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# Supporting Information

# Multifunctional Odorless Isocyano(triphenylphosphoranylidene)-acetates: Synthesis and Direct One-Pot Four-Component Ugi/Wittig Cyclization to Multisubstituted Oxazoles

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## Content

## 1. General Information:

Reactions were generally carried out in an appropriate round bottom flask with magnetic stirring. Unless otherwise noted, materials were purchased from commercial suppliers and used without further purification. Dichloromethane was used after distillation. Column chromatography purifications were performed under "flash" conditions using 400–630 mesh silica gel. Analytical thin-layer chromatography (TLC) was carried out on silica gel 60 F254 plates, which were visualized by exposure to ultraviolet light. Melting points were uncorrected. HRMS was measured on an Agilent 6224 TOF LC/MS spectrometer. NMR spectra were recorded in $CDCl_3$ on a Varian Mercury 600 spectrometer and resonances were relative to TMS. Data are reported as follows: chemical shift, multiplicity (s = single, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz) and integration. $^{13}C$ NMR spectra were recorded on a Varian Mercury 600 (150 MHz) with complete proton decoupling spectrophotometers ($CDCl_3$: 77.0 ppm).

## 2. Experimental Procedures and Characterization Data

### General procedure for the preparation of 3a-b.

Anhydrous $CH_2Cl_2$ (50 mL), $PPh_3$ (39 mmol, 10.2 g), $NEt_3$ (78 mmol, 7.9 g) and α-isocyano ester **2** (30 mmol) were placed in a reaction flask which had been dried with a heat-gun under high-vacuum. The homogeneous mixture was then cooled to 10-15 °C, and $CCl_4$ (39 mmol, 6.0 g) in dry $CH_2Cl_2$ (10 mL) was added dropwise over a period of about 30 minutes. The mixture was kept at the temperature for 8-12 h while the reaction progress was monitored by TLC. Upon completion of the reaction, the mixture was concentrated by rotary evaporation. Purification by silica flash chromatography with EtOAc/petroleum ether (1:3) as the eluent afforded the desired products **3**.

### Characterization Data

**3a: ethyl 2-isocyano-2-(triphenyl-λ$^5$-phosphanylidene)acetate**

White solid, yield 58%, mp 185-186 °C; $^1H$ NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.66-7.53 (m, 15H, Ar-H), 4.15 (q, $J$ = 6.6 Hz, 1.34H, 0.67$OCH_2$), 3.82 (q, $J$ = 7.2 Hz, 0.66H, 0.33$OCH_2$), 1.29 (t, $J$ = 6.6 Hz, 2H, 0.67$CH_3$), 0.54 (t, $J$ = 6.6 Hz, 1H, 0.33$CH_3$); $^{13}C$ NMR ($CDCl_3$, 150 MHz) δ (ppm) 168.7 (d, $^2J_{PC}$ = 23.6 Hz), 167.5 (Minor, d, $^2J_{PC}$ = 18.3 Hz), 162.0, 160.4 (Minor), 133.6, 133.5, 132.9, 129.0, 128.9, 124.1, 123.6, 123.0, 59.3, 58.5 (Minor), 49.8 (d, $^1J_{PC}$ = 157.7 Hz), 14.8, 13.8 (Minor); HRMS calculated for $[C_{23}H_{20}NO_2P+Na]^+$: 396.1124, found: 396.1129.

**3b: methyl 2-isocyano-2-(triphenyl-λ$^5$-phosphanylidene)acetate**

White solid, yield 53%, mp 191-192 °C; $^1H$ NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.66-7.52 (m, 15H, Ar-H), 3.71 (s, 2.4H, 0.8$CH_3$), 3.25 (s, 0.6H, 0.2$CH_3$); $^{13}C$ NMR ($CDCl_3$, 150 MHz) δ (ppm) 168.9 (d, $^2J_{PC}$ = 23.9 Hz), 162.1, 133.6, 133.5, 133.0, 129.0, 128.9, 123.3, 122.7, 50.8, 49.71 (Minor), 49.69 (d, $^1J_{PC}$ = 156.3 Hz); HRMS calculated for $[C_{22}H_{18}NO_2P+H]^+$: 360.1148, found: 360.1150.

### General procedure for the synthesis of 7a-q by using secondary amines.

To a magnetically stirred solution of aldehyde **4** (1 mmol), amine **5** (1 mmol) and isocyanide **3** (1 mmol) in anhydrous $CH_2Cl_2$ (5 mL) was added slowly a solution of acid **6** (1 mmol) in $CH_2Cl_2$ (5 mL) at room temperature. The mixture was stirred for 12-24 h, and the reaction progress was monitored by TLC. After completion, the $CH_2Cl_2$ solution was evaporated under reduced pressure, the residue was purified by silica gel chromatography with EtOAc/petroleum ether (1:15) as the eluent to afford products **7a-q**.

### Characterization Data

**7a: ethyl 2-((4-chlorophenyl)(diethylamino)methyl)-5-(4-fluorophenyl)oxazole-4-carboxylate**

Light yellow oil, yield 87%; $^1$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 8.05 (dd, $J_1$ = 5.4 Hz, $J_2$ = 8.4 Hz, 2H, Ar-H), 7.47 (d, $J$ = 8.4 Hz, 2H, Ar-H), 7.32 (d, $J$ = 8.4 Hz, 2H, Ar-H), 7.15 (t, $J$ = 8.4 Hz, 2H, Ar-H), 5.20 (s, 1H, CH), 4.43 (q, $J$ = 6.6 Hz, 2H, $OCH_2$), 2.70-2.53 (m, 4H, $2NCH_2$), 1.39 (t, $J$ = 7.2 Hz, 3H, $CH_3$), 1.03 (t, $J$ = 7.2 Hz, 6H, $2CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 164.5, 162.8, 162.1, 161.5, 154.9, 136.8, 133.7, 132.3, 130.7, 129.6, 128.7, 126.4, 123.2, 115.6, 63.4, 61.4, 43.8, 14.3, 11.9; HRMS calculated for $[C_{23}H_{24}ClFN_2O_3+Na]^+$: 453.1352, found: 453.1356.

**7b: methyl 5-(2-bromophenyl)-2-((4-chlorophenyl)(diethylamino)methyl)oxazole-4-carboxylate**

Light yellow oil, yield 81%; $^1$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.68 (d, $J$ = 8.4 Hz, 1H, Ar-H), 7.48-7.29 (m, 7H, Ar-H), 5.22 (s, 1H, CH), 3.82 (s, 3H, $OCH_3$), 2.71-2.54 (m, 4H, $2NCH_2$), 1.02 (t, $J$ = 6.6 Hz, 6H, $2CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 162.9, 161.6, 154.7, 136.6, 133.6, 133.0, 132.5, 131.7, 129.7, 128.8, 128.7, 128.5, 126.9, 123.5, 63.3, 52.1, 43.6, 11.8; HRMS calculated for $[C_{22}H_{22}BrClN_2O_3+H]^+$: 477.0575, found: 477.0600.

**7c: ethyl 5-(4-bromophenyl)-2-((diethylamino)(phenyl)methyl)oxazole-4-carboxylate**

White solid, yield 86%, mp 65-66 °C; $^1$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.93 (d, $J$ = 7.8 Hz, 2H, Ar-H), 7.58 (d, $J$ = 8.4 Hz, 2H, Ar-H), 7.50 (d, $J$ = 6.6 Hz, 2H, Ar-H), 7.35-7.28 (m, 3H, Ar-H), 5.22 (s, 1H, CH), 4.42 (q, $J$ = 6.0 Hz, 2H, $OCH_2$), 2.70-2.56 (m, 4H, $2NCH_2$), 1.39 (t, $J$ = 6.6 Hz, 3H, $CH_3$), 1.02 (t, $J$ = 6.6 Hz, 6H, $2CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 162.4, 162.1, 154.6, 138.1, 131.5, 129.9, 128.4, 128.3, 127.9, 126.9, 125.9, 124.6, 64.1, 61.4, 43.7, 14.3, 11.8; HRMS calculated for $[C_{23}H_{25}BrN_2O_3+H]^+$: 457.1121, found: 457.1144.

**7d: ethyl 2-((3-bromophenyl)(dibenzylamino)methyl)-5-(4-chlorophenyl)oxazole-4-carboxylate**

Light yellow oil, yield 78 %; $^1$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.91 (d, $J$ = 7.8 Hz, 2H, Ar-H), 7.69 (s, 1H, Ar-H), 7.46-7.20 (m, 15H, Ar-H), 5.24 (s, 1H, CH), 4.45 (q, $J$ = 6.6 Hz, 2H, $OCH_2$), 3.79 (d, $J$ = 14.4 Hz, 2H, $2CH_2^a$), 3.66 (d, $J$ = 13.8 Hz, 2H, $2CH_2^b$), 1.42 (t, $J$ = 7.2 Hz, 3H, $CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 162.0, 160.2, 154.6, 139.8, 138.4, 136.4, 131.5, 131.2, 130.1, 129.7, 128.7, 128.6, 128.3, 127.2, 127.1, 125.2, 122.7, 62.0, 61.5, 55.0, 14.3; HRMS calculated for $[C_{33}H_{28}BrClN_2O_3+Na]^+$: 637.0864, found: 637.0870.

**7e: ethyl 2-((4-chlorophenyl)(diethylamino)methyl)-5-phenyloxazole-4-carboxylate**

Light yellow oil, yield 88%; $^1$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 8.00 (d, $J$ = 6.0 Hz, 2H, Ar-H), 7.46-7.30 (m, 7H, Ar-H), 5.21 (s, 1H, CH), 4.42 (q, $J$ = 6.6 Hz, 2H, $OCH_2$), 2.69-2.54 (m, 4H, $2NCH_2$), 1.39 (t, $J$ = 6.6 Hz, 3H, $CH_3$), 1.02 (t, $J$ = 6.6 Hz, 6H, $2CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 162.0, 161.6, 155.7, 136.8, 133.5, 130.2, 129.5, 128.6, 128.4, 128.3, 126.9, 126.6, 63.3, 61.3, 43.7, 14.2, 11.9; HRMS calculated for $[C_{23}H_{25}ClN_2O_3+Na]^+$: 435.1446, found: 435.1449.

**7f: ethyl 5-(furan-2-yl)-2-(phenyl(piperidin-1-yl)methyl)oxazole-4-carboxylate**

Light yellow oil, yield 77%; $^1$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.60-7.27 (m, 8H, Ar-H), 6.57 (s, 1H, Ar-H), 4.76 (s, 1H, CH), 4.44 (q, $J$ = 6.6 Hz, 2H, $OCH_2$), 2.50-2.33 (m, 4H, $2NCH_2$), 1.60-1.40 (m, 9H, $3CH_2$ and $CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 161.5, 161.4, 147.4, 144.3, 142.1, 137.2, 128.5, 128.4, 127.9, 125.1, 115.2, 112.1, 69.1, 61.2, 52.5, 25.8, 24.2, 14.3; HRMS calculated for $[C_{22}H_{24}N_2O_4+Na]^+$: 403.1628, found: 403.1635.

**7g: ethyl 2-((diethylamino)(4-fluorophenyl)methyl)-5-(furan-2-yl)oxazole-4-carboxylate**

Light yellow oil, yield 79%; $^1$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.59-7.49 (m, 4H, Ar-H), 7.02 (t, $J$ = 7.8 Hz, 2H, Ar-H), 6.57 (s, 1H, Ar-H), 5.20 (s, 1H, CH), 4.44 (q, $J$ = 6.6 Hz, 2H, $OCH_2$), 2.68-2.57 (m, 4H, $2NCH_2$), 1.42 (t, $J$ = 6.6 Hz, 3H, $CH_3$), 1.02 (t, $J$ = 8.4 Hz, 6H, $2CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 163.1, 161.5, 161.4, 147.4, 144.4, 142.0, 133.7, 129.9, 129.8, 125.0, 115.3, 115.2, 115.1, 112.1, 63.1, 61.2, 43.6, 14.3, 11.8; HRMS calculated for $[C_{21}H_{23}FN_2O_4+Na]^+$: 409.1534, found: 409.1547.

**7h: ethyl 5-(4-chlorophenyl)-2-((dibenzylamino)(4-fluorophenyl)methyl)oxazole-4-carboxylate**

Light yellow oil, yield 82%; $^{1}$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.91 (d, *J* = 7.8 Hz, 2H, Ar-H), 7.52-7.05 (m, 16H, Ar-H), 5.25 (s, 1H, CH), 4.44 (q, *J* = 6.6 Hz, 2H, $OCH_2$), 3.78 (d, *J* = 13.8 Hz, 2H, $2CH_2^a$), 3.67 (d, *J* = 14.4 Hz, 2H, $2CH_2^b$), 1.41 (t, *J* = 6.6 Hz, 3H, $CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 163.2, 162.0, 161.6, 160.8, 154.4, 138.6, 136.3, 133.1, 130.2, 130.1, 129.7, 128.7, 128.6, 128.3, 127.1, 125.3, 115.5, 115.4, 61.9, 61.5, 54.9, 14.3; HRMS calculated for $[C_{33}H_{28}ClFN_2O_3 +H]^+$: 555.1845, found: 555.1854.

**7i: ethyl 5-(4-bromophenyl)-2-((4-chlorophenyl)(piperidin-1-yl)methyl)oxazole-4-carboxylate**

Light yellow oil, yield 80%; $^{1}$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.92 (d, *J* = 8.4 Hz, 2H, Ar-H), 7.59 (d, *J* = 8.4 Hz, 2H, Ar-H), 7.49 (d, *J* = 7.8 Hz, 2H, Ar-H), 7.32 (d, *J* = 7.8 Hz, 2H, Ar-H), 4.75 (s, 1H, CH), 4.42 (q, *J* = 3.6 Hz, 2H, $OCH_2$), 2.47-1.38 (m, 13H, $5CH_2$ and $CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 161.9, 161.4, 154.8, 135.9, 133.9, 131.6, 129.9, 129.7, 128.8, 127.0, 125.8, 124.8, 68.4, 61.5, 52.5, 25.9, 24.2, 14.3; HRMS calculated for $[C_{24}H_{24}BrClN_2O_3 +H]^+$: 503.0732, found: 503.0748.

**7j: ethyl 2-((4-chlorophenyl)(diethylamino)methyl)-5-(p-tolyl)oxazole-4-carboxylate**

Light yellow oil, yield 82%; $^{1}$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.90 (d, *J* = 6.6 Hz, 2H, Ar-H), 7.44 (d, *J* = 7.2 Hz, 2H, Ar-H), 7.31-7.26 (m, 4H, Ar-H), 5.19 (s, 1H, CH), 4.42 (q, *J* = 6.6 Hz, 2H, $OCH_2$), 2.67-2.54 (m, 4H, $2NCH_2$), 2.40 (s, 3H, $CH_3$), 1.38 (t, *J* = 7.2 Hz, 3H, $CH_3$), 1.02 (t, *J* = 7.2 Hz, 6H, $2CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 162.2, 161.3, 156.1, 140.6, 137.0, 133.6, 129.6, 129.0, 128.6, 128.4, 126.1, 124.2, 63.3, 61.3, 43.8, 21.5, 14.3, 12.0; HRMS calculated for $[C_{24}H_{27}ClN_2O_3 +Na]^+$: 449.1602, found: 449.1605.

**7k: ethyl 2-((4-chlorophenyl)(dipropylamino)methyl)-5-(p-tolyl)oxazole-4-carboxylate**

Light yellow oil, yield 78%; $^{1}$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.91 (d, *J* = 7.8 Hz, 2H, Ar-H), 7.39 (d, *J* = 7.8 Hz, 2H, Ar-H), 7.30-7.26 (m, 4H, Ar-H), 5.23 (s, 1H, CH), 4.42 (q, *J* = 7.2 Hz, 2H, $OCH_2$), 2.56-2.41 (m, 7H, $2CH_2$ and $CH_3$), 1.50-1.38 (m, 7H, $2CH_2$ and $CH_3$), 0.82 (t, *J* = 7.2 Hz, 6H, $2CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 162.2, 161.2, 156.0, 140.6, 137.1, 133.4, 132.0, 129.8, 129.0, 128.4, 128.3, 126.0, 124.2, 63.2, 61.2, 52.6, 21.4, 20.5, 14.3, 11.6; HRMS calculated for $[C_{26}H_{31}ClN_2O_3 +Na]^+$: 477.1915, found: 477.1920.

**7l: ethyl 2-((dibenzylamino)(4-fluorophenyl)methyl)-5-(p-tolyl)oxazole-4-carboxylate**

Light yellow oil, yield 81%; $^{1}$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.87 (d, *J* = 8.4 Hz, 2H, Ar-H), 7.50 (t, *J* = 8.4 Hz, 2H, Ar-H), 7.37-7.20 (m, 12H, Ar-H), 7.05 (t, *J* = 8.4 Hz, 2H, Ar-H), 5.26 (s, 1H, CH), 4.44 (q, *J* = 7.2 Hz, 2H, $OCH_2$), 3.82 (d, *J* = 13.8 Hz, 2H, $2CH_2^a$), 3.64 (d, *J* = 13.8 Hz, 2H, $2CH_2^b$), 2.41 (s, 3H, $CH_3$), 1.41 (t, *J* = 7.2 Hz, 3H, $CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 163.1, 162.2, 161.5, 160.3, 155.9, 140.6, 138.7, 133.3, 130.2, 130.1, 129.0, 128.7, 128.4, 128.3, 127.1, 126.3, 124.1, 115.4, 115.3, 61.4, 61.3, 54.9, 21.5, 14.3; HRMS calculated for $[C_{34}H_{31}FN_2O_3 +H]^+$: 535.2391, found: 535.2410.

**7m: ethyl 2-((3-bromophenyl)(diethylamino)methyl)-5-ethyloxazole-4-carboxylate**

Light yellow oil, yield 73%; $^{1}$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.65 (s, 1H, Ar-H), 7.40 (d, *J* = 7.8 Hz, 1H, Ar-H), 7.35 (d, *J* = 7.8 Hz, 1H, Ar-H), 7.19 (t, *J* = 7.8 Hz, 1H, Ar-H), 5.10 (s, 1H, CH), 4.39 (q, *J* = 6.6 Hz, 2H, $OCH_2$), 3.05 (q, *J* = 4.2 Hz, 2H, $CH_2$), 2.65-2.46 (m, 4H, $2CH_2$), 1.39 (t, *J* = 7.2 Hz, 3H, $CH_3$), 1.26 (t, *J* = 7.2 Hz, 3H, $CH_3$), 1.01 (t, *J* = 6.6 Hz, 6H, $2CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 162.1, 161.5, 160.9, 140.8, 131.1, 130.8, 129.8, 126.8, 126.3, 122.4, 63.3, 60.8, 43.7, 19.6, 14.3, 12.0, 11.8; HRMS calculated for $[C_{19}H_{25}BrN_2O_3 +H]^+$: 409.1121, found: 409.1131.

**7n: methyl 2-((benzyl(methyl)amino)(4-bromophenyl)methyl)-5-ethyloxazole-4-carboxylate**

Light yellow oil, yield 71%; $^{1}$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.49-7.25 (m, 9H, Ar-H), 4.90 (s, 1H, CH), 4.38 (q, *J* = 6.6 Hz, 2H, $OCH_2$), 3.56 (d, *J* = 13.2 Hz, 1H, $CH_2^a$), 3.46 (d, *J* = 13.2 Hz, 1H, $CH_2^b$), 3.05 (q, *J* = 7.2 Hz, 2H, $CH_2$), 2.13 (s, 3H, $CH_3$), 1.38 (t, *J* = 7.2 Hz, 3H, $CH_3$), 1.26 (t, *J* = 7.2 Hz, 3H, $CH_3$); $^{13}$C

NMR ($CDCl_3$, 150 MHz) δ (ppm) 162.1, 161.6, 160.5, 138.4, 136.8, 131.6, 130.1, 128.6, 128.2, 127.1, 126.4, 122.0, 66.6, 60.9, 59.0, 39.4, 19.7, 14.3, 12.0; HRMS calculated for $[C_{23}H_{25}BrN_2O_3 +H]^+$: 457.1121, found: 457.1128.

**7o: ethyl 2-((benzyl(methyl)amino)(4-bromophenyl)methyl)-5-(4-(trifluoromethyl)phenyl)oxazole-4-carboxylate**

Light yellow oil, yield 82%; $^1$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 8.14 (d, *J* = 7.2 Hz, 2H, Ar-H), 7.72 (d, *J* = 7.2 Hz, 2H, Ar-H), 7.51-7.24 (m, 9H, Ar-H), 5.01 (s, 1H, CH), 4.44 (q, *J* = 6.0 Hz, 2H, $OCH_2$), 3.65 (d, *J* = 13.8 Hz, 1H, $CH_2^a$), 3.54 (d, *J* = 13.2 Hz, 1H, $CH_2^b$), 2.22 (s, 3H, $CH_3$), 1.41 (t, *J* = 7.2 Hz, 3H, $CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 161.7, 161.6, 154.1, 138.1, 136.4, 131.9, 131.7, 130.1, 128.7, 128.6, 128.4, 128.3, 128.1, 127.2, 125.3, 125.2, 124.6, 122.3, 66.7, 61.7, 59.1, 39.6, 14.3; HRMS calculated for $[C_{28}H_{24}BrF_3N_2O_3 +H]^+$: 573.0995, found: 573.1010.

**7p: methyl 5-(2-bromophenyl)-2-((4-bromophenyl)(diethylamino)methyl)oxazole-4-carboxylate**

Light yellow oil, yield 84%; $^1$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.68 (d, *J* = 7.8 Hz, 1H, Ar-H), 7.48-7.34 (m, 7H, Ar-H), 5.20 (s, 1H, CH), 3.82 (s, 3H, $OCH_3$), 2.71-2.53 (m, 4H, $2NCH_2$), 1.02 (t, *J* = 6.6 Hz, 3H, $CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 162.8, 161.6, 154.6, 137.1, 133.0, 132.4, 131.7, 131.5, 130.0, 128.7, 128.6, 126.9, 123.5, 121.7, 63.3, 52.1, 43.6, 11.8; HRMS calculated for $[C_{22}H_{22}Br_2N_2O_3 +H]^+$: 521.0070, found: 521.0082.

**7q: methyl 5-(2-chlorophenyl)-2-((diethylamino)(p-tolyl)methyl)oxazole-4-carboxylate**

Light yellow oil, yield 82%; $^1$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.51-7.33 (m, 6H, Ar-H), 7.13 (d, *J* = 7.8 Hz, 2H, Ar-H), 5.19 (s, 1H, CH), 3.82 (s, 3H, $OCH_3$), 2.70-2.54 (m, 4H, $2NCH_2$), 2.32 (s, 3H, $CH_3$), 1.02 (t, *J* = 7.2 Hz, 6H, $2CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 163.8, 161.8, 153.2, 137.6, 134.9, 134.1, 132.3, 131.5, 129.8, 129.1, 128.8, 128.3, 126.7, 126.3, 63.9, 52.1, 43.5, 21.1, 11.6; HRMS calculated for $[C_{23}H_{25}ClN_2O_3 +Na]^+$: 435.1446, found: 435.1456.

## General procedure for the synthesis of 7r-v by using primary amines.

To a magnetically stirred solution of Schiff base (1 mmol) (prepared from aldehyde **4** and primary amine **5** in the presence of catalytic amount of HOAc) and isocyanide **3** (1 mmol) in anhydrous $CH_2Cl_2$ (5 mL) was added slowly a solution of acid **6** (1 mmol) in $CH_2Cl_2$ (5 mL) at room temperature. The mixture was stirred for 12-24 h, and the reaction progress was monitored by TLC. After completion, the $CH_2Cl_2$ solution was evaporated under reduced pressure, the residue was purified by silica gel chromatography with EtOAc/petroleum ether (1:15) as the eluent to afford products **7r-v**.

**7r: ethyl 2-((4-chlorophenyl)(p-tolylamino)methyl)-5-ethyloxazole-4-carboxylate**

White solid, yield 56%, mp 67-69 °C; $^1$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.43 (d, *J* = 7.2 Hz, 2H, Ar-H), 7.31 (d, *J* = 7.8 Hz, 2H, Ar-H), 6.94 (d, *J* = 7.2 Hz, 2H, Ar-H), 6.55 (d, *J* = 7.2 Hz, 2H, Ar-H), 5.65 (s, 1H, CH), 4.83 (s, 1H, NH), 4.38 (q, *J* = 6.6 Hz, 2H, $OCH_2$), 3.05-2.94 (m, 2H, $CH_2$), 2.20 (s, 3H, $CH_3$), 1.38 (t, *J* = 7.2 Hz, 3H, $CH_3$), 1.21 (t, *J* = 7.2 Hz, 3H, $CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 162.0, 161.4, 161.2, 143.4, 137.0, 134.0, 129.7, 129.0, 128.4, 127.9, 126.7, 113.8, 61.0, 56.0, 20.3, 19.6, 14.3, 11.9; HRMS calculated for $[C_{22}H_{23}ClN_2O_3 +Na]^+$: 421.1289, found: 421.1299.

**7s: ethyl 2-((4-bromophenyl)((4-chlorophenyl)amino)methyl)-5-ethyloxazole-4-carboxylate**

Light yellow oil, yield 61%; $^1$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.47 (d, *J* = 6.6 Hz, 2H, Ar-H), 7.36 (d, *J* = 7.2 Hz, 2H, Ar-H), 7.08 (d, *J* = 6.6 Hz, 2H, Ar-H), 6.54 (d, *J* = 7.8 Hz, 2H, Ar-H), 5.60 (s, 1H, CH), 5.05 (s, 1H, NH), 4.38 (q, *J* = 6.0 Hz, 2H, $OCH_2$), 3.04-2.95 (m, 2H, $CH_2$), 1.38 (t, *J* = 7.2 Hz, 3H, $CH_3$), 1.21 (t, *J* = 7.2 Hz, 3H, $CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 161.9, 161.6, 160.6, 144.2, 136.9, 132.2, 129.1, 128.7, 126.8, 123.4, 122.5, 114.7, 61.1, 55.9, 19.7, 14.3, 11.9; HRMS calculated for $[C_{21}H_{20}BrClN_2O_3$

+Na]$^+$: 485.0238, found: 485.0214.

**7t: ethyl 2-((3-chlorophenyl)((4-chlorophenyl)amino)methyl)-5-isopropyloxazole-4-carboxylate**

Light yellow oil, yield 64%; $^1$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.49 (s, 1H, Ar-H), 7.37-7.28 (m, 3H, Ar-H), 7.09 (d, *J* = 8.4 Hz, 2H, Ar-H), 6.56 (d, *J* = 9.0 Hz, 2H, Ar-H), 5.62 (d, *J* = 5.4 Hz, 1H, CH), 5.07 (d, *J* = 5.4 Hz, 1H, NH), 4.39 (q, *J* = 7.2 Hz, 2H, $OCH_2$), 3.74-3.69 (m, 1H, CH), 1.39 (t, *J* = 7.2 Hz, 3H, $CH_3$), 1.27 (d, *J* = 6.6 Hz, 3H, $CH_3$), 1.19 (d, *J* = 6.6 Hz, 3H, $CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 164.8, 161.9, 160.3, 144.2, 140.0, 134.9, 130.3, 129.1, 128.7, 127.1, 125.8, 125.1, 123.4, 114.7, 61.1, 55.9, 26.2, 20.6, 20.3, 14.3; HRMS calculated for [$C_{22}H_{22}Cl_2N_2O_3$ +Na]$^+$: 455.0900, found: 455.0903.

**7u: ethyl2-((4-chlorophenyl)((4-chlorophenyl)amino)methyl)-5-(p-tolyl)oxazole-4-carboxylate**

Light yellow oil, yield 52%; $^1$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.79 (d, *J* = 7.2 Hz, 2H, Ar-H), 7.47 (d, *J* = 7.2 Hz, 2H, Ar-H), 7.34 (d, *J* = 7.2 Hz, 2H, Ar-H), 7.25 (d, *J* = 7.2 Hz, 2H, Ar-H), 7.10 (d, *J* = 7.8 Hz, 2H, Ar-H), 6.58 (d, *J* = 7.2 Hz, 2H, Ar-H), 5.71 (d, *J* = 4.8 Hz, 1H, CH), 5.03 (d, *J* = 4.2 Hz, 1H, NH), 4.41 (q, *J* = 6.0 Hz, 2H, $OCH_2$), 2.40 (s, 3H, $CH_3$), 1.38 (t, *J* = 7.2 Hz, 3H, $CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 161.8, 160.7, 156.3, 144.2, 141.0, 136.3, 134.5, 129.3, 129.2, 129.1, 128.5, 128.4, 126.4, 123.7, 123.5, 114.8, 61.5, 55.9, 21.5, 14.3; HRMS calculated for [$C_{26}H_{22}Cl_2N_2O_3$ +Na]$^+$: 503.0900, found: 503.0899.

**7v: ethyl 2-((benzylamino)(4-chlorophenyl)methyl)-5-(4-fluorophenyl)oxazole-4-carboxylate**

Light yellow oil, yield 67%; $^1$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.97 (t, *J* = 7.2 Hz, 2H, Ar-H), 7.46-7.26 (m, 9H, Ar-H), 7.12 (t, *J* = 7.8 Hz, 2H, Ar-H), 5.10 (s, 1H, CH), 4.42 (q, *J* = 6.6 Hz, 2H, $OCH_2$), 3.84 (d, *J* = 13.2 Hz, 1H, $CH_2^a$), 3.77 (d, *J* = 13.2 Hz, 1H, $CH_2^b$), 2.06 (s, 1H, NH), 1.39 (t, *J* = 6.6 Hz, 3H, $CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 164.5, 162.9, 162.2, 162.0, 154.9, 139.0, 136.9, 134.2, 130.7, 130.6, 129.0, 128.9, 128.5, 128.3, 127.3, 126.6, 123.0, 115.6, 115.4, 61.5, 59.1, 51.5, 14.3; HRMS calculated for [$C_{26}H_{22}ClFN_2O_3$ +H]$^+$: 465.1376, found: 465.1388.

## General procedure for the synthesis of 8a-n.

To a magnetically stirred solution of isocyanides **3** (1 mmol) in anhydrous $CH_2Cl_2$ (5 mL) was added slowly a solution of acid **6** (1 mmol) in $CH_2Cl_2$ (5 mL) at room temperature. The mixture was stirred for 24-48 h, and the reaction progress was monitored by TLC. After completion, the $CH_2Cl_2$ solution was evaporated under reduced pressure, the residue was purified by silica gel chromatography with EtOAc/petroleum ether (1:10) as the eluent to afford products **8a-n**.

## Characterization Data

**8a: ethyl 5-phenyloxazole-4-carboxylate**[4]

Light yellow oil, yield 86%; $^1$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 8.06 (d, *J* = 5.4 Hz, 2H, Ar-H), 7.91 (s, 1H, Ar-H), 7.47-7.46 (m, 3H, Ar-H), 4.42 (q, *J* = 6.6 Hz, 2H, $OCH_2$), 1.40 (t, *J* = 6.6 Hz, 3H, $CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 161.8, 155.3, 148.9, 130.3, 128.3, 128.2, 126.6, 126.5, 61.3, 14.1; HRMS calculated for [$C_{12}H_{11}NO_3$ +Na]$^+$: 240.0631, found: 240.0643.

**8b: ethyl 5-(4-chlorophenyl)oxazole-4-carboxylate**[2]

White solid, yield 90%, mp 101-103 °C; $^1$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 8.07 (d, *J* = 8.4 Hz, 2H, Ar-H), 7.93 (s, 1H, Ar-H), 7.46 (d, *J* = 8.4 Hz, 2H, Ar-H), 4.43 (q, *J* = 7.2 Hz, 2H, $OCH_2$), 1.42 (t, *J* = 6.6 Hz, 3H, $CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 161.8, 154.4, 149.0, 136.5, 129.7, 128.7, 126.8, 125.1, 61.5, 14.2; HRMS calculated for [$C_{12}H_{10}ClNO_3$ +Na]$^+$: 274.0241, found: 274.0247.

**8c: ethyl 5-(4-bromophenyl)oxazole-4-carboxylate**[2]

White solid, yield 82%, mp 109-110 °C; $^1$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 8.00 (d, *J* = 8.4 Hz, 2H, Ar-H), 7.92 (s, 1H, Ar-H), 7.62 (d, *J* = 8.4 Hz, 2H, Ar-H), 4.43 (q, *J* = 7.2 Hz, 2H, $OCH_2$), 1.42 (t, *J* = 6.6

Hz, 3H, $CH_3$); $^{13}C$ NMR ($CDCl_3$, 150 MHz) δ (ppm) 161.8, 154.4, 149.0, 131.7, 129.9, 126.9, 125.5, 125.0, 61.6, 14.2; HRMS calculated for $[C_{12}H_{10}BrNO_3 + Na]^+$: 317.9736, found: 317.9744.

**8d: ethyl 5-(2,4-dichlorophenyl)oxazole-4-carboxylate**

White solid, yield 87%, mp 103-105 °C; $^1H$ NMR ($CDCl_3$, 600 MHz) δ (ppm) 8.01 (s, 1H, Ar-H), 7.54 (s, 1H, Ar-H), 7.48 (d, *J* = 8.4 Hz, 1H, Ar-H), 7.37 (d, *J* = 7.8 Hz, 1H, Ar-H), 4.32 (q, *J* = 7.2 Hz, 2H, $OCH_2$), 1.29 (t, *J* = 6.6 Hz, 3H, $CH_3$); $^{13}C$ NMR ($CDCl_3$, 150 MHz) δ (ppm) 160.9, 151.8, 150.4, 137.2, 135.0, 132.9, 129.8, 129.7, 126.9, 125.0, 61.4, 14.0; HRMS calculated for $[C_{12}H_9Cl_2NO_3 + Na]^+$: 307.9852, found: 307.9863.

**8e: ethyl 5-(*p*-tolyl)oxazole-4-carboxylate**[2]

White solid, yield 83%, mp 84-85 °C; $^1H$ NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.97 (d, *J* = 8.4 Hz, 2H, Ar-H), 7.89 (s, 1H, Ar-H), 7.28 (d, *J* = 7.8 Hz, 2H, Ar-H), 4.42 (q, *J* = 7.2 Hz, 2H, $OCH_2$), 2.41 (s, 3H, $CH_3$), 1.41 (t, *J* = 6.6 Hz, 3H, $CH_3$); $^{13}C$ NMR ($CDCl_3$, 150 MHz) δ (ppm) 161.9, 155.7, 148.6, 140.8, 129.0, 128.3, 126.0, 123.8, 61.3, 21.4, 14.2; HRMS calculated for $[C_{13}H_{13}NO_3 + Na]^+$: 254.0788, found: 254.0796.

**8f: ethyl 5-(4-methoxyphenyl)oxazole-4-carboxylate**

White solid, yield 74%, mp 68-69 °C (Lit.[4] mp 70-71 °C); $^1H$ NMR ($CDCl_3$, 600 MHz) δ (ppm) 8.07 (d, *J* = 8.4 Hz, 2H, Ar-H), 7.87 (s, 1H, Ar-H), 6.99 (d, *J* = 8.4 Hz, 2H, Ar-H), 4.42 (q, *J* = 7.2 Hz, 2H, $OCH_2$), 3.86 (s, 3H, $OCH_3$), 1.41 (t, *J* = 6.6 Hz, 3H, $CH_3$); $^{13}C$ NMR ($CDCl_3$, 150 MHz) δ (ppm) 162.0, 161.1, 155.7, 148.3, 130.0, 125.2, 119.1, 113.7, 61.2, 55.3, 14.2; HRMS calculated for $[C_{13}H_{13}NO_4 + Na]^+$: 270.0737, found: 270.0747.

**8g: ethyl 5-(3-nitrophenyl)oxazole-4-carboxylate**

White solid, yield 81%, mp 87-89 °C; $^1H$ NMR ($CDCl_3$, 600 MHz) δ (ppm) 9.04 (s, 1H, Ar-H), 8.51 (d, *J* = 7.2 Hz, 1H, Ar-H), 8.33 (d, *J* = 7.8 Hz, 1H, Ar-H), 8.03 (s, 1H, Ar-H), 7.70 (t, *J* = 8.4 Hz, 1H, Ar-H), 4.47 (q, *J* = 7.2 Hz, 2H, $OCH_2$), 1.44 (t, *J* = 6.6 Hz, 3H, $CH_3$); $^{13}C$ NMR ($CDCl_3$, 150 MHz) δ (ppm) 161.5, 152.6, 149.6, 148.1, 133.9, 129.6, 128.2, 128.1, 124.8, 123.3, 61.9, 14.1; HRMS calculated for $[C_{12}H_{10}N_2O_5 + Na]^+$: 285.0482, found: 285.0485.

**8h: ethyl 5-(furan-2-yl)oxazole-4-carboxylate**

White solid, yield 72%, mp 91-92 °C; $^1H$ NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.88 (s, 1H, Ar-H), 7.68-7.62 (m, 2H, Ar-H), 6.60 (s, 1H, Ar-H), 4.45 (q, *J* = 7.2 Hz, 2H, $OCH_2$), 1.44 (t, *J* = 7.2 Hz, 3H, $CH_3$); $^{13}C$ NMR ($CDCl_3$, 150 MHz) δ (ppm) 161.3, 148.4, 147.1, 144.6, 141.8, 124.9, 115.6. 112.2, 61.3, 14.2; HRMS calculated for $[C_{10}H_9NO_4 + Na]^+$: 230.0424, found: 230.0441.

**8i: ethyl 5-(2-chlorophenyl)oxazole-4-carboxylate**[2]

Light yellow oil, yield 82%; $^1H$ NMR ($CDCl_3$, 600 MHz) δ (ppm) 8.01 (s, 1H, Ar-H), 7.53-7.37 (m, 4H, Ar-H), 4.31 (q, *J* = 7.2 Hz, 2H, $OCH_2$), 1.26 (t, *J* = 7.2 Hz, 3H, $CH_3$); $^{13}C$ NMR ($CDCl_3$, 150 MHz) δ (ppm) 161.0, 152.9, 150.2, 134.2, 132.1, 131.6, 129.8, 129.4, 126.5, 126.4, 61.2, 13.9; HRMS calculated for $[C_{12}H_{10}ClNO_3 + Na]^+$: 274.0241, found: 274.0251.

**8j: methyl 5-(4-chlorophenyl)oxazole-4-carboxylate**

White solid, yield 80%, mp 111-113 °C(lit.[3] mp 113-115 °C); $^1H$ NMR ($CDCl_3$, 600 MHz) δ (ppm) 8.07 (d, *J* = 9.0 Hz, 2H, Ar-H), 7.93 (s, 1H, Ar-H), 7.46 (d, *J* = 8.4 Hz, 2H, Ar-H), 3.96 (s, 3H, $OCH_3$); $^{13}C$ NMR ($CDCl_3$, 150 MHz) δ (ppm) 162.2, 154.5, 149.0, 136.6, 129.6, 128.7, 126.5, 124.9, 52.4; HRMS calculated for $[C_{11}H_8ClNO_3 + Na]^+$:260.0085, found: 260.0089.

**8k: methyl 5-(*o*-tolyl)oxazole-4-carboxylate**

White solid, yield 85%, mp 98-100 °C; $^1H$ NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.97 (s, 1H, Ar-H), 7.45 (d, *J* = 7.2 Hz, 1H, Ar-H), 7.40 (t, *J* = 7.2 Hz, 1H, Ar-H), 7.32-7.27 (m, 2H, Ar-H), 3.84 (s, 3H, $CH_3$), 2.28 (s, 3H, $OCH_3$); $^{13}C$ NMR ($CDCl_3$, 150 MHz) δ (ppm) 161.7, 156.2, 149.7, 137.8, 130.7, 130.5, 130.3, 127.9, 126.3, 125.4, 52.0, 19.9; HRMS calculated for $[C_{12}H_{11}NO_3 + Na]^+$: 240.0631, found: 240.0644.

