Electronic Supplementary Information (ESI)

Copper-Triggered Three-Component Reaction of CF_3CHN_2, Nitriles, and Aldehydes: Highly Diastereoselective Synthesis of CF_3-Substituted Oxazolines and Vicinal Amino Alcohols

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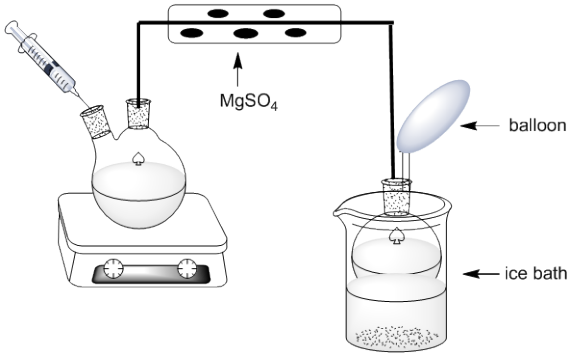
General information:

^{1}H, ^{13}C and ^{19}F NMR were recorded on a Bruker AVANCE III 400 M or Bruker AVANCE III 600 M spectrometer. Chemical shifts were reported in ppm from the solvent resonance as the internal standard ($CDCl_3$: δ_H = 7.26 ppm, δ_C = 77.16 ppm; DMSO-d_6: δ_H = 2.50 ppm, δ_C = 39.52 ppm). Multiplicity was indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (doublet of doublets), dt (doublet of triplets), dq (doublet of quartets). Coupling constants were reported in Hertz (Hz). High resolution mass spectrometry (HRMS) spectra were obtained on a Bruker miorOTOF-QII instrument. IR spectra were recorded on an AVATAR 360 FT-IR spectrometer. Melting points (MP) were measured on a WRS-1A digital melting point apparatus and are uncorrected. X-ray structural analysis was conducted on the XtaLAB mini instrument.

Materials: Tetrahydrofuran (THF) was distilled from sodium/benzophenone prior to use. All purchased reagents were used without further purification unless otherwise noted. Analytical thin layer chromatography was performed on 0.20 mm Qingdao Haiyang silica gel plates. Silica gel (200-300 mesh) (from Qingdao Haiyang Chem. Company, Ltd.) was used for flash chromatography. Standard reagents and solvents were purified according to known procedures.

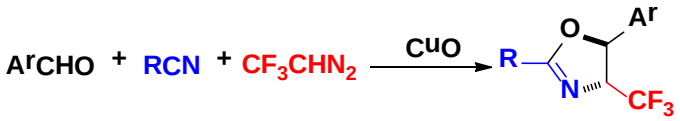
2,2,2-Trifluorodiazoethane (N_2CHCF_3) in nitrile was prepared as flows:



As shown in the figure: A solution of $NaNO_2$ (6.1 g) in 15 mL water was added slowly to the stirring solution of trifluoroethylamine hydrochloride (10.8 g) in 25 mL water at room temperature. And then the rapidly generated yellow gas was gradually blown off through a drying tube ($MgSO_4$) into a gas absorber containing 100 mL anhydrous solvent equipped with an ice bath. After about 2 hours later, there would be no gas bubbling any more. Then the apparatus was removed carefully. Finally the concentration of the stock solution was determined by ^{19}F-NMR analysis with dispersion method.

General procedures

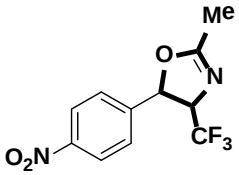
General procedure for the synthesis of the CF_3-substituted oxazolines:



1 2

A 10 mL sealed tube backfilled with argon was added CuO (0.04 mmol, 0.20 equiv), aldehyde (0.2 mmol, 1.0 equiv), and CF_3CHN_2 in nitrile (0.2 M, 2.0 equiv), then the reaction mixture was conducted at room temperature for 12 h. After the reaction was completed, the excess nitrile was evaporated under reduced pressure, the residue was chromatographed on silica gel (petroleum ether / ethyl acetate = 20 / 1) to afford the pure product **2**.

2-Methyl-5-(4-nitrophenyl)-4-(trifluoromethyl)-4,5-dihydrooxazole (2a):



43.9 mg; 80% yield; > 99:1 dr; light yellow solid; Mp: 82 – 84 ºC.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.28 (d, *J* = 8.3 Hz, 2H), 7.47 (d, *J* = 8.2 Hz, 2H), 5.61 (d, *J* = 6.6 Hz, 1H), 4.44 – 4.37 (m, 1H), 2.23 (s, 3H).

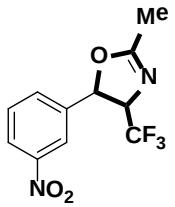
^{13}C NMR (150 MHz, $CDCl_3$): δ 169.45, 148.28, 145.57, 126.23, 124.57, 124.35 (q, *J* = 277.7 Hz), 79.64, 76.30 (q, *J* = 29.8 Hz), 14.14.

^{19}F NMR (565 MHz, $CDCl_3$): δ -75.77 (d, *J* = 6.9 Hz).

IR (KBr): ν: 2924, 2854, 1671, 1606, 1524, 1387, 1350, 1274, 1220, 1169, 1131, 997, 897, 840, 719, 504 cm^{-1}.

HRMS (ESI): found: m/z 273.0493 $[M-H]^-$; calcd. for $C_{11}H_9F_3N_2O_3$-H 273.0493.

2-Methyl-5-(3-nitrophenyl)-4-(trifluoromethyl)-4,5-dihydrooxazole (2b):



38.9 mg; 71% yield; > 99:1 dr; light yellow solid; Mp: 87 – 89 ºC.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.15 (m, 1H), 8.07 (s, 1H), 7.55 (d, *J* = 4.8 Hz, 2H), 5.53 (d, *J* = 6.7 Hz, 1H), 4.39 – 4.33 (m, 1H), 2.15 (s, 3H).

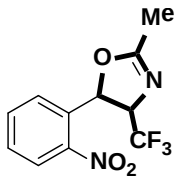
^{13}C NMR (150 MHz, $CDCl_3$): δ 169.38, 148.79, 140.80, 131.35, 130.49, 124.39 (q, *J* = 277.5 Hz), 123.98, 120.40, 79.57, 76.27 (q, *J* = 30.0 Hz), 13.99.

^{19}F NMR (565 MHz, $CDCl_3$): δ -75.82 (d, *J* = 6.8 Hz).

IR (KBr): ν: 2926, 2855, 1670, 1530, 1386, 1352, 1312, 1267, 1225, 1167, 1088, 927, 873, 831, 665, 516 cm^{-1}.

HRMS (ESI): found: m/z 273.0494 $[M-H]^-$; calcd. for $C_{11}H_9F_3N_2O_3$-H 273.0493.

2-Methyl-5-(2-nitrophenyl)-4-(trifluoromethyl)-4,5-dihydrooxazole (2c):



46.0 mg; 84% yield; > 99:1 dr; light yellow solid; Mp: 77 – 79 ºC.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.95 (d, *J* = 8.1 Hz, 1H), 7.68 (t, *J* = 7.6 Hz, 1H), 7.56 (t, *J* = 7.8 Hz, 1H), 7.39 (d, *J* = 7.8 Hz, 1H), 6.06 (d, *J* = 6.7 Hz, 1H), 4.61 (p, *J* = 6.5 Hz, 1H), 2.17 (s, 3H).

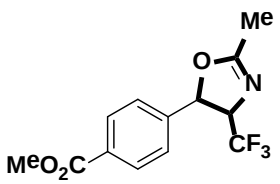
^{13}C NMR (151 MHz, $CDCl_3$): δ 169.51, 148.08, 133.77, 132.52, 130.24, 128.46, 124.35 (q, *J* = 276.0 Hz), 125.28, 77.23, 75.74 (q, *J* = 30.0 Hz), 13.87.

^{19}F NMR (565 MHz, $CDCl_3$): δ -75.27 (d, *J* = 6.9 Hz).

IR (KBr): ν: 2922, 2853, 1673, 1610, 1533, 1438, 1354, 1267, 1218, 1172, 1131, 1086, 983, 919, 786, 744, 627, 511 cm^{-1}.

HRMS (ESI): found: m/z 297.0459 $[M+Na]^+$; calcd. for $C_{11}H_9F_3N_2O_3$+Na 297.0457.

Methyl 4-(2-methyl-4-(trifluoromethyl)-4,5-dihydrooxazol-5-yl)benzoate (2d):



42.0 mg; 73% yield; > 99:1 dr; light yellow solid; Mp: 52 – 54 ºC.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.04 (d, *J* = 8.1 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 2H), 5.53 (d, *J* = 6.6 Hz, 1H), 4.41 – 4.35 (m, 1H), 3.90 (s, 3H), 2.17 (s, 3H).

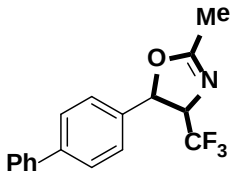
^{13}C NMR (150 MHz, $CDCl_3$): δ 169.41, 166.45, 143.48, 130.89, 130.50, 125.25, 124.53 (q, *J* = 277.5 Hz), 80.26, 76.22 (q, *J* = 30.0 Hz), 52.36, 14.01.

^{19}F NMR (565 MHz, $CDCl_3$): δ -75.94 (d, *J* = 6.9 Hz).

IR (KBr): ν: 2955, 2851, 1725, 1671, 1612, 1437, 1385, 1279, 1221, 1170, 1130, 994, 919, 851, 706, 672 cm^{-1}.

HRMS (ESI): found: m/z 310.0669 $[M+Na]^+$; calcd. for $C_{13}H_{12}F_3NO_3$+Na 310.0661.

5-([1,1'-Biphenyl]-4-yl)-2-methyl-4-(trifluoromethyl)-4,5-dihydrooxazole (2e):



47.0 mg; 77% yield; > 99:1 dr; white solid; Mp: 75 – 77 ºC.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.61 (d, *J* = 8.1 Hz, 2H), 7.57 (d, *J* = 7.5 Hz, 2H), 7.44 (t, *J* = 7.5 Hz, 2H), 7.35 (m, 3H), 5.54 (d, *J* = 6.6 Hz, 1H), 4.48 (m, 1H), 2.18 (s, 3H).

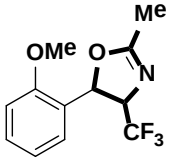
^{13}C NMR (150 MHz, $CDCl_3$): δ 169.52, 142.22, 140.40, 137.63, 129.03, 127.99, 127.85, 127.27, 125.99, 124.75 (q, *J* = 277.5 Hz), 80.82, 76.15 (q, *J* = 28.5 Hz), 14.13.

^{19}F NMR (565 MHz, $CDCl_3$): δ -75.87 (d, *J* = 7.1 Hz).

IR (KBr): ν: 2966, 2855, 1668, 1605, 1517, 1489, 1385, 1269, 1219, 1167, 1129, 1080, 991, 891, 832, 697, 504 cm^{-1}.

HRMS (ESI): found: m/z 328.0917 $[M+Na]^+$; calcd. for $C_{17}H_{14}F_3NO$+Na 328.0920.

5-(2-Methoxyphenyl)-2-methyl-4-(trifluoromethyl)-4,5-dihydrooxazole (2f):



37.9 mg; 73% yield; > 99:1 dr; light yellow solid; Mp: 188 – 191 ºC.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.27 (t, *J* = 7.4 Hz, 1H), 7.10 (d, *J* = 7.1 Hz, 1H), 6.89 (t, *J* = 7.2 Hz, 1H), 6.85 (d, *J* = 8.1 Hz, 1H), 5.62 (d, *J* = 5.9 Hz, 1H), 4.44 – 4.37 (m, 1H), 3.76 (s, 3H), 2.06

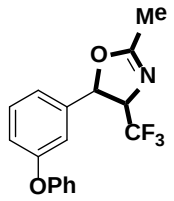
(s, 3H); **^{13}C NMR (150 MHz, $CDCl_3$):** δ 169.22, 157.01, 130.57, 127.66, 126.14, 124.99 (q, *J* = 277.5 Hz), 120.86, 111.16, 78.01, 74.50 (q, *J* = 30.0 Hz), 55.50, 14.05.

^{19}F NMR (565 MHz, $CDCl_3$): δ -76.07 (d, *J* = 6.9 Hz).

IR (KBr): ν: 2926, 1800, 1673, 1590, 1516, 1374, 1261, 1042, 939, 820, 681, 549, 469 cm^{-1}.

HRMS (ESI): found: m/z 260.0893 $[M+H]^+$; calcd. for $C_{12}H_{12}F_3NO_2$+H 260.0893.

2-Methyl-5-(3-phenoxyphenyl)-4-(trifluoromethyl)-4,5-dihydrooxazole (2g):



41.8 mg; 65% yield; > 99:1 dr; light yellow liquid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.34 (m, 3H), 7.13 (t, *J* = 7.4 Hz, 1H), 7.00 (m, 3H), 6.95 (m, 2H), 5.47 (d, *J* = 6.6 Hz, 1H), 4.43 (p, *J* = 6.7 Hz, 1H), 2.14 (s, 3H).

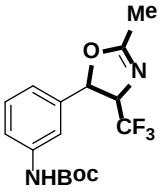
^{13}C NMR (150 MHz, $CDCl_3$): δ 169.41, 158.22, 156.66, 140.80, 130.69, 130.03, 124.63 (q, *J* = 277.5 Hz), 123.94, 119.85, 119.30, 118.89, 115.66, 80.48, 76.19 (q, *J* = 30.0 Hz), 14.03.

^{19}F NMR (565 MHz, $CDCl_3$): δ -75.91 (d, *J* = 7.1 Hz).

IR (KBr): ν: 2934, 1668, 1585, 1487, 1446, 1381, 1258, 1219, 1169, 1131, 995, 751, 692, 560, 468 cm^{-1}.

HRMS (ESI): found: m/z 322.1046 $[M+H]^+$; calcd. for $C_{17}H_{14}F_3NO_2$+Na 322.1049.

Tert-butyl(3-(2-methyl-4-(trifluoromethyl)-4,5-dihydrooxazol-5-yl)phenyl)carbamate (2h):



31.0 mg; 45% yield; > 99:1 dr; light yellow solid; Mp: 98 – 100 ºC.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.25 (m, 3H), 6.85 (d, *J* = 6.4 Hz, 1H), 6.67 (s, 1H), 5.38 (d, *J* = 5.8 Hz, 1H), 4.36 (m, 1H), 2.09 (s, 3H), 1.44 (s, 9H).

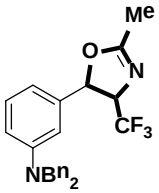
^{13}C NMR (150 MHz, $CDCl_3$): δ 169.49, 152.76, 139.67, 139.45, 129.97, 124.69 (q, *J* = 277.5 Hz), 119.76, 119.10, 115.42, 80.99, 80.84, 76.07 (q, *J* = 30.0 Hz), 28.45, 14.13.

^{19}F NMR (565 MHz, $CDCl_3$): δ -75.89 (d, *J* = 7.1 Hz).

IR (KBr): ν: 2918, 2550, 1728, 1667, 1595, 1496, 1446, 1368, 1276, 1222, 1161, 1132, 789, 698, 527 cm^{-1}.

HRMS (ESI): found: m/z 367.1245 $[M+Na]^+$; calcd. for $C_{16}H_{19}F_2N_2O_3$+Na 367.1240.

***N*,*N*-Dibenzyl-3-(2-methyl-4-(trifluoromethyl)-4,5-dihydrooxazol-5-yl)aniline (2i):**



60.3 mg; 71% yield; > 99:1 dr; light yellow solid; Mp: 89 – 91 ºC.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.32 (t, *J* = 7.5 Hz, 4H), 7.24 (m, 6H), 7.16 (t, *J* = 7.9 Hz, 1H), 6.71 (dd, *J* = 8.3, 2.0 Hz, 1H), 6.57 (d, *J* = 7.5 Hz, 1H), 6.54 (s, 1H), 5.33 (d, *J* = 6.3 Hz, 1H), 4.65 (s, 4H), 4.34 (p, *J* = 6.5 Hz, 1H), 1.99 (s, 3H).

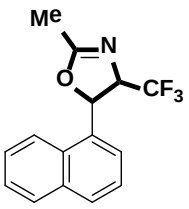
^{13}C NMR (150 MHz, $CDCl_3$): δ 169.38, 149.69, 139.90, 138.27, 130.13, 128.89, 127.22, 126.69, 124.71 (q, *J* = 277.5 Hz), 113.39, 113.15, 109.26, 81.17, 76.00 (q, *J* = 30.0 Hz), 54.83, 13.95.

^{19}F NMR (565 MHz, $CDCl_3$): δ -76.01 (d, *J* = 7.2 Hz).

IR (KBr): ν: 2926, 2858, 1668, 1603, 1499, 1451, 1357, 1273, 1219, 1166, 1128, 958, 885, 775, 676, 641, 524, 421 cm^{-1}.

HRMS (ESI): found: m/z 447.1657 $[M+Na]^+$; calcd. for $C_{25}H_{23}F_3N_2O$+Na 447.1655.

2-Methyl-5-(naphthalen-1-yl)-4-(trifluoromethyl)-4,5-dihydrooxazole (2j):



45.2 mg; 81% yield; > 99:1 dr; brown solid; Mp: 54 – 56 ºC.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.81 – 7.78 (m, 2H), 7.76 (d, *J* = 8.2 Hz, 1H), 7.47 – 7.41 (m, 2H), 7.36 (t, *J* = 7.7 Hz, 1H), 7.30 (d, *J* = 7.0 Hz, 1H), 6.07 (d, *J* = 6.5 Hz, 1H), 4.55 (p, *J* = 6.5 Hz, 1H), 2.13 (s, 3H).

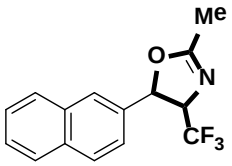
^{13}C NMR (151 MHz, $CDCl_3$): δ 169.82, 134.20, 133.13, 130.17, 130.03, 129.42, 127.19, 126.32, 125.37, 124.97 (q, *J* = 279.0 Hz), 124.73, 122.29, 79.36, 74.76 (q, *J* = 30.0 Hz), 14.18.

^{19}F NMR (565 MHz, $CDCl_3$): δ -75.25 (d, *J* = 6.9 Hz).

IR (KBr): ν: 2931, 2856, 1667, 1594, 1514, 1384, 1264, 1219, 1167, 1017, 973, 880, 705, 556, 523 cm^{-1}.

HRMS (ESI): found: m/z 302.0768 $[M+Na]^+$; calcd. for $C_{15}H_{12}F_3NO$+Na 302.0763.

2-Methyl-5-(naphthalen-2-yl)-4-(trifluoromethyl)-4,5-dihydrooxazole (2k):



43.0 mg; 77% yield; > 99:1 dr; light yellow solid; Mp: 43 – 45 ºC.

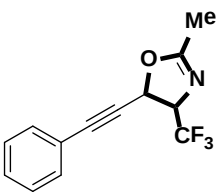
^{1}H NMR (600 MHz, $CDCl_3$): δ 7.85 (d, *J* = 8.5 Hz, 1H), 7.83 – 7.79 (m, 2H), 7.71 (s, 1H), 7.51 – 7.47 (m, 2H), 7.30 (dd, *J* = 8.5, 1.3 Hz, 1H), 5.65 (d, *J* = 6.7 Hz, 1H), 4.52 (p, *J* = 6.7 Hz, 1H), 2.20 (s, 3H). **^{13}C NMR (150 MHz, $CDCl_3$):** δ 169.52, 135.83, 133.52, 133.17, 129.50, 128.19, 127.90, 126.90, 126.86, 125.00, 124.76 (q, *J* = 277.5 Hz), 122.48, 81.15, 76.07 (q, *J* = 30.0 Hz), 14.10.

^{19}F NMR (565 MHz, $CDCl_3$): δ -75.79 (d, *J* = 6.6 Hz).

IR (KBr): ν: 2935, 2856, 1667, 1603, 1435, 1380, 1273, 1221, 1168, 1130, 995, 856, 711, 646, 517, 477 cm^{-1}.

HRMS (ESI): found: m/z 302.0770 $[M+Na]^+$; calcd. for $C_{15}H_{12}F_3NO$ +Na 302.0763.

2-Methyl-5-(phenylethynyl)-4-(trifluoromethyl)-4,5-dihydrooxazole (2l):



30.4 mg; 60% yield; 92:8 dr; light yellow liquid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.46 (d, *J* = 7.0 Hz, 2H), 7.37 (m, 1H), 7.33 (m, 2H), 5.34 (d, *J* = 6.7 Hz, 1H), 4.69 (p, *J* = 6.7 Hz, 1H), 2.11 (s, 3H).

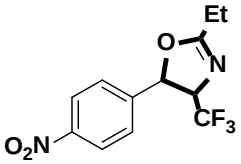
^{13}C NMR (150 MHz, $CDCl_3$): δ 169.06, 132.11, 129.57, 128.59, 124.22 (q, *J* = 277.5 Hz), 121.29, 88.51, 83.87, 75.51 (q, *J* = 30.0 Hz), 69.47 (q, *J* = 3.0 Hz), 14.14.

^{19}F NMR (565 MHz, $CDCl_3$): δ -76.02 (d, *J* = 7.0 Hz), -76.17 (d, *J* = 6.9 Hz).

IR (KBr): ν: 2964, 2871, 1668, 1495, 1378, 1264, 1223, 1176, 1136, 1012, 957, 913, 756, 691, 579, 527 cm^{-1}.

HRMS (ESI): found: m/z 276.0605 $[M+Na]^+$; calcd. for $C_{13}H_{10}F_3NO$+Na 276.0607.

2-Ethyl-5-(4-nitrophenyl)-4-(trifluoromethyl)-4,5-dihydrooxazole (2m):



43.8 mg; 76% yield; > 99:1 dr; light yellow solid; Mp: 133 – 135 ºC.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.26 (d, *J* = 8.6 Hz, 2H), 7.45 (d, *J* = 8.6 Hz, 2H), 5.59 (d, *J* = 6.6 Hz, 1H), 4.40 (p, *J* = 6.8 Hz, 1H), 2.52 (q, *J* = 7.5 Hz, 2H), 1.30 (t, *J* = 7.6 Hz, 3H).

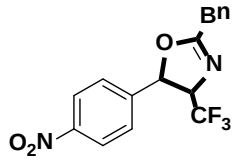
^{13}C NMR (150 MHz, $CDCl_3$): δ 173.43, 148.33, 145.80, 126.17, 124.53, 124.43 (q, *J* = 277.5 Hz), 79.40, 76.23 (q, *J* = 30.0 Hz), 21.71, 10.34.

^{19}F NMR (565 MHz, $CDCl_3$): δ -75.90 (d, *J* = 6.9 Hz).

IR (KBr): ν: 2927, 1665, 1605, 1525, 1349, 1273, 1173, 1734, 1034, 893, 842, 714, 660, 507 cm^{-1}.

HRMS (ESI): found: m/z 289.0798 $[M+H]^+$; calcd. for $C_{12}H_{11}F_3N_2O_3$+H 289.0795.

2-Benzyl-5-(4-nitrophenyl)-4-(trifluoromethyl)-4,5-dihydrooxazole (2n):



44.8 mg; 64% yield; > 99:1 dr; light yellow solid; Mp: 125 – 128 ºC.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.15 (d, *J* = 8.7 Hz, 2H), 7.39 – 7.31 (m, 5H), 7.21 (d, *J* = 8.6 Hz, 2H), 5.61 (d, *J* = 6.3 Hz, 1H), 4.41 (p, *J* = 6.7 Hz, 1H), 3.87 (d, *J* = 14.6 Hz, 1H), 3.79 (d, *J* = 14.6

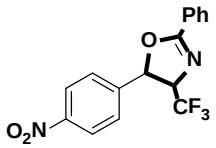
Hz, 1H). **^{13}C NMR (150 MHz, $CDCl_3$):** δ 170.86, 148.22, 145.58, 133.93, 129.13, 129.04, 127.81, 125.94, 124.43, 124.35 (q, *J* = 279.0 Hz), 79.61, 76.25 (q, *J* = 28.5 Hz), 34.89.

^{19}F NMR (565 MHz, $CDCl_3$): δ -75.78 (d, *J* = 7.0 Hz).

IR (KBr): ν: 2932, 2310, 1664, 1603, 1524, 1349, 1273, 1228, 1172, 1130, 996, 897, 840, 723, 452 cm^{-1}.

HRMS (ESI): found: m/z 349.0811 $[M-H]^-$; calcd. for $C_{17}H_{13}F_3N_2O_3$-H 349.0806.

5-(4-Nitrophenyl)-2-phenyl-4-(trifluoromethyl)-4,5-dihydrooxazole (2o):



57.8 mg; 86% yield; 95:5 dr; light yellow liquid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.28 (d, *J* = 8.5 Hz, 2H), 8.09 (d, *J* = 7.7 Hz, 2H), 7.60 (t, *J* = 7.3 Hz, 1H), 7.53 (d, *J* = 8.5 Hz, 2H), 7.49 (t, *J* = 7.7 Hz, 2H), 5.81 (d, *J* = 6.6 Hz, 1H), 4.63 (p, *J* = 6.7 Hz, 1H).

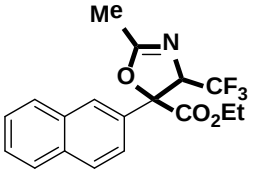
^{13}C NMR (150 MHz, $CDCl_3$): δ 167.55, 148.42, 145.74, 133.04, 129.11, 128.88, 126.33, 125.90, 124.60, 124.53 (q, *J* = 277.5 Hz), 79.77, (q, *J* = 1.5 Hz), 76.71 (q, *J* = 30.0 Hz).

^{19}F NMR (565 MHz, $CDCl_3$): δ -75.42 (d, *J* = 6.9 Hz), -80.34 (d, *J* = 4.5 Hz).

IR (KBr): ν: 2918, 2849, 1648, 1607, 1525, 1451, 1387, 1347, 1272, 1236, 1171, 1070, 1025, 985, 840, 776, 694, 513 cm^{-1}.

HRMS (ESI): found: m/z 337.0792 $[M+H]^+$; calcd. for $C_{16}H_{11}F_3N_2O_3$+H 337.0795.

Ethyl 2-methyl-5-(naphthalen-2-yl)-4-(trifluoromethyl)-4,5-dihydrooxazole-5-carboxylate (4):



49.9 mg; 71% yield; 80:20 dr; light yellow solid; Mp: 53 – 54 ºC.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.02 (s, 1H), 7.91 (d, *J* = 8.7 Hz, 1H), 7.89 – 7.84 (m, 2H), 7.68 (d, *J* = 8.2 Hz, 1H), 7.54 (m, 2H), 5.04 (q, *J* = 6.0 Hz, 1H), 4.28 – 4.16 (m, 2H), 2.29 (s, 3H), 1.24 (t, *J* = 7.1 Hz, 3H).

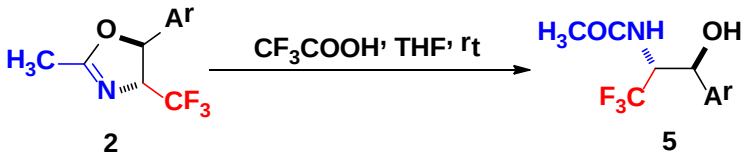
^{13}C NMR (150 MHz, $CDCl_3$): δ 168.26, 167.18, 135.80, 133.34, 132.81, 128.86, 128.57, 127.77, 127.18, 126.92, 124.68, 123.76 (q, *J* = 277.5 Hz), 123.40, 88.58, 78.87 (q, *J* = 30.0 Hz), 63.07, 14.30, 13.75.

^{19}F NMR (565 MHz, $CDCl_3$): δ -70.05 (d, *J* = 7.6 Hz).

IR (KBr): ν: 2933, 1749, 1682, 1596, 1509, 1438, 1369, 1283, 1243, 1170, 1137, 994, 946, 895, 815, 753, 521, 476 cm^{-1}.

HRMS (ESI): found: m/z 374.0979 $[M+Na]^+$; calcd. for $C_{18}H_{16}F_3NO_3$+Na 374.0974.

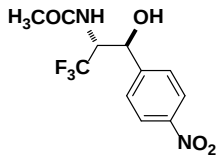
General procedure for the ring opening of the product (5):



2 5

To a solution of **2** (0.4 mmol) in THF was added CF_3COOH (120 μL, 4.0 equiv). The reaction mixture was stirred overnight at room temperature. After completion of the reaction, the mixture was quenched with saturated aqueous $NaHCO_3$ and extracted with EtOAc (10 mL) for three times. The combined organic extracts were washed with brine, and dried over Na_2SO_4. Concentration under vacuum gave the crude product, which was purified by column chromatography on silica gel to give the ring opening product **5**.

***N*-(1,1,1-Trifluoro-3-hydroxy-3-(4-nitrophenyl)propan-2-yl)acetamide (5a):**



113.4 mg; 97% yield; > 99:1 dr; white solid; Mp: 179 – 181 ºC.

^{1}H NMR (600 MHz, DMSO): δ 8.44 (d, *J* = 9.7 Hz, 1H), 8.18 (d, *J* = 8.5 Hz, 2H), 7.72 (d, *J* = 8.3 Hz, 2H), 6.30 (d, *J* = 3.9 Hz, 1H), 5.27 (s, 1H), 4.86 – 4.75 (m, 1H), 1.76 (s, 3H).

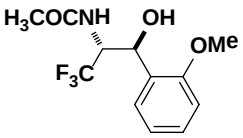
^{13}C NMR (150 MHz, DMSO): δ = 169.80, 149.22, 146.87, 127.58, 124.89 (q, *J* = 282.0 Hz), 122.84, 68.30 (q, *J* = 9.0 Hz), 54.22 (q, *J* = 28.5 Hz), 21.75.

^{19}F NMR (565 MHz, DMSO): δ -65.89 (d, *J* = 8.3 Hz).

IR (KBr): ν: 2917, 2849, 1743, 1661, 1597, 1516, 1341, 1252, 1174, 1128, 1077, 846, 718, 557, 474 cm^{-1}.

HRMS (ESI): found: m/z 291.0601 $[M-H]^-$; calcd. for $C_{11}H_{11}F_3N_2O_4$-H 291.0598.

***N*-(1,1,1-Trifluoro-3-hydroxy-3-(2-methoxyphenyl)propan-2-yl)acetamide (5b):**



101.0 mg; 91% yield; > 99:1 dr; white solid; Mp: 190 – 192 ºC.

^{1}H NMR (400 MHz, DMSO): δ 8.31 (d, *J* = 9.8 Hz, 1H), 7.46 (d, *J* = 7.2 Hz, 1H), 7.23 (t, *J* = 7.4 Hz, 1H), 6.94 (m, 2H), 5.91 (d, *J* = 5.1 Hz, 1H), 5.39 (d, *J* = 4.5 Hz, 1H), 4.70 (m, 1H), 3.81 (s, 3H), 1.74 (s, 3H).

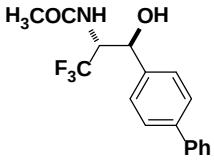
^{13}C NMR (100 MHz, DMSO): δ 170.06, 155.19, 129.32, 128.56, 127.18, 125.5 (q, *J* = 282.0 Hz), 120.00, 110.33, 63.37, 55.57, 52.77 (q, *J* = 27.0 Hz), 21.96.

^{19}F NMR (376 MHz, DMSO): δ -71.25 (d, *J* = 8.7 Hz).

IR (KBr): ν: 3734, 3428, 3284, 2930, 1667, 1600, 1524, 1433, 1385, 1252, 1142, 1024, 971, 752, 618, 557 cm^{-1}.

HRMS (ESI): found: m/z 300.0825 $[M+Na]^+$; calcd. for $C_{12}H_{14}F_3NO_3$+Na 300.0818.

***N*-(3-([1,1'-Biphenyl]-4-yl)-1,1,1-trifluoro-3-hydroxypropan-2-yl)acetamide (5c):**



121.5 mg; 94% yield; > 99:1 dr; white solid; Mp: 181 – 183 ºC.

^{1}H NMR (400 MHz, DMSO): δ 8.50 (d, *J* = 9.6 Hz, 1H), 7.66 (m, 7.8 Hz, 4H), 7.53 (d, *J* = 7.9 Hz, 2H), 7.46 (t, *J* = 7.4 Hz, 2H), 7.36 (t, *J* = 7.1 Hz, 1H), 6.10 (s, 1H), 5.18 (s, 1H), 4.84 – 4.70 (m, 1H), 1.84 (s, 3H).

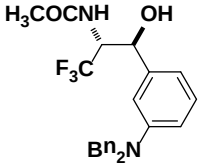
^{13}C NMR (100 MHz, DMSO): δ 170.06, 140.91, 139.88, 139.21, 129.01, 127.48, 126.99, 126.66, 126.17, 125.27 (q, *J* = 282.0 Hz), 68.69, 54.75 (q, *J* = 27.0 Hz), 22.07

^{19}F NMR (376 MHz, DMSO): δ -70.78 (d, *J* = 8.3 Hz).

IR (KBr): ν: 3732, 3285, 3033, 2891, 1669, 1519, 1374, 1261, 1173, 1132, 1073, 882, 832, 741, 692, 556 cm^{-1}.

HRMS (ESI): found: m/z 322.1061 $[M-H]^-$; calcd. for $C_{17}H_{16}F_3NO_2$-H 322.1060.

***N*-(3-(3-(Dibenzylamino)phenyl)-1,1,1-trifluoro-3-hydroxypropan-2-yl)acetamide (5d):**



168.1 mg; 95% yield; > 99:1 dr; white solid; Mp: 43 – 45 ºC.

^{1}H NMR (400 MHz, DMSO): δ 8.37 (d, *J* = 9.6 Hz, 1H), 7.33 (m, 4H), 7.29 – 7.22 (m, 6H), 7.06 – 6.98 (m, 2H), 6.67 (d, *J* = 7.4 Hz, 1H), 6.56 (d, *J* = 6.7 Hz, 1H), 5.93 (d, *J* = 4.3 Hz, 1H), 4.99 (s, 1H), 4.71 – 4.58 (m, 5H), 1.80 (s, 3H).

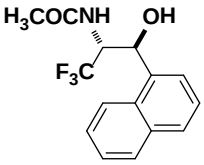
^{13}C NMR (100 MHz, DMSO): δ 169.88, 148.49, 142.58, 138.96, 128.58, 128.50, 126.85, 126.78, 125.25 (q, *J* = 282.0 Hz), 114.43, 111.59, 110.59, 69.19, 54.87 (q, *J* = 28.0 Hz), 22.03.

^{19}F NMR (376 MHz, DMSO): δ -71.00 (d, *J* = 8.4 Hz).

IR (KBr): ν: 3735, 3301, 3032, 2914, 1670, 1601, 1499, 1449, 1367, 1257, 1132, 1034, 965, 733, 697, 562 cm^{-1}.

HRMS (ESI): found: m/z 441.1792 $[M-H]^-$; calcd. for $C_{25}H_{25}F_3N_2O_2$-H 441.1795.

***N*-(1,1,1-Trifluoro-3-hydroxy-3-(naphthalen-1-yl)propan-2-yl)acetamide (5e):**



115.3 mg; 97% yield; > 99:1 dr; white solid; Mp: 232 – 234 ºC.

^{1}H NMR (400 MHz, DMSO): δ 8.55 (d, *J* = 9.6 Hz, 1H), 8.00 (m, 2H), 7.87 (d, *J* = 8.1 Hz, 1H), 7.77 (d, *J* = 7.1 Hz, 1H), 7.64 (t, *J* = 7.3 Hz, 1H), 7.55 (m, 2H), 6.25 (d, *J* = 4.4 Hz, 1H), 5.94 (d, *J* = 3.9 Hz, 1H), 4.87 – 4.76 (m, 1H), 1.79 (s, 3H).

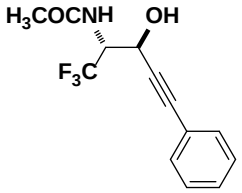
^{13}C NMR (100 MHz, DMSO): δ 170.44, 137.01, 133.58, 129.66, 129.54, 128.50, 127.11, 125.99, 125.83 (q, *J* = 282.0 Hz), 125.53, 124.92, 122.08, 65.44, 54.05 (q, *J* = 28.0 Hz), 22.28.

^{19}F NMR (376 MHz, DMSO): δ -71.12 (d, *J* = 8.6 Hz).

