630, 532, 453 cm^{-1}. The ee was determined by HPLC on Chiralpak OD-H (*n*-hexane/*i*-PrOH = 95/5, 1.0 mL/min, 254 nm), t_R(major) = 8.8 min, t_S(minor) = 14.4 min, 51% ee.



峰表

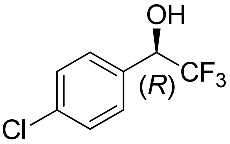
检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	8.818	1047013	50632	49.762	59.182
2	14.253	1057025	34921	50.238	40.818
总计		2104039	85553	100.000	100.000



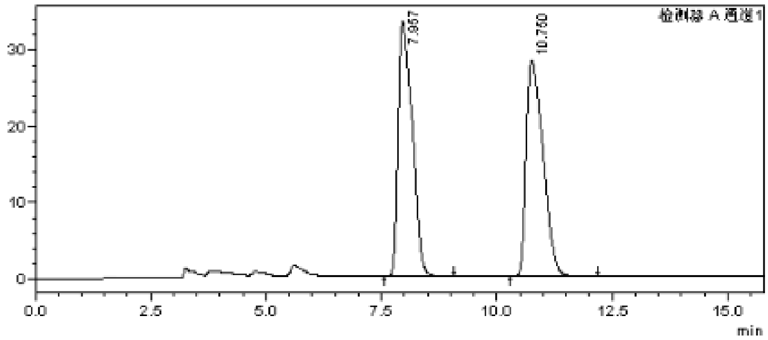
峰表
检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	8.789	1276445	60354	75.572	80.504
2	14.454	412595	14616	24.428	19.496
总计		1689040	74970	100.000	100.000



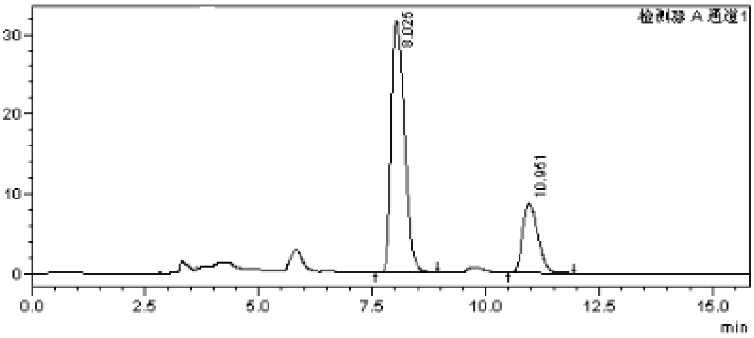
1-(4-chlorophenyl)-2,2,2-trifluoroethanol (2f)[10]

The reaction of **1f** (28.1 mg, 0.20 mmol), Me_3SiCF_3 (60.0 µL, 0.40 mmol), (IPr)CuF (1.9 mg, 0.004 mmol, 2 mol%), quaternary ammonium salts (**3e)** (2.6 mg, 0.004 mmol, 2 mol%) at –20 °C for 2 h gave **2f** as a colorless oil (35.0 mg, 83%) by flash chromatography (PE/EtOAc = 20/1). $[\alpha]_D^{25}$= –8.3 (*c* 0.13, CH_2Cl_2) [lit.[10] $[\alpha]_D^{20}$ = –8.8 (*c* 0.10, CH_2Cl_2, 50% ee)]; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.43–7.38 (m, 4H), 5.04–4.98 (m, 1H), 2.72 (d, *J* = 4.4 Hz, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 135.7, 132.4, 129.0, 128.9, 124.1 (q, *J* = 281.1 Hz), 72.3 (q, *J*= 32.1 Hz) ppm; IR (KBr) 3431, 2919, 1576, 1492, 1346, 1267, 1197, 1097, 870, 847, 811, 667, 586 cm^{-1}. The ee was determined by HPLC on Chiralpak OD-H (*n*-hexane/*i*-PrOH = 95/5, 1.0 mL/min, 254 nm), t_R(major) = 8.0 min, t_S(minor) = 10.9 min, 52% ee.



峰表
检测器 A Ch1 254nm

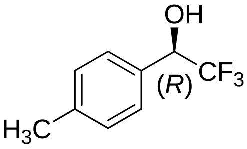
峰#	保留时间	面积	高度	面积 %	高度 %
1	7.957	717783	33528	49.967	54.193
2	10.750	718723	28340	50.033	45.807
总计		1436506	61867	100.000	100.000



峰表

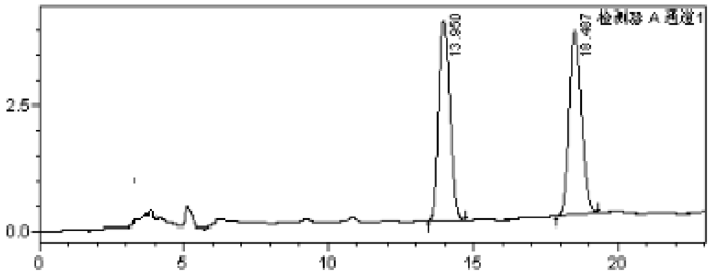
检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	8.025	646492	31579	76.085	78.474
2	10.951	203208	8662	23.915	21.526
总计		849700	40241	100.000	100.000



2,2,2-trifluoro-1-(p-tolyl)ethanol (2g)[10]

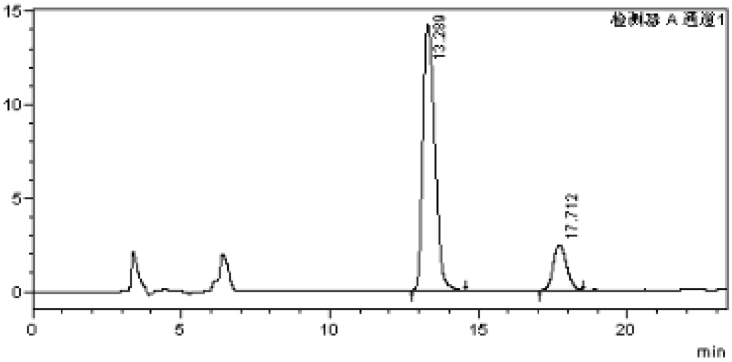
The reaction of **1g** (23.6 µL, 0.20 mmol), Me_3SiCF_3 (60.0 µL, 0.40 mmol), (IPr)CuF (1.9 mg, 0.004 mmol, 2 mol%), quaternary ammonium salts (**3e)** (2.6 mg, 0.004 mmol, 2 mol%) for 1 h gave **2g** as a colorless oil (33.4 mg, 88%) by flash chromatography (PE/EtOAc = 20/1). $[\alpha]_D^{25} = -12.7$ (*c* 0.18, CH_2Cl_2) [lit.[10] $[\alpha]_D^{20} = -18.4$ (*c* 0.43, CH_2Cl_2, 60% ee)]; ^1H NMR (400 MHz, $CDCl_3$): δ 7.36 (d, *J* = 8.0 Hz, 2H), 7.22 (d, *J* = 7.6 Hz, 2H), 4.97 (m, 1H), 2.73 (s, 1H), 2.38 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.6, 131.1, 129.4, 127.4, 124.3 (q, *J* = 280.9 Hz), 72.8 (q, *J* = 31.9 Hz), 21.3 ppm; IR (KBr) 3421, 3046, 2927, 2847, 1515, 1399, 1355, 1264, 1167, 1126, 1093, 1030, 1001, 877, 781, 698, 632, 538, 525, 455 cm^{-1}. The ee was determined by HPLC on Chiralpak OD-H (*n*-hexane/*i*-PrOH = 97/3, 1.0 mL/min, 254 nm), t_R(major) = 13.3 min, t_S(minor) = 17.7 min, 68% ee.



峰表

检测器 A Ch1 254nm

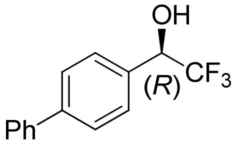
峰#	保留时间	面积	高度	面积 %	高度 %
1	13.950	107872	4001	49.707	52.245
2	18.487	109145	3657	50.293	47.755



峰表

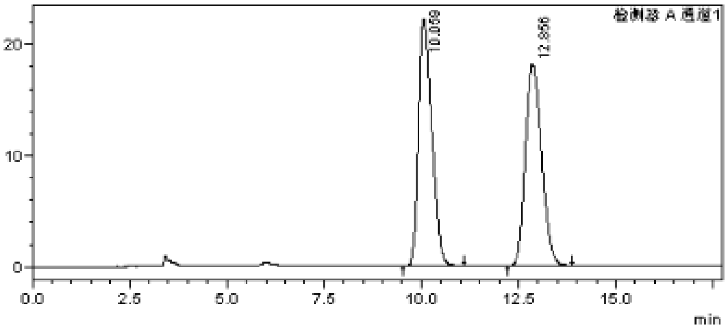
检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	13.289	390368	14187	83.988	85.451
2	17.712	74420	2416	16.012	14.549
总计		464787	16603	100.000	100.000



1-([1,1'-biphenyl]-4-yl)-2,2,2-trifluoroethanol (2h)[10]

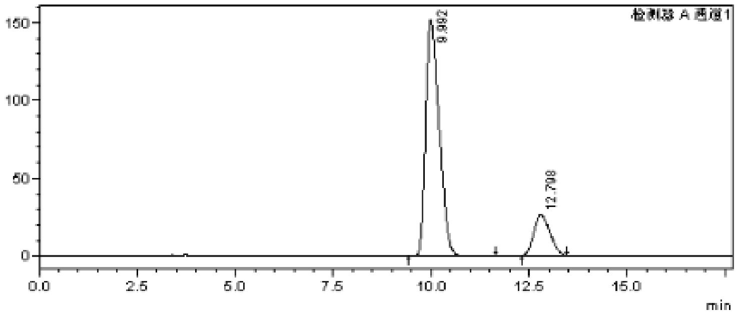
The reaction of **1h** (36.0 mg, 0.20 mmol), Me_3SiCF_3 (60.0 μL, 0.40 mmol), (IPr)CuF (1.9 mg, 0.004 mmol, 2 mol%), quaternary ammonium salts (**3e)** (2.6 mg, 0.004 mmol, 2 mol%) for 1 h gave **2h** as a white solid (45.4 mg, 90%) by flash chromatography (PE/EtOAc = 10/1). m.p. 113–114 °C; $[\alpha]_D^{28}$= –18.5 (*c* 0.40, CH_2Cl_2) [lit.[10] $[\alpha]_D^{20}$ = –7.1 (*c* 0.14, CH_2Cl_2, 56% ee)]; ^{1}H NMR (400 MHz, $CDCl_3$): δ7.65–7.54(m, 6H), 7.47–7.43 (m, 2H), 7.39–7.35 (m, 1H), 5.07 (m, 1H), 2.70 (d, *J* = 4.4 Hz, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 142.5, 140.3, 132.9, 128.9, 127.9, 127.7, 127.4, 127.2, 124.3 (q, *J*= 281.0 Hz), 72.7 (q, *J*= 32.0 Hz) ppm; IR (KBr) 3364, 1490, 1408, 1352, 1256, 1198, 1173, 1158, 1130, 1075, 1006, 855, 823, 764, 743, 726, 696 cm^{-1}. The ee was determined by HPLC on Daicel Chiralpak OD-H (hexane/iPrOH = 90/10, 1.0 mL/min, 254 nm), t_R(major) = 10.0 min, t_S(minor) = 12.8 min, 66% ee.



峰表

检测器 A Ch1 254nm

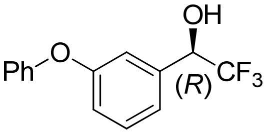
峰#	保留时间	面积	高度	面积 %	高度 %
1	10.059	527496	22150	50.068	55.040
2	12.856	526062	18093	49.932	44.960
总计		1053559	40243	100.000	100.000



峰表

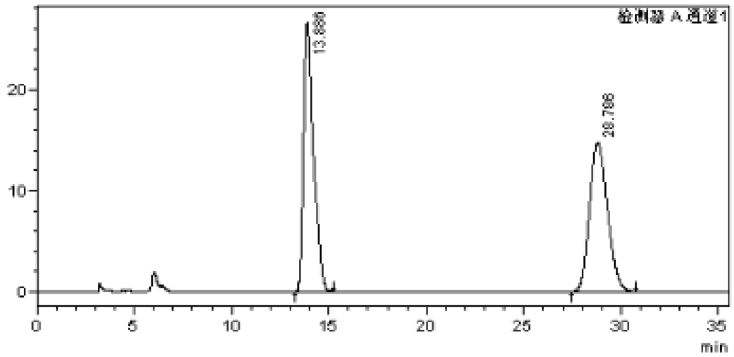
检测器 A Ch1 254nm

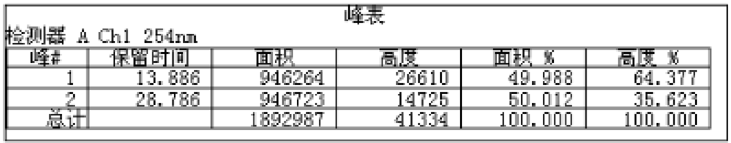
峰#	保留时间	面积	高度	面积 %	高度 %
1	9.992	3650280	152069	82.898	85.278
2	12.798	753059	26252	17.102	14.722
总计		4403339	178321	100.000	100.000



2,2,2-trifluoro-1-(3-phenoxyphenyl)ethanol (2i)[13]

The reaction of **1i** (34.5μL, 0.20 mmol), Me_3SiCF_3 (60.0 μL, 0.40 mmol), (IPr)CuF (1.9 mg, 0.004 mmol, 2 mol%), quaternary ammonium salts (**3e)** (2.6 mg, 0.004 mmol, 2 mol%) for 1 h gave **2i** as a colorless oil (46.6 mg, 87%) by flash chromatography (petroleum ether/EtOAc = 20/1). $[\alpha]_D^{25}$= –8.8 (*c* 0.50, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37–7.32 (m, 3H), 7.18 (d, *J* = 8.0 Hz, 1H), 7.14–7.10 (m, 2H), 7.04–7.00 (m, 3H), 4.96 (m, 1H), 2.75 (d, *J* = 4.0 Hz, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.3, 156.4, 135.6, 129.7, 129.6, 123.8 (q, *J* = 281.0 Hz), 123.4, 121.8, 119.3, 118.8, 117.5, 72.2 (q, *J* = 32.0 Hz) ppm; IR (KBr) 3447, 2926, 2843, 2357, 1606, 1491, 1458, 1438, 1262, 1170, 1126, 1044, 839, 788, 710, 631, 556 cm^{-1}. The ee was determined by HPLC on Chiralpak OD-H (*n*-hexane/*i*-PrOH = 95/5, 1.0 mL/min, 254 nm), t_R(major) = 13.9 min, t_S(minor) = 28.6 min, 60% ee.

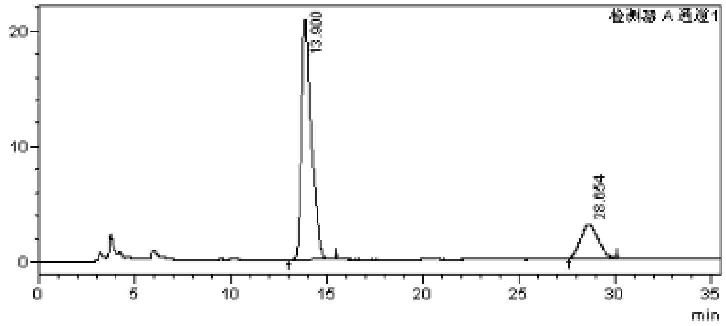


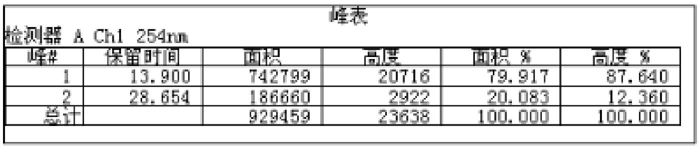


峰表

检测器 A Ch1 254nm

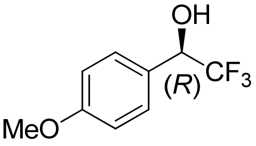
峰#	保留时间	面积	高度	面积 %	高度 %
1	13.886	946264	26610	49.988	64.377
2	28.786	946723	14725	50.012	35.623
总计		1892987	41334	100.000	100.000




峰表

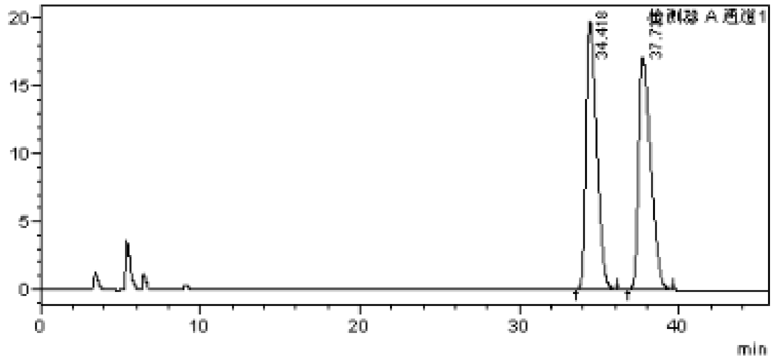
检测器 A Ch1 254nm

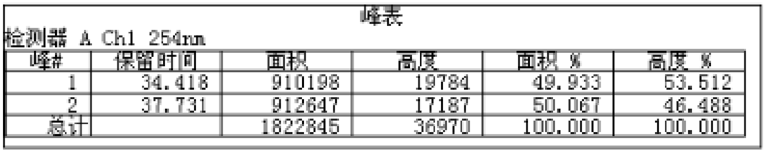
峰#	保留时间	面积	高度	面积 %	高度 %
1	13.900	742799	20716	79.917	87.640
2	28.654	186660	2922	20.083	12.360
总计		929459	23638	100.000	100.000



2,2,2-trifluoro-1-(4-methoxyphenyl)ethanol (2j)[10]

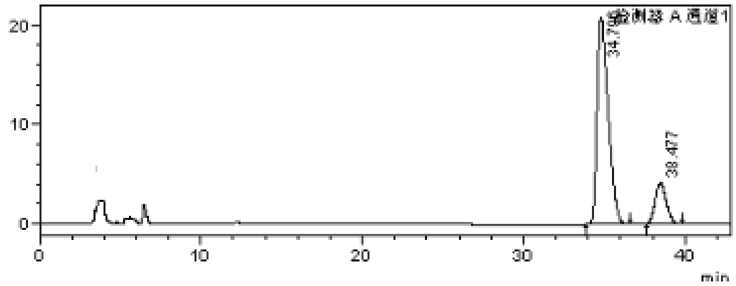
The reaction of **1j** (24.3μL, 0.20 mmol), Me_3SiCF_3 (60.0 μL, 0.40 mmol), (IPr)CuF (1.9 mg, 0.004 mmol, 2 mol%), quaternary ammonium salts (**3e)** (2.6 mg, 0.004 mmol, 2 mol%) for 1 h gave **2j** as a colorless oil (35.0 mg, 85%) by flash chromatography (PE/EtOAc = 20/1). $[\alpha]_D^{25}$= –13.6 (*c* 0.27, CH_2Cl_2) [lit.[10] $[\alpha]_D^{20}$ = –8.9 (*c* 1.00, CH_2Cl_2, 41% ee)]; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40 (d, *J* = 8.4 Hz, 2H), 6.93 (d, *J* = 8.4 Hz, 2H), 4.97 (q, *J* = 3.2 Hz, 1H), 3.82 (s, 3H), 2.58 (s, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.5, 128.8, 126.2, 124.4 (q, *J*= 281.0 Hz), 114.1, 72.5 (q, *J*= 32.0 Hz), 55.3 ppm; IR (KBr) 3445, 3008, 2918, 2842, 1614, 1587, 1517, 1465, 1444, 1356, 1252, 1207, 1171, 1127, 1075, 1031, 850, 819, 695, 589, 520 cm^{-1}. The ee was determined by HPLC on Chiralpak OJ-H (*n*-hexane/*i*-PrOH = 95/5, 1.0 mL/min, 254 nm), t_R(major) = 34.8 min, t_S(minor) = 38.5 min, 67% ee.

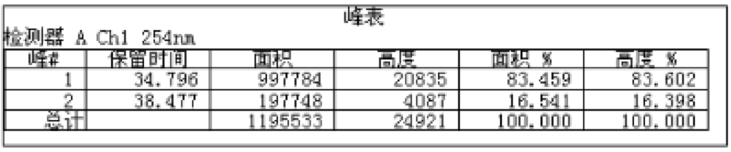



峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	34.418	910198	19784	49.933	53.512
2	37.731	912647	17187	50.067	46.488
总计		1822845	36970	100.000	100.000

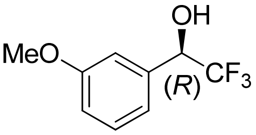




峰表

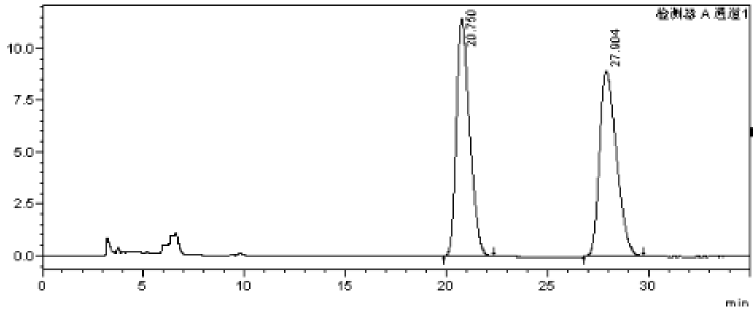
检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	34.796	997784	20835	83.459	83.602
2	38.477	197748	4087	16.541	16.398
总计		1195533	24921	100.000	100.000



2,2,2-trifluoro-1-(3-methoxyphenyl)ethanol (2k)[14]

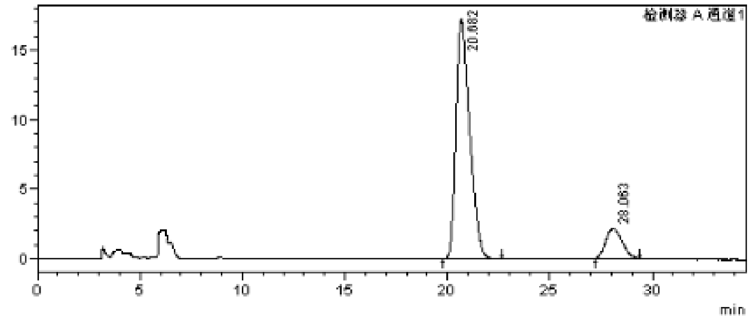
The reaction of **1k** (24.3 µL, 0.20 mmol), Me_3SiCF_3 (60.0 µL, 0.40 mmol), (IPr)CuF (1.9 mg, 0.004 mmol, 2 mol%), quaternary ammonium salts (**3e)** (2.6 mg, 0.004 mmol, 2 mol%) for 1 h gave **2k** as a colorless oil (36.7 mg, 89%) by flash chromatography (PE/EtOAc = 20/1). $[\alpha]_D^{25}$= –13.6 (*c* 0.13, CH_2Cl_2); ^1H NMR (400 MHz, $CDCl_3$): δ 7.38–7.30 (m, 1H), 7.04 (d, *J* = 7.6 Hz, 2H), 6.95–6.92 (m, 1H), 4.98 (m, 1H), 3.82 (s, 3H), 2.93 (s, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.8, 135.5, 129.7, 124.2 (q, *J*= 281.1 Hz), 119.8, 115.1, 113.0, 72.8 (q, *J*= 31.8 Hz), 55.4 ppm; IR (KBr) 3442, 2926, 2843, 1357, 1605, 1589, 1491, 1458, 1438, 1262, 1170, 1126, 1044, 933, 839, 788, 760, 710, 631, 556 cm^{-1}. The ee was determined by HPLC on Chiralpak OD-H (*n*-hexane/*i*-PrOH = 95/5, 1.0 mL/min, 254 nm), t_R(major) = 20.7 min, t_S(minor) = 28.0 min, 74% ee.

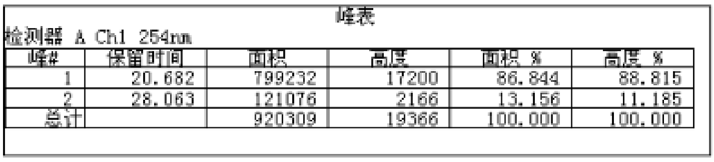


峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	20.750	522318	11420	50.074	56.131
2	27.904	520773	8925	49.926	43.869
总计		1043091	20345	100.000	100.000

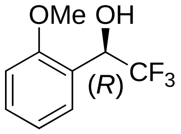




峰表

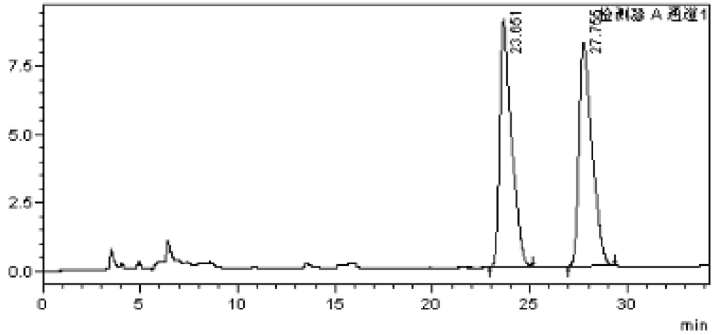
检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	20.682	799232	17200	86.844	88.815
2	28.063	121076	2166	13.156	11.185
总计		920309	19366	100.000	100.000



2,2,2-trifluoro-1-(2-methoxyphenyl)ethanol (2l)[11]

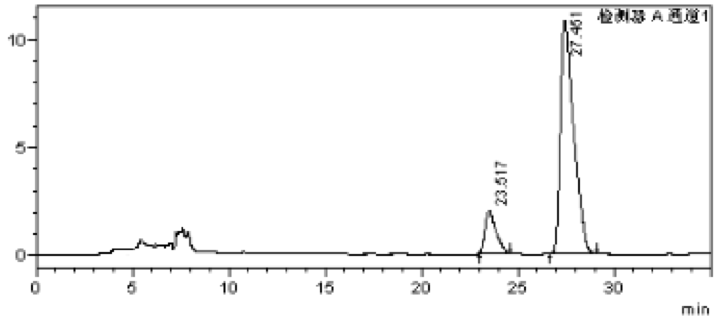
The reaction of **1l** (27.2 mg, 0.20 mmol), Me_3SiCF_3 (60.0 μL, 0.40 mmol), (IPr)CuF (1.9 mg, 0.004 mmol, 2 mol%), quaternary ammonium salts (**3e)** (2.6 mg, 0.004 mmol, 2 mol%) for 1 h gave **2l** as a colorless oil (36.1 mg, 88%) by flash chromatography (PE/EtOAc = 20/1). $[\alpha]_D^{25}$= –11.7 (*c* 0.24, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39–7.34 (m, 2H), 7.00 (dt, *J* = 7.6, 1.2 Hz, 1H), 6.94 (d, *J* = 8.4 Hz, 1H), 5.27 (m, 1H), 3.86 (s, 3H), 3.75 (q, *J* = 4.0 Hz, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.6, 130.6, 129.3, 124.7 (q, *J*= 282.0 Hz), 122.1, 121.1, 111.3, 69.9 (q, *J*= 32.5 Hz), 55.8 ppm; IR (KBr) 3441, 3012, 2946, 2845, 1605, 1591, 1496, 1466, 1442, 1358, 1249, 1171, 1131, 1027, 871, 829, 781, 627, 593, 574, 538, 498 cm^{-1}. The ee was determined by HPLC on Chiralpak OJ-H (*n*-hexane/*i*-PrOH = 97/3, 1.0 mL/min, 254 nm), t_S(minor) = 23.5 min, t_R(major) = 27.4 min, 74% ee.