**8l: ethyl 5-isopropyloxazole-4-carboxylate**[1]

Light yellow oil, yield 71%; $^{1}$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.78 (s, 1H, Ar-H), 4.39 (q, *J* = 7.2 Hz, 2H, $OCH_2$), 3.84-3.80 (m, 1H, CH), 1.41 (t, *J* = 7.2 Hz, 3H, $CH_3$), 1.31 (d, *J* = 7.2 Hz, 6H, $2CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 164.2, 161.9, 148.5, 125.1, 60.8, 25.8, 20.4, 14.1; HRMS calculated for $[C_9H_{13}NO_3 +Na]^+$: 206.0788, found: 206.0805.

**8m: ethyl 5-((4-chlorophenoxy)methyl)oxazole-4-carboxylate**

Light yellow oil, yield 83%; $^{1}$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.92 (s, 1H, Ar-H), 7.25 (d, *J* = 8.4 Hz, 2H, Ar-H), 6.94 (d, *J* = 8.4 Hz, 2H, Ar-H), 5.43 (s, 2H, $CH_2$), 4.43 (q, *J* = 7.2 Hz, 2H, $OCH_2$), 1.41 (t, *J* = 7.2 Hz, 3H, $CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 161.2, 156.2, 152.7, 150.6, 130.0, 129.4, 126.7, 116.1, 61.6, 59.8, 14.2; HRMS calculated for $[C_{13}H_{12}ClNO_4 +H]^+$: 282.0528, found: 282.0523.

**8n: ethyl 5-(9H-xanthen-9-yl)oxazole-4-carboxylate**

White solid, yield 78%, mp 128-129 °C; $^{1}$H NMR ($CDCl_3$, 600 MHz) δ (ppm) 7.60 (s, 1H, Ar-H), 7.29-7.01 (m, 8H, Ar-H), 6.43 (s, 1H, CH), 4.51 (q, *J* = 7.2 Hz, 2H, $OCH_2$), 1.48 (t, *J* = 7.2 Hz, 3H, $CH_3$); $^{13}$C NMR ($CDCl_3$, 150 MHz) δ (ppm) 162.1, 160.1, 151.2, 149.8, 129.1, 129.0, 126.4, 123.4, 119.1, 117.0, 61.4, 35.0, 14.3; HRMS calculated for $[C_{19}H_{15}NO_4 +Na]^+$:344.0893, found: 344.0903.

## References:

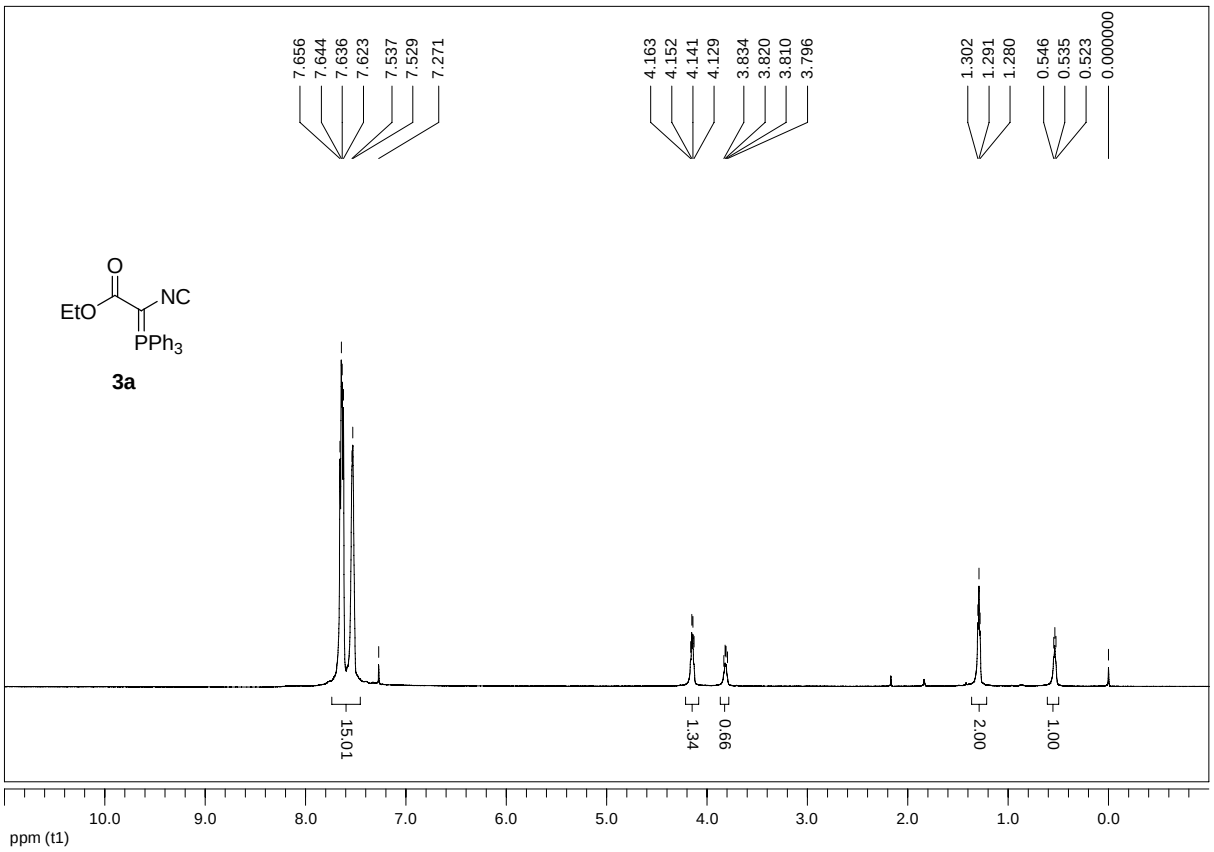

[1] R. Schröder, U. Schöllkopf, E. Blume and I. Hoppe, *Liebigs Ann. Chem.,* 1975, **3**, 533-546.

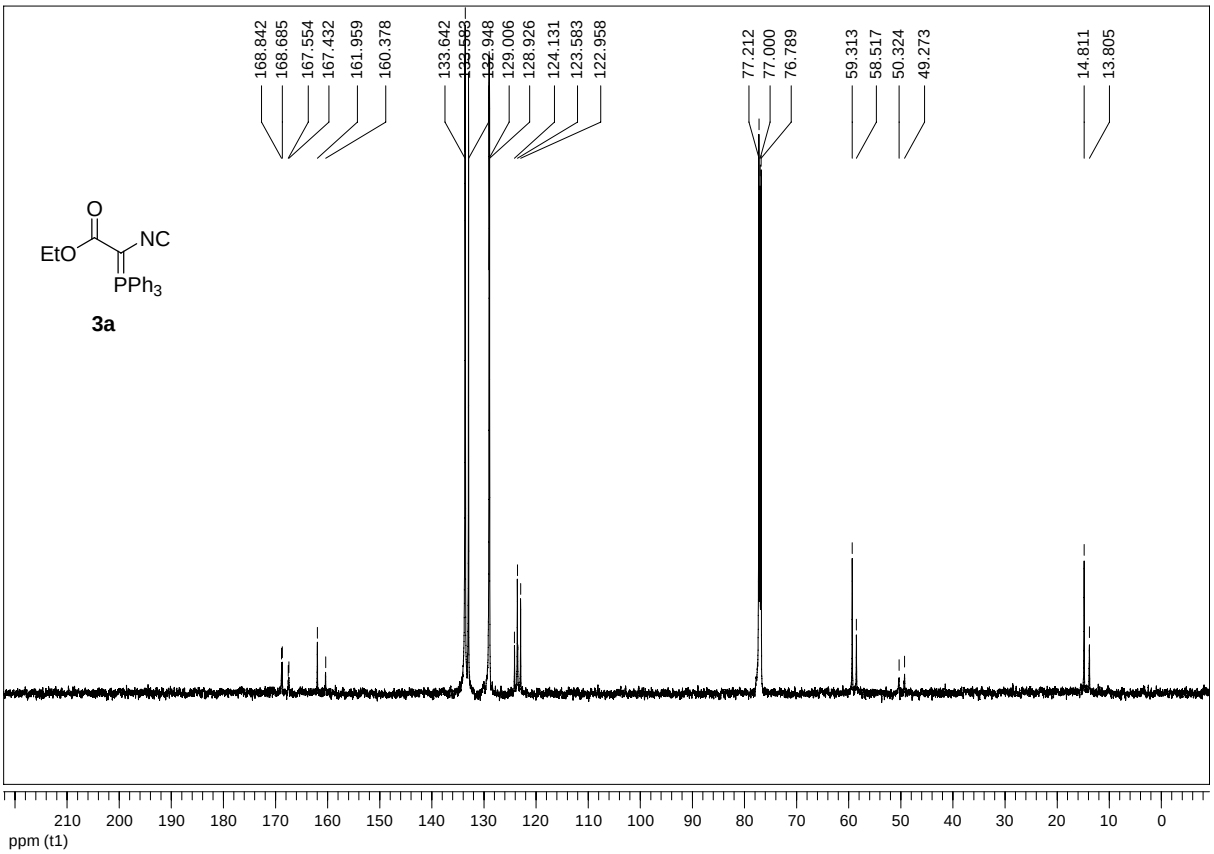
[2] Y. Ma, Z. Yan, C. Bian, K. Li, X. Zhang, M. Wang, X. Gao, H. Zhang and A. Lei, *Chem. Commun.,* 2015, **51**, 10524-10527.

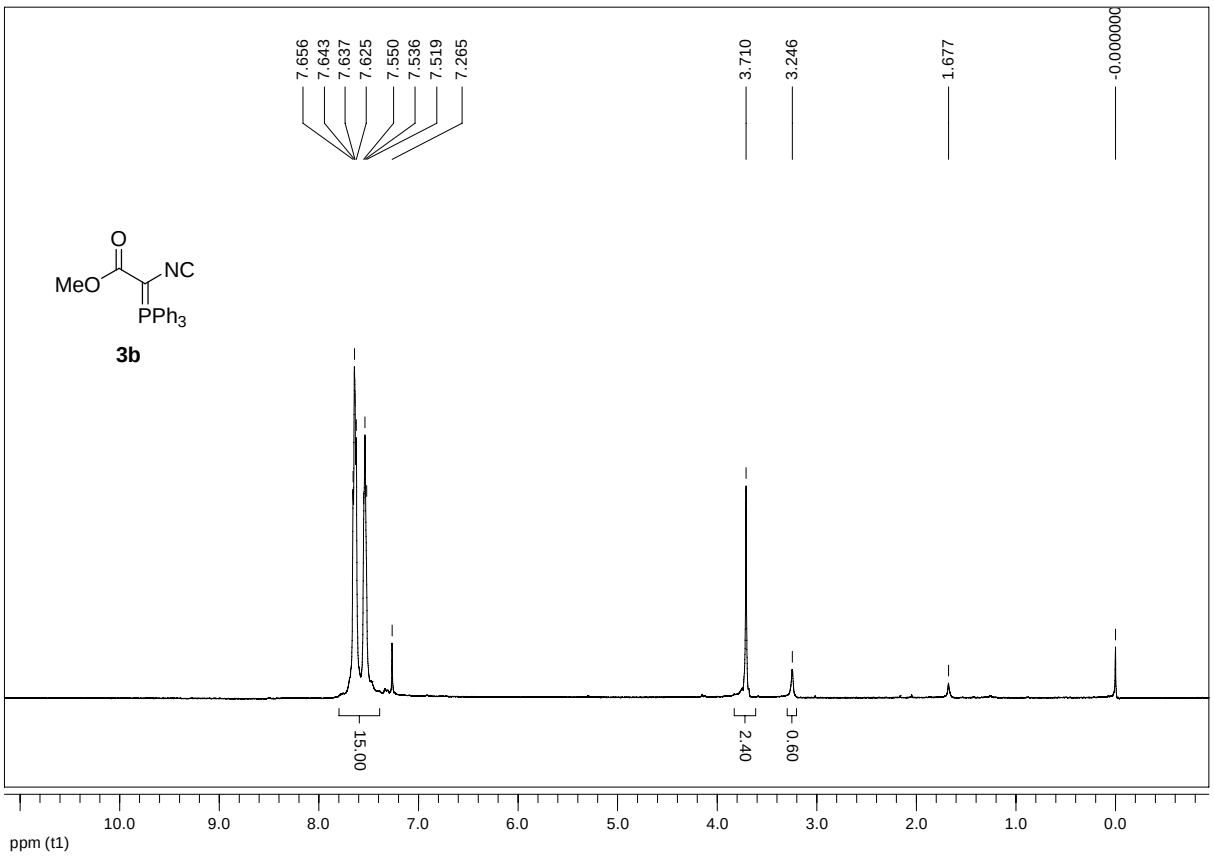
[3] J. R. Davies, P. D. Kane and C. J. Moody, *Tetrahedron,* 2004, **60**, 3967-3977.

[4] C. Verrier, C. Fiol-Petit, C. Hoarau and F. Marsais, *Org. Biomol. Chem.,* 2011, **9**, 6215-6218.

## 3. $^{1}H$ and $^{13}C$ NMR spectra of compounds 3a-b, 7a-v, 8a-n

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2.0
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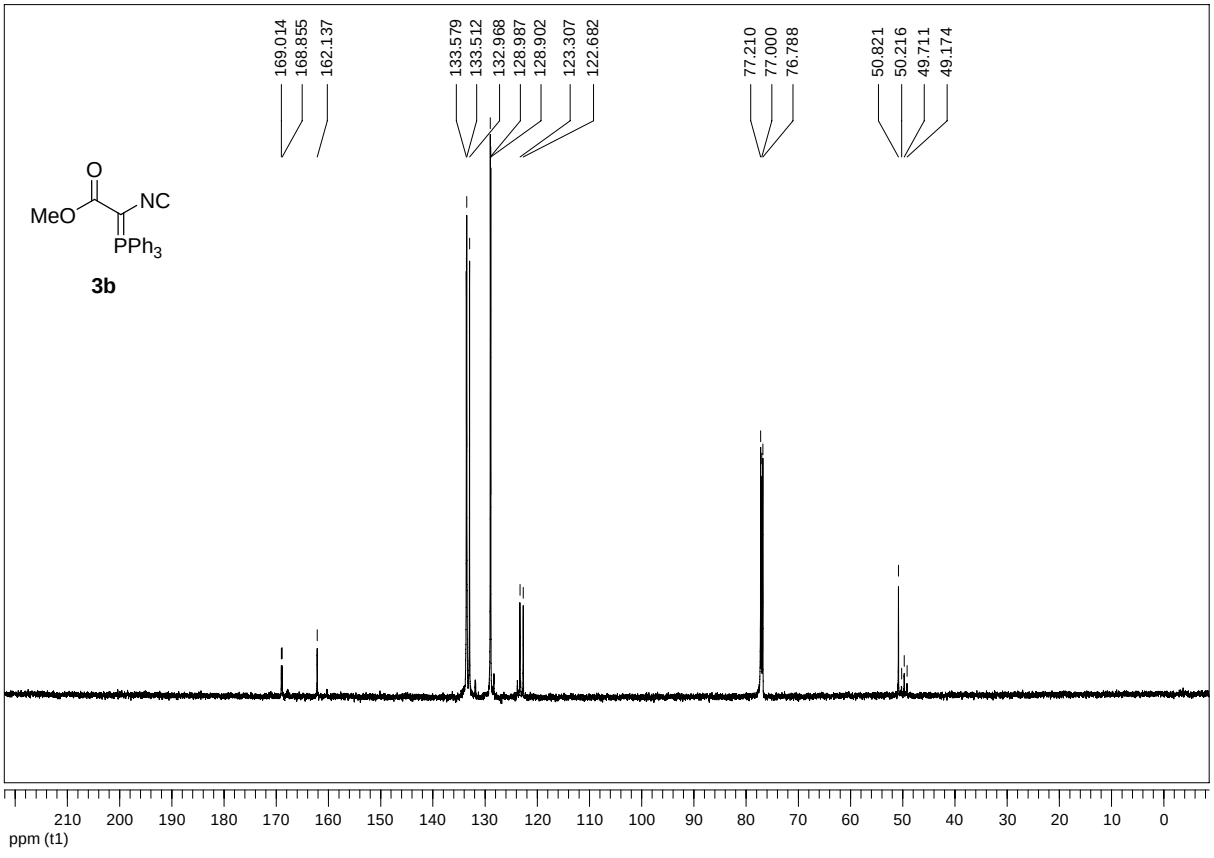
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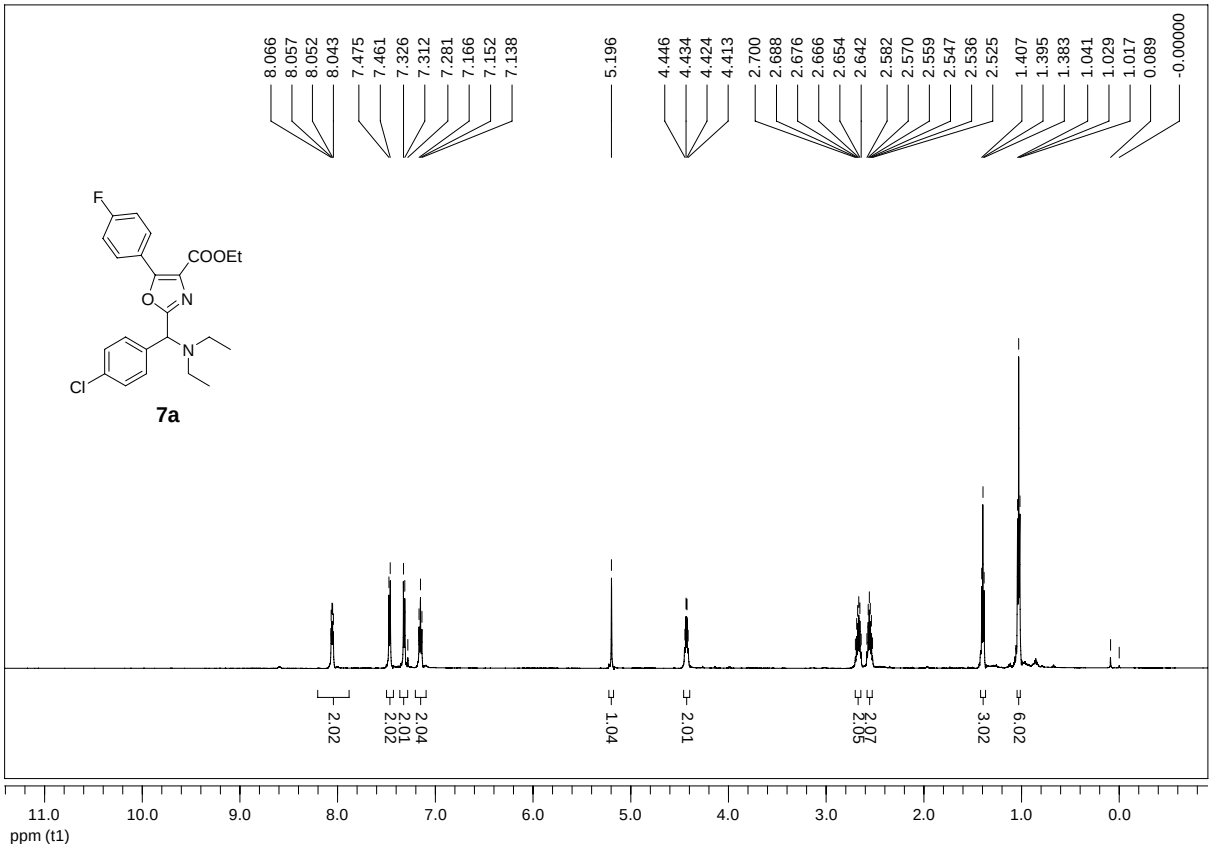
ppm (t1)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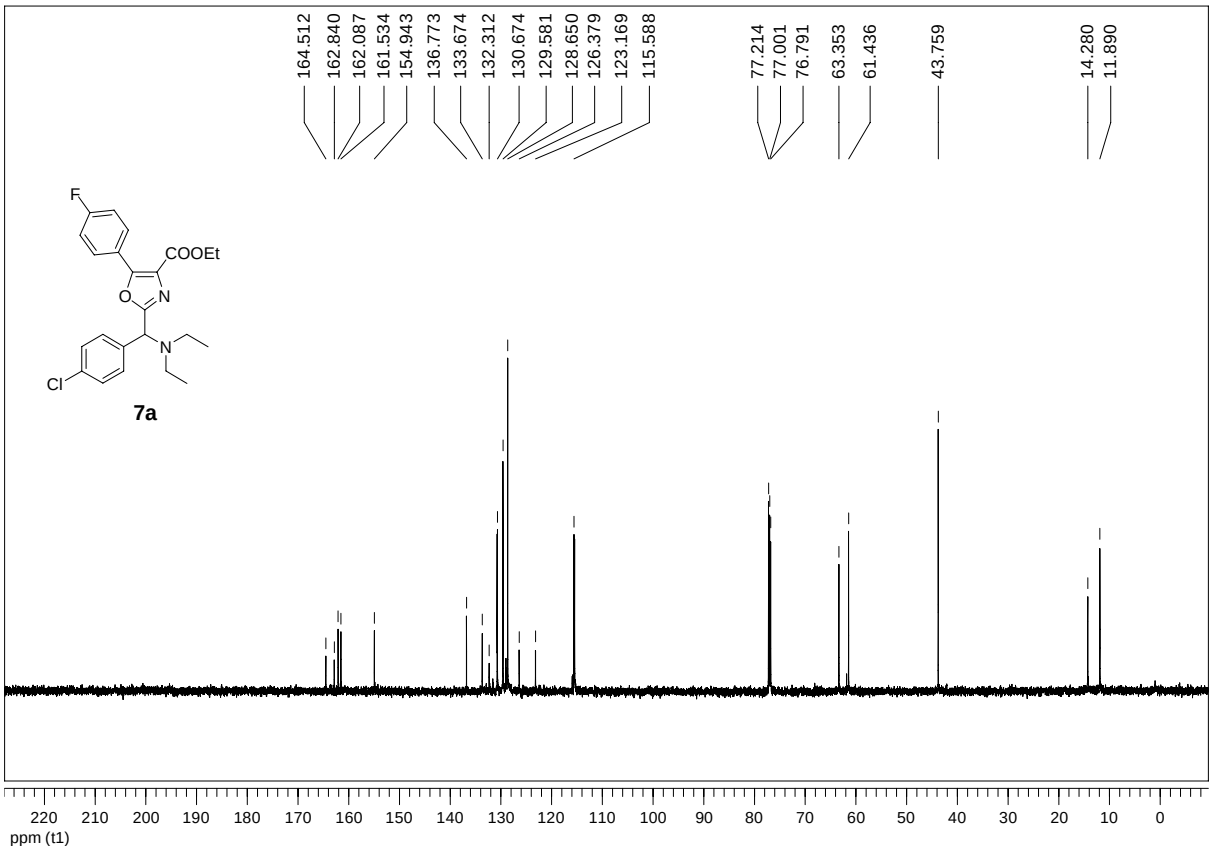
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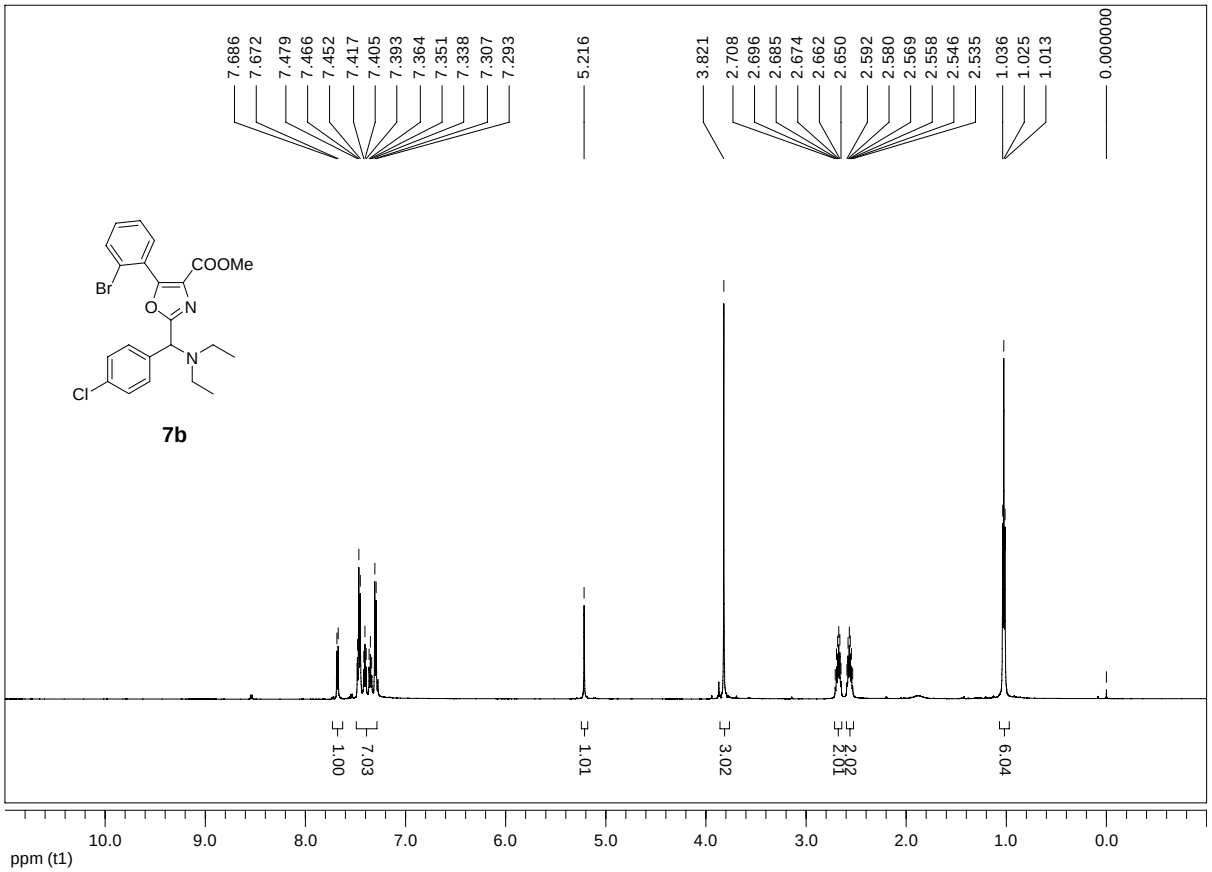
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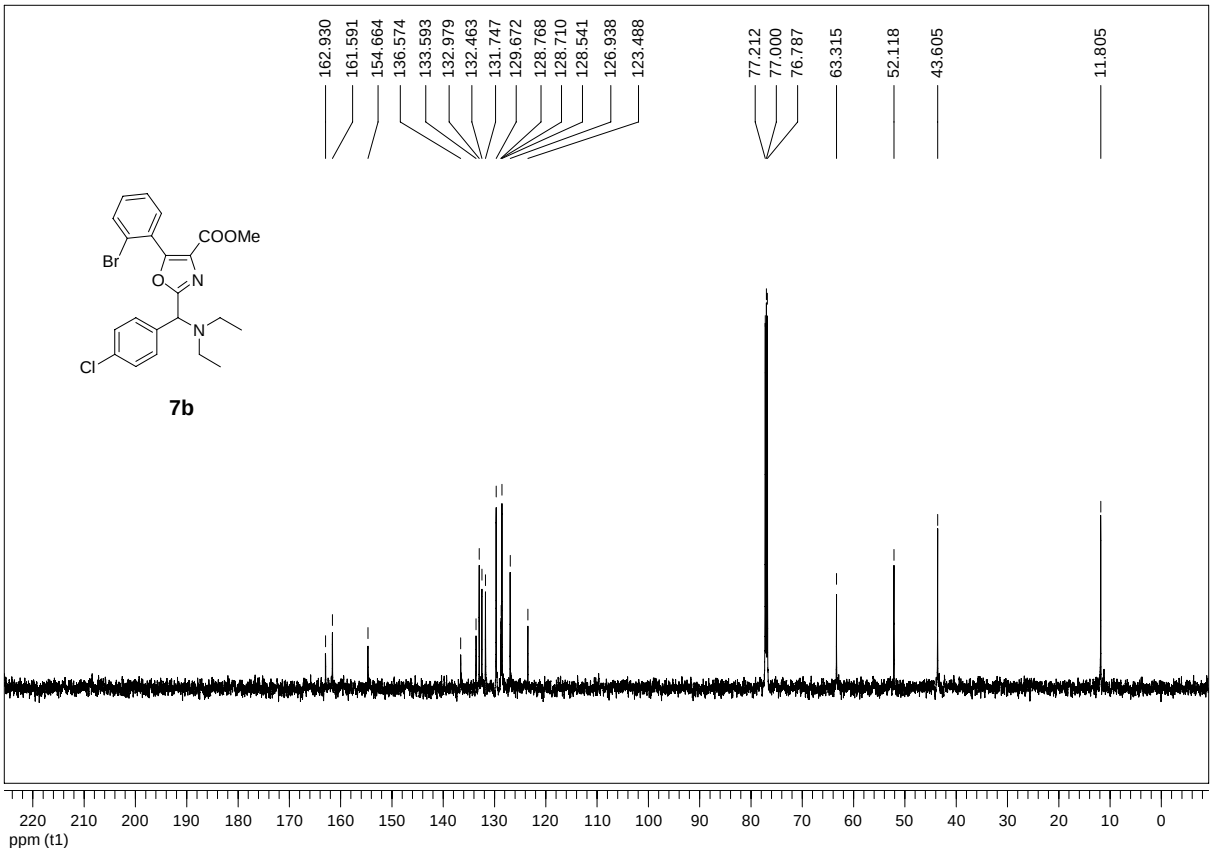
1.0
0.0
ppm (t1)

**7b**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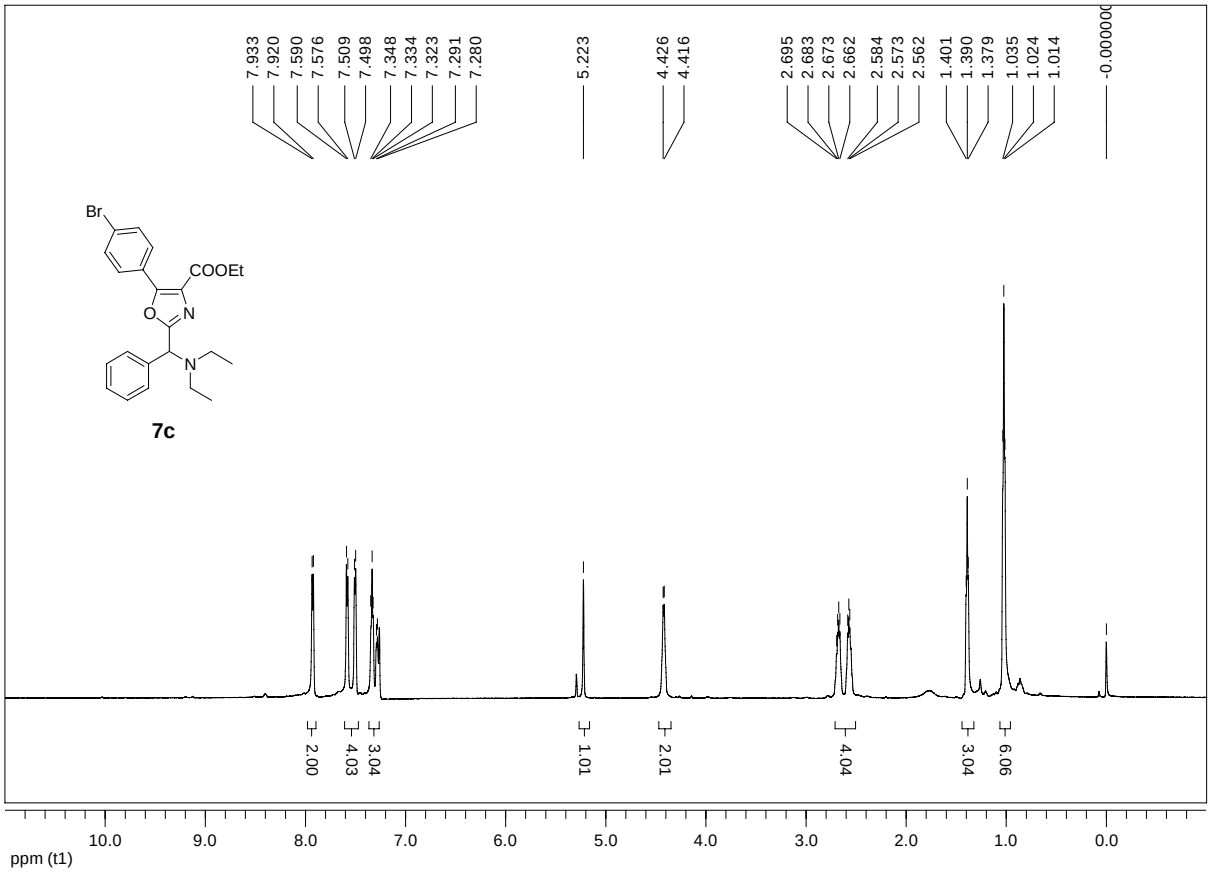
161.591
154.664
136.574
133.593
132.979
132.463
131.747
129.672
128.768
128.710
128.541
126.938
123.488
77.212
77.000
76.787
63.315
52.118
43.605
11.805
COOMe
Br
O
N
N
Cl
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