IR (KBr): ν: 3734, 3418, 3162, 3067, 2896, 1664, 1517, 1429, 1378, 1298, 1252, 1176, 1133, 1008, 774, 624, 558, cm^{-1}.

HRMS (ESI): found: m/z 320.0867 $[M+Na]^+$; calcd. for $C_{15}H_{14}F_3NO_2$+Na 320.0869.

***N*-(1,1,1-Trifluoro-3-hydroxy-5-phenylpent-4-yn-2-yl)acetamide (5f):**



97.6 mg; 90% yield; > 99:1 dr; white solid; Mp: 111 – 113 ºC.

^{1}H NMR (400 MHz, DMSO): δ 8.54 (d, *J* = 9.6 Hz, 1H), 7.38 (m, 5H), 6.24 (s, 1H), 4.96 – 4.77 (m, 2H), 1.99 (s, 3H).

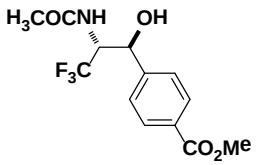
^{13}C NMR (100 MHz, DMSO): δ 170.29, 131.39, 128.92, 128.79, 124.51 (q, *J* = 284.0 Hz), 121.88, 87.92, 84.31, 59.45, 53.99 (q, *J* = 28.0 Hz), 22.31.

^{19}F NMR (376 MHz, DMSO): δ -70.22 (d, *J* = 8.3 Hz).

IR (KBr): ν: 3733, 3058, 2880, 2233, 1668, 1533, 1435, 1375, 1261, 1179, 1136, 1065, 905, 865, 765, 691, 526 cm^{-1}.

HRMS (ESI): found: m/z 270.0746 $[M-H]^-$; calcd. for $C_{13}H_{12}F_3NO_2$-H 270.0747.

Methyl 4-(2-acetamido-3,3,3-trifluoro-1-hydroxypropyl)benzoate (5g):



109.9 mg; 90% yield; > 99:1 dr; white solid; Mp: 191 – 193 ºC.

^{1}H NMR (400 MHz, DMSO): δ 8.44 (d, *J* = 9.7 Hz, 1H), 7.91 (d, *J* = 8.1 Hz, 2H), 7.57 (d, *J* = 8.1 Hz, 2H), 6.20 (d, *J* = 4.5 Hz, 1H), 5.20 (s, 1H), 4.82 – 4.68 (m, 1H), 3.83 (s, 3H), 1.75 (s, 3H).

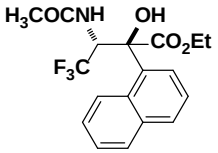
^{13}C NMR (100 MHz, DMSO): δ 169.92, 166.21, 147.08, 128.78, 126.68, 125.08 (q, *J* = 281.0 Hz), 68.62, 54.48 (q, *J* = 27.0 Hz), 52.11, 21.88.

^{19}F NMR (376 MHz, DMSO): δ -70.73 (d, *J* = 7.7 Hz).

IR (KBr): ν: 3736, 3679, 3219, 1705, 1661, 1522, 1435, 1378, 1264, 1202, 1147, 1015, 895, 850, 719, 512 cm^{-1}.

HRMS (ESI): found: m/z 304.0798 $[M-H]^-$; calcd. for $C_{13}H_{14}F_3NO_4$-H 304.0802.

Ethyl 3-acetamido-4,4,4-trifluoro-2-hydroxy-2-(naphthalen-1-yl)butanoate (5h):



133.0 mg; 90% yield; > 99:1 dr; white solid; Mp: 58 – 60 ºC.

^{1}H NMR (400 MHz, DMSO): δ 8.50 (d, *J* = 10.1 Hz, 1H), 8.14 (s, 1H), 7.88 (m, 3H), 7.65 (d, *J* = 8.7 Hz, 1H), 7.56 – 7.47 (m, 2H), 6.97 (s, 1H), 5.83 – 5.71 (m, 1H), 4.21 (q, *J* = 7.0 Hz, 2H), 1.51 (s, 3H), 1.18 (t, *J* = 7.1 Hz, 3H).

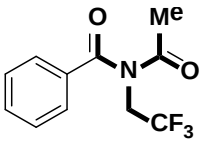
^{13}C NMR (100 MHz, DMSO): δ 171.48, 169.78, 136.33, 132.54, 132.27, 128.26, 127.46, 127.29, 126.58, 126.42, 125.25, 124.96(q, *J* = 282.0 Hz), 123.61, 78.89, 62.02, 54.85 (q, *J* = 27.0 Hz), 21.70, 13.82.

^{19}F NMR (376 MHz, DMSO): δ -67.78 (d, *J* = 7.6 Hz).

IR (KBr): ν: 3735, 3384, 3300, 2985, 1735, 1680, 1528, 1370, 1261, 1167, 1029, 862, 811, 759, 681, 578, 519 cm^{-1}.

HRMS (ESI): found: m/z 392.1084 $[M+Na]^+$; calcd. for $C_{18}H_{18}F_3NO_4$+Na 392.1080.

***N*-Acetyl-*N*-(2,2,2-trifluoroethyl)benzamide (2p):**



14.7 mg; 30% yield; light yellow liquid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, *J* = 7.5 Hz, 2H), 7.66 (t, *J* = 7.4 Hz, 1H), 7.54 (t, *J* = 7.6 Hz, 2H), 4.60 (q, *J* = 8.7 Hz, 2H), 2.07 (s, 3H).

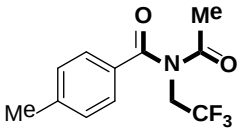
^{13}C NMR (100 MHz, $CDCl_3$): δ 173.42, 171.85, 134.93, 133.63, 129.38, 128.98, 124.06 (q, *J* = 279.0 Hz), 45.32 (q, *J* = 34.0 Hz), 26.02.

^{19}F NMR (376 MHz, $CDCl_3$): δ -70.33 (t, *J* = 8.6 Hz).

IR (KBr): ν: 3031, 2982, 1713, 1681, 1599, 1424, 1336, 1259, 1159, 1060, 935, 801, 743, 665, 612, 496 cm^{-1}.

HRMS (ESI): found: m/z 268.0553 $[M+Na]^+$; calcd. for $C_{11}H_{10}F_3NO_2$+Na 268.0556.

***N*-Acetyl-3-chloro-*N*-(2,2,2-trifluoroethyl)benzamide (2q):**



18.2 mg; 35% yield; light yellow liquid.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.60 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 7.9 Hz, 2H), 4.57 (q, *J* = 8.7 Hz, 2H), 2.44 (s, 3H), 2.03 (s, 3H).

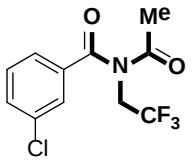
^{13}C NMR (150 MHz, $CDCl_3$): δ 173.40, 171.86, 144.91, 132.02, 130.07, 129.27, 124.08 (q, *J* = 277.5 Hz), 45.28 (q, *J* = 34.5 Hz), 25.98, 21.86.

^{19}F NMR (565 MHz, $CDCl_3$): δ -70.40 (t, *J* = 8.8 Hz).

IR (KBr): ν: 2967, 2931, 1713, 1681, 1609, 1336, 1259, 1159, 1062, 986, 794, 707, 657, 576, 496 cm^{-1}.

HRMS (ESI): found: m/z 282.0717 $[M+Na]^+$; calcd. for $C_{12}H_{12}F_3NO_2$+Na 282.0712.

***N*-Acetyl-4-methyl-*N*-(2,2,2-trifluoroethyl)benzamide (2r):**



10.1 mg; 18% yield; white solid; Mp: 53 – 55 ºC.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.76 (s, 1H), 7.69 (d, *J* = 7.9 Hz, 1H), 7.63 (d, *J* = 7.7 Hz, 1H), 7.56 (t, *J* = 7.8 Hz, 1H), 4.65 (q, *J* = 8.6 Hz, 2H), 2.20 (s, 3H).

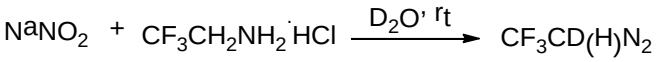
^{13}C NMR (150 MHz, $CDCl_3$): δ 172.06, 171.62, 136.50, 135.69, 133.56, 130.65, 128.83, 126.83, 123.92 (q, *J* = 277.5 Hz), 45.38 (q, *J* = 34.5 Hz), 26.01.

^{19}F NMR (565 MHz, $CDCl_3$): δ -70.33 (t, *J* = 8.6 Hz).

IR (KBr): ν: 2921, 2850, 1713, 1684, 1558, 1515, 1395, 1336, 1254, 1188, 980, 893, 745, 863 cm^{-1}.

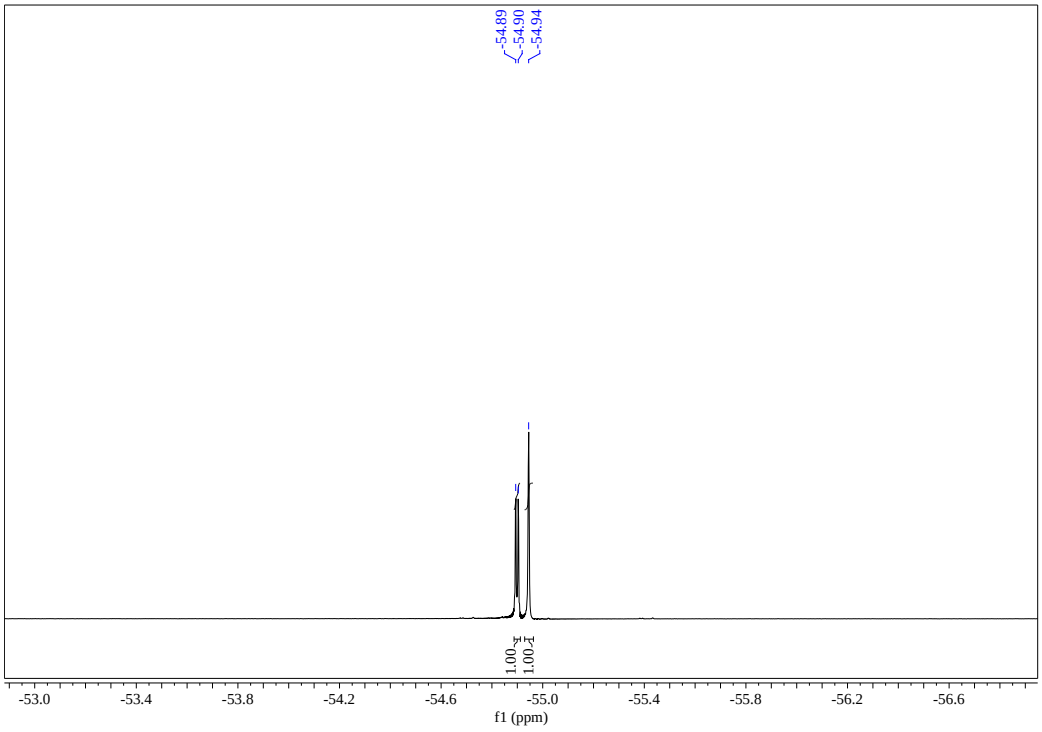
HRMS (ESI): found: m/z 302.0173 $[M+Na]^+$; calcd. for $C_{11}H_3ClF_3NO_2$+Na 302.0166.

General procedure for the synthesis of the $N_2CD(H)CF_3$:

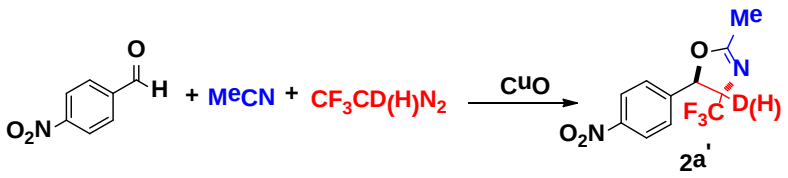


A solution of 2.0 g $NaNO_2$ in 5 mL D_2O was added slowly to the stirring solution of 3.6 g of tritluoroethylamine hydrochloride in 5 mL water at room temperature. And then the rapidly generated yellow gas was gradually blown off through a drying tube ($MgSO_4$) into a gas absorber containing 30 mL anhydrous solvent equipped with an ice bath. After about 2 hours later, there would be no gas bubbling any more. Then the apparatus was removed carefully. Finally the concentration of the stock solution was determined by ^{19}F-NMR analysis with dispersion method.

^{19}F NMR spectra of $N_2CD(H)CF_3$

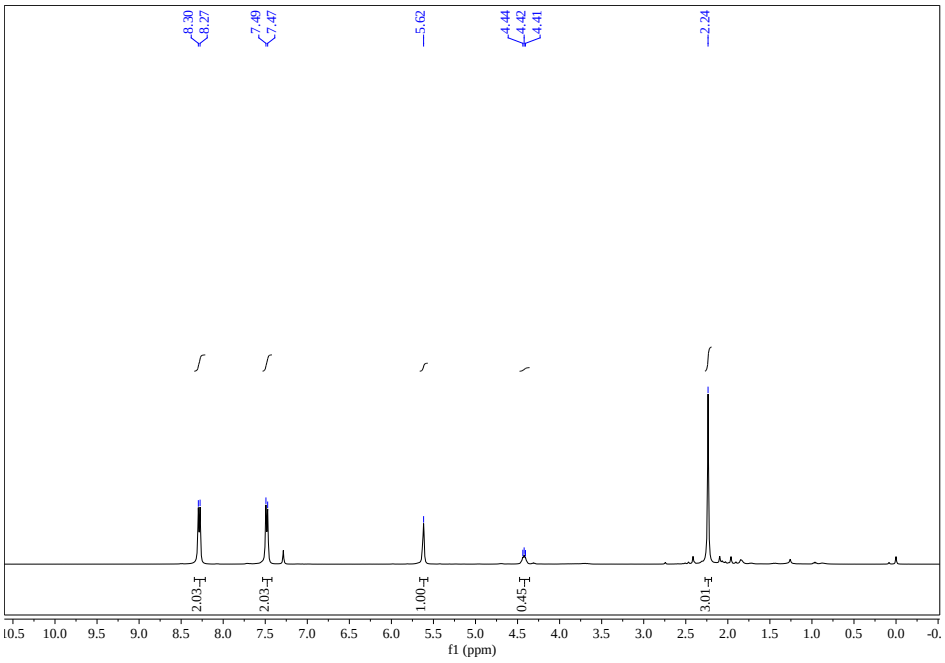


General procedure for D-labeling experiments:

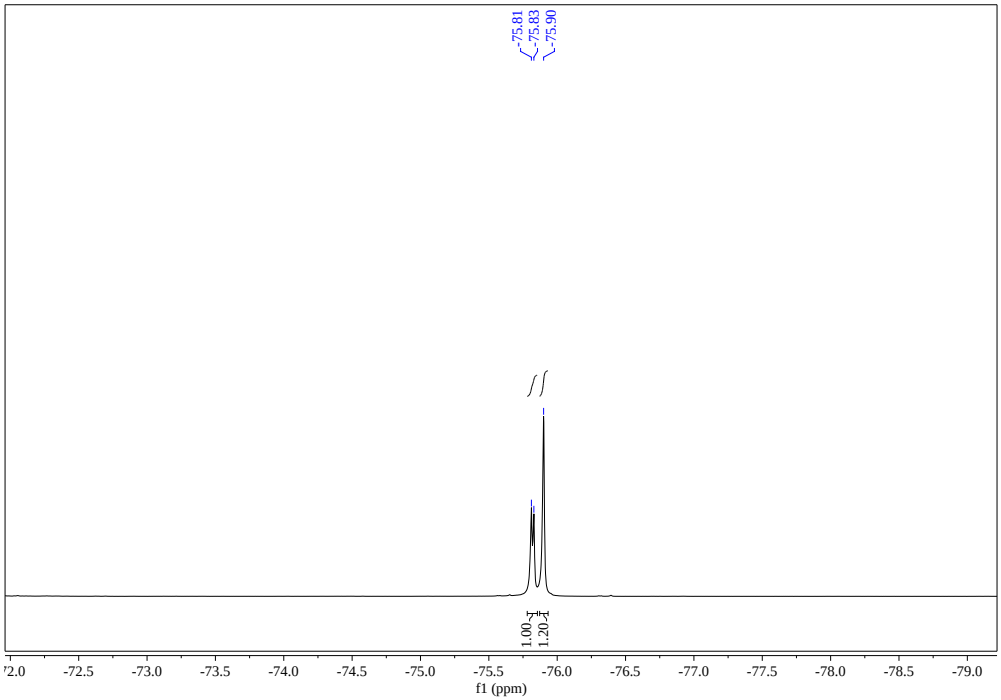


A 10 mL sealed tube backfilled with Ar was added CuO (0.04 mmol, 0.20 equiv), 4-nitrobenzaldehyde (0.2 mmol, 1.0 equiv), and $CF_3CD(H)N_2$ in acetonitrile (0.2 M, 2.0 equiv), then the reaction mixture was conducted at room temperature for 12 h. After the reaction was completed, the excess nitrile was evaporated under reduced pressure, the residue was chromatographed on silica gel (petroleum ether / AcOEt = 20/1) to afford the pure product **2a′**.

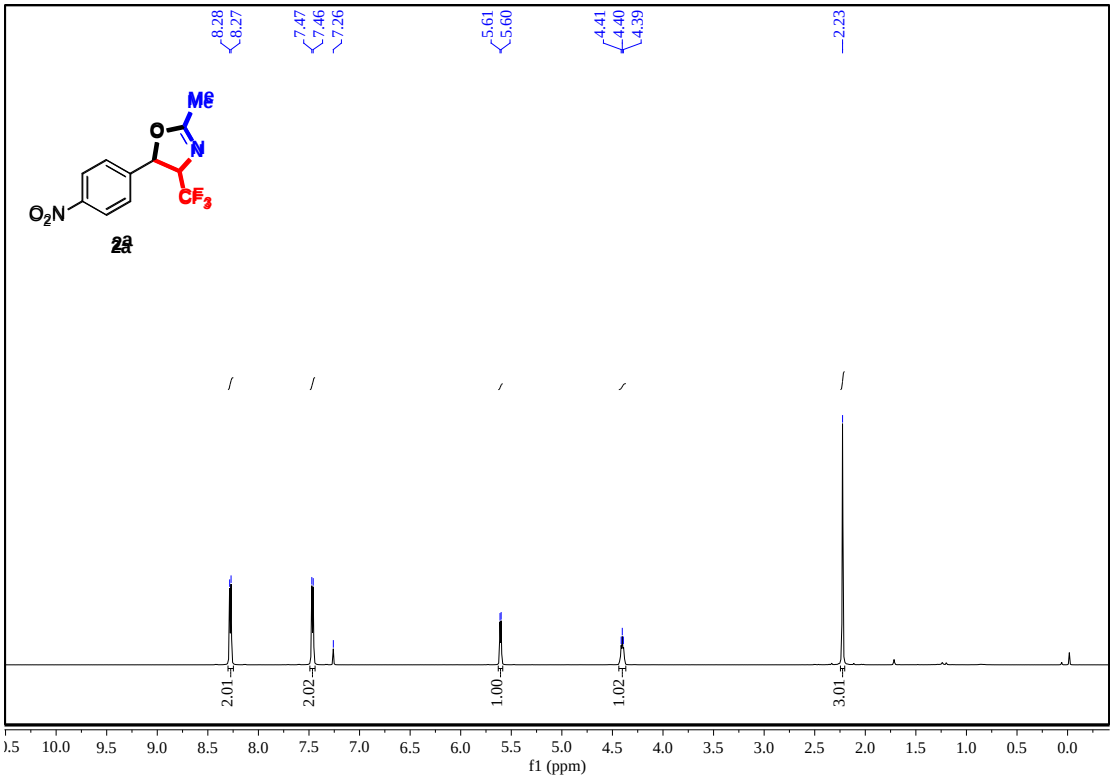
^{1}H NMR spectra of 2a′

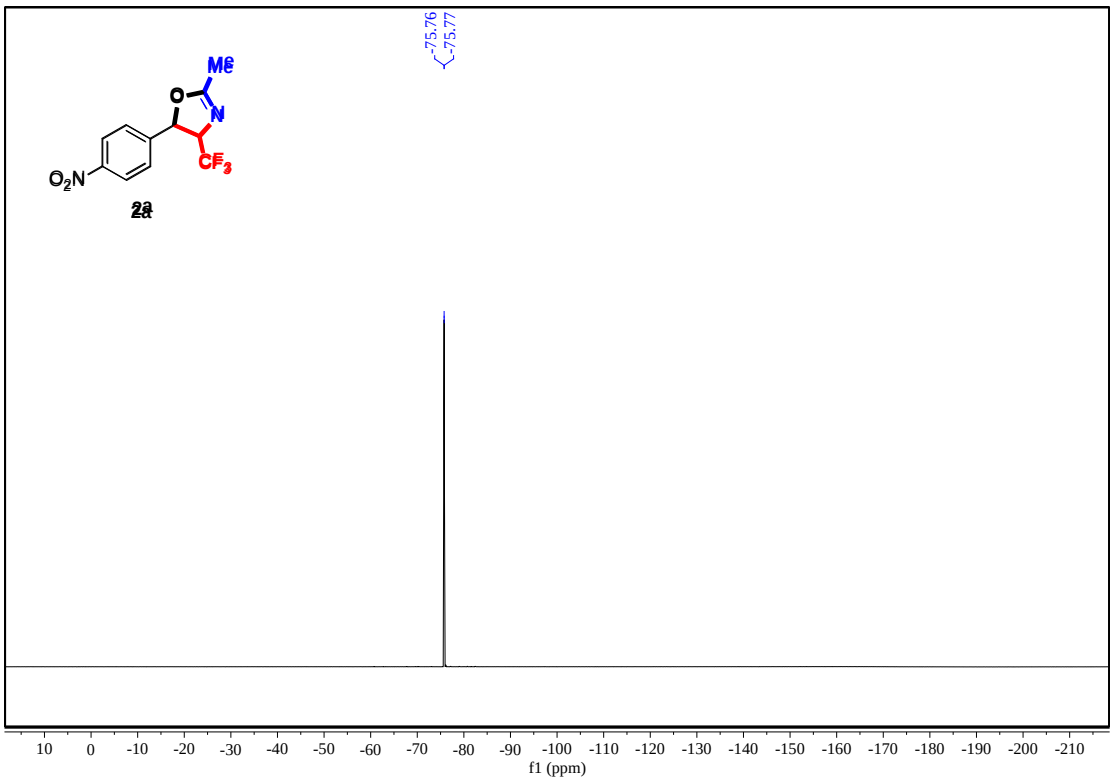


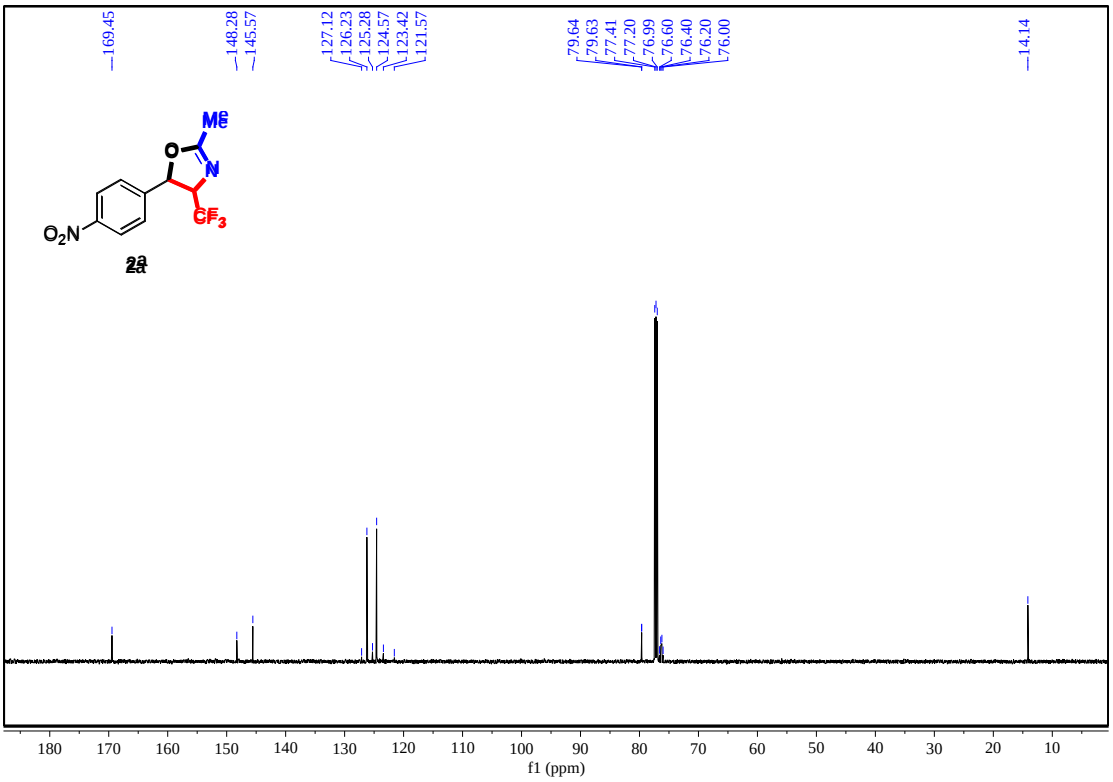
^{19}F NMR spectra of 2a′



Copies of NMR spectra of the products:






169.45
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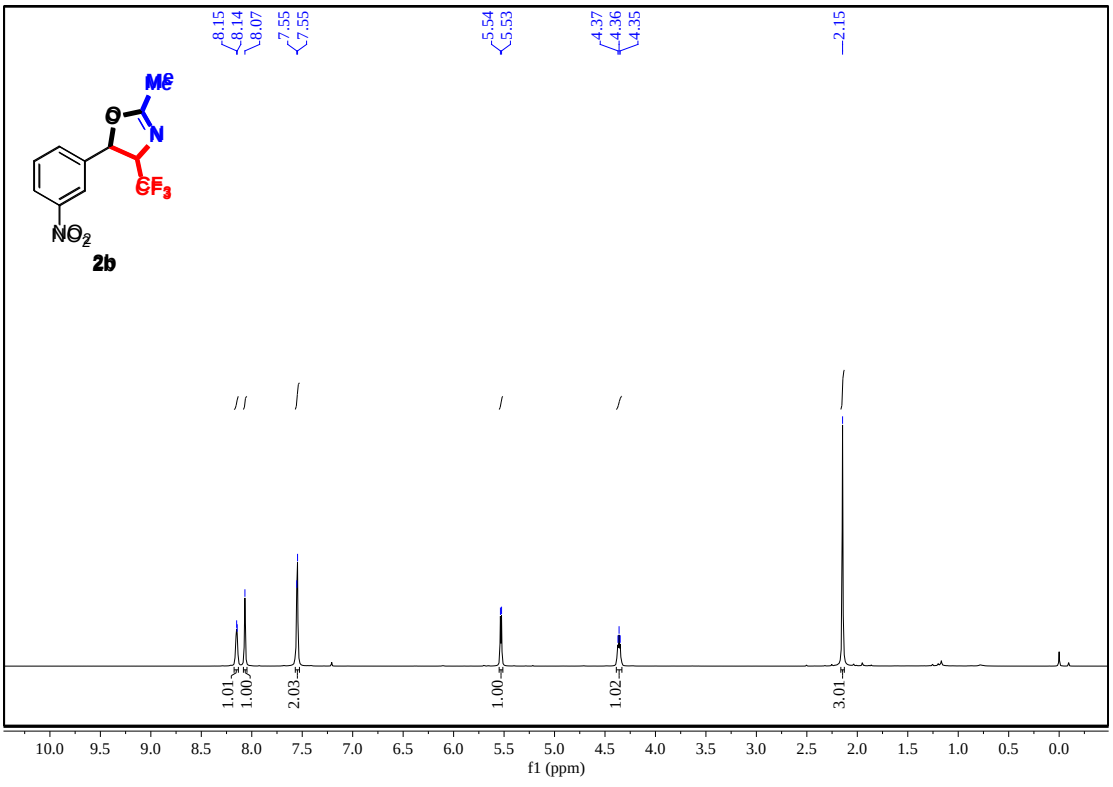
145.57
127.12
126.23
125.28
124.57
123.42
121.57
79.64
79.63
77.41
77.20
76.99
76.60
76.40
76.20
76.00
14.14
Me
O
N
CF3
O2N
2a
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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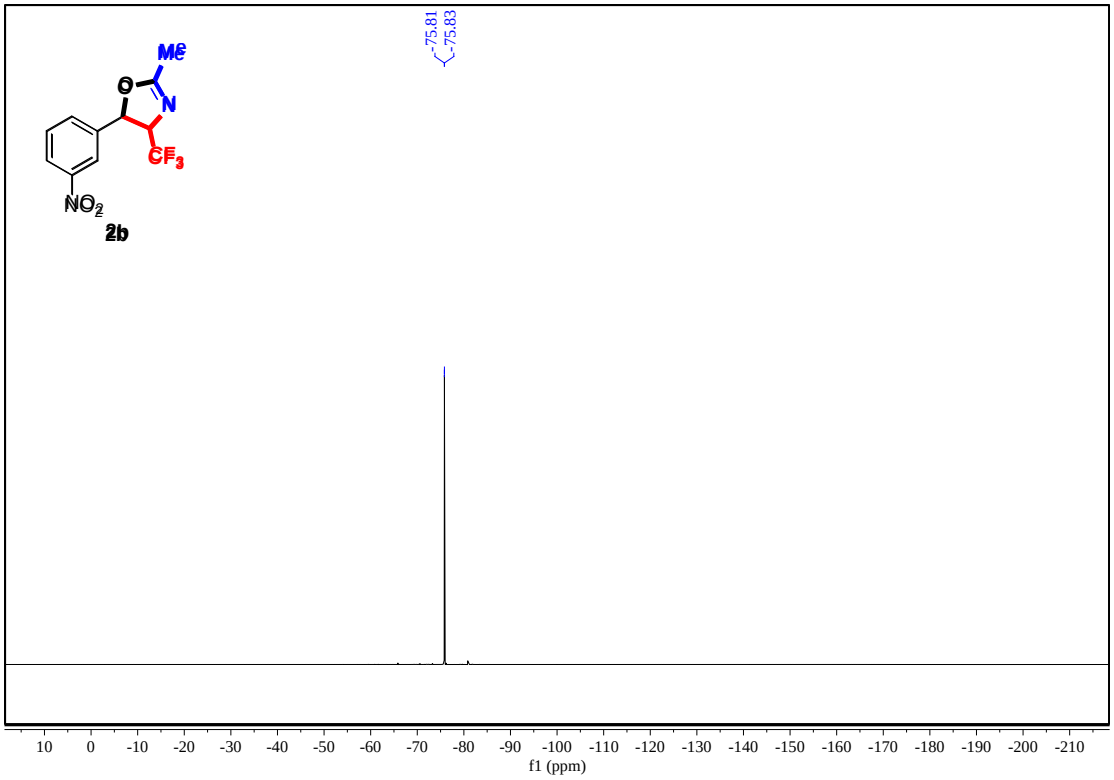
8.14
8.07
7.55
7.55
5.54
5.53
4.37
4.36
4.35
2.15
Me
O
N
CF3
NO2
2b
1.01
1.00
2.03
1.00
1.02
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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CF3
NO2
2b
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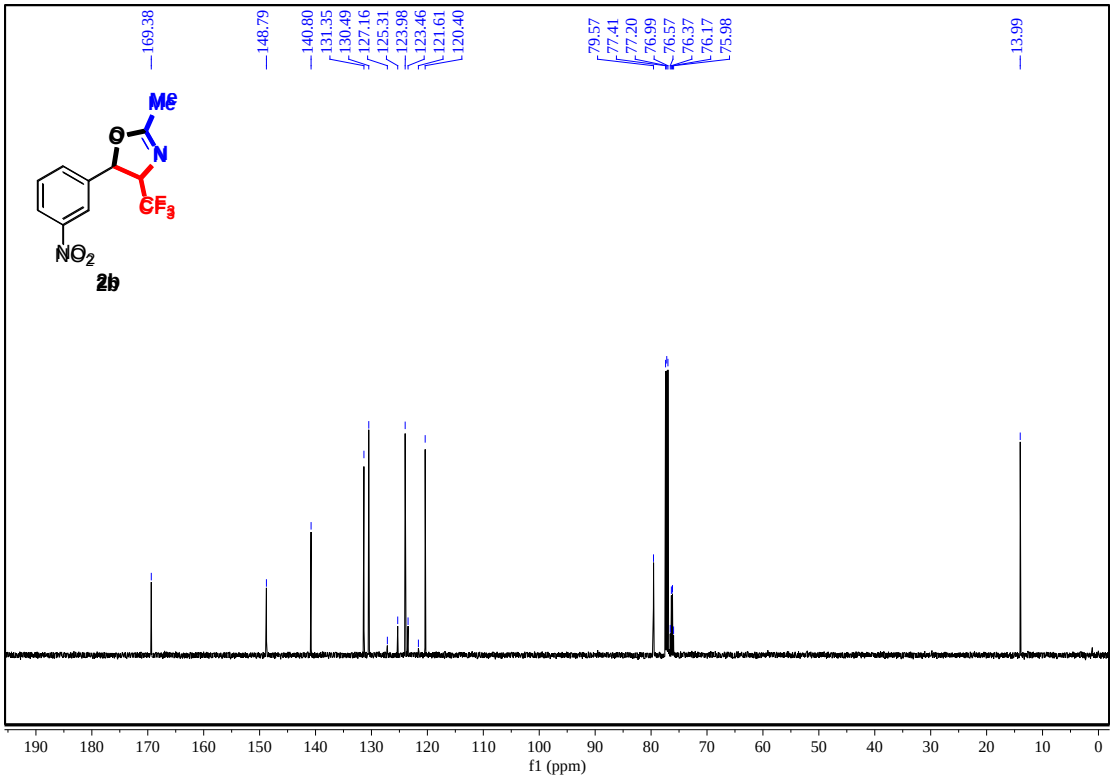
f1 (ppm)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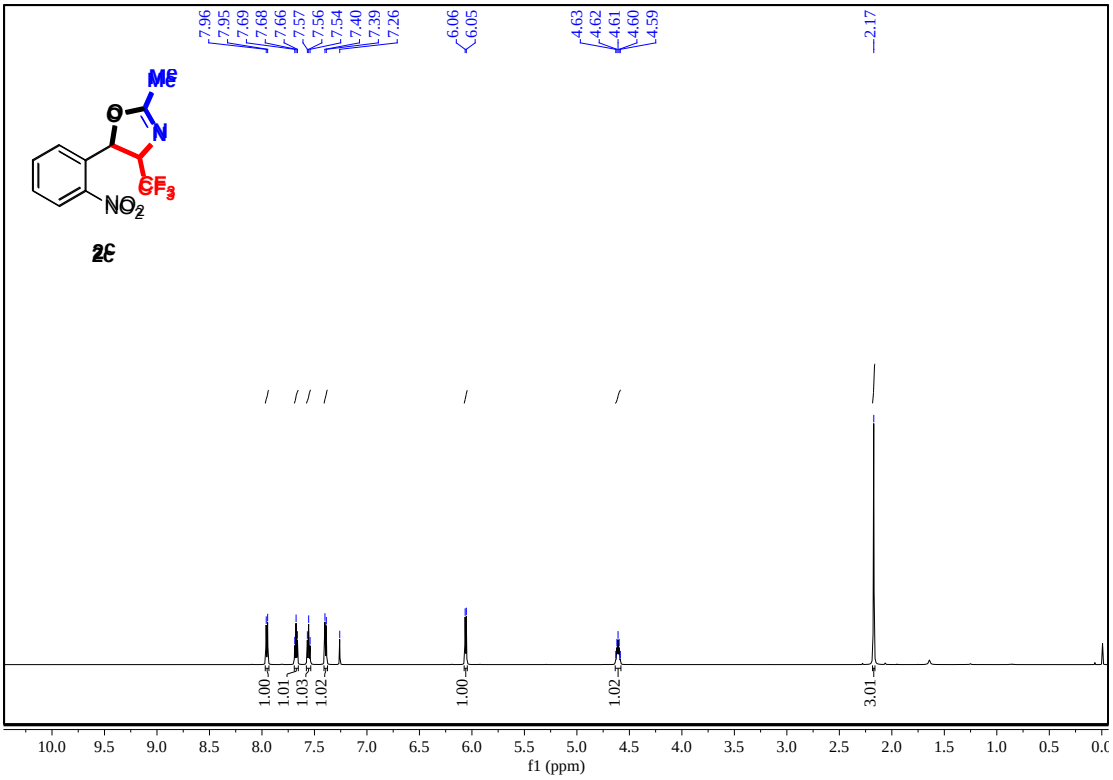
140.80
131.35
130.49
127.16
125.31
123.98
123.46
121.61
120.40
79.57
77.41
77.20
76.99
76.57
76.37
76.17
75.98
13.99
Me
O
N
CF3
NO2
2b
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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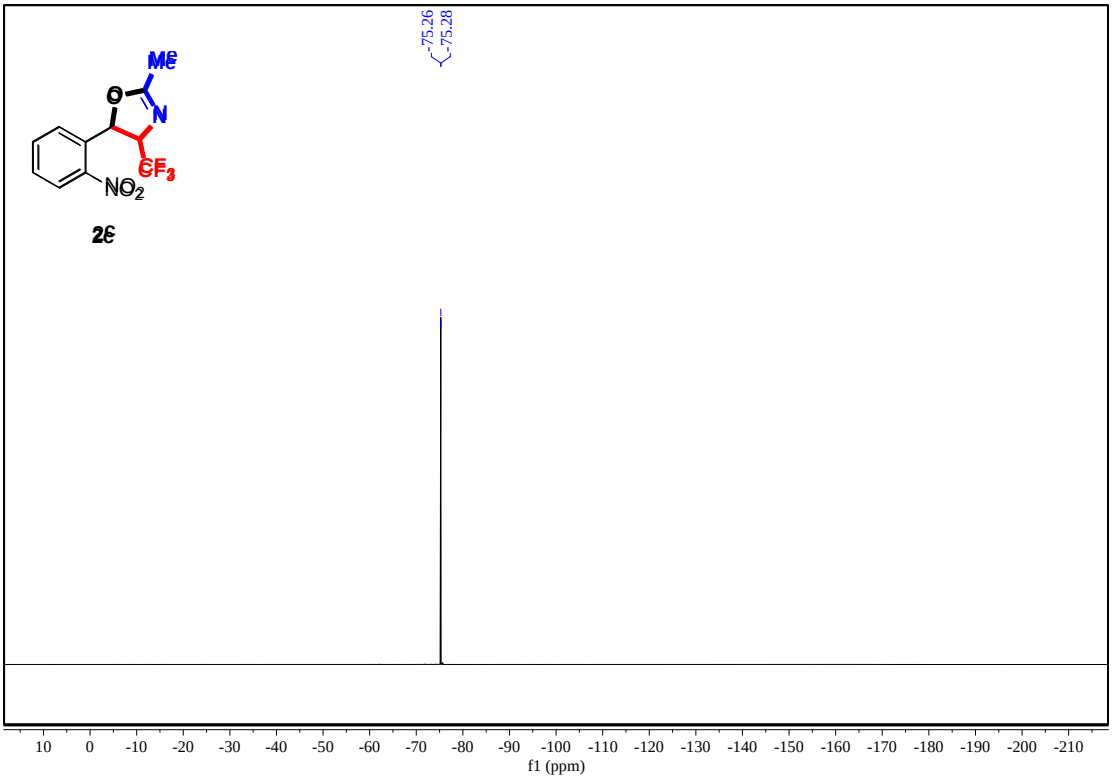
7.54
7.40
7.39
7.26
6.06
6.05
4.63
4.62
4.61
4.60
4.59
2.17
Me
O
N
CF3
NO2
2e
1.00
1.01
1.03
1.02
1.00
1.02
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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CF3
NO2
2e
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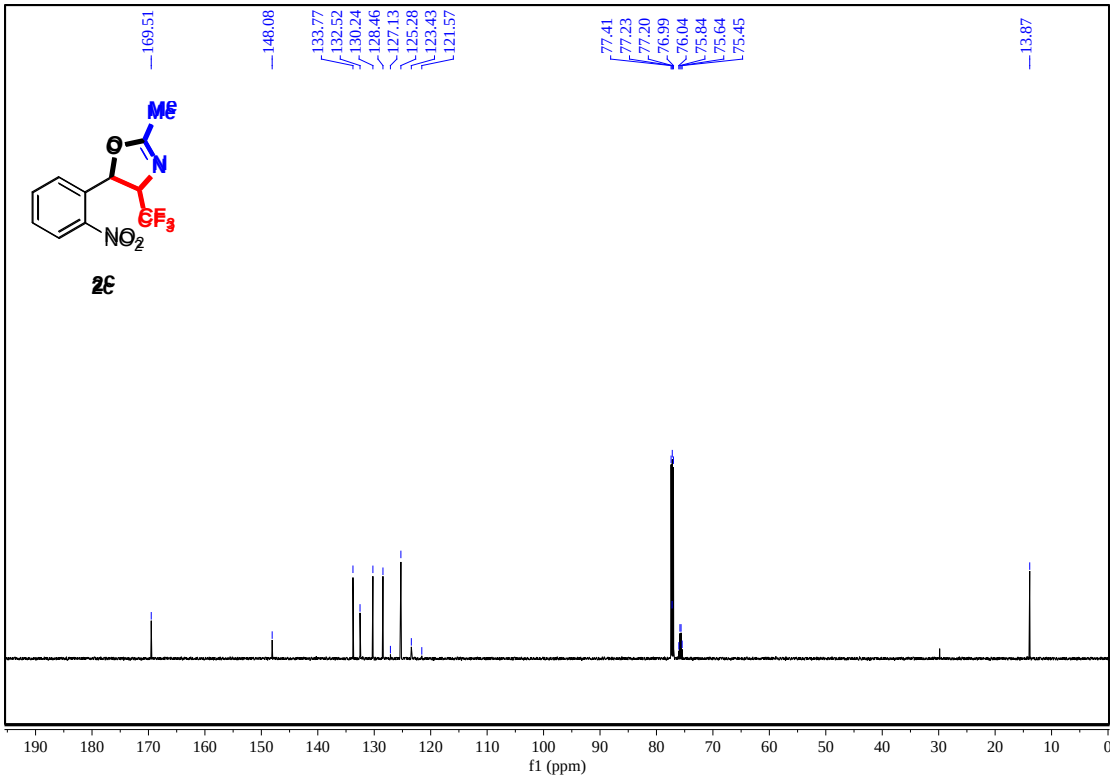
f1 (ppm)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127.13
125.28
123.43
121.57
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77.23
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76.99
76.04
75.84
75.64
75.45
13.87
Me
O
N
CF3
NO2
2c
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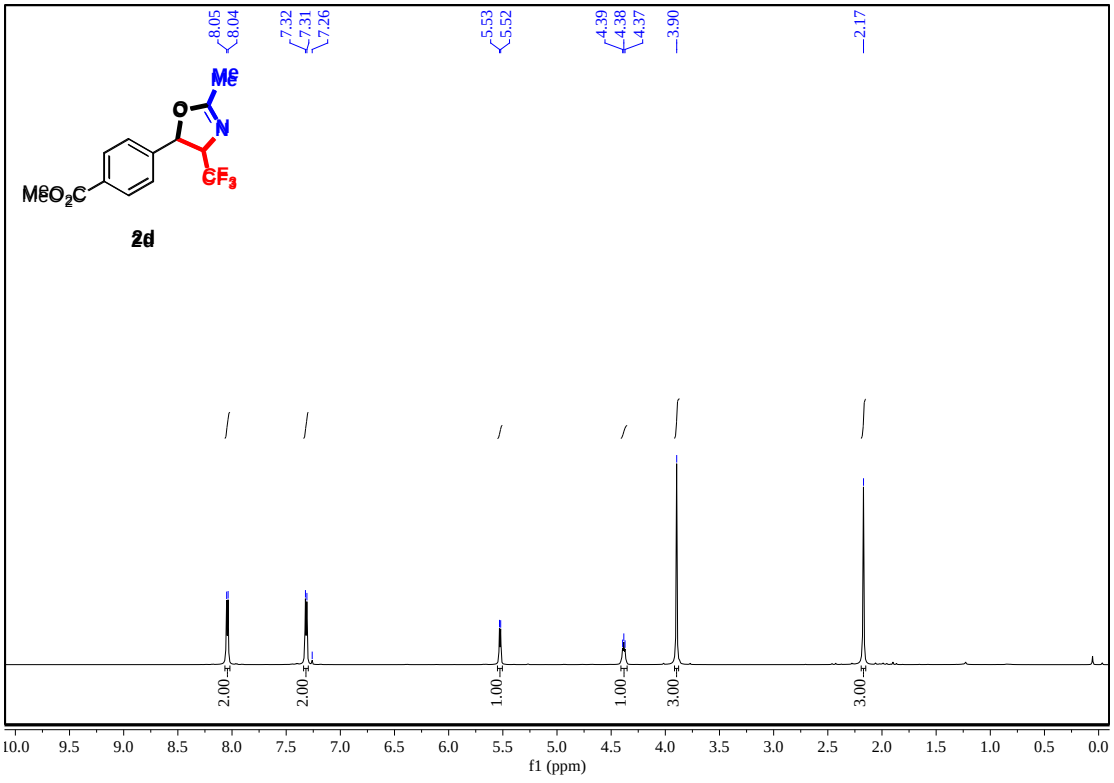
f1 (ppm)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8.04
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7.31
7.26
5.53
5.52
4.39
4.38
4.37
3.90
2.17
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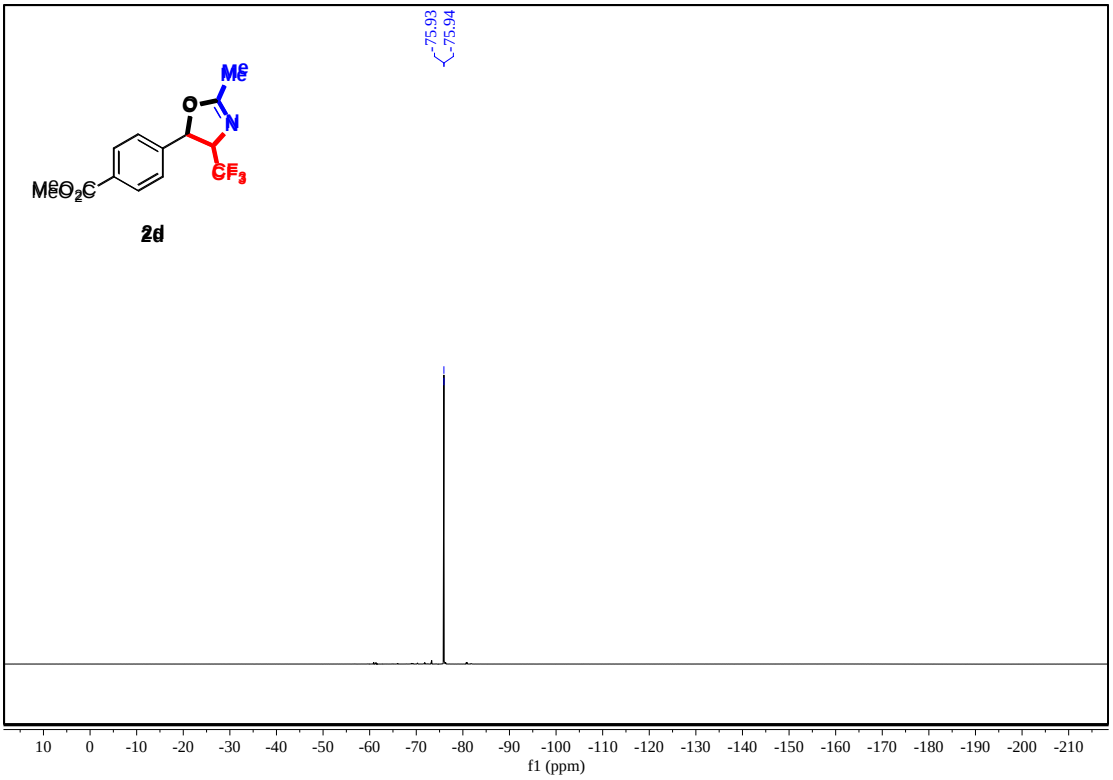
O
N
CF3
MeO2C
2d
2.00
2.00
1.00
1.00
3.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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CF3
MeO2C
2d
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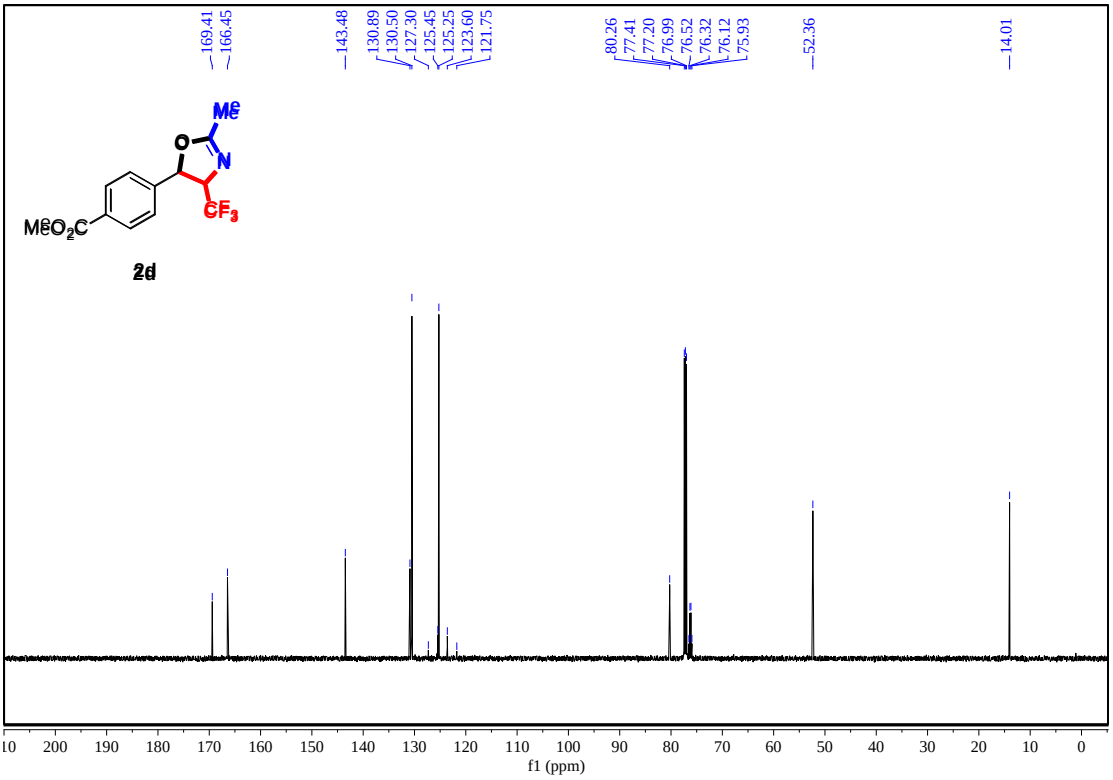
f1 (ppm)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125.25
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121.75
80.26
77.41
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76.99
76.52
76.32
76.12
75.93
52.36
14.01
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O
N
CF3
MeO2C
2d
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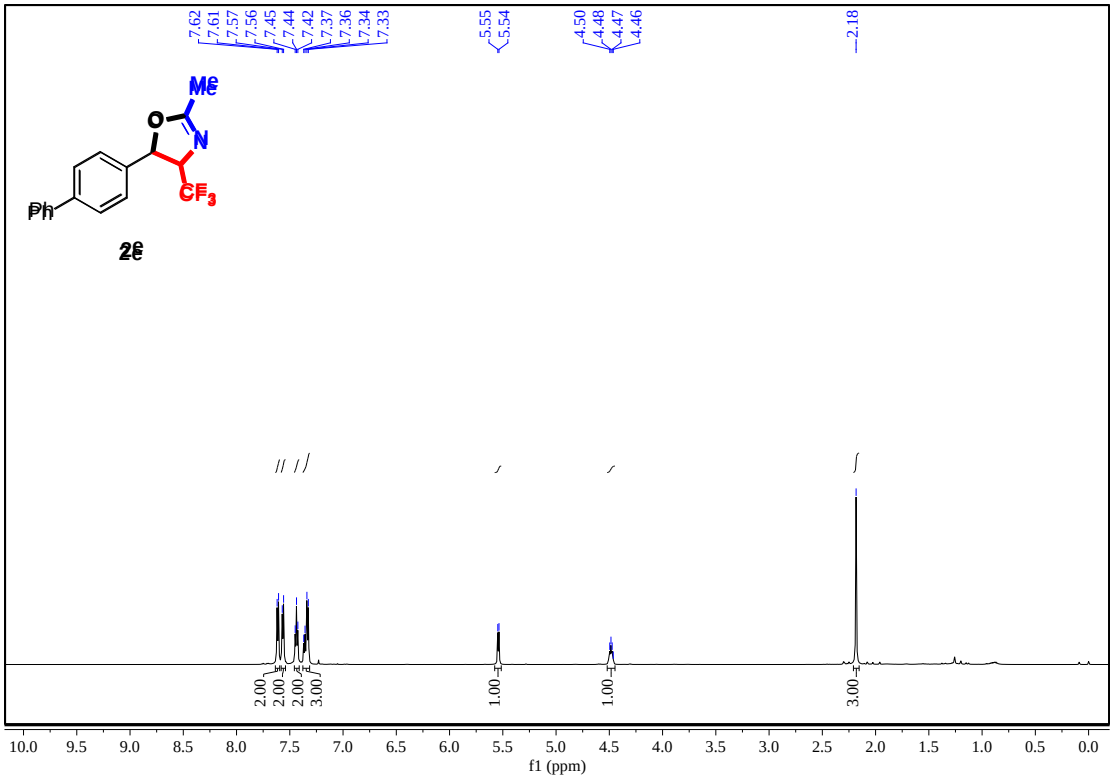
f1 (ppm)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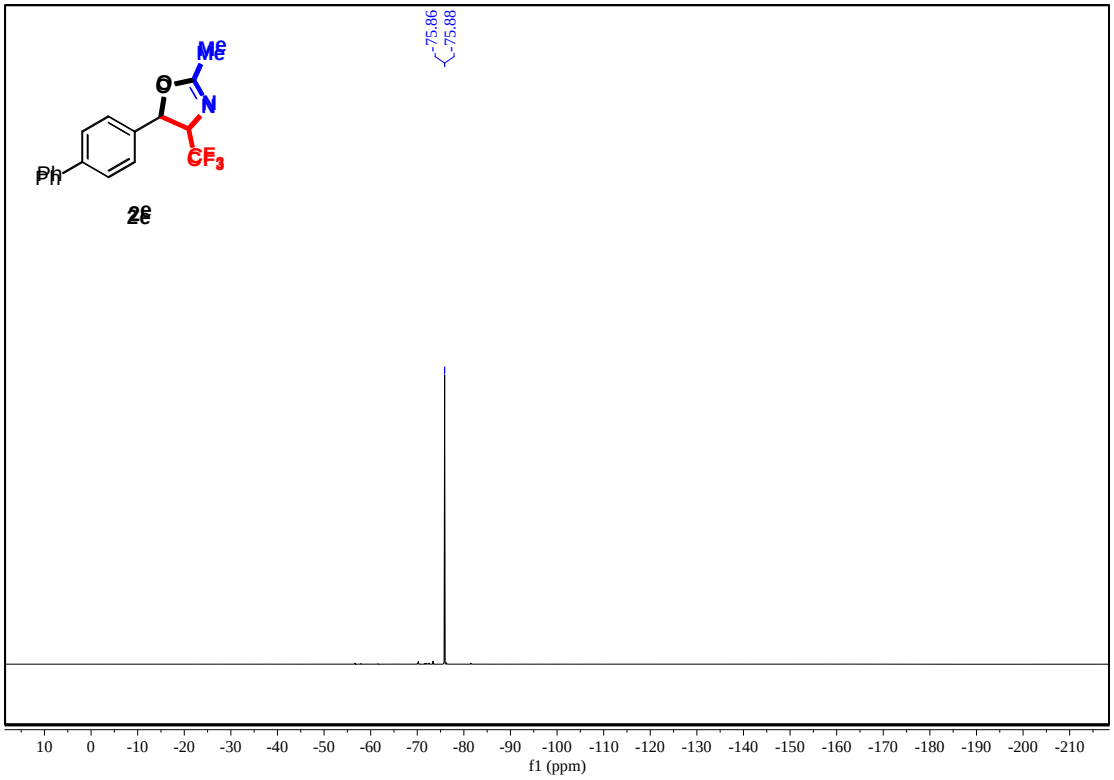
4.48
4.47
4.46
2.18
Me
O
N
CF3
Ph
2e
2.00
2.00
2.00
3.00
1.00
1.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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Ph
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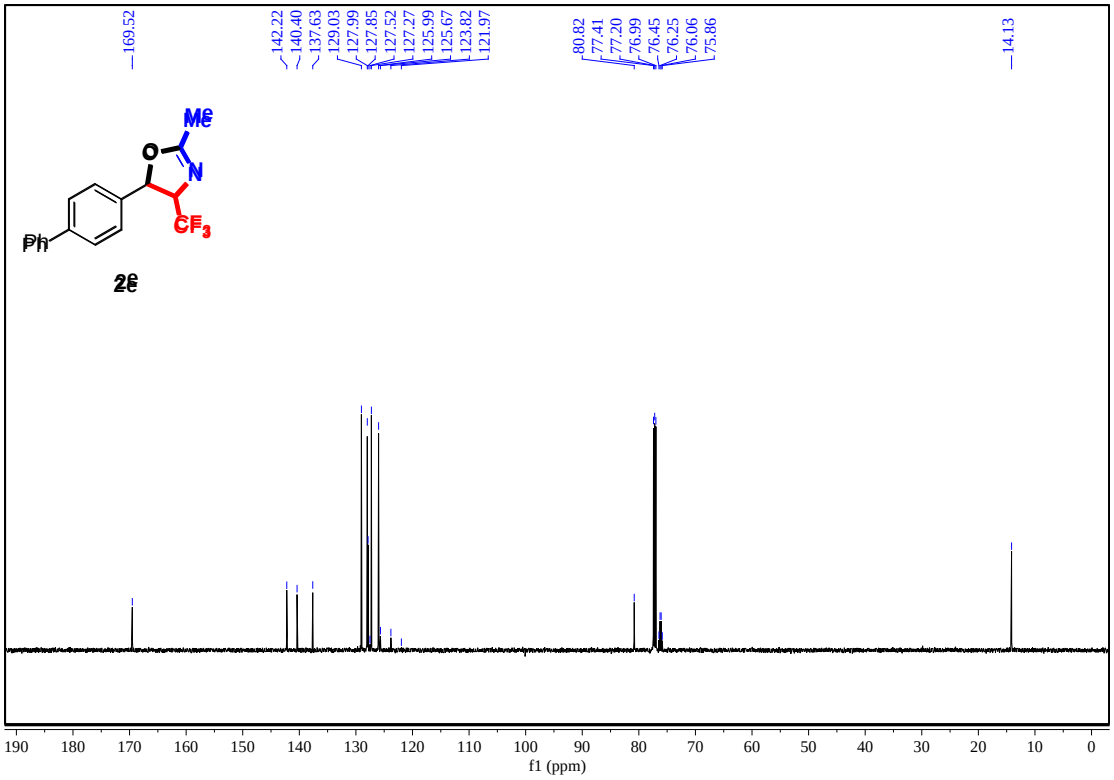
f1 (ppm)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80.82
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77.20
76.99
76.45
76.25
76.06
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Me
O
N
CF3
Ph
2e
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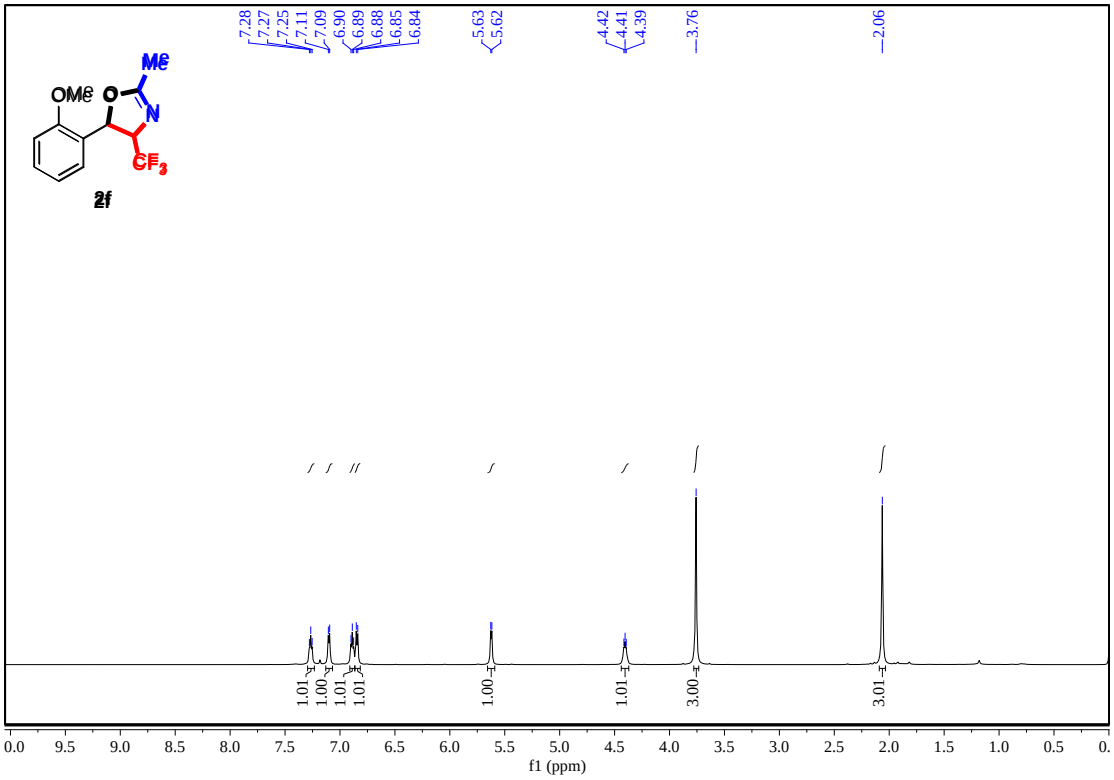
f1 (ppm)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4.41
4.39
3.76
2.06
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OMe
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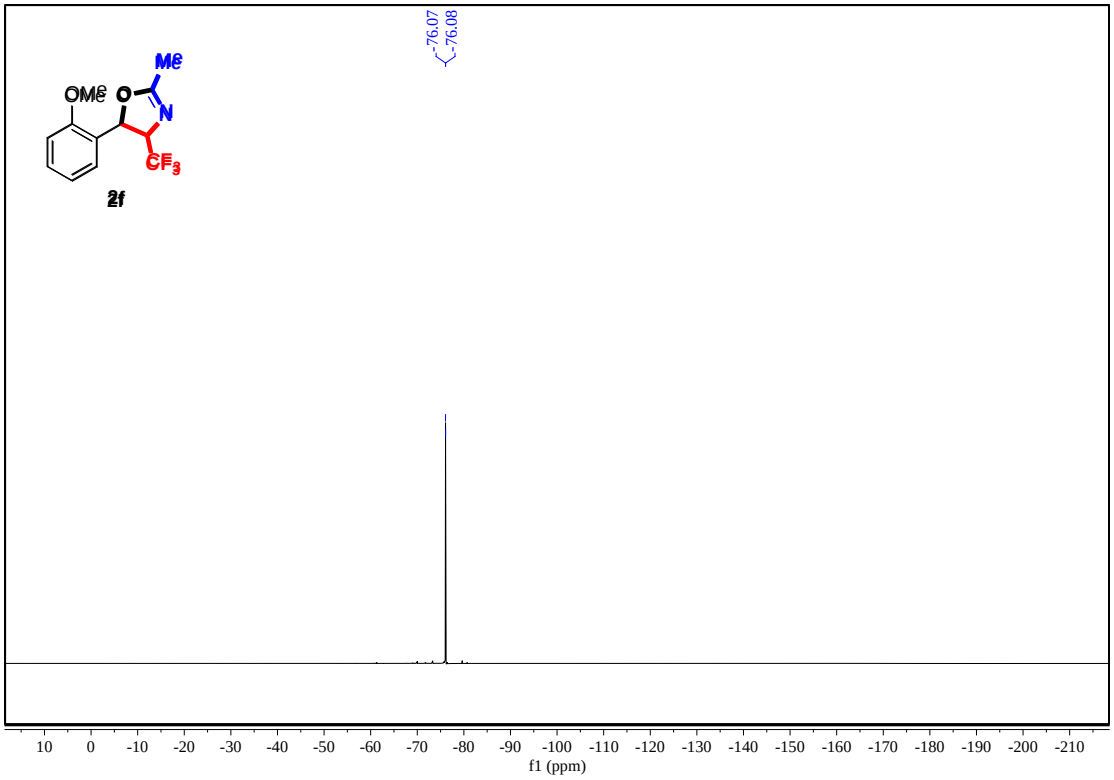
1.00
1.01
1.01
1.00
1.01
3.00
3.01
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
f1 (ppm)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N
CF3
2f
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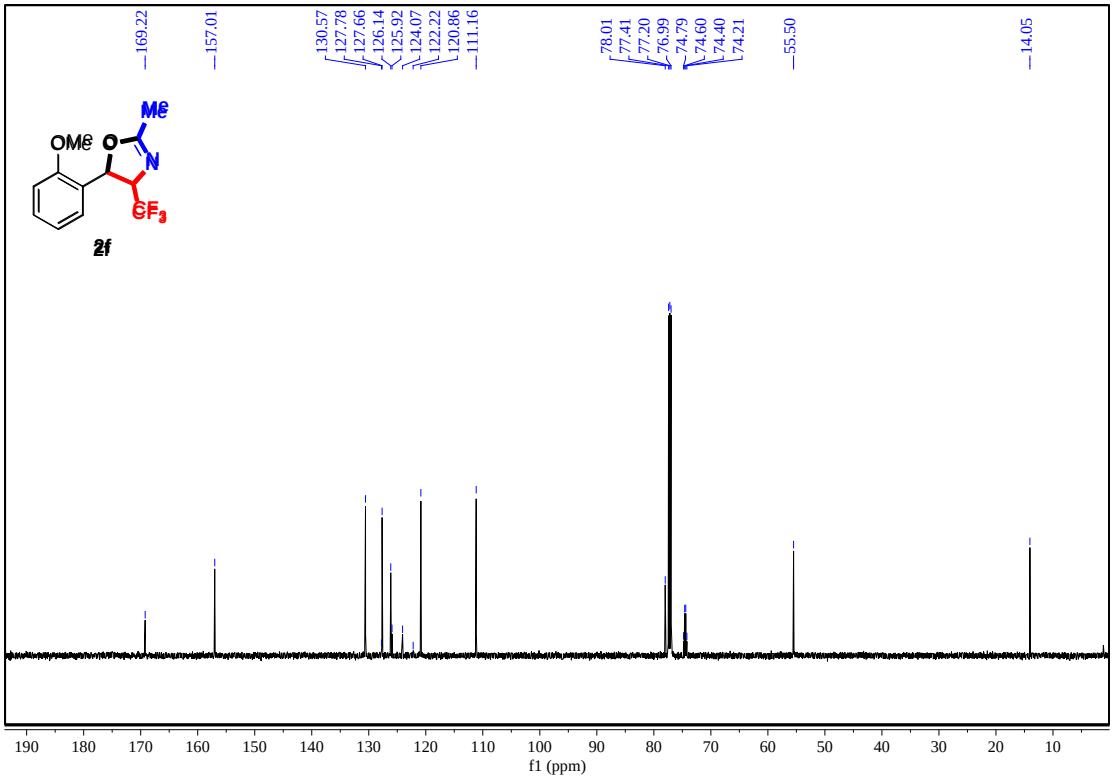
f1 (ppm)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76.99
74.79
74.60
74.40
74.21
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N
CF3
2f
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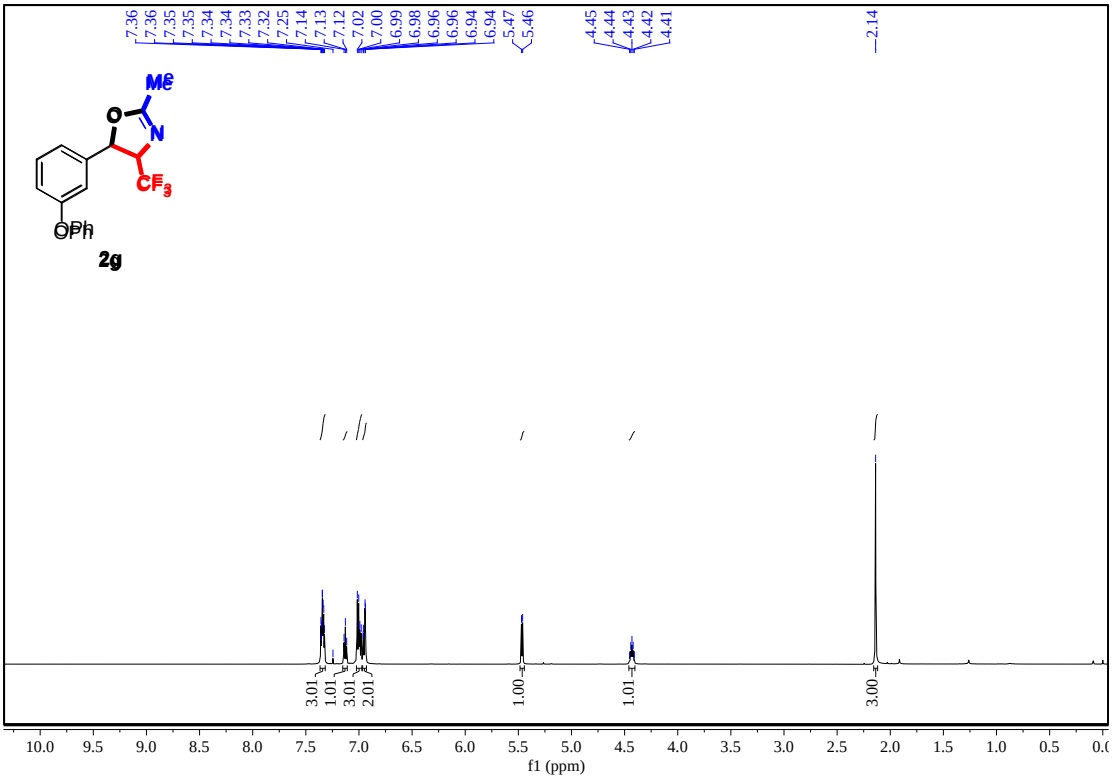
f1 (ppm)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6.98
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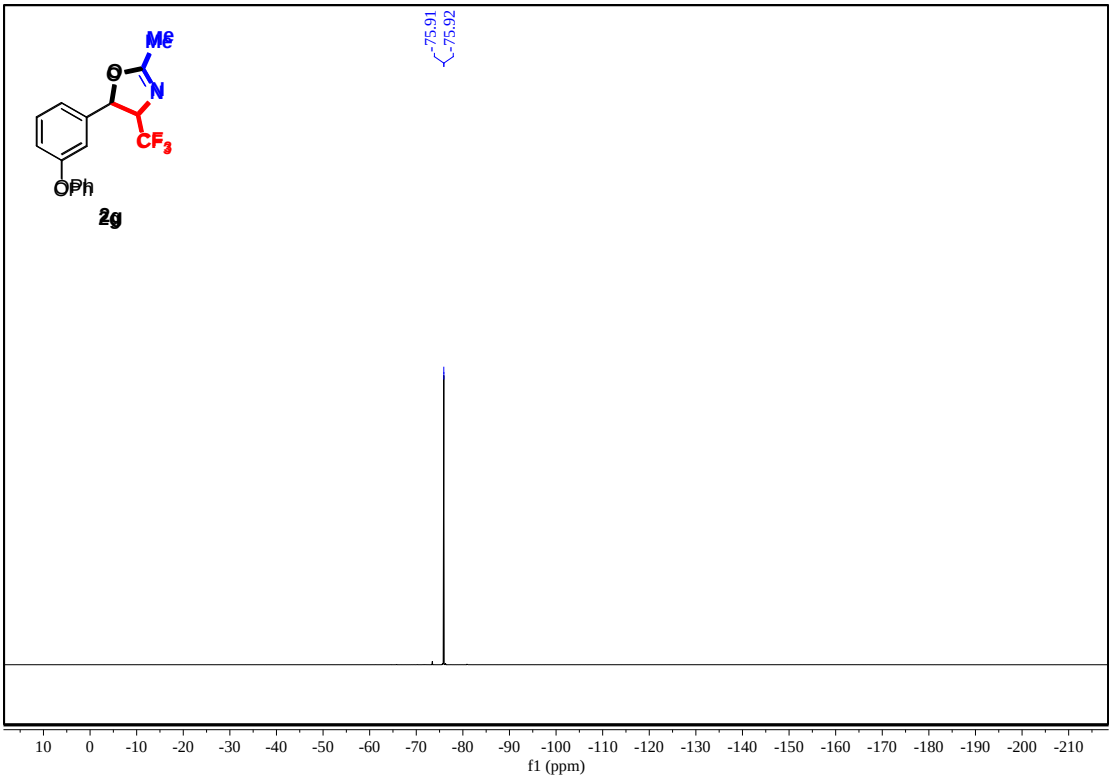
6.96
6.94
6.94
5.47
5.46
4.45
4.44
4.43
4.42
4.41
2.14
Me
O
N
CF3
OPh
2g
3.01
1.01
3.01
2.01
1.00
1.01
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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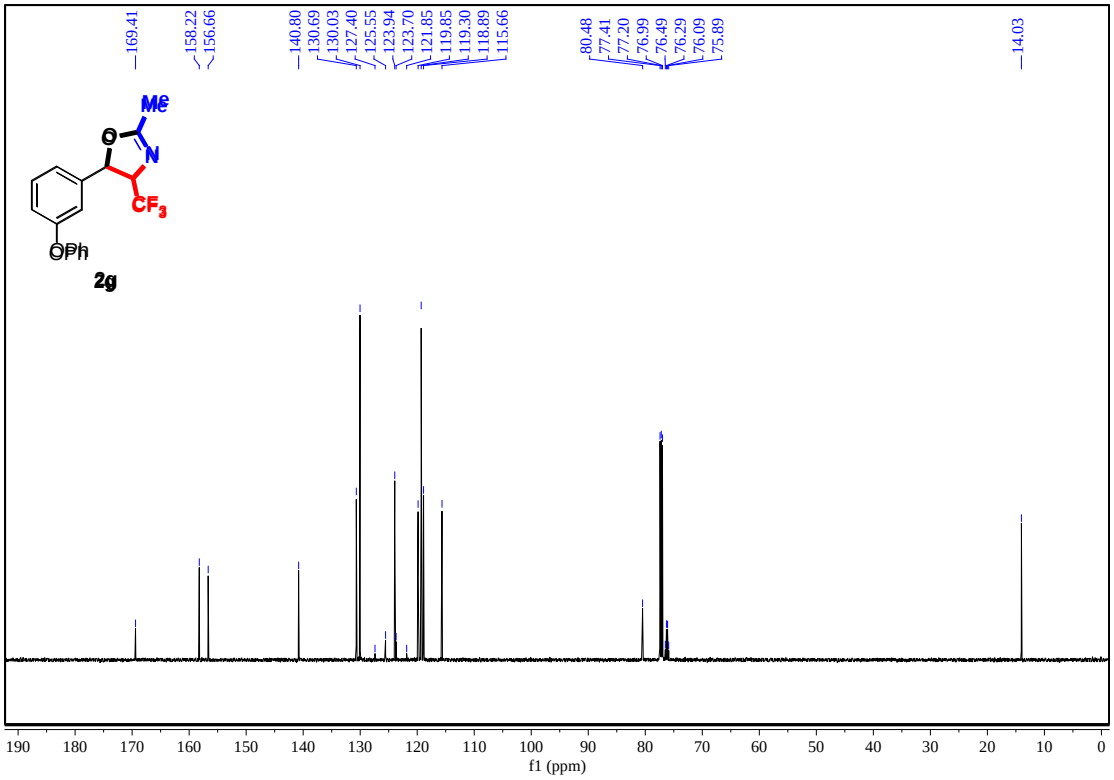
f1 (ppm)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115.66
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77.41
77.20
76.99
76.49
76.29
76.09
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14.03
Me
O
N
CF3
OPh
2g
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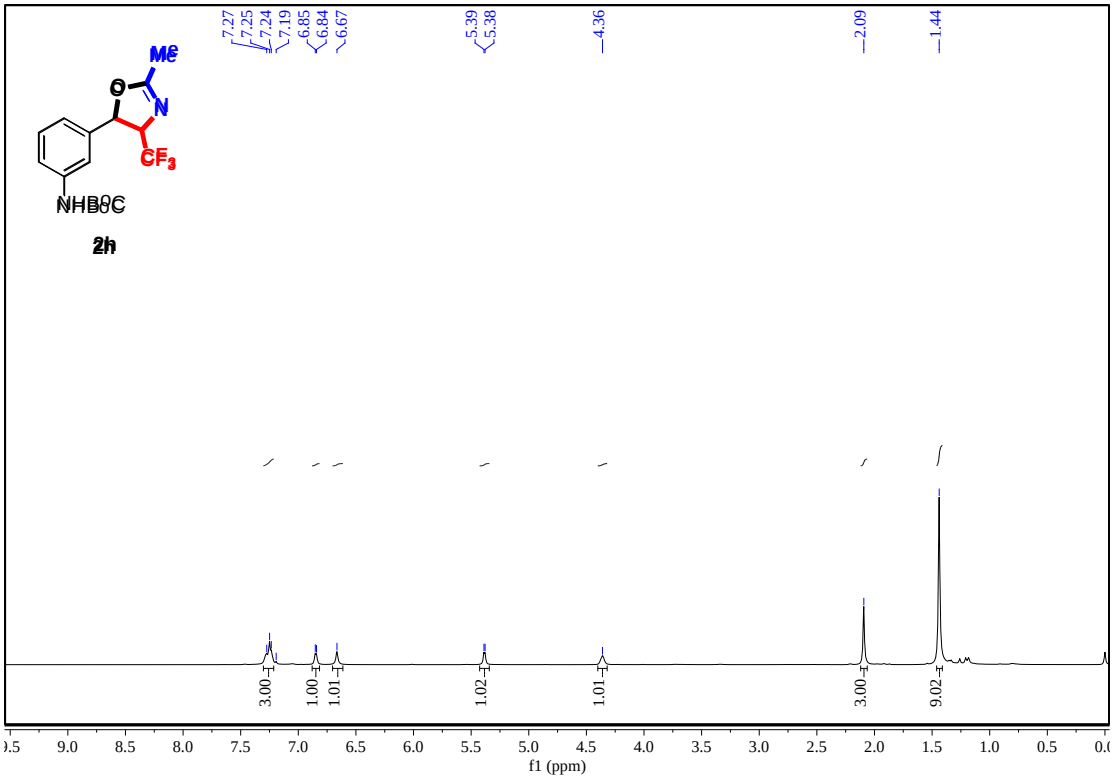
f1 (ppm)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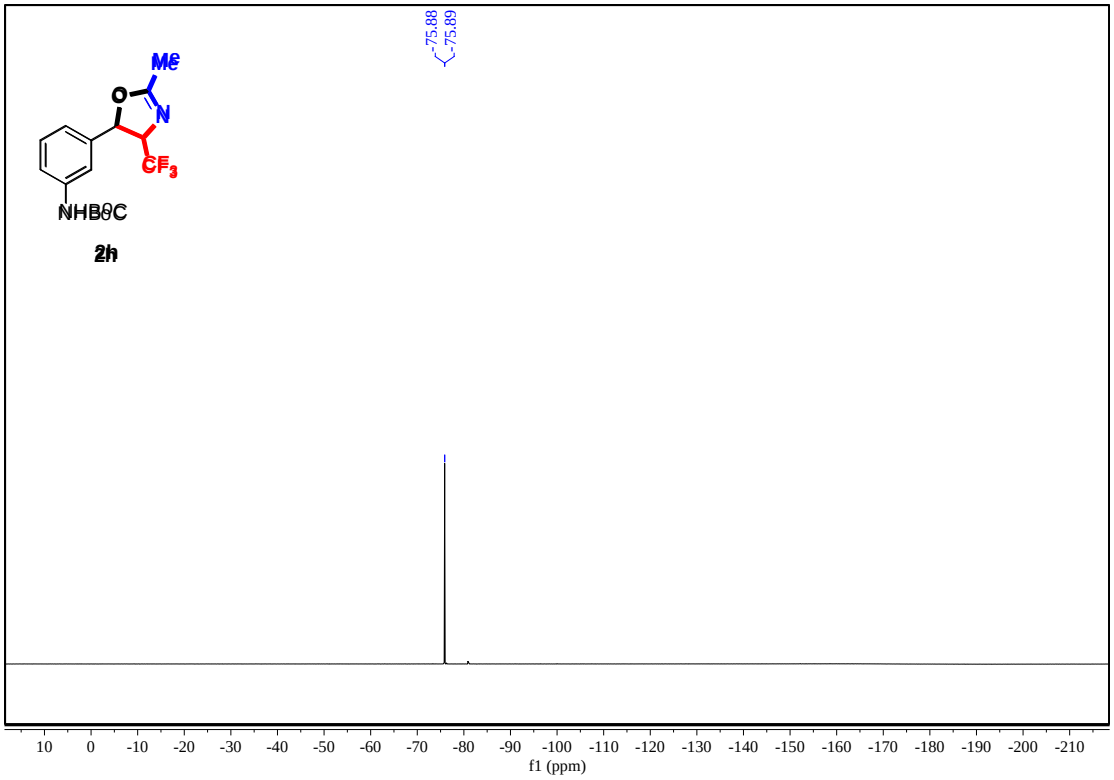
NHBOC
2h
3.00
1.00
1.01
1.02
1.01
3.00
9.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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2h
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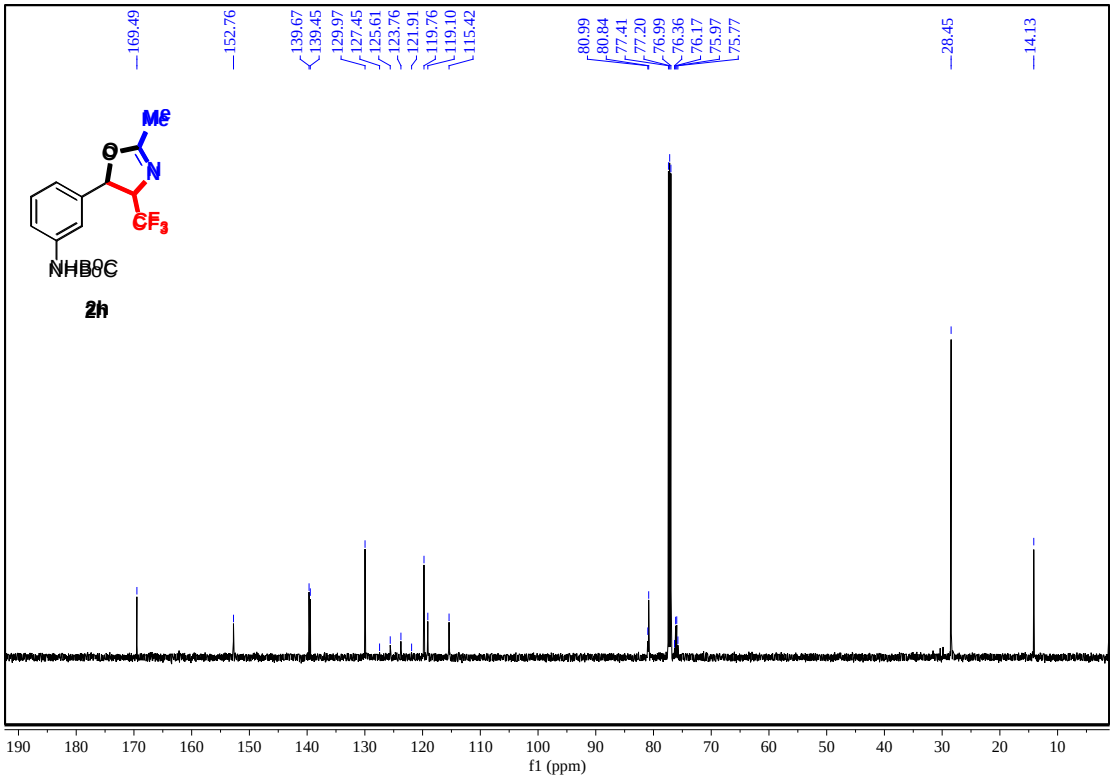
f1 (ppm)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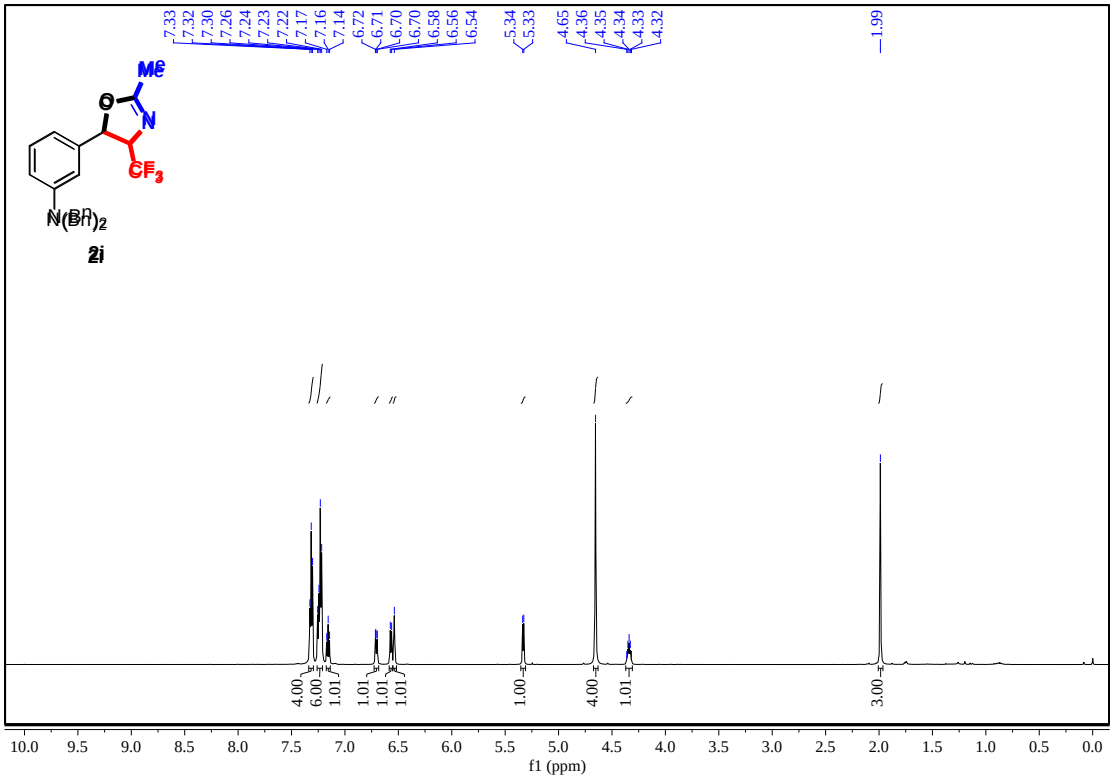
80.84
77.41
77.20
76.99
76.36
76.17
75.97
75.77
28.45
14.13
Me
O
N
CF3
NHBOC
2h
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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6.70
6.70
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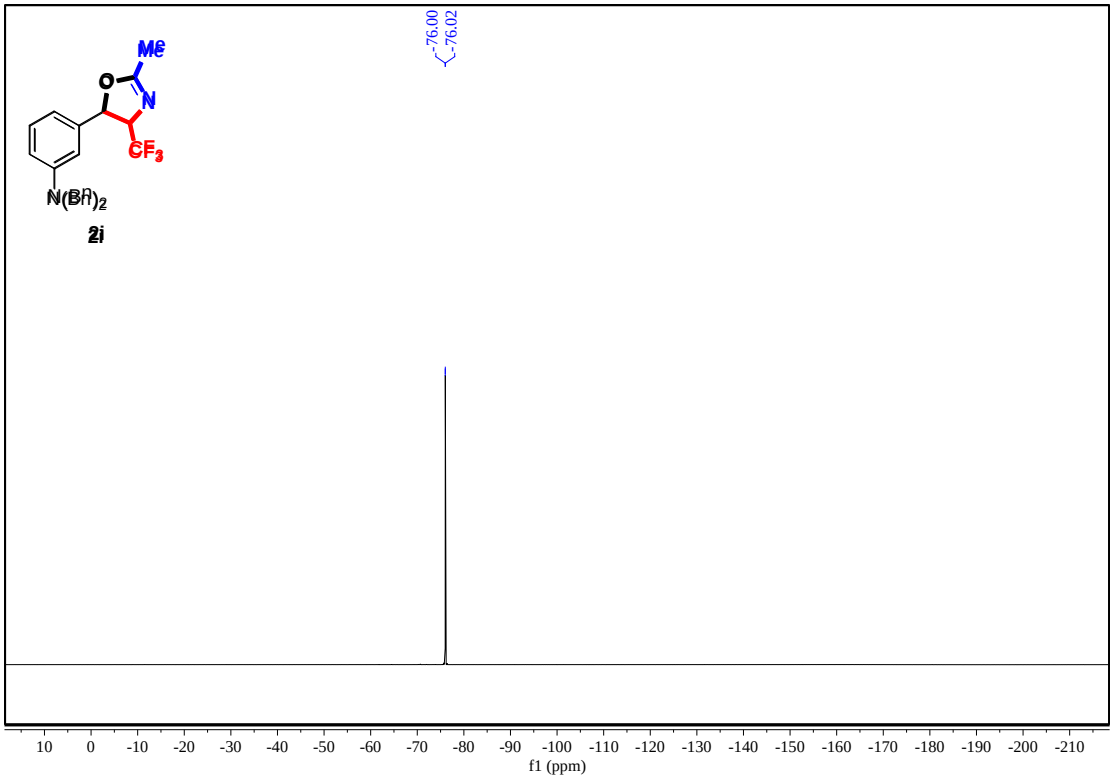
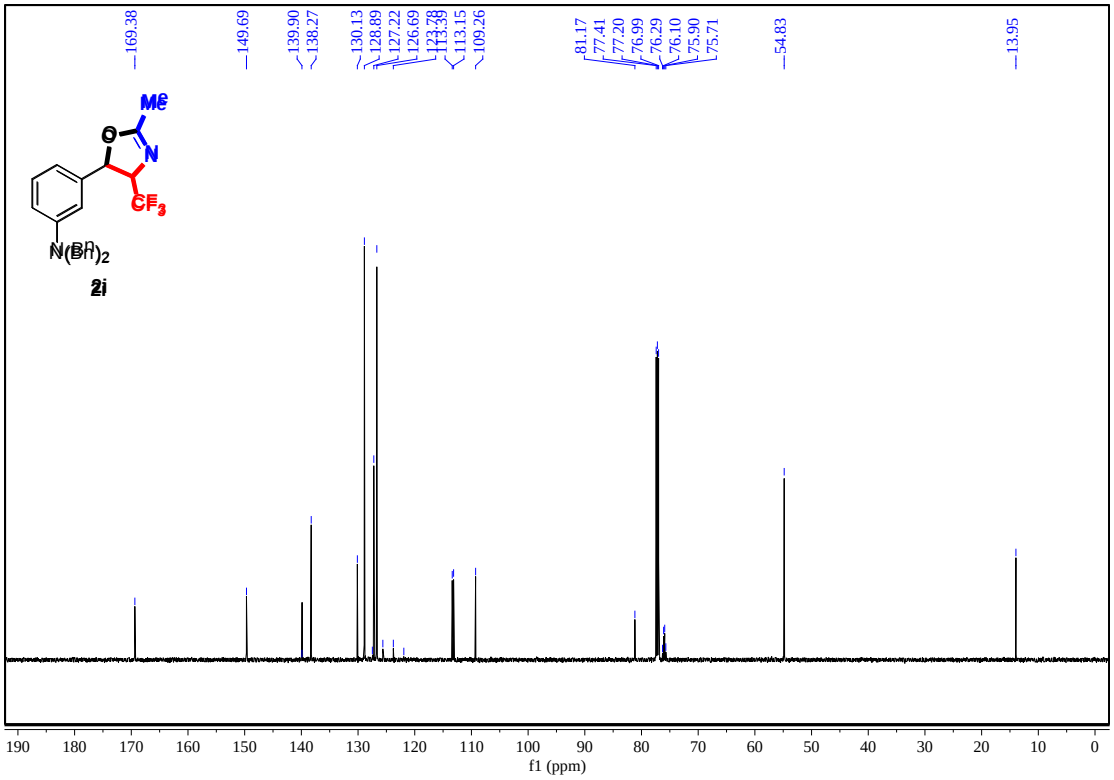
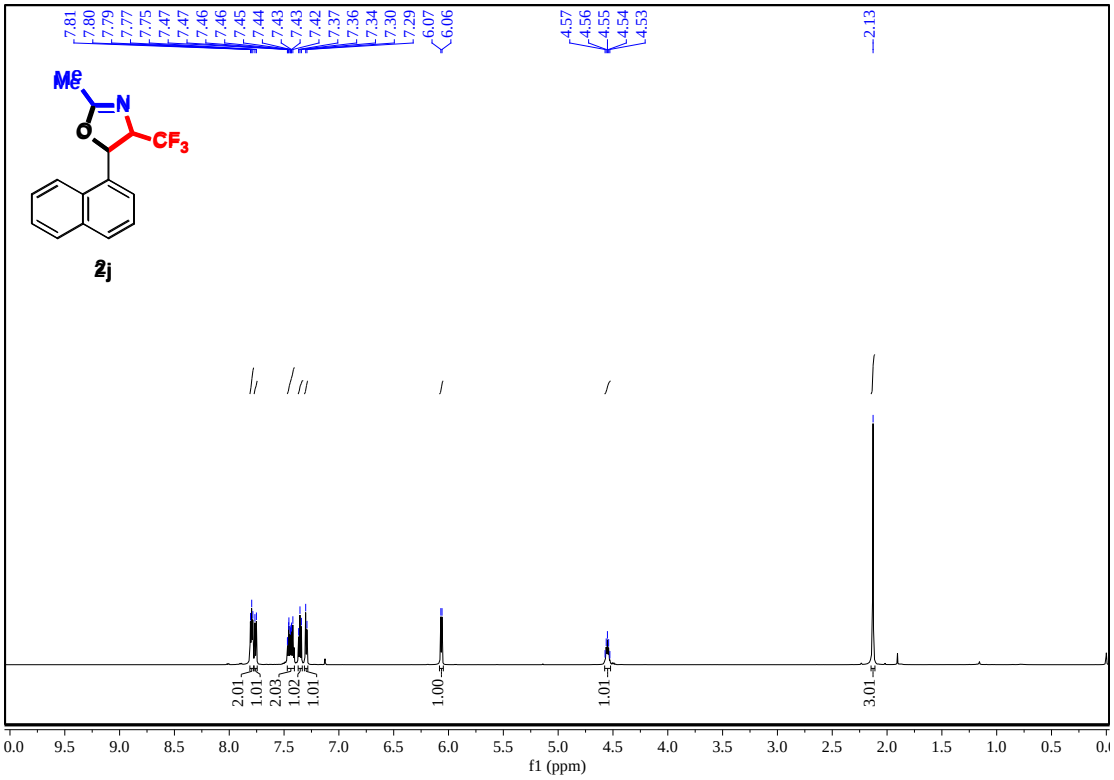
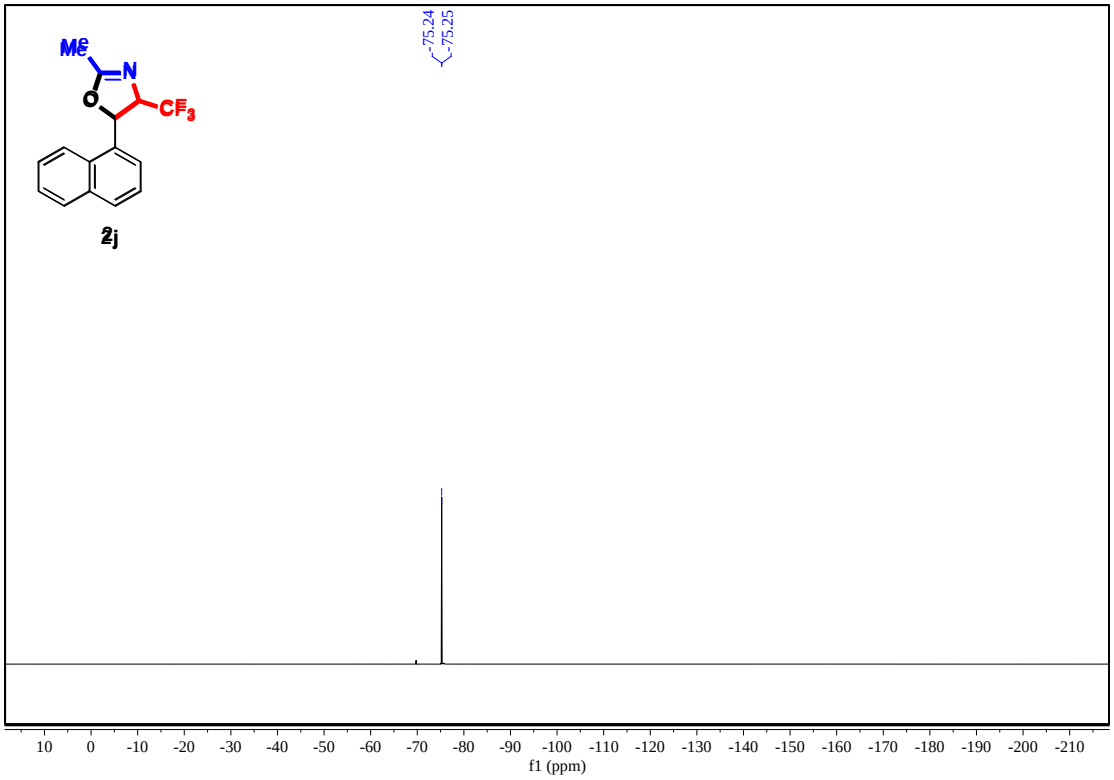
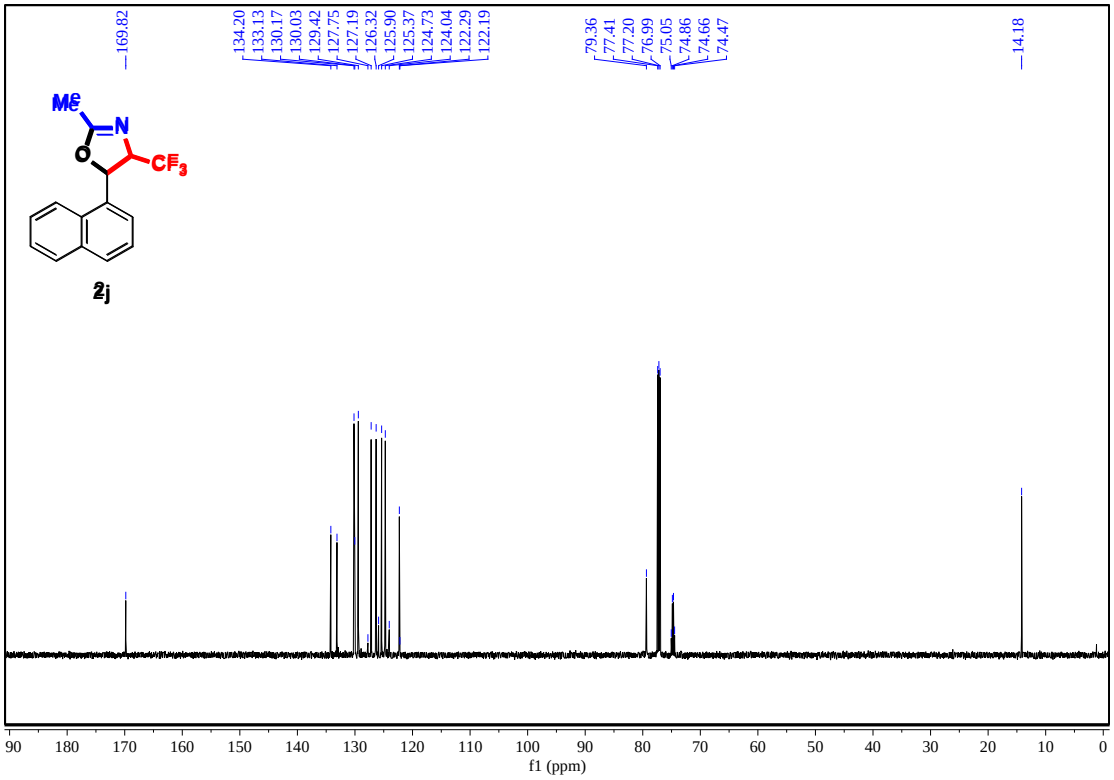
6.56
6.54
5.34
5.33
4.65
4.36
4.35
4.34
4.33
4.32
1.99
Me
O
N
CF3
N(Bn)2
2i
4.00
6.00
1.01
1.01
1.01
1.01
1.00
4.00
1.01
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