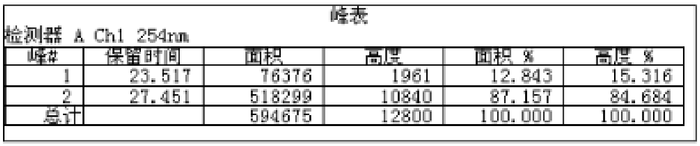


峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	23.651	383074	9068	50.037	52.589
2	27.755	382508	8175	49.963	47.411
总计		765582	17243	100.000	100.000

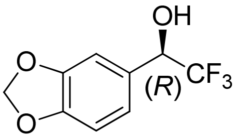




峰表

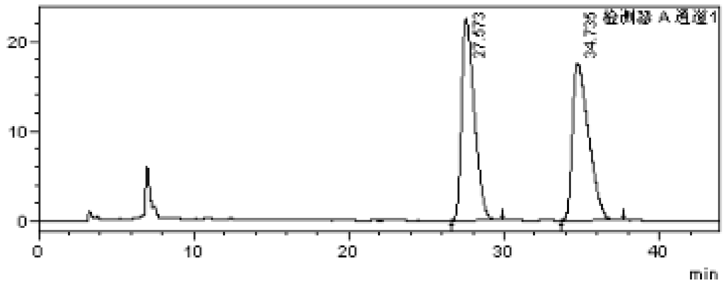
检测器 A Ch1 254nm

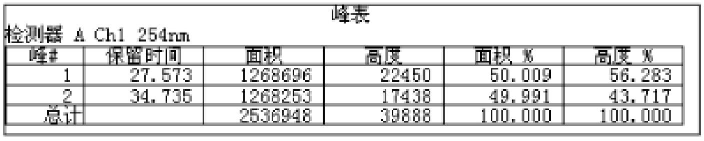
峰#	保留时间	面积	高度	面积 %	高度 %
1	23.517	76376	1961	12.843	15.316
2	27.451	518299	10840	87.157	84.684
总计		594675	12800	100.000	100.000



1-(benzo[d][1,3]dioxol-5-yl)-2,2,2-trifluoroethanol (2m)[10]

The reaction of **1m** (30.0 mg, 0.20 mmol), Me_3SiCF_3 (60.0 μL, 0.40 mmol), (IPr)CuF (1.9 mg, 0.004 mmol, 2 mol%), quaternary ammonium salts (**3e)** (2.6 mg, 0.004 mmol, 2 mol%) for 2 h gave **2m** as a colorless oil (40.5 mg, 92%) by flash chromatography (PE/EtOAc = 10/1). $[\alpha]_D^{25}$= –16.7 (*c* 0.48, CH_2Cl_2) [lit.[10] $[\alpha]_D^{20}$ = –7.8 (*c* 0.55, CH_2Cl_2, 46% ee)]; ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.96 (s. 1H), 6.91 (d, J = 8.4 Hz, 1H), 6.81 (d, J = 8.0 Hz, 1H), 5.97 (s, 2 H), 4.90 (m, 1H), 2.90 (d, J = 2.8 Hz, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.6, 148.0, 127.8, 124.3 (q, J= 281.0 Hz), 121.6, 108.3, 107.7, 101.4, 72.6 (q, J= 32.0 Hz) ppm; IR (KBr) 3454, 2906, 2772, 1855, 1602, 1506, 1492, 1448, 1351, 1251, 1170, 1124, 1040, 930, 872, 810, 793, 730, 704, 636, 654, 560 cm^{-1}. The ee was determined by HPLC on Chiralpak OD-H (*n*-hexane/*i*-PrOH = 97/3, 1.0 mL/min, 254 nm), t_R(major) = 27.9 min, t_S(minor) = 34.7 min, 81% ee.

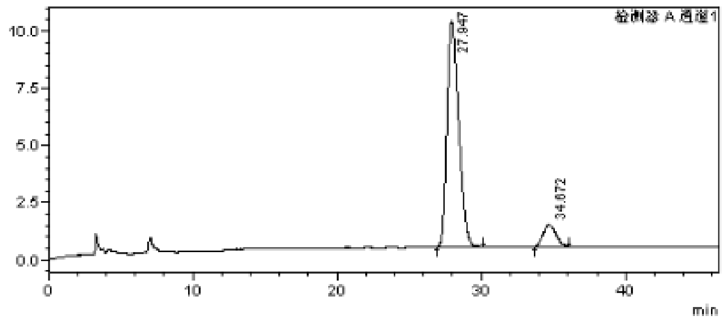


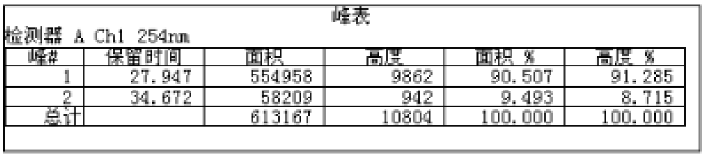


峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	27.573	1268696	22450	50.009	56.283
2	34.735	1268253	17438	49.991	43.717
总计		2536948	39888	100.000	100.000

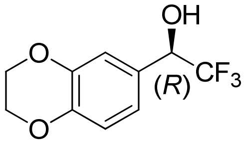




峰表

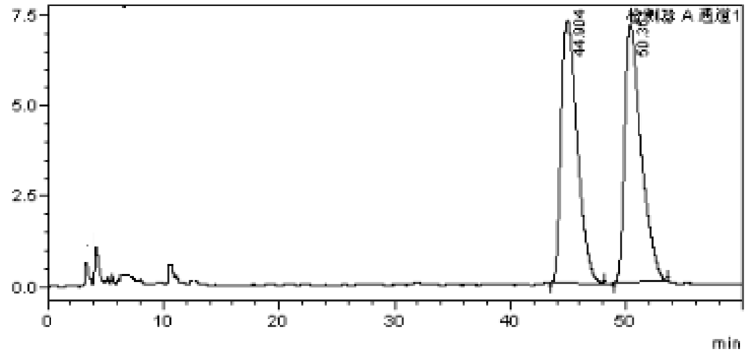
检测器 A Ch1 254nm

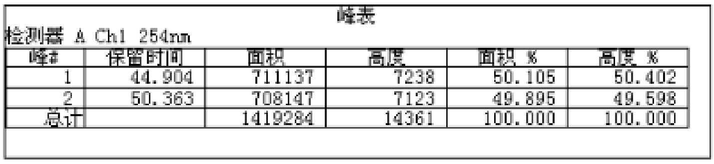
峰#	保留时间	面积	高度	面积 %	高度 %
1	27.947	554958	9862	90.507	91.285
2	34.672	58209	942	9.493	8.715
总计		613167	10804	100.000	100.000



1-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-2,2,2-trifluoroethanol (2n)[15]

The reaction of **1n** (32.8 mg, 0.20 mmol), Me_3SiCF_3 (60.0 µL, 0.40 mmol), (IPr)CuF (1.9 mg, 0.004 mmol, 2 mol%), quaternary ammonium salts (**3e)** (2.6 mg, 0.004 mmol, 2 mol%) for 2 h gave **2n** as a colorless oil (43.1 mg, 92%) by flash chromatography (PE/EtOAc = 10/1). $[\alpha]_D^{25}$= –16.3 (*c* 0.54, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ7.00 (s, 1H), 6.94 (d, *J* = 8.4 Hz, 1H), 6.88 (d, *J* = 8.4 Hz, 1H), 4.90 (m, 1H), 4.27(s, 4H), 2.90 (d, *J* = 4.0 Hz, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.6, 143.6, 127.2, 124.3 (q, *J*= 281.0 Hz), 120.6, 117.5, 116.6, 72.4 (q, *J*= 32.0 Hz), 64.4, 64.3 ppm; IR (KBr) 3458, 2928, 1539, 1511, 1461, 1437, 1314, 1291, 1260, 1171, 1125, 1067, 921, 888, 846, 816, 725, 703, 664 cm^{-1}. The ee was determined by HPLC on Chiralpak OD-H (*n*-hexane/*i*-PrOH = 97/3, 1.0 mL/min, 254 nm), t_S(minor) = 44.9 min, t_R(major) = 50.4 min, 79% ee.

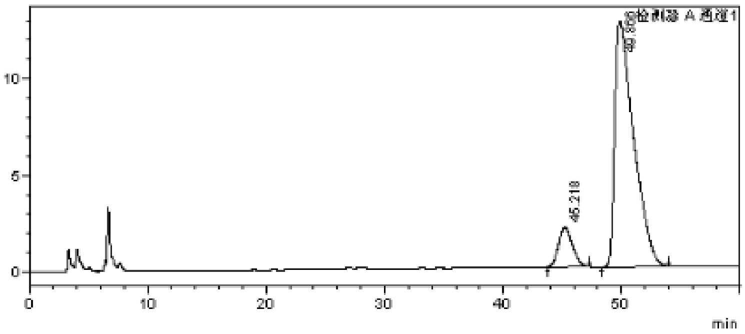




峰表

检测器 A Ch1 254nm

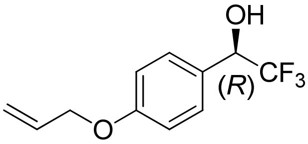
峰#	保留时间	面积	高度	面积 %	高度 %
1	44.904	711137	7238	50.105	50.402
2	50.363	708147	7123	49.895	49.598
总计		1419284	14361	100.000	100.000




峰表

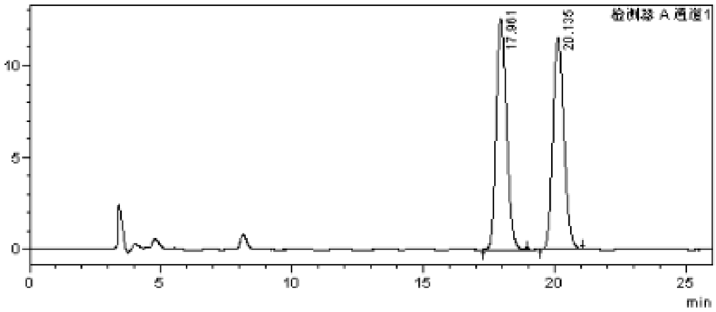
检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	45.218	166725	2018	10.599	13.704
2	49.866	1406348	12705	89.401	86.296
总计		1573073	14723	100.000	100.000



1-(4-(allyloxy)phenyl)-2,2,2-trifluoroethanol (2o)

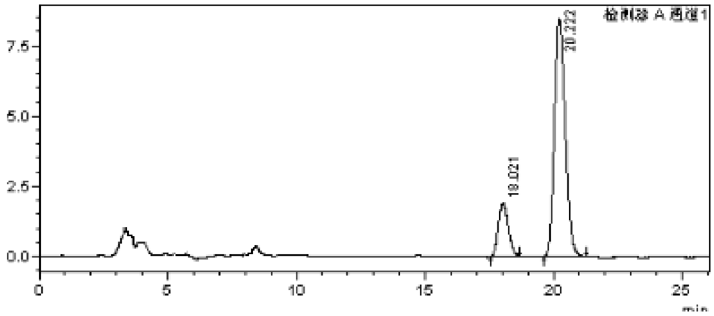
The reaction of **1o** (30.7 µL, 0.20 mmol), Me_3SiCF_3 (60.0 µL, 0.40 mmol), (IPr)CuF (1.9 mg, 0.004 mmol, 2 mol%), quaternary ammonium salts (**3e)** (2.6 mg, 0.004 mmol, 2 mol%) for 2 h gave **2o** as a white solid (37.1 mg, 80%) by flash chromatography (PE/EtOAc = 20/1). m.p. 49–50 °C; $[\alpha]_D^{25} = -19.3$ (c 0.20, CH_2Cl_2); ^1H NMR (400 MHz, $CDCl_3$): δ7.38 (d, J = 8.4 Hz, 2H), 6.95–6.92 (m, 2H), 6.10–6.00 (m, 1H), 5.41(qd, J = 1,6, 17.2 Hz, 1H), 5.29 (qd, J = 1.2, 10.8 Hz, 1H), 4.98–4.92 (m, 1H), 4.54 (td, J = 1.6, 5.2 Hz, 2H), 2.61 (br, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.5, 133.0, 128.8, 126.3, 124.4 (q, J= 281.0 Hz), 117.9, 114.9, 72.5 (q, J= 32.0 Hz), 68.9 ppm; IR (KBr) 3408, 2929, 2863, 1888, 1614, 1515, 1428, 1324, 1305, 1247, 1178, 1117, 1070, 1013, 940, 871, 802, 693, 589 cm^{-1}; Anal. Calcd. for $C_{11}H_{11}F_3O_2$: C, 56.90; H, 4.77; Found: C, 57.12; H, 4.87; The ee was determined by HPLC on Chiralpak AD-H (n-hexane/i-PrOH = 97/3, 1.0 mL/min, 254 nm), t_S(minor) = 18.0 min, t_R(major) = 20.2 min, 66% ee.

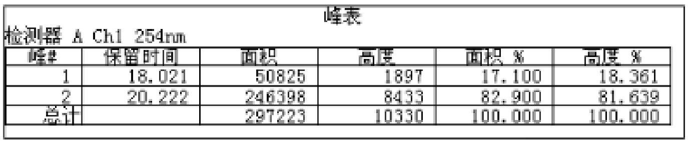



峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	17.961	342247	12535	50.479	52.062
2	20.135	335758	11542	49.521	47.938
总计		678005	24076	100.000	100.000

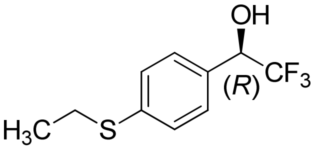




峰表

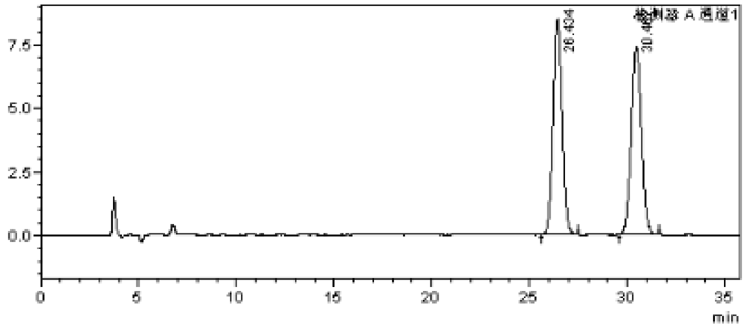
检测器 A Ch1 254nm

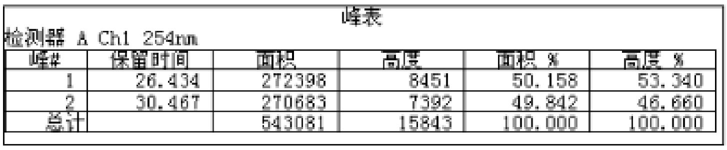
峰#	保留时间	面积	高度	面积 %	高度 %
1	18.021	50825	1897	17.100	18.361
2	20.222	246398	8433	82.900	81.639
总计		297223	10330	100.000	100.000



1-(4-(ethylthio)phenyl)-2,2,2-trifluoroethanol (2p)

The reaction of **1p** (30.2 μL, 0.20 mmol), Me_3SiCF_3 (60.0 μL, 0.40 mmol), (IPr)CuF (1.9 mg, 0.004 mmol, 2 mol%), quaternary ammonium salts (**3e)** (2.6 mg, 0.004 mmol, 2 mol%) for 1 h gave **2p** as a white solid (40.1 mg, 85%) by flash chromatography (PE/EtOAc = 10/1). m.p. 47–49 °C; $[\alpha]_D^{25} = -16.7$ (c 0.63, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37 (d, J = 8.4 Hz, 2H), 7.32 (d, J = 8.8 Hz, 2H), 4.93–4.50 (m, 1H), 2.96 (q, J = 7.2 Hz, 2H), 2.70 (s, 1H), 1.33 (t, J = 7.4 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.9, 131.1, 128.3, 127.9, 124.2 (q, J= 281.0 Hz), 72.5 (q, J= 32.0 Hz), 27.1, 14.2 ppm; IR (KBr) 3356, 2974, 2928, 2873, 1601, 1496, 1406, 1351, 1255, 1135, 1093, 1071, 1013, 868, 848, 811, 793, 680, 586, 496 cm^{-1}; Anal. Calcd. for $C_{10}H_{11}F_3OS$: C, 50.84; H, 4.69; Found: C, 51.23; H, 4.76; The ee was determined by HPLC on Chiralpak OJ-H (n-hexane/i-PrOH = 95/5, 1.0 mL/min, 254 nm), t_R(major) = 26.2 min, t_S(minor) = 30.2 min, 73% ee.

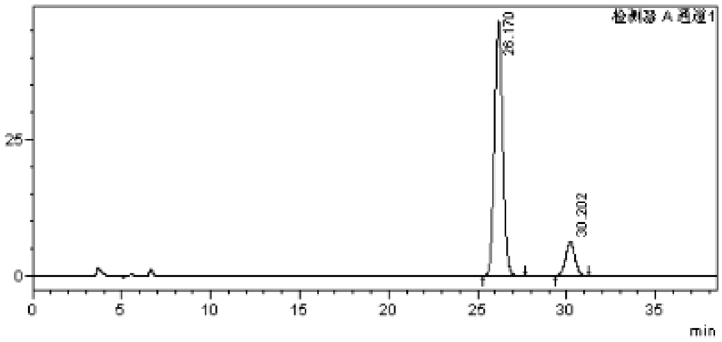


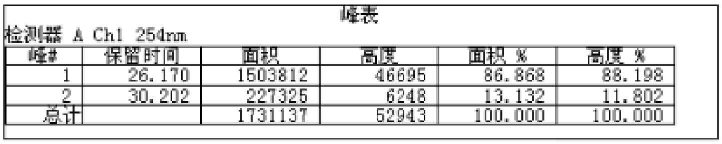


峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	26.434	272398	8451	50.158	53.340
2	30.467	270683	7392	49.842	46.660
总计		543081	15843	100.000	100.000





峰表

检测器 A Ch1 254nm

峰#	保留时间	面积	高度	面积 %	高度 %
1	26.170	1503812	46695	86.868	88.198
2	30.202	227325	6248	13.132	11.802
总计		1731137	52943	100.000	100.000

5 References

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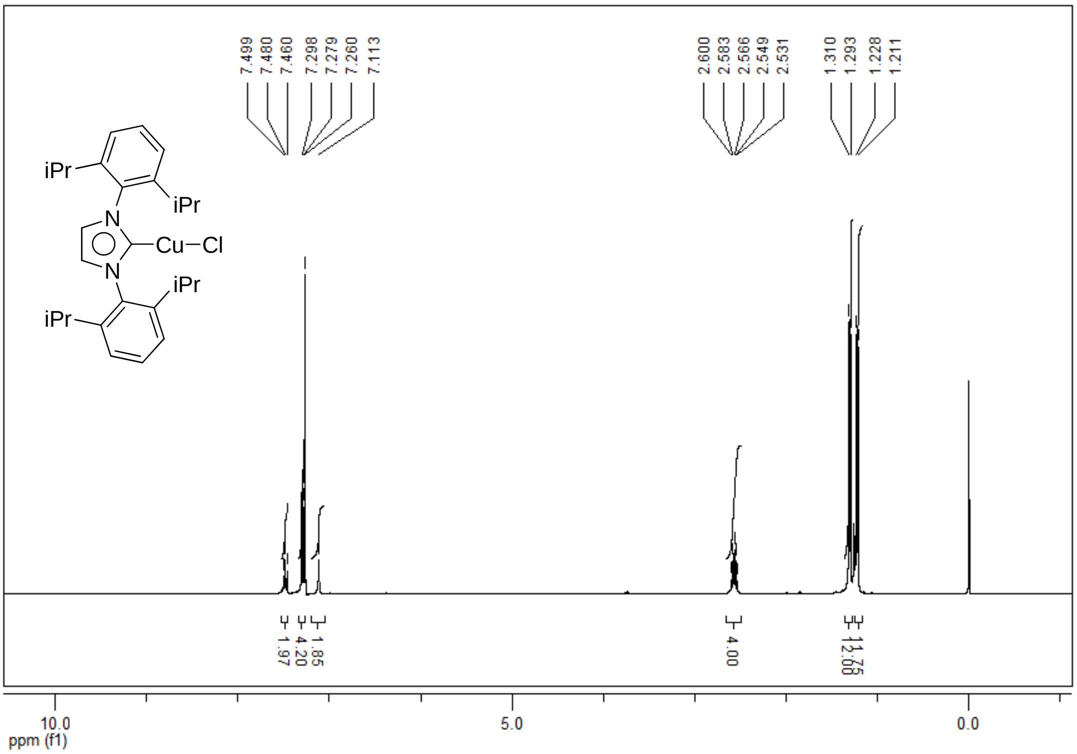
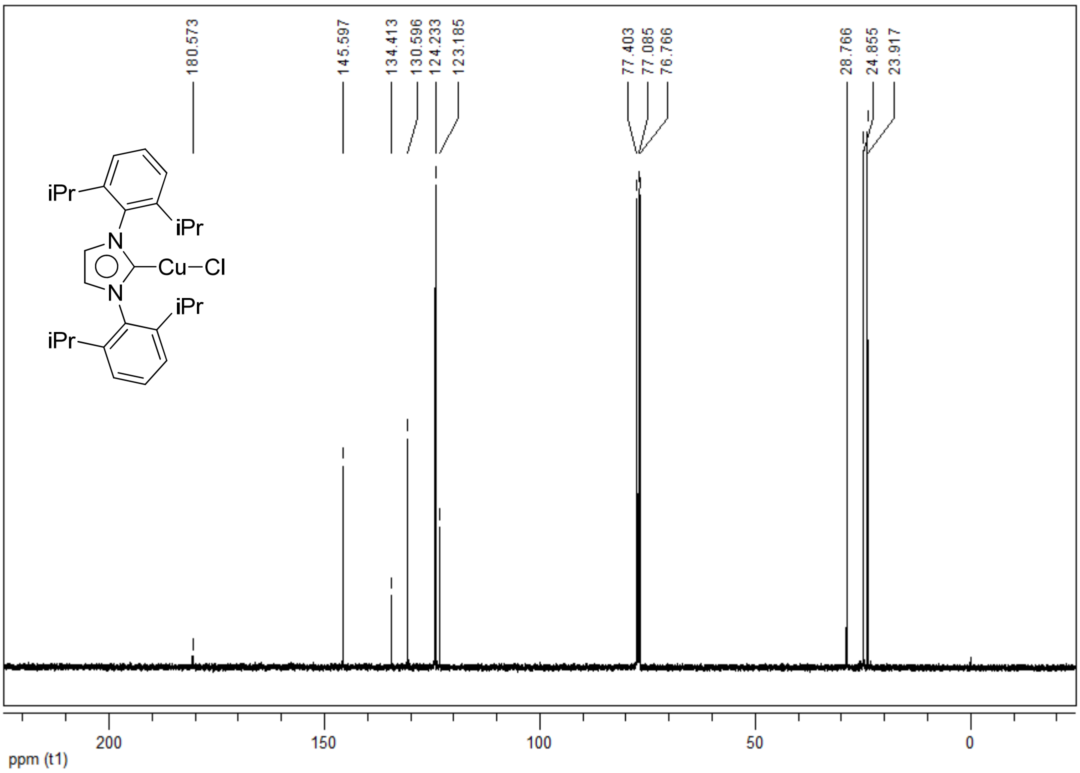
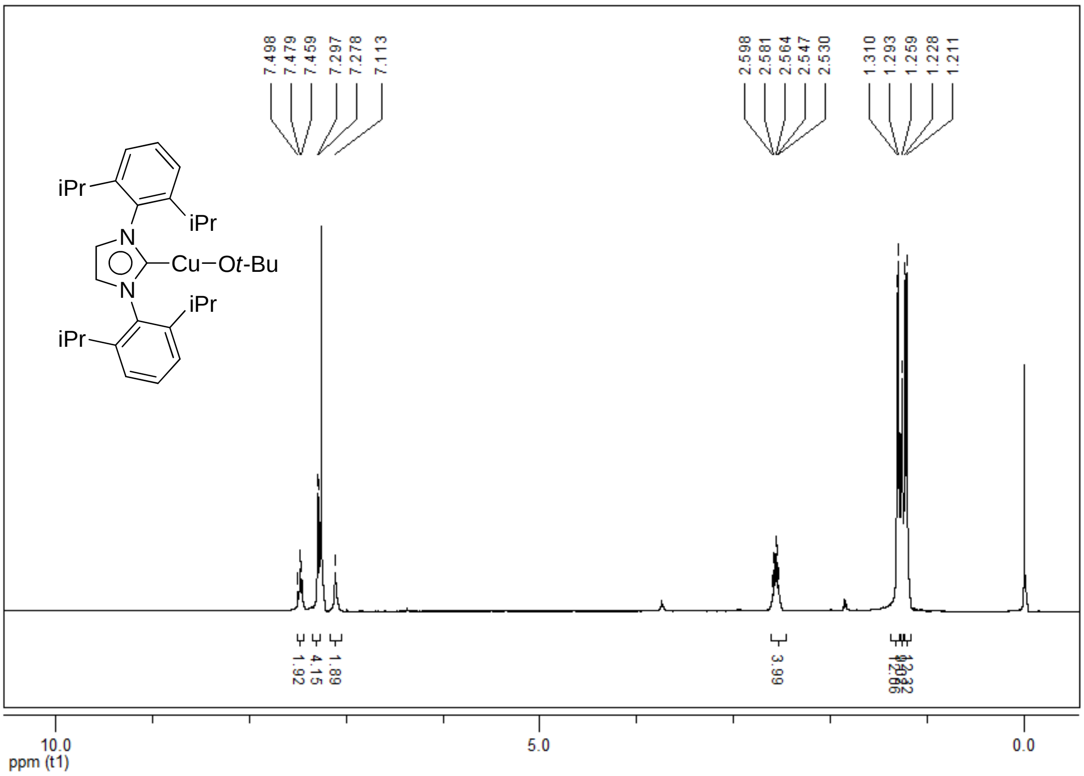
6 Copies of NMR spectra