**7b**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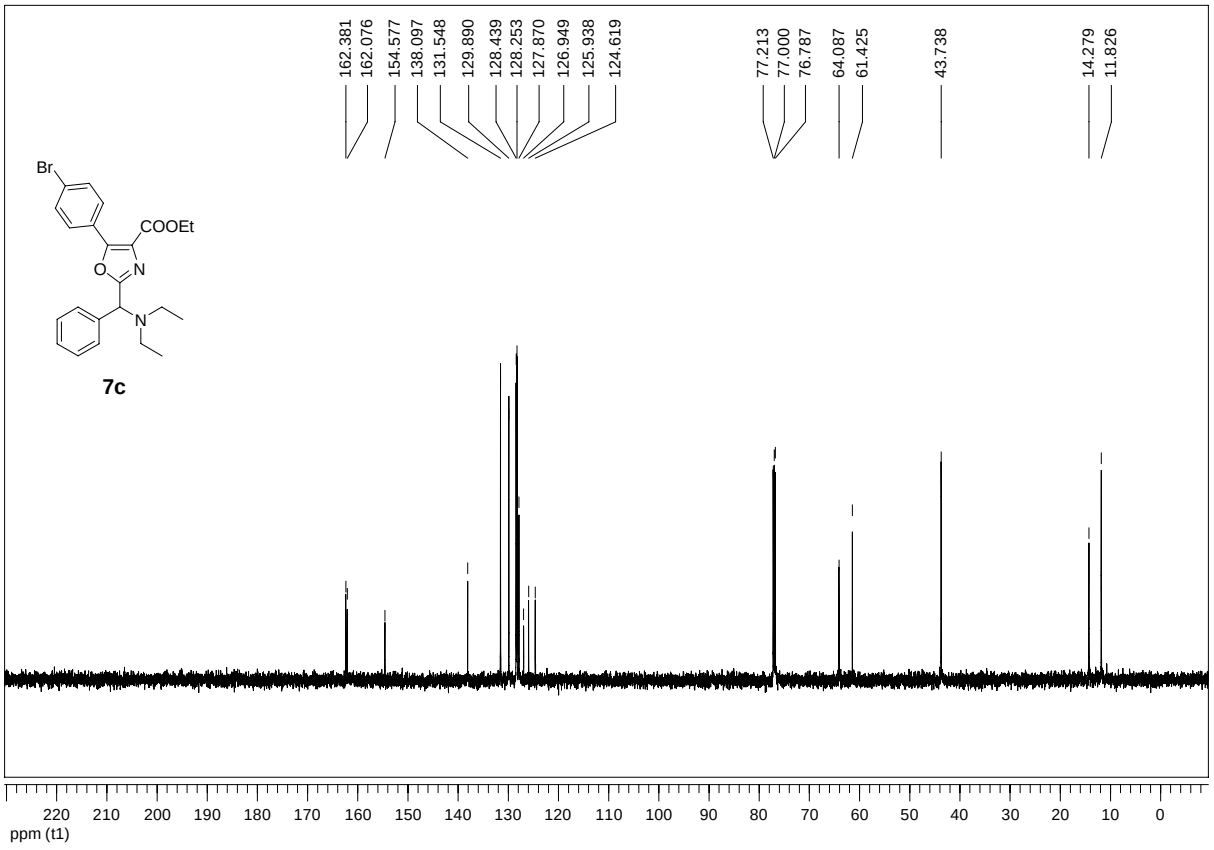
7.590
7.576
7.509
7.498
7.348
7.334
7.323
7.291
7.280
5.223
4.426
4.416
2.695
2.683
2.673
2.662
2.584
2.573
2.562
1.401
1.390
1.379
1.035
1.024
1.014
-0.000000
Br
COOEt
O
N
N
7c
2.00
4.03
3.04
1.01
2.01
4.04
3.04
9.06
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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154.577
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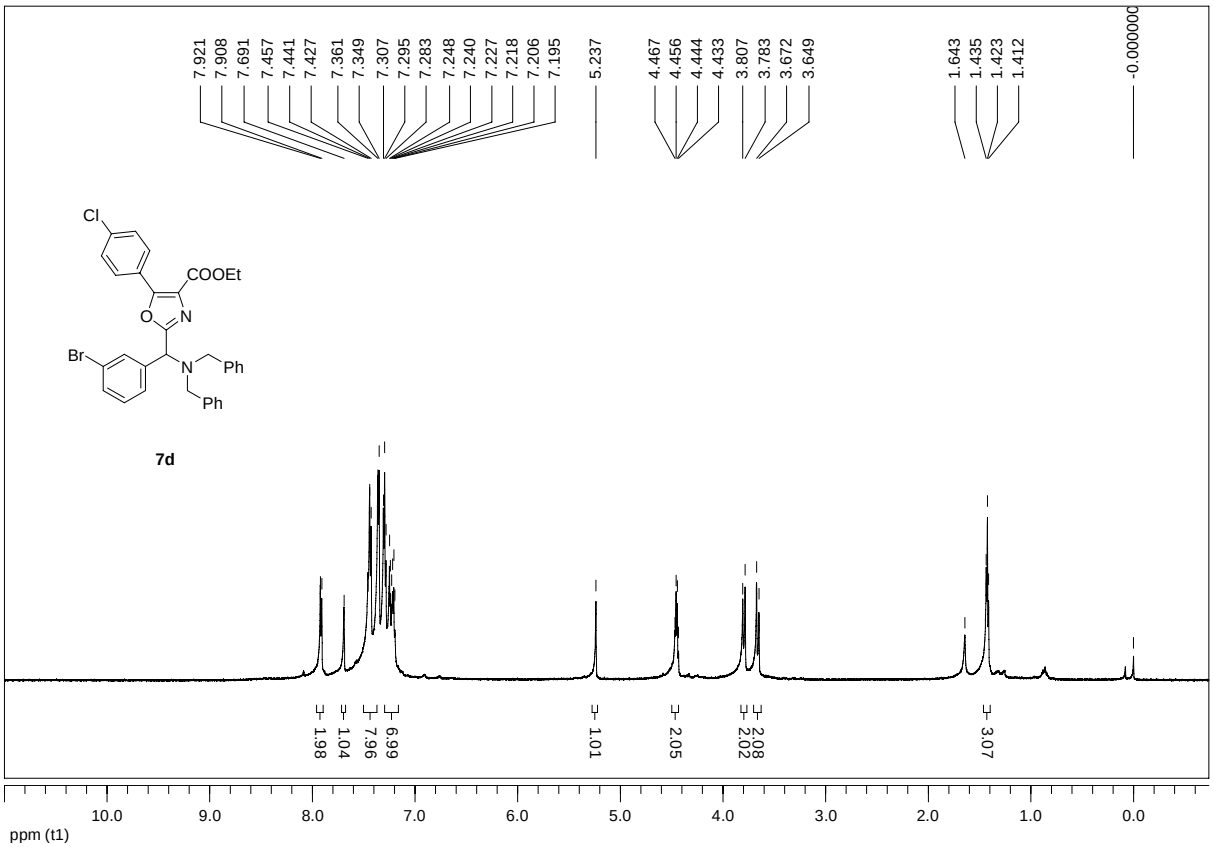
129.890
128.439
128.253
127.870
126.949
125.938
124.619
77.213
77.000
76.787
64.087
61.425
43.738
14.279
11.826
Br
COOEt
O
N
N
7c
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)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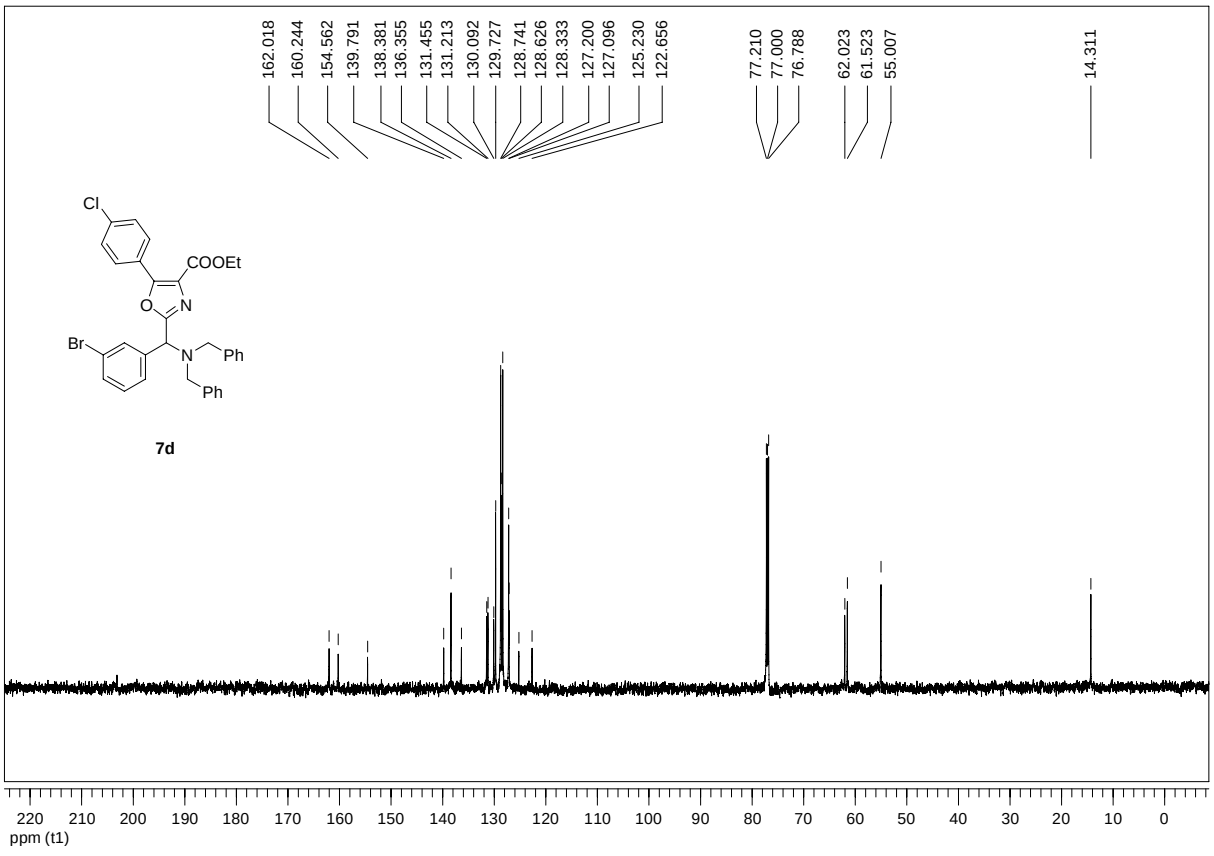
7.691
7.457
7.441
7.427
7.361
7.349
7.307
7.295
7.283
7.248
7.240
7.227
7.218
7.206
7.195
5.237
4.467
4.456
4.444
4.433
3.807
3.783
3.672
3.649
1.643
1.435
1.423
1.412
-0.000000
Cl
COOEt
O
N
Br
N
Ph
Ph
7d
1.98
1.04
7.96
6.99
1.01
2.05
2.02
2.08
3.07
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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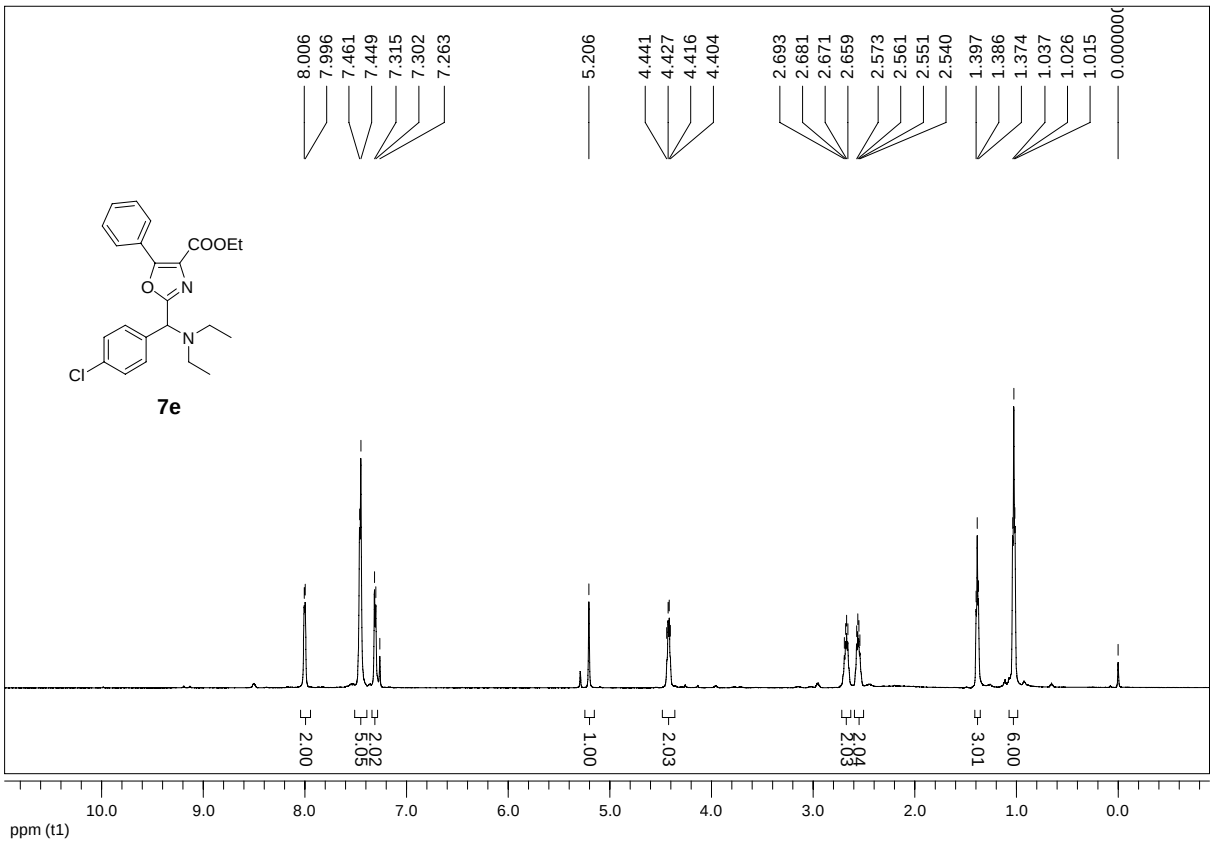
160.244
154.562
139.791
138.381
136.355
131.455
131.213
130.092
129.727
128.741
128.626
128.333
127.200
127.096
125.230
122.656
77.210
77.000
76.788
62.023
61.523
55.007
14.311
Cl
COOEt
O
N
Br
N
Ph
Ph
7d
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)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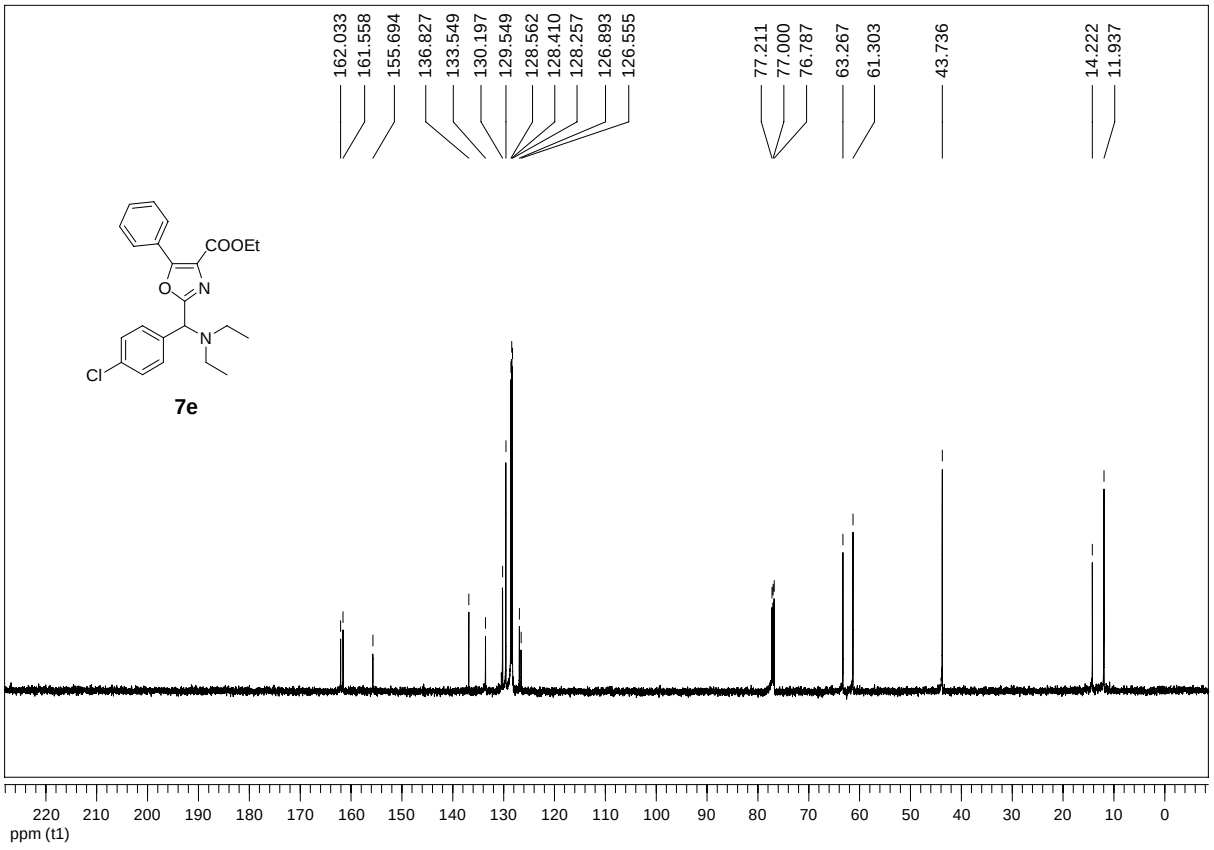
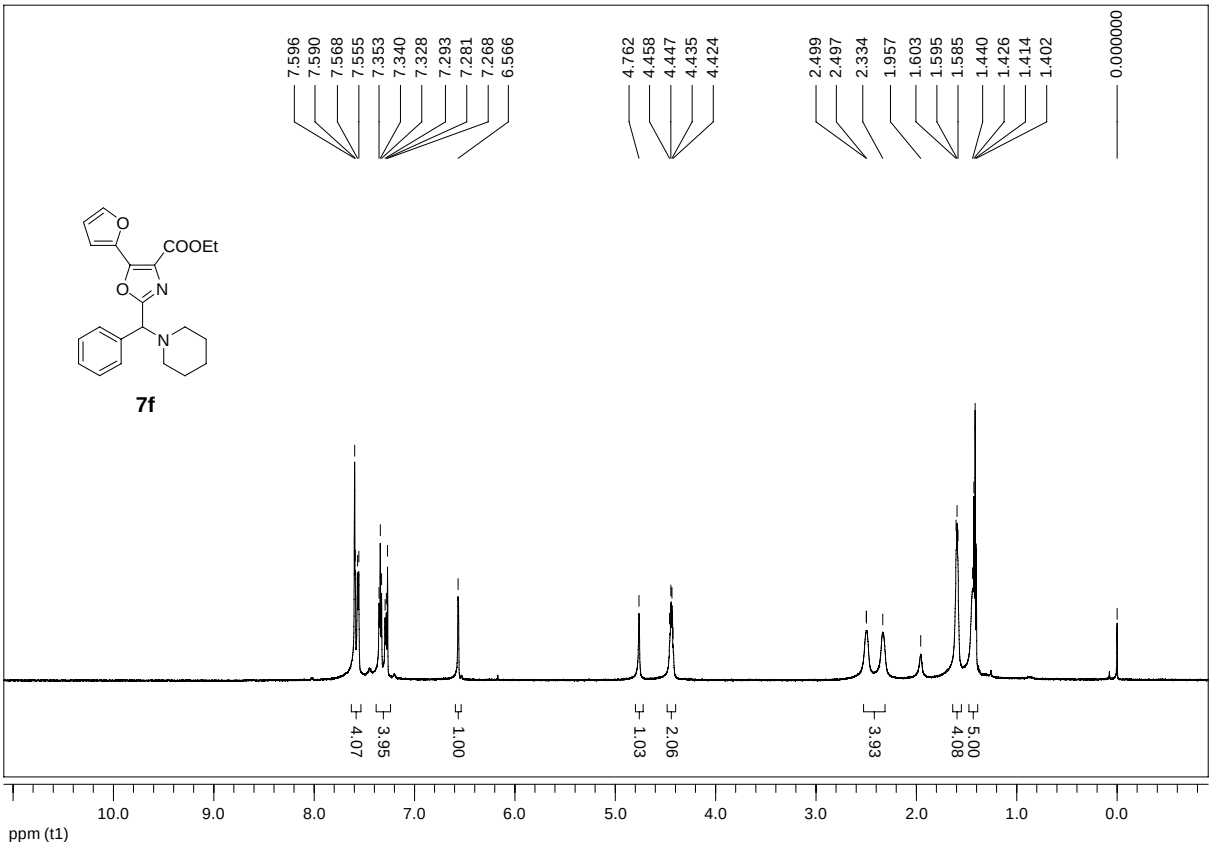
7.996
7.461
7.449
7.315
7.302
7.263
5.206
4.441
4.427
4.416
4.404
2.693
2.681
2.671
2.659
2.573
2.561
2.551
2.540
1.397
1.386
1.374
1.037
1.026
1.015
0.000000
COOEt
O
N
N
Cl
7e
2.00
5.05
2.02
1.00
2.03
2.03
2.04
3.01
6.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


162.033
161.558
155.694
136.827
133.549
130.197
129.549
128.562
128.410
128.257
126.893
126.555
77.211
77.000
76.787
63.267
61.303
43.736
14.222
11.937
COOEt
O
N
N
Cl
7e
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)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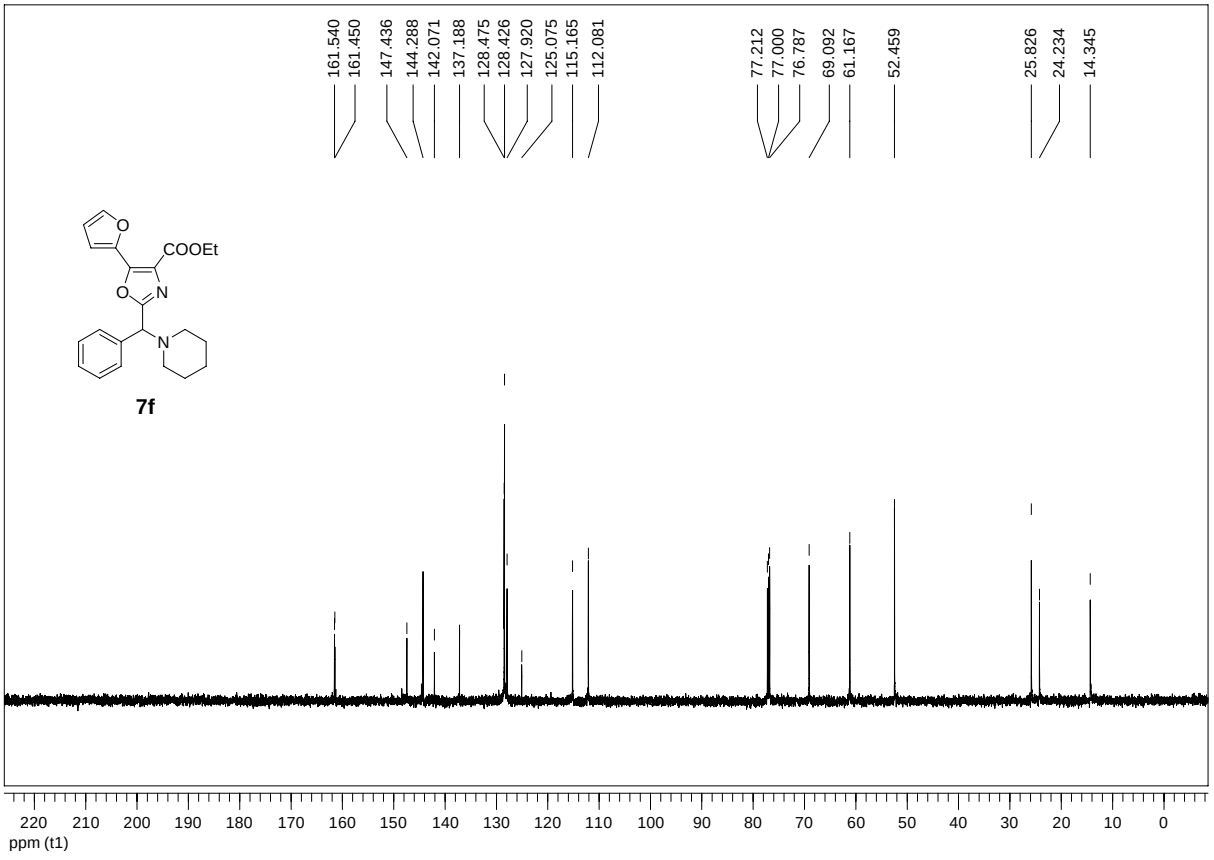
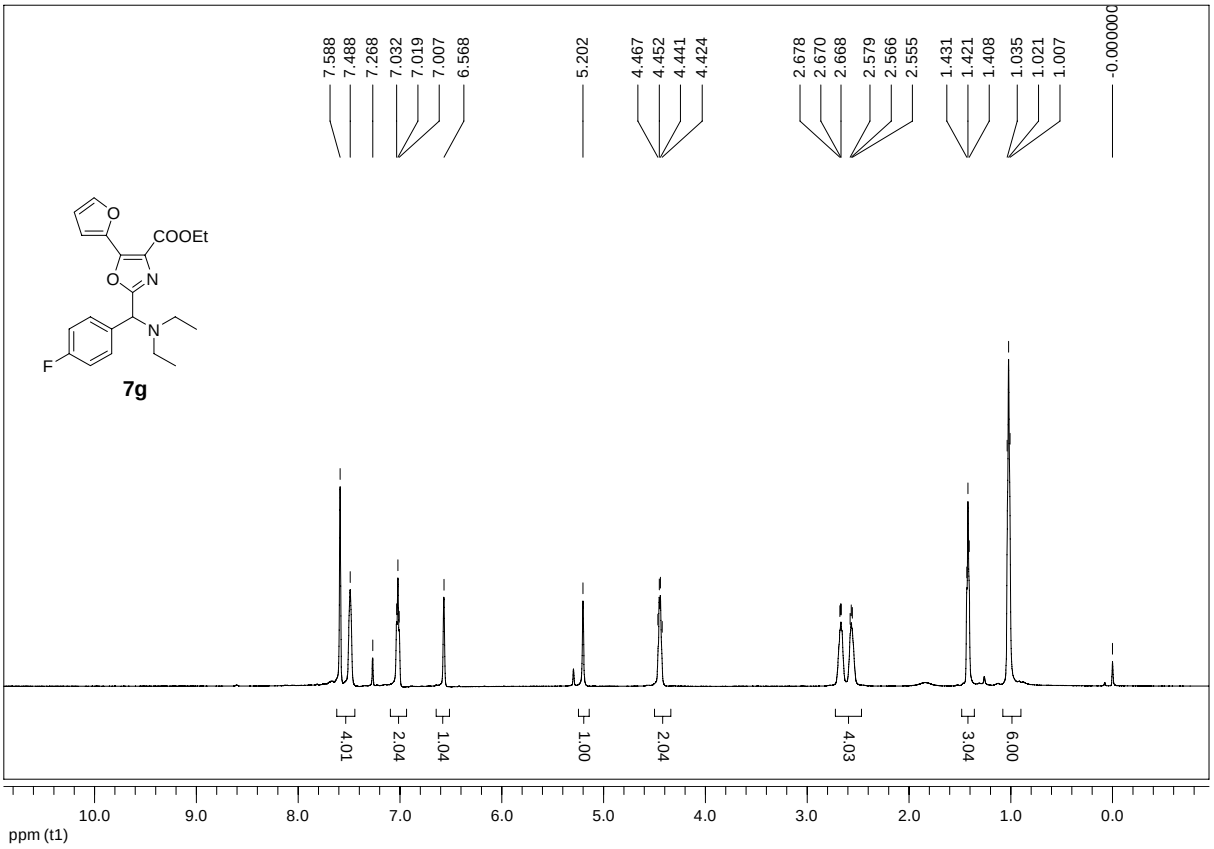
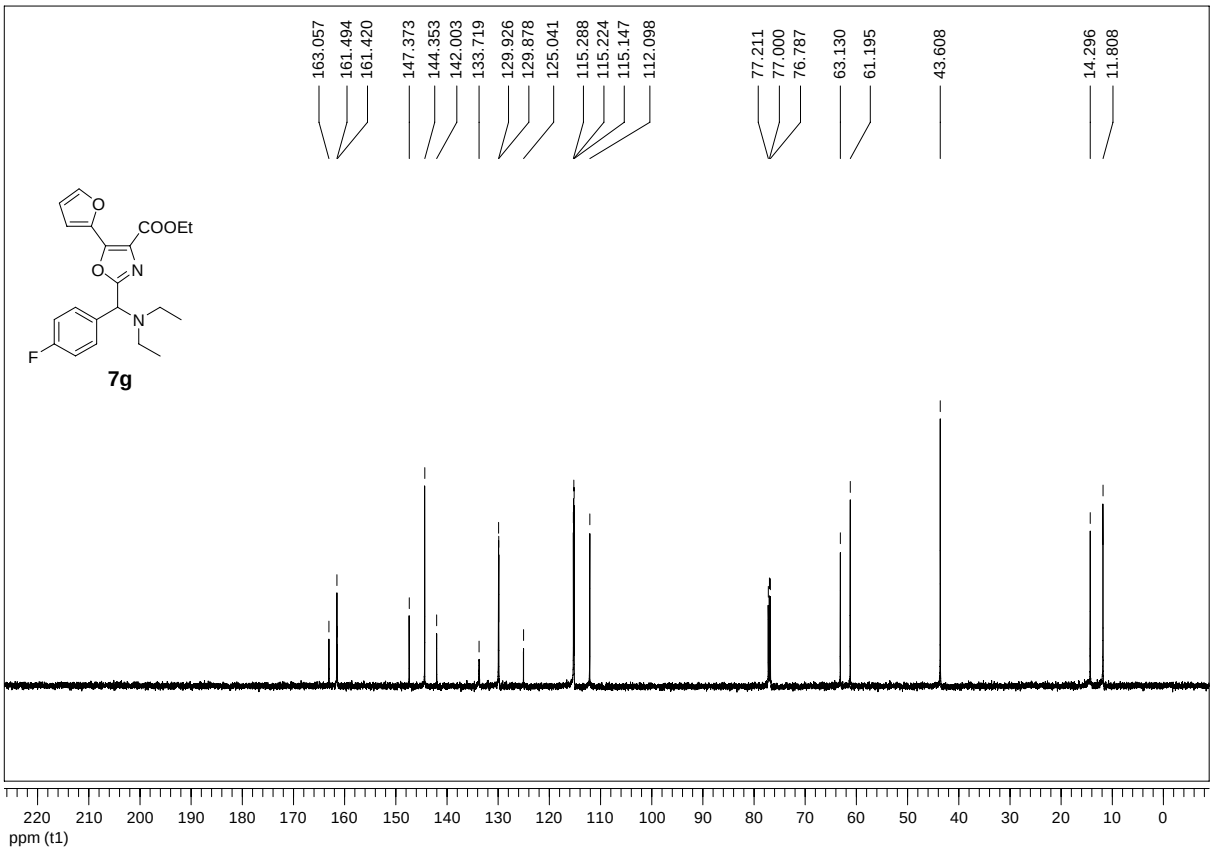
7.590
7.568
7.555
7.353
7.340
7.328
7.293
7.281
7.268
6.566
4.762
4.458
4.447
4.435
4.424
2.499
2.497
2.334
1.957
1.603
1.595
1.585
1.440
1.426
1.414
1.402
0.000000
COOEt
O
N
7f
4.07
3.95
1.00
1.03
2.06
3.93
5.08
5.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


161.540
161.450
147.436
144.288
142.071
137.188
128.475
128.426
127.920
125.075
115.165
112.081
77.212
77.000
76.787
69.092
61.167
52.459
25.826
24.234
14.345
COOEt
O
N
7f
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)


7.588
7.488
7.268
7.032
7.019
7.007
6.568
5.202
4.467
4.452
4.441
4.424
2.678
2.670
2.668
2.579
2.566
2.555
1.431
1.421
1.408
1.035
1.021
1.007
-0.000000
COOEt
O
N
F
7g
4.01
2.04
1.04
1.00
2.04
4.03
3.04
6.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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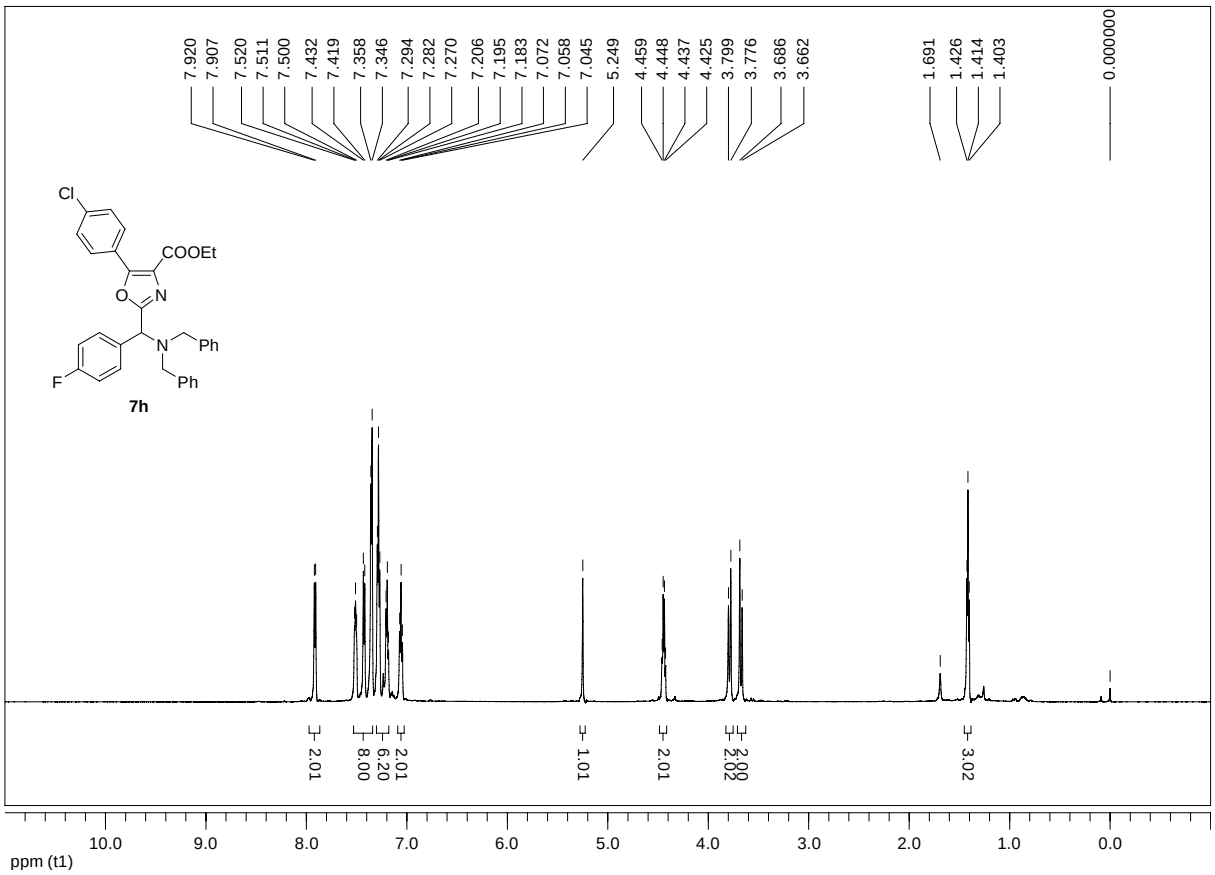
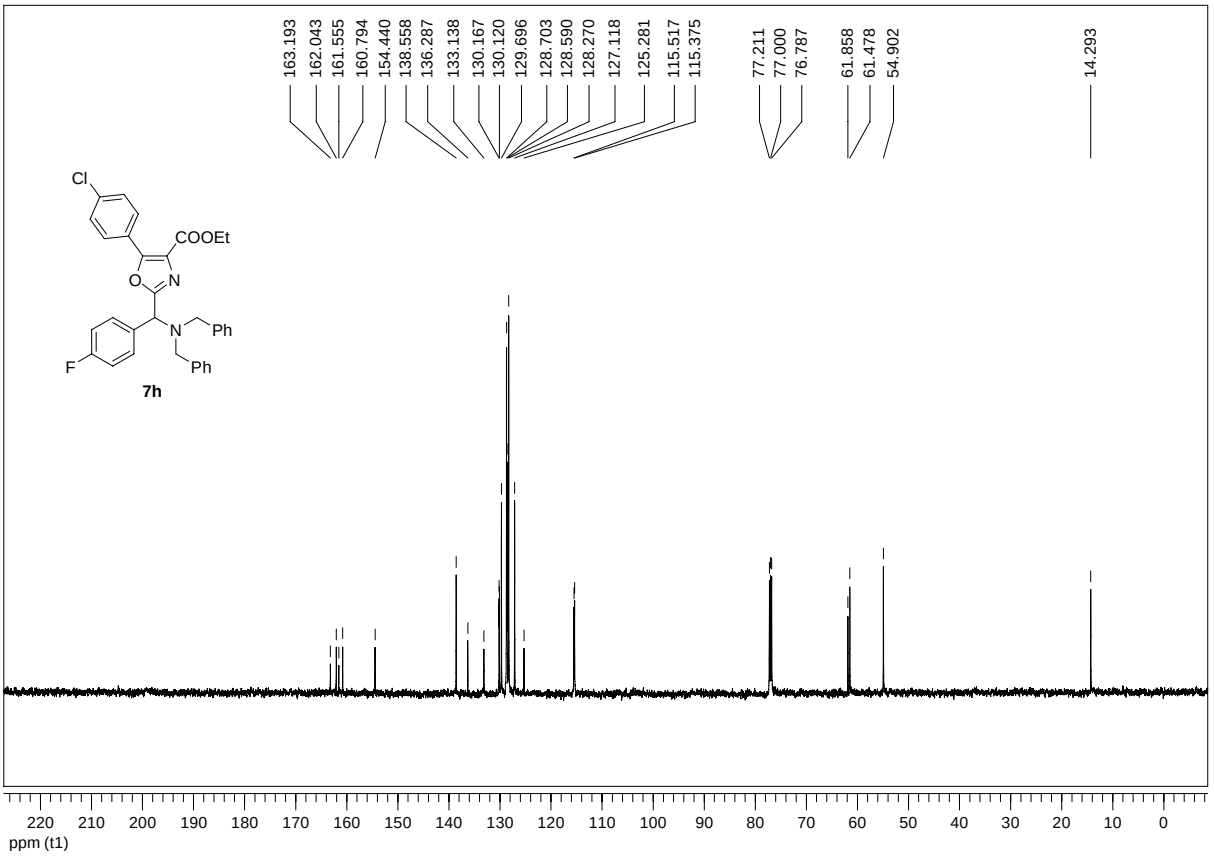
147.373
144.353
142.003
133.719
129.926
129.878
125.041
115.288
115.224
115.147
112.098
77.211
77.000
76.787
63.130
61.195
43.608
14.296
11.808
COOEt
O
N
F
7g
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)


7.920
7.907
7.520
7.511
7.500
7.432
7.419
7.358
7.346
7.294
7.282
7.270
7.206
7.195
7.183
7.072
7.058
7.045
5.249
4.459
4.448
4.437
4.425
3.799
3.776
3.686
3.662
1.691
1.426
1.414
1.403
0.000000
Cl
COOEt
O
N
N
Ph
Ph
F
7h
2.01
8.00
2.01
1.01
2.01
2.00
3.02
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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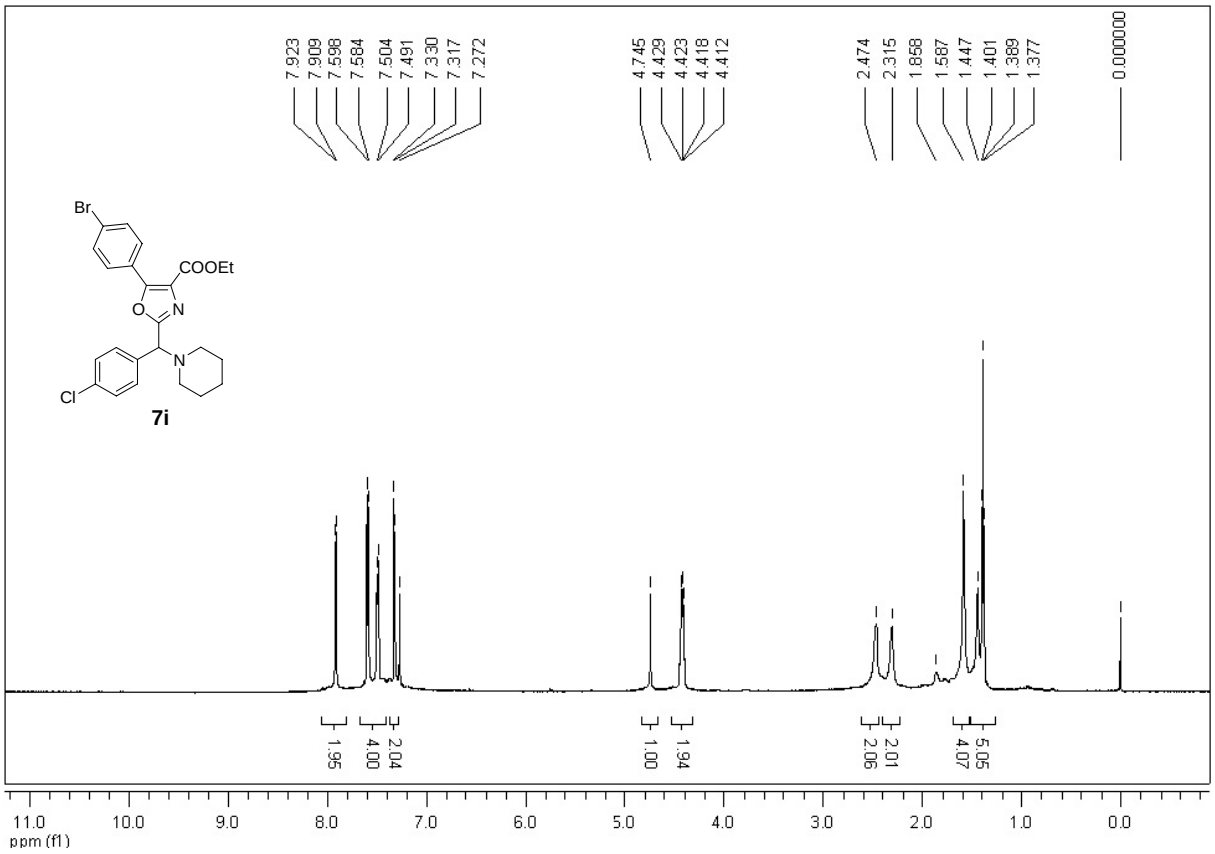
161.555
160.794
154.440
138.558
136.287
133.138
130.167
130.120
129.696
128.703
128.590
128.270
127.118
125.281
115.517
115.375
77.211
77.000
76.787
61.858
61.478
54.902
14.293
Cl
COOEt
O
N
N
Ph
Ph
F
7h
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)