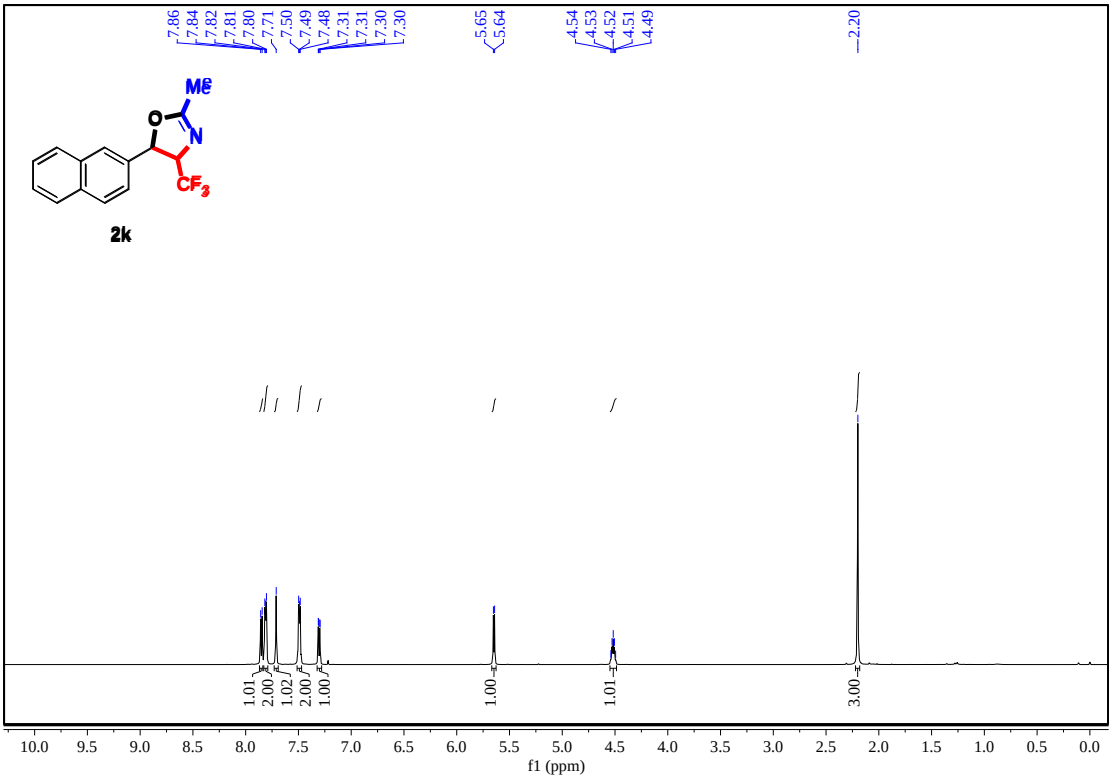

-76.00
-76.02
Me
O
N
CF3
N(Bn)2
2i
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

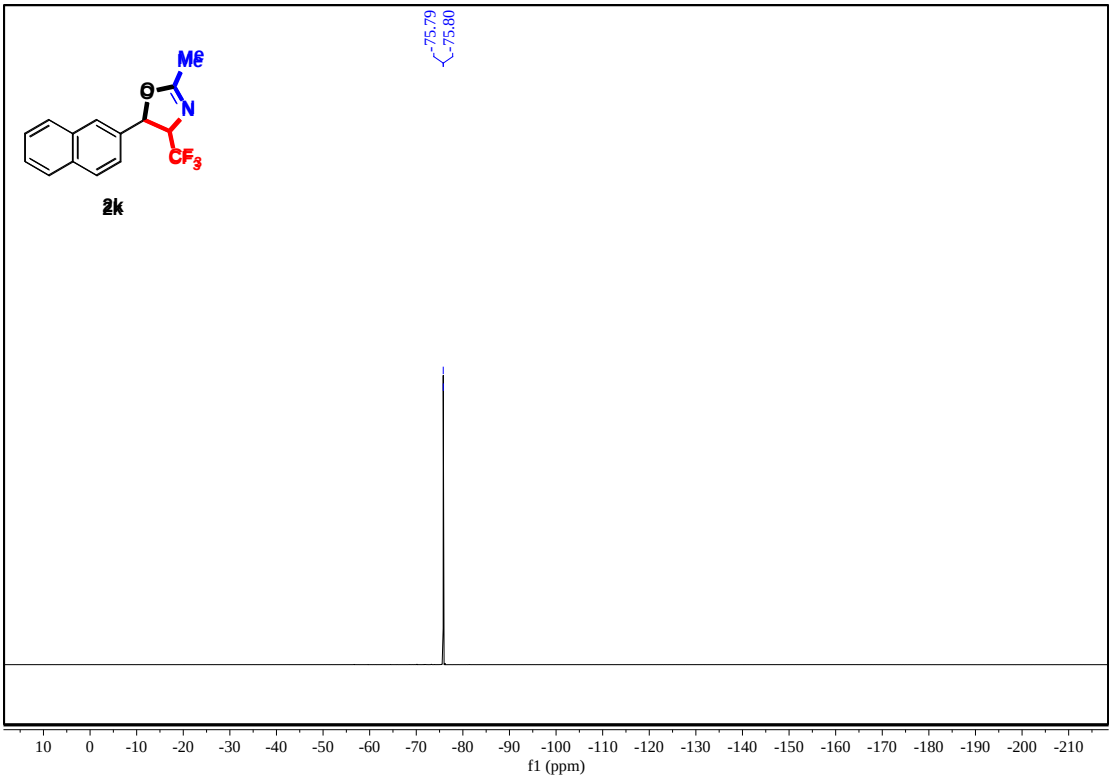

169.38
149.69
139.90
138.27
130.13
128.89
127.22
126.69
123.78
113.39
113.15
109.26
81.17
77.41
77.20
76.99
76.29
76.10
75.90
75.71
54.83
13.95
Me
O
N
CF3
N(Bn)2
2i
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

