Electronic Supplementary Material (ESI) for ChemComm.

Copper-catalyzed synthesis of dihydrooxazoles from *α,β*-unsaturated ketoximes and activated ketones

Binsen Rong, Gaochen Xu, Huan Yan, Sai Zhang, Qinghuan Wu, Ning Zhu, Jindian Duan* and Kai Guo*

College of Biotechnology and Pharmaceutical Engineering, State Key Laboratory of Materials-Oriented Chemical Engineering, Nanjing Tech University, Nanjing 211816, China.

E-mail: duanjd@njtech.edu.cn; guok@njtech.edu.cn

Supporting Information

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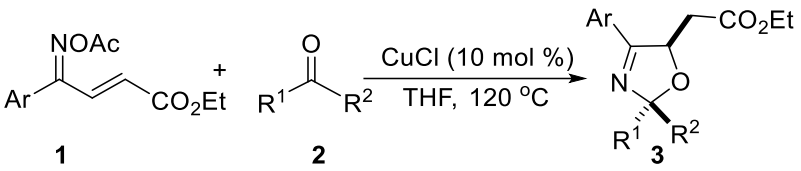
Experimental section

General

Unless otherwise noted, all experiments were performed under N_2 atmosphere. Commercial solvents and reagents were used without further purification. Thin-layer chromatography (TLC) was performed on silica gel plates (60F-254) using UV-light (254 nm). Flash chromatography was conducted on silica gel (200-300 mesh). NMR (400 MHz for ^{1}H NMR, 100 MHz for ^{13}C NMR) spectra were recorded in $CDCl_3$ with TMS as the internal standard. Chemical shifts are reported in ppm and coupling constants are given in Hz. Data for ^{1}H NMR are recorded as follows: chemical shift (ppm), multiplicity (s, singlet; d, doublet; t, triplet; q, quarter; m, multiplet； quint, quintet), coupling constant (Hz), integration. Data for ^{13}C NMR and ^{19}F NMR are reported in terms of chemical shift (δ, ppm). An Agilent 7890A GC instrument equipped with a split-splitless injector and a flame ionization detector (FID) was used for separation and determination of the compounds. Chromatographic separation of target analytes was performed by HP-5 Agilent fused-silica capillary column (30 m × 250 μm × 0.25 μm film thickness). N_2 (99.999%) was used as the carrier gas with a flow rate of 4.0 mL/min. Detector and injector temperatures were 300 and 280 °C, respectively. The GC oven temperature program was: 80 °C for 2 min, increased to 280 °C at a rate of 10 °C/min and then held at 280 °C for 8 min. High-resolution mass spectra (HRMS) were obtained on an Agilent mass spectrometer using ESI-TOF (electrospray ionization-time of flight).

A variety of ketoxime-enoates[1] were prepared using general procedures reported in the literatures.

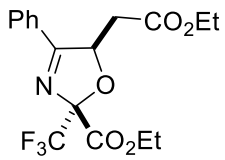
General procedure for the synthesis of 3



1 (0.4 mmol), **2** (0.2 mmol) and CuCl (2 mg, 0.02 mmol) were loaded into a 10 mL Schlenk tube equipped with a Teflon-coated magnetic stir bar. The Schlenk tube was placed under vacuum for 1 min and then N_2 was pumped into it. The solvent THF (2 mL, 0.1 M) was added into the Schlenk tube by syringe. The reaction mixture was stirred at 120 °C for 12 h. After completion of the reaction (detected by TLC), the reaction tube was allowed to cool to room temperature and the reaction solution was concentrated under vacuum. The crude products were purified by column chromatography on silica gel (Petroleum Ether/EtOAc) to give the products **3**.

Compounds characterization

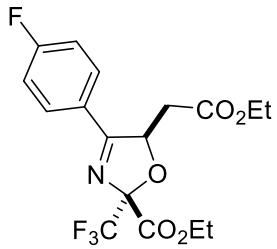
Ethyl-5-(2-ethoxy-2-oxoethyl)-4-phenyl-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3aa)



64.9 mg, 87% yield; white oil; dr 86:14; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.75 (d, *J* = 7.4 Hz, 2H), 7.51–7.47 (m, 1H), 7.41 (t, *J* = 7.3 Hz, 2H), 5.96 (dd, *J* = 7.6, 3.8 Hz, 1H), 4.27 (q, *J* = 7.0 Hz, 2H), 4.10 (q, *J* = 7.0 Hz, 2H), 2.89–2.78 (m, 2H), 1.28 (t, *J* = 7.0 Hz, 3H), 1.17 (t, *J* = 7.0 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 176.4, 169.5, 164.2, 132.9, 132.9, 129.1, 128.8, 121.6 (q, *J* = 286.1 Hz), 106.7 (q, *J* = 30.7 Hz), 85.5, 63.0, 61.3, 39.1, 14.0, 13.9 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.6 ppm; HRMS (ESI-TOF): m/z calcd for $C_{17}H_{19}F_3NO_5$

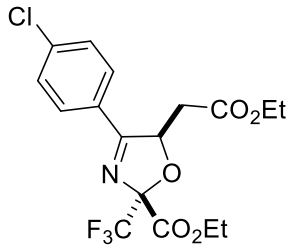
$[M+H]^+$ 374.1215, found 374.1230.

Ethyl-5-(2-ethoxy-2-oxoethyl)-4-(4-fluorophenyl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3ba)



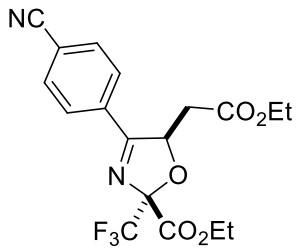
60.2 mg, 77% yield; white oil; dr 90:10; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88–7.85 (m, 2H), 7.18 (t, *J* = 8.6 Hz, 2H), 6.01 (dd, *J* = 6.5, 4.7 Hz, 1H), 4.36 (q, *J* = 7.1 Hz, 2H), 4.18 (q, *J* = 7.2 Hz, 2H), 2.95–2.86 (m, 2H), 1.36 (t, *J* = 7.1 Hz, 3H), 1.26 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 175.3, 169.5, 166.8, 164.1, 131.3 (d, *J* = 9.1 Hz), 125.2 (d, *J* = 3.3 Hz), 121.6 (q, *J* = 285.9 Hz), 116.5 (d, *J* = 22.1 Hz), 106.6 (q, *J* = 30.9 Hz), 85.4, 63.1, 61.4, 39.1, 14.1, 13.9 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.7, -104.8 ppm; HRMS (ESI-TOF): m/z calcd for $C_{17}H_{18}F_4NO_5$ $[M+H]^+$ 392.1121, found 392.1149.

Ethyl-4-(4-chlorophenyl)-5-(2-ethoxy-2-oxoethyl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3ca)



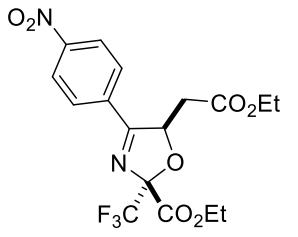
69.2 mg, 85% yield; white oil; dr 86:14; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.78 (d, *J* = 8.6 Hz, 2H), 7.47 (d, *J* = 8.6 Hz, 2H), 6.00 (dd, *J* = 6.4, 4.6 Hz, 1H), 4.36 (q, *J* = 7.1 Hz, 2H), 4.17 (q, *J* = 7.1 Hz, 2H), 2.94–2.85 (m, 2H), 1.36 (t, *J* = 7.1 Hz, 3H), 1.25 (t, *J* = 7.1 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 175.4, 169.4, 164.0, 139.3, 130.1, 129.5, 127.2, 121.5 (q, *J* = 286.0 Hz), 106.6 (q, *J* = 30.9 Hz), 85.4, 63.1, 61.4, 39.0, 14.0, 13.9 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.6 ppm; HRMS (ESI-TOF): m/z calcd for $C_{17}H_{18}ClF_3NO_5$ $[M+H]^+$ 408.0826, found 408.0858.

Ethyl-4-(4-cyanophenyl)-5-(2-ethoxy-2-oxoethyl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3da)



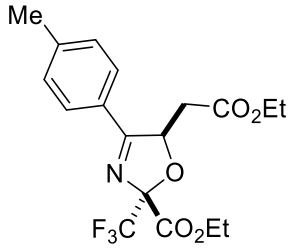
53.3 mg, 67% yield; white oil; dr 80:20; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.96 (d, *J* = 8.6 Hz, 2H), 7.80 (d, *J* = 8.5 Hz, 2H), 6.01 (dd, *J* = 6.3, 4.4 Hz, 1H), 4.37 (q, *J* = 7.1 Hz, 2H), 4.16 (q, *J* = 7.1 Hz, 2H), 2.97–2.85 (m, 2H), 1.37 (t, *J* = 7.1 Hz, 3H), 1.25 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 175.1, 169.1, 163.6, 132.8, 129.3, 127.4, 121.4 (q, *J* = 286.0 Hz), 117.7, 116.2, 106.7 (q, *J* = 31.0 Hz), 85.4, 63.3, 61.5, 38.6, 14.0, 13.9 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.5 ppm; HRMS (ESI-TOF): m/z calcd for $C_{18}H_{18}F_3N2O_5$ $[M+H]^+$ 399.1168, found 399.1172.

Ethyl-5-(2-ethoxy-2-oxoethyl)-4-(4-nitrophenyl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3ea)



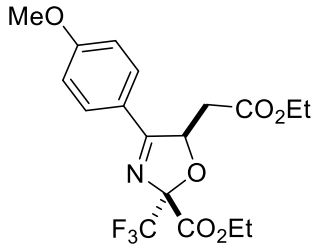
32.6 mg, 39% yield; white oil; dr 97:3; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.35 (d, *J* = 8.7 Hz, 2H), 8.03 (d, *J* = 8.7 Hz, 2H), 6.05–6.02 (m, 1H), 4.38 (q, *J* = 7.1 Hz, 2H), 4.16 (q, *J* = 7.1 Hz, 2H), 2.97–2.88 (m, 2H), 1.38 (t, *J* = 7.1 Hz, 3H), 1.25 (t, *J* = 7.1 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 174.9, 169.1, 163.6, 150.2, 134.4, 129.9, 124.2, 121.4 (q, *J* = 286.0 Hz), 106.7 (q, *J* = 31.0 Hz), 85.5, 63.4, 61.5, 38.5, 14.0, 13.9 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.6 ppm; HRMS (ESI-TOF): m/z calcd for $C_{17}H_{18}F_3N_2O_7$ $[M+H]^+$ 419.1066, found 419.1042.

Ethyl-5-(2-ethoxy-2-oxoethyl)-4-(p-tolyl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3fa)



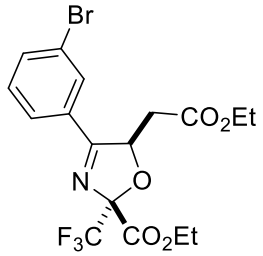
49.5 mg, 65% yield; white oil; dr 84:16; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.72 (d, *J* = 8.2 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 6.02 (dd, *J* = 7.6, 3.7 Hz, 1H), 4.35 (q, *J* = 7.1 Hz, 2H), 4.18 (q, *J* = 7.2 Hz, 2H), 1.25 (t, *J* = 7.1 Hz, 3H), 2.96–2.85 (m, 2H), 2.42 (s, 3H), 1.36 (t, *J* = 7.1 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 176.2, 169.6, 164.3, 143.8, 129.8, 126.9, 121.6 (q, *J* = 284.3 Hz), 106.6 (q, *J* = 30.8 Hz), 85.4, 63.0, 61.3, 39.3, 21.7, 14.1, 13.9 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.7 ppm; HRMS (ESI-TOF): m/z calcd for $C_{18}H_{21}F_3NO_5$ $[M+H]^+$ 388.1372, found 388.1397.

Ethyl-5-(2-ethoxy-2-oxoethyl)-4-(4-methoxyphenyl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3ga)



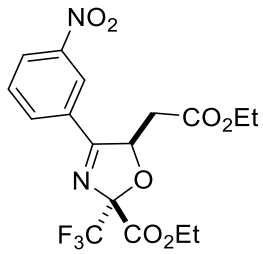
66.9 mg, 83% yield; white oil; dr 87:13; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.79 (d, *J* = 8.9 Hz, 2H), 6.97 (d, *J* = 8.9 Hz, 2H), 6.01 (dd, *J* = 7.4, 3.9 Hz, 1H), 4.34 (q, *J* = 7.1 Hz, 2H), 4.19 (q, *J* = 7.2 Hz, 2H), 3.87 (s, 3H), 2.97–2.86 (m, 2H), 1.36 (t, *J* = 7.1 Hz, 3H), 1.26 (t, *J* = 7.1 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 175.5, 169.7, 164.4, 163.3, 130.8, 121.6 (q, *J* = 285.9 Hz), 121.2, 114.5, 106.5 (q, *J* = 30.8 Hz), 85.2, 63.0, 61.3, 55.5, 39.4, 14.1, 13.9 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.7 ppm; HRMS (ESI-TOF): m/z calcd for $C_{18}H_{21}F_3NO_6$ $[M+H]^+$ 404.1321, found 404.1368.

Ethyl-4-(3-bromophenyl)-5-(2-ethoxy-2-oxoethyl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3ha)



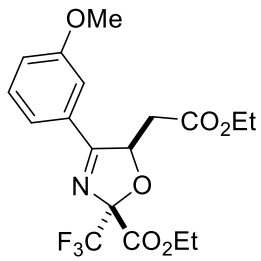
62.2 mg, 69% yield; white oil; dr 98:2; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.04 (t, *J* = 1.7 Hz, 1H), 7.70 (dd, *J* = 7.9, 1.4 Hz, 2H), 7.37 (t, *J* = 7.9 Hz, 1H), 5.99 (dd, *J* = 6.8, 4.3 Hz, 1H), 4.36 (q, *J* = 7.1 Hz, 2H), 4.18 (q, *J* = 7.1 Hz, 2H), 2.96–2.85 (d, 2H), 1.37 (t, *J* = 7.1 Hz, 3H), 1.26 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 175.3, 169.3, 163.9, 135.8, 131.6, 130.7, 130.6, 127.3, 123.3, 121.5 (q, *J* = 286.0 Hz), 106.6 (q, *J* = 31.0 Hz), 85.4, 63.2, 61.4, 38.9, 14.1, 13.9 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.6 ppm; HRMS (ESI-TOF): m/z calcd for $C_{17}H_{18}BrF_3NO_5$ $[M+H]^+$ 452.0320, found 452.0348.

Ethyl-5-(2-ethoxy-2-oxoethyl)-4-(3-nitrophenyl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3ia)



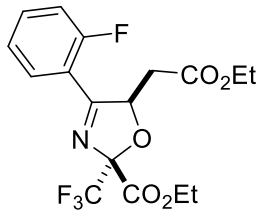
49.3 mg, 59% yield; white oil; dr 98:2; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.57–8.62 (m, 1H), 8.36 (d, *J* = 8.3 Hz, 1H), 8.12 (d, *J* = 7.8 Hz, 1H), 7.66 (t, *J* = 8.0 Hz, 1H), 5.97 (dd, *J* = 6.3, 4.4 Hz, 1H), 4.30 (q, *J* = 7.1 Hz, 2H), 4.10 (q, *J* = 7.1 Hz, 2H), 2.93–2.82 (m, 2H), 1.31 (t, *J* = 7.1 Hz, 3H), 1.18 (t, *J* = 7.1 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 174.7, 169.1, 163.6, 148.5, 134.4, 130.6, 130.4, 127.2, 123.6, 121.4 (q, *J* = 284.5 Hz), 106.6 (q, *J* = 31.1 Hz), 85.4, 63.4, 61.6, 38.6, 14.0, 13.9 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.5 ppm; HRMS (ESI-TOF): m/z calcd for $C_{17}H_{18}F_3N_2O_7$ $[M+H]^+$ 419.1066, found 419.1097.

Ethyl-5-(2-ethoxy-2-oxoethyl)-4-(3-methoxyphenyl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3ja)



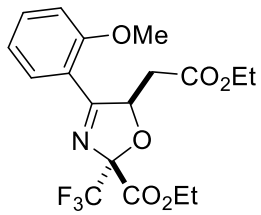
77.4 mg, 96% yield; white oil; dr 91:9; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.43–7.37 (m, 2H), 7.32–7.30 (m, 1H), 7.13–7.01 (m, 1H), 6.02 (dd, *J* = 7.6, 3.7 Hz, 1H), 4.36 (q, *J* = 7.1 Hz, 2H), 4.18 (q, *J* = 7.2 Hz, 2H), 3.86 (s, 3H), 2.98–2.85 (m, 2H), 1.37 (t, *J* = 7.1 Hz, 3H), 1.26 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 176.4, 169.6, 164.2, 160.0, 130.1, 130.0, 121.6 (q, *J* = 285.9 Hz), 121.2, 119.4, 113.3, 106.6 (q, *J* = 30.8 Hz), 85.6, 63.1, 61.3, 55.5, 39.2, 14.1, 13.9 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.6 ppm; HRMS (ESI-TOF): m/z calcd for $C_{18}H_{21}F_3NO_6$ $[M+H]^+$ 404.1321, found 404.1367.

Ethyl-5-(2-ethoxy-2-oxoethyl)-4-(2-fluorophenyl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3ka)



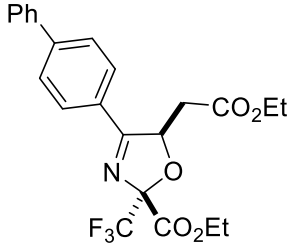
60.2 mg, 77% yield; white oil; dr 95:5; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.15–8.11 (m, 1H), 7.61–7.55 (m, 1H), 7.31 (d, *J* = 7.9 Hz, 1H), 7.18 (dd, *J* = 10.8, 8.8 Hz, 1H), 5.98–5.95 (m, 1H), 4.36 (q, *J* = 7.1 Hz, 2H), 4.18–4.10 (m, 2H), 2.95–2.78 (m, 2H), 1.37 (t, *J* = 7.1 Hz, 3H), 1.23 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 173.8, 169.4, 164.1, 161.0 (d, *J* = 253.4 Hz), 134.9 (d, *J* = 9.0 Hz), 131.5 (d, *J* = 2.8 Hz), 125.2 (d, *J* = 3.1 Hz), 121.6 (q, *J* = 284.5 Hz), 117.4 (d, *J* = 12.2 Hz), 116.5 (d, *J* = 22.0 Hz), 105.7 (q, *J* = 31.0 Hz), 86.9 (d, *J* = 8.2 Hz), 63.1, 61.2, 38.0 (d, *J* = 1.8 Hz), 14.1, 13.9 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.7, -110.3 ppm; HRMS (ESI-TOF): m/z calcd for $C_{17}H_{18}F_4NO_5$ $[M+H]^+$ 392.1121, found 392.1153.

Ethyl-5-(2-ethoxy-2-oxoethyl)-4-(2-methoxyphenyl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3la)



68.5 mg, 85% yield; white oil; dr 99:1; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.06 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.54–7.50 (m, 1H), 7.06 (t, *J* = 7.9 Hz, 1H), 6.98 (d, *J* = 8.4 Hz, 1H), 6.10 (dd, *J* = 7.6, 3.0 Hz, 1H), 4.35 (q, *J* = 7.2 Hz, 2H), 4.15 (q, *J* = 7.1 Hz, 2H), 3.89 (s, 3H), 2.86–2.70 (m, 2H), 1.36 (t, *J* = 7.1 Hz, 3H), 1.24 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 176.5, 170.0, 164.5, 158.0, 134.3, 131.8, 121.7 (q, *J* = 286.4 Hz), 121.4, 118.4, 111.4, 105.3 (q, *J* = 30.6 Hz), 87.4, 62.9, 61.0, 55.5, 38.2, 14.1, 13.9 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.7 ppm; HRMS (ESI-TOF): m/z calcd for $C_{18}H_{21}F_3NO_6$ $[M+H]^+$ 404.1321, found 404.1356.

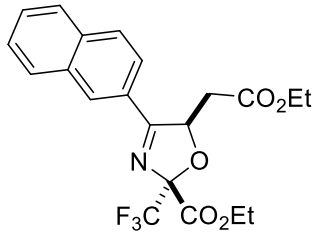
Ethyl-4-([1,1'-biphenyl]-4-yl)-5-(2-ethoxy-2-oxoethyl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3ma)



69.9 mg, 78% yield; white oil; dr 92:8; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90 (d, *J* = 8.2 Hz, 2H), 7.68 (d, *J* = 8.2 Hz, 2H), 7.59 (d, *J* = 7.4 Hz, 2H), 7.44 (t, *J* = 7.4 Hz, 2H), 7.37–7.35 (m, 1H), 6.10 (dd, *J* = 7.5, 3.5 Hz, 1H), 4.34 (q, *J* = 7.1 Hz, 2H), 4.17 (q, *J* = 7.1 Hz, 2H), 3.04–2.92 (m, 2H), 1.34 (t, *J* = 7.1 Hz, 3H), 1.24 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 176.2, 169.5, 164.2, 145.6, 139.5, 129.4, 129.0, 128.4, 127.6, 127.5, 127.1, 121.8 (q, *J* = 285.8 Hz), 106.7 (q, *J* = 30.7 Hz), 85.6, 63.0, 61.2, 39.2, 14.0, 13.8 ppm; ^{19}F NMR (376 MHz,

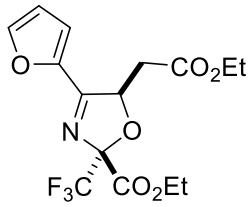
Chloroform-*d*) δ -78.5 ppm; HRMS (ESI-TOF): m/z calcd for $C_{23}H_{22}F_3NO_5$ $[M+H]^+$ 449.1450, found 449.1474.

Ethyl-5-(2-ethoxy-2-oxoethyl)-4-(naphthalen-2-yl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3na)



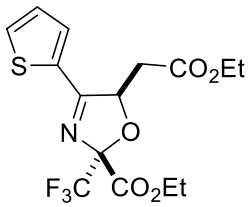
72.8 mg, 86% yield; white oil; dr 80:20; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.22 (s, 1H), 7.99–7.87 (m, 4H), 7.62–7.54 (m, 2H), 6.19 (dd, *J* = 7.7, 3.5 Hz, 1H), 4.38 (q, *J* = 7.1 Hz, 2H), 4.19 (q, *J* = 7.1 Hz, 2H), 3.06–2.94 (m, 2H), 1.38 (t, *J* = 7.1 Hz, 3H), 1.25 (t, *J* = 7.1 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 176.5, 169.7, 164.3, 135.3, 132.6, 130.0, 129.1, 129.0, 128.6, 127.9, 127.2, 126.2, 124.6, 121.6 (q, *J* = 286.0 Hz), 106.7 (q, *J* = 30.7 Hz), 85.6, 63.1, 61.3, 39.4, 14.1, 13.9 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.5 ppm; HRMS (ESI-TOF): m/z calcd for $C_{21}H_{21}F_3NO_5$ $[M+H]^+$ 424.1372, found 424.1389.

Ethyl-5-(2-ethoxy-2-oxoethyl)-4-(furan-2-yl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3oa)



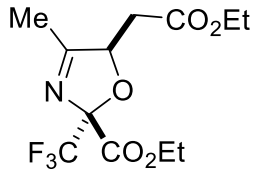
50.8 mg, 70% yield; white oil; dr 92:8; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.65 (d, *J* = 1.2 Hz, 1H), 7.29–7.28 (m, 1H), 6.62 (dd, *J* = 3.6, 1.7 Hz, 1H), 5.83 (dd, *J* = 7.9, 3.4 Hz, 1H), 4.34 (q, *J* = 7.1 Hz, 2H), 4.22–4.13 (m, 2H), 3.13–2.96 (m, 2H), 1.35 (t, *J* = 7.1 Hz, 3H), 1.26 (s, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.4, 165.9, 164.1, 146.8, 145.4, 121.5 (q, *J* = 286.2 Hz), 117.5, 112.8, 106.5 (q, *J* = 31.0 Hz), 85.6, 63.1, 61.2, 38.9, 14.0, 13.8 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.6 ppm; HRMS (ESI-TOF): m/z calcd for $C_{15}H_{17}F_3NO_6$ $[M+H]^+$ 364.1008, found 364.1036.

Ethyl-5-(2-ethoxy-2-oxoethyl)-4-(thiophen-2-yl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3pa)



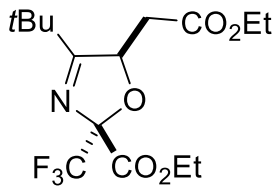
36.4 mg, 48% yield; white oil; dr 93:7; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.66 (d, *J* = 5.0 Hz, 1H), 7.52 (d, *J* = 3.7 Hz, 1H), 7.17–7.15 (m, 1H), 5.92 (dd, *J* = 7.3, 4.0 Hz, 1H), 4.34 (q, *J* = 7.1 Hz, 2H), 4.20 (q, *J* = 7.1 Hz, 2H), 3.07–2.95 (m, 2H), 1.35 (t, *J* = 7.1 Hz, 3H), 1.27 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.0, 169.4, 164.1, 132.9, 132.3, 128.3, 121.5 (q, *J* = 286.0 Hz), 106.2 (q, *J* = 31.0 Hz), 85.5, 63.1, 61.3, 39.8, 14.1, 13.8 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.6 ppm; HRMS (ESI-TOF): m/z calcd for $C_{15}H_{17}F_3NO_5S$ $[M+H]^+$ 380.0780, found 380.0792.

Ethyl-5-(2-ethoxy-2-oxoethyl)-4-methyl-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3qa)



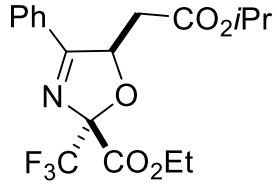
31.7 mg, 51% yield; white oil; dr 71:29; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 5.31–5.28 (m, 1H), 4.20–4.13 (m, 2H), 4.20–4.13 (m, 2H), 3.99–3.09 (m, 2H), 1.93 (s, 3H), 1.24–1.16 (m, 6H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 179.0, 169.1, 164.0, 121.5 (q, *J* = 284.4 Hz), 105.9 (q, *J* = 30.1 Hz), 87.5, 63.0, 61.3, 37.4, 15.8, 14.1, 13.9 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -79.0 ppm; HRMS (ESI-TOF): m/z calcd for $C_{12}H_{17}F_3NO_5$ $[M+H]^+$ 312.1059, found 312.1083.

Ethyl-4-(tert-buty-ethoxy-2-oxoethyl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3ra)



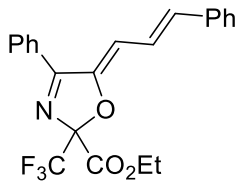
47.3 mg, 67% yield; white oil; dr 95:5; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 5.50 (dd, *J* = 8.4, 3.3 Hz, 1H), 4.31 (q, *J* = 7.1 Hz, 2H), 4.22–4.16 (m, 2H), 2.98–2.80 (m, 2H), 1.33–1.26 (m, 15H), ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 188.0, 169.3, 164.2, 121.5 (q, *J* = 285.6 Hz), 105.6 (q, *J* = 30.4 Hz), 85.9, 62.8, 61.2, 39.1, 35.5, 28.4, 14.1, 13.8 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -79.3 ppm; HRMS (ESI-TOF): m/z calcd for $C_{15}H_{23}F_3NO_5$ $[M+H]^+$ 354.1528, found 354.1556.

Ethyl-5-(2-isopropoxy-2-oxoethyl)-4-phenyl-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3sa)



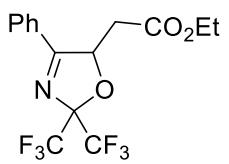
58.1 mg, 75% yield; white oil; dr 93:7; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.84–7.82 (m, 2H), 7.60–7.55 (m, 1H), 7.49 (t, *J* = 7.5 Hz, 2H), 6.04 (dd, *J* = 7.5, 3.9 Hz, 1H), 5.08–5.02 (m, 1H), 4.35 (q, *J* = 7.1 Hz, 2H), 2.94–2.83 (m, 2H), 1.36 (t, *J* = 7.1 Hz, 3H), 1.23 (t, *J* = 6.6 Hz, 6H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 176.5, 169.1, 164.2, 132.9, 129.1, 128.8, 121.6 (q, *J* = 285.9 Hz), 106.6 (q, *J* = 30.9 Hz), 117.3, 85.5, 68.9, 63.0, 39.4, 21.8, 13.9 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.66 ppm; HRMS (ESI-TOF): m/z calcd for $C_{18}H_{21}F_3NO_5$ $[M+H]^+$ 388.1372, found 388.1395.

Ethyl (*Z*)-4-phenyl-5-((*E*)-3-phenylallylidene)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3va)



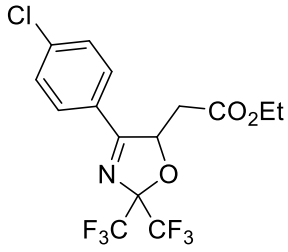
16.0 mg, 20% yield; white oil; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.80–7.78 (m, 2H), 7.59–7.47 (m, 5H), 7.36–7.27 (m, 3H), 7.25–7.20 (m, 1H), 6.76 (d, *J* = 15.8 Hz, 1H), 6.13 (d, *J* = 11.2 Hz, 1H), 4.44–4.31 (m, 2H), 1.36 (t, *J* = 7.1 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.8, 162.6, 152.0, 136.7, 136.7, 131.9, 129.6, 128.9, 128.8, 128.5, 126.9, 122.0, 120.9 (q, *J* = 284.6 Hz), 109.6, 104.9 (q, *J* = 31.4 Hz), 63.5, 14.0 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.2 ppm; HRMS (ESI-TOF): m/z calcd for $C_{22}H_{19}F_3NO_3$ $[M+H]^+$ 402.1317, found 402.1346.

Ethyl 2-(4-phenyl-2,2-bis(trifluoromethyl)-2,5-dihydrooxazol-5-yl)acetate (3ab)



59.0 mg, 80% yield; white oil; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.85–7.83 (m, 2H), 7.63–7.59 (m, 1H), 7.51 (t, *J* = 7.6 Hz, 2H), 6.11 (dd, *J* = 8.8, 2.7 Hz, 1H), 4.25–4.17 (m, 2H), 2.96–2.67 (m, 2H), 1.27 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 178.9, 169.2, 133.5, 129.2, 128.9, 128.2, 120.9 (q, *J* = 287.1 Hz, 2C), 106.0–104.7 (quint, *J* = 31.5 Hz), 86.3, 61.5, 39.1, 14.0 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.4 (q, *J* = 8.6 Hz), -77.8 (q, *J* = 8.7 Hz) ppm; HRMS (ESI-TOF): m/z calcd for $C_{15}H_{14}F_6NO_3$ $[M+H]^+$ 370.0878, found 370.0893.

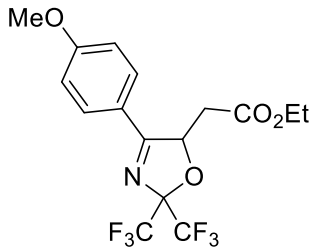
Ethyl 2-(4-(4-chlorophenyl)-2,2-bis(trifluoromethyl)-2,5-dihydrooxazol-5-yl)acetate (3cb)



58.8 mg, 73% yield; white oil; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.79 (d, *J* = 8.7 Hz, 2H), 7.49 (d, *J* = 8.6 Hz, 2H), 6.07 (dd, *J* = 8.3, 3.1 Hz, 1H), 4.25–4.17 (m, 2H), 2.92–2.68 (m, 2H), 1.27 (t, *J* = 7.1 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 177.8, 169.0, 140.0, 130.2, 129.6, 126.7, 120.8 (q, *J* = 285.4 Hz, 2C), 116.2–104.7 (quint, *J* = 31.5 Hz), 86.1, 61.6, 39.0, 14.0 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ

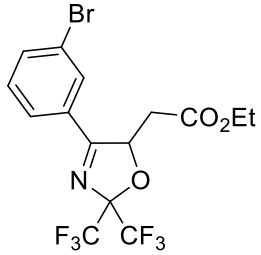
-78.4 (q, J = 8.6 Hz), -77.8 (q, J = 8.5 Hz) ppm; HRMS (ESI-TOF): m/z calcd for $C_{15}H_{13}ClF_6NO_3$ $[M+H]^+$ 404.0488, found 404.0497.

Ethyl 2-(4-(4-methoxyphenyl)-2,2-bis(trifluoromethyl)-2,5-dihydrooxazol-5-yl)acetate (3gb)



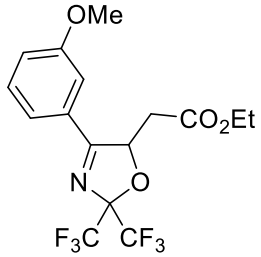
65.4 mg, 82% yield; white oil; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.80 (d, J = 8.9 Hz, 2H), 6.99 (d, J = 8.9 Hz, 2H), 6.06 (dd, J = 8.8, 2.6 Hz, 1H), 4.25–4.18 (m, 2H), 3.88 (s, 3H), 2.96–2.67 (m, 2H), 1.28 (t, J = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 177.8, 169.4, 163.7, 131.0, 120.9 (q, J = 286.9 Hz, 2C), 120.6, 114.6, 105.9–104.6 (quint, J = 31.3 Hz), 85.9, 61.5, 55.5, 39.4, 14.0 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.5 (q, J = 8.6 Hz), -77.9 (q, J = 8.7 Hz) ppm; HRMS (ESI-TOF): m/z calcd for $C_{16}H_{16}F_6NO_4$ $[M+H]^+$ 400.0984, found 400.1021.

Ethyl 2-(4-(3-bromophenyl)-2,2-bis(trifluoromethyl)-2,5-dihydrooxazol-5-yl)acetate (3hb)



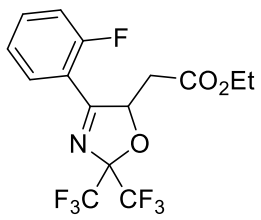
55.3 mg, 62% yield; white oil; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.04 (s, 1H), 7.75–7.71 (m, 2H), 7.39 (t, J = 7.9 Hz, 1H), 6.06 (dd, J = 8.3, 3.1 Hz, 1H), 4.25–4.18 (m, 2H), 2.93–2.69 (m, 2H), 1.28 (t, J = 7.1 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 177.8, 168.9, 136.4, 131.7, 130.7, 130.1, 127.4, 123.5, 120.7 (q, J = 287.1 Hz, 2C), 106.1–104.5 (quint, J = 31.5 Hz), 86.2, 61.7, 38.9, 14.0 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.3 (q, J = 8.7 Hz), -77.7 (q, J = 8.5 Hz) ppm; HRMS (ESI-TOF): m/z calcd for $C_{15}H_{13}BrF_6NO_3$ $[M+H]^+$ 447.9983, found 447.9989.

Ethyl 2-(4-(3-methoxyphenyl)-2,2-bis(trifluoromethyl)-2,5-dihydrooxazol-5-yl)acetate (3jb)



62.2 mg, 78% yield; white oil; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.42–7.38 (m, 2H), 7.31 (d, J = 7.7 Hz, 1H), 7.14 (dd, J = 8.2, 2.2 Hz, 1H), 6.08 (dd, J = 8.6, 2.9 Hz, 1H), 4.25–4.17 (m, 2H), 3.87 (s, 3H), 2.96–2.67 (m, 2H), 1.27 (t, J = 7.1 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 178.8, 169.2, 160.1, 130.2, 129.4, 121.3, 120.8 (q, J = 285.2 Hz, 2C), 119.9, 113.4, 106.0–104.7 (quint, J = 31.3 Hz), 86.3, 61.5, 55.6, 39.2, 14.1 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.4 (q, J = 8.6 Hz), -77.8 (q, J = 8.6 Hz) ppm; HRMS (ESI-TOF): m/z calcd for $C_{16}H_{16}F_6NO_4$ $[M+H]^+$ 400.0984, found 400.1033.

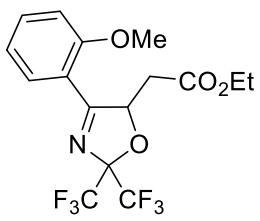
Ethyl 2-(4-(2-fluorophenyl)-2,2-bis(trifluoromethyl)-2,5-dihydrooxazol-5-yl)acetate (3kb)



40.9 mg, 53% yield; white oil; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.15–8.11 (m, 1H), 7.64–7.59 (m, 1H), 7.33 (t, J = 7.6 Hz, 1H), 7.22–7.18 (m, 1H), 6.05–6.03 (m, 1H), 4.19 (q, J = 7.2 Hz, 2H), 2.91–2.60 (m, 2H), 1.26 (t, J = 7.1 Hz, 1H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 176.3, 168.8, 161.1 (d, J = 254.0 Hz), 135.5 (d, J = 9.1 Hz), 131.4 (d, J = 2.6 Hz), 125.4 (d, J = 3.1 Hz), 120.9 (q, J = 285.4 Hz, 2C), 116.9 (d, J = 12.2 Hz), 116.6 (d, J = 21.9 Hz), 105.1–103.8 (quint, J = 31.5 Hz), 87.8, 61.4, 38.1 (d, J = 2.0 Hz), 14.0 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -109.7, -78.3 (q, J = 8.6 Hz), -77.8 (q, J = 8.6 Hz) ppm; HRMS (ESI-TOF): m/z calcd for $C_{15}H_{12}F_7NO_3$ $[M+H]^+$ 387.0705, found 387.0751.

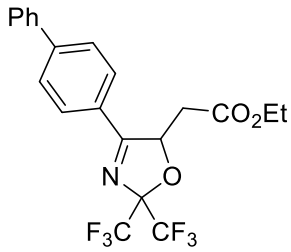
Ethyl 2-(4-(2-methoxyphenyl)-2,2-bis(trifluoromethyl)-2,5-dihydrooxazol-5-yl)acetate (3lb)

51.9 mg, 65% yield; white oil; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.99–7.97 (m, 1H), 7.49–7.45



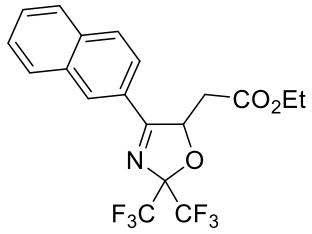
(m, 1H), 6.99 (t, *J* = 7.6 Hz, 1H), 6.90 (d, *J* = 8.4 Hz, 1H), 6.08 (d, *J* = 8.5 Hz, 1H), 4.14–4.08 (m, 2H), 3.81 (s, 3H), 2.75–2.41 (m, 2H), 1.18 (t, *J* = 7.1 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 178.9, 169.7, 158.1, 134.9, 131.7, 121.5, 121.0 (q, *J* = 285.0 Hz, 2C), 117.9, 111.5, 104.7–103.4 (quint, *J* = 31.3 Hz), 88.3, 61.2, 55.5, 38.3, 14.1 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.4 (q, *J* = 8.5 Hz), -78.1 (q, *J* = 8.5 Hz) ppm; HRMS (ESI-TOF): m/z calcd for $C_{16}H_{16}F_6NO_4$ $[M+H]^+$ 400.0984, found 400.1033.

Ethyl 2-(4-([1,1'-biphenyl]-4-yl)-2,2-bis(trifluoromethyl)-2,5-dihydrooxazol-5-yl)acetate (3mb)



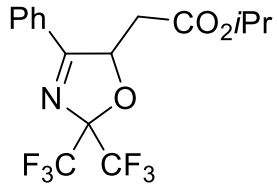
59.6 mg, 67% yield; white oil; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.91 (d, *J* = 8.3 Hz, 2H), 7.72 (d, *J* = 8.3 Hz, 2H), 7.62 (d, *J* = 7.3 Hz, 2H), 7.49 (t, *J* = 7.4 Hz, 2H), 7.42 (t, *J* = 7.3 Hz, 1H), 6.13 (dd, *J* = 8.7, 2.9 Hz, 1H), 4.27–4.19 (m, 2H), 3.00–2.70 (m, 2H), 1.28 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 178.5, 169.2, 146.3, 139.4, 129.5, 129.1, 128.6, 127.8, 127.2, 127.1, 120.9 (q, *J* = 287.0 Hz, 2C), 106.0–104.8 (quint, *J* = 31.3 Hz), 86.3, 61.6, 39.2, 14.1 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.4 (q, *J* = 8.6 Hz), -77.8 (q, *J* = 8.7 Hz) ppm; HRMS (ESI-TOF): m/z calcd for $C_{21}H_{18}F_6NO_3$ $[M+H]^+$ 446.1191, found 446.1209.

Ethyl 2-(4-(naphthalen-2-yl)-2,2-bis(trifluoromethyl)-2,5-dihydrooxazol-5-yl)acetate (3nb)



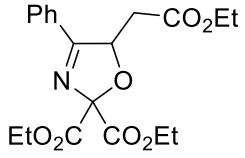
77.9 mg, 93% yield; white oil; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.13 (s, 1H), 7.89–7.78 (m, 4H), 7.55–7.44 (m, 2H), 6.16 (dd, *J* = 8.7, 2.9 Hz, 1H), 4.17–4.09 (m, 2H), 2.96–2.64 (m, 2H), 1.17 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 178.9, 169.3, 135.5, 132.5, 130.4, 129.3, 129.1, 128.9, 128.0, 127.4, 125.6, 124.5, 120.9 (q, *J* =285.2 Hz, 2C), 106.1–104.8 (quint, *J* = 31.5 Hz), 61.6, 39.4, 14.0 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.3 (q, *J* = 8.7 Hz), -77.7 (q, *J* = 8.7 Hz) ppm; HRMS (ESI-TOF): m/z calcd for $C_{19}H_{16}F_6NO_3$ $[M+H]^+$ 420.1034, found 420.1075.

Isopropyl 2-(4-phenyl-2,2-bis(trifluoromethyl)-2,5-dihydrooxazol-5-yl)acetate (3rb)



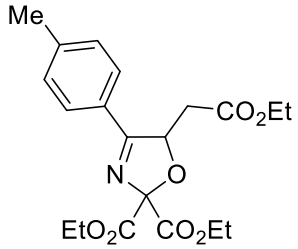
63.6 mg, 83% yield; white oil; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.85–7.83 (m, 2H), 7.63–7.58 (m, 1H), 7.52–7.49 (m, 2H), 6.10 (dd, *J* = 8.7, 2.9 Hz, 1H), 5.08 (p, *J* = 6.3 Hz, 1H), 2.64–2.93 (m, 2H), 1.27–1.22 (m, 6H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 179.0, 168.7, 133.4, 129.2, 129.0, 128.3, 120.5 (q, *J* = 286.3 Hz, 2C), 105.9–104.7 (quint, *J* = 31.3 Hz), 86.3, 69.2, 39.4, 21.7, 21.6 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.4 (q, *J* = 8.6 Hz), -77.9 (q, *J* = 8.6 Hz) ppm; HRMS (ESI-TOF): m/z calcd for $C_{16}H_{16}F_6NO_3$ $[M+H]^+$ 384.1034, found 384.1076.

Diethyl 5-(2-ethoxy-2-oxoethyl)-4-phenyloxazole-2,2(5*H*)-dicarboxylate (3ac)



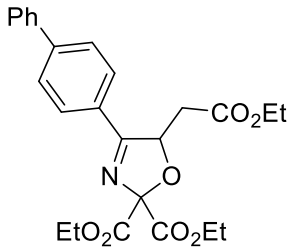
46.0 mg, 61% yield; white oil; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.75 (d, *J* = 7.2 Hz, 2H), 7.47–7.36 (m, 3H), 5.93 (dd, *J* = 7.3, 3.7 Hz, 1H), 4.29–4.20 (m, 4H), 4.06 (q, *J* = 7.1 Hz, 2H), 2.84–2.72 (m, 2H), 1.28–1.22 (m, 6H), 1.15 (t, *J* = 7.1 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 174.2, 169.7, 166.3, 166.1, 132.4, 129.3, 129.0, 128.7, 108.0, 84.3, 62.6, 61.2, 39.1, 14.0, 14.0, 14.0 ppm; HRMS (ESI-TOF): m/z calcd for $C_{19}H_{24}NO_7$ $[M+H]^+$ 378.1553, found 378.1587.

Diethyl 5-(2-ethoxy-2-oxoethyl)-4-(p-tolyl)oxazole-2,2(5*H*)-dicarboxylate (3fc)



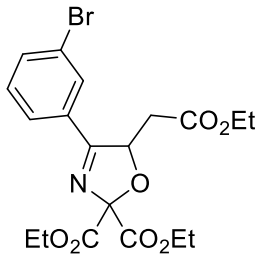
43.8 mg, 56% yield; white oil; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 (d, *J* = 8.2 Hz, 2H), 7.27 (d, *J* = 8.2 Hz, 2H), 5.98 (dd, *J* = 7.5, 3.7 Hz, 1H), 4.37–4.28 (m, 4H), 4.15 (q, *J* = 7.2 Hz, 2H), 2.91–2.79 (m, 2H), 2.41 (s, 3H), 1.36–1.30 (m, 6H), 1.24 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 174.0, 169.8, 166.5, 166.2, 143.1, 129.6, 128.7, 126.6, 108.0, 84.2, 62.5, 61.1, 21.6, 14.1, 14.0, 14.0 ppm; HRMS (ESI-TOF): m/z calcd for $C_{20}H_{26}NO_7$ $[M+H]^+$ 392.1709, found 392.1745.

Diethyl 4-([1,1'-biphenyl]-4-yl)-5-(2-ethoxy-2-oxoethyl)oxazole-2,2(5*H*)-dicarboxylate (3mc)



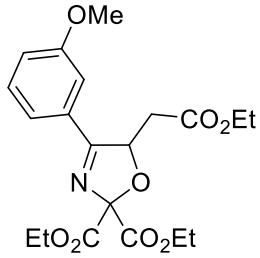
42.5 mg, 47% yield; white oil; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.91 (d, *J* = 8.3 Hz, 2H), 7.69 (d, *J* = 8.2 Hz, 2H), 7.61 (d, *J* = 7.4 Hz, 2H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.42–7.38 (m, 1H), 6.04 (dd, *J* = 7.4, 3.6 Hz, 1H), 4.38–4.29 (m, 4H), 4.17 (q, *J* = 7.1 Hz, 2H), 2.97–2.84 (m, 2H), 1.37–1.31 (m, 6H), 1.24 (t, *J* = 7.1 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 173.9, 169.8, 166.4, 166.1, 145.2, 139.7, 129.3, 129.0, 128.3, 128.1, 127.6, 127.2, 108.1, 84.3, 62.7, 61.2, 39.3, 14.1, 14.0, 14.0 ppm; HRMS (ESI-TOF): m/z calcd for $C_{25}H_{27}NO_7$ $[M+H]^+$ 453.1788, found 453.1824.

Diethyl 4-(3-bromophenyl)-5-(2-ethoxy-2-oxoethyl)oxazole-2,2(5*H*)-dicarboxylate (3hc)



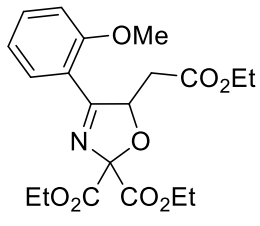
47.3 mg, 52% yield; white oil; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.07 (s, 1H), 7.68 (t, *J* = 8.7 Hz, 2H), 7.35 (t, *J* = 7.9 Hz, 1H), 5.96 (dd, *J* = 6.5, 4.3 Hz, 1H), 4.39–4.29 (m, 4H), 4.15 (q, *J* = 7.1 Hz, 1H), 2.91–2.81 (m, 2H), 1.37–1.31 (m, 6H), 1.24 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 173.0, 169.4, 166.0, 165.8, 135.3, 131.5, 131.3, 130.4, 127.2, 123.2, 108.0, 84.2, 62.7, 61.3, 38.9, 14.0, 14.0, 14.0 ppm; HRMS (ESI-TOF): m/z calcd for $C_{19}H_{23}NO_7$ $[M+H]^+$ 456.0658, found 456.0667.