7.923
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7.584
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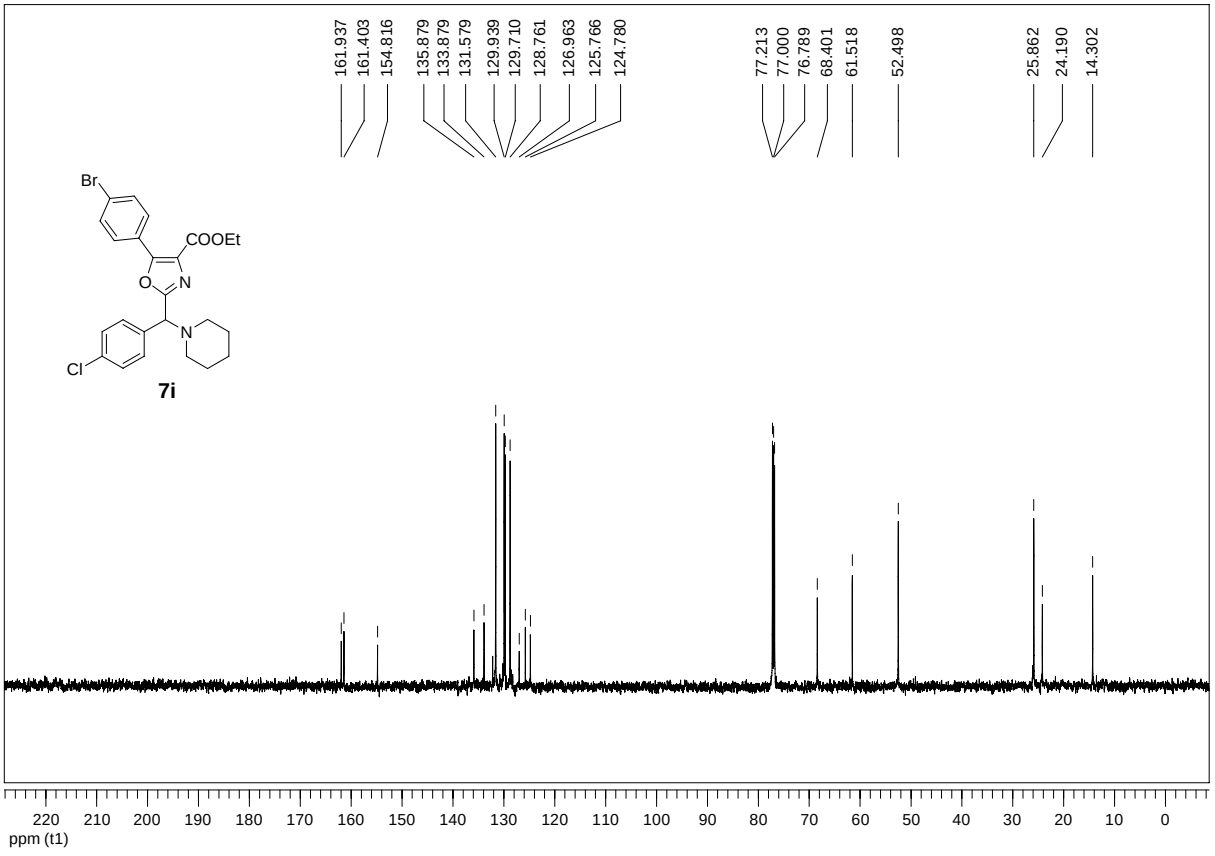
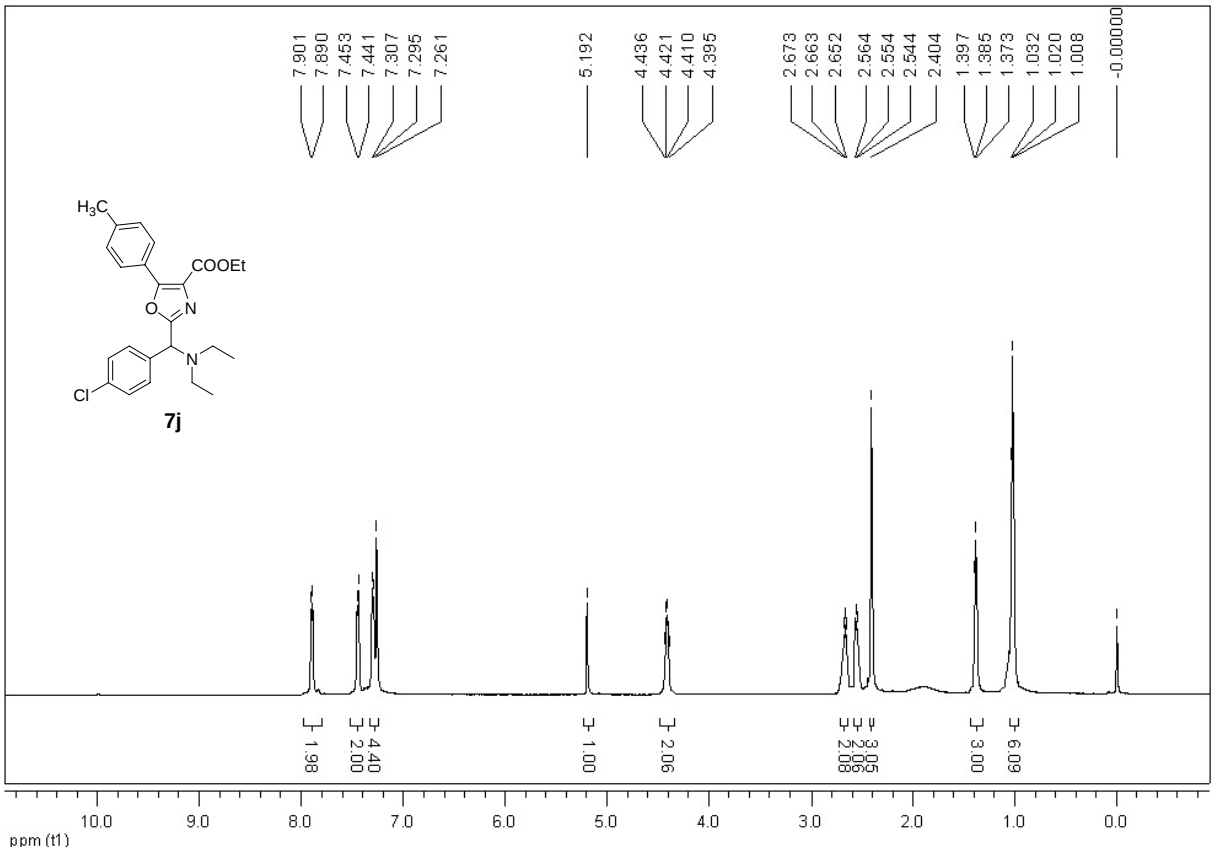
7.330
7.317
7.272
4.745
4.429
4.423
4.418
4.412
2.474
2.315
1.858
1.587
1.447
1.401
1.389
1.377
0.000000
Br
COOEt
O
N
N
Cl
7i
1.95
4.00
2.04
1.00
1.94
2.06
2.01
4.07
5.05
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)


161.937
161.403
154.816
135.879
133.879
131.579
129.939
129.710
128.761
126.963
125.766
124.780
77.213
77.000
76.789
68.401
61.518
52.498
25.862
24.190
14.302
Br
COOEt
O
N
N
Cl
7i
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)


7.901
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7.441
7.307
7.295
7.261
5.192
4.436
4.421
4.410
4.395
2.673
2.663
2.652
2.564
2.554
2.544
2.404
1.397
1.385
1.373
1.032
1.020
1.008
-0.00000
H3C
COOEt
O
N
N
Cl
7j
1.98
2.00
4.40
1.00
2.06
3.05
2.96
2.08
3.00
6.09
10.0
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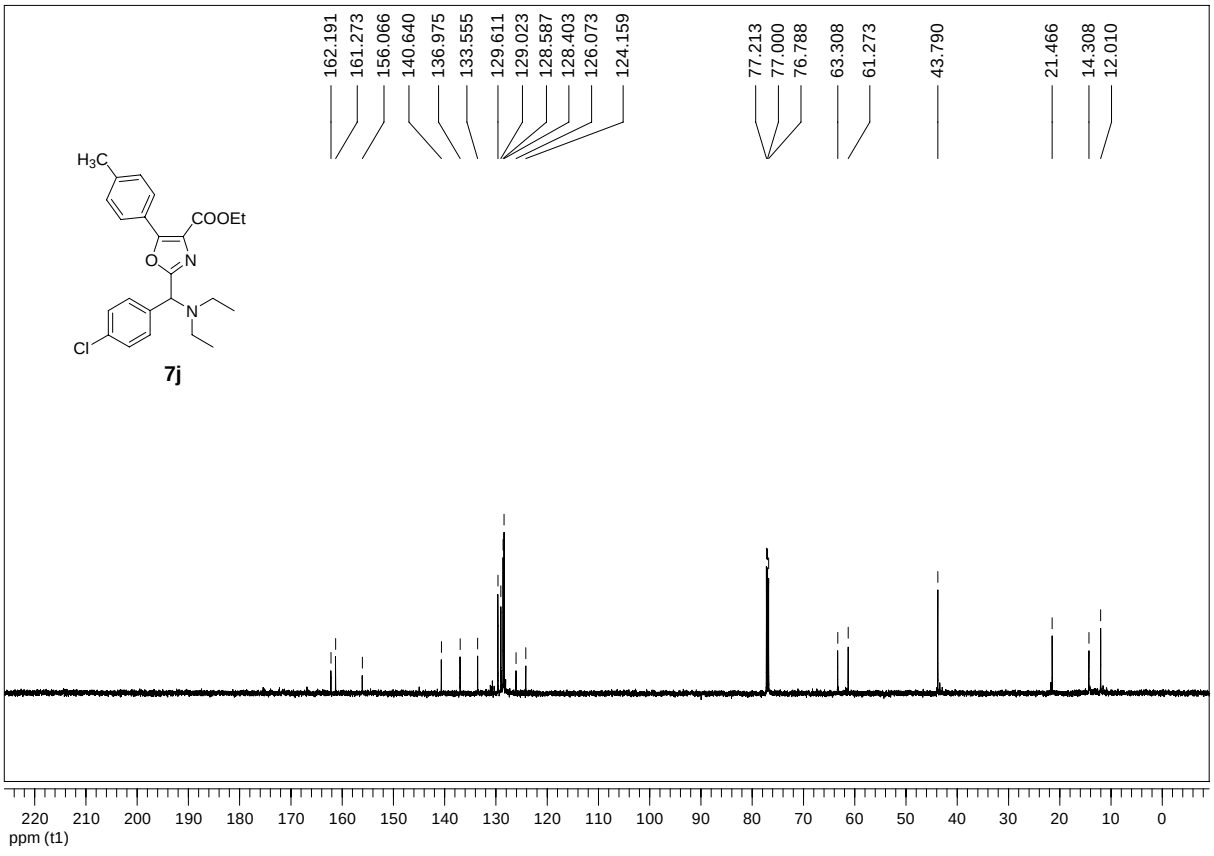
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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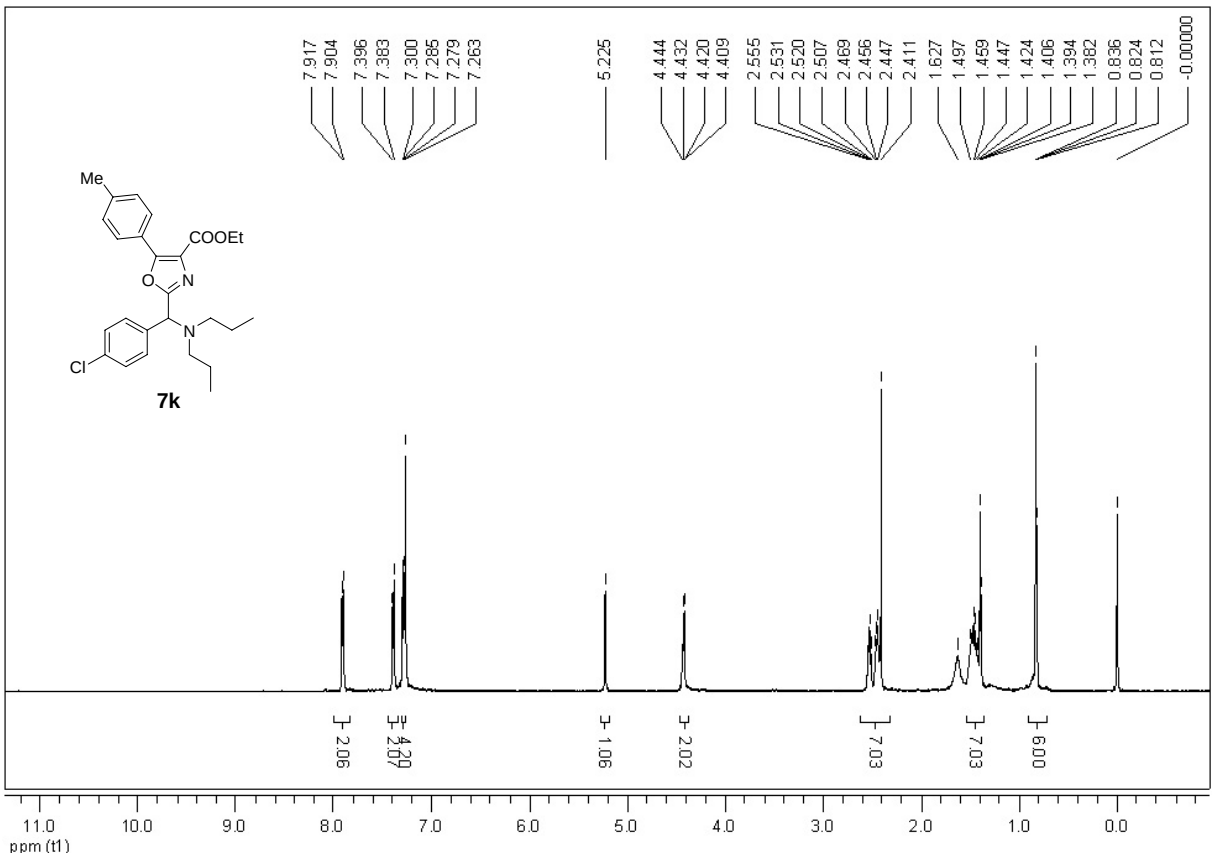
129.611
129.023
128.587
128.403
126.073
124.159
77.213
77.000
76.788
63.308
61.273
43.790
21.466
14.308
12.010
H3C
COOEt
O
N
N
Cl
7j
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)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7.300
7.285
7.279
7.263
5.225
4.444
4.432
4.420
4.409
2.555
2.531
2.520
2.507
2.469
2.456
2.447
2.411
1.627
1.497
1.459
1.447
1.424
1.406
1.394
1.382
0.836
0.824
0.812
-0.00000
Me
COOEt
O
N
N
Cl
7k
2.06
4.20
1.06
2.02
7.03
7.03
6.00
11.0
10.0
9.0
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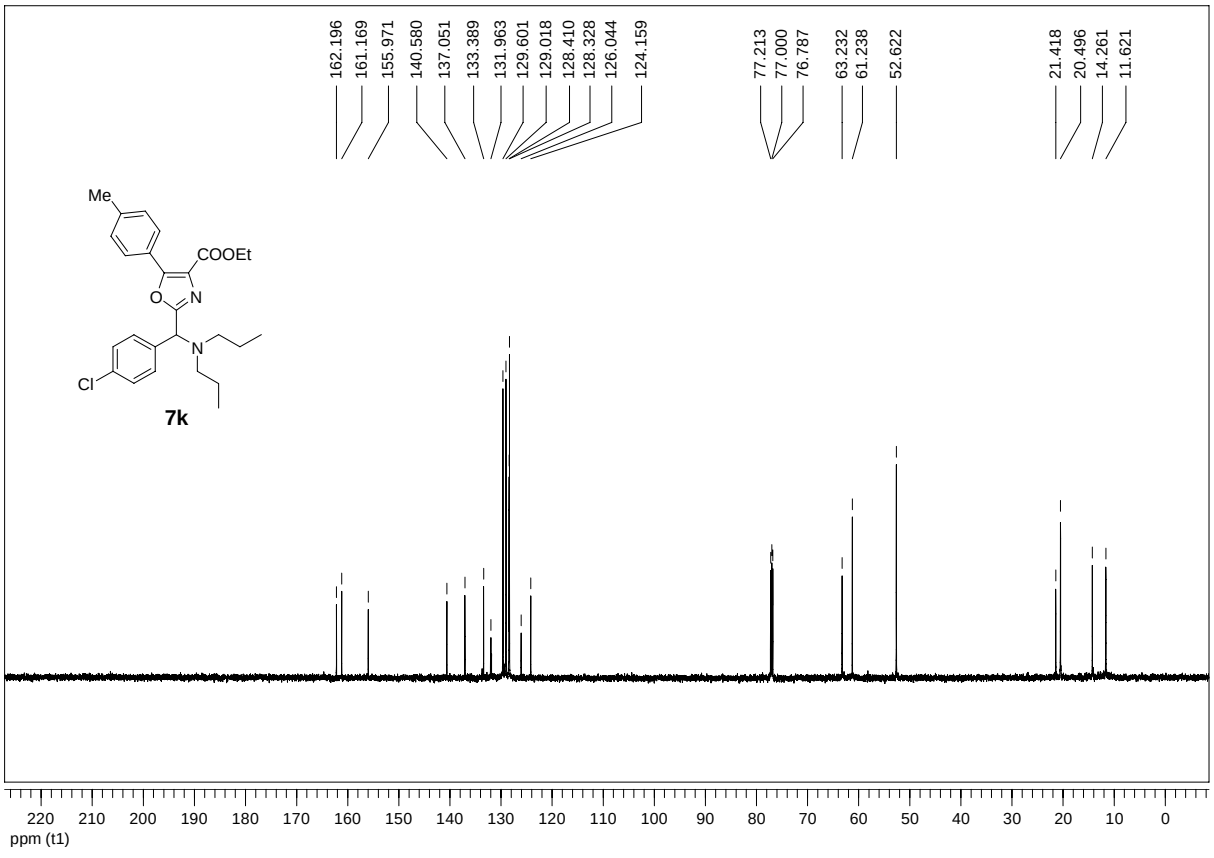
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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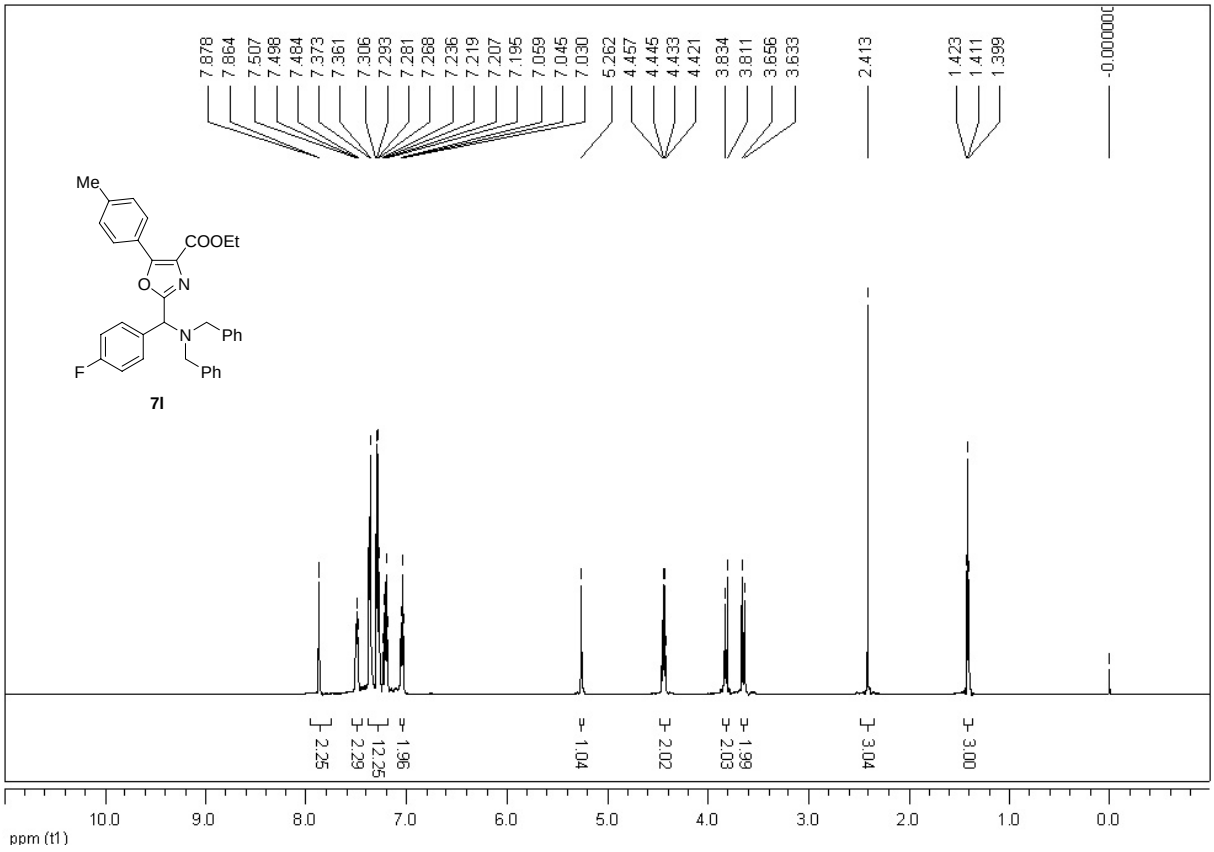
140.580
137.051
133.389
131.963
129.601
129.018
128.410
128.328
126.044
124.159
77.213
77.000
76.787
63.232
61.238
52.622
21.418
20.496
14.261
11.621
Me
COOEt
O
N
N
Cl
7k
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)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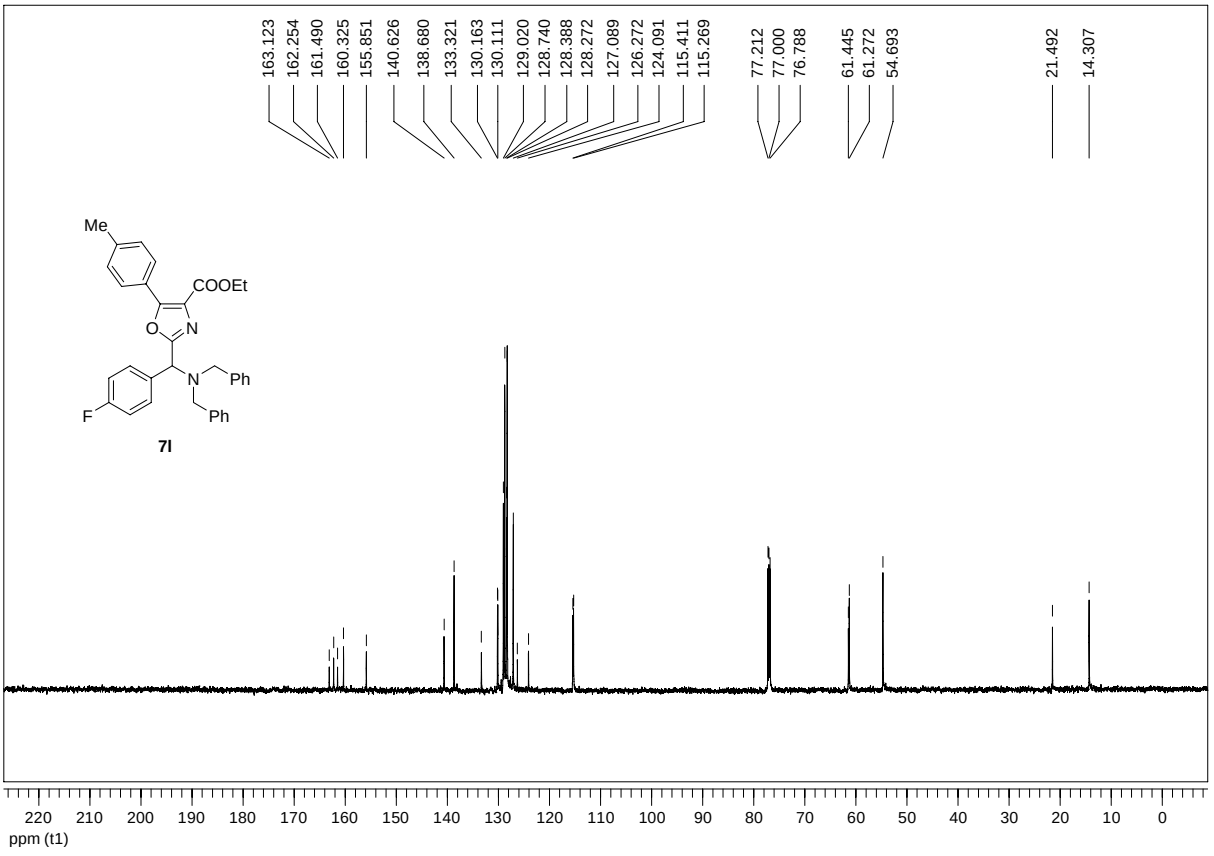
7.361
7.306
7.293
7.281
7.268
7.236
7.219
7.207
7.195
7.059
7.045
7.030
5.262
4.457
4.445
4.433
4.421
3.834
3.811
3.656
3.633
2.413
1.423
1.411
1.399
-0.000000
Me
COOEt
O
N
N
Ph
Ph
F
7l
2.25
2.29
12.25
1.96
1.04
2.02
2.03
1.99
3.04
3.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


163.123
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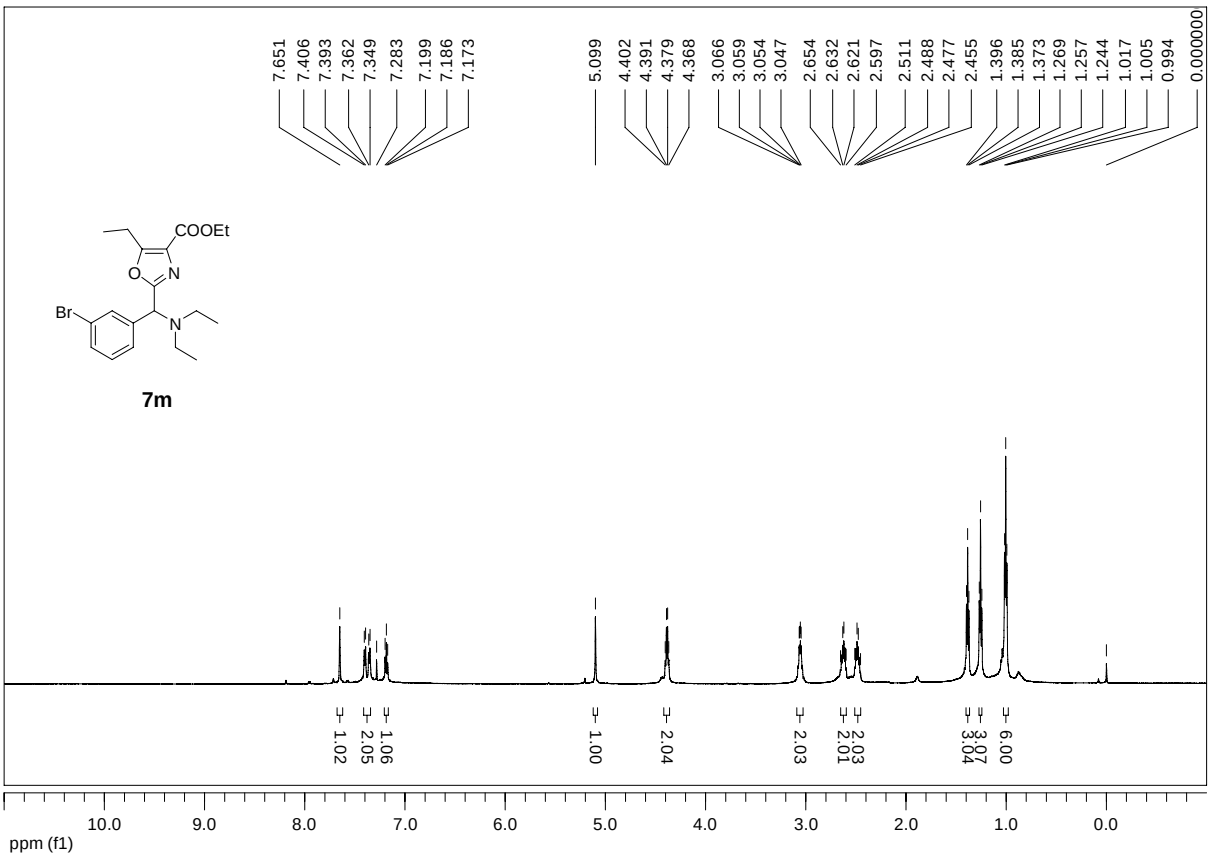
160.325
155.851
140.626
138.680
133.321
130.163
130.111
129.020
128.740
128.388
128.272
127.089
126.272
124.091
115.411
115.269
77.212
77.000
76.788
61.445
61.272
54.693
21.492
14.307
Me
COOEt
O
N
N
Ph
Ph
F
7l
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)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7.362
7.349
7.283
7.199
7.186
7.173
5.099
4.402
4.391
4.379
4.368
3.066
3.059
3.054
3.047
2.654
2.632
2.621
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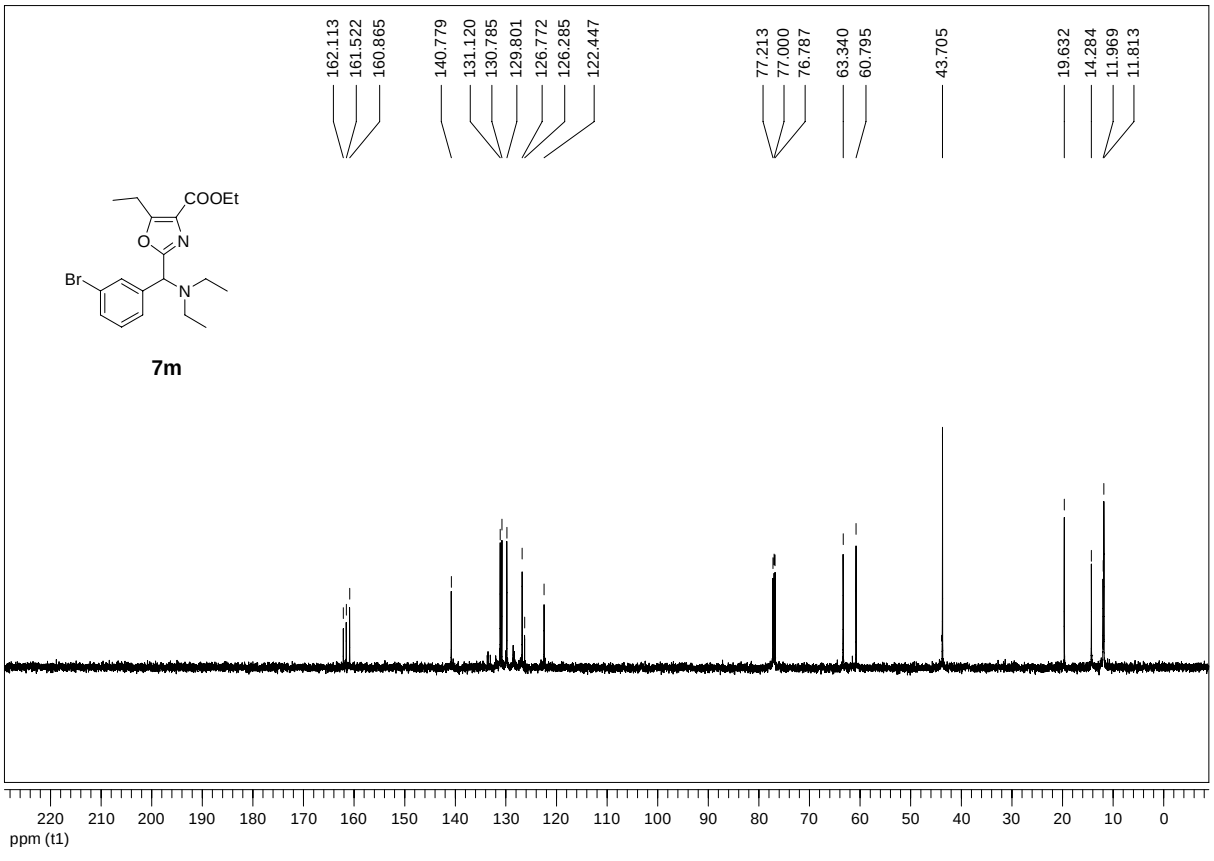
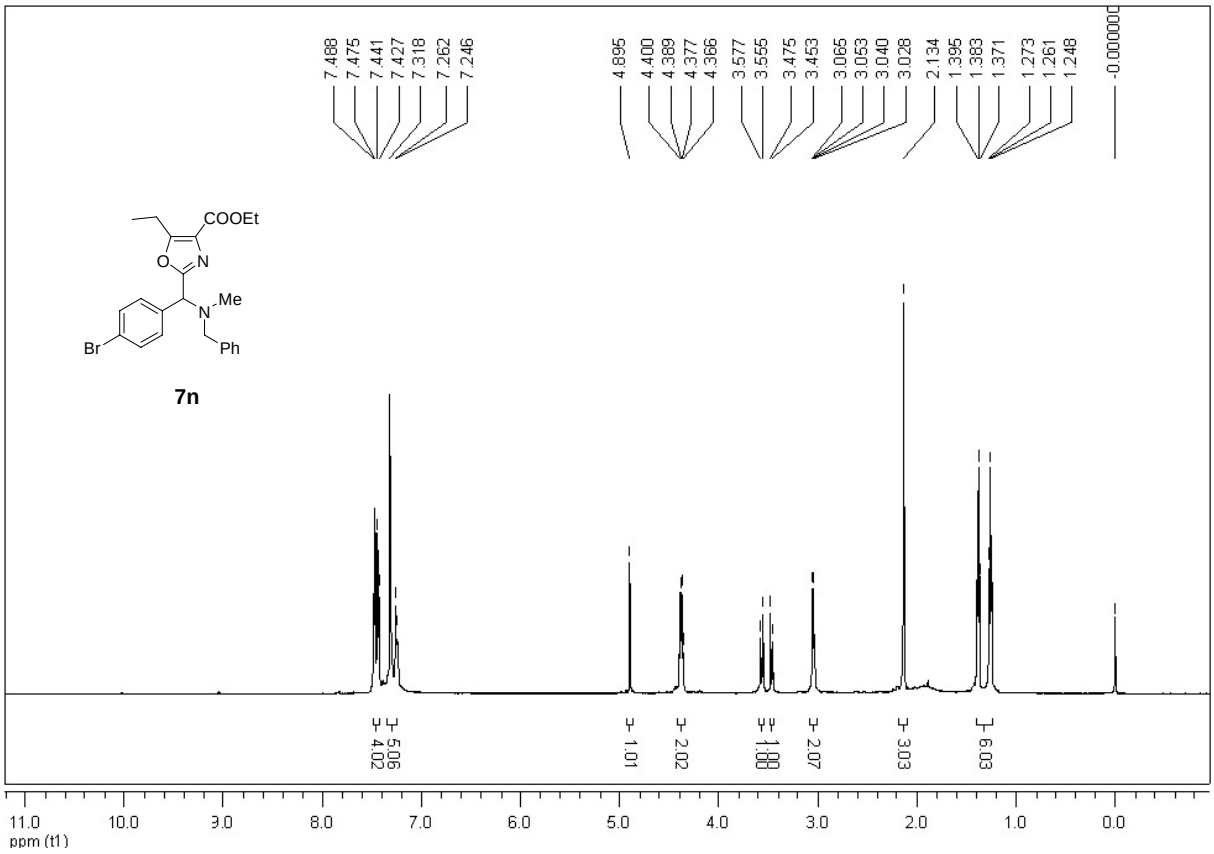
2.477
2.455
1.396
1.385
1.373
1.269
1.257
1.244
1.017
1.005
0.994
0.000000
COOEt
O
N
Br
N
1.02
2.05
1.06
1.00
2.04
2.03
2.01
2.03
3.04
3.07
6.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)

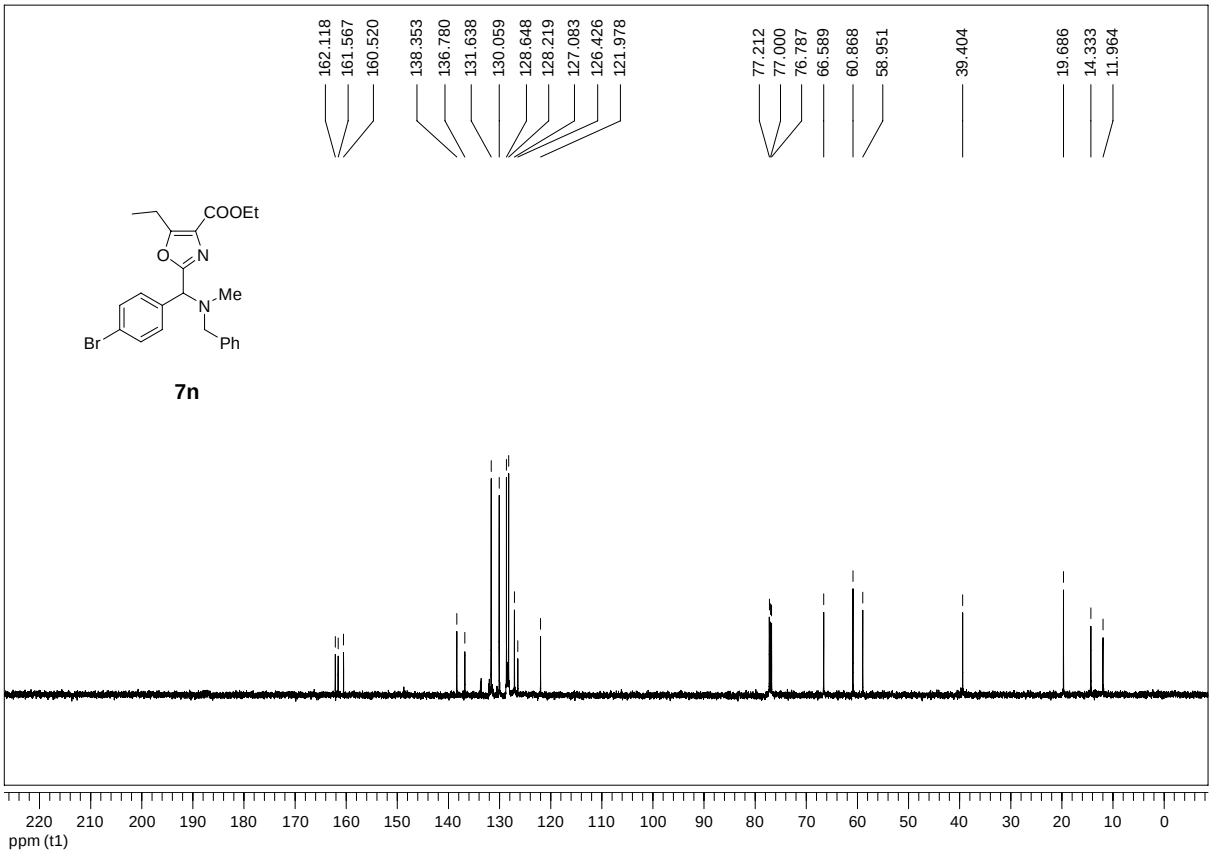
**7m**


162.113
161.522
160.865
140.779
131.120
130.785
129.801
126.772
126.285
122.447
77.213
77.000
76.787
63.340
60.795
43.705
19.632
14.284
11.969
11.813
COOEt
O
N
Br
N
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