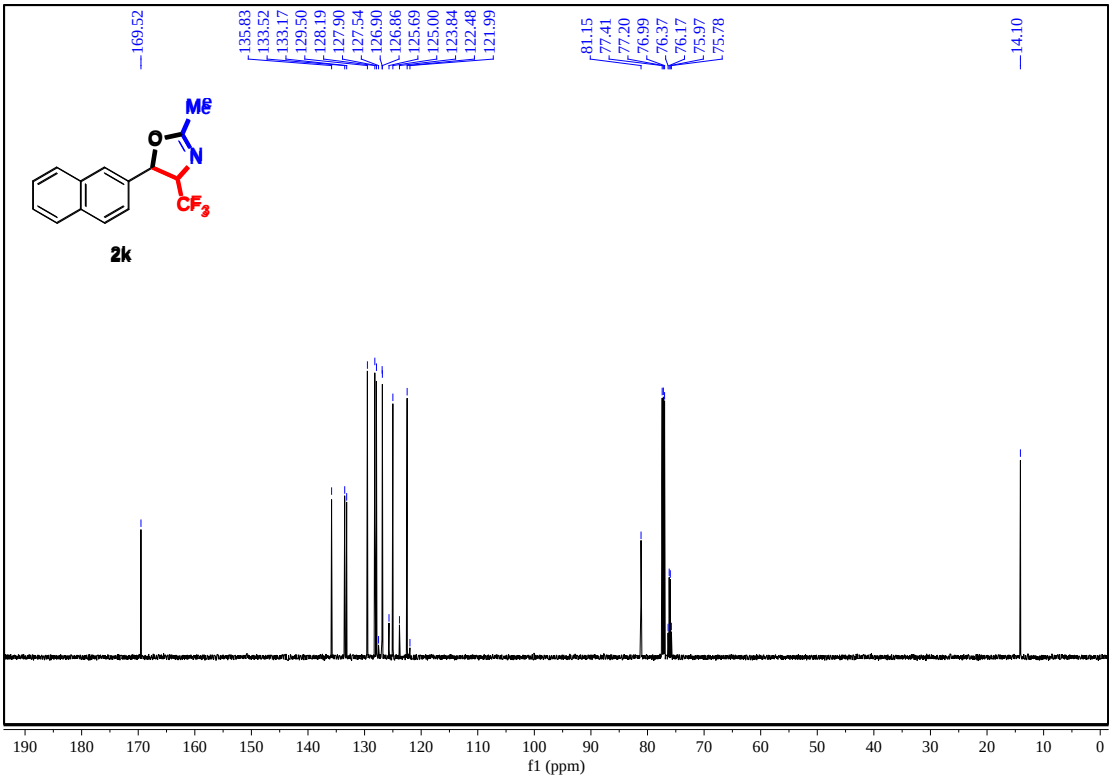

7.81
7.80
7.79
7.77
7.75
7.47
7.47
7.46
7.46
7.45
7.44
7.43
7.43
7.42
7.37
7.36
7.34
7.30
7.29
6.07
6.06
4.57
4.56
4.55
4.54
4.53
2.13
Me
N
O
CF3
2j
2.01
1.01
2.03
1.02
1.01
1.00
1.01
3.01
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

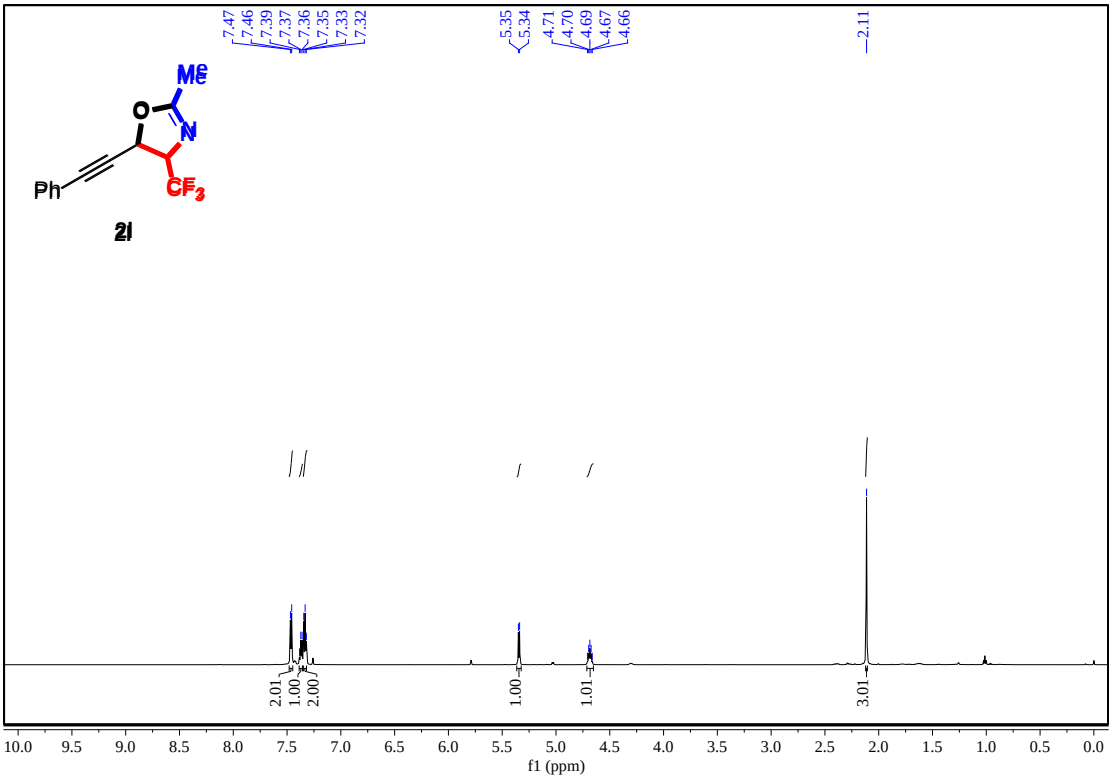

Me
N
O
CF3
2j
-75.24
-75.25
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

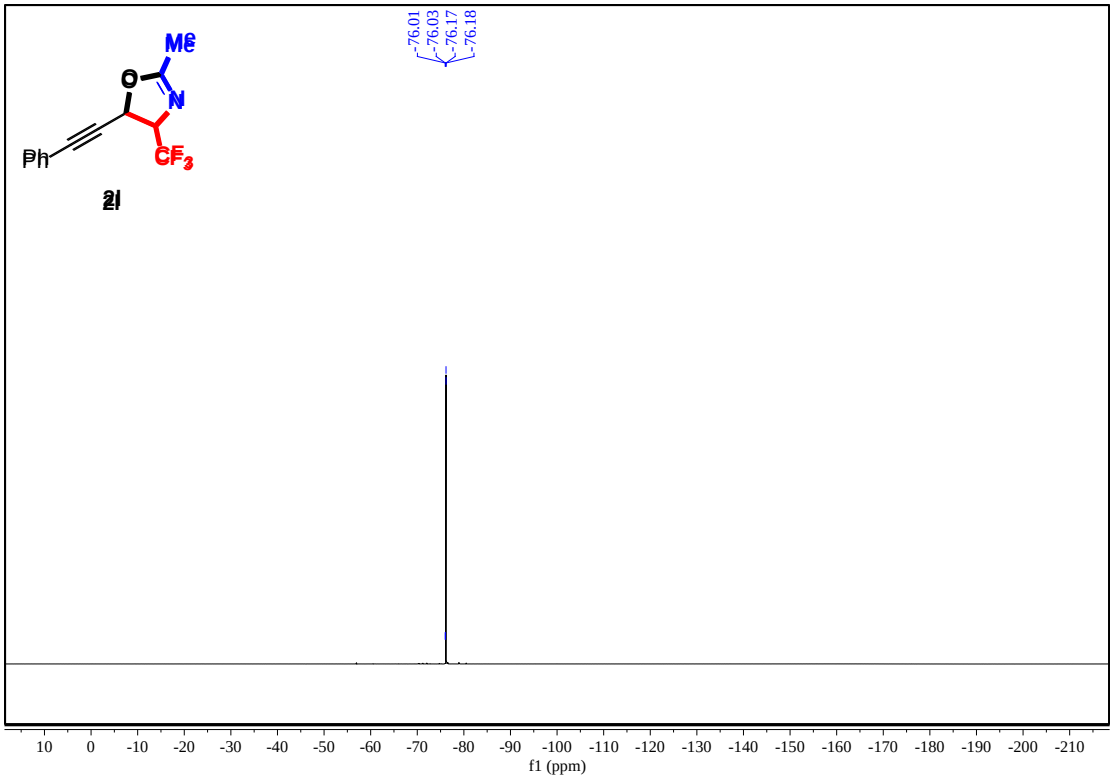

169.82
134.20
133.13
130.17
130.03
129.42
127.75
127.19
126.32
125.90
125.37
124.73
124.04
122.29
122.19
79.36
77.41
77.20
76.99
75.05
74.86
74.66
74.47
14.18
Me
N
O
CF3
2j
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.86
7.84
7.82
7.81
7.80
7.71
7.50
7.49
7.48
7.31
7.31
7.30
7.30
5.65
5.64
4.54
4.53
4.52
4.51
4.49
2.20
Me
O
N
CF3
2k
1.01
2.00
1.02
2.00
1.00
1.00
1.01
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

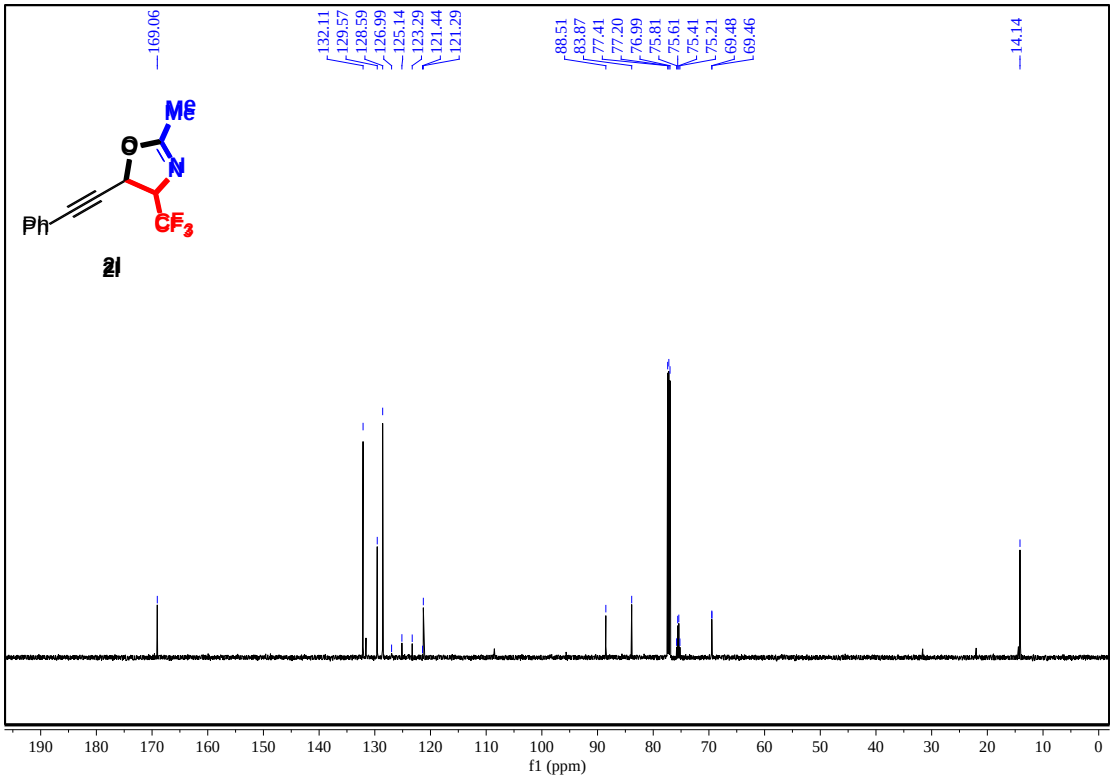

-75.79
-75.80
Me
O
N
CF3
2k
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


169.52
135.83
133.52
133.17
129.50
128.19
127.90
127.54
126.90
126.86
125.69
125.00
123.84
122.48
121.99
81.15
77.41
77.20
76.99
76.37
76.17
75.97
75.78
14.10
Me
O
N
CF3
2k
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

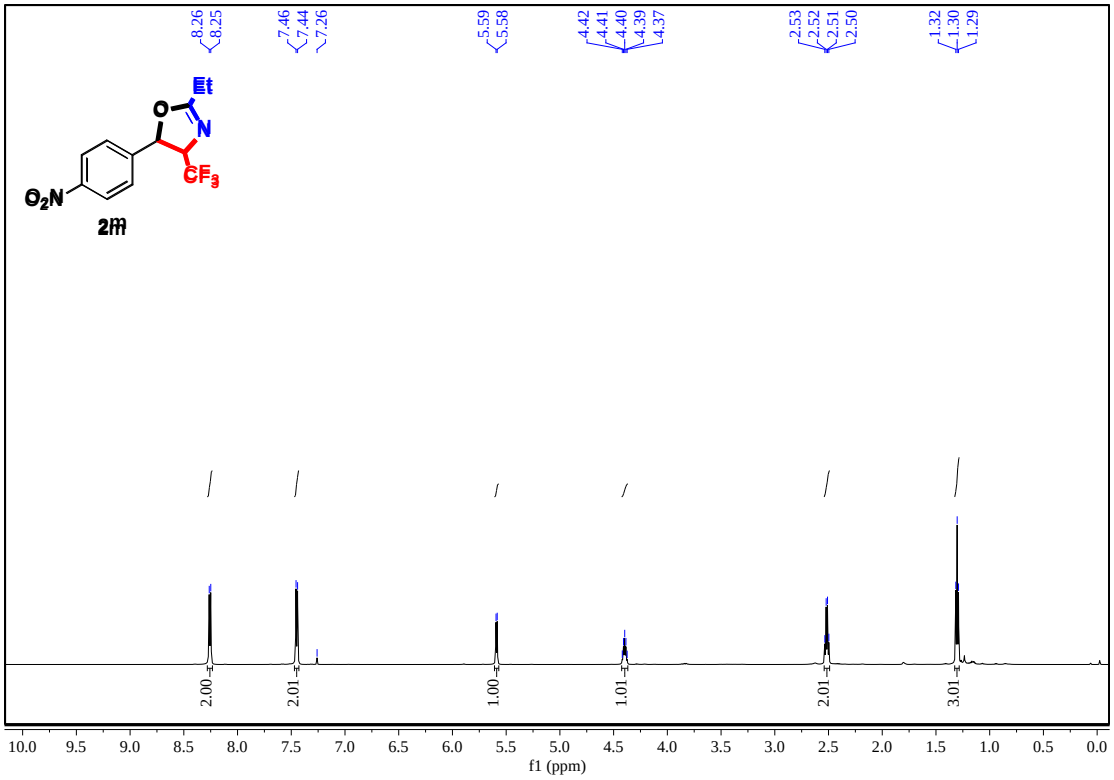

7.47
7.46
7.39
7.37
7.36
7.35
7.33
7.32
5.35
5.34
4.71
4.70
4.69
4.67
4.66
2.11
Me
O
N
Ph
CF3
2l
2.01
1.00
2.00
1.00
1.01
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

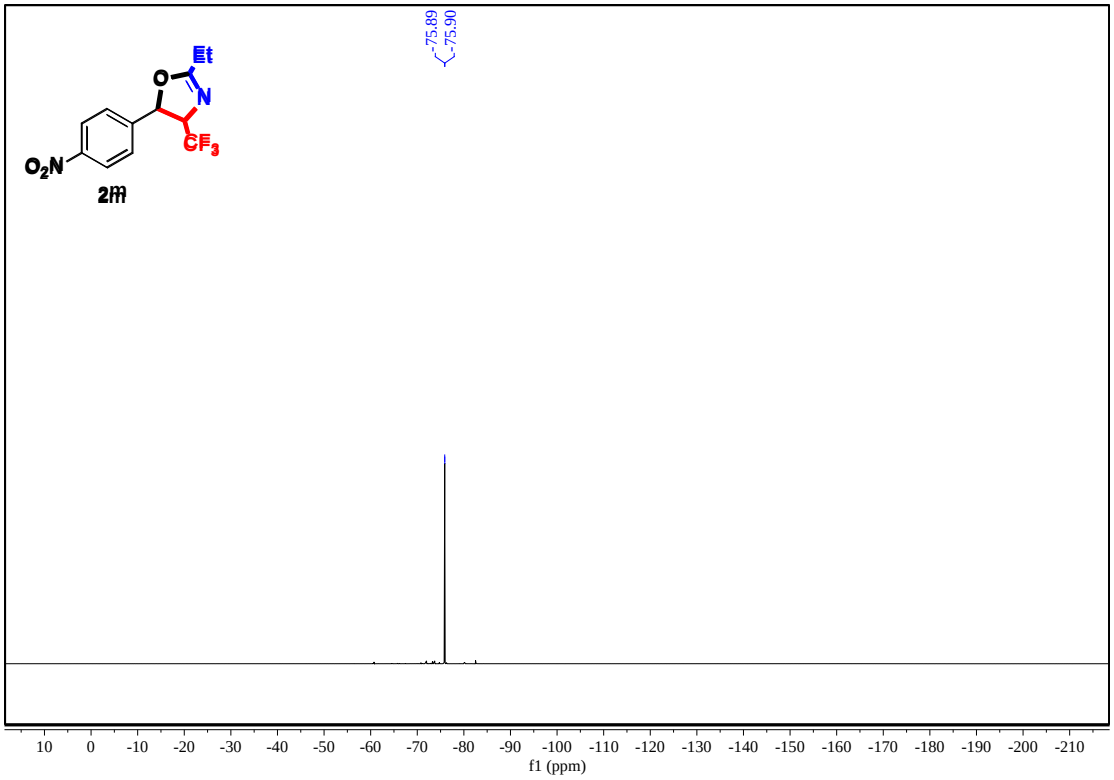

-76.01
-76.03
-76.17
-76.18
Me
O
N
Ph
CF3
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

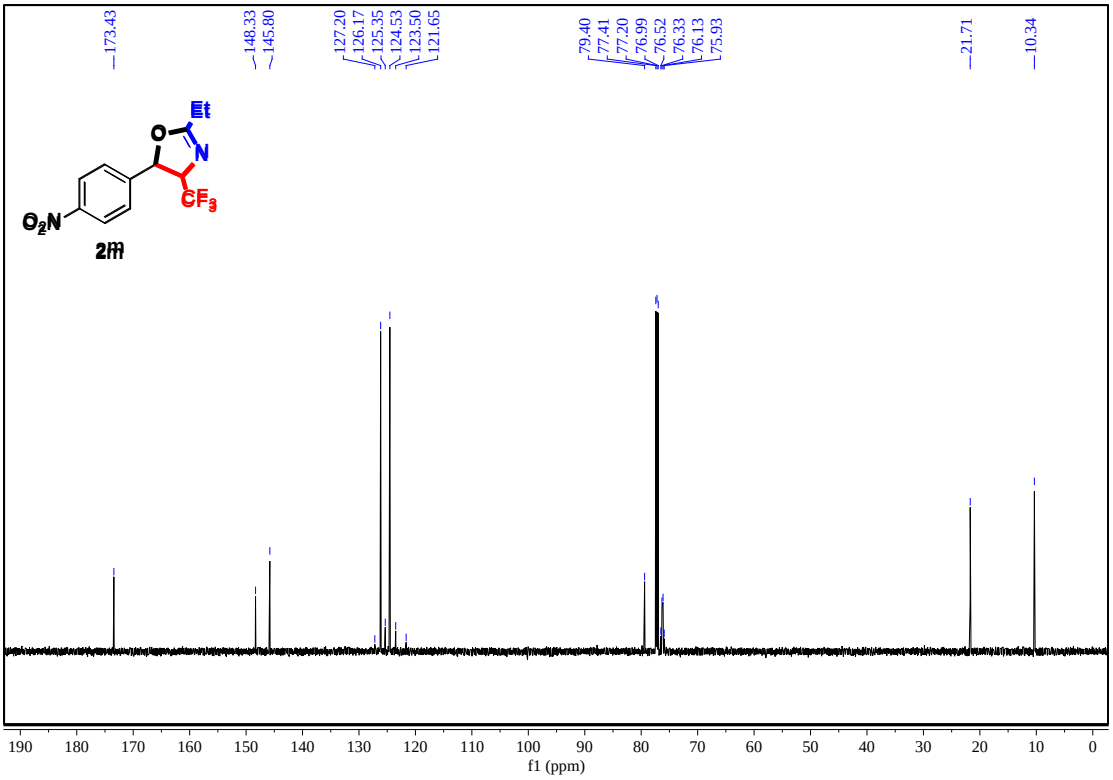
2l

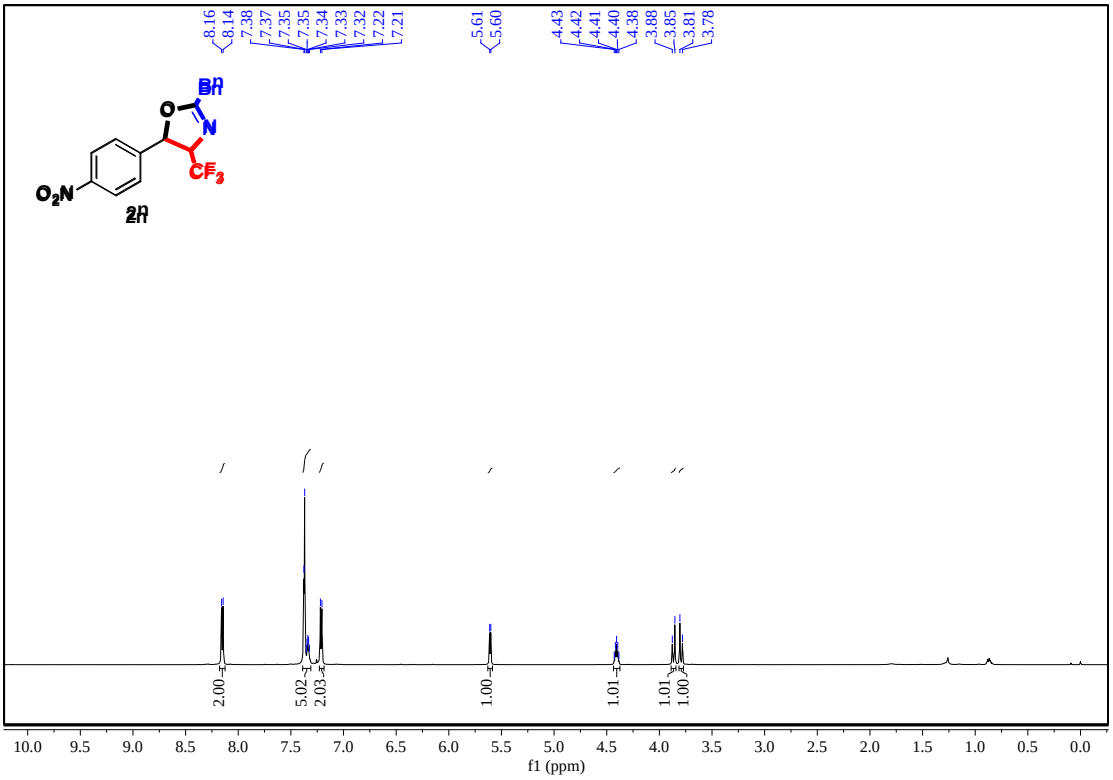

169.06
132.11
129.57
128.59
126.99
125.14
123.29
121.44
121.29
88.51
83.87
77.41
77.20
76.99
75.81
75.61
75.41
75.21
69.48
69.46
14.14
Me
O
N
Ph
CF3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

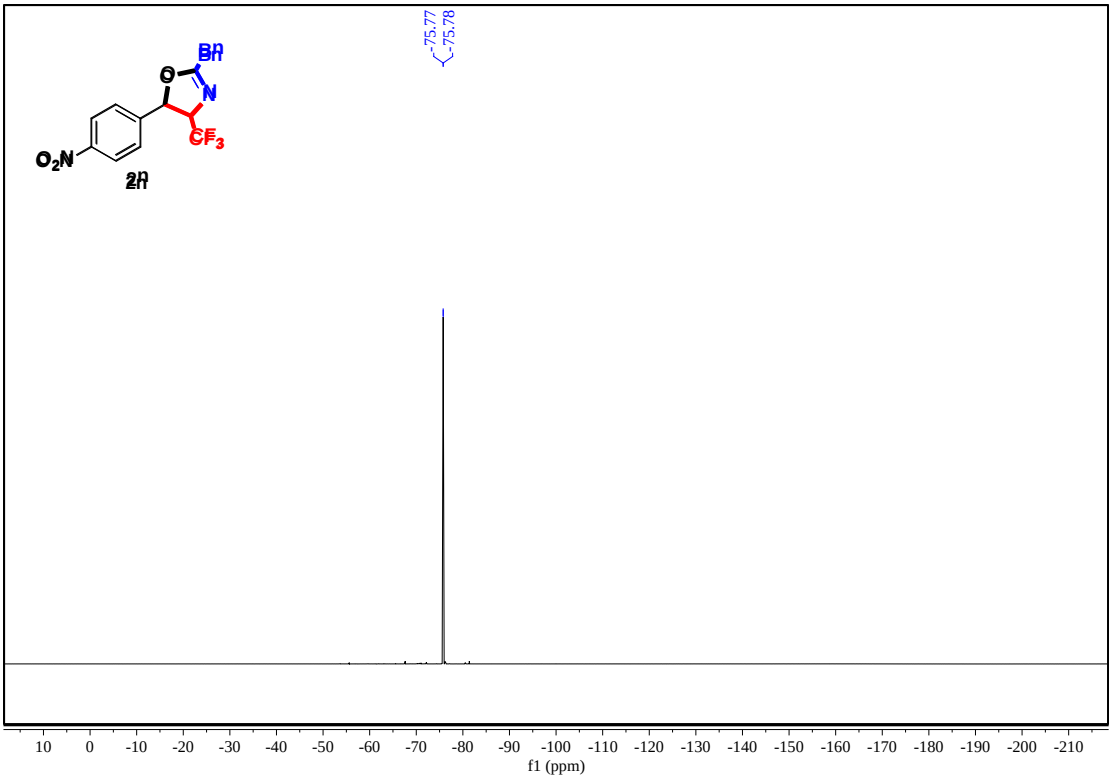
2l

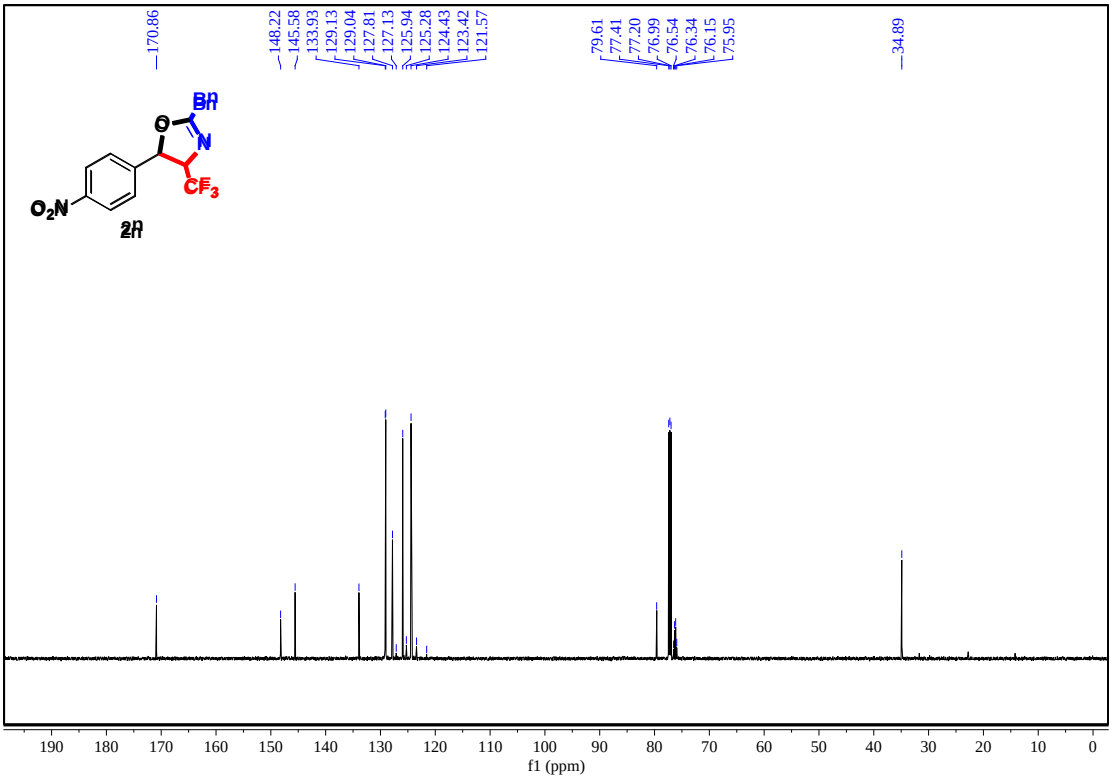

8.26
8.25
7.46
7.44
7.26
5.59
5.58
4.42
4.41
4.40
4.39
4.37
2.53
2.52
2.51
2.50
1.32
1.30
1.29
Et
O
N
CF3
O2N
2m
2.00
2.01
1.00
1.01
2.01
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

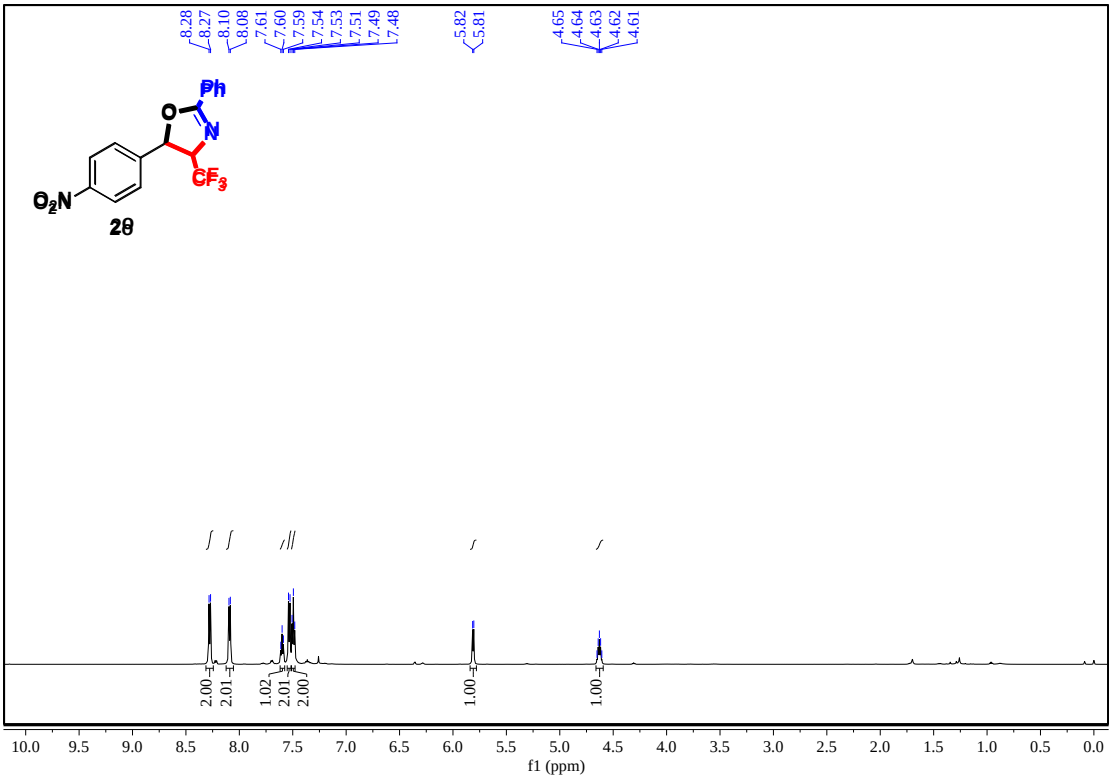

-75.89
-75.90
Et
O
N
CF3
O2N
2m
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

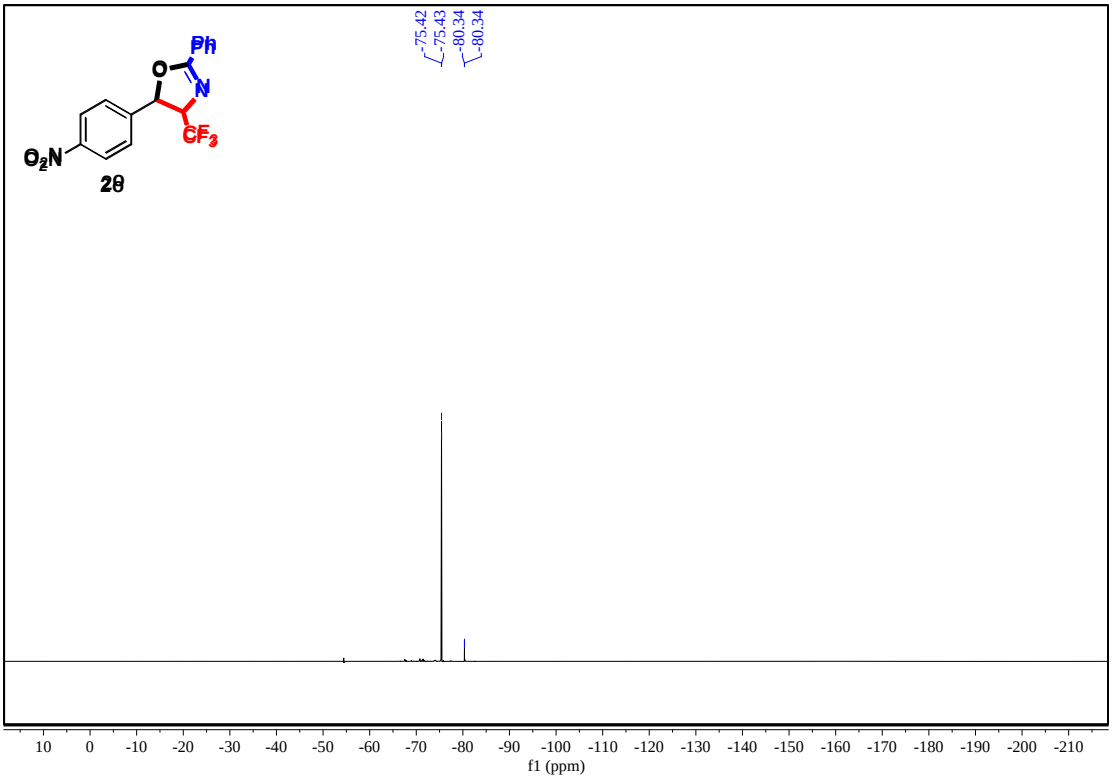

173.43
148.33
145.80
127.20
126.17
125.35
124.53
123.50
121.65
79.40
77.41
77.20
76.99
76.52
76.33
76.13
75.93
21.71
10.34
Et
O
N
CF3
O2N
2m
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

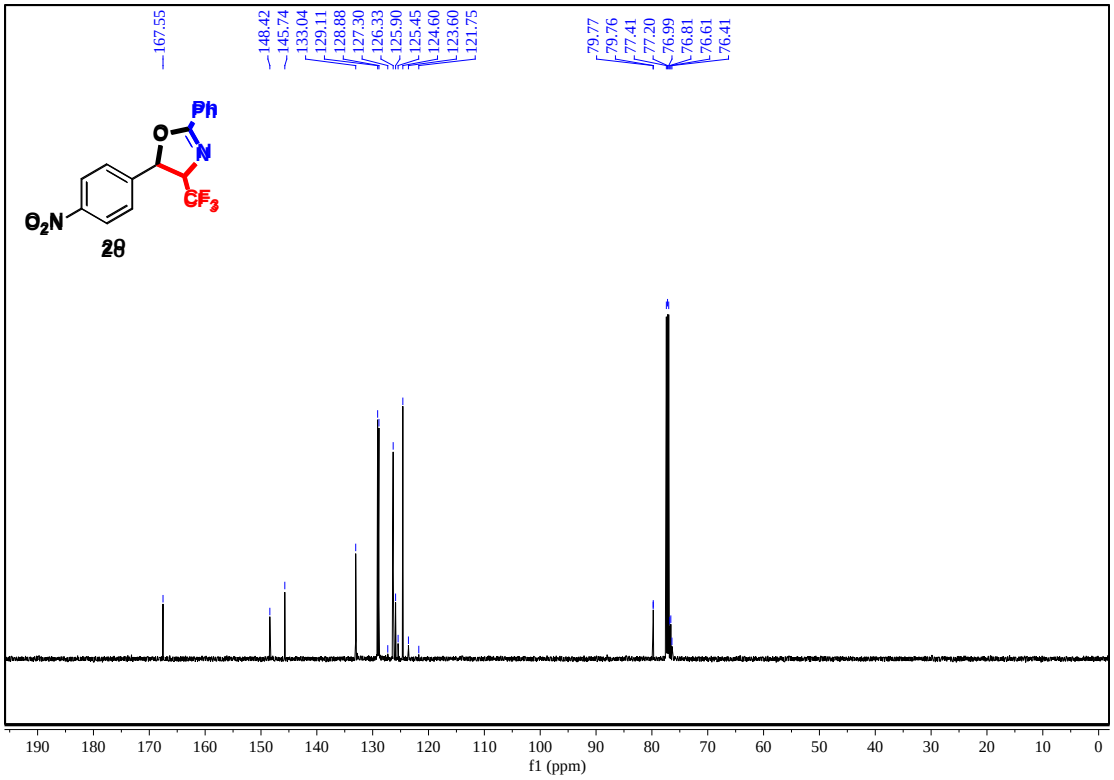

8.16
8.14
7.38
7.37
7.35
7.35
7.34
7.33
7.32
7.22
7.21
5.61
5.60
4.43
4.42
4.41
4.40
4.38
3.88
3.85
3.81
3.78
Bn
O
N
CF3
O2N
2n
2.00
5.02
2.03
1.00
1.01
1.01
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