Diethyl 5-(2-ethoxy-2-oxoethyl)-4-(3-methoxyphenyl)oxazole-2,2(5*H*)-dicarboxylate (3jc)



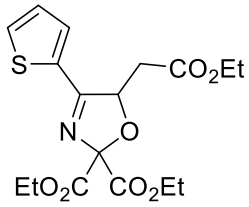
44.8 mg, 55% yield; white oil; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.38–7.37 (m, 1H), 7.30–7.21 (m, 2H), 7.01–6.99 (m, 1H), 5.91 (dd, *J* = 7.4, 3.7 Hz, 1H), 4.31–4.20 (m, 4H), 4.07 (q, *J* = 7.2 Hz, 2H), 3.78 (s, 3H), 2.82–2.73 (m, 2H), 1.29–1.23 (m, 6H), 1.16 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 174.2, 169.7, 166.3, 166.1, 160.0, 130.5, 129.9, 121.2, 119.1, 113.0, 108.0, 84.4, 62.6, 61.1, 55.6, 39.3, 14.1, 14.0, 14.0; HRMS (ESI-TOF): m/z calcd for $C_{20}H_{26}NO_8$ $[M+H]^+$ 408.1658, found 408.1697.

Diethyl 5-(2-ethoxy-2-oxoethyl)-4-(2-methoxyphenyl)oxazole-2,2(5*H*)-dicarboxylate (3lc)



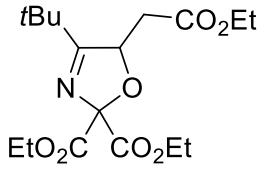
38.3 mg, 47% yield; white oil; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.08 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.50–7.46 (m, 1H), 7.06–7.02 (m, 1H), 6.95 (d, *J* = 8.3 Hz, 1H), 6.07 (dd, *J* = 7.3, 3.2 Hz, 1H), 4.36–4.27 (m, 4H), 4.12 (q, *J* = 7.1 Hz, 2H), 3.87 (s, 3H), 2.81–2.64 (m, 2H), 1.36–1.30 (m, 6H), 1.22 (t, *J* = 7.1 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 174.2, 170.1, 166.6, 166.4, 157.9, 133.7, 131.9, 121.3, 119.0, 111.3, 106.7, 86.2, 62.5, 62.4, 60.8, 55.4, 38.3, 14.1, 14.0 ppm; HRMS (ESI-TOF): m/z calcd for $C_{20}H_{26}NO_8$ $[M+H]^+$ 408.1658, found 408.1694.

Diethyl 5-(2-ethoxy-2-oxoethyl)-4-(thiophen-2-yl)oxazole-2,2(5*H*)-dicarboxylate (3pc)



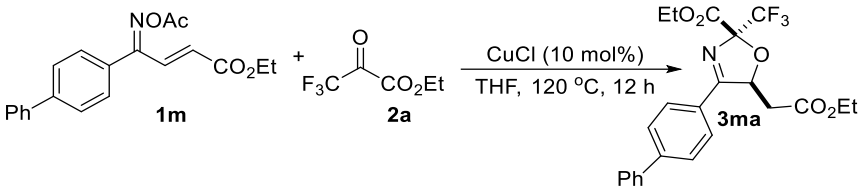
33.7 mg, 44% yield; white oil; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.62 (d, *J* = 5.0 Hz, 1H), 7.49 (d, *J* = 3.6 Hz, 1H), 7.06–7.20 (m, 1H), 5.88 (dd, *J* = 7.3, 3.8 Hz, 1H), 4.35–4.29 (m, 4H), 4.18 (q, *J* = 7.1 Hz, 2H), 3.02–2.90 (m, 2H), 1.35–1.30 (m, 6H), 1.25 (t, *J* = 7.1 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.7, 167.9, 166.3, 166.0, 132.9, 132.3, 131.8, 128.1, 107.6, 84.4, 63.5, 62.6, 61.2, 39.8, 14.1, 14.0, 13.9 ppm; HRMS (ESI-TOF): m/z calcd for $C_{17}H_{22}NO_7S$ $[M+H]^+$ 384.1117, found 384.1152.

Diethyl 4-(tert-butyl)-5-(2-ethoxy-2-oxoethyl)oxazole-2,2(5*H*)-dicarboxylate (3qc)



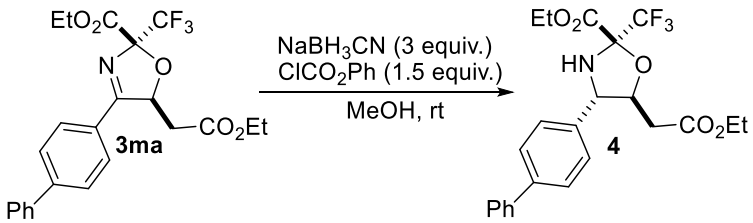
41.4 mg, 58% yield; white oil; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 1.27–1.19 (m, 18H), 2.89–2.67 (m, 2H), 4.24–4.08 (m, 6H), 5.40 (dd, *J* = 8.0, 3.4 Hz, 1H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 185.2, 169.4, 166.4, 166.2, 107.0, 84.6, 62.3, 61.0, 39.1, 35.3, 28.6, 14.1, 13.9, 13.9 ppm; HRMS (ESI-TOF): m/z calcd for $C_{17}H_{28}NO_7$ $[M+H]^+$ 358.1866, found 358.1888.

Scale-up synthesis of compound 3ma



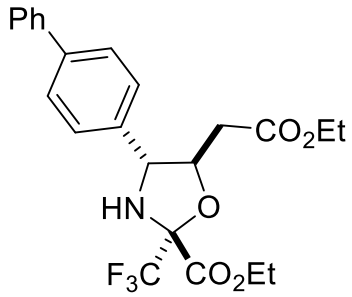
ketoxime-enoate **1m** (3.37 g, 10 mmol), ethyl trifluoropyruvate **2a** (0.85 g, 5 mmol) and CuCl (49 mg, 0.5 mmol) were loaded into a Schlenk tube equipped with a Teflon-coated magnetic stir bar. The Schlenk tube was placed under vacuum for 1 min and then N_2 was pumped into it. The solvent THF (40 mL) was added into the Schlenk tube by syringe. The reaction mixture was stirred at 120 ^{o}C for 12 h. Then the reaction tube was allowed to cool to room temperature and the reaction solution was concentrated under reduced pressure. The crude products were purified by column chromatography on silica gel (Petroleum Ether/EtOAc= 10:1) to give the product **3ma** 1.68 g (75% yield, 92:7 dr).

General procedure for the synthesis of 4



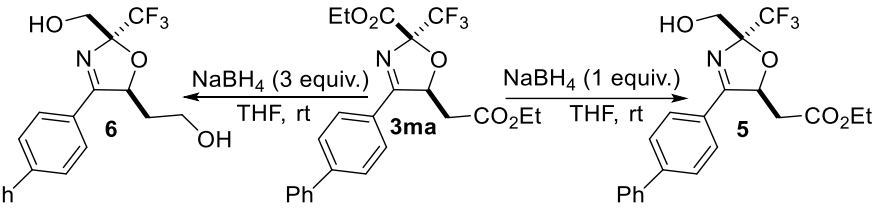
3ma (0.2 mmol), Phenyl chloroformate (0.3 mmol), and $NaBH_3CN$ (0.6 mmol) were loaded into a 10 mL Schlenk tube equipped with a Teflon-coated magnetic stir bar. The solvent MeOH (2 mL, 0.1 M) was added into the Schlenk tube by syringe. The reaction mixture was stirred at room temperature for 12 h. After completion of the reaction (detected by TLC), the reaction solution was concentrated under vacuum. The crude products were purified by column chromatography on silica gel (Petroleum Ether/EtOAc) to give the products **4**.

Ethyl-4-([1,1'-biphenyl]-4-yl)-5-(2-ethoxy-2-oxoethyl)-2-(trifluoromethyl)oxazolidine-2-carboxylate (4)



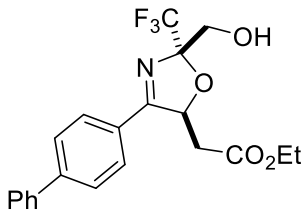
74.0 mg, 82% yield; white oil; dr 95:5; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.57 (t, *J* = 6.4 Hz, 4H), 7.52 (d, *J* = 8.2 Hz, 2H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.35 (t, *J* = 7.3 Hz, 1H), 4.53–4.34 (m, 4H), 4.10 – 3.95 (m, 2H), 3.67 (d, *J* = 6.1 Hz, 1H), 2.74–2.63 (m, 2H), 1.37 (t, *J* = 7.1 Hz, 3H), 1.15 (t, *J* = 7.1 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.4, 167.0, 141.6, 140.6, 136.0, 128.84, 127.9, 127.5, 127.1, 122.7 (q, *J* = 285.0 Hz), 91.7 (q, *J* = 32.7 Hz), 84.0, 65.0, 63.4, 60.9, 36.5, 14.0, 14.0 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -80.0 ppm; HRMS (ESI-TOF): m/z calcd for $C_{23}H_{25}F_3NO_5$ $[M+H]^+$ 452.1685, found 452.1721.

General procedure for the synthesis of 5 and 6



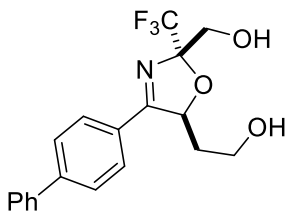
3ma (0.2 mmol, 1.0 equiv.), $NaBH_4$ (0.2 mmol, 1.0 equiv or 0.6 mmol, 3.0 equiv) were loaded into a 10 mL Schlenk tube equipped with a Teflon-coated magnetic stir bar. The solvent THF (2 mL, 0.1 M) was added into the Schlenk tube by syringe. The reaction mixture was stirred at room temperature for 12 h. After completion of the reaction (detected by TLC), the reaction solution was concentrated under vacuum. The crude products were purified by column chromatography on silica gel (Petroleum Ether/EtOAc) to give the products **5** or **6**.

Ethyl 2-(4-([1,1'-biphenyl]-4-yl)-2-(hydroxymethyl)-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl)acetate (5)



29.3 mg, 36% yield; white oil; dr 85:15; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.86 (d, *J* = 8.3 Hz, 2H), 7.68 (d, *J* = 8.2 Hz, 2H), 7.60 (d, *J* = 7.3 Hz, 2H), 7.47 (t, *J* = 7.4 Hz, 2H), 7.40 (t, *J* = 7.3 Hz, 1H), 5.88 (dd, *J* = 8.2, 3.3 Hz, 1H), 4.2–4.00 (m, 4H), 3.03–2.80 (m, 2H), 1.24 (t, *J* = 7.1 Hz, 3H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 174.9, 170.2, 145.3, 139.7, 129.0, 129.0, 128.3, 128.1, 127.6, 127.2, 123.0 (q, *J* = 285.4 Hz), 109.3 (q, *J* = 27.8 Hz), 83.8, 61.6, 61.5, 39.4, 14.1 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -79.9 ppm; HRMS (ESI-TOF): m/z calcd for $C_{21}H_{21}F_3NO_4$ $[M+H]^+$ 408.1423, found 408.1456.

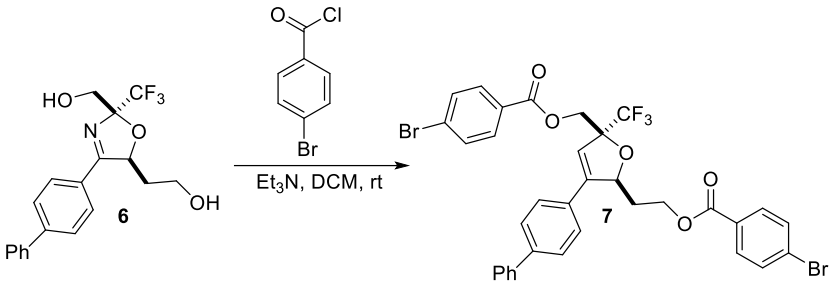
2-(4-([1,1'-Biphenyl]-4-yl)-2-(hydroxymethyl)-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl)ethan-1-ol (6)



63.5 mg, 87% yield; white oil; dr 85:15; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.76 (d, *J* = 8.3 Hz, 2H), 7.58 (d, *J* = 8.4 Hz, 2H), 7.51 (d, *J* = 7.1 Hz, 2H), 7.38 (t, *J* = 7.3 Hz, 2H), 7.33–7.29 (m, 1H), 5.61 (dd, *J* = 7.2, 3.6 Hz, 1H), 4.15 (d, *J* = 12.1 Hz, 1H), 3.93 (d, *J* = 12.1 Hz, 1H), 3.83–3.78 (m, 1H), 3.69–3.63 (m, 1H), 2.25–2.18 (m, 1H), 2.04–1.97 (m, 1H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 176.9, 145.1, 139.7, 129.0, 128.9, 128.7, 128.3, 127.6, 127.2, 123.2 (q, *J* = 286.0 Hz), 108.6 (q, *J* = 27.4

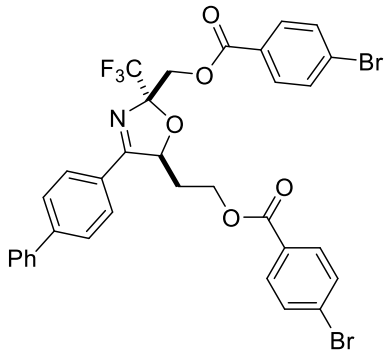
Hz), 86.4, 61.4, 59.0, 35.5 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -80.2 ppm; HRMS (ESI-TOF): m/z calcd for $C_{19}H_{19}F_3NO_3$ $[M+H]^+$ 366.1317, found 366.1354.

General procedure for the synthesis of 7



6 (0.2 mmol), 4-bromobenzoyl chloride (0.3 mmol), and Et_3N (0.3 mmol) were loaded into a 10 mL Schlenk tube equipped with a Teflon-coated magnetic stir bar. The solvent DCM (2 mL, 0.1 M) was added into the Schlenk tube by syringe. The reaction mixture was stirred at room temperature for 12 h. After completion of the reaction (detected by TLC), the reaction solution was concentrated under vacuum. The crude product was purified by column chromatography on silica gel (Petroleum Ether/EtOAc) to give the product **7**.

2-(4-([1,1'-Biphenyl]-4-yl)-2-(((4-bromobenzoyl)oxy)methyl)-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl)ethyl 4-bromobenzoate (7)



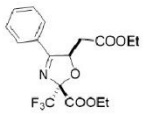
128.3 mg, 88% yield; white solid; mp 285–286 ºC; dr 87:13; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.89–7.82 (m, 4H), 7.72 (d, *J* = 8.5 Hz, 2H), 7.64–7.57 (m, 4H), 7.53–7.38 (m, 7H), 5.68 (dd, *J* = 8.9, 2.5 Hz, 1H), 4.92–4.84 (m, 2H), 4.50 (t, *J* = 6.2 Hz, 2H), 2.50–2.04 (m, 2H) ppm; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 175.8, 165.5, 165.0, 145.4, 139.5, 132.4, 132.0, 131.7, 131.2, 131.0, 129.1, 128.7, 128.4, 128.3, 128.3, 128.1, 127.6, 127.2, 122.9 (q, *J* = 286.0 Hz), 107.1 (q, *J* = 28.9 Hz), 85.1, 63.1, 61.3, 33.6 ppm; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.5 PPM; HRMS (ESI-TOF): m/z calcd for $C_{33}H_{25}Br_2F_3NO_5$ $[M+H]^+$ 730.0052, found 730.0098.

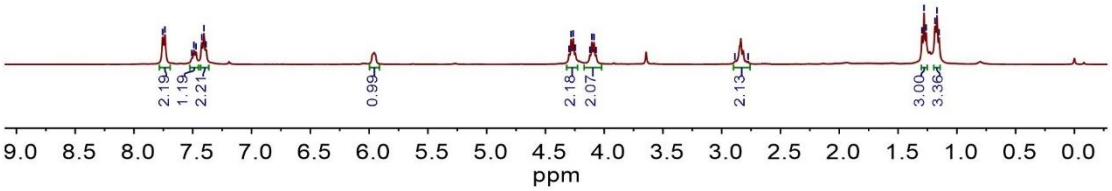
REFERENCES

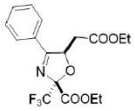
(1) J. Duan, L. Zhang, G. Xu, H. Chen, X. Ding, Y. Mao, B. Rong, N. Zhu and K. Guo, *J. Org. Chem.*, 2020, **85**, 8157.

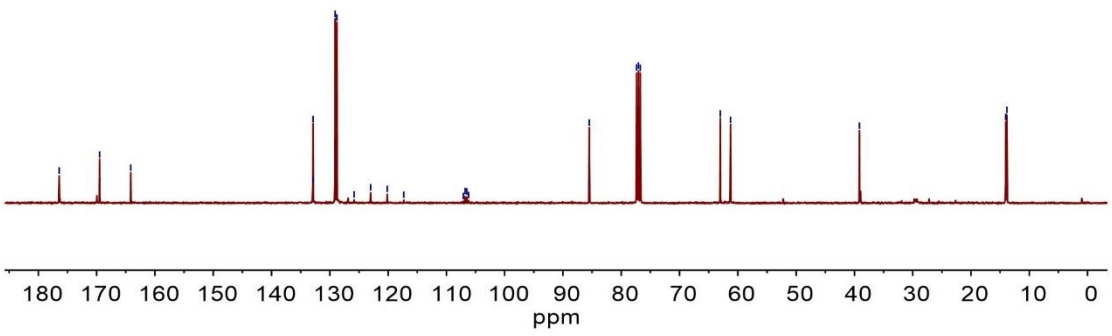
NMR spectra and GC chromatograms

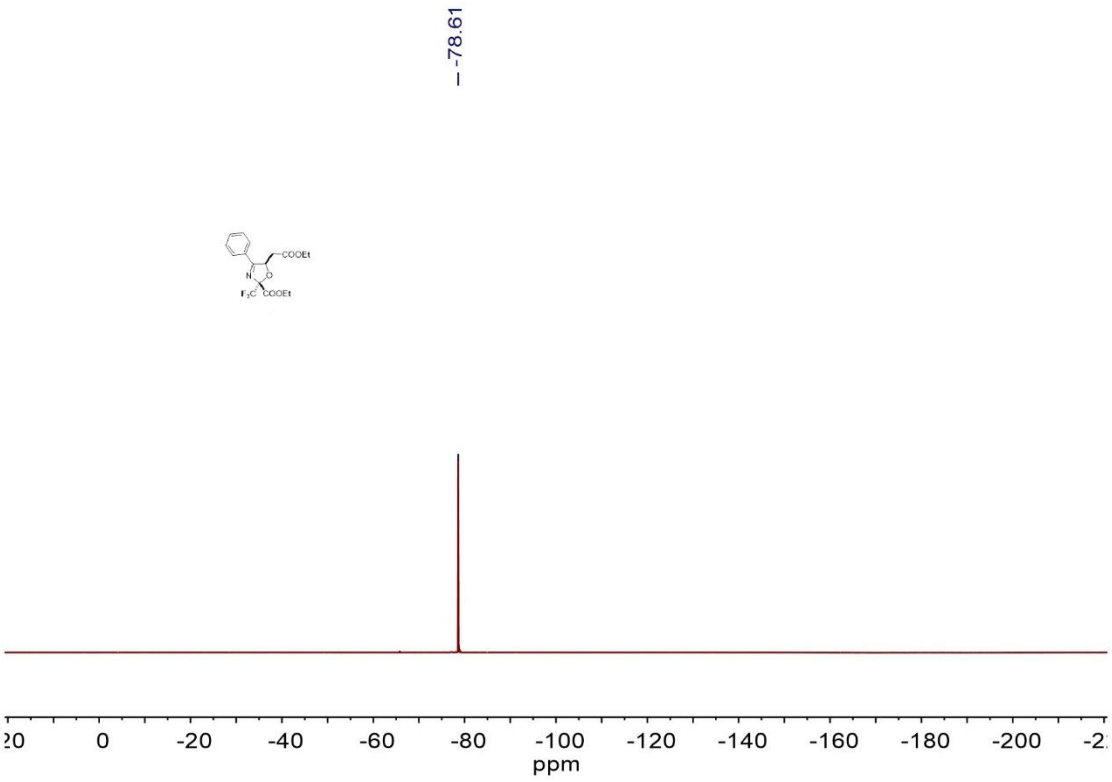
Ethyl-5-(2-ethoxy-2-oxoethyl)-4-phenyl-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3aa)

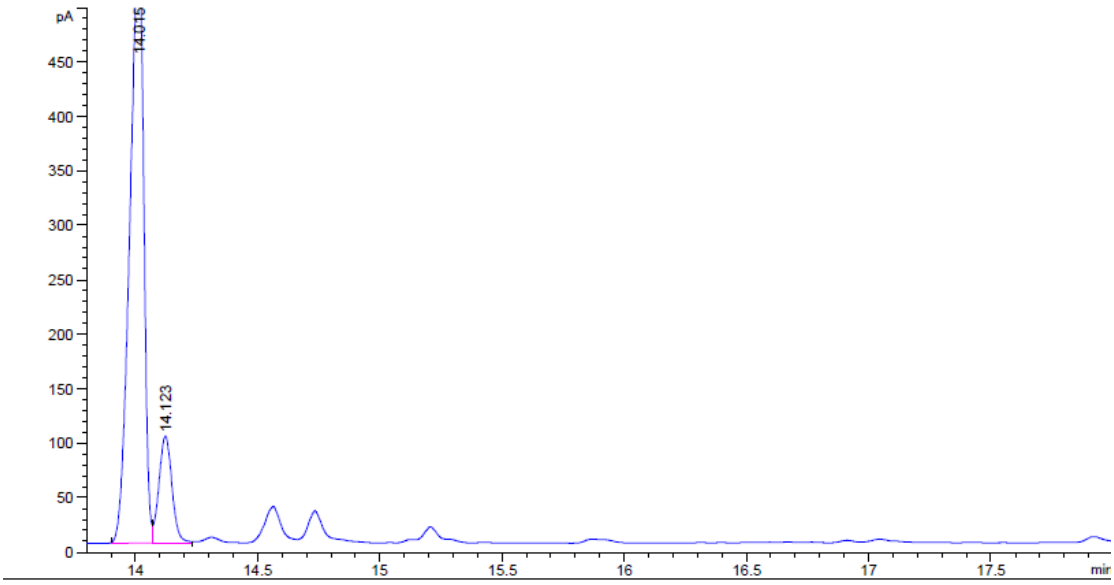






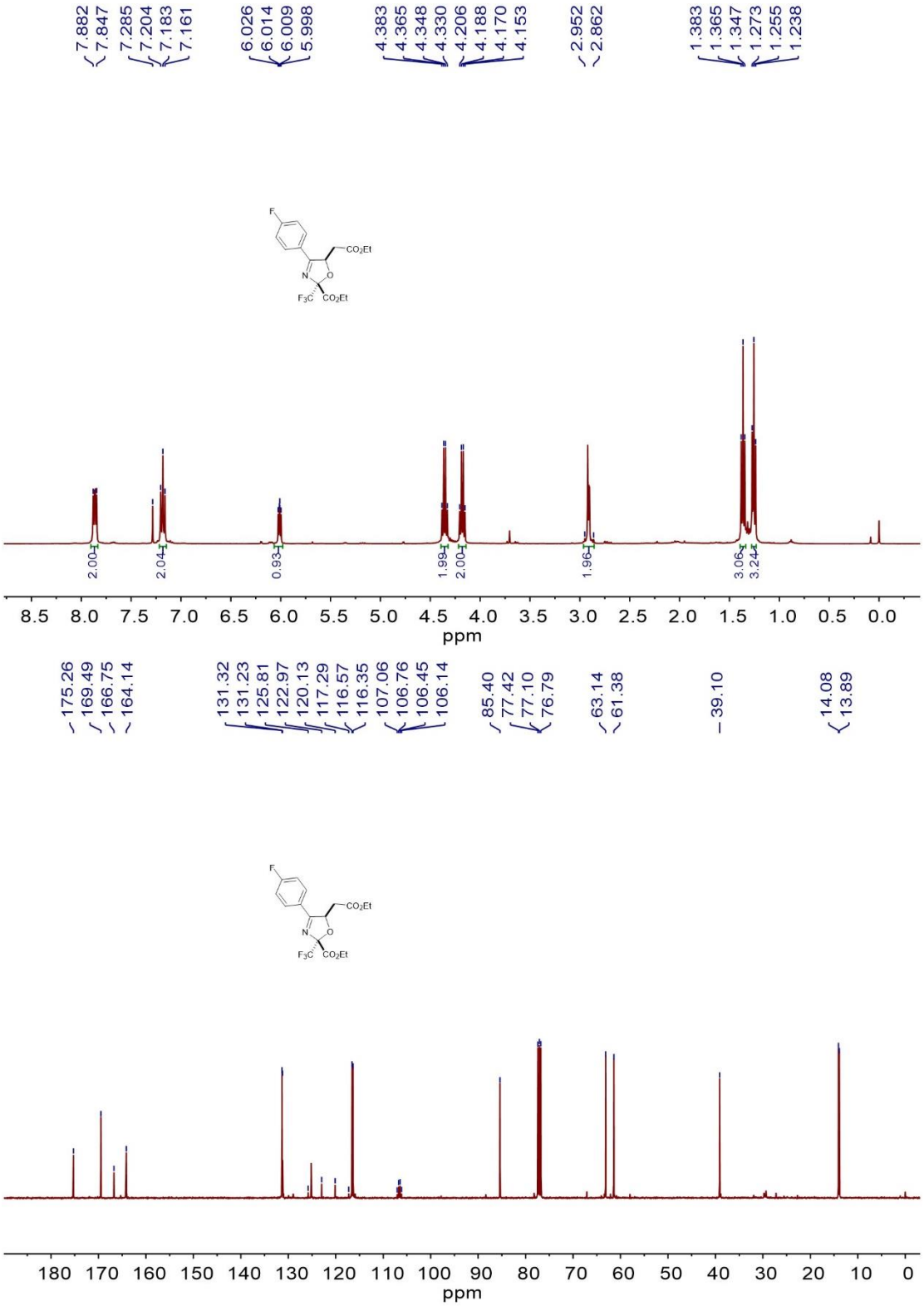


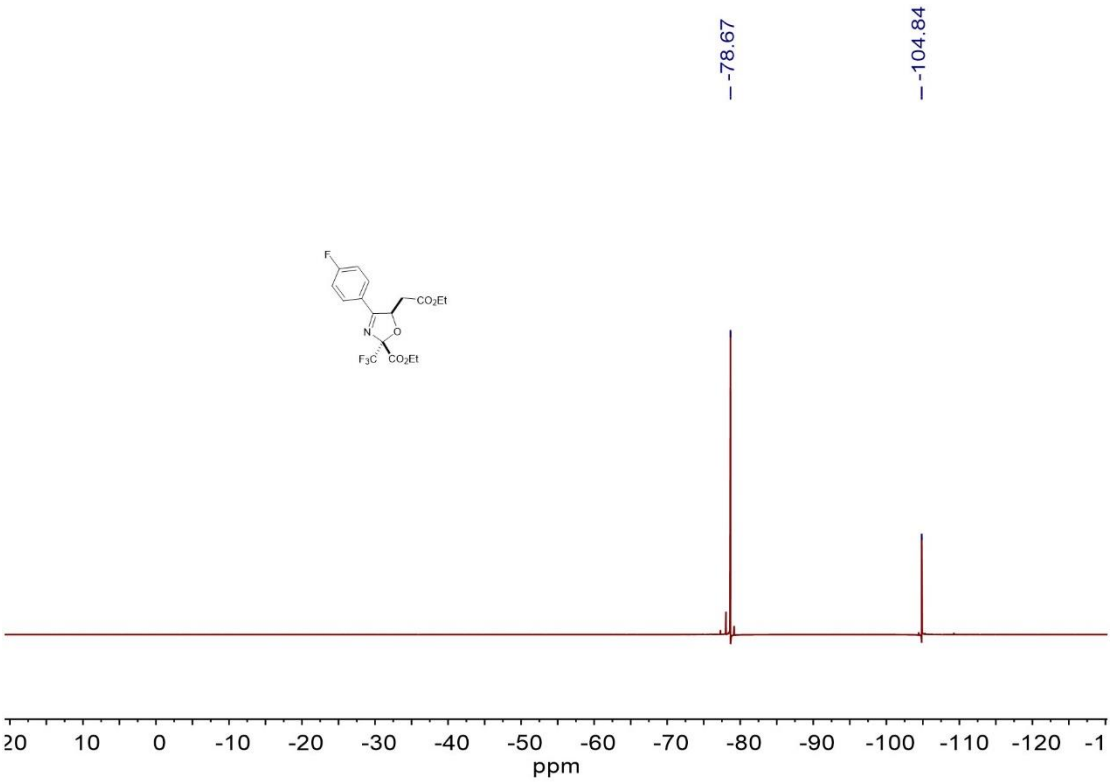


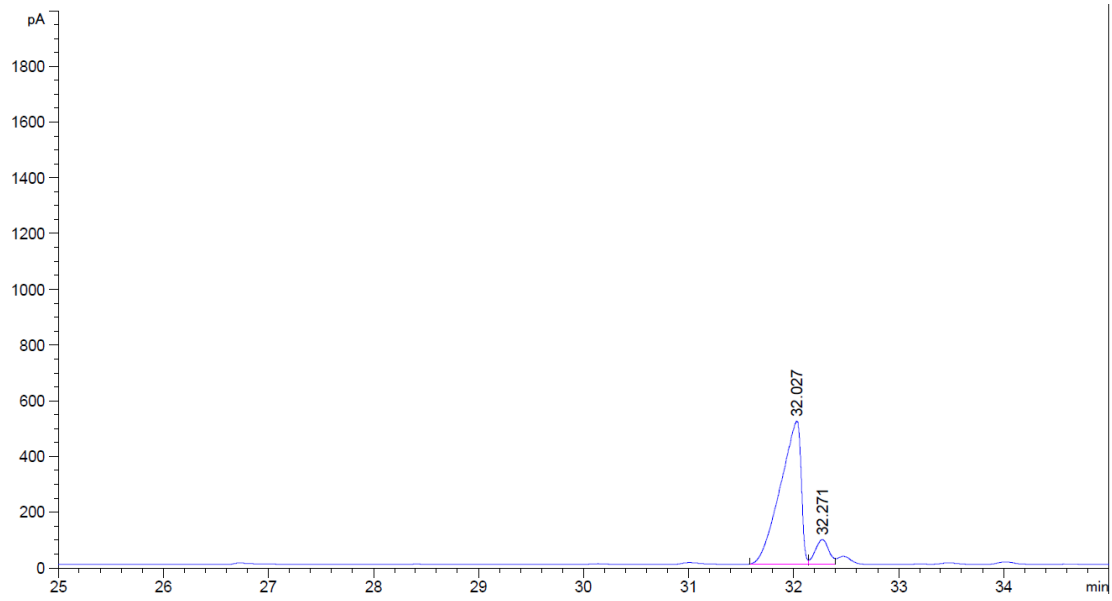


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [pA*s]	峰高 [pA]	峰面积 %
1	14.015	BV	0.0540	2174.84155	564.10565	85.66917
2	14.123	VB	0.0582	363.80991	98.19147	14.33083
总量：				2538.65146	662.29713	

Ethyl-5-(2-ethoxy-2-oxoethyl)-4-(4-fluorophenyl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3ba)

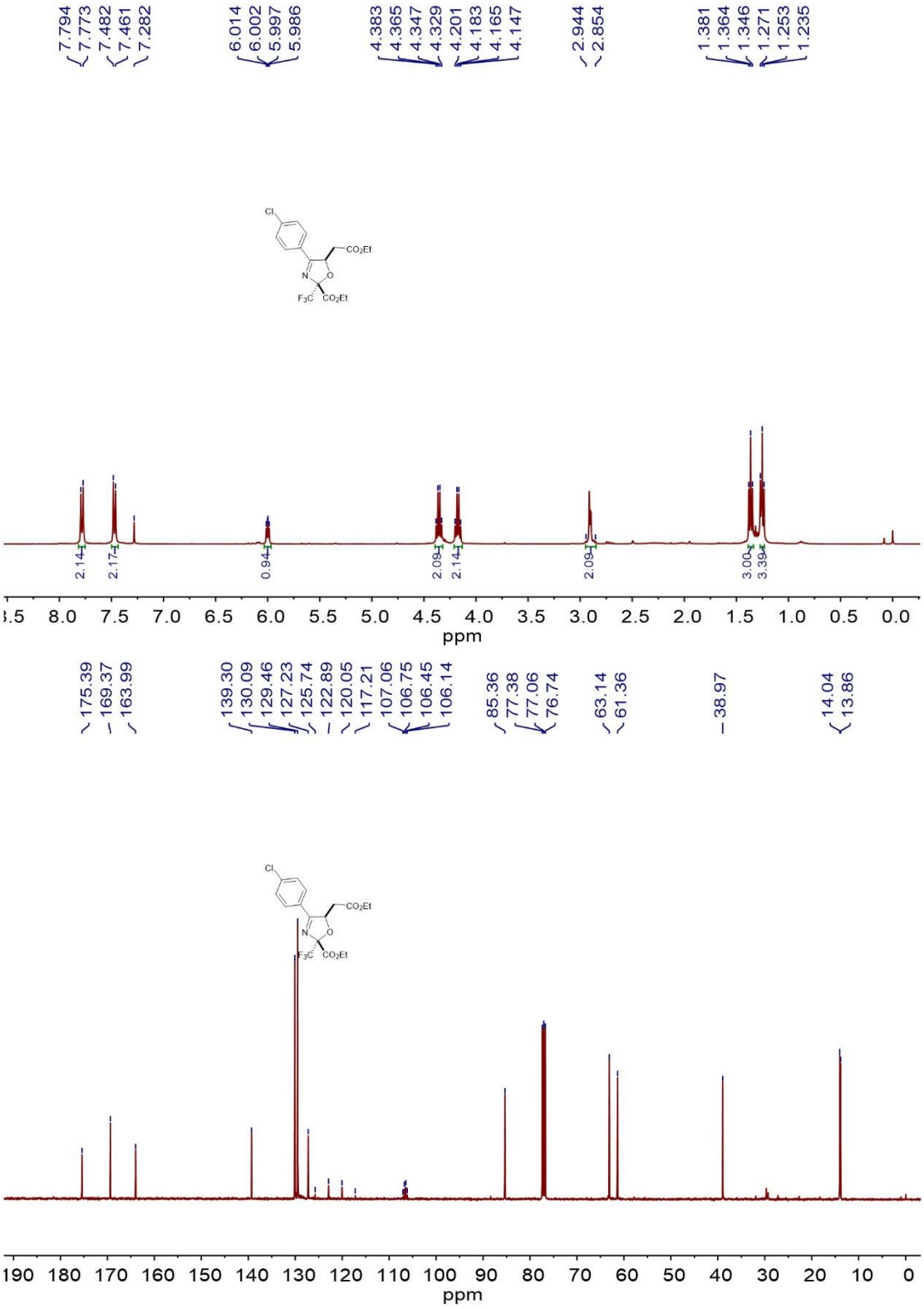


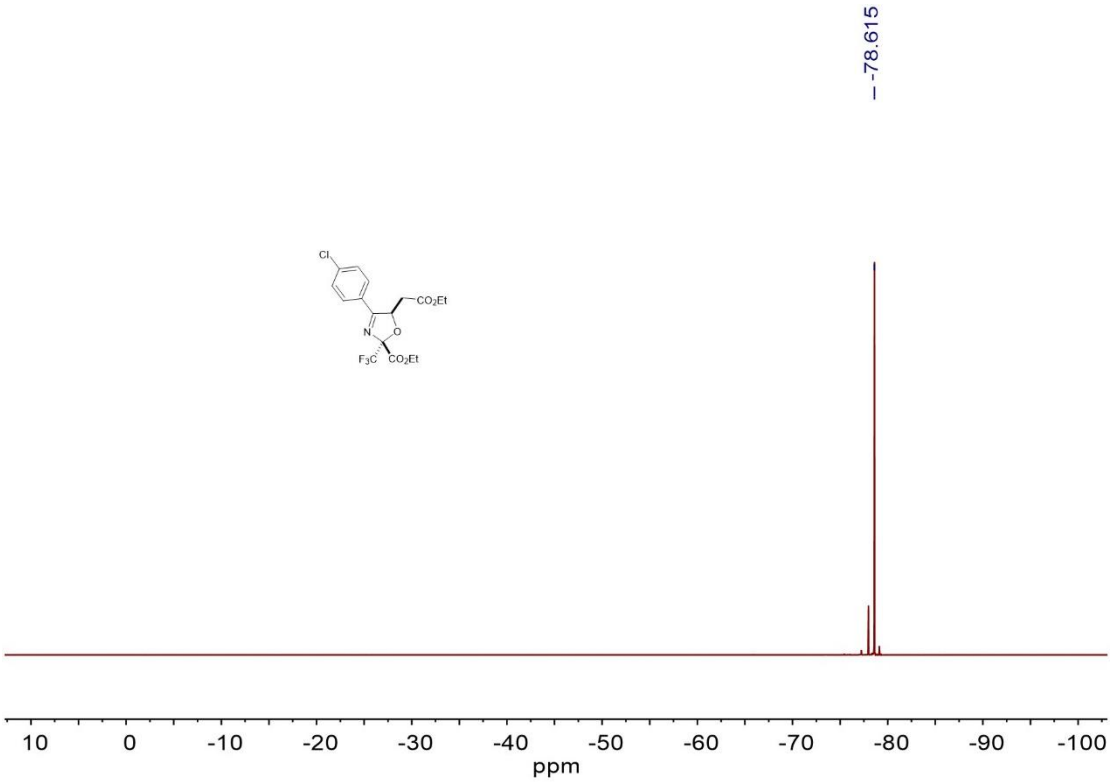


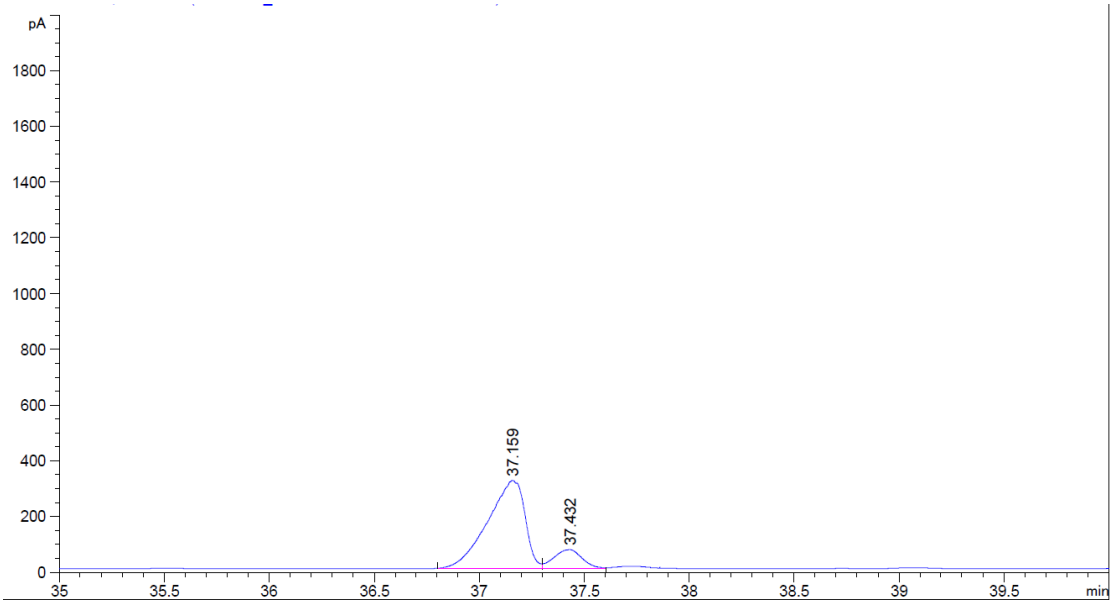


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [pA*s]	峰高 [pA]	峰面积 %
1	32.027	BV	0.1639	7086.56689	513.92224	89.82065
2	32.271	VV	0.1236	803.11841	89.53707	10.17935
总量 :				7889.68530	603.45931	

Ethyl -4-(4-chlorophenyl)-5-(2-ethoxy-2-oxoethyl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3ca)







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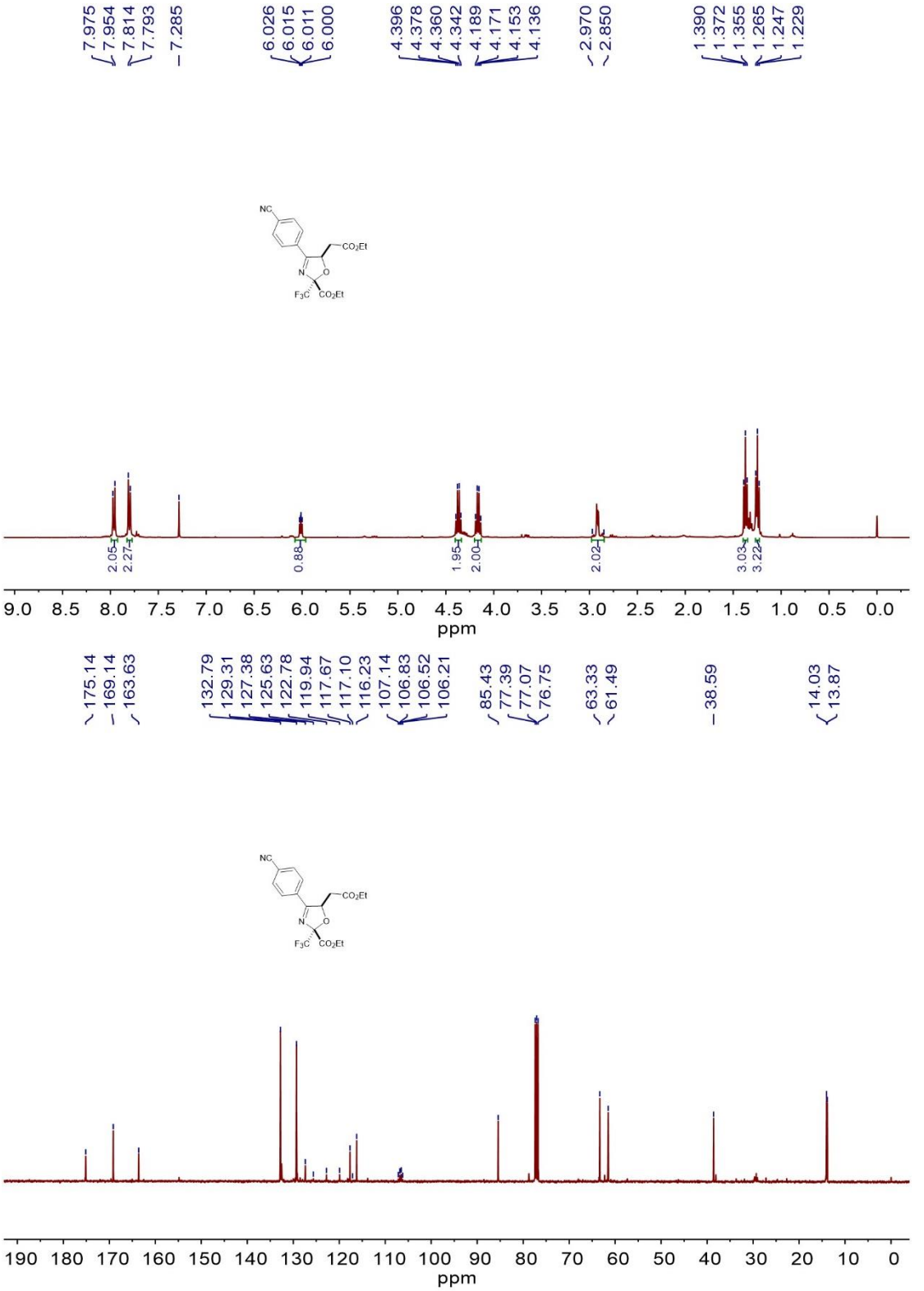
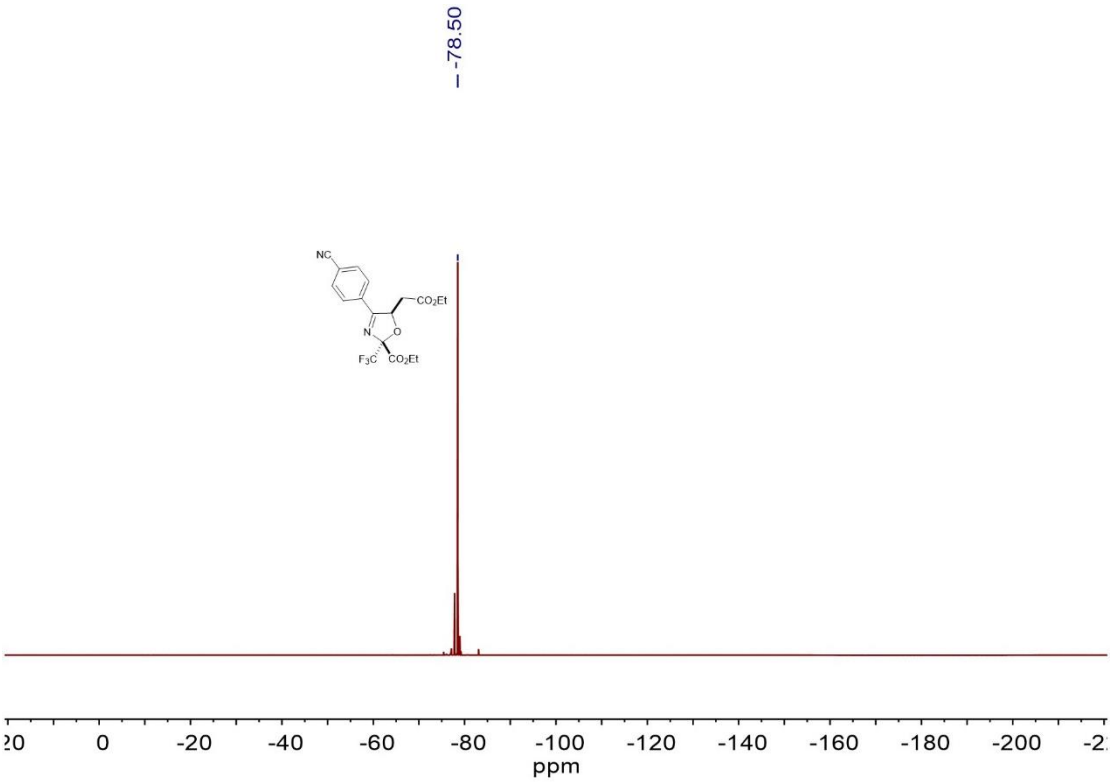
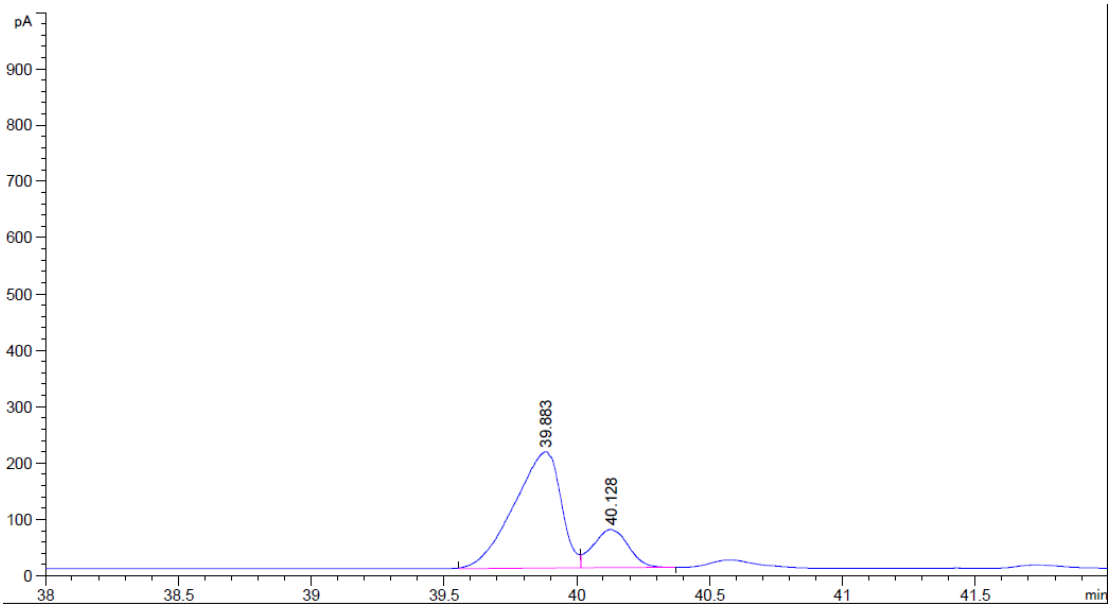
1	37.159	BV	0.1534	3920.65479	316.83633	85.98796
2	37.432	VV	0.1255	638.88464	68.06641	14.01204
总量 :				4559.53943	384.90274	