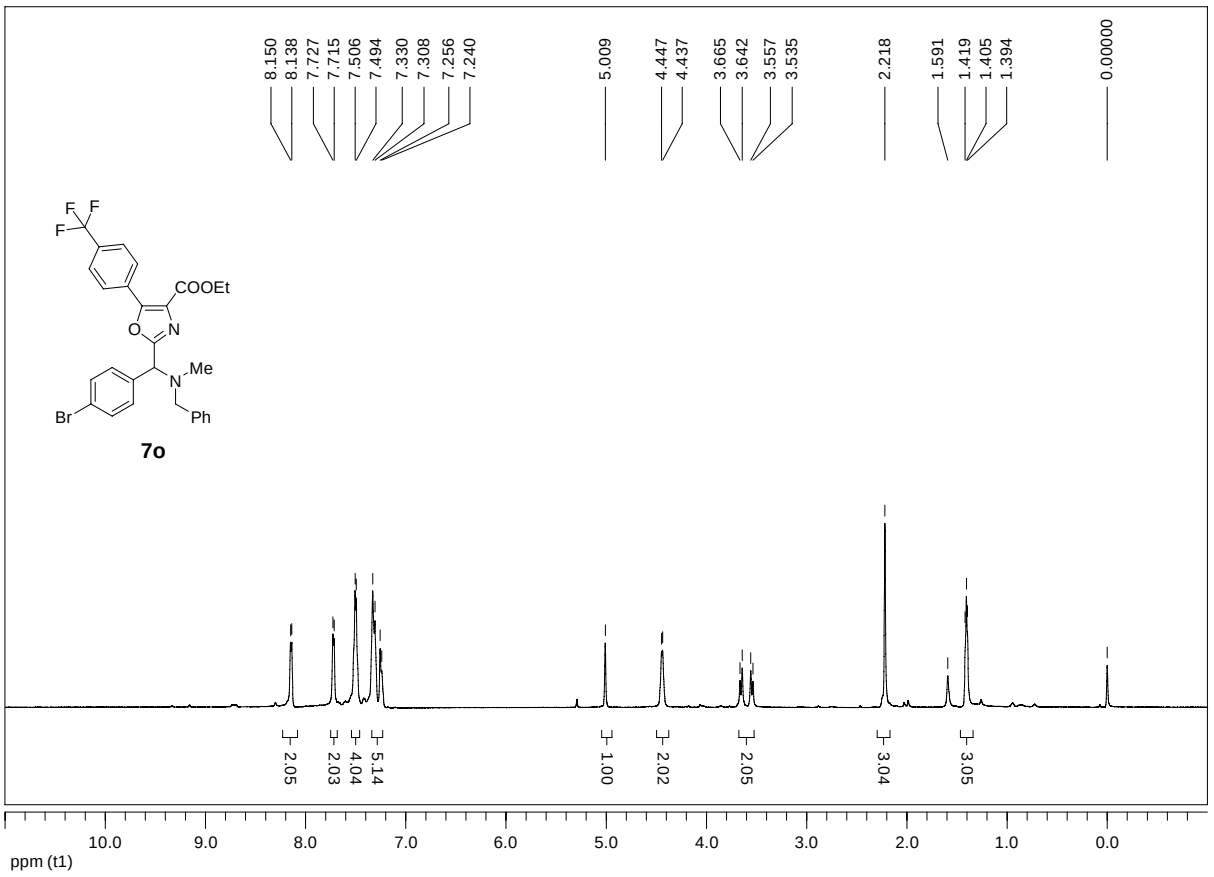
**7m**

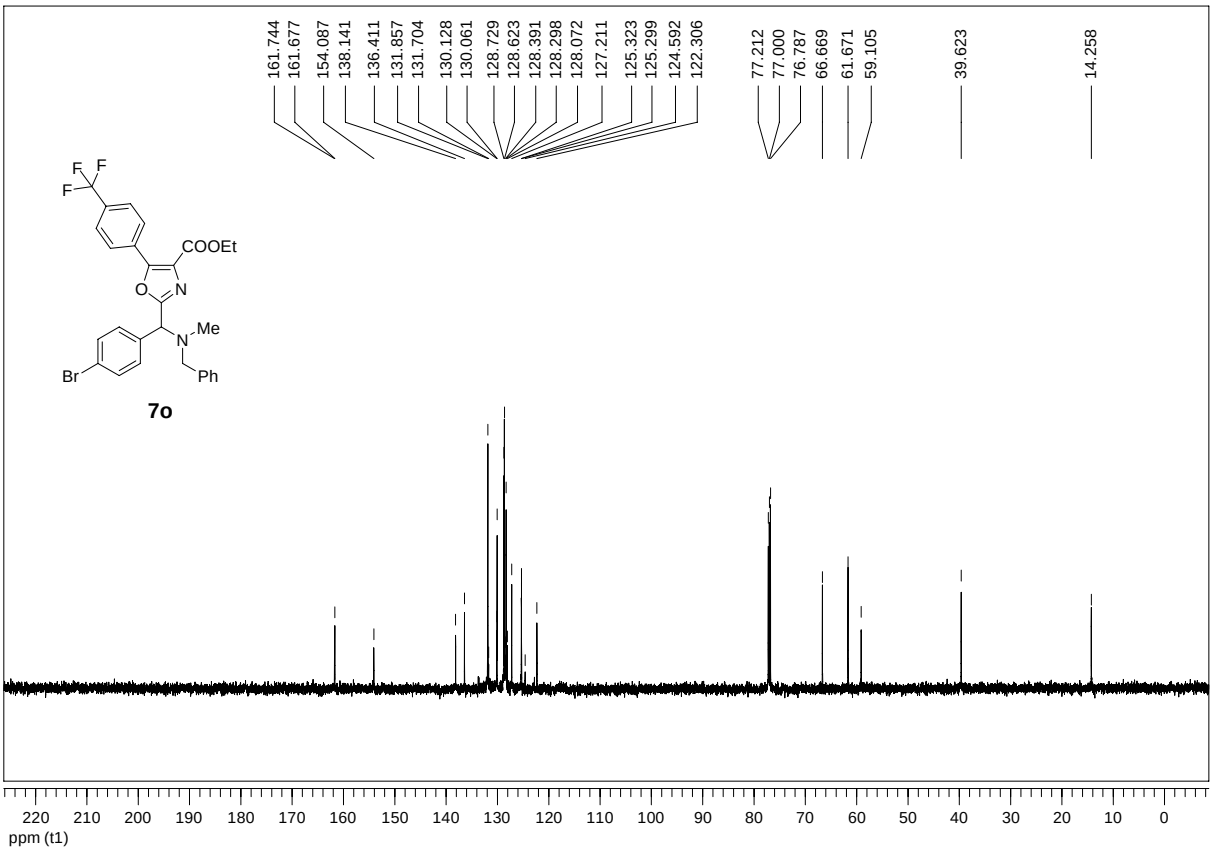

7.488
7.475
7.441
7.427
7.318
7.262
7.246
4.895
4.400
4.389
4.377
4.366
3.577
3.555
3.475
3.453
3.065
3.053
3.040
3.028
2.134
1.395
1.383
1.371
1.273
1.261
1.248
-0.000000
COOEt
O
N
Me
N
Br
Ph
5.06
4.02
1.01
2.02
1.00
2.07
3.03
6.03
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

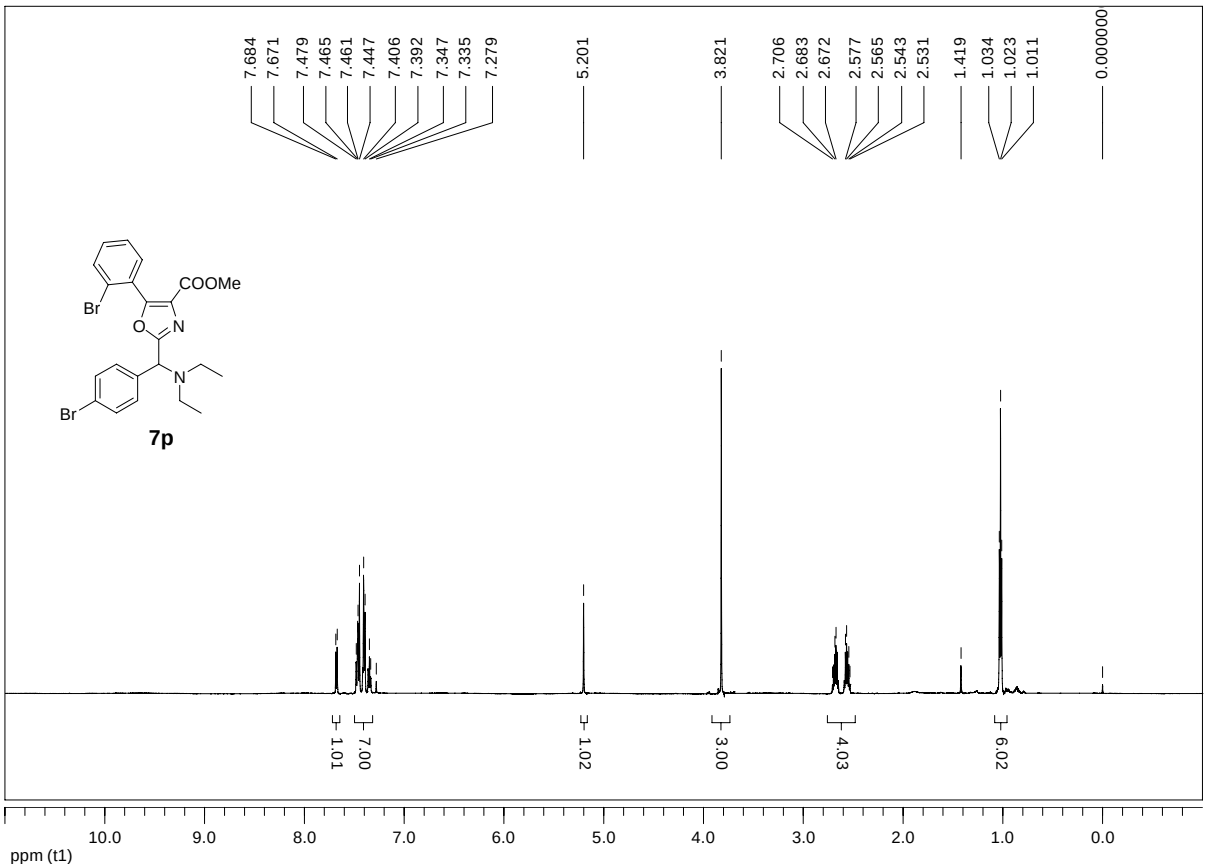
**7n**


162.118
161.567
160.520
138.353
136.780
131.638
130.059
128.648
128.219
127.083
126.426
121.978
77.212
77.000
76.787
66.589
60.868
58.951
39.404
19.686
14.333
11.964
COOEt
O
N
Me
N
Br
Ph
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

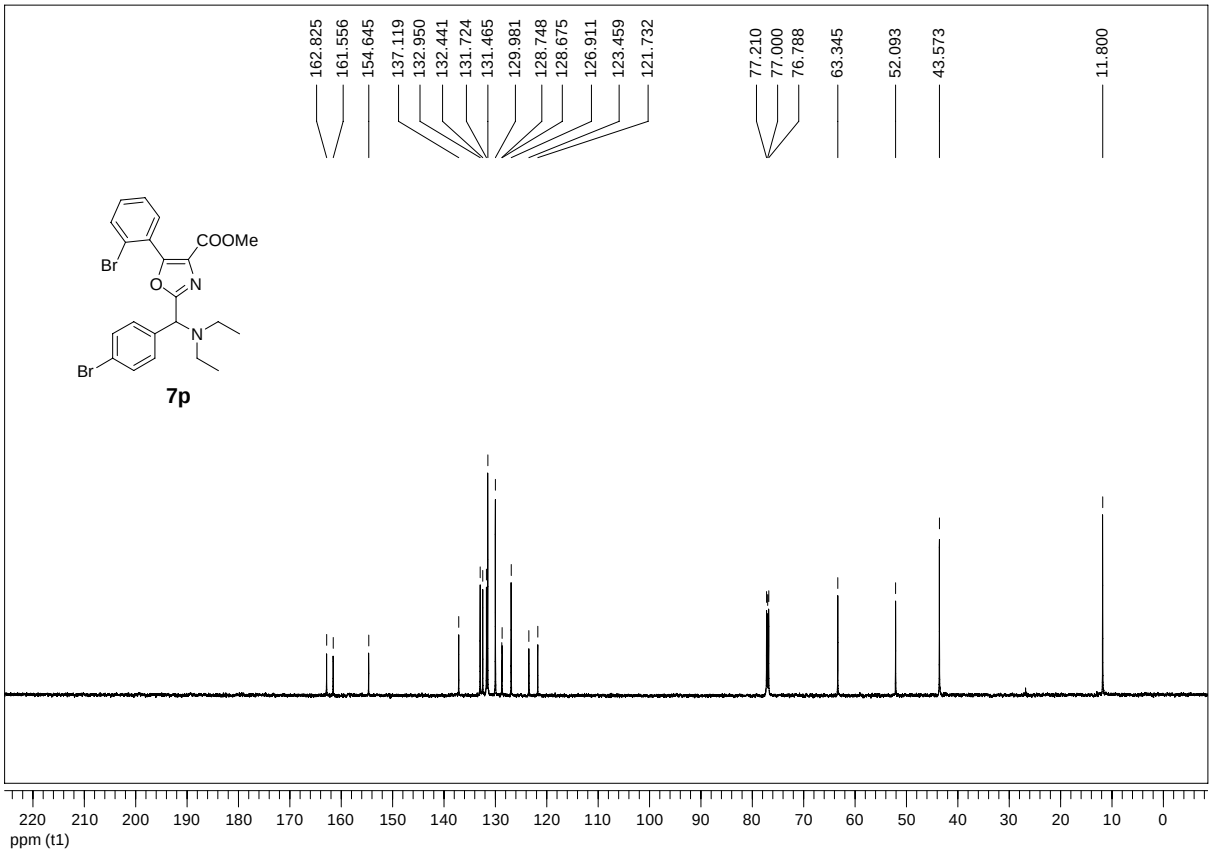
**7n**


8.150
8.138
7.727
7.715
7.506
7.494
7.330
7.308
7.256
7.240
5.009
4.447
4.437
3.665
3.642
3.557
3.535
2.218
1.591
1.419
1.405
1.394
0.00000
F
F
F
COOEt
O
N
N
Me
Ph
Br
7o
2.05
2.03
4.04
5.14
1.00
2.02
2.05
3.04
3.05
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

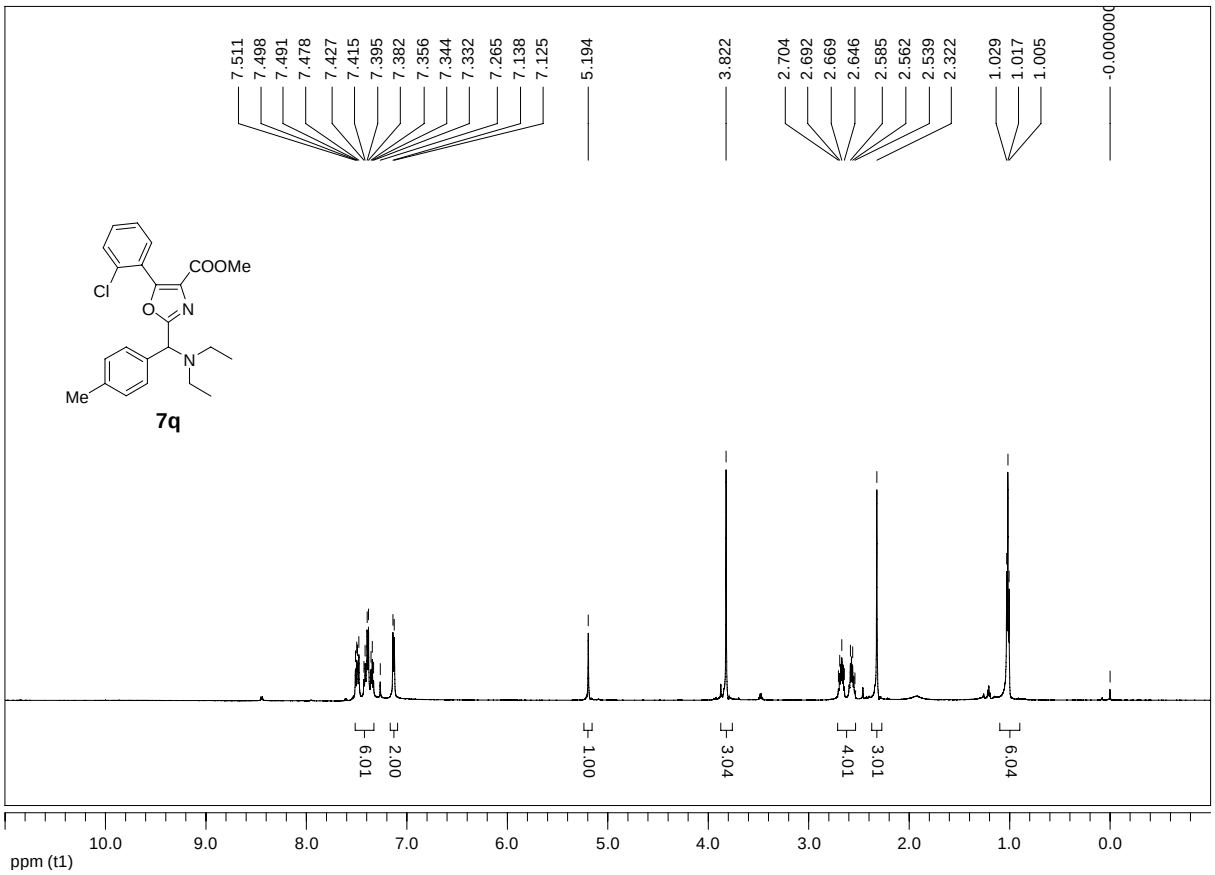

161.744
161.677
154.087
138.141
136.411
131.857
131.704
130.128
130.061
128.729
128.623
128.391
128.298
128.072
127.211
125.323
125.299
124.592
122.306
77.212
77.000
76.787
66.669
61.671
59.105
39.623
14.258
F
F
F
COOEt
O
N
N
Me
Ph
Br
7o
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

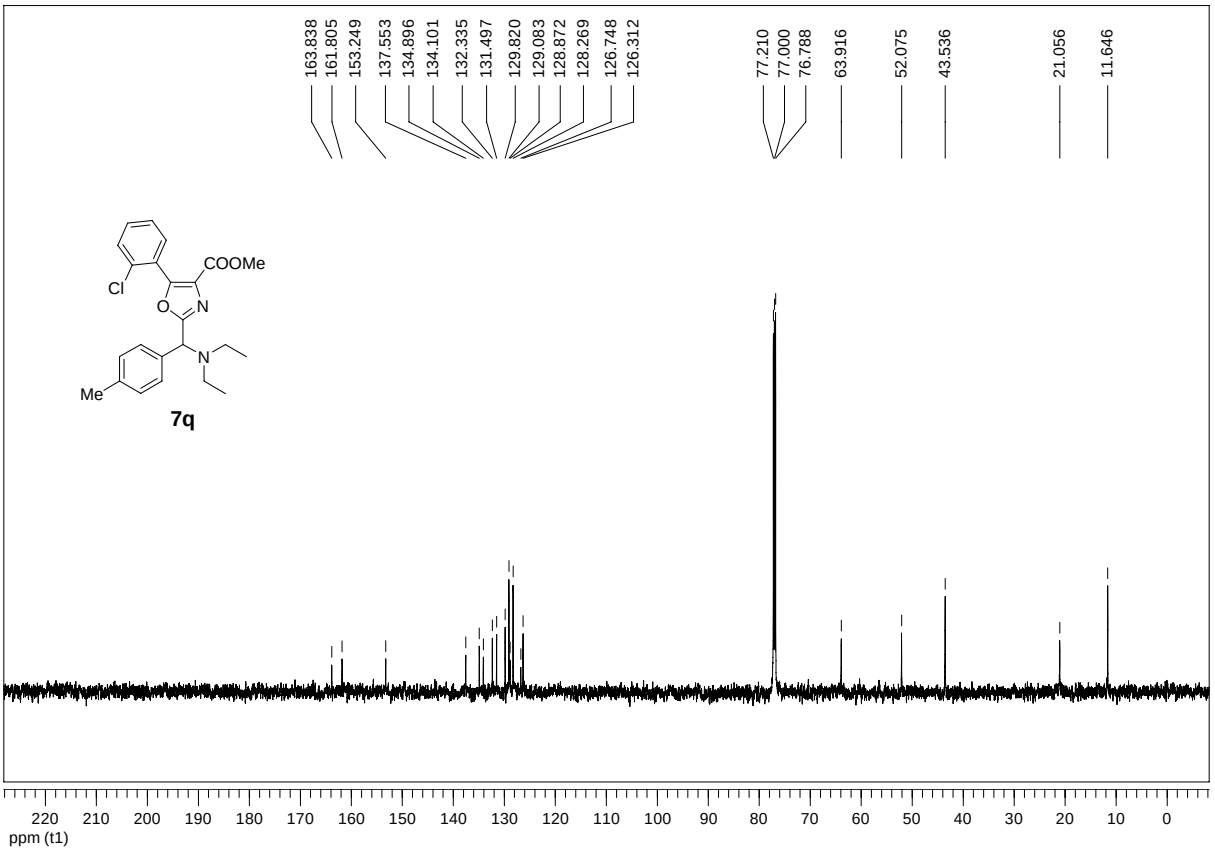

7.684
7.671
7.479
7.465
7.461
7.447
7.406
7.392
7.347
7.335
7.279
5.201
3.821
2.706
2.683
2.672
2.577
2.565
2.543
2.531
1.419
1.034
1.023
1.011
0.000000
COOMe
Br
O
N
N
Br
1.01
7.00
1.02
3.00
4.03
6.02
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

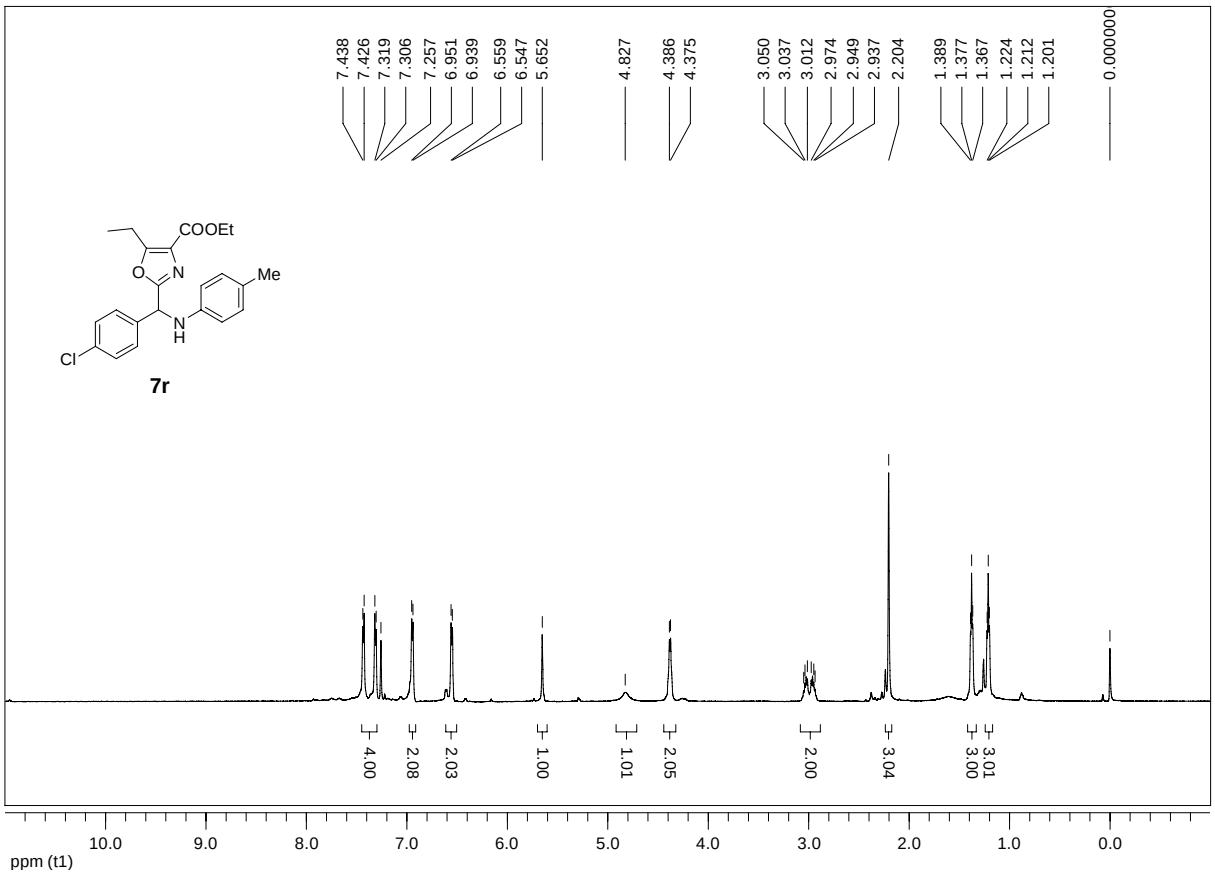
**7p**

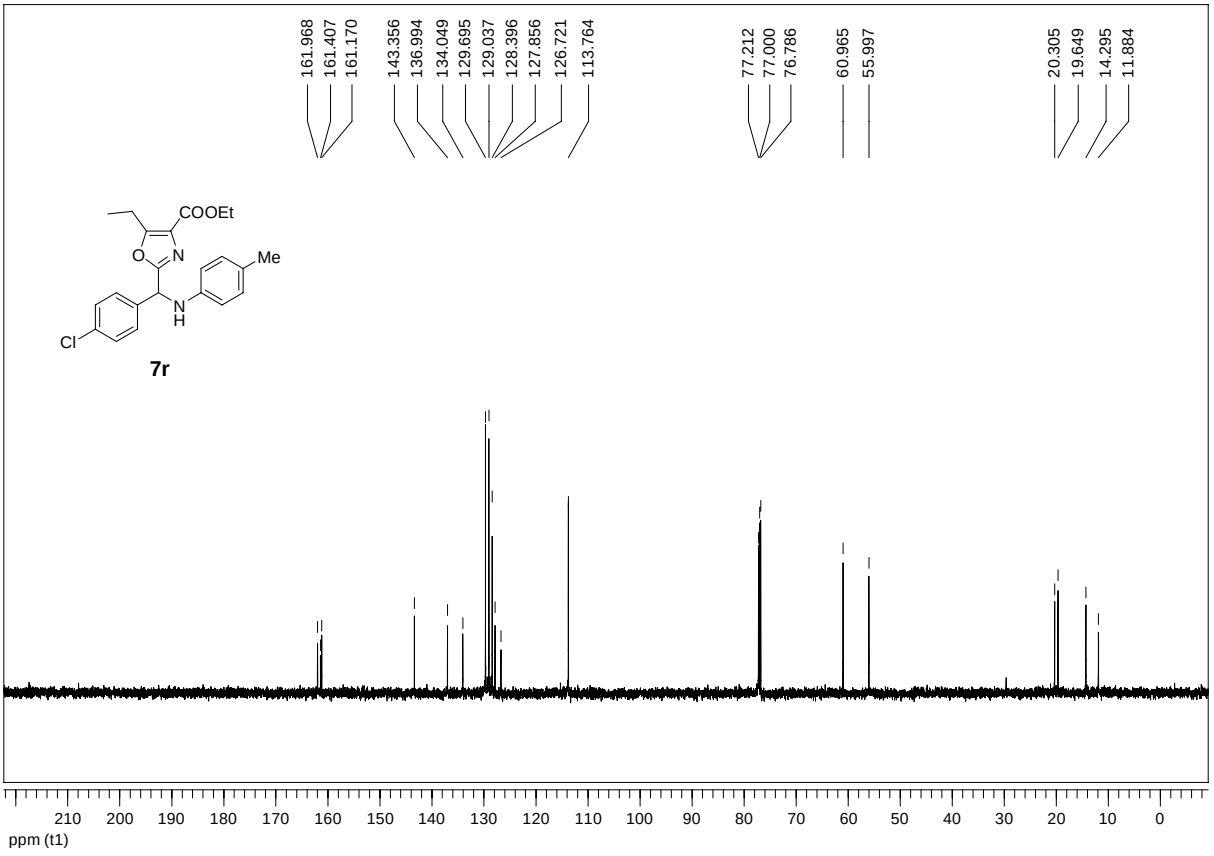

162.825
161.556
154.645
137.119
132.950
132.441
131.724
131.465
129.981
128.748
128.675
126.911
123.459
121.732
77.210
77.000
76.788
63.345
52.093
43.573
11.800
COOMe
Br
O
N
N
Br
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

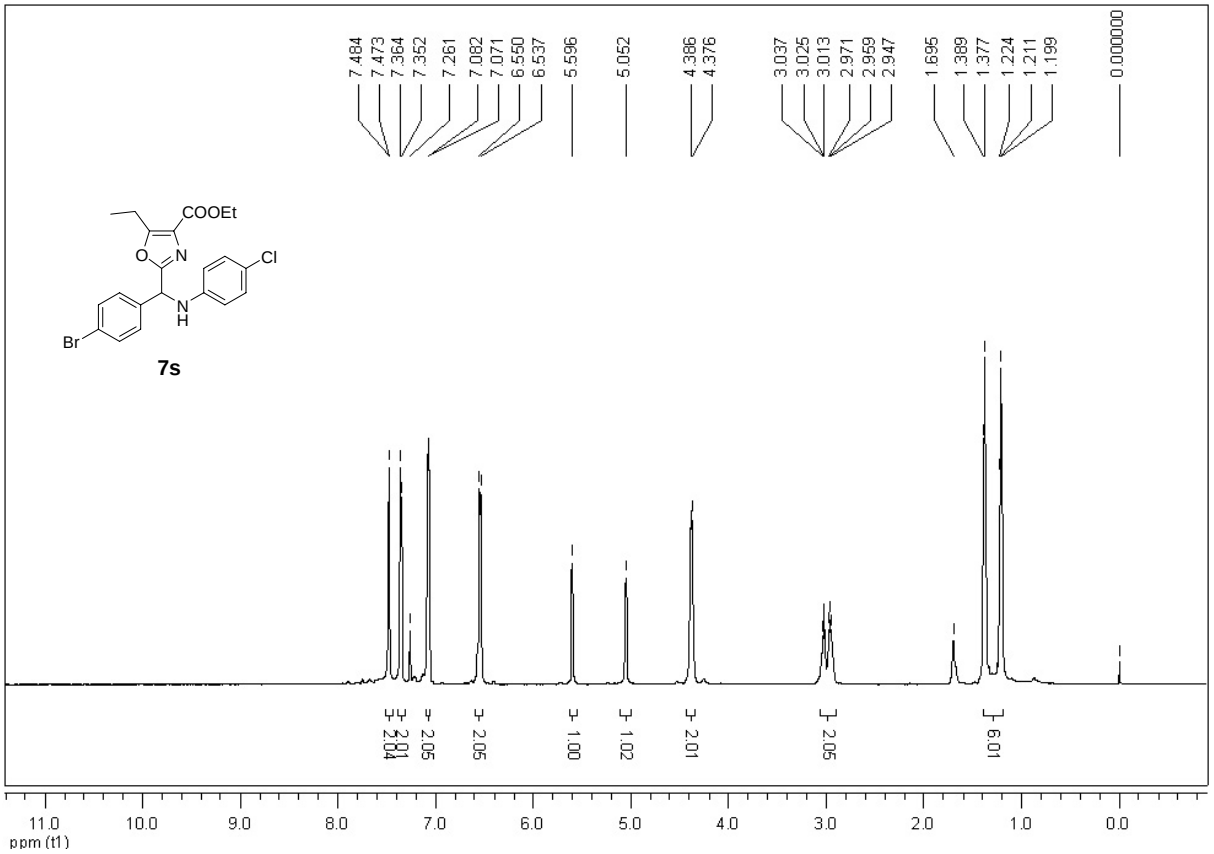
**7p**

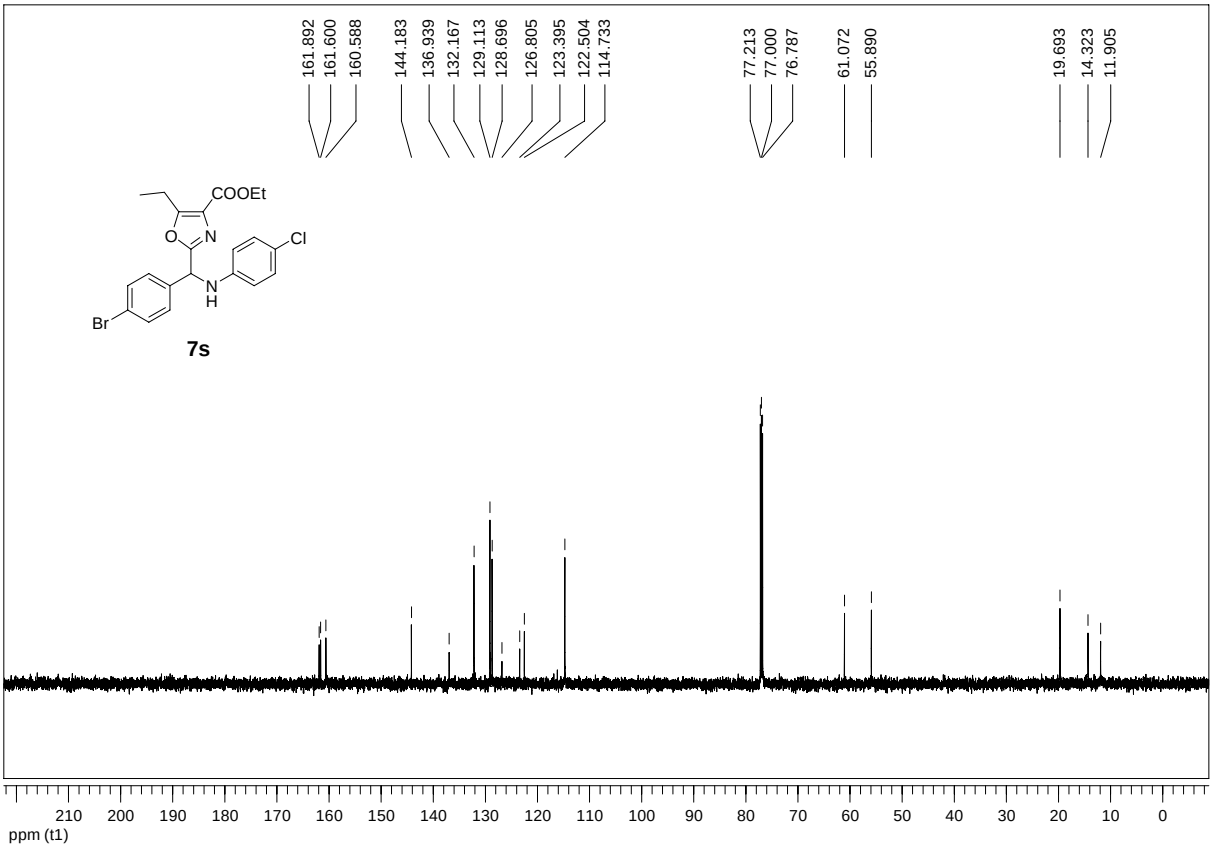

7.511
7.498
7.491
7.478
7.427
7.415
7.395
7.382
7.356
7.344
7.332
7.265
7.138
7.125
5.194
3.822
2.704
2.692
2.669
2.646
2.585
2.562
2.539
2.322
1.029
1.017
1.005
-0.000000
COOMe
Cl
O
N
N
Me
7q
6.01
2.00
1.00
3.04
4.01
3.01
6.04
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

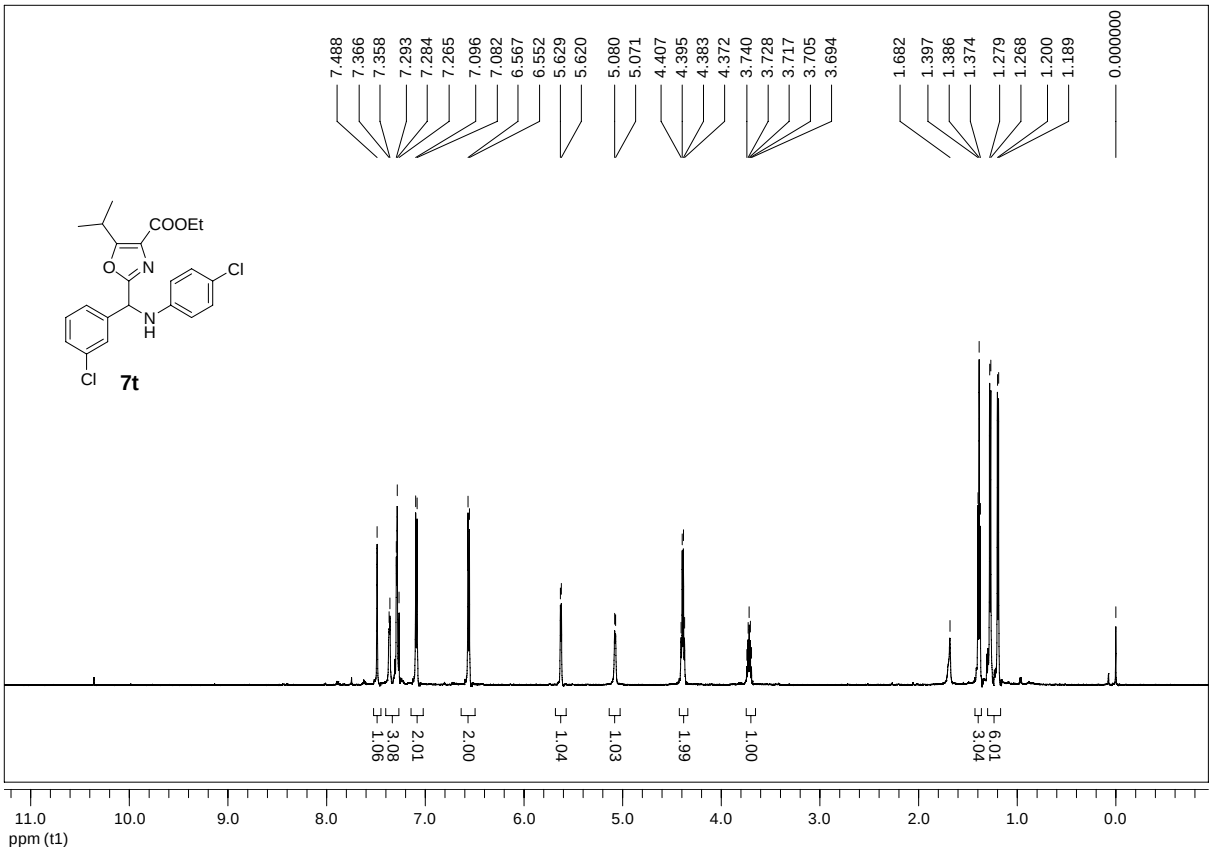

163.838
161.805
153.249
137.553
134.896
134.101
132.335
131.497
129.820
129.083
128.872
128.269
126.748
126.312
77.210
77.000
76.788
63.916
52.075
43.536
21.056
11.646
COOMe
Cl
O
N
N
Me
7q
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