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2.581
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2.547
2.530
1.310
1.293
1.259
1.228
1.211
iPr
iPr
N
N
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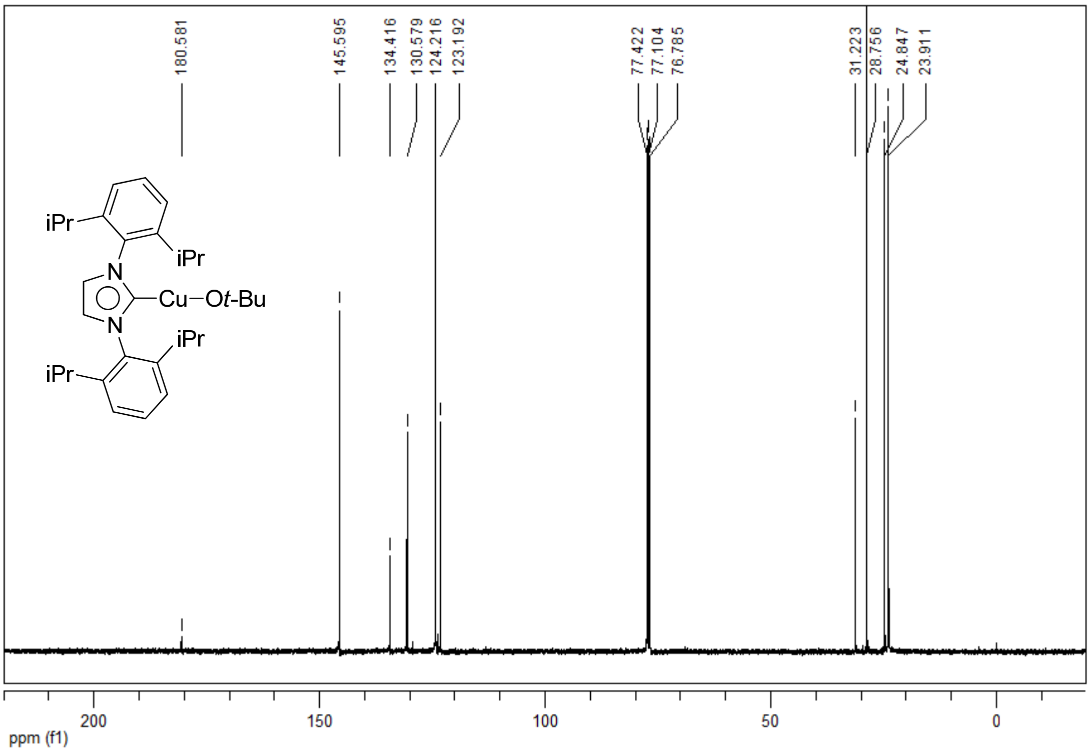
1.89
3.99
12.32
10.0
5.0
0.0
ppm (t1)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24.847
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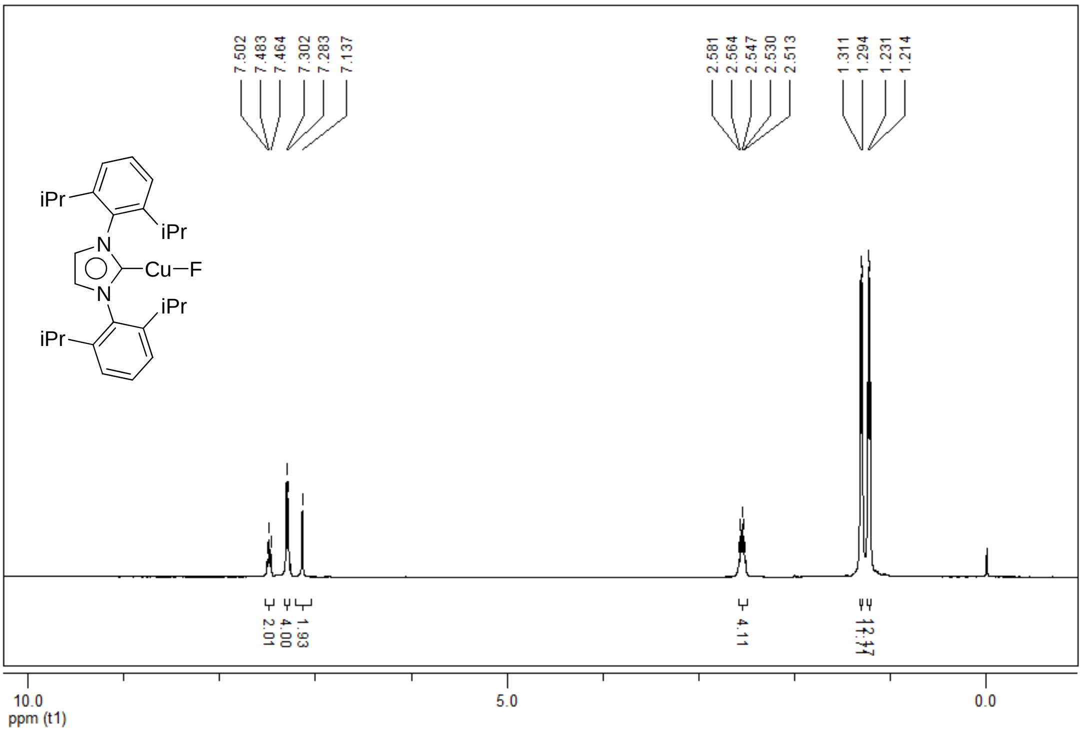
iPr
N
N
Cu−Ot-Bu
iPr
iPr
200
150
100
50
0
ppm (f1)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2.564
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2.530
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1.294
1.231
1.214
iPr
iPr
N
Cu–F
N
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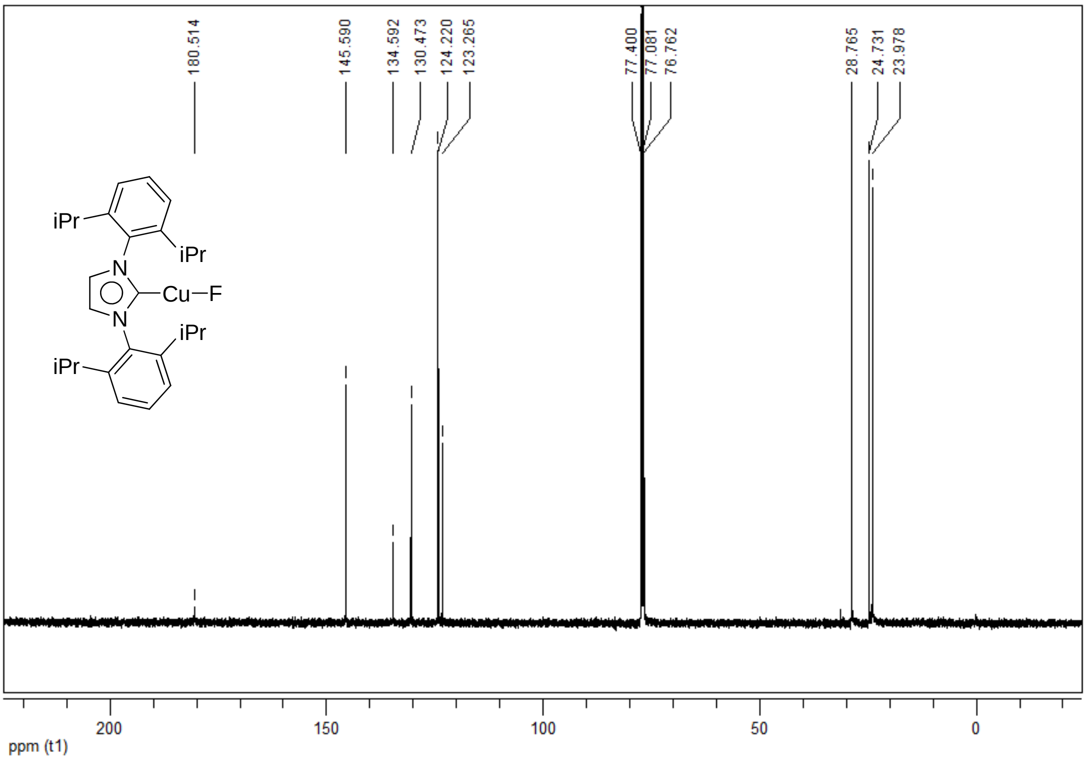
4.11
12.11
10.0
ppm (t1)
5.0
0.0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N
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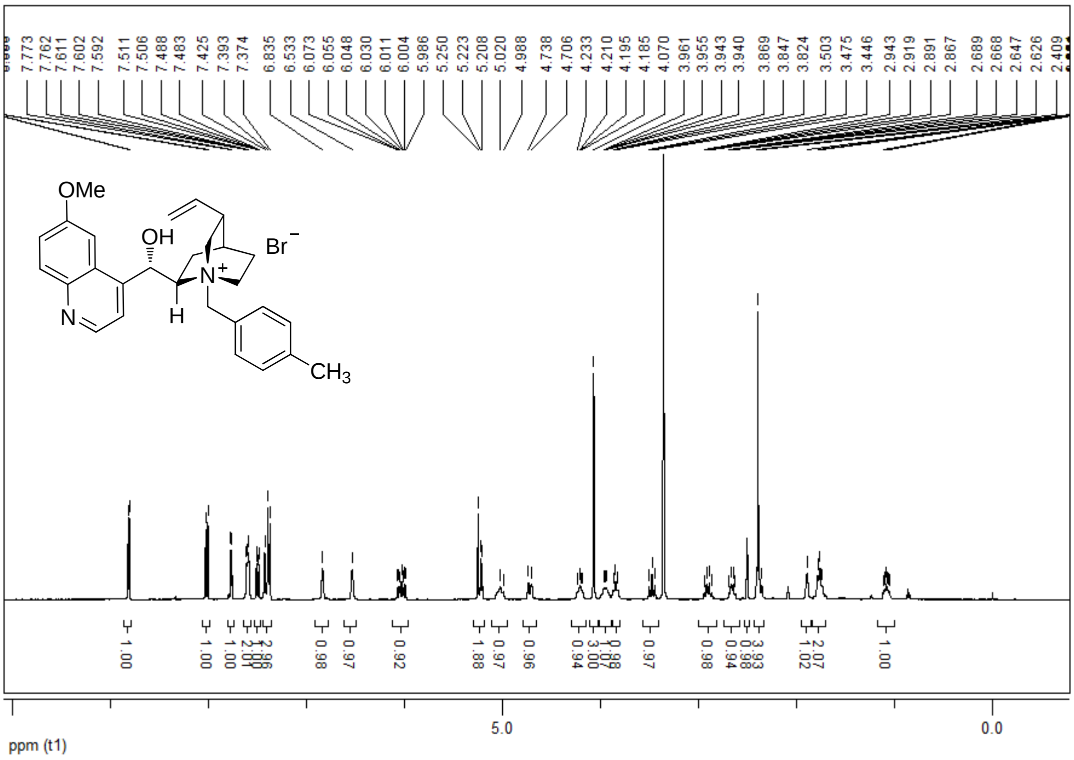
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6.533
6.073
6.055
6.048
6.030
6.011
6.004
5.986
5.250
5.223
5.208
5.020
4.988
4.738
4.706
4.233
4.210
4.195
4.185
4.070
3.961
3.955
3.943
3.940
3.869
3.847
3.824
3.503
3.475
3.446
2.943
2.919
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2.867
2.689
2.668
2.647
2.626
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N⁺
N
H
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1.00
2.01
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0.98
0.97
0.92
1.88
0.97
0.96
0.94
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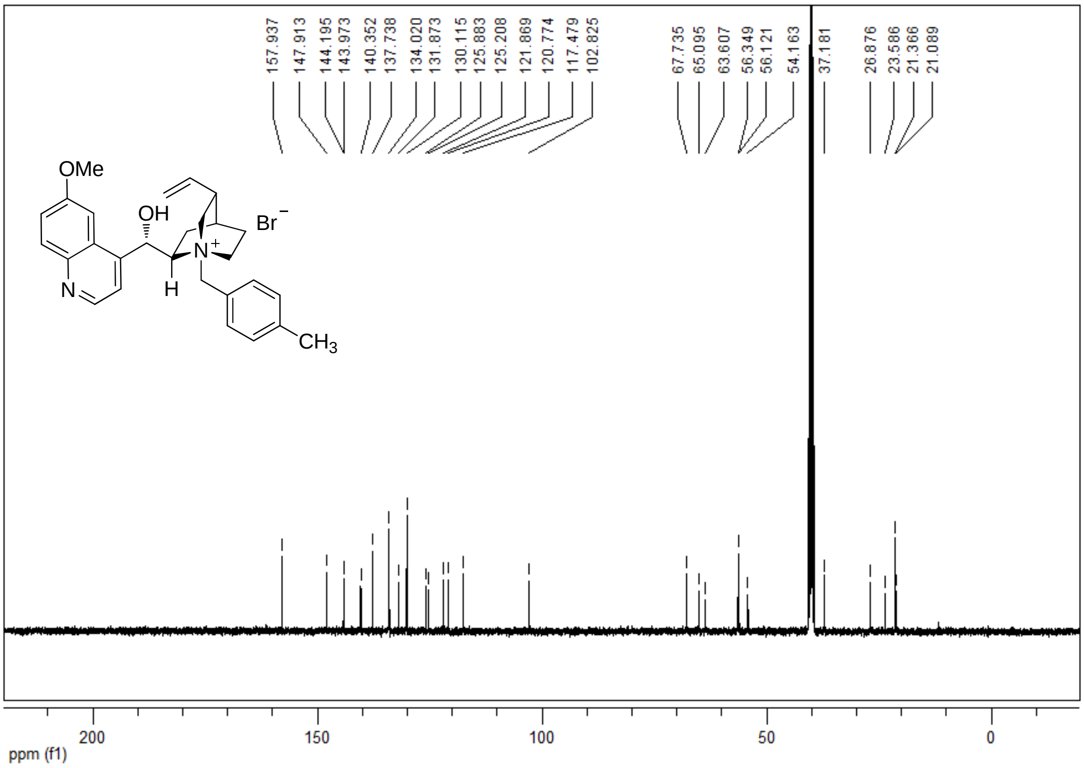
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117.479
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65.095
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37.181
26.876
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N⁺
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H
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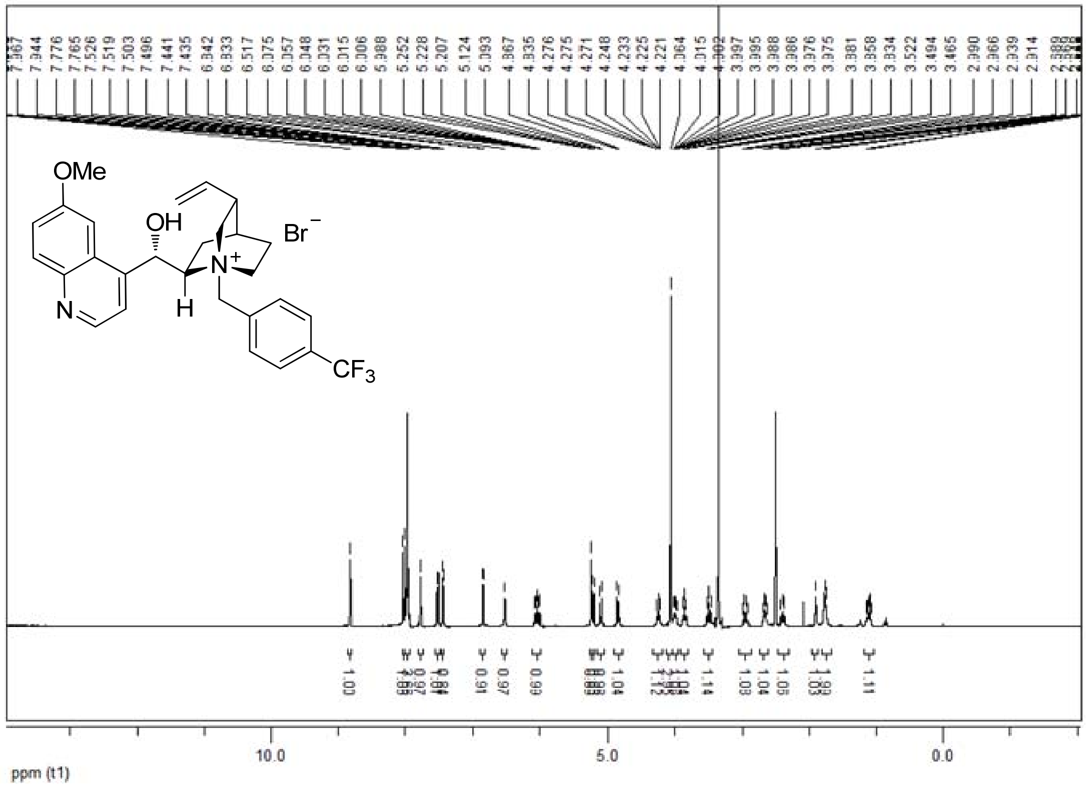
100
50
0
ppm (f1)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5.124
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4.335
4.276
4.275
4.271
4.248
4.233
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4.221
4.064
4.015
3.997
3.995
3.988
3.986
3.976
3.975
3.381
3.358
3.334
3.522
3.494
3.465
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2.939
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OH
Br−
N+
H
N
CF3
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0.91
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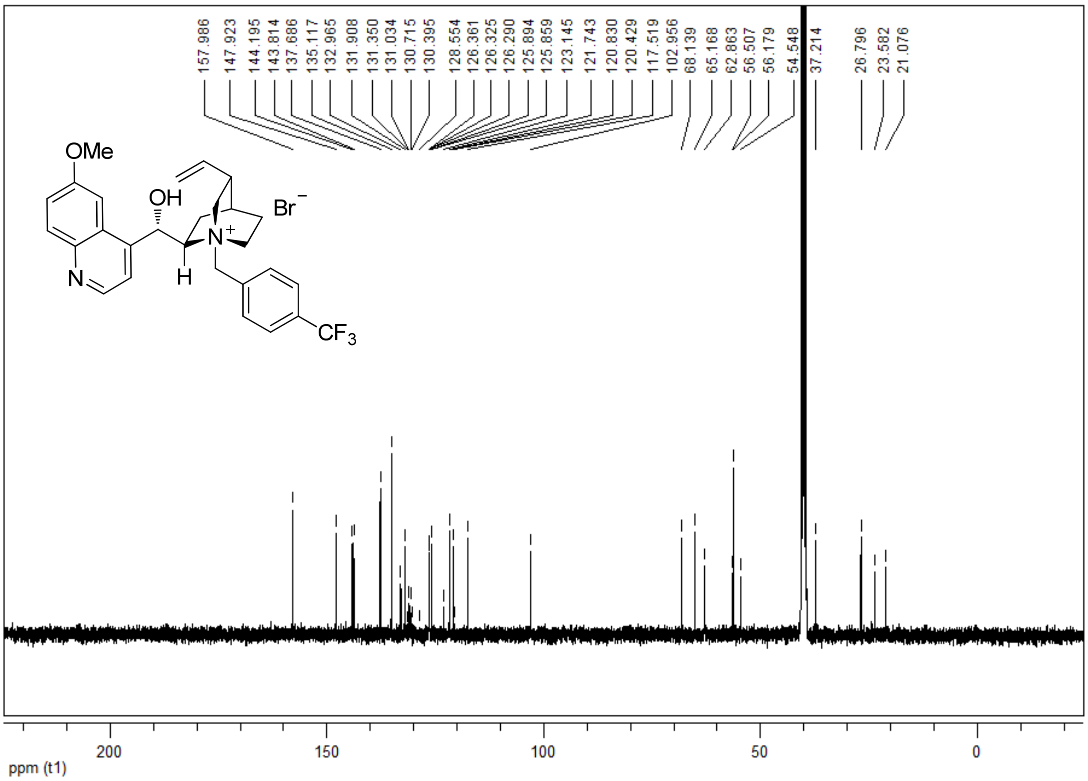
ppm (t1)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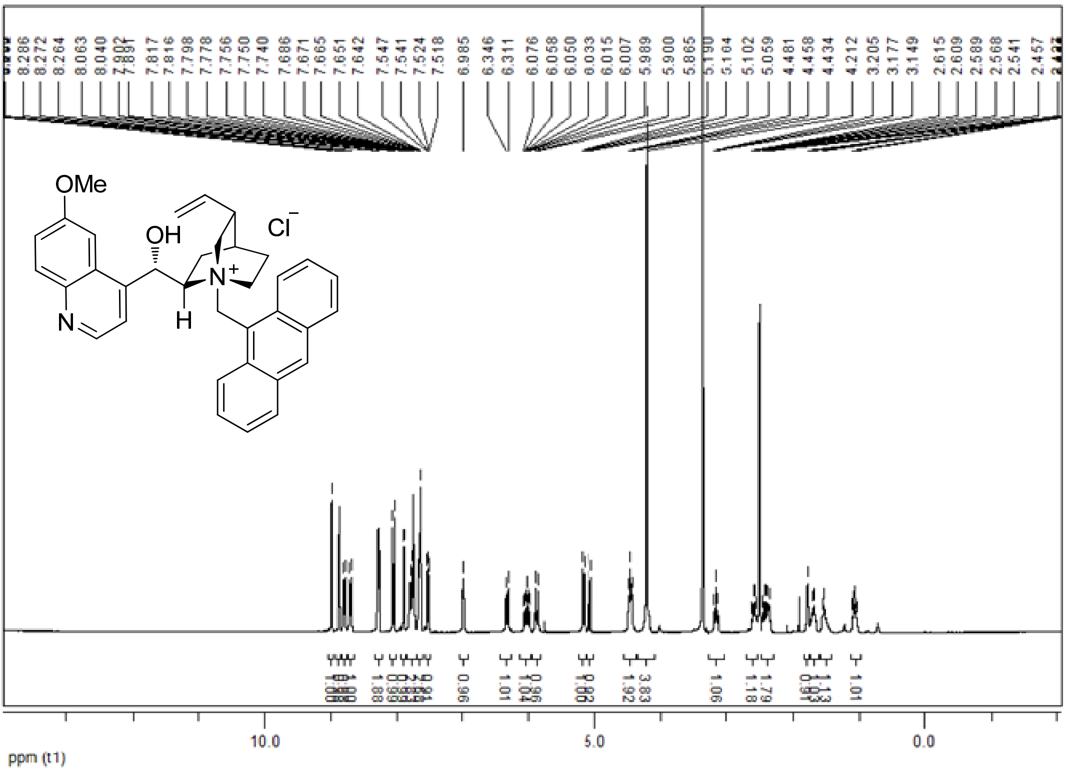
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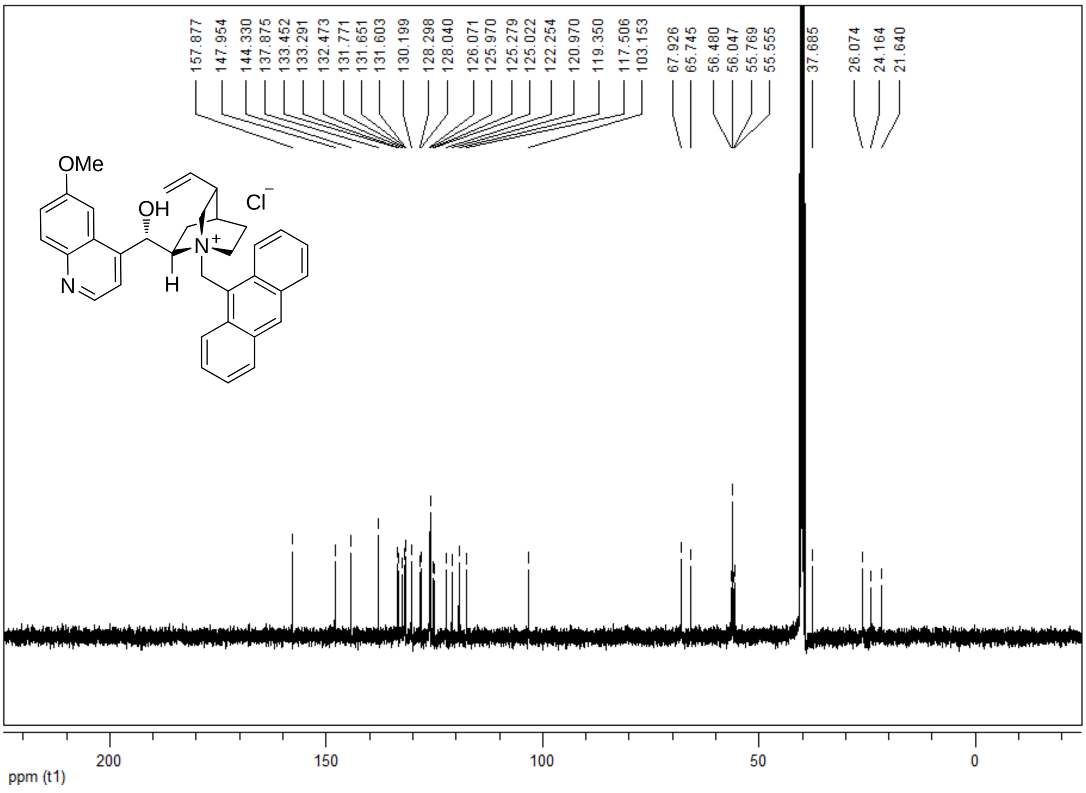
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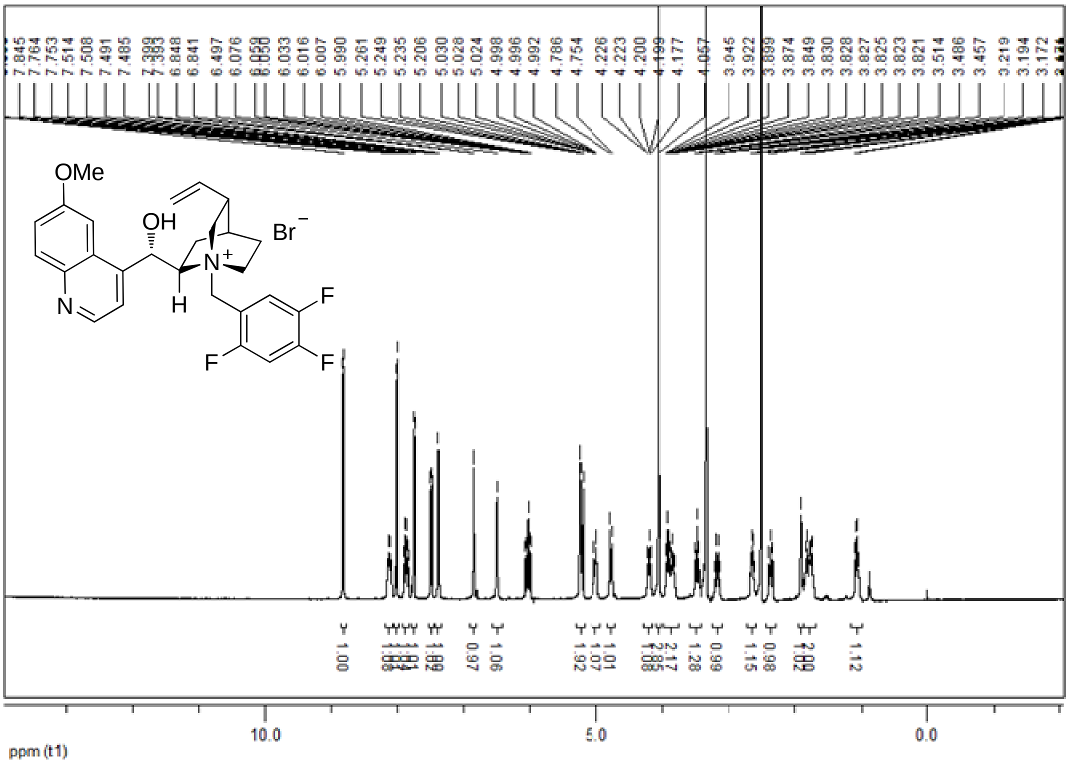
ppm (t1)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F
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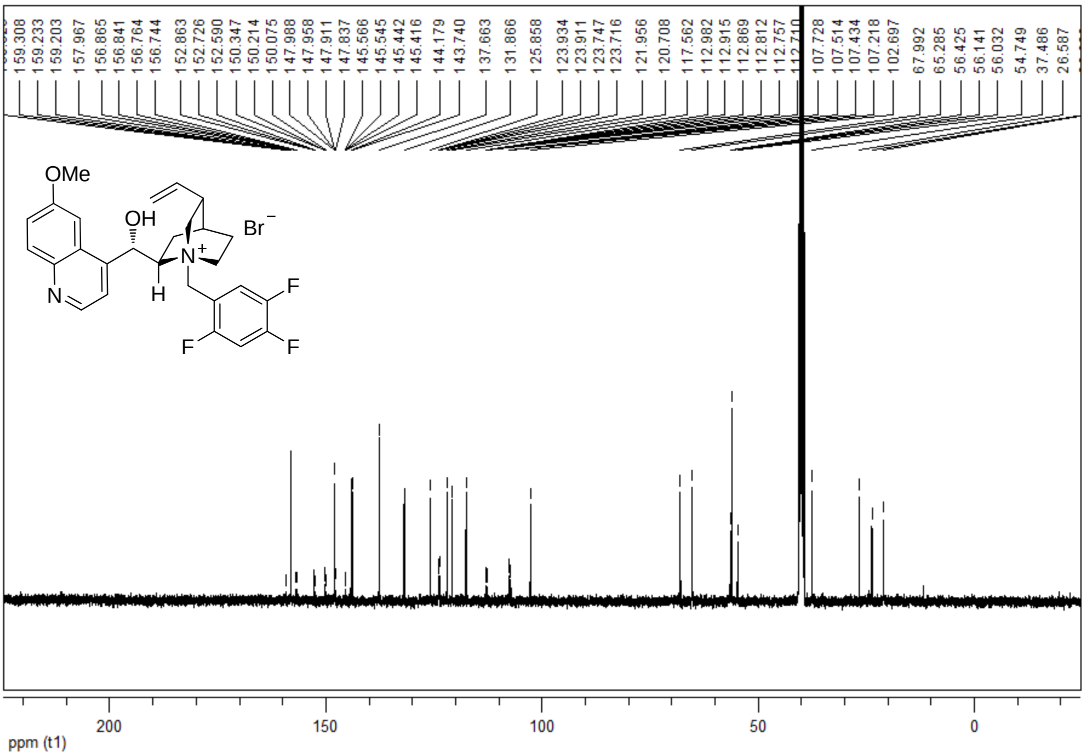
ppm (t1)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OH
Br−
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H
N
F
F
F
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100
50
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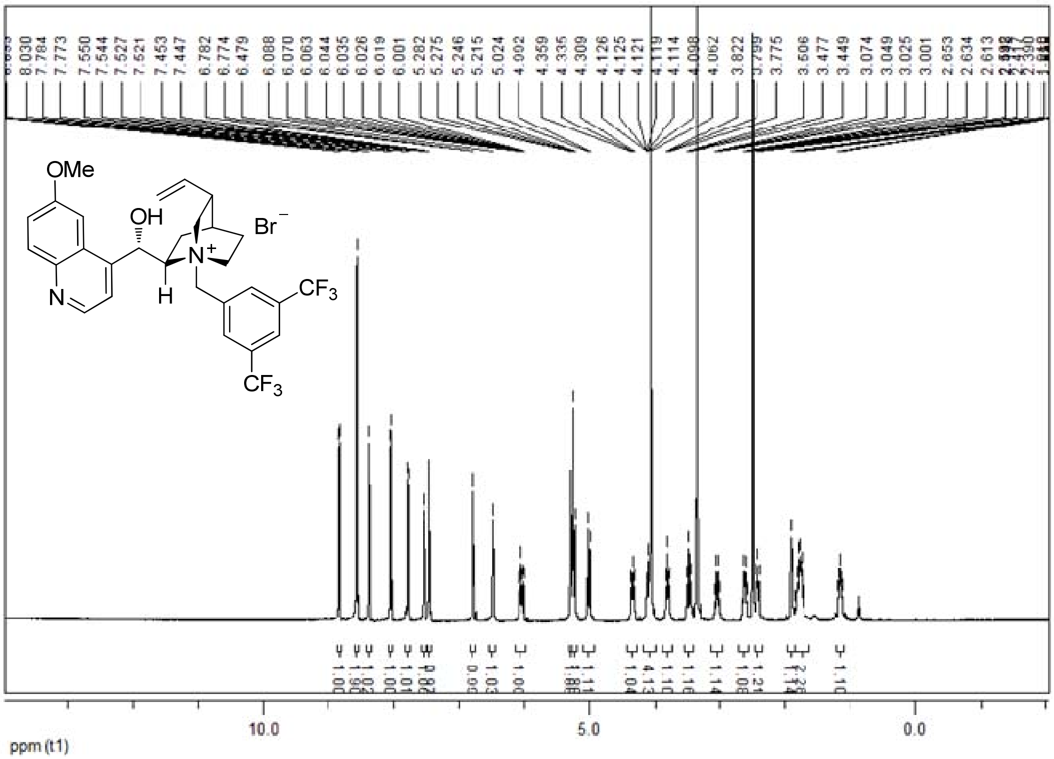
ppm (t1)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N⁺
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N
CF3
CF3
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1.02
1.00
1.01
1.03
1.00
1.11
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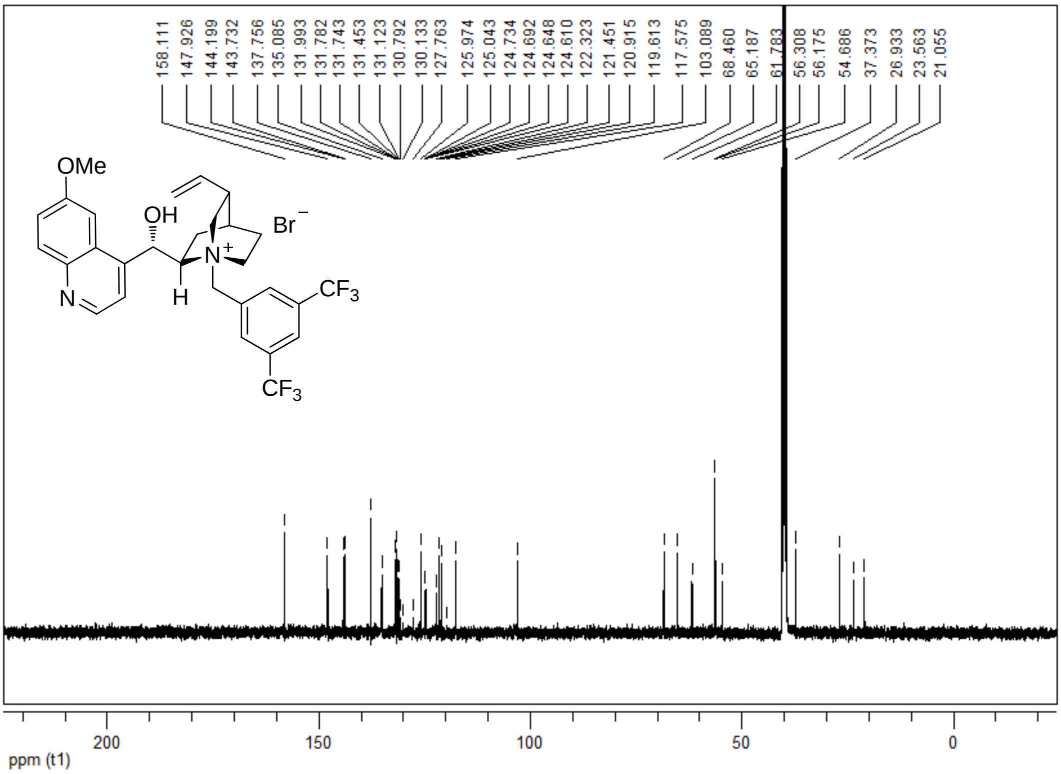
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CF3
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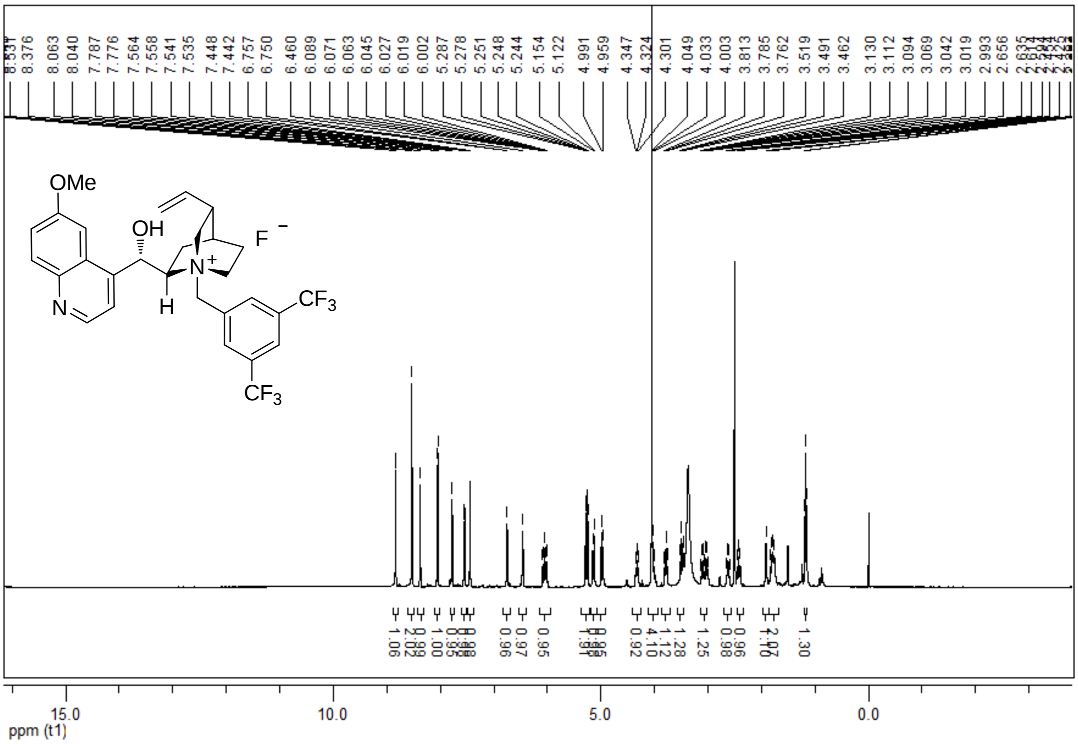
ppm (t1)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OH
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N+
N
H
CF3
CF3
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2.02
1.00
0.95
0.96
0.97
0.95
0.92
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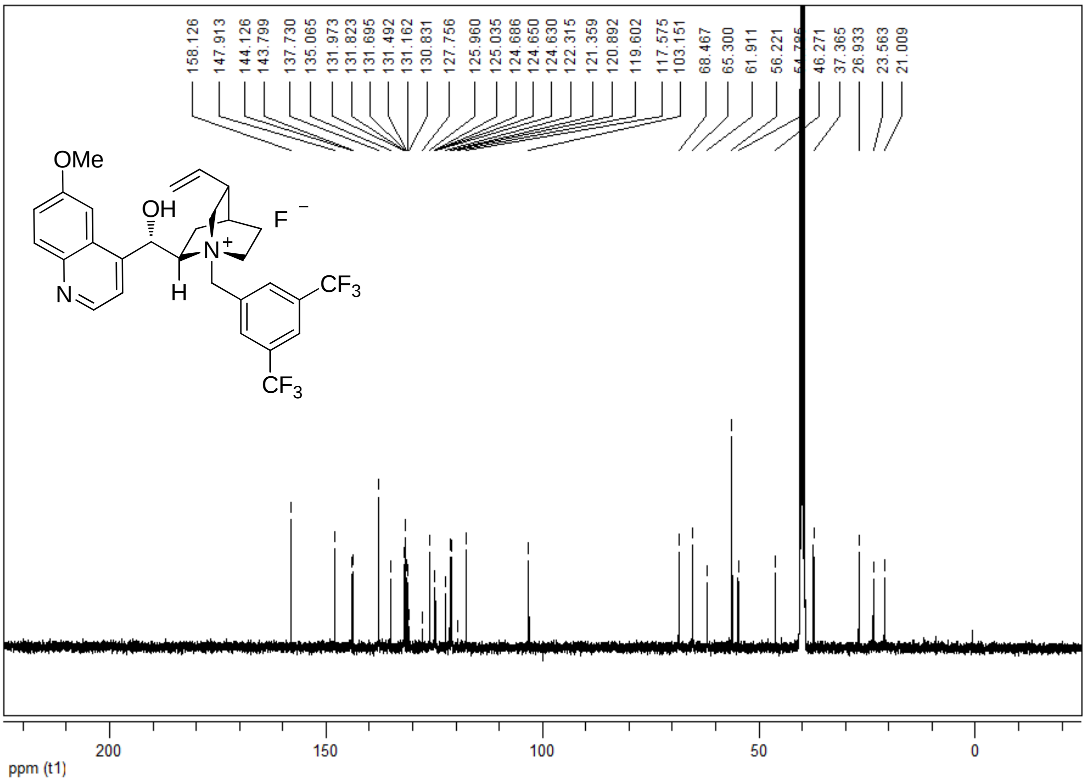
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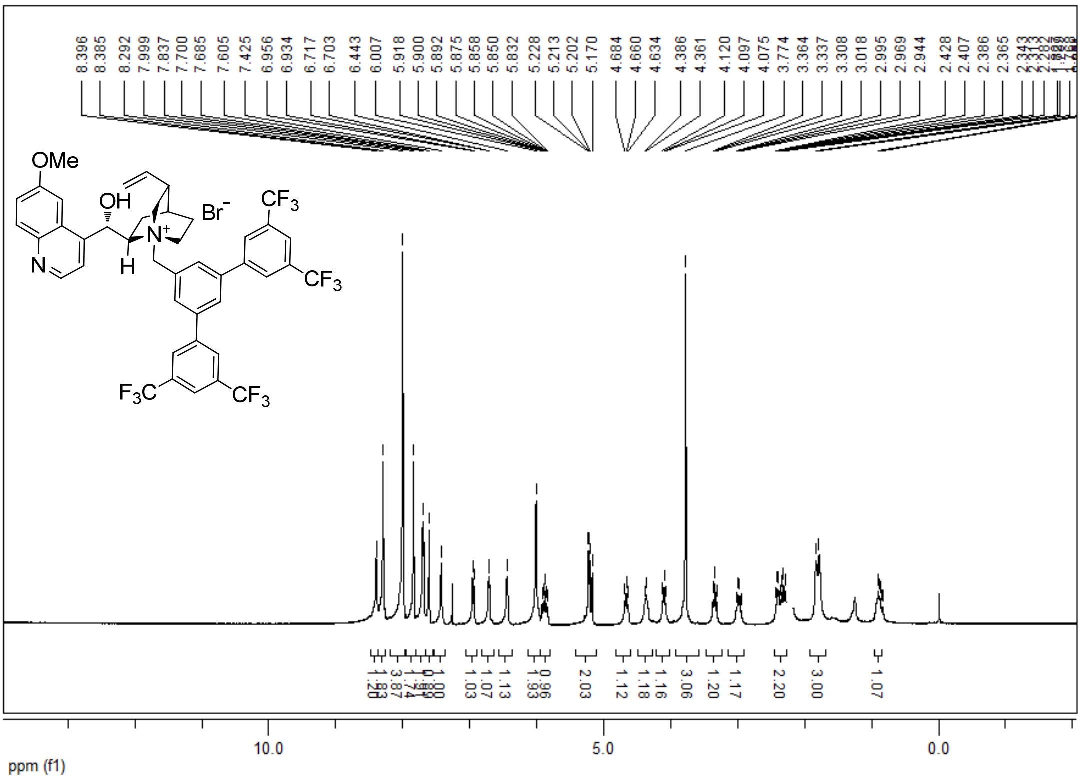
ppm (t1)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CF3
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1.12
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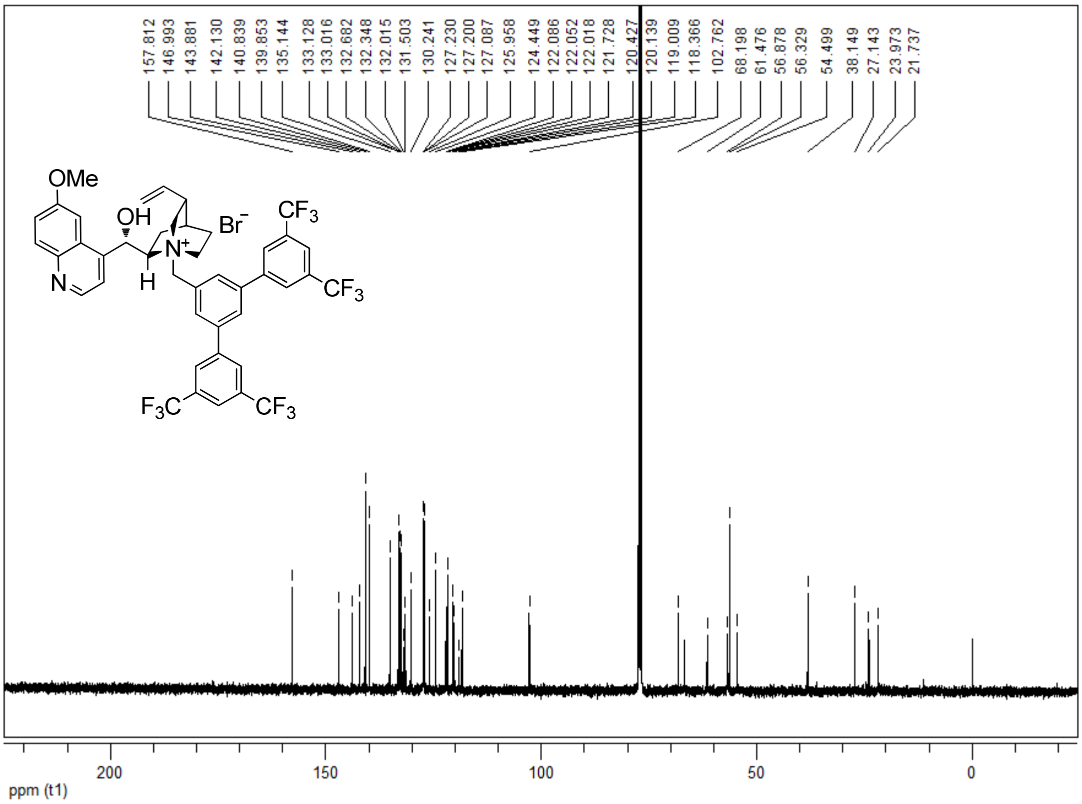
ppm (f1)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130.241
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127.200
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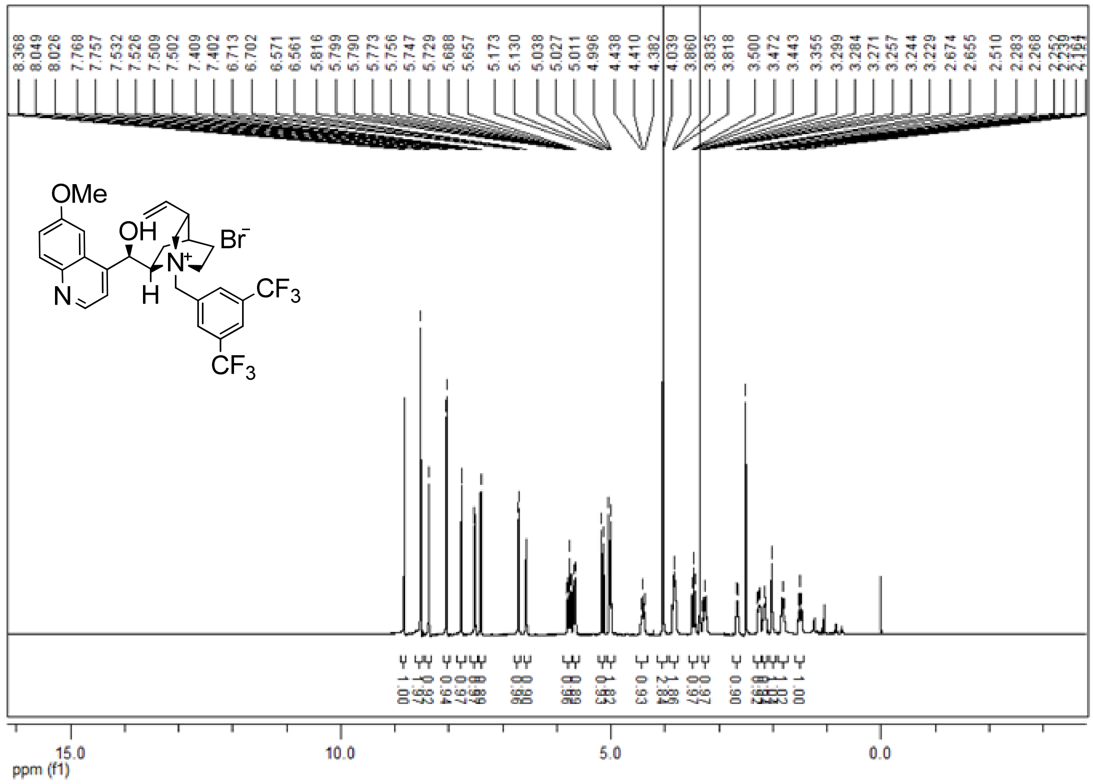
ppm (t1)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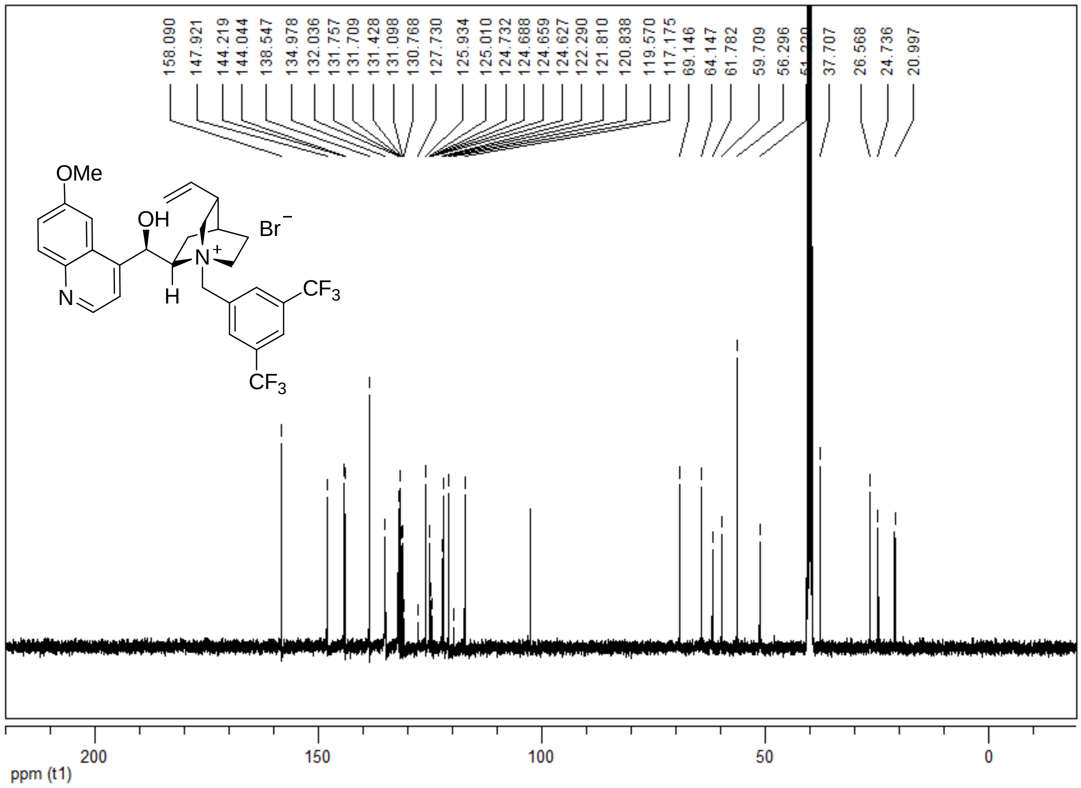
7.757
7.532
7.526
7.509
7.502
7.409
7.402
6.713
6.702
6.571
6.561
5.816
5.799
5.790
5.773
5.756
5.747
5.729
5.688
5.657
5.173
5.130
5.038
5.027
5.011
4.996
4.438
4.410
4.382
4.039
3.860
3.835
3.818
3.500
3.472
3.443
3.355
3.299
3.284
3.271
3.257
3.244
3.229
2.674
2.655
2.510
2.283
2.268
OMe
OH
Br⁻
N⁺
N
H
CF3
CF3
1.00
1.92
0.94
0.97
0.89
0.96
0.93
2.84
1.86
0.97
0.90
1.00
15.0
10.0
5.0
0.0
ppm (f1)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147.921
144.219
144.044
138.547
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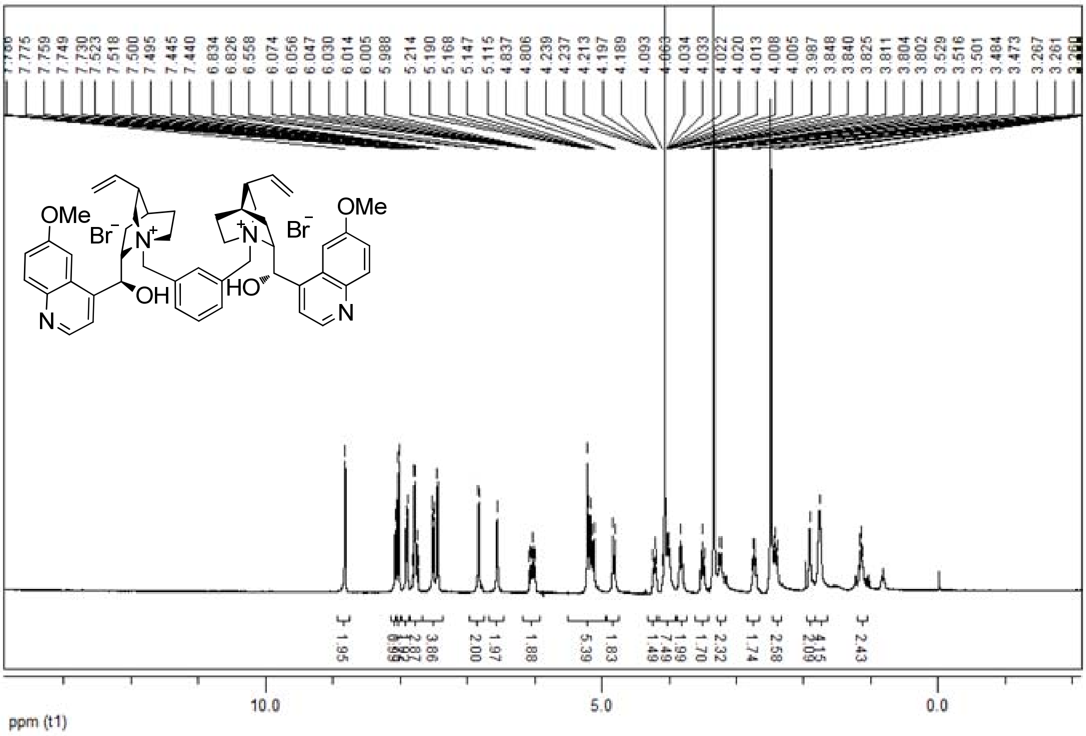
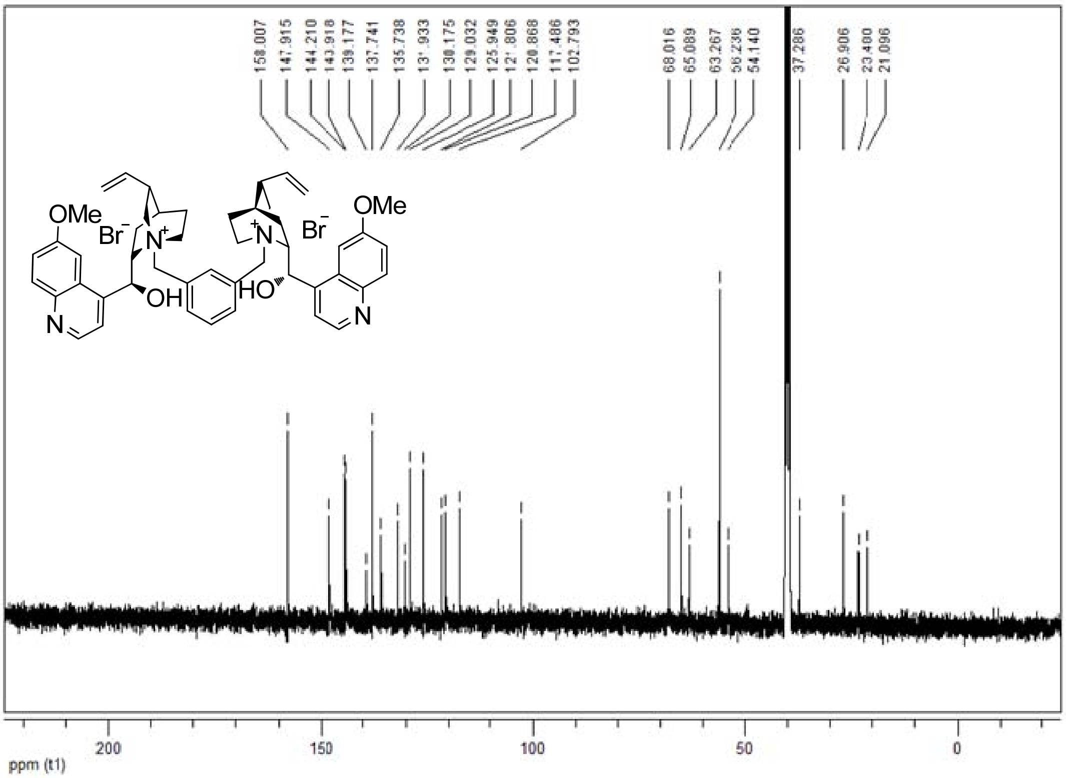
132.036
131.757
131.709
131.428
131.098
130.768
127.730
125.934
125.010
124.732
124.688
124.659
124.627
122.290
121.810
120.838
119.570
117.175
69.146
64.147
61.782
59.709
56.296
37.707
26.568
24.736
20.997
OMe
OH
Br⁻
N⁺
N
H
CF3
CF3
200
150
100
50
0
ppm (t1)