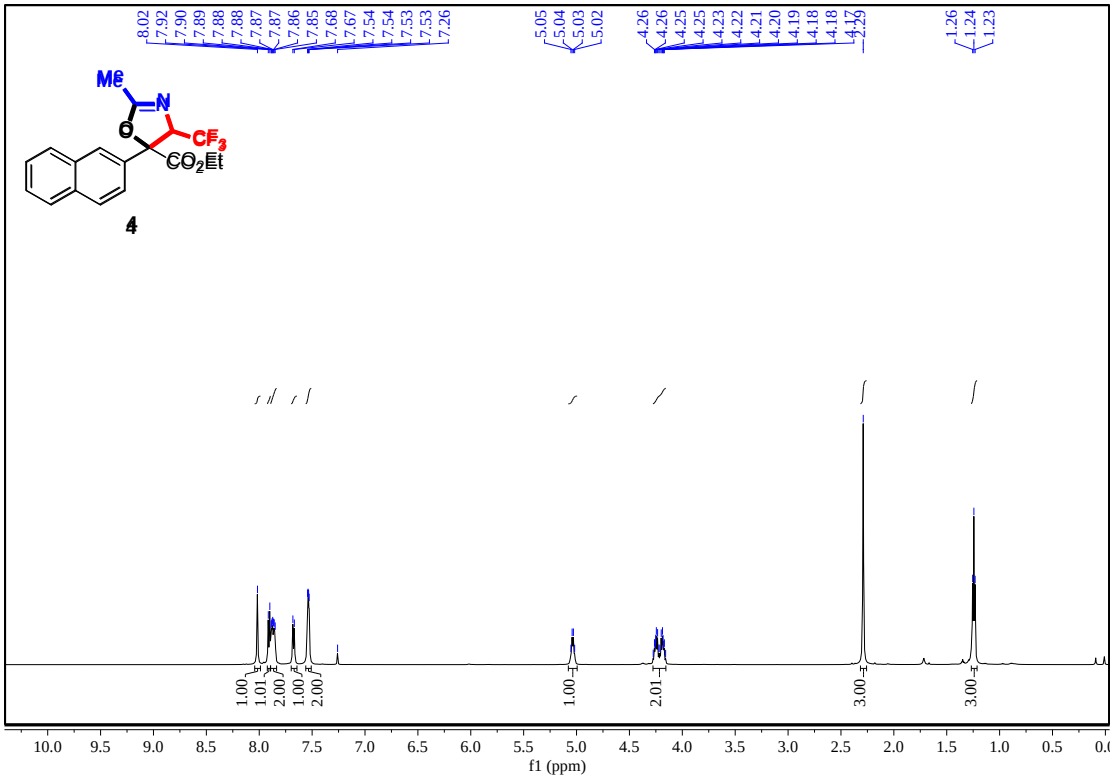

75.77
75.78
Bn
O
N
CF3
O2N
2n
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

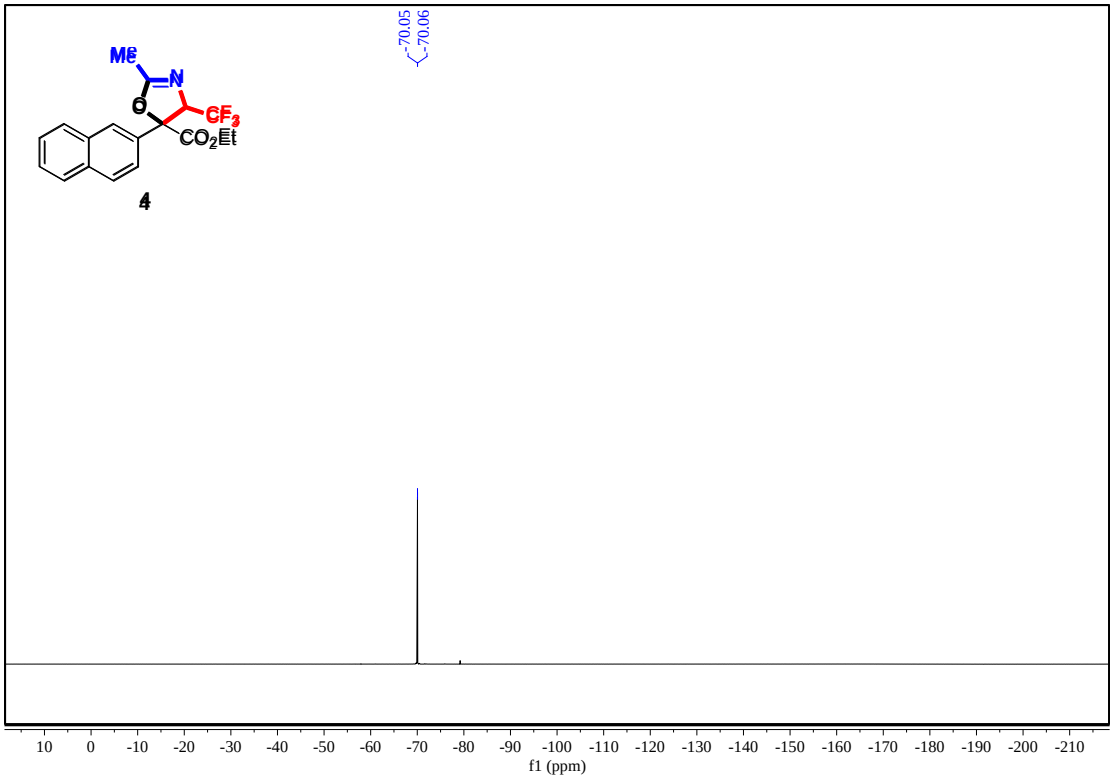

170.86
148.22
145.58
133.93
129.13
129.04
127.81
127.13
125.94
125.28
124.43
123.42
121.57
79.61
77.41
77.20
76.99
76.54
76.34
76.15
75.95
34.89
Bn
O
N
CF3
O2N
2n
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

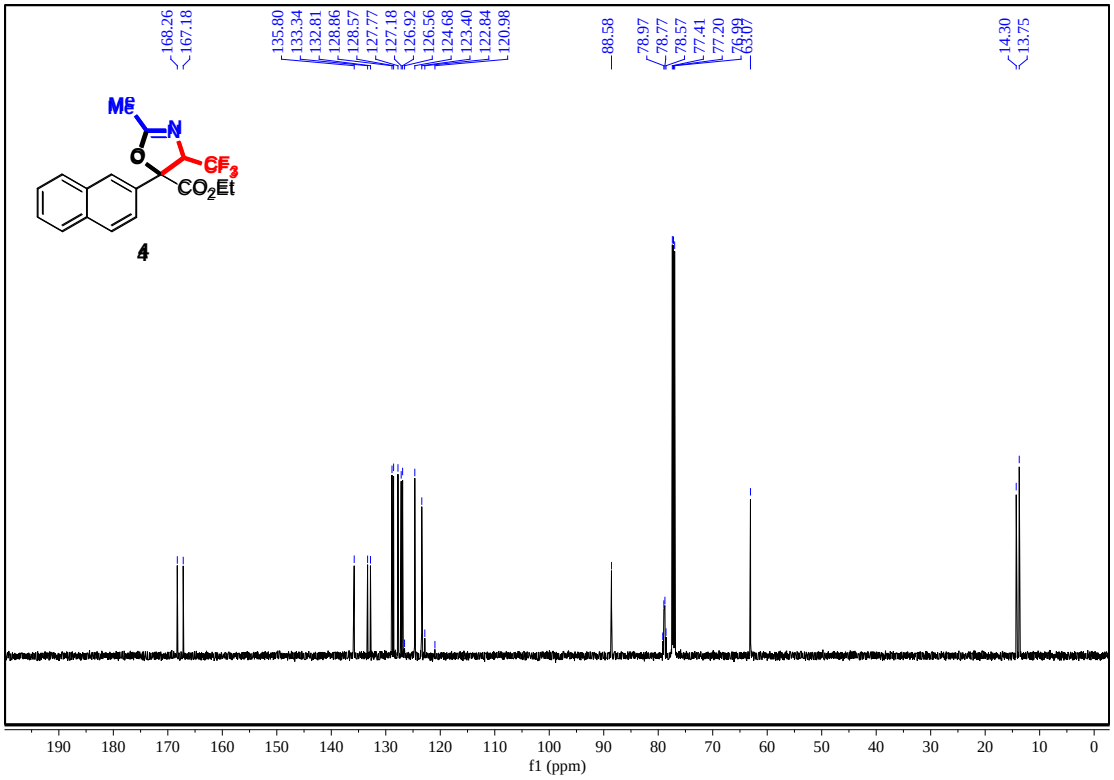

8.28
8.27
8.10
8.08
7.61
7.60
7.59
7.54
7.53
7.51
7.49
7.48
5.82
5.81
4.65
4.64
4.63
4.62
4.61
Ph
O
N
CF3
O2N
2θ
2.00
2.01
1.02
2.01
2.00
1.00
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

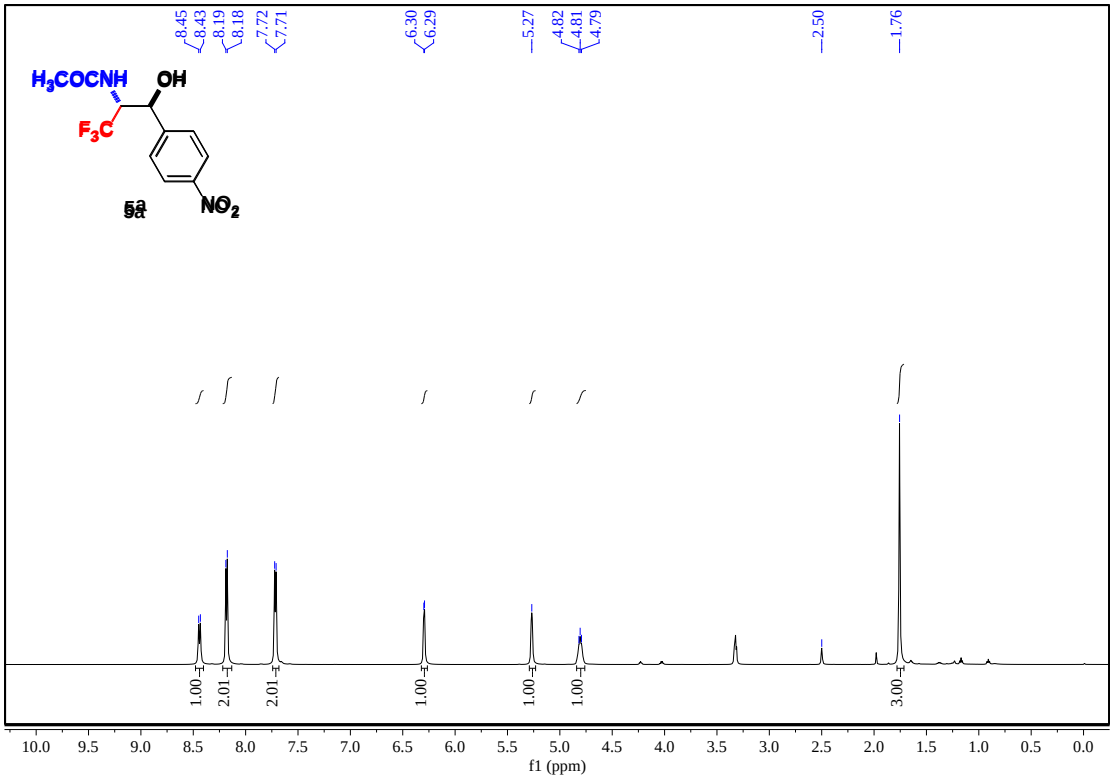

-75.42
-75.43
-80.34
-80.34
Ph
O
N
CF3
O2N
2θ
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

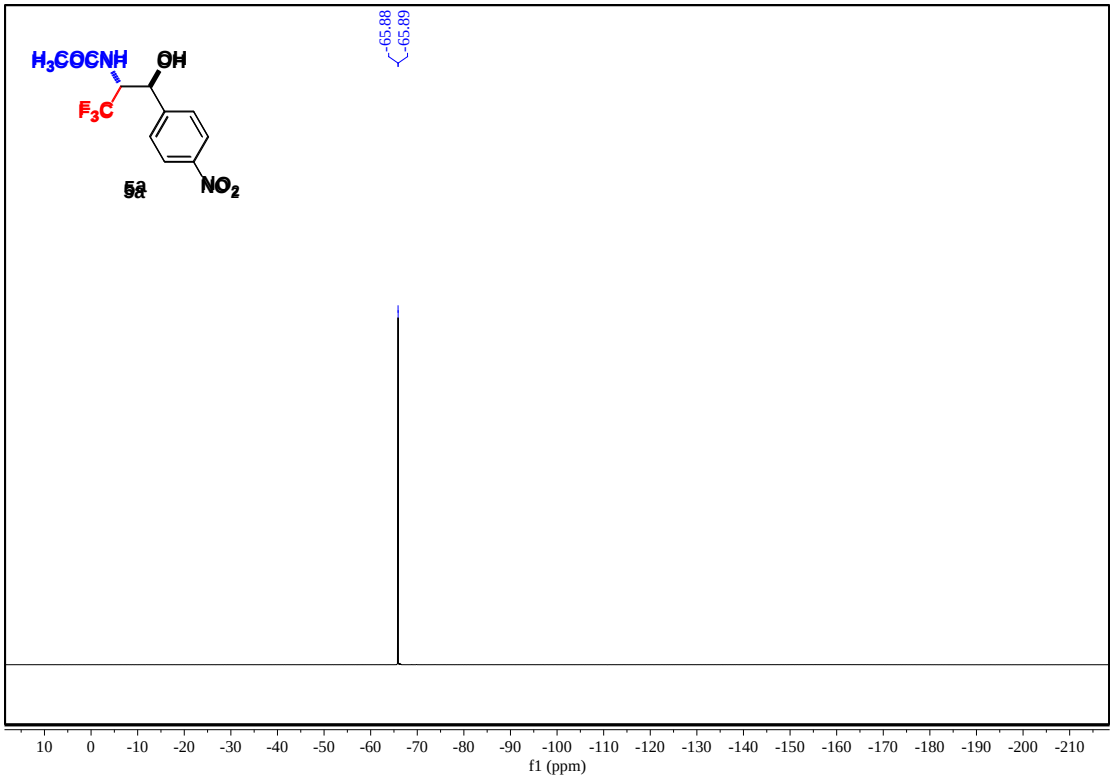

167.55
148.42
145.74
133.04
129.11
128.88
127.30
126.33
125.90
125.45
124.60
123.60
121.75
79.77
79.76
77.41
77.20
76.99
76.81
76.61
76.41
Ph
O
N
CF3
O2N
2θ
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

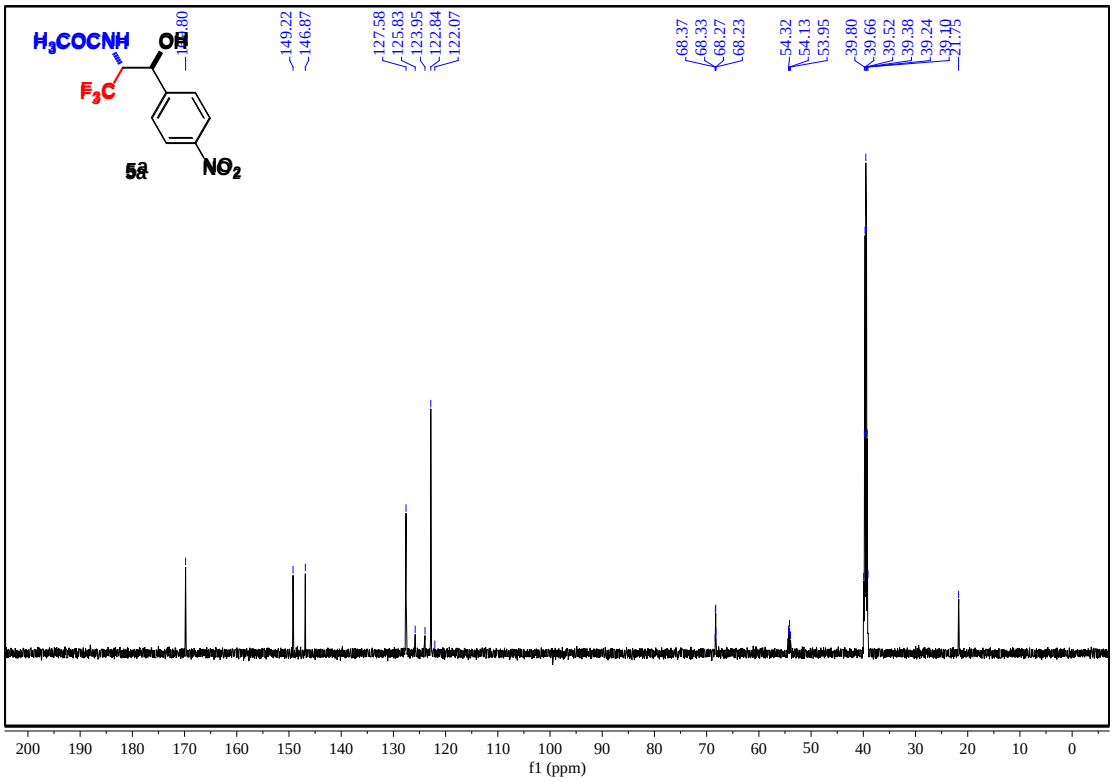

8.02
7.92
7.90
7.89
7.88
7.88
7.87
7.87
7.86
7.85
7.68
7.67
7.54
7.54
7.53
7.53
7.26
5.05
5.04
5.03
5.02
4.26
4.26
4.25
4.25
4.23
4.22
4.21
4.20
4.19
4.18
4.18
4.17
2.29
1.26
1.24
1.23
Me
N
O
CF2
CO2Et
4
1.00
1.01
2.00
1.00
2.00
1.00
2.01
3.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

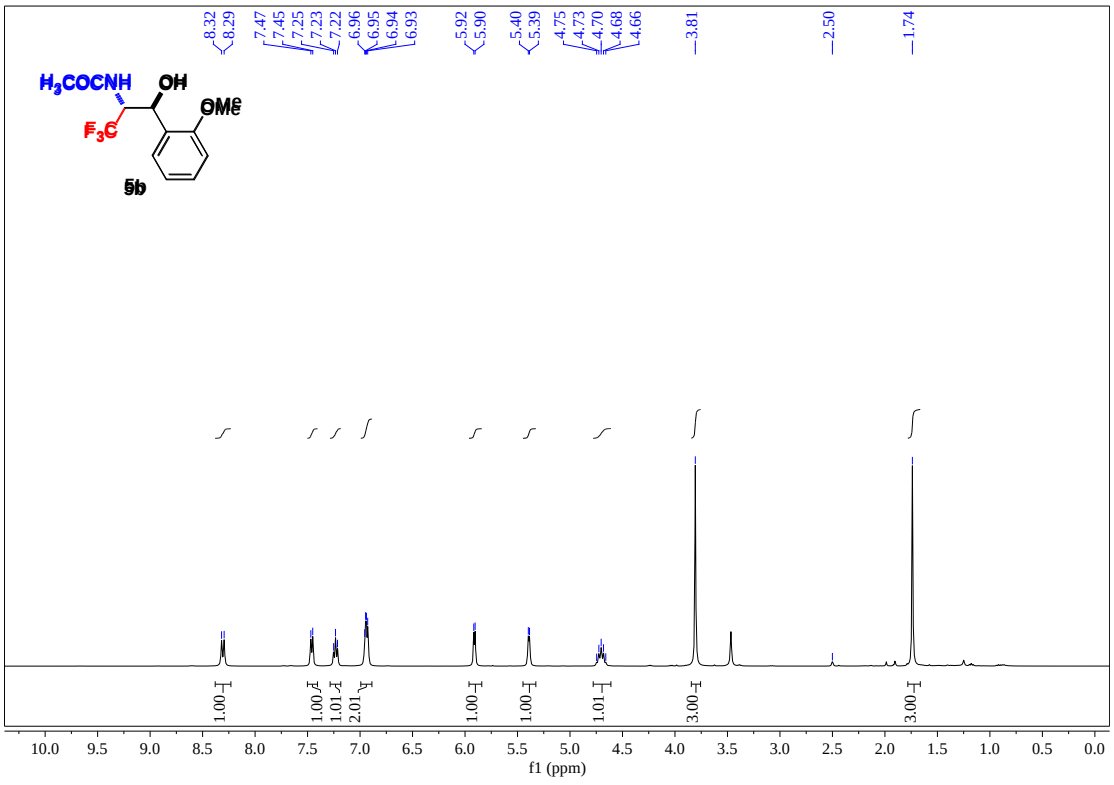

-70.05
-70.06
Me
N
O
CF3
CO2Et
4
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

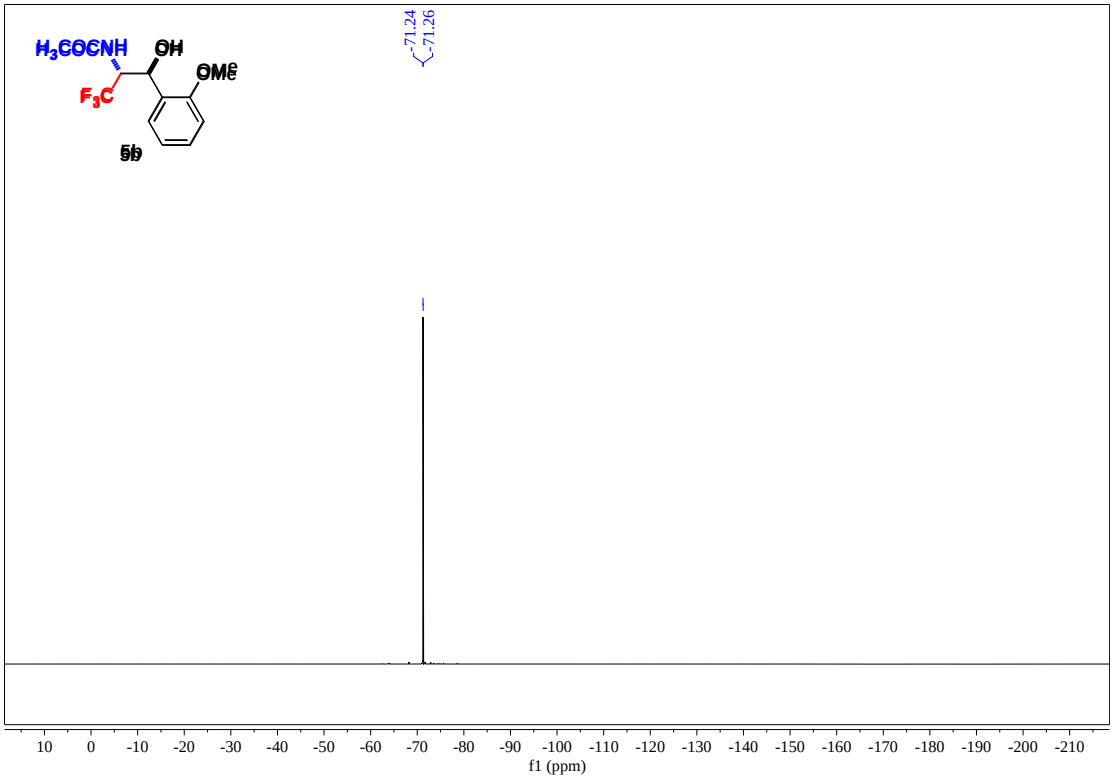

168.26
167.18
135.80
133.34
132.81
128.86
128.57
127.77
127.18
126.92
126.56
124.68
123.40
122.84
120.98
88.58
78.97
78.77
78.57
77.41
77.20
76.99
63.07
14.30
13.75
Me
N
O
CF3
CO2Et
4
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.45
8.43
8.19
8.18
7.72
7.71
6.30
6.29
5.27
4.82
4.81
4.79
2.50
1.76
H3COCNH
OH
F3C
NO2
1.00
2.01
2.01
1.00
1.00
1.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


-65.88
-65.89
H3COCNH
OH
F3C
NO2
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


H3COCNH
OH
F3C
NO2
5a
169.80
149.22
146.87
127.58
125.83
123.95
122.84
122.07
68.37
68.33
68.27
68.23
54.32
54.13
53.95
39.80
39.66
39.52
39.38
39.24
39.10
21.75
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


H3COCNH
OH
OMe
F3C
5b
8.32
8.29
7.47
7.45
7.25
7.23
7.22
6.96
6.95
6.94
6.93
5.92
5.90
5.40
5.39
4.75
4.73
4.70
4.68
4.66
3.81
2.50
1.74
1.00
1.00
1.01
2.01
1.00
1.00
1.01
3.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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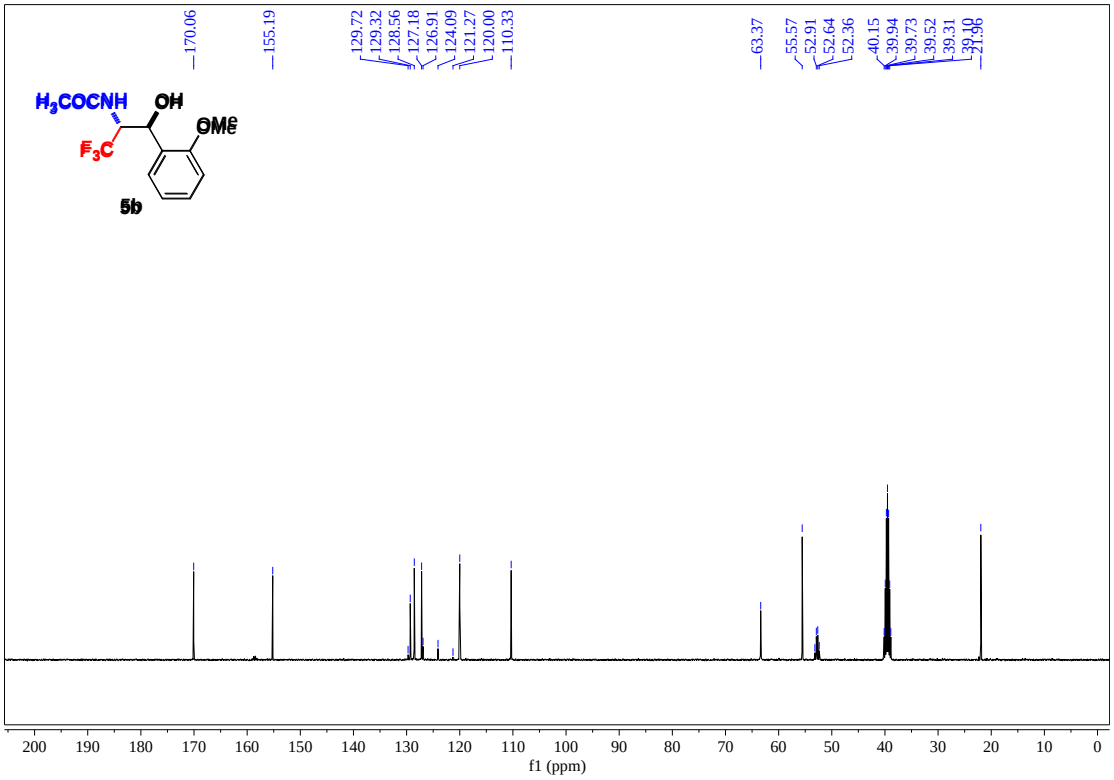
OH
OMe
F3C
5b
-71.24
-71.26
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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129.72
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128.56
127.18
126.91
124.09
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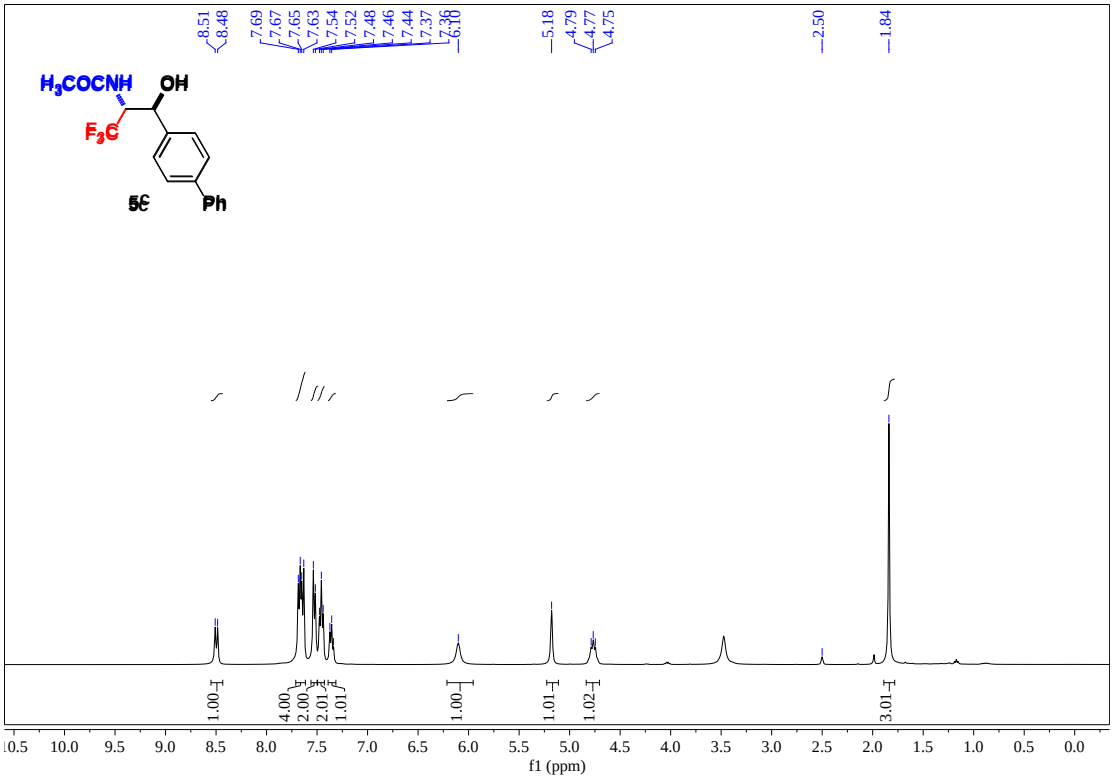
120.00
110.33
63.37
55.57
52.91
52.64
52.36
40.15
39.94
39.73
39.52
39.31
39.10
21.98
H3COCNH
OH
OMe
F3C
5b
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.48
7.69
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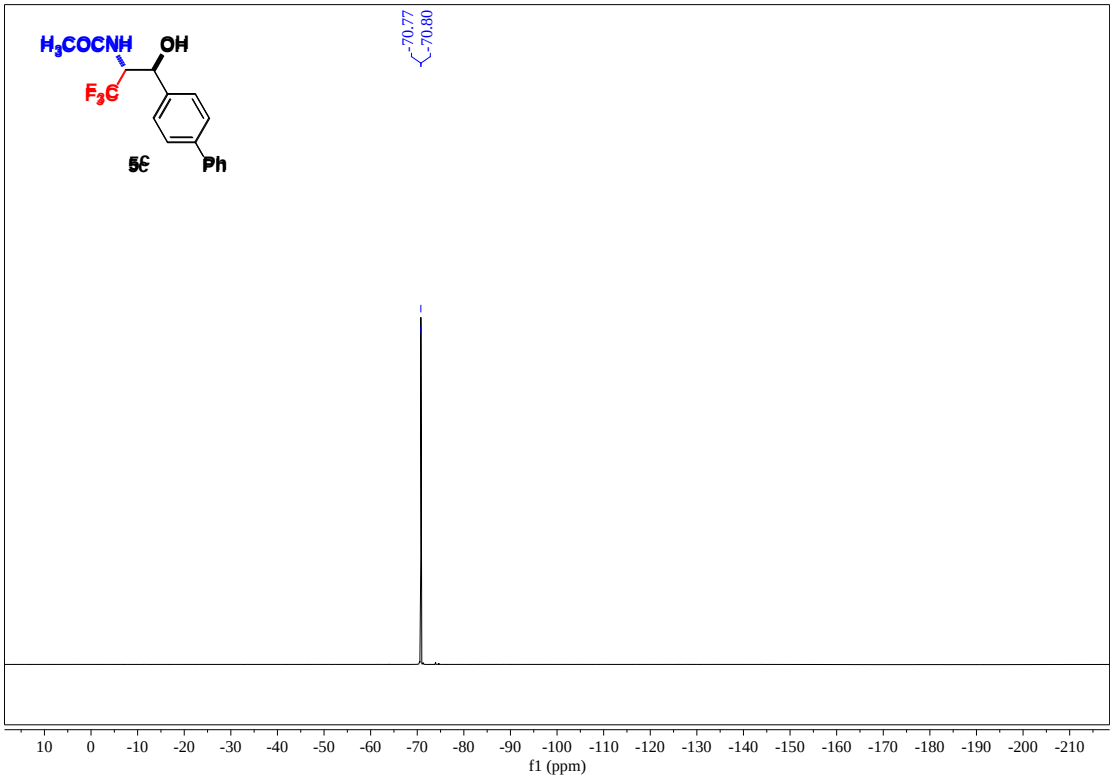
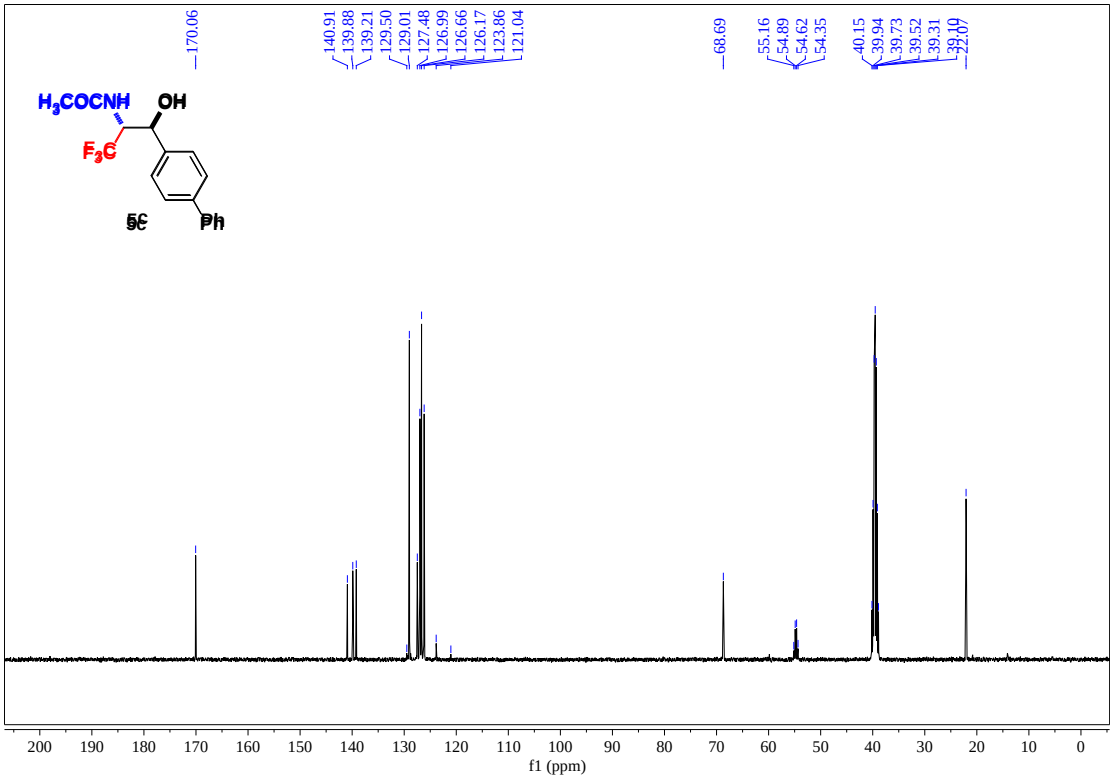
7.65
7.63
7.54
7.52
7.48
7.46
7.44
7.37
7.36
6.10
5.18
4.79
4.77
4.75
2.50
1.84
H3COCNH
OH
F3C
Ph
1.00
4.00
2.00
2.01
1.01
1.00
1.01
1.02
3.01
f1 (ppm)