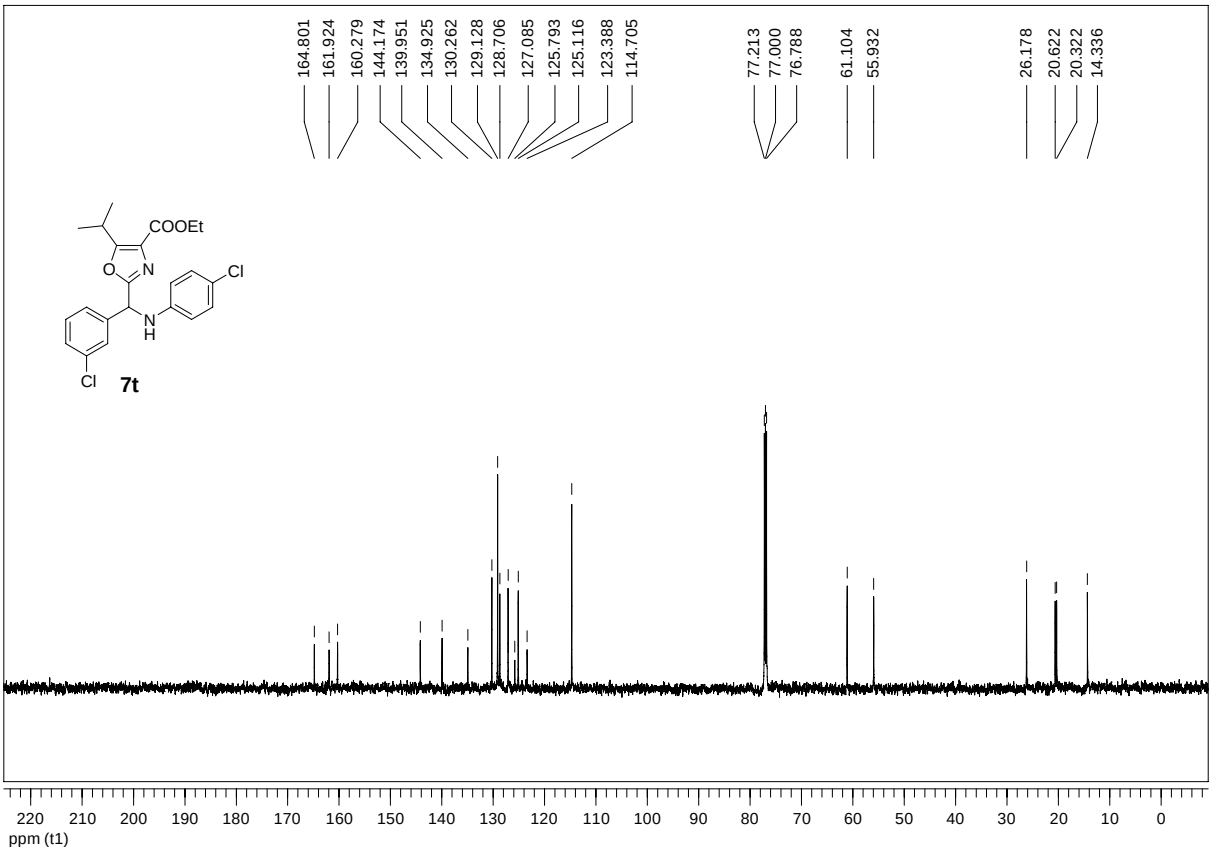

7.438
7.426
7.319
7.306
7.257
6.951
6.939
6.559
6.547
5.652
4.827
4.386
4.375
3.050
3.037
3.012
2.974
2.949
2.937
2.204
1.389
1.377
1.367
1.224
1.212
1.201
0.000000
COOEt
O
N
Me
NH
Cl
7r
4.00
2.08
2.03
1.00
1.01
2.05
2.00
3.04
3.00
3.01
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


161.968
161.407
161.170
143.356
136.994
134.049
129.695
129.037
128.396
127.856
126.721
113.764
77.212
77.000
76.786
60.965
55.997
20.305
19.649
14.295
11.884
COOEt
O
N
Me
NH
Cl
7r
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)


7.484
7.473
7.364
7.352
7.261
7.082
7.071
6.550
6.537
5.596
5.052
4.386
4.376
3.037
3.025
3.013
2.971
2.959
2.947
1.695
1.389
1.377
1.224
1.211
1.199
0.000000
COOEt
O
N
Cl
N
H
Br
7s
2.04
2.01
2.06
2.06
1.00
1.02
2.01
2.05
6.01
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


161.892
161.600
160.588
144.183
136.939
132.167
129.113
128.696
126.805
123.395
122.504
114.733
77.213
77.000
76.787
61.072
55.890
19.693
14.323
11.905
COOEt
O
N
Cl
N
H
Br
7s
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)


7.488
7.366
7.358
7.293
7.284
7.265
7.096
7.082
6.567
6.552
5.629
5.620
5.080
5.071
4.407
4.395
4.383
4.372
3.740
3.728
3.717
3.705
3.694
1.682
1.397
1.386
1.374
1.279
1.268
1.200
1.189
0.000000
COOEt
O
N
Cl
NH
Cl
7t
1.06
3.08
2.01
2.00
1.04
1.03
1.99
1.00
6.04
3.04
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


164.801
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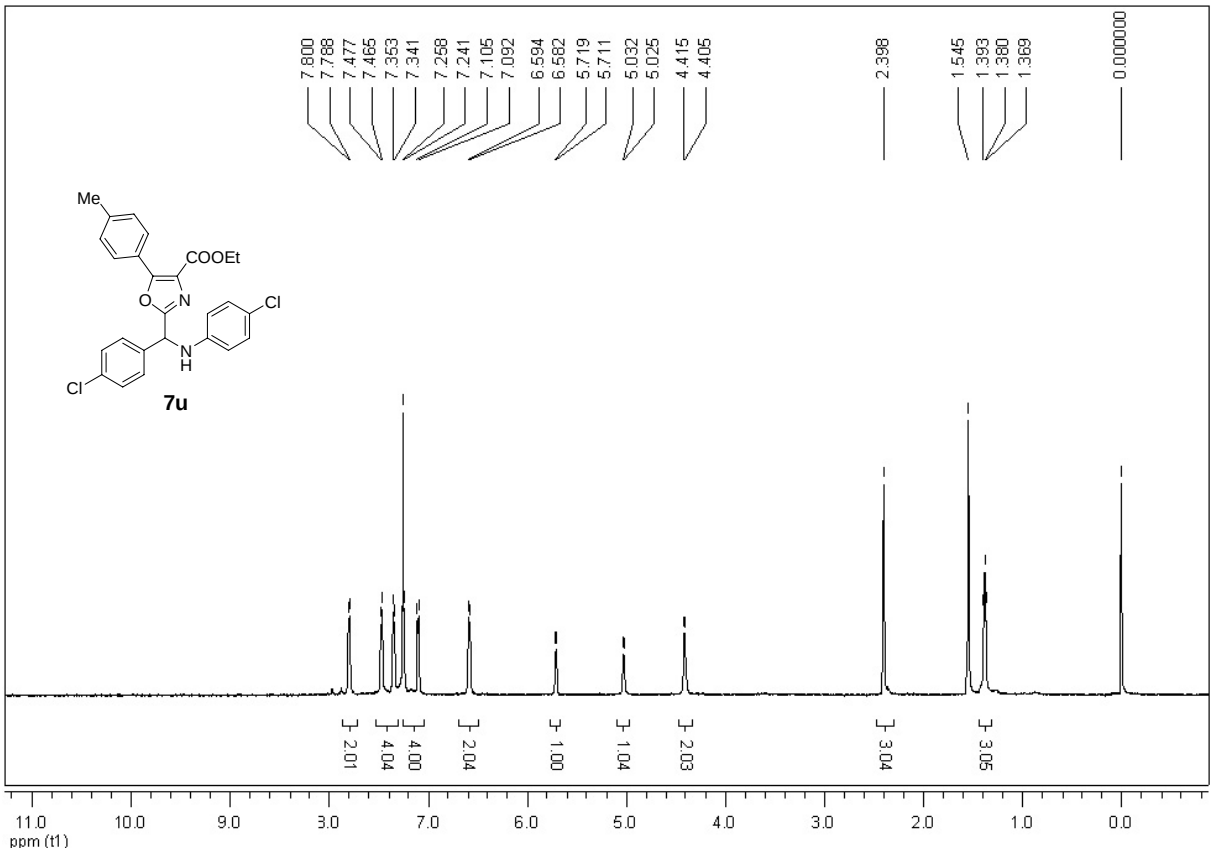
160.279
144.174
139.951
134.925
130.262
129.128
128.706
127.085
125.793
125.116
123.388
114.705
77.213
77.000
76.788
61.104
55.932
26.178
20.622
20.322
14.336
COOEt
O
N
Cl
NH
Cl
7t
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)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7.788
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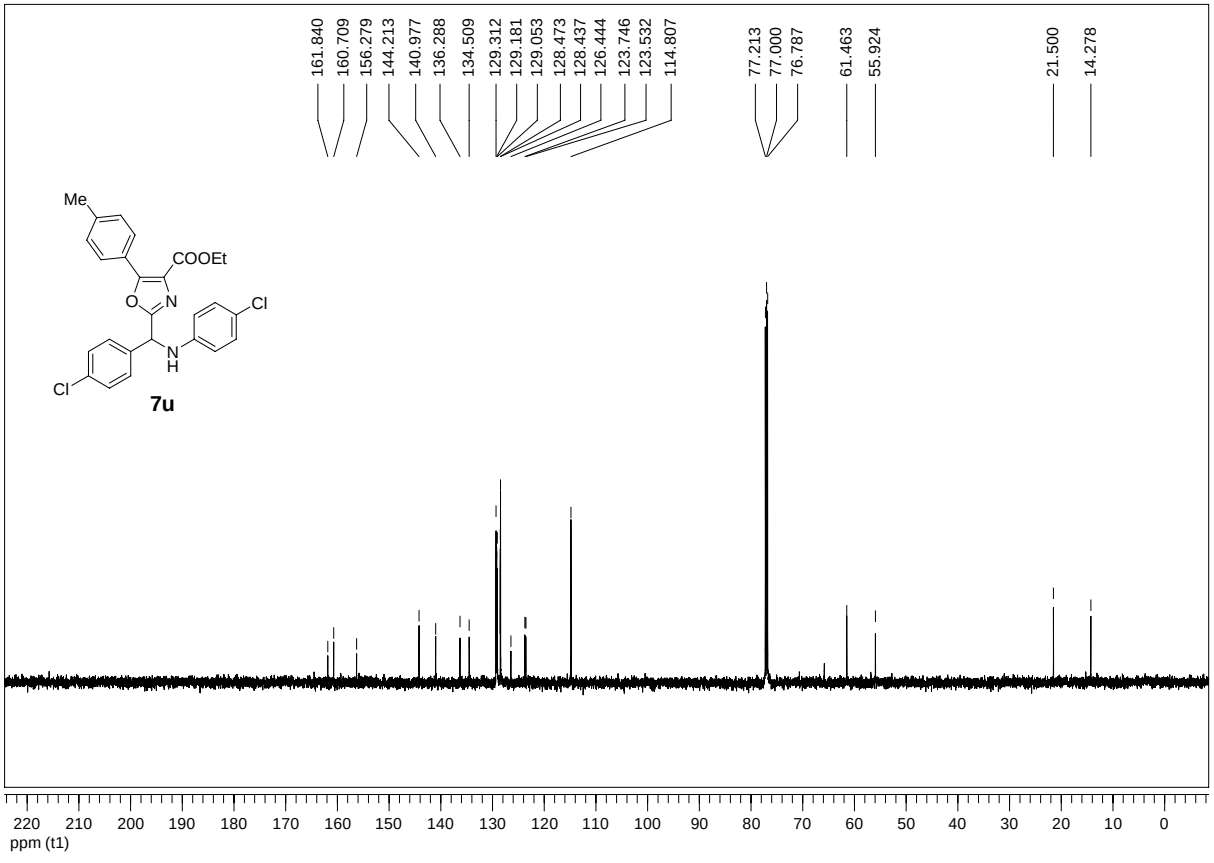
7.465
7.353
7.341
7.258
7.241
7.105
7.092
6.594
6.582
5.719
5.711
5.032
5.025
4.415
4.405
2.398
1.545
1.393
1.380
1.369
0.000000
Me
COOEt
O
N
Cl
N
H
Cl
7u
2.01
4.04
4.00
2.04
1.00
1.04
2.03
3.04
3.05
11.0
10.0
9.0
3.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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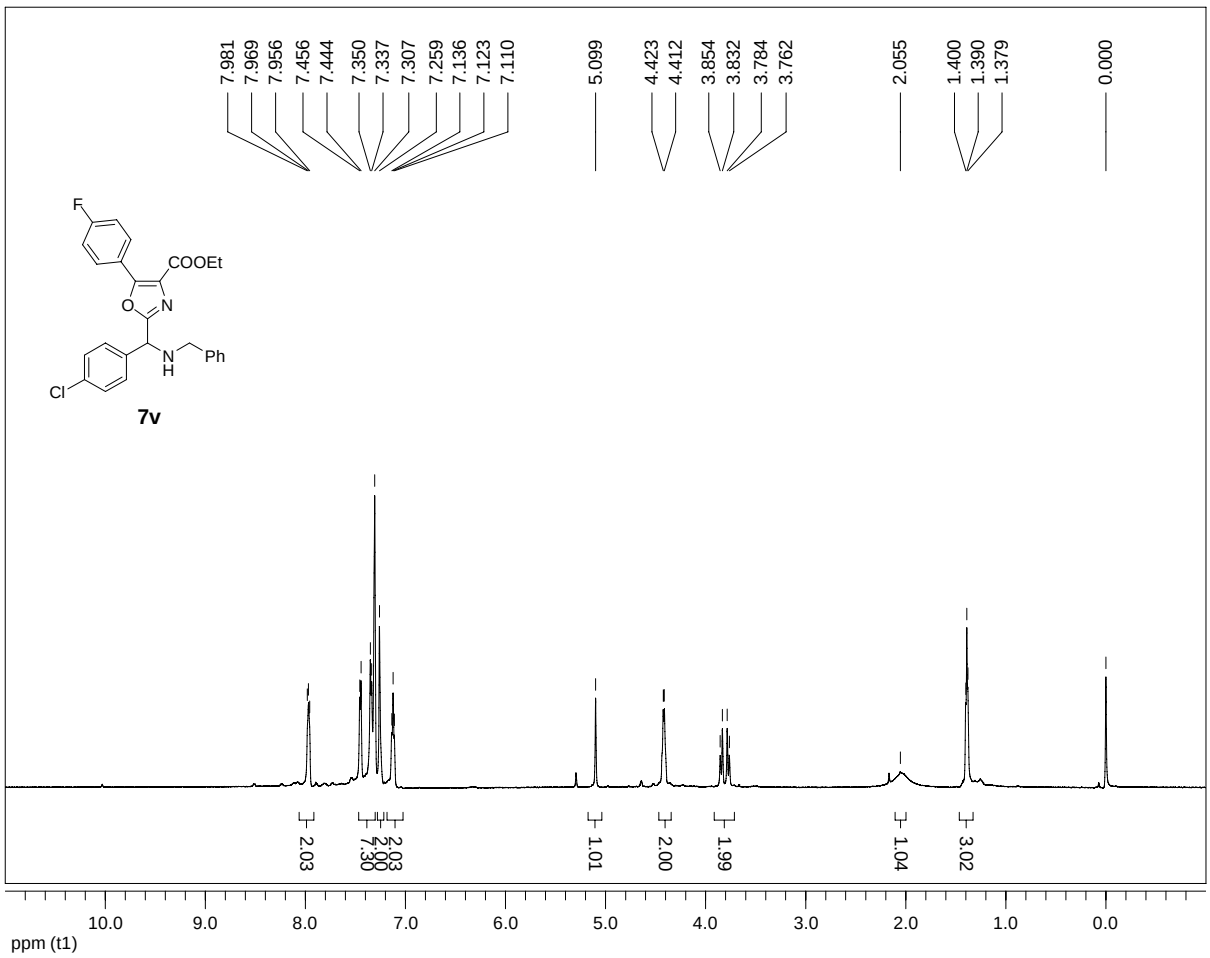
156.279
144.213
140.977
136.288
134.509
129.312
129.181
129.053
128.473
128.437
126.444
123.746
123.532
114.807
77.213
77.000
76.787
61.463
55.924
21.500
14.278
Me
COOEt
O
N
Cl
N
H
Cl
7u
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)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7.350
7.337
7.307
7.259
7.136
7.123
7.110
5.099
4.423
4.412
3.854
3.832
3.784
3.762
2.055
1.400
1.390
1.379
0.000
F
COOEt
O
N
N
H
Ph
Cl
7v
2.03
7.30
2.00
2.03
1.01
2.00
1.99
1.04
3.02
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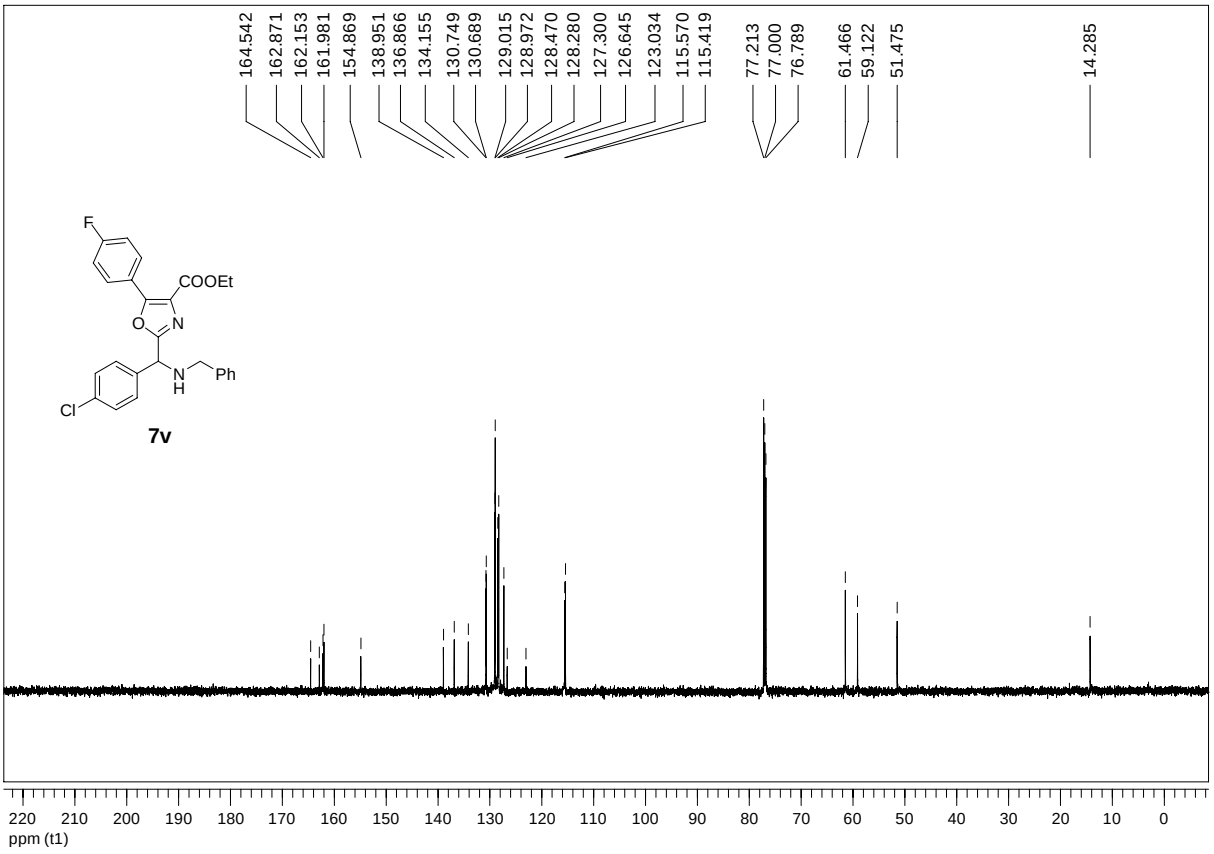
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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134.155
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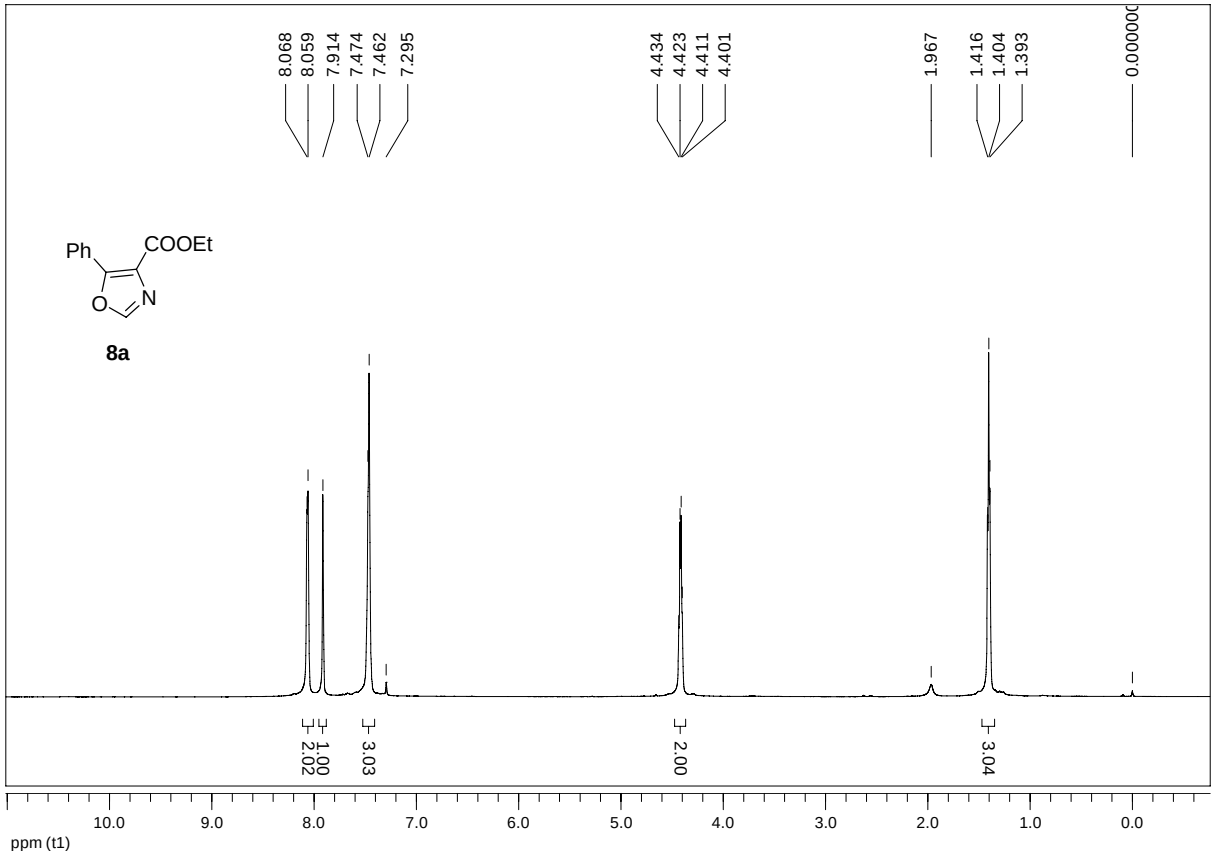
130.689
129.015
128.972
128.470
128.280
127.300
126.645
123.034
115.570
115.419
77.213
77.000
76.789
61.466
59.122
51.475
14.285
F
COOEt
O
N
N
H
Ph
Cl
7v
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)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8.059
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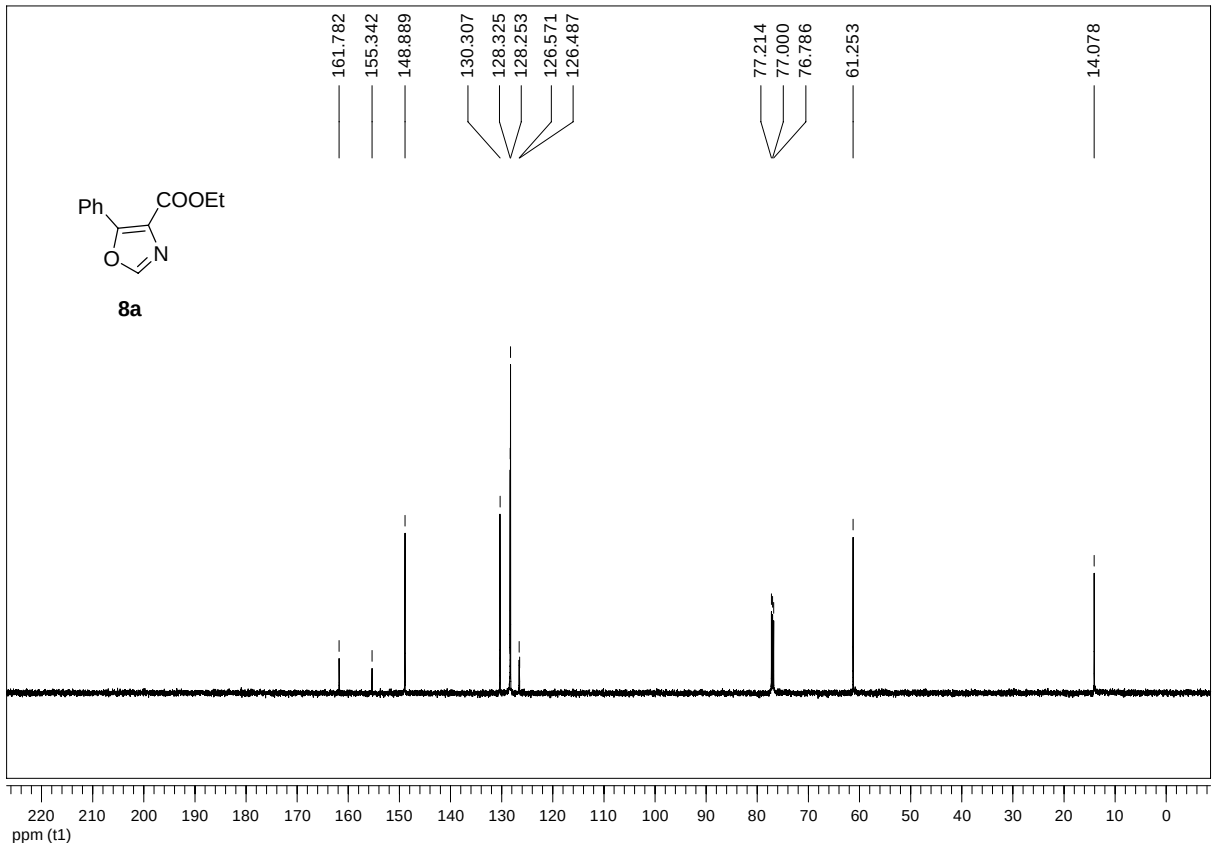
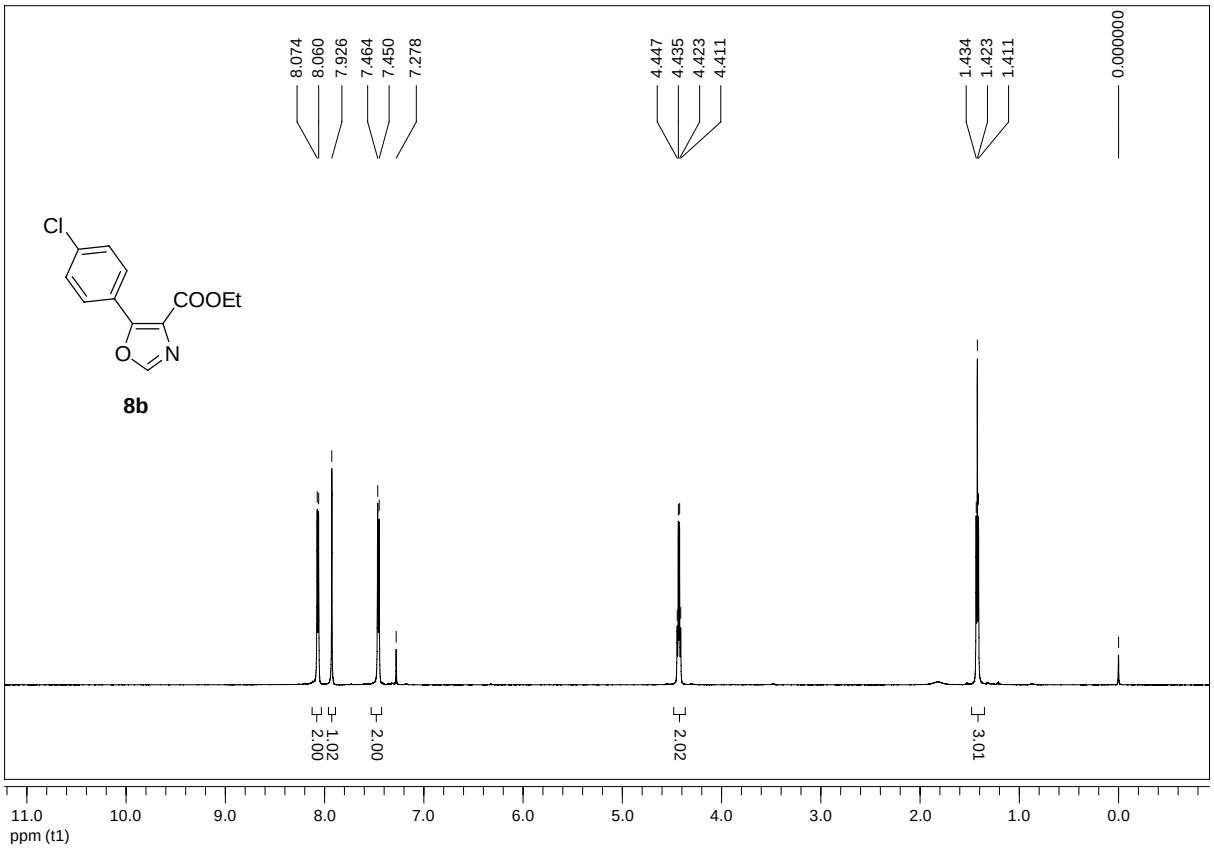
7.474
7.462
7.295
4.434
4.423
4.411
4.401
1.967
1.416
1.404
1.393
0.000000
Ph
COOEt
O
N
8a
2.22
1.00
3.03
2.00
3.04
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


161.782
155.342
148.889
130.307
128.325
128.253
126.571
126.487
77.214
77.000
76.786
61.253
14.078
Ph
COOEt
O
N
8a
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)


8.074
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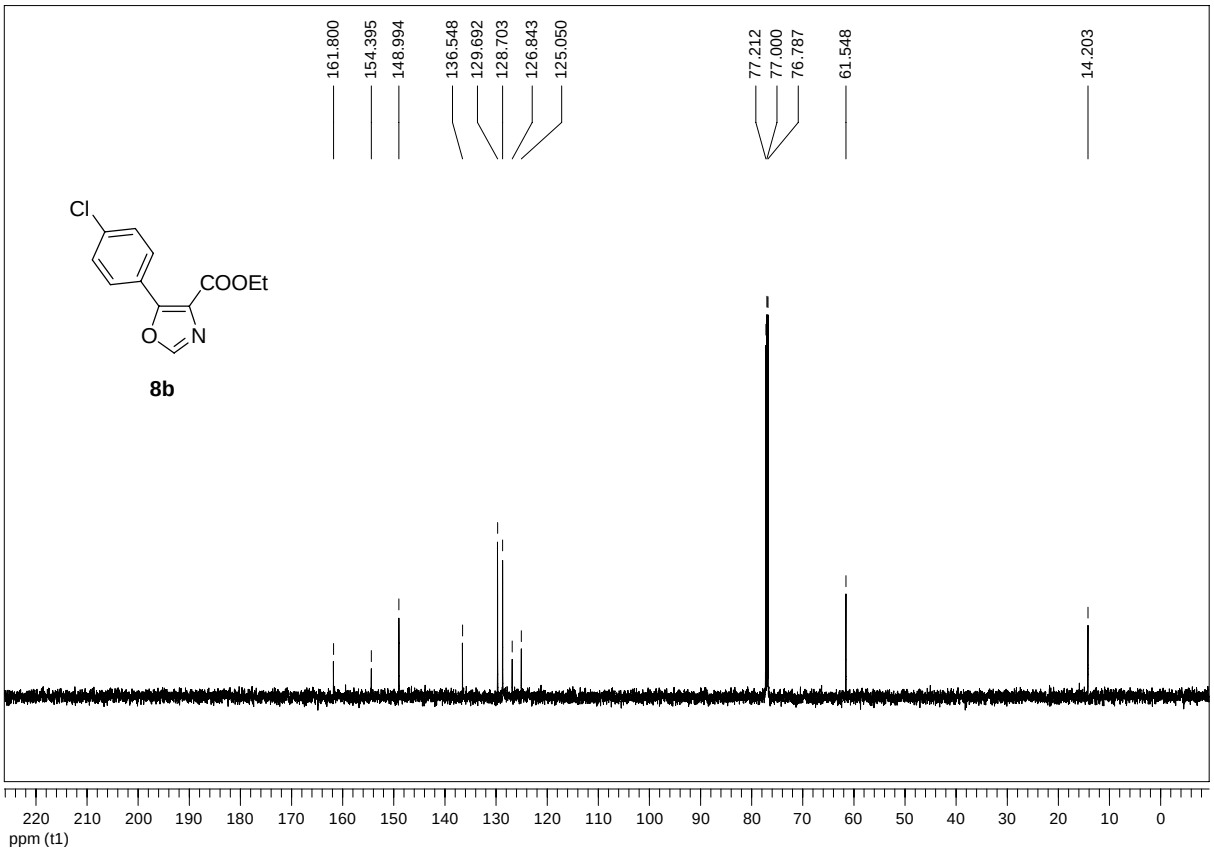
7.464
7.450
7.278
4.447
4.435
4.423
4.411
1.434
1.423
1.411
0.000000
Cl
COOEt
O
N
8b
2.00
1.02
2.00
2.02
3.01
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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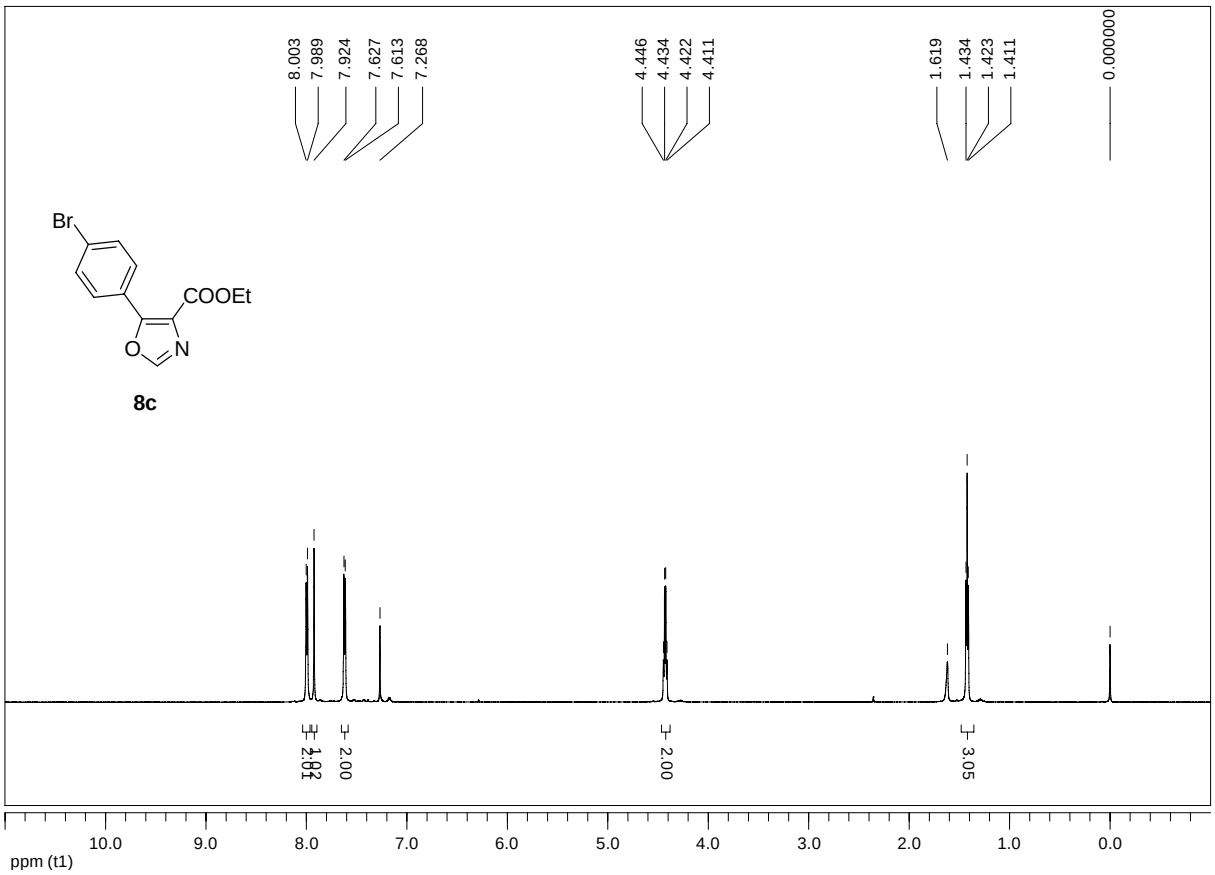
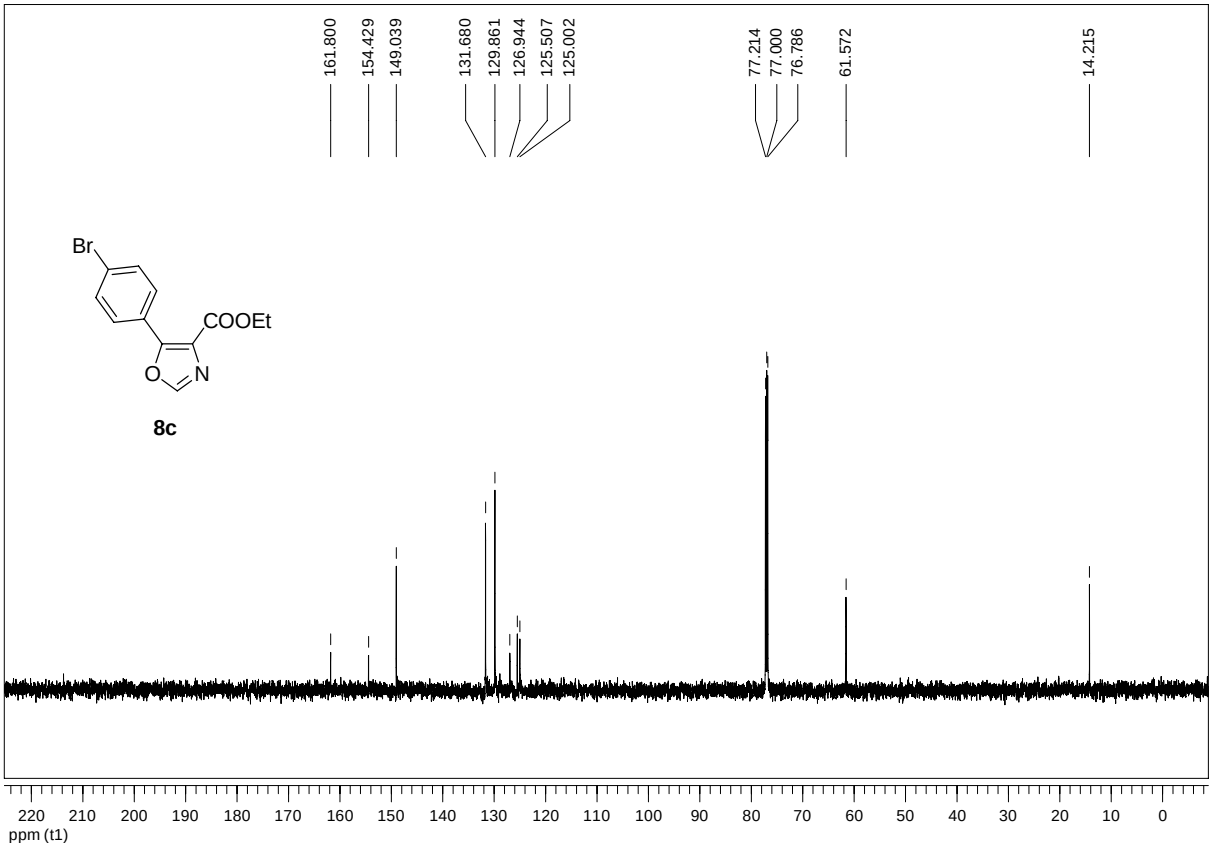
154.395
148.994
136.548
129.692
128.703
126.843
125.050
77.212
77.000
76.787
61.548
14.203
Cl
COOEt
O
N
8b
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)