7.786
7.775
7.759
7.749
7.730
7.523
7.518
7.500
7.495
7.445
7.440
6.834
6.826
6.558
6.074
6.056
6.047
6.030
6.014
6.005
5.988
5.214
5.190
5.168
5.147
5.115
4.837
4.806
4.239
4.237
4.213
4.197
4.189
4.093
4.063
4.034
4.033
4.022
4.020
4.013
4.008
4.005
3.987
3.848
3.840
3.825
3.811
3.804
3.802
3.529
3.516
3.501
3.484
3.473
3.267
3.261
3.260
OMe
Br⁻
N⁺
OH
N
HO
N⁺
Br⁻
OMe
N
1.95
3.86
2.00
1.97
1.88
5.39
1.83
1.49
7.49
1.99
1.70
2.32
1.74
2.58
2.09
4.15
2.43
10.0
5.0
0.0
ppm (t1)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144.210
143.918
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137.741
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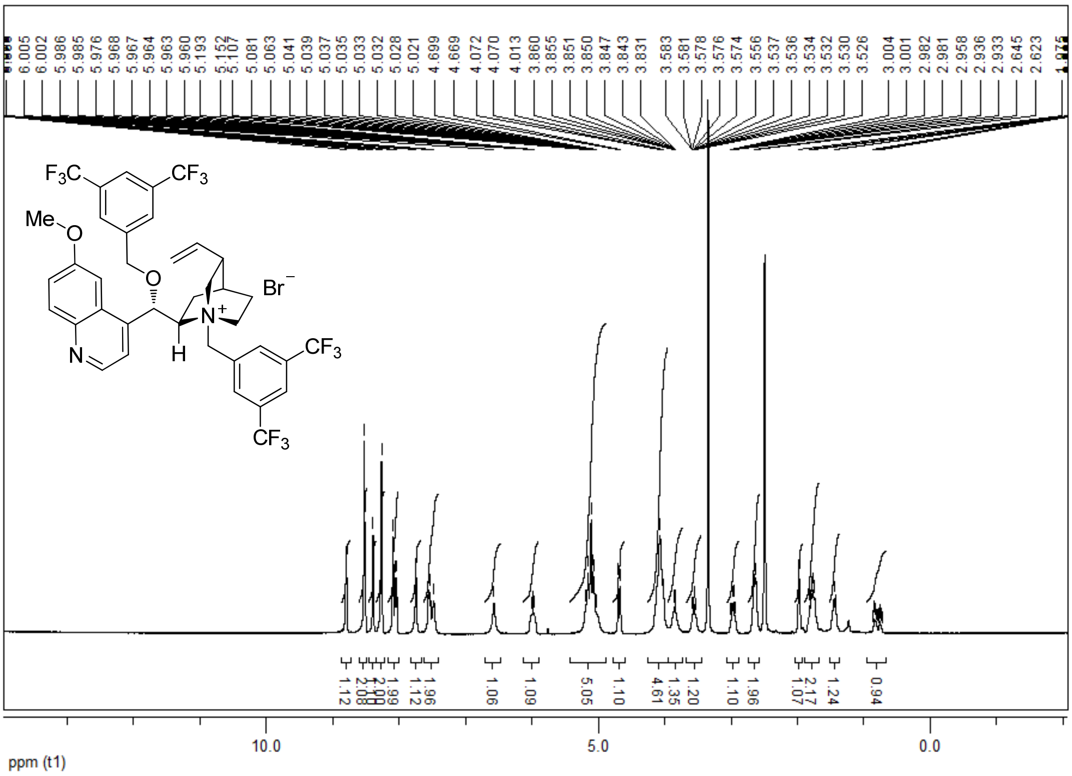
131.933
130.175
129.032
125.949
121.806
120.868
117.486
102.793
68.016
65.089
63.267
56.236
54.140
37.286
26.906
23.400
21.096
OMe
Br⁻
N⁺
OH
N
HO
N⁺
Br⁻
OMe
N
200
150
100
50
0
ppm (t1)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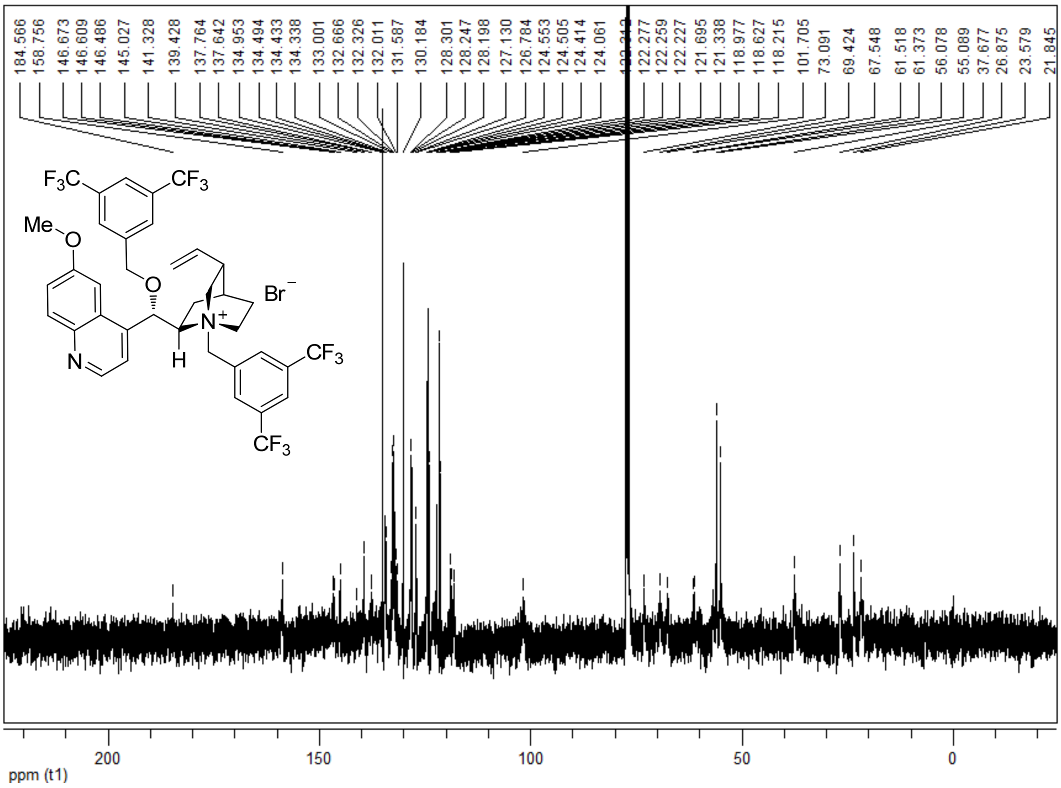
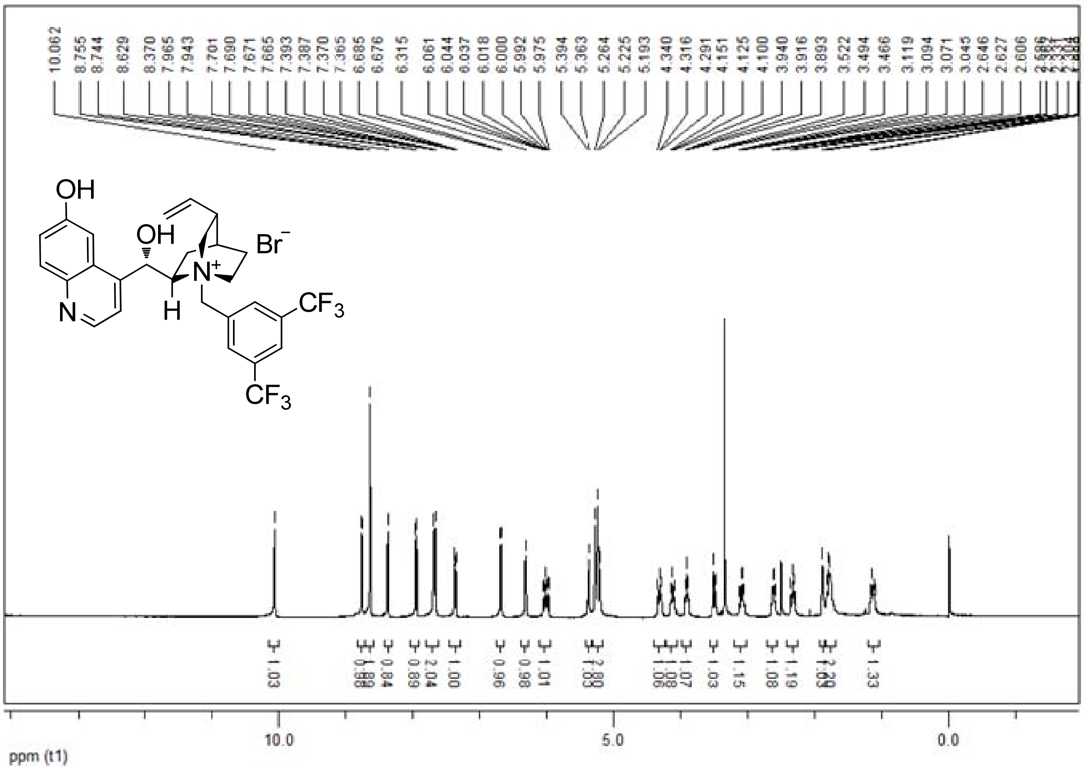
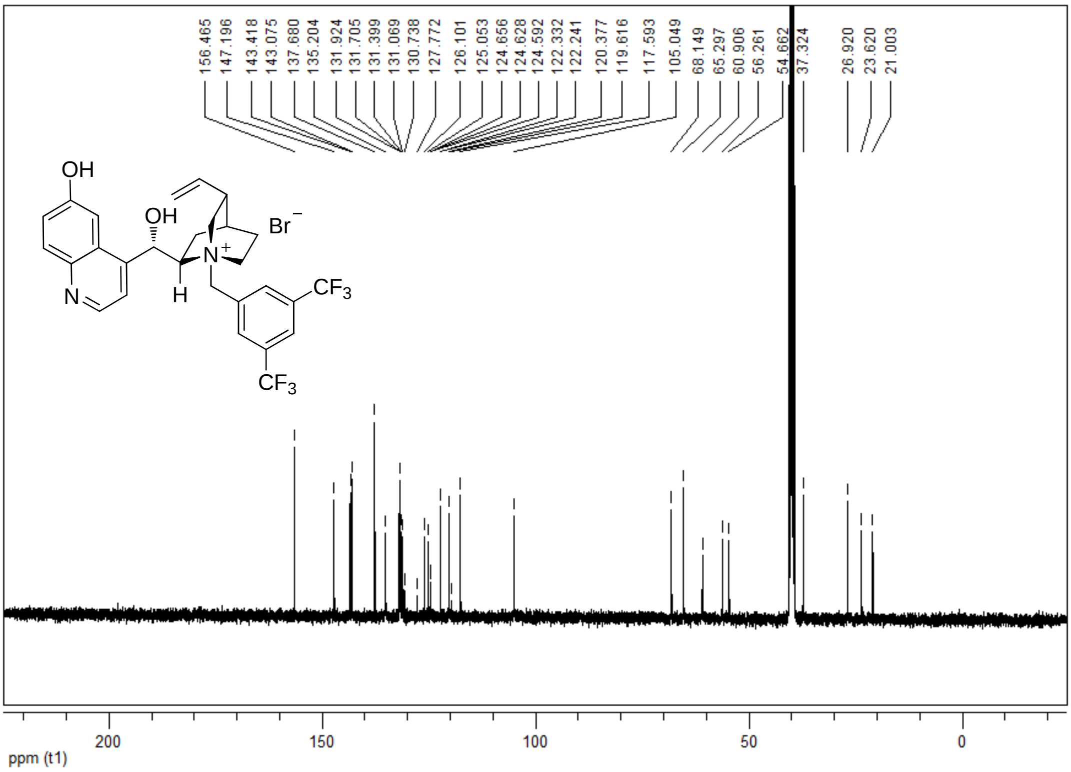
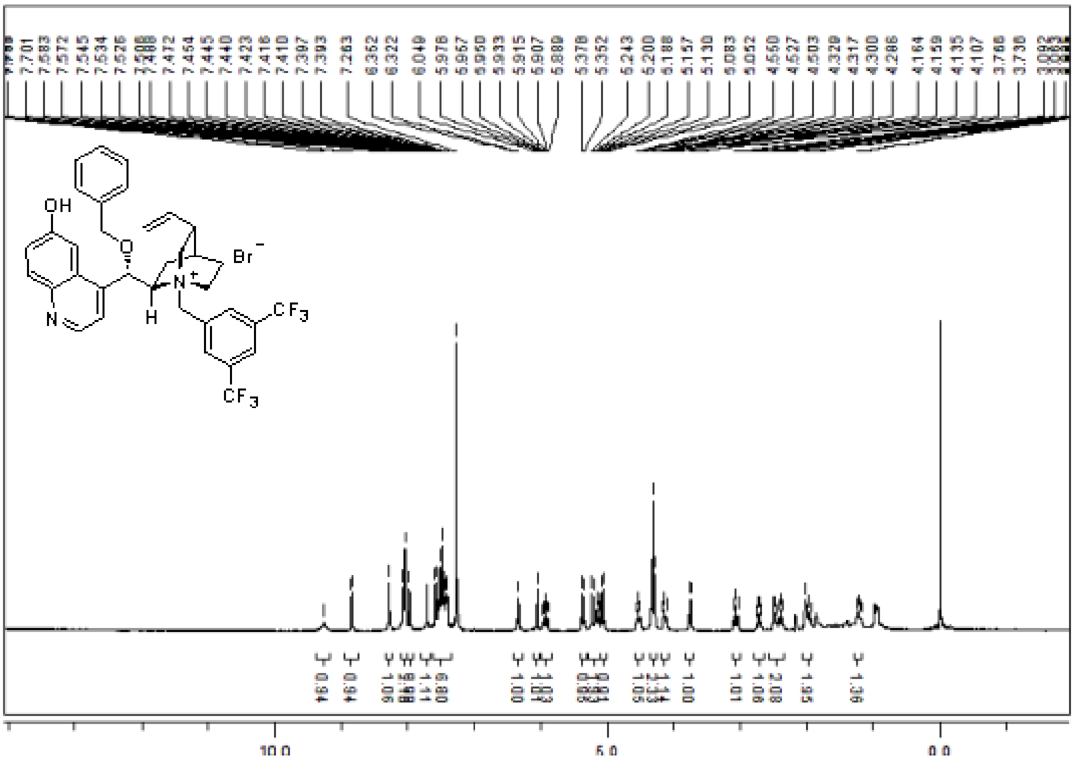
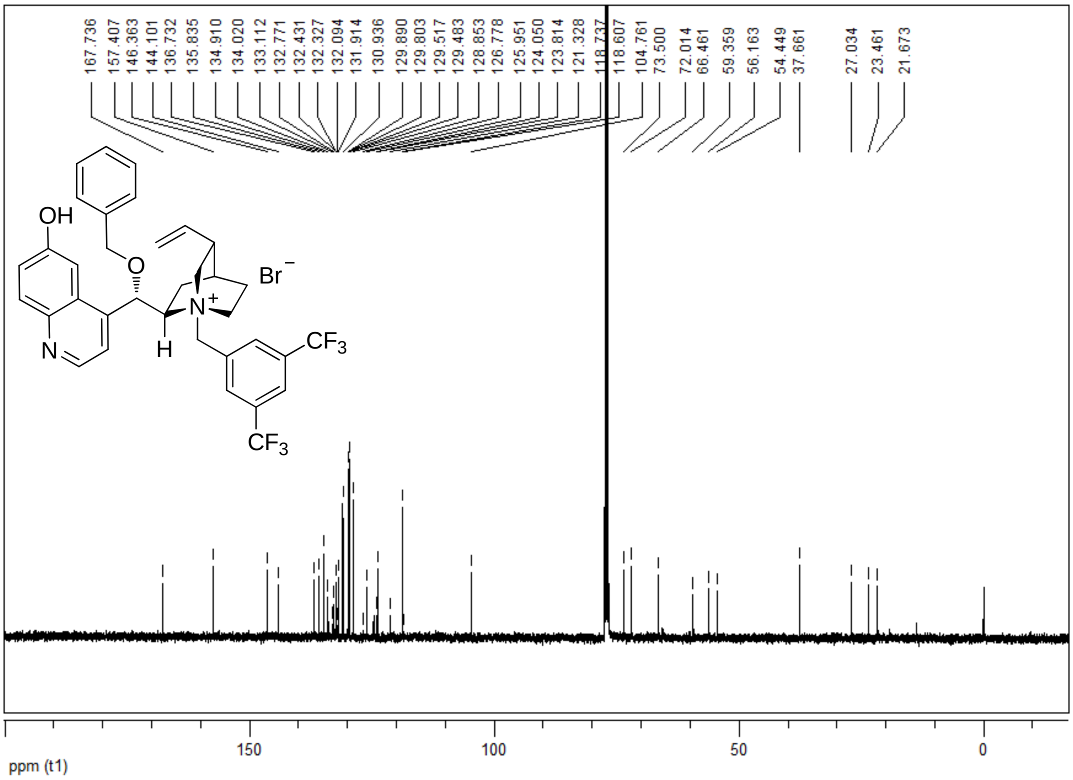
6.002
5.986
5.985
5.976
5.968
5.967
5.964
5.963
5.960
5.193
5.152
5.107
5.081
5.063
5.041
5.039
5.037
5.035
5.033
5.032
5.028
5.021
4.699
4.669
4.072
4.070
4.013
3.860
3.855
3.851
3.850
3.847
3.843
3.831
3.583
3.581
3.578
3.576
3.574
3.556
3.537
3.536
3.534
3.532
3.530
3.526
3.004
3.001
2.982
2.981
2.958
2.936
2.933
2.645
2.623
F3C
CF3
Me
O
O
Br−
N+
N
H
CF3
CF3
1.12
2.08
1.00
1.99
1.12
1.96
1.06
1.09
5.05
1.10
4.61
1.35
1.20
1.10
1.96
1.07
2.17
1.24
0.94
10.0
5.0
0.0
ppm (t1)