Ethyl-4-(4-cyanophenyl)-5-(2-ethoxy-2-oxoethyl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3da)

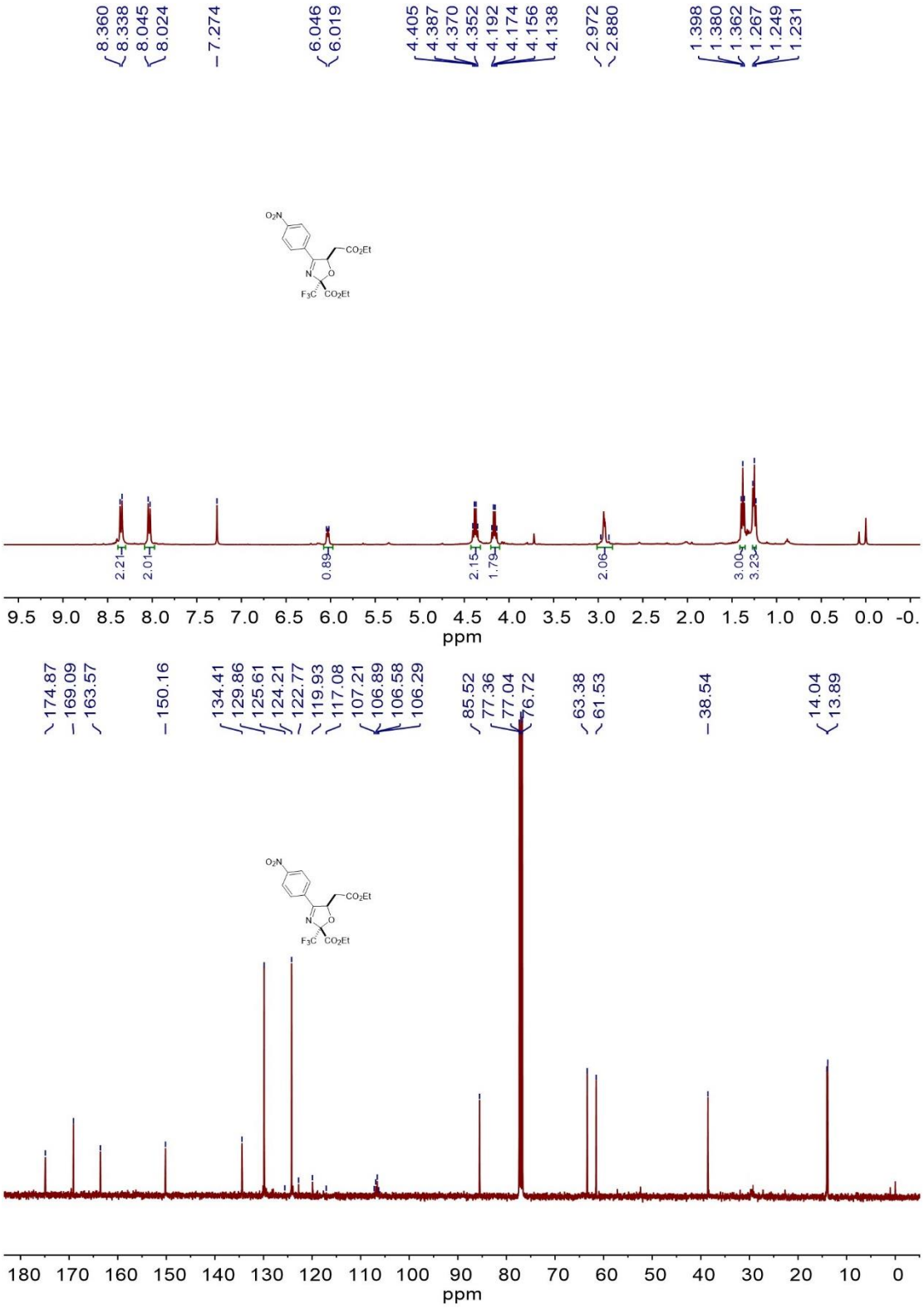


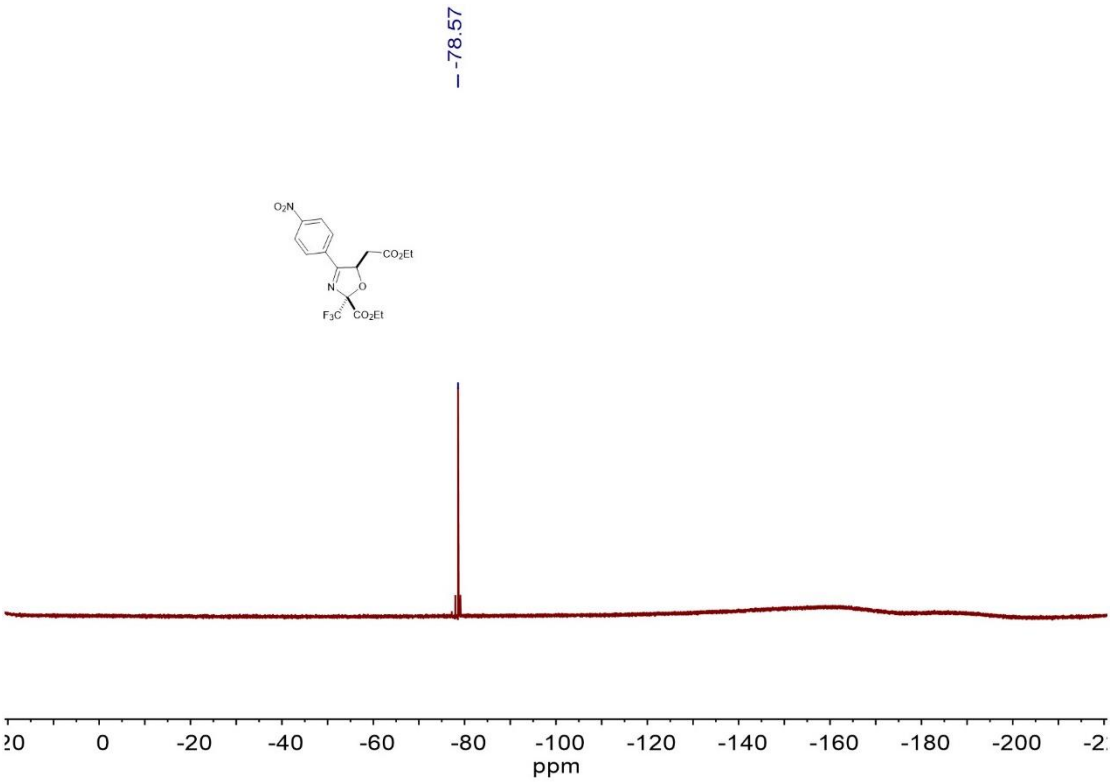


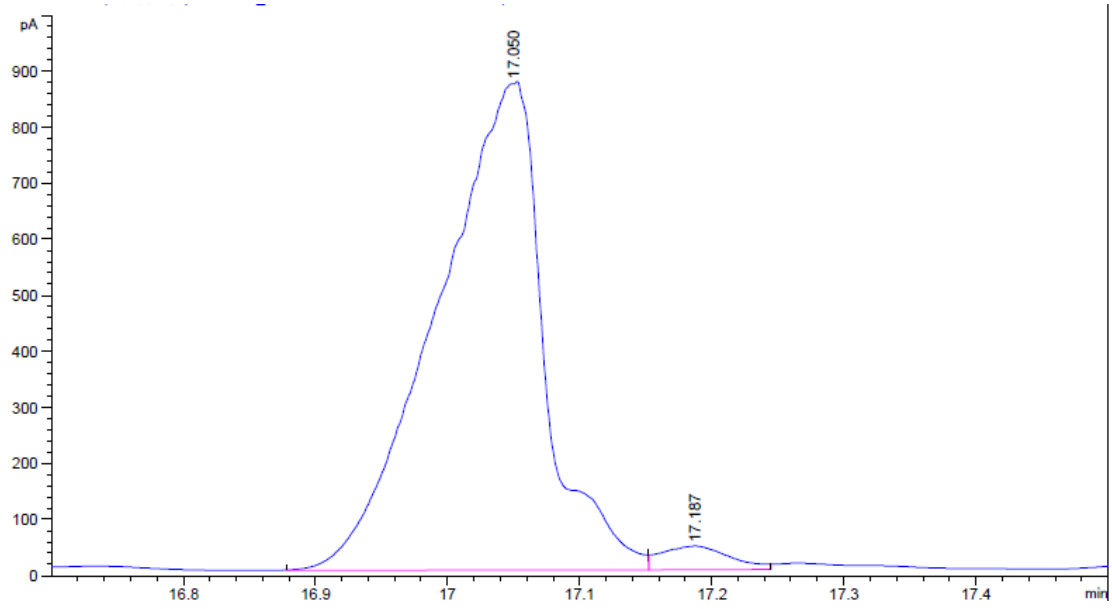


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [pA*s]	峰高 [pA]	峰面积 %
1	39.883	BV	0.1542	2534.45728	206.45010	80.15078
2	40.128	VB	0.1142	627.65472	67.70673	19.84922
总量 :				3162.11200	274.15683	

Ethyl-5-(2-ethoxy-2-oxoethyl)-4-(4-nitrophenyl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3ea)



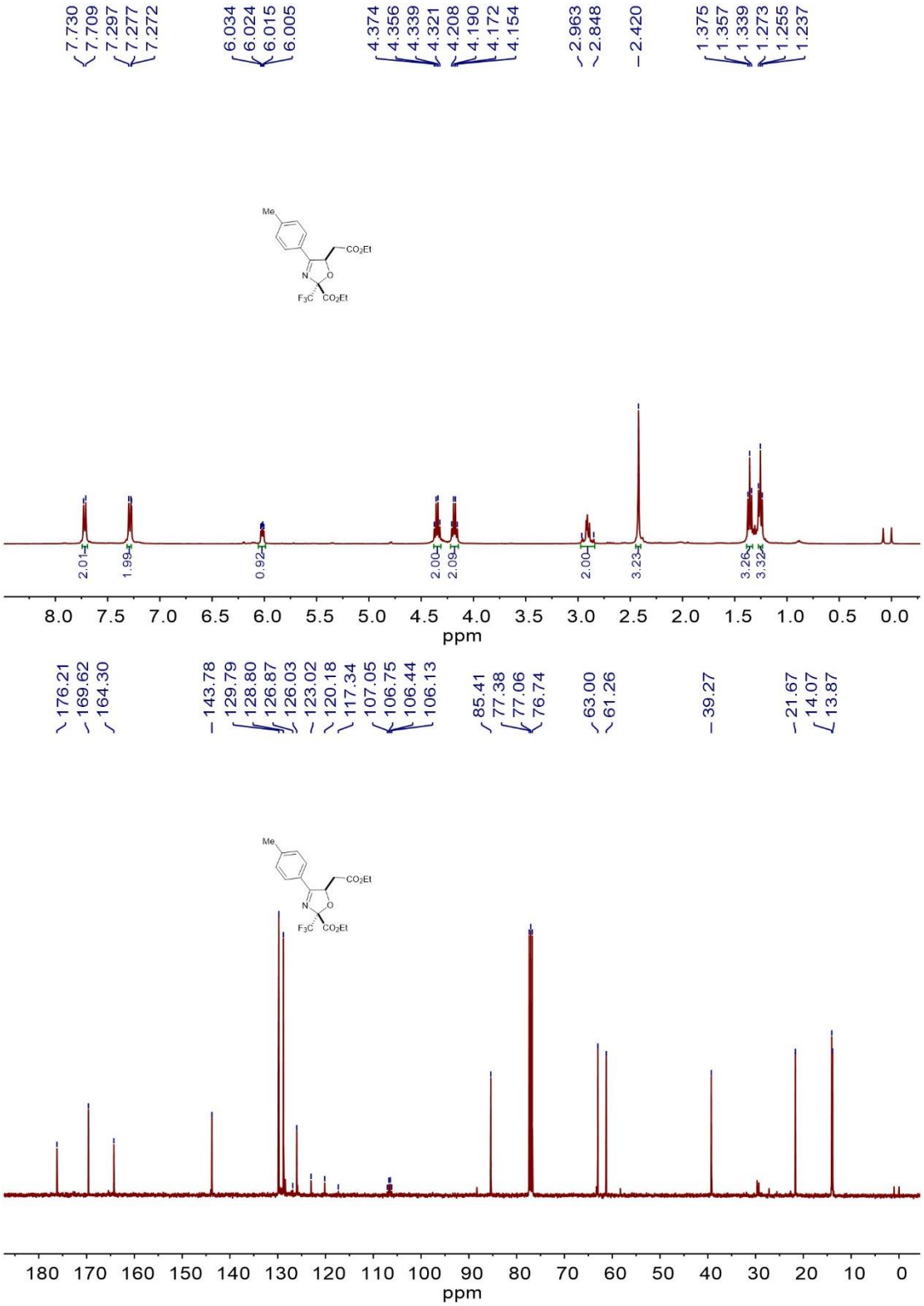


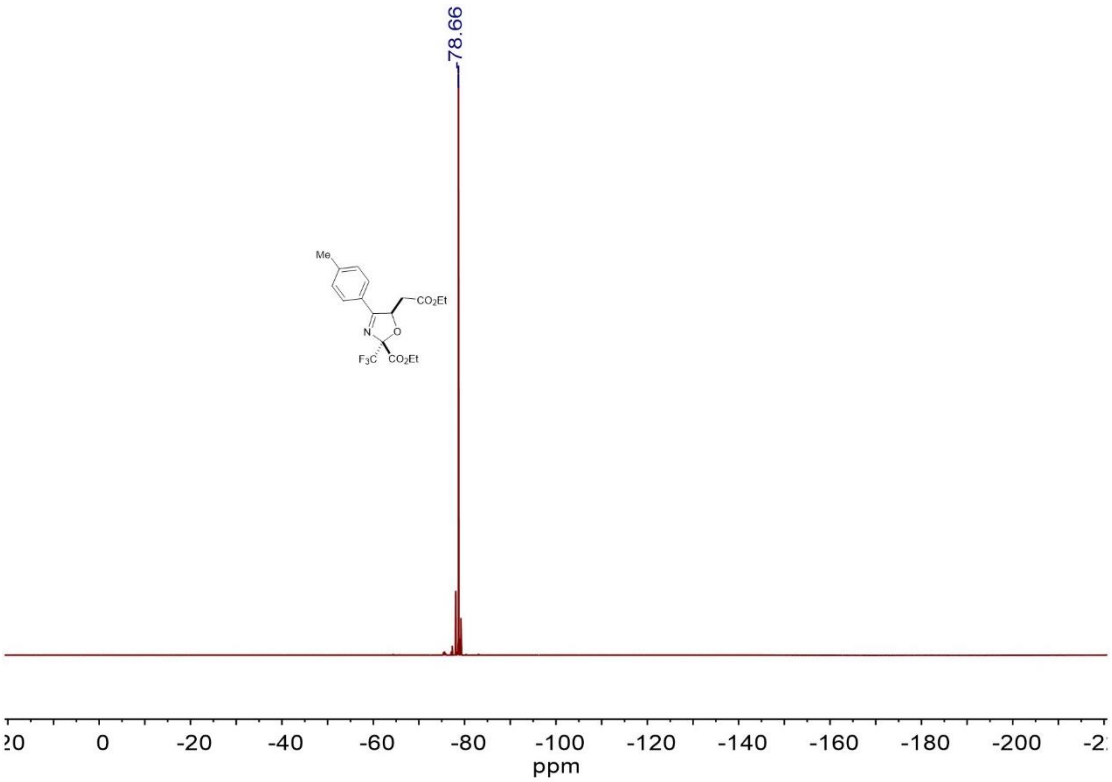


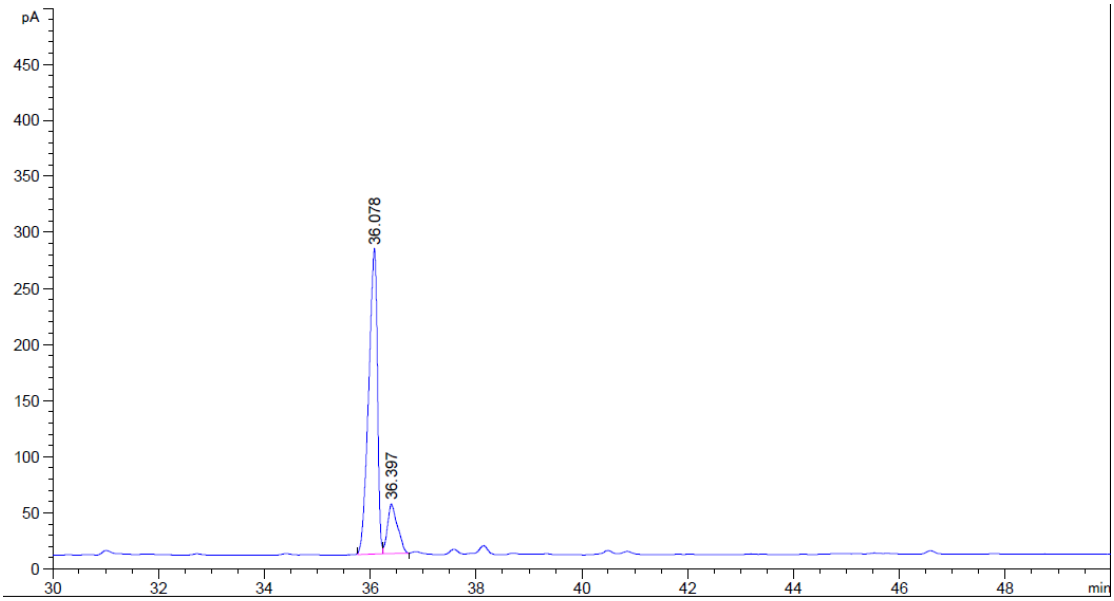
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [pA*s]	峰高 [pA]	峰面积 %
1	17.050	BV	0.0749	4913.46582	870.27124	96.99590
2	17.187	VV	0.0512	152.17706	42.07787	3.00410
总量：				5065.64288	912.34911	

Ethyl-5-(2-ethoxy-2-oxoethyl)-4-(p-tolyl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxyla

te (3fa)

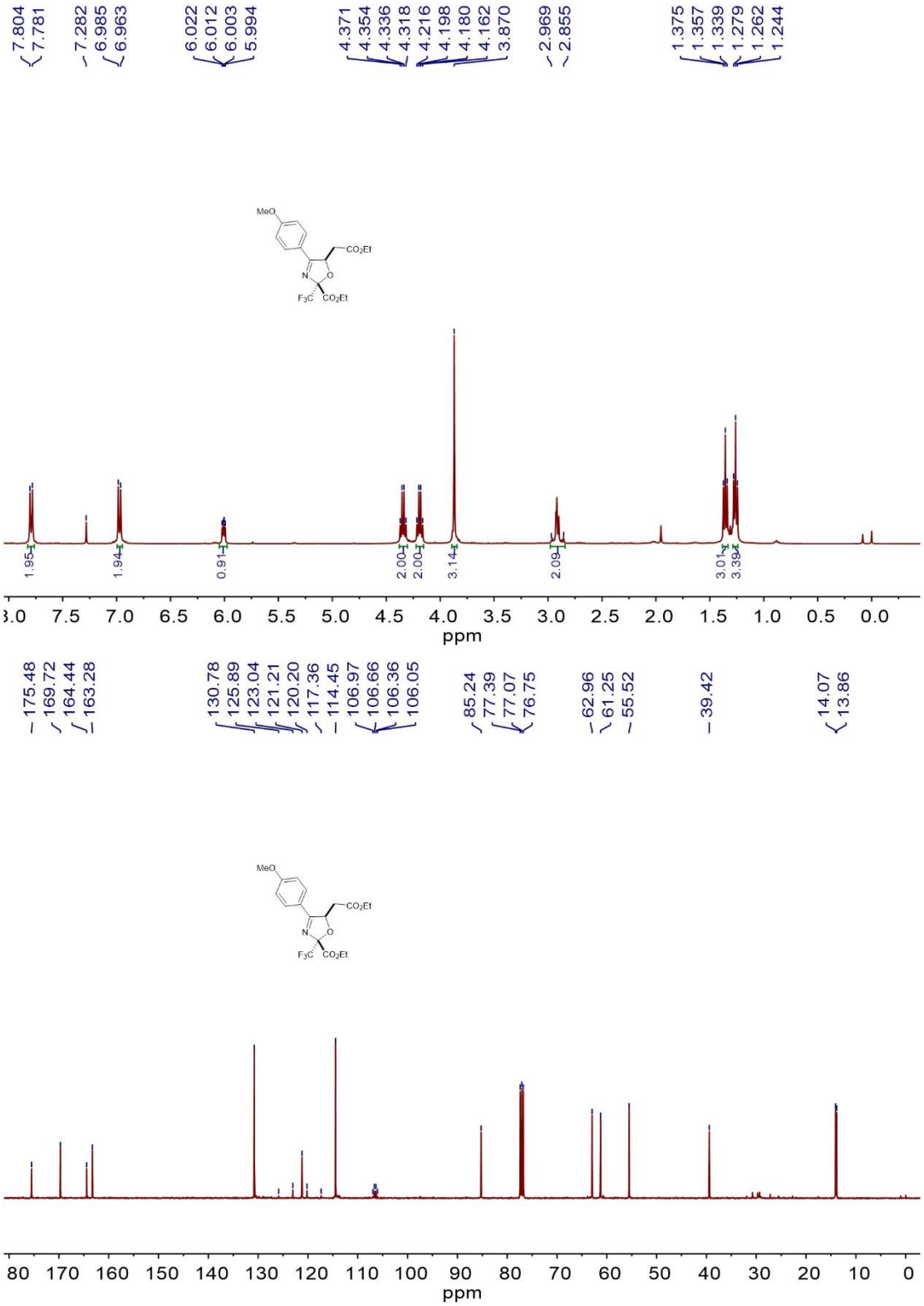


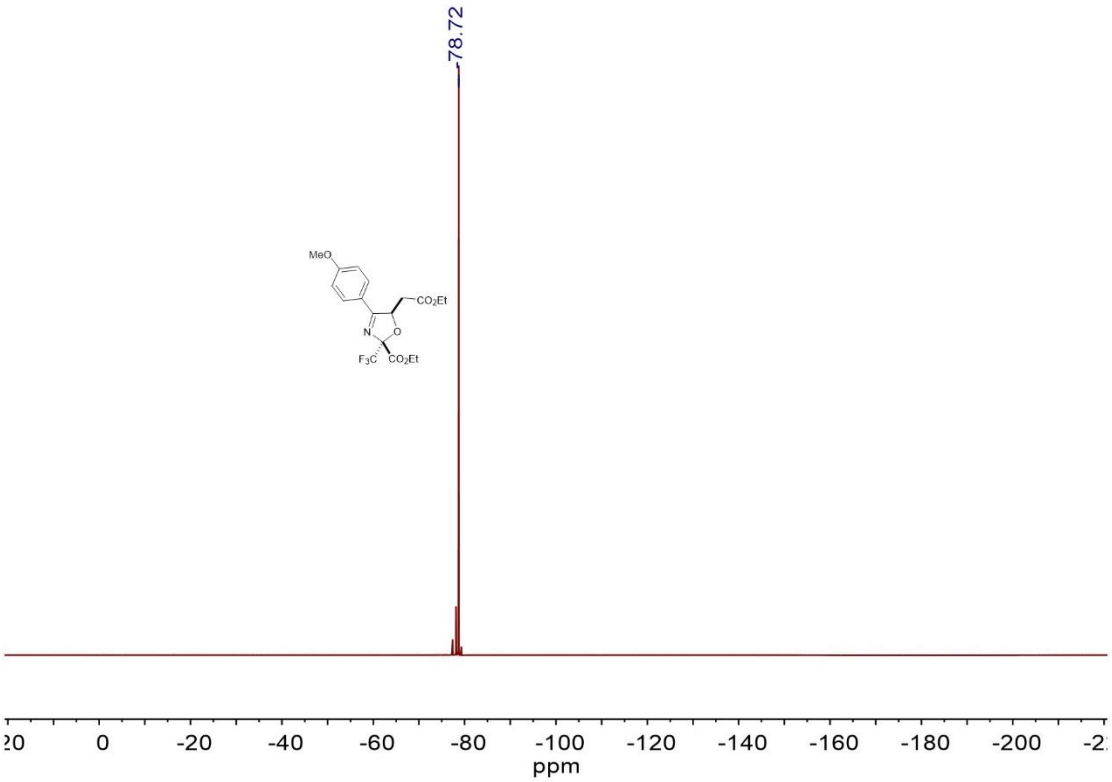


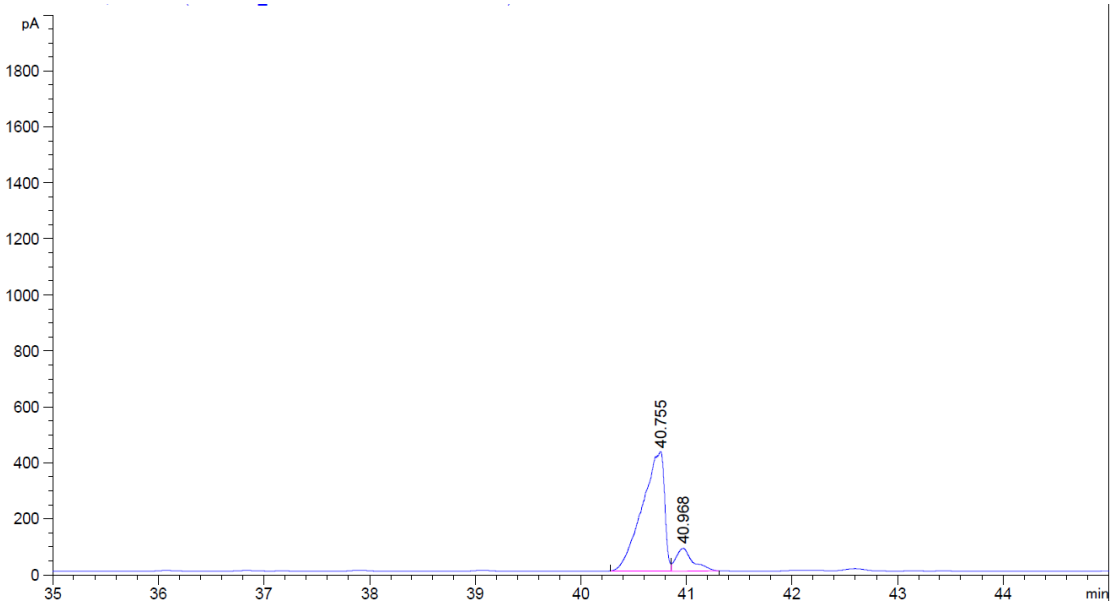


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [pA*s]	峰高 [pA]	峰面积 %
1	36.078	BV	0.1388	3140.76221	271.79196	84.41208
2	36.397	VB	0.1655	579.98737	44.37963	15.58792
总量：				3720.74957	316.17160	

Ethyl-5-(2-ethoxy-2-oxoethyl)-4-(4-methoxyphenyl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3ga)







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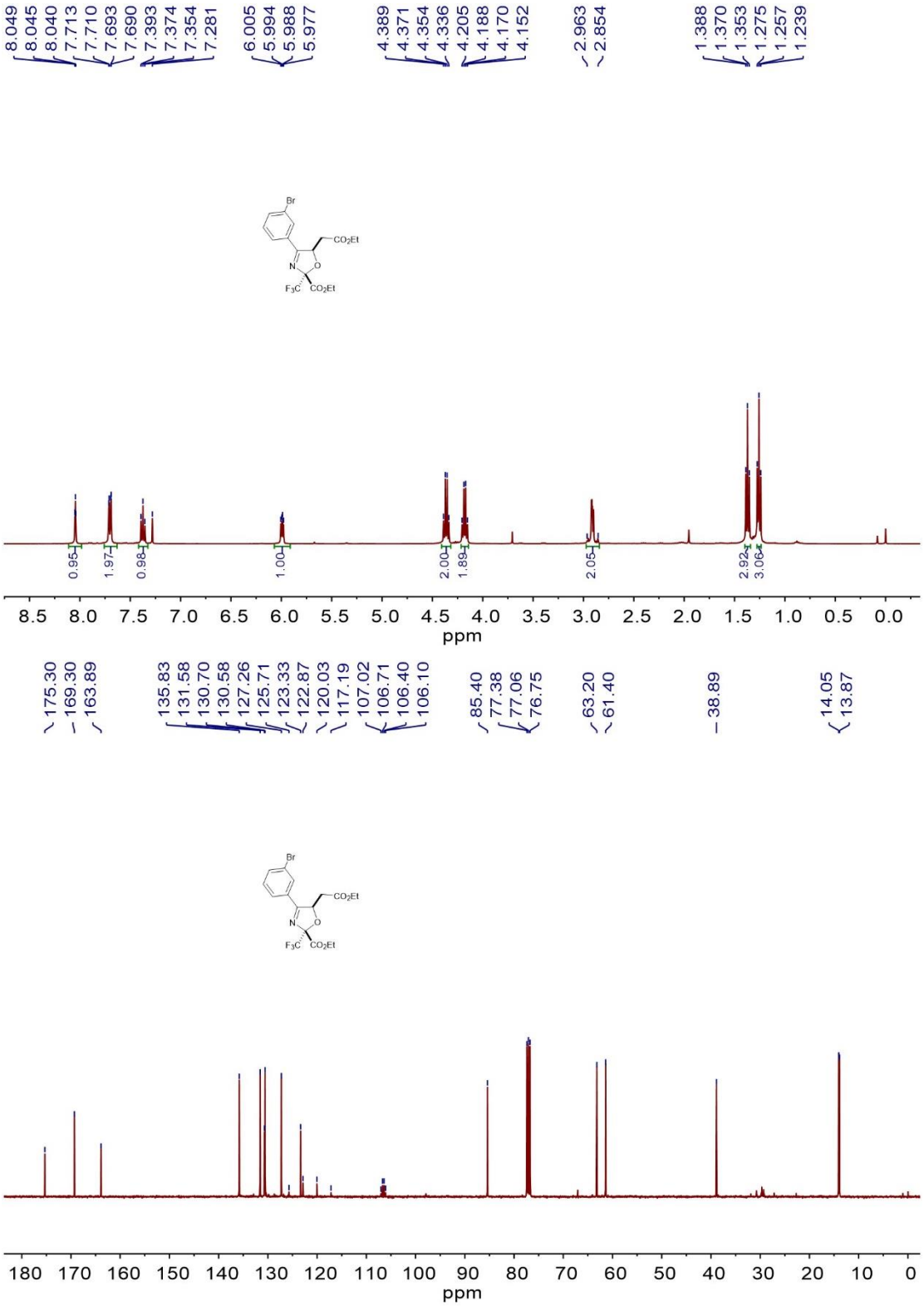
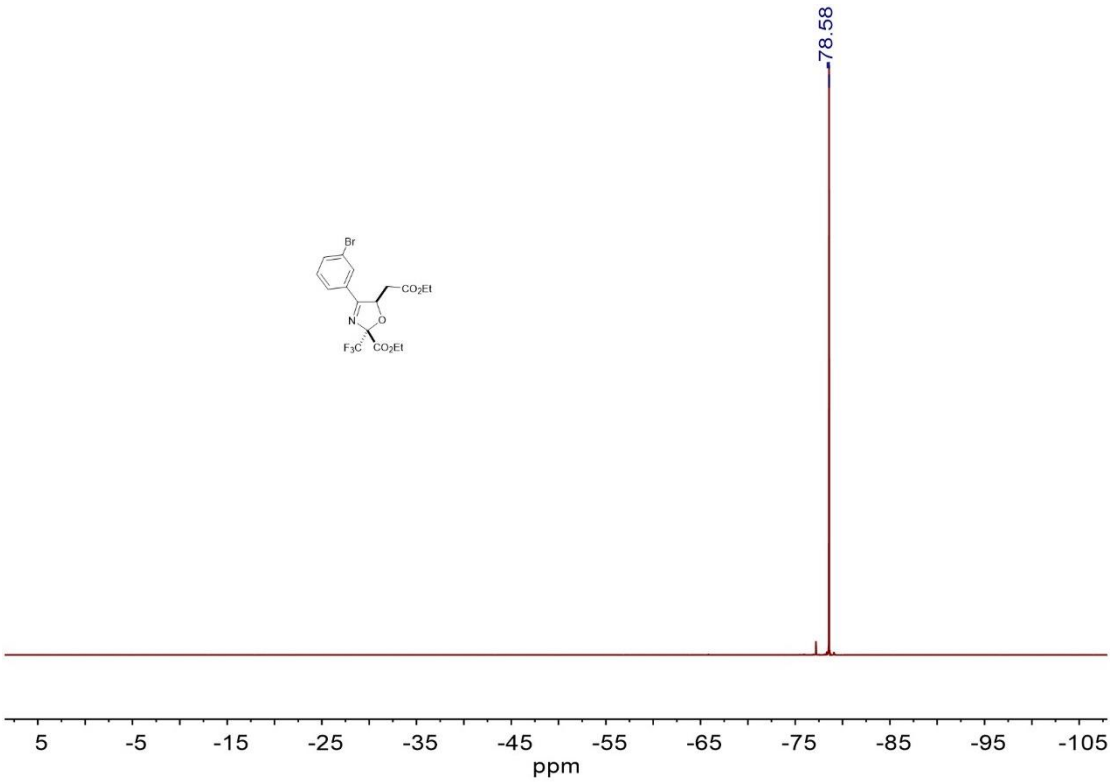
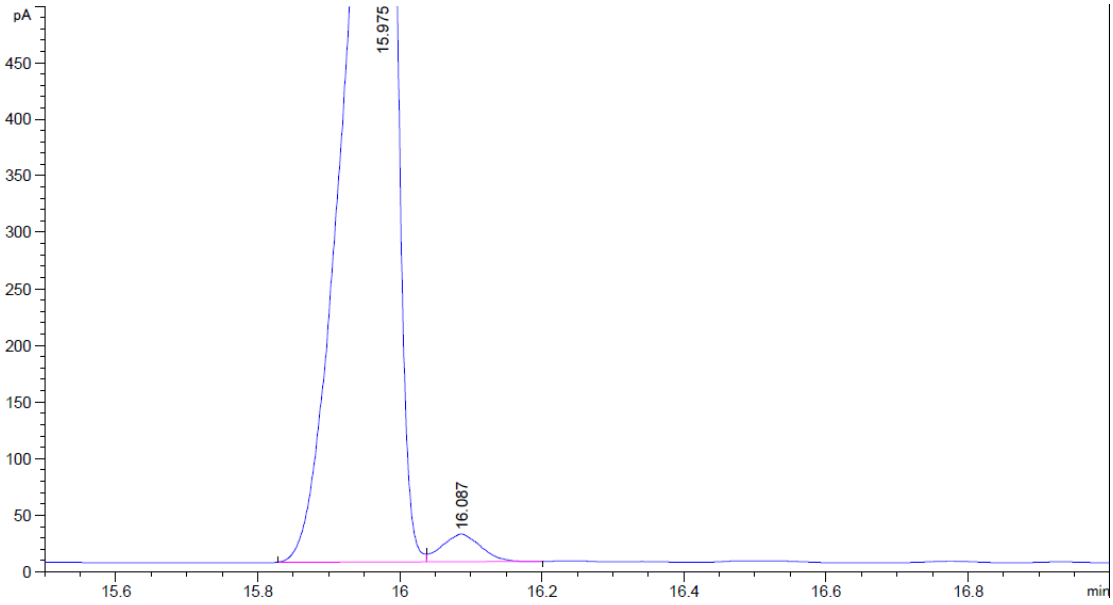
1	40.755	BV	0.1889	6258.93555	424.88953	87.45599
2	40.968	VB	0.1463	897.73322	81.02985	12.54401
总量 :				7156.66876	505.91937	

Ethyl-4-(3-bromophenyl)-5-(2-ethoxy-2-oxoethyl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3ha)

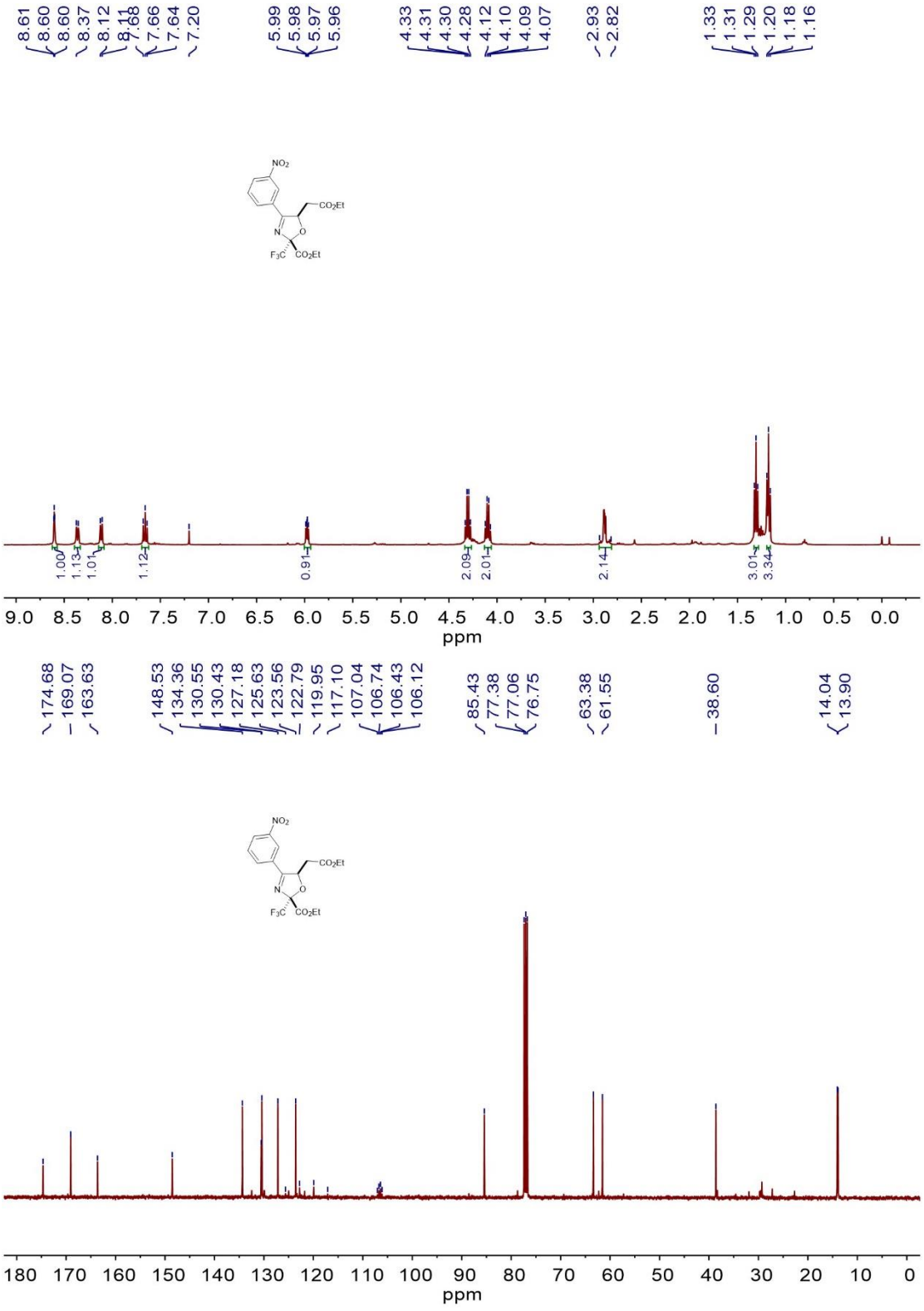


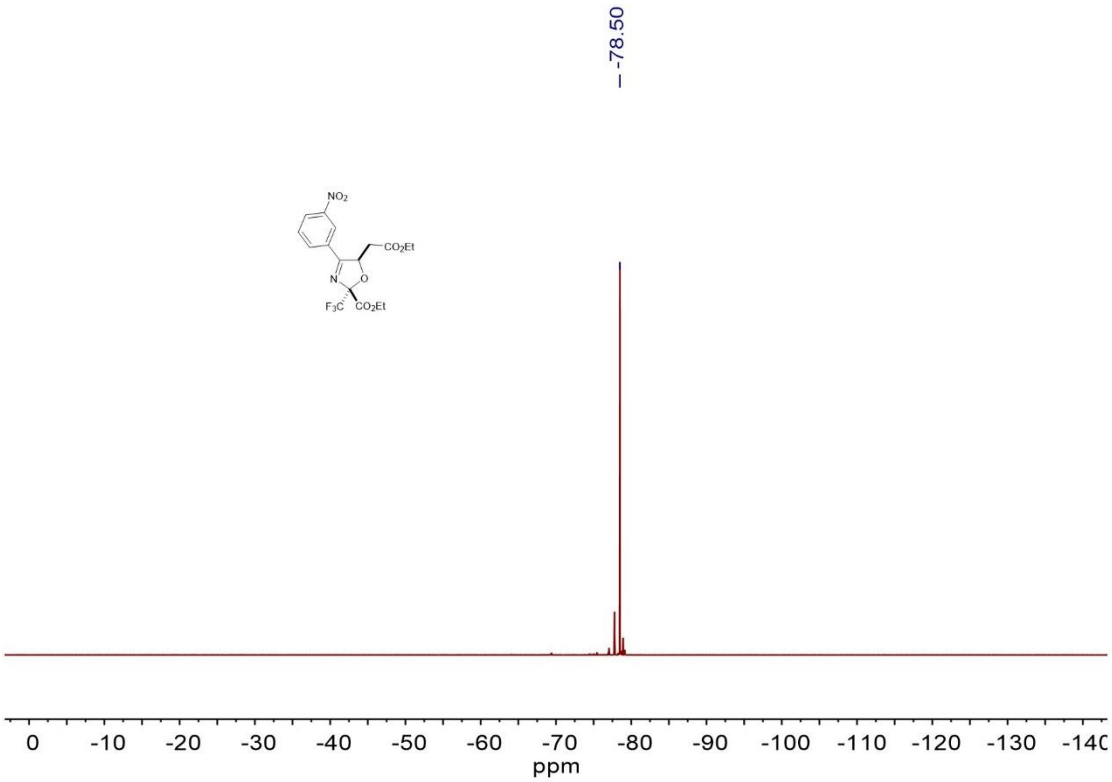


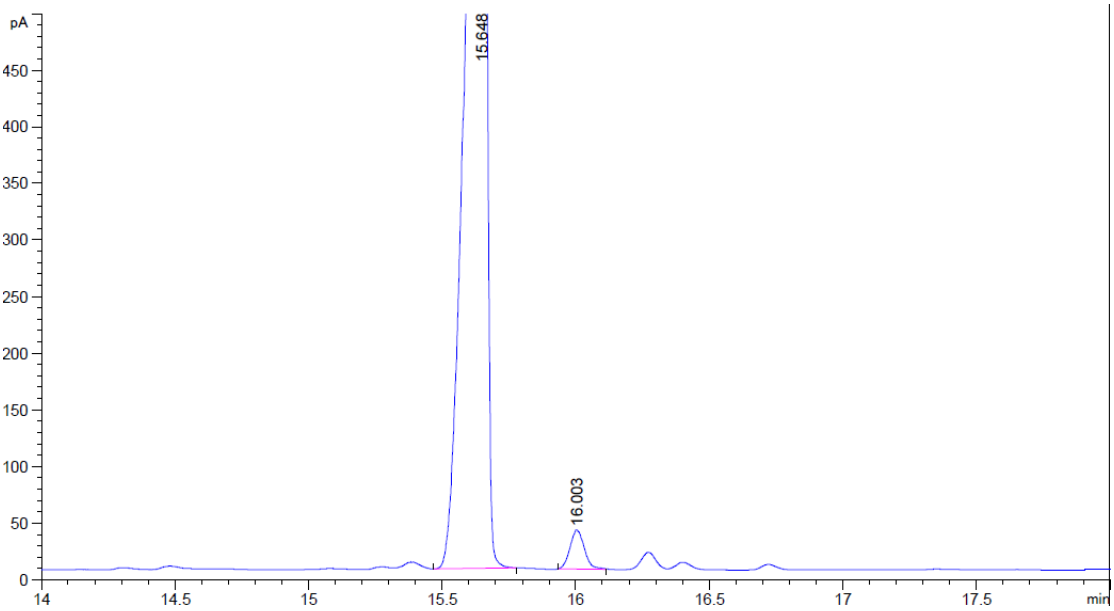


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [pA*s]	峰高 [pA]	峰面积 %
1	15.975	BV	0.0633	4212.67871	939.90503	97.84177
2	16.087	VB	0.0612	92.92463	24.52824	2.15823
总量 :				4305.60334	964.43327	

Ethyl-5-(2-ethoxy-2-oxoethyl)-4-(3-nitrophenyl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3ia)