-70.77
-70.80
H3COCNH
OH
F3C
Ph
f1 (ppm)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139.88
139.21
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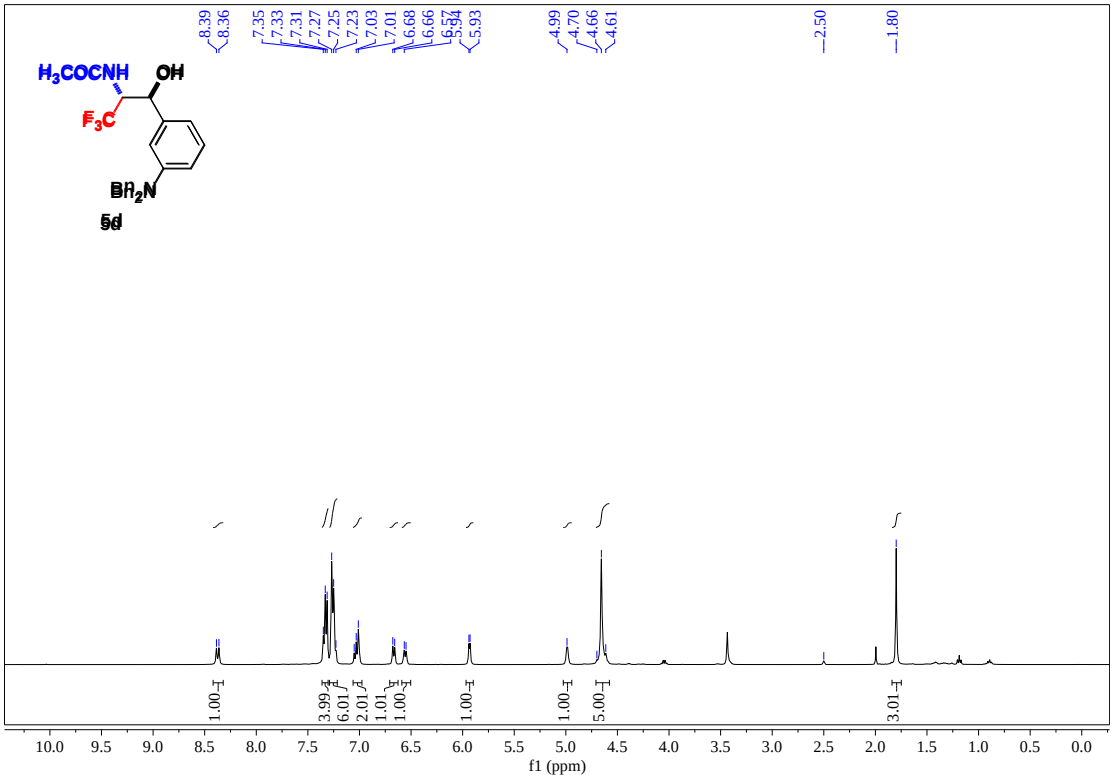
127.48
126.99
126.66
126.17
123.86
121.04
68.69
55.16
54.89
54.62
54.35
40.15
39.94
39.73
39.52
39.31
39.10
22.07
H3COCNH
OH
F3C
5c
Ph
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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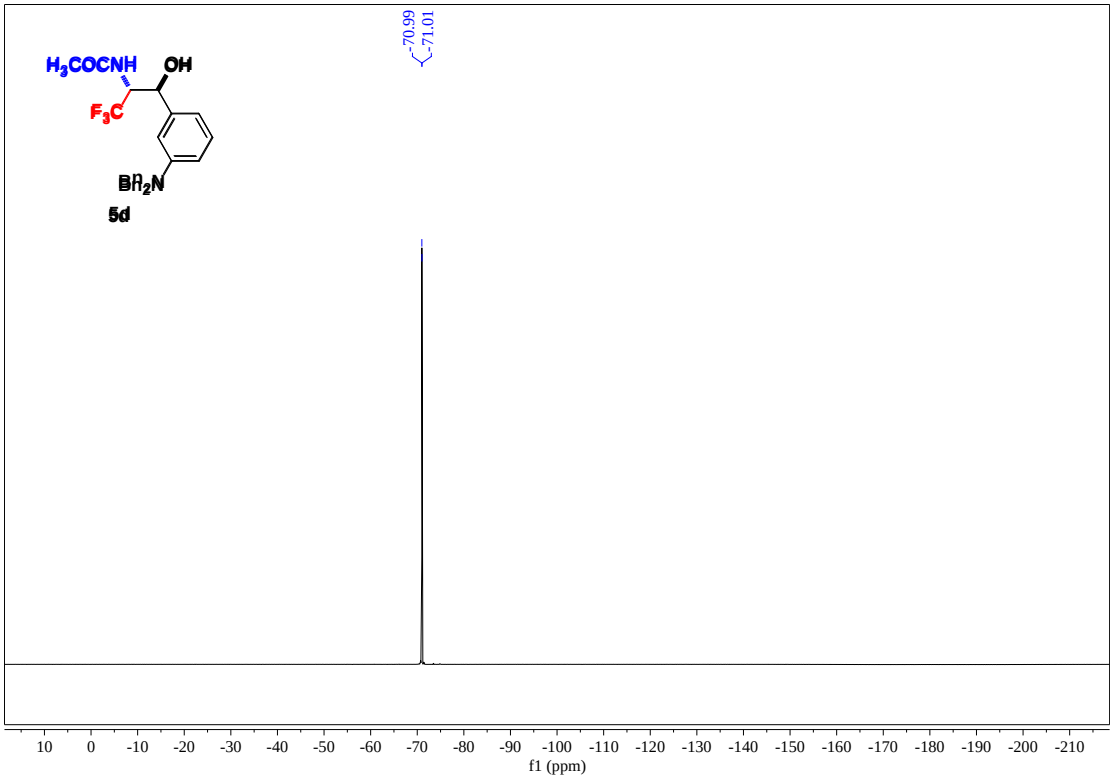
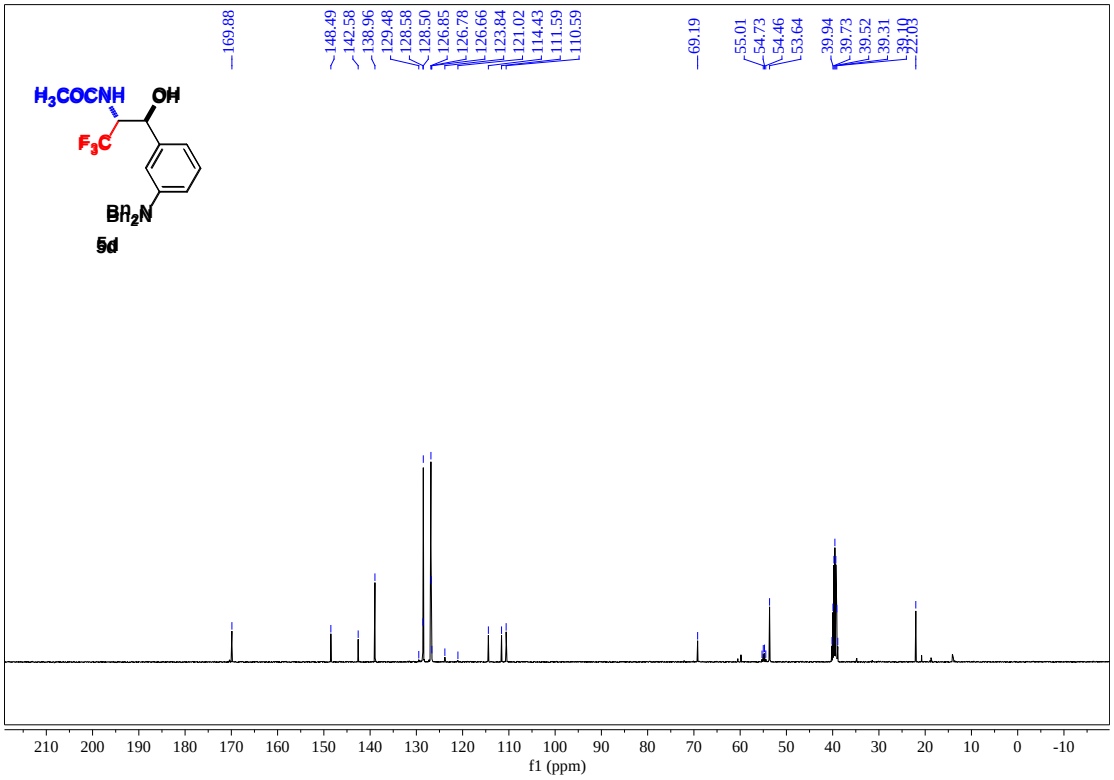
8.36
7.35
7.33
7.31
7.27
7.25
7.23
7.03
7.01
6.68
6.66
6.57
5.94
5.93
4.99
4.70
4.66
4.61
2.50
1.80
H3COCNH
OH
F3C
Bn2N
5d
1.00
3.99
6.01
2.01
1.01
1.00
1.00
1.00
5.00
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


-70.99
-71.01
H3COCNH
OH
F3C
Br2N
5d
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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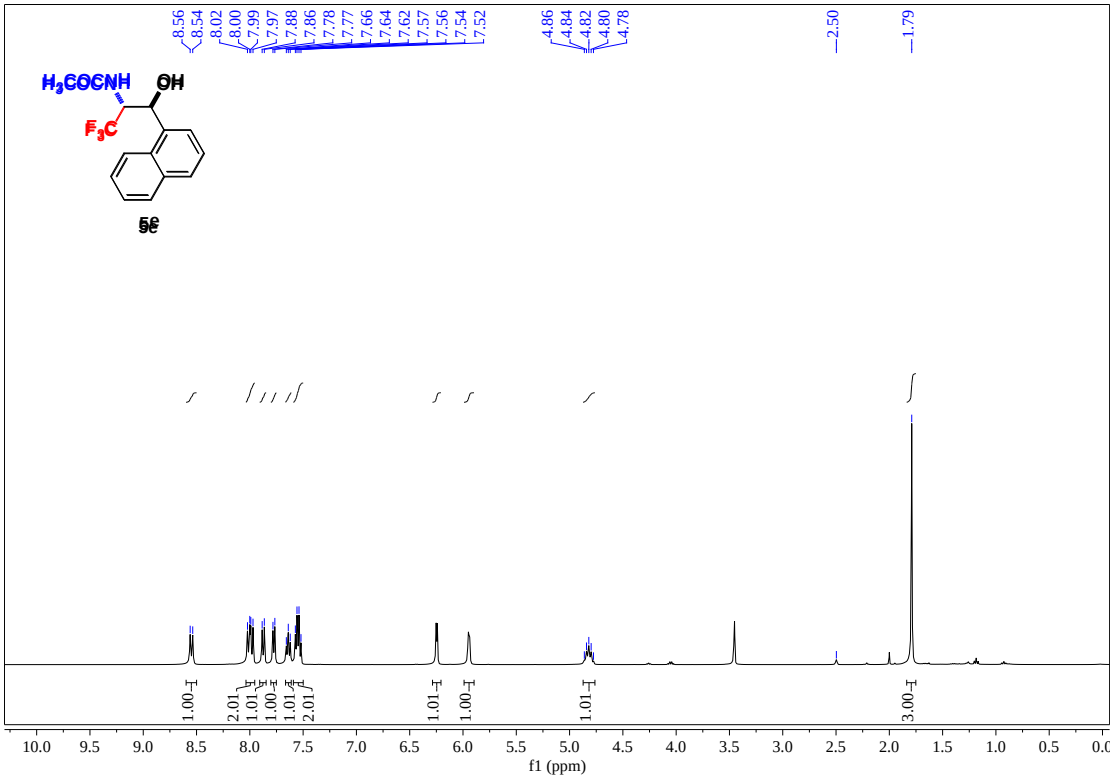
148.49
142.58
138.96
129.48
128.58
128.50
126.85
126.78
126.66
123.84
121.02
114.43
111.59
110.59
69.19
55.01
54.73
54.46
53.64
39.94
39.73
39.52
39.31
39.10
22.03
H3COCNH
OH
F3C
Br2N
5d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.54
8.02
8.00
7.99
7.97
7.88
7.86
7.78
7.77
7.66
7.64
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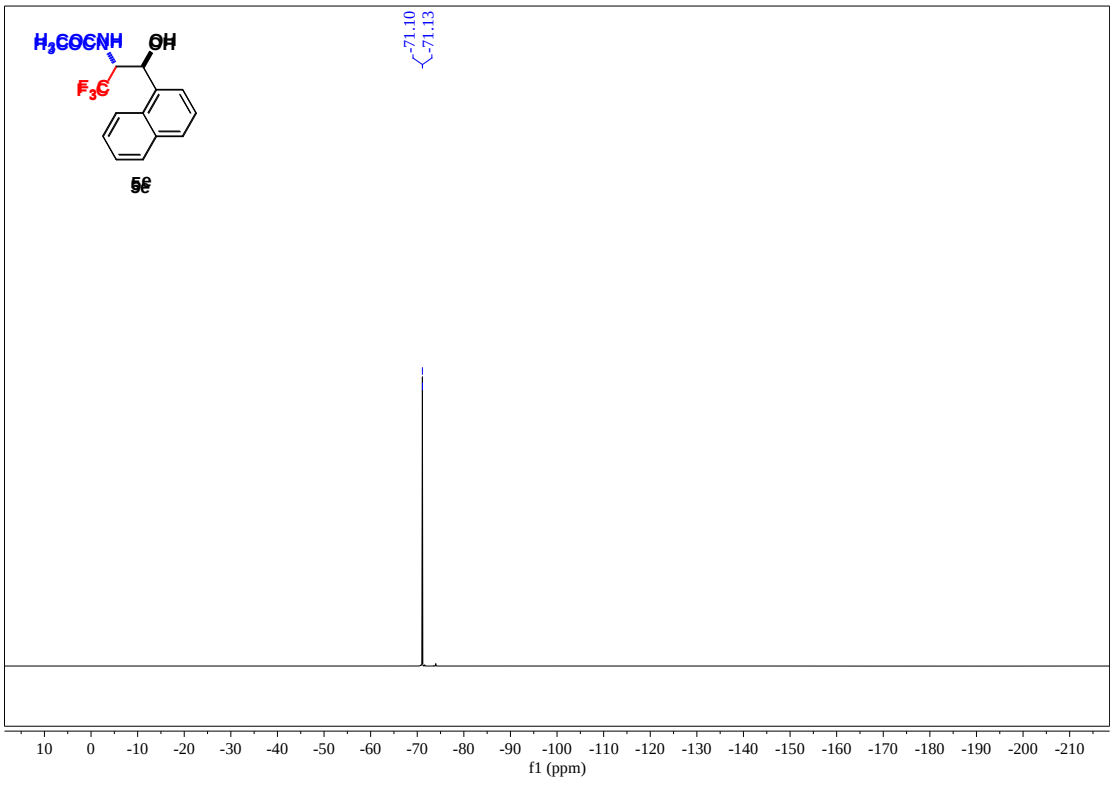
7.57
7.56
7.54
7.52
4.86
4.84
4.82
4.80
4.78
2.50
1.79
H3COCNH
OH
F3C
5e
1.00
2.01
1.01
1.00
1.01
2.01
1.01
1.00
1.01
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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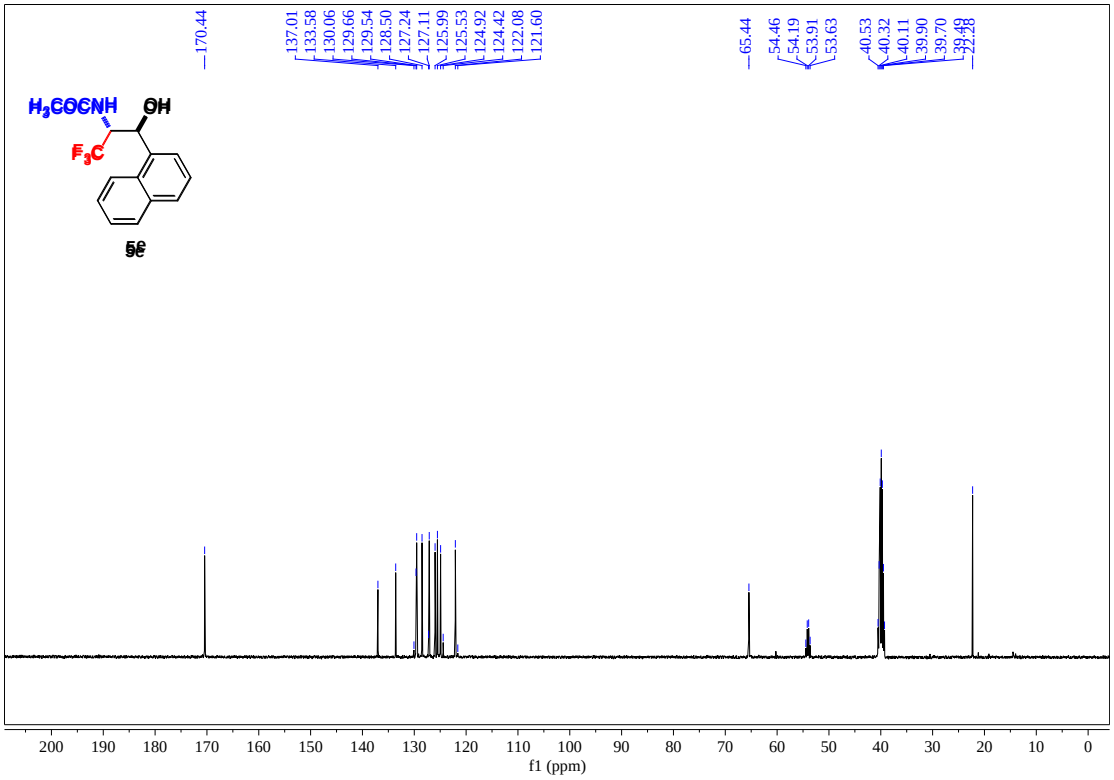
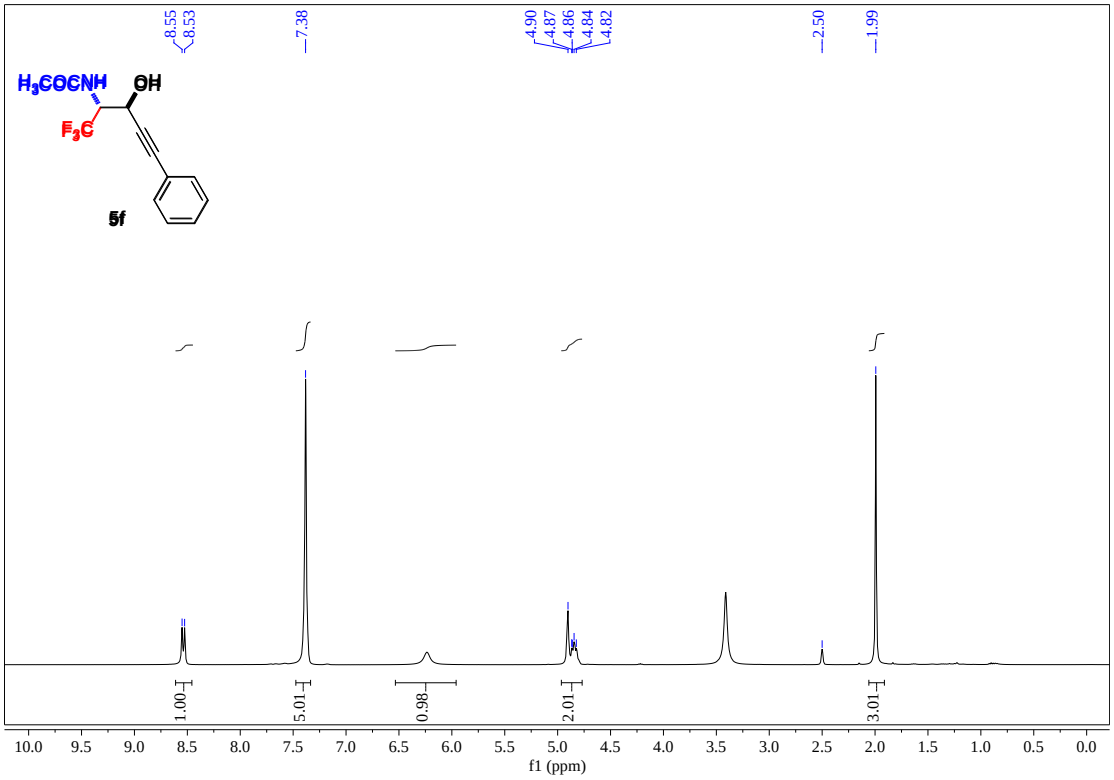
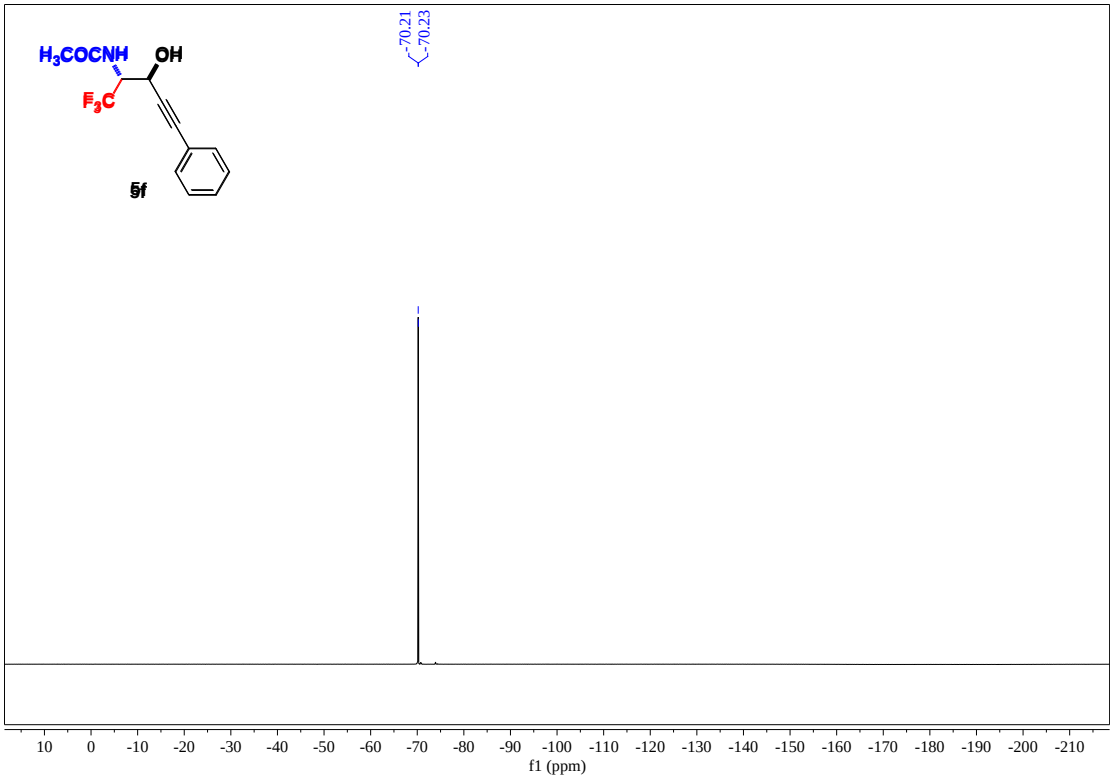
-71.13
H3COCNH
OH
F3C
5e
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