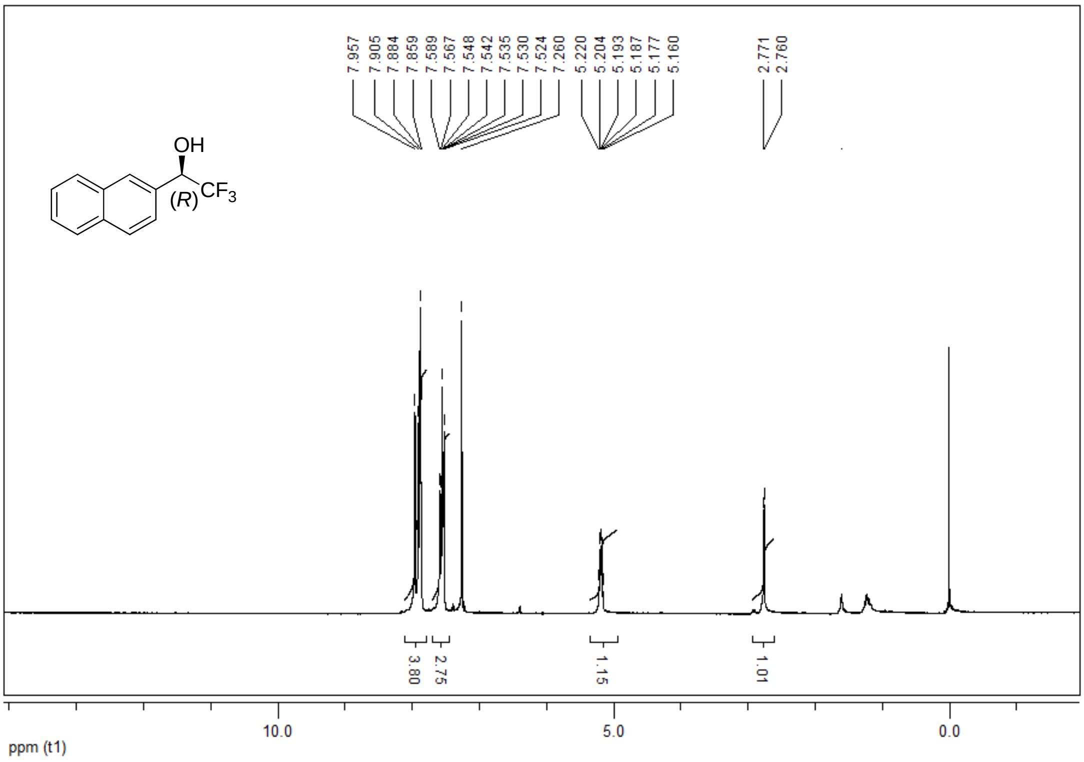

184.566
158.756
146.673
146.609
146.486
145.027
141.328
139.428
137.764
137.642
134.953
134.494
134.433
134.338
133.001
132.666
132.326
132.011
131.587
130.184
128.301
128.247
128.198
127.130
126.784
124.553
124.505
124.414
124.061
122.277
122.259
122.227
121.695
121.338
118.977
118.627
118.215
101.705
73.091
69.424
67.548
61.518
61.373
56.078
55.089
37.677
26.875
23.579
21.845
F3C
CF3
Me
O
O
Br−
N+
N
H
CF3
CF3
200
150
100
50
0
ppm (t1)

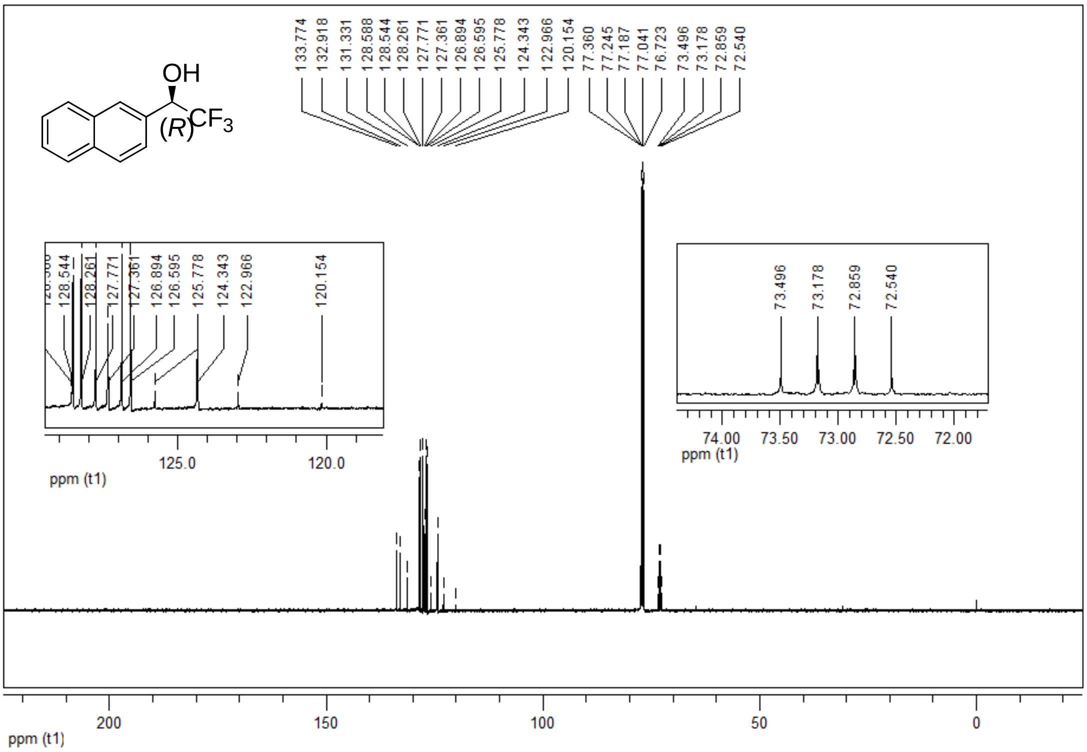

10.062
8.755
8.744
8.629
8.370
7.965
7.943
7.701
7.690
7.671
7.665
7.393
7.387
7.370
7.365
6.685
6.676
6.315
6.061
6.044
6.037
6.018
6.000
5.992
5.975
5.394
5.363
5.264
5.225
5.193
4.340
4.316
4.291
4.151
4.125
4.100
3.940
3.916
3.893
3.522
3.494
3.466
3.119
3.094
3.071
3.045
2.646
2.627
2.606
OH
OH
Br⁻
N⁺
N
H
CF3
CF3
1.03
0.84
0.89
2.04
1.00
0.96
0.98
1.01
2.80
1.07
1.03
1.15
1.08
1.19
1.33
10.0
5.0
0.0
ppm (t1)

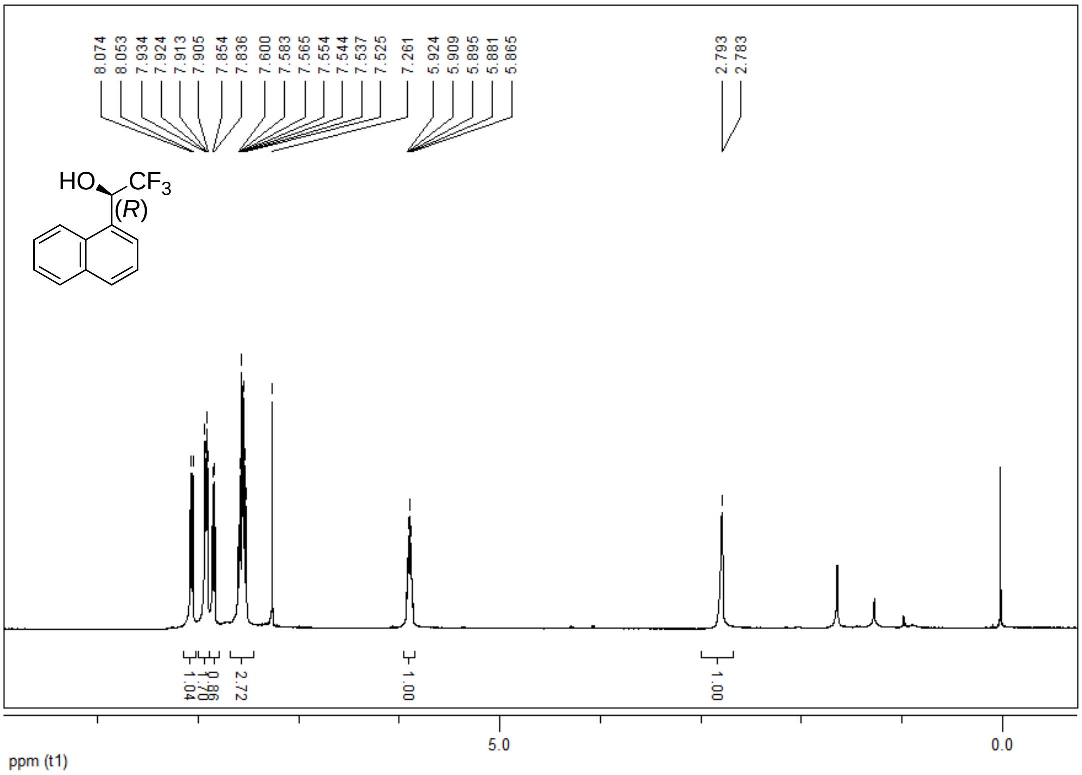

156.465
147.196
143.418
143.075
137.680
135.204
131.924
131.705
131.399
131.069
130.738
127.772
126.101
125.053
124.656
124.628
124.592
122.332
122.241
120.377
119.616
117.593
105.049
68.149
65.297
60.906
56.261
54.662
37.324
26.920
23.620
21.003
OH
OH
Br⁻
N⁺
N
H
CF3
CF3
200
150
100
50
0
ppm (t1)

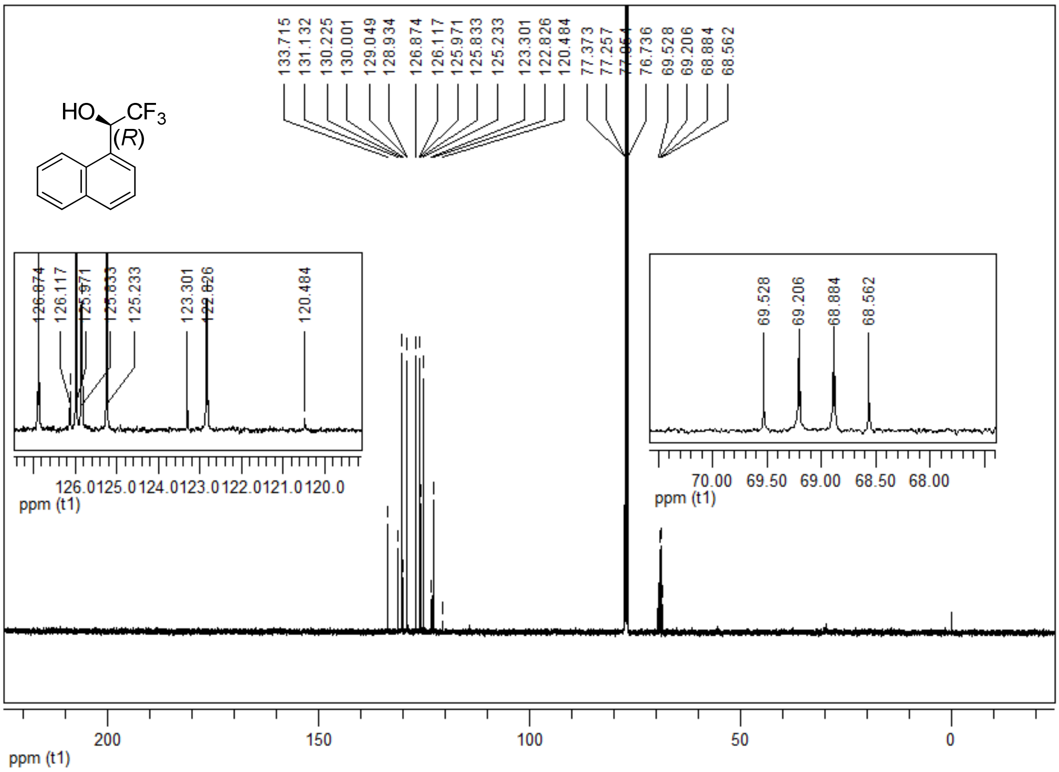

7.701
7.583
7.572
7.545
7.534
7.526
7.472
7.454
7.445
7.440
7.423
7.416
7.410
7.397
7.393
7.263
6.352
6.322
6.049
5.976
5.957
5.950
5.933
5.915
5.907
5.889
5.378
5.352
5.243
5.200
5.188
5.157
5.130
5.083
5.052
4.550
4.527
4.503
4.329
4.317
4.300
4.286
4.164
4.159
4.135
4.107
3.766
3.738
OH
O
Br⁻
N⁺
N
H
CF3
CF3
0.94
0.94
1.06
1.11
6.80
1.00
1.05
1.00
1.01
1.06
2.08
1.95
1.36
10.0
5.0
0.0