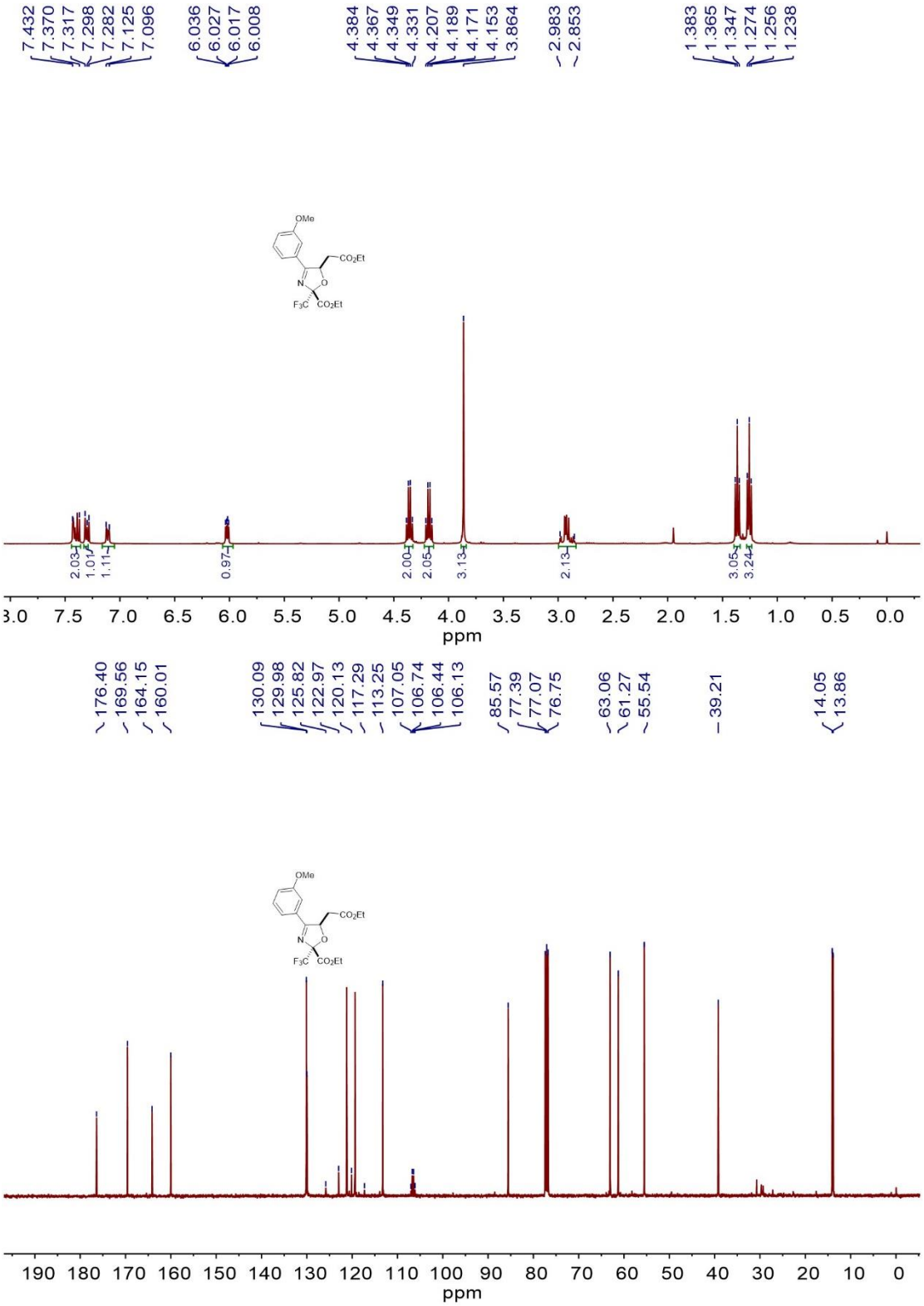


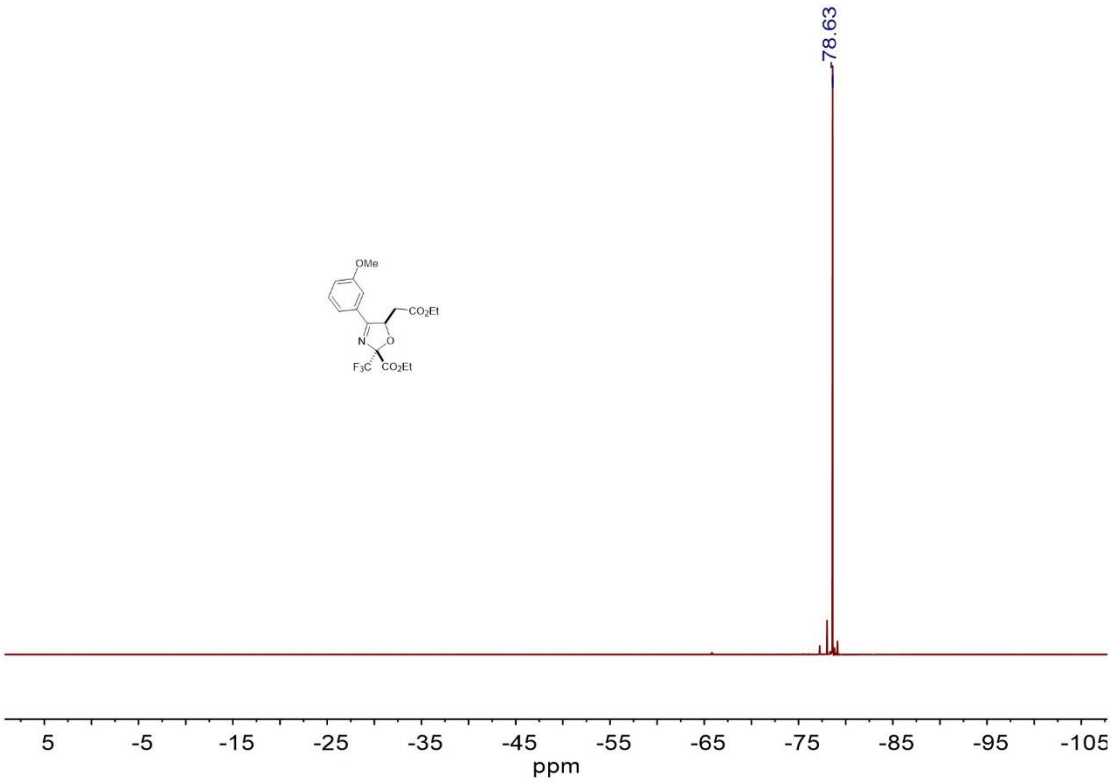


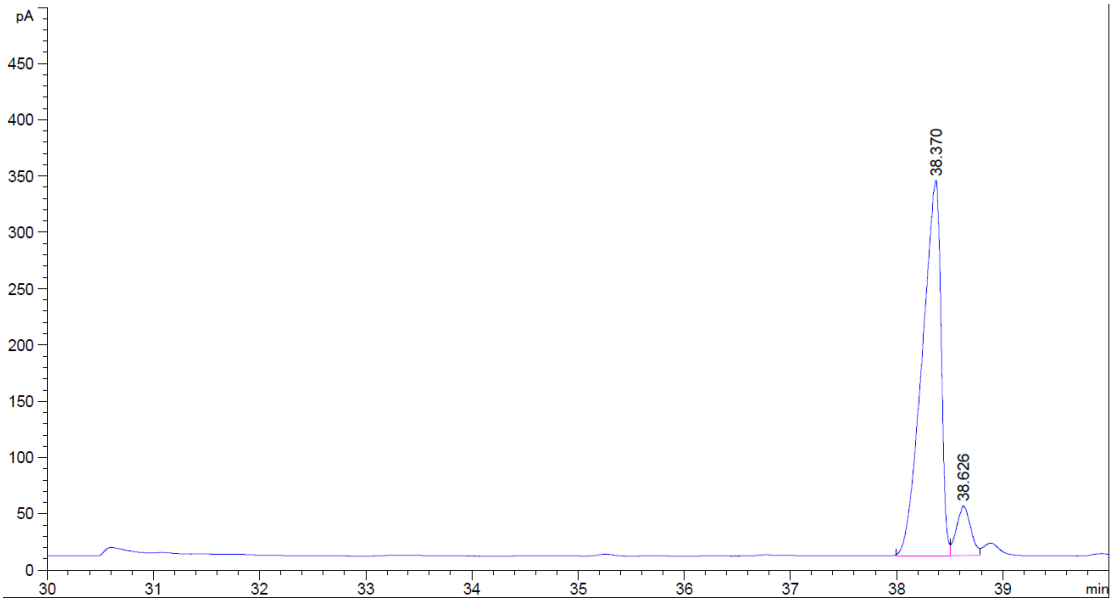


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [pA*s]	峰高 [pA]	峰面积 %
1	15.648	VB	0.0660	5176.13379	1077.56580	97.58221
2	16.003	BB	0.0592	128.24878	34.64323	2.41779
总量 :				5304.38257	1112.20902	

Ethyl-5-(2-ethoxy-2-oxoethyl)-4-(3-methoxyphenyl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3ja)

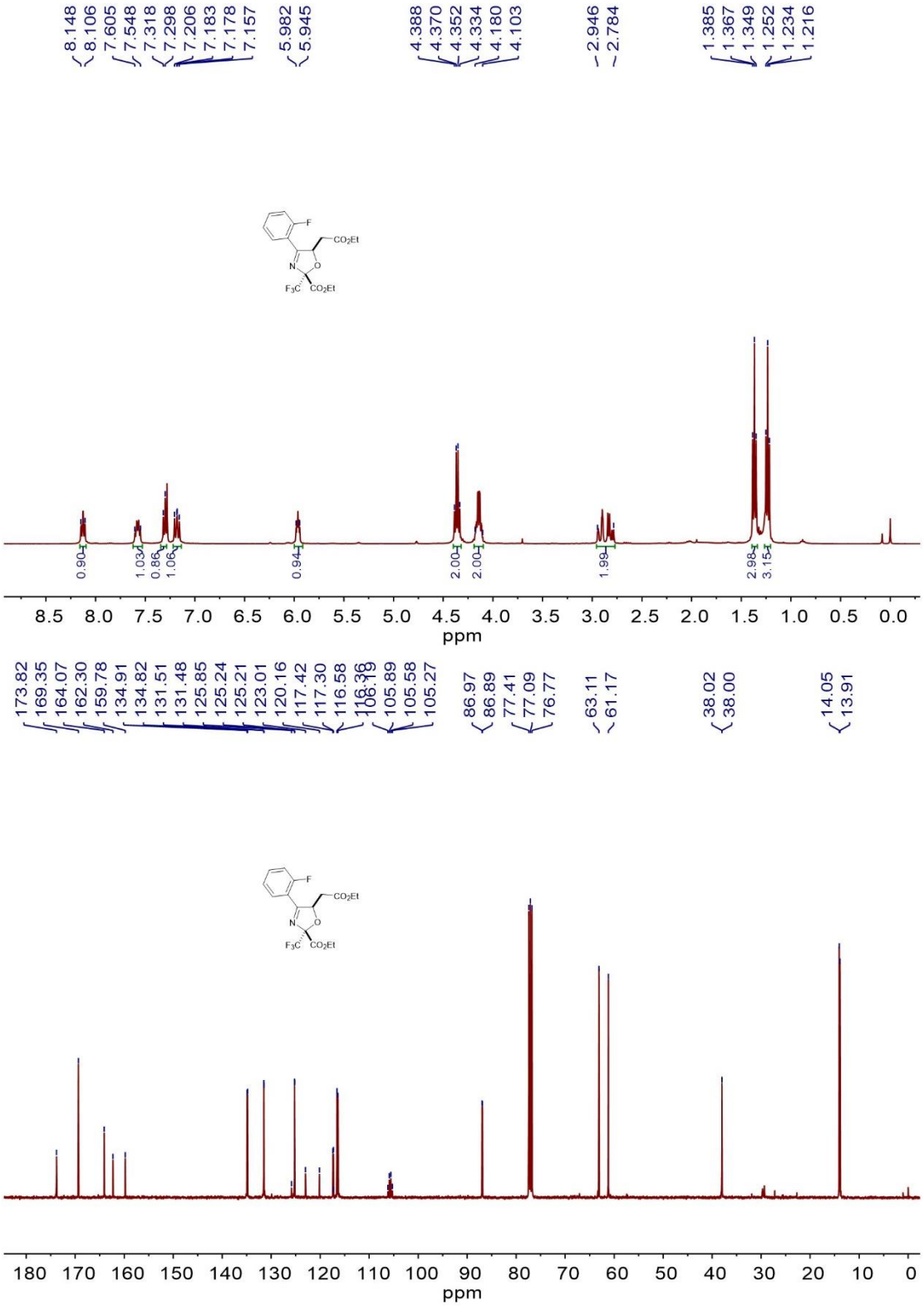


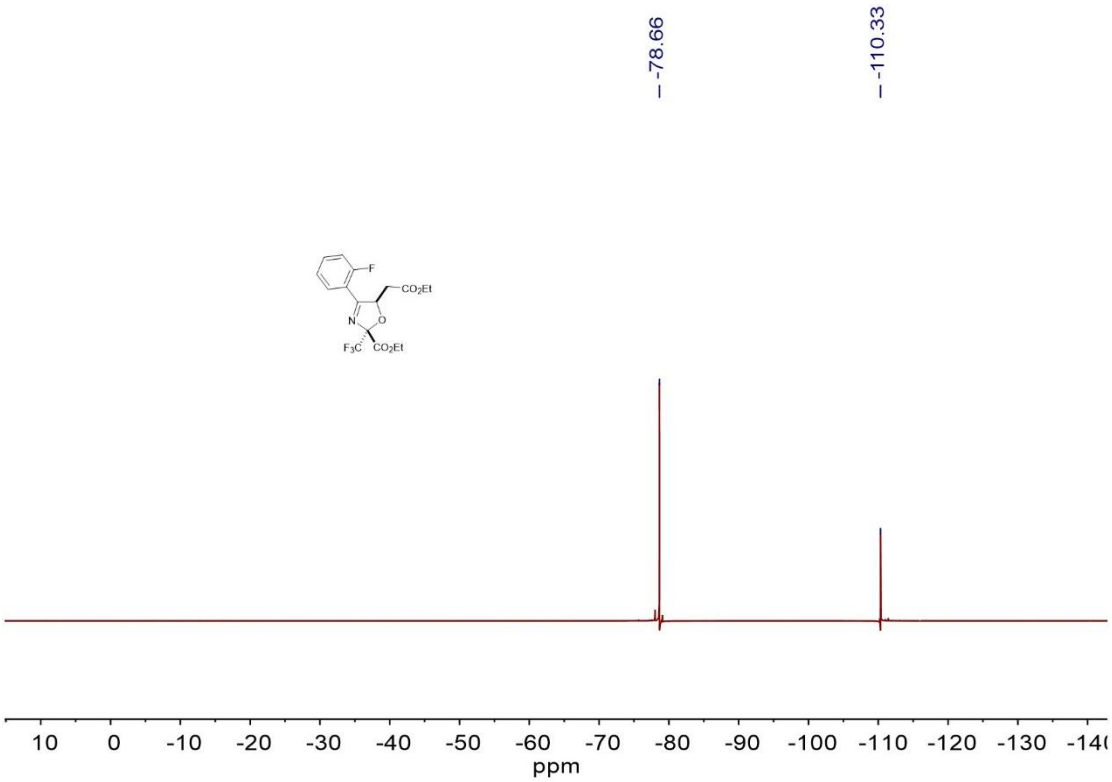


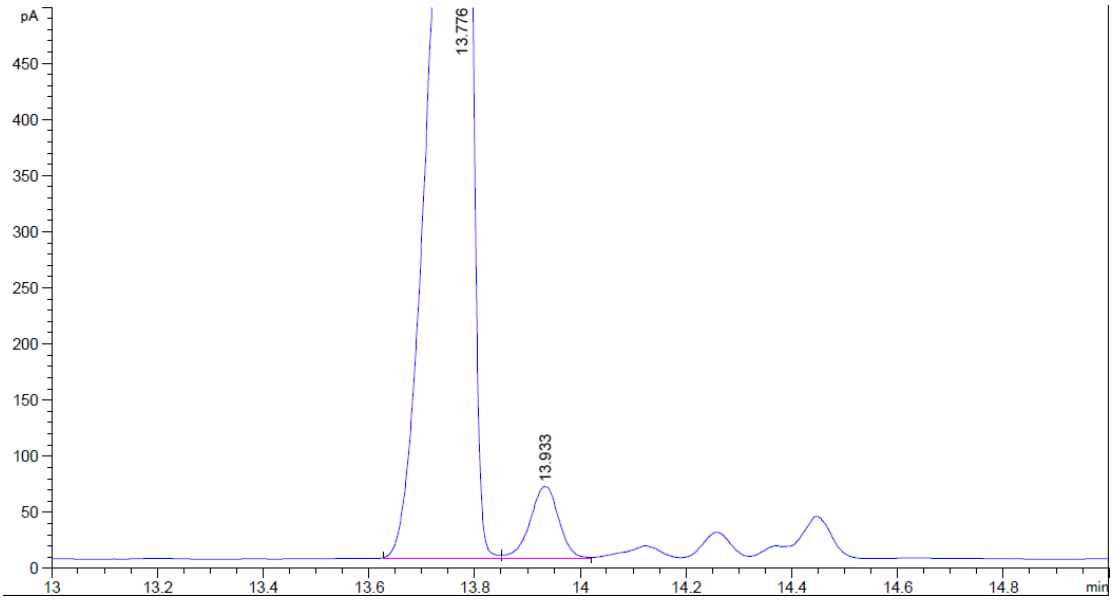


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [pA*s]	峰高 [pA]	峰面积 %
1	38.370	BV	0.1515	4097.33545	333.11636	90.90145
2	38.626	VV	0.1154	410.11258	44.14054	9.09855
总量：				4507.44803	377.25690	

Ethyl-5-(2-ethoxy-2-oxoethyl)-4-(2-fluorophenyl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3ka)



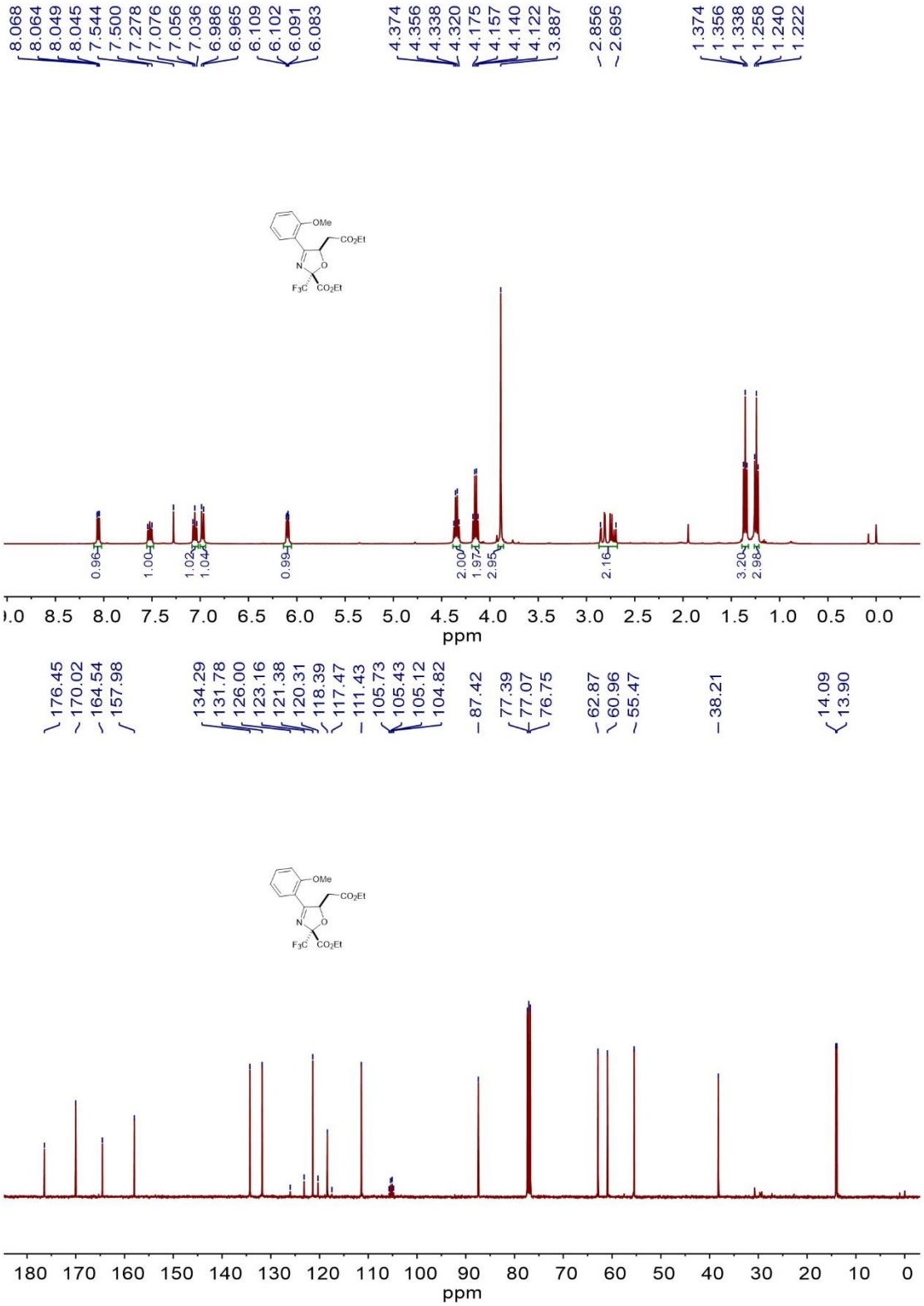


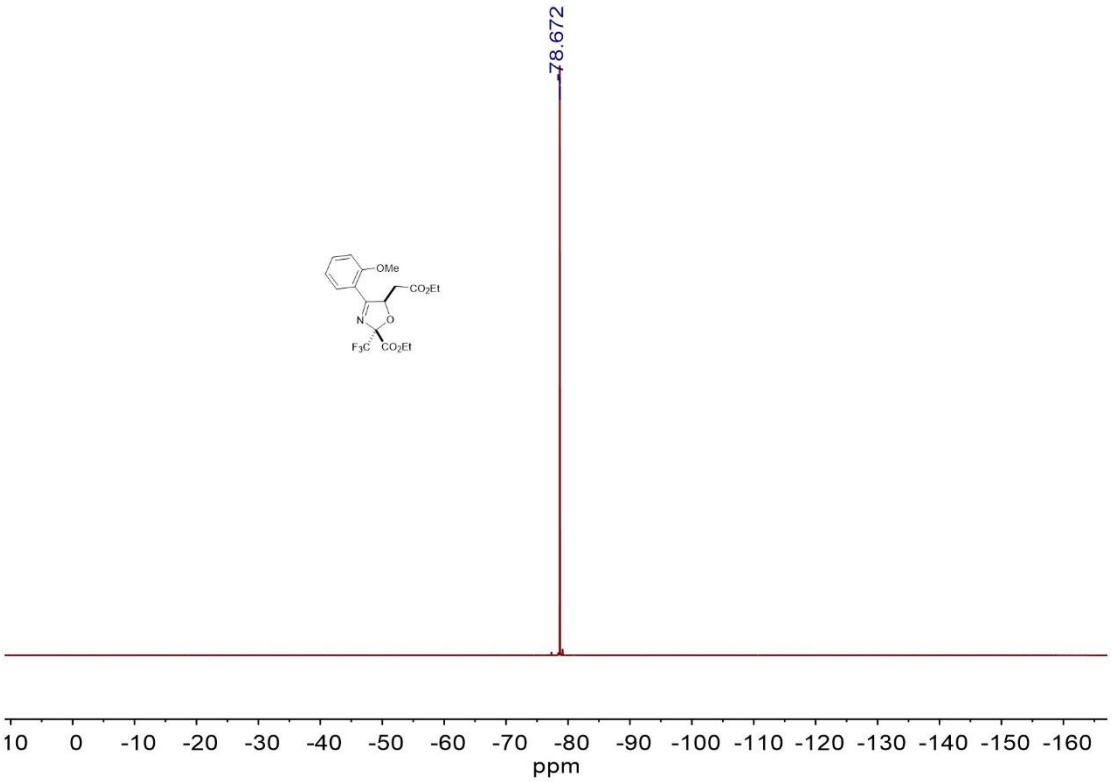


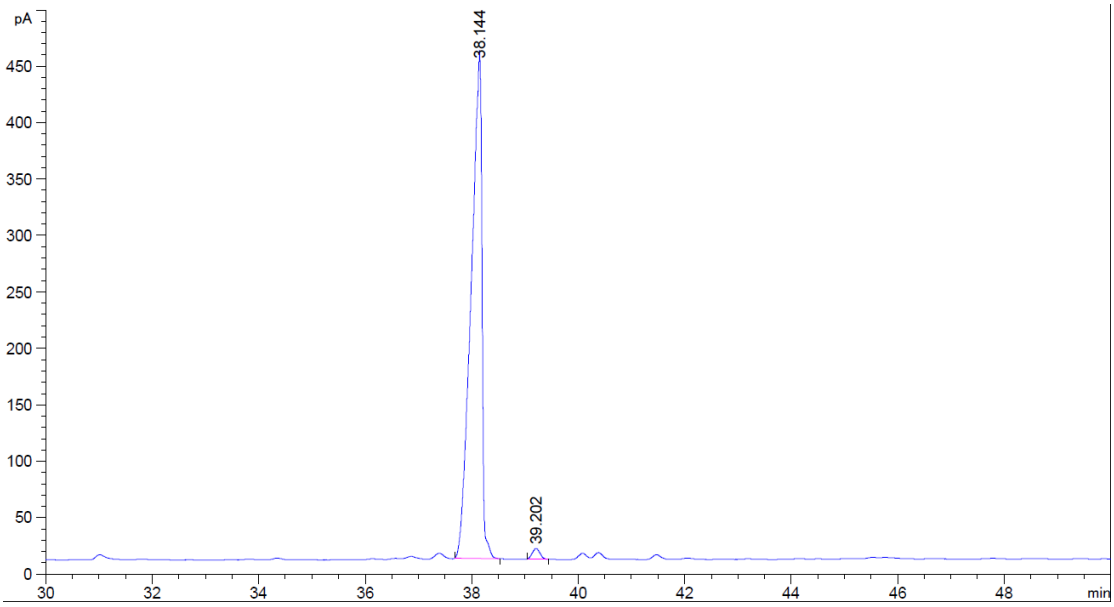
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [pA*s]	峰高 [pA]	峰面积 %
1	13.776	BV	0.0624	5098.03418	1134.19275	95.42802
2	13.933	VV	0.0573	244.24785	64.28325	4.57198

总量 : 5342.28203 1198.47600

Ethyl-5-(2-ethoxy-2-oxoethyl)-4-(2-methoxyphenyl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3la)

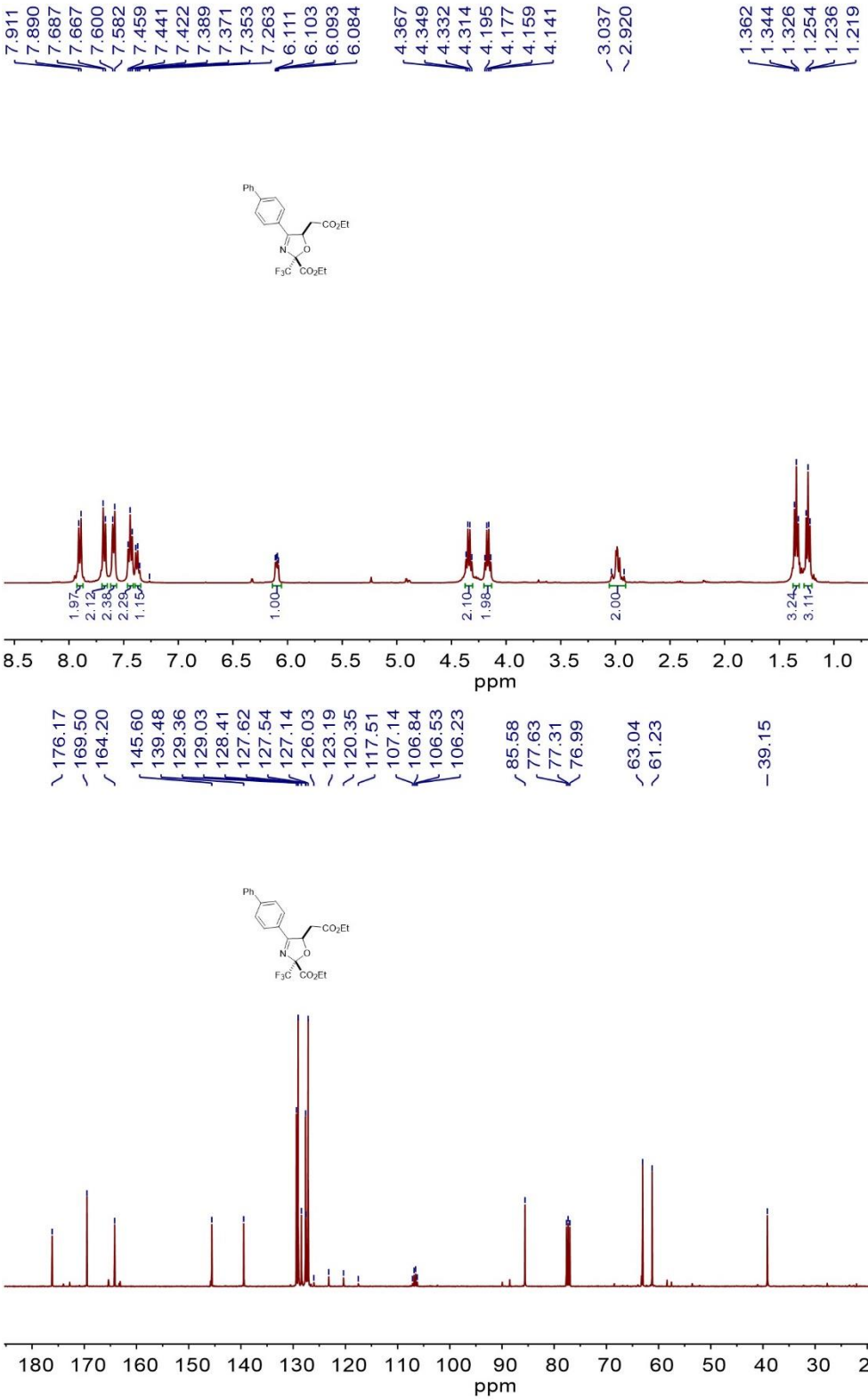


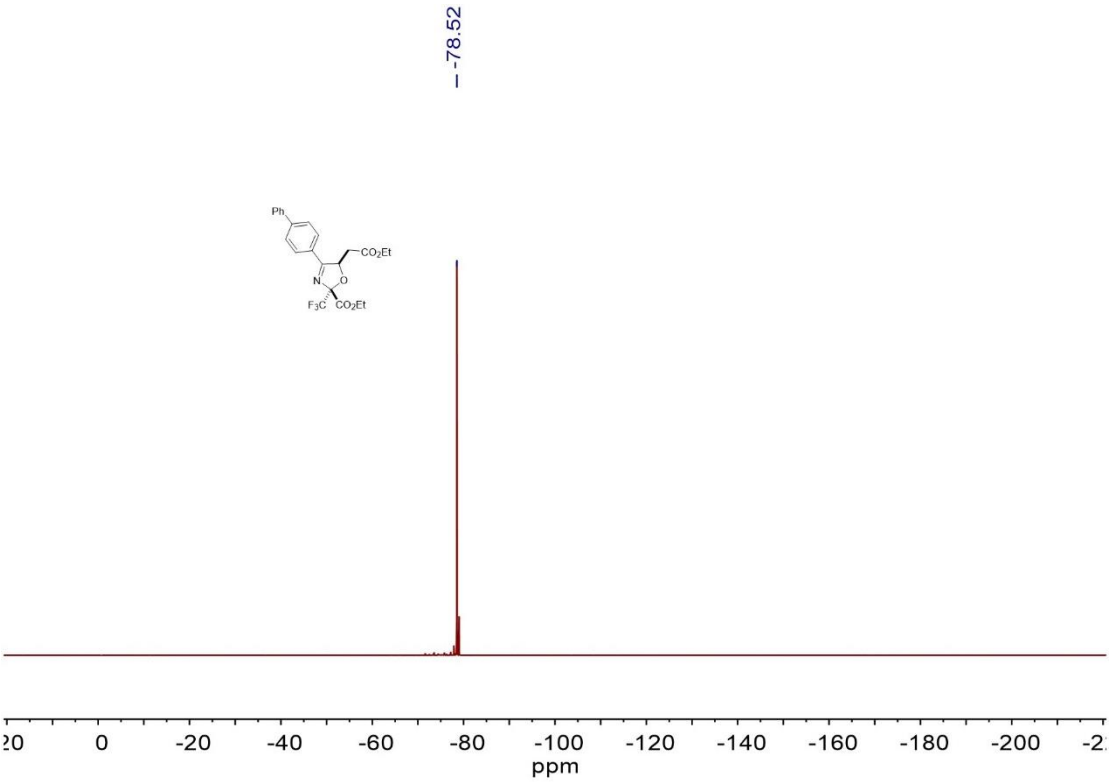


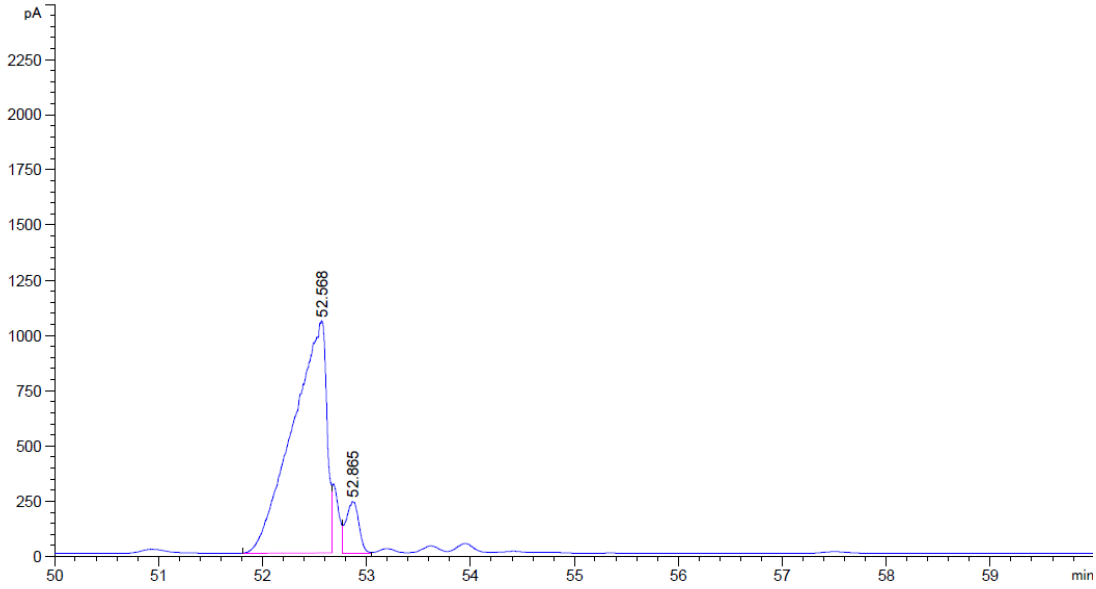


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [pA*s]	峰高 [pA]	峰面积 %
1	38.144	BB	0.1827	6347.10107	449.69666	98.51248
2	39.202	BB	0.1264	95.83975	9.60731	1.48752
总量 :				6442.94083	459.30396	

Ethyl-4-([1,1'-biphenyl]-4-yl)-5-(2-ethoxy-2-oxoethyl)-2-(trifluoromethyl)-2,5-dihydrooxazole -2-carboxylate (3ma)

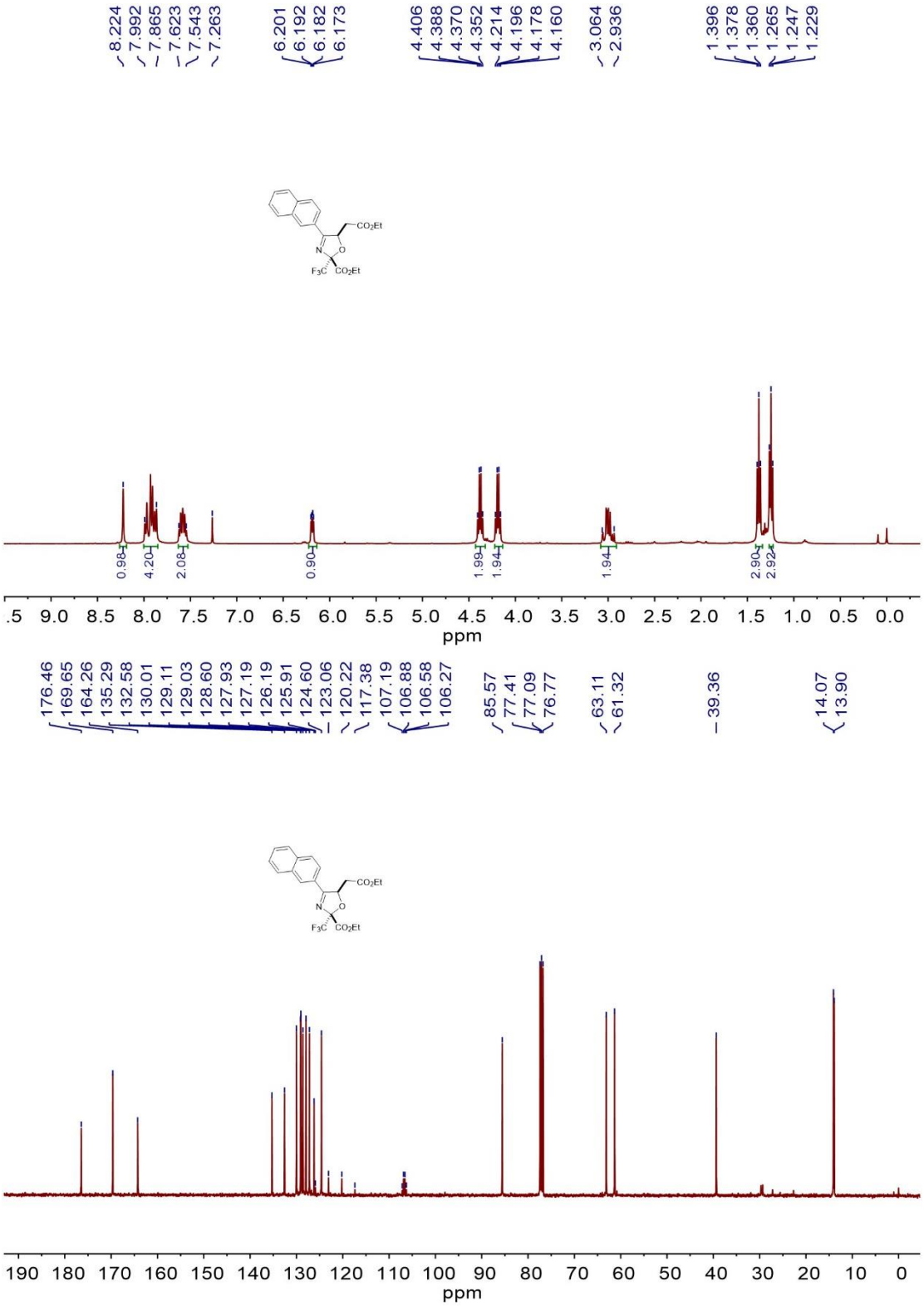


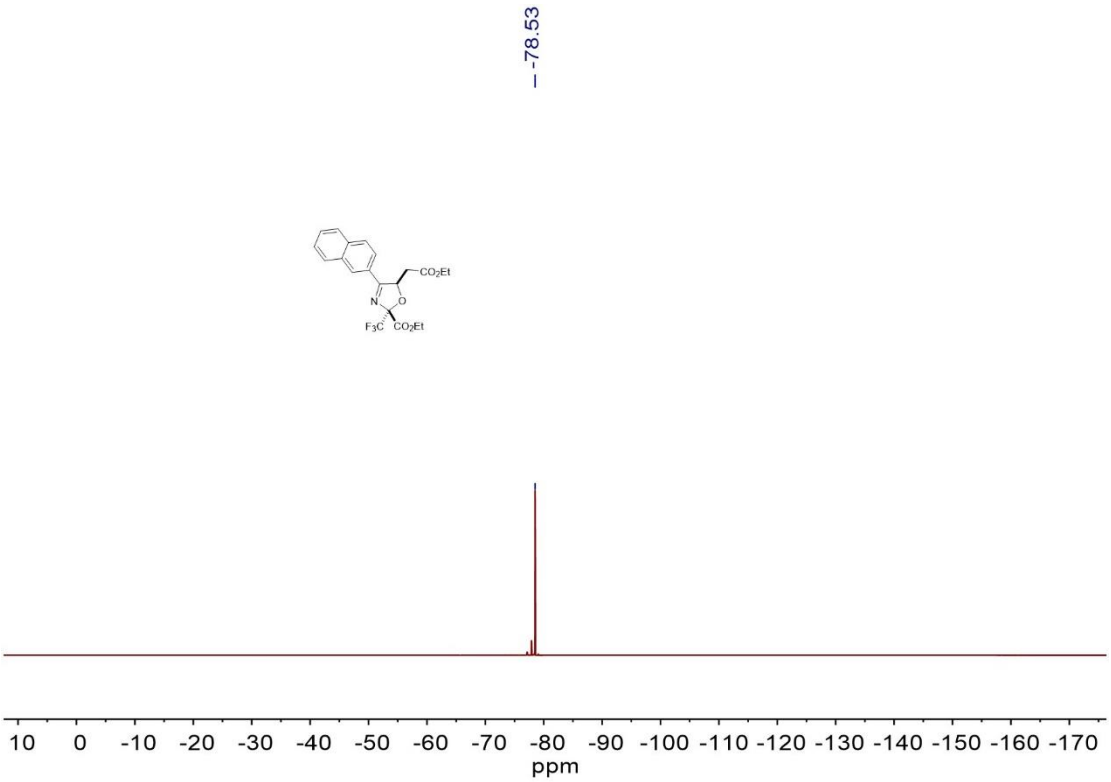


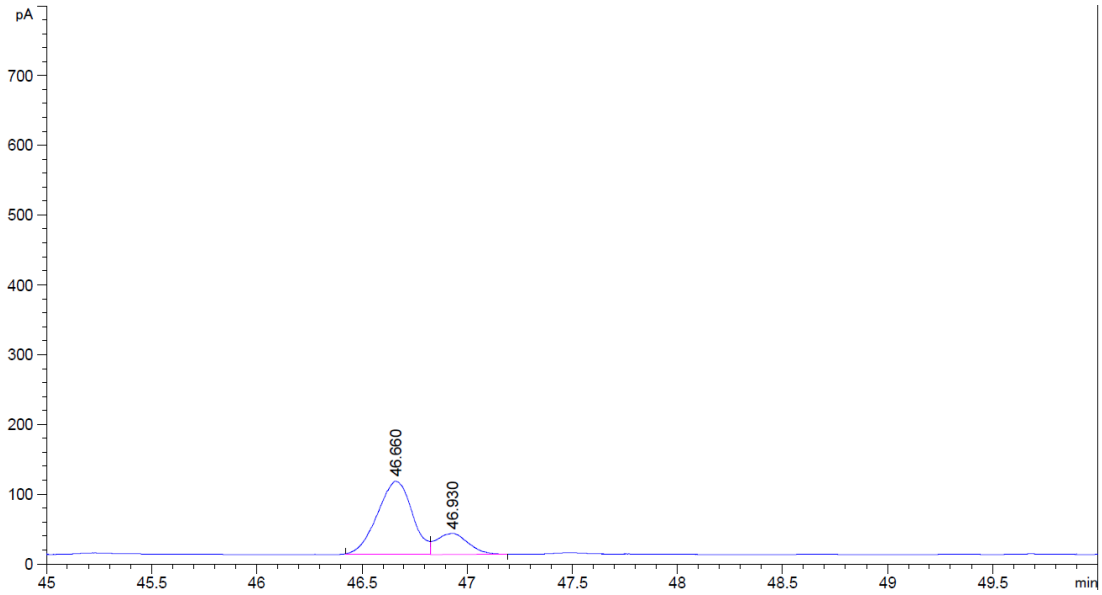


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [pA*s]	峰高 [pA]	峰面积 %
1	52.568	BV	0.2820	2.38122e4	1048.34778	92.36820
2	52.865	VV	0.1026	1967.44800	232.70560	7.63180
总量 :				2.57796e4	1281.05338	

Ethyl-5-(2-ethoxy-2-oxoethyl)-4-(naphthalen-2-yl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3na)