8.003
7.989
7.924
7.627
7.613
7.268
4.446
4.434
4.422
4.411
1.619
1.434
1.423
1.411
0.000000
Br
COOEt
O
N
8c
2.00
2.00
3.05
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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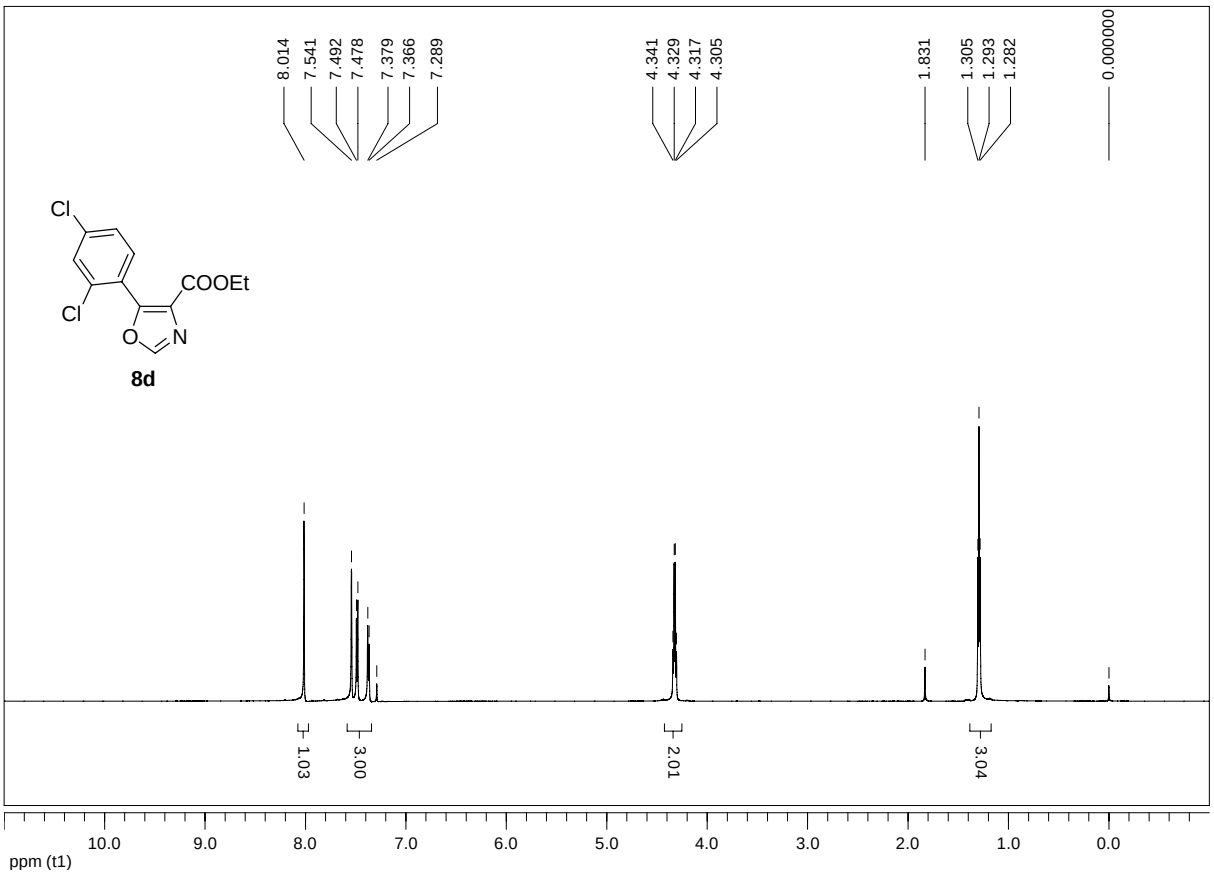
154.429
149.039
131.680
129.861
126.944
125.507
125.002
77.214
77.000
76.786
61.572
14.215
Br
COOEt
O
N
8c
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)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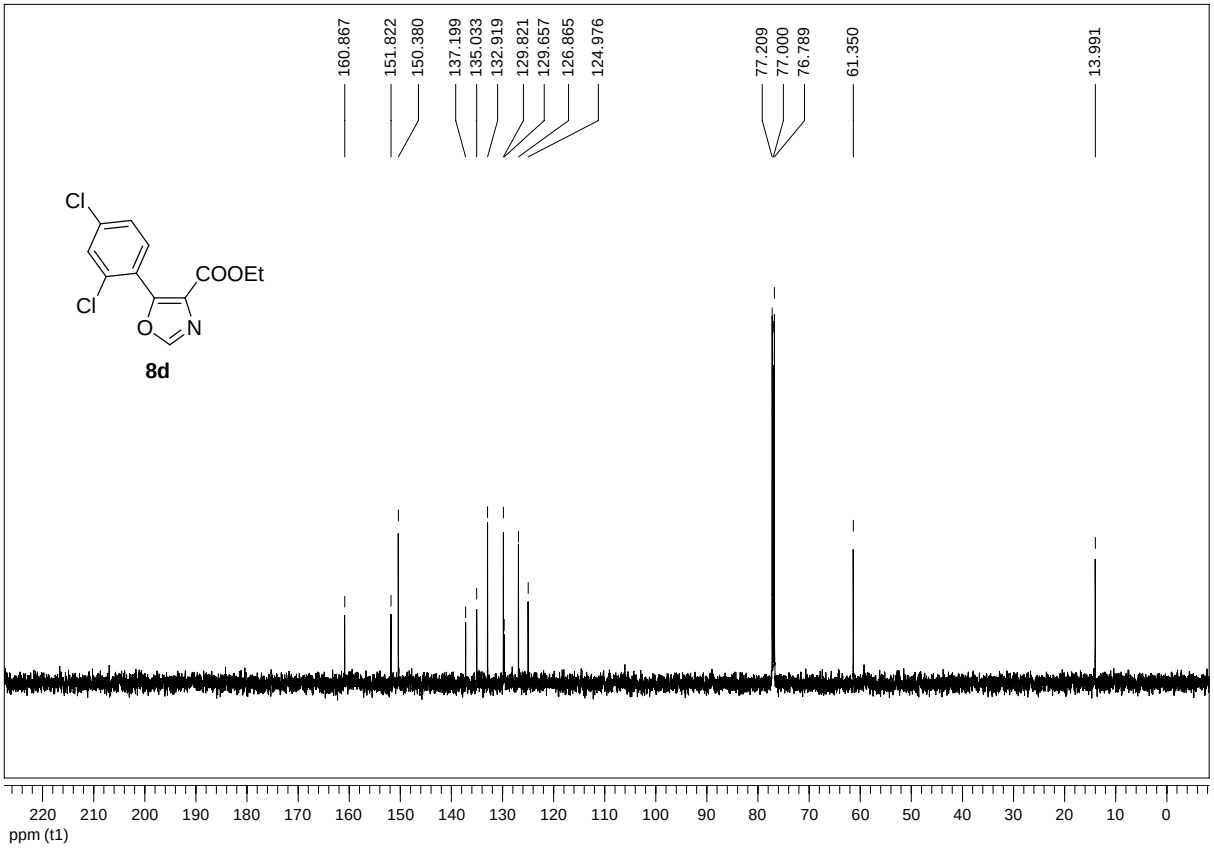
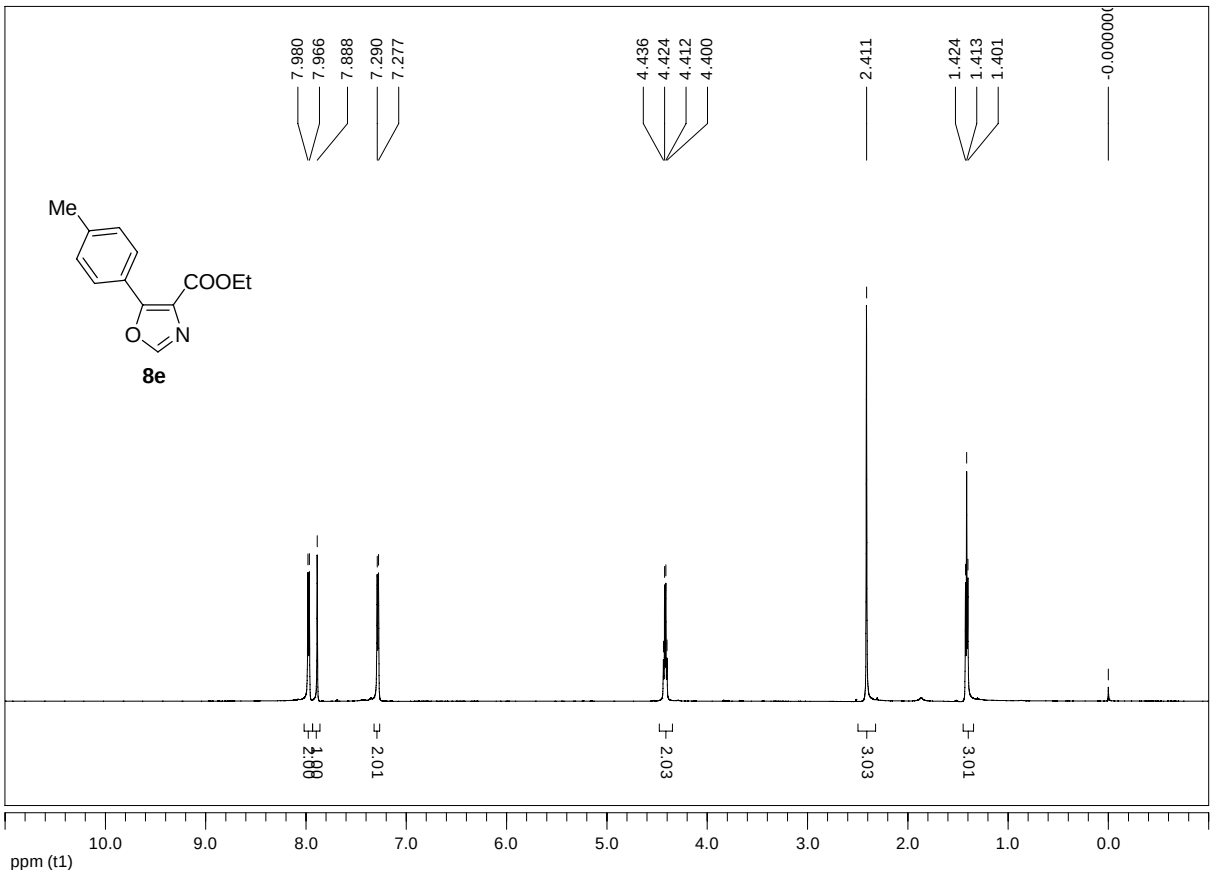
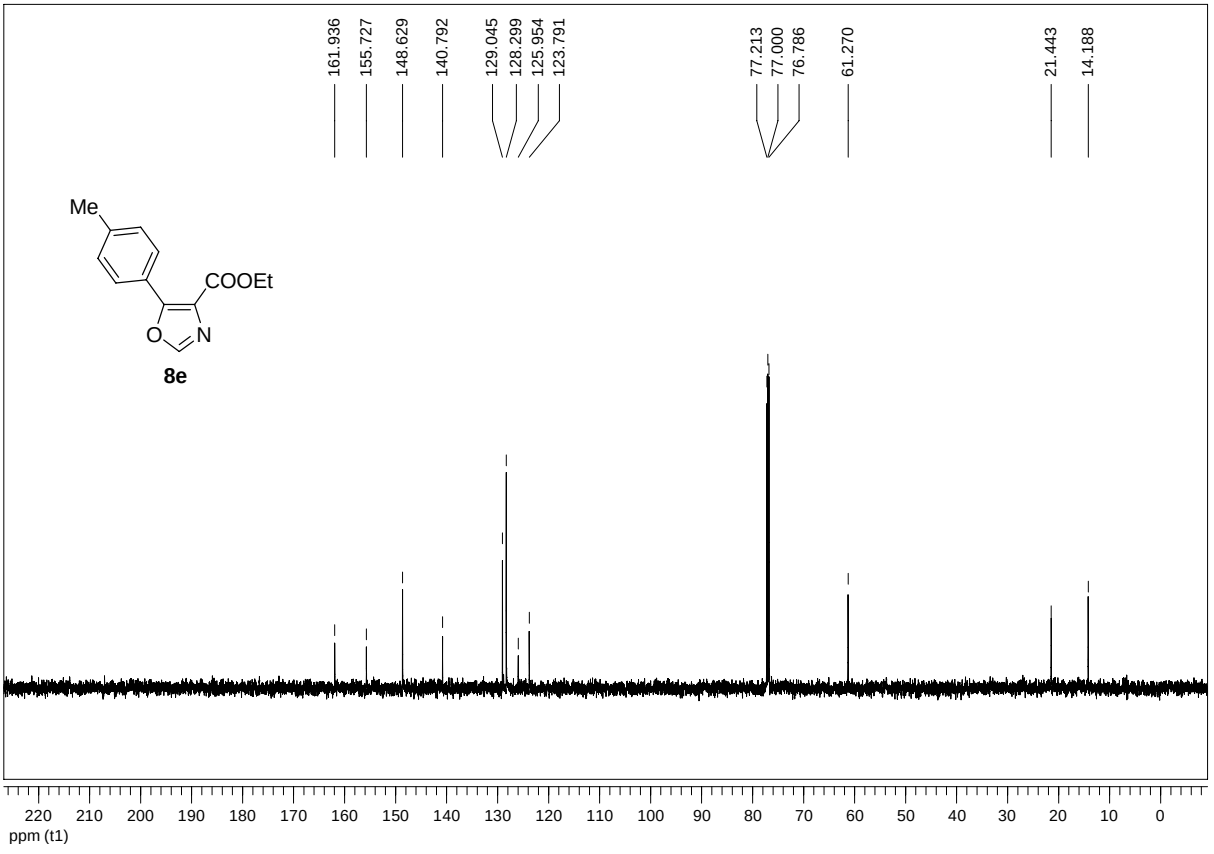
7.541
7.492
7.478
7.379
7.366
7.289
4.341
4.329
4.317
4.305
1.831
1.305
1.293
1.282
0.000000
Cl
Cl
COOEt
O
N
8d
1.03
3.00
2.01
3.04
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


160.867
151.822
150.380
137.199
135.033
132.919
129.821
129.657
126.865
124.976
77.209
77.000
76.789
61.350
13.991
Cl
Cl
COOEt
O
N
8d
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)


7.980
7.966
7.888
7.290
7.277
4.436
4.424
4.412
4.400
2.411
1.424
1.413
1.401
-0.000000
Me
COOEt
O
N
8e
2.00
2.01
2.03
3.03
3.01
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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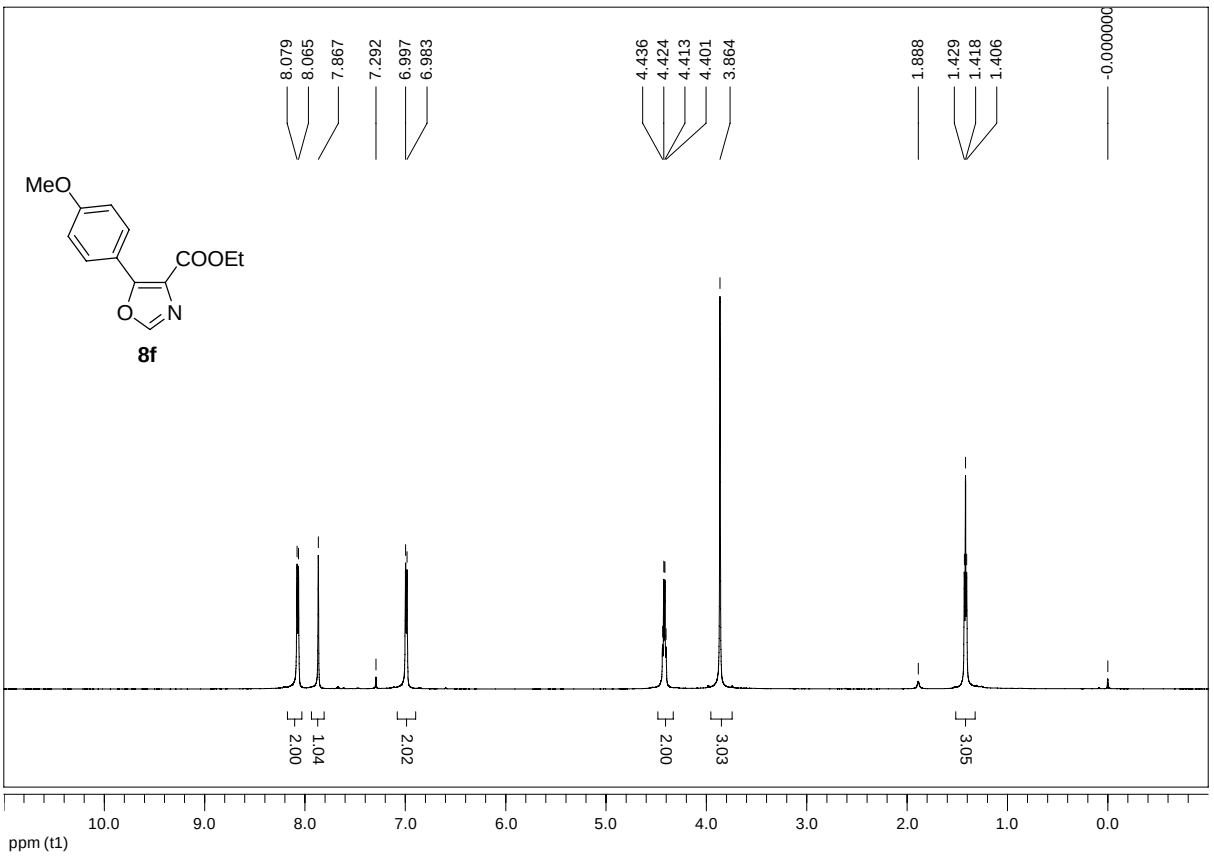
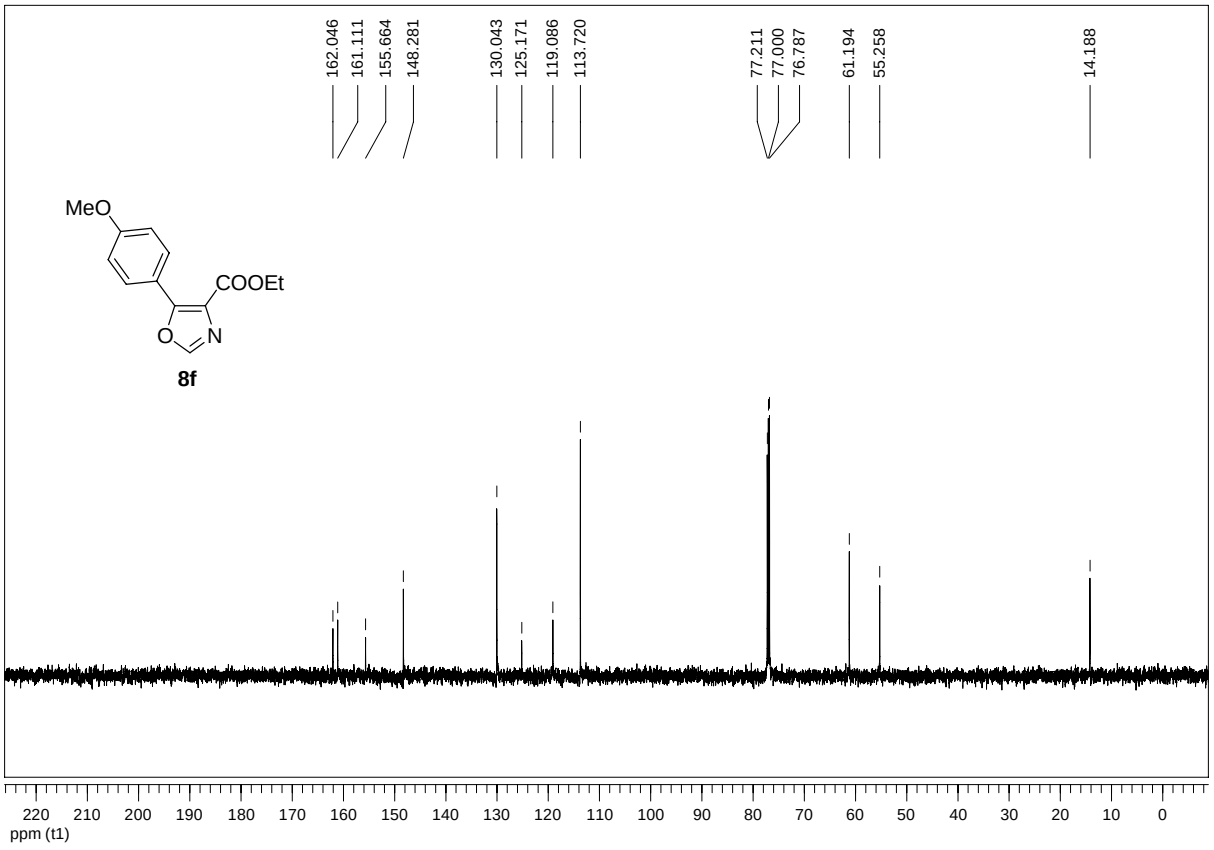
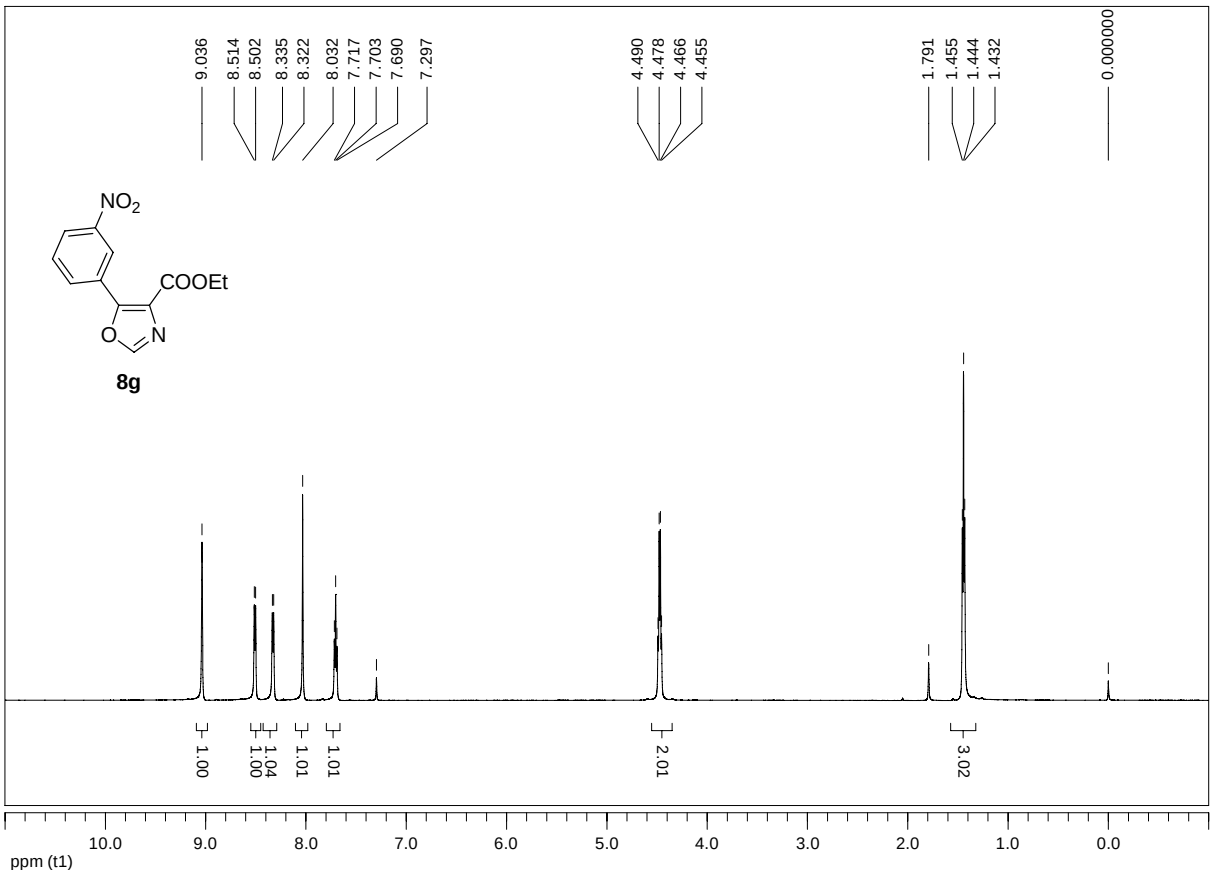
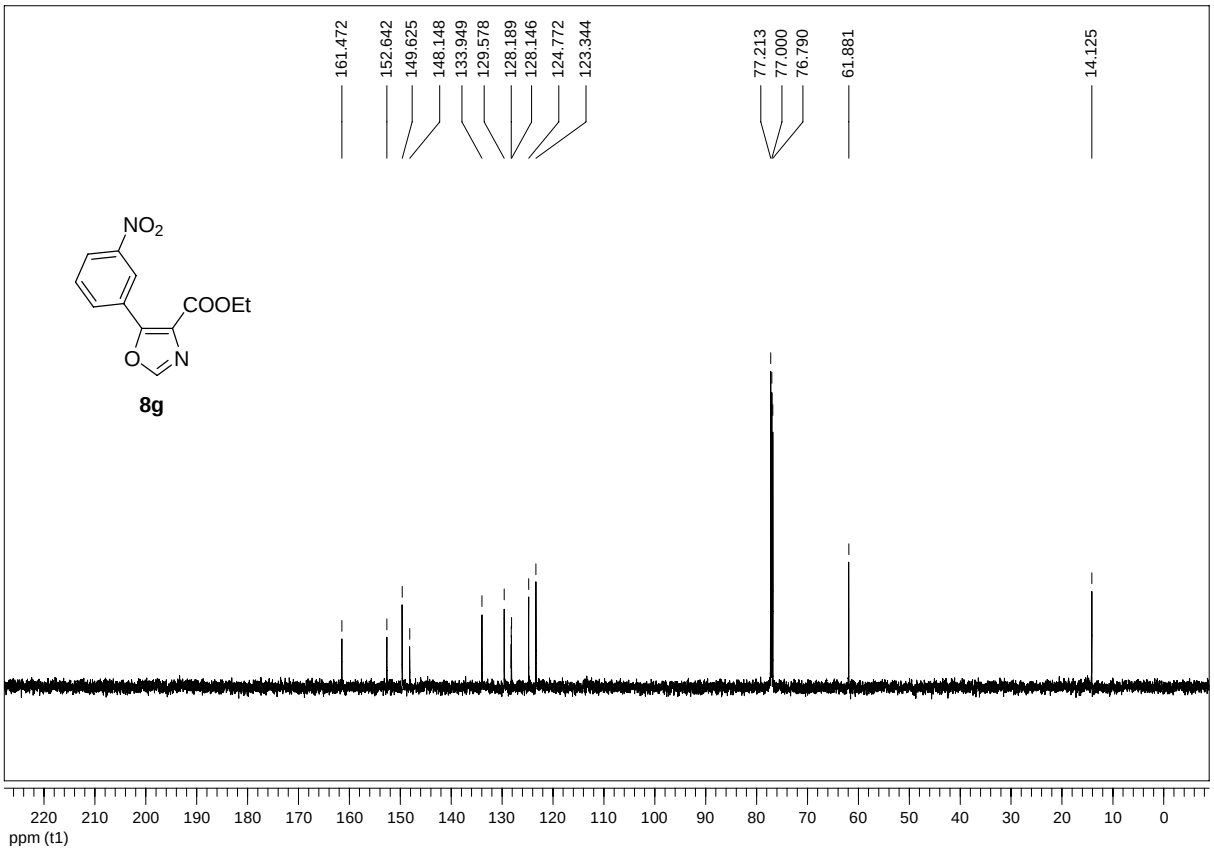
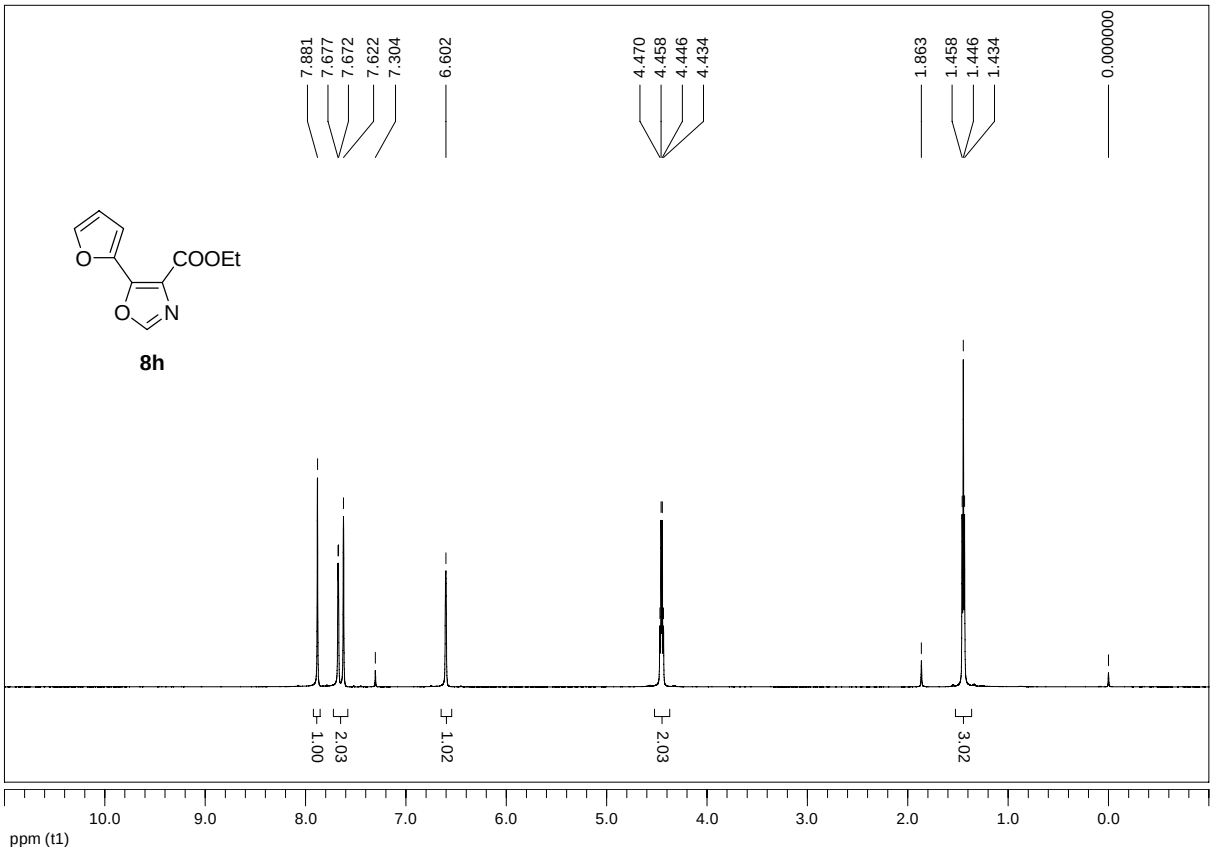
155.727
148.629
140.792
129.045
128.299
125.954
123.791
77.213
77.000
76.786
61.270
21.443
14.188
Me
COOEt
O
N
8e
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

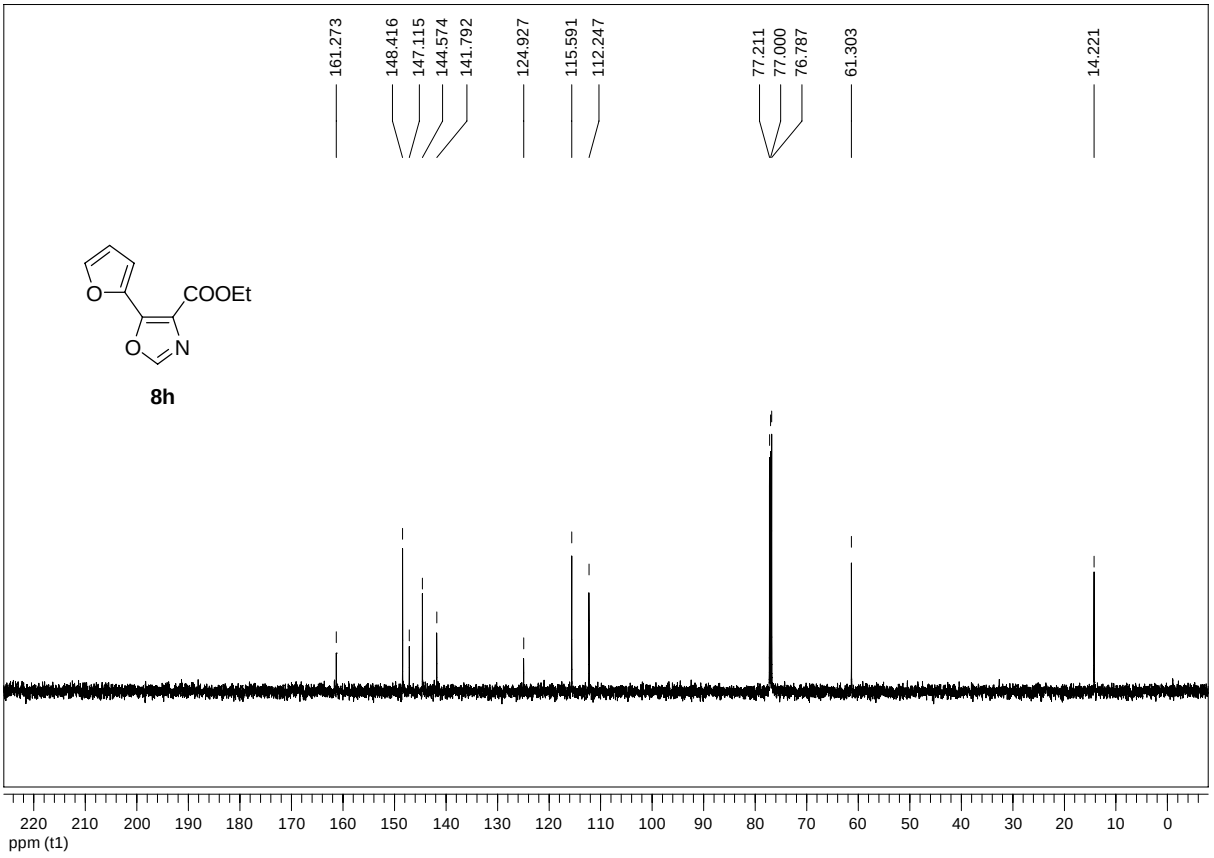

8.079
8.065
7.867
7.292
6.997
6.983
4.436
4.424
4.413
4.401
3.864
1.888
1.429
1.418
1.406
-0.000000
MeO
COOEt
O
N
8f
2.00
1.04
2.02
2.00
3.03
3.05
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

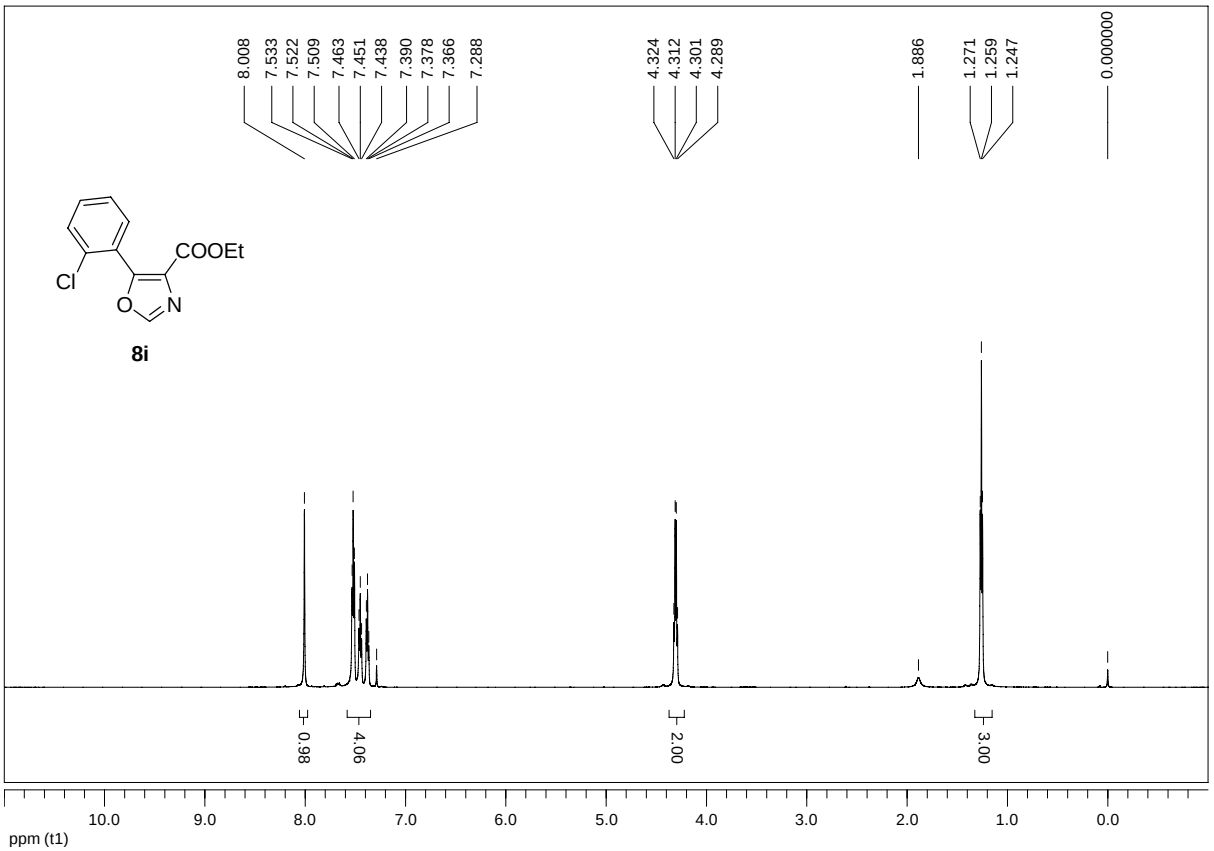

162.046
161.111
155.664
148.281
130.043
125.171
119.086
113.720
77.211
77.000
76.787
61.194
55.258
14.188
MeO
COOEt
O
N
8f
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