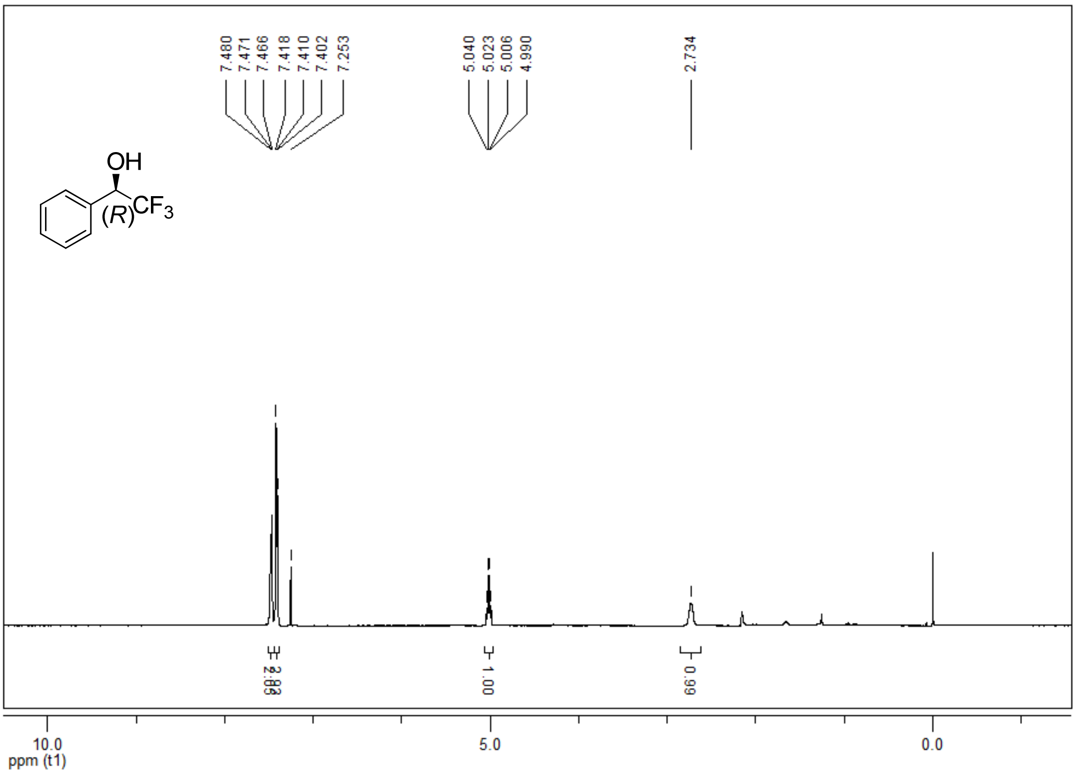

167.736
157.407
146.363
144.101
136.732
135.835
134.910
134.020
133.112
132.771
132.431
132.327
132.094
131.914
130.936
129.890
129.803
129.517
129.483
128.853
126.778
125.951
124.050
123.814
121.328
118.737
118.607
104.761
73.500
72.014
66.461
59.359
56.163
54.449
37.661
27.034
23.461
21.673
OH
O
Br⁻
N⁺
N
H
CF3
CF3
150
100
50
0
ppm (t1)

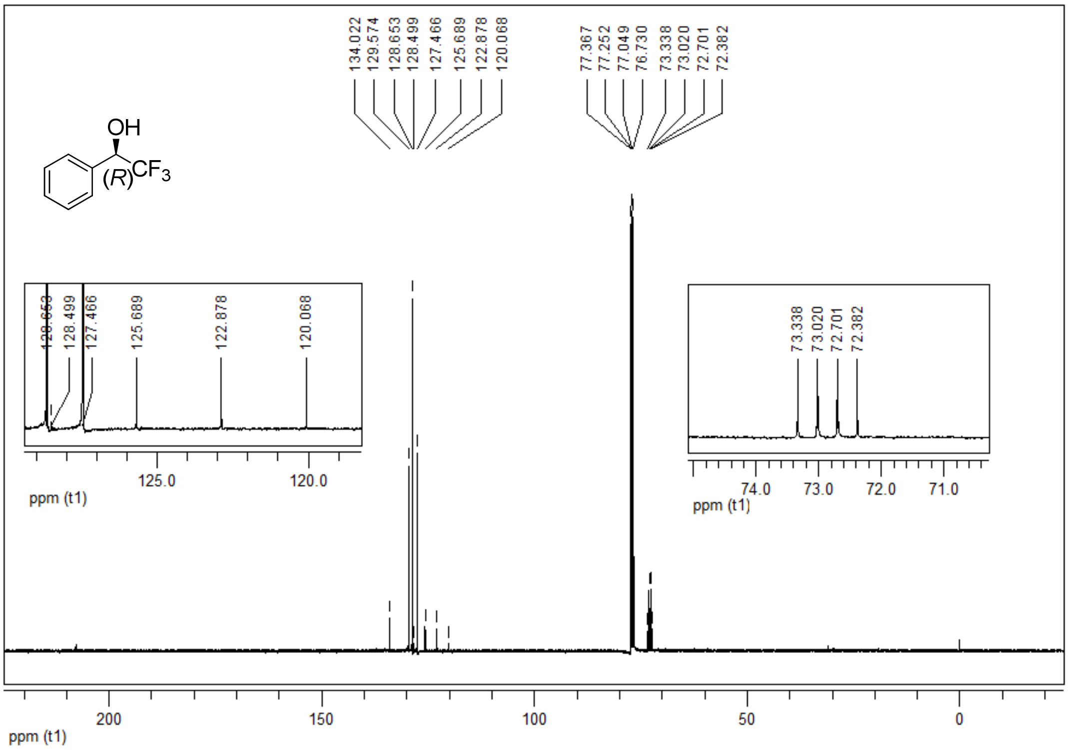

7.957
7.905
7.884
7.859
7.589
7.567
7.548
7.542
7.535
7.530
7.524
7.260
5.220
5.204
5.193
5.187
5.177
5.160
2.771
2.760
OH
(R)
CF3
3.80
2.75
1.15
1.01
10.0
5.0
0.0
ppm (t1)

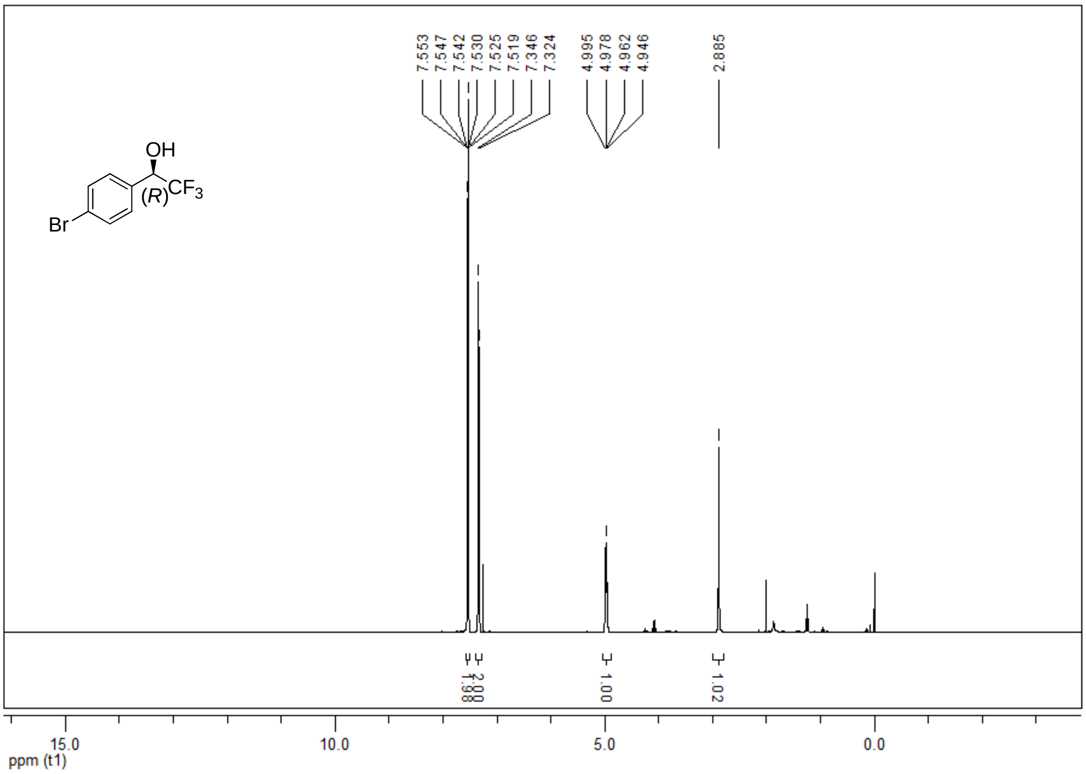

133.774
132.918
131.331
128.588
128.544
128.261
127.771
127.361
126.894
126.595
125.778
124.343
122.966
120.154
77.360
77.245
77.187
77.041
76.723
73.496
73.178
72.859
72.540
OH
(R)
CF3
128.544
128.261
127.771
127.361
126.894
126.595
125.778
124.343
122.966
120.154
125.0
120.0
ppm (t1)
73.496
73.178
72.859
72.540
74.00
73.50
73.00
72.50
72.00
ppm (t1)
200
150
100
50
0
ppm (t1)

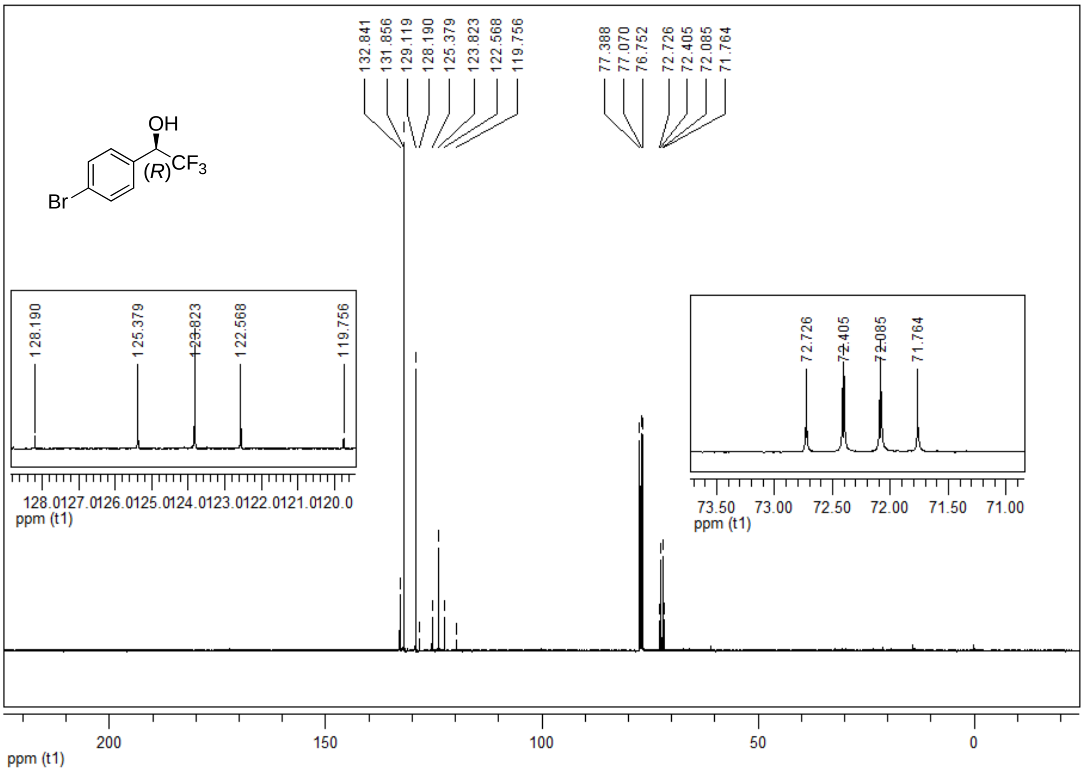

8.074
8.053
7.934
7.924
7.913
7.905
7.854
7.836
7.600
7.583
7.565
7.554
7.544
7.537
7.525
7.261
5.924
5.909
5.895
5.881
5.865
2.793
2.783
HO
CF3
(R)
1.04
1.70
0.86
2.72
1.00
1.00
5.0
0.0
ppm (t1)

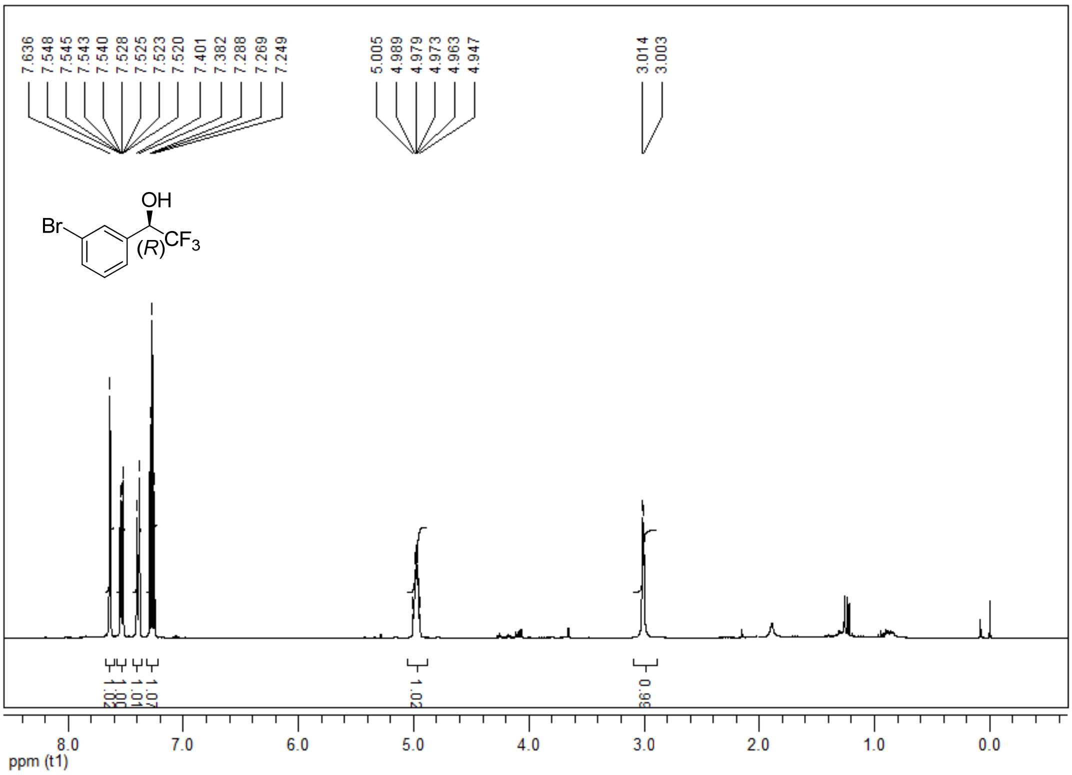

133.715
131.132
130.225
130.001
129.049
128.934
126.874
126.117
125.971
125.833
125.233
123.301
122.826
120.484
77.373
77.257
77.054
76.736
69.528
69.206
68.884
68.562
HO
CF3
(R)
126.874
126.117
125.971
125.833
125.233
123.301
122.826
120.484
126.0
125.0
124.0
123.0
122.0
121.0
120.0
ppm (t1)
69.528
69.206
68.884
68.562
70.00
69.50
69.00
68.50
68.00
ppm (t1)
200
150
100
50
0
ppm (t1)

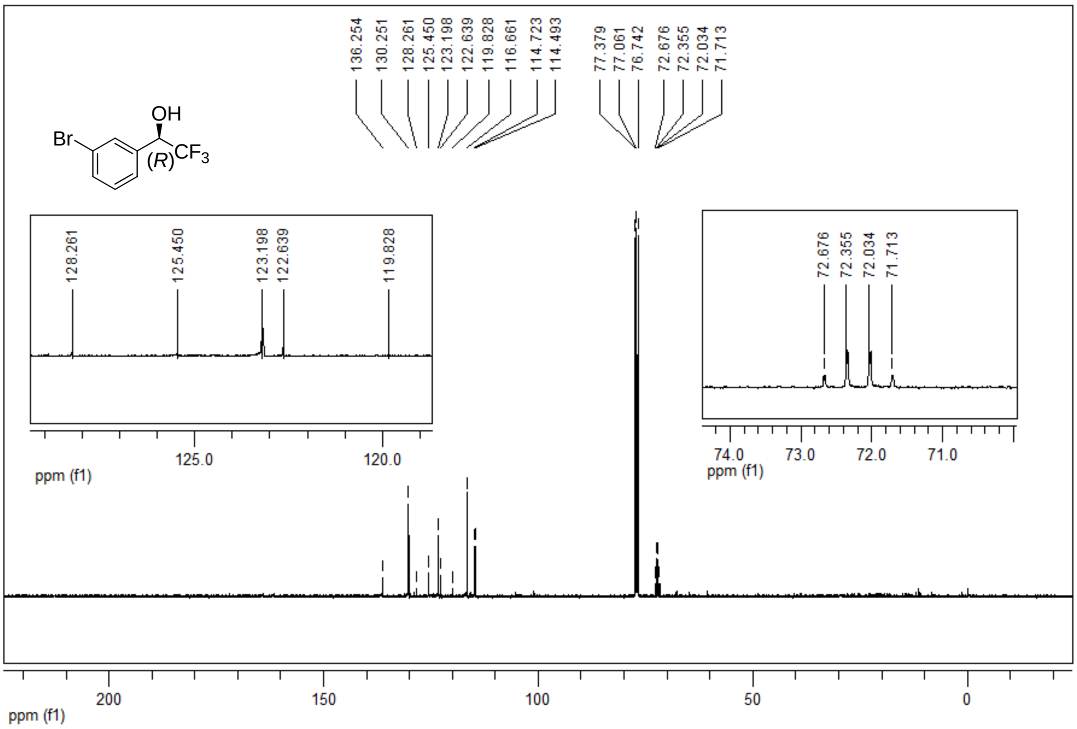

7.480
7.471
7.466
7.418
7.410
7.402
7.253
5.040
5.023
5.006
4.990
2.734
OH
(R)
CF3
2.86
2.03
1.00
0.99
10.0
5.0
0.0
ppm (t1)

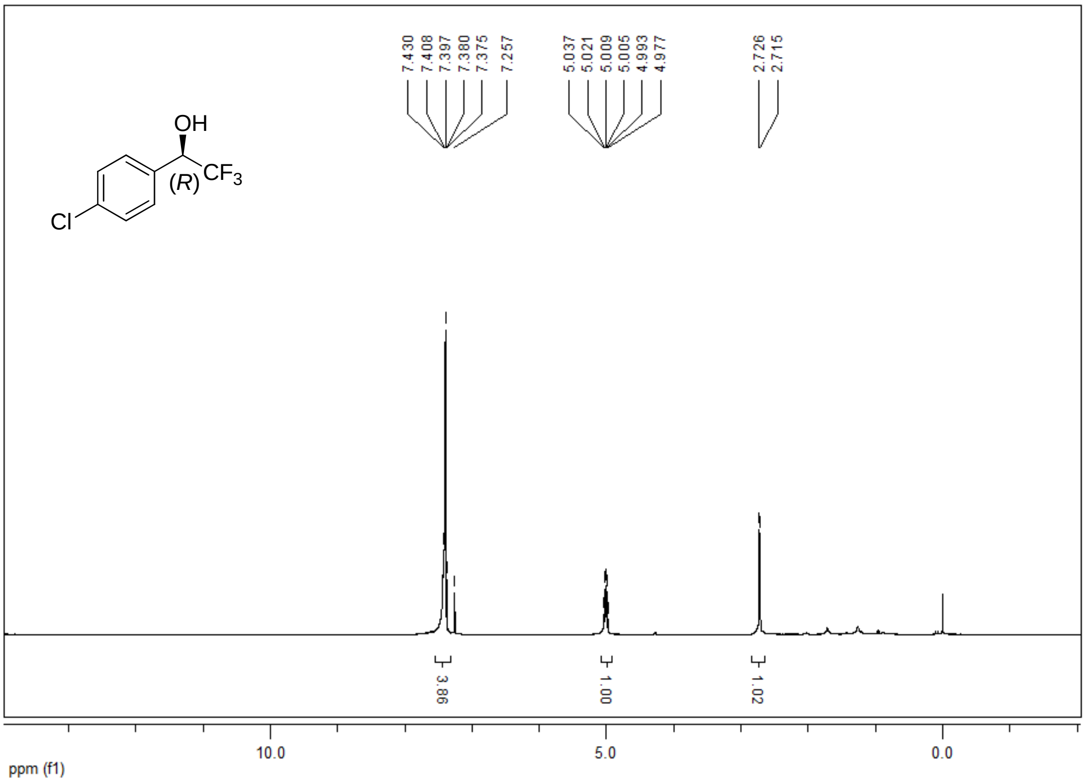

134.022
129.574
128.653
128.499
127.466
125.689
122.878
120.068
77.367
77.252
77.049
76.730
73.338
73.020
72.701
72.382
OH
(R)
CF3
128.653
128.499
127.466
125.689
122.878
120.068
125.0
120.0
ppm (t1)
73.338
73.020
72.701
72.382
74.0
73.0
72.0
71.0
ppm (t1)
200
150
100
50
0
ppm (t1)

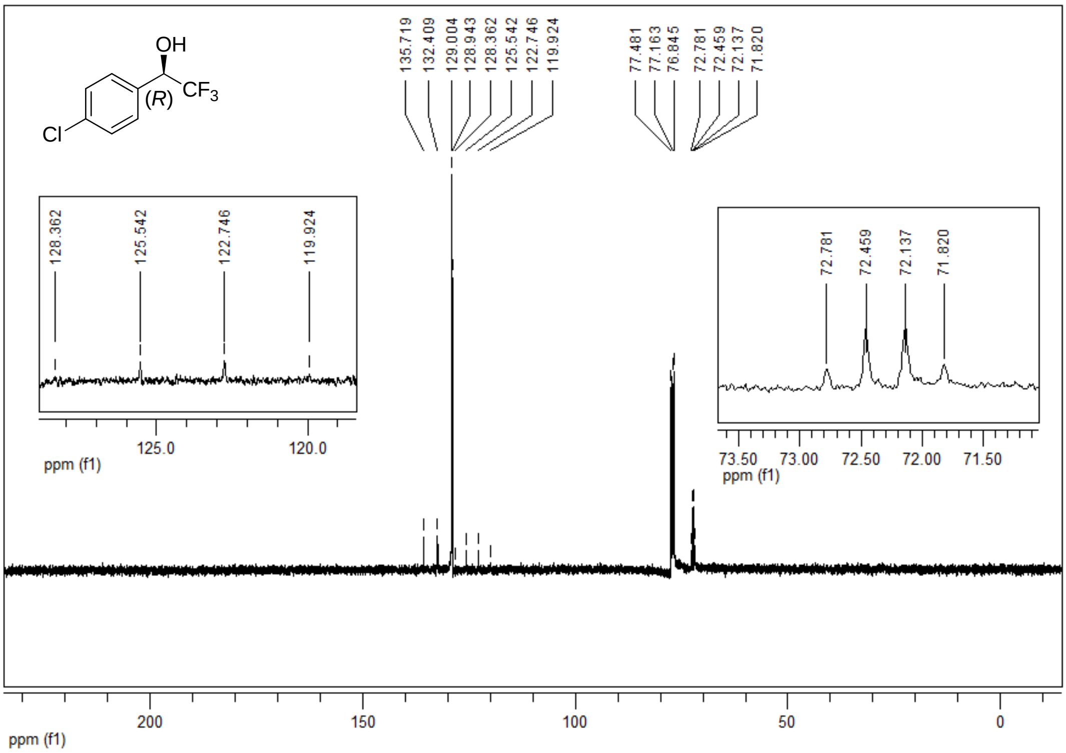

OH
(R)
CF3
Br
7.553
7.547
7.542
7.530
7.525
7.519
7.346
7.324
4.995
4.978
4.962
4.946
2.885
1.98
2.00
1.00
1.02
15.0
10.0
5.0
0.0
ppm (t1)

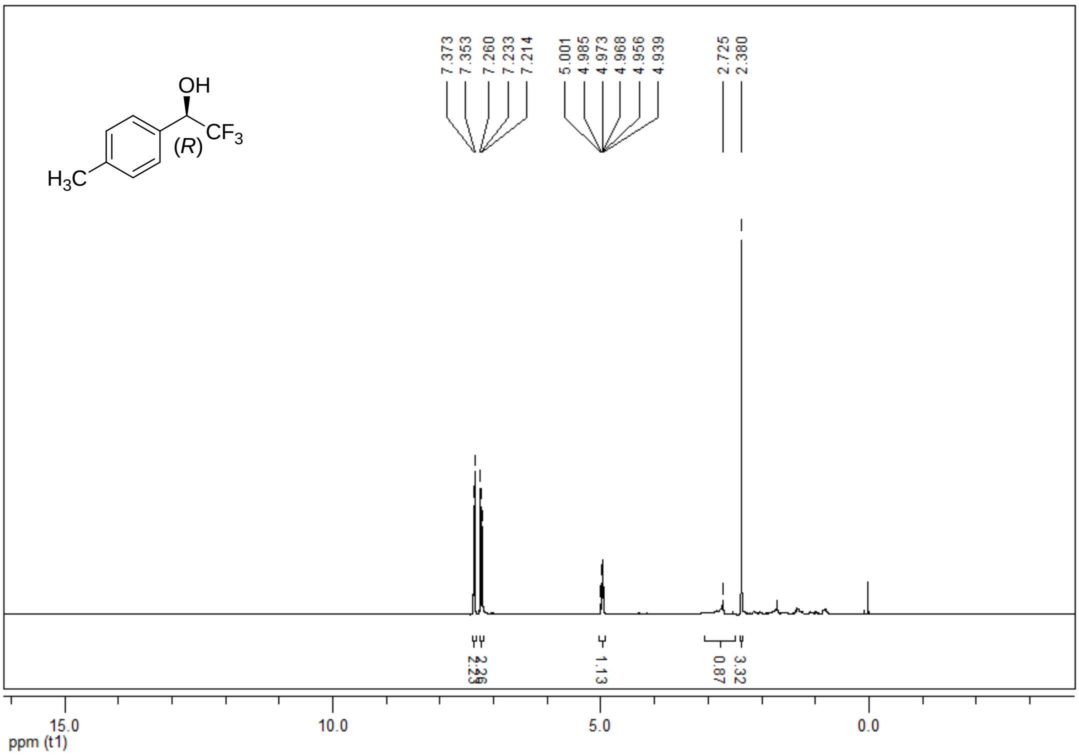

132.841
131.856
129.119
128.190
125.379
123.823
122.568
119.756
77.388
77.070
76.752
72.726
72.405
72.085
71.764
OH
(R)
CF3
Br
128.190
125.379
123.823
122.568
119.756
128.0127.0126.0125.0124.0123.0122.0121.0120.0
ppm (t1)
72.726
72.405
72.085
71.764
73.50
73.00
72.50
72.00
71.50
71.00
ppm (t1)
200
150
100
50
0
ppm (t1)

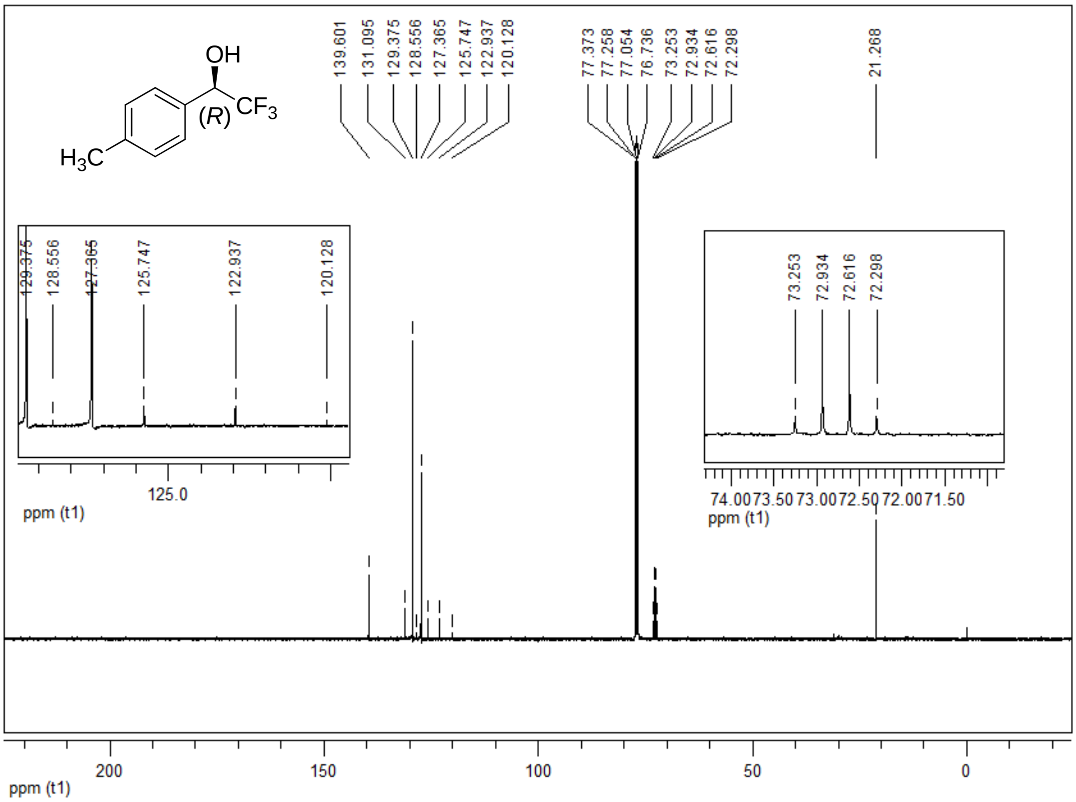

7.636
7.548
7.545
7.543
7.540
7.528
7.525
7.523
7.520
7.401
7.382
7.288
7.269
7.249
5.005
4.989
4.979
4.973
4.963
4.947
3.014
3.003
OH
Br
(R)
CF3
1.02
1.00
1.01
1.07
1.02
0.96
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