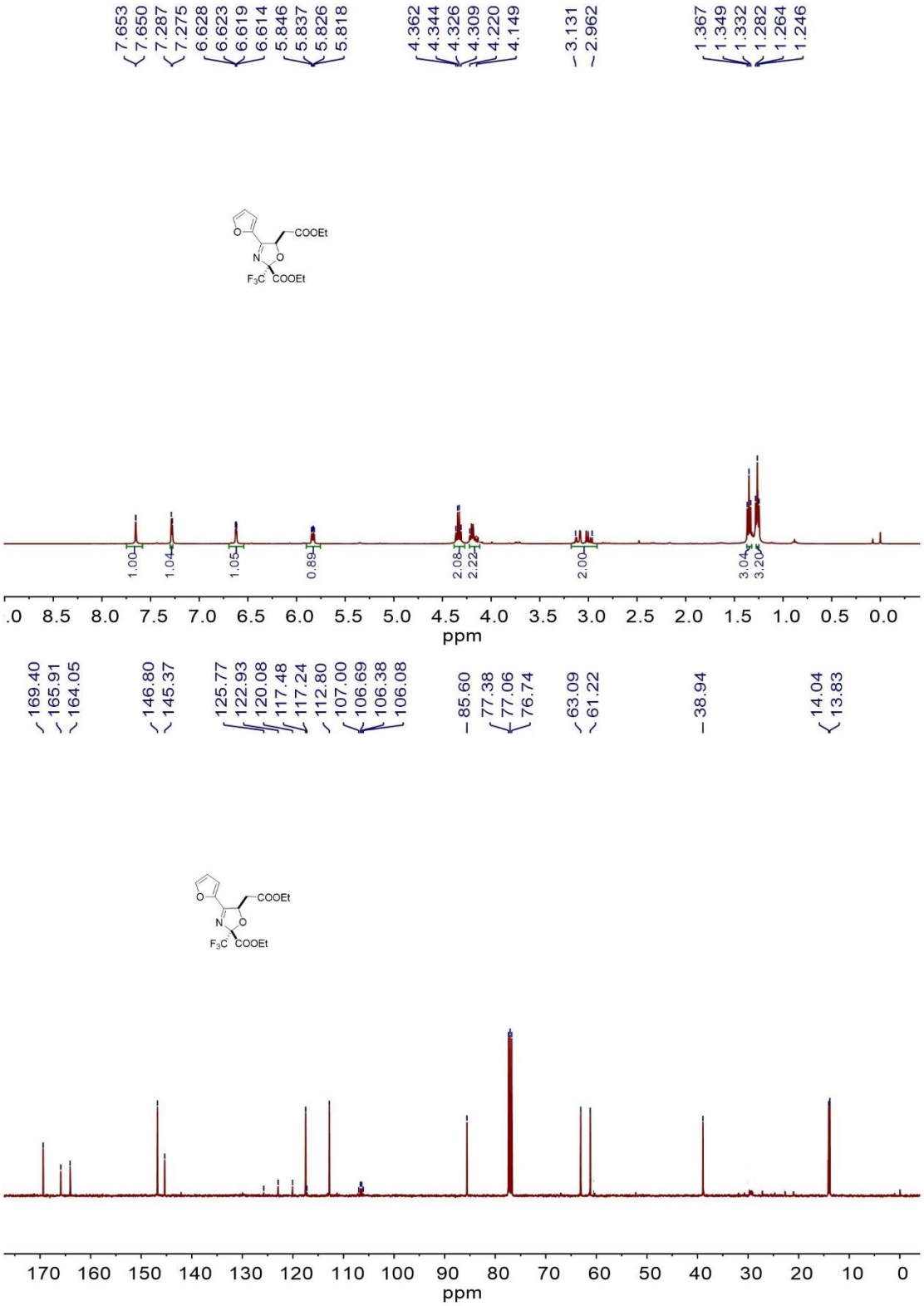


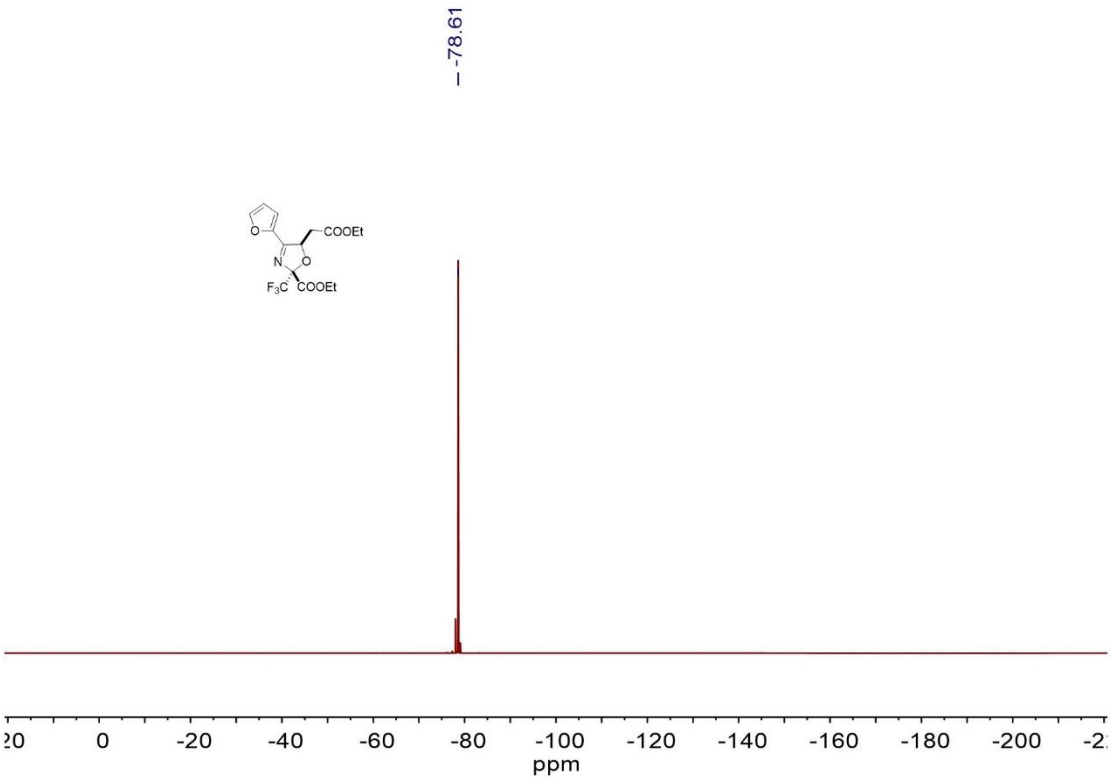


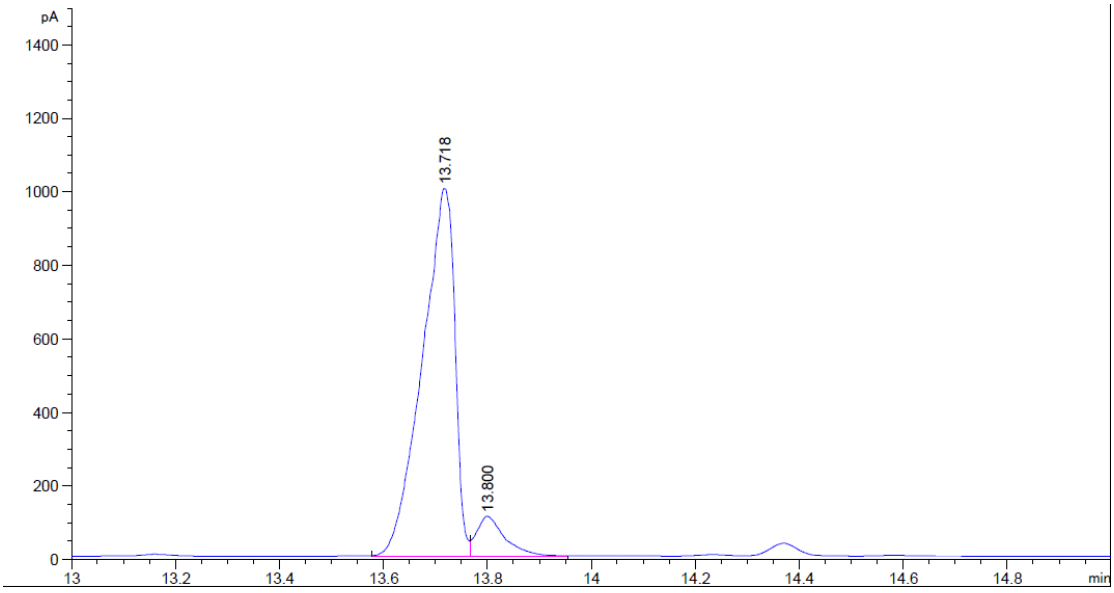


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [pA*s]	峰高 [pA]	峰面积 %
1	46.660	BV	0.1409	1215.53442	105.16164	79.55917
2	46.930	VB	0.1290	312.30249	30.10020	20.44083
总量：				1527.83691	135.26184	

Ethyl-5-(2-ethoxy-2-oxoethyl)-4-(furan-2-yl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3oa)



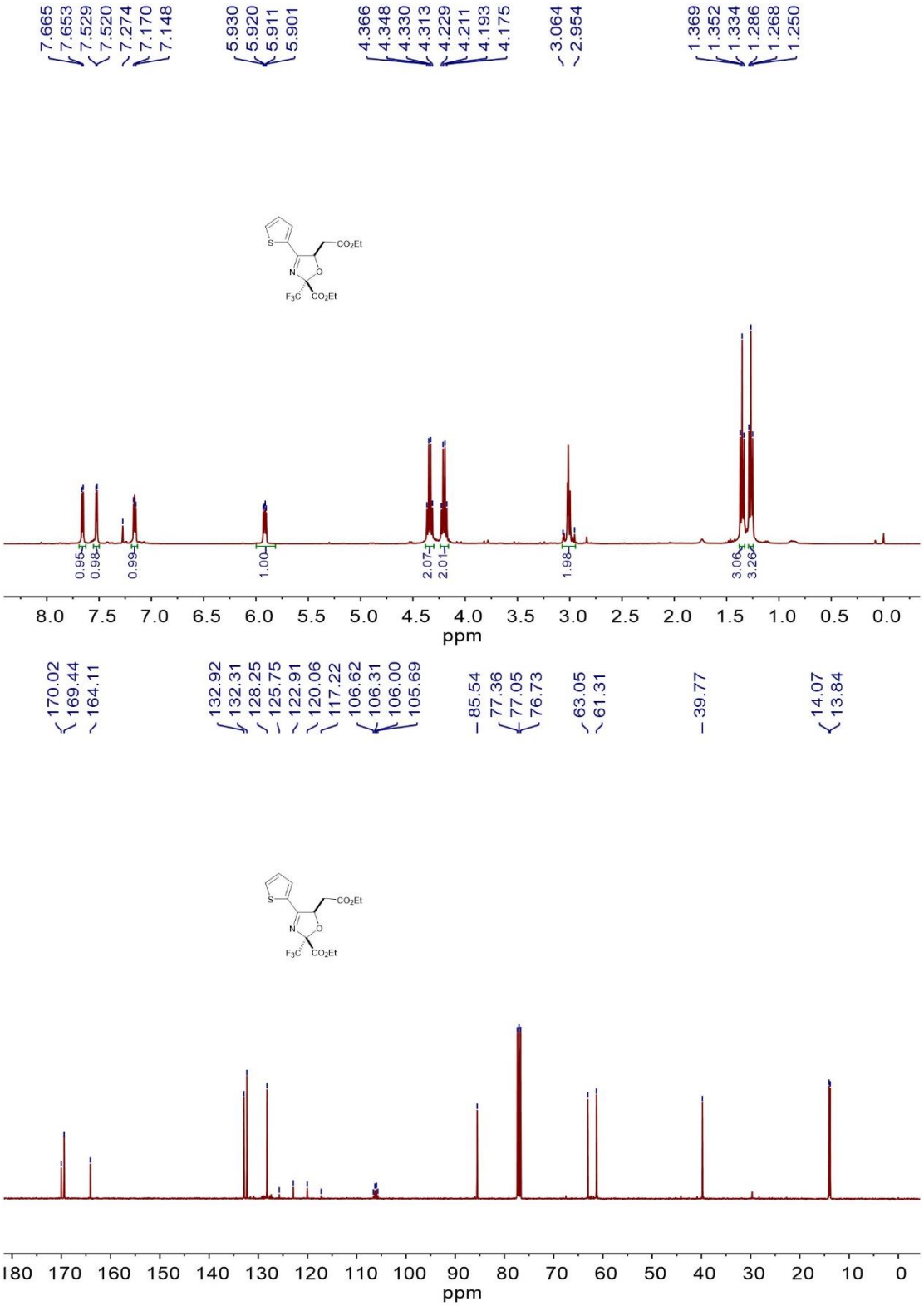


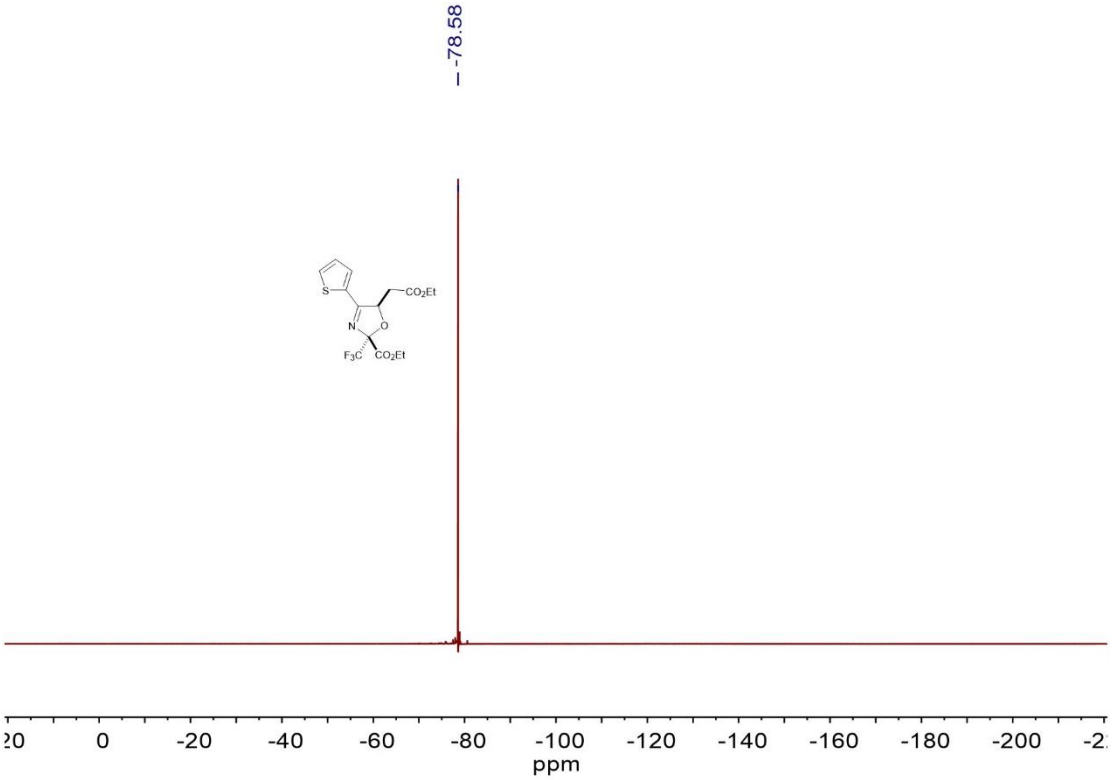


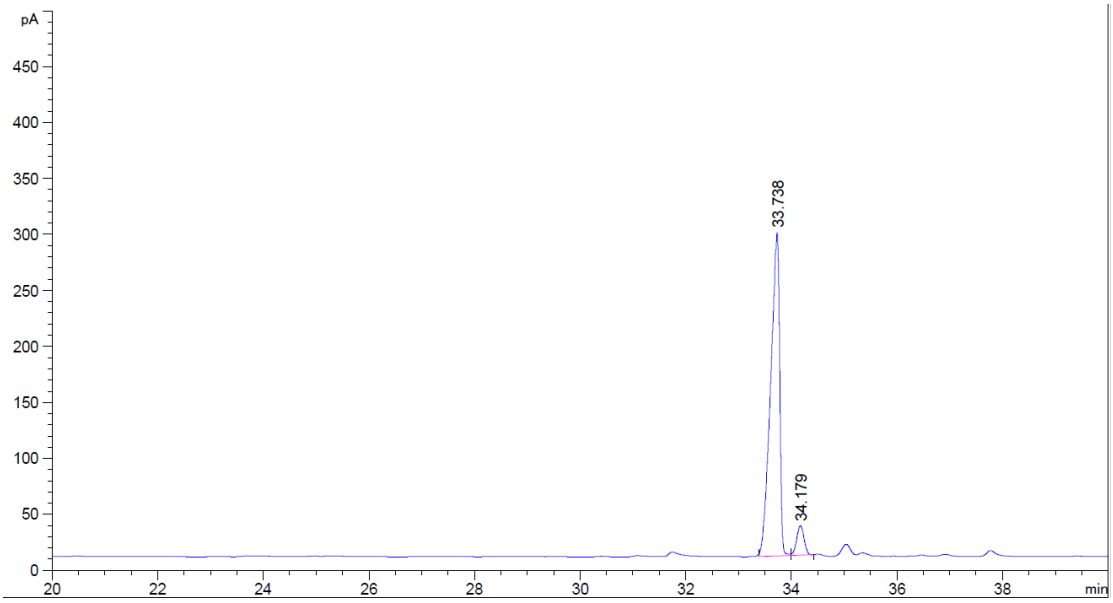
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [pA*s]	峰高 [pA]	峰面积 %
1	13.718	BV	0.0628	4353.12158	998.93317	91.52647
2	13.800	VB	0.0535	403.01230	108.14889	8.47353

总量 : 4756.13388 1107.08205

Ethyl-5-(2-ethoxy-2-oxoethyl)-4-(thiophen-2-yl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3pa)

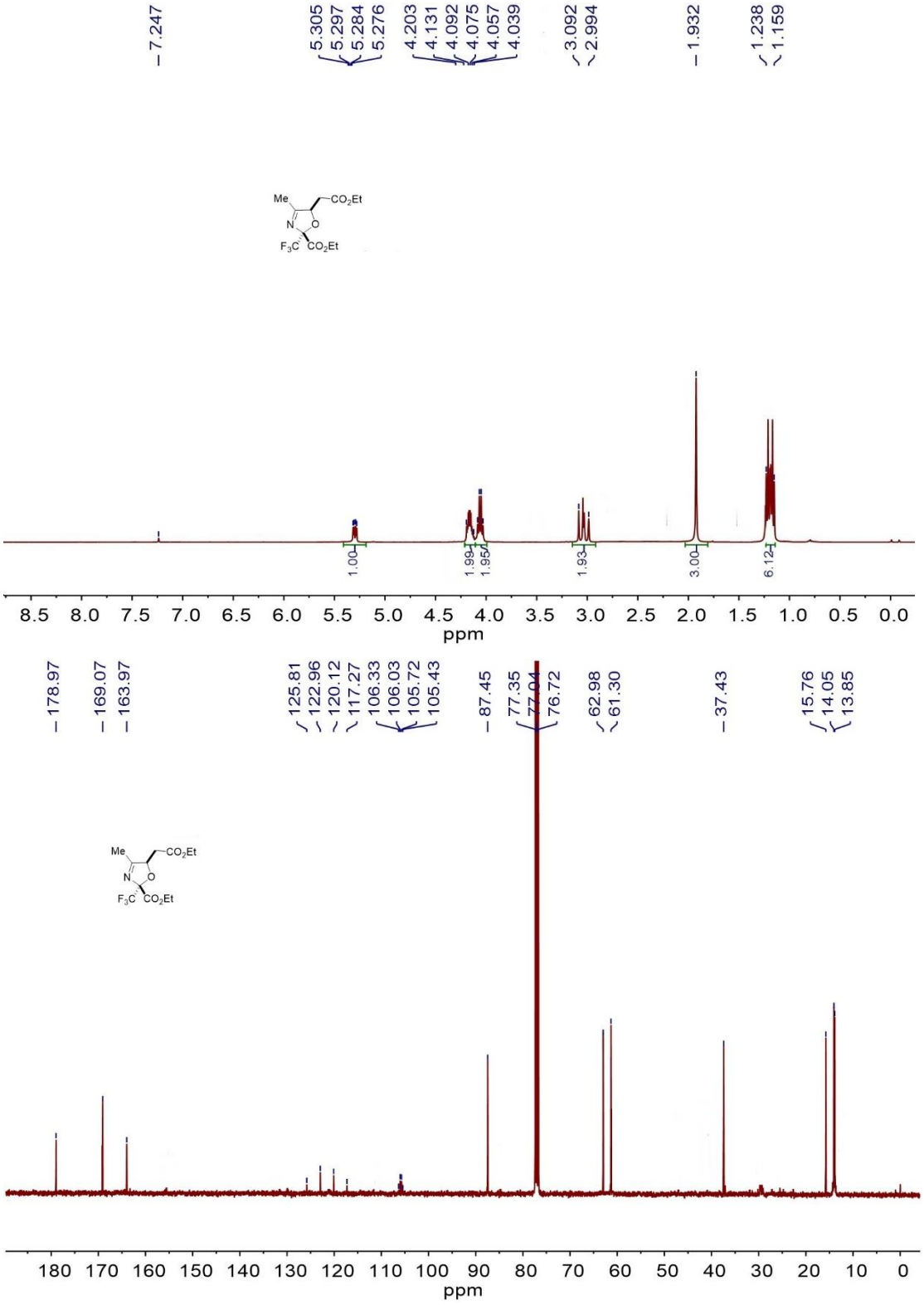


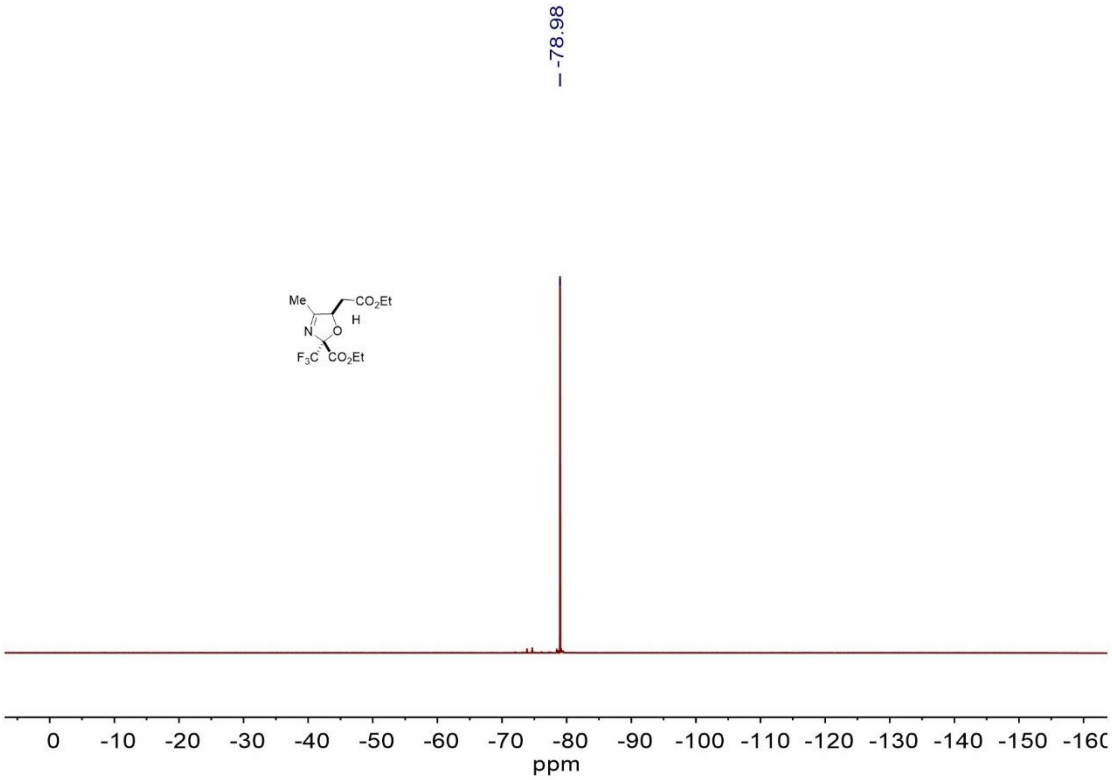


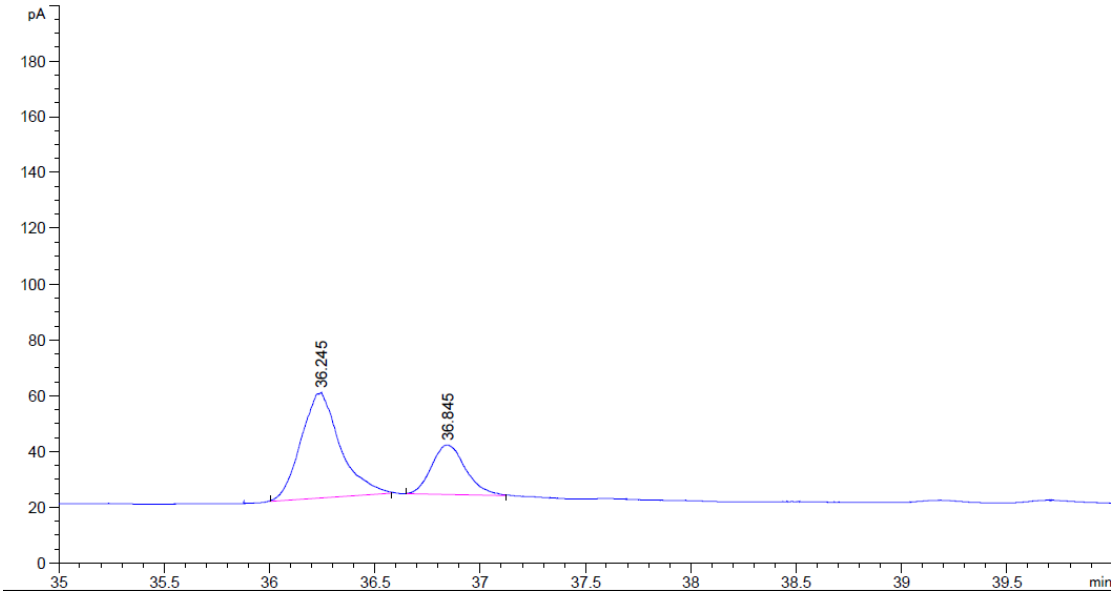


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [pA*s]	峰高 [pA]	峰面积 %
1	33.738	BV	0.1463	3429.69507	289.26007	93.12253
2	34.179	VB	0.1254	253.29671	26.30084	6.87747
总量：				3682.99178	315.56091	

Ethyl-5-(2-ethoxy-2-oxoethyl)-4-methyl-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3qa)

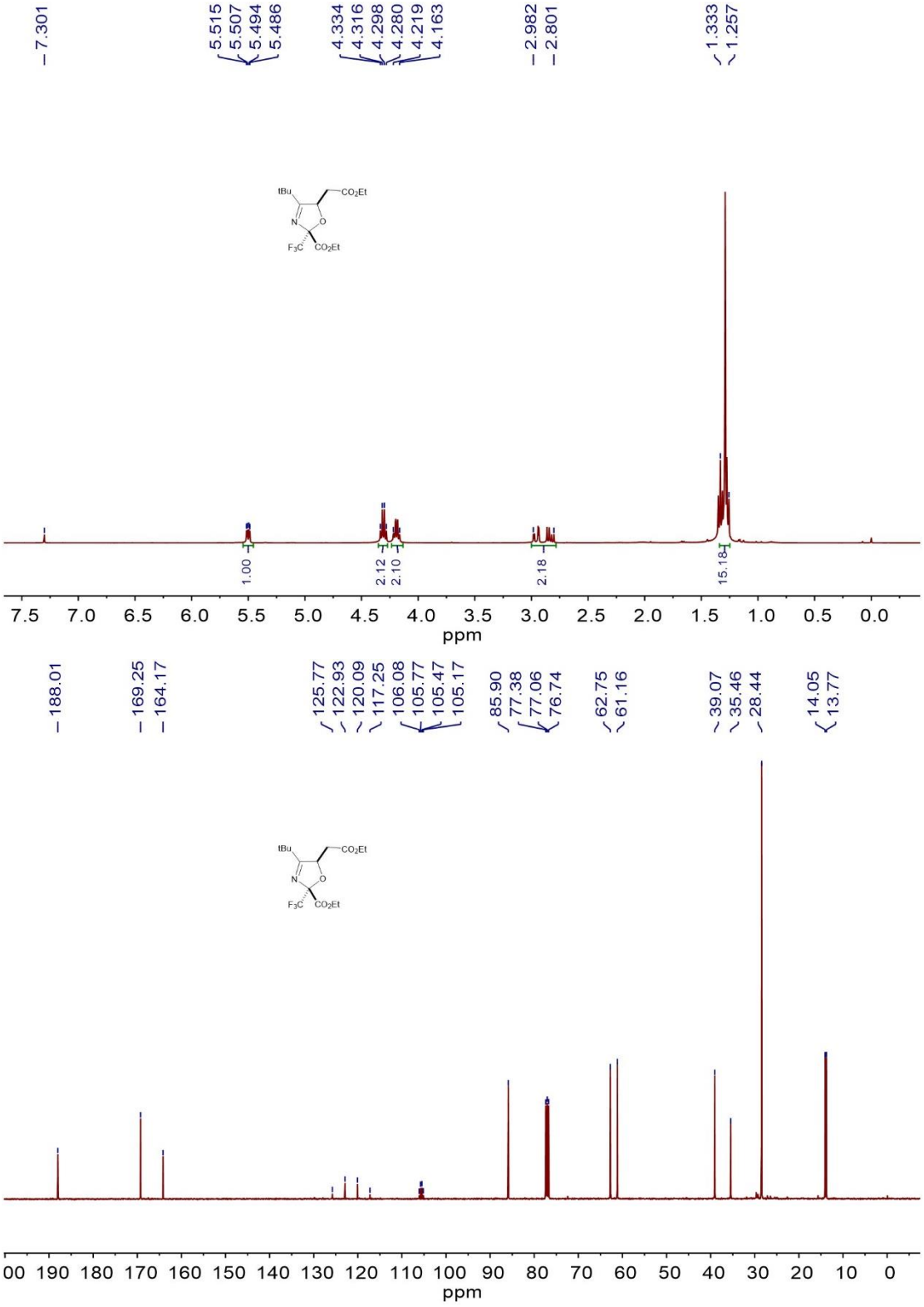


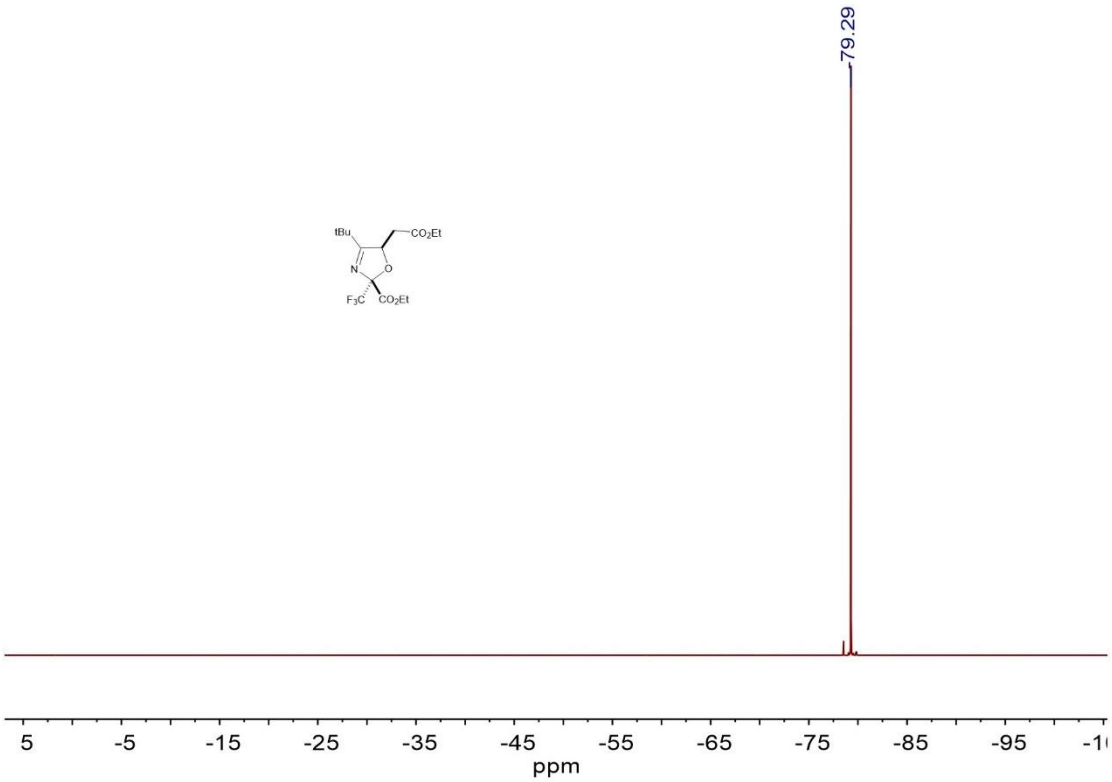


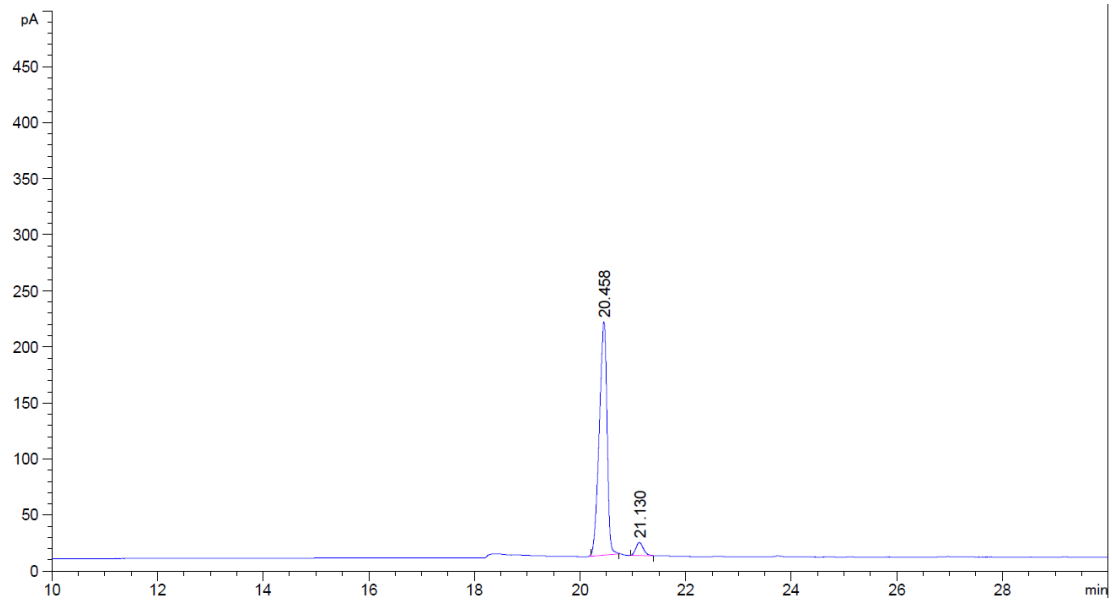


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [pA*s]	峰高 [pA]	峰面积 %
1	36.245	BB	0.1563	489.95367	37.76827	71.26432
2	36.845	BB	0.1477	197.56244	17.63446	28.73568
总量：				687.51611	55.40273	

Ethyl-4-(tert-butyl)-5-(2-ethoxy-2-oxoethyl)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3ra)

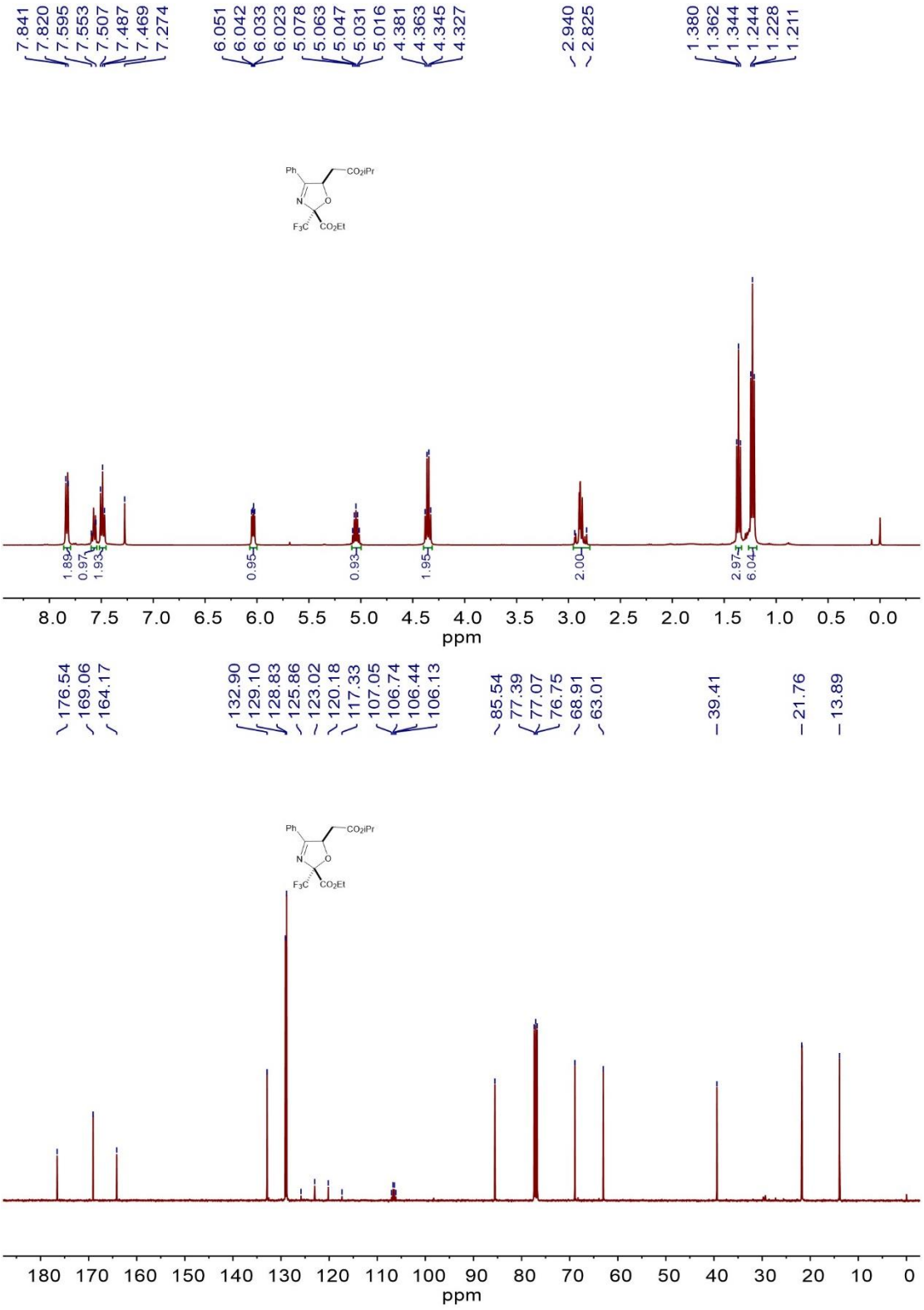


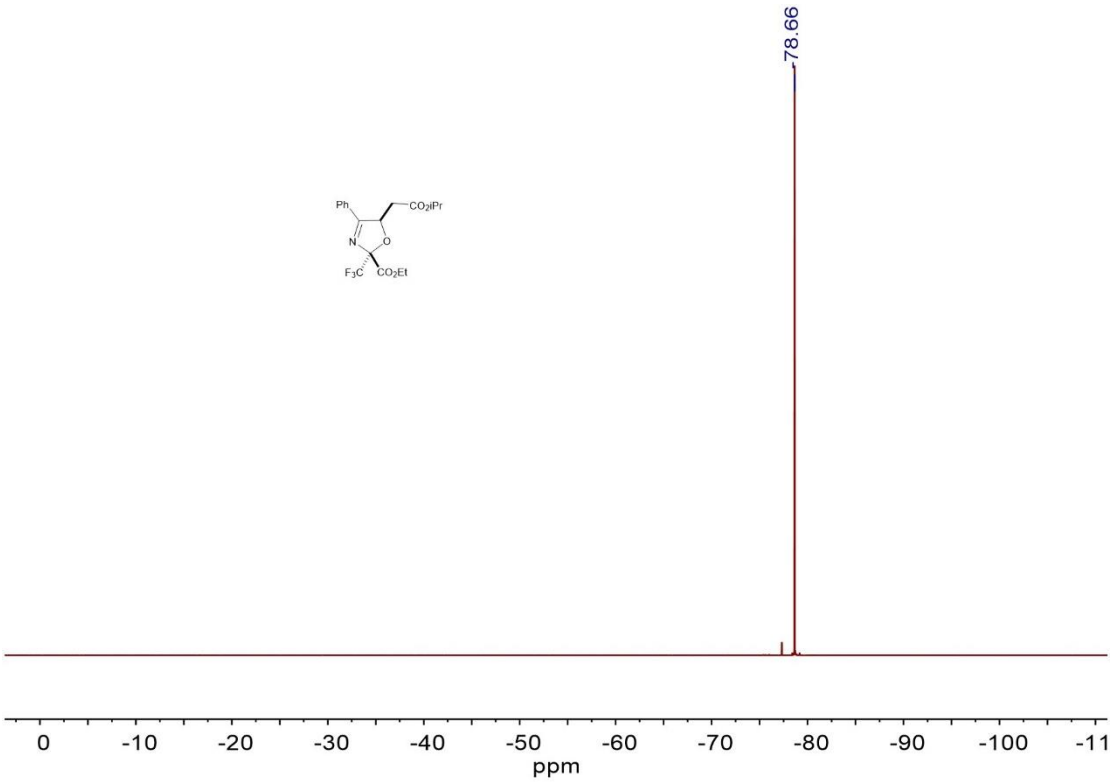


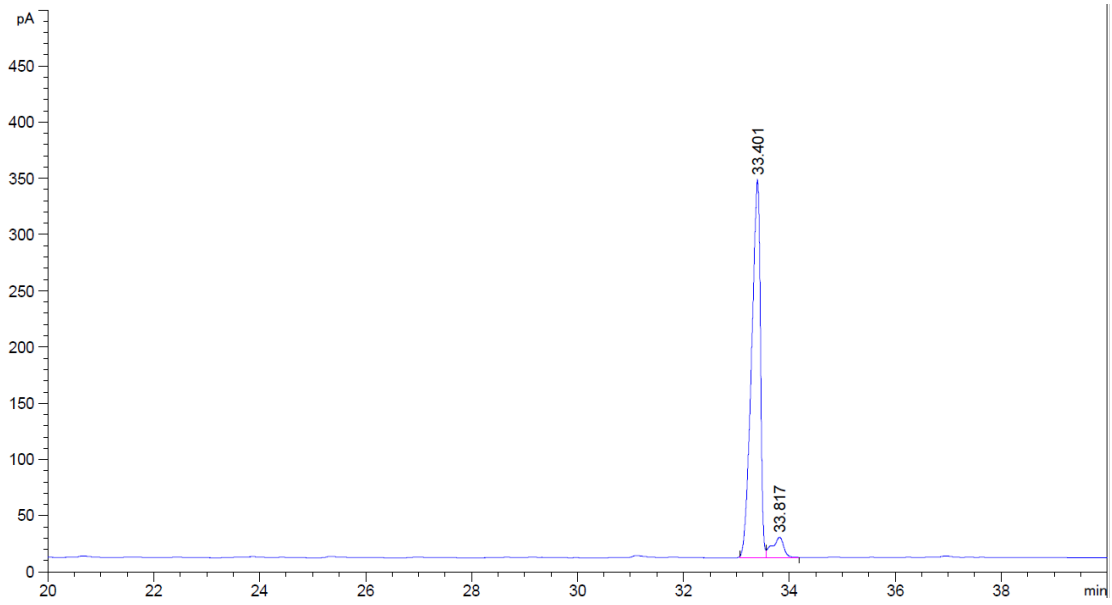


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [pA*s]	峰高 [pA]	峰面积 %
1	20.458	BB	0.1442	2124.58667	207.97144	94.87283
2	21.130	BB	0.1249	114.81816	11.65653	5.12717
总量：				2239.40483	219.62797	

Ethyl-5-(2-isopropoxy-2-oxoethyl)-4-phenyl-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3sa)