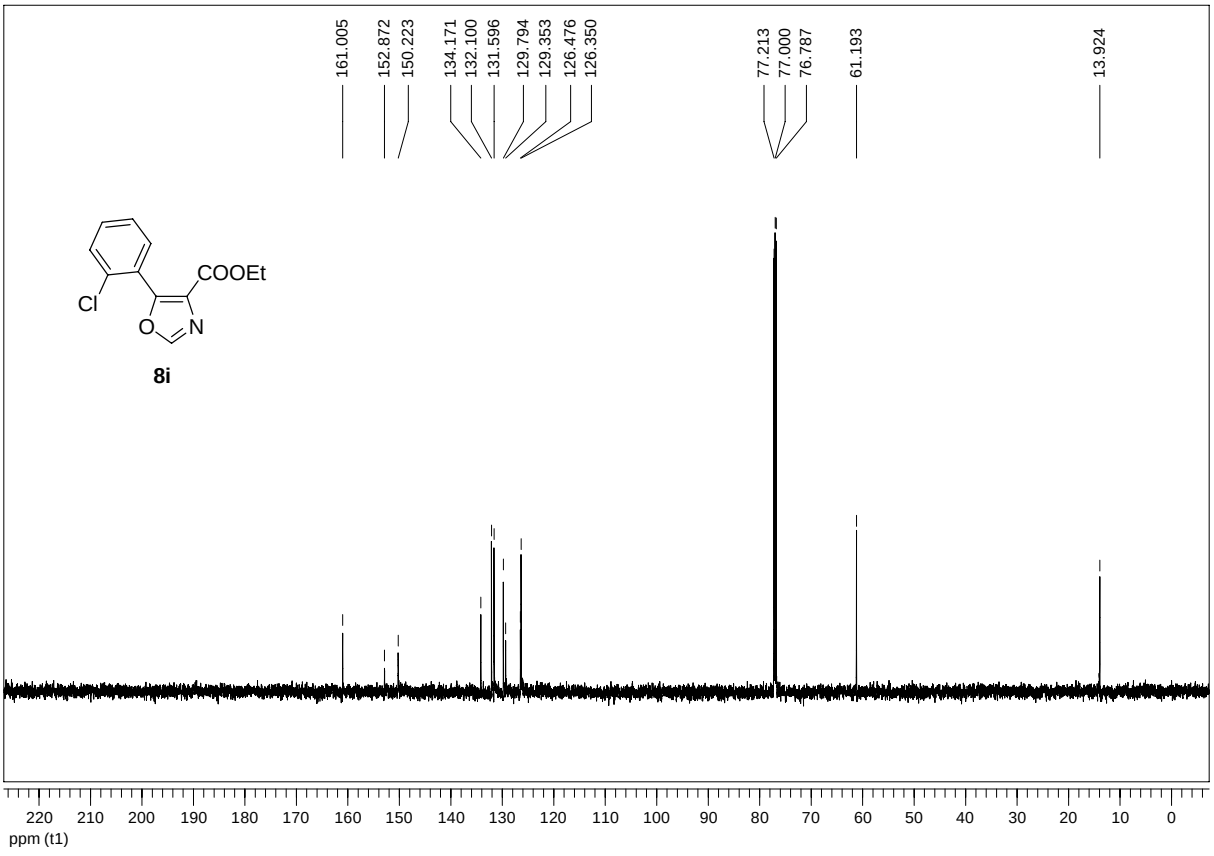

9.036
8.514
8.502
8.335
8.322
8.032
7.717
7.703
7.690
7.297
4.490
4.478
4.466
4.455
1.791
1.455
1.444
1.432
0.000000
NO2
COOEt
O
N
8g
1.00
1.00
1.04
1.01
1.01
2.01
3.02
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

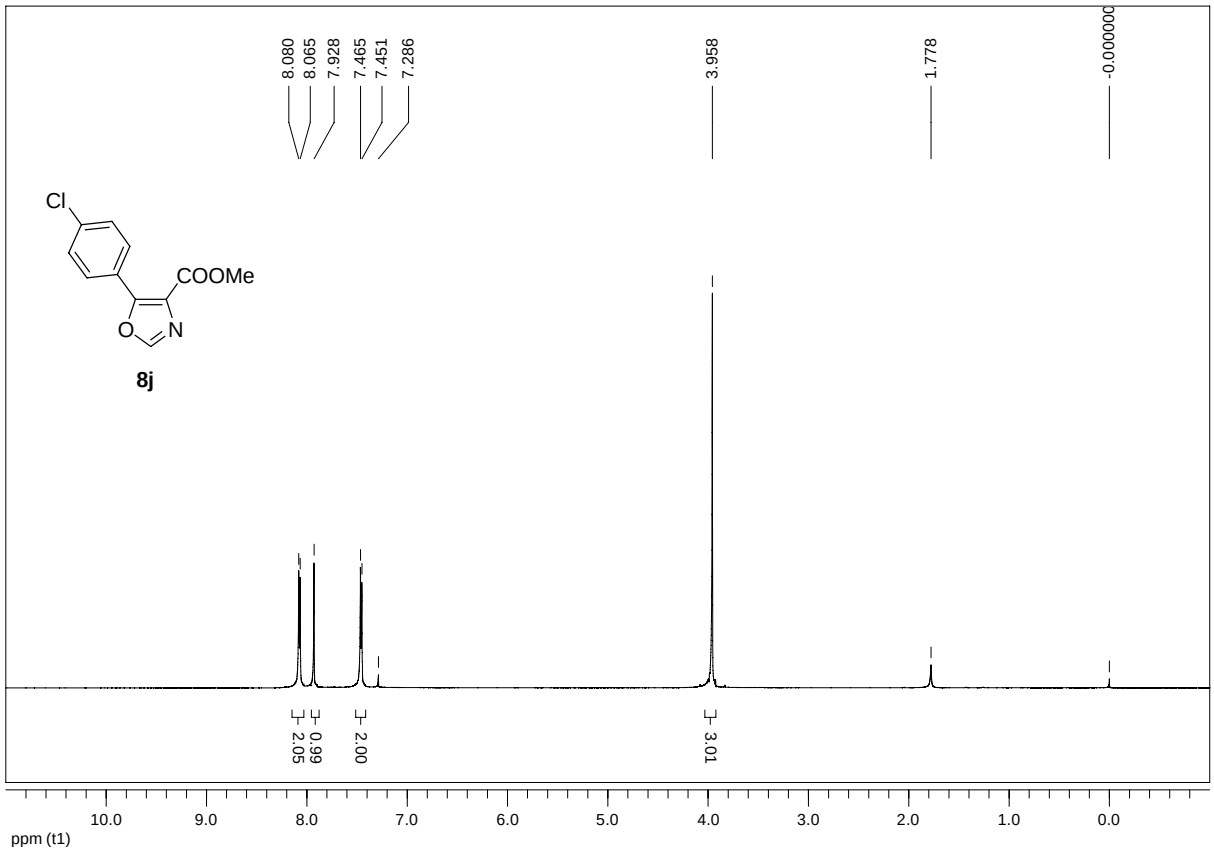

161.472
152.642
149.625
148.148
133.949
129.578
128.189
128.146
124.772
123.344
77.213
77.000
76.790
61.881
14.125
NO2
COOEt
O
N
8g
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

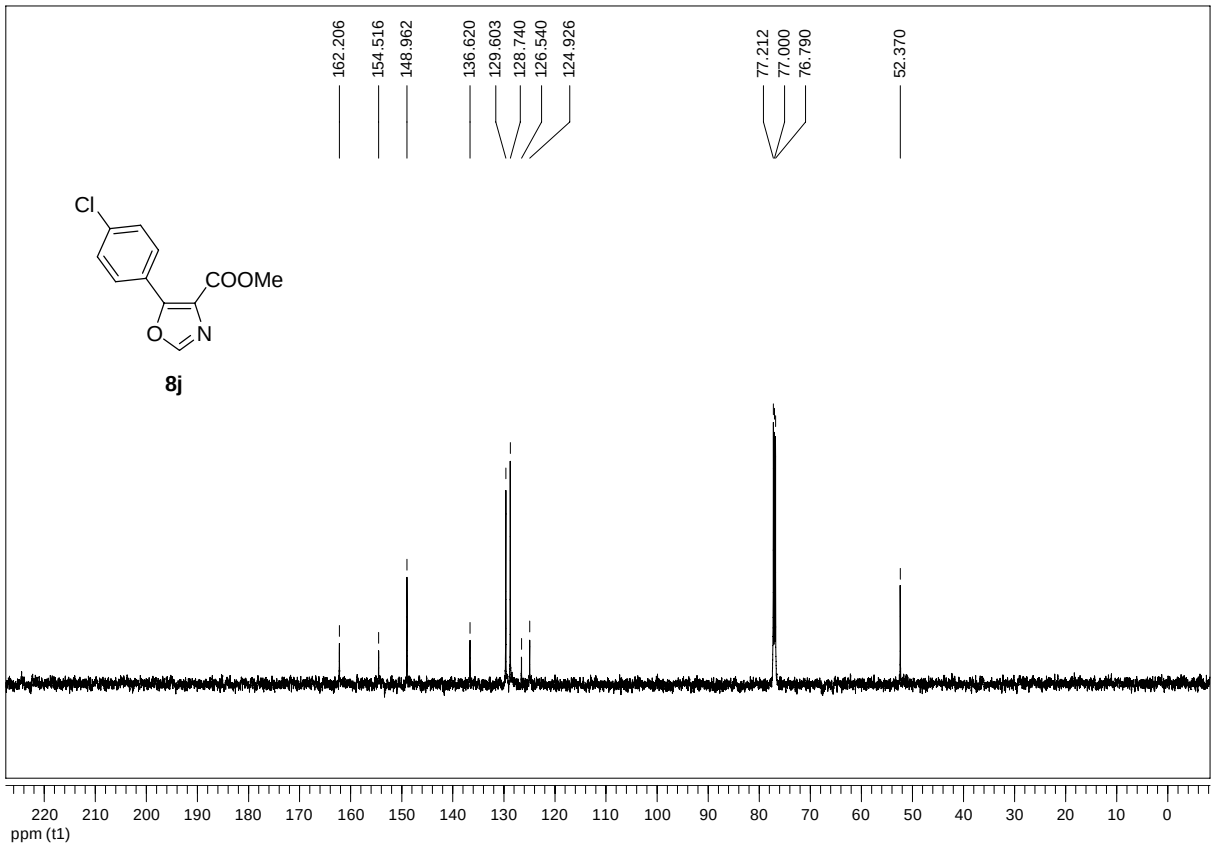

7.881
7.677
7.672
7.622
7.304
6.602
4.470
4.458
4.446
4.434
1.863
1.458
1.446
1.434
0.000000
COOEt
O
O
N
8h
1.00
2.03
1.02
2.03
3.02
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

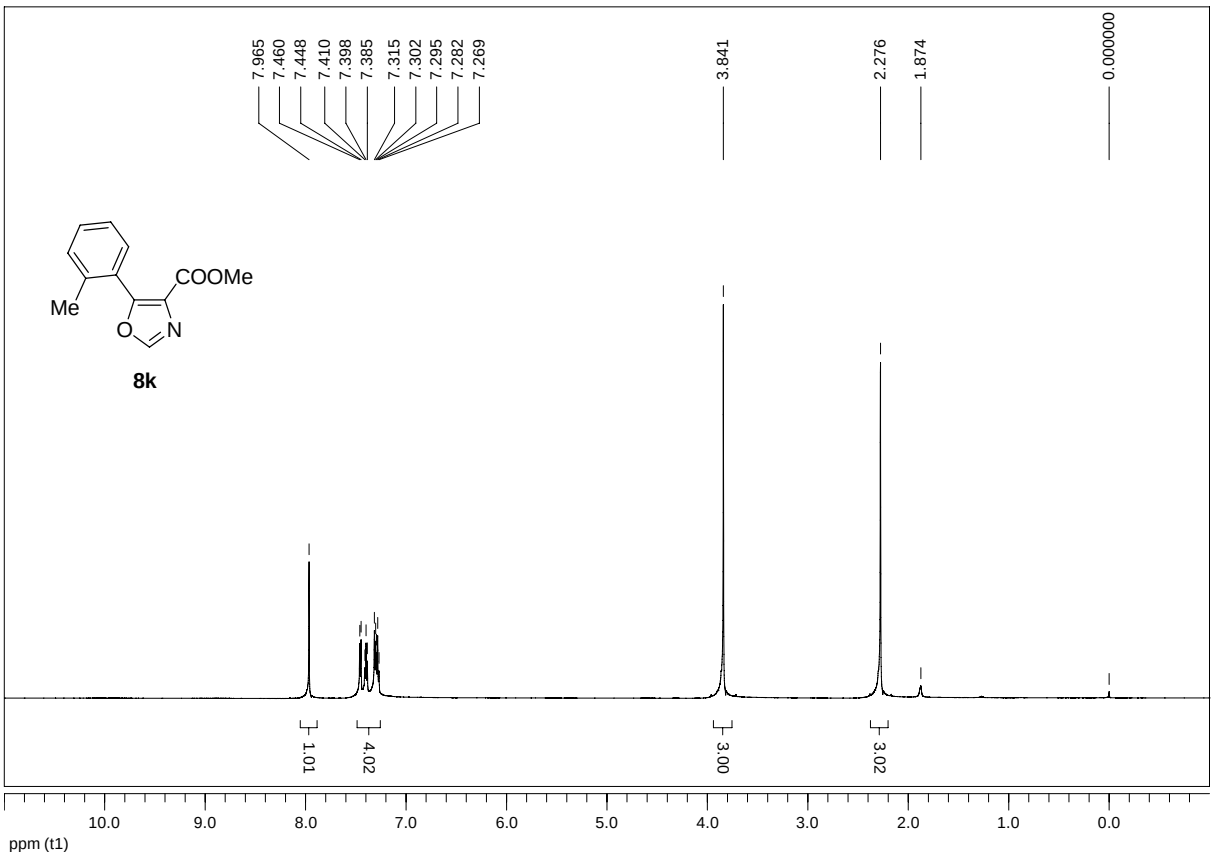

161.273
148.416
147.115
144.574
141.792
124.927
115.591
112.247
77.211
77.000
76.787
61.303
14.221
COOEt
O
O
N
8h
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

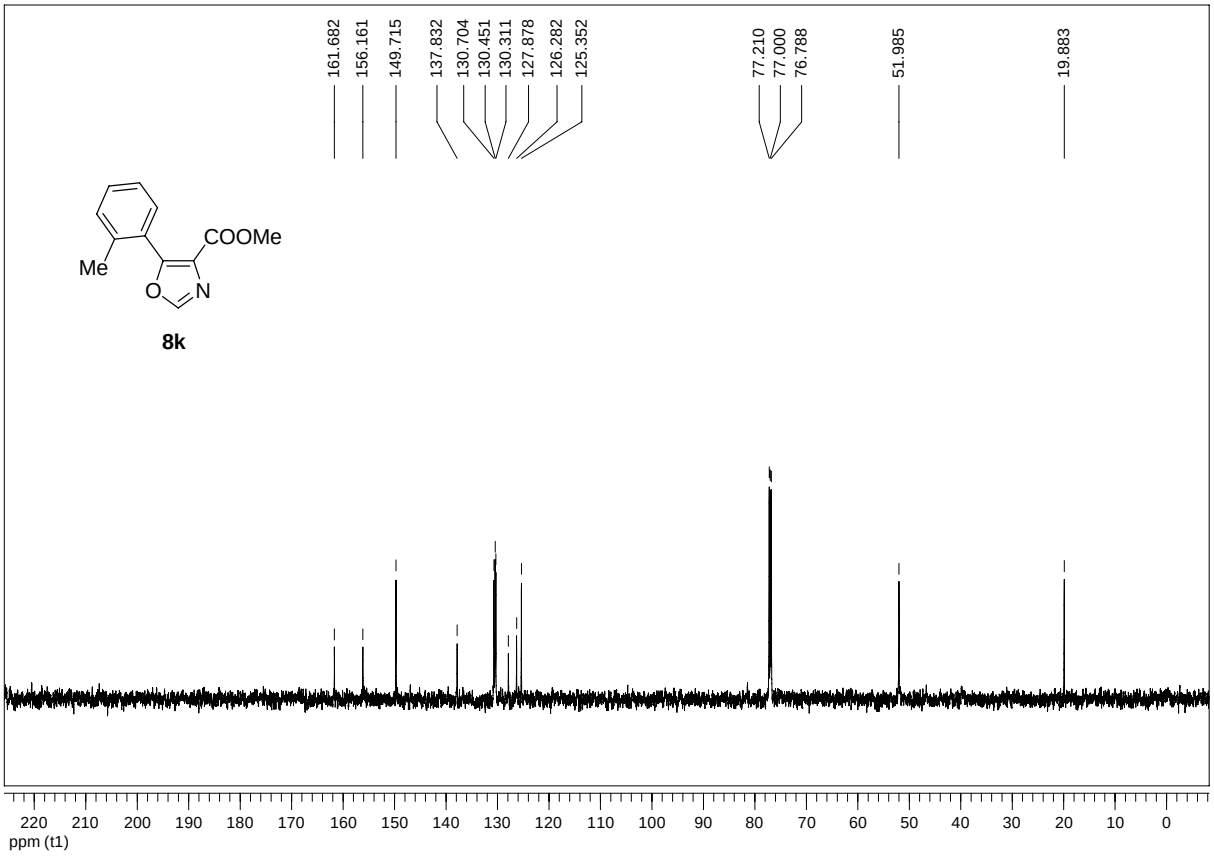

8.008
7.533
7.522
7.509
7.463
7.451
7.438
7.390
7.378
7.366
7.288
4.324
4.312
4.301
4.289
1.886
1.271
1.259
1.247
0.000000
COOEt
Cl
O
N
8i
0.98
4.06
2.00
3.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

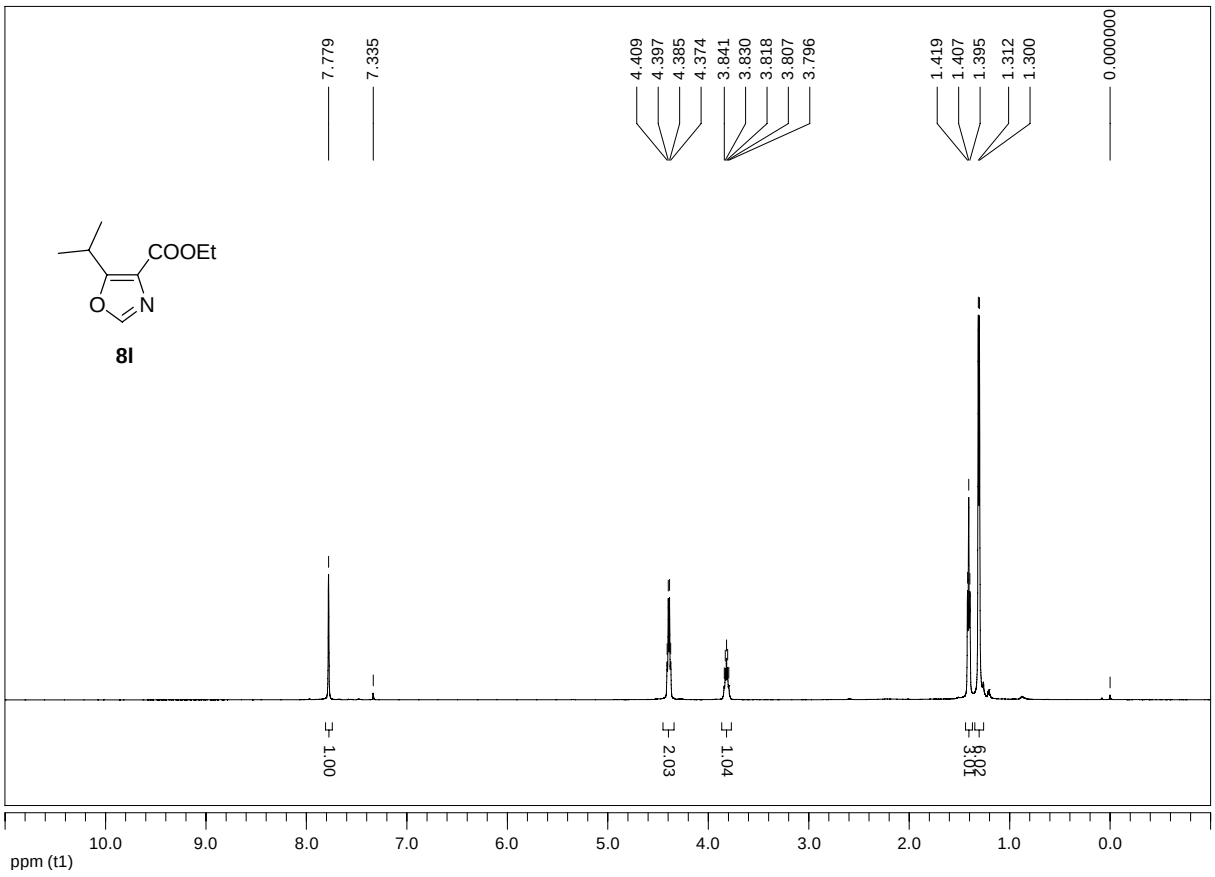

161.005
152.872
150.223
134.171
132.100
131.596
129.794
129.353
126.476
126.350
77.213
77.000
76.787
61.193
13.924
COOEt
Cl
O
N
8i
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

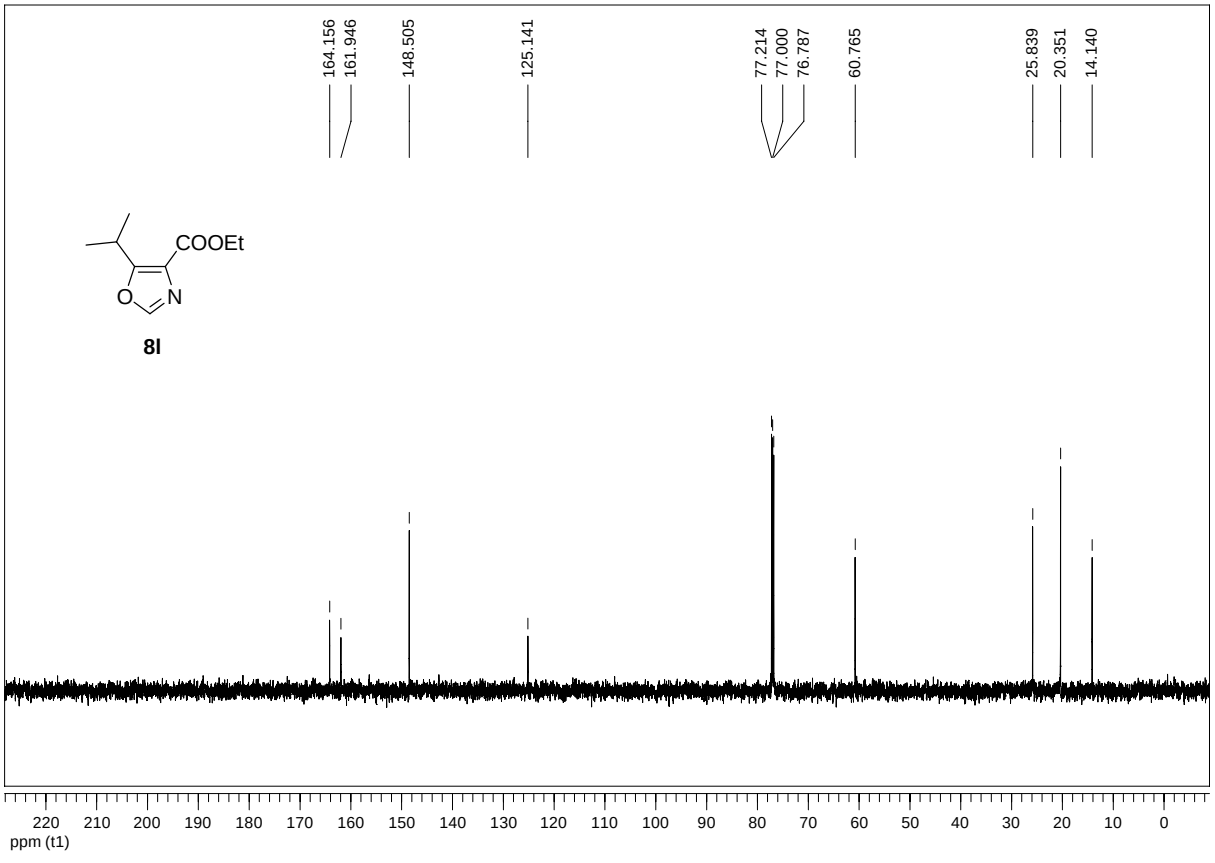

8.080
8.065
7.928
7.465
7.451
7.286
3.958
1.778
-0.000000
Cl
COOMe
O
N
8j
2.05
0.99
2.00
3.01
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

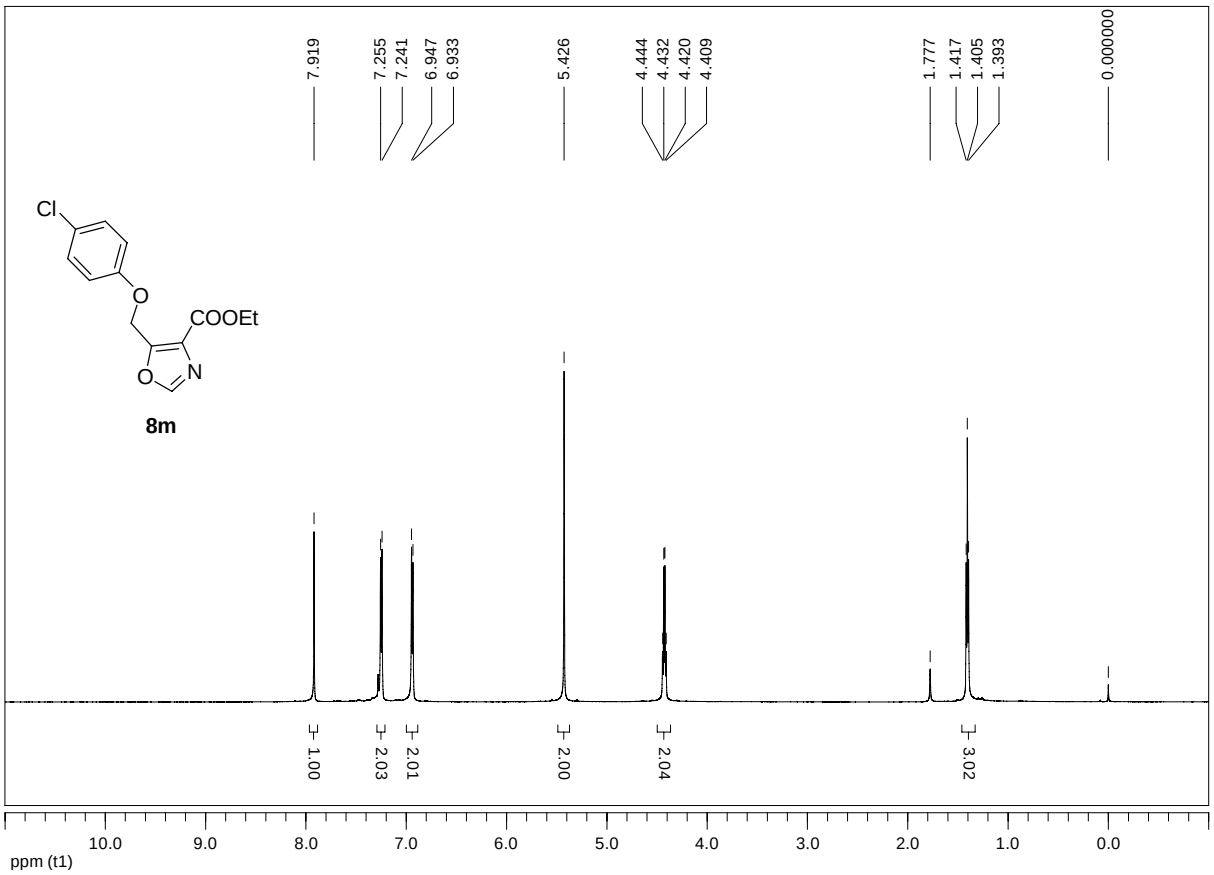

162.206
154.516
148.962
136.620
129.603
128.740
126.540
124.926
77.212
77.000
76.790
52.370
Cl
COOMe
O
N
8j
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

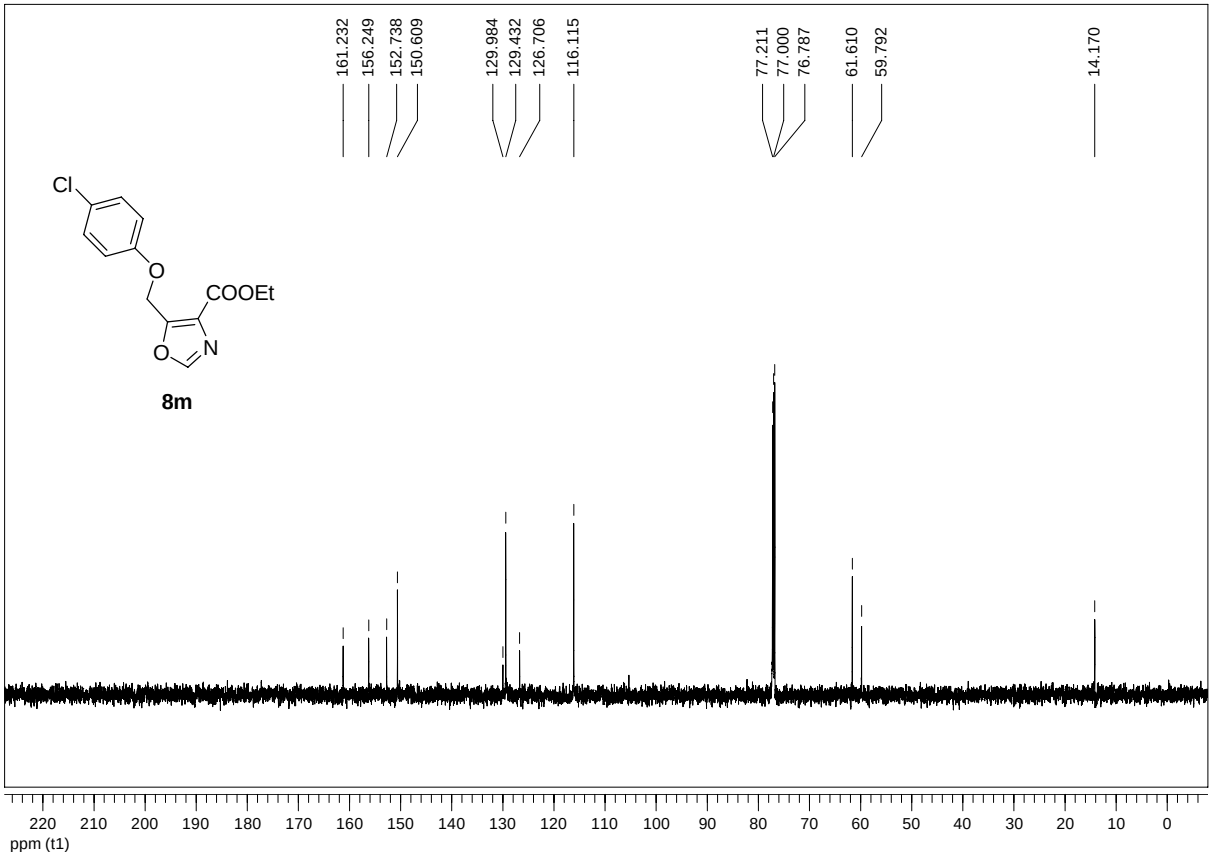

7.965
7.460
7.448
7.410
7.398
7.385
7.315
7.302
7.295
7.282
7.269
3.841
2.276
1.874
0.000000
COOMe
Me
O
N
8k
1.01
4.02
3.00
3.02
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

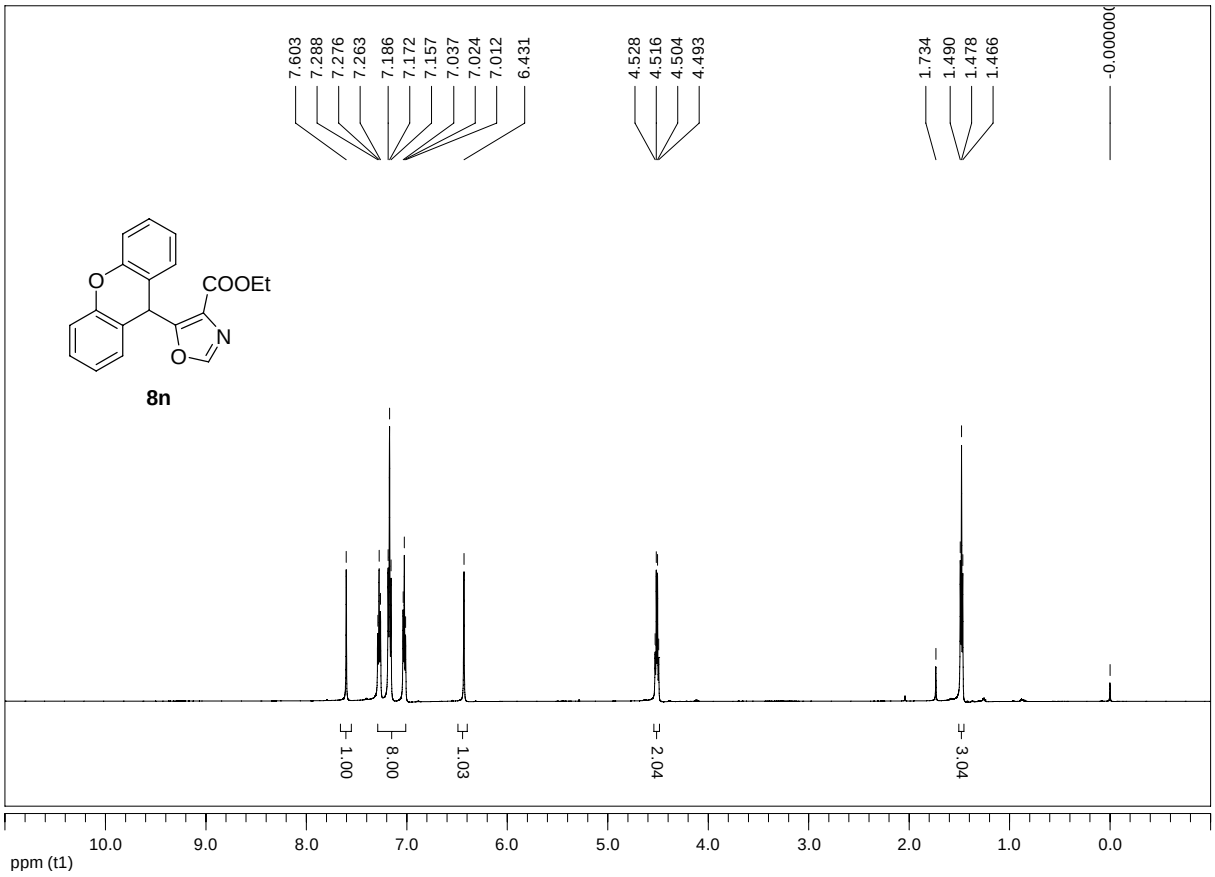

161.682
156.161
149.715
137.832
130.704
130.451
130.311
127.878
126.282
125.352
77.210
77.000
76.788
51.985
19.883
COOMe
Me
O
N
8k
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)

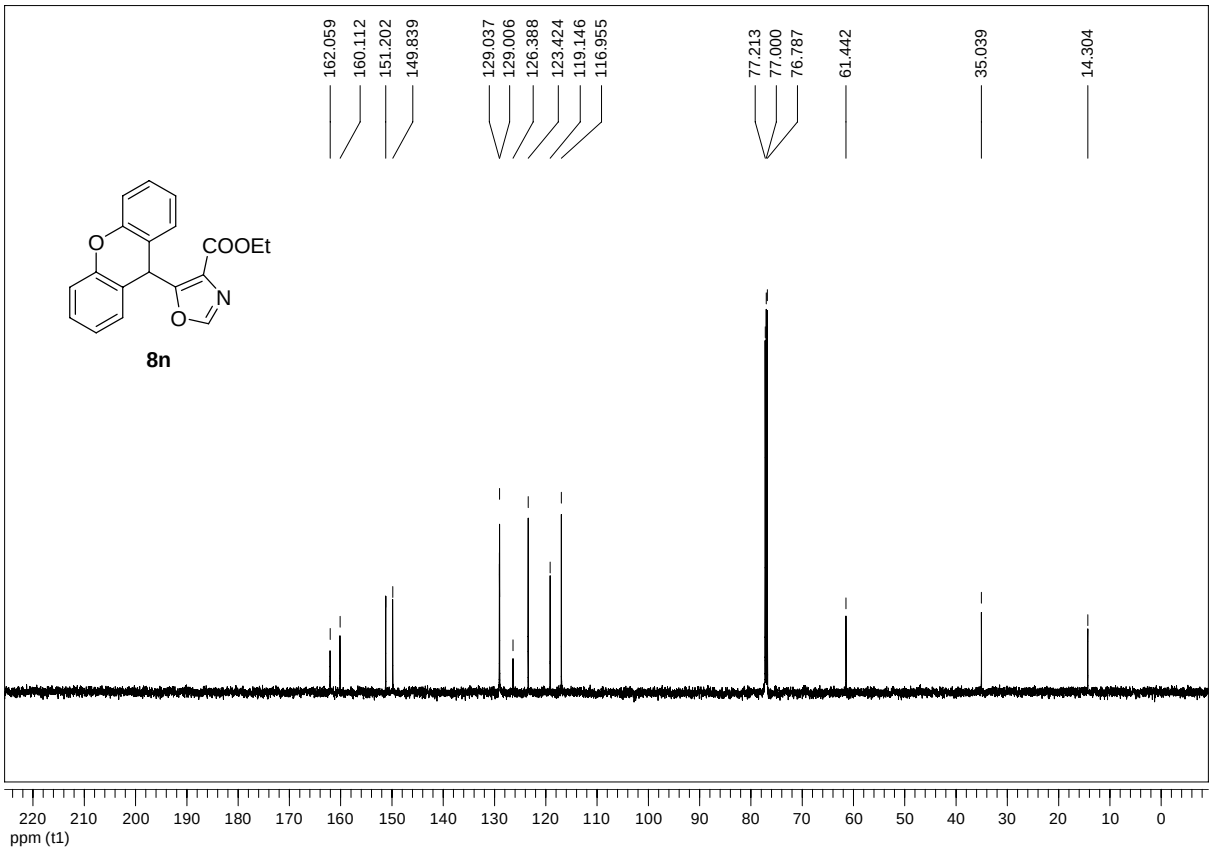

7.779
7.335
4.409
4.397
4.385
4.374
3.841
3.830
3.818
3.807
3.796
1.419
1.407
1.395
1.312
1.300
0.000000
COOEt
O
N
8l
1.00
2.03
1.04
6.01
3.02
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


164.156
161.946
148.505
125.141
77.214
77.000
76.787
60.765
25.839
20.351
14.140
COOEt
O
N
8l
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)


7.919
7.255
7.241
6.947
6.933
5.426
4.444
4.432
4.420
4.409
1.777
1.417
1.405
1.393
0.000000
Cl
O
COOEt
O
N
8m
1.00
2.03
2.01
2.00
2.04
3.02
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


161.232
156.249
152.738
150.609
129.984
129.432
126.706
116.115
77.211
77.000
76.787
61.610
59.792
14.170
Cl
O
COOEt
O
N
8m
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)


7.603
7.288
7.276
7.263
7.186
7.172
7.157
7.037
7.024
7.012
6.431
4.528
4.516
4.504
4.493
1.734
1.490
1.478
1.466
-0.000000
COOEt
O
N
O
8n
1.00
8.00
1.03
2.04
3.04
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


162.059
160.112
151.202
149.839
129.037
129.006
126.388
123.424
119.146
116.955
77.213
77.000
76.787
61.442
35.039
14.304
COOEt
O
N
O
8n
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm (t1)