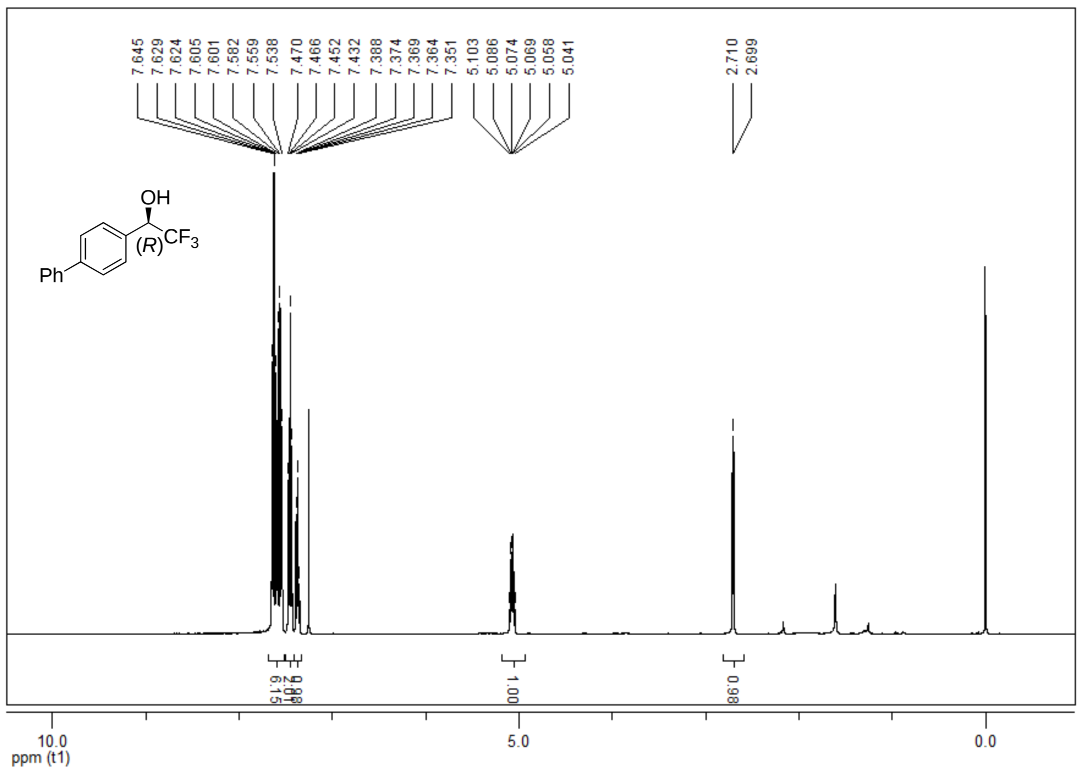

136.254
130.251
128.261
125.450
123.198
122.639
119.828
116.661
114.723
114.493
77.379
77.061
76.742
72.676
72.355
72.034
71.713
OH
Br
(R)
CF3
128.261
125.450
123.198
122.639
119.828
125.0
120.0
ppm (f1)
72.676
72.355
72.034
71.713
74.0
73.0
72.0
71.0
ppm (f1)
200
150
100
50
0
ppm (f1)

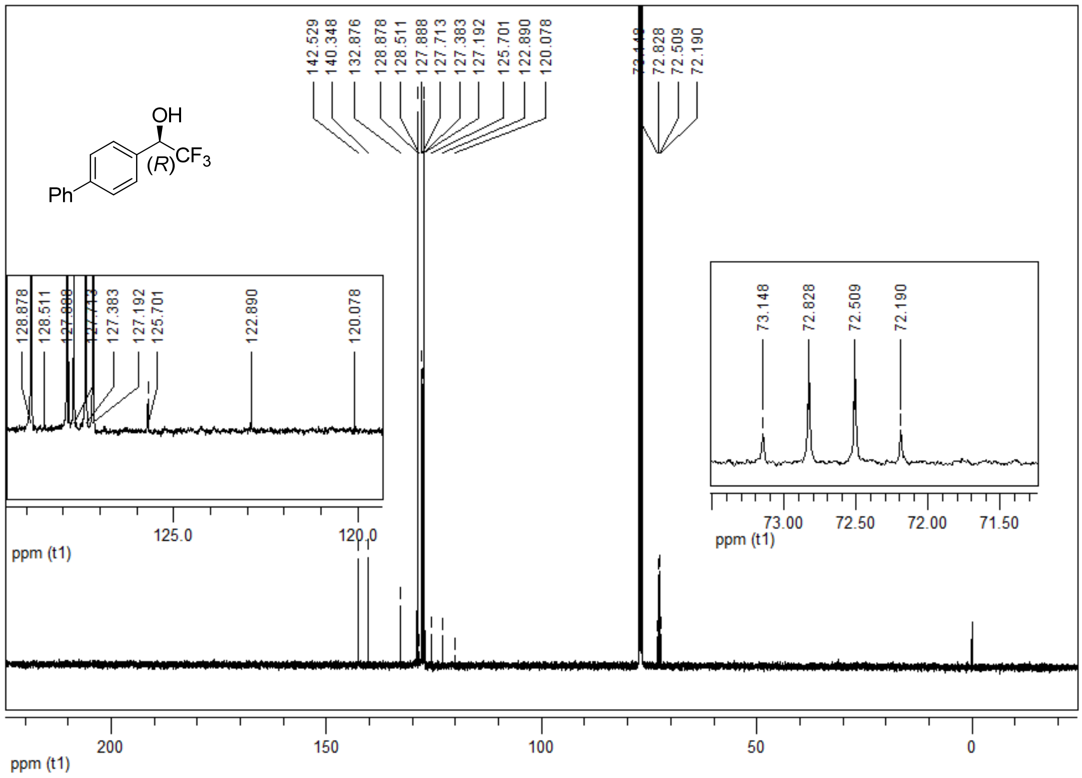

OH
CF3
(R)
Cl
7.430
7.408
7.397
7.380
7.375
7.257
5.037
5.021
5.009
5.005
4.993
4.977
2.726
2.715
3.86
1.00
1.02
10.0
5.0
0.0
ppm (f1)

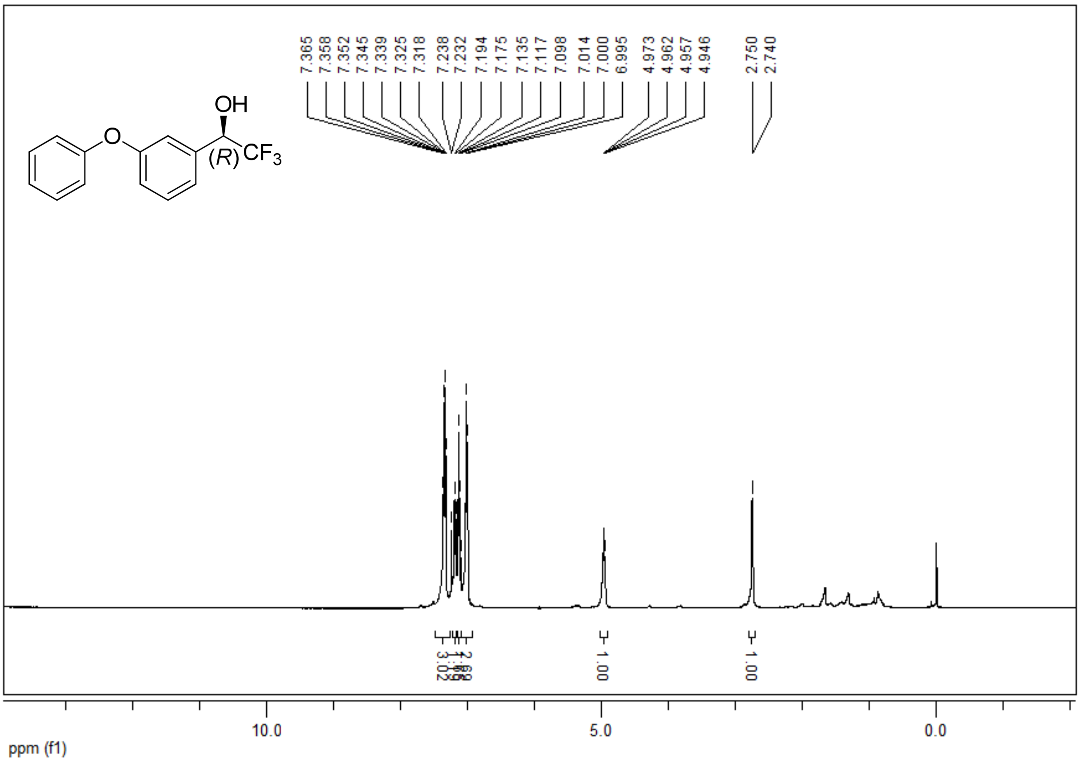

OH
CF3
(R)
Cl
135.719
132.409
129.004
128.943
128.362
125.542
122.746
119.924
77.481
77.163
76.845
72.781
72.459
72.137
71.820
128.362
125.542
122.746
119.924
125.0
120.0
ppm (f1)
72.781
72.459
72.137
71.820
73.50
73.00
72.50
72.00
71.50
ppm (f1)
200
150
100
50
0
ppm (f1)


OH
CF3
(R)
H3C
7.373
7.353
7.260
7.233
7.214
5.001
4.985
4.973
4.968
4.956
4.939
2.725
2.380
2.23
2.26
1.13
0.87
3.32
15.0
10.0
5.0
0.0
ppm (t1)


OH
CF3
(R)
H3C
139.601
131.095
129.375
128.556
127.365
125.747
122.937
120.128
77.373
77.258
77.054
76.736
73.253
72.934
72.616
72.298
21.268
125.0
ppm (t1)
74.00
73.50
73.00
72.50
72.00
71.50
ppm (t1)
200
150
100
50
0
ppm (t1)


7.645
7.629
7.624
7.605
7.601
7.582
7.559
7.538
7.470
7.466
7.452
7.432
7.388
7.374
7.369
7.364
7.351
5.103
5.086
5.074
5.069
5.058
5.041
2.710
2.699
OH
(R)
CF3
Ph
6.15
2.01
0.98
1.00
0.98
10.0
5.0
0.0
ppm (t1)


142.529
140.348
132.876
128.878
128.511
127.888
127.713
127.383
127.192
125.701
122.890
120.078
73.148
72.828
72.509
72.190
OH
(R)
CF3
Ph
125.0
120.0
ppm (t1)
73.00
72.50
72.00
71.50
200
150
100
50
0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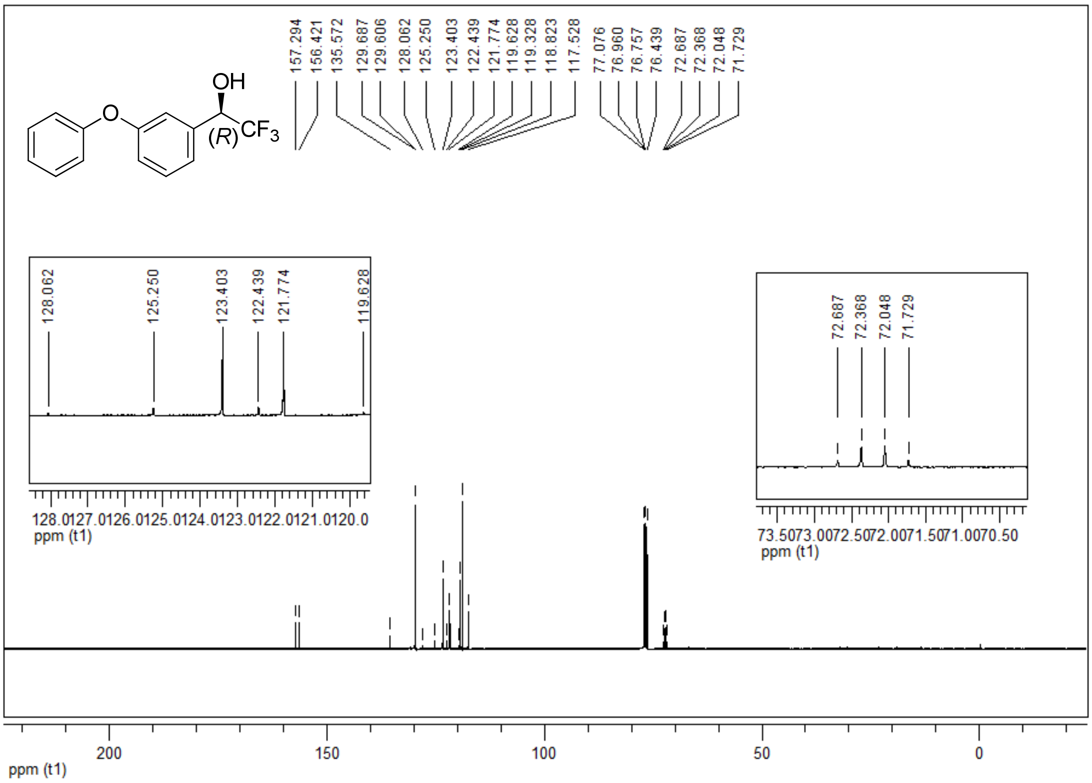
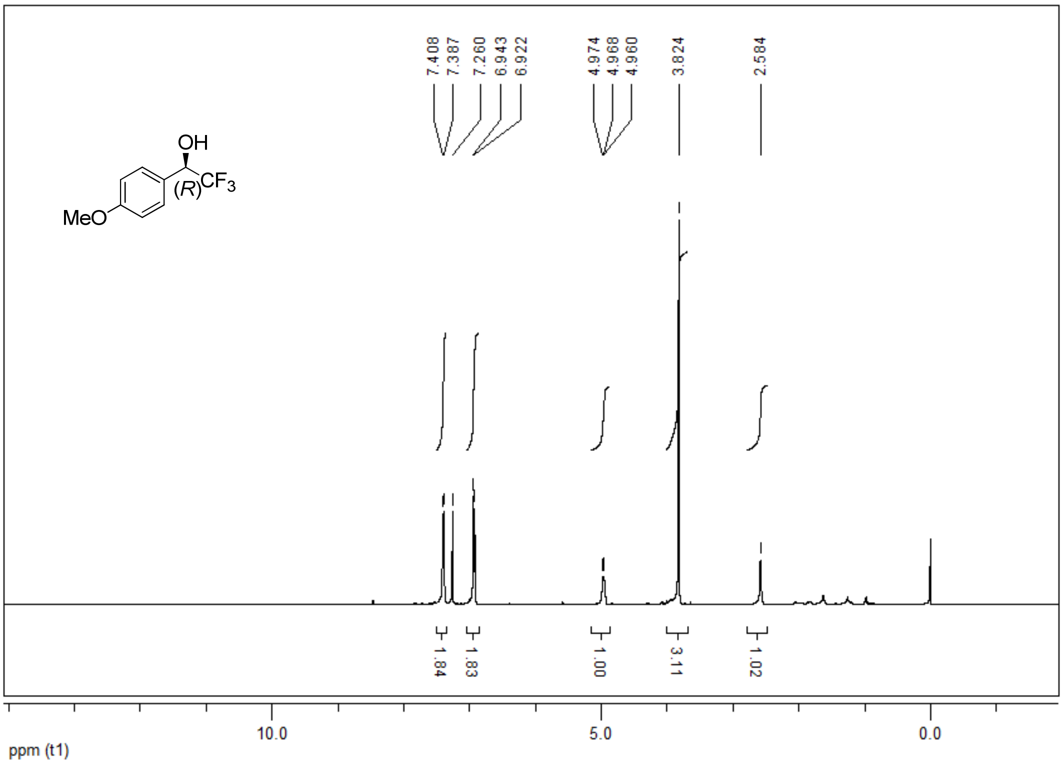
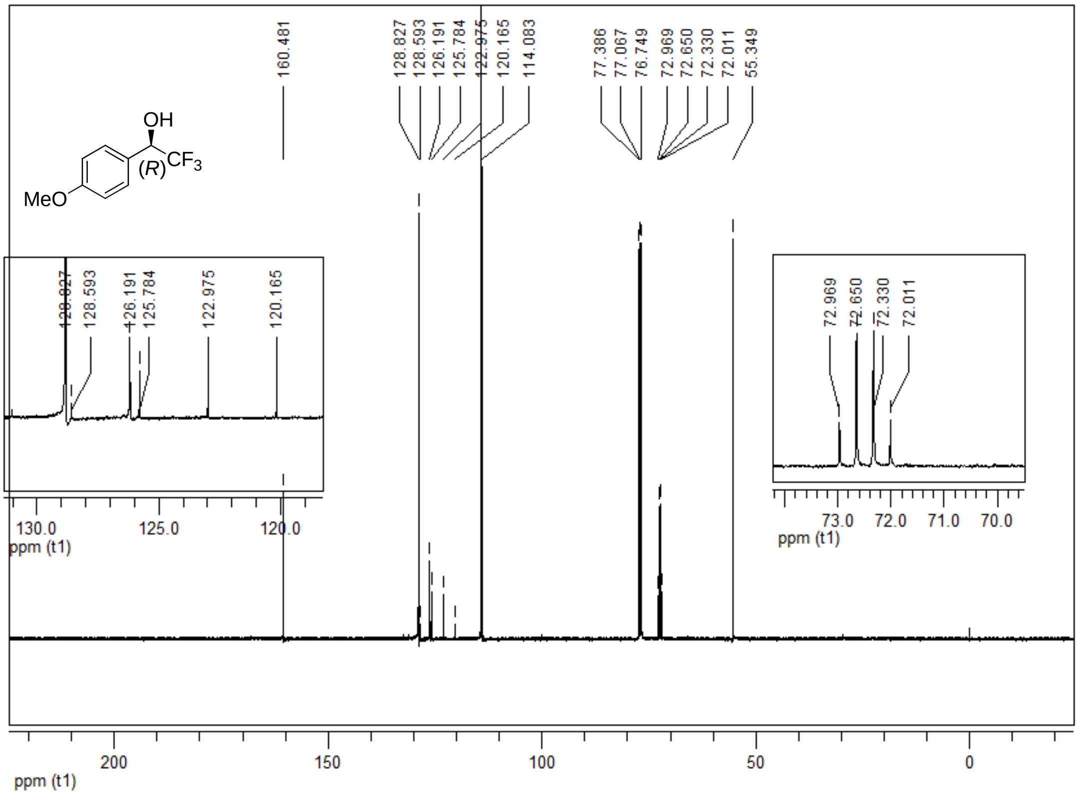
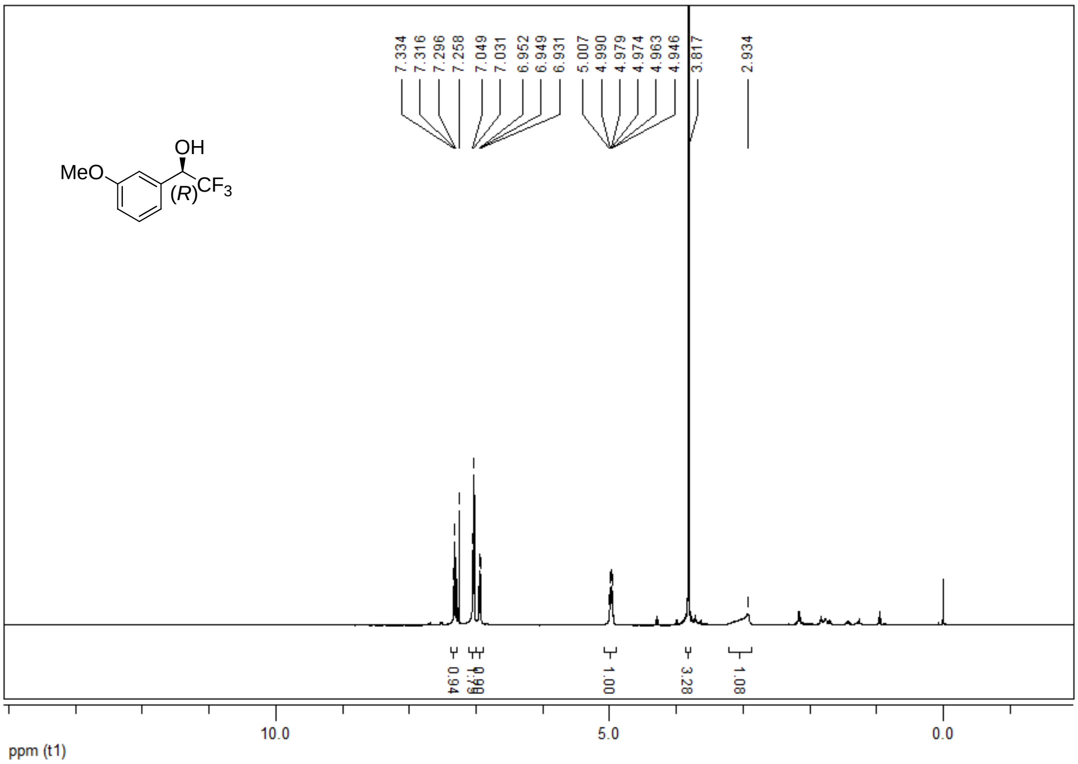
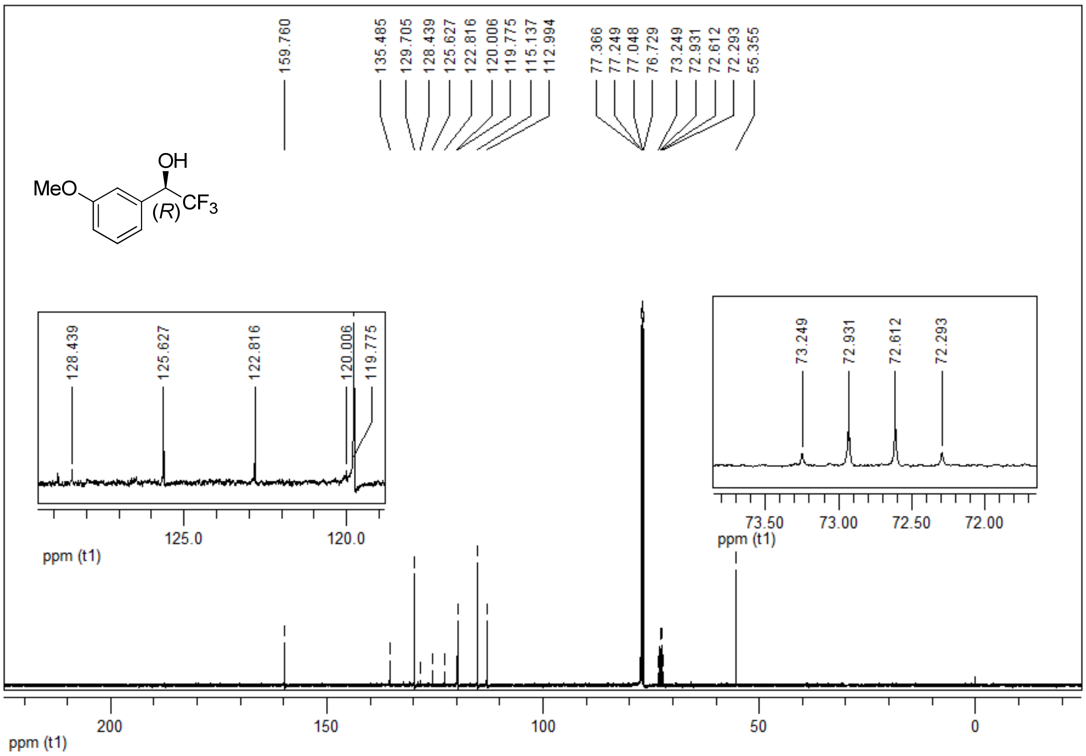
7.358
7.352
7.345
7.339
7.325
7.318
7.238
7.232
7.194
7.175
7.135
7.117
7.098
7.014
7.000
6.995
4.973
4.962
4.957
4.946
2.750
2.740
OH
O
(R)
CF3
3.02
1.00
1.00
10.0
5.0
0.0
ppm (f1)

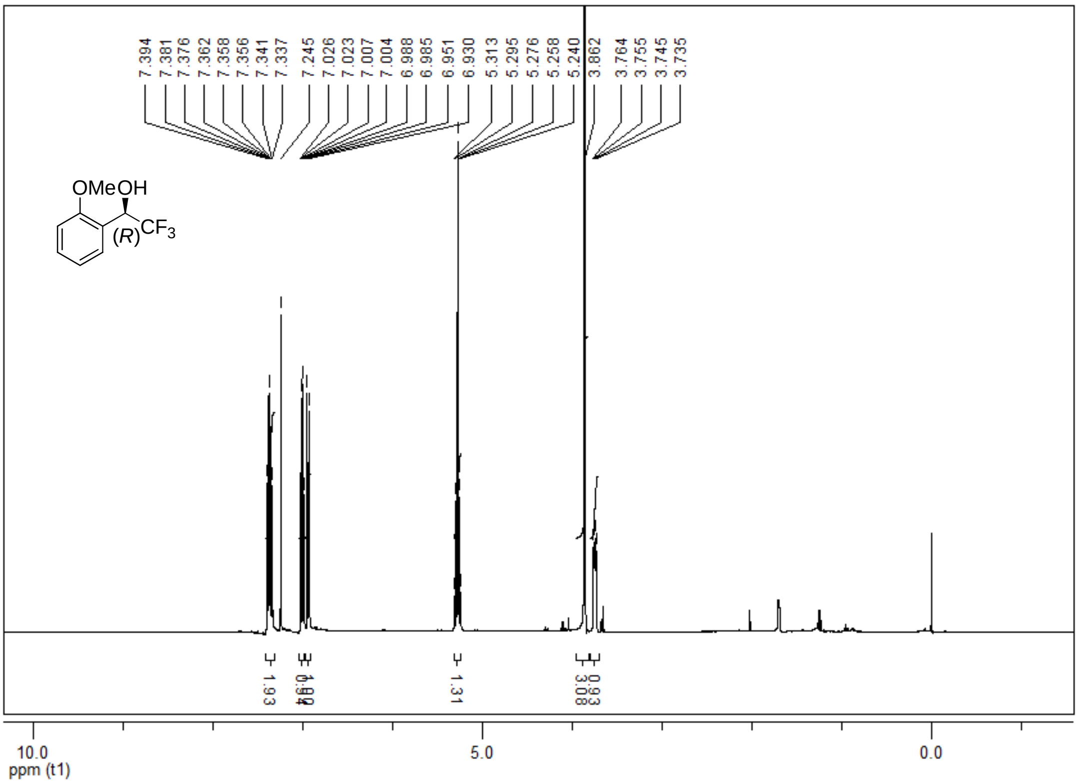

157.294
156.421
135.572
129.687
129.606
128.062
125.250
123.403
122.439
121.774
119.628
119.328
118.823
117.528
77.076
76.960
76.757
76.439
72.687
72.368
72.048
71.729
OH
O
(R)
CF3
128.062
125.250
123.403
122.439
121.774
119.628
128.0127.0126.0125.0124.0123.0122.0121.0120.0
ppm (t1)
72.687
72.368
72.048
71.729
73.5073.0072.5072.0071.5071.0070.50
ppm (t1)
200
150
100
50
0
ppm (t1)