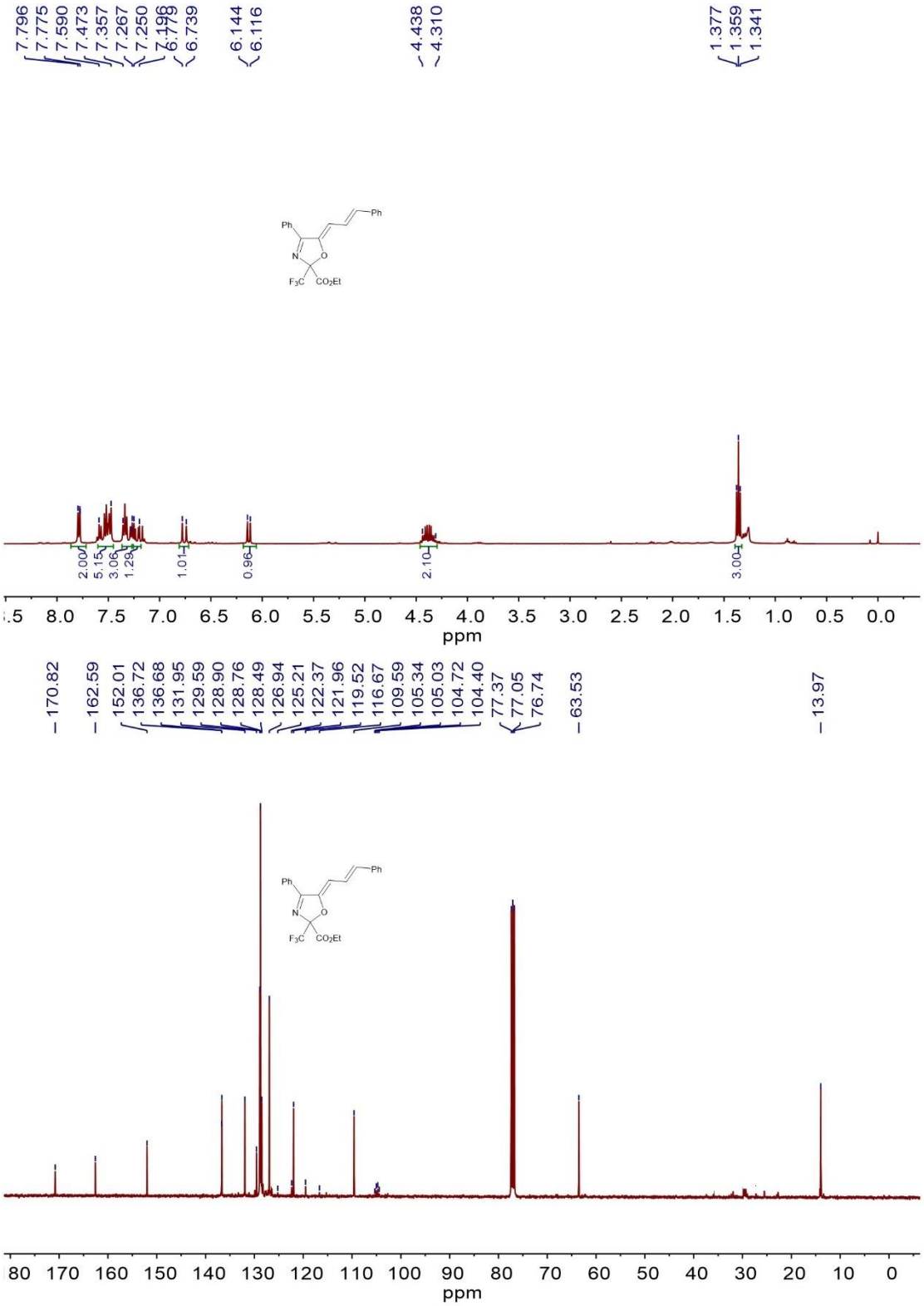


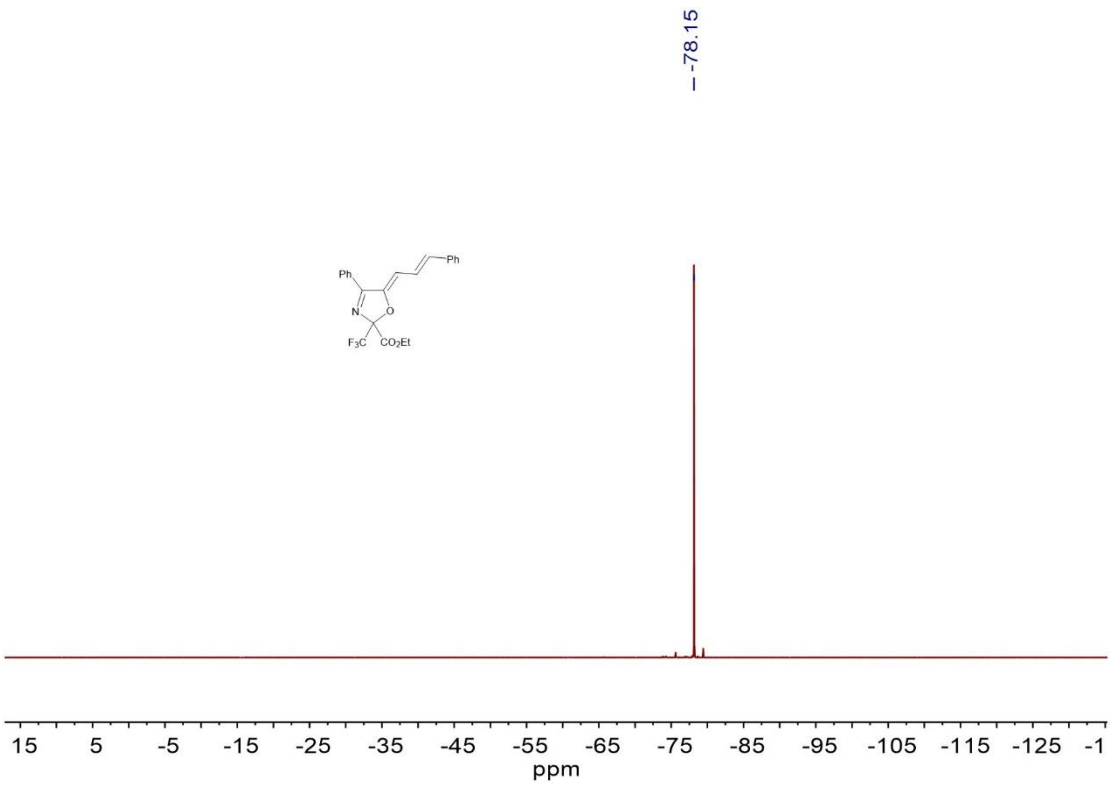




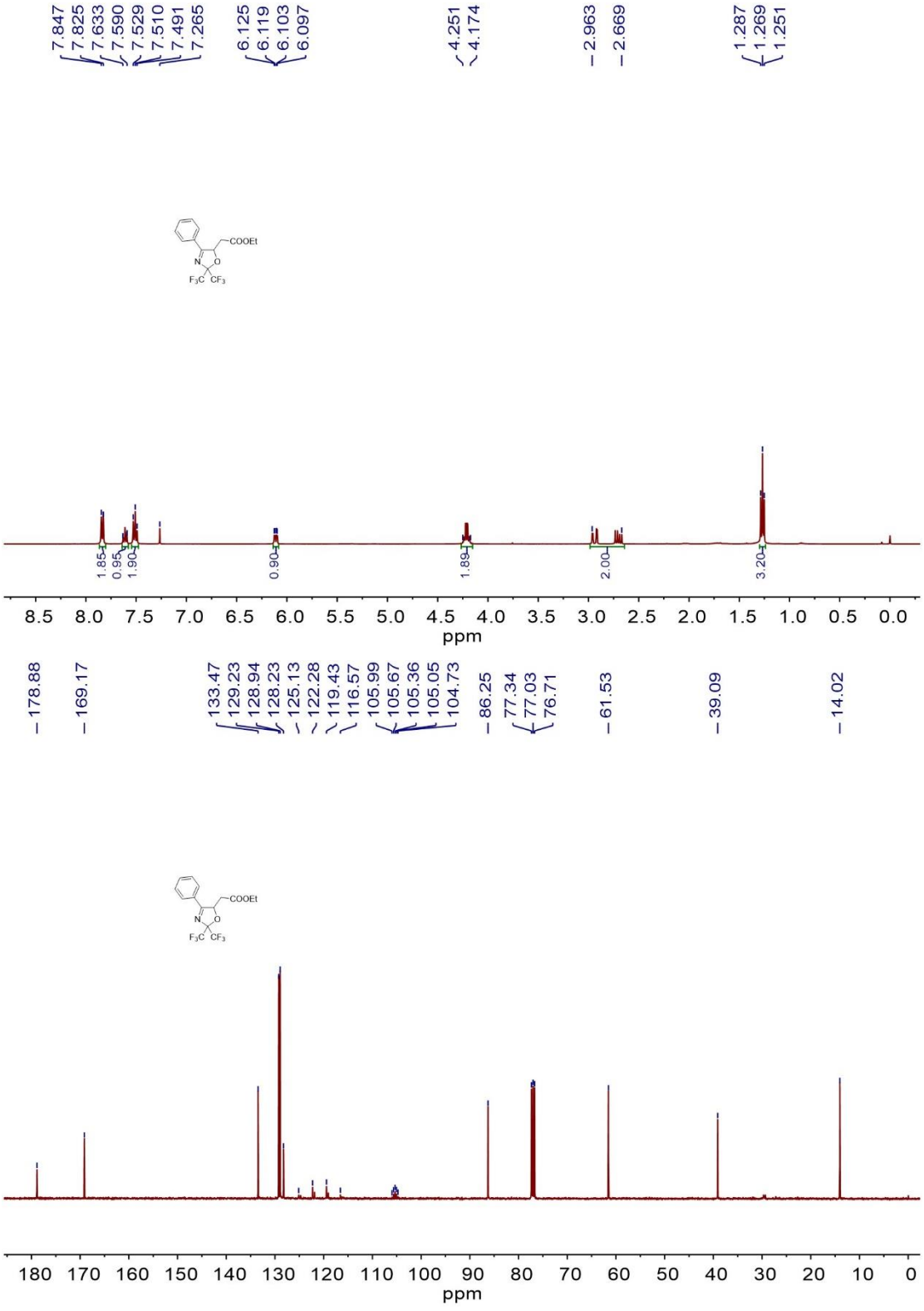
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [pA*s]	峰高 [pA]	峰面积 %
1	33.401	BV	0.1423	3900.56226	336.38861	93.38980
2	33.817	VB	0.1859	276.08472	18.20785	6.61020
总量：				4176.64697	354.59646	

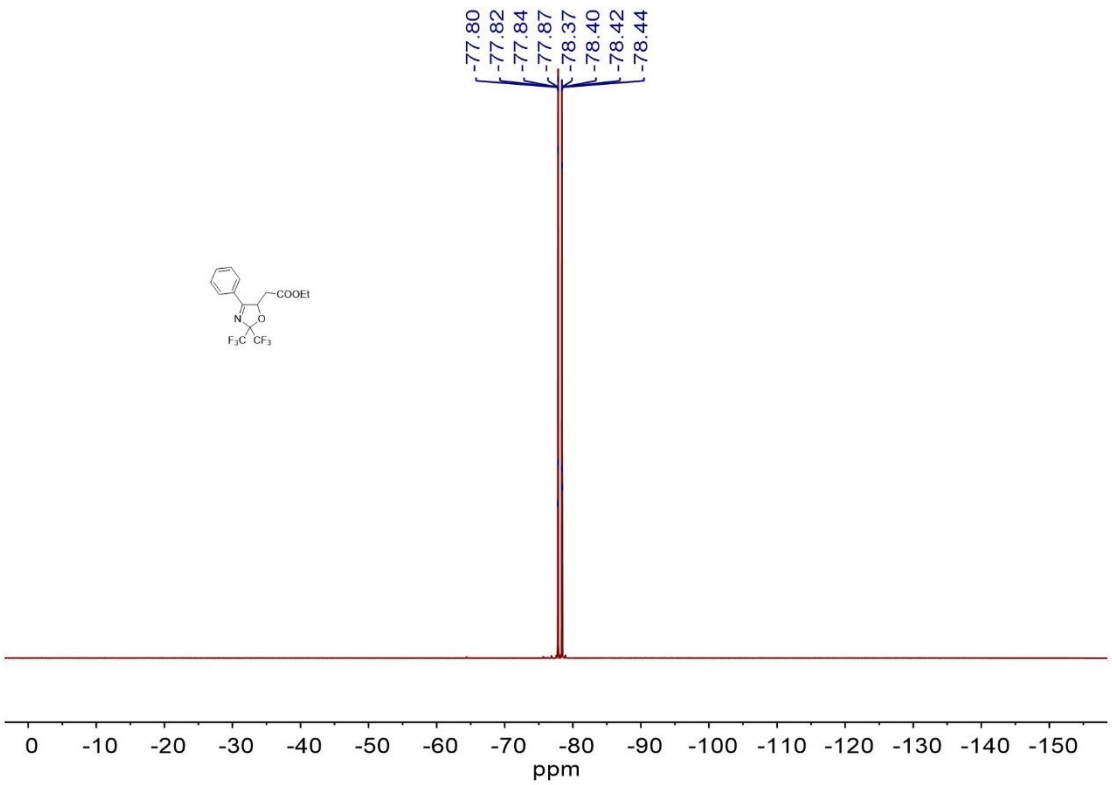
Ethyl (*Z*)-4-phenyl-5-((*E*)-3-phenylallylidene)-2-(trifluoromethyl)-2,5-dihydrooxazole-2-carboxylate (3va)



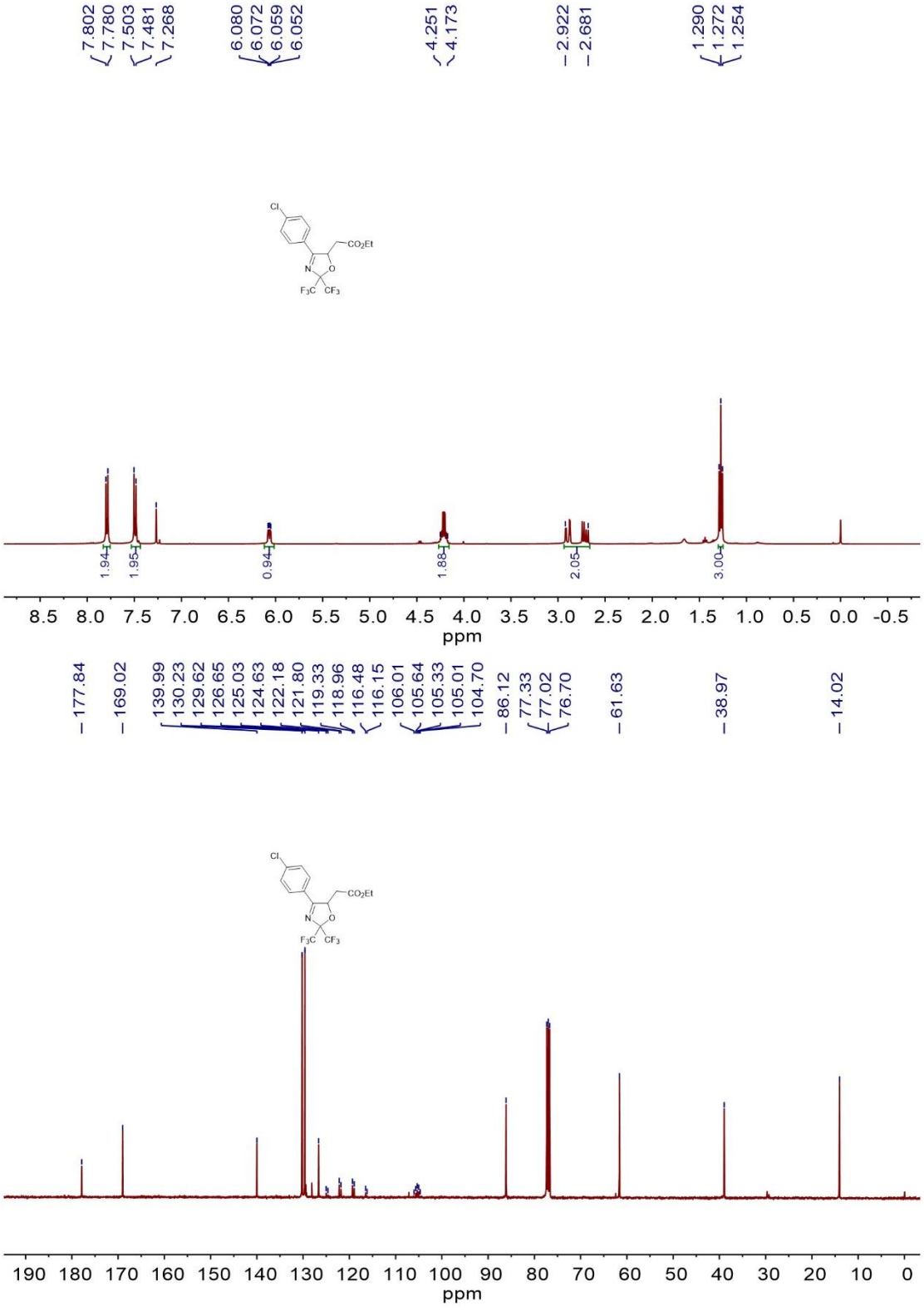

-78.15
Ph
Ph
N
O
F3C
CO2Et
15
5
-5
-15
-25
-35
-45
-55
-65
-75
-85
-95
-105
-115
-125
-1
ppm

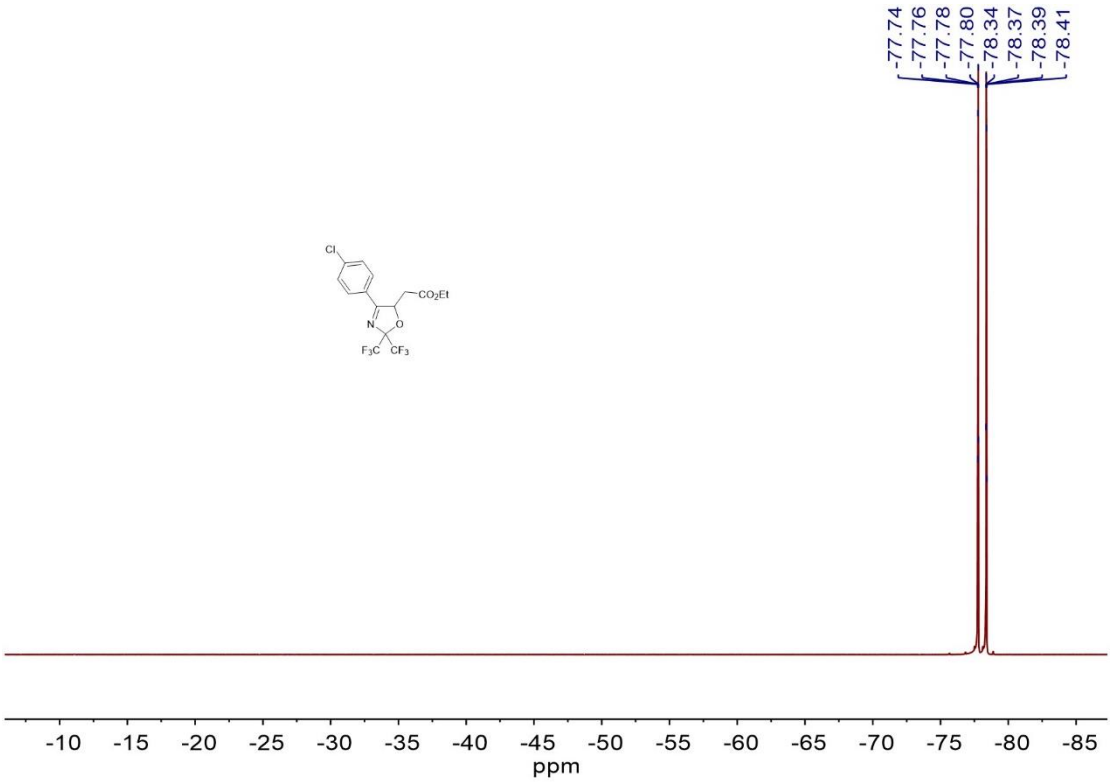
Ethyl 2-(4-phenyl-2,2-bis(trifluoromethyl)-2,5-dihydrooxazol-5-yl)acetate (3ab)



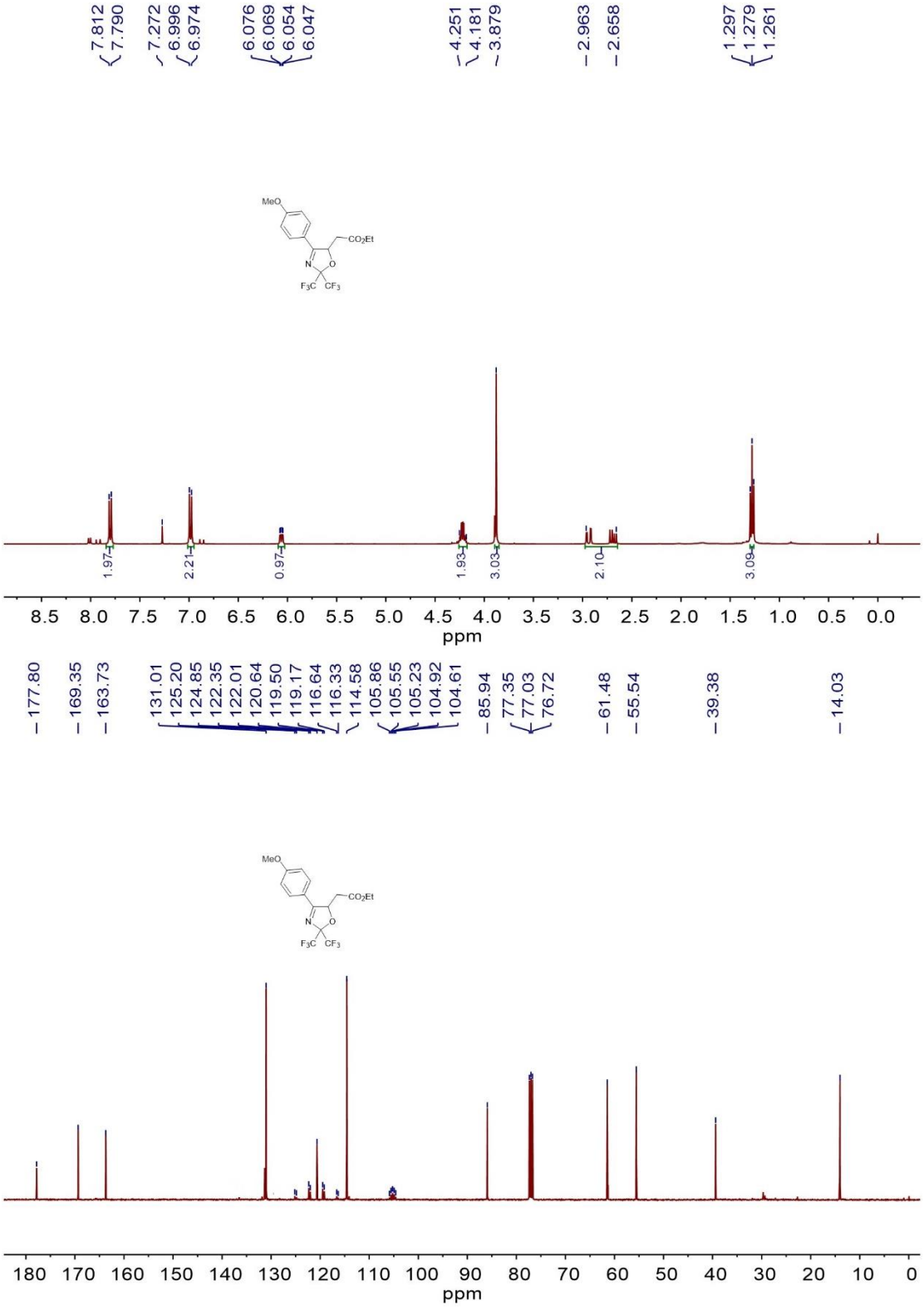

-77.80
-77.82
-77.84
-77.87
-78.37
-78.40
-78.42
-78.44
COOEt
N
O
F3C CF3
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150
ppm

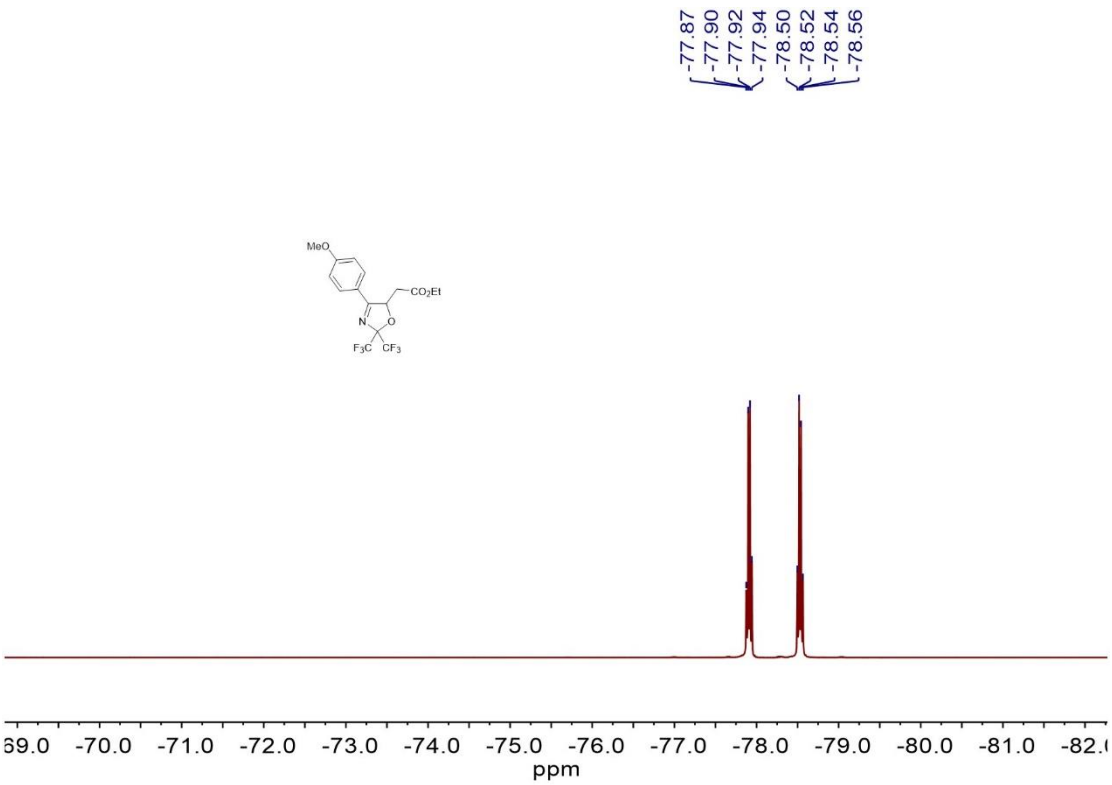
Ethyl 2-(4-(4-chlorophenyl)-2,2-bis(trifluoromethyl)-2,5-dihydrooxazol-5-yl)acetate (3cb)



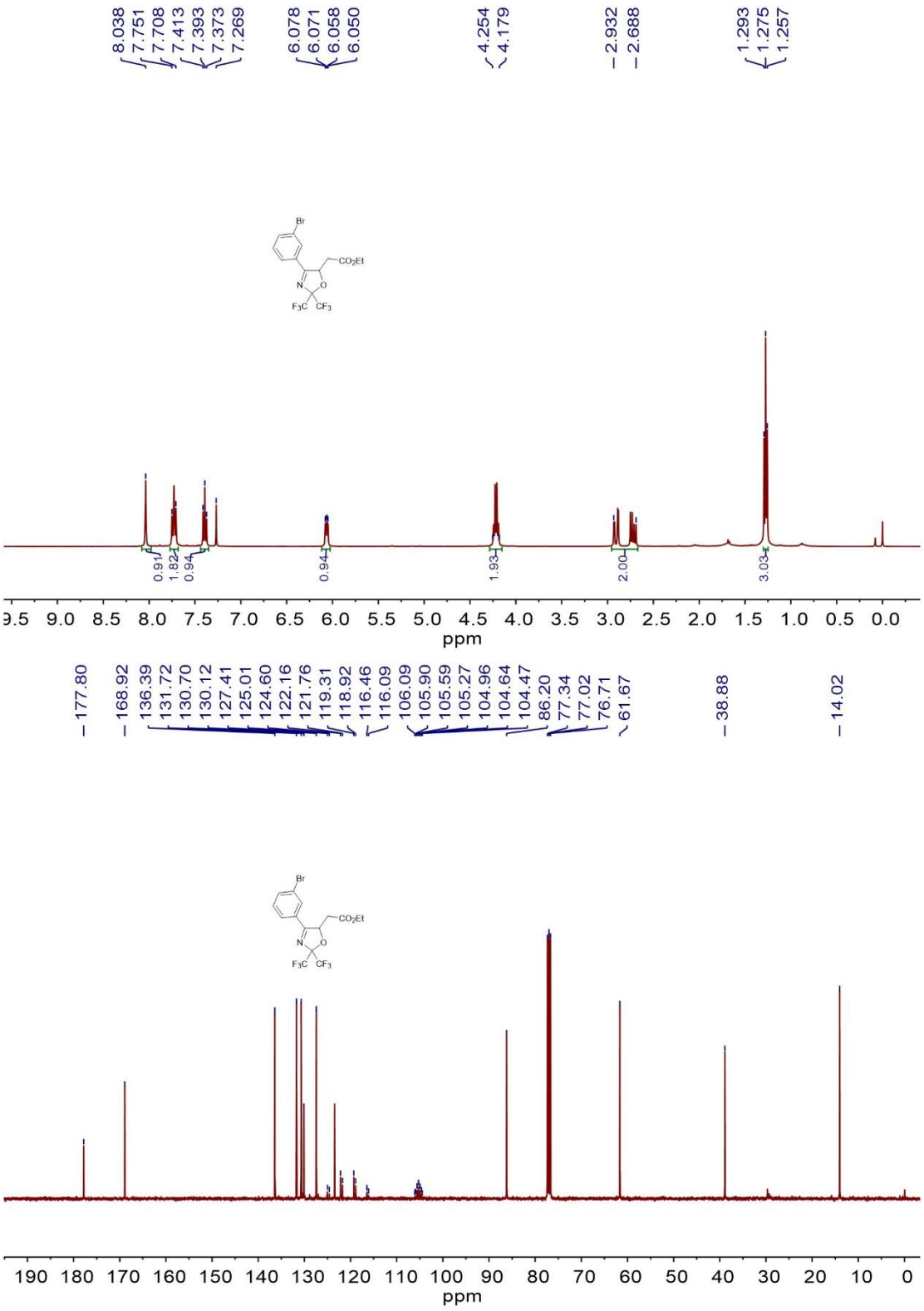

-77.74
-77.76
-77.78
-77.80
-78.34
-78.37
-78.39
-78.41
Cl
CO2Et
N
O
F3C
CF3
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
ppm

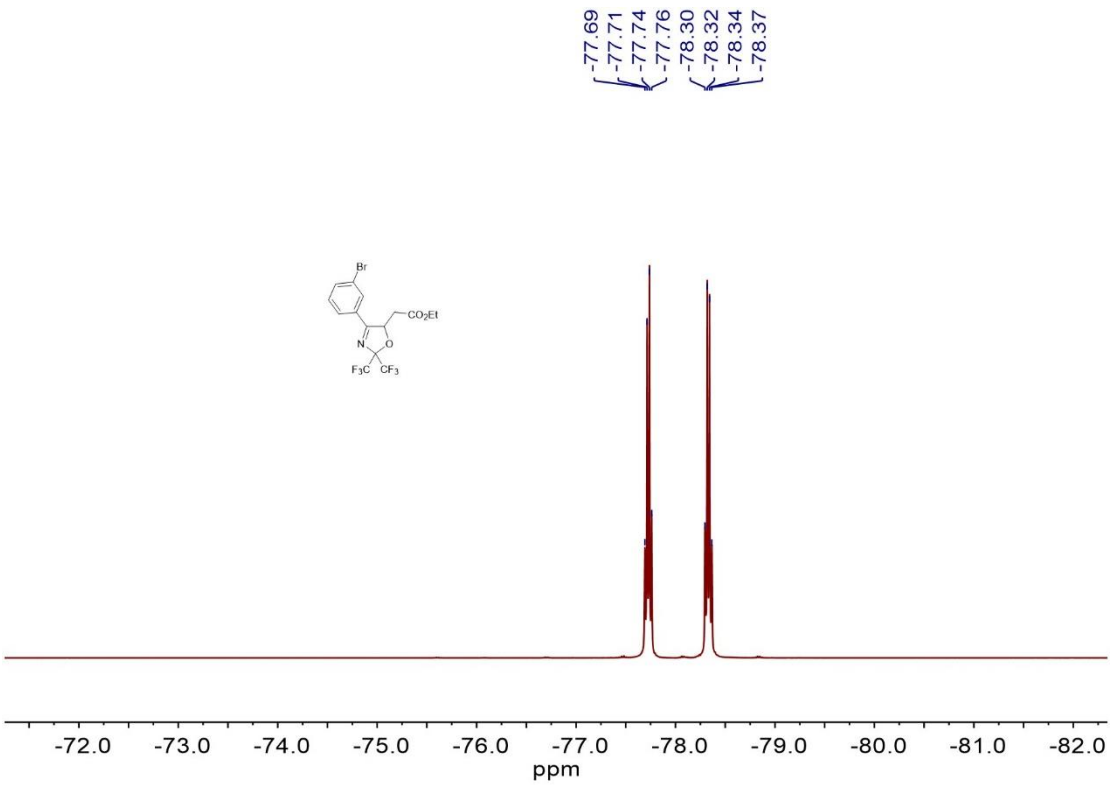
Ethyl 2-(4-(4-methoxyphenyl)-2,2-bis(trifluoromethyl)-2,5-dihydrooxazol-5-yl)acetate (3gb)



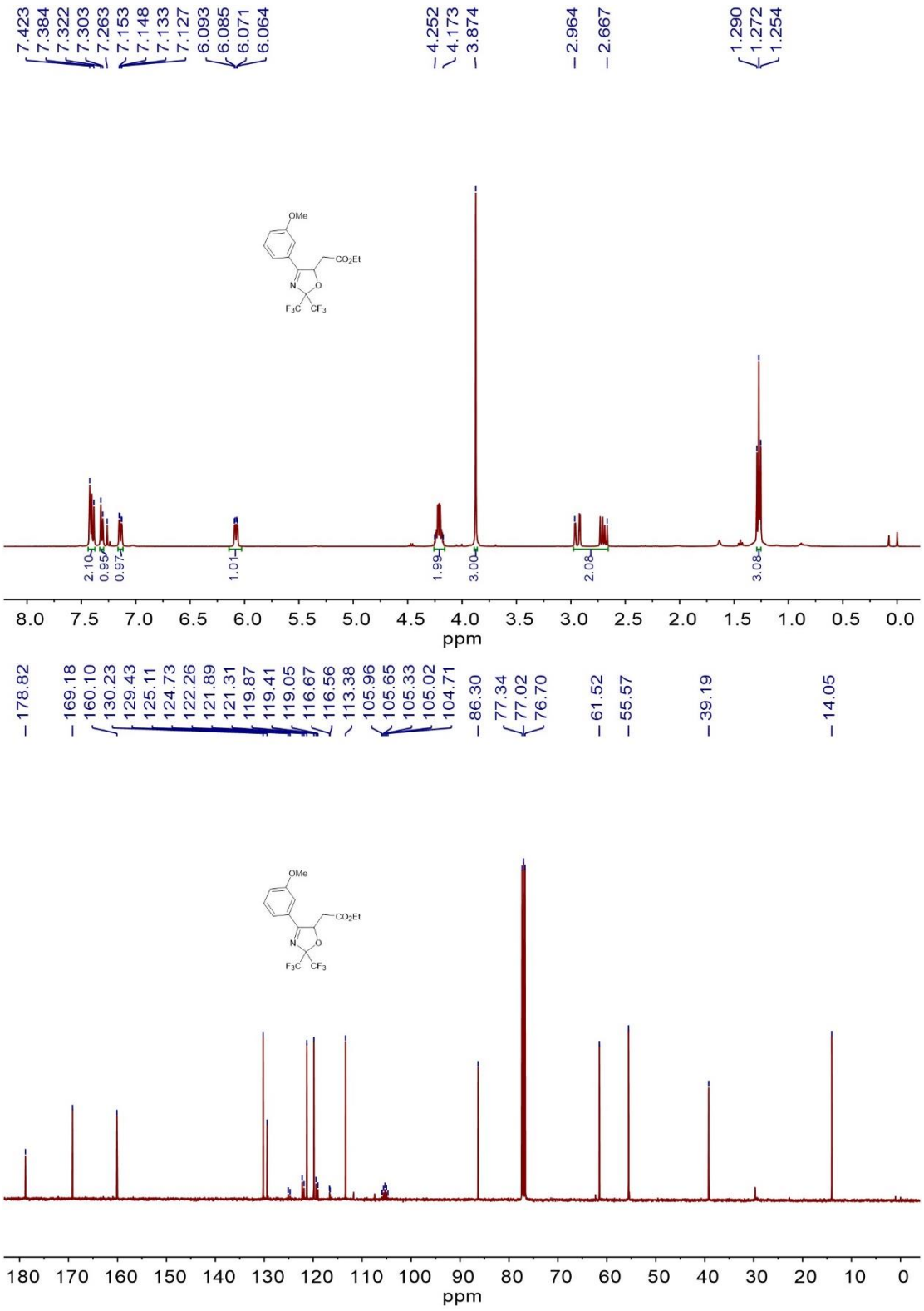

-77.87
-77.90
-77.92
-77.94
-78.50
-78.52
-78.54
-78.56
MeO
CO2Et
N
O
F3C
CF3
69.0
-70.0
-71.0
-72.0
-73.0
-74.0
-75.0
-76.0
-77.0
-78.0
-79.0
-80.0
-81.0
-82.
ppm

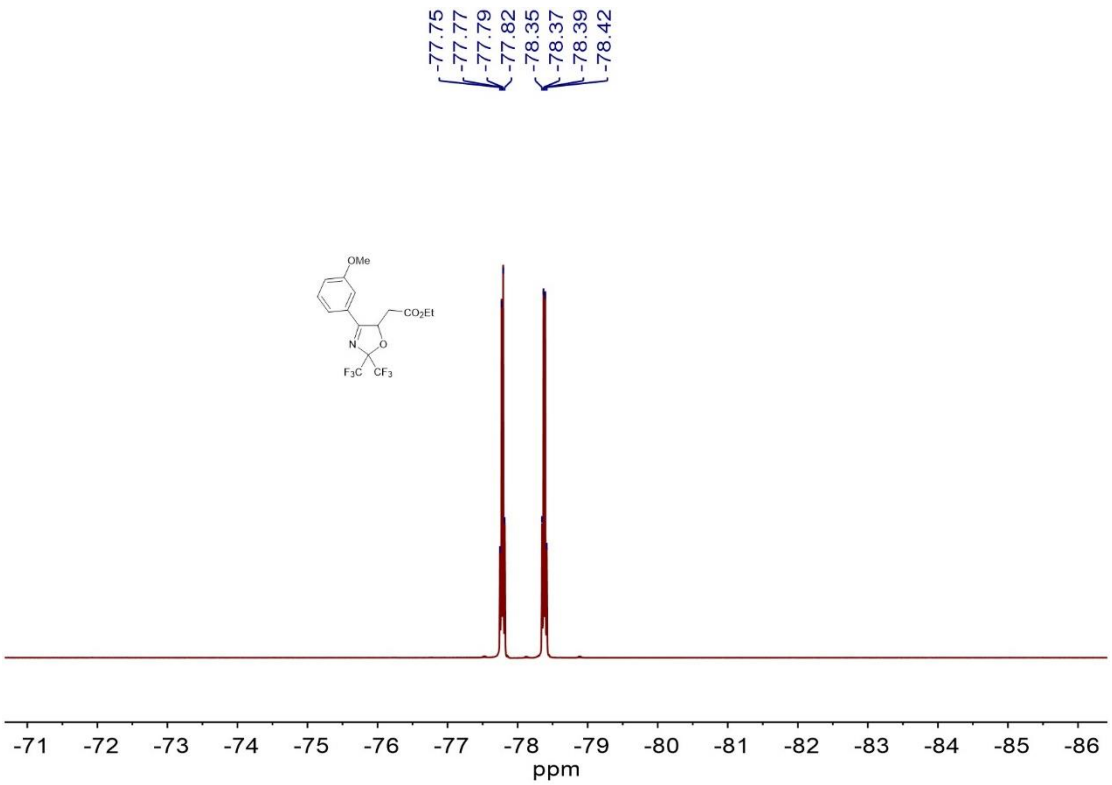
Ethyl 2-(4-(3-bromophenyl)-2,2-bis(trifluoromethyl)-2,5-dihydrooxazol-5-yl)acetate (3hb)



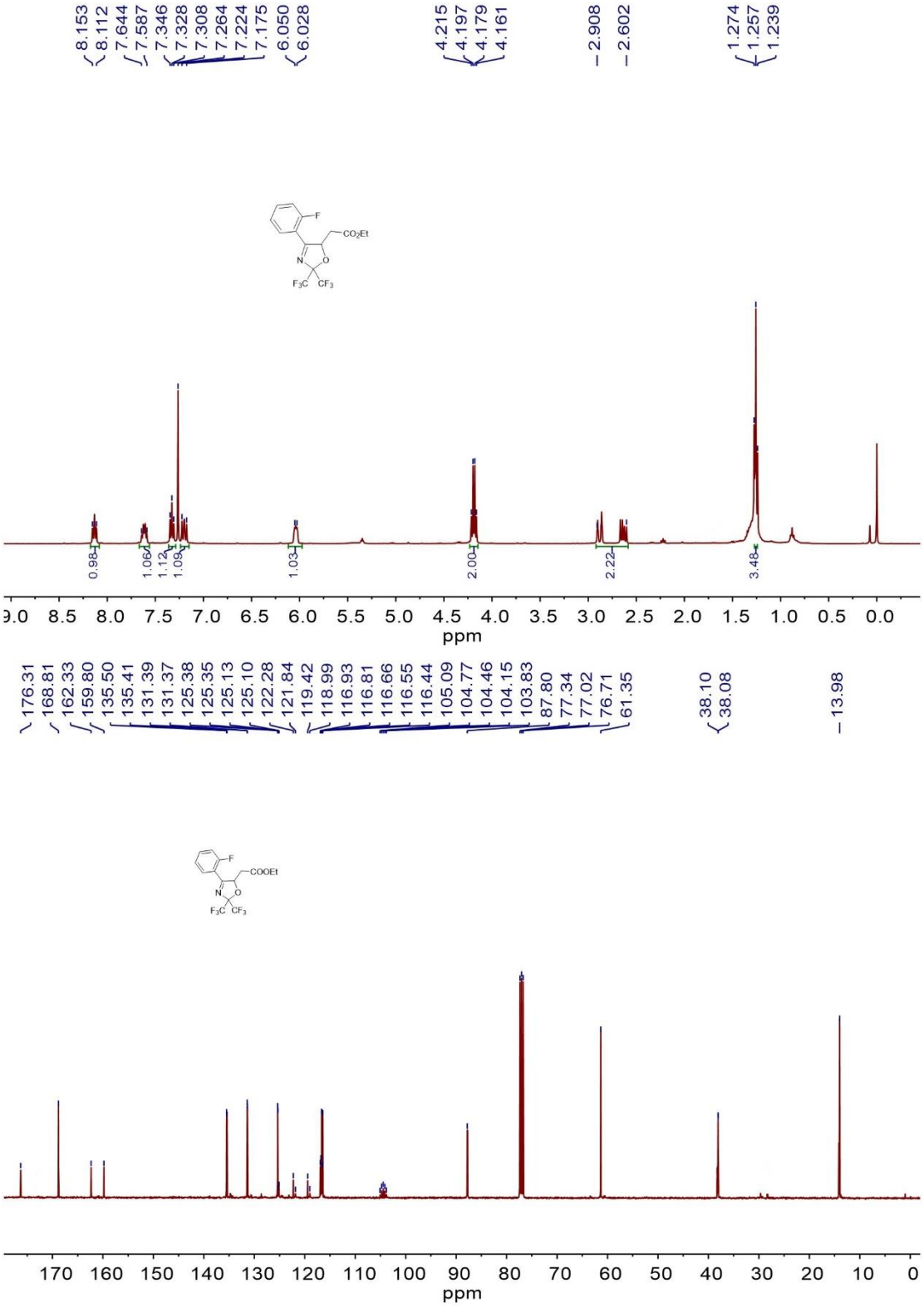

-77.69
-77.71
-77.74
-77.76
-78.30
-78.32
-78.34
-78.37
Br
CO2Et
N
O
F3C
CF3
-72.0
-73.0
-74.0
-75.0
-76.0
-77.0
-78.0
-79.0
-80.0
-81.0
-82.0
ppm

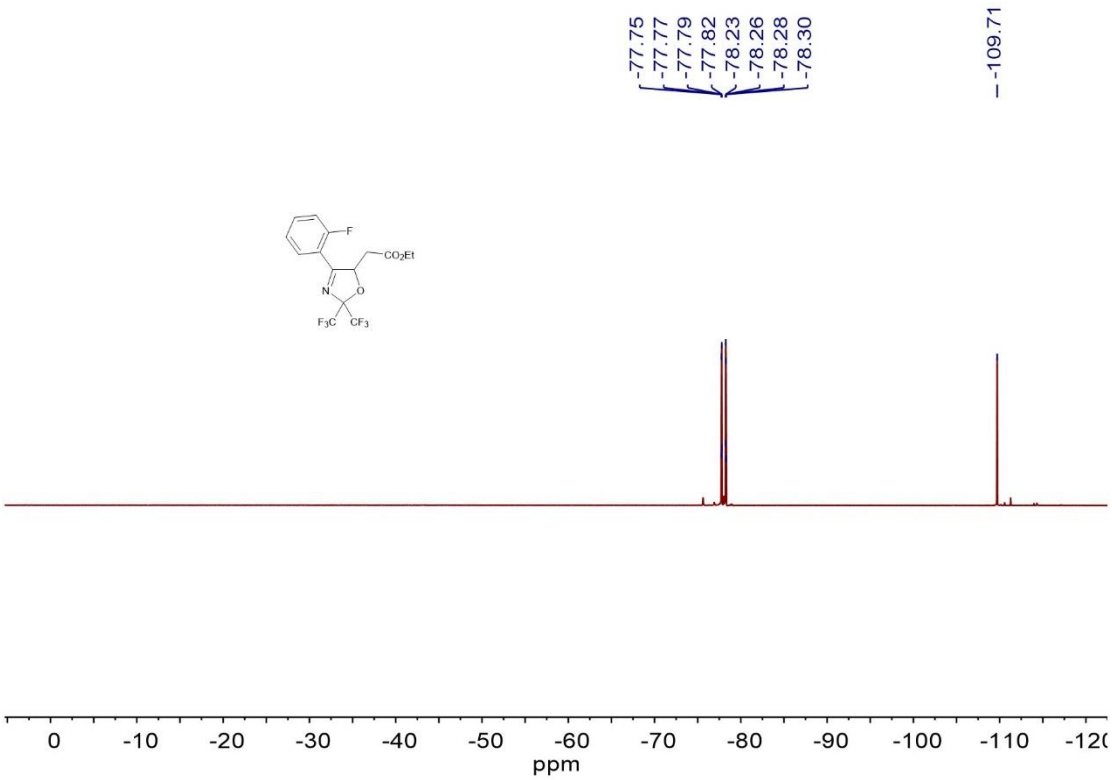
Ethyl 2-(4-(3-methoxyphenyl)-2,2-bis(trifluoromethyl)-2,5-dihydrooxazol-5-yl)acetate (3jb)



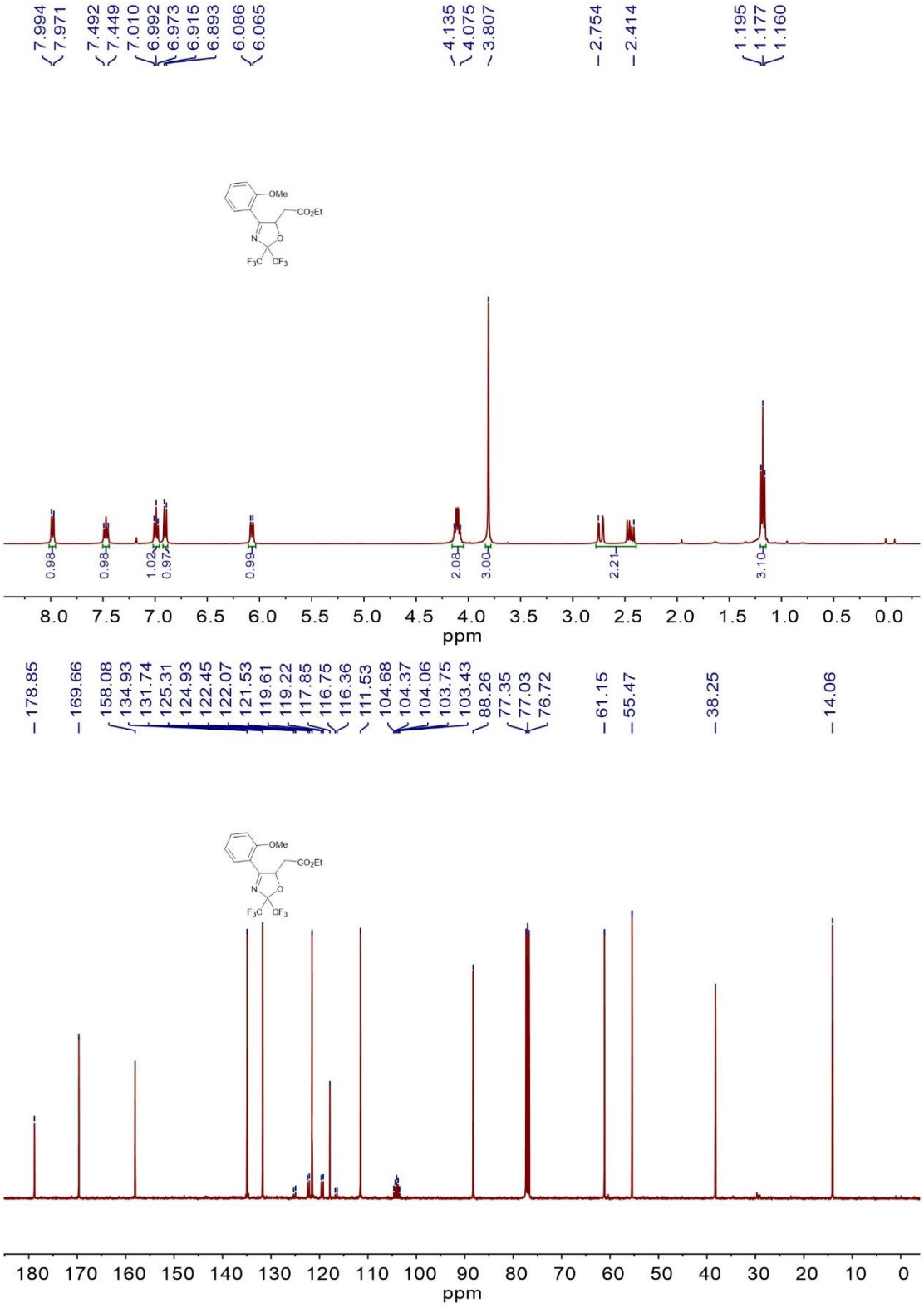

-77.75
-77.77
-77.79
-77.82
-78.35
-78.37
-78.39
-78.42
OMe
CO2Et
N
O
F3C
CF3
-71
-72
-73
-74
-75
-76
-77
-78
-79
-80
-81
-82
-83
-84
-85
-86
ppm