170.44
137.01
133.58
130.06
129.66
129.54
128.50
127.24
127.11
125.99
125.53
124.92
124.42
122.08
121.60
65.44
54.46
54.19
53.91
53.63
40.53
40.32
40.11
39.90
39.70
39.49
39.28
22.28
H3COCNH
OH
F3C
5e
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.55
8.53
7.38
4.90
4.87
4.86
4.84
4.82
2.50
1.99
H3COCNH
OH
F3C
5f
1.00
5.01
0.98
2.01
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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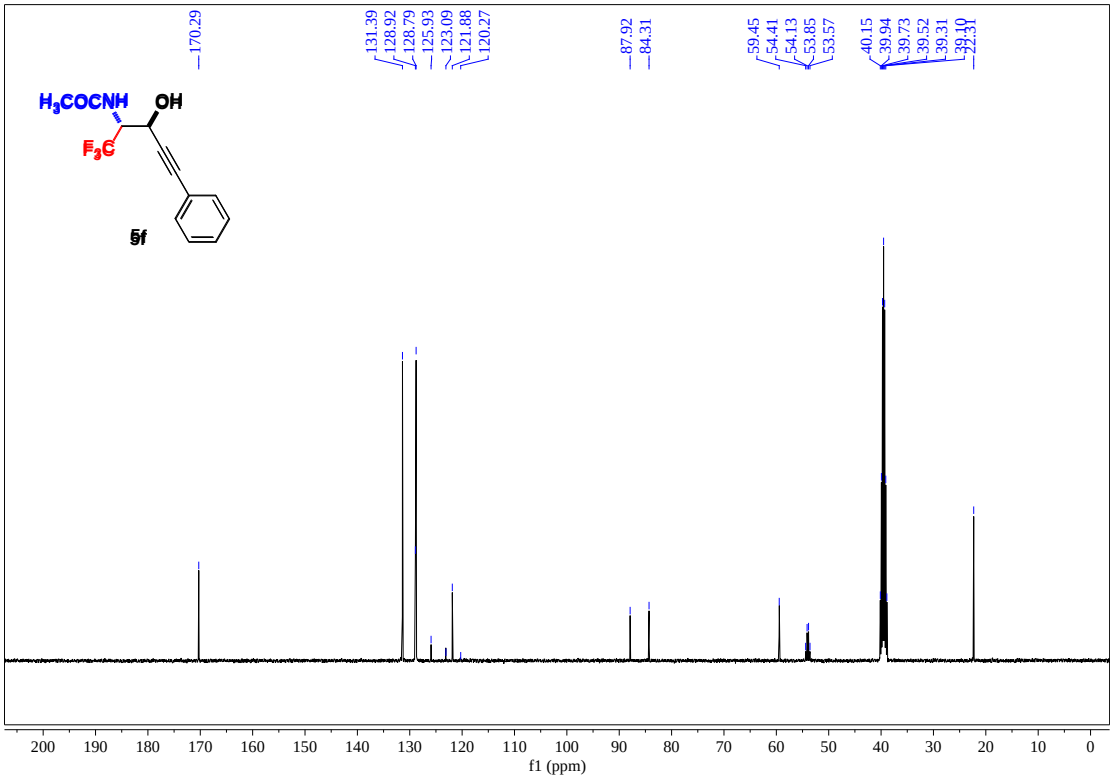
OH
F3C
5f
-70.21
-70.23
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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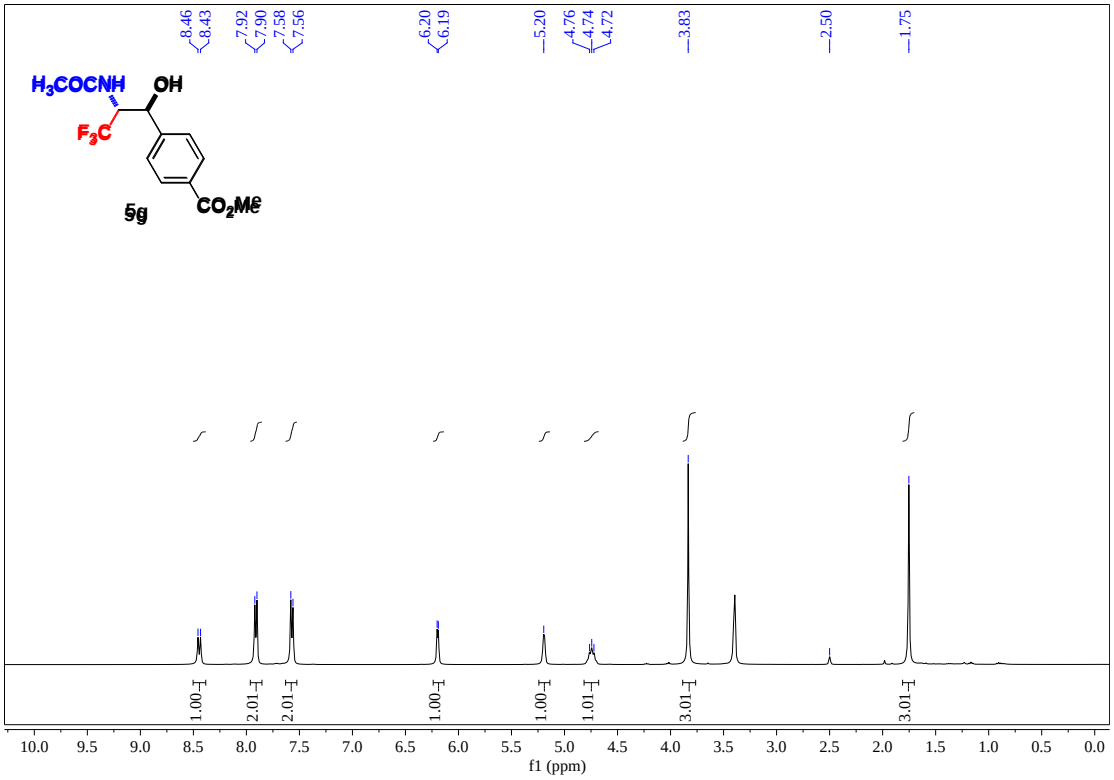
131.39
128.92
128.79
125.93
123.09
121.88
120.27
87.92
84.31
59.45
54.41
54.13
53.85
53.57
40.15
39.94
39.73
39.52
39.31
39.10
22.31
H3COCNH
OH
F3C
5f
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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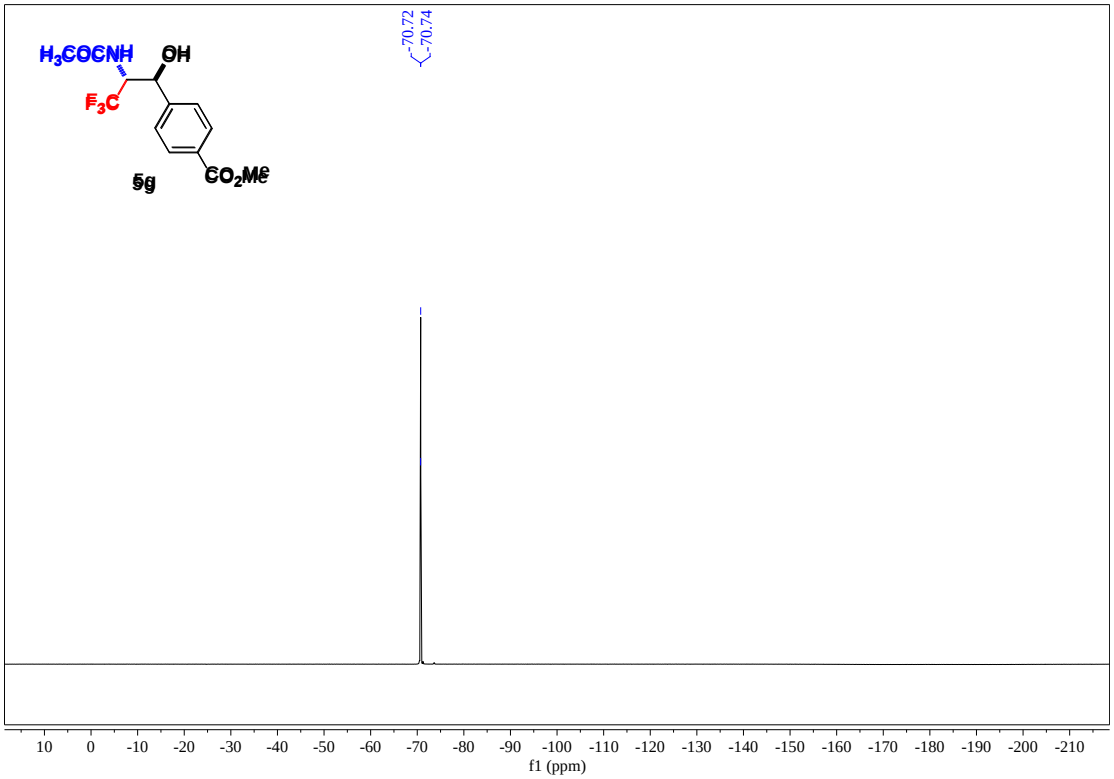
8.43
7.92
7.90
7.58
7.56
6.20
6.19
5.20
4.76
4.74
4.72
3.83
2.50
1.75
H3COCNH
OH
F3C
CO2Me
5g
1.00
2.01
2.01
1.00
1.00
1.01
3.01
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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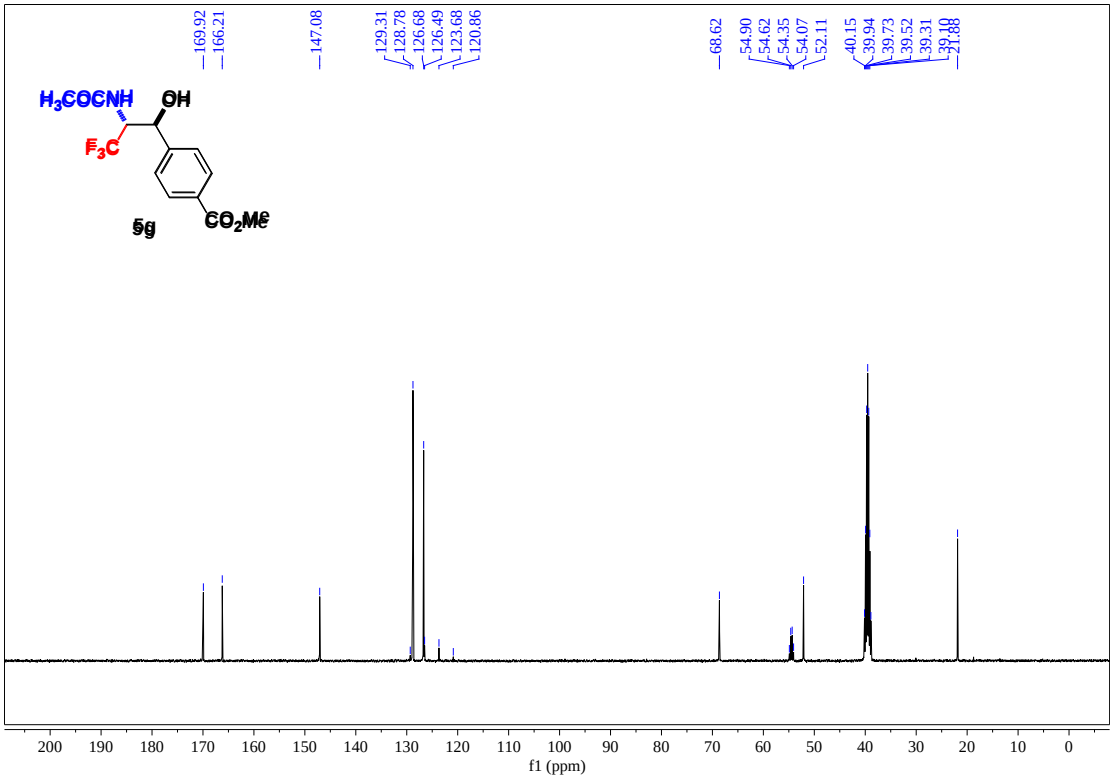
-70.74
H3COCNH
OH
F3C
CO2Me
5g
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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166.21
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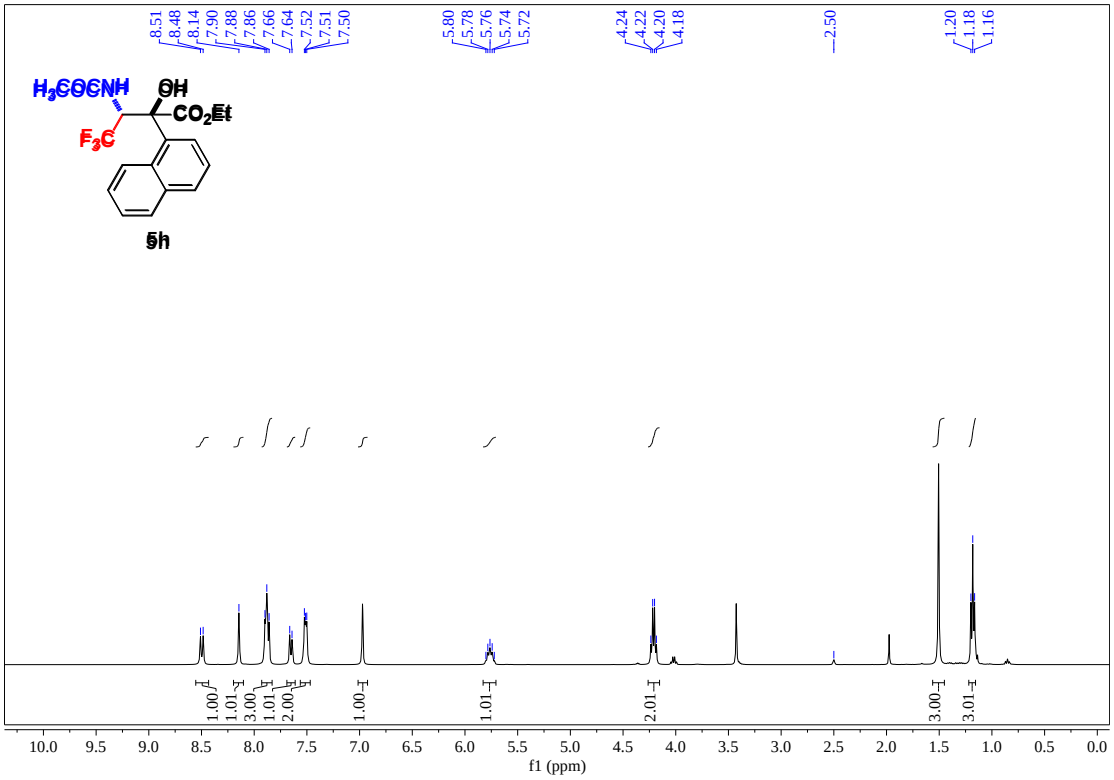
128.78
126.68
126.49
123.68
120.86
68.62
54.90
54.62
54.35
54.07
52.11
40.15
39.94
39.73
39.52
39.31
39.10
21.88
H3COCNH
OH
F3C
CO2Me
5g
f1 (ppm)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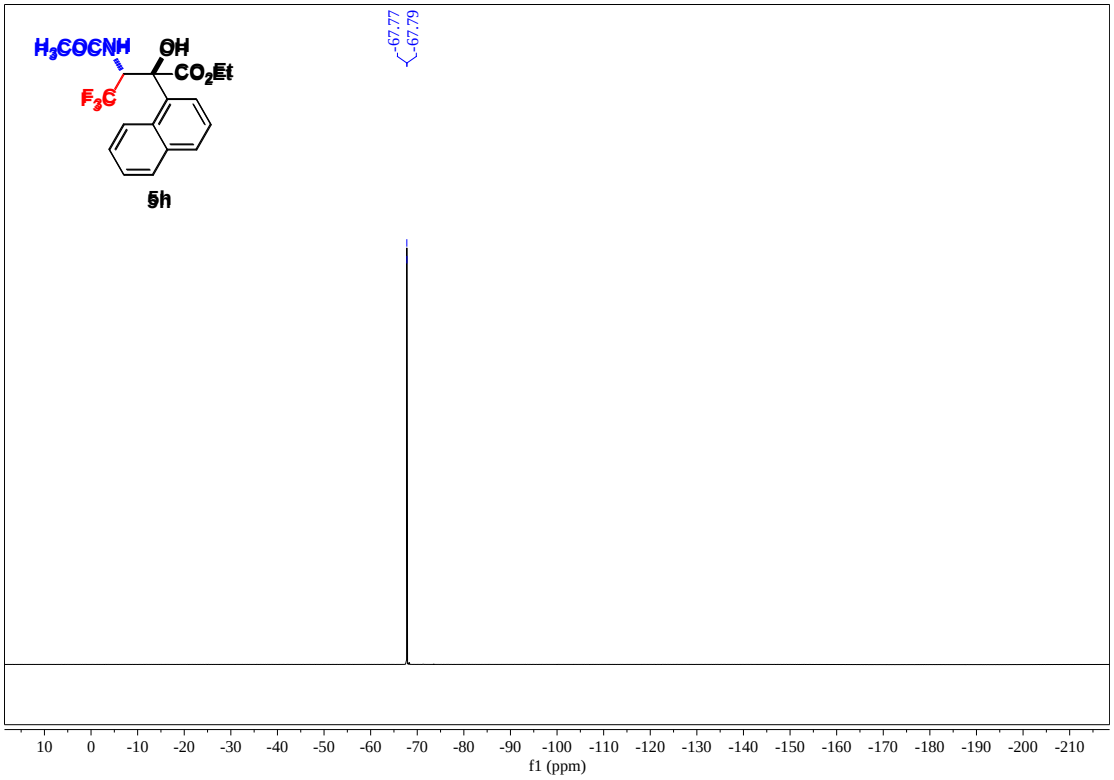
7.88
7.86
7.66
7.64
7.52
7.51
7.50
5.80
5.78
5.76
5.74
5.72
4.24
4.22
4.20
4.18
2.50
1.20
1.18
1.16
H3COCNH
OH
CO2Et
F3C
5h
1.00
1.01
3.00
1.01
2.00
1.00
1.01
2.01
3.00
3.01
f1 (ppm)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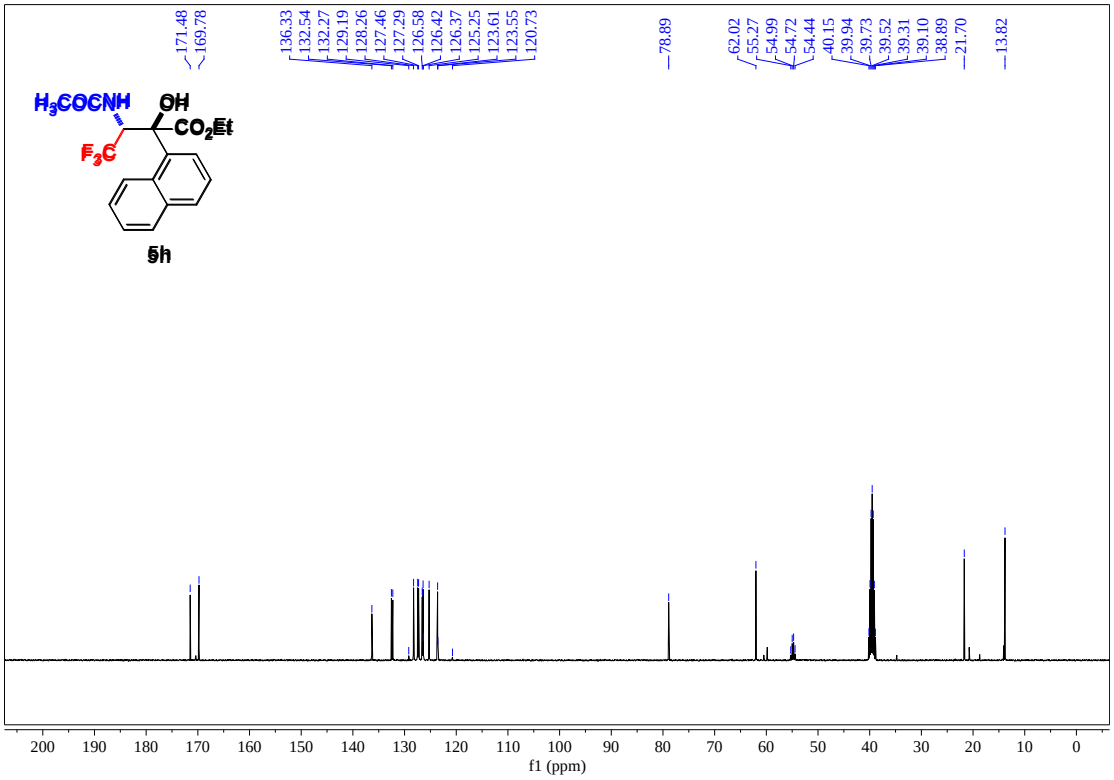
F3C
5h
-67.77
-67.79
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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126.58
126.42
126.37
125.25
123.61
123.55
120.73
78.89
62.02
55.27
54.99
54.72
54.44
40.15
39.94
39.73
39.52
39.31
39.10
38.89
21.70
13.82
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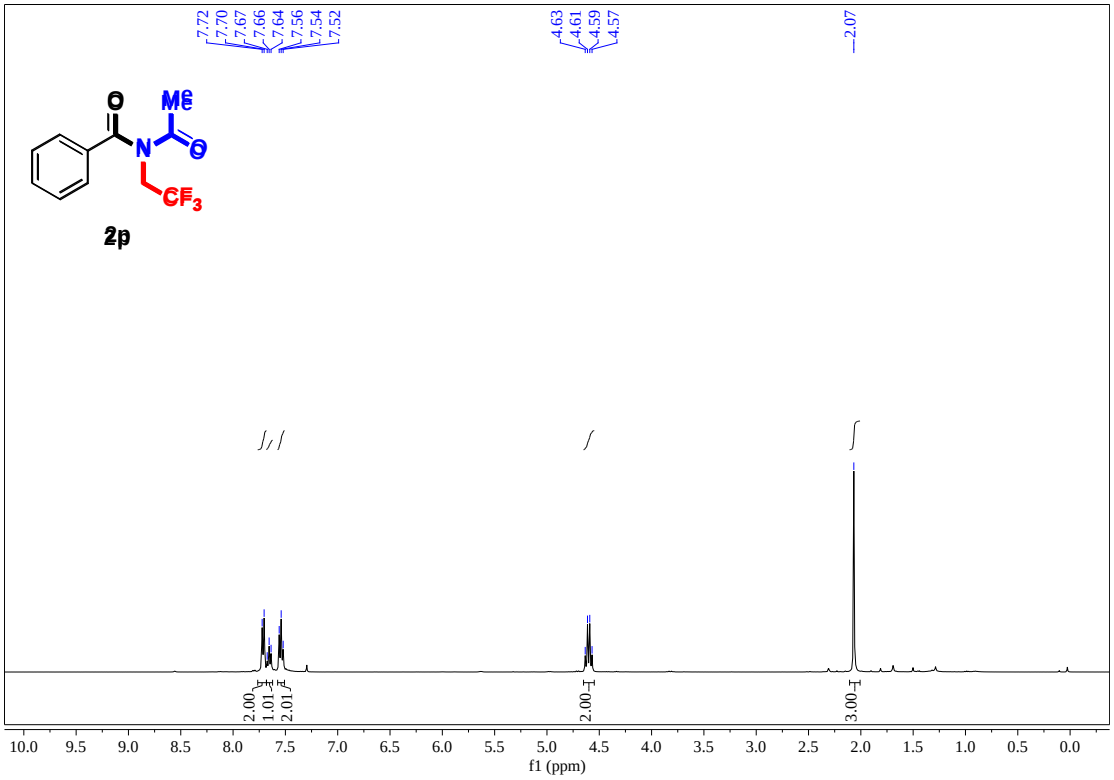
OH
CO2Et
F3C
5h
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.70
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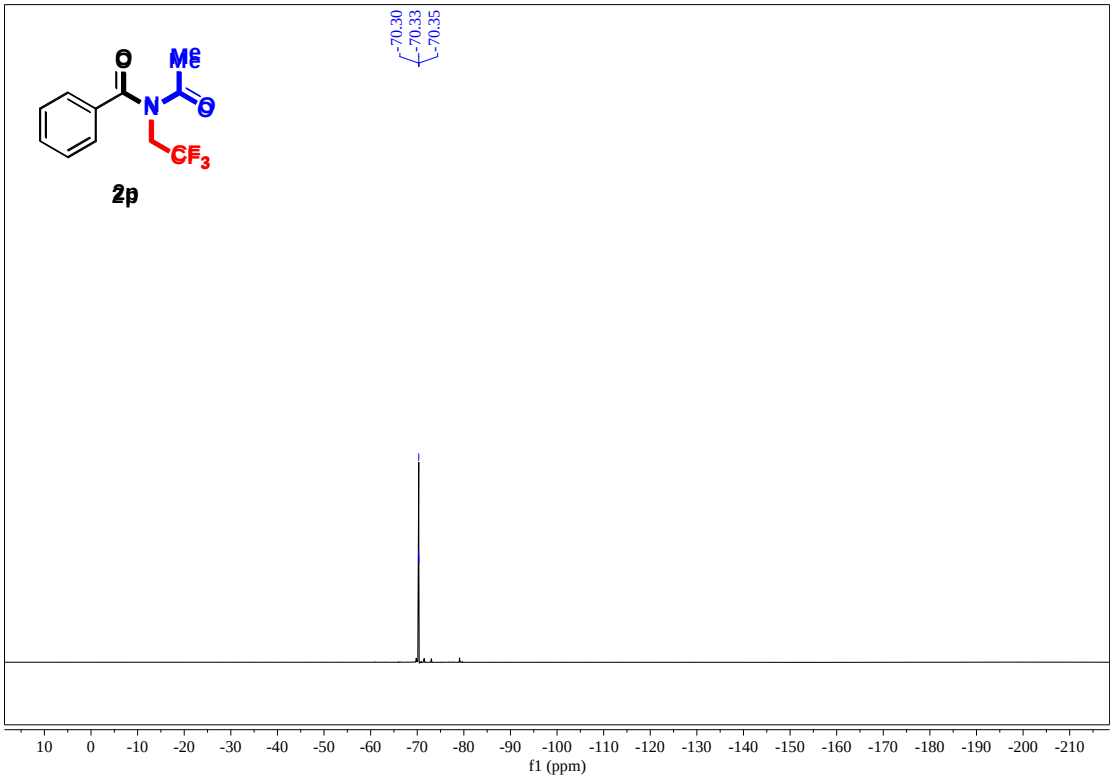
7.66
7.64
7.56
7.54
7.52
4.63
4.61
4.59
4.57
2.07
O
Me
N
O
CF3
2p
2.00
1.01
2.01
2.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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-70.35
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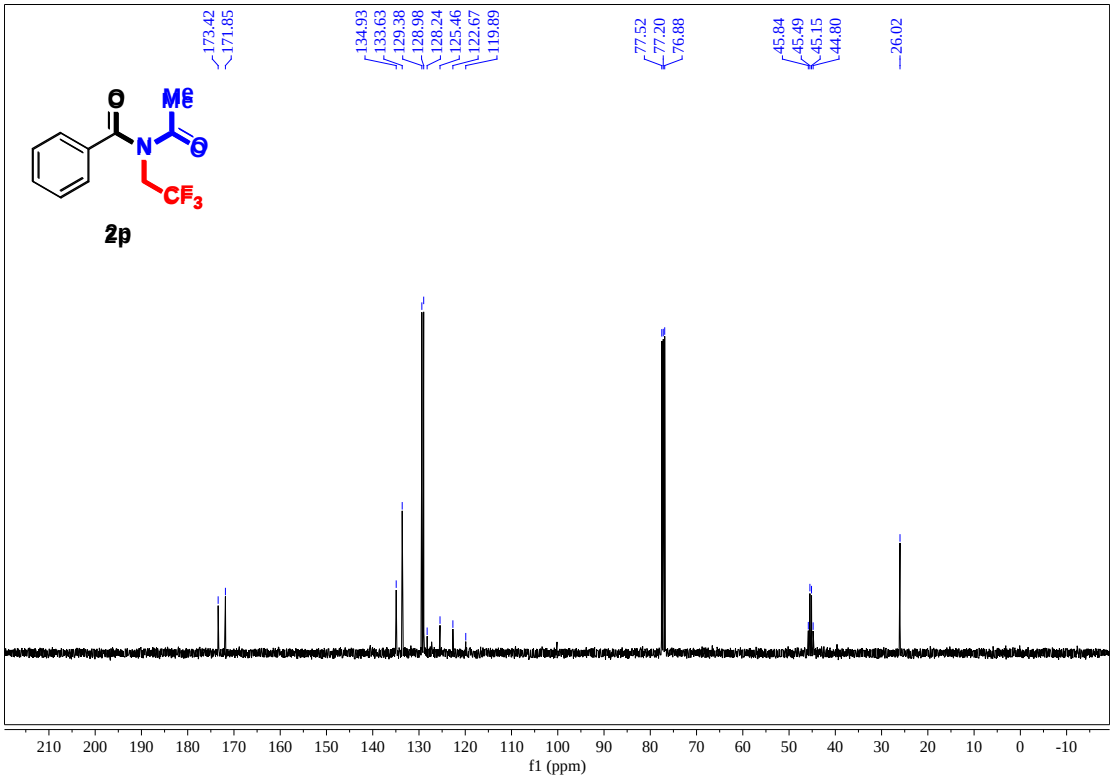
Me
N
O
CF3
2p
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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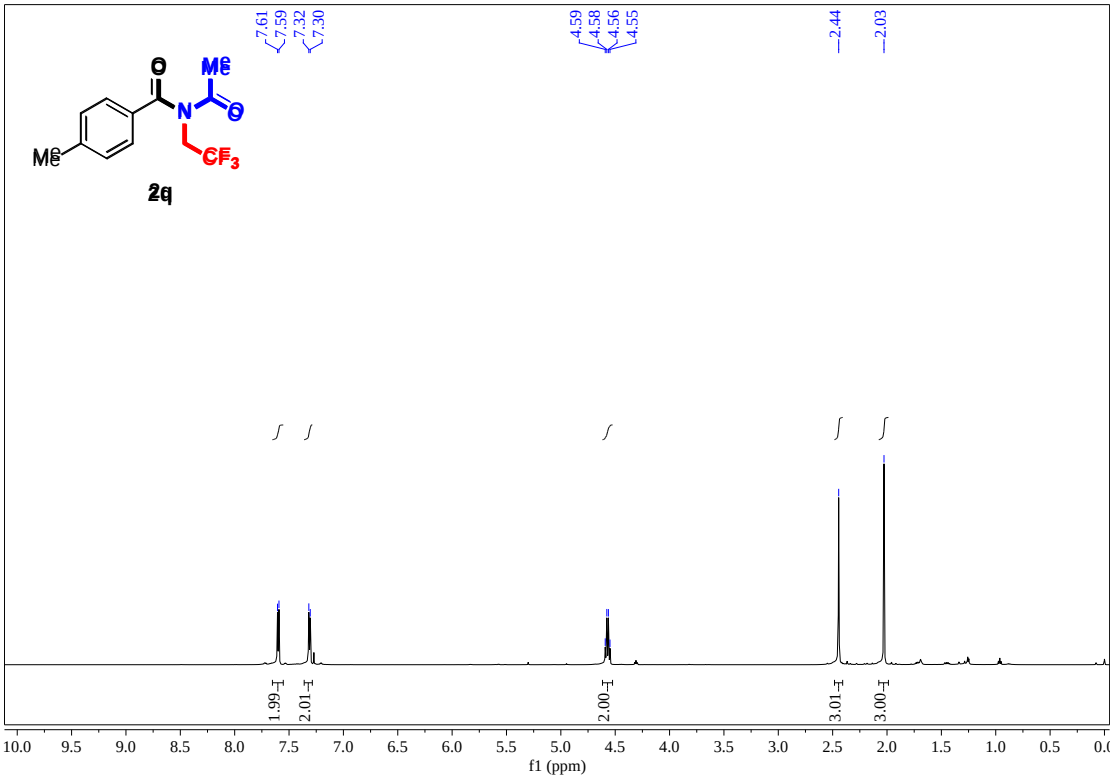
128.24
125.46
122.67
119.89
77.52
77.20
76.88
45.84
45.49
45.15
44.80
26.02
O
Me
N
O
CF3
2p
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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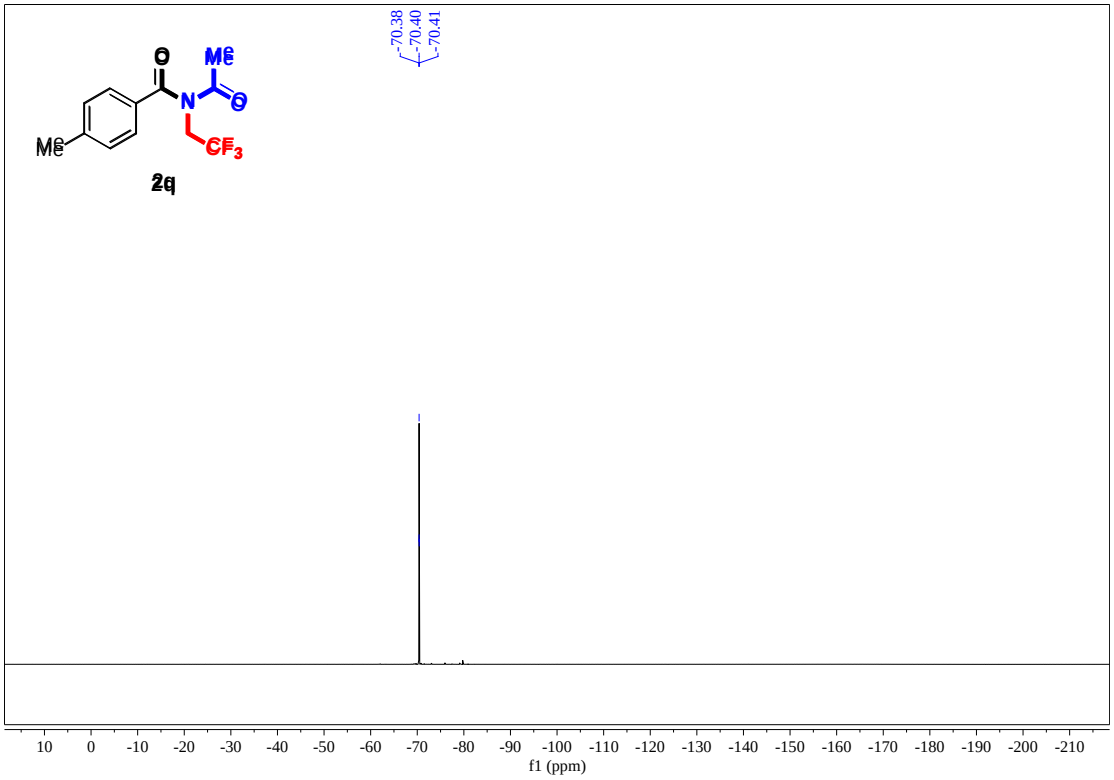
7.59
7.32
7.30
4.59
4.58
4.56
4.55
2.44
2.03
O
Me
N
O
CF3
Me
2q
1.99
2.01
2.00
3.01
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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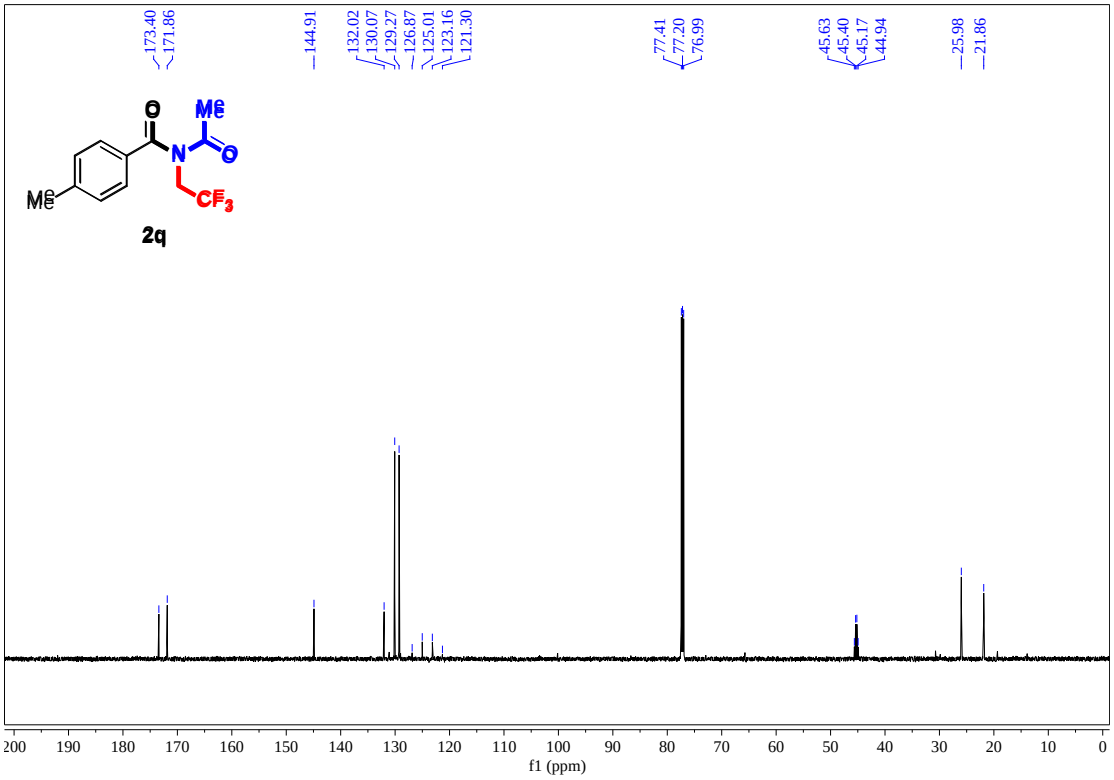
-70.40
-70.41
O
Me
N
O
Me
CF3
2q
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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144.91
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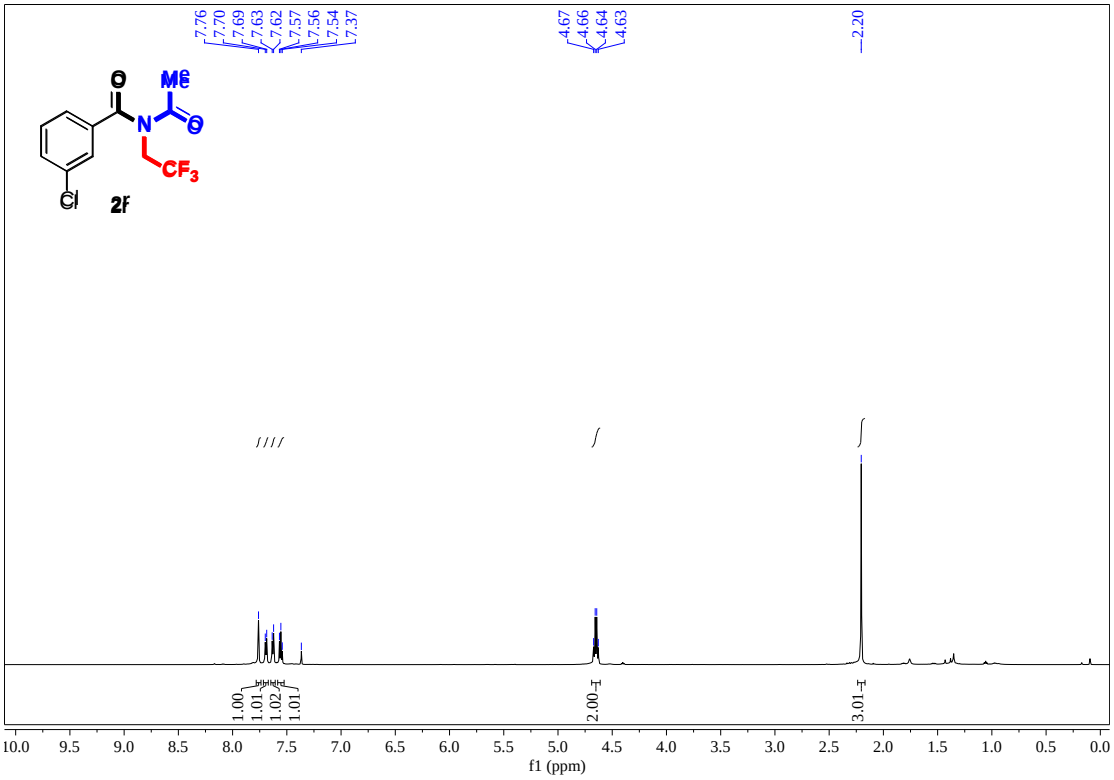
130.07
129.27
126.87
125.01
123.16
121.30
77.41
77.20
76.99
45.63
45.40
45.17
44.94
25.98
21.86
O
Me
N
O
Me
CF3
2q
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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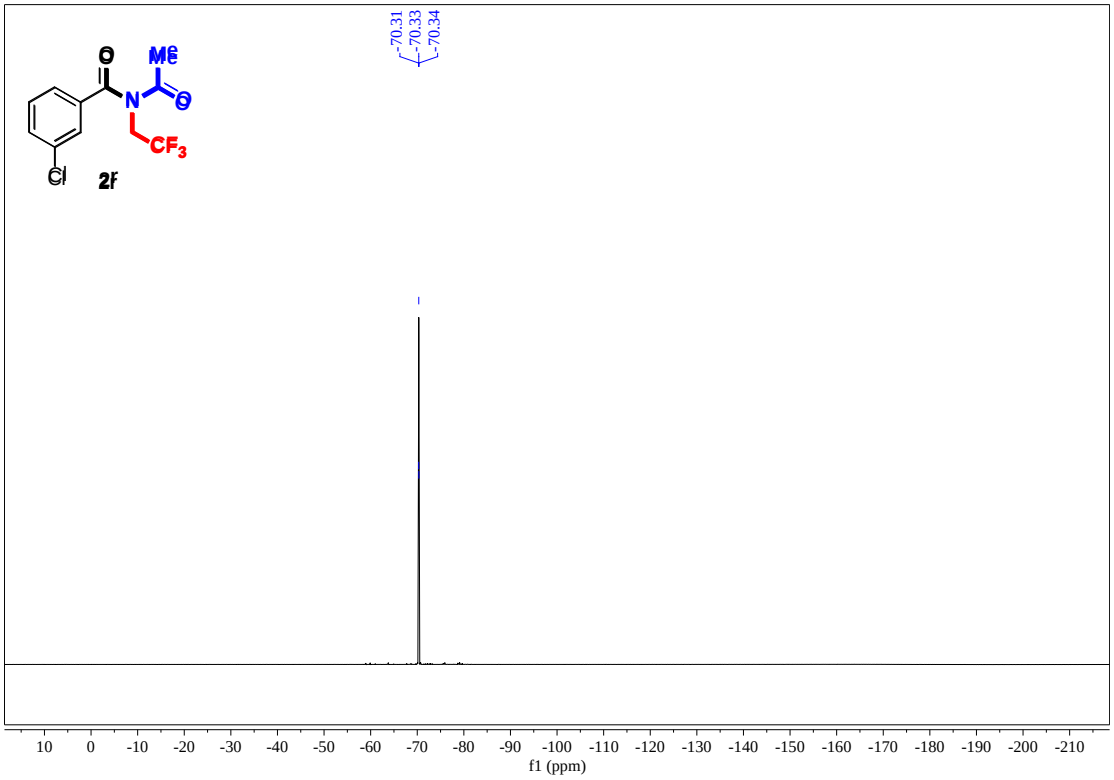
7.54
7.37
4.67
4.66
4.64
4.63
2.20
O
Me
N
O
CF3
Cl
2f
1.00
1.01
1.02
1.01
2.00
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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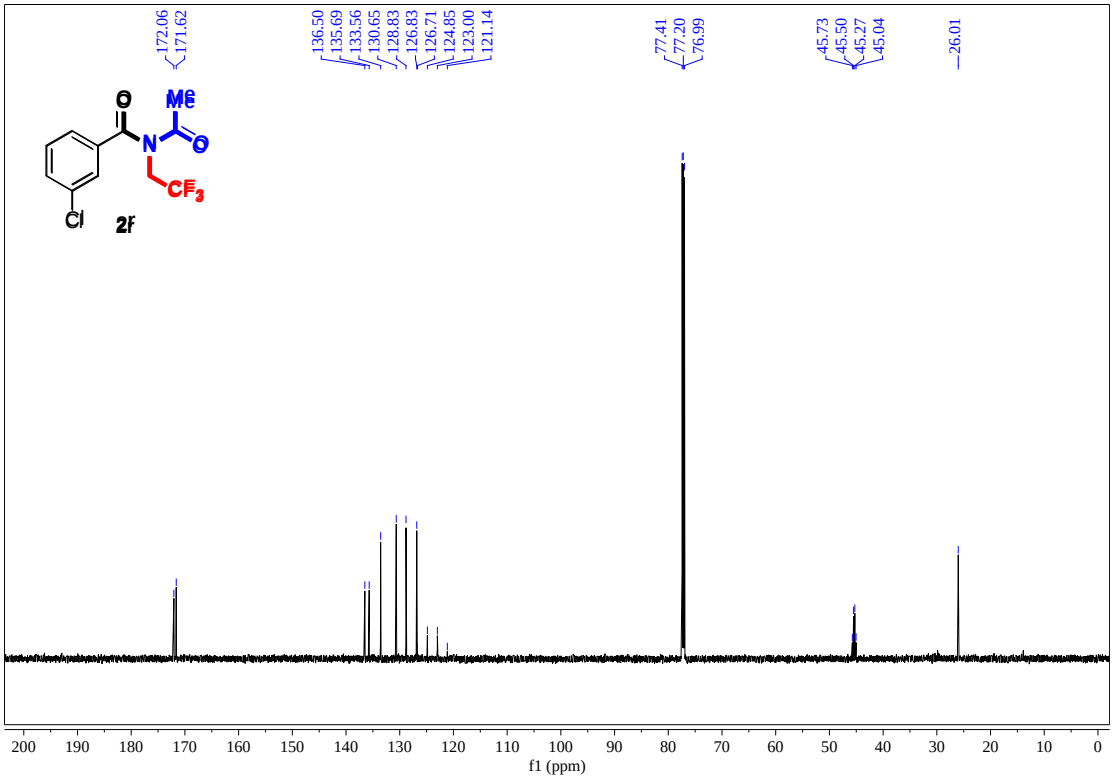
-70.33
-70.34
O
Me
N
O
CF3
Cl
2f
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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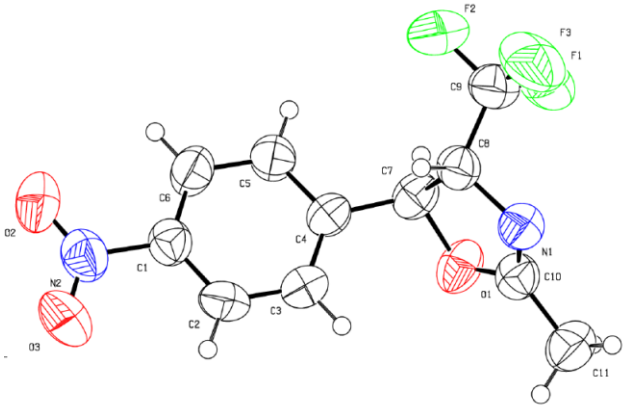
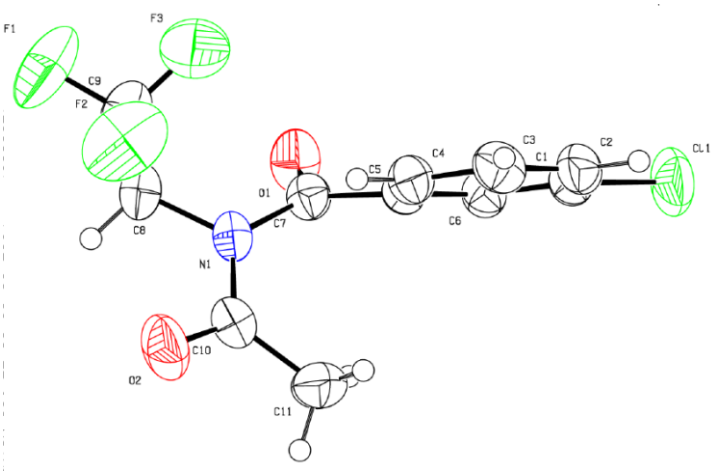
76.99
45.73
45.50
45.27
45.04
26.01
O
Me
N
O
CF3
Cl
2f
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

X-Ray analysis for the annulation products 2a and 2r:

CCDC 1042102 and 1042103 contain the supplementary crystallographic data for the products **2a** and **2r**. The data can be obtained free of charge from The Cambridge Crystallographic Data Center via http://www.ccdc.cam.ac.uk/deosit/



2a



2r