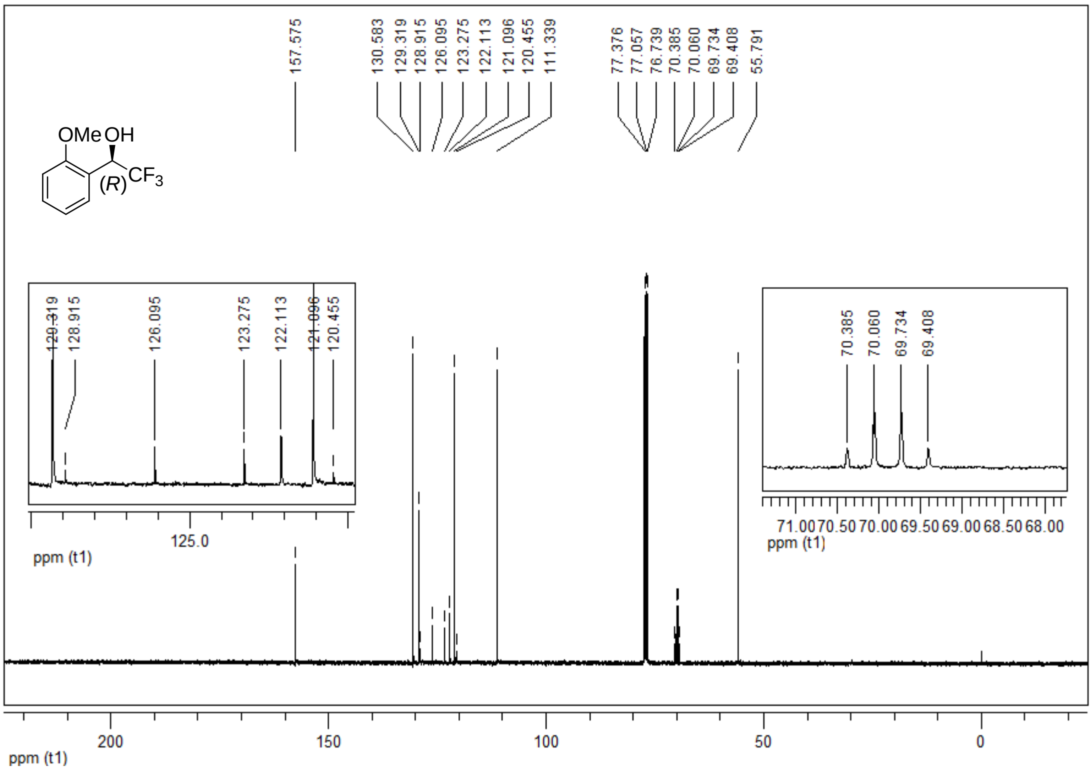

OH
(R)
CF3
MeO
7.408
7.387
7.260
6.943
6.922
4.974
4.968
4.960
3.824
2.584
1.84
1.83
1.00
3.11
1.02
10.0
5.0
0.0
ppm (t1)

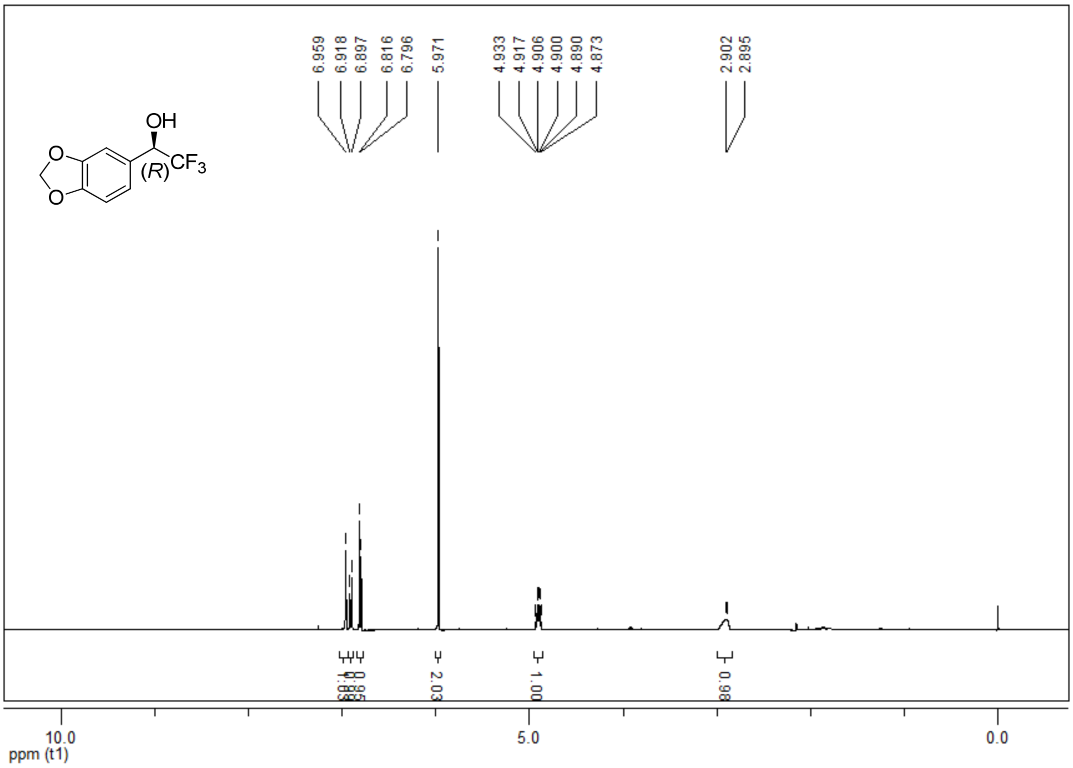

160.481
128.827
128.593
126.191
125.784
122.975
120.165
114.083
77.386
77.067
76.749
72.969
72.650
72.330
72.011
55.349
OH
(R)
CF3
MeO
128.827
128.593
126.191
125.784
122.975
120.165
130.0
125.0
120.0
ppm (t1)
72.969
72.650
72.330
72.011
73.0
72.0
71.0
70.0
ppm (t1)
200
150
100
50
0
ppm (t1)

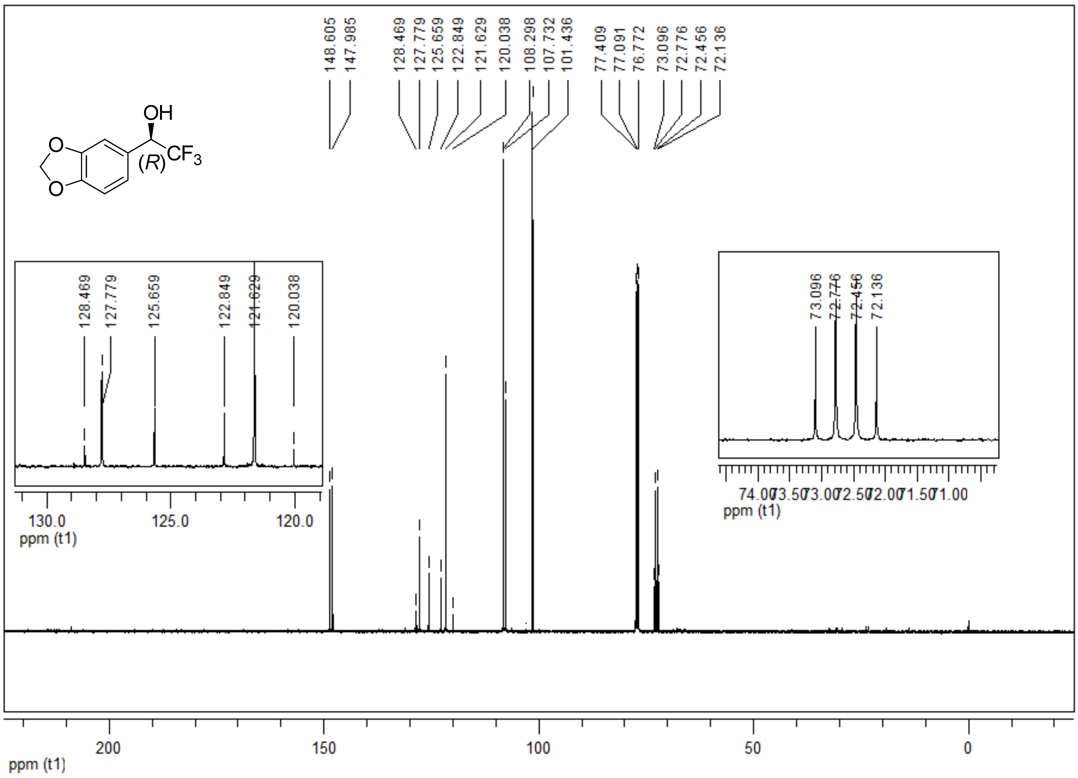

7.334
7.316
7.296
7.258
7.049
7.031
6.952
6.949
6.931
5.007
4.990
4.979
4.974
4.963
4.946
3.817
2.934
OH
MeO
(R)
CF3
0.94
1.79
0.99
1.00
3.28
1.08
10.0
5.0
0.0
ppm (t1)

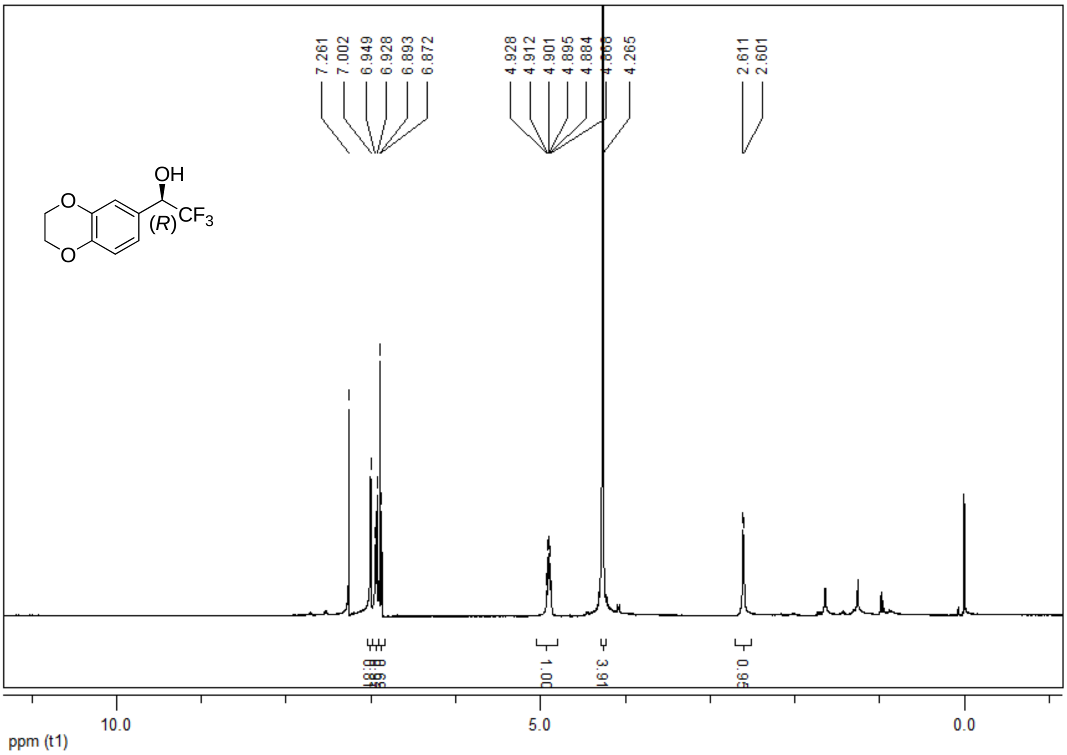

159.760
135.485
129.705
128.439
125.627
122.816
120.006
119.775
115.137
112.994
77.366
77.249
77.048
76.729
73.249
72.931
72.612
72.293
55.355
OH
MeO
(R)
CF3
128.439
125.627
122.816
120.006
119.775
125.0
120.0
ppm (t1)
73.249
72.931
72.612
72.293
73.50
73.00
72.50
72.00
ppm (t1)
200
150
100
50
0
ppm (t1)

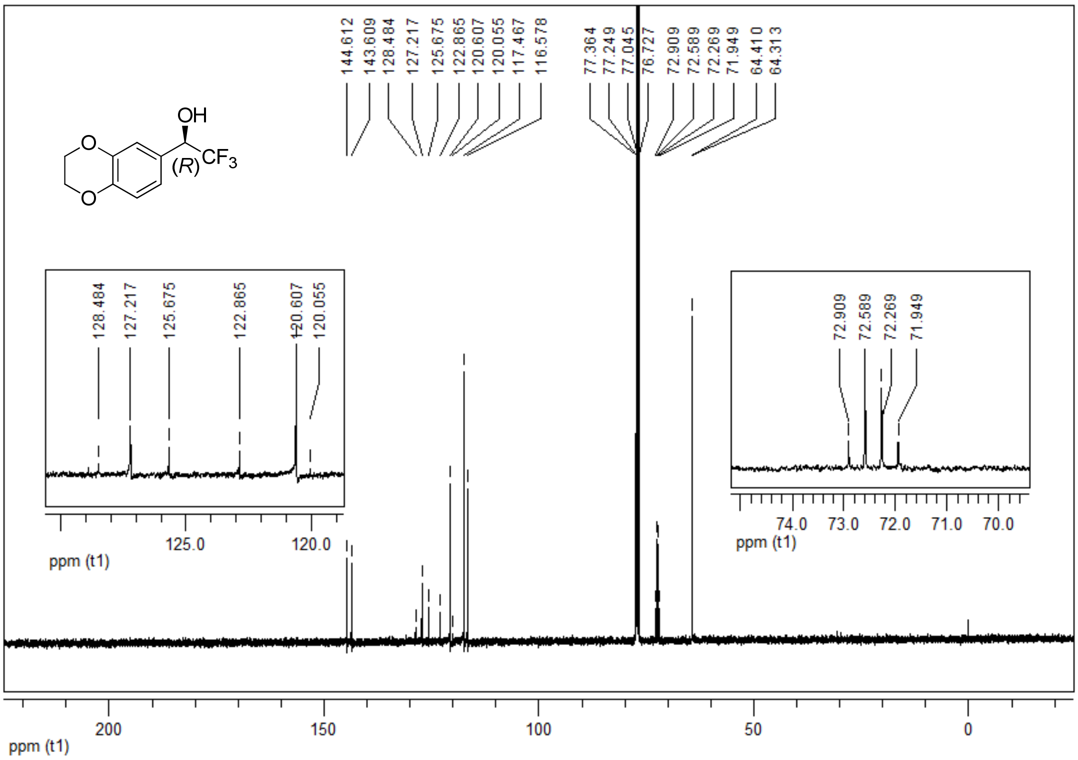

7.394
7.381
7.376
7.362
7.358
7.356
7.341
7.337
7.245
7.026
7.023
7.007
7.004
6.988
6.985
6.951
6.930
5.313
5.295
5.276
5.258
5.240
3.862
3.764
3.755
3.745
3.735
OMe
OH
(R)
CF3
1.93
1.31
3.08
0.93
10.0
5.0
0.0
ppm (t1)

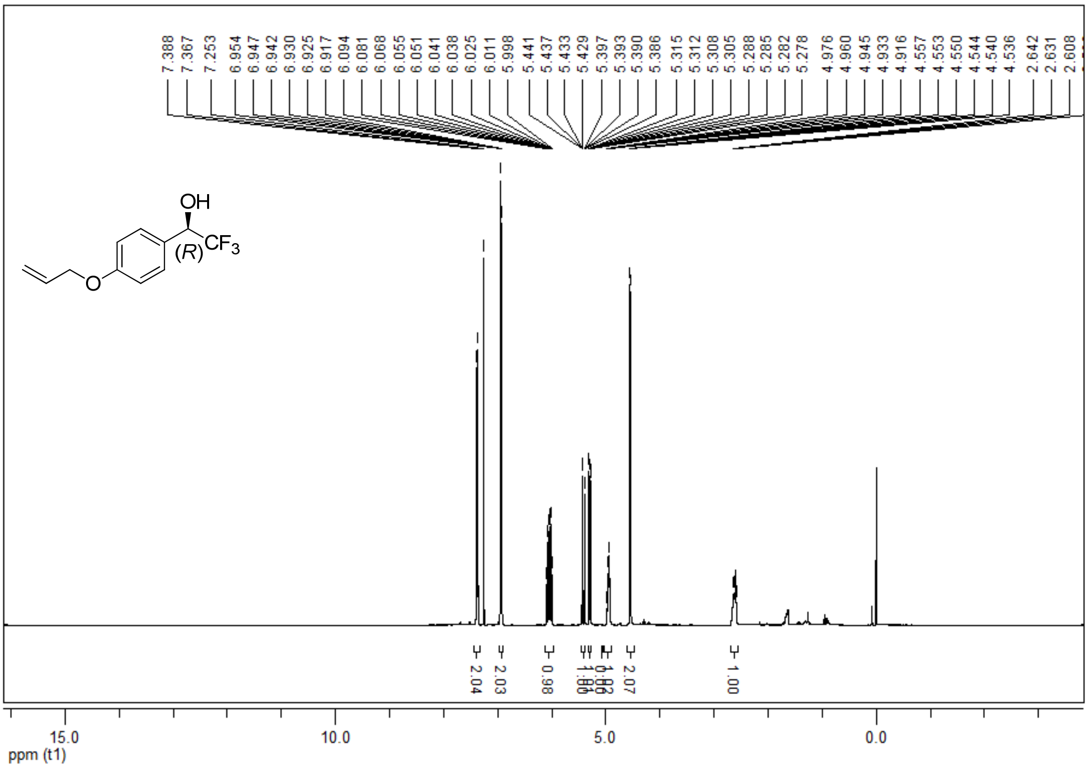

157.575
130.583
129.319
128.915
126.095
123.275
122.113
121.096
120.455
111.339
77.376
77.057
76.739
70.385
70.060
69.734
69.408
55.791
OMe
OH
(R)
CF3
129.319
128.915
126.095
123.275
122.113
121.096
120.455
125.0
ppm (t1)
70.385
70.060
69.734
69.408
71.00
70.50
70.00
69.50
69.00
68.50
68.00
ppm (t1)
200
150
100
50
0
ppm (t1)

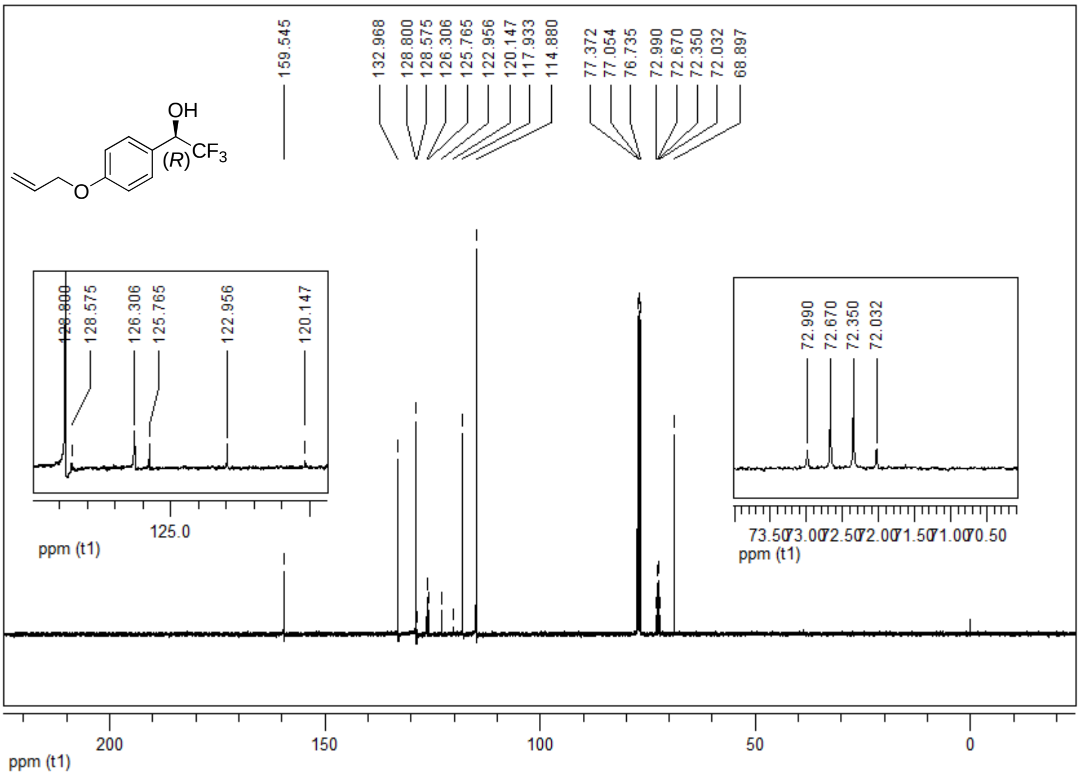

6.959
6.918
6.897
6.816
6.796
5.971
4.933
4.917
4.906
4.900
4.890
4.873
2.902
2.895
OH
CF3
(R)
O
O
1.03
0.96
2.03
1.00
0.98
10.0
5.0
0.0
ppm (t1)

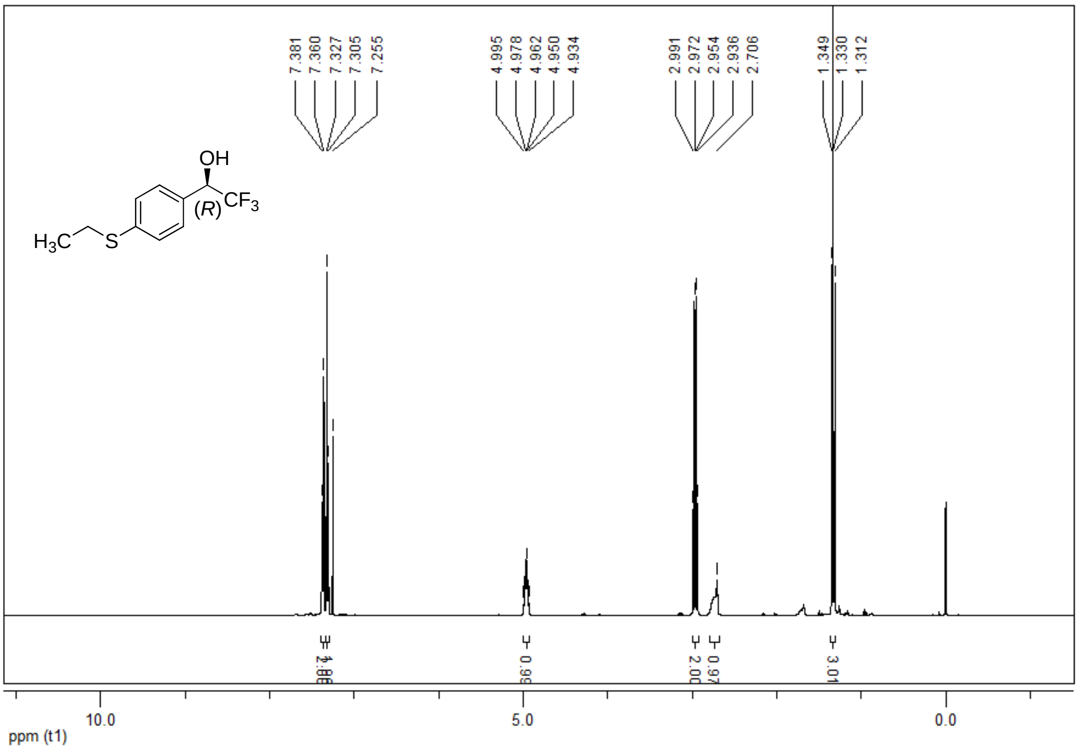

148.605
147.985
128.469
127.779
125.659
122.849
121.629
120.038
108.298
107.732
101.436
77.409
77.091
76.772
73.096
72.776
72.456
72.136
OH
CF3
(R)
O
O
130.0
125.0
120.0
74.00
73.50
73.00
72.50
72.00
71.50
71.00
200
150
100
50
0
ppm (t1)

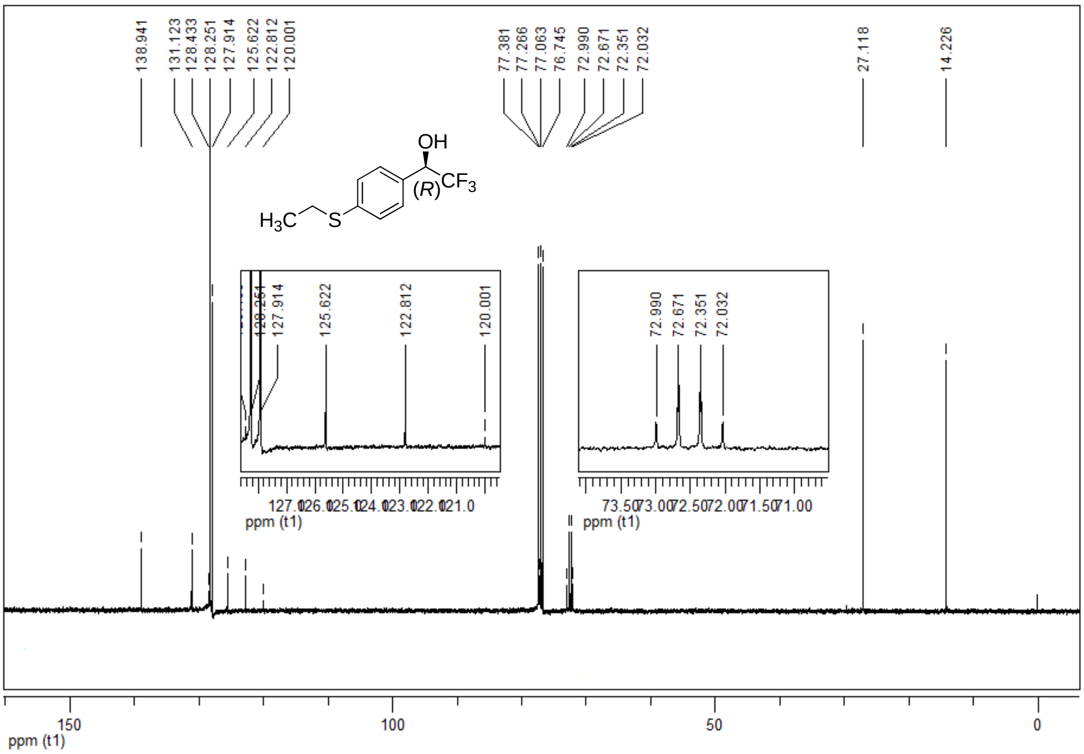

7.261
7.002
6.949
6.928
6.893
6.872
4.928
4.912
4.901
4.895
4.884
4.868
4.265
2.611
2.601
OH
O
O
(R)
CF3
1.00
3.91
0.95
10.0
5.0
0.0
ppm (t1)


144.612
143.609
128.484
127.217
125.675
122.865
120.607
120.055
117.467
116.578
77.364
77.249
77.045
76.727
72.909
72.589
72.269
71.949
64.410
64.313
OH
O
O
(R)
CF3
128.484
127.217
125.675
122.865
120.607
120.055
125.0
120.0
ppm (t1)
72.909
72.589
72.269
71.949
74.0
73.0
72.0
71.0
70.0
ppm (t1)
200
150
100
50
0
ppm (t1)


7.388
7.367
7.253
6.954
6.947
6.942
6.930
6.925
6.917
6.094
6.081
6.068
6.055
6.051
6.041
6.038
6.025
6.011
5.998
5.441
5.437
5.433
5.429
5.397
5.393
5.390
5.386
5.315
5.312
5.308
5.305
5.288
5.285
5.282
5.278
4.976
4.960
4.945
4.933
4.916
4.557
4.553
4.550
4.544
4.540
4.536
2.642
2.631
2.608
OH
(R)
CF3
O
2.04
2.03
0.98
2.07
1.00
15.0
10.0
5.0
0.0
ppm (t1)


159.545
132.968
128.800
128.575
126.306
125.765
122.956
120.147
117.933
114.880
77.372
77.054
76.735
72.990
72.670
72.350
72.032
68.897
OH
(R)
CF3
O
128.800
128.575
126.306
125.765
122.956
120.147
125.0
ppm (t1)
72.990
72.670
72.350
72.032
73.50
73.00
72.50
72.00
71.50
71.00
70.50
ppm (t1)
200
150
100
50
0
ppm (t1)


7.381
7.360
7.327
7.305
7.255
4.995
4.978
4.962
4.950
4.934
2.991
2.972
2.954
2.936
2.706
1.349
1.330
1.312
OH
(R)
CF3
H3C
S
0.99
2.00
0.97
3.01
10.0
5.0
0.0
ppm (t1)


138.941
131.123
128.433
128.251
127.914
125.622
122.812
120.001
77.381
77.266
77.063
76.745
72.990
72.671
72.351
72.032
27.118
14.226
OH
(R)
CF3
H3C
S
128.251
127.914
125.622
122.812
120.001
127.0
126.0
125.0
124.0
123.0
122.0
121.0
ppm (t1)
72.990
72.671
72.351
72.032
73.50
73.00
72.50
72.00
71.50
71.00
ppm (t1)
150
100
50
0
ppm (t1)