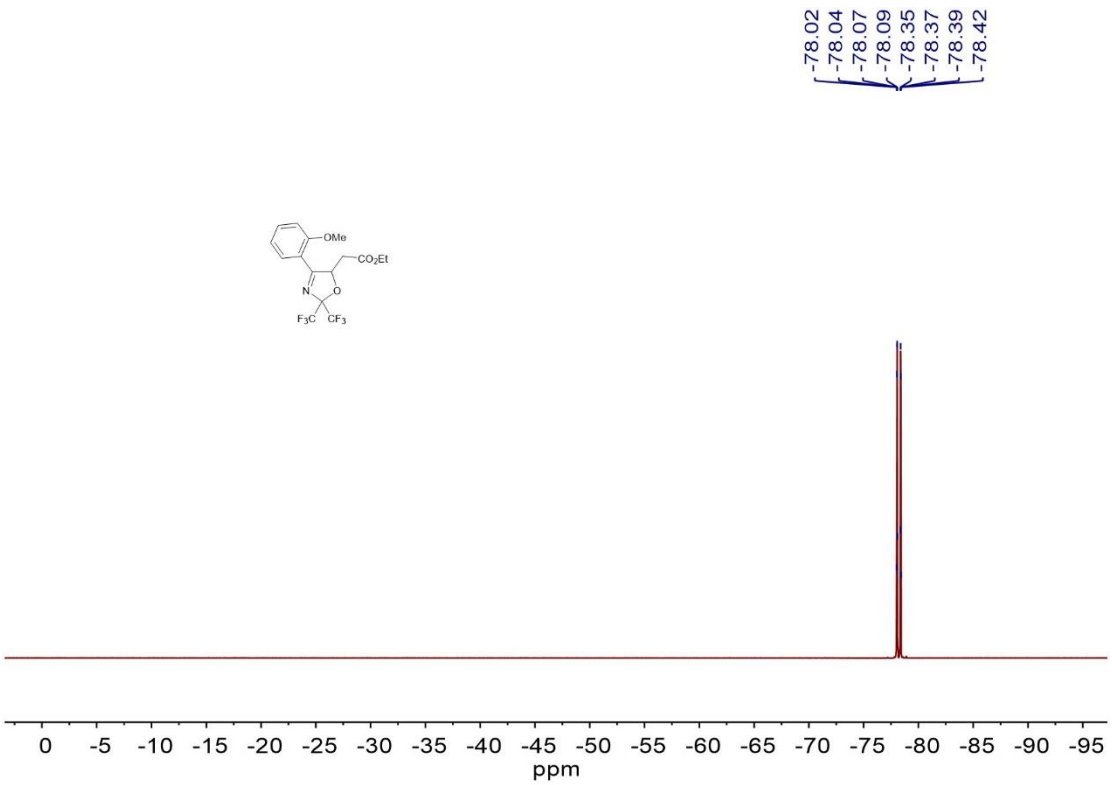
Ethyl 2-(4-(2-fluorophenyl)-2,2-bis(trifluoromethyl)-2,5-dihydrooxazol-5-yl)acetate (3kb)



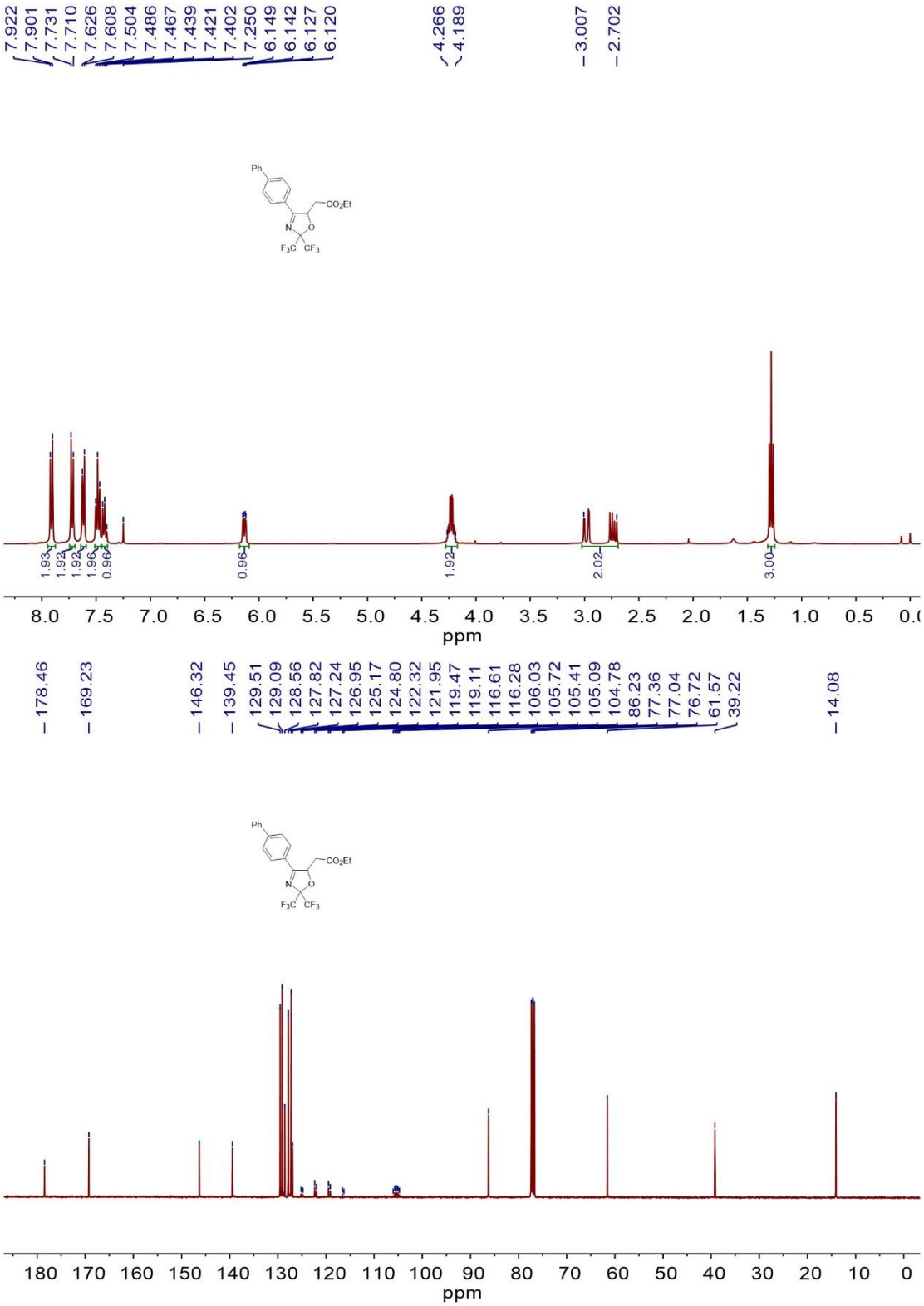

-77.75
-77.77
-77.79
-77.82
-78.23
-78.26
-78.28
-78.30
-109.71
F
CO2Et
N
O
F3C
CF3
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
ppm

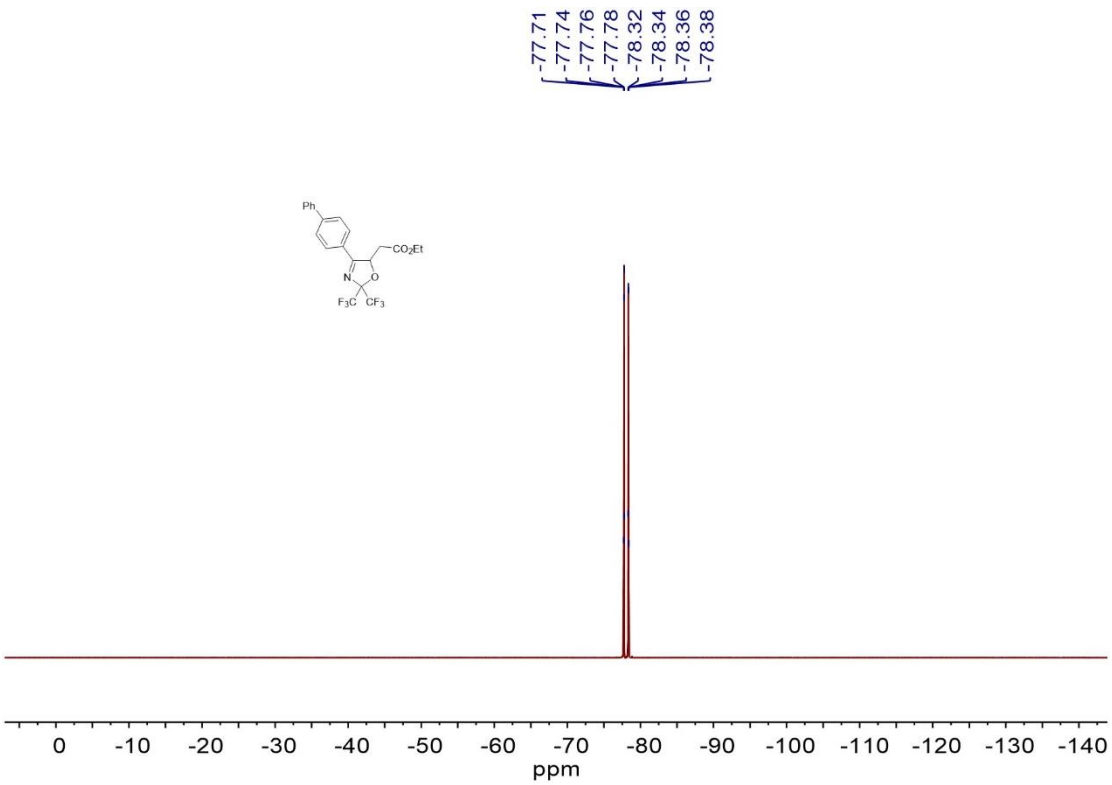
Ethyl 2-(4-(2-methoxyphenyl)-2,2-bis(trifluoromethyl)-2,5-dihydrooxazol-5-yl)acetate (3lb)



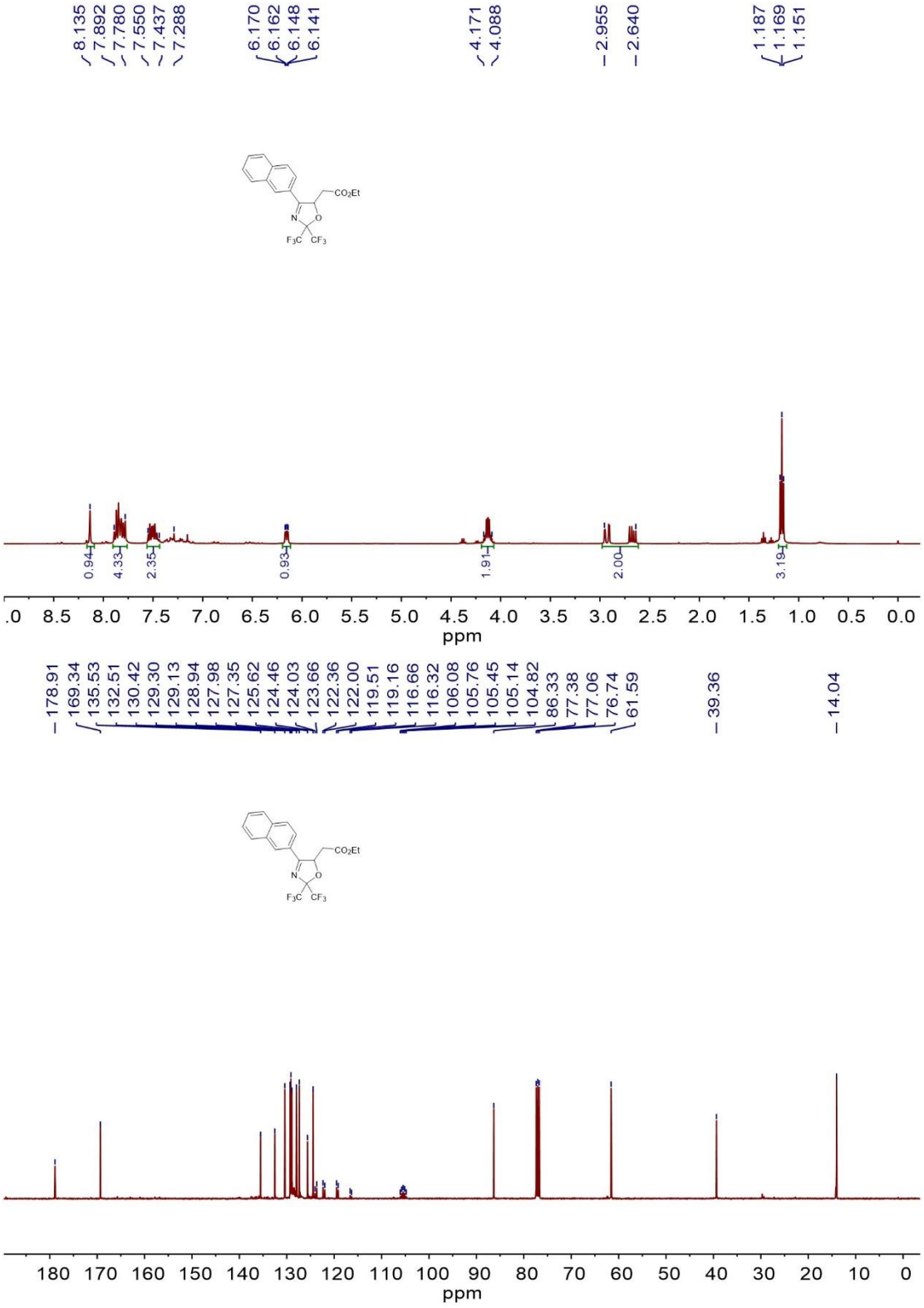

-78.02
-78.04
-78.07
-78.09
-78.35
-78.37
-78.39
-78.42
OMe
CO2Et
N
O
F3C
CF3
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
ppm

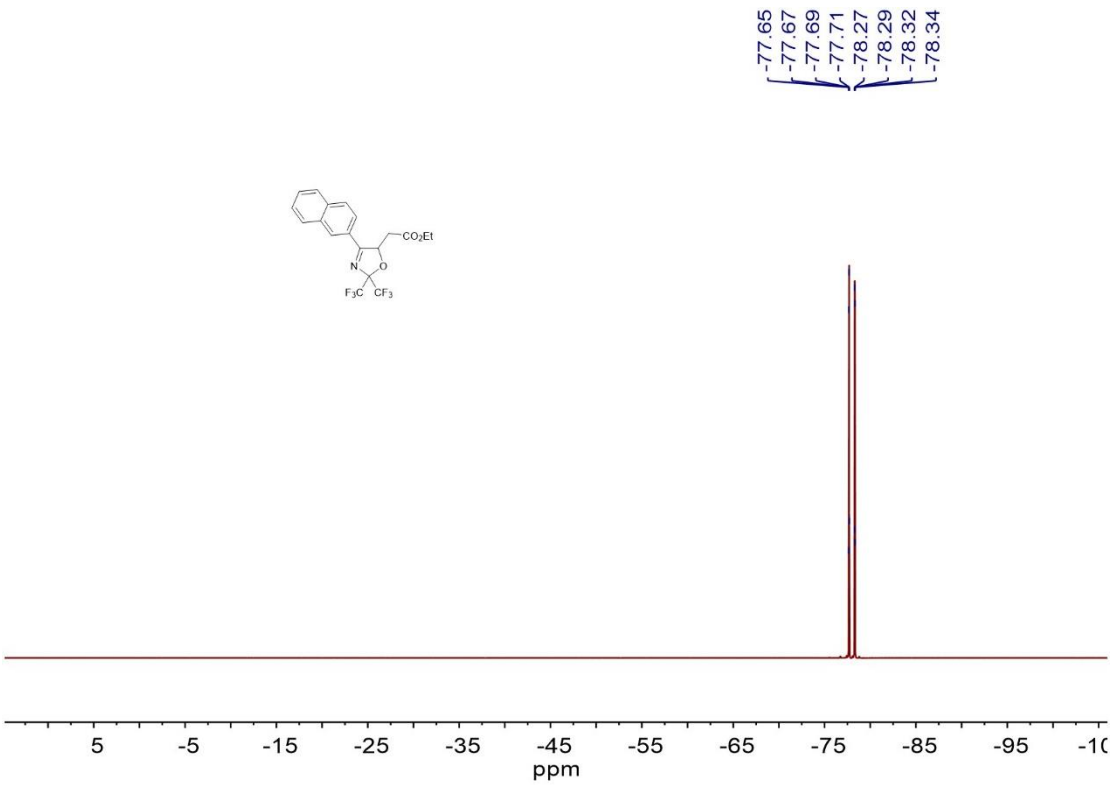
Ethyl 2-(4-([1,1'-biphenyl]-4-yl)-2,2-bis(trifluoromethyl)-2,5-dihydrooxazol-5-yl)acetate (3mb)



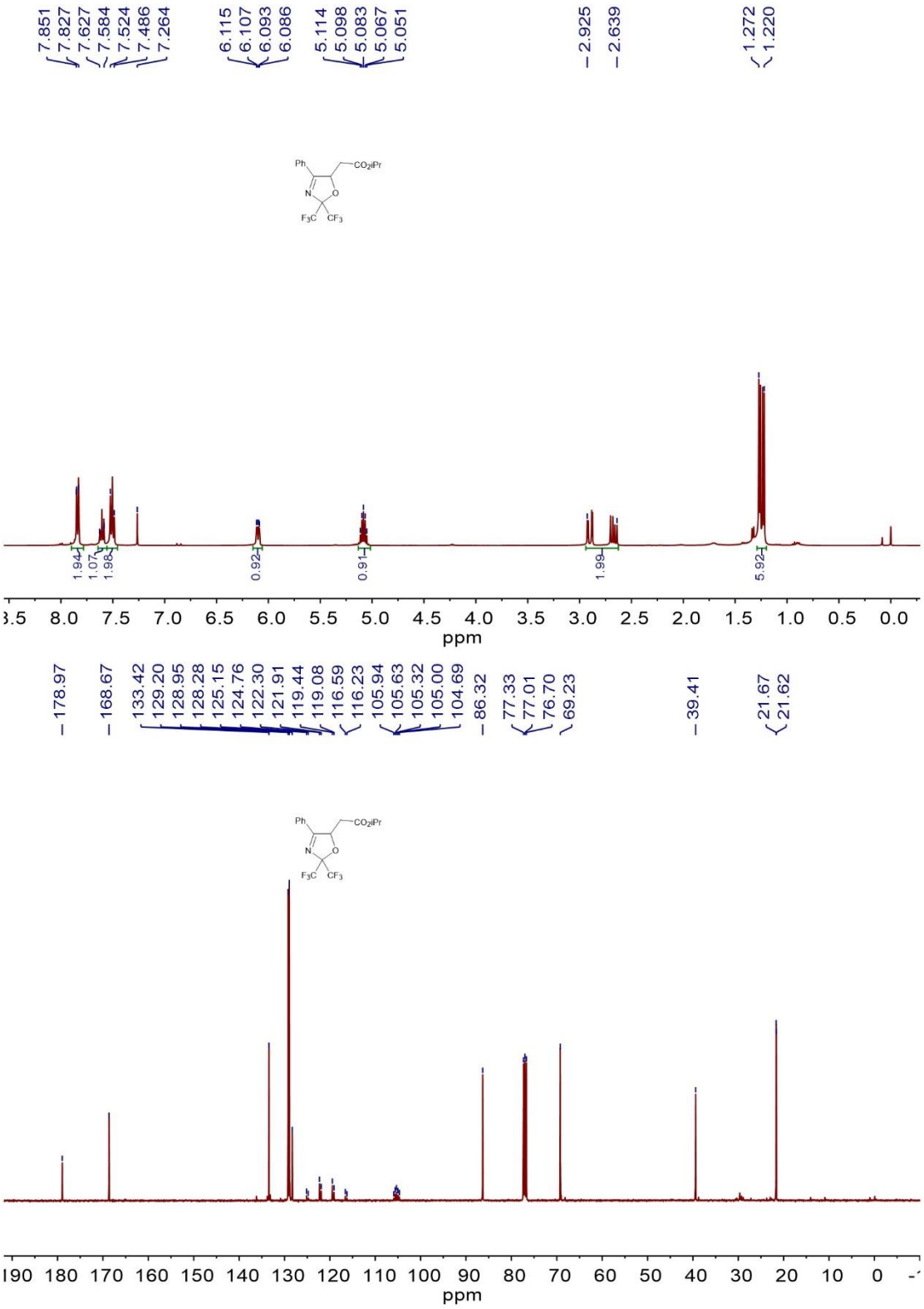

-77.71
-77.74
-77.76
-77.78
-78.32
-78.34
-78.36
-78.38
Ph
CO2Et
N
O
F3C
CF3
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
ppm

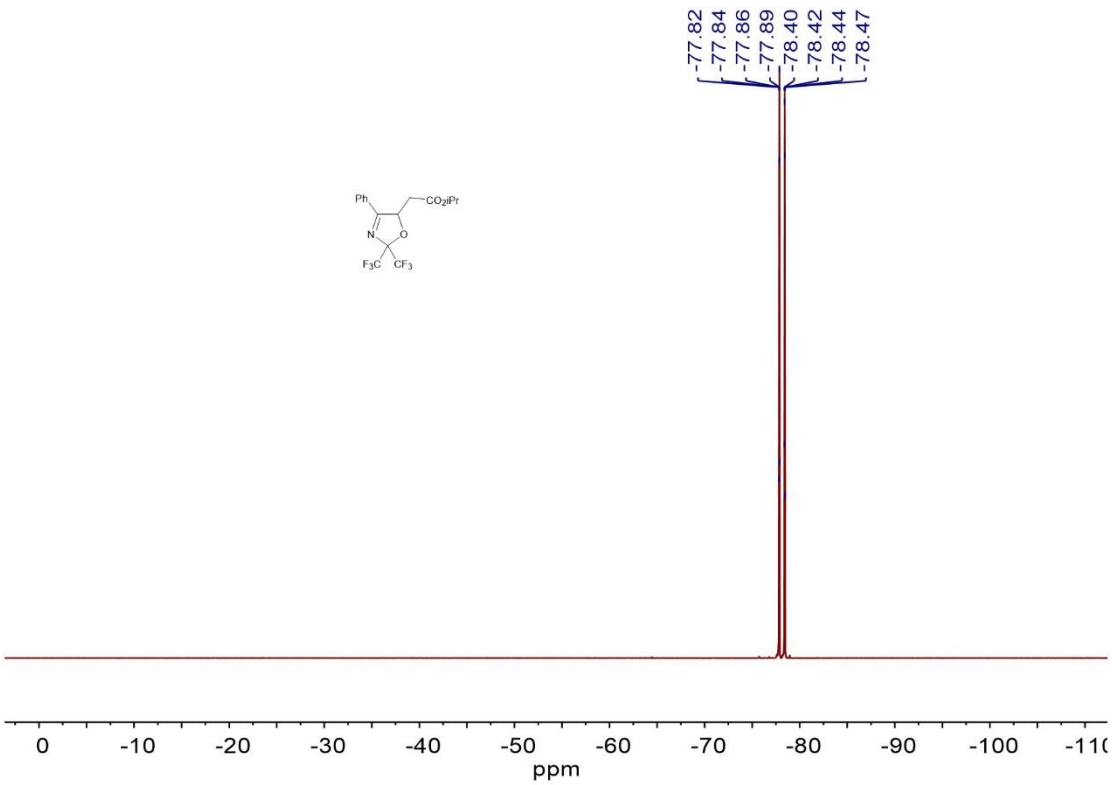
Ethyl 2-(4-(naphthalen-2-yl)-2,2-bis(trifluoromethyl)-2,5-dihydrooxazol-5-yl)acetate (3nb)



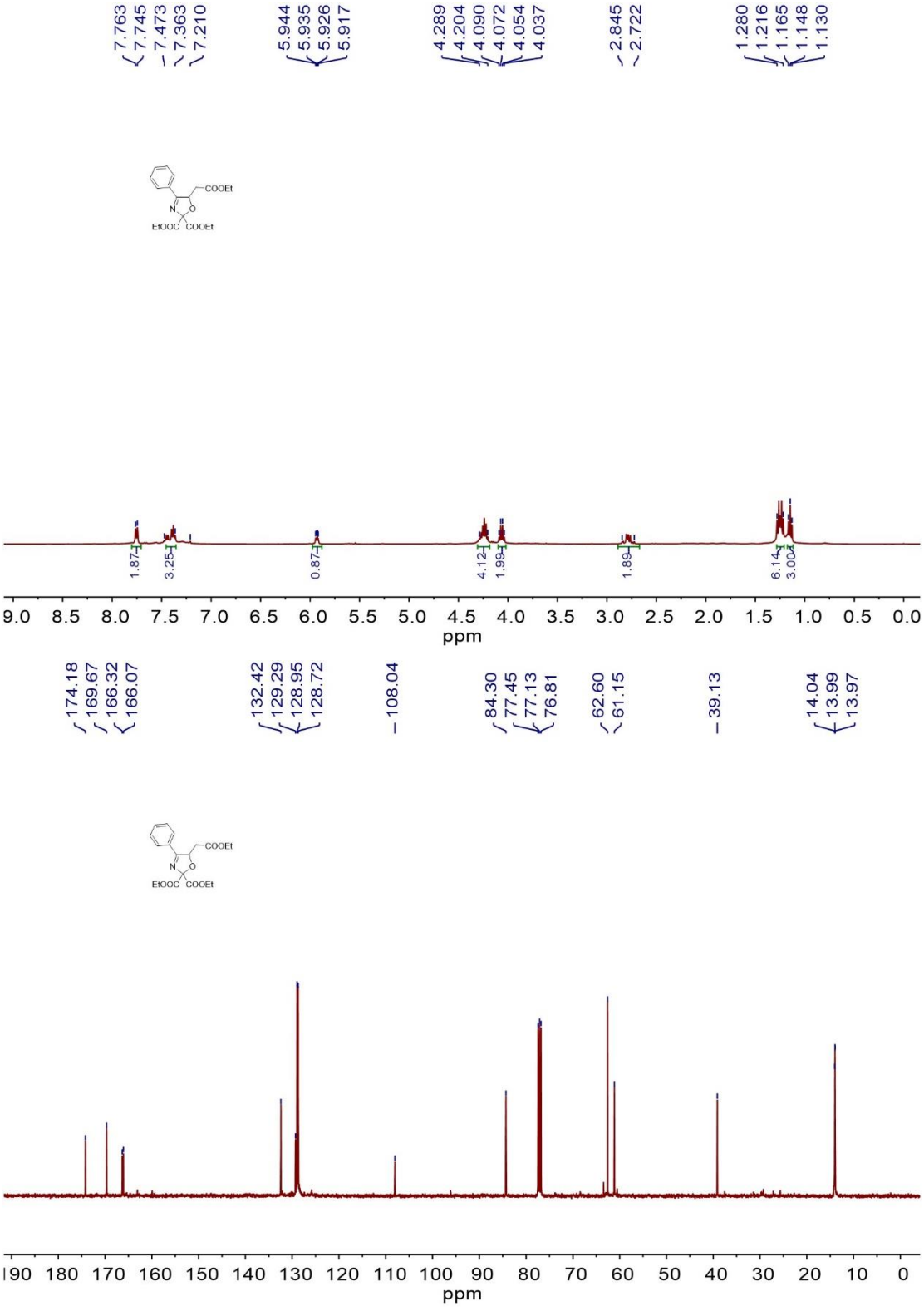

-77.65
-77.67
-77.69
-77.71
-78.27
-78.29
-78.32
-78.34
CO2Et
N
O
F3C
CF3
5
-5
-15
-25
-35
-45
-55
-65
-75
-85
-95
-10
ppm

Isopropyl 2-(4-phenyl-2,2-bis(trifluoromethyl)-2,5-dihydrooxazol-5-yl)acetate (3rb)

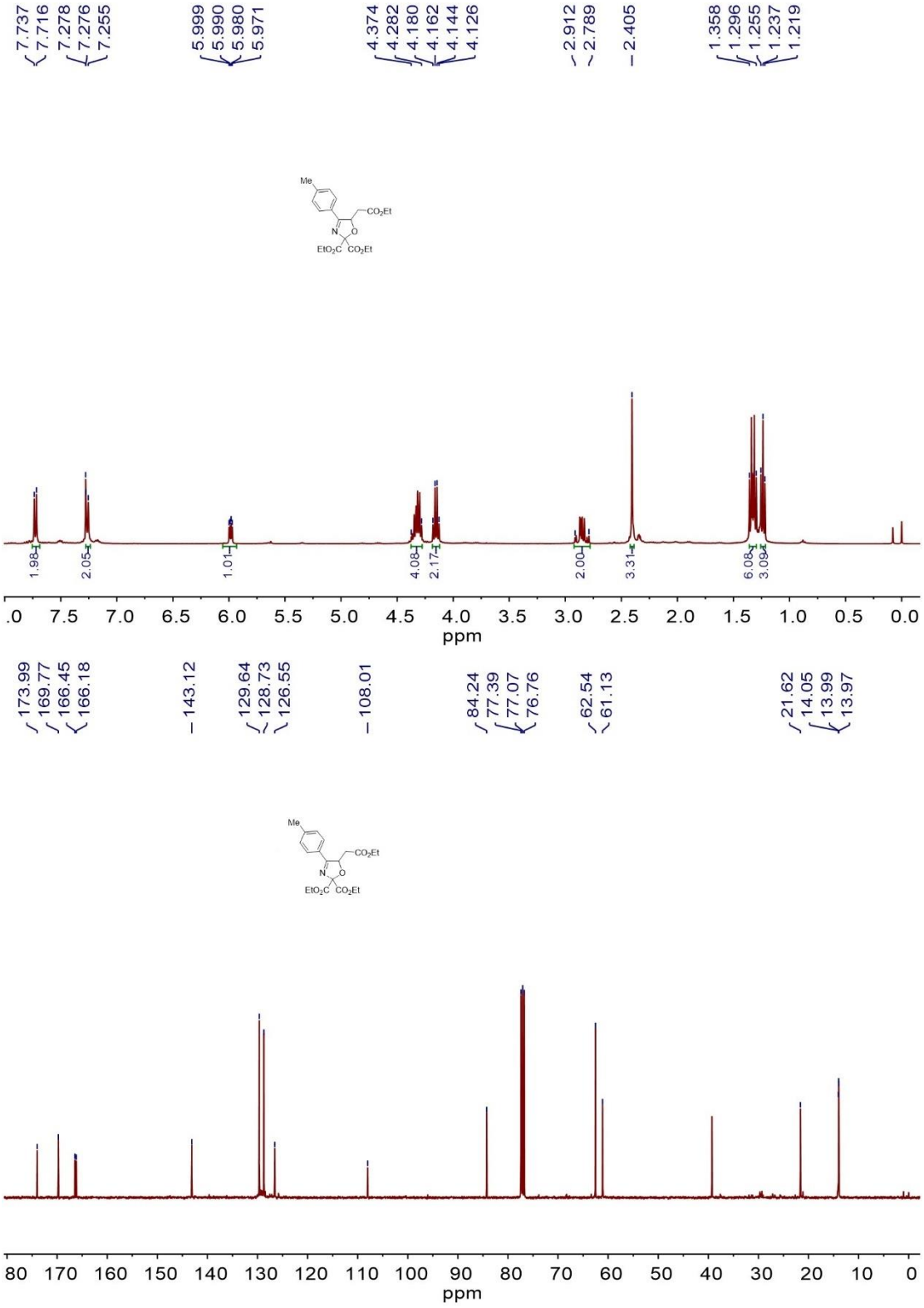



-77.82
-77.84
-77.86
-77.89
-78.40
-78.42
-78.44
-78.47
Ph
CO2iPr
N
O
F3C
CF3
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
ppm

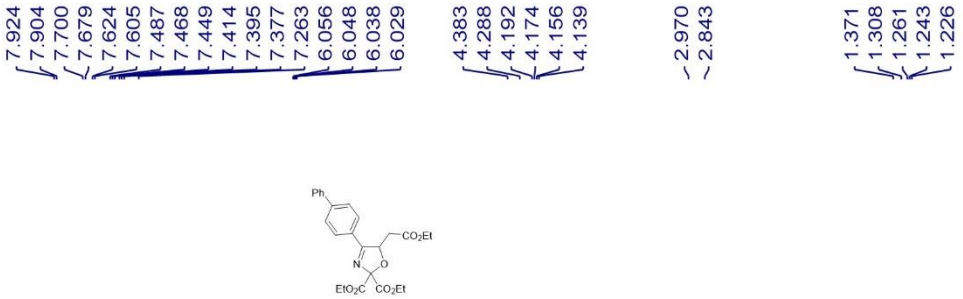
Diethyl 5-(2-ethoxy-2-oxoethyl)-4-phenyloxazole-2,2(5H)-dicarboxylate (3ac)

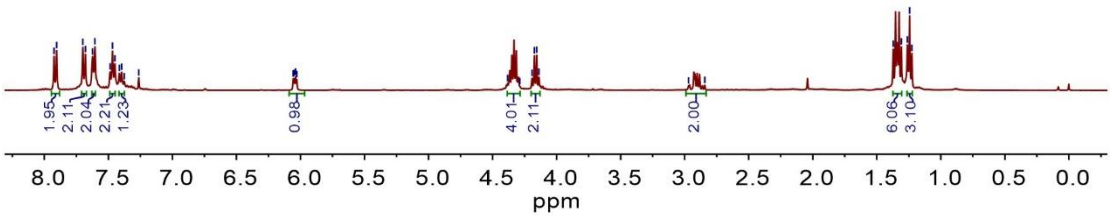


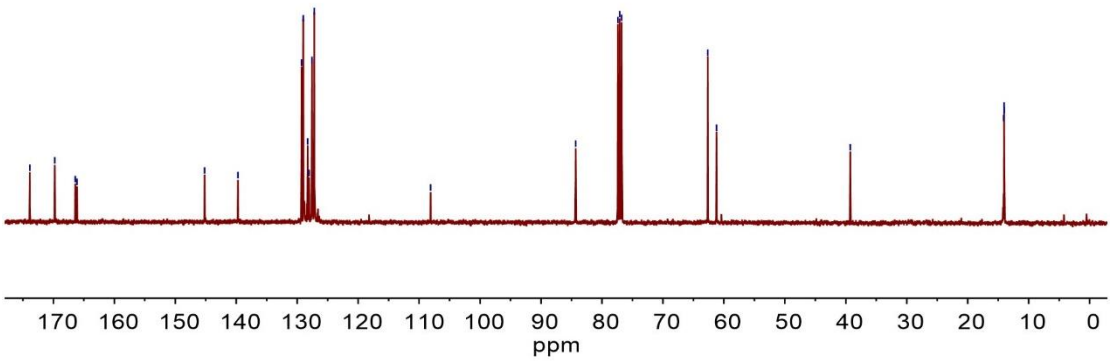
Diethyl 5-(2-ethoxy-2-oxoethyl)-4-(p-tolyl)oxazole-2,2(5H)-dicarboxylate (3fc)



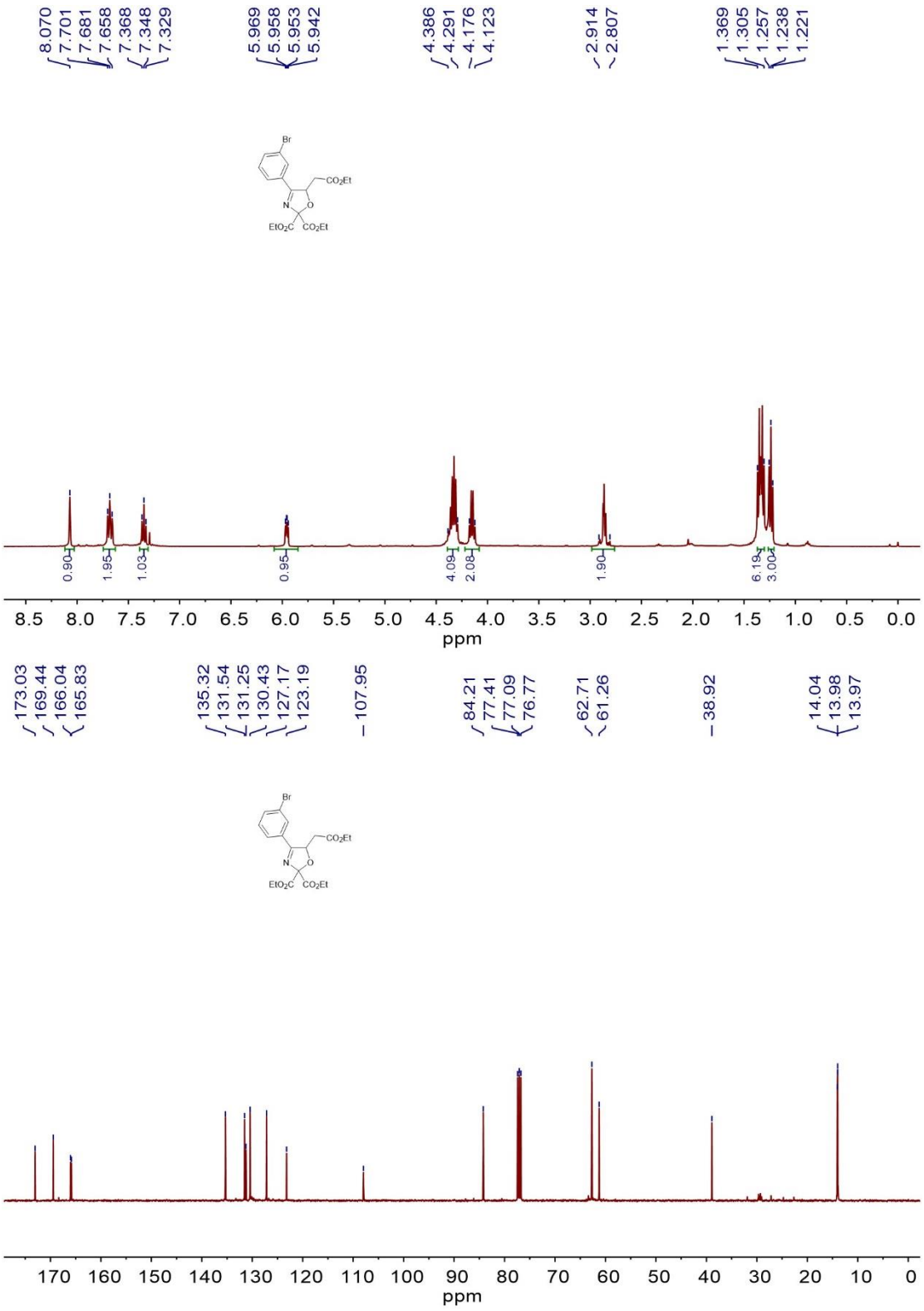
Diethyl 4-([1,1'-biphenyl]-4-yl)-5-(2-ethoxy-2-oxoethyl)oxazole-2,2(5H)-dicarboxylate (3mc)



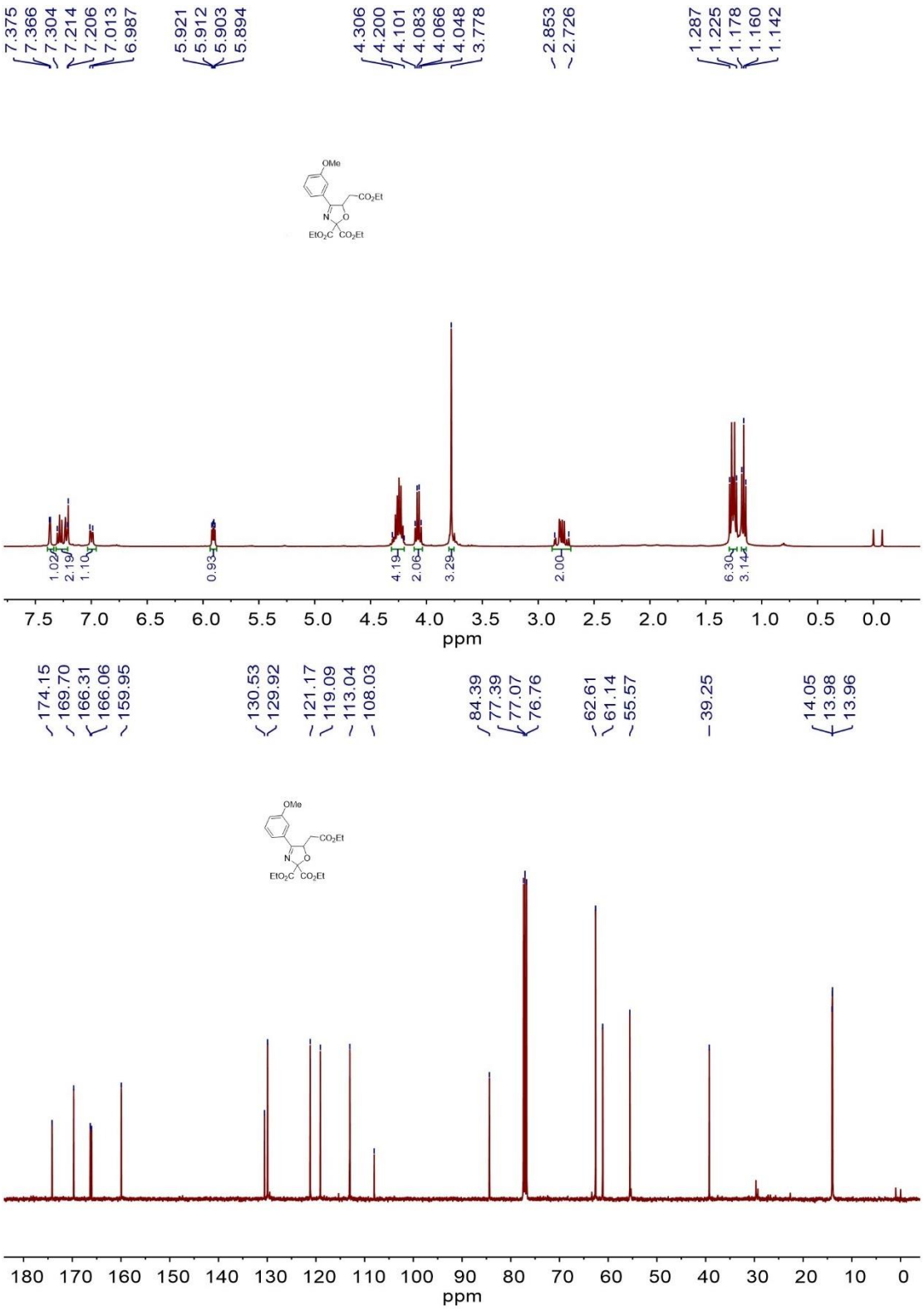




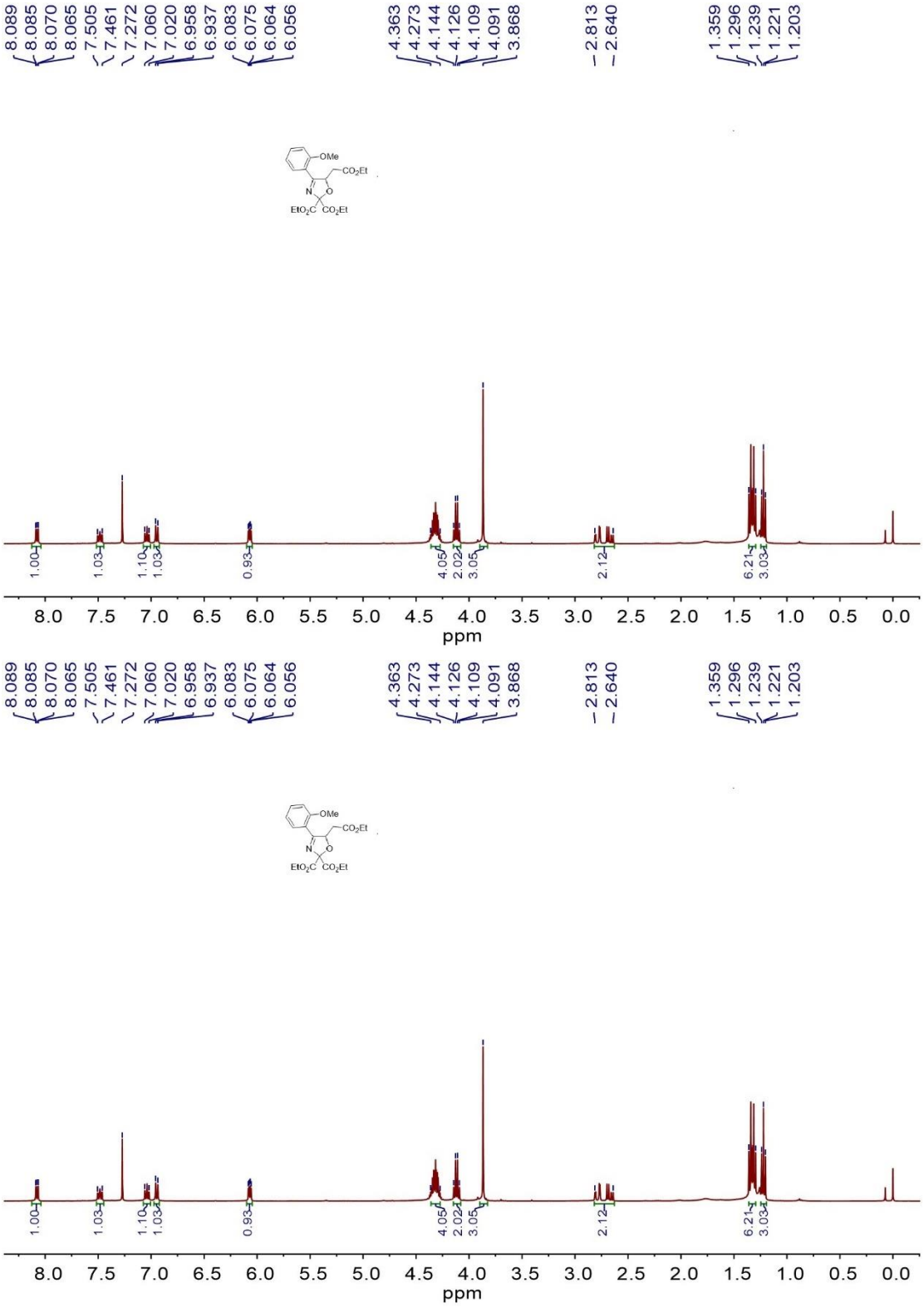
Diethyl 4-(3-bromophenyl)-5-(2-ethoxy-2-oxoethyl)oxazole-2,2(5H)-dicarboxylate (3hc)



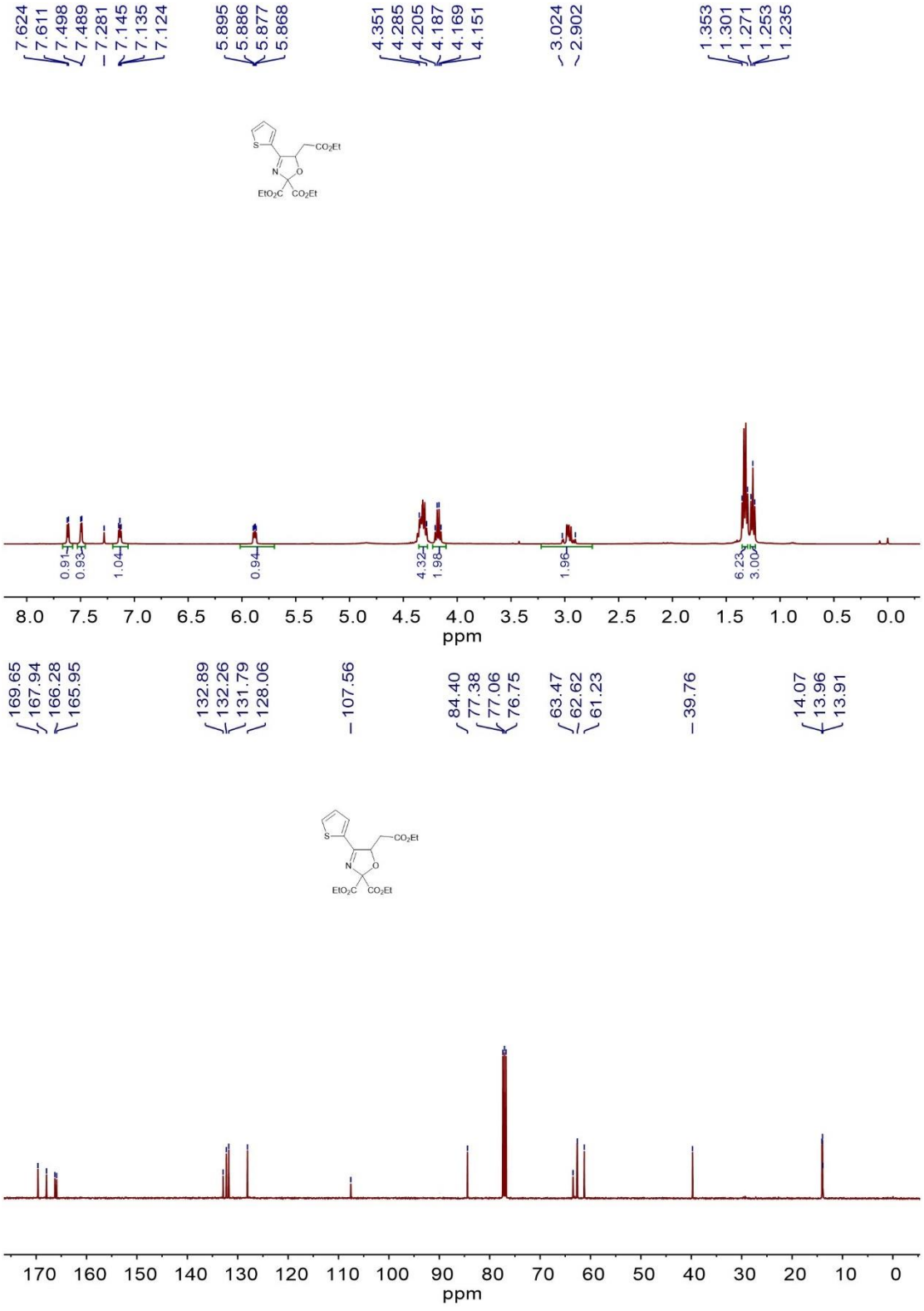
Diethyl 5-(2-ethoxy-2-oxoethyl)-4-(3-methoxyphenyl)oxazole-2,2(5H)-dicarboxylate (3jc)



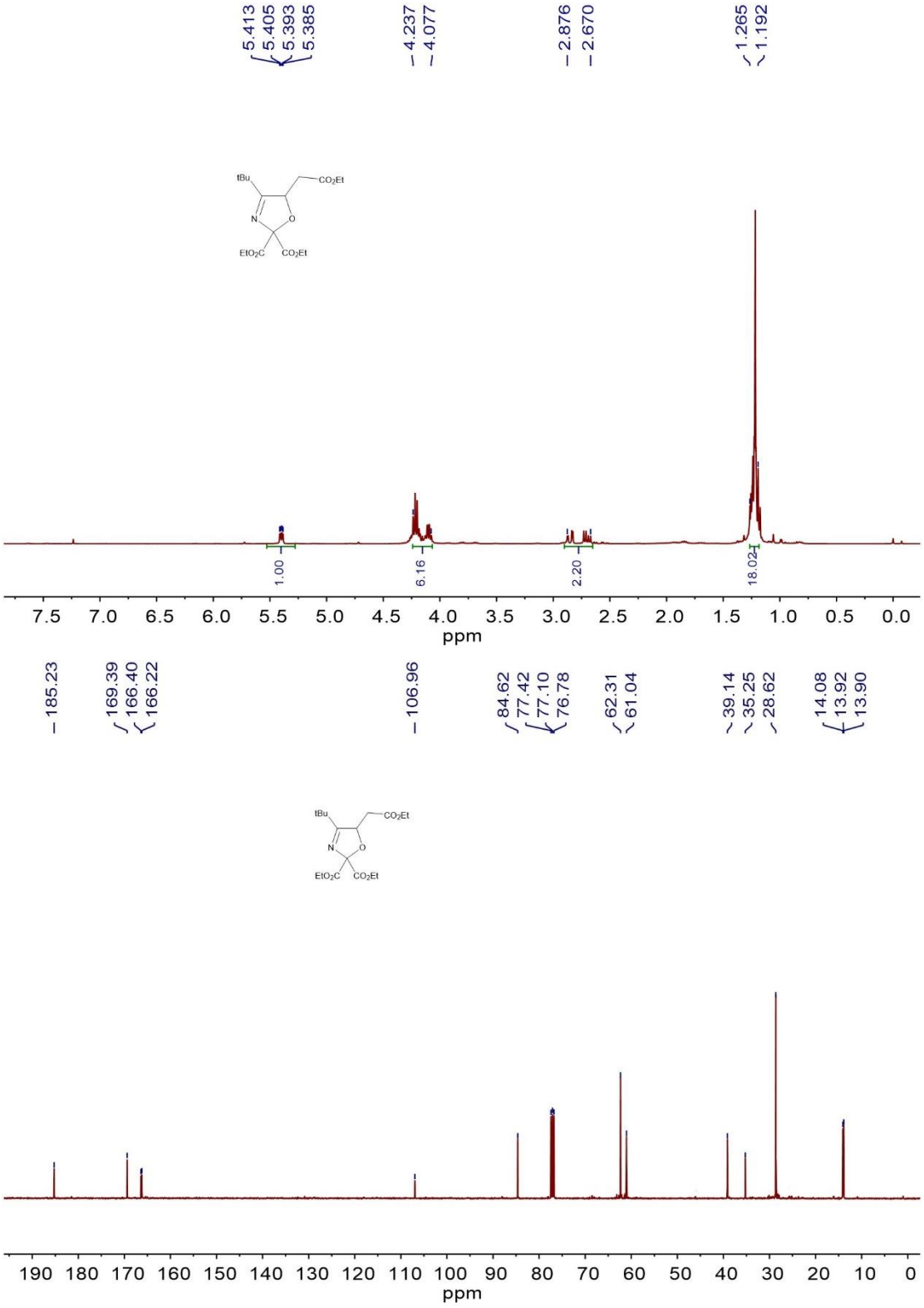
Diethyl 5-(2-ethoxy-2-oxoethyl)-4-(2-methoxyphenyl)oxazole-2,2(5H)-dicarboxylate (3lc)



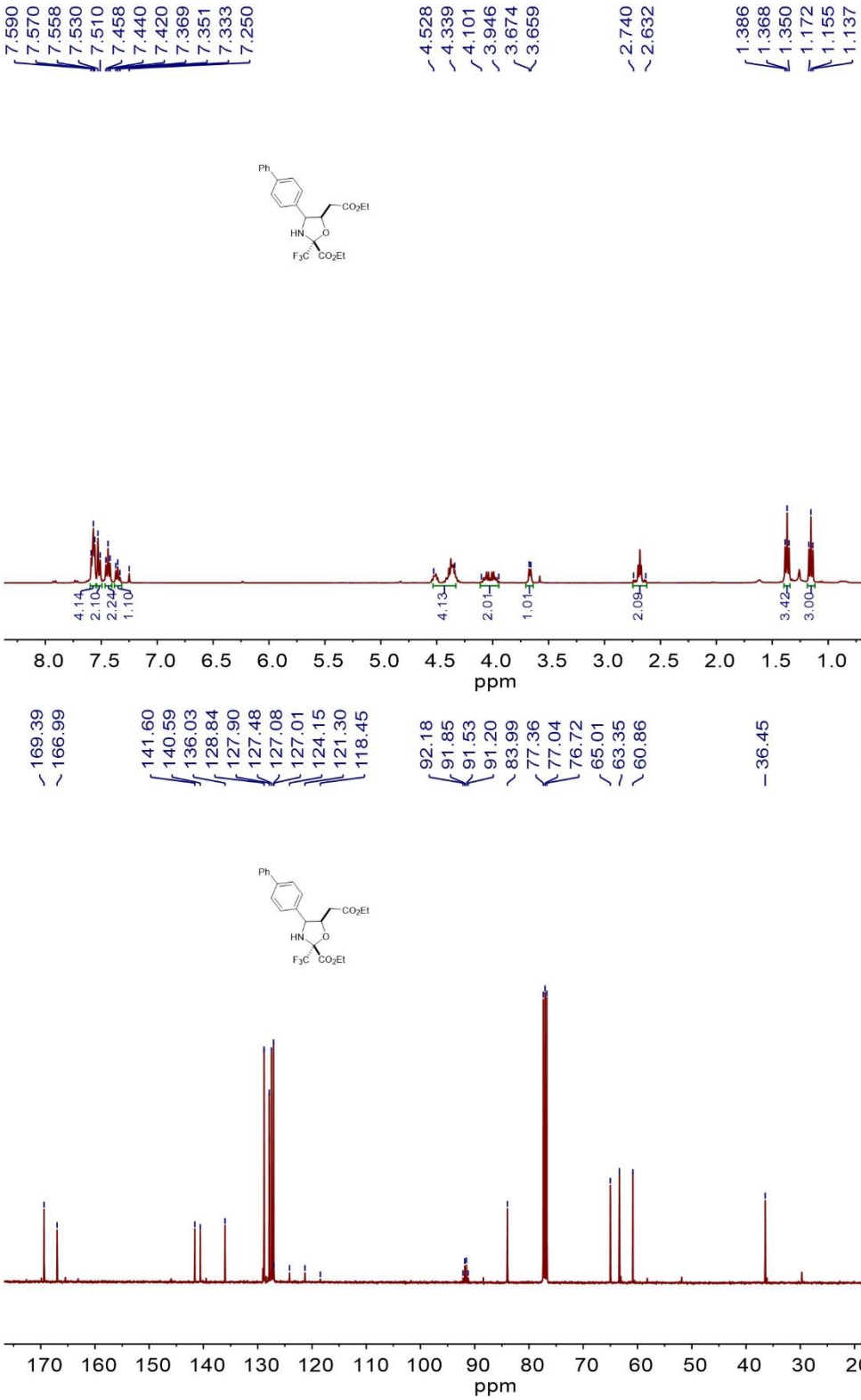
Diethyl 5-(2-ethoxy-2-oxoethyl)-4-(thiophen-2-yl)oxazole-2,2(5H)-dicarboxylate (3pc)

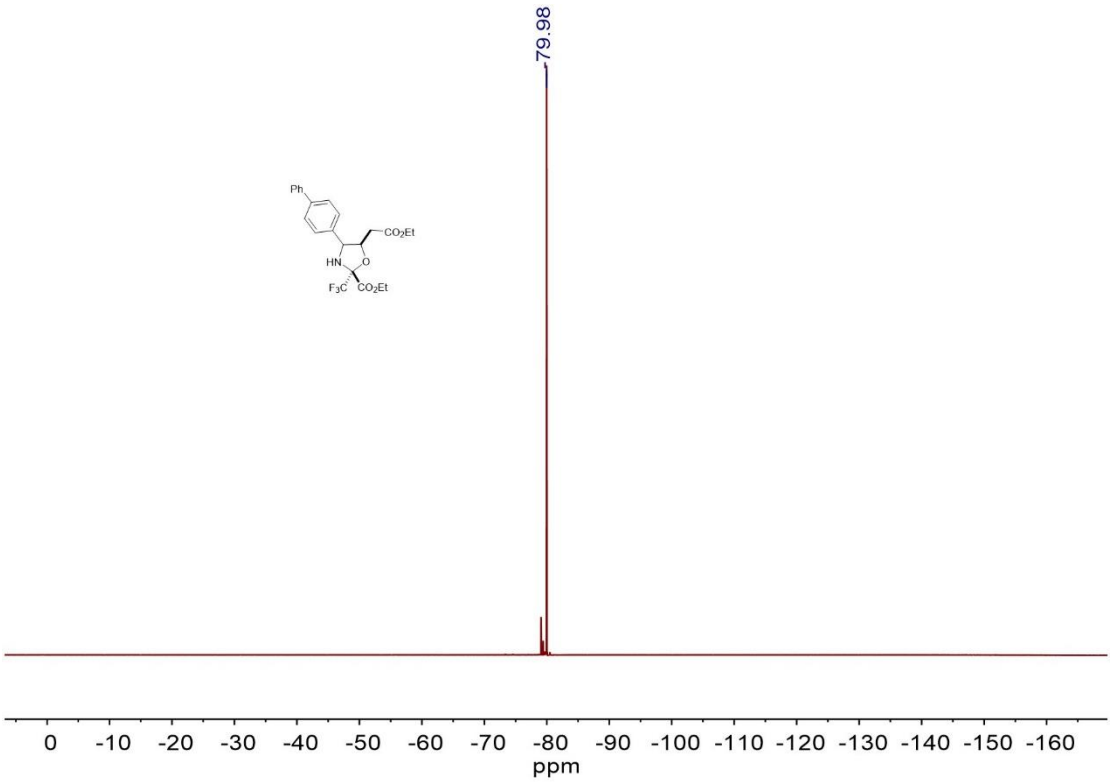


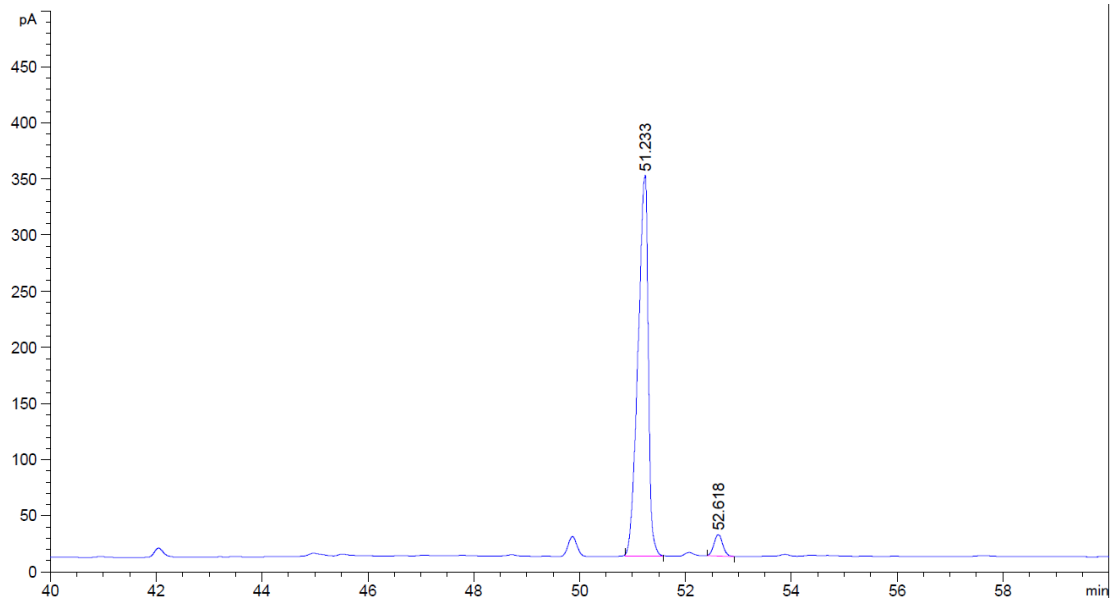
Diethyl 4-(tert-butyl)-5-(2-ethoxy-2-oxoethyl)oxazole-2,2(5H)-dicarboxylate (3qc)



Ethyl (2*R*,5*R*)-4-([1,1'-biphenyl]-4-yl)-5-(2-ethoxy-2-oxoethyl)-2-(trifluoromethyl)oxazolidine-2-carboxylate (4)

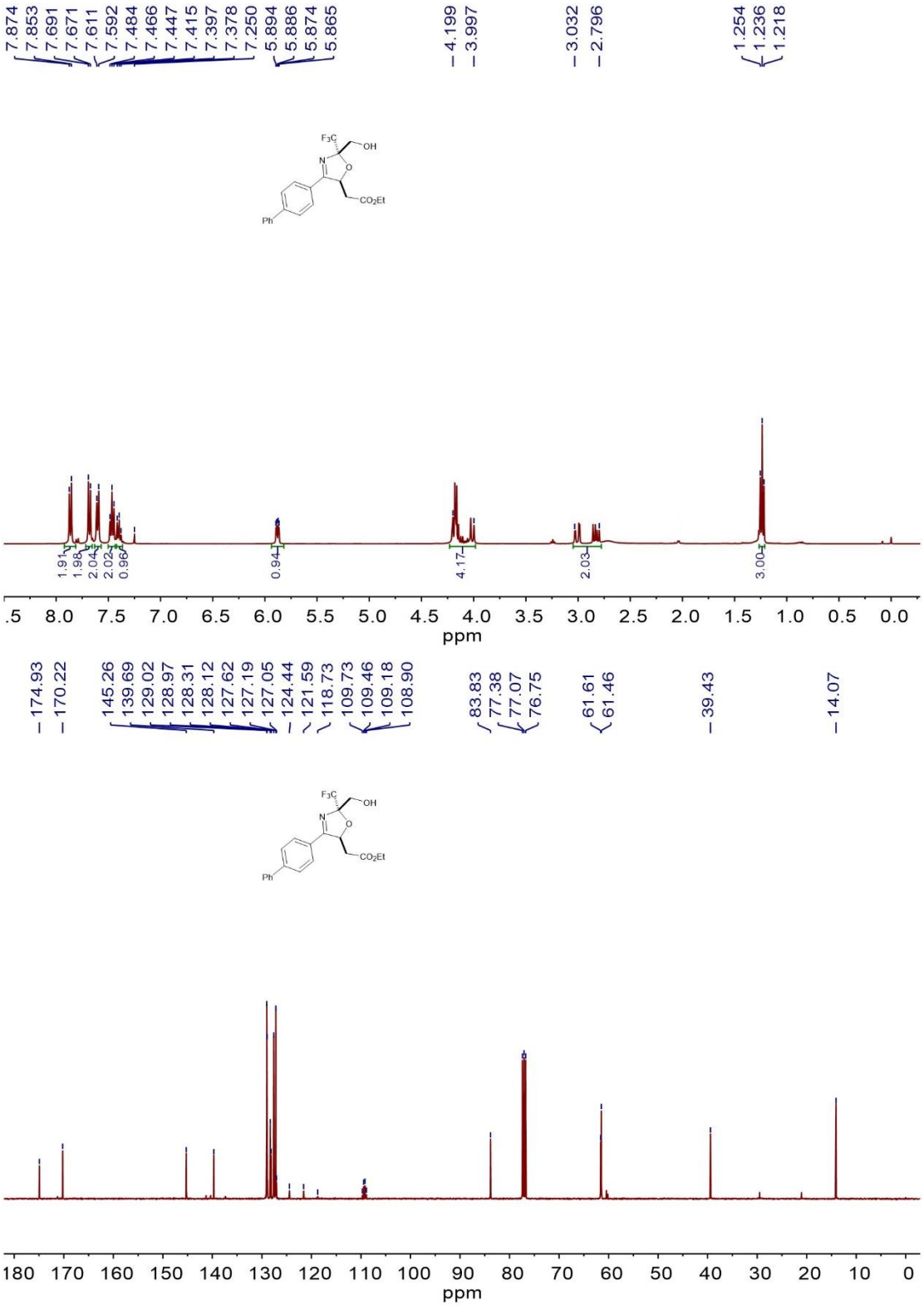


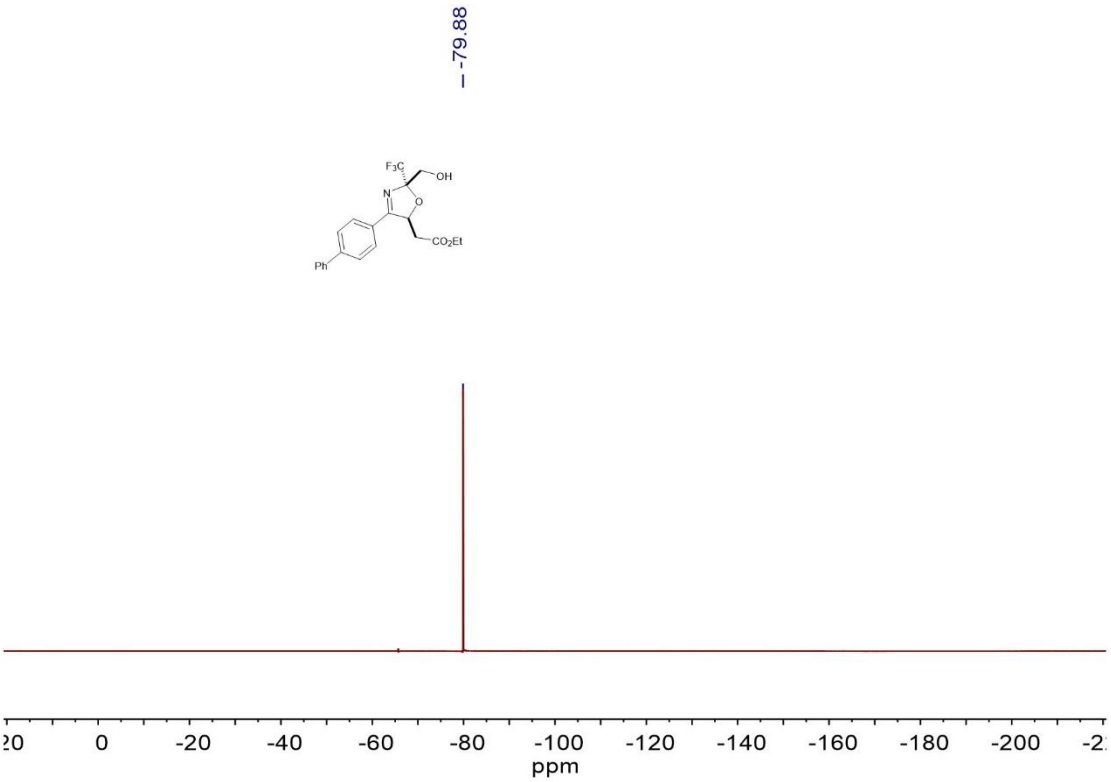


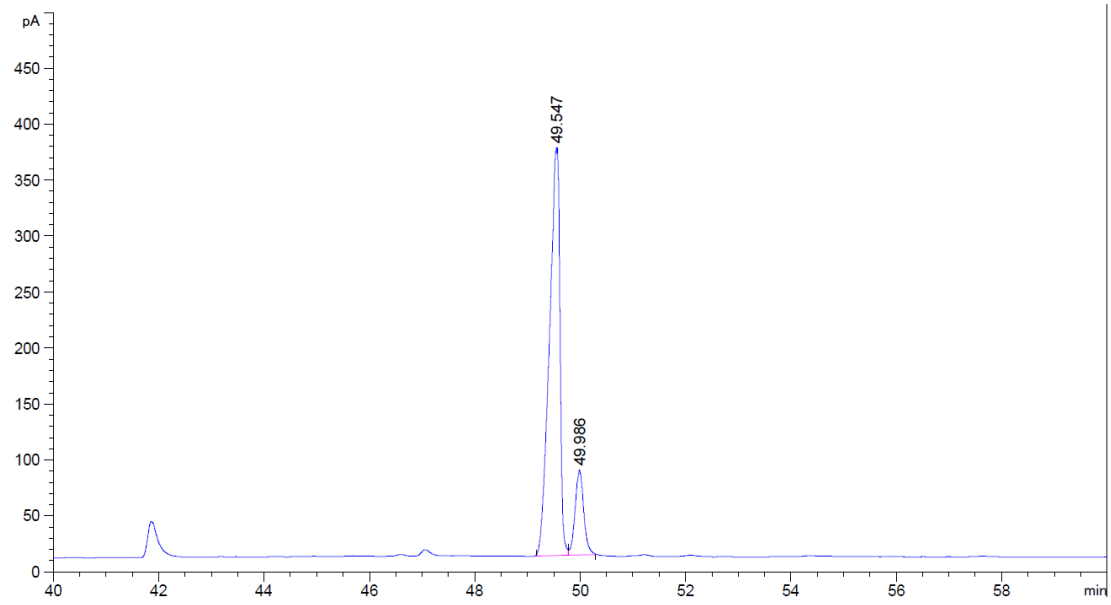


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [pA*s]	峰高 [pA]	峰面积 %
1	51.233	BB	0.1593	4571.69727	339.12363	95.45214
2	52.618	BB	0.1472	217.82051	18.65858	4.54786
总量：				4789.51778	357.78221	

Ethyl 2-4-([1,1'-biphenyl]-4-yl)-2-(hydroxymethyl)-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl)acetate (5)

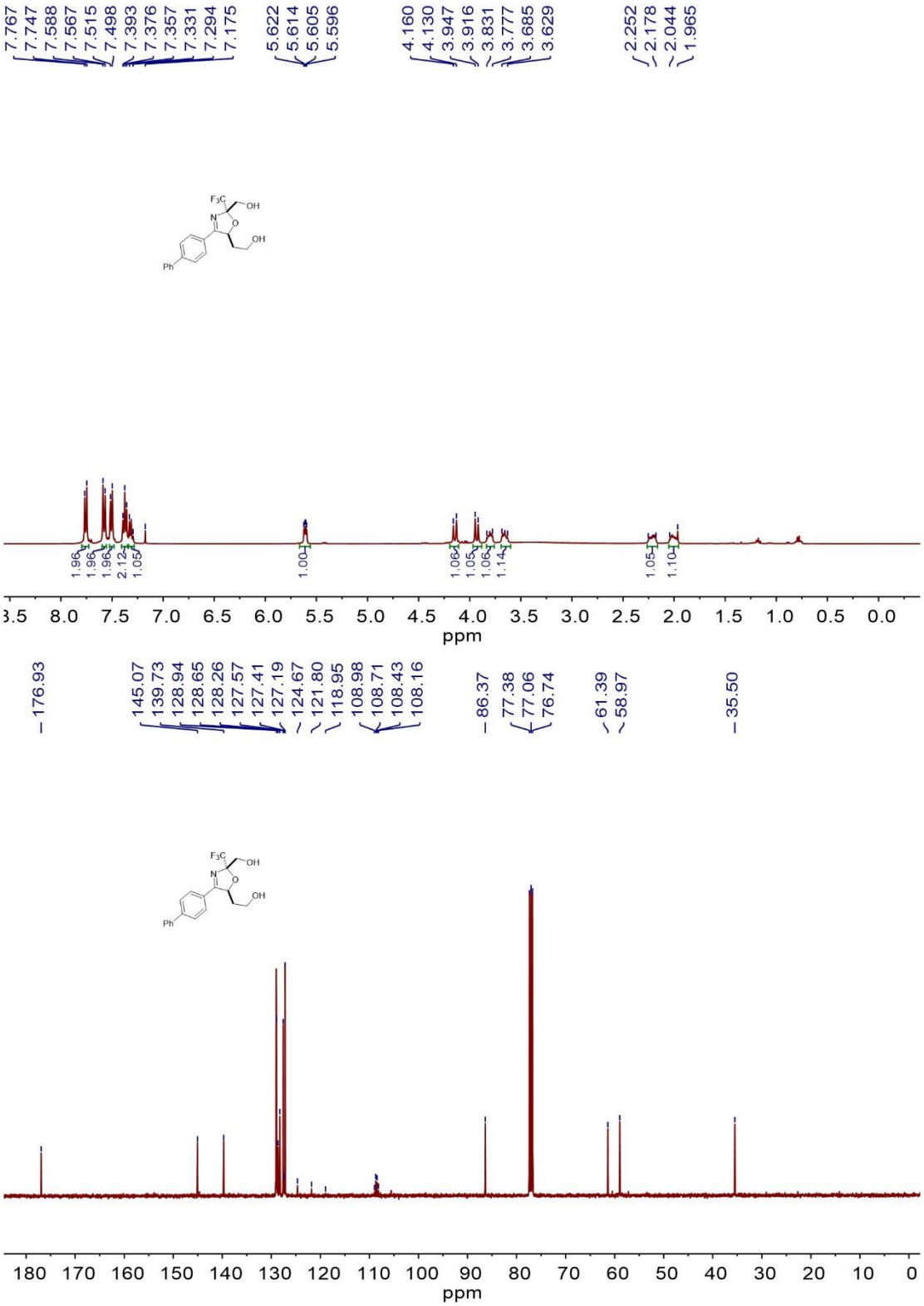


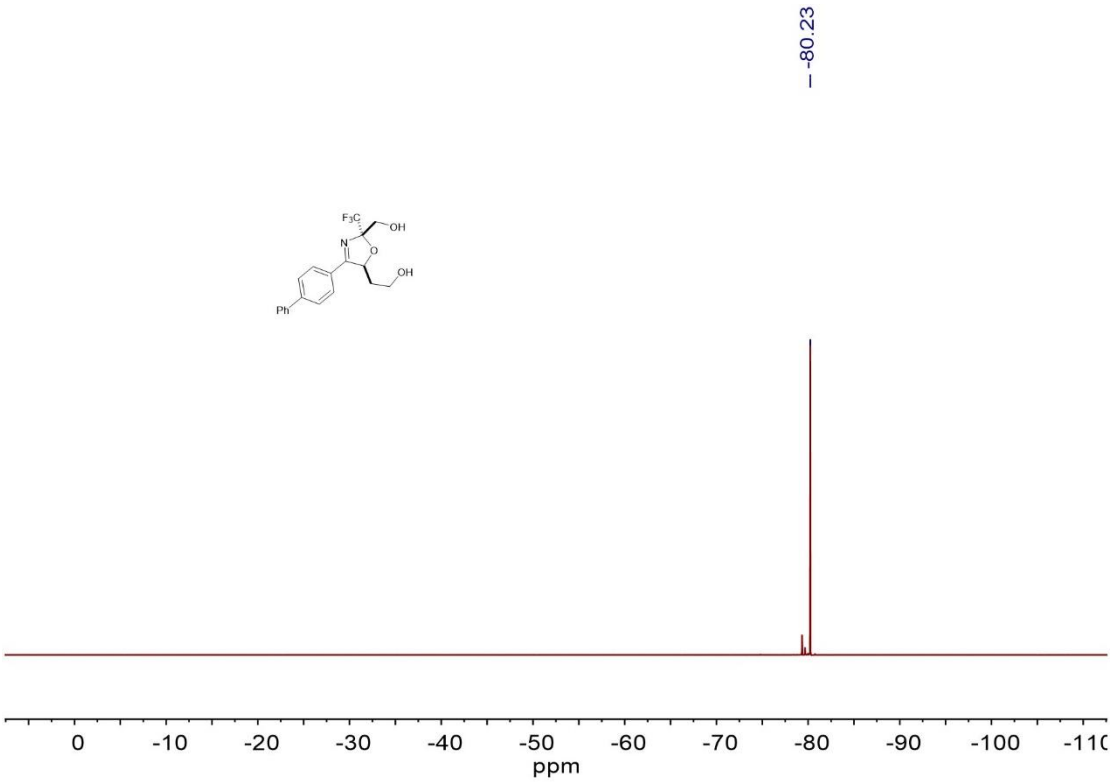


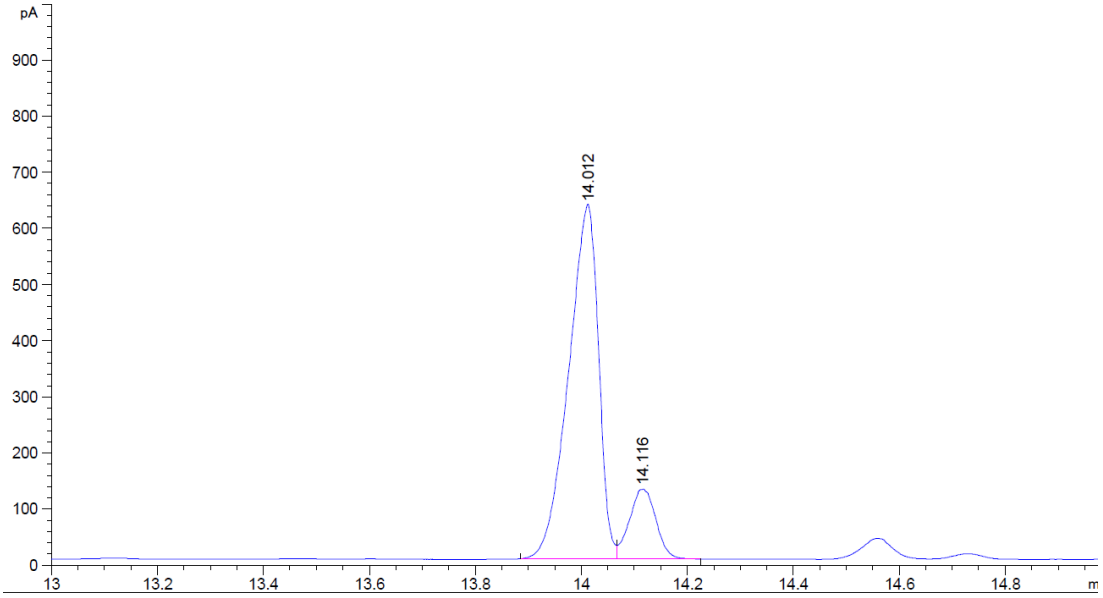


峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [pA*s]	峰高 [pA]	峰面积 %
1	49.547	BV	0.1657	5049.89941	364.35220	85.39638
2	49.986	VB	0.1417	863.58228	75.90038	14.60362
总量 :				5913.48169	440.25259	

2-4-([1,1'-Biphenyl]-4-yl)-2-(hydroxymethyl)-2-(trifluoromethyl)-2,5-dihydrooxazol-5-yl)ethan-1-ol (6)



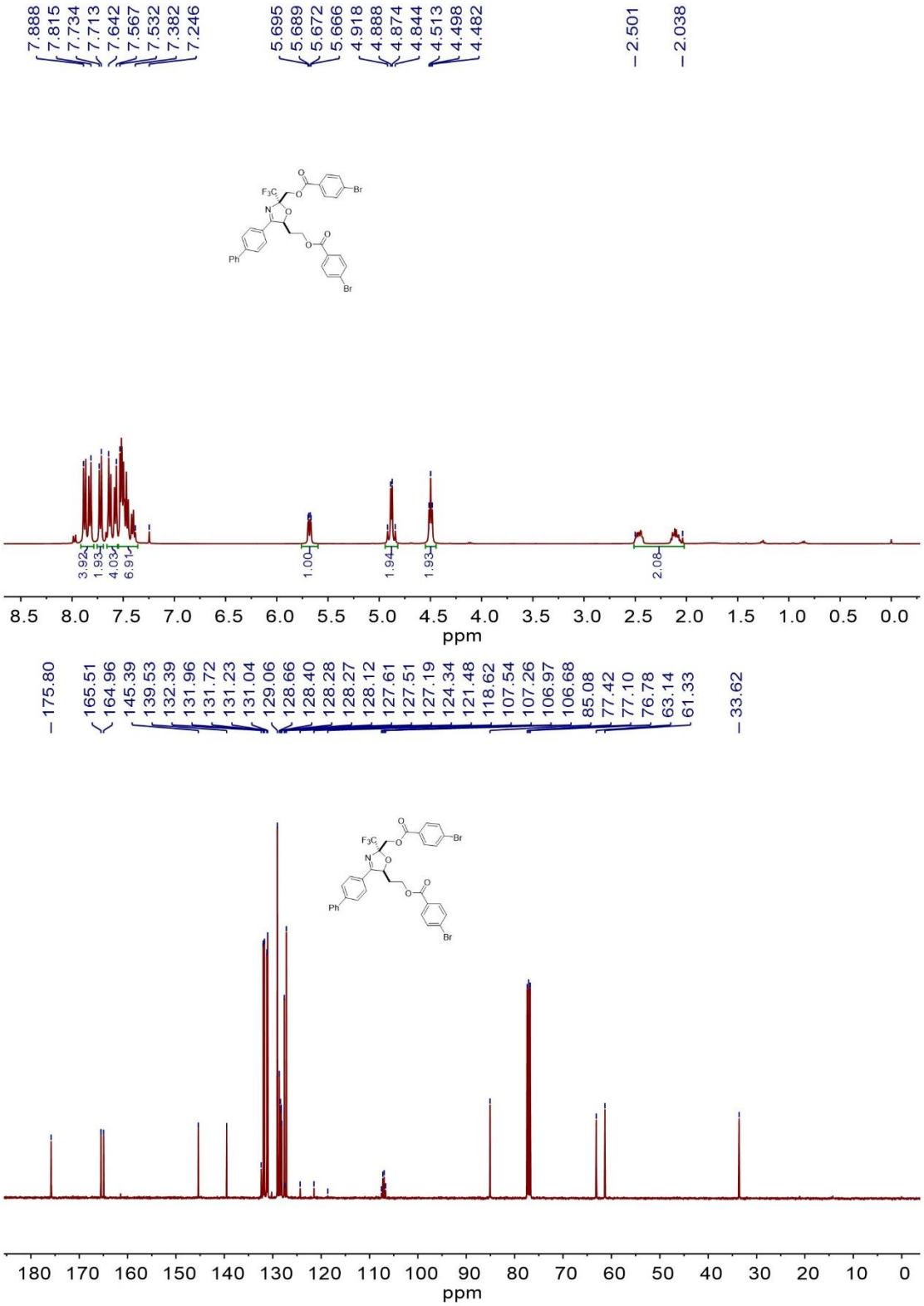


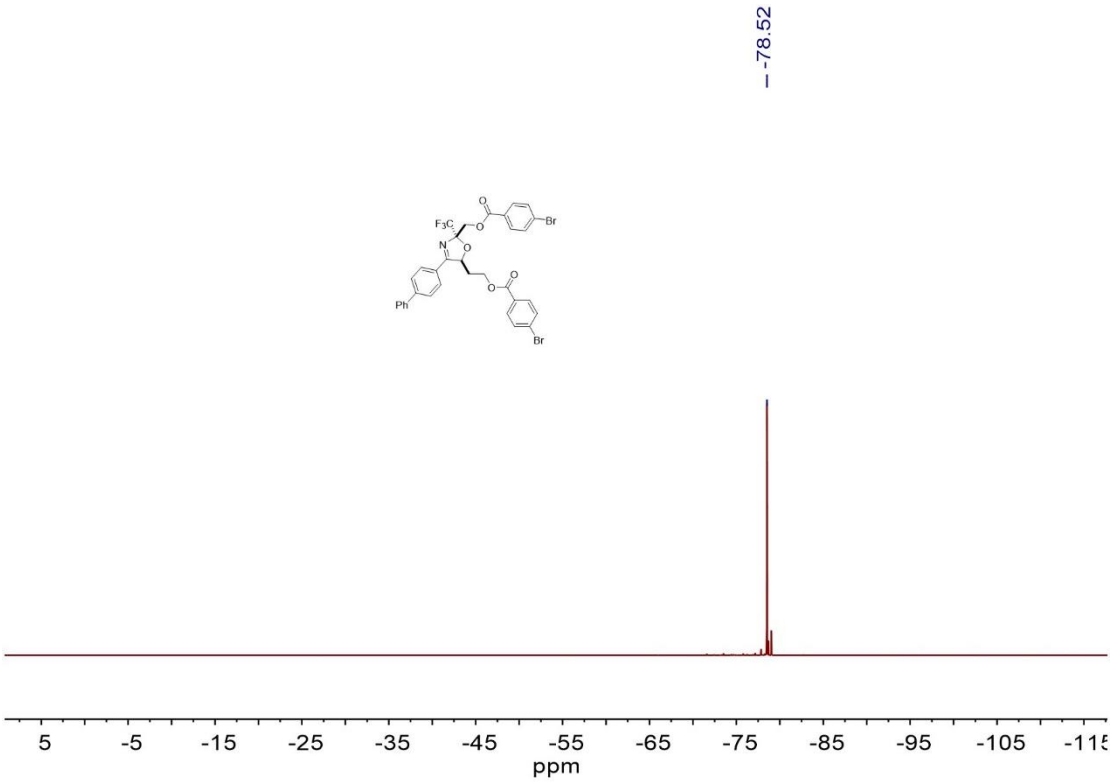


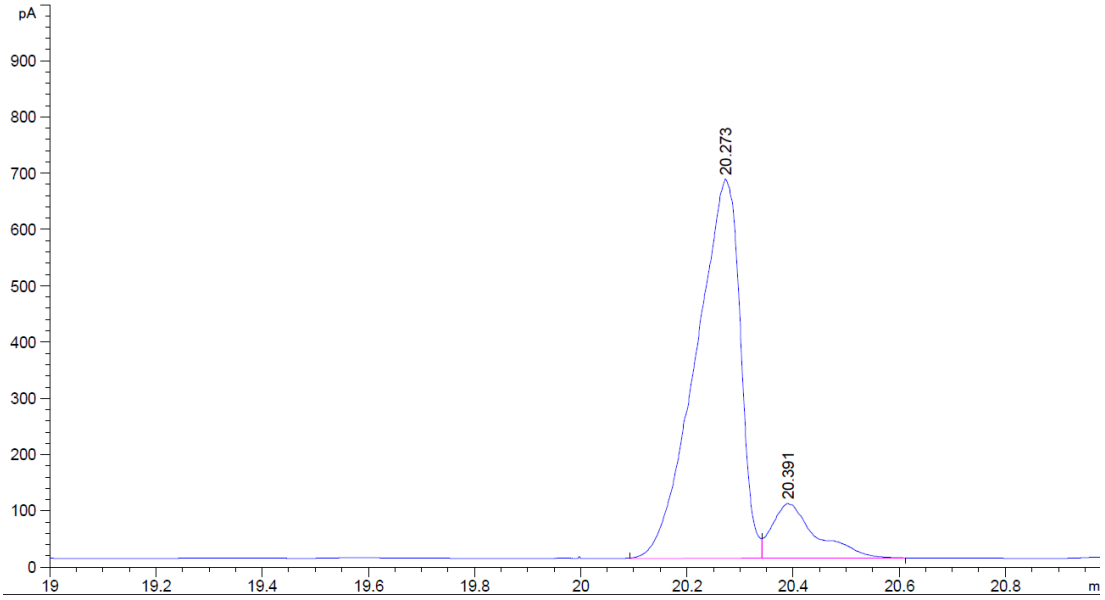
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [pA*s]	峰高 [pA]	峰面积 %
1	14.012	BV	0.0600	2484.77100	629.93262	85.06256
2	14.116	VB	0.0549	436.33899	124.58698	14.93744
总量 :				2921.10999	754.51959	

2-4-([1,1'-Biphenyl]-4-yl)-2-(((4-bromobenzoyl)oxy)methyl)-2-(trifluoromethyl)-2,5-dihydroo

xazol-5-yl)ethyl 4-bromobenzoate (7)







峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [pA*s]	峰高 [pA]	峰面积 %
1	20.273	BV	0.0830	3924.59473	673.43536	87.43310
2	20.391	VB	0.0799	564.08856	96.88893	12.56690
总量：				4488.68329	770.32430	

Crystal Structure and data for compound 7

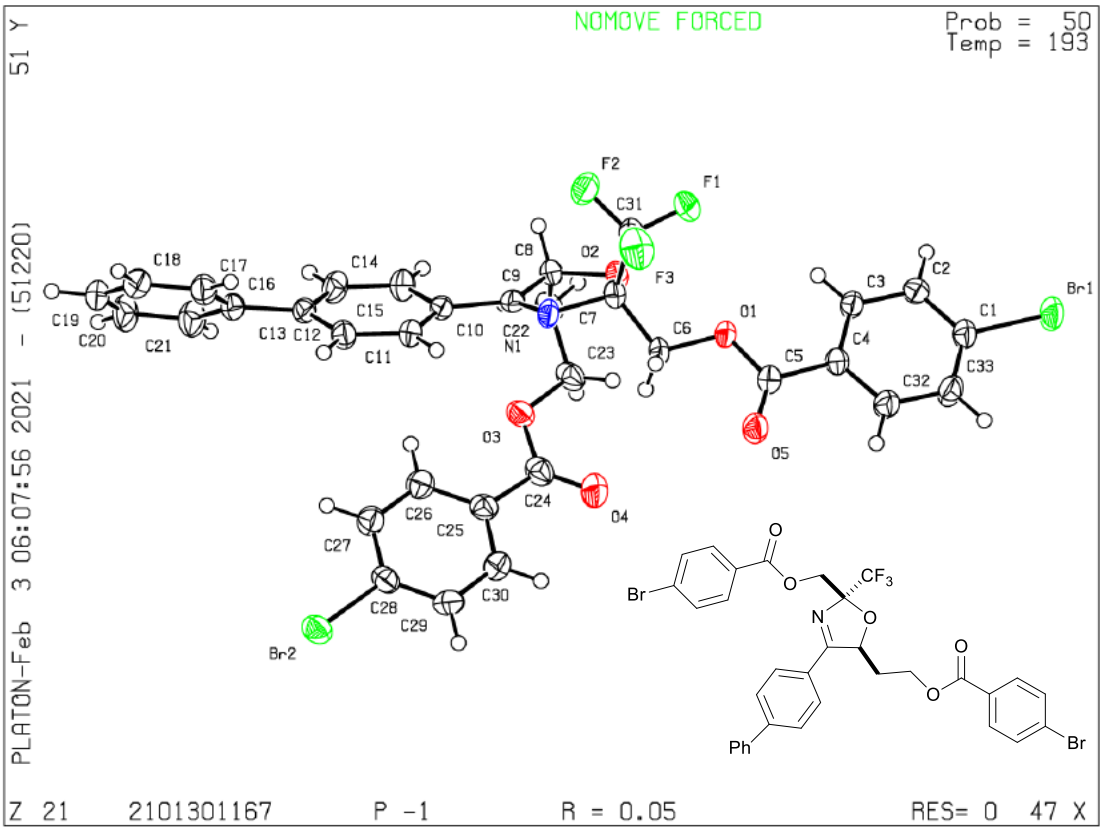


Table 1. Crystal data and structure refinement for **7**

Identification code	2101301167	
Empirical formula	C33 H24 Br2 F3 N O5	
Formula weight	731.35	
Temperature	193.01 K	
Wavelength	1.34139 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.3047(2) Å	a= 73.9880(10)°.
	b = 9.9702(2) Å	b= 80.7730(10)°.
	c = 17.0352(4) Å	g = 80.4190(10)°.
Volume	1486.89(6) $Å^3$	
Z	2	
Density (calculated)	1.634 Mg/m^3	
Absorption coefficient	2.736 mm^{-1}	
F(000)	732	
Crystal size	0.08 x 0.05 x 0.03 mm^3	
Theta range for data collection	4.047 to 54.932°.	
Index ranges	-11<=h<=11, -12<=k<=12, -20<=l<=20	
Reflections collected	17604	
Independent reflections	5621 [R(int) = 0.0541]	
Completeness to theta = 53.594°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7508 and 0.5632	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5621 / 0 / 397	
Goodness-of-fit on F^2	1.032	
Final R indices [I>2sigma(I)]	R1 = 0.0465, wR2 = 0.0957	
R indices (all data)	R1 = 0.0723, wR2 = 0.1098	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.879 and -0.815 $e.Å^{-3}$	